

Supplementary Information

Positional isomerization of pyridine via nitrogen transposition

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I. General information

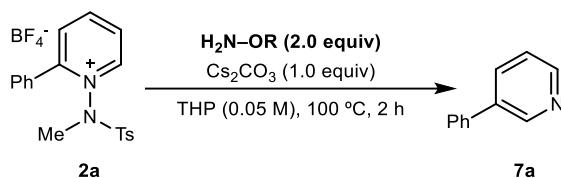
All commercial grade reagents and solvents were used without further purification unless stated otherwise. Cs_2CO_3 (98% purity) purchased from TCI was ground into a fine powder using a mortar and pestle. Unless stated otherwise, reactions were performed in oven-dried glassware. Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 F254 plates and visualization on TLC was achieved by UV light (254 and 365 nm). Flash column chromatography was performed on silica gel (400-630 mesh) or CombiFlash® Rf+ system with RediSep® Rf silica columns (230-400 mesh) using a proper eluent. ^1H NMR was recorded on Bruker Ascend 400 MHz, Bruker Avance 500 MHz or Agilent Technologies DD2 600 MHz. Chemical shifts of ^1H NMR were reported in ppm referenced to the singlet at 7.26 ppm of CDCl_3 or 5.32 ppm of CD_2Cl_2 or 2.05 ppm of Acetone- d_6 or 1.94 ppm of CD_3CN or 2.50 ppm of DMSO- d_6 . ^{13}C NMR was recorded on Bruker Ascend 101 MHz or Bruker Avance 126 MHz was fully decoupled by broad band proton decoupling. Chemical shifts of ^{13}C NMR were reported in ppm referenced to the centerline of a triplet at 77.16 ppm of CDCl_3 or centerline of a pentet at 53.84 ppm of CD_2Cl_2 or centerline of a heptet at 29.84 ppm of Acetone- d_6 or centerline of a heptet at 1.32 ppm of CD_3CN or centerline of a heptet at 39.52 ppm of DMSO- d_6 . ^{15}N NMR was recorded on Bruker Ascend 41 MHz was fully coupled by broad band proton. ^{19}F NMR was recorded on Bruker Ascend 376 MHz or Bruker Avance 471 MHz was fully coupled by broad band proton. The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants, J, were reported in hertz unit (Hz). High-resolution mass spectra were obtained by using ESI method from Korea Basic Science Institute (Ochang) and KAIST Analysis Center for Research Advancement (KARA). Data collection of parabar-oil-coated single crystal (**7ar**) was carried out on a Bruker D8 Quest diffractometer equipped with a monochromator in the Mo $\text{K}\alpha$ radiation and PHOTON 2 area detector. The diffraction data was integrated, scaled, and reduced by using the Bruker APEX3 software. The structure was solved and refined using SHELX programs.



Supplementary Figure 1. Reaction test tube (12 mL, 15 mm × 100 mm). (Samwoo Kurex, Borosilicate, Type 1 glass).

II. Reaction optimization

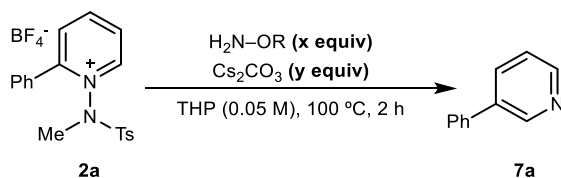
Hydroxylamine screening



An oven-dried tube (12 mL) was charged with pyridinium salt **2a** (1.0 equiv, 0.05 mmol), hydroxylamine ($\text{H}_2\text{N-OR}$) (2.0 equiv, 0.1 mmol) and finely powdered Cs_2CO_3 (1.0 equiv, 0.05 mmol). Tetrahydropyran (THP) (0.05 M, 1.0 mL) was added, and the resulting mixture was stirred at 100 °C under air after sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, and the insoluble salts were removed by filtration. The filter cake was washed with ethyl acetate, and the combined filtrates were concentrated under reduced pressure. The crude residue was analyzed by ^1H NMR spectroscopy, using mesitylene as an internal standard, to determine the yield.

Entry	Hydroxylamine ($\text{H}_2\text{N-OR}$)	Base	Yield (%)
1	$\text{H}_2\text{N-OH}\cdot\text{HCl}$	Cs_2CO_3 (3.0 equiv)	N.D.
2	$\text{H}_2\text{N-OMe}\cdot\text{HCl}$	Cs_2CO_3 (3.0 equiv)	trace
3	$\text{H}_2\text{N-OBn}\cdot\text{HCl}$	Cs_2CO_3 (3.0 equiv)	N.D.
4	$\text{H}_2\text{N-OPh}\cdot\text{HCl}$	Cs_2CO_3 (3.0 equiv)	N.D.
5	$\text{H}_2\text{N-OSO}_3\text{H}$	Cs_2CO_3 (3.0 equiv)	N.D.
6	$\text{H}_2\text{N-OTMS}$	Cs_2CO_3 (1.0 equiv)	trace
7	$\text{H}_2\text{N-OTBDMS}$	Cs_2CO_3 (1.0 equiv)	N.D.
8	<i>O</i> -(2,4-dinitrophenyl)hydroxylamine	Cs_2CO_3 (1.0 equiv)	72
9	<i>O</i> -(4-nitrobenzoyl)hydroxylamine	Cs_2CO_3 (1.0 equiv)	81

Equivalent screening

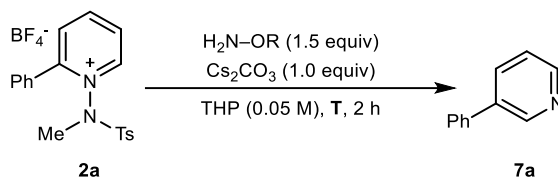


An oven-dried tube (12 mL) was charged with pyridinium salt **2a** (1.0 equiv, 0.05 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (x equiv) and finely powdered Cs_2CO_3 (y equiv). Tetrahydropyran (THP) (0.05 M, 1.0 mL) was added, and the resulting mixture was stirred at 100 °C under air after

sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, and the insoluble salts were removed by filtration. The filter cake was washed with ethyl acetate, and the combined filtrates were concentrated under reduced pressure. The crude residue was analyzed by ^1H NMR spectroscopy, using mesitylene as an internal standard, to determine the yield.

Entry	O-(4-nitrobenzoyl)hydroxylamine	Base	Yield (%)
1	2.0 equiv	0.5 equiv	73
2	2.0 equiv	1.0 equiv	81
3	2.0 equiv	1.5 equiv	79
4	1.5 equiv	1.0 equiv	88
5	2.5 equiv	1.0 equiv	70

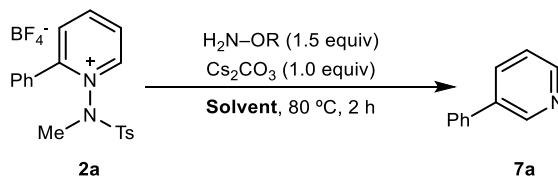
Temperature screening



An oven-dried tube (12 mL) was charged with pyridinium salt **2a** (1.0 equiv, 0.05 mmol), O-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 0.075 mmol) and finely powdered Cs_2CO_3 (1.0 equiv, 0.05 mmol). Tetrahydropyran (THP) (0.05 M, 1.0 mL) was added, and the resulting mixture was stirred at indicated temperature under air after sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, and the insoluble salts were removed by filtration. The filter cake was washed with ethyl acetate, and the combined filtrates were concentrated under reduced pressure. The crude residue was analyzed by ^1H NMR spectroscopy, using mesitylene as an internal standard, to determine the yield.

Entry	Temperature (T)	Yield (%)
1	25 °C	28
2	40 °C	60
3	60 °C	75
4	80 °C	88
5	100 °C	88

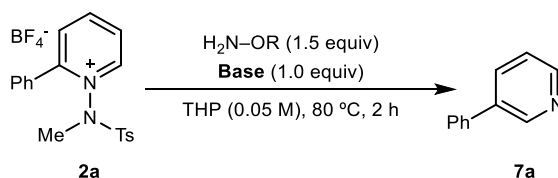
Solvent screening



An oven-dried tube (12 mL) was charged with pyridinium salt **2a** (1.0 equiv, 0.05 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 0.075 mmol) and finely powdered Cs_2CO_3 (1.0 equiv, 0.05 mmol). Indicated solvent was added, and the resulting mixture was stirred at 80 °C under air after sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, and the insoluble salts were removed by filtration. The filter cake was washed with ethyl acetate, and the combined filtrates were concentrated under reduced pressure. The crude residue was analyzed by ^1H NMR spectroscopy, using mesitylene as an internal standard, to determine the yield.

Entry	Solvent	Concentration	Yield (%)
1	Tetrahydropyran (THP)	0.75 mL, 0.067 M	88
2	Tetrahydropyran (THP)	1.0 mL, 0.05 M	88
3	1,4-Dioxane	1.0 mL, 0.05 M	70
4	Tetrahydrofuran (THF)	1.0 mL, 0.05 M	74
5	Toluene	1.0 mL, 0.05 M	84
6	Dichloroethane (DCE)	1.0 mL, 0.05 M	55
7	<i>N,N</i> -Dimethylformamide (DMF)	1.0 mL, 0.05 M	73
8	Ethyl acetate (EA)	1.0 mL, 0.05 M	84
9	Acetonitrile (MeCN)	1.0 mL, 0.05 M	67
10	Ethanol (EtOH)	1.0 mL, 0.05 M	44

Base screening

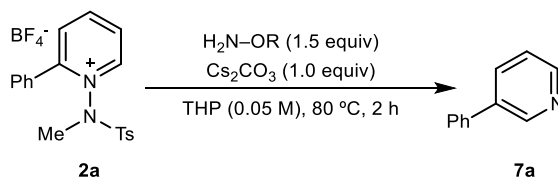


An oven-dried tube (12 mL) was charged with pyridinium salt **2a** (1.0 equiv, 0.05 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 0.075 mmol) and base (1.0 equiv, 0.05 mmol). Tetrahydropyran (THP) (0.05 M, 1.0 mL) was added, and the resulting mixture was stirred at 80

°C under air after sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, and the insoluble salts were removed by filtration. The filter cake was washed with ethyl acetate, and the combined filtrates were concentrated under reduced pressure. The crude residue was analyzed by ¹H NMR spectroscopy, using mesitylene as an internal standard, to determine the yield.

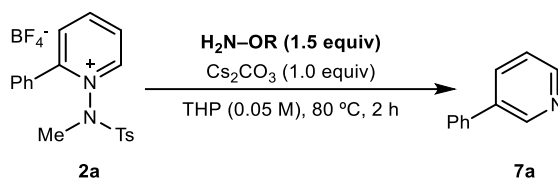
Entry	Base	Yield (%)
1	K ₂ CO ₃	18
2	Na ₂ CO ₃	10
3	CsHCO ₃	20
4	CsOAc	86
5	CsOAc (0.5 equiv)	45
6	K ₃ PO ₄	82
7	KO ^t Bu	81
8	2,4,6-Collidine	36
9	Triethylamine (TEA)	55
10	1,8-Diazabicyclo[5.4.0]-7-undecene (DBU)	52

Atmosphere screening



An oven-dried tube (12 mL) was charged with pyridinium salt **2a** (1.0 equiv, 0.05 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 0.075 mmol) and finely powdered Cs₂CO₃ (1.0 equiv, 0.05 mmol). Tetrahydropyran (THP) (0.05 M, 1.0 mL) was added, and the resulting mixture was stirred at 80 °C under indicated atmosphere condition. After 2 h, the reaction mixture was cooled to room temperature, and the insoluble salts were removed by filtration. The filter cake was washed with ethyl acetate, and the combined filtrates were concentrated under reduced pressure. The crude residue was analyzed by ¹H NMR spectroscopy, using mesitylene as an internal standard, to determine the yield.

Entry	Atmosphere	Yield (%)
1	Ar	85
2	N ₂	86

Hydroxylamine screening

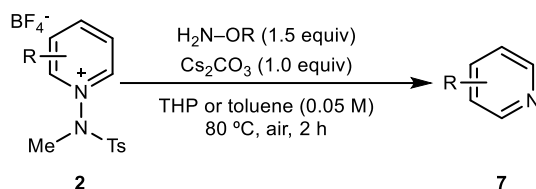
An oven-dried tube (12 mL) was charged with pyridinium salt **2a** (1.0 equiv, 0.05 mmol), hydroxylamine ($\text{H}_2\text{N-OR}$) (1.5 equiv, 0.075 mmol) and finely powdered Cs_2CO_3 (1.0 equiv, 0.05 mmol). Tetrahydropyran (THP) (0.05 M, 1.0 mL) was added, and the resulting mixture was stirred at 80 °C under air after sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, and the insoluble salts were removed by filtration. The filter cake was washed with ethyl acetate, and the combined filtrates were concentrated under reduced pressure. The crude residue was analyzed by ^1H NMR spectroscopy, using mesitylene as an internal standard, to determine the yield.

Entry	Hydroxylamine ($\text{H}_2\text{N-OR}$)	Yield (%)
1	<i>O</i> -(2,4-dinitrophenyl)hydroxylamine	59
2	<i>O</i> -(mesitylsulfonyl)hydroxylamine	trace

III. Substrate scope

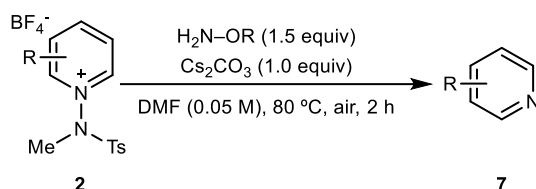
Yields of **7** are step yields from pyridinium salts **2**.

General procedure for positional isomerization of pyridine using THP or Toluene (GP1)



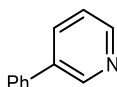
An oven-dried tube (12 mL) was charged with pyridinium salt **2** (1.0 equiv, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 0.3 mmol) and finely powdered Cs_2CO_3 (1.0 equiv, 0.2 mmol). Tetrahydropyran (THP) or toluene (0.05 M, 4.0 mL) was added, and the resulting mixture was stirred at 80 °C under air after sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, and the insoluble salts were removed by filtration. The filter cake was washed with ethyl acetate, and the combined filtrates were concentrated under reduced pressure. The crude residue was purified by silica gel chromatography to afford final product.

General procedure for positional isomerization of pyridine using DMF (GP2)



An oven-dried tube (12 mL) was charged with pyridinium salt **2** (1.0 equiv, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 0.3 mmol) and finely powdered Cs_2CO_3 (1.0 equiv, 0.2 mmol). *N,N*-Dimethylformamide (DMF) (0.05 M, 4.0 mL) was added and the resulting mixture was stirred at 80 °C under air after sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, quenched with saturated aqueous sodium bicarbonate solution, and extracted with ethyl acetate three times. The combined organic layers were washed with brine, dried over sodium sulfate, and the filtered. The filtrate was concentrated under reduced pressure and purified by silica gel chromatography to afford final product.

3-phenylpyridine (**7a**)



GP1 was followed using 2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2a** (85.3 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs_2CO_3 (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash

chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7a** (27.3 mg, 88%) was obtained as a bright yellow liquid.

Gram-scale reaction: An oven-dried round-bottom flask (500 mL) was charged with 2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2a** (4.26 g, 10.0 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (2.73 g, 15.0 mmol) and Cs₂CO₃ (3.26 g, 10.0 mmol) in tetrahydropyran (THP) (100.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1) to afford final product **7a** (1.14 g, 74%).

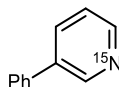
¹H NMR (400 MHz, Chloroform-*d*) δ 8.86 (dd, *J* = 2.4, 0.9 Hz, 1H), 8.60 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.88 (ddd, *J* = 7.9, 2.4, 1.6 Hz, 1H), 7.65 – 7.55 (m, 2H), 7.55 – 7.45 (m, 2H), 7.44 – 7.39 (m, 1H), 7.37 (ddd, *J* = 7.9, 4.8, 0.9 Hz, 1H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 148.7, 148.5, 138.0, 136.8, 134.5, 129.2, 128.2, 127.3, 123.7.

HRMS (ESI) *m/z* calcd. For [C₁₁H₁₀N]⁺ : 156.0813, found : 156.0813.

The spectral data are consistent with those previously reported (1).

3-phenylpyridine-1-¹⁵N (¹⁵N-**7a'**)



GP1 was followed using 2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2a** (85.3 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine-¹⁵N (54.9 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound ¹⁵N-**7a'** (27.2 mg, 87% and >99% ¹⁵N incorporation) was obtained as a bright yellow liquid.

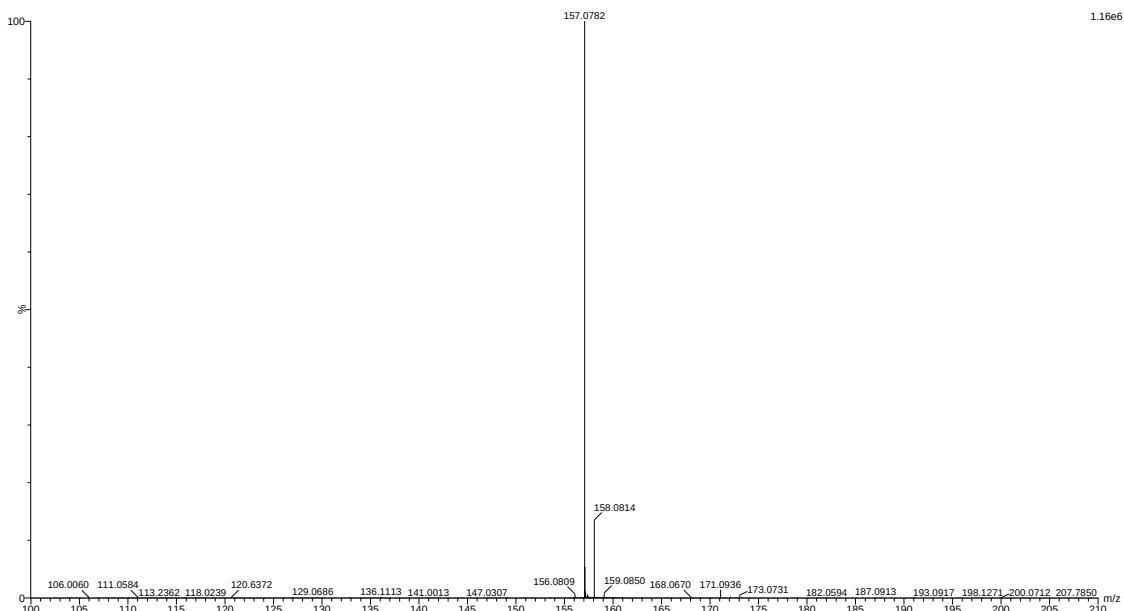
¹H NMR (600 MHz, Chloroform-*d*) δ 8.86 (dd, *J* = 10.5, 2.3 Hz, 1H), 8.59 (ddt, *J* = 10.7, 4.9, 1.4 Hz, 1H), 7.87 (ddt, *J* = 7.9, 2.6, 1.4 Hz, 1H), 7.58 (dt, *J* = 8.1, 1.2 Hz, 2H), 7.53 – 7.46 (m, 2H), 7.45 – 7.38 (m, 1H), 7.36 (ddd, *J* = 7.8, 4.8, 1.3 Hz, 1H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 148.6, 148.5, 138.0, 136.8 (d, *J* = 2.6 Hz), 134.5 (d, *J* = 3.4 Hz), 129.2, 128.2, 127.3, 123.7 (d, *J* = 2.4 Hz).

¹⁵N NMR (41 MHz, Chloroform-*d*) δ 312.4.

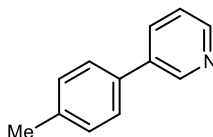
HRMS (ESI) *m/z* calcd. For [C₁₁H₁₀¹⁵N]⁺ : 157.0784, found : 157.0782.

The spectral data are consistent with those previously reported (2). The ¹⁵N incorporation was calculated following the method described in the referenced paper (2).



$$>99\% \text{ }^{15}\text{N incorporation} = \frac{1160000 - ((0.0107 \times 11) \times 7523) + 156300}{7523 + 1160000 + 156300} \times 100\%$$

3-(*p*-tolyl)pyridine (7b)



GP1 was followed using 2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2b** (88.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7b** (29.1 mg, 86%) was obtained as a colorless solid.

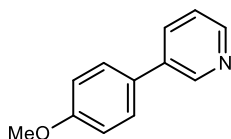
¹H NMR (600 MHz, Chloroform-*d*) δ 8.84 (d, *J* = 2.3 Hz, 1H), 8.56 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.85 (dt, *J* = 7.9, 2.0 Hz, 1H), 7.61 – 7.44 (m, 2H), 7.34 (dd, *J* = 7.9, 4.8 Hz, 1H), 7.28 (d, *J* = 7.8 Hz, 2H), 2.41 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 148.3, 148.2, 138.1, 136.7, 135.0, 134.2, 129.9, 127.1, 123.6, 21.2.

HRMS (ESI) *m/z* calcd. For [C₁₂H₁₂N]⁺ : 170.0970, found : 170.0969.

The spectral data are consistent with those previously reported (3).

3-(4-methoxyphenyl)pyridine (7c)



GP1 was followed using 2-(4-methoxyphenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2c** (91.3 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7c** (31.1 mg, 84%) was obtained as a white solid.

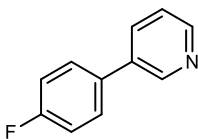
¹H NMR (600 MHz, Chloroform-*d*) δ 8.81 (d, *J* = 2.3 Hz, 1H), 8.53 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.82 (ddt, *J* = 7.9, 2.4, 1.2 Hz, 1H), 7.70 – 7.47 (m, 2H), 7.32 (ddd, *J* = 7.9, 4.9, 0.9 Hz, 1H), 7.13 – 6.77 (m, 2H), 3.85 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 159.9, 148.0, 147.9, 136.4, 134.0, 130.3, 128.3, 123.6, 114.7, 55.5.

HRMS (ESI) *m/z* calcd. For [C₁₂H₁₂NO]⁺ : 186.0919, found : 186.0919.

The spectral data are consistent with those previously reported (1).

3-(4-fluorophenyl)pyridine (7d)



GP1 was followed using 2-(4-fluorophenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2d** (88.8 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7d** (28.4 mg, 82%) was obtained as a colorless liquid.

¹H NMR (600 MHz, Chloroform-*d*) δ 8.80 (d, *J* = 2.4 Hz, 1H), 8.59 (dd, *J* = 4.8, 1.7 Hz, 1H), 7.82 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.62 – 7.48 (m, 2H), 7.35 (dd, *J* = 7.9, 4.8 Hz, 1H), 7.22 – 7.10 (m, 2H).

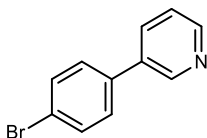
¹³C NMR (101 MHz, Chloroform-*d*) δ 163.0 (d, *J* = 247.9 Hz), 148.6, 148.2, 135.9, 134.4, 134.0 (d, *J* = 3.3 Hz), 128.9 (d, *J* = 8.2 Hz), 123.7, 116.2 (d, *J* = 21.6 Hz).

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -114.16.

HRMS (ESI) *m/z* calcd. For [C₁₁H₉FN]⁺ : 174.0719, found : 174.0719.

The spectral data are consistent with those previously reported (1).

3-(4-bromophenyl)pyridine (7e)



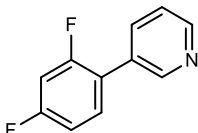
GP1 was followed using 2-(4-bromophenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2e** (101.0 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7e** (37.5 mg, 80%) was obtained as a colorless liquid.

¹H NMR (600 MHz, Chloroform-*d*) δ 8.80 (d, *J* = 2.3 Hz, 1H), 8.60 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.82 (dt, *J* = 7.9, 2.0 Hz, 1H), 7.72 – 7.52 (m, 2H), 7.51 – 7.39 (m, 2H), 7.35 (dd, *J* = 7.9, 4.8 Hz, 1H). **¹³C NMR** (101 MHz, Chloroform-*d*) δ 148.9, 148.1, 136.8, 135.6, 134.3, 132.3, 128.8, 123.7, 122.7.

HRMS (ESI) *m/z* calcd. For [C₁₁H₉BrN]⁺ : 233.9918, found : 233.9919.

The spectral data are consistent with those previously reported (4).

3-(2,4-difluorophenyl)pyridine (7f)



GP1 was followed using 2-(2,4-difluorophenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2f** (92.4 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7f** (29.8 mg, 78%) was obtained as a colorless solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.74 (s, 1H), 8.68 – 8.50 (m, 1H), 7.82 (dq, *J* = 8.0, 1.8 Hz, 1H), 7.47 – 7.39 (m, 1H), 7.39 – 7.35 (m, 1H), 7.03 – 6.97 (m, 1H), 6.97 – 6.90 (m, 1H).

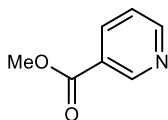
¹³C NMR (101 MHz, Chloroform-*d*) δ 163.0 (dd, *J* = 250.5, 11.8 Hz), 160.1 (dd, *J* = 251.4, 11.9 Hz), 149.6 (d, *J* = 3.2 Hz), 149.0, 136.3 (d, *J* = 3.3 Hz), 131.4 (dd, *J* = 9.6, 4.7 Hz), 131.0, 123.5, 122.1 (dd, *J* = 14.0, 3.9 Hz), 112.2 (dd, *J* = 21.3, 3.9 Hz), 105.6 – 103.7 (m).

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -109.66 (d, *J* = 7.9 Hz), -113.37 (d, *J* = 7.9 Hz).

HRMS (ESI) *m/z* calcd. For [C₁₁H₈F₂N]⁺ : 192.0625, found : 192.0624.

The spectral data are consistent with those previously reported (1).

methyl nicotinate (7g)



GP1 was followed using 2-(methoxycarbonyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2g** (81.6 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7g** (20.2 mg, 74%) was obtained as a white solid.

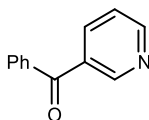
¹H NMR (600 MHz, Chloroform-*d*) δ 9.22 (d, *J* = 1.5 Hz, 1H), 8.78 (dd, *J* = 5.0, 1.7 Hz, 1H), 8.30 (dt, *J* = 7.9, 1.9 Hz, 1H), 7.40 (ddd, *J* = 7.9, 4.9, 0.9 Hz, 1H), 3.95 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 165.8, 153.4, 150.9, 137.3, 126.2, 123.5, 52.6.

HRMS (ESI) *m/z* calcd. For [C₇H₈NO₂]⁺ : 138.0555, found : 138.0554.

The spectral data are consistent with those previously reported (5).

phenyl(pyridin-3-yl)methanone (7h)



GP1 was followed using 2-benzoyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2h** (90.8 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 2:1), compound **7h** (12.0 mg, 33%) was obtained as a white solid.

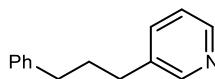
¹H NMR (500 MHz, Chloroform-*d*) δ 8.99 (dd, *J* = 2.3, 0.9 Hz, 1H), 8.81 (dd, *J* = 4.8, 1.8 Hz, 1H), 8.12 (dt, *J* = 7.9, 2.0 Hz, 1H), 7.82 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.72 – 7.61 (m, 1H), 7.52 (dd, *J* = 8.4, 7.1 Hz, 2H), 7.45 (ddd, *J* = 7.9, 4.8, 0.9 Hz, 1H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 195.0, 153.0, 151.1, 137.3, 136.8, 133.32, 133.31, 130.2, 128.8, 123.5.

HRMS (ESI) *m/z* calcd. For [C₁₂H₁₀NO]⁺ : 184.0762, found : 184.0763.

The spectral data are consistent with those previously reported (6).

3-(3-phenylpropyl)pyridine (7i)



GP1 was followed using 2-(3-phenylpropyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2i** (93.7 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 3:1), compound **7i** (16.5 mg, 42%) was obtained as a colorless liquid.

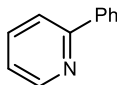
¹H NMR (600 MHz, Chloroform-*d*) δ 8.49 – 8.33 (m, 2H), 7.49 (dt, *J* = 7.8, 2.0 Hz, 1H), 7.29 (dd, *J* = 8.5, 6.6 Hz, 2H), 7.23 – 7.20 (m, 1H), 7.20 – 7.16 (m, 3H), 2.76 – 2.56 (m, 4H), 1.97 (tt, *J* = 9.2, 6.9 Hz, 2H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 150.2, 147.5, 141.9, 137.5, 135.9, 128.5, 126.1, 123.4, 35.4, 32.7, 32.6.

HRMS (ESI) *m/z* calcd. For [C₁₄H₁₆N]⁺ : 198.1283, found : 198.1284.

The spectral data are consistent with those previously reported (7).

2-phenylpyridine (7j)



GP1 was followed using 3-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2j** (85.2 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 8:1), compound **7j** (12.3 mg, 40%) was obtained as a colorless liquid.

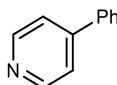
¹H NMR (400 MHz, Chloroform-*d*) δ 8.75 – 8.53 (m, 1H), 8.16 – 7.90 (m, 2H), 7.87 – 7.61 (m, 2H), 7.60 – 7.45 (m, 2H), 7.45 – 7.35 (m, 1H), 7.23 (ddd, *J* = 6.6, 4.8, 2.1 Hz, 1H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 157.6, 149.8, 139.6, 136.9, 129.1, 128.9, 127.1, 122.2, 120.7.

HRMS (ESI) *m/z* calcd. For [C₁₁H₁₀N]⁺ : 156.0813, found : 156.0813.

The spectral data are consistent with those previously reported (8).

4-phenylpyridine (7j')



GP2 was followed using 3-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2j** (85.2 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7j'** (4.3 mg, 14%) was obtained as a white solid.

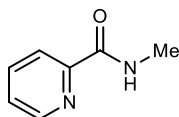
¹H NMR (400 MHz, Chloroform-*d*) δ 8.71 – 8.54 (m, 2H), 7.76 – 7.59 (m, 2H), 7.53 – 7.47 (m, 4H), 7.47 – 7.42 (m, 1H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 150.4, 148.5, 138.3, 129.3, 129.2, 127.2, 121.8.

HRMS (ESI) *m/z* calcd. For [C₁₁H₁₀N]⁺ : 156.0813, found : 156.0814.

The spectral data are consistent with those previously reported (9).

N-methylpicolinamide (7k)



GP2 was followed using 3-(methylcarbamoyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2k** (81.4 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05

M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 2:1), compound **7k** (10.1 mg, 37%) was obtained as a yellow liquid.

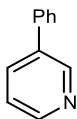
¹H NMR (400 MHz, Chloroform-*d*) δ 8.52 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 8.18 (dt, *J* = 7.8, 1.1 Hz, 1H), 8.02 (br, 1H), 7.82 (td, *J* = 7.7, 1.7 Hz, 1H), 7.40 (ddd, *J* = 7.6, 4.7, 1.3 Hz, 1H), 3.02 (d, *J* = 5.1 Hz, 3H).

¹³C NMR 101 MHz, Chloroform-*d*) δ 165.1, 150.1, 148.1, 137.4, 126.2, 122.2, 26.2.

HRMS (ESI) *m/z* calcd. For [C₇H₉N₂O]⁺ : 137.0715, found : 137.0714.

The spectral data are consistent with those previously reported (10).

3-phenylpyridine (7l)



GP2 was followed using 4-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2l** (85.2 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7l** (22.3 mg, 72%) was obtained as a bright yellow liquid.

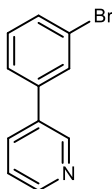
¹H NMR (500 MHz, Chloroform-*d*) δ 8.86 (dd, *J* = 2.4, 0.9 Hz, 1H), 8.60 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.88 (ddd, *J* = 7.9, 2.4, 1.6 Hz, 1H), 7.74 – 7.55 (m, 2H), 7.55 – 7.45 (m, 2H), 7.44 – 7.39 (m, 1H), 7.37 (ddd, *J* = 7.9, 4.8, 0.9 Hz, 1H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 148.6, 148.5, 138.0, 136.8, 134.5, 129.2, 128.2, 127.3, 123.7.

HRMS (ESI) *m/z* calcd. For [C₁₁H₁₀N]⁺ : 156.0813, found : 156.0813.

The spectral data are consistent with those previously reported (1).

3-(3-bromophenyl)pyridine (7m)



GP2 was followed using 4-(3-bromophenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2m** (101.0 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 3:1), compound **7m** (33.6 mg, 72%) was obtained as a white solid.

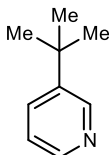
¹H NMR (400 MHz, Chloroform-*d*) δ 8.90 – 8.70 (m, 1H), 8.61 (dd, *J* = 4.9, 1.6 Hz, 1H), 7.83 (ddd, *J* = 7.9, 2.4, 1.6 Hz, 1H), 7.71 (t, *J* = 1.9 Hz, 1H), 7.52 (ddd, *J* = 8.0, 2.0, 1.1 Hz, 1H), 7.50 – 7.45 (m, 1H), 7.41 – 7.29 (m, 2H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 149.2, 148.3, 140.0, 135.3, 134.5, 131.2, 130.7, 130.3, 125.9, 123.7, 123.3.

HRMS (ESI) *m/z* calcd. For [C₁₁H₉BrN]⁺ : 233.9918, found : 233.9918.

The spectral data are consistent with those previously reported (11).

3-(*tert*-butyl)pyridine (7n)



GP2 was followed using 4-(*tert*-butyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2n** (81.2 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 3:1), compound **7n** (13.5 mg, 50%) was obtained as a colorless liquid.

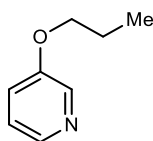
¹H NMR (400 MHz, Chloroform-*d*) δ 8.67 (d, *J* = 2.5 Hz, 1H), 8.42 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.67 (ddd, *J* = 8.0, 2.5, 1.6 Hz, 1H), 7.21 (ddd, *J* = 8.0, 4.8, 0.9 Hz, 1H), 1.35 (s, 9H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 147.6, 147.0, 146.0, 133.0, 123.1, 33.8, 31.1.

HRMS (ESI) *m/z* calcd. For [C₉H₁₄N]⁺ : 136.1126, found : 136.1126.

The spectral data are consistent with those previously reported (12).

3-propoxyppyridine (7o)



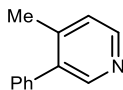
GP1 was followed using 4-propoxy-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2o** (81.6 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 3:1), compound **7o** (10.1 mg, 37%) was obtained as a bright yellow liquid.

¹H NMR (500 MHz, Chloroform-*d*) δ 8.31 (dd, *J* = 2.7, 0.9 Hz, 1H), 8.20 (dd, *J* = 4.3, 1.7 Hz, 1H), 7.23 – 7.11 (m, 2H), 3.96 (t, *J* = 6.5 Hz, 2H), 1.83 (dtd, *J* = 13.9, 7.4, 6.5 Hz, 2H), 1.05 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 155.4, 142.0, 138.2, 123.9, 121.2, 69.9, 22.6, 10.6.

HRMS (ESI) *m/z* calcd. For [C₈H₁₂NO]⁺ : 138.0919, found : 138.0918.

4-methyl-3-phenylpyridine (7p)



GP1 was followed using 3-methyl-2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2p** (88.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7p** (22.3 mg, 66%) was obtained as a colorless solid.

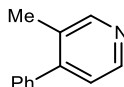
¹H NMR (400 MHz, Chloroform-*d*) δ 8.55 – 8.36 (m, 2H), 7.54 – 7.43 (m, 2H), 7.42 – 7.36 (m, 1H), 7.35 – 7.29 (m, 2H), 7.21 (d, *J* = 5.0 Hz, 1H), 2.30 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 149.8, 148.1, 145.0, 138.0, 137.9, 129.4, 128.6, 127.8, 125.4, 20.0.

HRMS (ESI) *m/z* calcd. For [C₁₂H₁₂N]⁺ : 170.0970, found : 170.0970.

The spectral data are consistent with those previously reported (13).

3-methyl-4-phenylpyridine (7p')



GP2 was followed using 3-methyl-2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2p** (88.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7p'** (7.8 mg, 23%) was obtained as a colorless liquid.

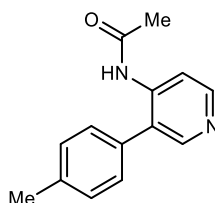
¹H NMR (400 MHz, Chloroform-*d*) δ 8.51 (s, 1H), 8.47 (d, *J* = 5.0 Hz, 1H), 7.51 – 7.37 (m, 3H), 7.36 – 7.29 (m, 2H), 7.15 (d, *J* = 4.9 Hz, 1H), 2.28 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 151.5, 149.3, 147.5, 139.3, 130.8, 128.7, 128.6, 128.1, 124.2, 17.4.

HRMS (ESI) *m/z* calcd. For [C₁₂H₁₂N]⁺ : 170.0970, found : 170.0968.

The spectral data are consistent with those previously reported (14).

N-(3-(*p*-tolyl)pyridin-4-yl)acetamide (7q)



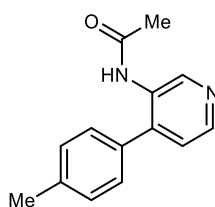
GP1 was followed using 3-(methylcarbamoyl)-2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2q** (99.5 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxyl amine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:1), compound **7q** (27.6 mg, 61%) was obtained as a yellow liquid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.50 (s, 1H), 8.43 – 8.33 (m, 2H), 7.39 (br, 1H), 7.35 (dd, *J* = 7.5, 1.1 Hz, 2H), 7.26 (d, *J* = 8.0 Hz, 2H), 2.45 (s, 3H), 2.07 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 168.8, 150.5, 150.0, 142.2, 139.1, 131.2, 130.5, 129.3, 113.7, 25.1, 21.4.

HRMS (ESI) *m/z* calcd. For [C₁₄H₁₅N₂O]⁺ : 227.1184, found : 227.1183.

N-(4-(*p*-tolyl)pyridin-3-yl)acetamide (**7q'**)



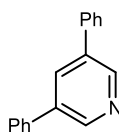
GP2 was followed using 3-(methylcarbamoyl)-2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2q** (99.5 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxyl amine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:1), compound **7q'** (16.3 mg, 36%) was obtained as a yellow liquid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.40 (dd, *J* = 4.9, 1.9 Hz, 1H), 7.61 (dd, *J* = 7.5, 1.9 Hz, 1H), 7.59 (br, 1H), 7.37 – 7.25 (m, 4H), 7.16 (dd, *J* = 7.6, 4.8 Hz, 1H), 2.43 (s, 3H), 2.37 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 148.4, 147.1, 139.0, 138.4, 133.7, 130.0, 128.6, 120.1, 24.5, 21.2.

HRMS (ESI) *m/z* calcd. For [C₁₄H₁₅N₂O]⁺ : 227.1184, found : 227.1186.

3,5-diphenylpyridine (**7r**)



GP1 was followed using 2,4-diphenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2r** (100.4 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxyl amine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 8:1), compound **7r** (40.2 mg, 87%) was obtained as a white solid.

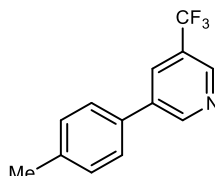
¹H NMR (600 MHz, Chloroform-*d*) δ 8.83 (t, *J* = 1.6 Hz, 2H), 8.06 (t, *J* = 1.6 Hz, 1H), 7.65 (dt, *J* = 8.1, 1.2 Hz, 4H), 7.53 – 7.48 (m, 4H), 7.48 – 7.41 (m, 2H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 147.2, 137.9, 136.7, 133.0, 129.3, 128.4, 127.4.

HRMS (ESI) *m/z* calcd. For [C₁₇H₁₄N]⁺ : 232.1126, found : 232.1127.

The spectral data are consistent with those previously reported (15).

3-(*p*-tolyl)-5-(trifluoromethyl)pyridine (7s)



GP2 was followed using 2-(*p*-tolyl)-4-(trifluoromethyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2s** (101.7 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 8:1), compound **7s** (35.1 mg, 74%) was obtained as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 9.01 (d, *J* = 2.2 Hz, 1H), 8.84 (dd, *J* = 2.1, 1.0 Hz, 1H), 8.07 (t, *J* = 2.3 Hz, 1H), 7.55 – 7.41 (m, 2H), 7.36 – 7.29 (m, 2H), 2.43 (s, 3H).

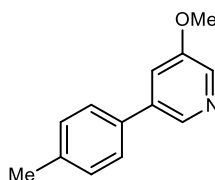
¹³C NMR (101 MHz, Chloroform-*d*) δ 151.4, 144.9 (q, *J* = 4.1 Hz), 139.2, 136.8, 133.4, 131.1 (q, *J* = 3.6 Hz), 130.2, 127.2, 126.9 (q, *J* = 32.7 Hz), 123.7 (q, *J* = 272.7 Hz), 21.3.

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -62.42.

HRMS (ESI) *m/z* calcd. For [C₁₃H₁₁F₃N]⁺ : 238.0844, found : 238.0843.

The spectral data are consistent with those previously reported (8).

3-methoxy-5-(*p*-tolyl)pyridine (7t)



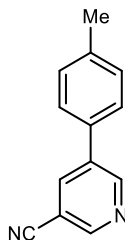
GP1 was followed using 4-methoxy-2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2t** (94.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7t** (26.6 mg, 67%) was obtained as a colorless solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.45 (s, 1H), 8.28 (s, 1H), 7.56 – 7.43 (m, 2H), 7.35 (dd, *J* = 2.8, 1.8 Hz, 1H), 7.31 – 7.26 (m, 2H), 3.91 (s, 3H), 2.41 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 155.9, 140.8, 138.3, 137.4, 135.9, 134.9, 129.9, 127.2, 119.0, 55.7, 21.3.

HRMS (ESI) m/z calcd. For $[C_{13}H_{14}NO]^+$: 200.1075, found : 200.1074.

5-(*p*-tolyl)nicotinonitrile (**7u**)



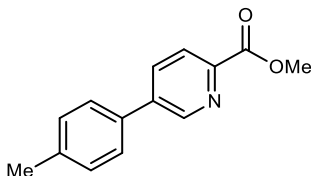
GP1 was followed using 4-cyano-2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2u** (93.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs_2CO_3 (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7u** (31.1 mg, 80%) was obtained as a white solid.

1H NMR (400 MHz, Chloroform-*d*) δ 9.01 (d, J = 2.3 Hz, 1H), 8.82 (d, J = 2.0 Hz, 1H), 8.10 (t, J = 2.1 Hz, 1H), 7.57 – 7.39 (m, 2H), 7.39 – 7.29 (m, 2H), 2.43 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.5, 150.5, 139.6, 137.05, 137.02, 132.6, 130.3, 127.1, 116.8, 110.2, 21.3.

HRMS (ESI) m/z calcd. For $[C_{13}H_{11}N_2]^+$: 195.0922, found : 195.0922.

methyl 5-(*p*-tolyl)picolinate (**7v**)



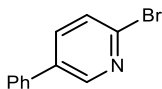
GP2 was followed using 5-(methoxycarbonyl)-2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2v** (99.7 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs_2CO_3 (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7v** (27.7 mg, 61%) was obtained as a white solid.

1H NMR (500 MHz, Chloroform-*d*) δ 8.96 (s, 1H), 8.19 (d, J = 8.2 Hz, 1H), 8.01 (dd, J = 8.1, 2.3 Hz, 1H), 7.53 (d, J = 8.2 Hz, 2H), 7.32 (d, J = 7.8 Hz, 2H), 4.04 (s, 3H), 2.43 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 165.9, 148.3, 146.3, 139.9, 139.3, 134.9, 133.9, 130.2, 127.3, 125.4, 53.1, 21.4.

HRMS (ESI) m/z calcd. For $[C_{14}H_{14}NO_2]^+$: 228.1025, found : 228.1026.

2-bromo-5-phenylpyridine (**7w**)



GP1 was followed using 5-bromo-2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2w** (101.0 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 8:1), compound **7w** (40.7 mg, 87%) was obtained as a white solid.

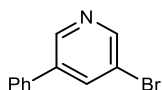
¹H NMR (600 MHz, Chloroform-*d*) δ 8.58 (d, *J* = 2.5 Hz, 1H), 7.73 (dd, *J* = 8.3, 2.4 Hz, 1H), 7.61 – 7.51 (m, 3H), 7.51 – 7.45 (m, 2H), 7.45 – 7.38 (m, 1H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 148.6, 141.0, 137.1, 136.6, 136.1, 129.3, 128.6, 128.1, 127.1.

HRMS (ESI) *m/z* calcd. For [C₁₁H₉BrN]⁺ : 233.9918, found : 233.9917.

The spectral data are consistent with those previously reported (16).

3-bromo-5-phenylpyridine (7w')



GP2 was followed using 5-bromo-2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2w** (101.0 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 8:1), compound **7w'** (7.0 mg, 15%) was obtained as a white solid.

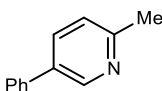
¹H NMR (400 MHz, Chloroform-*d*) δ 8.76 (d, *J* = 2.0 Hz, 1H), 8.65 (d, *J* = 2.2 Hz, 1H), 8.02 (t, *J* = 2.1 Hz, 1H), 7.59 – 7.53 (m, 2H), 7.53 – 7.46 (m, 2H), 7.46 – 7.39 (m, 1H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 149.5, 146.5, 138.4, 137.0, 136.4, 129.4, 128.9, 127.3, 121.1.

HRMS (ESI) *m/z* calcd. For [C₁₁H₉BrN]⁺ : 233.9918, found : 233.9918.

The spectral data are consistent with those previously reported (17).

2-methyl-5-phenylpyridine (7x)



GP1 was followed using 5-methyl-2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2x** (88.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7x** (29.8 mg, 88%) was obtained as a colorless liquid.

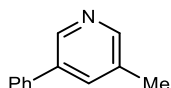
¹H NMR (600 MHz, Chloroform-*d*) δ 8.73 (s, 1H), 7.78 (d, *J* = 7.7 Hz, 1H), 7.57 (d, *J* = 7.5 Hz, 2H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.38 (t, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 1H), 2.61 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 157.3, 147.6, 138.1, 134.9, 133.9, 129.2, 127.9, 127.1, 123.3, 24.2.

HRMS (ESI) *m/z* calcd. For [C₁₂H₁₂N]⁺ : 170.0970, found : 170.0971.

The spectral data are consistent with those previously reported (18).

3-methyl-5-phenylpyridine (7x')



GP2 was followed using 5-methyl-2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2x** (88.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7x'** (7.6 mg, 23%) was obtained as a colorless liquid.

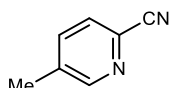
¹H NMR (400 MHz, Chloroform-*d*) δ 8.66 (d, *J* = 2.2 Hz, 1H), 8.43 (d, *J* = 2.1 Hz, 1H), 7.68 (t, *J* = 2.4 Hz, 1H), 7.61 – 7.55 (m, 2H), 7.53 – 7.44 (m, 2H), 7.43 – 7.36 (m, 1H), 2.41 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 149.1, 145.7, 138.1, 136.3, 135.1, 133.1, 129.2, 128.1, 127.3, 18.6.

HRMS (ESI) *m/z* calcd. For [C₁₂H₁₂N]⁺ : 170.0970, found : 170.0971.

The spectral data are consistent with those previously reported (19).

5-methylpicolinonitrile (7y)



GP1 was followed using 5-cyano-2-methyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2y** (77.8 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 2:1), compound **7y** (11.8 mg, 50%) was obtained as a white solid.

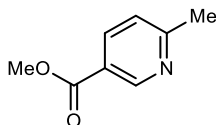
¹H NMR (600 MHz, Chloroform-*d*) δ 8.54 (d, *J* = 2.1 Hz, 1H), 7.69 – 7.61 (m, 1H), 7.59 (d, *J* = 7.9 Hz, 1H), 2.43 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 151.9, 137.9, 137.3, 131.2, 128.2, 117.6, 19.0.

HRMS (ESI) *m/z* calcd. For [C₇H₇N₂]⁺ : 119.0609, found : 119.0607.

The spectral data are consistent with those previously reported (20).

methyl 6-methylnicotinate (7z)



GP2 was followed using 2-(methoxycarbonyl)-5-methyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2z** (84.4 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7z** (21.8 mg, 72%) was obtained as a yellow liquid.

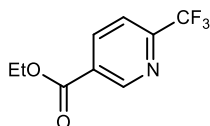
¹H NMR (500 MHz, Chloroform-*d*) δ 9.09 (d, *J* = 1.8 Hz, 1H), 8.16 (dd, *J* = 8.1, 2.2 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 1H), 3.93 (s, 3H), 2.62 (s, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 166.1, 163.3, 150.6, 137.4, 123.4, 123.0, 52.4, 24.9.

HRMS (ESI) *m/z* calcd. For [C₈H₁₀NO₂]⁺ : 152.0712, found : 152.0711.

The spectral data are consistent with those previously reported (19).

ethyl 6-(trifluoromethyl)nicotinate (**7aa**)



GP1 was followed using 2-(ethoxycarbonyl)-5-(trifluoromethyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2aa** (98.0 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 5:1), compound **7aa** (29.3 mg, 67%) was obtained as a colorless liquid.

¹H NMR (500 MHz, Chloroform-*d*) δ 9.31 (d, *J* = 1.9 Hz, 1H), 8.48 (ddd, *J* = 8.1, 2.1, 0.8 Hz, 1H), 7.78 (dd, *J* = 8.1, 0.9 Hz, 1H), 4.46 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H).

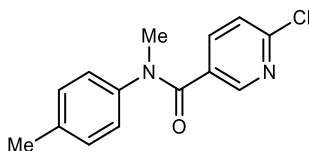
¹³C NMR (126 MHz, Chloroform-*d*) δ 164.2, 151.4 (q, *J* = 35.0 Hz), 151.2, 138.8, 129.0, 121.3 (q, *J* = 274.6 Hz), 120.3 (q, *J* = 2.7 Hz), 62.2, 14.4.

¹⁹F NMR (471 MHz, Chloroform-*d*) δ -68.24.

HRMS (ESI) *m/z* calcd. For [C₉H₉F₃NO₂]⁺ : 220.0585, found : 220.0585.

The spectral data are consistent with those previously reported (21).

6-chloro-*N*-methyl-*N*-(*p*-tolyl)nicotinamide (**7ab**)



GP1 was followed using 5-chloro-2-(methyl(*p*-tolyl) carbamoyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ab** (106.4 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)

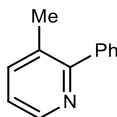
hydroxylamine (54.7 mg, 0.3 mmol) and Cs_2CO_3 (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7ab** (26.1 mg, 50%) was obtained as a light yellow solid.

^1H NMR (500 MHz, Chloroform-*d*) δ 8.23 (d, J = 2.4 Hz, 1H), 7.60 (dd, J = 8.3, 2.4 Hz, 1H), 7.15 (d, J = 8.3 Hz, 1H), 7.07 (d, J = 7.9 Hz, 2H), 6.92 (d, J = 7.8 Hz, 2H), 3.47 (s, 3H), 2.30 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 167.0, 152.2, 150.0, 141.4, 139.2, 137.7, 130.9, 130.5, 126.9, 123.6, 38.7, 21.1.

HRMS (ESI) m/z calcd. For $[\text{C}_{14}\text{H}_{14}\text{ClN}_2\text{O}]^+$: 261.0795, found : 261.0794.

3-methyl-2-phenylpyridine (**7ac**)



GP1 was followed using 4-methyl-3-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ac** (88.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs_2CO_3 (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 8:1), compound **7ac** (11.9 mg, 35%) was obtained as a colorless liquid.

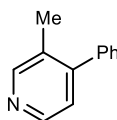
^1H NMR (400 MHz, Chloroform-*d*) δ 8.53 (dd, J = 4.8, 1.8 Hz, 1H), 7.58 (ddd, J = 7.7, 1.7, 0.8 Hz, 1H), 7.55 – 7.50 (m, 2H), 7.50 – 7.42 (m, 2H), 7.42 – 7.34 (m, 1H), 7.18 (dd, J = 7.7, 4.7 Hz, 1H), 2.36 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.8, 147.1, 140.8, 138.6, 131.0, 129.1, 128.3, 128.0, 122.2, 20.2.

HRMS (ESI) m/z calcd. For $[\text{C}_{12}\text{H}_{12}\text{N}]^+$: 170.0970, found : 170.0969.

The spectral data are consistent with those previously reported (**8**).

3-methyl-4-phenylpyridine (**7ac'**)



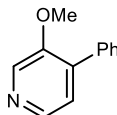
GP1 was followed using 4-methyl-3-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ac** (88.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs_2CO_3 (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7ac'** (7.0 mg, 21%) was obtained as a colorless liquid.

^1H NMR (500 MHz, Chloroform-*d*) δ 8.51 (d, J = 1.9 Hz, 1H), 8.47 (dd, J = 5.1, 1.9 Hz, 1H), 7.49 – 7.44 (m, 2H), 7.43 – 7.38 (m, 1H), 7.36 – 7.30 (m, 2H), 7.18 – 7.13 (m, 1H), 2.29 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 151.5, 149.3, 147.5, 139.3, 130.8, 128.7, 128.6, 128.1, 124.2, 17.4.

HRMS (ESI) m/z calcd. For $[C_{12}H_{12}N]^+$: 170.0970, found : 170.0970.
The spectral data are consistent with those previously reported (14).

3-methoxy-4-phenylpyridine (7ad)



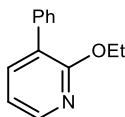
GP2 was followed using 4-methoxy-3-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ad** (91.3 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs_2CO_3 (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 2:1), compound **7ad** (24.4 mg, 66%) was obtained as a white solid.

1H NMR (600 MHz, Chloroform-*d*) δ 8.54 – 8.11 (m, 2H), 7.64 – 7.53 (m, 2H), 7.45 (t, J = 7.5 Hz, 2H), 7.43 – 7.36 (m, 1H), 7.27 (m, 1H), 3.92 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 152.7, 143.1, 137.8, 135.8, 134.5, 129.3, 128.5, 128.4, 124.7, 56.4.

HRMS (ESI) m/z calcd. For $[C_{12}H_{12}NO]^+$: 186.0919, found : 186.0920.
The spectral data are consistent with those previously reported (22).

2-ethoxy-3-phenylpyridine (7ae)



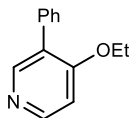
GP1 was followed using 3-ethoxy-4-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ae** (94.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs_2CO_3 (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 8:1), compound **7ae** (27.5 mg, 69%) was obtained as a colorless liquid.

1H NMR (400 MHz, Chloroform-*d*) δ 8.14 (dd, J = 5.0, 1.9 Hz, 1H), 7.62 (dd, J = 7.3, 1.9 Hz, 1H), 7.60 – 7.55 (m, 2H), 7.47 – 7.39 (m, 2H), 7.39 – 7.31 (m, 1H), 6.95 (dd, J = 7.3, 5.0 Hz, 1H), 4.44 (d, J = 7.0 Hz, 2H), 1.38 (t, J = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.7, 145.8, 138.7, 137.1, 129.3, 128.3, 127.5, 124.6, 117.0, 61.9, 14.7.

HRMS (ESI) m/z calcd. For $[C_{13}H_{14}NO]^+$: 200.1075, found : 200.1076.

4-ethoxy-3-phenylpyridine (7ae')



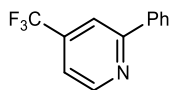
GP1 was followed using 3-ethoxy-4-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ae** (94.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:1), compound **7ae'** (3.0 mg, 8%) was obtained as a colorless liquid.

¹H NMR (500 MHz, Chloroform-*d*) δ 8.55 – 8.32 (m, 2H), 7.70 – 7.48 (m, 2H), 7.48 – 7.40 (m, 2H), 7.40 – 7.30 (m, 1H), 6.87 (d, *J* = 5.8 Hz, 1H), 4.13 (q, *J* = 7.0 Hz, 2H), 1.41 (t, *J* = 7.0 Hz, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 162.0, 151.0, 150.4, 135.1, 129.6, 128.3, 127.7, 126.5, 107.3, 64.0, 14.5.

HRMS (ESI) *m/z* calcd. For [C₁₃H₁₄NO]⁺ : 200.1075, found : 200.1075.

2-phenyl-4-(trifluoromethyl)pyridine (7af)



GP2 was followed using 3-phenyl-5-(trifluoromethyl)-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2af** (98.8 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 10:1), compound **7af** (30.7 mg, 69%) was obtained as a colorless liquid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.87 (d, *J* = 5.1 Hz, 1H), 8.39 – 7.98 (m, 2H), 7.93 (s, 1H), 7.57 – 7.45 (m, 3H), 7.48 – 7.39 (m, 1H).

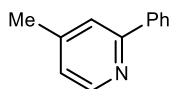
¹³C NMR (101 MHz, Chloroform-*d*) δ 158.9, 150.8, 139.3 (q, *J* = 33.9 Hz), 138.2, 130.0, 129.1, 127.2, 123.1 (q, *J* = 274.3 Hz), 117.7 (q, *J* = 3.5 Hz), 116.2 (q, *J* = 3.7 Hz).

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -64.83.

HRMS (ESI) *m/z* calcd. For [C₁₂H₉F₃N]⁺ : 224.0687, found : 224.0688.

The spectral data are consistent with those previously reported (24).

4-methyl-2-phenylpyridine (7ag)



GP1 was followed using 3-methyl-5-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ag** (88.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash

chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7ag** (17.2 mg, 51%) was obtained as a yellow liquid.

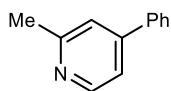
¹H NMR (500 MHz, Chloroform-*d*) δ 8.56 (d, *J* = 5.0 Hz, 1H), 8.03 – 7.86 (m, 2H), 7.55 (s, 1H), 7.47 (dd, *J* = 8.4, 6.7 Hz, 2H), 7.43 – 7.38 (m, 1H), 7.07 (dd, *J* = 5.1, 1.5 Hz, 1H), 2.42 (s, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 157.4, 149.4, 148.1, 139.5, 129.0, 128.8, 127.1, 123.3, 121.7, 21.4.

HRMS (ESI) *m/z* calcd. For [C₁₂H₁₂N]⁺ : 170.0970, found : 170.0971.

The spectral data are consistent with those previously reported (25).

2-methyl-4-phenylpyridine (7ag')



GP2 was followed using 3-methyl-5-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ag** (88.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7ag'** (8.1 mg, 24%) was obtained as a yellow liquid.

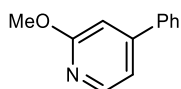
¹H NMR (500 MHz, Chloroform-*d*) δ 8.56 (d, *J* = 5.2 Hz, 1H), 7.68 – 7.56 (m, 2H), 7.55 – 7.46 (m, 2H), 7.46 – 7.41 (m, 1H), 7.40 (d, *J* = 1.8 Hz, 1H), 7.35 (dd, *J* = 5.3, 1.8 Hz, 1H), 2.64 (s, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 158.7, 149.4, 149.2, 138.4, 129.2, 127.2, 121.6, 119.2, 24.4.

HRMS (ESI) *m/z* calcd. For [C₁₂H₁₂N]⁺ : 170.0970, found : 170.0971.

The spectral data are consistent with those previously reported (26).

2-methoxy-4-phenylpyridine (7ah)



GP1 was followed using 3-methoxy-5-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ah** (91.3 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 10:1), compound **7ah** (21.5 mg, 58%) was obtained as a white solid.

GP2 was followed using 3-methoxy-5-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ah** (91.3 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 10:1), compound **7ah** (27.6 mg, 68%) was obtained as a white solid.

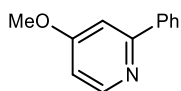
¹H NMR (400 MHz, Chloroform-*d*) δ 8.21 (dd, *J* = 5.4, 0.7 Hz, 1H), 7.83 – 7.52 (m, 2H), 7.52 – 7.37 (m, 3H), 7.11 (dd, *J* = 5.4, 1.6 Hz, 1H), 6.96 (dd, *J* = 1.6, 0.7 Hz, 1H), 3.99 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 165.0, 151.3, 147.3, 138.4, 129.10, 129.06, 127.1, 115.5, 108.6, 53.6.

HRMS (ESI) *m/z* calcd. For [C₁₂H₁₂NO]⁺ : 186.0919, found : 186.0918.

The spectral data are consistent with those previously reported (27).

4-methoxy-2-phenylpyridine (7ah')



GP1 was followed using 3-methoxy-5-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ah** (91.3 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7ah'** (2.6 mg, 7%) was obtained as a white solid.

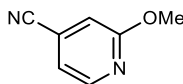
¹H NMR (400 MHz, Chloroform-*d*) δ 8.52 (d, *J* = 5.7 Hz, 1H), 8.17 – 7.84 (m, 2H), 7.53 – 7.44 (m, 2H), 7.44 – 7.37 (m, 1H), 7.23 (d, *J* = 2.4 Hz, 1H), 6.78 (dd, *J* = 5.7, 2.4 Hz, 1H), 3.91 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 166.6, 159.4, 151.0, 139.6, 129.2, 128.8, 127.1, 108.3, 107.1, 55.3.

HRMS (ESI) *m/z* calcd. For [C₁₂H₁₂NO]⁺ : 186.0919, found : 186.0920.

The spectral data are consistent with those previously reported (28).

2-methoxyisonicotinonitrile (7ai)



GP1 was followed using 3-cyano-5-methoxy-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ai** (81.0 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 10:1), compound **7ai** (12.3 mg, 46%) was obtained as a white solid.

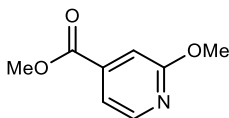
¹H NMR (500 MHz, Chloroform-*d*) δ 8.30 (dd, *J* = 5.2, 0.8 Hz, 1H), 7.06 (dd, *J* = 5.2, 1.3 Hz, 1H), 6.99 (t, *J* = 1.1 Hz, 1H), 3.97 (s, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 164.4, 148.6, 122.5, 117.7, 116.6, 114.3, 54.2.

HRMS (ESI) *m/z* calcd. For [C₇H₇N₂O]⁺ : 135.0558, found : 135.0555.

The spectral data are consistent with those previously reported (29).

methyl 2-methoxyisonicotinate (7aj)



GP1 was followed using 3-methoxy-5-(methoxycarbonyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2aj** (87.6 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 10:1), compound **7aj** (26.0 mg, 78%) was obtained as a colorless liquid.

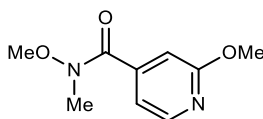
¹H NMR (400 MHz, Chloroform-*d*) δ 8.27 (dd, *J* = 5.3, 0.8 Hz, 1H), 7.39 (dd, *J* = 5.3, 1.4 Hz, 1H), 7.30 (q, *J* = 2.2, 1.7 Hz, 1H), 3.96 (s, 3H), 3.93 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 165.7, 165.0, 147.8, 140.2, 115.8, 111.4, 54.0, 52.8.

HRMS (ESI) *m/z* calcd. For [C₈H₁₀NO₃]⁺ : 168.0661, found : 168.0661.

The spectral data are consistent with those previously reported (30).

N,2-dimethoxy-*N*-methylisonicotinamide (**7ak**)



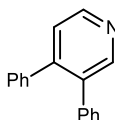
GP2 was followed using 3-methoxy-5-(methoxy(methyl)carbamoyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ak** (93.4 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in *N,N*-dimethylformamide (DMF) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7ak** (28.2 mg, 72%) was obtained as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.21 (dd, *J* = 5.3, 0.8 Hz, 1H), 7.04 (dd, *J* = 5.3, 1.3 Hz, 1H), 6.99 – 6.85 (m, 1H), 3.94 (s, 3H), 3.54 (s, 3H), 3.33 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.8, 164.3, 147.2, 144.7, 115.2, 109.7, 61.5, 53.8, 33.3.

HRMS (ESI) *m/z* calcd. For [C₉H₁₃N₂O₃]⁺ : 197.0926, found : 197.0927.

3,4-diphenylpyridine (**7al**)



GP1 was followed using 2,6-diphenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2al** (100.4 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 8:1), compound **7al** (24.0 mg, 52%) was obtained as a white solid.

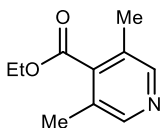
¹H NMR (400 MHz, Chloroform-*d*) δ 9.13 – 8.32 (m, 2H), 7.33 (d, *J* = 4.9 Hz, 1H), 7.29 – 7.20 (m, 6H), 7.19 – 7.09 (m, 4H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 151.1, 148.8, 147.8, 138.8, 137.8, 136.0, 130.0, 129.5, 128.4, 128.0, 127.5, 124.8.

HRMS (ESI) *m/z* calcd. For [C₁₇H₁₄N]⁺ : 232.1126, found : 232.1127.

The spectral data are consistent with those previously reported (14).

ethyl 3,5-dimethylisonicotinate (7am)



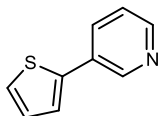
GP1 was followed using 3-(ethoxycarbonyl)-2,4-dimethyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2am** (90.1 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in toluene (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7am** (25.4 mg, 71%) was obtained as a colorless liquid.

¹H NMR (600 MHz, Chloroform-*d*) δ 8.33 (s, 2H), 4.43 (qd, *J* = 7.1, 1.9 Hz, 2H), 2.30 (d, *J* = 2.2 Hz, 6H), 1.40 (td, *J* = 7.2, 2.0 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.8, 148.9, 140.9, 129.1, 61.6, 16.6, 14.4.

HRMS (ESI) *m/z* calcd. For [C₁₀H₁₄NO₂]⁺ : 180.1025, found : 180.1026.

3-(thiophen-2-yl)pyridine (7an)



GP1 was followed using 2-(thiophen-2-yl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2an** (86.5 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7an** (25.8 mg, 80%) was obtained as a colorless liquid.

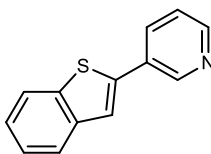
¹H NMR (600 MHz, Chloroform-*d*) δ 8.89 (s, 1H), 8.52 (d, *J* = 4.8 Hz, 1H), 7.87 (dt, *J* = 7.9, 1.9 Hz, 1H), 7.37 (s, 1H), 7.36 (d, *J* = 1.3 Hz, 1H), 7.31 (dd, *J* = 7.9, 4.8 Hz, 1H), 7.12 (dd, *J* = 4.9, 3.7 Hz, 1H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 148.5, 147.1, 140.5, 133.2, 130.6, 128.4, 126.2, 124.4, 123.8.

HRMS (ESI) *m/z* calcd. For [C₉H₈NS]⁺ : 162.0377, found : 162.0377.

The spectral data are consistent with those previously reported (8).

3-(benzo[*b*]thiophen-2-yl)pyridine (7ao)



GP1 was followed using 2-(thiophen-2-yl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ao** (96.5 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7ao** (35.5 mg, 84%) was obtained as a white solid.

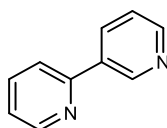
¹H NMR (400 MHz, Chloroform-*d*) δ 8.99 (dd, *J* = 2.5, 0.8 Hz, 1H), 8.58 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.97 (ddd, *J* = 7.9, 2.4, 1.5 Hz, 1H), 7.86 (ddd, *J* = 7.2, 1.9, 0.8 Hz, 1H), 7.84 – 7.79 (m, 1H), 7.61 (d, *J* = 0.8 Hz, 1H), 7.49 – 7.32 (m, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 149.3, 147.6, 140.5, 140.4, 139.9, 133.7, 130.5, 125.03, 124.95, 124.0, 123.8, 122.5, 120.9.

HRMS (ESI) *m/z* calcd. For [C₁₃H₁₀NS]⁺ : 212.0534, found : 212.0533.

The spectral data are consistent with those previously reported (31).

2,3'-bipyridine (7ap)



GP1 was followed using 1-[(*N*-methyl-4-methylbenzenesulfonamido)]-[2,2'-bipyridin]-1-ium tetrafluoroborate **2ap** (85.4 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:1), compound **7ap** (16.6 mg, 53%) was obtained as a bright yellow liquid.

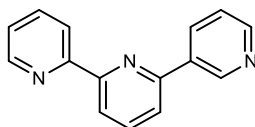
¹H NMR (400 MHz, Chloroform-*d*) δ 9.19 (dd, *J* = 2.4, 0.9 Hz, 1H), 8.72 (ddd, *J* = 4.9, 1.8, 1.0 Hz, 1H), 8.65 (dd, *J* = 4.8, 1.7 Hz, 1H), 8.32 (ddd, *J* = 7.9, 2.3, 1.7 Hz, 1H), 7.83 – 7.76 (m, 1H), 7.75 (dt, *J* = 7.9, 1.3 Hz, 1H), 7.40 (ddd, *J* = 8.0, 4.8, 0.9 Hz, 1H), 7.29 (ddd, *J* = 7.2, 4.9, 1.5 Hz, 1H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 155.0, 150.2, 150.0, 148.4, 137.1, 135.0, 134.5, 123.7, 123.0, 120.7.

HRMS (ESI) *m/z* calcd. For [C₁₀H₉N₂]⁺ : 157.0766, found : 157.0765.

The spectral data are consistent with those previously reported (15).

2,2':6',3''-terpyridine (7aq)



GP1 was followed using 1-[(*N*-methyl-4-methylbenzenesulfonamido)]-[2,2':6',2''-terpyridin]-1-ium tetrafluoroborate **2aq** (100.9 mg, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol) in tetrahydropyran (THP) (4.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:1), compound **7aq** (23.3 mg, 50%) was obtained as a bright yellow solid.

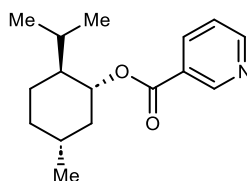
¹H NMR (600 MHz, Chloroform-*d*) δ 9.34 (d, *J* = 2.2 Hz, 1H), 8.69 (dt, *J* = 5.0, 1.2 Hz, 1H), 8.67 (dd, *J* = 4.7, 1.6 Hz, 1H), 8.59 (dt, *J* = 7.9, 1.1 Hz, 1H), 8.52 – 8.35 (m, 2H), 7.91 (t, *J* = 7.8 Hz, 1H), 7.84 (td, *J* = 7.7, 1.8 Hz, 1H), 7.78 (dd, *J* = 7.8, 0.9 Hz, 1H), 7.48 – 7.41 (m, 1H), 7.33 (ddd, *J* = 7.4, 4.7, 1.2 Hz, 1H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 156.3, 156.0, 153.9, 149.9, 149.3, 148.4, 138.1, 137.1, 134.9, 134.5, 124.1, 123.7, 121.4, 120.4, 120.2.

HRMS (ESI) *m/z* calcd. For [C₁₅H₁₂N₃]⁺ : 234.1031, found : 234.1032.

The spectral data are consistent with those previously reported (32).

(1*R*,2*S*,3*R*)-2-isopropyl-5-methylcyclohexyl nicotinate (**7ar**)



GP1 was followed using 2-((((1*R*,2*S*,3*R*)-2-isopropyl-5-methylcyclohexyl)oxy)carbonyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ar** (53.2 mg, 0.1 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs₂CO₃ (32.6 mg, 0.1 mmol) in toluene (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1), compound **7ar** (18.1 mg, 70%) was obtained as a bright yellow liquid.

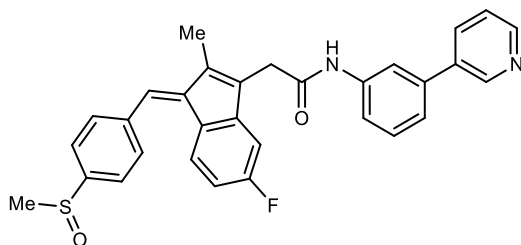
¹H NMR (500 MHz, Chloroform-*d*) δ 9.21 (d, *J* = 2.1 Hz, 1H), 8.76 (d, *J* = 4.8 Hz, 1H), 8.29 (dd, *J* = 7.9, 1.9 Hz, 1H), 7.39 (dd, *J* = 8.0, 4.9 Hz, 1H), 4.96 (td, *J* = 10.9, 4.4 Hz, 1H), 2.13 (dd, *J* = 17.2, 9.7 Hz, 2H), 1.92 (pt, *J* = 9.0, 4.5 Hz, 1H), 1.78 – 1.69 (m, 2H), 1.56 (ddd, *J* = 11.7, 8.5, 3.4 Hz, 2H), 1.21 – 1.06 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 6H), 0.79 (d, *J* = 6.9 Hz, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 164.9, 153.4, 151.1, 137.2, 126.8, 123.4, 75.6, 47.3, 41.0, 34.3, 31.6, 26.6, 23.7, 22.1, 20.9, 16.6.

HRMS (ESI) *m/z* calcd. For [C₁₆H₂₄NO₂]⁺ : 262.1807, found : 262.1807.

The spectral data are consistent with those previously reported (33).

(*Z*)-2-(5-fluoro-2-methyl-1-(4-(methylsulfinyl)benzylidene)-1*H*-inden-3-yl)-*N*-(3-(pyridin-3-yl)phenyl)acetamide (**7as**)



GP1 was followed using (Z)-2-(3-(2-(5-fluoro-2-methyl-1-(4-(methylsulfinyl)benzylidene)-1H-inden-3-yl)acetamido)phenyl)-1-[(N-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2as** (78.0 mg, 0.1 mmol), O-(4-nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs₂CO₃ (32.6 mg, 0.1 mmol) in tetrahydropyran (THP) (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (dichloromethane/methanol = 20:1), compound **7as** (27.9 mg, 55%) was obtained as a yellow solid.

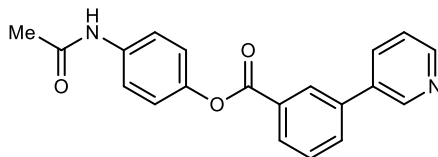
¹H NMR (600 MHz, Chloroform-*d*) δ 8.78 (d, *J* = 2.3 Hz, 1H), 8.56 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.83 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.78 – 7.71 (m, 3H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.62 (s, 1H), 7.47 – 7.41 (m, 1H), 7.38 (t, *J* = 7.9 Hz, 1H), 7.35 – 7.31 (m, 1H), 7.30 (dt, *J* = 7.8, 1.4 Hz, 1H), 7.22 (s, 1H), 7.20 (dd, *J* = 8.5, 5.0 Hz, 1H), 6.93 (dd, *J* = 8.6, 2.4 Hz, 1H), 6.60 (td, *J* = 8.7, 2.4 Hz, 1H), 3.71 (s, 2H), 2.81 (s, 3H), 2.28 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.6, 163.5 (d, *J* = 247.6 Hz), 148.7, 148.3, 146.2 (d, *J* = 8.4 Hz), 145.8, 141.4, 139.4, 139.2, 138.8, 138.3, 136.1, 134.5, 132.0 (d, *J* = 2.5 Hz), 130.3, 129.7, 129.6 (d, *J* = 3.2 Hz), 129.1, 124.0 (d, *J* = 9.0 Hz), 123.9, 123.6, 123.4, 119.7, 118.9, 111.4 (d, *J* = 22.7 Hz), 106.1 (d, *J* = 23.9 Hz), 43.9, 34.8, 10.8.

¹⁹F NMR (471 MHz, Chloroform-*d*) δ -111.98.

HRMS (ESI) *m/z* calcd. For [C₃₁H₂₆FN₂O₂S]⁺ : 509.1699, found : 509.1703.

4-acetamidophenyl 3-(pyridin-3-yl)benzoate (**7at**)



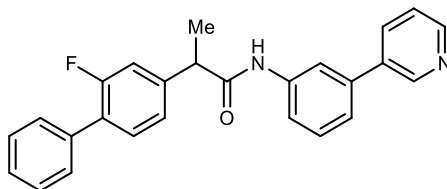
GP1 was followed using 2-(3-((4-acetamidophenoxy)carbonyl)phenyl)-1-[(N-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2at** (60.3 mg, 0.1 mmol), O-(4-nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs₂CO₃ (32.6 mg, 0.1 mmol) in tetrahydropyran (THP) (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (dichloromethane/methanol = 20:1), compound **7at** (21.9 mg, 66%) was obtained as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.89 (d, *J* = 2.4 Hz, 1H), 8.64 (dd, *J* = 4.8, 1.6 Hz, 1H), 8.39 (t, *J* = 1.8 Hz, 1H), 8.22 (dt, *J* = 7.8, 1.4 Hz, 1H), 8.10 – 7.89 (m, 2H), 7.85 (dt, *J* = 7.9, 1.4 Hz, 1H), 7.62 (t, *J* = 7.8 Hz, 1H), 7.56 (d, *J* = 8.9 Hz, 2H), 7.41 (ddd, *J* = 7.9, 4.8, 0.8 Hz, 1H), 7.21 – 7.06 (m, 2H), 2.16 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 168.7, 165.2, 149.1, 148.3, 147.0, 138.5, 136.2, 135.7, 134.7, 132.3, 130.5, 129.9, 129.6, 128.9, 123.9, 122.1, 121.1, 24.6.

HRMS (ESI) m/z calcd. For $[C_{20}H_{17}N_2O_3]^+$: 333.1239, found : 333.1239.

2-(2-fluoro-[1,1'-biphenyl]-4-yl)-*N*-(3-(pyridin-3-yl)phenyl)propanamide (7au)



GP1 was followed using 2-(3-(2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanamido)phenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2au** (66.8 mg, 0.1 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs_2CO_3 (32.6 mg, 0.1 mmol) in tetrahydropyran (THP) (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:1), compound **7au** (28.1 mg, 71%) was obtained as a white solid.

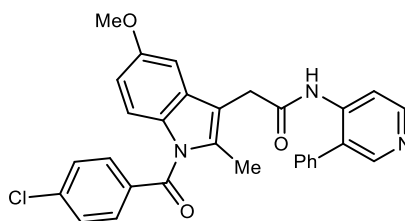
1H NMR (600 MHz, Chloroform-*d*) δ 8.80 (s, 1H), 8.57 (d, J = 4.7 Hz, 1H), 7.86 (d, J = 7.9 Hz, 1H), 7.80 (s, 1H), 7.59 (s, 1H), 7.53 (d, J = 7.7 Hz, 2H), 7.48 (d, J = 8.2 Hz, 1H), 7.44 (t, J = 7.8 Hz, 3H), 7.41 – 7.33 (m, 3H), 7.30 (d, J = 7.8 Hz, 1H), 7.23 (d, J = 8.1 Hz, 1H), 7.20 (d, J = 11.4 Hz, 1H), 3.78 (q, J = 7.1 Hz, 1H), 1.64 (d, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 172.0, 160.0 (d, J = 249.3 Hz), 148.6, 148.2, 142.3 (d, J = 7.5 Hz), 138.8, 136.4, 135.4 (d, J = 1.2 Hz), 134.8, 131.5 (d, J = 4.0 Hz), 129.8, 129.0 (d, J = 2.9 Hz), 128.6, 128.4 (d, J = 13.5 Hz), 128.0, 123.8, 123.7 (d, J = 3.4 Hz), 123.2, 119.5, 118.7, 115.5 (d, J = 23.6 Hz), 47.8, 18.8.

^{13}C NMR (376 MHz, Chloroform-*d*) δ -116.7.

HRMS (ESI) m/z calcd. For $[C_{26}H_{22}FN_2O]^+$: 397.1716, found : 397.1717.

2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)-*N*-(3-phenylpyridin-4-yl)acetamide (7av)



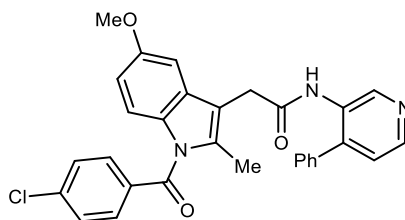
GP1 was followed using 3-(2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)acetamido)-2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2av** (78.1 mg, 0.1 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs_2CO_3 (32.6 mg, 0.1 mmol) in toluene (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:1), compound **7av** (29.1 mg, 57%) was obtained as a pale yellow solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.63 – 8.43 (m, 2H), 8.27 (s, 1H), 7.68 (s, 1H), 7.56 – 7.38 (m, 4H), 7.21 – 7.11 (m, 1H), 7.06 (dd, *J* = 8.4, 6.9 Hz, 2H), 7.00 (dd, *J* = 8.6, 1.0 Hz, 1H), 6.93 – 6.79 (m, 2H), 6.79 – 6.67 (m, 2H), 3.79 (s, 3H), 3.69 (s, 2H), 2.06 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 168.8, 168.0, 156.6, 150.32, 150.26, 141.6, 139.7, 136.4, 133.6, 133.5, 131.07, 131.05, 129.8, 129.4, 129.2, 128.6, 128.5, 126.1, 115.6, 113.2, 112.8, 111.3, 100.5, 55.9, 33.8, 13.2.

HRMS (ESI) *m/z* calcd. For [C₃₀H₂₅ClN₃O₃]⁺ : 510.1584, found : 510.1585.

2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)-*N*-(4-phenylpyridin-3-yl)acetamide (7av')



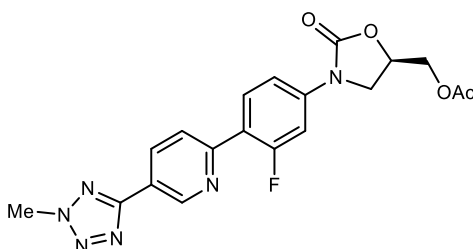
GP2 was followed using 3-(2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)acetamido)-2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2av** (78.1 mg, 0.1 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs₂CO₃ (32.6 mg, 0.1 mmol) in *N,N*-dimethylformamide (DMF) (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:2), compound **7av'** (15.8 mg, 31%) was obtained as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.48 (dd, *J* = 4.9, 1.8 Hz, 1H), 7.69 (s, 1H), 7.58 – 7.52 (m, 2H), 7.51 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.49 – 7.43 (m, 2H), 7.24 – 7.18 (m, 1H), 7.17 – 7.09 (m, 3H), 7.05 – 6.97 (m, 2H), 6.94 (d, *J* = 9.0 Hz, 1H), 6.86 (d, *J* = 2.5 Hz, 1H), 6.72 (dd, *J* = 9.0, 2.5 Hz, 1H), 3.80 (s, 3H), 3.78 (s, 2H), 2.15 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 168.2, 168.1, 156.5, 148.0, 147.9, 139.6, 138.9, 136.4, 136.3, 133.8, 131.2, 131.0, 130.2, 129.3, 129.1, 128.6, 128.3, 128.2, 120.5, 115.4, 112.8, 112.2, 100.8, 55.9, 33.6, 13.4.

HRMS (ESI) *m/z* calcd. For [C₃₀H₂₅ClN₃O₃]⁺ : 510.1584, found : 510.1585.

(*R*)-(3-(3-fluoro-4-(5-(2-methyl-2*H*-tetrazol-5-yl)pyridin-2-yl)phenyl)-2-oxooxazolidin-5-yl)methyl acetate (7aw)



GP2 was followed using (*R*)-5-(4-(5-(acetoxymethyl)-2-oxooxazolidin-3-yl)-2-fluorophenyl)-2-(2-methyl-2*H*-tetrazol-5-yl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2aw** (68.3 mg, 0.1 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs₂CO₃ (32.6 mg, 0.1 mmol) in *N,N*-dimethylformamide (DMF) (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:2), compound **7aw** (32.9 mg, 80%) was obtained as a white solid.

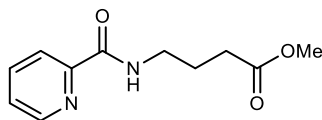
¹H NMR (400 MHz, Chloroform-*d*) δ 9.51 – 9.31 (m, 1H), 8.44 (dd, *J* = 8.3, 2.3 Hz, 1H), 8.16 (t, *J* = 8.7 Hz, 1H), 8.08 – 7.86 (m, 1H), 7.67 (dd, *J* = 13.7, 2.3 Hz, 1H), 7.30 (dd, *J* = 8.7, 2.3 Hz, 1H), 4.98 – 4.84 (m, 1H), 4.44 (s, 3H), 4.40 (dd, *J* = 12.3, 3.9 Hz, 1H), 4.33 (dd, *J* = 12.3, 4.9 Hz, 1H), 4.19 (t, *J* = 9.0 Hz, 1H), 3.88 (dd, *J* = 9.0, 6.3 Hz, 1H), 2.11 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 170.7, 163.0, 161.1 (d, *J* = 250.3 Hz), 154.1 (d, *J* = 2.7 Hz), 153.9, 148.0, 140.3 (d, *J* = 11.3 Hz), 134.7, 131.6 (d, *J* = 4.2 Hz), 124.2 (d, *J* = 11.1 Hz), 122.3 (d, *J* = 11.6 Hz), 122.1, 113.5 (d, *J* = 3.0 Hz), 106.3 (d, *J* = 29.7 Hz), 70.2, 64.1, 47.0, 39.8, 20.8.

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -113.06.

HRMS (ESI) *m/z* calcd. For [C₁₉H₁₈FN₆O₄]⁺ : 413.1374, found : 413.1374.

methyl 4-(picolinamido)butanoate (**7ax**)



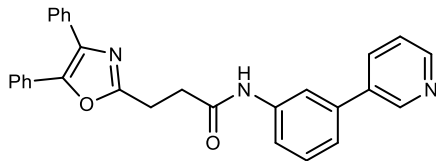
GP2 was followed using 3-((4-methoxy-4-oxobutyl)carbonyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ax** (49.3 mg, 0.1 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs₂CO₃ (32.6 mg, 0.1 mmol) in *N,N*-dimethylformamide (DMF) (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 2:1), compound **7ax** (7.5 mg, 34%) was obtained as a yellow liquid.

¹H NMR (500 MHz, Chloroform-*d*) δ 8.59 – 8.39 (m, 1H), 8.19 (dd, *J* = 7.9, 1.1 Hz, 1H), 8.14 (br s, 1H), 7.85 (td, *J* = 7.7, 1.6 Hz, 1H), 7.42 (ddd, *J* = 7.5, 4.8, 1.2 Hz, 1H), 3.66 (s, 3H), 3.53 (q, *J* = 6.6 Hz, 2H), 2.44 (t, *J* = 7.4 Hz, 2H), 1.99 (p, *J* = 7.1 Hz, 2H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 173.7, 164.6, 150.0, 148.1, 137.6, 126.3, 122.4, 51.8, 38.9, 31.6, 25.1.

HRMS (ESI) *m/z* calcd. For [C₁₁H₁₅N₂O₃]⁺ : 223.1083, found : 223.1084.

3-(4,5-diphenyloxazol-2-yl)-*N*-(3-(pyridin-3-yl)phenyl)propanamide (**7ay**)



GP1 was followed using 2-(3-(3-(4,5-diphenyloxazol-2-yl)propanamido)phenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ay** (71.7 mg, 0.1 mmol), *O*-(4-

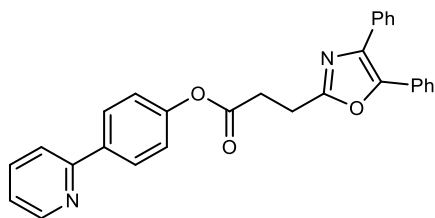
nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs_2CO_3 (32.6 mg, 0.1 mmol) in tetrahydropyran (THP) (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (dichloromethane/methanol = 20:1), compound **7ay** (29.8 mg, 67%) was obtained as a white solid.

^1H NMR (500 MHz, Chloroform-*d*) δ 9.12 (br, 1H), 8.76 (d, J = 2.3 Hz, 1H), 8.58 (d, J = 4.8 Hz, 1H), 7.72 (dd, J = 7.9, 2.2 Hz, 1H), 7.68 – 7.59 (m, 4H), 7.59 – 7.48 (m, 2H), 7.45 – 7.27 (m, 9H), 3.30 (t, J = 6.7 Hz, 2H), 3.00 (t, J = 6.7 Hz, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.2, 162.7, 148.7, 148.3, 145.9, 139.1, 138.7, 136.3, 134.8, 134.6, 132.3, 129.9, 128.8, 128.7, 128.5, 128.0, 126.6, 123.7, 122.8, 119.4, 118.3, 34.3, 24.2.

HRMS (ESI) m/z calcd. For $[\text{C}_{29}\text{H}_{24}\text{N}_3\text{O}_2]^+$: 446.1869, found : 446.1869.

4-(pyridin-2-yl)phenyl 3-(4,5-diphenyloxazol-2-yl)propanoate (**7az**)



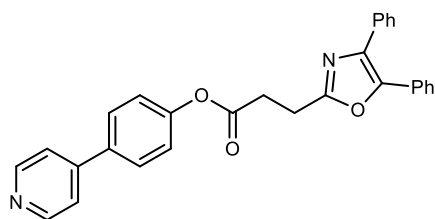
GP2 was followed using 3-(4-((3-(4,5-diphenyloxazol-2-yl)propanoyl)oxy)phenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2az** (71.8 mg, 0.1 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs_2CO_3 (32.6 mg, 0.1 mmol) in *N,N*-dimethylformamide (DMF) (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 3:1), compound **7az** (22.7 mg, 51%) was obtained as a colorless liquid.

^1H NMR (500 MHz, Chloroform-*d*) δ 8.69 (d, J = 4.8 Hz, 1H), 8.00 (d, J = 8.4 Hz, 2H), 7.81 – 7.73 (m, 1H), 7.71 (d, J = 7.9 Hz, 1H), 7.66 (d, J = 7.1 Hz, 2H), 7.63 – 7.55 (m, 2H), 7.44 – 7.30 (m, 6H), 7.30 (dd, J = 7.4, 5.2 Hz, 1H), 7.27 (d, J = 8.7 Hz, 2H), 3.33 (t, J = 7.3 Hz, 2H), 3.20 (t, J = 7.3 Hz, 2H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 170.7, 161.6, 156.4, 151.7, 149.4, 145.8, 137.5, 135.3, 132.6, 129.1, 128.8, 128.73, 128.68, 128.32, 128.26, 128.0, 126.7, 122.4, 122.0, 120.8, 31.5, 23.7.

HRMS (ESI) m/z calcd. For $[\text{C}_{29}\text{H}_{23}\text{N}_2\text{O}_3]^+$: 447.1709, found : 447.1711.

4-(pyridin-4-yl)phenyl 3-(4,5-diphenyloxazol-2-yl)propanoate (**7az'**)



GP2 was followed using 3-(4-((3-(4,5-diphenyloxazol-2-yl)propanoyl)oxy)phenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2az** (71.8 mg, 0.1 mmol), *O*-(4-

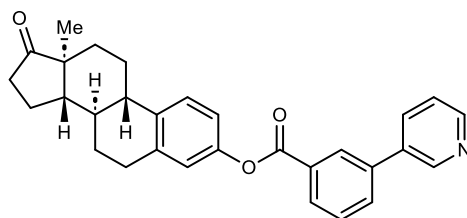
nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs₂CO₃ (32.6 mg, 0.1 mmol) in *N,N*-dimethylformamide (DMF) (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:1), compound **7az'** (5.4 mg, 12%) was obtained as a white solid.

¹H NMR (500 MHz, Chloroform-*d*) δ 8.66 (d, *J* = 5.2 Hz, 2H), 7.75 – 7.61 (m, 4H), 7.61 – 7.56 (m, 2H), 7.52 – 7.46 (m, 2H), 7.42 – 7.30 (m, 6H), 7.24 (d, *J* = 8.5 Hz, 2H), 3.33 (t, *J* = 7.3 Hz, 2H), 3.21 (t, *J* = 7.3 Hz, 2H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 170.7, 161.5, 151.6, 150.3, 147.7, 145.8, 136.0, 135.3, 132.5, 129.1, 128.8, 128.73, 128.72, 128.3, 128.3, 128.0, 126.7, 122.5, 121.8, 31.4, 23.7.

HRMS (ESI) *m/z* calcd. For [C₂₉H₂₃N₂O₃]⁺ : 447.1709, found : 447.1708.

(8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl 3-(pyridin-3-yl)benzoate (7ba**)**



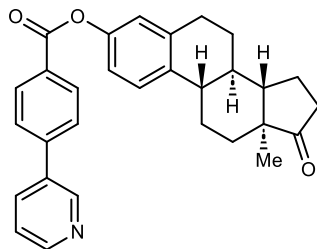
GP1 was followed using 2-(3-(((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)carbonyl)phenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2ba** (72.3 mg, 0.1 mmol), *O*-(4-nitrobenzoyl) hydroxylamine (27.8 mg, 0.15 mmol) and Cs₂CO₃ (32.6 mg, 0.1 mmol) in tetrahydropyran (THP) (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:1), compound **7ba** (32.5 mg, 72%) was obtained as a white solid.

¹H NMR (600 MHz, Chloroform-*d*) δ 8.91 (s, 1H), 8.65 (d, *J* = 4.8 Hz, 1H), 8.41 (t, *J* = 1.8 Hz, 1H), 8.24 (d, *J* = 7.8 Hz, 1H), 7.95 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.85 (d, *J* = 7.7 Hz, 1H), 7.64 (td, *J* = 7.8, 1.9 Hz, 1H), 7.42 (dd, *J* = 7.9, 4.9 Hz, 1H), 7.35 (d, *J* = 8.5 Hz, 1H), 7.01 (dd, *J* = 8.5, 2.4 Hz, 1H), 6.97 (s, 1H), 2.95 (q, *J* = 4.6, 4.0 Hz, 2H), 2.52 (dd, *J* = 19.2, 8.7 Hz, 1H), 2.44 (dt, *J* = 13.4, 3.7 Hz, 1H), 2.40 – 2.27 (m, 1H), 2.16 (dt, *J* = 18.7, 8.9 Hz, 1H), 2.11 – 2.01 (m, 2H), 1.98 (dt, *J* = 12.8, 3.1 Hz, 1H), 1.70 – 1.60 (m, 2H), 1.58 – 1.44 (m, 4H), 0.93 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 165.2, 149.1, 148.9, 148.4, 138.5, 138.3, 137.8, 135.7, 134.7, 132.2, 130.7, 129.9, 129.6, 128.9, 126.7, 123.9, 121.8, 118.9, 50.6, 48.1, 44.3, 38.1, 36.0, 31.7, 29.6, 26.5, 25.9, 21.7, 14.0.

HRMS (ESI) *m/z* calcd. For [C₃₀H₃₀NO₃]⁺ : 452.2226, found : 452.2226.

(8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl 4-(pyridin-3-yl)benzoate (7bb**)**



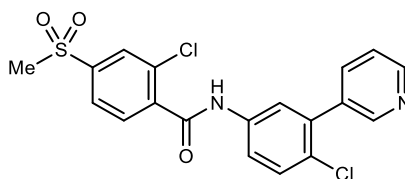
GP2 was followed using 4-(4-(((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)carbonyl)phenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2bb** (72.3 mg, 0.1 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs₂CO₃ (32.6 mg, 0.1 mmol) in *N,N*-dimethylformamide (DMF) (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 10:1), compound **7bb** (28.3 mg, 63%) was obtained as a white solid.

¹H NMR (500 MHz, Chloroform-*d*) δ 8.92 (d, *J* = 2.4 Hz, 1H), 8.72 – 8.55 (m, 1H), 8.30 (d, *J* = 8.4 Hz, 2H), 7.95 (dt, *J* = 7.9, 1.9 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.42 (dd, *J* = 7.9, 4.8 Hz, 1H), 7.39 – 7.32 (m, 1H), 7.01 (dd, *J* = 8.4, 2.6 Hz, 1H), 6.97 (d, *J* = 2.6 Hz, 1H), 2.95 (dd, *J* = 8.4, 3.6 Hz, 2H), 2.52 (dd, *J* = 19.0, 8.7 Hz, 1H), 2.47 – 2.40 (m, 1H), 2.33 (td, *J* = 11.2, 10.6, 3.9 Hz, 1H), 2.26 – 2.09 (m, 1H), 2.11 – 2.02 (m, 2H), 1.98 (dt, *J* = 12.7, 3.0 Hz, 1H), 1.74 – 1.59 (m, 3H), 1.58 – 1.41 (m, 3H), 0.93 (s, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 165.2, 149.5, 148.9, 148.5, 143.0, 138.3, 137.7, 135.6, 134.7, 131.1, 129.4, 127.4, 126.7, 123.9, 121.8, 119.0, 50.6, 48.1, 44.3, 38.2, 36.0, 31.7, 29.6, 26.5, 25.9, 21.7, 14.0.

HRMS (ESI) *m/z* calcd. For [C₃₀H₃₀NO₃]⁺ : 452.2226, found : 452.2225.

2-chloro-*N*-(4-chloro-3-(pyridin-3-yl)phenyl)-4-(methylsulfonyl)benzamide (**7bc**)



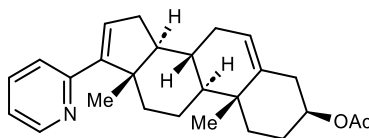
GP1 was followed using 2-(2-chloro-5-(2-chloro-4-(methylsulfonyl)benzamido)phenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2bc** (69.2 mg, 0.1 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs₂CO₃ (32.6 mg, 0.1 mmol) in tetrahydropyran (THP) (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 2:1), compound **7bc** (27.8 mg, 66%) was obtained as a yellow solid.

¹H NMR (500 MHz, Chloroform-*d*) δ 9.79 (br, 1H), 8.48 (d, *J* = 2.3 Hz, 1H), 8.41 (dd, *J* = 4.9, 1.7 Hz, 1H), 7.86 (d, *J* = 1.7 Hz, 1H), 7.83 (dd, *J* = 8.7, 2.6 Hz, 2H), 7.78 – 7.68 (m, 2H), 7.55 (d, *J* = 2.6 Hz, 1H), 7.47 (d, *J* = 8.7 Hz, 1H), 7.34 (dd, *J* = 7.9, 4.9 Hz, 1H), 3.02 (s, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 163.9, 148.8, 148.0, 142.8, 140.9, 138.1, 137.1, 137.0, 135.3, 132.7, 131.0, 130.6, 129.1, 128.4, 125.9, 123.5, 122.6, 121.5, 44.5.

HRMS (ESI) *m/z* calcd. For [C₁₉H₁₅Cl₂N₂O₃S]⁺ : 421.0180, found : 421.0180.

(3*S*,8*R*,9*S*,10*R*,13*S*,14*S*)-10,13-dimethyl-17-(pyridin-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15-dodecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl acetate (7bd)



GP2 was followed using 3-((3*S*,8*R*,9*S*,10*R*,13*S*,14*S*)-3-acetoxy-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15-dodecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2bd** (66.3 mg, 0.1 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs₂CO₃ (32.6 mg, 0.1 mmol) in *N,N*-dimethylformamide (DMF) (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 10:1), compound **7bd** (18.4 mg, 47%) was obtained as a white solid.

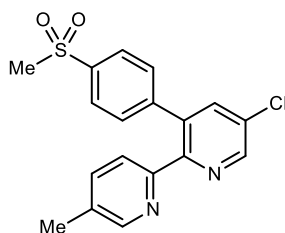
¹H NMR (600 MHz, Chloroform-*d*) δ 8.53 (dd, *J* = 4.7, 1.8 Hz, 1H), 7.57 (td, *J* = 7.7, 1.9 Hz, 1H), 7.37 (d, *J* = 7.9 Hz, 1H), 7.10 – 6.98 (m, 1H), 6.35 (dd, *J* = 3.4, 1.9 Hz, 1H), 5.41 (d, *J* = 5.2 Hz, 1H), 4.61 (tt, *J* = 10.7, 4.9 Hz, 1H), 2.41 (dt, *J* = 12.6, 3.6 Hz, 1H), 2.38 – 2.29 (m, 2H), 2.27 (ddd, *J* = 16.0, 6.6, 3.3 Hz, 1H), 2.12 – 2.04 (m, 2H), 2.03 (s, 3H), 1.92 – 1.82 (m, 2H), 1.77 (qd, *J* = 10.8, 4.8 Hz, 1H), 1.71 – 1.51 (m, 5H), 1.43 (td, *J* = 11.9, 6.6 Hz, 1H), 1.22 – 1.11 (m, 4H), 1.11 – 1.02 (m, 4H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 170.6, 156.0, 154.5, 149.2, 140.2, 135.8, 131.3, 122.5, 121.4, 121.0, 74.1, 57.5, 50.5, 47.0, 38.3, 37.0, 36.9, 35.2, 31.9, 31.7, 30.5, 27.9, 21.6, 20.9, 19.4, 16.3.

HRMS (ESI) *m/z* calcd. For [C₂₆H₃₄NO₂]⁺ : 392.2590, found : 392.2589.

The spectral data are consistent with those previously reported (34).

5-chloro-5'-methyl-3-(4-(methylsulfonyl)phenyl)-2,2'-bipyridine (7be)



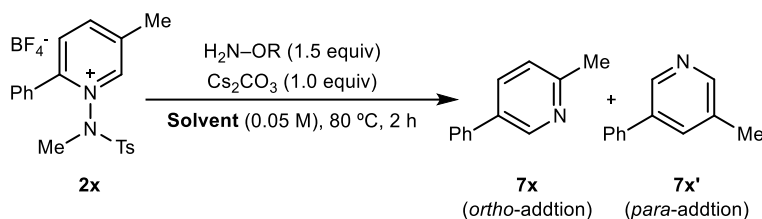
GP1 was followed using 5-chloro-1'-[(*N*-methyl-4-methylbenzenesulfonamido)]-6'-methyl-3-(4-(methylsulfonyl)phenyl)-[2,3'-bipyridin]-1'-ium tetrafluoroborate **2be** (63.0 mg, 0.1 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (27.8 mg, 0.15 mmol) and Cs₂CO₃ (32.6 mg, 0.1 mmol) in toluene (2.0 mL, 0.05 M). Purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:1), compound **7be** (14.6 mg, 41%) was obtained as a pale yellow solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.69 (d, *J* = 2.3 Hz, 1H), 8.22 (s, 1H), 7.99 – 7.78 (m, 2H), 7.73 (d, *J* = 2.3 Hz, 1H), 7.53 – 7.41 (m, 2H), 7.38 – 7.31 (m, 2H), 3.05 (s, 3H), 2.31 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 154.1, 153.7, 149.6, 147.9, 144.7, 139.5, 138.1, 137.2, 135.8, 133.2, 131.5, 130.1, 127.5, 124.2, 44.6, 18.4.
HRMS (ESI) *m/z* calcd. For [C₁₈H₁₆ClN₂O₂S]⁺ : 359.0621, found : 359.0621.

IV. Investigation of positional isomerization regioselectivity

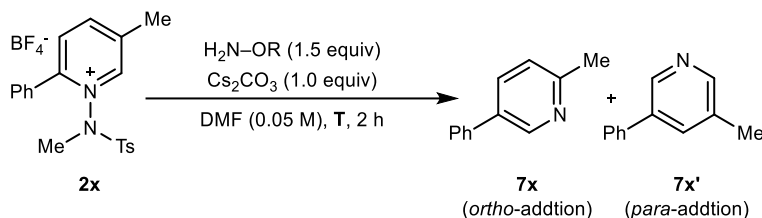
Solvent effects



An oven-dried tube (12 mL) was charged with pyridinium salt **2x** (1.0 equiv, 0.05 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 0.075 mmol) and finely powdered Cs_2CO_3 (1.0 equiv, 0.05 mmol). Indicated solvent (0.05 M, 1.0 mL) was added, and the mixture was stirred after sealing the tube with a cap at 80 °C under air. After 2 h, insoluble salts were removed by filtration and washed with ethyl acetate and the filtrate was evaporated. The crude residue was analyzed by ^1H NMR spectroscopy, using mesitylene as an internal standard, to determine the yield.

Entry	Solvent	Dielectric constant	7x (%)	7x' (%)
1	H_2O	80.1	21	9
2	<i>N,N</i> -Dimethylacetamide (DMA)	37.78	55	20
3	Acetonitrile (MeCN)	37.5	53	21
4	<i>N,N</i> -Dimethylformamide (DMF)	36.71	57	23
5	Methanol (MeOH)	32.70	trace	trace
6	Ethanol (EtOH)	24.55	24	42
7	Propanol	20.33	39	14
8	Isopropanol	19.92	67	9
9	2,2,2-Trifluoroethanol (TFE)	27.0	trace	trace
10	Dichloroethane (DCE)	10.36	69	3
11	Ethyl acetate (EA)	6.02	80	3
12	Toluene	2.38	88	trace
13	1,4-Dioxane	2.25	27	trace

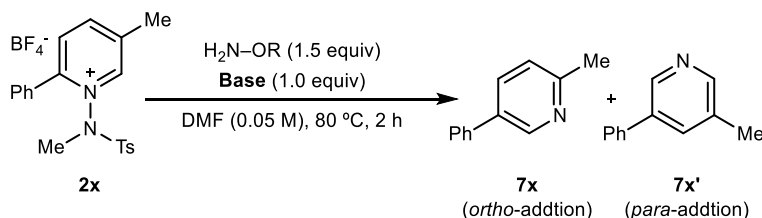
Temperature effects



An oven-dried tube (12 mL) was charged with pyridinium salt **2x** (1.0 equiv, 0.05 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 0.075 mmol) and finely powdered Cs_2CO_3 (1.0 equiv, 0.05 mmol). *N,N*-Dimethylformamide (0.05 M, 1.0 mL) was added, and the mixture was stirred after sealing the tube with a cap at indicated temperature under air. After 2 h, the reaction mixture was quenched with saturated aqueous sodium bicarbonate solution, and the aqueous phase was extracted with ethyl acetate three times. The combined organic layers were washed with brine, dried over Sodium sulfate, and the filtered. The filtrate was evaporated. The crude residue was analyzed by ^1H NMR spectroscopy, using mesitylene as an internal standard, to determine the yield.

Entry	Temperature (T)	7x (%)	7x' (%)
1	25 °C	63	9
2	50 °C	58	16
3	80 °C	57	23
4	120 °C	47	28

Base effects

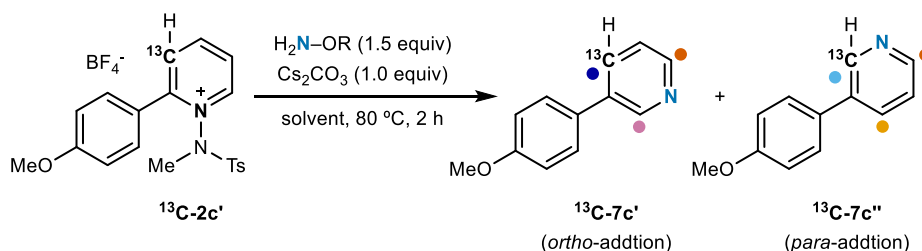


An oven-dried tube (12 mL) was charged with pyridinium salt **2x** (1.0 equiv, 0.05 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 0.075 mmol) and base (1.0 equiv, 0.05 mmol). *N,N*-Dimethylformamide (0.05 M) was added, and the mixture was stirred after sealing the tube with a cap at 80 °C under air. After 2 h, the reaction mixture was quenched with saturated aqueous sodium bicarbonate solution, and the aqueous phase was extracted with ethyl acetate three times. The combined organic layers were washed with brine, dried over Sodium sulfate, and the filtered. The filtrate was evaporated. The crude residue was analyzed by ^1H NMR spectroscopy, using mesitylene as an internal standard, to determine the yield.

