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SUPPLEMENTARY INFORMATION

https://doi.org/10.1038/s41586-018-0056-8

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Nanoscale synthesis and affinity ranking

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Supporting Information

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This supplementary information document contains general information, experimental procedures, supplementary tables and images, and compound data, and spectra. Source data for experiments are available as Excel spreadsheets for each Figure and Extended Data Figure. These documents contain processed LC-MS reaction screening data, library information, and processed affinity-based ranking data.

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1. General Information

1.1. Materials, Reagents, Analytical, and Protein Targets

All reagents used in this disclosure were purchased from commercial suppliers (when possible) and used as-is. Reagents and intermediates that were not commercially available were prepared as described in this manuscript or prepared according to published procedures. Anhydrous solvents were purchased from Sigma-Aldrich or Acros, in sealed bottles and were either degassed before use or moved to a nitrogen atmosphere glove box and used without further purification. Reactions, screens, and libraries were typically set up in an MBraun glove box under an N_2 atmosphere (oxygen and water levels usually < 1 ppm). Scaled up bench-scale reactions were set up in the glove box in 1-dram vials, then sealed and moved to a fume hood and stirred for 16 to 24 hours. Products were purified (when necessary) using silica gel column chromatography (Isco RediSep® normal-phase chromatography) or by preparative-scale reverse-phase HPLC.

Product isolation from a reaction mixture by preparative-scale reverse-phase HPLC was carried out using an Agilent 1200 HPLC-MSD system consisting of a 6130B single quadrupole mass-selective detector (MSD), G1315B diode array detector (DAD), G2258A autosampler, two G1361A preparative pumps, one G1379A quaternary pump with degasser, one G1312A binary pump, and three G1364B fraction collectors from Agilent Technologies (Agilent Technologies, Palo Alto, CA). System control and data analysis was performed using Agilent's ChemStation software, revision B.03.01-SR.1. A Waters SunFire C18 OBD Prep Column, 100Å, 5 µm, 19 mm X 150 mm column was used as the stationary phase (Waters Corporation, Milford, MA, USA). Gradient elution was carried out using water with 0.1% trifluoroacetic acid (solvent A) and acetonitrile with 0.1% trifluoroacetic acid (solvent B) as a mobile phase. Purification under basic conditions employed water with 0.1% NH_4OAc (solvent A) and acetonitrile with 0.1% NH_4OAc (solvent B) as the mobile phase. Electrospray (ESI) mass-triggered fraction collection was employed using positive ion polarity scanning to monitor for the target mass. Products with basic functionality that were purified under acidic conditions were assumed to be TFA salts when calculating yield.

Time (min)	% MeCN (solvent B)	Flow rate (mL/min)
0.0	2	25
3.0	2	35
33.0	95	35
33.1	100	40
36.1	100	50
36.8/end	2	25

NMR spectra were acquired on a Bruker Avance 600 MHz spectrometer equipped with a sample changer. Chemical shifts are reported as parts per million (ppm) downfield from tetramethylsilane and referenced to solvent (e.g. DMSO-d_6). NMR data are represented as follows: chemical shift, multiplicity (s = singlet, br s = broad singlet, d = doublet, dd = doublet of doublet, t = triplet, q = quartet, m = multiplet, etc.), coupling constant, and integration. Coupling constants (*J*) are given in Hertz (Hz). For products isolated as TFA salts the ^{13}C NMR signals for trifluoroacetate are sometimes, but not always visible in product ^{13}C NMR spectra. High-resolution mass spectrometry for characterization and affinity-based ranking were acquired using a Thermo Scientific™ Q Exactive™ Hybrid Quadrupole-Orbitrap high-resolution, accurate-mass (HRAM) Mass Spectrometer. A Waters ACQUITY QDa mass detector was used (ESI positive ionization mode, looking for $[M+H]^+$) for product detection in high-throughput LC-MS reaction screening (details below). Residual palladium levels in pooled ASMS libraries were measured by inductively coupled plasma mass spectrometry (ICP-MS) and reported as parts per million (ppm). Instrument used: Agilent 7700 Quadruple ICP-MS (EA-12).

All half maximal inhibitory concentration values (IC_{50}, reported in nM or µM) for compounds presented in the manuscript and supporting information targeting mitogen-activated protein kinase-activated protein kinase 2 (MK2 or MAPKAPK2) and checkpoint kinase 1 (CHK1 or CHEK1), were measured using the Invitrogen SelectScreen® Biochemical Kinase Profiling Service (Thermo Fisher Scientific Corp., Madison, WI, USA). Previously reported compounds that were synthesized and subjected to affinity ranking were also measured using the SelectScreen® Biochemical Kinase Profiling Service for consistency.

Recombinant extracellular signal-regulated kinase 2, pERK2 (6His-humERK2(4-360)/pT7-5, 42307 Da without the first Met and 2P by Mass Spectrometry), was prepared by expression in Escherichia Coli cells BL21 (DE3) cells by the Merck & Co., Inc.

structural chemistry group and purified by affinity chromatography according to standard procedures. Checkpoint kinase 1, CHK1 (6His-humCHK1(2-274), 31410 Da), was produced in insect cells for crystallization by the Merck & Co., Inc. structural chemistry group and purified by affinity chromatography according to standard procedures (*J. Biol. Chem.* **2002**, *277*, 46609-46615). Mitogen-activated protein kinase-activated protein kinase 2, MK2 or MAPKAPK2, was purchased from Carna Biosciences, Inc. (Chuo-ku, Kobe, Japan) at a concentration of 687 µg/mL in storage buffer. According to the product description: full-length human MAPKAPK2 was prepared using a baculovirus expression system and purified by using glutathione sepharose chromatography and Ni-NTA chromatography.

1.2. High-Throughput Experimentation

Nanomole-scale synthesis (1 µL volume reactions in a 1,536-well microplate) was performed using the TTP Labtech Mosquito® HTS liquid handling robot inside a glove box under an N_2 atmosphere. In all cases, a 384-well source plate was created containing all required reagents, catalysts, and building blocks (Greiner polypropylene deepwell 384-well plate, cat. no. 784201). The Mosquito® was used to dispense from the source plate into the 1,536-well reaction plate (Analytical Sales and Services, 20 µL polypropylene plate, cat. no. 15020). After the nano-scale reactions were quenched, 1 µL of each quenched reaction was transferred, using the Mosquito®, from the reaction plate to a 384-well analytical plate (Greiner polypropylene deepwell 384-well plate, cat. no. 784201) and diluted with DMSO (multiple 384-well analytical plates were required when the total number of reactions exceeded 384). Images are shown below of key components of this miniaturized synthesis and screening platform for reference. For a detailed step-by-step reaction setup guide to nanomole-scale HTE using the TTP Labtech Mosquito®, including images, see the preceding publication (Santanilla, A. B. et al. *Science* **2015**, *347*, 49–53).[8]

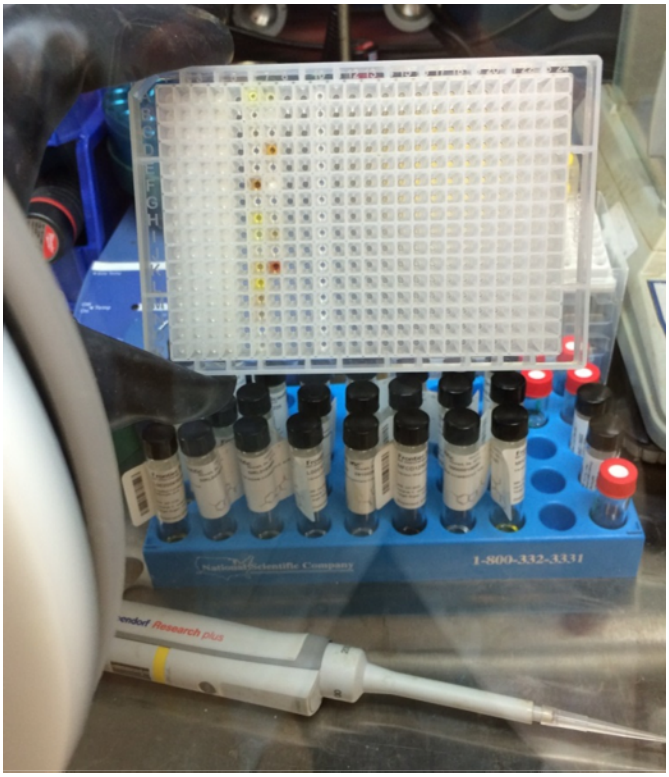


Figure 1. A source plate containing reagent stock solutions. Stock solutions were dispensed into a Greiner polypropylene deepwell 384-well plate in a predetermined order for reaction assembly using Mosquito® HTS

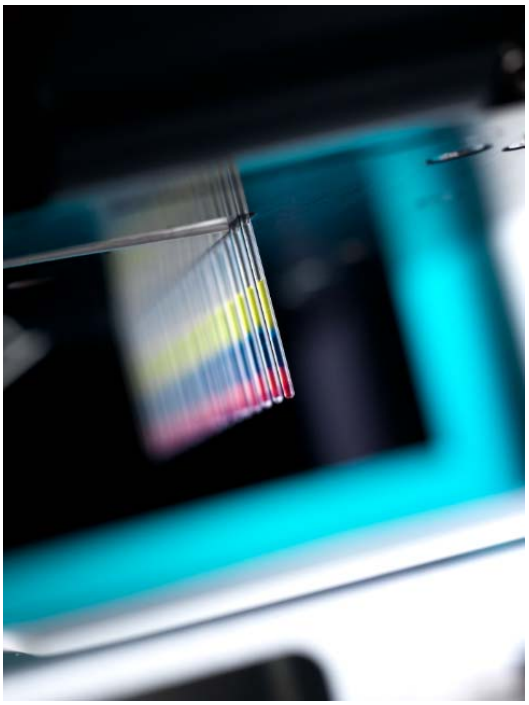


Figure 2. TTP Labtech Mosquito® HTS liquid handling robot, equipped with 1200 nL tips, utilizing the multi-aspiration feature to prepare reactions from reagent stock solutions (Image credit: TTP Labtech).

High-throughput analytical reaction screening was performed with a Waters *I*-class ACQUITY UPLC-MS (Waters Corporation, Milford, MA, USA) equipped with in-line photodiode array detector (PDA) and QDa mass detector (ESI positive ionization mode). One µL sample injections were taken from 384-well plates (samples diluted in DMSO, 1 µL quenched reaction into 60 µL DMSO). A partial loop injection mode was used with the needle placement at 1.0 mm from bottom of the wells and a 0.2 µL air gap at pre-aspiration and post-aspiration. Column used: Waters Cortecs UPLC C18+ column, 2.1mm x 50 mm with (Waters #186007114) with Waters Cortecs UPLC C18+ VanGuard Pre-column 2.1mm x 5 mm (Waters #186007125), Mobile Phase A: 0.1 % formic acid in Optima LC/MS-grade water, Mobile Phase B: 0.1% formic acid in Optima LC/MS-grade MeCN. Flow rate: 1 mL/min. Column temperature: 45 ˚C. The PDA sampling rate was 20 points/sec. The QDa detector monitored *m/z* 150-750 with a scan time of 0.06 seconds and a cone voltage of 30 V. 1 minute and 2 minute methods were used when possible, but the method was tailored for improved resolution when necessary. Sample method gradients:

1 minute method.

Time (min)	% MeCN (solvent B)	Flow rate (mL/min)
0.0	5	1
0.75	100	1
0.98	100	1
0.99/end	5	1

2 minute method.

Time (min)	% MeCN (solvent B)	Flow rate (mL/min)
0.0	5	1
1.5	100	1
1.96	100	1
1.98/end	5	1

Sample custom method.

Time (min)	% MeCN (solvent B)	Flow rate (mL/min)
0.0	5	1
0.55	40	1
1.02	100	1
1.35	100	1
1.37/end	5	1

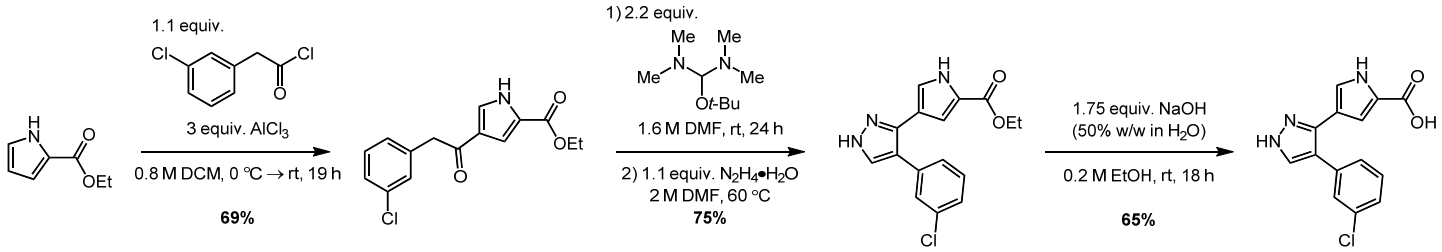
After LC-MS data acquisition, sample data were processed using Virscidian Analytical Studio software (version 4.8). Product UV peak area (210 nm or 248 nm) was used to judge reaction efficiency (relative to remaining starting material, relative to an internal standard, or by plugging into a standard curve).

For affinity ranking by ASMS, the crude reaction mixtures were transferred from the 1,536-well reaction plate to 384-well LDV diamond plates (Labcyte Echo® qualified, LP-0200) and further diluted to 10 mM final concentration with DMSO.

Data visualization was typically performed using the TIBCO® Spotfire® software suite (Build version 7.0.2.8) or in Rstudio (Version 1.0.143). All heat maps, scatter plots, bar charts, and other visualizations presented herein were constructed in Spotfire® after importing data from Microsoft Excel (2010, version 14.0.7177.5000).

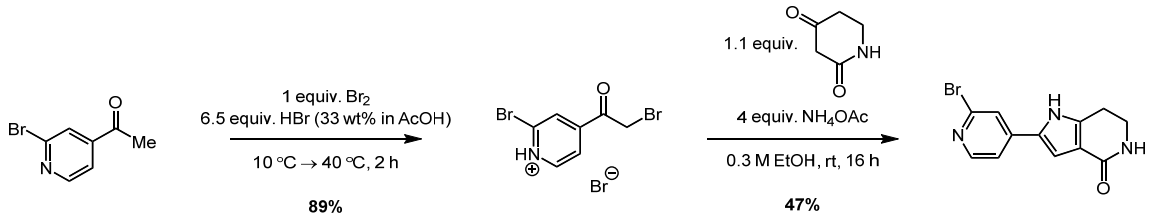
2. Substrate Synthesis

Synthesis of 4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrole-2-carboxylic acid (1)



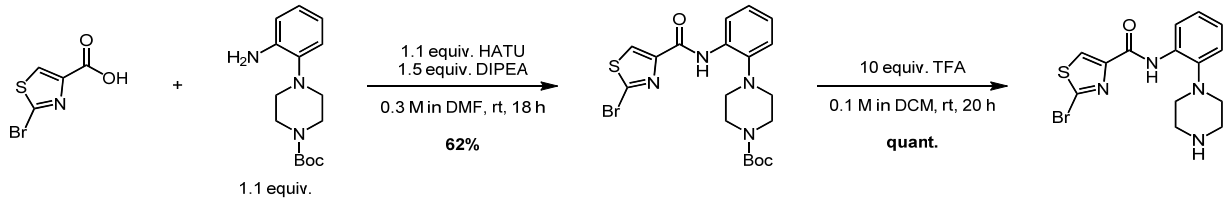
The pyrrole-2-caboxylic acid core was prepared according to published literature procedures and spectral data for the final product were in agreement with reported literature values.[6] Analytical data for **1**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.69 (br s, 2H), 11.93 (br s, 1H), 7.73 (s, 1H), 7.41 (s, 1H), 7.36 (m, 2H), 7.30 (d, *J* = 7.6 Hz, 1H), 7.02 (s, 1H), 6.79 (s, 1H); **HRMS**: *m/z* calculated for $C_{14}H_{11}ClN_3O_2$ [M+H]+ 288.05345, found 288.05362.

Synthesis of 2-(2-bromopyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (4):



Prepared according to published route, however substituting 1-(2-bromopyridin-4-yl)ethan-1-one (shown above) in place of 1-(2-chloropyridin-4-yl)ethan-1-one.[7] The procedure was not otherwise altered. Analytical data for **4**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.00 (s, 1H), 8.24 (d, *J* = 5.2 Hz, 1H), 7.86 (s, 1H), 7.65 (d, *J* = 4.9 Hz, 1H), 7.12 (s, 1H), 7.10 (s, 1H), 3.39 (t, *J* = 5.5 Hz, 2H), 2.83 (t, *J* = 6.7 Hz, 2H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 164.6, 150.5, 142.4, 142.0, 139.8, 127.0, 120.6, 117.2, 116.0, 108.0, 40.0, 21.8; **HRMS**: *m/z* calculated for $C_{12}H_{11}BrN_3O$ [M+H]+ 292.00802, found 292.00769.

Synthesis of 2-bromo-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (7):



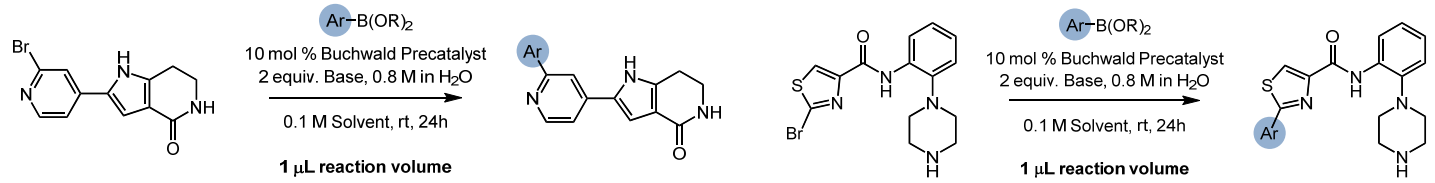
Prepared according to a published route, spectral data were in agreement with reported literature values.[5] Analytical data for **7**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.26 (s, 1H), 8.46 (s, 1H), 8.36 (d, *J* = 7.8 Hz, 1H), 7.25 (d, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.3 Hz, 1H), 7.11 (t, *J* = 7.1 Hz, 1H), 2.95 (m, 4H), 2.76 (m, 4H); **HRMS**: *m/z* calculated for $C_{14}H_{16}BrN_4OS$ [M+H]+ 367.02229, found 367.02277.

3. Reaction Optimization via Nanomole-Scale High-Throughput Experimentation (HTE)

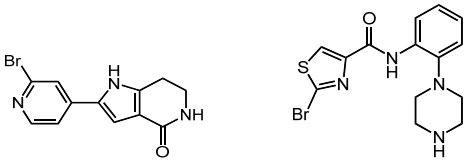
3.1. General HTE Procedure and HTE Notes

All reactions were prepared at the 1 µL scale (0.1 M, 100 nmol) or 1.2 µL scale (0.1 M, 120 nmol) using the TTP Labtech Mosquito®HTS liquid handling robot inside an N_2 atmosphere glove box. For each screen a 384-well polypropylene source plate was prepared with stock solutions of all reagents, catalysts, substrates, etc. The TTPLabTech Mosquito®HTS was used to dispense from the 384-well source plate into the 1,536-well reaction plate (mixing upon dispense, 3×750 nL). After dispensing the reaction plate was sealed, centrifuged, and allowed to sit at ambient temperature in the glove box for 18 to 24 hours. The next morning the reactions were quenched by the addition of 3×1 µL 0.5 M AcOH in DMSO (containing PhPh internal standard) to each reaction well, mixing upon dispense. 1 µL of each quenched reaction (4 µL total volume) was transferred from the 1,536 plate reaction well into a 384-well analytical plate containing 60 µL DMSO per well. The plate was sealed, shaken, then analyzed by LC-MS. For screens where the total number of reactions was greater than 384, multiple 384-well analytical plates were prepared. For example, a 1,536 reaction screen requires four 384-well analytical plates. For additional background and instruction on liquid-handling robot enabled nanomole-scale HTE and reaction screening, consult the referenced seminal publication.[8]

3.2. Nanomole-Scale Suzuki Cross-Coupling Reaction Screen

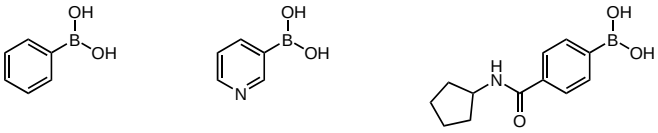


Two aryl halide cores examined (0.4 M stock in NMP): 2-(2-bromopyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (left, **4**) and 2-bromo-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (right, **7**)**. 4 equiv. H_2O added to each core stock solution in advance of source plate preparation.**

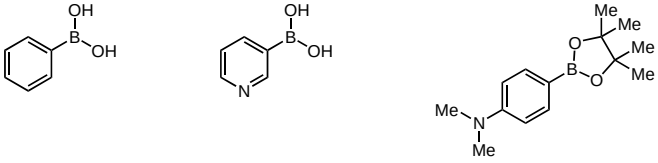


Three aryl boronic acids (esters) tested per core (1.5 equiv., 0.6 M stock in NMP):

phenylboronic acid (MFCD00002103), 3-pyridylboronic acid (MFCD00674177), [4-(cyclopentylcarbamoyl)phenyl]boronic acid (MFCD03788418) tested against 2-(2-bromopyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one.

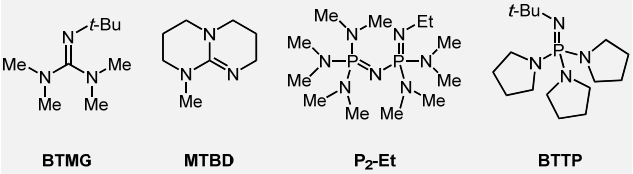


phenylboronic acid (MFCD00002103), 3-pyridylboronic acid (MFCD00674177), N,N-dimethyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (MFCD05663854) tested against 2-bromo-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide.



Eight palladium Buchwald precatalysts tested for each reaction (10 mol % loading, 0.04 M stock in NMP): XPhos G3, *t*-BuXphos G3, *t*-Bu_3P G2, DTBPF G3, SPhos G2, RuPhos G3, BrettPhos G3, and APhos G3

Fourteen solvent (+cosolvent) / base combinations tested per reaction (2 equiv., 0.8 M stock in solvent):



BTMG = 2-*tert*-Butyl-1,1,3,3-tetramethylguanidine

MTBD = 7-Methyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene

P_2-Et = 1-Ethyl-2,2,4,4,4-pentakis(dimethylamino)-2λ5,4λ5-catenadi(phosphazene)

BTTP = *tert*-Butylimino-tri(pyrrolidino)phosphorane

1. P_2-Et dispensed in NMP (column 9) Final reaction solvent: NMP
2. BTTP dispensed in NMP. (column 10) Final reaction solvent: NMP
3. BTMG dispensed in NMP (column 11) Final reaction solvent: NMP
4. MTBD dispensed in NMP (column 12) Final reaction solvent: NMP
5. P_2-Et dispensed in 40% *t*-AmOH/NMP (column 13) Final reaction solvent: 10% *t*-AmOH/NMP
6. BTTP dispensed in 40% *t*-AmOH/NMP (column 14) Final reaction solvent: 10% *t*-AmOH/NMP
7. BTMG dispensed in 40% *t*-AmOH/NMP (column 15) Final reaction solvent: 10% *t*-AmOH/NMP)
8. MTBD dispensed in 40% *t*-AmOH/NMP (column 16) Final reaction solvent: 10% *t*-AmOH/NMP
9. P_2-Et dispensed in H_2O (column 17) Final reaction solvent: 25% H_2O/NMP
10. BTTP dispensed in H_2O (column 18) Final reaction solvent: 25% H_2O/NMP
11. BTMG dispensed in H_2O (column 19) Final reaction solvent: 25% H_2O/NMP
12. MTBD dispensed in H_2O (column 20) Final reaction solvent: 25% H_2O/NMP
13. K_3PO_4 dispensed in H_2O (column 21) Final reaction solvent: 25% H_2O/NMP
14. Cs_2CO_3 dispensed in H_2O (column 22) Final reaction solvent: 25% H_2O/NMP

Source plate arrayed according to Figure 3below.

Synthesis	Core	Building Blocks	NMP Wash	Catalyst 1	Catalyst 2	Catalyst 3	Catalyst 4	NMP Wash	P2-Et in NMP	BTTP in NMP	BTMG in NMP	MTBD in NMP	P2-Et in NMP/tAmOH	BTTP in NMP/tAmOH	BTMG in NMP/tAmOH	MTBD in NMP/tAmOH	P2-Et in water	BTTP in water	BTMG in water	MTBD in water	K3PO4 in water	Cs2CO3 in water	23	24
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22		
A	Pyrydyl Core	MFCD00002103	NMP	Xphos G3	tBuXphos G3	tBu3P G2	DTBPF G3	NMP	P2-Et	BTTP	BTMG	MTBD	AmOH P2Et	AmOH BTTP	AmOH BTMG	AmOH MTBD	aq P2Et	aq BTTP	aq BTMG	aq MTBD	aq K3PO4	aq Cs2CO3			
B	Pyrydyl Core	MFCD00002103	NMP	Sphos G2	RuPhos G3	BrettPhos G3	Aphos G3	NMP	P2-Et	BTTP	BTMG	MTBD	AmOH P2Et	AmOH BTTP	AmOH BTMG	AmOH MTBD	aq P2Et	aq BTTP	aq BTMG	aq MTBD	aq K3PO4	aq Cs2CO3			
C	Pyrydyl Core	MFCD00674177	NMP	Xphos G3	tBuXphos G3	tBu3P G2	DTBPF G3	NMP	P2-Et	BTTP	BTMG	MTBD	AmOH P2Et	AmOH BTTP	AmOH BTMG	AmOH MTBD	aq P2Et	aq BTTP	aq BTMG	aq MTBD	aq K3PO4	aq Cs2CO3			
D	Pyrydyl Core	MFCD00674177	NMP	Sphos G2	RuPhos G3	BrettPhos G3	Aphos G3	NMP	P2-Et	BTTP	BTMG	MTBD	AmOH P2Et	AmOH BTTP	AmOH BTMG	AmOH MTBD	aq P2Et	aq BTTP	aq BTMG	aq MTBD	aq K3PO4	aq Cs2CO3			
E	Pyrydyl Core	MFCD03788418	NMP	Xphos G3	tBuXphos G3	tBu3P G2	DTBPF G3	NMP	P2-Et	BTTP	BTMG	MTBD	AmOH P2Et	AmOH BTTP	AmOH BTMG	AmOH MTBD	aq P2Et	aq BTTP	aq BTMG	aq MTBD	aq K3PO4	aq Cs2CO3			
F	Pyrydyl Core	MFCD03788418	NMP	Sphos G2	RuPhos G3	BrettPhos G3	Aphos G3	NMP	P2-Et	BTTP	BTMG	MTBD	AmOH P2Et	AmOH BTTP	AmOH BTMG	AmOH MTBD	aq P2Et	aq BTTP	aq BTMG	aq MTBD	aq K3PO4	aq Cs2CO3			
G																								
H																								
I	Thiazole Core	MFCD00002103	NMP	Xphos G3	tBuXphos G3	tBu3P G2	DTBPF G3	NMP	P2-Et	BTTP	BTMG	MTBD	AmOH P2Et	AmOH BTTP	AmOH BTMG	AmOH MTBD	aq P2Et	aq BTTP	aq BTMG	aq MTBD	aq K3PO4	aq Cs2CO3			
J	Thiazole Core	MFCD00002103	NMP	Sphos G2	RuPhos G3	BrettPhos G3	Aphos G3	NMP	P2-Et	BTTP	BTMG	MTBD	AmOH P2Et	AmOH BTTP	AmOH BTMG	AmOH MTBD	aq P2Et	aq BTTP	aq BTMG	aq MTBD	aq K3PO4	aq Cs2CO3			
K	Thiazole Core	MFCD00674177	NMP	Xphos G3	tBuXphos G3	tBu3P G2	DTBPF G3	NMP	P2-Et	BTTP	BTMG	MTBD	AmOH P2Et	AmOH BTTP	AmOH BTMG	AmOH MTBD	aq P2Et	aq BTTP	aq BTMG	aq MTBD	aq K3PO4	aq Cs2CO3			
L	Thiazole Core	MFCD00674177	NMP	Sphos G2	RuPhos G3	BrettPhos G3	Aphos G3	NMP	P2-Et	BTTP	BTMG	MTBD	AmOH P2Et	AmOH BTTP	AmOH BTMG	AmOH MTBD	aq P2Et	aq BTTP	aq BTMG	aq MTBD	aq K3PO4	aq Cs2CO3			
M	Thiazole Core	MFCD05663854	NMP	Xphos G3	tBuXphos G3	tBu3P G2	DTBPF G3	NMP	P2-Et	BTTP	BTMG	MTBD	AmOH P2Et	AmOH BTTP	AmOH BTMG	AmOH MTBD	aq P2Et	aq BTTP	aq BTMG	aq MTBD	aq K3PO4	aq Cs2CO3			
N	Thiazole Core	MFCD05663854	NMP	Sphos G2	RuPhos G3	BrettPhos G3	Aphos G3	NMP	P2-Et	BTTP	BTMG	MTBD	AmOH P2Et	AmOH BTTP	AmOH BTMG	AmOH MTBD	aq P2Et	aq BTTP	aq BTMG	aq MTBD	aq K3PO4	aq Cs2CO3			
O																								
P																								

Figure 3. Suzuki Reaction Screen Source Plate

TTP Labtech Mosquito®HTS liquid handling robot used to generate reaction plate containing all possible reaction conditions per aryl halide core/boronic acid building block combination. 8 catalysts × 14 solvent/base combinations = 112 reaction conditions. 6 core/building block combinations × 112 conditions = 672 reaction screen. Results of this screen plotted below as a heat map arrayed by reaction conditions. Reactions are represented by product peak area versus internal standard (PhPh) peak area ratio.

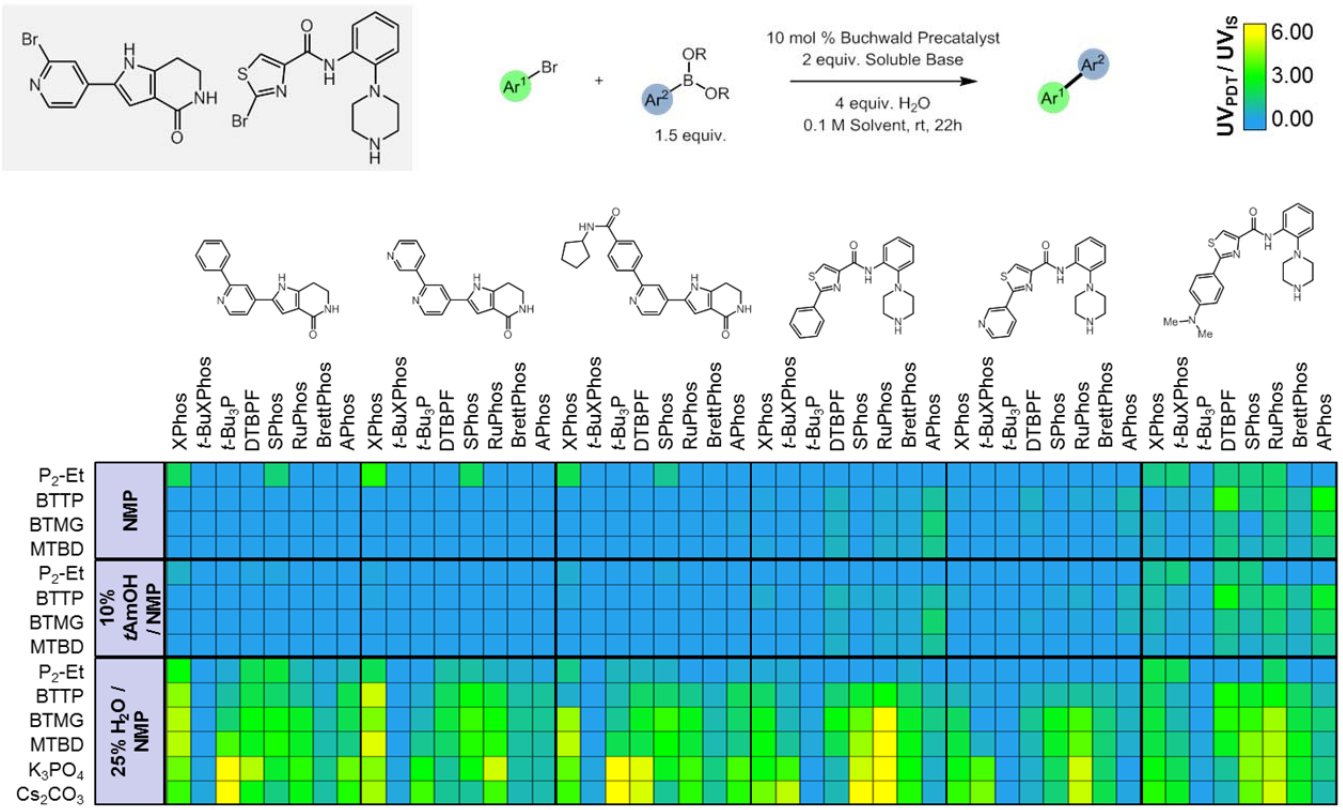
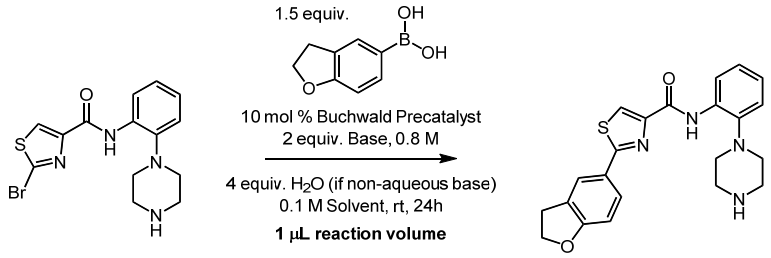


Figure 4. Suzuki Coupling Screen Heat Map

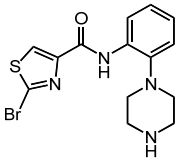
Continued optimization around each aryl halide core, focusing on solvent (+cosolvent) and catalyst/ligand yielded the optimized Suzuki coupling conditions displayed in the manuscript and supporting information. Tabulated reaction data are provided in supplementary Excel tables.

3.3. Supplementary Suzuki Cross-Coupling Screen on 2-Bromothiazole Core 7 to form D6

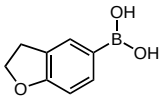


Three solvents tested: NMP, DMSO, and DMF

One aryl halide core examined (0.4 M stock in each solvent): 2-bromo-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (**7**). **4 equiv. H_2O added to each core stock solution in advance of source plate preparation.**

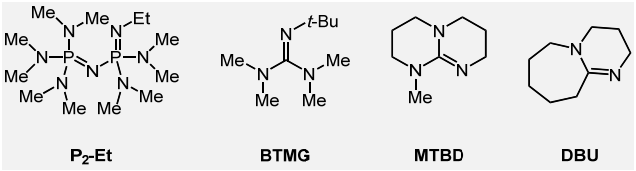


One boronic acid tested (1.5 equiv., 0.6 M stock in each solvent): 2,3-dihydrobenzofuran-5-boronic acid (MFCD02681979)



Six palladium Buchwald precatalysts tested (10 mol % loading, 0.04 M stock in each solvent): XPhos G3, *t*-BuXphos G3, SPhos G2, RuPhos G3, BrettPhos G3, and APhos G3

Nine solvent (+cosolvent) / base combinations tested per reaction (2 equiv., 0.8 M stock in solvent, column indicated):



DBU = 1,8-Diazabicyclo[5.4.0]undec-7-ene

1. P_2-Et dispensed in H_2O (column 11) Final reaction solvent: 25% H_2O in NMP, DMSO, or DMF
2. BTMG dispensed in H_2O (column 12) Final reaction solvent: 25% H_2O in NMP, DMSO, or DMF
3. MTBD dispensed in H_2O (column 13) Final reaction solvent: 25% H_2O in NMP, DMSO, or DMF
4. DBU dispensed in H_2O (column 14) Final reaction solvent: 25% H_2O in NMP, DMSO, or DMF
5. K_3PO_4 dispensed in H_2O (column 15) Final reaction solvent: 25% H_2O in NMP, DMSO, or DMF
6. Cs_2CO_3 dispensed in H_2O (column 16) Final reaction solvent: 25% H_2O in NMP, DMSO, or DMF
7. P_2-Et dispensed in NMP, DMSO, or DMF (column 17) Final reaction solvent: NMP, DMSO, or DMF
8. BTMG dispensed in NMP, DMSO, or DMF (column 18) Final reaction solvent: NMP, DMSO, or DMF
9. DBU dispensed in NMP, DMSO, or DMF (column 19) Final reaction solvent: NMP, DMSO, or DMF

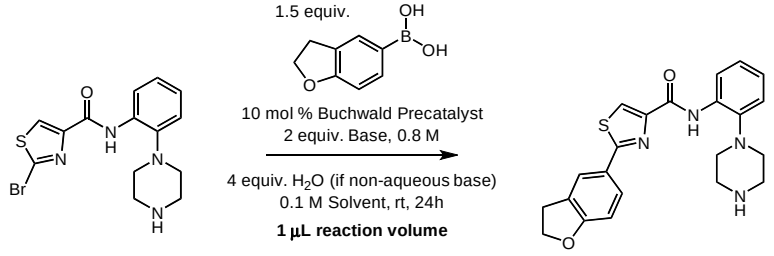
Source plate arrayed according to Figure 5 below.

		CHK1 Core		Building Block			Wash Solvent	Catalyst 1	Catalyst 2	Wash Solvent		Base 1	Base 2	Base 3	Base 4	Base 5	Base 6	Base 7	Base 8	Base 9					
		20 uL		20 uL			50 uL	30 uL	30 uL	50 uL		35 uL	35 uL	35 uL	35 uL	35 uL	35 uL	35 uL	35 uL	35 uL					
Solvent		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
NMP	A	Core NMP		MFCD02681979			NMP	Xphos G3	tBuXphos G3	NMP		aq. P2Et	aq. BTMG	aq. MTBD	aq. DBU	aq. K3PO4	aq. Cs2Co3	P2Et NMP	BTMG NMP	DBU NMP					
NMP	B	Core NMP		MFCD02681979			NMP	Sphos G2	RuPhos G3	NMP		aq. P2Et	aq. BTMG	aq. MTBD	aq. DBU	aq. K3PO4	aq. Cs2Co3	P2Et NMP	BTMG NMP	DBU NMP					
NMP	C	Core NMP		MFCD02681979			NMP	BrettPhos G3	Aphos G3	NMP		aq. P2Et	aq. BTMG	aq. MTBD	aq. DBU	aq. K3PO4	aq. Cs2Co3	P2Et NMP	BTMG NMP	DBU NMP					
DMSO	D	Core DMSO		MFCD02681979			DMSO	Xphos G3	tBuXphos G3	DMSO		aq. P2Et	aq. BTMG	aq. MTBD	aq. DBU	aq. K3PO4	aq. Cs2Co3	P2Et DMSO	BTMG DMSO	DBU DMSO					
DMSO	E	Core DMSO		MFCD02681979			DMSO	Sphos G2	RuPhos G3	DMSO		aq. P2Et	aq. BTMG	aq. MTBD	aq. DBU	aq. K3PO4	aq. Cs2Co3	P2Et DMSO	BTMG DMSO	DBU DMSO					
DMSO	F	Core DMSO		MFCD02681979			DMSO	BrettPhos G3	Aphos G3	DMSO		aq. P2Et	aq. BTMG	aq. MTBD	aq. DBU	aq. K3PO4	aq. Cs2Co3	P2Et DMSO	BTMG DMSO	DBU DMSO					
DMF	G	Core DMF		MFCD02681979			DMF	Xphos G3	tBuXphos G3	DMF		aq. P2Et	aq. BTMG	aq. MTBD	aq. DBU	aq. K3PO4	aq. Cs2Co3	P2Et DMF	BTMG DMF	DBU DMF					
DMF	H	Core DMF		MFCD02681979			DMF	Sphos G2	RuPhos G3	DMF		aq. P2Et	aq. BTMG	aq. MTBD	aq. DBU	aq. K3PO4	aq. Cs2Co3	P2Et DMF	BTMG DMF	DBU DMF					
DMF	I	Core DMF		MFCD02681979			DMF	BrettPhos G3	Aphos G3	DMF		aq. P2Et	aq. BTMG	aq. MTBD	aq. DBU	aq. K3PO4	aq. Cs2Co3	P2Et DMF	BTMG DMF	DBU DMF					
	J																								
	K																								
	L																								
	M																								
	N																								
	O																								
	P																								

Figure 5. Source Plate Map for Supplementary Suzuki Cross-Coupling Screen

TTP Labtech Mosquito®HTS liquid handling robot was used to generate reaction plate containing all possible reaction conditions per aryl halide core/amine nucleophile building block combination. 6 catalysts × 3 main solvents × 9 base/cosolvent combinations = 162 reaction conditions. 1 core/building block combination × 162 conditions = 162 reaction screen. Results of this screen are plotted below as a heat map arrayed by reaction conditions. Reactions are represented by product peak area versus internal standard (PhPh) peak area ratio. Tabulated reaction data are provided in supplementary Excel tables.

Note: An additional boronic ester building block was originally included in this screen in Column 4 of the source plate, however analytical instrumentation errors prevented proper analysis of the series using that building block, leaving the screen and results shown.



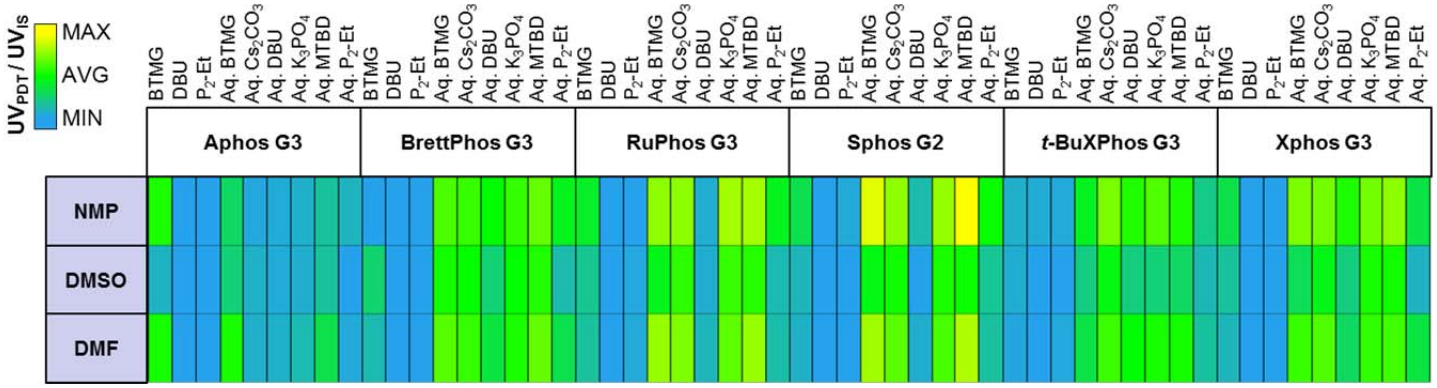
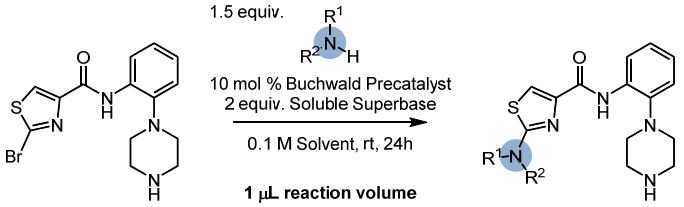


Figure 6. Supplementary Suzuki Cross-Coupling Heat Map

3.4. First Nanomole-Scale Buchwald-Hartwig Amination Screen on 2-Bromothiazole Core 7

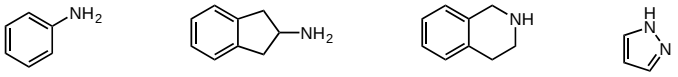


Two smaller C-N coupling optimization screens were performed, testing a range of amine nucleophiles in a system with core 2-bromo-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (above, **7**).

Two solvents tested: NMP and DMSO

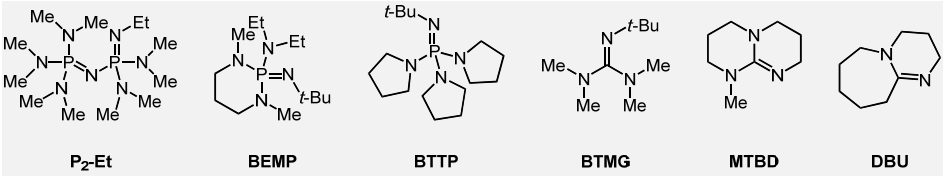
Four amine building blocks tested (1.5 equiv., 0.6 M stock in NMP and DMSO):

- aniline (MFCD00007629)
- 2,3-dihydro-1H-inden-2-amine (MFCD00082597)
- 1,2,3,4-tetrahydroisoquinoline (MFCD00006896)
- pyrazole (MFCD00005234)
- Benzylamine and isoindoline were part of this experiment but were excluded from visualization due to presence in next optimization experiment



Eight Buchwald precatalysts tested for each reaction (10 mol % loading, 0.04 M stock in NMP and DMSO): XPhos G3, tBuXphos G3, BrettPhos G3, tBuBrettPhos G3, RuPhos G3, RockPhos G3, JackiePhos G3, CPhos G3

Six organic-soluble superbases tested for each reaction (2 equiv., 0.8 M stock in NMP and DMSO):



BEMP = 2-*tert*-Butylimino-2-diethylamino-1,3-dimethylperhydro-1,3,2-diazaphosphorine

1. P_2-Et (column 12)
2. BEMP (column 13)
3. BTTP (column 14)
4. BTMG (column 15)
5. MTBD (column 16)
6. DBU (column 17)

6 bases × 2 solvents = 12 solvent/base combinations. Source plate arrayed according to Figure 7 below.

Synthesis	Solvent	Core		Building block		Catalyst 1	catalyst 2	catalyst 3	catalyst 4		Wash solvent		P2-Et	BEMP	BTTP	BTMG	MTBD	DBU							
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	NMP	Core NMP		MFCD00007629 NMP		Xphos G3	tBuXphos G3	BrettPhos G3	tBuBrettphos G3		NMP		P2-Et NMP	BEMP NMP	BTTP NMP	BTMG NMP	MTBD NMP	DBU NMP							
B	NMP	Core NMP		MFCD00007629 NMP		RuPhos G3	RockPhos G3	JackiePhos G3	Cphos G3		NMP		P2-Et NMP	BEMP NMP	BTTP NMP	BTMG NMP	MTBD NMP	DBU NMP							
C	NMP	Core NMP		MFCD00082597 NMP		Xphos G3	tBuXphos G3	BrettPhos G3	tBuBrettphos G3		NMP		P2-Et NMP	BEMP NMP	BTTP NMP	BTMG NMP	MTBD NMP	DBU NMP							
D	NMP	Core NMP		MFCD00082597 NMP		RuPhos G3	RockPhos G3	JackiePhos G3	Cphos G3		NMP		P2-Et NMP	BEMP NMP	BTTP NMP	BTMG NMP	MTBD NMP	DBU NMP							
E	NMP	Core NMP		MFCD00006896 NMP		Xphos G3	tBuXphos G3	BrettPhos G3	tBuBrettphos G3		NMP		P2-Et NMP	BEMP NMP	BTTP NMP	BTMG NMP	MTBD NMP	DBU NMP							
F	NMP	Core NMP		MFCD00006896 NMP		RuPhos G3	RockPhos G3	JackiePhos G3	Cphos G3		NMP		P2-Et NMP	BEMP NMP	BTTP NMP	BTMG NMP	MTBD NMP	DBU NMP							
G	NMP	Core NMP		MFCD00005234 NMP		Xphos G3	tBuXphos G3	BrettPhos G3	tBuBrettphos G3		NMP		P2-Et NMP	BEMP NMP	BTTP NMP	BTMG NMP	MTBD NMP	DBU NMP							
H	NMP	Core NMP		MFCD00005234 NMP		RuPhos G3	RockPhos G3	JackiePhos G3	Cphos G3		NMP		P2-Et NMP	BEMP NMP	BTTP NMP	BTMG NMP	MTBD NMP	DBU NMP							
I	DMSO	Core DMSO		MFCD00007629 DMSO		Xphos G3	tBuXphos G3	BrettPhos G3	tBuBrettphos G3		DMSO		P2-Et DMSO	BEMP DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO	DBU DMSO							
J	DMSO	Core DMSO		MFCD00007629 DMSO		RuPhos G3	RockPhos G3	JackiePhos G3	Cphos G3		DMSO		P2-Et DMSO	BEMP DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO	DBU DMSO							
K	DMSO	Core DMSO		MFCD00082597 DMSO		Xphos G3	tBuXphos G3	BrettPhos G3	tBuBrettphos G3		DMSO		P2-Et DMSO	BEMP DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO	DBU DMSO							
L	DMSO	Core DMSO		MFCD00082597 DMSO		RuPhos G3	RockPhos G3	JackiePhos G3	Cphos G3		DMSO		P2-Et DMSO	BEMP DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO	DBU DMSO							
M	DMSO	Core DMSO		MFCD00006896 DMSO		Xphos G3	tBuXphos G3	BrettPhos G3	tBuBrettphos G3		DMSO		P2-Et DMSO	BEMP DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO	DBU DMSO							
N	DMSO	Core DMSO		MFCD00006896 DMSO		RuPhos G3	RockPhos G3	JackiePhos G3	Cphos G3		DMSO		P2-Et DMSO	BEMP DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO	DBU DMSO							
O	DMSO	Core DMSO		MFCD00005234 DMSO		Xphos G3	tBuXphos G3	BrettPhos G3	tBuBrettphos G3		DMSO		P2-Et DMSO	BEMP DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO	DBU DMSO							
P	DMSO	Core DMSO		MFCD00005234 DMSO		RuPhos G3	RockPhos G3	JackiePhos G3	Cphos G3		DMSO		P2-Et DMSO	BEMP DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO	DBU DMSO							

Figure 7. Source Plate for Buchwald-Hartwig Amination Screen 1

TTP Labtech Mosquito®HTS liquid handling robot was used to generate reaction plate containing all possible reaction conditions per aryl halide core/amine nucleophile building block combination. 8 catalysts × 12 solvent/base combinations = 96 reaction conditions. 4 core/building block combinations × 96 conditions = 384 reaction screen. Results of this screen are plotted below as a heat map arrayed by reaction conditions. Reactions are represented by product peak area versus internal standard (PhPh) peak area ratio. Tabulated reaction data are provided in supplementary Excel tables.

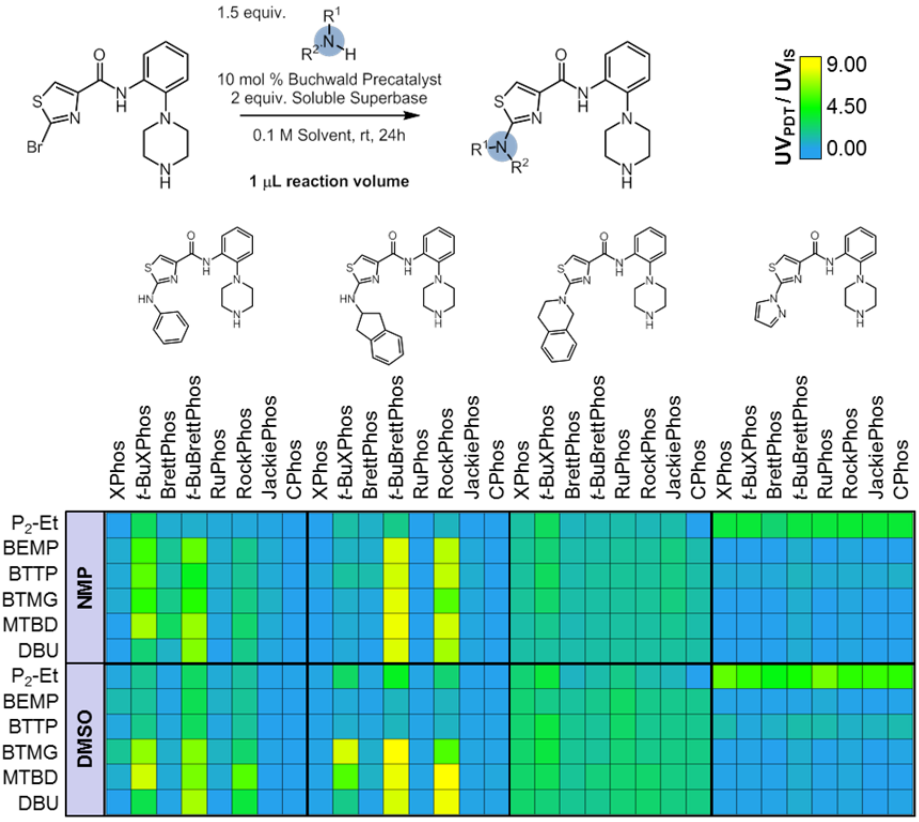
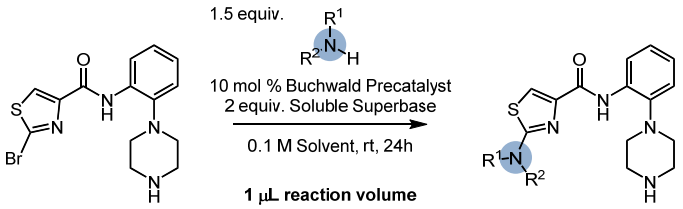


Figure 8. C-N Coupling Screen 1 Heat Map Array by Condition

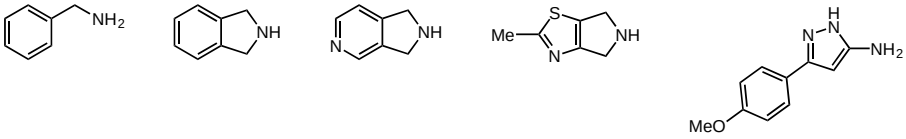
3.5. Second Nanomole-Scale Buchwald-Hartwig Amination Screen on 2-Bromothiazole Core 7



Three solvents tested: NMP, DMF, and DMSO

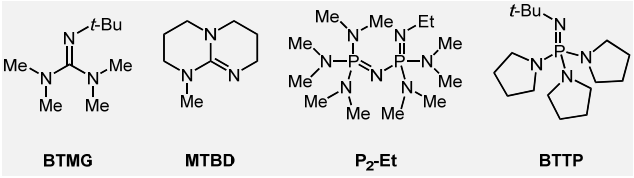
Five amine building blocks tested (1.5 equiv., 0.6 M stock in solvent):

- benzylamine (MFCD00008106)
- isoindoline (MFCD00605324)
- 2,3-dihydro-1H-pyrrolo[3,4-c]pyridine (MFCD06858479)
- 2-methyl-5,6-dihydro-4H-pyrrolo[3,4-d]thiazole (MFCD06738528)
- 3-(4-methoxyphenyl)-1H-pyrazol-5-amine (MFCD00462192)



Six Buchwald precatalysts tested for each reaction (10 mol % loading, 0.04 M stock in solvent): tBuXphos G3, BrettPhos G3, tBuBrettPhos G3, AdBrettPhos G3, RuPhos G3, RockPhos G3

Four organic-soluble superbases tested for each reaction (2 equiv., 0.8 M stock in solvent):



1. P_2-Et (column 14)
2. BTTP (column 15)
3. BTMG (column 16)
4. MTBD (column 17)

4 bases × 3 solvents = 12 solvent/base combinations. Source plate arrayed according to Figure 9 below.

		Bromide Core		Building Blocks		tBuXphos G3	BrettPhos G3	tBuBrettPhos G3	AdBrettPhos G3	RuPhos G3	RockPhos G3		Wash Solvent		P2-Et Base	BTTP Base	BTMG Base	MTBD Base								
Row	Solvent	Vol / well:	15 uL		30 uL		25 uL	25 uL	25 uL	25 uL	25 uL	25 uL		50 uL		30 uL	30 uL	30 uL	30 uL								
			1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
NMP	A		Core NMP		MFCD00008106 NMP		tBuXphos G3 NMP	BrettPhos G3 NMP	tBuBrettPhos G3 NMP	AdBrettPhos G3 NMP	Ruphos G3 NMP	RockPhos G3 NMP		NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP								
DMSO	B		Core DMSO		MFCD00008106 DMSO		tBuXphos G3 DMSO	BrettPhos G3 DMSO	tBuBrettPhos G3 DMSO	AdBrettPhos G3 DMSO	Ruphos G3 DMSO	RockPhos G3 DMSO		DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO								
DMF	C		Core DMF		MFCD00008106 DMF		tBuXphos G3 DMF	BrettPhos G3 DMF	tBuBrettPhos G3 DMF	AdBrettPhos G3 DMF	Ruphos G3 DMF	RockPhos G3 DMF		DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF								
NMP	D		Core NMP		MFCD00605324 NMP		tBuXphos G3 NMP	BrettPhos G3 NMP	tBuBrettPhos G3 NMP	AdBrettPhos G3 NMP	Ruphos G3 NMP	RockPhos G3 NMP		NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP								
DMSO	E		Core DMSO		MFCD00605324 DMSO		tBuXphos G3 DMSO	BrettPhos G3 DMSO	tBuBrettPhos G3 DMSO	AdBrettPhos G3 DMSO	Ruphos G3 DMSO	RockPhos G3 DMSO		DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO								
DMF	F		Core DMF		MFCD00605324 DMF		tBuXphos G3 DMF	BrettPhos G3 DMF	tBuBrettPhos G3 DMF	AdBrettPhos G3 DMF	Ruphos G3 DMF	RockPhos G3 DMF		DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF								
NMP	G		Core NMP		MFCD06858479 NMP		tBuXphos G3 NMP	BrettPhos G3 NMP	tBuBrettPhos G3 NMP	AdBrettPhos G3 NMP	Ruphos G3 NMP	RockPhos G3 NMP		NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP								
DMSO	H		Core DMSO		MFCD06858479 DMSO		tBuXphos G3 DMSO	BrettPhos G3 DMSO	tBuBrettPhos G3 DMSO	AdBrettPhos G3 DMSO	Ruphos G3 DMSO	RockPhos G3 DMSO		DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO								
DMF	I		Core DMF		MFCD06858479 DMF		tBuXphos G3 DMF	BrettPhos G3 DMF	tBuBrettPhos G3 DMF	AdBrettPhos G3 DMF	Ruphos G3 DMF	RockPhos G3 DMF		DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF								
NMP	J		Core NMP		MFCD06738528 NMP		tBuXphos G3 NMP	BrettPhos G3 NMP	tBuBrettPhos G3 NMP	AdBrettPhos G3 NMP	Ruphos G3 NMP	RockPhos G3 NMP		NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP								
DMSO	K		Core DMSO		MFCD06738528 DMSO		tBuXphos G3 DMSO	BrettPhos G3 DMSO	tBuBrettPhos G3 DMSO	AdBrettPhos G3 DMSO	Ruphos G3 DMSO	RockPhos G3 DMSO		DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO								
DMF	L		Core DMF		MFCD06738528 DMF		tBuXphos G3 DMF	BrettPhos G3 DMF	tBuBrettPhos G3 DMF	AdBrettPhos G3 DMF	Ruphos G3 DMF	RockPhos G3 DMF		DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF								
NMP	M		Core NMP		MFCD00462192 NMP		tBuXphos G3 NMP	BrettPhos G3 NMP	tBuBrettPhos G3 NMP	AdBrettPhos G3 NMP	Ruphos G3 NMP	RockPhos G3 NMP		NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP								
DMSO	N		Core DMSO		MFCD00462192 DMSO		tBuXphos G3 DMSO	BrettPhos G3 DMSO	tBuBrettPhos G3 DMSO	AdBrettPhos G3 DMSO	Ruphos G3 DMSO	RockPhos G3 DMSO		DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO								
DMF	O		Core DMF		MFCD00462192 DMF		tBuXphos G3 DMF	BrettPhos G3 DMF	tBuBrettPhos G3 DMF	AdBrettPhos G3 DMF	Ruphos G3 DMF	RockPhos G3 DMF		DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF								
	P																									

Figure 9. C-N Coupling Screen 2 Source Plate Map

TTP Labtech Mosquito®HTS liquid handling robot was used to generate reaction plate containing all possible reaction conditions per aryl halide core/amine nucleophile building block combination. 6 catalysts × 12 solvent/base combinations = 72 reaction conditions. 5 core/building block combinations × 72 conditions = 360 reaction screen. Results of this screen are plotted below as a heat map arrayed by reaction conditions. Reactions are represented by product peak area versus internal standard (PhPh) peak area ratio. Tabulated reaction data are provided in supplementary Excel tables.

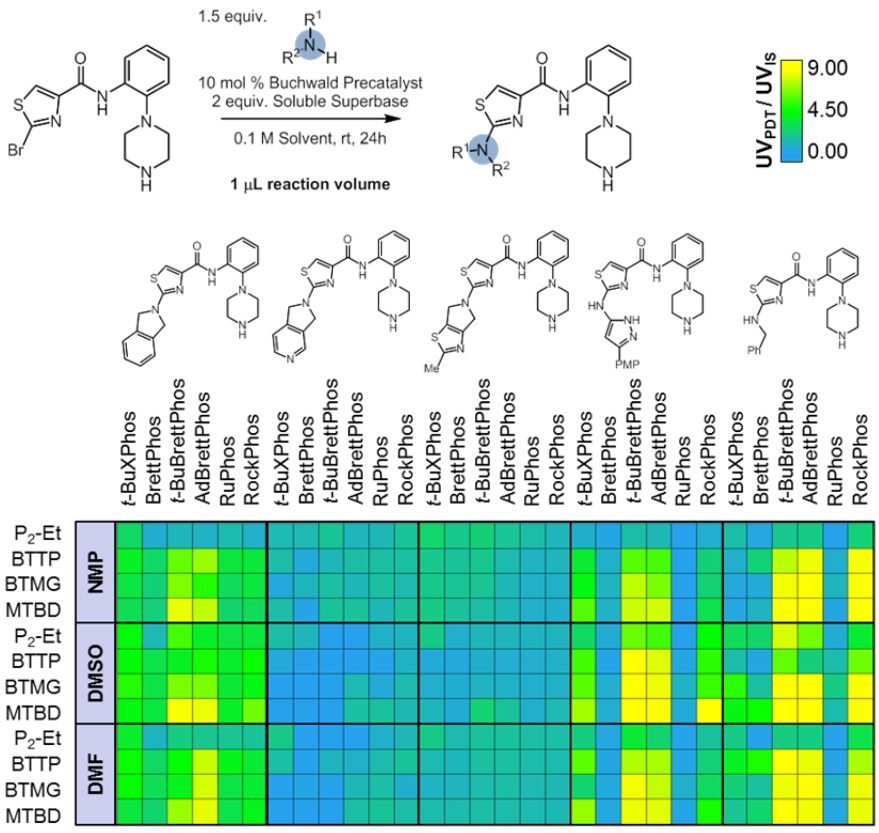
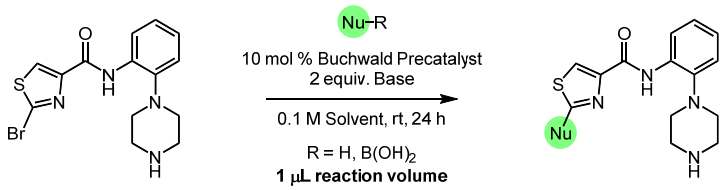


Figure 10. C-N Coupling Screen 2 Heat Map

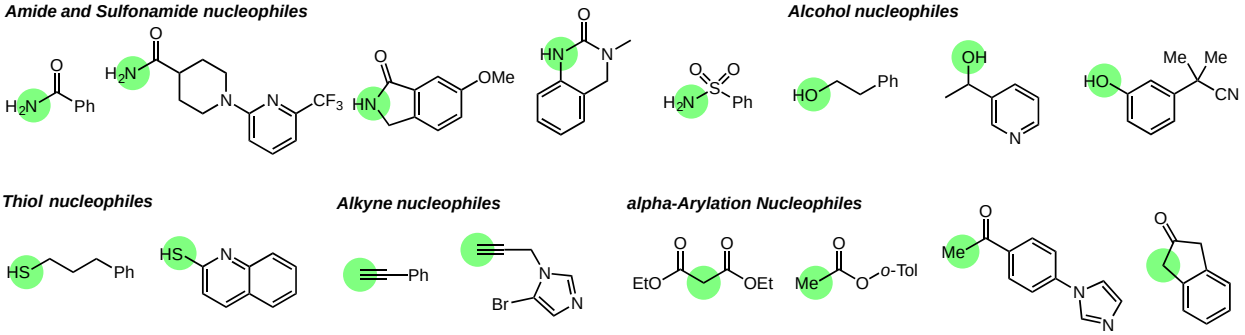
3.6. Nanomole-Scale 2-Bromothiazole Diverse Nucleophile Coupling Screen on 7



Three solvents tested: NMP, DMSO, and DMF

Sixteen nucleophile building blocks tested (1.5 equiv., 0.6 M stock in solvent)

1.	Benzamide (MFCD00007968)	amide C-N coupling
2.	1-(6-(trifluoromethyl)pyridin-2-yl)piperidine-4-carboxamide	amide C-N coupling
3.	6-methoxyisoindolin-1-one (MFCD08234735)	amide C-N coupling
4.	3-methyl-3,4-dihydroquinazolin-2(1H)-one (MFCD00192043)	urea C-N coupling
5.	Benzenesulfonamide (MFCD00007930)	sulfonamide C-N coupling
6.	2-phenylethan-1-ol (MFCD00002886)	C-O coupling
7.	1-(pyridin-3-yl)ethan-1-ol (MFCD01691686)	C-O coupling
8.	2-(3-hydroxyphenyl)-2-methylpropanenitrile (MFCD19694707)	C-O coupling
9.	3-phenylpropane-1-thiol (MFCD00004903)	C-S coupling
10.	quinoline-2-thiol (MFCD00006751)	C-S coupling
11.	phenylacetylene (MFCD00008570)	Sonogashira coupling
12.	5-bromo-1-(prop-2-yn-1-yl)-1H-imidazole	Sonogashira coupling
13.	diethyl malonate (MFCD00009195)	ester α-arylation
14.	*o*-tolyl acetate (MFCD00053704)	ester α-arylation
15.	1-(4-(1H-imidazol-1-yl)phenyl)ethan-1-one (MFCD00005282)	ketone α-arylation
16.	1,3-dihydro-2H-inden-2-one (MFCD00003792)	ketone α-arylation



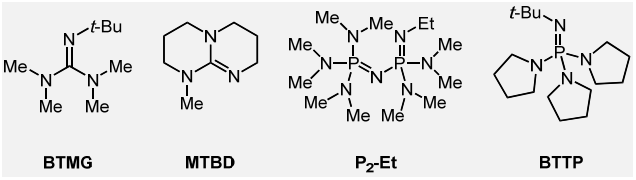
Seven (+blank) or eight Buchwald precatalysts tested for each reaction (10 mol % loading, 0.04 M stock):

	Coupling type / bond formed				
	C-N coupling	**C-O coupling**	**C-S coupling**	**Sonogashira coupling**	**alpha-arylation**
catalyst 1	BLANK/no cat.	BLANK/no cat.	BLANK/no cat.	Xphos G3	cataCXium® A G3
catalyst 2	BrettPhos G3	RuPhos G3	BINAP G3	BrettPhos G3	BINAP G3
catalyst 3	tBuBrettPhos G3	tBuBrettPhos G3	tBuBrettPhos G3	tBuBrettPhos G3	tBuBrettPhos G3
catalyst 4	AdBrettPhos G3	AdBrettPhos G3	AdBrettPhos G3	RuPhos G3	AdBrettPhos G3
catalyst 5	RockPhos G3	RockPhos G3	RockPhos G3	Aphos G3	RockPhos G3
catalyst 6	tBuXphos G3	tBuXphos G3	tBuXphos G3	tBuXphos G3	tBuXphos G3
catalyst 7	JackiePhos G3	DTBPF G3	DTBPF G3	tBu3P G3	tBu3P G3
catalyst 8	XantPhos G3	BINAP G3	XantPhos G3	XantPhos G3	XantPhos G3

Catalyst 1 – column 6 Catalyst 2 – column 7 Catalyst 3 – column 8 Catalyst 4 – column 9

Catalyst 5 – column 10 Catalyst 6 – column 11 Catalyst 7 – column 12 Catalyst 8 – column 13

Four organic-soluble superbases tested for each reaction (2 equiv., 0.8 M stock in solvent):



1. P_2-Et (column 16)
2. BTTP (column 17)
3. BTMG (column 18)
4. MTBD (column 19)

4 bases × 3 solvents × 8 catalysts = 96 solvent/base/catalyst combinations. Source plates arrayed according to below. In total three source plates were prepared: one for each solvent (NMP, DMSO, DMF). Available space on the 384-well source plate necessitated this approach.

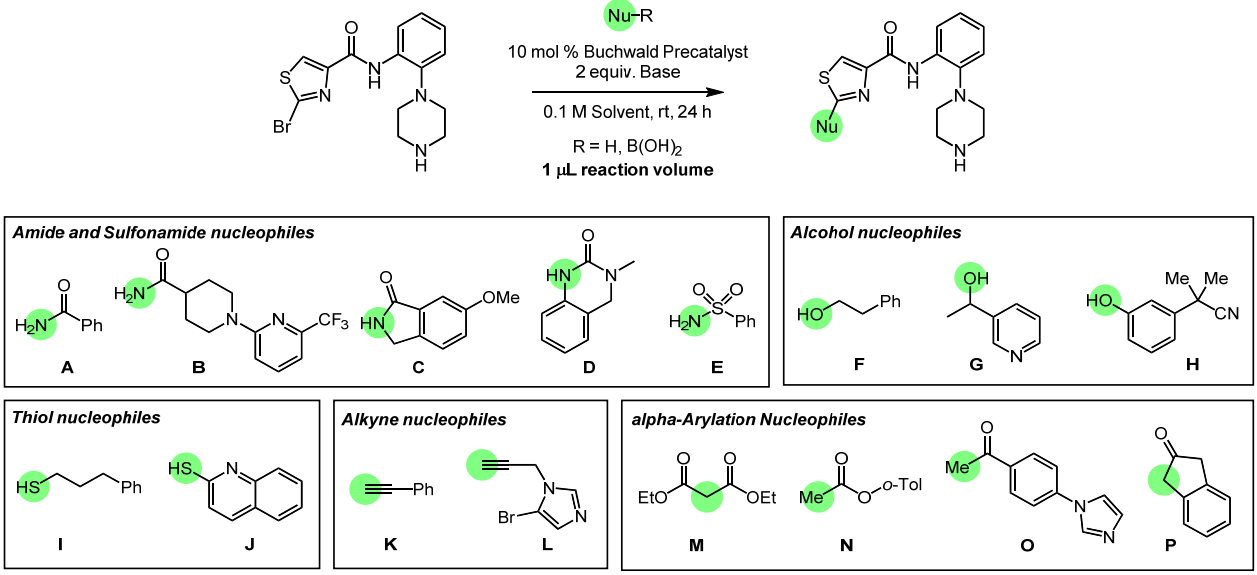
			Core		Building block		Wash solvent	catalyst 1	catalyst 2	catalyst 3	catalyst 4	catalyst 5	catalyst 6	catalyst 7	catalyst 8	Wash solvent		Base 1	Base 2	Base 3	Base 4					
			16 uL		30 uL		50 uL	20 uL	20 uL	20 uL	20 uL	20 uL	20 uL	20 uL	20 uL	50 uL		25 uL	25 uL	25 uL	25 uL					
	Solvent	Row	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
C-N Coupling	DMSO	A	Core DMSO		MFCD00007968		DMSO	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
C-N Coupling	DMSO	B	Core DMSO		CM00576334		DMSO	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
C-N Coupling	DMSO	C	Core DMSO		MFCD08234735		DMSO	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
C-N Coupling	DMSO	D	Core DMSO		MFCD00192043		DMSO	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
C-N Coupling	DMSO	E	Core DMSO		MFCD00007930		DMSO	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
C-O Coupling	DMSO	F	Core DMSO		MFCD00002886		DMSO	BLANK	RuPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	BINAP	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
C-O Coupling	DMSO	G	Core DMSO		MFCD01691686		DMSO	BLANK	RuPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	BINAP	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
C-O Coupling	DMSO	H	Core DMSO		MFCD19694707		DMSO	BLANK	RuPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	BINAP	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
C-S Coupling	DMSO	I	Core DMSO		MFCD00004903		DMSO	BLANK	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	XantPhos	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
C-S Coupling	DMSO	J	Core DMSO		MFCD00006751		DMSO	BLANK	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	XantPhos	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
Sonogashira	DMSO	K	Core DMSO		MFCD00008570		DMSO	XPphs	BrettPhos	tBuBrettPhos	RuPhos	Aphos	tBuXphos	tBu3P	XantPhos	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
Sonogashira	DMSO	L	Core DMSO		L00491220100ON		DMSO	XPphs	BrettPhos	tBuBrettPhos	RuPhos	Aphos	tBuXphos	tBu3P	XantPhos	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
alpha-arylation	DMSO	M	Core DMSO		MFCD00009195		DMSO	CatacXium A	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	tBu3P	XantPhos	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
alpha-arylation	DMSO	N	Core DMSO		MFCD00053704		DMSO	CatacXium A	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	tBu3P	XantPhos	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
alpha-arylation	DMSO	O	Core DMSO		MFCD00005282		DMSO	CatacXium A	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	tBu3P	XantPhos	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					
alpha-arylation	DMSO	P	Core DMSO		MFCD00003792		DMSO	CatacXium A	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	tBu3P	XantPhos	DMSO		P2-Et DMSO	BTTP DMSO	BTMG DMSO	MTBD DMSO					

			Core		Building block		Wash solvent	catalyst 1	catalyst 2	catalyst 3	catalyst 4	catalyst 5	catalyst 6	catalyst 7	catalyst 8	Wash solvent		Base 1	Base 2	Base 3	Base 4					
			16 uL		30 uL		50 uL	20 uL	20 uL	20 uL	20 uL	20 uL	20 uL	20 uL	20 uL	50 uL		25 uL	25 uL	25 uL	25 uL					
	Solvent	Row	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
C-N Coupling	NMP	A	Core NMP		MFCD00007968		NMP	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
C-N Coupling	NMP	B	Core NMP		CM00576334		NMP	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
C-N Coupling	NMP	C	Core NMP		MFCD08234735		NMP	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
C-N Coupling	NMP	D	Core NMP		MFCD00192043		NMP	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
C-N Coupling	NMP	E	Core NMP		MFCD00007930		NMP	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
C-O Coupling	NMP	F	Core NMP		MFCD00002886		NMP	BLANK	RuPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	BINAP	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
C-O Coupling	NMP	G	Core NMP		MFCD01691686		NMP	BLANK	RuPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	BINAP	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
C-O Coupling	NMP	H	Core NMP		MFCD19694707		NMP	BLANK	RuPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	BINAP	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
C-S Coupling	NMP	I	Core NMP		MFCD00004903		NMP	BLANK	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	XantPhos	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
C-S Coupling	NMP	J	Core NMP		MFCD00006751		NMP	BLANK	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	XantPhos	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
Sonogashira	NMP	K	Core NMP		MFCD00008570		NMP	XPphs	BrettPhos	tBuBrettPhos	RuPhos	Aphos	tBuXphos	tBu3P	XantPhos	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
Sonogashira	NMP	L	Core NMP		L00491220100ON		NMP	XPphs	BrettPhos	tBuBrettPhos	RuPhos	Aphos	tBuXphos	tBu3P	XantPhos	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
alpha-arylation	NMP	M	Core NMP		MFCD00009195		NMP	CatacXium A	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	tBu3P	XantPhos	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
alpha-arylation	NMP	N	Core NMP		MFCD00053704		NMP	CatacXium A	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	tBu3P	XantPhos	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
alpha-arylation	NMP	O	Core NMP		MFCD00005282		NMP	CatacXium A	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	tBu3P	XantPhos	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					
alpha-arylation	NMP	P	Core NMP		MFCD00003792		NMP	CatacXium A	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	tBu3P	XantPhos	NMP		P2-Et NMP	BTTP NMP	BTMG NMP	MTBD NMP					

			Core		Building block		Wash solvent	catalyst 1	catalyst 2	catalyst 3	catalyst 4	catalyst 5	catalyst 6	catalyst 7	catalyst 8	Wash solvent		Base 1	Base 2	Base 3	Base 4					
			16 uL		30 uL		50 uL	20 uL	20 uL	20 uL	20 uL	20 uL	20 uL	20 uL	20 uL	50 uL		25 uL	25 uL	25 uL	25 uL					
	Solvent	Row	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
C-N Coupling	DMF	A	Core DMF		MFCD00007968		DMF	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
C-N Coupling	DMF	B	Core DMF		CM00576334		DMF	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
C-N Coupling	DMF	C	Core DMF		MFCD08234735		DMF	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
C-N Coupling	DMF	D	Core DMF		MFCD00192043		DMF	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
C-N Coupling	DMF	E	Core DMF		MFCD00007930		DMF	BLANK	BrettPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	JackiePhos	XantPhos	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
C-O Coupling	DMF	F	Core DMF		MFCD00002886		DMF	BLANK	RuPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	BINAP	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
C-O Coupling	DMF	G	Core DMF		MFCD01691686		DMF	BLANK	RuPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	BINAP	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
C-O Coupling	DMF	H	Core DMF		MFCD19694707		DMF	BLANK	RuPhos	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	BINAP	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
C-S Coupling	DMF	I	Core DMF		MFCD00004903		DMF	BLANK	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	XantPhos	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
C-S Coupling	DMF	J	Core DMF		MFCD00006751		DMF	BLANK	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	DTBPF	XantPhos	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
Sonogashira	DMF	K	Core DMF		MFCD00008570		DMF	XPphs	BrettPhos	tBuBrettPhos	RuPhos	Aphos	tBuXphos	tBu3P	XantPhos	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
Sonogashira	DMF	L	Core DMF		L00491220100ON		DMF	XPphs	BrettPhos	tBuBrettPhos	RuPhos	Aphos	tBuXphos	tBu3P	XantPhos	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
alpha-arylation	DMF	M	Core DMF		MFCD00009195		DMF	CatacXium A	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	tBu3P	XantPhos	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
alpha-arylation	DMF	N	Core DMF		MFCD00053704		DMF	CatacXium A	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	tBu3P	XantPhos	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
alpha-arylation	DMF	O	Core DMF		MFCD00005282		DMF	CatacXium A	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	tBu3P	XantPhos	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					
alpha-arylation	DMF	P	Core DMF		MFCD00003792		DMF	CatacXium A	BINAP	tBuBrettPhos	AdBrettPhos	RockPhos	tBuXphos	tBu3P	XantPhos	DMF		P2-Et DMF	BTTP DMF	BTMG DMF	MTBD DMF					

Figure 11. Nucleophile Screen Source Plates: DMSO (1), NMP (2), and DMF (3)

TTP Labtech Mosquito®HTS liquid handling robot was used to generate a 1,536 reaction plate containing all desired reaction conditions per aryl halide core/ nucleophile building block combination. 8 catalyst columns × 12 solvent/base combinations = 96 reaction conditions. 16 core/building block combinations × 96 conditions = 1,536 reaction screen. Results of this screen are plotted below as a heat map arrayed by nucleophile and reaction conditions after quenching. Reactions are represented by percent yield calculated from standard curves generated from isolated product standards. Tabulated reaction data are provided in supplementary Excel tables.



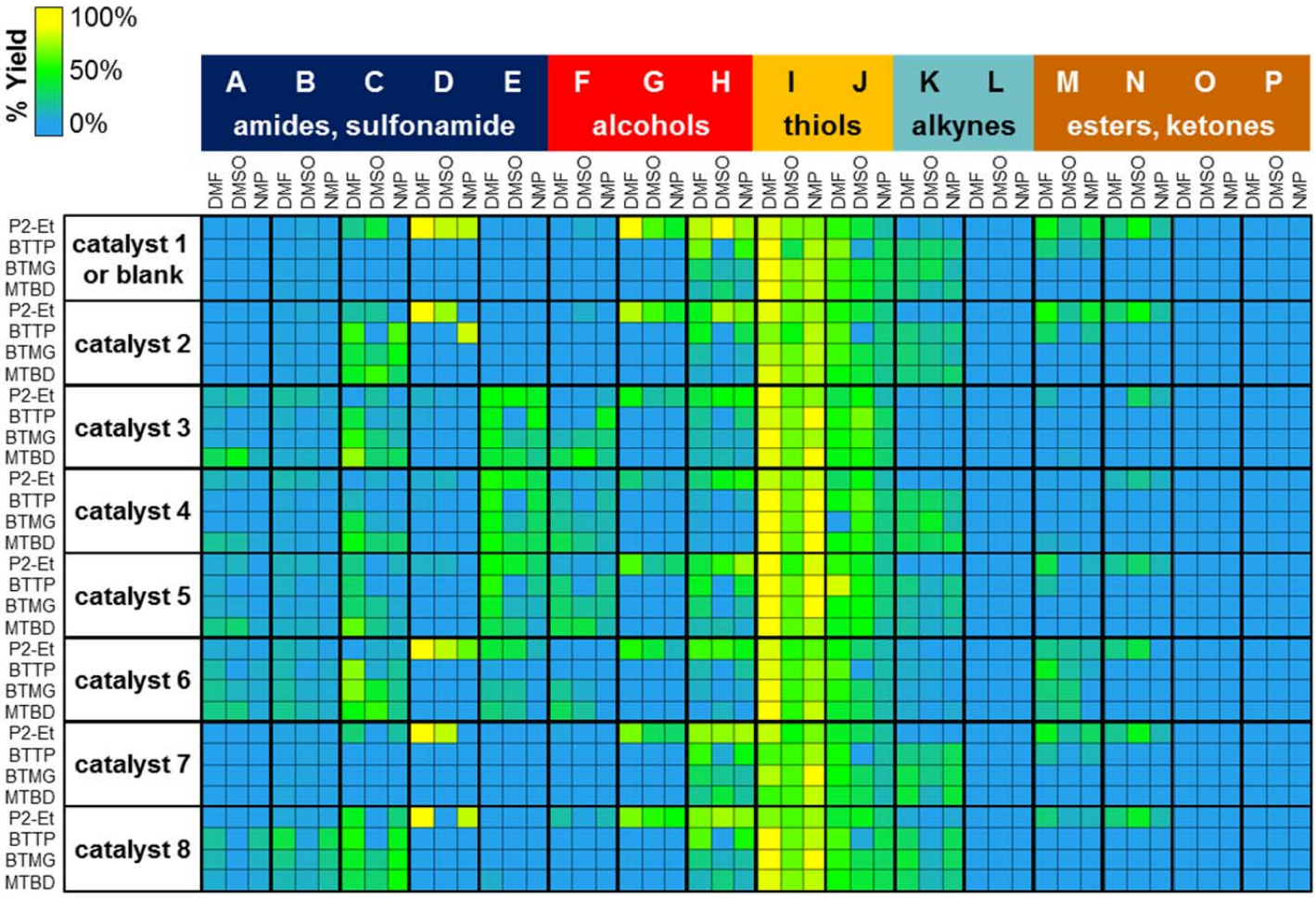


Figure 12. Nanomole-Scale Diverse Nucleophile Coupling Screen Heat Map

3.7. Circlize Optimization Visualization for the Coupling of Nucleophiles to a 2-Bromothiazole Core 7

To construct the outer optimization ring of the 2-bromo-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide coupling library circlize visualization shown in the manuscript and supporting information, data from many of the optimization reaction screens described above were combined and grouped by nucleophile class. Suzuki cross coupling data was collected from 3.3 Supplementary Suzuki Cross-Coupling Screen on 2-Bromothiazole Core, aryl amination data using aryl and aliphatic amines was collected rom 3.5 Second Nanomole-Scale Buchwald-Hartwig Amination Screen on 2-Bromothiazole Core , and data using amides, sulfonamides, alkynes, alcohols, and thiols as nucleophiles was collected from 3.6 Nanomole-Scale 2-Bromothiazole Diverse Nucleophile Coupling Screen.

Conditions were selected for library synthesis (384 member library, see Section 7) according to the following logic:

1. **Objective 1.** SYNTHESIZE EVERY MOLECULE. Reaction conditions selected to ensure each product can be formed. In some instances, this meant including in our four preferred reaction conditions one catalyst-base pair that worked for just one or two monomers.

2. **Objective 2.** SELECT CONDITIONS WITH HIGHEST AVERAGE YIELD. The reaction conditions that gave good conversion to product for the broadest diversity of monomers were selected. Ideally, the top four conditions producing the highest average yield were included but, some were replaced if necessary to satisfy Objective 1.

3. **Objective 3.** MINIMIZE DIVERSITY OF SOLVENTS. Ideally, each functional group class could be carried out in a single solvent. This greatly simplified the experimental preparation of reaction arrays produced from stock solutions.

4. **Objective 4.** MAXIMIZE CATALYST-BASE DIVERSITY. In cases where the highest average yield was comparable with two very similar catalysts, such as tBuBrettPhos and AdBrettPhos, one redundant catalyst was replaced with another more diverse catalyst that also produced a high average yield.

4. General Procedure for an Affinity-Based Rank Ordering Experiment

4.1. Affinity Selection Mass Spectrometry (ASMS) Instrumentation and Methods

Automated pooling: A LABCYTE Echo® 555 Liquid Handler was used to dispense from Echo® qualified 384-well LDV diamond plates into 384-well destination plates.

Instrumentation: ASMS SEC-based affinity selection-mass spectrometry instrument configured and utilized as previously described.[1–4] Components listed here: Agilent 1260 system equipped with cooled autosampler, two UV detectors, 1 binary RPC capillary pump, 3 isocratic pumps (for SEC wash, SEC buffer, and RPC wash), and a Thermo Scientific™ Q Exactive™ Quadrupole-Orbitrap high-resolution, accurate-mass (HRAM) mass spectrometer detector.

ASMS Size Exclusion Chromatography step (SEC):

Injection volume: 2 µL (duplicate injections standard)

SEC buffer: 0.7 M or 1.0 M NH_4AOc pH 7.5 or pH 8 (concentration and pH are target dependent)

SEC buffer flow rate: 0.3 mL/min

SEC wash: 70:30 MeCN/water

SEC wash flow rate: 0.3 mL/min

ASMS Reverse Phase Chromatography step (RPC):

RPC column: Higgins C_{18} 0.5 mm x 50 mm, 5 µm with two column switching

RPC mobile phase A: 0.2% formic acid in water

RPC mobile phase B: 0.2% formic acid in MeCN

RPC wash: 0.2% formic acid in water at 0.1 mL/min

RPC flow rate: 20 µL/min

Four minute RPC gradient:

Time (min)	% MeCN (solvent B)	Flow rate (µL/min)
0.0	0	20
0.5	0	20
2.5	99	20
3.5	99	20
3.6/end	0	20

4.2. Library Pooling Techniques

Libraries were synthesized in a single compound per well or container, either at nanomole-scale, micromole-scale, or millimole-scale. In advance of affinity-based ranking the discrete reactions/library members were pooled together (typically 12-24 compounds per pool). Library pools were mass encoded (no two compounds possessing the same molecular formula in the same pool) to ensure one's ability to accurately differentiate each library member. Multiple library pools were generated when mass redundancy existed in the library.

Automated library pooling was accomplished using the LABCYTE Echo® 555 Liquid Handler, capable of nanoliter volume transfers through acoustic dispensing. Quenched and diluted reaction plates were transferred to Echo® qualified 384-well LDV diamond plates (described above, each compound approximately 10 mM in DMSO after dilution) and taken to the Echo® 555 Liquid Handler where discrete reactions/compounds were pooled into compound sets (pools) using the Cherry Pick feature. 10 nL transfer volumes were used along with a Labcyte 384-well polypropylene (384PP) StdV plate as the destination plate. The library pools were diluted with DMSO in accordance with the specified affinity-based rank ordering procedure herein.

Example pool dilution:

Source well concentrations 10 mM, destination pool concentration 40 µM per compound

20-member pool with 10 nL Echo® dispense volumes = 200 nL total dispense volume

Dilution factor: 1:250 dilution per compound (2.5 µL final pool volume)

DMSO used to dilute pool: 2.5 µL — 0.2 µL = 2.3 µL

For smaller libraries where automated library pooling was not necessary, compound pooling was accomplished using manual pipetting (transfer volume of 1 µL from the desired wells on a 384-well LDV diamond source plate to a destination microcentrifuge tube). The library pools were diluted with DMSO in accordance with the specified affinity-based rank ordering procedure herein.

Example pool dilution:

Source well concentrations 10 mM, destination pool concentration 40 µM per compound

18-member pool with 1 µL dispense volumes = 18 µL total dispense volume

Dilution factor: 1:250 dilution per compound (250 µL final pool volume)

DMSO used to dilute pool: 250 µL — 18 µL = 232 µL

4.3. General Affinity Ranking Competition Experiment Procedure

A general affinity selection-mass spectrometry based library rank ordering procedure is described below. The protein and compound concentrations described are those which were most often used the competition experiment, however experimental considerations occasionally required modifications be made to better serve a library of interest. Such modifications included lowering compound concentration (e.g. 1:500 dilution per compound with DMSO rather than 1:250), lowering protein concentration to induce greater

competition (e.g. 10 µM versus 5 µM), or utilizing an alternative negative control protein. Procedural modifications are noted in each individual experiment.

1. **Prepare buffers:** protein dilution buffer and library dilution buffer stock solutions were prepared (target dependent, described herein, 1 M dithiothreitol (DTT) stock solution was thawed beforehand if necessary).
2. **Prepare pools:** library pool(s) were assembled as described above and diluted 1:20 with library dilution buffer (example: final pool concentration of 2 µM per compound from a 40 µM per compound DMSO pool).
3. **Target protein preparation:** Target protein was removed from the freezer and thawed on ice. Once thawed, target protein was diluted to prepare 4X protein stock using protein dilution buffer (typically 40 µM for an affinity ranking competition experiment starting at 10 µM but ultimately method/target dependent).
4. **Negative control protein preparation:** Invertase (Sigma Aldrich cat. no. I4504) was removed from refrigerator, weighed into a centrifuge tube, then 20 µM and 10 µM Invertase stock solutions were prepared by diluting with protein dilution buffer (exact desired concentrations are again ultimately method/target dependent).
5. **Prepare highest protein level:** 4X protein stock was diluted 1:1 with 20 µM invertase stock.
6. **Serial dilution:** carry out serial dilution of protein from previously prepared highest protein level using 10 µM Invertase stock. Seven protein levels were constructed, with the final (eighth) position reserved for negative control (invertase only).

Level	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Invertase	10 µM	10 µM	10 µM	10 µM	10 µM	10 µM	10 µM	10 µM
Target	20 µM	10 µM	5 µM	2.5 µM	1.25 µM	0.62 µM	0.31 µM	0 µM

7. **Affinity Ranking**: Dilute previously prepared pool (2 µM per compound) 1:1 with each of the eight protein levels (3 µL + 3 µL = 6 µL total per well) in a 96-well plate to assemble the affinity-based competition experiment as shown below. Aspirate to mix. After completion of all pipetting steps the plate sat at ambient temperature for 30 minutes before moving to a cooled LC-MS autosampler for analysis. This step was done for each pool (separately) for experiments where multiple pools were used. Final concentrations of all components were as follows:

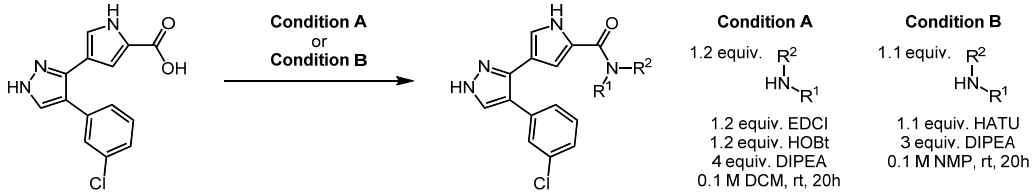
Level	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Per Cmpd.	1 µM	1 µM	1 µM	1 µM	1 µM	1 µM	1 µM	1 µM
Invertase	5 µM	5 µM	5 µM	5 µM	5 µM	5 µM	5 µM	5 µM
Target	10 µM	5 µM	2.5 µM	1.25 µM	0.62 µM	0.31 µM	0.16 µM	0 µM

5. Synthesis and Rank Ordering of an Extracellular Signal-Regulated Kinase 2 (pERK2) Amide Library

The below described library was initially disclosed by a medicinal chemistry group targeting ERK2.[6] Reproducing this library, but at a significantly miniaturized scale, was attractive to us from the perspective of workflow validation. The library contains species ranging from highly potent (<10 nM) to weak/inactive (>10,000 nM) and would serve as a good test of our ability to differentiate between high affinity, moderate, and weak compounds. Finally, these amides could be easily prepared and purified on scale, providing a direct comparison between the crude nano-scale workflow and a traditional synthesis/purification/ranking workflow.

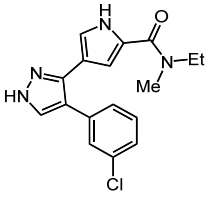
5.1. Bench-Scale Synthesis of pERK2 Amides

General Amide Coupling Procedure



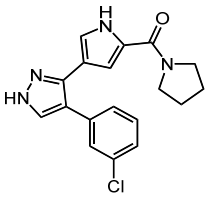
Amides were prepared according to published procedures (at the 0.05 mmol or 0.1 mmol scale) with the reaction stoichiometry shown above.[6] All examples were previously reported.[6] Reactions were stirred at room temperature after addition of all reagents for 18 hours. Reactions were quenched, diluted with EtOAc and water, and the organic phase was separated. The aqueous phase was washed with EtOAc, then the combined organics were washed twice with brine and dried with $MgSO_4$. The crude extract was concentrated by rotavap to afford a residue, which was submitted for purification by RP-HPLC. Amine building blocks were purchased from commercial vendors. After purification and characterization the amide products were dissolved in DMSO to a concentration of 10 mM. For some examples in this library, rotamers resulted in ^{1}H NMR peak broadening.

4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-ethyl-N-methyl-1H-pyrrole-2-carboxamide (A1)



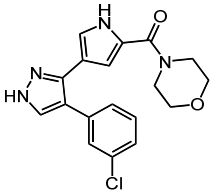
The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 8 mg (49% yield) of the title compound as a colorless residue. Spectral data were in agreement with reported literature values. Analytical data for **A1**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.63 (br s, 1H), 7.74 (s, 1H), 7.44 (s, 1H), 7.37 (m, 2H), 7.29 (m, 1H), 7.00 (s, 1H), 6.56 (br s, 1H), 3.48 (apparent s, 2H), 3.03 (br s, 3H), 1.07 (t, *J* = 7.0 Hz, 3H); **HRMS** (ESI): *m/z* calculated for $C_{17}H_{18}ClN_4O$ [M+H]+ 329.11639, found 329.11621

(4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrol-2-yl)(pyrrolidin-1-yl)methanone (A2)



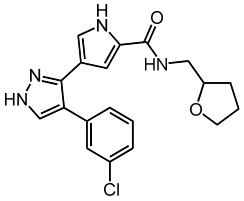
The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 9.4 mg (55% yield) of the title compound as an off-white residue. Spectral data were in agreement with reported literature values. Analytical data for **A2**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.65 (s, 1H), 7.74 (s, 1H), 7.45 (s, 1H), 7.37 (m, 2H), 7.29 (m, 1H), 6.98 (s, 1H), 6.69 (s, 1H), 3.57 (s, 2H), 3.46 (s, 2H), 1.91 (m, 2H), 1.80 (m, 2H); **HRMS** (ESI): *m/z* calculated for $C_{18}H_{18}ClN_4O$ [M+H]+ 341.11639, found 341.11627

(4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrol-2-yl)(morpholino)methanone (A3)



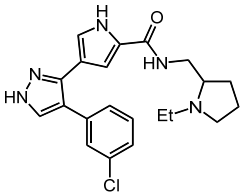
The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 11.1 mg (62% yield) of the title compound as an off-white residue. Spectral data were in agreement with reported literature values. Analytical data for **A3**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.71 (s, 1H), 7.75 (s, 1H), 7.43 (s, 1H), 7.37 (d, *J* = 4.5 Hz, 2H), 7.30 (s, 1H), 6.99 (s, 1H), 6.53 (s, 1H), 3.64 (s, 4H), 3.59 (m, 4H); **HRMS** (ESI): *m/z* calculated for $C_{18}H_{18}ClN_4O_2$ [M+H]+ 357.1113, found 357.11172

4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-((tetrahydrofuran-2-yl)methyl)-1H-pyrrole-2-carboxamide (A4)



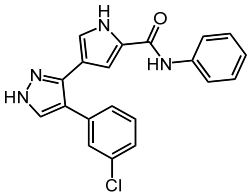
The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 11 mg (59% yield) of the title compound as an off-white residue. Spectral data were in agreement with reported literature values. Analytical data for **A4**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 11.65 (s, 1H), 8.12 (t, *J* = 5.5 Hz, 1H), 7.77 (s, 1H), 7.42 (s, 1H), 7.34 (d, *J* = 4.5 Hz, 2H), 7.26 (m, 1H), 6.93 (br s, 1H), 6.89 (s, 1H), 3.90 (m, 1H), 3.74 (q, *J* = 7.0 Hz, 1H), 3.60 (q, *J* = 7.2 Hz, 1H), 3.24 (m, 2H), 1.85 (m, 1H), 1.79 (m, 2H), 1.55 (m, 1H);. **HRMS** (ESI): *m/z* calculated for $C_{19}H_{20}ClN_4O_2$ [M+H]+ 371.12695, found 371.12671

4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-((1-ethylpyrrolidin-2-yl)methyl)-1H-pyrrole-2-carboxamide (A5)



The desired product was prepared at the 0.05 mmol scale using **Condition A** to yield 20.6 mg (80% yield) of the title compound as an off-white solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **A5**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.79 (s, 1H), 9.12 (s, 1H), 8.43 (apparent d, *J* = 5.5 Hz, 1H), 7.80 (s, 1H), 7.42 (s, 1H), 7.35 (d, *J* = 4.4 Hz, 2H), 7.28 (s, 1H), 6.99 (s, 1H), 6.90 (s, 1H), 3.53 (m, 5H), 3.08 (m, 2H), 2.10 (m, 1H), 1.96 (m, 1H), 1.84 (m, 1H), 1.79 (m, 1H), 1.23 (t, *J* = 7.1 Hz, 3H); **HRMS** (ESI): *m/z* calculated for $C_{21}H_{25}ClN_5O$ [M+H]+ 398.17424, found 398.17462

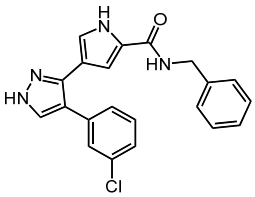
4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-phenyl-1H-pyrrole-2-carboxamide (A6)



The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 6.8 mg (29% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **A6**: **^{1}H NMR** (600

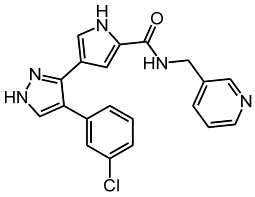
MHz, DMSO-d_6) 11.88 (s, 1H), 9.83 (s, 1H), 7.83 (s, 1H), 7.71 (d, *J* = 7.8 Hz, 2H), 7.45 (s, 1H), 7.36 (m, 2H), 7.30 (m, 3H), 7.21 (s, 1H), 7.04 (m, 2H); **HRMS** (ESI): *m/z* calculated for $C_{20}H_{16}ClN_4O$ [M+H]+ 363.10074, found 363.10135

***N*-benzyl-4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrole-2-carboxamide (A7)**



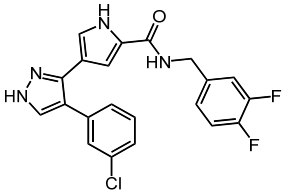
The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 8.9 mg (47% yield) of the title compound as an off-white residue. Spectral data were in agreement with reported literature values. Analytical data for **A7**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.70 (s, 1H), 8.63 (t, *J* = 5.7 Hz, 1H), 7.78 (s, 1H), 7.43 (s, 1H), 7.35 (m, 2H), 7.29 (m, 5H), 7.22 (t, *J* = 6.9 Hz, 1H), 6.96 (br s, 1H), 6.93 (s, 1H), 4.41 (d, *J* = 5.8 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{21}H_{18}ClN_4O$ [M+H]+ 377.11639, found 377.11603

4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(pyridin-3-ylmethyl)-1H-pyrrole-2-carboxamide (A8)



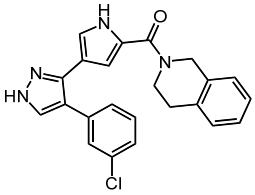
The desired product was prepared at the 0.1 mmol scale using **Condition A** to yield 15.5 mg (32% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **A8**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.75 (s, 1H), 8.79 (t, *J* = 5.6 Hz, 1H), 8.74 (s, 1H), 8.70 (d, *J* = 4.7 Hz, 1H), 8.21 (d, *J* = 7.7 Hz, 1H), 7.81 (m, 2H), 7.43 (s, 1H), 7.35 (d, *J* = 4.3 Hz, 1H), 7.27 (br s, 1H), 6.98 (s, 1H), 6.93 (s, 1H), 4.54 (d, *J* = 5.6 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{20}H_{17}ClN_5O$ [M+H]+ 378.11164, found 378.11197

4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(3,4-difluorobenzyl)-1H-pyrrole-2-carboxamide (A9)



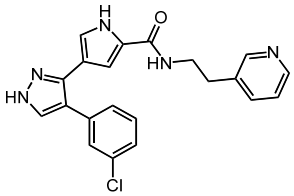
The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 10.9 mg (53% yield) of the title compound as an off-white residue. Spectral data were in agreement with reported literature values. Analytical data for **A9**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.72 (s, 1H), 8.67 (t, *J* = 5.6 Hz, 1H), 7.79 (s, 1H), 7.43 (s, 1H), 7.32 (m, 5H), 7.12 (s, 1H), 6.97 (s, 1H), 6.92 (s, 1H), 4.38 (d, *J* = 5.6 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{21}H_{16}ClF_2N_4O$ [M+H]+ 413.09755, found 413.09373

(4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrol-2-yl)(3,4-dihydroisoquinolin-2(1H)-yl)methanone (A10)



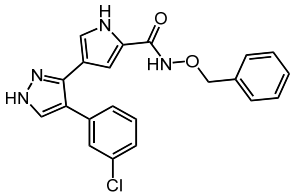
The desired product was prepared at the 0.1 mmol scale using **Condition A** to yield 13.7 mg (27% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **A10**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.75 (s, 1H), 7.76 (s, 1H), 7.46 (s, 1H), 7.39 (m, 2H), 7.32 (m, 1H), 7.18 (s, 4H), 7.02 (s, 1H), 6.67 (s, 1H), 4.78 (br s, 2H), 3.85 (apparent s, 2H), 2.85 (t, *J* = 5.3 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{23}H_{20}ClN_4O$ [M+H]+ 403.13204, found 403.13232

4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(2-(pyridin-3-yl)ethyl)-1H-pyrrole-2-carboxamide (A11)



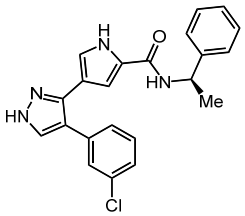
The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 11.2 mg (57% yield) of the title compound as an off-white residue. Spectral data were in agreement with reported literature values. Analytical data for **A11**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.63 (s, 1H), 8.76 (s, 1H), 8.72 (d, J = 5.1 Hz, 1H), 8.30 (d, *J* = 7.8 Hz, 1H), 8.17 (t, *J* = 5.3 Hz, 1H), 7.86 (m, 1H), 7.79 (s, 1H), 7.41 (s, 1H), 7.34 (m, 2H), 7.27 (d, *J* = 6.8 Hz, 1H), 6.93 (s, 1H), 6.80 (s, 1H), 3.53 (q, *J* = 6.1 Hz, 2H), 2.98 (t, *J* = 6.4 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{21}H_{19}ClN_5O$ [M+H]+ 392.12729, found 392.12759

N-(benzyloxy)-4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrole-2-carboxamide (A12)



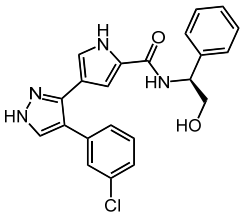
The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 19.3 mg (98% yield) of the title compound as an off-white residue. Spectral data were in agreement with reported literature values. Analytical data for **A12**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.81 (s, 1H), 11.36 (br s, 1H), 7.78 (s, 1H), 7.37 (m, 8H), 7.27 (d, *J* = 7.2 Hz, 1H), 7.00 (s, 1H), 6.78 (s, 1H), 4.86 (s, 2H); **HRMS** (ESI): *m/z* calculated for $C_{21}H_{18}ClN_4O_2$ [M+H]+ 393.11130, found 393.11115

(R)-4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(1-phenylethyl)-1H-pyrrole-2-carboxamide (A13)



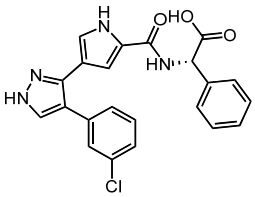
The desired product was prepared at the 0.05 mmol scale using **Condition A** to yield 9 mg (36% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **A13**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.63 (s, 1H), 8.41 (d, *J* = 8.2 Hz, 1H), 7.79 (s, 1H), 7.44 (s, 1H), 7.35 (m, 4H), 7.29 (m, 3H), 7.20 (t, *J* = 7.1 Hz, 1H), 7.04 (s, 1H), 6.93 (br s, 1H), 5.12 (p, *J* = 7.0 Hz, 1H), 1.42 (d, *J* = 7.0 Hz, 3H); **HRMS** (ESI): *m/z* calculated for $C_{22}H_{20}ClN_4O$ [M+H]+ 391.13204, found 391.13278

(S)-4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(2-hydroxy-1-phenylethyl)-1H-pyrrole-2-carboxamide (2)



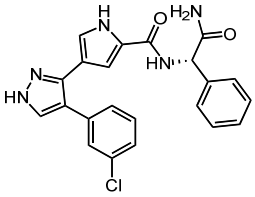
The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 10.8 mg (53% yield) of the title compound as an off-white residue. Spectral data were in agreement with reported literature values. Analytical data for **2**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.64 (s, 1H), 8.31 (d, *J* = 8.2 Hz, 1H), 7.80 (s, 1H), 7.45 (s, 1H), 7.35 (m, 4H), 7.29 (m, 3H), 7.21 (t, *J* = 7.1 Hz, 1H), 7.06 (s, 1H), 6.93 (s, 1H), 5.03 (q, *J* = 7.1 Hz, 1H), 3.63 (m, 2H) **HRMS** (ESI): *m/z* calculated for $C_{22}H_{20}ClN_4O_2$ [M+H]+ 407.12695, found 407.12704

(S)-2-(4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrole-2-carboxamido)-2-phenylacetic acid (3)



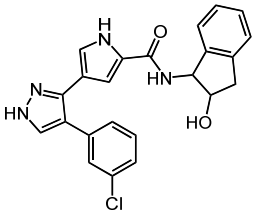
The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 7.9 mg (38% yield) of the title compound as an off-white solid. Spectral data were in agreement with reported literature values. Analytical data for **3**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.74 (s, 1H), 8.64 (d, *J* = 7.5 Hz, 1H), 7.79 (s, 1H), 7.45 (m, 3H), 7.34 (m, 5H), 7.26 (br s, 1H), 7.11 (s, 1H), 6.97 (s, 1H), 5.55 (d, *J* = 7.5 Hz, 1H); **HRMS** (ESI): *m/z* calculated for $C_{22}H_{18}ClN_4O_3$ [M+H]+ 421.10622, found 421.10645

(S)-N-(2-amino-2-oxo-1-phenylethyl)-4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrole-2-carboxamide (A14)



The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 13.2 mg (58% yield) of the title compound as an off-white solid. Spectral data were in agreement with reported literature values. Analytical data for **A14**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.80 (s, 1H), 8.36 (d, *J* = 8.1 Hz, 1H), 7.78 (s, 1H), 7.69 (s, 1H), 7.46 (m, 3H), 7.34 (m, 4H), 7.28 (m, 2H), 7.21 (s, 1H), 7.08 (s, 1H), 6.97 (s, 1H), 5.60 (d, *J* = 8.1 Hz, 1H); **HRMS** (ESI): *m/z* calculated for $C_{22}H_{19}ClN_5O_2$ [M+H]+ 420.1222, found 420.12231

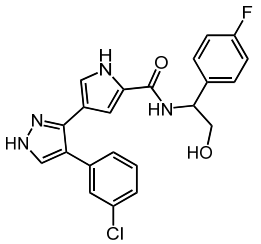
4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(2-hydroxy-2,3-dihydro-1H-inden-1-yl)-1H-pyrrole-2-carboxamide (A15)



The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 11.6 mg (55% yield) of the title compound as an off-white residue. Spectral data were in agreement with reported literature values. Analytical data for **A15**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.70 (br s, 1H), 8.34 (d, *J* = 8.5 Hz, 1H), 7.75 (br s, 1H), 7.39 (s, 1H), 7.31 (m, 2H), 7.21 (m, 1H), 7.14 (m, 3H), 7.04 (d, *J* = 7.1

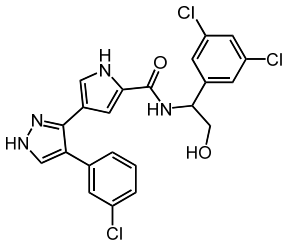
Hz, 1H), 6.95 (br s, 2H), 5.21 (t, *J* = 7.7 Hz, 1H), 4.30 (q, *J* = 7.2 Hz, 1H), 3.10 (dd, *J* = 15.4, *J* = 7.2 Hz, 1H), 2.68 (dd, *J* = 15.3, *J* = 7.7 Hz, 1H); **HRMS** (ESI): *m/z* calculated for $C_{23}H_{20}ClN_4O_2$ [M+H]+ 419.12695, found 419.12741

4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(1-(4-fluorophenyl)-2-hydroxyethyl)-1H-pyrrole-2-carboxamide (A16)



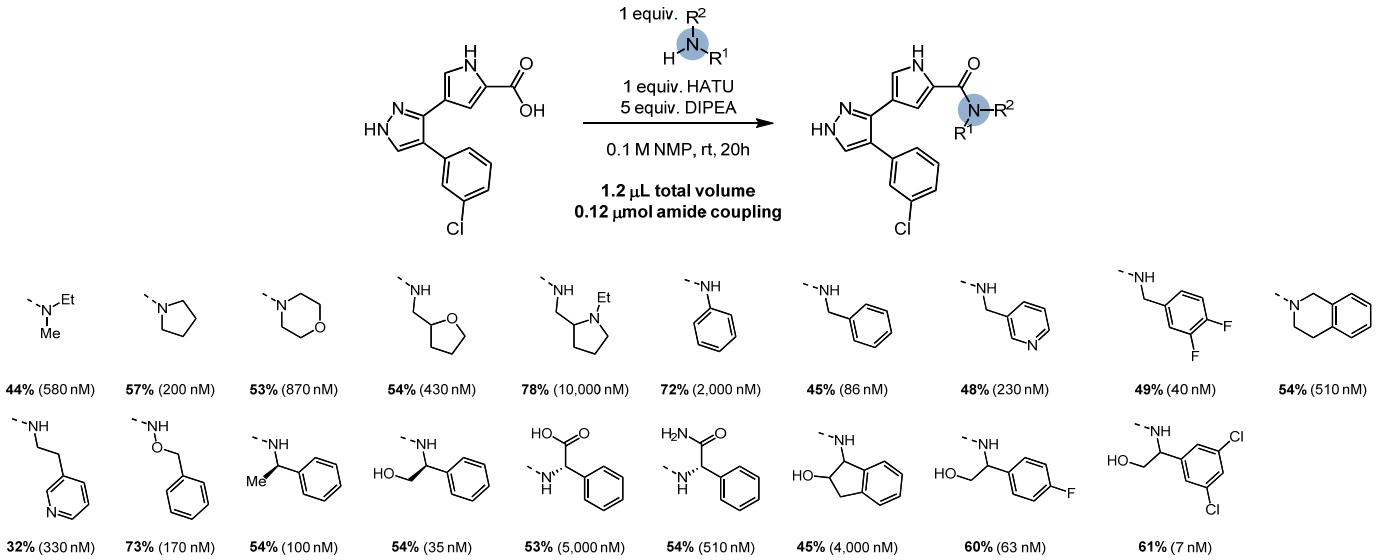
The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 7.1 mg (26% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **A16**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.65 (s, 1H), 8.32 (d, *J* = 7.9 Hz, 1H), 7.80 (s, 1H), 7.44 (s, 1H), 7.37 (m, 4H), 7.28 (br s, 1H), 7.12 (t, *J* = 8.3 Hz, 2H), 7.05 (s, 1H), 6.93 (s, 1H), 5.02 (apparent q, *J* = 6.7 Hz, 1H), 3.61 (m, 2H); **HRMS** (ESI): *m/z* calculated for $C_{22}H_{19}ClFN_4O_2$ [M+H]+ 425.11753, found 425.11639

4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(1-(3,5-dichlorophenyl)-2-hydroxyethyl)-1H-pyrrole-2-carboxamide (A17)



The desired product was prepared at the 0.05 mmol scale using **Condition B** to yield 3.6 mg (12% yield) of the title compound as an off-white solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **A17**: **^{1}H NMR** (600 MHz, DMSO-d_6) 11.69 (s, 1H), 8.38 (d, *J* = 7.8 Hz, 1H), 7.80 (s, 1H), 7.46 (d, *J* = 13.5 Hz, 2H), 7.41 (s, 2H), 7.35 (m, 2H), 7.28 (d, *J* = 5.6 Hz, 1H), 7.06 (s, 1H), 6.95 (s, 1H), 5.02 (apparent q, *J* = 6.7 Hz, 1H), 3.63 (m, 2H); **HRMS** (ESI): *m/z* calculated for $C_{22}H_{18}Cl_3N_4O_2$ [M+H]+ 475.04901, found 475.04852

5.2. Nanomole-Scale Amide Synthesis



All chemistry and nanoliter pipetting was done in an N_2 atmosphere glove box (yields shown calculated using standard curves).

Stock solutions of the carboxylic acid core (0.4 M in NMP), amine building blocks (0.4 M in NMP), HATU coupling agent (0.4 M in NMP), and DIPEA (2.0 M in NMP) were prepared. A source plate was constructed, using the reagent stock solutions, according to the diagram below by pipetting 15 µL of the correct stock solution into the indicated wells shown (Figure 13). The TTP Labtech Mosquito® was used to assemble the reaction mixtures using the multi-aspiration and dispense mixing.

1. 297 nL was drawn up from the Core column (column 1)
2. 297 nL was then drawn from the HATU column (column 3)
3. 6 nL NMP pipette tip wash (column 5)
4. 297 nL was drawn up from the correct building block column (column 7 or 8)
5. 6 nL NMP pipette tip wash (column 11)
6. 297 nL was then drawn up from the DIPEA stock solution column (13) which was immediately followed by dispense mixing (3×800 nL) into the 1,536-well reaction plate to ensure all reagents are adequately combined.
7. This procedure was repeated to assemble a second (backup) copy of this library (see supplementary Excel tables).
8. The 1,536-plate was sealed and briefly centrifuged before sitting at ambient temperature for 20 hours.

The next morning, the reactions were quenched by the addition of 1 µL H_2O and 2×1 µL DMSO to each reaction well. The reactions were further diluted with DMSO (to approximately 10 mM assuming complete conversion to product) and transferred to a 384-well LDV diamond plate in preparation for affinity-based ranking. 1 µL was drawn from each quenched and diluted crude reaction mixture and transferred a 384-well plate containing 60 µL DMSO per well for analysis by LC-MS. The crude reaction percent yields shown above were calculated using standard curves generated from an isolated sample of each product.

Synthesis Plate																				
	Core	Core	HATU	HATU	Wash Solvent	Wash Solvent	Monomers	Monomers	Monomers		Wash Solvent	Wash Solvent	Base	Base						
	12 uL	12 uL	20 uL	20 uL	50 uL	50 uL	25 uL	25 uL	25 uL		50 uL	50 uL	25 uL	25 uL						
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
A	Core [0.4 NMP]	Core [0.4 NMP]	HATU [0.4 NMP]	HATU [0.4 NMP]	NMP	NMP	MFCD00009030	MFCD00191604	MFCD00064403		NMP	NMP	DIPEA [2.0 NMP]	DIPEA [2.0 NMP]						
B	Core [0.4 NMP]		HATU [0.4 NMP]		NMP		MFCD00005249	MFCD00221709			NMP		DIPEA [2.0 NMP]							
C	Core [0.4 NMP]		HATU [0.4 NMP]		NMP		MFCD00005972	MFCD00064405			NMP		DIPEA [2.0 NMP]							
D	Core [0.4 NMP]		HATU [0.4 NMP]		NMP		MFCD00005373	MFCD00064404			NMP		DIPEA [2.0 NMP]							
E	Core [0.4 NMP]		HATU [0.4 NMP]		NMP		MFCD00003178	BLANK			NMP		DIPEA [2.0 NMP]							
F	Core [0.4 NMP]		HATU [0.4 NMP]		NMP		MFCD00007629	MFCD00270568			NMP		DIPEA [2.0 NMP]							
G	Core [0.4 NMP]		HATU [0.4 NMP]		NMP		MFCD00008106	MFCD00053472			NMP		DIPEA [2.0 NMP]							
H	Core [0.4 NMP]		HATU [0.4 NMP]		NMP		MFCD00006412	MFCD09253714			NMP		DIPEA [2.0 NMP]							
I	Core [0.4 NMP]		HATU [0.4 NMP]		NMP		MFCD00010145	BLANK			NMP		DIPEA [2.0 NMP]							
J	Core [0.4 NMP]		HATU [0.4 NMP]		NMP		MFCD00006896	MFCD02683179			NMP		DIPEA [2.0 NMP]							
K																				
L																				
M																				
N																				
O																				
P																				

Figure 13. ERK2 Amide Coupling Source Plate Map

Chromatograms are shown below for the quenched and diluted crude nanomole-scale reactions producing **A9** and **3** (green peak is the carboxylic acid core, red peaks are the amide products).

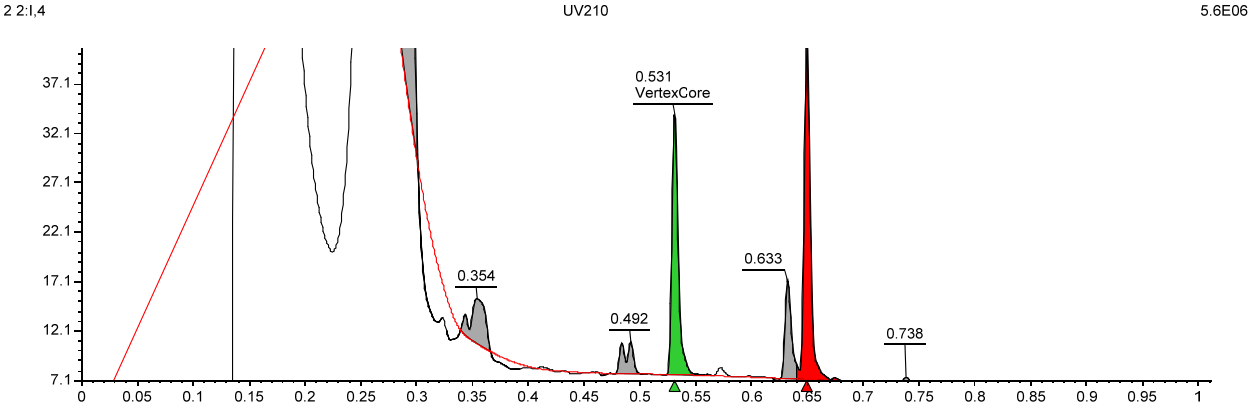


Figure 14. Chromatogram of Crude Nanomole-Scale Reaction Producing Product A9

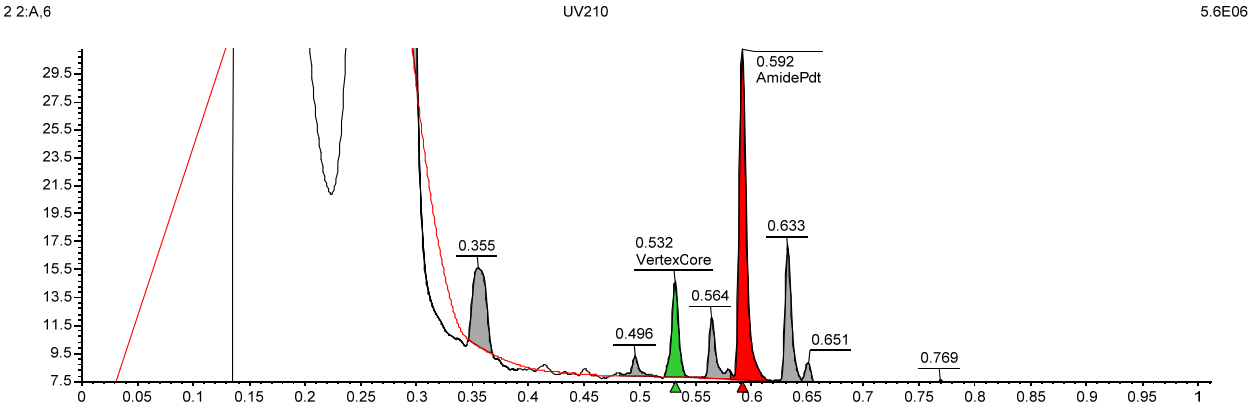


Figure 15. Chromatogram of Crude Nanomole-Scale Reaction Producing Product 3

5.3. Affinity Ranking of the pERK2 Amide Library

Pool Prep. A pool comprised of the purified amide library (19 compounds) was created by transferring 1 µL of each respective 10 mM solution into a centrifuge tube. This mixture was then diluted with DMSO to 250 µL (1:250 dilution per compound) to give a per compound concentration of 40 µM (760 µM total compound concentration). This pool was stored at -20 ˚C when not in use. A pool of quenched crude nanomole-scale reaction mixtures was prepared in a similar fashion: 1 µL was transferred from each well of the quenched reaction plate that contained product (approx. 10 mM assuming complete conversion to product, 19 total transfers) to a

centrifuge tube. This crude library mixture was then diluted with DMSO to 250 µL (1:250 dilution per compound) to give a per compound concentration of approximately 40 µM. This pool was stored at -20 ˚C when not in use.

Pool	Treatment	Sample ID	Crude Reaction Well	Mass	Formula	Protein	Reported Ki (nM)
Pool 1	Purified	0378493_0086_022	A4	328.10909	C17H17ClN4O	pERK2	580
Pool 1	Purified	0378493_0086_023	B4	340.10909	C18H17ClN4O	pERK2	200
Pool 1	Purified	0378493_0086_024	C4	356.104	C18H17ClN4O2	pERK2	870
Pool 1	Purified	0378493_0086_025	D4	370.11965	C19H19ClN4O2	pERK2	430
Pool 1	Purified	0378493_0086_026	E4	397.16694	C21H24ClN5O	pERK2	10000
Pool 1	Purified	0378493_0086_027	F4	362.09344	C20H15ClN4O	pERK2	2000
Pool 1	Purified	0378493_0086_028	G4	376.10909	C21H17ClN4O	pERK2	86
Pool 1	Purified	0378493_0086_029	H4	377.10434	C20H16ClN5O	pERK2	230
Pool 1	Purified	0378493_0086_030	I4	412.09025	C21H15ClF2N4O	pERK2	40
Pool 1	Purified	0378493_0086_031	J4	402.12474	C23H19ClN4O	pERK2	510
Pool 1	Purified	0378493_0086_032	A5	391.11999	C21H18ClN5O	pERK2	330
Pool 1	Purified	0378493_0086_033	B5	392.104	C21H17ClN4O2	pERK2	170
Pool 1	Purified	0378493_0086_034	C5	390.12474	C22H19ClN4O	pERK2	100
Pool 1	Purified	0378493_0086_035	D5	406.11965	C22H19ClN4O2	pERK2	35
Pool 1	Purified	0378493_0086_042	A6	420.09892	C22H17ClN4O3	pERK2	5000
Pool 1	Purified	0378493_0086_037	F5	419.1149	C22H19Cl2N5O2	pERK2	510
Pool 1	Purified	0378493_0086_038	G5	418.11965	C23H19ClN4O2	pERK2	4000
Pool 1	Purified	0378493_0086_039	H5	424.11023	C22H18ClFN4O2	pERK2	63
Pool 1	Purified	0378493_0086_041	J5	474.04171	C22H17Cl3N4O2	pERK2	7
Pool	**Treatment**	**Sample ID**	**Crude Reaction Well**	**Mass**	**Formula**	**Protein**	**Reported Ki (nM)**
Pool 2	Crude	0378493_0086_Std01	N/A	328.10909	C17H17ClN4O	pERK2	580
Pool 2	Crude	0378493_0086_Std02	N/A	340.10909	C18H17ClN4O	pERK2	200
Pool 2	Crude	0378493_0086_Std03	N/A	356.104	C18H17ClN4O2	pERK2	870
Pool 2	Crude	0378493_0086_Std04	N/A	370.11965	C19H19ClN4O2	pERK2	430
Pool 2	Crude	0378493_0086_Std05	N/A	397.16694	C21H24ClN5O	pERK2	10000
Pool 2	Crude	0378493_0086_Std06	N/A	362.09344	C20H15ClN4O	pERK2	2000

Pool 2	Crude	0378493_0086_Std07	N/A	376.10909	C21H17ClN4O	pERK2	86
Pool 2	Crude	0378493_0086_Std08	N/A	377.10434	C20H16ClN5O	pERK2	230
Pool 2	Crude	0378493_0086_Std09	N/A	412.09025	C21H15ClF2N4O	pERK2	40
Pool 2	Crude	0378493_0086_Std10	N/A	402.12474	C23H19ClN4O	pERK2	510
Pool 2	Crude	0378493_0086_Std11	N/A	391.11999	C21H18ClN5O	pERK2	330
Pool 2	Crude	0378493_0086_Std12	N/A	392.104	C21H17ClN4O2	pERK2	170
Pool 2	Crude	0378493_0086_Std13	N/A	390.12474	C22H19ClN4O	pERK2	100
Pool 2	Crude	0378493_0086_Std14	N/A	406.11965	C22H19ClN4O2	pERK2	35
Pool 2	Crude	0378493_0086_Std15	N/A	420.09892	C22H17ClN4O3	pERK2	5000
Pool 2	Crude	0378493_0086_Std16	N/A	419.1149	C22H19Cl2N5O2	pERK2	510
Pool 2	Crude	0378493_0086_Std17	N/A	418.11965	C23H19ClN4O2	pERK2	4000
Pool 2	Crude	0378493_0086_Std18	N/A	424.11023	C22H18ClFN4O2	pERK2	63
Pool 2	Crude	0378493_0086_Std20	N/A	474.04171	C22H17Cl3N4O2	pERK2	7

Competition Experiment Prep. All work was done at 0 ˚C unless otherwise noted. pERK2 stock (internal preparation: 58.6 µM stock solution in 25 mM Tris, pH 8.0, 260 mM NaCl, 10 % glycerol, 1mM EDTA, 5mM DTT) was removed from a -78 ˚C freezer and warmed to approximately 0 ˚C. Protein dilution buffer was prepared (61 mM Hepes pH 7.50, 250 mM NaCl, 12 mM $MgCl_2$, 0.25% CHAPS, 2.5 mM dithiothreitol) along with library dilution buffer (50.0 mM Hepes pH 7.50, 150 mM NaCl). The two pools were thawed and aliquots were removed. The pool aliquots were then separately diluted 1:20 with library dilution buffer and stored at ambient temperature (4 µL DMSO pool into 76 µL library dilution buffer, to yield a final concentration of 2 µM/compound). Invertase (negative control, Sigma Aldrich cat. no. I4504) was weighed into a centrifuge tube and diluted to 20 µM (then to 10 µM) with protein dilution buffer. Separately, stock pERK2 was diluted to 40 µM with protein dilution buffer in advance of the serial dilution. A pERK2 serial dilution was then performed (with diluted invertase solution) in a 96-well plate to arrive at the following pERK2/Invertase protein levels:

Invertase	10 µM	10 µM	10 µM	10 µM	10 µM	10 µM	10 µM	10 µM
pERK2	20 µM	10 µM	5 µM	2.5 µM	1.25 µM	0.62 µM	0.31 µM	0 µM

Finally, a 1:1 dilution of the appropriate protein solution (3 µL) with the buffered library pool prepared above (3 µL) in a new 96-well plate provided the affinity ranking experiment samples with desired protein and compound concentrations. As two pools were tested (1 crude pool and 1 purified pool), this step resulted in two affinity ranking experiment sequences: one where the dilution was done with the pool of purified compounds and one where the dilution was done with the crude compound pool. The serial dilution performed above was used to prepare both affinity ranking sequences. The protein/compound mixtures were warmed to room temperature then allowed to incubate for 30 minutes. After 30 minutes, the 96-well plate was moved to an LC-MS autosampler (cooled to 4 ˚C) for analysis. Final component concentrations are shown below.

Lib. Size	19	19	19	19	19	19	19	19
Per Cmpd.	1 µM	1 µM	1 µM	1 µM	1 µM	1 µM	1 µM	1 µM
Invertase	5 µM	5 µM	5 µM	5 µM	5 µM	5 µM	5 µM	5 µM
pERK2	10 µM	5 µM	2.5 µM	1.25 µM	0.62 µM	0.31 µM	0.16 µM	0 µM

Chromatography conditions

SEC Running Buffer: 1 M NH_4OAc, pH 7.5

Flow Rate: 0.3 mL / min

Negative Control: 5 µM Invertase

See attached Excel file for raw affinity-based rank ordering data.

Table 1. Affinity-Based Rank Ordering Results

Pool	**Treatment**	**Sample Name**	**Mass**	**Formula**	**Protein**	**Reported Ki (nM)**	**Protein Conc. Where Binding First Observed**
Pool 1	Crude	0378493_0086_022	328.10909	C17H17ClN4O	pERK2	580	5.00µM Erk2_act
Pool 1	Crude	0378493_0086_023	340.10909	C18H17ClN4O	pERK2	200	5.00µM Erk2_act
Pool 1	Crude	0378493_0086_024	356.104	C18H17ClN4O2	pERK2	870	10.00µM Erk2_act
Pool 1	Crude	0378493_0086_025	370.11965	C19H19ClN4O2	pERK2	430	5.00µM Erk2_act
Pool 1	Crude	0378493_0086_026	397.16694	C21H24ClN5O	pERK2	10000	ASMS Binding Not Observed
Pool 1	Crude	0378493_0086_027	362.09344	C20H15ClN4O	pERK2	2000	ASMS Binding Not Observed
Pool 1	Crude	0378493_0086_028	376.10909	C21H17ClN4O	pERK2	86	2.50µM Erk2_act
Pool 1	Crude	0378493_0086_029	377.10434	C20H16ClN5O	pERK2	230	10.00µM Erk2_act
Pool 1	Crude	0378493_0086_030	412.09025	C21H15ClF2N4O	pERK2	40	1.25µM Erk2_act
Pool 1	Crude	0378493_0086_031	402.12474	C23H19ClN4O	pERK2	510	ASMS Binding Not Observed
Pool 1	Crude	0378493_0086_032	391.11999	C21H18ClN5O	pERK2	330	5.00µM Erk2_act
Pool 1	Crude	0378493_0086_033	392.104	C21H17ClN4O2	pERK2	170	5.00µM Erk2_act
Pool 1	Crude	0378493_0086_034	390.12474	C22H19ClN4O	pERK2	100	0.62µM Erk2_act
Pool 1	Crude	0378493_0086_035	406.11965	C22H19ClN4O2	pERK2	35	0.16µM Erk2_act
Pool 1	Crude	0378493_0086_042	420.09892	C22H17ClN4O3	pERK2	5000	ASMS Binding Not Observed
Pool 1	Crude	0378493_0086_037	419.1149	C22H19Cl2N5O2	pERK2	510	ASMS Binding Not Observed
Pool 1	Crude	0378493_0086_038	418.1196	C23H19ClN4O	pERK2	4000	ASMS Binding Not Observed

			5	2			
Pool 1	Crude	0378493_0086_039	424.11023	C22H18ClFN4O2	pERK2	63	0.16µM Erk2_act
Pool 1	Crude	0378493_0086_041	474.04171	C22H17Cl3N4O2	pERK2	7	1.25µM Erk2_act
Pool	**Treatment**	**Sample Name**	**Mass**	**Formula**	**Protein**	**Reported Ki (nM)**	**Protein Conc. Where Binding First Observed**
Pool 2	Purified	0378493_0086_Std01	328.10909	C17H17ClN4O	pERK2	580	5.00µM Erk2_act
Pool 2	Purified	0378493_0086_Std02	340.10909	C18H17ClN4O	pERK2	200	5.00µM Erk2_act
Pool 2	Purified	0378493_0086_Std03	356.104	C18H17ClN4O2	pERK2	870	10.00µM Erk2_act
Pool 2	Purified	0378493_0086_Std04	370.11965	C19H19ClN4O2	pERK2	430	5.00µM Erk2_act
Pool 2	Purified	0378493_0086_Std05	397.16694	C21H24ClN5O	pERK2	10000	ASMS Binding Not Observed
Pool 2	Purified	0378493_0086_Std06	362.09344	C20H15ClN4O	pERK2	2000	ASMS Binding Not Observed
Pool 2	Purified	0378493_0086_Std07	376.10909	C21H17ClN4O	pERK2	86	2.50µM Erk2_act
Pool 2	Purified	0378493_0086_Std08	377.10434	C20H16ClN5O	pERK2	230	10.00µM Erk2_act
Pool 2	Purified	0378493_0086_Std09	412.09025	C21H15ClF2N4O	pERK2	40	0.62µM Erk2_act
Pool 2	Purified	0378493_0086_Std10	402.12474	C23H19ClN4O	pERK2	510	ASMS Binding Not Observed
Pool 2	Purified	0378493_0086_Std11	391.11999	C21H18ClN5O	pERK2	330	5.00µM Erk2_act
Pool 2	Purified	0378493_0086_Std12	392.104	C21H17ClN4O2	pERK2	170	5.00µM Erk2_act
Pool 2	Purified	0378493_0086_Std13	390.12474	C22H19ClN4O	pERK2	100	0.62µM Erk2_act
Pool 2	Purified	0378493_0086_Std14	406.11965	C22H19ClN4O2	pERK2	35	0.31µM Erk2_act
Pool 2	Purified	0378493_0086_Std15	420.09892	C22H17ClN4O3	pERK2	5000	ASMS Binding Not Observed
Pool 2	Purified	0378493_0086_Std16	419.1149	C22H19Cl2N5O2	pERK2	510	ASMS Binding Not Observed
Pool 2	Purified	0378493_0086_Std17	418.11965	C23H19ClN4O2	pERK2	4000	ASMS Binding Not Observed
Pool 2	Purified	0378493_0086_Std18	424.11023	C22H18ClFN4O2	pERK2	63	0.31µM Erk2_act
Pool 2	Purified	0378493_0086_Std20	474.04171	C22H17Cl3N4O2	pERK2	7	0.62µM Erk2_act

Plots displaying the general correlation between activity assay K_i (plotted on a log scale) [6] and the lowest pERK2 concentration at which ASMS binding was observed (protein level) are shown below:

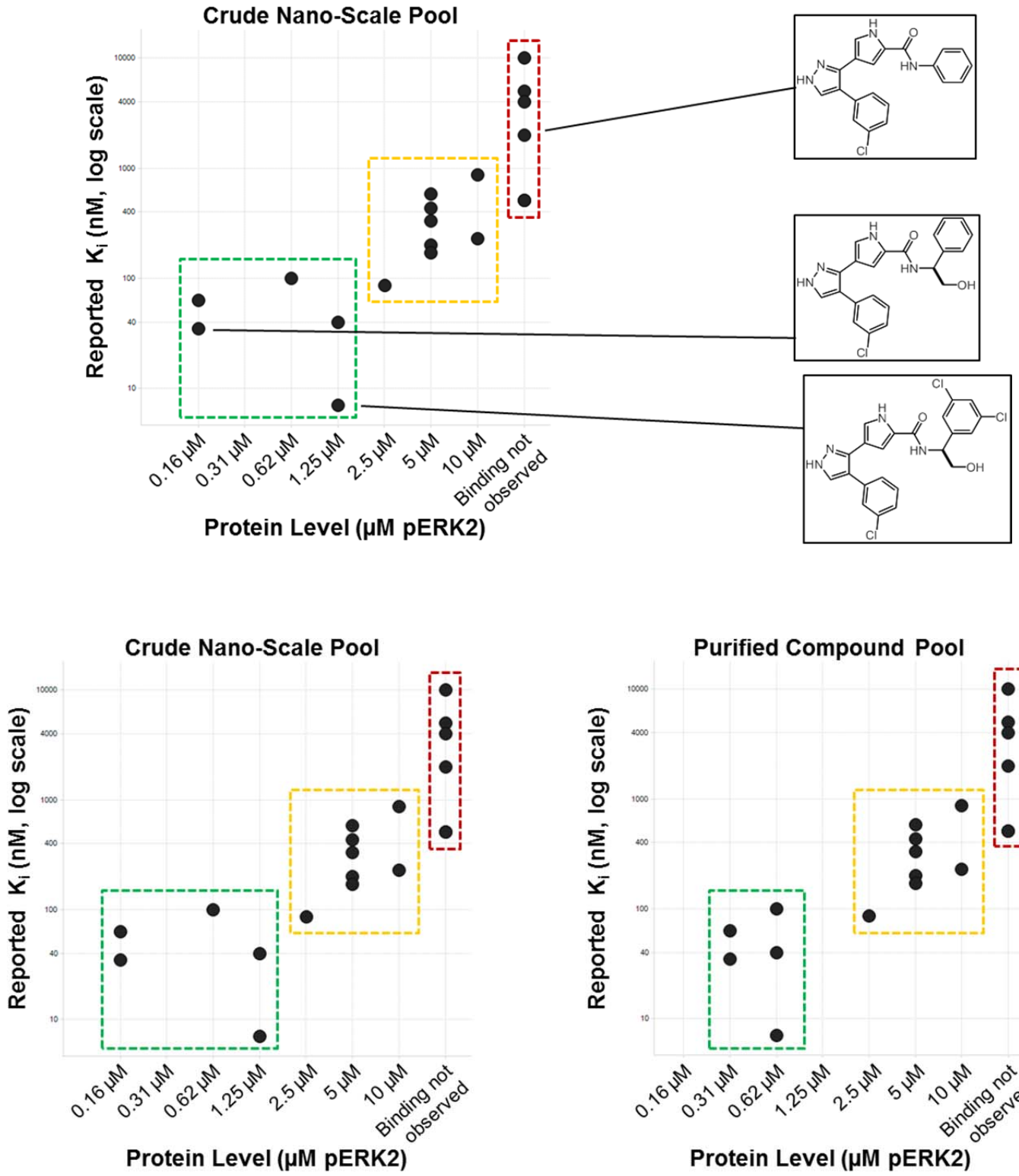


Figure 16. Affinity-Based Ranking of pERK2 Amide Library Comparison: Nano-Scale Crude Library Versus Purified Library

5.4. ASMS Quality Control (QC) Data

Prior to the affinity-based ranking experiment, ASMS QC (LC-HRMS) was performed to confirm that all 19 library members were present and could be detected by mass within the crude pool. When compounds detected in the QC experiment are not observed to

bind in the subsequent affinity-based ranking assay, we concluded that those compounds were successfully synthesized and tested, but do not bind to the protein with sufficient affinity for detection in the ASMS system.

Table 2. ERK2 Amide ASMS QC Data

Condition	Reaction ID	Compound ID	Base Mass	QC data (MS signal intensity)
Crude reaction	0378493_0086_022	**A1**	328.10909	72956001.3
Crude reaction	0378493_0086_023	**A2**	340.10909	93177424.6
Crude reaction	0378493_0086_024	**A3**	356.104	101352294.9
Crude reaction	0378493_0086_025	**A4**	370.11965	86147576.83
Crude reaction	0378493_0086_026	**A5**	397.16694	44643578.2
Crude reaction	0378493_0086_027	**A6**	362.09344	35366764.07
Crude reaction	0378493_0086_028	**A7**	376.10909	54353797.02
Crude reaction	0378493_0086_029	**A8**	377.10434	11906919.7
Crude reaction	0378493_0086_030	**A9**	412.09025	19176416.81
Crude reaction	0378493_0086_031	**A10**	402.12474	10528827.65
Crude reaction	0378493_0086_032	**A11**	391.11999	6854152.21
Crude reaction	0378493_0086_033	**A12**	392.104	67933663.41
Crude reaction	0378493_0086_034	**A13**	390.12474	91363196.19
Crude reaction	0378493_0086_035	**2**	406.11965	65368865.72
Crude reaction	0378493_0086_042	**3**	420.09892	94348340.58
Crude reaction	0378493_0086_037	**A14**	419.1149	1464876.4
Crude reaction	0378493_0086_038	**A15**	418.11965	34803186.33
Crude reaction	0378493_0086_039	**A16**	424.11023	68404830.67
Crude reaction	0378493_0086_041	**A17**	474.04171	13730935.88

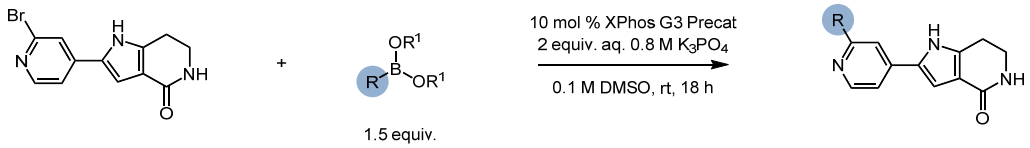
6. Synthesis and Rank Ordering of a Suzuki Coupling Library Targeting Mitogen-Activated Protein Kinase-Activated Protein Kinase 2 (MK2)

The library below was previously described in a *J. Med. Chem.* article and in a patent.[7,12] Reproducing a selection of compounds from this extensive library, at a miniaturized scale, was attractive to us from the perspective of workflow and result validation. The library contains species ranging from highly potent (<10 nM) to weak/inactive (>10,000 nM) and would serves as a good test of this platforms ability to differentiate high affinity, moderate, and weak compounds from each other in crude mixtures. Finally, this was an opportunity to construct a miniaturized library using a complex catalytic transformation, showcasing the screening capabilities of the nano-scale synthesis platform, and to highlight the value of utilizing multiple conditions in synthesis to ensure good to high library yields are ultimately achieved.

The 18-member Suzuki coupling library was initially prepared and purified at the 0.05 mmol bench-scale for a direct comparison to the crude nano-scale library. The purified compounds were submitted to Invitrogen as 10 mM DMSO solutions for biochemical evaluation against MK2 (IC_{50} values reported).

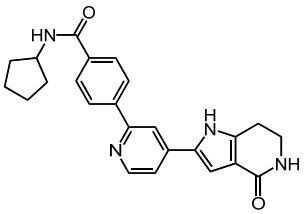
6.1. Bench-Scale Synthesis of MK2 Validation Library

General Procedure for 2-(2-bromopyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one Suzuki Cross-Coupling



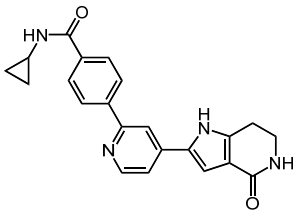
The aryl bromide core above was weighed into a 1-dram vial (1 equiv., 0.05 mmol scale) equipped with a magnetic stir bar. The desired boronic acid or [pinacol] boronic ester building block (1.5 equiv., 0.075 mmol) was next weighed and dispensed into the same 1-dram vial. The vial was moved to a glove box where DMSO was added and the reagents dissolved. Next, Xphos G3 precatalyst (10 mol %, 0.005 mmol) was added as a stock solution in DMSO, followed by aqueous 0.8 M K_3PO_4 (2 equiv.). The vial was sealed, removed from the glove box, and stirred at room temperature for 18 hours. The next morning, aliquots were taken of all reactions and progress was determined by LC-MS. Upon completion, reactions were diluted with DMSO (1.5 mL), filtered, and submitted for purification by RP-HPLC. Products were returned as TFA salts unless otherwise noted. After purification and characterization the coupling products were dissolved in DMSO to a concentration of 10 mM. All members of this library were previously disclosed as part of an MK-2 campaign article or accompanying patent.[7,12]

***N*-cyclopentyl-4-(4-(4-oxo-4,5,6,7-tetrahydro-1H-pyrrolo[3,2-c]pyridin-2-yl)pyridin-2-yl)benzamide (B1)**



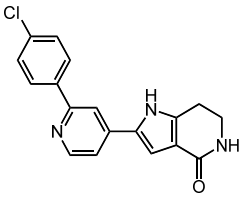
The title compound was prepared using the standard conditions described above and [4-(cyclopentylcarbamoyl)phenyl]boronic acid (MFCD03788418) as the building block. The desired product was prepared at the 0.033 mmol scale and purified by RP-HPLC to yield 12 mg (71% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **B1**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.01 (br s, 1H), 8.58 (d, *J* = 4.9 Hz, 1H), 8.37 (d, *J* = 7.0 Hz, 1H), 8.28 (s, 1H), 8.24 (d, *J* = 8.0 Hz, 2H), 7.96 (d, *J* = 8.0 Hz, 2H), 7.60 (d, *J* = 4.7 Hz, 1H), 7.19 (s, 1H), 7.07 (s, 1H), 4.25 (apparent d, *J* = 6.6 Hz, 1H), 3.42 (br s, 2H), 2.87 (t, *J* = 6.5 Hz, 2H), 1.90 (br s, 2H), 1.71 (br s, 2H), 1.54 (br s, 4H); **HRMS** (ESI): *m/z* calculated for $C_{24}H_{25}N_4O_2$ [M+H]+ 401.19723, found 401.19375. Measured IC_{5o} (MK2, Invitrogen) 73.9 nM

***N*-cyclopropyl-4-(4-(4-oxo-4,5,6,7-tetrahydro-1H-pyrrolo[3,2-c]pyridin-2-yl)pyridin-2-yl)benzamide (5)**



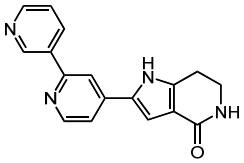
The title compound was prepared using the standard conditions described above and [4-(cyclopropylcarbamoyl)phenyl]boronic acid (MFCD03788419) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 16.6 mg (89% yield) of the title compound as a yellow solid. Spectral data were in agreement with reported literature values. Analytical data for **5**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.01 (br s, 1H), 8.57 (d, *J* = 5.1 Hz, 1H), 8.53 (d, *J* = 3.7 Hz, 1H), 8.28 (s, 1H), 8.24 (d, *J* = 8.2 Hz, 2H), 7.94 (d, *J* = 8.2 Hz, 2H), 7.60 (d, *J* = 4.7 Hz, 1H), 7.20 (s, 1H), 7.08 (s, 1H), 3.42 (t, *J* = 5.6 Hz, 2H), 2.87 (t, *J* = 6.4 Hz, 3H), 0.71 (apparent q, *J* = 5.5 Hz, 2H), 0.60 (br s, 2H); **HRMS** (ESI): *m/z* calculated for $C_{22}H_{21}N_4O_2$ [M+H]+ 373.16593, found 373.16559. Measured IC_{50} (MK2, Invitrogen) 59.3 nM

2-(2-(4-chlorophenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B2)



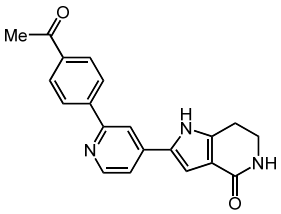
The title compound was prepared using the standard conditions described above and (4-chlorophenyl)boronic acid (MFCD00039137) as the building block. The desired product was prepared at the 0.033 mmol scale and purified by RP-HPLC to yield 1.8 mg (12% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **B2**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.22 (s, 1H), 8.61 (d, *J* = 5.6 Hz, 1H), 8.33 (s, 1H), 8.14 (d, *J* = 8.4 Hz, 2H), 7.77 (m, 1H), 7.65 (d, *J* = 8.3 Hz, 2H), 7.39 (s, 1H), 7.16 (s, 1H), 3.43 (t, *J* = 6.3 Hz, 2H), 2.89 (t, *J* = 6.7 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{18}H_{15}ClN_3O$ [M+H]+ 324.08984, found 324.08936. Measured IC_{50} (MK2, Invitrogen) 367 nM

2-([2,3'-bipyridin]-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B3)



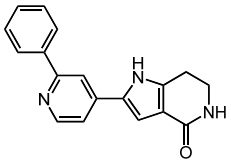
The title compound was prepared using the standard conditions described above and 3-pyridylboronic acid (MFCD00674177) as the building block. The desired product was prepared at the 0.033 mmol scale and purified by RP-HPLC to yield 3.3 mg (25% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **B3**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.03 (s, 1H), 9.35 (s, 1H), 8.69 (d, *J* = 3.9 Hz, 1H), 8.61 (d, *J* = 5.2 Hz, 1H), 8.56 (d, *J* = 7.1 Hz, 1H), 8.34 (s, 1H), 7.67 (d, *J* = 4.4 Hz, 1H), 7.62 (m, 1H), 7.26 (s, 1H), 7.09 (s, 1H), 3.42 (t, obscured by water, *J* = 6.0 Hz, 2H), 2.87 (t, *J* = 6.7 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{17}H_{15}N_4O$ [M+H]+ 291.12406, found 291.12439. Measured IC_{50} (MK2, Invitrogen) 231.5 nM

2-(2-(4-acetylphenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B4)



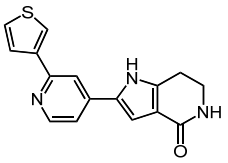
The title compound was prepared using the standard conditions described above and (4-acetylphenyl)boronic acid (MFCD01074667) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 16.5 mg (74% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **B4**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.11 (s, 1H), 8.62 (d, *J* = 5.2 Hz, 1H), 8.35 (s, 1H), 8.30 (d, *J* = 8.1 Hz, 2H), 8.10 (d, *J* = 8.1 Hz, 2H), 7.70 (s, 1H), 7.28 (s, 1H), 7.11 (s, 1H), 3.43 (t, *J* = 6.0 Hz, 2H), 2.88 (t, *J* = 6.7 Hz, 2H), 2.64 (s, 3H); **HRMS** (ESI): *m/z* calculated for $C_{20}H_{18}N_3O_2$ [M+H]+ 332.13938, found 332.13922. Measured IC_{50} (MK2, Invitrogen) 132 nM

2-(2-phenylpyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B5)



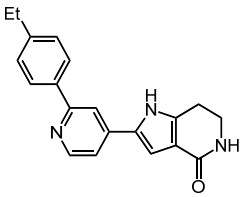
The title compound was prepared using the standard conditions described above and phenylboronic acid (MFCD00002103) as the building block. The desired product was prepared at the 0.033 mmol scale and purified by RP-HPLC to yield 10.5 mg (79% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **B5**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.22 (br s, 1H), 8.60 (d, *J* = 5.5 Hz, 1H), 8.31 (s, 1H), 8.11 (d, *J* = 7.3 Hz, 2H), 7.77 (br s, 1H), 7.56 (m, 3H), 7.38 (br s, 1H), 7.16 (s, 1H), 3.43 (t, *J* = 5.9 Hz, 3H), 2.89 (t, *J* = 6.7 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{18}H_{16}N_3O$ [M+H]+ 290.12881, found 290.12885. Measured IC_{50} (MK2, Invitrogen) 373.5 nM

2-(2-(thiophen-3-yl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B6)



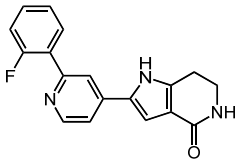
The title compound was prepared using the standard conditions described above and 3-thienylboronic acid (MFCD00151851) as the building block. The desired product was prepared at the 0.033 mmol scale and purified by RP-HPLC to yield 13.8 mg (100% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **B6**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.21 (br s, 1H), 8.54 (d, *J* = 5.5 Hz, 1H), 8.39 (br s, 1H), 8.31 (br s, 1H), 7.87 (d, *J* = 4.6 Hz, 1H), 7.78 (s, 1H), 7.72 (br s, 1H), 7.44 (br s, 1H), 7.17 (s, 1H), 3.43 (t, *J* = 5.8 Hz, 2H), 2.90 (t, *J* = 6.6 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{16}H_{14}N_3OS$ [M+H]+ 296.08523, found 296.08484. Measured IC_{50} (MK2, Invitrogen) 399 nM

2-(2-(4-ethylphenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B7)



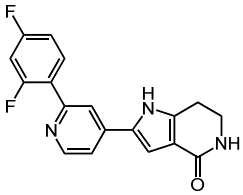
The title compound was prepared using the standard conditions described above and (4-ethylphenyl)boronic acid (MFCD00859377) as the building block. The desired product was prepared at the 0.033 mmol scale and purified by RP-HPLC to yield 10.3 mg (72% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **B7**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 11.98 (br s, 1H), 8.52 (d, *J* = 5.1 Hz, 1H), 8.17 (s, 1H), 8.08 (d, *J* = 7.9 Hz, 2H), 7.54 (d, *J* = 4.8 Hz, 1H), 7.34 (d, *J* = 7.9 Hz, 2H), 7.14 (s, 1H), 7.06 (br s, 1H), 3.42 (t, *J* = 5.6 Hz, 2H), 2.86 (t, *J* = 6.7 Hz, 2H), 2.67 (q, *J* = 7.3 Hz, 2H), 1.22 (t, *J* = 7.5 Hz, 3H); **HRMS** (ESI): *m/z* calculated for $C_{20}H_{20}N_3O$ [M+H]+ 318.16011, found 318.15967. Measured IC_{50} (MK2, Invitrogen) 409.5 nM

2-(2-(2-fluorophenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B8)



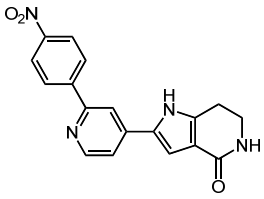
The title compound was prepared using the standard conditions described above and (2-fluorophenyl)boronic acid (MFCD00674013) as the building block. The desired product was prepared at the 0.033 mmol scale and purified by RP-HPLC to yield 12.7 mg (91% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **B8**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.19 (s, 1H), 8.65 (d, *J* = 5.4 Hz, 1H), 8.09 (s, 1H), 7.86 (t, *J* = 7.5 Hz, 1H), 7.79 (s, 1H), 7.57 (m, 1H), 7.40 (m, 2H), 7.25 (s, 1H), 7.15 (s, 1H), 3.41 (t, *J* = 5.9 Hz, 2H), 2.87 (t, *J* = 6.7 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{18}H_{15}FN_3O$ [M+H]+ 308.11939, found 308.11917. Measured IC_{50} (MK2, Invitrogen) 665 nM

2-(2-(2,4-difluorophenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B9)



The title compound was prepared using the standard conditions described above and 2-(2,4-difluorophenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (MFCD05663880) as the building block. The desired product was prepared at the 0.075 mmol scale and purified by RP-HPLC to yield 18.7 mg (57% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **B9**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.19 (s, 1H), 8.65 (d, *J* = 5.5 Hz, 1H), 8.08 (s, 1H), 7.93 (q, *J* = 8.5 Hz, 1H), 7.79 (br s, 1H), 7.50 (t, *J* = 9.5 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.26 (s, 1H), 7.16 (s, 1H), 3.41 (t, *J* = 6.2 Hz, 2H), 2.87 (t, *J* = 6.7 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{18}H_{14}F_2N_3O$ [M+H]+ 326.10997, found 326.10974. Measured IC_{50} (MK2, Invitrogen) 1029 nM

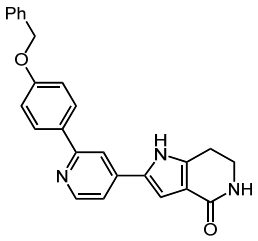
2-(2-(4-nitrophenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B10)



The title compound was prepared using the standard conditions described above and (4-nitrophenyl)boronic acid (MFCD00161360) as the building block. The desired product was prepared at the 0.033 mmol scale and purified by RP-HPLC to yield 2.2 mg (15% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data

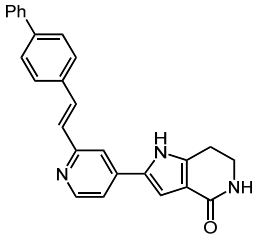
for **B10**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.11 (s, 1H), 8.65 (d, *J* = 5.0 Hz, 1H), 8.43 (d, *J* = 8.4 Hz, 2H), 8.40 (s, 1H), 8.38 (d, *J* = 8.4 Hz, 2H), 7.72 (d, *J* = 4.4 Hz, 1H), 7.29 (s, 1H), 7.09 (d, J = 13.1 Hz, 1H), 3.43 (t, *J* = 6.1 Hz, 2H), 2.88 (t, *J* = 6.5 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{18}H_{15}N_4O_3$ [M+H]+ 335.11389, found 335.11337. Measured IC_{50} (MK2, Invitrogen) 421 nM

2-(2-(4-(benzyloxy)phenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B11)



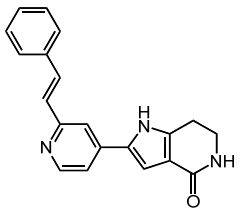
The title compound was prepared using the standard conditions described above and (4-benzyloxyphenyl)boronic acid (MFCD01075705) as the building block. The desired product was prepared at the 0.075 mmol scale and purified by RP-HPLC to yield 12 mg (31% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **B11**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 11.96 (s, 1H), 8.49 (d, *J* = 4.5 Hz, 1H), 8.12 (m, 3H), 7.48 (m, 3H), 7.40 (t, *J* = 7.0 Hz, 2H), 7.34 (d, J = 6.9 Hz, 1H), 7.13 (m, 3H), 7.05 (s, 1H), 5.18 (s, 2H), 3.42 (br s, 2H), 2.86 (t, *J* = 6.1 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{25}H_{22}N_3O_2$ [M+H]+ 396.17068, found 396.17102. Measured IC_{50} (MK2, Invitrogen) 1790 nM

(*E*)-2-(2-(2-([1,1'-biphenyl]-4-yl)vinyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B12)



The title compound was prepared using the standard conditions described above and [(E)-2-(4-phenylphenyl)vinyl]boronic acid (MFCD04974059) as the building block. The desired product was prepared at the 0.033 mmol scale and purified by RP-HPLC to yield 11.7 mg (70% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **B12**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.35 (s, 1H), 8.60 (d, *J* = 5.9 Hz, 1H), 8.34 (br s, 1H), 7.96 (d, *J* = 16.3 Hz, 1H), 7.81 (m, 3H), 7.75 (m, 4H), 7.49 (t, *J* = 7.4 Hz, 3H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.32 (d, *J* = 16.3 Hz, 1H), 7.24 (s, 1H), 3.44 (t, *J* = 5.6 Hz, 2H), 2.92 (t, *J* = 6.6 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{26}H_{22}N_3O$ [M+H]+ 392.17576, found 392.17508. Measured IC_{50} (MK2, Invitrogen) 4435 nM

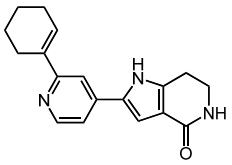
(*E*)-2-(2-styrylpyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B13)



The title compound was prepared using the standard conditions described above and [(E)-styryl]boronic acid (MFCD00963621) as the building block. The desired product was prepared at the 0.033 mmol scale and purified by RP-HPLC to yield 9.7 mg (68% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **B13**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 11.94 (s, 1H), 8.47 (d, *J* = 4.5 Hz, 1H), 7.84 (s, 1H), 7.69 (d, *J* = 16.2 Hz, 1H), 7.65 (d, *J* = 7.4 Hz, 2H), 7.47 (d, *J* = 4.3 Hz, 1H), 7.41 (t, *J* = 7.1 Hz, 2H), 7.32 (t, *J* = 6.9 Hz, 1H), 7.25 (d, *J* = 16.1 Hz, 1H), 7.06 (d, J = 7.3 Hz, 2H), 3.41 (s,

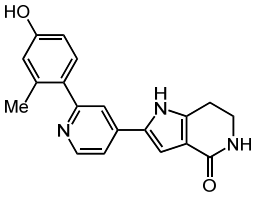
2H), 2.85 (t, *J* = 6.2 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{20}H_{18}N_3O$ [M+H]+ 316.14446, found 316.14474. Measured IC_{50} (MK2, Invitrogen) 172.5 nM

2-(2-(cyclohex-1-en-1-yl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B14)



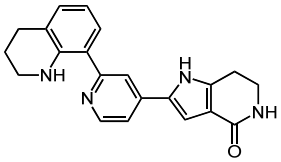
The title compound was prepared using the standard conditions described above and 2-(cyclohexen-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (MFCD05663845) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 5 mg (34% yield) of the title compound as a yellow solid. Spectral data were in agreement with reported literature values. Analytical data for **B14**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.47 (s, 1H), 8.48 (d, *J* = 6.3 Hz, 1H), 8.08 (s, 1H), 7.90 (d, *J* = 5.7 Hz, 1H), 7.57 (s, 1H), 7.25 (s, 1H), 6.86 (s, 1H), 3.43 (t, *J* = 5.7 Hz, 2H), 2.91 (t, *J* = 6.7 Hz, 2H), 2.30 (br s, 2H), 1.76 (m, 2H), 1.64 (m, 2H); **HRMS** (ESI): *m/z* calculated for $C_{18}H_{20}N_3O$ [M+H]+ 294.16011, found 294.15964. Measured IC_{50} (MK2, Invitrogen) 3110 nM

2-(2-(4-hydroxy-2-methylphenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (6)



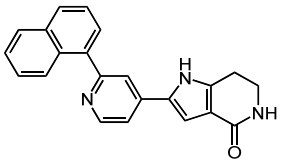
The title compound was prepared using 3-methyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenol (1.5 equiv., MFCD16994280) as the building block, *t*-Bu_3P G2 precatalyst (10 mol %), aqueous 0.8 M K_3PO_4 (2 equiv.), and NMP as the reaction solvent. The reaction was carried out at the 0.12 mmol scale (aryl bromde core), stirred overnight, and purified by RP-HPLC to yield 45.0 mg (87% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **6**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.45 (s, 1H), 10.05 (br s, 1H), 8.62 (d, *J* = 6.2 Hz, 1H), 8.05 (s, 1H), 7.99 (d, *J* = 5.3 Hz, 1H), 7.54 (s, 1H), 7.35 (d, *J* = 8.2 Hz, 1H), 7.26 (s, 1H), 6.80 (m, 2H), 3.42 (t, *J* = 5.6 Hz, 2H), 2.90 (t, *J* = 6.6 Hz, 2H), 2.30 (s, 3H); **HRMS** (ESI): *m/z* calculated for $C_{19}H_{18}N_3O_2$ [M+H]+ 320.13938, found 320.13925. Measured IC_{50} (MK2, Invitrogen) 3405 nM

2-(2-(1,2,3,4-tetrahydroquinolin-8-yl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B15)



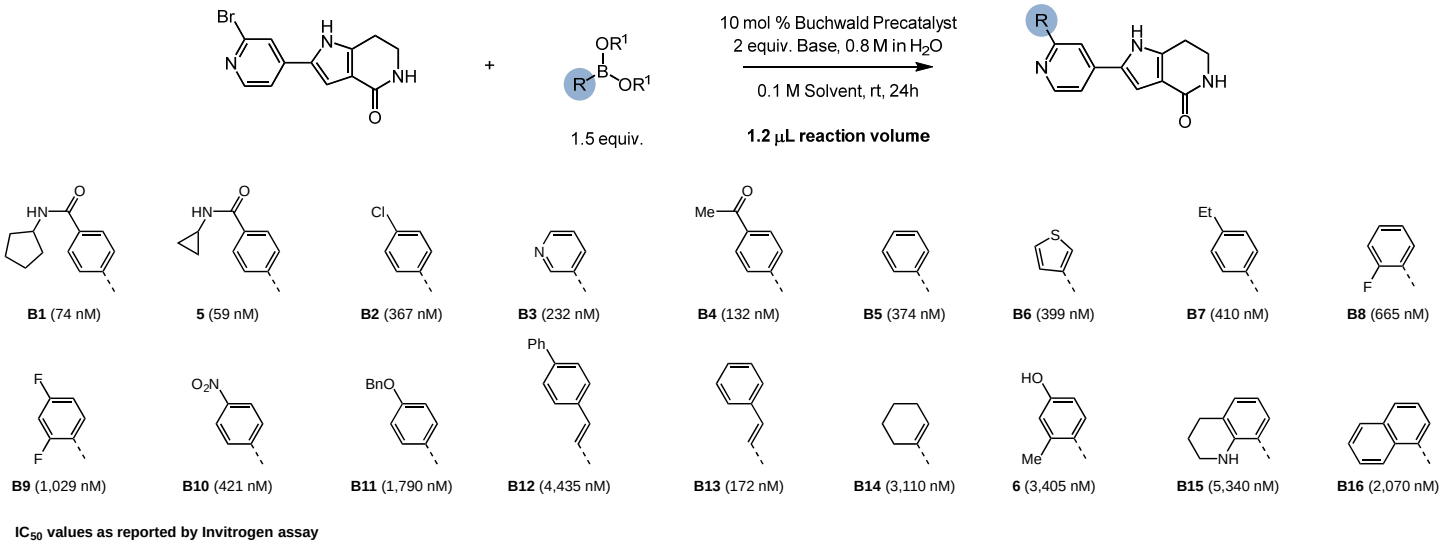
The title compound was prepared using the standard conditions described above and 8-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,2,3,4-tetrahydroquinoline (MFCD18383813) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 16.3 mg (71% yield) of the title compound as a yellow solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **B15**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.00 (s, 1H), 8.46 (d, *J* = 4.9 Hz, 2H), 7.99 (s, 1H), 7.54 (d, *J* = 7.7 Hz, 1H), 7.50 (d, *J* = 4.8 Hz, 1H), 7.08 (s, 1H), 7.05 (s, 1H), 6.92 (d, *J* = 7.1 Hz, 1H), 6.53 (t, *J* = 7.5 Hz, 1H), 3.41 (q, *J* = 4.8 Hz, 2H), 3.33 (m, 2H, obscured by water), 2.85 (t, *J* = 6.8 Hz, 2H), 2.75 (t, *J* = 6.1 Hz, 2H), 1.81 (m, 2H); **HRMS** (ESI): *m/z* calculated for $C_{21}H_{21}N_4O$ [M+H]+ 345.17101, found 345.17096. Measured IC_{50} (MK2, Invitrogen) 5340 nM

2-(2-(naphthalen-1-yl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B16)



The title compound was prepared using the standard conditions described above and 1-naphthylboronic acid (MFCD00019722) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 9.3 mg (55% yield) of the title compound as a yellow solid. Spectral data were in agreement with reported literature values. Analytical data for **B16**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 11.99 (s, 1H), 8.64 (d, *J* = 5.3 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 8.01 (m, 2H), 7.90 (s, 1H), 7.65 (m, 3H), 7.53 (m, 2H), 7.09 (s, 1H), 7.06 (s, 1H), 3.40 (m, 2H), 2.83 (t, *J* = 6.8 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{22}H_{18}N_3O$ [M+H]+ 340.14446, found 340.14423. Measured IC_{50} (MK2, Invitrogen) 2070 nM

6.2. Nanomole-Scale Suzuki Coupling Library on 4



List of boronic acid and boronic ester building blocks used in this study (MDL numbers): MFCD03788418, MFCD03788419, MFCD00039137, MFCD00674177, MFCD01074667, MFCD00002103, MFCD00151851, MFCD00859377, MFCD00674013, MFCD05663880, MFCD00161360, MFCD01075705, MFCD04974059, MFCD00963621, MFCD05663845, MFCD16994280, MFCD18383813, MFCD00019722

8 unique reaction conditions were screened in the synthesis of the above-depicted library (2 solvents, 2 aqueous bases, 2 Buchwald precatalysts). Solvents used: DMSO and NMP. Bases used: aqueous 0.8 M K_3PO_4 and aqueous 0.8 M 2-*tert*-butyl-1,1,3,3-tetramethylguanidine (BTMG, Aldrich #20615-5ML). Catalysts used: Chloro[(tri-*tert*-butylphosphine)-2-(2-aminobiphenyl)] palladium(II) G2 precatalyst (*t*-Bu_3P G2, Aldrich #756482-500MG) and (2-Dicyclohexylphosphino-2',4',6'-triisopropyl-1,1'-biphenyl)[2-(2'-amino-1,1'-biphenyl)]palladium(II) methanesulfonate G3 precatalyst (XPhos G3, Aldrich #763381-1G).