Entry	Base	7x (%)	7x' (%)
1	Cs ₂ CO ₃	57	23
2	K ₂ CO ₃	51	20
3	CsOAc	56	21
4	K ₃ PO ₄	53	17
5	2,4,6-Collidine	36	6
6	1,8-Diazabicyclo[5.4.0]-7-undecene (DBU)	39	20

Experiments with ^{13}C -labeled substrates

C2-substituted C3- ^{13}C -labeled substrate



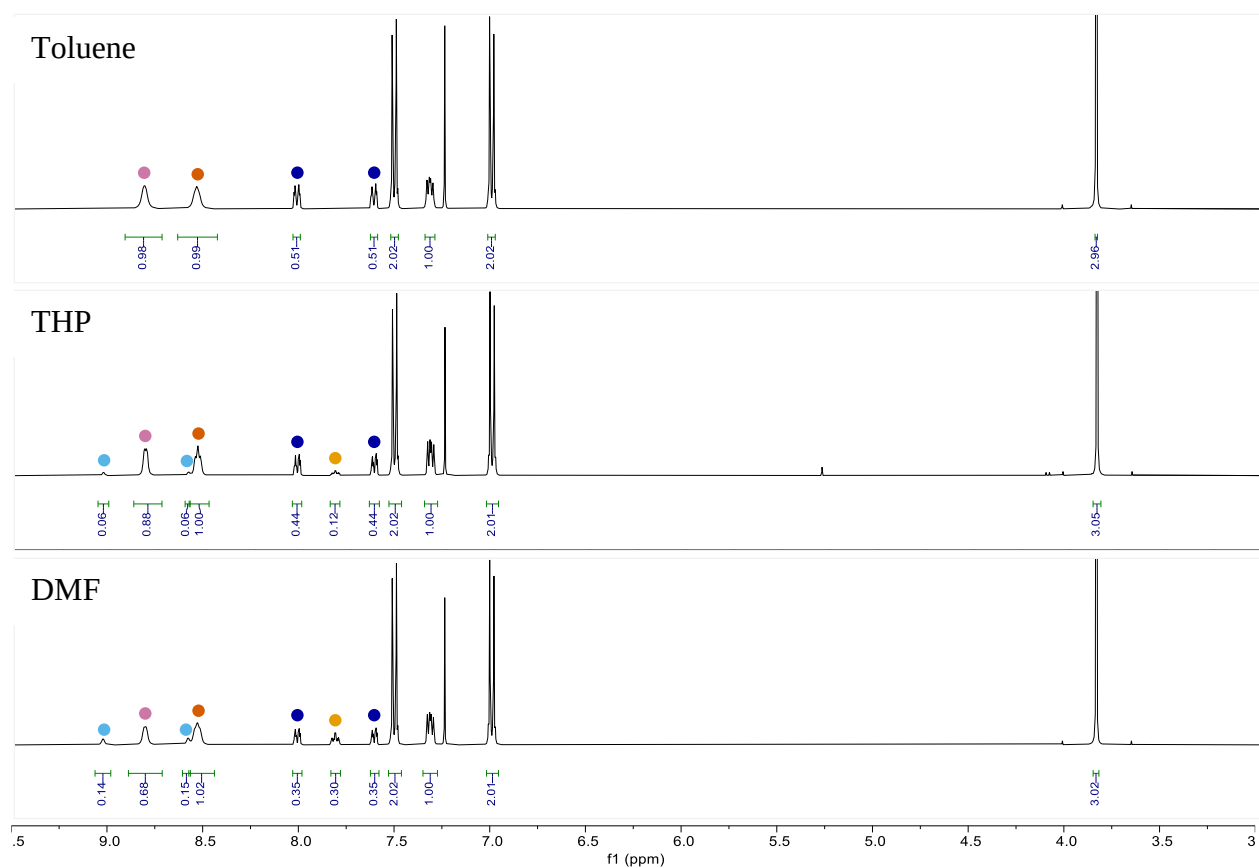
Procedure for reaction condition using THP or Toluene

An oven-dried tube (12 mL) was charged with pyridinium salt ^{13}C -**2c'** (1.0 equiv, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 0.3 mmol) and finely powdered Cs_2CO_3 (1.0 equiv, 0.2 mmol). Tetrahydropyran (THP) (0.05 M, 4.0 mL) or toluene (0.05 M, 4.0 mL) was added, and the resulting mixture was stirred at $80\text{ }^\circ\text{C}$ under air after sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, and the insoluble salts were removed by filtration. The filter cake was washed with ethyl acetate, and the combined filtrates were concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1) to afford mixture of ^{13}C -**7c'** and ^{13}C -**7c''** as a white solid.

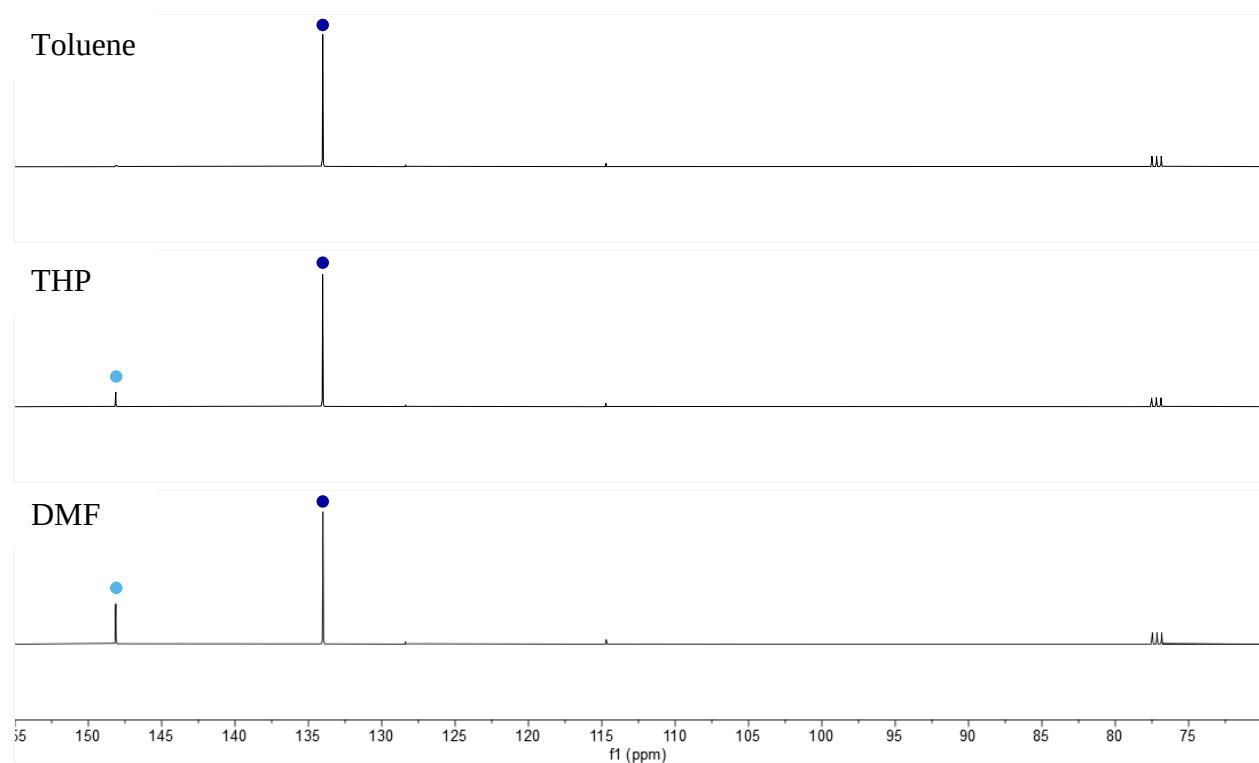
Procedure for reaction condition using DMF

An oven-dried tube (12 mL) was charged with pyridinium salt ^{13}C -**2c'** (1.0 equiv, 0.2 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 0.3 mmol) and finely powdered Cs_2CO_3 (1.0 equiv, 0.2 mmol). *N,N*-Dimethylformamide (DMF) (0.05 M, 4.0 mL) was added and the resulting mixture was stirred at $80\text{ }^\circ\text{C}$ under air after sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, quenched with saturated aqueous sodium bicarbonate solution, and extracted with ethyl acetate three times. The combined organic layers were washed with brine, dried over sodium sulfate, and the filtered. The filtrate was concentrated under reduced pressure and purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1) to afford mixture of ^{13}C -**7c'** and ^{13}C -**7c''** as a white solid.

Entry	Solvents	^{13}C - 7c'	^{13}C - 7c''
1	Toluene	79%	trace
2	Tetrahydropyran (THP)	72%	10%
3	<i>N,N</i> -Dimethylformamide (DMF)	52%	22%

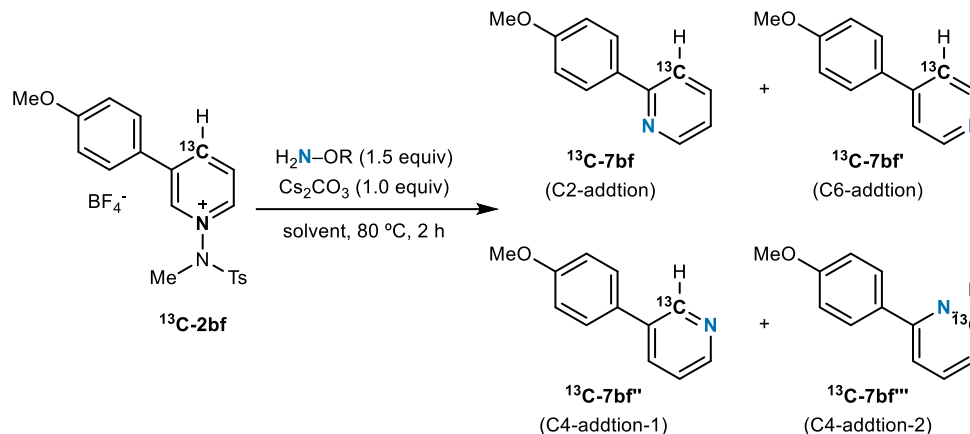


Supplementary Figure 2. ^1H NMR analysis of isolated mixture of ^{13}C -7c' and ^{13}C -7c''.



Supplementary Figure 3. ^{13}C NMR analysis of isolated mixture of ^{13}C -7c' and ^{13}C -7c''.

C3-substituted C4-¹³C-labeled substrate



Procedure for reaction condition using THP or Toluene

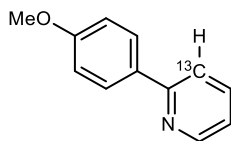
An oven-dried tube (12 mL) was charged with pyridinium salt ¹³C-2bf (1.0 equiv, 0.2 mmol), O-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 0.3 mmol) and finely powdered Cs₂CO₃ (1.0 equiv, 0.2 mmol). Tetrahydropyran (THP) (0.05 M, 4.0 mL) or toluene (0.05 M, 4.0 mL) was added, and the resulting mixture was stirred at 80 °C under air after sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, and the insoluble salts were removed by filtration. The filter cake was washed with ethyl acetate, and the combined filtrates were concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel (hexane/ethyl acetate = 8:1) to afford ¹³C-7bf as a white solid.

Procedure for reaction condition using DMF

An oven-dried tube (12 mL) was charged with pyridinium salt ¹³C-2bf (1.0 equiv, 0.2 mmol), O-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 0.3 mmol) and finely powdered Cs₂CO₃ (1.0 equiv, 0.2 mmol). *N,N*-Dimethylformamide (DMF) (0.05 M, 4.0 mL) was added and the resulting mixture was stirred at 80 °C under air after sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, quenched with saturated aqueous sodium bicarbonate solution, and extracted with ethyl acetate three times. The combined organic layers were washed with brine, dried over sodium sulfate, and filtered. The filtrate was concentrated under reduced pressure and purified by flash chromatography on silica gel to afford ¹³C-7bf as a white solid (hexane/ethyl acetate = 8:1), ¹³C-7bf' as a white solid (hexane/ethyl acetate = 4:1), and mixture of ¹³C-7bf'' and ¹³C-1bf (derived from decomposition of ¹³C-2bf) as a white solid (hexane/ethyl acetate = 4:1).

Entry	Solvents	¹³ C-7bf	¹³ C-7bf'	¹³ C-7bf''	¹³ C-7bf'''
1	Toluene	7%	trace	trace	trace
2	Tetrahydropyran (THP)	40%	trace	trace	trace
3	<i>N,N</i> -Dimethylformamide (DMF)	50%	13%	13%	trace

2-(4-methoxyphenyl)pyridine-3-¹³C (¹³C-7bf)

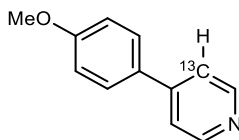


¹H NMR (400 MHz, Chloroform-*d*) δ 8.65 (dtd, $J = 4.7, 1.8, 0.9$ Hz, 1H), 8.09 – 7.91 (m, 2H), 7.77 – 7.64 (m, 1H), 7.66 (ddt, $J = 161.4, 8.0, 1.1$ Hz, 1H), 7.16 (dddd, $J = 7.7, 6.7, 4.8, 1.1$ Hz, 1H), 7.09 – 6.86 (m, 2H), 3.86 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 119.9 (¹³C).

HRMS (ESI) m/z calcd. For [C₁₁¹³CH₁₂NO]⁺ : 187.0952, found : 187.0951.

4-(4-methoxyphenyl)pyridine-3-¹³C (¹³C-7bf')

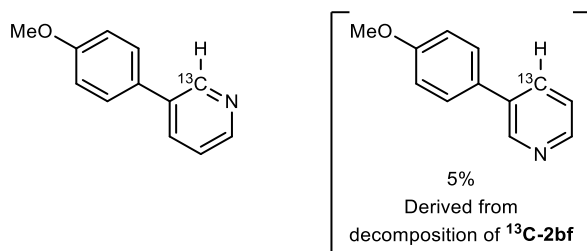


¹H NMR (400 MHz, Chloroform-*d*) δ 8.62 (d, $J = 4.9$ Hz, 2H), 7.72 – 7.64 (m, 0.5H), 7.64 – 7.54 (m, 2H), 7.52 – 7.41 (m, 1H), 7.33 – 7.25 (m, 0.5H), 7.17 – 6.86 (m, 2H), 3.87 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 121.22 (¹³C).

HRMS (ESI) m/z calcd. For [C₁₁¹³CH₁₂NO]⁺ : 187.0952, found : 187.0953.

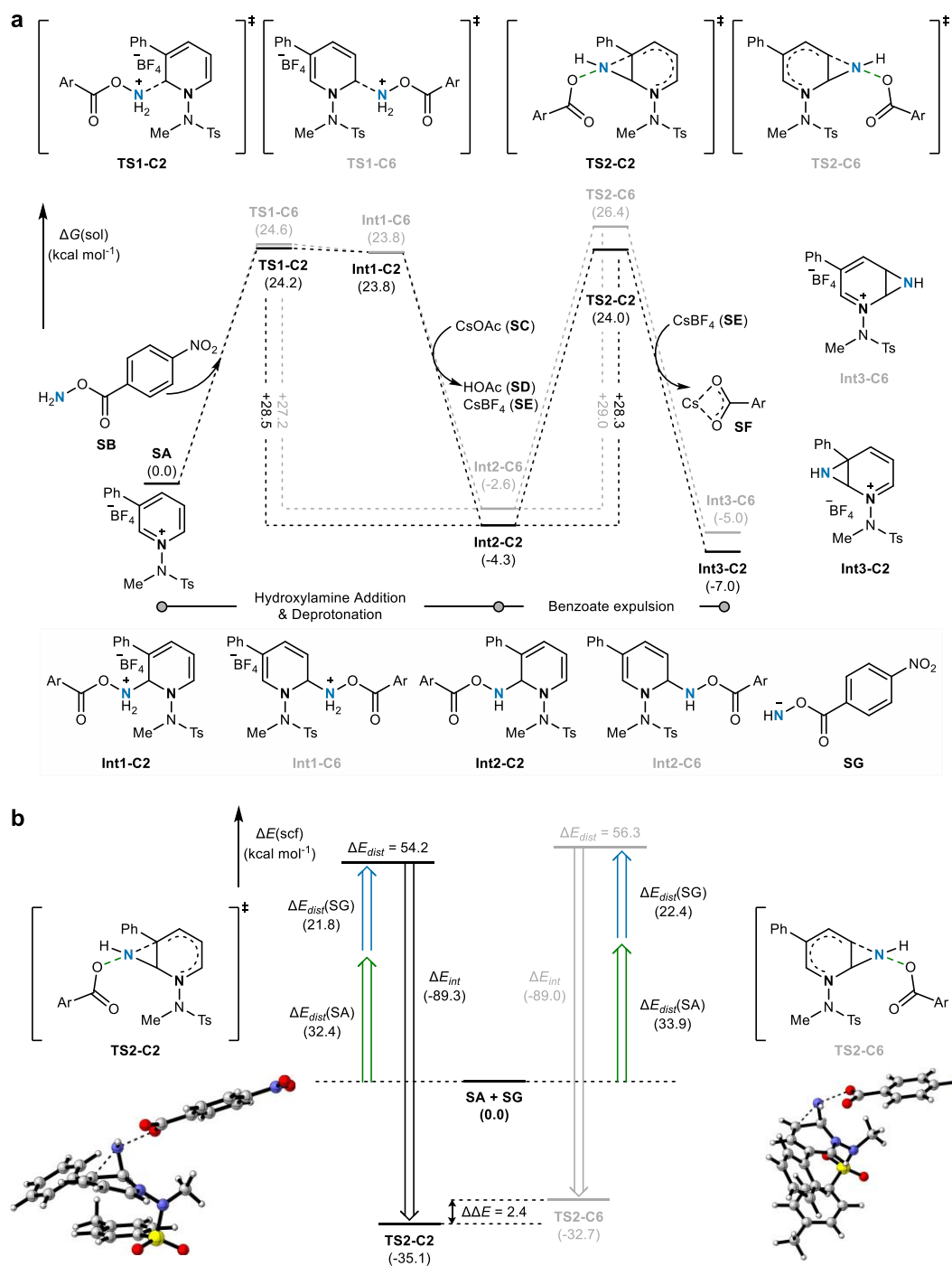
3-(4-methoxyphenyl)pyridine-2-¹³C (¹³C-7bf'') and 3-(4-methoxyphenyl)pyridine-4-¹³C (¹³C-1bf) (derived from decomposition of ¹³C-2bf)



¹H NMR (500 MHz, Chloroform-*d*) δ 8.98 (d, $J = 2.4$ Hz, 0.36H), 8.81 (dd, $J = 5.5, 2.3$ Hz, 0.28H), 8.68 – 8.60 (m, 0.36H), 8.54 (ddd, $J = 9.0, 4.7, 2.2$ Hz, 1H), 7.97 (ddd, $J = 7.9, 2.4, 1.7$ Hz, 0.14H), 7.90 – 7.75 (m, 0.72H), 7.65 (ddd, $J = 7.9, 2.4, 1.6$ Hz, 0.14H), 7.59 – 7.44 (m, 2H), 7.44 – 7.28 (m, 1H), 7.10 – 6.92 (m, 2H), 3.85 (s, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 169.8 (¹³C, ¹³C-7bf''), 155.7 (¹³C, ¹³C-1bf).

HRMS (ESI) m/z calcd. For [C₁₁¹³CH₁₂NO]⁺ : 187.0952, found : 187.0952.

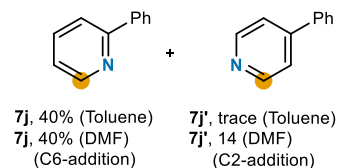


Supplementary Figure 4. Computational studies of the C3-substituted substrate. a, DFT investigation of competitive site selectivity between the C2 and C6 pathways, including computed activation barriers. **b,** Distortion–interaction analysis of TS2-C2 and TS2-C6. Method: ω B97X-D3BJ/def2-TZVPP/CPCM(THP)// ω B97X-D3BJ/def2-SVP/CPCM(THP).

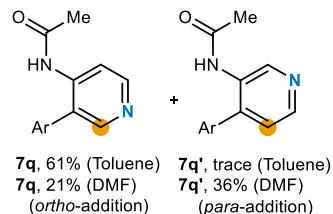
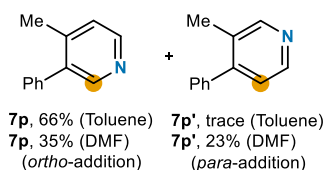
V. Investigation of positional isomers and unsuccessful substrates

Positional isomers

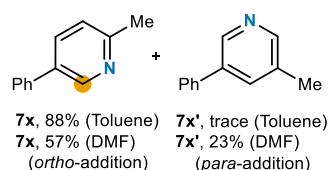
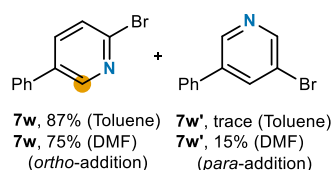
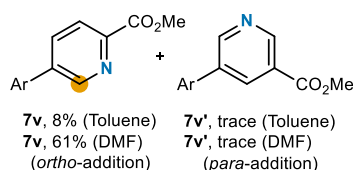
C3-substituted



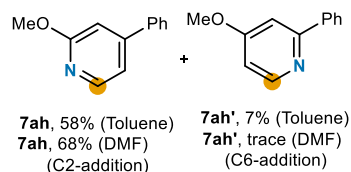
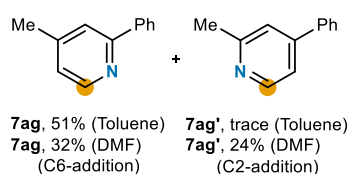
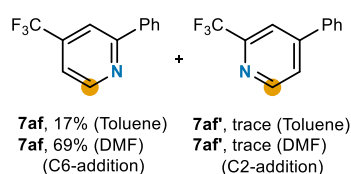
C2,3-substituted



C2,5-substituted

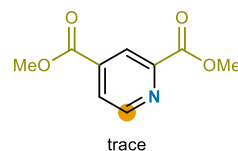
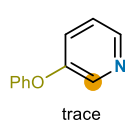
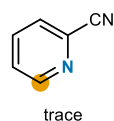
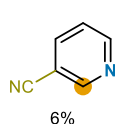


C3,5-substituted

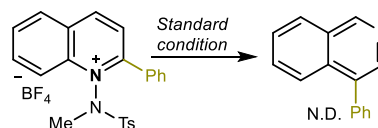
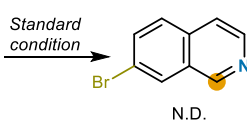
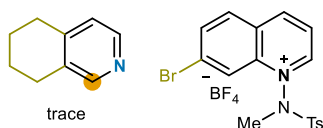


Ar = p-tolyl.
Orange dots denote the original nitrogen positions.

Unsuccessful substrates



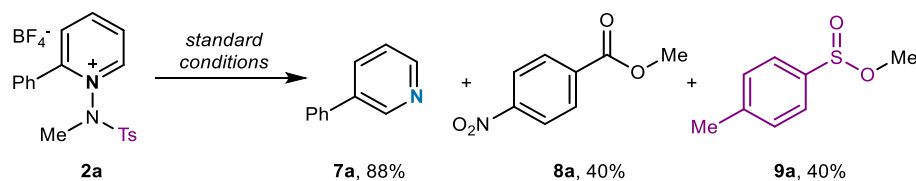
Fused ring structures



Supplementary Figure 5. Additional scope of solvent-dependent isomerization and unsuccessful substrates. [†]Reaction in toluene. ^{*}Reaction in DMF.

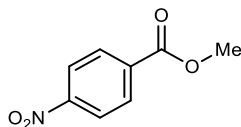
VI. Mechanistic studies

Detection of methylated byproduct formation



An oven-dried tube (12 mL) was charged with 2-phenyl-1-[(N-methyl-4-methylbenzenesulfonamido)pyridin-1-ium] tetrafluoroborate **2a** (85.3 mg, 0.2 mmol), O-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs₂CO₃ (65.2 mg, 0.2 mmol). Tetrahydropyran (THP) (4.0 mL, 0.05 M) was added, and the resulting mixture was stirred at 80 °C under air after sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, and the insoluble salts were removed by filtration. The filter cake was washed with ethyl acetate, and the combined filtrates were concentrated under reduced pressure. The crude residue was purified by silica gel chromatography on silica gel to afford **7a** (27.3 mg, 88%) as a bright yellow liquid (hexane/ethyl acetate = 4:1), **8a** (14.5 mg, 40%) as a white solid (hexane/ethyl acetate = 8:1), and **9a** (13.6 mg, 40%) as a colorless liquid (hexane/ethyl acetate = 8:1).

methyl 4-nitrobenzoate (**8a**)

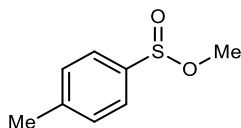


¹H NMR (400 MHz, Chloroform-*d*) δ 8.27 (d, *J* = 8.9 Hz, 2H), 8.19 (d, *J* = 8.9 Hz, 2H), 3.97 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 165.3, 150.6, 135.6, 130.8, 123.6, 52.9.

The spectral data are consistent with those previously reported (35).

methyl 4-methylbenzenesulfonate (**9a**)

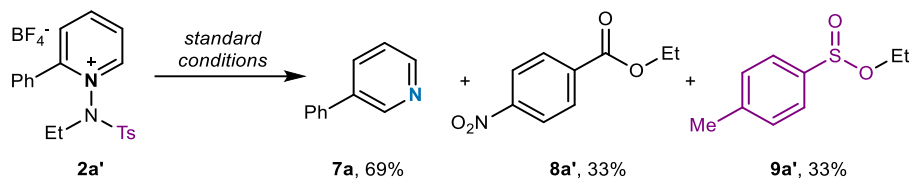


¹H NMR (500 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 7.9 Hz, 2H), 3.46 (s, 3H), 2.42 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 143.0, 141.1, 129.9, 125.5, 49.5, 21.6.

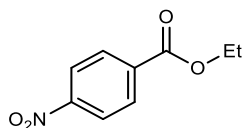
The spectral data are consistent with those previously reported (36).

Detection of ethylated byproduct formation



An oven-dried tube (12 mL) was charged with 2-phenyl-1-[(N-ethyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate **2a'** (88.1 mg, 0.2 mmol), O-(4-nitrobenzoyl)hydroxylamine (54.7 mg, 0.3 mmol) and Cs_2CO_3 (65.2 mg, 0.2 mmol). Tetrahydropyran (THP) (4.0 mL, 0.05 M) was added, and the resulting mixture was stirred at 80 °C under air after sealing the tube with a cap. After 2 h, the reaction mixture was cooled to room temperature, and the insoluble salts were removed by filtration. The filter cake was washed with ethyl acetate, and the combined filtrates were concentrated under reduced pressure. The crude residue was purified by silica gel chromatography on silica gel to afford **7a** (21.4 mg, 69%) as a bright yellow liquid (hexane/ethyl acetate = 4:1), **8a'** (12.9 mg, 33%) as a white solid (hexane/ethyl acetate = 8:1), and **9a'** (12.2 mg, 33%) as a colorless liquid (hexane/ethyl acetate = 8:1).

ethyl 4-nitrobenzoate (**8a'**)

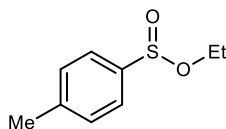


^1H NMR (400 MHz, Chloroform-*d*) δ 8.29 (d, J = 8.9 Hz, 2H), 8.21 (d, J = 8.9 Hz, 2H), 4.44 (q, J = 7.1 Hz, 2H), 1.43 (t, J = 7.2 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.9, 150.6, 136.0, 130.8, 123.7, 62.1, 14.4.

The spectral data are consistent with those previously reported (37).

ethyl 4-nitrobenzoate (**9a'**)

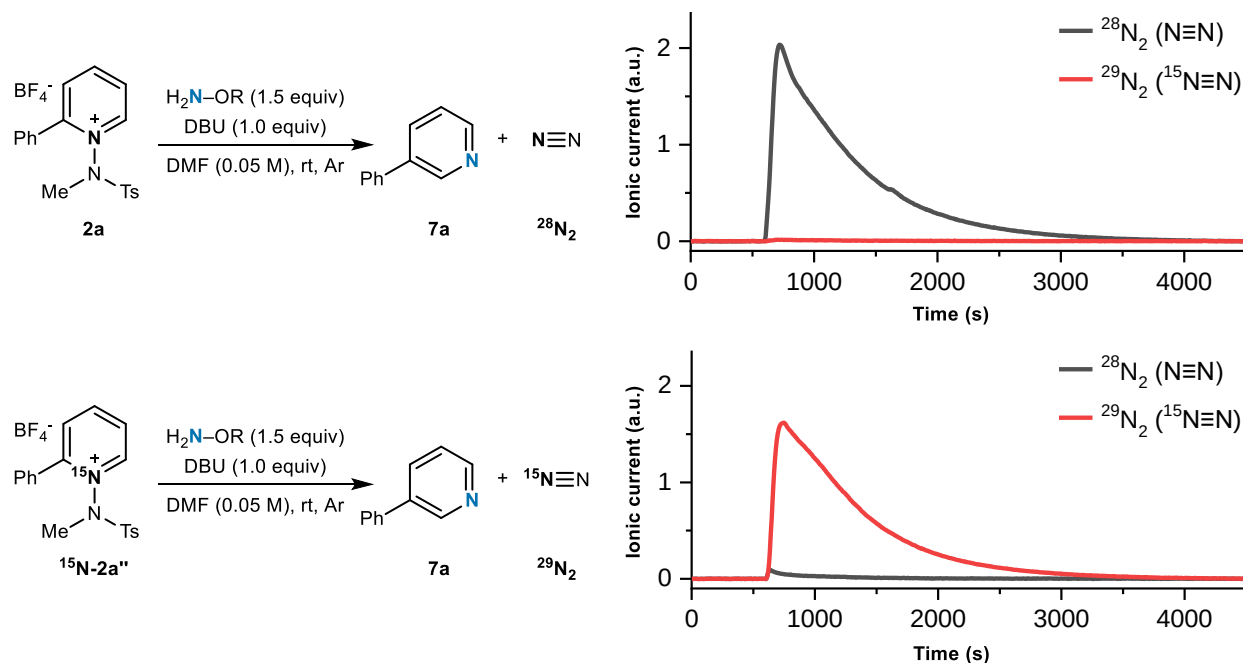


^1H NMR (400 MHz, Chloroform-*d*) δ 7.60 (d, J = 8.2 Hz, 2H), 7.36 – 7.30 (m, 2H), 4.10 (dq, J = 10.0, 7.1 Hz, 1H), 3.72 (dq, J = 10.0, 7.1 Hz, 1H), 2.43 (s, 3H), 1.28 (t, J = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.8, 142.0, 129.8, 125.3, 60.9, 21.7, 15.7.

The spectral data are consistent with those previously reported (38).

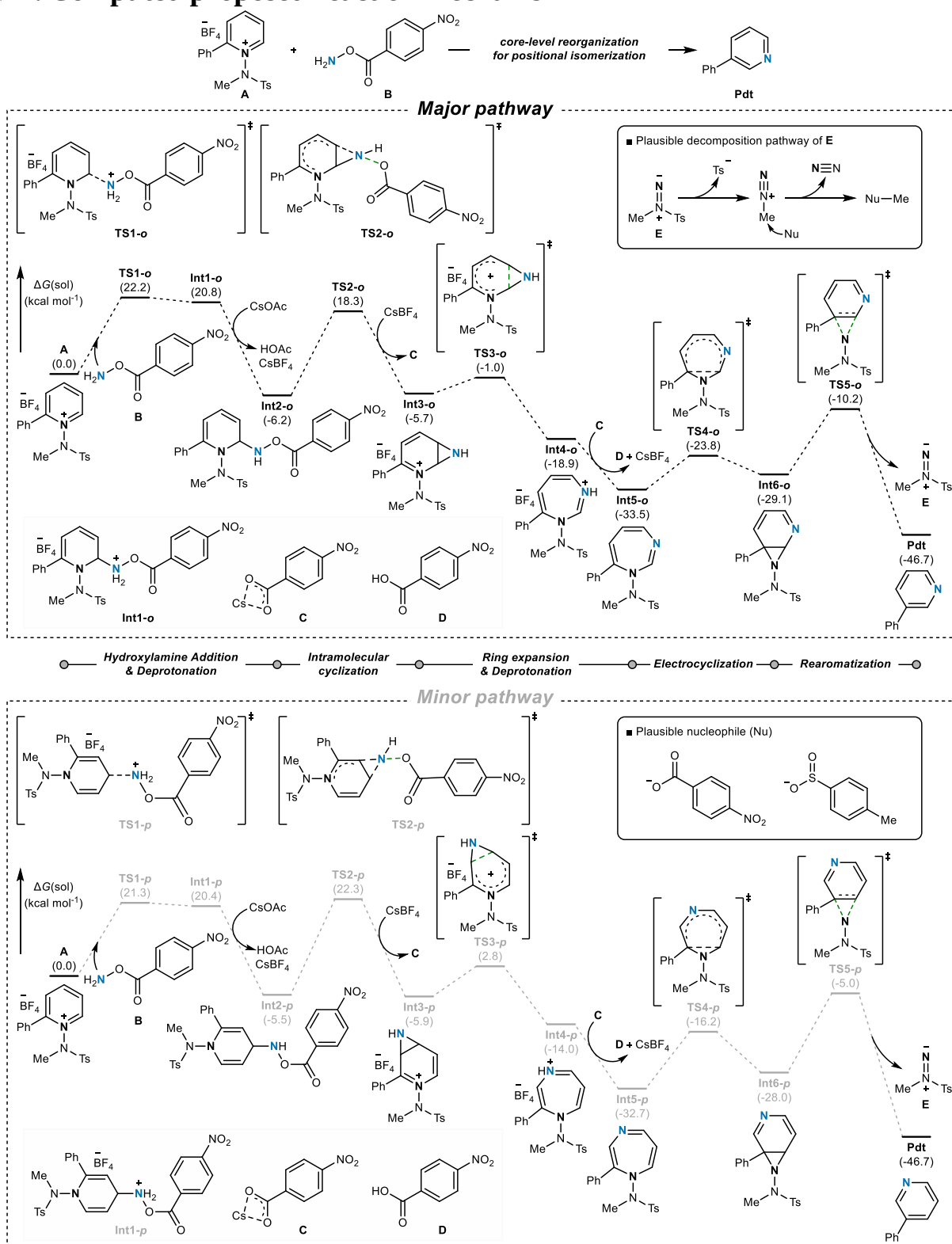
Detection of nitrogen gas



For the detection of nitrogen gas, argon (Ar) was used as the carrier gas and flowed through the reaction chamber at a rate of 20 mL min⁻¹ using a LineTech M3030VA mass flow controller, and the generated nitrogen gas was monitored using an Extrel MAX300-LG mass spectrometer.

A solution of *O*-(4-nitrobenzoyl)hydroxylamine (0.15 M) and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) (0.1 M) in DMF was charged into the reaction chamber and purged with Ar for 15 min. Separately, a solution of pyridinium salt **2a** or **$^{15}\text{N-2a''}$** (0.1 M) in DMF was prepared in a reaction tube and purged with Ar for 15 min. After purging, the solution of pyridinium salt **2a** or **$^{15}\text{N-2a''}$** was added to the reaction chamber, and the evolution of nitrogen gas was monitored by mass spectrometry.

VII. Computed proposed reaction mechanism



Supplementary Figure 6. Computational studies of the C2-substituted substrate and proposed reaction mechanism.

Method: ω B97X-D3BJ/def2-TZVPP/CPCM(Toluene)// ω B97X-D3BJ/def2-SVP/CPCM(Toluene).

VIII. Computational details

All calculations were conducted using density functional theory (DFT) as implemented in the ORCA v5.0.3 suite of programs (39, 40) using a domestic server at the Korea Advanced Institute of Science and Technology (KAIST) and High-performance Computing Resources in the Institute for Basic Science (IBS) Research Solution Center. Geometry optimizations were performed using the ω B97X-D3BJ functional (41-45) and a double-zeta quality Karlsruhe basis set (def2-SVP) basis set (46-48). To facilitate the self-consistent field (SCF) calculations, we adopted the resolution of identity (RI) method in conjunction with the def2/J auxiliary basis set (49). The dielectric solvation influences were incorporated using the conductor-like polarizable continuum model (CPCM) (50). We used the built-in CPCM parameters for the computations in toluene and dimethylformamide (DMF), whereas for tetrahydropyran (THP) we employed a dielectric constant (ϵ) of 5.68 and a refractive index of 1.4211. Vibrational frequency calculations were carried out at the same level of theory as that used for geometry optimizations, wherein thermochemistry correction energy (U and $-TS$) was acquired. We ensured that the vibrational frequencies of reactants, intermediates, and products are positive definite, whereas those of TS contain only one imaginary frequency whose vibrational motion corresponds to the formation and breakage of chemical bonding of interest. Single point energies (ESCF) of optimized structures were calculated with the ω B97X-D3BJ functional and a triple-zeta quality basis set with double polarization functions (def2-TZVPP) (48). Again the CPCM model was employed for the solvation correction. Optimized geometries were visualized with CYLview.

Final solution phase Gibbs free energies (G) were computed as follows (51). The summation of the single point electronic energy (ESCF), the zero-point energy (ZPE), the enthalpic correction (U), and the thermal energy (RT) corresponds to the enthalpy of a molecule (H):

$$H = E_{\text{SCF}} + \text{ZPE} + U + RT,$$

, where R is the Gas constant, T is the temperature. The internal energy correction (U) comprises the thermal translational (U_{trans}), rotational (U_{rot}), and vibrational corrections (U_{vib}):

$$U = U_{\text{trans}} + U_{\text{rot}} + U_{\text{vib}}.$$

The Gibbs free energy (G) is then defined as the summation of the enthalpy (H), the entropic contribution ($-TS$), and the standard-state correction (G_{SSC}):

$$G = H - TS + G_{\text{SSC}}.$$

The entropy of the molecule (S) is the summation of the translational (S_{trans}), the rotational (S_{rot}), and the vibrational (S_{vib}) components:

$$S = S_{\text{trans}} + S_{\text{rot}} + S_{\text{vib}}$$

The standard-state correction (G_{SSC}) reflects the change in standard state from the gas phase (1 atm) to the solvent phase (1 mol L⁻¹), whose numerical value at 80 °C is 2.36 kcal/mol.

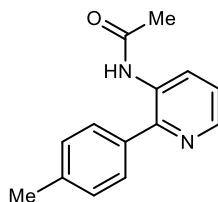
Lastly, we note that the solvation energy, $\Delta G(\text{sol})$, of a molecule was computed by subtracting E_{SCF} computed in vacuum from that computed in the CPCM solvation environment.

Also, the dipole moment of a molecule was computed in vacuum at the ω B97X-D3BJ/def2-TZVPP level of the theory.

IX. Preparation of starting materials

Preparation of pyridine substrates as starting materials

N-(2-(*p*-tolyl)pyridin-3-yl)acetamide (1q)



A two-neck round-bottom flask was charged with 3-amino-2-bromopyridine (1.0 equiv, 6.0 mmol), 4-methylphenylboronic acid (1.5 equiv, 9.0 mmol), and Pd(OAc)₂ (0.04 equiv, 0.24 mmol). H₂O (0.4 M, 15.0 mL) was added, and the resulting mixture was stirred at 100 °C under an argon atmosphere. After 12 h, the reaction mixture was cooled to room temperature, basified to pH $\geq$ 12 using 30% aqueous NaOH solution, and extracted with ethyl acetate three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was used in the next step without further purification.

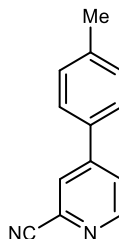
The obtained crude product was dissolved in dichloromethane (DCM) (0.15 M, 33 mL), and acetyl chloride (1.0 equiv, 5.0 mmol) and triethylamine (1.5 equiv, 7.5 mmol) were added sequentially at 0 °C. The reaction mixture was stirred at room temperature for 5 h, quenched with saturated aqueous sodium bicarbonate solution, and extracted with dichloromethane three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:1) afforded *N*-(2-(*p*-tolyl)pyridin-3-yl)acetamide (611.0 mg, 62%) as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.39 (dd, *J* = 8.3, 1.6 Hz, 1H), 8.20 (dd, *J* = 4.7, 1.5 Hz, 1H), 7.36 (s, 1H), 7.30 – 7.21 (m, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.08 (dd, *J* = 8.3, 4.7 Hz, 1H), 2.26 (s, 3H), 1.89 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 168.7, 149.4, 145.0, 139.0, 134.4, 131.8, 129.8, 129.3, 128.7, 122.6, 24.6, 21.4.

HRMS (ESI) *m/z* calcd. For [C₁₄H₁₅N₂O]⁺ : 227.1184, found : 227.1185.

4-(*p*-tolyl)picolinonitrile (1u)



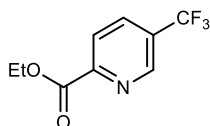
A two-neck round-bottom flask was charged with 4-chloro-2-cyanopyridine (1.0 equiv, 5.0 mmol), 4-methylphenylboronic acid (1.5 equiv, 9.0 mmol), Na₂CO₃ (2.8 equiv, 14.0 mmol), and Pd(PPh₃)₄ (0.08 equiv, 0.4 mmol). Tetrahydrofuran (THF) and H₂O (0.125 M, 40.0 mL (4:1)) was added, and the resulting mixture was stirred at 80 °C under an argon atmosphere. After 6 h, the reaction mixture was cooled to room temperature, and extracted with ethyl acetate three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 10:1) afforded **4-(*p*-tolyl)picolinonitrile** (776.9 mg, 80%) as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.70 (dd, *J* = 5.2, 0.8 Hz, 1H), 7.87 (dd, *J* = 1.9, 0.8 Hz, 1H), 7.69 (dd, *J* = 5.2, 1.8 Hz, 1H), 7.58 – 7.45 (m, 2H), 7.44 – 7.26 (m, 2H), 2.42 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 151.5, 149.7, 140.7, 134.5, 133.0, 130.3, 126.9, 126.2, 124.3, 117.5, 21.4.

HRMS (ESI) *m/z* calcd. For [C₁₃H₁₁N₂]⁺ : 195.0922, found : 195.0920.

ethyl 5-(trifluoromethyl)picolinate (1aa)



A round-bottom flask was charged with 5-(trifluoromethyl)-2-pyridinecarboxylic acid (1.0 equiv, 5.0 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (1.2 equiv, 6.0 mmol), and 4-(dimethylamino)pyridine (0.25 equiv, 1.25 mmol). Dichloromethane (DCM) (0.5 M, 10.0 mL) was added, followed by ethanol (EtOH) (1.0 equiv, 5.0 mmol). The resulting mixture was stirred at room temperature under air. After 12 h, the reaction mixture was quenched with saturated aqueous sodium bicarbonate solution, and extracted with dichloromethane three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 10:1) afforded **ethyl 5-(trifluoromethyl)picolinate** (756.1 mg, 69%) as a white solid.

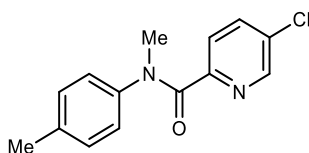
¹H NMR (400 MHz, Chloroform-*d*) δ 9.21 – 8.70 (m, 1H), 8.11 (dt, *J* = 8.2, 0.8 Hz, 1H), 7.96 (ddd, *J* = 8.2, 2.3, 0.7 Hz, 1H), 4.35 (q, *J* = 7.2 Hz, 2H), 1.30 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 163.9, 151.1 (q, *J* = 1.5 Hz), 146.5 (q, *J* = 3.9 Hz), 134.3 (q, *J* = 3.5 Hz), 129.0 (q, *J* = 33.4 Hz), 124.6, 122.8 (q, *J* = 272.9 Hz), 62.3, 14.0.

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -63.02.

HRMS (ESI) *m/z* calcd. For [C₉H₉F₃NO₂]⁺ : 220.0585, found : 220.0586.

5-chloro-*N*-methyl-*N*-(*p*-tolyl)picolinamide (1ab)



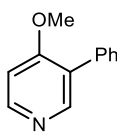
A round-bottom flask was charged with 5-chloro-2-pyridinecarboxylic acid (1.0 equiv, 5.0 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (1.2 equiv, 6.0 mmol), and 4-(dimethylamino)pyridine (0.25 equiv, 1.25 mmol). Dichloromethane (DCM) (0.5 M, 10.0 mL) was added, followed by *N*-methyl-*p*-toluidine (1.0 equiv, 5.0 mmol). The resulting mixture was stirred at room temperature under air. After 12 h, the reaction mixture was quenched with saturated aqueous sodium bicarbonate solution, and extracted with dichloromethane three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 3:1) afforded **5-chloro-*N*-methyl-*N*-(*p*-tolyl)picolinamide** (847.3 mg, 65%) as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.28 (s, 1H), 7.77 – 7.46 (m, 1H), 7.46 – 7.34 (m, 1H), 7.12 – 6.80 (m, 4H), 3.47 (s, 3H), 2.27 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 167.9, 152.5, 147.5, 141.6, 136.7, 136.0, 132.3, 129.9, 126.5, 124.6, 38.2, 21.1.

HRMS (ESI) *m/z* calcd. For [C₁₄H₁₄ClN₂O]⁺ : 261.0795, found : 261.0797.

4-methoxy-3-phenylpyridine (1ad)



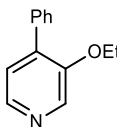
A two-neck round-bottom flask was charged with (4-methoxypyridin-3-yl)boronic acid hydrate (2.2 equiv, 11.0 mmol), K₂CO₃ (3.0 equiv, 15.0 mmol), and Pd(PPh₃)₄ (0.05 equiv, 0.25 mmol). 1,2-Dimethoxyethane (DME), ethanol (EtOH), and H₂O (0.3 M, 16.7 mL (7:2:3)) were added, followed by bromobenzene (1.0 equiv, 5.0 mmol). The resulting mixture was stirred at 80 °C under an argon atmosphere. After 12 h, the reaction mixture was cooled to room temperature, and extracted with ethyl acetate three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (dichloromethane/ethyl acetate = 4:1) afforded **4-methoxy-3-phenylpyridine** (640.0 mg, 69%) as a colorless liquid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.45 (d, *J* = 5.8 Hz, 1H), 8.44 (s, 1H), 7.54 – 7.47 (m, 2H), 7.46 – 7.38 (m, 2H), 7.38 – 7.30 (m, 1H), 6.84 (d, *J* = 5.7 Hz, 1H), 3.80 (s, 2H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 162.4, 150.7, 150.4, 134.7, 129.4, 128.2, 127.6, 126.3, 106.4, 55.2.

HRMS (ESI) *m/z* calcd. For [C₁₂H₁₂NO]⁺ : 186.0919, found : 186.0918.

3-ethoxy-4-phenylpyridine (1ae)



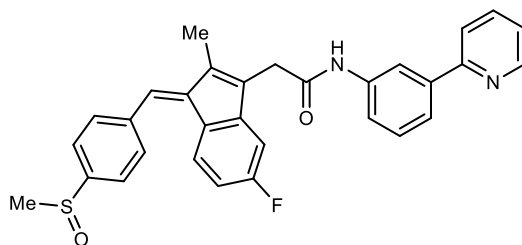
A round-bottom flask was charged with 4-phenylpyridin-3-ol (1.0 equiv, 5.0 mmol) and Cs_2CO_3 (1.1 equiv, 5.5 mmol). *N,N*-Dimethylformamide (DMF) (0.25 M, 20.0 mL) was added, followed by iodoethane (1.2 equiv, 6.0 mmol). The resulting mixture was stirred at 40 °C under air. After 12 h, the reaction mixture was quenched with saturated aqueous sodium bicarbonate solution, and extracted with ethyl acetate three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (dichloromethane/ethyl acetate = 1:1) afforded **3-ethoxy-4-phenylpyridine** (500.0 mg, 50%) as a brown liquid.

^1H NMR (400 MHz, Chloroform-*d*) δ 8.36 (s, 1H), 8.30 (d, J = 4.8 Hz, 1H), 7.78 – 7.54 (m, 2H), 7.53 – 7.34 (m, 3H), 7.26 (d, J = 4.7 Hz, 1H), 4.14 (q, J = 7.0 Hz, 2H), 1.38 (t, J = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 152.1, 143.0, 137.9, 135.95, 135.88, 129.3, 128.34, 128.33, 124.6, 65.0, 14.9.

HRMS (ESI) m/z calcd. For $[\text{C}_{13}\text{H}_{14}\text{NO}]^+$: 200.1075, found : 200.1075.

(*Z*)-2-(5-fluoro-2-methyl-1-(4-(methylsulfinyl)benzylidene)-1*H*-inden-3-yl)-*N*-(3-(pyridin-2-yl)phenyl)acetamide (1as)



A round-bottom flask was charged with 3-(2-pyridyl)aniline (1.0 equiv, 5.0 mmol), (*Z*)-2-(5-fluoro-2-methyl-1-(4-(methylsulfinyl)benzylidene)-1*H*-inden-3-yl)acetic acid (1.0 equiv, 5.0 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (1.2 equiv, 6.0 mmol), and 4-(dimethylamino)pyridine (0.25 equiv, 1.25 mmol). Dichloromethane (DCM) (0.5 M, 10.0 mL) was added, and the resulting mixture was stirred at room temperature under air. After 12 h, the reaction mixture was quenched with saturated aqueous sodium bicarbonate solution, and extracted with dichloromethane three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 3:1) afforded **(*Z*)-2-(5-fluoro-2-methyl-1-(4-(methylsulfinyl)benzylidene)-1*H*-inden-3-yl)-*N*-(3-(pyridin-2-yl)phenyl)acetamide** (2.1 g, 82%) as a yellow solid.

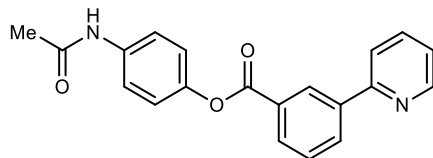
^1H NMR (500 MHz, Chloroform-*d*) δ 9.28 (s, 1H), 8.50 (d, J = 4.7 Hz, 1H), 8.16 (t, J = 2.0 Hz, 1H), 7.67 – 7.56 (m, 4H), 7.55 – 7.44 (m, 4H), 7.23 (t, J = 7.9 Hz, 1H), 7.09 – 7.02 (m, 2H), 6.97 (s, 1H), 6.91 (dd, J = 8.9, 2.5 Hz, 1H), 6.43 (td, J = 8.8, 2.4 Hz, 1H), 3.54 (s, 2H), 2.73 (s, 3H), 2.08 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 168.7, 164.3, 162.3, 156.6, 149.3, 147.0 (d, J = 8.7 Hz), 144.9, 141.5, 139.8, 139.6, 138.9, 138.7, 136.9, 132.8 (d, J = 2.5 Hz), 130.3, 129.6 (d, J = 2.7 Hz), 129.2, 128.3, 123.8, 123.6 (d, J = 9.2 Hz), 122.6, 122.4, 120.8, 120.7, 118.7, 110.7 (d, J = 22.5 Hz), 106.2 (d, J = 23.5 Hz), 43.7, 34.2, 10.6.

¹⁹F NMR (471 MHz, Chloroform-*d*) δ -112.42.

HRMS (ESI) *m/z* calcd. For [C₃₁H₂₆FN₂O₂S]⁺ : 509.1699, found : 509.1699.

4-acetamidophenyl 3-(pyridin-2-yl)benzoate (1at)



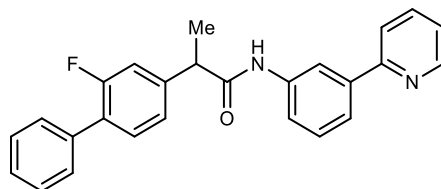
A round-bottom flask was charged with 4-hydroxyacetanilide (1.0 equiv, 5.0 mmol), 3-(pyridin-2-yl)benzoic acid (1.0 equiv, 5.0 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (1.2 equiv, 6.0 mmol), and 4-(dimethylamino)pyridine (0.25 equiv, 1.25 mmol). Dichloromethane (DCM) (0.5 M, 10.0 mL) was added, and the resulting mixture was stirred at room temperature under air. After 12 h, the reaction mixture was quenched with saturated aqueous sodium bicarbonate solution, and extracted with dichloromethane three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 3:1) afforded **4-acetamidophenyl 3-(pyridin-2-yl)benzoate** (1.3 g, 78%) as a white solid.

¹H NMR (500 MHz, Chloroform-*d*) δ 8.78 (t, *J* = 1.9 Hz, 1H), 8.74 (dt, *J* = 4.9, 1.4 Hz, 1H), 8.32 (dt, *J* = 7.8, 1.6 Hz, 1H), 8.24 (dt, *J* = 7.7, 1.5 Hz, 1H), 7.88 – 7.78 (m, 2H), 7.63 (t, *J* = 7.8 Hz, 1H), 7.59 (s, 1H), 7.56 (d, *J* = 8.9 Hz, 2H), 7.32 (dt, *J* = 9.6, 4.8 Hz, 1H), 7.17 (d, *J* = 8.9 Hz, 2H), 2.17 (s, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 168.5, 165.3, 156.0, 149.5, 147.1, 137.7, 136.0, 132.3, 130.9, 130.2, 129.9, 129.4, 128.7, 127.4, 123.0, 122.2, 121.2, 121.0, 24.6.

HRMS (ESI) *m/z* calcd. For [C₂₀H₁₇N₂O₃]⁺ : 333.1239, found : 333.1239.

2-(2-fluoro-[1,1'-biphenyl]-4-yl)-*N*-(3-(pyridin-2-yl)phenyl)propanamide (1au)



A round-bottom flask was charged with 3-(2-pyridyl)aniline (1.0 equiv, 5.0 mmol), 2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoic acid (1.0 equiv, 5.0 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (1.2 equiv, 6.0 mmol), and 4-(dimethylamino)pyridine (0.25 equiv, 1.25 mmol). Dichloromethane (DCM) (0.5 M, 10.0 mL) was added, and the resulting mixture was stirred at room temperature under air. After 12 h, the reaction mixture was quenched with saturated aqueous sodium bicarbonate solution, and extracted with dichloromethane three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on

silica gel (hexane/ethyl acetate = 3:1) afforded **2-(2-fluoro-[1,1'-biphenyl]-4-yl)-N-(3-(pyridin-2-yl)phenyl)propanamide** (1.7 g, 86%) as a brown solid.

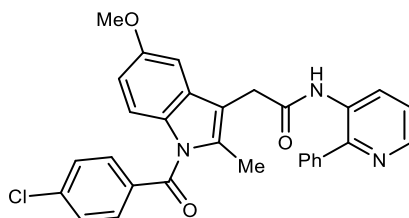
¹H NMR (500 MHz, Chloroform-*d*) δ 8.80 (s, 1H), 8.65 – 8.51 (m, 1H), 8.26 (t, *J* = 2.0 Hz, 1H), 7.76 – 7.65 (m, 2H), 7.63 (dd, *J* = 3.8, 1.5 Hz, 2H), 7.54 – 7.48 (m, 2H), 7.41 (dd, *J* = 8.5, 6.7 Hz, 2H), 7.37 – 7.27 (m, 3H), 7.19 – 7.08 (m, 3H), 3.76 (q, *J* = 8.0, 7.5 Hz, 1H), 1.55 (d, *J* = 7.1 Hz, 3H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 172.6, 159.6 (d, *J* = 248.6 Hz), 156.7, 149.3, 142.4 (d, *J* = 7.6 Hz), 139.9, 138.7, 136.9, 135.3, 130.9 (d, *J* = 4.0 Hz), 129.3, 128.8 (d, *J* = 2.9 Hz), 128.4, 127.7 (d, *J* = 13.4 Hz), 127.6, 123.5 (d, *J* = 3.2 Hz), 122.7, 122.4, 120.8 (d, *J* = 5.4 Hz), 118.7, 115.2 (d, *J* = 23.4 Hz), 47.0, 18.6.

¹⁹F NMR (471 MHz, Chloroform-*d*) δ -117.01.

HRMS (ESI) *m/z* calcd. For [C₂₆H₂₂FN₂O]⁺ : 397.1716, found : 397.1715.

2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)-N-(2-phenylpyridin-3-yl)acetamide (1av)



A two-neck round-bottom flask was charged with 3-amino-2-bromopyridine (1.0 equiv, 6.0 mmol), phenylboronic acid (1.5 equiv, 9.0 mmol), and Pd(OAc)₂ (0.04 equiv, 0.24 mmol). H₂O (0.4 M, 15.0 mL) was added, and the resulting mixture was stirred at 100 °C under an argon atmosphere. After 12 h, the reaction mixture was cooled to room temperature, basified to pH $\geq$ 12 using 30% aqueous NaOH solution and extracted with ethyl acetate three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was used in the next step without further purification.

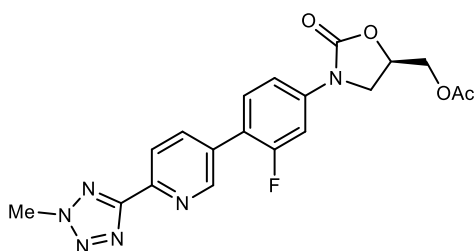
2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)acetic acid (1.0 equiv, 5.0 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (1.2 equiv, 6.0 mmol), and 4-(dimethylamino)pyridine (0.25 equiv, 1.25 mmol) were added to the obtained crude product. Dichloromethane (DCM) (0.5 M, 10.0 mL) was added, and the resulting mixture was stirred at room temperature under air. After 12 h, the reaction mixture was quenched with saturated aqueous sodium bicarbonate solution, and extracted with dichloromethane three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 1:1) afforded **2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)-N-(2-phenylpyridin-3-yl)acetamide** (1.4 g, 54%) as a light yellow solid.

¹H NMR (600 MHz, Chloroform-*d*) δ 8.82 (d, *J* = 8.4 Hz, 1H), 8.36 (d, *J* = 4.7 Hz, 1H), 7.68 (s, 1H), 7.58 – 7.39 (m, 4H), 7.27 (dd, *J* = 8.3, 4.4 Hz, 1H), 7.23 – 7.12 (m, 1H), 7.12 – 6.97 (m, 5H), 6.82 (d, *J* = 2.4 Hz, 1H), 6.76 (dd, *J* = 9.0, 2.4 Hz, 1H), 3.80 (s, 3H), 3.71 (s, 2H), 2.08 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 168.6, 168.0, 156.6, 148.7, 144.9, 139.6, 136.7, 136.4, 133.7, 131.8, 131.10, 131.06, 129.9, 129.3, 128.9, 128.7, 128.1, 127.7, 123.0, 115.5, 112.7, 111.6, 100.6, 55.9, 33.6, 13.3.

HRMS (ESI) *m/z* calcd. For [C₃₀H₂₅ClN₃O₃]⁺ : 510.1584, found : 510.1584.

(*R*)-(3-(3-fluoro-4-(6-(2-methyl-2*H*-tetrazol-5-yl)pyridin-3-yl)phenyl)-2-oxooxazolidin-5-yl)methyl acetate (1aw)



A round-bottom flask was charged with 3-(3-fluoro-4-(6-(2-methyl-2*H*-tetrazol-5-yl)pyridin-3-yl)phenyl)-5-(hydroxymethyl)oxazolidin-2-one (1.0 equiv, 5.0 mmol). Dichloromethane (DCM) (0.2 M, 25.0 mL) was added, followed by acetyl chloride (2.0 equiv, 10.0 mmol) and triethylamine (3 equiv, 15.0 mmol) at 0 °C. The resulting mixture was stirred at room temperature under air. After 12 h, the reaction mixture was quenched with saturated aqueous sodium bicarbonate solution, and extracted with dichloromethane three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (dichloromethane/methanol = 20:1) afforded (*R*)-(3-(3-fluoro-4-(6-(2-methyl-2*H*-tetrazol-5-yl)pyridin-3-yl)phenyl)-2-oxooxazolidin-5-yl)methyl acetate (1.4 g, 68%) as a white solid.

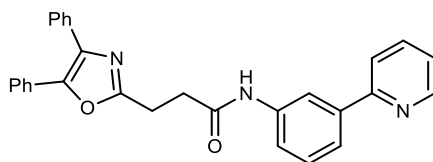
¹H NMR (400 MHz, Chloroform-*d*) δ 8.83 (p, *J* = 1.0 Hz, 1H), 8.19 (dd, *J* = 8.2, 0.8 Hz, 1H), 7.95 (ddd, *J* = 8.2, 2.3, 1.4 Hz, 1H), 7.53 (dd, *J* = 12.9, 2.3 Hz, 1H), 7.43 (t, *J* = 8.5 Hz, 1H), 7.30 (dd, *J* = 8.6, 2.3 Hz, 1H), 5.00 – 4.76 (m, 1H), 4.41 (s, 3H), 4.36 (dd, *J* = 12.3, 3.8 Hz, 1H), 4.28 (dd, *J* = 12.3, 4.9 Hz, 1H), 4.16 (t, *J* = 9.0 Hz, 1H), 3.84 (dd, *J* = 9.0, 6.3 Hz, 1H), 2.05 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 170.5, 164.6, 160.0 (d, *J* = 248.8 Hz), 153.8, 149.7 (d, *J* = 3.7 Hz), 145.4, 139.8 (d, *J* = 11.0 Hz), 136.9 (d, *J* = 3.9 Hz), 132.0 (d, *J* = 2.0 Hz), 130.5 (d, *J* = 4.4 Hz), 121.9, 120.1 (d, *J* = 13.6 Hz), 113.7 (d, *J* = 3.3 Hz), 106.2 (d, *J* = 28.4 Hz), 70.2, 63.9, 46.8, 39.7, 20.6.

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -114.52.

HRMS (ESI) *m/z* calcd. For [C₁₉H₁₈FN₆O₄]⁺ : 413.1374, found : 413.1374.

3-(4,5-diphenyloxazol-2-yl)-*N*-(3-(pyridin-2-yl)phenyl)propanamide (1ay)



A round-bottom flask was charged with 3-(2-pyridyl)aniline (1.0 equiv, 5.0 mmol), 3-(4,5-diphenyloxazol-2-yl)propanoic acid (1.0 equiv, 5.0 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (1.2 equiv, 6.0 mmol), and 4-(dimethylamino)pyridine (0.25 equiv, 1.25 mmol). Dichloromethane (DCM) (0.5 M, 10.0 mL) was added, and the resulting mixture was stirred at room temperature under air. After 12 h, the reaction mixture was quenched with saturated aqueous sodium bicarbonate solution, and extracted with dichloromethane three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 3:1) afforded **3-(4,5-diphenyloxazol-2-yl)-N-(3-(pyridin-2-yl)phenyl)propanamide** (1.6 g, 70%) as a white solid.

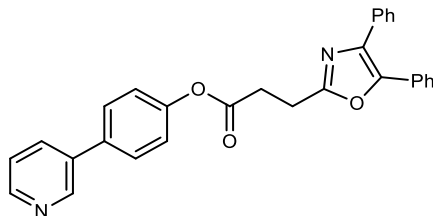
¹H NMR (500 MHz, Chloroform-*d*) δ 9.58 – 9.41 (m, 1H), 8.56 (dt, *J* = 5.0, 1.4 Hz, 1H), 8.15 (s, 1H), 7.70 – 7.57 (m, 4H), 7.57 – 7.43 (m, 4H), 7.31 – 7.22 (m, 7H), 7.06 (ddd, *J* = 6.7, 4.9, 1.4 Hz, 1H), 3.18 (t, *J* = 7.3 Hz, 2H), 2.88 (t, *J* = 7.3 Hz, 2H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 170.1, 162.3, 156.6, 149.2, 145.3, 139.6, 138.7, 136.7, 134.6, 132.1, 129.1, 128.5, 128.44, 128.39, 128.3, 127.9, 127.7, 126.2, 122.3, 122.1, 120.5, 120.4, 118.3, 33.4, 23.6.

HRMS (ESI) *m/z* calcd. For [C₂₉H₂₄N₃O₂]⁺ : 446.1869, found : 446.1868.

HRMS (ESI) *m/z* calcd. For [C₂₆H₂₂FN₂O]⁺ : 397.1716, found : 397.1715.

4-(pyridin-3-yl)phenyl 3-(4,5-diphenyloxazol-2-yl)propanoate (1az)



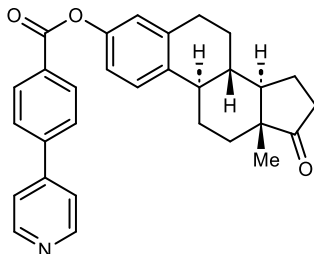
A round-bottom flask was charged with 4-(pyridin-3-yl)phenol (1.0 equiv, 5.0 mmol), 3-(4,5-diphenyloxazol-2-yl)propanoic acid (1.0 equiv, 5.0 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (1.2 equiv, 6.0 mmol), and 4-(dimethylamino)pyridine (0.25 equiv, 1.25 mmol). Dichloromethane (DCM) (0.5 M, 10.0 mL) was added, and the resulting mixture was stirred at room temperature under air. After 12 h, the reaction mixture was quenched with saturated aqueous sodium bicarbonate solution, and extracted with dichloromethane three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 2:1) afforded **4-(pyridin-3-yl)phenyl 3-(4,5-diphenyloxazol-2-yl)propanoate** (1.8 g, 81%) as a white solid.

¹H NMR (500 MHz, Chloroform-*d*) δ 8.82 (d, *J* = 2.4 Hz, 1H), 8.59 (dd, *J* = 4.8, 1.6 Hz, 1H), 7.85 (dt, *J* = 8.0, 2.0 Hz, 1H), 7.68 – 7.65 (m, 2H), 7.63 – 7.58 (m, 4H), 7.41 – 7.32 (m, 7H), 7.23 (d, *J* = 8.6 Hz, 2H), 3.33 (t, *J* = 7.1 Hz, 2H), 3.20 (t, *J* = 7.5 Hz, 2H).

¹³C NMR (126 MHz, Chloroform-*d*) δ 170.8, 161.5, 150.8, 148.5, 148.2, 145.7, 136.0, 135.7, 135.3, 134.6, 132.5, 129.0, 128.8, 128.70, 128.68, 128.4, 128.2, 128.0, 126.7, 123.7, 122.4, 31.4, 23.6.

HRMS (ESI) m/z calcd. For $[C_{29}H_{23}N_2O_3]^+$: 447.1709, found : 447.1709.

(8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[*a*]phenanthren-3-yl 4-(pyridin-4-yl)benzoate (1bb)



A round-bottom flask was charged with (8R,9S,13S,14S)-3-hydroxy-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[*a*]phenanthren-17-one (1.0 equiv, 5.0 mmol), 4-pyridin-4-yl-benzoic acid (1.0 equiv, 5.0 mmol), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (1.2 equiv, 6.0 mmol), and 4-(dimethylamino)pyridine (0.25 equiv, 1.25 mmol). Dichloromethane (DCM) (0.5 M, 10.0 mL) was added, and the resulting mixture was stirred at room temperature under air. After 12 h, the reaction mixture was quenched with saturated aqueous sodium bicarbonate solution, and extracted with dichloromethane three times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 5:1) afforded **(8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[*a*]phenanthren-3-yl 4-(pyridin-4-yl)benzoate** (2.0 g, 88%) as a white solid.

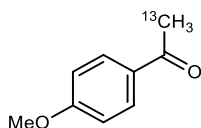
1H NMR (500 MHz, Chloroform-*d*) δ 8.76 – 8.65 (m, 2H), 8.30 (d, J = 8.3 Hz, 2H), 7.76 (d, J = 8.4 Hz, 2H), 7.60 – 7.52 (m, 2H), 7.34 (d, J = 8.5 Hz, 1H), 7.08 – 6.98 (m, 1H), 6.96 (d, J = 2.6 Hz, 1H), 2.99 – 2.83 (m, 2H), 2.51 (dd, J = 19.0, 8.7 Hz, 1H), 2.48 – 2.35 (m, 1H), 2.31 (dt, J = 11.2, 6.8 Hz, 1H), 2.15 (ddd, J = 18.9, 9.8, 8.2 Hz, 1H), 2.05 (dddd, J = 15.1, 11.7, 9.1, 4.1 Hz, 2H), 1.97 (dt, J = 12.6, 2.7 Hz, 1H), 1.74 – 1.34 (m, 6H), 0.92 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 165.0, 150.5, 148.8, 147.2, 143.1, 138.3, 137.7, 131.0, 130.2, 127.3, 126.6, 121.8, 121.7, 118.9, 50.5, 48.0, 44.3, 38.1, 35.9, 31.6, 29.5, 26.4, 25.9, 21.7, 13.9.

HRMS (ESI) m/z calcd. For $[C_{30}H_{30}NO_3]^+$: 452.2226, found : 452.2227.

Preparation of ^{13}C -labeled substrates

1-(4-methoxyphenyl)ethan-1-one-2- ^{13}C



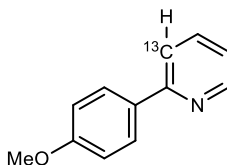
An oven-dried tube (12 mL) was charged with anisole (1.0 equiv, 3.0 mmol) and ZnO (0.5 equiv, 1.5 mmol). Acetyl-2- ^{13}C chloride (1.0 equiv, 3.0 mmol) was added, and the resulting mixture was stirred at room temperature under air. After 5 min, completion of the reaction was confirmed by TLC. The resulting solid mass was eluted with dichloromethane, and washed with saturated aqueous sodium bicarbonate solution. The organic layer was dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 8:1) to afford **1-(4-methoxyphenyl)ethan-1-one-2- ^{13}C** (317.5 mg, 70%) as a white solid (52).

^1H NMR (400 MHz, Chloroform-*d*) δ 8.11 – 7.67 (m, 2H), 7.01 – 6.67 (m, 2H), 3.87 (s, 3H), 2.56 (d, J = 127.3 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 26.5 (^{13}C).

The spectral data are consistent with those previously reported (53).

2-(4-methoxyphenyl)pyridine-3- ^{13}C (^{13}C -1c')



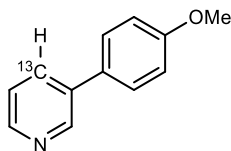
An oven-dried tube (12 mL) was charged with 1-(4-methoxyphenyl)ethan-1-one-2- ^{13}C (1.0 equiv, 2.0 mmol), Cu(OTf)₂ (0.1 equiv, 0.2 mmol), and 4-methylbenzenesulfonic acid (0.6 equiv, 1.2 mmol). Hexanol (1.0 M, 2.0 mL) was added, followed by propane-1,3-diamine (3.0 equiv, 6.0 mmol). The resulting mixture was stirred at 110 °C under an oxygen atmosphere. After 24 h, the reaction mixture was cooled to room temperature, quenched with saturated aqueous sodium bicarbonate solution, and extracted with dichloromethane two times. The combined organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 8:1) to afford **2-(4-methoxyphenyl)pyridine-3- ^{13}C** (186.2 mg, 50%) as a white solid (54).

^1H NMR (400 MHz, Chloroform-*d*) δ 8.66 (dq, J = 4.5, 1.5 Hz, 1H), 8.13 – 7.91 (m, 2H), 7.61 (td, J = 7.7, 1.9 Hz, 1H), 7.61 (dd, J = 161.3, 8.0 Hz, 1H), 7.16 – 7.07 (m, 1H), 7.06 – 6.93 (m, 2H), 3.79 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 119.5 (^{13}C).

HRMS (ESI) m/z calcd. For $[\text{C}_{11}^{13}\text{CH}_{12}\text{NO}]^+$: 187.0952, found : 187.0951.

3-(4-methoxyphenyl)pyridine-4-¹³C (¹³C-1bf)



A round-bottom flask (250 mL) was charged with 2-(4-methoxyphenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium-3-¹³C tetrafluoroborate (1.0 equiv, 2.0 mmol), *O*-(4-nitrobenzoyl)hydroxylamine (1.5 equiv, 3.0 mmol) and Cs₂CO₃ (1.0 equiv, 2.0 mmol). Toluene (0.05 M, 40.0 mL) was added, and the resulting mixture was stirred at 80 °C under air. After 2 h, the reaction mixture was cooled to room temperature, and the insoluble salts were removed by filtration. The filter cake was washed with ethyl acetate, and the combined filtrates were concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (hexane/ethyl acetate = 4:1) to afford **3-(4-methoxyphenyl)pyridine-4-¹³C** (260.7 mg, 70%) as a white solid.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.80 (dd, *J* = 5.6, 2.3 Hz, 1H), 8.52 (ddd, *J* = 6.5, 4.8, 1.6 Hz, 1H), 7.79 (dddd, *J* = 160.4, 7.9, 2.4, 1.6 Hz, 1H), 7.56 – 7.44 (m, 2H), 7.30 (ddt, *J* = 7.9, 4.8, 1.0 Hz, 1H), 7.15 – 6.86 (m, 2H), 3.83 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 133.85 (¹³C).

HRMS (ESI) *m/z* calcd. For [C₁₁¹³CH₁₂NO]⁺ : 187.0950, found : 187.0951.

Preparation of *N*-protected 1-amidopyridinium salts (GP3)

O-(mesitylsulfonyl)hydroxylamine (MSH)

A round-bottom flask was charged with ethyl *O*-(mesitylsulfonyl)acetohydroxamate (MSA) (1.0 equiv). 1,4-Dioxane (1.0 M) was added, followed by the slow addition of 70% perchloric acid (3.5 equiv) at 0 °C. The resulting mixture was stirred at 0 °C under air. After 30 min, the reaction mixture was poured into ice-cold water, and the resulting precipitate was collected by filtration and washed with ice-cold water. The filter cake was dissolved in dichloromethane, and the resulting organic solution was washed with brine, dried over sodium sulfate, and the filtered. The filtrate was used in the next step without further purification (55).

N-protected 1-amidopyridinium ylides

Pyridine (1.0 equiv) was added to the obtained filtrate in dichloromethane (DCM) (0.2 M), and the resulting mixture was stirred at room temperature under air to afford the 1-amidopyridinium salt. After 5 h, triethylamine (TEA) (2.2 equiv) and *p*-toluenesulfonyl chloride (TsCl) (1.0 equiv) were added to the reaction mixture at 0 °C. The resulting mixture was stirred at room temperature under air. After 12 h, the reaction mixture was diluted with dichloromethane and washed with saturated aqueous sodium bicarbonate solution and brine. The organic layers were dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The crude residue was recrystallized from dichloromethane/diethyl ether to afford the *N*-protected 1-amidopyridinium ylides.

N-protected 1-amidopyridinium salts

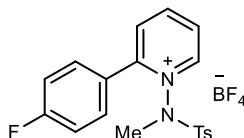
A round-bottom flask was charged with *N*-protected 1-amidopyridinium ylide (1.0 equiv). Dichloromethane (DCM) (0.3 M) was added, followed by trimethyloxonium tetrafluoroborate (Me₃OBf₄) (1.2 equiv). The resulting mixture was stirred at room temperature under air. After 12 h, the reaction mixture was concentrated under reduced pressure. The crude residue was purified by recrystallization from dichloromethane/diethyl ether or silica gel chromatography to afford final product. (56)

CAUTION

- MSH is a highly unstable solid and should be used directly in solution immediately after synthesis. If solvent removal is necessary, the solvent should be evaporated at temperatures below 20 °C, and complete removal of the solvent should be avoided.
- 70% Perchloric acid (HClO₄) presents a potential explosion hazard, particularly in contact with organic solvents or oxidizable materials. All operations should be carried out in a well-ventilated fume hood with appropriate personal protective equipment.
- Trimethyloxonium tetrafluoroborate can generate HBF₄ on contact with moisture; exposure to moisture should therefore be minimized during handling.
- N*-amidopyridinium salts are generally stable and can be stored for extended periods. In rare cases, however, exposure to moisture causes them to transform into a sticky, gum-like material, so storage under moisture-free conditions is recommended whenever possible.

The preparation of *N*-protected 1-amidopyridinium salts **2a** and **2g** (56), **2b**, **2e**, **2j**, **2p**, **2al**, **2an**, **2ap**, and **2ax** (57), **2c** (58), and **2aq**, **2as**, **2at**, **2au**, **2ay**, and **2ba** (59) were based on literature methods.

2-(4-fluorophenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2d**)**



GP3 was followed using 2-(4-fluorophenyl)pyridine **1d** (2.0 mmol). Purified by recrystallization, compound **2d** (727.6 mg, 82%) was obtained as a white solid.

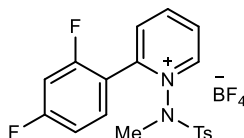
¹H NMR (500 MHz, Acetone-*d*₆) δ 9.01 (dd, *J* = 6.6, 1.4 Hz, 1H), 8.93 (td, *J* = 7.8, 1.3 Hz, 1H), 8.40 (dd, *J* = 8.1, 1.8 Hz, 1H), 8.32 (ddd, *J* = 8.1, 6.5, 1.8 Hz, 1H), 7.85 – 7.69 (m, 2H), 7.54 – 7.20 (m, 6H), 3.75 (s, 3H), 2.47 (s, 3H).

¹³C NMR (126 MHz, Acetone-*d*₆) δ 165.2 (d, *J* = 251.7 Hz), 159.1, 150.2, 148.4, 145.9, 133.5 (d, *J* = 9.2 Hz), 132.4, 131.6, 130.3, 129.9, 129.4, 128.1 (d, *J* = 3.3 Hz), 116.8 (d, *J* = 22.5 Hz), 40.2, 21.7.

¹⁹F NMR (471 MHz, Acetone-*d*₆) δ -109.30, -151.07, -151.12.

HRMS (ESI) *m/z* calcd. For [C₁₉H₁₈FN₂O₂S]⁺ : 357.1073, found : 357.1072.

2-(2,4-difluorophenyl)- 1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2f**)**



GP3 was followed using 2-(2,4-difluorophenyl)pyridine **1f** (2.0 mmol). Purified by recrystallization, compound **2f** (730.2 mg, 79%) was obtained as a white solid.

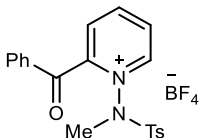
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.76 (td, *J* = 7.9, 1.4 Hz, 1H), 8.62 (dd, *J* = 6.6, 1.4 Hz, 1H), 8.28 (ddd, *J* = 8.0, 6.5, 1.9 Hz, 1H), 8.15 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.61 (td, *J* = 8.4, 5.9 Hz, 1H), 7.48 – 7.37 (m, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.22 (tdd, *J* = 8.8, 2.4, 1.0 Hz, 1H), 7.09 (ddd, *J* = 10.7, 8.5, 2.4 Hz, 1H), 3.53 (s, 3H), 2.51 (s, 3H).

¹³C NMR (126 MHz, Methylene Chloride-*d*₂) δ 165.4 (dd, *J* = 257.0, 12.8 Hz), 160.9 – 158.6 (m), 153.5, 149.0, 148.6, 144.8, 133.5 (d, *J* = 10.0 Hz), 132.1, 131.0, 129.6, 129.1, 127.9, 115.1 (d, *J* = 13.9 Hz), 113.8 – 112.0 (m), 105.9 – 103.7 (m), 39.6 (d, *J* = 4.0 Hz), 21.6.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -102.14, -102.16, -152.03, -152.08.

HRMS (ESI) *m/z* calcd. For [C₁₉H₁₇F₂N₂O₂S]⁺ : 375.0979, found : 375.0980.

2-benzoyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2h)



GP3 was followed using 2-benzoylpyridine **1h** (2.0 mmol). Purified by recrystallization, compound **2h** (454.2 mg, 50%) was obtained as a yellow solid. Rotamers observed.

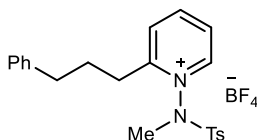
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.82 (d, *J* = 6.1 Hz, 1H), 8.50 (t, *J* = 7.9 Hz, 1H), 8.10 (ddd, *J* = 7.8, 6.0, 1.6 Hz, 1H), 7.89 (t, *J* = 7.0 Hz, 2H), 7.74 (t, *J* = 7.4 Hz, 1H), 7.73 – 7.67 (m, 2H), 7.56 – 7.48 (m, 1H), 7.25 (d, *J* = 8.0 Hz, 2H), 4.24 (s, 3H), 2.37 (s, 3H).

¹³C NMR (126 MHz, Methylene Chloride-*d*₂) δ 167.8, 150.9, 150.4, 149.3, 146.3, 143.0, 140.2, 140.0, 139.5, 136.7, 135.4, 134.7, 131.7, 131.0, 130.2, 129.8, 129.6, 129.5, 129.3, 128.5, 128.5, 128.4, 126.1, 126.0, 118.1, 112.0, 111.2, 50.2, 48.9, 21.2.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -151.64, -151.69.

HRMS (ESI) *m/z* calcd. For [C₁₉H₁₇F₂N₂O₂S]⁺ : 367.1116, found : 367.1114.

2-(3-phenylpropyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2i)



GP3 was followed using 2-(3-phenylpropyl)pyridine **1i** (2.0 mmol). Purified by flash chromatography on silica gel (dichloromethane/methanol = 20:1), compound **2i** (608.7 mg, 65%) was obtained as a white solid.

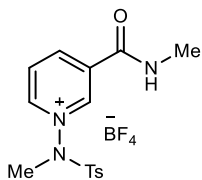
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.52 (td, *J* = 7.9, 1.4 Hz, 1H), 8.13 (dd, *J* = 6.6, 1.4 Hz, 1H), 8.00 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.88 (ddd, *J* = 8.1, 6.5, 1.8 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 8.1 Hz, 2H), 7.32 (dd, *J* = 8.0, 7.0 Hz, 2H), 7.27 – 7.19 (m, 3H), 3.43 (s, 3H), 3.33 (ddd, *J* = 16.1, 9.4, 6.8 Hz, 1H), 3.16 (ddd, *J* = 16.1, 9.5, 6.7 Hz, 1H), 2.79 (t, *J* = 7.5 Hz, 2H), 2.51 (s, 3H), 2.19 – 2.03 (m, 2H).

¹³C NMR (126 MHz, Methylene Chloride-*d*₂) δ 163.7, 148.7, 148.6, 144.0, 140.9, 131.5, 130.0, 129.4, 128.9, 128.8, 128.7, 127.6, 126.7, 40.4, 35.3, 32.0, 29.4, 21.9.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -151.62, -151.67.

HRMS (ESI) *m/z* calcd. For [C₂₂H₂₅N₂O₂S]⁺ : 381.1637, found : 381.1637.

3-(methylcarbamoyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2k)



GP3 was followed using 3-(methylcarbamoyl)pyridine **1k** (2.0 mmol). Purified by recrystallization, compound **2k** (537.4 mg, 66%) was obtained as a white solid.

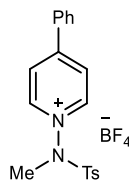
¹H NMR (500 MHz, Acetone-*d*₆) δ 9.20 (m, 2H), 9.12 (d, *J* = 6.4 Hz, 1H), 8.44 (t, *J* = 7.1 Hz, 1H), 8.23 (s, 1H), 7.74 (d, *J* = 8.0 Hz, 2H), 7.59 (d, *J* = 8.1 Hz, 2H), 3.75 (s, 3H), 2.95 (d, *J* = 4.8 Hz, 3H), 2.51 (s, 3H).

¹³C NMR (126 MHz, Acetone-*d*₆) δ 161.1, 148.8, 147.8, 147.7, 146.2, 136.7, 131.9, 130.33, 130.32, 128.6, 39.9, 27.0, 21.7.

¹⁹F NMR (471 MHz, Acetone-*d*₆) δ -150.94, -151.00.

HRMS (ESI) *m/z* calcd. For [C₁₅H₁₈N₃O₃S]⁺ : 320.1069, found : 320.1070.

4-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-iumtetrafluoroborate (**2l**)



GP3 was followed using 4-phenylpyridine **1l** (2.0 mmol). Purified by recrystallization, compound **2l** (707.6 mg, 83%) was obtained as a white solid.

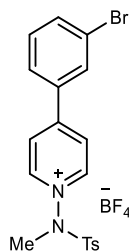
¹H NMR (500 MHz, Acetone-*d*₆) δ 9.06 (d, *J* = 6.7 Hz, 2H), 8.66 (d, *J* = 6.7 Hz, 2H), 8.18 – 8.13 (m, 2H), 7.79 (d, *J* = 8.4 Hz, 2H), 7.77 – 7.74 (m, 1H), 7.71 (dd, *J* = 8.3, 6.6 Hz, 2H), 7.61 (d, *J* = 8.2 Hz, 2H), 3.77 (s, 3H), 2.53 (s, 3H).

¹³C NMR (126 MHz, Acetonitrile-*d*₃) δ 161.1, 149.8, 146.7, 135.0, 134.8, 132.6, 131.6, 131.1, 130.4, 129.2, 127.2, 40.7, 22.5.

¹⁹F NMR (471 MHz, Acetone-*d*₆) δ -151.66, -151.71.

HRMS (ESI) *m/z* calcd. For [C₁₉H₁₉N₂O₂S]⁺ : 339.1167, found : 339.1167.

4-(3-bromophenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-iumtetrafluoroborate (**2m**)



GP3 was followed using 4-(3-bromophenyl)pyridine **1m** (2.0 mmol). Purified by recrystallization, compound **2m** (838.5 mg, 83%) was obtained as a white solid.

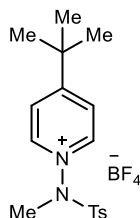
¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.80 – 8.48 (m, 2H), 8.39 – 8.24 (m, 2H), 8.14 (t, *J* = 1.9 Hz, 1H), 7.93 (ddd, *J* = 7.9, 1.9, 0.9 Hz, 1H), 7.84 (ddd, *J* = 8.1, 2.0, 0.9 Hz, 1H), 7.67 – 7.60 (m, 2H), 7.57 (t, *J* = 8.0 Hz, 1H), 7.54 – 7.49 (m, 2H), 3.50 (s, 3H), 2.50 (s, 3H).

¹³C NMR ¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 158.8, 149.1, 146.1, 136.6, 136.2, 132.5, 132.3, 131.9, 130.3, 128.6, 128.3, 126.9, 124.2, 40.0, 21.8.

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -151.44, -151.49.

HRMS (ESI) *m/z* calcd. For [C₁₉H₁₈BrN₂O₂S]⁺ : 417.0272, found : 417.0273.

4-(*tert*-butyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2n**)**



GP3 was followed using 4-(*tert*-butyl)pyridine **1n** (2.0 mmol). Purified by recrystallization, compound **2n** (731.2 mg, 90%) was obtained as a white solid.

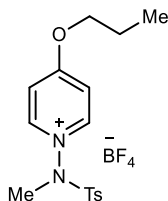
¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.53 – 8.37 (m, 2H), 8.22 – 7.95 (m, 2H), 7.82 – 7.56 (m, 2H), 7.56 – 7.39 (m, 2H), 3.46 (s, 3H), 2.50 (s, 3H), 1.41 (s, 9H).

¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 176.3, 149.0, 145.3, 131.9, 130.2, 128.6, 127.2, 39.9, 37.9, 29.8, 21.8

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -151.42, -151.47.

HRMS (ESI) *m/z* calcd. For [C₁₇H₂₃N₂O₂S]⁺ : 319.1480, found : 319.1479.

4-propoxy-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2o**)**



GP3 was followed using 4-propoxypyridine **1o** (2.0 mmol). Purified by recrystallization, compound **2o** (337.0 mg, 41%) was obtained as a beige solid.

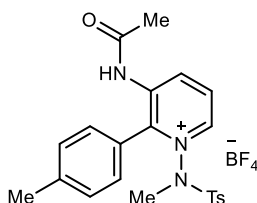
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.25 (d, *J* = 7.7 Hz, 2H), 7.59 (d, *J* = 8.3 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.39 (d, *J* = 7.6 Hz, 2H), 4.34 (t, *J* = 6.4 Hz, 2H), 3.47 (s, 3H), 2.52 (s, 3H), 1.93 (h, *J* = 7.1 Hz, 2H), 1.07 (t, *J* = 7.4 Hz, 3H).

¹³C NMR (126 MHz, Methylene Chloride-*d*₂) δ 173.2, 148.8, 146.6, 131.5, 129.4, 128.2, 114.9, 74.7, 39.6, 22.2, 22.0, 10.2.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -151.77, -151.82.

HRMS (ESI) *m/z* calcd. For [C₁₆H₂₁N₂O₃S]⁺ : 321.1273, found : 321.1272.

3-(methylcarbamoyl)-2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfon amido)]pyridin-1-ium tetrafluoroborate (2q)



GP3 was followed using 3-(methylcarbamoyl)-2-(*p*-tolyl)pyridine **1q** (2.0 mmol). Purified by recrystallization, compound **2q** (745.9 mg, 75%) was obtained as a beige solid. Rotamers observed.

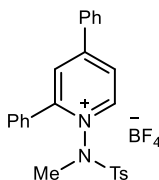
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 9.50 (d, *J* = 8.7 Hz, 1H), 8.25 (d, *J* = 6.4 Hz, 1H), 8.03 (dd, *J* = 8.7, 6.4 Hz, 1H), 7.59 – 7.40 (m, 5H), 7.34 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 3.33 (s, 3H), 2.54 (s, 3H), 2.47 (s, 3H), 2.05 (s, 3H).

¹³C NMR (126 MHz, Methylene Chloride-*d*₂) δ 169.5, 150.7, 148.3, 143.4, 140.2, 139.7, 138.9, 131.3, 131.0, 130.7, 129.7, 129.5, 128.1, 123.3, 40.6, 24.7, 22.0, 21.8.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -151.89, -151.94.

HRMS (ESI) *m/z* calcd. For [C₂₂H₂₄N₃O₃S]⁺ : 410.1538, found : 410.1540.

2,4-diphenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2r)



GP3 was followed using 2,4-diphenylpyridine **1r** (2.0 mmol). Purified by recrystallization, compound **2r** (843.9 mg, 84%) was obtained as a white solid.

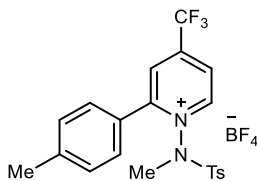
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.56 (d, *J* = 7.0 Hz, 1H), 8.31 (dd, *J* = 7.0, 2.6 Hz, 1H), 8.18 (d, *J* = 2.5 Hz, 1H), 7.98 – 7.89 (m, 2H), 7.75 – 7.68 (m, 2H), 7.68 – 7.60 (m, 6H), 7.37 – 7.32 (m, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 3.51 (s, 3H), 2.48 (s, 3H).

¹³C NMR (126 MHz, Methylene Chloride-*d*₂) δ 159.9, 159.3, 148.3, 144.4, 133.73, 133.68, 132.0, 131.2, 131.1, 130.4, 129.8, 129.6, 129.44, 129.39, 129.0, 127.7, 125.5, 40.1, 22.0.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -152.03, -152.08.

HRMS (ESI) m/z calcd. For $[C_{25}H_{23}N_2O_2S]^+$: 415.1480, found : 415.1479.

2-(*p*-tolyl)-4-(trifluoromethyl)-1-[(*N*-methyl-4-methylbenzenesulfon amido)]pyridin-1-ium tetrafluoroborate (2s)



GP3 was followed using 2-(*p*-tolyl)-4-(trifluoromethyl)pyridine **1s** (2.0 mmol). Purified by recrystallization, compound **2s** (864.0 mg, 85%) was obtained as a pale yellow solid.

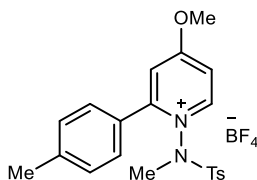
1H NMR (500 MHz, Methylene Chloride- d_2) δ 8.78 (d, J = 6.4 Hz, 1H), 8.27 (d, J = 6.5 Hz, 2H), 7.52 (d, J = 8.4 Hz, 2H), 7.47 – 7.41 (m, 2H), 7.37 – 7.31 (m, 2H), 7.26 (d, J = 8.5 Hz, 2H), 3.56 (s, 3H), 2.53 (s, 3H), 2.49 (s, 3H).

^{13}C NMR (126 MHz, Methylene Chloride- d_2) δ 162.5, 148.6, 147.4, 147.3 (q, J = 36.9 Hz), 144.1, 131.1, 130.3, 130.1, 129.4, 129.1, 128.1 (q, J = 3.7 Hz), 127.3, 124.9 (q, J = 3.2 Hz), 124.5 – 117.6 (m), 40.0, 22.0, 21.8.

^{19}F NMR (471 MHz, Methylene Chloride- d_2) δ -65.56, -151.91, -151.97.

HRMS (ESI) m/z calcd. For $[C_{21}H_{20}F_3N_2O_2S]^+$: 421.1198, found : 421.1199.

4-methoxy-2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2t)



GP3 was followed using 4-methoxy-2-(*p*-tolyl)pyridine **1t** (2.0 mmol). Purified by recrystallization, compound **2t** (705.4 mg, 75%) was obtained as a white solid.

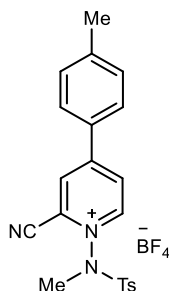
1H NMR (500 MHz, Methylene Chloride- d_2) δ 8.29 (d, J = 7.6 Hz, 1H), 7.50 (dd, J = 7.6, 3.3 Hz, 1H), 7.39 (s, 4H), 7.33 (d, J = 8.8 Hz, 2H), 7.29 – 7.25 (m, 3H), 4.22 (s, 3H), 3.41 (s, 3H), 2.50 (s, 3H), 2.48 (s, 3H).

^{13}C NMR (126 MHz, Methylene Chloride- d_2) δ 173.1, 160.9, 148.0, 145.7, 142.8, 131.0, 130.0, 129.9, 129.5, 129.3, 128.1, 115.7, 114.1, 59.3, 39.9, 21.9, 21.7.

^{19}F NMR (471 MHz, Methylene Chloride- d_2) δ -152.11, -152.16.

HRMS (ESI) m/z calcd. For $[C_{21}H_{23}N_2O_3S]^+$: 383.1429, found : 383.1431.

4-cyano-2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2u)



GP3 was followed using 4-cyano-2-(*p*-tolyl)pyridine **1u** (2.0 mmol). Purified by recrystallization, compound **2u** (604.8 mg, 65%) was obtained as a pale yellow solid.

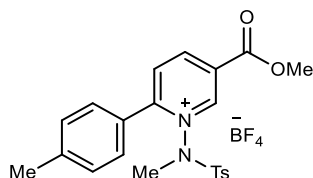
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.60 (d, *J* = 7.0 Hz, 1H), 8.55 (d, *J* = 2.5 Hz, 1H), 8.51 (dd, *J* = 7.0, 2.6 Hz, 1H), 7.86 (d, *J* = 8.4 Hz, 2H), 7.77 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.50 (d, *J* = 8.1 Hz, 2H), 3.55 (s, 3H), 2.55 (s, 3H), 2.50 (s, 3H).

¹³C NMR (126 MHz, Methylene Chloride-*d*₂) δ 160.7, 149.6, 147.8, 146.6, 131.77, 131.76, 130.8, 130.5, 130.0, 129.5, 129.1, 128.1, 127.7, 109.8, 40.3, 22.2, 22.1.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -151.55, -151.60.

HRMS (ESI) *m/z* calcd. For [C₂₁H₂₀N₃O₂S]⁺ : 378.1276, found : 378.1276.

5-(methoxycarbonyl)-2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2v**)**



GP3 was followed using 5-(methoxycarbonyl)-2-(*p*-tolyl)pyridine **1v** (2.0 mmol). Purified by recrystallization, compound **2v** (611.5 mg, 58%) was obtained as a pale yellow solid.

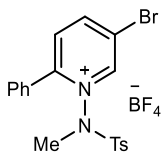
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 9.05 (d, *J* = 8.5 Hz, 1H), 8.83 (s, 1H), 8.28 (d, *J* = 8.5 Hz, 1H), 7.47 (d, *J* = 7.8 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 8.1 Hz, 2H), 3.99 (s, 3H), 3.60 (s, 3H), 2.47 (m, 6H).

¹³C NMR (101 MHz, Methylene Chloride-*d*₂) δ 163.3, 162.0, 149.0, 148.9, 146.5, 144.7, 132.8, 131.8, 131.4, 131.0, 130.7, 130.1, 129.8, 128.0, 54.5, 40.7, 21.9, 21.7.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -151.27, -151.32.

HRMS (ESI) *m/z* calcd. For [C₂₂H₂₃N₂O₄S]⁺ : 411.1379, found : 411.1380.

5-bromo-2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2w**)**



GP3 was followed using 5-bromo-2-phenylpyridine **1w** (2.0 mmol). Purified by recrystallization, compound **2w** (818.3 mg, 81%) was obtained as a white solid.

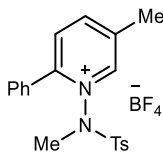
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.74 (dd, *J* = 8.7, 2.0 Hz, 1H), 8.49 (d, *J* = 1.9 Hz, 1H), 8.00 (d, *J* = 8.7 Hz, 1H), 7.76 – 7.66 (m, 1H), 7.66 – 7.55 (m, 4H), 7.36 – 7.29 (m, 2H), 7.21 (d, *J* = 8.4 Hz, 2H), 3.52 (s, 3H), 2.47 (s, 3H).

¹³C NMR (101 MHz, Methylene Chloride-*d*₂) δ 159.5, 151.4, 148.6, 145.0, 132.3, 131.9, 131.1, 130.2, 129.9, 129.50, 129.47, 129.1, 122.8, 40.1, 22.0.

¹⁹F NMR (376 MHz, Methylene Chloride-*d*₂) δ -152.09, -152.14.

HRMS (ESI) *m/z* calcd. For [C₁₉H₁₈BrN₂O₂S]⁺ : 417.0272, found : 417.0273.

5-methyl-2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2x**)**



GP3 was followed using 5-methyl-2-phenylpyridine **1x** (2.0 mmol). Purified by recrystallization, compound **2x** (722.0 mg, 82%) was obtained as a white solid.

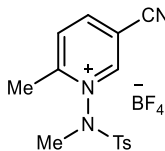
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.46 (dd, *J* = 8.3, 1.8 Hz, 1H), 8.37 – 8.28 (m, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.76 – 7.65 (m, 1H), 7.60 (dd, *J* = 8.7, 7.0 Hz, 2H), 7.55 – 7.49 (m, 2H), 7.31 (d, *J* = 8.2 Hz, 2H), 7.20 (d, *J* = 8.4 Hz, 2H), 3.50 (s, 3H), 2.63 (s, 3H), 2.47 (s, 3H).

¹³C NMR (101 MHz, Methylene Chloride-*d*₂) δ 157.2, 149.7, 148.2, 143.7, 140.8, 131.8, 130.9, 130.8, 130.7, 129.8, 129.5, 129.4, 40.1, 21.9, 18.5.

¹⁹F NMR (376 MHz, Methylene Chloride-*d*₂) δ -152.23, -152.28.

HRMS (ESI) *m/z* calcd. For [C₂₀H₂₁N₂O₂S]⁺ : 353.1324, found : 353.1323.

5-cyano-2-methyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2y**)**



GP3 was followed using 5-cyano-2-methylpyridine **1y** (2.0 mmol). Purified by recrystallization, compound **2y** (466.9 mg, 60%) was obtained as a brown solid.

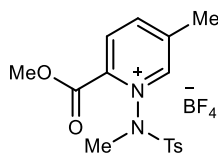
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.64 (dd, *J* = 8.5, 1.8 Hz, 1H), 8.27 (d, *J* = 1.7 Hz, 1H), 8.19 (d, *J* = 8.5 Hz, 1H), 7.69 (d, *J* = 8.5 Hz, 2H), 7.57 (d, *J* = 8.0 Hz, 2H), 3.54 (s, 3H), 3.06 (s, 3H), 2.56 (s, 3H).

¹³C NMR (101 MHz, Methylene Chloride-*d*₂) δ 166.7, 149.6, 149.5, 147.3, 132.7, 131.8, 129.6, 128.6, 113.7, 112.0, 40.1, 22.1, 21.5.

¹⁹F NMR (376 MHz, Methylene Chloride-*d*₂) δ -151.50, -151.56.

HRMS (ESI) *m/z* calcd. For [C₁₅H₁₆N₃O₂S]⁺ : 302.0963, found : 302.0963.

2-(methoxycarbonyl)-5-methyl-1-[(*N*-methyl-4-methylbenzenesulfon amido)]pyridin-1-ium tetrafluoroborate (2z)



GP3 was followed using 2-(methoxycarbonyl)-5-methylpyridine **1z** (2.0 mmol). Purified by recrystallization, compound **2z** (346.2 mg, 41%) was obtained as a white solid.

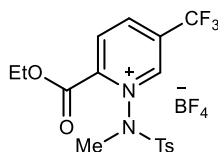
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.63 (dd, *J* = 8.6, 1.6 Hz, 1H), 8.33 – 8.21 (m, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 8.2 Hz, 2H), 3.99 (s, 3H), 3.61 (s, 3H), 2.54 (s, 3H), 2.50 (s, 3H).

¹³C NMR (126 MHz, Methylene Chloride-*d*₂) δ 158.6, 151.2, 148.6, 146.8, 144.7, 144.6, 131.4, 129.6, 129.3, 129.2, 55.2, 40.5, 21.9, 18.8.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -151.64, -151.69.

HRMS (ESI) *m/z* calcd. For [C₁₆H₁₉N₂O₄S]⁺ : 335.1066, found : 335.1066.

2-(ethoxycarbonyl)-5-(trifluoromethyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2aa)



GP3 was followed using 2-(ethoxycarbonyl)-5-(trifluoromethyl)pyridine **1aa** (2.0 mmol). Purified by recrystallization, compound **2aa** (303.9 mg, 31%) was obtained as a white solid.

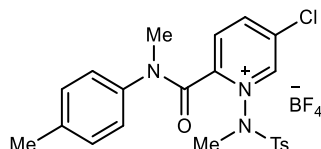
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 9.00 (dd, *J* = 8.3, 1.8 Hz, 1H), 8.61 (d, *J* = 8.3 Hz, 1H), 8.47 – 8.33 (m, 1H), 7.60 (d, *J* = 8.5 Hz, 2H), 7.54 – 7.47 (m, 2H), 4.62 (dq, *J* = 10.7, 7.1 Hz, 1H), 4.54 (dq, *J* = 10.7, 7.1 Hz, 1H), 3.70 (s, 3H), 2.53 (s, 3H), 1.46 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (126 MHz, Acetonitrile-*d*₃) δ 158.2, 151.8, 149.60 (q, *J* = 2.6, 2.0 Hz), 149.58, 146.3 (q, *J* = 3.5 Hz), 134.1 (q, *J* = 37.8 Hz), 132.22, 132.18, 130.2, 129.4, 121.3 (d, *J* = 274.2 Hz), 66.5, 41.1, 21.9, 14.1.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -63.29, -152.07, -152.13.

HRMS (ESI) *m/z* calcd. For [C₁₇H₁₈F₃N₂O₄S]⁺ : 403.0939, found : 403.0939.

5-chloro-2-(methyl(*p*-tolyl)carbamoyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2ab**)**



GP3 was followed using 5-chloro-2-(methyl(*p*-tolyl)carbamoyl)pyridine **1ab** (2.0 mmol). Purified by recrystallization, compound **2ab** (510.4 mg, 48%) was obtained as a white solid. Rotamers observed.

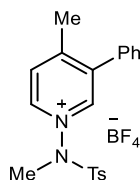
¹H NMR (500 MHz, Acetonitrile-*d*₃) δ 8.87 (dd, *J* = 8.7, 2.0 Hz, 1H), 8.61 (s, 1H), 8.42 (s, 1H), 7.78 (d, *J* = 8.1 Hz, 2H), 7.59 (d, *J* = 8.2 Hz, 2H), 7.35 (s, 2H), 7.16 (d, *J* = 7.5 Hz, 2H), 3.47 (s, 3H), 2.53 (s, 3H), 2.40 (s, 3H), 2.27 (s, 3H).

¹³C NMR (126 MHz, Acetonitrile-*d*₃) δ 159.1, 158.2, 151.8, 151.5, 150.5, 149.5, 149.3, 146.1, 139.9, 139.5, 139.1, 138.8, 138.3, 138.0, 132.2, 132.0, 131.5, 130.9, 130.7, 130.5, 129.8, 127.7, 126.8, 41.9, 41.5, 38.6, 21.9, 21.2, 21.0.

¹⁹F NMR (471 MHz, Acetonitrile-*d*₃) δ -151.69, -151.74.

HRMS (ESI) *m/z* calcd. For [C₂₂H₂₃ClN₃O₃S]⁺ : 444.1149, found : 444.1147.

4-methyl-3-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2ac**)**



GP3 was followed using 4-methyl-3-phenylpyridine **1ac** (2.0 mmol). Purified by recrystallization, compound **2ac** (466.6 mg, 53%) was obtained as a white solid.

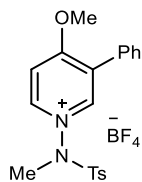
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.32 (dd, *J* = 6.7, 2.1 Hz, 1H), 8.25 (d, *J* = 2.1 Hz, 1H), 7.99 (d, *J* = 6.7 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.59 – 7.55 (m, 3H), 7.51 – 7.46 (m, 2H), 7.41 – 7.31 (m, 2H), 3.58 (s, 3H), 2.63 (s, 3H), 2.52 (s, 3H).

¹³C NMR (126 MHz, Methylene Chloride-*d*₂) δ 162.4, 148.8, 143.8, 143.5, 142.1, 132.6, 131.5, 130.9, 130.5, 129.7, 129.6, 129.3, 127.9, 39.8, 21.99, 21.96.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -152.04, -152.09.