All chemistry and nanoliter pipetting was done under an N_2 atmosphere in a glove box. Stock solutions of the pyridyl bromide core (0.4 M in NMP and DMSO), boronic acid/ester building blocks (0.6 M in NMP and DMSO), Buchwald palladium precatalysts (0.04 M in NMP and DMSO), and bases (K_3PO_4 and BTMG, 0.8 M in H_2O) were prepared in the glove box. A source plate was constructed using the reagent stock solutions, according to the diagram below, by pipetting 15-20 μL of the correct component stock into the wells shown in Figure 17. The TTP Labtech Mosquito® was used to assemble the reaction mixtures, utilizing the multi-aspiration feature and dispense mixing.

1. 297 nL was drawn up from the desired core column (NMP: column 1, DMSO: column 2)
2. 297 nL was drawn from the desired building block column (NMP: columns 4-5, DMSO columns 6-7)
3. 6 nL Tip wash (NMP column 9, DMSO column 10)
4. 297 nL was drawn up from the desired catalyst column (NMP: columns 11-12, DMSO columns 13-14)
5. 6 nL Tip wash (NMP column 15, DMSO column 16)
6. 297 nL was drawn up from the desired aqueous base column (K_3PO_4 in column 18, BTMG in column 19).
7. This was immediately followed by dispense mixing (3×800 nL) into the 1,536-well reaction plate to ensure all reagents were adequately combined.
8. This process was done 8 times to cover all possible reaction conditions (8 total: 2 solvents × 2 bases × 2 catalysts).
9. The 1,536-plate was sealed and briefly centrifuged before sitting at ambient temperature for 24 hours.

The next morning, the reactions were quenched by addition of 3×1.2 µL 0.5 M AcOH in DMSO to each reaction well. The reactions were further diluted (to approximately 10 mM assuming complete conversion to product) with DMSO and transferred to a 384-well LDV diamond plate for affinity-based ranking. 1 µL of the quenched and diluted crude reaction was drawn up for analysis by LC-MS (1 µL crude ~10 mM reaction into 60 µL DMSO followed by shaking). Screening results are represented as a heat map (Figure 18). Colors represent a percent yield gradient (blue-green-yellow = 0% to 50% to 100% yield), where values were calculated using standard curves created from isolated products. Highlighted wells were used to create the crude pool for ASMS ranking and were selected based upon product yield and substrate conversion. NOTE: elevated yields (above 100% as determined by standard curves) shown for some reactions in DMSO are likely the result of diminished solubility of the pyridyl bromide core in DMSO as a 0.4 M stock solution, causing more of the core (limiting reagent) to be charged into the reaction drop.

	NMP Core	DMSO Core		NMP Mono	NMP Mono	DMSO Mono	DMSO Mono		Wash	Wash	Cat 1 NMP	Cat 2 NMP	Cat 1 DMSO	Cat 2 DMSO	Wash	Wash		Aq Base	Aq Base					
	16 uL	16 uL		30 uL	30 uL	30 uL	30 uL		50 uL	50 uL	30 uL	30 uL	30 uL	30 uL	50 uL	50 uL		30 uL	30 uL					
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
A	Core NMP	Core DMSO		MFCD03788418	MFCD05663880	MFCD03788418	MFCD05663880		NMP	DMSO	Xphos G3 NMP	tBu3P G2 NMP	Xphos G3 DMSO	tBu3P G2 DMSO	NMP	DMSO		aq K3PO4	aq BTMG					
B	Core NMP	Core DMSO		MFCD03788419	MFCD00161360	MFCD03788419	MFCD00161360		NMP	DMSO	Xphos G3 NMP	tBu3P G2 NMP	Xphos G3 DMSO	tBu3P G2 DMSO	NMP	DMSO		aq K3PO4	aq BTMG					
C	Core NMP	Core DMSO		MFCD00039137	MFCD01075705	MFCD00039137	MFCD01075705		NMP	DMSO	Xphos G3 NMP	tBu3P G2 NMP	Xphos G3 DMSO	tBu3P G2 DMSO	NMP	DMSO		aq K3PO4	aq BTMG					
D	Core NMP	Core DMSO		MFCD00674177	MFCD04974059	MFCD00674177	MFCD04974059		NMP	DMSO	Xphos G3 NMP	tBu3P G2 NMP	Xphos G3 DMSO	tBu3P G2 DMSO	NMP	DMSO		aq K3PO4	aq BTMG					
E	Core NMP	Core DMSO		MFCD01074667	MFCD00963621	MFCD01074667	MFCD00963621		NMP	DMSO	Xphos G3 NMP	tBu3P G2 NMP	Xphos G3 DMSO	tBu3P G2 DMSO	NMP	DMSO		aq K3PO4	aq BTMG					
F	Core NMP	Core DMSO		MFCD00002103	MFCD05663845	MFCD00002103	MFCD05663845		NMP	DMSO	Xphos G3 NMP	tBu3P G2 NMP	Xphos G3 DMSO	tBu3P G2 DMSO	NMP	DMSO		aq K3PO4	aq BTMG					
G	Core NMP	Core DMSO		MFCD00151851	MFCD16994280	MFCD00151851	MFCD16994280		NMP	DMSO	Xphos G3 NMP	tBu3P G2 NMP	Xphos G3 DMSO	tBu3P G2 DMSO	NMP	DMSO		aq K3PO4	aq BTMG					
H	Core NMP	Core DMSO		MFCD00859377	MFCD18383813	MFCD00859377	MFCD18383813		NMP	DMSO	Xphos G3 NMP	tBu3P G2 NMP	Xphos G3 DMSO	tBu3P G2 DMSO	NMP	DMSO		aq K3PO4	aq BTMG					
I	Core NMP	Core DMSO		MFCD00674013	MFCD00019722	MFCD00674013	MFCD00019722		NMP	DMSO	Xphos G3 NMP	tBu3P G2 NMP	Xphos G3 DMSO	tBu3P G2 DMSO	NMP	DMSO		aq K3PO4	aq BTMG					
J																								
K																								
L																								
M																								
N																								
O																								
P																								

Figure 17. MK2 Suzuki Cross-Coupling Source Plate Map

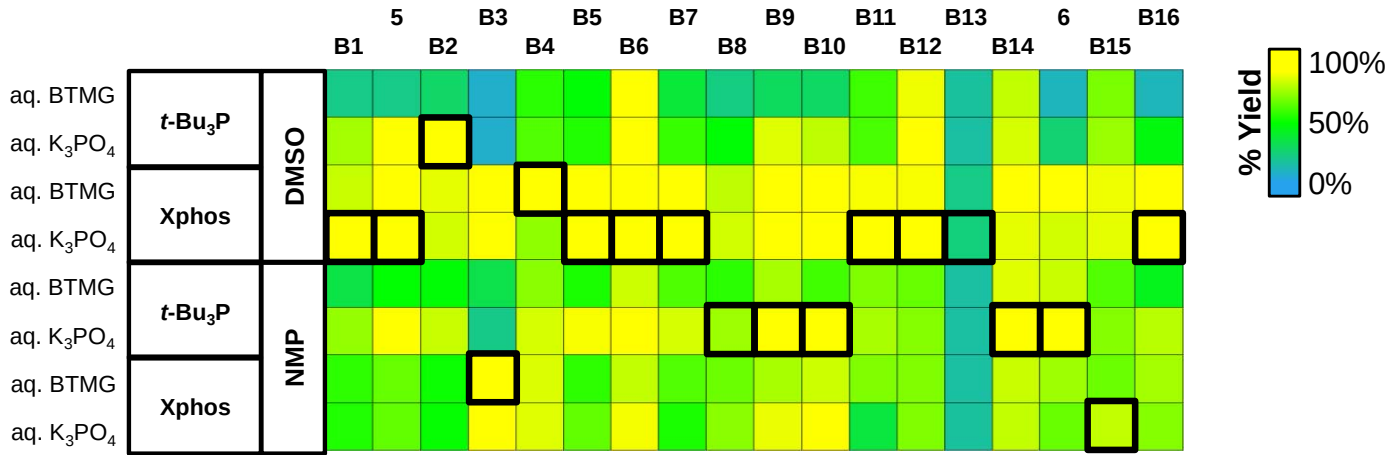


Figure 18. Nanomole-Scale Suzuki Coupling Library Heat Map

Chromatograms are presented below for the quenched and diluted crude nanomole-scale reactions producing **5** and **6** (blue peaks are the cross-coupling products).

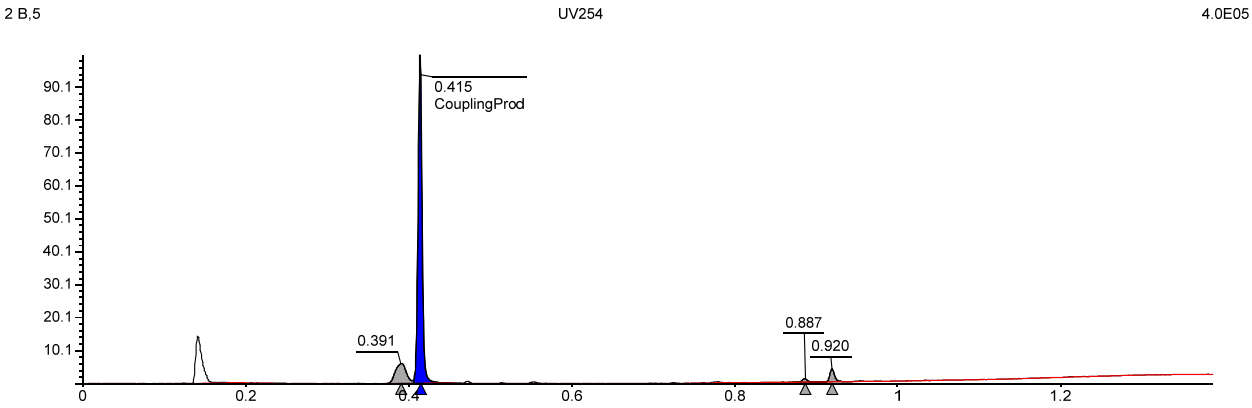


Figure 19. Chromatogram of Crude Nanomole-Scale Reaction Producing 5. Conditions: XPhos G3 / aq. K_3PO_4 / DMSO

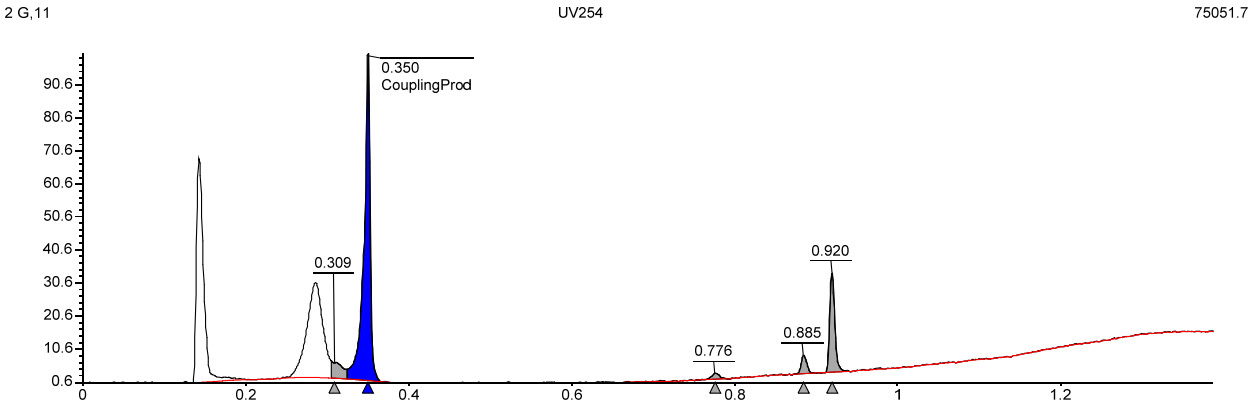


Figure 20. Chromatogram of Crude Nanomole-Scale Reaction Producing 6. Conditions: *t*-Bu_3P G3 / aq. K_3PO_4 / NMP

6.3. Affinity Ranking of the MK2 Coupling Products

Pool Prep. A pool comprised of the purified cross-coupling library (18 compounds purified by RP-HPLC and diluted to 10 mM in DMSO) was created by transferring 1 µL of each respective 10 mM solution into a centrifuge tube (18 transfers total, 18 µL total). This mixture was then diluted with DMSO to 500 µL (1:500 dilution per compound) to give a per compound concentration of 20 µM (360 µM total compound concentration). This pool was stored at -20 ˚C when not in use. A pool of quenched crude nanomole-scale reaction mixtures was prepared in a similar fashion: 1 µL was transferred from each well of the quenched reaction indicated above in Figure 18 (approx. 10 mM assuming complete conversion to product, 18 total transfers, 18 µL total) to a centrifuge tube. This crude library mixture was then diluted with DMSO to 500 µL (1:500 dilution per compound) to give a per compound concentration of approximately 20 µM. This pool was stored at -20 ˚C when not in use. Crude reactions to use in the pooling step were selected in the basis of product UV peak area (yield) and absence of starting material (relative conversion).

Table 3. MK2 Suzuki Library Pools for Affinity-Based Rank Ordering

Pool ID	Sample Name	Catalyst	Base	Solvent	Source Wells	Mass	Formula	Target	Invitrogen IC50 (nM)
Pool 1 Crude	0378493_0088_ASMS_2017_005	Xphos	K3PO4	25%H2O_DMSO	A5	400.18993	C24H24N4O2	MK2	73.9
Pool 1 Crude	0378493_0088_ASMS_2017_013	Xphos	K3PO4	25%H2O_DMSO	B5	372.15863	C22H20N4O2	MK2	59.3
Pool 1 Crude	0378493_0088_ASMS_2017_023	tBu3P	K3PO4	25%H2O_DMSO	C7	323.08254	C18H14ClN3O	MK2	367
Pool 1 Crude	0378493_0088_ASMS_2017_026	Xphos	BTMG	25%H2O_NMP	D2	290.11676	C17H14N4O	MK2	231.5

Pool 1 Crude	0378493_0088_ASMS_2017_038	Xphos	BTMG	25%H2O_DMSO	E6	331.13208	C20H17N3O2	MK2	132
Pool 1 Crude	0378493_0088_ASMS_2017_045	Xphos	K3PO4	25%H2O_DMSO	F5	289.12151	C18H15N3O	MK2	373.5
Pool 1 Crude	0378493_0088_ASMS_2017_053	Xphos	K3PO4	25%H2O_DMSO	G5	295.07793	C16H13N3OS	MK2	399
Pool 1 Crude	0378493_0088_ASMS_2017_061	Xphos	K3PO4	25%H2O_DMSO	H5	317.15281	C20H19N3O	MK2	409.5
Pool 1 Crude	0378493_0088_ASMS_2017_067	tBu3P	K3PO4	25%H2O_NMP	I3	307.11209	C18H14FN3O	MK2	665
Pool 1 Crude	0378493_0088_ASMS_2017_075	tBu3P	K3PO4	25%H2O_NMP	A11	325.10267	C18H13F2N3O	MK2	1029
Pool 1 Crude	0378493_0088_ASMS_2017_083	tBu3P	K3PO4	25%H2O_NMP	B11	334.10659	C18H14N4O3	MK2	421
Pool 1 Crude	0378493_0088_ASMS_2017_093	Xphos	K3PO4	25%H2O_DMSO	C13	395.16338	C25H21N3O2	MK2	1790
Pool 1 Crude	0378493_0088_ASMS_2017_101	Xphos	K3PO4	25%H2O_DMSO	D13	391.16846	C26H21N3O	MK2	4435
Pool 1 Crude	0378493_0088_ASMS_2017_109	Xphos	K3PO4	25%H2O_DMSO	E13	315.13716	C20H17N3O	MK2	172.5
Pool 1 Crude	0378493_0088_ASMS_2017_115	tBu3P	K3PO4	25%H2O_NMP	F11	293.15281	C18H19N3O	MK2	3110
Pool 1 Crude	0378493_0088_ASMS_2017_123	tBu3P	K3PO4	25%H2O_NMP	G11	319.13208	C19H17N3O2	MK2	3405
Pool 1 Crude	0378493_0088_ASMS_2017_129	Xphos	K3PO4	25%H2O_NMP	H9	344.16371	C21H20N4O	MK2	5340
Pool 1 Crude	0378493_0088_ASMS_2017_141	Xphos	K3PO4	25%H2O_DMSO	I13	339.13716	C22H17N3O	MK2	2070
Pool ID	**Sample Name**	**Catalyst**	**Base**	**Solvent**	**Source Wells**	**Mass**	**Formula**	**Target**	**Invitrogen IC50 (nM)**
Pool 2 Purified	0378493_0088_std1-mk2_pdt_01	**N/A**	**N/A**	**N/A**	Std Plate	400.18993	C24H24N4O2	MK2	73.9
Pool 2 Purified	0378493_0088_std2-mk2_pdt_02	**N/A**	**N/A**	**N/A**	Std Plate	372.15863	C22H20N4O2	MK2	59.3
Pool 2 Purified	0378493_0088_std3-mk2_pdt_03	**N/A**	**N/A**	**N/A**	Std Plate	323.08254	C18H14ClN3O	MK2	367
Pool 2 Purified	0378493_0088_std4-mk2_pdt_04	**N/A**	**N/A**	**N/A**	Std Plate	290.11676	C17H14N4O	MK2	231.5
Pool 2 Purified	0378493_0088_std5-mk2_pdt_05	**N/A**	**N/A**	**N/A**	Std Plate	331.13208	C20H17N3O2	MK2	132
Pool 2 Purified	0378493_0088_std6-mk2_pdt_06	**N/A**	**N/A**	**N/A**	Std Plate	289.12151	C18H15N3O	MK2	373.5
Pool 2 Purified	0378493_0088_std7-mk2_pdt_07	**N/A**	**N/A**	**N/A**	Std Plate	295.07793	C16H13N3OS	MK2	399
Pool 2 Purified	0378493_0088_std8-mk2_pdt_08	**N/A**	**N/A**	**N/A**	Std Plate	317.15281	C20H19N3O	MK2	409.5
Pool 2 Purified	0378493_0088_std9-mk2_pdt_09	**N/A**	**N/A**	**N/A**	Std Plate	307.11209	C18H14FN3O	MK2	665
Pool 2 Purified	0378493_0088_std10-mk2_pdt_10	**N/A**	**N/A**	**N/A**	Std Plate	325.10267	C18H13F2N3O	MK2	1029
Pool 2 Purified	0378493_0088_std11-mk2_pdt_11	**N/A**	**N/A**	**N/A**	Std Plate	334.10659	C18H14N4O3	MK2	421
Pool 2 Purified	0378493_0088_std12-mk2_pdt_12	**N/A**	**N/A**	**N/A**	Std Plate	395.16338	C25H21N3O2	MK2	1790
Pool 2	0378493_0088_std13-	**N/A**	**N/A**	**N/A**	Std	391.168	C26H21N3	MK2	4435

Purified	mk2_pdt_13				Plate	46	O		
Pool 2 Purified	0378493_0088_std14-mk2_pdt_14	**N/A**	**N/A**	**N/A**	Std Plate	315.13716	C20H17N3O	MK2	172.5
Pool 2 Purified	0378493_0088_std15-mk2_pdt_15	**N/A**	**N/A**	**N/A**	Std Plate	293.15281	C18H19N3O	MK2	3110
Pool 2 Purified	0378493_0088_std16-mk2_pdt_16	**N/A**	**N/A**	**N/A**	Std Plate	319.13208	C19H17N3O2	MK2	3405
Pool 2 Purified	0378493_0088_std17-mk2_pdt_17	**N/A**	**N/A**	**N/A**	Std Plate	344.16371	C21H20N4O	MK2	5340
Pool 2 Purified	0378493_0088_std18-mk2_pdt_18	**N/A**	**N/A**	**N/A**	Std Plate	339.13716	C22H17N3O	MK2	2070

Competition Experiment Prep. All work was done at 0 ˚C unless otherwise noted. MK2 (purchased from Carna Biosciences, Inc., #02-142, lot 10CBS0101F: 9.5 µM stock solution in 50 mM HEPES, pH 7.5, 200 mM NaCl, 5 mM $MgCl_2$, 10 mM DTT, 5% glycerol) was removed from a -78 ˚C freezer and warmed to approximately 0 ˚C on ice. Protein dilution buffer was prepared (54 mM Hepes pH 7.5, 150 mM NaCl, 6.2 mM $MgCl_2$, 1mM dithiothreitol) along with library dilution buffer (54 mM Hepes pH 7.5, 150 mM NaCl, 6.2 mM $MgCl_2$, 1mM dithiothreitol). Invertase (negative control, Sigma Aldrich cat. no. I4504) was weighed into a centrifuge tube and diluted to 10 µM with protein dilution buffer. The two pools were thawed and aliquots were removed. The pool aliquots were then separately diluted 1:20 with 10 µM invertase stock and stored at ambient temperature until use (2 µL of a DMSO pool into 38 µL 10 µM invertase stock, to yield a final concentration of 1 µM/compound and 9.5 µM invertase). Next, a serial dilution was performed to from the 9.5 µM MK2 stock to generate the MK2 protein levels for the competition experiment. Serial dilution was performed in a 96-well plate using protein dilution buffer to arrive at the following MK2 protein levels.

MK2 Conc.	9.5 µM	4.75 µM	2.38 µM	1.19 µM	0.60 µM	0.30 µM	0.15 µM	0 µM
Final Vol. (µL)	20	20	20	20	20	20	40	20

Finally, a 1:1 dilution of the appropriate MK2 protein stock (3 µL) with the buffered library/invertase solution prepared above (3 µL) in a new 96-well plate provided an affinity-based ranking experiment with the desired protein and compound concentrations (0.5 µM/compound, 4.8 µM invertase, variable MK2 concentration). Two pools were tested (see Table 3): one pool derived from crude reactions and one derived from purified compounds for direct comparison. This resulted in two unique affinity ranking sequences where the final 1:1 protein/library dilution was performed separately with each pool. The serial dilution performed above was used to prepare all affinity ranking experiment sequences. The protein/compound mixtures were then warmed to room temperature then allowed to incubate for 30 minutes. After 30 minutes, the 96-well plate was moved to an LC-MS autosampler (cooled to 4 ˚C) for analysis. Final component concentrations are shown below.

Lib. Size	18	18	18	18	18	18	18	18
Per Cmpd.	0.5 µM	0.5 µM	0.5 µM	0.5 µM	0.5 µM	0.5 µM	0.5 µM	0.5 µM
Invertase	4.8 µM	4.8 µM	4.8 µM	4.8 µM	4.8 µM	4.8 µM	4.8 µM	4.8 µM
MK2	4.75 µM	2.38 µM	1.19 µM	0.60 µM	0.30 µM	0.15 µM	0.08 µM	0 µM

Chromatography conditions

SEC Running Buffer: 1 M NH_4OAc, pH 8.0

Flow Rate: 0.3 mL / min

Negative Control: 5 µM Invertase

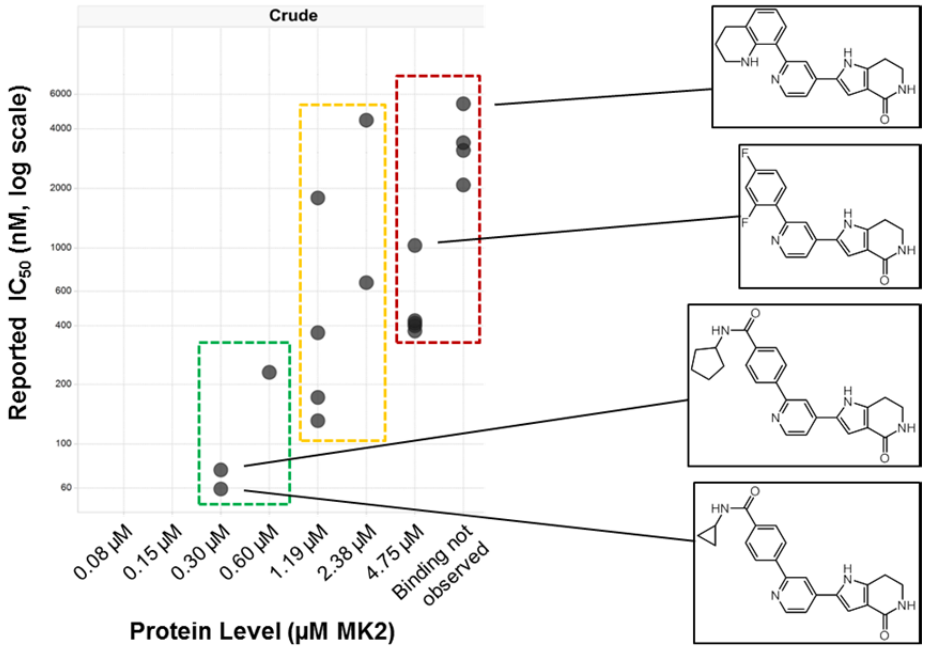
See attached Excel for raw affinity-based rank ordering data

Table 4. MK2 Suzuki Coupling Library – Affinity Ranking Results

Pool	Prep	Per Cmpd. Conc.	Exact Mass	Formula	Sample Ref	Invitrogen Avg. IC50 (nM)	Protein Conc. Where Binding First Observed
Pool 1 Crude	Crude	0.5 uM	400.18993	C24H24N4O2	0378493_0088_ASMS_2017_005	73.9	0.3µM MK2
Pool 1 Crude	Crude	0.5 uM	372.15863	C22H20N4O2	0378493_0088_ASMS_2017_013	59.3	0.3µM MK2
Pool 1 Crude	Crude	0.5 uM	323.08254	C18H14ClN3O	0378493_0088_ASMS_2017_023	367	1.19µM MK2
Pool 1 Crude	Crude	0.5 uM	290.11676	C17H14N4O	0378493_0088_ASMS_2017_026	231.5	0.6µM MK2
Pool 1 Crude	Crude	0.5 uM	331.13208	C20H17N3O2	0378493_0088_ASMS_2017_038	132	1.19µM MK2
Pool 1 Crude	Crude	0.5 uM	289.12151	C18H15N3O	0378493_0088_ASMS_2017_045	373.5	4.75µM MK2
Pool 1 Crude	Crude	0.5 uM	295.07793	C16H13N3OS	0378493_0088_ASMS_2017_053	399	4.75µM MK2
Pool 1 Crude	Crude	0.5 uM	317.15281	C20H19N3O	0378493_0088_ASMS_2017_061	409.5	4.75µM MK2
Pool 1 Crude	Crude	0.5 uM	307.11209	C18H14FN3O	0378493_0088_ASMS_2017_067	665	2.38µM MK2
Pool 1 Crude	Crude	0.5 uM	325.10267	C18H13F2N3O	0378493_0088_ASMS_2017_075	1029	4.75µM MK2
Pool 1 Crude	Crude	0.5 uM	334.10659	C18H14N4O3	0378493_0088_ASMS_2017_083	421	4.75µM MK2
Pool 1 Crude	Crude	0.5 uM	395.16338	C25H21N3O2	0378493_0088_ASMS_2017_093	1790	1.19µM MK2
Pool 1 Crude	Crude	0.5 uM	391.16846	C26H21N3O	0378493_0088_ASMS_2017_101	4435	2.38µM MK2
Pool 1 Crude	Crude	0.5 uM	315.13716	C20H17N3O	0378493_0088_ASMS_2017_109	172.5	1.19µM MK2
Pool 1 Crude	Crude	0.5 uM	293.15281	C18H19N3O	0378493_0088_ASMS_2017_115	3110	Binding Not Observed
Pool 1 Crude	Crude	0.5 uM	319.13208	C19H17N3O2	0378493_0088_ASMS_2017_123	3405	Binding Not Observed
Pool 1 Crude	Crude	0.5 uM	344.16371	C21H20N4O	0378493_0088_ASMS_2017_129	5340	Binding Not Observed
Pool 1 Crude	Crude	0.5 uM	339.13716	C22H17N3O	0378493_0088_ASMS_2017_141	2070	Binding Not Observed
Pool	**Prep**	**Per Cmpd. Conc.**	**Exact Mass**	**Formula**	**Sample Ref**	**Invitrogen Avg. IC50 (nM)**	**Protein Conc. Where Binding First Observed**
Pool 2 Purified	Purified	0.5 uM	400.18993	C24H24N4O2	0378493_0088_std1-mk2_pdt_01	73.9	0.3µM MK2
Pool 2 Purified	Purified	0.5 uM	372.15863	C22H20N4O2	0378493_0088_std2-mk2_pdt_02	59.3	0.3µM MK2
Pool 2 Purified	Purified	0.5 uM	323.08254	C18H14ClN3O	0378493_0088_std3-mk2_pdt_03	367	2.38µM MK2
Pool 2 Purified	Purified	0.5 uM	290.11676	C17H14N4O	0378493_0088_std4-mk2_pdt_04	231.5	1.19µM MK2
Pool 2 Purified	Purified	0.5 uM	331.13208	C20H17N3O2	0378493_0088_std5-mk2_pdt_05	132	1.19µM MK2

Pool 2 Purified	Purified	0.5 uM	289.12151	C18H15N3O	0378493_0088_std6-mk2_pdt_06	373.5	4.75µM MK2
Pool 2 Purified	Purified	0.5 uM	295.07793	C16H13N3OS	0378493_0088_std7-mk2_pdt_07	399	4.75µM MK2
Pool 2 Purified	Purified	0.5 uM	317.15281	C20H19N3O	0378493_0088_std8-mk2_pdt_08	409.5	4.75µM MK2
Pool 2 Purified	Purified	0.5 uM	307.11209	C18H14FN3O	0378493_0088_std9-mk2_pdt_09	665	Binding Not Observed
Pool 2 Purified	Purified	0.5 uM	325.10267	C18H13F2N3O	0378493_0088_std10-mk2_pdt_10	1029	4.75µM MK2
Pool 2 Purified	Purified	0.5 uM	334.10659	C18H14N4O3	0378493_0088_std11-mk2_pdt_11	421	4.75µM MK2
Pool 2 Purified	Purified	0.5 uM	395.16338	C25H21N3O2	0378493_0088_std12-mk2_pdt_12	1790	1.19µM MK2
Pool 2 Purified	Purified	0.5 uM	391.16846	C26H21N3O	0378493_0088_std13-mk2_pdt_13	4435	4.75µM MK2
Pool 2 Purified	Purified	0.5 uM	315.13716	C20H17N3O	0378493_0088_std14-mk2_pdt_14	172.5	0.6µM MK2
Pool 2 Purified	Purified	0.5 uM	293.15281	C18H19N3O	0378493_0088_std15-mk2_pdt_15	3110	Binding Not Observed
Pool 2 Purified	Purified	0.5 uM	319.13208	C19H17N3O2	0378493_0088_std16-mk2_pdt_16	3405	Binding Not Observed
Pool 2 Purified	Purified	0.5 uM	344.16371	C21H20N4O	0378493_0088_std17-mk2_pdt_17	5340	Binding Not Observed
Pool 2 Purified	Purified	0.5 uM	339.13716	C22H17N3O	0378493_0088_std18-mk2_pdt_18	2070	Binding Not Observed

Plots displaying the general correlation between activity assay IC_{50} (plotted on a log scale) and the lowest MK2 concentration at which ASMS binding was observed (protein level, all 18 library members plotted together) are shown below:



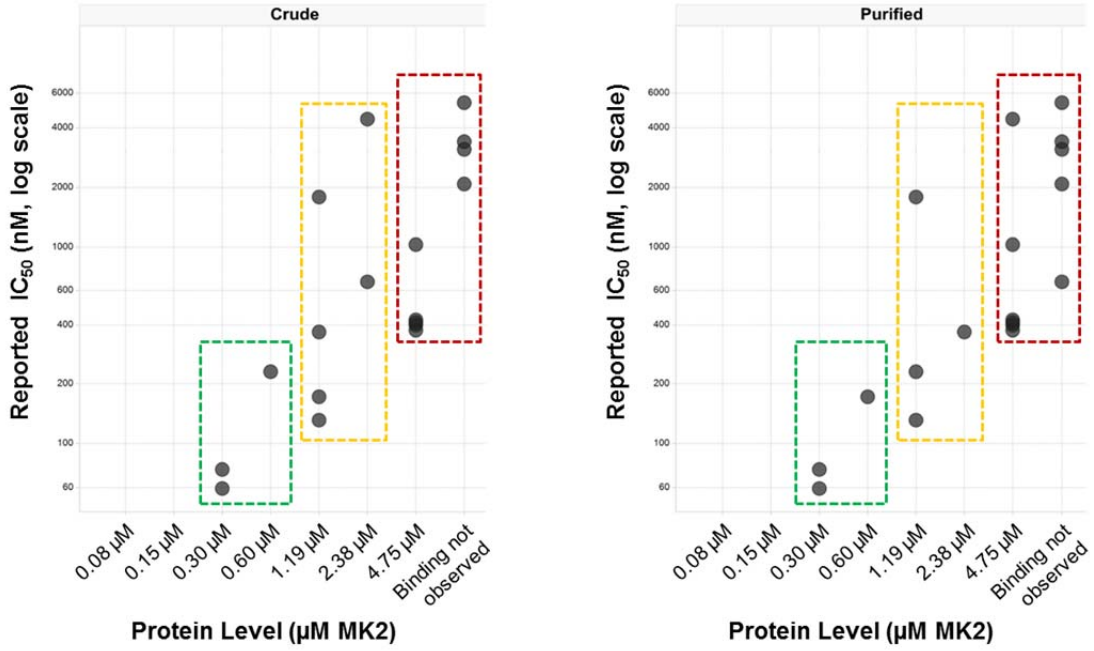


Figure 21. MK2 Suzuki Library Affinity-Based Ranking Results: Crude Nano-Scale Versus Purified

6.4. ASMS Quality Control (QC)

Prior to the affinity-based rank ordering experiment, ASMS QC (LC-HRMS) was performed to confirm that all 18 library members were present and could be detected in the crude pool. When compounds detected in the QC experiment are not observed to bind in the subsequent affinity-based ranking assay, we concluded that those compounds were successfully synthesized and tested, but do not bind to the protein with sufficient affinity for detection in the ASMS system. ASMS QC detected 17 of 18 crude library members, the final library member was confirmed separately.

Table 5. MK2 Biaryl ASMS QC Data

Condition	Product ID	Mass	QC data (MS Response)
Crude reaction	**B1**	400.18993	116541235.9
Crude reaction	**5**	372.15863	266432612
Crude reaction	**B2**	323.08254	164800932.4
Crude reaction	**B3**	290.11676	111142394
Crude reaction	**B4**	331.13208	14733961.07
Crude reaction	**B5**	289.12151	252230205
Crude reaction	**B6**	295.07793	327886882
Crude reaction	**B7**	317.15281	332203329
Crude reaction	**B8**	307.11209	330486720
Crude reaction	**B9**	325.10267	378817253
Crude reaction	**B10**	334.10659	3842642
Crude reaction	**B11**	395.16338	71311514
Crude reaction	**B12**	391.16846	2964132.2
Crude reaction	**B13**	315.13716	182221253
Crude reaction	**B14**	293.15281	N/A*
Crude reaction	**6**	319.13208	323633818
Crude reaction	**B15**	344.16371	83610873.65
Crude reaction	**B16**	339.13716	244071930

*Was detected in earlier binding experiment and synthesis of desired product was confirmed by reaction QC LC-MS

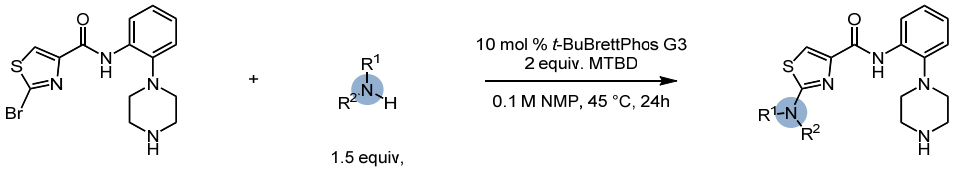
7. Synthesis and Rank Ordering of a Mixed Coupling Library Targeting Checkpoint Kinase 1 (CHK1)

The library described below was initially described in two publications reporting a Suzuki cross-coupling library and Buchwald-Hartwig aryl amination library.[5,13] Reproducing a selection of compounds from library, at a miniaturized scale, was attractive to us again from the perspective of workflow and result validation. The library contains species ranging from highly potent (<10 nM) to weak/inactive (>10,000 nM) and serves as a good test of our ability to differentiate high affinity, moderate, and weak compounds from each other in crude mixtures. Furthermore, this library showcases two different catalytic transformations side-by-side in nanomole-scale library synthesis: Suzuki coupling and Buchwald-Hartwig Amination. This library provided an opportunity to showcase the screening capabilities of the nano-scale synthesis platform and to highlight the value of utilizing multiple conditions in library synthesis to achieve high yields.

Suzuki coupling and aryl amination products were prepared and purified at the 0.05 mmol bench-scale to for direct comparison for the crude nano-scale library. Additionally, the crude nano-scale library was compared side-by-side to a crude library treated with SiliCycle Inc. SiliaMetS® Dimercaptotriazine (DMT) silica-bound metal scavenger to exclude interference in the affinity ranking assay by residual palladium.

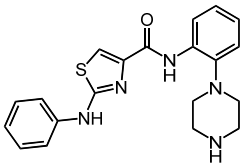
7.1. Bench-Scale Synthesis of CHK1 Inhibitor Validation Library

General procedure for C-N coupling to 2-bromo-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide:



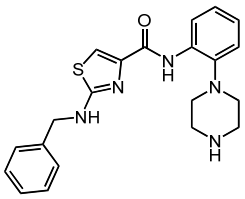
The aryl bromide above core was weighed into a 1-dram vial (1 equiv., 0.05 mmol scale) equipped with a magnetic stir bar. The vial was moved to a glove box where NMP was added and the core dissolved. The desired amine building block (1.5 equiv., 0.075 mmol) was next added the vial, followed by *t*-BuBrettPhos G3 precatalyst (10 mol %, 0.005 mmol, added as a stock solution in NMP). Finally, 7-Methyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene (MTBD, added as a solution in NMP, 0.1 mmol, 2 equiv.) was added and the vial was sealed. The vial was removed from the glove box and stirred at 35-45 ˚C for 24 hours. The next morning, aliquots were taken of all reactions and progress was determined by LC-MS. Upon completion, reactions were diluted with DMSO (1.5 mL), filtered, and submitted for purification by RP-HPLC. Products were returned as TFA salts unless otherwise noted. After purification and characterization the coupling products were dissolved in DMSO to a concentration of 10 mM. All members of this validation library were previously reported.[13]

2-(phenylamino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C1)



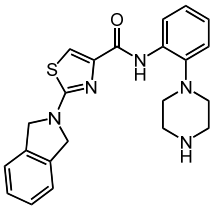
The title compound was prepared using the standard conditions described above and aniline (MFCD00007629) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 10 mg (41% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C1**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.44 (s, 1H), 9.74 (s, 1H), 8.86 (br s, 2H), 8.29 (d, *J* = 7.9 Hz, 1H), 7.73 (s, 1H), 7.67 (d, *J* = 8.0 Hz, 2H), 7.40 (t, *J* = 7.8 Hz, 3H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 1H), 7.05 (t, *J* = 7.3 Hz, 1H), 3.21 (br s, 4H), 3.07 (s, 4H); **HRMS** (ESI): *m/z* calculated for $C_{20}H_{22}N_5OS$ [M+H]+ 380.15398, found 380.15359. Measured IC_{50} (CHK1, Invitrogen) 193 nM.

2-(benzylamino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C2, D1)



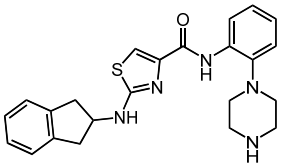
The title compound was prepared using the standard conditions described above and benzylamine (MFCD00008106) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 23.1 mg (91% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C2**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.96 (s, 1H), 9.03 (br s, 2H), 8.43 (s, 1H), 8.38 (d, *J* = 8.0 Hz, 1H), 7.46 (s, 1H), 7.42 (d, *J* = 7.5 Hz, 2H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.27 (m, 2H), 7.19 (t, *J* = 7.7 Hz, 1H), 7.11 (t, *J* = 7.6 Hz, 1H), 4.54 (d, *J* = 4.5 Hz, 2H), 3.30 (br s, 4H), 3.05 (m, 4H); **HRMS** (ESI): *m/z* calculated for $C_{21}H_{24}N_5OS$ [M+H]+ 394.16963, found 394.16974. Measured IC_{5o} (CHK1, Invitrogen) >10000 nM.

2-(isoindolin-2-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (43 / C3 / D2)



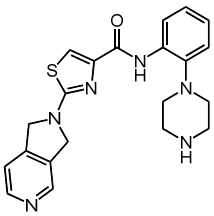
The title compound was prepared using the standard conditions described above and isoindoline (MFCD00605324) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 9.4 mg (36% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **43**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.05 (s, 1H), 9.09 (br s, 2H), 8.41 (d, *J* = 8.0 Hz, 1H), 7.63 (s, 1H), 7.47 (m, 2H), 7.34 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.28 (d, *J* = 7.8 Hz, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.11 (t, *J* = 7.5 Hz, 1H), 4.83 (s, 4H), 3.39 (br s, 4H), 3.08 (t, *J* = 4.4 Hz, 4H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 166.5, 158.5, 146.5, 140.4, 136.3, 132.8, 127.5, 125.6, 123.9, 123.2, 120.7, 118.7, 113.5, 55.2, 48.7, 44.2, 40.0, 39.8, 39.7, 39.5, 39.3, 39.2, 39.0; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{24}N_5OS$ [M+H]+ 406.16963, found 406.16968. Measured IC_{5o} (CHK1, Invitrogen) 17.2 nM.

2-((2,3-dihydro-1H-inden-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C4)



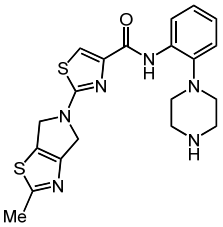
The title compound was prepared using the standard conditions described above and indan-2-amine (MFCD00082597) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 9.8 mg (37% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C4**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.89 (s, 1H), 8.99 (br s, 2H), 8.40 (d, *J* = 8.0 Hz, 1H), 8.23 (d, *J* = 6.1 Hz, 1H), 7.47 (s, 1H), 7.29 (t, *J* = 7.6 Hz, 3H), 7.19 (m, 3H), 7.13 (t, *J* = 7.5 Hz, 1H), 4.55 (m, 1H), 3.38 (dd, *J* = 16.2, *J* = 6.7 Hz, 2H), 3.31 (br s, 4H), 3.08 (s, 4H), 2.97 (dd, *J* = 16.2, *J* = 2.4 Hz, 2H); **HRMS** (ESI): *m/z* calculated for $C_{23}H_{26}N_5OS$ [M+H]+ 420.18528, found 420.18463. Measured IC_{5o} (CHK1, Invitrogen) 7170 nM.

2-(1,3-dihydro-2H-pyrrolo[3,4-c]pyridin-2-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C5, D3)



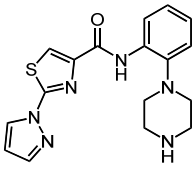
The title compound was prepared using the standard conditions described above and 2,3-dihydro-1H-pyrrolo[3,4-c]pyridine (MFCD06858479) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 6.4 mg (25% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C5**: **^{1}H NMR** (600 MHz, DMSO-d6) δ 10.07 (s, 1H), 9.08 (br s, 2H), 8.79 (s, 1H), 8.66 (d, *J* = 5.1 Hz, 1H), 8.43 (d, *J* = 8.0 Hz, 1H), 7.69 (m, *J* = 8.8 Hz, 2H), 7.32 (d, *J* = 7.8 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 4.950 (s, 2H), 4.947 (s, 2H), 3.42 (br s, 4H), 3.11 (s, 4H); **HRMS** (ESI): *m/z* calculated for $C_{21}H_{23}N_6OS$ [M+H]+ 407.16488, found 407.16452. Measured IC_{50} (CHK1, Invitrogen) 209 nM.

2-(2-methyl-4,6-dihydro-5H-pyrrolo[3,4-d]thiazol-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C6, D4)



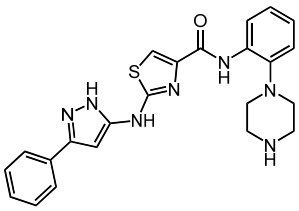
The title compound was prepared using the standard conditions described above and 2-methyl-5,6-dihydro-4H-pyrrolo[3,4-d]thiazole (MFCD06738528) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 4.7 mg (17% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C6**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.97 (s, 1H), 8.95 (br s, 2H), 8.41 (d, *J* = 8.0 Hz, 1H), 7.67 (s, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.21 (t, *J* = 7.7 Hz, 1H), 7.13 (t, *J* = 7.5 Hz, 1H), 4.83 (s, 2H), 4.70 (s, 2H), 3.37 (br s, 4H), 3.08 (s, 4H), 2.72 (s, 3H); **HRMS** (ESI): *m/z* calculated for $C_{20}H_{23}N_6OS_2$ [M+H]+ 427.13695, found 427.13623. Measured IC_{50} (CHK1, Invitrogen) 361 nM.

N-(2-(piperazin-1-yl)phenyl)-2-(1H-pyrazol-1-yl)thiazole-4-carboxamide (C7)



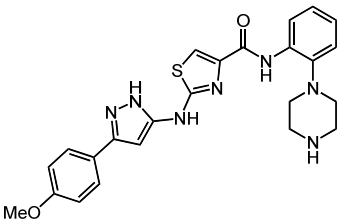
The title compound was prepared using the conditions described above, P_2-Et as the base, and 1H-pyrazole (MFCD00005234) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 9.5 mg (41% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C7**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.90 (s, 1H), 9.01 (br s, 2H), 8.57 (d, *J* = 2.3 Hz, 1H), 8.37 (d, *J* = 7.9 Hz, 1H), 8.29 (s, 1H), 7.97 (s, 1H), 7.31 (d, *J* = 7.7 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.4 Hz, 1H), 6.71 (s, 1H), 3.36 (br s, 4H), 3.09 (m, 4H); **HRMS** (ESI): *m/z* calculated for $C_{17}H_{19}N_6OS$ [M+H]+ 355.13358, found 355.13354. Measured IC_{50} (CHK1, Invitrogen) 233 nM.

2-((3-phenyl-1H-pyrazol-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C8)



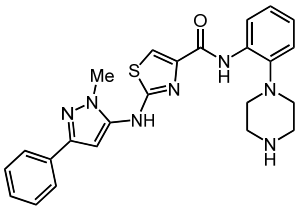
The title compound was prepared using the standard conditions described above and 3-phenyl-1H-pyrazol-5-amine as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 22.4 mg (80% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C8**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.99 (br s, 1H), 10.76 (s, 1H), 10.00 (s, 1H), 8.83 (br s, 2H), 8.32 (d, *J* = 7.9 Hz, 1H), 7.73 (m, 3H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.3 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 6.41 (s, 1H), 3.38 (s, 4H), 3.07 (s, 4H); **HRMS** (ESI): *m/z* calculated for $C_{23}H_{24}N_7OS$ [M+H]+ 446.17578, found 446.17621. Measured IC_{50} (CHK1, Invitrogen) 18.8 nM.

2-((3-(4-methoxyphenyl)-1H-pyrazol-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (8, D5)



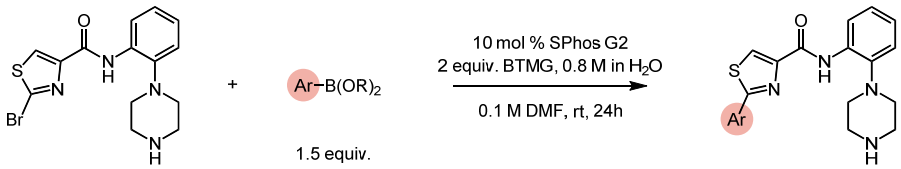
The title compound was prepared using the standard conditions described above and 3-(4-methoxyphenyl)-1H-pyrazol-5-amine (MFCD00462192) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 25.2 mg (85% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **8**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.80 (br s, 1H), 10.66 (s, 1H), 9.98 (s, 1H), 8.88 (br s, 2H), 8.30 (d, *J* = 7.9 Hz, 1H), 7.68 (s, 1H), 7.63 (d, *J* = 8.6 Hz, 2H), 7.24 (d, *J* = 7.8 Hz, 1H), 7.18 (t, *J* = 7.6 Hz, 1H), 7.11 (t, *J* = 7.5 Hz, 1H), 7.01 (d, *J* = 8.6 Hz, 2H), 6.28 (s, 1H), 3.77 (s, 3H), 3.36 (s, 4H), 3.05 (s, 4H); **HRMS** (ESI): *m/z* calculated for $C_{24}H_{26}N_7O_2S$ [M+H]+ 476.18634, found 476.18616. Measured IC_{50} (CHK1, Invitrogen) 23.2 nM.

2-((1-methyl-3-phenyl-1H-pyrazol-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C9)



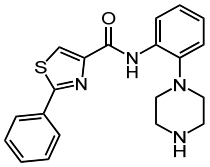
The title compound was prepared using the standard conditions described above (with heating to 50 ˚C) and 2-methyl-5-phenyl-pyrazol-3-amine (MFCD00067874) as the building block. The desired product was prepared at the 0.06 mmol scale and purified by RP-HPLC to yield 32.7 mg (95% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C9**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.40 (br s, 1H), 9.93 (s, 1H), 8.81 (br s, 2H), 8.28 (d, *J* = 7.9 Hz, 1H), 7.80 (d, *J* = 7.6 Hz, 2H), 7.75 (s, 1H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.25 (m, 3H), 7.15 (d, *J* = 7.6 Hz, 1H), 6.98 (s, 1H), 3.82 (s, 3H), 3.12 (s, 4H), 3.01 (s, 4H); **HRMS** (ESI): *m/z* calculated for $C_{24}H_{26}N_7OS$ [M+H]+ 460.19143, found 460.19168. Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

General procedure for Suzuki coupling to 2-bromo-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide:



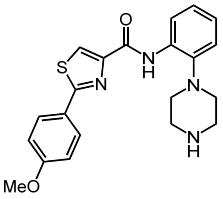
The aryl bromide core above was weighed into a 1-dram vial (1 equiv., 0.05 mmol scale) equipped with a magnetic stir bar. The desired boronic acid or pinacol boronic ester building block (1.5 equiv., 0.075 mmol) was next weighed and dispensed into the same 1-dram vial. The vial was moved to a glove box where DMF was added and the reagents dissolved. Next, SPhos G2 precatalyst (10 mol %, 0.005 mmol) was added as a stock solution in DMF, followed by aqueous 0.8 M 2-tert-Butyl-1,1,3,3-tetramethylguanidine (BTMG, 2 equiv.). The vial was sealed, removed from the glove box, and stirred at room temperature for 24 hours. The next morning, aliquots were taken of all reactions and progress was determined by LC-MS. Upon completion, reactions were diluted with DMSO (1.5 mL), filtered, and submitted for purification by RP-HPLC. Products were returned as TFA salts unless otherwise noted. After purification and characterization the coupling products were dissolved in DMSO to a concentration of 10 mM. All members of this validation library were previously reported.[5]

2-phenyl-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C10)



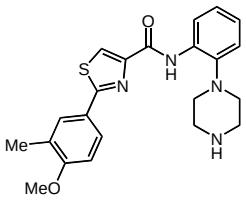
The title compound was prepared using the standard conditions described above and phenylboronic acid (MFCD00002103) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 14.4 mg (60% yield) of the title compound as an off-white solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C10**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.26 (s, 1H), 9.05 (br s, 2H), 8.55 (s, 1H), 8.43 (d, *J* = 7.9 Hz, 1H), 8.05 (d, *J* = 7.0 Hz, 2H), 7.62 (m, 3H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.4 Hz, 1H), 3.33 (m, obscured, 4H), 3.11 (br m, 4H); **HRMS** (ESI): *m/z* calculated for $C_{20}H_{21}N_4OS$ [M+H]+ 365.14308, found 365.14316. Measured IC_{50} (CHK1, Invitrogen) 197 nM.

2-(4-methoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C11)



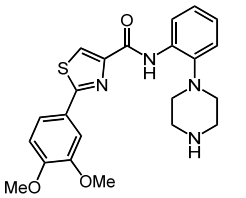
The title compound was prepared using the standard conditions described above and (4-methoxyphenyl)boronic acid (MFCD00039139) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 15.3 mg (60% yield) of the title compound as an off-white solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C11**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.26 (s, 1H), 9.05 (br s, 2H), 8.45 (s, 1H), 8.43 (d, *J* = 8.0 Hz, 1H), 7.99 (d, *J* = 8.6 Hz, 2H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.16 (m, 3H), 3.86 (s, 3H), 3.33 (br s, obscured, 4H), 3.11 (br s, 4H); **HRMS** (ESI): *m/z* calculated for $C_{21}H_{23}N_4O_2S$ [M+H]+ 395.15365, found 395.15323. Measured IC_{50} (CHK1, Invitrogen) 114 nM.

2-(4-methoxy-3-methylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C12, E38)



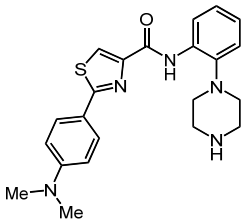
The title compound was prepared using the standard conditions described above and (4-methoxy-3-methyl-phenyl)boronic acid (MFCD02179464) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 19.8 mg (76% yield) of the title compound as an off-white solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C12/E38**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.25 (s, 1H), 8.96 (br s, 2H), 8.44 (s, 1H), 8.40 (d, *J* = 7.9 Hz, 1H), 7.88 (d, *J* = 8.3 Hz, 1H), 7.84 (s, 1H), 7.33 (d, *J* = 7.7 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.16 (m, 2H), 3.89 (s, 3H), 3.33 (br s, 4H), 3.11 (br s, 4H), 2.26 (s, 3H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 168.0, 159.6, 158.0, 150.0, 140.7, 132.6, 128.5, 127.1, 125.6, 125.5, 124.5, 124.3, 120.8, 119.2, 111.1, 111.0, 55.6, 48.7, 44.1, 16.1; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{25}N_4O_2S$ [M+H]+ 409.16927, found 409.16953; 384-Member crude library ASMS protein concentration first observed: 2.5 µM CHK1;Measured IC_{50} (CHK1, Invitrogen) 190 nM.

2-(3,4-dimethoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C13)



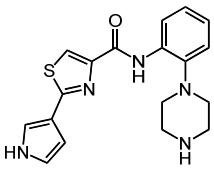
The title compound was prepared using the standard conditions described above and (3,4-dimethoxyphenyl)boronic acid (MFCD01074574) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 19.8 mg (74% yield) of the title compound as an off-white solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C13**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.14 (s, 1H), 8.98 (br s, 2H), 8.47 (s, 1H), 8.37 (d, *J* = 7.9 Hz, 1H), 7.62 (m, 1H), 7.51 (s, 1H), 7.31 (d, *J* = 7.7 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.9 Hz, 2H), 3.89 (s, 3H), 3.86 (s, 3H), 3.29 (s, 4H), 3.10 (s, 4H); **HRMS** (ESI): *m/z* calculated for $C_{22}H_{25}N_4O_3S$ [M+H]+ 425.16421, found 425.16345. Measured IC_{50} (CHK1, Invitrogen) 682 nM.

2-(4-(dimethylamino)phenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C14)



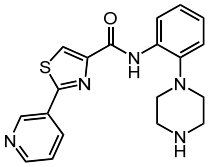
The title compound was prepared using the standard conditions described above and N,N-dimethyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (MFCD05663854) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 19.9 mg (76% yield) of the title compound as an off-white solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C14**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.26 (s, 1H), 9.08 (s, 2H), 8.43 (d, *J* = 7.9 Hz, 1H), 8.32 (s, 1H), 7.84 (d, *J* = 8.7 Hz, 2H), 7.33 (d, *J* = 7.7 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 7.4 Hz, 1H), 6.86 (d, *J* = 8.7 Hz, 2H), 3.36 (s, obscured, 4H), 3.11 (s, 4H), 3.03 (s, 6H); **HRMS** (ESI): *m/z* calculated for $C_{22}H_{26}N_5OS$ [M+H]+ 408.18528, found 408.18442. Measured IC_{50} (CHK1, Invitrogen) 60.1 nM.

N-(2-(piperazin-1-yl)phenyl)-2-(1H-pyrrol-3-yl)thiazole-4-carboxamide (C15)



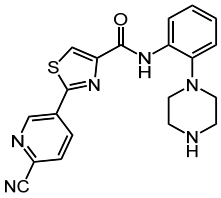
The title compound was prepared using the standard conditions described above and 3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-pyrrole (MFCD11109266) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 11.7 mg (50% yield) of the title compound as an off-white solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C15**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 11.41 (s, 1H), 10.14 (s, 1H), 9.05 (br s, 2H), 8.40 (s, 1H), 8.23 (s, 1H), 7.54 (s, 1H), 7.29 (s, 1H), 7.23 (s, 1H), 7.15 (t, *J* = 7.5 Hz, 1H), 6.91 (m, 1H), 6.59 (s, 1H), 3.35 (br s, 4H), 3.10 (br s, 4H); **HRMS** (ESI): *m/z* calculated for $C_{18}H_{20}N_5OS$ [M+H]+ 354.13833, found 354.13809. Measured IC_{50} (CHK1, Invitrogen) 140 nM.

N-(2-(piperazin-1-yl)phenyl)-2-(pyridin-3-yl)thiazole-4-carboxamide (C16)



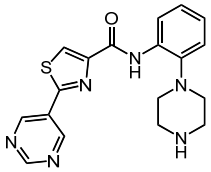
The title compound was prepared using the standard conditions described above and 3-pyridylboronic acid (MFCD00674177) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 15.4 mg (64% yield) of the title compound as an off-white solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C16**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.19 (s, 1H), 9.26 (s, 1H), 8.99 (br s, 2H), 8.78 (d, *J* = 4.1 Hz, 1H), 8.64 (s, 1H), 8.43 (d, *J* = 7.9 Hz, 1H), 8.40 (d, *J* = 7.9 Hz, 1H), 7.65 (dd, *J* = 7.7, *J* = 4.9 Hz, 1H), 7.32 (d, *J* = 7.7 Hz, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 7.4 Hz, 1H), 3.31 (br s, 4H), 3.10 (s, 4H); **HRMS** (ESI): *m/z* calculated for $C_{19}H_{20}N_5OS$ [M+H]+ 366.13833, found 366.13730. Measured IC_{50} (CHK1, Invitrogen) 3350 nM.

2-(6-cyanopyridin-3-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C17)



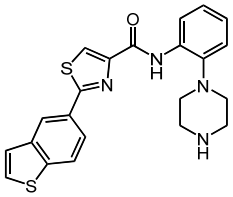
The title compound was prepared using the standard conditions described above and 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine-2-carbonitrile (MFCD06657825) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 5 mg (20% yield) of the title compound as an off-white residue (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C17**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.19 (s, 1H), 9.42 (s, 1H), 8.94 (br s, 2H), 8.75 (s, 1H), 8.68 (d, *J* = 8.0 Hz, 1H), 8.38 (d, *J* = 7.8 Hz, 1H), 8.26 (d, *J* = 7.9 Hz, 1H), 7.32 (d, *J* = 7.7 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 3.30 (br s, obscured, 4H), 3.09 (br s, 4H); **HRMS** (ESI): *m/z* calculated for $C_{20}H_{19}N_6OS$ [M+H]+ 391.13358, found 391.13315. Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

N-(2-(piperazin-1-yl)phenyl)-2-(pyrimidin-5-yl)thiazole-4-carboxamide (9)



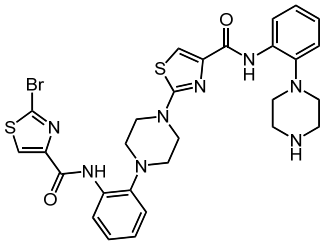
The title compound was prepared using the conditions described below and pyrimidin-5-ylboronic acid (MFCD03002366) as the building block. RuPhos G3 (10 mol %) precatalyst was used with aqueous 0.8 M tribasic potassium phosphate at 35 ˚C. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 18.9 mg (79% yield) of the title compound as an off-white solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **9**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.12 (s, 1H), 9.45 (s, 2H), 9.38 (s, 1H), 9.00 (br s, 2H), 8.71 (s, 1H), 8.37 (d, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 7.7 Hz, 1H), 7.24 (t, *J* = 7.5 Hz, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 3.29 (br s, 4H), 3.10 (br s, 4H); **HRMS** (ESI): *m/z* calculated for $C_{18}H_{19}N_6OS$ [M+H]+ 367.13358, found 367.13381. Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

2-(benzo[b]thiophen-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C18, E51)



The title compound was prepared using RuPhos G3 (10 mol %), aq. 0.8 M K_3PO_4, and NMP and 2-(benzothiophen-5-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (MFCD05664405) as the building block. The desired product was prepared at the 0.05 mmol scale and purified by RP-HPLC to yield 18.3 mg (68% yield) of the title compound as an off-white solid (TFA salt). Spectral data were in agreement with reported literature values. Analytical data for **C18/E51**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.29 (s, 1H), 9.00 (br s, 2H), 8.58 (s, 1H), 8.56 (s, 1H), 8.42 (d, *J* = 7.8 Hz, 1H), 8.24 (d, *J* = 8.3 Hz, 1H), 8.07 (d, *J* = 8.3 Hz, 1H), 7.93 (d, *J* = 4.8 Hz, 1H), 7.65 (d, *J* = 4.8 Hz, 1H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.26 (t, *J* = 7.5 Hz, 1H), 7.18 (t, *J* = 7.3 Hz, 1H), 3.36 (br s, 4H), 3.12 (br s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 168.2, 158.0, 150.2, 141.4, 140.8, 140.1, 132.6, 129.4, 128.7, 125.6, 125.5, 124.7, 124.3, 123.9, 121.9, 121.8, 120.8, 119.2, 48.8, 44.1; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{21}N_4OS_2$ [M+H]+ 421.11515, found 421.11453. Measured IC_{50} (CHK1, Invitrogen) 33.1 nM. ASMS protein concentration first observed in crude 384-member library: 1.25 µM CHK1.

2-bromo-N-(2-(4-(4-((2-(piperazin-1-yl)phenyl)carbamoyl)thiazol-2-yl)piperazin-1-yl)phenyl)thiazole-4-carboxamide (C19)



Dimer impurity formed from the coupling of one equivalent of thiazole bromide core to the free secondary amine of another equivalent of thiazole bromide core. This impurity was occasionally observed, in small quantities, in crude palladium-catalyzed amination reactions where the desired aryl amination process was inefficient. Formation of this impurity is due to the use of the free secondary amine core in nanomole-scale library synthesis rather than a core incorporating a protecting group (and requiring a nanomole-scale deprotection step). Control experiments using P_2-Et, BTMG, or MTBD but excluding the palladium precatalyst showed formation of this dimer suggesting that it may be produced from an S_NAr pathway rather than a metal-mediated process (example chromatograms shown below). The mass balance of these control reactions was unconsumed aryl halide core and addition of exogenous amine nucleophiles (e.g. benzylamine to form **C2**) resulted in trace or no formation of desired coupling product in

contrast to the higher yields observed when using a palladium precatalyst (comparisons shown below). In reaction optimization and library synthesis using **1**, this species is monitored and identified as "Dimer" or "CNDimer." Analytical data for **C19**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.40 (s, 1H), 10.02 (s, 1H), 8.80 (br s, 2H), 8.47 (s, 1H), 8.39 (m, 2H), 7.67 (s, 1H), 7.35 (d, *J* = 7.8 Hz, 1H), 7.23 (m, 3H), 7.12 (m, 2H), 3.77 (br s, 4H), 3.22 (br s, 4H), 3.10 (m, 4H), 3.02 (m, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 170.4, 158.3, 156.7, 149.3, 146.0, 141.0, 140.4, 137.3, 132.9, 132.6, 129.6, 125.8, 125.5, 124.2, 124.0, 121.2, 121.0, 118.75, 118.4, 114.3, 50.8, 48.9, 48.8, 44.1; **HRMS** (ESI): *m/z* calculated for $C_{28}H_{30}BrN_8O_2S_2$ [M+H]+ 653.11110, found 653.11086.

Crude reaction chromatogram legend

Free amine 2-bromothiazole core (**green**, retention time 0.522 min)

Desired aryl amination products (**red** peaks)

Dimer impurity / product (**orange**, retention time 0.856 min)

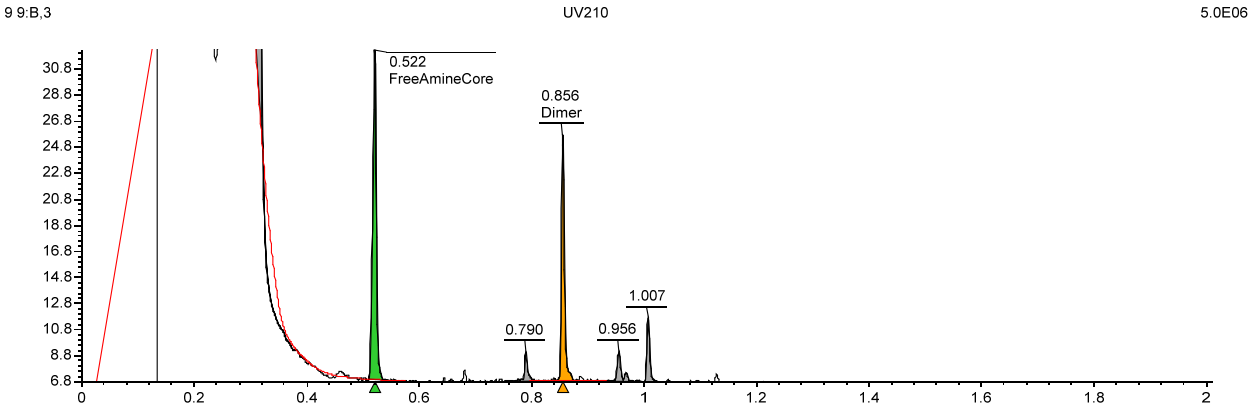


Figure 22. Control reaction crude chromatogram – no catalyst, reaction to form C2 (conditions: 1.5 equiv. benzylamine, 2 equiv. MTBD base, no catalyst)

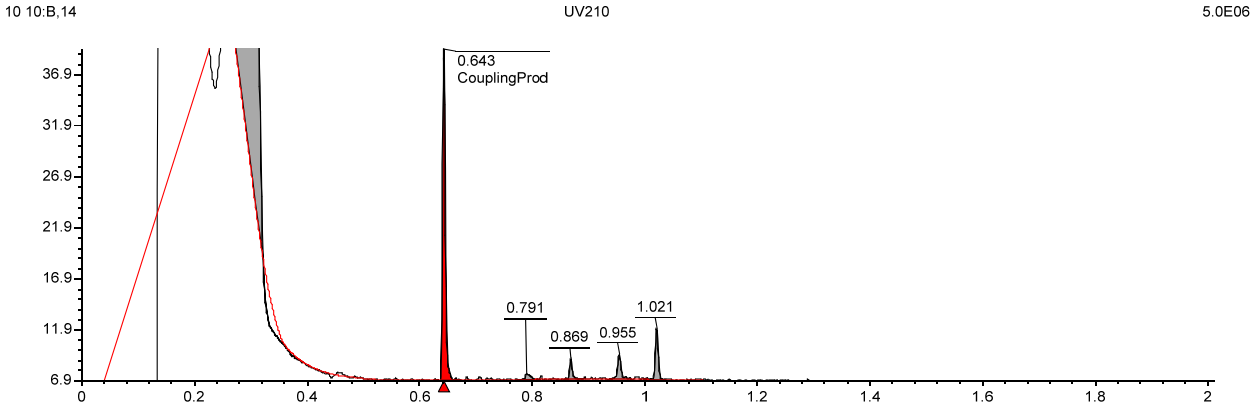


Figure 23. Comparison crude chromatogram, reaction forming C2 (conditions: 1.5 equiv. benzylamine, 2 equiv. MTBD base, 10 mol % *t*-BuBrettPhos G3)

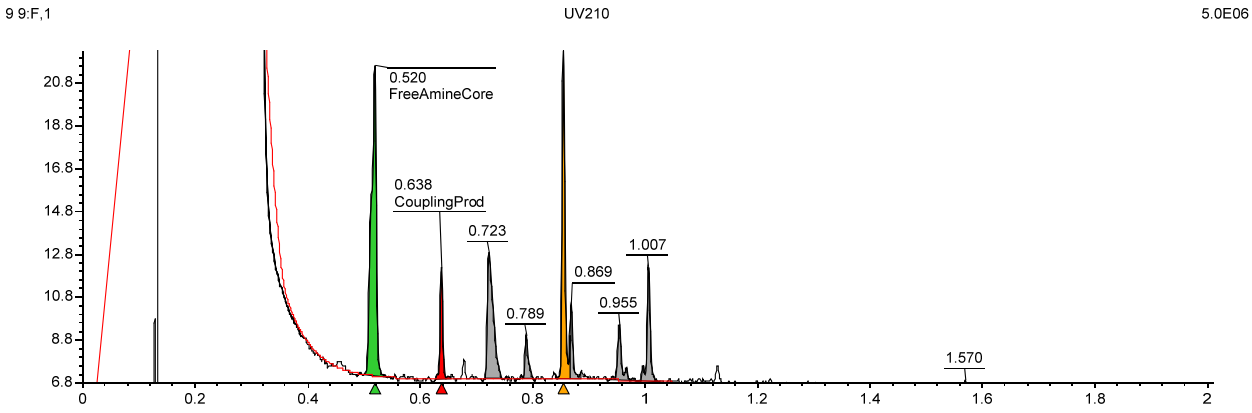


Figure 24. Control reaction crude chromatogram – no catalyst, reaction to form C6 (conditions: 1.5 equiv. 2-methyl-5,6-dihydro-4H-pyrrolo[3,4-d]thiazole, 2 equiv. P_2-Et, no catalyst)

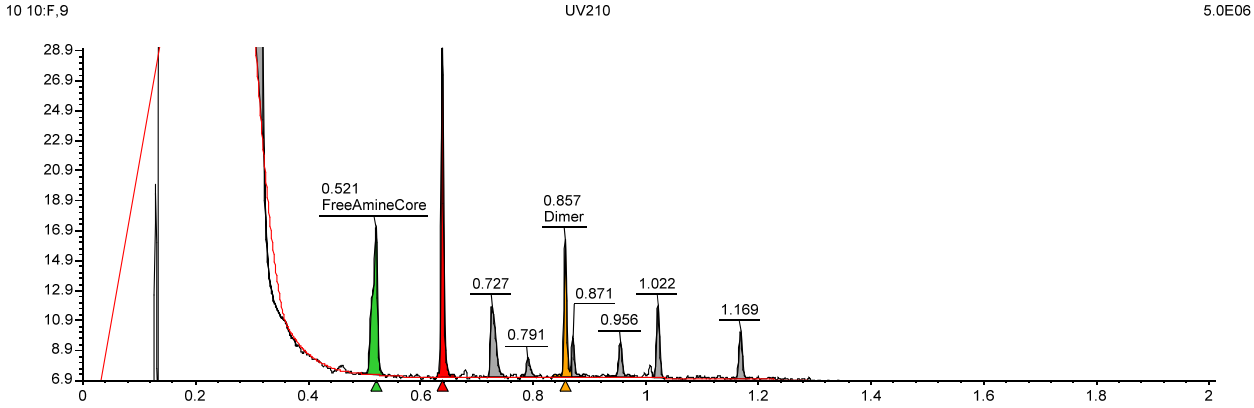
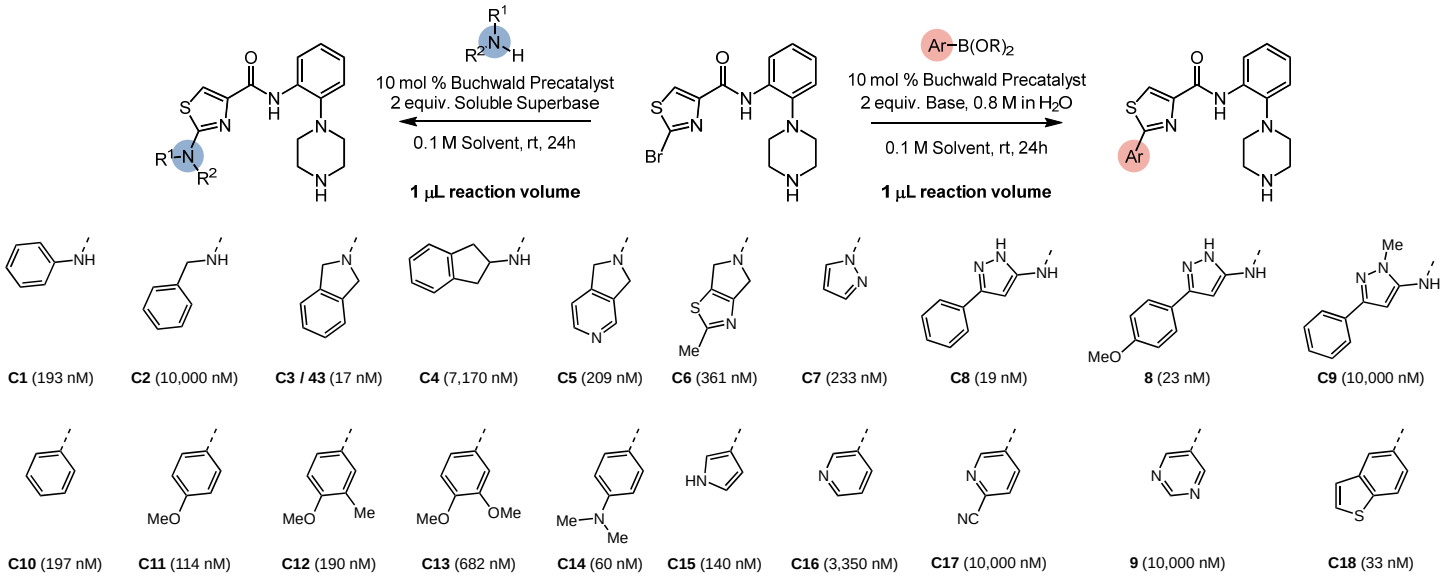


Figure 25. Comparison chromatogram, reaction forming C6 (conditions: 1.5 equiv. 2-methyl-5,6-dihydro-4H-pyrrolo[3,4-d]thiazole, 2 equiv. P_2-Et, 10 mol % *t*-BuXPhos G3)

7.2. Nanomole-Scale Mixed Coupling Library



List of boronic acid and boronic ester building blocks used in this study for the Suzuki cross coupling library (MDL numbers): MFCD00002103, MFCD00039139, MFCD02179464, MFCD01074574, MFCD05663854, MFCD11109266, MFCD00674177, MFCD06657825, MFCD03002366, MFCD05664405

List of amine building blocks used in this study for the Buchwald-Hartwig amination library (MDL numbers): MFCD00007629, MFCD00008106, MFCD00605324, MFCD00082597, MFCD06858479, MFCD06738528, MFCD00005234, MFCD00191749, MFCD00462192, MFCD00067874

8 unique reaction conditions were screened in the synthesis of the above-depicted 10-member Suzuki cross-coupling library (2 solvents, 2 aqueous bases, 2 Buchwald precatalysts). Solvents used: DMF and NMP. Bases used: aqueous 0.8 M K_3PO_4 and aqueous 0.8 M 2-*tert*-butyl-1,1,3,3-tetramethylguanidine (BTMG, Aldrich #20615-5ML). Catalysts used: (2-Dicyclohexylphosphino-2',6'-diisopropoxy-1,1'-biphenyl)[2-(2'-amino-1,1'-biphenyl)]palladium(II) methanesulfonate (RuPhos G3 precatalyst, Aldrich # 763403) and Chloro(2-dicyclohexylphosphino-2',6'-dimethoxy-1,1'-biphenyl)[2-(2'-amino-1,1'-biphenyl)]palladium(II) (Sphos G2 precatalyst, Aldrich # 753009).

12 unique reaction conditions were screened in the synthesis of the above-depicted 10-member Buchwald-Hartwig amination library (1 solvent, 3 organic-soluble bases, 4 Buchwald precatalysts). Solvents used: NMP. Bases used (0.8 M in NMP): 2-*tert*-butyl-1,1,3,3-tetramethylguanidine (BTMG, Aldrich #20615-5ML), 7-Methyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene (MTBD, Aldrich #359505-5ML), and phosphazene base P_2-Et (Aldrich #79417-5ML). Catalysts used: [(2-Di-tert-butylphosphino-2',4',6'-triisopropyl-1,1'-biphenyl)-2-(2'-amino-1,1'-biphenyl)] palladium(II) methanesulfonate (*t*-BuXPhos G3 precatalyst, Aldrich # 762229), [(2-Di-tert-butylphosphino-3,6-dimethoxy-2',4',6'-triisopropyl-1,1'-biphenyl)-2-(2'-amino-1,1'-biphenyl)]palladium(II) methanesulfonate (*t*-BuBrettPhos G3 precatalyst, Aldrich # 745979), [2-(Di-1-adamantylphosphino)-2',4',6'-triisopropyl-3,6-dimethoxybiphenyl][2-(2'-amino-1,1'-biphenyl)]palladium(II) methanesulfonate (AdBrettPhos G3 precatalyst, Aldrich #776106), and [(2-Di-tert-butylphosphino-3-methoxy-6-methyl-2',4',6'-triisopropyl-1,1'-biphenyl)-2-(2-aminobiphenyl)]palladium(II) methanesulfonate (RockPhos G3 precatalyst, Aldrich #773905).

All chemistry and nanoliter pipetting was performed in an N_2 atmosphere glove box.

Suzuki Coupling Prep: Stock solutions of the thiazole bromide core (0.4 M in NMP and DMF), boronic acid/ester building blocks (0.6 M in NMP and DMF), Buchwald palladium precatalysts (0.04 M in NMP and DMF), and bases (K_3PO_4 and BTMG, 0.8 M in H_2O) were prepared in a glove box under an N_2 atmosphere. A source plate was constructed using the reagent stock solutions, according to the diagram below, by pipetting 20-25 µL of the correct component stock solution into the wells indicated below in Figure 26.

384-Well Source Plate Suzuki Coupling Library

	Core 1	Core 2	3	Building block NMP 4	Building block DMF 5	6	NMP Wash 7	DMF Wash 8	Sphos NMP 9	RuPhos NMP 10	Sphos DMF 11	RuPhos DMF 12	NMP Wash 13	DMF Wash 14	15	aq. K3PO4 16	aq. BTMG 17	18	19	20	21	22	23	24
A	Core NMP	Core DMF		MFCD00002103	MFCD00002103		NMP	DMF	Sphos G3	RuPhos G3	Sphos G3	RuPhos G3	NMP	DMF		aq K3PO4	aq BTMG							
B	Core NMP	Core DMF		MFCD00033133	MFCD00033133		NMP	DMF	Sphos G3	RuPhos G3	Sphos G3	RuPhos G3	NMP	DMF		aq K3PO4	aq BTMG							
C	Core NMP	Core DMF		MFCD02173464	MFCD02173464		NMP	DMF	Sphos G3	RuPhos G3	Sphos G3	RuPhos G3	NMP	DMF		aq K3PO4	aq BTMG							
D	Core NMP	Core DMF		MFCD01074574	MFCD01074574		NMP	DMF	Sphos G3	RuPhos G3	Sphos G3	RuPhos G3	NMP	DMF		aq K3PO4	aq BTMG							
E	Core NMP	Core DMF		MFCD05663854	MFCD05663854		NMP	DMF	Sphos G3	RuPhos G3	Sphos G3	RuPhos G3	NMP	DMF		aq K3PO4	aq BTMG							
F	Core NMP	Core DMF		MFCD11103266	MFCD11103266		NMP	DMF	Sphos G3	RuPhos G3	Sphos G3	RuPhos G3	NMP	DMF		aq K3PO4	aq BTMG							
G	Core NMP	Core DMF		MFCD00674177	MFCD00674177		NMP	DMF	Sphos G3	RuPhos G3	Sphos G3	RuPhos G3	NMP	DMF		aq K3PO4	aq BTMG							
H	Core NMP	Core DMF		MFCD06657825	MFCD06657825		NMP	DMF	Sphos G3	RuPhos G3	Sphos G3	RuPhos G3	NMP	DMF		aq K3PO4	aq BTMG							
I	Core NMP	Core DMF		MFCD03002366	MFCD03002366		NMP	DMF	Sphos G3	RuPhos G3	Sphos G3	RuPhos G3	NMP	DMF		aq K3PO4	aq BTMG							
J	Core NMP	Core DMF		MFCD05664405	MFCD05664405		NMP	DMF	Sphos G3	RuPhos G3	Sphos G3	RuPhos G3	NMP	DMF		aq K3PO4	aq BTMG							
K																								
L																								
M																								
N																								
O																								
P																								

Figure 26. CHK1 Suzuki Coupling Source Plate Map

Buchwald-Hartwig Amination Prep: Stock solutions of the thiazole bromide core (0.4 M in NMP), amine building blocks (0.6 M in NMP), Buchwald palladium precatalysts (0.04 M in NMP), and bases (BTMG, MTBD, and P_2-Et, 0.8 M in NMP) were prepared in a glove box under an N_2 atmosphere. A source plate was constructed using the reagent stock solutions, according to the diagram below, by pipetting 20-25 µL of the correct component stock solution into the wells indicated below in Figure 27.

384-Well Source Plate Buchwald-Hartwig Amination Library

	Core 1	2	Building block NMP 3	4	NMP Wash 5	6	tBuXphos NMP 7	tBuBrettPhos NMP 8	AdBrettPhos NMP 9	RockPhos NMP 10	11	NMP Wash 12	13	P2-Et Base 14	BTMG Base 15	MTBD Base 16	17	18	19	20	21	22	23	24
A	Core NMP		MFCD00007629		NMP		tBuXphos G3	tBuBrettPhos G3	AdBrettPhos G3	RockPhos G3		NMP		P2-Et	BTMG	MTBD								
B	Core NMP		MFCD00008106		NMP		tBuXphos G3	tBuBrettPhos G3	AdBrettPhos G3	RockPhos G3		NMP		P2-Et	BTMG	MTBD								
C	Core NMP		MFCD00605324		NMP		tBuXphos G3	tBuBrettPhos G3	AdBrettPhos G3	RockPhos G3		NMP		P2-Et	BTMG	MTBD								
D	Core NMP		MFCD00082597		NMP		tBuXphos G3	tBuBrettPhos G3	AdBrettPhos G3	RockPhos G3		NMP		P2-Et	BTMG	MTBD								
E	Core NMP		MFCD06858479		NMP		tBuXphos G3	tBuBrettPhos G3	AdBrettPhos G3	RockPhos G3		NMP		P2-Et	BTMG	MTBD								
F	Core NMP		MFCD06738528		NMP		tBuXphos G3	tBuBrettPhos G3	AdBrettPhos G3	RockPhos G3		NMP		P2-Et	BTMG	MTBD								
G	Core NMP		MFCD00005234		NMP		tBuXphos G3	tBuBrettPhos G3	AdBrettPhos G3	RockPhos G3		NMP		P2-Et	BTMG	MTBD								
H	Core NMP		MFCD00191749		NMP		tBuXphos G3	tBuBrettPhos G3	AdBrettPhos G3	RockPhos G3		NMP		P2-Et	BTMG	MTBD								
I	Core NMP		MFCD00462192		NMP		tBuXphos G3	tBuBrettPhos G3	AdBrettPhos G3	RockPhos G3		NMP		P2-Et	BTMG	MTBD								
J	Core NMP		MFCD00067874		NMP		tBuXphos G3	tBuBrettPhos G3	AdBrettPhos G3	RockPhos G3		NMP		P2-Et	BTMG	MTBD								
K																								
L																								
M																								
N																								
O																								
P																								

Figure 27. CHK1 Buchwald-Hartwig Amination Source Plate Map

The TTP Labtech Mosquito® was used to assemble the reaction mixtures using the multi-aspiration feature with dispense mixing.

1. 297 nL was drawn up from the desired thiazole core column (Suzuki coupling NMP: 1, DMF: 2)
2. 297 nL drawn from the desired building block column (Suzuki coupling NMP: 4, DMF: 5),
3. 6 nL tip wash (NMP: 7, DMF: 8)
4. 297 nL was drawn up from the desired catalyst column (Suzuki coupling NMP: 9-10, DMF 11-12)
5. 6 nL tip wash (NMP: 13, DMF: 14)
6. 297 nL was drawn up from the desired aqueous base column (16-17).
7. Dispense mixing (3×800 nL) into the 1,536-well reaction plate to ensure all reagents were adequately combined.
8. This process was repeated 8 times to cover all possible Suzuki coupling reaction conditions from the Suzuki coupling source plate (8 total: 2 solvents × 2 bases × 2 catalysts). This process was then preformed using the Buckwald-Hartwig amination plate to assemble the nano-scale C-N coupling library. A total of 12 dispenses were performed from the Buchwald-Hartwig amination plate to cover all reaction conditions (12 total: 1 solvent × 3 bases × 4 catalysts).
9. The 1,536-plate was sealed and briefly centrifuged before sitting at ambient temperature for 24 hours.

The next morning, the reactions were quenched by addition of 3×1.2 µL 0.5 M AcOH in DMSO to each reaction well. The reactions were further diluted (to approximately 10 mM assuming complete conversion to product) with DMSO and transferred to a 384-well LDV diamond plate for affinity-based ranking. 1 µL of the quenched and diluted crude reaction was drawn up for analysis by LC-MS (1 µL crude ~10 mM reaction into 60 µL DMSO followed by shaking). Screening results are shown below as heat maps (Suzuki coupling left, C-N coupling on right, Figure 28). Colors represent a percent yield gradient (blue-green-yellow = 0% to 50% to 100% yield), where values were calculated using a standard curves created for each respective product. Highlighted wells were used to create the crude pool for ASMS ranking and were selected based upon product yield and substrate conversion.

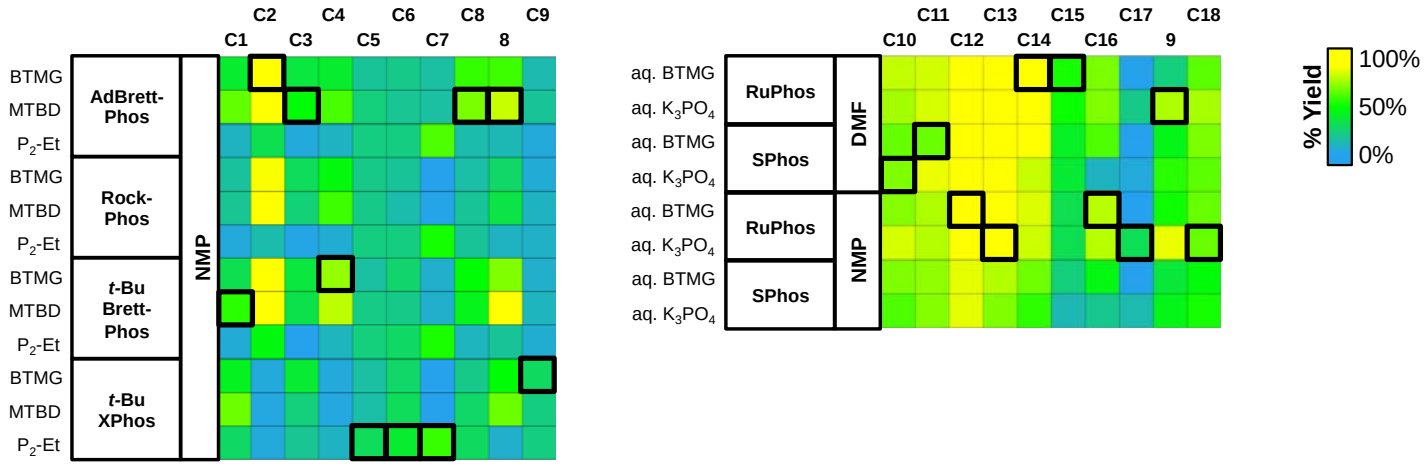


Figure 28. CHK1 Mixed Coupling Library Crude Reaction Heat Maps by Conditions

Chromatograms are shown below for the quenched and diluted crude nanomole-scale reactions producing **C8** and **9** (the green peak is unconsumed aryl bromide core, the red peaks are the desired coupling products, and the orange peak is dimer byproduct **C19**).

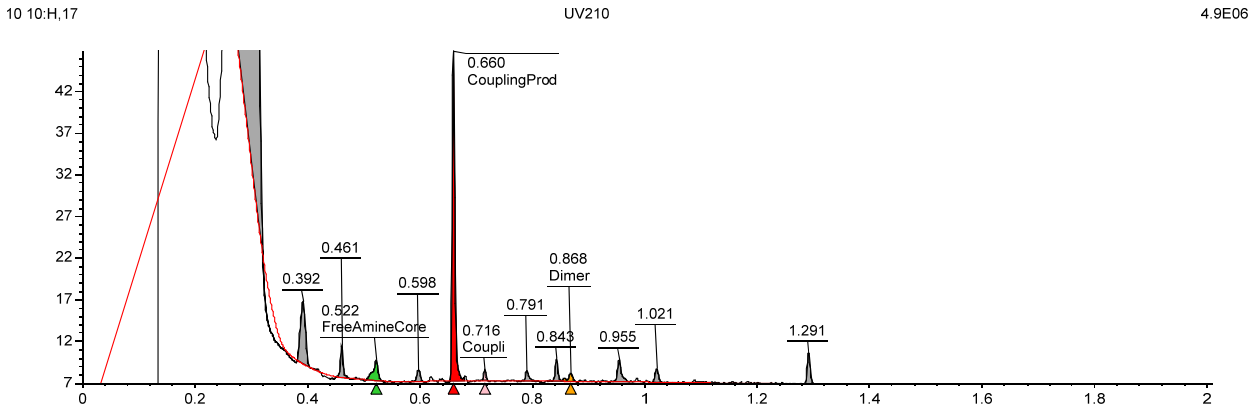


Figure 29. Chromatogram of Crude Nanomole-Scale Reaction Producing C8. Conditions: AdBrettPhos G3 / MTBD / NMP

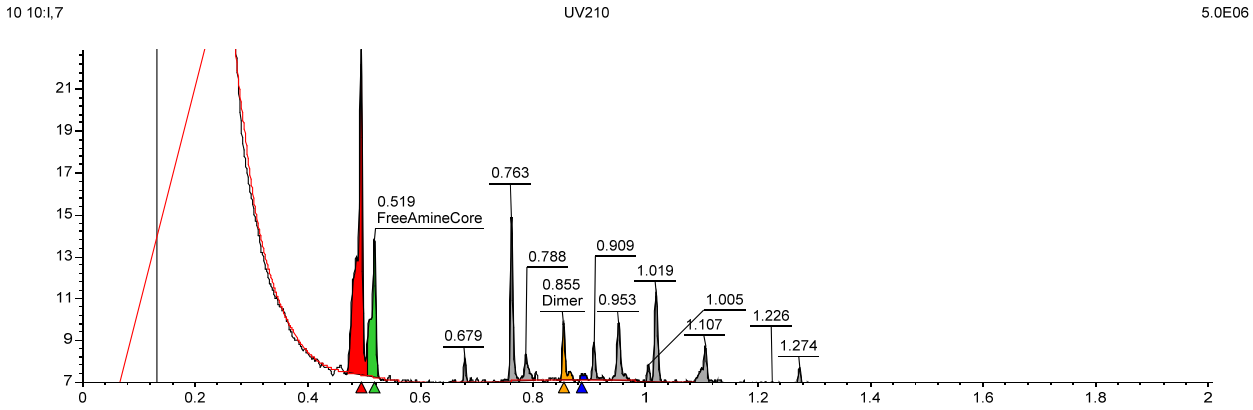


Figure 30. Chromatogram of Crude Nanomole-Scale Reaction Producing 9. Conditions: RuPhos G3 / aq. K_3PO_4 / DMF

7.3. Affinity Ranking Competition Experiment: Crude Library vs. DMT Resin Treated Library vs. Purified Library

Pool Prep. A pool comprised of the purified coupling library (10 Suzuki cross-coupling members and 10 aryl amination members, 20 total compounds) was created by transferring 1 µL of each respective 10 mM solution into a centrifuge tube (20 transfers total, 20 µL). This mixture was then diluted with DMSO to 250 µL (1:250 dilution per compound) to give a per compound concentration of 40 µM (800 µM total compound concentration). This pool was stored at -20 ˚C when not in use. A pool of quenched crude nanomole-scale reaction mixtures was prepared in a similar fashion: 1 µL was transferred from each well of the quenched reaction plate indicated above in Figure 28 (approx. 10 mM assuming complete conversion to product, 20 total transfers, 20 µL) to a centrifuge tube. This crude library mixture was then diluted with DMSO to 250 µL (1:250 dilution per compound) to give a per compound concentration of approximately 40 µM. This pool was stored at -20 ˚C when not in use. Crude reactions used in the pooling step were selected in the basis of product UV peak area (yield) and absence of starting material (relative conversion). A SiliaMetS® Dimercaptotriazine (DMT) scavenger-treated pool was constructed using the same crude reactions indicated above for the crude reaction pool, however diluting with a DMSO suspension of the SiliaMetS® Dimercaptotriazine (DMT) silica-bound metal scavenger (5 equiv. resin relative to palladium loading). This pool was centrifuged before use. Baseline residual palladium concentrations were acquired for the crude, treated, and purified pools using ICP-MS and are reported below.

Table 6. Residual Pool Palladium Concentrations

Pool	Pd conc. (ppm)
Purified product pool	<1
SiliaMetS® DMT treated pool	2.5
Crude reaction pool	4.3

Table 7. CHK1 Library Pools: Crude, Treated, Purified

Pool	Sample Name	Catalyst	Base	Solvent	Source Wells	Mass	Formula	Target	Invitrogen IC50 (nM)	Percent Yield
Pool 1 Crude	0378493_0089_005	Sphos G2	aq. K3PO4	DMF	A5	364.13578	C20H20N4OS	CHK1	197	89
Pool 1 Crude	0378493_0089_014	Sphos G2	aq. BTMG	DMF	B6	394.14635	C21H22N4O2S	CHK1	114	100
Pool 1 Crude	0378493_0089_020	RuPhos G3	aq. BTMG	NMP	C4	408.162	C22H24N4O2S	CHK1	190	100
Pool 1 Crude	0378493_0089_027	RuPhos G3	aq. K3PO4	NMP	D3	424.15691	C22H24N4O3S	CHK1	682	100
Pool 1 Crude	0378493_0089_040	RuPhos G3	aq. BTMG	DMF	E8	407.17798	C22H25N5OS	CHK1	60.1	100
Pool 1 Crude	0378493_0089_048	RuPhos G3	aq. BTMG	DMF	F8	353.13103	C18H19N5OS	CHK1	140	88
Pool 1 Crude	0378493_0089_052	RuPhos G3	aq. BTMG	NMP	G4	365.13103	C19H19N5OS	CHK1	3350	80
Pool 1 Crude	0378493_0089_059	RuPhos G3	aq. K3PO4	NMP	H3	390.12628	C20H18N6OS	CHK1	10000	54
Pool 1 Crude	0378493_0089_071	RuPhos G3	aq. K3PO4	DMF	I7	366.12628	C18H18N6OS	CHK1	10000	61
Pool 1 Crude	0378493_0089_075	RuPhos G3	aq. K3PO4	NMP	J3	420.10785	C22H20N4OS2	CHK1	33.1	100
Pool 1 Crude	0378493_0089_086	tBuBrettPhos G3	MTBD	NMP	A14	379.14668	C20H21N5OS	CHK1	193	100
Pool 1 Crude	0378493_0089_100	AdBrettPhos G3	BTMG	NMP	B16	393.16233	C21H23N5OS	CHK1	10000	100
Pool 1 Crude	0378493_0089_113	AdBrettPhos G3	MTBD	NMP	C17	405.16233	C22H23N5OS	CHK1	17.2	91
Pool 1 Crude	0378493_0089_121	tBuBrettPhos G3	BTMG	NMP	D13	419.17798	C23H25N5OS	CHK1	7170	100
Pool 1 Crude	0378493_0089_129	tBuXphos G3	P2-Et	NMP	E9	406.15758	C21H22N6OS	CHK1	209	48
Pool 1 Crude	0378493_0089_141	tBuXphos G3	P2-Et	NMP	F9	426.12965	C20H22N6OS2	CHK1	361	47
Pool 1 Crude	0378493_0089_153	tBuXphos G3	P2-Et	NMP	G9	354.12628	C17H18N6OS	CHK1	233	93
Pool 1 Crude	0378493_0089_173	AdBrettPhos G3	MTBD	NMP	H17	445.16848	C23H23N7OS	CHK1	18.8	93
Pool 1 Crude	0378493_0089_185	AdBrettPhos G3	MTBD	NMP	I17	475.17904	C24H25N7O2S	CHK1	23.2	100
Pool 1 Crude	0378493_0089_190	tBuXphos G3	BTMG	NMP	J10	459.18413	C24H25N7OS	CHK1	10000	48
Pool	**Sample Name**	**Catalyst**	**Base**	**Solvent**	**Source Wells**	**Mass**	**Formula**	**Target**	**Invitrogen IC50 (nM)**	**Percent Yield**
Pool 2 Resin Treated	0378493_0089_005	Sphos G2	aq. K3PO4	DMF	A5	364.13578	C20H20N4OS	CHK1	197	89
Pool 2 Resin Treated	0378493_0089_014	Sphos G2	aq. BTMG	DMF	B6	394.14635	C21H22N4O2S	CHK1	114	100
Pool 2 Resin	0378493_0089_020	RuPhos G3	aq. BTMG	NMP	C4	408.162	C22H24N4O2S	CHK1	190	100

Treated										
Pool 2 Resin Treated	0378493_0089_027	RuPhos G3	aq. K3PO4	NMP	D3	424.15691	C22H24N4O3S	CHK1	682	100
Pool 2 Resin Treated	0378493_0089_040	RuPhos G3	aq. BTMG	DMF	E8	407.17798	C22H25N5OS	CHK1	60.1	100
Pool 2 Resin Treated	0378493_0089_048	RuPhos G3	aq. BTMG	DMF	F8	353.13103	C18H19N5OS	CHK1	140	88
Pool 2 Resin Treated	0378493_0089_052	RuPhos G3	aq. BTMG	NMP	G4	365.13103	C19H19N5OS	CHK1	3350	80
Pool 2 Resin Treated	0378493_0089_059	RuPhos G3	aq. K3PO4	NMP	H3	390.12628	C20H18N6OS	CHK1	10000	54
Pool 2 Resin Treated	0378493_0089_071	RuPhos G3	aq. K3PO4	DMF	I7	366.12628	C18H18N6OS	CHK1	10000	61
Pool 2 Resin Treated	0378493_0089_075	RuPhos G3	aq. K3PO4	NMP	J3	420.10785	C22H20N4OS2	CHK1	33.1	100
Pool 2 Resin Treated	0378493_0089_086	tBuBrettPhos G3	MTBD	NMP	A14	379.14668	C20H21N5OS	CHK1	193	100
Pool 2 Resin Treated	0378493_0089_100	AdBrettPhos G3	BTMG	NMP	B16	393.16233	C21H23N5OS	CHK1	10000	100
Pool 2 Resin Treated	0378493_0089_113	AdBrettPhos G3	MTBD	NMP	C17	405.16233	C22H23N5OS	CHK1	17.2	91
Pool 2 Resin Treated	0378493_0089_121	tBuBrettPhos G3	BTMG	NMP	D13	419.17798	C23H25N5OS	CHK1	7170	100
Pool 2 Resin Treated	0378493_0089_129	tBuXphos G3	P2-Et	NMP	E9	406.15758	C21H22N6OS	CHK1	209	48
Pool 2 Resin Treated	0378493_0089_141	tBuXphos G3	P2-Et	NMP	F9	426.12965	C20H22N6OS2	CHK1	361	47
Pool 2 Resin Treated	0378493_0089_153	tBuXphos G3	P2-Et	NMP	G9	354.12628	C17H18N6OS	CHK1	233	93
Pool 2 Resin Treated	0378493_0089_173	AdBrettPhos G3	MTBD	NMP	H17	445.16848	C23H23N7OS	CHK1	18.8	93
Pool 2 Resin Treated	0378493_0089_185	AdBrettPhos G3	MTBD	NMP	I17	475.17904	C24H25N7O2S	CHK1	23.2	100
Pool 2 Resin Treated	0378493_0089_190	tBuXphos G3	BTMG	NMP	J10	459.18413	C24H25N7OS	CHK1	10000	48
Pool	**Sample Name**	**Catalyst**	**Base**	**Solvent**	**Source Wells**	**Mass**	**Formula**	**Target**	**Invitrogen IC50 (nM)**	**Percent Yield**
Pool 3	0378493_0083_0	N/A	N/A	N/A	N/A	364.135	C20H20N4O	CHK1	197	10 mM

Purified	2					78	S			DMSO stock
Pool 3 Purified	0378493_0083_03	N/A	N/A	N/A	N/A	394.14635	C21H22N4O2S	CHK1	114	10 mM DMSO stock
Pool 3 Purified	0378493_0083_04	N/A	N/A	N/A	N/A	408.162	C22H24N4O2S	CHK1	190	10 mM DMSO stock
Pool 3 Purified	0378493_0083_05	N/A	N/A	N/A	N/A	424.15691	C22H24N4O3S	CHK1	682	10 mM DMSO stock
Pool 3 Purified	0378493_0083_06	N/A	N/A	N/A	N/A	407.17798	C22H25N5OS	CHK1	60.1	10 mM DMSO stock
Pool 3 Purified	0378493_0083_08	N/A	N/A	N/A	N/A	353.13103	C18H19N5OS	CHK1	140	10 mM DMSO stock
Pool 3 Purified	0378493_0083_11	N/A	N/A	N/A	N/A	365.13103	C19H19N5OS	CHK1	3350	10 mM DMSO stock
Pool 3 Purified	0378493_0083_12	N/A	N/A	N/A	N/A	390.12628	C20H18N6OS	CHK1	10000	10 mM DMSO stock
Pool 3 Purified	0378493_0083_13	N/A	N/A	N/A	N/A	366.12628	C18H18N6OS	CHK1	10000	10 mM DMSO stock
Pool 3 Purified	0378493_0083_14	N/A	N/A	N/A	N/A	420.10785	C22H20N4OS2	CHK1	33.1	10 mM DMSO stock
Pool 3 Purified	0378493_0105	N/A	N/A	N/A	N/A	379.14668	C20H21N5OS	CHK1	193	10 mM DMSO stock
Pool 3 Purified	0378493_0106	N/A	N/A	N/A	N/A	393.16233	C21H23N5OS	CHK1	10000	10 mM DMSO stock
Pool 3 Purified	0378493_0107	N/A	N/A	N/A	N/A	405.16233	C22H23N5OS	CHK1	17.2	10 mM DMSO stock
Pool 3 Purified	0378493_0108	N/A	N/A	N/A	N/A	419.17798	C23H25N5OS	CHK1	7170	10 mM DMSO stock
Pool 3 Purified	0378493_0109	N/A	N/A	N/A	N/A	406.15758	C21H22N6OS	CHK1	209	10 mM DMSO stock
Pool 3 Purified	0378493_0110	N/A	N/A	N/A	N/A	426.12965	C20H22N6OS2	CHK1	361	10 mM DMSO stock
Pool 3 Purified	0378493_0111	N/A	N/A	N/A	N/A	354.12628	C17H18N6OS	CHK1	233	10 mM DMSO stock
Pool 3 Purified	0378493_0112	N/A	N/A	N/A	N/A	445.16848	C23H23N7OS	CHK1	18.8	10 mM DMSO stock
Pool 3 Purified	0378493_0113	N/A	N/A	N/A	N/A	475.17904	C24H25N7O2S	CHK1	23.2	10 mM DMSO stock

Pool 3 Purified	0378493_0114	N/A	N/A	N/A	N/A	459.18413	C24H25N7OS	CHK1	10000	10 mM DMSO stock

Competition Experiment Prep. All work was done at 0 ˚C unless otherwise noted. CHK1 (internal preparation: 50 µM stock solution in 25 mM Hepes, pH 7.5, 300 mM NaCl, 5 mM DTT, 5% glycerol) was removed from a -78 ˚C freezer and warmed to approximately 0 ˚C on ice. Protein dilution buffer was prepared (56.5 mM Hepes pH 7.5, 200 mM NaCl, 5 mM dithiothreitol) along with library dilution buffer (56.5 mM Hepes pH 7.5, 200 mM NaCl, 5 mM dithiothreitol). Invertase (Sigma Aldrich cat. no. I4504) was weighed into a centrifuge tube and diluted to 20 µM with protein dilution buffer (and then separately to 10 µM) in preparation for the serial dilution. The three previously prepared pools were thawed, aliquots removed and diluted 1:20 with library dilution buffer (4 µL DMSO pool into 76 µL library dilution buffer to give final concentrations of 2 µM/compound). The diluted pools were stored at ambient temperature prior to use. Next, a serial dilution of CHK1 was performed. The CHK1 stock was diluted with protein dilution buffer to 40 µM, then diluted 1:1 with 20 µM invertase (to populate the first protein level). The CHK1 serial dilution was then performed in a 96-well plate, using the 10 µM invertase stock, to arrive at the following CHK1/invertase protein levels:

CHK1 Conc.	20 µM	10 µM	5 µM	2.5 µM	1.25 µM	0.62 µM	0.31 µM	0 µM
Invertase Conc.	10 µM	10 µM	10 µM	10 µM	10 µM	10 µM	10 µM	10 µM
Final Vol. (µL)	15	15	15	15	15	15	30	15

Finally, a 1:1 dilution of the appropriate CHK1 protein stock (3 µL) with the desired buffered library (3 µL) in a new 96-well plate provided an affinity-based ranking experiment with the desired protein and compound concentrations (1 µM/compound, 5 µM invertase, variable CHK1 concentration). Three pools were tested (crude pool, DMT resin treated crude pool, and purified pool) which resulted in three unique affinity ranking sequences: one where the 1:1 dilution was done with the purified library pool, one using the resin treated pool, and finally one using the crude reaction mixture pool. The serial dilution performed above was used to prepare all affinity ranking sequences. The protein/compound mixtures were warmed to room temperature then allowed to incubate for 30 minutes. After 30 minutes, the 96-well plate was moved to an LC-MS autosampler (cooled to 4 ˚C) for analysis. Final component concentrations are shown below.

Lib. Size	20	20	20	20	20	20	20	20
Per Cmpd.	1 µM	1 µM	1 µM	1 µM	1 µM	1 µM	1 µM	1 µM
Invertase Conc.	5 µM	5 µM	5 µM	5 µM	5 µM	5 µM	5 µM	5 µM
CHK1 Conc.	10 µM	5 µM	2.5 µM	1.25 µM	0.62 µM	0.31 µM	0.16 µM	0 µM

Chromatography conditions

SEC Running Buffer: 1 M NH_4OAc, pH 8.0

Flow Rate: 0.3 mL / min

Negative Control: 5 µM Invertase

Table 8. Affinity-Based Ranking Results

Pool	Treatment	Sample Name	Invitrogen Avg. IC50 (nM)	Well	Mass	Formula	Protein Conc. Where Binding First Observed
Pool 1 Crude	Crude	0378493_0089_005	197	A5	364.13578	C20H20N4OS	10.00µM CHK1
Pool 1 Crude	Crude	0378493_0089_014	114	B6	394.14635	C21H22N4O2S	10.00µM CHK1
Pool 1 Crude	Crude	0378493_0089_020	190	C4	408.162	C22H24N4O2S	5.00µM CHK1
Pool 1 Crude	Crude	0378493_0089_027	682	D3	424.15691	C22H24N4O3S	ASMS Binding Not Observed
Pool 1 Crude	Crude	0378493_0089_040	60.1	E8	407.17798	C22H25N5OS	5.00µM CHK1
Pool 1 Crude	Crude	0378493_0089_048	140	F8	353.13103	C18H19N5OS	10.00µM CHK1
Pool 1 Crude	Crude	0378493_0089_052	3350	G4	365.13103	C19H19N5OS	ASMS Binding Not Observed
Pool 1 Crude	Crude	0378493_0089_059	10000	H3	390.12628	C20H18N6OS	ASMS Binding Not Observed
Pool 1 Crude	Crude	0378493_0089_071	10000	I7	366.12628	C18H18N6OS	ASMS Binding Not Observed
Pool 1 Crude	Crude	0378493_0089_075	33.1	J3	420.10785	C22H20N4OS2	1.25µM CHK1
Pool 1 Crude	Crude	0378493_0089_086	193	A14	379.14668	C20H21N5OS	ASMS Binding Not Observed
Pool 1 Crude	Crude	0378493_0089_100	10000	B16	393.16233	C21H23N5OS	ASMS Binding Not Observed
Pool 1 Crude	Crude	0378493_0089_113	17.2	C17	405.16233	C22H23N5OS	2.50µM CHK1
Pool 1 Crude	Crude	0378493_0089_121	7170	D13	419.17798	C23H25N5OS	ASMS Binding Not Observed
Pool 1 Crude	Crude	0378493_0089_129	209	E9	406.15758	C21H22N6OS	ASMS Binding Not Observed
Pool 1 Crude	Crude	0378493_0089_141	361	F9	426.12965	C20H22N6OS2	ASMS Binding Not Observed
Pool 1 Crude	Crude	0378493_0089_153	233	G9	354.12628	C17H18N6OS	10.00µM CHK1
Pool 1 Crude	Crude	0378493_0089_173	18.8	H17	445.16848	C23H23N7OS	1.25µM CHK1
Pool 1 Crude	Crude	0378493_0089_185	23.2	I17	475.17904	C24H25N7O2S	1.25µM CHK1
Pool 1 Crude	Crude	0378493_0089_190	10000	J10	459.18413	C24H25N7OS	ASMS Binding Not Observed
Pool	**Treatment**	**Sample Name**	**Invitrogen Avg. IC50 (nM)**	**Well**	**Mass**	**Formula**	**Protein Conc. Where Binding First Observed**
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_005	197	A5	364.13578	C20H20N4OS	10.00µM CHK1
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_014	114	B6	394.14635	C21H22N4O2S	10.00µM CHK1
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_020	190	C4	408.162	C22H24N4O2S	5.00µM CHK1
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_027	682	D3	424.15691	C22H24N4O3S	ASMS Binding Not Observed

Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_040	60.1	E8	407.17798	C22H25N5OS	5.00µM CHK1
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_048	140	F8	353.13103	C18H19N5OS	ASMS Binding Not Observed
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_052	3350	G4	365.13103	C19H19N5OS	ASMS Binding Not Observed
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_059	10000	H3	390.12628	C20H18N6OS	ASMS Binding Not Observed
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_071	10000	I7	366.12628	C18H18N6OS	ASMS Binding Not Observed
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_075	33.1	J3	420.10785	C22H20N4OS2	2.50µM CHK1
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_086	193	A14	379.14668	C20H21N5OS	ASMS Binding Not Observed
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_100	10000	B16	393.16233	C21H23N5OS	ASMS Binding Not Observed
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_113	17.2	C17	405.16233	C22H23N5OS	2.50µM CHK1
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_121	7170	D13	419.17798	C23H25N5OS	ASMS Binding Not Observed
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_129	209	E9	406.15758	C21H22N6OS	ASMS Binding Not Observed
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_141	361	F9	426.12965	C20H22N6OS2	ASMS Binding Not Observed
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_153	233	G9	354.12628	C17H18N6OS	10.00µM CHK1
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_173	18.8	H17	445.16848	C23H23N7OS	1.25µM CHK1
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_185	23.2	I17	475.17904	C24H25N7O2S	1.25µM CHK1
Pool 2 Resin Treated	DMT Resin Treated	0378493_0089_190	10000	J10	459.18413	C24H25N7OS	ASMS Binding Not Observed
Pool	**Treatment**	**Sample Name**	**Invitrogen Avg. IC50 (nM)**	**Well**	**Mass**	**Formula**	**Protein Conc. Where Binding First Observed**
Pool 3 Purified	Purified	0378493_0083_02	197	N/A	364.13578	C20H20N4OS	10.00µM CHK1
Pool 3 Purified	Purified	0378493_0083_03	114	N/A	394.14635	C21H22N4O2S	10.00µM CHK1
Pool 3 Purified	Purified	0378493_0083_04	190	N/A	408.162	C22H24N4O2S	10.00µM CHK1
Pool 3 Purified	Purified	0378493_0083_05	682	N/A	424.15691	C22H24N4O3S	ASMS Binding Not Observed
Pool 3 Purified	Purified	0378493_0083_06	60.1	N/A	407.17798	C22H25N5OS	5.00µM CHK1
Pool 3 Purified	Purified	0378493_0083_08	140	N/A	353.13103	C18H19N5OS	10.00µM CHK1
Pool 3 Purified	Purified	0378493_0083_11	3350	N/A	365.13103	C19H19N5OS	ASMS Binding Not Observed
Pool 3 Purified	Purified	0378493_0083_12	10000	N/A	390.12628	C20H18N6OS	ASMS Binding Not Observed
Pool 3 Purified	Purified	0378493_0083_13	10000	N/A	366.12628	C18H18N6OS	ASMS Binding Not Observed
Pool 3 Purified	Purified	0378493_0083_14	33.1	N/A	420.10785	C22H20N4OS2	2.50µM CHK1

Pool 3 Purified	Purified	0378493_0105	193	N/A	379.1466 8	C20H21N5OS	ASMS Binding Not Observed
Pool 3 Purified	Purified	0378493_0106	10000	N/A	393.1623 3	C21H23N5OS	ASMS Binding Not Observed
Pool 3 Purified	Purified	0378493_0107	17.2	N/A	405.1623 3	C22H23N5OS	2.50µM CHK1
Pool 3 Purified	Purified	0378493_0108	7170	N/A	419.1779 8	C23H25N5OS	ASMS Binding Not Observed
Pool 3 Purified	Purified	0378493_0109	209	N/A	406.1575 8	C21H22N6OS	10.00µM CHK1
Pool 3 Purified	Purified	0378493_0110	361	N/A	426.1296 5	C20H22N6OS 2	ASMS Binding Not Observed
Pool 3 Purified	Purified	0378493_0111	233	N/A	354.1262 8	C17H18N6OS	10.00µM CHK1
Pool 3 Purified	Purified	0378493_0112	18.8	N/A	445.1684 8	C23H23N7OS	1.25µM CHK1
Pool 3 Purified	Purified	0378493_0113	23.2	N/A	475.1790 4	C24H25N7O2 S	2.50µM CHK1
Pool 3 Purified	Purified	0378493_0114	10000	N/A	459.1841 3	C24H25N7OS	ASMS Binding Not Observed

Plots displaying the general correlation between activity assay IC_{50} (plotted on a log scale) and the lowest CHK1 concentration at which ASMS binding was observed (protein level, for 20 library members) are shown below. The three plots represent the three different pool preparations: crude pool (left), DMT resin treated pool (middle), and purified compound pool (right):

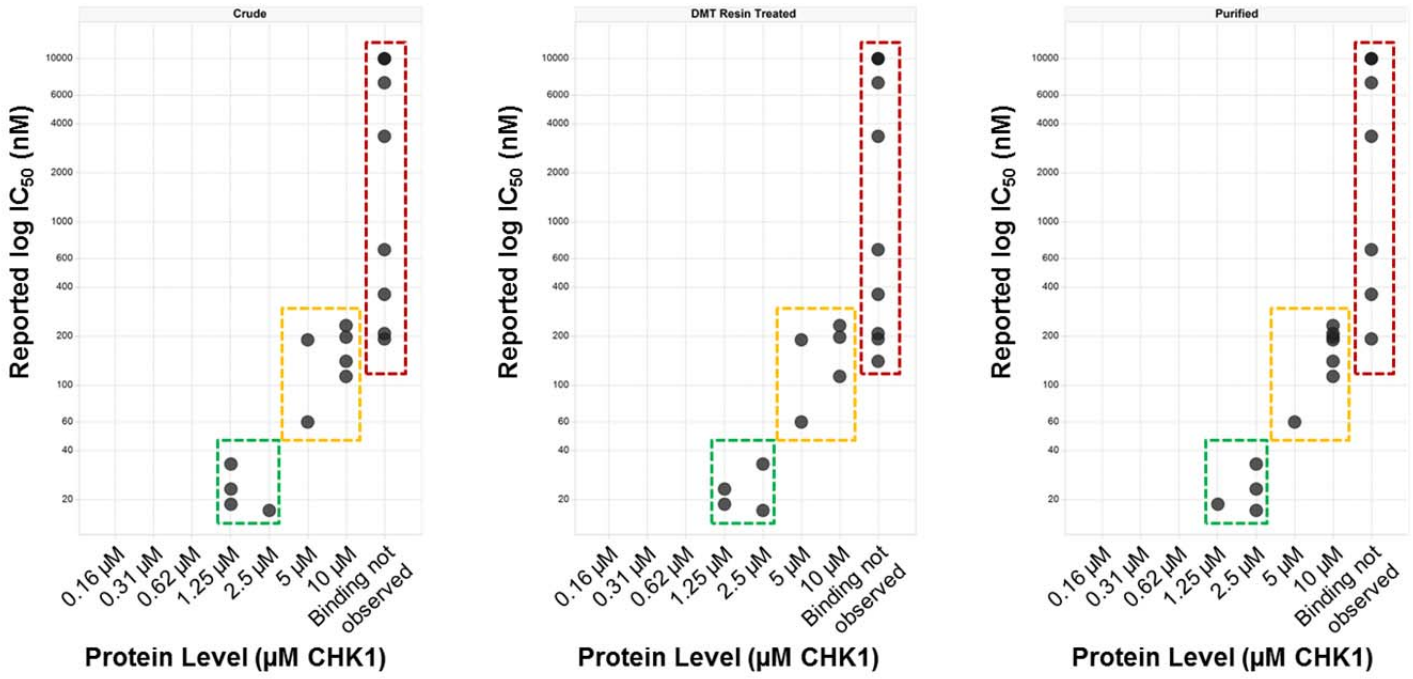
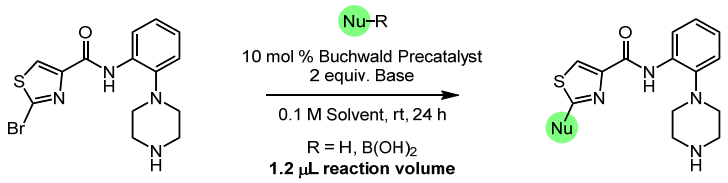


Figure 31. CHK1 Mixed Coupling Library Affinity Ranking Results

Note: in the SilaMetS DMT resin treated pool some library members (masses 407.18, 408.16, 420.11, and 475.18) were observed at lower protein concentrations than those indicated above. It was determined that these data points may not represent binding of the library members to the desired target, but rather possibly background binding or experimental breakthrough (a rare occurrence but sometime observed). These points were excluded for various reasons listed below:

1. Abnormal affinity ranking behavior at lower levels than indicated above. Signal strength remained constant and low rather than increasing as protein concentration increased, suggesting possible background binding to invertase.
2. Presence of these compounds was not constant in the affinity ranking experiment; there were gaps (protein levels) where these species were absent between levels where they were present.
3. Generally very low signal strength (<20000)
4. See excel supplementary Excel data tables, data points in question are highlighted. Data were retained when normal affinity ranking behavior was observed: general increase in signal strength with increasing protein concentration).

8. 384-Member Mixed Coupling Library Targeting CHK1



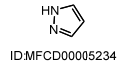
Previous screening campaigns revealed coupling reactions amenable to miniaturization to the nanomole-scale: Suzuki cross coupling to forge C-C bonds, Buchwald-Hartwig aryl amination (using aliphatic amines, aryl amines, amides, and sulfonamides) for form C-N bonds, C-O coupling/S_NAr, C-S coupling/S_NAr, and the Sonogashira coupling. A 384-member library was constructed around these reactions and the aryl bromide core above. Available building blocks to couple to thiazole bromide core **1** (above) were selected based on the following criteria:

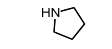
1. Building block falls under one of the reactions described above and previously studied (Section 3)
2. Building block is commercially available
3. Building block results in a product with a relatively high Quantitative Estimate of Drug-likeness (QED) score,[14] >0.5 when possible. See supplementary Excel tables for nucleophile building block order and descriptions.

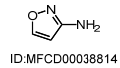
8.1. Library Design and Plate Preparation

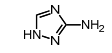
The 384 nucleophile structures shown below were used as the building blocks to generate the inner heatmap of Figure 3. MFCD's are shown as identifiers here to link to commercial availability. In Figure 3, these building blocks are listed as Nuc_1 to Nuc_384. Please see Supplementary Data File Source Data for Figure 3.xlsx to map MFCD identifiers to each Nuc_#.

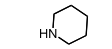
Amine Building Blocks

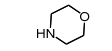

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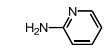

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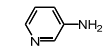

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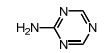

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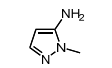

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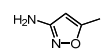

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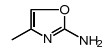

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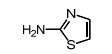

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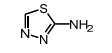

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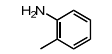

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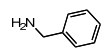

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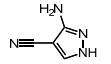

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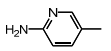

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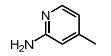

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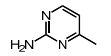

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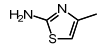

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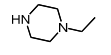

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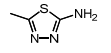

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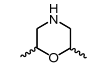

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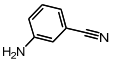

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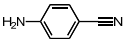

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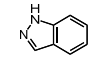

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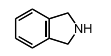

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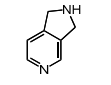

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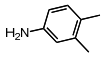

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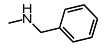

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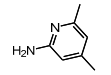

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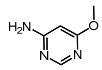

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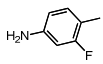

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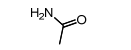
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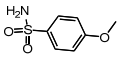
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Amide and Sulfonamide Building Blocks


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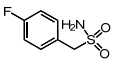

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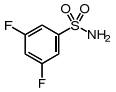

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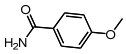

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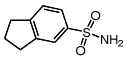

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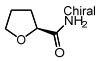

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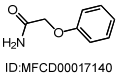

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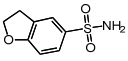

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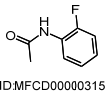

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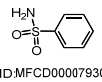

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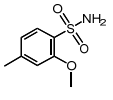

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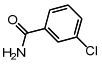

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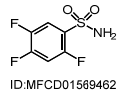

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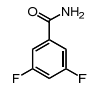

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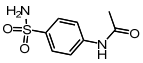

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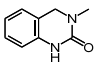

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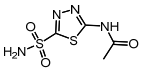

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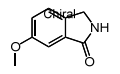

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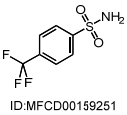

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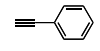
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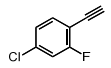
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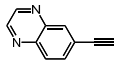
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Alkyne / Sonogashira Building Blocks

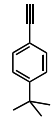

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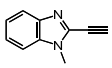

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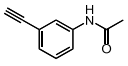

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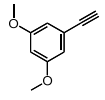

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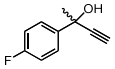

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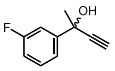

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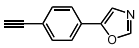

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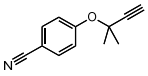

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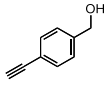

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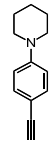

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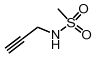

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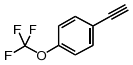

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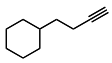

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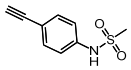

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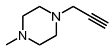

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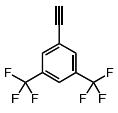

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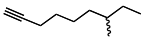

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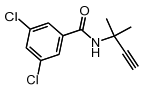

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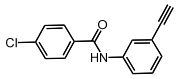

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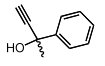

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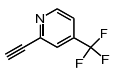

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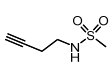

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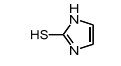

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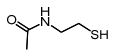

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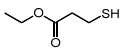

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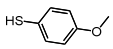

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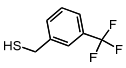

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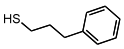

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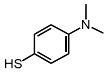

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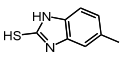

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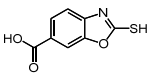

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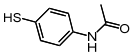

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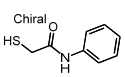

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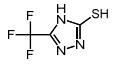

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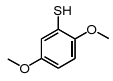

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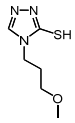

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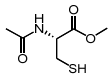

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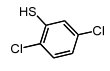

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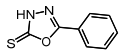

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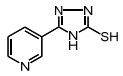

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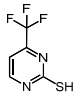

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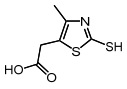

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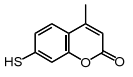

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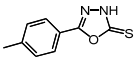

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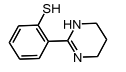

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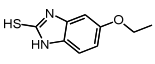

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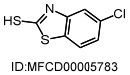

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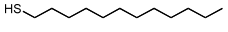

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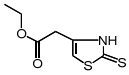

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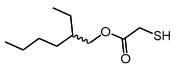

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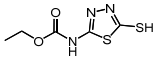

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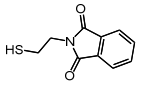

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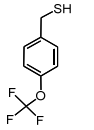

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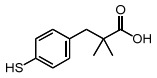

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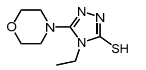

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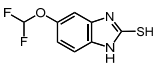

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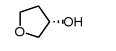
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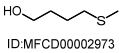
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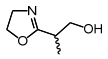
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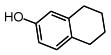
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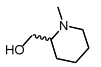

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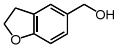

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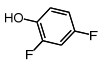

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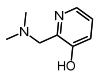

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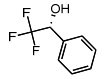

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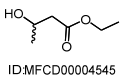

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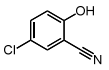

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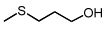

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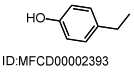

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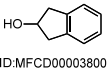

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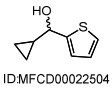

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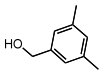

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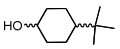

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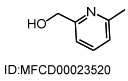

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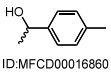

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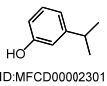

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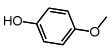

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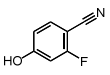

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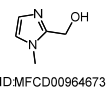

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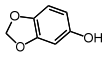

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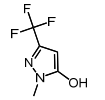

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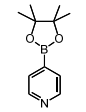
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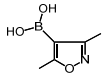

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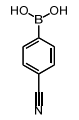

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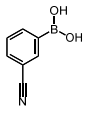

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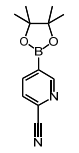

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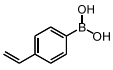

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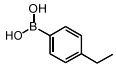

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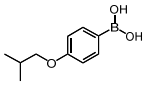

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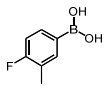

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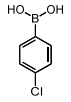

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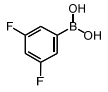

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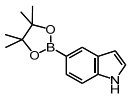

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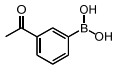

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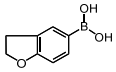

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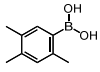

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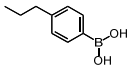

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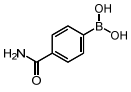

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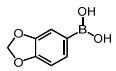

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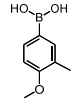

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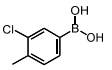

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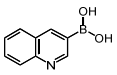

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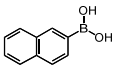

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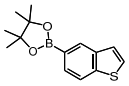

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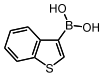

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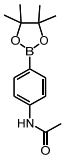

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Nucleophile building blocks were dissolved in the desired solvent (NMP or DMF depending on transformation) to 0.6 M. The nucleophile stock solutions were then transferred via pipette to a polypropylene 384-well nucleophile source plate for storage and dispensing. The nucleophile plate map is described below in Table 9 (from supplementary Excel tables).

Table 9. Nucleophile Source Plate Map

Well	Nucleophile Type / Chemistry	Building Block ID	BB MW	BB Formula	Qty Ordered (mg)	Solvent to 0.6M (µL)	Solvent
A1	Amine	MFCD00005234	68.03745	C3H4N2	8.5	199.8	NMP
B1	Amine	MFCD00005249	71.0735	C4H9N	8.88	199.5	NMP
C1	Amine	MFCD00038814	84.03236	C3H4N2O	10.5	197.8	NMP
D1	Amine	MFCD00005230	84.0436	C2H4N4	10.51	197.8	NMP
E1	Amine	MFCD00005979	85.08915	C5H11N	10.64	197.7	NMP
F1	Amine	MFCD00005972	87.06841	C4H9NO	10.88	197.5	NMP
G1	Amine	MFCD00006312	94.0531	C5H6N2	11.76	196.6	NMP
H1	Amine	MFCD00006400	94.0531	C5H6N2	11.76	196.6	NMP
I1	Amine	MFCD00023179	96.0436	C3H4N4	12.01	196.3	NMP
J1	Amine	MFCD00068156	97.064	C4H7N3	12.13	196.2	NMP
K1	Amine	MFCD00003155	98.04801	C4H6N2O	12.26	196.1	NMP
L1	Amine	MFCD00126682	98.04801	C4H6N2O	12.26	196.1	NMP
M1	Amine	MFCD00005325	100.00952	C3H4N2S	12.5	195.8	NMP
N1	Amine	MFCD00003107	101.00477	C2H3N3S	12.63	195.7	NMP
O1	Amine	MFCD00007730	107.0735	C7H9N	13.38	195	NMP
P1	Amine	MFCD00008106	107.0735	C7H9N	13.38	195	NMP
A2	Amine	MFCD00005237	108.0436	C4H4N4	13.51	194.8	NMP
B2	Amine	MFCD00006328	108.06875	C6H8N2	13.51	194.8	NMP
C2	Amine	MFCD00006321	108.06875	C6H8N2	13.51	194.8	NMP
D2	Amine	MFCD00006101	109.064	C5H7N3	13.63	194.7	NMP
E2	Amine	MFCD00005329	114.02517	C4H6N2S	14.25	194.1	NMP
F2	Amine	MFCD00059912	114.1157	C6H14N2	14.26	194.1	NMP
G2	Amine	MFCD00003110	115.02042	C3H5N3S	14.38	194	NMP
H2	Amine	MFCD00005973	115.09971	C6H13NO	14.39	193.9	NMP
I2	Amine	MFCD00007756	118.0531	C7H6N2	14.76	193.6	NMP
J2	Amine	MFCD00007821	118.0531	C7H6N2	14.76	193.6	NMP
K2	Amine	MFCD00005691	118.0531	C7H6N2	14.76	193.6	NMP
L2	Amine	MFCD00605324	119.0735	C8H9N	14.88	193.5	NMP
M2	Amine	MFCD06858479	120.06875	C7H8N2	15.01	193.3	NMP
N2	Amine	MFCD00007810	121.08915	C8H11N	15.14	193.2	NMP
O2	Amine	MFCD00008289	121.08915	C8H11N	15.14	193.2	NMP
P2	Amine	MFCD00006322	122.0844	C7H10N2	15.26	193.1	NMP
A3	Amine	MFCD00007688	123.06841	C7H9NO	15.38	193	NMP
B3	Amine	MFCD00706298	124.00952	C5H4N2S	15.5	192.8	NMP
C3	Amine	MFCD00833386	124.06366	C6H8N2O	15.51	192.8	NMP
D3	Amine	MFCD00129983	125.05891	C5H7N3O	15.63	192.7	NMP
E3	Amine	MFCD00007762	125.06408	C7H8FN	15.63	192.7	NMP

F3	Amine	MFCD00017942	125.06408	C7H8FN	15.63	192.7	NMP
G3	Amine	MFCD00020961	111.06841	C6H9NO	13.88	194.5	NMP
H3	Amine	MFCD00167971	128.13135	C7H16N2	16.02	192.3	NMP
I3	Amine	MFCD00003111	129.03607	C4H7N3S	16.13	192.2	NMP
J3	Amine	MFCD00007761	129.03901	C6H5F2N	16.13	192.2	NMP
K3	Amine	MFCD00005679	132.06875	C8H8N2	16.51	191.8	NMP
L3	Amine	MFCD00005596	133.064	C7H7N3	16.63	191.7	NMP
M3	Amine	MFCD00182045	133.064	C7H7N3	16.63	191.7	NMP
N3	Amine	MFCD00082598	133.08915	C9H11N	16.64	191.7	NMP
O3	Amine	MFCD00082597	133.08915	C9H11N	16.64	191.7	NMP
P3	Amine	MFCD00006896	133.08915	C9H11N	16.64	191.7	NMP
A4	Amine	MFCD00182850	134.04801	C7H6N2O	16.76	191.6	NMP
B4	Amine	MFCD03407353	134.04801	C7H6N2O	16.76	191.6	NMP
C4	Amine	MFCD03617969	135.06841	C8H9NO	16.88	191.5	NMP
D4	Amine	MFCD08447400	135.07965	C7H9N3	16.88	191.5	NMP
E4	Amine	MFCD00008291	135.1048	C9H13N	16.89	191.4	NMP
F4	Amine	MFCD00007860	136.10005	C8H12N2	17.01	191.3	NMP
G4	Amine	MFCD00005832	137.04768	C7H7NO2	17.13	191.2	NMP
H4	Amine	MFCD00075057	137.08406	C8H11NO	17.14	191.2	NMP
I4	Amine	MFCD00008399	137.08406	C8H11NO	17.14	191.2	NMP
J4	Amine	MFCD04629633	139.07973	C8H10FN	17.38	191	NMP
K4	Amine	MFCD04623547	139.07973	C8H10FN	17.38	191	NMP
L4	Amine	MFCD06738528	140.04082	C6H8N2S	17.51	190.8	NMP
M4	Amine	MFCD00000614	141.03453	C7H8ClN	17.63	190.7	NMP
N4	Amine	MFCD00075040	141.05899	C7H8FNO	17.63	190.7	NMP
O4	Amine	MFCD00001953	146.0844	C9H10N2	18.26	190.1	NMP
P4	Amine	MFCD00083522	147.02958	C6H4F3N	18.38	190	NMP
A5	Amine	MFCD00001736	147.1048	C10H13N	18.39	189.9	NMP
B5	Amine	MFCD00130046	147.1048	C10H13N	18.39	189.9	NMP
C5	Amine	MFCD00006824	151.06333	C8H9NO2	18.88	189.5	NMP
D5	Amine	MFCD04115407	151.09971	C9H13NO	18.89	189.4	NMP
E5	Amine	MFCD00008392	153.07898	C8H11NO2	19.13	189.2	NMP
F5	Amine	MFCD00068002	153.1266	C8H15N3	19.14	189.2	NMP
G5	Amine	MFCD00022851	154.05647	C7H10N2S	19.26	189.1	NMP
H5	Amine	MFCD00007771	157.02944	C7H8ClNO	19.63	188.7	NMP
I5	Amine	MFCD00007774	160.9799	C6H5Cl2N	20.12	188.2	NMP
J5	Amine	MFCD00064396	161.04523	C7H6F3N	20.13	188.2	NMP
K5	Amine	MFCD00173960	162.04048	C6H5F3N2	20.26	188.1	NMP
L5	Amine	MFCD00005957	162.1157	C10H14N2	20.26	188.1	NMP
M5	Amine	MFCD00006216	163.11095	C9H13N3	20.39	187.9	NMP
N5	Amine	MFCD00038011	154.147	C9H18N2	19.27	189.1	NMP
O5	Amine	MFCD00003109	168.99215	C3H2F3N3S	21.12	187.2	NMP
P5	Amine	MFCD12828134	169.07031	C9H9F2N	21.13	187.2	NMP
A6	Amine	MFCD00025353	171.0354	C7H9NO2S	21.38	187	NMP

B6	Amine	MFCD07369717	175.06088	C8H8F3N	21.88	186.5	NMP
C6	Amine	MFCD00040737	176.13135	C11H16N2	22.02	186.3	NMP
D6	Amine	MFCD00159799	177.03607	C8H7N3S	22.13	186.2	NMP
E6	Amine	MFCD00128282	192.07212	C10H12N2S	24.01	184.3	NMP
F6	Amine	MFCD00047408	178.11061	C10H14N2O	22.26	186.1	NMP
G6	Amine	MFCD00005787	180.03573	C8H8N2OS	22.5	185.8	NMP
H6	Amine	MFCD00038831	180.08988	C9H12N2O2	22.51	185.8	NMP
I6	Amine	MFCD00005960	180.10628	C10H13FN2	22.51	185.8	NMP
J6	Amine	MFCD00053557	183.9862	C7H5ClN2S	23	185.3	NMP
K6	Amine	MFCD00462192	189.09021	C10H11N3O	23.64	184.7	NMP
L6	Amine	MFCD07772854	191.14225	C11H17N3	23.89	184.4	NMP
M6	Amine	MFCD00040733	192.12626	C11H16N2O	24.02	184.3	NMP
N6	Amine	MFCD00171470	160.0749	C8H8N4	20.01	188.3	NMP
O6	Amine	MFCD00005968	197.15281	C10H19N3O	24.64	183.7	NMP
P6	Amine	MFCD00114706	231.09833	C10H12F3N3	28.89	179.4	NMP
A7	Amide	MFCD00008023	59.03711	C2H5NO	7.38	201	DMF
B7	Amide	MFCD00008019	87.06841	C4H9NO	10.88	197.5	DMF
C7	Amide	MFCD00041894	87.06841	C4H9NO	10.88	197.5	DMF
D7	Amide	MFCD00008011	101.0841	C5H11NO	12.64	195.7	DMF
E7	Amide	MFCD04039924	115.0633	C5H9NO2	14.38	194	DMF
F7	Amide	MFCD00007968	121.0528	C7H7NO	15.13	193.2	DMF
G7	Amide	MFCD00006384	136.0637	C7H8N2O	17.01	191.3	DMF
H7	Amide	MFCD00006395	122.048	C6H6N2O	15.26	193.1	DMF
I7	Amide	MFCD00006432	122.048	C6H6N2O	15.26	193.1	DMF
J7	Amide	MFCD00010425	127.0092	C5H5NOS	15.88	192.5	DMF
K7	Amide	MFCD00001814	160.0637	C9H8N2O	20.01	188.3	DMF
L7	Amide	MFCD00009693	127.0997	C7H13NO	15.89	192.4	DMF
M7	Amide	MFCD00008002	135.0684	C8H9NO	16.88	191.5	DMF
N7	Amide	MFCD00007944	136.0637	C7H8N2O	17.01	191.3	DMF
O7	Amide	MFCD00007983	139.0433	C7H6FNO	17.38	191	DMF
P7	Amide	MFCD00007970	139.0433	C7H6FNO	17.38	191	DMF
A8	Amide	MFCD00016892	142.0201	C5H6N2OS	17.75	190.6	DMF
B8	Amide	MFCD00079246	142.0742	C6H10N2O2	17.76	190.6	DMF
C8	Amide	MFCD00008287	149.0841	C9H11NO	18.64	189.7	DMF
D8	Amide	MFCD00007995	151.0633	C8H9NO2	18.88	189.5	DMF
E8	Amide	MFCD00017140	151.0633	C8H9NO2	18.88	189.5	DMF
F8	Amide	MFCD00000315	153.059	C8H8FNO	19.13	189.2	DMF
G8	Amide	MFCD00014799	155.0138	C7H6ClNO	19.38	189	DMF
H8	Amide	MFCD00061138	157.0339	C7H5F2NO	19.63	188.7	DMF
I8	Amide	MFCD00192043	162.0793	C9H10N2O	20.26	188.1	DMF
J8	Amide	MFCD08234735	163.0633	C9H9NO2	20.38	188	DMF
K8	Amide	MFCD00007977	165.079	C9H11NO2	20.63	187.7	DMF
L8	Amide	MFCD00085105	165.079	C9H11NO2	20.63	187.7	DMF
M8	Amide	MFCD00834989	181.0739	C9H11NO3	22.63	185.7	DMF

N8	Amide	MFCD00040579	190.1106	C11H14N2O	23.76	184.6	DMF
O8	Amide	MFCD00007971	211.0057	C7H2F5NO	26.38	182	DMF
P8	Amide	MFCD03011716	236.042	C11H9FN2OS	29.51	178.8	DMF
A9	Sulfonamide	MFCD00007940	95.0041	CH5NO2S	11.88	196.5	DMF
B9	Sulfonamide	MFCD03265410	109.01975	C2H7NO2S	13.63	194.7	DMF
C9	Sulfonamide	MFCD08705286	121.01975	C3H7NO2S	15.13	193.2	DMF
D9	Sulfonamide	MFCD11501466	135.0354	C4H9NO2S	16.88	191.5	DMF
E9	Sulfonamide	MFCD02179404	137.05105	C4H11NO2S	17.13	191.2	DMF
F9	Sulfonamide	MFCD00007930	157.01975	C6H7NO2S	19.63	188.7	DMF
G9	Sulfonamide	MFCD08690712	158.015	C5H6N2O2S	19.75	188.6	DMF
H9	Sulfonamide	MFCD02091382	161.0259	C4H7N3O2S	20.13	188.2	DMF
I9	Sulfonamide	MFCD00185853	162.97617	C4H5NO2S2	20.37	188	DMF
J9	Sulfonamide	MFCD11043141	162.99148	C2H4F3NO2S	20.37	188	DMF
K9	Sulfonamide	MFCD09734097	167.02523	C4H9NO4S	20.88	187.5	DMF
L9	Sulfonamide	MFCD00011692	171.0354	C7H9NO2S	21.38	187	DMF
M9	Sulfonamide	MFCD00041893	171.0354	C7H9NO2S	21.38	187	DMF
N9	Sulfonamide	MFCD00661363	172.03065	C6H8N2O2S	21.5	186.8	DMF
O9	Sulfonamide	MFCD00178767	182.015	C7H6N2O2S	22.75	185.6	DMF
P9	Sulfonamide	MFCD03094593	182.015	C7H6N2O2S	22.75	185.6	DMF
A10	Sulfonamide	MFCD00025392	187.03031	C7H9NO3S	23.38	185	DMF
B10	Sulfonamide	MFCD09731823	189.02598	C7H8FNO2S	23.63	184.7	DMF
C10	Sulfonamide	MFCD02091379	193.00091	C6H5F2NO2S	24.13	184.2	DMF
D10	Sulfonamide	MFCD00021245	197.05105	C9H11NO2S	24.63	183.7	DMF
E10	Sulfonamide	MFCD03069322	199.03031	C8H9NO3S	24.88	183.5	DMF
F10	Sulfonamide	MFCD01318156	201.04596	C8H11NO3S	25.13	183.2	DMF
G10	Sulfonamide	MFCD01569462	210.99148	C6H4F3NO2S	26.37	182	DMF
H10	Sulfonamide	MFCD00035784	214.04121	C8H10N2O3S	26.76	181.6	DMF
I10	Sulfonamide	MFCD00003105	221.98813	C4H6N4O3S2	27.75	180.6	DMF
J10	Sulfonamide	MFCD00159251	225.00713	C7H6F3NO2S	28.13	180.2	DMF
K10	Sulfonamide	MFCD00177161	230.89823	C4H3Cl2NO2S2	28.86	179.5	DMF
L10	Sulfonamide	MFCD00798381	241.00205	C7H6F3NO3S	30.13	178.2	DMF
M10	Sulfonamide	MFCD01317542	245.03579	C9H11NO5S	30.63	177.7	DMF
N10	Sulfonamide	MFCD00035707	253.05211	C10H11N3O3S	31.63	176.7	DMF
O10	Sulfonamide	MFCD00079454	275.0286	C10H13NO4S2	34.38	174	DMF
P10	Sulfonamide	MFCD01935138	292.99452	C8H5F6NO2S	36.62	171.7	DMF
A11	Alkyne	MFCD00008570	102.04695	C8H6	12.76	195.6	NMP
B11	Alkyne	MFCD01936255	104.03745	C6H4N2	13	195.3	NMP
C11	Alkyne	MFCD06421422	106.0531	C6H6N2	13.26	195.1	NMP
D11	Alkyne	MFCD08703531	156.06875	C10H8N2	19.51	188.8	NMP
E11	Alkyne	MFCD04974089	106.0531	C6H6N2	13.26	195.1	NMP
F11	Alkyne	MFCD00001513	108.0939	C8H12	13.51	194.8	NMP
G11	Alkyne	MFCD00039881	111.1048	C7H13N	13.89	194.4	NMP
H11	Alkyne	MFCD03095259	121.03278	C7H4FN	15.13	193.2	NMP
I11	Alkyne	MFCD05664205	132.05751	C9H8O	16.51	191.8	NMP

J11	Alkyne	MFCD14631470	133.01975	C4H7NO2S	16.63	191.7	NMP
K11	Alkyne	MFCD07369939	136.1252	C10H16	17.02	191.3	NMP
L11	Alkyne	MFCD09910338	138.1157	C8H14N2	17.26	191.1	NMP
M11	Alkyne	MFCD00049120	138.14085	C10H18	17.27	191.1	NMP
N11	Alkyne	MFCD11109424	142.07825	C11H10	17.76	190.6	NMP
O11	Alkyne	MFCD00004454	146.07316	C10H10O	18.26	190.1	NMP
P11	Alkyne	MFCD19643101	147.0354	C5H9NO2S	18.38	190	NMP
A12	Alkyne	MFCD08703530	153.99856	C8H4ClF	19.25	189.1	NMP
B12	Alkyne	MFCD08435845	154.0531	C10H6N2	19.26	189.1	NMP
C12	Alkyne	MFCD00190197	158.10955	C12H14	19.76	188.6	NMP
D12	Alkyne	MFCD00831583	159.06841	C10H9NO	19.88	188.5	NMP
E12	Alkyne	MFCD03839985	162.06808	C10H10O2	20.26	188.1	NMP
F12	Alkyne	MFCD08276766	164.06374	C10H9FO	20.51	187.8	NMP
G12	Alkyne	MFCD07369730	164.06374	C10H9FO	20.51	187.8	NMP
H12	Alkyne	MFCD08435847	169.05276	C11H7NO	21.13	187.2	NMP
I12	Alkyne	MFCD00174270	185.08406	C12H11NO	23.14	185.2	NMP
J12	Alkyne	MFCD03839993	185.12045	C13H15N	23.14	185.2	NMP
K12	Alkyne	MFCD03094333	186.02925	C9H5F3O	23.25	185.1	NMP
L12	Alkyne	MFCD03012027	195.0354	C9H9NO2S	24.38	184	NMP
M12	Alkyne	MFCD01861850	238.02172	C10H4F6	29.75	178.6	NMP
N12	Alkyne	MFCD00055346	255.02177	C12H11Cl2NO	31.88	176.5	NMP
O12	Alkyne	MFCD00176067	255.04509	C15H10ClNO	31.88	176.5	NMP
P12	Alkyne	MFCD13189722	171.02958	C8H4F3N	21.38	187	NMP
A13	Thiol	MFCD00005188	100.00952	C3H4N2S	12.5	195.8	DMF
B13	Thiol	MFCD00005229	101.00477	C2H3N3S	12.63	195.7	DMF
C13	Thiol	MFCD00022449	116.97069	C3H3NS2	14.62	193.7	DMF
D13	Thiol	MFCD00037831	119.04048	C4H9NOS	14.88	193.5	DMF
E13	Thiol	MFCD00055027	126.02517	C5H6N2S	15.75	192.6	DMF
F13	Thiol	MFCD03789243	128.04082	C5H8N2S	16.01	192.3	DMF
G13	Thiol	MFCD00004896	134.04015	C5H10O2S	16.76	191.6	DMF
H13	Thiol	MFCD00004849	140.02959	C7H8OS	17.5	190.8	DMF
I13	Thiol	MFCD00042435	192.02206	C8H7F3S	24	184.3	DMF
J13	Thiol	MFCD00004903	152.06597	C9H12S	19.01	189.3	DMF
K13	Thiol	MFCD01658123	153.06122	C8H11NS	19.13	189.2	DMF
L13	Thiol	MFCD03789242	156.07212	C7H12N2S	19.51	188.8	DMF
M13	Thiol	MFCD00010617	164.04082	C8H8N2S	20.51	187.8	DMF
N13	Thiol	MFCD09259279	194.99901	C8H5NO3S	24.37	184	DMF
O13	Thiol	MFCD00004848	167.04048	C8H9NOS	20.88	187.5	DMF
P13	Thiol	MFCD00014451	167.04048	C8H9NOS	20.88	187.5	DMF
A14	Thiol	MFCD11205085	168.99215	C3H2F3N3S	21.12	187.2	DMF
B14	Thiol	MFCD00052738	170.04015	C8H10O2S	21.26	187.1	DMF
C14	Thiol	MFCD06654964	173.06228	C6H11N3OS	21.63	186.7	DMF
D14	Thiol	MFCD00237476	177.04596	C6H11NO3S	22.13	186.2	DMF
E14	Thiol	MFCD00004831	177.94108	C6H4Cl2S	22.24	186.1	DMF

F14	Thiol	MFCD00030467	178.02008	C8H6N2OS	22.25	186.1	DMF
G14	Thiol	MFCD00207933	178.03132	C7H6N4S	22.25	186.1	DMF
H14	Thiol	MFCD00115113	179.9969	C5H3F3N2S	22.5	185.8	DMF
I14	Thiol	MFCD01750430	188.99182	C6H7NO2S2	23.62	184.7	DMF
J14	Thiol	MFCD00467591	192.0245	C10H8O2S	24	184.3	DMF
K14	Thiol	MFCD01067387	192.03573	C9H8N2OS	24	184.3	DMF
L14	Thiol	MFCD00052612	192.07212	C10H12N2S	24.01	184.3	DMF
M14	Thiol	MFCD01326487	194.05138	C9H10N2OS	24.26	184.1	DMF
N14	Thiol	MFCD00005783	200.94737	C7H4ClNS2	25.12	183.2	DMF
O14	Thiol	MFCD00004885	202.17552	C12H26S	25.27	183.1	DMF
P14	Thiol	MFCD00142794	203.00747	C7H9NO2S2	25.38	183	DMF
A15	Thiol	MFCD00022081	204.1184	C10H20O2S	25.51	182.8	DMF
B15	Thiol	MFCD01925225	204.99797	C5H7N3O2S2	25.62	182.7	DMF
C15	Thiol	MFCD00023091	207.0354	C10H9NO2S	25.88	182.5	DMF
D15	Thiol	MFCD00052327	208.01697	C8H7F3OS	26	182.3	DMF
E15	Thiol	MFCD02683322	210.07145	C11H14O2S	26.26	182.1	DMF
F15	Thiol	MFCD07314189	214.08883	C8H14N4OS	26.76	181.6	DMF
G15	Thiol	MFCD00467504	216.01689	C8H6F2N2OS	27	181.3	DMF
H15	Thiol	MFCD01313795	218.01255	C8H5F3N2S	27.25	181.1	DMF
I15	Thiol	MFCD00085109	218.05138	C11H10N2OS	27.26	181.1	DMF
J15	Thiol	MFCD01116594	233.09867	C12H15N3S	29.14	179.2	DMF
K15	Thiol	MFCD00603728	235.05278	C9H9N5OS	29.38	179	DMF
L15	Thiol	MFCD00105100	247.11432	C13H17N3S	30.89	177.4	DMF
M15	Thiol	MFCD00022414	253.05613	C15H11NOS	31.63	176.7	DMF
N15	Thiol	MFCD02180672	258.04385	C11H9F3N2S	32.26	176.1	DMF
O15	Thiol	MFCD00006751	161.02992	C9H7NS	20.13	188.2	DMF
P15	Thiol	MFCD06201755	154.00885	C7H6O2S	19.25	189.1	DMF
A16	Alcohol	MFCD00064327	88.05243	C4H8O2	11.01	197.3	DMF
B16	Alcohol	MFCD00006378	95.03711	C5H5NO	11.88	196.5	DMF
C16	Alcohol	MFCD00001366	100.08882	C6H12O	12.51	195.8	DMF
D16	Alcohol	MFCD00005372	102.06808	C5H10O2	12.76	195.6	DMF
E16	Alcohol	MFCD00036560	106.04524	C4H10OS	13.26	195.1	DMF
F16	Alcohol	MFCD00006339	109.05276	C6H7NO	13.63	194.7	DMF
G16	Alcohol	MFCD00082538	109.05276	C6H7NO	13.63	194.7	DMF
H16	Alcohol	MFCD00002254	112.03244	C6H5FO	14	194.3	DMF
I16	Alcohol	MFCD00077775	112.05243	C6H8O2	14.01	194.3	DMF
J16	Alcohol	MFCD00964673	112.06366	C5H8N2O	14.01	194.3	DMF
K16	Alcohol	MFCD00005454	114.01394	C5H6OS	14.25	194.1	DMF
L16	Alcohol	MFCD00077792	115.06333	C5H9NO2	14.38	194	DMF
M16	Alcohol	MFCD00006495	115.09971	C6H13NO	14.39	193.9	DMF
N16	Alcohol	MFCD00011727	115.09971	C6H13NO	14.39	193.9	DMF
O16	Alcohol	MFCD00002145	119.03711	C7H5NO	14.88	193.5	DMF
P16	Alcohol	MFCD00002252	119.03711	C7H5NO	14.88	193.5	DMF
A17	Alcohol	MFCD00002973	120.06089	C5H12OS	15.01	193.3	DMF

B17	Alcohol	MFCD00002237	122.07316	C8H10O	15.26	193.1	DMF
C17	Alcohol	MFCD00004622	122.07316	C8H10O	15.26	193.1	DMF
D17	Alcohol	MFCD00077844	176.0449	C8H7F3O	22.01	186.3	DMF
E17	Alcohol	MFCD00002393	122.07316	C8H10O	15.26	193.1	DMF
F17	Alcohol	MFCD04972322	123.06841	C7H9NO	15.38	193	DMF
G17	Alcohol	MFCD00023520	123.06841	C7H9NO	15.38	193	DMF
H17	Alcohol	MFCD00002185	124.05243	C7H8O2	15.51	192.8	DMF
I17	Alcohol	MFCD00002332	124.05243	C7H8O2	15.51	192.8	DMF
J17	Alcohol	MFCD00042296	126.04809	C7H7FO	15.76	192.6	DMF
K17	Alcohol	MFCD00072599	126.06808	C7H10O2	15.76	192.6	DMF
L17	Alcohol	MFCD00464226	127.06333	C6H9NO2	15.88	192.5	DMF
M17	Alcohol	MFCD00151326	127.09971	C7H13NO	15.89	192.4	DMF
N17	Alcohol	MFCD00001447	128.12012	C8H16O	16.02	192.3	DMF
O17	Alcohol	MFCD00006379	128.99814	C5H4ClNO	16.12	192.2	DMF
P17	Alcohol	MFCD00006235	128.99814	C5H4ClNO	16.12	192.2	DMF
A18	Alcohol	MFCD03427228	129.07898	C6H11NO2	16.13	192.2	DMF
B18	Alcohol	MFCD00006494	129.11536	C7H15NO	16.14	192.2	DMF
C18	Alcohol	MFCD00009715	130.02302	C6H4F2O	16.25	192.1	DMF
D18	Alcohol	MFCD00004545	132.07864	C6H12O3	16.51	191.8	DMF
E18	Alcohol	MFCD00003800	134.07316	C9H10O	16.76	191.6	DMF
F18	Alcohol	MFCD00004648	136.08882	C9H12O	17.01	191.3	DMF
G18	Alcohol	MFCD00016860	136.08882	C9H12O	17.01	191.3	DMF
H18	Alcohol	MFCD00002301	136.08882	C9H12O	17.01	191.3	DMF
I18	Alcohol	MFCD00192177	137.02769	C7H4FNO	17.13	191.2	DMF
J18	Alcohol	MFCD00005827	138.03169	C7H6O3	17.25	191.1	DMF
K18	Alcohol	MFCD00004515	140.06374	C8H9FO	17.51	190.8	DMF
L18	Alcohol	MFCD03086098	143.04048	C6H9NOS	17.88	190.5	DMF
M18	Alcohol	MFCD00005339	143.04048	C6H9NOS	17.88	190.5	DMF
N18	Alcohol	MFCD00012132	177.11536	C11H15NO	22.14	186.2	DMF
O18	Alcohol	MFCD00544189	147.06841	C9H9NO	18.38	190	DMF
P18	Alcohol	MFCD06797471	148.06366	C8H8N2O	18.51	189.8	DMF
A19	Alcohol	MFCD00001738	148.08882	C10H12O	18.51	189.8	DMF
B19	Alcohol	MFCD02169755	150.06808	C9H10O2	18.76	189.6	DMF
C19	Alcohol	MFCD00006347	152.09496	C8H12N2O	19.01	189.3	DMF
D19	Alcohol	MFCD00219003	152.99814	C7H4ClNO	19.12	189.2	DMF
E19	Alcohol	MFCD00022504	154.04524	C8H10OS	19.26	189.1	DMF
F19	Alcohol	MFCD00001473	156.15142	C10H20O	19.52	188.8	DMF
G19	Alcohol	MFCD00070774	158.01346	C7H7ClO2	19.75	188.6	DMF
H19	Alcohol	MFCD00274321	158.05432	C8H8F2O	19.76	188.6	DMF
I19	Alcohol	MFCD00002299	162.02925	C7H5F3O	20.25	188.1	DMF
J19	Alcohol	MFCD00139833	166.0354	C5H5F3N2O	20.75	187.6	DMF
K19	Alcohol	MFCD00085094	166.0354	C5H5F3N2O	20.75	187.6	DMF
L19	Alcohol	MFCD08276849	169.07389	C8H11NO3	21.13	187.2	DMF
M19	Alcohol	MFCD06199341	205.07389	C11H11NO3	25.63	182.7	DMF

N19	Alcohol	MFCD00044708	256.01702	C11H10Cl2N2O	32	176.3	DMF
O19	Alcohol	MFCD00038714	152.08373	C9H12O2	19.01	189.3	DMF
P19	Alcohol	MFCD00006503	191.13101	C12H17NO	23.89	184.4	DMF
A20	Suzuki	MFCD01319007	112.03317	C4H5BO3	14	194.3	NMP
B20	Suzuki	MFCD07368251	112.04441	C3H5BN2O2	14.01	194.3	NMP
C20	Suzuki	MFCD02020768	112.04441	C3H5BN2O2	14.01	194.3	NMP
D20	Suzuki	MFCD00002103	122.05391	C6H7BO2	15.26	193.1	NMP
E20	Suzuki	MFCD01319051	205.12741	C11H16BNO2	25.64	182.7	NMP
F20	Suzuki	MFCD00674177	123.04916	C5H6BNO2	15.38	193	NMP
G20	Suzuki	MFCD03002366	124.04441	C4H5BN2O2	15.51	192.8	NMP
H20	Suzuki	MFCD00040198	136.06956	C7H9BO2	17.01	191.3	NMP
I20	Suzuki	MFCD02677945	141.05972	C5H8BNO3	17.63	190.7	NMP
J20	Suzuki	MFCD04039882	142.02598	C5H7BO2S	17.75	190.6	NMP
K20	Suzuki	MFCD01318968	147.04916	C7H6BNO2	18.38	190	NMP
L20	Suzuki	MFCD01318967	147.04916	C7H6BNO2	18.38	190	NMP
M20	Suzuki	MFCD06657825	230.12266	C12H15BN2O2	28.77	179.6	NMP
N20	Suzuki	MFCD00239441	148.06956	C8H9BO2	18.51	189.8	NMP
O20	Suzuki	MFCD01009693	150.08521	C8H11BO2	18.76	189.6	NMP
P20	Suzuki	MFCD02093075	150.08521	C8H11BO2	18.76	189.6	NMP
A21	Suzuki	MFCD00859377	150.08521	C8H11BO2	18.76	189.6	NMP
B21	Suzuki	MFCD00161359	152.06447	C7H9BO3	19.01	189.3	NMP
C21	Suzuki	MFCD06798083	194.11142	C10H15BO3	24.26	184.1	NMP
D21	Suzuki	MFCD03428512	154.06014	C7H8BFO2	19.26	189.1	NMP
E21	Suzuki	MFCD01863527	154.06014	C7H8BFO2	19.26	189.1	NMP
F21	Suzuki	MFCD00039137	156.01494	C6H6BClO2	19.5	188.8	NMP
G21	Suzuki	MFCD01318138	158.03507	C6H5BF2O2	19.75	188.6	NMP
H21	Suzuki	MFCD03789263	243.14306	C14H18BNO2	30.39	177.9	NMP
I21	Suzuki	MFCD01321263	164.06447	C8H9BO3	20.51	187.8	NMP
J21	Suzuki	MFCD01074678	164.06447	C8H9BO3	20.51	187.8	NMP
K21	Suzuki	MFCD02681979	164.06447	C8H9BO3	20.51	187.8	NMP
L21	Suzuki	MFCD03427049	164.10086	C9H13BO2	20.51	187.8	NMP
M21	Suzuki	MFCD00859261	164.10086	C9H13BO2	20.51	187.8	NMP
N21	Suzuki	MFCD03411940	165.05972	C7H8BNO3	20.63	187.7	NMP
O21	Suzuki	MFCD01009695	166.04374	C7H7BO4	20.76	187.6	NMP
P21	Suzuki	MFCD02179465	166.08012	C8H11BO3	20.76	187.6	NMP
A22	Suzuki	MFCD02179464	166.08012	C8H11BO3	20.76	187.6	NMP
B22	Suzuki	MFCD04039010	170.03059	C7H8BClO2	21.25	187.1	NMP
C22	Suzuki	MFCD02094728	170.05505	C7H8BFO3	21.26	187.1	NMP
D22	Suzuki	MFCD02183527	173.06481	C9H8BNO2	21.63	186.7	NMP
E22	Suzuki	MFCD00236051	172.06956	C10H9BO2	21.51	186.8	NMP
F22	Suzuki	MFCD05664405	260.10423	C14H17BO2S	32.51	175.8	NMP
G22	Suzuki	MFCD01114669	178.02598	C8H7BO2S	22.25	186.1	NMP
H22	Suzuki	MFCD02093722	261.15362	C14H20BNO3	32.64	175.7	NMP
I22	Suzuki	MFCD04971190	261.19001	C15H24BNO2	32.65	175.7	NMP

J22	Suzuki	MFCD01009696	180.05939	C8H9BO4	22.51	185.8	NMP
K22	Suzuki	MFCD08690229	262.14887	C13H19BN2O3	32.77	175.6	NMP
L22	Suzuki	MFCD03427050	180.09577	C9H13BO3	22.51	185.8	NMP
M22	Suzuki	MFCD00196832	180.09577	C9H13BO3	22.51	185.8	NMP
N22	Suzuki	MFCD01074590	182.07504	C8H11BO4	22.76	185.6	NMP
O22	Suzuki	MFCD01318985	184.06554	C6H9BN2O4	23.01	185.3	NMP
P22	Suzuki	MFCD06798077	184.0707	C8H10BFO3	23.01	185.3	NMP
A23	Suzuki	MFCD04039888	186.0255	C7H8BClO3	23.25	185.1	NMP
B23	Suzuki	MFCD00151855	190.04129	C7H6BF3O2	23.76	184.6	NMP
C23	Suzuki	MFCD00151854	190.04129	C7H6BF3O2	23.76	184.6	NMP
D23	Suzuki	MFCD02179463	194.11142	C10H15BO3	24.26	184.1	NMP
E23	Suzuki	MFCD06411285	198.08635	C9H12BFO3	24.76	183.6	NMP
F23	Suzuki	MFCD01630820	200.03146	C7H9BO4S	25	183.3	NMP
G23	Suzuki	MFCD05865163	198.08635	C9H12BFO3	24.76	183.6	NMP
H23	Suzuki	MFCD01074648	206.03621	C7H6BF3O3	25.75	182.6	NMP
I23	Suzuki	MFCD07784336	208.03187	C7H5BF4O2	26	182.3	NMP
J23	Suzuki	MFCD00093312	214.08012	C12H11BO3	26.76	181.6	NMP
K23	Suzuki	MFCD02093926	178.11651	C10H15BO2	22.26	186.1	NMP
L23	Suzuki	MFCD01075707	216.07579	C12H10BFO2	27.01	181.3	NMP
M23	Suzuki	MFCD07367523	244.13831	C13H17BN2O2	30.52	177.8	NMP
N23	Suzuki	MFCD03839356	173.06481	C9H8BNO2	21.63	186.7	NMP
O23	Suzuki	MFCD04115667	184.0707	C8H10BFO3	23.01	185.3	NMP
P23	Suzuki	MFCD04974065	214.0568	C9H12BClO3	26.76	181.6	NMP
A24	Suzuki	MFCD03095047	154.06014	C7H8BFO2	19.26	189.1	NMP
B24	Suzuki	MFCD12545934	245.13356	C12H16BN3O2	30.64	177.7	NMP
C24	Suzuki	MFCD04038760	202.09136	C10H11BN2O2	25.26	183.1	NMP
D24	Suzuki	MFCD05663852	222.15396	C11H19BN2O2	27.77	180.6	NMP
E24	Suzuki	MFCD03453668	219.14306	C12H18BNO2	27.39	180.9	NMP
F24	Suzuki	MFCD01074603	138.04882	C6H7BO3	17.26	191.1	NMP
G24	Suzuki	MFCD02093724	248.15838	C14H21BO3	31.02	177.3	NMP
H24	Suzuki	MFCD04039879	178.08012	C9H11BO3	22.26	186.1	NMP
I24	Suzuki	MFCD00963621	148.06956	C8H9BO2	18.51	189.8	NMP
J24	Suzuki	MFCD01074578	148.06956	C8H9BO2	18.51	189.8	NMP
K24	Suzuki	MFCD03427005	216.05694	C9H8BF3O2	27.01	181.3	NMP
L24	Suzuki	MFCD02093725	166.06014	C8H8BFO2	20.76	187.6	NMP
M24	Suzuki	MFCD01074615	154.11651	C8H15BO2	19.26	189.1	NMP
N24	Suzuki	MFCD06202527	162.08521	C9H11BO2	20.26	188.1	NMP
O24	Suzuki	MFCD03092930	182.05728	C8H11BO2S	22.76	185.6	NMP
P24	Suzuki	MFCD04974115	170.05505	C7H8BFO3	21.26	187.1	NMP

8.2. Nanomole-Scale Library Synthesis – Variable Reaction Conditions

Conditions identified from reaction screening and optimization:

Nucleophile Type	Catalyst 1	Catalyst 2	Base 1	Base 2	Solvent	Number of Conditions
Amine	*t*-BuXPhos G3	*t*-BuBrettPhos G3	P2-Et	MTBD	NMP	4
Amide	*t*-BuXPhos G3	*t*-BuBrettPhos G3	MTBD	BTMG	DMF	4
Sulfonamide	*t*-BuBrettPhos G3	RockPhos G3	P2-Et	MTBD	DMF	4
Alkyne / Sonogashira	RuPhos G3	*t*-Bu3P	BTTP	MTBD	NMP	4
Thiol	Blank / No Cat.	AdBrettPhos	P2-Et	BTMG	DMF	4
Alcohol	Blank / No Cat.	RockPhos G3	P2-Et	MTBD	DMF	4
Suzuki	RuPhos G3	SPhos G2	aq. BTMG	aq. K_3PO_4	NMP	4

Coupling Library Prep: Stock solutions of thiazole bromide core **1** (0.3 M in NMP and DMF), the Buchwald palladium precatalysts indicated above (0.06 M in NMP and/or DMF), and bases indicated above (P_2-Et, BTTP, and MTBD 0.8 M in NMP, P_2-Et, MTBD, BTMG 0.8 M in DMF, K_3PO_4 and BTMG, 0.8 M in H_2O) were prepared in a glove box under an N_2 atmosphere. A source plate was constructed using the reagent stock solutions, according to Figure 32 below, by pipetting 20-25 µL of the correct component stock solution into the 384-well plate wells.