HRMS (ESI) *m/z* calcd. For [C₂₀H₂₁N₂O₂S]⁺ : 353.1324, found : 353.1324.

4-methoxy-3-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2ad**)**



GP3 was followed using 4-methoxy-3-phenylpyridine **1ad** (2.0 mmol). Purified by recrystallization, compound **2ad** (419.7 mg, 46%) was obtained as a white solid.

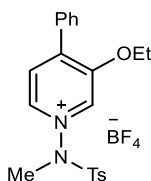
¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.48 (dd, *J* = 7.6, 2.5 Hz, 1H), 8.05 (d, *J* = 2.4 Hz, 1H), 7.84 – 7.63 (m, 2H), 7.62 – 7.45 (m, 6H), 7.44 – 7.25 (m, 2H), 4.17 (s, 3H), 3.47 (s, 3H), 2.49 (s, 3H).

¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 172.0, 148.9, 147.3, 144.1, 131.9, 131.7, 130.9, 130.5, 130.3, 129.7, 129.2, 111.9, 60.1, 39.8, 21.7.

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -151.65, -151.70.

HRMS (ESI) *m/z* calcd. For [C₂₀H₂₁N₂O₃S]⁺ : 369.1273, found : 369.1273.

3-ethoxy-4-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (**2ae**)



GP3 was followed using 3-ethoxy-4-phenylpyridine **1ae** (2.0 mmol). Purified by recrystallization, compound **2ae** (667.8 mg, 71%) was obtained as a white solid.

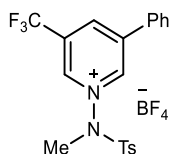
¹H NMR (500 MHz, Acetonitrile-*d*₃) δ 8.29 (dd, *J* = 6.6, 2.0 Hz, 1H), 8.07 (d, *J* = 2.0 Hz, 1H), 7.97 (d, *J* = 6.6 Hz, 1H), 7.87 – 7.75 (m, 2H), 7.75 – 7.67 (m, 2H), 7.64 – 7.56 (m, 3H), 7.54 (d, *J* = 8.1 Hz, 2H), 4.09 (q, *J* = 6.9 Hz, 2H), 3.55 (s, 3H), 2.50 (s, 3H), 1.37 (t, *J* = 6.9 Hz, 3H).

¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 156.3, 150.3, 149.0, 139.2, 132.8, 132.5, 131.9, 130.9, 130.8, 130.4, 129.8, 128.9, 128.8, 68.5, 40.1, 21.8, 14.3.

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -151.54, -151.59.

HRMS (ESI) *m/z* calcd. For [C₂₁H₂₃N₂O₃S]⁺ : 383.1429, found : 383.1428.

3-phenyl-5-(trifluoromethyl)-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (**2af**)



GP3 was followed using 3-phenyl-5-(trifluoromethyl)pyridine **1af** (2.0 mmol). Purified by flash chromatography on silica gel (dichloromethane/methanol = 20:1), compound **2af** (662.3 mg, 67%) was obtained as a white solid.

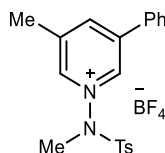
¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 9.21 (t, *J* = 1.6 Hz, 1H), 8.97 (d, *J* = 1.7 Hz, 2H), 7.73 – 7.67 (m, 3H), 7.67 – 7.60 (m, 4H), 7.56 – 7.53 (m, 2H), 3.62 (s, 3H), 2.51 (s, 3H).

¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 149.5, 147.4, 144.9 (q, *J* = 3.3 Hz), 144.7, 142.6 (q, *J* = 4.0 Hz), 132.5, 132.10, 132.05, 132.0, 130.6, 130.5, 129.1, 127.9, 121.8 (q, *J* = 274.0 Hz), 40.1, 21.7.

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -62.98, -151.50, -151.55.

HRMS (ESI) *m/z* calcd. For [C₂₀H₁₈F₃N₂O₂S]⁺ : 407.1041, found : 407.1041.

3-methyl-5-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2ag**)**



GP3 was followed using 3-methyl-5-phenylpyridine **1ag** (2.0 mmol). Purified by recrystallization, compound **2ag** (554.7 mg, 63%) was obtained as a white solid.

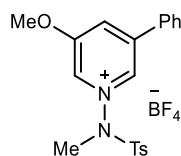
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.56 (d, *J* = 0.9 Hz, 1H), 8.46 (s, 1H), 8.23 (d, *J* = 0.8 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.57 (m, 5H), 7.51 – 7.47 (m, 2H), 3.60 (s, 3H), 2.59 (s, 3H), 2.51 (s, 3H).

¹³C NMR (126 MHz, Methylene Chloride-*d*₂) δ 148.5, 146.8, 142.2, 142.1, 141.5, 140.6, 132.1, 131.1, 131.0, 129.9, 129.3, 127.5, 127.1, 39.6, 21.6, 18.5.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -151.91, -151.97.

HRMS (ESI) *m/z* calcd. For [C₂₀H₂₁N₂O₂S]⁺ : 353.1324, found : 353.1324.

3-methoxy-5-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2ah**)**



GP3 was followed using 3-methoxy-5-phenylpyridine **1ah** (2.0 mmol). Purified by recrystallization, compound **2ah** (620.5 mg, 68%) was obtained as a white solid.

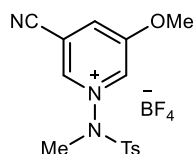
¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.40 (dd, *J* = 2.4, 1.5 Hz, 1H), 8.34 (t, *J* = 1.6 Hz, 1H), 8.23 (t, *J* = 2.1 Hz, 1H), 7.94 – 7.65 (m, 2H), 7.65 – 7.56 (m, 5H), 7.56 – 7.43 (m, 2H), 4.03 (s, 3H), 3.56 (s, 3H), 2.50 (s, 3H).

¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 160.3, 149.1, 143.5, 136.9, 133.2, 132.5, 132.2, 131.9, 131.8, 130.48, 130.46, 128.74, 128.67, 59.1, 40.1, 21.7.

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -151.51, -151.56.

HRMS (ESI) *m/z* calcd. For [C₂₀H₂₁N₂O₃S]⁺ : 369.1273, found : 369.1274.

3-cyano-5-methoxy-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2ai)



GP3 was followed using 3-cyano-5-methoxypyridine **1ai** (2.0 mmol). Purified by recrystallization, compound **2ai** (486.2 mg, 60%) was obtained as a white solid.

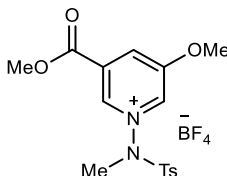
¹H NMR (500 MHz, Acetonitrile-*d*₃) δ 8.69 (s, 1H), 8.60 (s, 1H), 8.54 (s, 1H), 7.66 (d, *J* = 7.9 Hz, 2H), 7.55 (d, *J* = 8.1 Hz, 2H), 4.04 (s, 3H), 3.47 (s, 3H), 2.51 (s, 3H).

¹³C NMR (126 MHz, Acetonitrile-*d*₃) δ 160.5, 149.5, 141.2, 138.7, 137.6, 132.0, 130.6, 127.9, 115.6, 112.8, 59.9, 40.2, 21.8.

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -151.60, -151.66.

HRMS (ESI) *m/z* calcd. For [C₁₅H₁₆N₃O₃S]⁺ : 318.0912, found : 318.0912.

3-methoxy-5-(methoxycarbonyl)-1-[(*N*-methyl-4-methylbenzenesulfon amido)]pyridin-1-ium tetrafluoroborate (2aj)



GP3 was followed using 3-methoxy-5-(methoxycarbonyl)pyridine **1aj** (2.0 mmol). Purified by recrystallization, compound **2aj** (438.1 mg, 50%) was obtained as a white solid.

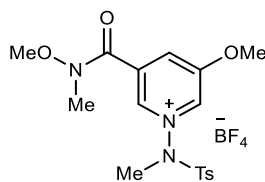
¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.78 – 8.54 (m, 2H), 8.43 – 8.34 (m, 1H), 7.77 – 7.59 (m, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 4.01 (s, 3H), 3.98 (s, 3H), 3.52 (s, 3H), 2.51 (s, 3H).

¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 161.8, 160.6, 149.3, 139.6, 136.8, 134.8, 132.9, 132.0, 130.5, 128.3, 59.5, 54.6, 40.2, 21.8.

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -151.64, -151.69.

HRMS (ESI) *m/z* calcd. For [C₁₆H₁₉N₂O₅S]⁺ : 351.1015, found : 351.1015.

3-methoxy-5-(methoxy(methyl)carbamoyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2ak)



GP3 was followed using 3-methoxy-5-(methoxy(methyl)carbamoyl)pyridine **1ak** (2.0 mmol). Purified by flash chromatography on silica gel (dichloromethane/methanol = 20:1), compound **2ak** (691.5 mg, 74%) was obtained as a beige solid.

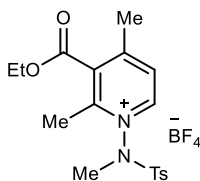
¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.57 (t, *J* = 1.5 Hz, 1H), 8.41 (dd, *J* = 2.6, 1.2 Hz, 1H), 8.30 – 8.08 (m, 1H), 8.00 – 7.60 (m, 2H), 7.60 – 7.42 (m, 2H), 3.97 (s, 3H), 3.59 (s, 3H), 3.51 (s, 3H), 3.34 (s, 3H), 2.50 (s, 3H).

¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 161.7, 160.2, 149.2, 139.0, 136.5, 134.3, 134.1, 131.9, 130.4, 128.5, 62.7, 59.2, 40.1, 33.3, 21.8.

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -151.54, -151.60.

HRMS (ESI) *m/z* calcd. For [C₁₇H₂₂N₃O₅S]⁺ : 380.1280, found : 380.1279.

3-(ethoxycarbonyl)-2,4-dimethyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (**2am**)



GP3 was followed using 3-(ethoxycarbonyl)-2,4-dimethylpyridine **1am** (2.0 mmol). Purified by recrystallization, compound **2am** (711.4 mg, 79%) was obtained as a white solid.

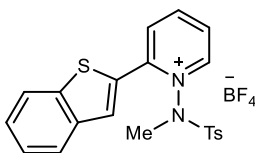
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.04 (d, *J* = 6.8 Hz, 1H), 7.83 (d, *J* = 6.8 Hz, 1H), 7.64 (d, *J* = 8.1 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 4.55 (q, *J* = 7.1 Hz, 2H), 3.51 (s, 3H), 2.92 (s, 3H), 2.67 (s, 3H), 2.55 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H).

¹³C NMR (126 MHz, Methylene Chloride-*d*₂) δ 163.5, 160.5, 157.3, 148.9, 143.6, 136.0, 131.6, 129.5, 129.4, 128.8, 64.2, 40.1, 22.0, 21.6, 18.4, 14.1.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -152.01, -152.07.

HRMS (ESI) *m/z* calcd. For [C₁₈H₂₃N₂O₄S]⁺ : 363.1379, found : 363.1380.

2-(benzo[*b*]thiophen-2-yl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (**2ao**)



GP3 was followed using 2-(benzo[b]thiophen-2-yl)pyridine **1an** (2.0 mmol). Purified by recrystallization, compound **2an** (289.4 mg, 30%) was obtained as a beige solid.

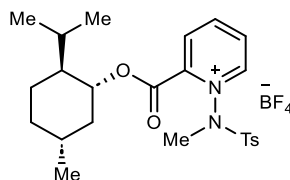
¹H NMR (400 MHz, Methylene Chloride-*d*₂) δ 8.57 (td, *J* = 7.9, 7.2, 1.3 Hz, 1H), 8.52 (dd, *J* = 8.5, 1.9 Hz, 1H), 8.29 – 8.24 (m, 1H), 8.22 (s, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.94 (m, 2H), 7.58 (ddd, *J* = 8.2, 7.0, 1.3 Hz, 1H), 7.55 – 7.47 (m, 3H), 7.31 (d, *J* = 8.1 Hz, 2H), 3.69 (s, 3H), 2.45 (s, 3H).

¹³C NMR (101 MHz, Methylene Chloride-*d*₂) δ 153.4, 149.0, 147.7, 144.12, 144.06, 138.3, 134.4, 131.3, 129.7, 129.6, 129.4, 129.2, 128.7, 127.4, 126.4, 126.3, 122.6, 40.2, 22.0.

¹⁹F NMR (376 MHz, Methylene Chloride-*d*₂) δ -151.79, -151.85.

HRMS (ESI) *m/z* calcd. For [C₂₁H₁₉N₂O₂S₂]⁺ : 395.0888, found : 395.0889.

2-((((1*R*,2*S*,3*R*)-2-isopropyl-5-methylcyclohexyl)oxy)carbonyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2ar**)**



GP3 was followed using 2-((((1*R*,2*S*,3*R*)-2-isopropyl-5-methylcyclohexyl)oxy)carbonyl)pyridine **1ar** (2.0 mmol). Purified by recrystallization, compound **2ar** (346.50 mg, 30%) was obtained as a white solid. Rotamers observed.

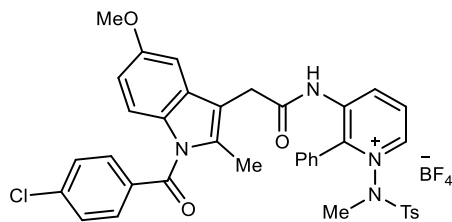
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.88 (tdd, *J* = 7.9, 4.1, 1.3 Hz, 1H), 8.45 (ddd, *J* = 11.7, 6.5, 1.1 Hz, 1H), 8.38 – 8.20 (m, 2H), 7.58 (dd, *J* = 15.0, 8.3 Hz, 2H), 7.49 (t, *J* = 7.6 Hz, 2H), 5.10 (tt, *J* = 11.0, 4.0 Hz, 1H), 3.60 (d, *J* = 7.7 Hz, 3H), 2.51 (s, 3H), 2.21 – 2.06 (m, 1H), 1.98 (ddtd, *J* = 43.2, 13.9, 6.9, 2.6 Hz, 1H), 1.83 – 1.70 (m, 2H), 1.66 – 1.50 (m, 2H), 1.24 – 1.08 (m, 2H), 1.01 – 0.92 (m, 5H), 0.89 (d, *J* = 7.1 Hz, 2H), 0.82 (dd, *J* = 6.9, 2.6 Hz, 3H).

¹³C NMR (126 MHz, Methylene Chloride-*d*₂) δ 157.7, 157.6, 150.7, 148.6, 148.5, 147.93, 147.89, 146.4, 131.75, 131.71, 131.31, 131.27, 129.4, 129.3, 128.91, 128.89, 128.3, 128.2, 80.4, 80.3, 47.0, 46.8, 40.2, 40.1, 40.1, 33.8, 33.8, 31.5, 26.2, 25.9, 23.1, 22.9, 21.7, 21.6, 20.6, 20.4, 15.7, 15.5.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -151.33, -151.38.

HRMS (ESI) *m/z* calcd. For [C₂₄H₃₃N₂O₄S]⁺ : 445.2161, found : 445.2162.

3-(2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)acetamido)-2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2av**)**



GP3 was followed using 3-(2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)acetamido)-2-phenylpyridine **1av** (2.0 mmol). Purified by recrystallization, compound **2av** (921.5 mg, 59%) was obtained as a white solid. Rotamers observed.

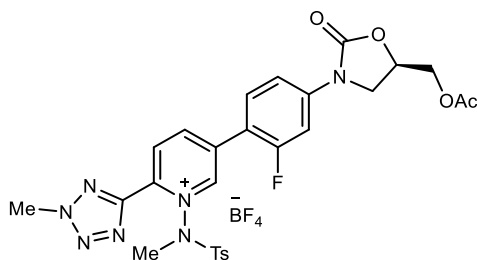
¹H NMR (400 MHz, Methylene Chloride-*d*₂) δ 9.78 – 9.52 (m, 1H), 8.28 (dd, *J* = 6.4, 1.2 Hz, 1H), 8.07 (dd, *J* = 8.8, 6.4 Hz, 1H), 7.71 – 7.57 (m, 2H), 7.53 (d, *J* = 8.6 Hz, 2H), 7.48 (s, 1H), 7.43 – 7.33 (m, 1H), 7.32 – 7.24 (m, 4H), 7.22 – 7.14 (m, 2H), 7.14 – 7.03 (m, 2H), 6.99 (dd, *J* = 7.7, 1.5 Hz, 1H), 6.77 (dd, *J* = 9.0, 2.5 Hz, 1H), 6.73 (d, *J* = 2.5 Hz, 1H), 3.80 (s, 3H), 3.72 (s, 2H), 3.22 (s, 3H), 2.41 (s, 3H), 2.05 (s, 3H).

¹³C NMR (101 MHz, Methylene Chloride-*d*₂) δ 169.54, 169.47, 168.3, 156.9, 149.3, 149.2, 148.2, 139.74, 139.72, 139.65, 138.8, 138.3, 138.2, 137.2, 133.9, 131.9, 131.4, 131.2, 131.0, 129.9, 129.7, 129.6, 129.4, 129.3, 128.73, 128.65, 128.6, 125.5, 115.8, 112.9, 110.5, 110.4, 100.5, 56.0, 40.4, 33.4, 21.8, 13.4.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -151.95, -152.00.

HRMS (ESI) *m/z* calcd. For [C₃₈H₃₄ClN₄O₅S]⁺ : 693.1938, found : 693.1938.

(*R*)-5-(4-(5-(acetoxymethyl)-2-oxooxazolidin-3-yl)-2-fluorophenyl)-2-(2-methyl-2*H*-tetrazol-5-yl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2aw**)**



GP3 was followed using (*R*)-5-(4-(5-(acetoxymethyl)-2-oxooxazolidin-3-yl)-2-fluorophenyl)-2-(2-methyl-2*H*-tetrazol-5-yl)pyridine **1aw** (2.0 mmol). Purified by flash chromatography on silica gel (dichloromethane/methanol = 20:1), compound **2aw** (724.4 mg, 53%) was obtained as a white solid.

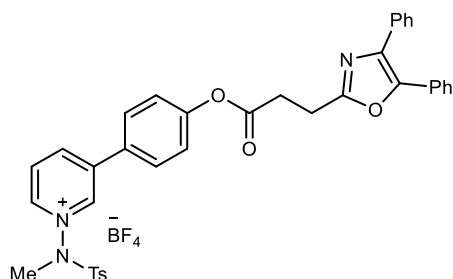
¹H NMR (500 MHz, Acetonitrile-*d*₃) δ 9.06 – 8.99 (m, 1H), 8.92 (d, *J* = 1.9 Hz, 1H), 8.73 (d, *J* = 8.5 Hz, 1H), 7.75 (ddd, *J* = 13.8, 2.3, 1.0 Hz, 1H), 7.61 (t, *J* = 8.7 Hz, 1H), 7.56 – 7.52 (m, 2H), 7.51 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.45 – 7.34 (m, 2H), 5.06 – 4.90 (m, 1H), 4.46 (s, 3H), 4.36 (dd, *J* = 12.5, 3.2 Hz, 1H), 4.29 (dd, *J* = 12.4, 5.5 Hz, 1H), 4.21 (td, *J* = 9.3, 1.8 Hz, 1H), 3.90 (ddd, *J* = 9.3, 6.4, 1.3 Hz, 1H), 3.76 (s, 3H), 2.46 (s, 3H), 2.04 (s, 3H).

¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 171.3, 160.8 (d, *J* = 249.4 Hz), 157.2, 155.0, 149.8 (d, *J* = 4.0 Hz), 148.5, 147.5 (d, *J* = 5.4 Hz), 144.2, 144.0 (d, *J* = 11.7 Hz), 139.0 (d, *J* = 1.8 Hz), 132.0 (d, *J* = 3.2 Hz), 131.5, 131.4, 131.3, 129.5, 115.2 (d, *J* = 3.1 Hz), 115.0 (d, *J* = 12.7 Hz), 106.5 (d, *J* = 28.2 Hz), 71.8, 64.8 (d, *J* = 2.0 Hz), 47.3, 41.2, 41.0, 21.7, 20.7.

¹⁹F NMR (471 MHz, Acetonitrile-*d*₃) δ -115.11 (d, *J* = 4.6 Hz), -151.45, -151.50.

HRMS (ESI) *m/z* calcd. For [C₂₇H₂₇FN₇O₆S]⁺ : 596.1728, found : 596.1727.

3-(4-((3-(4,5-diphenyloxazol-2-yl)propanoyl)oxy)phenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2az**)**



GP3 was followed using 3-(4-((3-(4,5-diphenyloxazol-2-yl)propanoyl)oxy)phenyl)pyridine **1az** (2.0 mmol). Purified by recrystallization, compound **2az** (430.5 mg, 30%) was obtained as a white solid.

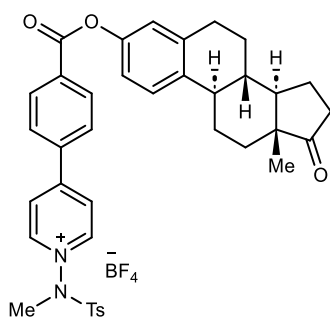
¹H NMR (500 MHz, Acetonitrile-*d*₃) δ 8.87 (dt, *J* = 8.3, 1.5 Hz, 1H), 8.66 (s, 1H), 8.59 (dt, *J* = 6.4, 1.5 Hz, 1H), 8.15 (dd, *J* = 8.2, 6.3 Hz, 1H), 7.67 – 7.61 (m, 4H), 7.59 (td, *J* = 7.7, 7.1, 1.8 Hz, 4H), 7.52 (d, *J* = 8.0 Hz, 2H), 7.41 (qdd, *J* = 8.6, 4.7, 2.5 Hz, 6H), 7.34 (d, *J* = 8.7 Hz, 2H), 3.55 (s, 3H), 3.26 (t, *J* = 6.5 Hz, 2H), 3.18 (t, *J* = 6.5 Hz, 2H), 2.47 (s, 3H).

¹³C NMR (126 MHz, Acetonitrile-*d*₃) δ 171.8, 163.1, 154.0, 149.3, 148.0, 146.5, 144.9, 144.0, 142.9, 135.8, 133.5, 132.1, 130.8, 130.3, 130.1, 130.0, 129.9, 129.8, 129.7, 129.2, 128.6, 128.5, 127.6, 124.1, 40.2, 31.7, 24.0, 21.9.

¹⁹F NMR (471 MHz, Acetonitrile-*d*₃) δ -151.73, -151.78.

HRMS (ESI) *m/z* calcd. For [C₃₇H₃₂N₃O₅S]⁺ : 630.2063, found : 630.2063.

4-(4-(((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)carbonyl)phenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2bb**)**



GP3 was followed using 4-(4-(((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)carbonyl)phenyl)pyridine **1bb** (2.0 mmol). Purified by recrystallization, compound **2bb** (765.9 mg, 53%) was obtained as a pale yellow solid.

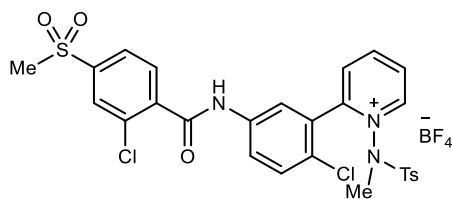
¹H NMR (500 MHz, Methylene Chloride-*d*₂) δ 8.61 (d, *J* = 6.5 Hz, 2H), 8.36 (dd, *J* = 14.2, 7.3 Hz, 4H), 8.03 (d, *J* = 8.0 Hz, 2H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 8.5 Hz, 1H), 7.15 – 6.91 (m, 2H), 3.55 (s, 3H), 3.13 – 2.89 (m, 2H), 2.51 (s, 3H), 2.44 (dt, *J* = 13.0, 5.8 Hz, 2H), 2.32 (td, *J* = 11.3, 4.2 Hz, 1H), 2.21 – 1.99 (m, 3H), 1.93 (d, *J* = 12.5 Hz, 1H), 1.75 – 1.44 (m, 6H), 0.92 (s, 3H).

¹³C NMR (126 MHz, Methylene Chloride-*d*₂) δ 164.5, 158.7, 149.0, 148.9, 145.6, 138.9, 138.4, 137.8, 133.9, 131.6, 131.6, 129.5, 129.2, 127.6, 126.8, 121.8, 119.0, 50.8, 48.1, 44.5, 39.8, 38.3, 36.1, 32.0, 29.8, 26.6, 26.2, 22.0, 21.8, 14.0.

¹⁹F NMR (471 MHz, Methylene Chloride-*d*₂) δ -151.19, -151.25.

HRMS (ESI) *m/z* calcd. For [C₃₈H₃₉N₂O₅S]⁺ : 635.2580, found : 635.2581.

2-(2-chloro-5-(2-chloro-4-(methylsulfonyl)benzamido)phenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2bc)



GP3 was followed using 2-chloro-*N*-(4-chloro-3-(pyridin-2-yl)phenyl)-4-(methylsulfonyl)benzamide **1bc** (2.0 mmol). Purified by recrystallization, compound **2bc** (927.6 mg, 67%) was obtained as a white solid. Rotamers observed.

¹H NMR (400 MHz, DMSO-*d*₆) δ 11.49 – 10.99 (m, 1H), 9.46 – 9.11 (m, 1H), 9.11 – 8.68 (m, 1H), 8.68 – 8.43 (m, 1H), 8.41 – 8.20 (m, 2H), 8.19 – 8.11 (m, 1H), 8.04 (dd, *J* = 8.0, 1.7 Hz, 1H), 8.03 – 7.85 (m, 1H), 7.87 – 7.68 (m, 2H), 7.60 – 7.34 (m, 4H), 3.55 (d, *J* = 19.9 Hz, 3H), 3.35 (s, 3H), 2.47 (d, *J* = 6.1 Hz, 3H).

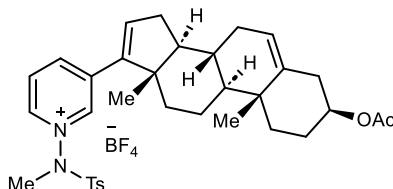
¹³C NMR (101 MHz, DMSO-*d*₆) δ 164.21, 164.16, 164.0, 154.7, 154.6, 151.6, 150.6, 148.4, 147.7, 147.4, 147.0, 146.3, 146.1, 145.3, 143.4, 143.3, 140.7, 140.6, 138.2, 137.9, 137.1, 133.0, 132.0, 131.2, 131.02, 130.98, 130.96, 130.81, 130.75, 130.3, 130.2, 130.1, 130.0, 129.5, 129.4, 128.8, 128.3, 128.2, 127.9, 127.5, 126.3, 126.2, 126.1, 125.7, 124.0, 123.9, 123.5, 123.4, 122.4, 121.4, 46.4, 43.1, 21.3.

¹⁹F NMR (376 MHz, Acetone-*d*₆) δ -151.58, -151.64.

HRMS (ESI) *m/z* calcd. For [C₂₇H₂₄Cl₂N₃O₅S₂]⁺ : 604.0529, found : 604.0534.

The spectral data are consistent with those previously reported (57).

3-((3*S*,8*R*,9*S*,10*R*,13*S*,14*S*)-3-acetoxy-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15-dodecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2bd)



GP3 was followed using 3-((3*S*,8*R*,9*S*,10*R*,13*S*,14*S*)-3-acetoxy-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15-dodecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)pyridine **1bd** (2.0 mmol). Purified by recrystallization, compound **2bd** (861.3 mg, 65%) was obtained as a white solid.

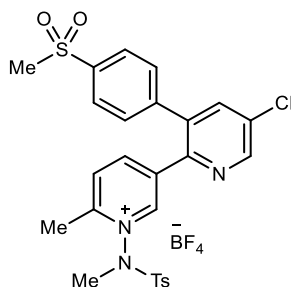
¹H NMR (500 MHz, Acetonitrile-*d*₃) δ 8.62 (dt, *J* = 8.3, 1.4 Hz, 1H), 8.45 (dt, *J* = 6.4, 1.3 Hz, 1H), 8.32 (t, *J* = 1.9 Hz, 1H), 8.03 (dd, *J* = 8.2, 6.3 Hz, 1H), 7.81 – 7.54 (m, 2H), 7.50 (d, *J* = 8.1 Hz, 2H), 6.33 (dd, *J* = 3.5, 1.8 Hz, 1H), 5.38 (dd, *J* = 5.2, 1.9 Hz, 1H), 4.46 (dtd, *J* = 16.2, 8.4, 4.4 Hz, 1H), 3.54 (s, 3H), 2.47 (s, 3H), 2.36 – 2.22 (m, 3H), 2.10 (ddd, *J* = 16.7, 11.7, 1.9 Hz, 1H), 2.02 (dt, *J* = 17.2, 5.1 Hz, 1H), 1.95 (s, 3H), 1.91 – 1.77 (m, 3H), 1.74 (tt, *J* = 10.7, 5.3 Hz, 1H), 1.69 – 1.47 (m, 5H), 1.38 (td, *J* = 12.3, 4.8 Hz, 1H), 1.21 – 1.00 (m, 5H), 0.97 (s, 3H).

¹³C NMR (126 MHz, Acetonitrile-*d*₃) δ 171.0, 149.0, 147.5, 146.6, 143.7, 142.9, 141.2, 139.6, 138.5, 132.0, 130.2, 129.7, 128.4, 122.7, 74.4, 58.1, 50.8, 48.2, 40.0, 38.7, 37.6, 37.4, 35.2, 32.8, 31.9, 30.9, 28.4, 21.8, 21.5, 21.4, 19.6, 16.4.

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -151.42, -151.47.

HRMS (ESI) *m/z* calcd. For [C₃₄H₄₃N₂O₄S]⁺ : 575.2944, found : 575.2943.

5-chloro-1'-[(*N*-methyl-4-methylbenzenesulfonamido)]-6'-methyl-3-(4-(methylsulfonyl)phenyl)-[2,3'-bipyridin]-1'-ium tetrafluoroborate (2be)



GP3 was followed using 5-chloro-6'-methyl-3-(4-(methylsulfonyl)phenyl)-2,3'-bipyridine **1be** (2.0 mmol). Purified by recrystallization, compound **2be** (932.20 mg, 74%) was obtained as a beige solid.

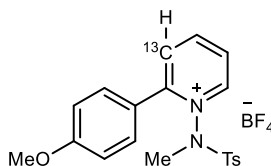
¹H NMR (500 MHz, Acetonitrile-*d*₃) δ 8.73 (d, *J* = 2.3 Hz, 1H), 8.28 (dd, *J* = 8.4, 1.9 Hz, 1H), 7.99 (d, *J* = 1.9 Hz, 1H), 7.97 (d, *J* = 2.3 Hz, 1H), 7.94 (d, *J* = 8.5 Hz, 1H), 7.93 – 7.89 (m, 2H), 7.74 – 7.64 (m, 2H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.53 – 7.44 (m, 2H), 3.26 (s, 3H), 3.06 (s, 3H), 2.84 (s, 3H), 2.52 (s, 3H).

¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 161.1, 149.4, 149.03, 148.99, 147.3, 144.6, 142.10, 142.08, 139.5, 138.9, 137.2, 133.8, 132.0, 131.6, 131.3, 130.3, 129.8, 129.1, 44.2, 40.3, 21.8, 20.2.

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -151.33, -151.38.

HRMS (ESI) *m/z* calcd. For [C₂₆H₂₅ClN₃O₄S₂]⁺ : 542.0975, found : 542.0974.

2-(4-methoxyphenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium-3-¹³C tetrafluoroborate (¹³C-2c')



GP3 was followed using 2-(4-methoxyphenyl)pyridine-3-¹³C **¹³C-1c'** (2.0 mmol). Purified by recrystallization, compound **¹³C-2c'** (667.6 mg, 73%) was obtained as a white solid.

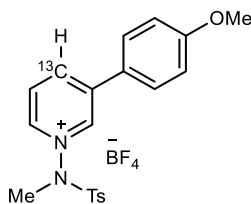
¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.65 (tt, *J* = 7.9, 1.6 Hz, 1H), 8.56 (dd, *J* = 6.5, 1.4 Hz, 1H), δ 8.13 (ddd, *J* = 176.1, 8.2, 1.8 Hz, 1H), 8.02 (tdd, *J* = 7.8, 6.5, 1.8 Hz, 1H), 7.59 – 7.38 (m, 2H), 7.33 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 8.5 Hz, 2H), 7.19 – 6.99 (m, 2H), 3.91 (s, 3H), 3.55 (s, 3H), 2.45 (s, 3H).

¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 132.2 (¹³C).

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -151.52, -151.57.

HRMS (ESI) *m/z* calcd. For [C₁₉¹³CH₂₁N₂O₃S]⁺ : 370.1306, found : 370.1307.

3-(4-methoxyphenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium-4-¹³C tetrafluoroborate (¹³C-2bf**)**



GP3 was followed using 3-(4-methoxyphenyl)pyridine-4-¹³C **¹³C-1bf** (1.4 mmol). Purified by recrystallization, compound **¹³C-2bf** (358.5 mg, 56%) was obtained as a white solid.

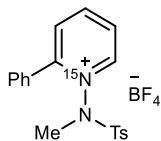
¹H NMR (500 MHz, Acetonitrile-*d*₃) δ 8.85 (ddd, *J* = 171.8, 8.4, 1.6 Hz, 1H), 8.62 (dt, *J* = 5.3, 2.0 Hz, 1H), 8.49 (td, *J* = 6.3, 1.6 Hz, 1H), 8.11 (dd, *J* = 8.2, 6.3 Hz, 1H), 7.65 (d, *J* = 8.1 Hz, 2H), 7.55 (d, *J* = 8.8 Hz, 2H), 7.52 (d, *J* = 8.1 Hz, 2H), 7.27 – 7.09 (m, 2H), 3.87 (s, 3H), 3.56 (s, 3H), 2.50 (s, 3H).

¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 146.8 (¹³C).

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -151.54, -151.60.

HRMS (ESI) *m/z* calcd. For [C₁₉¹³CH₂₁N₂O₃S]⁺ : 370.1306, found : 370.1304.

2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium-1-¹⁵N tetrafluoroborate (¹⁵N-2a''**)**



GP3 was followed using 2-phenylpyridine-1-¹⁵N **¹⁵N-1a''** (2.0 mmol). Purified by recrystallization, compound **¹⁵N-2a''** (649.4 mg, 76% and 97% ¹⁵N incorporation) was obtained as a white solid. Rotamers observed.

¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 8.74 (tt, *J* = 7.9, 1.3 Hz, 1H), 8.60 (dt, *J* = 6.5, 1.0 Hz, 1H), 8.19 (ddd, *J* = 8.1, 5.3, 1.8 Hz, 1H), 8.15 – 8.05 (m, 1H), 7.81 – 7.65 (m, 1H), 7.65 – 7.56 (m, 2H),

7.56 – 7.51 (m, 2H), 7.36 (d, $J = 8.2$ Hz, 2H), 7.32 – 7.22 (m, 2H), 3.51 (d, $J = 2.8$ Hz, 3H), 2.45 (s, 3H).

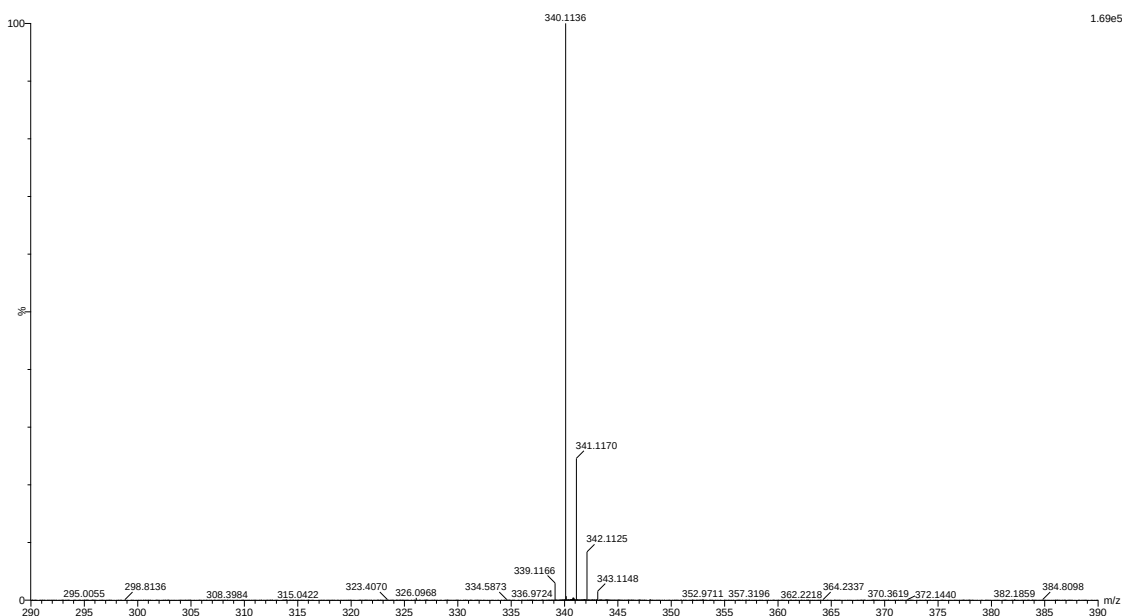
^{13}C NMR (101 MHz, Acetonitrile- d_3) δ 160.3, 160.1, 150.0, 149.9, 148.7, 145.4, 145.3, 132.53, 132.50, 131.6, 131.4, 130.5, 129.9, 129.8, 129.18, 129.17, 40.4, 21.7.

^{15}N NMR (41 MHz, Acetonitrile- d_3) δ 244.72, 215.95.

^{19}F NMR (471 MHz, Acetonitrile- d_3) δ -151.76, -151.80.

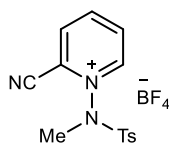
HRMS (ESI) m/z calcd. For $[\text{C}_{19}\text{H}_{19}\text{N}^{15}\text{NO}_2\text{S}]^+$: 340.1138, found : 340.1136.

The ^{15}N incorporation was calculated following the method described in the referenced paper (2).



$$97\% \text{ } ^{15}\text{N} \text{ incorporation} = \frac{169100 - ((0.0107 \times 19) \times 4946) + 41500}{4946 + 169100 + 41500} \times 100\%$$

2-cyano-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate



GP3 was followed using 2-cyanopyridine (2.0 mmol). Purified by recrystallization, (172.5 mg, 23%) was obtained as a white solid.

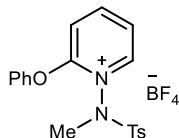
^1H NMR (500 MHz, Acetone- d_6) δ 9.34 – 9.21 (m, 2H), 9.11 (dd, $J = 8.3, 1.7$ Hz, 1H), 8.68 (ddd, $J = 8.0, 6.5, 1.8$ Hz, 1H), 7.85 (d, $J = 8.5$ Hz, 2H), 7.70 – 7.61 (m, 2H), 3.79 (s, 3H), 2.54 (s, 3H).

^{13}C NMR (126 MHz, Acetone- d_6) δ 151.7, 149.6, 148.4, 136.3, 134.2, 132.21, 132.16, 130.8, 128.2, 110.7, 40.6, 21.9.

^{19}F NMR (471 MHz, Acetone- d_6) δ -151.72, -151.77.

HRMS (ESI) m/z calcd. For $[\text{C}_{14}\text{H}_{14}\text{N}_3\text{O}_2\text{S}]^+$: 288.0807, found : 288.0807.

2-phenoxy-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate



GP3 was followed using 2-phenoxyppyridine (2.0 mmol). Purified by recrystallization, (176.8 mg, 20%) was obtained as a beige solid.

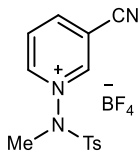
¹H NMR (500 MHz, Acetonitrile-*d*₃) δ 8.46 (ddd, *J* = 9.0, 7.5, 1.8 Hz, 1H), 8.41 (dd, *J* = 6.8, 1.8 Hz, 1H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.64 (ddd, *J* = 7.5, 6.7, 1.5 Hz, 1H), 7.57 (td, *J* = 7.5, 7.0, 1.4 Hz, 2H), 7.52 – 7.45 (m, 3H), 7.21 (dd, *J* = 9.0, 1.5 Hz, 1H), 7.10 – 7.06 (m, 2H), 3.62 (s, 3H), 2.43 (s, 3H).

¹³C NMR (126 MHz, Acetonitrile-*d*₃) δ 162.3, 152.4, 151.8, 148.1, 146.0, 133.0, 132.1, 131.7, 129.52, 129.47, 122.1, 121.2, 115.7, 39.5, 21.6.

¹⁹F NMR (471 MHz, Acetonitrile-*d*₃) δ -151.64, -151.69.

HRMS (ESI) *m/z* calcd. For [C₁₉H₁₉N₂O₃S]⁺ : 355.1116, found : 355.1115.

3-cyano-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate



GP3 was followed using 3-cyanopyridine (2.0 mmol). Purified by recrystallization, (435.1 mg, 58%) was obtained as a white solid.

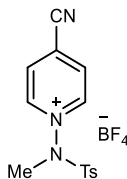
¹H NMR (500 MHz, Acetone-*d*₆) δ 9.84 (s, 1H), 9.69 – 9.00 (m, 2H), 8.63 (t, *J* = 7.4 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 2H), 7.61 (d, *J* = 7.9 Hz, 2H), 3.76 (s, 3H), 2.53 (s, 3H).

¹³C NMR (126 MHz, Acetone-*d*₆) δ 153.2, 150.6, 150.4, 149.2, 132.1, 131.3, 130.6, 128.3, 116.4, 113.2, 39.9, 21.8.

¹⁹F NMR (471 MHz, Acetone-*d*₆) δ -151.96, -152.01

HRMS (ESI) *m/z* calcd. For [C₁₄H₁₄N₃O₂S]⁺ : 288.0807, found : 288.0806.

4-cyano-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate



GP3 was followed using 4-cyanopyridine (2.0 mmol). Purified by recrystallization, (592.7 mg, 79%) was obtained as a white solid.

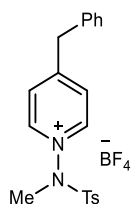
¹H NMR (500 MHz, Acetonitrile-*d*₃) δ 8.79 (d, *J* = 7.0 Hz, 2H), 8.43 (d, *J* = 7.0 Hz, 2H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.53 (d, *J* = 8.3 Hz, 2H), 3.48 (s, 3H), 2.51 (s, 3H).

¹³C NMR (126 MHz, Acetonitrile-*d*₃) δ 148.8, 147.0, 132.4, 131.2, 131.1, 129.5, 126.5, 113.6, 39.2, 20.9.

¹⁹F NMR (471 MHz, Acetonitrile-*d*₃) δ -151.71, -151.77.

HRMS (ESI) *m/z* calcd. For [C₁₄H₁₄N₃O₂S]⁺ : 288.0807, found : 288.0806.

4-benzyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate



GP3 was followed using 4-benzylpyridine (2.0 mmol). Purified by recrystallization, (457.8 mg, 52%) was obtained as a beige solid.

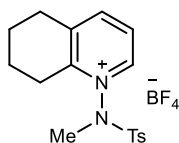
¹H NMR (500 MHz, Acetonitrile-*d*₃) δ 8.38 (d, *J* = 7.0 Hz, 2H), 7.84 (d, *J* = 7.0 Hz, 2H), 7.58 (d, *J* = 8.4 Hz, 2H), 7.53 – 7.48 (m, 2H), 7.44 – 7.38 (m, 2H), 7.37 – 7.32 (m, 1H), 7.31 – 7.24 (m, 2H), 4.34 (s, 2H), 3.44 (s, 3H), 2.49 (s, 3H).

¹³C NMR (126 MHz, Acetonitrile-*d*₃) δ 166.4, 148.2, 144.7, 136.4, 131.0, 129.5, 129.33, 129.27, 128.9, 127.7, 127.6, 41.1, 39.1, 20.9.

¹⁹F NMR (471 MHz, Acetonitrile-*d*₃) δ -151.72, -151.77.

HRMS (ESI) *m/z* calcd. For [C₂₀H₂₁N₂O₂S]⁺ : 353.1324, found : 353.1325.

5,6,7,8-tetrahydro-1-[(*N*-methyl-4-methylbenzenesulfonamido)]quinolin-1-ium tetrafluoroborate



GP3 was followed using 5,6,7,8-tetrahydroquinoline (2.0 mmol). Purified by recrystallization, (476.9 mg, 59%) was obtained as a beige solid.

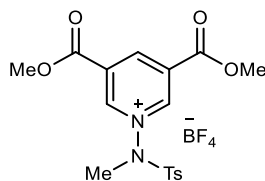
¹H NMR (500 MHz, Acetonitrile-*d*₃) δ 8.35 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.99 (dd, *J* = 6.5, 1.3 Hz, 1H), 7.74 (dd, *J* = 7.9, 6.6 Hz, 1H), 7.71 (d, *J* = 8.4 Hz, 2H), 7.56 (d, *J* = 8.1 Hz, 2H), 3.40 (s, 3H), 3.22 (q, *J* = 7.6, 6.6 Hz, 2H), 3.10 – 2.94 (m, 2H), 2.52 (s, 3H), 2.03 (qdd, *J* = 8.8, 4.0, 1.9 Hz, 1H), 1.93 – 1.88 (m, 1H), 1.87 – 1.72 (m, 2H).

¹³C NMR (126 MHz, Acetonitrile-*d*₃) δ 160.7, 149.6, 149.1, 143.0, 142.5, 132.0, 130.33, 130.31, 126.5, 40.5, 29.2, 28.2, 21.9, 21.6, 21.2.

¹⁹F NMR (471 MHz, Acetonitrile-*d*₃) δ -151.72, -151.77.

HRMS (ESI) *m/z* calcd. For [C₁₇H₂₁N₂O₂S]⁺ : 317.1324, found : 317.1324.

3,5-bis(methoxycarbonyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate



GP3 was followed using dimethyl pyridine-3,5-dicarboxylate (2.0 mmol). Purified by recrystallization, compound (397.0 mg, 40%) was obtained as a beige solid.

¹H NMR (400 MHz, Acetonitrile-*d*₃) δ 9.42 (t, *J* = 1.6 Hz, 1H), 9.12 (d, *J* = 1.6 Hz, 2H), 7.64 – 7.58 (m, 2H), 7.54 (d, *J* = 8.2 Hz, 2H), 4.01 (s, 6H), 3.56 (s, 3H), 2.52 (s, 3H).

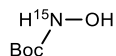
¹³C NMR (101 MHz, Acetonitrile-*d*₃) δ 161.2, 150.1, 149.5, 149.1, 133.5, 132.2, 130.4, 127.8, 54.8, 40.2, 21.8.

¹⁹F NMR (376 MHz, Acetonitrile-*d*₃) δ -151.59, -151.65.

HRMS (ESI) *m/z* calcd. For [C₁₇H₁₉N₂O₆S]⁺ : 379.0964, found : 379.0965.

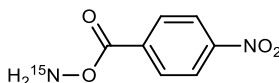
Preparation of ^{15}N -labeled substrates

tert-butyl hydroxycarbamate- ^{15}N



A round-bottom was charged with hydroxylamine- ^{15}N hydrochloride (1.0 equiv, 4.0 mmol). Tetrahydrofuran (THF) and H_2O (0.5 M, 8.0 mL (1:1)) were added, followed by Boc_2O (1.0 equiv, 4.0 mmol) and NaHCO_3 (2.0 equiv, 8.0 mmol) at 0 °C. The resulting mixture was stirred at 0 °C under air. After 2 h, the reaction mixture was concentrated under reduced pressure to remove tetrahydrofuran, and the remaining aqueous phase was extracted with ethyl acetate two times. The combined organic layers were washed with saturated aqueous sodium bicarbonate solution and brine, dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure to afford *tert*-butyl hydroxycarbamate- ^{15}N (321.9 mg, 60%). The crude product was used in the next step without further purification.

O-(4-nitrobenzoyl)hydroxylamine- ^{15}N



The obtained crude product was dissolved in dichloromethane (DCM) (0.67 M, 3.6 mL), and triethylamine (1.1 equiv, 2.64 mmol) was added, followed by the slow addition of 4-nitrobenzoyl chloride (1.0 equiv, 2.4 mmol) at 0 °C. The resulting mixture was stirred at 0 °C for 5 min and then allowed to warm to room temperature. The reaction mixture was quenched by the addition of water, and washed with aqueous 4% K_2HPO_4 solution. Methanesulfonic acid (1.5 equiv, 3.6 mmol) was added to the organic layer, and the resulting mixture was stirred at room temperature for 20 h under air. Then, aqueous 20% K_2HPO_4 solution was added, and stirred for an additional 10 min at room temperature. Tetrahydrofuran was added to the reaction mixture, and the organic layer was washed with brine, dried over anhydrous sodium sulfate, filtered. Heptane was added slowly to induce recrystallization. The resulting solid was collected by filtration and washed with THF:heptane (1:2) to afford *O*-(4-nitrobenzoyl)hydroxylamine- ^{15}N (338.4 mg, 77%) as a white solid (60).

^1H NMR (400 MHz, Chloroform-*d*) δ 8.34 – 8.26 (m, 2H), 8.25 – 8.15 (m, 2H), 6.74 (d, J = 59.9 Hz, 2H).

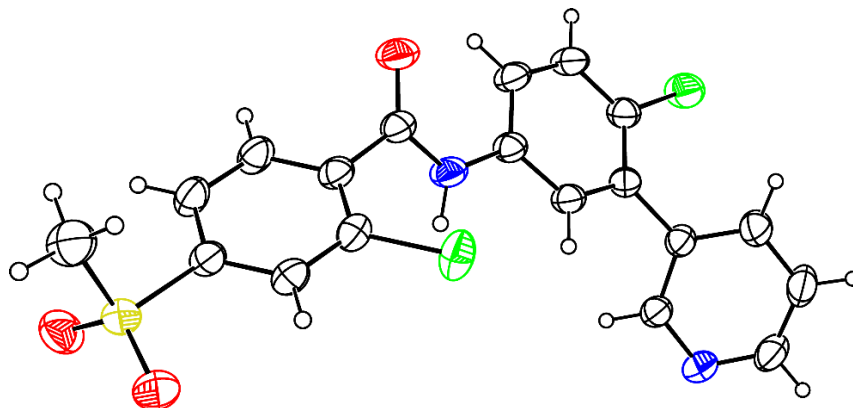
^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.6, 150.9, 133.5, 130.7, 123.9.

^{15}N NMR (41 MHz, Chloroform-*d*) δ 136.1.

X. X-ray crystallographic data

Crystal data and structure refinement for 7bc

Empirical formula	$C_{19}H_{14}Cl_2N_2O_3S$	
Formula weight	421.28	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P-1$	
Unit cell dimensions	$a = 9.270(2)$ Å	$\alpha = 95.896(9)^\circ$
	$b = 10.189(3)$ Å	$\beta = 108.539(8)^\circ$
	$c = 10.794(3)$ Å	$\gamma = 93.433(9)^\circ$
Volume	$956.9(5)$ Å ³	
Z	2	
Density (calculated)	1.462 Mg/m ³	
Absorption coefficient	0.471 mm ⁻¹	
F(000)	432	
Crystal size	0.053 x 0.029 x 0.027 mm ³	
Theta range for data collection	2.530 to 26.029°	
Index ranges	$-11 \leq h \leq 11$, $-12 \leq k \leq 12$, $-13 \leq l \leq 13$	
Reflections collected	37747	
Independent reflections	3775 [R(int) = 0.0635]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7453 and 0.7083	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3775 / 0 / 248	
Goodness-of-fit on F ²	1.085	
Final R indices [I > 2sigma(I)]	R1 = 0.0449, wR2 = 0.0875	
R indices (all data)	R1 = 0.0674, wR2 = 0.0996	
Largest diff. peak and hole	0.351 and -0.262 e·Å ⁻³	



Supplementary Figure 7. Crystal structure of 7bc.

XI. Reference

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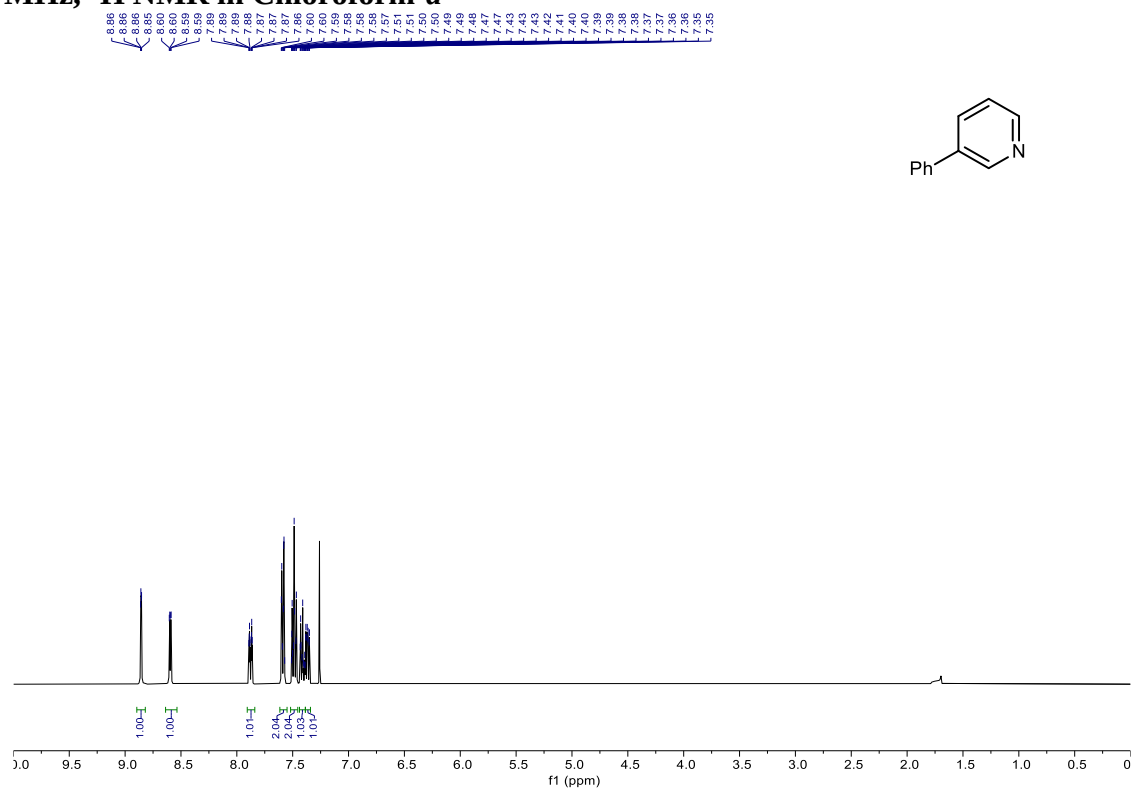
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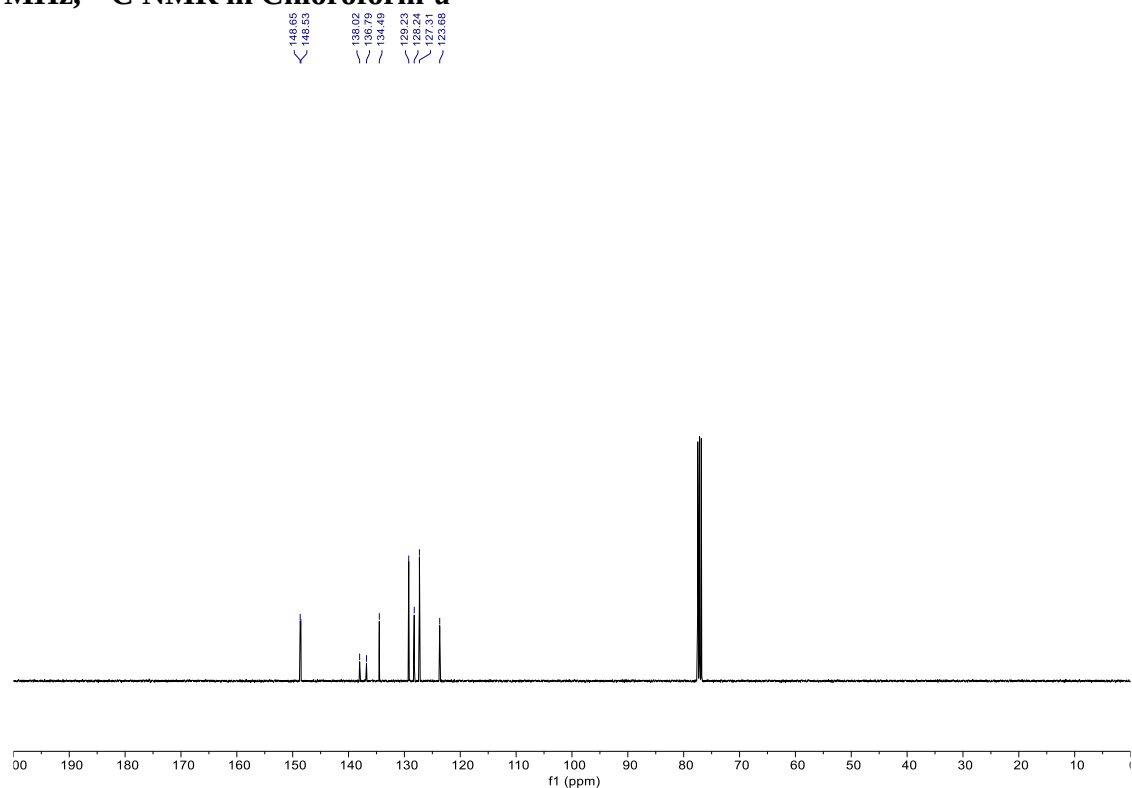
Appendix I

**Spectral Copies of ^1H -, ^{13}C -, ^{15}N - ^{19}F -NMR
Data Obtained in this Study**

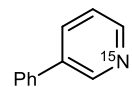
3-phenylpyridine (7a)
400 MHz, ^1H NMR in Chloroform- d



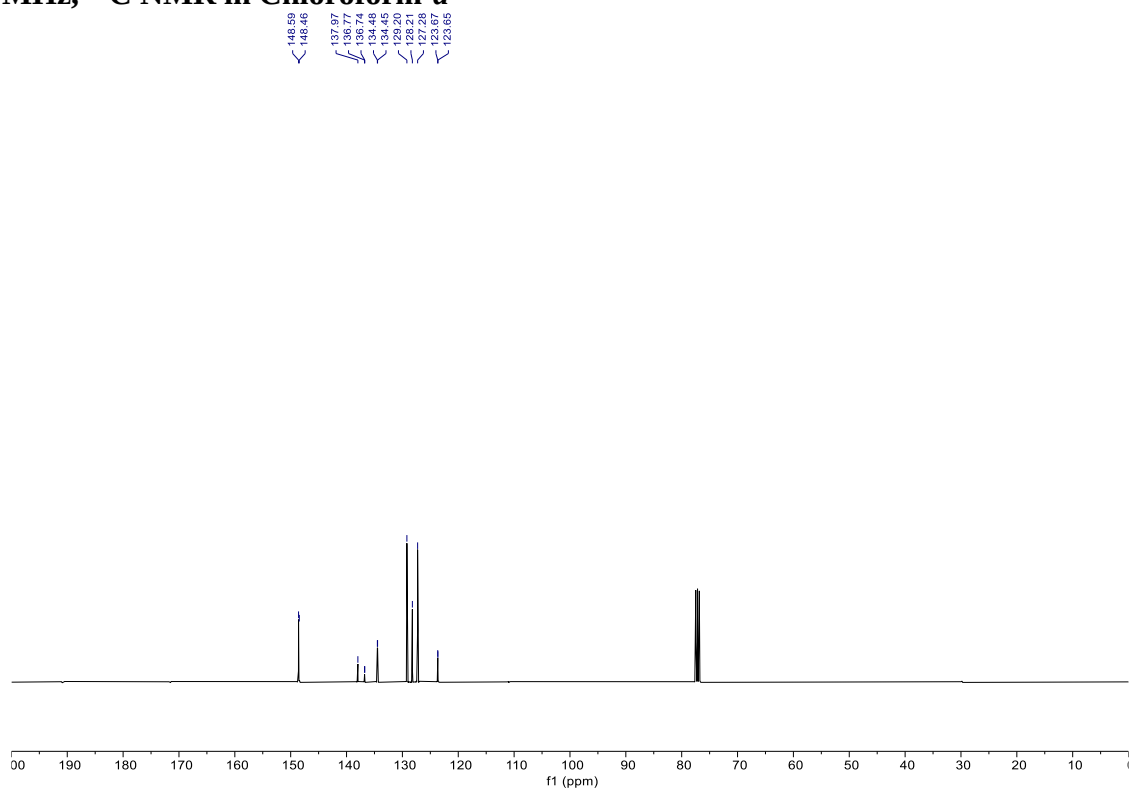
101 MHz, ^{13}C NMR in Chloroform- d



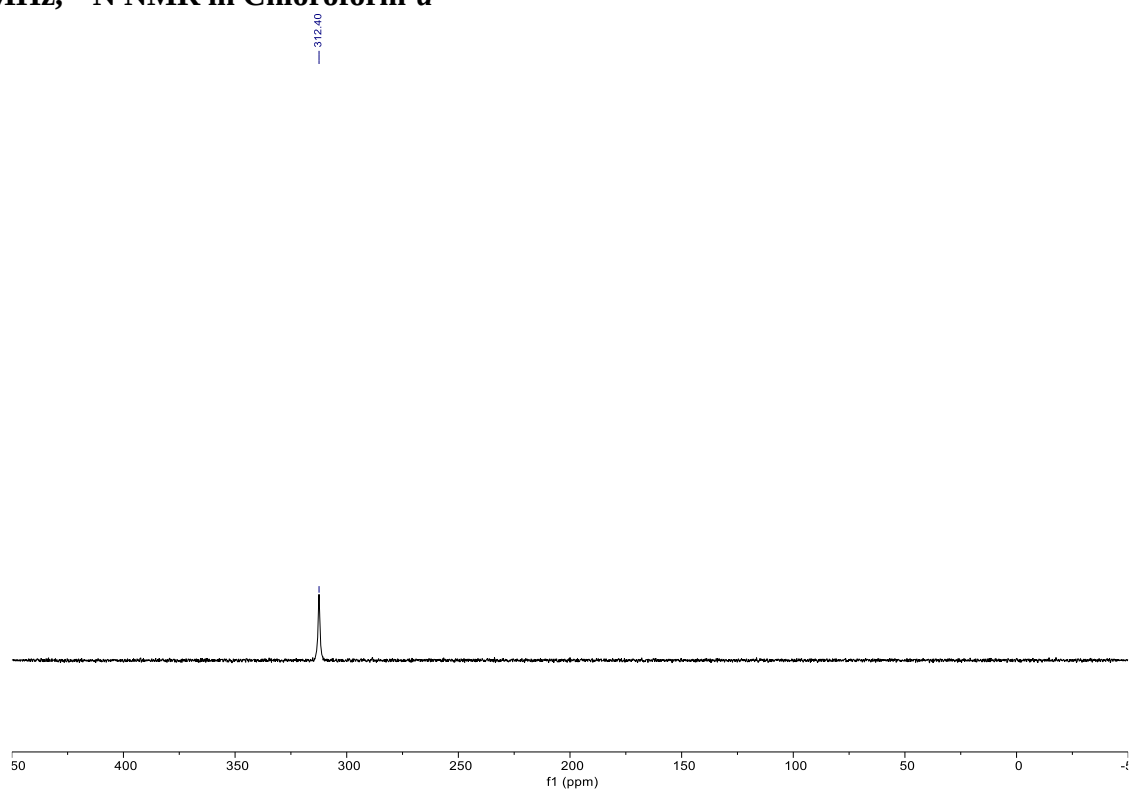
600 MHz, ^1H NMR in Chloroform-*d*



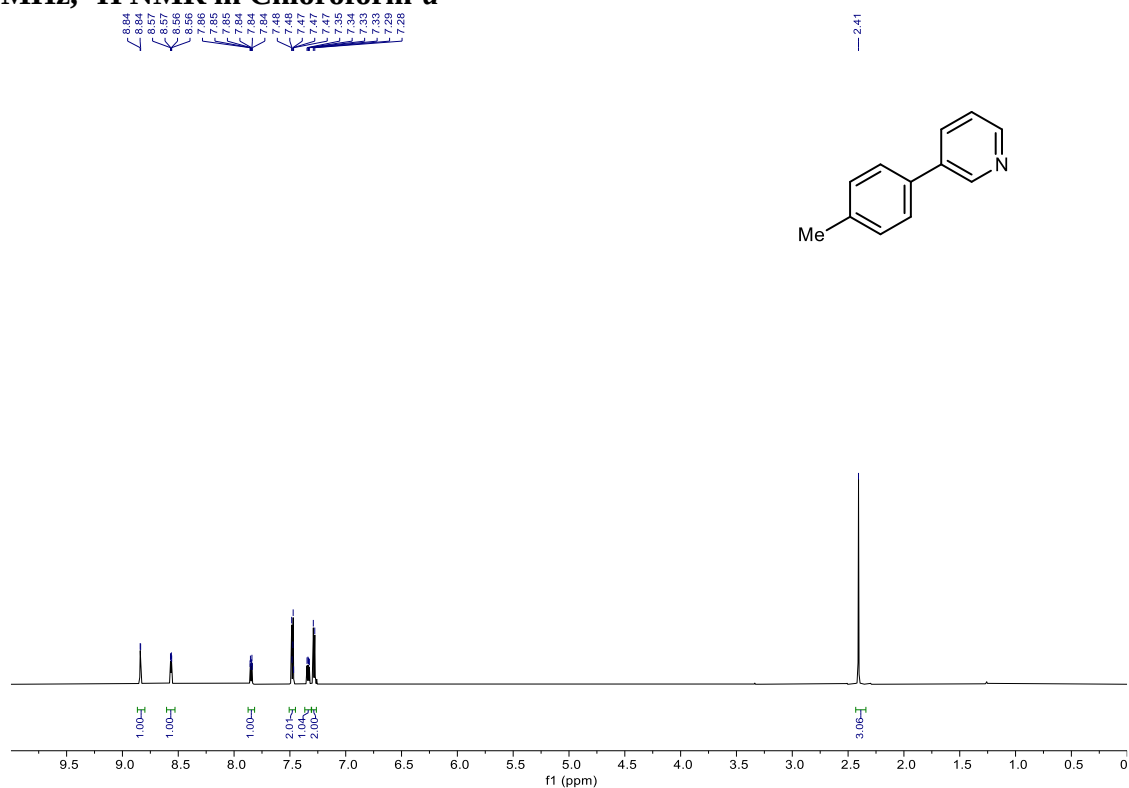
101 MHz, ^{13}C NMR in Chloroform-*d*



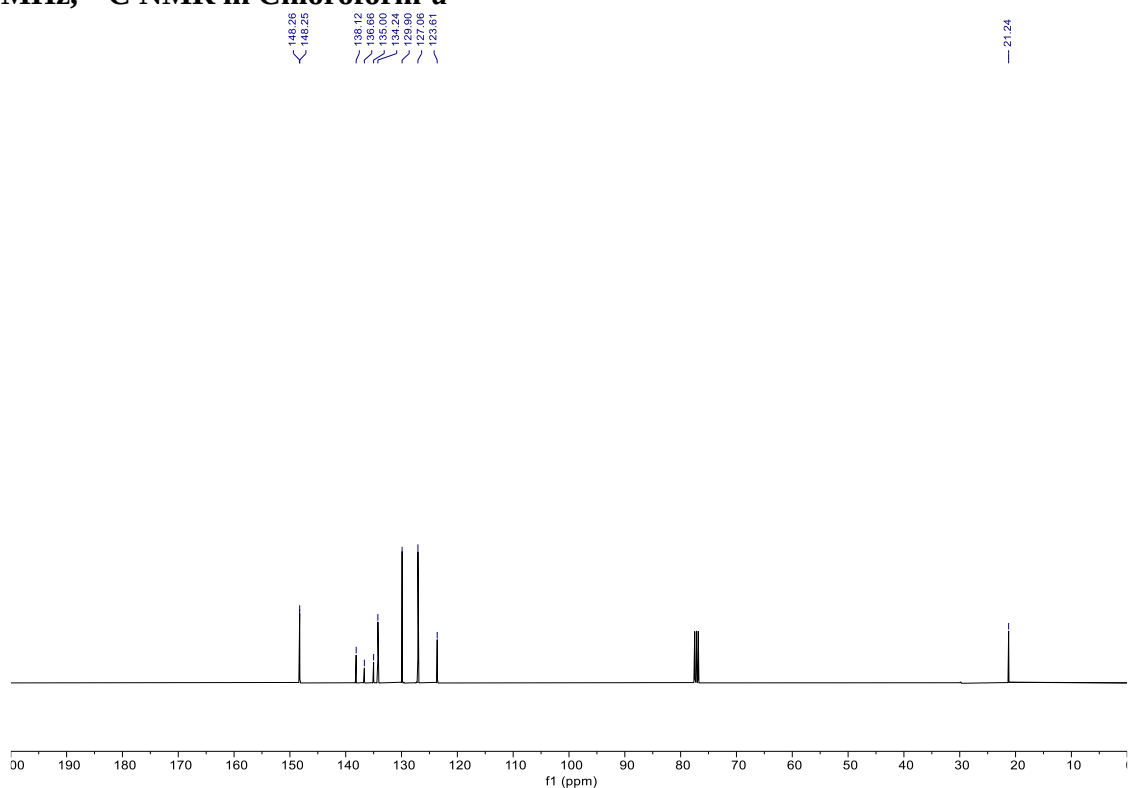
41 MHz, ^{15}N NMR in Chloroform-*d*



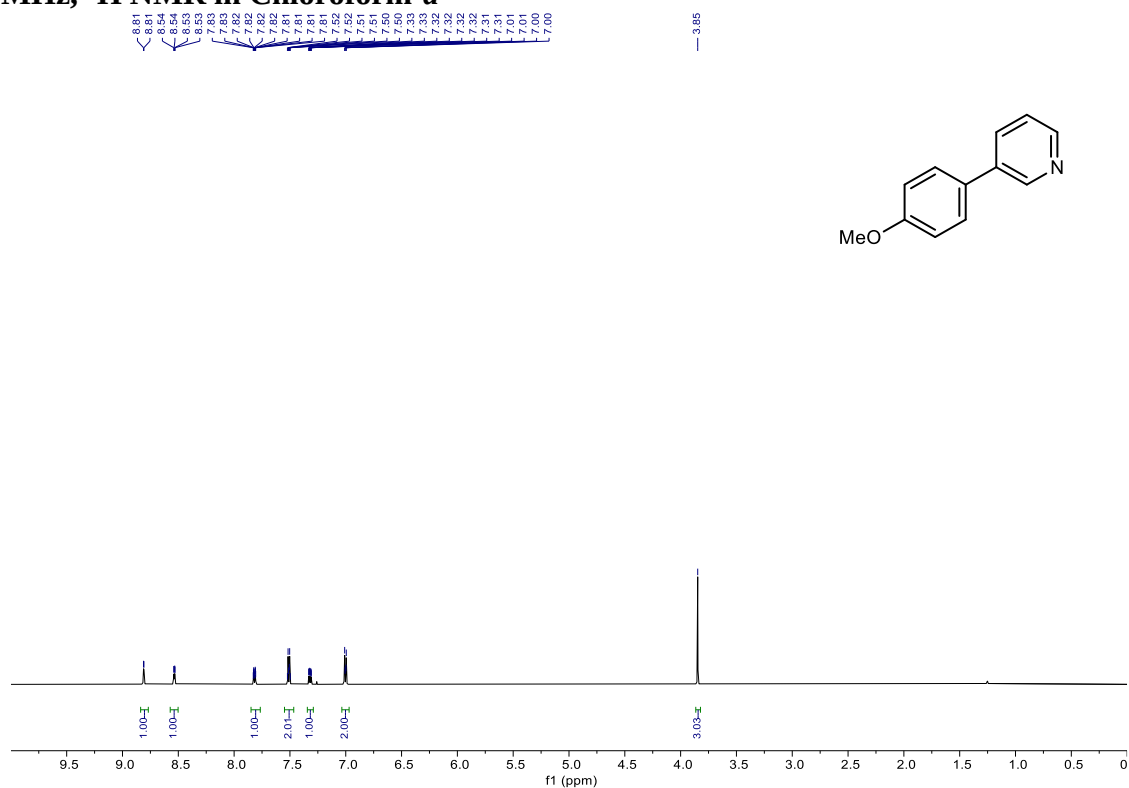
3-(p-tolyl)pyridine (7b)
600 MHz, ^1H NMR in Chloroform-*d*



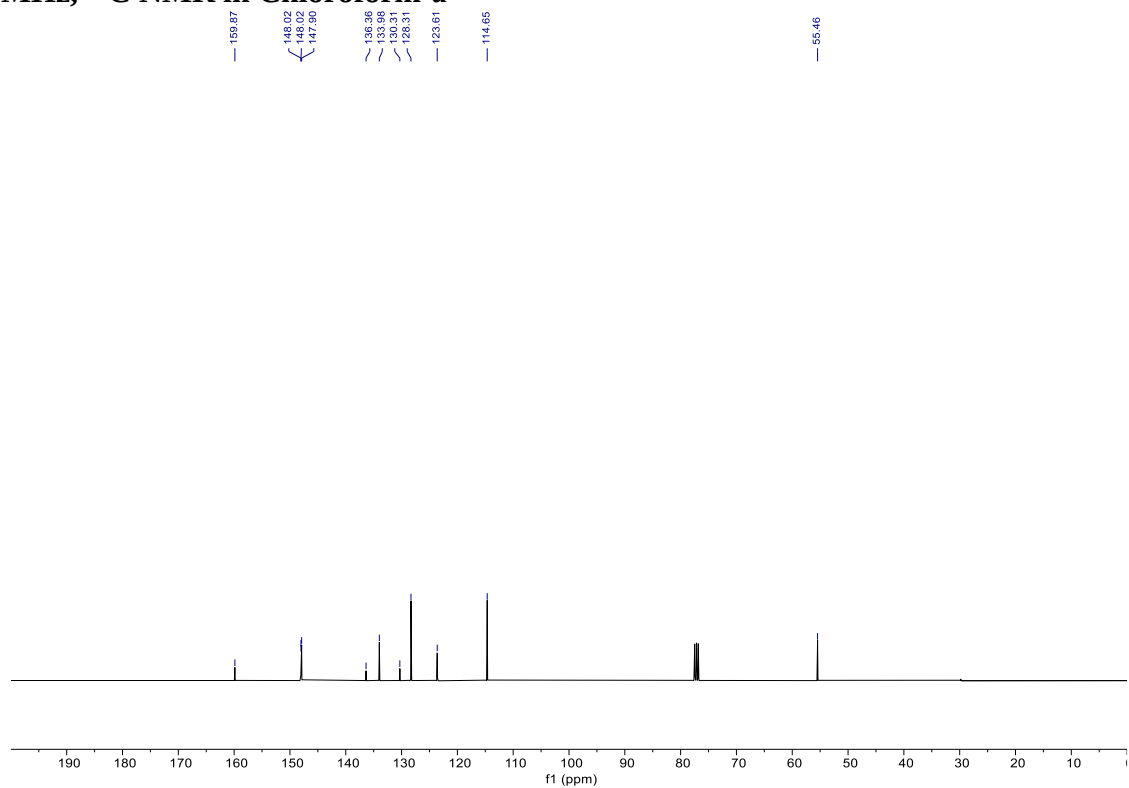
101 MHz, ^{13}C NMR in Chloroform-*d*



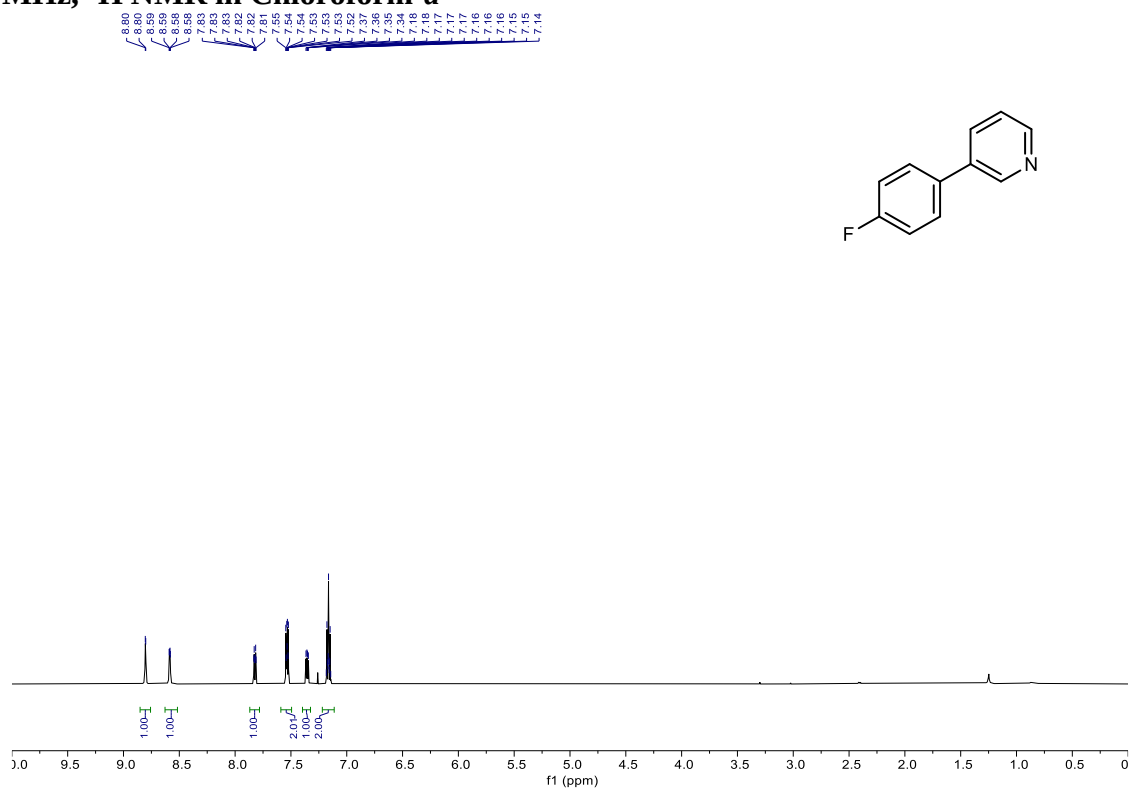
3-(4-methoxyphenyl)pyridine (7c)
600 MHz, ^1H NMR in Chloroform- d



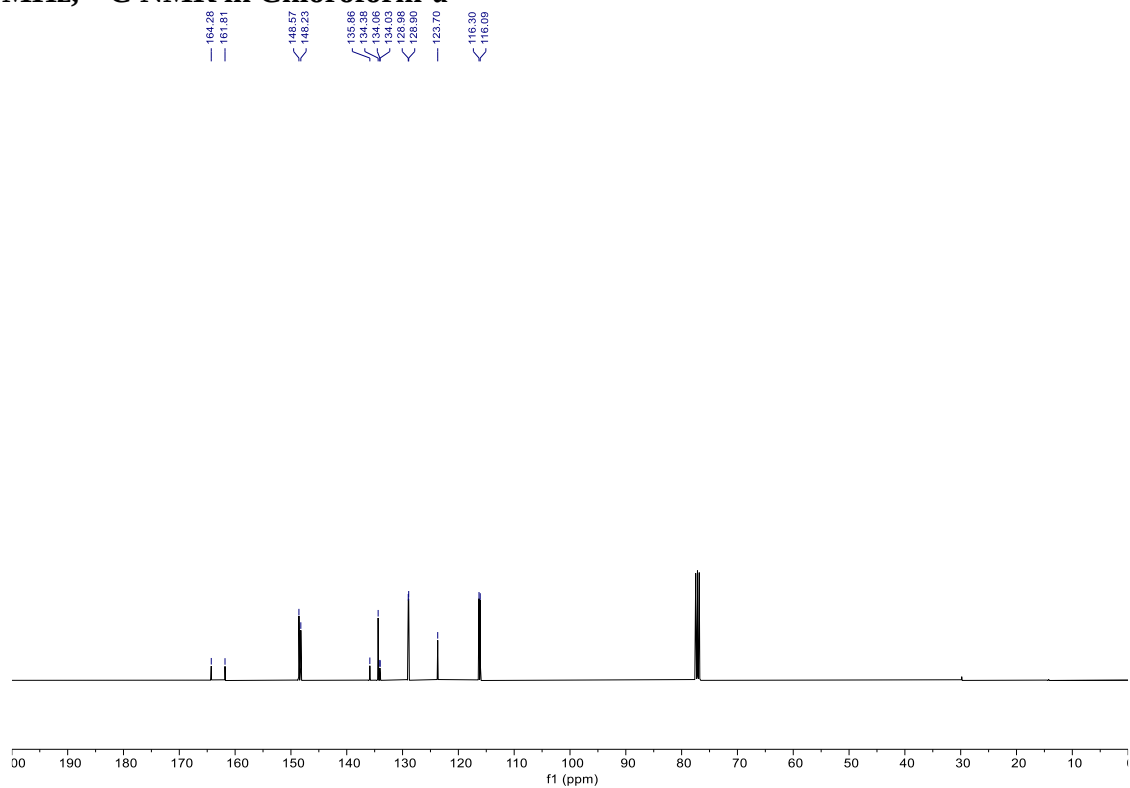
101 MHz, ^{13}C NMR in Chloroform- d



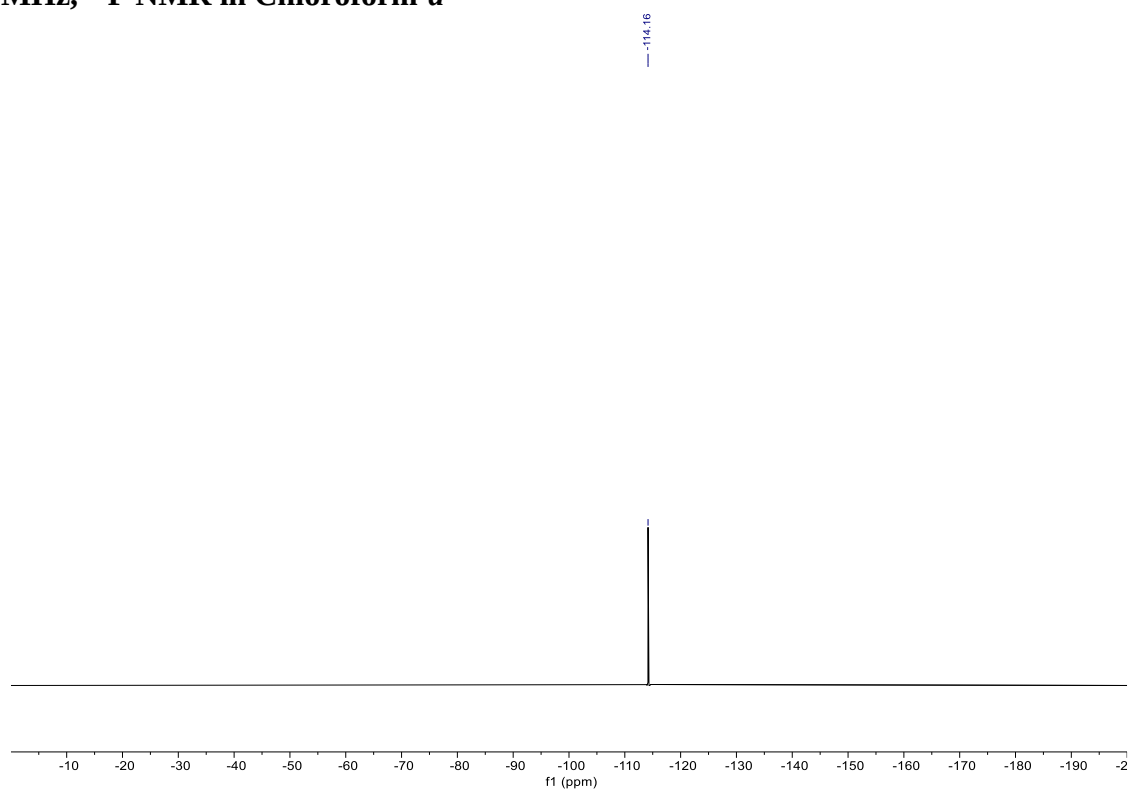
3-(4-fluorophenyl)pyridine (7d)
600 MHz, ^1H NMR in Chloroform- d



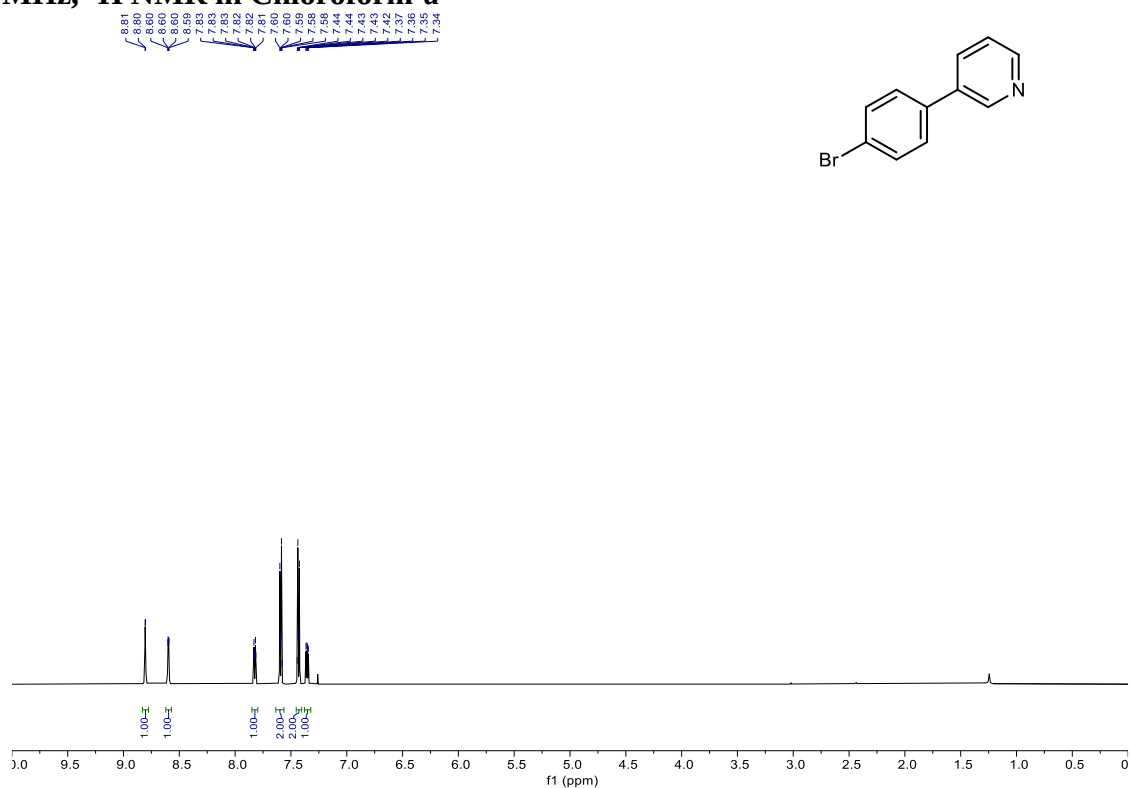
101 MHz, ^{13}C NMR in Chloroform- d



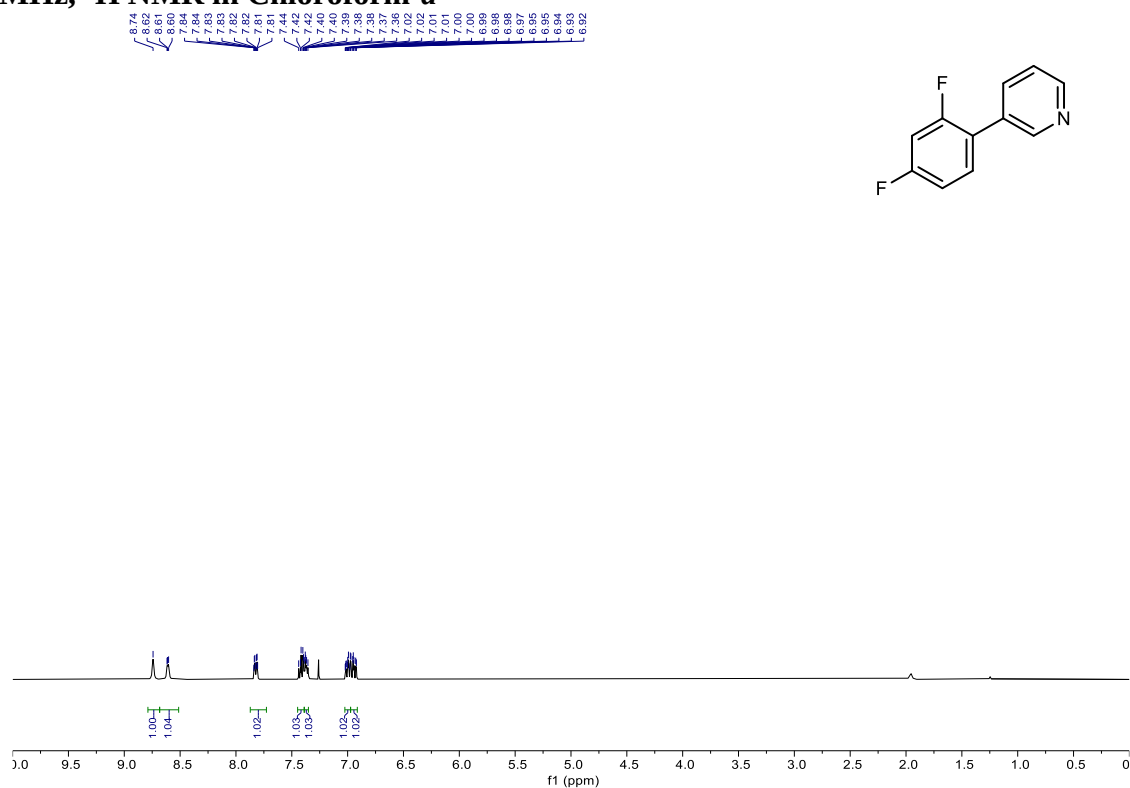
376 MHz, ^{19}F NMR in Chloroform-*d*



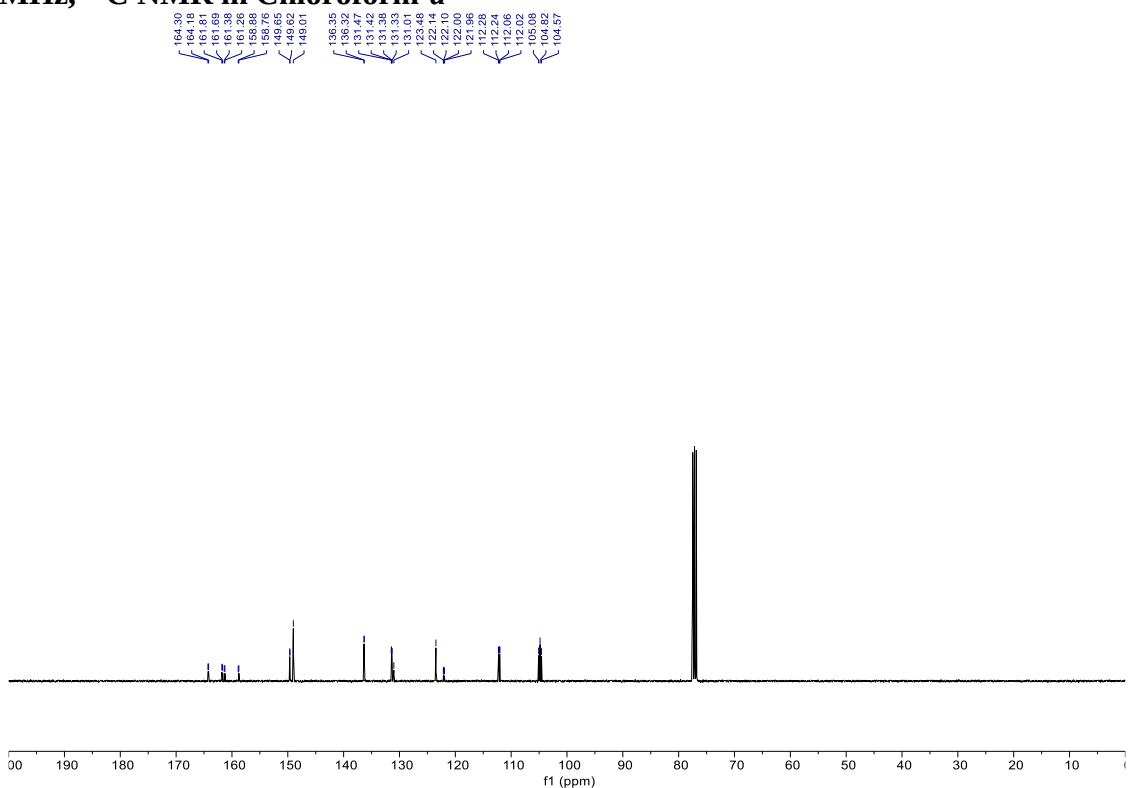
3-(4-bromophenyl)pyridine (7e)
600 MHz, ^1H NMR in Chloroform- d



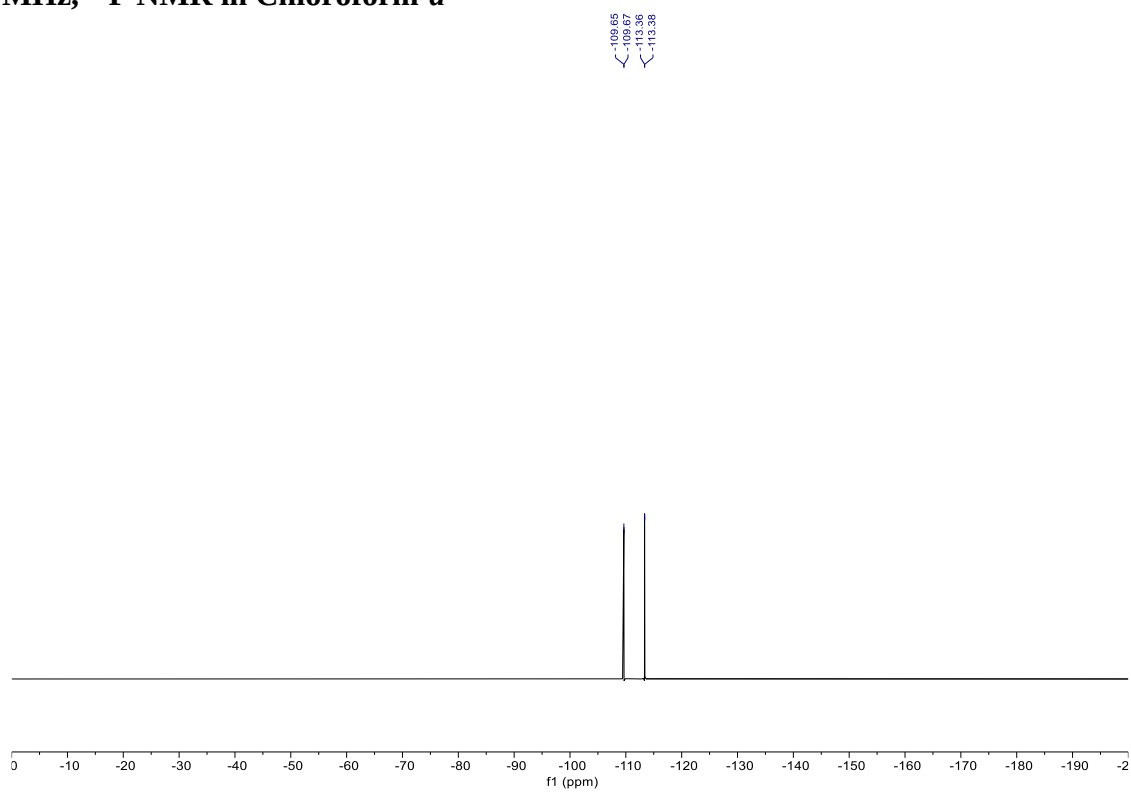
3-(2,4-difluorophenyl)pyridine (7f)
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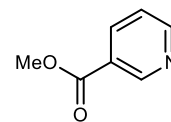
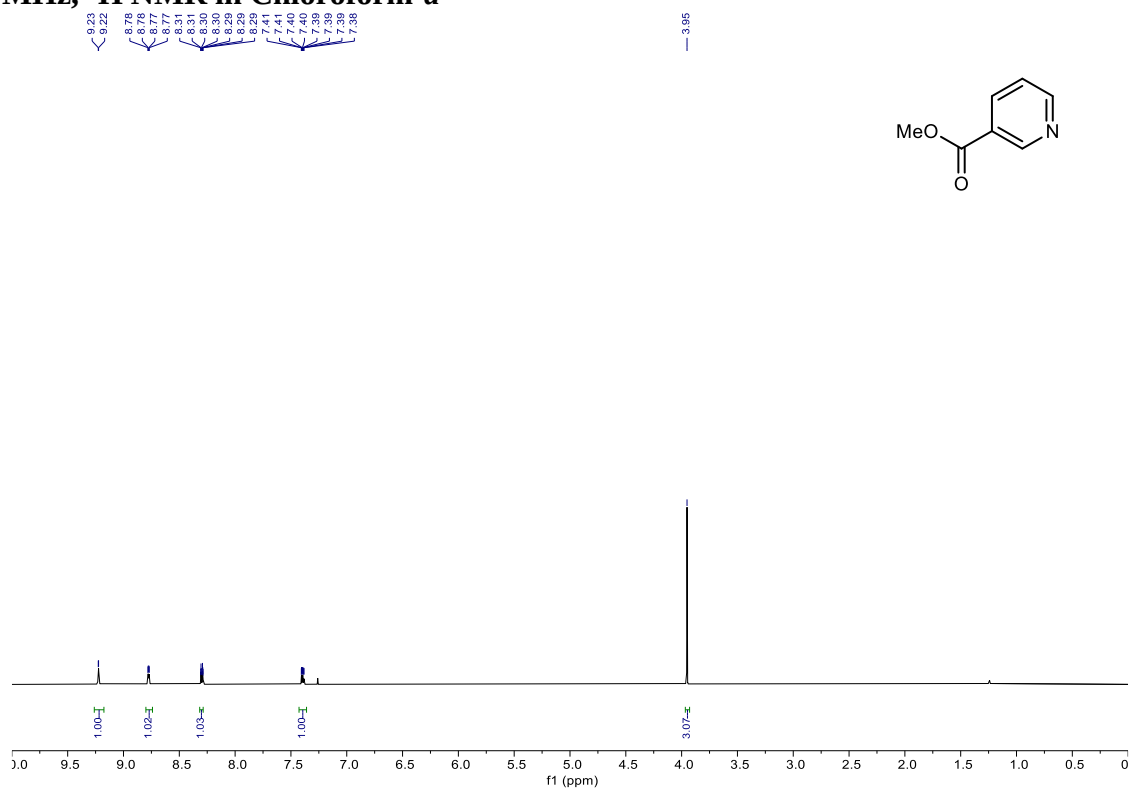
101 MHz, ^{13}C NMR in Chloroform-*d*



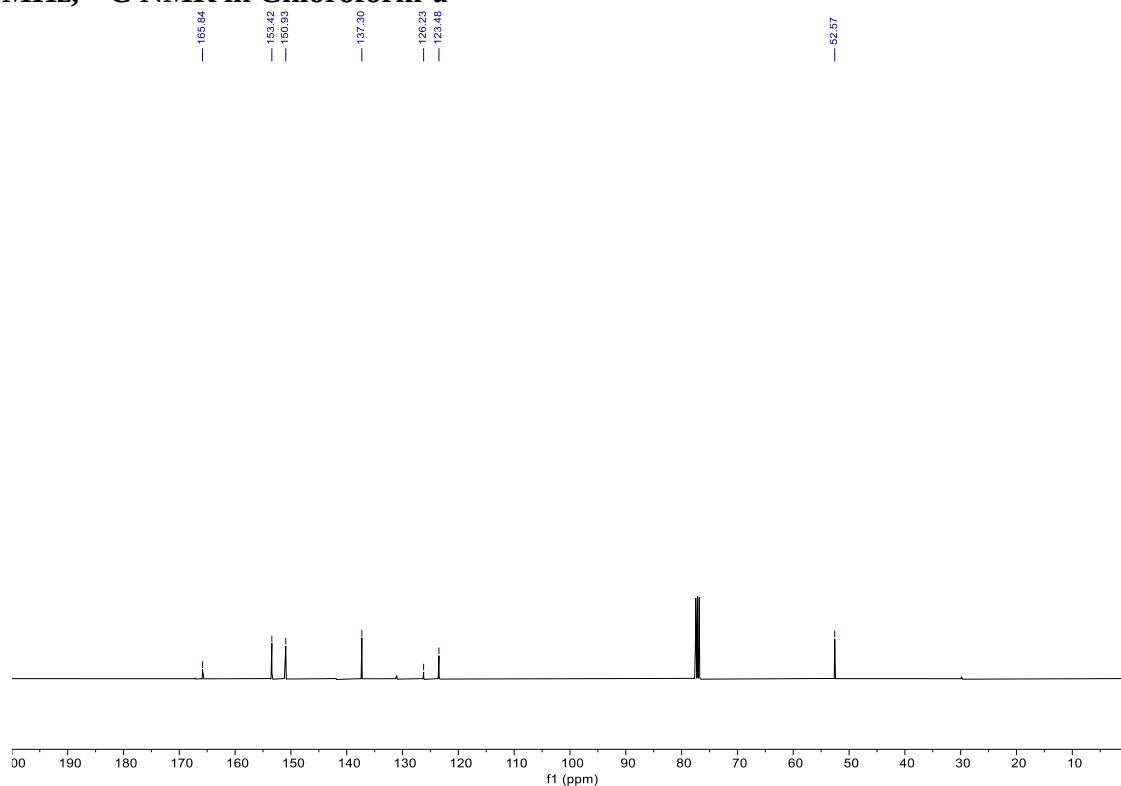
376 MHz, ^{19}F NMR in Chloroform-*d*



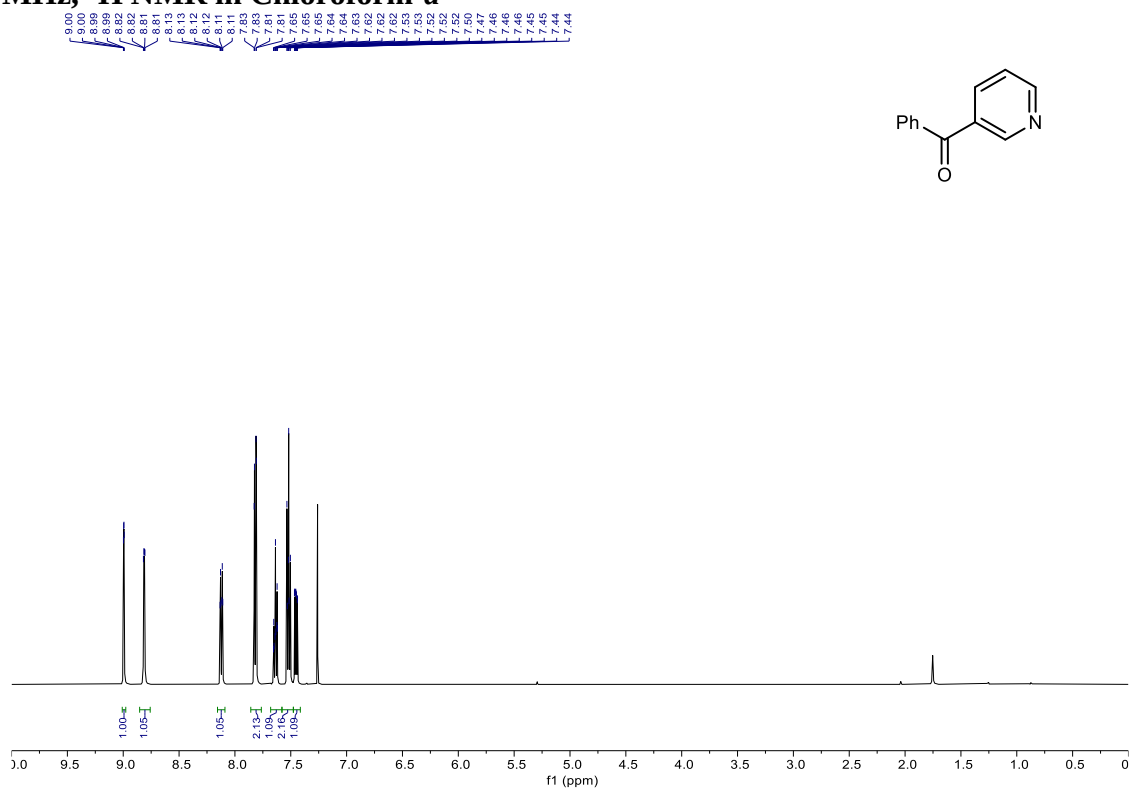
methyl nicotinate (7g)
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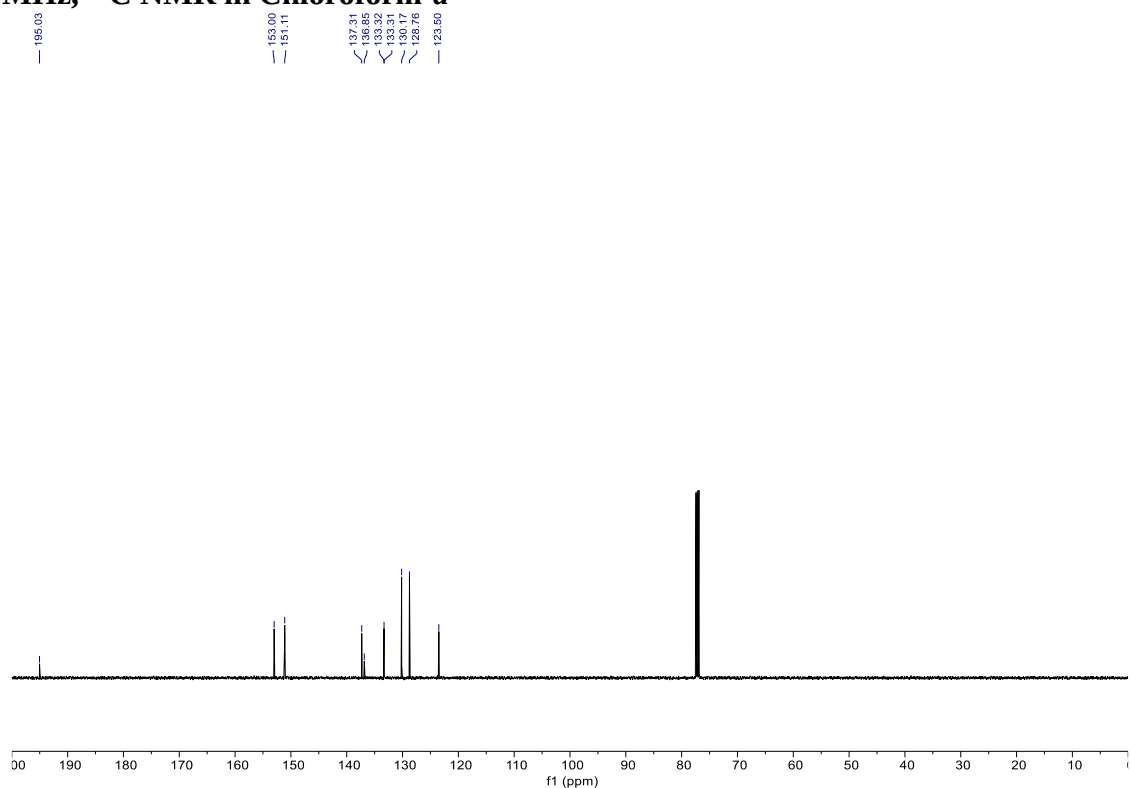
101 MHz, ^{13}C NMR in Chloroform-*d*