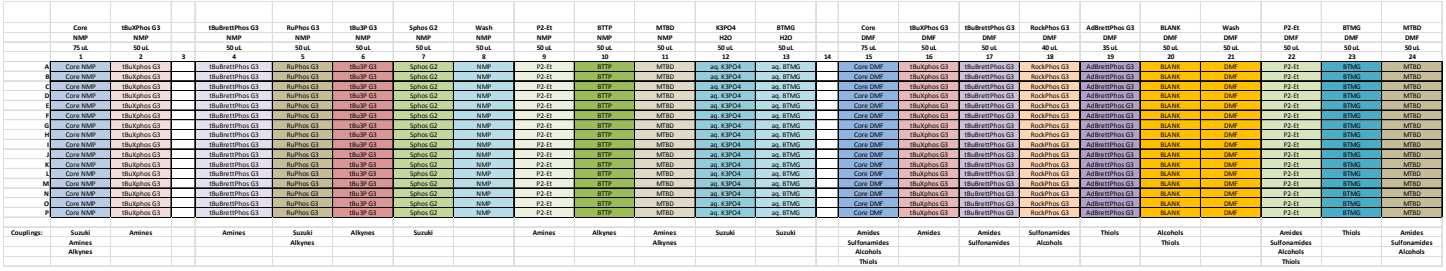


Figure 32. Reagent Source Map

A separate reagent and building block source plate was constructed for aliphatic and aryl amine nucleophiles due to the volatility of some of the selected building blocks. This was done to minimize Mosquito dispense time and to more quickly seal the reaction plate. The plate map for the amine nucleophile rerun experiment is shown below in Figure 33.

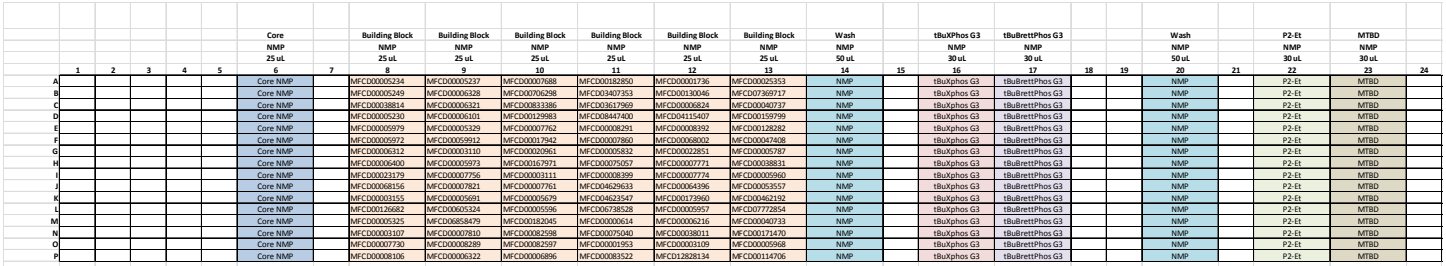


Figure 33. Amine Building Block Backup Plate

The TTP Labtech Mosquito® was used to assemble the reaction mixtures using the multi-aspiration feature with dispense mixing.

1. 300 nL was drawn up from each well of the nucleophile building block source plate and dispensed into the 1,536-well reaction plate. This was repeated four times so each of the 384 building blocks was present in four well wells.

2. 400 nL drawn from the desired core column (NMP: column 1, DMF: column 15)
3. 200 nL was drawn up from the desired catalyst column (see plate maps)
4. 10 nL tip wash (NMP: column 8, DMF: column 21)
5. 300 nL was drawn up from the desired base column (see plate maps).
6. Dispense mixing (3×800 nL) into the 1,536-well reaction plate to ensure all reagents were adequately combined.
7. This process was repeated to cover all relevant conditions for each coupling class. Four reaction conditions were tested with each coupling class resulting in 1,536 total reactions at 1.2 µL (120 nmol) each.
8. The 1,536-plate was sealed and briefly centrifuged before sitting at ambient temperature for 24 hours.
9. This process was repeated for the separate amine nucleophile source plate however using the reagent columns indicated in Figure 33.

The next morning, the reactions were quenched by addition of 3×1.2 µL 0.5 M AcOH in DMSO to each reaction well. The reactions were further diluted (to approximately 10 mM assuming complete conversion to product) with DMSO and transferred to 384-well LDV diamond plates (four total) for affinity-based ranking. 1 µL of the quenched and diluted crude reaction was drawn up for analysis by LC-MS (1 µL crude ~10 mM reaction into 60 µL DMSO followed by shaking). Reaction results are shown below as a heat map. Colors represent a relative percent conversion gradient (blue-green-yellow = 0% to 50% to 100% conversion), where values were calculated using the UV peak area of product and the UV peak area of the limiting reagent aryl halide core. The grid is separated based on nucleophile type.

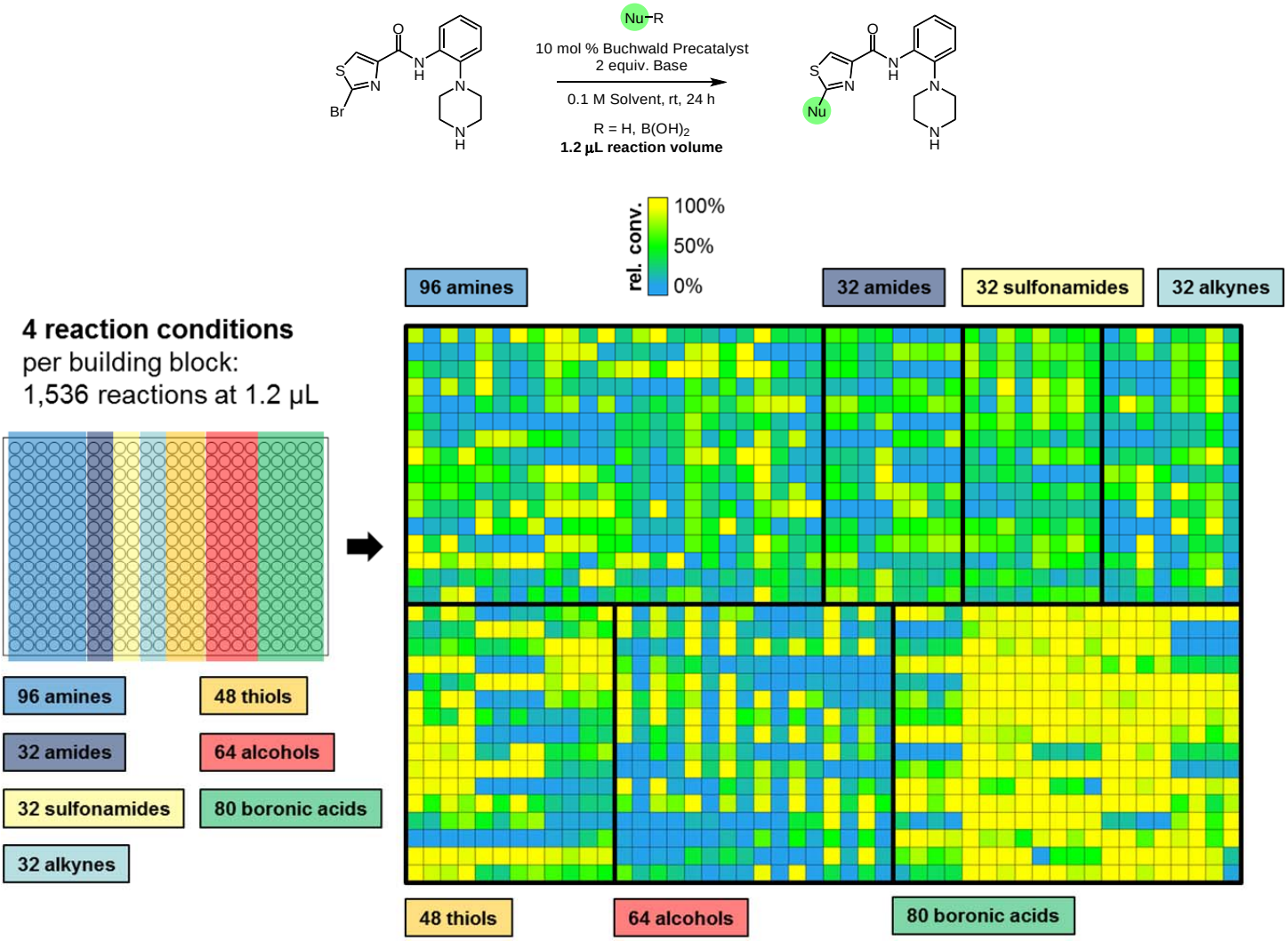


Figure 34. Nanomole-Scale 384-Member Library Synthesis

345/384 products produced in sufficient quantity to deliver to ASMS affinity-based rank ordering method. 39/384 products were not produced or produced in yields too low to carry on. See Figure 35 for 345 highlighted reactions that were delivered to ASMS rank ordering method. See supplementary Excel data tables for reaction details.

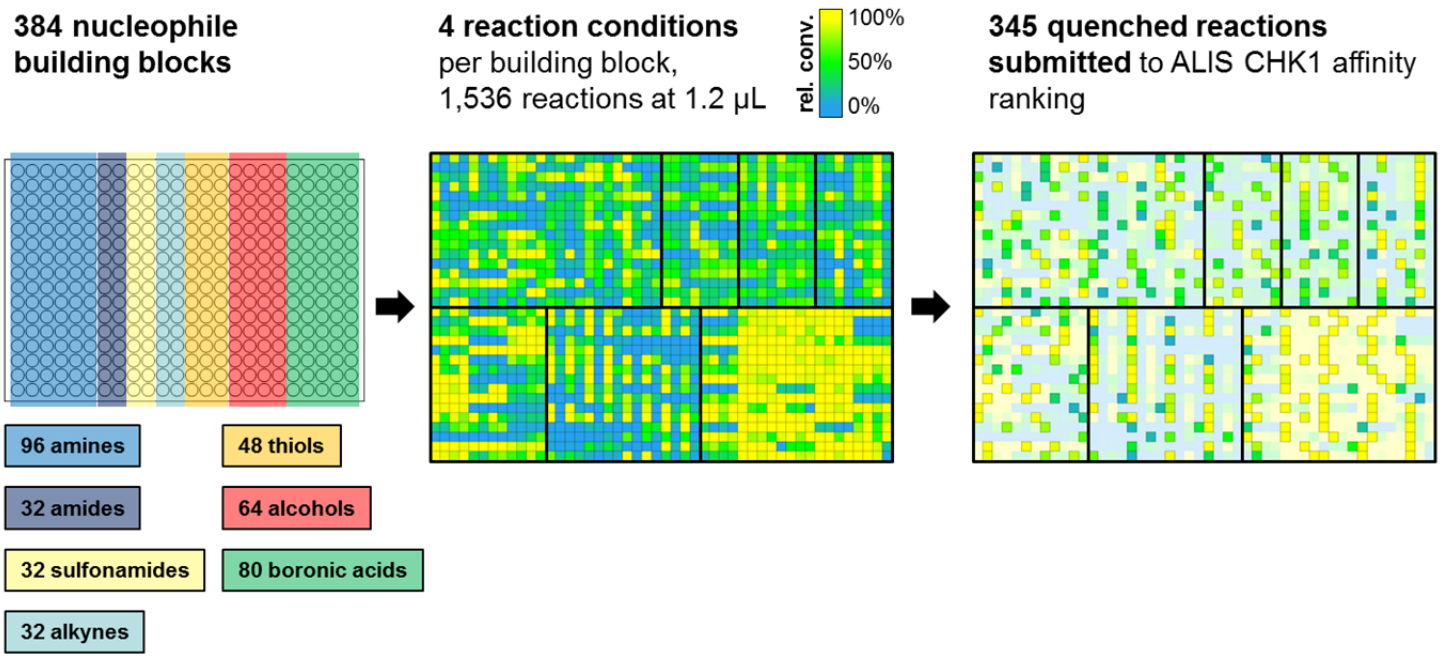


Figure 35. Reaction Selection for ASMS Affinity-Based Rank Ordering

Representative crude reaction chromatograms for the coupling products highlighted in this manuscript are shown below (blue peaks represent the desired coupling products and the teal peak represents unconsumed aryl bromide core).

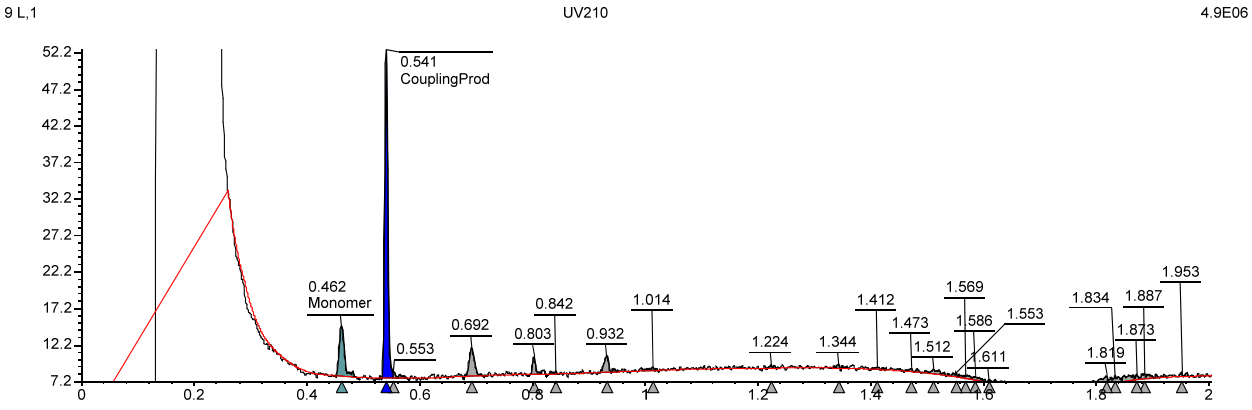


Figure 36. Chromatogram of Crude Nanomole-Scale Reaction Producing 35. Conditions: No catalyst / P_2-Et / DMF

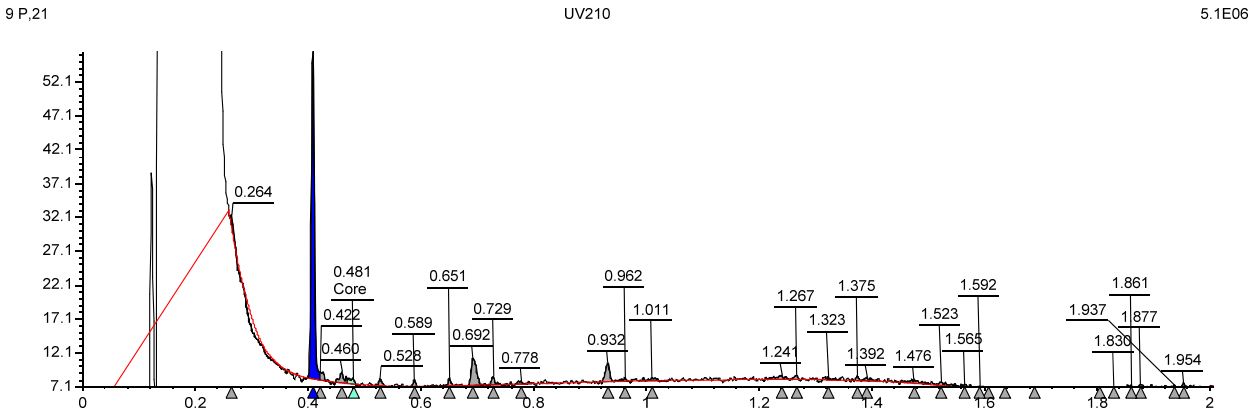


Figure 37. Chromatogram of Crude Nanomole-Scale Reaction Producing 36. Conditions: No catalyst / P_2-Et / DMF

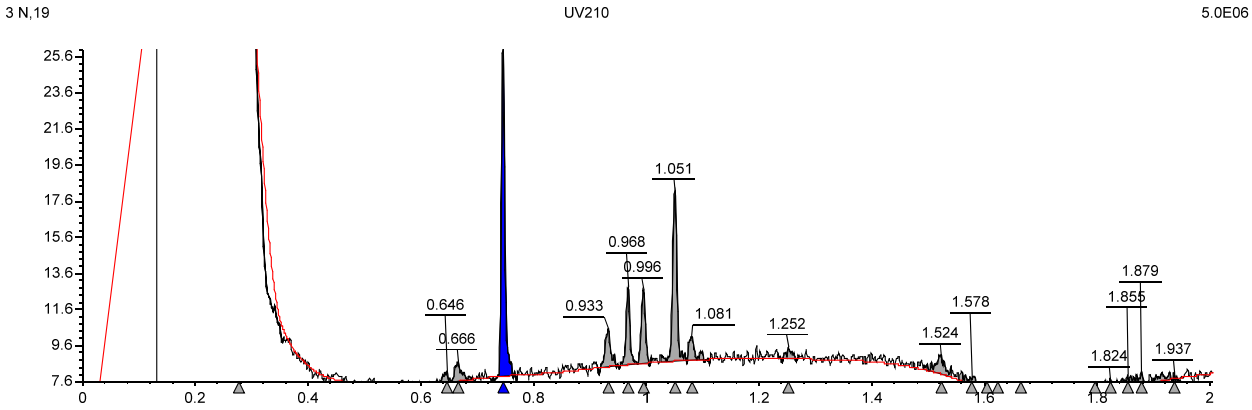


Figure 38. Chromatogram of Crude Nanomole-Scale Reaction Producing 37. Conditions: RuPhos G3 / BTTP / NMP

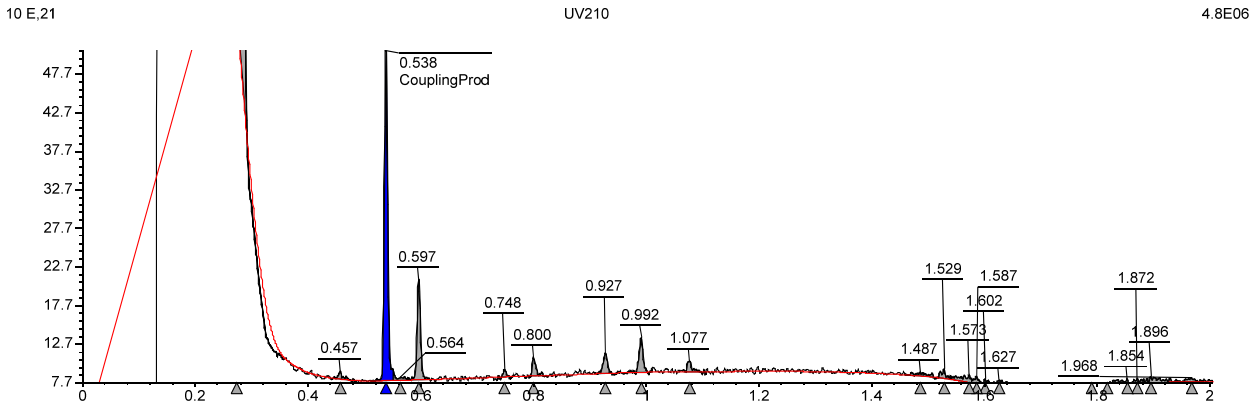


Figure 39. Chromatogram of Crude Nanomole-Scale Reaction Producing 38. Conditions: RuPhos G3 / aq. K_3PO_4 / NMP

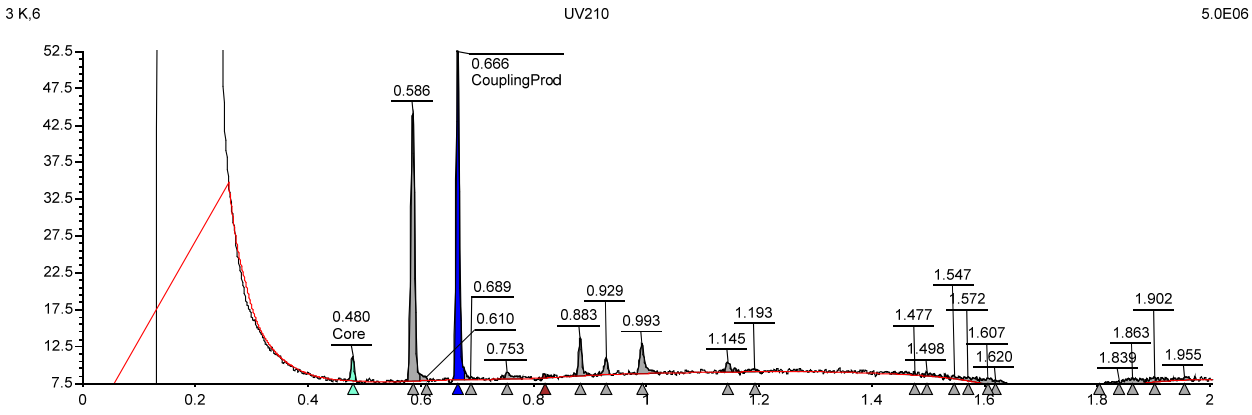


Figure 40. Chromatogram of Crude Nanomole-Scale Reaction Producing 39. Conditions: *t*-BuXPhos G3 / MTBD / DMF

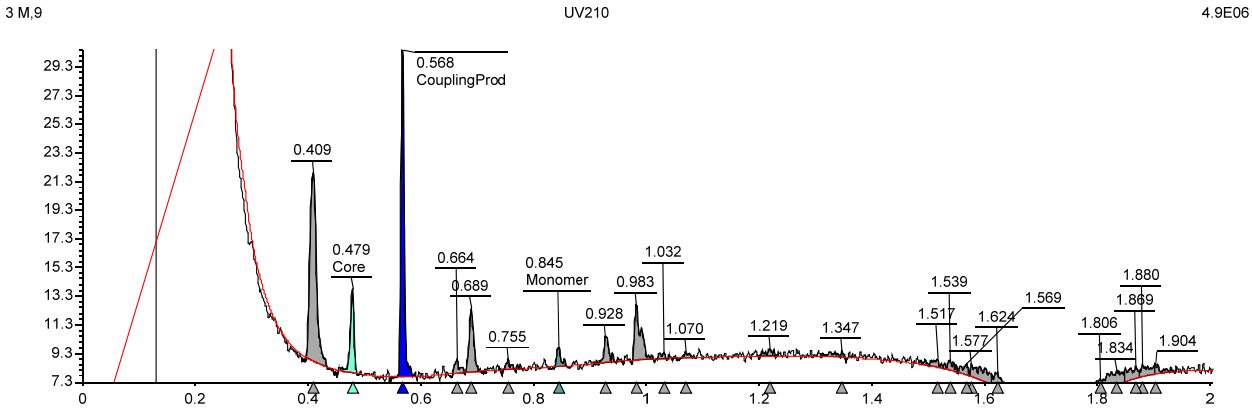


Figure 41. Chromatogram of Crude Nanomole-Scale Reaction Producing 40. Conditions: *t*-BuBrettPhos G3 / P_2-Et / DMF

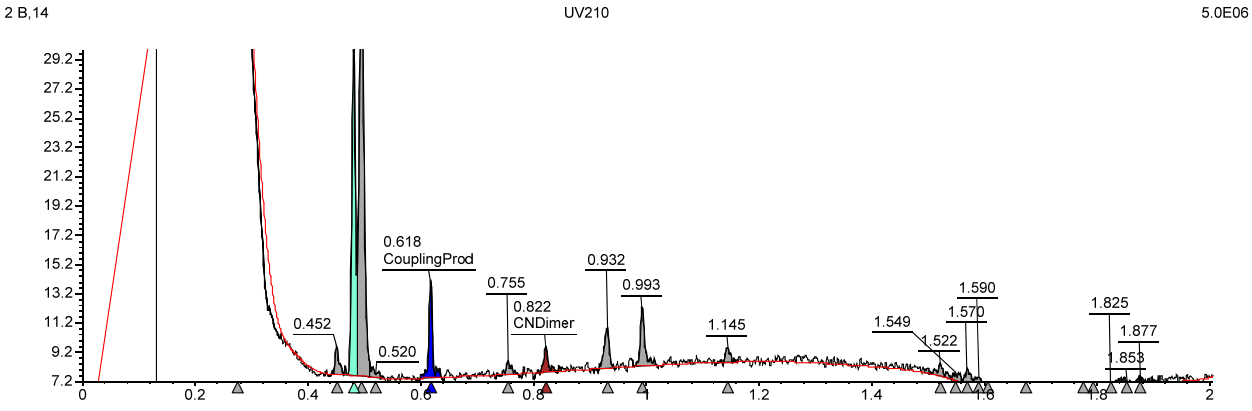


Figure 42. Chromatogram of Crude Nanomole-Scale Reaction Producing 41. Conditions: *t*-BuXPhos G3 / MTBD / NMP

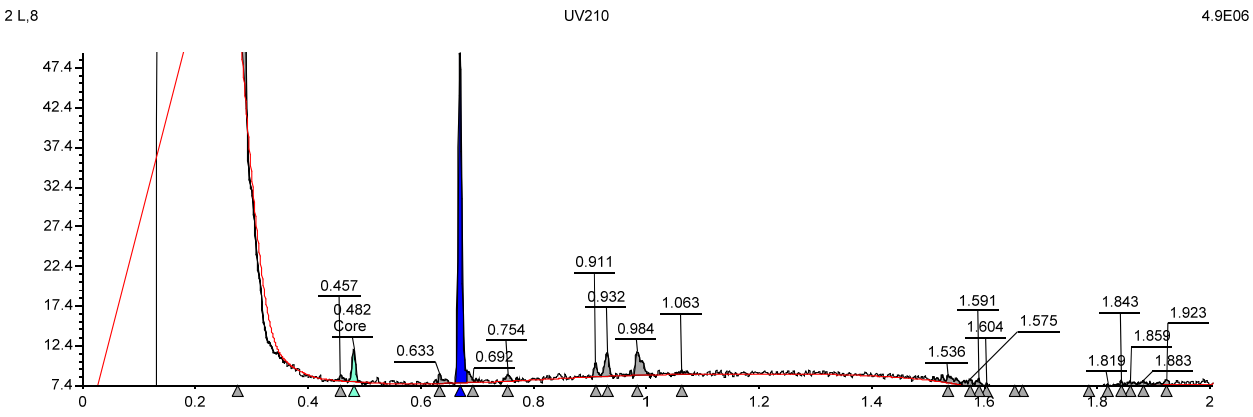


Figure 43. Chromatogram of Crude Nanomole-Scale Reaction Producing 43. Conditions: *t*-BuBrettPhos G3 / MTBD / NMP

8.3. Nanomole-Scale Library Synthesis – Single Set of Reaction Conditions: *t*-XPhos G3 / P_2-Et / NMP

10 mol % *t*-BuXPhos G3, 1.5 equiv. nucleophile, and 2 equiv. P_2-Et were identified as general, homogenous, nano-scale compatible reaction conditions in related systems.[8,15] These conditions were tested against the 384-member nucleophile library described above for comparison to the screening-based approach from Section 8.2. A source plate was prepared using a 384-well polypropylene plate, dispensing all reagent stock solutions inside a glovebox under N_2. A 0.4 M stock solution of thiazole bromide core **1** was prepared inside a glove box using NMP and dispensed into column 1 (25 µL/well). Next, a 0.4 M stock solution of thiazole bromide core **1** containing 4 equiv. H_2O (for Suzuki cross-coupling reactions) was prepared using NMP and dispensed into column 3 inside the glove box (25 µL/well). *t*BuXPhos G3 precatalyst was weighed out, moved to the glove box, dissolved in NMP (to 0.04 M) and dispensed into column 5 (25 µL/well). Finally, a 0.8 M stock solution of P_2-Et in NMP was prepared and dispensed into source plate column 7.

The TTP Labtech Mosquito® was used to assemble the reaction mixtures using the multi-aspiration feature with dispense mixing.

1. 300 nL was drawn up from each well of the nucleophile building block source plate and dispensed into the 1,536-well reaction plate.
2. 300 nL drawn from the desired core column (column 1: no water, column 3: with water, for Suzuki)
3. 300 nL was drawn up from the *t*-BuXphos catalyst column (column 5)
4. 300 nL was drawn up from the P_2-Et base column (column 7).
5. Dispense mixing (3×800 nL) into the 1,536-well reaction plate to ensure all reagents were adequately combined.
6. This process was repeated to cover all columns of the nucleophile source plate resulting in 384 reactions assembled at 1.2 µL (120 nmol) each.
7. The 1,536-plate was sealed and briefly centrifuged before sitting at ambient temperature for 24 hours.

The next morning, the reactions were quenched by addition of 3×1.2 µL 0.5 M AcOH in DMSO to each reaction well. The reactions were further diluted (to approximately 10 mM assuming complete conversion to product) with DMSO. 1 µL of the quenched and diluted crude reaction was drawn up for analysis by LC-MS (1 µL crude ~10 mM reaction into 60 µL DMSO followed by shaking). Reaction results are shown below as a heat map. Colors represent a relative percent conversion gradient (blue-green-yellow = 0% to 50% to 100% conversion), where values were calculated using the UV peak area of product and the UV peak area of the limiting reagent aryl halide core. The grid is separated based on nucleophile type. A direct comparison from the screening experiment, filtered down to the best reaction for each nucleophile, communicates the advantage of testing multiple reaction conditions and tailoring the screen to reaction class (Figure 44). On the left below are displayed the best reaction for each of the 384 nucleophiles (plotted as a 16 × 24 heat map) and on the right are displayed the results when subjecting the same library to just the *t*-BuXPhos G3/P_2-Et/NMP reaction conditions.

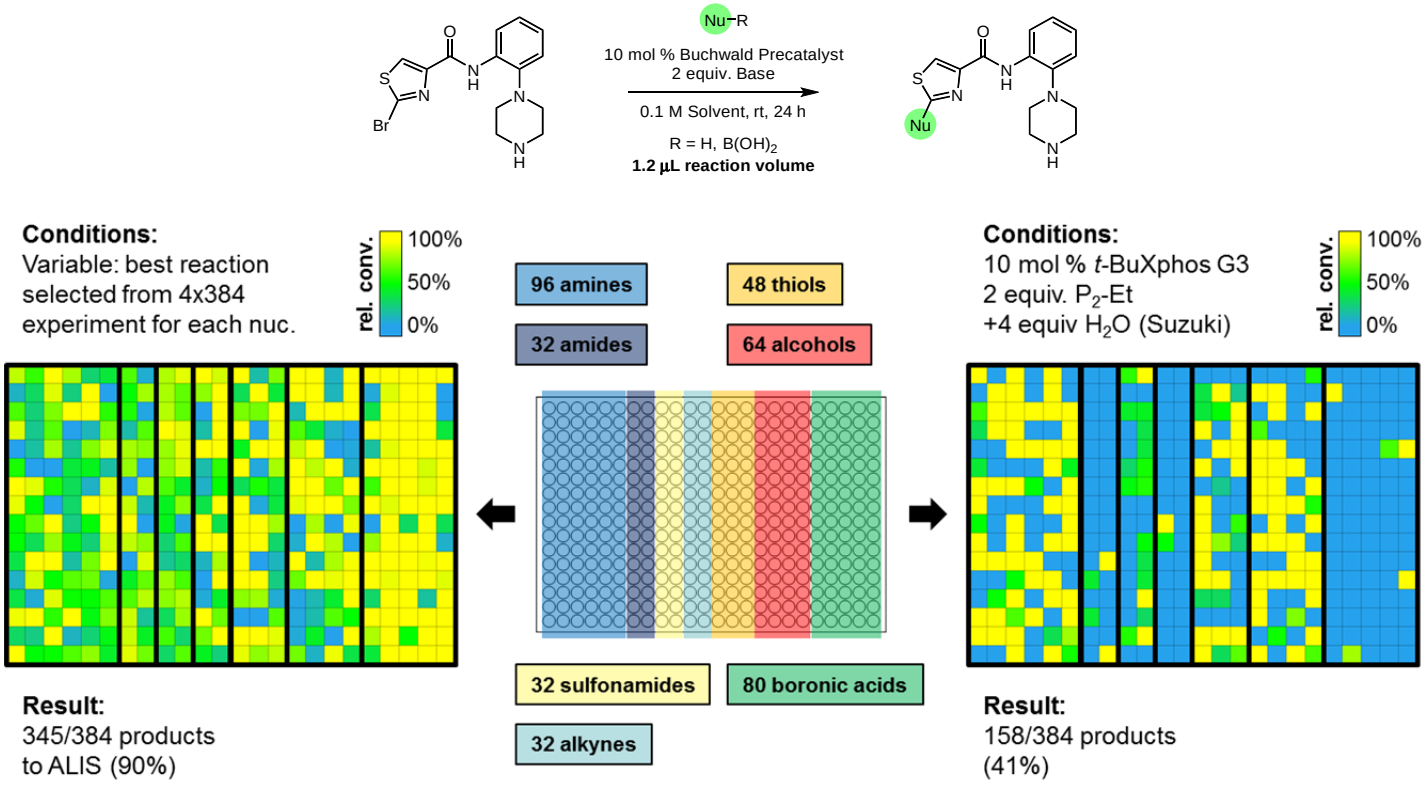


Figure 44. Single Set of Reaction Conditions Versus Reaction Screening

When testing *t*-BuXPhos G3/P_2-Et/NMP across all 384 nucleophiles, 158/384 (41%) possible products were detected by LC-MS. When optimizing the reaction conditions and testing multiple sets of conditions the number of products detected increased to 345/384 (90%). Notable differences include amide nucleophiles, alkynes, and Suzuki cross-couplings where optimization through high throughput reaction screening lead to improved reaction conditions. *t*-BuXPhos G3/P_2-Et/NMP was still effective for amines, some sulfonamides, thiols, and alcohols as shown above in Figure 44, *t*-BuXPhos G3 and/or P_2-Et were used for these nucleophile classes when testing multiple reaction conditions as well.

8.4. Affinity-Based Ranking Experiments

Pool Prep. 24 Pools were comprised of 12-18 crude coupling products along with 3-5 purified standards of known CHK1 IC_{50}'s. The purified standards utilized in this experiment were from the same series and should bind to the same pocket. Pools were demarcated by nucleophile type (22 total pools) then finally by yield (2 pools comprised of low yielding crude reactions). Automated library pooling was accomplished using the LABCYTE Echo® 555 acoustic dispensing liquid handler and 10 nL dispense volumes. After acoustic dispensing the crude pools were diluted with DMSO to 2.5 µL (1:250 dilution per compound, assuming 10 mM product concentration in each reaction) to give a per compound concentration of 40 µM. This pool was stored at -20 ˚C when not in use. See supplementary excel tables for pool design, composition, and standards used.

Available standards (all were used unless mass overlap was present):

Affinity Ranking Standards	Chemistry		Plate	Source Wells	Mass	Formula	Target	Invitrogen IC50 (nM)	Source
Control-01	Suzuki		Ctrl	D1	353.13103	C18H19N5OS	CHK1	140	10 mM Stock
Control-02	Amine		Ctrl	C1	379.14668	C20H21N5OS	CHK1	193	10 mM Stock
Control-03	Suzuki		Ctrl	B1	424.15691	C22H24N4O3S	CHK1	682	10 mM Stock
Control-04	Amine		Ctrl	F1	445.16848	C23H23N7OS	CHK1	18.8	10 mM Stock
Control-05	Amine		Ctrl	A1	459.18413	C24H25N7OS	CHK1	10000	10 mM Stock

24 total ASMS pools assembled using acoustic dispensing (see supplementary excel tables for more detail):

Pool	Sample Name	Chemistry	Catalyst	Base	Solvent	Source Plate	Source Wells	Mass
1	0378493_0152_re_0001	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	A1	354.12628
1	0378493_0152_re_0032	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	H4	380.14193
1	0378493_0152_re_0056	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	N4	387.0936
1	0378493_0152_re_0076	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	C8	394.15758
1	0378493_0152_re_0100	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	I8	404.14193
1	0378493_0152_re_0128	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	P8	408.17323
1	0378493_0152_re_0148	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	E12	411.15291
1	0378493_0152_re_0178	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	M10	419.15283
1	0378493_0152_re_0198	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	B14	420.13684
1	0378493_0152_re_0229	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	J13	425.16856
1	0378493_0152_re_0260	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	A20	433.19363
1	0378493_0152_re_0310	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	N18	440.23583
1	0378493_0152_re_0297	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	K17	448.12931
1	0378493_0152_re_0322	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	A22	457.12423
1	0378493_0152_re_0353	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	I21	466.19511
1	0378493_0152_re_0378	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	O22	483.24164
1	Control-01	Suzuki	N/A	N/A	N/A	Standards	D1	353.13103
1	Control-02	Amine	N/A	N/A	N/A	Standards	C1	379.14668
1	Control-03	Suzuki	N/A	N/A	N/A	Standards	B1	424.15691
1	Control-04	Amine	N/A	N/A	N/A	Standards	F1	445.16848
1	Control-05	Amine	N/A	N/A	N/A	Standards	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
2	0378493_0152_re_0009	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	C1	370.12119
2	0378493_0152_re_0034	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	I2	382.13243

2	0378493_0152_re_0060	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	O4	393.16233
2	0378493_0152_re_0078	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	D6	395.15283
2	0378493_0152_re_0102	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	J6	404.14193
2	0378493_0152_re_0132	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	A12	409.15725
2	0378493_0152_re_0162	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	I10	415.1249
2	0378493_0152_re_0184	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	N12	419.17798
2	0378493_0152_re_0204	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	C16	421.15725
2	0378493_0152_re_0237	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	L13	426.12965
2	0378493_0152_re_0264	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	B20	433.19363
2	0378493_0152_re_0288	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	H20	443.11827
2	0378493_0152_re_0301	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	L17	448.20453
2	0378493_0152_re_0330	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	C22	462.22018
2	0378493_0152_re_0357	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	J21	470.07503
2	0378493_0152_re_0382	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	P22	517.18716
2	Control-01	Suzuki	N/A	N/A	N/A	Standards	D1	353.13103
2	Control-02	Amine	N/A	N/A	N/A	Standards	C1	379.14668
2	Control-03	Suzuki	N/A	N/A	N/A	Standards	B1	424.15691
2	Control-04	Amine	N/A	N/A	N/A	Standards	F1	445.16848
2	Control-05	Amine	N/A	N/A	N/A	Standards	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
3	0378493_0152_re_0015	Amine	tBuBrettPhos G3	P2-Et	NMP	Plate 5	D3	370.13243
3	0378493_0152_re_0040	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	J4	383.15283
3	0378493_0152_re_0064	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	P4	393.16233
3	0378493_0152_re_0153	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	G9	397.15725
3	0378493_0152_re_0107	Amine	tBuBrettPhos G3	P2-Et	NMP	Plate 5	K7	404.14193
3	0378493_0152_re_0134	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	B10	410.09835
3	0378493_0152_re_0168	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	J12	415.12784
3	0378493_0152_re_0188	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	O12	419.17798
3	0378493_0152_re_0214	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	F14	422.18888
3	0378493_0152_re_0241	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	M13	427.12336
3	0378493_0152_re_0268	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	C20	437.15216
3	0378493_0152_re_0376	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	N24	446.16373
3	0378493_0152_re_0306	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	M18	449.19978
3	0378493_0152_re_0333	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	D21	463.1249
3	0378493_0152_re_0364	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	K24	475.17904

3	Control-01	Suzuki	N/A	N/A	N/A	Standards	D1	353.13103
3	Control-02	Amine	N/A	N/A	N/A	Standards	C1	379.14668
3	Control-03	Suzuki	N/A	N/A	N/A	Standards	B1	424.15691
3	Control-04	Amine	N/A	N/A	N/A	Standards	F1	445.16848
3	Control-05	Amine	N/A	N/A	N/A	Standards	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
4	0378493_0152_re_0021	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	F1	373.15725
4	0378493_0152_re_0044	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	K4	384.13684
4	0378493_0152_re_0068	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	A8	394.13243
4	0378493_0152_re_0090	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	G6	401.10925
4	0378493_0152_re_0112	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	L8	405.16233
4	0378493_0152_re_0140	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	C12	410.15249
4	0378493_0152_re_0172	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	K12	418.15758
4	0378493_0152_re_0190	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	P10	419.17798
4	0378493_0152_re_0218	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	G14	423.13651
4	0378493_0152_re_0248	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	N16	427.14782
4	0378493_0152_re_0276	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	E20	439.16781
4	0378493_0152_re_0292	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	I20	447.06874
4	0378493_0152_re_0315	Amine	tBuBrettPhos G3	P2-Et	NMP	Plate 5	O19	455.08098
4	0378493_0152_re_0345	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	G21	466.12457
4	0378493_0152_re_0338	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	E22	478.16095
4	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
4	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
4	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
4	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
4	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
5	0378493_0152_re_0025	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	G1	380.14193
5	0378493_0152_re_0050	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	M2	386.09835
5	0378493_0152_re_0072	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	B8	394.15758
5	0378493_0152_re_0093	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	H5	401.18855
5	0378493_0152_re_0120	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	N8	407.17798
5	0378493_0152_re_0141	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	D9	411.14774
5	0378493_0152_re_0174	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	L10	419.15283
5	0378493_0152_re_0194	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	A14	420.13684
5	0378493_0152_re_0224	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	H16	423.1729

5	0378493_0152_re_0256	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	P16	433.11842
5	0378493_0152_re_0278	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	F18	439.21543
5	0378493_0152_re_0296	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	J20	447.13407
5	0378493_0152_re_0317	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	P17	455.15914
5	0378493_0152_re_0349	Amine	tBuXPhos G3	P2-Et	NMP	Plate 5	H21	466.17871
5	0378493_0152_re_0370	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	M22	478.21509
5	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
5	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
5	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
5	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
5	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
6	0378493_0152_0385	Amide	tBuXPhos G3	BTMG	DMF	Plate 2	A1	345.12595
6	0378493_0152_0393	Amide	tBuXPhos G3	BTMG	DMF	Plate 2	C1	373.15725
6	0378493_0152_0408	Amide	tBuBrettPhos G3	MTBD	DMF	Plate 2	F4	407.1416
6	0378493_0152_0420	Amide	tBuBrettPhos G3	MTBD	DMF	Plate 2	I4	408.13684
6	0378493_0152_0430	Amide	tBuXPhos G3	MTBD	DMF	Plate 2	L2	413.18855
6	0378493_0152_0438	Amide	tBuXPhos G3	MTBD	DMF	Plate 2	N2	422.15249
6	0378493_0152_0446	Amide	tBuXPhos G3	MTBD	DMF	Plate 2	P2	425.13217
6	0378493_0152_0462	Amide	tBuXPhos G3	MTBD	DMF	Plate 2	D6	437.15216
6	0378493_0152_0476	Amide	tBuBrettPhos G3	MTBD	DMF	Plate 2	G8	441.10262
6	0378493_0152_0490	Amide	tBuXPhos G3	MTBD	DMF	Plate 2	K6	451.16781
6	0378493_0152_0500	Amide	tBuBrettPhos G3	MTBD	DMF	Plate 2	M8	467.16273
6	0378493_0152_0508	Amide	tBuBrettPhos G3	MTBD	DMF	Plate 2	O8	497.09449
6	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
6	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
6	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
6	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
6	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
7	0378493_0152_0390	Amide	tBuXPhos G3	MTBD	DMF	Plate 2	B2	373.15725
7	0378493_0152_0402	Amide	tBuXPhos G3	MTBD	DMF	Plate 2	E2	401.15216
7	0378493_0152_0416	Amide	tBuBrettPhos G3	MTBD	DMF	Plate 2	H4	408.13684
7	0378493_0152_0424	Amide	tBuBrettPhos G3	MTBD	DMF	Plate 2	J4	413.09802
7	0378493_0152_0436	Amide	tBuBrettPhos G3	MTBD	DMF	Plate 2	M4	421.15725
7	0378493_0152_0444	Amide	tBuBrettPhos G3	MTBD	DMF	Plate 2	O4	425.13217

7	0378493_0152_0456	Amide	tBuBrettPhos G3	MTBD	DMF	Plate 2	B8	428.16306
7	0378493_0152_0467	Amide	tBuBrettPhos G3	BTMG	DMF	Plate 2	E7	437.15216
7	0378493_0152_0488	Amide	tBuBrettPhos G3	MTBD	DMF	Plate 2	J8	449.15216
7	0378493_0152_0495	Amide	tBuBrettPhos G3	BTMG	DMF	Plate 2	L7	451.16781
7	0378493_0152_0503	Amide	tBuBrettPhos G3	BTMG	DMF	Plate 2	N7	476.19944
7	0378493_0152_0512	Amide	tBuBrettPhos G3	MTBD	DMF	Plate 2	P8	522.13079
7	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
7	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
7	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
7	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
7	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
8	0378493_0152_0515	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	A11	381.09293
8	0378493_0152_0521	Sulfonamide	tBuBrettPhos G3	P2-Et	DMF	Plate 2	C9	407.10858
8	0378493_0152_0531	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	E11	423.13988
8	0378493_0152_0539	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	G11	444.10383
8	0378493_0152_0547	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	I11	449.065
8	0378493_0152_0561	Sulfonamide	tBuBrettPhos G3	P2-Et	DMF	Plate 2	M9	457.12423
8	0378493_0152_0571	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	O11	468.10383
8	0378493_0152_0577	Sulfonamide	tBuBrettPhos G3	P2-Et	DMF	Plate 2	A13	473.11915
8	0378493_0152_0587	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	C15	479.08974
8	0378493_0152_0593	Sulfonamide	tBuBrettPhos G3	P2-Et	DMF	Plate 2	E13	485.11915
8	0378493_0152_0603	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	G15	497.08032
8	0378493_0152_0615	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	J15	511.09597
8	0378493_0152_0623	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	L15	527.09088
8	0378493_0152_0629	Sulfonamide	tBuBrettPhos G3	P2-Et	DMF	Plate 2	N13	539.14094
8	0378493_0152_0640	Sulfonamide	RockPhos G3	MTBD	DMF	Plate 2	P16	579.08335
8	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
8	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
8	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
8	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
8	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
9	0378493_0152_0517	Sulfonamide	tBuBrettPhos G3	P2-Et	DMF	Plate 2	B9	395.10858
9	0378493_0152_0527	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	D11	421.12423
9	0378493_0152_0535	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	F11	443.10858

9	0378493_0152_0543	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	H11	447.11473
9	0378493_0152_0559	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	L11	457.12423
9	0378493_0152_0567	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	N11	458.11948
9	0378493_0152_0575	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	P11	468.10383
9	0378493_0152_0582	Sulfonamide	tBuBrettPhos G3	MTBD	DMF	Plate 2	B14	475.11481
9	0378493_0152_0589	Sulfonamide	tBuBrettPhos G3	P2-Et	DMF	Plate 2	D13	483.13988
9	0378493_0152_0597	Sulfonamide	tBuBrettPhos G3	P2-Et	DMF	Plate 2	F13	487.1348
9	0378493_0152_0605	Sulfonamide	tBuBrettPhos G3	P2-Et	DMF	Plate 2	H13	500.13004
9	0378493_0152_0618	Sulfonamide	tBuBrettPhos G3	MTBD	DMF	Plate 2	K14	516.98706
9	0378493_0152_0627	Sulfonamide	RockPhos G3	P2-Et	DMF	Plate 2	M15	531.12462
9	0378493_0152_0633	Sulfonamide	tBuBrettPhos G3	P2-Et	DMF	Plate 2	O13	561.11743
9	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
9	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
9	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
9	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
9	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
10	0378493_0152_0643	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	A19	388.13578
10	0378493_0152_0658	Alkyne	tBu3P G3	MTBD	NMP	Plate 2	E18	392.14193
10	0378493_0152_0675	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	I19	418.14635
10	0378493_0152_0695	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	N19	428.16708
10	0378493_0152_0703	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	P19	433.12423
10	0378493_0152_0711	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	B23	440.14193
10	0378493_0152_0719	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	D23	445.15725
10	0378493_0152_0727	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	F23	450.15257
10	0378493_0152_0735	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	H23	455.1416
10	0378493_0152_0766	Alkyne	tBu3P G3	MTBD	NMP	Plate 2	P22	457.11842
10	0378493_0152_0741	Alkyne	tBu3P G3	BTTP	NMP	Plate 2	J21	471.20928
10	0378493_0152_0749	Alkyne	tBu3P G3	BTTP	NMP	Plate 2	L21	481.12423
10	0378493_0152_0758	Alkyne	tBu3P G3	MTBD	NMP	Plate 2	N22	541.1106
10	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
10	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
10	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
10	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
11	0378493_0152_0647	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	B19	390.12628
11	0378493_0152_0670	Alkyne	tBu3P G3	MTBD	NMP	Plate 2	H18	407.12161
11	0378493_0152_0679	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	J19	419.10858
11	0378493_0152_0699	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	O19	432.162

11	0378493_0152_0707	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	A23	440.08739
11	0378493_0152_0715	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	C23	444.19838
11	0378493_0152_0723	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	E23	448.15691
11	0378493_0152_0731	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	G23	450.15257
11	0378493_0152_0739	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	I23	471.1729
11	0378493_0152_0747	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	K23	472.11808
11	0378493_0152_0754	Alkyne	tBu3P G3	MTBD	NMP	Plate 2	M22	524.11055
11	0378493_0152_0763	Alkyne	RuPhos G3	BTTP	NMP	Plate 2	O23	541.13392
11	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
11	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
11	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
11	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
12	0378493_0152_0769	Thiol	Blank / No Cat	P2-Et	DMF	Plate 3	A1	386.09835
12	0378493_0152_0782	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	D2	405.12932
12	0378493_0152_0798	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	H2	426.11842
12	0378493_0152_0959	Thiol	AdBrettPhos G3	P2-Et	DMF	Plate 3	P11	440.09768
12	0378493_0152_0820	Thiol	AdBrettPhos G3	BTMG	DMF	Plate 3	M4	450.12965
12	0378493_0152_0838	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	B6	456.12898
12	0378493_0152_0857	Thiol	Blank / No Cat	P2-Et	DMF	Plate 3	G5	464.12015
12	0378493_0152_0870	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	J6	478.11333
12	0378493_0152_0896	Thiol	AdBrettPhos G3	BTMG	DMF	Plate 3	P8	489.0963
12	0378493_0152_0906	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	C10	493.12423
12	0378493_0152_0917	Thiol	Blank / No Cat	P2-Et	DMF	Plate 3	F9	500.17766
12	0378493_0152_0932	Thiol	AdBrettPhos G3	BTMG	DMF	Plate 3	I12	504.14022
12	0378493_0152_0952	Thiol	AdBrettPhos G3	BTMG	DMF	Plate 3	N12	544.13269
12	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
12	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
12	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
12	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
12	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
13	0378493_0152_0776	Thiol	AdBrettPhos G3	BTMG	DMF	Plate 3	B4	387.0936
13	0378493_0152_0786	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	E2	412.114

13	0378493_0152_0806	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	J2	438.1548
13	0378493_0152_0813	Thiol	Blank / No Cat	P2-Et	DMF	Plate 3	L1	442.16095
13	0378493_0152_0826	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	O2	453.12932
13	0378493_0152_0844	Thiol	AdBrettPhos G3	BTMG	DMF	Plate 3	C8	459.15111
13	0378493_0152_0867	Thiol	AdBrettPhos G3	P2-Et	DMF	Plate 3	I7	475.08065
13	0378493_0152_0884	Thiol	AdBrettPhos G3	BTMG	DMF	Plate 3	M8	480.14022
13	0378493_0152_0898	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	A10	490.20723
13	0378493_0152_0910	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	D10	494.1058
13	0378493_0152_0924	Thiol	AdBrettPhos G3	BTMG	DMF	Plate 3	G12	502.10572
13	0378493_0152_0933	Thiol	Blank / No Cat	P2-Et	DMF	Plate 3	J9	519.1875
13	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
13	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
13	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
13	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
13	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
14	0378493_0152_0779	Thiol	AdBrettPhos G3	P2-Et	DMF	Plate 3	C3	403.05952
14	0378493_0152_0789	Thiol	Blank / No Cat	P2-Et	DMF	Plate 3	F1	414.12965
14	0378493_0152_0809	Thiol	Blank / No Cat	P2-Et	DMF	Plate 3	K1	439.15005
14	0378493_0152_0953	Thiol	Blank / No Cat	P2-Et	DMF	Plate 3	O9	447.11875
14	0378493_0152_0830	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	P2	453.12932
14	0378493_0152_0850	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	E6	464.02991
14	0378493_0152_0804	Thiol	AdBrettPhos G3	BTMG	DMF	Plate 3	I4	478.11089
14	0378493_0152_0890	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	O6	488.26435
14	0378493_0152_0902	Thiol	Blank / No Cat	BTMG	DMF	Plate 3	B10	491.0868
14	0378493_0152_0913	Thiol	Blank / No Cat	P2-Et	DMF	Plate 3	E9	496.16028
14	0378493_0152_0927	Thiol	AdBrettPhos G3	P2-Et	DMF	Plate 3	H11	504.10139
14	0378493_0152_0944	Thiol	AdBrettPhos G3	BTMG	DMF	Plate 3	L12	533.20315
14	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
14	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668

14	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
14	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
14	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
15	0378493_0152_0961	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	A13	374.14126
15	0378493_0152_0977	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	E13	392.13407
15	0378493_0152_0989	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	H13	398.12127
15	0378493_0152_1021	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	P13	405.12595
15	0378493_0152_1033	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	C17	408.162
15	0378493_0152_1049	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	G17	409.15725
15	0378493_0152_1061	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	J17	412.13692
15	0378493_0152_1097	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	C21	416.11185
15	0378493_0152_1117	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	H21	422.17765
15	0378493_0152_1133	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	L21	429.12932
15	0378493_0152_1149	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	P21	434.15249
15	0378493_0152_1161	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 4	C1	438.18379
15	0378493_0152_1185	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 4	I1	448.11808
15	0378493_0152_1213	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 4	P1	477.21985
15	0378493_0152_1201	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 4	M1	491.16273
15	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
15	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
15	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
15	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
15	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
16	0378493_0152_0965	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	B13	381.12595
16	0378493_0152_0981	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	F13	395.1416
16	0378493_0152_1001	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	K13	400.10277
16	0378493_0152_1025	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	A17	406.14972
16	0378493_0152_1041	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	E17	408.162
16	0378493_0152_1053	Alcohol	Blank / No	P2-Et	DMF	Plate 3	H17	410.14126

			Cat					
16	0378493_0152_1069	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	L17	413.15216
16	0378493_0152_1109	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	F21	422.17765
16	0378493_0152_1125	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	J21	424.12053
16	0378493_0152_1140	Alcohol	RockPhos G3	MTBD	DMF	Plate 3	M24	429.12932
16	0378493_0152_1153	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 4	A1	434.17765
16	0378493_0152_1177	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 4	G1	444.10229
16	0378493_0152_1193	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 4	K1	452.12423
16	0378493_0152_1207	Alcohol	RockPhos G3	P2-Et	DMF	Plate 4	N3	542.10585
16	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
16	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
16	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
16	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
16	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
17	0378493_0152_0973	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	D13	388.15691
17	0378493_0152_0985	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	G13	395.1416
17	0378493_0152_1008	Alcohol	RockPhos G3	MTBD	DMF	Plate 3	L16	401.15216
17	0378493_0152_1029	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	B17	408.162
17	0378493_0152_1045	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	F17	409.15725
17	0378493_0152_1057	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	I17	410.14126
17	0378493_0152_1081	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	O17	415.08697
17	0378493_0152_1113	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	G21	422.17765
17	0378493_0152_1129	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	K21	426.15257
17	0378493_0152_1157	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 4	B1	436.15691
17	0378493_0152_1209	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 4	O1	438.17256
17	0378493_0152_1181	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 4	H1	444.14315
17	0378493_0152_1197	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 4	L1	455.16273
17	0378493_0152_1141	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	N21	463.2042
17	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
17	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
17	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691

17	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
17	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
18	0378493_0152_1217	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	A5	354.11505
18	0378493_0152_1245	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	H5	378.15143
18	0378493_0152_1257	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	K5	389.13103
18	0378493_0152_1274	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	O6	392.16708
18	0378493_0152_1474	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	A22	396.14201
18	0378493_0152_1309	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	H9	403.14668
18	0378493_0152_1321	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	K9	406.14635
18	0378493_0152_1518	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	L22	408.14201
18	0378493_0152_1354	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	C14	412.13692
18	0378493_0152_1370	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	G14	420.10785
18	0378493_0152_1380	Suzuki	Sphos G2	aq. BTMG	NMP	Plate 4	I16	421.19363
18	0378493_0152_1530	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	O22	424.13915
18	0378493_0152_1411	Suzuki	Sphos G2	aq. K3PO4	NMP	Plate 4	A19	428.10737
18	0378493_0152_1434	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	G18	440.16822
18	0378493_0152_1469	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	P17	456.13867
18	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
18	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
18	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
19	0378493_0152_1227	Suzuki	Sphos G2	aq. K3PO4	NMP	Plate 4	C7	354.12628
19	0378493_0152_1489	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	E21	379.14668
19	0378493_0152_1262	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	L6	389.13103
19	0378493_0152_1278	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	P6	392.16708
19	0378493_0152_1297	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	E9	396.14201
19	0378493_0152_1457	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	M17	404.14193
19	0378493_0152_1329	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	M9	406.18273
19	0378493_0152_1498	Suzuki	RuPhos G3	aq.	NMP	Plate 4	G22	408.162

				BTMG				
19	0378493_0152_1534	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	P22	412.13692
19	0378493_0152_1365	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	F13	420.10785
19	0378493_0152_1381	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	J13	422.14126
19	0378493_0152_1398	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	N14	424.15691
19	0378493_0152_1414	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	B18	432.12317
19	0378493_0152_1426	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	E18	440.16822
19	0378493_0152_1446	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	J18	456.162
19	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
19	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
19	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
20	0378493_0152_1229	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	D5	364.13578
20	0378493_0152_1494	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	F22	380.1307
20	0378493_0152_1265	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	M5	390.12628
20	0378493_0152_1281	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	A9	392.16708
20	0378493_0152_1522	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	M22	396.19838
20	0378493_0152_1526	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	N22	404.16708
20	0378493_0152_1327	Suzuki	Sphos G2	aq. K3PO4	NMP	Plate 4	L11	406.18273
20	0378493_0152_1344	Suzuki	Sphos G2	aq. BTMG	NMP	Plate 4	P12	408.162
20	0378493_0152_1361	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	E13	414.15143
20	0378493_0152_1502	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	H22	420.162
20	0378493_0152_1385	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	K13	422.15249
20	0378493_0152_1404	Suzuki	Sphos G2	aq. BTMG	NMP	Plate 4	O16	426.14741
20	0378493_0152_1417	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	C17	432.12317
20	0378493_0152_1429	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	F17	442.11333
20	0378493_0152_1514	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	K22	458.13882
20	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
20	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
20	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413

Pool	Sample Name	Chemistry	Catalyst	Base	Solvent	Source Plate	Source Wells	Mass
21	0378493_0152_1238	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	F6	365.13103
21	0378493_0152_1485	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	D21	382.15758
21	0378493_0152_1269	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	N5	390.15143
21	0378493_0152_1288	Suzuki	Sphos G2	aq. BTMG	NMP	Plate 4	B12	394.14635
21	0378493_0152_1303	Suzuki	Sphos G2	aq. K3PO4	NMP	Plate 4	F11	398.09681
21	0378493_0152_1313	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	I9	406.14635
21	0378493_0152_1333	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	N9	407.1416
21	0378493_0152_1346	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	A14	408.162
21	0378493_0152_1357	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	D13	415.14668
21	0378493_0152_1450	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	K18	420.19838
21	0378493_0152_1389	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	L13	422.17765
21	0378493_0152_1405	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	P13	426.15257
21	0378493_0152_1289	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	C9	436.1933
21	0378493_0152_1439	Suzuki	Sphos G2	aq. K3PO4	NMP	Plate 4	H19	448.11808
21	0378493_0152_1454	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	L18	458.15766
21	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
21	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
21	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
22	0378493_0152_1241	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	G5	366.12628
22	0378493_0152_1254	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	J6	384.10785
22	0378493_0152_1505	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	I21	390.15143
22	0378493_0152_1293	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	D9	396.14201
22	0378493_0152_1305	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	G9	400.11694
22	0378493_0152_1319	Suzuki	Sphos G2	aq. K3PO4	NMP	Plate 4	J11	406.14635
22	0378493_0152_1339	Suzuki	Sphos G2	aq. K3PO4	NMP	Plate 4	O11	408.12561
22	0378493_0152_1351	Suzuki	Sphos G2	aq. K3PO4	NMP	Plate 4	B15	412.11246
22	0378493_0152_1462	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	N18	415.14668

22	0378493_0152_1373	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	H13	421.15725
22	0378493_0152_1393	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	M13	422.17765
22	0378493_0152_1465	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	O17	426.15257
22	0378493_0152_1422	Suzuki	RuPhos G3	aq. BTMG	NMP	Plate 4	D18	436.1933
22	0378493_0152_1444	Suzuki	Sphos G2	aq. BTMG	NMP	Plate 4	I20	450.11374
22	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
22	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
22	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
23 Low Yields	0378493_0152_re_0007	Amine	tBuBrettPhos G3	P2-Et	NMP	Plate 5	B3	357.16233
23 Low Yields	0378493_0152_re_0046	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	L2	384.13684
23 Low Yields	0378493_0152_re_0082	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	E6	400.114
23 Low Yields	0378493_0152_re_0122	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	O6	407.17798
23 Low Yields	0378493_0152_re_0210	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	E14	421.19363
23 Low Yields	0378493_0152_re_0226	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	I14	423.1729
23 Low Yields	0378493_0152_0397	Amide	tBuXPhos G3	BTMG	DMF	Plate 2	D1	387.1729
23 Low Yields	0378493_0152_0451	Amide	tBuBrettPhos G3	BTMG	DMF	Plate 2	A7	428.10892
23 Low Yields	0378493_0152_0549	Sulfonamide	tBuBrettPhos G3	P2-Et	DMF	Plate 2	J9	449.08032
23 Low Yields	0378493_0152_0654	Alkyne	tBu3P G3	MTBD	NMP	Plate 2	D18	442.15758
23 Low Yields	0378493_0152_0682	Alkyne	tBu3P G3	MTBD	NMP	Plate 2	K18	422.21403
23 Low Yields	0378493_0152_0835	Thiol	AdBrettPhos G3	P2-Et	DMF	Plate 3	A7	455.08098
23 Low Yields	0378493_0152_0939	Thiol	AdBrettPhos G3	P2-Et	DMF	Plate 3	K11	521.14161
23 Low Yields	0378493_0152_0969	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	C13	386.17765
23 Low Yields	0378493_0152_1000	Alcohol	RockPhos G3	MTBD	DMF	Plate 3	J16	398.15249
23 Low Yields	0378493_0152_1037	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	D17	462.13373
23 Low Yields	0378493_0152_1101	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	D21	418.16748
23 Low Yields	0378493_0152_1511	Suzuki	Sphos G2	aq. K3PO4	NMP	Plate 4	J23	390.15143
23 Low Yields	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
23 Low Yields	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668

23 Low Yields	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
23 Low Yields	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
23 Low Yields	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413
Pool	**Sample Name**	**Chemistry**	**Catalyst**	**Base**	**Solvent**	**Source Plate**	**Source Wells**	**Mass**
24 Low Yields	0378493_0152_re_0234	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	K14	425.16856
24 Low Yields	0378493_0152_re_0250	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	O14	432.17323
24 Low Yields	0378493_0152_re_0270	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	D18	437.18855
24 Low Yields	0378493_0152_re_0282	Amine	tBuXPhos G3	MTBD	NMP	Plate 5	G18	440.1453
24 Low Yields	0378493_0152_re_0344	Amine	tBuBrettPhos G3	MTBD	NMP	Plate 5	F24	464.19944
24 Low Yields	0378493_0152_0478	Amide	tBuXPhos G3	MTBD	DMF	Plate 2	H6	443.12275
24 Low Yields	0378493_0152_0556	Sulfonamide	RockPhos G3	MTBD	DMF	Plate 2	K12	453.11406
24 Low Yields	0378493_0152_0662	Alkyne	tBu3P G3	MTBD	NMP	Plate 2	F18	394.18273
24 Low Yields	0378493_0152_0668	Alkyne	RuPhos G3	MTBD	NMP	Plate 2	G20	397.19363
24 Low Yields	0378493_0152_0795	Thiol	AdBrettPhos G3	P2-Et	DMF	Plate 3	G3	420.12898
24 Low Yields	0378493_0152_0879	Thiol	AdBrettPhos G3	P2-Et	DMF	Plate 3	L7	478.16095
24 Low Yields	0378493_0152_1068	Alcohol	RockPhos G3	MTBD	DMF	Plate 3	K20	412.15691
24 Low Yields	0378493_0152_1073	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	M17	413.18855
24 Low Yields	0378493_0152_1079	Alcohol	RockPhos G3	P2-Et	DMF	Plate 3	N19	414.20895
24 Low Yields	0378493_0152_1085	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	P17	415.08697
24 Low Yields	0378493_0152_1093	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 3	B21	415.2042
24 Low Yields	0378493_0152_1173	Alcohol	Blank / No Cat	P2-Et	DMF	Plate 4	F1	442.24025
24 Low Yields	0378493_0152_1233	Suzuki	RuPhos G3	aq. K3PO4	NMP	Plate 4	E5	365.13103
24 Low Yields	Control-01	Suzuki	N/A	N/A	N/A	Control	D1	353.13103
24 Low Yields	Control-02	Amine	N/A	N/A	N/A	Control	C1	379.14668
24 Low Yields	Control-03	Suzuki	N/A	N/A	N/A	Control	B1	424.15691
24 Low Yields	Control-04	Amine	N/A	N/A	N/A	Control	F1	445.16848
24 Low Yields	Control-05	Amine	N/A	N/A	N/A	Control	A1	459.18413

Competition Experiment Prep. All work was done at 0 ˚C unless otherwise noted. CHK1 (internal preparation: 50 µM stock solution in 25 mM Hepes, pH 7.5, 300 mM NaCl, 5 mM DTT, 5% glycerol) was removed from a -78 ˚C freezer and warmed to approximately 0 ˚C on ice. Protein dilution buffer was prepared (56.5 mM Hepes pH 7.5, 200 mM NaCl, 5 mM DTT) along with library dilution buffer (56.5 mM Hepes pH 7.5, 200 mM NaCl, 5 mM DTT). Invertase (Sigma Aldrich cat. no. I4504) was weighed into a centrifuge tube and diluted to 20 µM with protein dilution buffer. Approximately half of the 20 µM invertase stock was reserved while the remainder was diluted to 10 µM with protein dilution buffer in preparation for the serial dilution. The pools were thawed and 2 µL aliquots were removed and diluted 1:20 with library dilution buffer (2 µL DMSO pool into 38 µL library dilution buffer to give final concentrations of 2 µM/compound). The diluted pools were stored at ambient temperature prior to use. Next, a serial dilution of CHK1 was performed. The CHK1 stock was diluted with protein dilution buffer to 40 µM, then diluted 1:1 with 20 µM invertase (to populate the first protein level). The CHK1 serial dilution was then performed in a 96-well plate, using the 10 µM invertase stock, to arrive at the following CHK1/invertase protein concentrations:

CHK1 Conc.	20 µM	10 µM	5 µM	2.5 µM	1.25 µM	0.62 µM	0.31 µM	0 µM
Invertase Conc.	10 µM	10 µM	10 µM	10 µM	10 µM	10 µM	10 µM	10 µM
Final Vol. (µL)	30	30	30	30	30	30	60	30

Finally, a 1:1 dilution of the appropriate CHK1 protein stock (3 µL) with the desired buffered library (3 µL) in a new 96-well plate provided an affinity ranking experiment with the desired protein and compound concentrations (1 µM/compound, 5 µM invertase, variable CHK1 concentration). This final 1:1 mixing step was done separately for each of the 24 crude reaction pools. The serial dilution depicted above was followed to prepare all competition experiments. The protein/compound mixtures were warmed to room temperature then allowed to incubate for 30 minutes. After 30 minutes, the 96-well plate was moved to an LC-MS autosampler (cooled to 4 ˚C) for analysis. Final component concentrations are shown below.

Pool Size	12 to 23	12 to 23	12 to 23	12 to 23	12 to 23	12 to 23	12 to 23	12 to 23
Per Cmpd.	1 µM	1 µM	1 µM	1 µM	1 µM	1 µM	1 µM	1 µM
Invertase Conc.	5 µM	5 µM	5 µM	5 µM	5 µM	5 µM	5 µM	5 µM
CHK1 Conc.	10 µM	5 µM	2.5 µM	1.25 µM	0.62 µM	0.31 µM	0.16 µM	0 µM

Chromatography conditions

SEC Running Buffer: 1 M NH_4OAc, pH 8.0

Flow Rate: 0.3 mL / min

Negative Control: 5 µM Invertase

ASMS affinity-based rank ordering results:

Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
1	0378493_0152_re_0001	Amine	Plate 5	A1	354.12628	C17H18N6OS	87.3	5.00µM CHK1
1	0378493_0152_re_0032	Amine	Plate 5	H4	380.14193	C19H20N6OS	95.5	ASMS Binding Not Observed
1	0378493_0152_re_005	Amine	Plate 5	N4	387.0936	C16H17N7OS2	96.6	ASMS Binding

	6							Not Observed
1	0378493_0152_re_0076	Amine	Plate 5	C8	394.15758	C20H22N6OS	24.8	ASMS Binding Not Observed
1	0378493_0152_re_0100	Amine	Plate 5	I8	404.14193	C21H20N6OS	70	ASMS Binding Not Observed
1	0378493_0152_re_0128	Amine	Plate 5	P8	408.17323	C21H24N6OS	48.3	ASMS Binding Not Observed
1	0378493_0152_re_0148	Amine	Plate 5	E12	411.15291	C21H22FN5OS	82.5	ASMS Binding Not Observed
1	0378493_0152_re_0178	Amine	Plate 5	M10	419.15283	C21H21N7OS	93.7	0.31µM CHK1
1	0378493_0152_re_0198	Amine	Plate 5	B14	420.13684	C21H20N6O2S	23.3	2.50µM CHK1
1	0378493_0152_re_0229	Amine	Plate 5	J13	425.16856	C22H24FN5OS	44.9	ASMS Binding Not Observed
1	0378493_0152_re_0260	Amine	Plate 5	A20	433.19363	C24H27N5OS	26.3	ASMS Binding Not Observed
1	0378493_0152_re_0310	Amine	Plate 5	N18	440.23583	C23H32N6OS	46.7	ASMS Binding Not Observed
1	0378493_0152_re_0297	Amine	Plate 5	K17	448.12931	C20H19F3N6OS	72.7	ASMS Binding Not Observed
1	0378493_0152_re_0322	Amine	Plate 5	A22	457.12423	C21H23N5O3S2	37.7	ASMS Binding Not Observed
1	0378493_0152_re_0353	Amine	Plate 5	I21	466.19511	C24H27FN6OS	100	ASMS Binding Not Observed
1	0378493_0152_re_0378	Amine	Plate 5	O22	483.24164	C24H33N7O2S	46.1	ASMS Binding Not Observed
1	Control-01	Suzuki	Standards	D1	353.13103	C18H19N5OS	10 mM Stock	5.00µM CHK1
1	Control-02	Amine	Standards	C1	379.14668	C20H21N5OS	10 mM Stock	10.00µM CHK1
1	Control-03	Suzuki	Standards	B1	424.15691	C22H24N4O3S	10 mM Stock	ASMS Binding Not Observed
1	Control-04	Amine	Standards	F1	445.16848	C23H23N7OS	10 mM Stock	2.50µM CHK1
1	Control-05	Amine	Standards	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
2	0378493_0152_re_0009	Amine	Plate 5	C1	370.12119	C17H18N6O2S	64.5	5.00µM CHK1
2	0378493_0152_re_0034	Amine	Plate 5	I2	382.13243	C17H18N8OS	50	ASMS Binding Not Observed
2	0378493_0152_re_0060	Amine	Plate 5	O4	393.16233	C21H23N5OS	29.2	ASMS Binding Not Observed
2	0378493_0152_re_0078	Amine	Plate 5	D6	395.15283	C19H21N7OS	20.4	ASMS Binding Not Observed
2	0378493_0152_re_0102	Amine	Plate 5	J6	404.14193	C21H20N6OS	31.8	ASMS Binding Not Observed
2	0378493_0152_re_0132	Amine	Plate 5	A12	409.15725	C21H23N5O2S	100	ASMS Binding Not Observed
2	0378493_0152_re_0162	Amine	Plate 5	I10	415.1249	C18H21N7OS2	100	ASMS Binding Not Observed
2	0378493_0152_re_018	Amine	Plate 5	N12	419.1779	C23H25N5OS	58.1	ASMS Binding

	4				8			Not Observed
2	0378493_0152_re_0204	Amine	Plate 5	C16	421.15725	C22H23N5O2S	100	ASMS Binding Not Observed
2	0378493_0152_re_0237	Amine	Plate 5	L13	426.12965	C20H22N6OS2	67.2	ASMS Binding Not Observed
2	0378493_0152_re_0264	Amine	Plate 5	B20	433.19363	C24H27N5OS	100	ASMS Binding Not Observed
2	0378493_0152_re_0288	Amine	Plate 5	H20	443.11827	C21H22ClN5O2S	100	ASMS Binding Not Observed
2	0378493_0152_re_0301	Amine	Plate 5	L17	448.20453	C24H28N6OS	71.2	ASMS Binding Not Observed
2	0378493_0152_re_0330	Amine	Plate 5	C22	462.22018	C25H30N6OS	57.7	ASMS Binding Not Observed
2	0378493_0152_re_0357	Amine	Plate 5	J21	470.07503	C21H19ClN6OS2	90.9	5.00µM CHK1
2	0378493_0152_re_0382	Amine	Plate 5	P22	517.18716	C24H26F3N7OS	41.5	ASMS Binding Not Observed
2	Control-01	Suzuki	Standards	D1	353.13103	C18H19N5OS	10 mM Stock	10.00µM CHK1
2	Control-02	Amine	Standards	C1	379.14668	C20H21N5OS	10 mM Stock	ASMS Binding Not Observed
2	Control-03	Suzuki	Standards	B1	424.15691	C22H24N4O3S	10 mM Stock	ASMS Binding Not Observed
2	Control-04	Amine	Standards	F1	445.16848	C23H23N7OS	10 mM Stock	2.50µM CHK1
2	Control-05	Amine	Standards	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
3	0378493_0152_re_0015	Amine	Plate 5	D3	370.13243	C16H18N8OS	93.8	ASMS Binding Not Observed
3	0378493_0152_re_0040	Amine	Plate 5	J4	383.15283	C18H21N7OS	50	ASMS Binding Not Observed
3	0378493_0152_re_0064	Amine	Plate 5	P4	393.16233	C21H23N5OS	100	ASMS Binding Not Observed
3	0378493_0152_re_0153	Amine	Plate 5	G9	397.15725	C20H23N5O2S	55.2	ASMS Binding Not Observed
3	0378493_0152_re_0107	Amine	Plate 5	K7	404.14193	C21H20N6OS	100	0.63µM CHK1
3	0378493_0152_re_0134	Amine	Plate 5	B10	410.09835	C19H18N6OS2	93.8	ASMS Binding Not Observed
3	0378493_0152_re_0168	Amine	Plate 5	J12	415.12784	C20H19F2N5OS	80	ASMS Binding Not Observed
3	0378493_0152_re_0188	Amine	Plate 5	O12	419.17798	C23H25N5OS	100	ASMS Binding Not Observed
3	0378493_0152_re_0214	Amine	Plate 5	F14	422.18888	C22H26N6OS	38	ASMS Binding Not Observed
3	0378493_0152_re_0241	Amine	Plate 5	M13	427.12336	C21H22ClN5OS	52	ASMS Binding Not Observed
3	0378493_0152_re_0268	Amine	Plate 5	C20	437.15216	C22H23N5O3S	100	10.00µM CHK1
3	0378493_0152_re_0376	Amine	Plate 5	N24	446.16373	C22H22N8OS	75.5	ASMS Binding Not Observed
3	0378493_0152_re_030	Amine	Plate 5	M18	449.1997	C23H27N7OS	49.3	ASMS Binding

	6				8			Not Observed
3	0378493_0152_re_0333	Amine	Plate 5	D21	463.1249	C22H21N7OS2	75.1	ASMS Binding Not Observed
3	0378493_0152_re_0364	Amine	Plate 5	K24	475.17904	C24H25N7O2S	100	5.00µM CHK1
3	Control-01	Suzuki	Standards	D1	353.13103	C18H19N5OS	10 mM Stock	ASMS Binding Not Observed
3	Control-02	Amine	Standards	C1	379.14668	C20H21N5OS	10 mM Stock	ASMS Binding Not Observed
3	Control-03	Suzuki	Standards	B1	424.15691	C22H24N4O3S	10 mM Stock	ASMS Binding Not Observed
3	Control-04	Amine	Standards	F1	445.16848	C23H23N7OS	10 mM Stock	2.50µM CHK1
3	Control-05	Amine	Standards	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
4	0378493_0152_re_0021	Amine	Plate 5	F1	373.15725	C18H23N5O2S	54.9	ASMS Binding Not Observed
4	0378493_0152_re_0044	Amine	Plate 5	K4	384.13684	C18H20N6O2S	34.7	2.50µM CHK1
4	0378493_0152_re_0068	Amine	Plate 5	A8	394.13243	C18H18N8OS	60.2	ASMS Binding Not Observed
4	0378493_0152_re_0090	Amine	Plate 5	G6	401.10925	C17H19N7OS2	94.1	ASMS Binding Not Observed
4	0378493_0152_re_0112	Amine	Plate 5	L8	405.16233	C22H23N5OS	91.2	5.00µM CHK1
4	0378493_0152_re_0140	Amine	Plate 5	C12	410.15249	C20H22N6O2S	74.8	ASMS Binding Not Observed
4	0378493_0152_re_0172	Amine	Plate 5	K12	418.15758	C22H22N6OS	100	ASMS Binding Not Observed
4	0378493_0152_re_0190	Amine	Plate 5	P10	419.17798	C23H25N5OS	51.1	ASMS Binding Not Observed
4	0378493_0152_re_0218	Amine	Plate 5	G14	423.13651	C21H21N5O3S	31.9	10.00µM CHK1
4	0378493_0152_re_0248	Amine	Plate 5	N16	427.14782	C21H22FN5O2S	100	ASMS Binding Not Observed
4	0378493_0152_re_0276	Amine	Plate 5	E20	439.16781	C22H25N5O3S	76	ASMS Binding Not Observed
4	0378493_0152_re_0292	Amine	Plate 5	I20	447.06874	C20H19Cl2N5OS	48.4	ASMS Binding Not Observed
4	0378493_0152_re_0315	Amine	Plate 5	O19	455.08098	C17H16F3N7OS2	26.2	ASMS Binding Not Observed
4	0378493_0152_re_0345	Amine	Plate 5	G21	466.12457	C22H22N6O2S2	92.5	0.31µM CHK1
4	0378493_0152_re_0338	Amine	Plate 5	E22	478.16095	C24H26N6OS2	93.1	ASMS Binding Not Observed
4	Control-01	Suzuki	Control	D1	353.13103	C18H19N5OS	10 mM Stock	ASMS Binding Not Observed
4	Control-02	Amine	Control	C1	379.14668	C20H21N5OS	10 mM Stock	ASMS Binding Not Observed
4	Control-03	Suzuki	Control	B1	424.15691	C22H24N4O3S	10 mM Stock	ASMS Binding Not Observed
4	Control-04	Amine	Control	F1	445.1684	C23H23N7OS	10 mM	2.50µM CHK1

					8		Stock	
4	Control-05	Amine	Control	A1	459.1841 3	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
5	0378493_0152_re_0025	Amine	Plate 5	G1	380.1419 3	C19H20N6OS	100	ASMS Binding Not Observed
5	0378493_0152_re_0050	Amine	Plate 5	M2	386.0983 5	C17H18N6OS2	35.5	ASMS Binding Not Observed
5	0378493_0152_re_0072	Amine	Plate 5	B8	394.1575 8	C20H22N6OS	29.8	10.00µM CHK1
5	0378493_0152_re_0093	Amine	Plate 5	H5	401.1885 5	C20H27N5O2S	48.7	ASMS Binding Not Observed
5	0378493_0152_re_0120	Amine	Plate 5	N8	407.1779 8	C22H25N5OS	100	ASMS Binding Not Observed
5	0378493_0152_re_0141	Amine	Plate 5	D9	411.1477 4	C19H21N7O2S	67.3	ASMS Binding Not Observed
5	0378493_0152_re_0174	Amine	Plate 5	L10	419.1528 3	C21H21N7OS	50	ASMS Binding Not Observed
5	0378493_0152_re_0194	Amine	Plate 5	A14	420.1368 4	C21H20N6O2S	83	ASMS Binding Not Observed
5	0378493_0152_re_0224	Amine	Plate 5	H16	423.1729	C22H25N5O2S	28.1	ASMS Binding Not Observed
5	0378493_0152_re_0256	Amine	Plate 5	P16	433.1184 2	C20H18F3N5OS	65.7	ASMS Binding Not Observed
5	0378493_0152_re_0278	Amine	Plate 5	F18	439.2154 3	C22H29N7OS	44.1	ASMS Binding Not Observed
5	0378493_0152_re_0296	Amine	Plate 5	J20	447.1340 7	C21H20F3N5OS	24.8	ASMS Binding Not Observed
5	0378493_0152_re_0317	Amine	Plate 5	P17	455.1591 4	C23H23F2N5OS	77.7	ASMS Binding Not Observed
5	0378493_0152_re_0349	Amine	Plate 5	H21	466.1787 1	C23H26N6O3S	100	ASMS Binding Not Observed
5	0378493_0152_re_0370	Amine	Plate 5	M22	478.2150 9	C25H30N6O2S	65.4	ASMS Binding Not Observed
5	Control-01	Suzuki	Control	D1	353.1310 3	C18H19N5OS	10 mM Stock	10.00µM CHK1
5	Control-02	Amine	Control	C1	379.1466 8	C20H21N5OS	10 mM Stock	10.00µM CHK1
5	Control-03	Suzuki	Control	B1	424.1569 1	C22H24N4O3S	10 mM Stock	ASMS Binding Not Observed
5	Control-04	Amine	Control	F1	445.1684 8	C23H23N7OS	10 mM Stock	2.50µM CHK1
5	Control-05	Amine	Control	A1	459.1841 3	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
6	0378493_0152_0385	Amide	Plate 2	A1	345.1259 5	C16H19N5O2S	65.1	ASMS Binding Not Observed
6	0378493_0152_0393	Amide	Plate 2	C1	373.1572 5	C18H23N5O2S	55.7	ASMS Binding Not Observed
6	0378493_0152_0408	Amide	Plate 2	F4	407.1416	C21H21N5O2S	79.1	1.25µM CHK1
6	0378493_0152_0420	Amide	Plate 2	I4	408.1368 4	C20H20N6O2S	100	ASMS Binding Not Observed

6	0378493_0152_0430	Amide	Plate 2	L2	413.1885 5	C21H27N5O2S	42.3	ASMS Binding Not Observed
6	0378493_0152_0438	Amide	Plate 2	N2	422.1524 9	C21H22N6O2S	90.2	1.25µM CHK1
6	0378493_0152_0446	Amide	Plate 2	P2	425.1321 7	C21H20FN5O2S	94.4	ASMS Binding Not Observed
6	0378493_0152_0462	Amide	Plate 2	D6	437.1521 6	C22H23N5O3S	65.8	1.25µM CHK1
6	0378493_0152_0476	Amide	Plate 2	G8	441.1026 2	C21H20ClN5O2S	85.6	2.50µM CHK1
6	0378493_0152_0490	Amide	Plate 2	K6	451.1678 1	C23H25N5O3S	93.6	0.16µM CHK1
6	0378493_0152_0500	Amide	Plate 2	M8	467.1627 3	C23H25N5O4S	85.9	ASMS Binding Not Observed
6	0378493_0152_0508	Amide	Plate 2	O8	497.0944 9	C21H16F5N5O2S	42.7	ASMS Binding Not Observed
6	Control-01	Suzuki	Control	D1	353.1310 3	C18H19N5OS	10 mM Stock	ASMS Binding Not Observed
6	Control-02	Amine	Control	C1	379.1466 8	C20H21N5OS	10 mM Stock	ASMS Binding Not Observed
6	Control-03	Suzuki	Control	B1	424.1569 1	C22H24N4O3S	10 mM Stock	5.00µM CHK1
6	Control-04	Amine	Control	F1	445.1684 8	C23H23N7OS	10 mM Stock	ASMS Binding Not Observed
6	Control-05	Amine	Control	A1	459.1841 3	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
7	0378493_0152_0390	Amide	Plate 2	B2	373.1572 5	C18H23N5O2S	48.8	ASMS Binding Not Observed
7	0378493_0152_0402	Amide	Plate 2	E2	401.1521 6	C19H23N5O3S	82.4	ASMS Binding Not Observed
7	0378493_0152_0416	Amide	Plate 2	H4	408.1368 4	C20H20N6O2S	89.2	2.50µM CHK1
7	0378493_0152_0424	Amide	Plate 2	J4	413.0980 2	C19H19N5O2S2	87.6	1.25µM CHK1
7	0378493_0152_0436	Amide	Plate 2	M4	421.1572 5	C22H23N5O2S	65.4	2.50µM CHK1
7	0378493_0152_0444	Amide	Plate 2	O4	425.1321 7	C21H20FN5O2S	89.6	1.25µM CHK1
7	0378493_0152_0456	Amide	Plate 2	B8	428.1630 6	C20H24N6O3S	81.8	ASMS Binding Not Observed
7	0378493_0152_0467	Amide	Plate 2	E7	437.1521 6	C22H23N5O3S	77.1	10.00µM CHK1
7	0378493_0152_0488	Amide	Plate 2	J8	449.1521 6	C23H23N5O3S	78.1	0.16µM CHK1
7	0378493_0152_0495	Amide	Plate 2	L7	451.1678 1	C23H25N5O3S	69.4	10.00µM CHK1
7	0378493_0152_0503	Amide	Plate 2	N7	476.1994 4	C25H28N6O2S	18.2	ASMS Binding Not Observed
7	0378493_0152_0512	Amide	Plate 2	P8	522.1307 9	C25H23FN6O2S2	71.9	ASMS Binding Not Observed
7	Control-01	Suzuki	Control	D1	353.1310 3	C18H19N5OS	10 mM Stock	ASMS Binding Not Observed

7	Control-02	Amine	Control	C1	379.14668	C20H21N5OS	10 mM Stock	ASMS Binding Not Observed
7	Control-03	Suzuki	Control	B1	424.15691	C22H24N4O3S	10 mM Stock	ASMS Binding Not Observed
7	Control-04	Amine	Control	F1	445.16848	C23H23N7OS	10 mM Stock	2.50µM CHK1
7	Control-05	Amine	Control	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
8	0378493_0152_0515	Sulfonamide	Plate 2	A11	381.09293	C15H19N5O3S2	84.3	ASMS Binding Not Observed
8	0378493_0152_0521	Sulfonamide	Plate 2	C9	407.10858	C17H21N5O3S2	85.2	ASMS Binding Not Observed
8	0378493_0152_0531	Sulfonamide	Plate 2	E11	423.13988	C18H25N5O3S2	79.6	ASMS Binding Not Observed
8	0378493_0152_0539	Sulfonamide	Plate 2	G11	444.10383	C19H20N6O3S2	64.7	ASMS Binding Not Observed
8	0378493_0152_0547	Sulfonamide	Plate 2	I11	449.065	C18H19N5O3S3	44.8	ASMS Binding Not Observed
8	0378493_0152_0561	Sulfonamide	Plate 2	M9	457.12423	C21H23N5O3S2	76.9	ASMS Binding Not Observed
8	0378493_0152_0571	Sulfonamide	Plate 2	O11	468.10383	C21H20N6O3S2	63	ASMS Binding Not Observed
8	0378493_0152_0577	Sulfonamide	Plate 2	A13	473.11915	C21H23N5O4S2	94.6	ASMS Binding Not Observed
8	0378493_0152_0587	Sulfonamide	Plate 2	C15	479.08974	C20H19F2N5O3S2	67.8	ASMS Binding Not Observed
8	0378493_0152_0593	Sulfonamide	Plate 2	E13	485.11915	C22H23N5O4S2	95.7	ASMS Binding Not Observed
8	0378493_0152_0603	Sulfonamide	Plate 2	G15	497.08032	C20H18F3N5O3S2	41	ASMS Binding Not Observed
8	0378493_0152_0615	Sulfonamide	Plate 2	J15	511.09597	C21H20F3N5O3S2	63.9	ASMS Binding Not Observed
8	0378493_0152_0623	Sulfonamide	Plate 2	L15	527.09088	C21H20F3N5O4S2	64.1	ASMS Binding Not Observed
8	0378493_0152_0629	Sulfonamide	Plate 2	N13	539.14094	C24H25N7O4S2	80	ASMS Binding Not Observed
8	0378493_0152_0640	Sulfonamide	Plate 2	P16	579.08335	C22H19F6N5O3S2	66.8	ASMS Binding Not Observed
8	Control-01	Suzuki	Control	D1	353.13103	C18H19N5OS	10 mM Stock	5.00µM CHK1
8	Control-02	Amine	Control	C1	379.14668	C20H21N5OS	10 mM Stock	10.00µM CHK1
8	Control-03	Suzuki	Control	B1	424.15691	C22H24N4O3S	10 mM Stock	10.00µM CHK1
8	Control-04	Amine	Control	F1	445.16848	C23H23N7OS	10 mM Stock	0.63µM CHK1
8	Control-05	Amine	Control	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
9	0378493_0152_0517	Sulfonamid	Plate 2	B9	395.1085	C16H21N5O3S2	82.8	ASMS Binding

		e			8			Not Observed
9	0378493_0152_0527	Sulfonamide	Plate 2	D11	421.12423	C18H23N5O3S2	100	ASMS Binding Not Observed
9	0378493_0152_0535	Sulfonamide	Plate 2	F11	443.10858	C20H21N5O3S2	78.3	ASMS Binding Not Observed
9	0378493_0152_0543	Sulfonamide	Plate 2	H11	447.11473	C18H21N7O3S2	43.3	ASMS Binding Not Observed
9	0378493_0152_0559	Sulfonamide	Plate 2	L11	457.12423	C21H23N5O3S2	79.8	ASMS Binding Not Observed
9	0378493_0152_0567	Sulfonamide	Plate 2	N11	458.11948	C20H22N6O3S2	31	ASMS Binding Not Observed
9	0378493_0152_0575	Sulfonamide	Plate 2	P11	468.10383	C21H20N6O3S2	28.7	ASMS Binding Not Observed
9	0378493_0152_0582	Sulfonamide	Plate 2	B14	475.11481	C21H22FN5O3S2	68.6	ASMS Binding Not Observed
9	0378493_0152_0589	Sulfonamide	Plate 2	D13	483.13988	C23H25N5O3S2	94.1	ASMS Binding Not Observed
9	0378493_0152_0597	Sulfonamide	Plate 2	F13	487.1348	C22H25N5O4S2	91.7	ASMS Binding Not Observed
9	0378493_0152_0605	Sulfonamide	Plate 2	H13	500.13004	C22H24N6O4S2	77	ASMS Binding Not Observed
9	0378493_0152_0618	Sulfonamide	Plate 2	K14	516.98706	C18H17Cl2N5O3S3	28.5	ASMS Binding Not Observed
9	0378493_0152_0627	Sulfonamide	Plate 2	M15	531.12462	C23H25N5O6S2	85.2	ASMS Binding Not Observed
9	0378493_0152_0633	Sulfonamide	Plate 2	O13	561.11743	C24H27N5O5S3	26.7	ASMS Binding Not Observed
9	Control-01	Suzuki	Control	D1	353.13103	C18H19N5OS	10 mM Stock	2.50µM CHK1
9	Control-02	Amine	Control	C1	379.14668	C20H21N5OS	10 mM Stock	10.00µM CHK1
9	Control-03	Suzuki	Control	B1	424.15691	C22H24N4O3S	10 mM Stock	10.00µM CHK1
9	Control-04	Amine	Control	F1	445.16848	C23H23N7OS	10 mM Stock	0.63µM CHK1
9	Control-05	Amine	Control	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
10	0378493_0152_0643	Alkyne	Plate 2	A19	388.13578	C22H20N4OS	100	ASMS Binding Not Observed
10	0378493_0152_0658	Alkyne	Plate 2	E18	392.14193	C20H20N6OS	100	ASMS Binding Not Observed
10	0378493_0152_0675	Alkyne	Plate 2	I19	418.14635	C23H22N4O2S	100	10.00µM CHK1
10	0378493_0152_0695	Alkyne	Plate 2	N19	428.16708	C25H24N4OS	100	5.00µM CHK1
10	0378493_0152_0703	Alkyne	Plate 2	P19	433.12423	C19H23N5O3S2	43.1	ASMS Binding Not Observed
10	0378493_0152_0711	Alkyne	Plate 2	B23	440.14193	C24H20N6OS	100	ASMS Binding Not Observed
10	0378493_0152_0719	Alkyne	Plate 2	D23	445.15725	C24H23N5O2S	100	10.00µM CHK1
10	0378493_0152_0727	Alkyne	Plate 2	F23	450.1525	C24H23FN4O2S	58.9	ASMS Binding

					7			Not Observed
10	0378493_0152_0735	Alkyne	Plate 2	H23	455.1416	C25H21N5O2S	100	ASMS Binding Not Observed
10	0378493_0152_0766	Alkyne	Plate 2	P22	457.11842	C22H18F3N5OS	24.4	ASMS Binding Not Observed
10	0378493_0152_0741	Alkyne	Plate 2	J21	471.20928	C27H29N5OS	100	10.00µM CHK1
10	0378493_0152_0749	Alkyne	Plate 2	L21	481.12423	C23H23N5O3S2	100	5.00µM CHK1
10	0378493_0152_0758	Alkyne	Plate 2	N22	541.1106	C26H25Cl2N5O2S	70.6	ASMS Binding Not Observed
10	Control-01	Suzuki	Control	D1	353.13103	C18H19N5OS	10 mM Stock	5.00µM CHK1
10	Control-02	Amine	Control	C1	379.14668	C20H21N5OS	10 mM Stock	5.00µM CHK1
10	Control-03	Suzuki	Control	B1	424.15691	C22H24N4O3S	10 mM Stock	10.00µM CHK1
10	Control-05	Amine	Control	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
11	0378493_0152_0647	Alkyne	Plate 2	B19	390.12628	C20H18N6OS	77.9	ASMS Binding Not Observed
11	0378493_0152_0670	Alkyne	Plate 2	H18	407.12161	C21H18FN5OS	35.1	ASMS Binding Not Observed
11	0378493_0152_0679	Alkyne	Plate 2	J19	419.10858	C18H21N5O3S2	100	ASMS Binding Not Observed
11	0378493_0152_0699	Alkyne	Plate 2	O19	432.162	C24H24N4O2S	72.1	ASMS Binding Not Observed
11	0378493_0152_0707	Alkyne	Plate 2	A23	440.08739	C22H18ClFN4OS	90.9	ASMS Binding Not Observed
11	0378493_0152_0715	Alkyne	Plate 2	C23	444.19838	C26H28N4OS	100	ASMS Binding Not Observed
11	0378493_0152_0723	Alkyne	Plate 2	E23	448.15691	C24H24N4O3S	100	ASMS Binding Not Observed
11	0378493_0152_0731	Alkyne	Plate 2	G23	450.15257	C24H23FN4O2S	51	ASMS Binding Not Observed
11	0378493_0152_0739	Alkyne	Plate 2	I23	471.1729	C26H25N5O2S	34.6	ASMS Binding Not Observed
11	0378493_0152_0747	Alkyne	Plate 2	K23	472.11808	C23H19F3N4O2S	83.3	ASMS Binding Not Observed
11	0378493_0152_0754	Alkyne	Plate 2	M22	524.11055	C24H18F6N4OS	41.5	ASMS Binding Not Observed
11	0378493_0152_0763	Alkyne	Plate 2	O23	541.13392	C29H24ClN5O2S	100	ASMS Binding Not Observed
11	Control-01	Suzuki	Control	D1	353.13103	C18H19N5OS	10 mM Stock	2.50µM CHK1
11	Control-02	Amine	Control	C1	379.14668	C20H21N5OS	10 mM Stock	5.00µM CHK1
11	Control-03	Suzuki	Control	B1	424.15691	C22H24N4O3S	10 mM Stock	5.00µM CHK1
11	Control-05	Amine	Control	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source**	**Sourc**	**Mass**	**Formula**	**%Conv**	**Protein Conc.**

			Plate	e Wells			.	First Observed
12	0378493_0152_0769	Thiol	Plate 3	A1	386.0983 5	C17H18N6OS2	100	ASMS Binding Not Observed
12	0378493_0152_0782	Thiol	Plate 3	D2	405.1293 2	C18H23N5O2S2	100	ASMS Binding Not Observed
12	0378493_0152_0798	Thiol	Plate 3	H2	426.1184 2	C21H22N4O2S2	100	0.00µM CHK1
12	0378493_0152_0959	Thiol	Plate 3	P11	440.0976 8	C21H20N4O3S2	86.9	10.00µM CHK1
12	0378493_0152_0820	Thiol	Plate 3	M4	450.1296 5	C22H22N6OS2	77.4	ASMS Binding Not Observed
12	0378493_0152_0838	Thiol	Plate 3	B6	456.1289 8	C22H24N4O3S2	100	0.00µM CHK1
12	0378493_0152_0857	Thiol	Plate 3	G5	464.1201 5	C21H20N8OS2	54.6	ASMS Binding Not Observed
12	0378493_0152_0870	Thiol	Plate 3	J6	478.1133 3	C24H22N4O3S2	100	0.16µM CHK1
12	0378493_0152_0896	Thiol	Plate 3	P8	489.0963	C21H23N5O3S3	77.8	ASMS Binding Not Observed
12	0378493_0152_0906	Thiol	Plate 3	C10	493.1242 3	C24H23N5O3S2	100	ASMS Binding Not Observed
12	0378493_0152_0917	Thiol	Plate 3	F9	500.1776 6	C22H28N8O2S2	82.3	ASMS Binding Not Observed
12	0378493_0152_0932	Thiol	Plate 3	I12	504.1402 2	C25H24N6O2S2	81.6	10.00µM CHK1
12	0378493_0152_0952	Thiol	Plate 3	N12	544.1326 9	C25H23F3N6OS2	66	ASMS Binding Not Observed
12	Control-01	Suzuki	Control	D1	353.1310 3	C18H19N5OS	10 mM Stock	2.50µM CHK1
12	Control-02	Amine	Control	C1	379.1466 8	C20H21N5OS	10 mM Stock	5.00µM CHK1
12	Control-03	Suzuki	Control	B1	424.1569 1	C22H24N4O3S	10 mM Stock	10.00µM CHK1
12	Control-04	Amine	Control	F1	445.1684 8	C23H23N7OS	10 mM Stock	0.31µM CHK1
12	Control-05	Amine	Control	A1	459.1841 3	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
13	0378493_0152_0776	Thiol	Plate 3	B4	387.0936	C16H17N7OS2	32.4	ASMS Binding Not Observed
13	0378493_0152_0786	Thiol	Plate 3	E2	412.114	C19H20N6OS2	44.3	ASMS Binding Not Observed
13	0378493_0152_0806	Thiol	Plate 3	J2	438.1548	C23H26N4OS2	100	0.00µM CHK1
13	0378493_0152_0813	Thiol	Plate 3	L1	442.1609 5	C21H26N6OS2	100	ASMS Binding Not Observed
13	0378493_0152_0826	Thiol	Plate 3	O2	453.1293 2	C22H23N5O2S2	100	0.00µM CHK1
13	0378493_0152_0844	Thiol	Plate 3	C8	459.1511 1	C20H25N7O2S2	72.4	ASMS Binding Not Observed
13	0378493_0152_0867	Thiol	Plate 3	I7	475.0806 5	C20H21N5O3S3	100	ASMS Binding Not Observed
13	0378493_0152_0884	Thiol	Plate 3	M8	480.1402	C23H24N6O2S2	80.9	0.16µM CHK1

					2			
13	0378493_0152_0898	Thiol	Plate 3	A10	490.2072 3	C24H34N4O3S2	74.1	0.16µM CHK1
13	0378493_0152_0910	Thiol	Plate 3	D10	494.1058	C22H21F3N4O2S2	96.3	0.00µM CHK1
13	0378493_0152_0924	Thiol	Plate 3	G12	502.1057 2	C22H20F2N6O2S2	37	ASMS Binding Not Observed
13	0378493_0152_0933	Thiol	Plate 3	J9	519.1875	C26H29N7OS2	27.7	0.00µM CHK1
13	Control-01	Suzuki	Control	D1	353.1310 3	C18H19N5OS	10 mM Stock	2.50µM CHK1
13	Control-02	Amine	Control	C1	379.1466 8	C20H21N5OS	10 mM Stock	10.00µM CHK1
13	Control-03	Suzuki	Control	B1	424.1569 1	C22H24N4O3S	10 mM Stock	5.00µM CHK1
13	Control-04	Amine	Control	F1	445.1684 8	C23H23N7OS	10 mM Stock	0.31µM CHK1
13	Control-05	Amine	Control	A1	459.1841 3	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
14	0378493_0152_0779	Thiol	Plate 3	C3	403.0595 2	C17H17N5OS3	73.5	ASMS Binding Not Observed
14	0378493_0152_0789	Thiol	Plate 3	F1	414.1296 5	C19H22N6OS2	100	ASMS Binding Not Observed
14	0378493_0152_0809	Thiol	Plate 3	K1	439.1500 5	C22H25N5OS2	100	0.16µM CHK1
14	0378493_0152_0953	Thiol	Plate 3	O9	447.1187 5	C23H21N5OS2	94.8	ASMS Binding Not Observed
14	0378493_0152_0830	Thiol	Plate 3	P2	453.1293 2	C22H23N5O2S2	95.4	ASMS Binding Not Observed
14	0378493_0152_0850	Thiol	Plate 3	E6	464.0299 1	C20H18Cl2N4OS2	100	ASMS Binding Not Observed
14	0378493_0152_0804	Thiol	Plate 3	I4	478.1108 9	C22H21F3N4OS2	100	ASMS Binding Not Observed
14	0378493_0152_0890	Thiol	Plate 3	O6	488.2643 5	C26H40N4OS2	100	0.16µM CHK1
14	0378493_0152_0902	Thiol	Plate 3	B10	491.0868	C19H21N7O3S3	38.4	ASMS Binding Not Observed
14	0378493_0152_0913	Thiol	Plate 3	E9	496.1602 8	C25H28N4O3S2	100	ASMS Binding Not Observed
14	0378493_0152_0927	Thiol	Plate 3	H11	504.1013 9	C22H19F3N6OS2	36.9	ASMS Binding Not Observed
14	0378493_0152_0944	Thiol	Plate 3	L12	533.2031 5	C27H31N7OS2	22.8	ASMS Binding Not Observed
14	Control-01	Suzuki	Control	D1	353.1310 3	C18H19N5OS	10 mM Stock	5.00µM CHK1
14	Control-02	Amine	Control	C1	379.1466 8	C20H21N5OS	10 mM Stock	5.00µM CHK1
14	Control-03	Suzuki	Control	B1	424.1569 1	C22H24N4O3S	10 mM Stock	5.00µM CHK1
14	Control-04	Amine	Control	F1	445.1684 8	C23H23N7OS	10 mM Stock	1.25µM CHK1
14	Control-05	Amine	Control	A1	459.1841 3	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed

Pool	Sample Name	Chemistry	Source Plate	Source Wells	Mass	Formula	%Conv.	Protein Conc. First Observed
15	0378493_0152_0961	Alcohol	Plate 3	A13	374.14126	C18H22N4O3S	100	ASMS Binding Not Observed
15	0378493_0152_0977	Alcohol	Plate 3	E13	392.13407	C18H24N4O2S2	88.5	ASMS Binding Not Observed
15	0378493_0152_0989	Alcohol	Plate 3	H13	398.12127	C20H19FN4O2S	94.9	ASMS Binding Not Observed
15	0378493_0152_1021	Alcohol	Plate 3	P13	405.12595	C21H19N5O2S	72.2	ASMS Binding Not Observed
15	0378493_0152_1033	Alcohol	Plate 3	C17	408.162	C22H24N4O2S	100	ASMS Binding Not Observed
15	0378493_0152_1049	Alcohol	Plate 3	G17	409.15725	C21H23N5O2S	100	ASMS Binding Not Observed
15	0378493_0152_1061	Alcohol	Plate 3	J17	412.13692	C21H21FN4O2S	100	5.00µM CHK1
15	0378493_0152_1097	Alcohol	Plate 3	C21	416.11185	C20H18F2N4O2S	100	ASMS Binding Not Observed
15	0378493_0152_1117	Alcohol	Plate 3	H21	422.17765	C23H26N4O2S	100	ASMS Binding Not Observed
15	0378493_0152_1133	Alcohol	Plate 3	L21	429.12932	C20H23N5O2S2	95.8	ASMS Binding Not Observed
15	0378493_0152_1149	Alcohol	Plate 3	P21	434.15249	C22H22N6O2S	96.9	ASMS Binding Not Observed
15	0378493_0152_1161	Alcohol	Plate 4	C1	438.18379	C22H26N6O2S	100	ASMS Binding Not Observed
15	0378493_0152_1185	Alcohol	Plate 4	I1	448.11808	C21H19F3N4O2S	97.1	ASMS Binding Not Observed
15	0378493_0152_1213	Alcohol	Plate 4	P1	477.21985	C26H31N5O2S	35.1	ASMS Binding Not Observed
15	0378493_0152_1201	Alcohol	Plate 4	M1	491.16273	C25H25N5O4S	100	ASMS Binding Not Observed
15	Control-01	Suzuki	Control	D1	353.13103	C18H19N5OS	10 mM Stock	2.50µM CHK1
15	Control-02	Amine	Control	C1	379.14668	C20H21N5OS	10 mM Stock	5.00µM CHK1
15	Control-03	Suzuki	Control	B1	424.15691	C22H24N4O3S	10 mM Stock	10.00µM CHK1
15	Control-04	Amine	Control	F1	445.16848	C23H23N7OS	10 mM Stock	0.63µM CHK1
15	Control-05	Amine	Control	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
16	0378493_0152_0965	Alcohol	Plate 3	B13	381.12595	C19H19N5O2S	100	ASMS Binding Not Observed
16	0378493_0152_0981	Alcohol	Plate 3	F13	395.1416	C20H21N5O2S	100	ASMS Binding Not Observed
16	0378493_0152_1001	Alcohol	Plate 3	K13	400.10277	C19H20N4O2S2	100	ASMS Binding Not Observed
16	0378493_0152_1025	Alcohol	Plate 3	A17	406.14972	C19H26N4O2S2	100	ASMS Binding Not Observed
16	0378493_0152_1041	Alcohol	Plate 3	E17	408.162	C22H24N4O2S	100	5.00µM CHK1

16	0378493_0152_1053	Alcohol	Plate 3	H17	410.14126	C21H22N4O3S	100	ASMS Binding Not Observed
16	0378493_0152_1069	Alcohol	Plate 3	L17	413.15216	C20H23N5O3S	100	ASMS Binding Not Observed
16	0378493_0152_1109	Alcohol	Plate 3	F21	422.17765	C23H26N4O2S	100	ASMS Binding Not Observed
16	0378493_0152_1125	Alcohol	Plate 3	J21	424.12053	C21H20N4O4S	85.6	ASMS Binding Not Observed
16	0378493_0152_1140	Alcohol	Plate 3	M24	429.12932	C20H23N5O2S2	40.1	ASMS Binding Not Observed
16	0378493_0152_1153	Alcohol	Plate 4	A1	434.17765	C24H26N4O2S	100	ASMS Binding Not Observed
16	0378493_0152_1177	Alcohol	Plate 4	G1	444.10229	C21H21ClN4O3S	100	ASMS Binding Not Observed
16	0378493_0152_1193	Alcohol	Plate 4	K1	452.12423	C19H19F3N6O2S	98.1	ASMS Binding Not Observed
16	0378493_0152_1207	Alcohol	Plate 4	N3	542.10585	C25H24Cl2N6O2S	50	ASMS Binding Not Observed
16	Control-01	Suzuki	Control	D1	353.13103	C18H19N5OS	10 mM Stock	5.00µM CHK1
16	Control-02	Amine	Control	C1	379.14668	C20H21N5OS	10 mM Stock	5.00µM CHK1
16	Control-03	Suzuki	Control	B1	424.15691	C22H24N4O3S	10 mM Stock	10.00µM CHK1
16	Control-04	Amine	Control	F1	445.16848	C23H23N7OS	10 mM Stock	1.25µM CHK1
16	Control-05	Amine	Control	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
17	0378493_0152_0973	Alcohol	Plate 3	D13	388.15691	C19H24N4O3S	65.4	ASMS Binding Not Observed
17	0378493_0152_0985	Alcohol	Plate 3	G13	395.1416	C20H21N5O2S	100	ASMS Binding Not Observed
17	0378493_0152_1008	Alcohol	Plate 3	L16	401.15216	C19H23N5O3S	70.6	ASMS Binding Not Observed
17	0378493_0152_1029	Alcohol	Plate 3	B17	408.162	C22H24N4O2S	100	2.50µM CHK1
17	0378493_0152_1045	Alcohol	Plate 3	F17	409.15725	C21H23N5O2S	87.1	ASMS Binding Not Observed
17	0378493_0152_1057	Alcohol	Plate 3	I17	410.14126	C21H22N4O3S	83.6	ASMS Binding Not Observed
17	0378493_0152_1081	Alcohol	Plate 3	O17	415.08697	C19H18ClN5O2S	42.1	ASMS Binding Not Observed
17	0378493_0152_1113	Alcohol	Plate 3	G21	422.17765	C23H26N4O2S	70.1	ASMS Binding Not Observed
17	0378493_0152_1129	Alcohol	Plate 3	K21	426.15257	C22H23FN4O2S	83.6	2.50µM CHK1
17	0378493_0152_1157	Alcohol	Plate 4	B1	436.15691	C23H24N4O3S	100	ASMS Binding Not Observed
17	0378493_0152_1209	Alcohol	Plate 4	O1	438.17256	C23H26N4O3S	100	ASMS Binding Not Observed
17	0378493_0152_1181	Alcohol	Plate 4	H1	444.14315	C22H22F2N4O2S	74	ASMS Binding Not Observed
17	0378493_0152_1197	Alcohol	Plate 4	L1	455.1627	C22H25N5O4S	100	ASMS Binding

					3			Not Observed
17	0378493_0152_1141	Alcohol	Plate 3	N21	463.2042	C25H29N5O2S	66.1	ASMS Binding Not Observed
17	Control-01	Suzuki	Control	D1	353.13103	C18H19N5OS	10 mM Stock	2.50µM CHK1
17	Control-02	Amine	Control	C1	379.14668	C20H21N5OS	10 mM Stock	5.00µM CHK1
17	Control-03	Suzuki	Control	B1	424.15691	C22H24N4O3S	10 mM Stock	5.00µM CHK1
17	Control-04	Amine	Control	F1	445.16848	C23H23N7OS	10 mM Stock	0.63µM CHK1
17	Control-05	Amine	Control	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
18	0378493_0152_1217	Suzuki	Plate 4	A5	354.11505	C18H18N4O2S	100	10.00µM CHK1
18	0378493_0152_1245	Suzuki	Plate 4	H5	378.15143	C21H22N4OS	100	2.50µM CHK1
18	0378493_0152_1257	Suzuki	Plate 4	K5	389.13103	C21H19N5OS	100	ASMS Binding Not Observed
18	0378493_0152_1274	Suzuki	Plate 4	O6	392.16708	C22H24N4OS	84	ASMS Binding Not Observed
18	0378493_0152_1474	Suzuki	Plate 4	A22	396.14201	C21H21FN4OS	100	ASMS Binding Not Observed
18	0378493_0152_1309	Suzuki	Plate 4	H9	403.14668	C22H21N5OS	94.1	0.63µM CHK1
18	0378493_0152_1321	Suzuki	Plate 4	K9	406.14635	C22H22N4O2S	100	2.50µM CHK1
18	0378493_0152_1518	Suzuki	Plate 4	L22	408.14201	C22H21FN4OS	94	10.00µM CHK1
18	0378493_0152_1354	Suzuki	Plate 4	C14	412.13692	C21H21FN4O2S	100	1.25µM CHK1
18	0378493_0152_1370	Suzuki	Plate 4	G14	420.10785	C22H20N4OS2	100	5.00µM CHK1
18	0378493_0152_1380	Suzuki	Plate 4	I16	421.19363	C23H27N5OS	30	ASMS Binding Not Observed
18	0378493_0152_1530	Suzuki	Plate 4	O22	424.13915	C22H24N4OS2	100	10.00µM CHK1
18	0378493_0152_1411	Suzuki	Plate 4	A19	428.10737	C21H21ClN4O2S	100	10.00µM CHK1
18	0378493_0152_1434	Suzuki	Plate 4	G18	440.16822	C23H25FN4O2S	93.9	ASMS Binding Not Observed
18	0378493_0152_1469	Suzuki	Plate 4	P17	456.13867	C23H25ClN4O2S	100	ASMS Binding Not Observed
18	Control-01	Suzuki	Control	D1	353.13103	C18H19N5OS	10 mM Stock	5.00µM CHK1
18	Control-04	Amine	Control	F1	445.16848	C23H23N7OS	10 mM Stock	1.25µM CHK1
18	Control-05	Amine	Control	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**

19	0378493_0152_1227	Suzuki	Plate 4	C7	354.1262 8	C17H18N6OS	34.6	ASMS Binding Not Observed
19	0378493_0152_1489	Suzuki	Plate 4	E21	379.1466 8	C20H21N5OS	100	0.63µM CHK1
19	0378493_0152_1262	Suzuki	Plate 4	L6	389.1310 3	C21H19N5OS	100	10.00µM CHK1
19	0378493_0152_1278	Suzuki	Plate 4	P6	392.1670 8	C22H24N4OS	38	ASMS Binding Not Observed
19	0378493_0152_1297	Suzuki	Plate 4	E9	396.1420 1	C21H21FN4OS	95.1	10.00µM CHK1
19	0378493_0152_1457	Suzuki	Plate 4	M17	404.1419 3	C21H20N6OS	16.7	2.50µM CHK1
19	0378493_0152_1329	Suzuki	Plate 4	M9	406.1827 3	C23H26N4OS	100	ASMS Binding Not Observed
19	0378493_0152_1498	Suzuki	Plate 4	G22	408.162	C22H24N4O2S	100	2.50µM CHK1
19	0378493_0152_1534	Suzuki	Plate 4	P22	412.1369 2	C21H21FN4O2S	100	2.50µM CHK1
19	0378493_0152_1365	Suzuki	Plate 4	F13	420.1078 5	C22H20N4OS2	100	1.25µM CHK1
19	0378493_0152_1381	Suzuki	Plate 4	J13	422.1412 6	C22H22N4O3S	100	10.00µM CHK1
19	0378493_0152_1398	Suzuki	Plate 4	N14	424.1569 1	C22H24N4O3S	100	1.25µM CHK1
19	0378493_0152_1414	Suzuki	Plate 4	B18	432.1231 7	C21H19F3N4OS	100	ASMS Binding Not Observed
19	0378493_0152_1426	Suzuki	Plate 4	E18	440.1682 2	C23H25FN4O2S	100	ASMS Binding Not Observed
19	0378493_0152_1446	Suzuki	Plate 4	J18	456.162	C26H24N4O2S	100	ASMS Binding Not Observed
19	Control-01	Suzuki	Control	D1	353.1310 3	C18H19N5OS	10 mM Stock	5.00µM CHK1
19	Control-04	Amine	Control	F1	445.1684 8	C23H23N7OS	10 mM Stock	1.25µM CHK1
19	Control-05	Amine	Control	A1	459.1841 3	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
20	0378493_0152_1229	Suzuki	Plate 4	D5	364.1357 8	C20H20N4OS	100	5.00µM CHK1
20	0378493_0152_1494	Suzuki	Plate 4	F22	380.1307	C20H20N4O2S	100	5.00µM CHK1
20	0378493_0152_1265	Suzuki	Plate 4	M5	390.1262 8	C20H18N6OS	28	ASMS Binding Not Observed
20	0378493_0152_1281	Suzuki	Plate 4	A9	392.1670 8	C22H24N4OS	100	5.00µM CHK1
20	0378493_0152_1522	Suzuki	Plate 4	M22	396.1983 8	C22H28N4OS	100	ASMS Binding Not Observed
20	0378493_0152_1526	Suzuki	Plate 4	N22	404.1670 8	C23H24N4OS	100	ASMS Binding Not Observed
20	0378493_0152_1327	Suzuki	Plate 4	L11	406.1827 3	C23H26N4OS	96.3	1.25µM CHK1
20	0378493_0152_1344	Suzuki	Plate 4	P12	408.162	C22H24N4O2S	100	ASMS Binding Not Observed
20	0378493_0152_1361	Suzuki	Plate 4	E13	414.1514 3	C24H22N4OS	100	1.25µM CHK1

20	0378493_0152_1502	Suzuki	Plate 4	H22	420.162	C23H24N4O2S	100	5.00µM CHK1
20	0378493_0152_1385	Suzuki	Plate 4	K13	422.15249	C21H22N6O2S	100	ASMS Binding Not Observed
20	0378493_0152_1404	Suzuki	Plate 4	O16	426.14741	C20H22N6O3S	50	5.00µM CHK1
20	0378493_0152_1417	Suzuki	Plate 4	C17	432.12317	C21H19F3N4OS	100	ASMS Binding Not Observed
20	0378493_0152_1429	Suzuki	Plate 4	F17	442.11333	C21H22N4O3S2	91.5	ASMS Binding Not Observed
20	0378493_0152_1514	Suzuki	Plate 4	K22	458.13882	C23H21F3N4OS	100	ASMS Binding Not Observed
20	Control-01	Suzuki	Control	D1	353.13103	C18H19N5OS	10 mM Stock	5.00µM CHK1
20	Control-04	Amine	Control	F1	445.16848	C23H23N7OS	10 mM Stock	1.25µM CHK1
20	Control-05	Amine	Control	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
21	0378493_0152_1238	Suzuki	Plate 4	F6	365.13103	C19H19N5OS	100	ASMS Binding Not Observed
21	0378493_0152_1485	Suzuki	Plate 4	D21	382.15758	C19H22N6OS	37.1	ASMS Binding Not Observed
21	0378493_0152_1269	Suzuki	Plate 4	N5	390.15143	C22H22N4OS	100	5.00µM CHK1
21	0378493_0152_1288	Suzuki	Plate 4	B12	394.14635	C21H22N4O2S	93.6	2.50µM CHK1
21	0378493_0152_1303	Suzuki	Plate 4	F11	398.09681	C20H19ClN4OS	100	2.50µM CHK1
21	0378493_0152_1313	Suzuki	Plate 4	I9	406.14635	C22H22N4O2S	100	ASMS Binding Not Observed
21	0378493_0152_1333	Suzuki	Plate 4	N9	407.1416	C21H21N5O2S	100	10.00µM CHK1
21	0378493_0152_1346	Suzuki	Plate 4	A14	408.162	C22H24N4O2S	100	2.50µM CHK1
21	0378493_0152_1357	Suzuki	Plate 4	D13	415.14668	C23H21N5OS	100	ASMS Binding Not Observed
21	0378493_0152_1450	Suzuki	Plate 4	K18	420.19838	C24H28N4OS	97.8	ASMS Binding Not Observed
21	0378493_0152_1389	Suzuki	Plate 4	L13	422.17765	C23H26N4O2S	100	ASMS Binding Not Observed
21	0378493_0152_1405	Suzuki	Plate 4	P13	426.15257	C22H23FN4O2S	100	0.63µM CHK1
21	0378493_0152_1289	Suzuki	Plate 4	C9	436.1933	C24H28N4O2S	100	ASMS Binding Not Observed
21	0378493_0152_1439	Suzuki	Plate 4	H19	448.11808	C21H19F3N4O2S	100	ASMS Binding Not Observed
21	0378493_0152_1454	Suzuki	Plate 4	L18	458.15766	C26H23FN4OS	100	ASMS Binding Not Observed
21	Control-01	Suzuki	Control	D1	353.13103	C18H19N5OS	10 mM Stock	5.00µM CHK1
21	Control-04	Amine	Control	F1	445.16848	C23H23N7OS	10 mM Stock	0.63µM CHK1
21	Control-05	Amine	Control	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed

Pool	Sample Name	Chemistry	Source Plate	Source Wells	Mass	Formula	%Conv.	Protein Conc. First Observed
22	0378493_0152_1241	Suzuki	Plate 4	G5	366.1262 8	C18H18N6OS	61.4	ASMS Binding Not Observed
22	0378493_0152_1254	Suzuki	Plate 4	J6	384.1078 5	C19H20N4OS2	79.5	10.00µM CHK1
22	0378493_0152_1505	Suzuki	Plate 4	I21	390.1514 3	C22H22N4OS	32.3	10.00µM CHK1
22	0378493_0152_1293	Suzuki	Plate 4	D9	396.1420 1	C21H21FN4OS	100	1.25µM CHK1
22	0378493_0152_1305	Suzuki	Plate 4	G9	400.1169 4	C20H18F2N4OS	100	ASMS Binding Not Observed
22	0378493_0152_1319	Suzuki	Plate 4	J11	406.1463 5	C22H22N4O2S	100	5.00µM CHK1
22	0378493_0152_1339	Suzuki	Plate 4	O11	408.1256 1	C21H20N4O3S	100	10.00µM CHK1
22	0378493_0152_1351	Suzuki	Plate 4	B15	412.1124 6	C21H21ClN4OS	100	5.00µM CHK1
22	0378493_0152_1462	Suzuki	Plate 4	N18	415.1466 8	C23H21N5OS	100	ASMS Binding Not Observed
22	0378493_0152_1373	Suzuki	Plate 4	H13	421.1572 5	C22H23N5O2S	100	5.00µM CHK1
22	0378493_0152_1393	Suzuki	Plate 4	M13	422.1776 5	C23H26N4O2S	100	ASMS Binding Not Observed
22	0378493_0152_1465	Suzuki	Plate 4	O17	426.1525 7	C22H23FN4O2S	100	ASMS Binding Not Observed
22	0378493_0152_1422	Suzuki	Plate 4	D18	436.1933	C24H28N4O2S	100	ASMS Binding Not Observed
22	0378493_0152_1444	Suzuki	Plate 4	I20	450.1137 4	C21H18F4N4OS	100	ASMS Binding Not Observed
22	Control-01	Suzuki	Control	D1	353.1310 3	C18H19N5OS	10 mM Stock	5.00µM CHK1
22	Control-04	Amine	Control	F1	445.1684 8	C23H23N7OS	10 mM Stock	1.25µM CHK1
22	Control-05	Amine	Control	A1	459.1841 3	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
23 Low Yields	0378493_0152_re_0007	Amine	Plate 5	B3	357.1623 3	C18H23N5OS	8.8	ASMS Binding Not Observed
23 Low Yields	0378493_0152_re_0046	Amine	Plate 5	L2	384.1368 4	C18H20N6O2S	8.5	ASMS Binding Not Observed
23 Low Yields	0378493_0152_re_0082	Amine	Plate 5	E6	400.114	C18H20N6OS2	15.9	ASMS Binding Not Observed
23 Low Yield	0378493_0152_re_0122	Amine	Plate 5	O6	407.1779 8	C22H25N5OS	22.6	ASMS Binding Not Observed

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23 Low Yields	0378493_0152_re_0210	Amine	Plate 5	E14	421.19363	C23H27N5OS	19.1	ASMS Binding Not Observed
23 Low Yields	0378493_0152_re_0226	Amine	Plate 5	I14	423.1729	C22H25N5O2S	22.6	ASMS Binding Not Observed
23 Low Yields	0378493_0152_0397	Amide	Plate 2	D1	387.1729	C19H25N5O2S	14.2	ASMS Binding Not Observed
23 Low Yields	0378493_0152_0451	Amide	Plate 2	A7	428.10892	C19H20N6O2S2	6.1	ASMS Binding Not Observed
23 Low Yields	0378493_0152_0549	Sulfonamide	Plate 2	J9	449.08032	C16H18F3N5O3S2	26.4	ASMS Binding Not Observed
23 Low Yields	0378493_0152_0654	Alkyne	Plate 2	D18	442.15758	C24H22N6OS	14.9	ASMS Binding Not Observed
23 Low Yields	0378493_0152_0682	Alkyne	Plate 2	K18	422.21403	C24H30N4OS	9	ASMS Binding Not Observed
23 Low Yields	0378493_0152_0835	Thiol	Plate 3	A7	455.08098	C17H16F3N7OS2	14.4	ASMS Binding Not Observed
23 Low Yields	0378493_0152_0939	Thiol	Plate 3	K11	521.14161	C23H23N9O2S2	9.9	ASMS Binding Not Observed
23 Low Yields	0378493_0152_0969	Alcohol	Plate 3	C13	386.17765	C20H26N4O2S	12.1	ASMS Binding Not Observed
23 Low Yields	0378493_0152_1000	Alcohol	Plate 3	J16	398.15249	C19H22N6O2S	6.8	ASMS Binding Not Observed
23 Low Yields	0378493_0152_1037	Alcohol	Plate 3	D17	462.13373	C22H21F3N4O2S	38.7	ASMS Binding Not Observed
23 Low Yields	0378493_0152_1101	Alcohol	Plate 3	D21	418.16748	C20H26N4O4S	6.9	ASMS Binding Not Observed
23 Low Yield	0378493_0152_1511	Suzuki	Plate 4	J23	390.15143	C22H22N4OS	7.3	ASMS Binding Not Observed

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23 Low Yields	Control-01	Suzuki	Control	D1	353.13103	C18H19N5OS	10 mM Stock	2.50µM CHK1
23 Low Yields	Control-02	Amine	Control	C1	379.14668	C20H21N5OS	10 mM Stock	5.00µM CHK1
23 Low Yields	Control-03	Suzuki	Control	B1	424.15691	C22H24N4O3S	10 mM Stock	10.00µM CHK1
23 Low Yields	Control-04	Amine	Control	F1	445.16848	C23H23N7OS	10 mM Stock	0.63µM CHK1
23 Low Yields	Control-05	Amine	Control	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed
Pool	**Sample Name**	**Chemistry**	**Source Plate**	**Source Wells**	**Mass**	**Formula**	**%Conv.**	**Protein Conc. First Observed**
24 Low Yields	0378493_0152_re_0234	Amine	Plate 5	K14	425.16856	C22H24FN5OS	15.6	ASMS Binding Not Observed
24 Low Yields	0378493_0152_re_0250	Amine	Plate 5	O14	432.17323	C23H24N6OS	9	ASMS Binding Not Observed
24 Low Yields	0378493_0152_re_0270	Amine	Plate 5	D18	437.18855	C23H27N5O2S	10.7	ASMS Binding Not Observed
24 Low Yields	0378493_0152_re_0282	Amine	Plate 5	G18	440.1453	C21H24N6OS2	8.2	ASMS Binding Not Observed
24 Low Yields	0378493_0152_re_0344	Amine	Plate 5	F24	464.19944	C24H28N6O2S	15.7	ASMS Binding Not Observed
24 Low Yields	0378493_0152_0478	Amide	Plate 2	H6	443.12275	C21H19F2N5O2S	12.6	5.00µM CHK1
24 Low Yields	0378493_0152_0556	Sulfonamide	Plate 2	K12	453.11406	C18H23N5O5S2	19	ASMS Binding Not Observed
24 Low Yields	0378493_0152_0662	Alkyne	Plate 2	F18	394.18273	C22H26N4OS	13.9	ASMS Binding Not Observed

24 Low Yields	0378493_0152_0668	Alkyne	Plate 2	G20	397.19363	C21H27N5OS	8.3	ASMS Binding Not Observed
24 Low Yields	0378493_0152_0795	Thiol	Plate 3	G3	420.12898	C19H24N4O3S2	32.1	ASMS Binding Not Observed
24 Low Yields	0378493_0152_0879	Thiol	Plate 3	L7	478.16095	C24H26N6OS2	100	ASMS Binding Not Observed
24 Low Yields	0378493_0152_1068	Alcohol	Plate 3	K20	412.15691	C21H24N4O3S	13.7	ASMS Binding Not Observed
24 Low Yields	0378493_0152_1073	Alcohol	Plate 3	M17	413.18855	C21H27N5O2S	12.5	ASMS Binding Not Observed
24 Low Yields	0378493_0152_1079	Alcohol	Plate 3	N19	414.20895	C22H30N4O2S	13.8	ASMS Binding Not Observed
24 Low Yields	0378493_0152_1085	Alcohol	Plate 3	P17	415.08697	C19H18ClN5O2S	8.7	ASMS Binding Not Observed
24 Low Yields	0378493_0152_1093	Alcohol	Plate 3	B21	415.2042	C21H29N5O2S	10.8	ASMS Binding Not Observed
24 Low Yields	0378493_0152_1173	Alcohol	Plate 4	F1	442.24025	C24H34N4O2S	7	ASMS Binding Not Observed
24 Low Yields	0378493_0152_1233	Suzuki	Plate 4	E5	365.13103	C19H19N5OS	16.4	ASMS Binding Not Observed
24 Low Yields	Control-01	Suzuki	Control	D1	353.13103	C18H19N5OS	10 mM Stock	5.00µM CHK1
24 Low Yields	Control-02	Amine	Control	C1	379.14668	C20H21N5OS	10 mM Stock	5.00µM CHK1
24 Low Yields	Control-03	Suzuki	Control	B1	424.15691	C22H24N4O3S	10 mM Stock	10.00µM CHK1
24 Low Yields	Control-04	Amine	Control	F1	445.16848	C23H23N7OS	10 mM Stock	0.31µM CHK1

24 Low Yields	Control-05	Amine	Control	A1	459.18413	C24H25N7OS	10 mM Stock	ASMS Binding Not Observed

The combined results of this affinity-based competition experiment are plotted below in Figure 45. Plate position was used to separate compounds from each other in addition to nucleophile class. Three examples are shown of high affinity compounds that appeared at low protein concentrations. Pool standards were omitted from this plot for clarity. Protein concentration at which ASMS binding was first observed was used as a guide for the selection of species from this library to scale up and isolate for result confirmation. Compounds were chosen to cover a range of expected activity (based on ASMS binding) and to cover a range of chemistry. High, moderate, and low affinity examples were chosen from all coupling types and are described in Section 8.6.

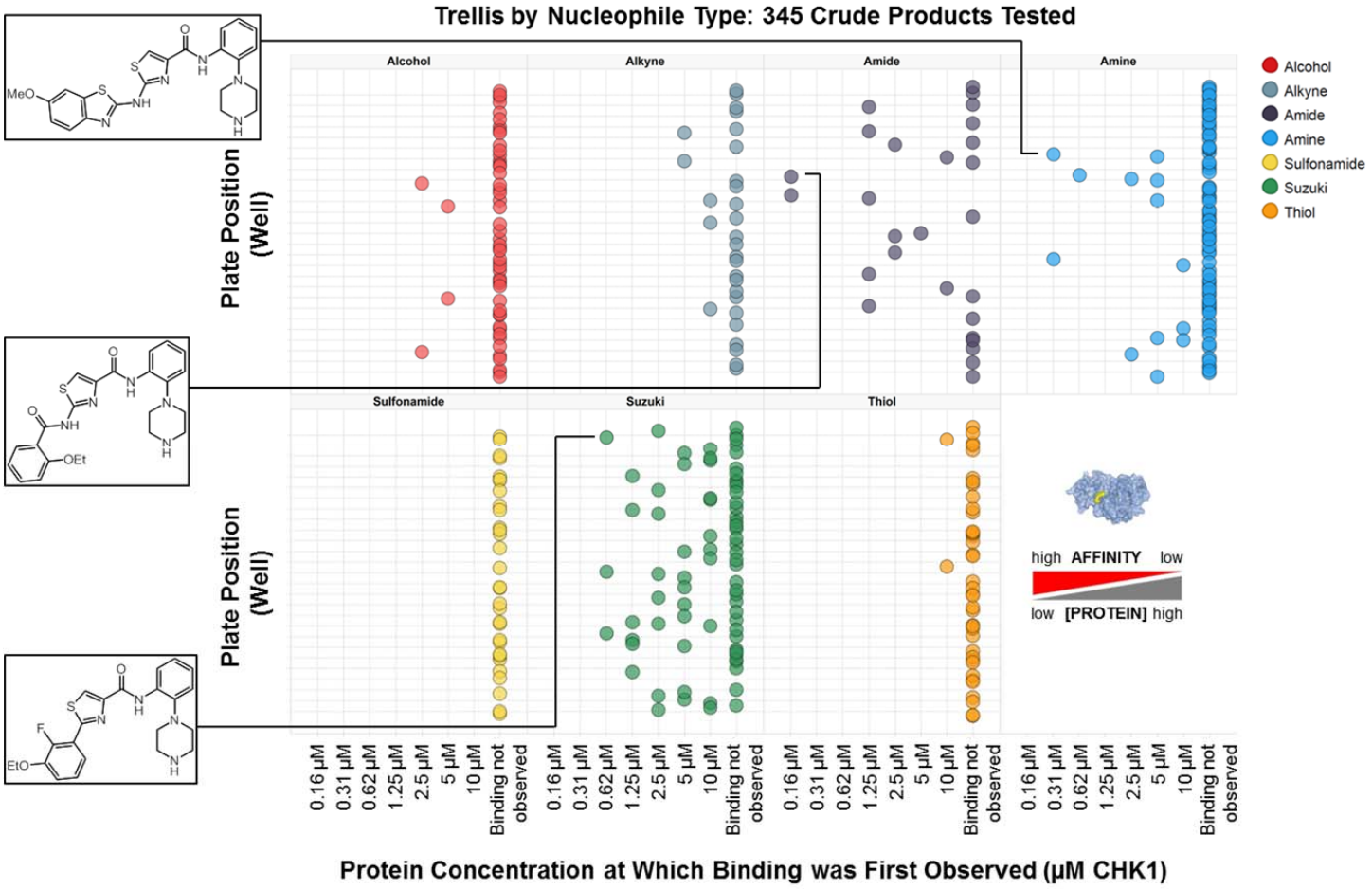


Figure 45. 345-Member Crude Library Affinity Ranking Competition Experiment.

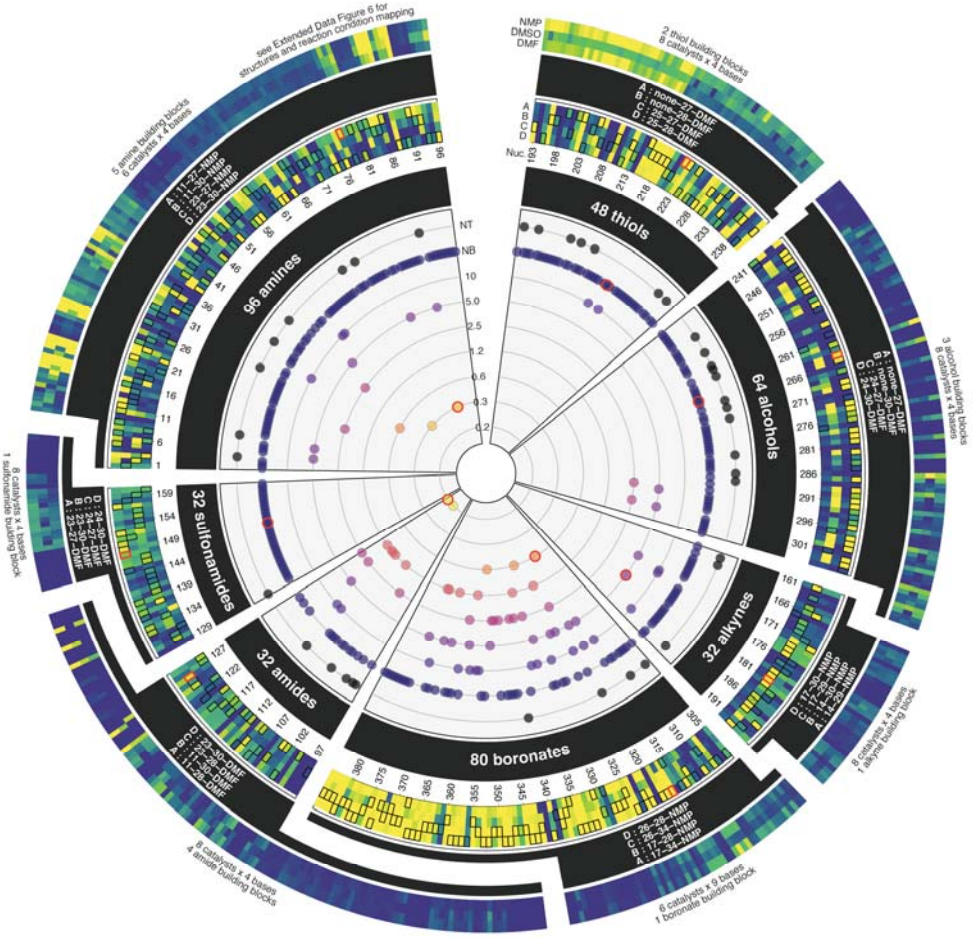
Note: it was observed that some of the products produced from S_NAr reactions with thiol nucleophiles bound to invertase, resulting in false positive results in the affinity-based competition experiment. This was confirmed by subjecting these compounds to the affinity ranking assay in presence of invertase but omitting CHK1. These data points were excluded from the table shown above for the following reasons related to invertase background binding:

1. Abnormal affinity ranking behavior at lower protein concentrations. Signal strength remained constant and low or fluctuated up and down, rather than increasing as protein concentration increased.
2. Presence of these compounds was not constant in the affinity-based ranking experiment; there were gaps (protein levels) where some species were absent between levels where they were present.
3. Very low MS signal intensity

See supplementary excel data tables, data points in question are highlighted. Data were retained when normal affinity ranking behavior was observed: general increase in signal strength with increasing protein concentration).

8.5. CHK1 384-Member Coupling Library Reaction Optimization/Library Synthesis/Affinity Ranking Circlize Visualization

The data from this expanded CHK1 library were visualized using the circlize package in R. A reprint of the graphic generated in R for Figure 3 is shown below along with the script used to generate this image.[16]



pdf("circles-trim-01-18-18.pdf", useDingbats = FALSE)

#open and assign

library(circlize)

library(viridis)

library(dplyr)

```
#selections

pick = as.character(c(39, 40, 37, 35, 36, 38, 41))

chk2 = read.csv("prelim-screening-csv-05-25-17.csv", header = TRUE, sep = ",")

chkf2 = subset(chk2, chk2$Study != "C-N Coupling Screen 1" & chk2$Study != "Suzuki Coupling Screen 1")

factors2 = factor(chkf2$Chemistry)

lev = c("Thiol", "Alcohol", "Alkyne", "Boronate", "Amide", "Sulfonamide", "Amine")

lev2 = factor(factors2, levels = lev)

a2 = data.frame(chkf2$Experiment, lev2, chkf2$Building.Block, chkf2$Solvent, chkf2$Base, chkf2$Catalyst, chkf2$Percent.Yield)

id2 = rep(1:nrow(a2))

a2 = cbind(a2, id2)

chkr2 = data.frame(transform(chkf2, chkf2.rank = ave(a2$id2, chkf2$Solvent, FUN = function(x) rank(x, ties.method = "first"))))

ranky2 = c(chkr2$chkf2.rank)

sol = as.numeric(a2$chkf2.Solvent)

a2 = cbind(a2, sol, ranky2)

nam2 = c(chkr2$Rank..Experiment..)

spot2 = as.numeric(c(a2$Catalyst, a2$Building.Block, a2$Base))


col_fun = colorRamp2(c(-20:100), viridis(121))

col_fun2 = colorRamp2(c(-20:100), viridis(121), transparency = 1)

tccol = plasma(8, alpha = 0.5, begin = 1, end = 0)


par(mar = c(0.3, 0.3, 0.3, 0.3), lwd = 0.5, cex = 0.7)

circos.par(track.height = 0.067, cell.padding = c(0, 0, 0, 0), start.degree = 82.5, gap.degree = c(rep(3, 6), 15))

xlim = do.call("rbind", tapply(chkr2$chkf2.rank, a2$lev2, range))

xlim[, 1] = xlim[, 1] - 0.5

xlim[, 2] = xlim[, 2] + 0.5

circos.initialize(a2$lev2, xlim = xlim)


circos.trackPlotRegion(ylim = c(0, 3), bg.border = "grey16",
```

```
        panel.fun = function(x, y) {

          sector.index = get.cell.meta.data("sector.index")

          a2_subset = a2[a2$lev2 == sector.index, ]

          nr = max(a2_subset$sol)

          circos.text(mean(get.cell.meta.data("xlim")), 4, paste(length(unique(a2_subset$chkf2.Catalyst)), " catalysts x ", length(unique(a2_subset$chkf2.Base)), " bases", sep = ""), sector.index = get.cell.meta.data("sector.index"), cex = 0.6, font = 1, col = "grey16", facing = "bending", niceFacing = TRUE)

          circos.text(mean(get.cell.meta.data("xlim")), 4.9, paste(length(unique(a2_subset$chkf2.Building.Block)), " ", tolower(get.cell.meta.data("sector.index")), " building block", ifelse(length(unique(a2_subset$chkf2.Building.Block)) == 1, "", "s"), sep = ""), sector.index = get.cell.meta.data("sector.index"), cex = 0.6, font = 1, col = "grey16", facing = "bending", niceFacing = TRUE)

          circos.rect(a2_subset$ranky2 - 0.5, nr - a2_subset$sol, a2_subset$ranky2 + 0.5, nr - a2_subset$sol + 1, border = col_fun(a2_subset$chkf2.Percent.Yield), col = col_fun(a2_subset$chkf2.Percent.Yield))

        })

circos.text(427.5, 2.5, "NMP", sector.index = "Thiol", cex = 0.6, font = 1, col = "grey16", facing = "bending", niceFacing = TRUE)

circos.text(426.7, 1.5, "DMSO", sector.index = "Thiol", cex = 0.6, font = 1, col = "grey16", facing = "bending", niceFacing = TRUE)

circos.text(427.3, 0.5, "DMF", sector.index = "Thiol", cex = 0.6, font = 1, col = "grey16", facing = "bending", niceFacing = TRUE)

circos.text(100, 4.9, "see Extended Data Figure 6 for", sector.index = "Amine", cex = 0.6, font = 1, col = "grey16", facing = "bending", niceFacing = TRUE)

circos.text(100, 4, "structures and reaction condition mapping", sector.index = "Amine", cex = 0.6, font = 1, col = "grey16", facing = "bending", niceFacing = TRUE)


circos.trackPlotRegion(ylim = c(0, 1), bg.col = "grey16", bg.border = "grey16", track.height = 0.02, cell.padding = c(0, 0, 0, 0), track.margin = c(0, 0))


circos.clear()


par(new = TRUE)


# open and assign

chk = read.csv("big-library-csv-01-15-18.csv", header = TRUE, sep = ",")


compoundA = c("AdBrettPhos", "Blank", "RockPhos", "RuPhos", "SPhos", "tBu3P", "tBuBrettPhos", "tBuXphos", "aqBTMG", "aqK3PO4", "BTMG", "BTTP", "MTBD", "P2Et")
```

```
compoundB = c("25", "none", "24", "17", "26", "14", "23", "11", "28", "34", "28", "29", "30", "27")

compoundC = c(rep("Catalyst", 8), rep("Base", 6))

compound = data.frame("REAGENT" = compoundA, "NUMBER" = compoundB, "CLASS" = compoundC)

comp = data.frame(Expt.Sample = chk$Expt.Sample, factors = chk$Chemistry, catalyst = chk$Catalyst, base = chk$Base, solvent = chk$Solvent)

comp2 = filter(compound, CLASS == "Catalyst")

comp3 = inner_join(comp, comp2, by = c("catalyst" = "REAGENT"))

comp4 = filter(compound, CLASS == "Base")

comp5 = inner_join(comp3, comp4, by = c("base" = "REAGENT"))

comp6 = select(mutate(comp5, condition = paste(comp5$NUMBER.x, "-", comp5$NUMBER.y, "-", comp5$solvent, sep = "")), Expt.Sample, condition)

chk = merge(chk, comp6, ID = 'Expt.Sample')


chkr = data.frame(transform(chk, chk.rank = ave(as.numeric(condition), Product.ID, FUN = function(x) rank(x,

                                                                    ties.method = "first"))))

id = as.numeric(gsub("Pdt_", "", chkr$Product.ID))

factors = factor(chkr$Chemistry, levels = lev)

tested = chkr$Submitted.to.PT.ALIS

y = c(chkr$Rel....Conv.)

y[is.na(y)] = 0

ranky = c(chkr$chk.rank)

logp = c(chkr$calc_ClogP)

pt = c(chkr$Updated.Protein.Level)

pt2 = c(as.character(chk$Updated.Protein.Level.Numeric))


#data frame

a = data.frame(id, logp, factors, y, ranky, pt, pt2, catalyst = comp$catalyst, base = comp$base, solvent = comp$solvent, tested)

a[is.na(a)] = 0

a_pick = data.frame(factors = unique(factors), pick)

a = merge(a, a_pick, ID = 'factors')
```

```
a = arrange(a, factors, logp, id)


a_list = data.frame(summarise(group_by(a, factors), min.id = min(id), count.id = length(id) / 4))

aa = distinct(a, factors, logp, id, pt2)

aa2 = data.frame(transform(aa, aa.rank = ave(as.numeric(row.names(aa)), aa$factors, FUN = function(x) rank(x, ties.method = "first"))))

aa3 = select(mutate(merge(aa2, a_list, ID = 'factors'), aa.id = aa.rank + min.id - 1), id, aa.id)

aa4 = merge(a, aa3, ID = 'id')

aa4 = arrange(aa4, factors, logp, id)

aa5 = data.frame(id = c(174, 123, 373, 288, 087, 141, 204), catalyst = c("RuPhos", "tBuXphos", "RuPhos", "Blank", "tBuXphos", "tBuBrettPhos", "Blank"), base = c("BTTP", "MTBD", "aqK3PO4", rep("P2Et", 4)), solvent = c("NMP", "DMF", "NMP", "DMF", "NMP", "DMF", "DMF"))

aa5 = right_join(aa4, aa5, by = c('id', 'catalyst', 'base', 'solvent'))


# circlize heatmap

par(mar = c(4, 4, 4, 4), lwd = 0.5, cex = 0.7)

circos.par(cell.padding = c(0, 0, 0.01, 0), start.degree = 82.5, gap.degree = c(rep(3,6), 15))

xlim = do.call("rbind", tapply(id, factors, range))

xlim[, 1] = xlim[, 1] - 0.5

xlim[, 2] = xlim[, 2] + 0.5

circos.initialize(aa4$factors, xlim = xlim)


circos.trackPlotRegion(ylim = c(0, 1), bg.col = "grey16", bg.border = "grey16", track.height = 0.02)


#Amine

L1 = 8.9

L2 = 96.5

BB = "Amine"

circos.rect(L1, 0, L2, 6, col = "grey16", border = "grey16")

for(i in c(max(ranky):min(ranky))) {
```

```
  condition.text = as.character(unique(select(subset(chkr, factors == BB & chk.rank == i), condition)))

  circos.text(mean(c(L1, L2)), 8.5 - 1.8*i, paste(as.character(LETTERS[i]), ":", condition.text), col = "white", cex = 0.6, font = 2, facing = "bending", niceFacing = TRUE)

}


#Thiol

L1 = 114.1

L2 = 160.9

BB = "Thiol"

circos.rect(L1, 0, L2, 6, col = "grey16", border = "grey16")

for(i in c(max(ranky):min(ranky))) {

  condition.text = as.character(unique(select(subset(chkr, factors == BB & chk.rank == i), condition)))

  circos.text(mean(c(L1, L2)), 8.5 - 1.8*i, paste(as.character(LETTERS[i]), ":", condition.text), col = "white", cex = 0.6, font = 2, facing = "bending", niceFacing = TRUE)

}


#Alcohol

L1 = 165.5

L2 = 230

BB = "Alcohol"

circos.rect(L1, 0, L2, 6, col = "grey16", border = "grey16")

for(i in c(max(ranky):min(ranky))) {

  condition.text = as.character(unique(select(subset(chkr, factors == BB & chk.rank == i), condition)))

  circos.text(mean(c(L1, L2)), 8.5 - 1.8*i, paste(as.character(LETTERS[i]), ":", condition.text), col = "white", cex = 0.6, font = 2, facing = "bending", niceFacing = TRUE)

}


#Alkyne

L1 = 238

L2 = 261.3
```

```
BB = "Alkyne"

circos.rect(L1, 0, L2, 6, col = "grey16", border = "grey16")

for(i in c(max(ranky):min(ranky))) {

  condition.text = as.character(unique(select(subset(chkr, factors == BB & chk.rank == i), condition)))

  circos.text(mean(c(L1, L2)), 8.5 - 1.8*i, paste(as.character(LETTERS[i]), ":", condition.text), col = "white", cex = 0.6, font = 2, facing =
"bending", niceFacing = TRUE)

}


#Boronate

L1 = 268

L2 = 304.3

BB = "Boronate"

circos.rect(L1, 0, L2, 6, col = "grey16", border = "grey16")

for(i in c(max(ranky):min(ranky))) {

  condition.text = as.character(unique(select(subset(chkr, factors == BB & chk.rank == i), condition)))

  circos.text(mean(c(L1, L2)), 8.5 - 1.8*i, paste(as.character(LETTERS[i]), ":", condition.text), col = "white", cex = 0.6, font = 2, facing =
"bending", niceFacing = TRUE)

}


#Amide

L1 = 352

L2 = 384.2

BB = "Amide"

circos.rect(L1, 0, L2, 6, col = "grey16", border = "grey16")

for(i in c(max(ranky):min(ranky))) {

  condition.text = as.character(unique(select(subset(chkr, factors == BB & chk.rank == i), condition)))

  circos.text(mean(c(L1, L2)), 8.5 - 1.8*i, paste(as.character(LETTERS[i]), ":", condition.text), col = "white", cex = 0.6, font = 2, facing =
"bending", niceFacing = TRUE)

}
```

```
#Sulfonamide

L1 = 404.75

L2 = 420

BB = "Sulfonamide"

circos.rect(L1, 0, L2, 6, col = "grey16", border = "grey16")

for(i in c(max(ranky):min(ranky))) {

  condition.text = as.character(unique(select(subset(chkr, factors == BB & chk.rank == i), condition)))

  circos.text(mean(c(L1, L2)), 8.5 - 1.8*i, paste(as.character(LETTERS[i]), ":", condition.text), col = "white", cex = 0.6, font = 2, facing = "bending", niceFacing = TRUE)

}



circos.trackPlotRegion(ylim = c(0, 4), track.height = 0.11, track.margin = c(0, 0), bg.border = "grey16",

                panel.fun = function(x, y) {

                  sector.index = get.cell.meta.data("sector.index")

                  a_subset = aa4[aa4$factors == sector.index, ]

                  nr = max(a_subset$ranky)

                  circos.rect(a_subset$aa.id - 0.5, nr - a_subset$ranky, a_subset$aa.id + 0.5, nr - a_subset$ranky + 1, border = col_fun(a_subset$y), col = col_fun(a_subset$y))

                  circos.axis(h = 0, labels = seq(from = min(a_subset$aa.id), to = max(a_subset$aa.id), by = 5), labels.facing = "clockwise", labels.cex = 0.6, major.at = seq(from = min(a_subset$aa.id), to = max(a_subset$aa.id), by = 5), major.tick = TRUE, minor.tick = FALSE, direction = "inside", lwd = 0, major.tick.length = 0.2)

                  aa4 = subset(aa4, aa4$tested != "Untagged")

                  a_subset = aa4[aa4$factors == sector.index, ]

                  circos.rect(a_subset$aa.id - 0.5, nr - a_subset$ranky, a_subset$aa.id + 0.5, nr - a_subset$ranky + 1, border = ifelse(a_subset$id == "172", col_fun(a_subset$y), "black"), col = col_fun(a_subset$y))

                  a_subset = aa5[aa5$factors == sector.index, ]

                  nr = 4

                  circos.rect(a_subset$aa.id - 0.5, nr - a_subset$ranky, a_subset$aa.id + 0.5, nr - a_subset$ranky + 1, border = "red", lwd = 1.1, col = col_fun(a_subset$y))

                })

circos.text(191, 3.5, "A", sector.index = "Thiol", cex = 0.6, font = 1, col = "grey16", facing = "bending", niceFacing = TRUE)
```

```
circos.text(191, 2.5, "B", sector.index = "Thiol", cex = 0.6, font = 1, col = "grey16", facing = "bending", niceFacing = TRUE)

circos.text(191, 1.5, "C", sector.index = "Thiol", cex = 0.6, font = 1, col = "grey16", facing = "bending", niceFacing = TRUE)

circos.text(191, 0.5, "D", sector.index = "Thiol", cex = 0.6, font = 1, col = "grey16", facing = "bending", niceFacing = TRUE)


circos.trackPlotRegion(ylim = c(0, 1), track.height = 0.035, bg.col = NULL, bg.border = col_fun2(a$y))

circos.text(190, 0.5, "Nuc.", sector.index = "Thiol", cex = 0.6, font = 1, col = "grey16", facing = "bending", niceFacing = TRUE)


# circlize pt plot

circos.trackPlotRegion(ylim = c(0, 1), bg.col = "grey16", bg.border = "grey16", track.height = 0.10, track.margin = c(0.01, 0.01),

                panel.fun = function(x, y) {

                  circos.text(mean(get.cell.meta.data("xlim")), 0.5, tolower(paste(max(get.cell.meta.data("xlim")) -
min(get.cell.meta.data("xlim")), " ", get.cell.meta.data("sector.index"), "s", sep = "")), cex = 0.9, font = 2, col = "white", facing =
"bending", niceFacing = TRUE)

                })

circos.trackPlotRegion(aa4$factors, y = aa4$pt, track.height = 0.60, track.margin = c(0, 0), cell.padding = c(0.05, 0, 0.05, 0), bg.col =
"grey96")

for(k in levels(as.factor(aa4$pt))) {

  circos.trackLines(aa4$factors, aa4$aa.id, rep(as.numeric(k), 1536), col = 'grey75')

}

circos.trackPoints(aa4$factors, aa4$aa.id, aa4$pt, col = 'grey75', cex = 1.2, pch = 1)

circos.trackPoints(aa4$factors, aa4$aa.id, aa4$pt, col = adjustcolor(colorRampPalette(c(tccol, bias = 1))(9)[as.numeric(cut(aa4$pt,

                                                                breaks = 9))], alpha.f = 0.2), pch = 20, cex = 1.6)

circos.trackPoints(aa5$factors, aa5$aa.id, aa5$pt, col = 'red', cex = 1.2, pch = 1)

circos.trackPoints(aa5$factors, aa5$aa.id, aa5$pt, col = 'red', cex = 1.4, pch = 1)

circos.text(rep(100, 9), unique(aa4$pt), c("NB","NT", "10", "2.5", "5.0", "0.6", "1.2", "0.2", "0.3"), sector.index = "Amine", cex = 0.6,
font = 1, col = "grey16", facing = "bending", niceFacing = TRUE)

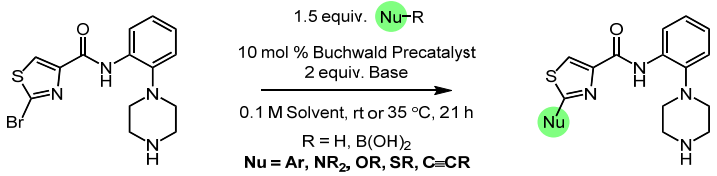


circos.clear()

dev.off()
```

8.6. Compound Selection for Scale Up, IC_{50} Measurement, Confirmation

General procedure for the coupling of various nucleophiles to 2-bromo-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide:



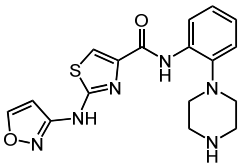
General procedure: The aryl bromide core above was weighed into a 1-dram vial (18.3 mg, 1 equiv., 0.05 mmol scale) equipped with a magnetic stir bar. The vial was moved to a glove box where solvent was added and the core dissolved. The desired monomer building block (1.5 equiv., 0.075 mmol in desired solvent) was next added the vial, followed by the correct G2/G3 precatalyst (10 mol %, 0.005 mmol, added as a stock solution in solvent). Finally, the base was added as a 0.8 M stock solution in reaction solvent to the reaction and the vial was sealed (0.1 mmol, 2 equiv., added in water for Suzuki cross-coupling reactions or in NMP/DMF for other coupling reactions). The vial was removed from the glove box and stirred at temperature ranging from ambient temperature to 35 ˚C for 21 hours. The next morning, aliquots were taken of all reactions and progress was determined by LC-MS. Upon completion, reactions were diluted with DMSO (1.5 mL), filtered, and submitted for purification by RP-HPLC. Products were returned as TFA salts unless otherwise noted. After purification and characterization the coupling products were dissolved in DMSO to a concentration of 10 mM.