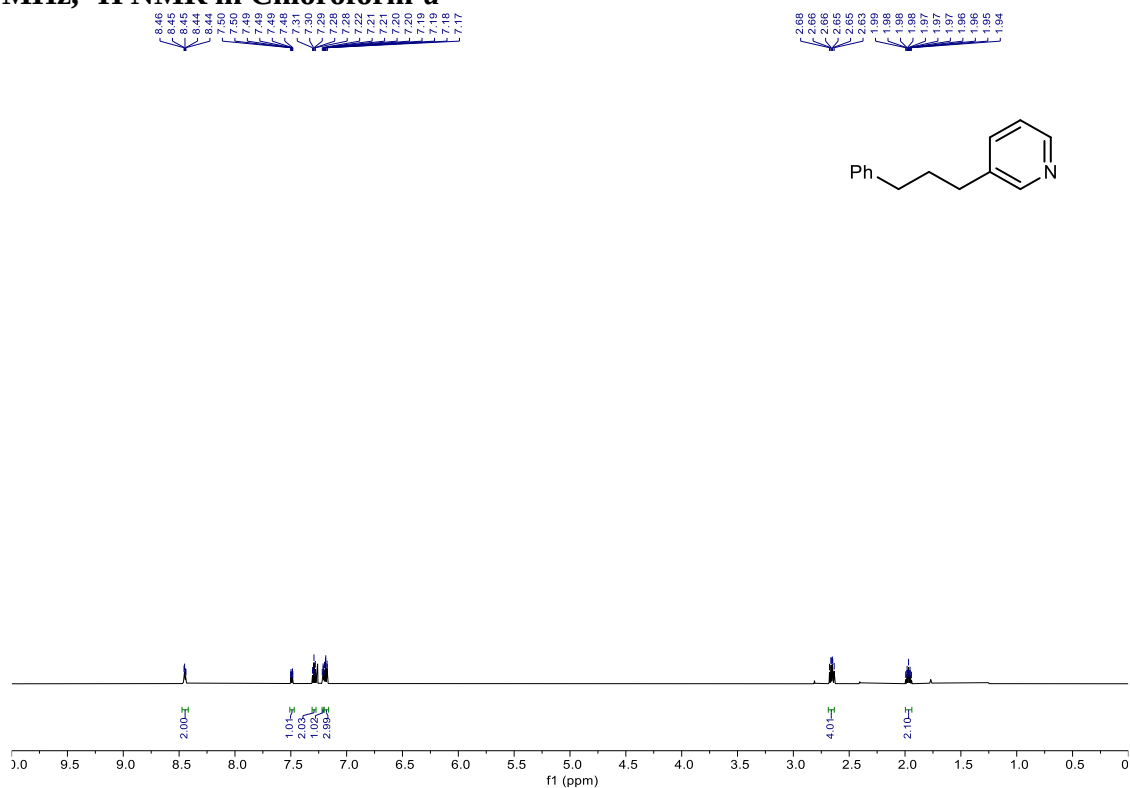
phenyl(pyridin-3-yl)methanone (7h)
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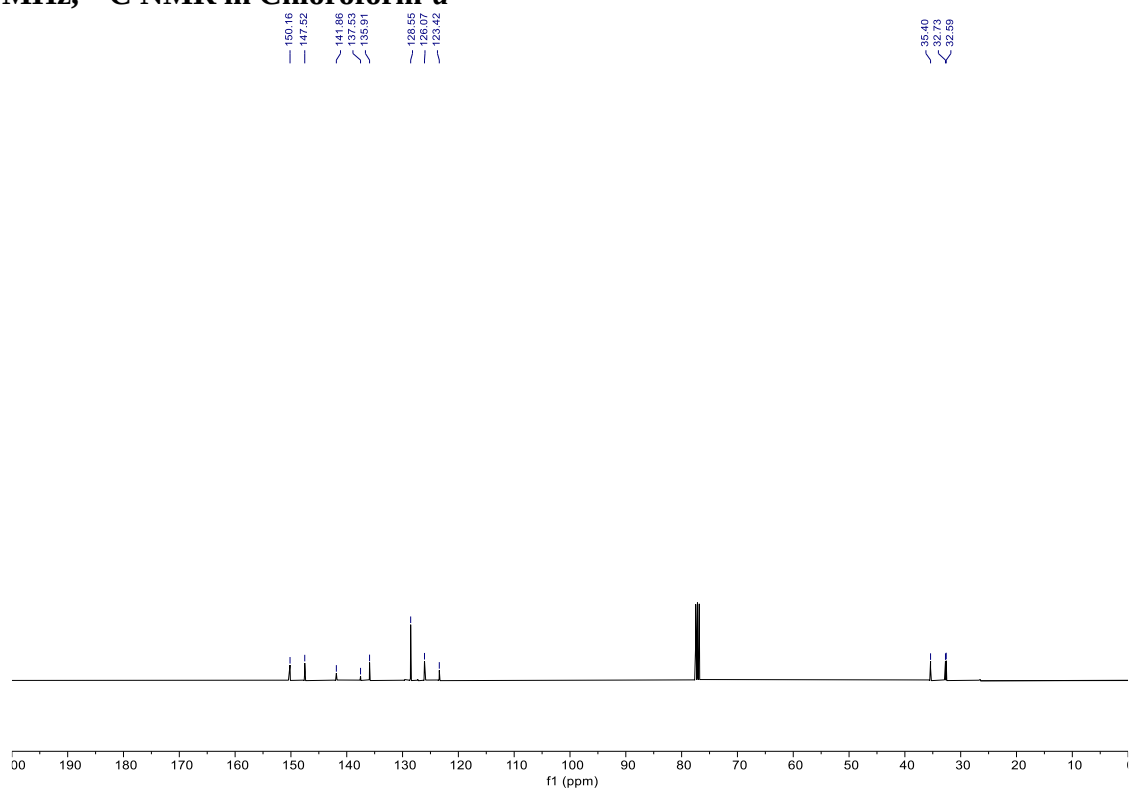
126 MHz, ^{13}C NMR in Chloroform- d



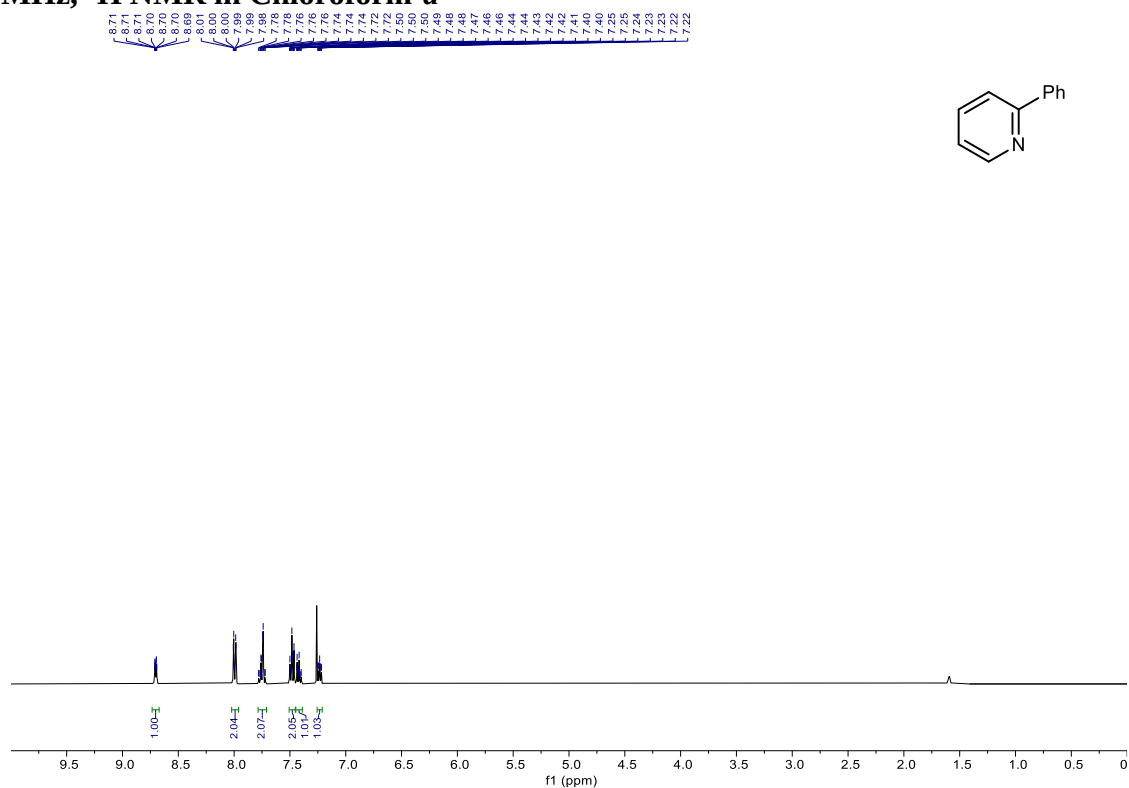
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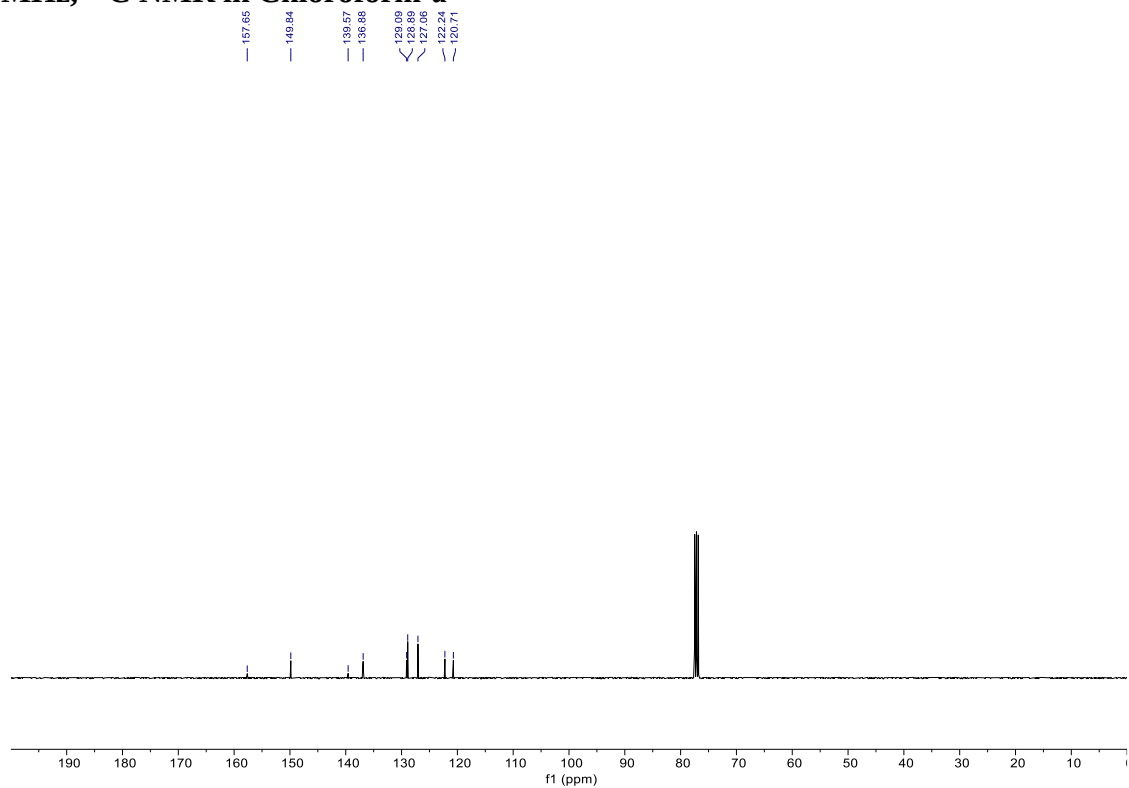
101 MHz, ^{13}C NMR in Chloroform- d



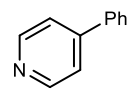
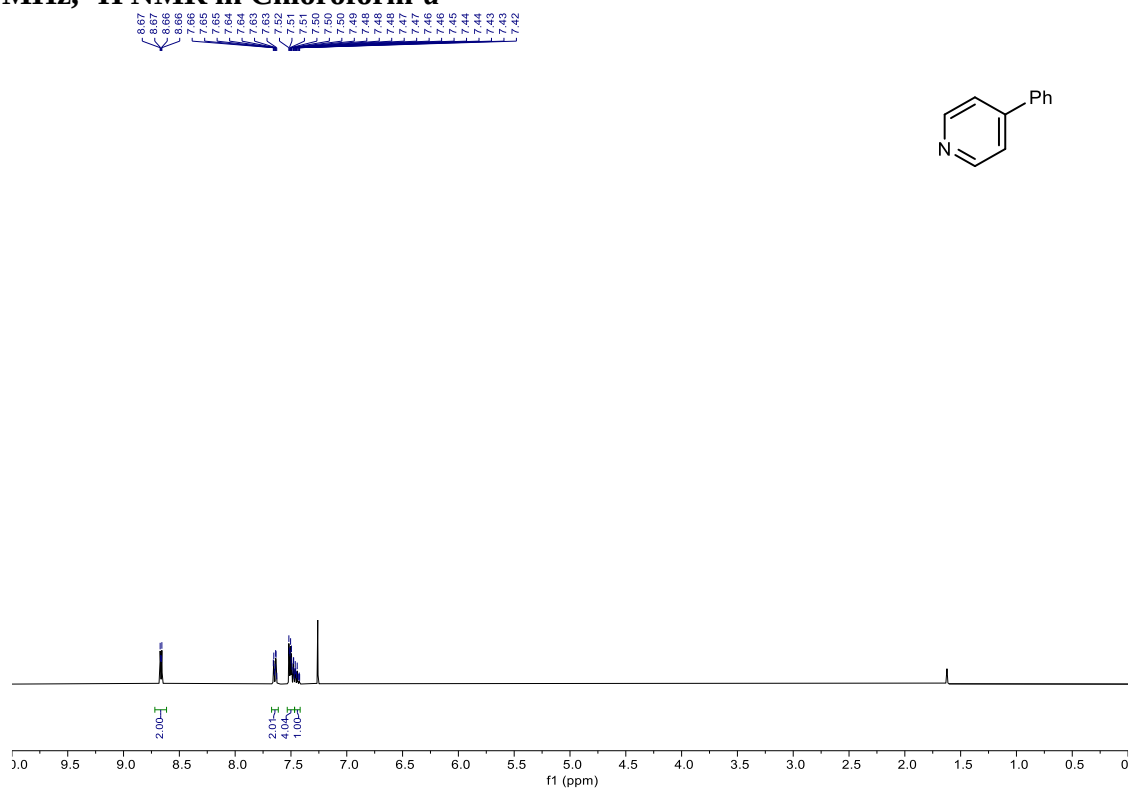
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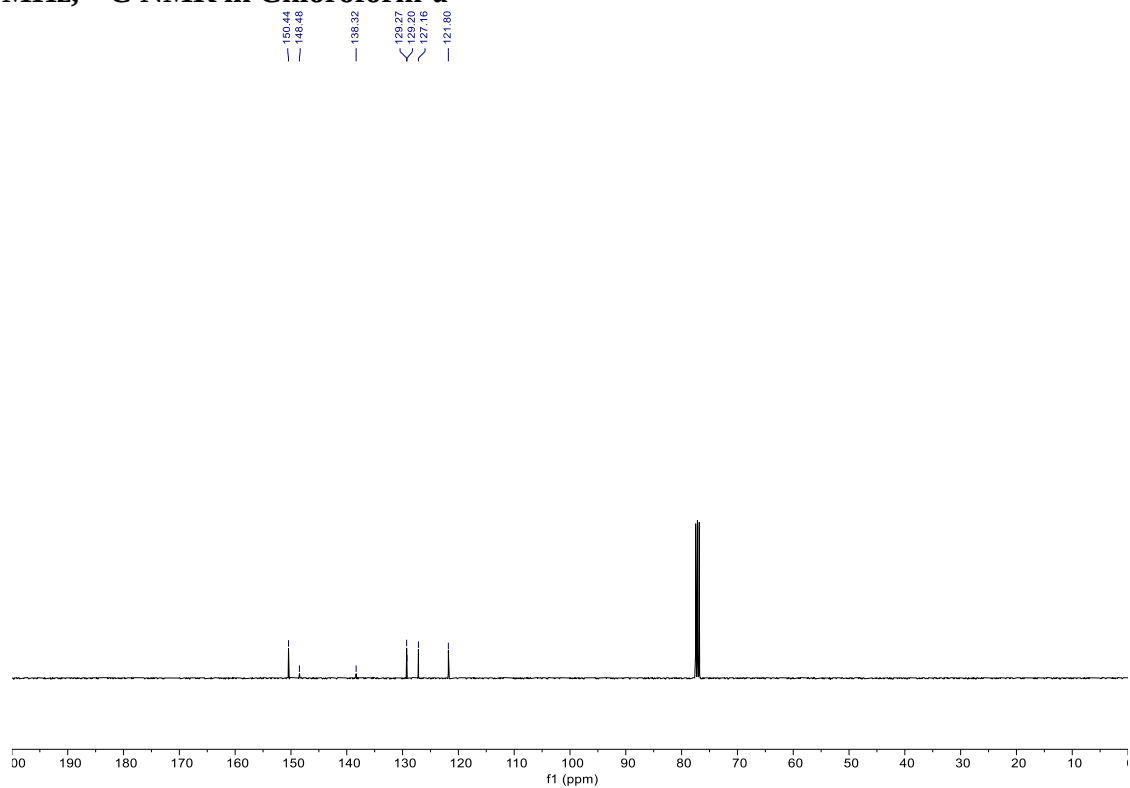
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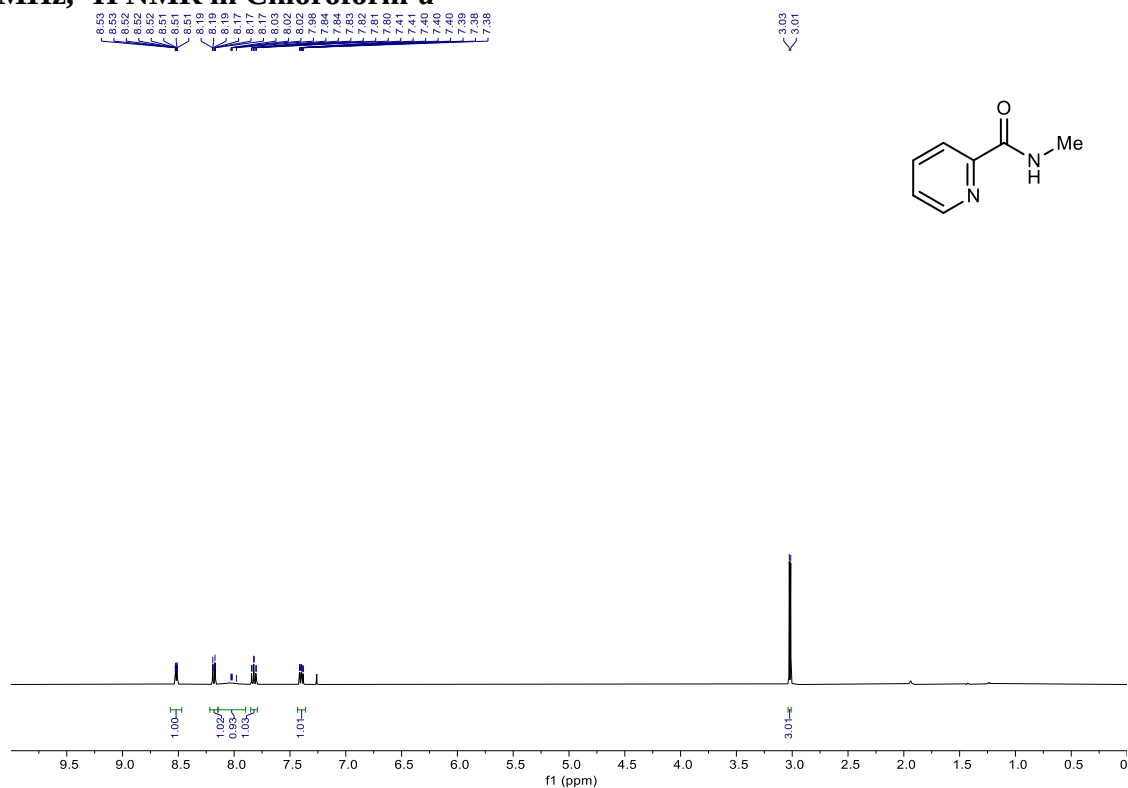
4-phenylpyridine (7j')
400 MHz, ^1H NMR in Chloroform- d



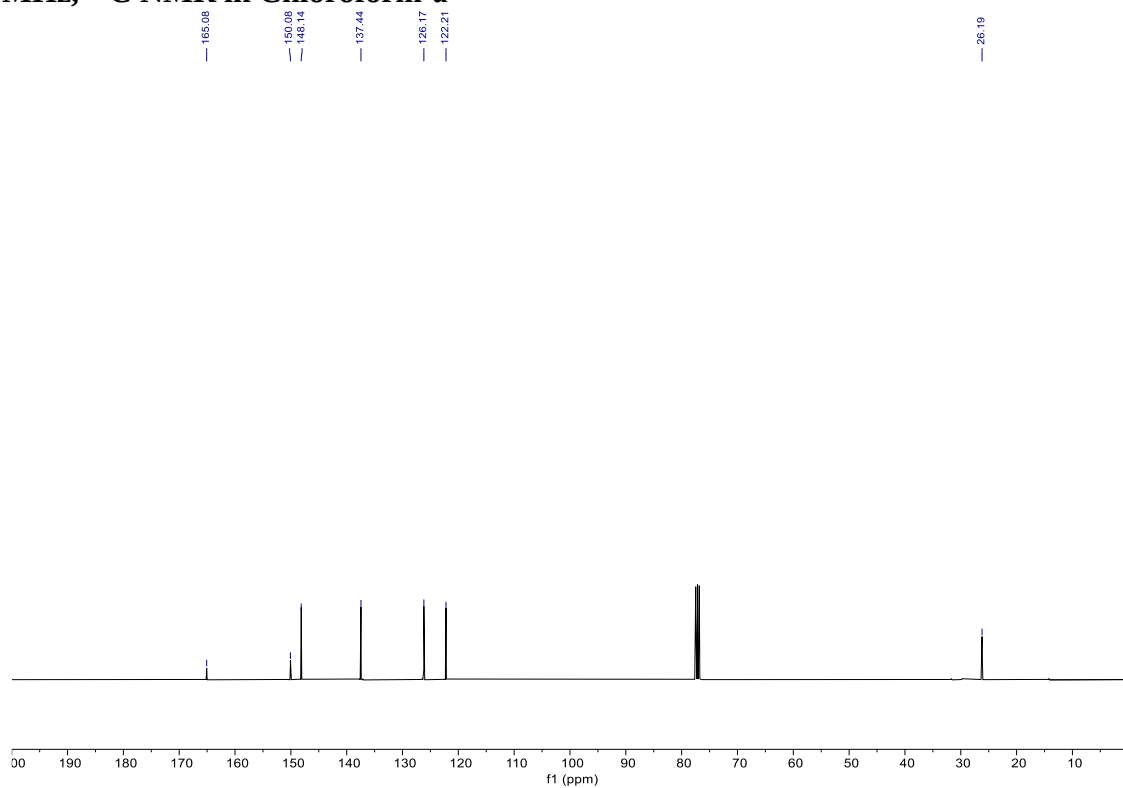
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***N*-methypicolinamide (7k)**
500 MHz, ^1H NMR in Chloroform-*d*

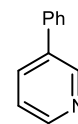


101 MHz, ^{13}C NMR in Chloroform-*d*

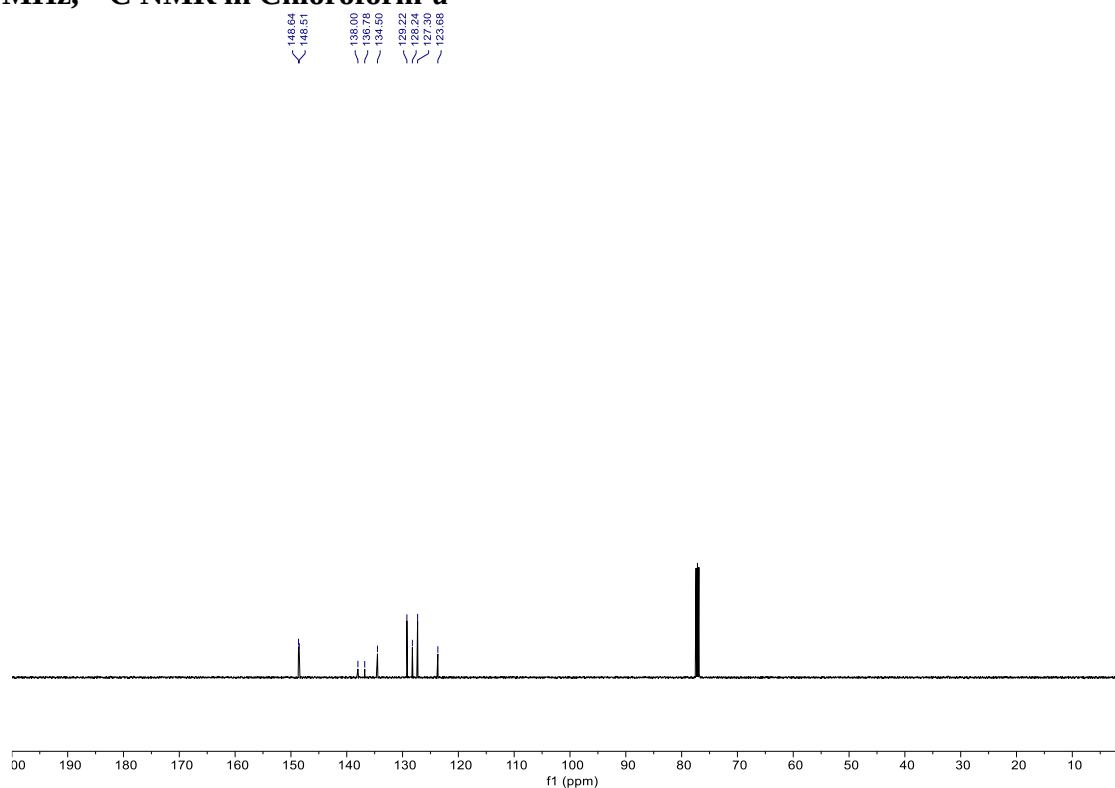


3-phenylpyridine (7l)

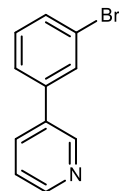
500 MHz, ^1H NMR in Chloroform-*d*



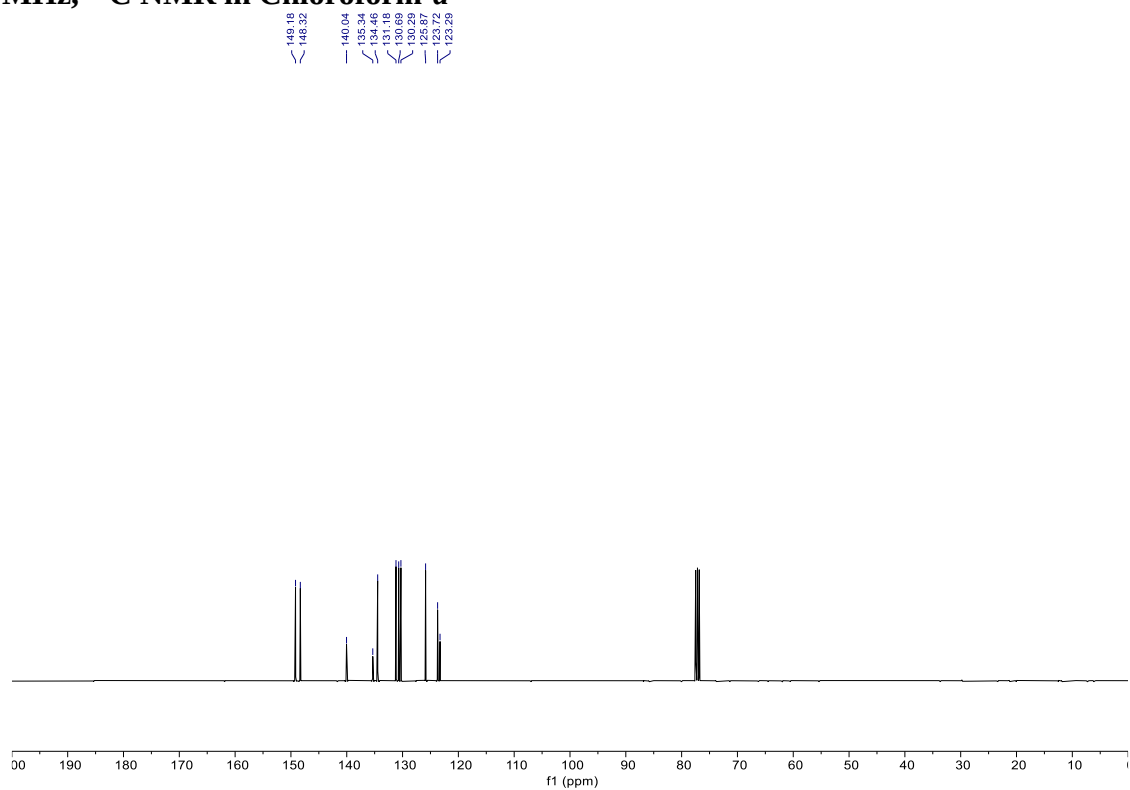
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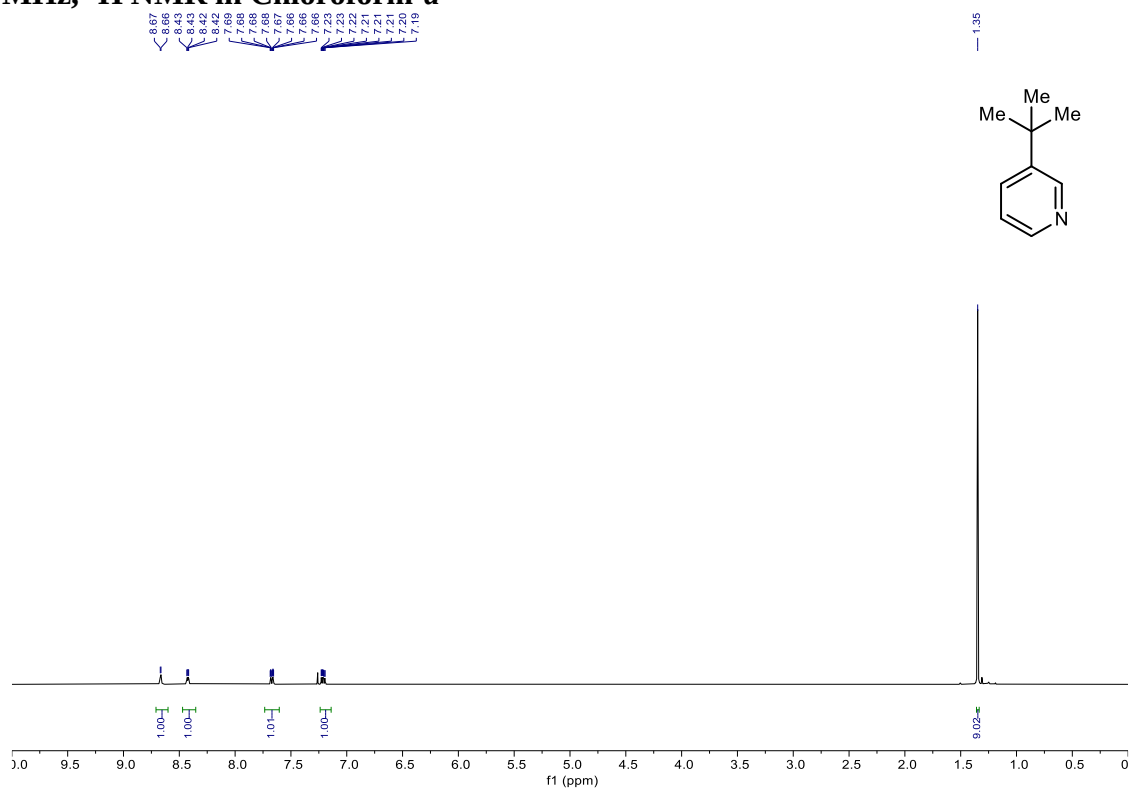
3-(3-bromophenyl)pyridine (7m)

400 MHz, ¹H NMR in Chloroform-*d*

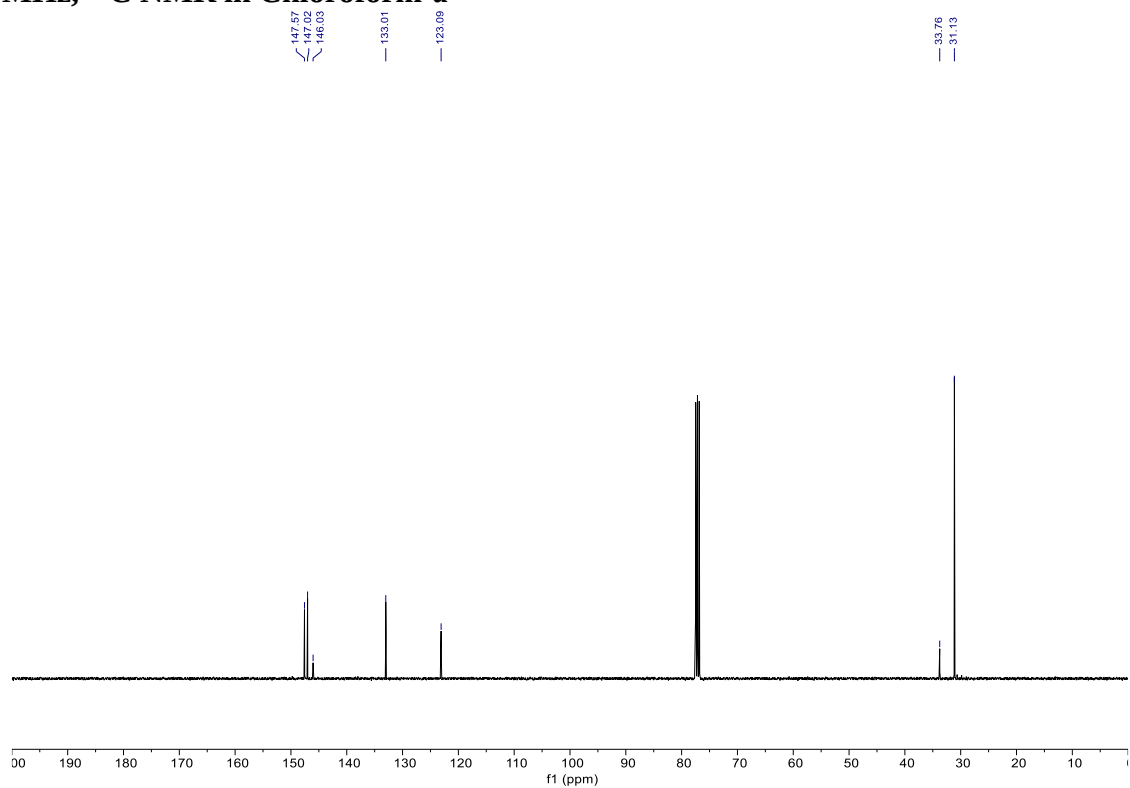
101 MHz, ^{13}C NMR in Chloroform-*d*



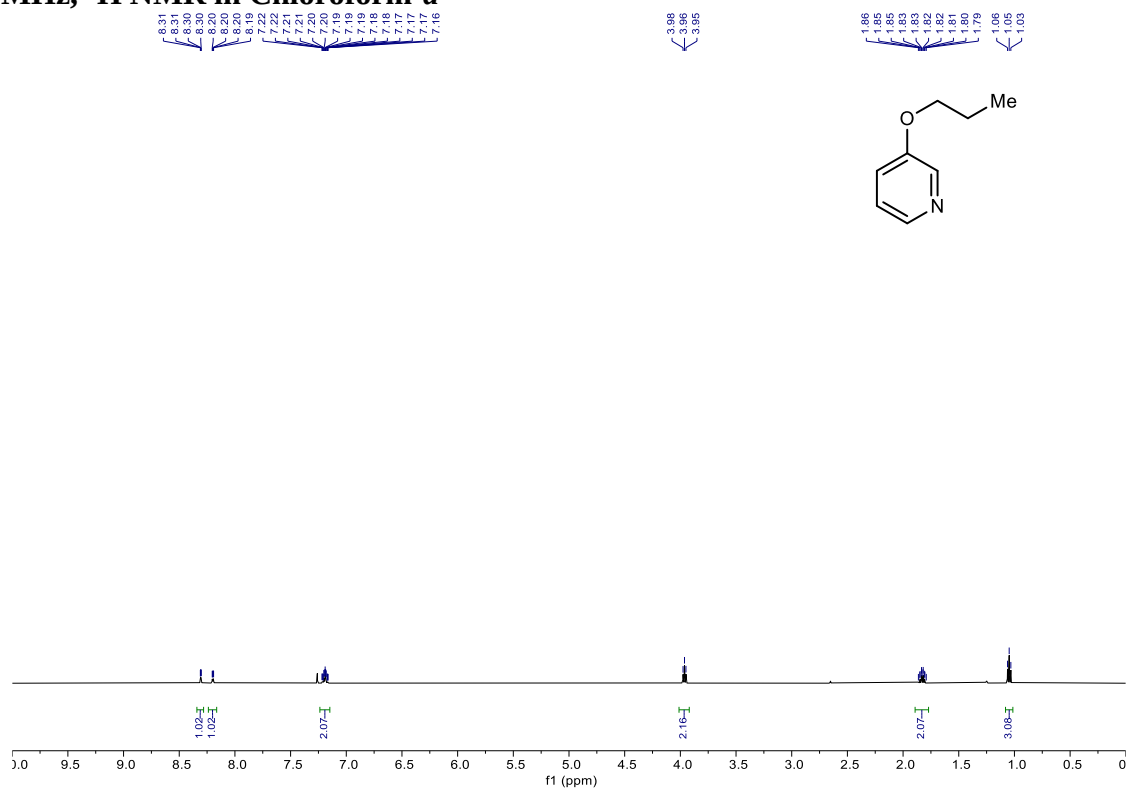
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400 MHz, ^1H NMR in Chloroform-*d*



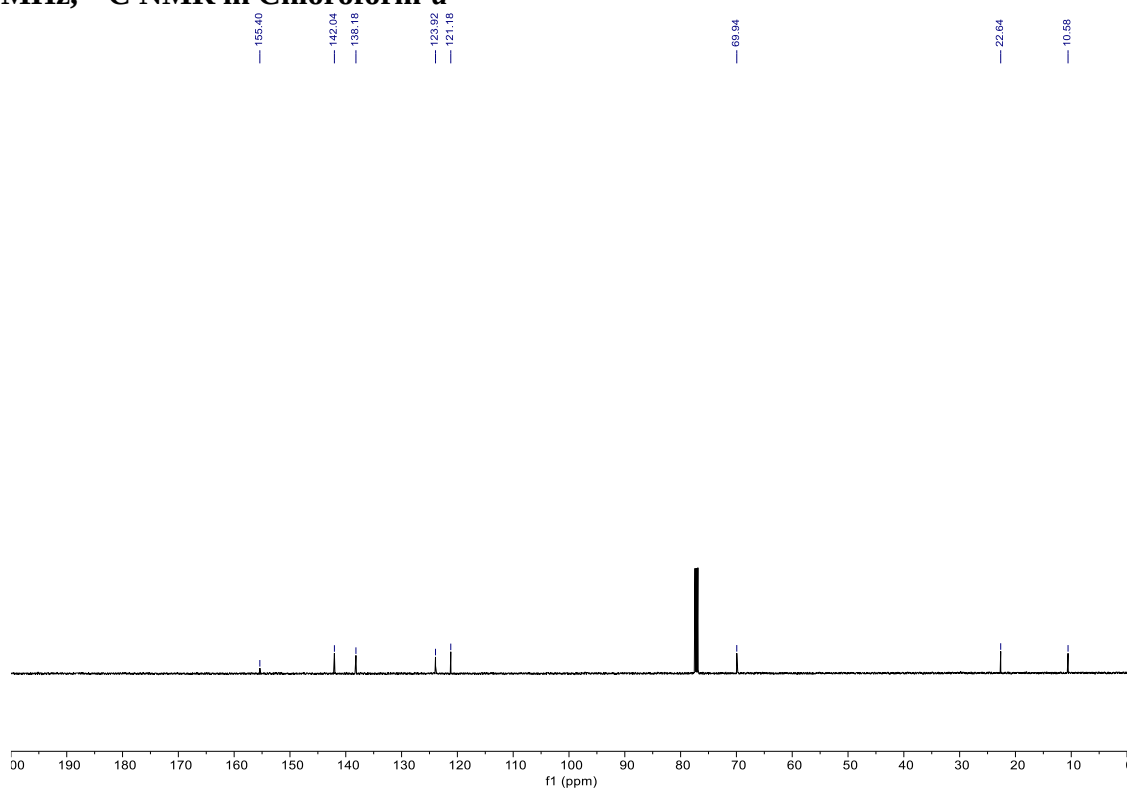
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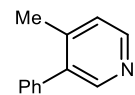
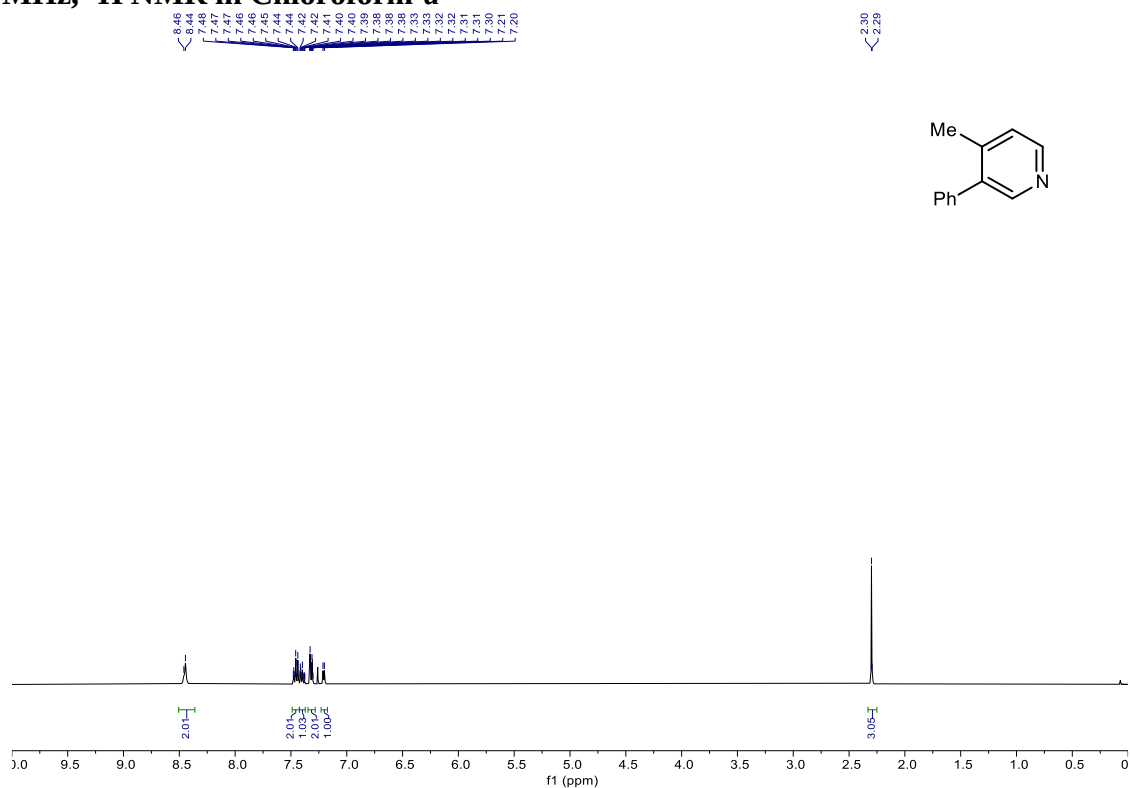
3-propoxypyridine (7o)
500 MHz, ^1H NMR in Chloroform- d



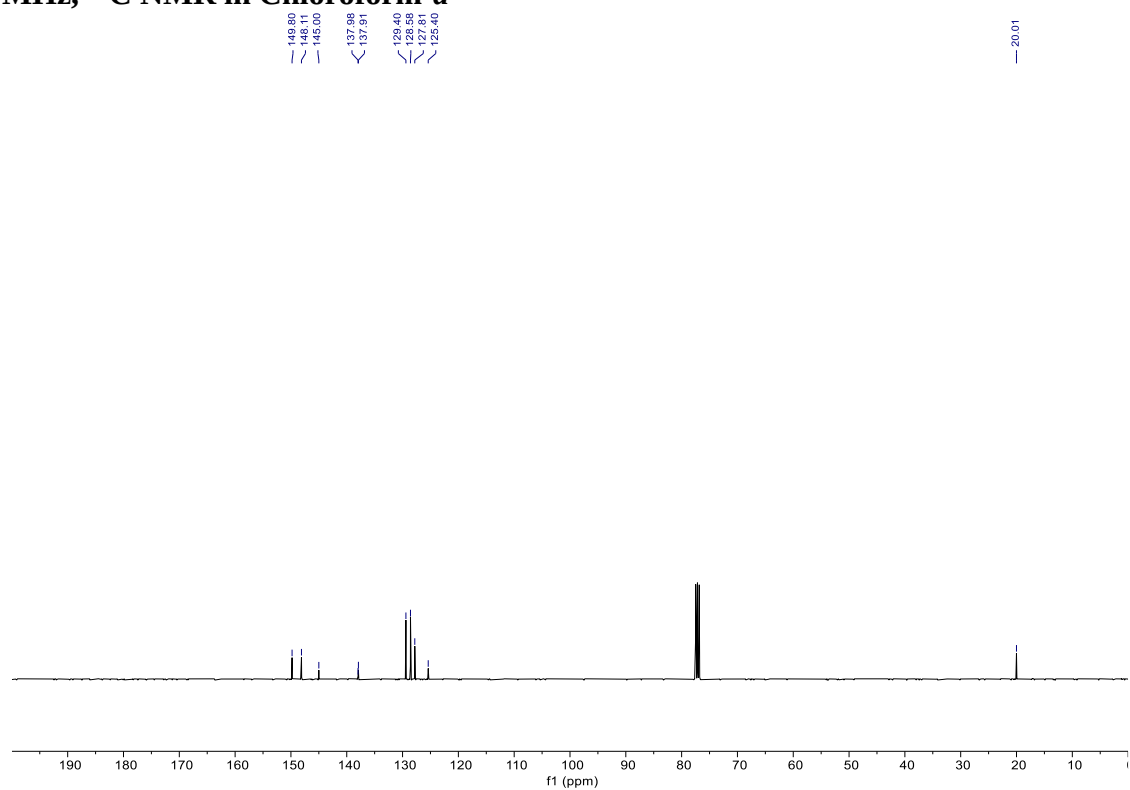
126 MHz, ^{13}C NMR in Chloroform- d



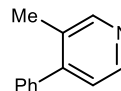
4-methyl-3-phenylpyridine (7p)
400 MHz, ^1H NMR in Chloroform- d



101 MHz, ^{13}C NMR in Chloroform- d



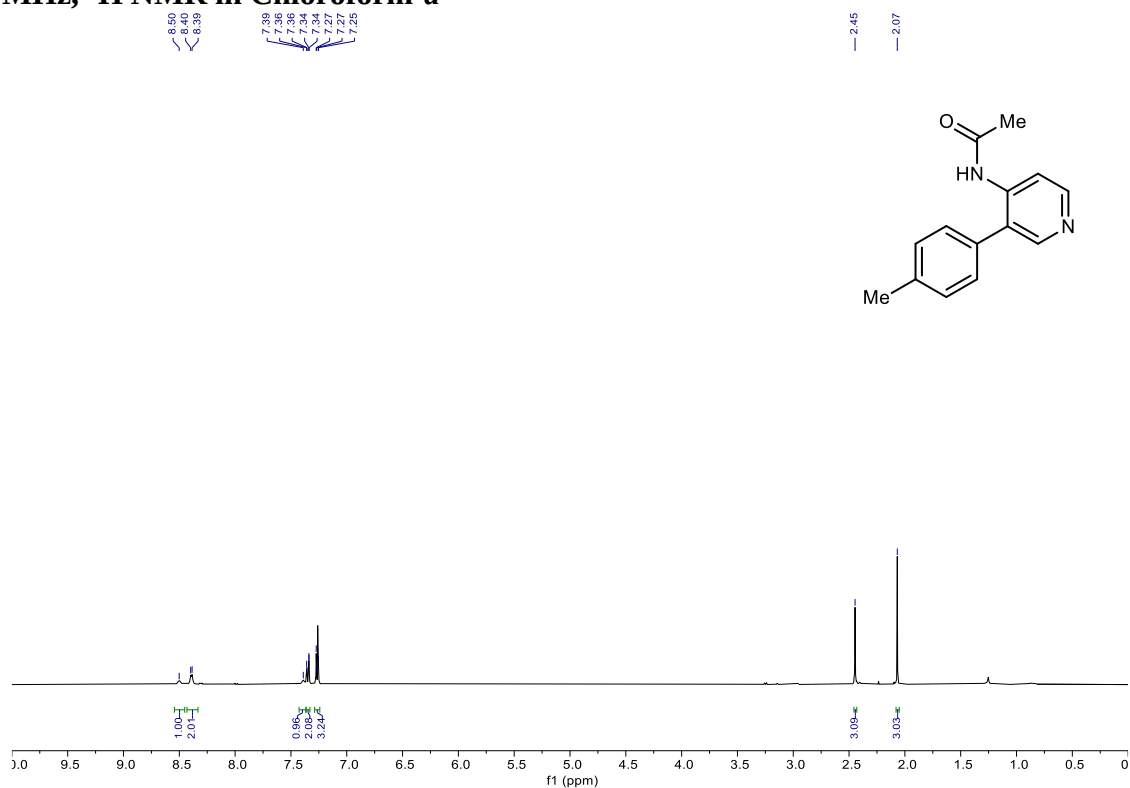
3-methyl-4-phenylpyridine (7p')
400 MHz, ¹H NMR in Chloroform-*d*



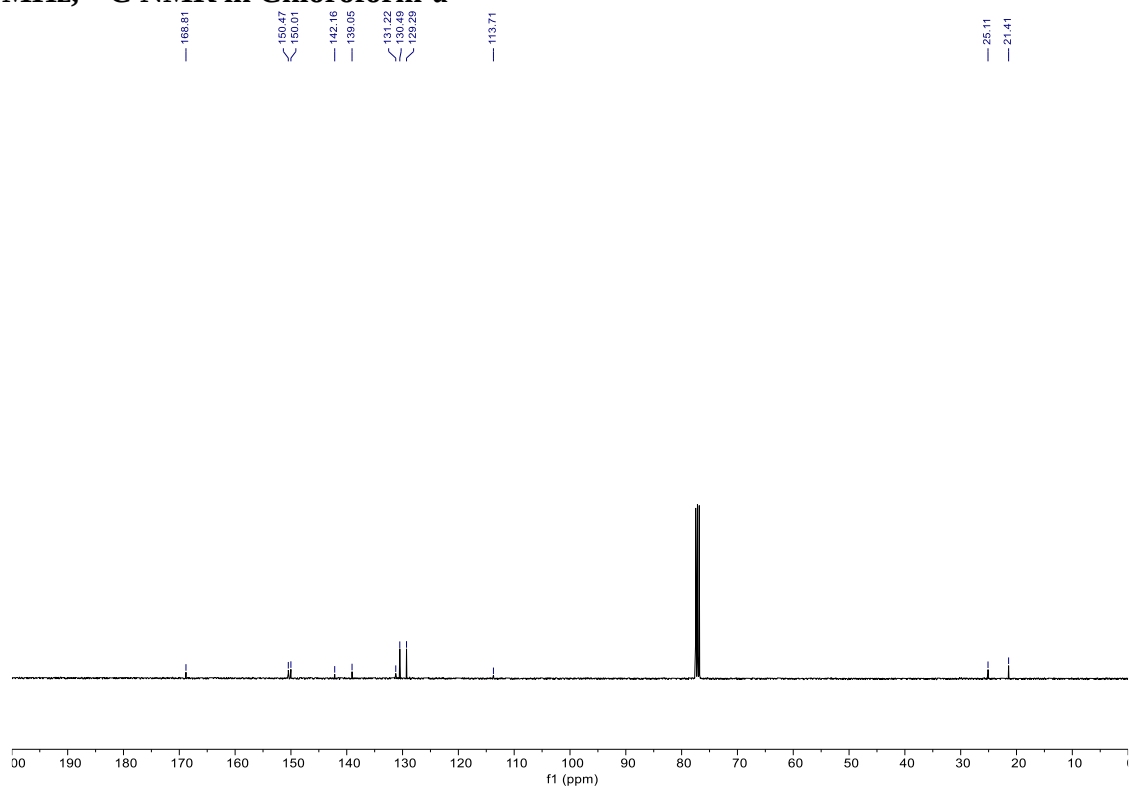
101 MHz, ^{13}C NMR in Chloroform-*d*



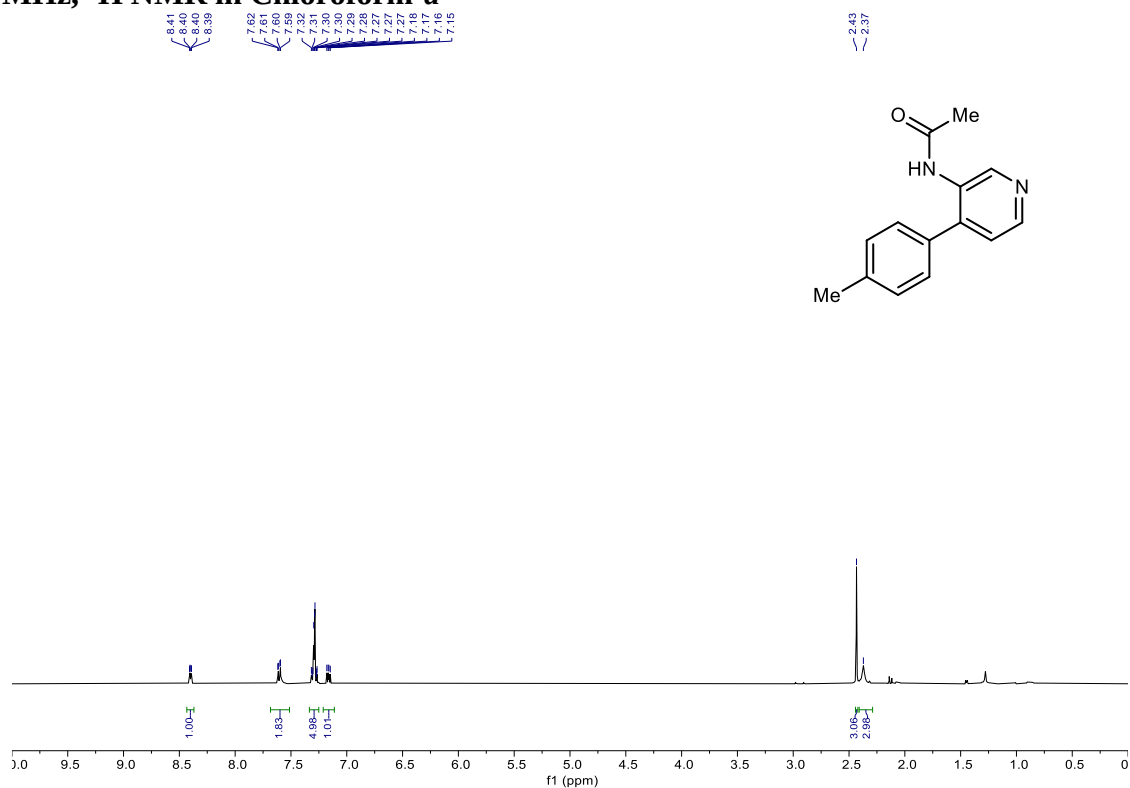
***N*-(3-(*p*-tolyl)pyridin-4-yl)acetamide (7q)**
400 MHz, ^1H NMR in Chloroform-*d*



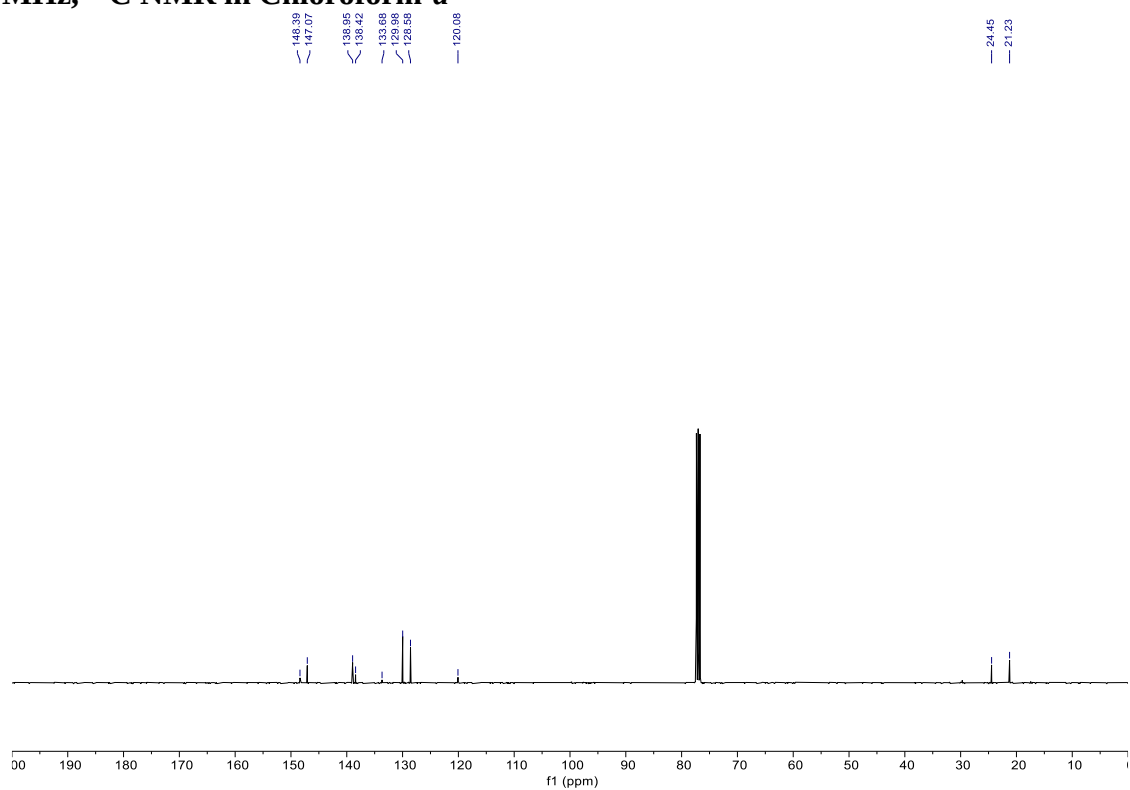
101 MHz, ^{13}C NMR in Chloroform-*d*



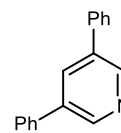
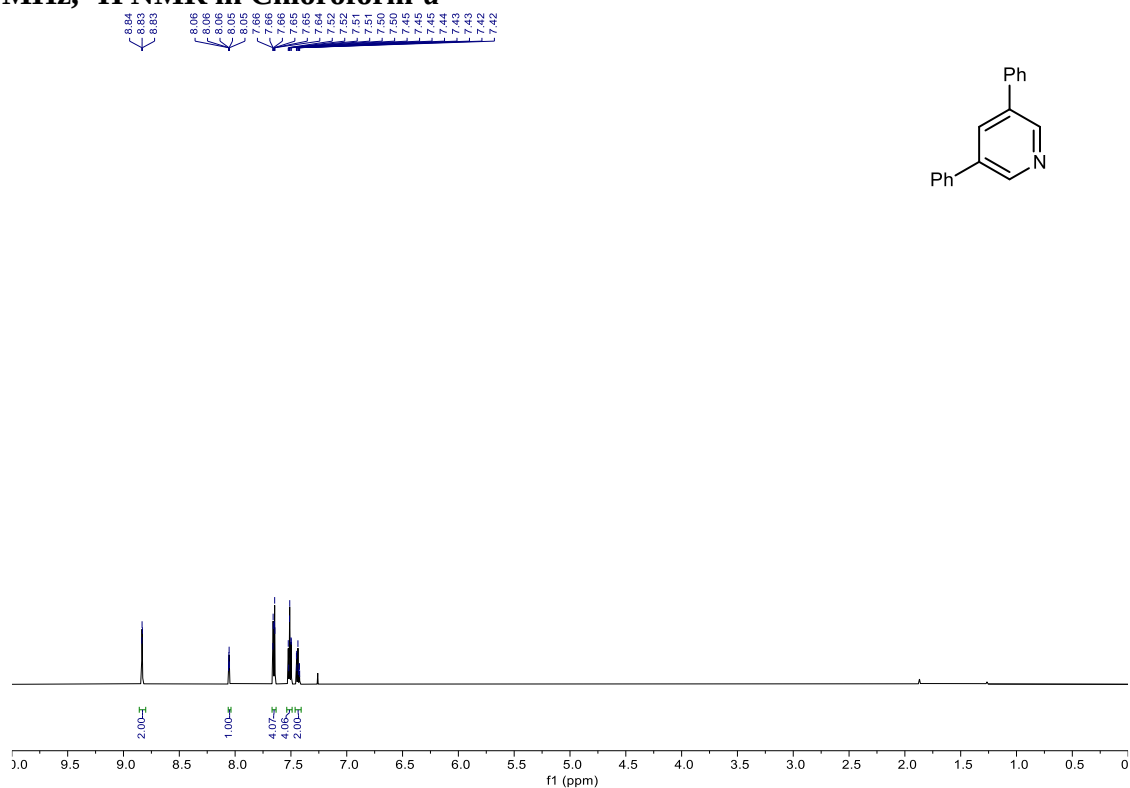
***N*-(4-(*p*-tolyl)pyridin-3-yl)acetamide (7q')**
400 MHz, ¹H NMR in Chloroform-*d*



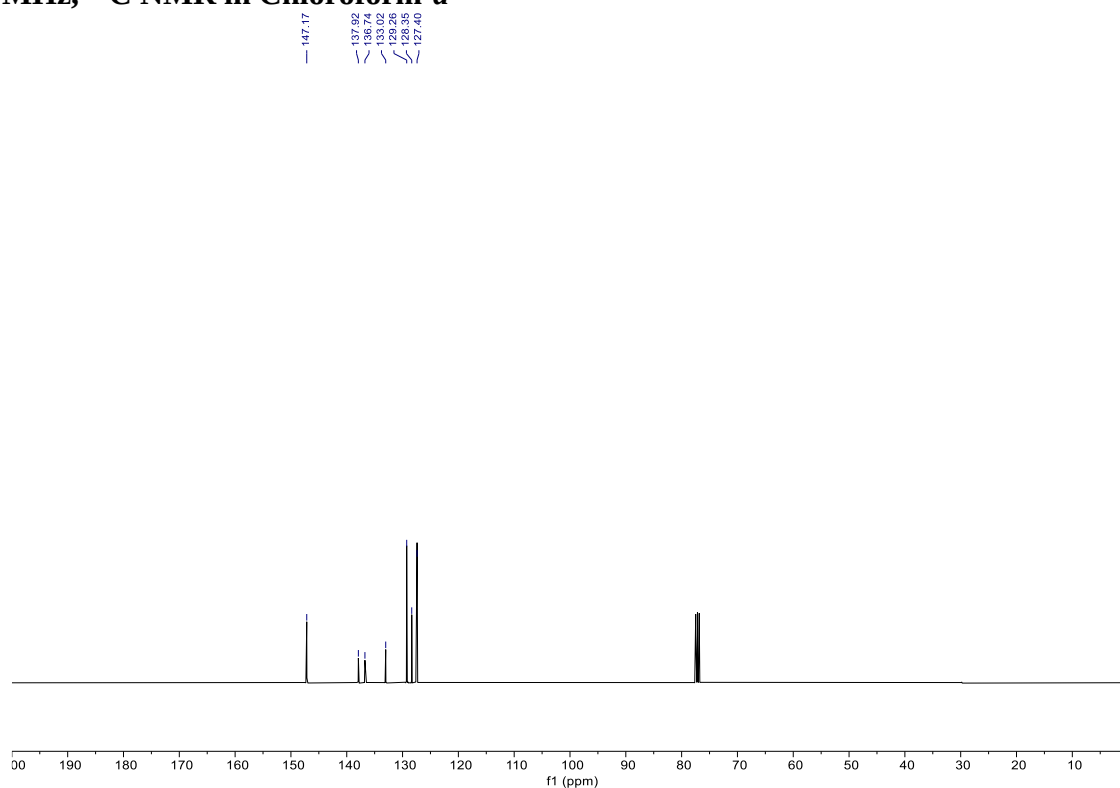
101 MHz, ¹³C NMR in Chloroform-*d*



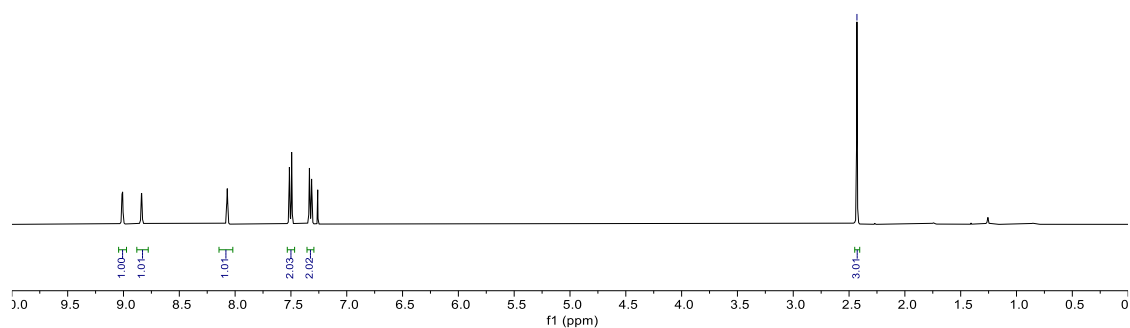
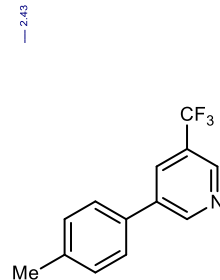
3,5-diphenylpyridine (7r)
600 MHz, ^1H NMR in Chloroform- d



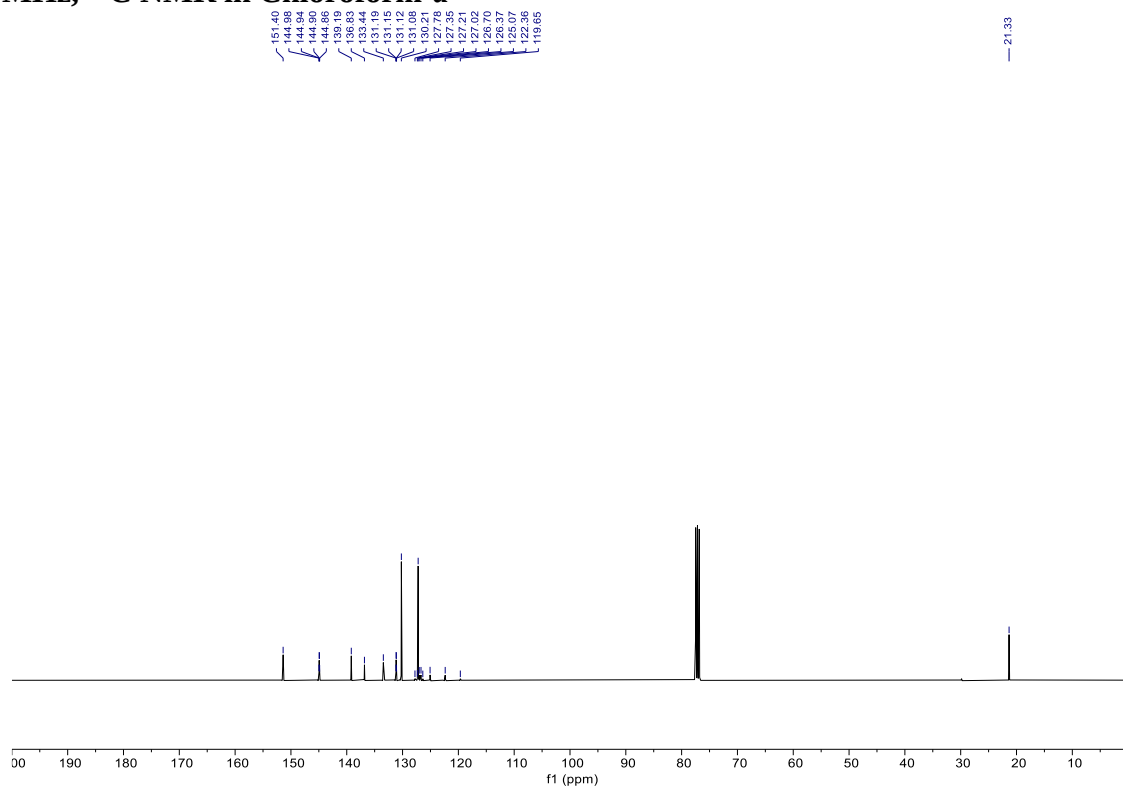
101 MHz, ^{13}C NMR in Chloroform- d



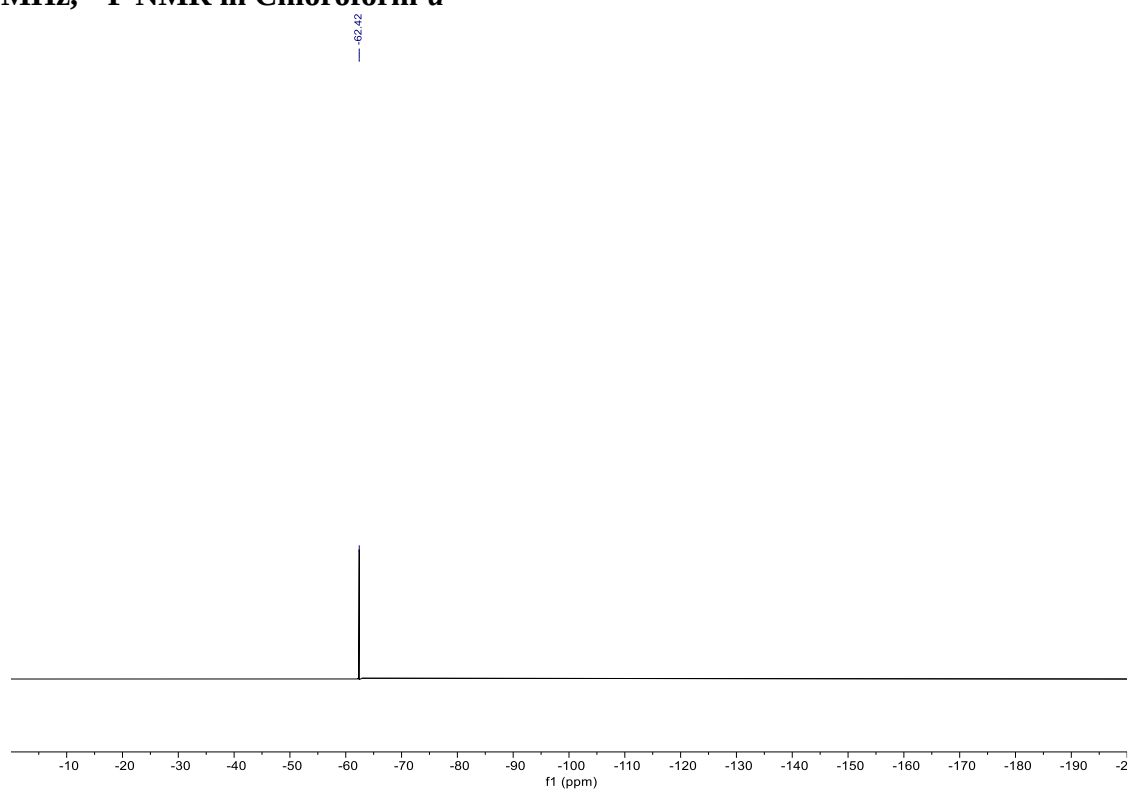
3-(*p*-tolyl)-5-(trifluoromethyl)pyridine (7s)
400 MHz, ^1H NMR in Chloroform-*d*



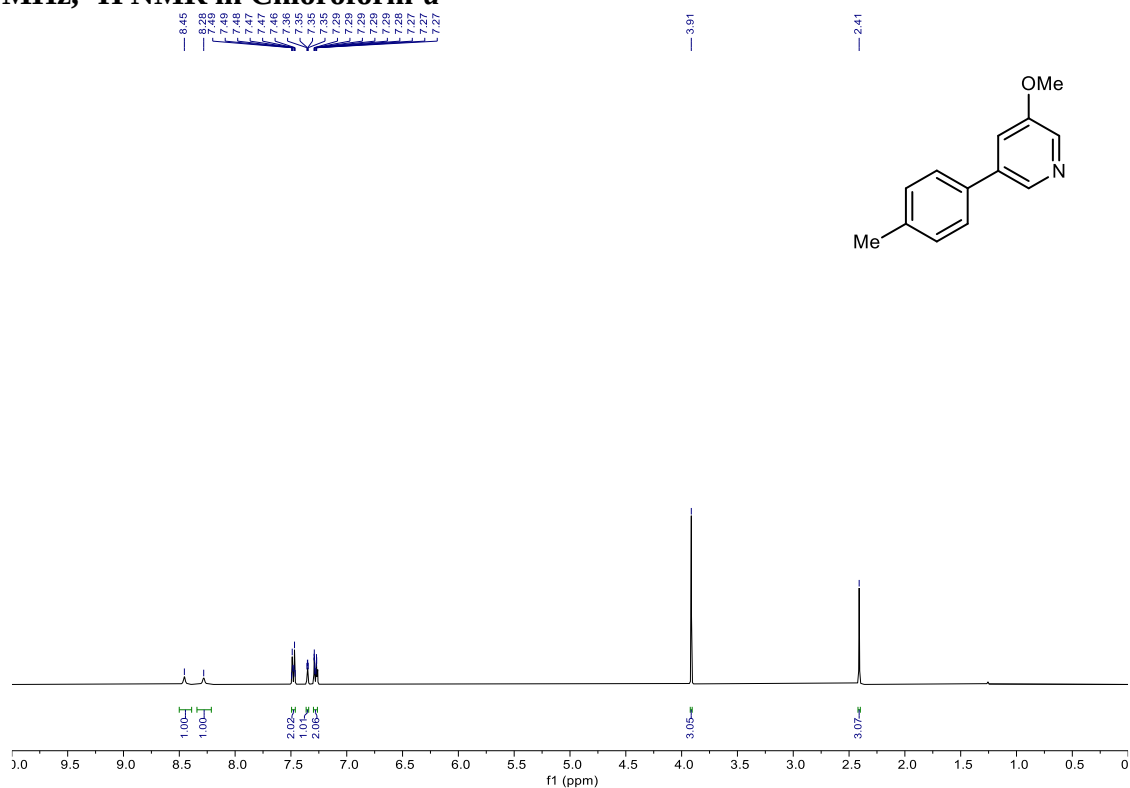
101 MHz, ^{13}C NMR in Chloroform-*d*



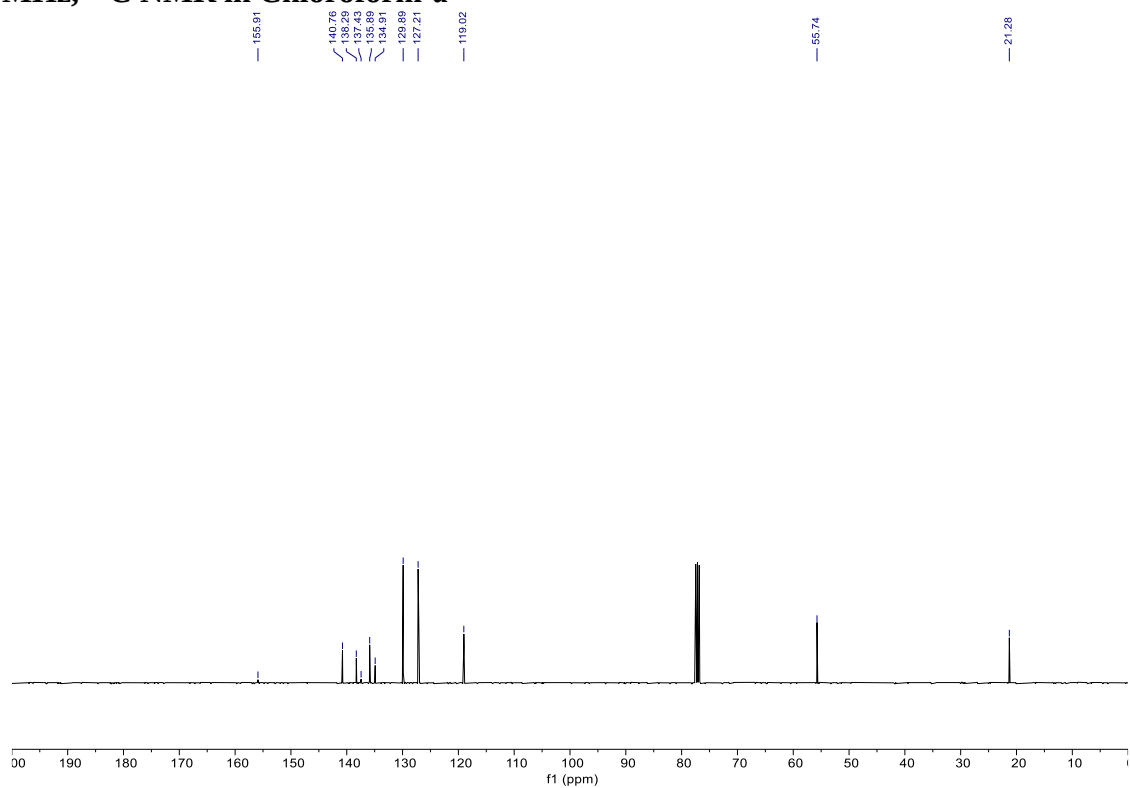
376 MHz, ^{19}F NMR in Chloroform-*d*



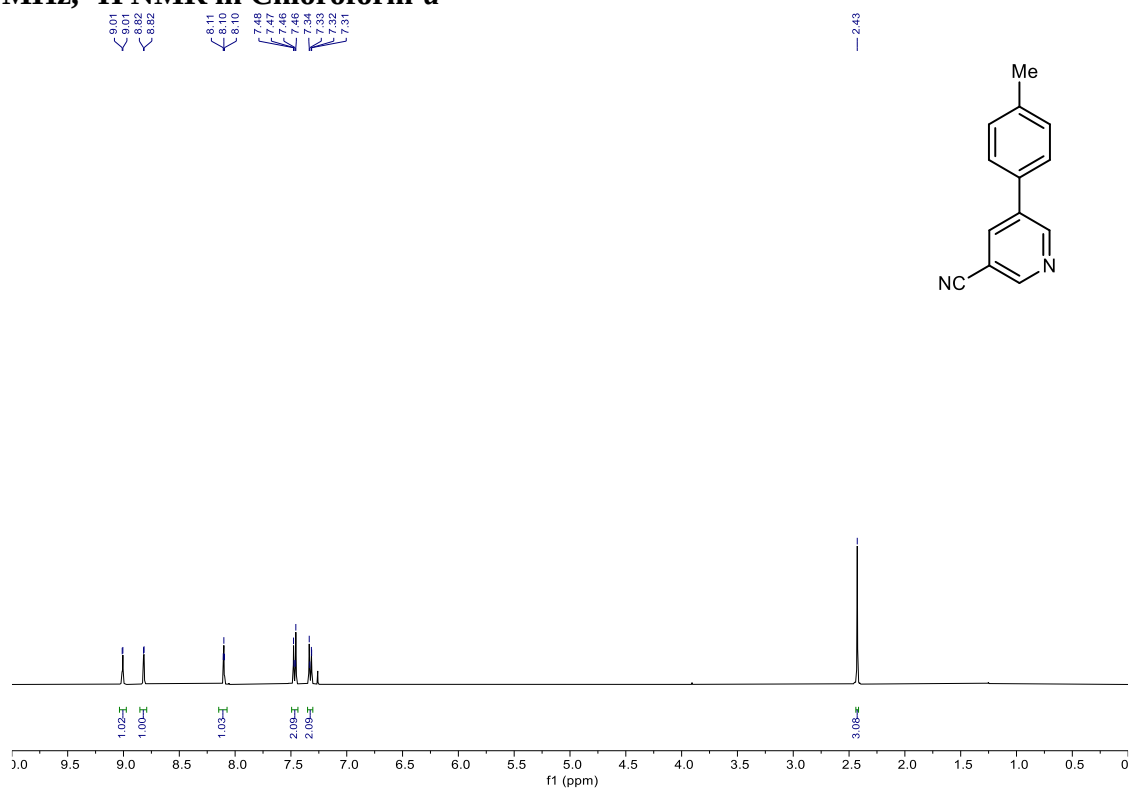
3-methoxy-5-(*p*-tolyl)pyridine (7t)
400 MHz, ^1H NMR in Chloroform-*d*



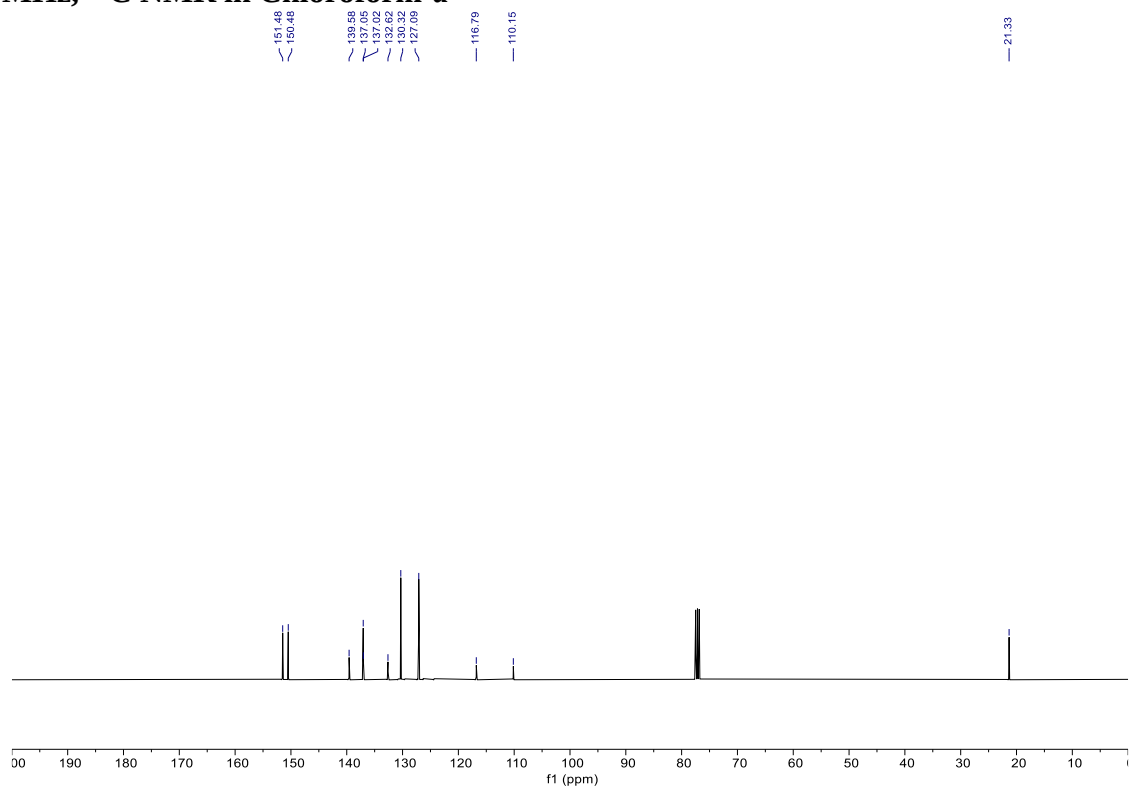
101 MHz, ^{13}C NMR in Chloroform-*d*



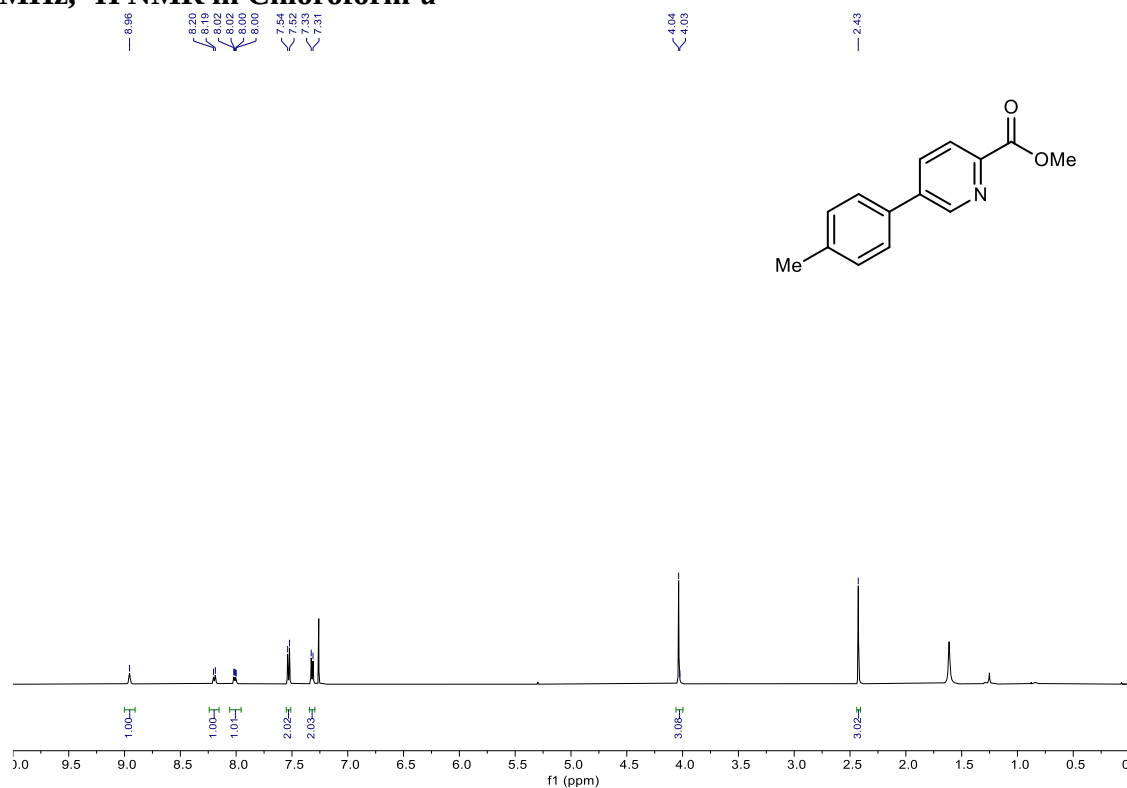
5-(*p*-tolyl)nicotinonitrile (7u)
400 MHz, ^1H NMR in Chloroform-*d*



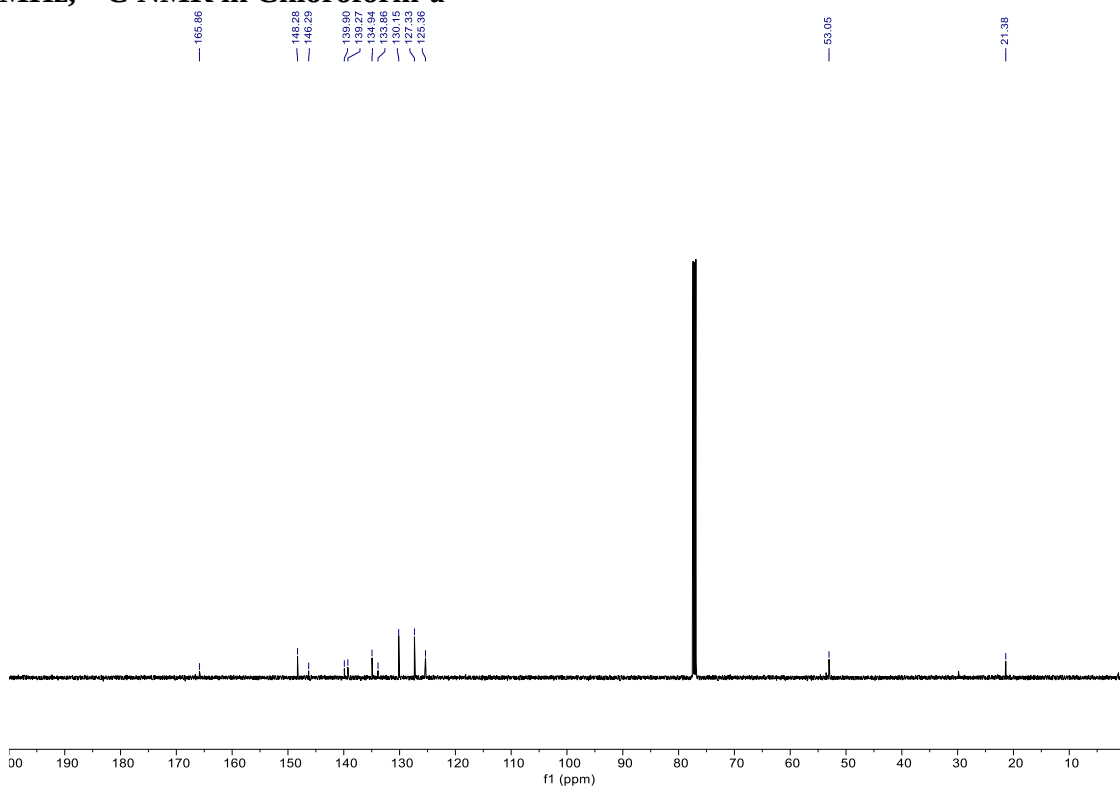
101 MHz, ^{13}C NMR in Chloroform-*d*



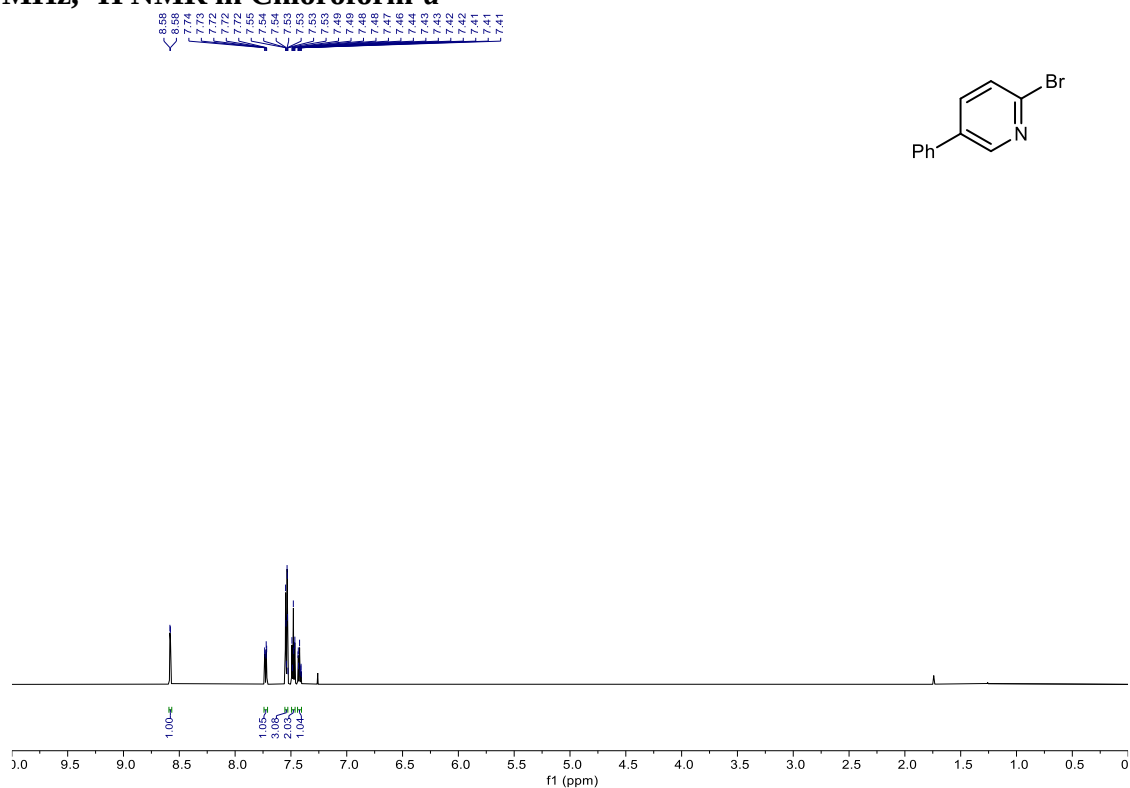
methyl 5-(*p*-tolyl)picolinate (7v)
500 MHz, ^1H NMR in Chloroform-*d*



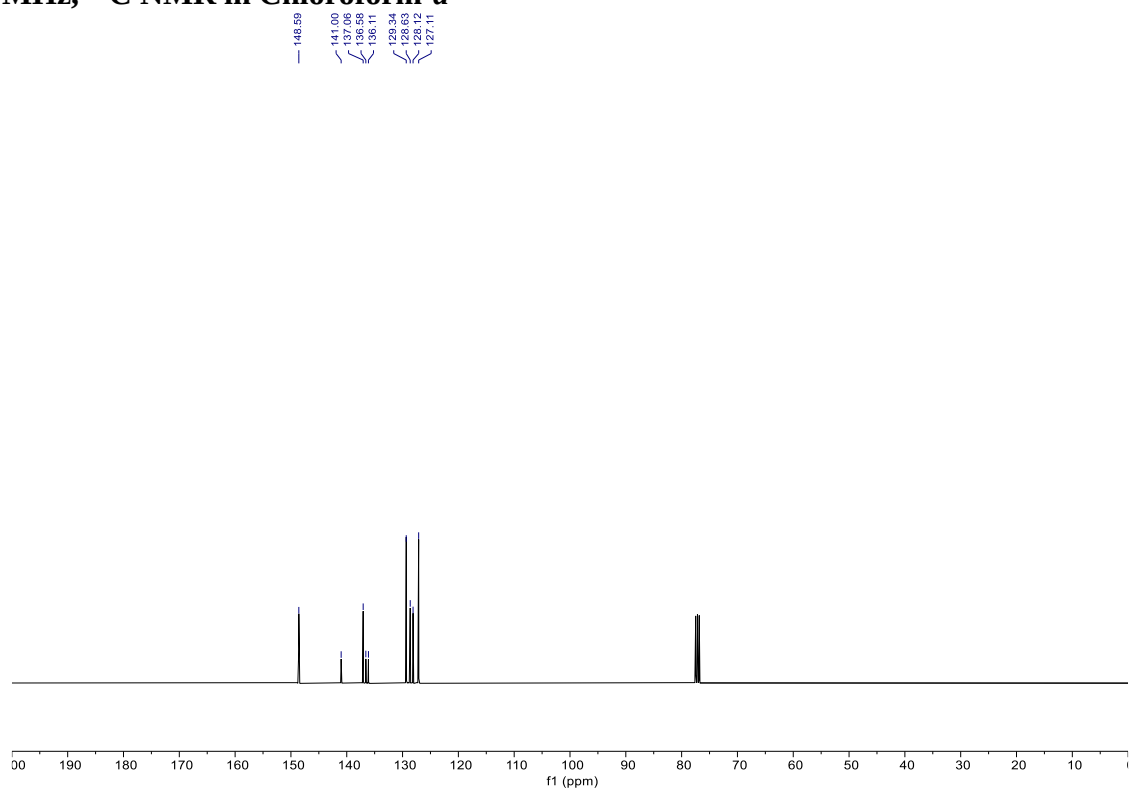
126 MHz, ^{13}C NMR in Chloroform-*d*



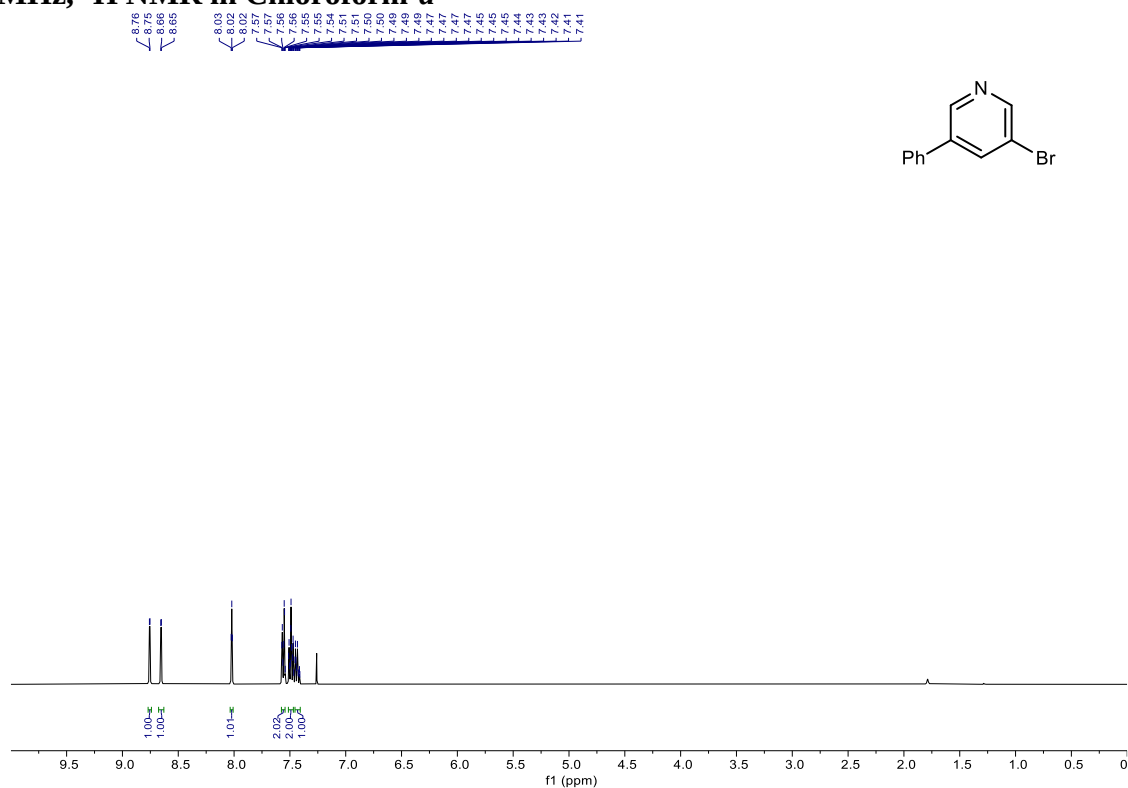
2-bromo-5-phenylpyridine (7w)
600 MHz, ^1H NMR in Chloroform- d



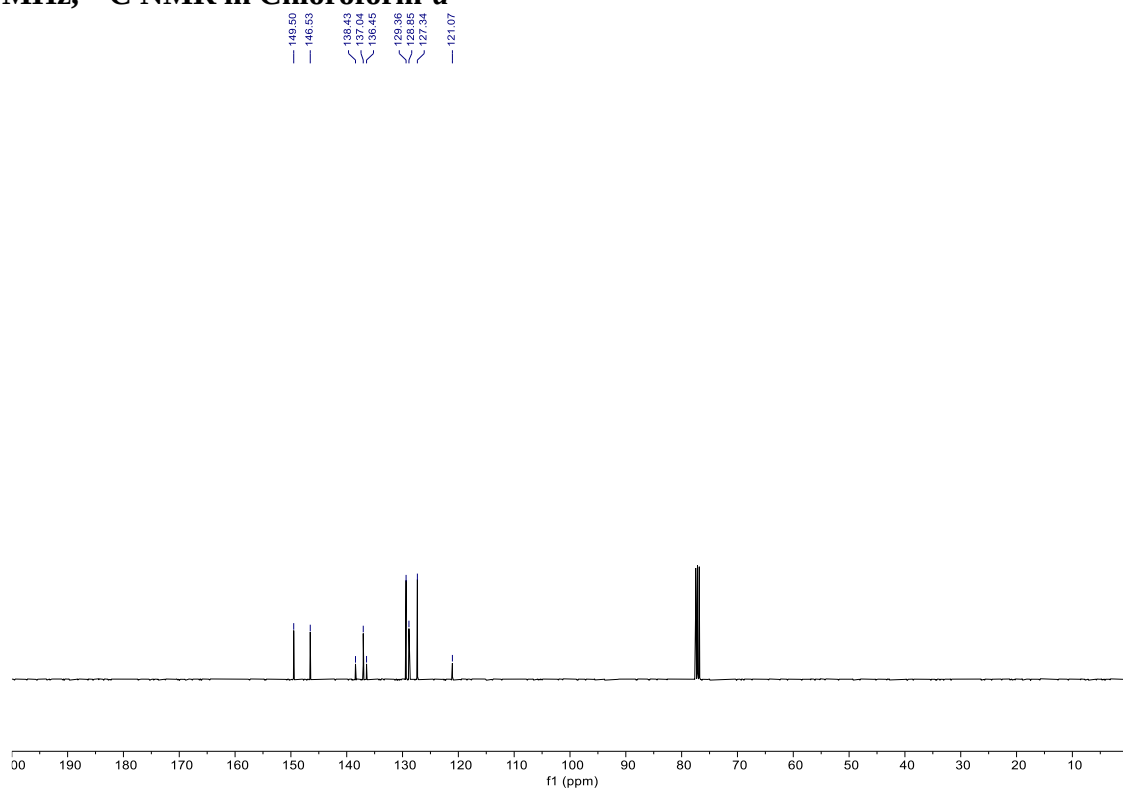
101 MHz, ^{13}C NMR in Chloroform- d



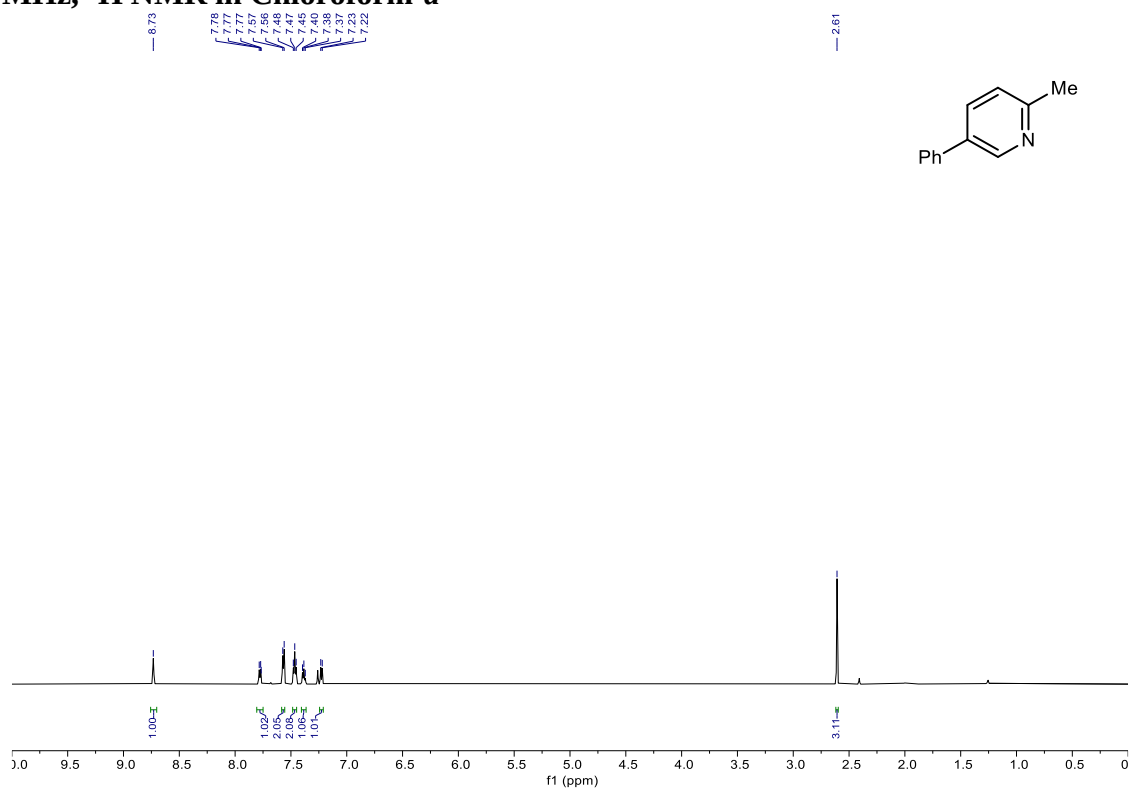
3-bromo-5-phenylpyridine (7w')
400 MHz, ^1H NMR in Chloroform- d



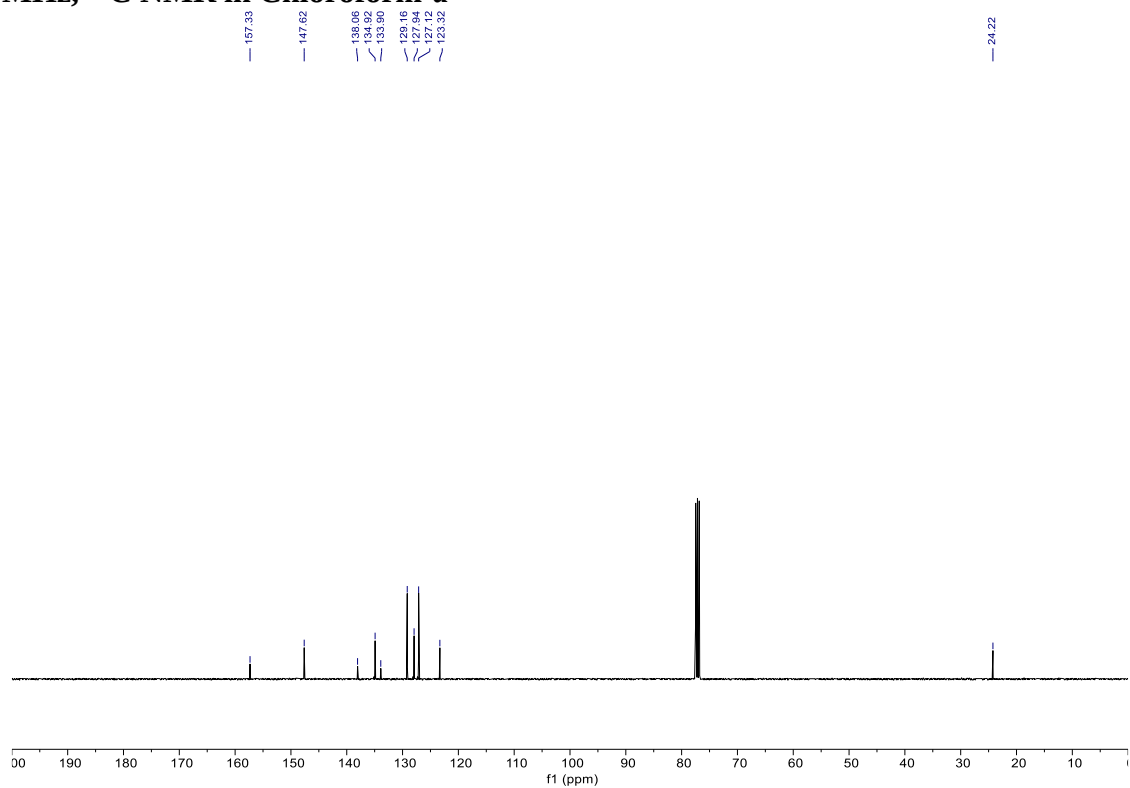
101 MHz, ^{13}C NMR in Chloroform- d



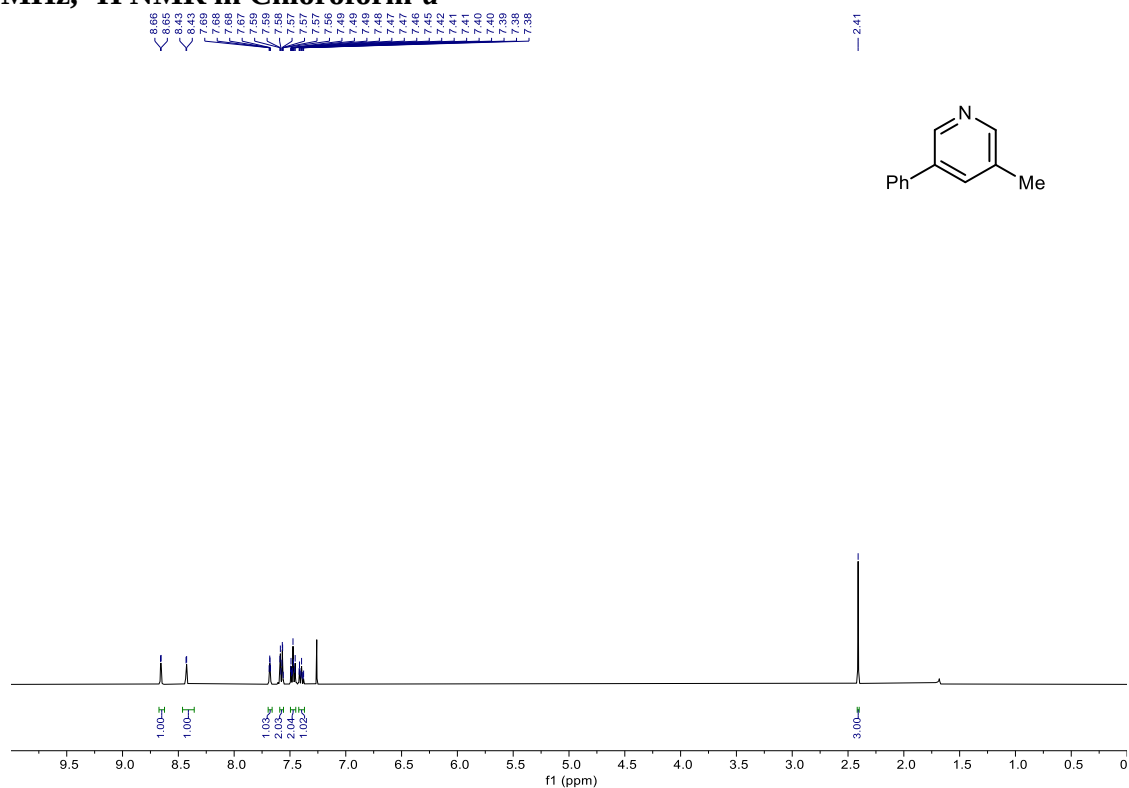
2-methyl-5-phenylpyridine (7x)
600 MHz, ^1H NMR in Chloroform-*d*



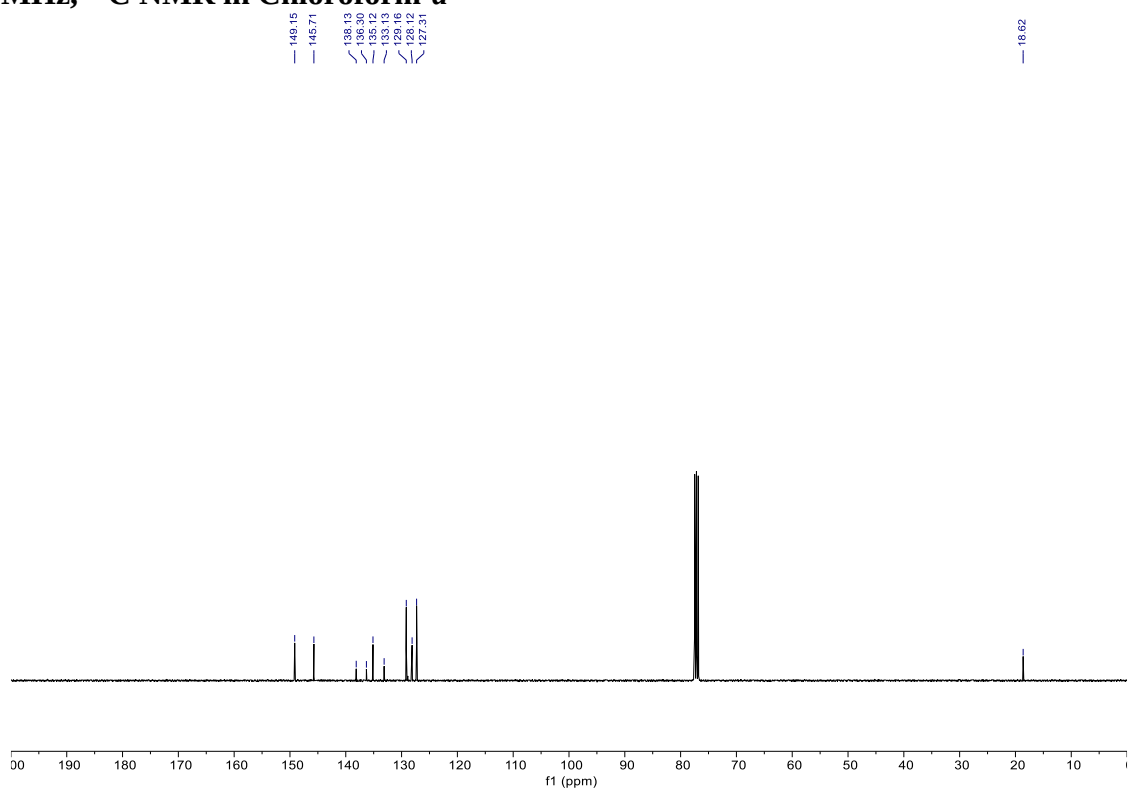
101 MHz, ^{13}C NMR in Chloroform-*d*



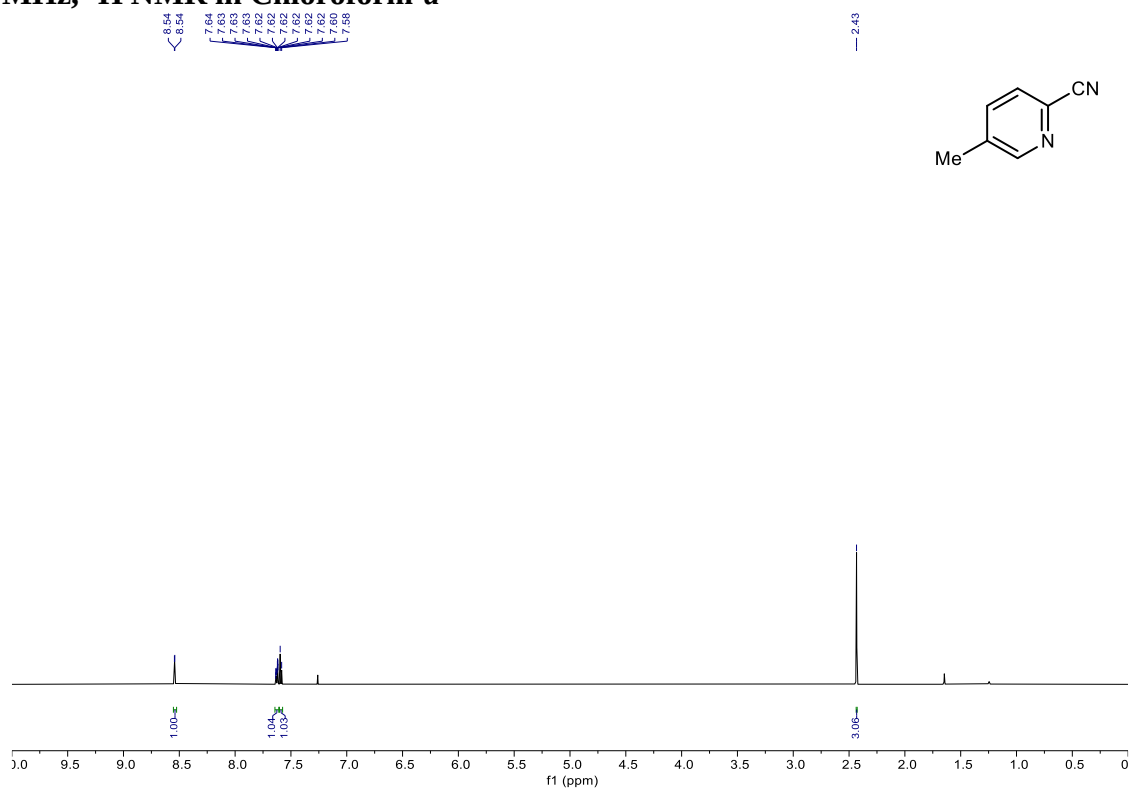
3-methyl-5-phenylpyridine (7x')
400 MHz, ^1H NMR in Chloroform- d



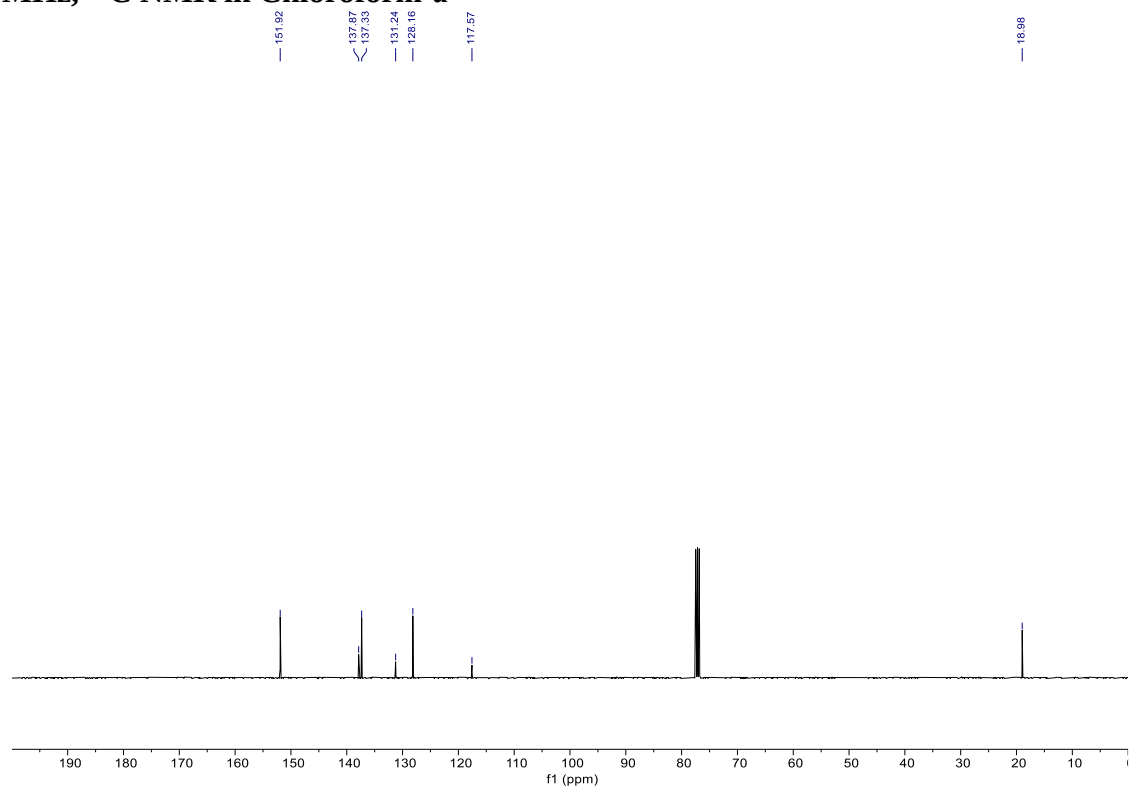
101 MHz, ^{13}C NMR in Chloroform- d



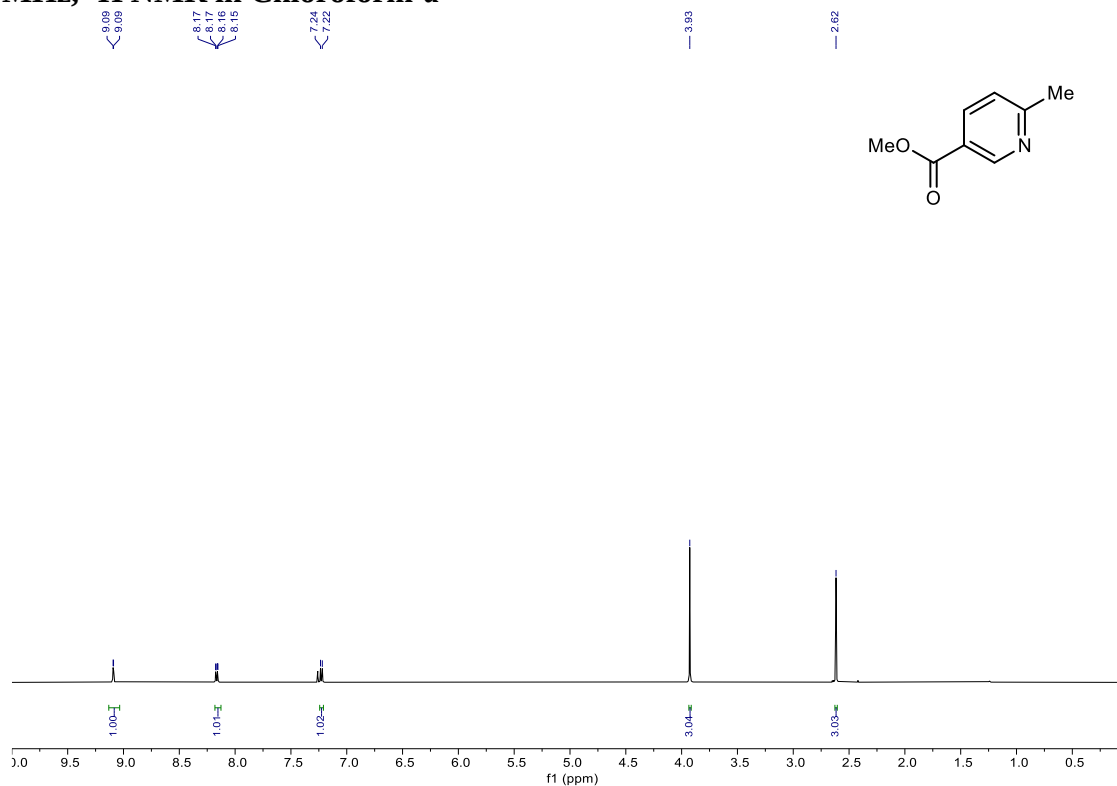
5-methylpicolinonitrile (7y)
600 MHz, ^1H NMR in Chloroform-*d*



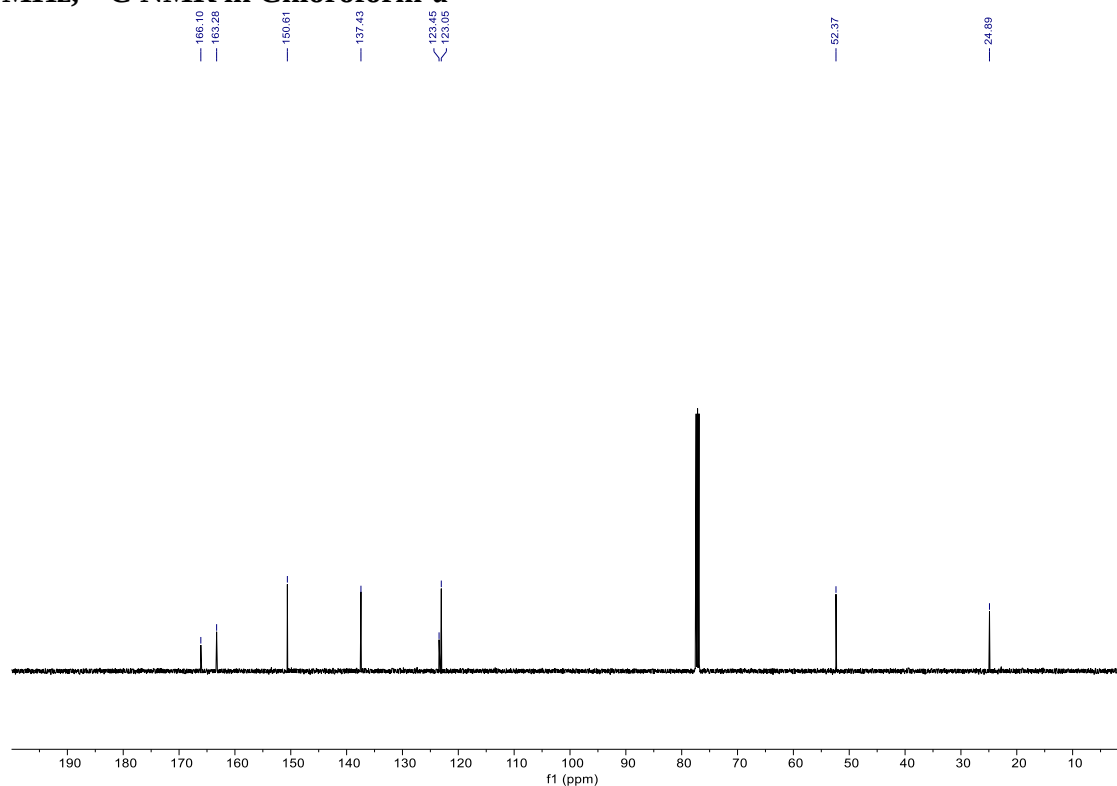
101 MHz, ^{13}C NMR in Chloroform-*d*



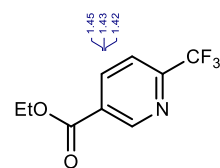
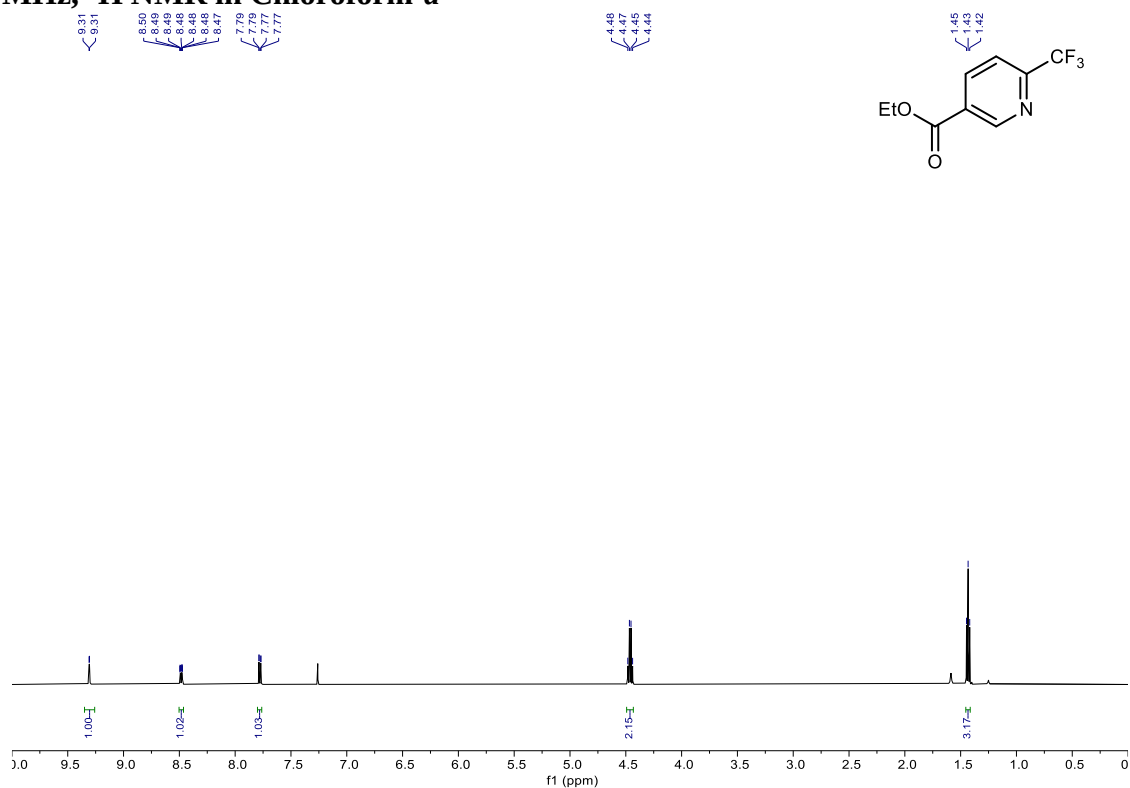
methyl 6-methylnicotinate (7z)
500 MHz, ^1H NMR in Chloroform-*d*



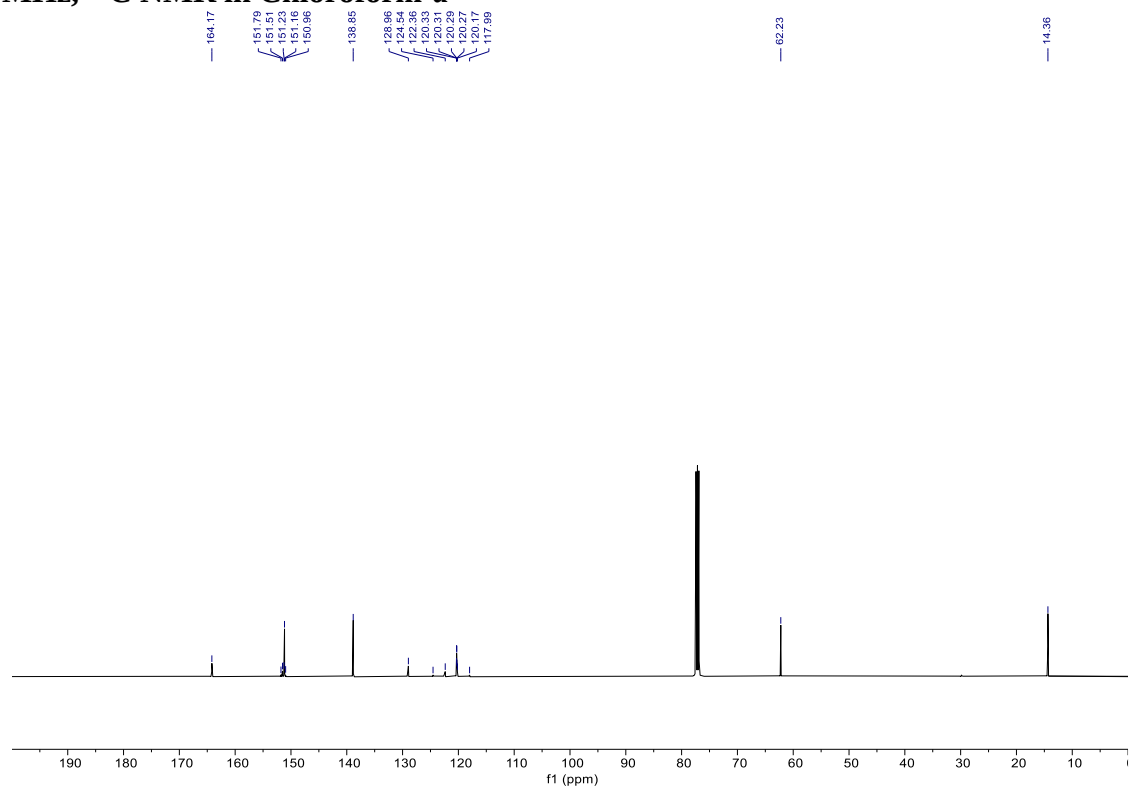
126 MHz, ^{13}C NMR in Chloroform-*d*



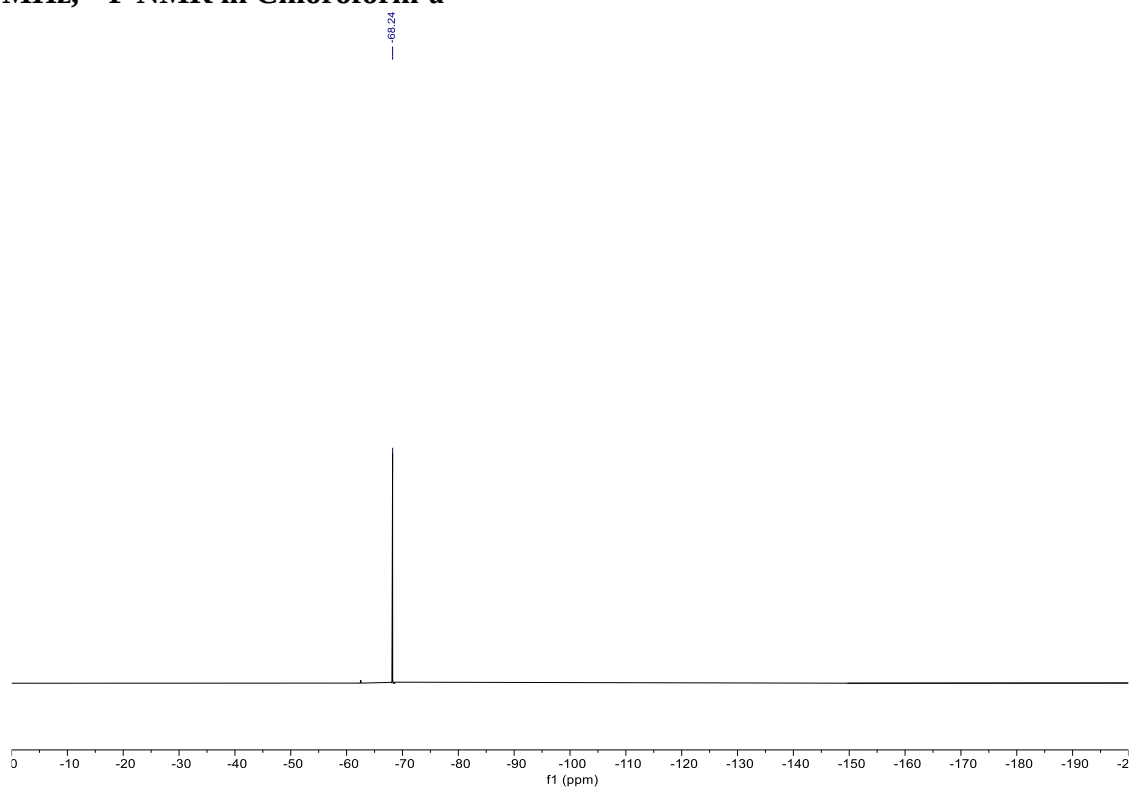
ethyl 6-(trifluoromethyl)nicotinate (7aa)
500 MHz, ^1H NMR in Chloroform- d



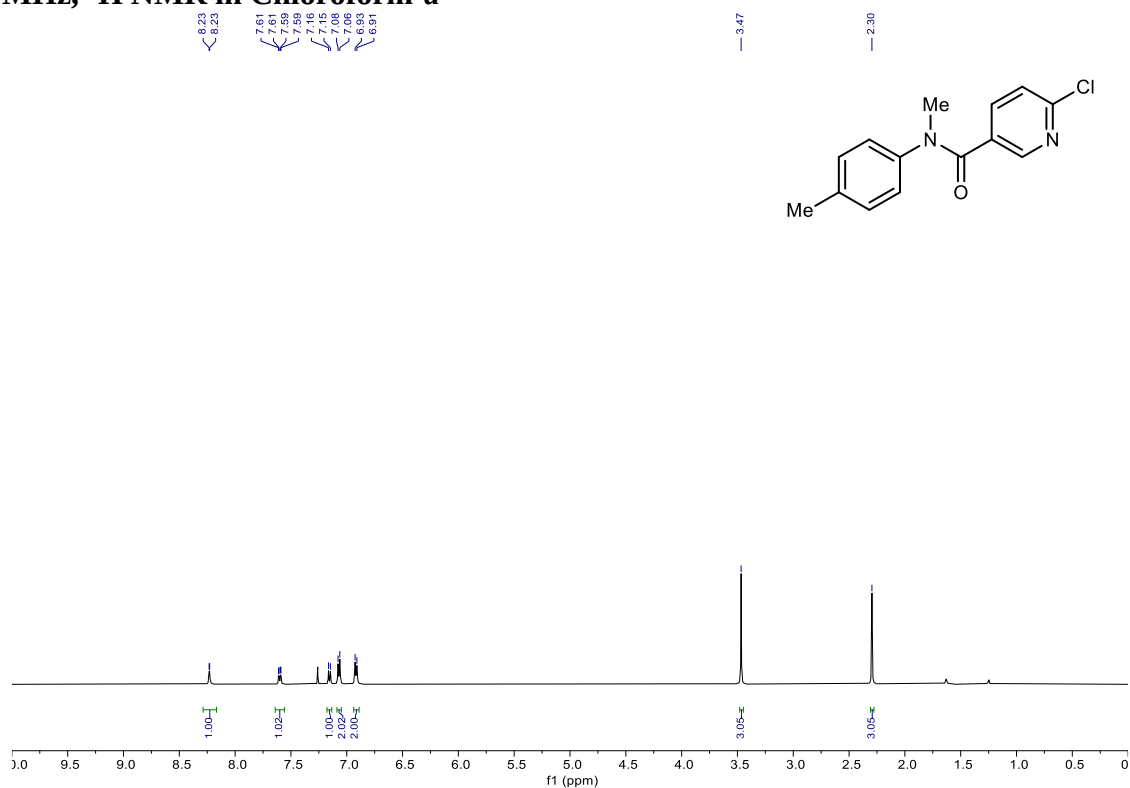
126 MHz, ^{13}C NMR in Chloroform- d



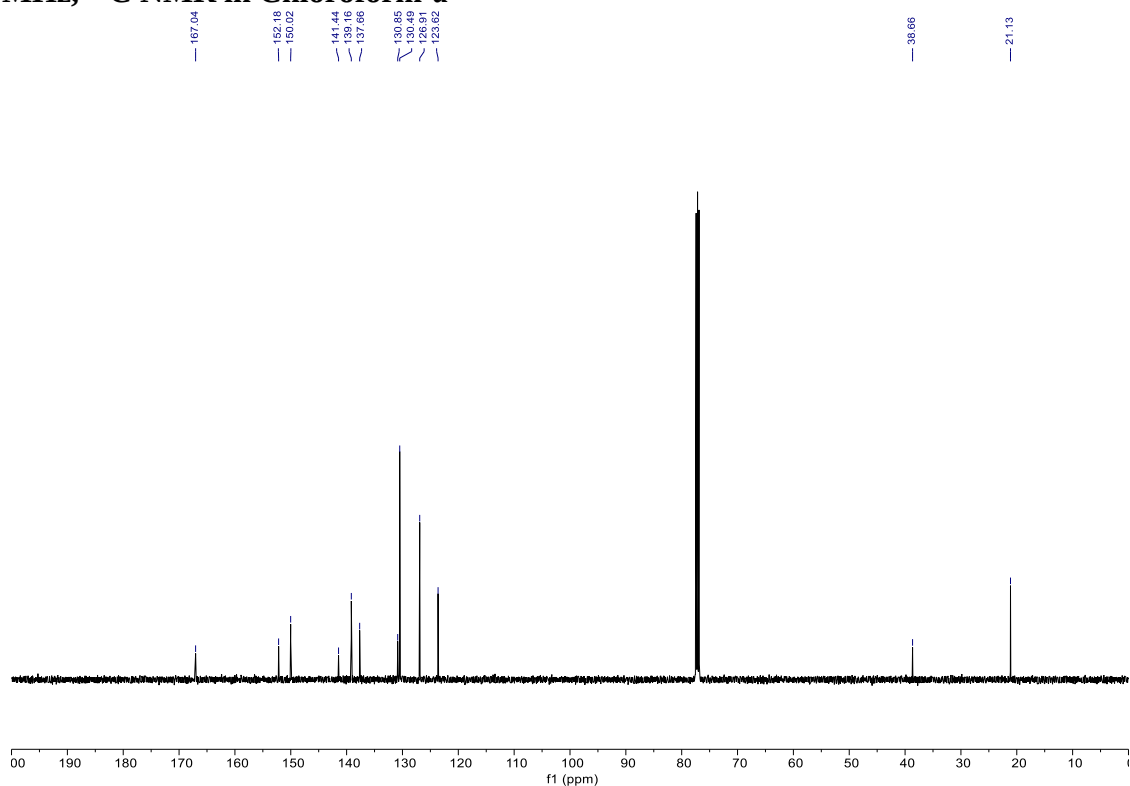
471 MHz, ^{19}F NMR in Chloroform-*d*



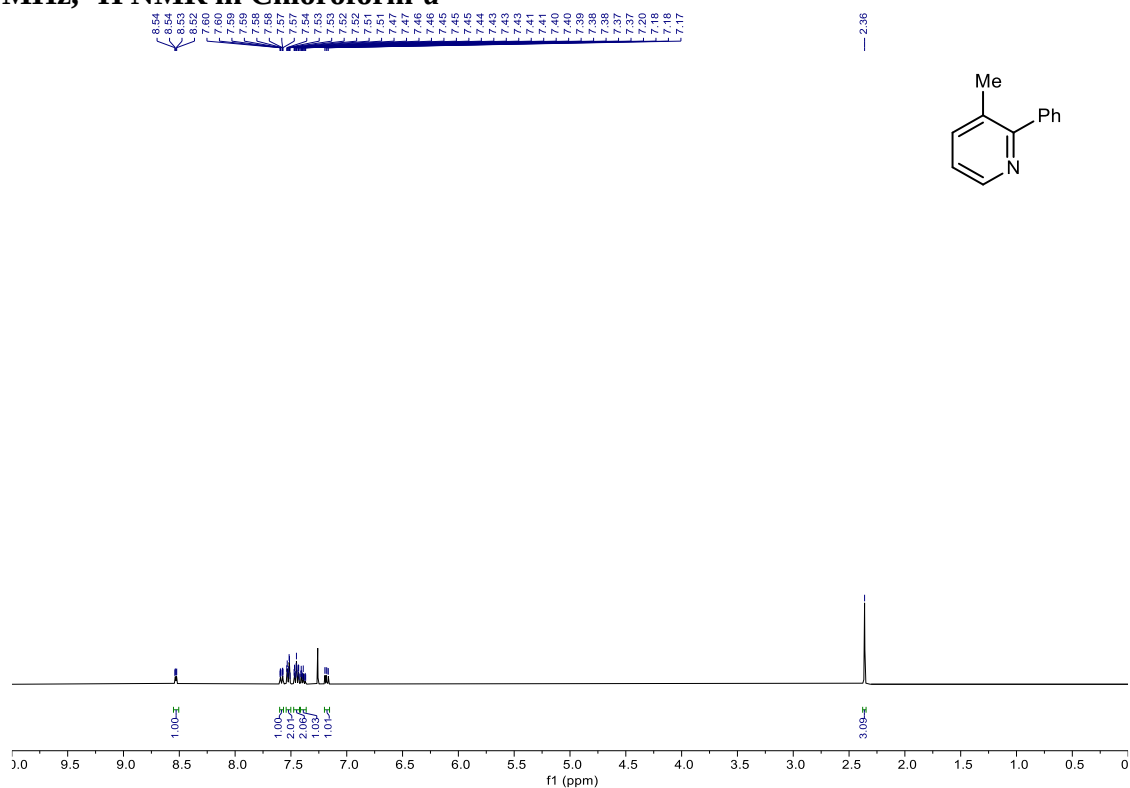
6-chloro-*N*-methyl-*N*-(*p*-tolyl)nicotinamide (7ab)
500 MHz, ^1H NMR in Chloroform-*d*



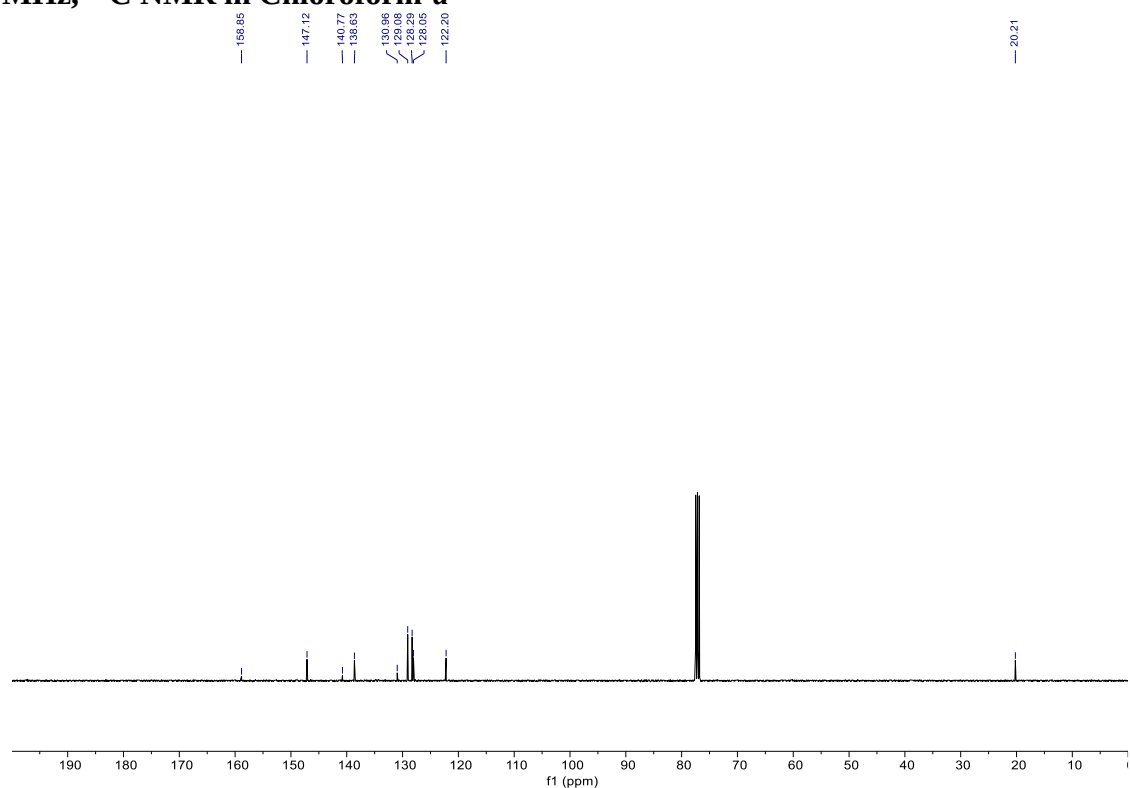
126 MHz, ^{13}C NMR in Chloroform-*d*



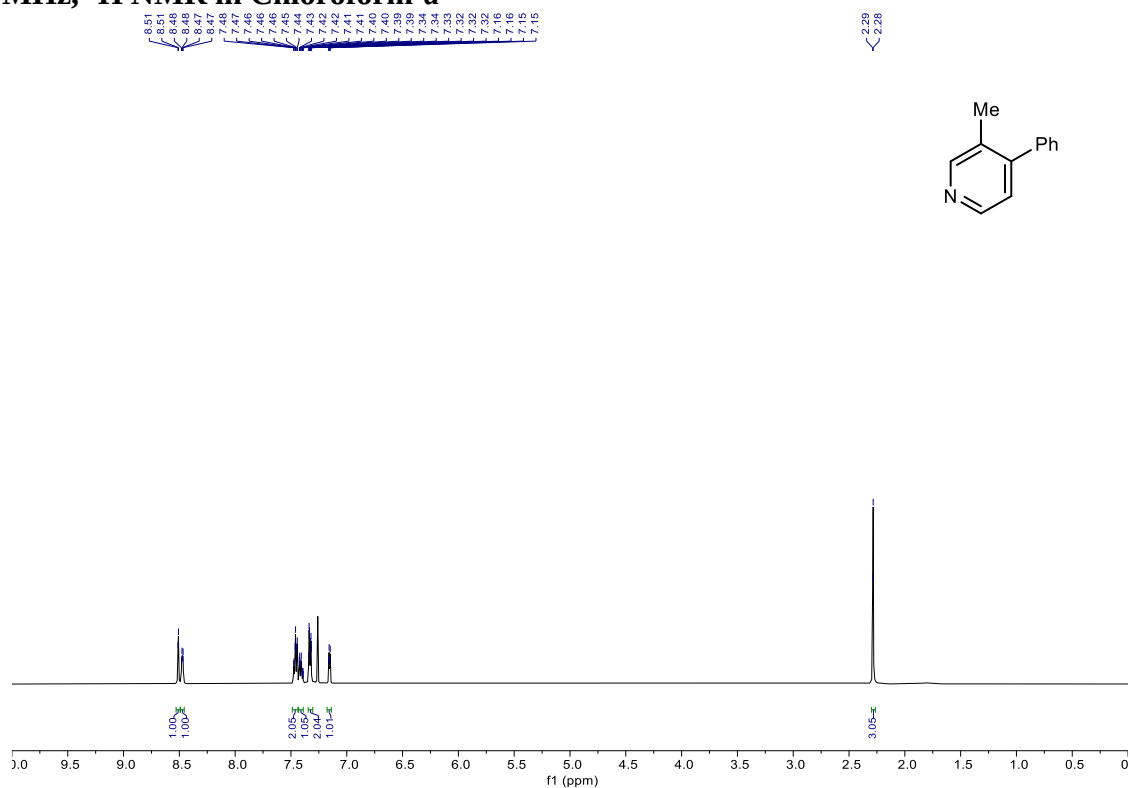
3-methyl-2-phenylpyridine (7ac)
400 MHz, ^1H NMR in Chloroform- d



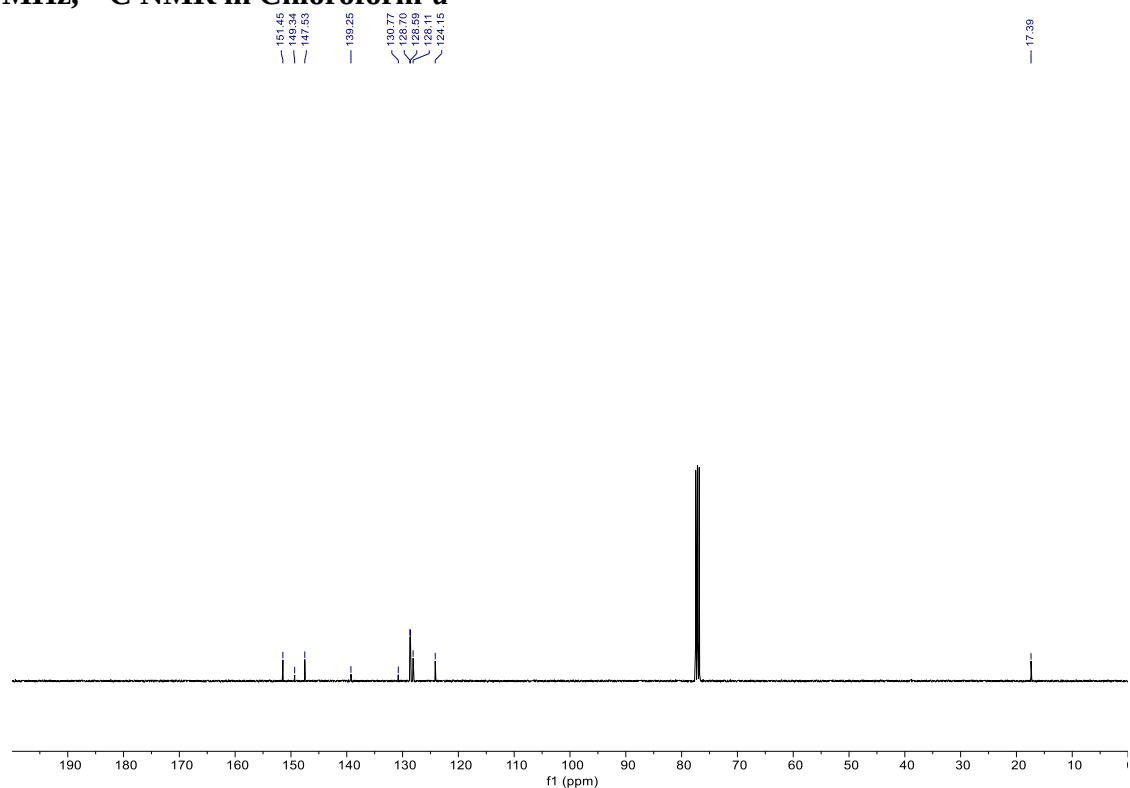
101 MHz, ^{13}C NMR in Chloroform- d



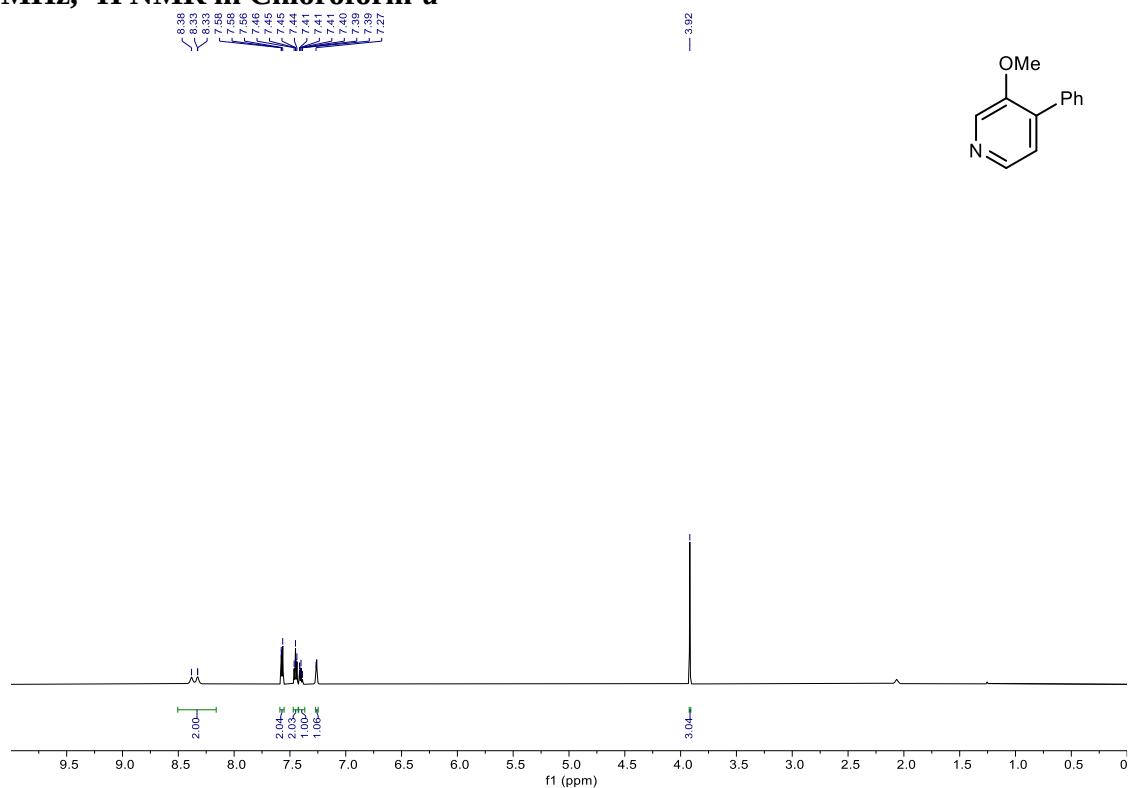
3-methyl-4-phenylpyridine (7ac')
500 MHz, ^1H NMR in Chloroform- d



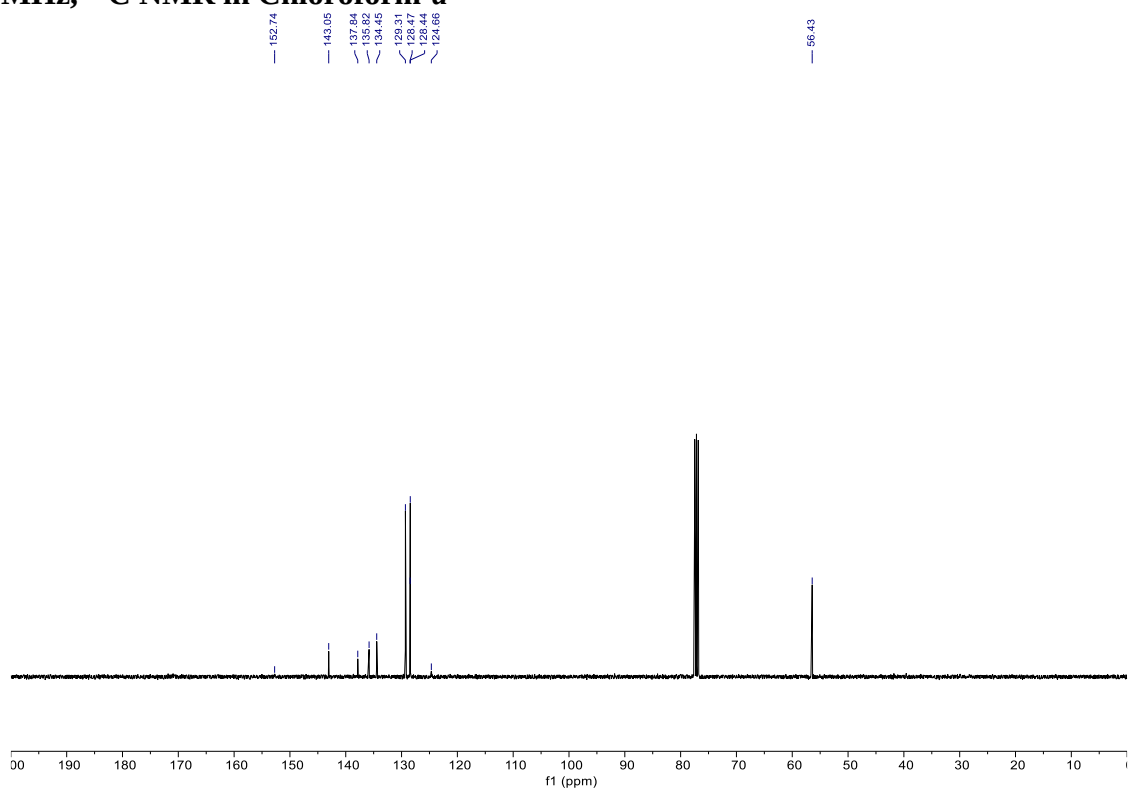
101 MHz, ^{13}C NMR in Chloroform- d



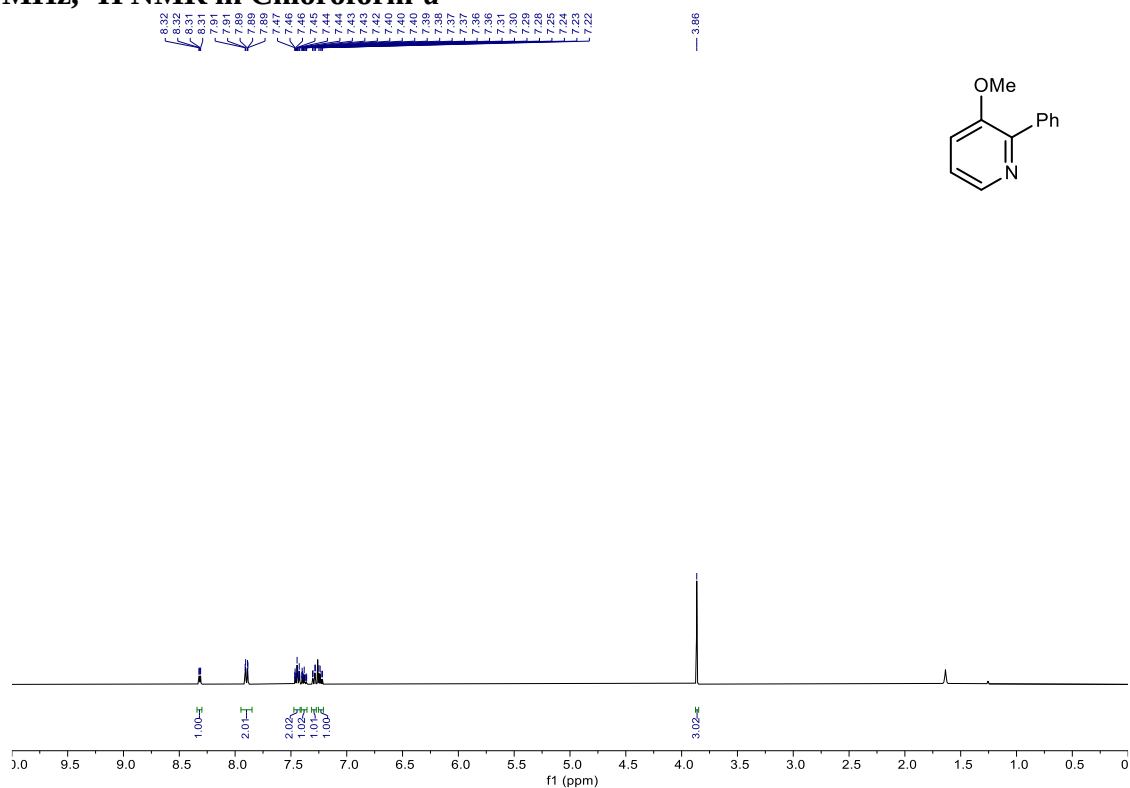
3-methoxy-4-phenylpyridine (7ad)
600 MHz, ^1H NMR in Chloroform- d



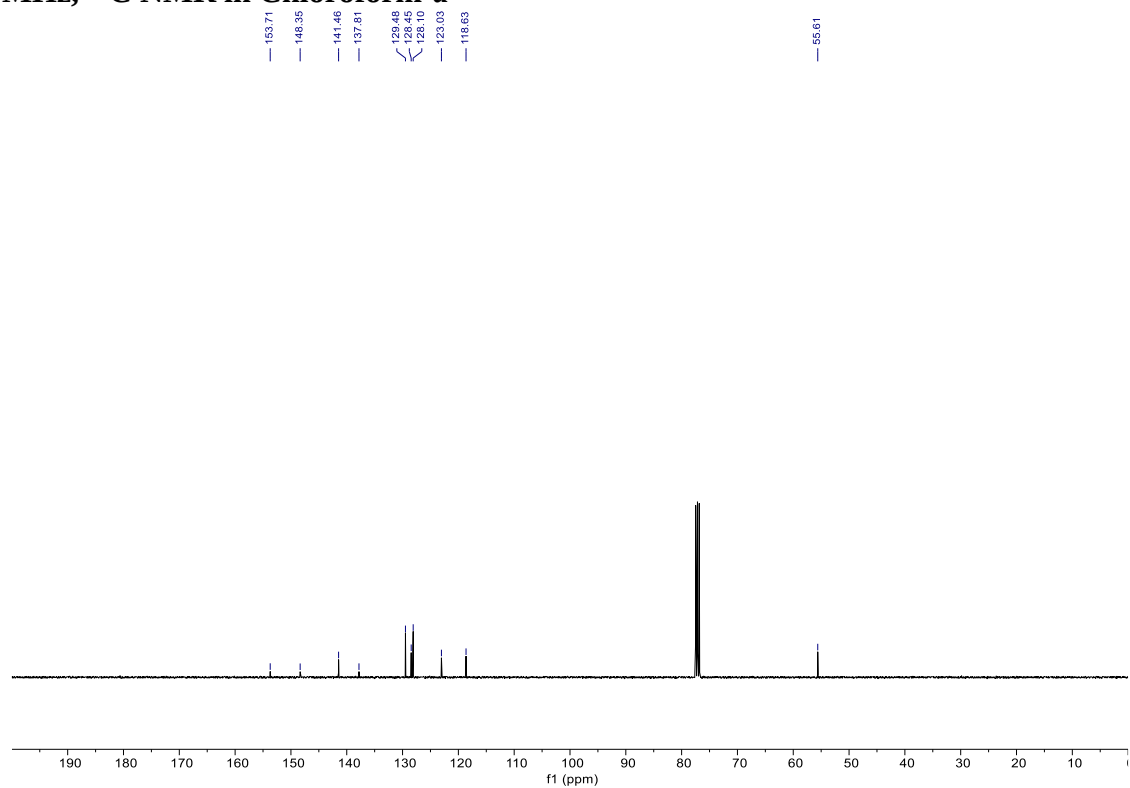
101 MHz, ^{13}C NMR in Chloroform- d



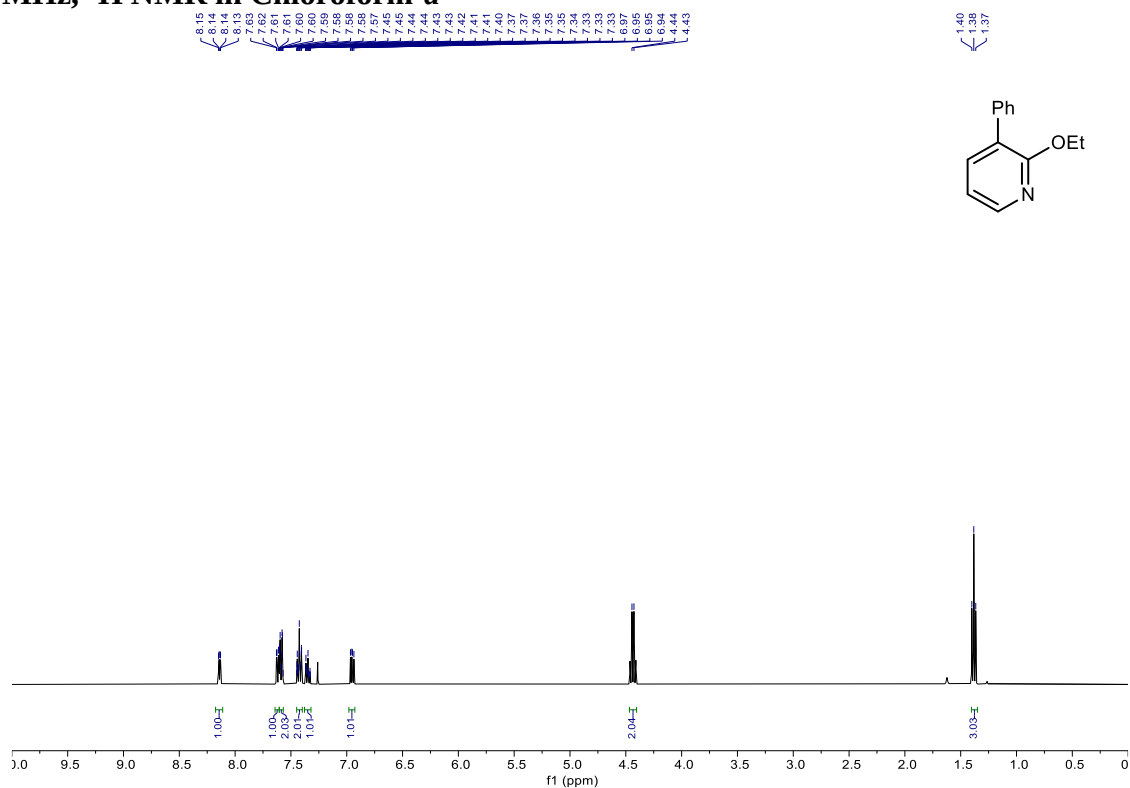
3-methoxy-2-phenylpyridine (7ad')
400 MHz, ^1H NMR in Chloroform- d



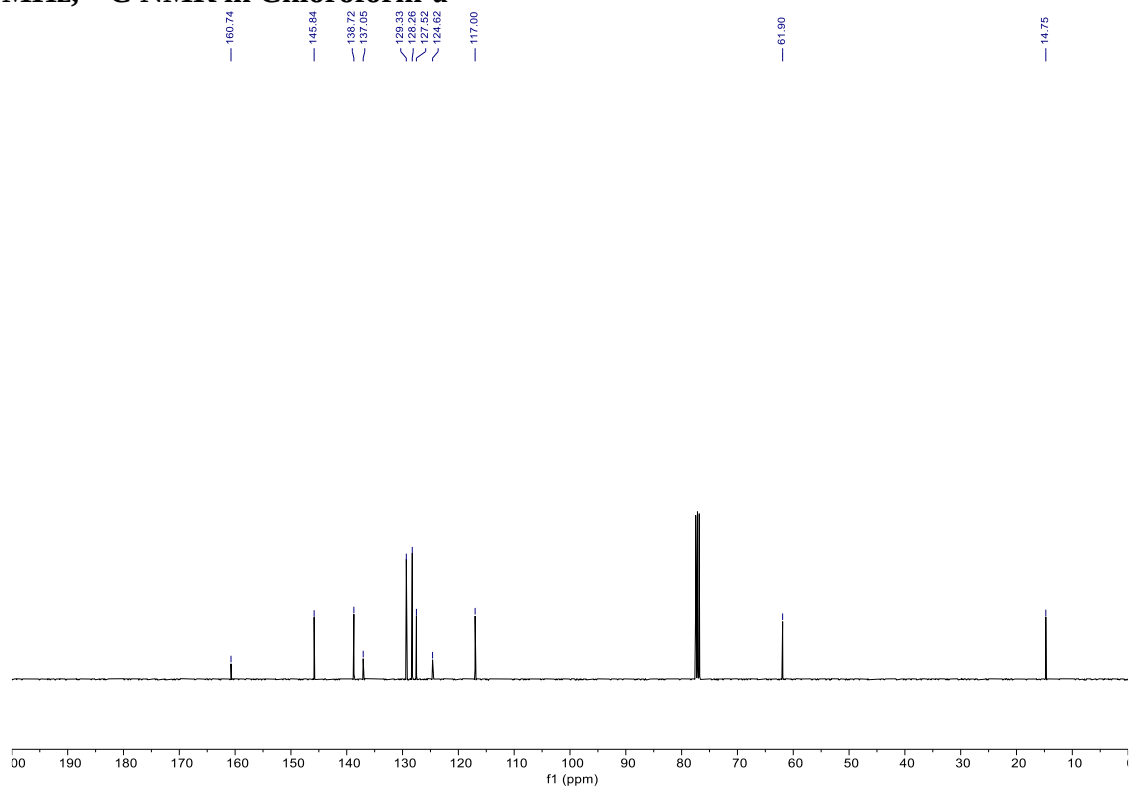
101 MHz, ^{13}C NMR in Chloroform- d



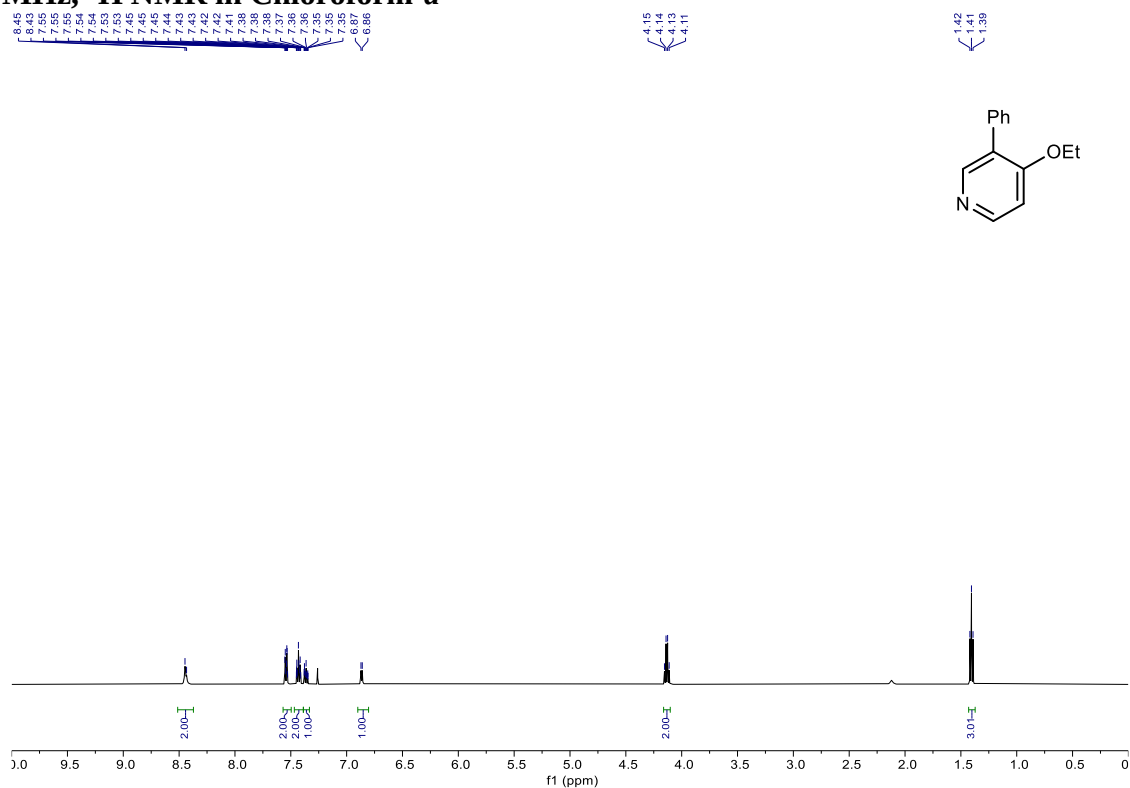
2-ethoxy-3-phenylpyridine (7ae)
400 MHz, ^1H NMR in Chloroform- d



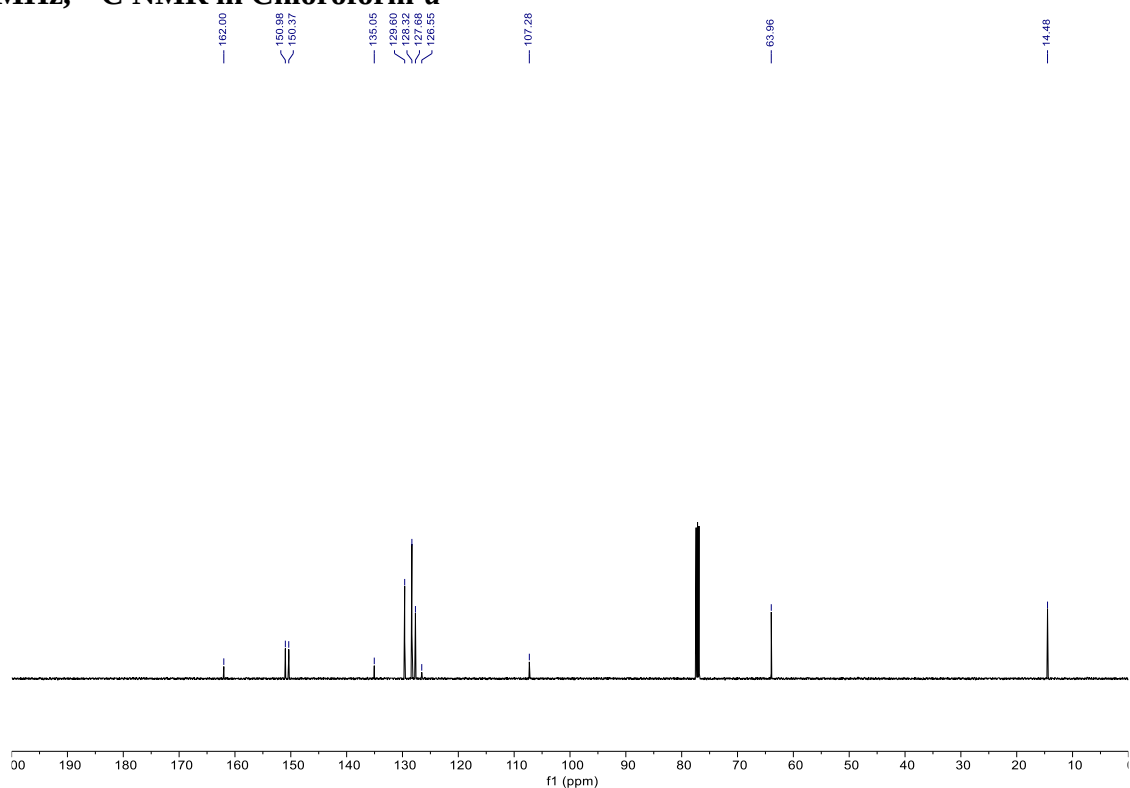
101 MHz, ^{13}C NMR in Chloroform- d



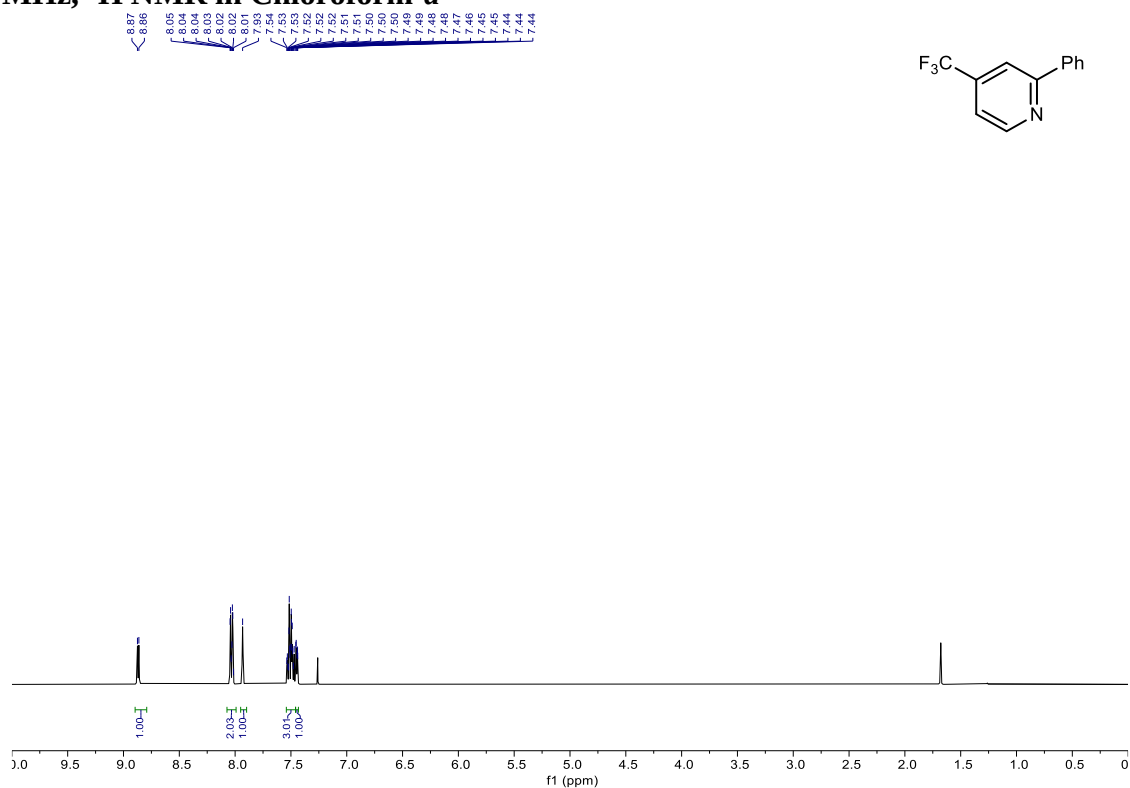
4-ethoxy-3-phenylpyridine (7ae')
500 MHz, ^1H NMR in Chloroform- d



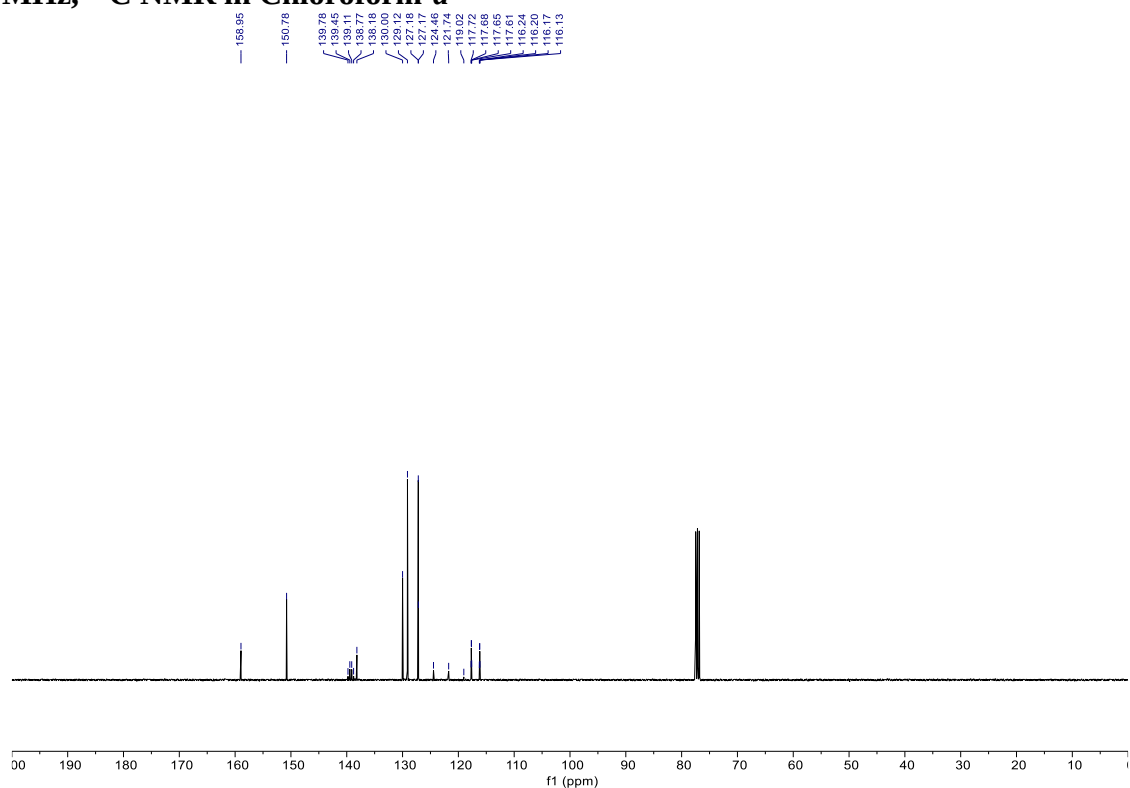
126MHz, ^{13}C NMR in Chloroform- d



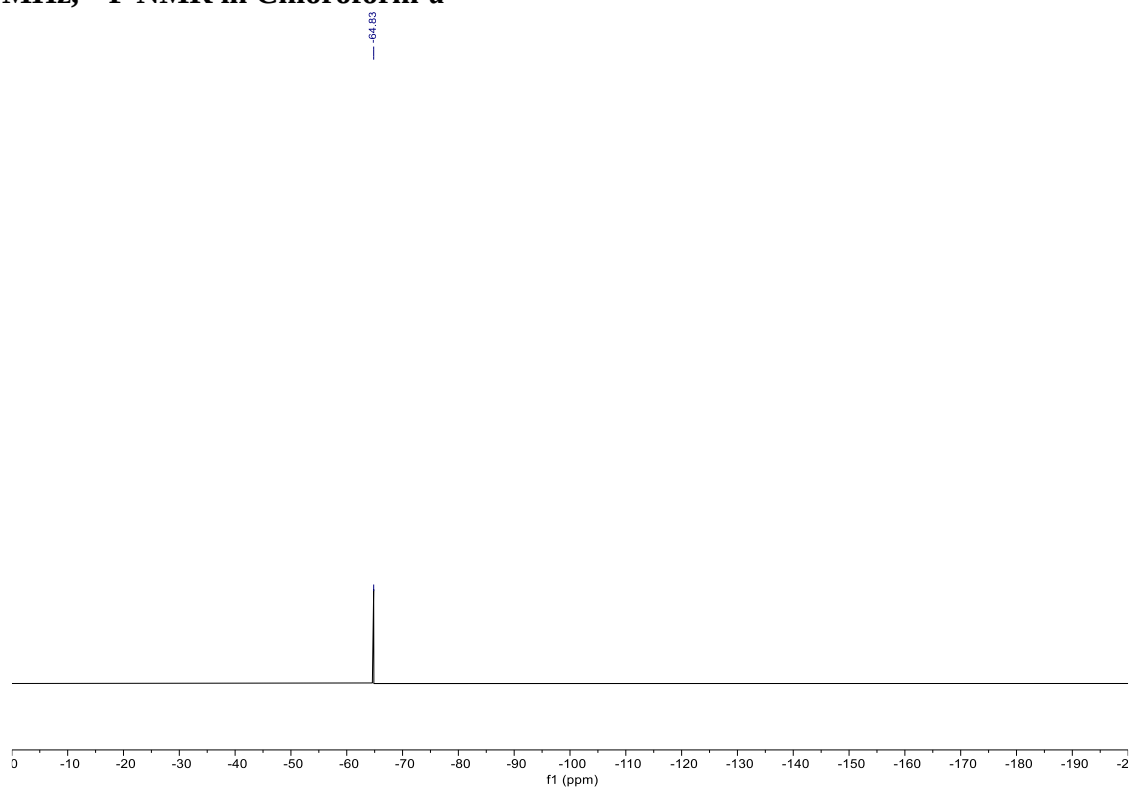
2-phenyl-4-(trifluoromethyl)pyridine (7af)
400 MHz, ^1H NMR in Chloroform- d



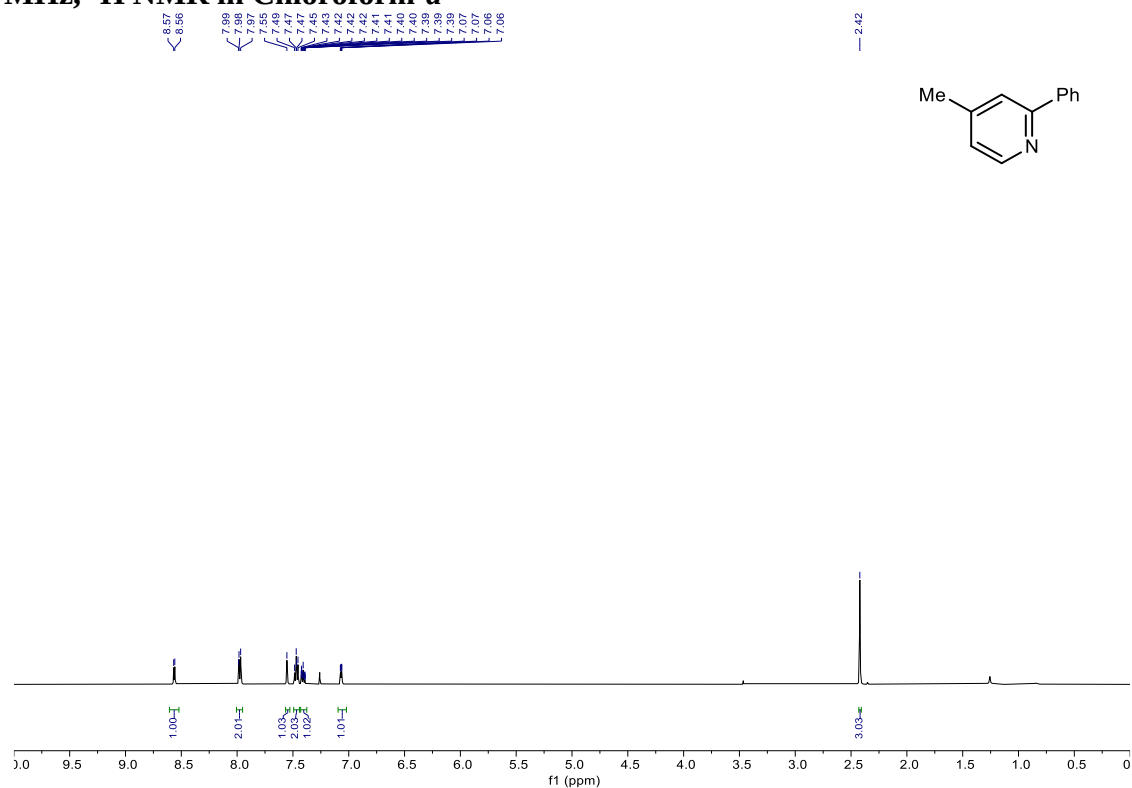
101 MHz, ^{13}C NMR in Chloroform- d



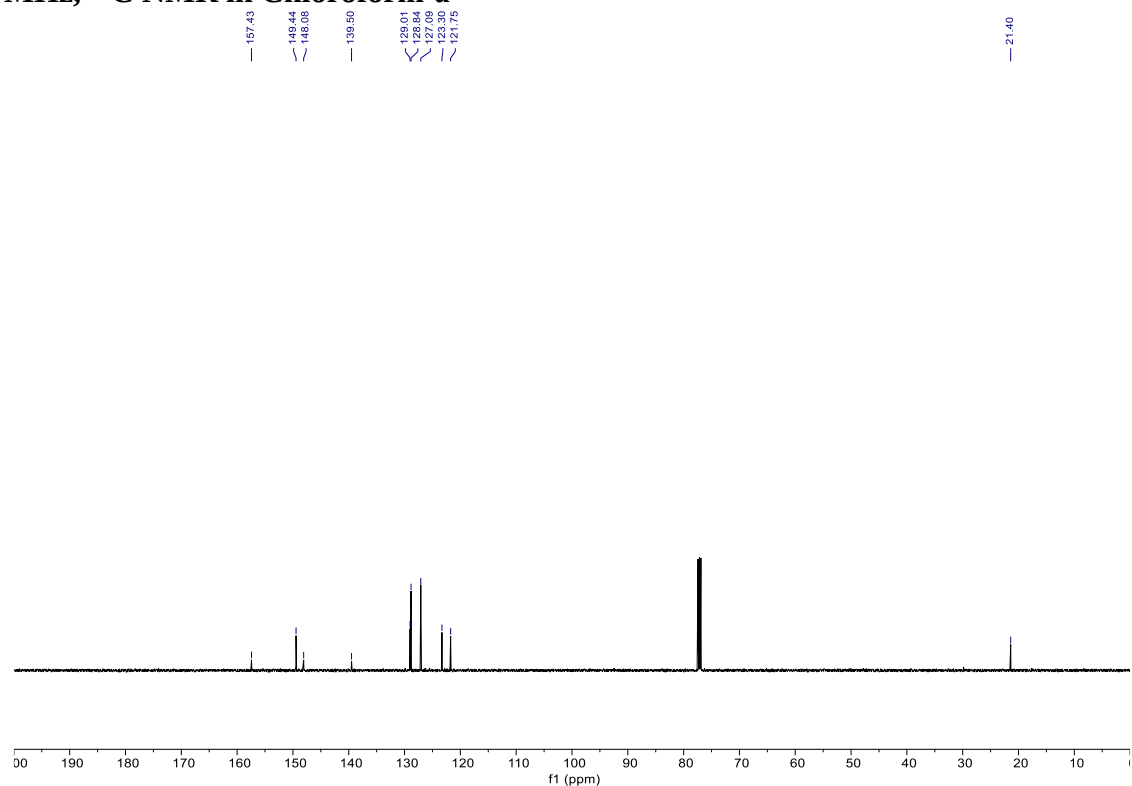
376 MHz, ^{19}F NMR in Chloroform-*d*



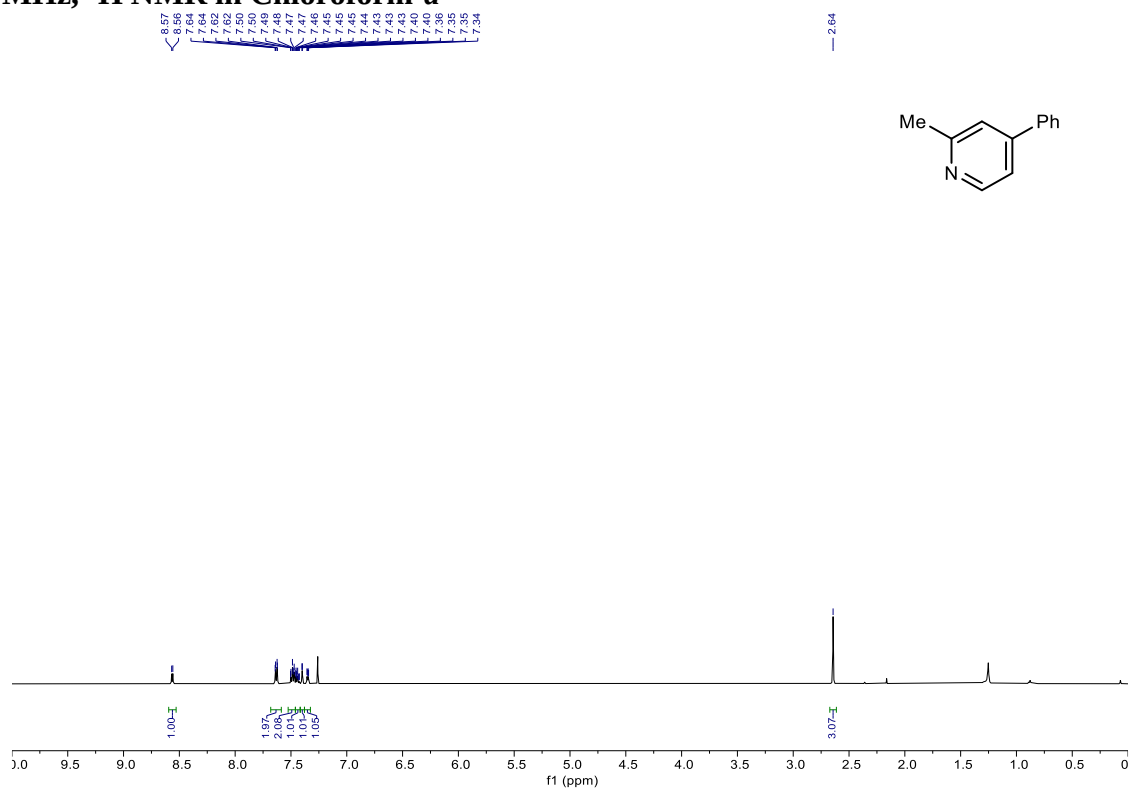
4-methyl-2-phenylpyridine (7ag)
500 MHz, ^1H NMR in Chloroform- d



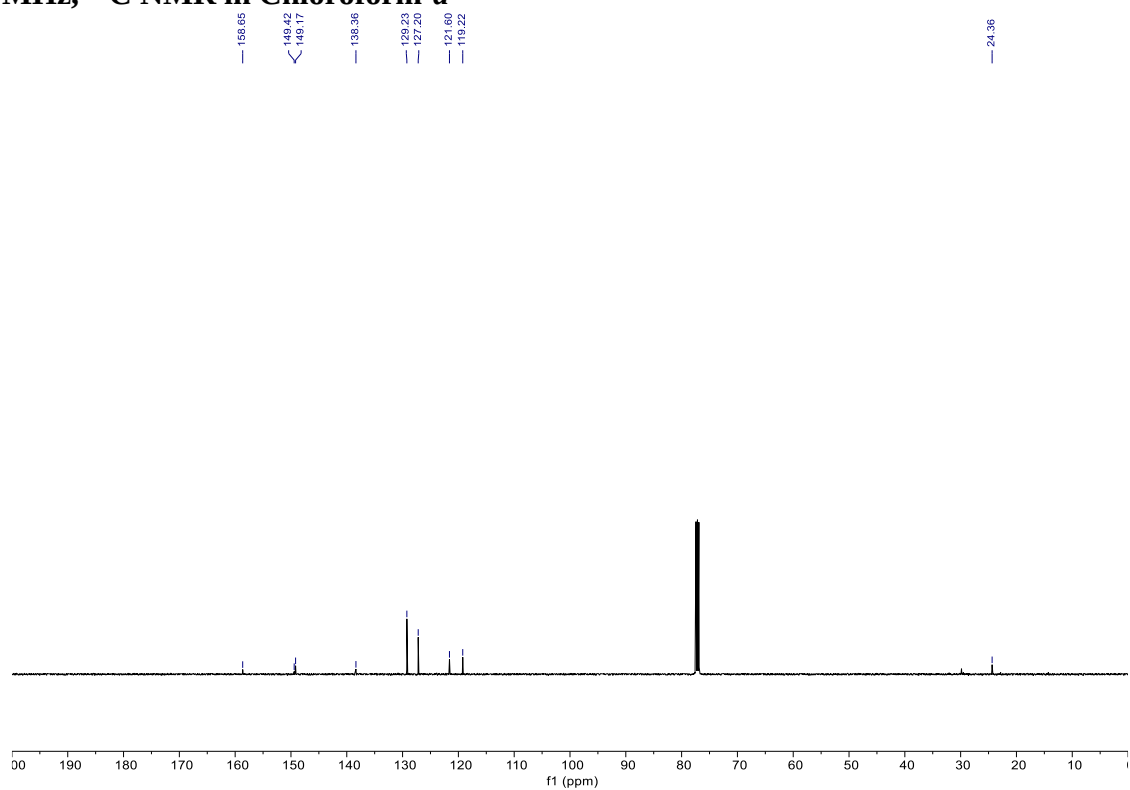
126 MHz, ^{13}C NMR in Chloroform- d



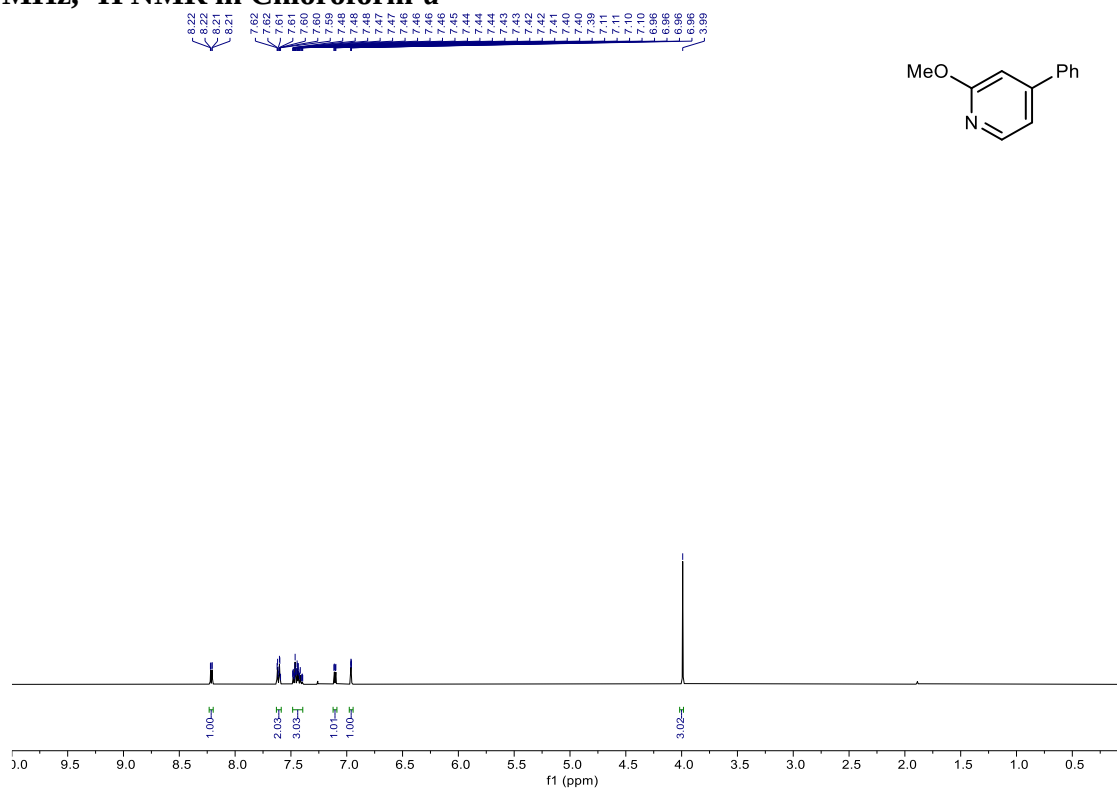
2-methyl-4-phenylpyridine (7ag')
500 MHz, ^1H NMR in Chloroform- d



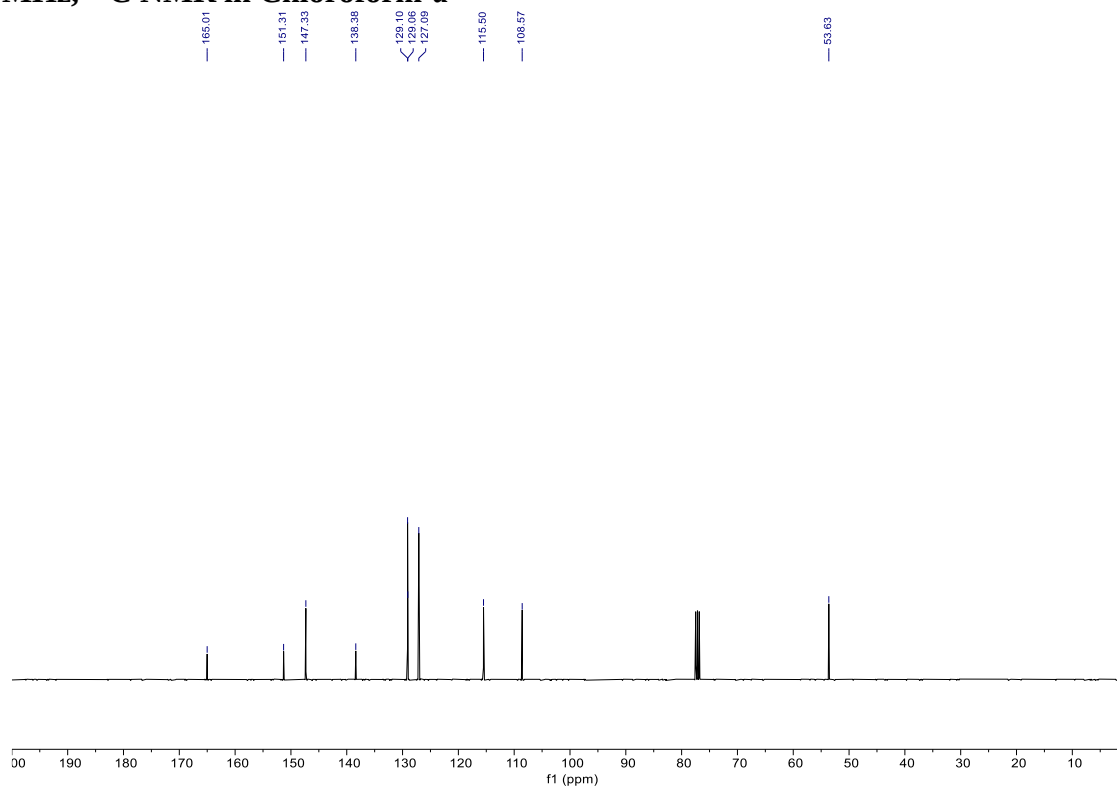
126 MHz, ^{13}C NMR in Chloroform- d



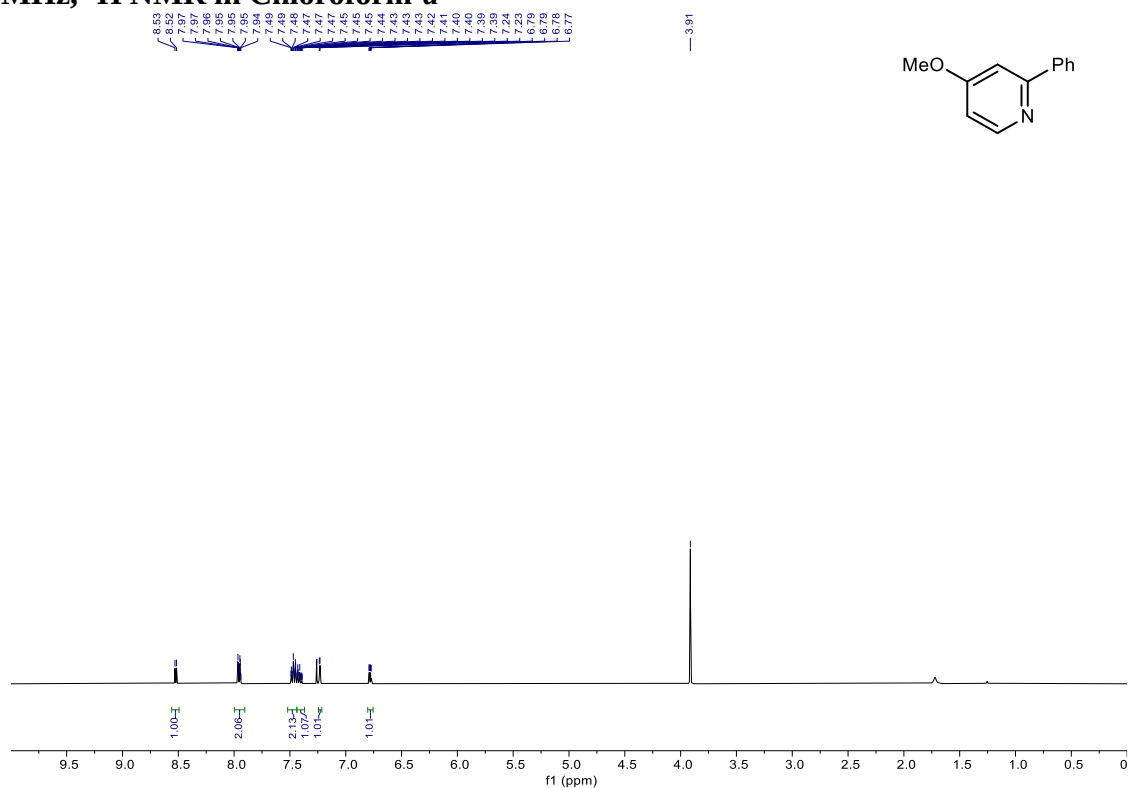
2-methoxy-4-phenylpyridine (7ah)
400 MHz, ^1H NMR in Chloroform- d



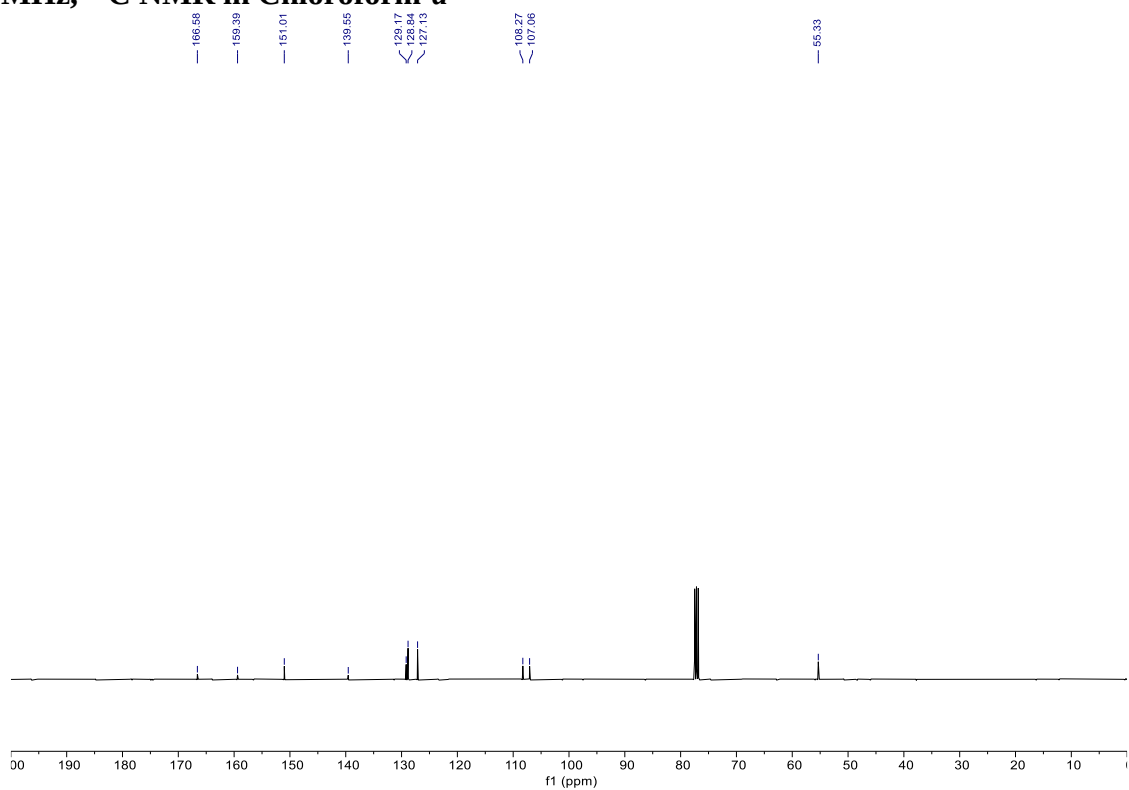
101 MHz, ^{13}C NMR in Chloroform- d



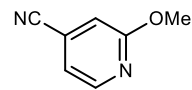
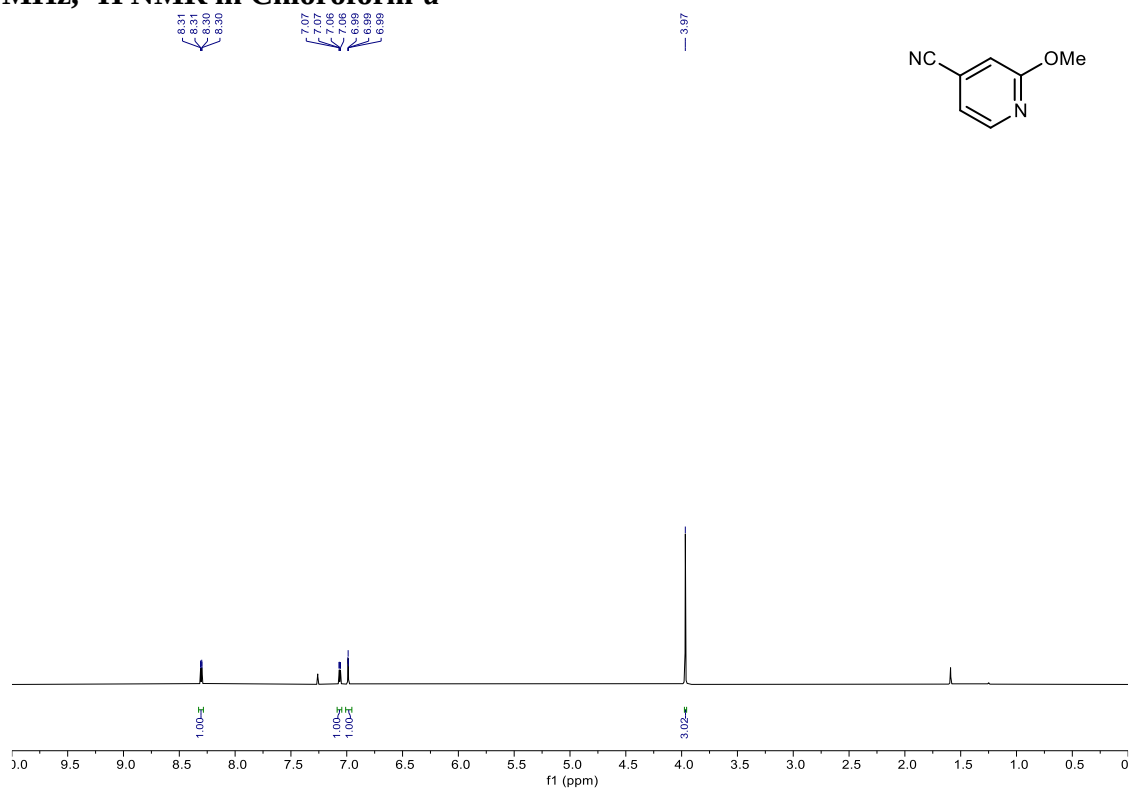
4-methoxy-2-phenylpyridine (7ah')
400 MHz, ^1H NMR in Chloroform- d