Workup: For challenging separations the following procedure was performed[8]: the reaction was concentrated and taken up in 2-MeTHF. The crude reaction was then quenched with sat. aq. NH_4Cl and product extracted twice with 2-MeTHF. The combined organics were washed with brine, dried with $MgSO_4$, and concentrated. The crude residue was then taken up in DMSO, filtered, and submitted for purification by preparatory RP-HPLC.

Compound selections: Examples were selected to capture a range of expected activity against CHK1 and to cover all reaction types that were tested. Examples present at the lowest protein concentrations (expected to be potent binders/inhibitors) were chosen along with uncompetitive examples that were either not observed or only observed at higher protein concentrations to show a correlation between affinity ranking result and CHK1 activity. For transformations that did not produce highly competitive binders of CHK1 (e.g. sulfonamide C-N coupling, C-O coupling, Sonogashira coupling) selections were made from the library of weak/uncompetitive members.

Note: Many of the compounds scaled up in this library were fully characterized after the synthesis/purification/DMSO dilution/ submission to the *in vitro* CHK1 assay workflow. Before acquisition of ^{1}H and ^{13}C NMR spectra the DMSO was removed via centrifugal evaporator andproducts were redissolved in DMSO-d_6. However, trace residual DMSO was still visible in some spectra. ^{1}H signal: 2.53 ppm (s), ^{13}C signal: 40.4 ppm (s).[17]

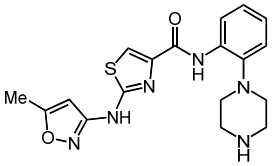
2-(isoxazol-3-ylamino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E1)



The title compound was prepared using isoxazol-3-amine (0.075 mmol, 1.5 equiv., MFCD00038814), *t*-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), P_2-Et (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol

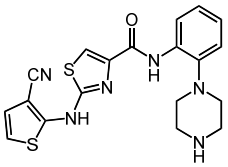
scale and stirred for 21 hours at 35 ˚C. The product was purified by RP-HPLC to yield 3.9 mg (21% yield) of the title compound as a off-white residue. Analytical data for **E1**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 11.34 (s, 1H), 9.92 (s, 1H), 8.91 (br s, 2H), 8.84 (s, 1H), 8.33 (d, *J* = 7.9 Hz, 1H), 7.91 (s, 1H), 7.28 (d, *J* = 7.7 Hz, 1H), 7.21 (t, *J* = 7.5 Hz, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 6.54 (s, 1H), 3.37 (br s, 4H), 3.07 (br s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 161.2, 160.4, 158.1, 157.7, 145.0, 140.8, 132.4, 125.3, 124.2, 120.4, 119.4, 117.4, 97.3, 48.6, 43.7; **HRMS** (ESI): *m/z* calculated for $C_{17}H_{19}N_6O_2S$ [M+H]+ 371.12847, found 371.12790. ASMS protein concentration first observed: 5.0 µM CHK1; Measured IC_{5o} (CHK1, Invitrogen) 83.6 nM.

2-((5-methylisoxazol-3-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (44)



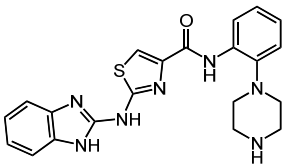
The title compound was prepared using 5-methylisoxazol-3-amine (0.075 mmol, 1.5 equiv., MFCD00003155), *t*-BuBrettPhos (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at 35 ˚C. The product was purified by RP-HPLC to yield 6.7 mg (27% yield) of the title compound as a off-white residue (TFA salt). Analytical data for **44**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 11.23 (br s, 1H), 9.89 (s, 1H), 8.76 (br s, 2H), 8.30 (d, *J* = 7.9 Hz, 1H), 7.88 (s, 1H), 7.27 (d, *J* = 7.7 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 6.24 (s, 1H), 3.35 (s, 4H), 3.06 (s, 4H), 2.40 (s, 3H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 169.8, 161.2, 158.3, 158.1, 144.9, 140.8, 132.3, 125.2, 124.2, 120.3, 119.4, 117.2, 94.2, 48.6, 43.7, 12.11 **HRMS** (ESI): *m/z* calculated for $C_{18}H_{21}N_6O_2S$ [M+H]+ 385.14412, found 385.14362; ASMS protein concentration first observed: 2.5 µM CHK1; Measured IC_{5o} (CHK1, Invitrogen) 17.9 nM.

2-((3-cyanothiophen-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E2)



The title compound was prepared using 2-aminothiophene-3-carbonitrile (0.075 mmol, 1.5 equiv., MFCD00706298), *t*-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at 35 ˚C. The product was purified by RP-HPLC to yield 18.9 mg (72% yield) of the title compound as a white solid (TFA salt). Analytical data for **E2**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.26 (s, 1H), 9.54 (s, 1H), 8.71 (br s, 2H), 8.20 (d, *J* = 7.8 Hz, 1H), 7.92 (s, 1H), 7.29 (d, *J* = 7.7 Hz, 1H), 7.22 (t, *J* = 7.4 Hz, 2H), 7.18 (t, *J* = 7.3 Hz, 1H), 7.11 (d, *J* = 4.9 Hz, 1H), 3.17 (s, 4H), 3.06 (s, 4H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 161.2, 157.9, 152.4, 144.5, 141.5, 131.8, 125.6, 125.0, 124.7, 120.7, 120.1, 118.0, 116.2, 115.1, 90.3, 48.5, 43.5; **HRMS** (ESI): *m/z* calculated for $C_{19}H_{19}N_6OS_2$ [M+H]+ 411.10563, found 411.10474; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{5o} (CHK1, Invitrogen) 784 nM.

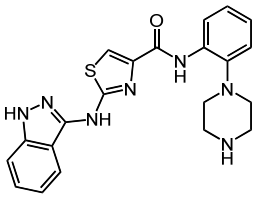
2-((1H-benzo[d]imidazol-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E3)



The title compound was prepared using 1H-benzo[d]imidazol-2-amine (0.075 mmol, 1.5 equiv., MFCD00005596), *t*-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at 35 ˚C. The product was purified by RP-HPLC to yield 15.9 mg (60% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E3**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 11.94 (br s, 1H), 10.06 (s,

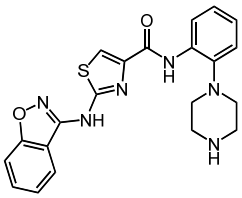
1H), 8.56 (br s, 2H), 8.10 (d, *J* = 7.6 Hz, 1H), 7.70 (s, 1H), 7.32 (dd, *J* = 5.5, *J* = 3.2 Hz, 2H), 7.25 (dd, *J* = 7.6, *J* = 1.3 Hz, 1H), 7.20 (m, 2H), 7.13 (m, 2H), 3.10 (br s, 4H), 3.05 (m, 4H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 158.6, 158.4, 158.2, 158.0, 157.8, 148.87, 142.8, 132.3, 124.8, 121.9, 120.4, 115.9, 48.1, 43.7, 40.4, 39.9; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{22}N_7OS$ [M+H]+ 420.16011, found 420.16022; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

2-((1H-indazol-3-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E4)



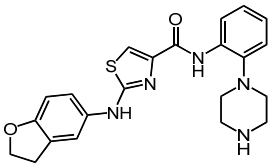
The title compound was prepared using 1H-indazol-3-amine (0.075 mmol, 1.5 equiv., MFCD00182045), *t*-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at 35 ˚C. The product was purified by RP-HPLC to yield 12.7 mg (61% yield) of the title compound as a white solid (TFA salt). Analytical data for **E4**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.86 (s, 1H), 8.69 (br s, 2H), 8.47 (d, *J* = 8.2 Hz, 1H), 8.30 (d, *J* = 7.8 Hz, 1H), 8.04 (s, 1H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.4 Hz, 1H), 7.33 (d, *J* = 7.7 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.19 (t, *J* = 7.4 Hz, 1H), 6.69 (s, 2H), 3.25 (s, 4H), 3.11 (s, 4H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 161.6, 158.2, 153.1, 146.8, 142.7, 138.0, 132.6, 129.6, 124.6, 124.2, 122.6, 121.5, 120.7, 119.2, 119.2, 118.4, 112.8, 53.4, 45.9; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{22}N_7OS$ [M+H]+ 420.16011, found 420.16028. ASMS protein concentration first observed: 0.31 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 4.6 nM.

2-(benzo[d]isoxazol-3-ylamino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E5)



The title compound was prepared using benzo[d]isoxazol-3-amine (0.075 mmol, 1.5 equiv., MFCD03407353), t-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at 35 ˚C. The product was purified by RP-HPLC to yield 3.2 mg (12% yield) of the title compound as a white solid (TFA salt). Analytical data for **E5**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.05 (br s, 1H), 9.96 (s, 1H), 8.83 (br s, 2H), 8.30 (d, *J* = 7.9 Hz, 1H), 8.17 (d, *J* = 7.9 Hz, 1H), 8.03 (s, 1H), 7.72 (d, *J* = 3.2 Hz, 2H), 7.45 (m, 1H), 7.29 (d, *J* = 7.7 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 1H), 3.44 (br s, 4H), 3.09 (br s, 4H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 162.2, 160.4, 158.1, 152.9, 145.1, 140.9, 132.2, 131.3, 125.2, 124.3, 123.4, 121.8, 120.2, 119.7, 118.3, 114.9, 110.1, 48.6, 43.6; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{21}N_6O_2S$ [M+H]+ 421.14412, found 421.14359; ASMS protein concentration first observed: 2.5 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 15.3 nM.

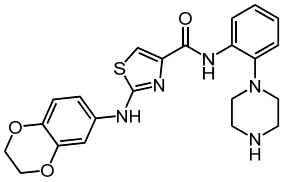
2-((2,3-dihydrobenzofuran-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E6)



The title compound was prepared using 2,3-dihydrobenzofuran-5-amine (0.075 mmol, 1.5 equiv., MFCD03617969), *t*-BuBrettPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at 35 ˚C. The product was purified by RP-HPLC to yield 24.5 mg (91% yield) of the

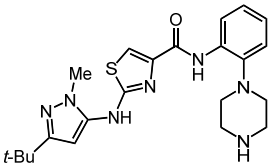
title compound as a white solid (TFA salt). Analytical data for **E6**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.04 (s, 1H), 9.79 (s, 1H), 8.70 (br s, 2H), 8.26 (d, *J* = 7.9 Hz, 1H), 7.60 (s, 1H), 7.48 (d, *J* = 8.2 Hz, 1H), 7.30 (s, 1H), 7.27 (d, *J* = 7.7 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 6.82 (d, *J* = 8.4 Hz, 1H), 6.54 (s, 1H), 4.52 (t, *J* = 8.6 Hz, 2H), 3.23 (s, 4H), 3.19 (t, *J* = 8.6 Hz, 2H), 3.05 (s, 4H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 165.4, 158.2, 155.7, 145.5, 140.9, 133.9, 132.2, 128.4, 125.2, 124.2, 120.2, 119.8, 118.3, 116.5, 113.4, 109.1, 71.0, 48.5, 43.8, 29.4; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{24}N_5O_2S$ [M+H]+ 422.16452, found 422.16467; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 303 nM.

2-((2,3-dihydrobenzo[b][1,4]dioxin-6-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E7)



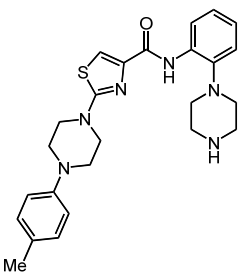
The title compound was prepared using 2,3-dihydrobenzo[b][1,4]dioxin-6-amine (0.075 mmol, 1.5 equiv., MFCD00006824), *t*-BuBrettPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at 35 ˚C. The product was purified by RP-HPLC to yield 22.5 mg (82% yield) of the title compound as a white solid (TFA salt). Analytical data for **E7**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.27 (s, 1H), 9.64 (s, 1H), 8.75 (br s, 2H), 8.26 (d, *J* = 7.9 Hz, 1H), 7.68 (s, 1H), 7.46 (s, 1H), 7.27 (d, *J* = 7.7 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 1H), 6.92 (d, *J* = 8.6 Hz, 1H), 6.88 (d, *J* = 8.7 Hz, 1H), 4.23 (d, *J* = 6.6 Hz, 4H), 3.26 (s, 4H), 3.06 (s, 4H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 164.1, 158.2, 145.4, 143.3, 141.0, 138.6, 134.6, 132.0, 125.1, 124.4, 120.1, 120.0, 117.5, 114.1, 110.7, 106.0, 64.2, 63.8, 48.5, 43.6; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{24}N_5O_3S$ [M+H]+ 438.15944, found 438.15906; ASMS protein concentration first observed: 10.0 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 165 nM.

2-((3-(tert-butyl)-1-methyl-1H-pyrazol-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E8)



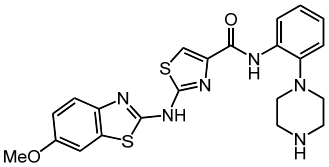
The title compound was prepared using 3-(tert-butyl)-1-methyl-1H-pyrazol-5-amine (0.075 mmol, 1.5 equiv., MFCD00068002), *t*-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at 35 ˚C. The product was purified by RP-HPLC to yield 7.8 mg (28% yield) of the title compound as a white solid (TFA salt). Analytical data for **E8**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.01 (s, 1H), 9.90 (s, 1H), 8.77 (br s, 2H), 8.25 (d, *J* = 7.9 Hz, 1H), 7.67 (s, 1H), 7.26 (d, *J* = 7.7 Hz, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 6.24 (s, 1H), 3.68 (s, 3H), 3.32 (s, 4H), 3.05 (s, 4H), 1.23 (s, 9H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 166.5, 159.5, 158.1, 145.6, 140.8, 138.6, 132.3, 125.3, 124.2, 120.3, 119.4, 114.7, 94.4, 48.5, 43.8, 35.0, 31.0, 30.3; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{30}N_7OS$ [M+H]+ 440.22271, found 440.22287; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

N-(2-(piperazin-1-yl)phenyl)-2-(4-(p-tolyl)piperazin-1-yl)thiazole-4-carboxamide (E9)



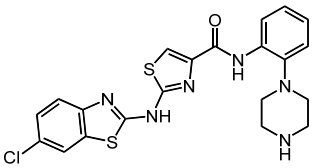
The title compound was prepared using 1-(p-tolyl)piperazine (0.075 mmol, 1.5 equiv., MFCD00040737), *t*-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at 35 ˚C. The product was purified by RP-HPLC to yield 10.7 mg (37% yield) of the title compound as a white solid (TFA salt). Analytical data for **E9**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.05 (s, 1H), 9.05 (br s, 2H), 8.41 (d, *J* = 8.0 Hz, 1H), 7.70 (s, 1H), 7.30 (d, *J* = 7.8 Hz, 1H), 7.21 (t, *J* = 7.7 Hz, 1H), 7.13 (t, *J* = 7.5 Hz, 1H), 7.08 (d, *J* = 8.2 Hz, 2H), 6.92 (d, *J* = 8.3 Hz, 2H), 3.65 (s, 4H), 3.32 (s, 4H), 3.27 (s, 4H), 3.06 (s, 4H), 2.21 (s, 3H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 170.4, 158.3, 148.6, 145.9, 140.4, 132.8, 129.5, 128.6, 125.7, 124.0, 120.8, 118.8, 116.4, 114.0, 48.7, 48.3, 48.0, 44.1, 20.1; **HRMS** (ESI): *m/z* calculated for $C_{25}H_{31}N_6OS$ [M+H]+ 463.22746, found 463.22690; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{5o} (CHK1, Invitrogen) 2140 nM.

2-((6-methoxybenzo[d]thiazol-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (41)



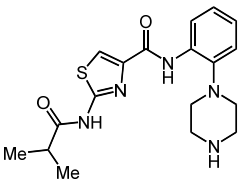
The title compound was prepared using 6-methoxybenzo[d]thiazol-2-amine (0.075 mmol, 1.5 equiv., MFCD00005787), *t*-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), P_2-Et (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at 35 ˚C. The product was purified by RP-HPLC to yield 7 mg (24% yield) of the title compound as a off-white solid (TFA salt). Analytical data for **41**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.92 (s, 1H), 8.33 (d, *J* = 7.7 Hz, 1H), 7.77 (s, 1H), 7.43 (m, 2H), 7.25 (d, *J* = 7.5 Hz, 1H), 7.14 (m, 2H), 6.94 (d, *J* = 8.5 Hz, 1H), 3.77 (s, 3H), 3.12 (br s, 4H), 2.90 (br s, 4H) **^{13}C NMR** (151 MHz, DMSO-d_6) δ 161.2, 159.1, 155.7, 145.2, 142.6, 132.9, 131.4, 125.0, 124.6, 120.6, 120.1, 118.6, 117.1, 114.3, 106.3, 56.1, 51.8, 45.4, 40.5; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{23}N_6O_2S_2$ [M+H]+ 467.13184, found 467.13046; ASMS protein concentration first observed: 0.31 μM CHK1; Measured IC_{5o} (CHK1, Invitrogen) 6.2 nM.

2-((6-chlorobenzo[d]thiazol-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E10)



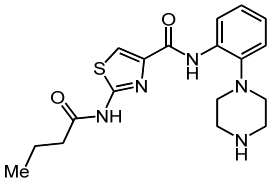
The title compound was prepared using 6-chlorobenzo[d]thiazol-2-amine (0.075 mmol, 1.5 equiv., MFCD00053557), *t*-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), P_2-Et (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at 35 ˚C. The product was purified by RP-HPLC to yield 3.5 mg (15% yield) of the title compound as an off-white solid. Analytical data for **E10**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.14 (s, 1H), 8.82 (br s, 2H), 8.37 (d, *J* = 7.8 Hz, 1H), 8.21 (s, 1H), 7.28 (d, *J* = 9.1 Hz, 2H), 7.21 (t, *J* = 7.5 Hz, 1H), 7.14 (m, 2H), 6.96 (d, *J* = 8.6 Hz, 1H), 3.36 (br s, 4H), 3.08 (br s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 158.2, 156.2, 156.1, 143.5, 142.9, 135.6, 132.2, 128.4, 126.4, 124.8, 124.4, 124.4, 122.0, 121.8, 120.4, 119.9, 116.3, 52.4, 45.6; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{20}ClN_6OS_2$ [M+H]+ 471.08230, found 471.08228; ASMS protein concentration first observed: 5.0 μM CHK1; Measured IC_{5o} (CHK1, Invitrogen) 13 nM.

2-isobutyramido-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E11)



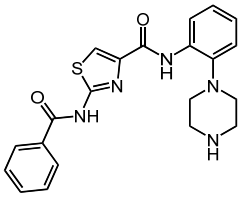
The title compound was prepared using isobutyramide (0.075 mmol, 1.5 equiv., MFCD00008019), *t*-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 5.9 mg (24% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E11**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.05 (br s, 1H), 9.82 (s, 1H), 8.81 (br s, 2H), 8.28 (d, *J* = 7.9 Hz, 1H), 8.00 (s, 1H), 7.27 (d, *J* = 7.7 Hz, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.4 Hz, 1H), 3.37 (s, 4H), 3.06 (br s, 4H), 2.81 (dt, *J* = 13.5, 6.7 Hz, 1H), 1.17 (d, *J* = 6.7 Hz, 6H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 175.9, 158.2, 158.1, 144.0, 140.9, 132.1, 125.2, 124.3, 124.0, 120.2, 119.7, 118.9, 48.5, 43.7, 33.9, 19.2; **HRMS** (ESI): *m/z* calculated for $C_{18}H_{24}N_5O_2S$ [M+H]+ 374.16452, found 374.16376; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 342 nM.

2-butyramido-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E12)



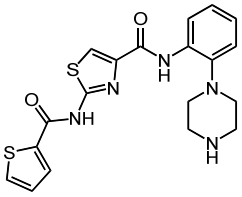
The title compound was prepared using butyramide (0.075 mmol, 1.5 equiv., MFCD00041894), *t*-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), BTMG (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 6.5 mg (27% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E12**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.06 (s, 1H), 9.83 (s, 1H), 8.87 (br s, 2H), 8.29 (d, *J* = 7.8 Hz, 1H), 7.99 (s, 1H), 7.27 (d, *J* = 7.6 Hz, 1H), 7.21 (t, *J* = 7.4 Hz, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 3.37 (br s, 4H), 3.06 (br s, 4H), 2.53 (apparent s, 2H, obscured by DMSO), 1.66 (q, *J* = 7.2 Hz, 2H), 0.93 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 171.8, 158.1, 158.0, 143.9, 140.8, 132.1, 125.2, 124.2, 120.2, 119.6, 118.8, 48.7, 43.7, 36.8, 18.0, 13.5; **HRMS** (ESI): *m/z* calculated for $C_{18}H_{24}N_5O_2S$ [M+H]+ 374.16452, found 374.16501; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 426 nM.

2-benzamido-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E13, D7)



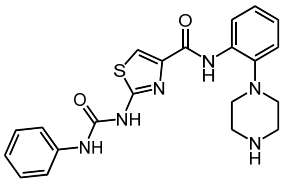
The title compound was prepared using benzamide (0.075 mmol, 1.5 equiv., MFCD00007968), *t*-BuBrettPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 15.7 mg (60% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E13**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.68 (br s, 1H), 9.95 (s, 1H), 8.96 (br s, 2H), 8.31 (d, *J* = 7.9 Hz, 1H), 8.10 (d, *J* = 9.4 Hz, 3H), 7.70 (t, *J* = 7.3 Hz, 1H), 7.60 (t, *J* = 7.5 Hz, 2H), 7.28 (d, *J* = 7.7 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.4 Hz, 1H), 3.44 (s, 4H), 3.09 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 165.8, 158.6, 158.1, 144.2, 140.89, 133.0, 132.1, 131.7, 128.8, 128.4, 125.2, 124.3, 120.2, 119.6, 119.3, 48.6, 43.6; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{22}N_5O_2S$ [M+H]+ 408.14887, found 408.14899; ASMS protein concentration first observed: 1.25 μM CHK1; Measured IC_{50} (CHK1, Invitrogen) 15.7 nM.

N-(2-(piperazin-1-yl)phenyl)-2-(thiophene-2-carboxamido)thiazole-4-carboxamide (42)



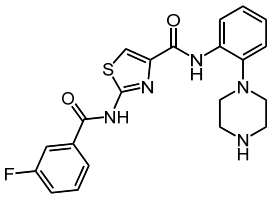
The title compound was prepared using thiophene-2-carboxamide (0.075 mmol, 1.5 equiv., MFCD00010425), *t*-BuBrettPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 19.1 mg (72% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **42**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.71 (br s, 1H), 9.91 (s, 1H), 8.78 (br s, 2H), 8.27 (d, *J* = 7.9 Hz, 1H), 8.24 (d, *J* = 3.1 Hz, 1H), 8.07 (s, 1H), 8.06 (d, *J* = 4.7 Hz, 1H), 7.30 (m, 2H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 7.4 Hz, 1H), 3.41 (s, 4H), 3.07 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 160.1, 158.2, 158.1, 144.2, 141.0, 136.4, 134.4, 132.1, 131.6, 128.6, 125.2, 124.3, 120.2, 119.8, 119.4, 48.6, 43.6; **HRMS** (ESI): *m/z* calculated for $C_{19}H_{20}N_5O_2S_2$ [M+H]+ 414.10529, found 414.10489; ASMS protein concentration first observed: 1.25 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 17 nM.

2-(3-phenylureido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E14)



The title compound was prepared using 1-phenylurea (0.075 mmol, 1.5 equiv., MFCD00007944), *t*-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 16 mg (60% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E14**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 11.25 (br s, 1H), 9.91 (s, 1H), 9.90 (s, 1H), 8.71 (br s, 2H), 8.31 (d, *J* = 7.9 Hz, 1H), 7.91 (s, 1H), 7.53 (d, *J* = 7.9 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.26 (d, *J* = 7.7 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 7.4 Hz, 1H), 7.05 (t, *J* = 7.2 Hz, 1H), 6.53 (s, 1H), 3.40 (br s, 4H), 3.06 (br s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 159.6, 158.2, 151.8, 144.1, 140.8, 138.5, 132.3, 129.0, 125.3, 124.1, 120.3, 119.4, 118.8, 118.2, 48.6, 43.9; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{23}N_6O_2S$ [M+H]+ 423.15977, found 423.15909; ASMS protein concentration first observed: 1.25 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 10.5 nM.

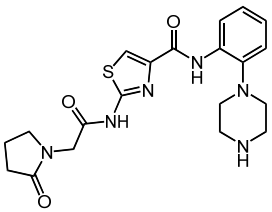
2-(3-fluorobenzamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E15)



The title compound was prepared using 3-fluorobenzamide (0.075 mmol, 1.5 equiv., MFCD00007983), *t*-BuBrettPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 18.9 mg (70% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E15**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.75 (br s, 1H), 9.91 (s, 1H), 8.77 (br s, 2H), 8.28 (d, *J* = 7.9 Hz, 1H), 8.11 (s, 1H), 7.97 (d, *J* = 7.7 Hz, 1H), 7.94 (d, *J* = 9.5 Hz, 1H), 7.65 (q, *J* = 7.5 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 1H), 7.29 (d, *J* = 7.7 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.16 (t, *J* = 7.4 Hz, 1H), 3.41 (s, 4H), 3.07 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 164.5 (d, *J* = 2.8 Hz), 162.9, 161.0, 158.4, 158.1, 144.3, 141.0, 134.0 (d, *J* = 6.7 Hz), 132.1, 131.0 (d, *J* = 8.3 Hz), 125.2,

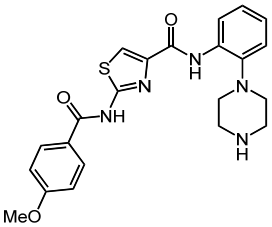
124.6 (d, *J* = 2.8 Hz), 124.4, 120.2, 120.0 (d, *J* = 21.2 Hz), 119.6 (d, *J* = 29.5 Hz), 115.2 (d, *J* = 23.3 Hz), 48.6, 43.7; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{21}FN_5O_2S$ [M+H]+ 426.13945, found 426.13864; ASMS protein concentration first observed: 1.25 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 28.4 nM.

2-(2-(2-oxopyrrolidin-1-yl)acetamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E16)



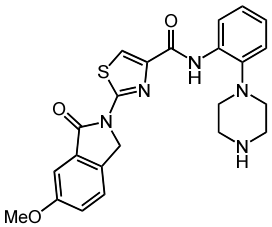
The title compound was prepared using 2-(2-oxopyrrolidin-1-yl)acetamide (0.075 mmol, 1.5 equiv., MFCD00079246), *t*-BuBrettPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 21.7 mg (80% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E16**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.39 (s, 1H), 9.83 (s, 1H), 8.85 (br s, 2H), 8.28 (d, *J* = 7.9 Hz, 1H), 8.03 (s, 1H), 7.28 (d, *J* = 7.8 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.4 Hz, 1H), 4.25 (s, 2H), 3.50 (t, *J* = 6.9 Hz, 2H), 3.35 (s, 4H, obscured by water), 3.06 (s, 4H), 2.29 (t, *J* = 8.0 Hz, 2H), 2.01 (p, *J* = 7.5 Hz, 2H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 175.0, 167.8, 158.0, 157.7, 144.1, 140.9, 132.1, 125.2, 124.3, 120.2, 119.7, 119.1, 48.6, 47.6, 44.9, 43.8, 29.8, 17.7; **HRMS** (ESI): *m/z* calculated for $C_{20}H_{25}N_6O_3S$ [M+H]+ 429.17034, found 429.17078; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

2-(4-methoxybenzamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E17)



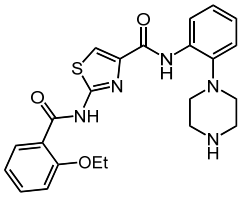
The title compound was prepared using 4-methoxybenzamide (0.075 mmol, 1.5 equiv., MFCD00007995), *t*-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 8.5 mg (31% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E17**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.48 (s, 1H), 9.94 (s, 1H), 8.84 (br s, 2H), 8.29 (d, *J* = 7.9 Hz, 1H), 8.12 (d, *J* = 8.6 Hz, 2H), 8.06 (s, 1H), 7.28 (d, *J* = 7.7 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 1H), 7.11 (d, *J* = 8.6 Hz, 2H), 3.87 (s, 3H), 3.43 (s, 4H), 3.08 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 165.0, 163.0, 158.8, 158.2, 144.2, 140.9, 132.1, 130.5, 125.2, 124.3, 123.7, 120.2, 119.7, 119.1, 114.0, 55.59, 48.6, 43.6; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{24}N_5O_3S$ [M+H]+ 438.15944, found 438.15976; ASMS protein concentration first observed: 1.25 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 13.6 nM.

2-(6-methoxy-1-oxoisoindolin-2-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E18, D9)



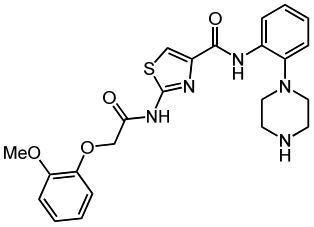
The title compound was prepared using 6-methoxyisoindolin-1-one (0.075 mmol, 1.5 equiv., MFCD08234735), *t*-BuBrettPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 13.2 mg (47% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E18**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.05 (s, 1H), 9.09 (br s, 2H), 8.44 (d, *J* = 8.0 Hz, 1H), 8.15 (s, 1H), 7.75 (d, *J* = 8.8 Hz, 1H), 7.39 (s, 2H), 7.34 (d, *J* = 7.7 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 1H), 5.23 (s, 2H), 3.87 (s, 3H), 3.43 (s, 4H), 3.11 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 166.5, 159.9, 158.1, 157.4, 144.2, 140.6, 134.0, 132.7, 131.0, 125.7, 125.6, 124.2, 121.6, 120.9, 119.9, 119.0, 106.6, 55.8, 50.1, 48.8, 44.2; **HRMS** (ESI): *m/z* calculated for $C_{23}H_{24}N_5O_3S$ [M+H]+ 450.15944, found 450.15869; ASMS protein concentration first observed: 0.16 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 3.9 nM.

2-(2-ethoxybenzamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (39)



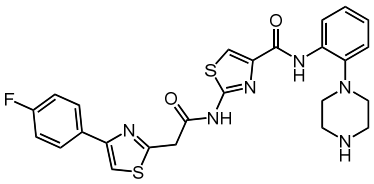
The title compound was prepared using 2-ethoxybenzamide (0.075 mmol, 1.5 equiv., MFCD00007977), *t*-BuXPhos G3 (0.005 mmol, 10 mol %, precatalyst), MEBD (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 14.6 mg (52% yield) of the title compound as an off- off-white residue (TFA salt). Analytical data for **39**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 11.99 (s, 1H), 9.80 (s, 1H), 8.82 (br s, 2H), 8.35 (d, *J* = 7.9 Hz, 1H), 8.08 (s, 1H), 7.74 (d, *J* = 7.4 Hz, 1H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.25 (m, 3H), 7.14 (m, 2H), 4.24 (q, *J* = 6.7 Hz, 2H), 3.33 (s, 4H, obscured by water peak), 3.07 (s, 4H), 1.39 (t, *J* = 6.8 Hz, 3H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 164.9, 158.2, 158.0, 156.4, 144.3, 140.8, 133.6, 132.3, 130.2, 125.3, 124.3, 122.0, 120.8, 120.4, 119.6, 119.4, 113.4, 64.5, 48.7, 43.8, 14.7; **HRMS** (ESI): *m/z* calculated for $C_{23}H_{26}N_5O_3S$ [M+H]+ 452.17509, found 452.17477; ASMS protein concentration first observed: 0.16 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 4.9 nM.

2-(2-(2-methoxyphenoxy)acetamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E19)



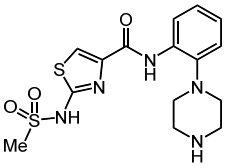
The title compound was prepared using 2-(2-methoxyphenoxy)acetamide (0.075 mmol, 1.5 equiv., MFCD00834989), *t*-BuBrettPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 19.8 mg (68% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E19**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.40 (br s, 1H), 9.82 (s, 1H), 8.82 (br s, 2H), 8.29 (d, *J* = 7.9 Hz, 1H), 8.05 (s, 1H), 7.28 (d, *J* = 7.7 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.4 Hz, 1H), 7.03 (d, *J* = 7.8 Hz, 1H), 6.96 (dd, *J* = 15.3, 7.6 Hz, 2H), 6.88 (t, *J* = 7.5 Hz, 1H), 4.92 (s, 2H), 3.79 (s, 3H), 3.36 (s, 4H), 3.06 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 167.6, 158.1, 157.6, 149.2, 147.2, 144.1, 140.9, 132.1, 125.2, 124.3, 122.2, 120.6, 120.3, 119.7, 119.3, 114.4, 112.6, 67.2, 55.6, 48.6, 43.8; **HRMS** (ESI): *m/z* calculated for $C_{23}H_{26}N_5O_4S$ [M+H]+ 468.17000, found 468.16928; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 650 nM.

2-(2-(4-(4-fluorophenyl)thiazol-2-yl)acetamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E20)



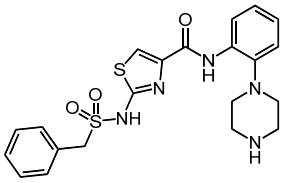
The title compound was prepared using 2-(4-(4-fluorophenyl)thiazol-2-yl)acetamide (0.075 mmol, 1.5 equiv., MFCD03011716), *t*-BuBrettPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at 35 ˚C. The product was purified by RP-HPLC to yield 9.1 mg (29% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E20**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.58 (s, 1H), 9.86 (s, 1H), 8.97 (br s, 2H), 8.30 (d, *J* = 7.9 Hz, 1H), 8.09 (s, 1H), 8.05 (s, 1H), 7.97 (dd, *J* = 8.0, 5.8 Hz, 2H), 7.27 (t, *J* = 9.0 Hz, 3H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.5 Hz, 1H), 4.47 (s, 2H), 3.40 (br s, 4H), 3.08 (br s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 167.6, 162.1, 161.5 (d, *J* = 245.6 Hz), 158.3 (d, *J* = 33.6 Hz), 158.1, 157.8, 152.6, 144.2, 140.9, 132.2, 130.6 (d, *J* = 3.0 Hz), 128.0 (d, *J* = 8.3 Hz), 125.3, 124.3, 120.3, 119.6, 119.3, 115.7 (d, *J* = 21.6 Hz), 115.2, 48.6, 43.8; **HRMS** (ESI): *m/z* calculated for $C_{25}H_{24}FN_6O_2S_2$ [M+H]+ 523.13807, found 523.13708; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 918 nM.

2-(methylsulfonamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E21)



The title compound was prepared using methanesulfonamide (0.075 mmol, 1.5 equiv., MFCD00007940), RockPhos G3 (0.005 mmol, 10 mol %, precatalyst), P_2-Et (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 12.8 mg (52% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E21**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.20 (br s, 1H), 9.89 (s, 1H), 8.82 (br s, 2H), 8.30 (s, 1H), 7.97 (s, 1H), 7.28 (dd, *J* = 7.9, *J* = 1.2 Hz, 1H), 7.21 (m, 1H), 7.15 (td, *J* = 7.7, *J* = 1.4 Hz, 1H), 3.33 (br s, 7H), 3.03 (m, 4H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 158.1 (q, *J* = 33.9 Hz, TFA), 157.5, 141.1, 132.5, 125.5, 124.4, 120.7, 119.7, 119.3, 118.4, 116.4 (q, *J* = 295.6 Hz, TFA), 48.8, 43.5, 40.5; **HRMS** (ESI): *m/z* calculated for $C_{15}H_{20}N_5O_3S_2$ [M+H]+ 382.10021, found 382.10378; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

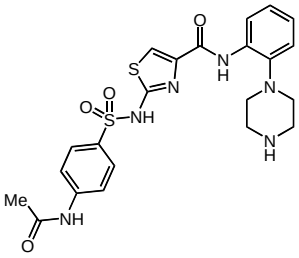
2-((phenylmethyl)sulfonamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (40)



The title compound was prepared using phenylmethanesulfonamide (0.075 mmol, 1.5 equiv., MFCD00041893), *t*-BuBrettPhos G3 (0.005 mmol, 10 mol %, precatalyst), P_2-Et (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at 35 ˚C. The product was purified by RP-HPLC to yield 17.6 mg (62% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **40**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.30 (br s, 1H), 9.89 (s, 1H), 8.90 (br s, 2H), 8.27 (s, 1H), 7.90 (s, 1H), 7.34 (s, 3H), 7.28 (m, 3H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.16 (t, *J* = 7.4 Hz, 1H), 4.75 (br s, 2H), 3.36 (br s, 4H), 3.05 (br s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 158.2 (q, J = 33.8 Hz, TFA), 157.4, 141.4, 132.4, 130.9, 129.2, 128.5, 125.4, 124.6,

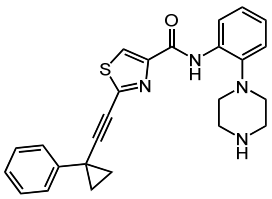
120.7, 120.0, 117.6, 115.3, 57.7, 48.8, 43.5; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{24}N_5O_3S_2$ [M+H]+ 458.13151, found 458.13098; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{5o} (CHK1, Invitrogen) >10000 nM.

2-((4-acetamidophenyl)sulfonamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E22)



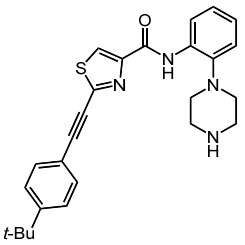
The title compound was prepared using N-(4-sulfamoylphenyl)acetamide (0.075 mmol, 1.5 equiv., MFCD00035784), *t*-BuBrettPhos G3 (0.005 mmol, 10 mol %, precatalyst), P_2-Et (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 21.1 mg (69% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E22**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 12.69 (br s, 1H), 10.32 (s, 1H), 9.82 (s, 1H), 8.88 (br s, 2H), 8.17 (d, *J* = 6.0 Hz, 1H), 7.84 (d, *J* = 8.8 Hz, 2H), 7.72 (d, *J* = 8.7 Hz, 2H), 7.26 (dd, *J* = 7.8, *J* = 1.2 Hz, 1H), 7.18 (td, *J* = 7.7, *J* = 1.3 Hz, 1H), 7.14 (td, *J* = 7.6, *J* = 1.4 Hz, 1H), 3.34 (s, 4H), 3.03 (m, 4H), 2.04 (s, 3H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 169.5, 158.6 (q, J = 32.0 Hz, TFA), 157.7, 149.8, 143.8, 141.8, 132.6, 130.3, 128.4, 126.0, 125.7, 125.0, 121.2, 120.9, 120.5, 119.0, 117.44 (d, J = 298.9 Hz, TFA), 49.1, 44.0, 24.6; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{24}N_6O_4S_2$ [M+H]+ 501.13732, found 501.13742; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{5o} (CHK1, Invitrogen) >10000 nM.

2-((1-phenylcyclopropyl)ethynyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (37)



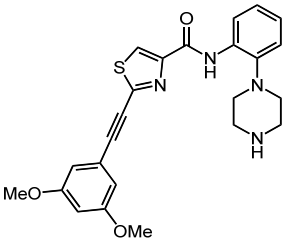
The title compound was prepared using (1-ethynylcyclopropyl)benzene (0.075 mmol, 1.5 equiv., MFCD11109424), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), BTTP (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at ambient temperature. The product was purified by RP-HPLC to yield 5.4 mg (20% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **37**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.98 (s, 1H), 9.01 (s, 2H), 8.53 (s, 1H), 8.32 (d, *J* = 7.9 Hz, 1H), 7.41 (d, *J* = 7.6 Hz, 2H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.25 (m, 3H), 7.16 (t, *J* = 7.5 Hz, 1H), 3.31 (br s, 4H), 3.09 (br s, 4H), 1.70 (m, 2H), 1.54 (m, 2H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 158.1, 157.4, 149.7, 148.4, 140.9, 139.8, 132.2, 128.7, 127.2, 126.6, 125.4, 124.5, 120.6, 119.5, 100.8, 70.8, 48.6, 43.8, 20.9, 16.0; **HRMS** (ESI): *m/z* calculated for $C_{25}H_{25}N_4OS$ [M+H]+ 429.17436, found 429.17413; ASMS protein concentration first observed: 5.0 µM CHK1; Measured IC_{5o} (CHK1, Invitrogen) 6570 nM.

2-((4-(tert-butyl)phenyl)ethynyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E23)



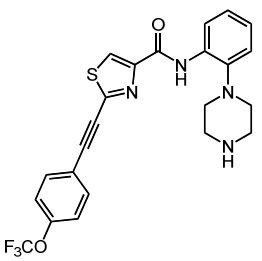
The title compound was prepared using 1-(*tert*-butyl)-4-ethynylbenzene (0.075 mmol, 1.5 equiv., MFCD00190197), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), BTTP (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at ambient temperature. The product was purified by RP-HPLC to yield 7.3 mg (26% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E23**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.08 (s, 1H), 8.93 (s, 2H), 8.61 (s, 1H), 8.35 (d, *J* = 7.9 Hz, 1H), 7.67 (d, J = 7.9 Hz, 2H), 7.52 (d, *J* = 7.9 Hz, 2H), 7.30 (d, *J* = 7.7 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.4 Hz, 1H), 3.35 (br s, 4H, close to water), 3.10 (br s, 4H), 1.30 (s, 9H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 157.4, 153.51, 150.1, 148.1, 140.8, 132.3, 132.0, 127.6, 125.8, 125.4, 124.4, 120.6, 119.3, 117.0, 94.9, 80.9, 48.6, 43.9, 40.0, 39.8, 39.7, 39.5, 39.3, 39.2, 39.0, 34.8, 30.8; **HRMS** (ESI): *m/z* calculated for $C_{26}H_{29}N_4OS$ [M+H]+ 445.20566, found 445.20554; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 1910 nM.

2-((3,5-dimethoxyphenyl)ethynyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E24)



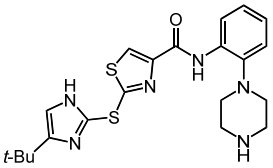
The title compound was prepared using 1-ethynyl-3,5-dimethoxybenzene (0.075 mmol, 1.5 equiv., MFCD03839985), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), BTTP (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at ambient temperature. The product was purified by RP-HPLC to yield 6.8 mg (24% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E24**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.03 (s, 1H), 8.85 (br s, 2H), 8.63 (s, 1H), 8.33 (d, *J* = 7.9 Hz, 1H), 7.30 (d, *J* = 7.7 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.4 Hz, 1H), 6.89 (s, 2H), 6.70 (s, 1H), 6.53 (s, 1H), 3.80 (s, 6H), 3.32 (s, 4H, under water), 3.10 (br s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 160.5, 157.3, 150.1, 147.9, 140.8, 132.2, 128.0, 125.4, 124.5, 121.3, 120.6, 119.4, 110.0, 103.1, 94.7, 80.8, 55.6, 48.5, 43.9; **HRMS** (ESI): *m/z* calculated for $C_{24}H_{25}N_4O_3S$ [M+H]+ 449.16419, found 449.16251; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 1150 nM.

N-(2-(piperazin-1-yl)phenyl)-2-((4-(trifluoromethoxy)phenyl)ethynyl)thiazole-4-carboxamide (E25)



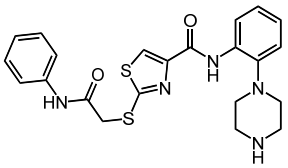
The title compound was prepared using 1-ethynyl-4-(trifluoromethoxy)benzene (0.075 mmol, 1.5 equiv., MFCD03094333), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), BTTP (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at ambient temperature. The product was purified by RP-HPLC to yield 3.9 mg (13% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E25**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.08 (s, 1H), 8.91 (br s, 2H), 8.65 (s, 1H), 8.34 (d, *J* = 7.9 Hz, 1H), 7.89 (d, *J* = 8.5 Hz, 2H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.30 (d, *J* = 7.7 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.5 Hz, 1H), 3.35 (br s, 4H, close to water), 3.10 (br s, 4H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 157.3, 150.2, 149.4, 147.6, 140.8, 134.4, 132.2, 128.1, 125.4, 124.4, 121.5, 120.6, 119.9 (q, *J* = 257.9 Hz), 119.3, 119.2, 93.0, 82.0, 48.5, 43.9; **HRMS** (ESI): *m/z* calculated for $C_{23}H_{20}F_3N_4O_2S$ [M+H]+ 473.12536, found 473.12463; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 1840 nM.

2-((4-(tert-butyl)-1H-imidazol-2-yl)thio)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (35)



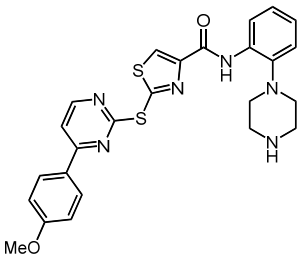
The title compound was prepared using 4-(*tert*-butyl)-1H-imidazole-2-thiol (0.075 mmol, 1.5 equiv., MFCD03789242), P_2-Et (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent (no palladium precatalyst). The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at ambient temperature. The product was purified by RP-HPLC to yield 27.2 mg (98% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **35**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.05 (s, 1H), 8.96 (br s, 2H), 8.34 (s, 1H), 7.30 (d, *J* = 7.7 Hz, 1H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.15 (m, 2H), 3.35 (s, 4H), 3.09 (s, 4H), 1.27 (s, 9H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 166.9, 158.2, 157.9, 157.3, 149.5, 140.6, 132.4, 130.04, 126.5, 125.5, 124.3, 120.7, 118.9, 48.5, 44.0, 40.4, 29.8; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{27}N_6OS_2$ [M+H]+ 443.16823, found 443.16782; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

2-((2-oxo-2-(phenylamino)ethyl)thio)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E26)



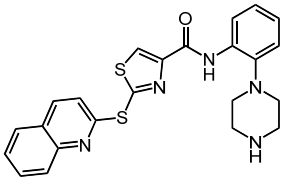
The title compound was prepared using 2-mercapto-N-phenylacetamide (0.075 mmol, 1.5 equiv., MFCD00014451), BTMG (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent (no palladium precatalyst). The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at ambient temperature. The product was purified by RP-HPLC to yield 9.8 mg (35% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E26**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.42 (s, 1H), 10.03 (s, 1H), 8.87 (br s, 2H), 8.41 (s, 1H), 8.33 (d, *J* = 7.9 Hz, 1H), 7.56 (d, *J* = 7.9 Hz, 2H), 7.29 (q, *J* = 7.5 Hz, 3H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.5 Hz, 1H), 7.06 (t, *J* = 7.3 Hz, 1H), 4.31 (s, 2H), 3.33 (s, 4H), 3.06 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 165.8, 165.6, 157.8, 149.9, 141.2, 139.0, 132.8, 129.3, 126.4, 126.0, 124.8, 124.3, 121.1, 119.7, 119.6, 49.0, 44.4, 40.9; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{24}N_5O_2S_2$ [M+H]+ 454.13659, found 454.13364; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

2-((4-(4-methoxyphenyl)pyrimidin-2-yl)thio)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E27)



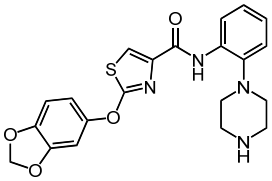
The title compound was prepared using 4-(4-methoxyphenyl)pyrimidine-2-thiol (0.075 mmol, 1.5 equiv., MFCD00085109), AdBrettPhos G3 (0.005 mmol, 10 mol %, precatalyst), BTMG (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at ambient temperature. The product was purified by RP-HPLC to yield 12.2 mg (39% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E27**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.22 (s, 1H), 8.89 (br s, 2H), 8.80 (d, *J* = 5.3 Hz, 1H), 8.69 (s, 1H), 8.39 (d, *J* = 8.0 Hz, 1H), 8.20 (d, *J* = 8.6 Hz, 2H), 7.97 (d, *J* = 5.3 Hz, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.8 Hz, 1H), 7.12 (d, *J* = 8.6 Hz, 2H), 3.85 (s, 3H), 3.35 (s, 4H), 3.08 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 166.2, 164.0, 162.5, 158.8, 158.4, 157.4, 148.7, 140.5, 132.5, 129.3, 128.3, 127.1, 125.6, 124.2, 120.8, 118.7, 114.7, 114.0, 55.6, 48.5, 44.0; **HRMS** (ESI): *m/z* calculated for $C_{25}H_{25}N_6O_2S_2$ [M+H]+ 505.14749, found 505.14725; ASMS protein concentration first observed: 10.0 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

N-(2-(piperazin-1-yl)phenyl)-2-(quinolin-2-ylthio)thiazole-4-carboxamide (E28, D16)



The title compound was prepared using quinoline-2-thiol (0.075 mmol, 1.5 equiv., MFCD00006751), , P_2-Et (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent (no palladium precatalyst). The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at ambient temperature. The product was purified by RP-HPLC to yield 17 mg (61% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E28**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.20 (s, 1H), 9.02 (br s, 2H), 8.65 (s, 1H), 8.45 (d, *J* = 8.6 Hz, 1H), 8.39 (d, *J* = 7.9 Hz, 1H), 8.06 (dd, *J* = 14.0, 8.3 Hz, 2H), 7.86 (t, *J* = 7.6 Hz, 1H), 7.66 (t, *J* = 7.4 Hz, 1H), 7.62 (d, *J* = 8.6 Hz, 1H), 7.30 (d, *J* = 7.8 Hz, 1H), 7.23 (t, *J* = 7.7 Hz, 1H), 7.15 (t, *J* = 7.5 Hz, 1H), 3.35 (s, 4H), 3.10 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 158.8, 157.5, 153.3, 148.4, 147.0, 140.6, 138.1, 132.5, 131.1, 128.4, 127.6, 127.1, 127.0, 126.4, 125.6, 124.2, 120.7, 120.1, 118.8, 48.6, 44.0; **HRMS** (ESI): *m/z* calculated for $C_{23}H_{22}N_5OS_2$ [M+H]+ 448.12603, found 448.12549; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

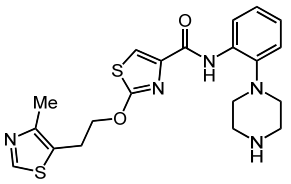
2-(benzo[d][1,3]dioxol-5-yloxy)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E29)



The title compound was prepared using benzo[d][1,3]dioxol-5-ol (0.075 mmol, 1.5 equiv., MFCD00005827), , P_2-Et (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent (no palladium precatalyst). The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at ambient temperature. The product was purified by RP-HPLC to yield 10.5 mg (39% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E29**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.82 (s, 1H), 8.84 (br s, 2H), 8.34 (d, *J* = 8.0 Hz, 1H), 7.95 (s, 1H), 7.28 (d, *J* = 7.8 Hz, 1H), 7.21 (t, *J* = 7.7 Hz, 1H), 7.19 (s, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 8.4 Hz, 1H), 6.94 (m, 1H), 6.13 (s, 2H), 3.27 (s, 4H), 3.06 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 174.0, 157.6, 149.3, 148.4, 146.0, 143.6,

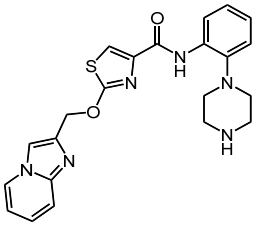
140.6, 132.3, 125.5, 124.3, 120.6, 119.3, 119.0, 113.5, 108.7, 102.9, 102.3, 48.5, 43.9; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{21}N_4O_4S$ [M+H]+ 425.12780, found 425.12799; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 5730 nM.

2-(2-(4-methylthiazol-5-yl)ethoxy)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E30)



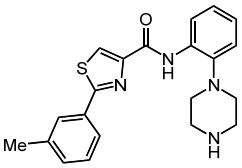
The title compound was prepared using 2-(4-methylthiazol-5-yl)ethan-1-ol (0.075 mmol, 1.5 equiv., MFCD00005339), RockPhos G3 (0.005 mmol, 10 mol %, precatalyst), MTBD (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at ambient temperature. The product was purified by RP-HPLC to yield 16.9 mg (62% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **E30**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.84 (s, 1H), 8.92 (br s, 2H), 8.86 (s, 1H), 8.38 (d, *J* = 8.0 Hz, 1H), 7.89 (s, 1H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.5 Hz, 1H), 4.70 (t, *J* = 5.5 Hz, 2H), 3.36 (t, *J* = 5.4 Hz, 2H), 3.30 (s, 4H), 3.07 (s, 4H), 2.34 (s, 3H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 173.1, 157.8, 151.1, 149.5, 143.0, 140.6, 132.6, 127.0, 125.6, 124.2, 120.9, 119.0, 118.3, 72.2, 48.7, 44.1, 25.3, 14.8; **HRMS** (ESI): *m/z* calculated for $C_{20}H_{24}N_5O_2S_2$ [M+H]+ 430.13659, found 430.13693; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

2-(imidazo[1,2-a]pyridin-2-ylmethoxy)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (36)



The title compound was prepared using imidazo[1,2-a]pyridin-2-ylmethanol (0.075 mmol, 1.5 equiv., MFCD03789242), P_2-Et (0.1 mmol, 2 equiv., base), and DMF as the reaction solvent (no palladium precatalyst). The reaction was carried out at the 0.05 mmol scale and stirred for 21 hours at ambient temperature. The product was purified by RP-HPLC to yield 21 mg (77% yield) of the title compound as an off-white residue (TFA salt). Analytical data for **36**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.90 (s, 1H), 8.96 (br s, 2H), 8.75 (d, *J* = 6.1 Hz, 1H), 8.41 (d, *J* = 7.9 Hz, 1H), 8.32 (s, 1H), 7.95 (s, 1H), 7.78 (d, *J* = 8.7 Hz, 1H), 7.62 (br s, 1H), 7.32 (d, *J* = 7.7 Hz, 1H), 7.23 (m, 2H), 7.16 (t, *J* = 7.4 Hz, 1H), 5.78 (s, 2H), 3.33 (br s, 4H), 3.08 (br s, 4H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 172.9, 157.8 (q, *J* = 34.4 Hz, TFA), 157.7, 143.1, 143.0, 140.5, 137.4, 132.5, 127.5, 127.4, 125.4, 124.0, 120.7, 119.1, 118.2, 116.1 (q, *J* = 295.5 Hz, TFA) 115.5, 113.495 113.2, 66.80, 48.5, 43.9; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{23}N_6O_2S$ [M+H]+ 435.15977, found 435.16003; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

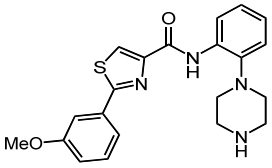
N-(2-(piperazin-1-yl)phenyl)-2-(m-tolyl)thiazole-4-carboxamide (E31)



The title compound was prepared using m-tolylboronic acid (0.075 mmol, 1.5 equiv., MFCD00040198), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M K_3PO_4 (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 17.1 mg (69% yield)

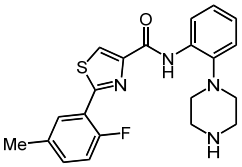
of the title compound as an off-white solid (TFA salt). Analytical data for **E31**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.25 (s, 1H), 9.00 (br s, 2H), 8.54 (s, 1H), 8.40 (d, *J* = 7.9 Hz, 1H), 7.86 (d, *J* = 9.4 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.41 (d, *J* = 7.3 Hz, 1H), 7.33 (d, *J* = 7.7 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.17 (t, *J* = 7.4 Hz, 1H), 3.32 (br s, 4H), 3.11 (br s, 4H), 2.44 (s, 3H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 168.0, 158.0, 150.2, 140.8, 139.2, 132.5, 131.7, 129.6, 126.9, 125.6, 125.5, 124.3, 123.4, 120.8, 119.2, 48.7, 44.1, 21.0; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{23}N_4OS$ [M+H]+ 379.15871, found 379.15802; ASMS protein concentration first observed: 2.5 μM CHK1; Measured IC_{50} (CHK1, Invitrogen) 134 nM.

2-(3-methoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E32)



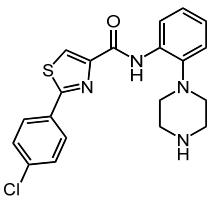
The title compound was prepared using (3-methoxyphenyl)boronic acid (0.075 mmol, 1.5 equiv., MFCD00161359), SPhos G2 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M BTMG (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 18.9 mg (74% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E32**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.20 (s, 1H), 8.95 (br s, 2H), 8.56 (s, 1H), 8.38 (d, *J* = 7.8 Hz, 1H), 7.64 (d, *J* = 7.4 Hz, 1H), 7.54 (m, 2H), 7.32 (d, *J* = 7.7 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.18 (t, *J* = 7.4 Hz, 2H), 3.87 (s, 3H), 3.30 (br s, 4H), 3.10 (br s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 167.7, 160.0, 158.0, 150.2, 140.9, 133.5, 132.4, 130.9, 125.8, 125.5, 124.4, 120.8, 119.5, 118.6, 116.9, 111.5, 55.5, 48.7, 44.1; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{23}N_4O_2S$ [M+H]+ 395.15632, found 395.15268; ASMS protein concentration first observed: 2.5 μM CHK1; Measured IC_{50} (CHK1, Invitrogen) 270 nM.

2-(2-fluoro-5-methylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E33)



The title compound was prepared using (2-fluoro-5-methylphenyl)boronic acid (0.075 mmol, 1.5 equiv., MFCD03428512), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M K_3PO_4 (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 17.3 mg (68% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E33**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.25 (s, 1H), 8.90 (br s, 2H), 8.65 (s, 1H), 8.37 (d, *J* = 7.9 Hz, 1H), 8.11 (d, *J* = 6.4 Hz, 1H), 7.45 (s, 1H), 7.39 (m, 1H), 7.33 (d, *J* = 7.7 Hz, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 3.29 (s, 4H), 3.10 (s, 4H), 2.44 (s, 3H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 159.6 (d, *J* = 239.4 Hz), 157.9, 156.7, 149.4, 141.0, 135.1, 133.1 (d, *J* = 8.0 Hz), 132.4, 128.4, 126.5 (d, *J* = 8.0 Hz), 125.6, 124.4, 120.8, 119.5, 119.4 (d, *J* = 11.2 Hz), 116.5 (d, *J* = 21.4 Hz), 48.7, 44.1, 20.3; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{22}FN_4OS$ [M+H]+ 397.14929, found 397.14841; ASMS protein concentration first observed: 1.25 μM CHK1; Measured IC_{50} (CHK1, Invitrogen) 85.3 nM.

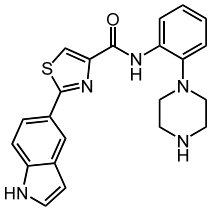
2-(4-chlorophenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E34)



The title compound was prepared using (4-chlorophenyl)boronic acid (0.075 mmol, 1.5 equiv., MFCD00039137), SPhos G2 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M K_3PO_4 (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried

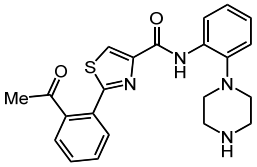
out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 16.3 mg (64% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E34**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.28 (s, 1H), 9.00 (br s, 2H), 8.58 (s, 1H), 8.43 (d, *J* = 8.0 Hz, 1H), 8.08 (d, *J* = 8.3 Hz, 2H), 7.69 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.5 Hz, 1H), 3.33 (br s, 4H), 3.10 (br s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 166.5, 157.8, 150.3, 140.7, 135.6, 132.6, 131.0, 129.8, 128.0, 126.2, 125.7, 124.3, 121.0, 119.0, 48.8, 44.1; **HRMS** (ESI): *m/z* calculated for $C_{20}H_{20}ClN_4OS$ [M+H]+ 399.10409, found 399.10287; ASMS protein concentration first observed: 2.5 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 269 nM.

2-(1H-indol-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E35)



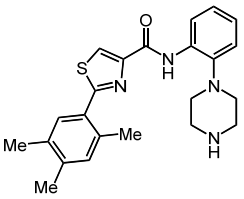
The title compound was prepared using 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole (0.075 mmol, 1.5 equiv., MFCD03789263), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M K_3PO_4 (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 15.7 mg (61% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E35**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 11.52 (s, 1H), 10.31 (s, 1H), 9.01 (br s, 2H), 8.43 (d, *J* = 9.0 Hz, 2H), 8.24 (s, 1H), 7.83 (d, *J* = 8.3 Hz, 1H), 7.62 (d, *J* = 8.3 Hz, 1H), 7.50 (s, 1H), 7.34 (d, *J* = 7.7 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.17 (t, *J* = 7.4 Hz, 1H), 6.64 (s, 1H), 3.37 (br s, 4H), 3.13 (br s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 170.0, 158.2, 149.9, 140.7, 137.3, 132.7, 128.0, 127.3, 125.7, 124.2, 124.0, 123.6, 120.8, 119.2, 119.1, 119.08, 112.7, 102.5, 48.8, 44.2; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{22}N_5OS$ [M+H]+ 404.15396, found 404.15283; ASMS protein concentration first observed: 0.63 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 11.6 nM.

2-(2-acetylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E36)



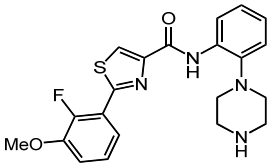
The title compound was prepared using (2-acetylphenyl)boronic acid (0.075 mmol, 1.5 equiv., MFCD01321263), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M K_3PO_4 (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 21.3 mg (82% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E36**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 9.70 (s, 1H), 8.81 (br s, 2H), 8.67 (s, 1H), 8.37 (d, *J* = 7.9 Hz, 1H), 7.89 (m, 1H), 7.69 (m, 2H), 7.62 (m, 1H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.3 Hz, 1H), 3.29 (s, 4H), 3.04 (s, 4H), 2.31 (s, 3H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 203.6, 166.4, 157.9, 150.1, 141.0, 140.5, 132.1, 131.1, 130.8, 129.8, 129.3, 127.9, 127.5, 125.3, 124.6, 120.5, 119.9, 48.8, 43.2, 30.4; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{23}N_4O_2S$ [M+H]+ 407.15362, found 407.15341; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) >10000 nM.

N-(2-(piperazin-1-yl)phenyl)-2-(2,4,5-trimethylphenyl)thiazole-4-carboxamide (E37)



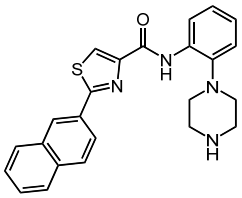
The title compound was prepared using (2,4,5-trimethylphenyl)boronic acid (0.075 mmol, 1.5 equiv., MFCD03427049), SPhos G2 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M K_3PO_4 (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 16.2 mg (62% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E37**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.08 (s, 1H), 8.84 (br s, 2H), 8.57 (s, 1H), 8.41 (d, *J* = 7.9 Hz, 1H), 7.62 (s, 1H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.21 (s, 1H), 7.17 (d, *J* = 7.7 Hz, 1H), 3.20 (s, 4H), 3.07 (s, 4H), 2.61 (s, 3H), 2.29 (s, 3H), 2.27 (s, 3H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 168.0, 158.2, 149.7, 140.8, 138.9, 134.8, 133.1, 132.9, 132.4, 130.6, 128.9, 125.7, 125.6, 124.4, 120.7, 119.4, 48.7, 43.9, 20.8, 19.2, 18.8; **HRMS** (ESI): *m/z* calculated for $C_{23}H_{27}N_4OS$ [M+H]+ 407.19001, found 407.18906; ASMS protein concentration first observed: 1.25 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 911 nM.

2-(2-fluoro-3-methoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E39)



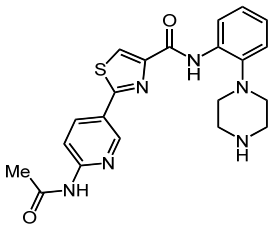
The title compound was prepared using (2-fluoro-3-methoxyphenyl)boronic acid (0.075 mmol, 1.5 equiv., MFCD02094728), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M BTMG (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 18.6 mg (71% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E39**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.28 (s, 1H), 8.95 (br s, 2H), 8.67 (s, 1H), 8.41 (d, *J* = 7.9 Hz, 1H), 7.83 (d, *J* = 7.7 Hz, 1H), 7.44 (m, 2H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 3.93 (s, 3H), 3.32 (s, 4H, under water), 3.10 (s, 4H); **^{13}C NMR** (151 MHz, DMSO-d_6) δ 160.15 (d, *J* = 3.8 Hz), 157.9, 149.4 (d, *J* = 251.9 Hz), 149.3, 148.0 (d, *J* = 9.7 Hz), 140.8, 132.6, 126.8 (d, *J* = 8.3 Hz), 125.7, 125.6 (d, *J* = 4.0 Hz), 124.4, 120.9, 120.4 (d, *J* = 8.4 Hz), 119.2, 118.7, 115.8, 56.5, 48.8, 44.1; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{22}FN_4O_2S$ [M+H]+ 413.14420, found 413.14301; ASMS protein concentration first observed: 1.25 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 56.1 nM.

2-(naphthalen-2-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E40)



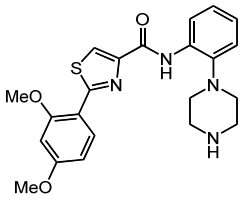
The title compound was prepared using naphthalen-2-ylboronic acid (0.075 mmol, 1.5 equiv., MFCD00236051), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M K_3PO_4 (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 13.8 mg (52% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E40**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.31 (s, 1H), 9.00 (br s, 2H), 8.65 (s, 1H), 8.60 (s, 1H), 8.43 (d, *J* = 7.9 Hz, 1H), 8.20 (d, *J* = 8.4 Hz, 1H), 8.15 (m, 2H), 8.01 (d, *J* = 6.9 Hz, 1H), 7.65 (m, 2H), 7.35 (d, *J* = 7.7 Hz, 1H), 7.26 (t, *J* = 7.6 Hz, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 3.37 (br s, 4H), 3.13 (br s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 167.9, 158.0, 150.4, 140.8, 133.9, 132.9, 132.6, 129.6, 129.4, 129.0, 127.8, 127.8, 127.3, 126.4, 125.9, 125.6, 124.4, 123.1, 120.9, 119.3, 48.8, 44.2; **HRMS** (ESI): *m/z* calculated for $C_{24}H_{23}N_4OS$ [M+H]+ 415.15871, found 415.15771; ASMS protein concentration first observed: 1.25 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 33.1 nM.

2-(6-acetamidopyridin-3-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E41)



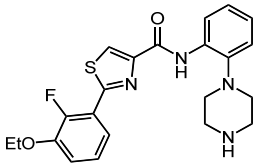
The title compound was prepared using *N*-(5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridin-2-yl)acetamide (0.075 mmol, 1.5 equiv., MFCD08690229), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M K_3PO_4 (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 22.3 mg (83% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E41**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.87 (s, 1H), 10.14 (s, 1H), 8.95 (s, 1H), 8.89 (br s, 2H), 8.56 (s, 1H), 8.40 (t, *J* = 6.6 Hz, 2H), 8.36 (d, *J* = 8.7 Hz, 1H), 7.32 (d, *J* = 7.7 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 3.31 (s, 4H), 3.10 (s, 4H), 2.15 (s, 3H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 169.7, 164.9, 157.9, 153.7, 150.3, 146.4, 140.8, 135.6, 132.4, 125.7, 125.5, 124.4, 124.0, 120.8, 119.4, 113.6, 48.7, 44.1, 24.0; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{23}N_6O_2S$ [M+H]+ 423.15977, found 423.15924; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 2950 nM.

2-(2,4-dimethoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E42)



The title compound was prepared using (2,4-dimethoxyphenyl)boronic acid (0.075 mmol, 1.5 equiv., MFCD01074590), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M BTMG (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 16.3 mg (61% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E42**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.33 (s, 1H), 9.00 (br s, 2H), 8.44 (s, 1H), 8.42 (s, 1H), 8.30 (d, *J* = 8.7 Hz, 1H), 7.33 (d, *J* = 7.8 Hz, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.5 Hz, 1H), 6.88 (d, *J* = 8.7 Hz, 1H), 6.85 (s, 1H), 4.05 (s, 3H), 3.89 (s, 3H), 3.33 (br s, 4H, under water), 3.11 (br s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 162.5, 162.2, 158.3, 157.9, 148.2, 140.7, 132.8, 128.4, 125.7, 124.5, 124.2, 120.9, 119.1, 113.7, 107.6, 98.5, 56.21, 55.7, 48.8, 44.2; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{25}N_4O_3S$ [M+H]+ 425.16419, found 425.16302; ASMS protein concentration first observed: 1.25 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 1860 nM.

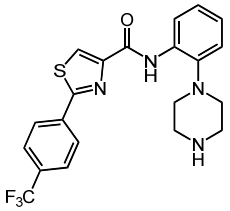
2-(3-ethoxy-2-fluorophenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (45)



The title compound was prepared using (3-ethoxy-2-fluorophenyl)boronic acid (0.075 mmol, 1.5 equiv., MFCD06798077), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M K_3PO_4 (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 8.3 mg (31% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **45**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.28 (s, 1H), 8.92 (br s, 2H), 8.67 (s, 1H), 8.41 (d, *J* = 7.9 Hz, 1H), 7.83 (d, *J* = 7.6 Hz, 1H), 7.42 (d, *J* = 6.0 Hz, 2H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 4.20 (q, *J* = 6.8 Hz, 2H), 3.32 (s, 4H, under water), 3.10 (s, 4H), 1.39 (t, *J* = 6.9 Hz, 3H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 160.2 (d, *J* = 4.1 Hz), 157.9, 149.6 (d, *J* = 252.1 Hz), 149.3, 147.3 (d, *J* = 10.5 Hz), 140.8, 132.6, 126.8 (d, *J*

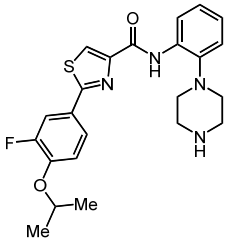
= 8.9 Hz), 125.7, 125.6 (d, *J* = 4.1 Hz), 124.4, 121.0, 120.5 (d, *J* = 8.5 Hz), 119.2, 118.5, 116.6, 64.8, 48.8, 44.1, 14.6; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{24}FN_4O_2S$ [M+H]+ 427.15985, found 427.15933; ASMS protein concentration first observed: 0.63 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 51.8 nM.

N-(2-(piperazin-1-yl)phenyl)-2-(4-(trifluoromethyl)phenyl)thiazole-4-carboxamide (E43)



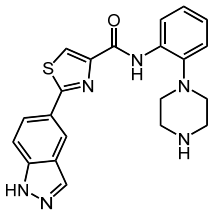
The title compound was prepared using (4-(trifluoromethyl)phenyl)boronic acid (0.075 mmol, 1.5 equiv., MFCD00151855), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M BTMG (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 9 mg (33% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E43**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.28 (s, 1H), 9.02 (br s, 2H), 8.66 (s, 1H), 8.44 (d, *J* = 8.0 Hz, 1H), 8.28 (d, *J* = 8.0 Hz, 2H), 7.99 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.26 (t, *J* = 7.6 Hz, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 3.36 (br s, 4H), 3.11 (br s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 166.0, 157.8, 150.6, 140.7, 135.7, 132.6, 130.5 (q, J = 31.9 Hz), 127.0, 126.7, 126.66, 125.7, 124.4, 123.6 (q, *J* = 189.1 Hz, approximate), 121.0, 119.1, 48.8, 44.1; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{20}F_3N_4OS$ [M+H]+ 433.13044, found 433.12915; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 1330 nM.

2-(3-fluoro-4-isopropoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E44)



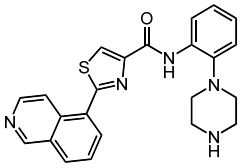
The title compound was prepared using (3-fluoro-4-isopropoxyphenyl)boronic acid (0.075 mmol, 1.5 equiv., MFCD05865163), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M BTMG (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 18.4 mg (66% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E44**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.22 (s, 1H), 8.97 (br s, 2H), 8.50 (s, 1H), 8.37 (d, *J* = 7.9 Hz, 1H), 7.90 (d, *J* = 11.8 Hz, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.38 (t, *J* = 8.5 Hz, 1H), 7.32 (d, *J* = 7.7 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.5 Hz, 1H), 4.77 (p, *J* = 5.9 Hz, 1H), 3.31 (s, 4H), 3.10 (s, 4H), 1.35 (d, *J* = 5.9 Hz, 6H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 166.5 (d, *J* = 2.1 Hz), 157.9, 152.4 (d, *J* = 245.4 Hz), 150.1, 147.6 (d, *J* = 10.1 Hz), 140.9, 132.5, 125.6, 125.4, 125.1 (d, *J* = 6.8 Hz), 124.4, 123.2 (d, *J* = 3.1 Hz), 120.8, 119.4, 116.8, 114.3 (d, *J* = 20.5 Hz), 71.4, 48.7, 44.1, 21.7; **HRMS** (ESI): *m/z* calculated for $C_{23}H_{26}FN_4O_2S$ [M+H]+ 441.17550, found 441.17395; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 910 nM.

2-(1H-indazol-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E45)



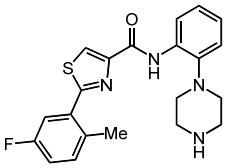
The title compound was prepared using 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indazole (0.075 mmol, 1.5 equiv., MFCD07367523), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M K_3PO_4 (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 4.8 mg (19% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E45**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 13.44 (s, 1H), 10.27 (s, 1H), 8.99 (br s, 2H), 8.46 (s, 1H), 8.45 (s, 1H), 8.40 (d, *J* = 8.0 Hz, 1H), 8.25 (s, 1H), 8.03 (d, *J* = 8.7 Hz, 1H), 7.74 (d, *J* = 8.7 Hz, 1H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 3.33 (s, 4H), 3.09 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 168.7, 158.0, 150.0, 140.7, 135.0, 132.7, 125.7, 125.0, 124.8, 124.3, 124.1, 123.2, 120.9, 119.7, 119.1, 111.6, 48.8, 44.2; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{21}N_6OS$ [M+H]+ 405.14921, found 405.14859; ASMS protein concentration first observed: 2.5 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 22.8 nM.

2-(isoquinolin-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E46)



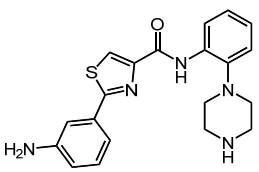
The title compound was prepared using isoquinolin-5-ylboronic acid (0.075 mmol, 1.5 equiv., MFCD03839356), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M BTMG (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 24.4 mg (92% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E46**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.19 (s, 1H), 9.56 (s, 1H), 8.80 (d, *J* = 5.8 Hz, 1H), 8.72 (m, 2H), 8.59 (br s, 2H), 8.44 (t, *J* = 7.2 Hz, 2H), 8.35 (d, *J* = 7.1 Hz, 1H), 7.90 (t, *J* = 7.7 Hz, 1H), 7.30 (d, *J* = 7.7 Hz, 1H), 7.26 (t, *J* = 7.7 Hz, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 3.05 (s, 4H), 2.99 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 166.0, 158.0, 152.9, 150.6, 144.0, 140.8, 133.4, 132.5, 132.1, 131.2, 128.7, 128.0, 127.6, 127.0, 125.5, 124.4, 120.7, 119.4, 118.0, 48.5, 43.8; **HRMS** (ESI): *m/z* calculated for $C_{23}H_{22}N_5OS$ [M+H]+ 416.15396, found 416.15347; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 768 nM.

2-(5-fluoro-2-methylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E47)



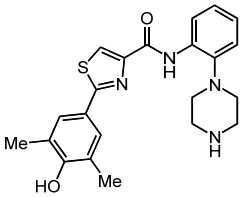
The title compound was prepared using (5-fluoro-2-methylphenyl)boronic acid (0.075 mmol, 1.5 equiv., MFCD03095047), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M BTMG (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 17.1 mg (67% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E47**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.11 (s, 1H), 8.88 (br s, 2H), 8.68 (s, 1H), 8.39 (d, *J* = 7.9 Hz, 1H), 7.74 (m, 1H), 7.49 (m, 1H), 7.33 (m, 2H), 7.25 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.5 Hz, 1H), 3.20 (s, 4H), 3.08 (s, 4H), 2.63 (s, 3H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 166.0 (d, *J* = 2.5 Hz), 160.5 (d, *J* = 242.8 Hz), 158.0, 149.7, 140.9, 133.8 (d, *J* = 8.1 Hz), 133.0 (d, *J* = 7.7 Hz), 132.4, 132.0 (d, *J* = 3.2 Hz), 126.8, 125.6, 124.5, 120.8, 119.5, 117.1 (d, *J* = 20.5 Hz), 116.0 (d, *J* = 23.5 Hz), 48.7, 43.8, 20.6; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{22}FN_4OS$ [M+H]+ 397.14929, found 397.14819; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 1380 nM.

2-(3-aminophenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (38)



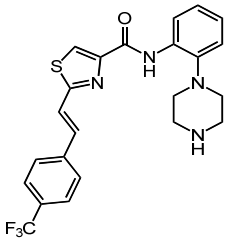
The title compound was prepared using 3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)aniline (0.075 mmol, 1.5 equiv., MFCD03453668), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M K_3PO_4 (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 24.2 mg (98% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **38**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.18 (s, 1H), 8.94 (br s, 2H), 8.48 (s, 1H), 8.40 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.35 – 7.29 (m, 1H), 7.29 – 7.22 (m, 3H), 7.20 (s, 1H), 7.17 (td, *J* = 7.7, 1.3 Hz, 1H), 6.78 (d, *J* = 7.9 Hz, 1H), 3.33 (br s, 4H), 3.17 – 3.05 (m, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 168.8, 158.1, 158.0, 150.1, 140.7, 132.8, 132.5, 130.3, 125.6, 125.0, 124.3, 120.7, 119.2, 116.7, 113.9, 111.5, 48.7, 44.1; **HRMS** (ESI): *m/z* calculated for $C_{20}H_{22}N_5OS$ [M+H]+ 380.15396, found 380.15356; ASMS protein concentration first observed: 0.63 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 50.9 nM.

2-(4-hydroxy-3,5-dimethylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E48)



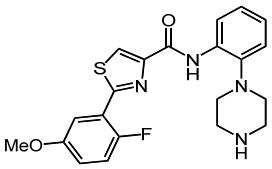
The title compound was prepared using 2,6-dimethyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenol (0.075 mmol, 1.5 equiv., MFCD02093724), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M BTMG (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 10.1 mg (39% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E48**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.23 (s, 1H), 9.02 (s, 1H), 8.88 (br s, 2H), 8.39 (s, 1H), 8.36 (d, *J* = 7.9 Hz, 1H), 7.63 (s, 2H), 7.31 (d, *J* = 7.7 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.4 Hz, 1H), 3.30 (s, 4H), 3.10 (s, 4H), 2.27 (s, 6H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 168.4, 158.1, 156.2, 149.8, 140.8, 132.5, 126.6, 125.5, 125.3, 124.3, 124.0, 123.4, 120.6, 119.3, 48.8, 44.2, 16.7; **HRMS** (ESI): *m/z* calculated for $C_{22}H_{25}N_4O_2S$ [M+H]+ 409.16927, found 409.16904; ASMS protein concentration first observed: 2.5 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 41.2 nM.

(*E*)-N-(2-(piperazin-1-yl)phenyl)-2-(4-(trifluoromethyl)styryl)thiazole-4-carboxamide (E49)



The title compound was prepared using (*E*)-(4-(trifluoromethyl)styryl)boronic acid (0.075 mmol, 1.5 equiv., MFCD03427005), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M BTMG (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 11.4 mg (40% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E49**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.16 (s, 1H), 8.84 (br s, 2H), 8.51 (s, 1H), 8.38 (d, *J* = 7.9 Hz, 1H), 7.98 (d, *J* = 7.8 Hz, 2H), 7.80 (d, *J* = 7.9 Hz, 2H), 7.75 (d, *J* = 16.3 Hz, 1H), 7.70 (d, *J* = 16.3 Hz, 1H), 7.31 (d, *J* = 7.7 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 7.4 Hz, 1H), 3.40 (s, 4H), 3.10 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 166.4, 157.8, 150.2, 140.6, 139.3, 134.3, 132.4, 128.2, 125.7, 125.67, 125.6, 125.4, 124.3, 124.1 (q, *J* = 272.9 Hz, approximate), 123.4, 120.6, 119.1, 48.6, 43.9; **HRMS** (ESI): *m/z* calculated for $C_{23}H_{22}F_3N_4OS$ [M+H]+ 459.14609, found 459.14566; ASMS protein concentration first observed: ASMS CHK1 binding not observed; Measured IC_{50} (CHK1, Invitrogen) 774 nM.

2-(2-fluoro-5-methoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E50)



The title compound was prepared using (2-fluoro-5-methoxyphenyl)boronic acid (0.075 mmol, 1.5 equiv., MFCD04974115), RuPhos G3 (0.005 mmol, 10 mol %, precatalyst), aq. 0.8 M BTMG (0.1 mmol, 2 equiv., base), and NMP as the reaction solvent. The reaction was carried out at the 0.05 mmol scale and stirred for 20 hours at ambient temperature. The product was purified by RP-HPLC to yield 10.4 mg (40% yield) of the title compound as an off-white solid (TFA salt). Analytical data for **E50**: **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.18 (s, 1H), 8.89 (br s, 2H), 8.66 (s, 1H), 8.31 (d, *J* = 7.9 Hz, 1H), 7.74 (s, 1H), 7.44 (t, *J* = 9.8 Hz, 1H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.24 (t, *J* = 7.5 Hz, 1H), 7.19 (q, *J* = 7.5, 6.2 Hz, 2H), 3.87 (s, 3H), 3.25 (s, 4H), 3.09 (s, 4H); **^{13}C NMR** (126 MHz, DMSO-d_6) δ 160.5 (d, *J* = 5.8 Hz), 153.8 (d, *J* = 243.7 Hz), 158.0, 156.0, 149.5, 141.4, 132.2, 126.8 (d, *J* = 8.0 Hz), 125.4, 124.6, 120.7, 120.3 (d, *J* = 13.5 Hz), 120.2, 118.2 (d, *J* = 8.5 Hz), 117.8 (d, *J* = 23.5 Hz), 112.4, 56.0, 48.6, 44.0; **HRMS** (ESI): *m/z* calculated for $C_{21}H_{22}FN_4O_2S$ [M+H]+ 413.14420, found 413.14304; ASMS protein concentration first observed: 2.5 µM CHK1; Measured IC_{50} (CHK1, Invitrogen) 96.9 nM.

8.7. Scaled Up Library Plots

Plots displaying the general correlation between activity assay IC_{50} (plotted on a log scale) and the lowest CHK1 concentration at which ASMS binding was observed (protein level) for scaled up examples from the big library experiment are shown below.

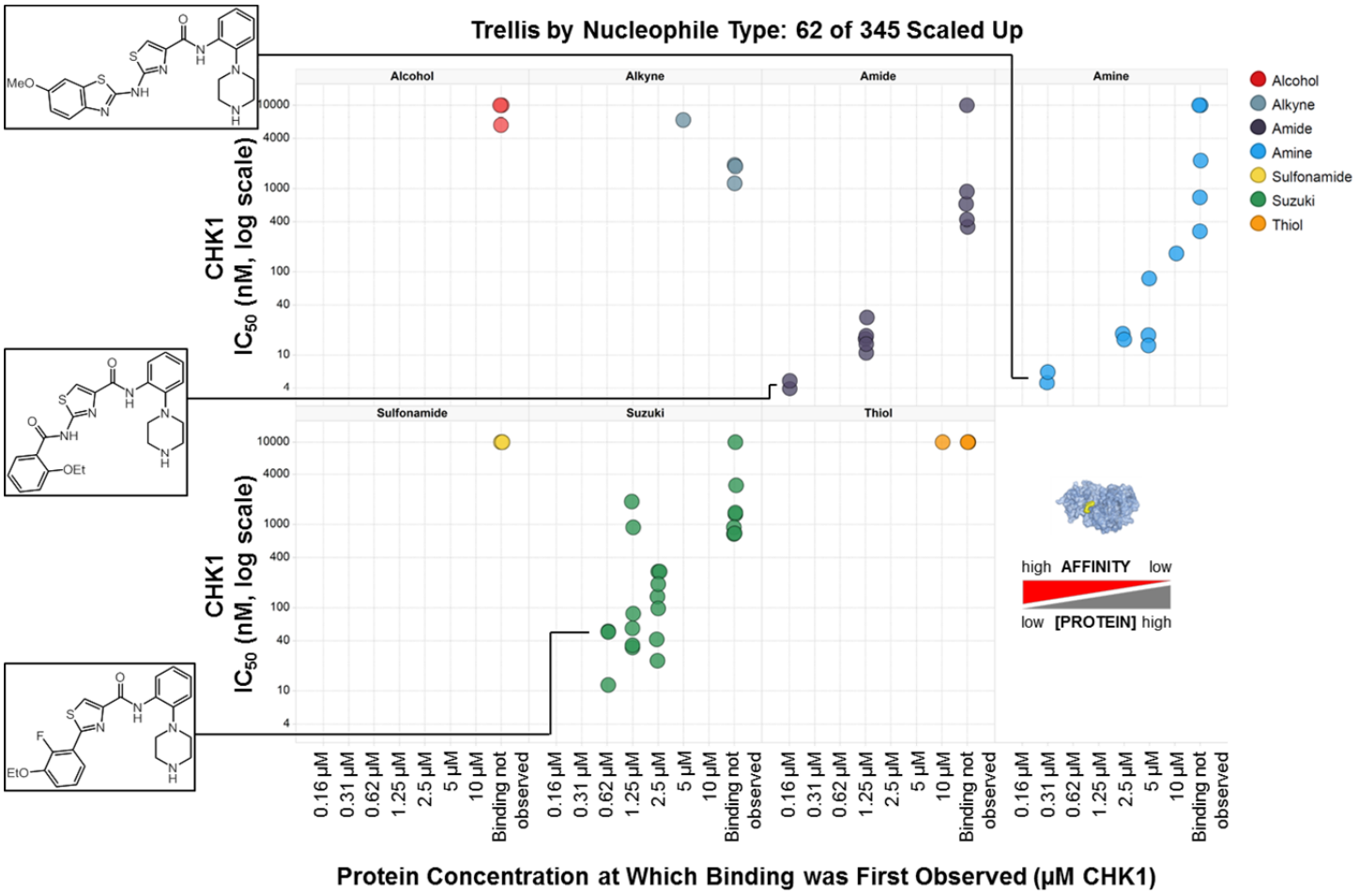


Figure 46. Trellis by Chemistry – Scaled up and Purified Examples: Affinity Ranking Protein Concentration at Which Binding was First Observed Versus CHK1 Activity.

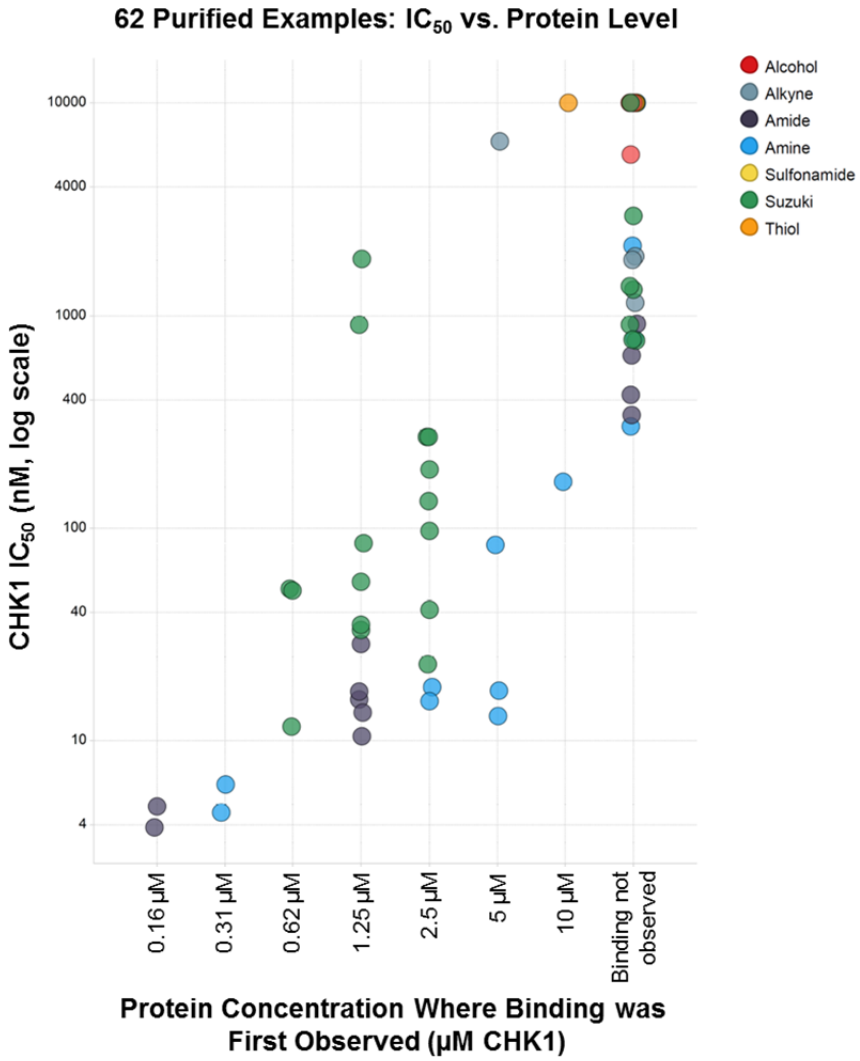


Figure 47. 62-Member Scaled Up and Purified Library Plotted Together.

9. TTP Labtech Mosquito® Protocols

9.1. Mosquito® Protocol for Suzuki Cross-Coupling Screen, Section 3.2

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C9-9, R1, S1) to (P3, C1-1, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C9-9, R1, S1) to (P3, C3-3, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C9-9, R1, S1) to (P3, C5-5, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C9-9, R1, S1) to (P3, C7-7, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C10-10, R1, S1) to (P3, C9-9, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C10-10, R1, S1) to (P3, C11-11, R1, S1)

Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C10-10, R1, S1) to (P3, C13-13, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C10-10, R1, S1) to (P3, C15-15, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C11-11, R1, S1) to (P3, C17-17, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C11-11, R1, S1) to (P3, C19-19, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C11-11, R1, S1) to (P3, C21-21, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C11-11, R1, S1) to (P3, C23-23, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C12-12, R1, S1) to (P3, C25-25, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C12-12, R1, S1) to (P3, C27-27, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C12-12, R1, S1) to (P3, C29-29, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C12-12, R1, S1) to (P3, C31-31, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Pause indefinitely - then home deck

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C13-13, R1, S1) to (P3, C33-33, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C13-13, R1, S1) to (P3, C35-35, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C13-13, R1, S1) to (P3, C37-37, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C13-13, R1, S1) to (P3, C39-39, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C41-41, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C43-43, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C45-45, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C47-47, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C2-2, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C4-4, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C6-6, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C8-8, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C10-10, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C12-12, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C14-14, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C16-16, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Pause indefinitely - then home deck

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C18-18, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C20-20, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C22-22, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C24-24, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C26-26, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C28-28, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C30-30, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C32-32, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C34-34, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C36-36, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C38-38, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first

Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C40-40, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C20-20, R1, S1) to (P3, C42-42, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C20-20, R1, S1) to (P3, C44-44, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C20-20, R1, S1) to (P3, C46-46, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C20-20, R1, S1) to (P3, C48-48, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C21-21, R1, S1) to (P3, C1-1, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C21-21, R1, S1) to (P3, C3-3, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C21-21, R1, S1) to (P3, C5-5, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C21-21, R1, S1) to (P3, C7-7, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C4)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C22-22, R1, S1) to (P3, C9-9, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C22-22, R1, S1) to (P3, C11-11, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C22-22, R1, S1) to (P3, C13-13, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C2)

Multi-aspirate 5nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 5nL from (P1, C8)

Copy 250nL from (P1, C22-22, R1, S1) to (P3, C15-15, R2, S1)
 Source (row, column) spacing: (1, 1)
 Destination (row, column) spacing: (2, 2)
 Contact first
 Change tips always
 Dispense Mix cycles 3, volume 750nL

9.2. Mosquito® Protocol for Supplementary Suzuki Cross-Coupling Screen, Section 3.3

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C11-11, R1, S1) to (P3, C1-1, R1, S1)
 Source (row, column) spacing: (1, 1)
 Destination (row, column) spacing: (2, 2)
 Contact first
 Change tips always
 Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C11-11, R1, S1) to (P3, C3-3, R1, S1)
 Source (row, column) spacing: (1, 1)
 Destination (row, column) spacing: (2, 2)
 Contact first
 Change tips always
 Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C12-12, R1, S1) to (P3, C5-5, R1, S1)
 Source (row, column) spacing: (1, 1)
 Destination (row, column) spacing: (2, 2)
 Contact first
 Change tips always
 Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C12-12, R1, S1) to (P3, C7-7, R1, S1)
 Source (row, column) spacing: (1, 1)
 Destination (row, column) spacing: (2, 2)
 Contact first
 Change tips always
 Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C13-13, R1, S1) to (P3, C9-9, R1, S1)
 Source (row, column) spacing: (1, 1)

Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C13-13, R1, S1) to (P3, C11-11, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C13-13, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C15-15, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C17-17, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C19-19, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C21-21, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C23-23, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C2-2, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C4-4, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C6-6, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C8-8, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C10-10, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C6)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C9)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C12-12, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

9.3. Mosquito® Protocol for Buchwald-Hartwig Amination Screen, Section 3.4

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C12-12, R1, S1) to (P3, C1-1, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C13-13, R1, S1) to (P3, C3-3, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C5-5, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C7-7, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C9-9, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C11-11, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C12-12, R1, S1) to (P3, C13-13, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C13-13, R1, S1) to (P3, C15-15, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C17-17, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C19-19, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C21-21, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C23-23, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C12-12, R1, S1) to (P3, C25-25, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C13-13, R1, S1) to (P3, C27-27, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C29-29, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C31-31, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C33-33, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C35-35, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C12-12, R1, S1) to (P3, C37-37, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C13-13, R1, S1) to (P3, C39-39, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C41-41, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C43-43, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C45-45, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C10)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C47-47, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

9.4. Mosquito® Protocol for Buchwald-Hartwig Amination Screen, Section 3.5

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C1-1, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C3-3, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C5-5, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C5)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C7-7, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C9-9, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C11-11, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C13-13, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C15-15, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C17-17, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C19-19, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C21-21, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C23-23, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C25-25, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C27-27, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C29-29, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C31-31, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C33-33, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C35-35, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C37-37, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C39-39, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C14-14, R1, S1) to (P3, C41-41, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C15-15, R1, S1) to (P3, C43-43, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C45-45, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C12)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C47-47, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

9.5. Mosquito® Protocol for 2-Bromothiazole Mixed Coupling Screen, Section 3.6

DMSO Plate

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C1-1, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C3-3, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C5-5, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C7-7, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)

Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C9-9, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C11-11, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C13-13, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C15-15, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C17-17, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C19-19, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C21-21, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C23-23, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C25-25, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C27-27, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C29-29, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C31-31, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C33-33, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C35-35, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C37-37, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C39-39, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C41-41, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C43-43, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C45-45, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C47-47, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C2-2, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C4-4, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C6-6, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C8-8, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C10-10, R1, S1)
Source (row, column) spacing: (1, 1)

Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C12-12, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C14-14, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C16-16, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

NMP Plate

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C18-18, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C20-20, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C22-22, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C24-24, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C26-26, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C28-28, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C30-30, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C32-32, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C34-34, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C36-36, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C38-38, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C40-40, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C42-42, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C44-44, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C46-46, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first

Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C48-48, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C1-1, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C3-3, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C5-5, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C7-7, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C9-9, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C11-11, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C13-13, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C15-15, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C17-17, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C19-19, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C21-21, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C23-23, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C25-25, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C27-27, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C29-29, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C31-31, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

DMF Plate

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C33-33, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C35-35, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C37-37, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C6)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C39-39, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C41-41, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C43-43, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C45-45, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C7)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C47-47, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C2-2, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C4-4, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C6-6, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C8-8, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C10-10, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C12-12, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C14-14, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C16-16, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C18-18, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C20-20, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C22-22, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C24-24, R2, S1)

Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C26-26, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C28-28, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C30-30, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C32-32, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C34-34, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C36-36, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C38-38, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C40-40, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C16-16, R1, S1) to (P3, C42-42, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C17-17, R1, S1) to (P3, C44-44, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C18-18, R1, S1) to (P3, C46-46, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 250nL from (P1, C1)

Multi-aspirate 250nL from (P1, C3)

Multi-aspirate 10nL from (P1, C5)

Multi-aspirate 250nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Copy 250nL from (P1, C19-19, R1, S1) to (P3, C48-48, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

9.6. Mosquito® Protocol for pERK2 Amide Library, Section 5.3

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C7)

Multi-aspirate 6nL from (P1, C11)

Copy 297nL from (P1, C13-13, R1, S1) to (P3, C1-1, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C8)

Multi-aspirate 6nL from (P1, C11)

Copy 297nL from (P1, C13-13, R1, S1) to (P3, C3-3, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C4)

Copy 6nL from (P1, C6-6, R1, S1) to (P3, C5-5, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 400nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C7)

Multi-aspirate 6nL from (P1, C11)

Copy 297nL from (P1, C13-13, R1, S1) to (P3, C7-7, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C8)

Multi-aspirate 6nL from (P1, C11)

Copy 297nL from (P1, C13-13, R1, S1) to (P3, C9-9, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C4)

Copy 6nL from (P1, C6-6, R1, S1) to (P3, C11-11, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 400nL

After 15 minutes:
Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 297nL from (P1, C9)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C14-14, R1, S1) to (P3, C5-5, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 600nL

Multi-aspirate 297nL from (P1, C9)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C14-14, R1, S1) to (P3, C11-11, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 600nL

9.7. Mosquito® Protocol for MK2 Suzuki Cross-Coupling Library, Section 6.2

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C4)

Multi-aspirate 6nL from (P1, C9)

Multi-aspirate 297nL from (P1, C11)

Multi-aspirate 6nL from (P1, C15)

Copy 297nL from (P1, C18-18, R1, S1) to (P3, C1-1, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C4)

Multi-aspirate 6nL from (P1, C9)

Multi-aspirate 297nL from (P1, C11)

Multi-aspirate 6nL from (P1, C15)

Copy 297nL from (P1, C19-19, R1, S1) to (P3, C3-3, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C4)

Multi-aspirate 6nL from (P1, C9)

Multi-aspirate 297nL from (P1, C12)

Multi-aspirate 6nL from (P1, C15)

Copy 297nL from (P1, C18-18, R1, S1) to (P3, C5-5, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C4)

Multi-aspirate 6nL from (P1, C9)

Multi-aspirate 297nL from (P1, C12)

Multi-aspirate 6nL from (P1, C15)

Copy 297nL from (P1, C19-19, R1, S1) to (P3, C7-7, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C6)

Multi-aspirate 6nL from (P1, C10)

Multi-aspirate 297nL from (P1, C13)

Multi-aspirate 6nL from (P1, C16)

Copy 297nL from (P1, C18-18, R1, S1) to (P3, C9-9, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C6)

Multi-aspirate 6nL from (P1, C10)

Multi-aspirate 297nL from (P1, C13)

Multi-aspirate 6nL from (P1, C16)

Copy 297nL from (P1, C19-19, R1, S1) to (P3, C11-11, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C6)

Multi-aspirate 6nL from (P1, C10)

Multi-aspirate 297nL from (P1, C14)

Multi-aspirate 6nL from (P1, C16)

Copy 297nL from (P1, C18-18, R1, S1) to (P3, C13-13, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C6)

Multi-aspirate 6nL from (P1, C10)

Multi-aspirate 297nL from (P1, C14)

Multi-aspirate 6nL from (P1, C16)

Copy 297nL from (P1, C19-19, R1, S1) to (P3, C15-15, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C5)

Multi-aspirate 6nL from (P1, C9)

Multi-aspirate 297nL from (P1, C11)

Multi-aspirate 6nL from (P1, C15)

Copy 297nL from (P1, C18-18, R1, S1) to (P3, C17-17, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C5)

Multi-aspirate 6nL from (P1, C9)

Multi-aspirate 297nL from (P1, C11)

Multi-aspirate 6nL from (P1, C15)

Copy 297nL from (P1, C19-19, R1, S1) to (P3, C19-19, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)

Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C5)

Multi-aspirate 6nL from (P1, C9)

Multi-aspirate 297nL from (P1, C12)

Multi-aspirate 6nL from (P1, C15)

Copy 297nL from (P1, C18-18, R1, S1) to (P3, C21-21, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C5)

Multi-aspirate 6nL from (P1, C9)

Multi-aspirate 297nL from (P1, C12)

Multi-aspirate 6nL from (P1, C15)

Copy 297nL from (P1, C19-19, R1, S1) to (P3, C23-23, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C7)

Multi-aspirate 6nL from (P1, C10)

Multi-aspirate 297nL from (P1, C13)

Multi-aspirate 6nL from (P1, C16)

Copy 297nL from (P1, C18-18, R1, S1) to (P3, C25-25, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C7)

Multi-aspirate 6nL from (P1, C10)

Multi-aspirate 297nL from (P1, C13)

Multi-aspirate 6nL from (P1, C16)

Copy 297nL from (P1, C19-19, R1, S1) to (P3, C27-27, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C7)

Multi-aspirate 6nL from (P1, C10)

Multi-aspirate 297nL from (P1, C14)

Multi-aspirate 6nL from (P1, C16)

Copy 297nL from (P1, C18-18, R1, S1) to (P3, C29-29, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C7)

Multi-aspirate 6nL from (P1, C10)

Multi-aspirate 297nL from (P1, C14)

Multi-aspirate 6nL from (P1, C16)

Copy 297nL from (P1, C19-19, R1, S1) to (P3, C31-31, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

9.8. Mosquito® Protocol for CHK1 Mixed Coupling Validation Library, Section 7.2

Suzuki Cross-Coupling Source Plate

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C4)

Multi-aspirate 6nL from (P1, C7)

Multi-aspirate 297nL from (P1, C9)

Multi-aspirate 6nL from (P1, C13)

Copy 297nL from (P1, C16-16, R1, S1) to (P3, C1-1, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C4)

Multi-aspirate 6nL from (P1, C7)

Multi-aspirate 297nL from (P1, C9)

Multi-aspirate 6nL from (P1, C13)

Copy 297nL from (P1, C17-17, R1, S1) to (P3, C3-3, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C4)

Multi-aspirate 6nL from (P1, C7)

Multi-aspirate 297nL from (P1, C10)

Multi-aspirate 6nL from (P1, C13)

Copy 297nL from (P1, C16-16, R1, S1) to (P3, C5-5, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C4)

Multi-aspirate 6nL from (P1, C7)

Multi-aspirate 297nL from (P1, C10)

Multi-aspirate 6nL from (P1, C13)

Copy 297nL from (P1, C17-17, R1, S1) to (P3, C7-7, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C5)

Multi-aspirate 6nL from (P1, C8)

Multi-aspirate 297nL from (P1, C11)

Multi-aspirate 6nL from (P1, C14)

Copy 297nL from (P1, C16-16, R1, S1) to (P3, C9-9, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C5)

Multi-aspirate 6nL from (P1, C8)

Multi-aspirate 297nL from (P1, C11)

Multi-aspirate 6nL from (P1, C14)

Copy 297nL from (P1, C17-17, R1, S1) to (P3, C11-11, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C5)

Multi-aspirate 6nL from (P1, C8)

Multi-aspirate 297nL from (P1, C12)

Multi-aspirate 6nL from (P1, C14)

Copy 297nL from (P1, C16-16, R1, S1) to (P3, C13-13, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 297nL from (P1, C2)

Multi-aspirate 297nL from (P1, C5)

Multi-aspirate 6nL from (P1, C8)

Multi-aspirate 297nL from (P1, C12)

Multi-aspirate 6nL from (P1, C14)

Copy 297nL from (P1, C17-17, R1, S1) to (P3, C15-15, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Buchwald-Hartwig Amination Source Plate

Tape pitch 4.5mm

Crystallography deck

Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C7)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C14-14, R1, S1) to (P3, C17-17, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C7)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C15-15, R1, S1) to (P3, C19-19, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C7)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C16-16, R1, S1) to (P3, C21-21, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first

Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C8)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C14-14, R1, S1) to (P3, C23-23, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C8)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C15-15, R1, S1) to (P3, C25-25, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C8)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C16-16, R1, S1) to (P3, C27-27, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C9)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C14-14, R1, S1) to (P3, C29-29, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C9)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C15-15, R1, S1) to (P3, C31-31, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C9)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C16-16, R1, S1) to (P3, C33-33, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C10)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C14-14, R1, S1) to (P3, C35-35, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C10)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C15-15, R1, S1) to (P3, C37-37, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

Multi-aspirate 297nL from (P1, C1)

Multi-aspirate 297nL from (P1, C3)

Multi-aspirate 6nL from (P1, C5)

Multi-aspirate 297nL from (P1, C10)

Multi-aspirate 6nL from (P1, C12)

Copy 297nL from (P1, C16-16, R1, S1) to (P3, C39-39, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 750nL

9.9. Mosquito® Protocol for CHK1 384-Member Mixed Coupling Library, Section 8

9.9.1. Variable Condition Screen: 1,536 Reaction, 384-Member Coupling Library, Section 8.2

Dispensing from 384-well nucleophile building block plate to 1,536 reaction plate

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Aliquot 300nL from (P1, C1, R1, S1) to (P3, C1-7, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C2, R1, S1) to (P3, C9-15, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C3, R1, S1) to (P3, C17-23, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C4, R1, S1) to (P3, C25-31, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C5, R1, S1) to (P3, C33-39, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C6, R1, S1) to (P3, C41-47, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)

Contact first
Change tips always

Aliquot 300nL from (P1, C7, R1, S1) to (P3, C2-8, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C8, R1, S1) to (P3, C10-16, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C9, R1, S1) to (P3, C18-24, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C10, R1, S1) to (P3, C26-32, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C11, R1, S1) to (P3, C34-40, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C12, R1, S1) to (P3, C42-48, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C13, R1, S1) to (P3, C1-7, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C14, R1, S1) to (P3, C9-15, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C15, R1, S1) to (P3, C17-23, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C16, R1, S1) to (P3, C25-31, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C17, R1, S1) to (P3, C33-39, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C18, R1, S1) to (P3, C41-47, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C19, R1, S1) to (P3, C2-8, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C20, R1, S1) to (P3, C10-16, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C21, R1, S1) to (P3, C18-24, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C22, R1, S1) to (P3, C26-32, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C23, R1, S1) to (P3, C34-40, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Aliquot 300nL from (P1, C24, R1, S1) to (P3, C42-48, R2, S1)

Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)

Dispensing from 384-well reagent source plate to 1,536-well reaction plate

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C2)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C9-9, R1, S1) to (P3, C1-1, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C2)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C3-3, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C4)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C9-9, R1, S1) to (P3, C5-5, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C4)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C7-7, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C2)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C9-9, R1, S1) to (P3, C9-9, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C2)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C11-11, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C4)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C9-9, R1, S1) to (P3, C13-13, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C4)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C15-15, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C2)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C9-9, R1, S1) to (P3, C17-17, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C2)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C19-19, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C4)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C9-9, R1, S1) to (P3, C21-21, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C4)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C23-23, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C2)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C9-9, R1, S1) to (P3, C25-25, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C2)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C27-27, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C4)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C9-9, R1, S1) to (P3, C29-29, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C4)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C31-31, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C2)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C9-9, R1, S1) to (P3, C33-33, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C2)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C35-35, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C4)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C9-9, R1, S1) to (P3, C37-37, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C4)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C39-39, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C2)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C9-9, R1, S1) to (P3, C41-41, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C2)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C43-43, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C4)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C9-9, R1, S1) to (P3, C45-45, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C4)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C47-47, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C16)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C23-23, R1, S1) to (P3, C2-2, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C16)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C4-4, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C17)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C23-23, R1, S1) to (P3, C6-6, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C17)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C8-8, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C16)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C23-23, R1, S1) to (P3, C10-10, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C16)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C12-12, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C17)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C23-23, R1, S1) to (P3, C14-14, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C17)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C16-16, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C17)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C18-18, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C17)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C20-20, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C18)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C22-22, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C18)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C24-24, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C17)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C26-26, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C17)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C28-28, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C18)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C30-30, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C18)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C32-32, R1, S1)

Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C6)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C10-10, R1, S1) to (P3, C34-34, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C6)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C36-36, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C10-10, R1, S1) to (P3, C38-38, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C40-40, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C6)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C10-10, R1, S1) to (P3, C42-42, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C6)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C44-44, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C10-10, R1, S1) to (P3, C46-46, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C11-11, R1, S1) to (P3, C48-48, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)

Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C1-1, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C23-23, R1, S1) to (P3, C3-3, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C19)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C5-5, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C19)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C23-23, R1, S1) to (P3, C7-7, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C9-9, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C23-23, R1, S1) to (P3, C11-11, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C19)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C13-13, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C19)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C23-23, R1, S1) to (P3, C15-15, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C17-17, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C23-23, R1, S1) to (P3, C19-19, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C19)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C21-21, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C19)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C23-23, R1, S1) to (P3, C23-23, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C25-25, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C27-27, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C18)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C29-29, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C18)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C31-31, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C33-33, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C35-35, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C18)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C37-37, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C18)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C39-39, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C41-41, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C43-43, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C18)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C45-45, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C18)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C47-47, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C2-2, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C20)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C4-4, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C18)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C22-22, R1, S1) to (P3, C6-6, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C15)

Multi-aspirate 200nL from (P1, C18)

Multi-aspirate 10nL from (P1, C21)

Copy 300nL from (P1, C24-24, R1, S1) to (P3, C8-8, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C12-12, R1, S1) to (P3, C10-10, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C13-13, R1, S1) to (P3, C12-12, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C7)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C12-12, R1, S1) to (P3, C14-14, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C7)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C13-13, R1, S1) to (P3, C16-16, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C12-12, R1, S1) to (P3, C18-18, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C13-13, R1, S1) to (P3, C20-20, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C7)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C12-12, R1, S1) to (P3, C22-22, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C7)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C13-13, R1, S1) to (P3, C24-24, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C12-12, R1, S1) to (P3, C26-26, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C13-13, R1, S1) to (P3, C28-28, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C7)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C12-12, R1, S1) to (P3, C30-30, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C7)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C13-13, R1, S1) to (P3, C32-32, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C12-12, R1, S1) to (P3, C34-34, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C13-13, R1, S1) to (P3, C36-36, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C7)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C12-12, R1, S1) to (P3, C38-38, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C7)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C13-13, R1, S1) to (P3, C40-40, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C12-12, R1, S1) to (P3, C42-42, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C5)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C13-13, R1, S1) to (P3, C44-44, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C7)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C12-12, R1, S1) to (P3, C46-46, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 400nL from (P1, C1)

Multi-aspirate 200nL from (P1, C7)

Multi-aspirate 10nL from (P1, C8)

Copy 300nL from (P1, C13-13, R1, S1) to (P3, C48-48, R2, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

9.9.2. Variable Condition Screen: 96 Amine Building Block / C-N Coupling Rerun, Section 8.2

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C16)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C1-1, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C16)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C3-3, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C17)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C5-5, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C17)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C7-7, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C16)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C9-9, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C16)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C11-11, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)

Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C17)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C13-13, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C17)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C15-15, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C16)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C17-17, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C16)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C19-19, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C17)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C21-21, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C17)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C23-23, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C16)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C25-25, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C16)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C27-27, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C17)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C29-29, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C17)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C31-31, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C16)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C33-33, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C16)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C35-35, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C17)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C37-37, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C17)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C39-39, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C16)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C41-41, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C16)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C43-43, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C17)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C45-45, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C17)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C47-47, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C18)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C2-2, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C8)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C18)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C4-4, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C18)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C6-6, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C9)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C18)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C8-8, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C18)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C10-10, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C10)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C18)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C12-12, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C18)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C14-14, R1, S1)
Source (row, column) spacing: (1, 1)

Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C11)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C18)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C16-16, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C18)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C18-18, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C12)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C18)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C20-20, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C18)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C22-22, R1, S1) to (P3, C22-22, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

Multi-aspirate 295nL from (P1, C6)

Multi-aspirate 295nL from (P1, C13)

Multi-aspirate 10nL from (P1, C14)

Multi-aspirate 295nL from (P1, C18)

Multi-aspirate 10nL from (P1, C20)

Copy 295nL from (P1, C23-23, R1, S1) to (P3, C24-24, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

9.9.3. Single Condition Screen: 384 Building Blocks × P_2-Et/*t*-BuXPhos G3, Section 8.3

Tape pitch 4.5mm

Crystallography deck
Position:
1: Greiner 384 Polypro Deepwell Conical
2: [no plate]
3: Greiner 1536 Polypro

Copy 300nL from (P1, C1-24, R1, S1) to (P3, C1-47, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always

Pause indefinitely - then home deck

Multi-aspirate 300nL from (P1, C1)

Multi-aspirate 300nL from (P1, C5)

Aliquot 300nL from (P1, C7, R1, S1) to (P3, C1-37, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

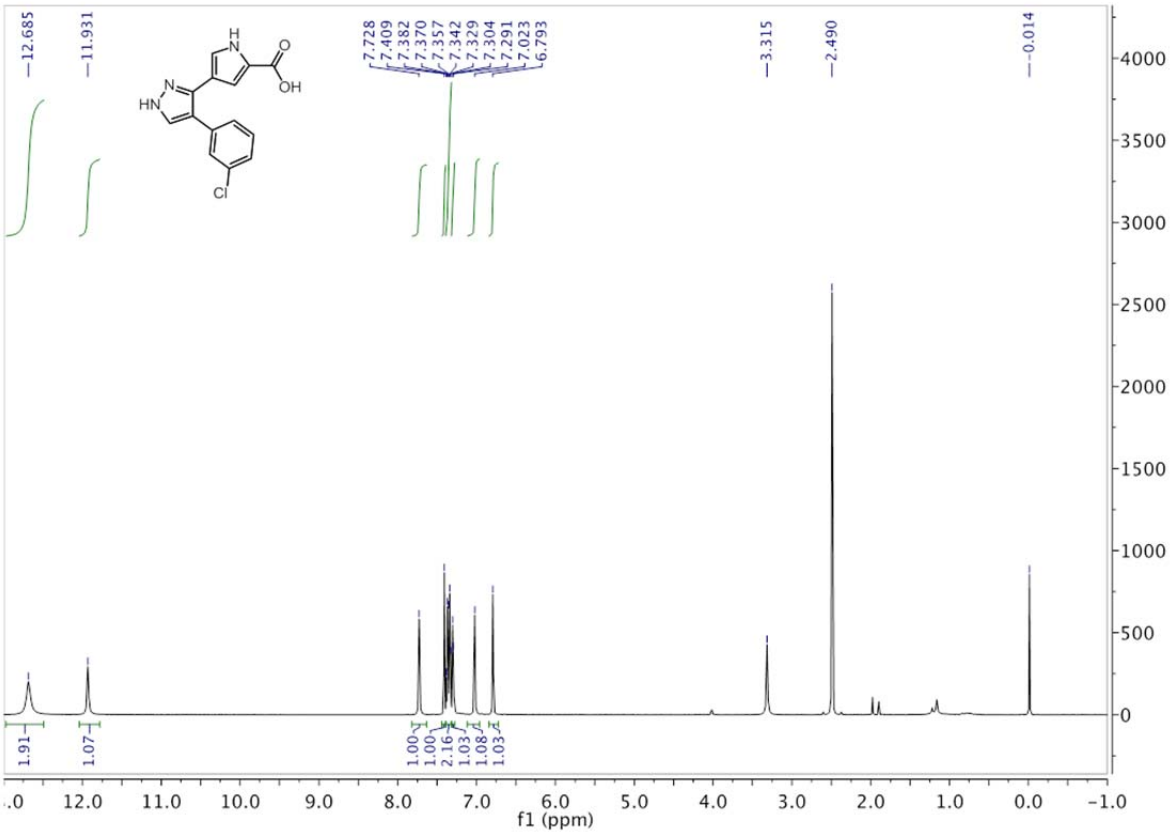
Multi-aspirate 300nL from (P1, C2)

Multi-aspirate 300nL from (P1, C5)

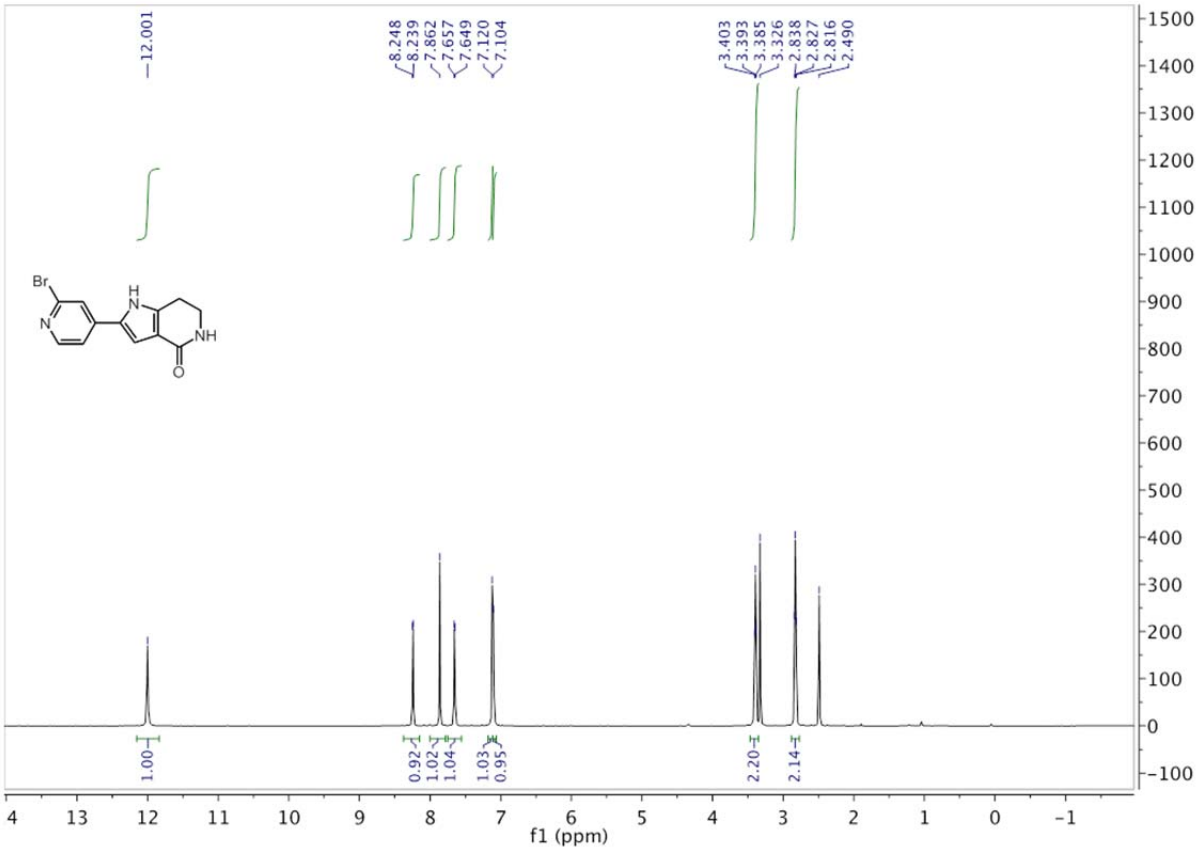
Aliquot 300nL from (P1, C7, R1, S1) to (P3, C39-47, R1, S1)
Source (row, column) spacing: (1, 1)
Destination (row, column) spacing: (2, 2)
Contact first
Change tips always
Dispense Mix cycles 3, volume 800nL

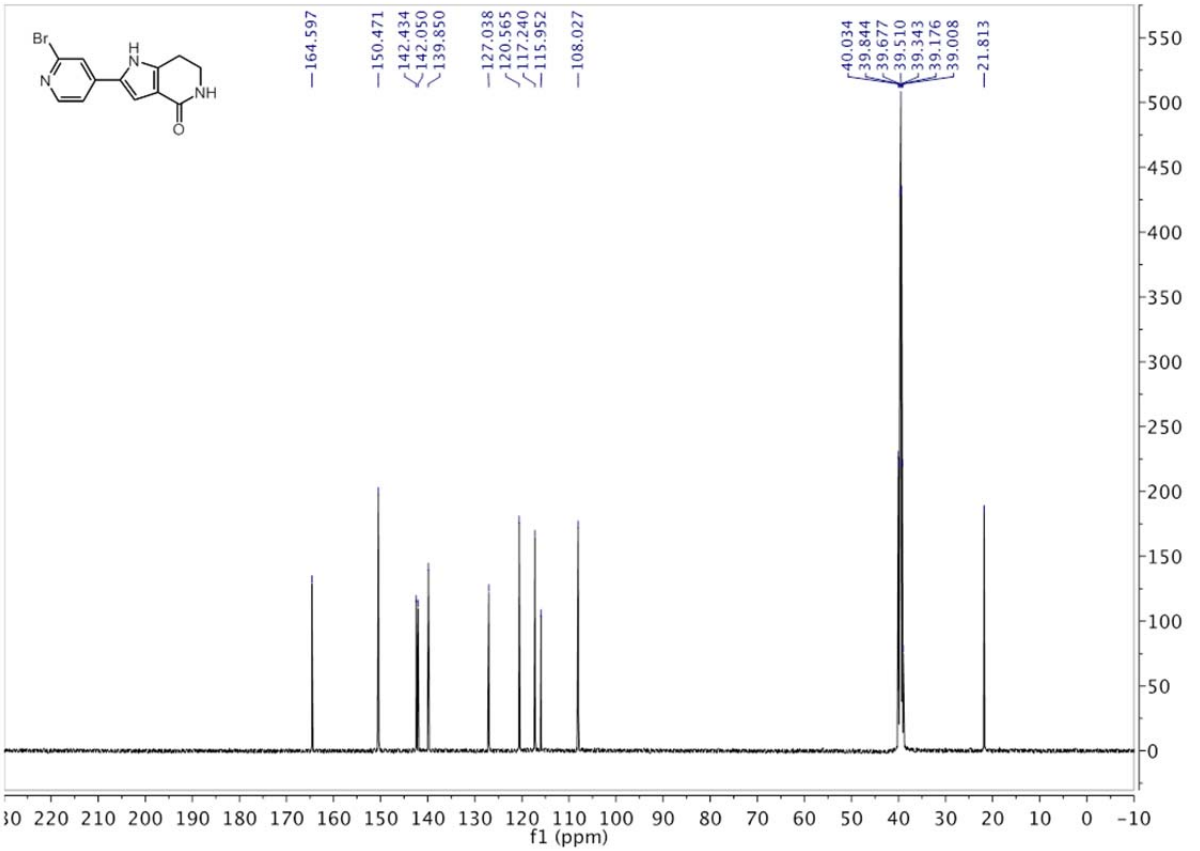
^{1}H and ^{13}C NMR Spectra

4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrole-2-carboxylic acid (1)

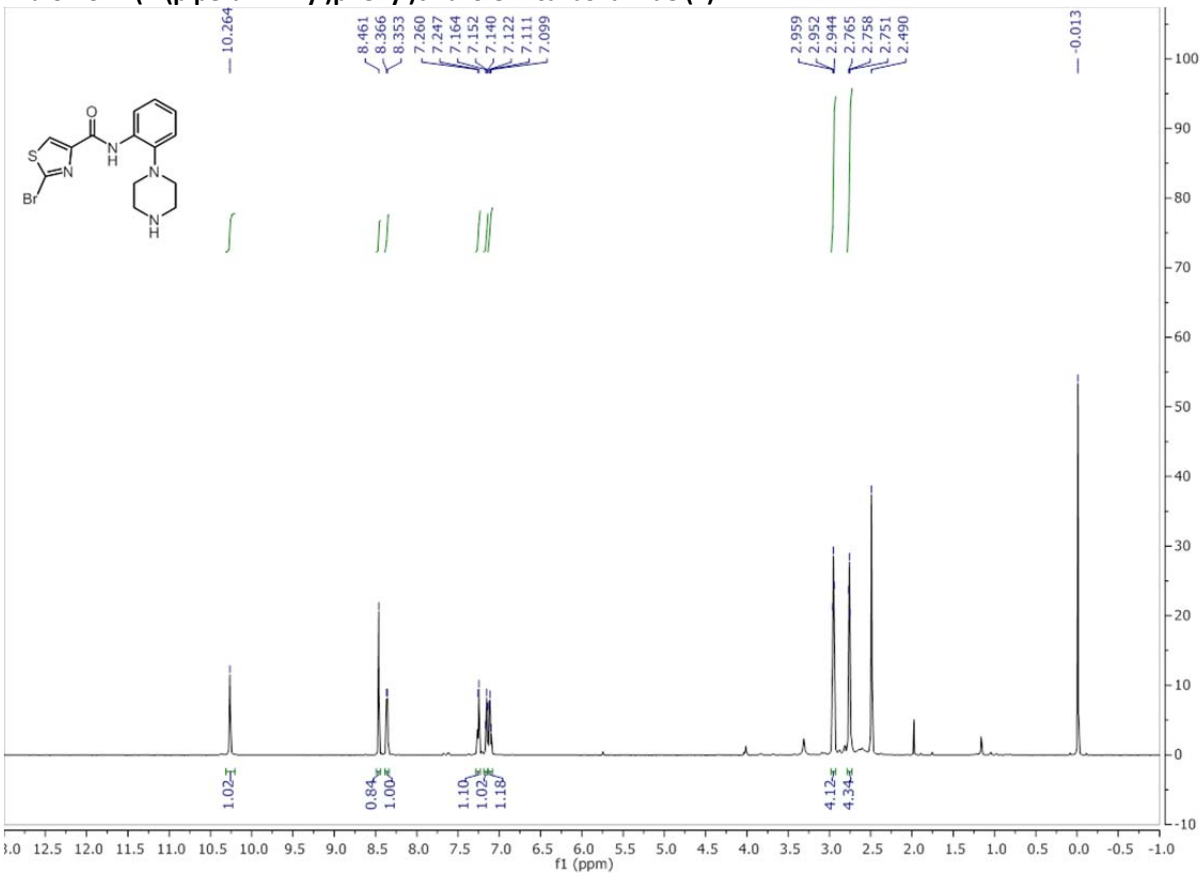


2-(2-bromopyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (4)

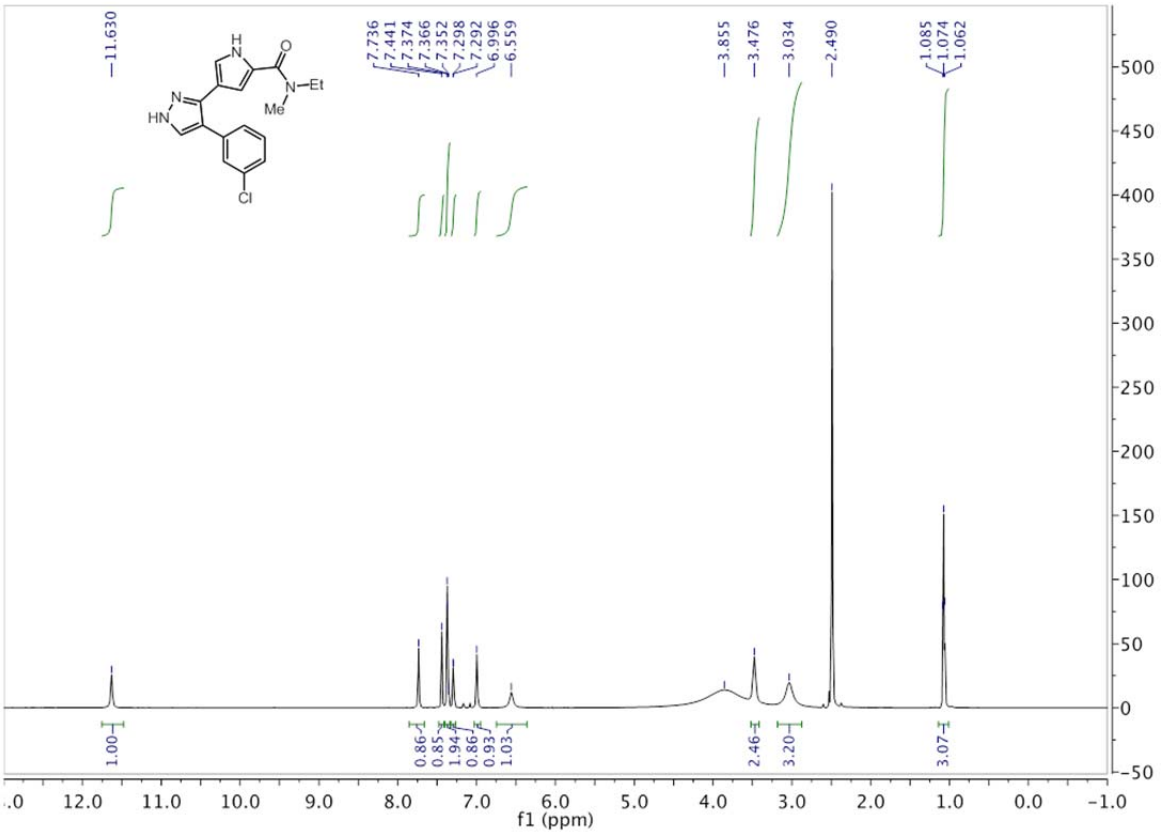




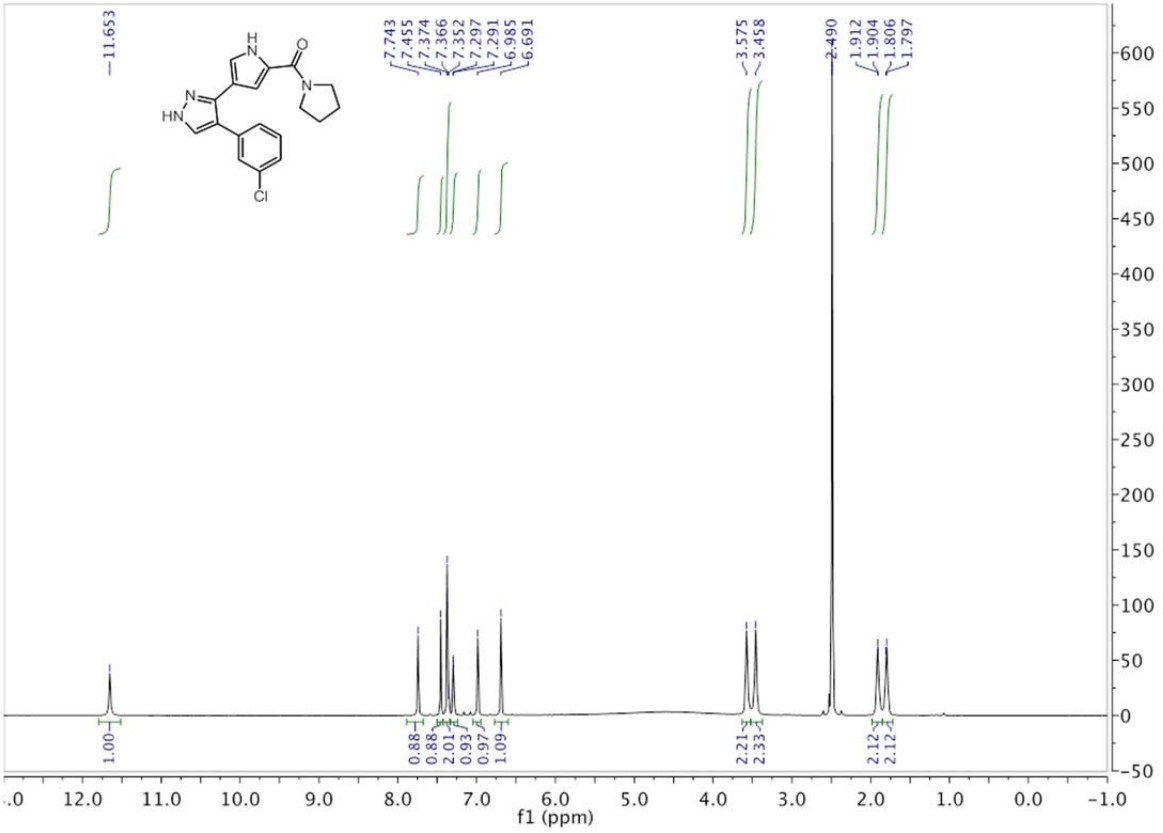
2-bromo-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (7)



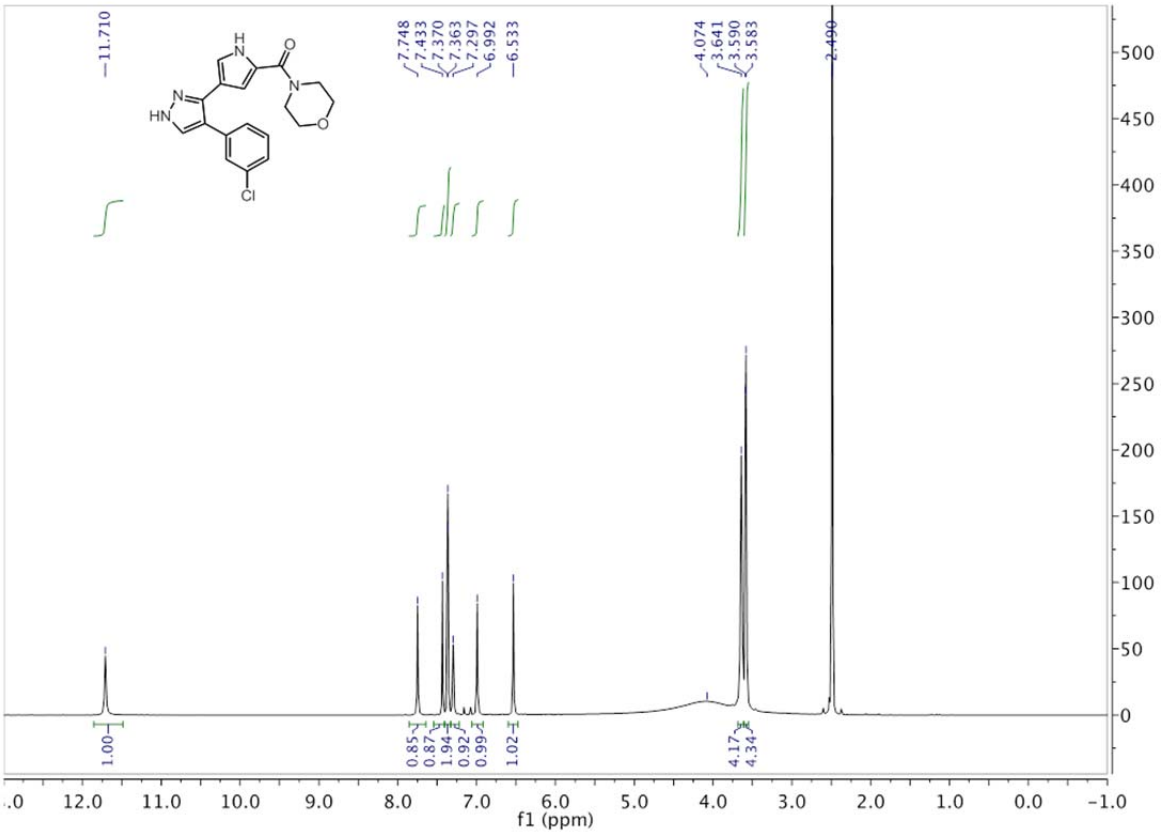
4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-ethyl-N-methyl-1H-pyrrole-2-carboxamide (A1)



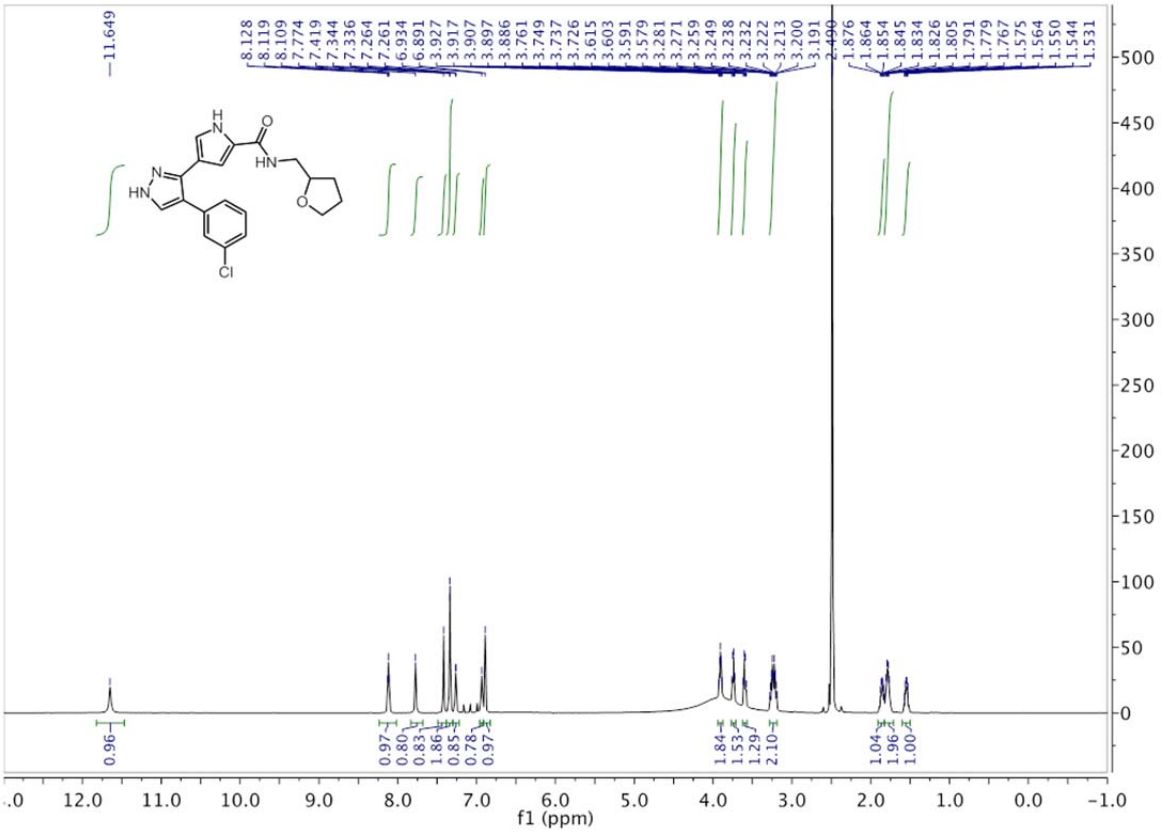
(4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrol-2-yl)(pyrrolidin-1-yl)methanone (A2)



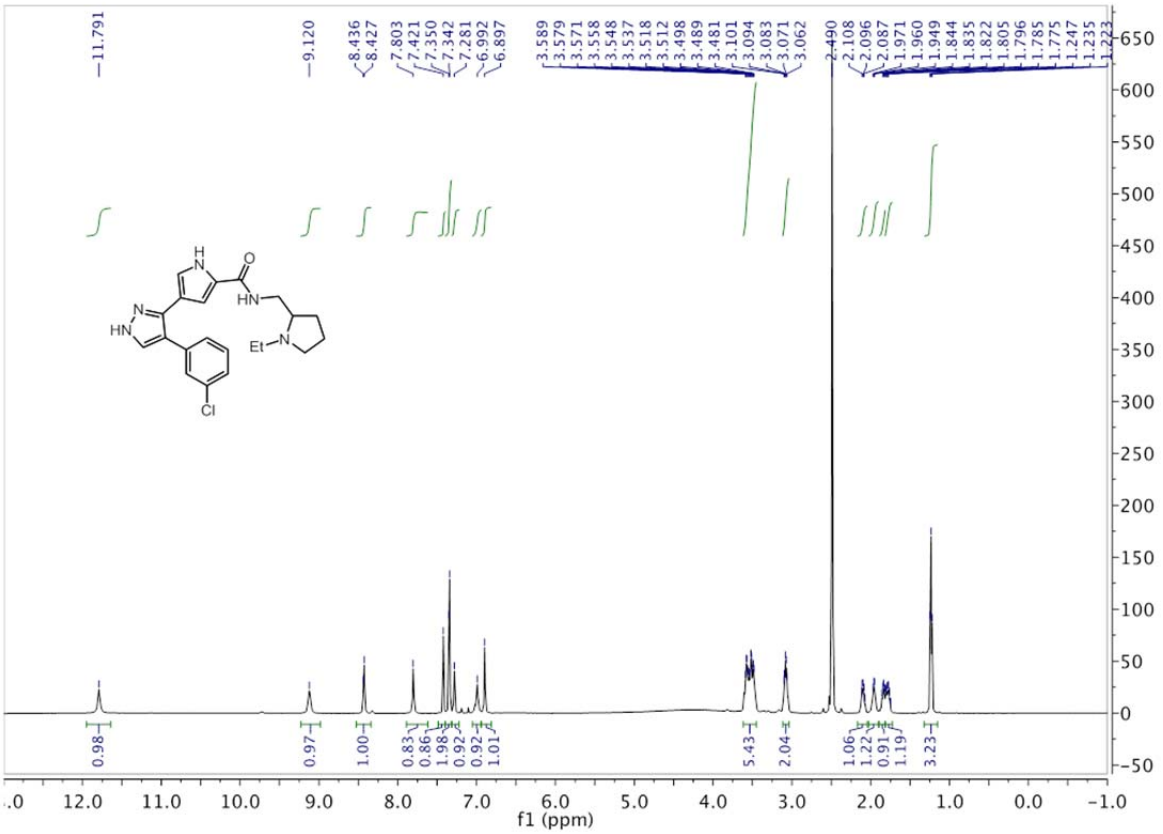
(4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrol-2-yl)(morpholino)methanone (A3)



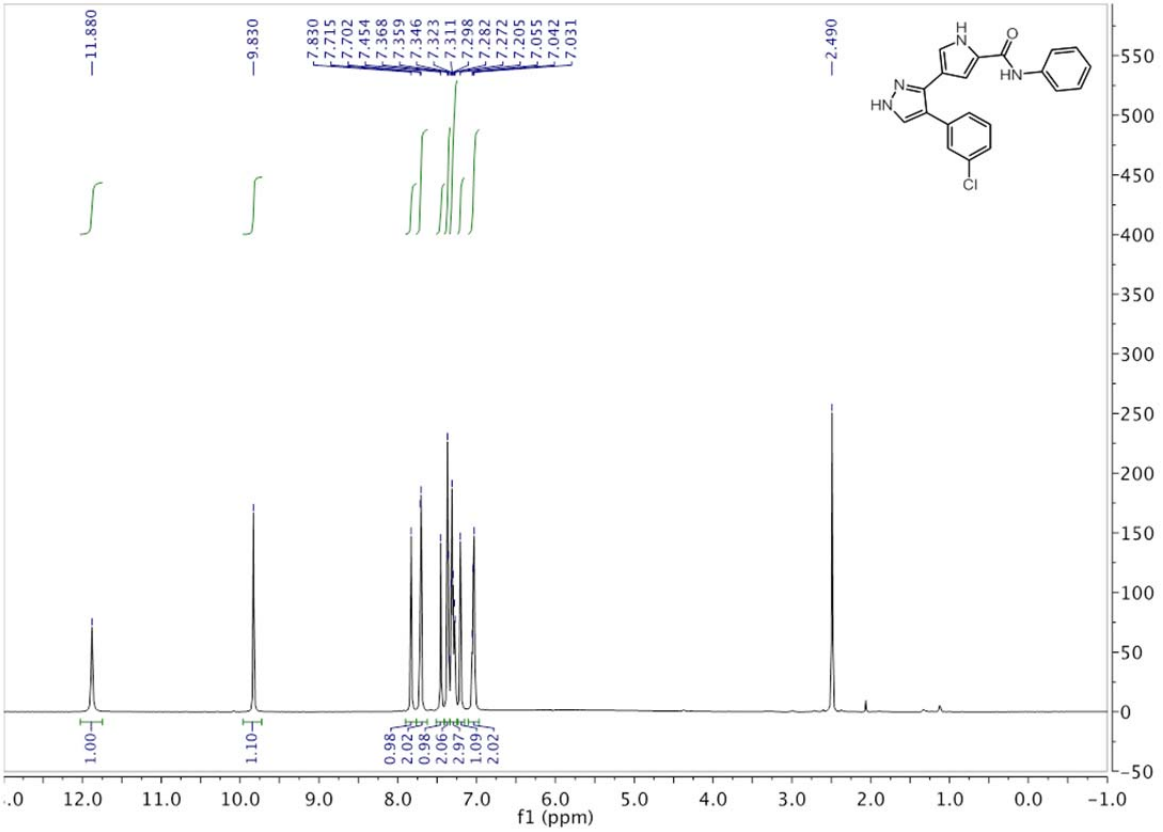
4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-((tetrahydrofuran-2-yl)methyl)-1H-pyrrole-2-carboxamide (A4)



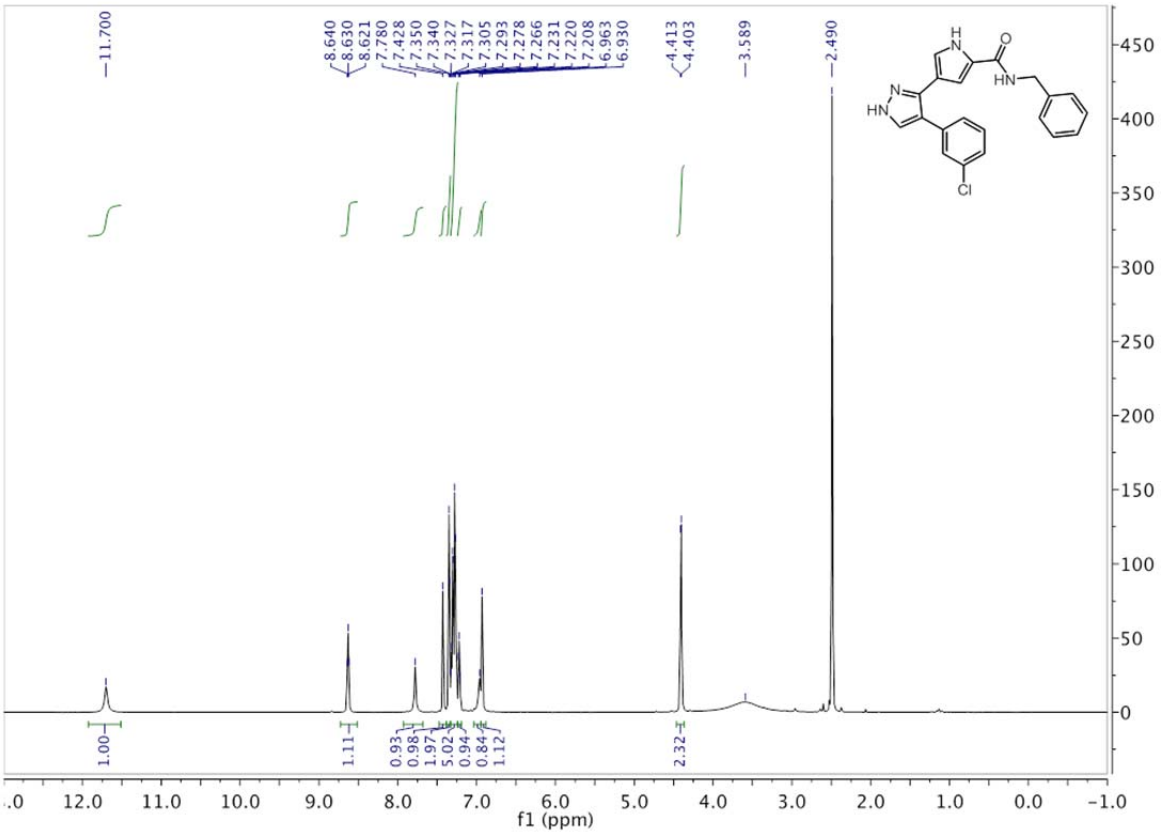
4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-((1-ethylpyrrolidin-2-yl)methyl)-1H-pyrrole-2-carboxamide (A5)



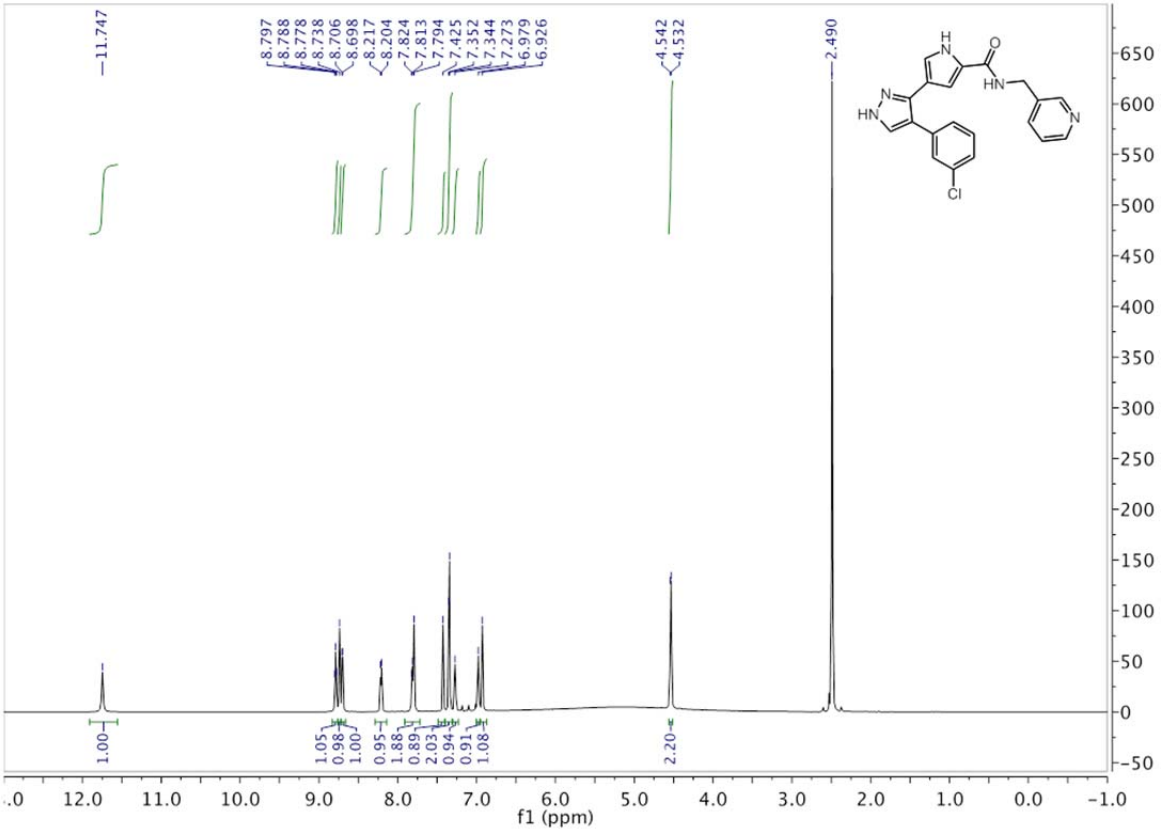
4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-phenyl-1H-pyrrole-2-carboxamide (A6)



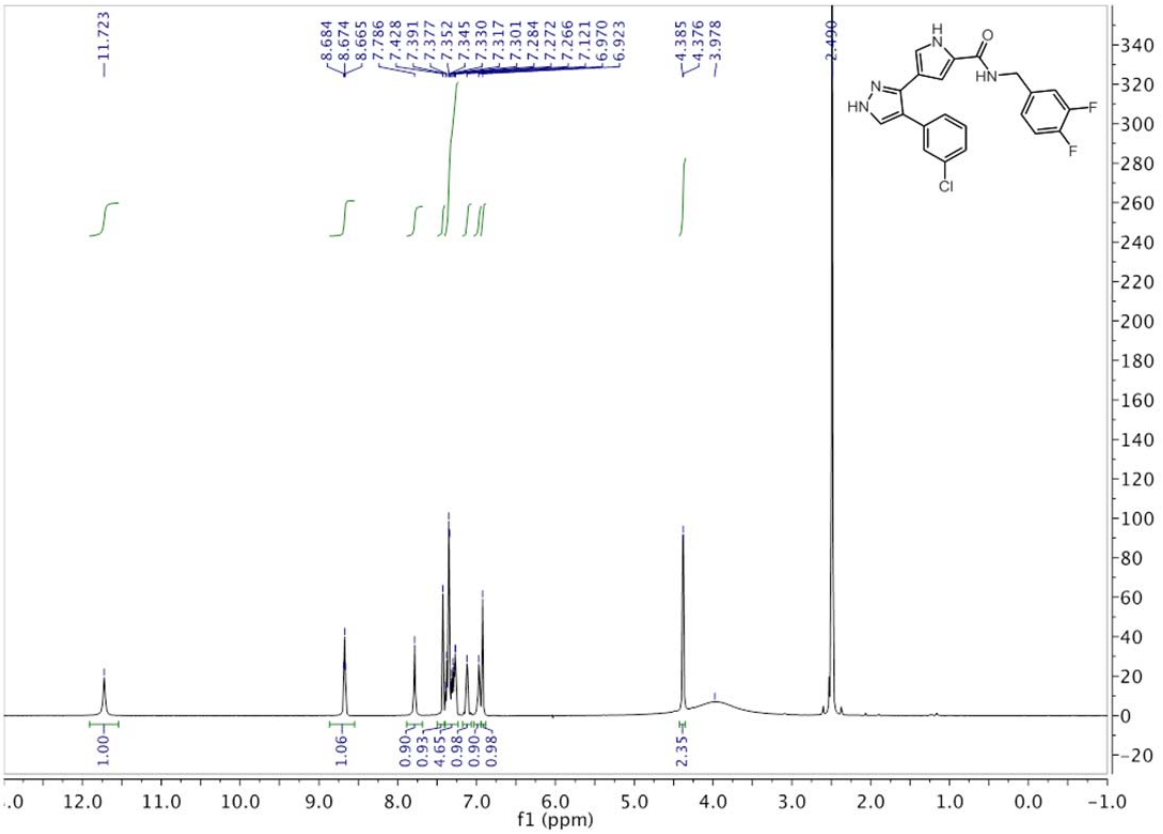
N-benzyl-4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrole-2-carboxamide (A7)



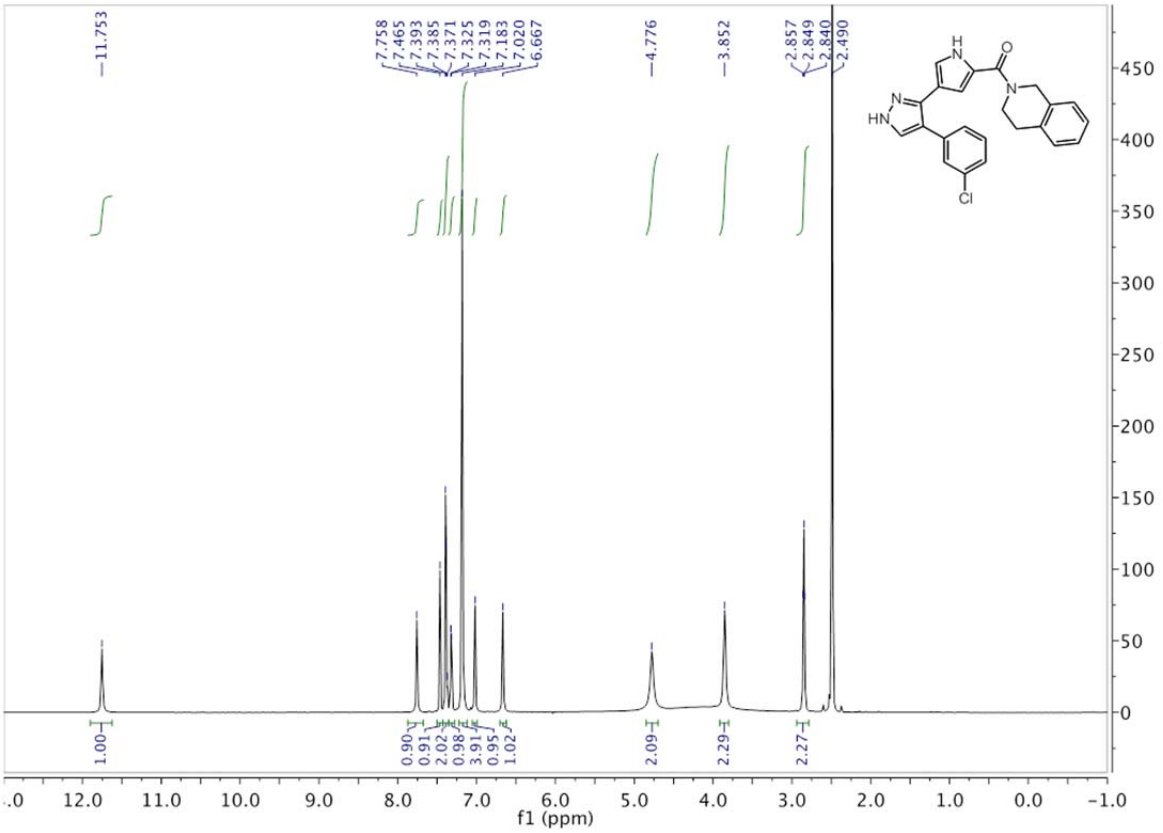
4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(pyridin-3-ylmethyl)-1H-pyrrole-2-carboxamide (A8)



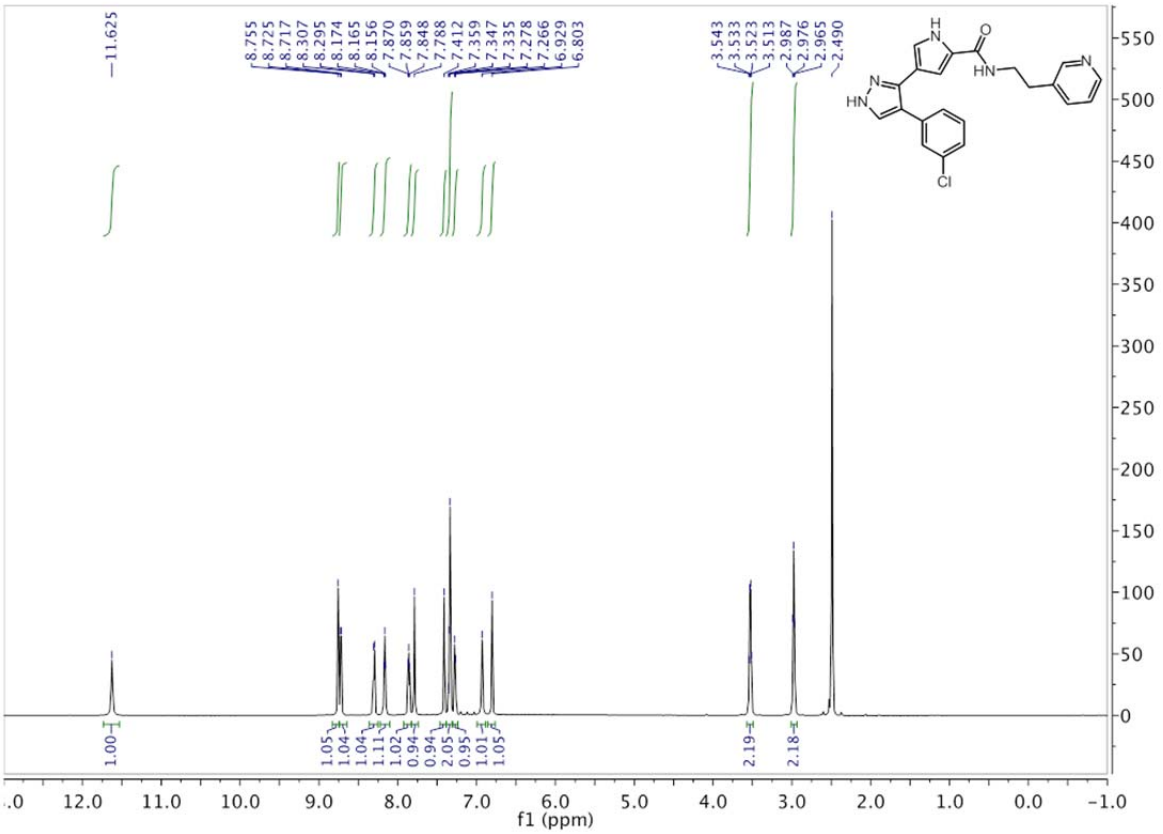
4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(3,4-difluorobenzyl)-1H-pyrrole-2-carboxamide (A9)



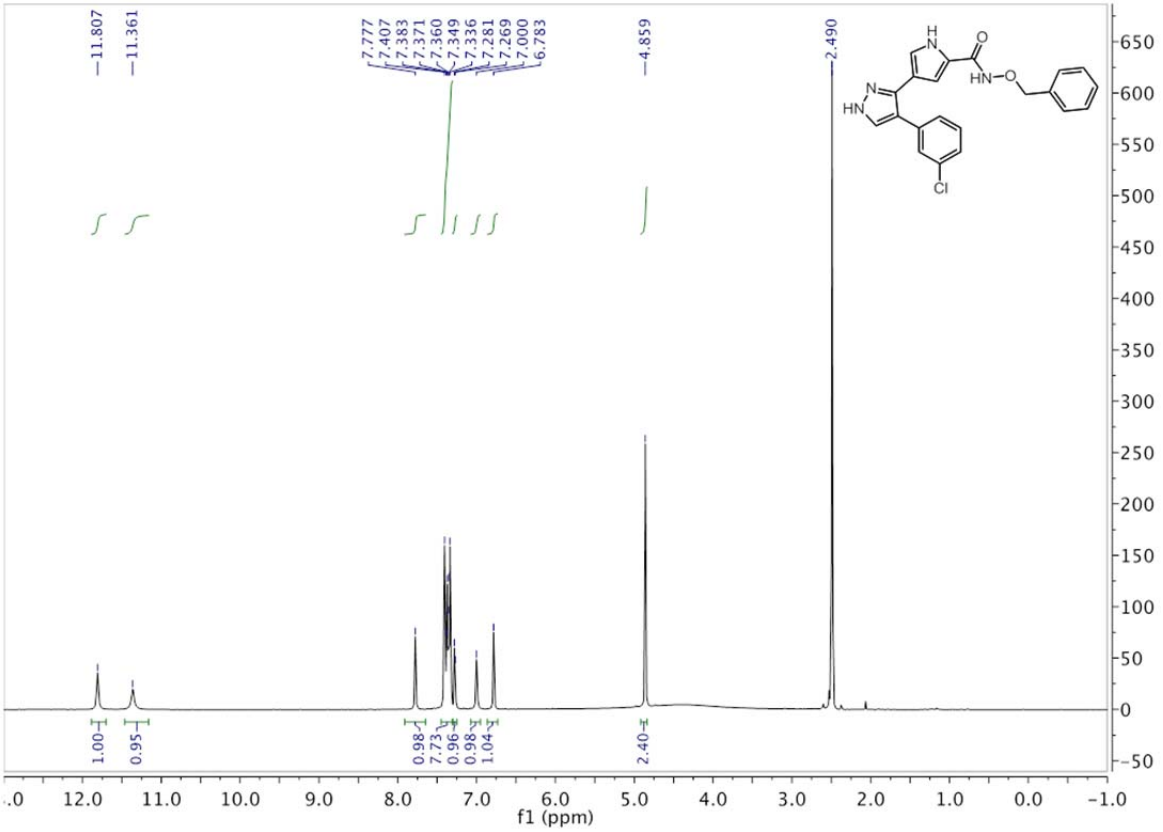
(4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrol-2-yl)(3,4-dihydroisoquinolin-2(1H)-yl)methanone (A10)



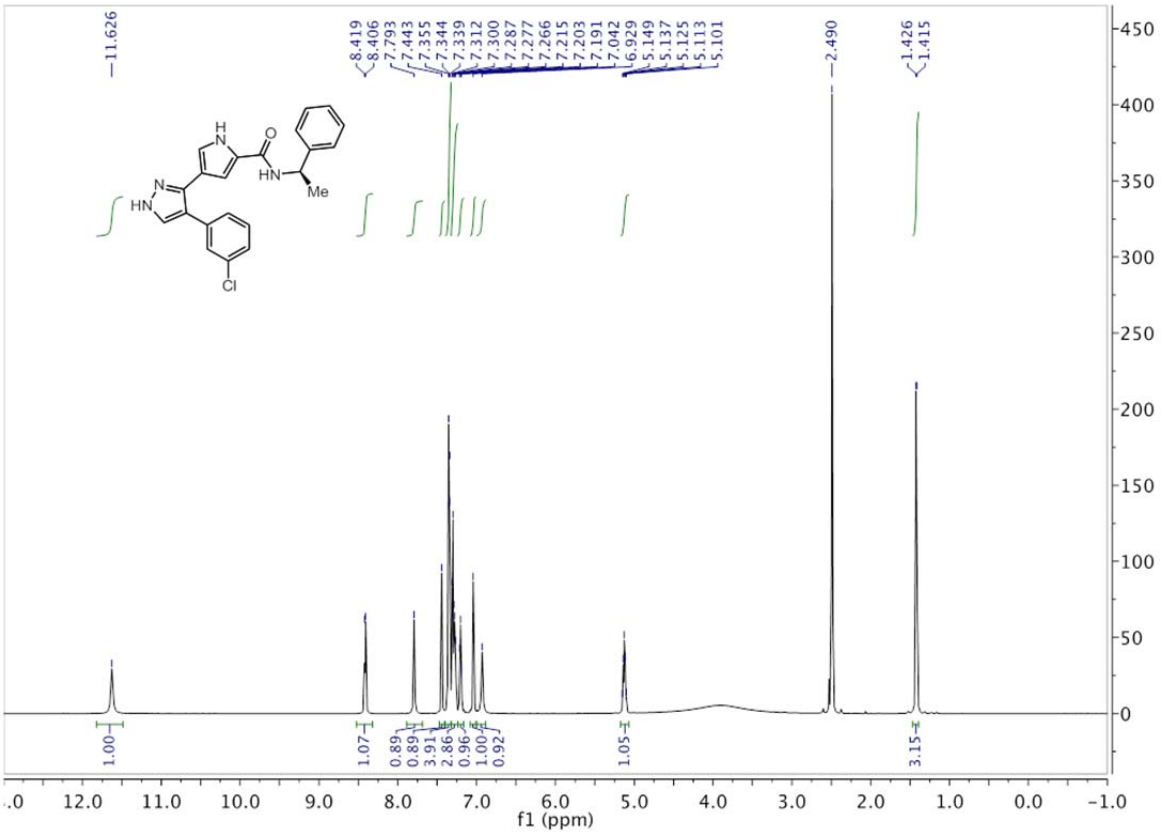
4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(2-(pyridin-3-yl)ethyl)-1H-pyrrole-2-carboxamide (A11)



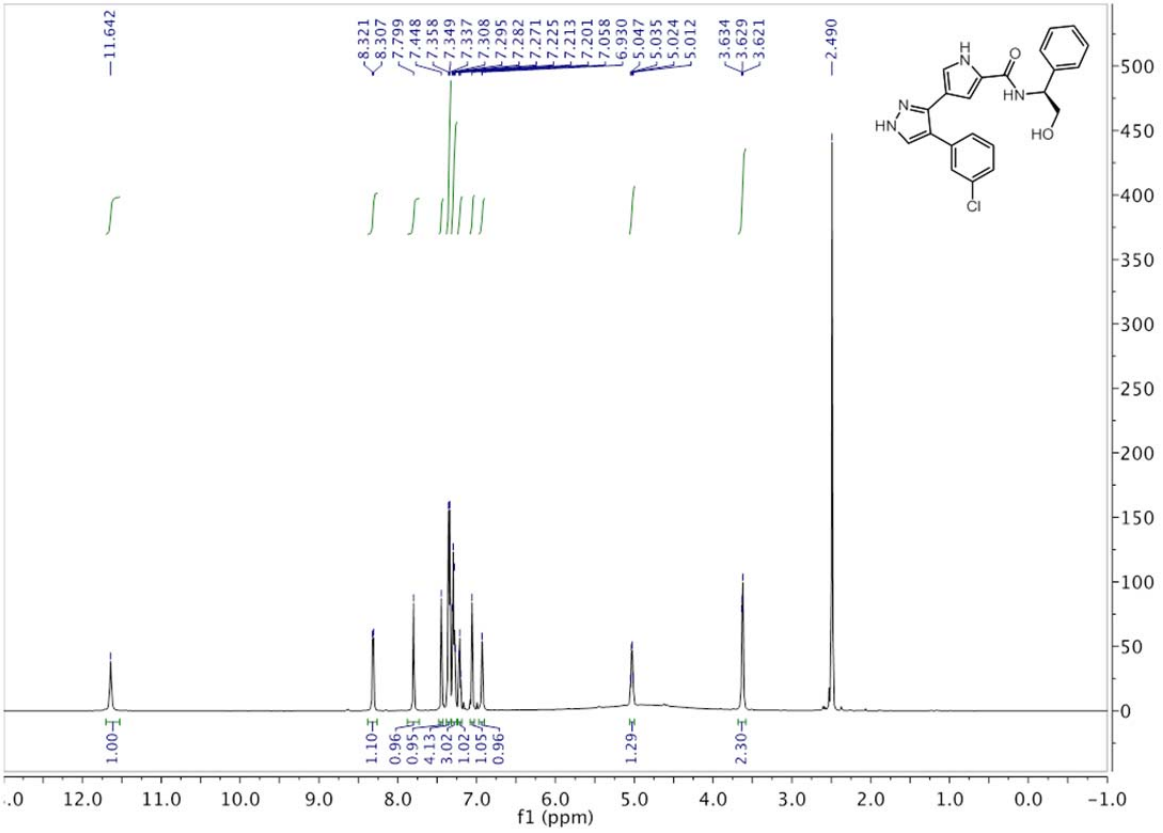
N-(benzyloxy)-4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrole-2-carboxamide (A12)



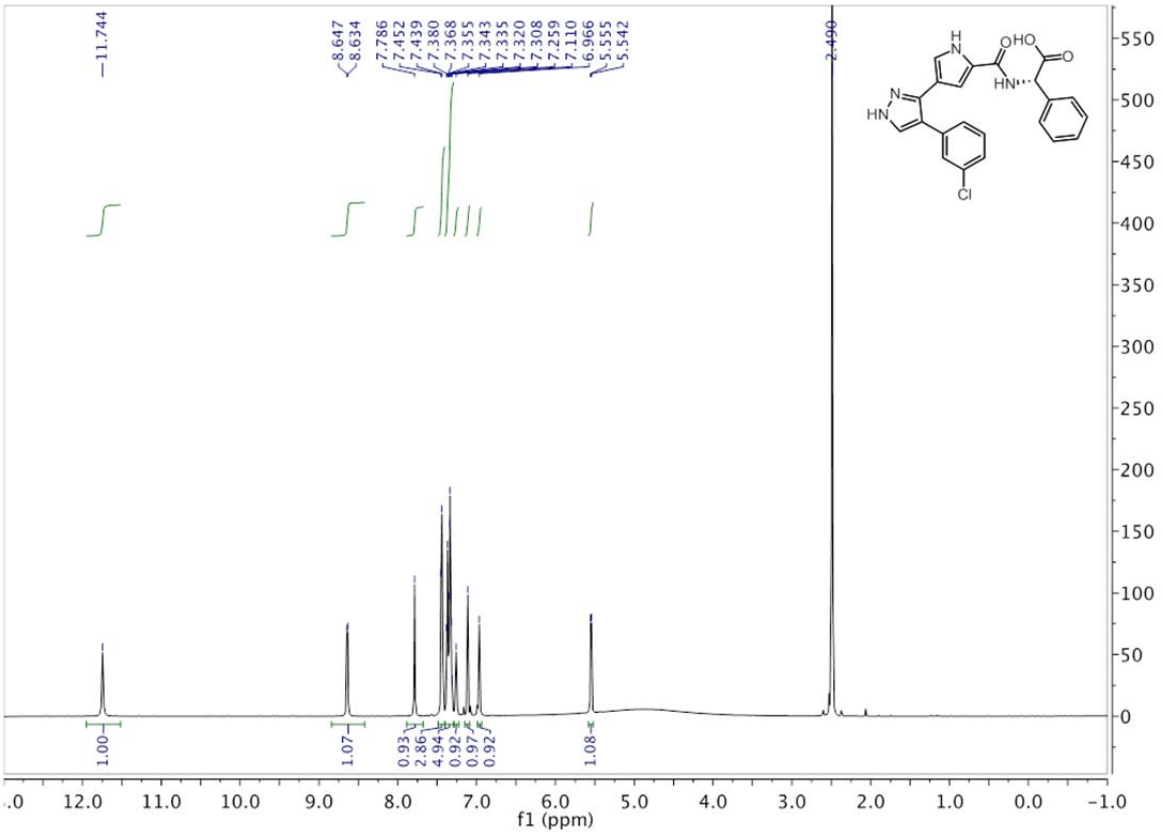
(R)-4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(1-phenylethyl)-1H-pyrrole-2-carboxamide (A13)



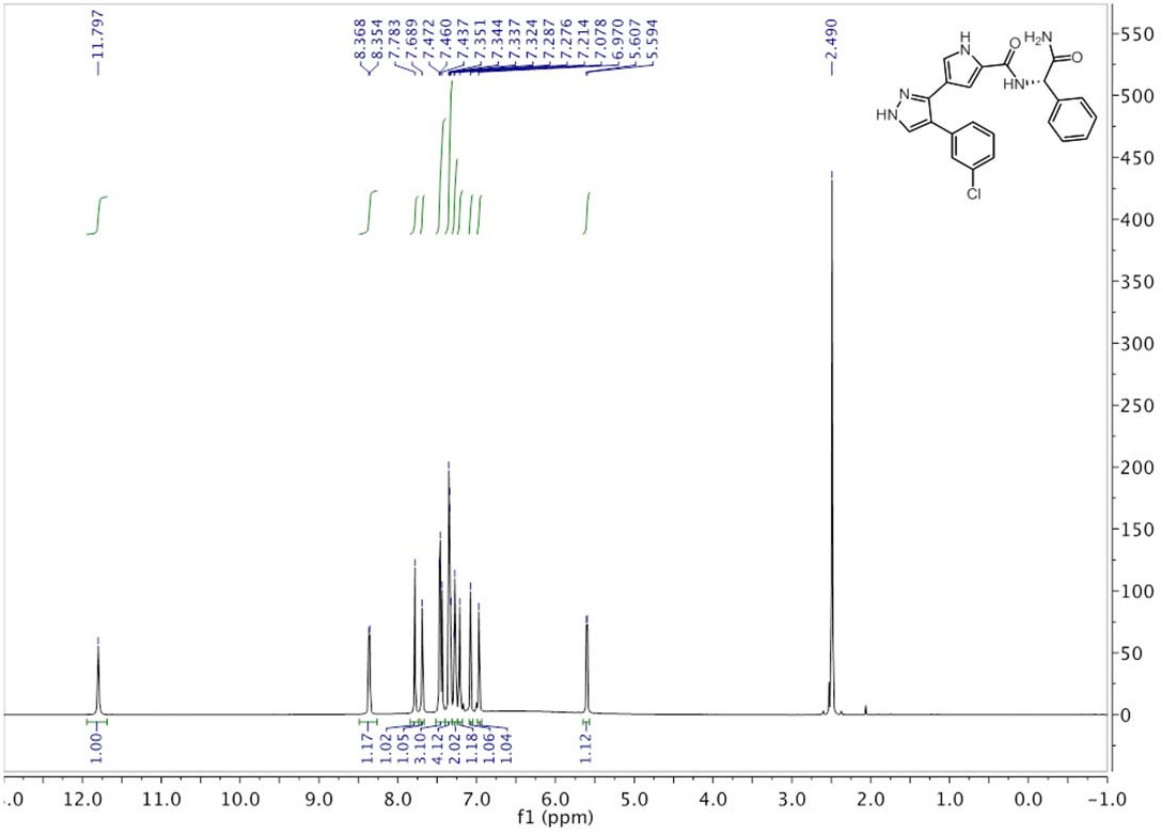
(S)-4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(2-hydroxy-1-phenylethyl)-1H-pyrrole-2-carboxamide (2)



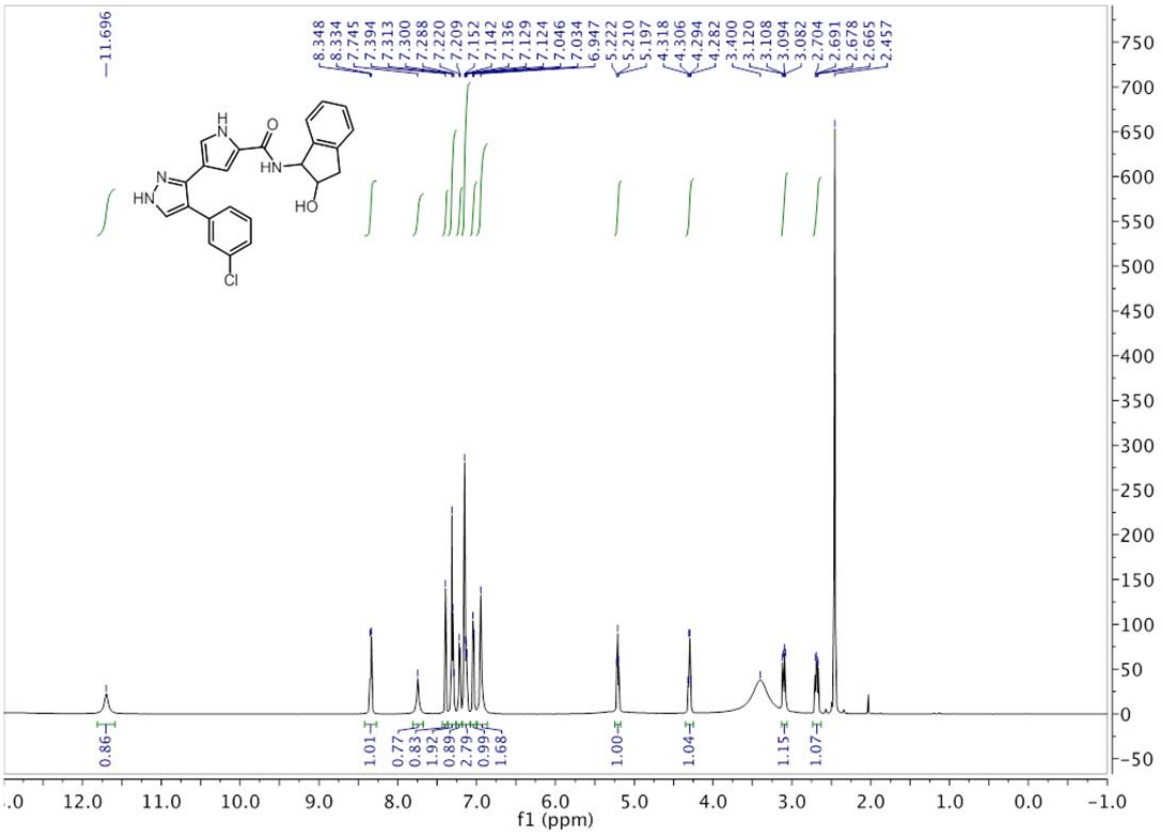
(S)-2-(4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrole-2-carboxamido)-2-phenylacetic acid (3)



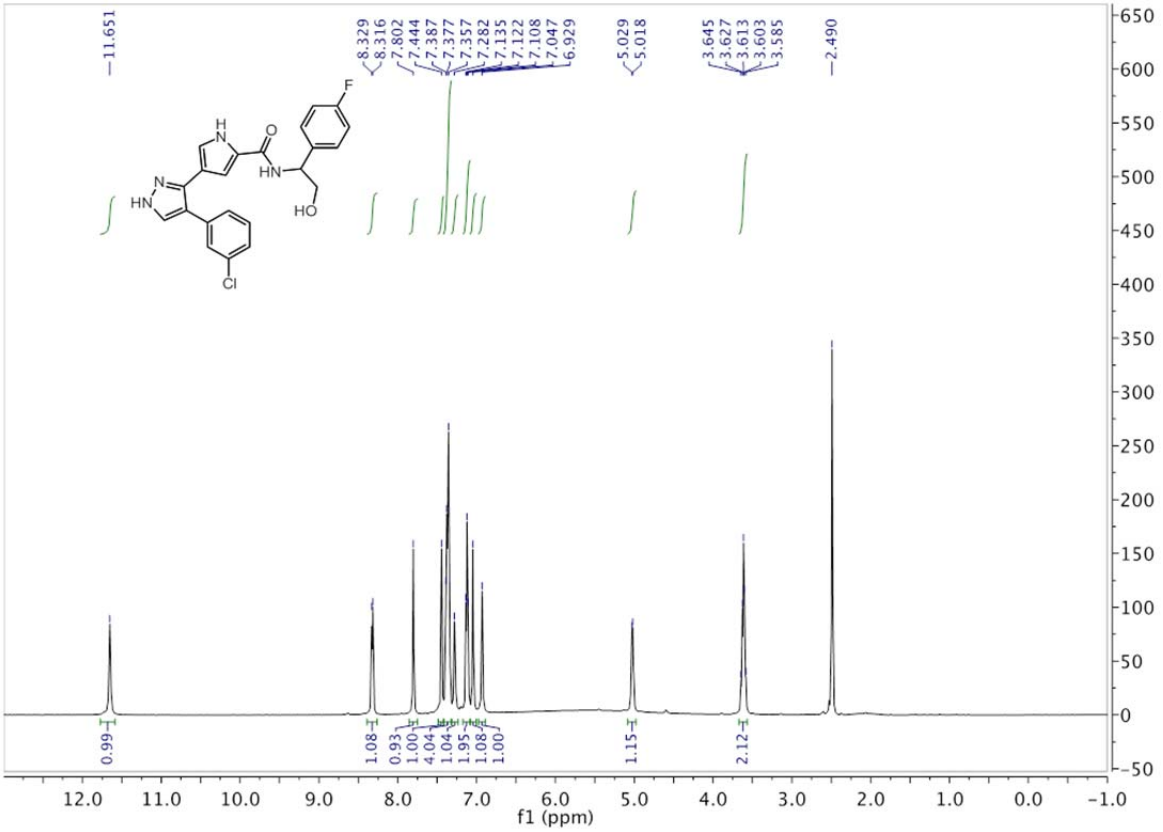
(S)-N-(2-amino-2-oxo-1-phenylethyl)-4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-1H-pyrrole-2-carboxamide (A14)



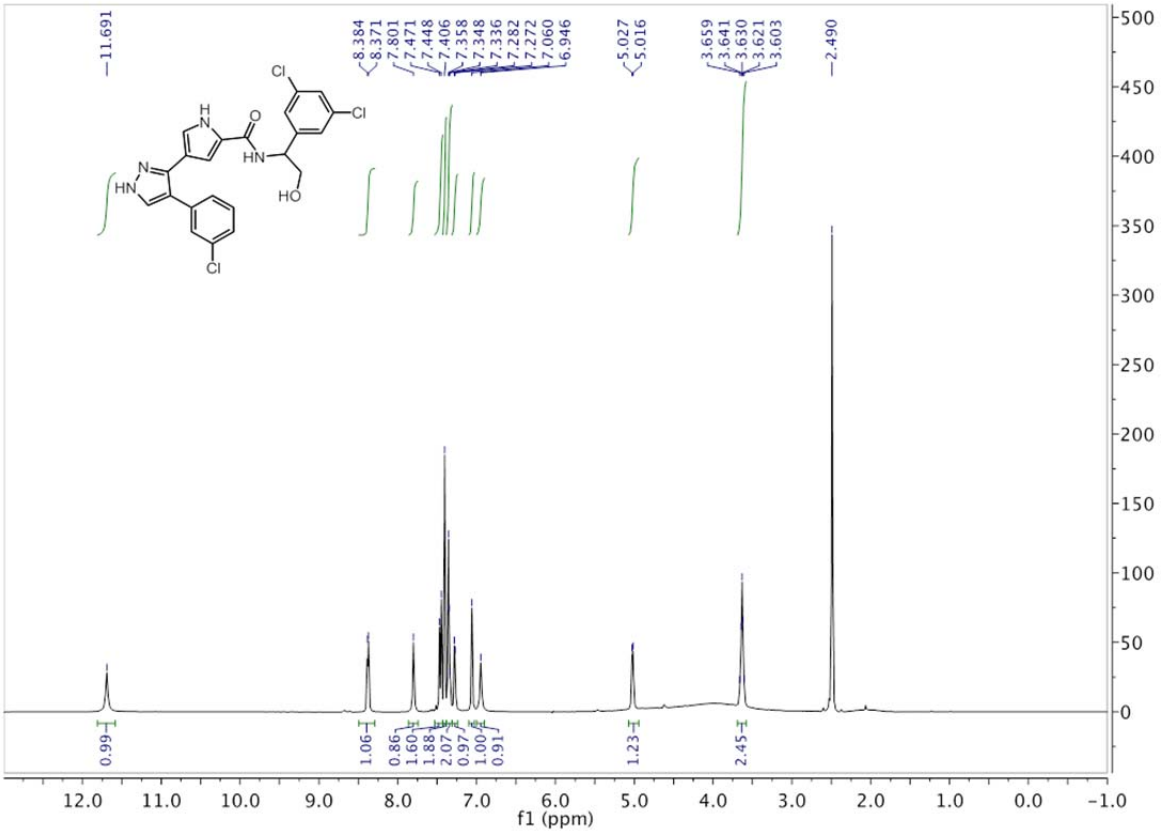
4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(2-hydroxy-2,3-dihydro-1H-inden-1-yl)-1H-pyrrole-2-carboxamide (A15)



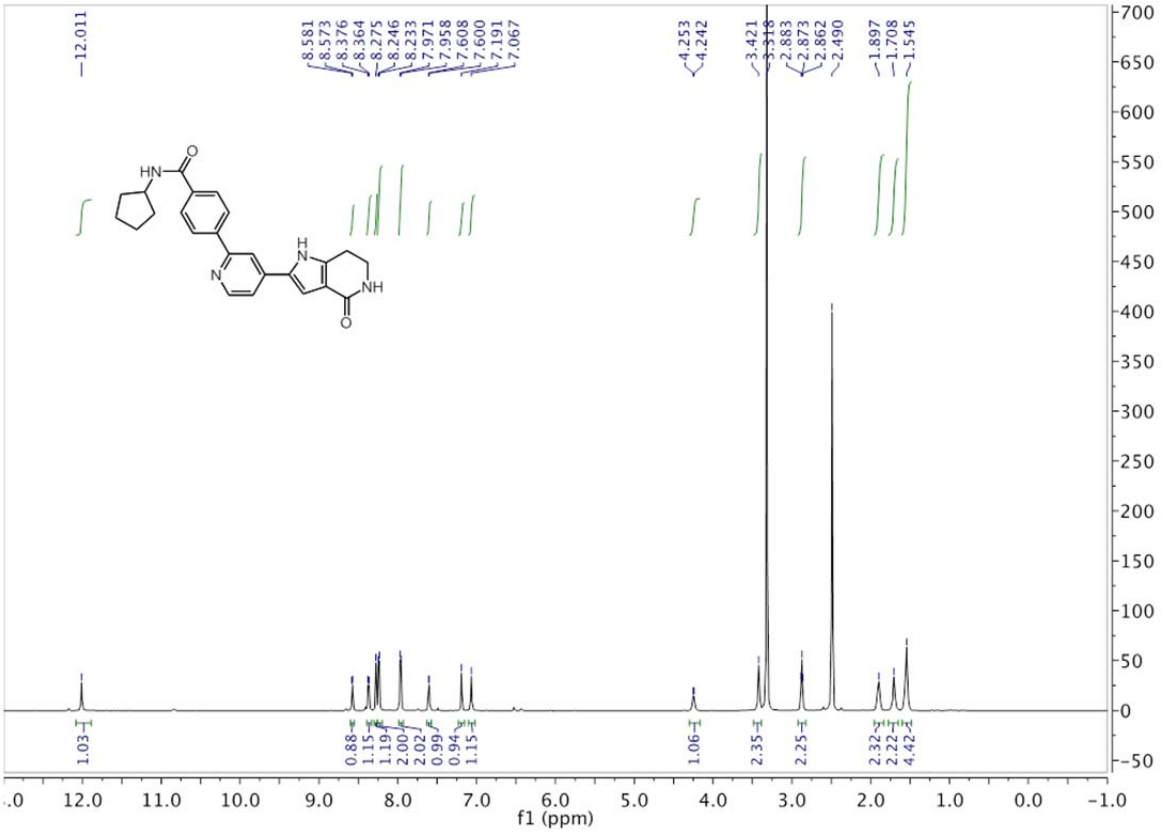
4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(1-(4-fluorophenyl)-2-hydroxyethyl)-1H-pyrrole-2-carboxamide (A16)



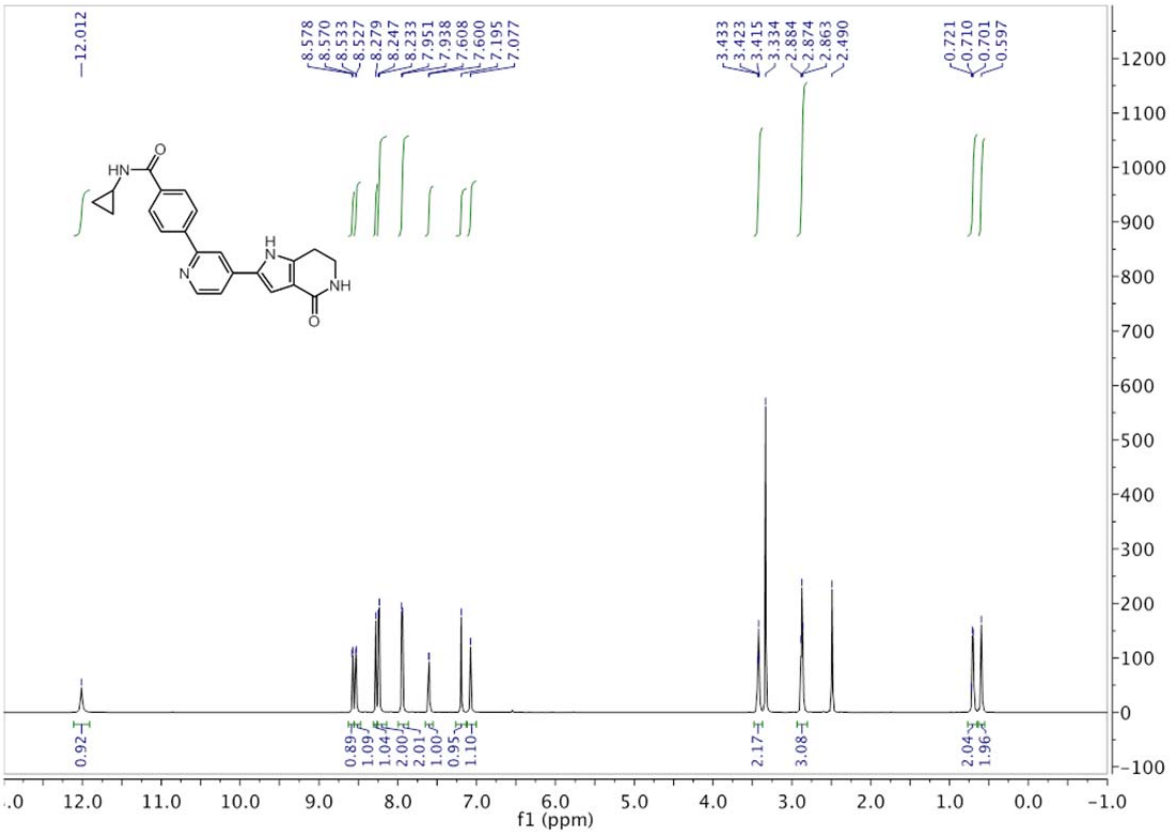
4-(4-(3-chlorophenyl)-1H-pyrazol-3-yl)-N-(1-(3,5-dichlorophenyl)-2-hydroxyethyl)-1H-pyrrole-2-carboxamide (A17)



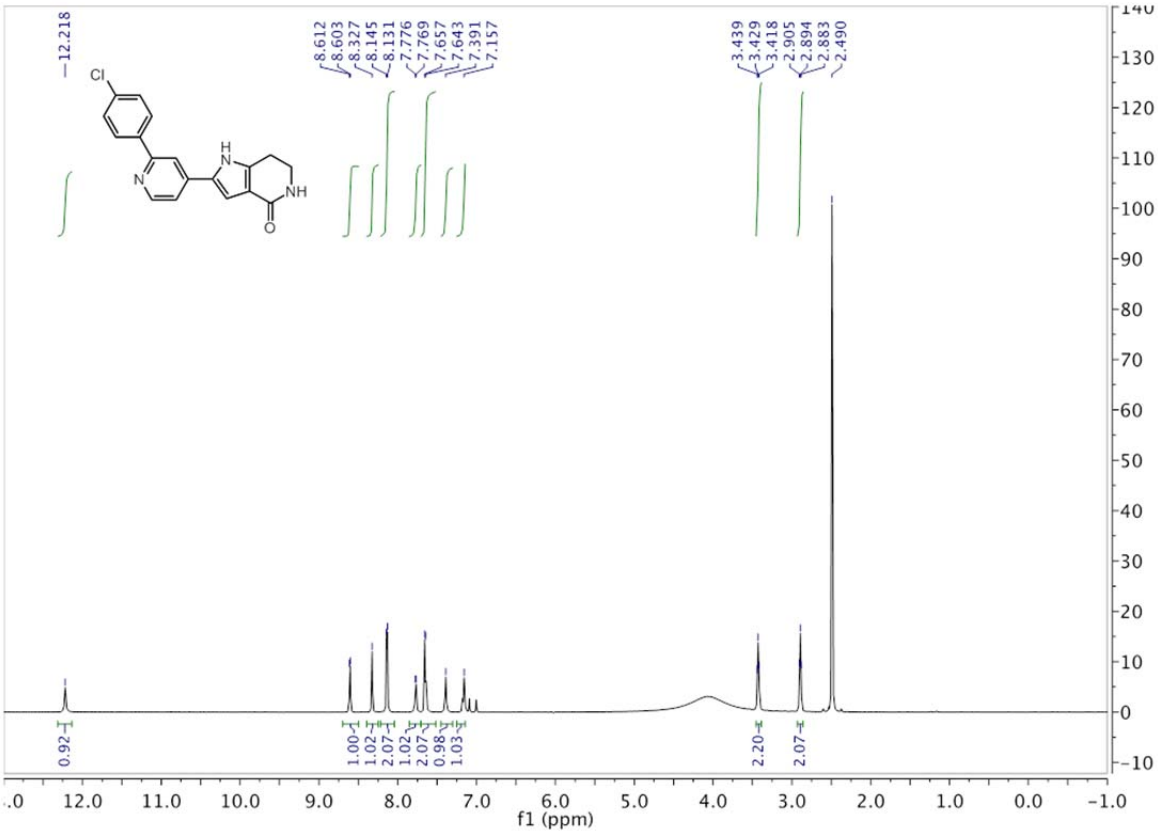
N-cyclopentyl-4-(4-(4-oxo-4,5,6,7-tetrahydro-1H-pyrrolo[3,2-c]pyridin-2-yl)pyridin-2-yl)benzamide (B1)



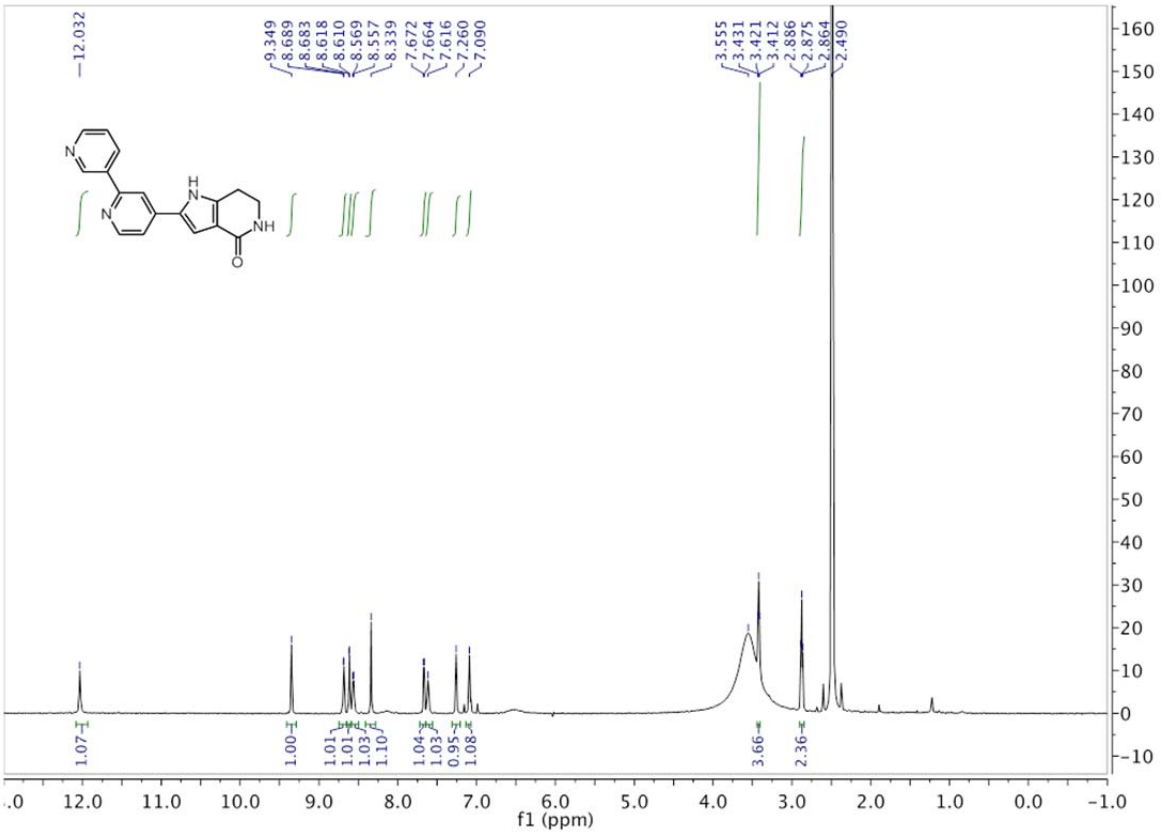
N-cyclopropyl-4-(4-(4-oxo-4,5,6,7-tetrahydro-1H-pyrrolo[3,2-c]pyridin-2-yl)pyridin-2-yl)benzamide (5)



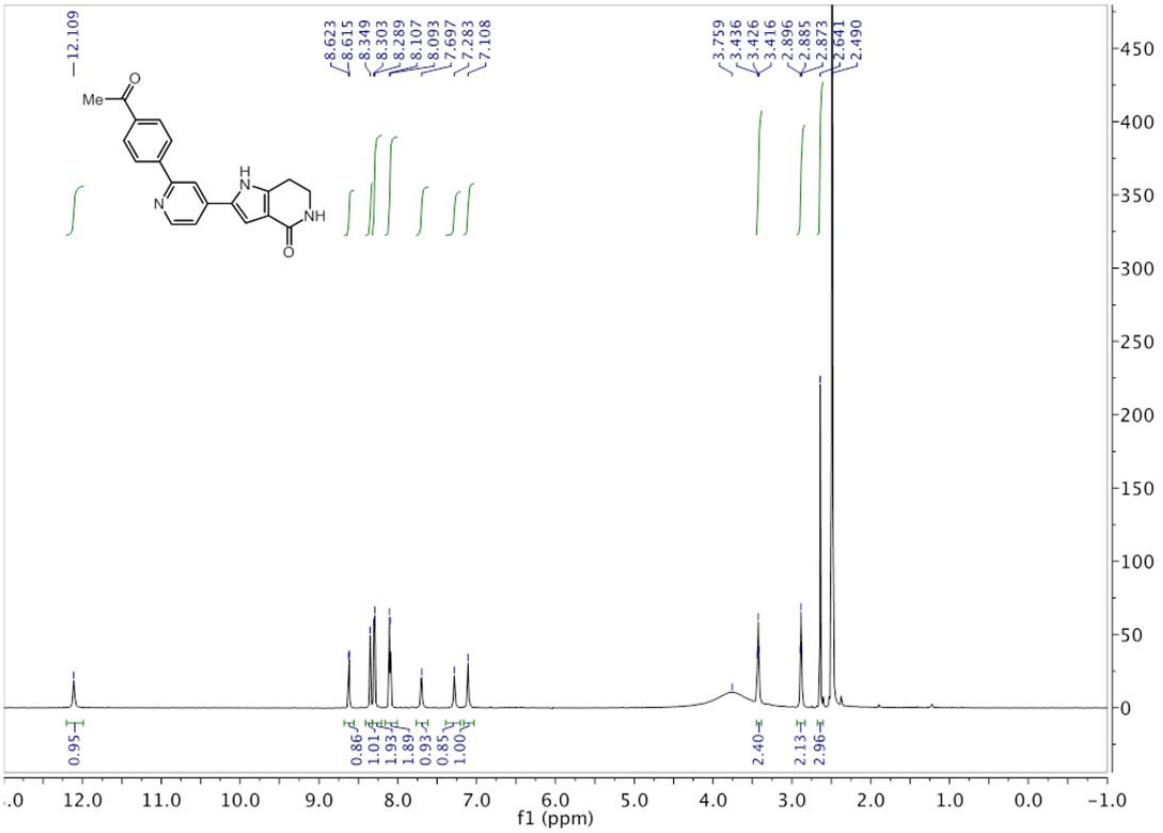
2-(2-(4-chlorophenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B2)



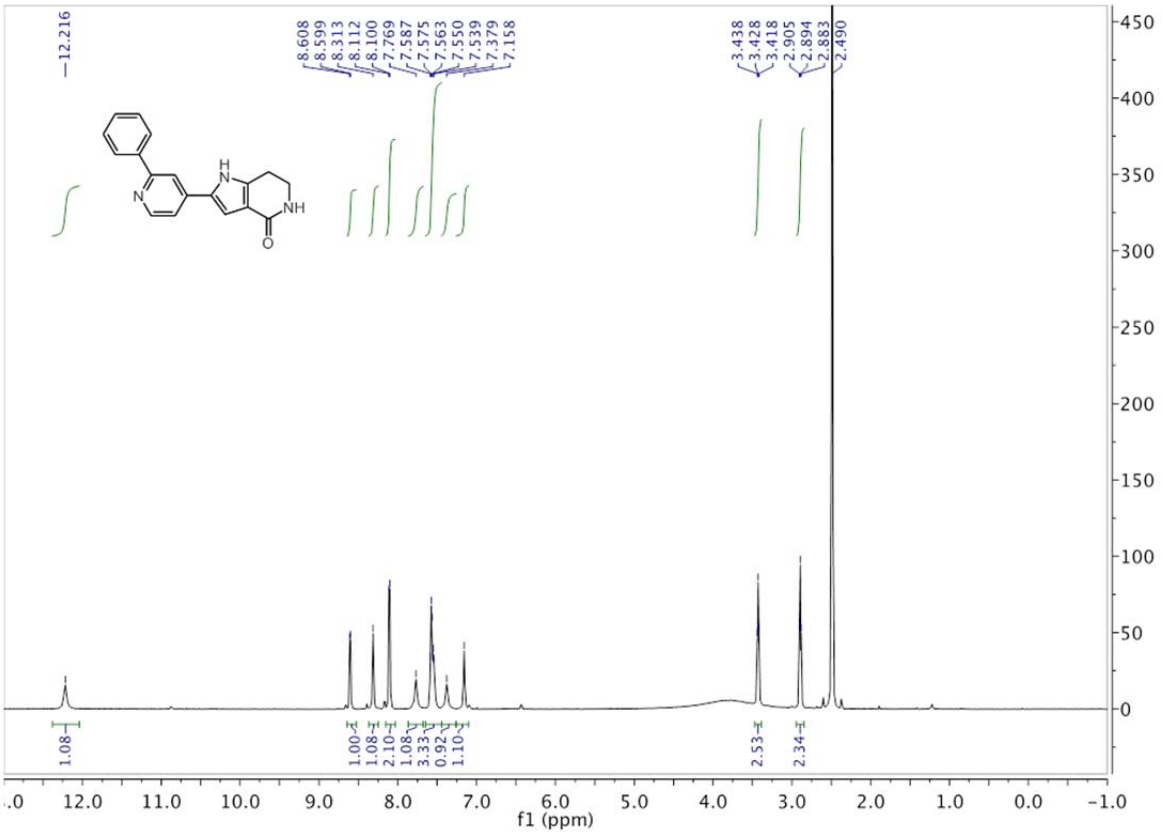
2-([2,3'-bipyridin]-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B3)



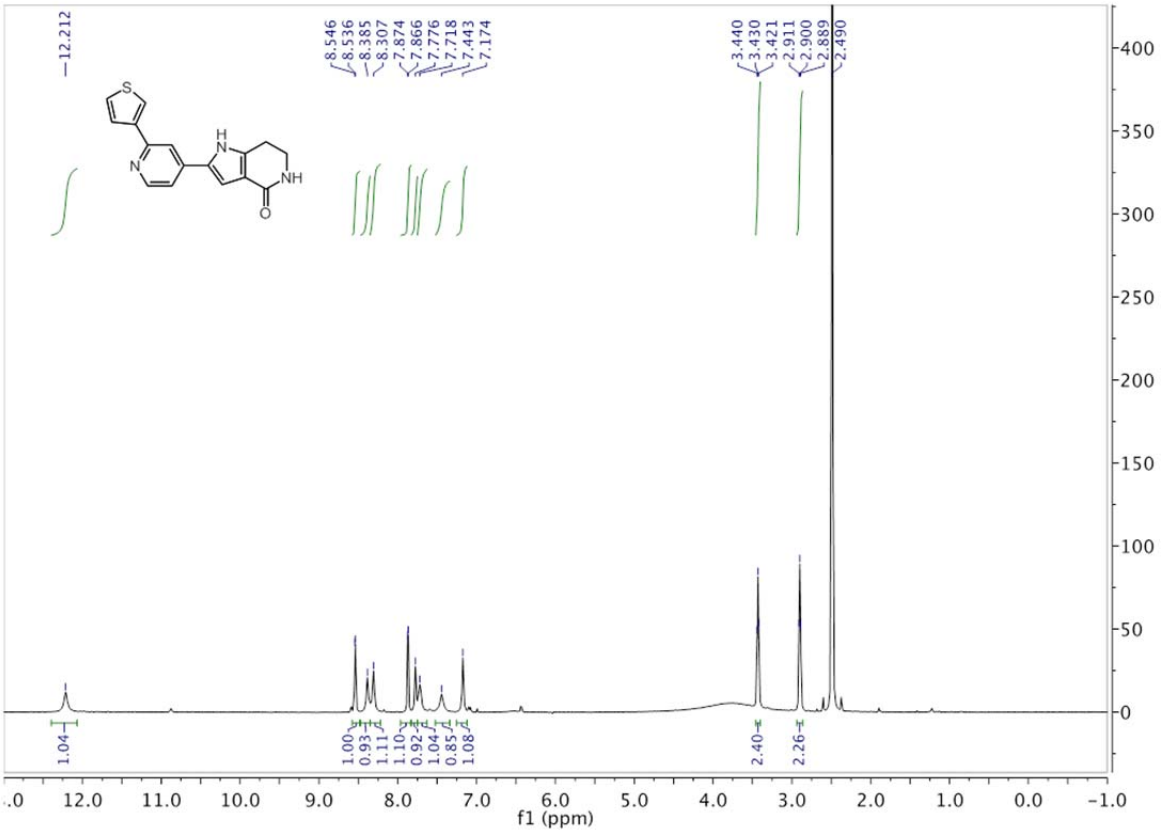
2-(2-(4-acetylphenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B4)



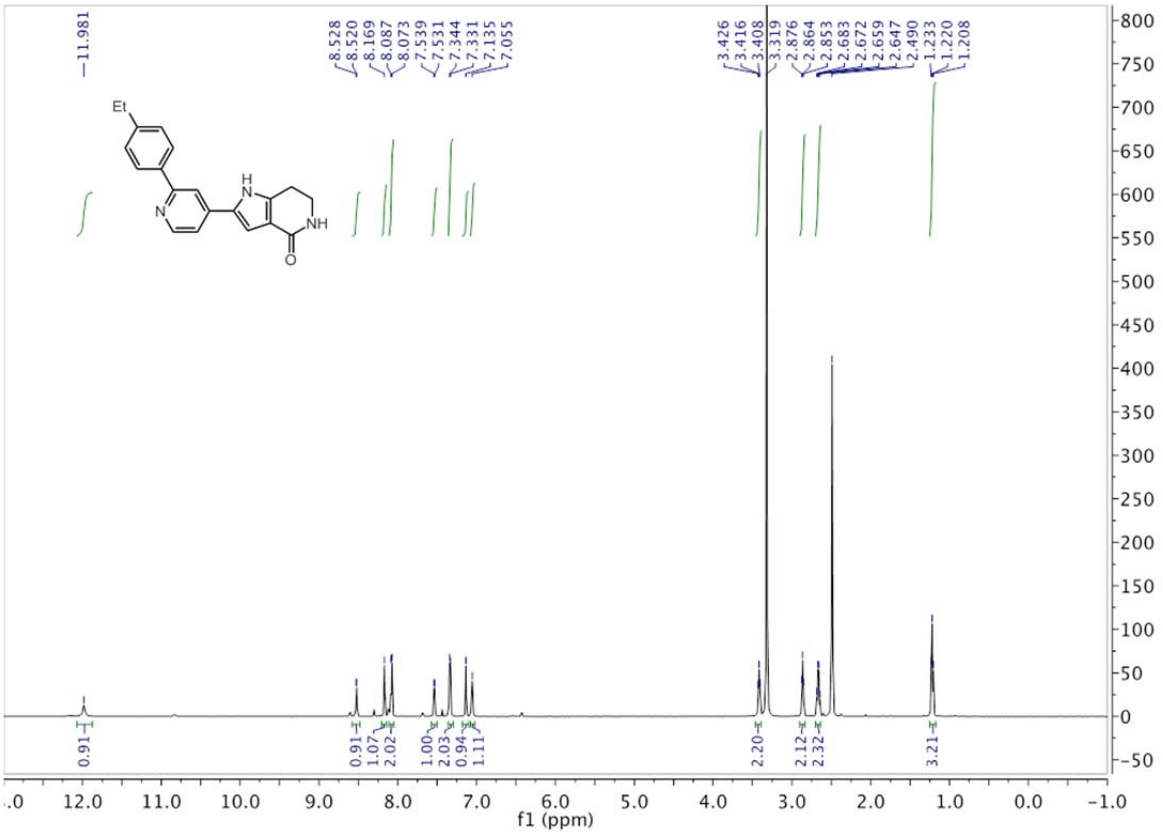
2-(2-phenylpyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B5)



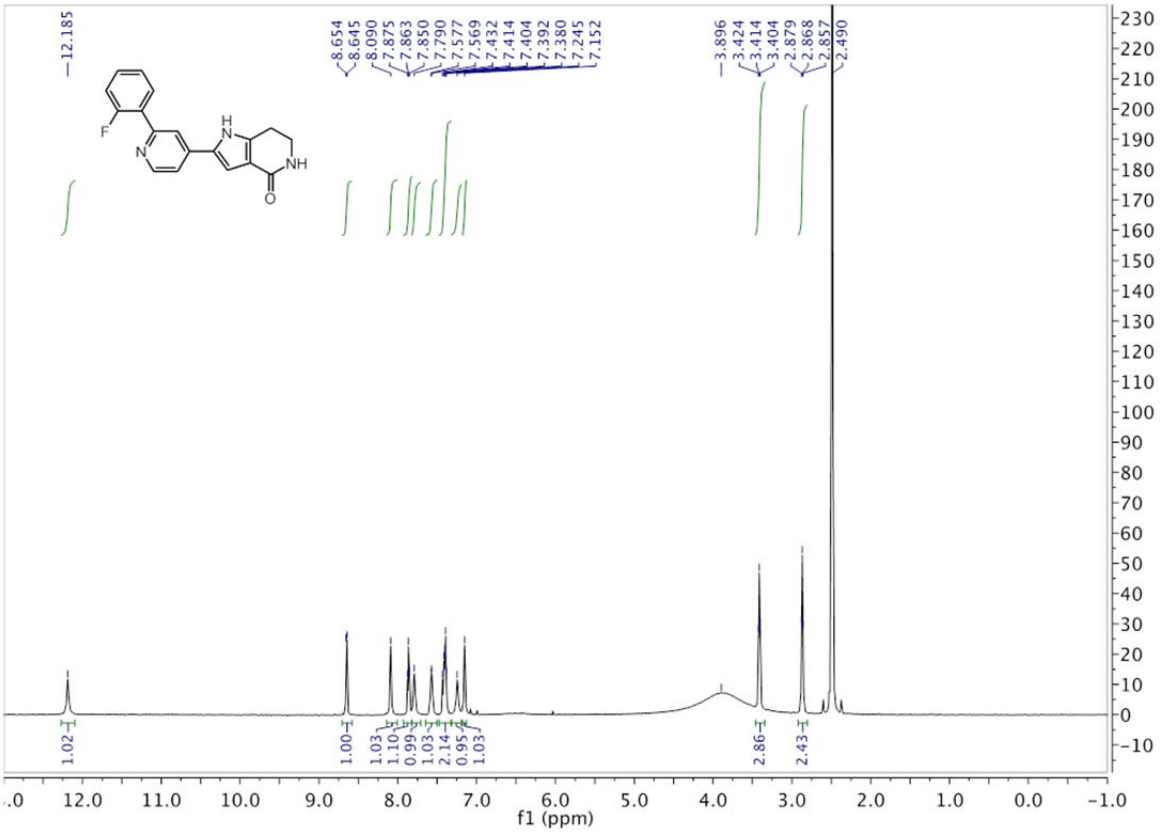
2-(2-(thiophen-3-yl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B6)



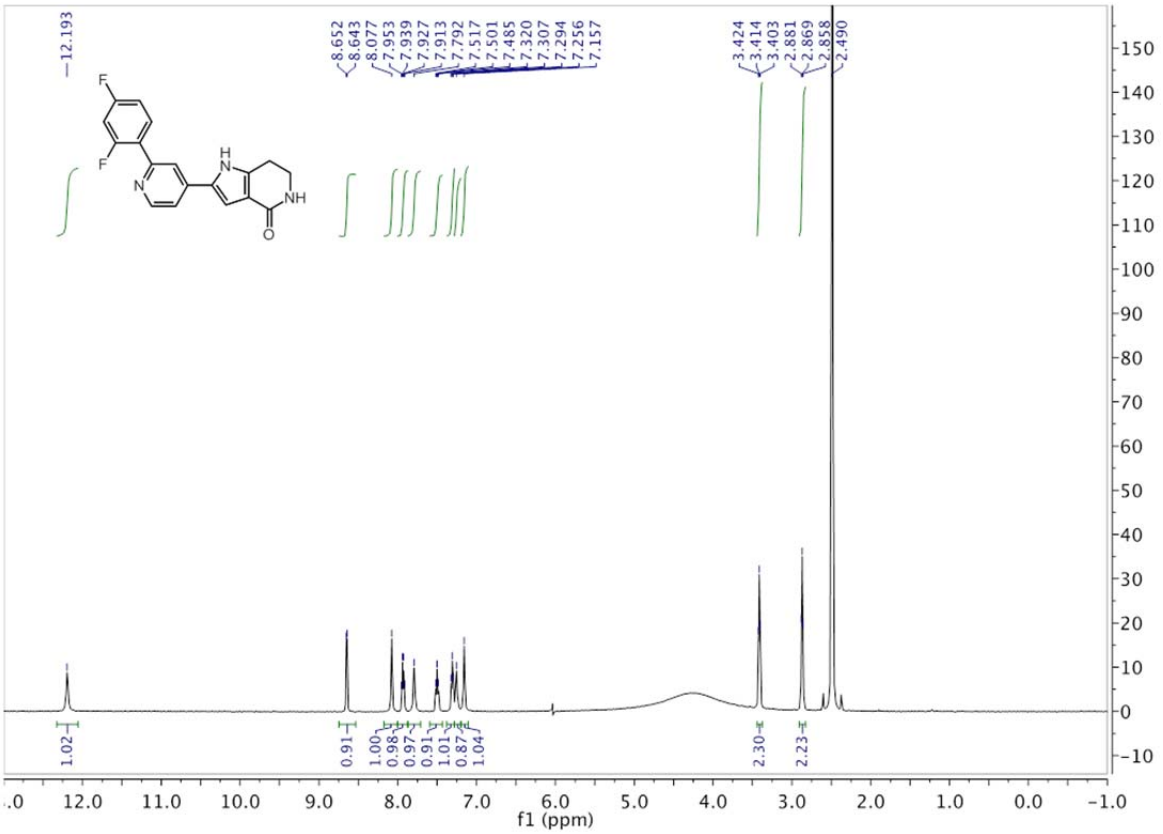
2-(2-(4-ethylphenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B7)



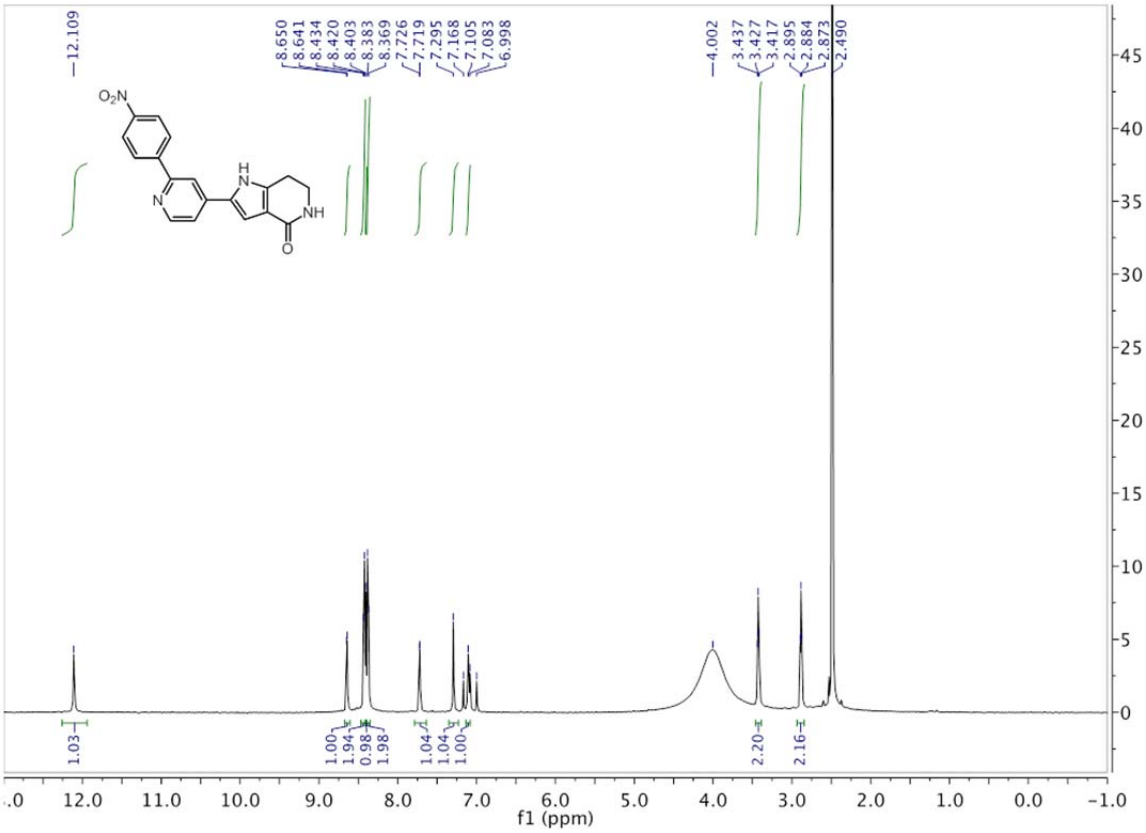
2-(2-(2-fluorophenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B8)



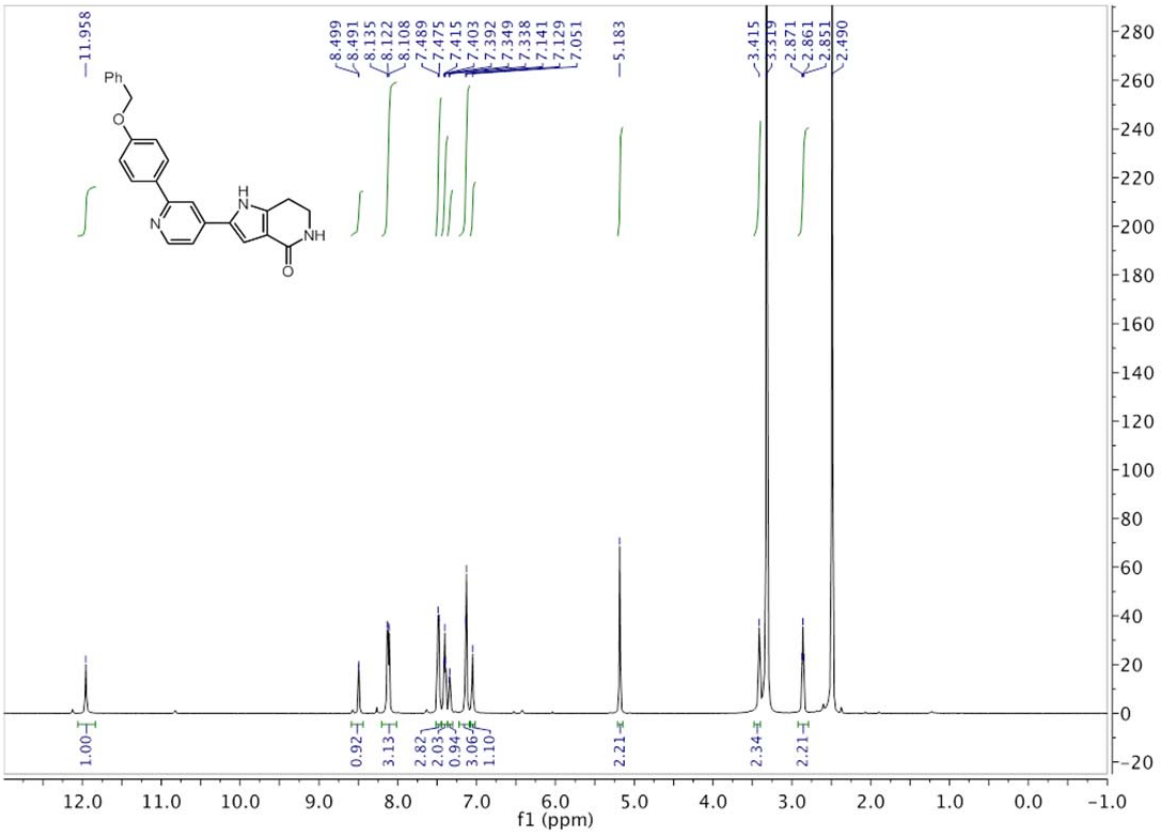
2-(2-(2,4-difluorophenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B9)



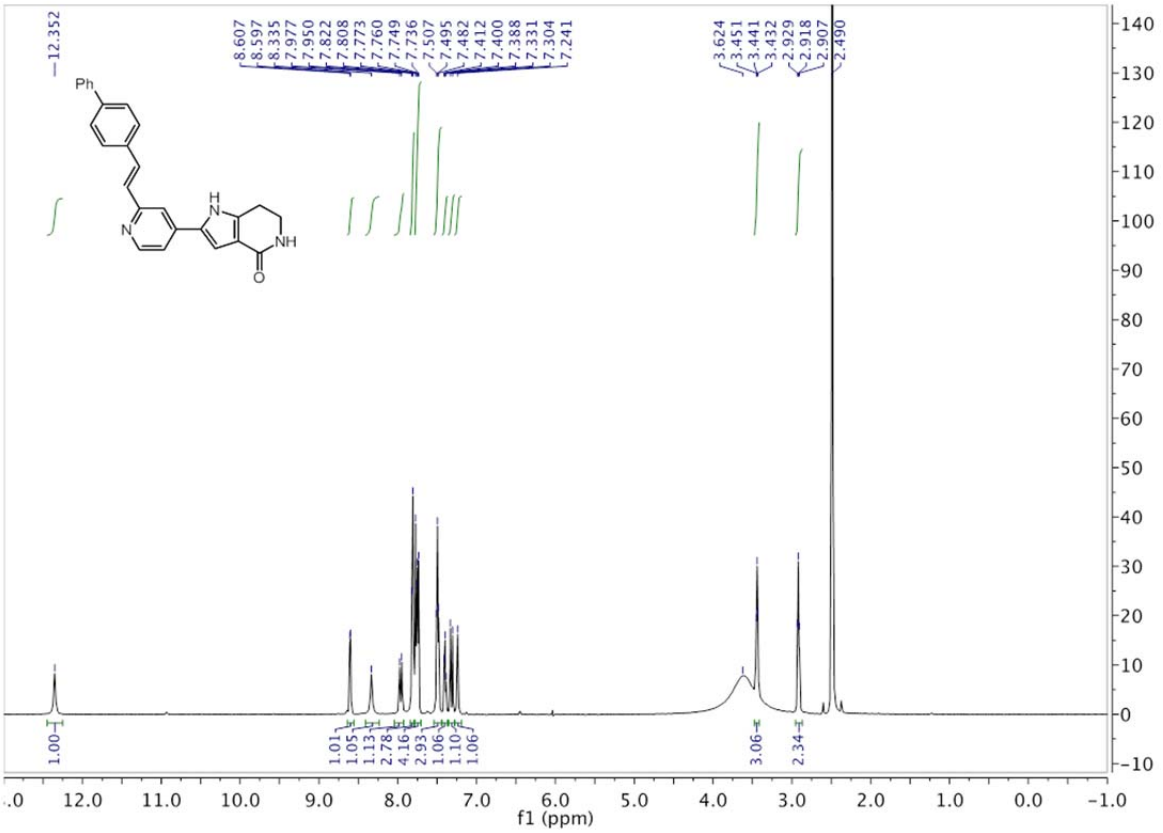
2-(2-(4-nitrophenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B10)



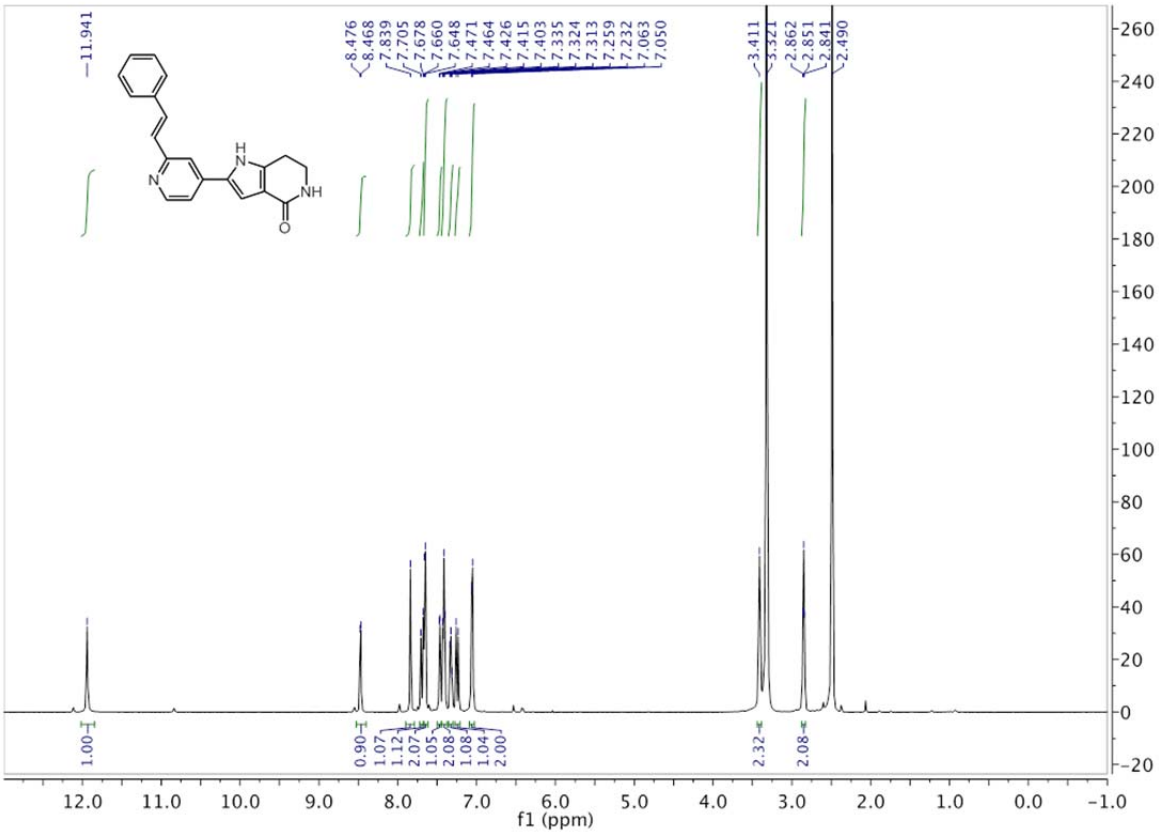
2-(2-(4-(benzyloxy)phenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B11)



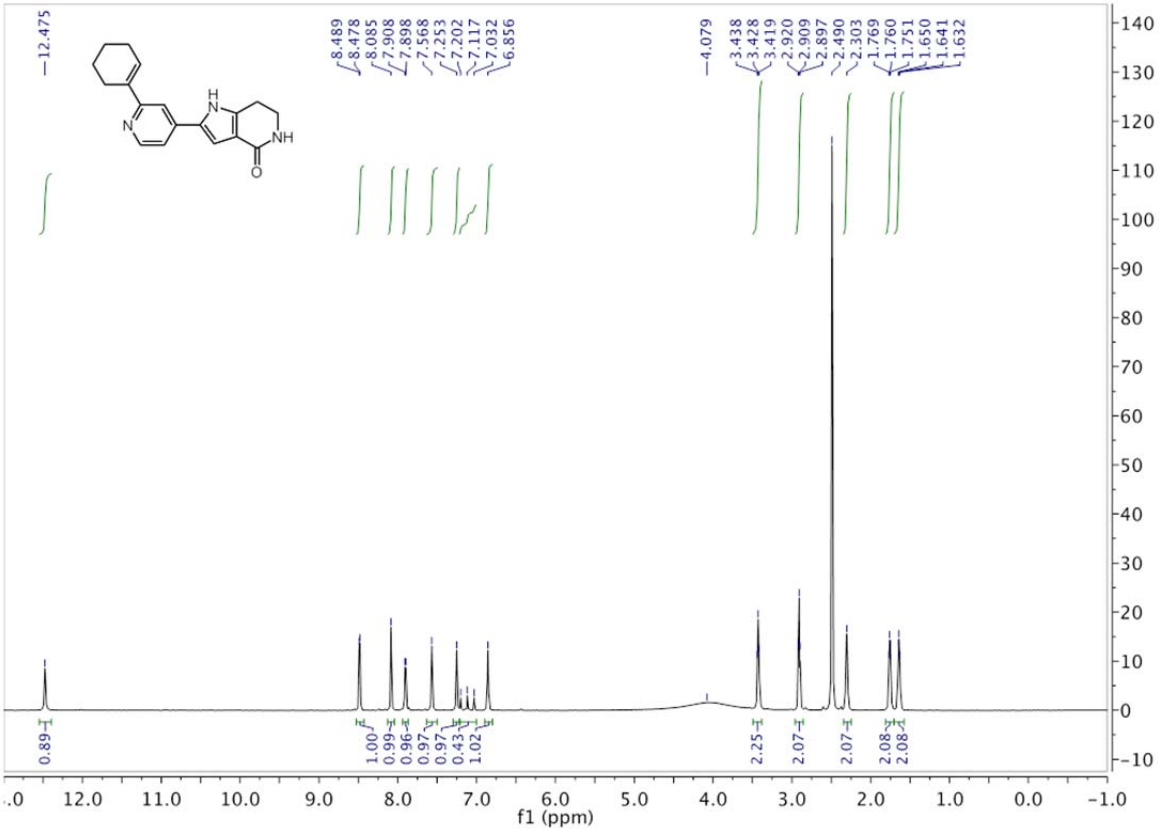
(E)-2-(2-(2-([1,1'-biphenyl]-4-yl)vinyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B12)



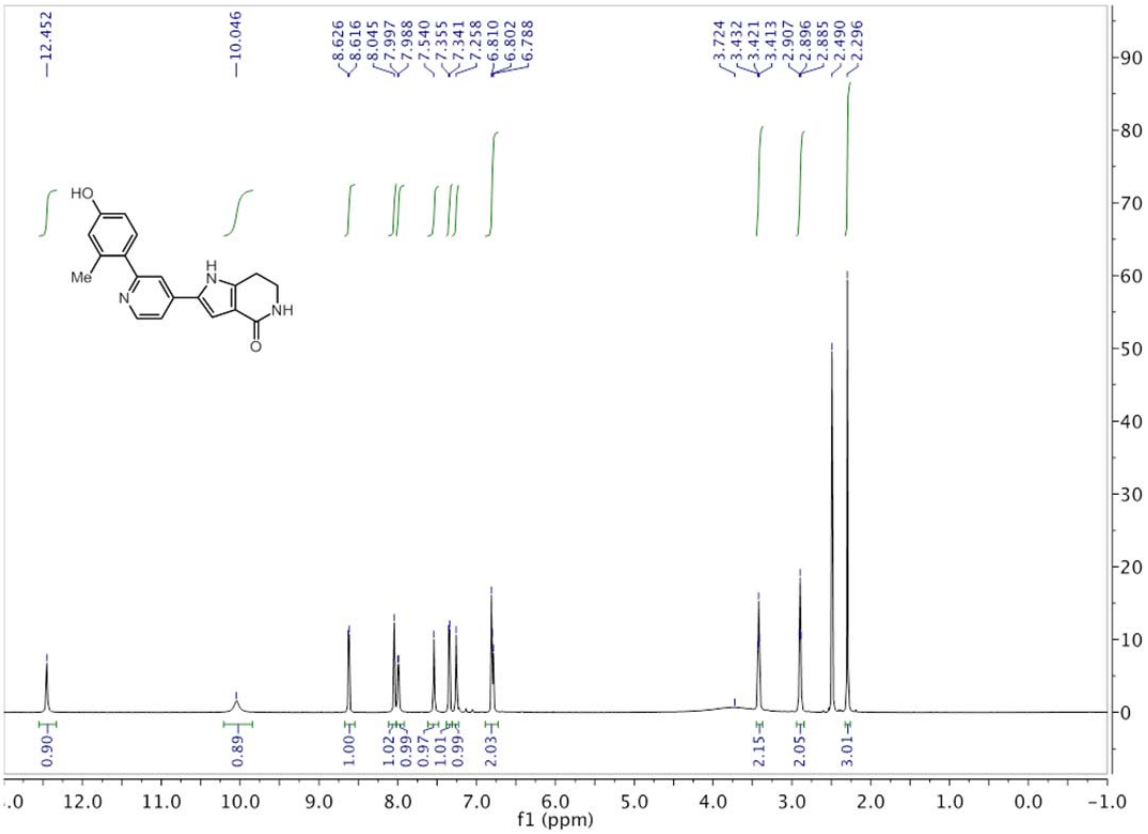
(E)-2-(2-styrylpyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B13)



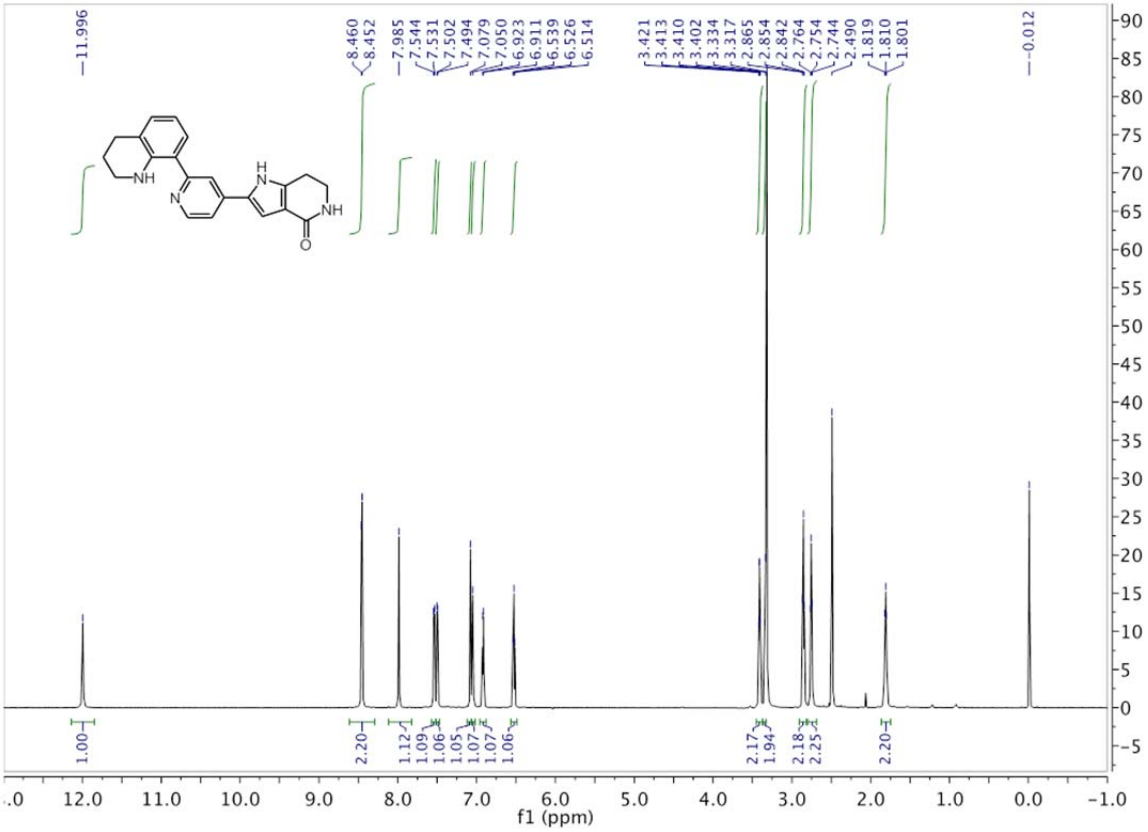
2-(2-(cyclohex-1-en-1-yl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B14)



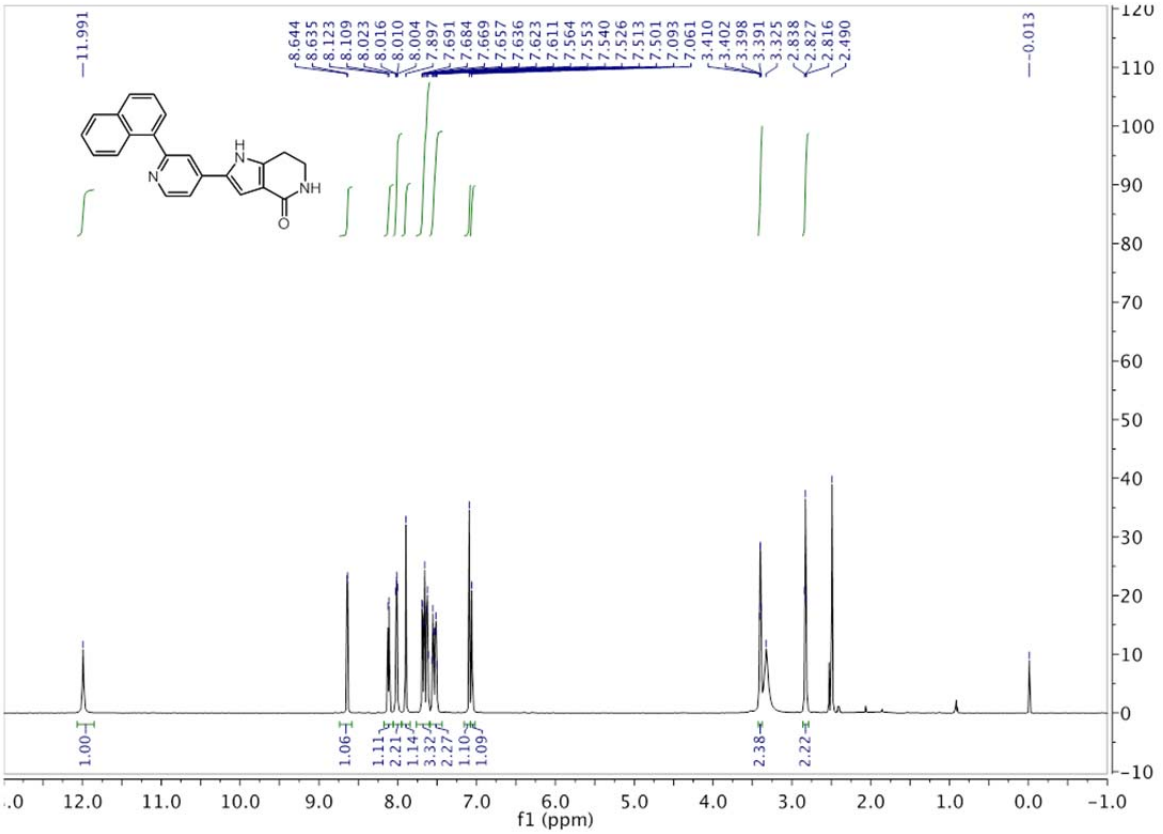
2-(2-(4-hydroxy-2-methylphenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (6)



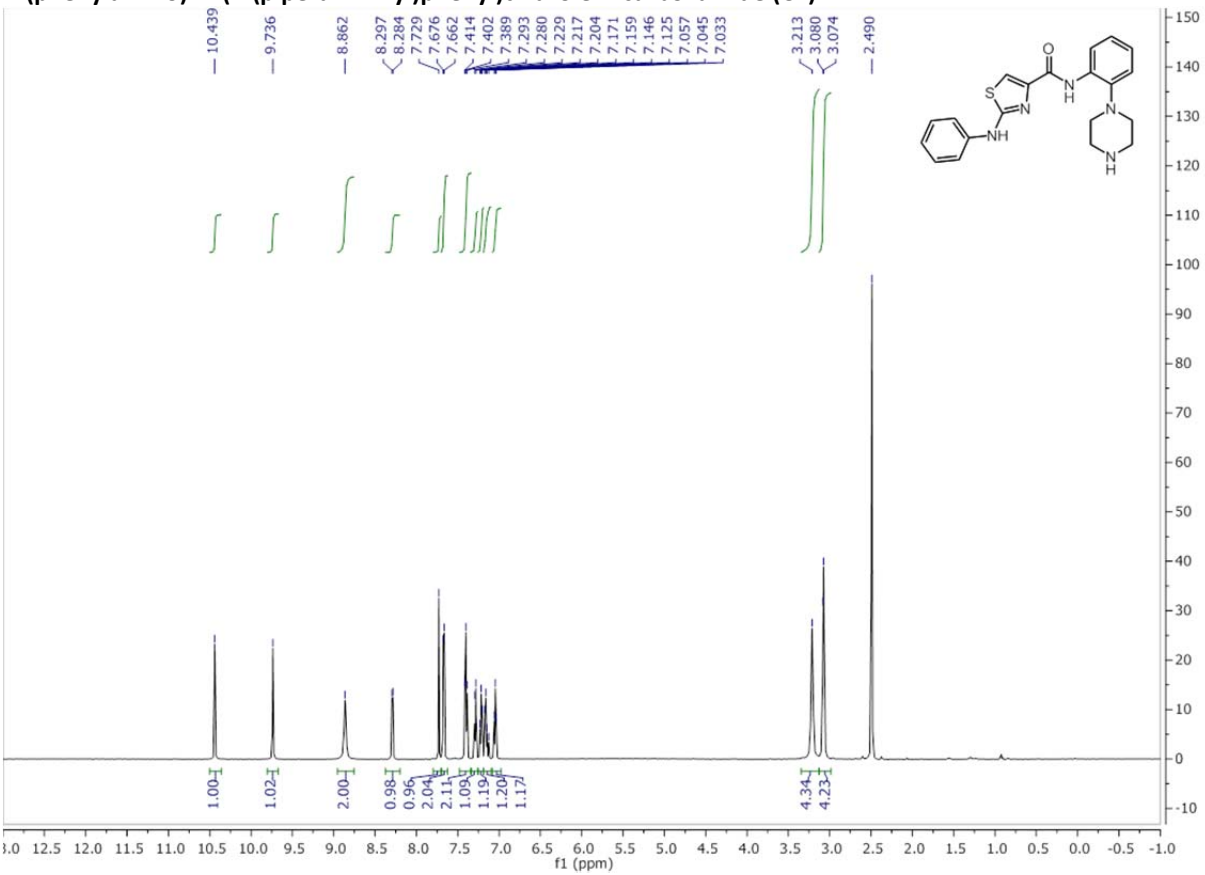
2-(2-(1,2,3,4-tetrahydroquinolin-8-yl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B15)



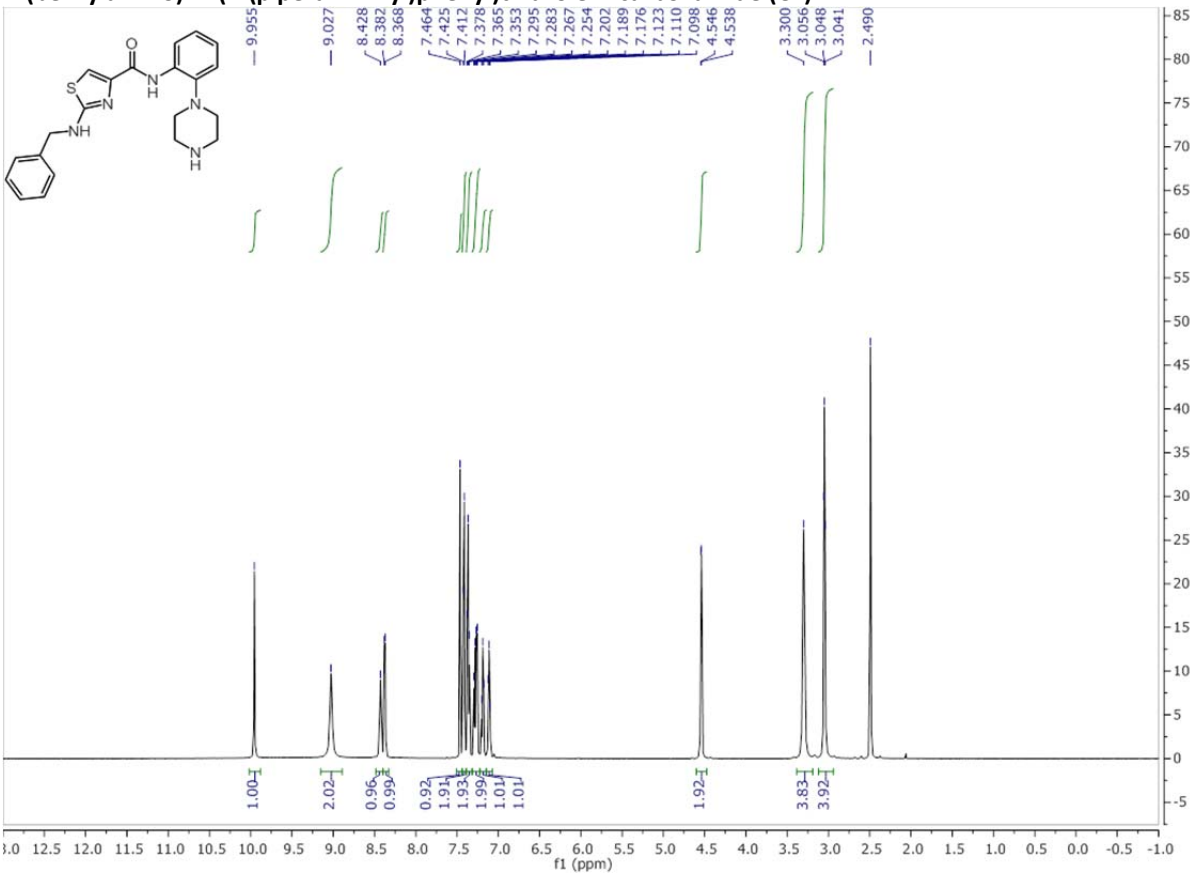
2-(2-(naphthalen-1-yl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B16)



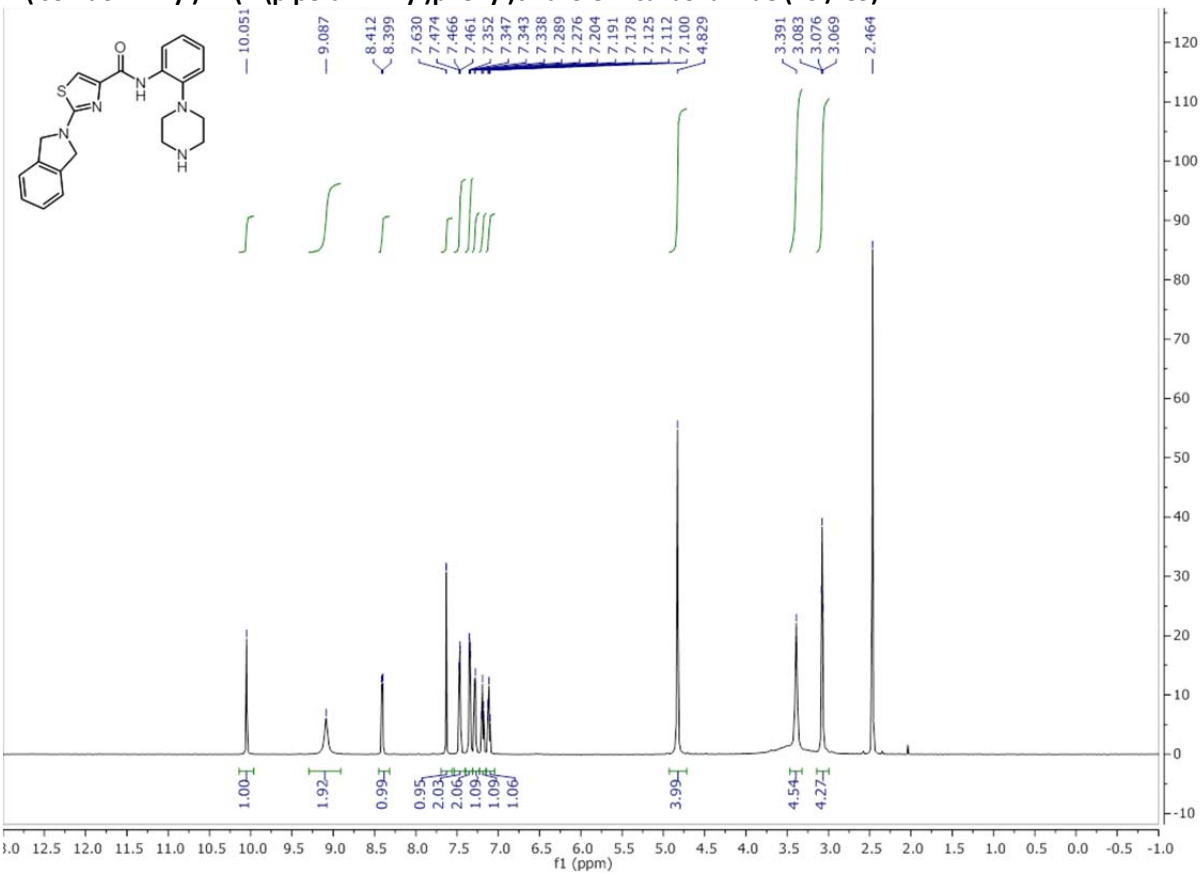
2-(phenylamino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C1)

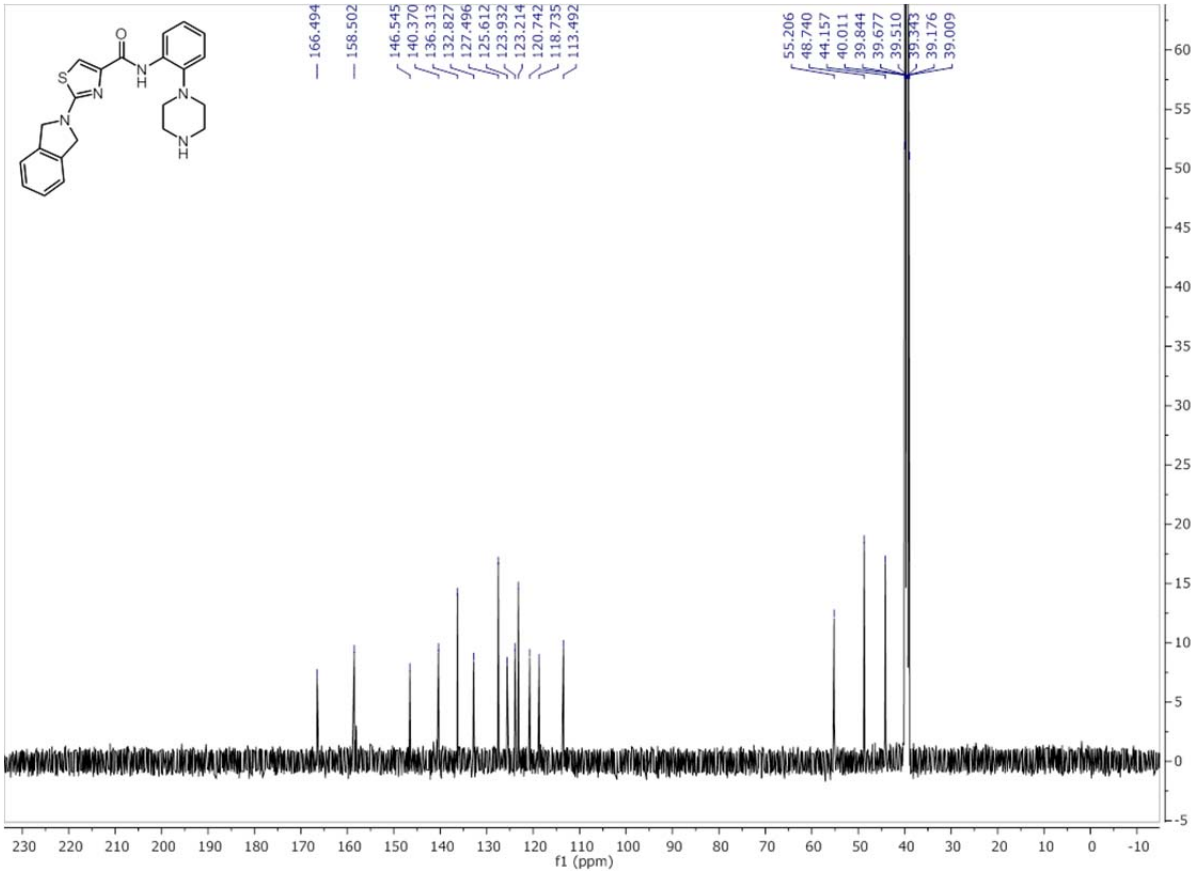


2-(benzylamino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C2)

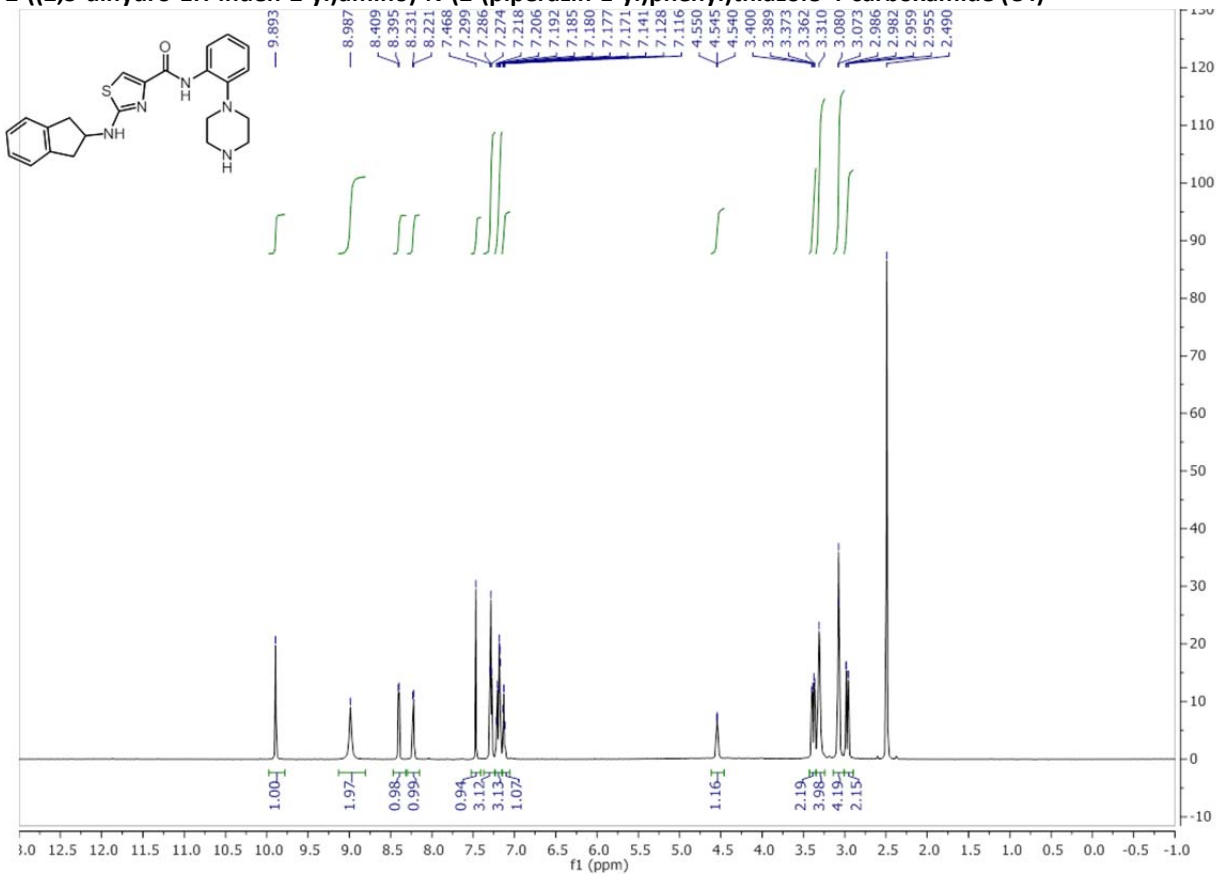


2-(isoindolin-2-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (43 / C3)

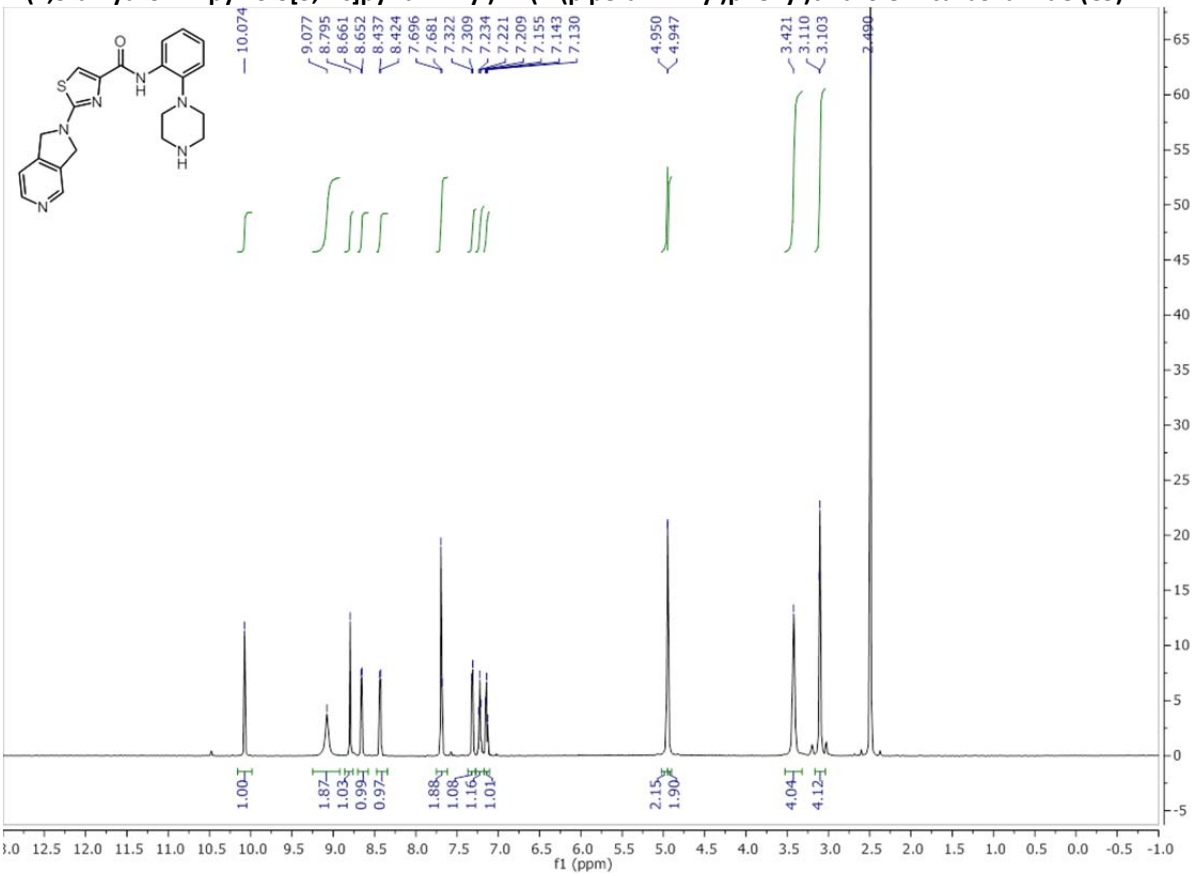




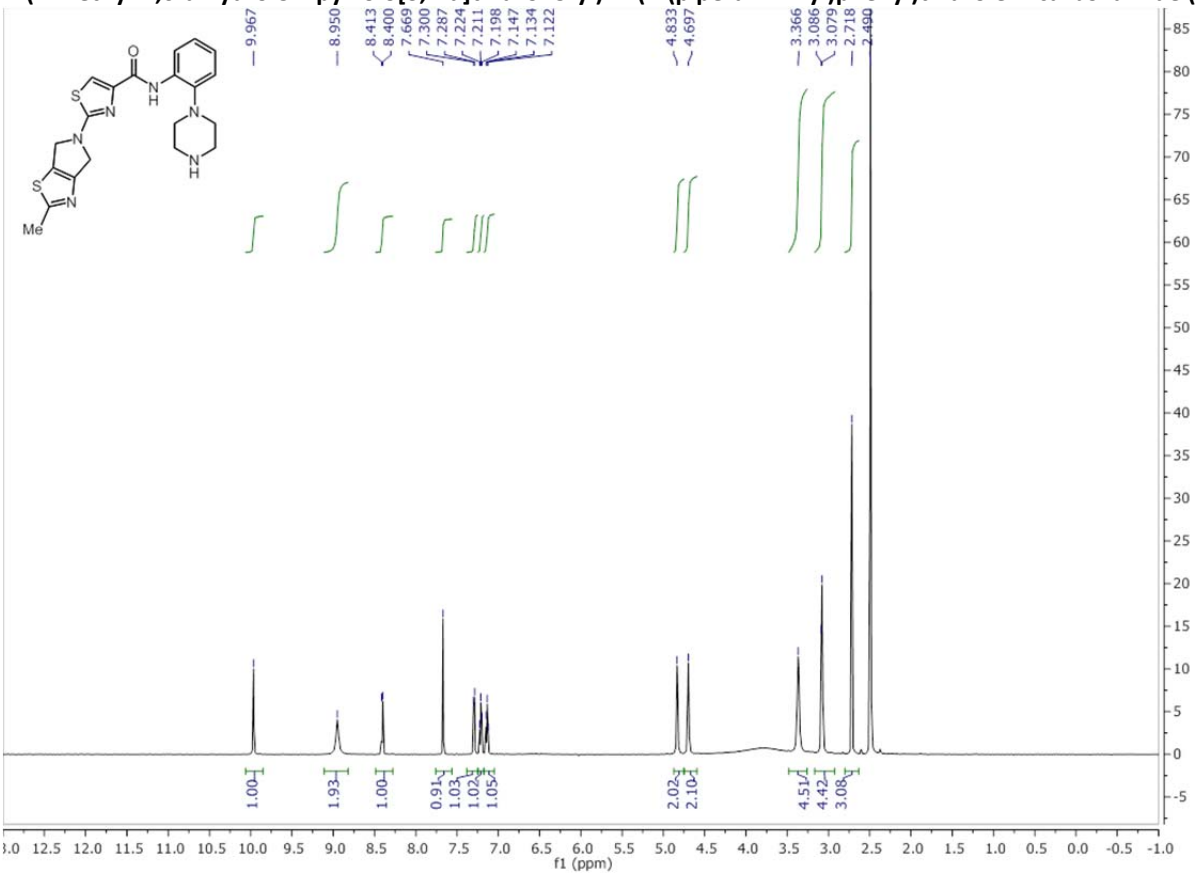
2-((2,3-dihydro-1H-inden-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C4)



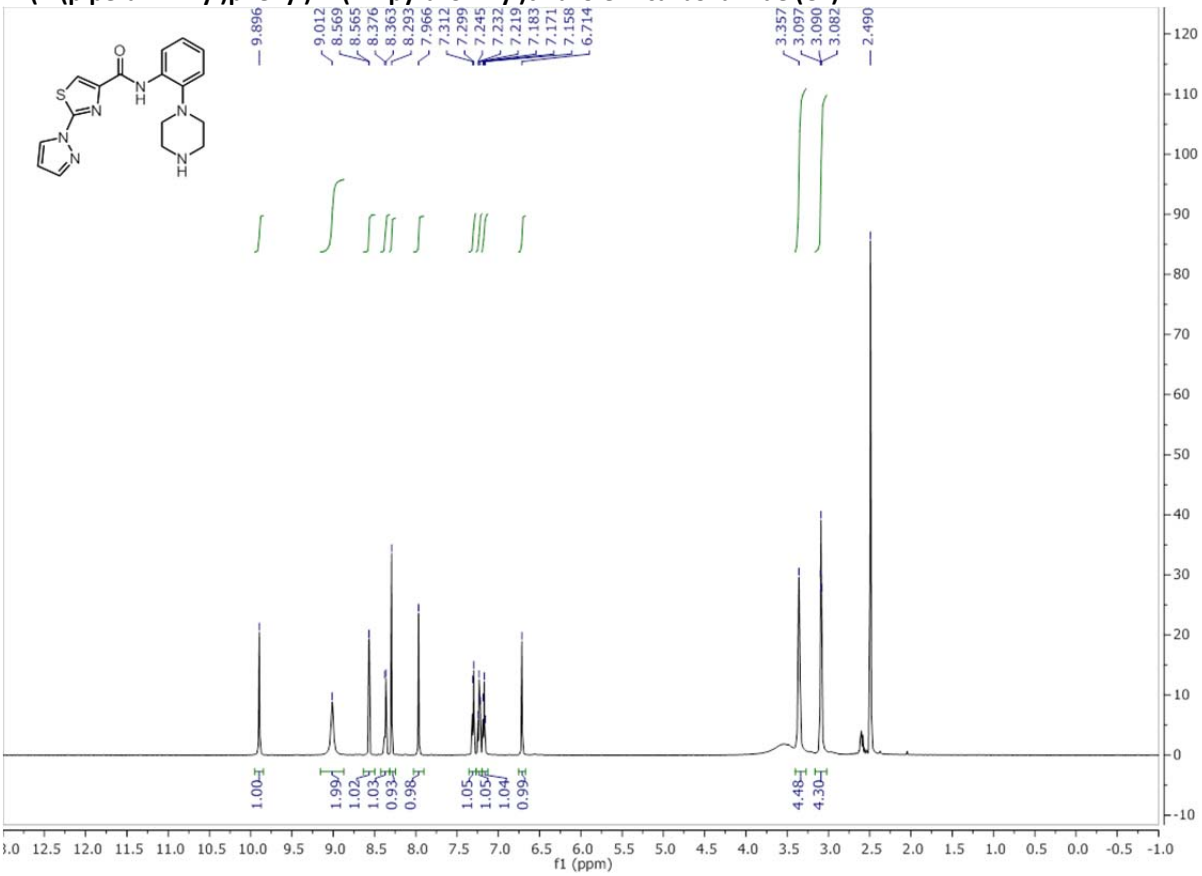
2-(1,3-dihydro-2H-pyrrolo[3,4-c]pyridin-2-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C5)



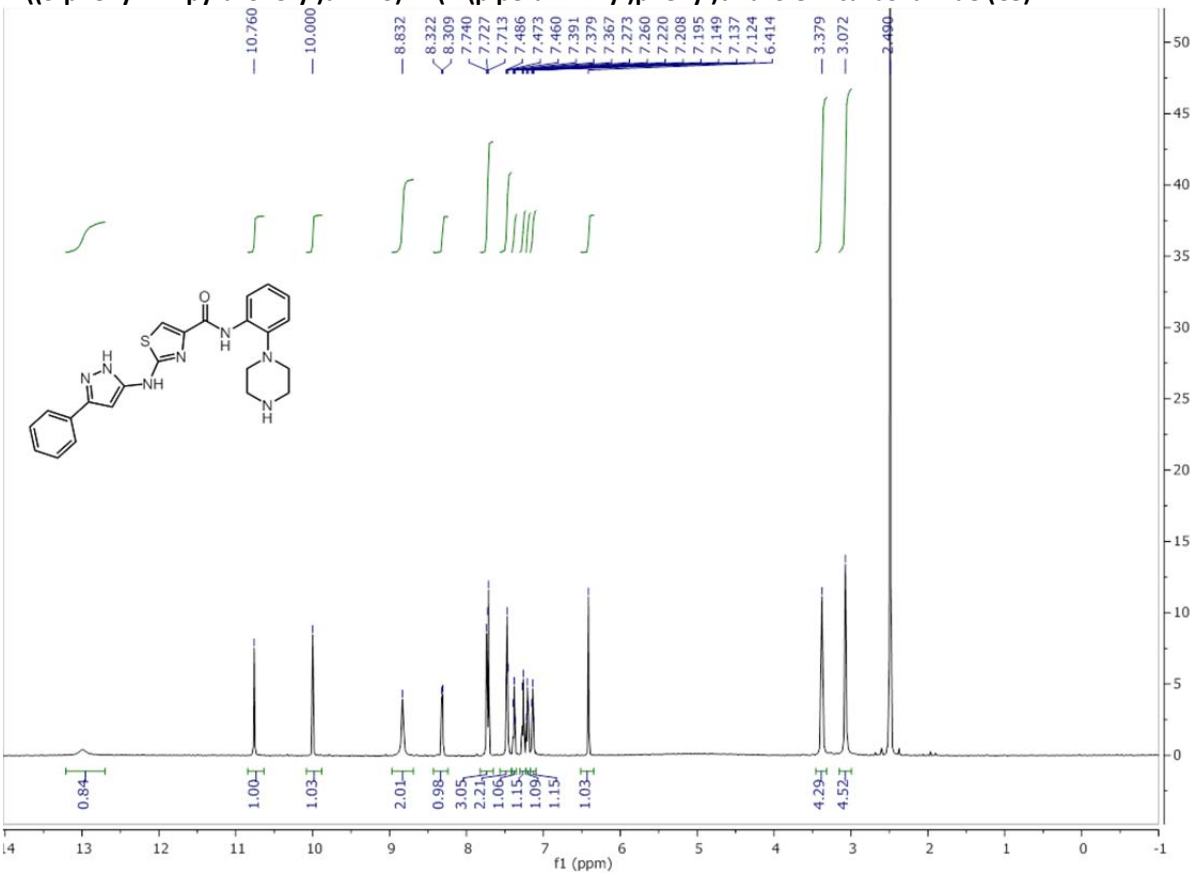
2-(2-methyl-4,6-dihydro-5H-pyrrolo[3,4-d]thiazol-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C6)



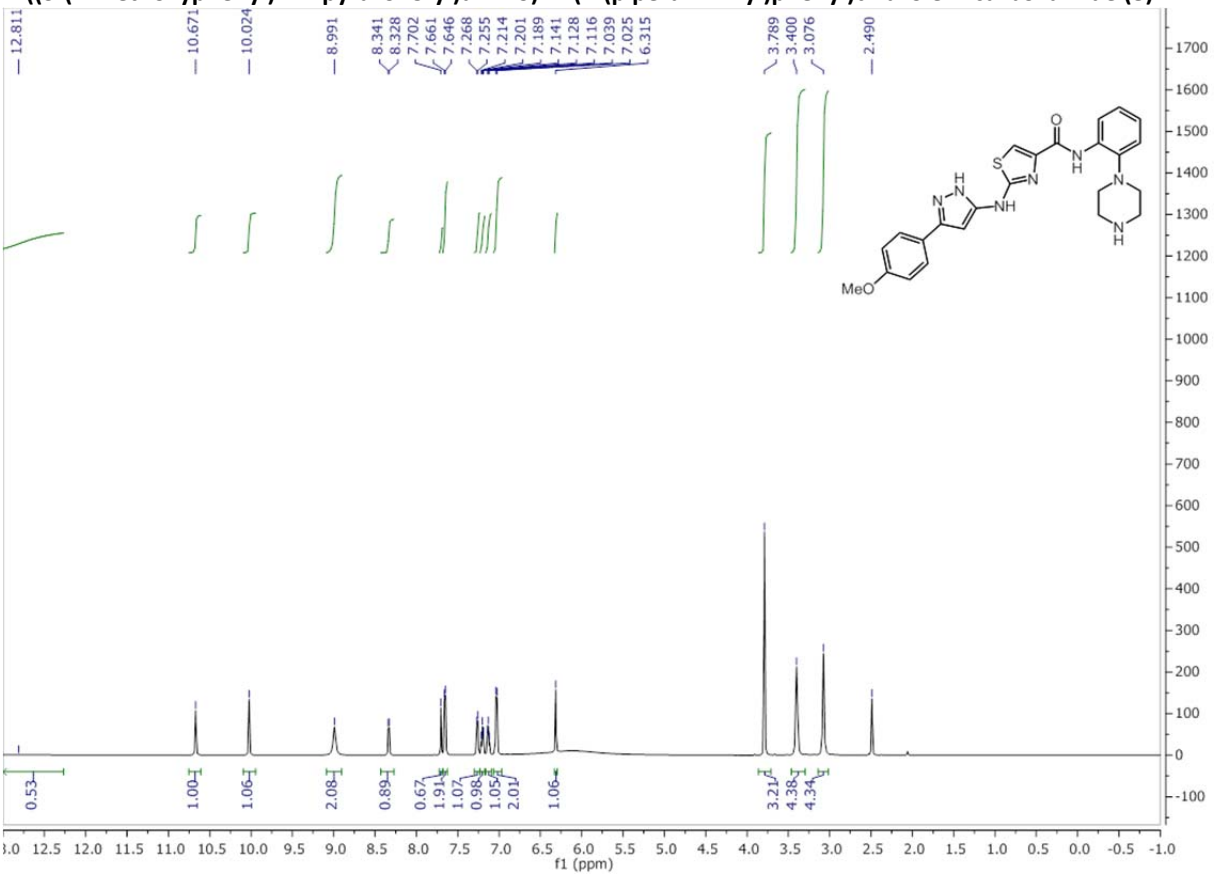
N-(2-(piperazin-1-yl)phenyl)-2-(1H-pyrazol-1-yl)thiazole-4-carboxamide (C7)



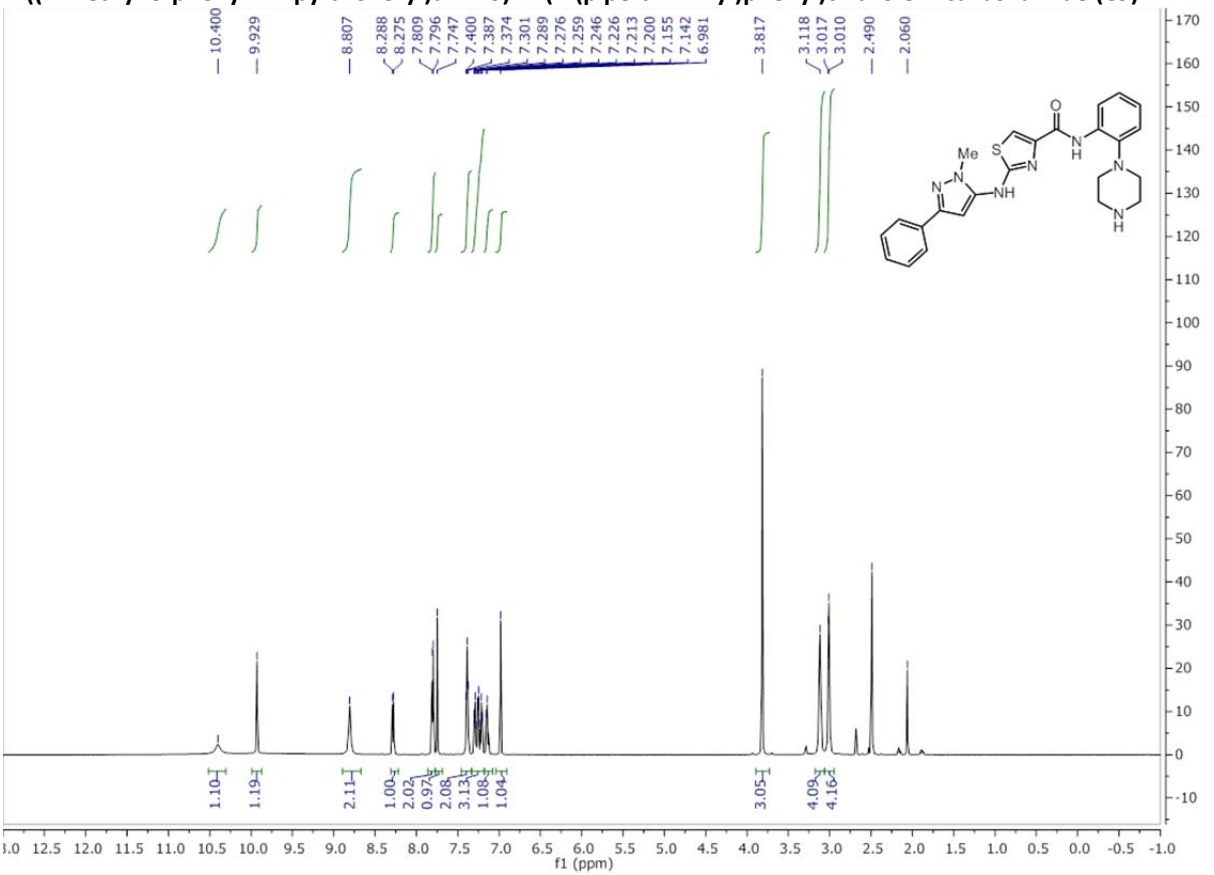
2-((3-phenyl-1H-pyrazol-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C8)



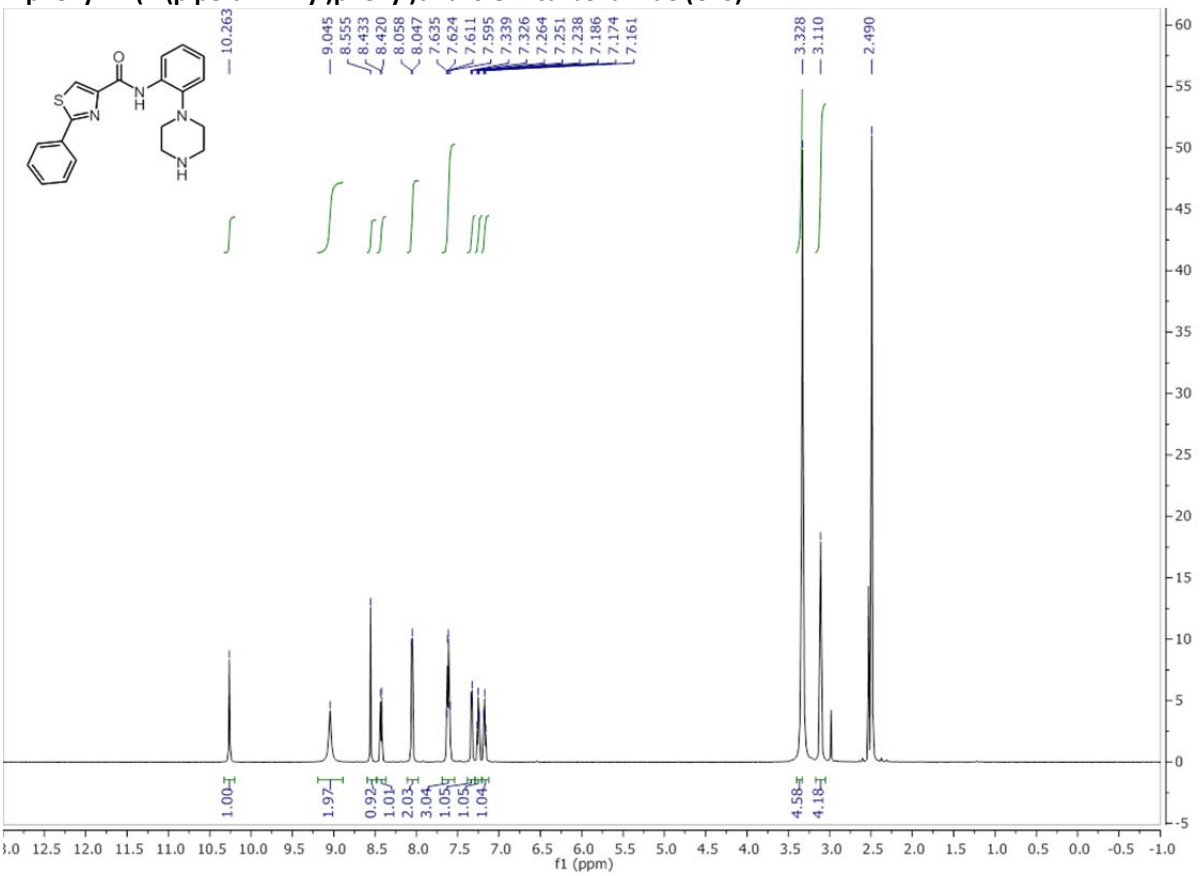
2-((3-(4-methoxyphenyl)-1H-pyrazol-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (8)



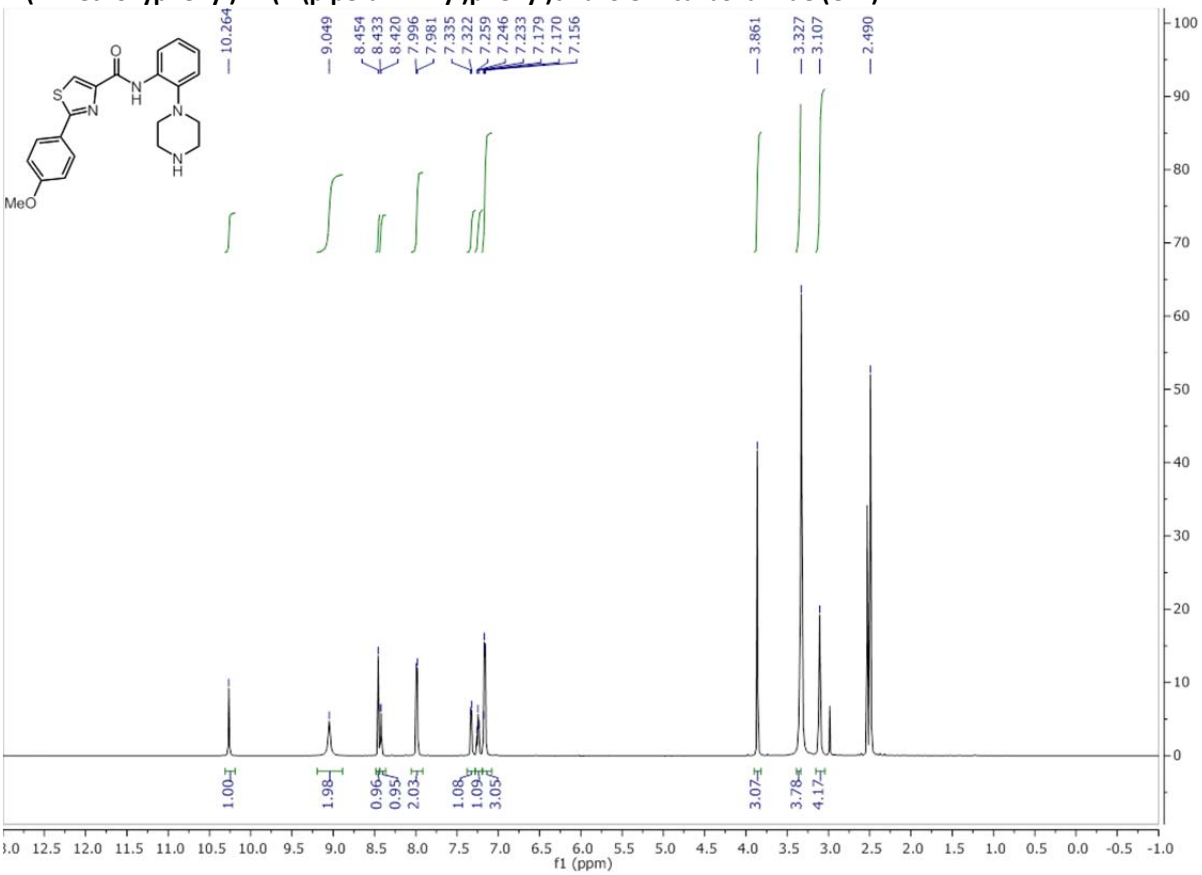
2-((1-methyl-3-phenyl-1H-pyrazol-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C9)



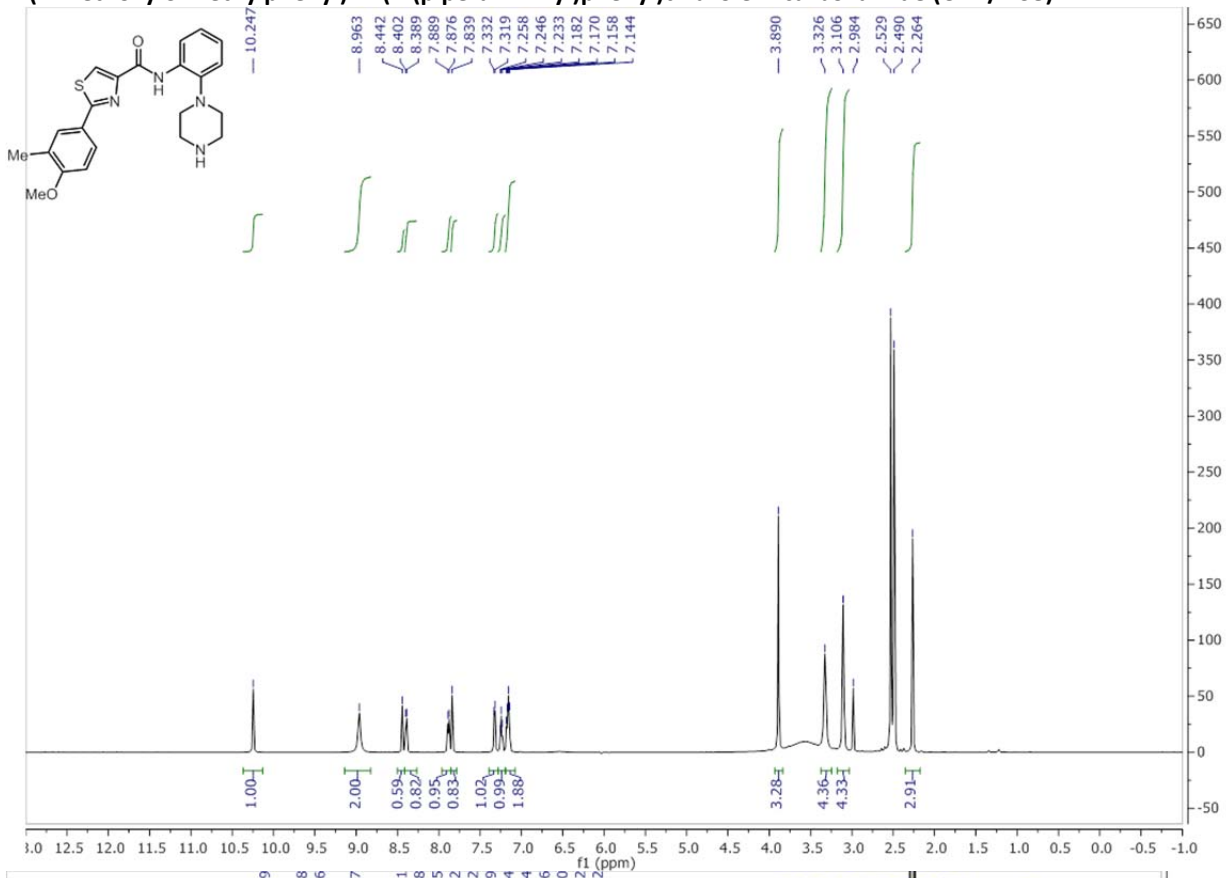
2-phenyl-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C10)

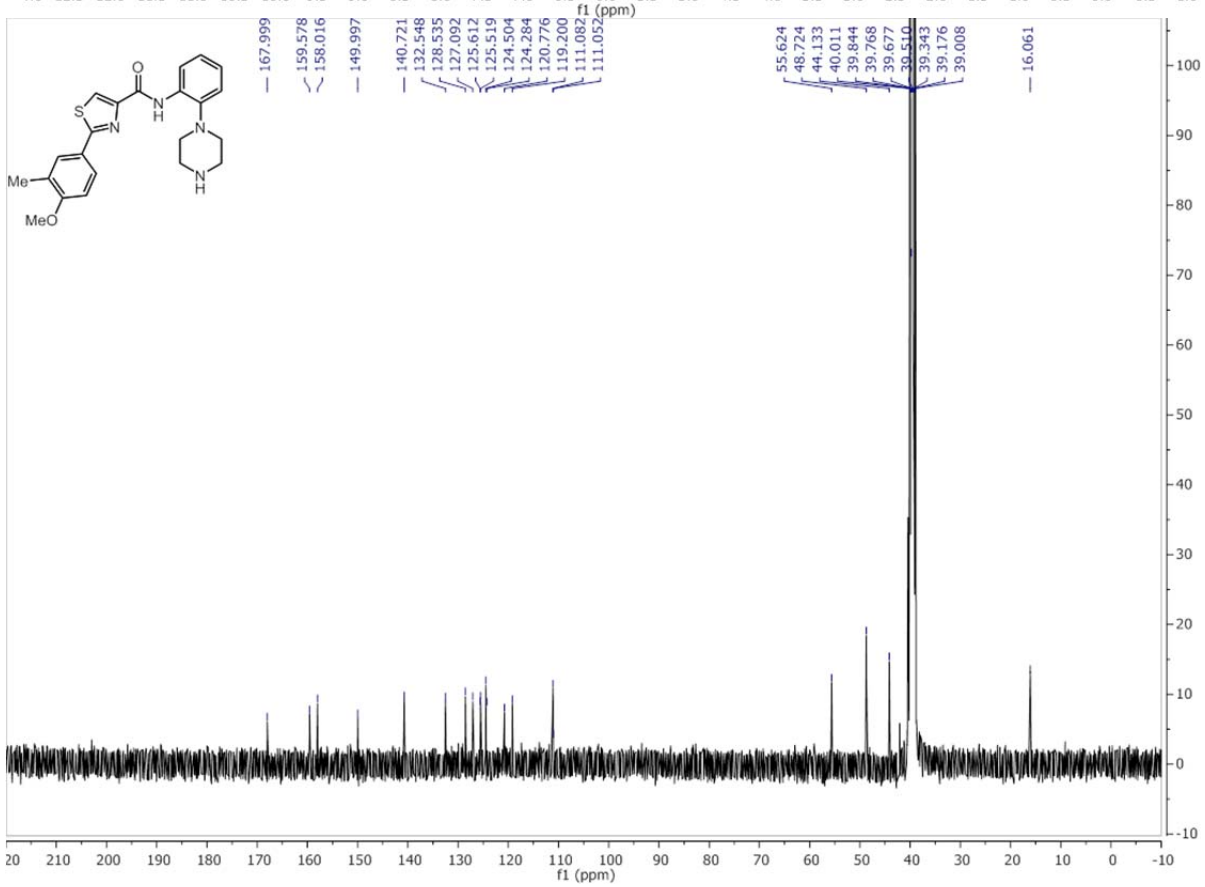


2-(4-methoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C11)

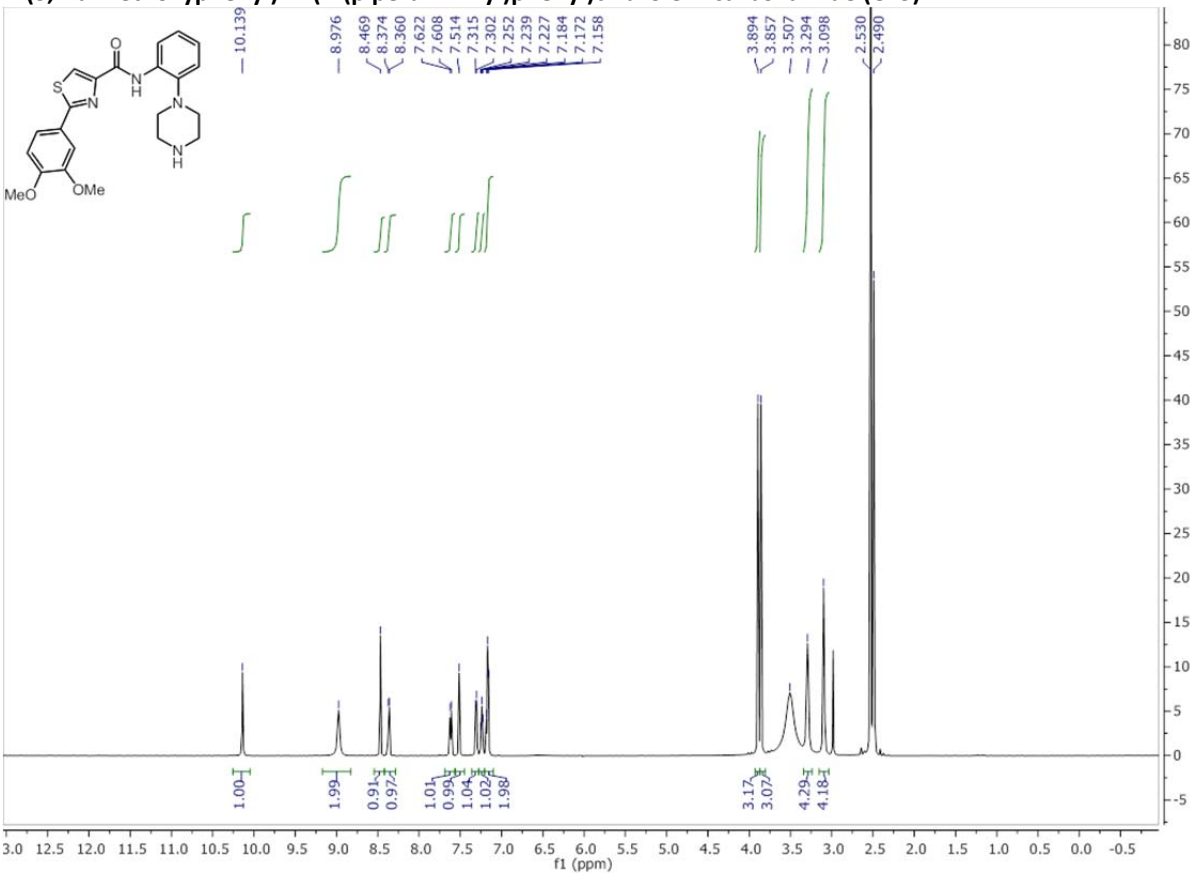


2-(4-methoxy-3-methylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C12 / E38)

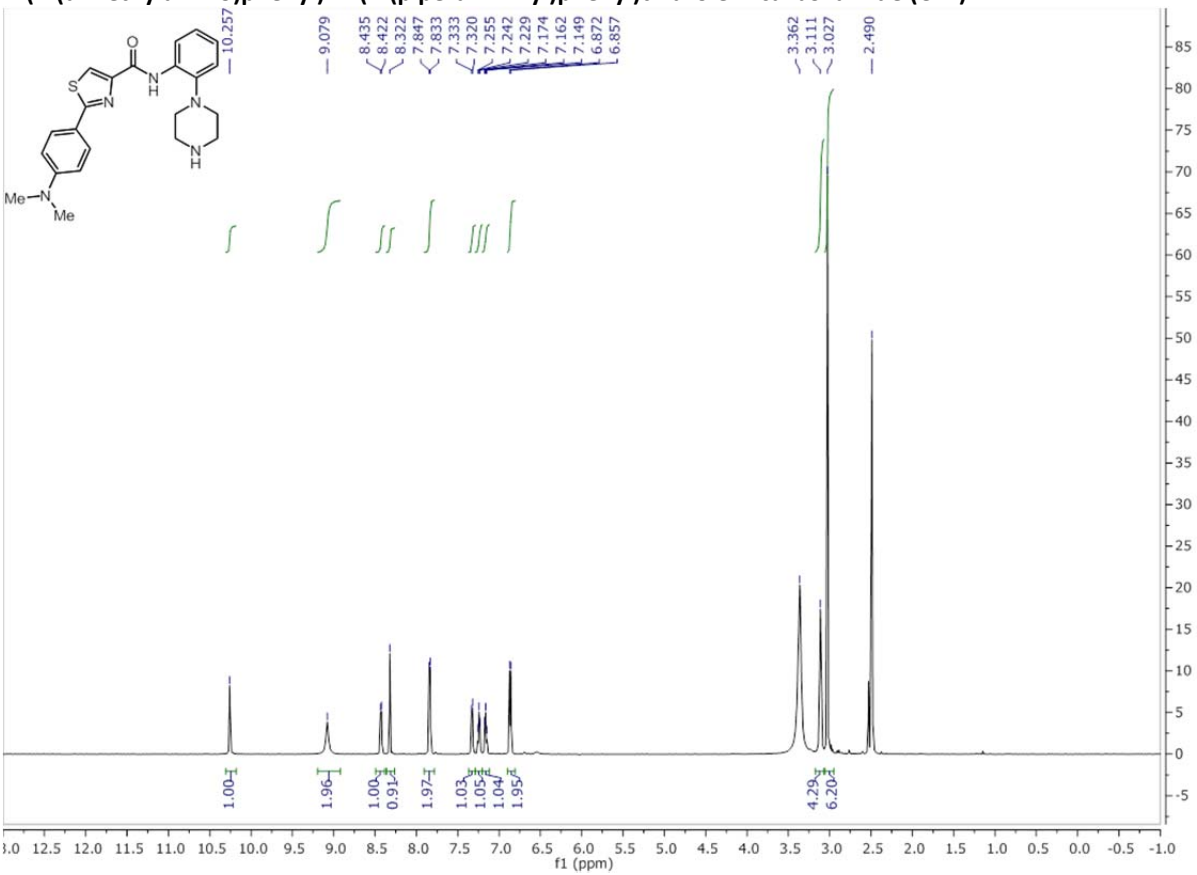




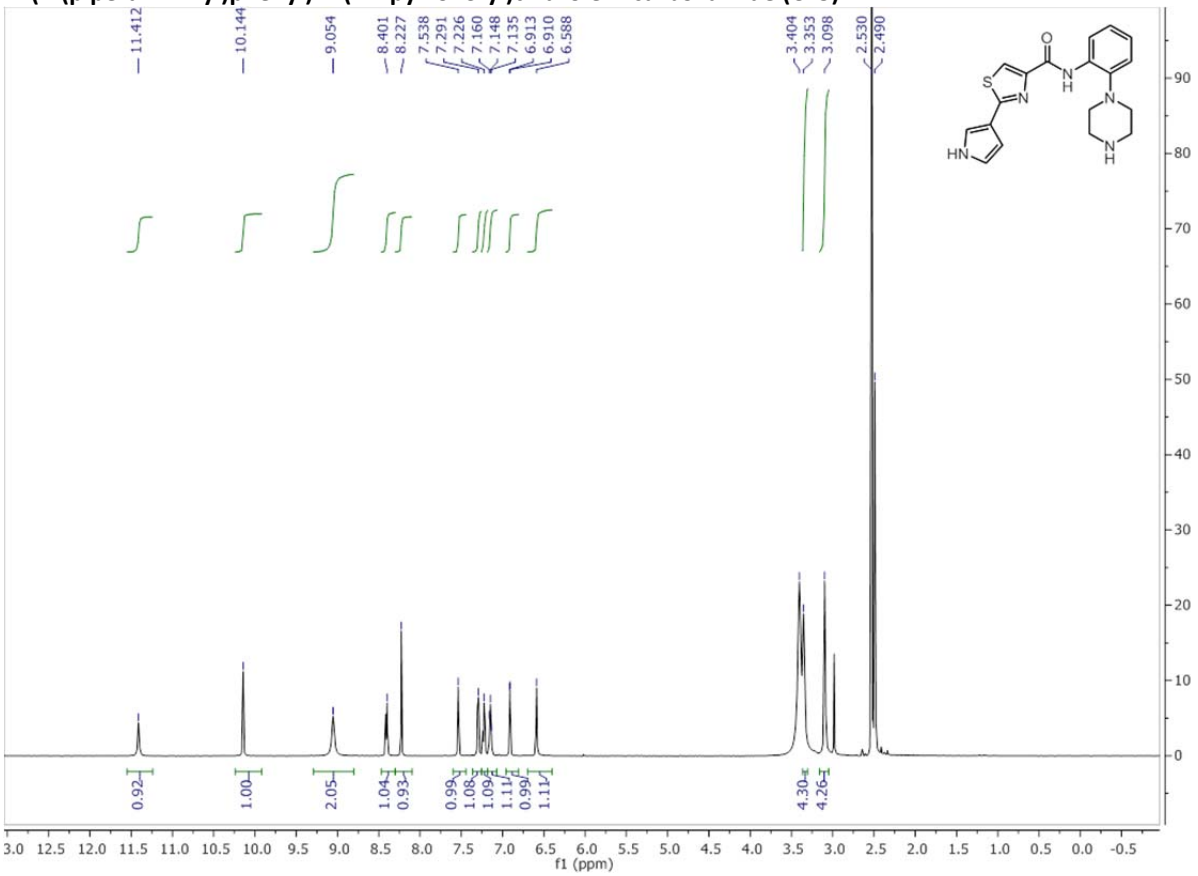
2-(3,4-dimethoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C13)



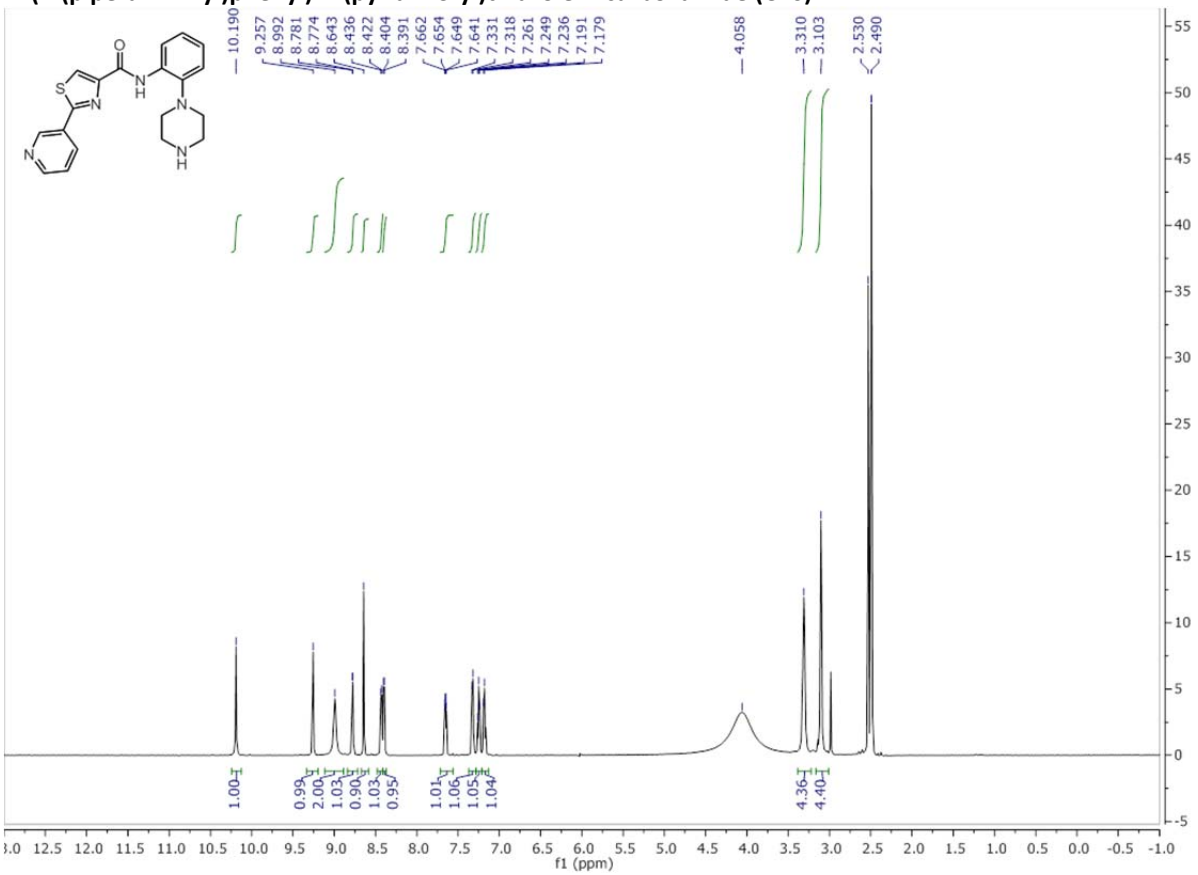
2-(4-(dimethylamino)phenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C14)



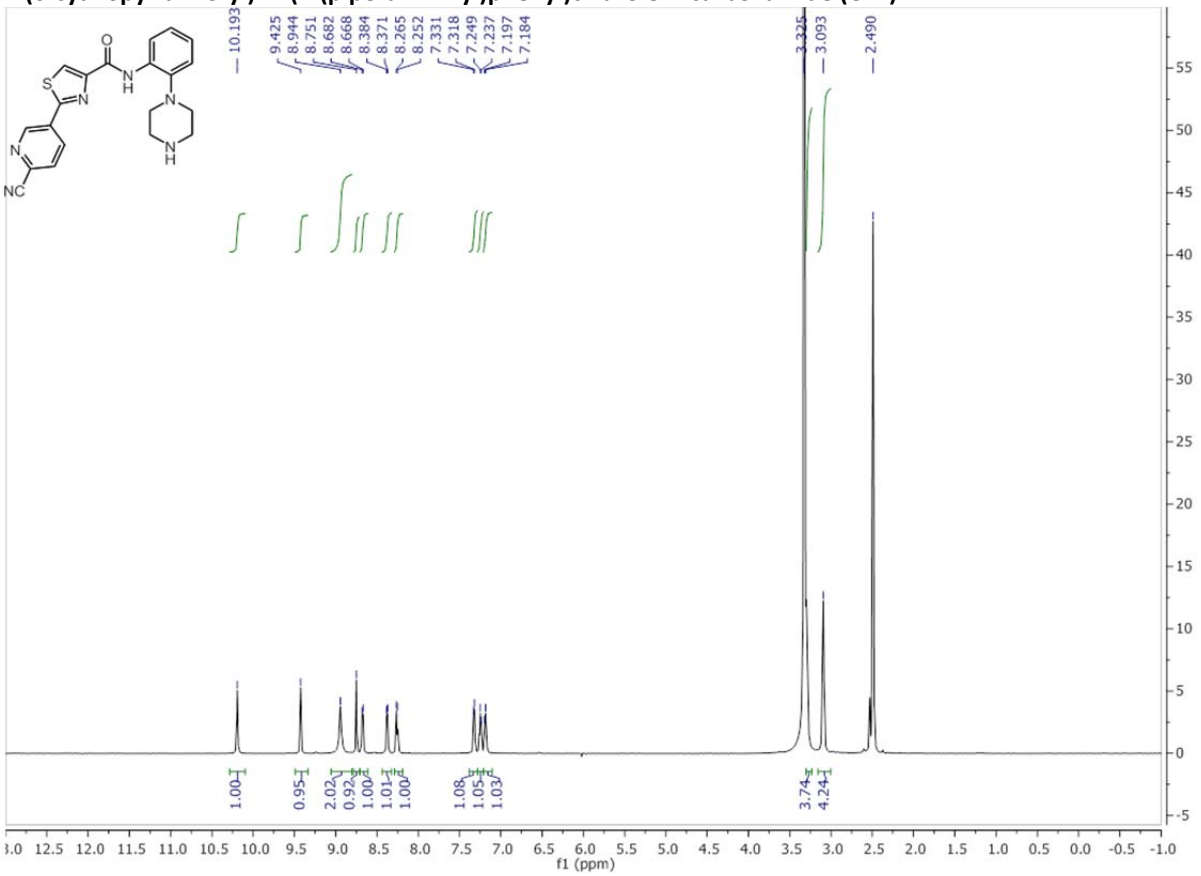
N-(2-(piperazin-1-yl)phenyl)-2-(1H-pyrrol-3-yl)thiazole-4-carboxamide (C15)



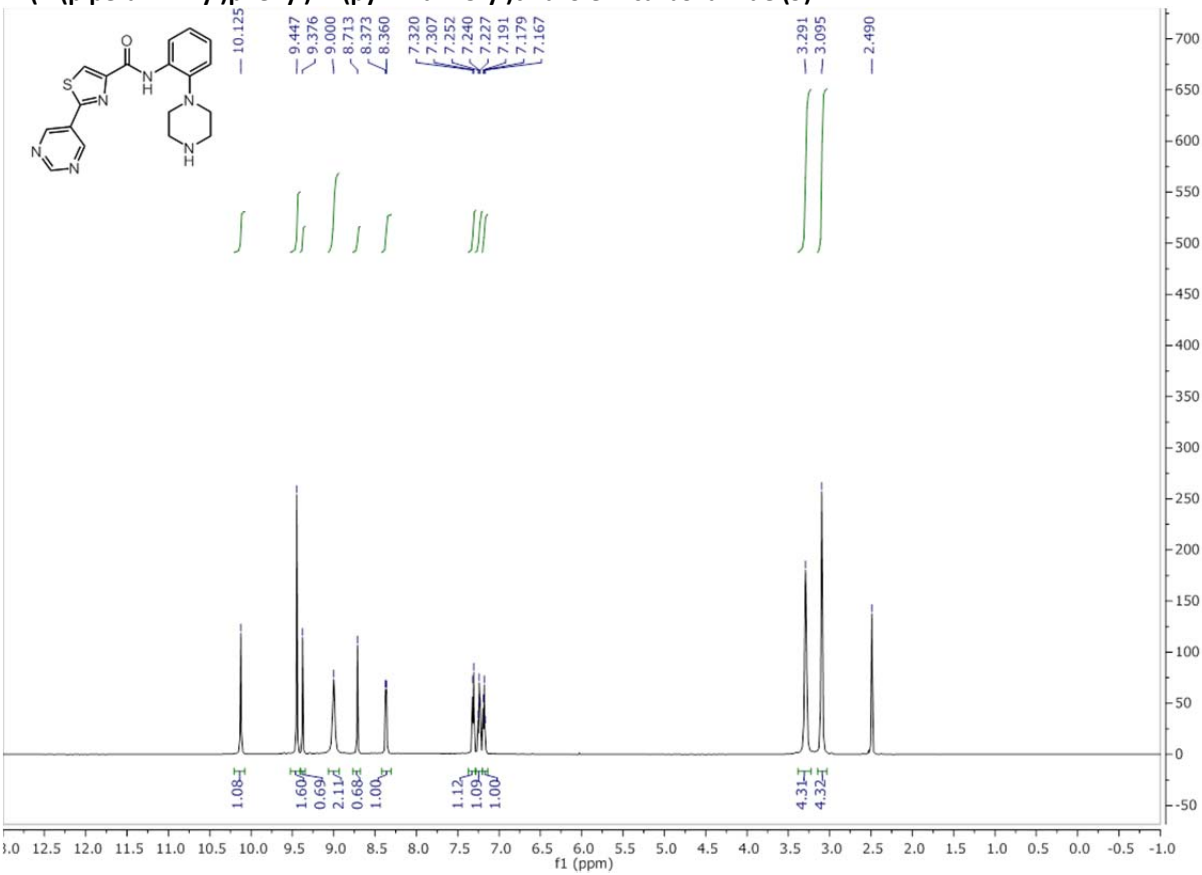
N-(2-(piperazin-1-yl)phenyl)-2-(pyridin-3-yl)thiazole-4-carboxamide (C16)



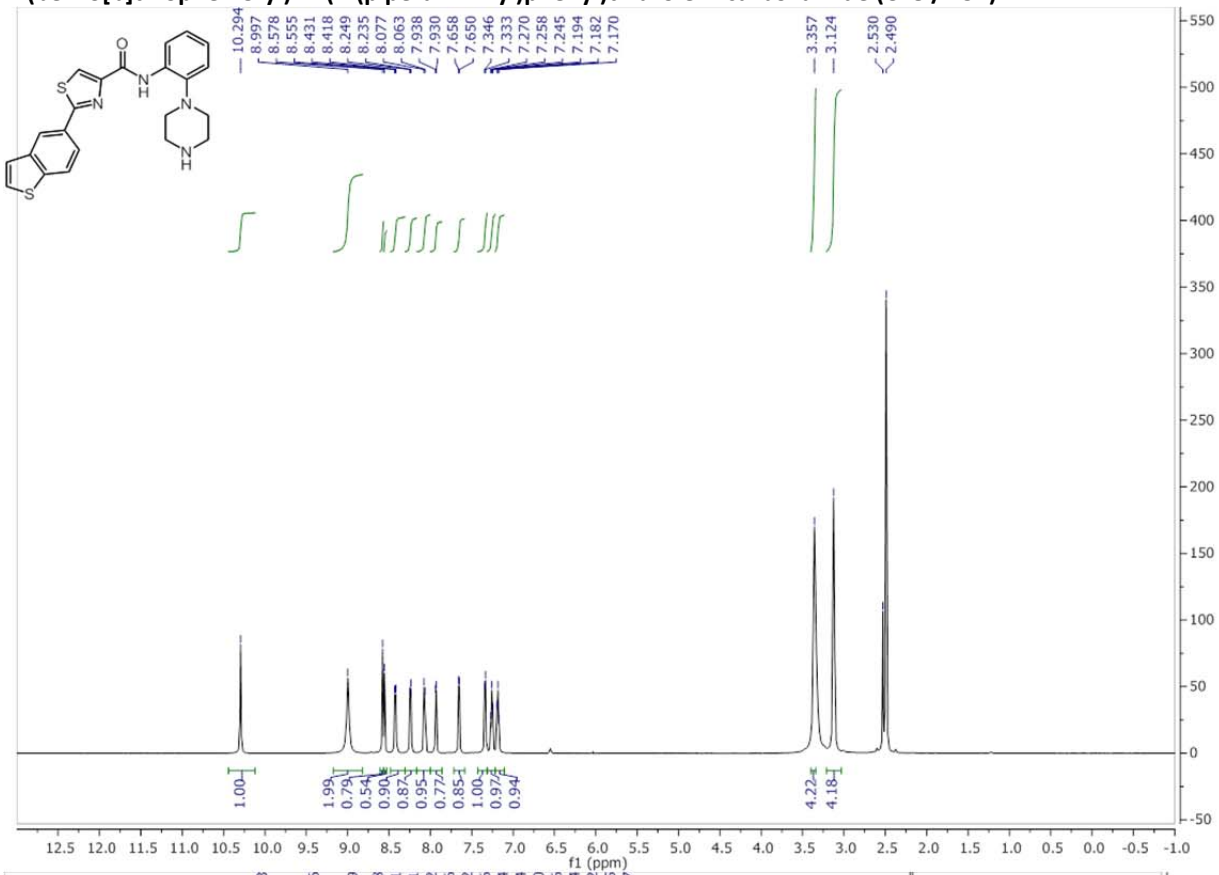
2-(6-cyanopyridin-3-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C17)

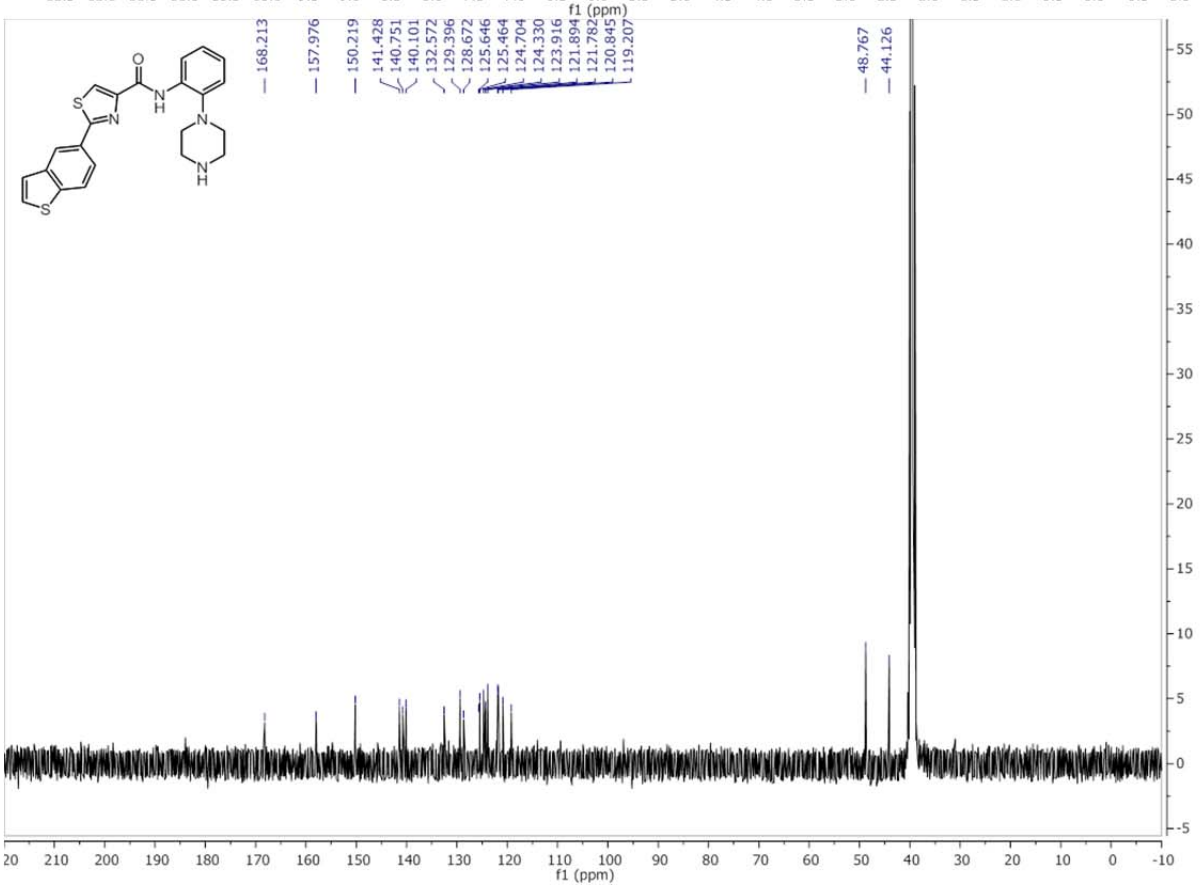


N-(2-(piperazin-1-yl)phenyl)-2-(pyrimidin-5-yl)thiazole-4-carboxamide (9)