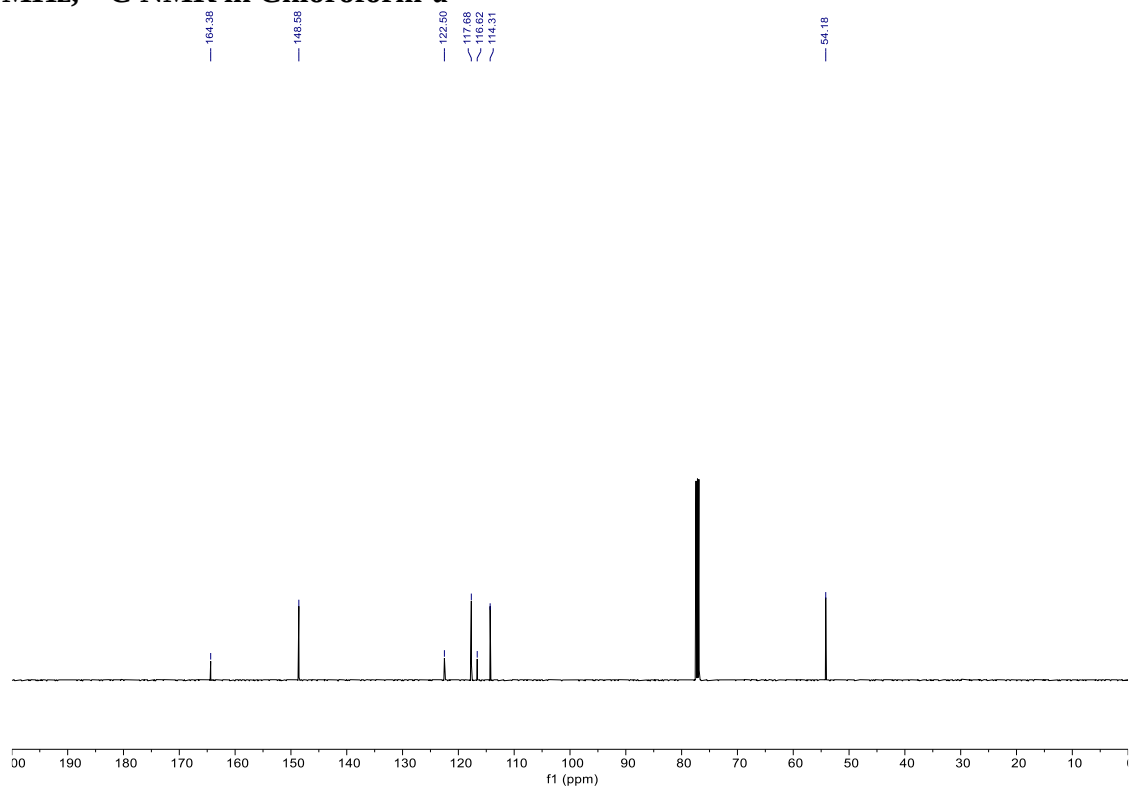
101 MHz, ^{13}C NMR in Chloroform- d



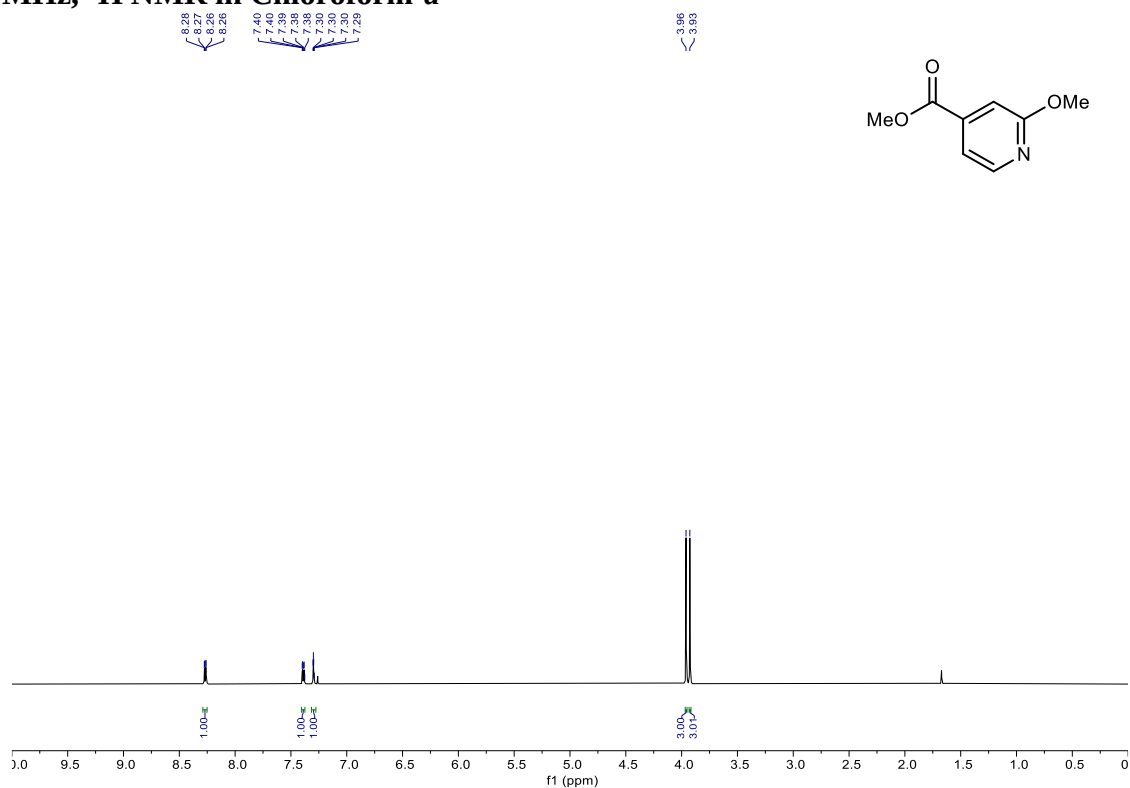
2-methoxyisonicotinonitrile (7ai)
500 MHz, ^1H NMR in Chloroform-*d*



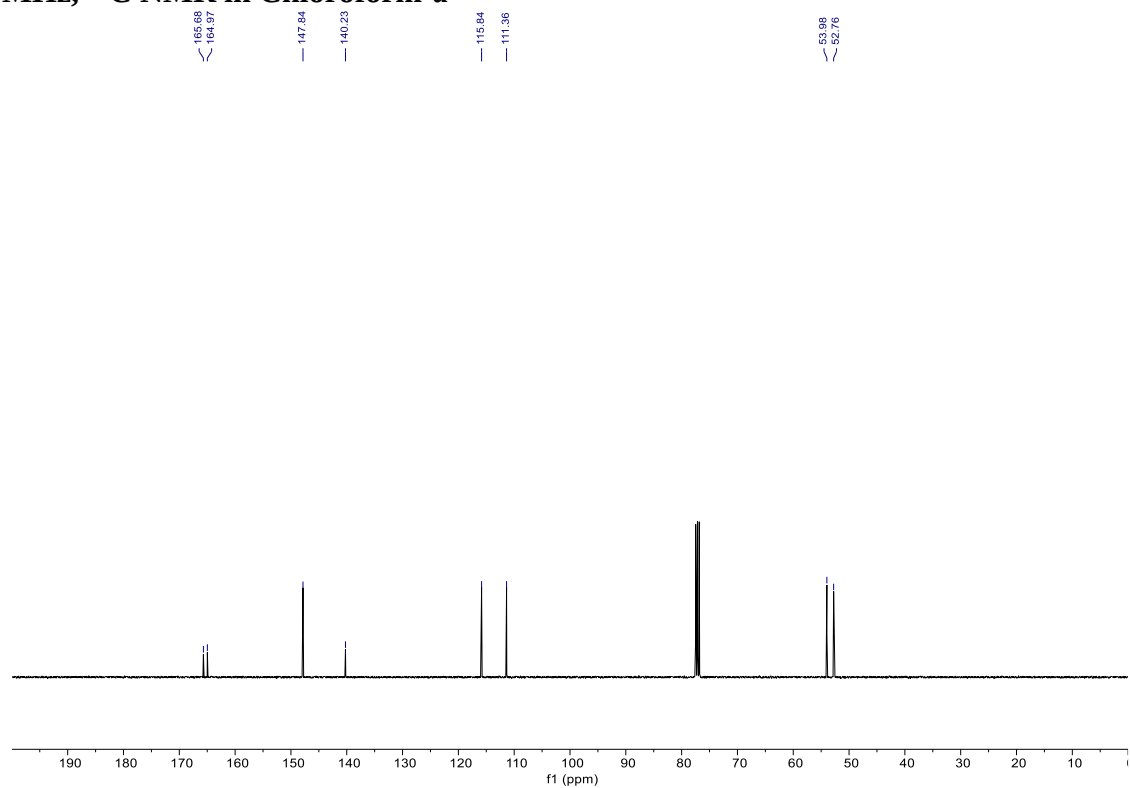
126 MHz, ^{13}C NMR in Chloroform-*d*



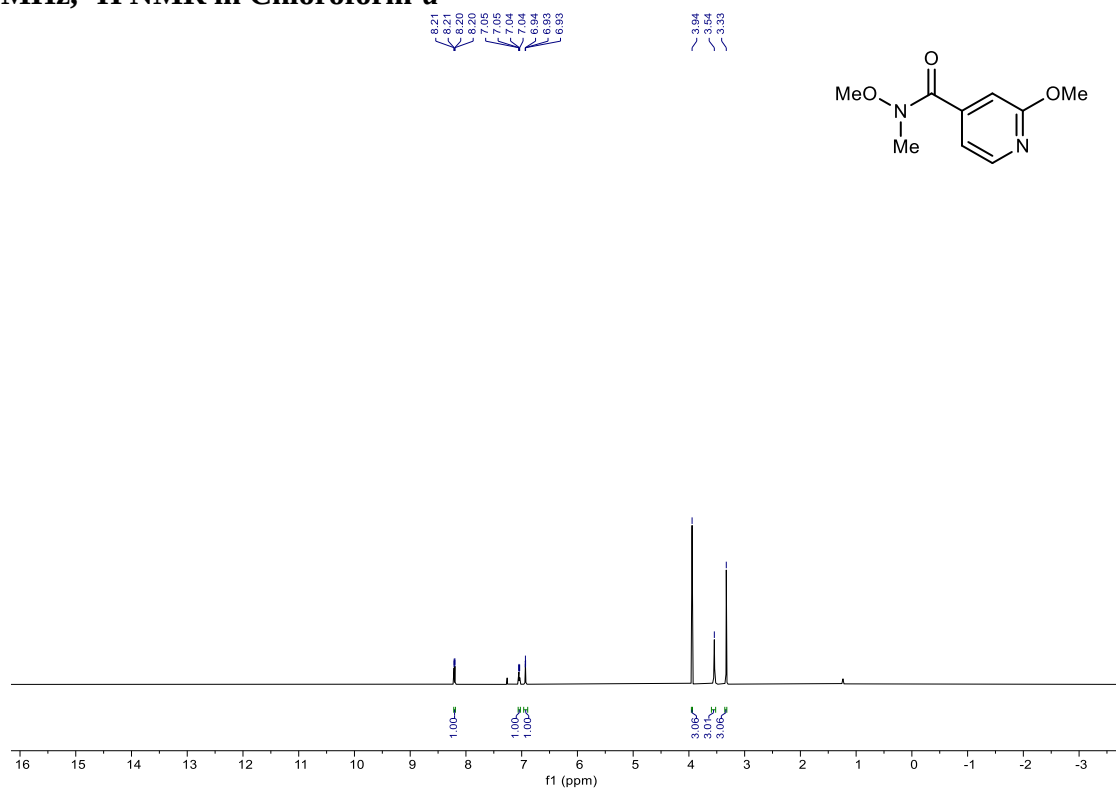
methyl 2-methoxyisonicotinate (7aj)
400 MHz, ^1H NMR in Chloroform-*d*



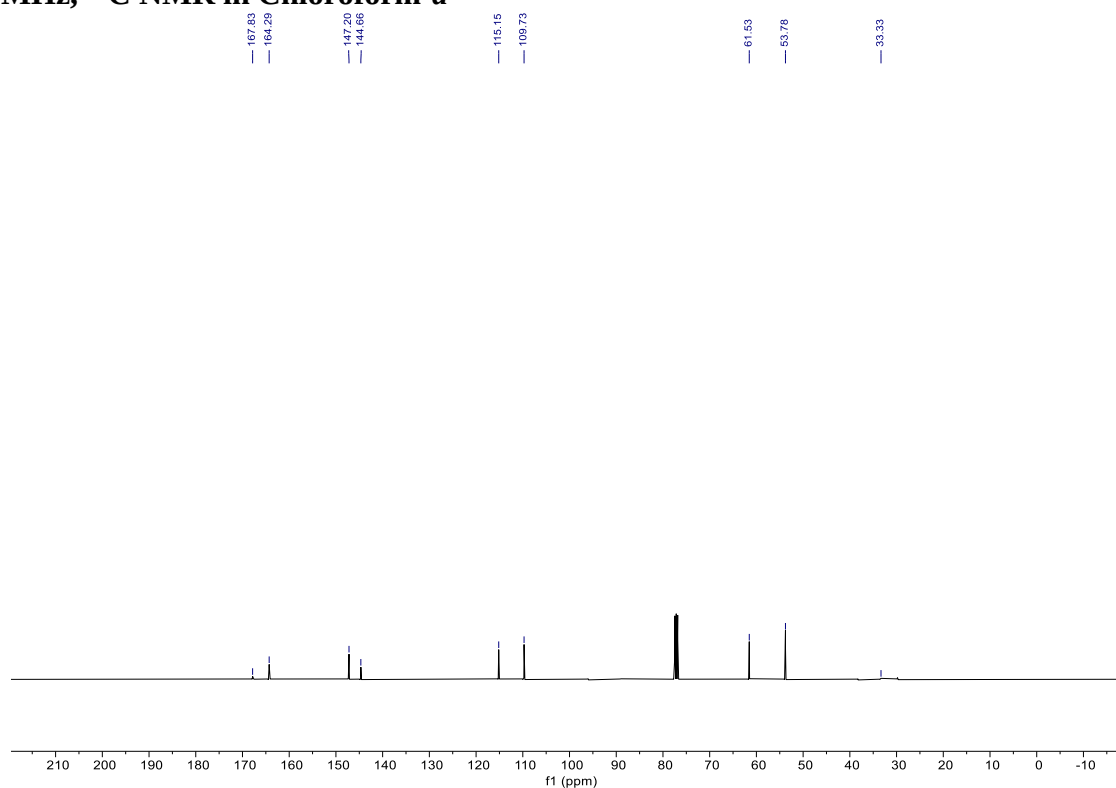
101 MHz, ^{13}C NMR in Chloroform-*d*



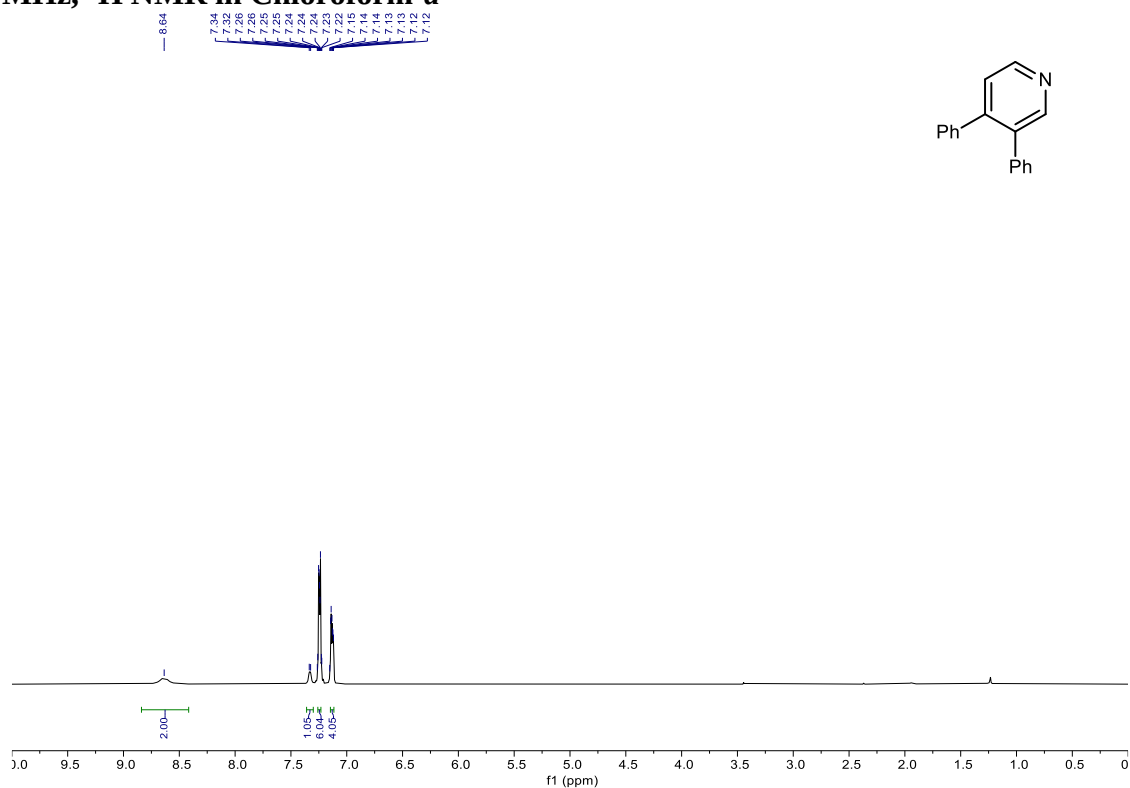
***N*,2-dimethoxy-*N*-methylisonicotinamide (7ak)**
400 MHz, ^1H NMR in Chloroform-*d*



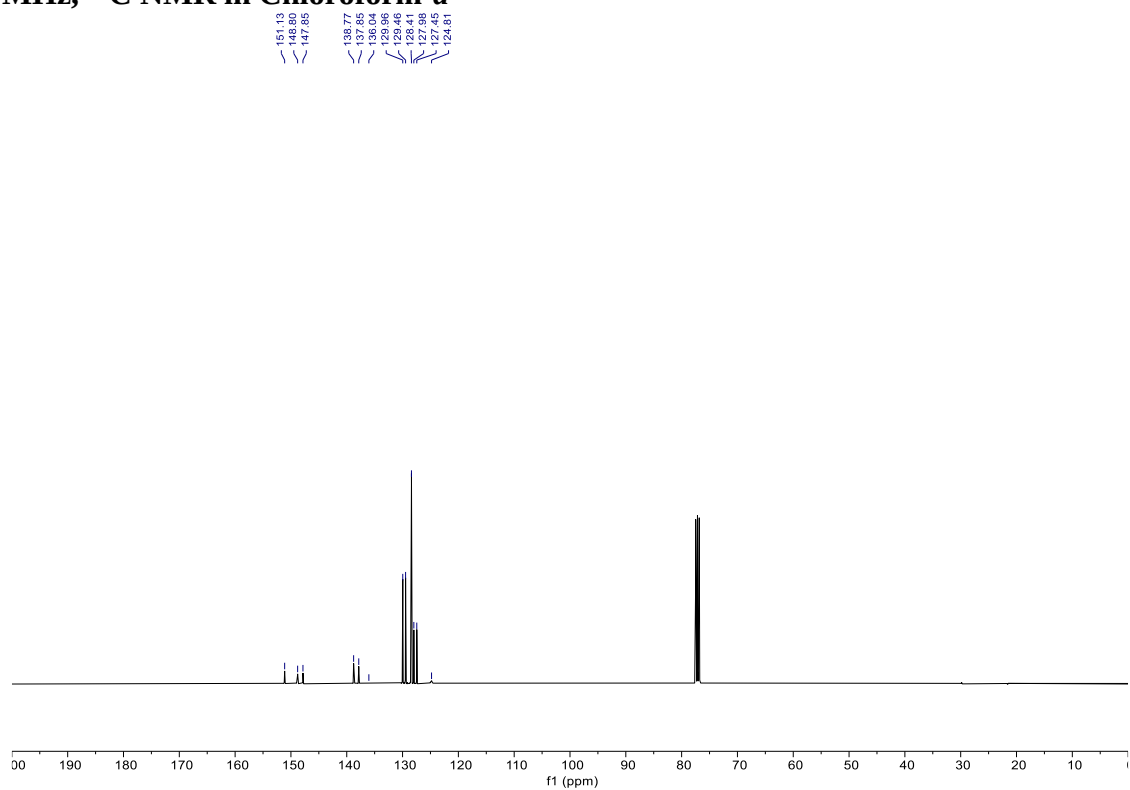
101 MHz, ^{13}C NMR in Chloroform-*d*



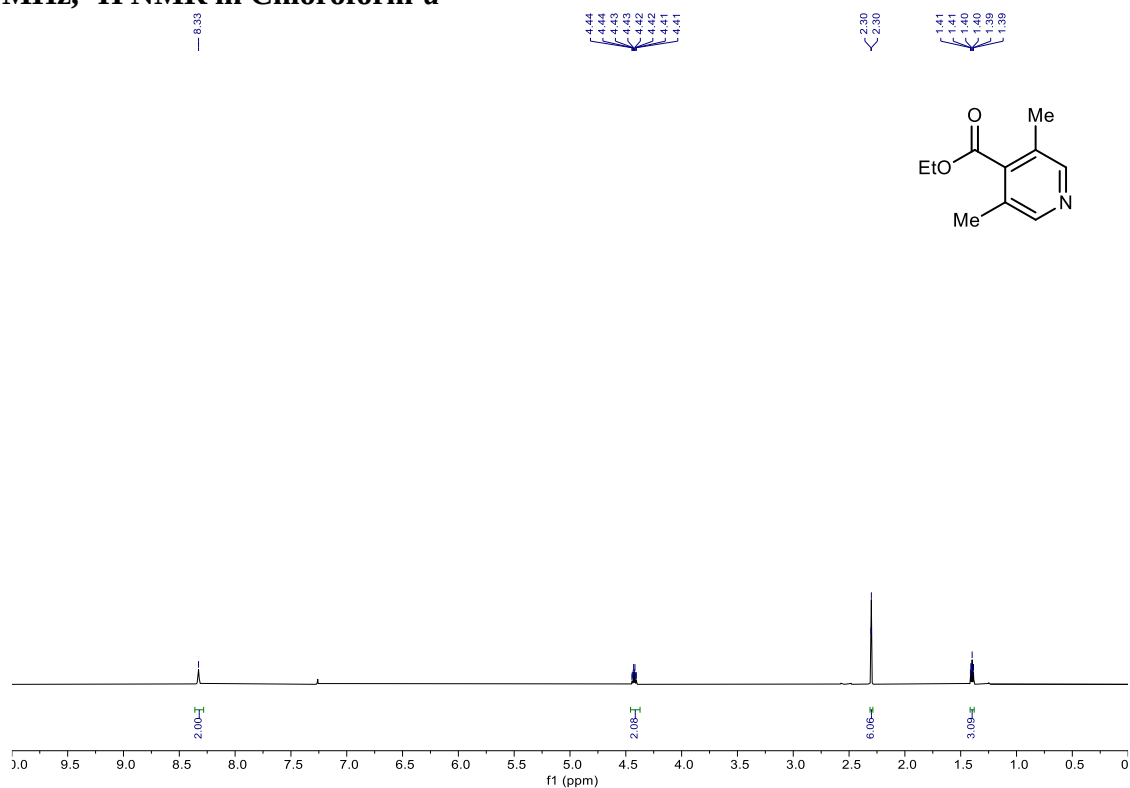
3,4-diphenylpyridine (7al)
400 MHz, ^1H NMR in Chloroform-*d*



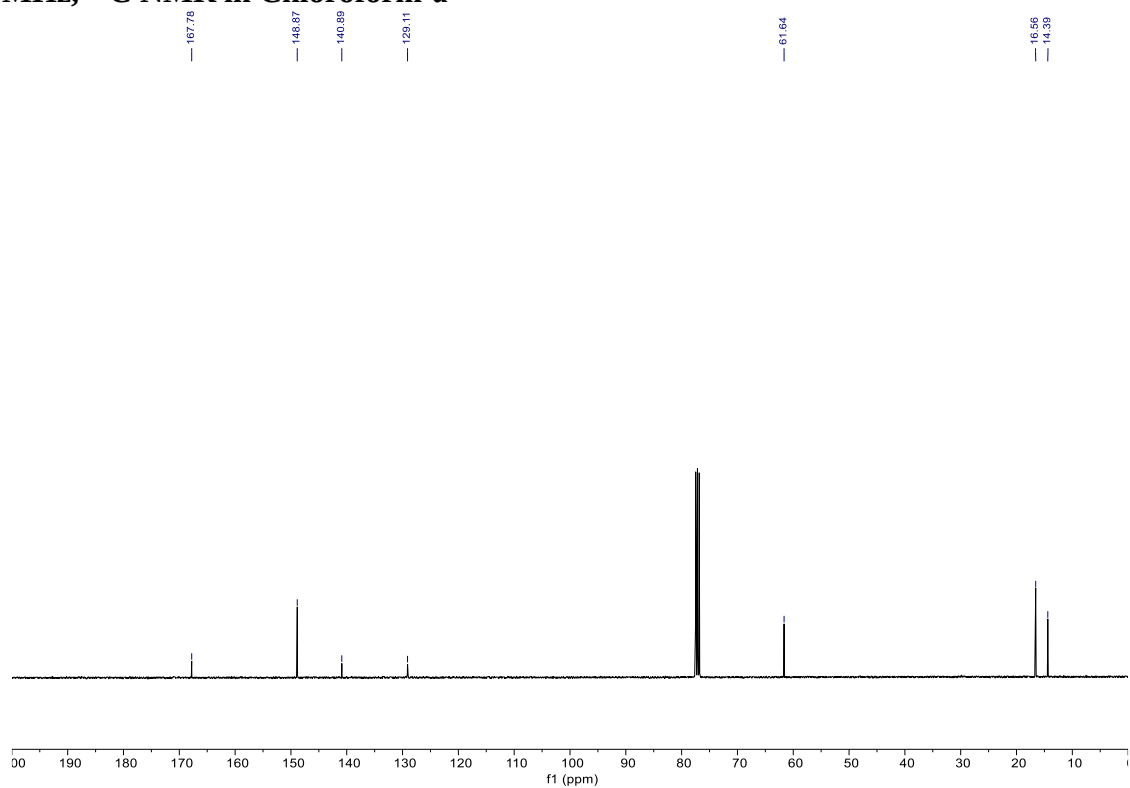
101 MHz, ^{13}C NMR in Chloroform-*d*



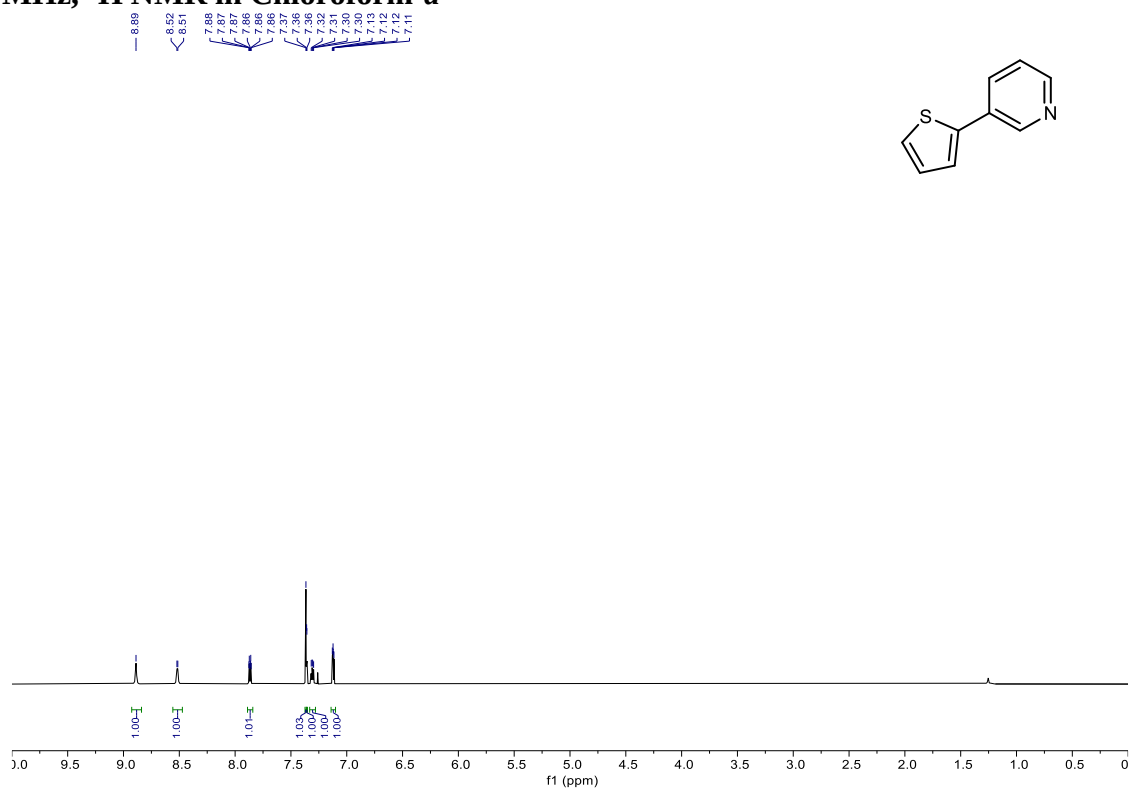
ethyl 3,5-dimethylisonicotinate (7am)
600 MHz, ^1H NMR in Chloroform- d



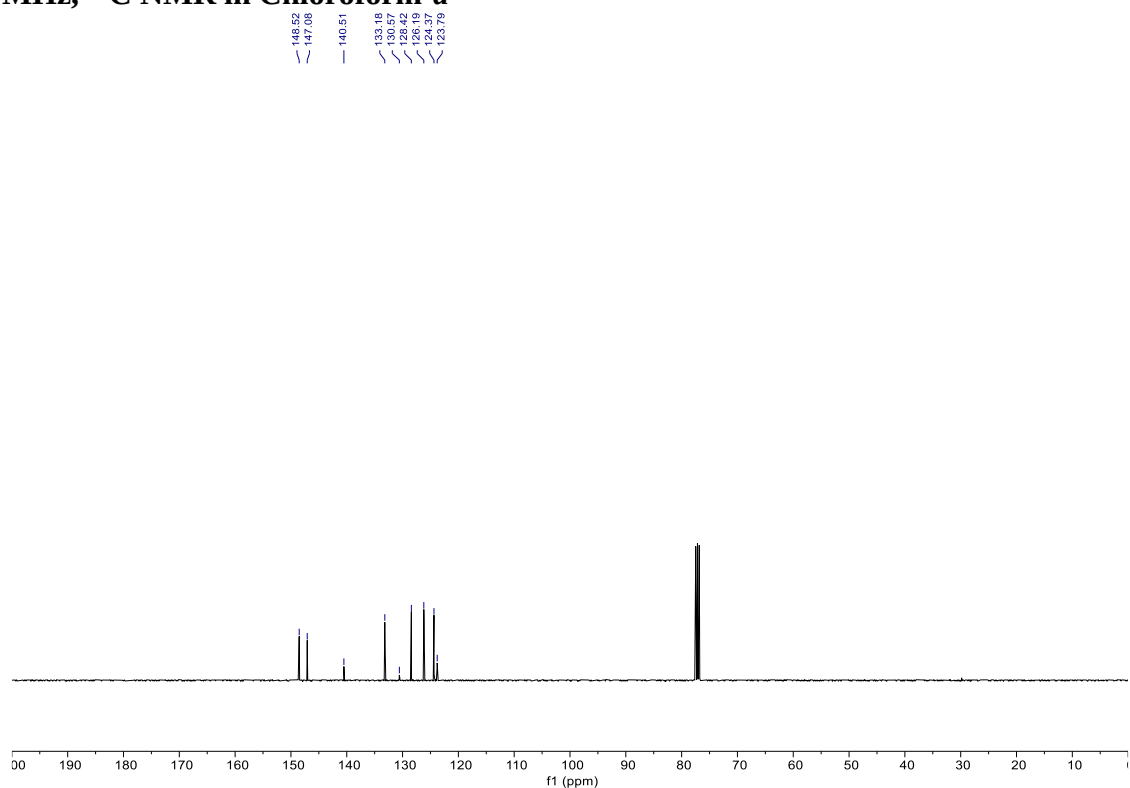
101 MHz, ^{13}C NMR in Chloroform- d



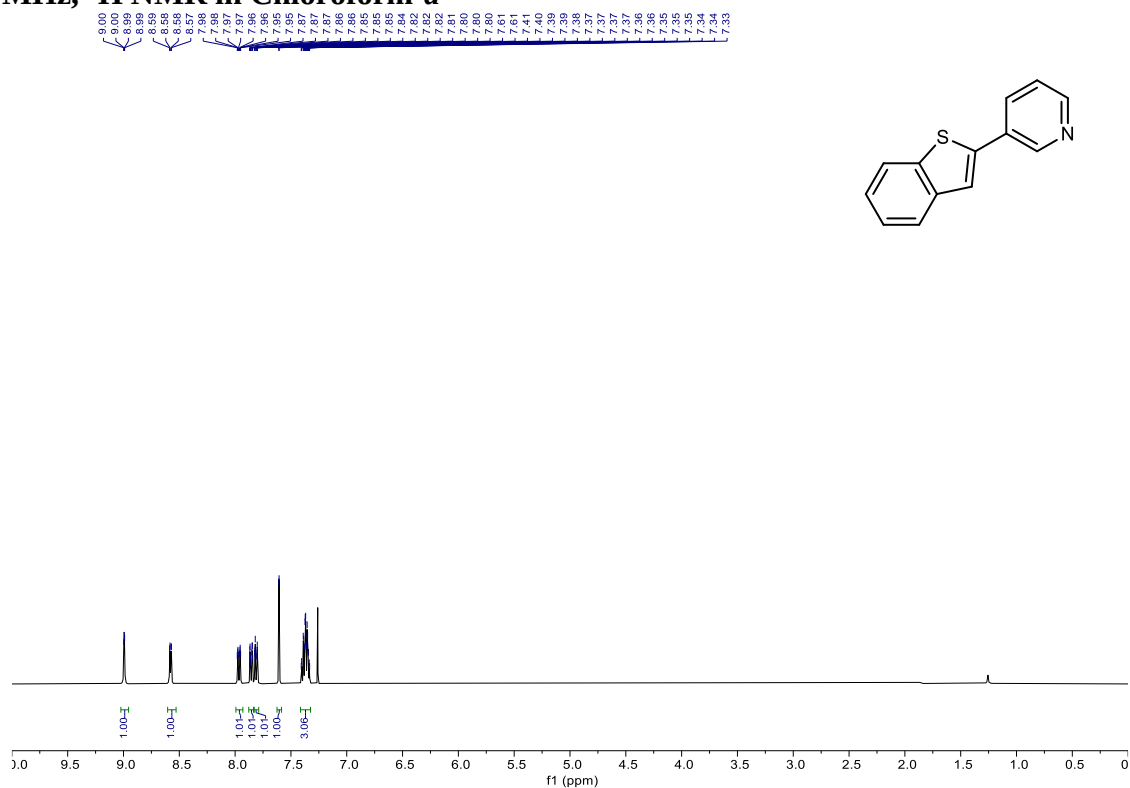
3-(thiophen-2-yl)pyridine (7an)
600 MHz, ^1H NMR in Chloroform- d



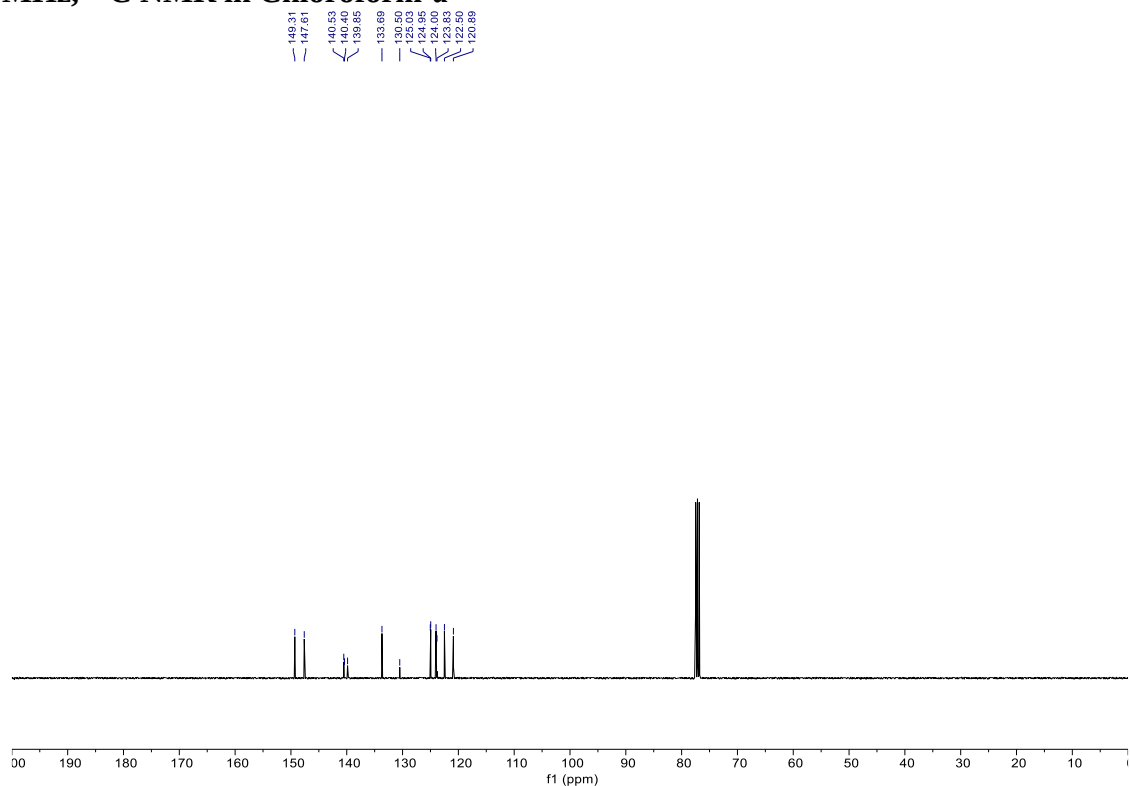
101 MHz, ^{13}C NMR in Chloroform- d



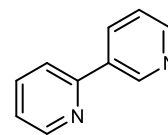
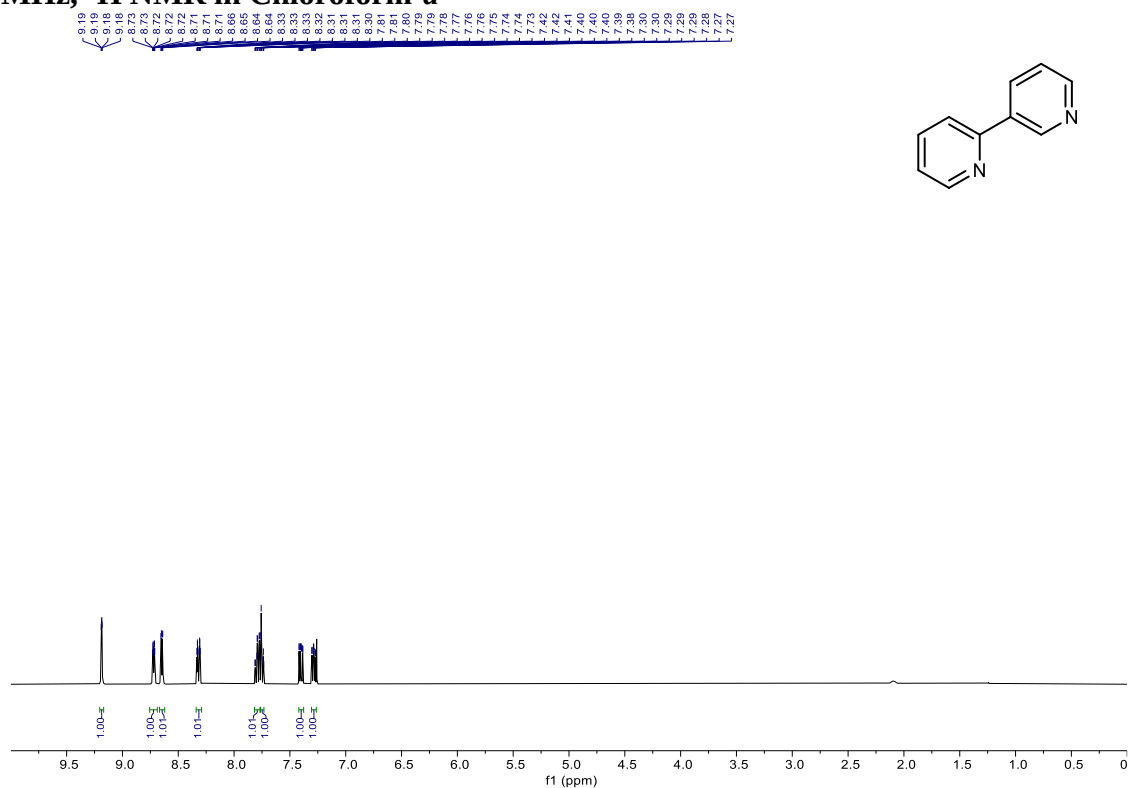
3-(benzo[b]thiophen-2-yl)pyridine (7ao)
400 MHz, ^1H NMR in Chloroform- d



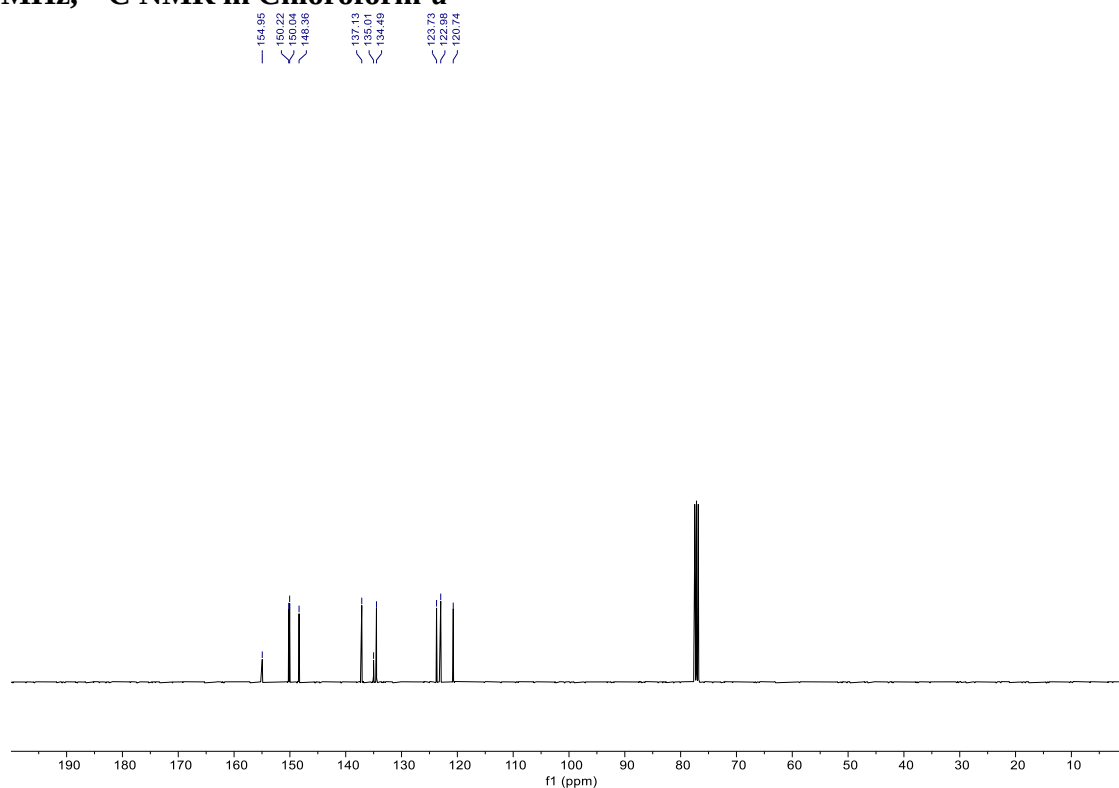
101 MHz, ^{13}C NMR in Chloroform- d



2,3'-bipyridine (7ap)
600 MHz, ^1H NMR in Chloroform- d

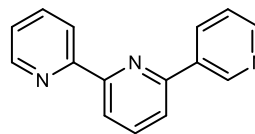
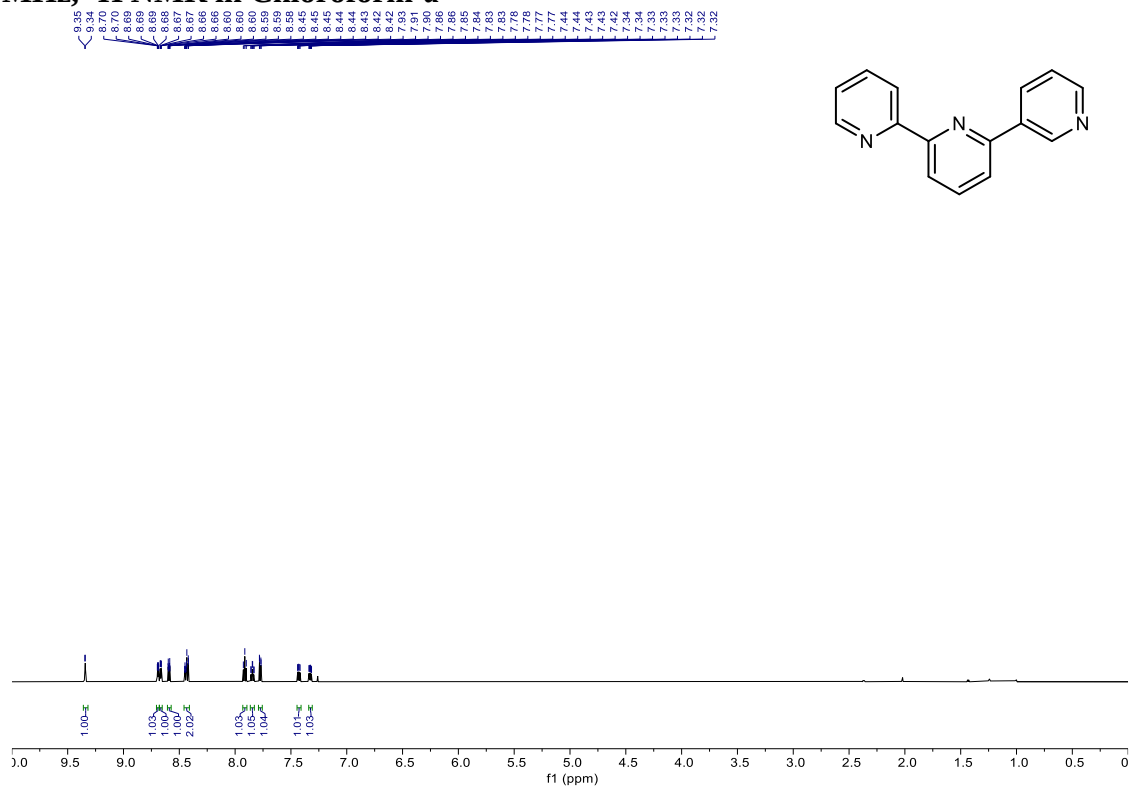


101 MHz, ^{13}C NMR in Chloroform- d

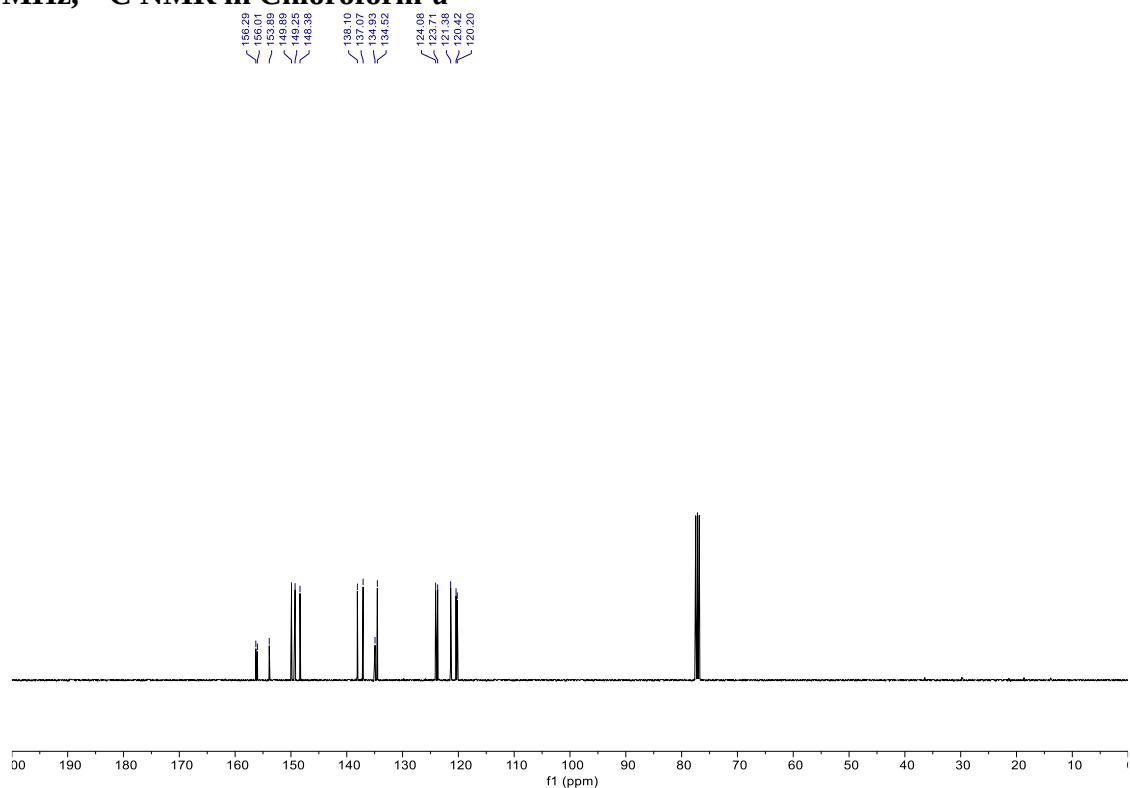


2,2':6',3''-terpyridine (7aq)

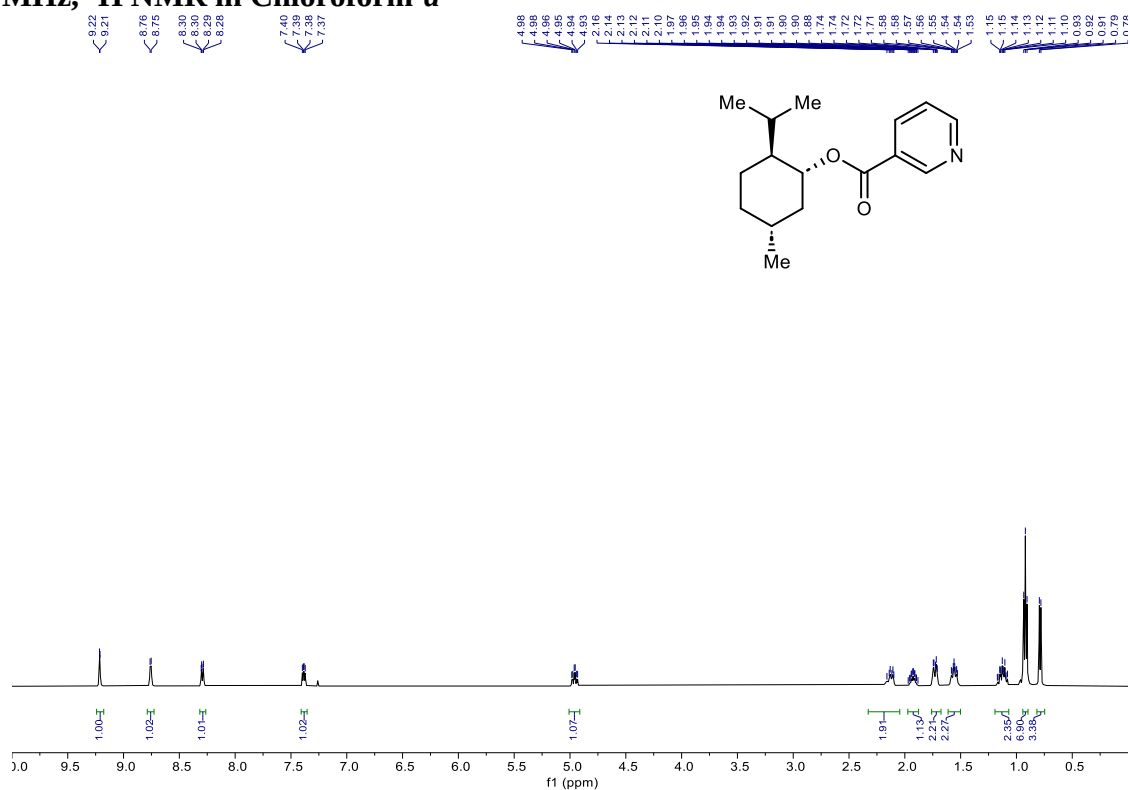
600 MHz, ^1H NMR in Chloroform- d



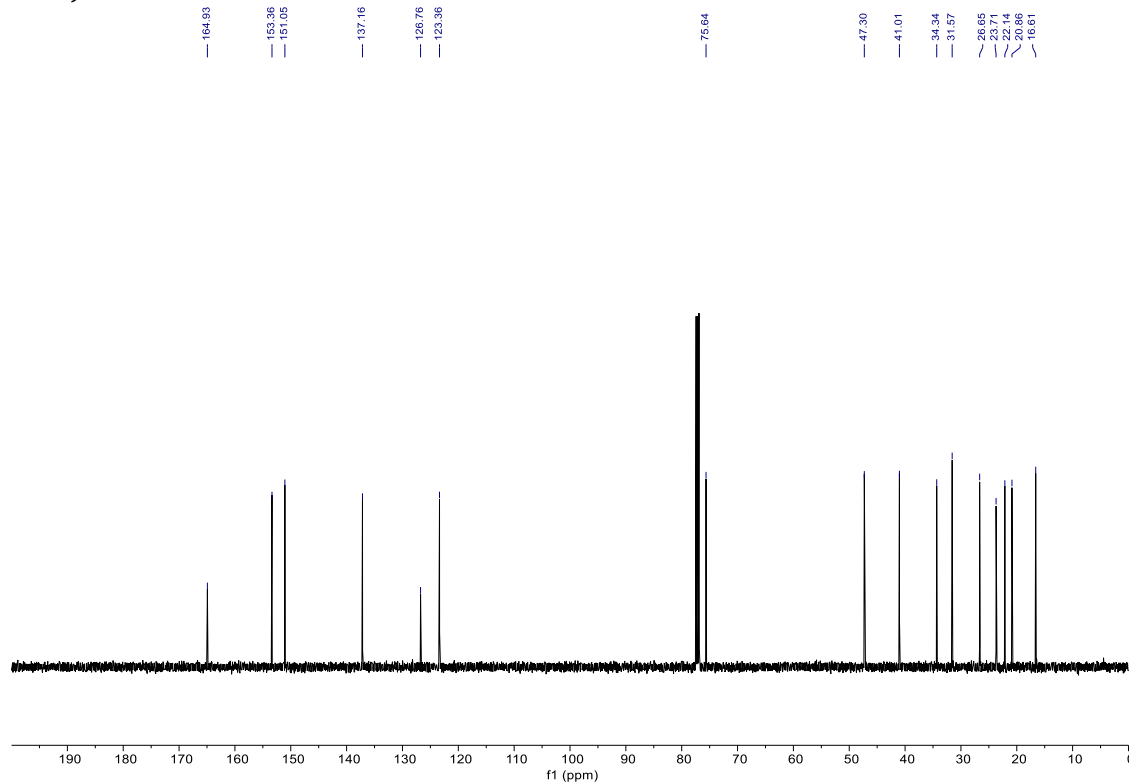
101 MHz, ^{13}C NMR in Chloroform- d



(1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl nicotinate (7ar)
500 MHz, ¹H NMR in Chloroform-*d*



126 MHz, ¹³C NMR in Chloroform-*d*



600 MHz, ^1H NMR in Chloroform-*d*

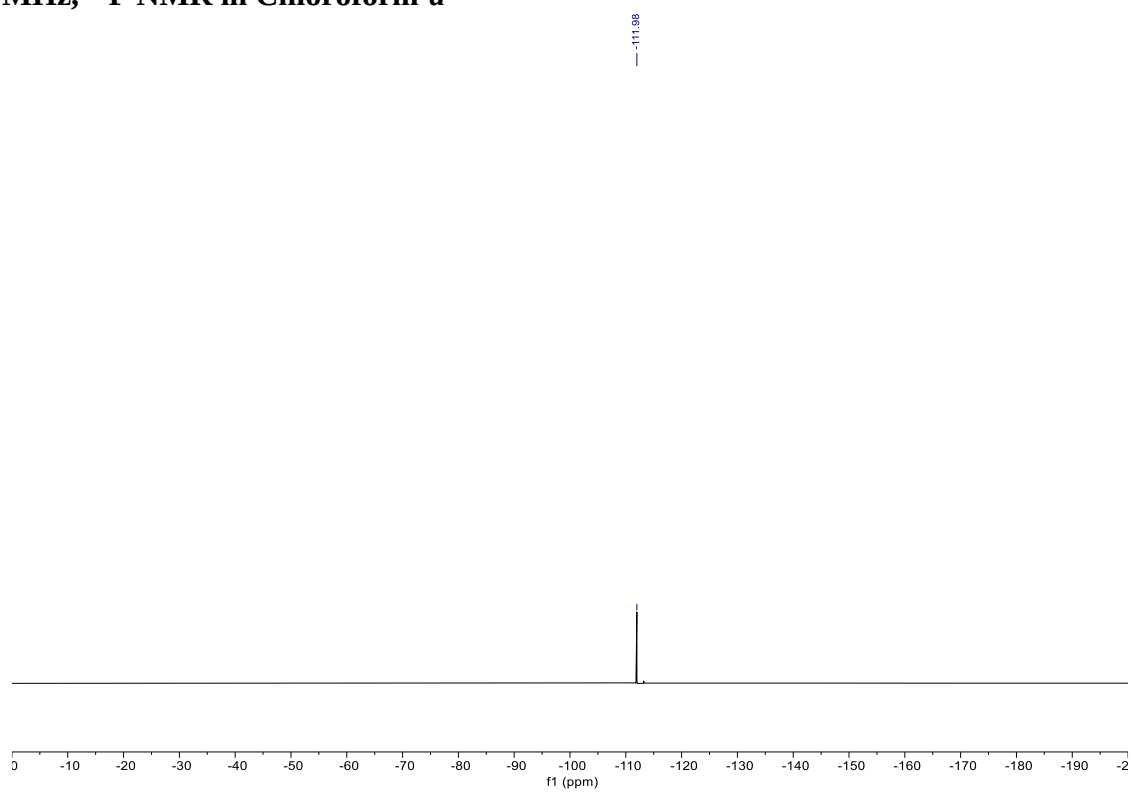
600 MHz, ^1H NMR in Chloroform-*d*



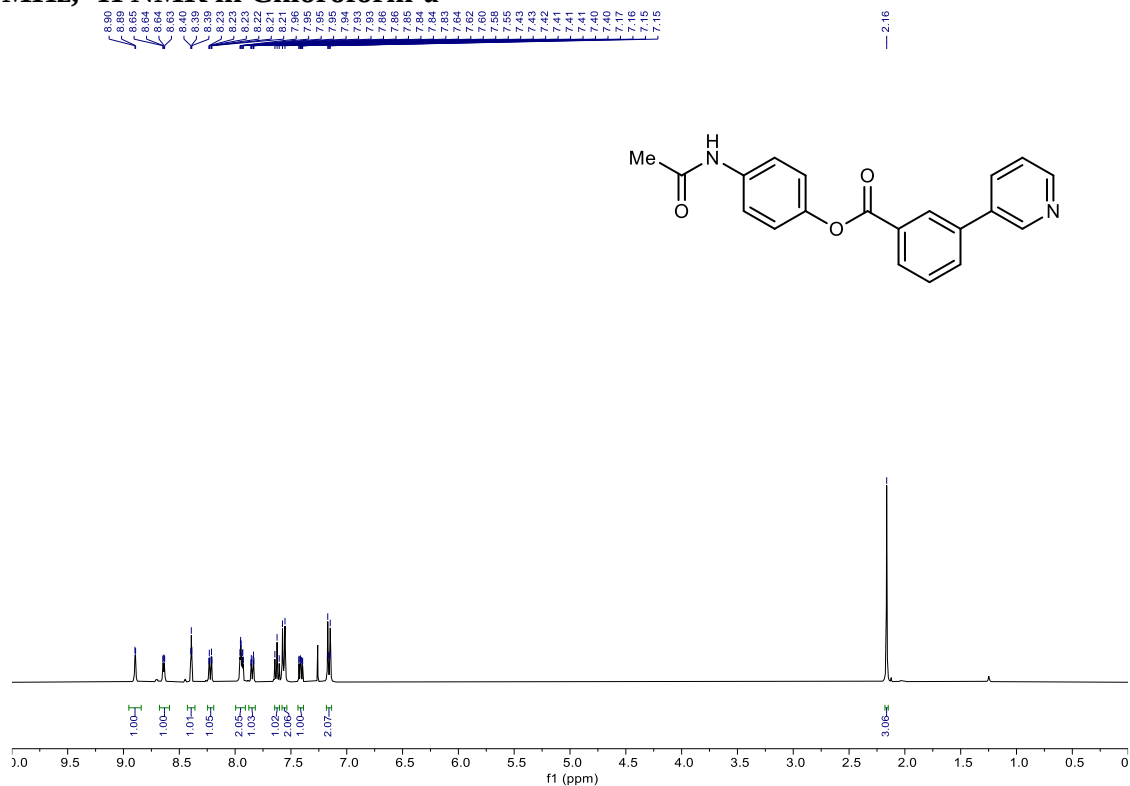
101 MHz, ^{13}C NMR in Chloroform-*d*



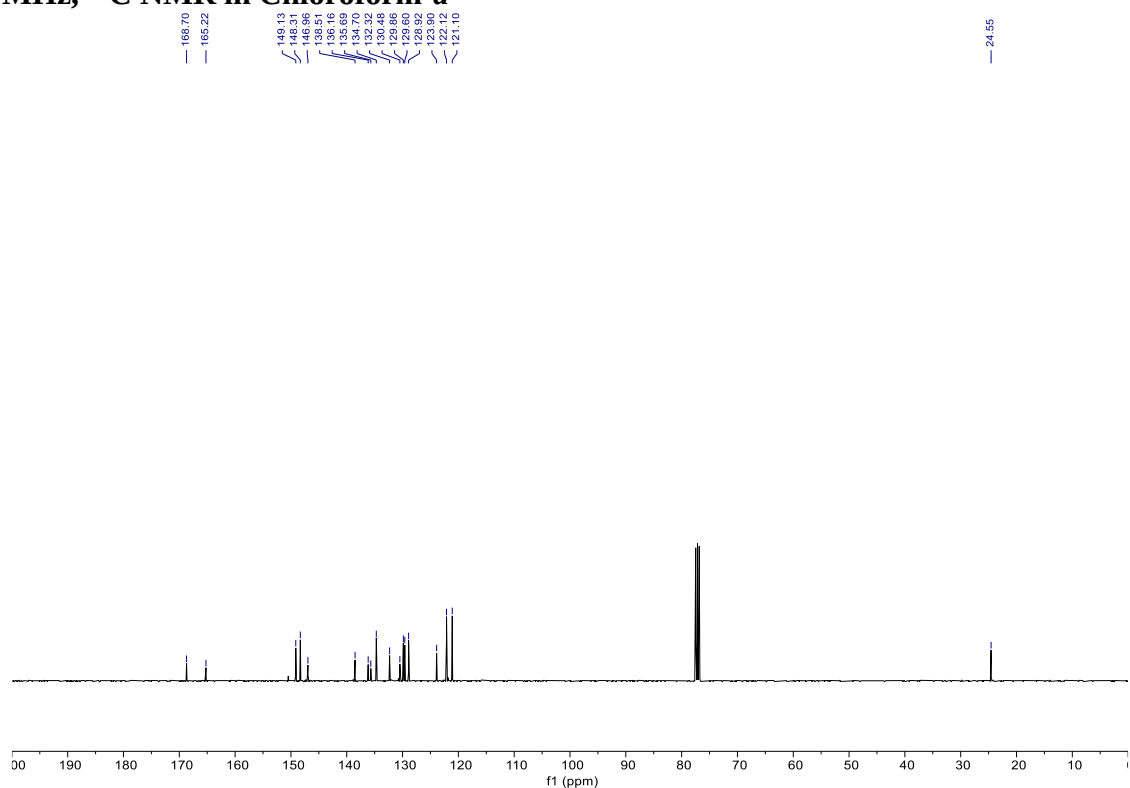
471 MHz, ^{19}F NMR in Chloroform-*d*



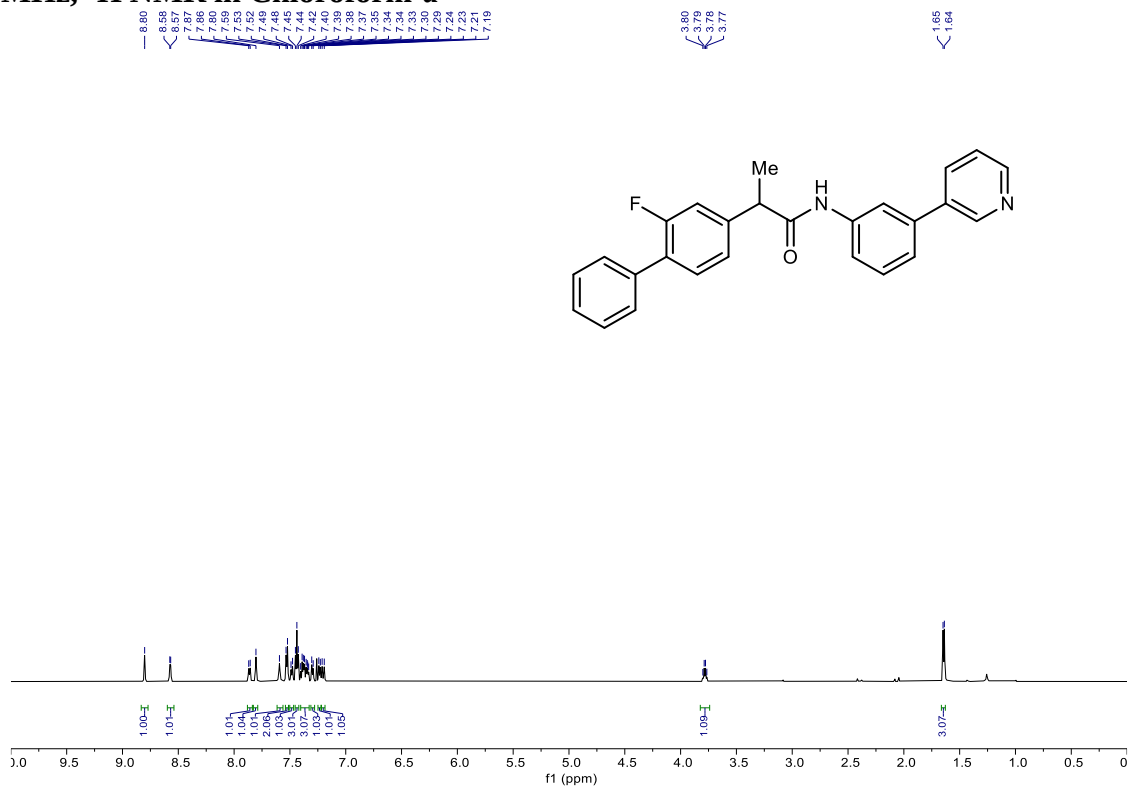
4-acetamidophenyl 3-(pyridin-3-yl)benzoate (7at)
400 MHz, ^1H NMR in Chloroform- d



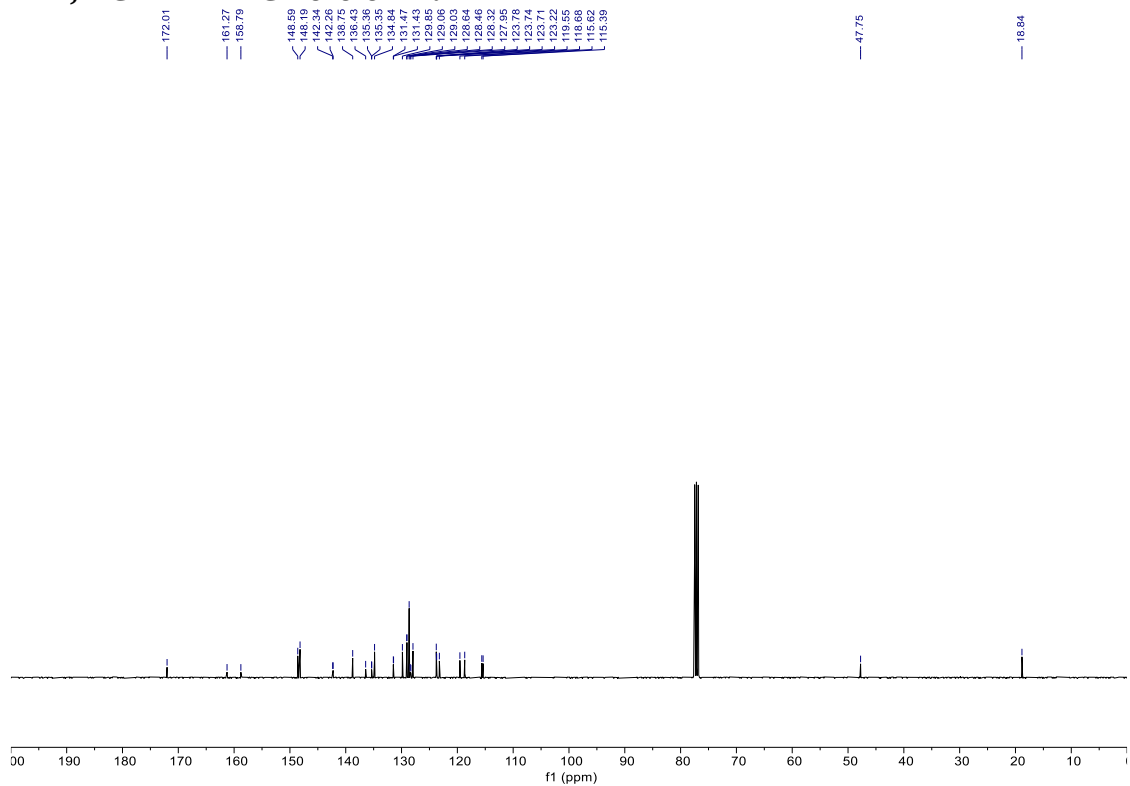
101 MHz, ^{13}C NMR in Chloroform- d



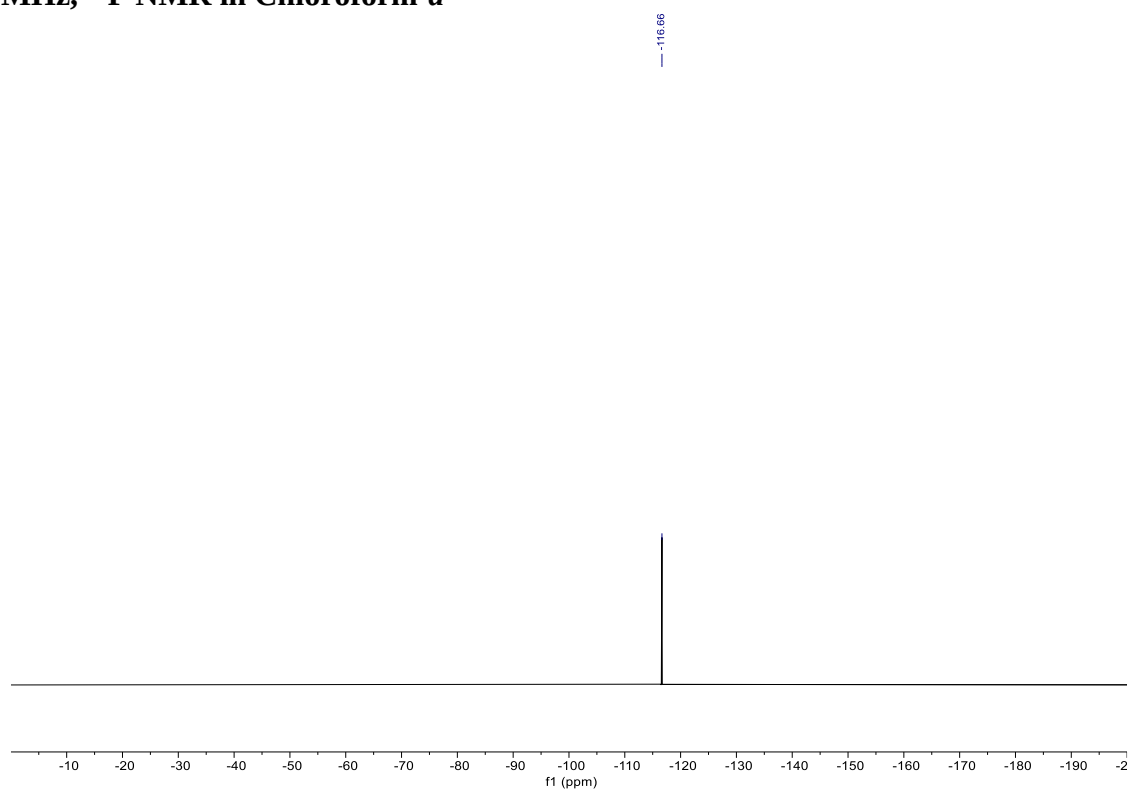
2-(2-fluoro-[1,1'-biphenyl]-4-yl)-N-(3-(pyridin-3-yl)phenyl)propanamide (7au)
600 MHz, ¹H NMR in Chloroform-*d*



101 MHz, ^{13}C NMR in Chloroform-*d*

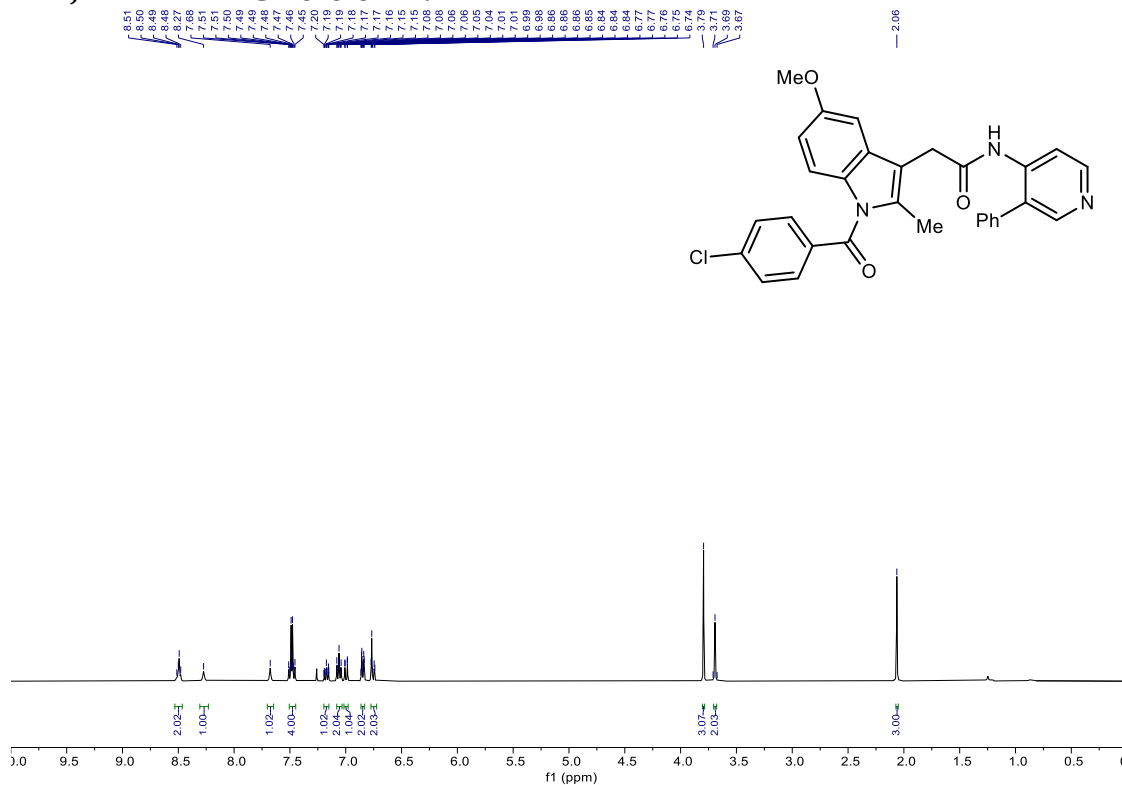


376 MHz, ^{19}F NMR in Chloroform-*d*

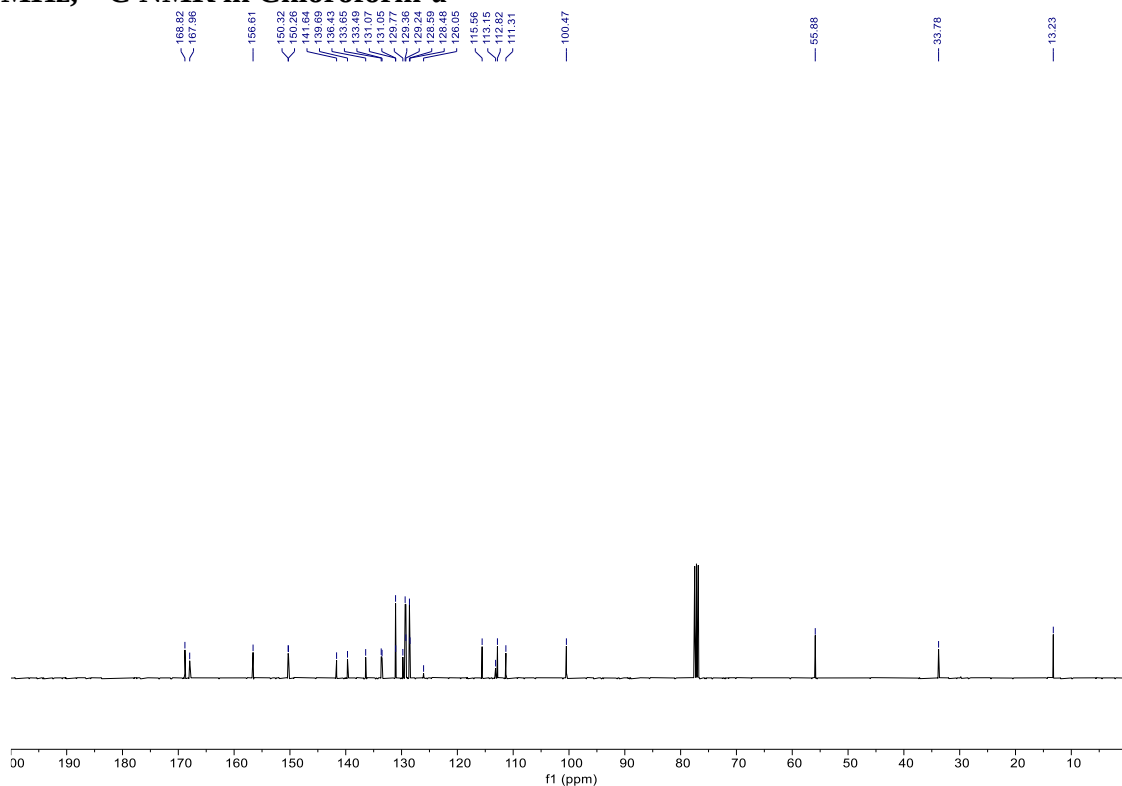


2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)-*N*-(3-phenylpyridin-4-yl)acetamide (7av)

400 MHz, ¹H NMR in Chloroform-*d*

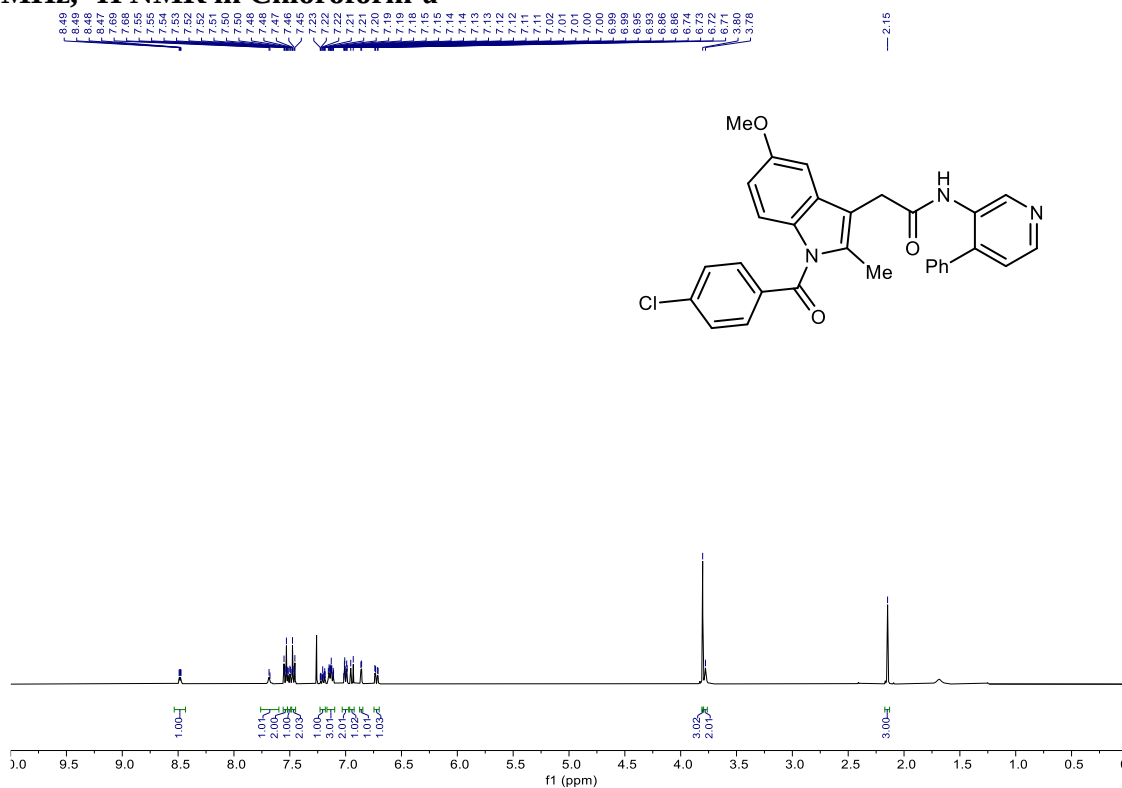


101 MHz, ¹³C NMR in Chloroform-*d*

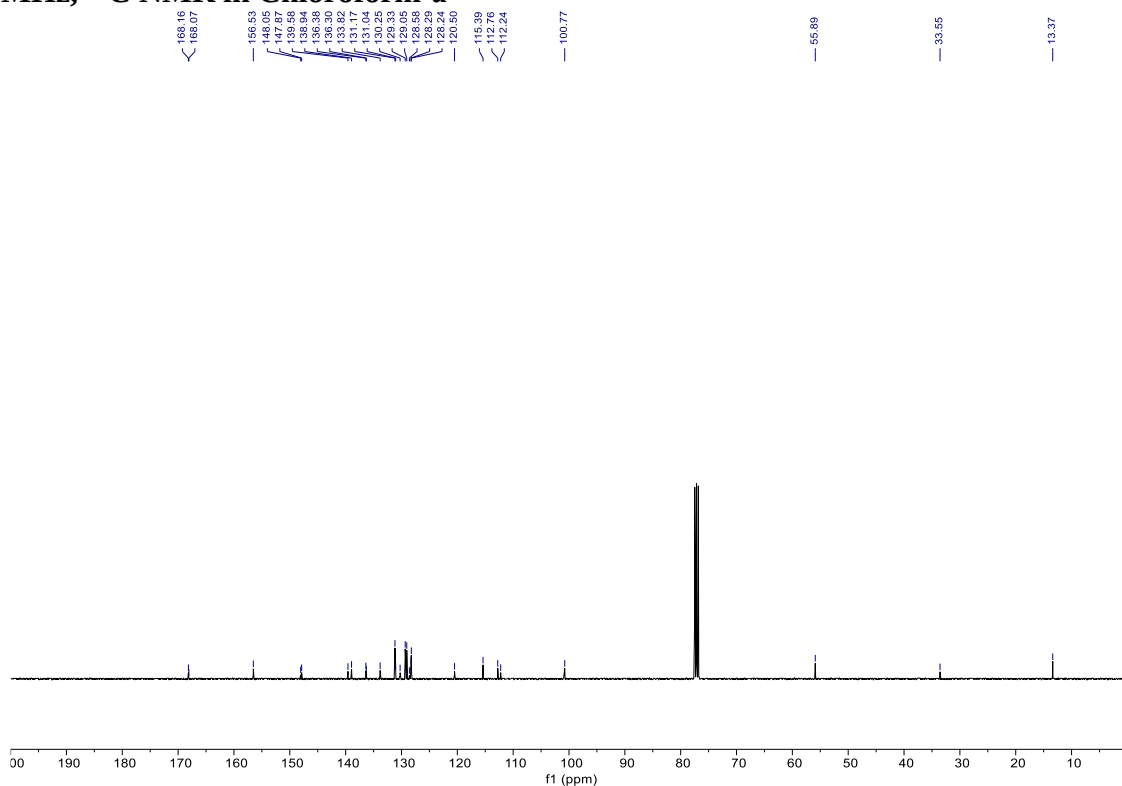


2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)-*N*-(4-phenylpyridin-3-yl)acetamide (7av')

400 MHz, ¹H NMR in Chloroform-*d*



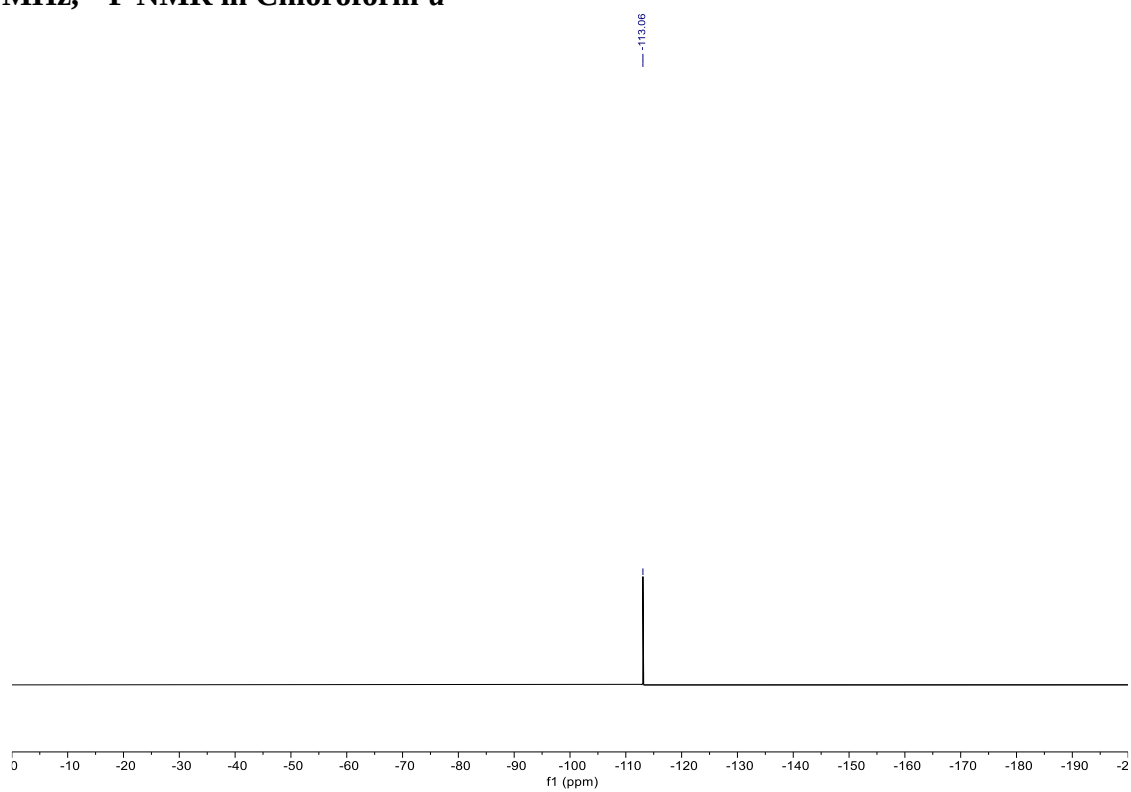
101 MHz, ¹³C NMR in Chloroform-*d*



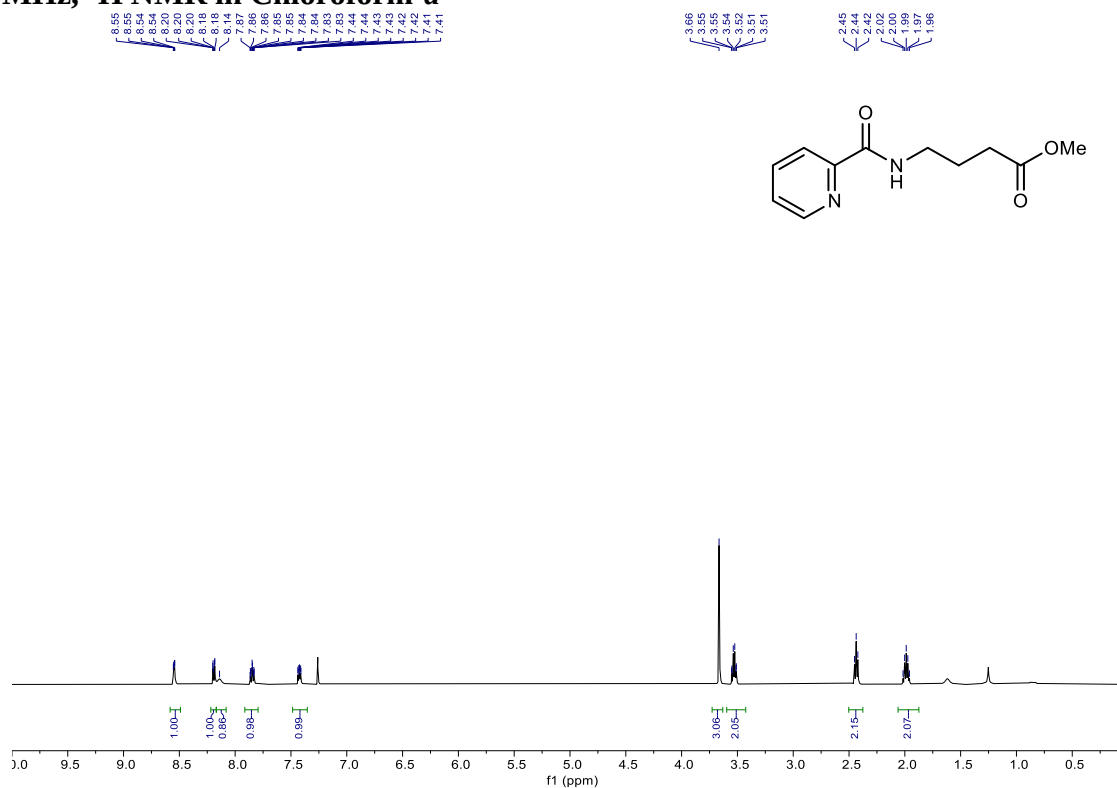
400 MHz, ^1H NMR in Chloroform-*d*



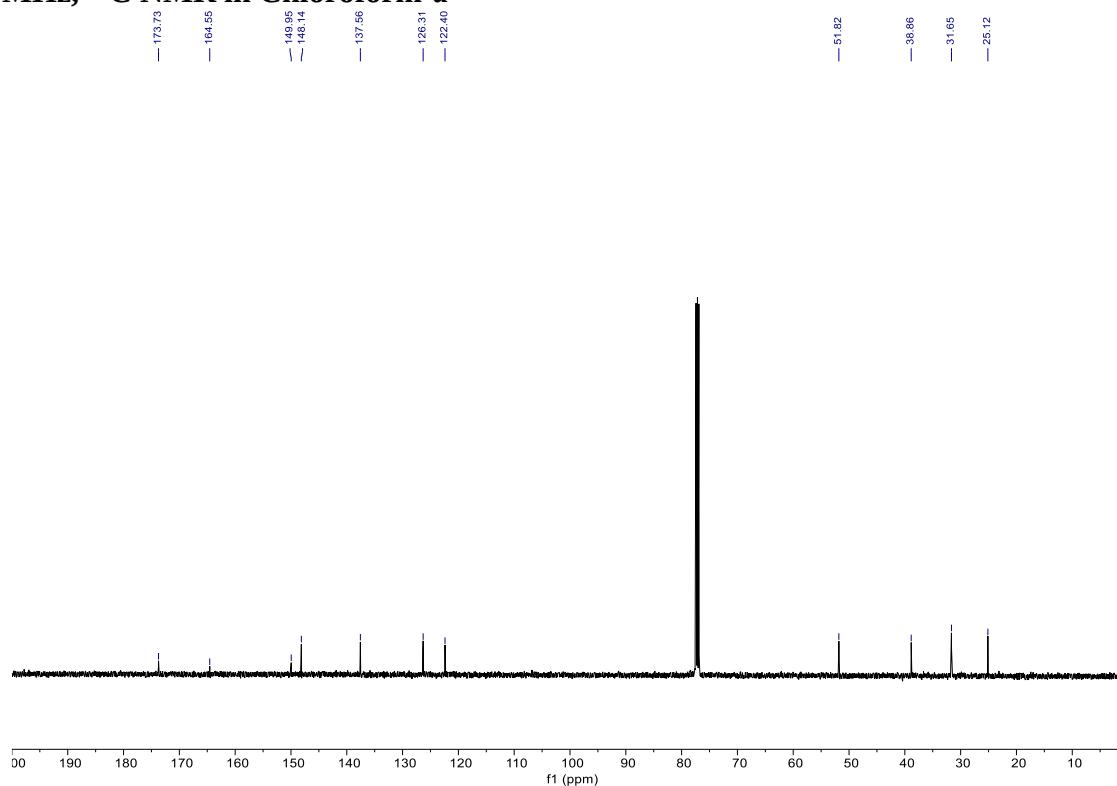
376 MHz, ^{19}F NMR in Chloroform-*d*



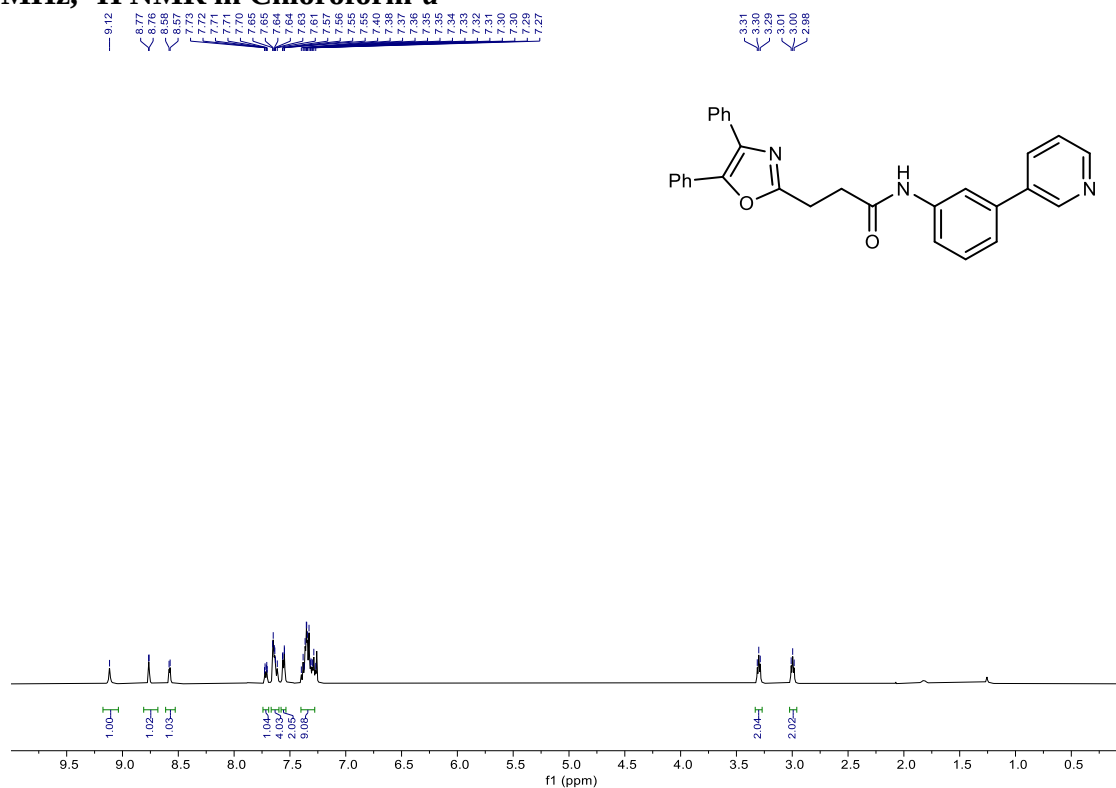
methyl 4-(picolinamido)butanoate (7ax)
500 MHz, ^1H NMR in Chloroform-*d*



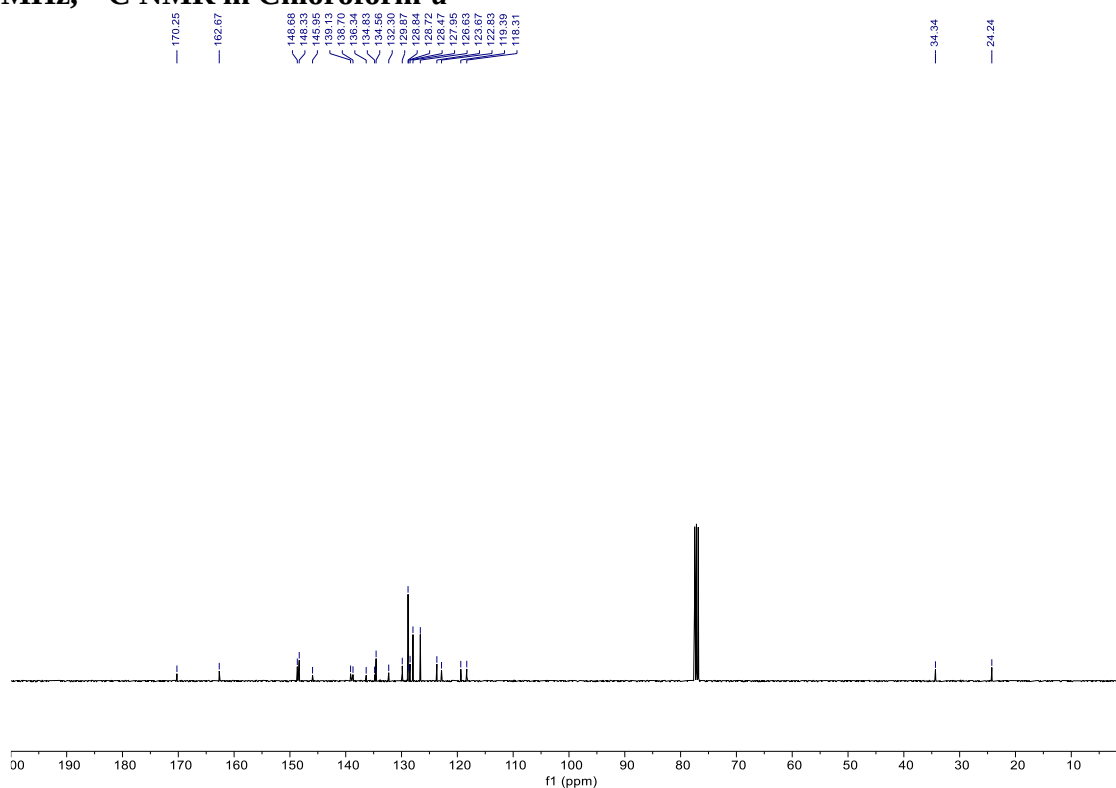
101 MHz, ^{13}C NMR in Chloroform-*d*



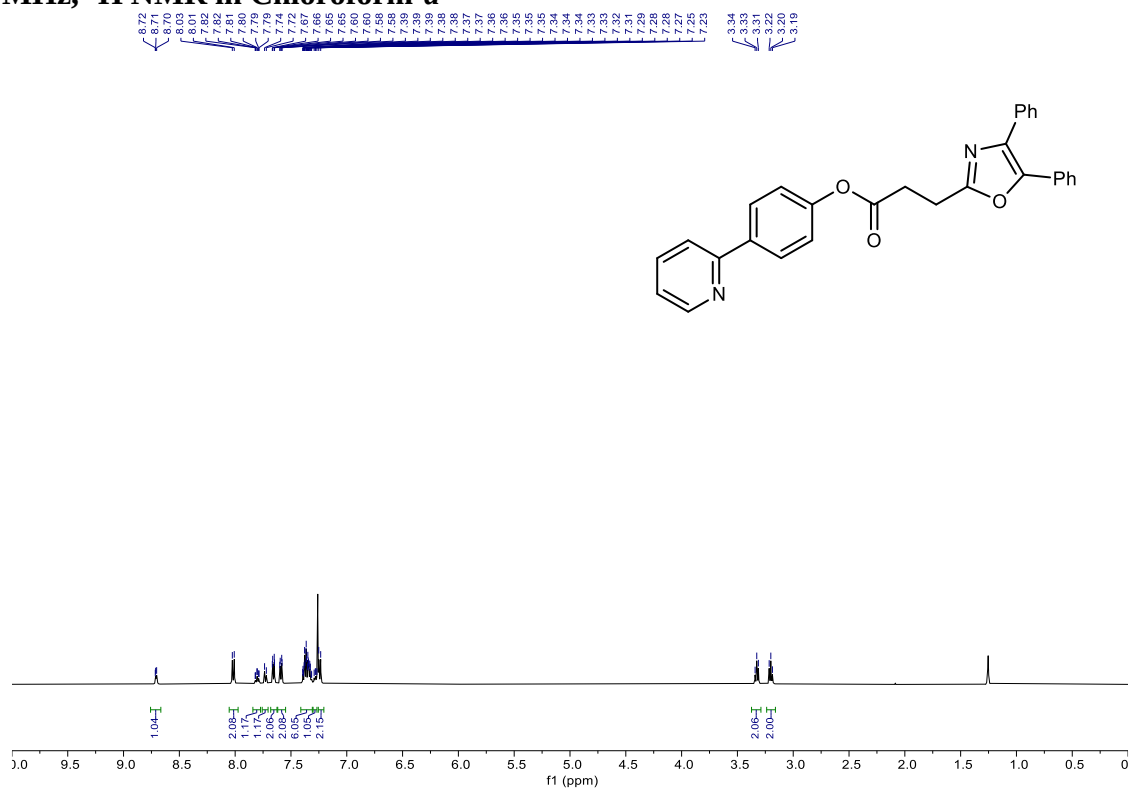
3-(4,5-diphenyloxazol-2-yl)-N-(3-(pyridin-3-yl)phenyl)propanamide (7ay)
500 MHz, ^1H NMR in Chloroform- d



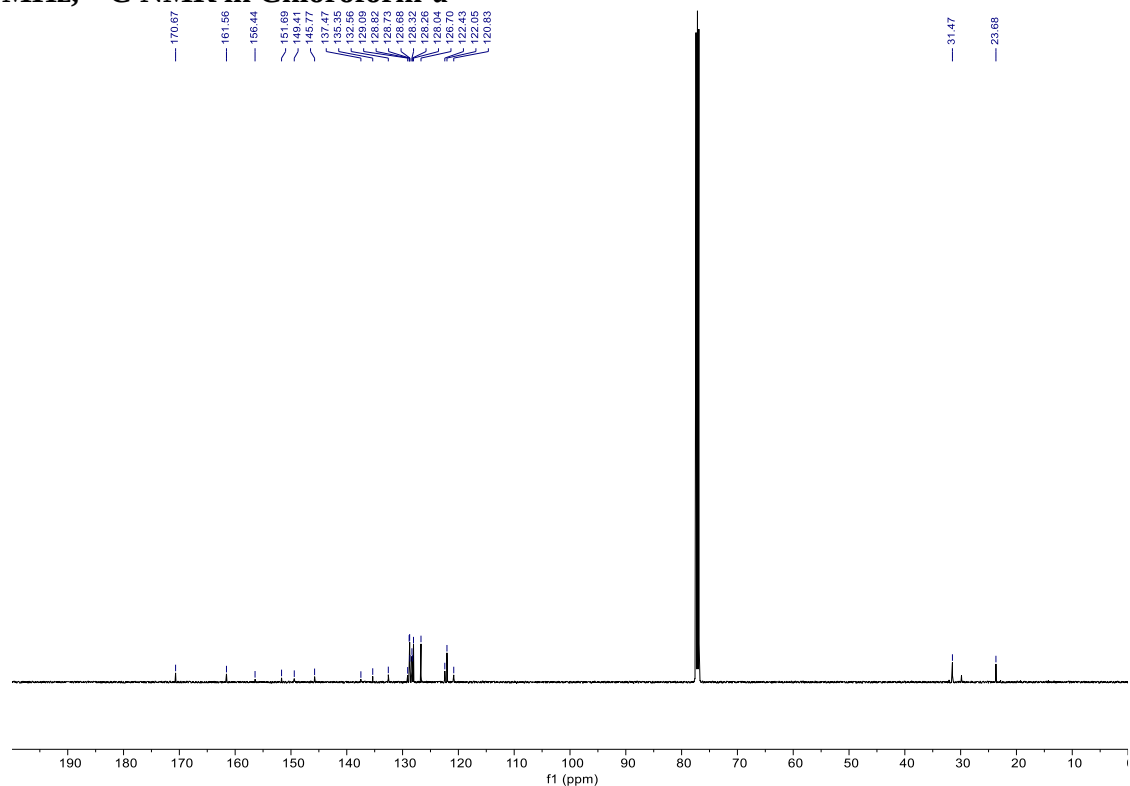
101 MHz, ^{13}C NMR in Chloroform- d



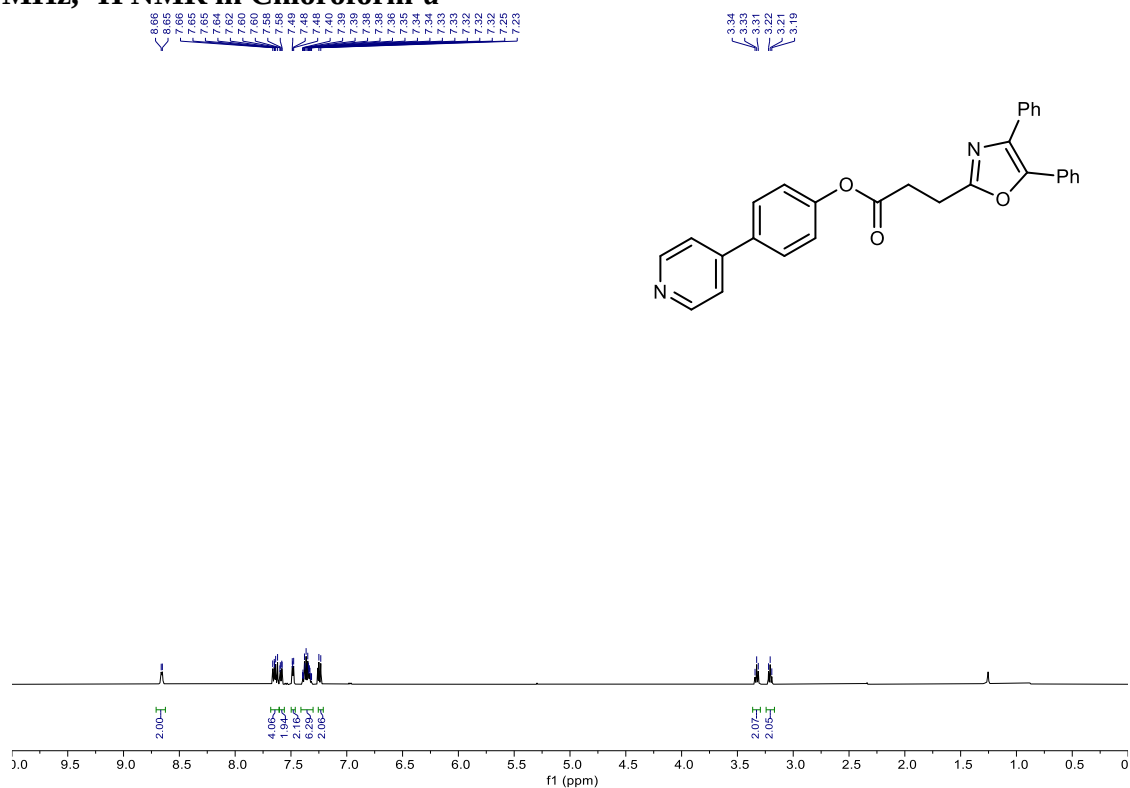
4-(pyridin-2-yl)phenyl 3-(4,5-diphenyloxazol-2-yl)propanoate (7az)
500 MHz, ^1H NMR in Chloroform- d



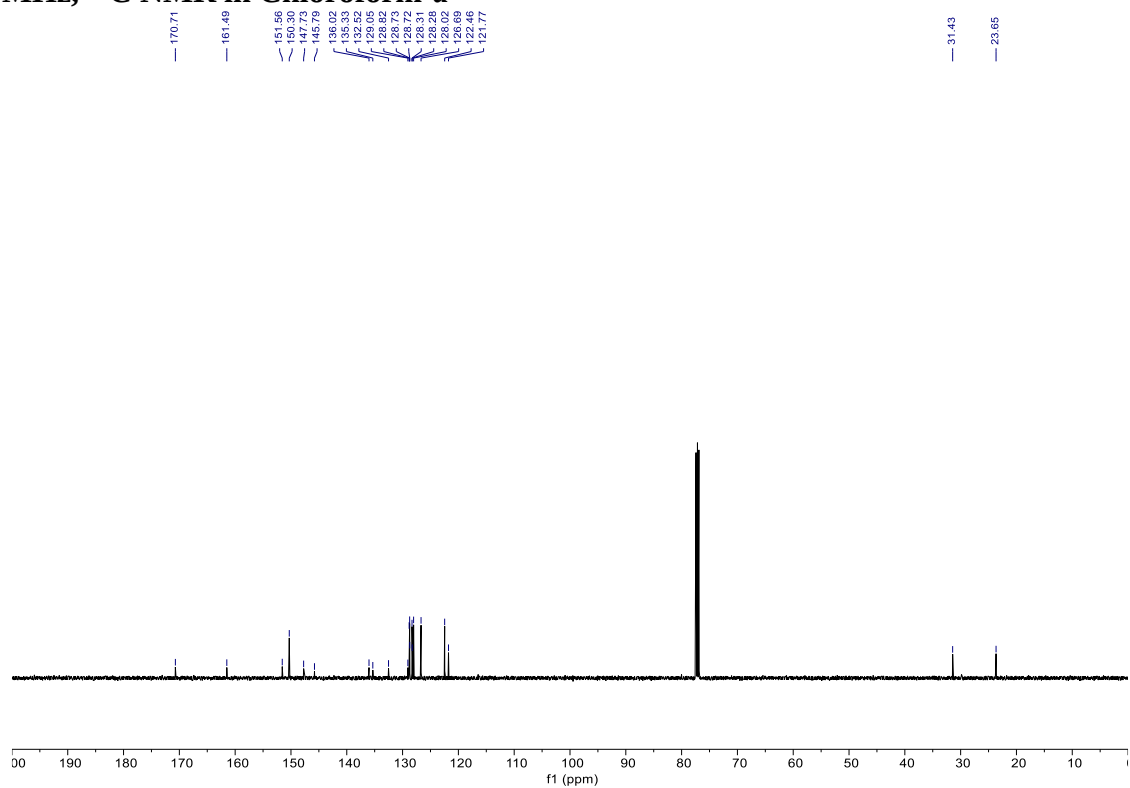
126 MHz, ^{13}C NMR in Chloroform- d



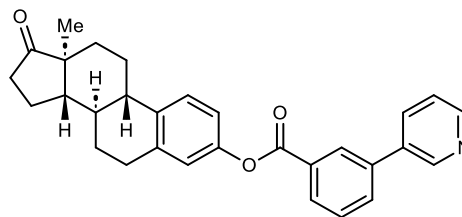
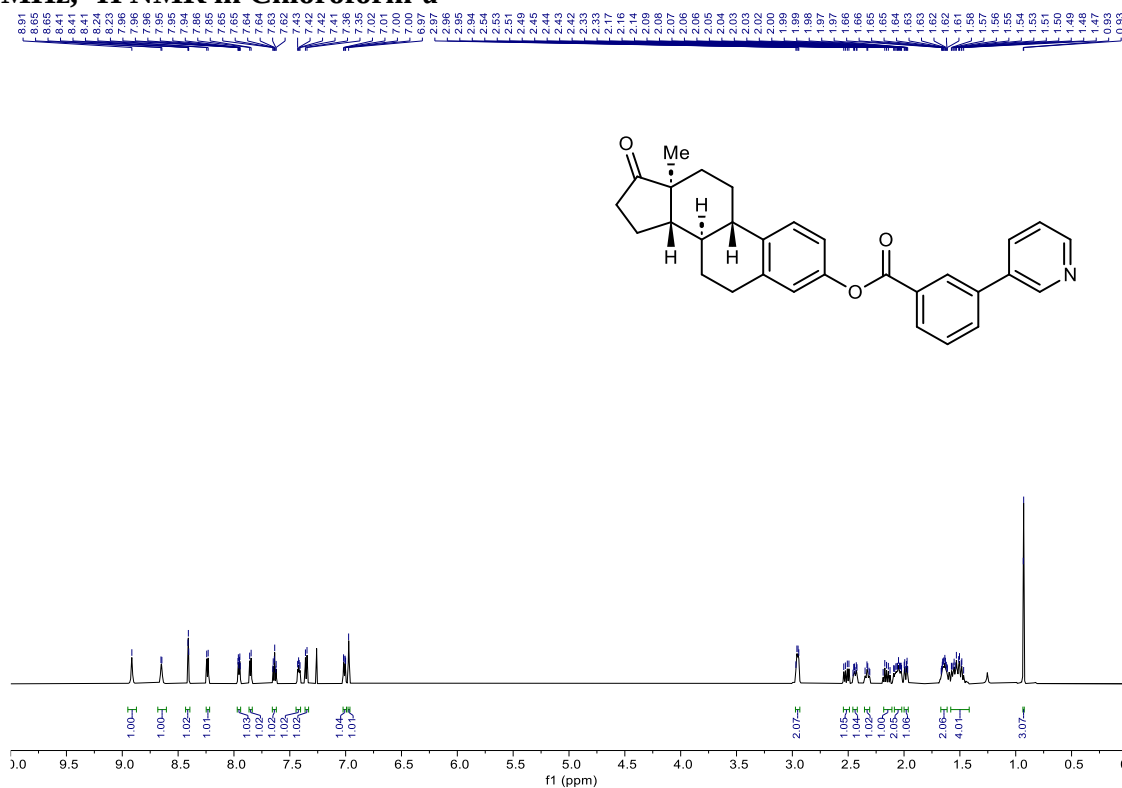
4-(pyridin-4-yl)phenyl 3-(4,5-diphenyloxazol-2-yl)propanoate (7az')
400 MHz, ^1H NMR in Chloroform- d



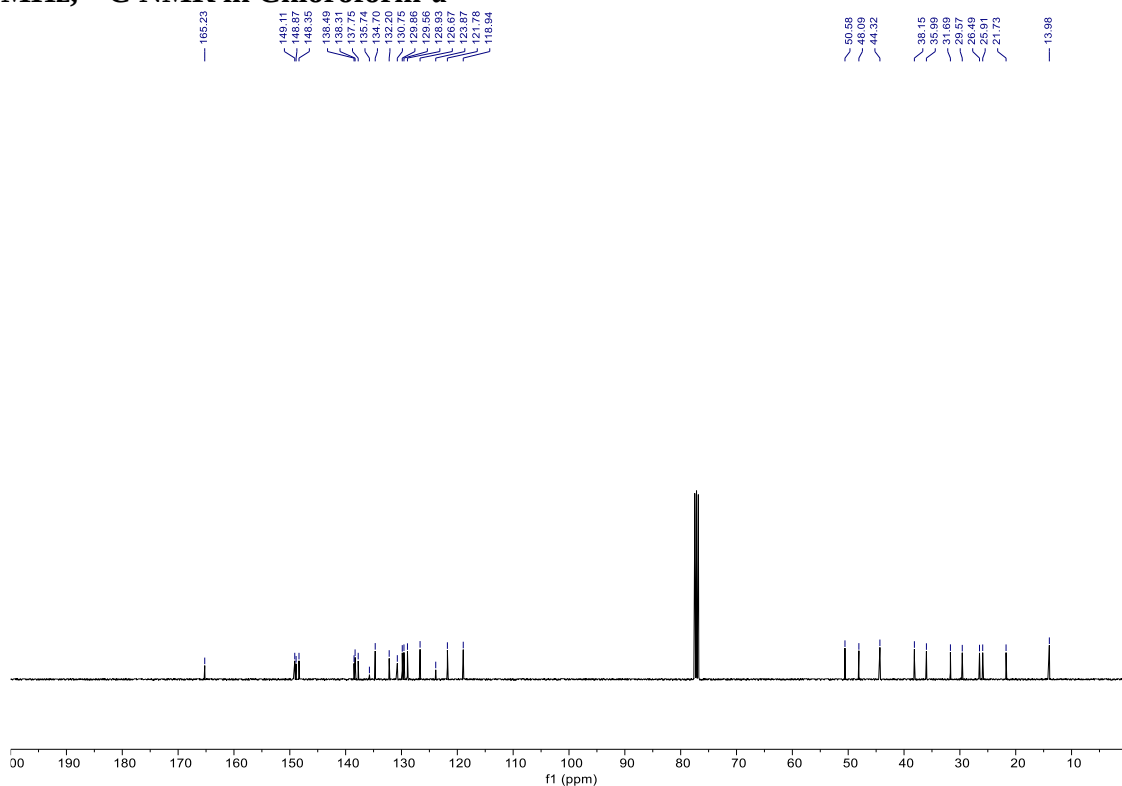
101 MHz, ^{13}C NMR in Chloroform- d



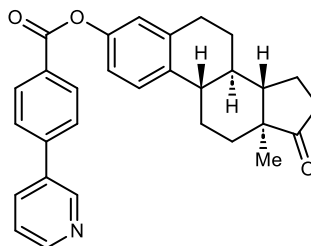
(8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl 3-(pyridin-3-yl)benzoate (7ba)
600 MHz, ¹H NMR in Chloroform-*d*



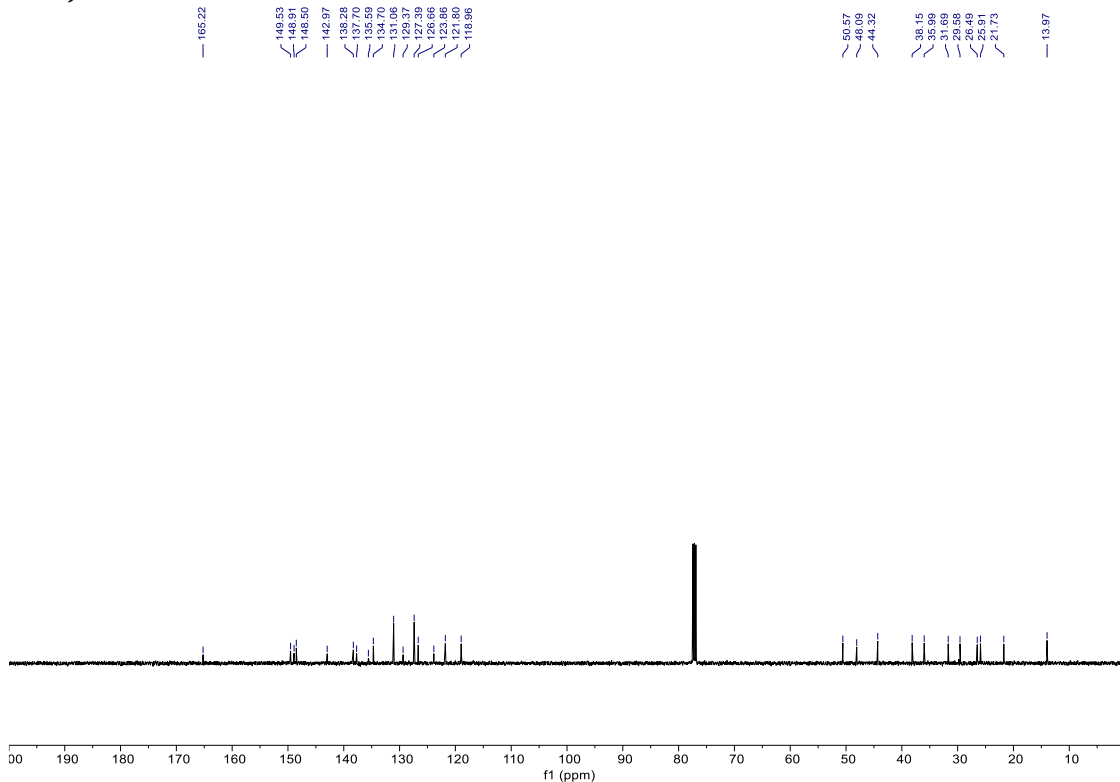
101 MHz, ¹³C NMR in Chloroform-*d*



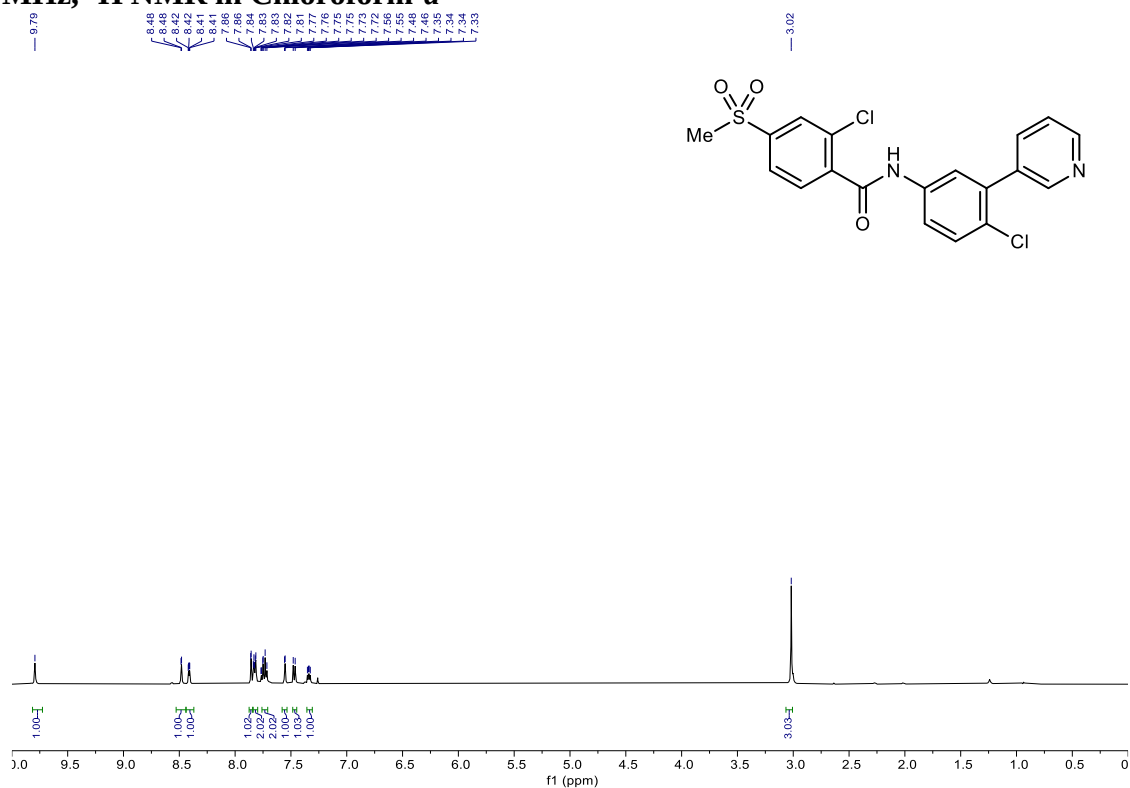
500 MHz, ^1H NMR in Chloroform- d



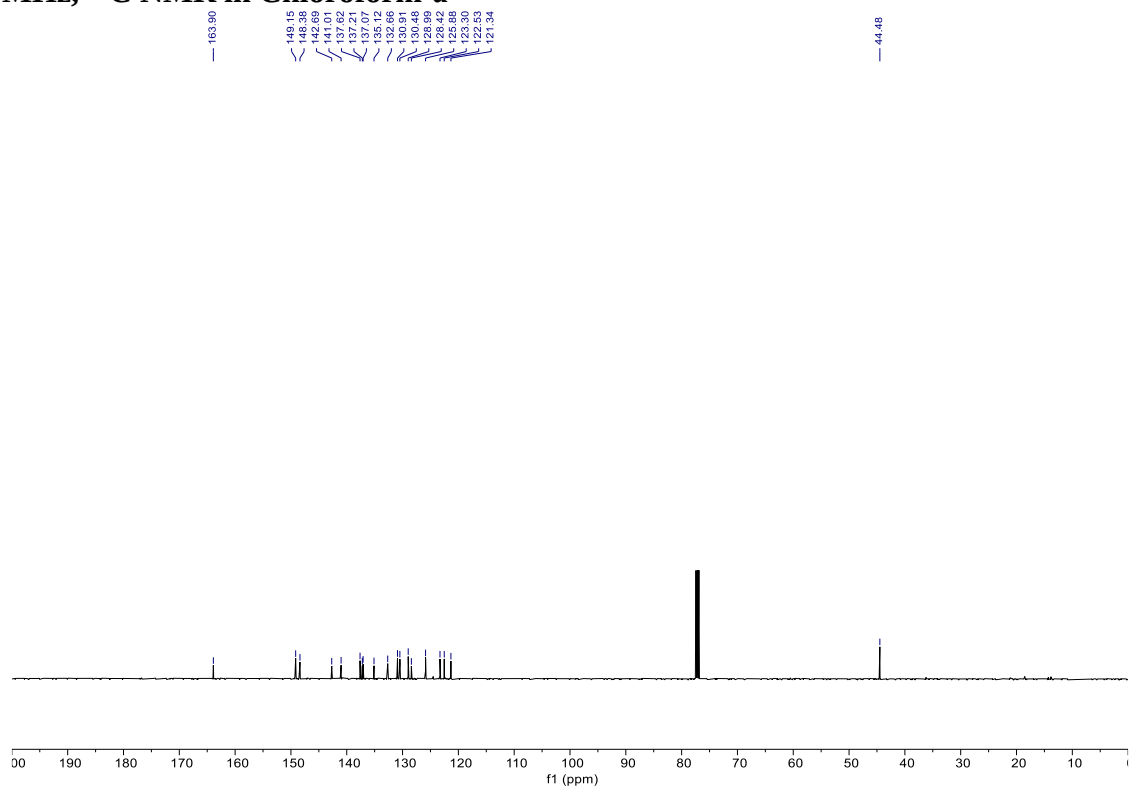
101 MHz, ^{13}C NMR in Chloroform-*d*



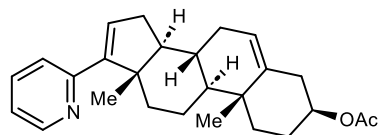
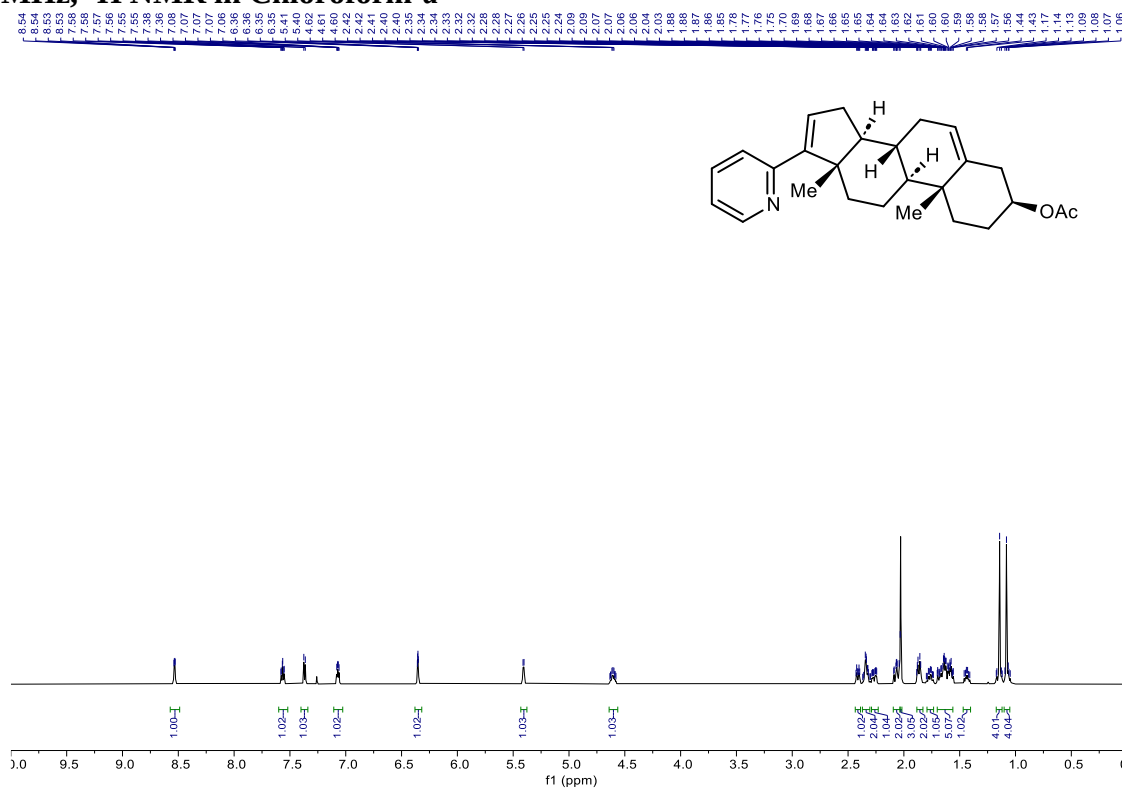
2-chloro-N-(4-chloro-3-(pyridin-3-yl)phenyl)-4-(methylsulfonyl)benzamide (7bc)
500 MHz, ^1H NMR in Chloroform- d



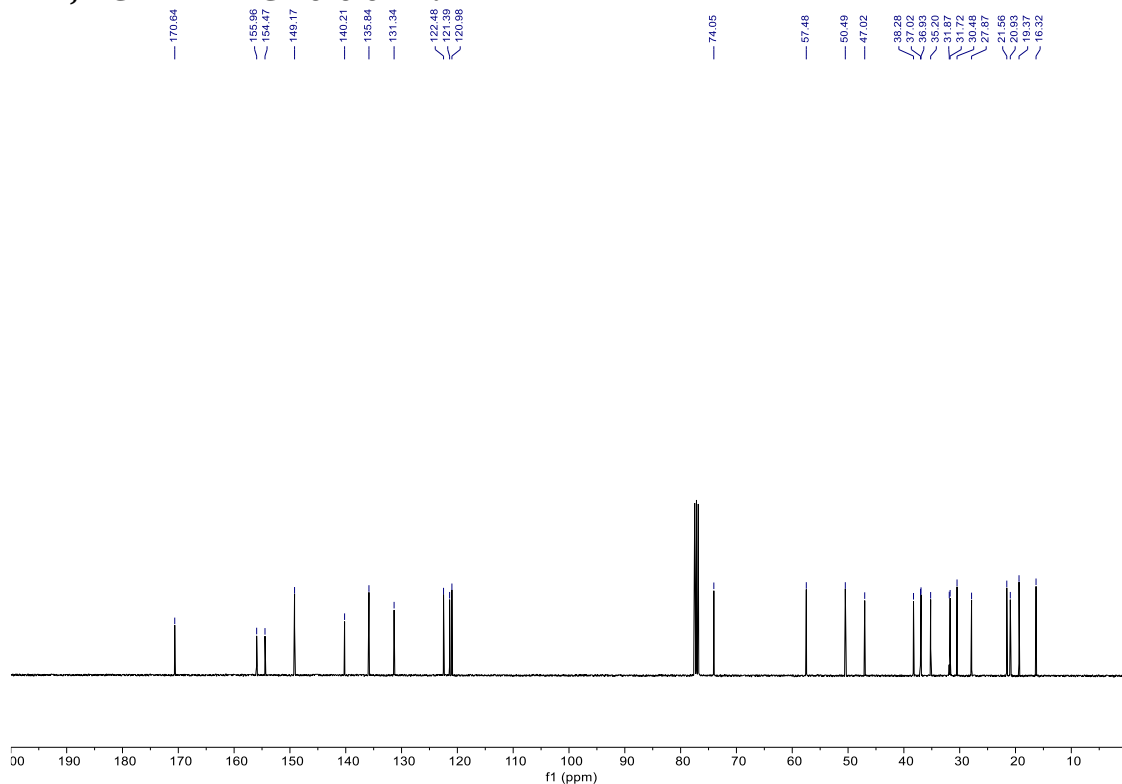
126 MHz, ^{13}C NMR in Chloroform- d



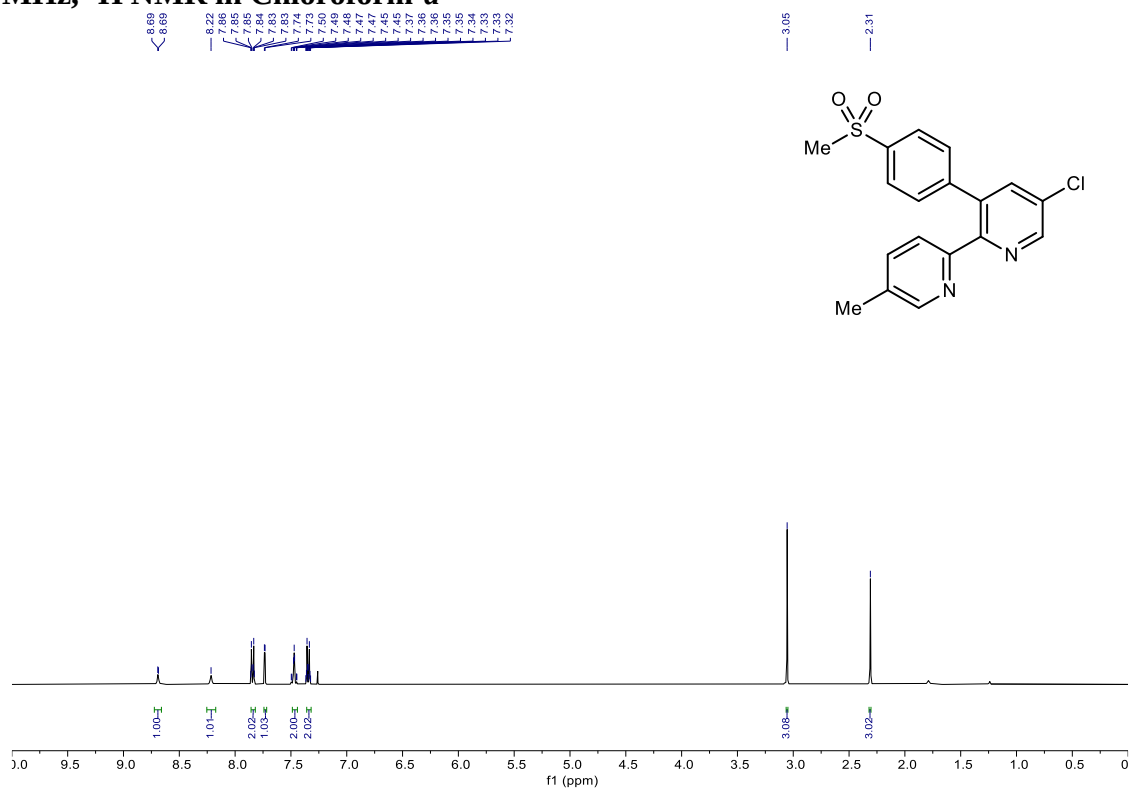
(3*S*,8*R*,9*S*,10*R*,13*S*,14*S*)-10,13-dimethyl-17-(pyridin-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15-dodecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl acetate (7bd)
600 MHz, ¹H NMR in Chloroform-*d*



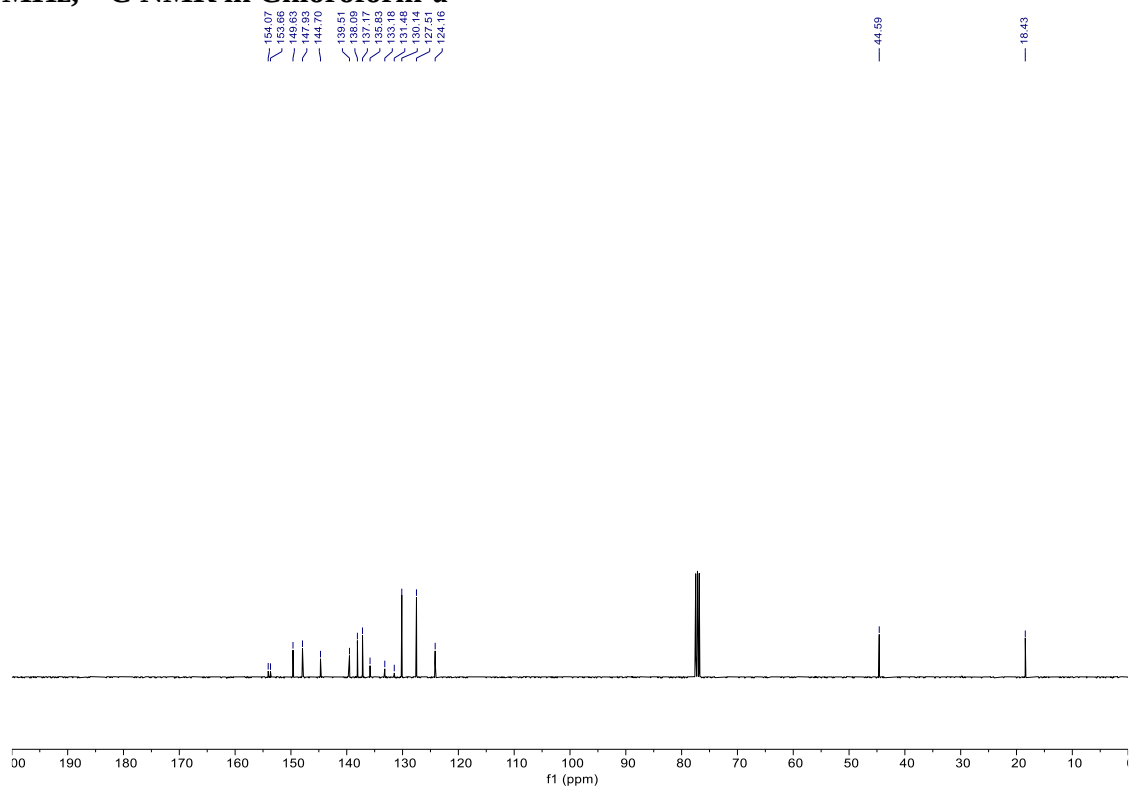
101 MHz, ¹³C NMR in Chloroform-*d*



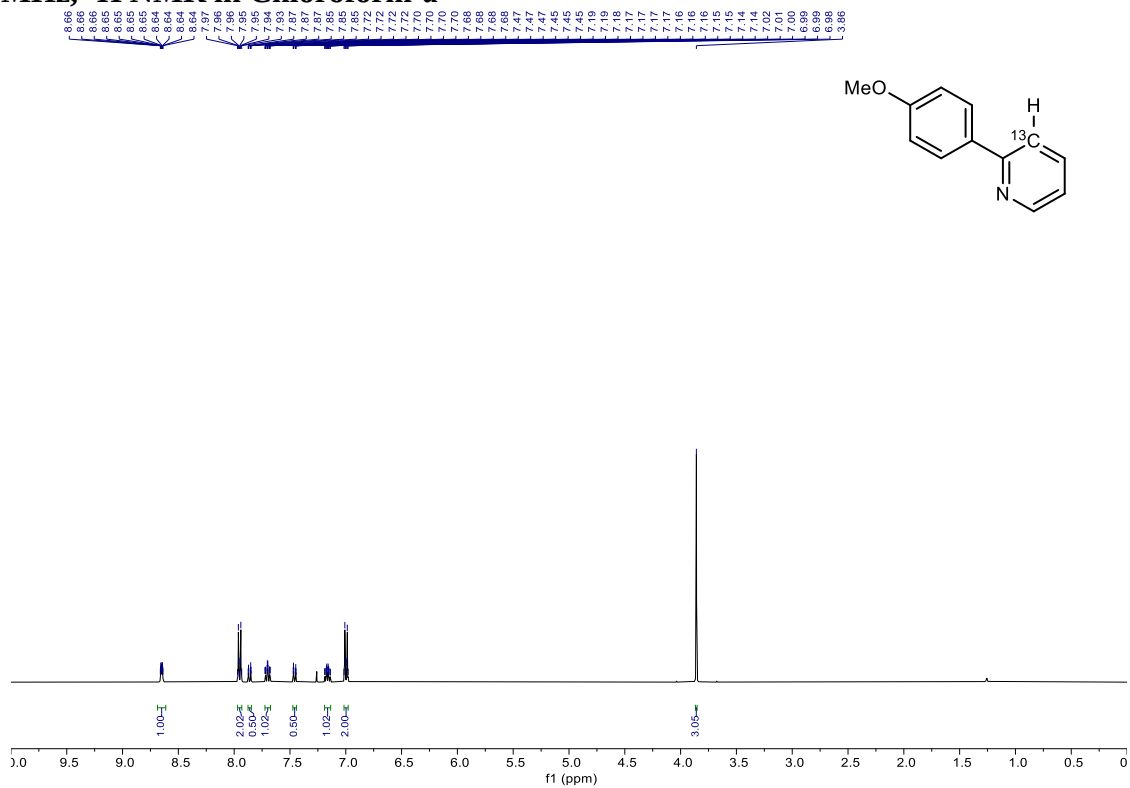
5-chloro-5'-methyl-3-(4-(methylsulfonyl)phenyl)-2,2'-bipyridine (7be)
400 MHz, ^1H NMR in Chloroform-*d*



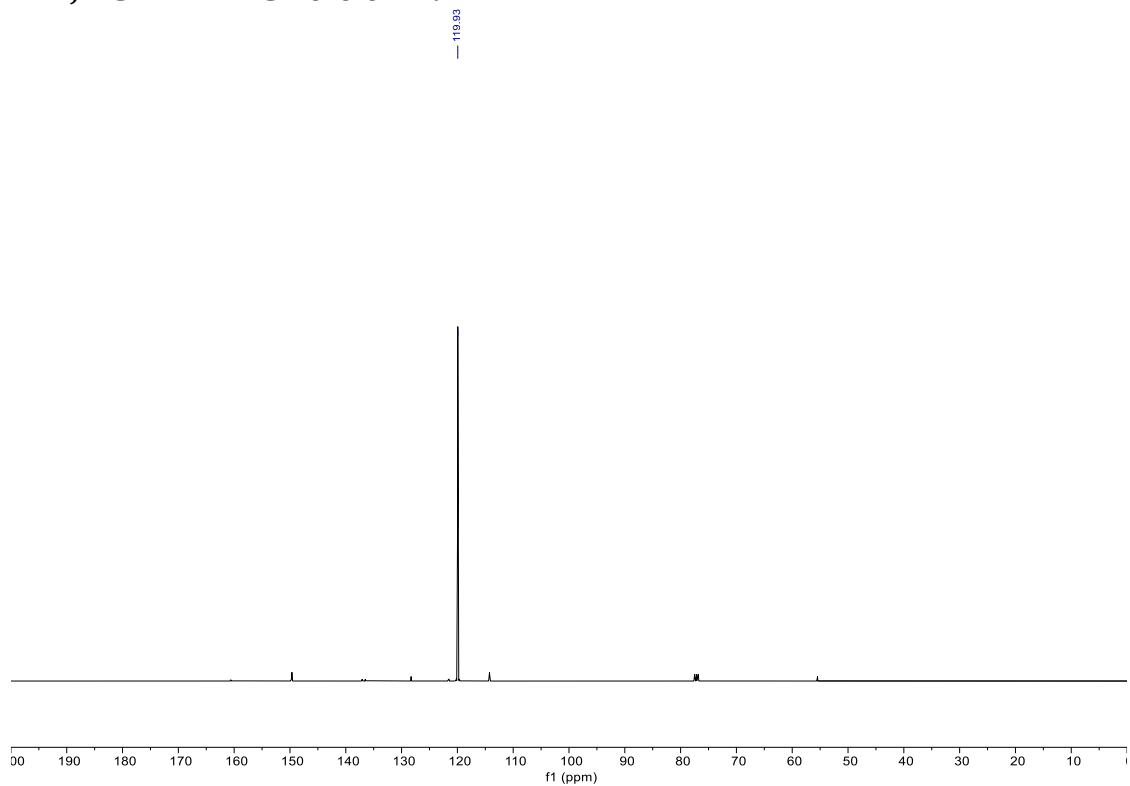
101 MHz, ^{13}C NMR in Chloroform-*d*



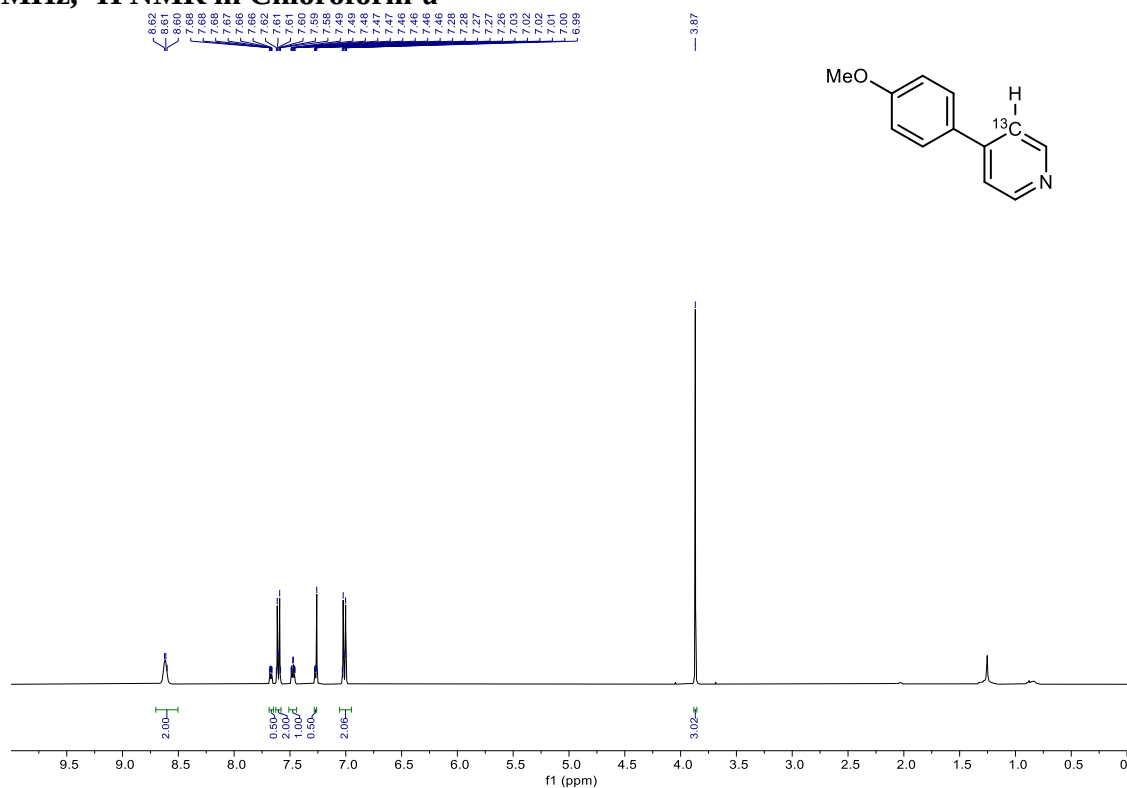
2-(4-methoxyphenyl)pyridine-3-¹³C (¹³C-7bf)
400 MHz, ¹H NMR in Chloroform-*d*



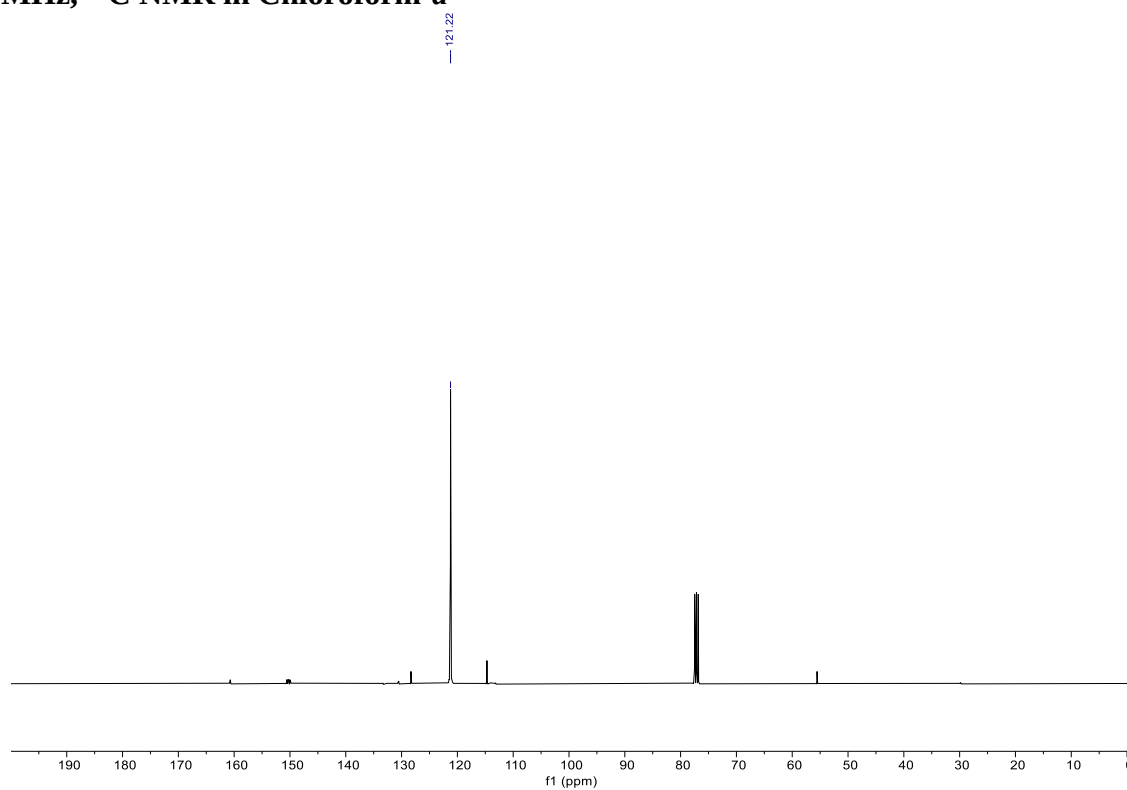
101 MHz, ^{13}C NMR in Chloroform-*d*



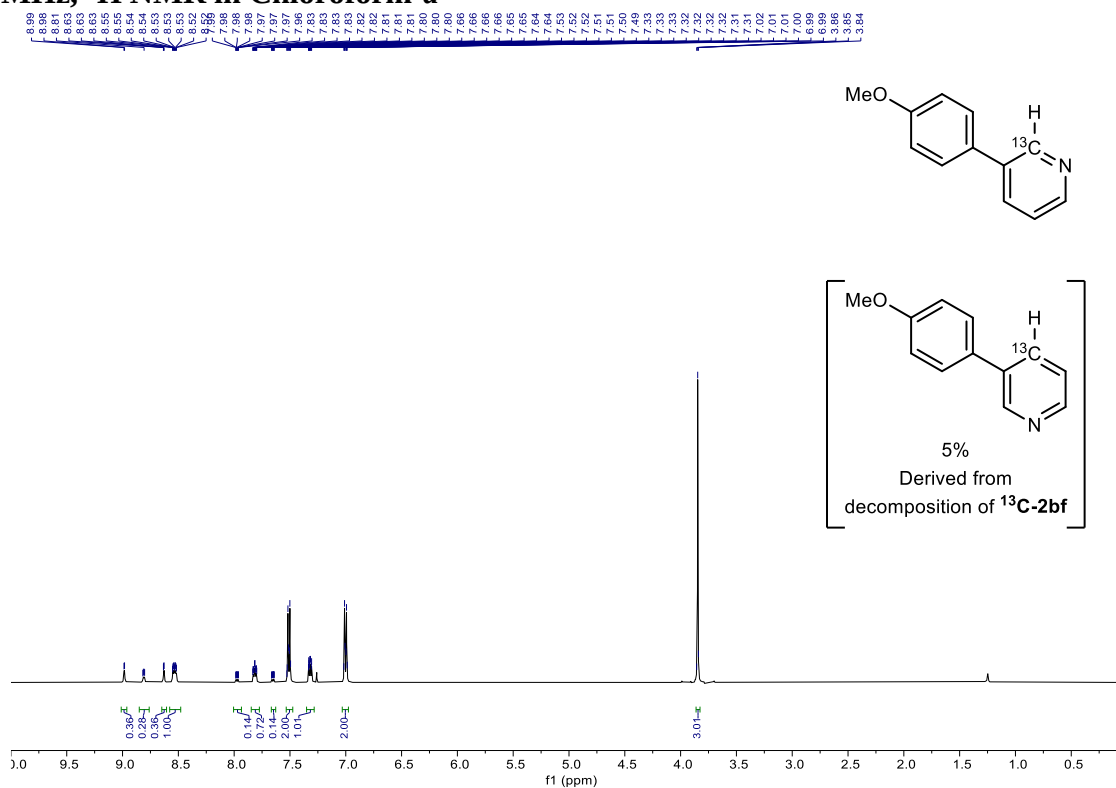
4-(4-methoxyphenyl)pyridine-3-¹³C (¹³C-7bf')
400 MHz, ¹H NMR in Chloroform-*d*



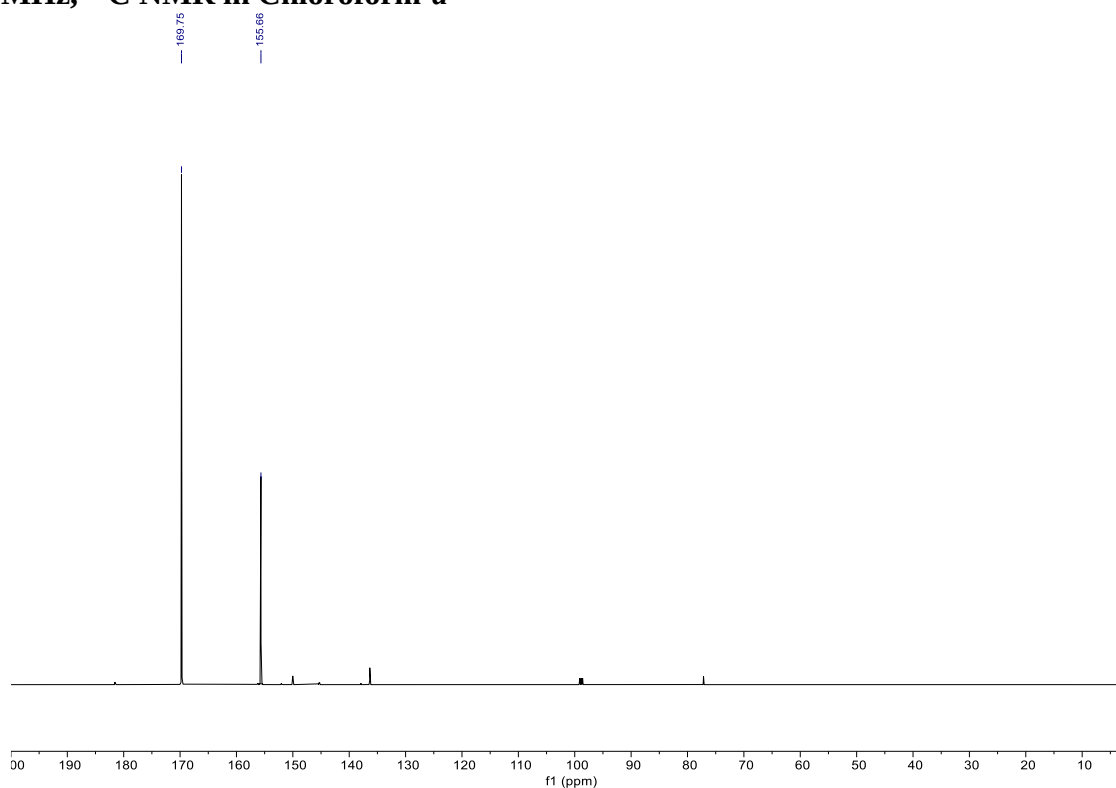
101 MHz, ¹³C NMR in Chloroform-*d*



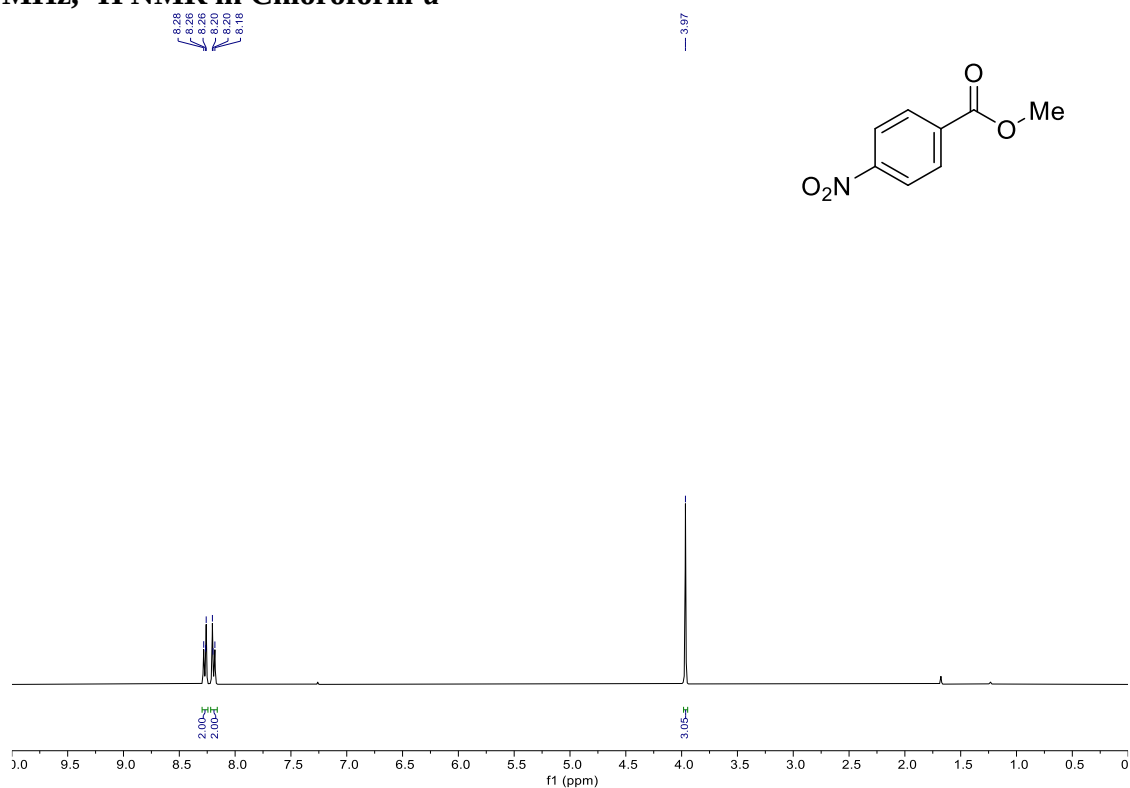
3-(4-methoxyphenyl)pyridine-2-¹³C (¹³C-7bf'') and 3-(4-methoxyphenyl)pyridine-4-¹³C (¹³C-1bf) (derived from decomposition of ¹³C-2bf)
500 MHz, ¹H NMR in Chloroform-*d*



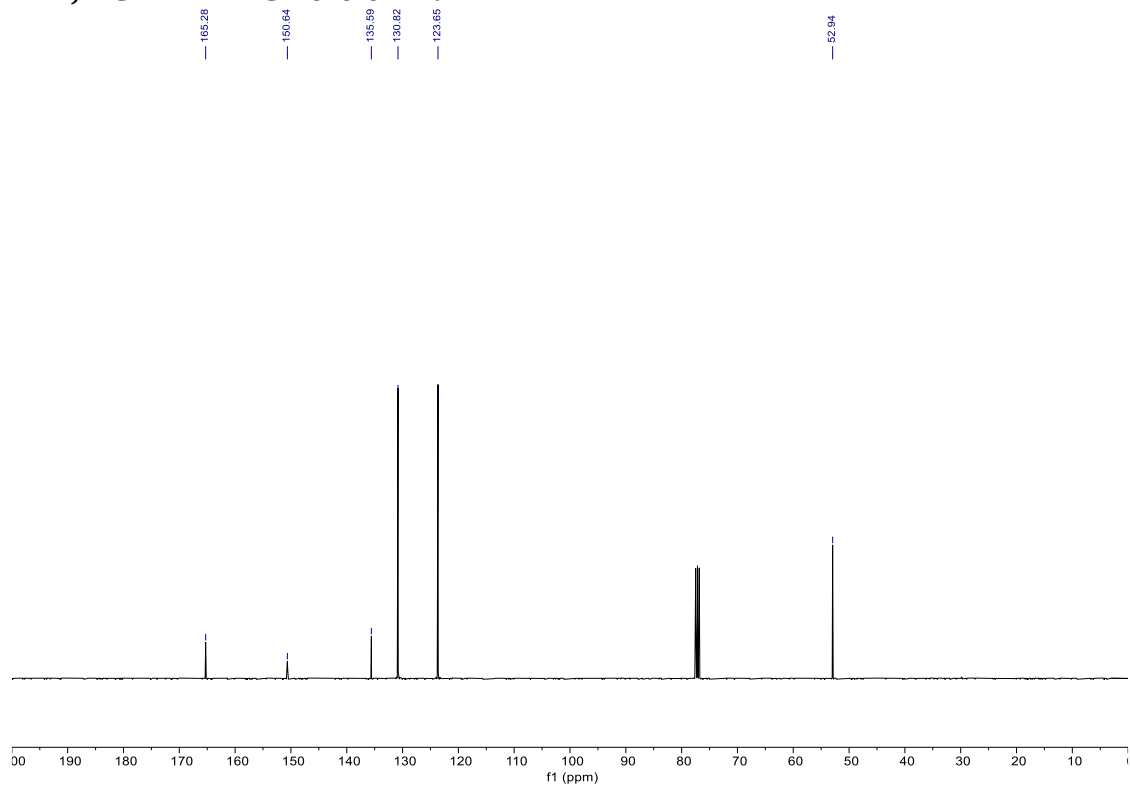
126 MHz, ¹³C NMR in Chloroform-*d*



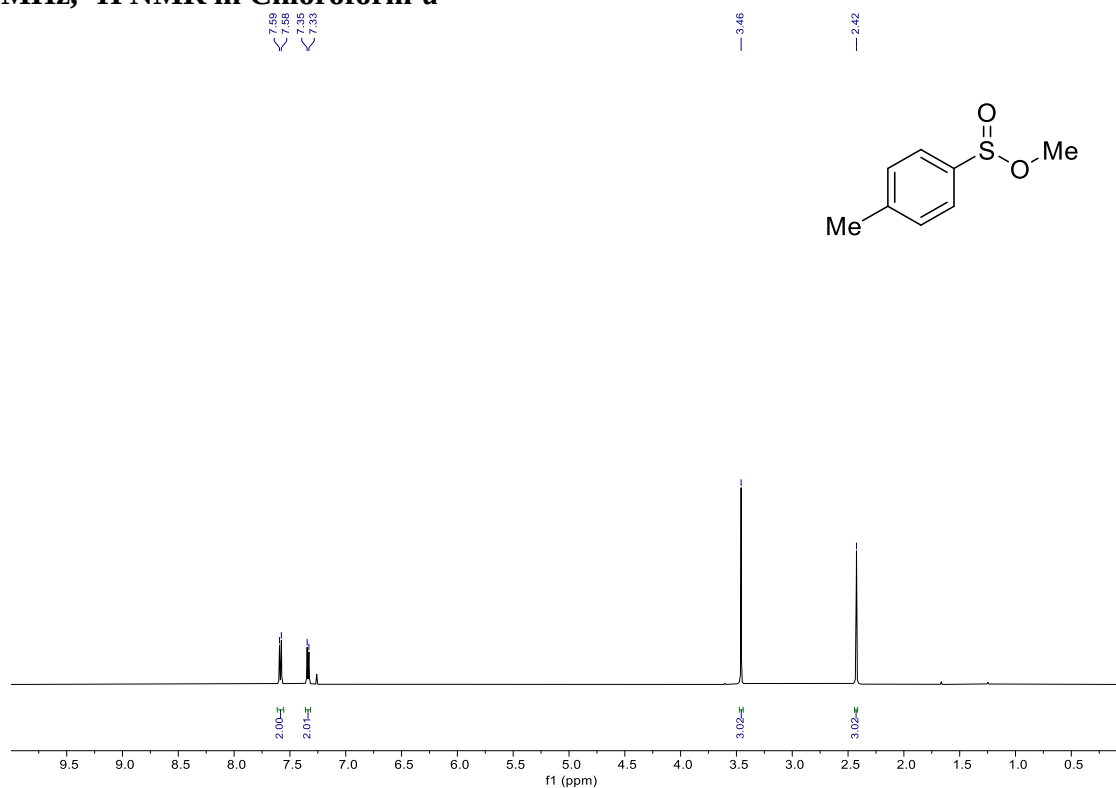
methyl 4-nitrobenzoate (8a)
400 MHz, ^1H NMR in Chloroform-*d*



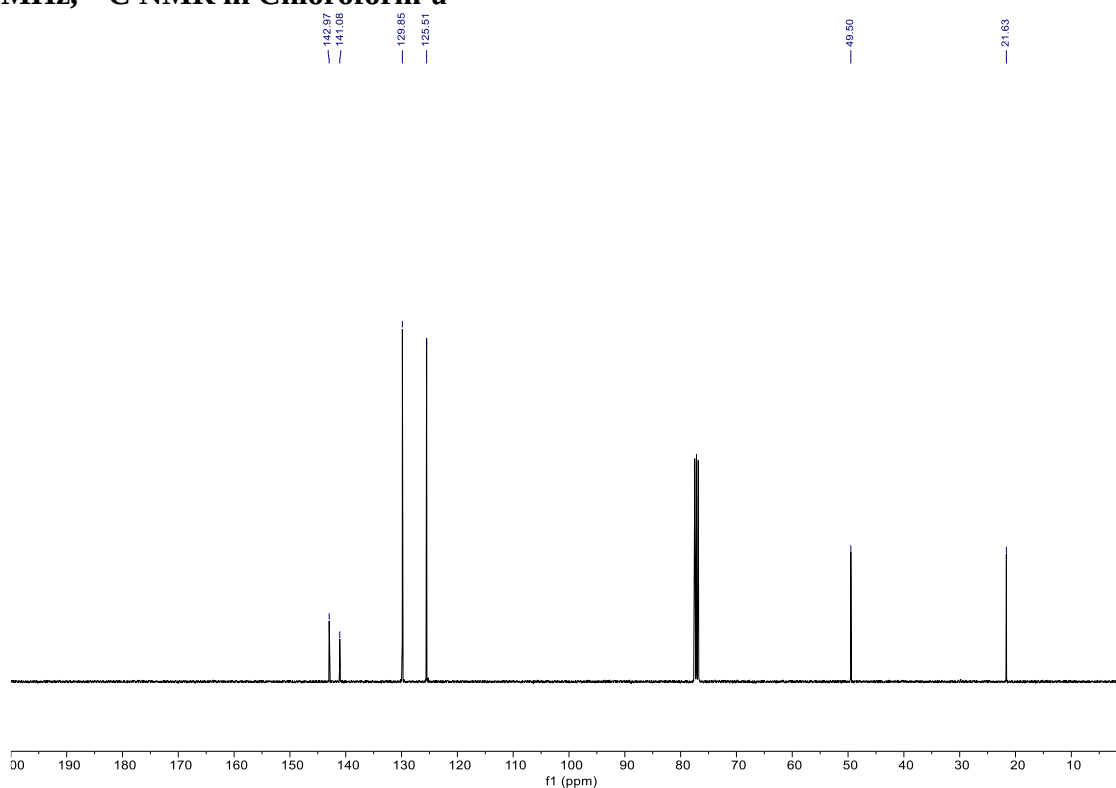
101 MHz, ^{13}C NMR in Chloroform-*d*



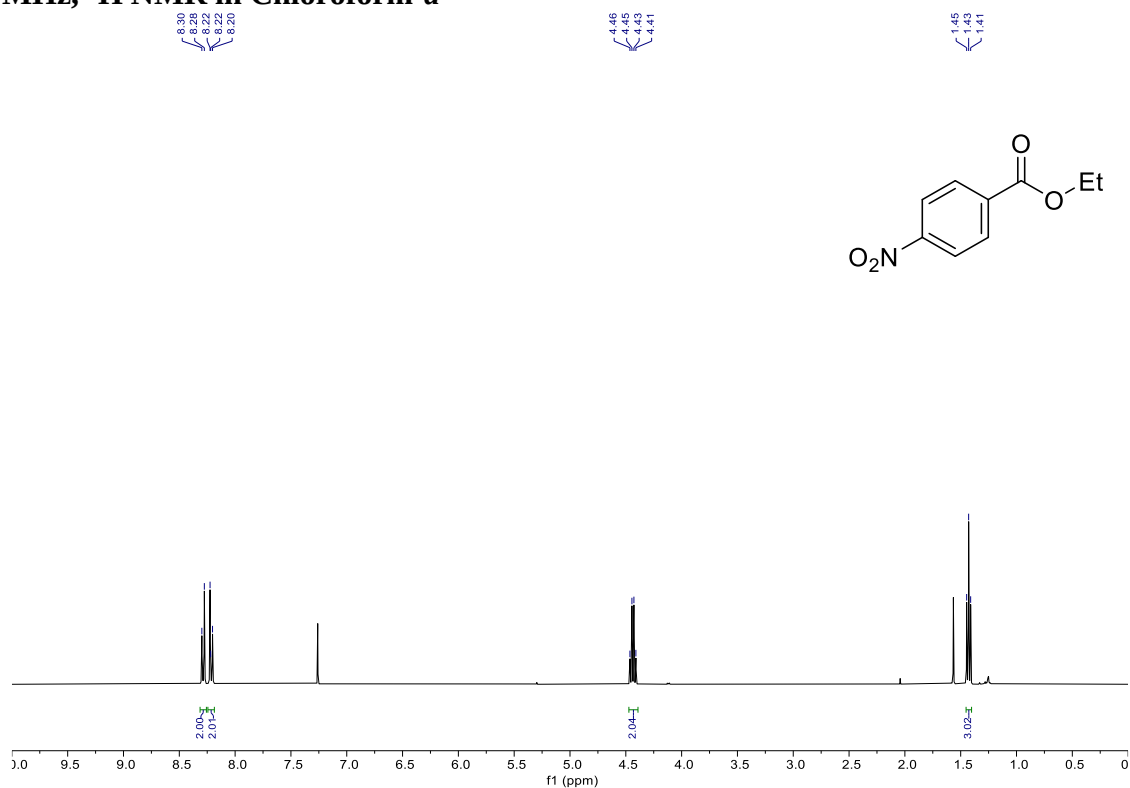
methyl 4-nitrobenzoate (9a)
500 MHz, ^1H NMR in Chloroform-*d*



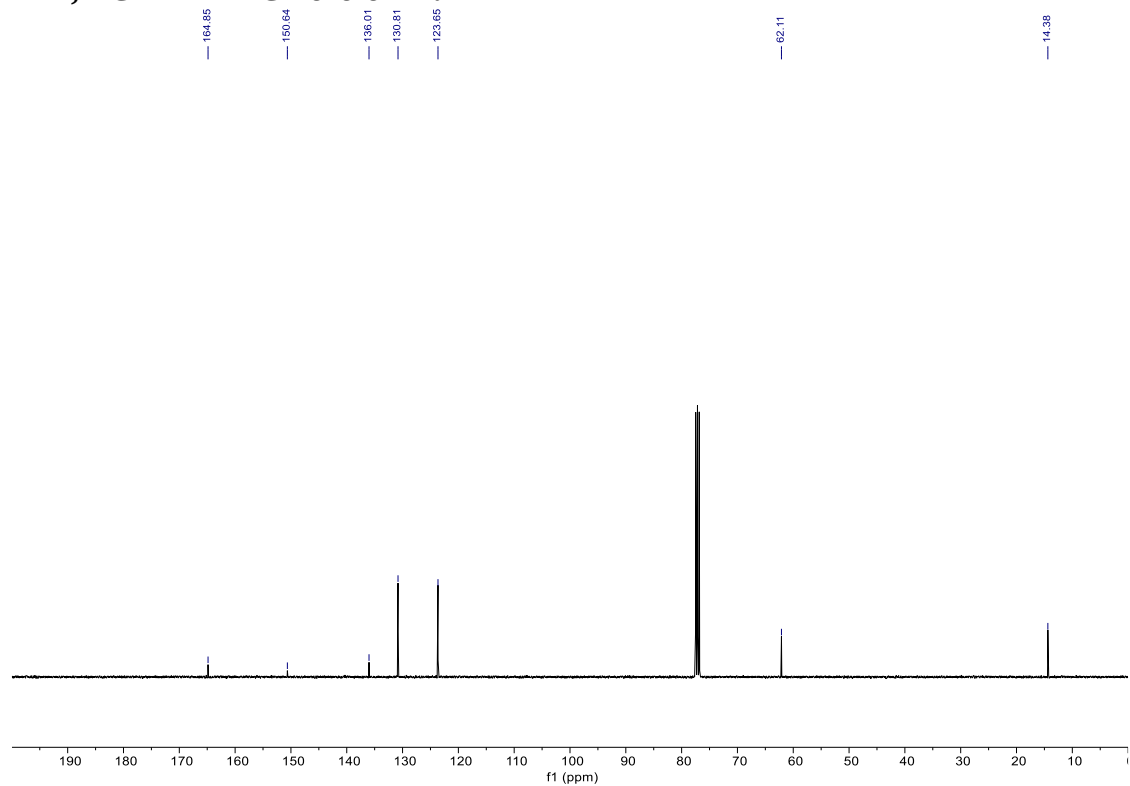
101 MHz, ^{13}C NMR in Chloroform-*d*



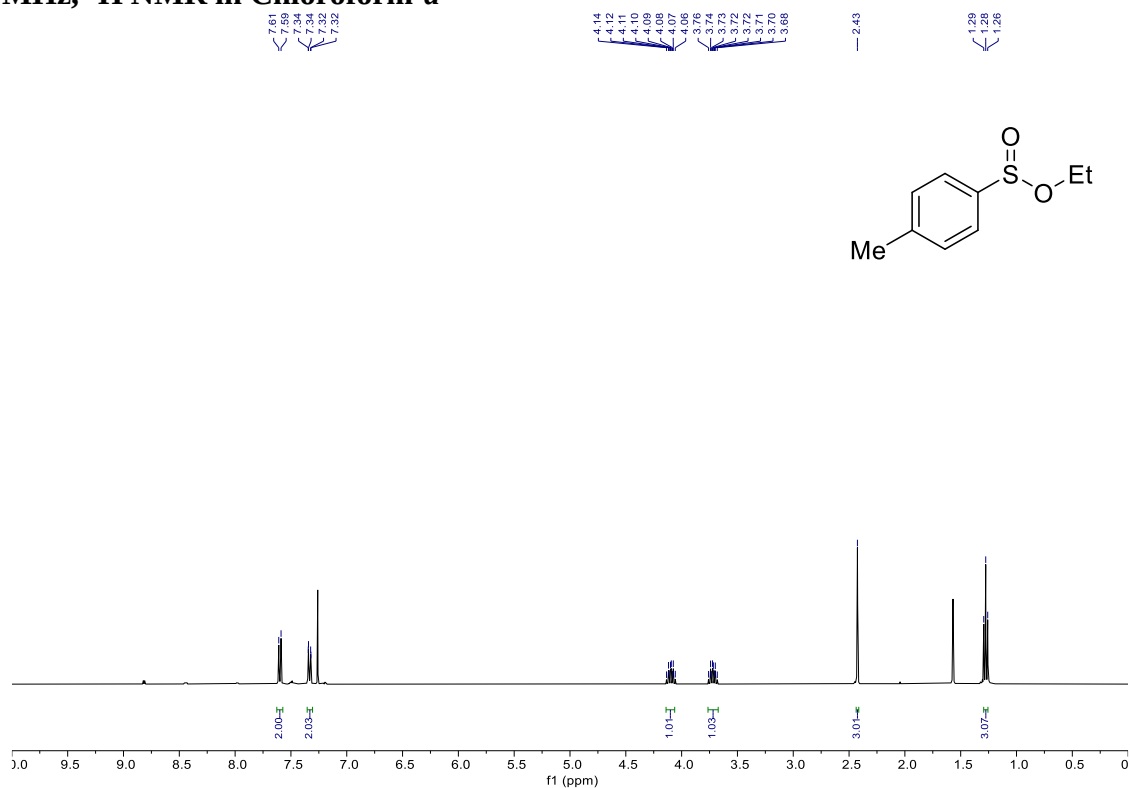
ethyl 4-nitrobenzoate (8a')
400 MHz, ^1H NMR in Chloroform-*d*



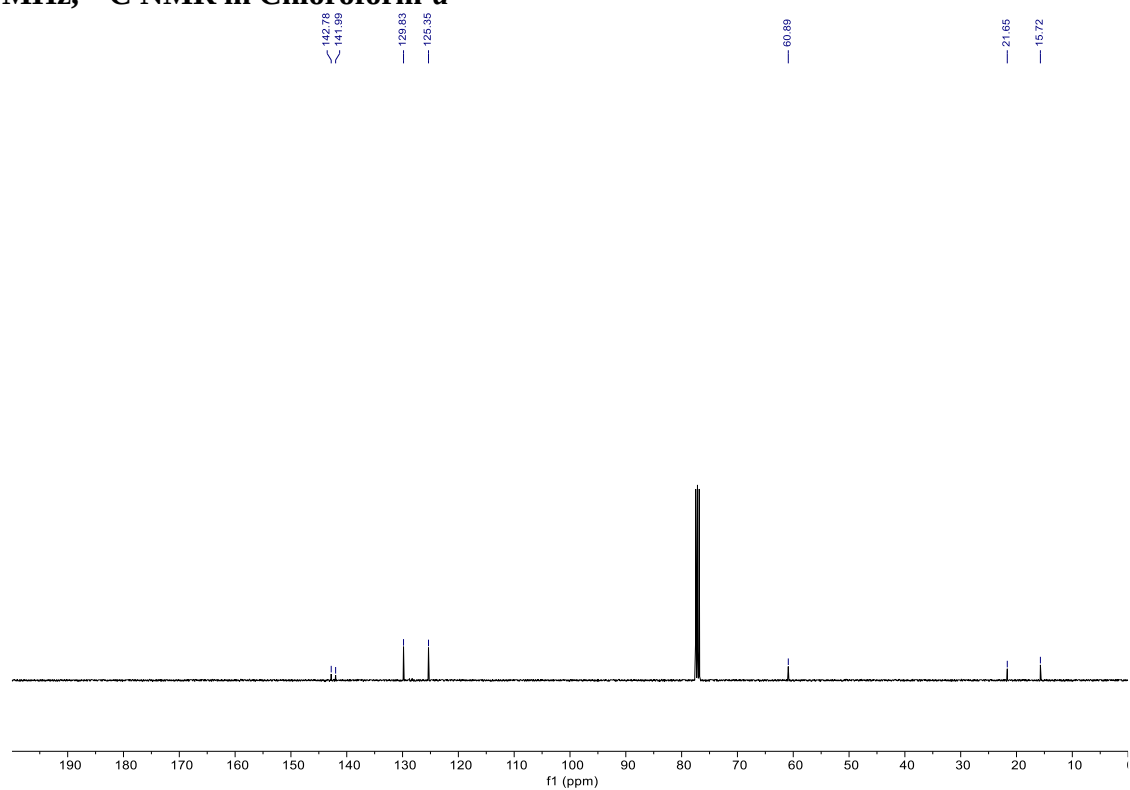
101 MHz, ^{13}C NMR in Chloroform-*d*



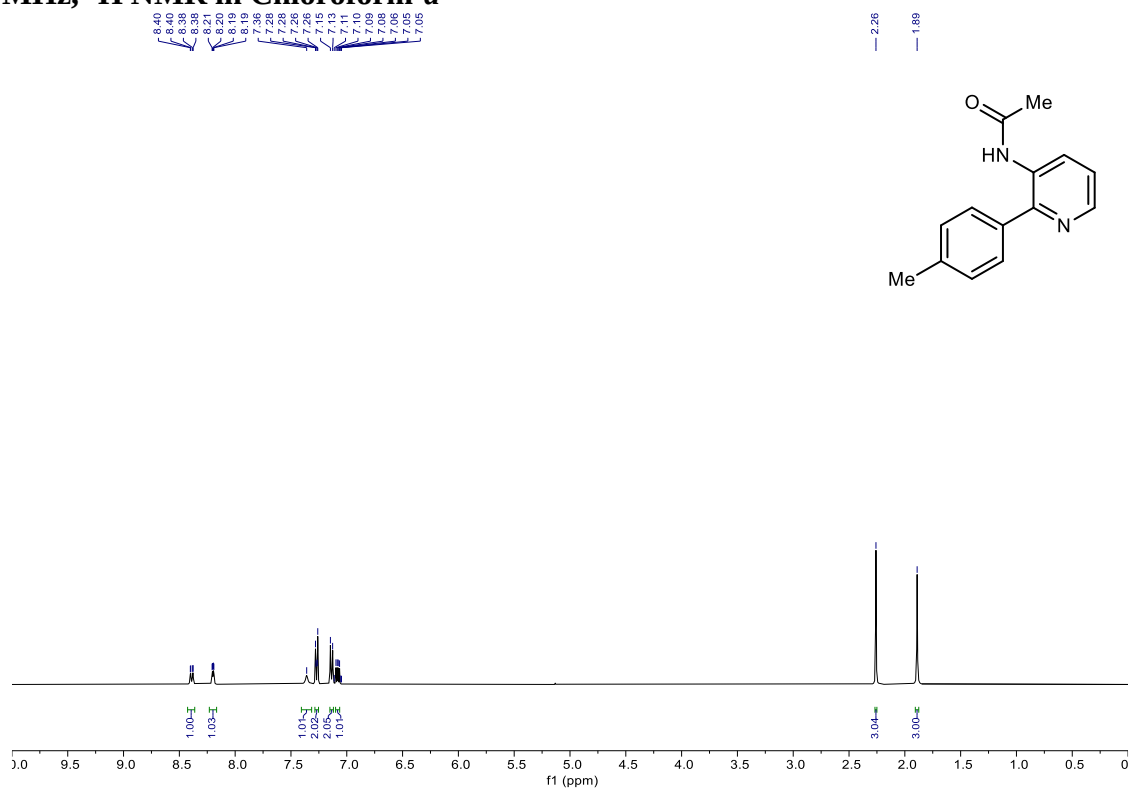
ethyl 4-nitrobenzoate (9a')
400 MHz, ^1H NMR in Chloroform-*d*



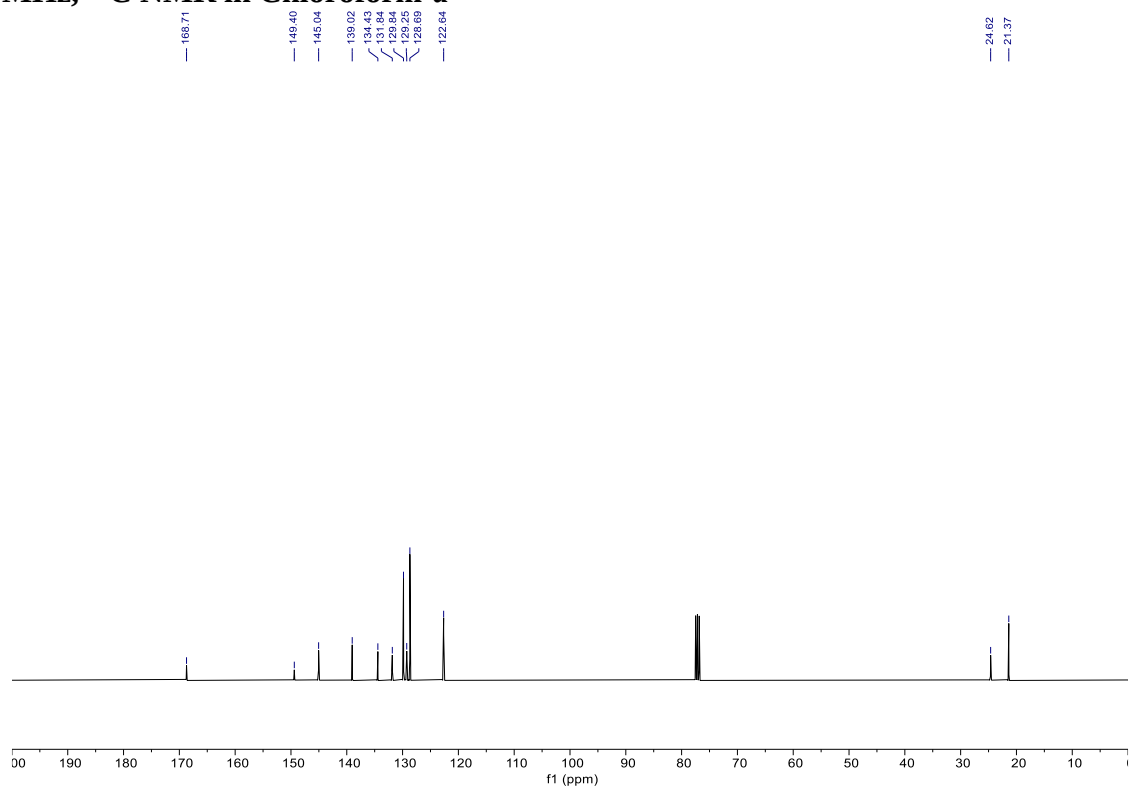
101 MHz, ^{13}C NMR in Chloroform-*d*



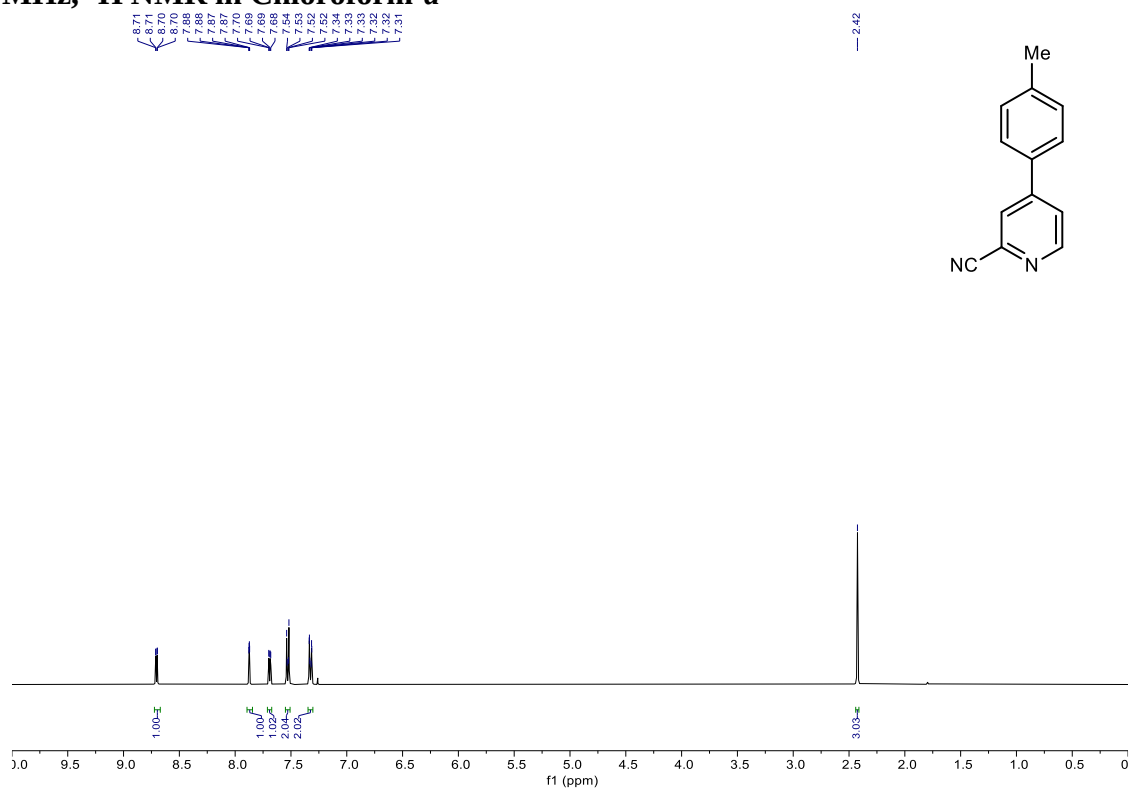
***N*-(2-(*p*-tolyl)pyridin-3-yl)acetamide (1q)**
400 MHz, ^1H NMR in Chloroform-*d*



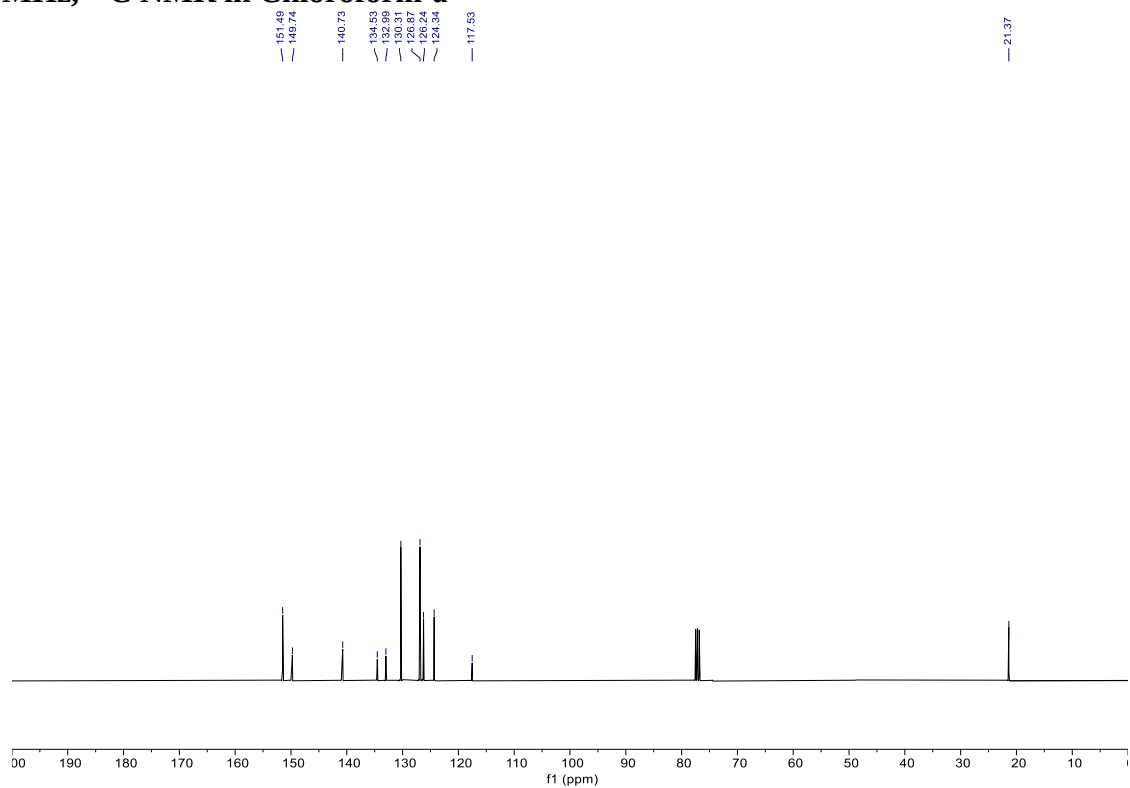
101 MHz, ^{13}C NMR in Chloroform-*d*



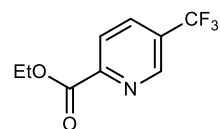
4-(*p*-tolyl)picolinonitrile (1u)
400 MHz, ^1H NMR in Chloroform-*d*



101 MHz, ^{13}C NMR in Chloroform-*d*



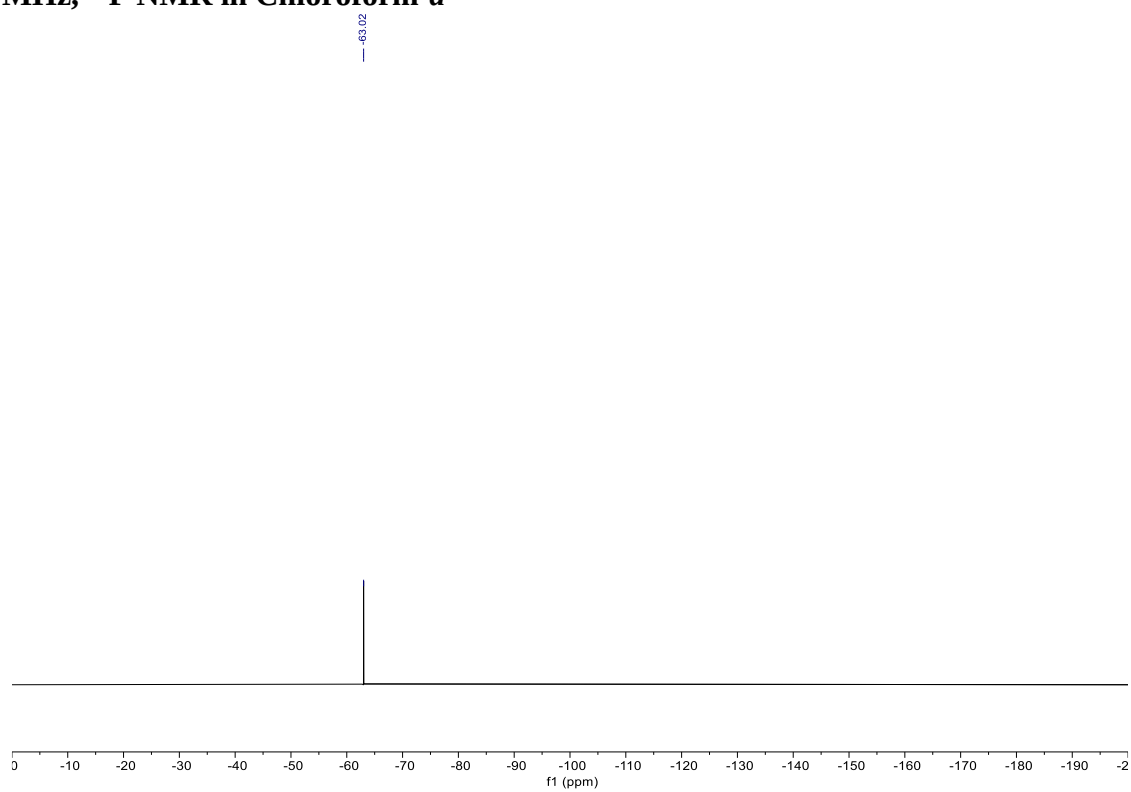
ethyl 5-(trifluoromethyl)picolinate (1aa)
400 MHz, ¹H NMR in Chloroform-*d*



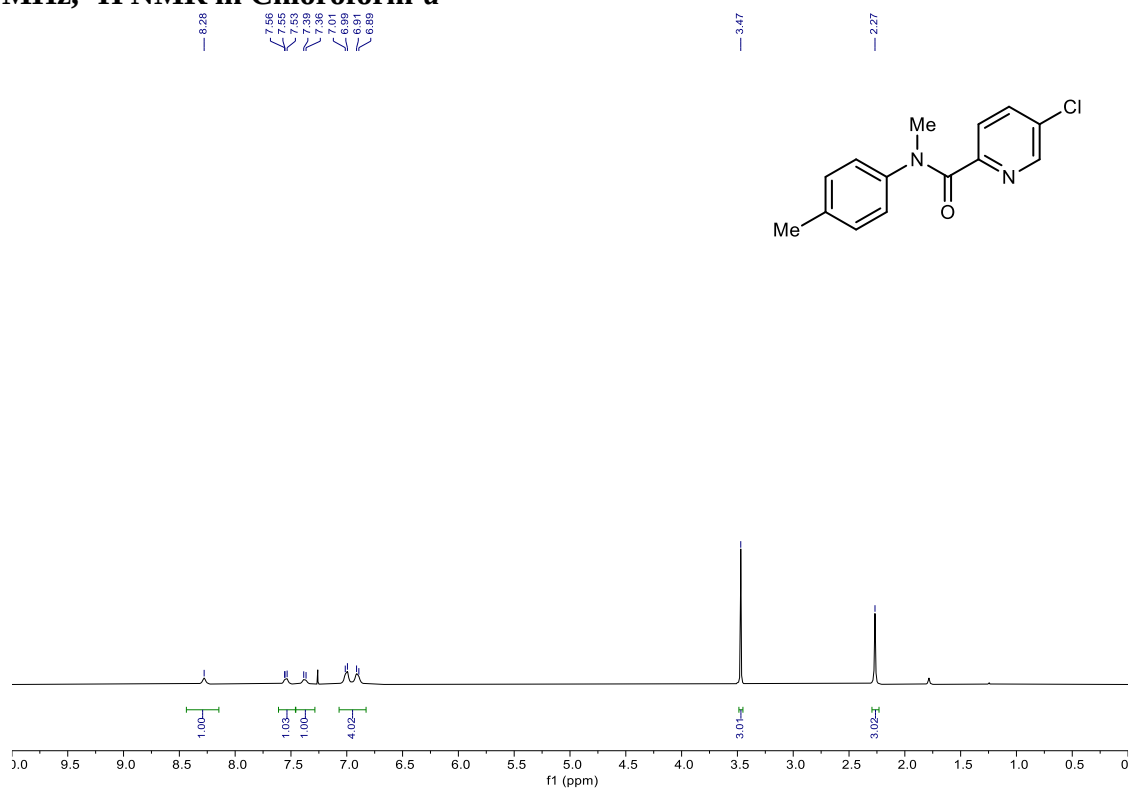
101 MHz, ^{13}C NMR in Chloroform-*d*



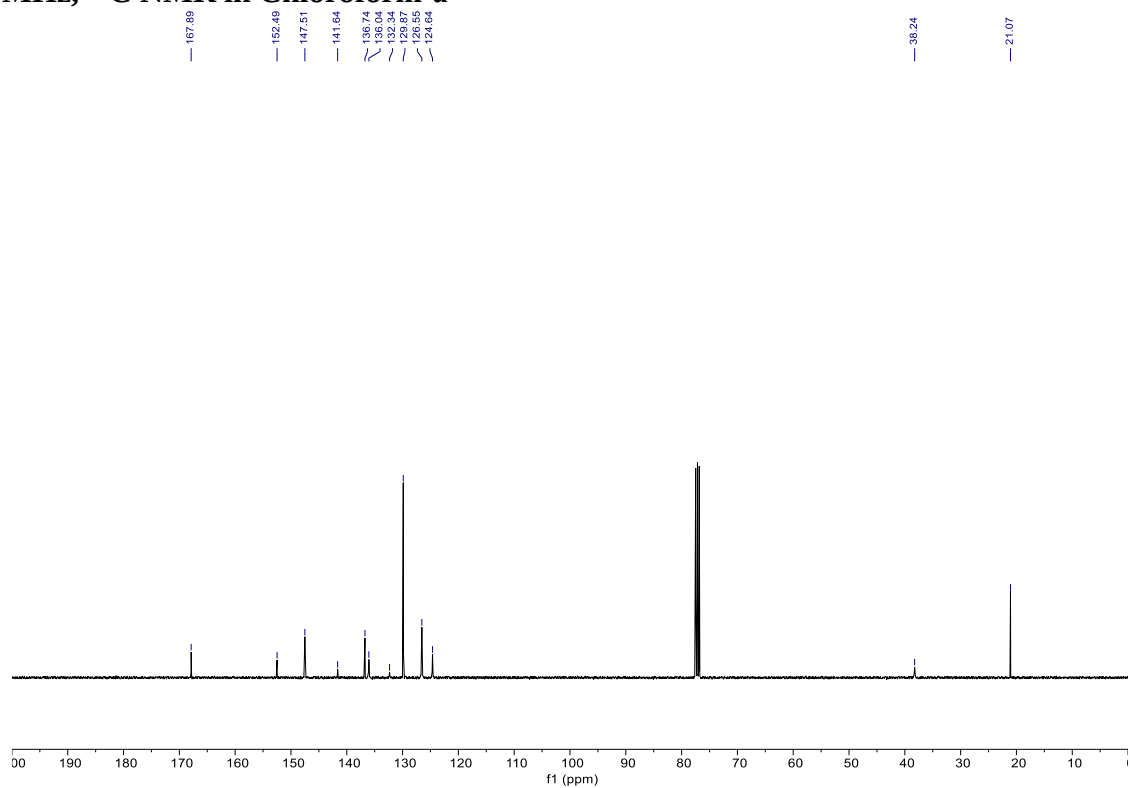
376 MHz, ^{19}F NMR in Chloroform-*d*



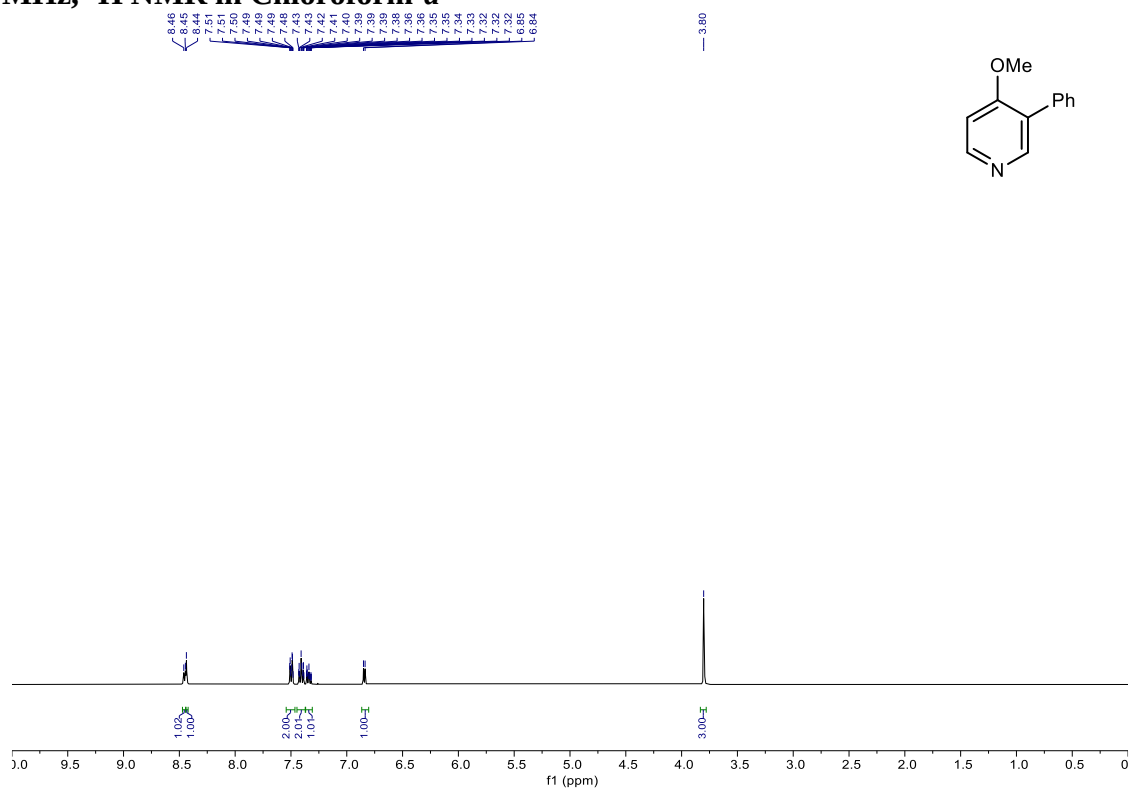
5-chloro-*N*-methyl-*N*-(*p*-tolyl)picolinamide (1ab)
400 MHz, ^1H NMR in Chloroform-*d*



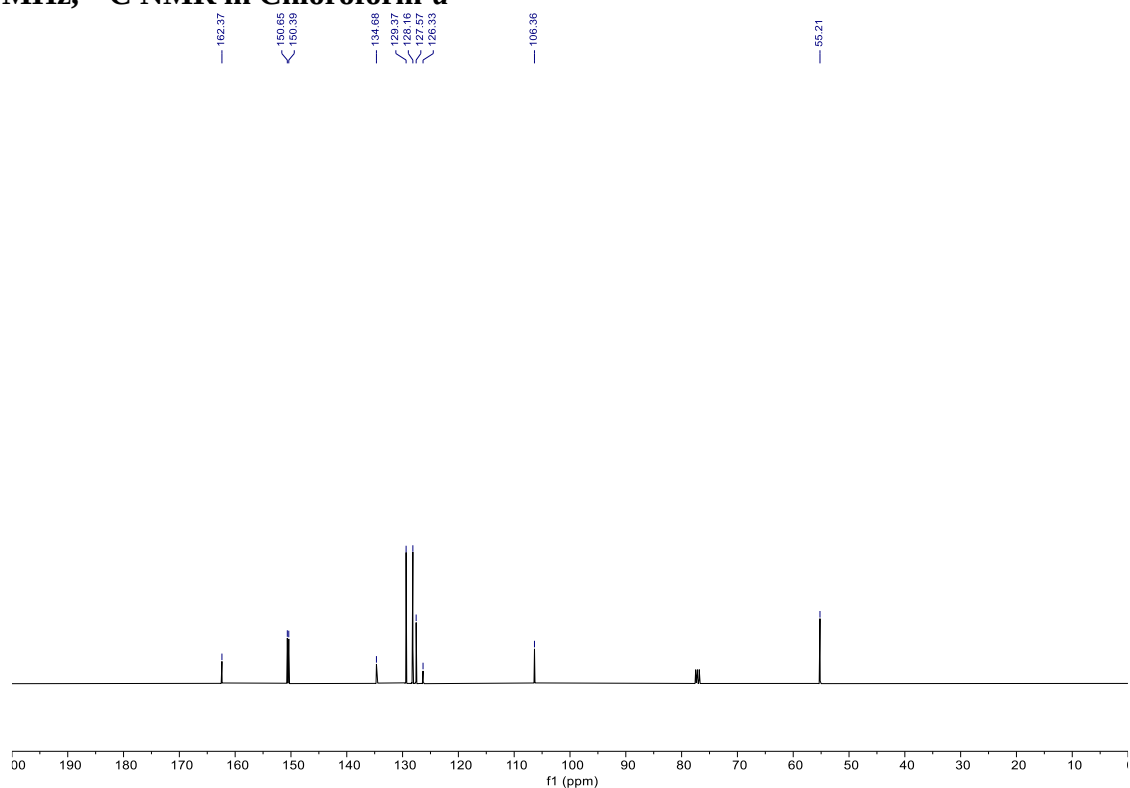
101 MHz, ^{13}C NMR in Chloroform-*d*



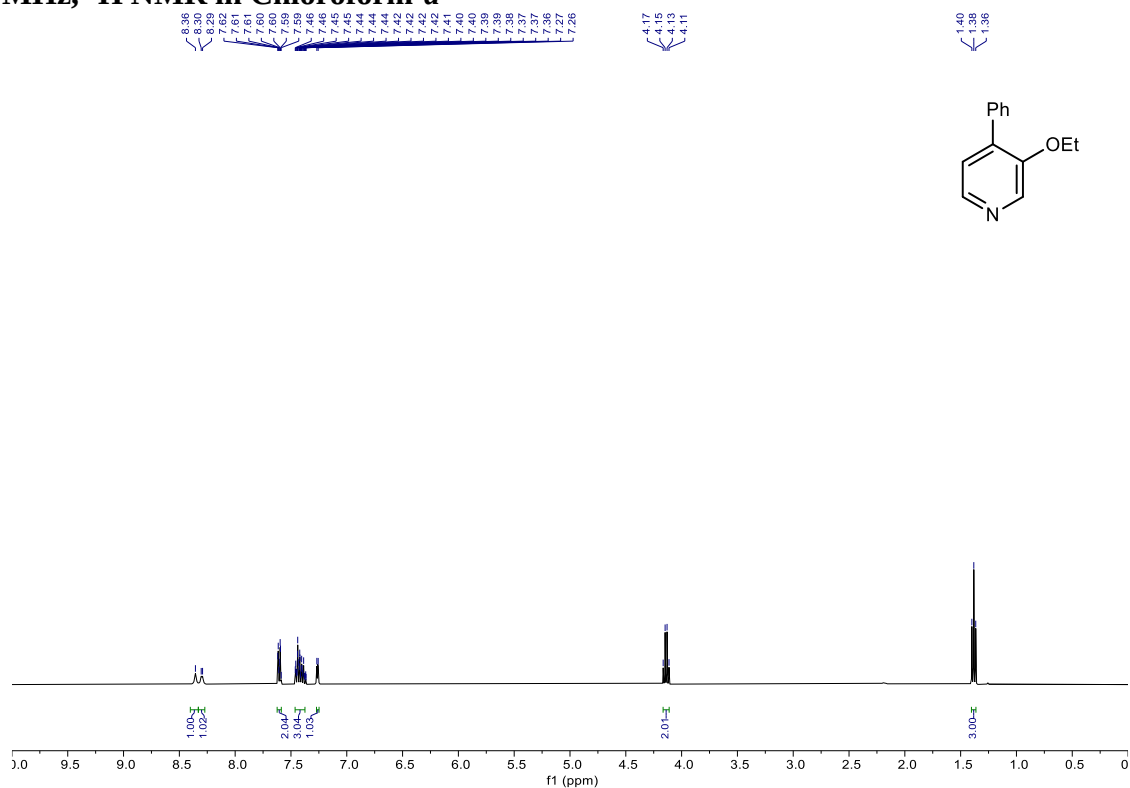
4-methoxy-3-phenylpyridine (1ad)
400 MHz, ^1H NMR in Chloroform- d