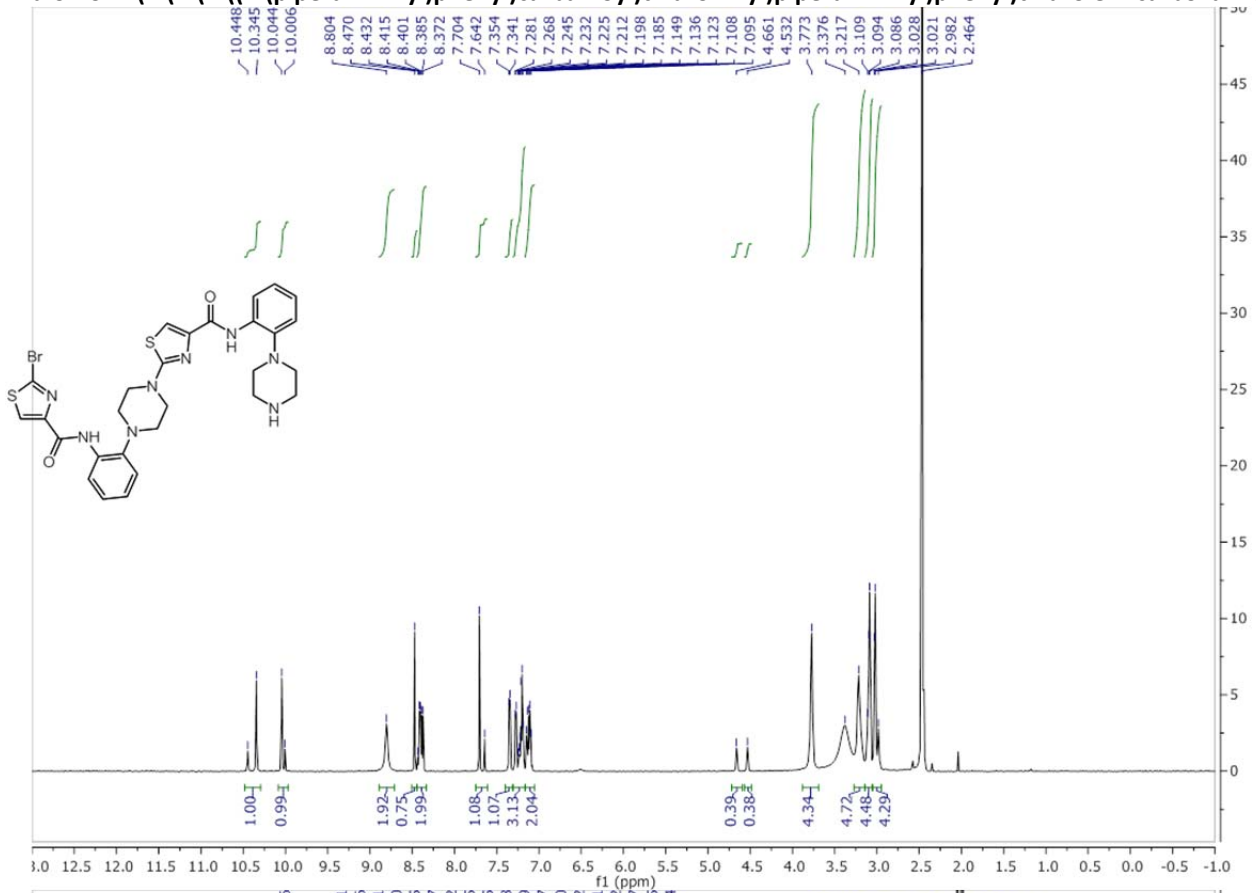


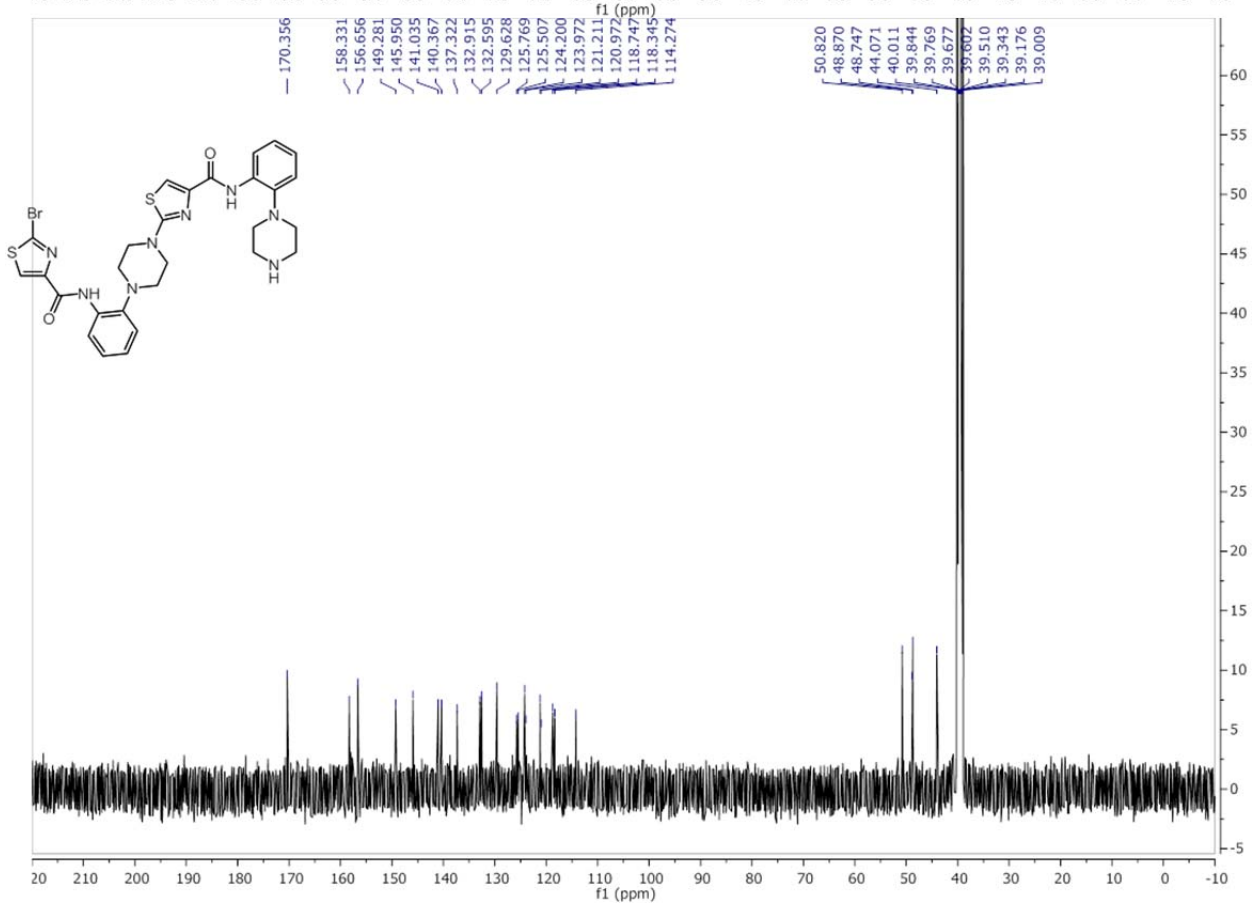
2-(benzo[b]thiophen-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C18 / E51)



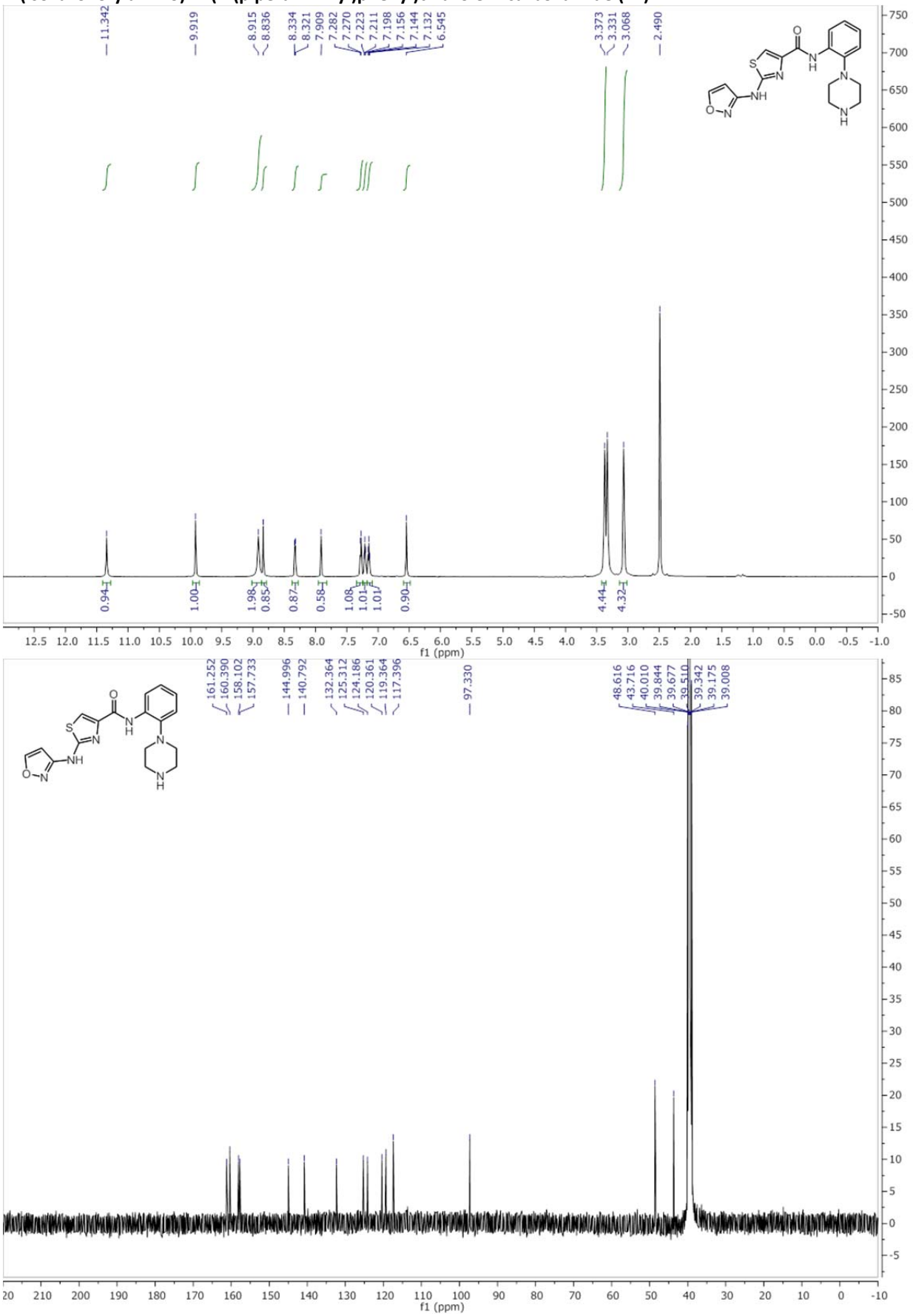


2-bromo-N-(2-(4-(4-((2-(piperazin-1-yl)phenyl)carbamoyl)thiazol-2-yl)piperazin-1-yl)phenyl)thiazole-4-carboxamide (C19)

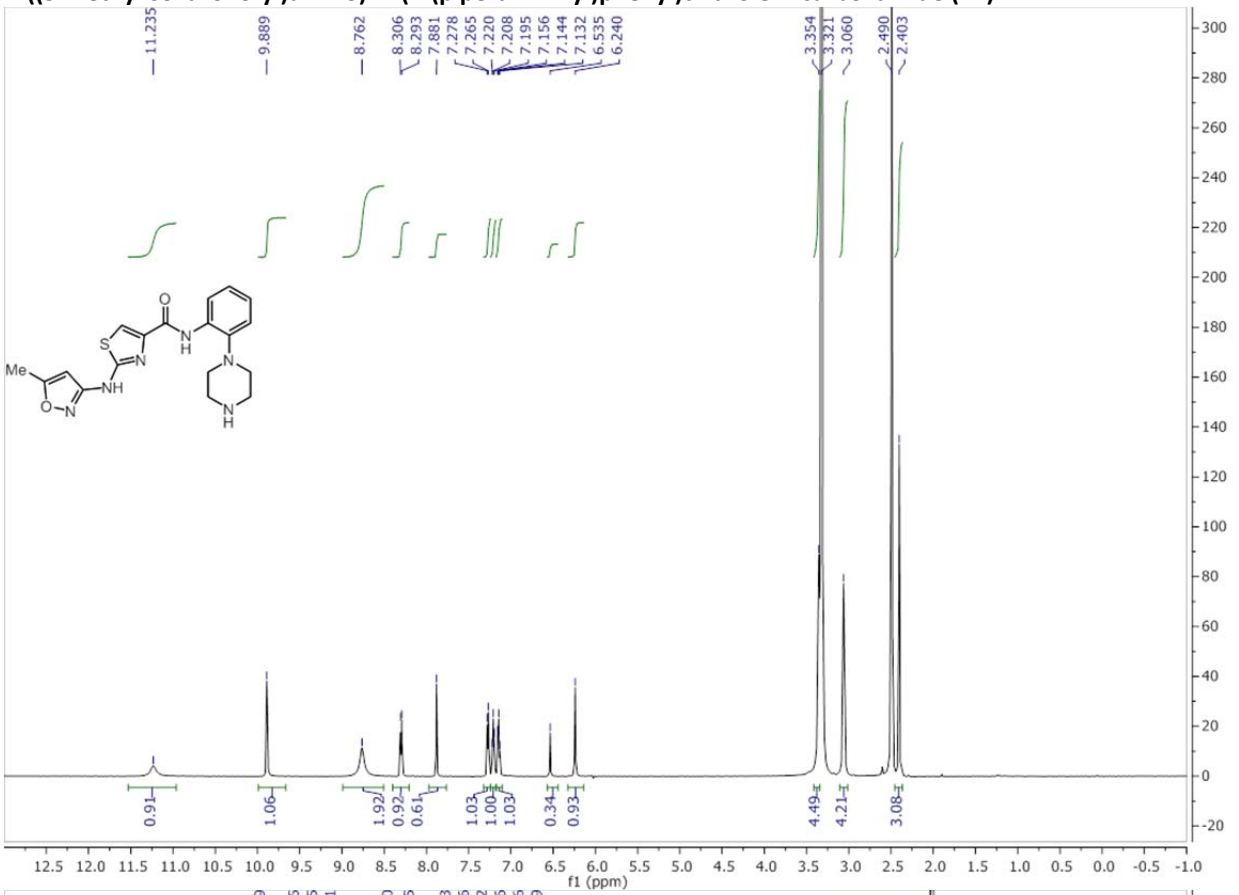


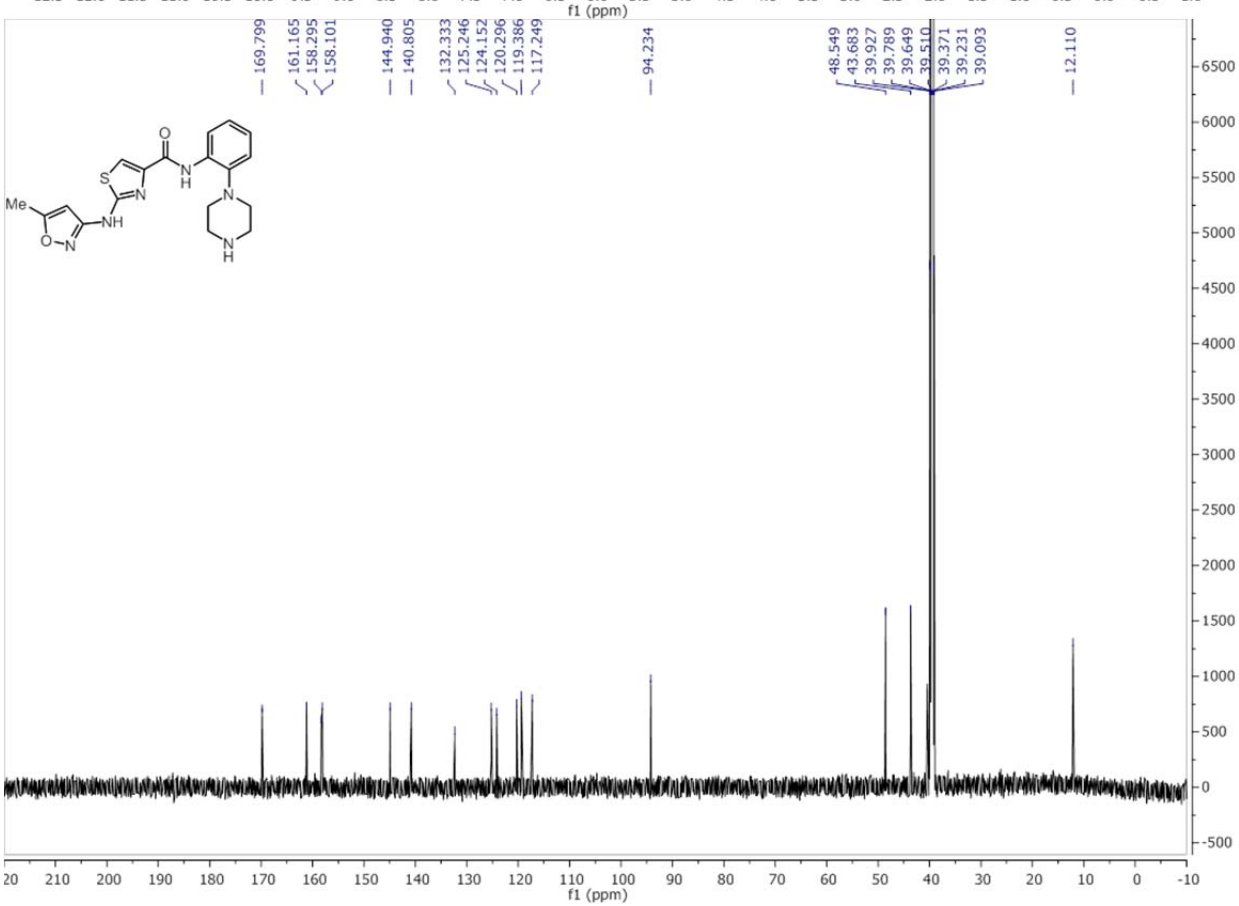


2-(isoxazol-3-ylamino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E1)

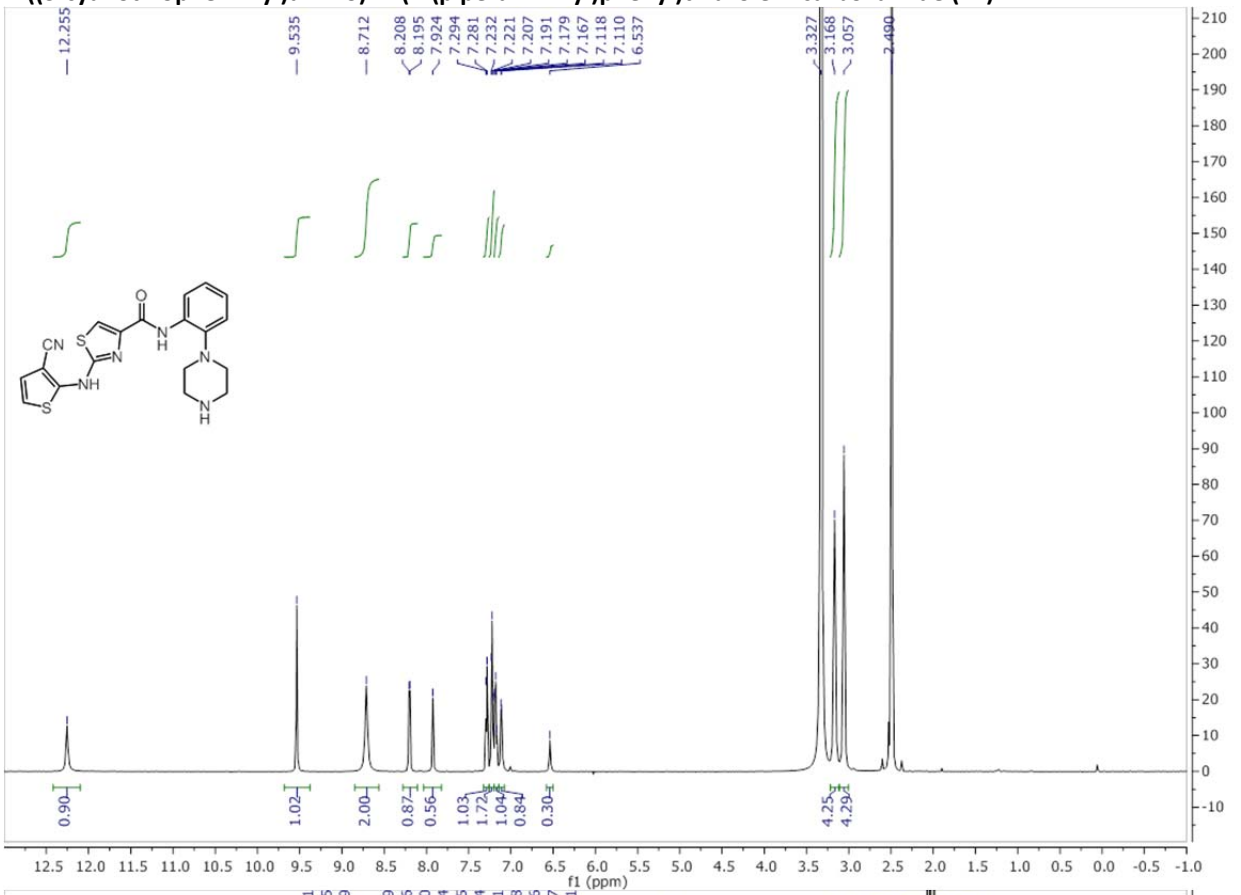


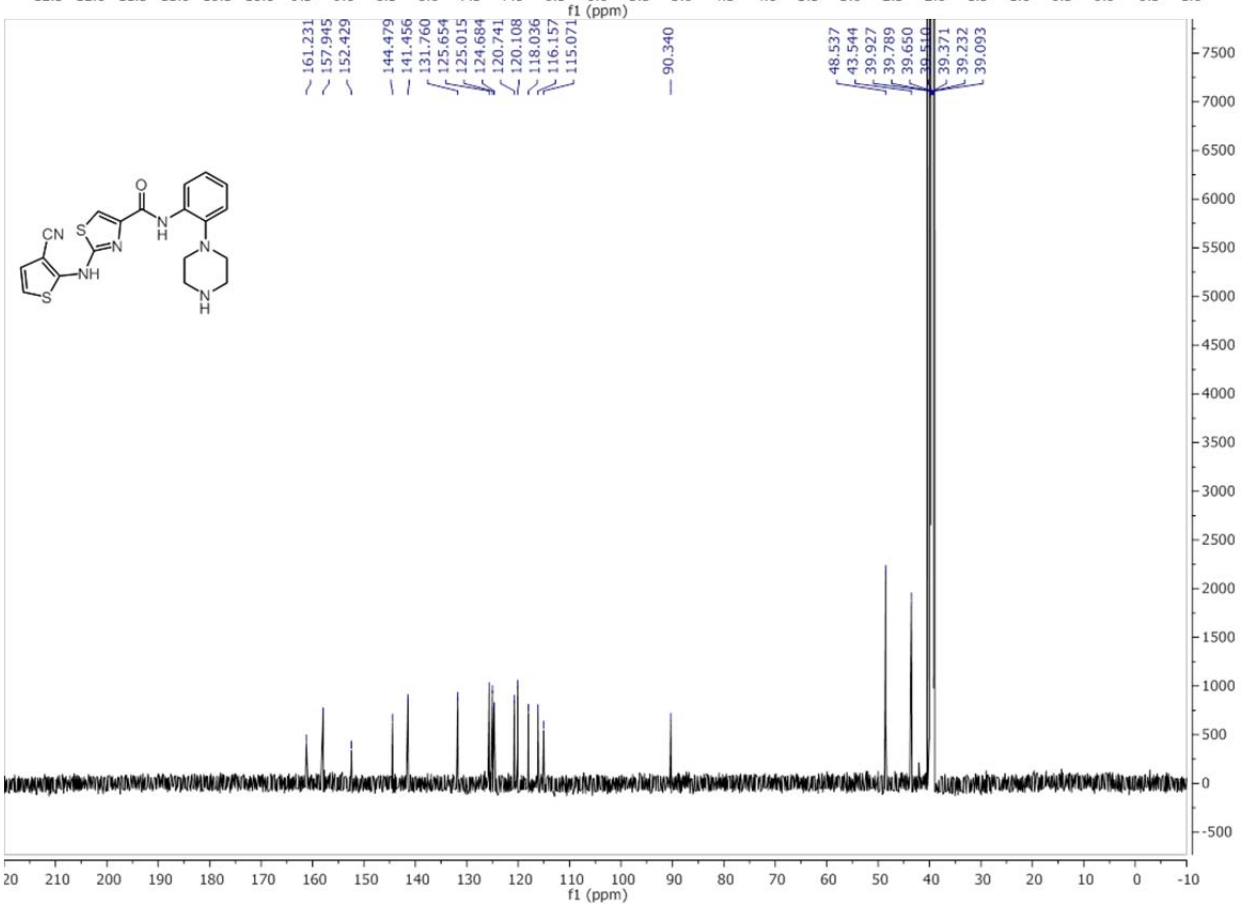
2-((5-methylisoxazol-3-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (44)



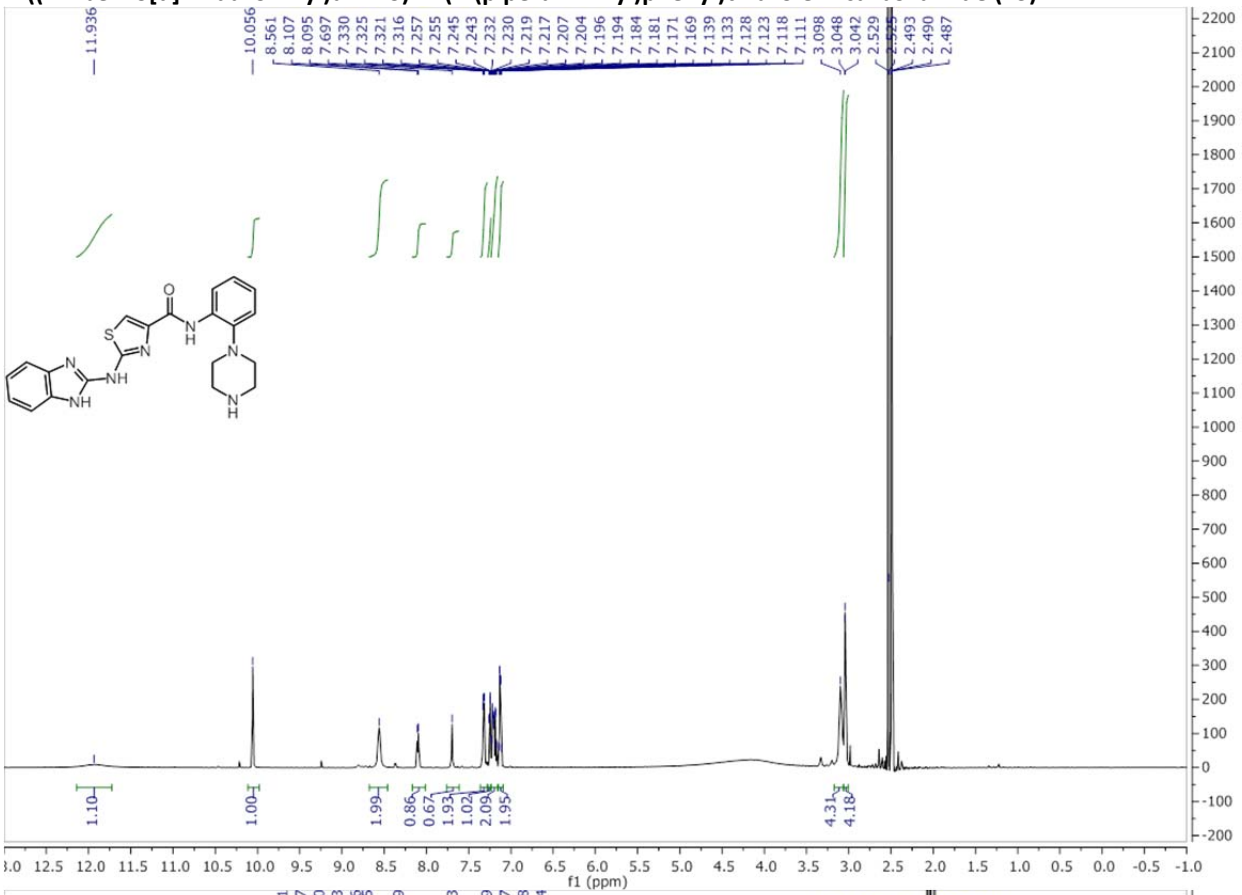


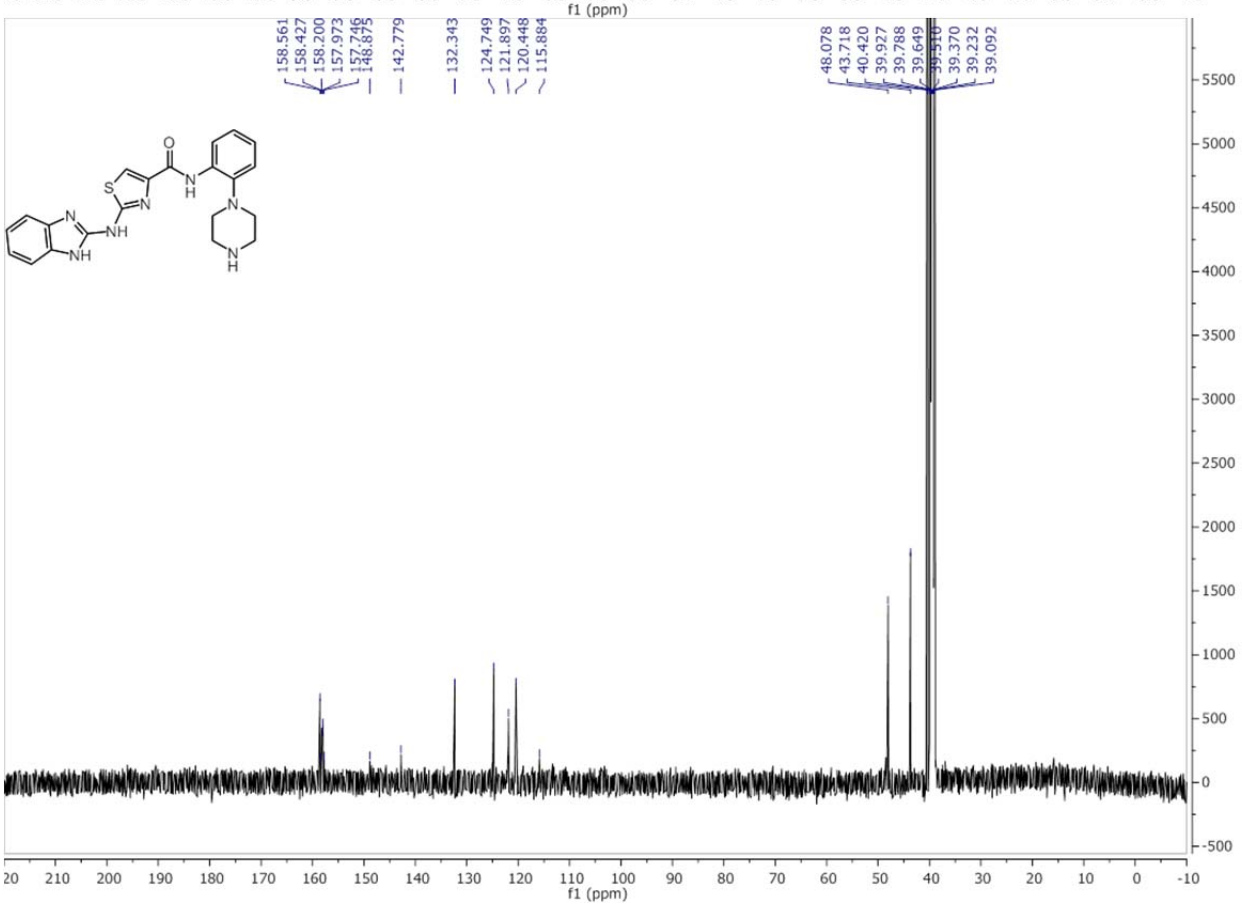
2-((3-cyanothiophen-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E2)



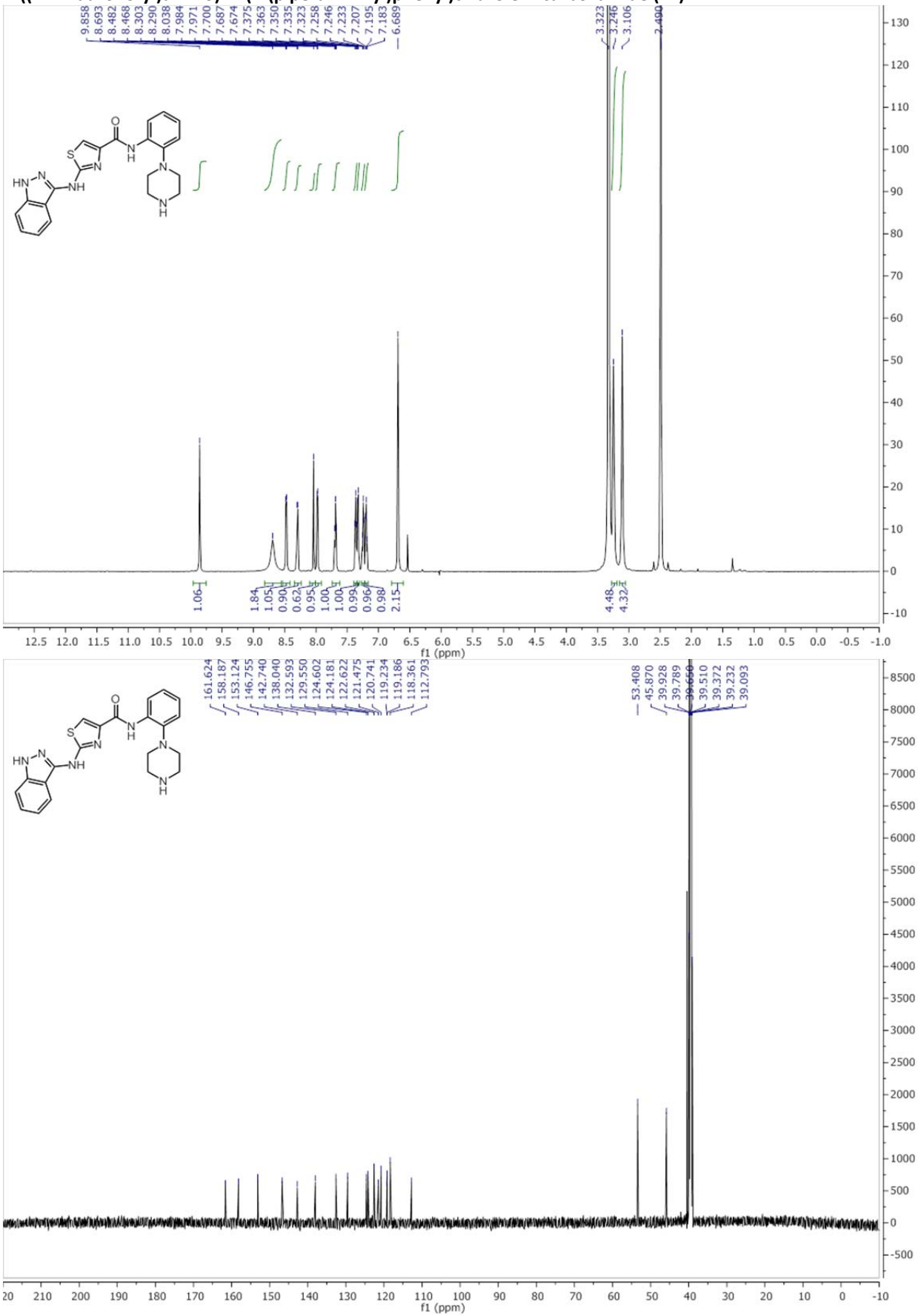


2-((1H-benzo[d]imidazol-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E3)

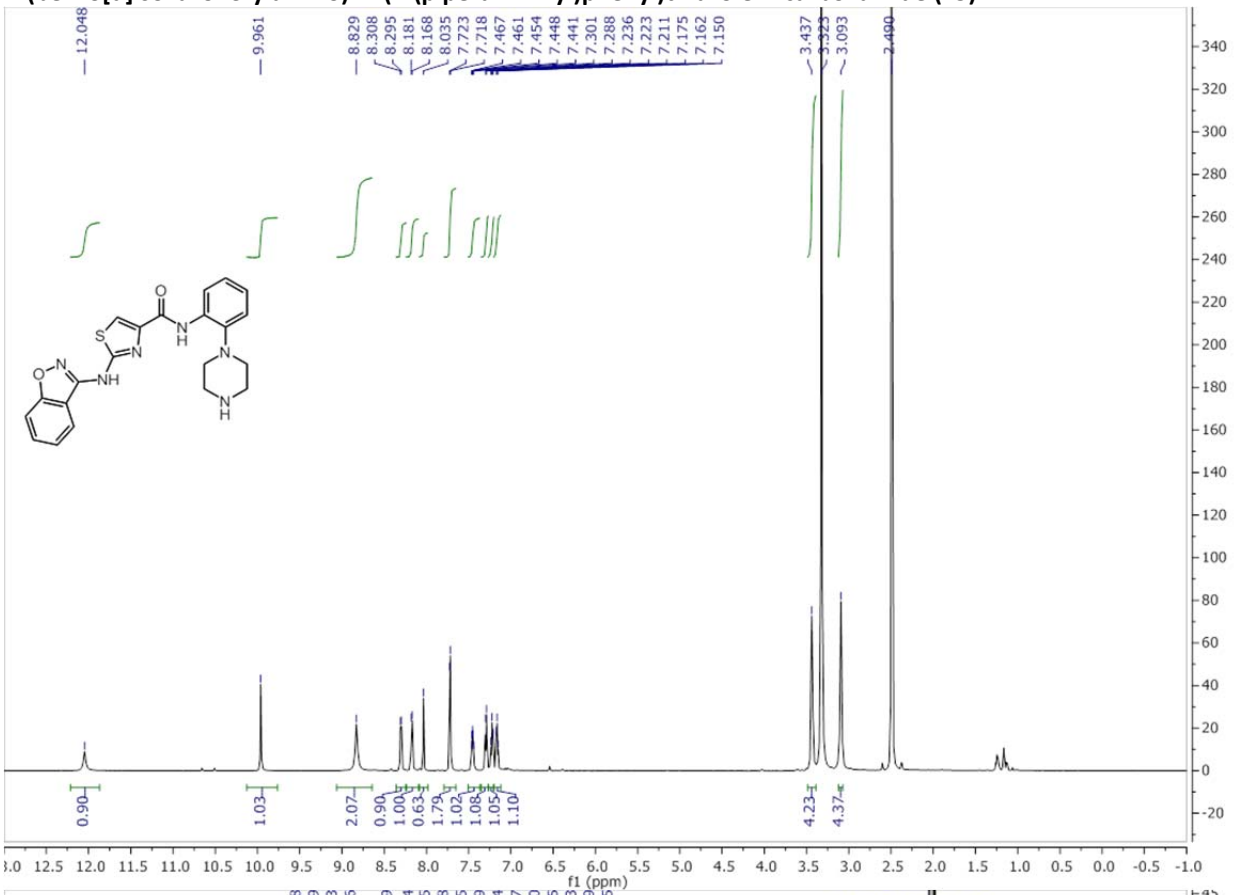


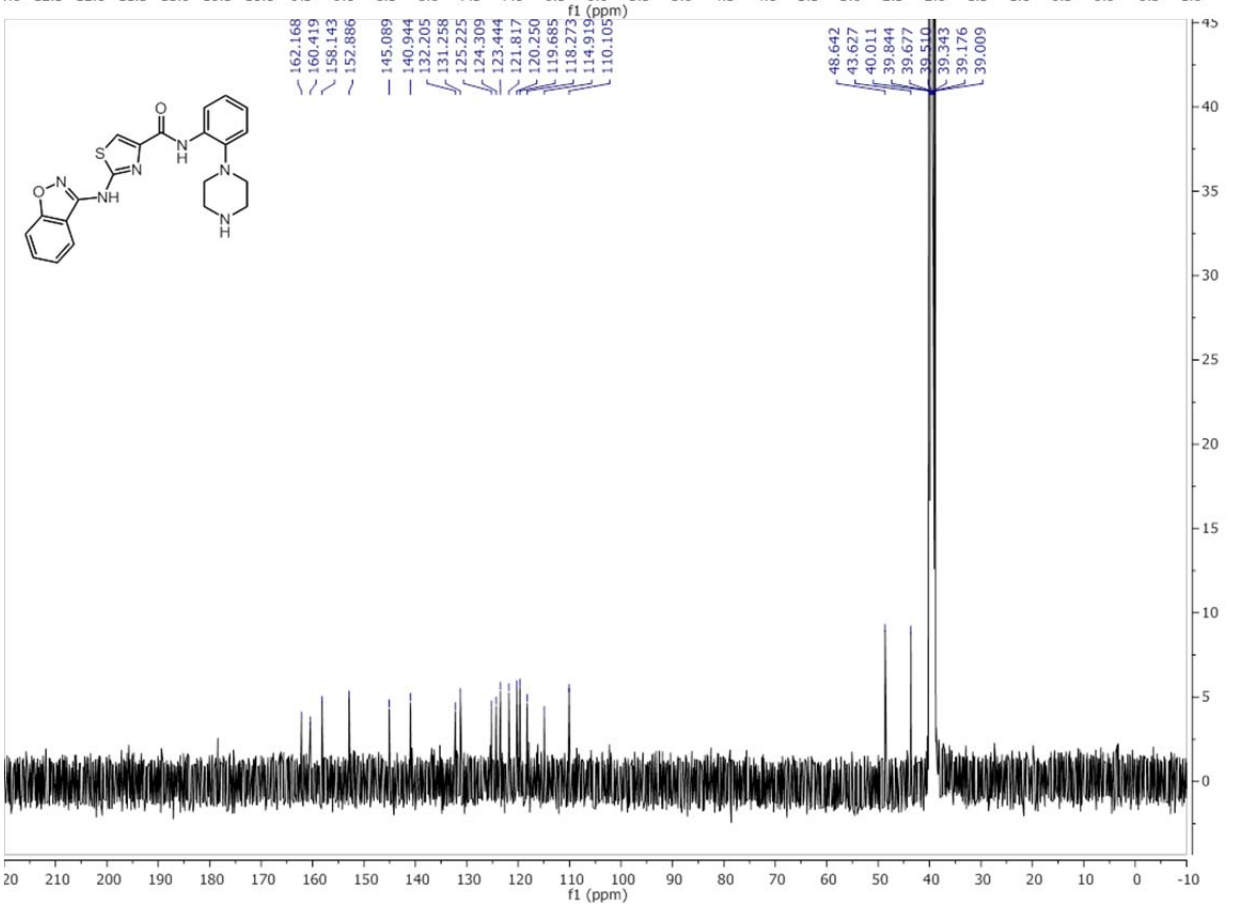


2-((1H-indazol-3-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E4)

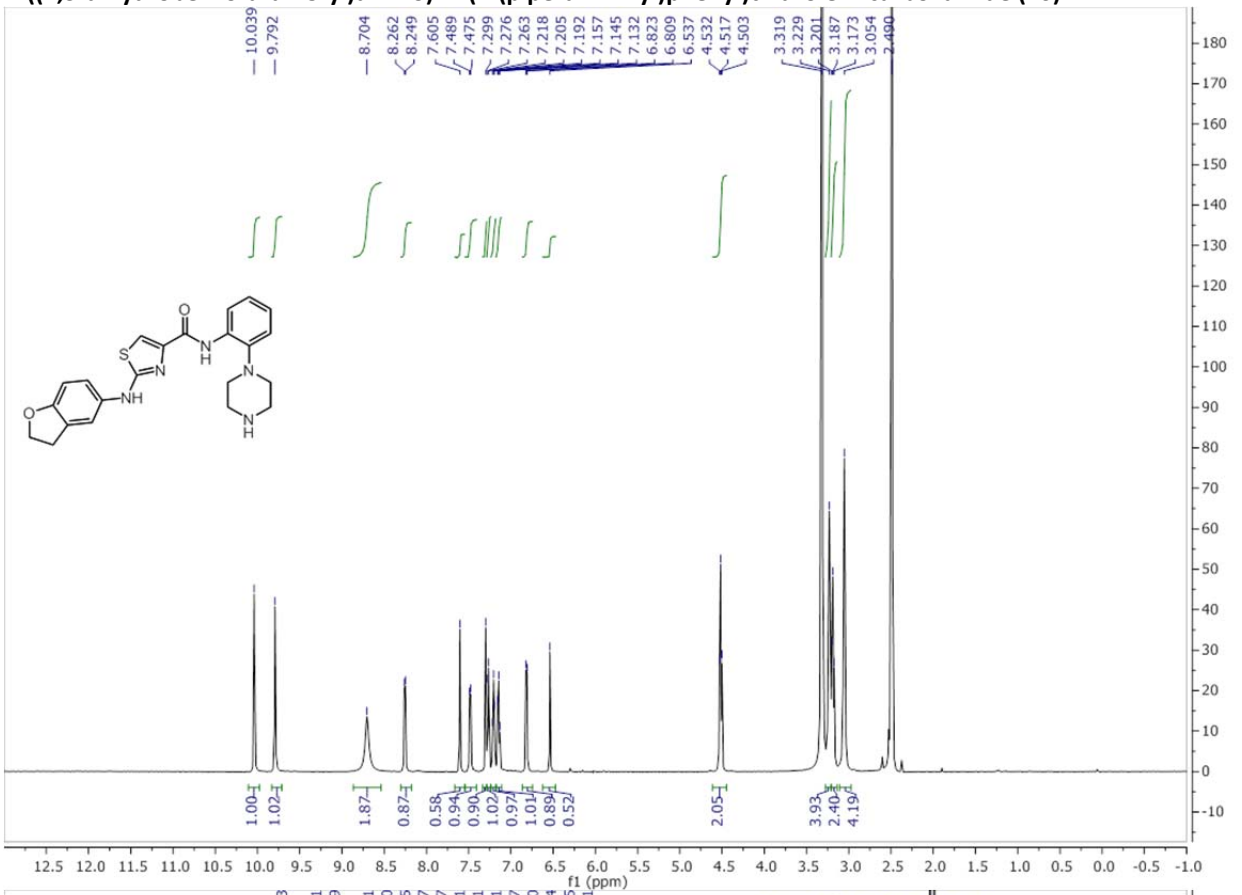


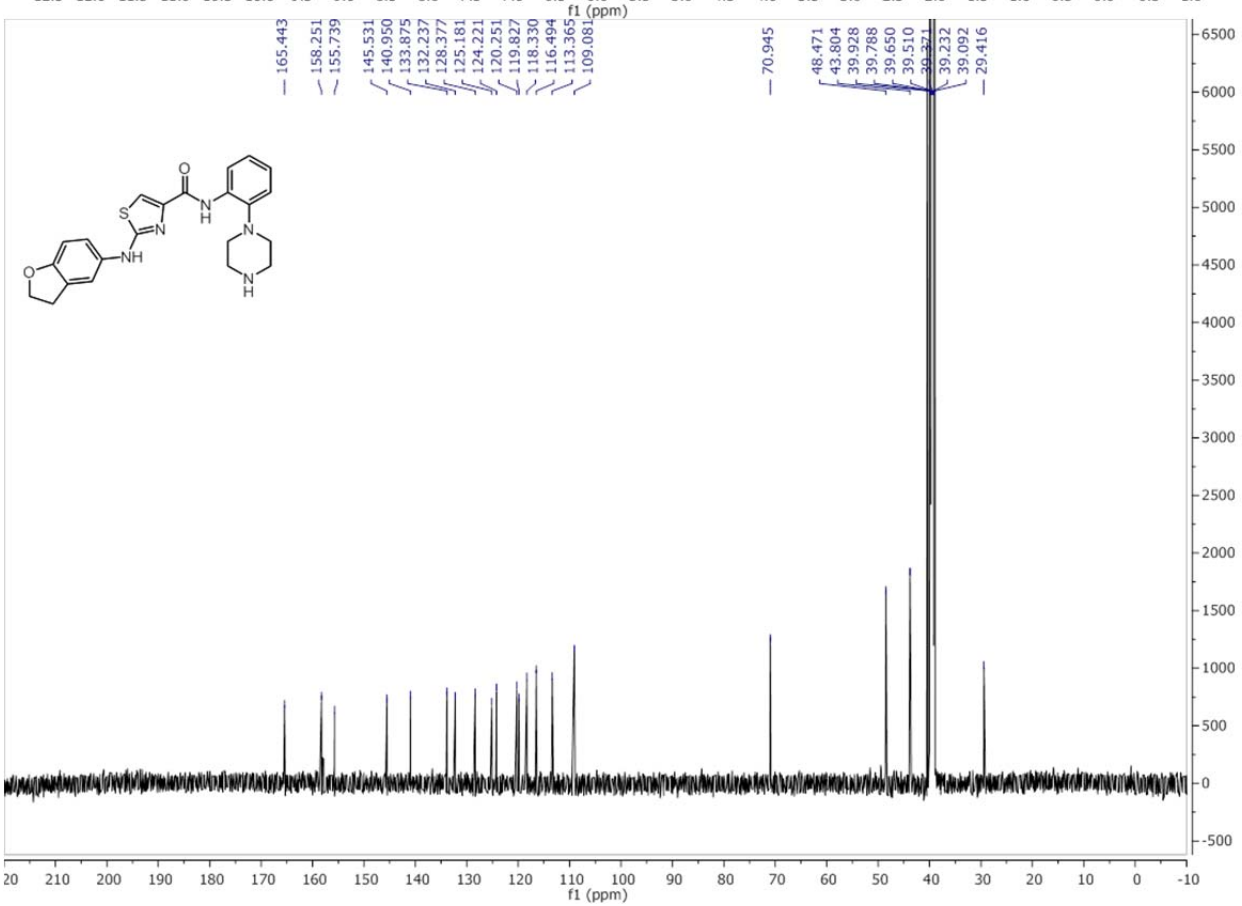
2-(benzo[d]isoxazol-3-ylamino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E5)



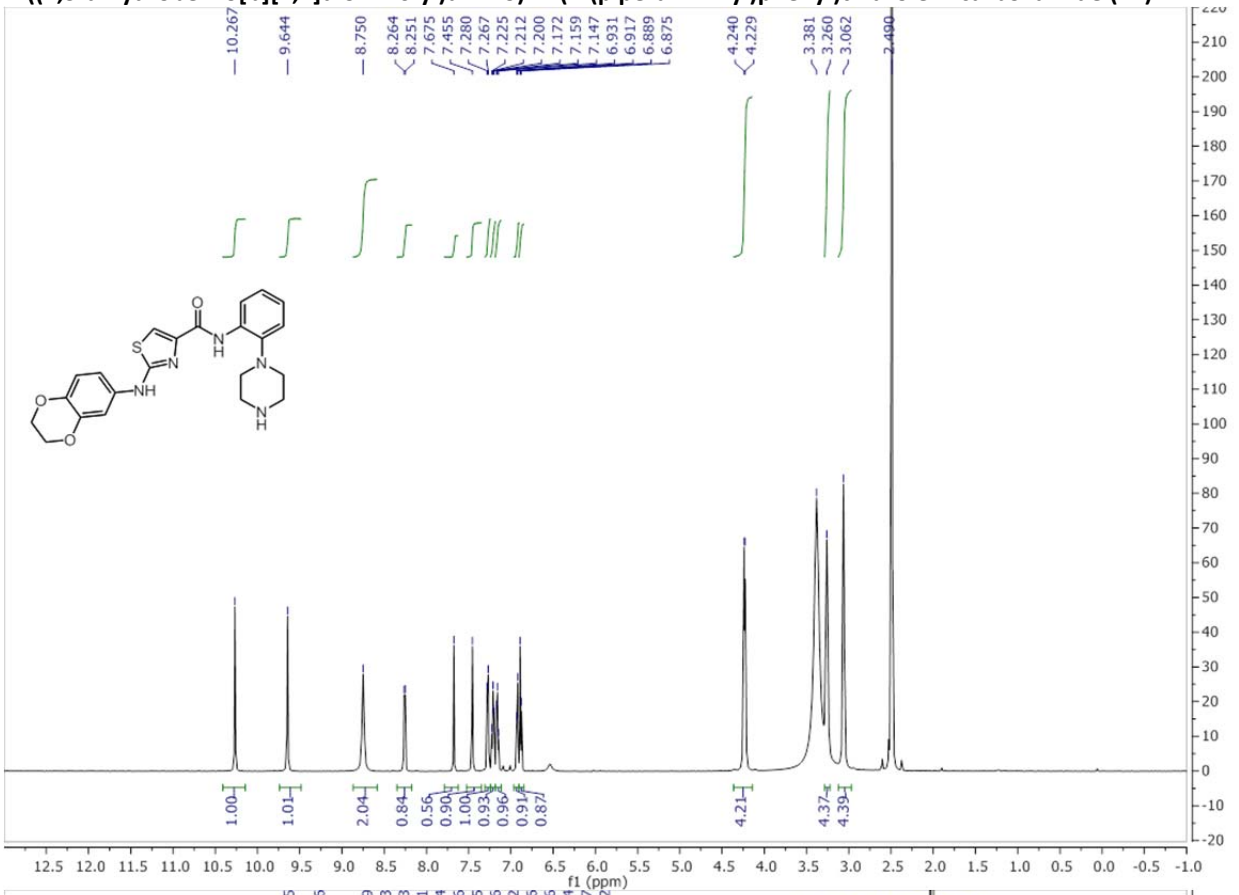


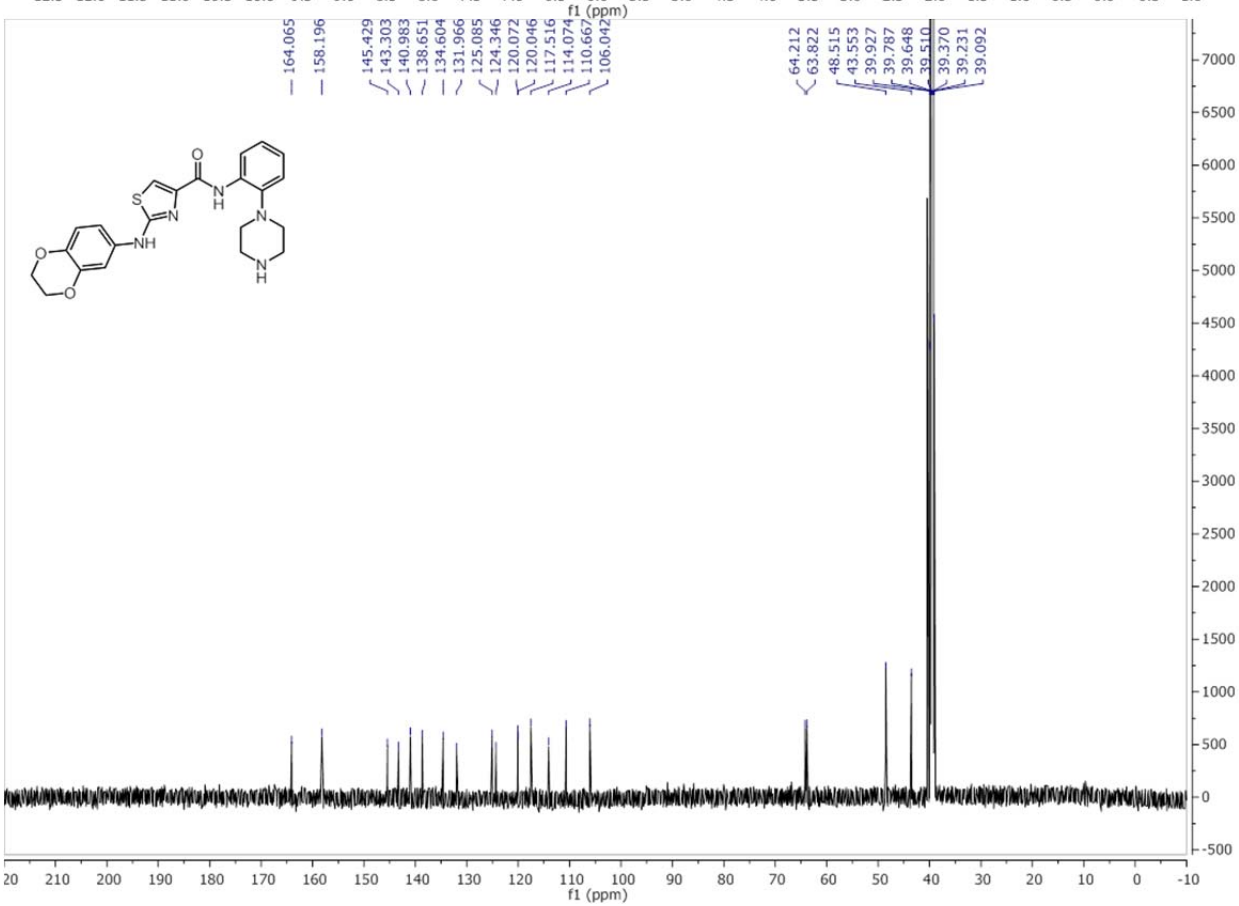
2-((2,3-dihydrobenzofuran-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E6)



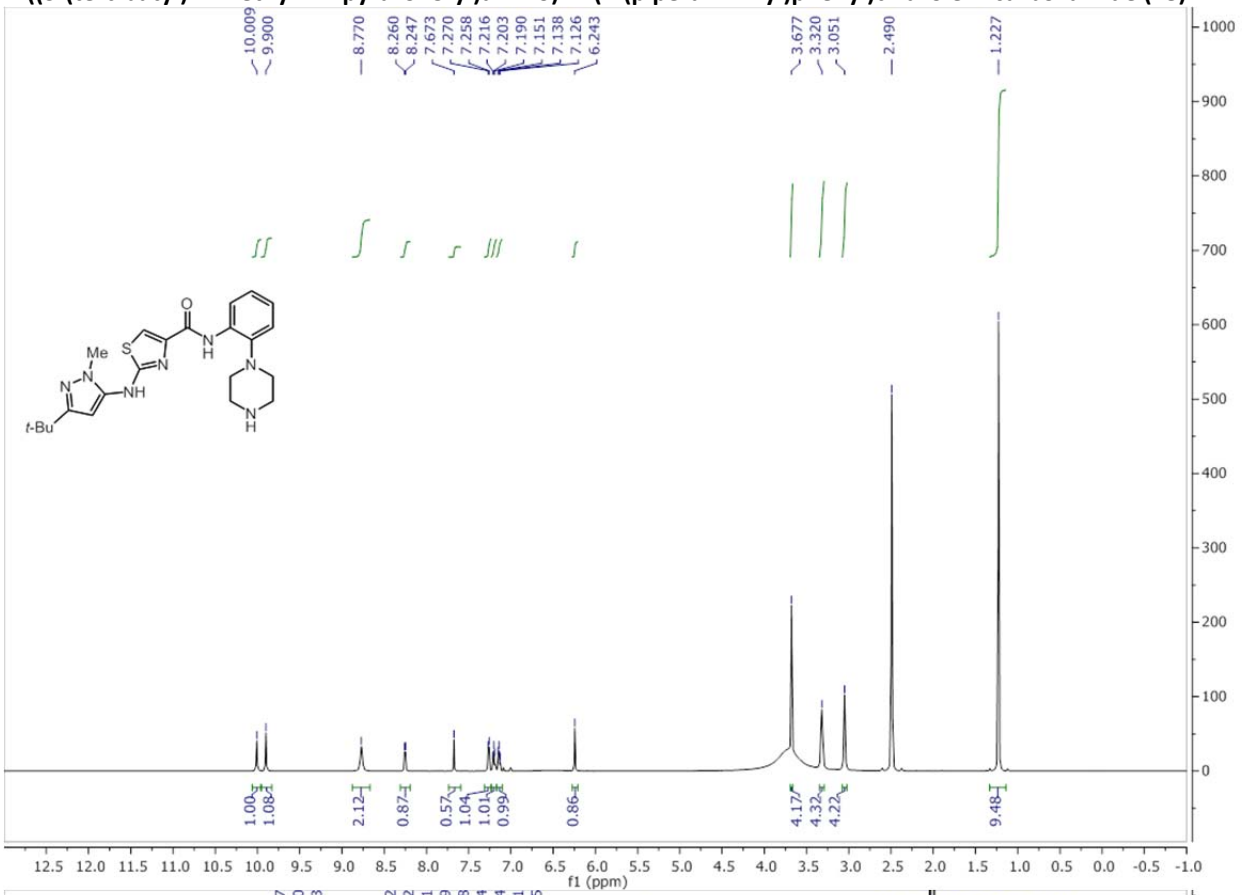


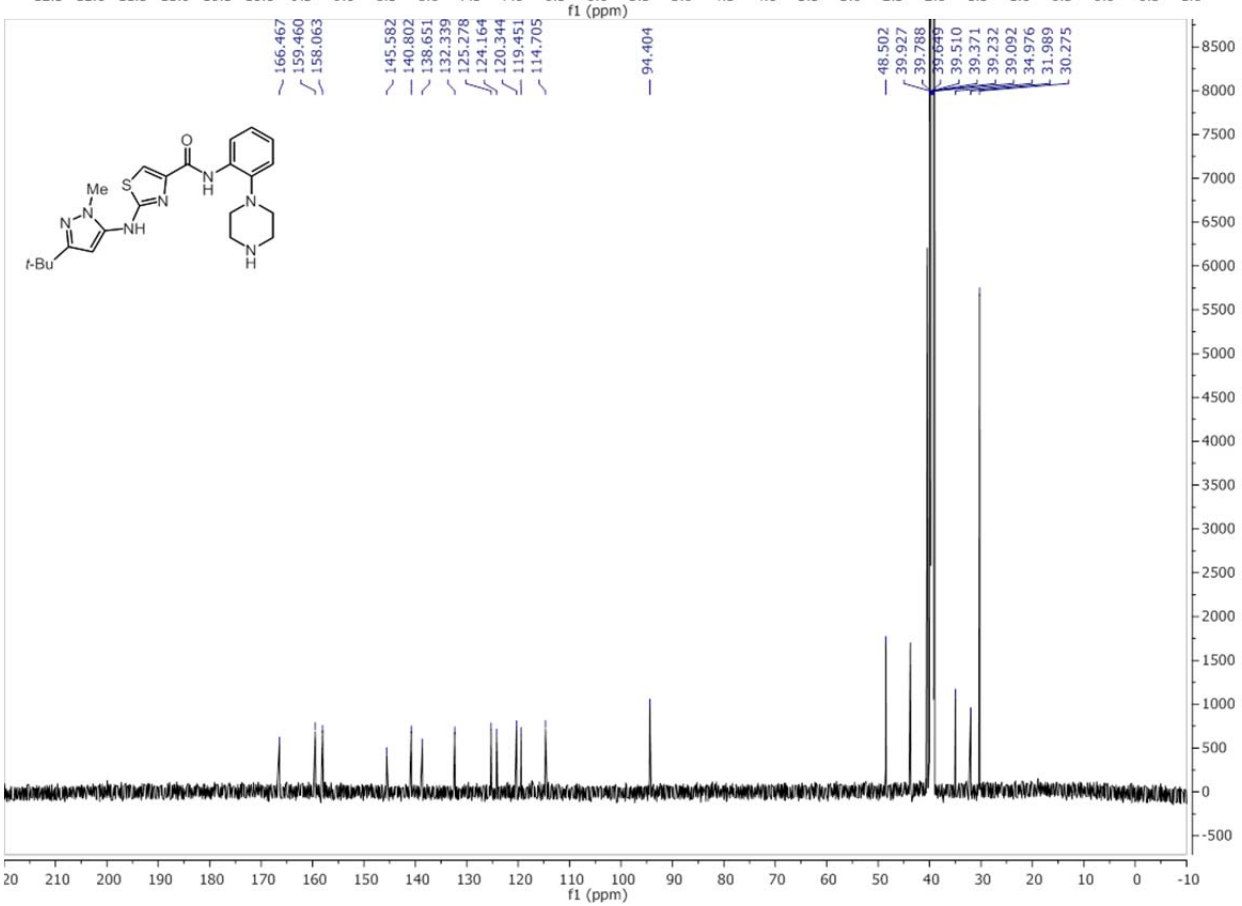
2-((2,3-dihydrobenzo[b][1,4]dioxin-6-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E7)



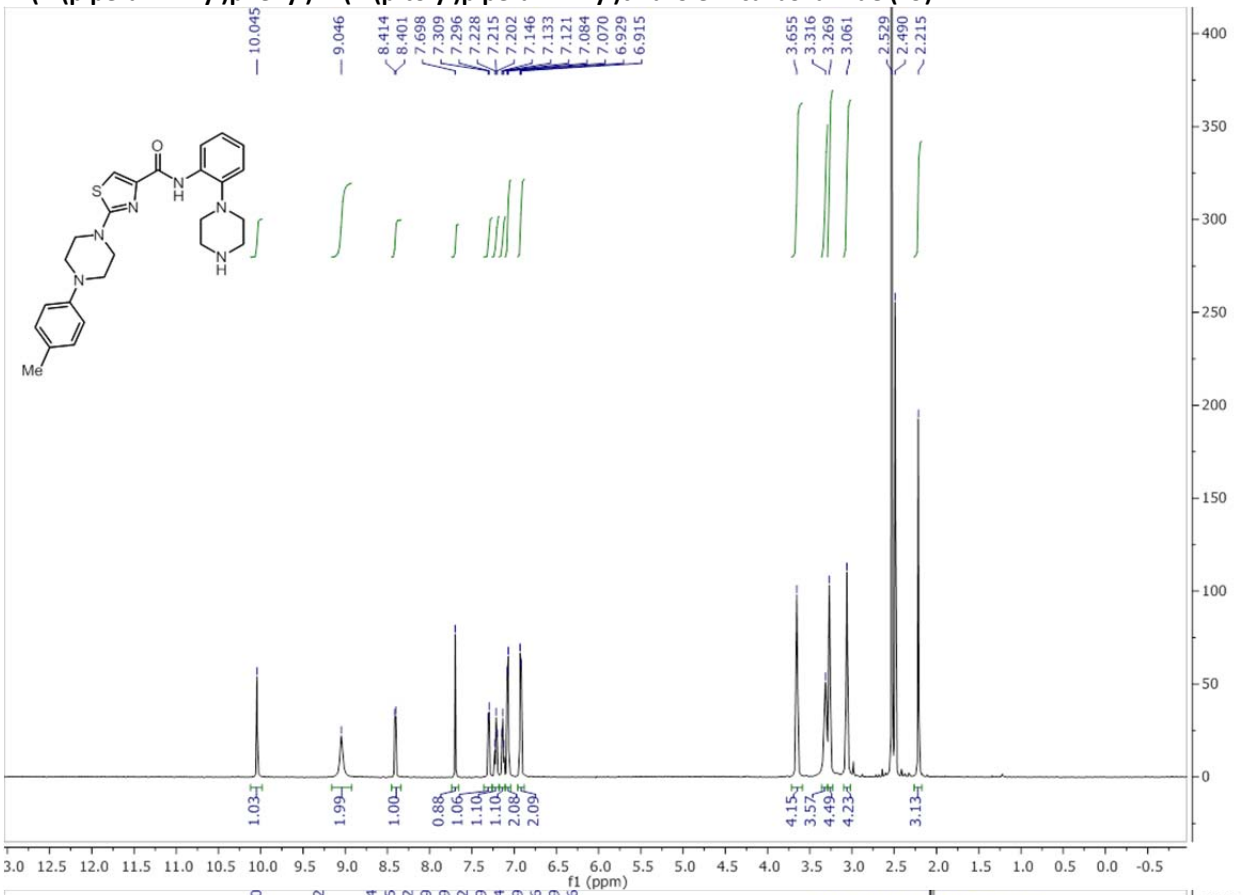


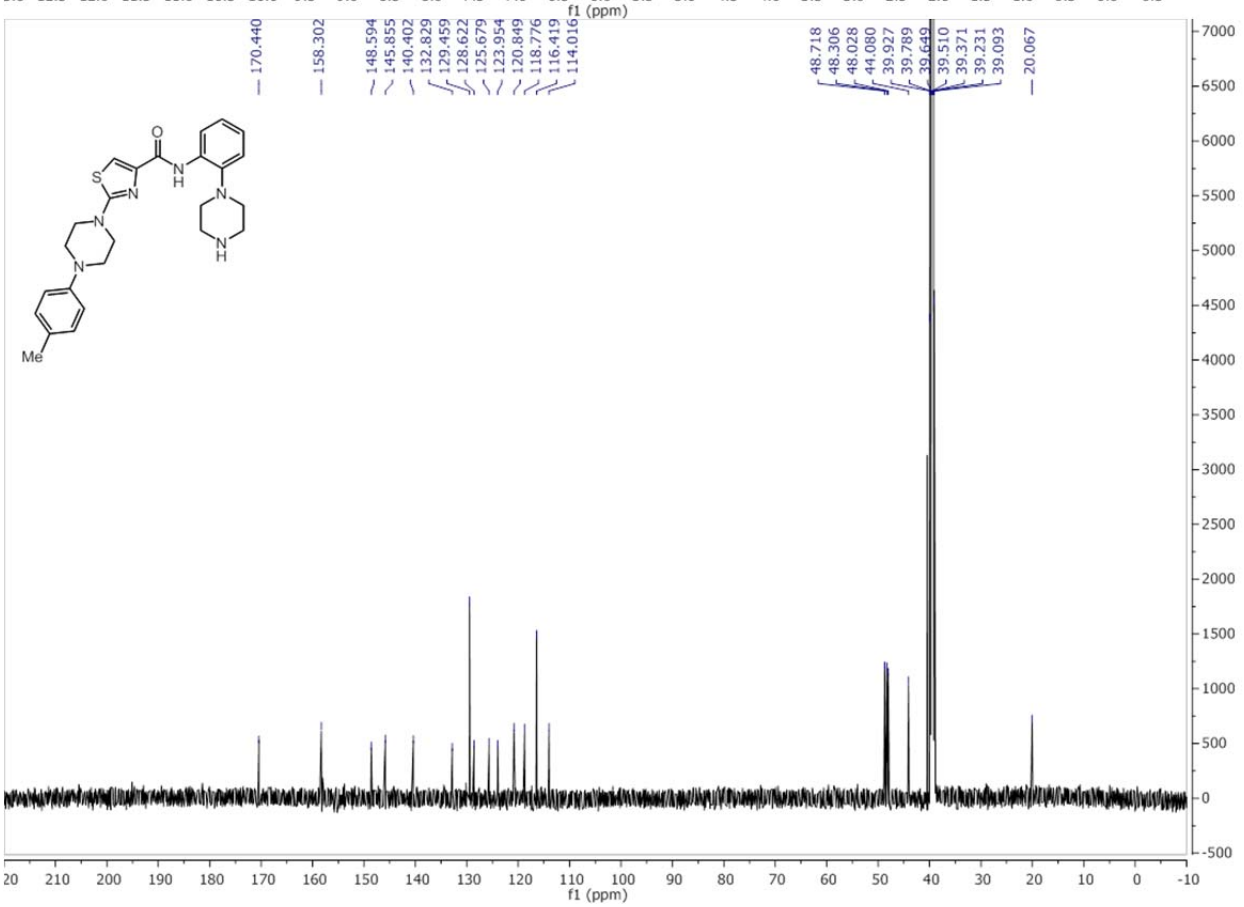
2-((3-(tert-butyl)-1-methyl-1H-pyrazol-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E8)



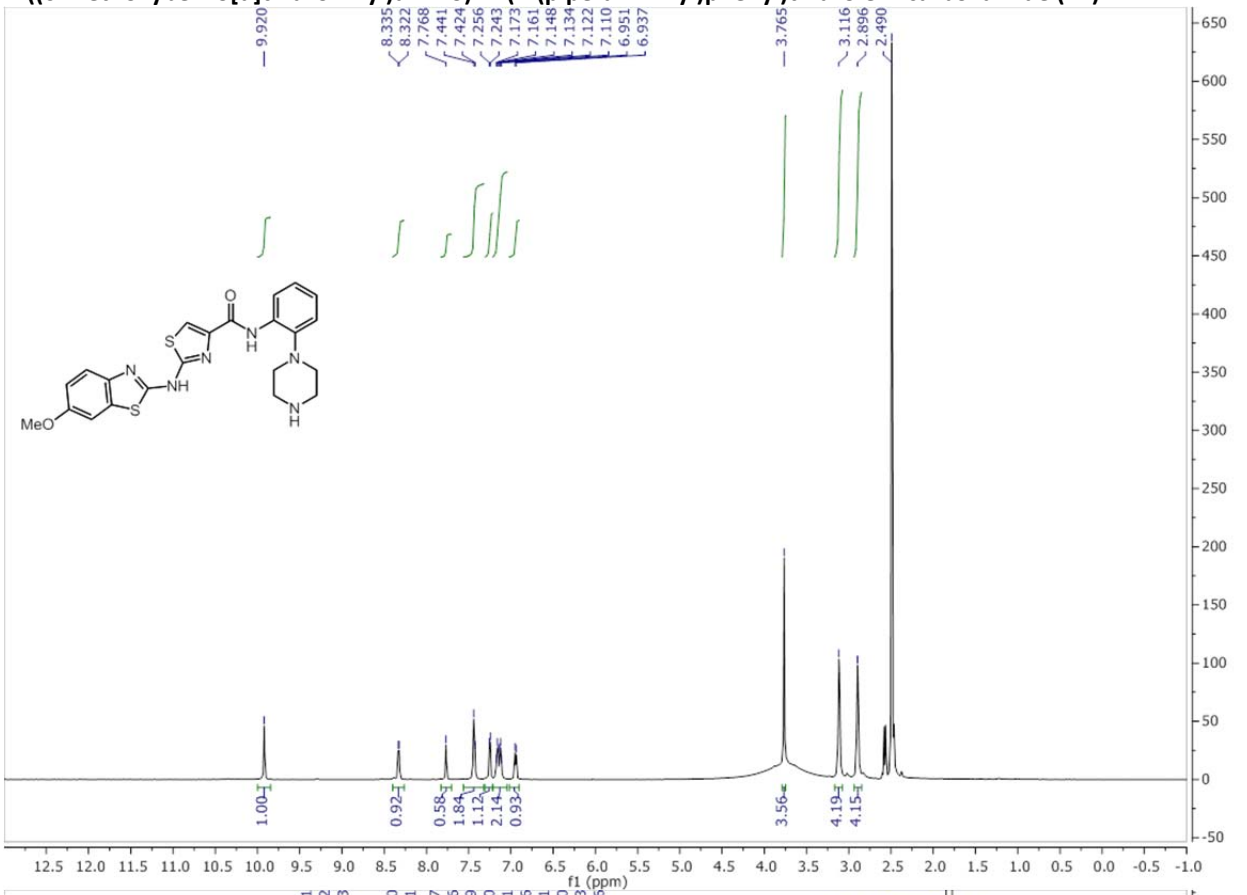


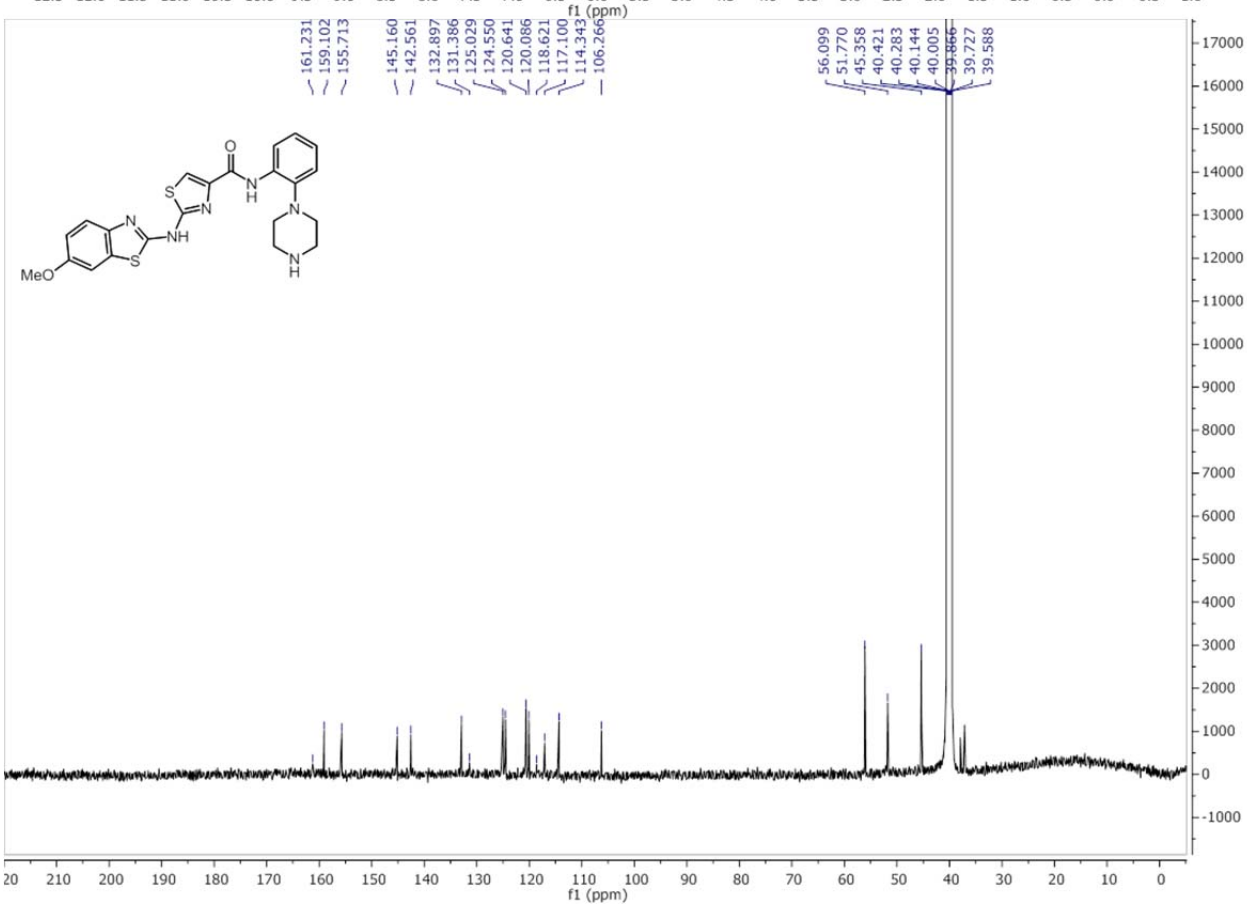
N-(2-(piperazin-1-yl)phenyl)-2-(4-(p-tolyl)piperazin-1-yl)thiazole-4-carboxamide (E9)



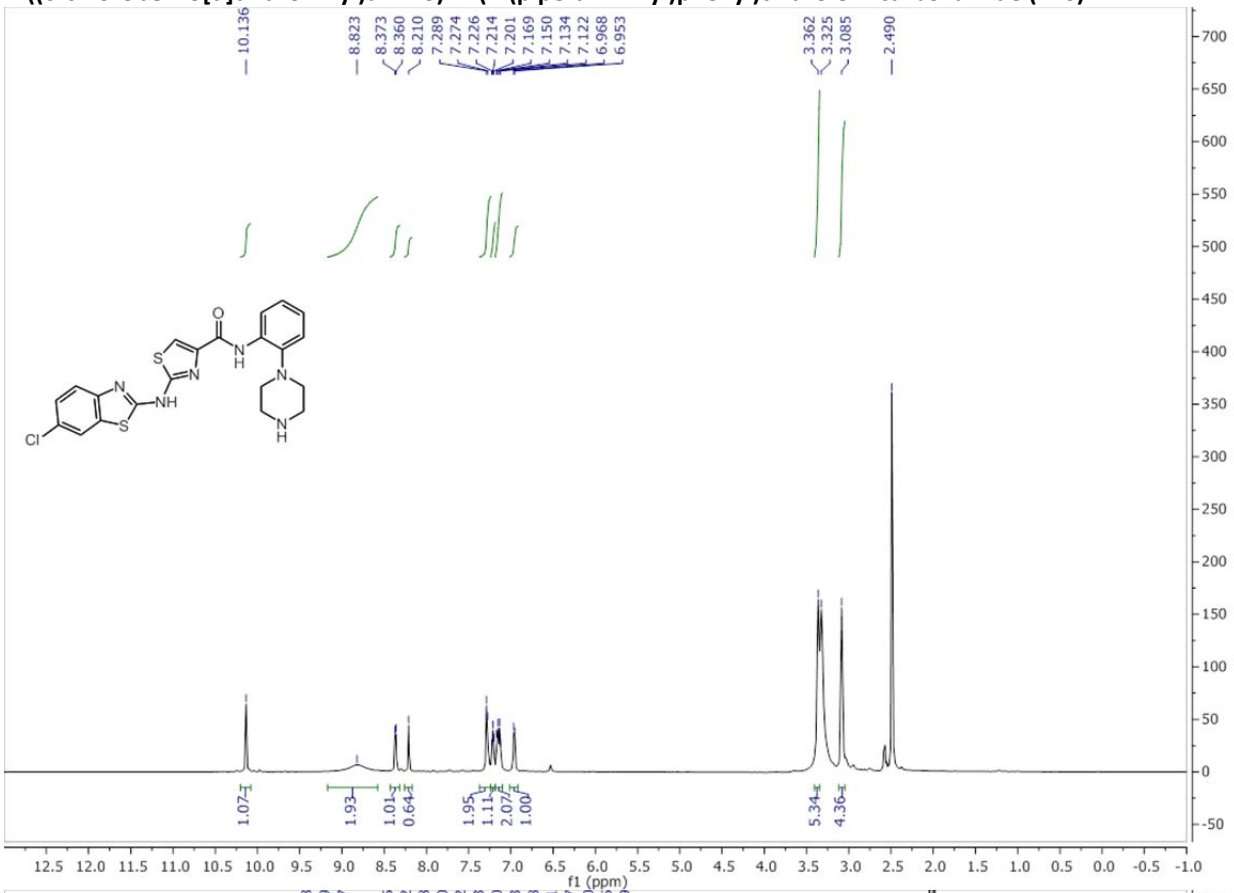


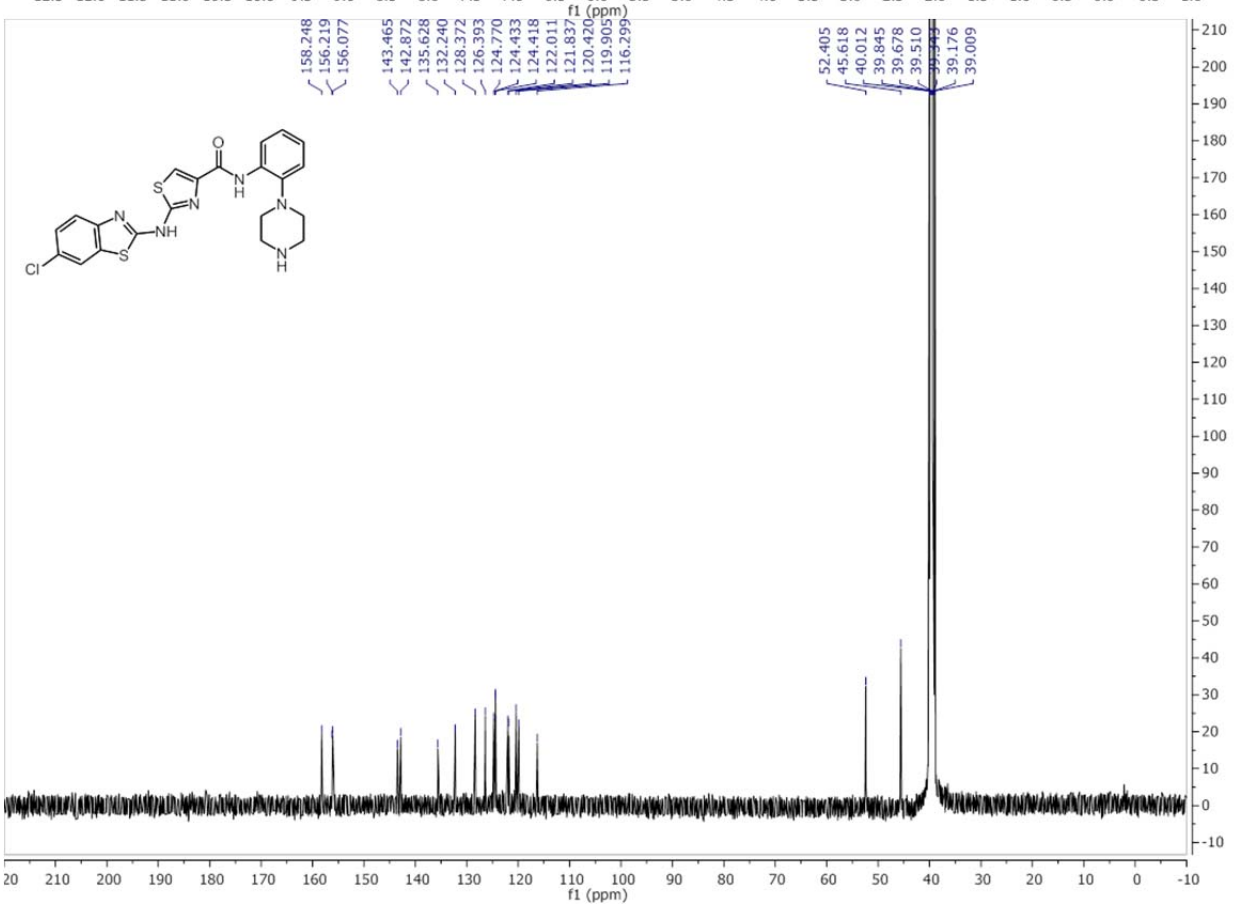
2-((6-methoxybenzo[d]thiazol-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (41)



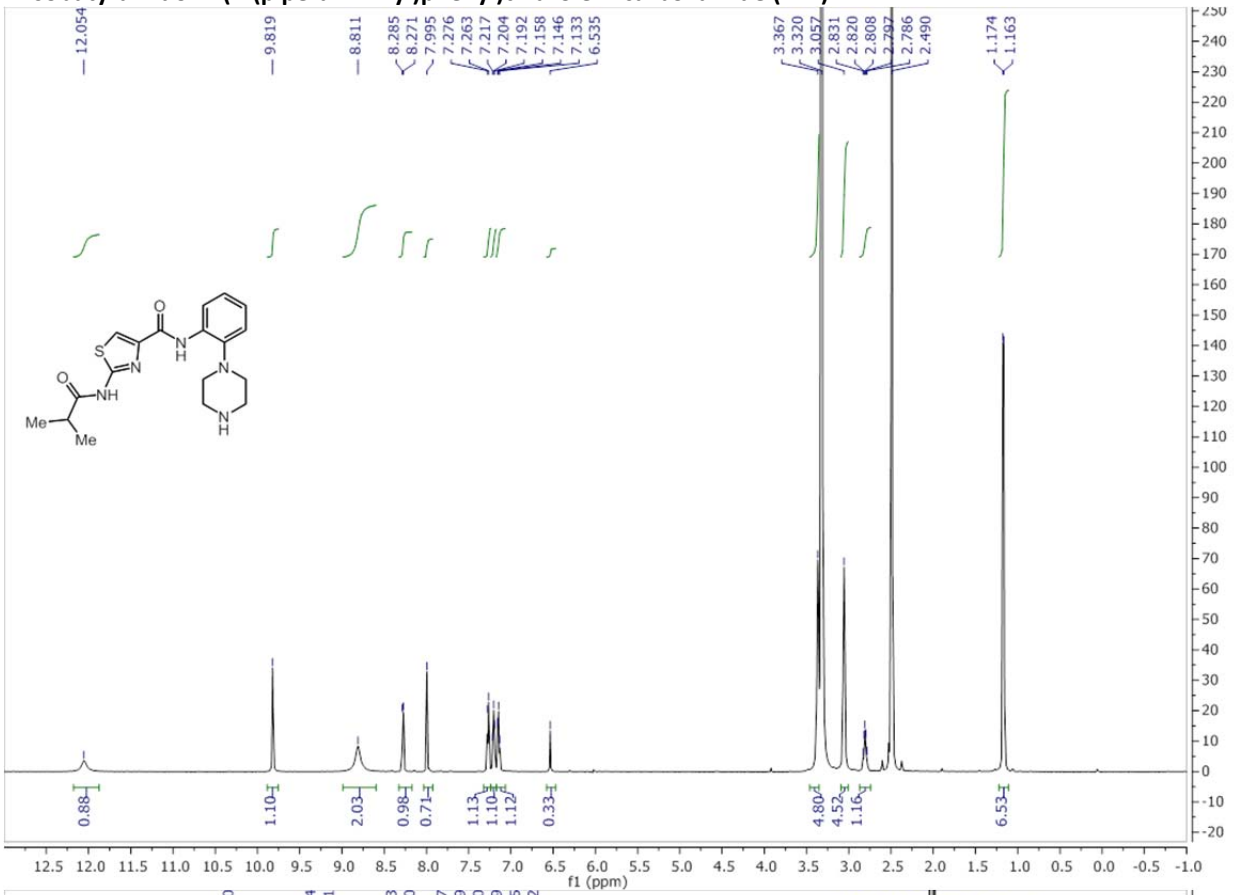


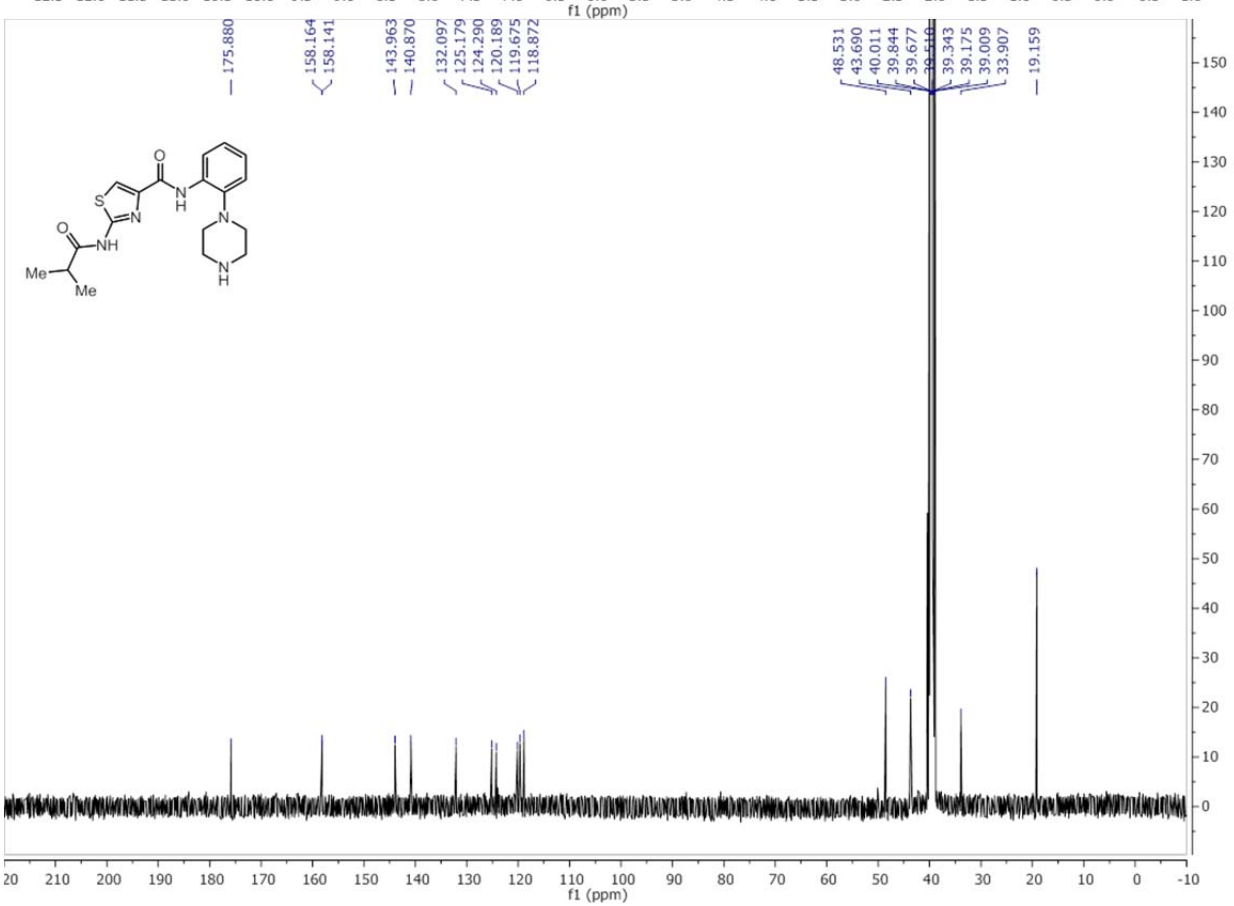
2-((6-chlorobenzo[d]thiazol-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E10)



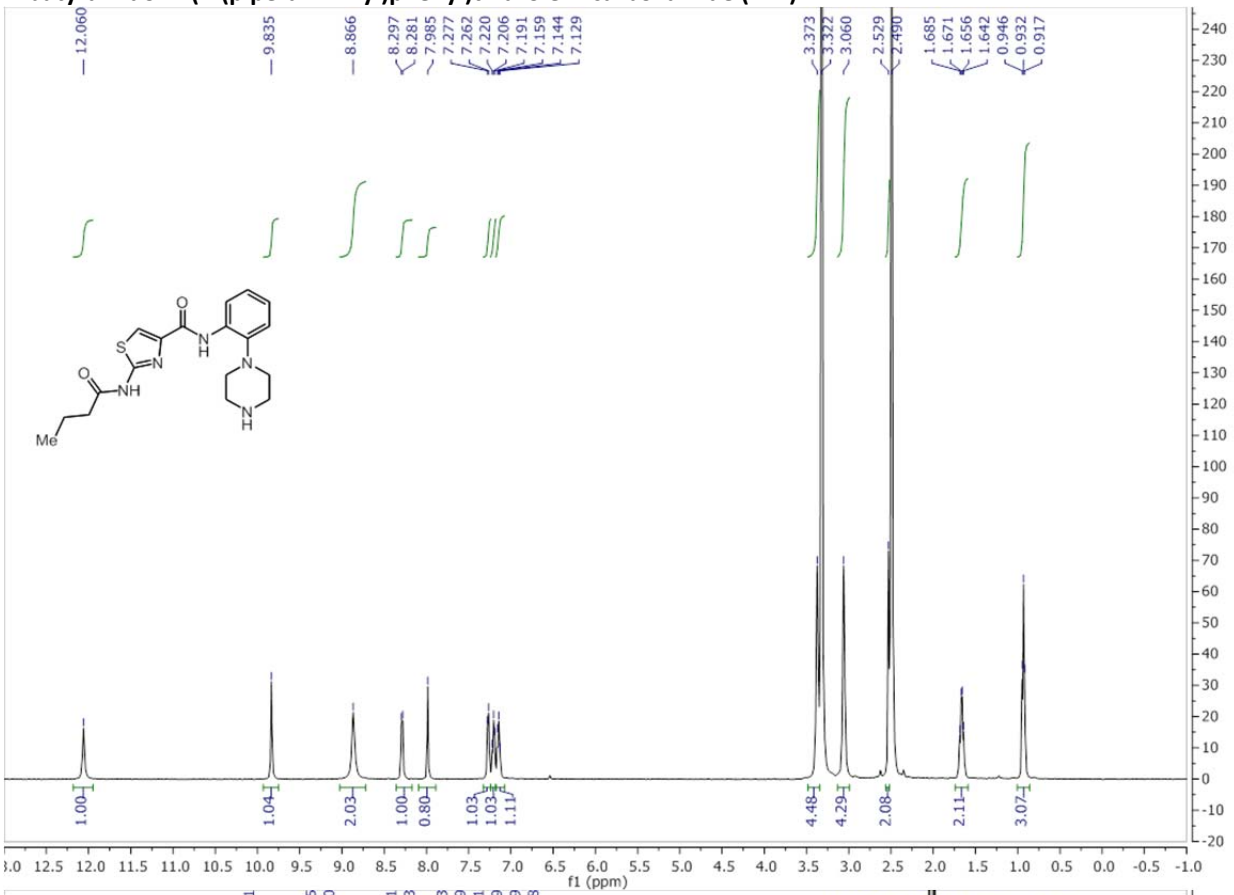


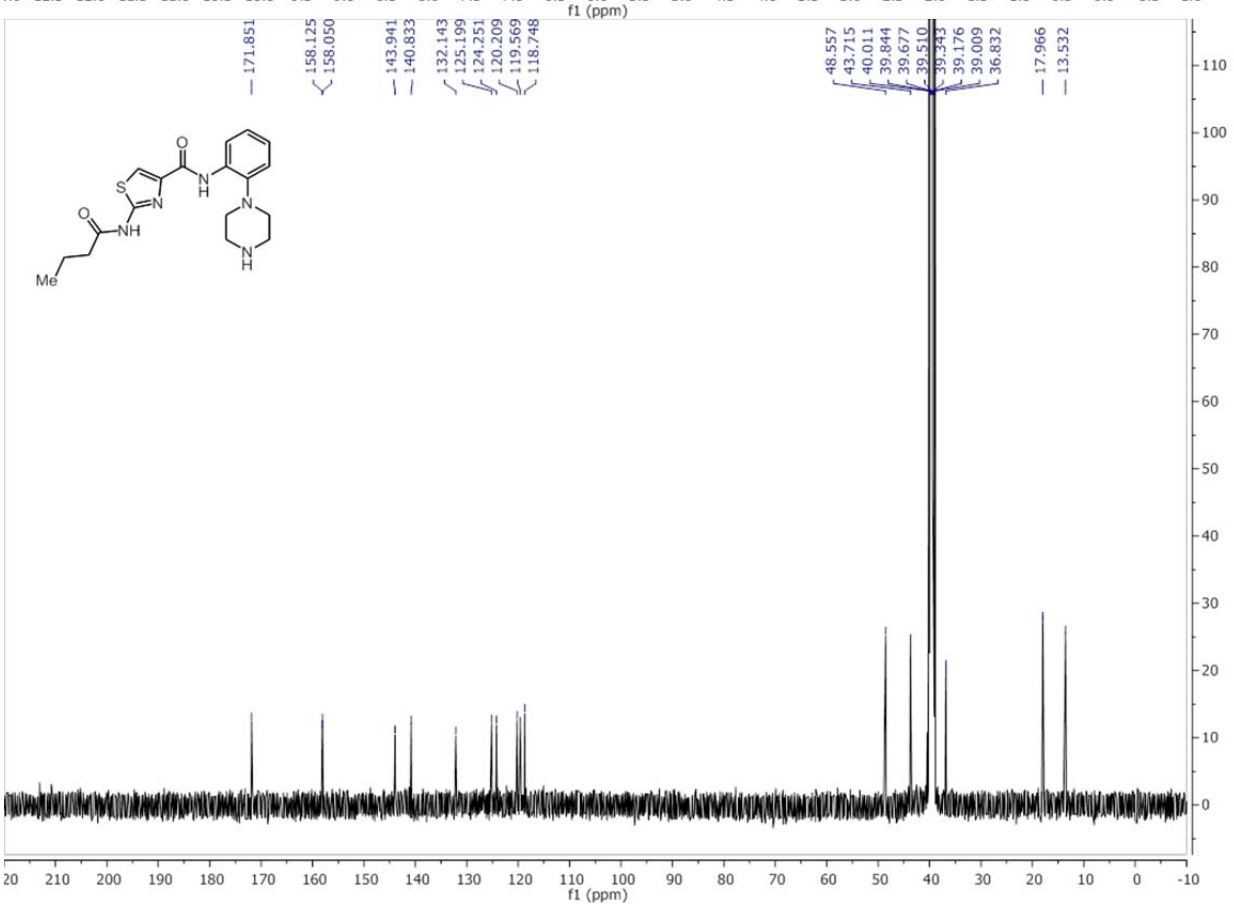
2-isobutyramido-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E11)



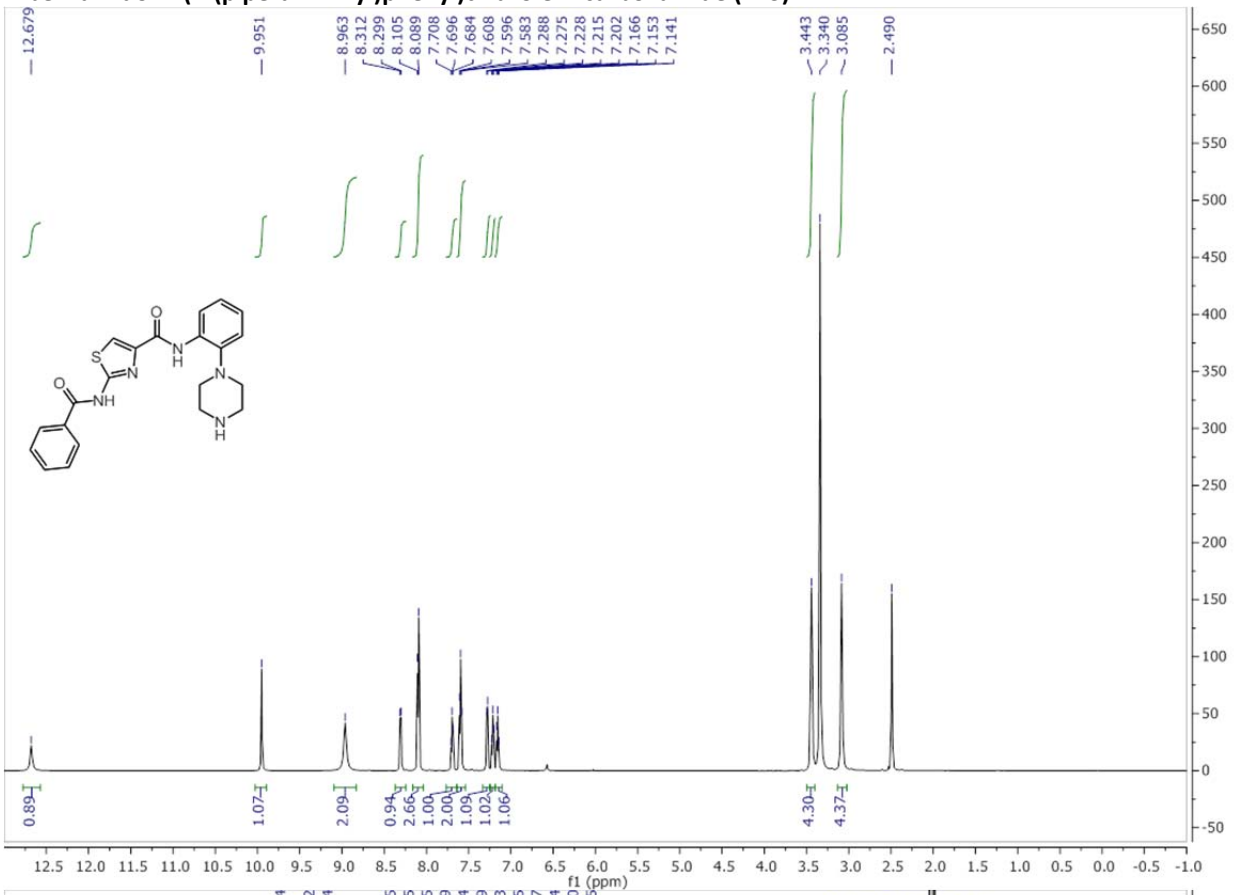


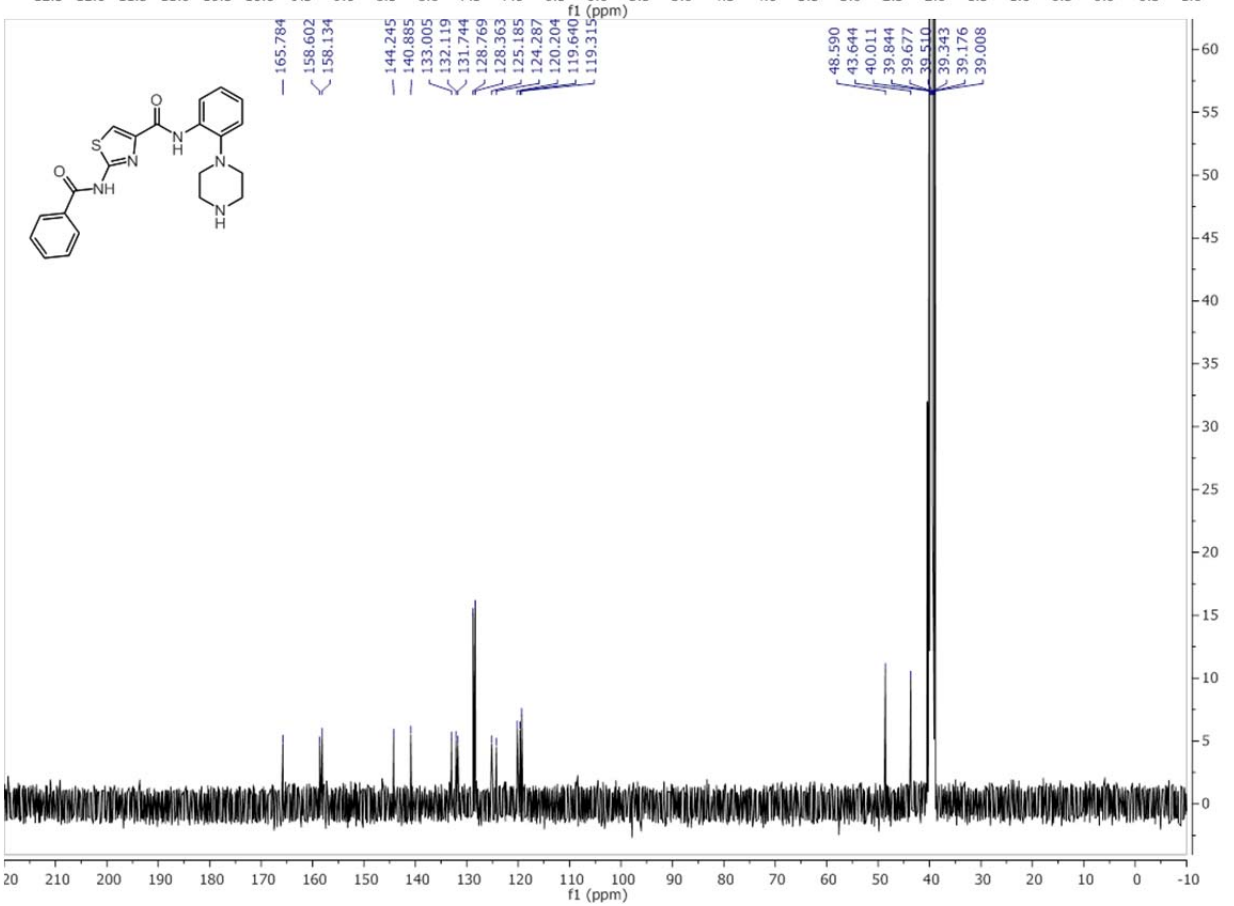
2-butyramido-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E12)



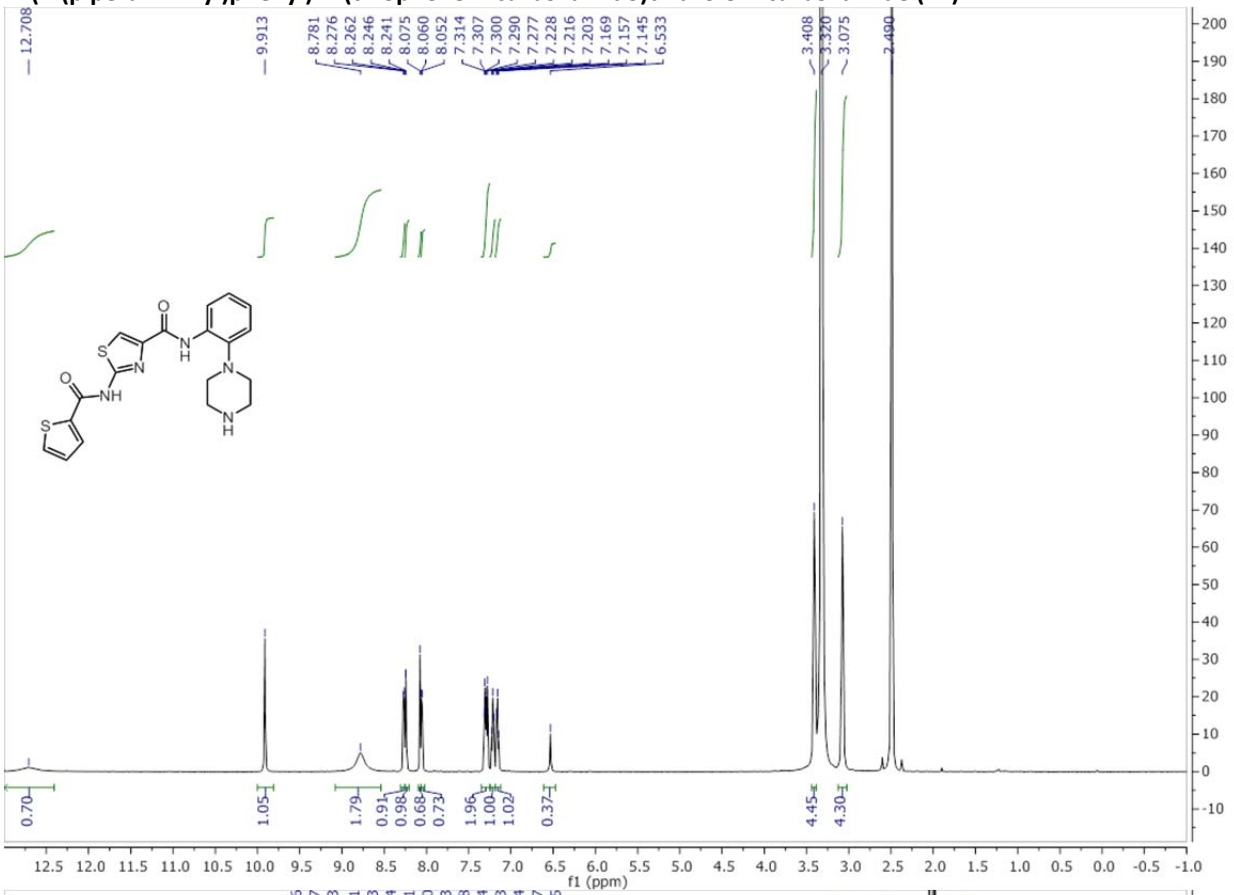


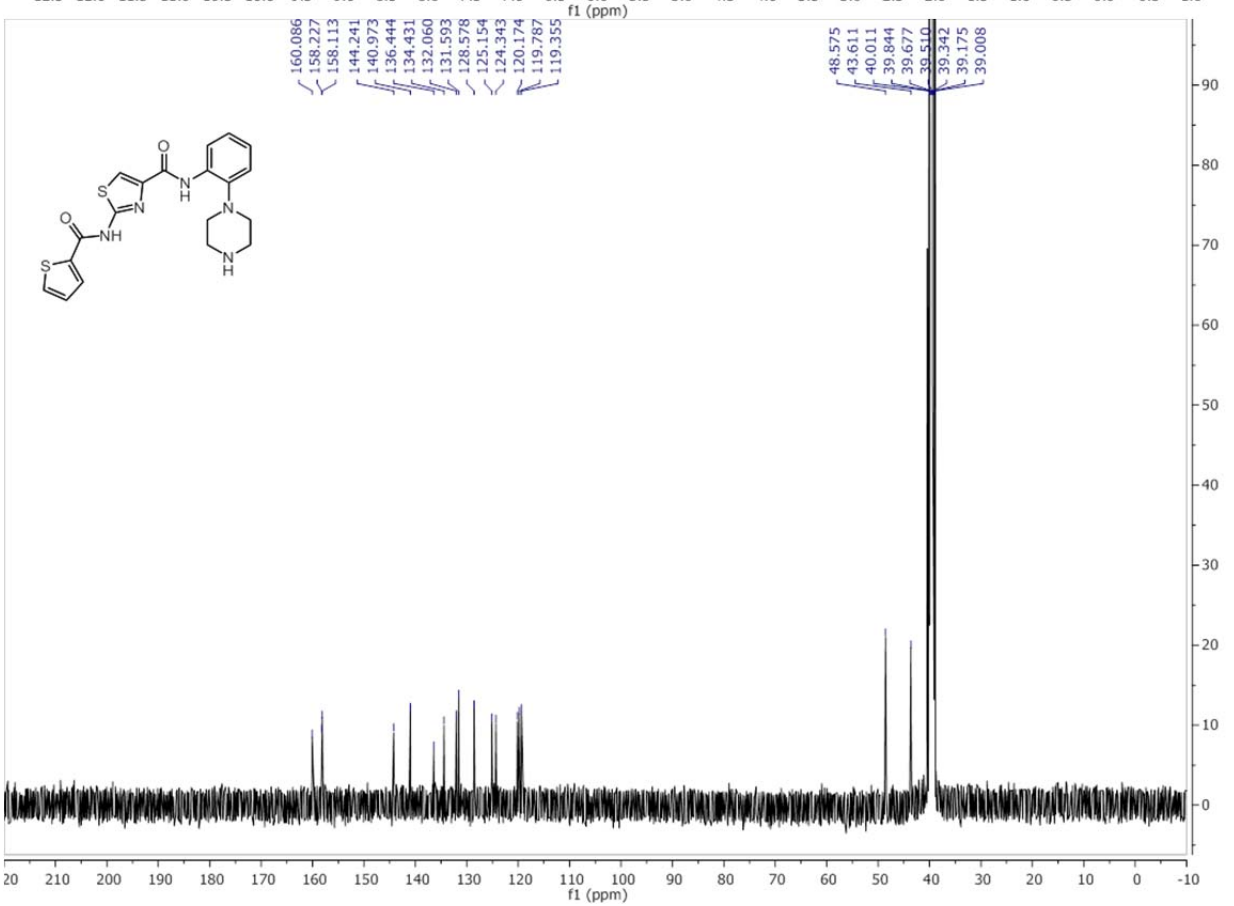
2-benzamido-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E13)



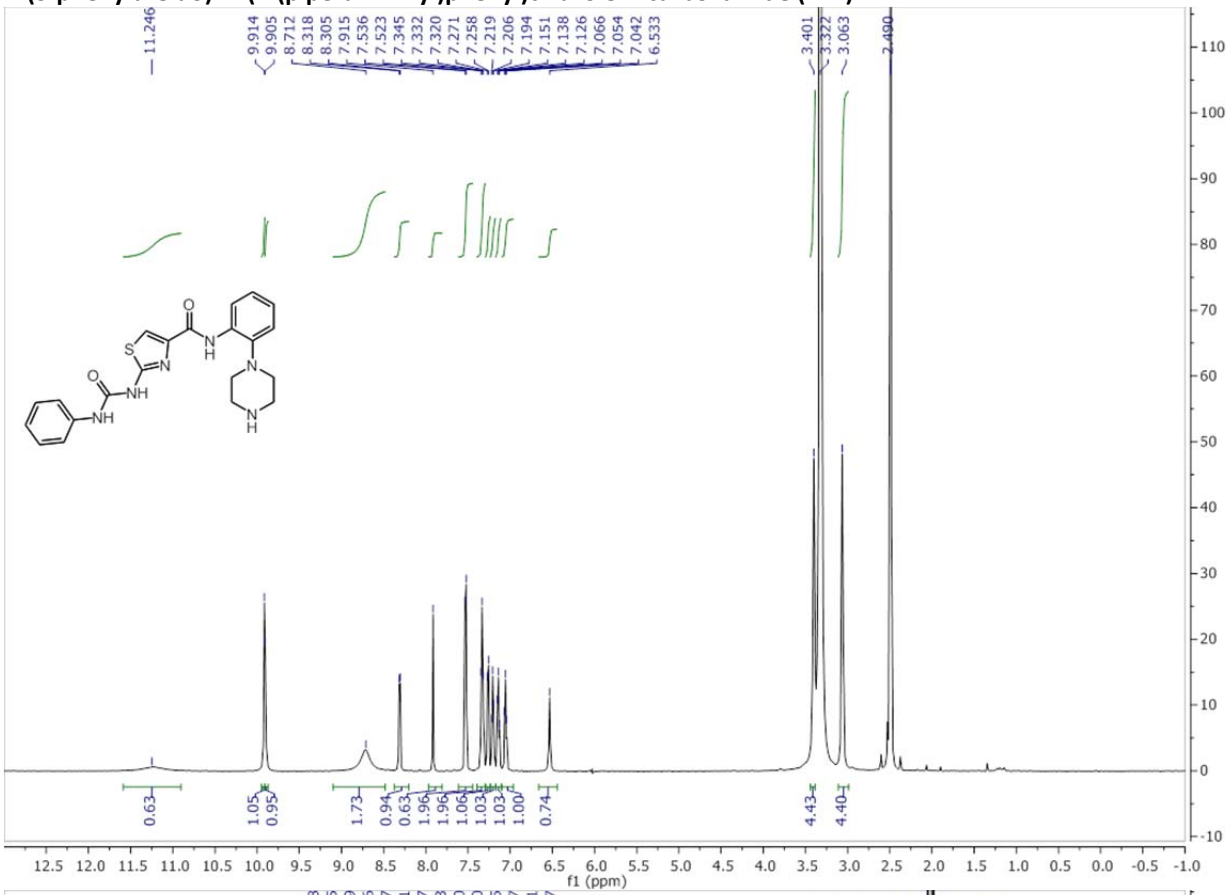


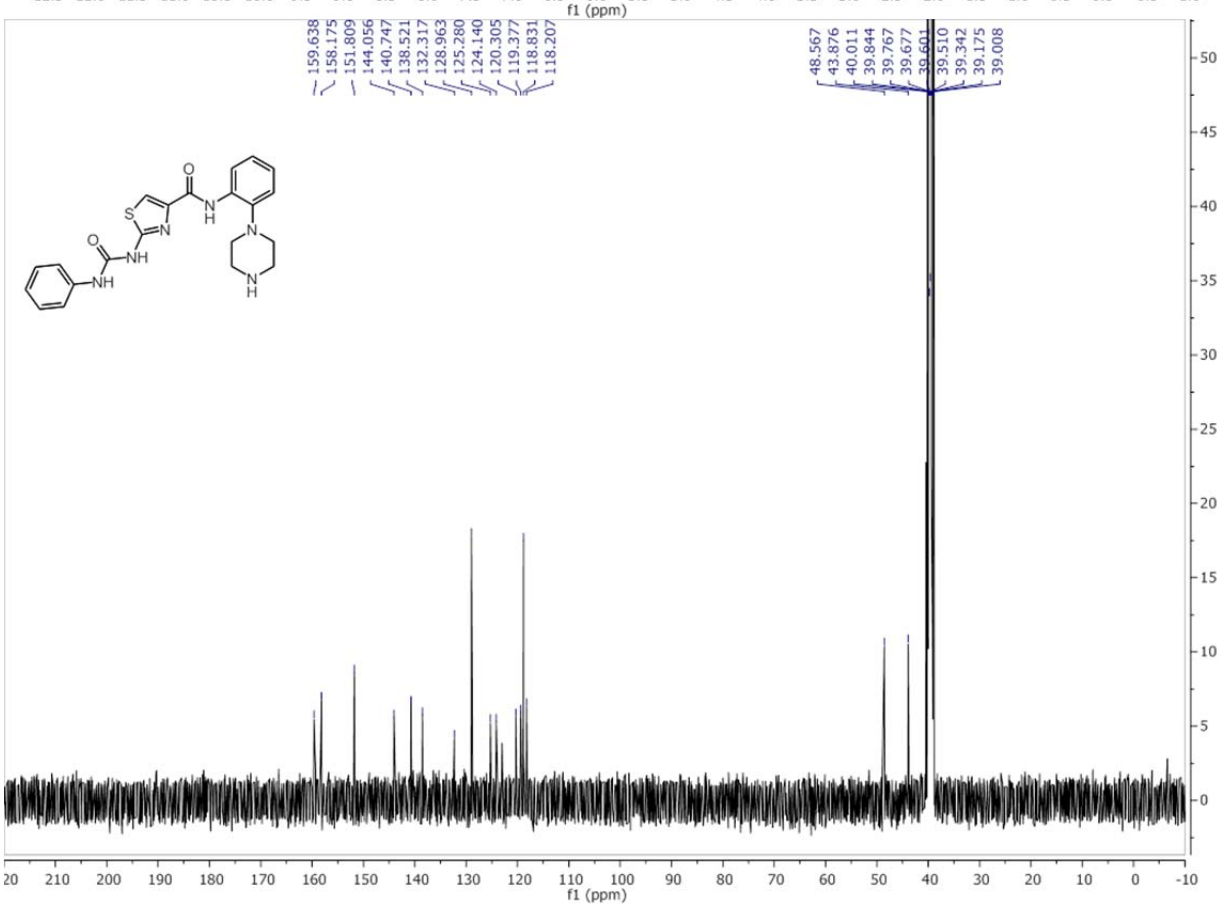
N-(2-(piperazin-1-yl)phenyl)-2-(thiophene-2-carboxamido)thiazole-4-carboxamide (42)



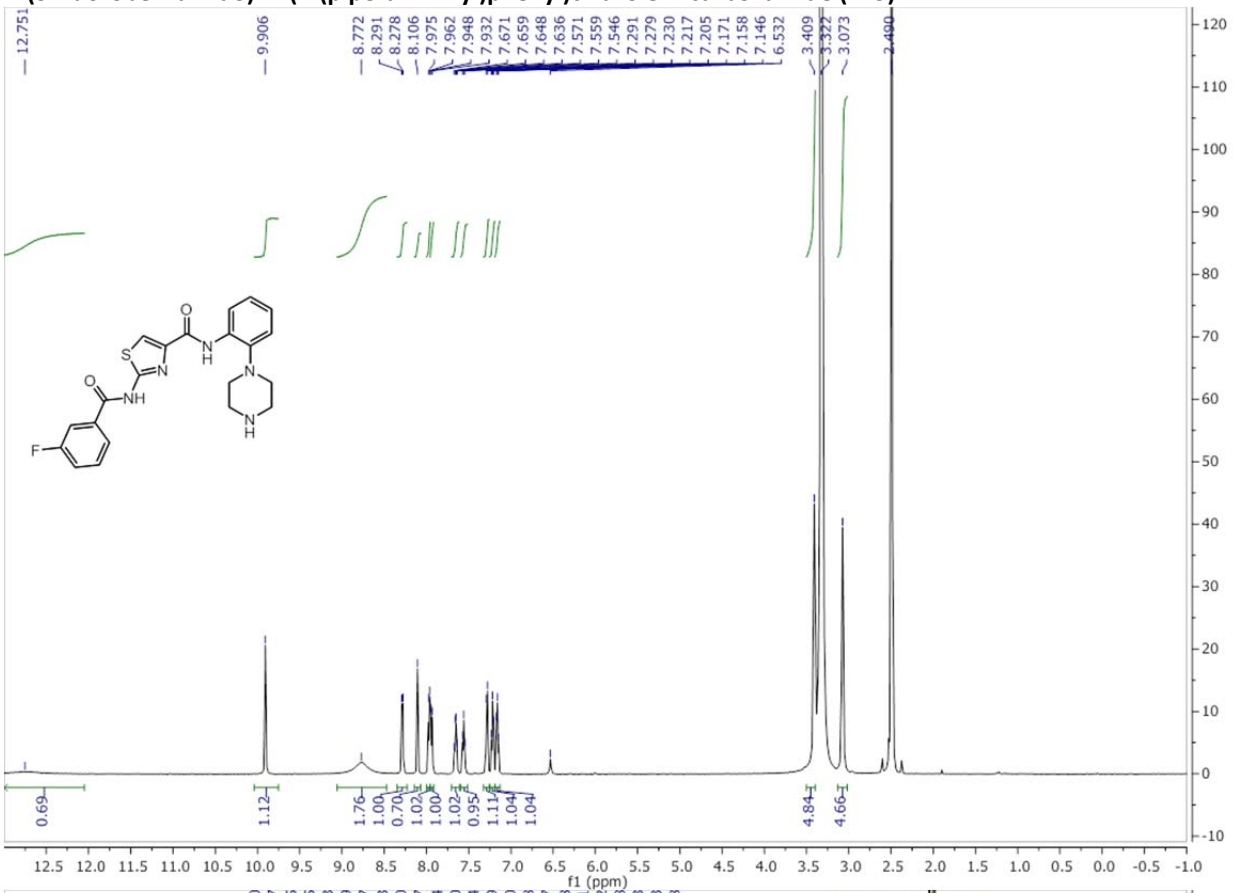


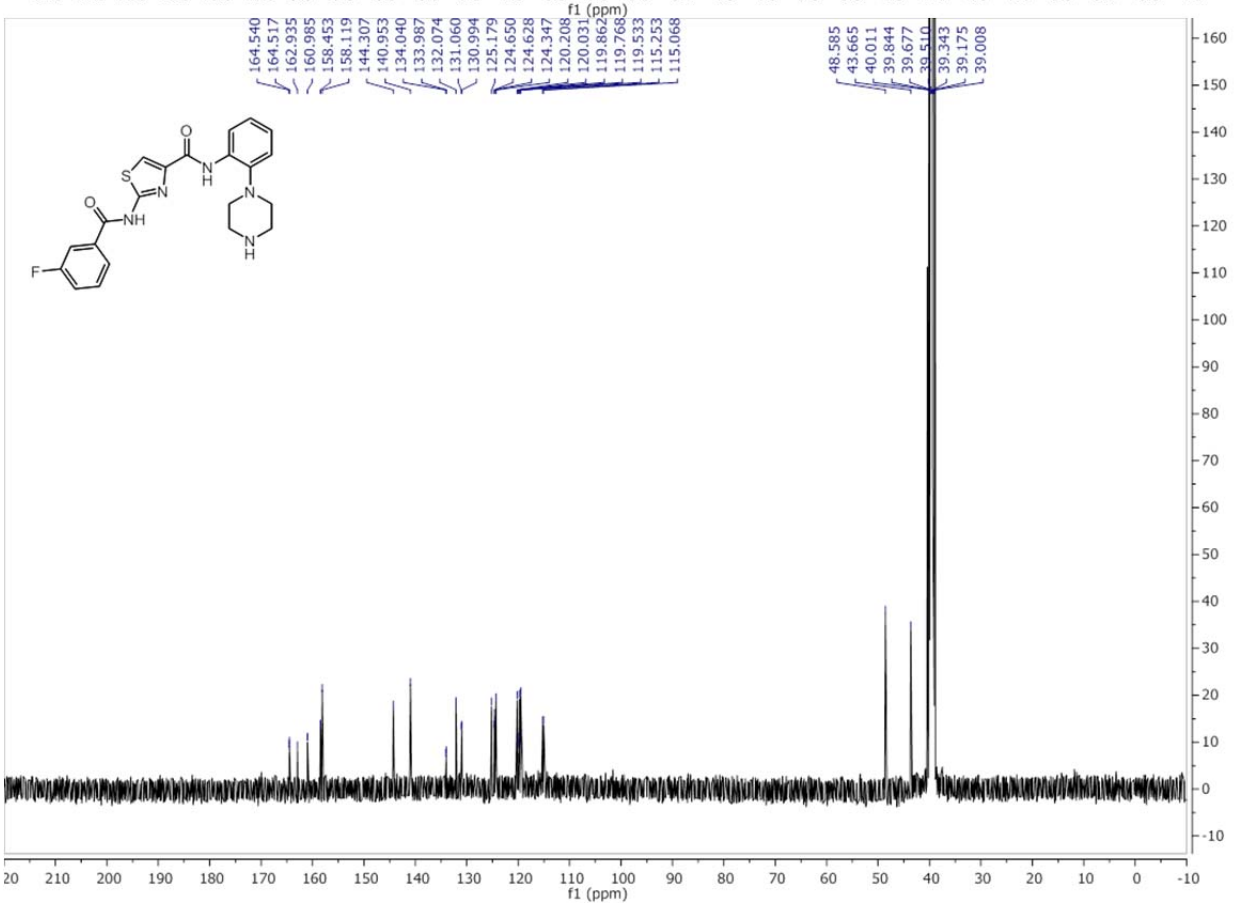
2-(3-phenylureido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E14)



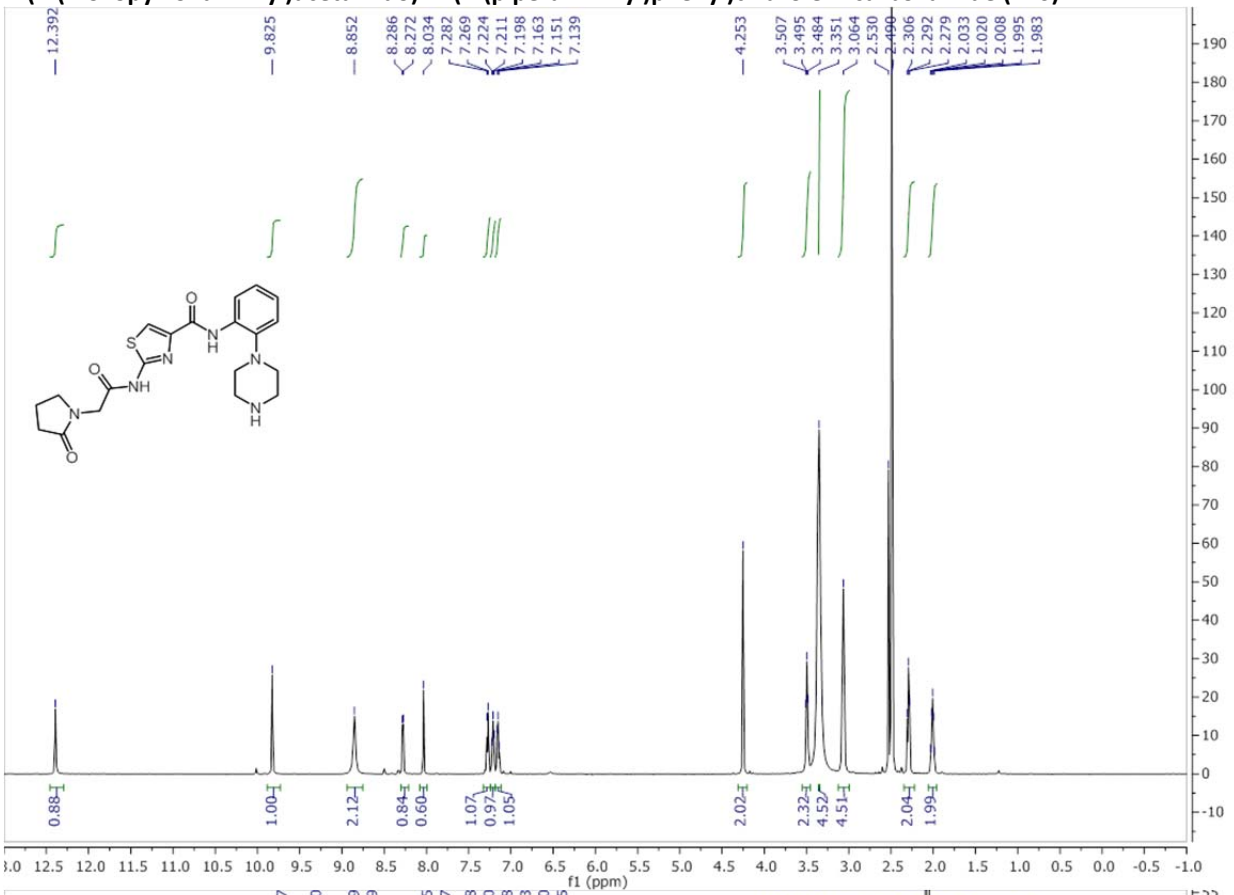


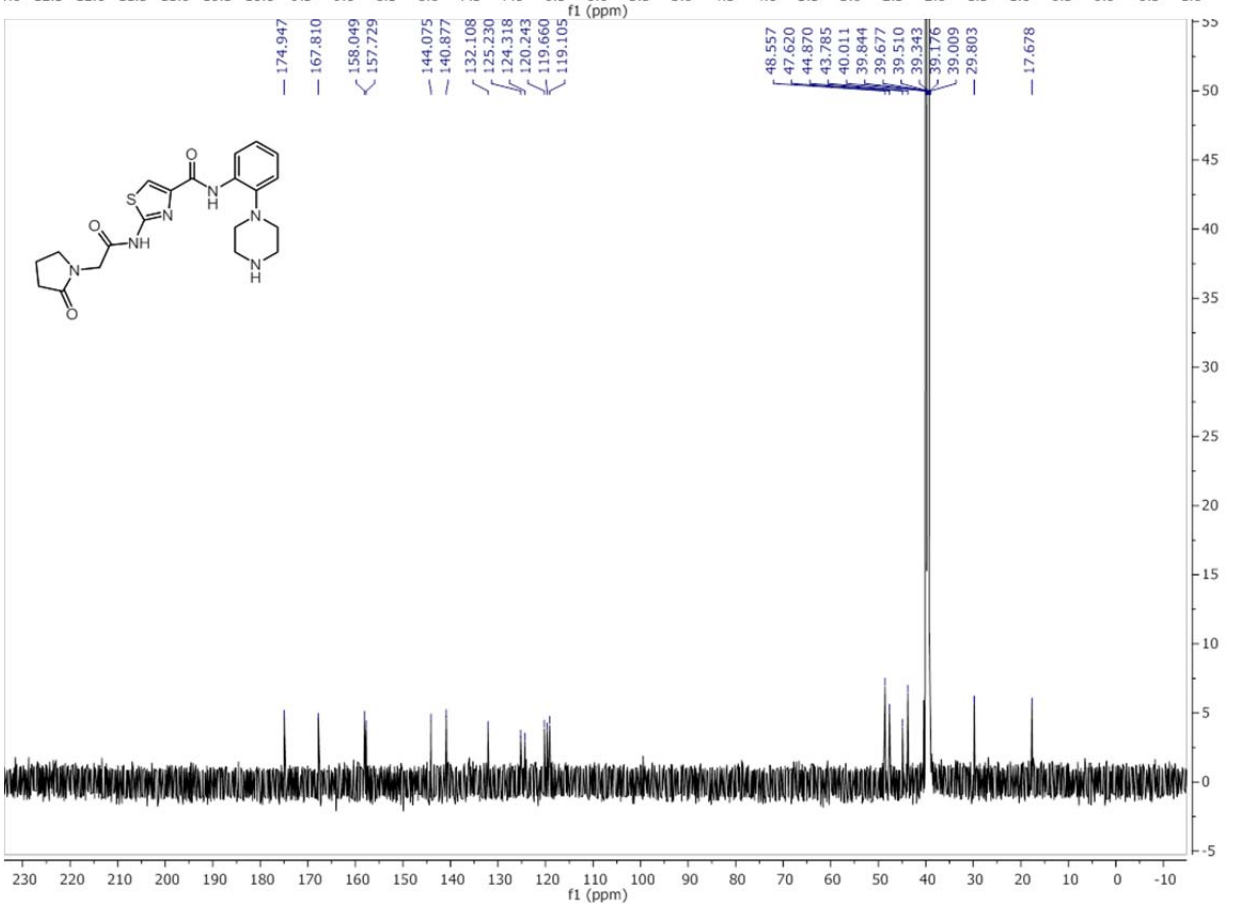
2-(3-fluorobenzamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E15)



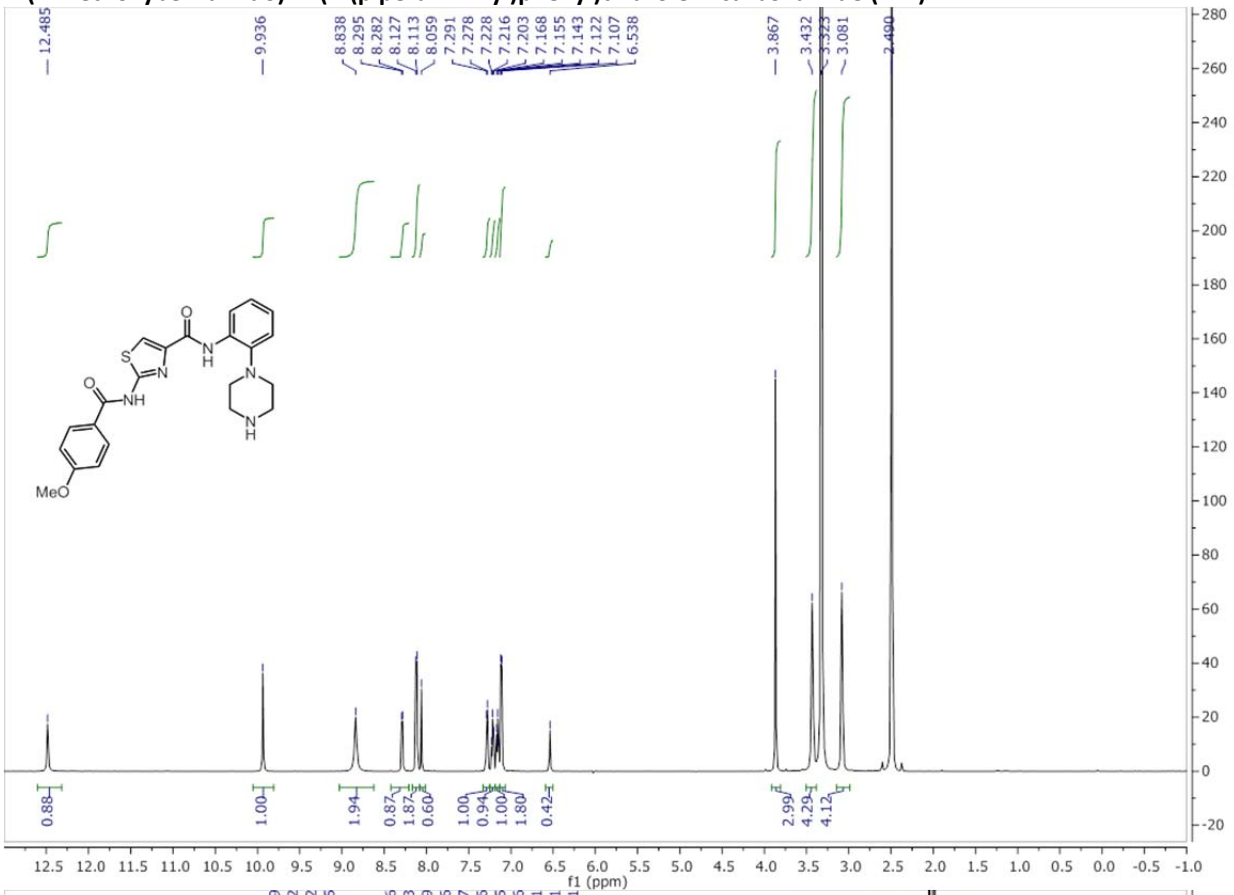


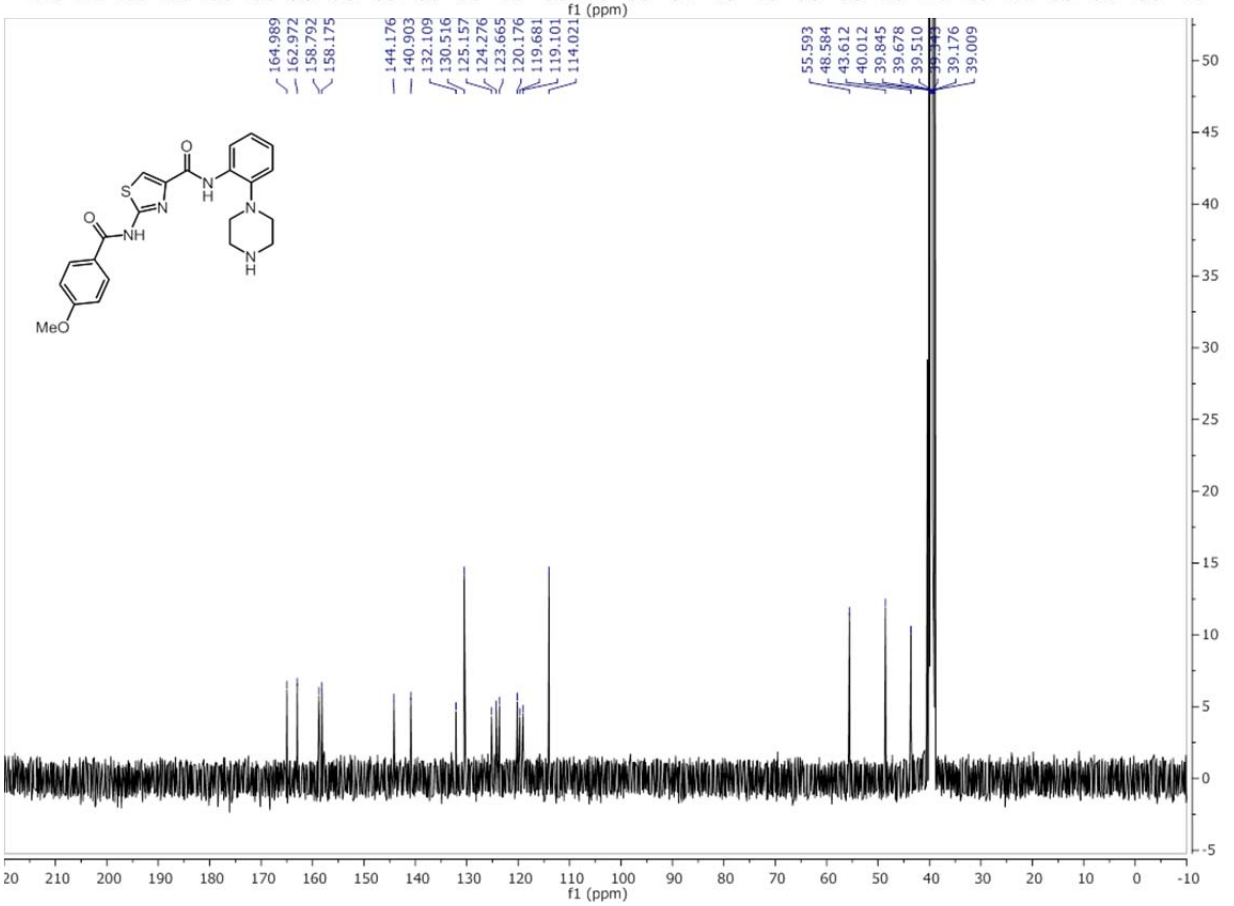
2-(2-(2-oxopyrrolidin-1-yl)acetamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E16)



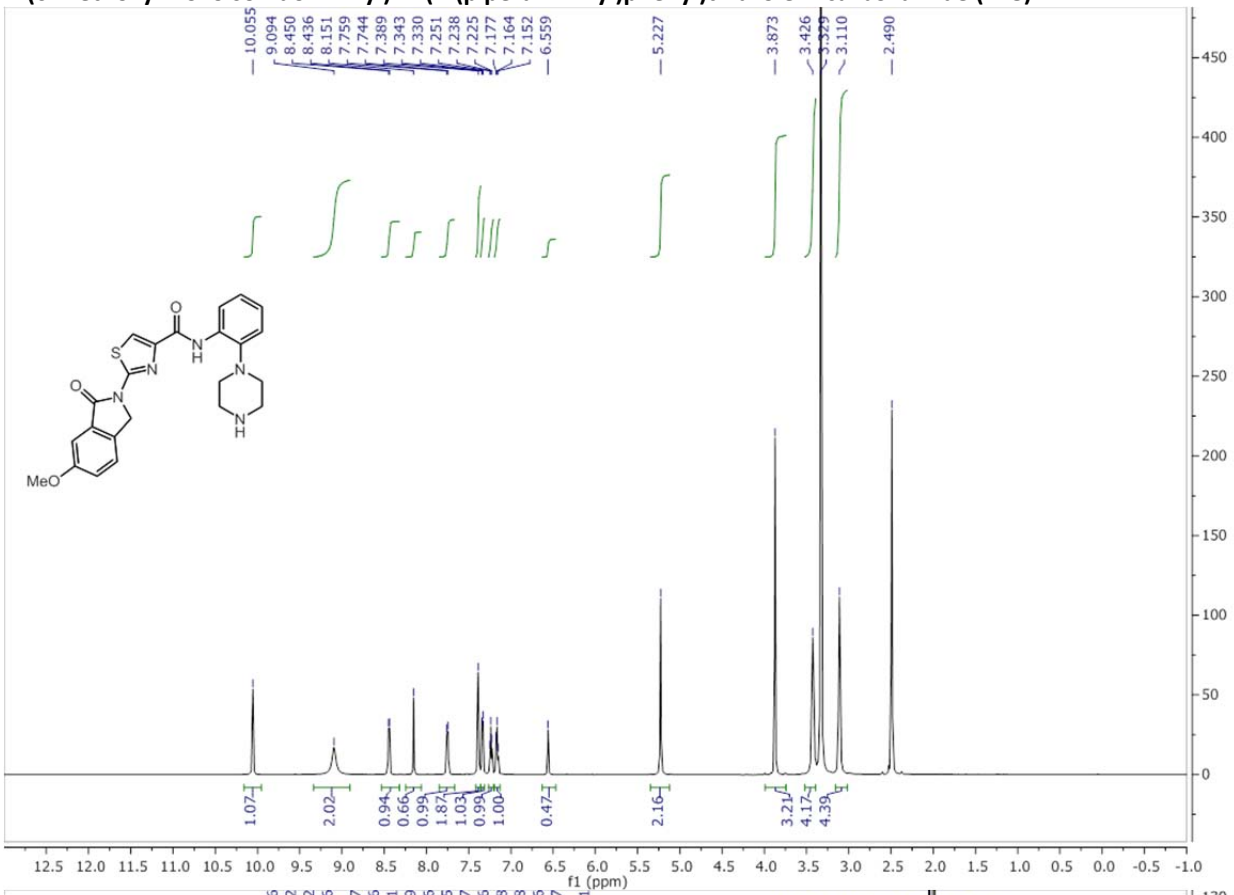


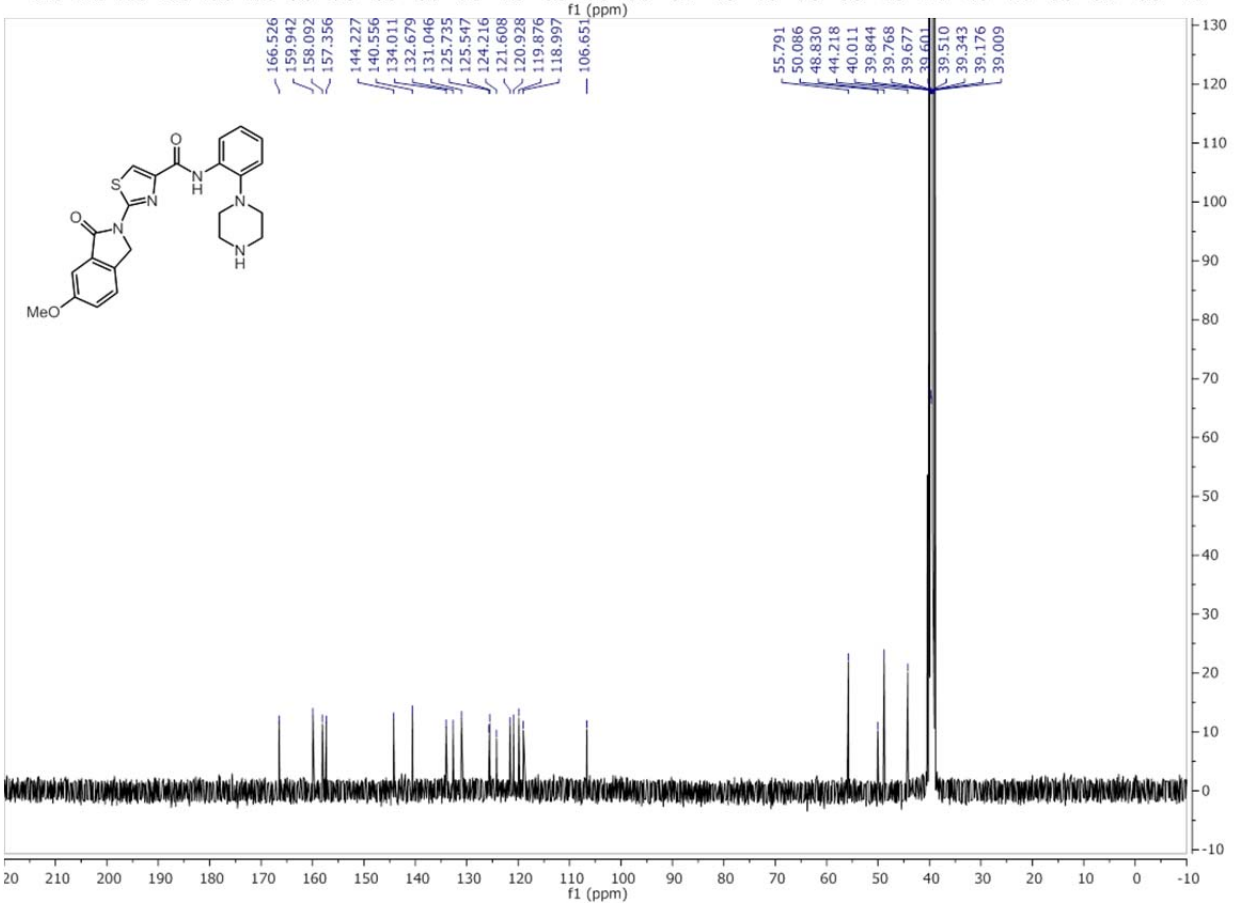
2-(4-methoxybenzamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E17)



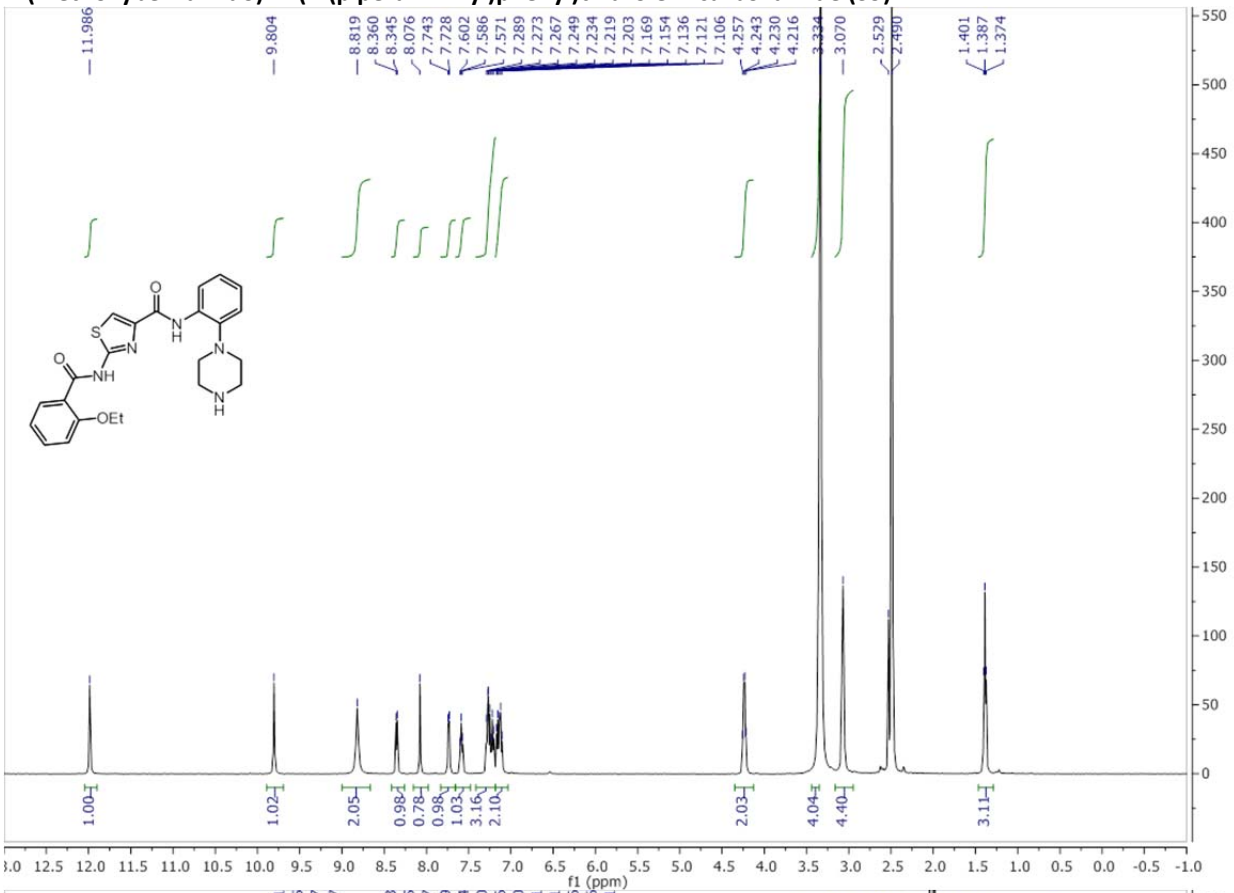


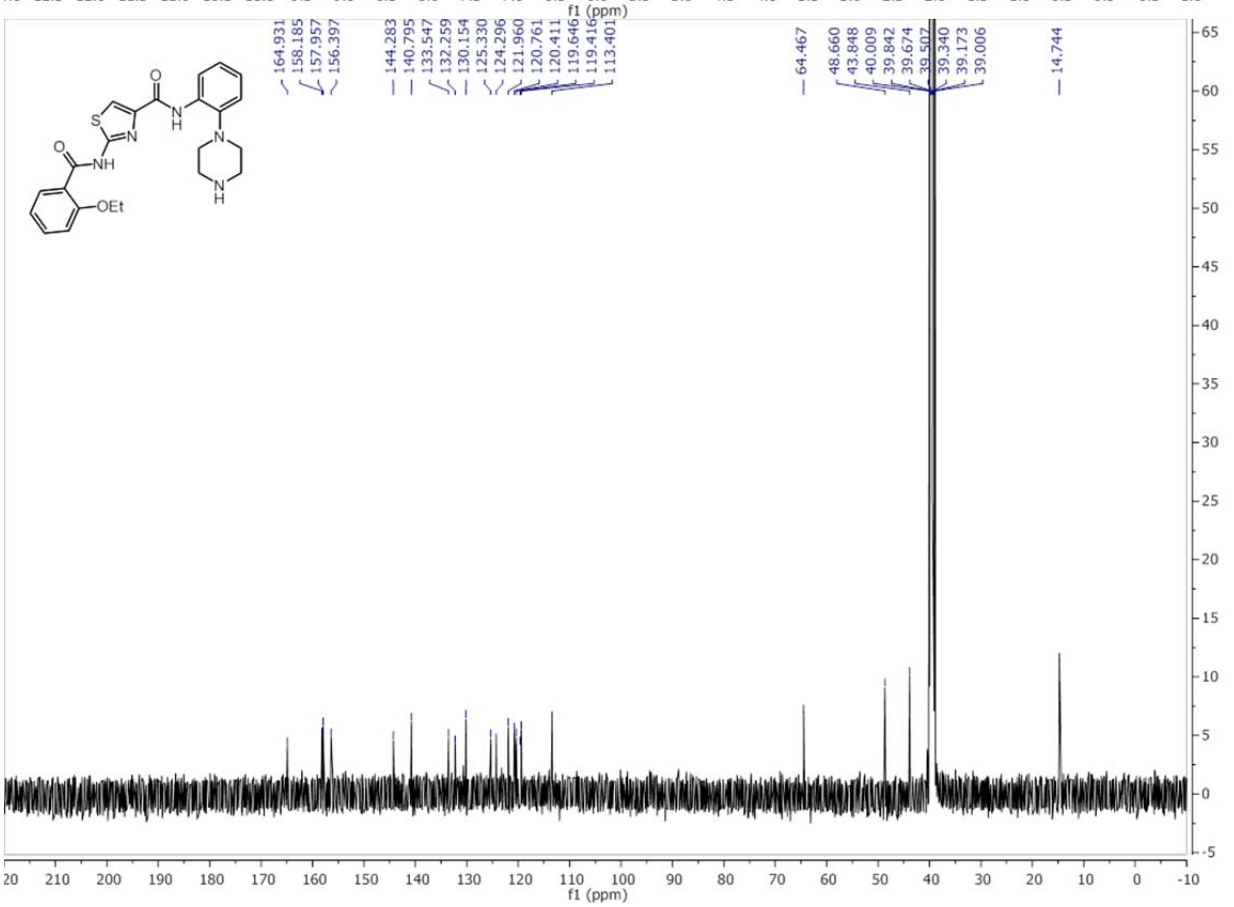
2-(6-methoxy-1-oxoisoindolin-2-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E18)



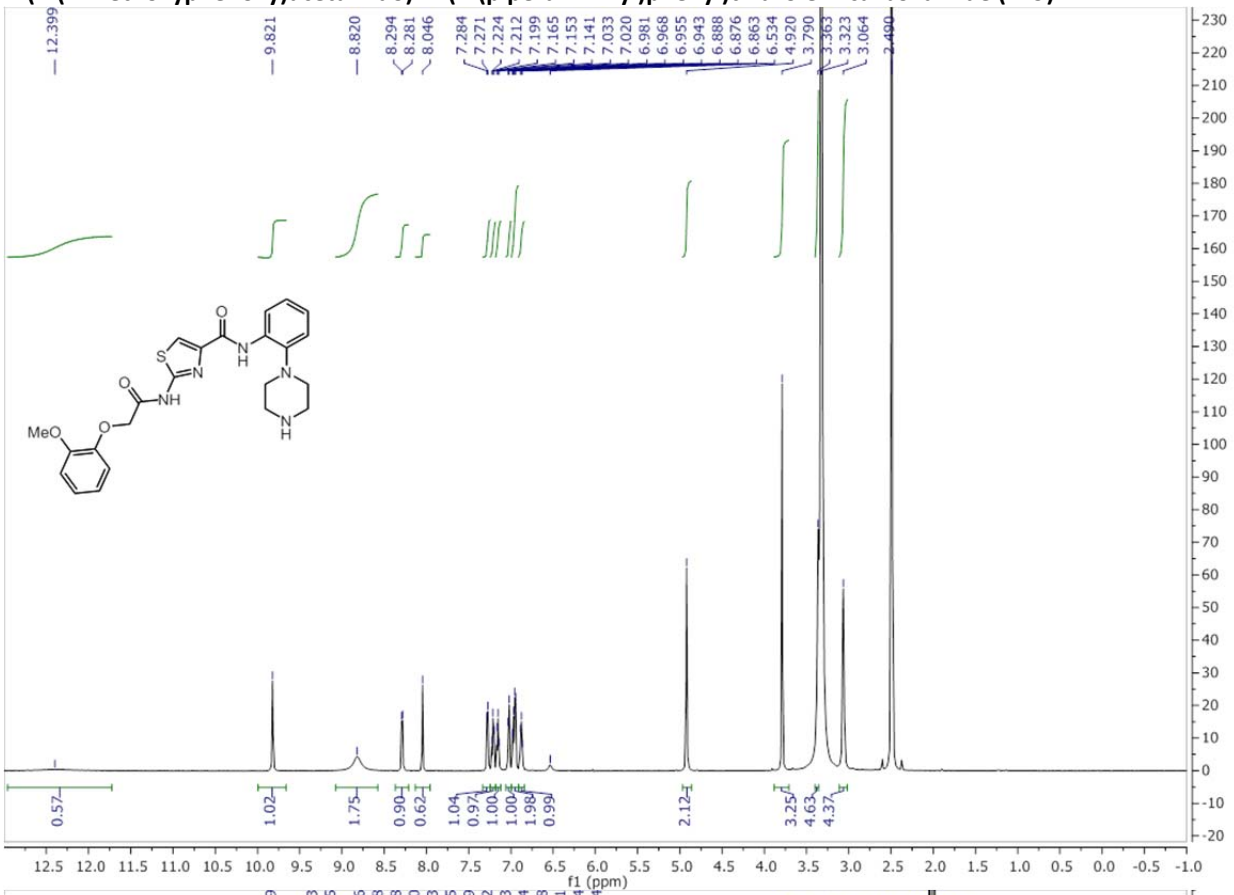


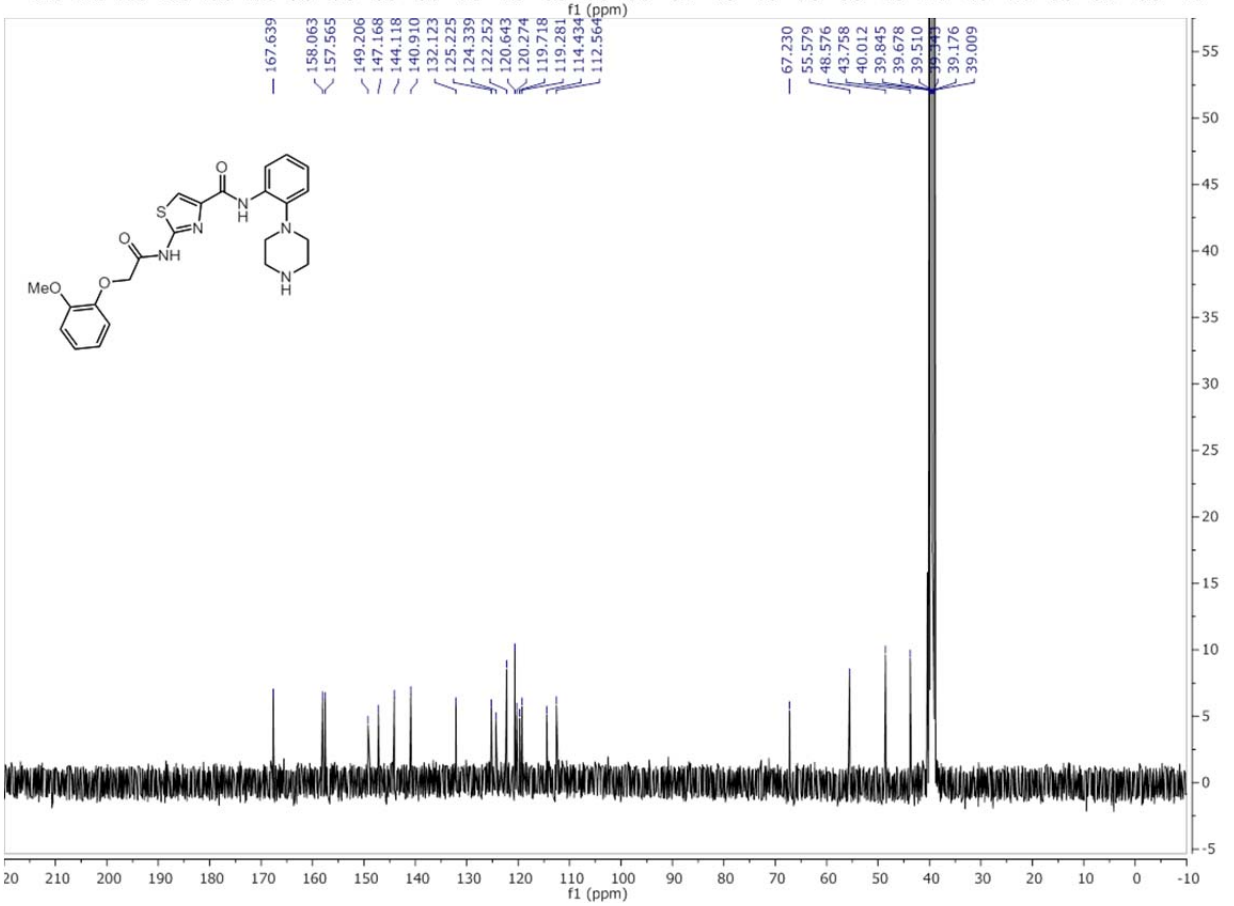
2-(2-ethoxybenzamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (39)



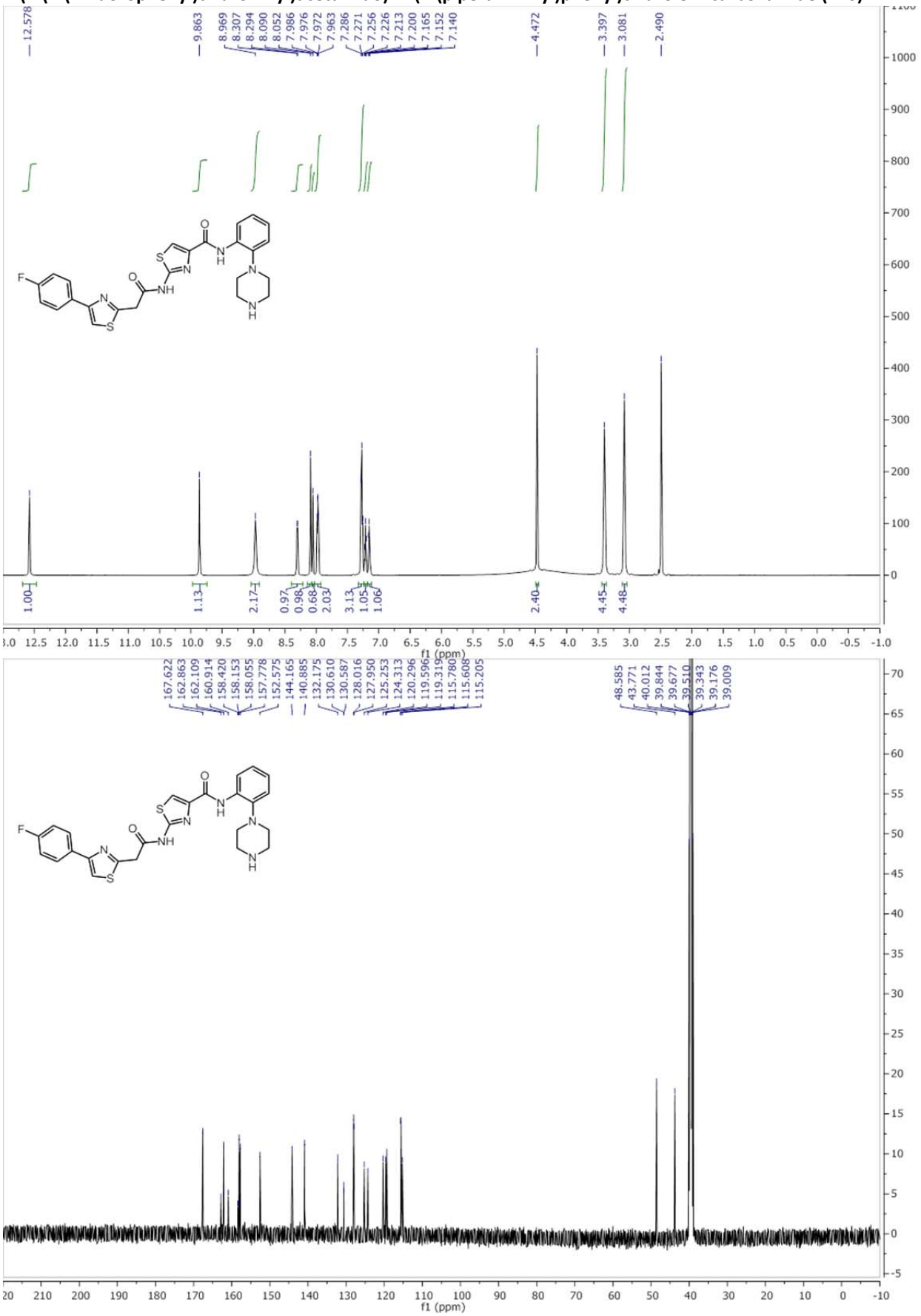


2-(2-(2-methoxyphenoxy)acetamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E19)

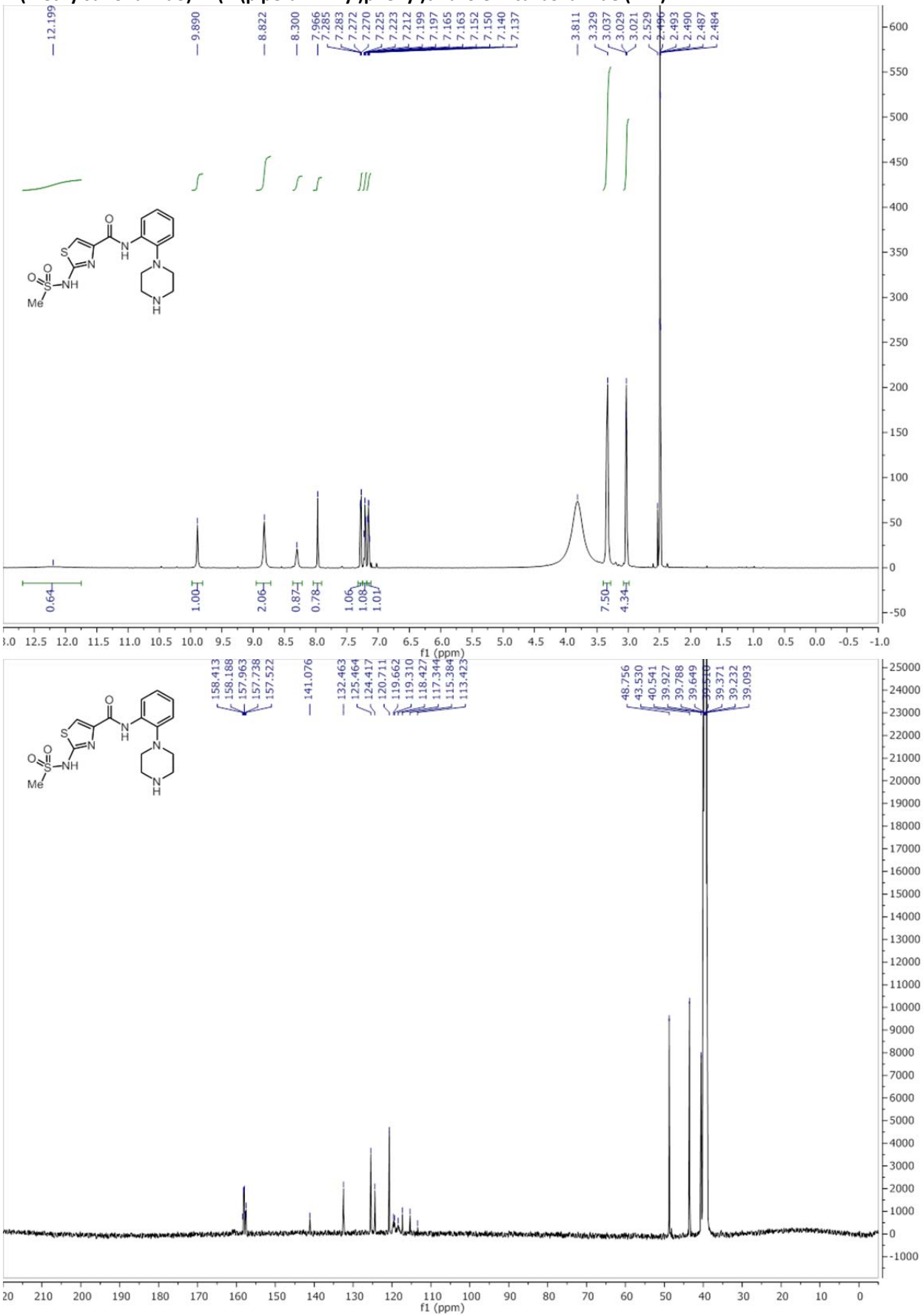




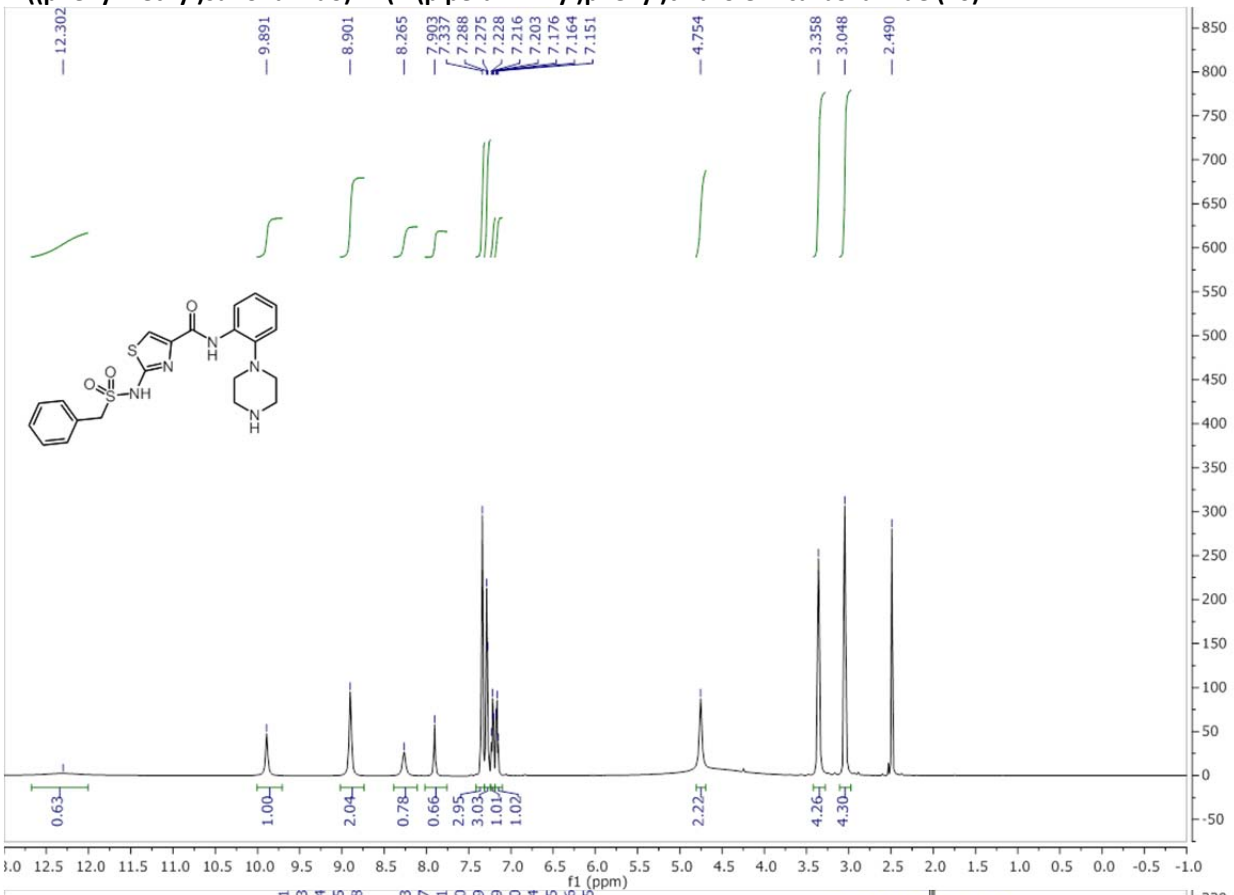
2-(2-(4-(4-fluorophenyl)thiazol-2-yl)acetamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E20)

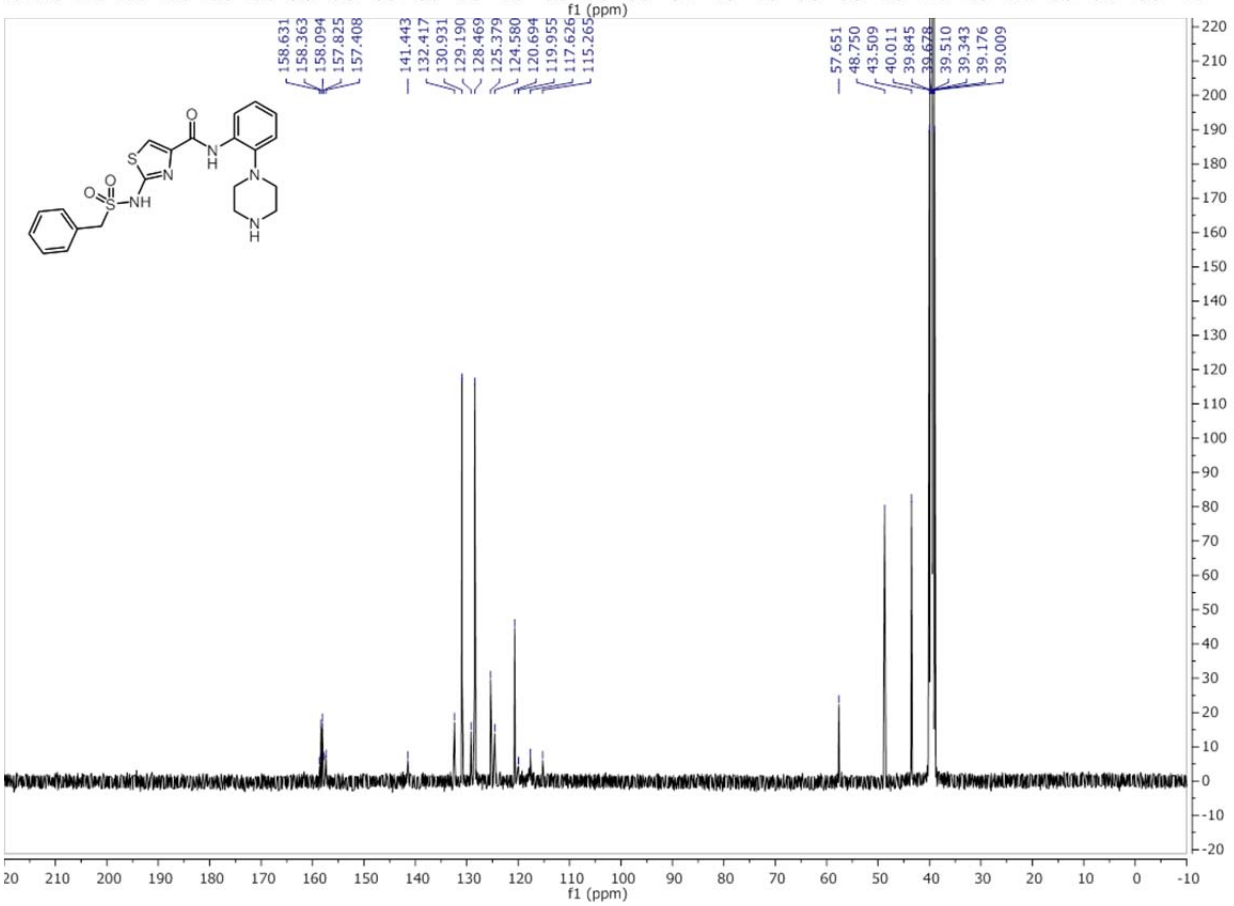


2-(methylsulfonamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E21)

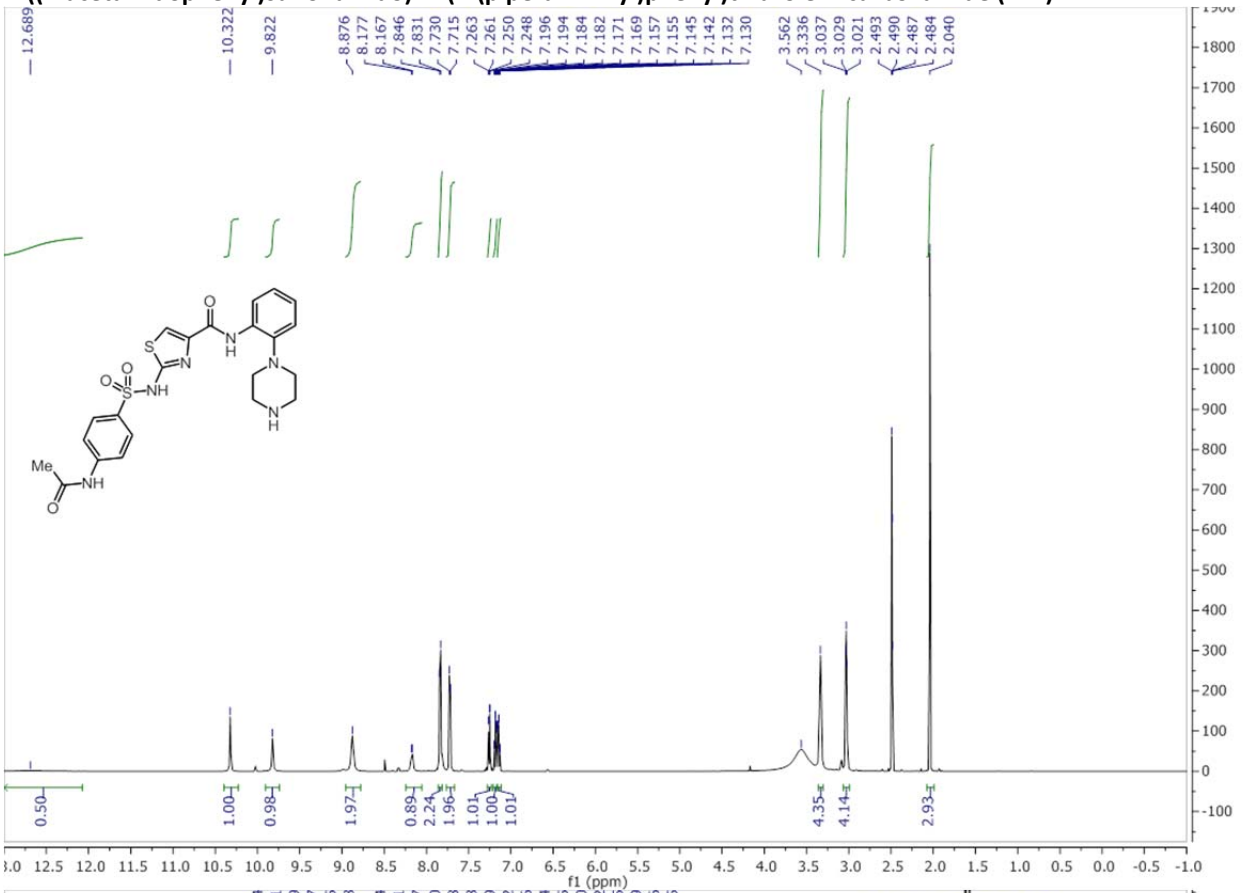


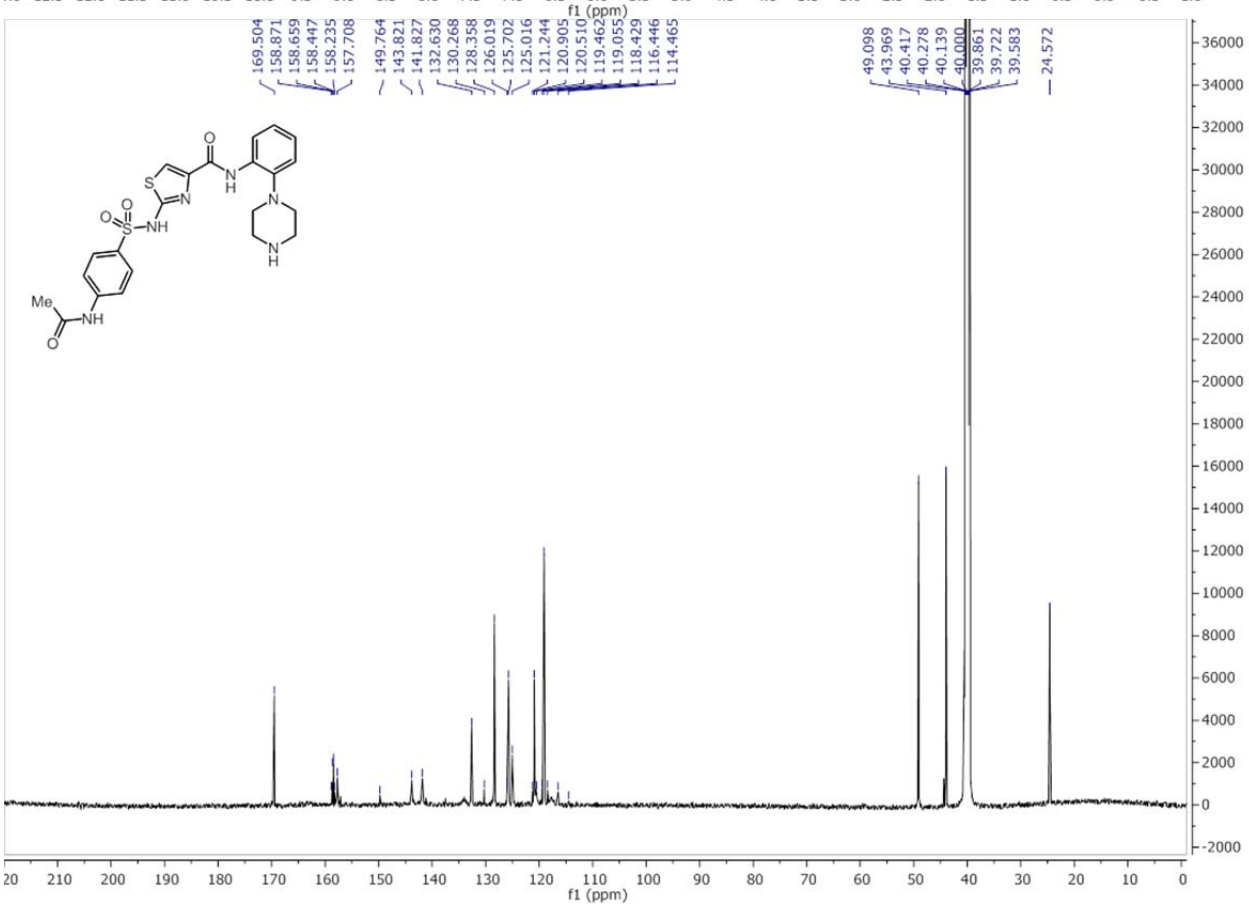
2-((phenylmethyl)sulfonamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (40)



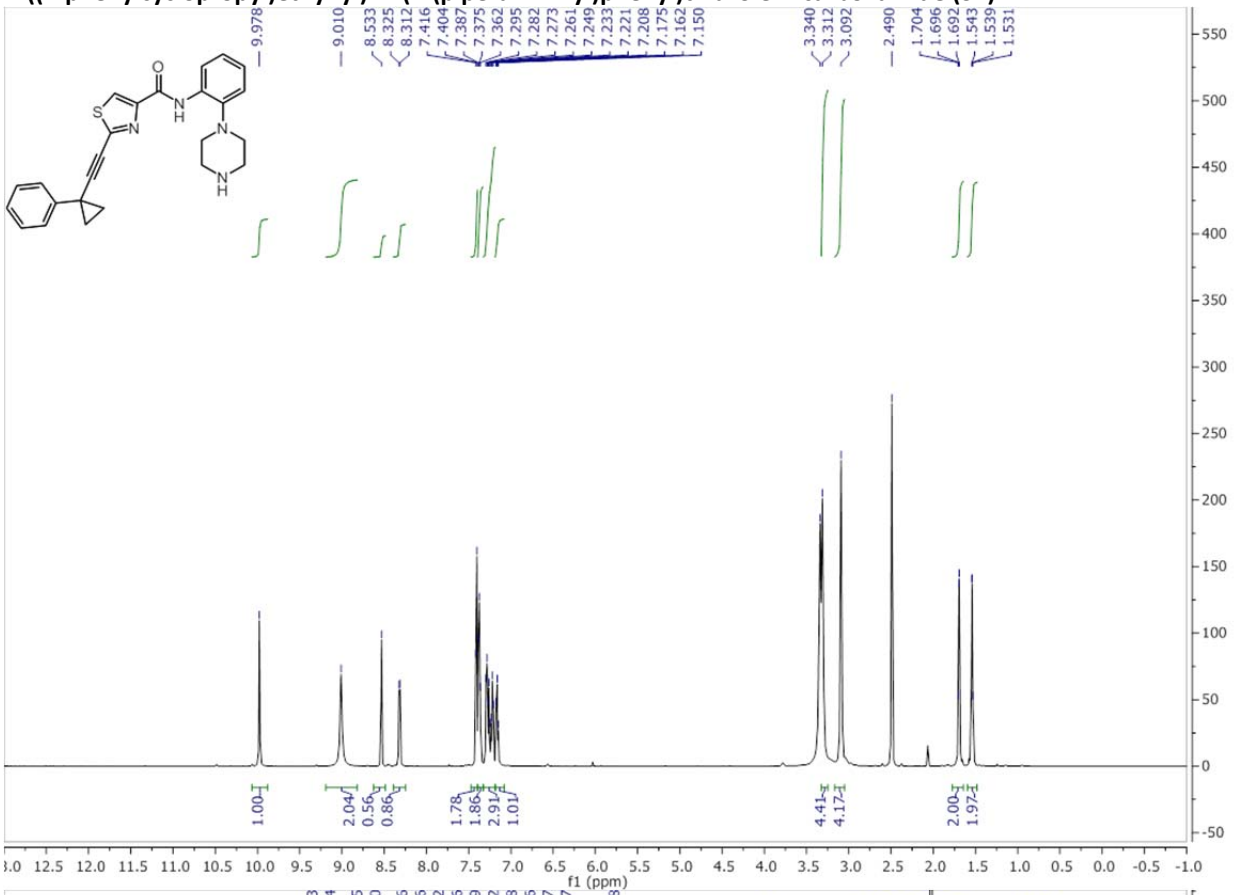


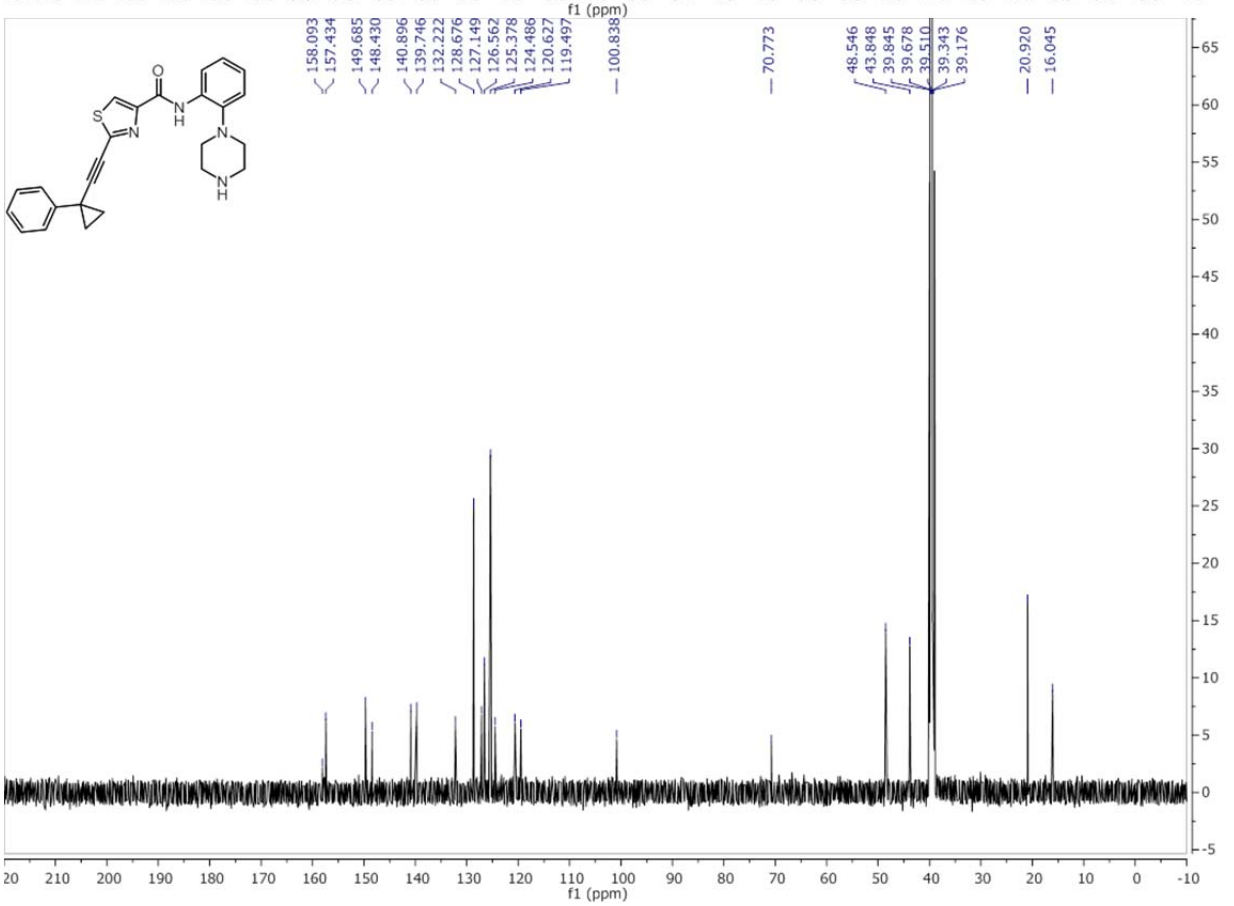
2-((4-acetamidophenyl)sulfonamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E22)



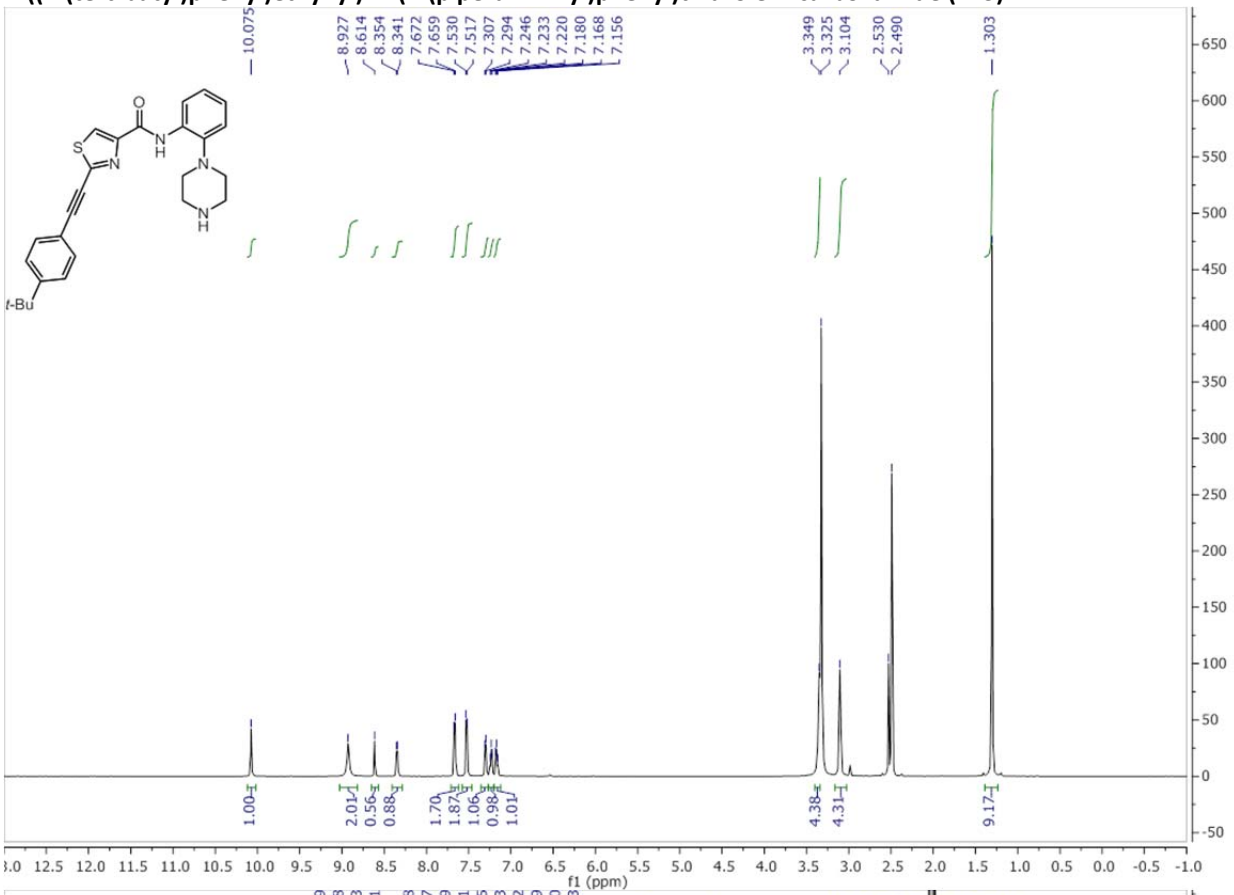


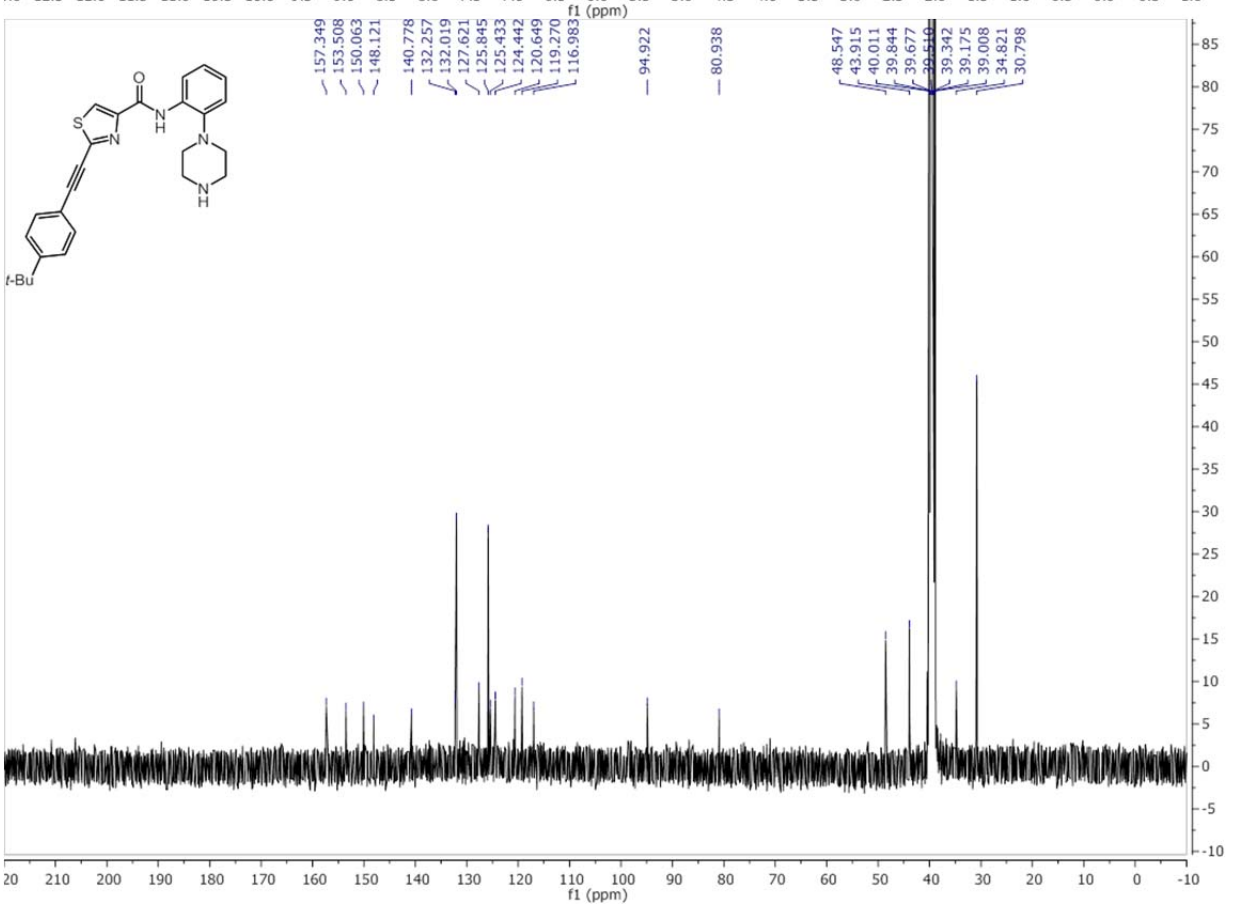
2-((1-phenylcyclopropyl)ethynyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (37)



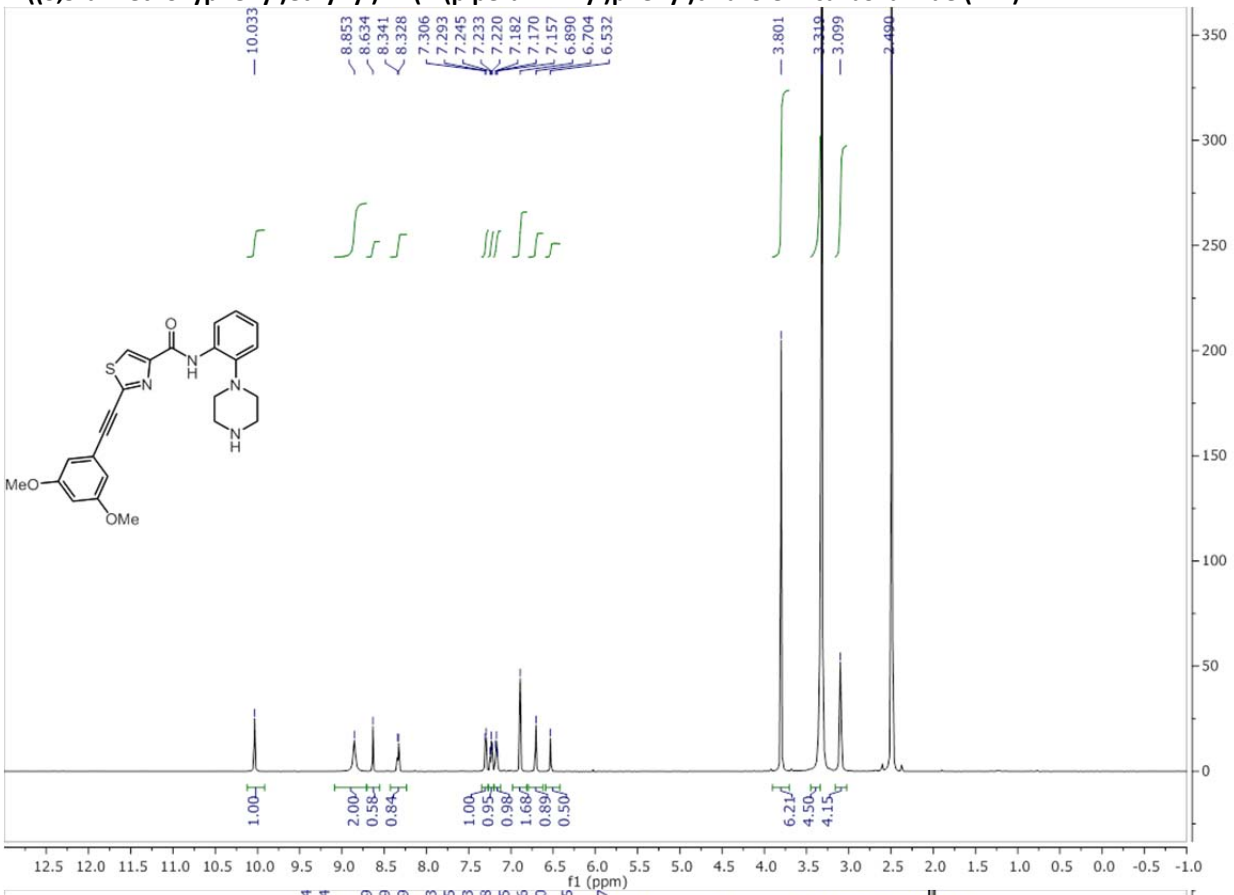


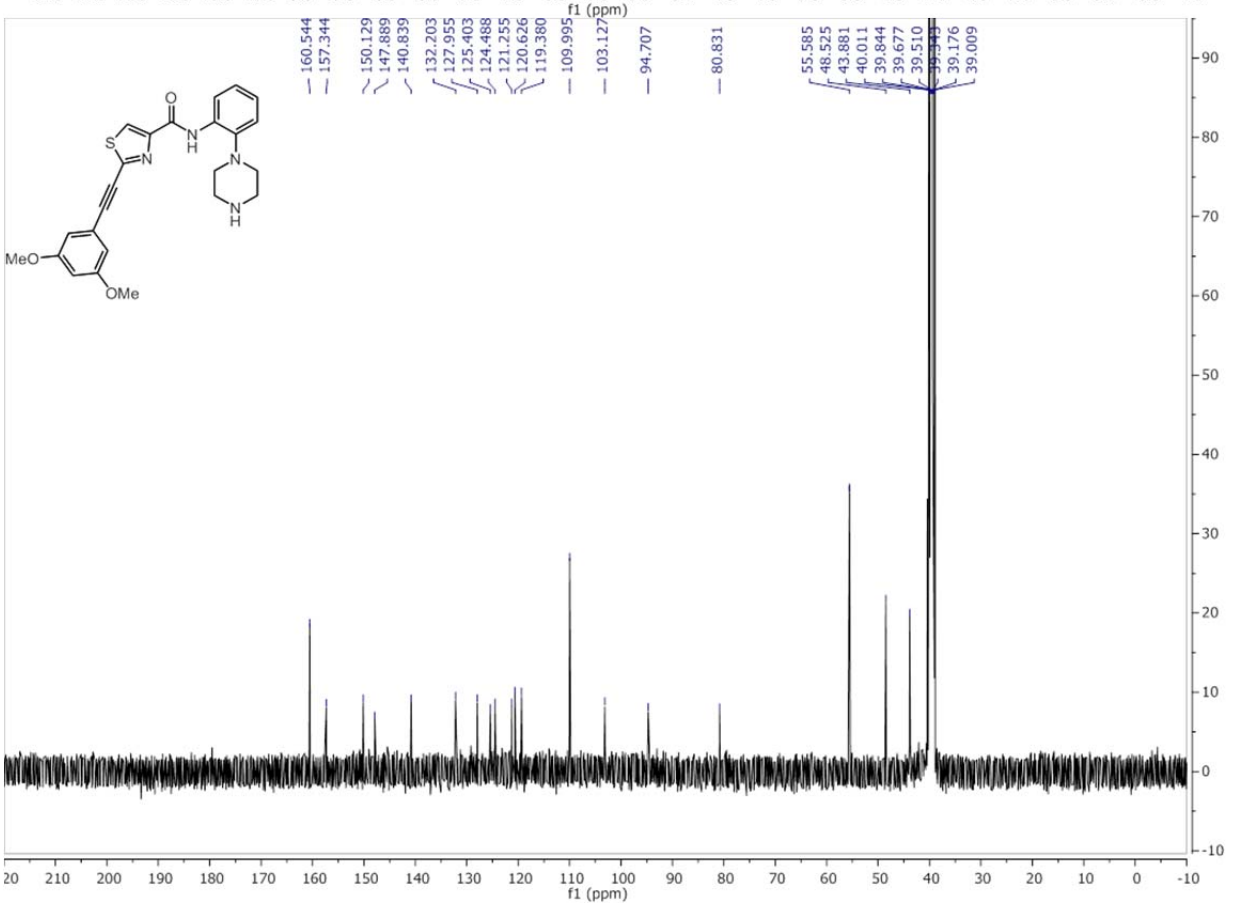
2-((4-(tert-butyl)phenyl)ethynyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E23)



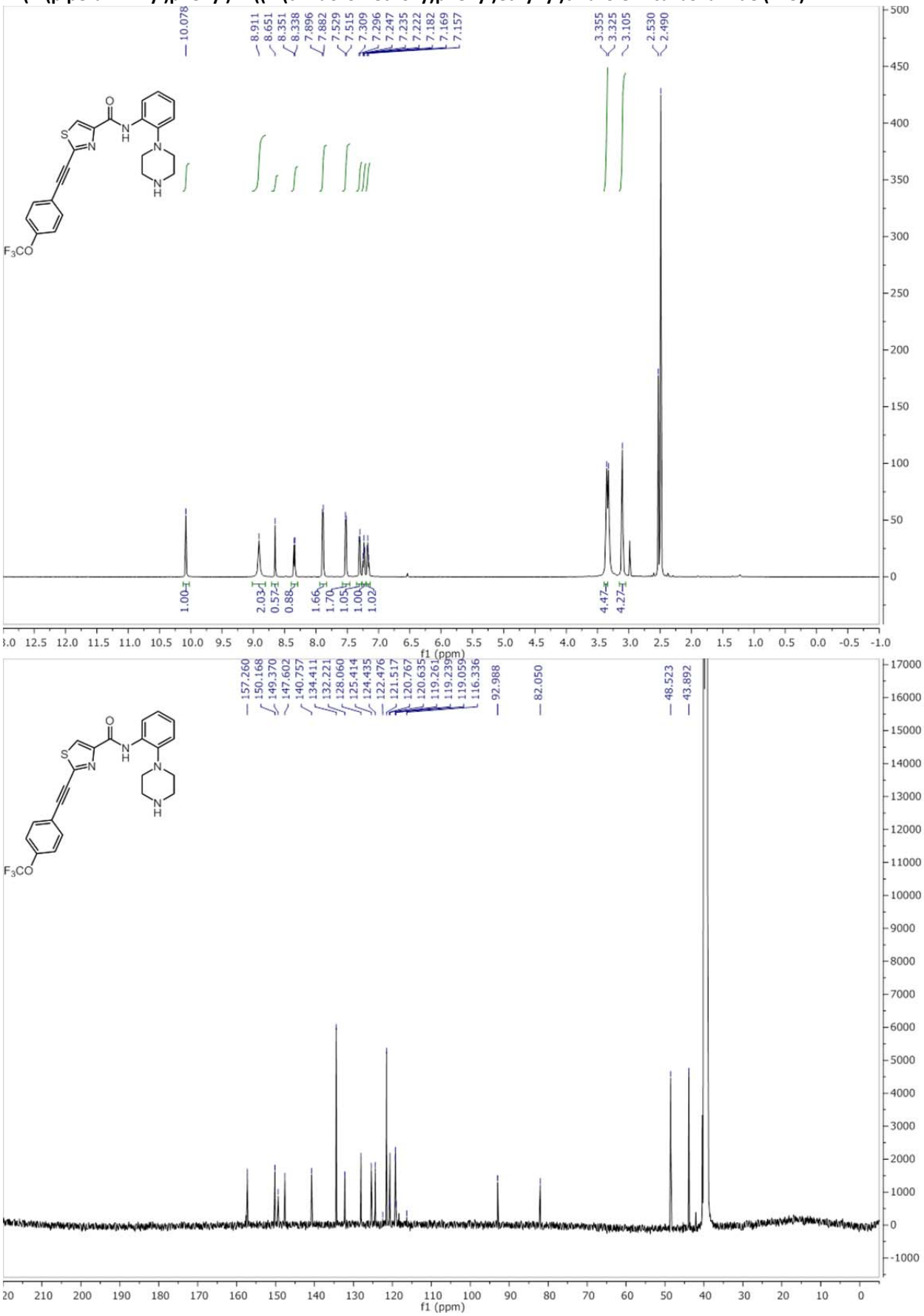


2-((3,5-dimethoxyphenyl)ethynyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E24)

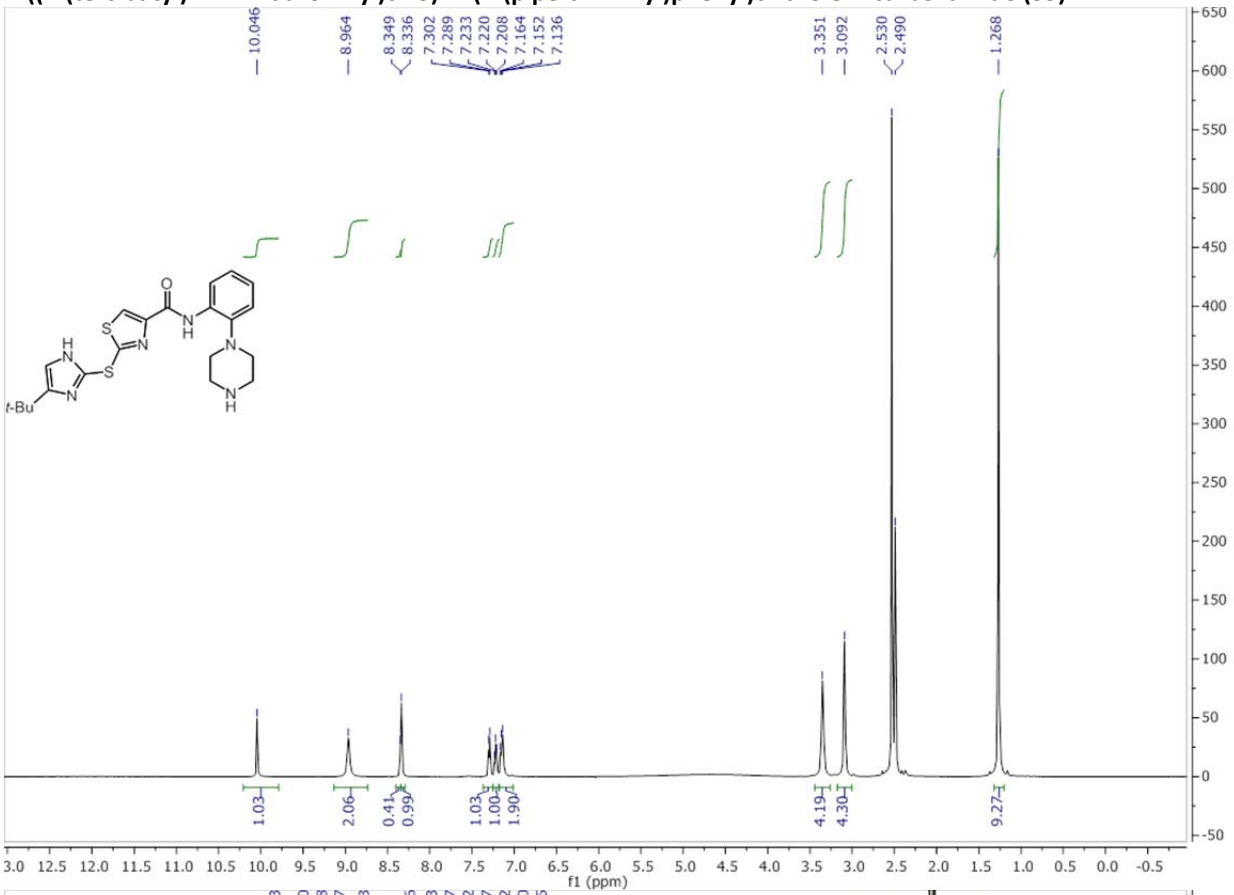


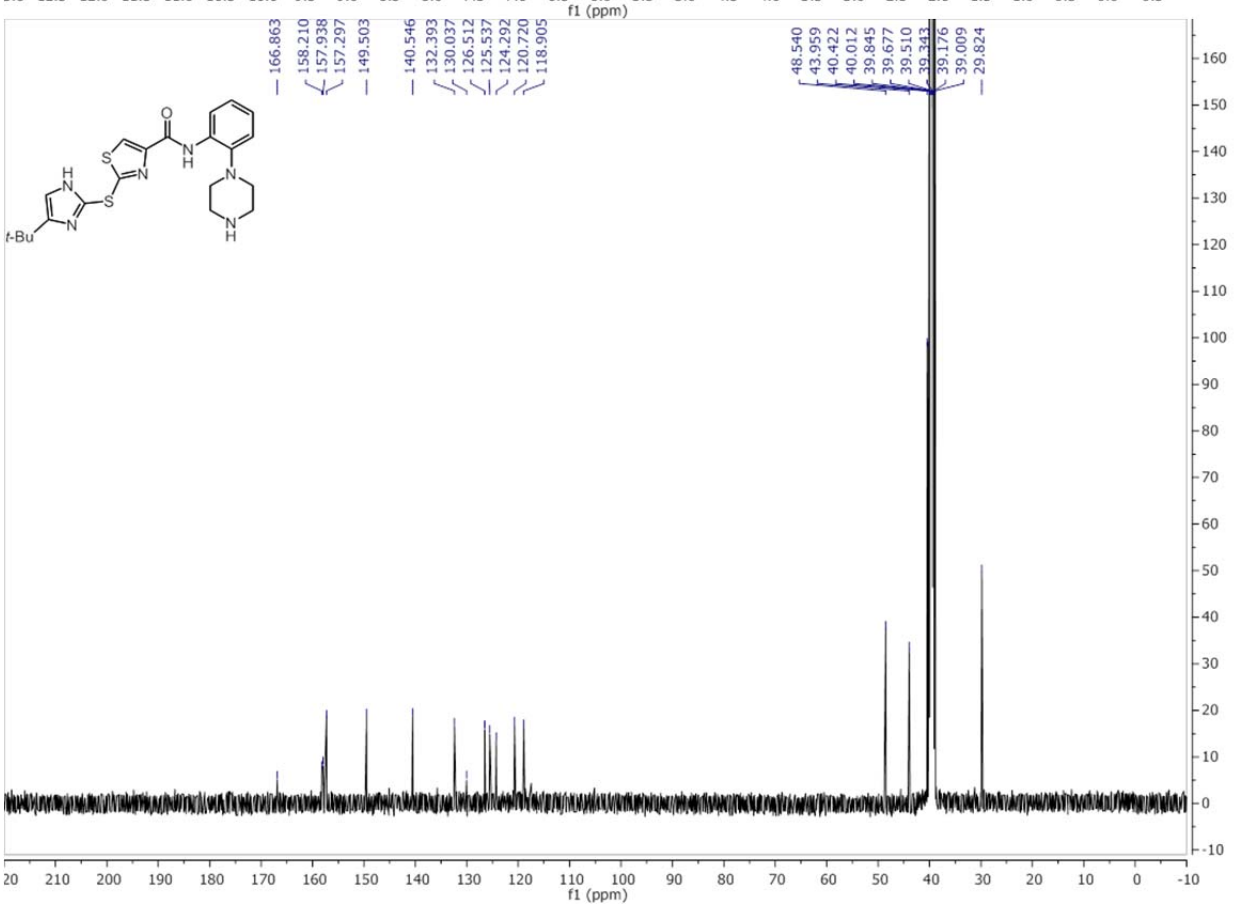


N-(2-(piperazin-1-yl)phenyl)-2-((4-(trifluoromethoxy)phenyl)ethynyl)thiazole-4-carboxamide (E25)

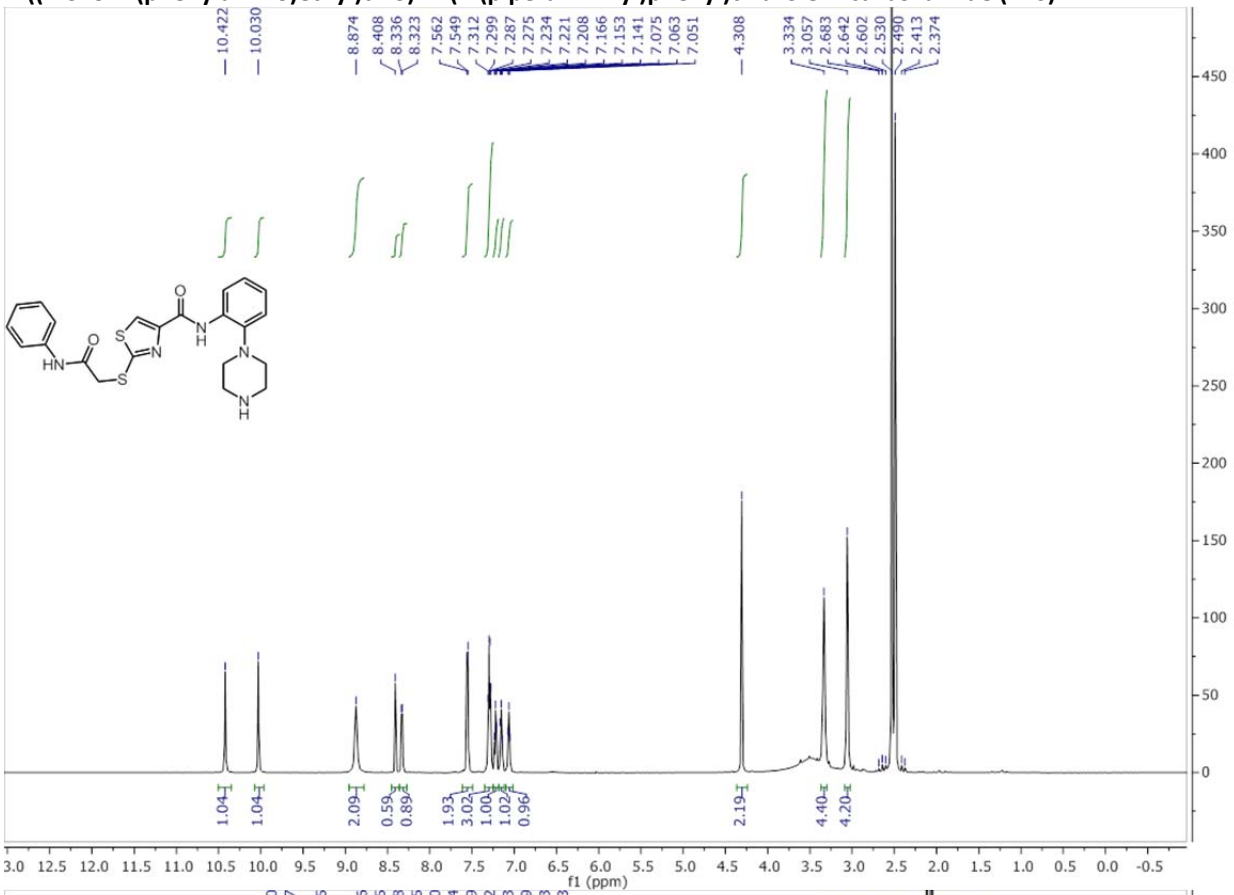


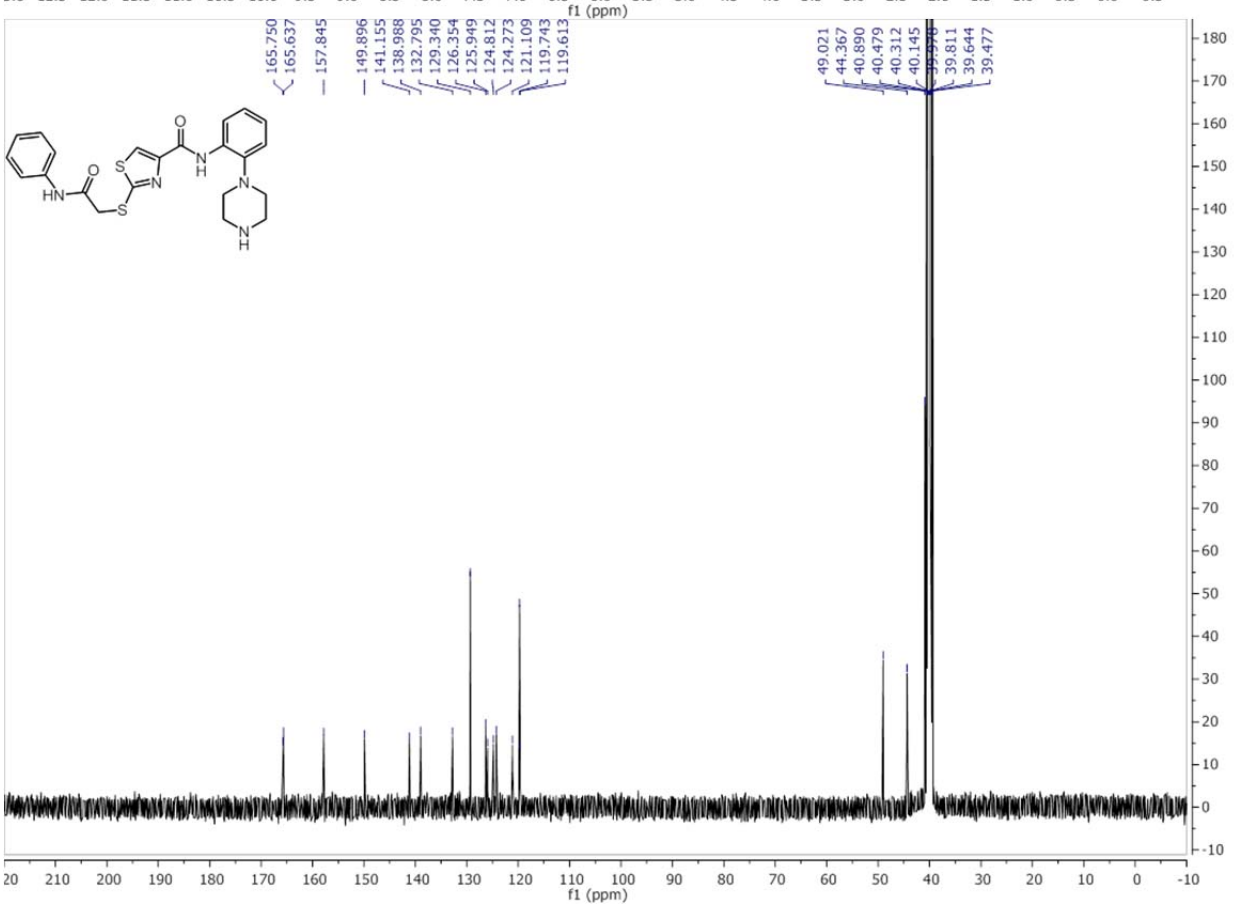
2-((4-(tert-butyl)-1H-imidazol-2-yl)thio)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (35)



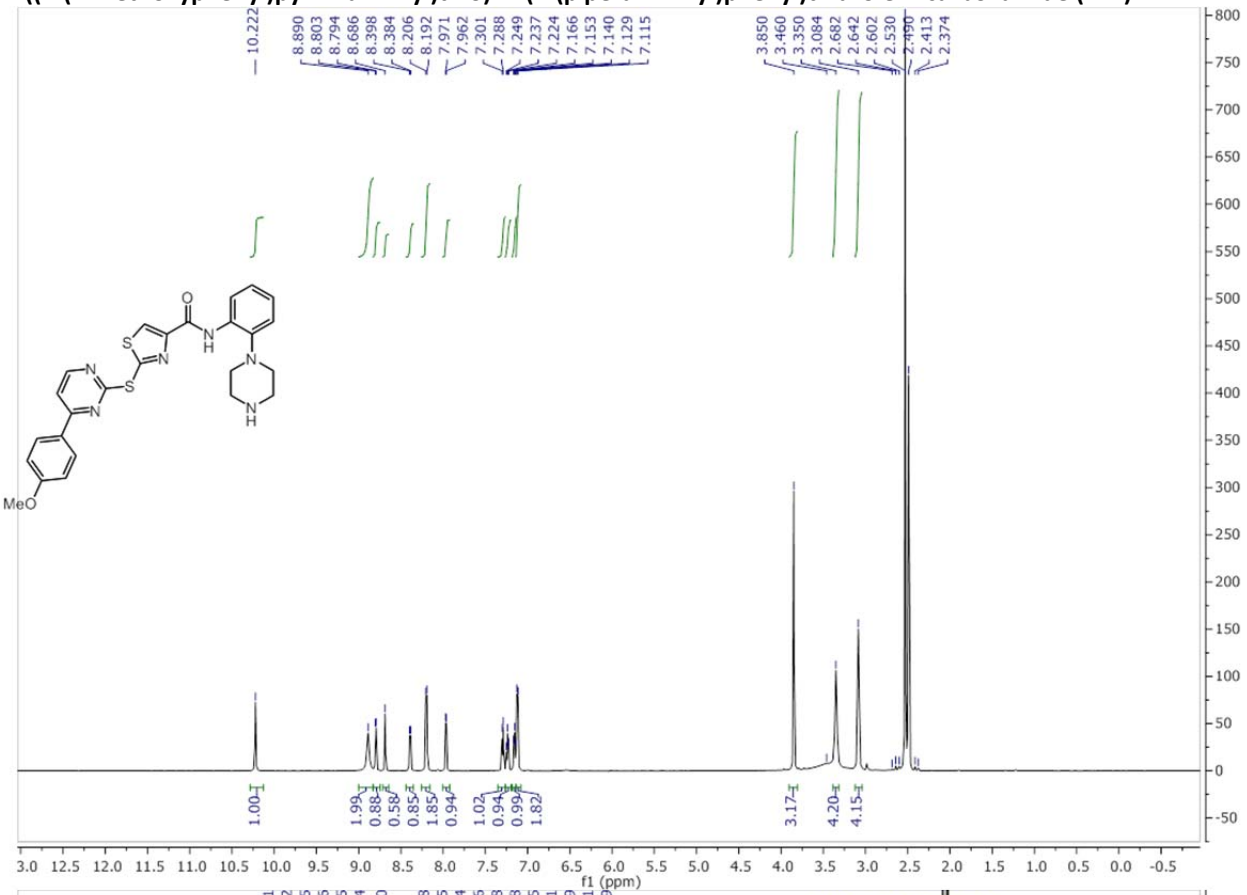


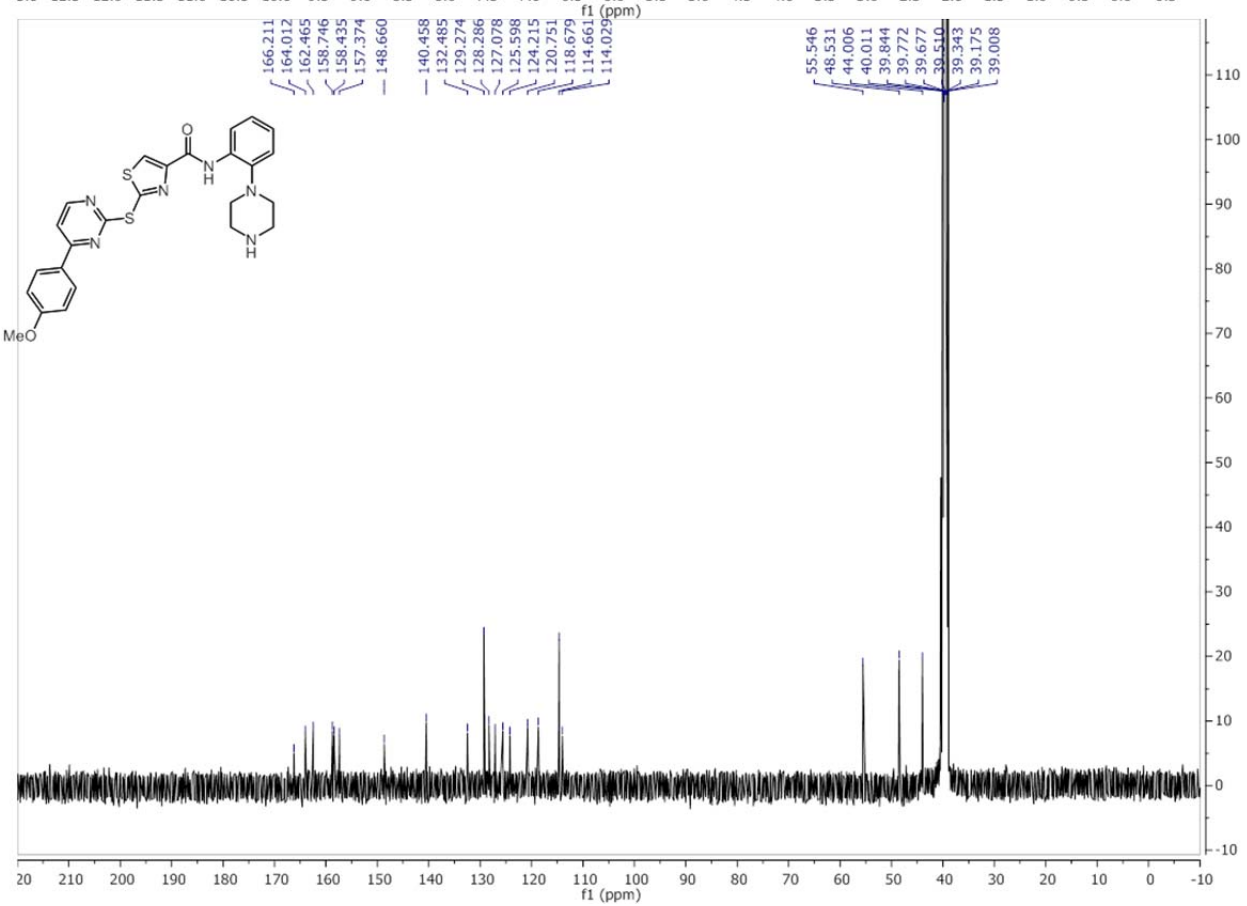
2-((2-oxo-2-(phenylamino)ethyl)thio)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E26)



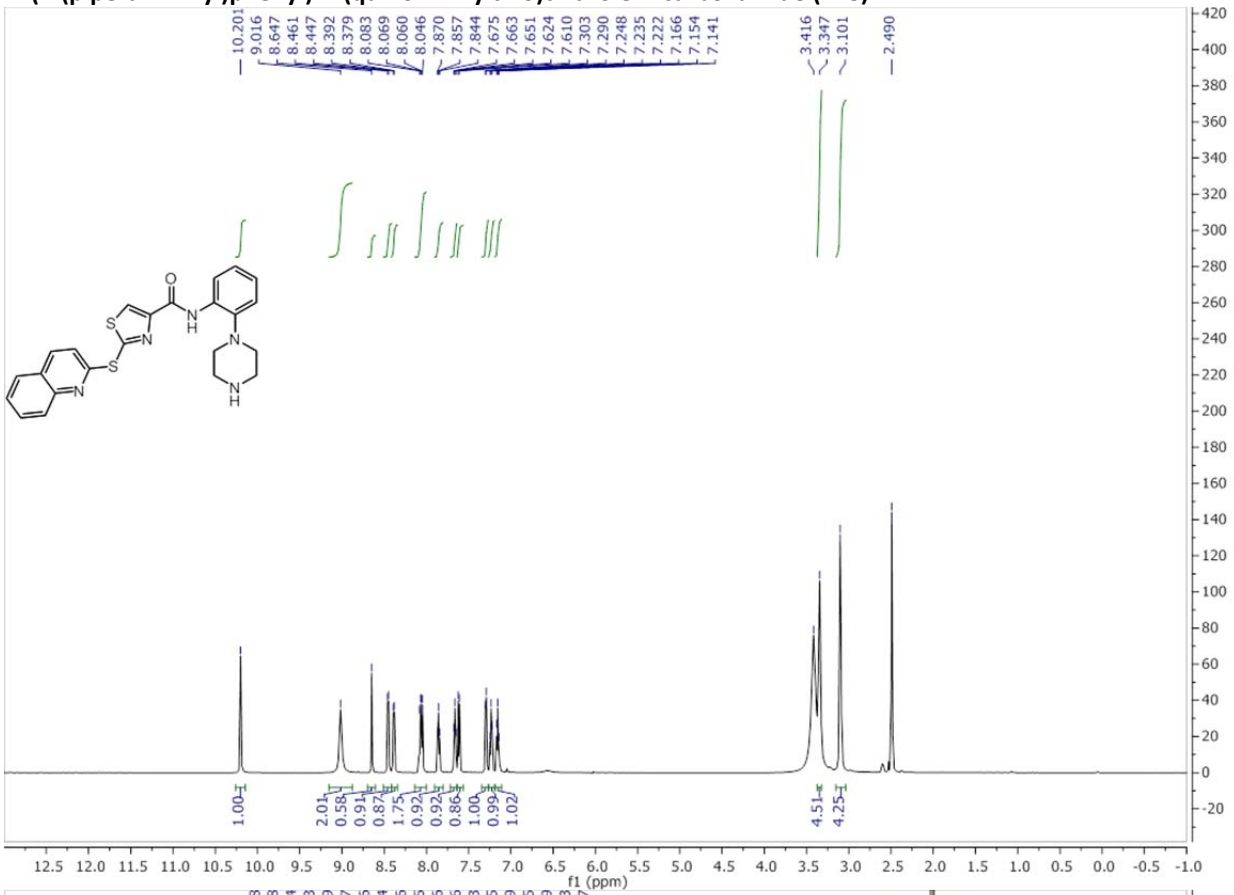


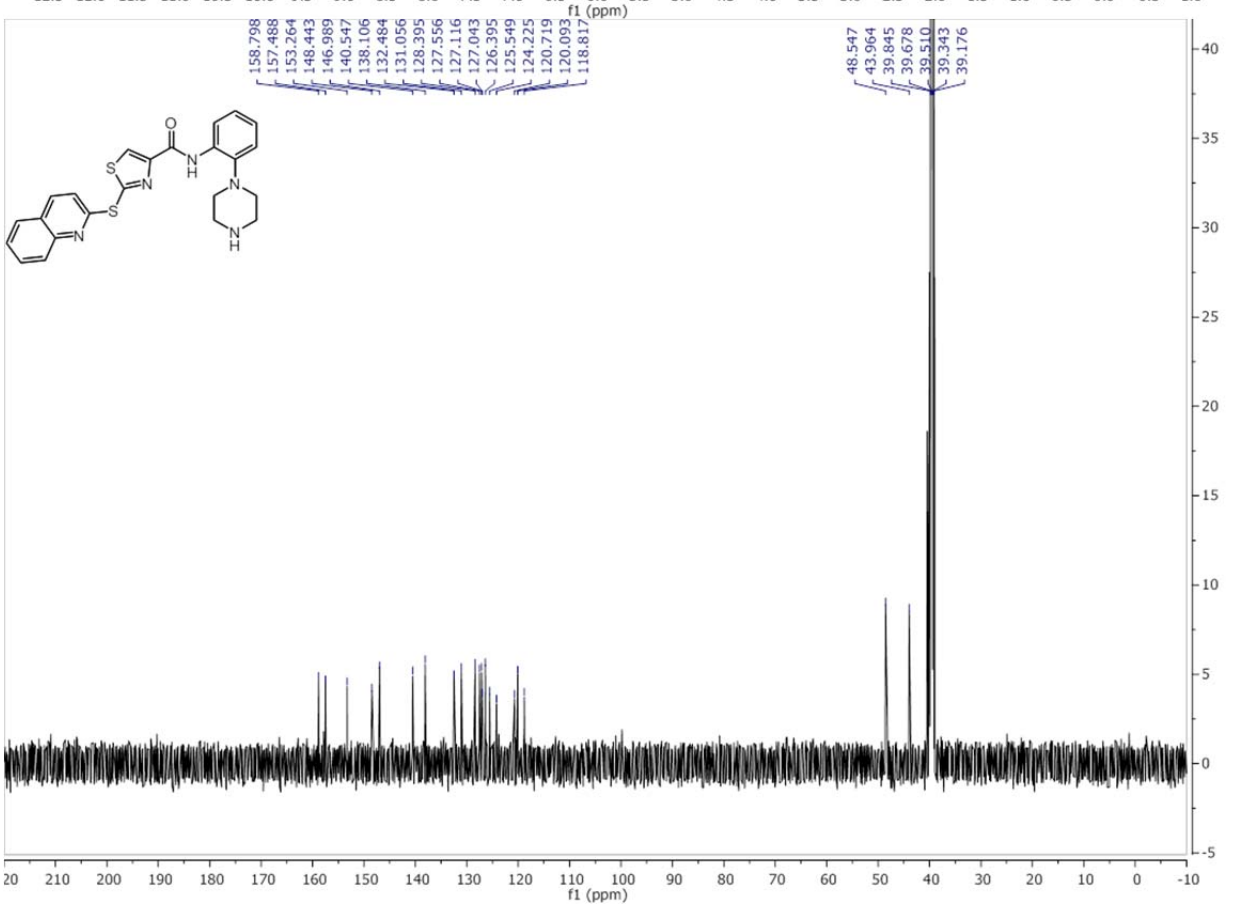
2-((4-(4-methoxyphenyl)pyrimidin-2-yl)thio)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E27)



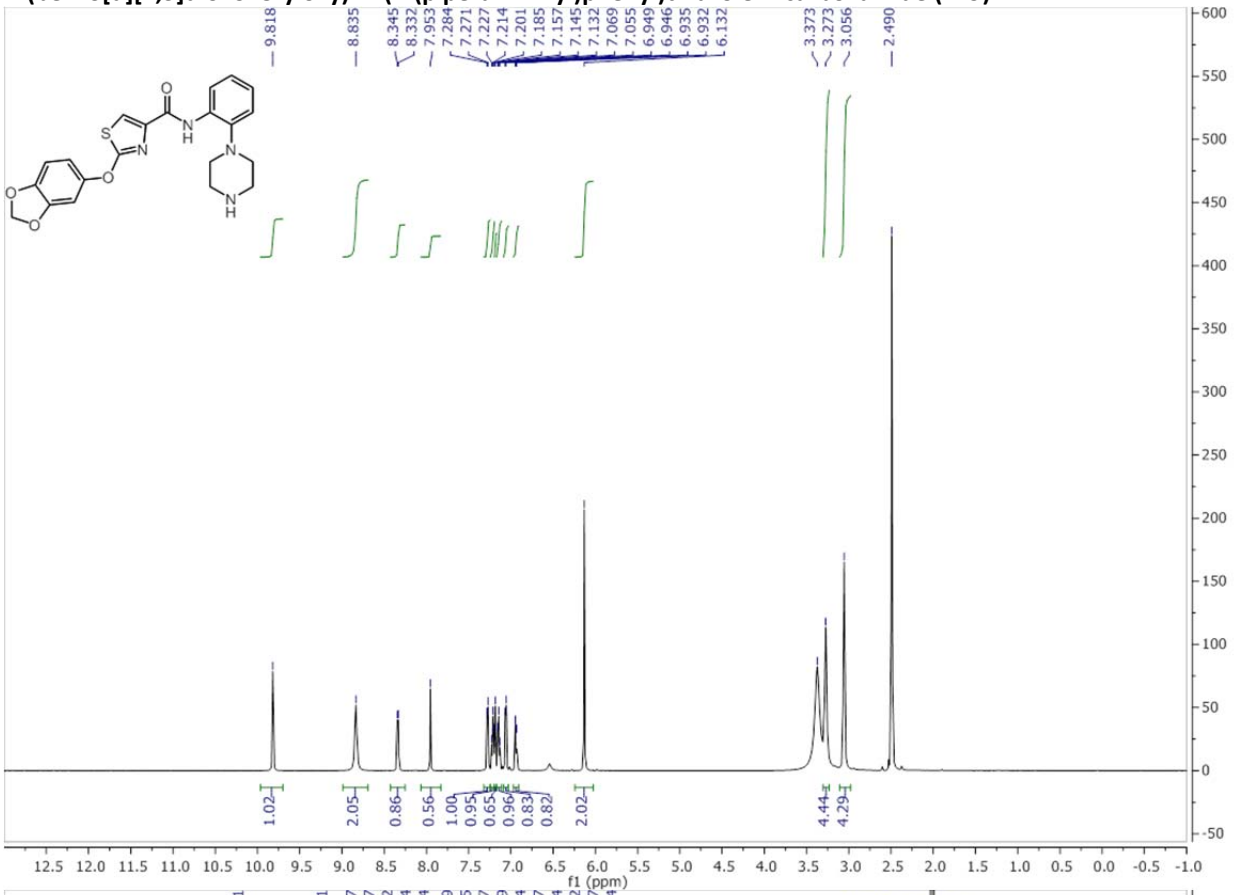


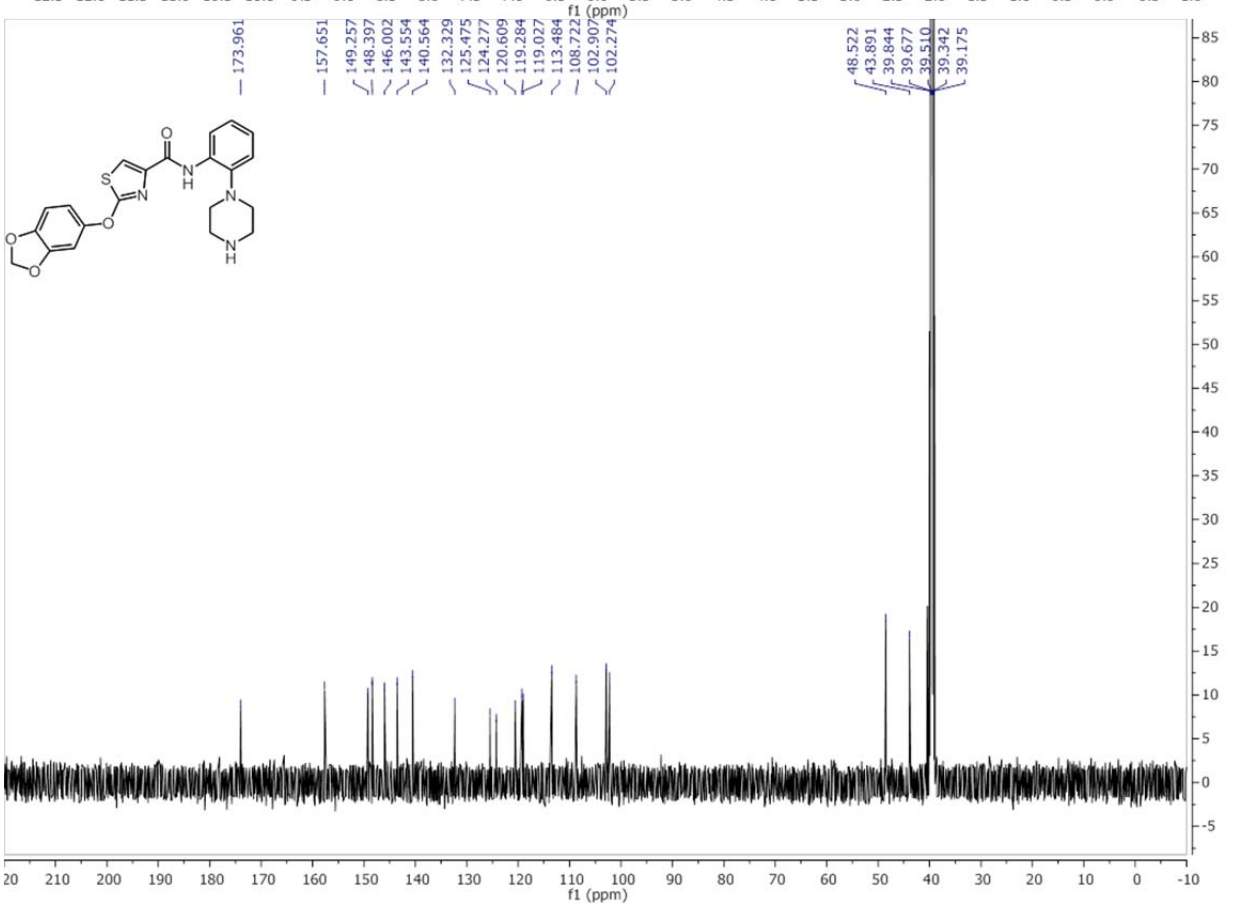
N-(2-(piperazin-1-yl)phenyl)-2-(quinolin-2-ylthio)thiazole-4-carboxamide (E28)



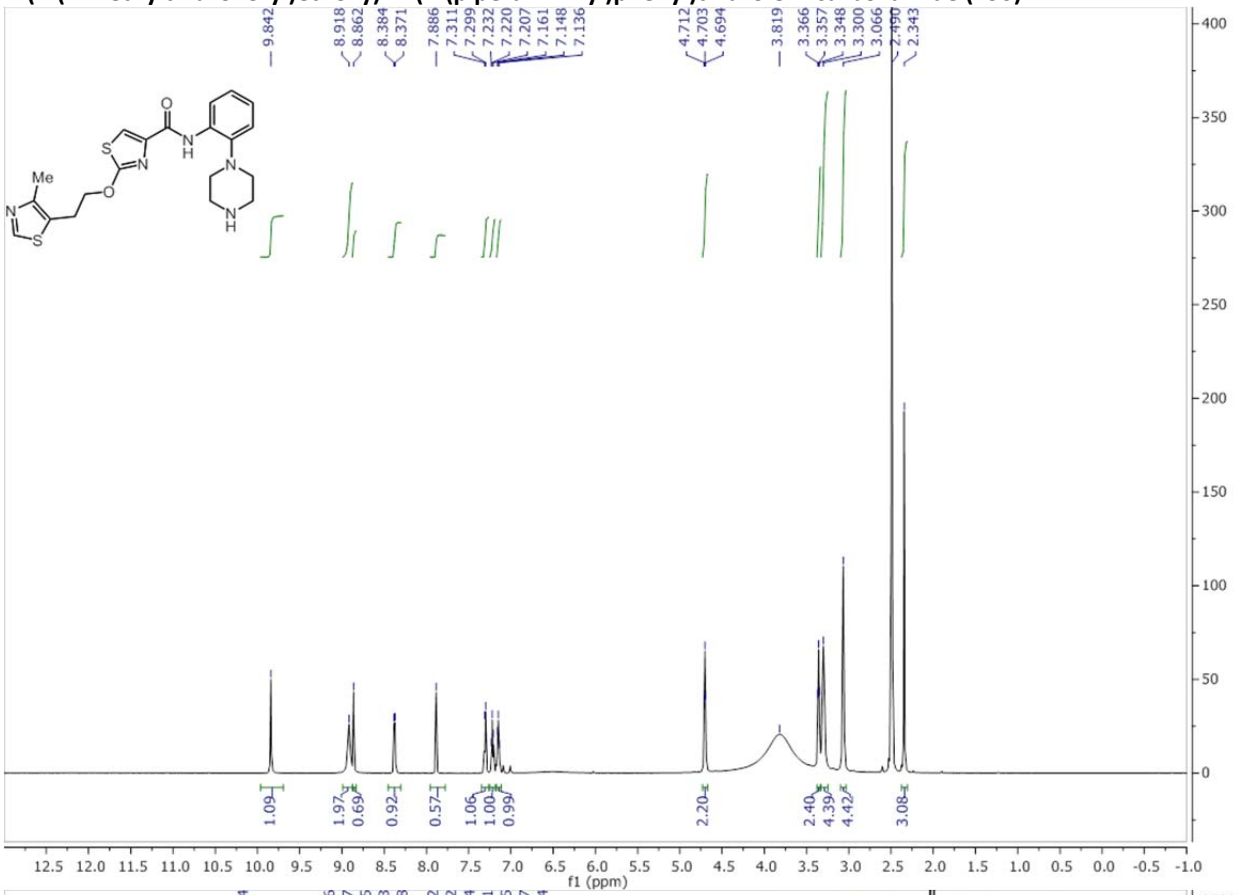


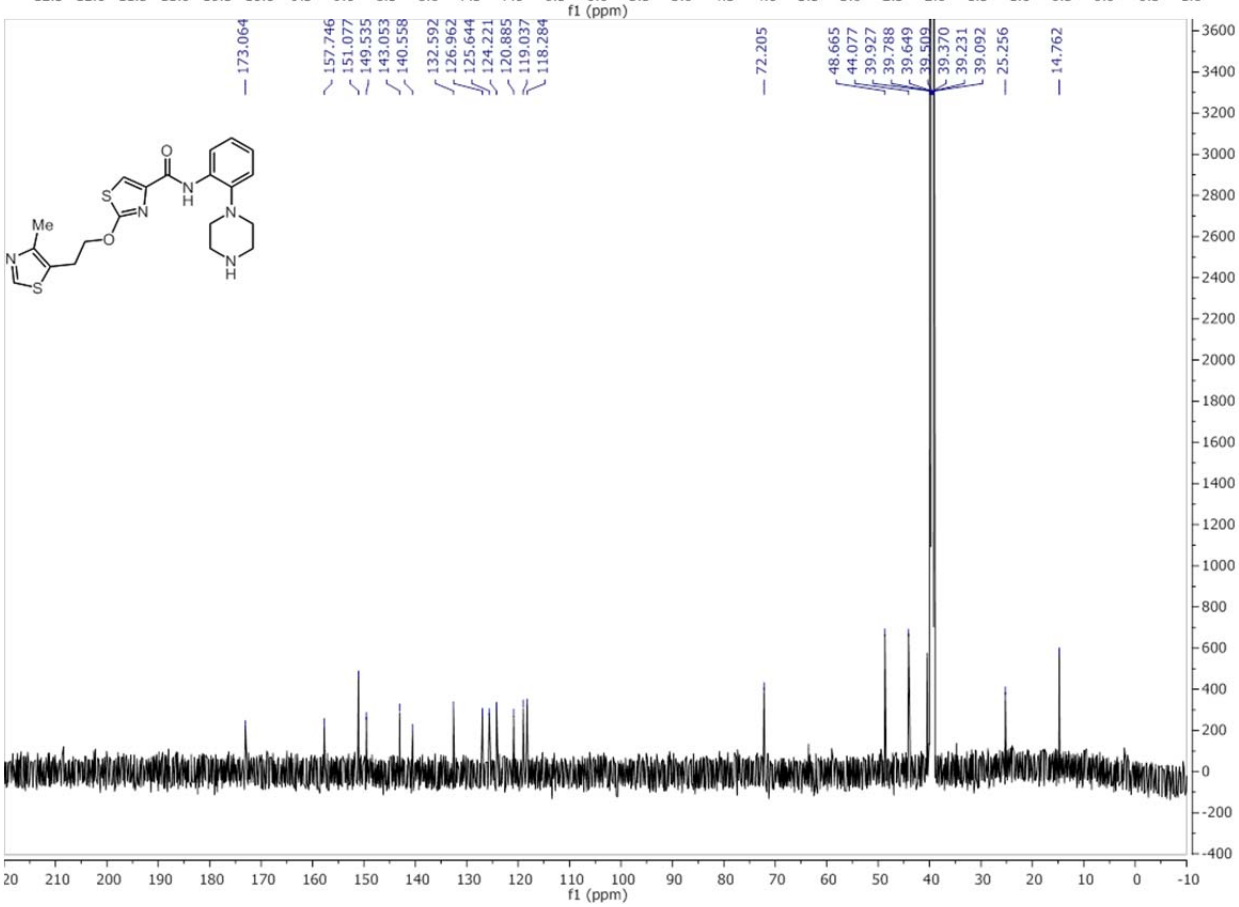
2-(benzo[d][1,3]dioxol-5-yloxy)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E29)



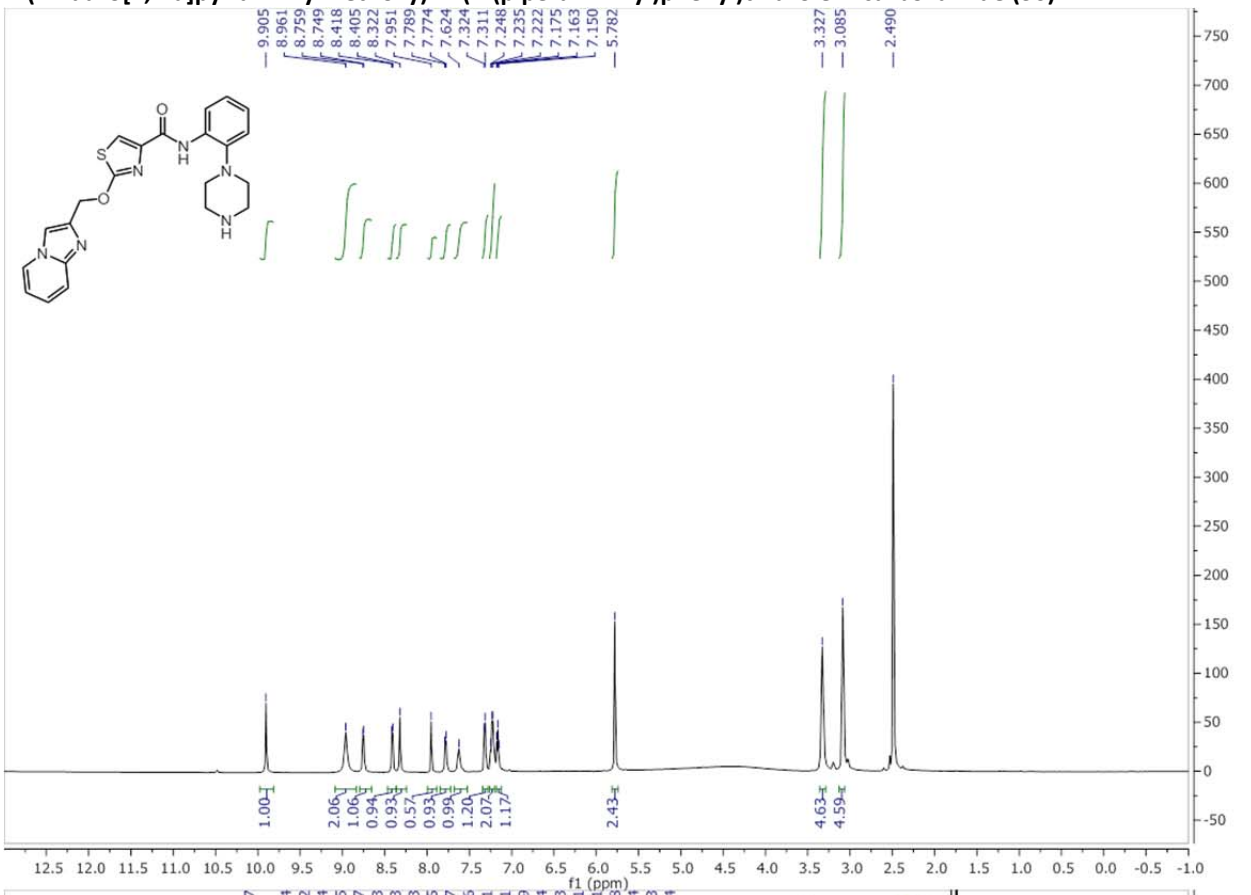


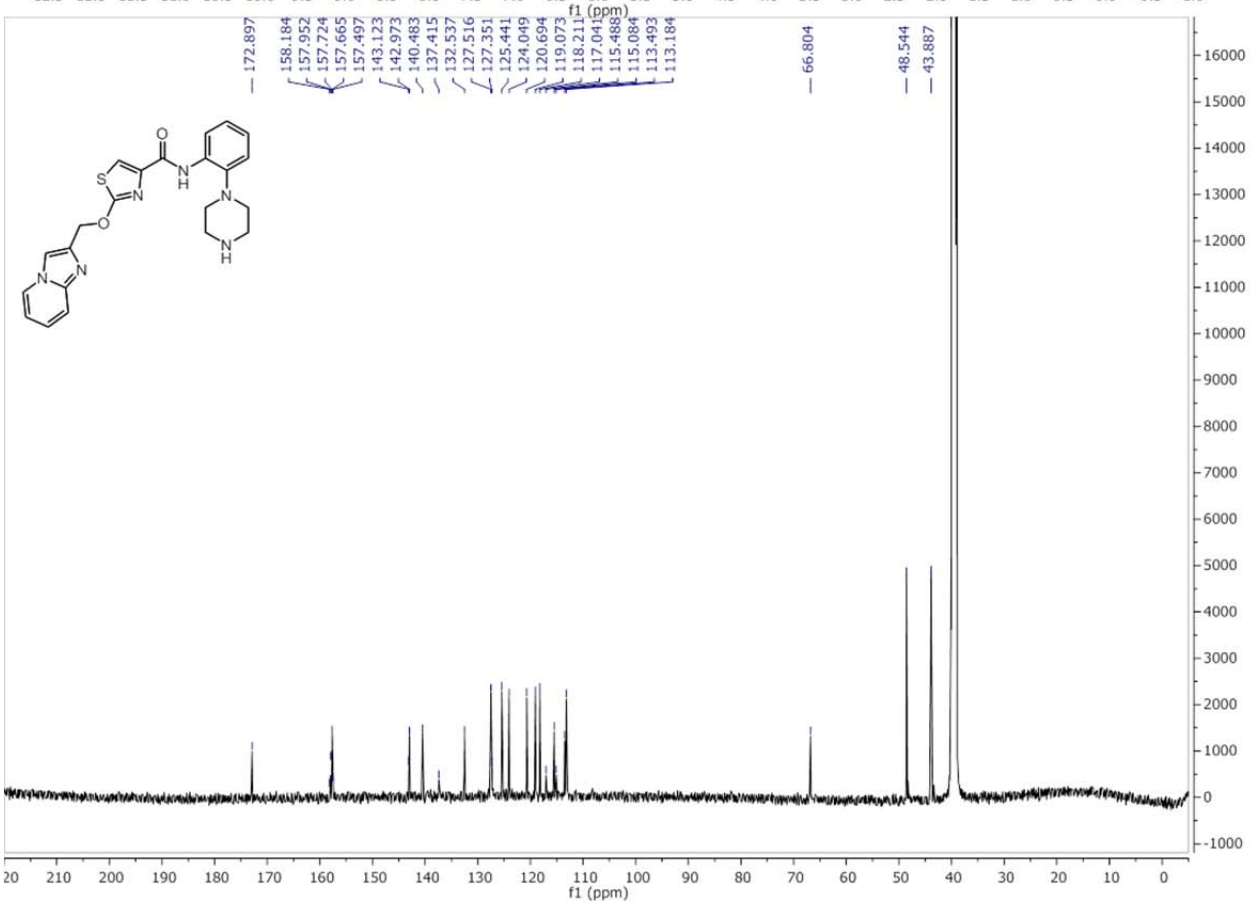
2-(2-(4-methylthiazol-5-yl)ethoxy)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E30)



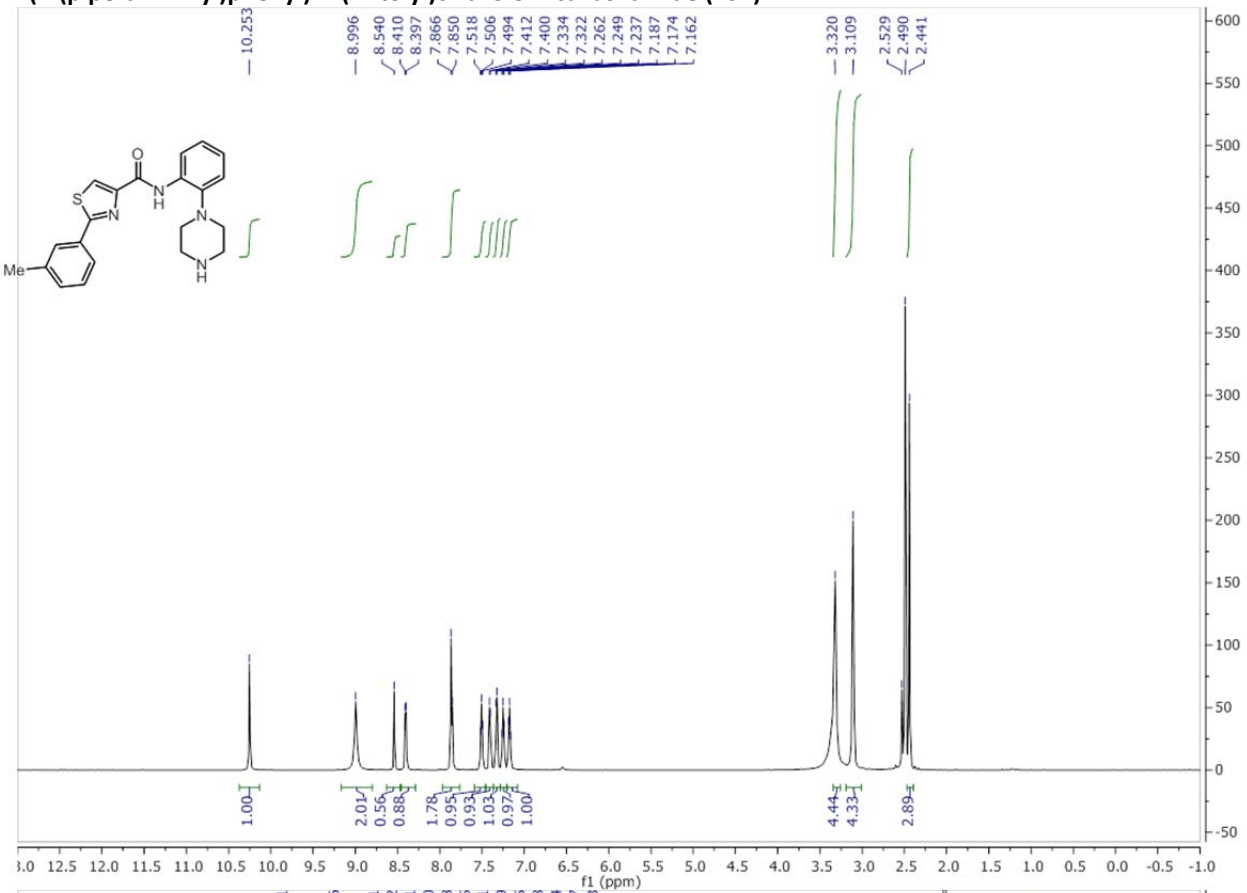


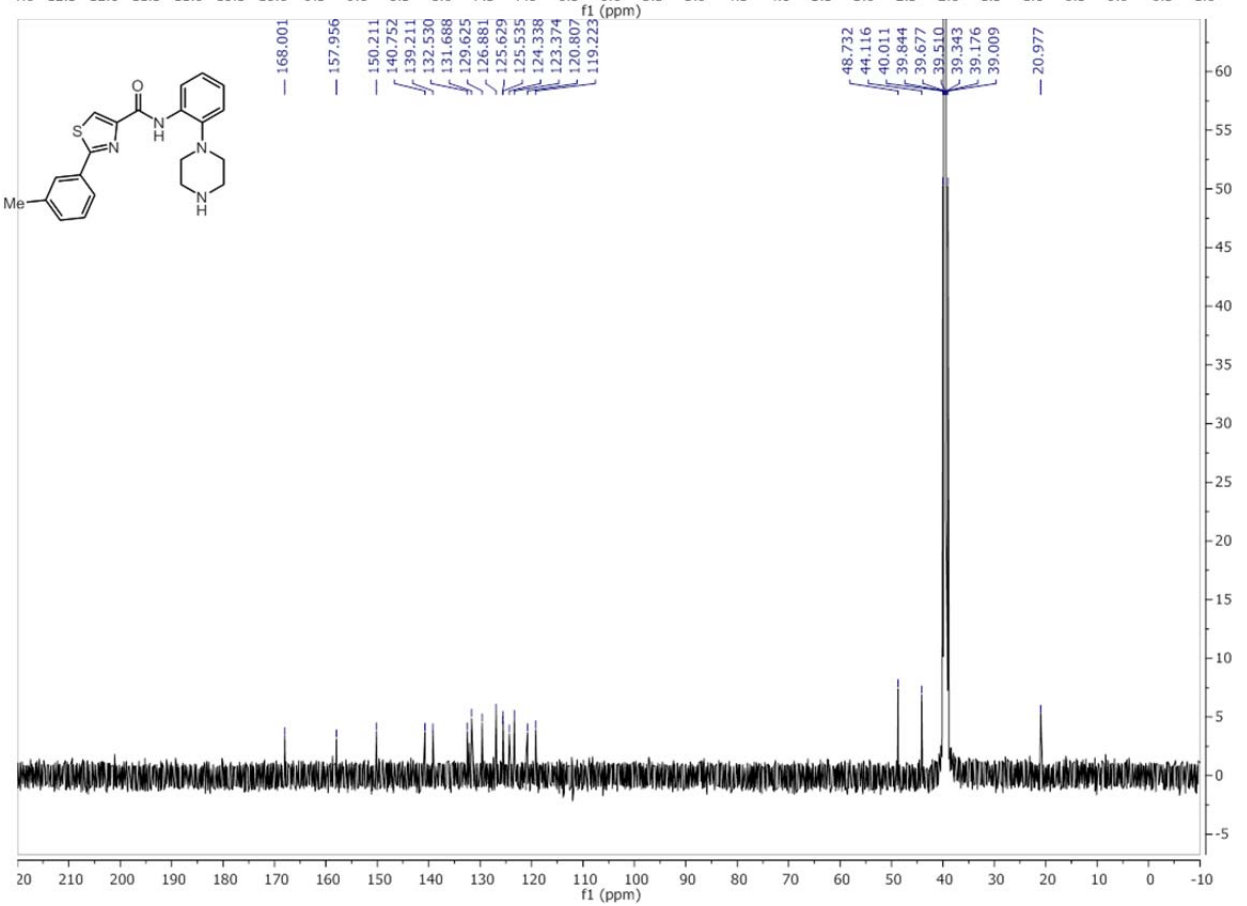
2-(imidazo[1,2-a]pyridin-2-ylmethoxy)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (36)



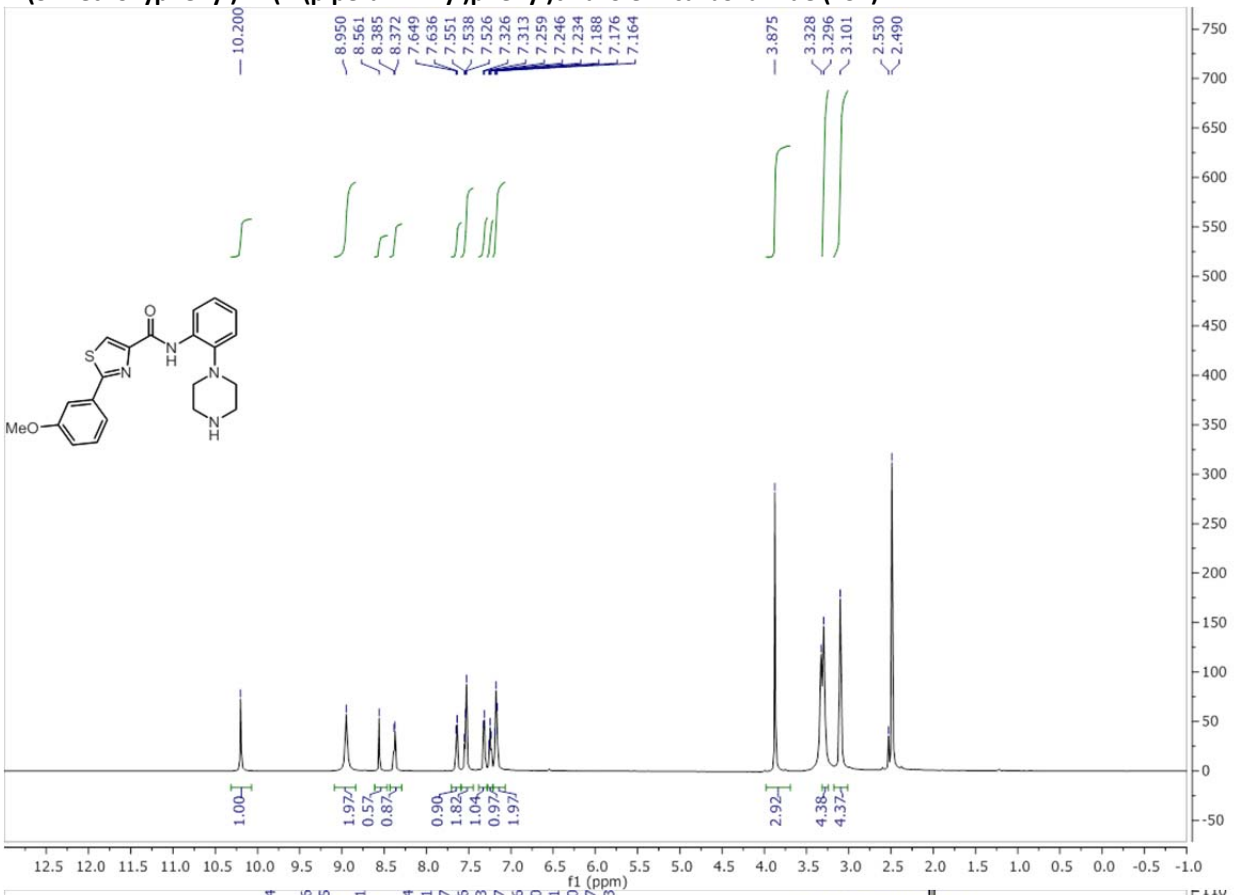


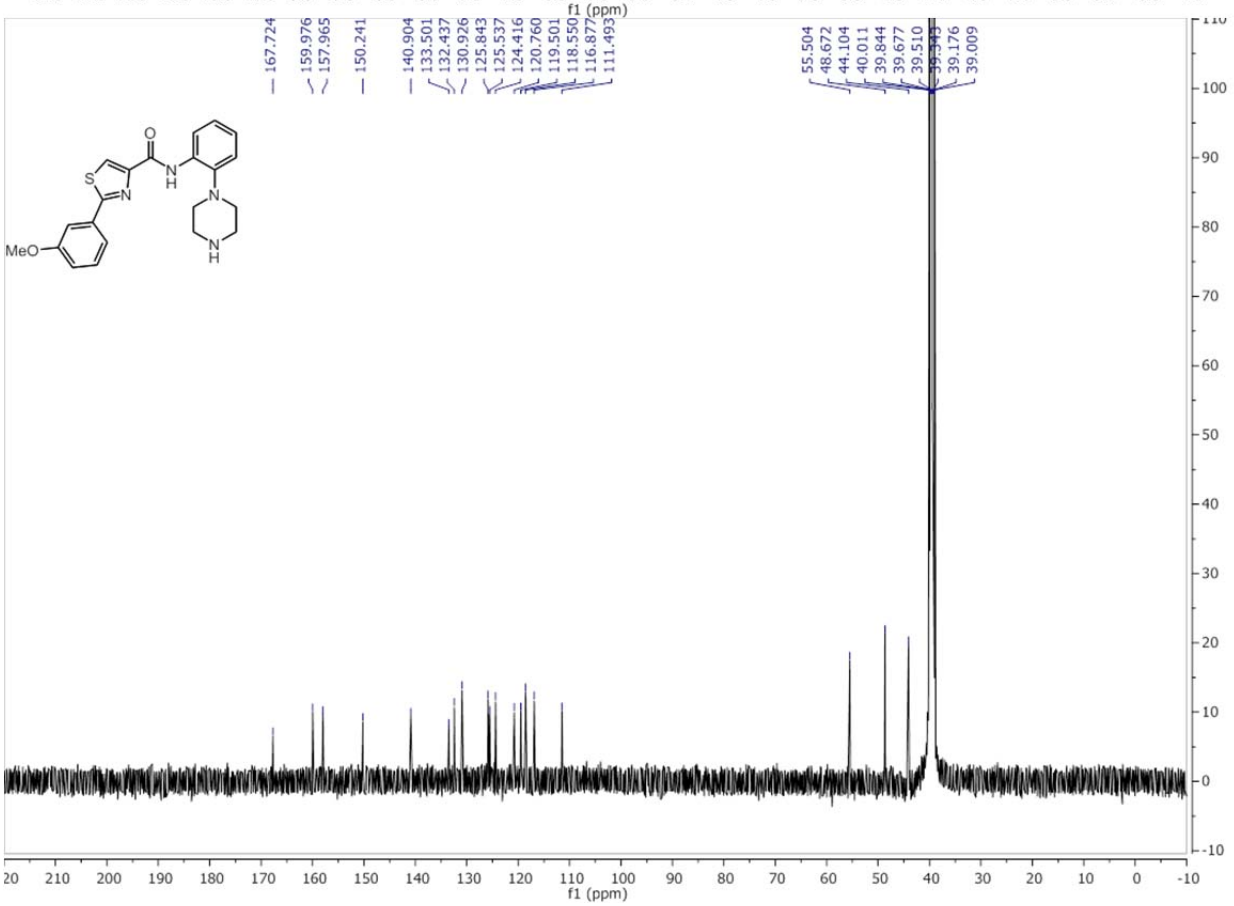
N-(2-(piperazin-1-yl)phenyl)-2-(m-tolyl)thiazole-4-carboxamide (E31)



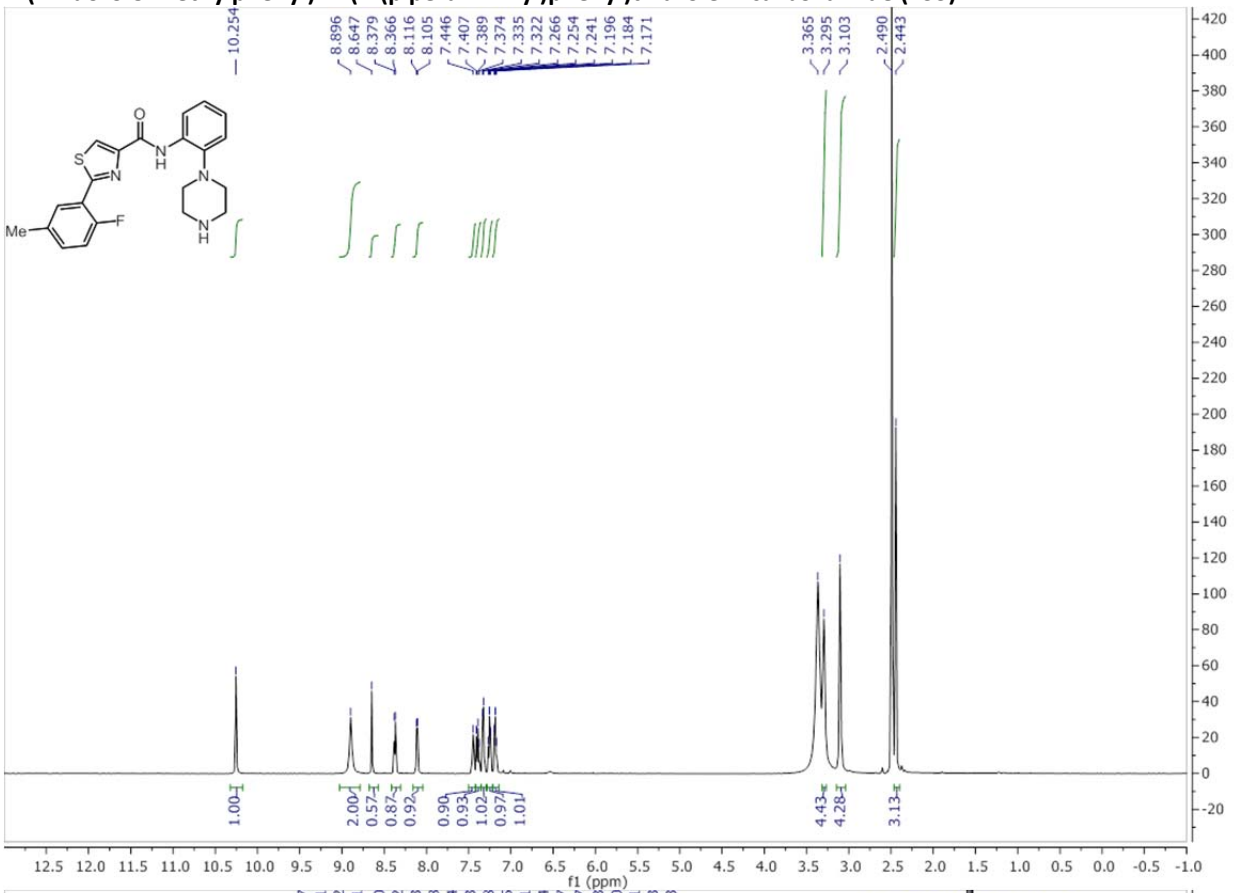


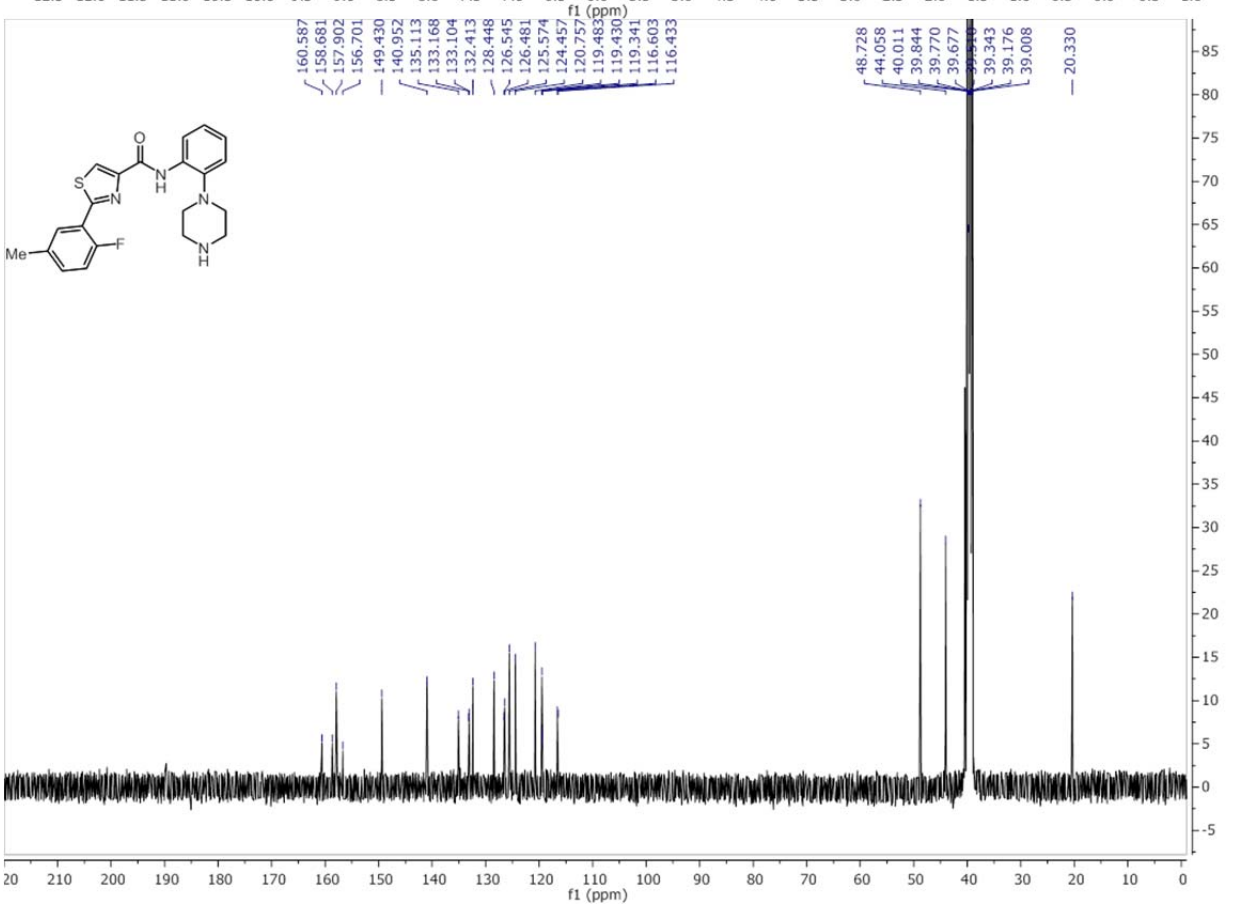
2-(3-methoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E32)



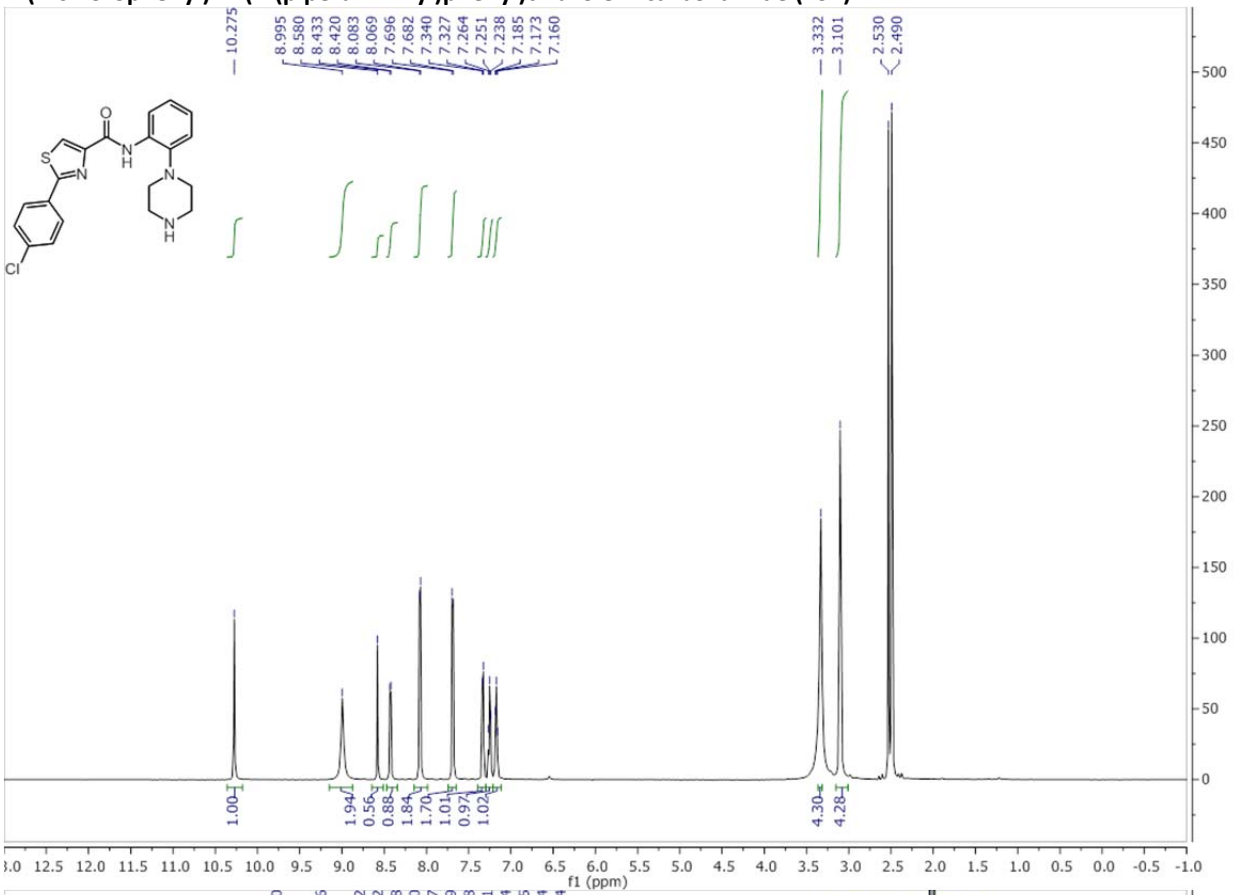


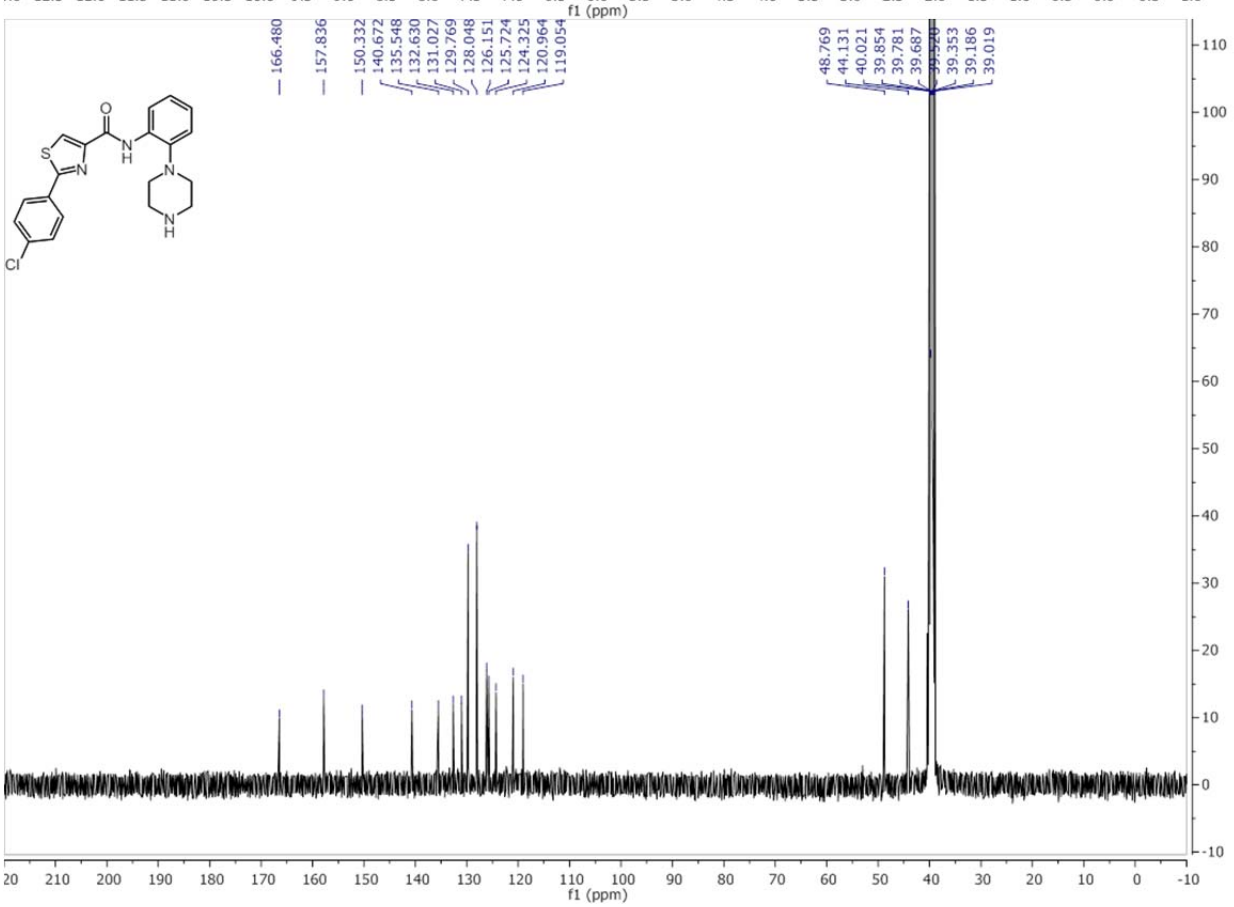
2-(2-fluoro-5-methylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E33)



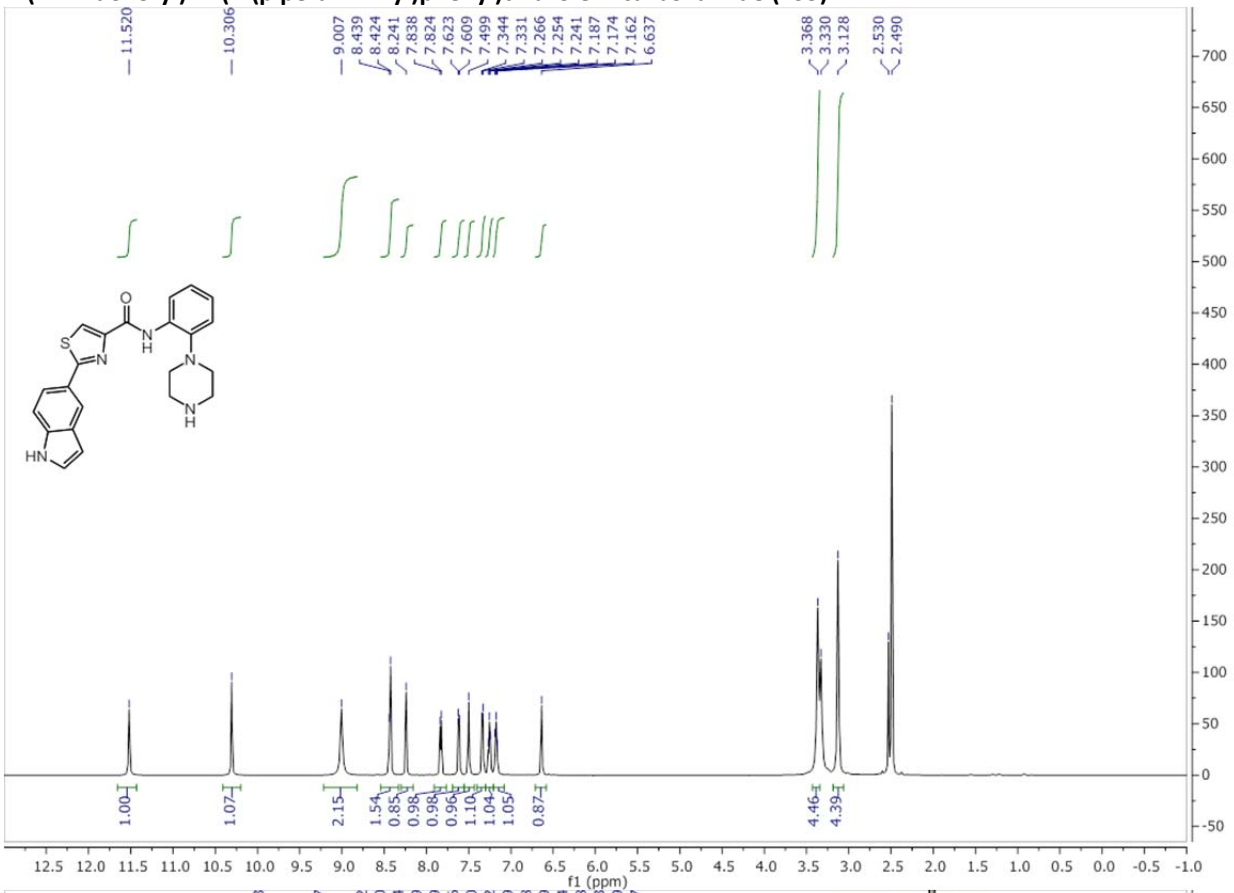


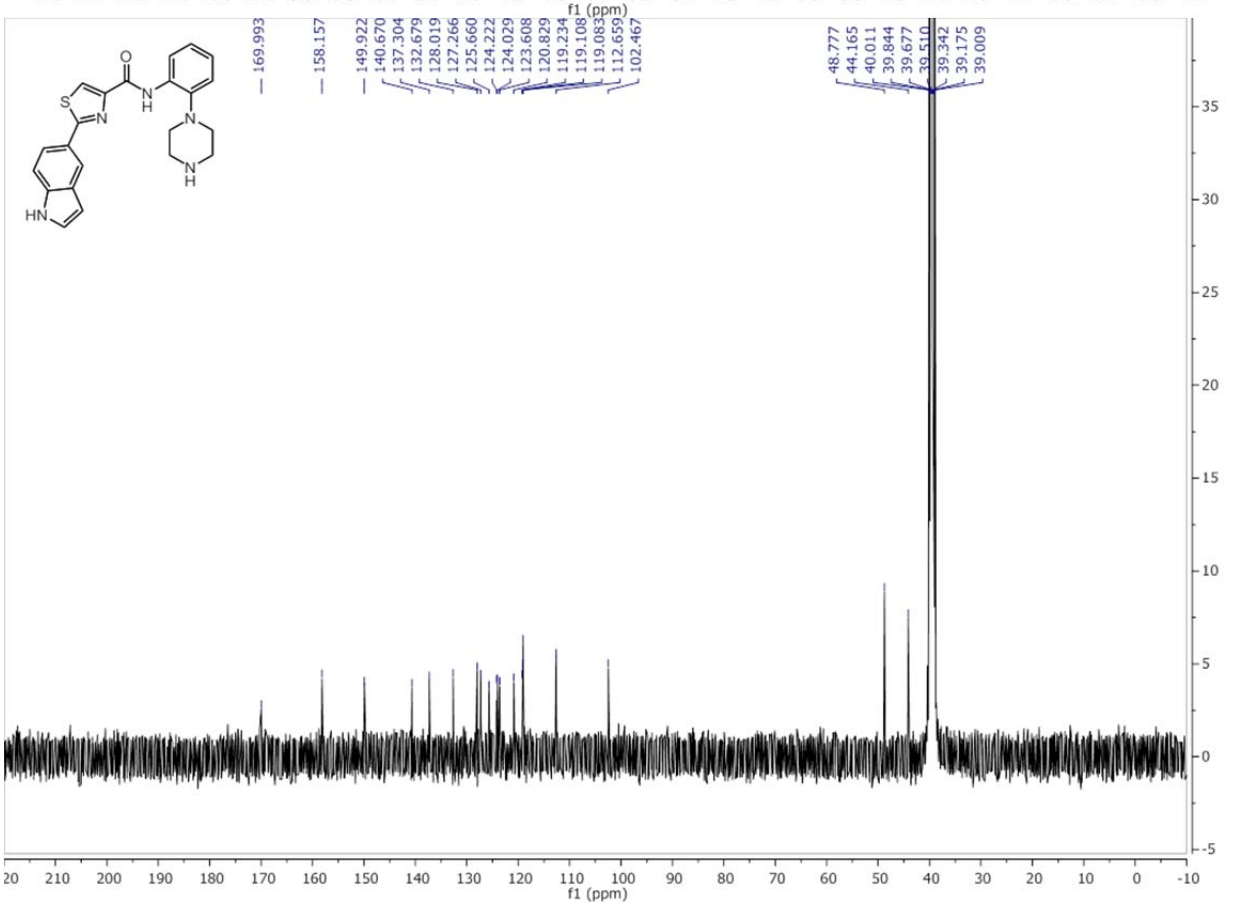
2-(4-chlorophenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E34)



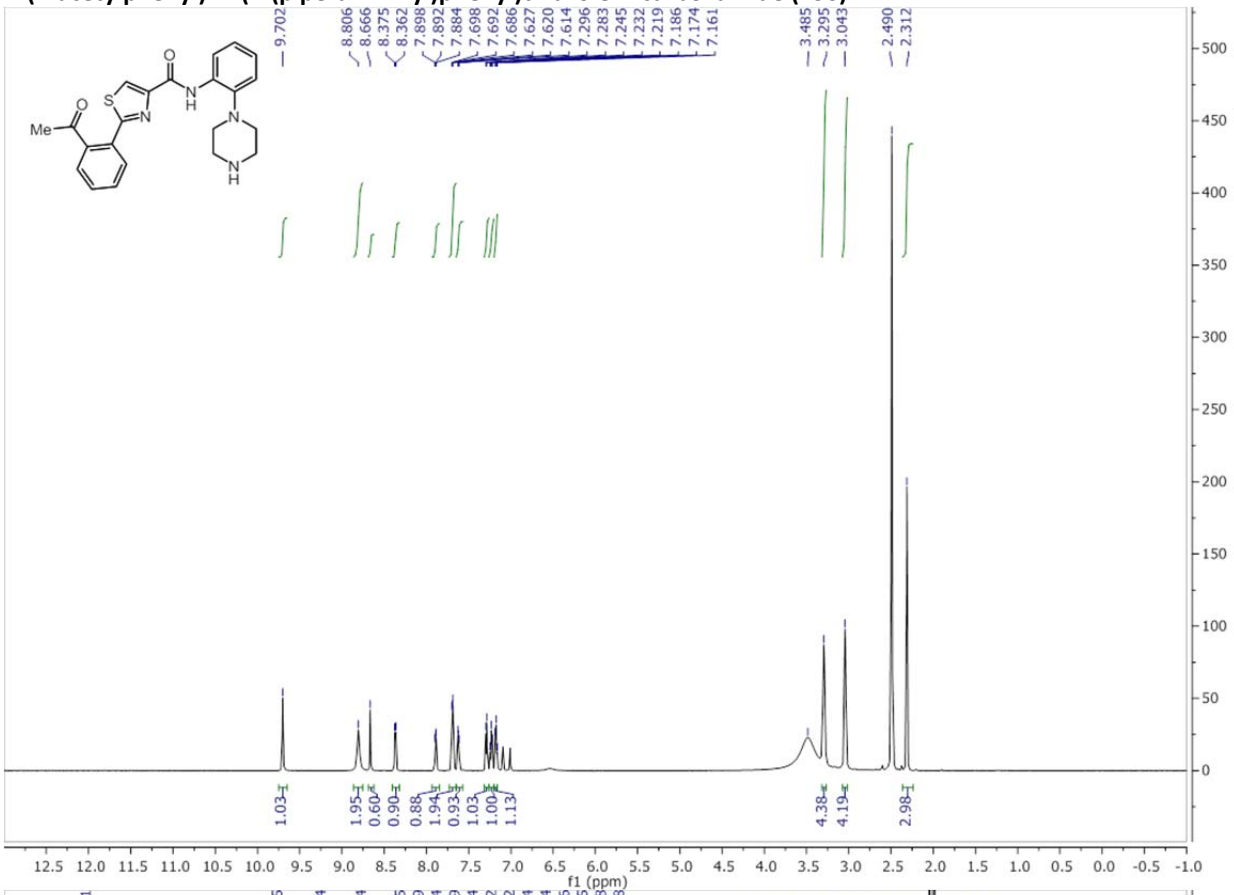


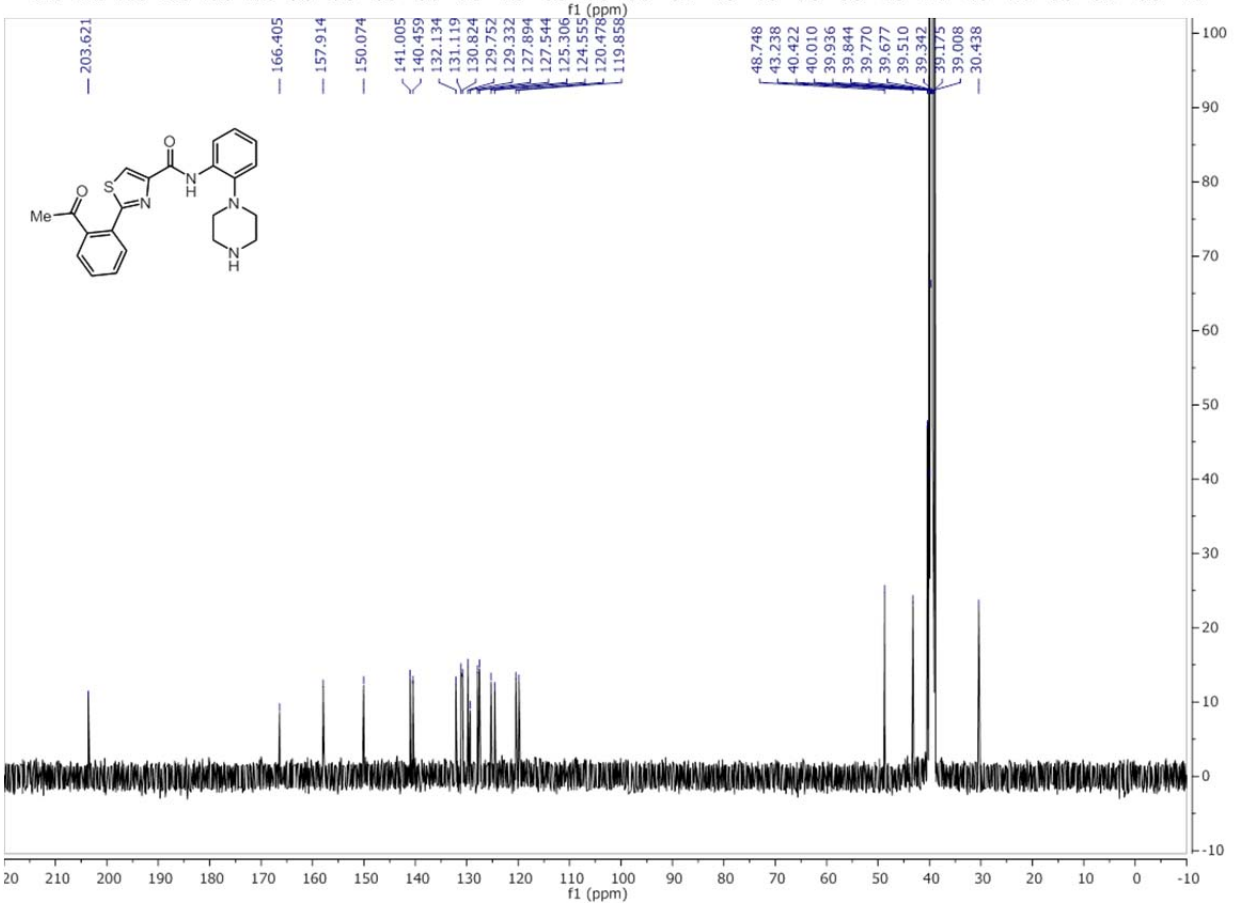
2-(1H-indol-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E35)



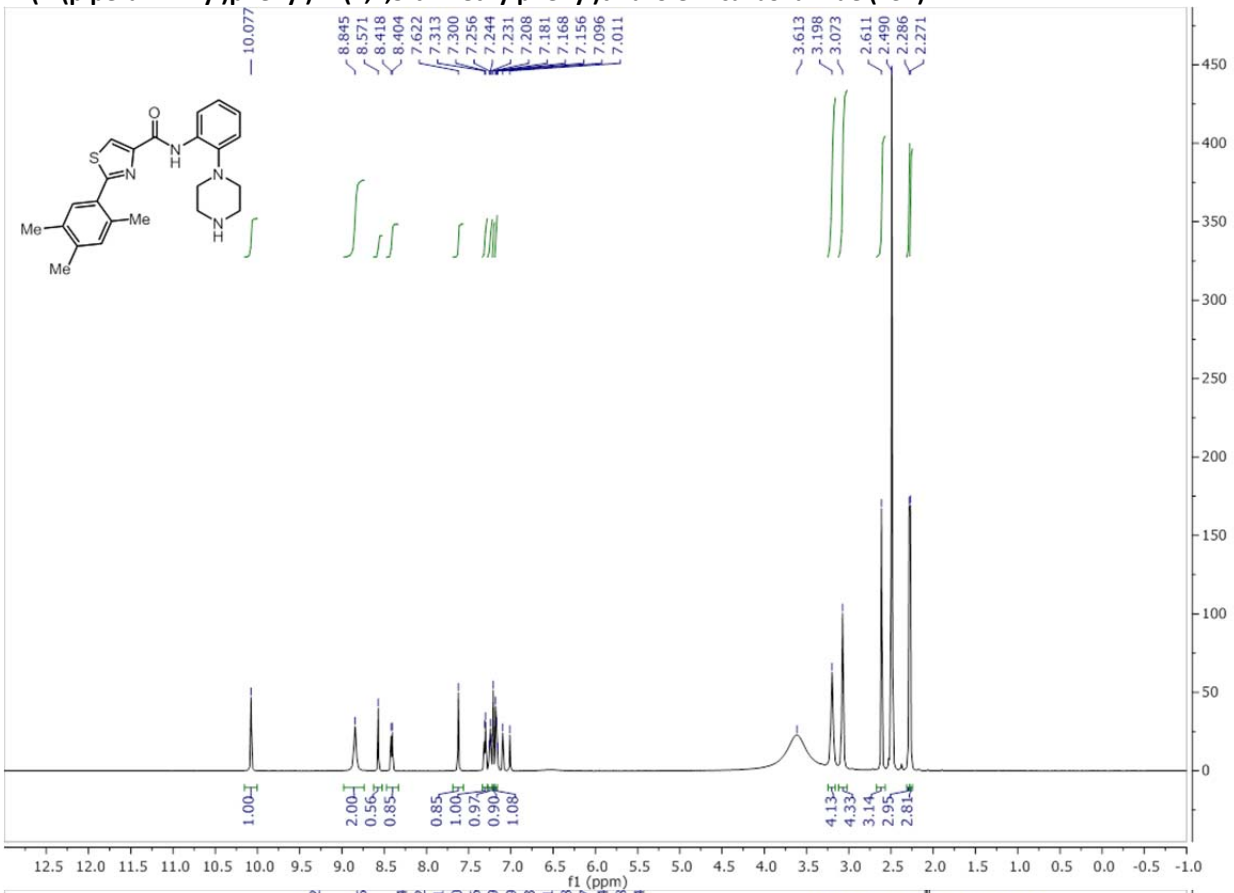


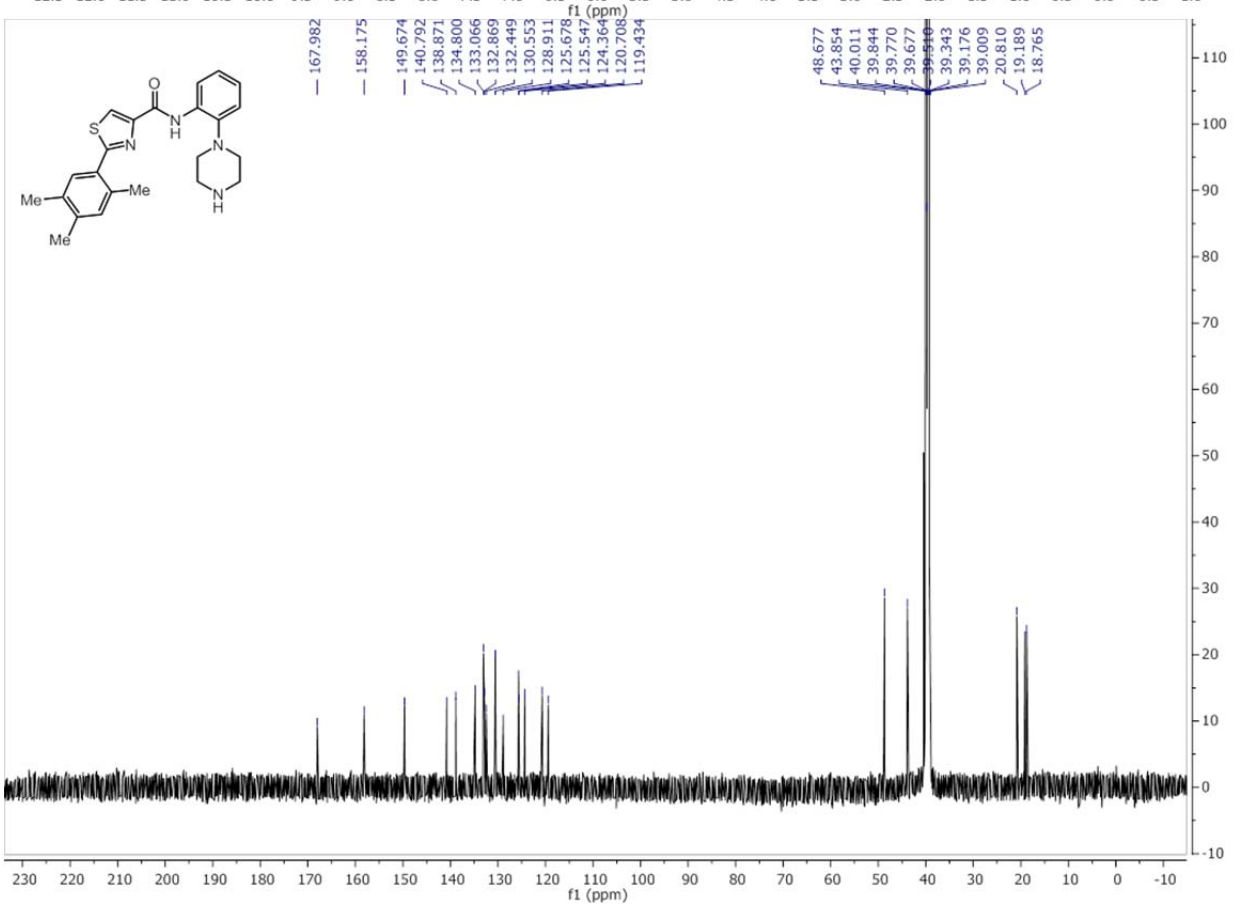
2-(2-acetylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E36)



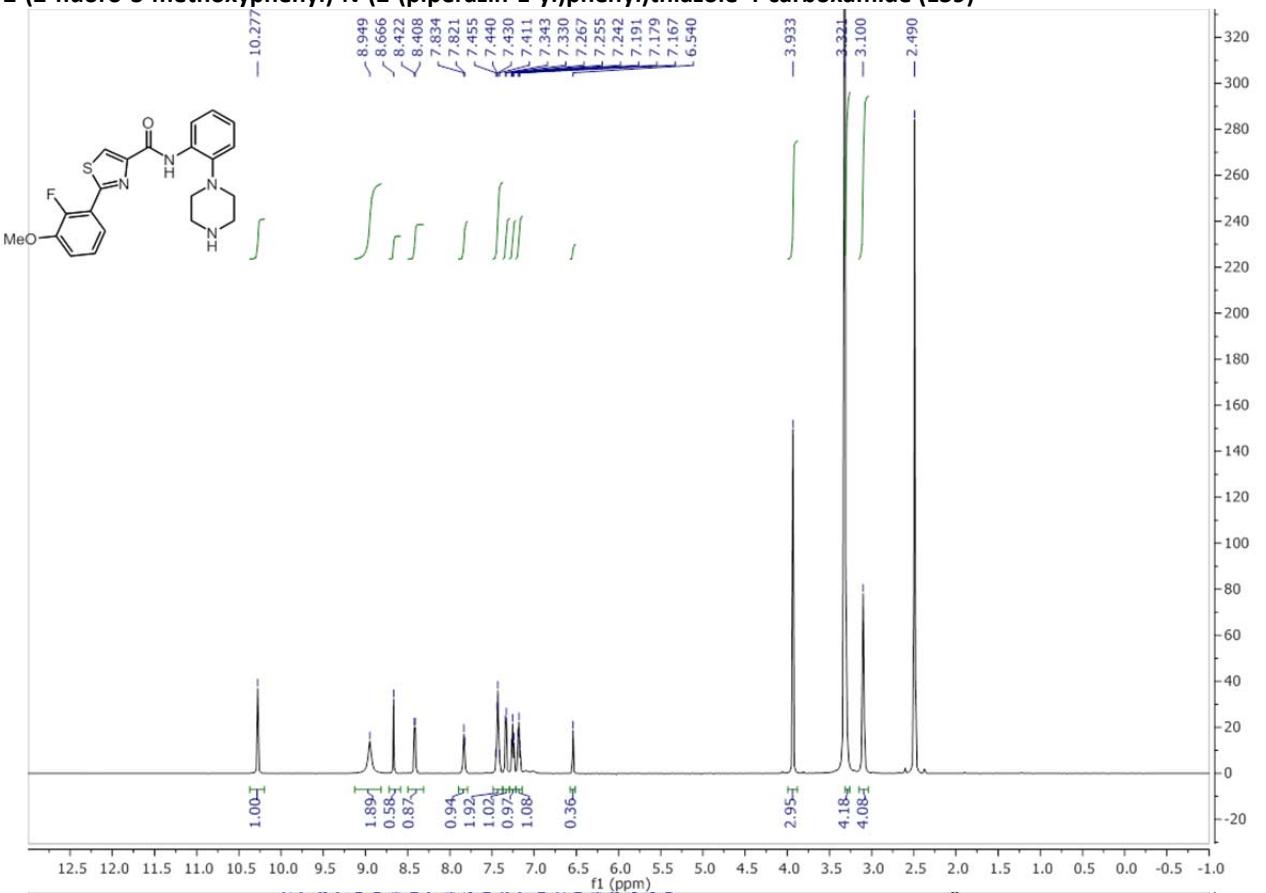


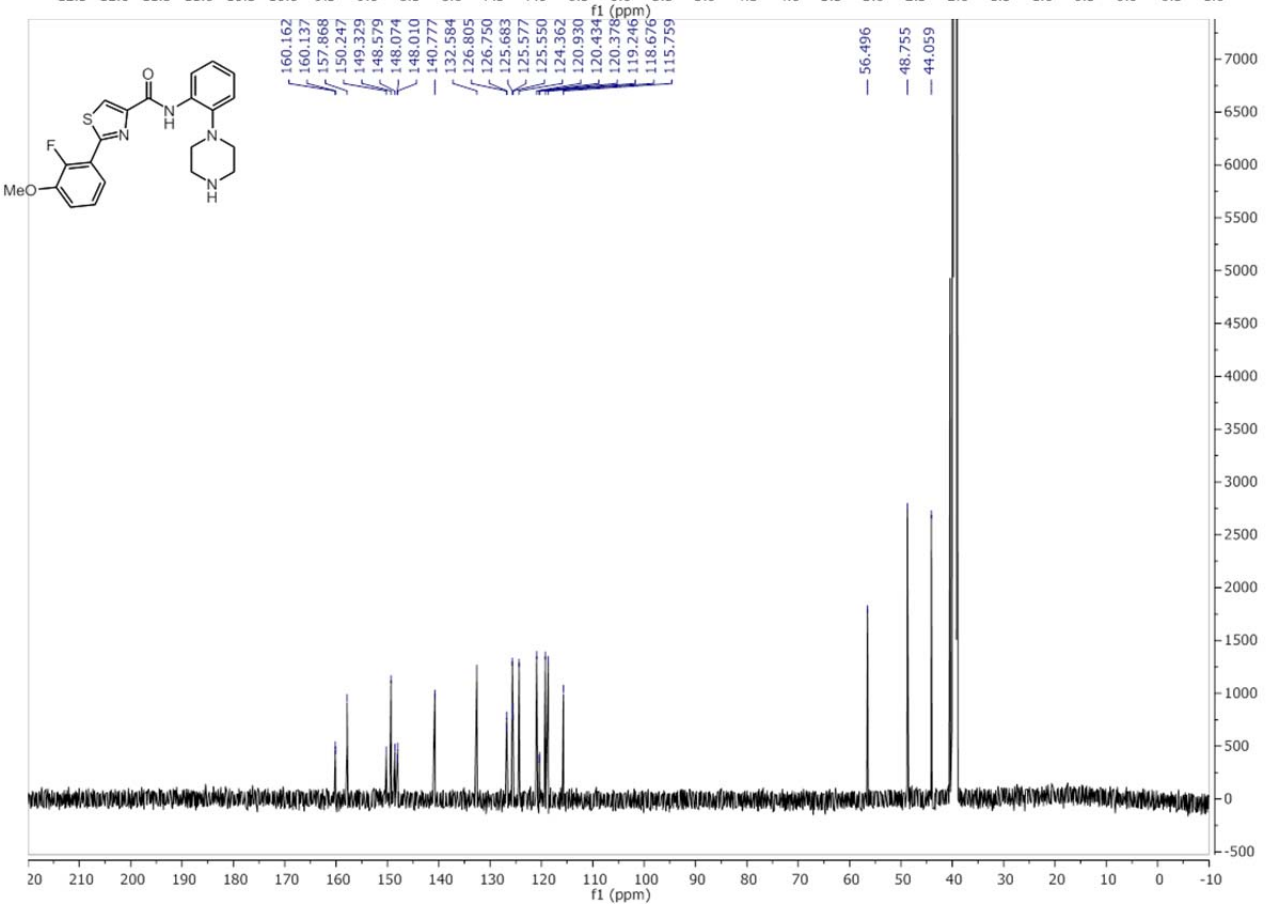
N-(2-(piperazin-1-yl)phenyl)-2-(2,4,5-trimethylphenyl)thiazole-4-carboxamide (E37)



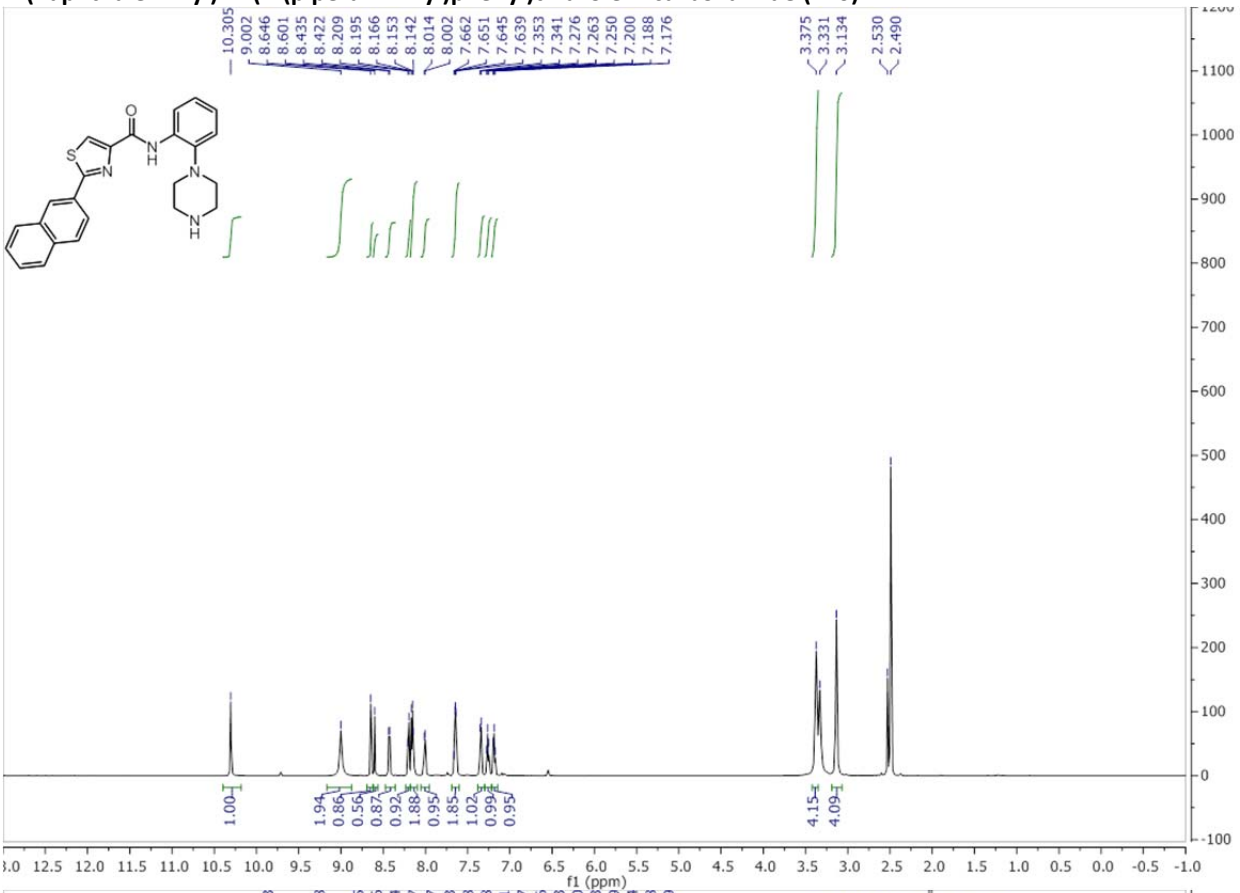


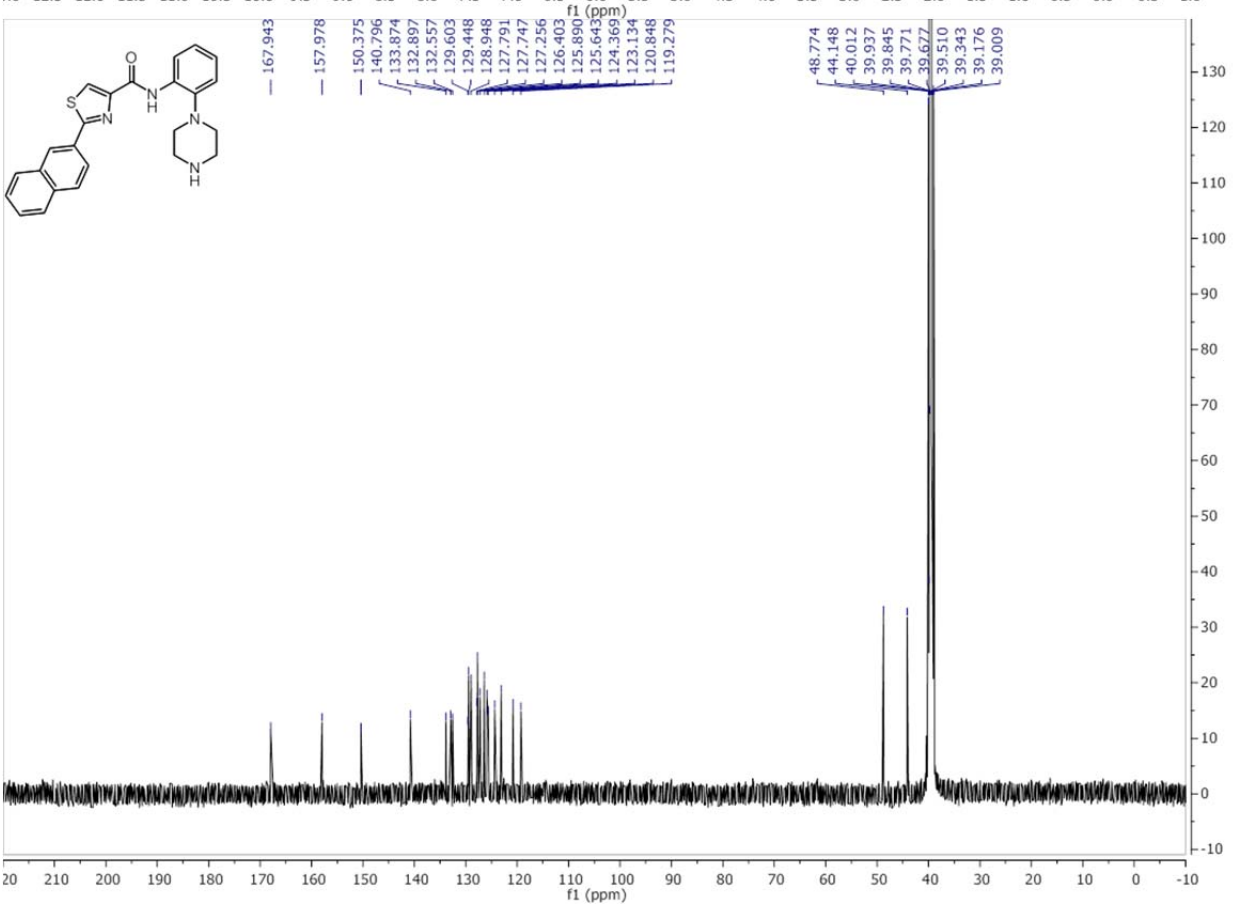
2-(2-fluoro-3-methoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E39)



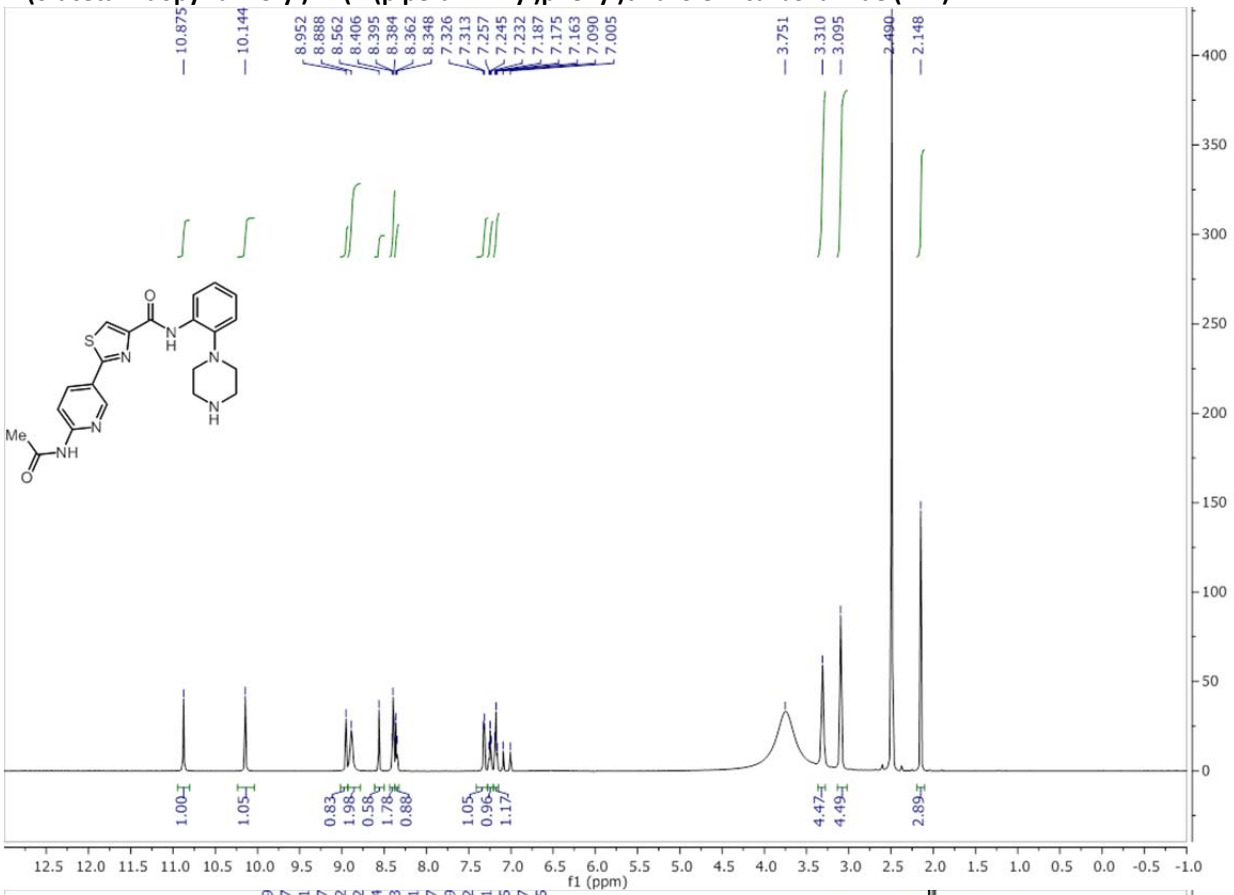


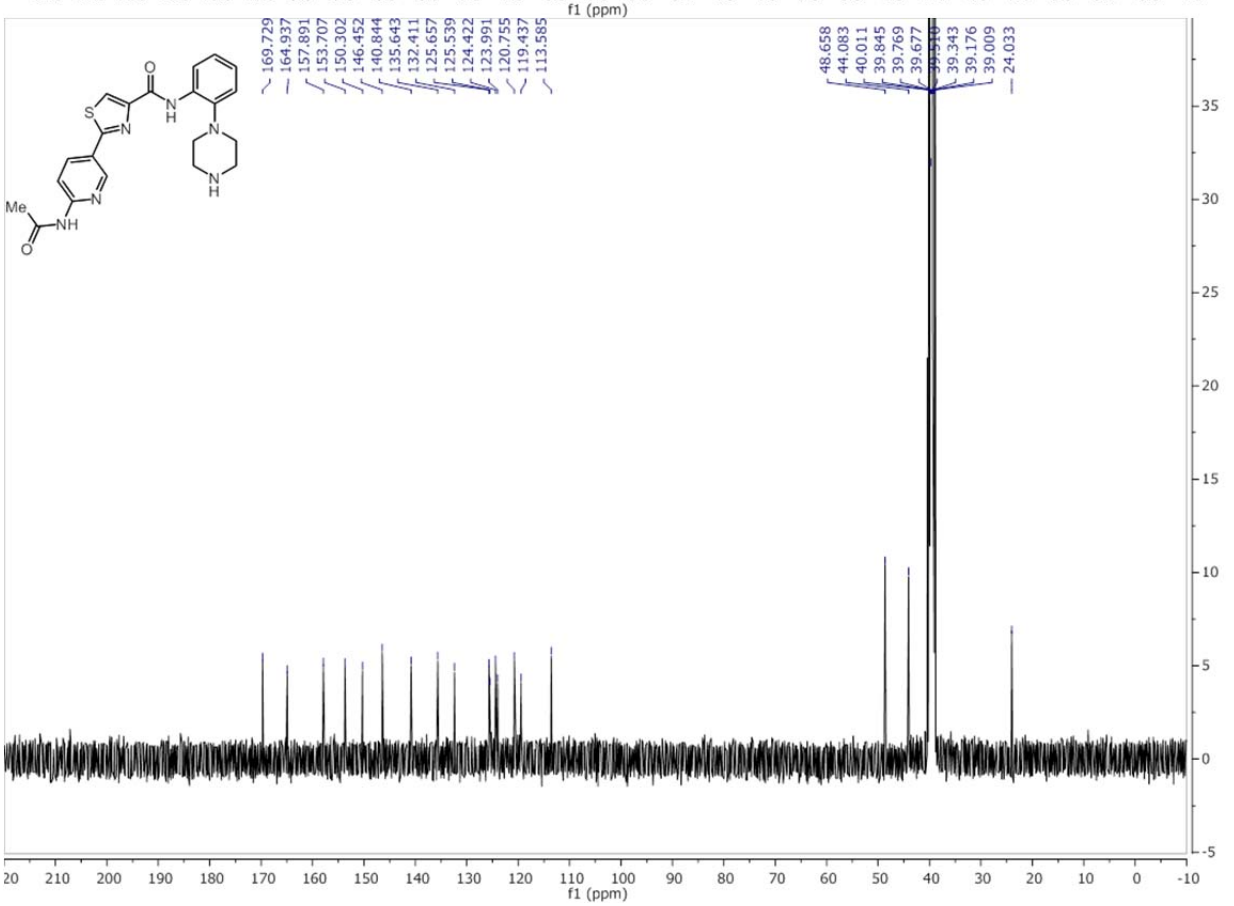
2-(naphthalen-2-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E40)



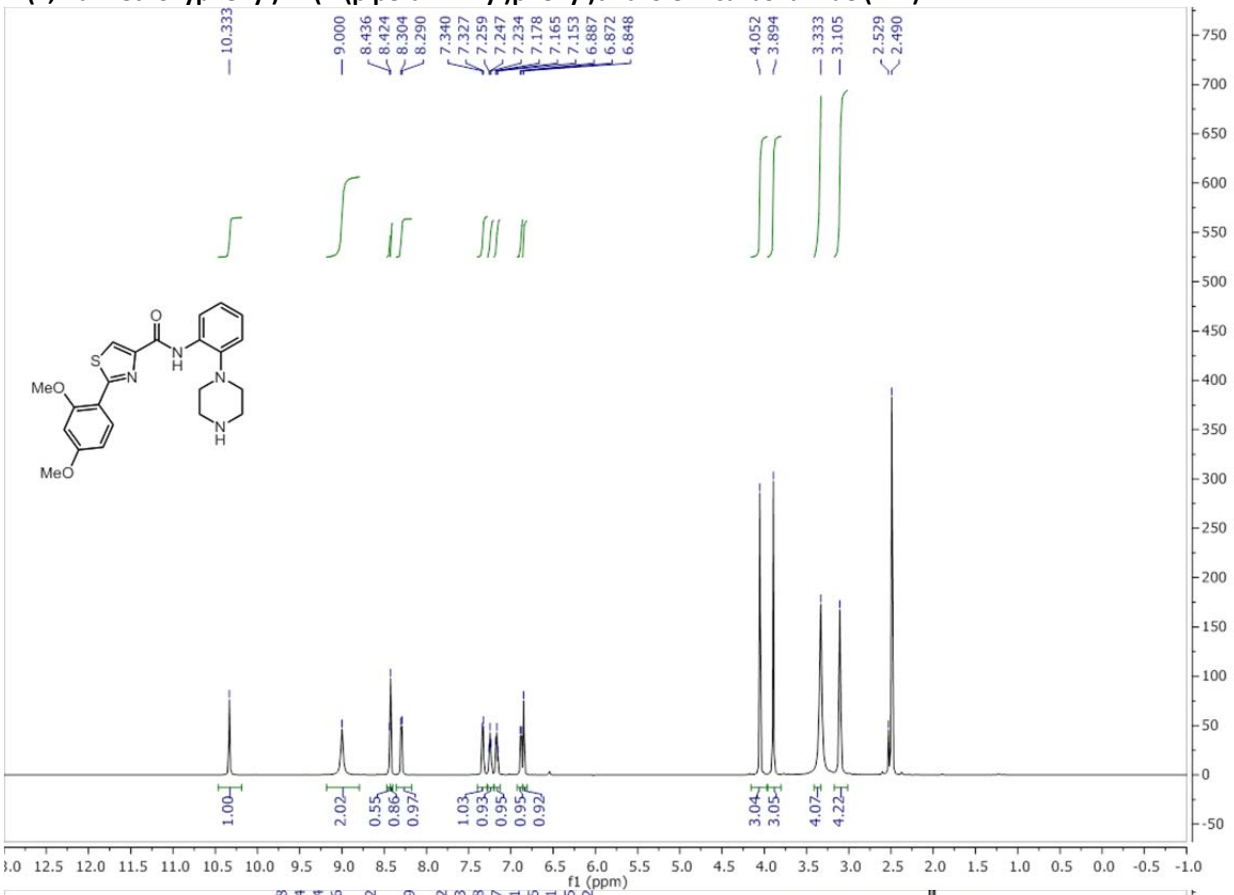


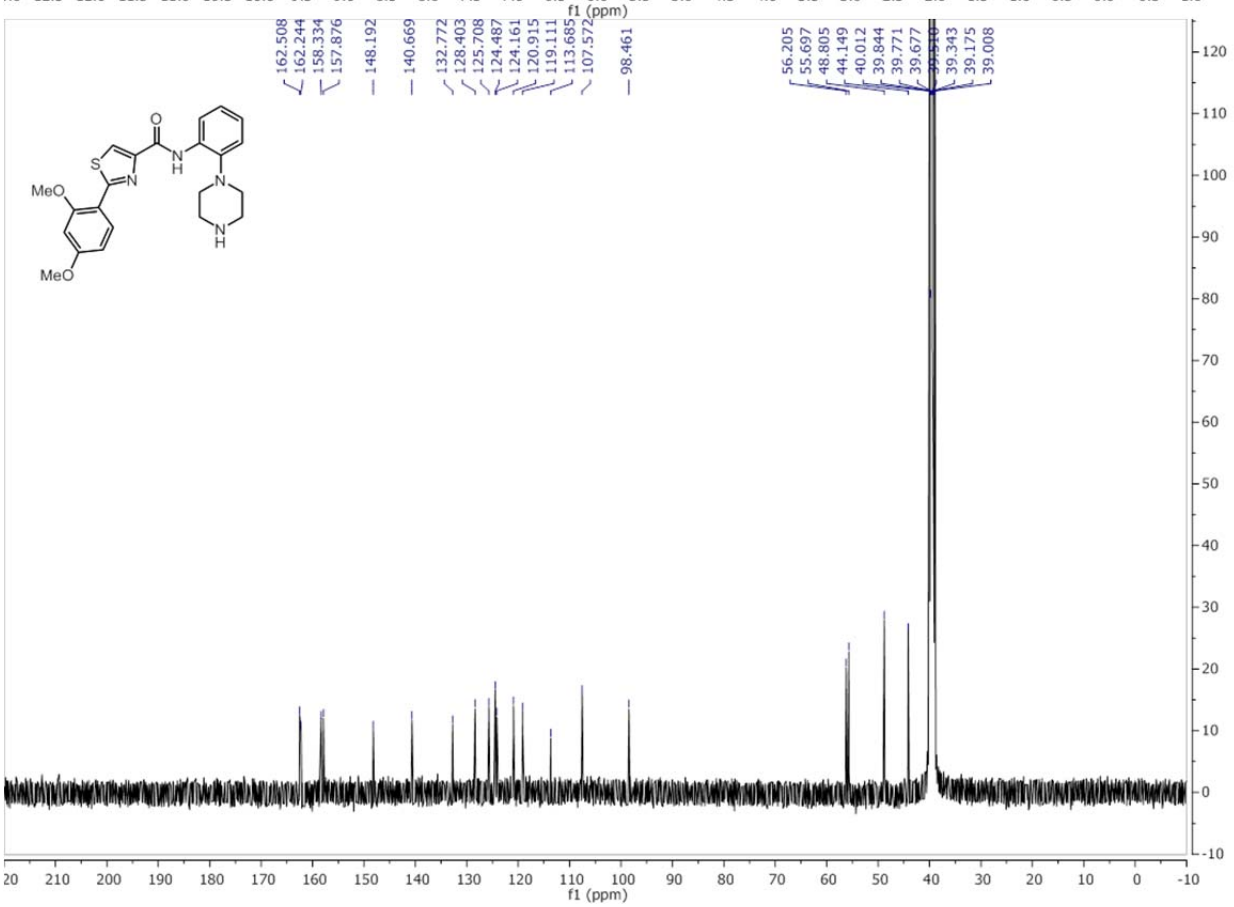
2-(6-acetamidopyridin-3-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E41)



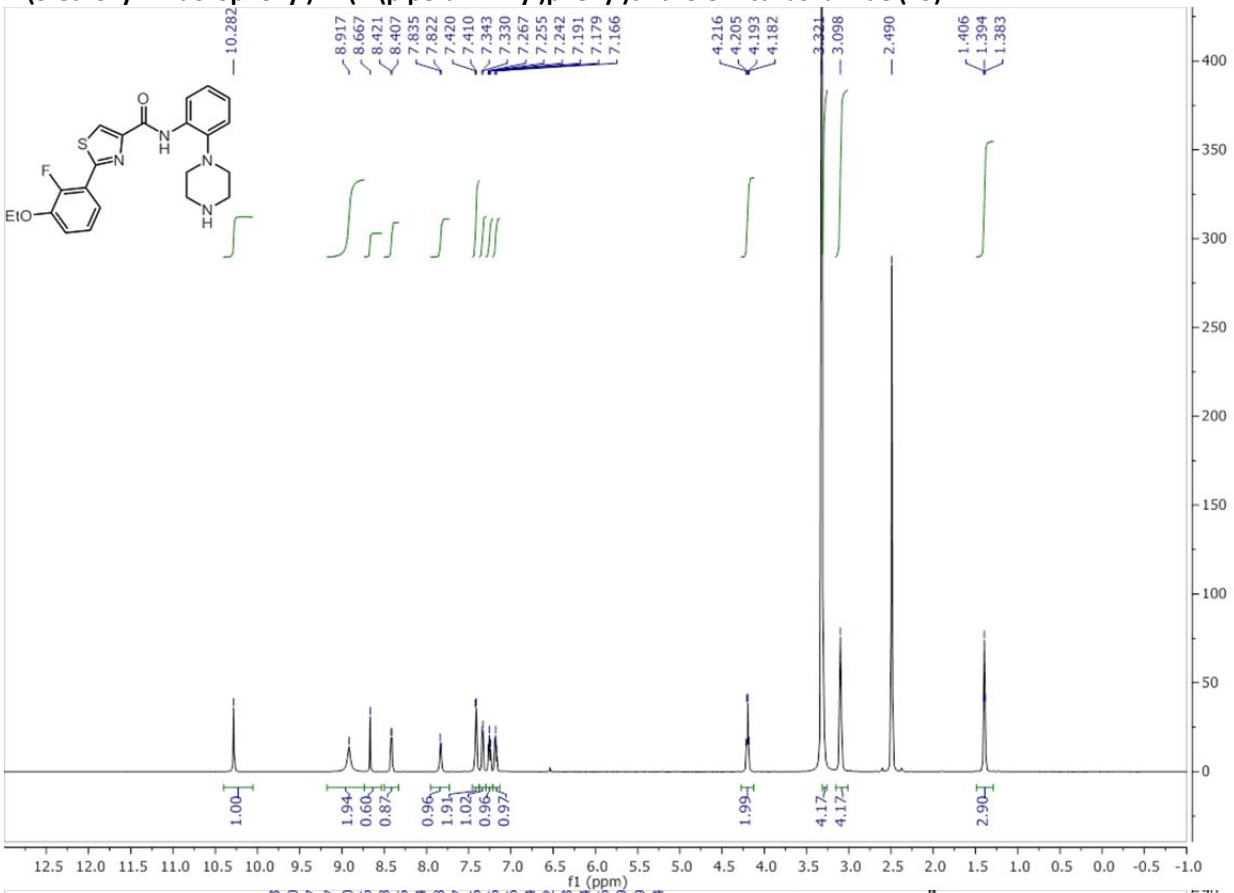


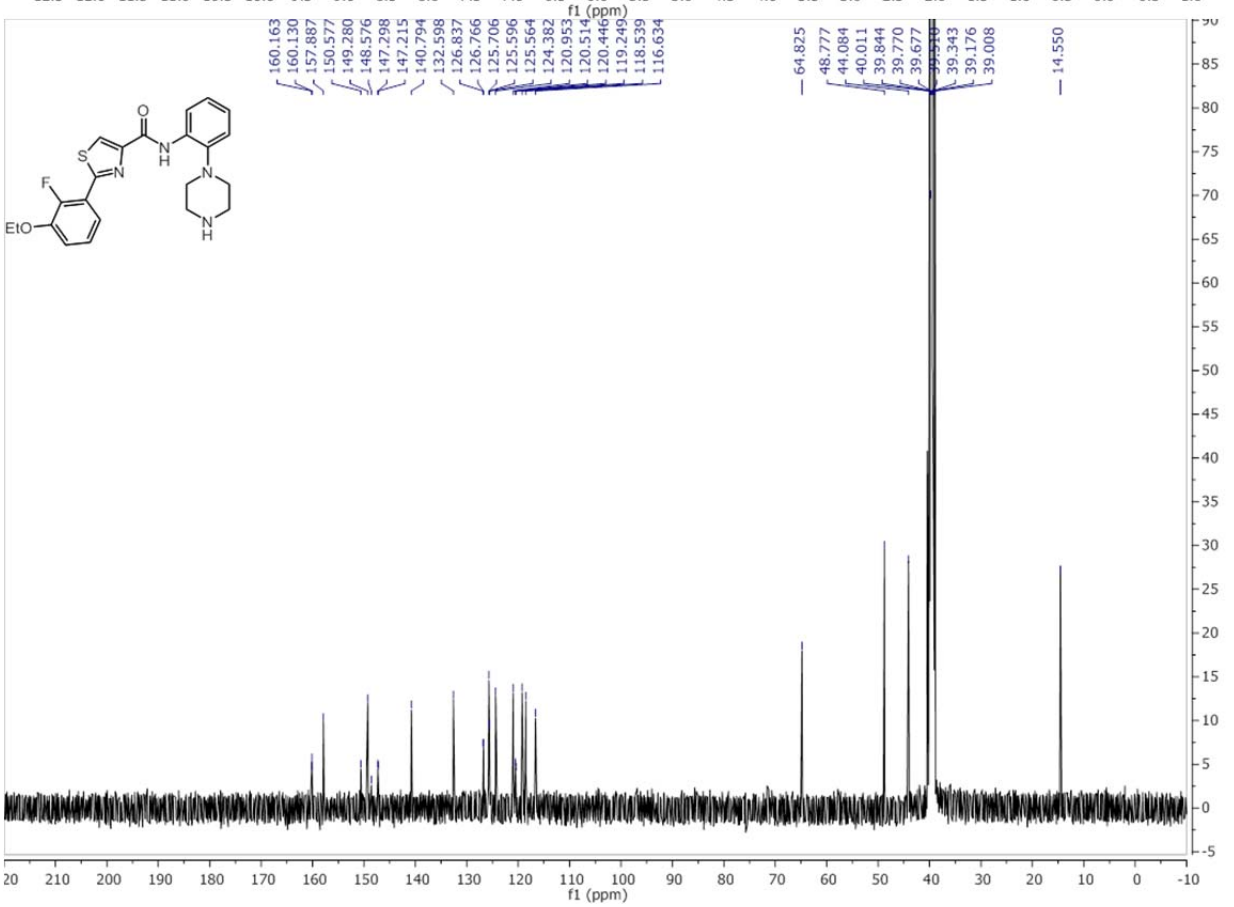
2-(2,4-dimethoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E42)



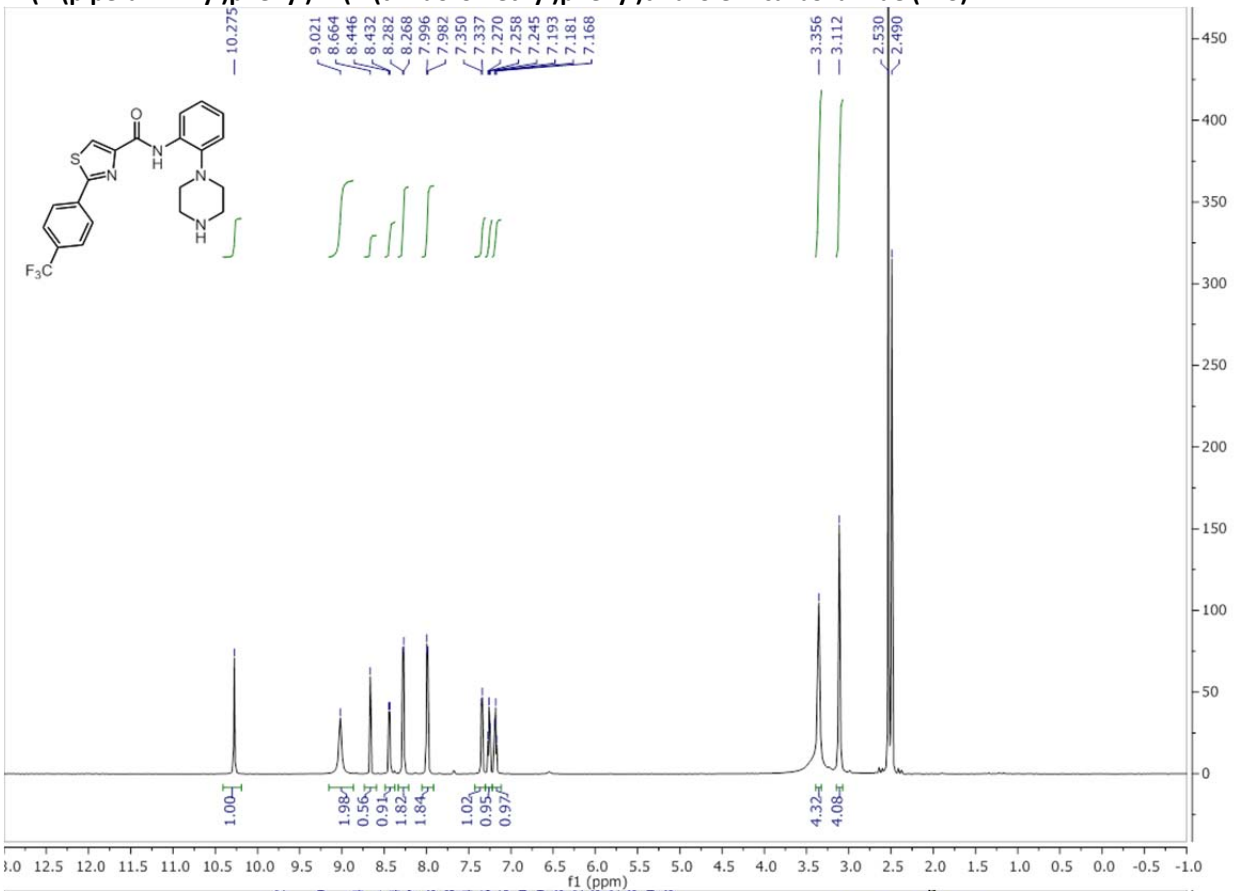


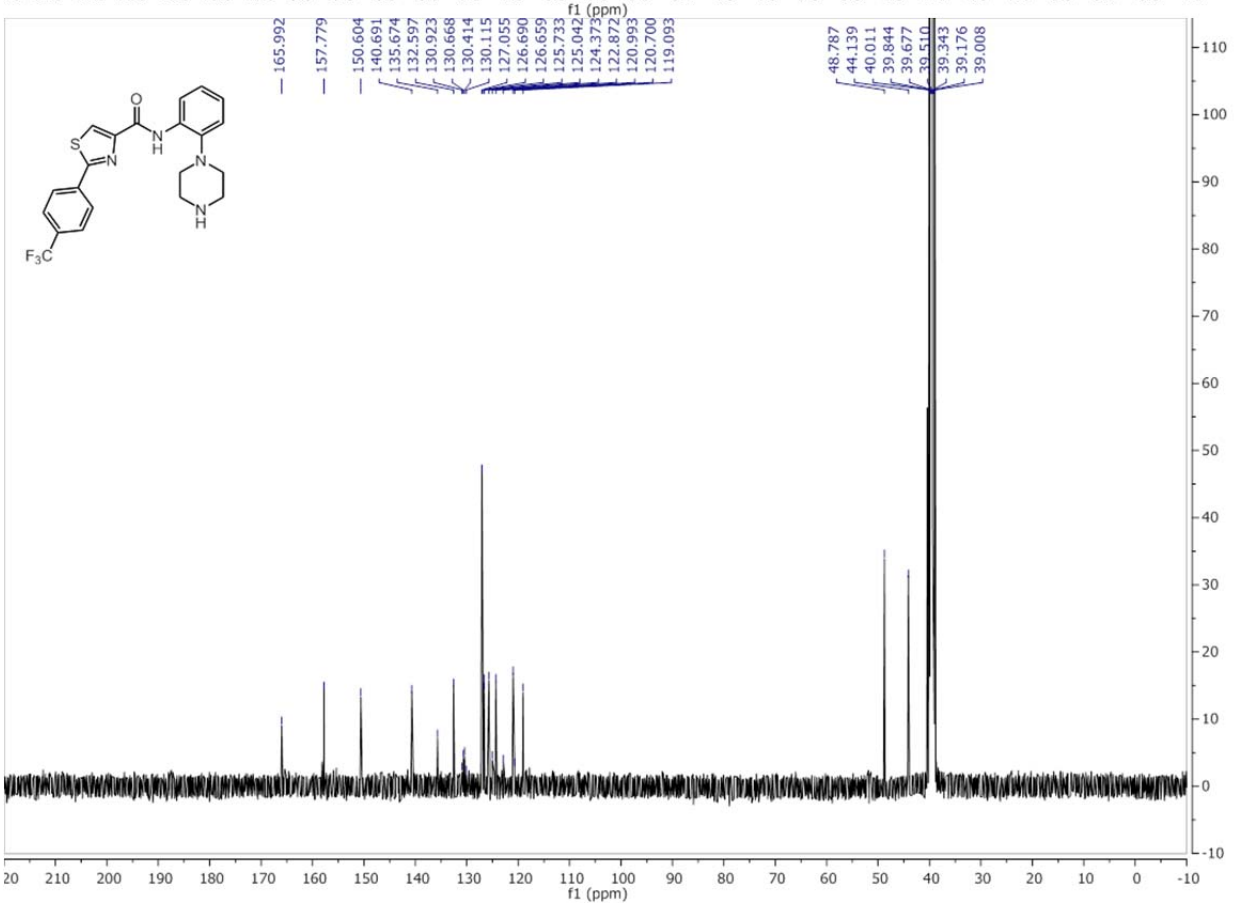
2-(3-ethoxy-2-fluorophenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (45)



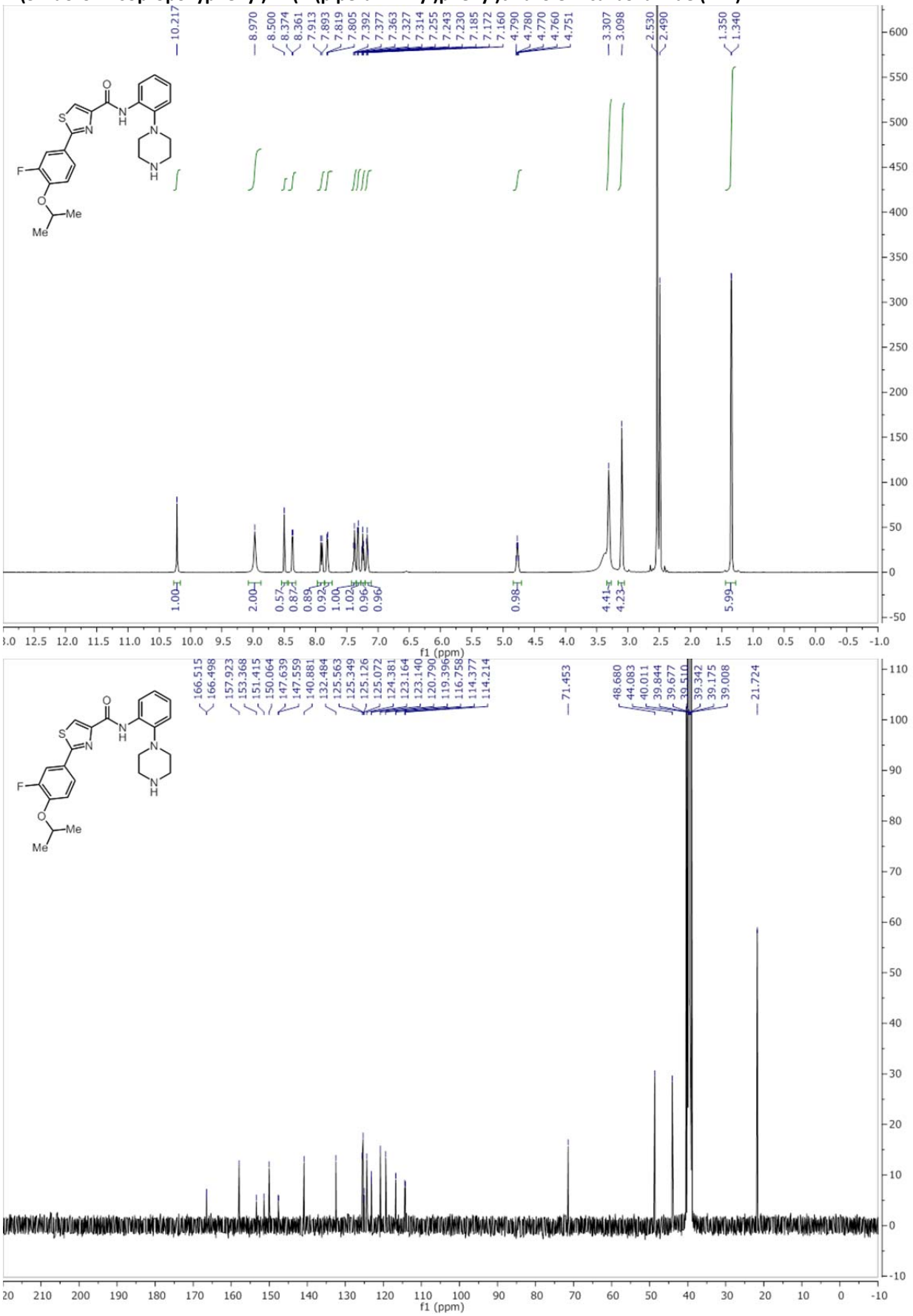


N-(2-(piperazin-1-yl)phenyl)-2-(4-(trifluoromethyl)phenyl)thiazole-4-carboxamide (E43)

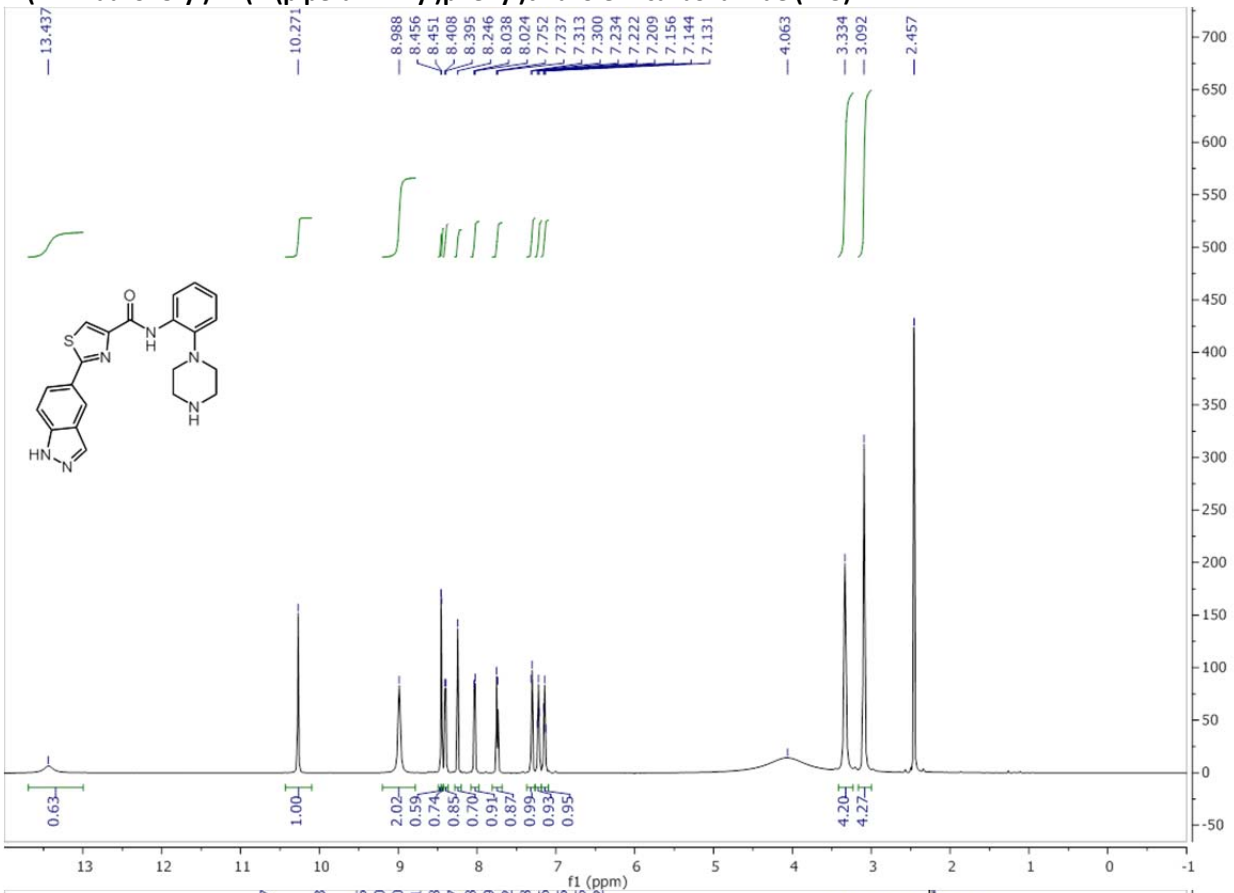


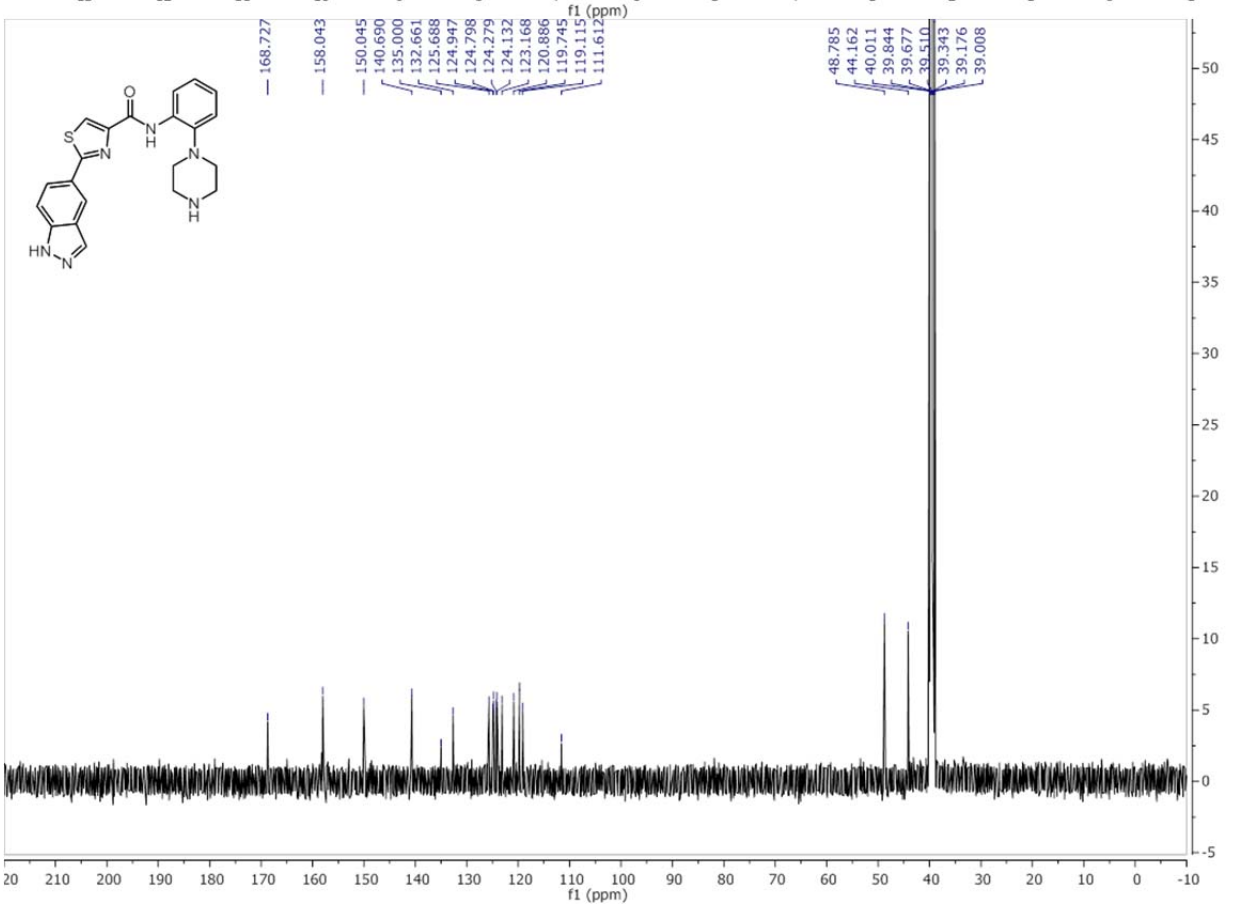


2-(3-fluoro-4-isopropoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E44)

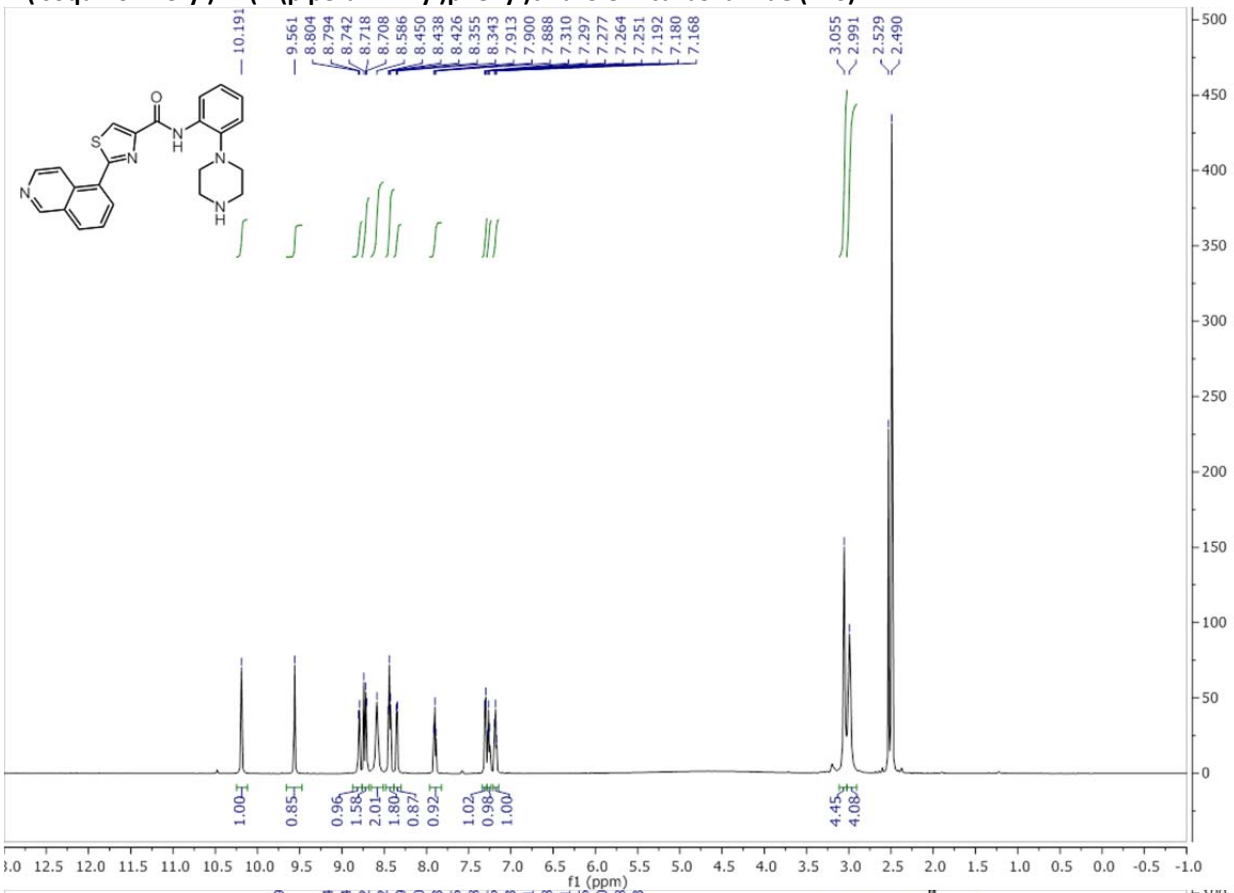


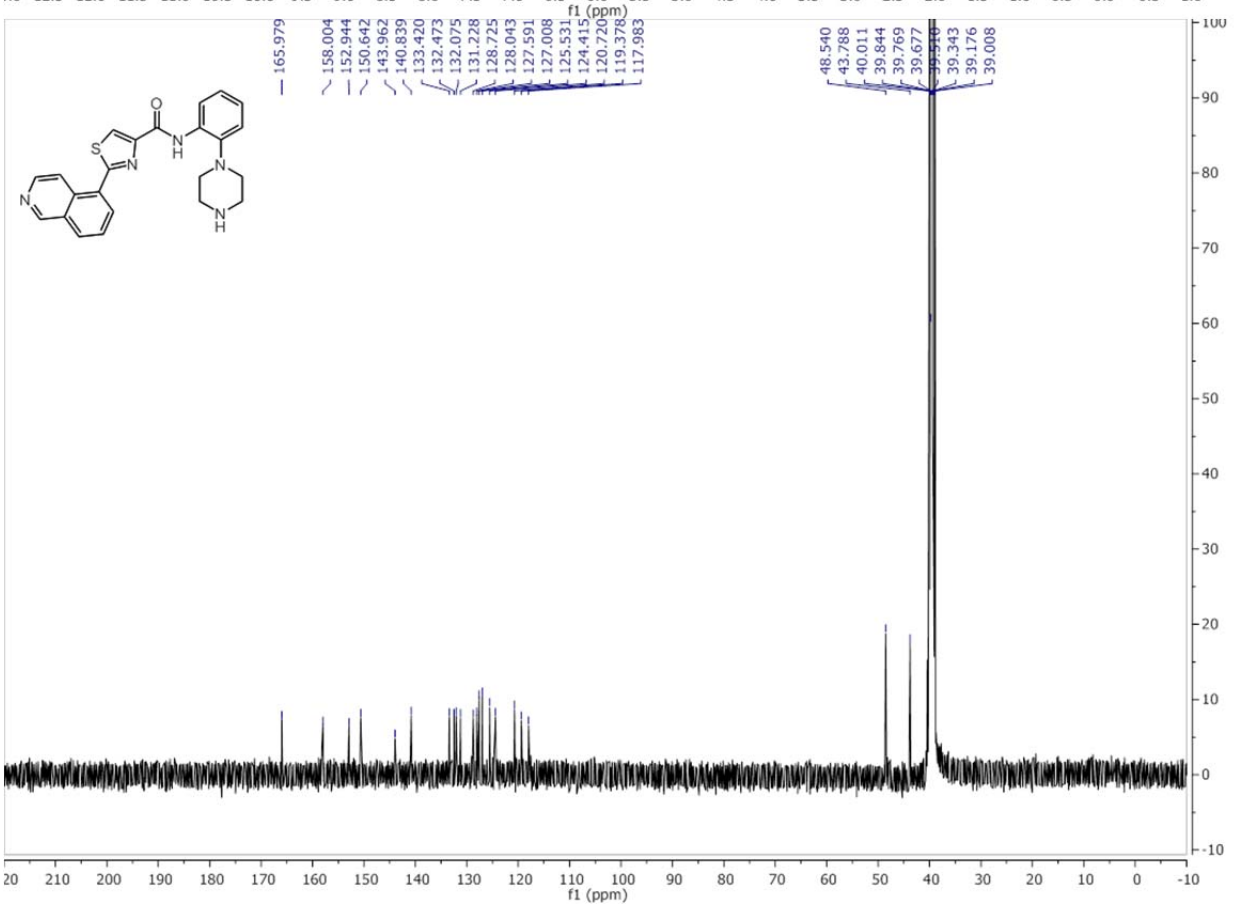
2-(1H-indazol-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E45)



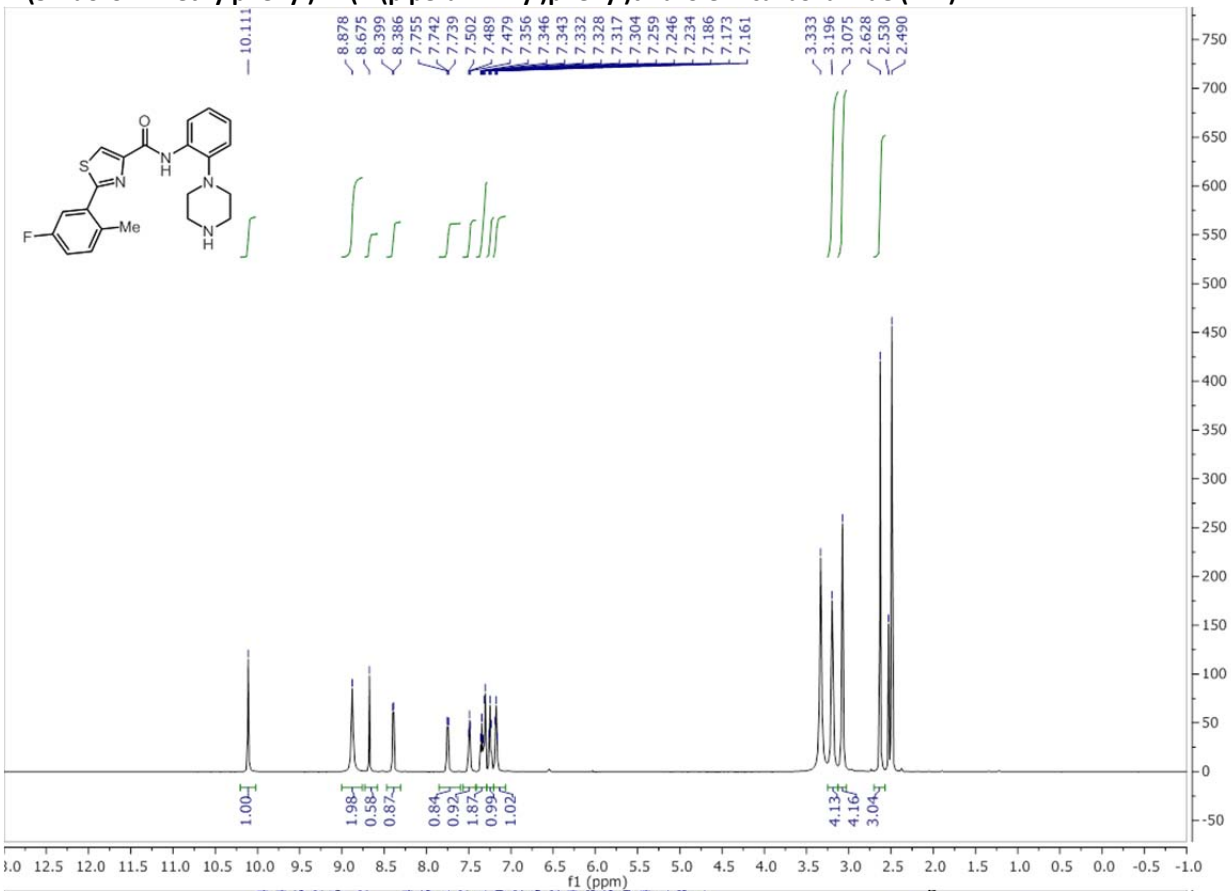


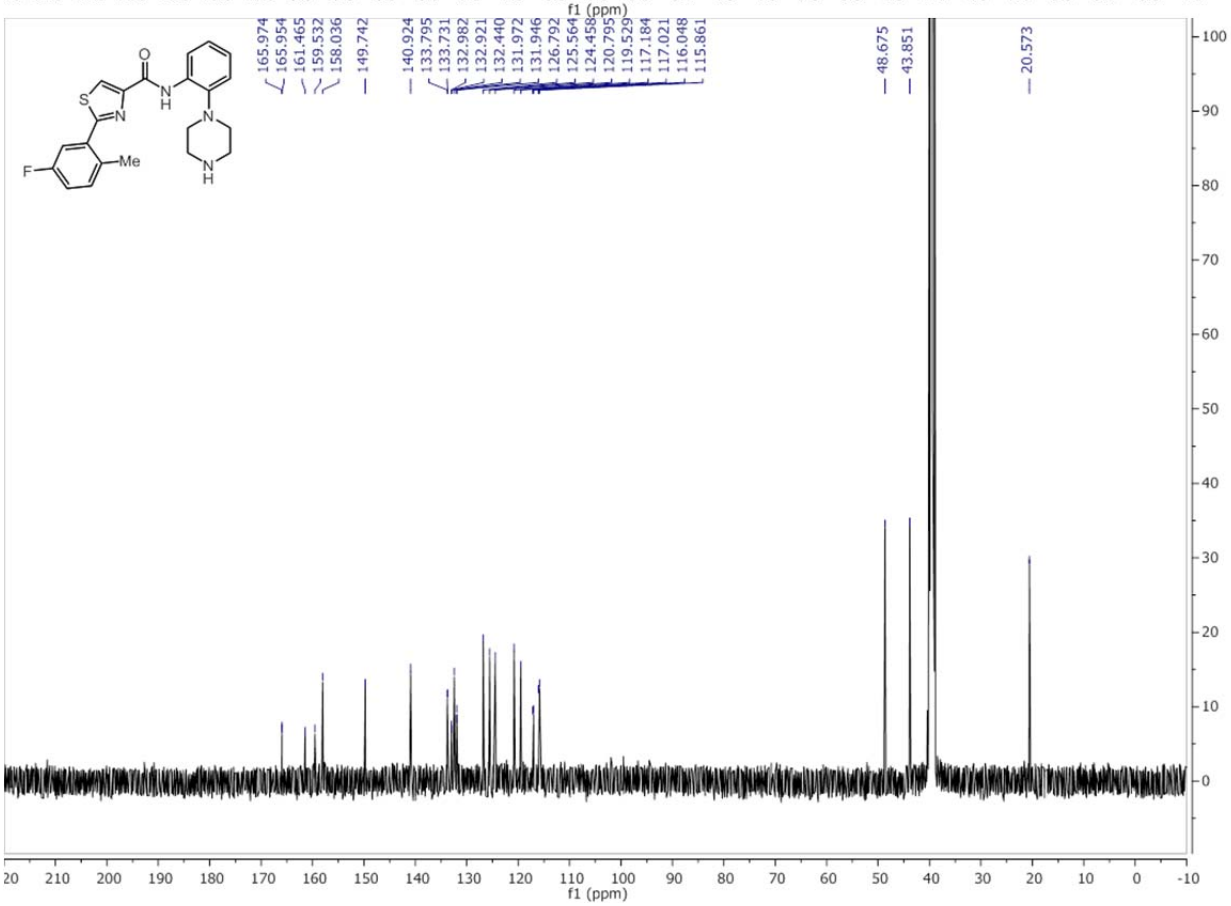
2-(isoquinolin-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E46)



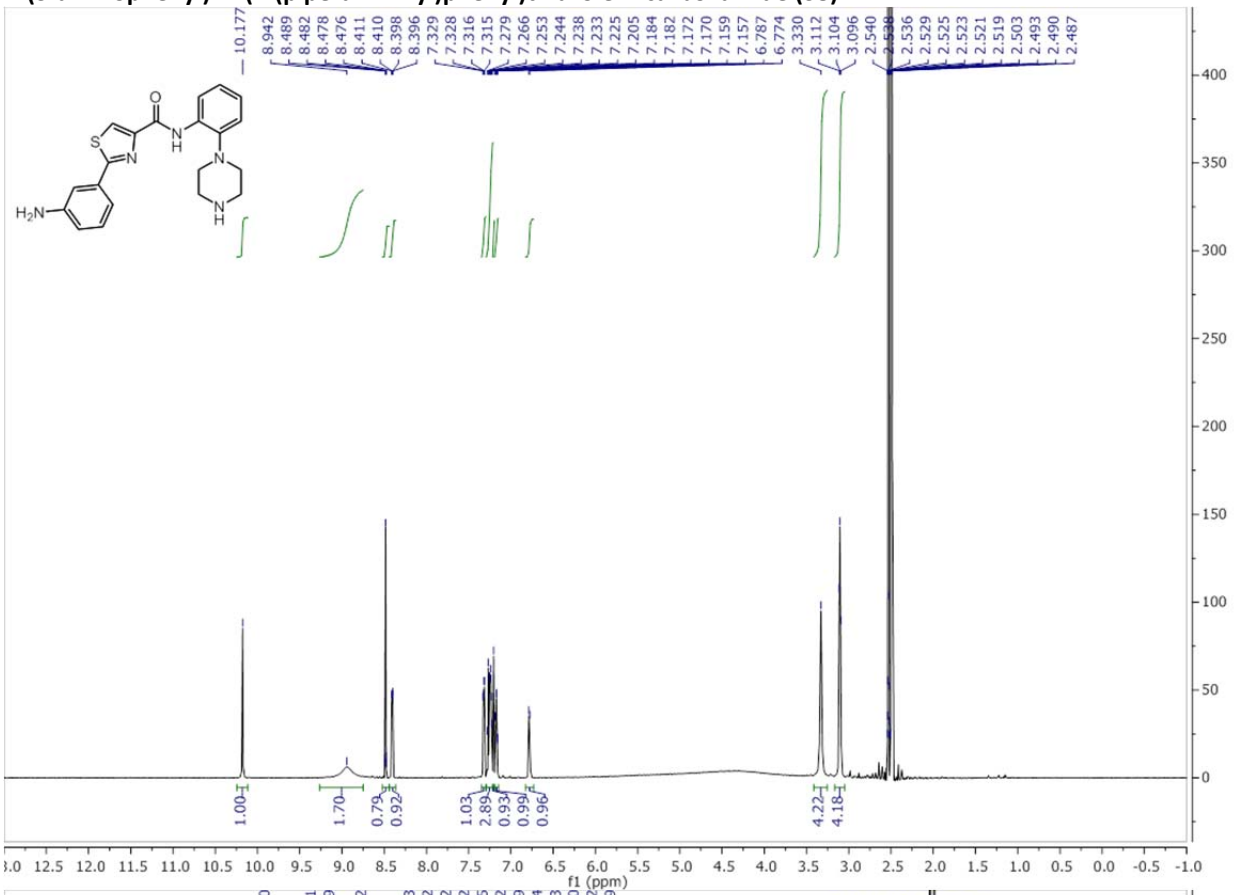


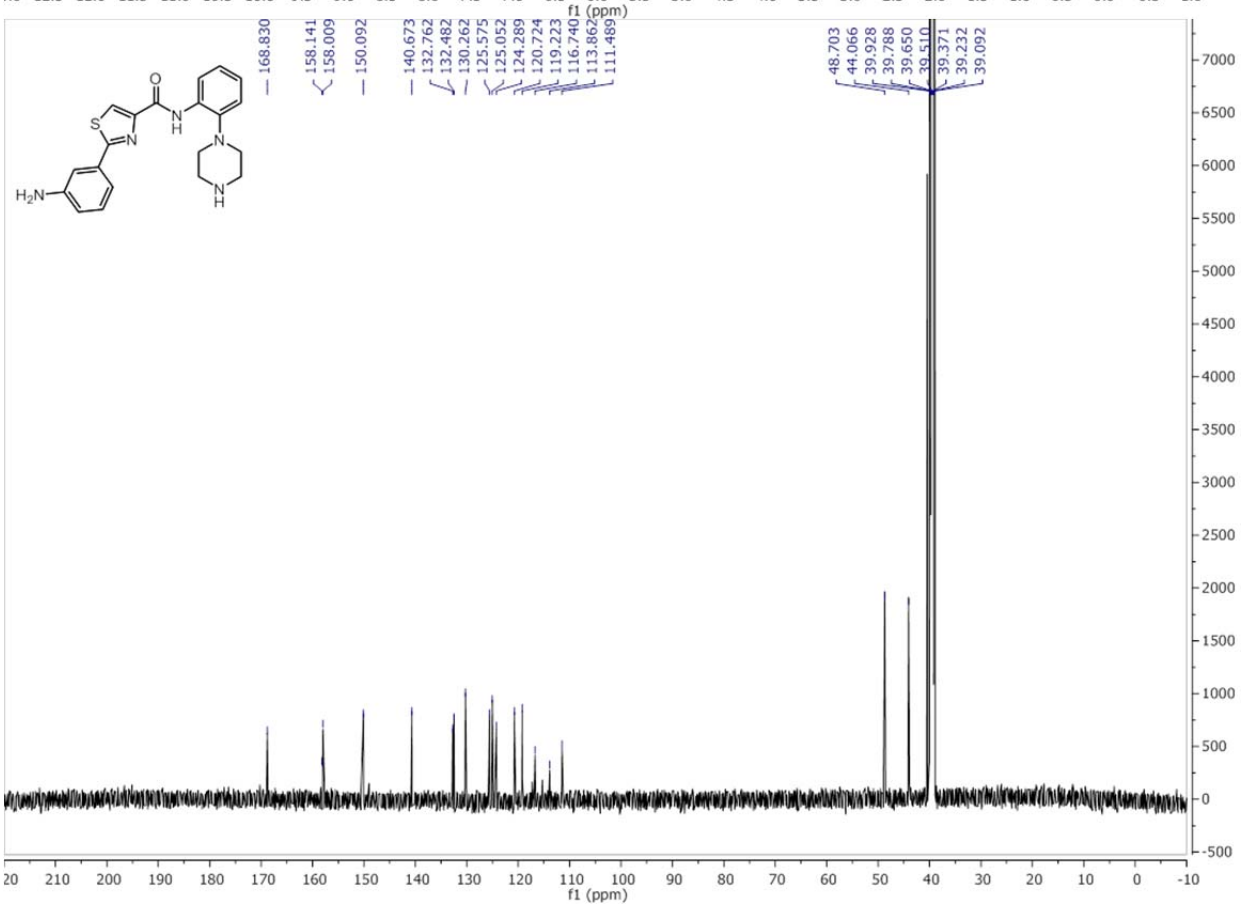
2-(5-fluoro-2-methylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E47)



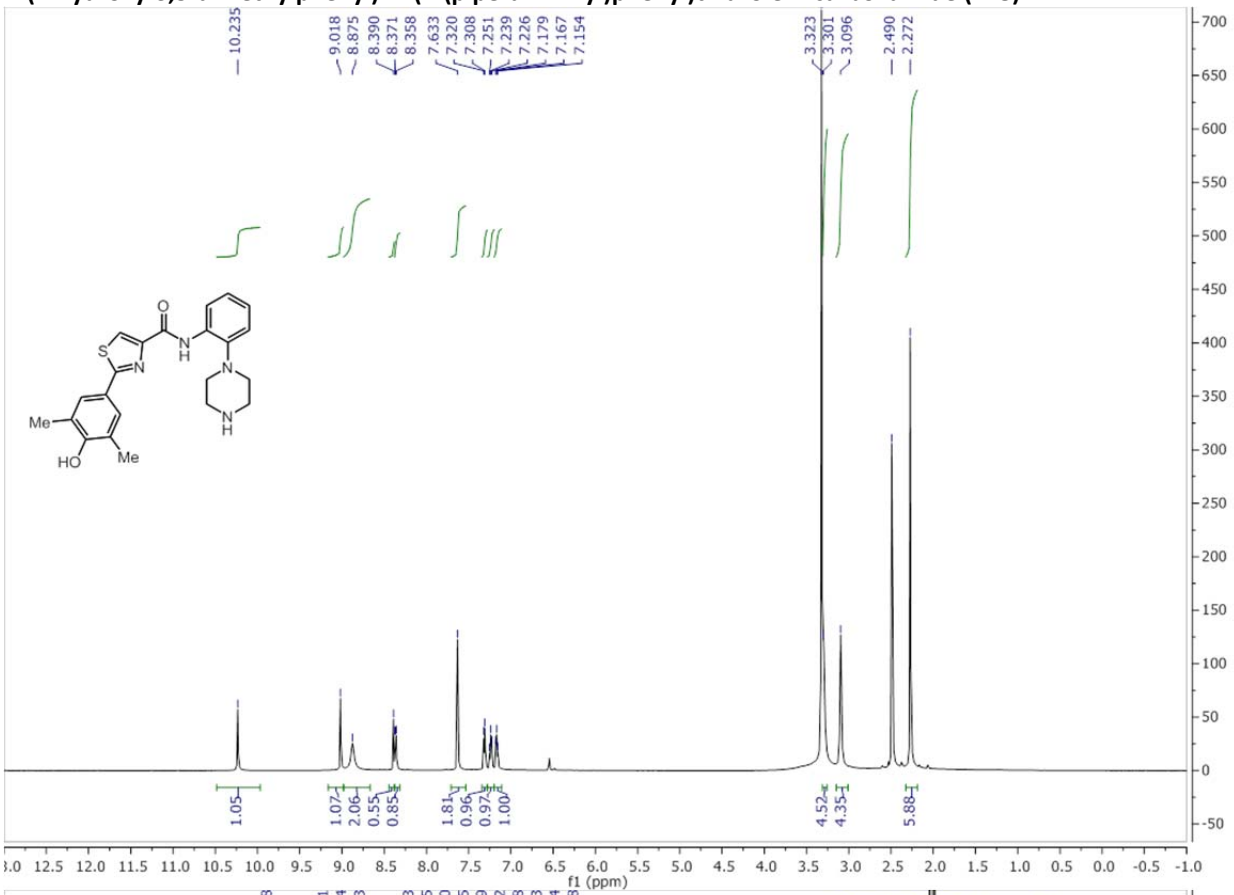


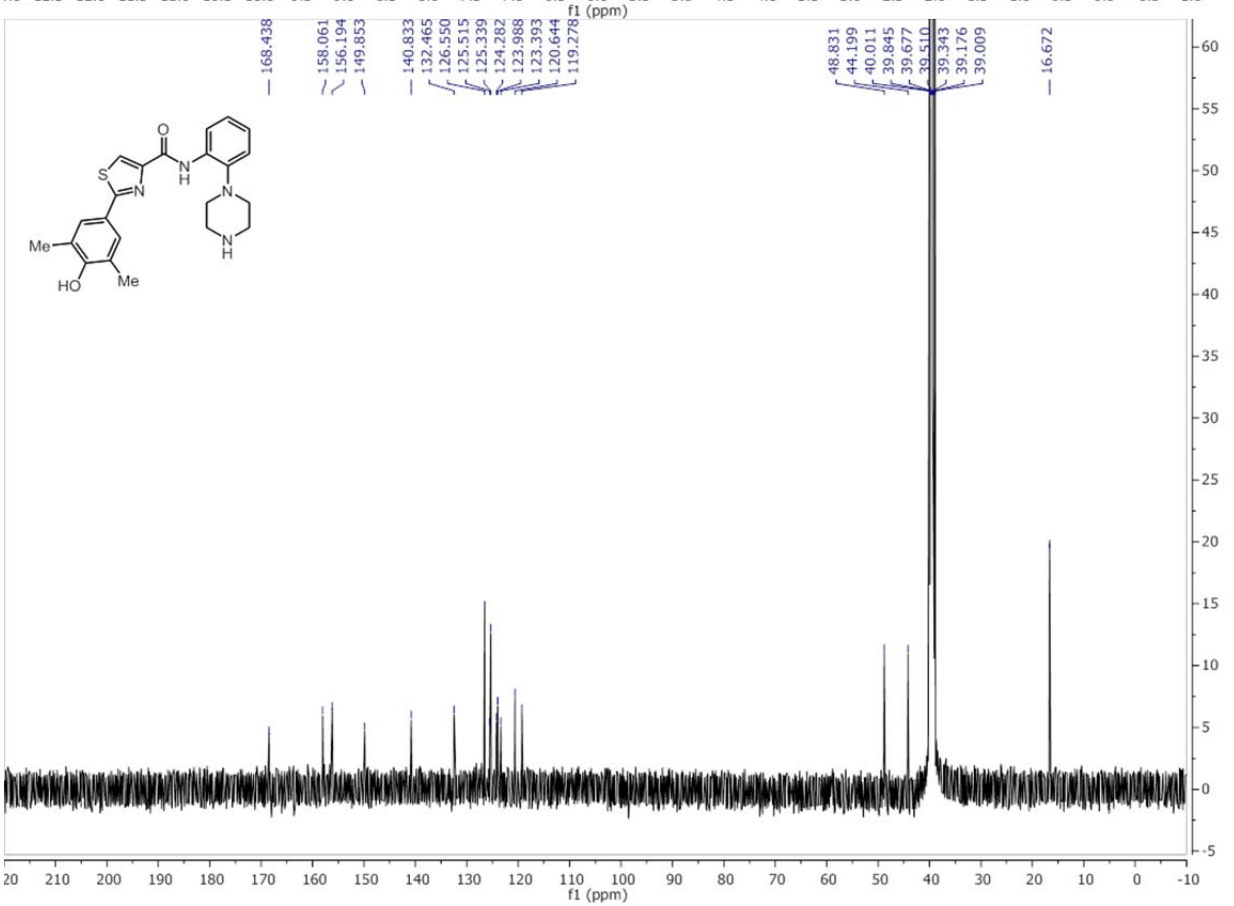
2-(3-aminophenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (38)



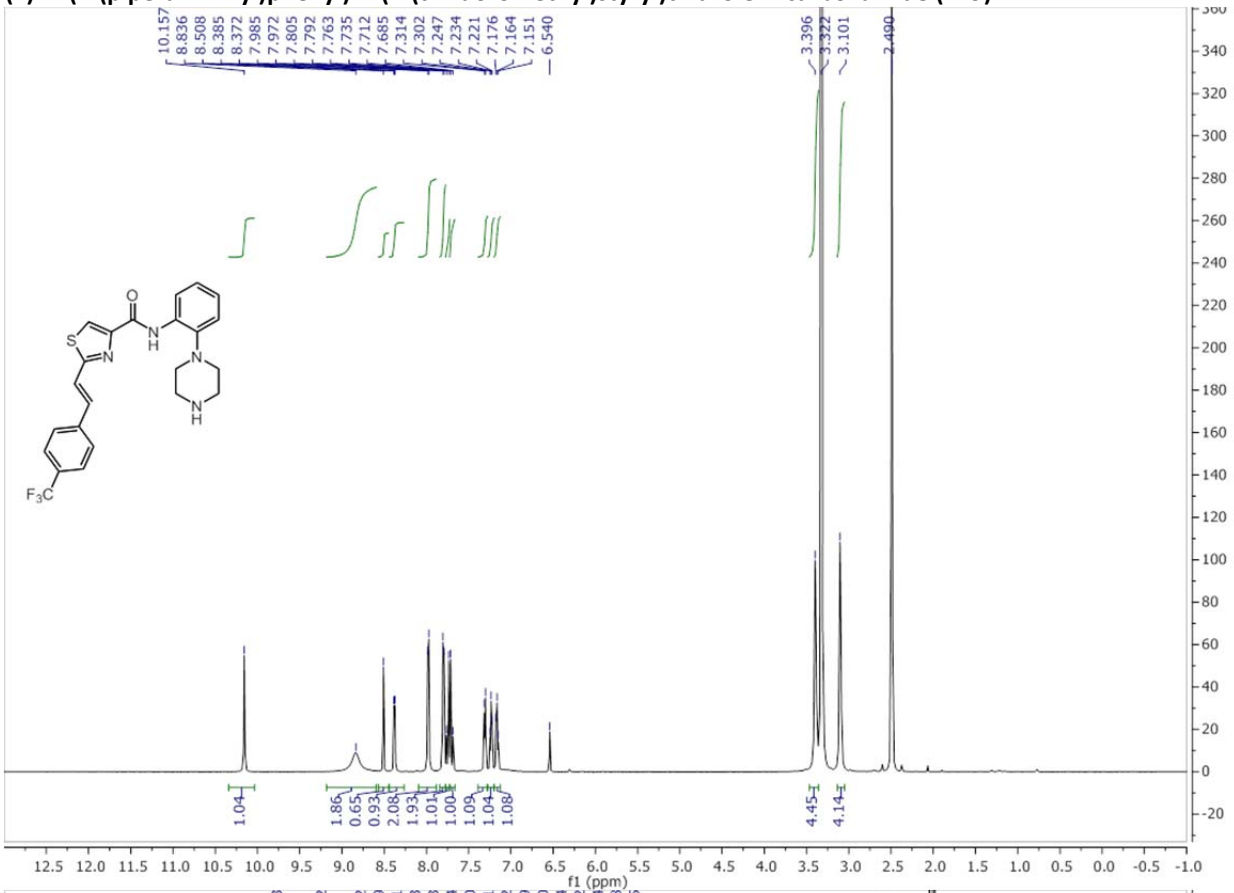


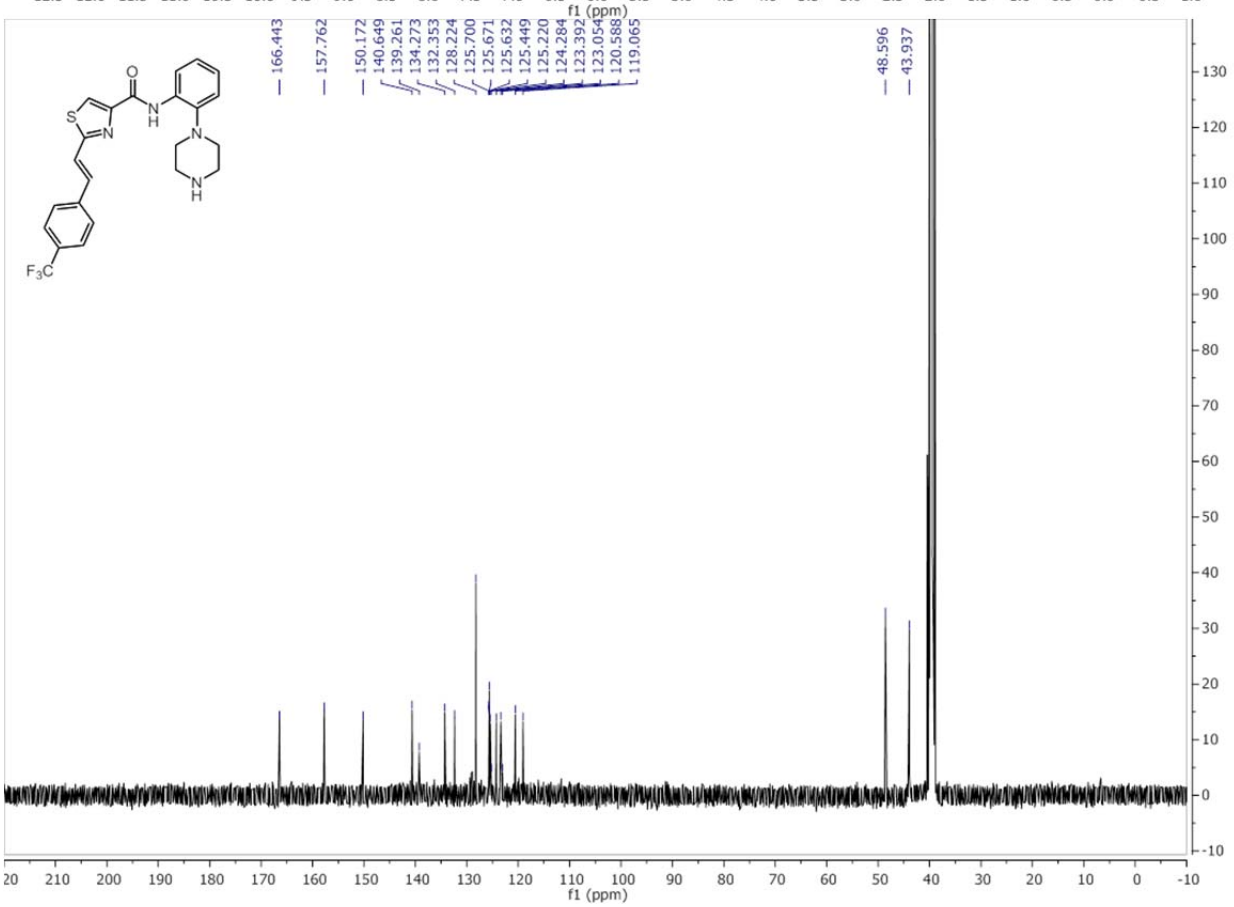
2-(4-hydroxy-3,5-dimethylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E48)



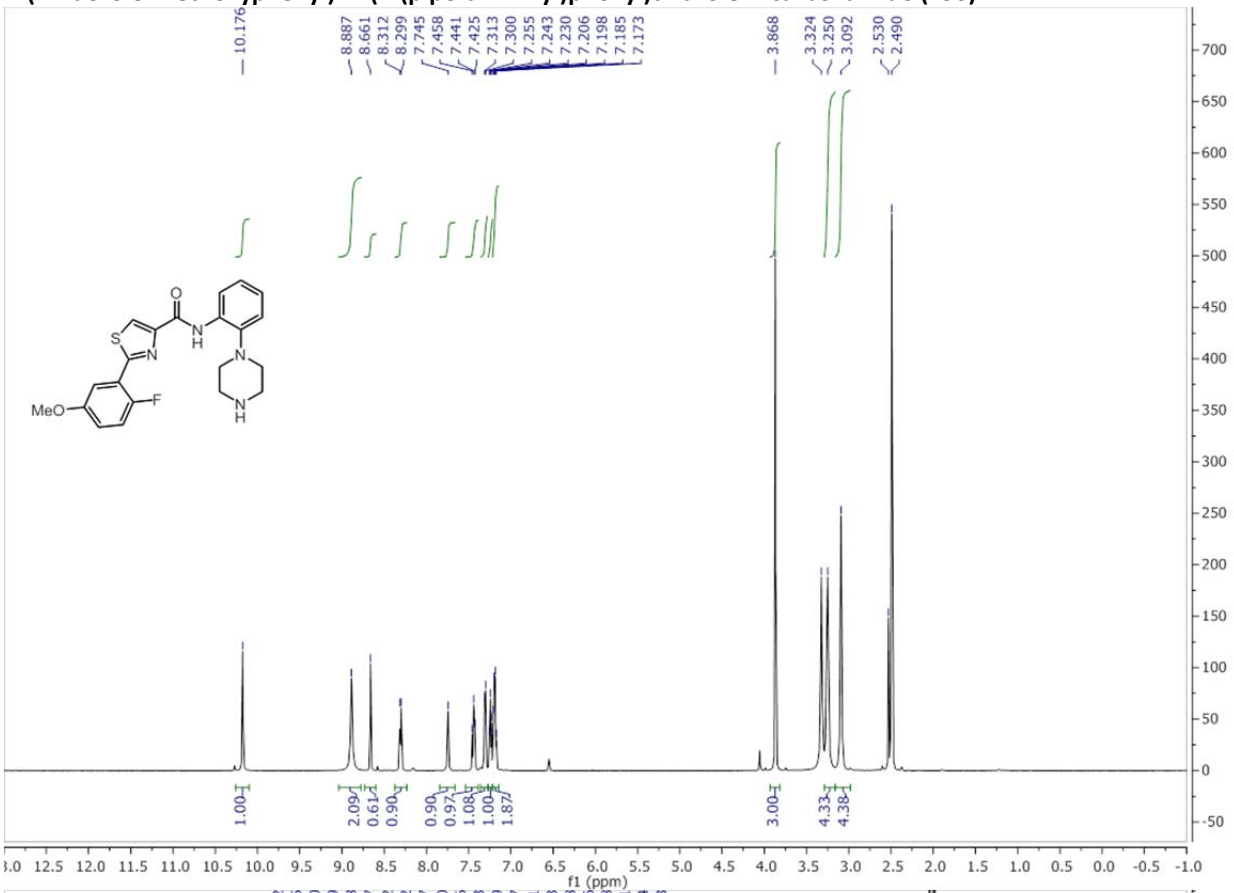


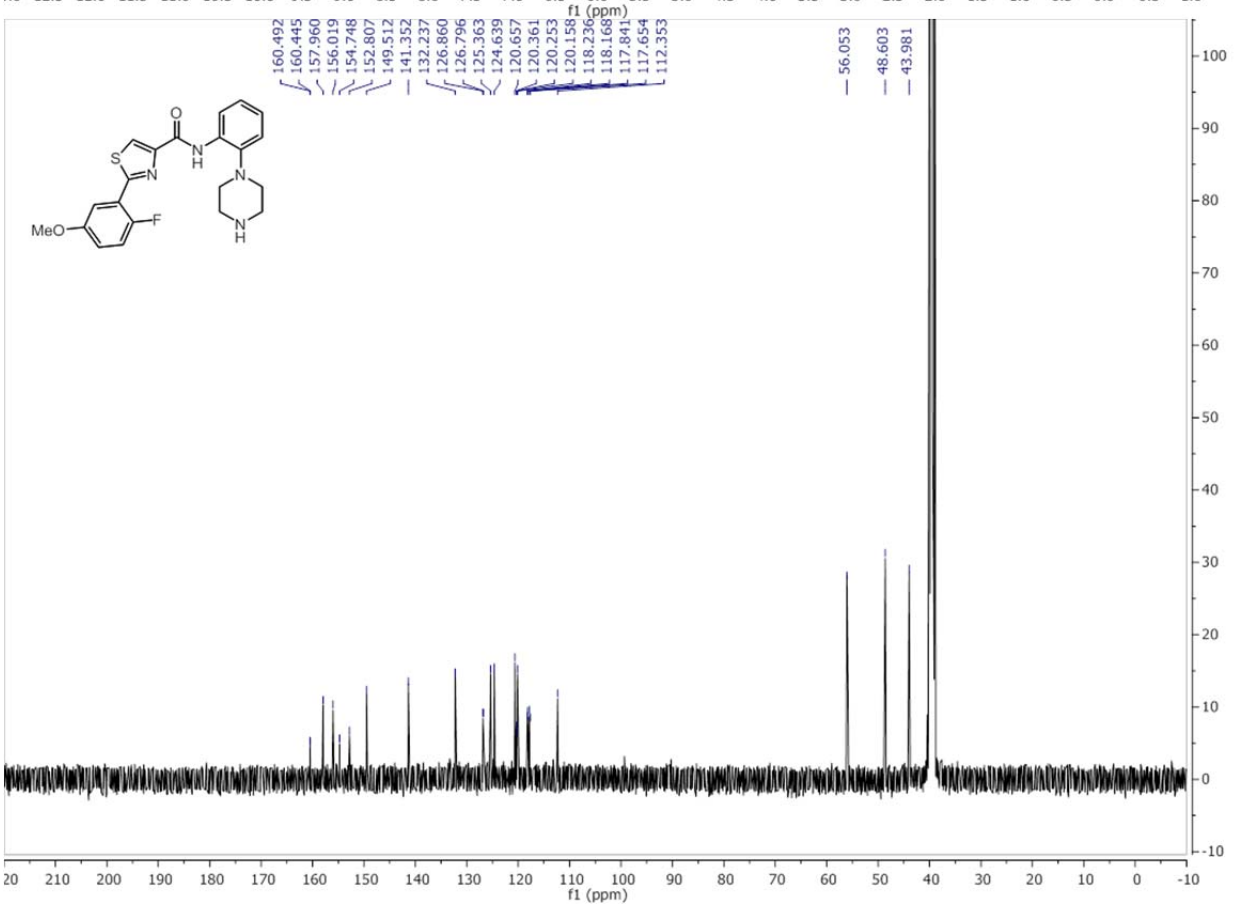
(E)-N-(2-(piperazin-1-yl)phenyl)-2-(4-(trifluoromethyl)styryl)thiazole-4-carboxamide (E49)





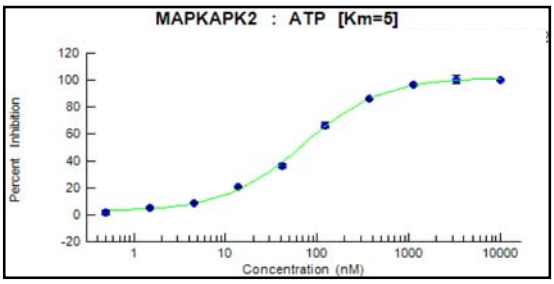
2-(2-fluoro-5-methoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E50)

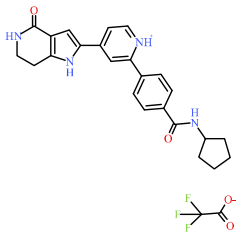




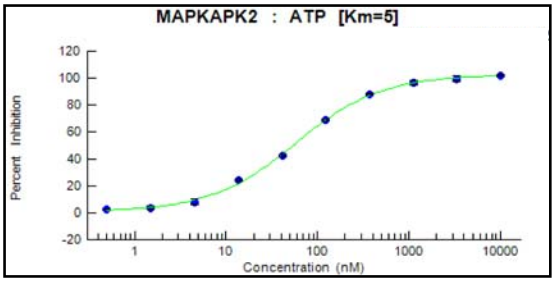
11. Invitrogen IC_{50} Titration Curves

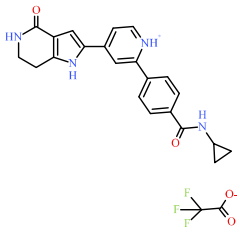
***N*-cyclopentyl-4-(4-(4-oxo-4,5,6,7-tetrahydro-1H-pyrrolo[3,2-c]pyridin-2-yl)pyridin-2-yl)benzamide (B1)**



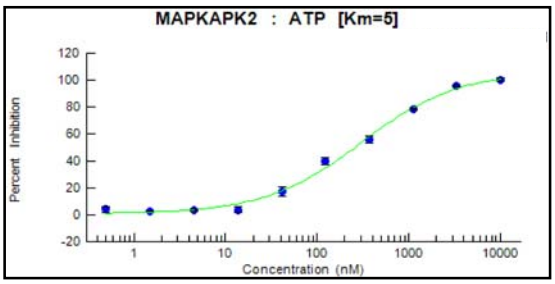


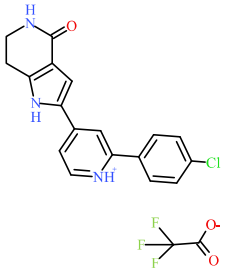
***N*-cyclopropyl-4-(4-(4-oxo-4,5,6,7-tetrahydro-1H-pyrrolo[3,2-c]pyridin-2-yl)pyridin-2-yl)benzamide (5)**



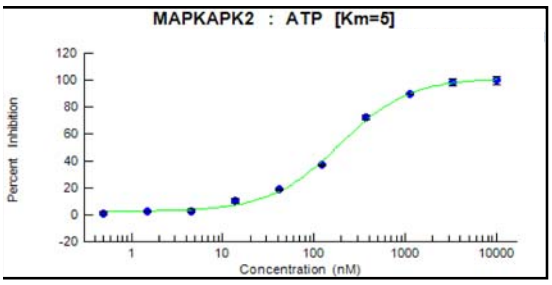


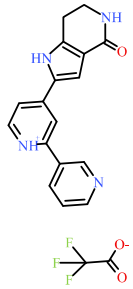
2-(2-(4-chlorophenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B2)



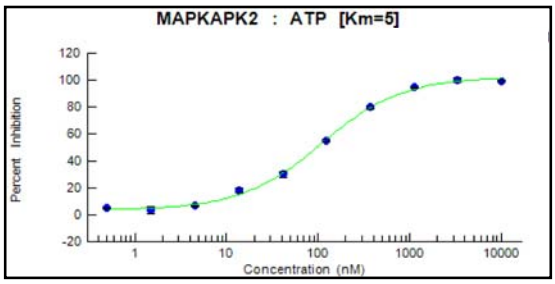


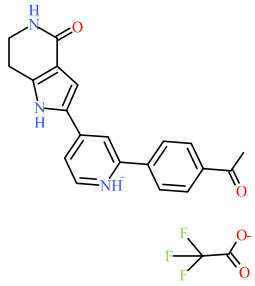
2-([2,3'-bipyridin]-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B3)



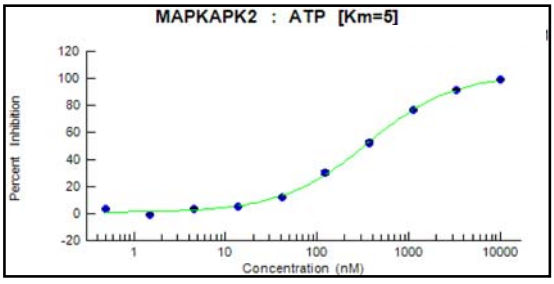


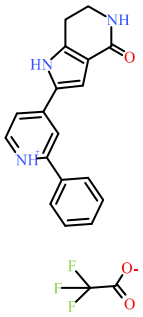
2-(2-(4-acetylphenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B4)



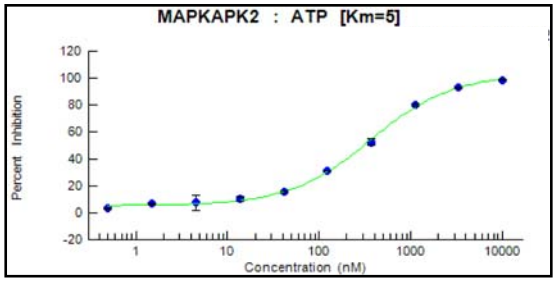


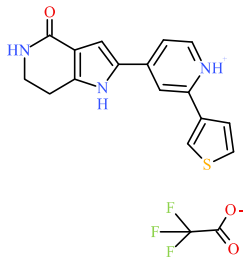
2-(2-phenylpyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B5)



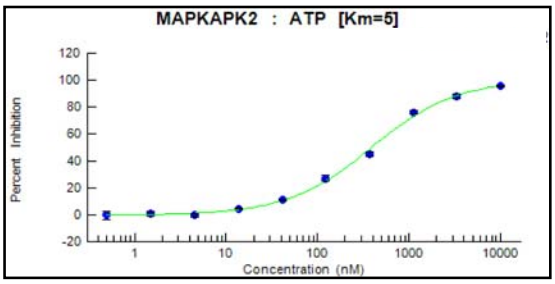


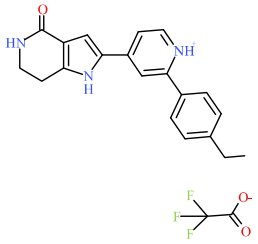
2-(2-(thiophen-3-yl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B6)



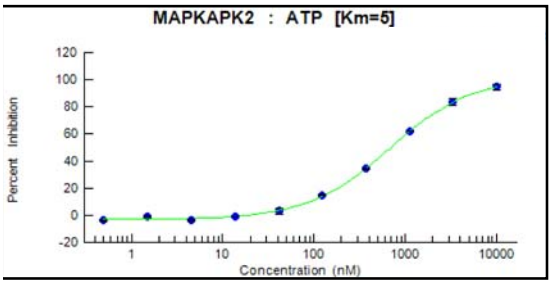


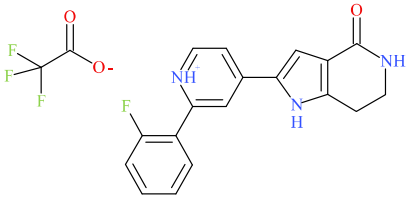
2-(2-(4-ethylphenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B7)



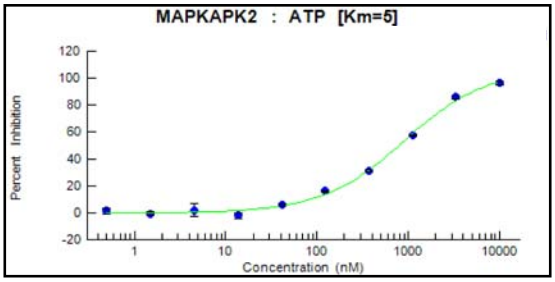


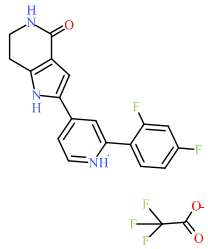
2-(2-(2-fluorophenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B8)



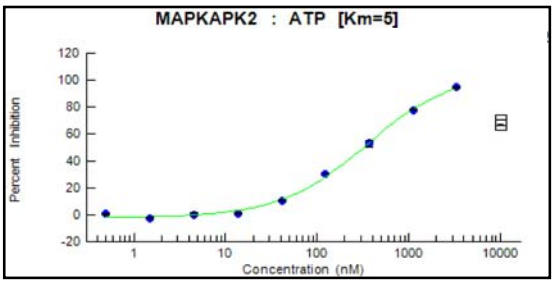


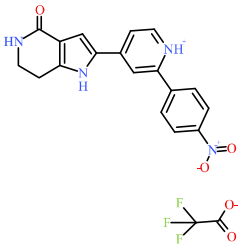
2-(2-(2,4-difluorophenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B9)



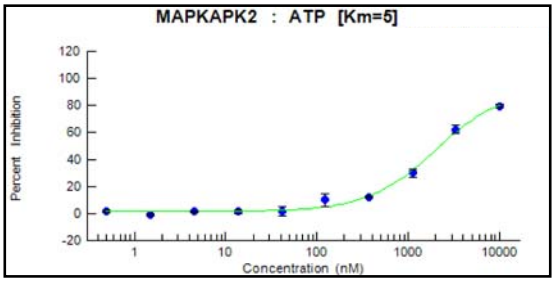


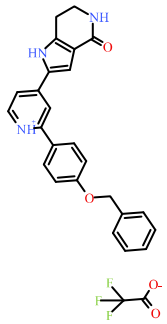
2-(2-(4-nitrophenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B10)



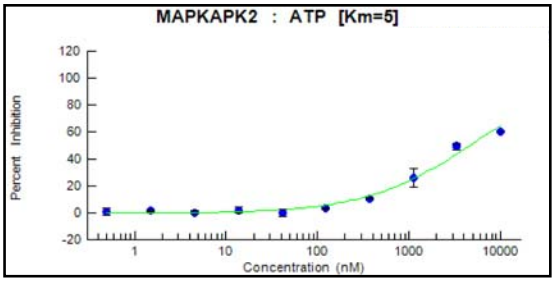


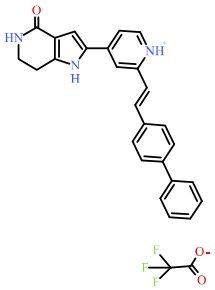
2-(2-(4-(benzyloxy)phenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B11)



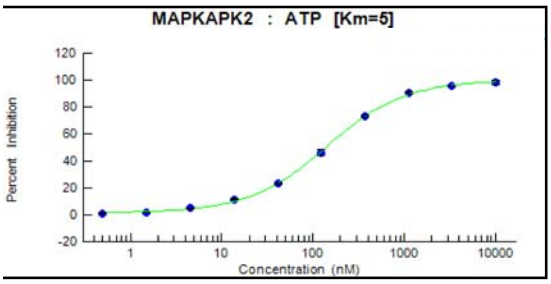


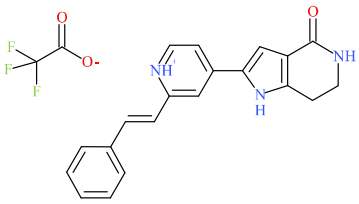
(*E*)-2-(2-(2-([1,1'-biphenyl]-4-yl)vinyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B12)



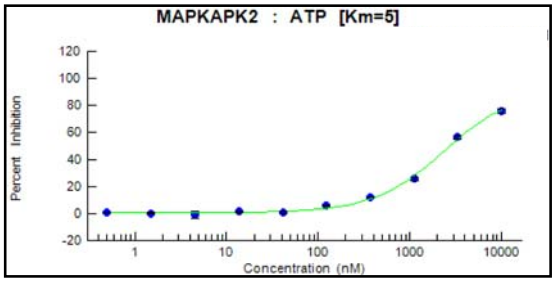


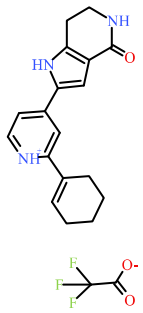
(*E*)-2-(2-styrylpyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B13)



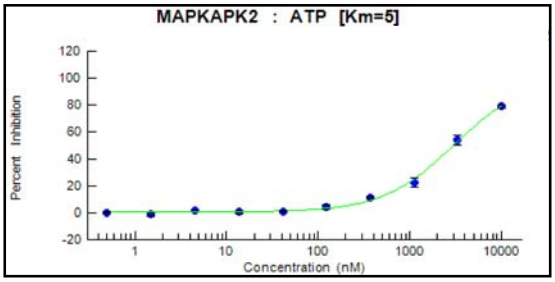


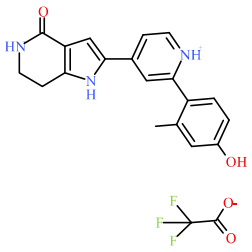
2-(2-(cyclohex-1-en-1-yl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B14)



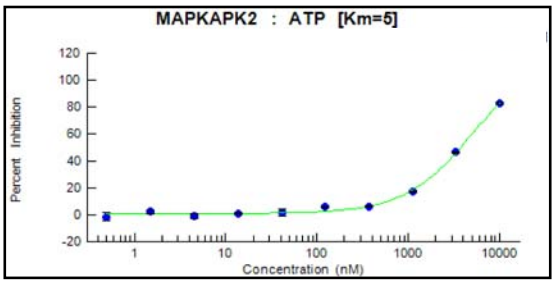


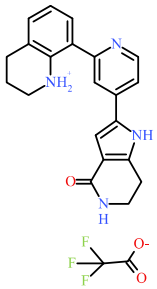
2-(2-(4-hydroxy-2-methylphenyl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (6)



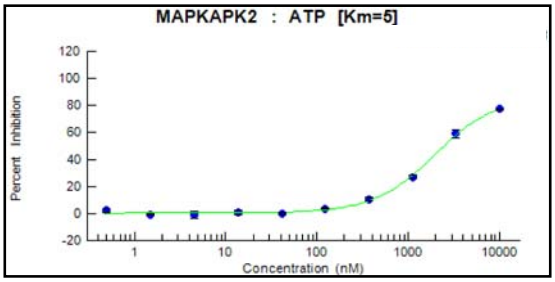


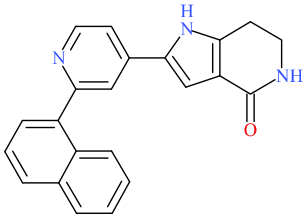
2-(2-(1,2,3,4-tetrahydroquinolin-8-yl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B15)



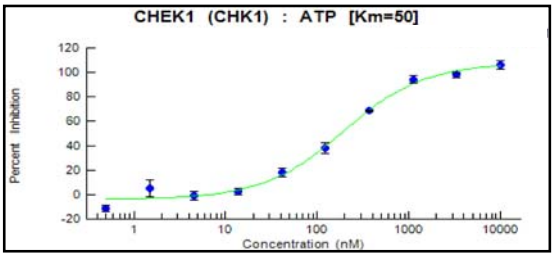


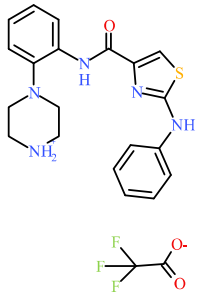
2-(2-(naphthalen-1-yl)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one (B16)



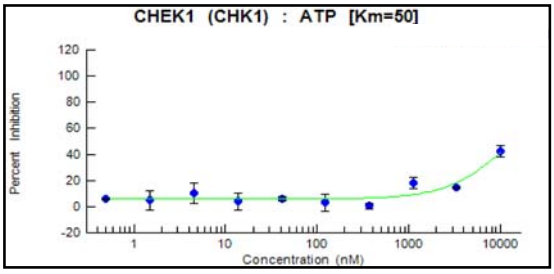


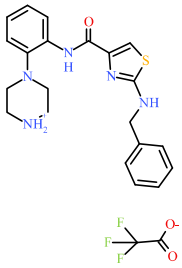
2-(phenylamino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C1)



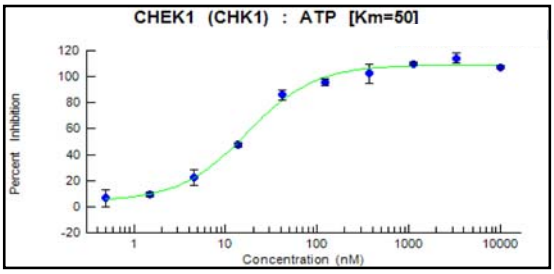


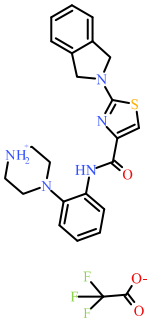
2-(benzylamino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide(C2)



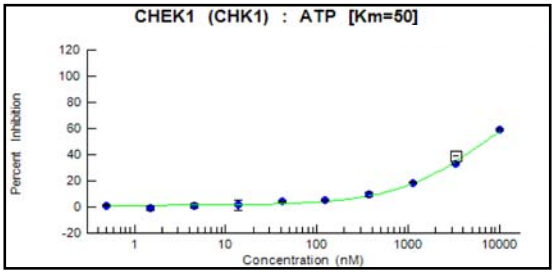


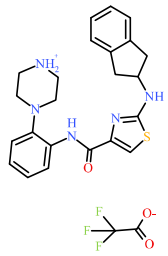
2-(isoindolin-2-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (43)



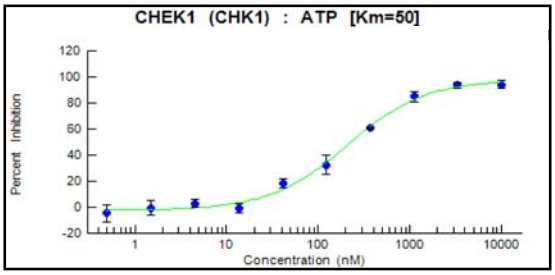


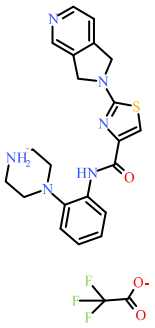
2-((2,3-dihydro-1H-inden-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C4)



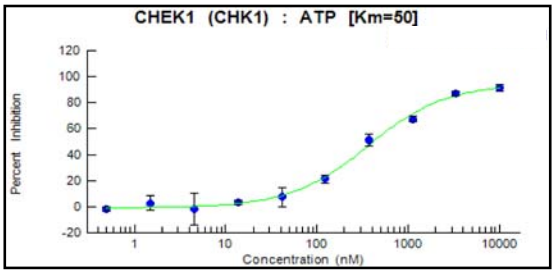


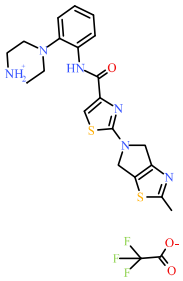
2-(1,3-dihydro-2H-pyrrolo[3,4-c]pyridin-2-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C5)



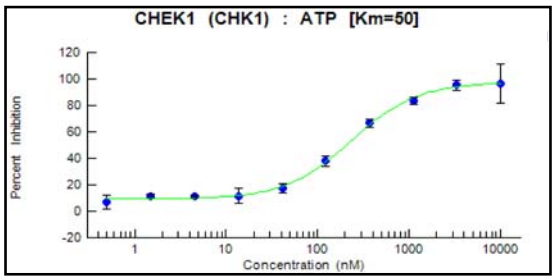


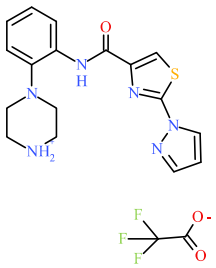
2-(2-methyl-4,6-dihydro-5H-pyrrolo[3,4-d]thiazol-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C6)



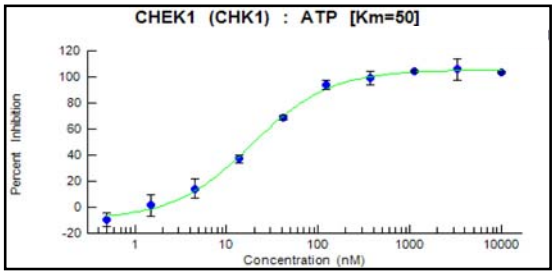


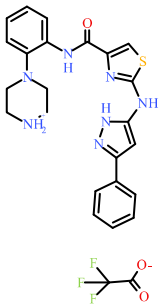
N-(2-(piperazin-1-yl)phenyl)-2-(1H-pyrazol-1-yl)thiazole-4-carboxamide (C7)



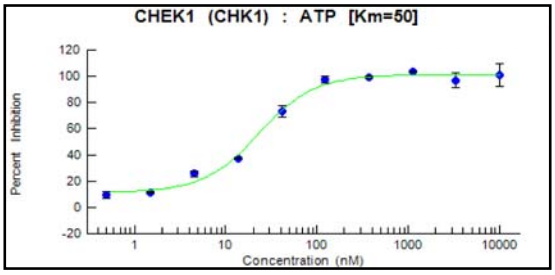


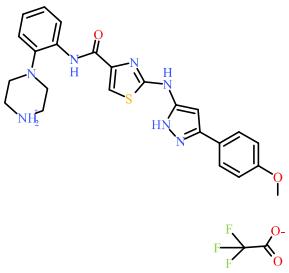
2-((3-phenyl-1H-pyrazol-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C8)



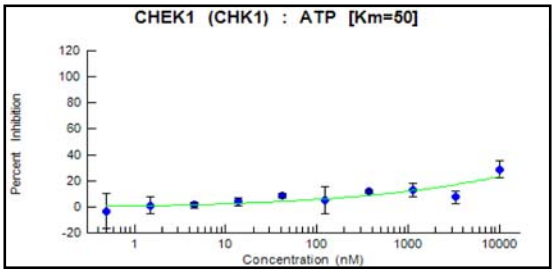


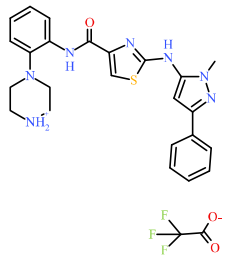
2-((3-(4-methoxyphenyl)-1H-pyrazol-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (8)



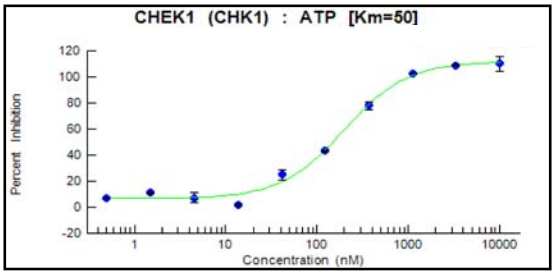


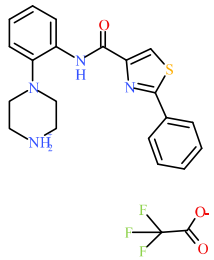
2-((1-methyl-3-phenyl-1H-pyrazol-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C9)



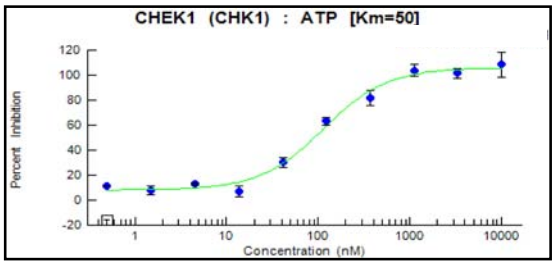


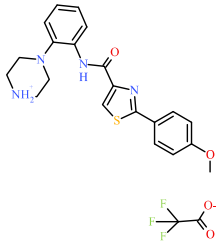
2-phenyl-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C10)



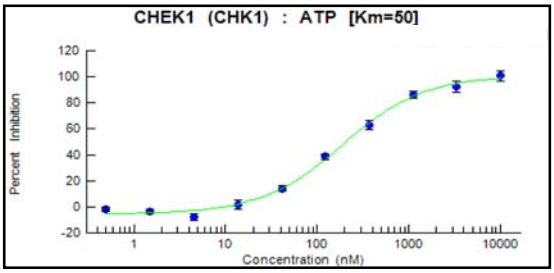


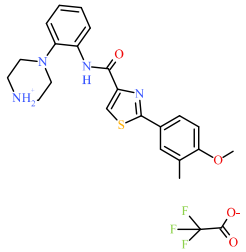
2-(4-methoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C11)



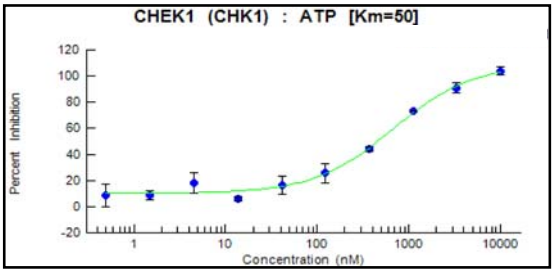


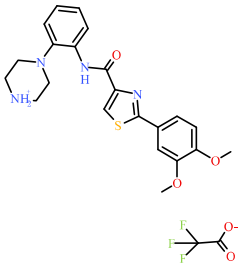
2-(4-methoxy-3-methylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C12)



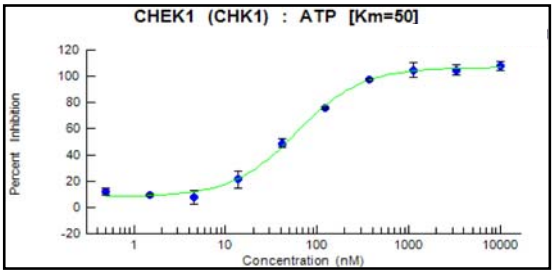


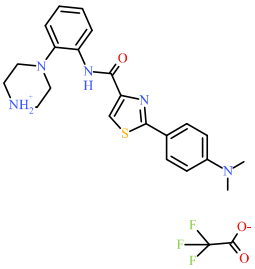
2-(3,4-dimethoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C13)



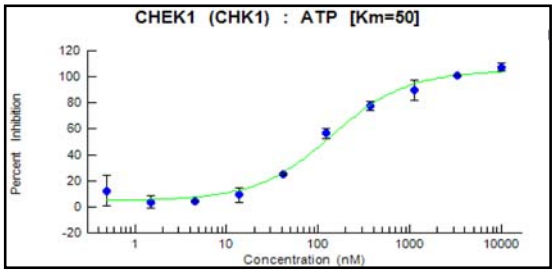


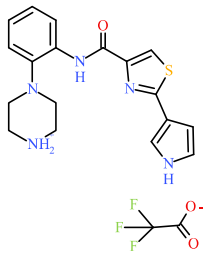
2-(4-(dimethylamino)phenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C14)



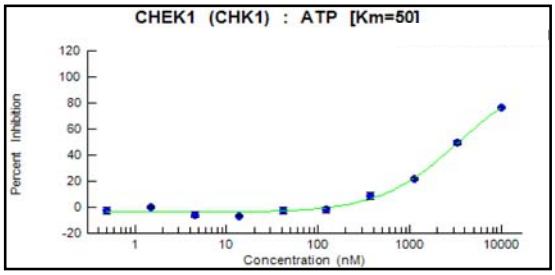


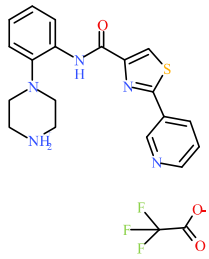
N-(2-(piperazin-1-yl)phenyl)-2-(1H-pyrrol-3-yl)thiazole-4-carboxamide (C15)



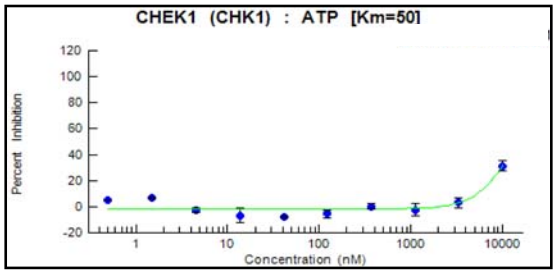


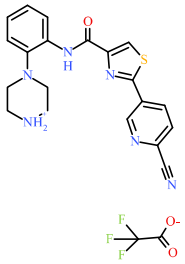
N-(2-(piperazin-1-yl)phenyl)-2-(pyridin-3-yl)thiazole-4-carboxamide (C16)



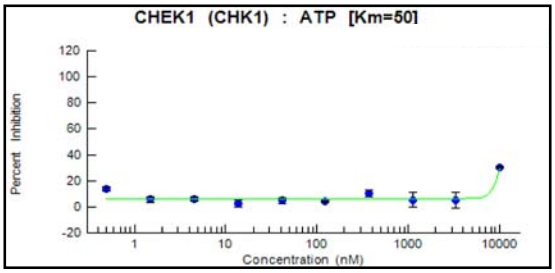


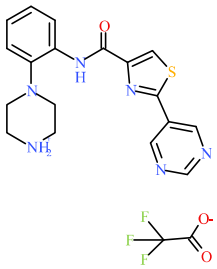
2-(6-cyanopyridin-3-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C17)



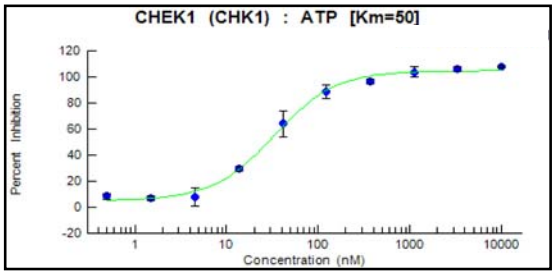


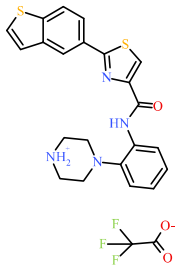
N-(2-(piperazin-1-yl)phenyl)-2-(pyrimidin-5-yl)thiazole-4-carboxamide (9)



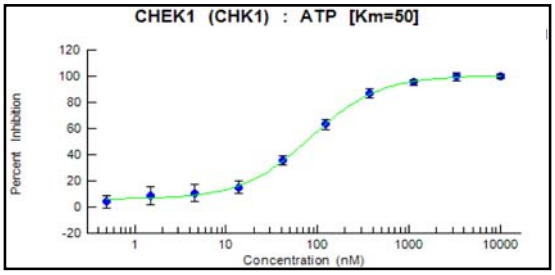


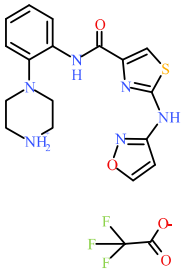
2-(benzo[b]thiophen-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (C18)



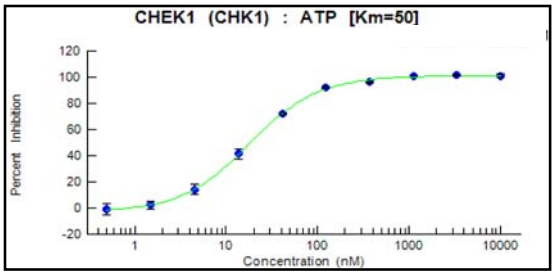


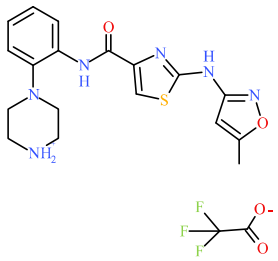
2-(isoxazol-3-ylamino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E1)



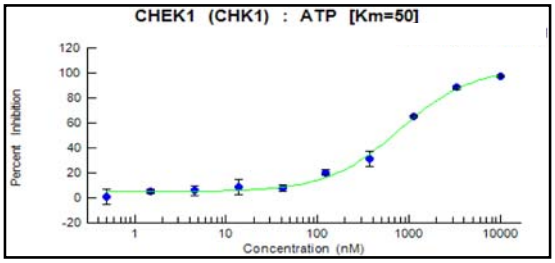


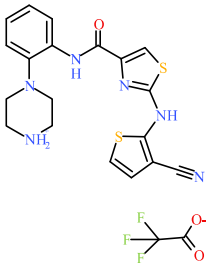
2-((5-methylisoxazol-3-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (44)



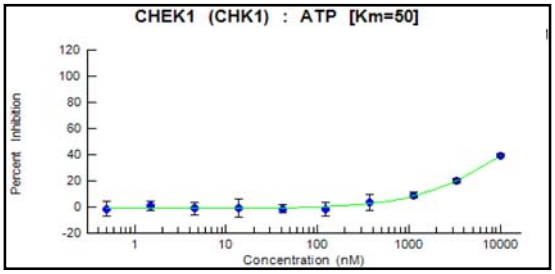


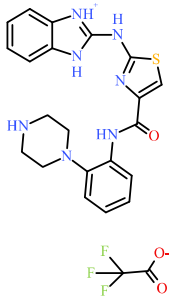
2-((3-cyanothiophen-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E2)



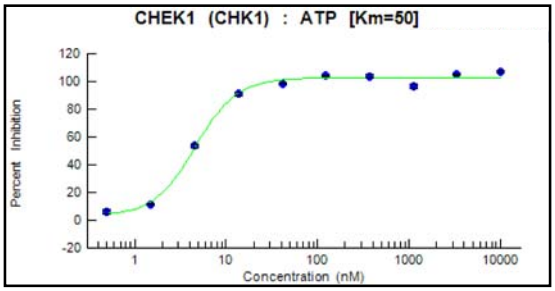


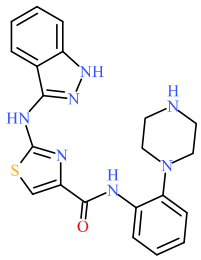
2-((1H-benzo[d]imidazol-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E3)



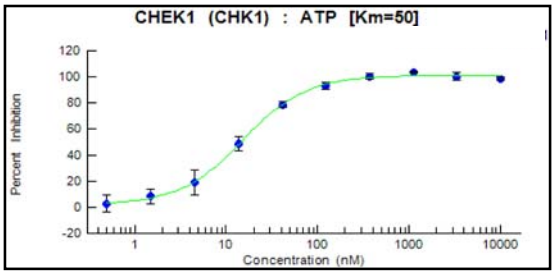


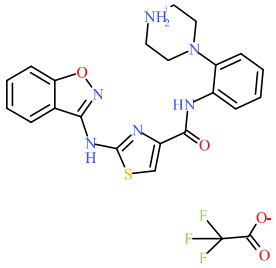
2-((1H-indazol-3-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E4)



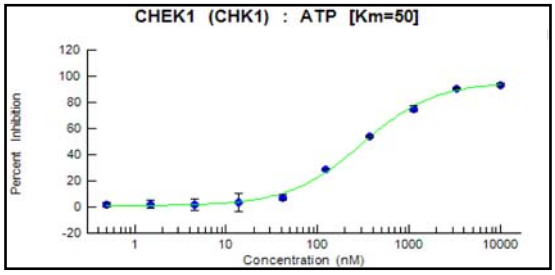


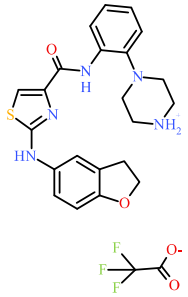
2-(benzo[d]isoxazol-3-ylamino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E5)



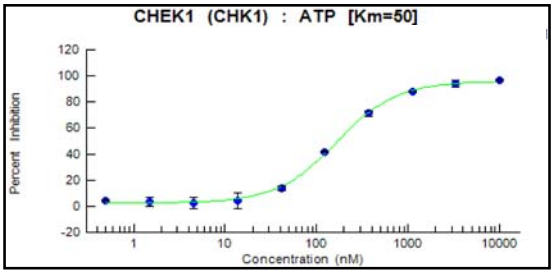


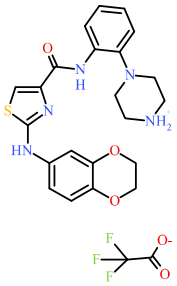
2-((2,3-dihydrobenzofuran-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E6)



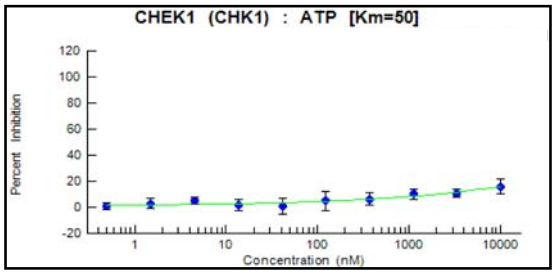


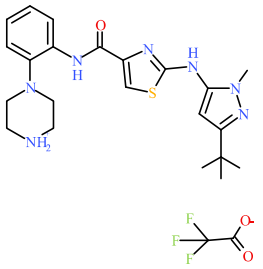
2-((2,3-dihydrobenzo[b][1,4]dioxin-6-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E7)



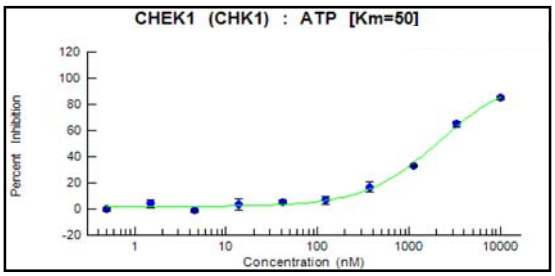


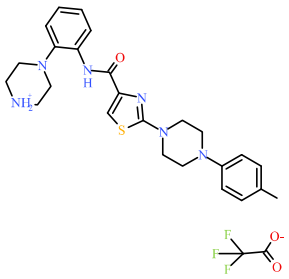
2-((3-(tert-butyl)-1-methyl-1H-pyrazol-5-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E8)



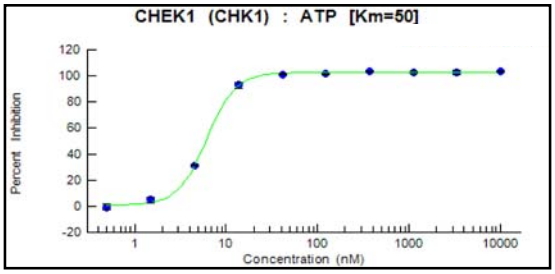


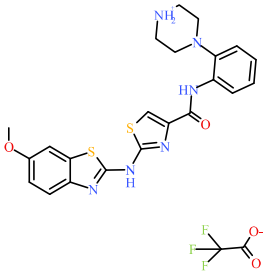
N-(2-(piperazin-1-yl)phenyl)-2-(4-(p-tolyl)piperazin-1-yl)thiazole-4-carboxamide (E9)



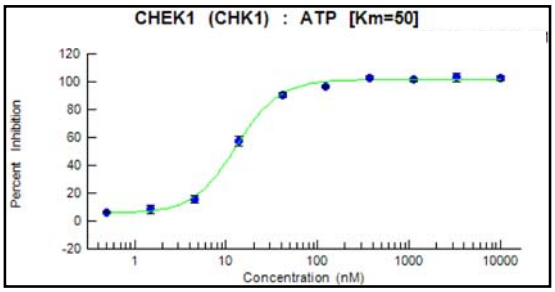


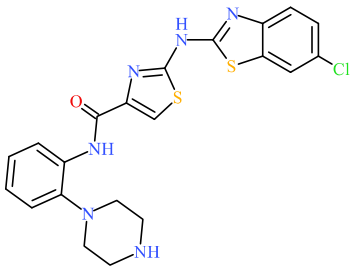
2-((6-methoxybenzo[d]thiazol-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (41)



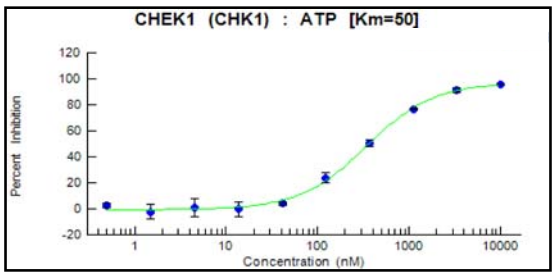


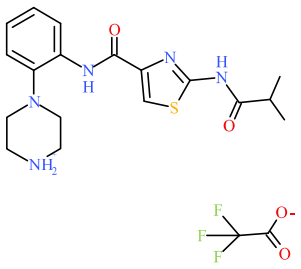
2-((6-chlorobenzo[d]thiazol-2-yl)amino)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E10)



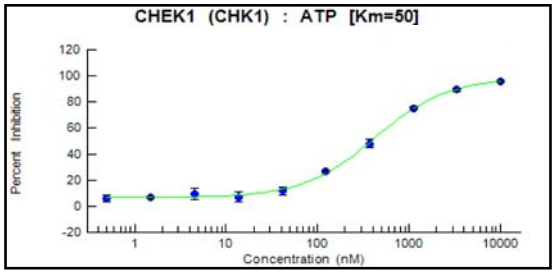


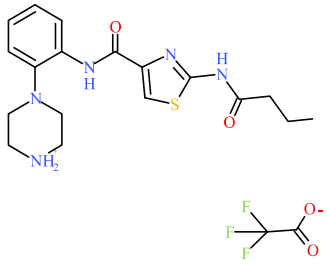
2-isobutyramido-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E11)



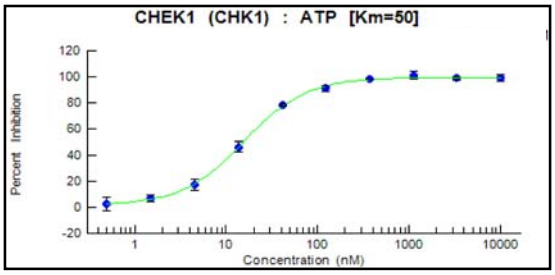


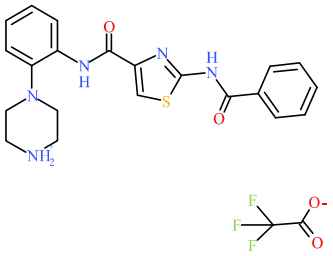
2-butyramido-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E12)



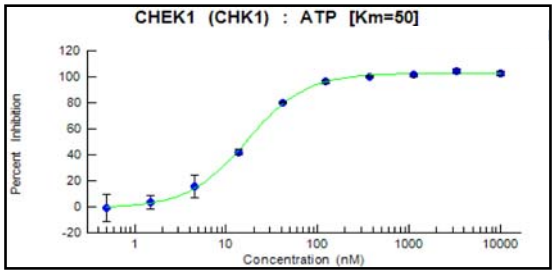


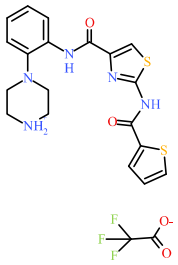
2-benzamido-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E13)



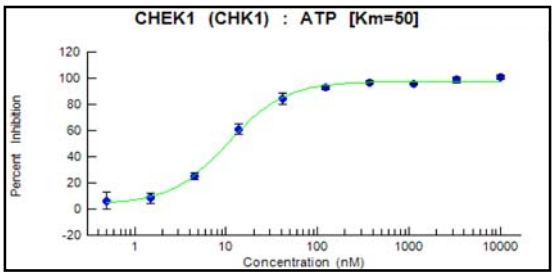


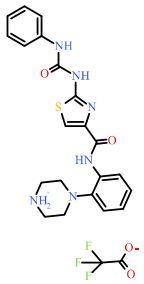
N-(2-(piperazin-1-yl)phenyl)-2-(thiophene-2-carboxamido)thiazole-4-carboxamide (42)



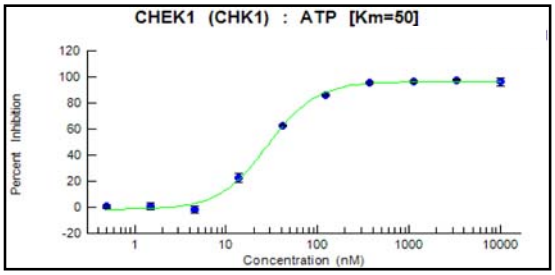


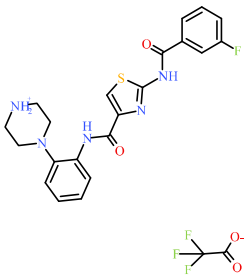
2-(3-phenylureido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E14)



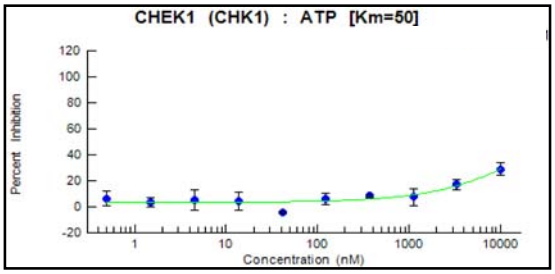


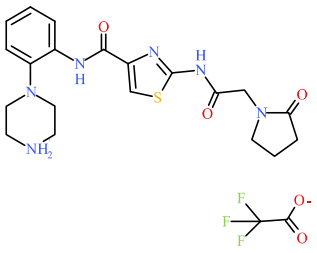
2-(3-fluorobenzamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E15)



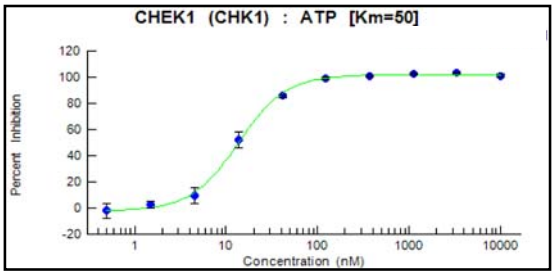


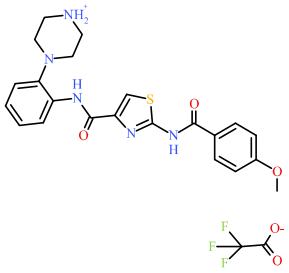
2-(2-(2-oxopyrrolidin-1-yl)acetamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E16)



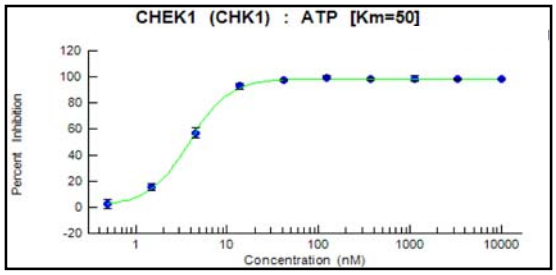


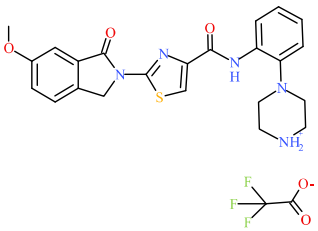
2-(4-methoxybenzamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E17)



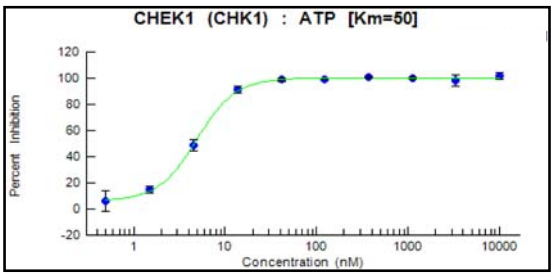


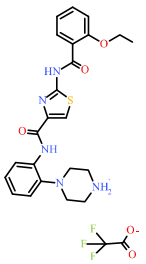
2-(6-methoxy-1-oxoisoindolin-2-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E18)



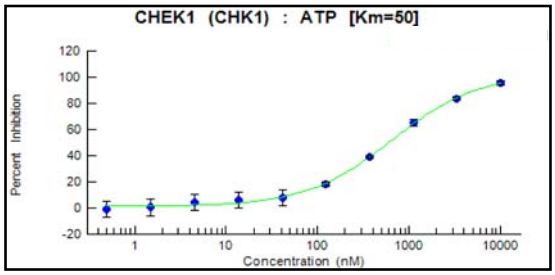


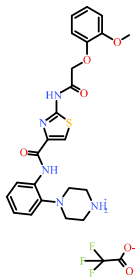
2-(2-ethoxybenzamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (39)



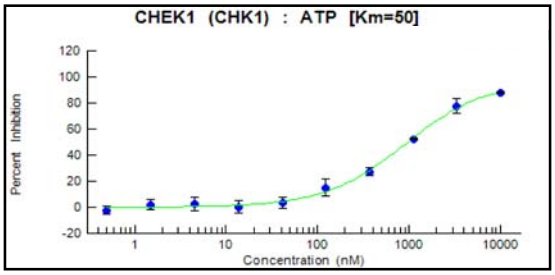


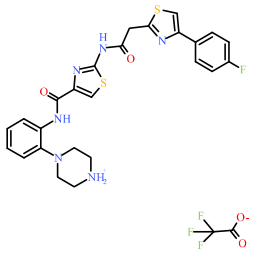
2-(2-(2-methoxyphenoxy)acetamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E19)



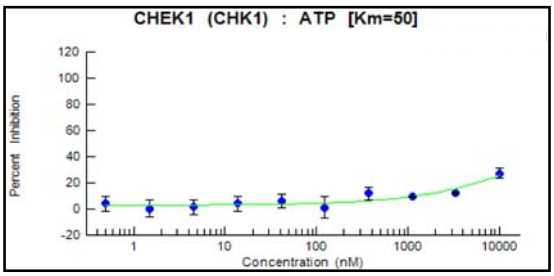


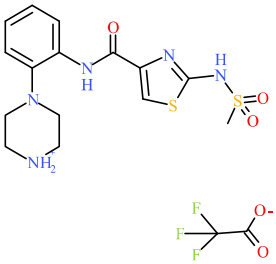
2-(2-(4-(4-fluorophenyl)thiazol-2-yl)acetamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E20)



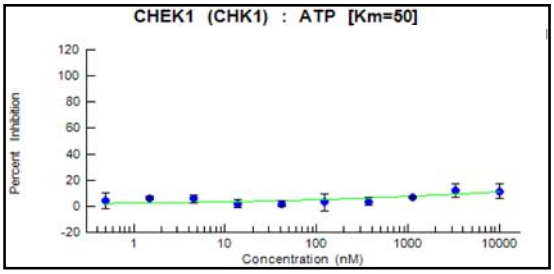


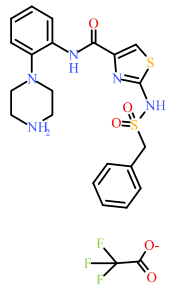
2-(methylsulfonamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E21)



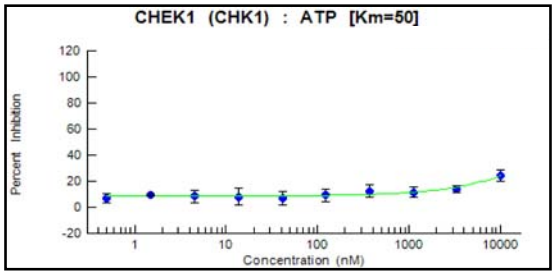


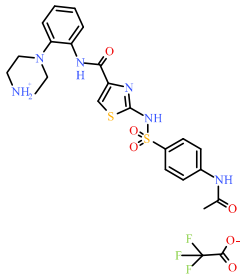
2-((phenylmethyl)sulfonamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (40)



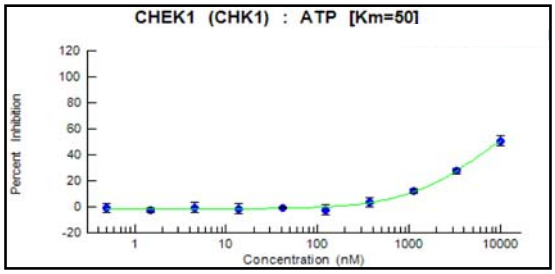


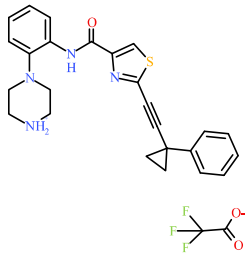
2-((4-acetamidophenyl)sulfonamido)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E22)



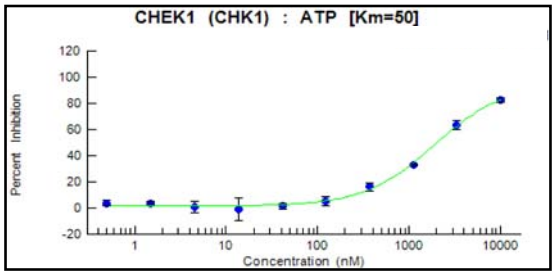


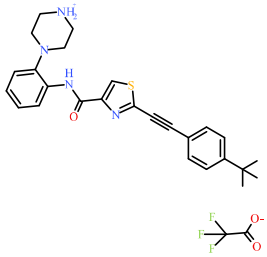
2-((1-phenylcyclopropyl)ethynyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (37)



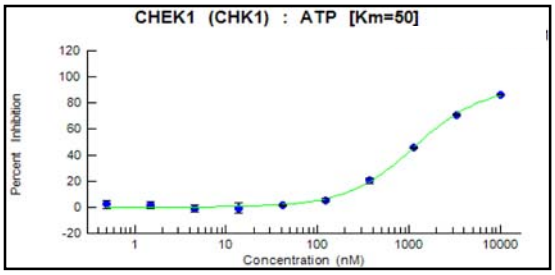


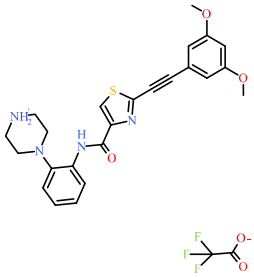
2-((4-(tert-butyl)phenyl)ethynyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E23)



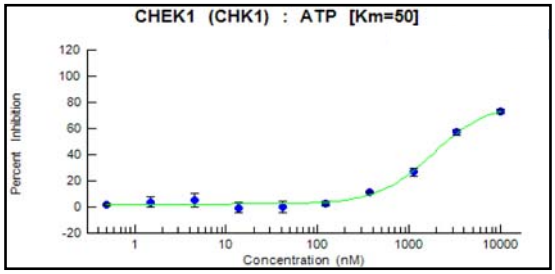


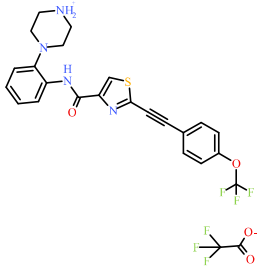
2-((3,5-dimethoxyphenyl)ethynyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E24)



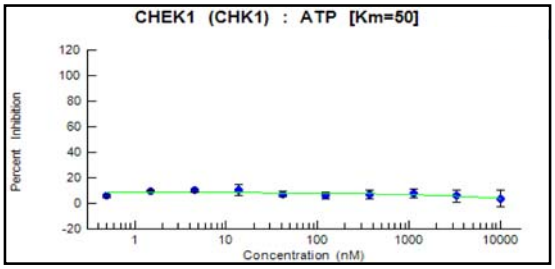


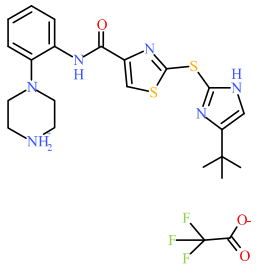
N-(2-(piperazin-1-yl)phenyl)-2-((4-(trifluoromethoxy)phenyl)ethynyl)thiazole-4-carboxamide (E25)



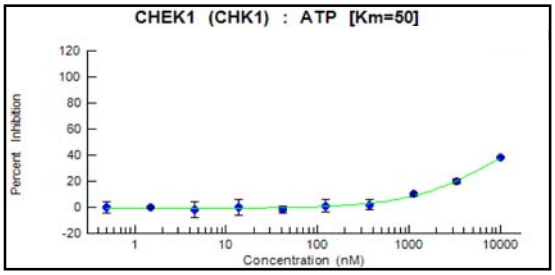


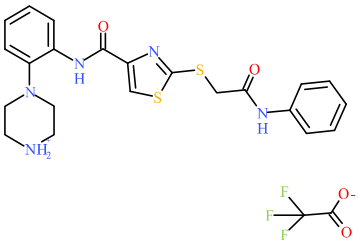
2-((4-(tert-butyl)-1H-imidazol-2-yl)thio)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (35)



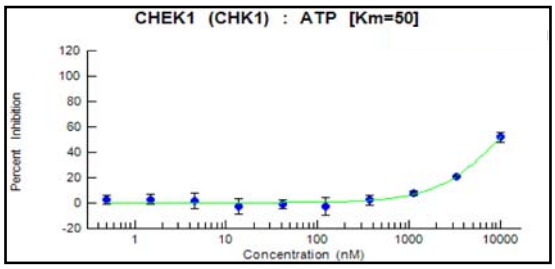


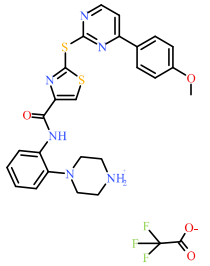
2-((2-oxo-2-(phenylamino)ethyl)thio)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E26)



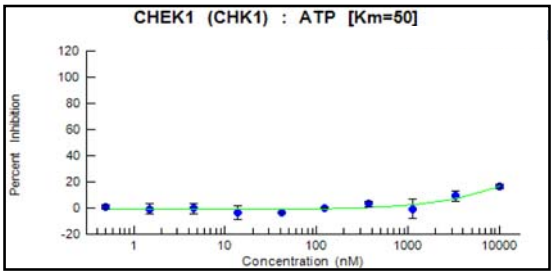


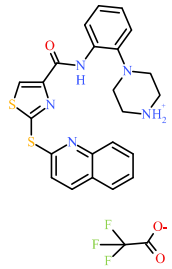
2-((4-(4-methoxyphenyl)pyrimidin-2-yl)thio)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E27)



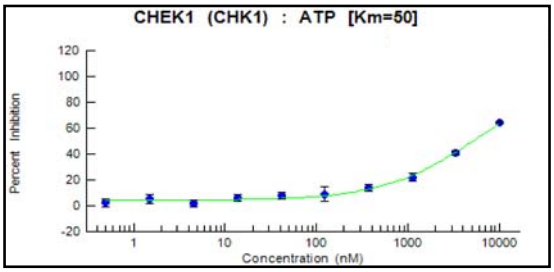


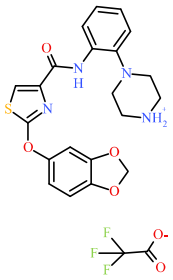
N-(2-(piperazin-1-yl)phenyl)-2-(quinolin-2-ylthio)thiazole-4-carboxamide (E28)



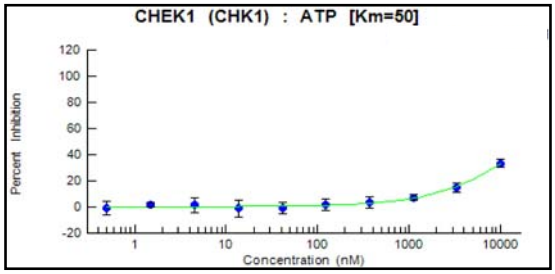


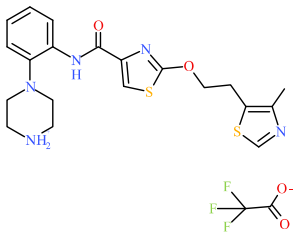
2-(benzo[d][1,3]dioxol-5-yloxy)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E29)



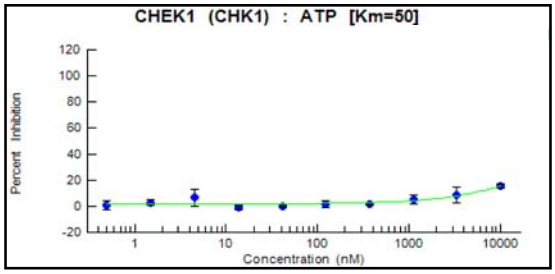


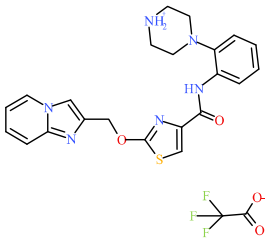
2-(2-(4-methylthiazol-5-yl)ethoxy)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E30)



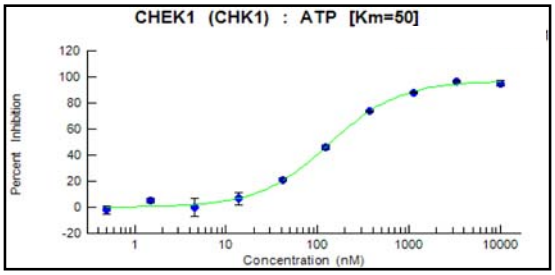


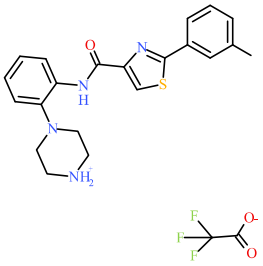
2-(imidazo[1,2-a]pyridin-2-ylmethoxy)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (36)



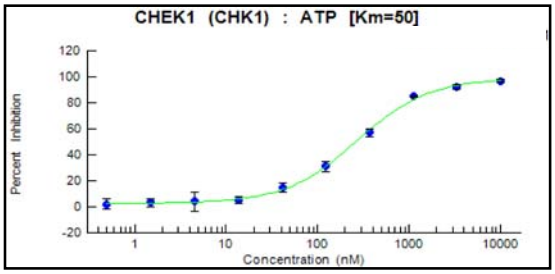


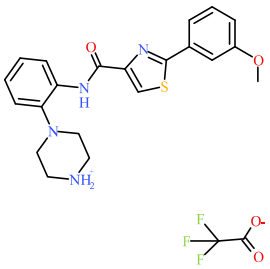
N-(2-(piperazin-1-yl)phenyl)-2-(m-tolyl)thiazole-4-carboxamide (E31)



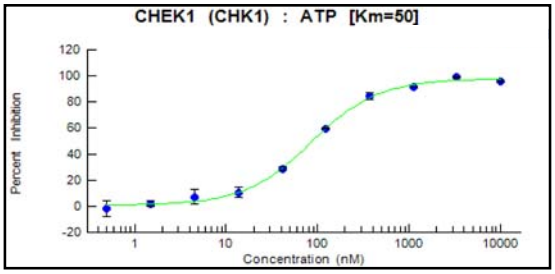


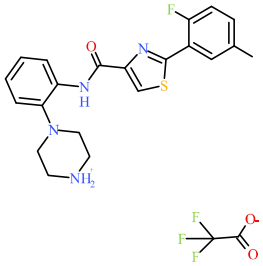
2-(3-methoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E32)



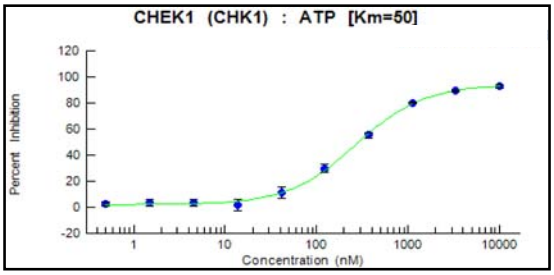


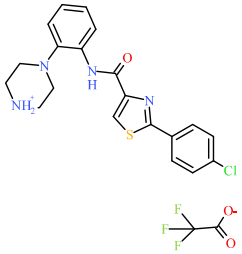
2-(2-fluoro-5-methylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E33)



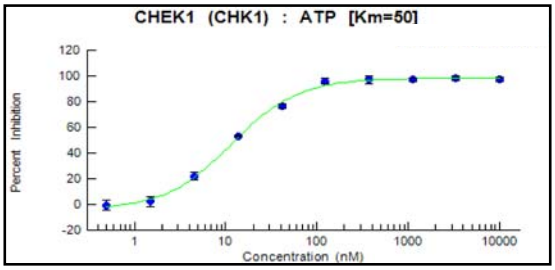


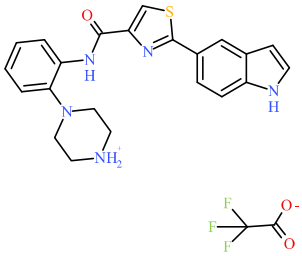
2-(4-chlorophenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E34)



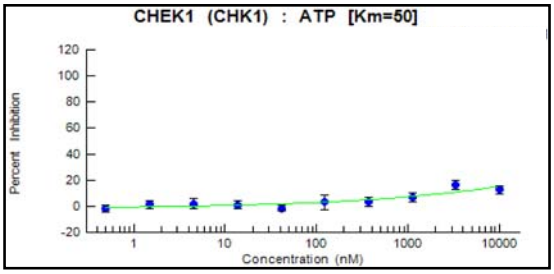


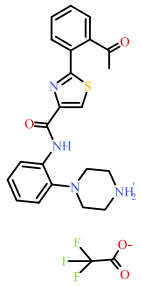
2-(1H-indol-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E35)



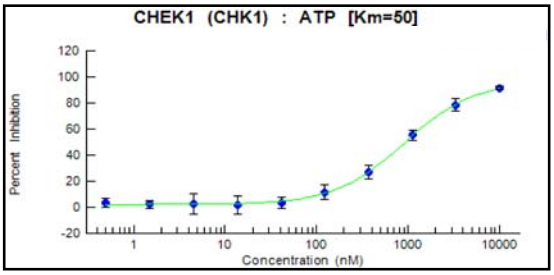


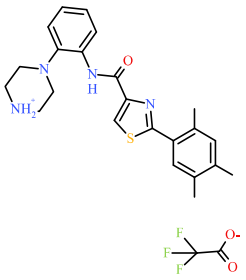
2-(2-acetylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E36)



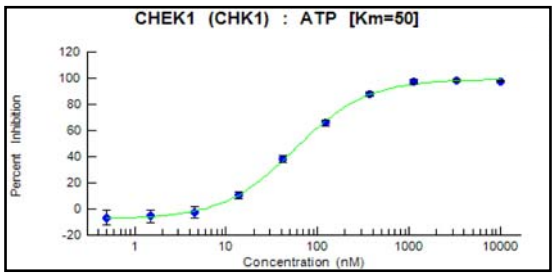


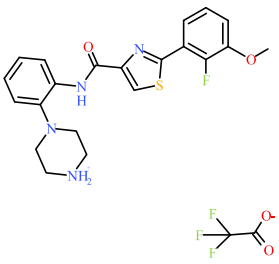
N-(2-(piperazin-1-yl)phenyl)-2-(2,4,5-trimethylphenyl)thiazole-4-carboxamide (E37)



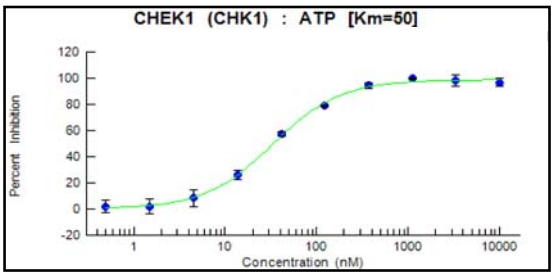


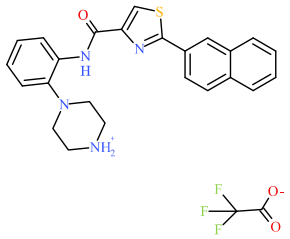
2-(2-fluoro-3-methoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E39)



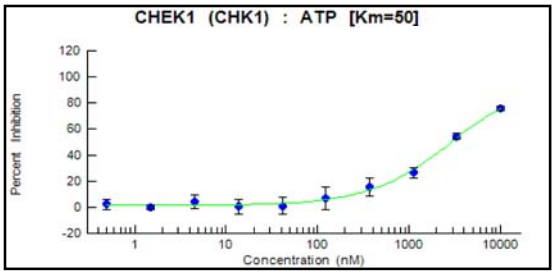


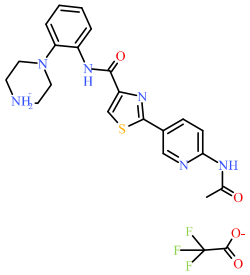
2-(naphthalen-2-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E40)



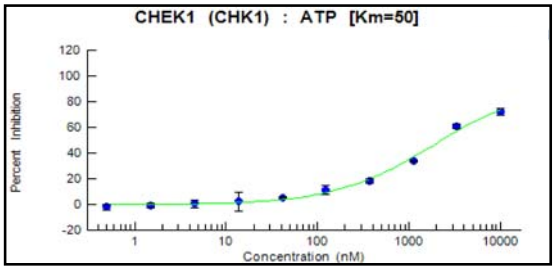


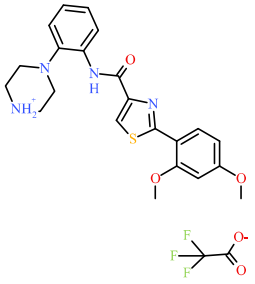
2-(6-acetamidopyridin-3-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E41)



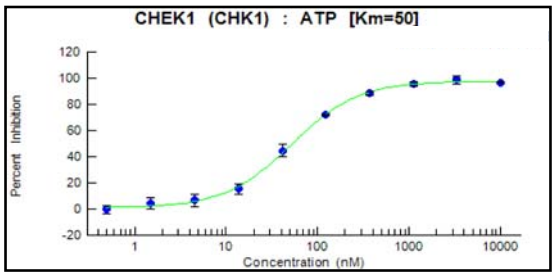


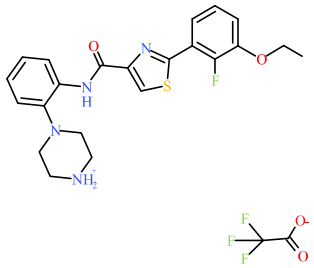
2-(2,4-dimethoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E42)



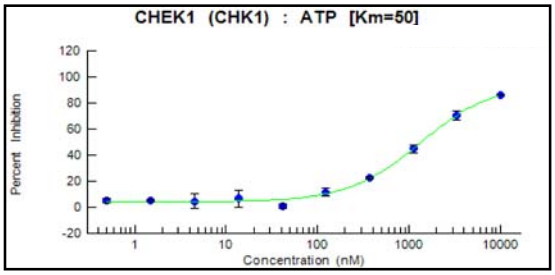


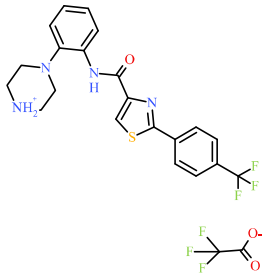
2-(3-ethoxy-2-fluorophenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (45)



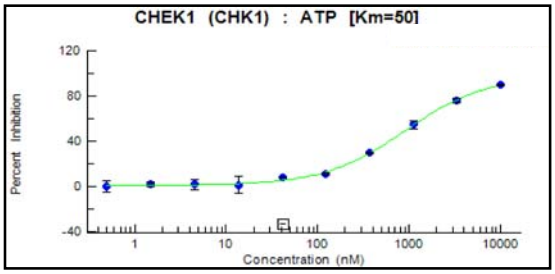


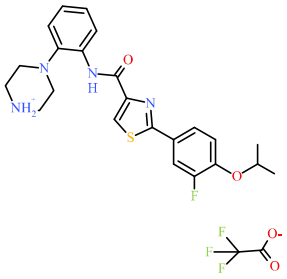
N-(2-(piperazin-1-yl)phenyl)-2-(4-(trifluoromethyl)phenyl)thiazole-4-carboxamide (E43)



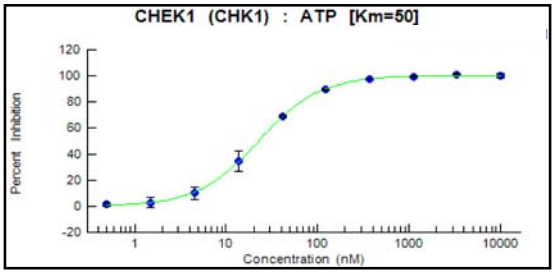


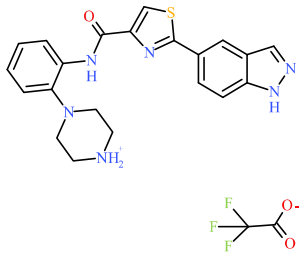
2-(3-fluoro-4-isopropoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E44)



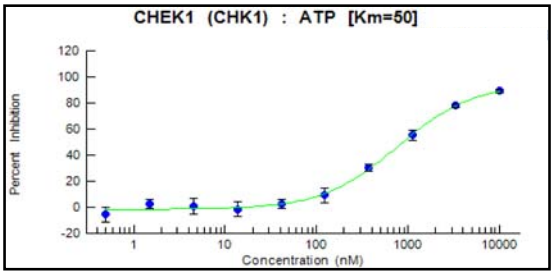


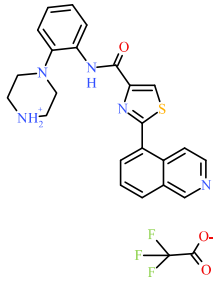
2-(1H-indazol-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E45)



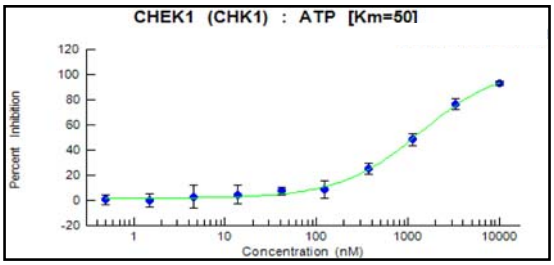


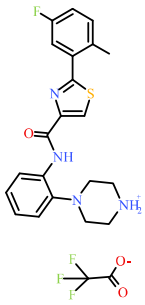
2-(isoquinolin-5-yl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E46)



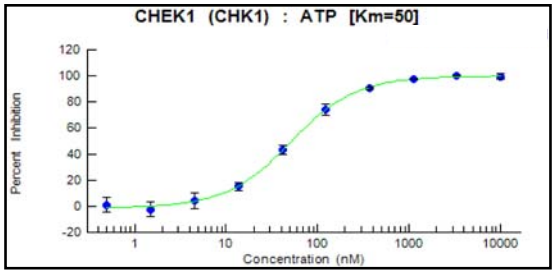


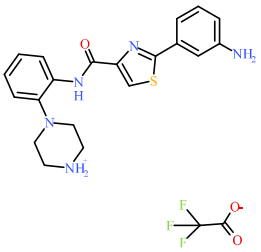
2-(5-fluoro-2-methylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E47)



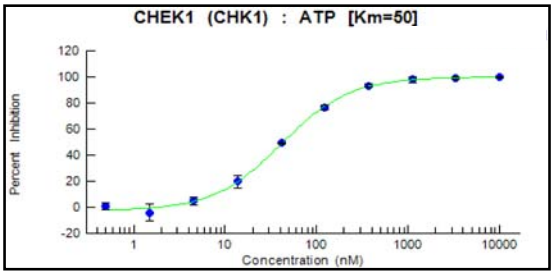


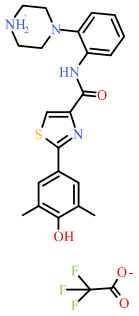
2-(3-aminophenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (38)



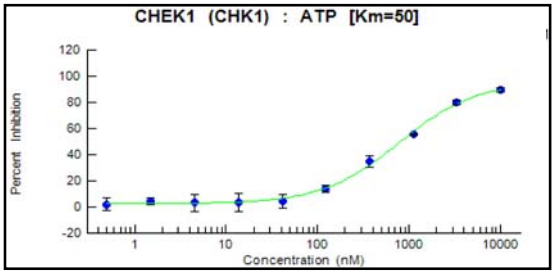


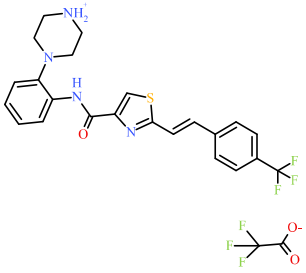
2-(4-hydroxy-3,5-dimethylphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E48)



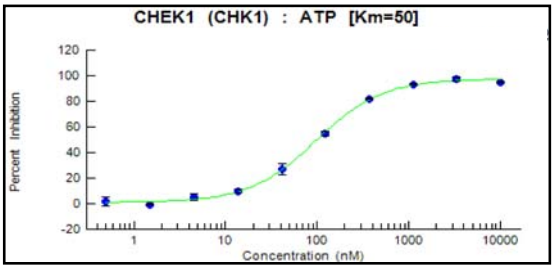


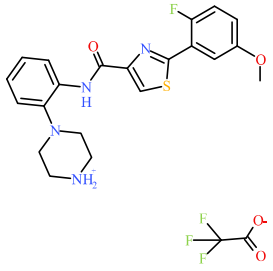
(*E*)-N-(2-(piperazin-1-yl)phenyl)-2-(4-(trifluoromethyl)styryl)thiazole-4-carboxamide (E49)





2-(2-fluoro-5-methoxyphenyl)-N-(2-(piperazin-1-yl)phenyl)thiazole-4-carboxamide (E50)





12. References

(1) Annis, D. A.; Athanasopoulos, J.; Curran, P. J.; Felsch, J. S.; Kalghatgi, K.; Lee, W. H.; Nash, H. M.; Orminati, J.-P. A.; Rosner, K. E.; Shipps Jr., G. W.; Thaddupathy, G. R. A.; Tyler, A. N.; Vilenchik, L.; Wagner, C. R.; Wintner, E. A. *Int. J. Mass Spectrom.* **2004**, *238* (2), 77–83.

(2) Annis, D. A.; Nazef, N.; Chuang, C.-C.; Scott, M. P.; Nash, H. M. *J. Am. Chem. Soc.* **2004**, *126* (47), 15495–15503.

(3) Annis, D. A.; Shipps, G. W.; Deng, Y.; Popovici-Müller, J.; Siddiqui, M. A.; Curran, P. J.; Gowen, M.; Windsor, W. T. *Anal. Chem.* **2007**, *79* (12), 4538–4542.

(4) Annis, D. A.; Nickbarg, E.; Yang, X.; Ziebell, M. R.; Whitehurst, C. E. *Curr. Opin. Chem. Biol.* **2007**, *11* (5), 518–526.

(5) Huang, X.; Cheng, C. C.; Fischmann, T. O.; Duca, J. S.; Yang, X.; Richards, M.; Shipps, G. W. *ACS Med. Chem. Lett.* **2012**, *3* (2), 123–128.

(6) Aronov, A. M.; Baker, C.; Bemis, G. W.; Cao, J.; Chen, G.; Ford, P. J.; Germann, U. A.; Green, J.; Hale, M. R.; Jacobs, M.; Janetka, J. W.; Maltais, F.; Martinez-Botella, G.; Namchuk, M. N.; Straub, J.; Tang, Q.; Xie, X. *J. Med. Chem.* **2007**, *50* (6), 1280–1287.

(7) Anderson, D. R.; Meyers, M. J.; Vernier, W. F.; Mahoney, M. W.; Kurumbail, R. G.; Caspers, N.; Poda, G. I.; Schindler, J. F.; Reitz, D. B.; Mourey, R. J. *J. Med. Chem.* **2007**, *50* (11), 2647–2654.

(8) Santanilla, A. B.; Regalado, E. L.; Pereira, T.; Shevlin, M.; Bateman, K.; Campeau, L.-C.; Schneeweis, J.; Berritt, S.; Shi, Z.-C.; Nantermet, P.; Liu, Y.; Helmy, R.; Welch, C. J.; Vachal, P.; Davies, I. W.; Cernak, T.; Dreher, S. D. *Science* **2015**, *347* (6217), 49–53.

(9) Mattson, R. J.; Pham, K. M.; Leuck, D. J.; Cowen, K. A. *J. Org. Chem.* **1990**, *55* (8), 2552–2554.

(10) Abdel-Magid, A. F.; Carson, K. G.; Harris, B. D.; Maryanoff, C. A.; Shah, R. D. *J. Org. Chem.* **1996**, *61* (11), 3849–3862.

(11) Neidigh, K. A.; Avery, M. A.; Williamson, J. S.; Bhattacharyya, S. *J. Chem. Soc. [Perkin 1]* **1998**, No. 16, 2527–2532.

(12) Vernier, W.; Anderson, D.; Phillion, D.; Meyers, M.; Hegde, S.; Reitz, D.; Buchler, I.; Mahoney, M.; Rogers, T.; Poda, G.; Singh, M.; Wu, K.; Xie, J. Mitogen activated protein kinase-activated protein kinase-2 inhibiting compounds. US20040209897 A1, October 21, 2004.

(13) Huang, X.; Cheng, C. C.; Fischmann, T. O.; Duca, J. S.; Richards, M.; Tadikonda, P. K.; Reddy, P. A.; Zhao, L.; Arshad Siddiqui, M.; Parry, D.; Davis, N.; Seghezzi, W.; Wiswell, D.; Shipps Jr., G. W. *Bioorg. Med. Chem. Lett.* **2013**, *23* (9), 2590–2594.

(14) Bickerton, G. R.; Paolini, G. V.; Besnard, J.; Muresan, S.; Hopkins, A. L. *Nat. Chem.* **2012**, *4* (2), 90–98.

(15) Buitrago Santanilla, A.; Christensen, M.; Campeau, L.-C.; Davies, I. W.; Dreher, S. D. *Org. Lett.* **2015**, *17* (13), 3370–3373.

(16) Gu, Z.; Gu, L.; Eils, R.; Schlesner, M.; Brors, B. *Bioinformatics* **2014**, *30* (19), 2811–2812.

(17) Gottlieb, H. E.; Kotlyar, V.; Nudelman, A. *J. Org. Chem.* **1997**, *62* (21), 7512–7515.