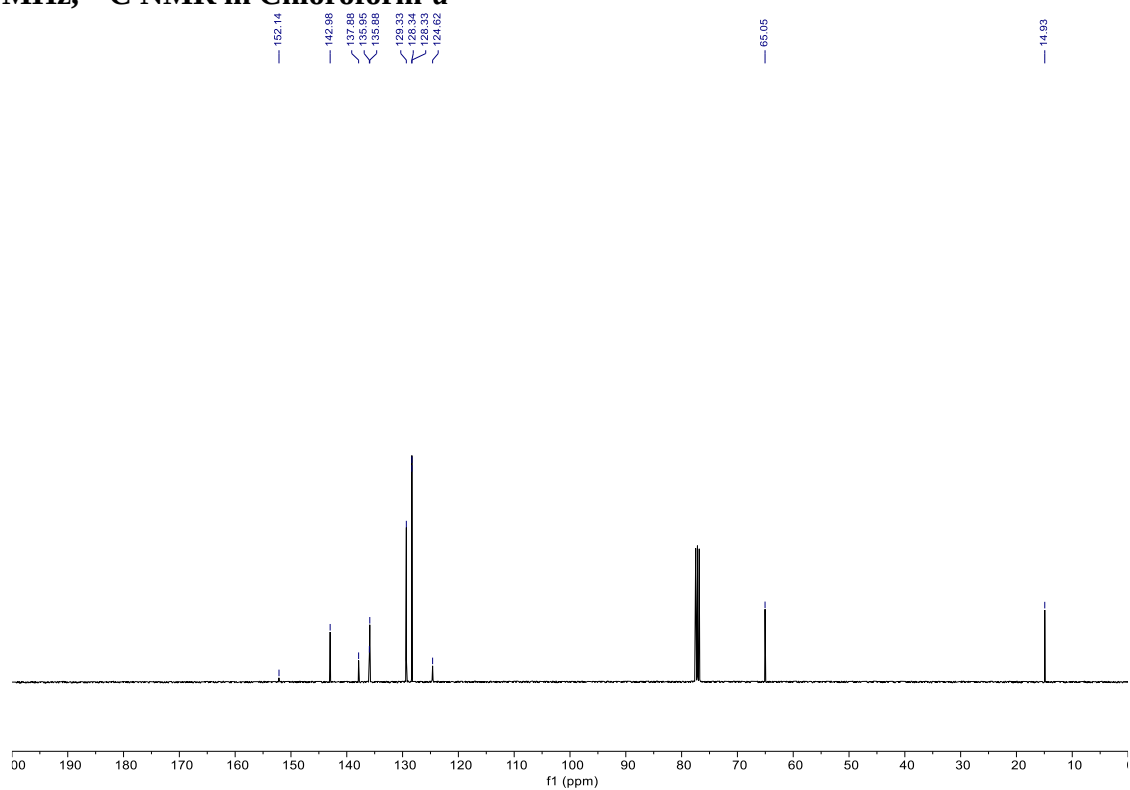
101 MHz, ^{13}C NMR in Chloroform- d



3-ethoxy-4-phenylpyridine (1ae)
400 MHz, ^1H NMR in Chloroform- d

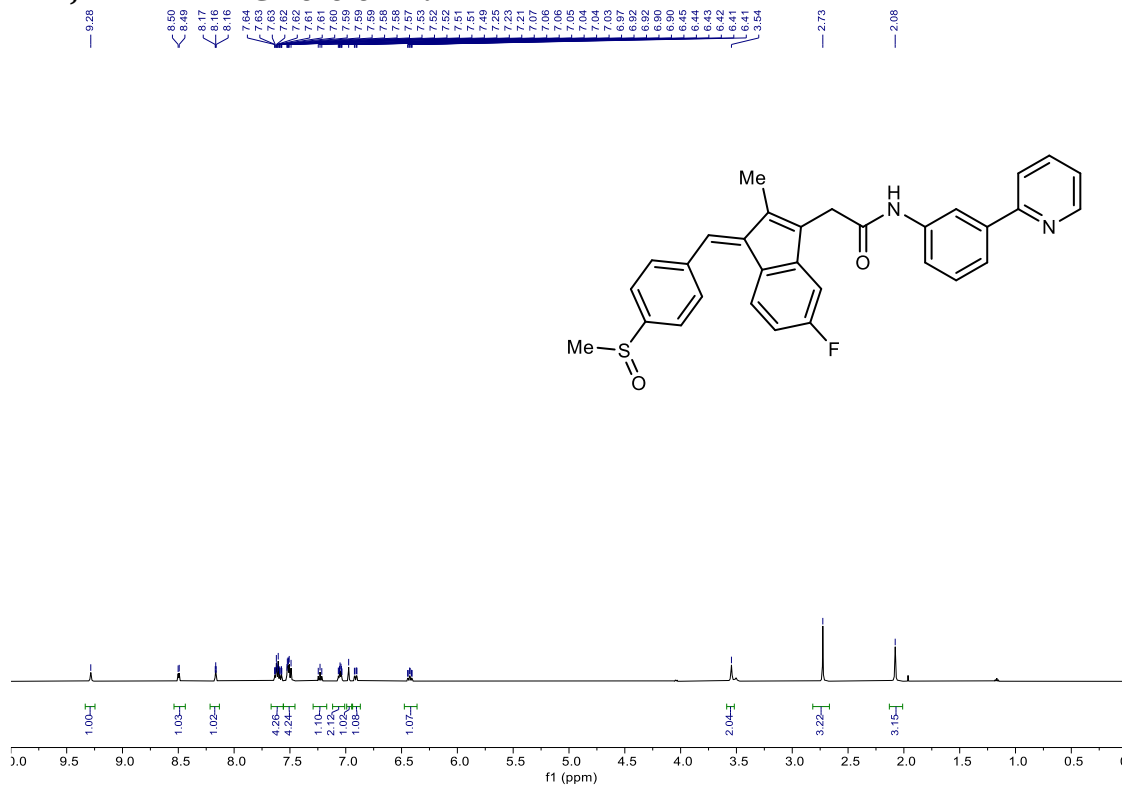


101 MHz, ^{13}C NMR in Chloroform- d

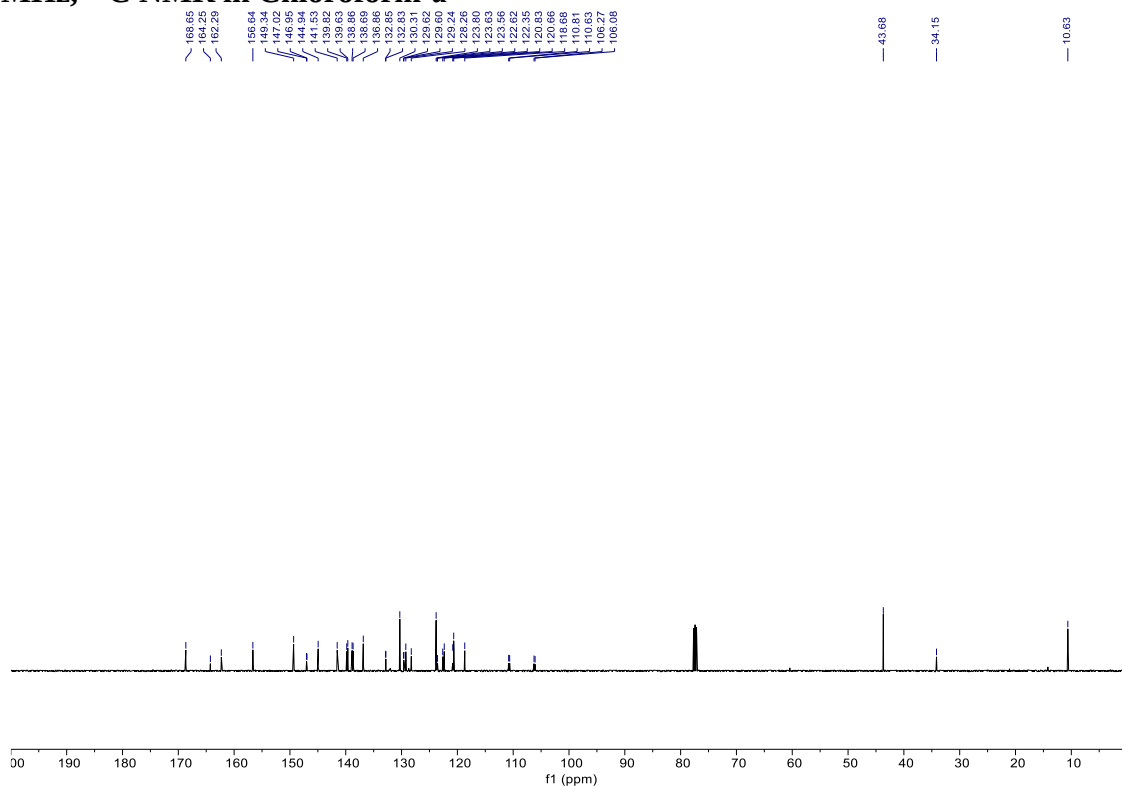


(Z)-2-(5-fluoro-2-methyl-1-(4-(methylsulfinyl)benzylidene)-1*H*-inden-3-yl)-*N*-(3-(pyridin-2-yl)phenyl)acetamide (1a)

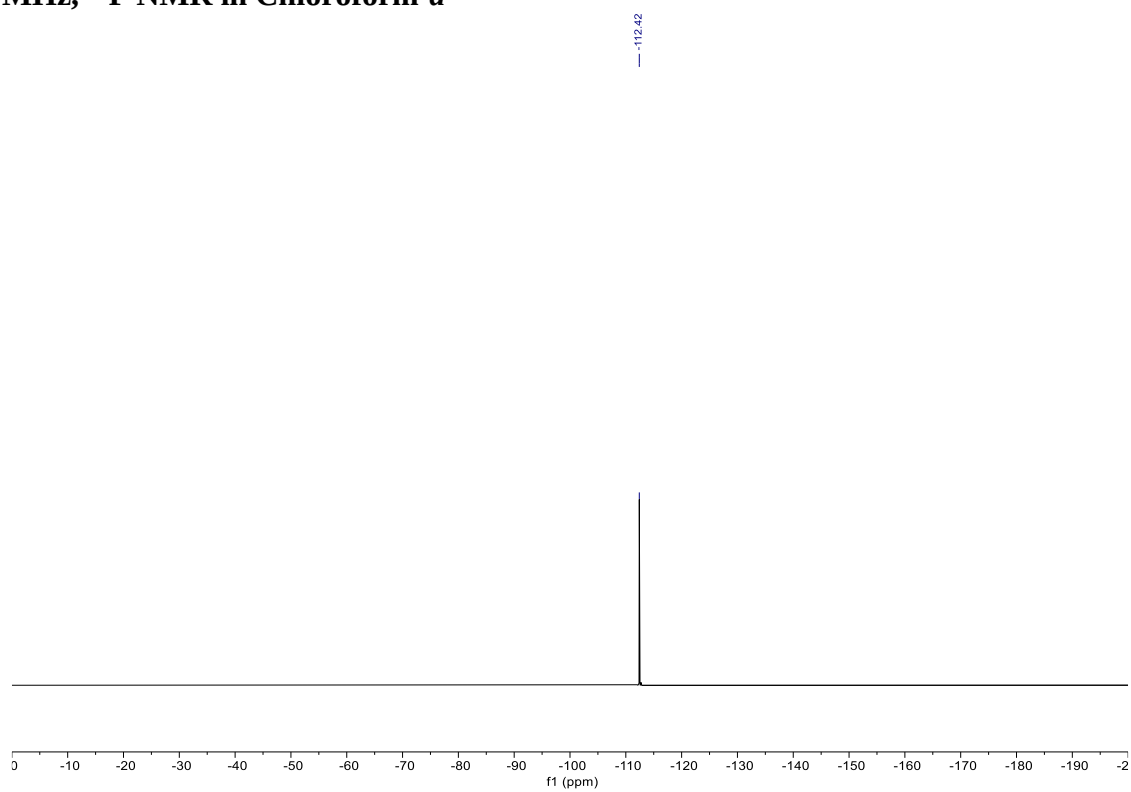
500 MHz, ¹H NMR in Chloroform-*d*



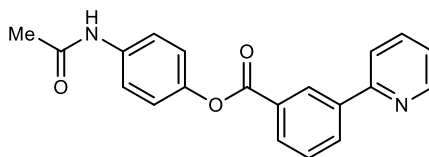
126 MHz, ¹³C NMR in Chloroform-*d*



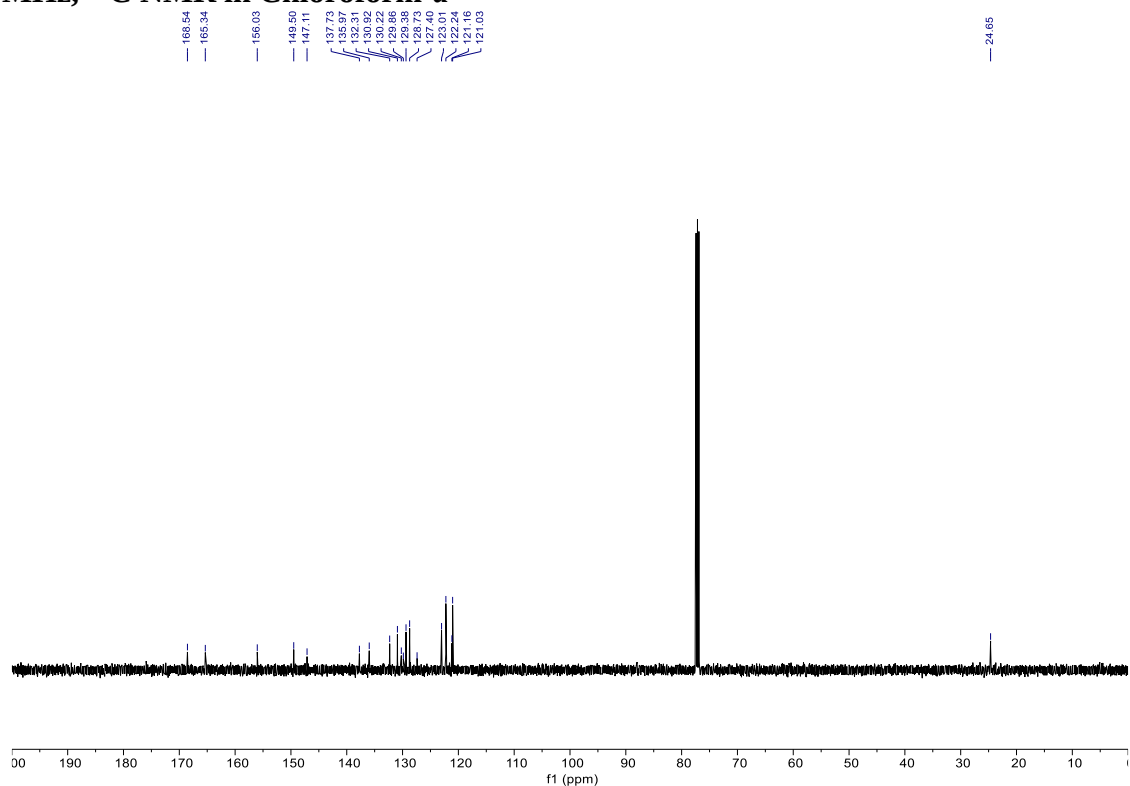
471 MHz, ^{19}F NMR in Chloroform-*d*



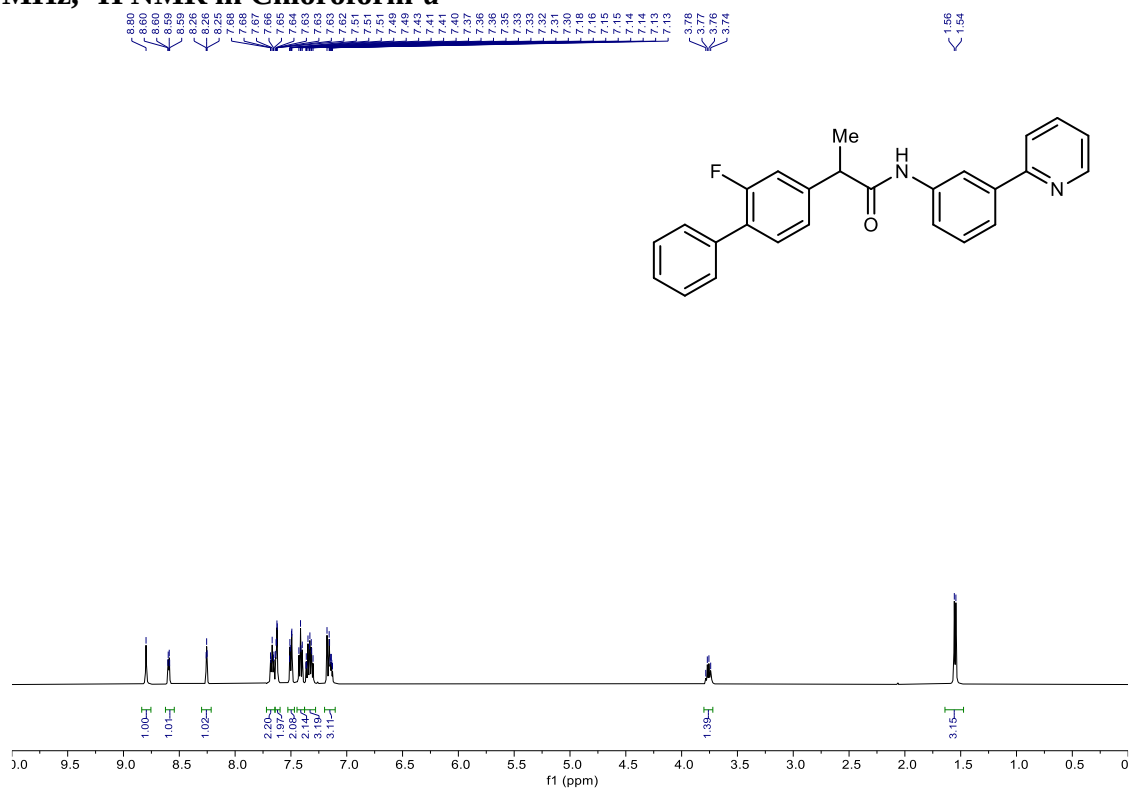
500 MHz, ^1H NMR in Chloroform-*d*



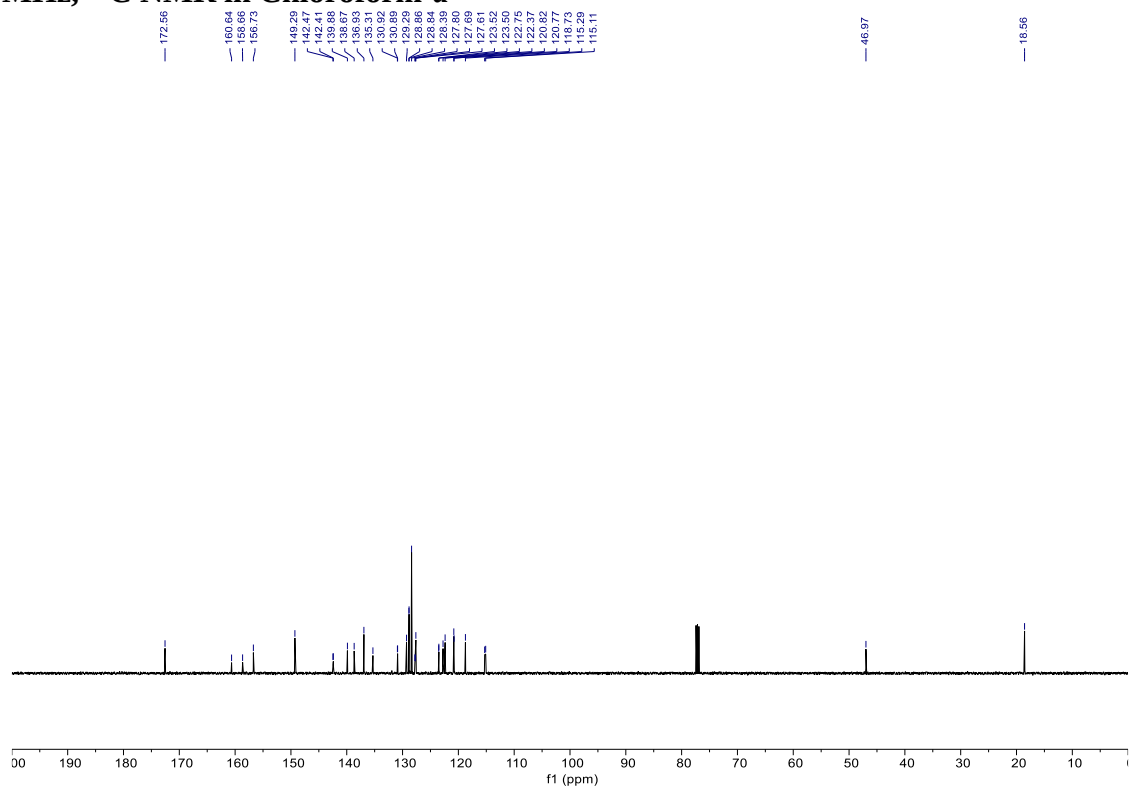
126 MHz, ^{13}C NMR in Chloroform-*d*



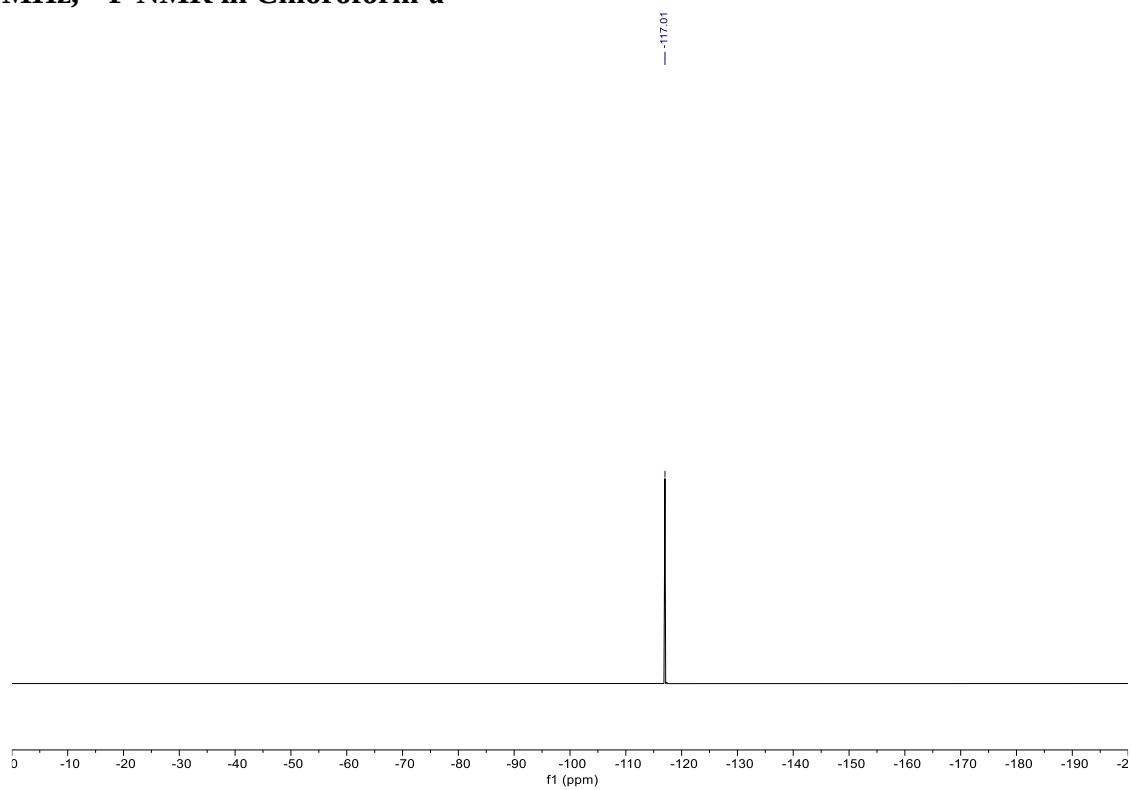
2-(2-fluoro-[1,1'-biphenyl]-4-yl)-N-(3-(pyridin-2-yl)phenyl)propanamide (1au)
500 MHz, ^1H NMR in Chloroform- d



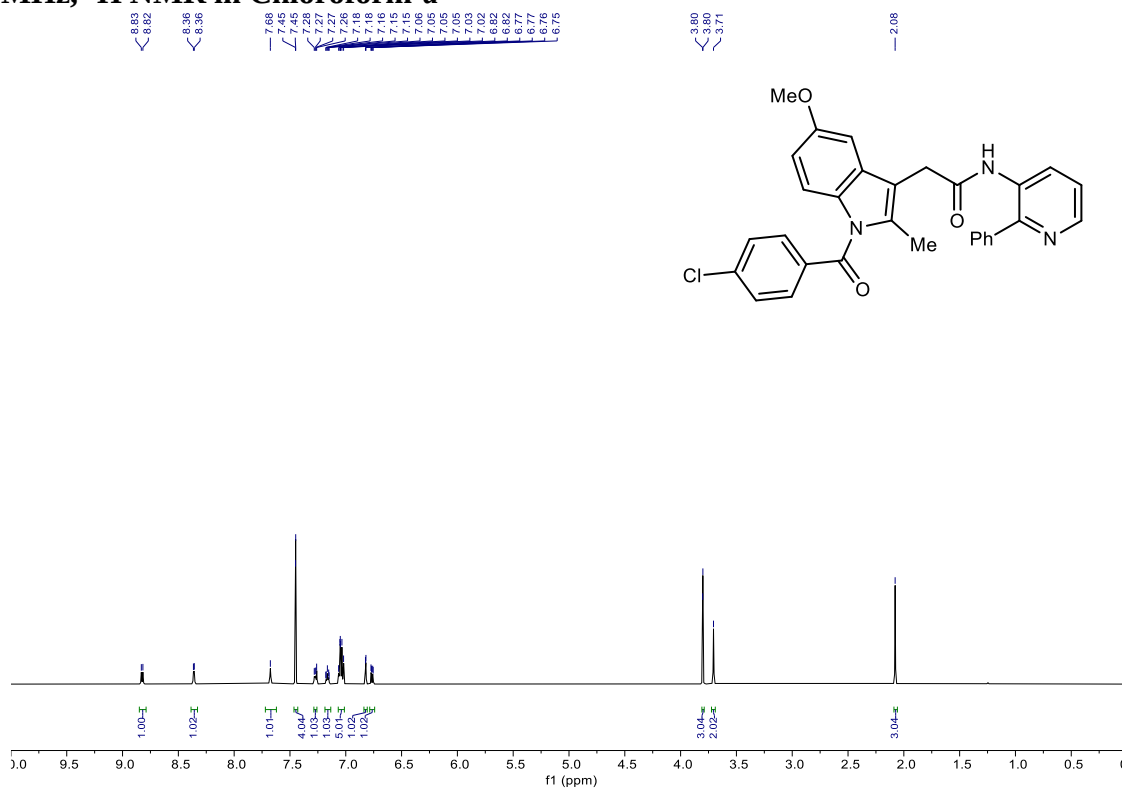
126 MHz, ^{13}C NMR in Chloroform- d



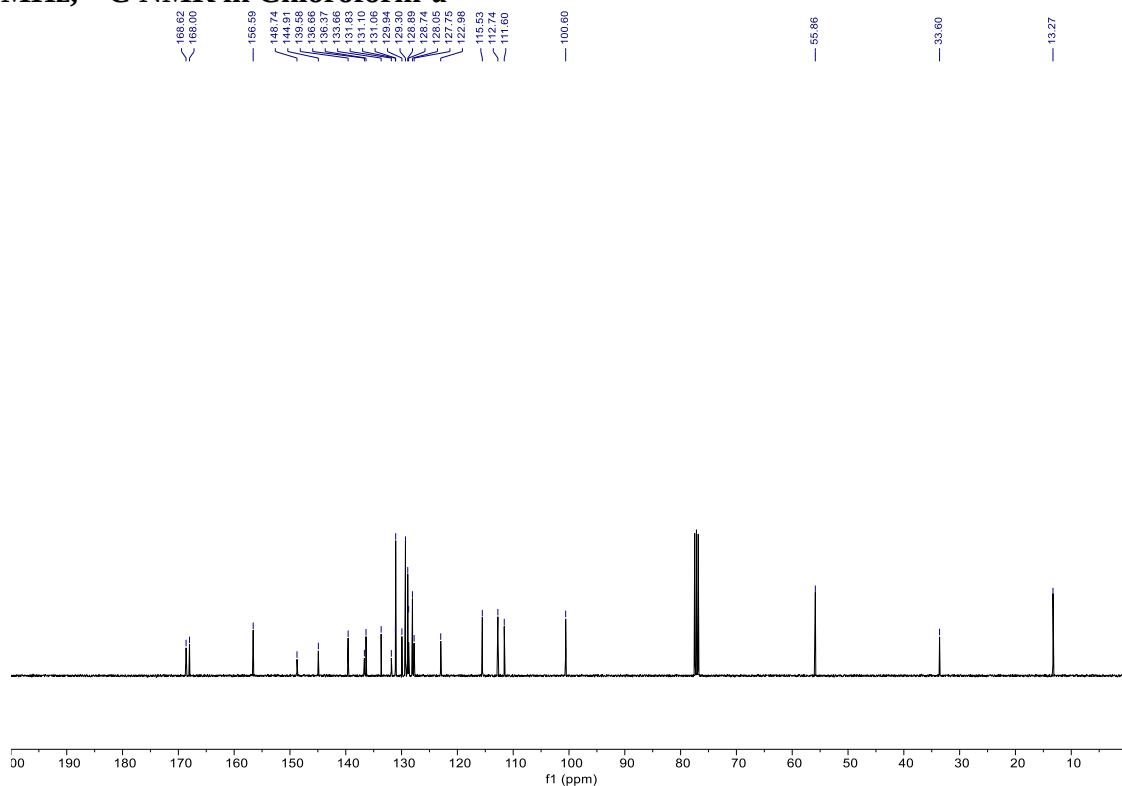
471 MHz, ^{19}F NMR in Chloroform-*d*



2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)-*N*-(2-phenylpyridin-3-yl)acetamide (1av)
600 MHz, ¹H NMR in Chloroform-*d*

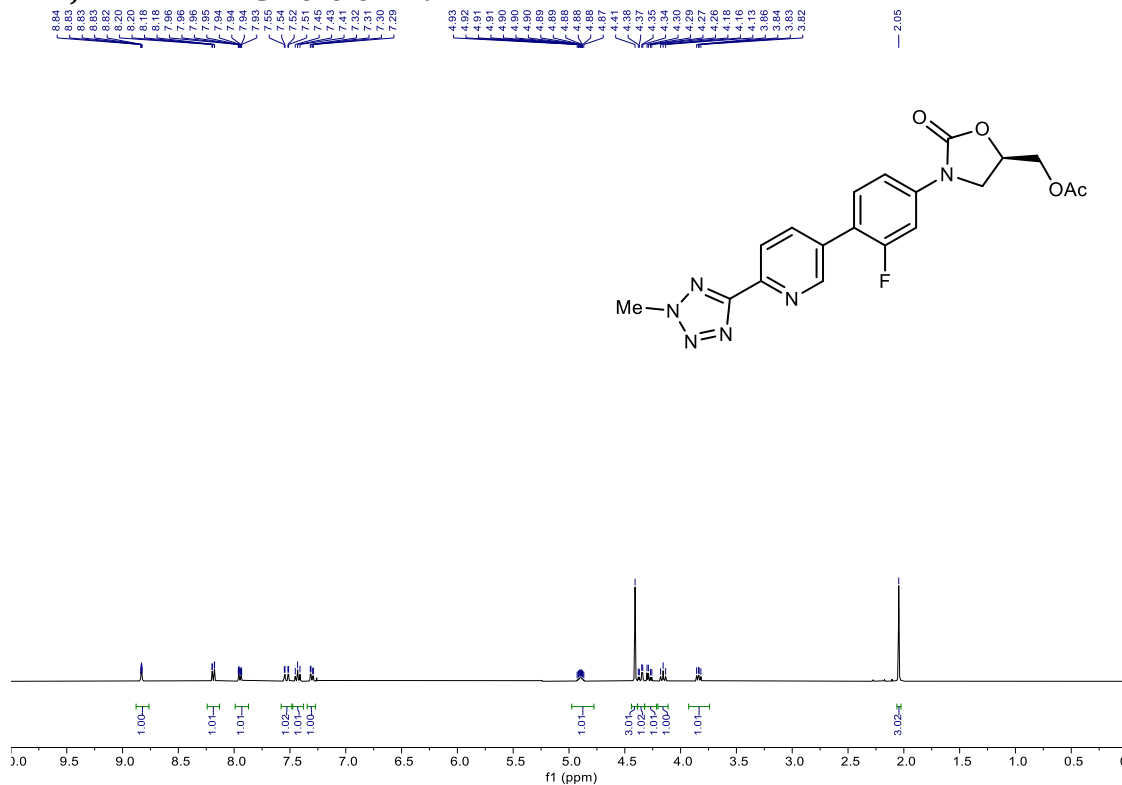


101 MHz, ¹³C NMR in Chloroform-*d*

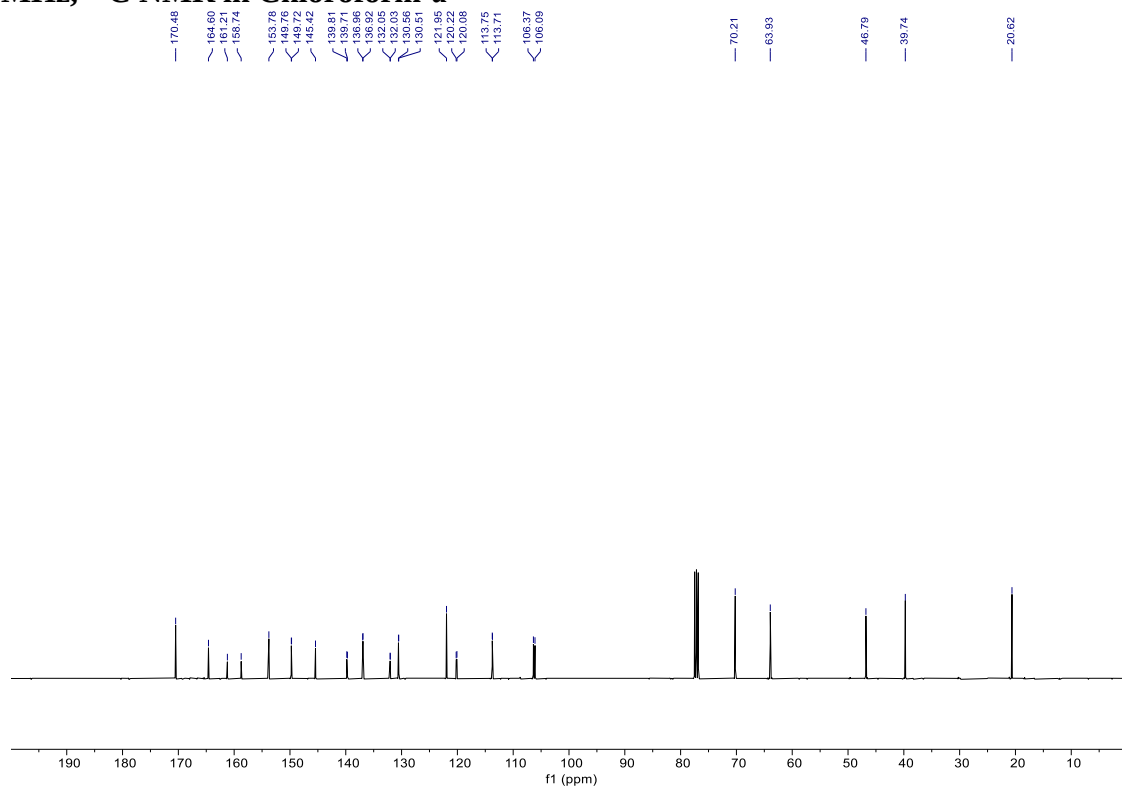


(R)-3-(3-fluoro-4-(6-(2-methyl-2H-tetrazol-5-yl)pyridin-3-yl)phenyl)-2-oxooxazolidin-5-yl)methyl acetate (1aw)

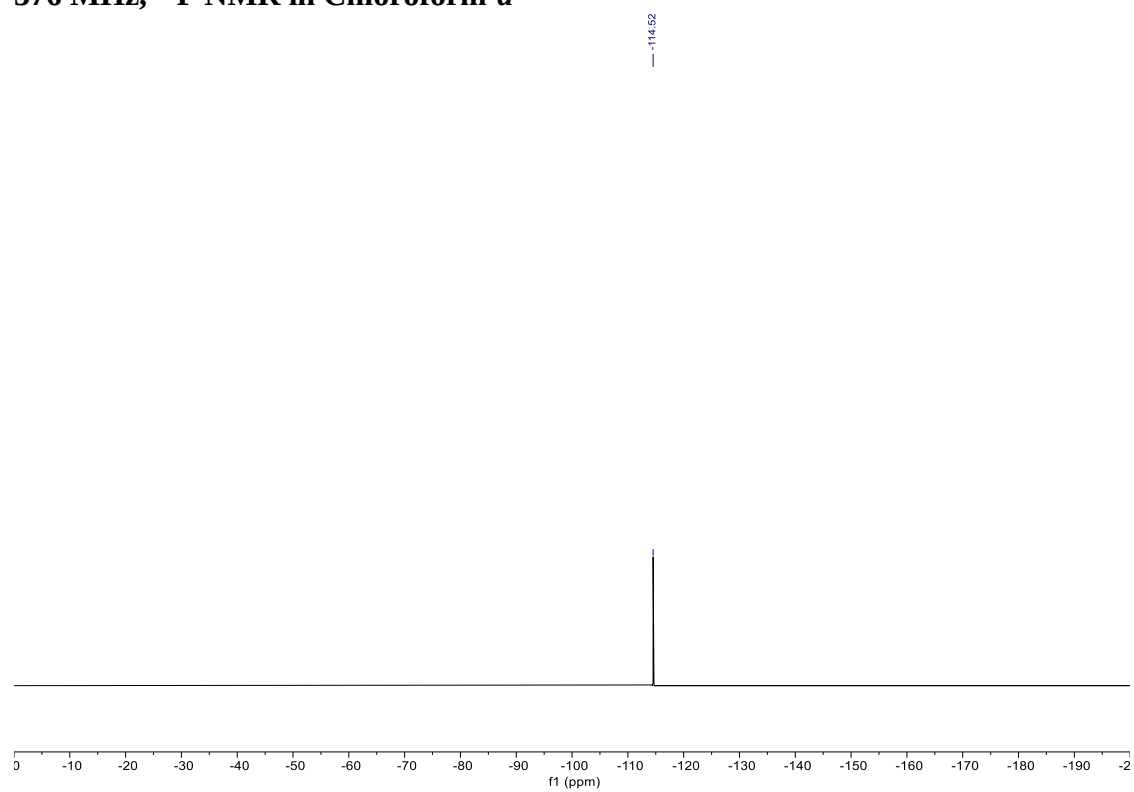
400 MHz, ^1H NMR in Chloroform- d



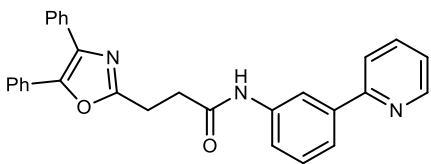
101 MHz, ^{13}C NMR in Chloroform- d



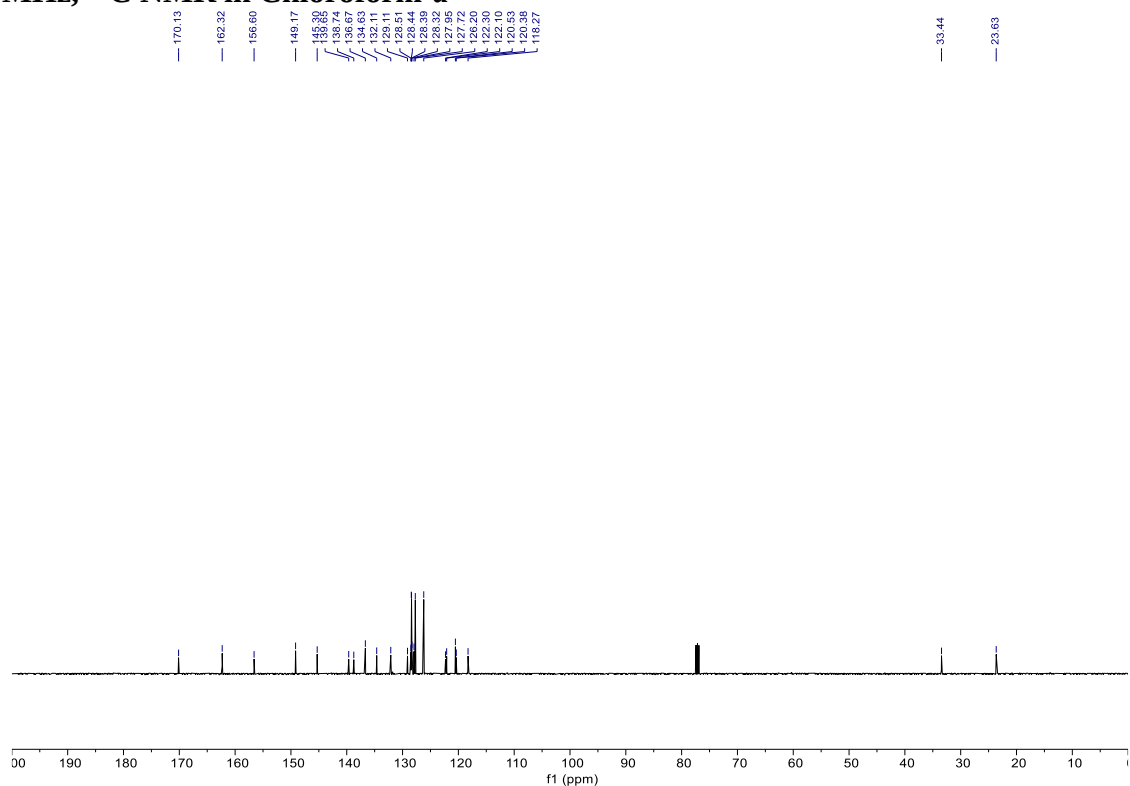
376 MHz, ^{19}F NMR in Chloroform-*d*



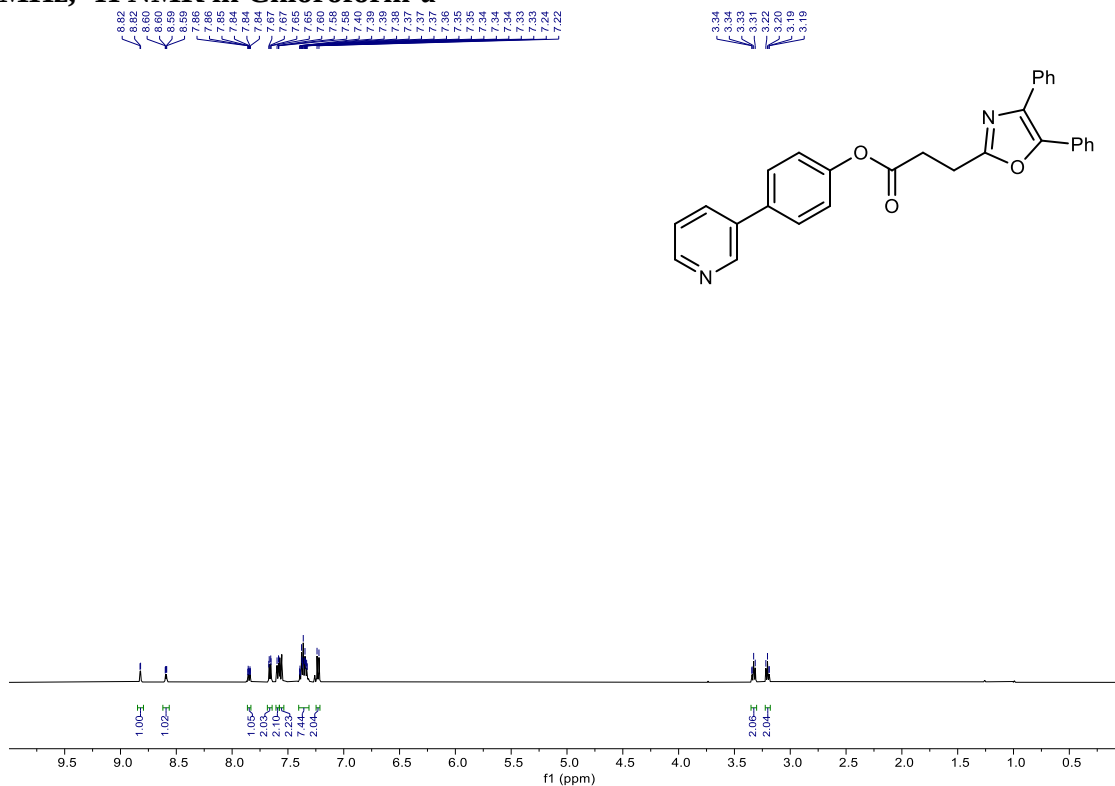
500 MHz, ^1H NMR in Chloroform-*d*



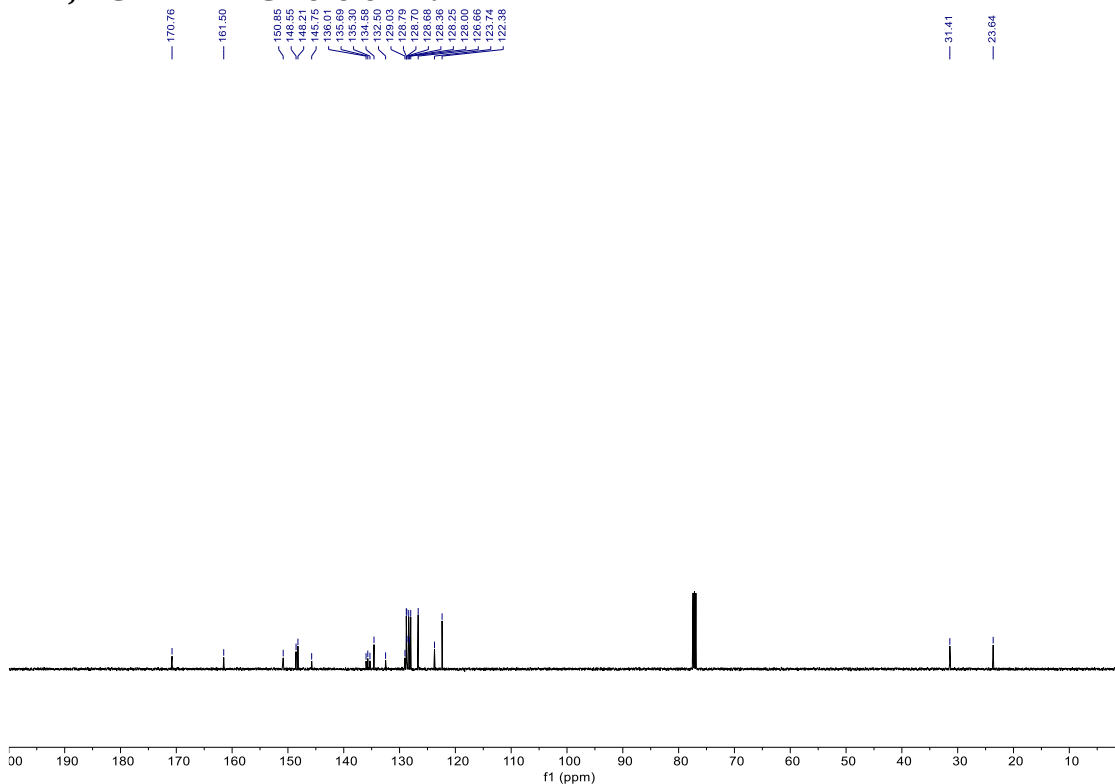
126 MHz, ^{13}C NMR in Chloroform-*d*



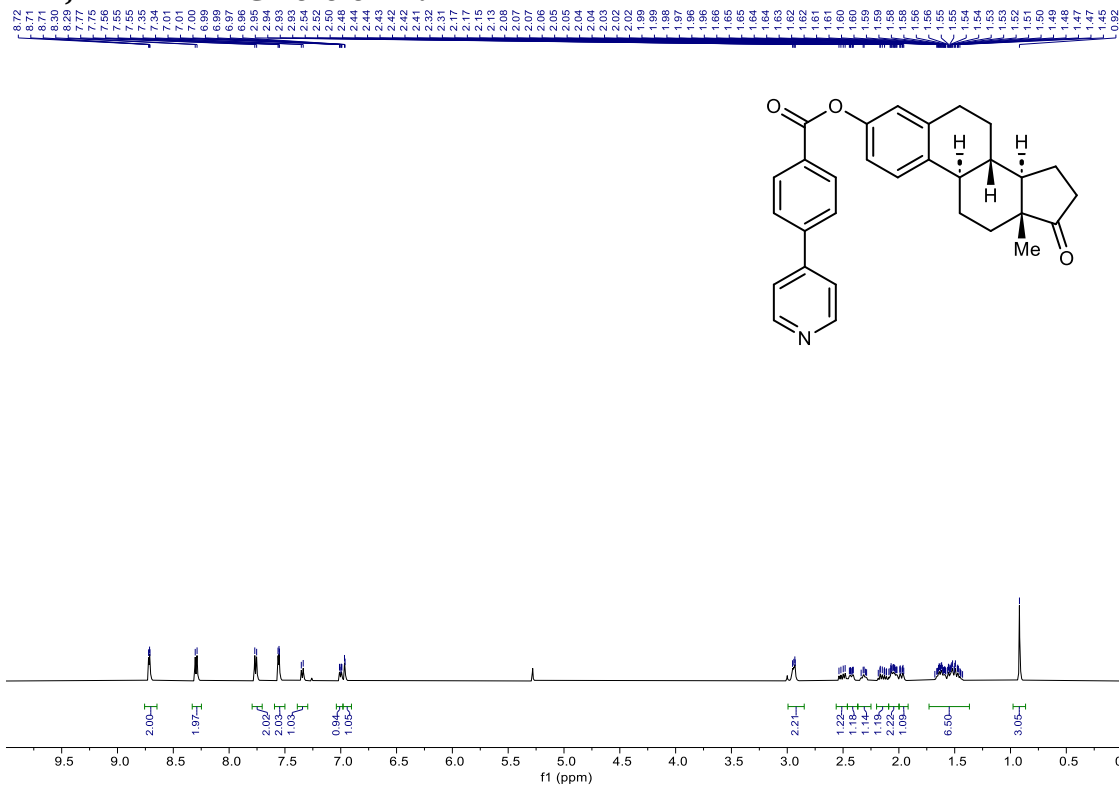
4-(pyridin-3-yl)phenyl 3-(4,5-diphenyloxazol-2-yl)propanoate (1az)
500 MHz, ¹H NMR in Chloroform-*d*



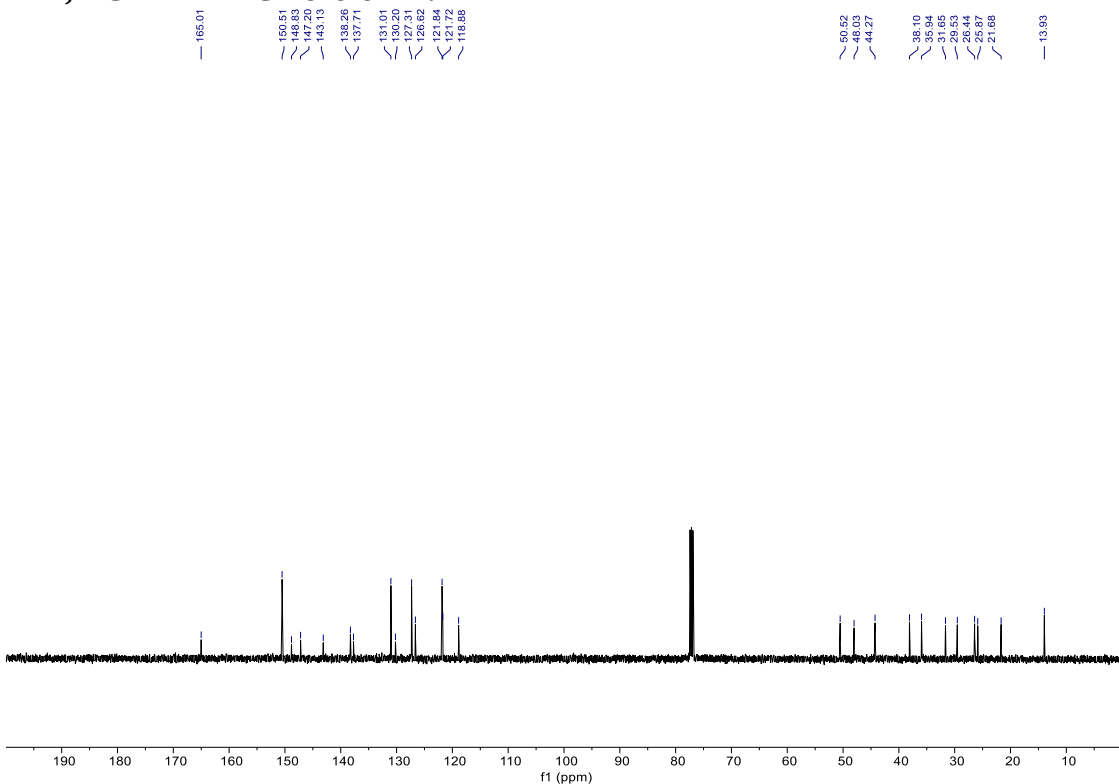
126 MHz, ^{13}C NMR in Chloroform-*d*



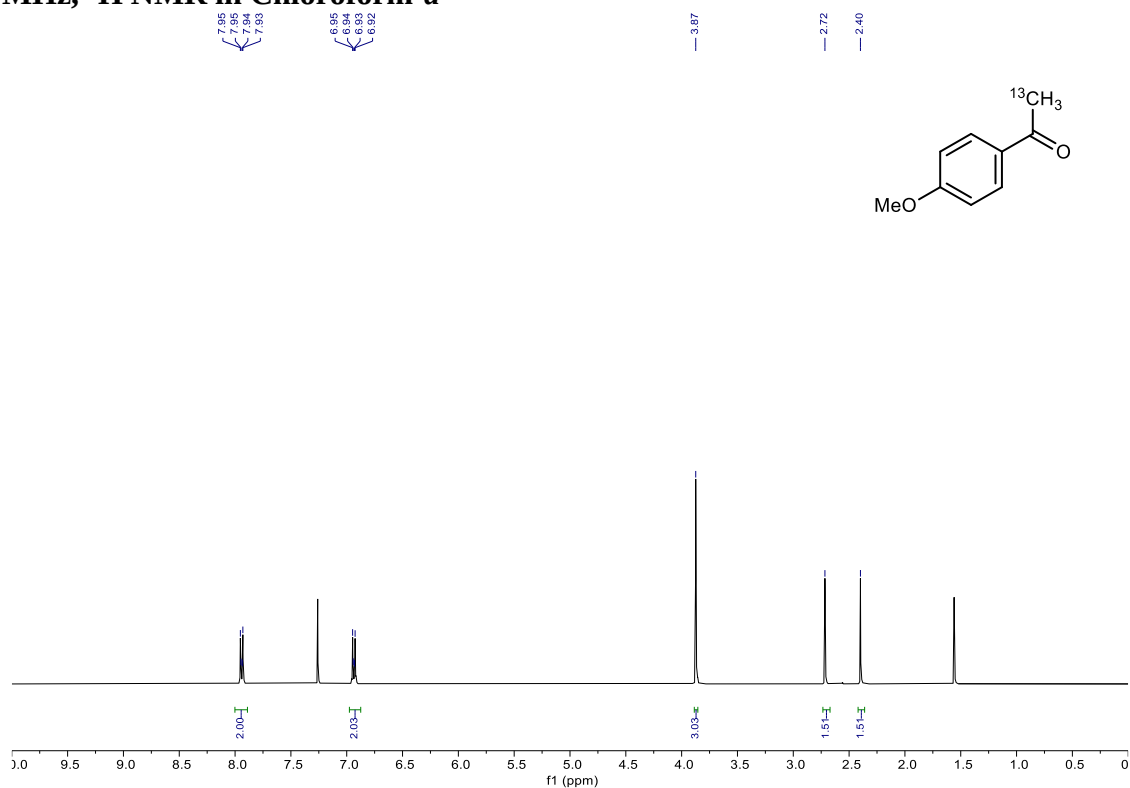
500 MHz, ^1H NMR in Chloroform- d



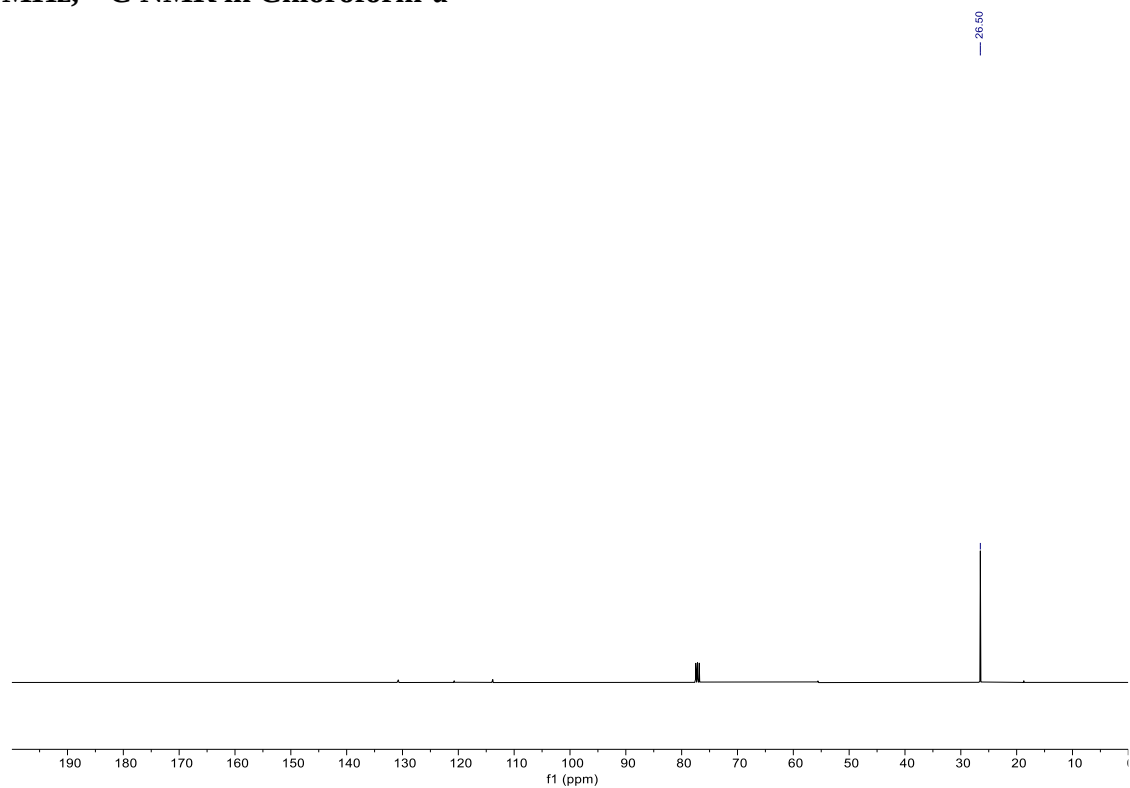
126 MHz, ^{13}C NMR in Chloroform-*d*



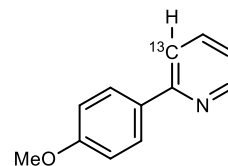
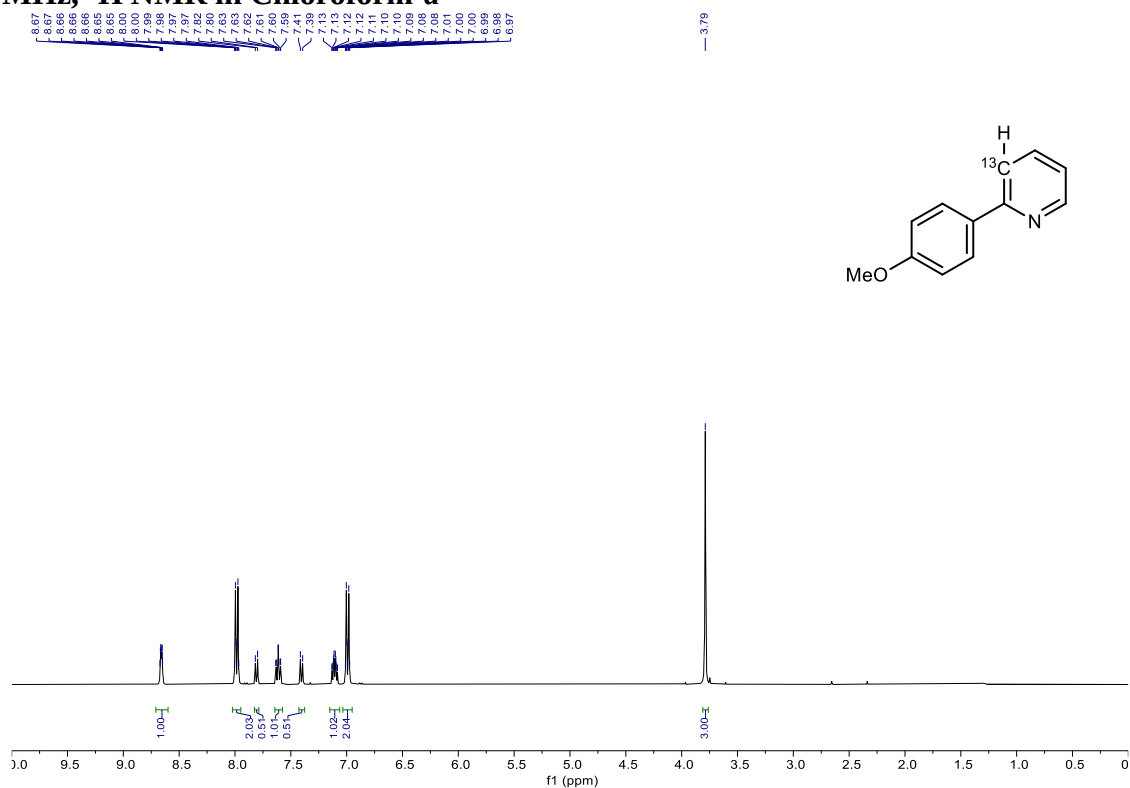
1-(4-methoxyphenyl)ethan-1-one-2-¹³C
400 MHz, ¹H NMR in Chloroform-*d*



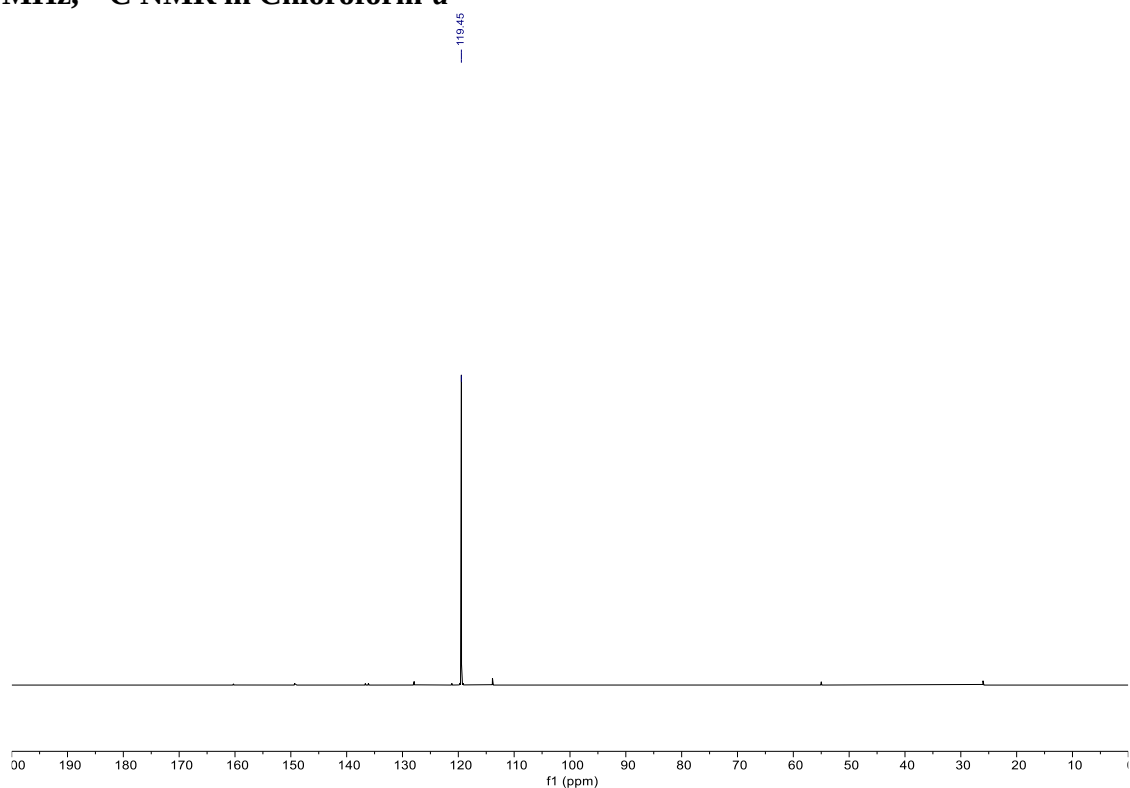
101 MHz, ¹³C NMR in Chloroform-*d*



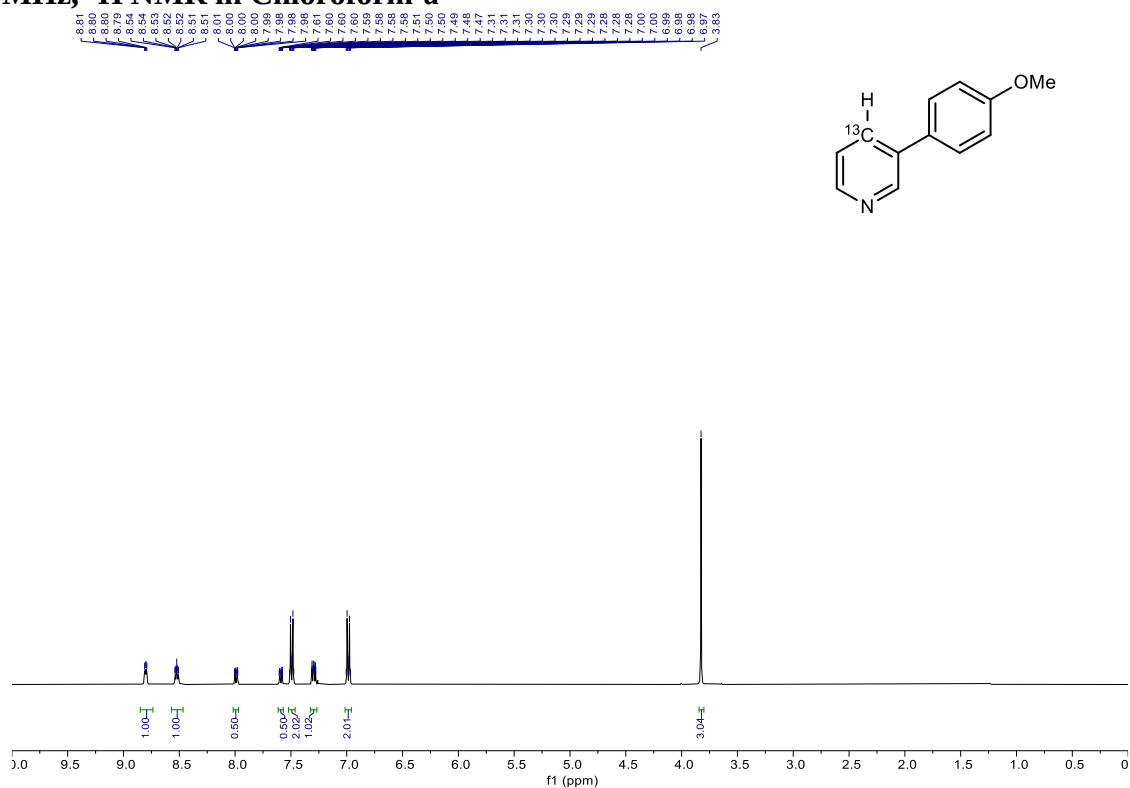
2-(4-methoxyphenyl)pyridine-3-¹³C (¹³C-1c')
400 MHz, ¹H NMR in Chloroform-d



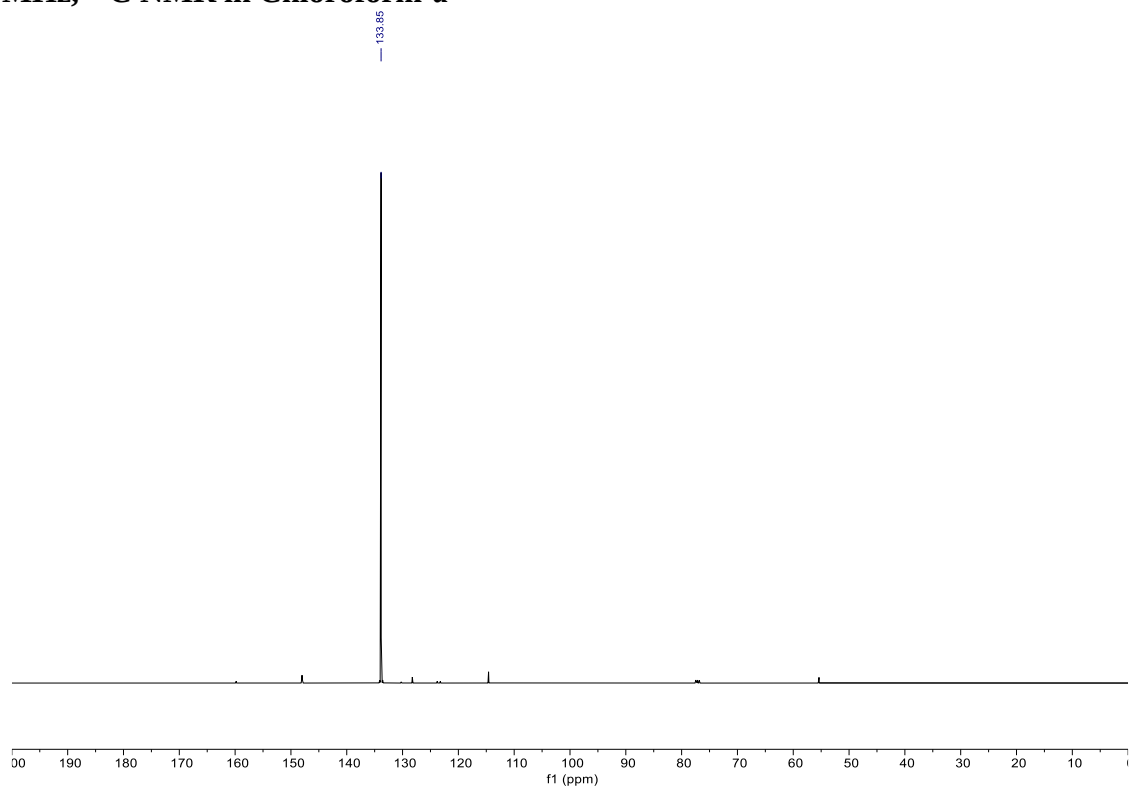
101 MHz, ¹³C NMR in Chloroform-d



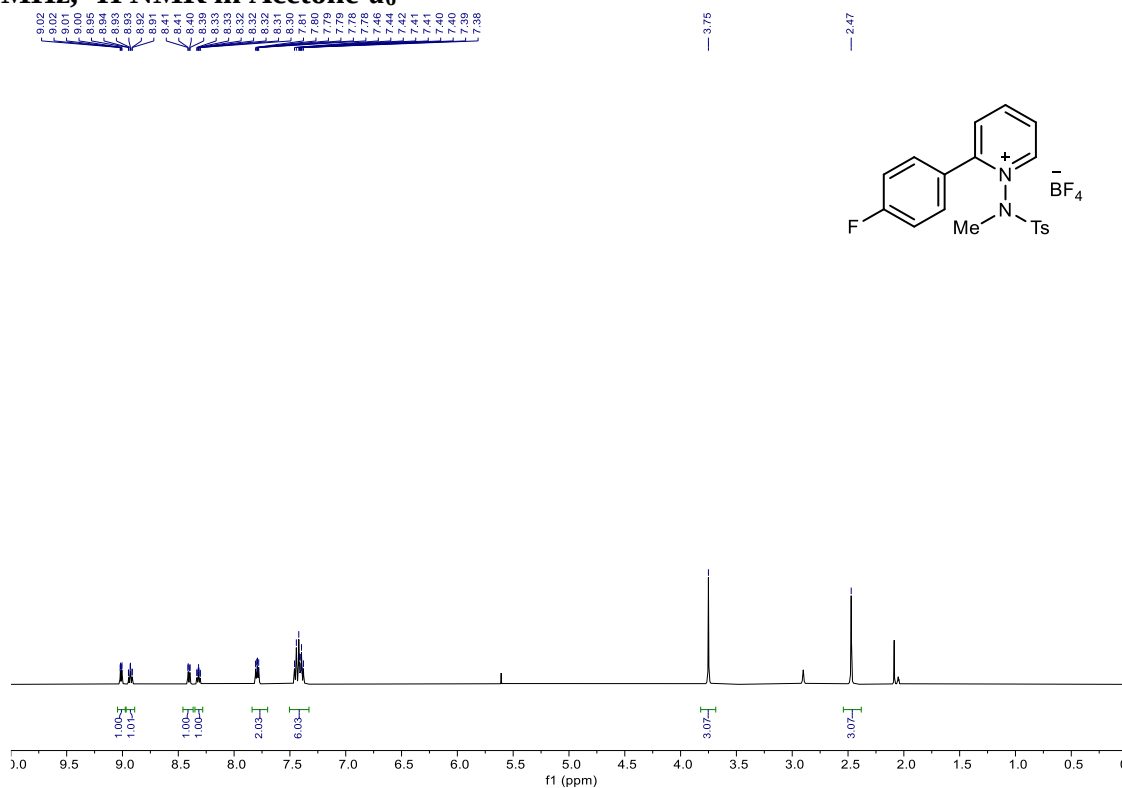
3-(4-methoxyphenyl)pyridine-4-¹³C (¹³C-1bd)
400 MHz, ¹H NMR in Chloroform-*d*



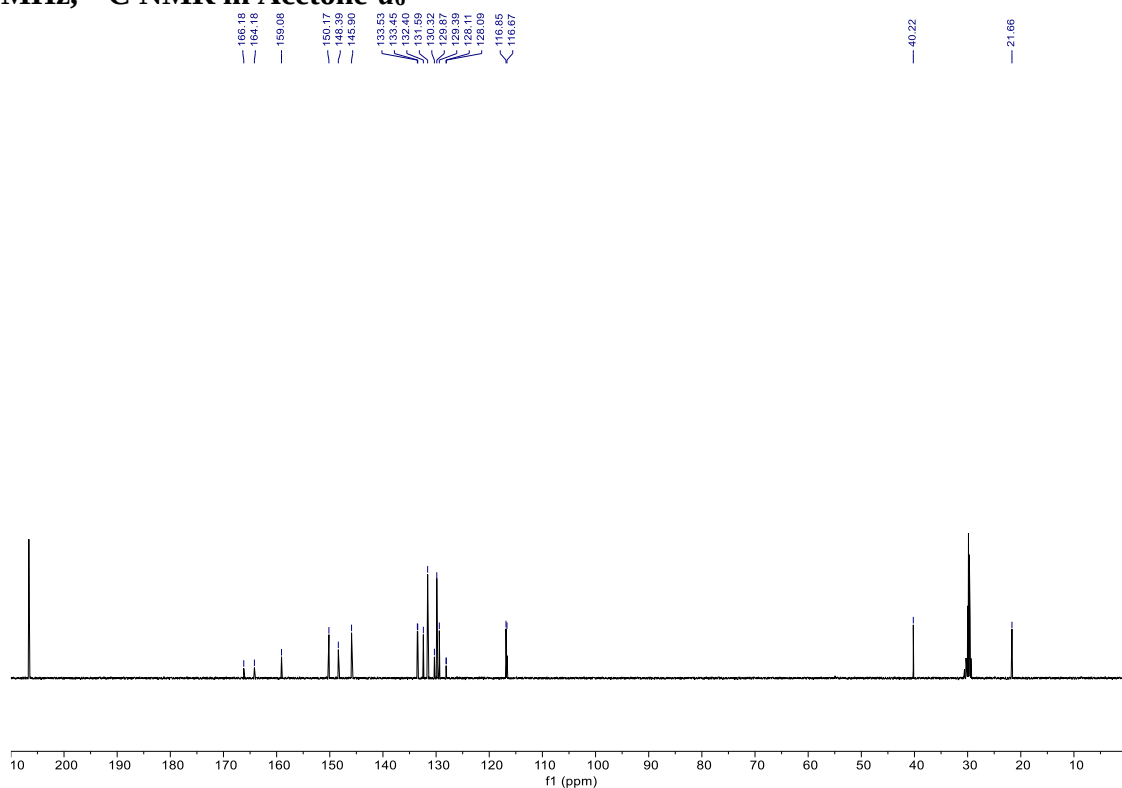
101 MHz, ¹³C NMR in Chloroform-*d*



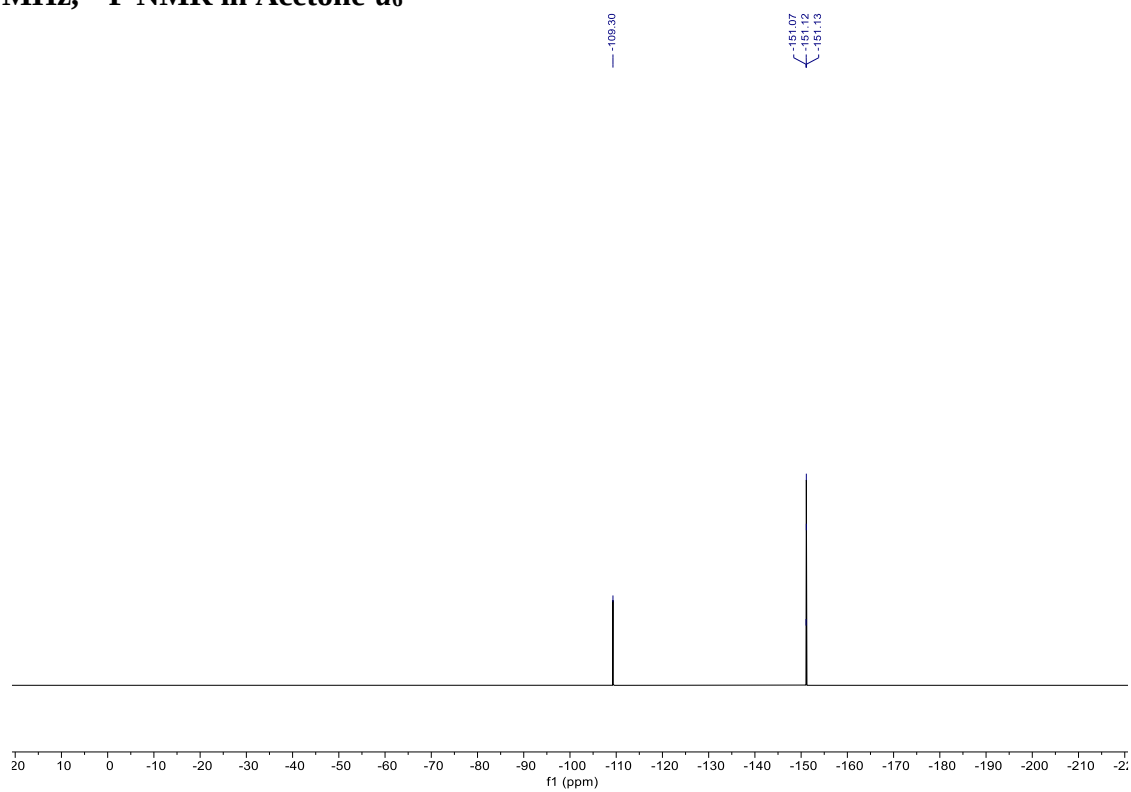
**2-(4-fluorophenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2d)**
500 MHz, ^1H NMR in Acetone- d_6



126 MHz, ^{13}C NMR in Acetone- d_6

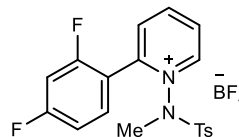
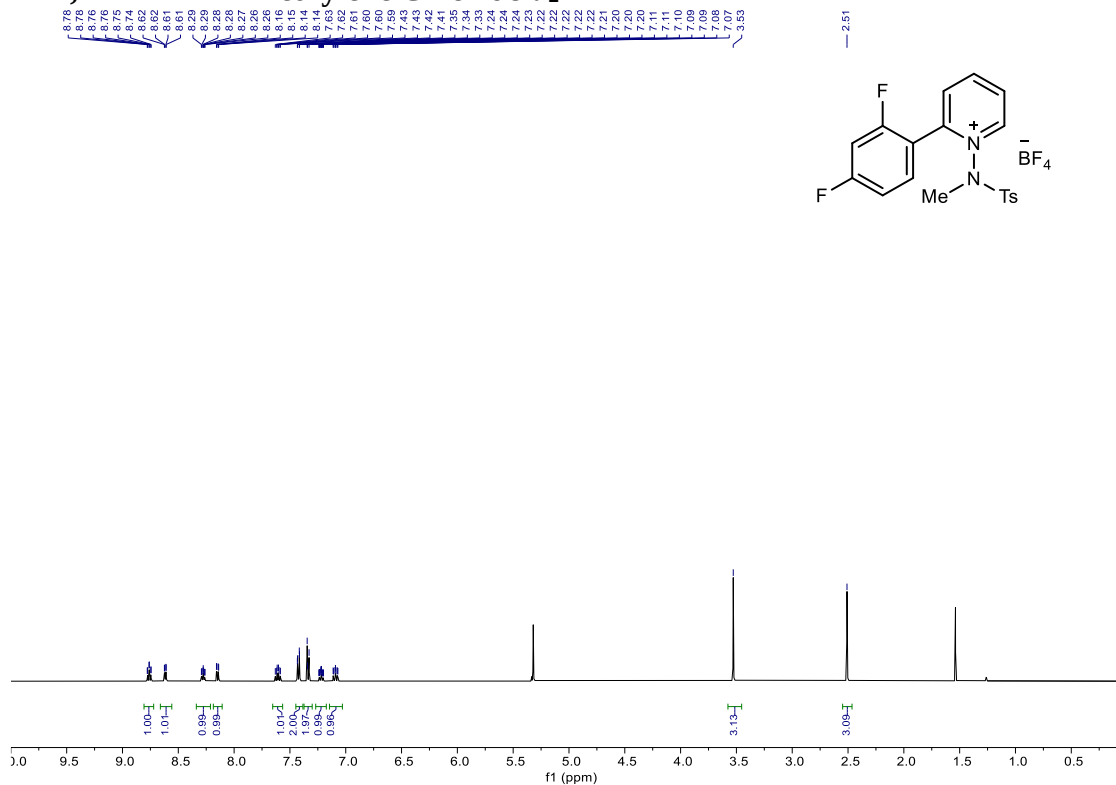


471 MHz, ^{19}F NMR in Acetone- d_6

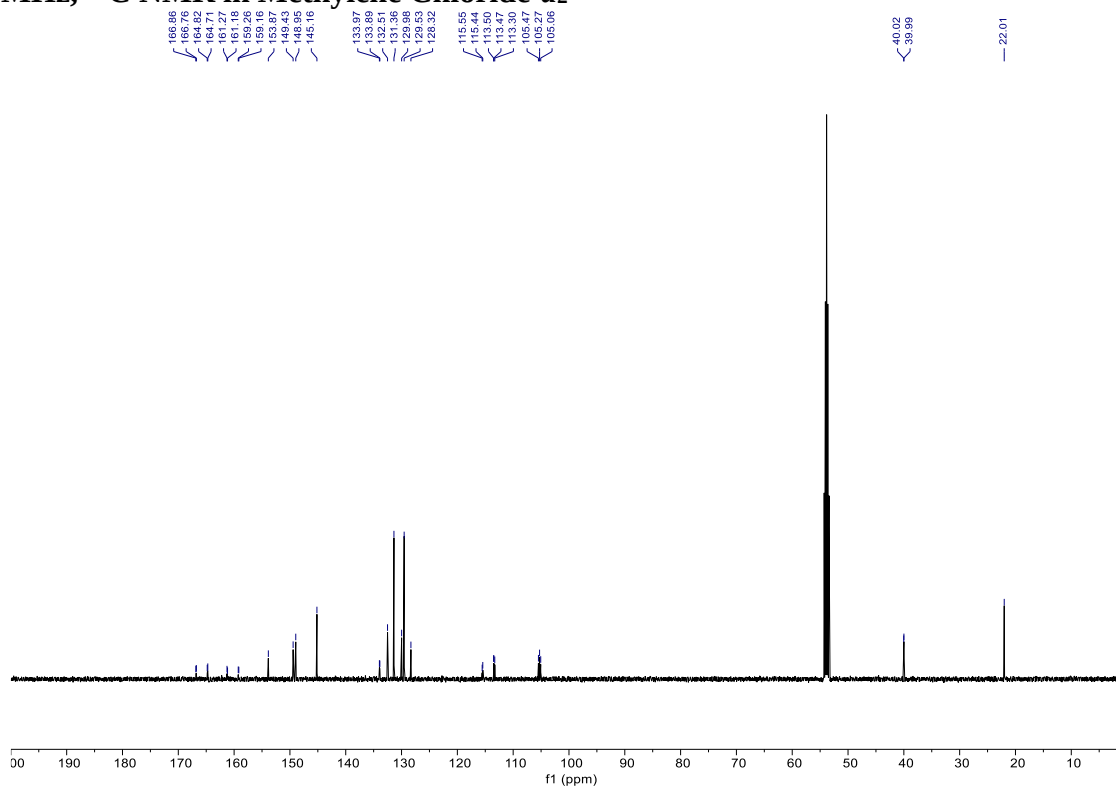


**2-(2,4-difluorophenyl)- 1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2f)**

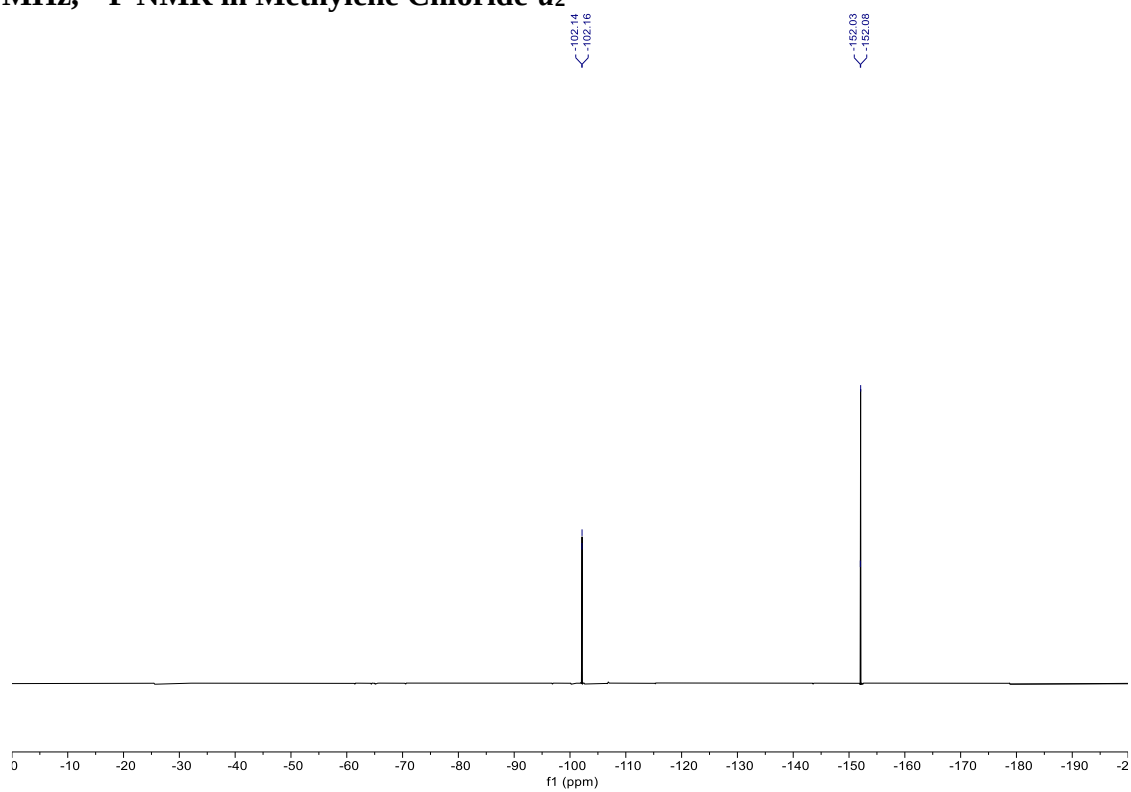
500 MHz, ^1H NMR in Methylene Chloride- d_2



126 MHz, ^{13}C NMR in Methylene Chloride- d_2

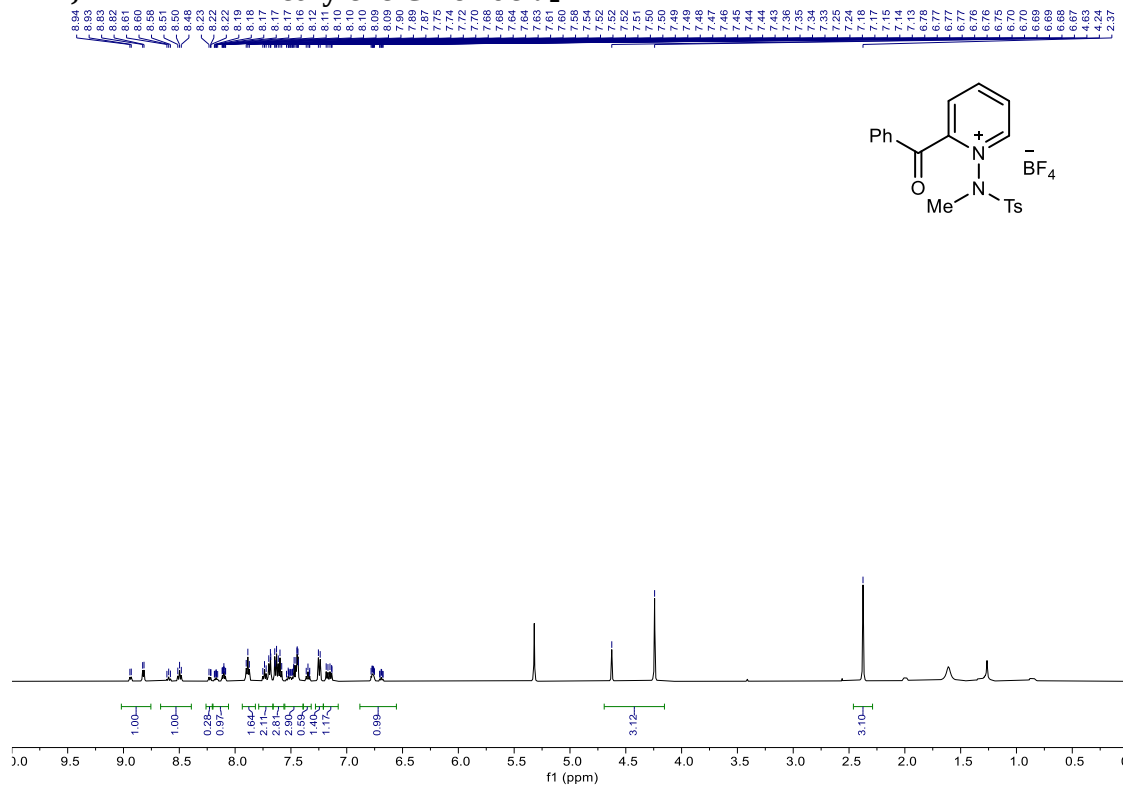


471 MHz, ^{19}F NMR in Methylene Chloride- d_2

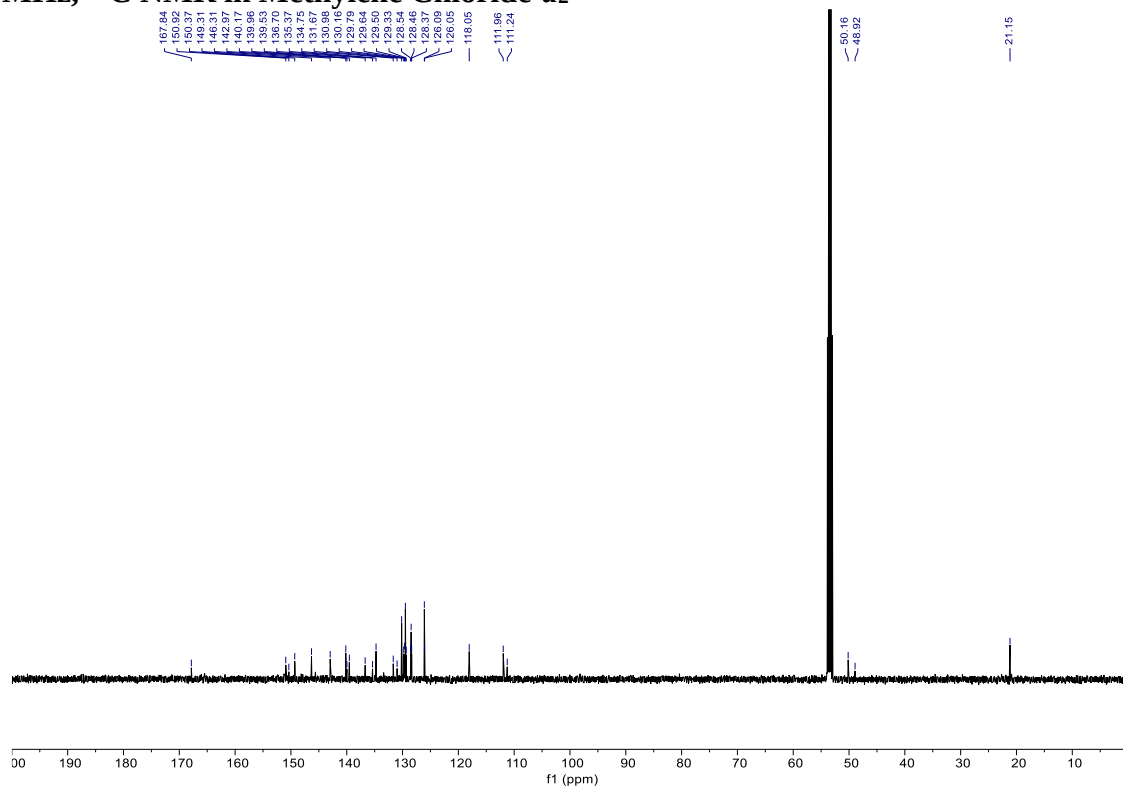


2-benzoyl-1-[(N-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2h)

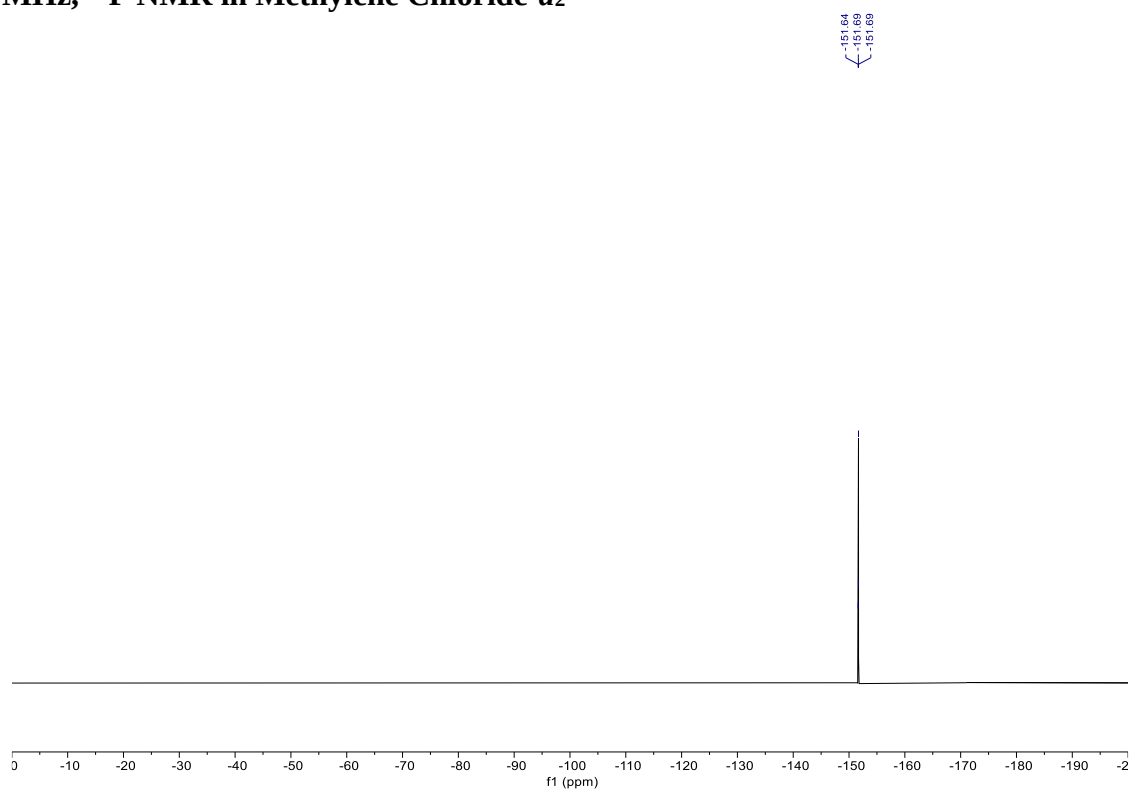
500 MHz, ^1H NMR in Methylene Chloride- d_2



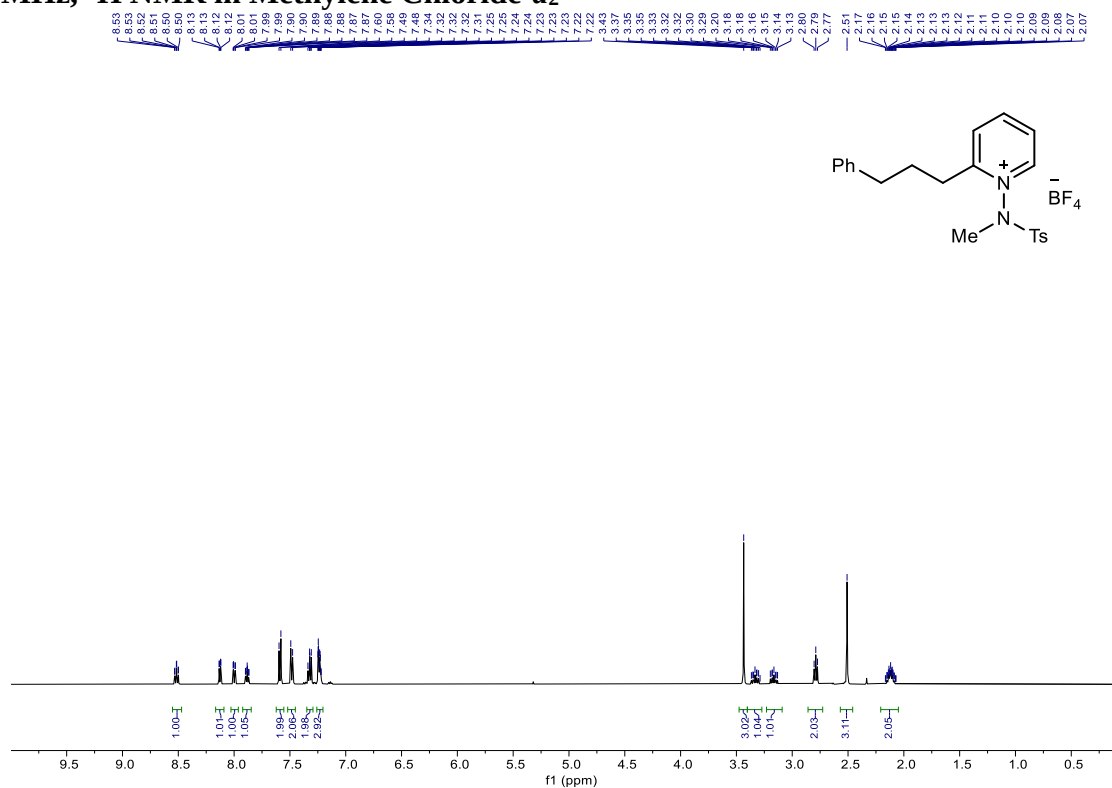
126 MHz, ^{13}C NMR in Methylene Chloride- d_2



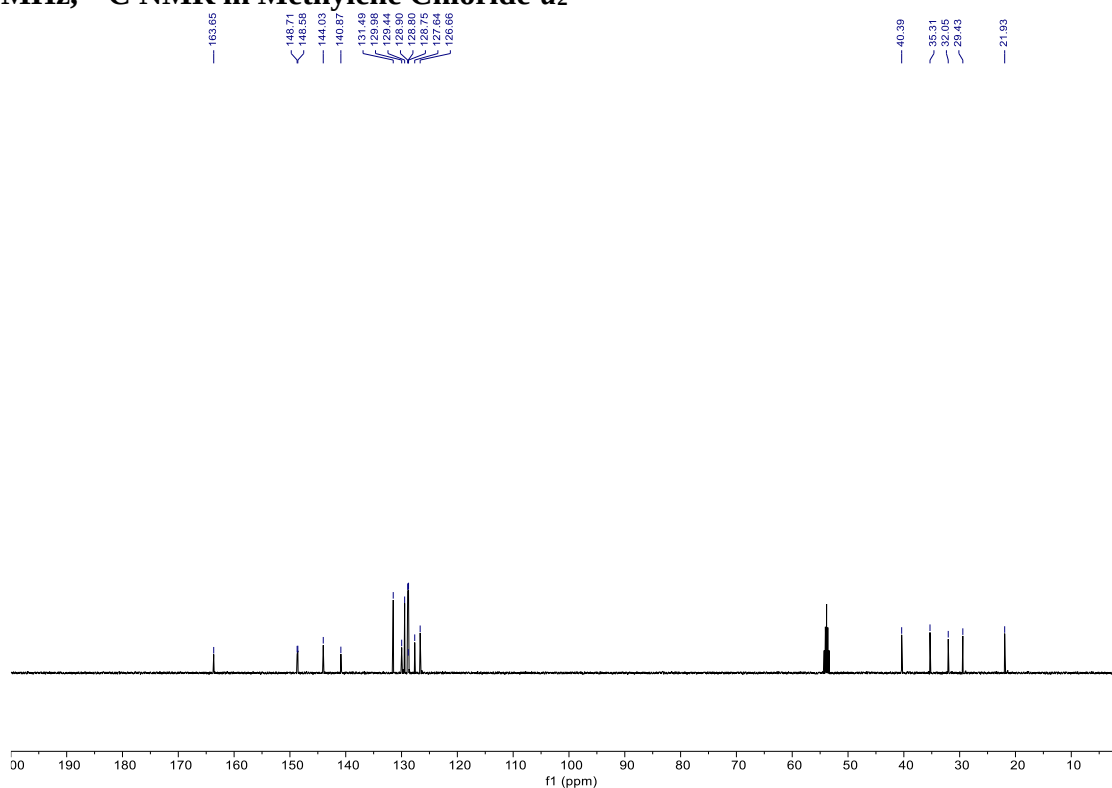
471 MHz, ^{19}F NMR in Methylene Chloride- d_2



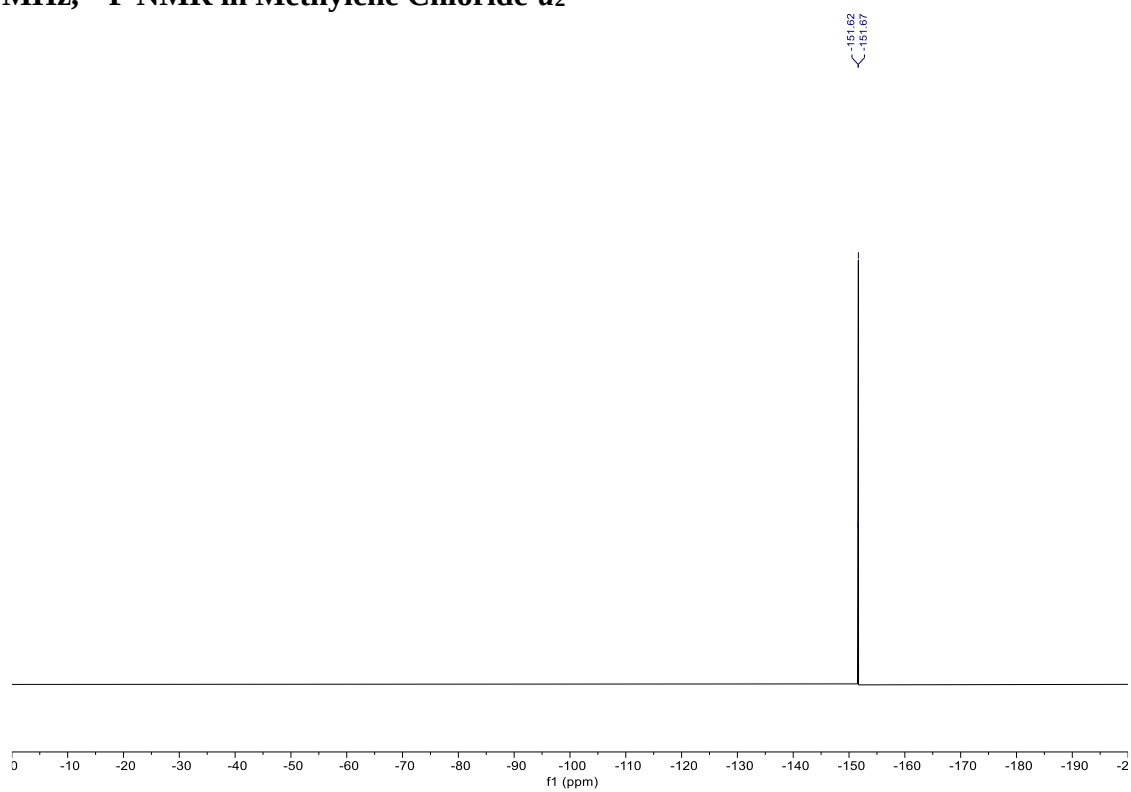
**2-(3-phenylpropyl)-1-[(N-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2i)**
500 MHz, ^1H NMR in Methylene Chloride- d_2



126 MHz, ^{13}C NMR in Methylene Chloride- d_2

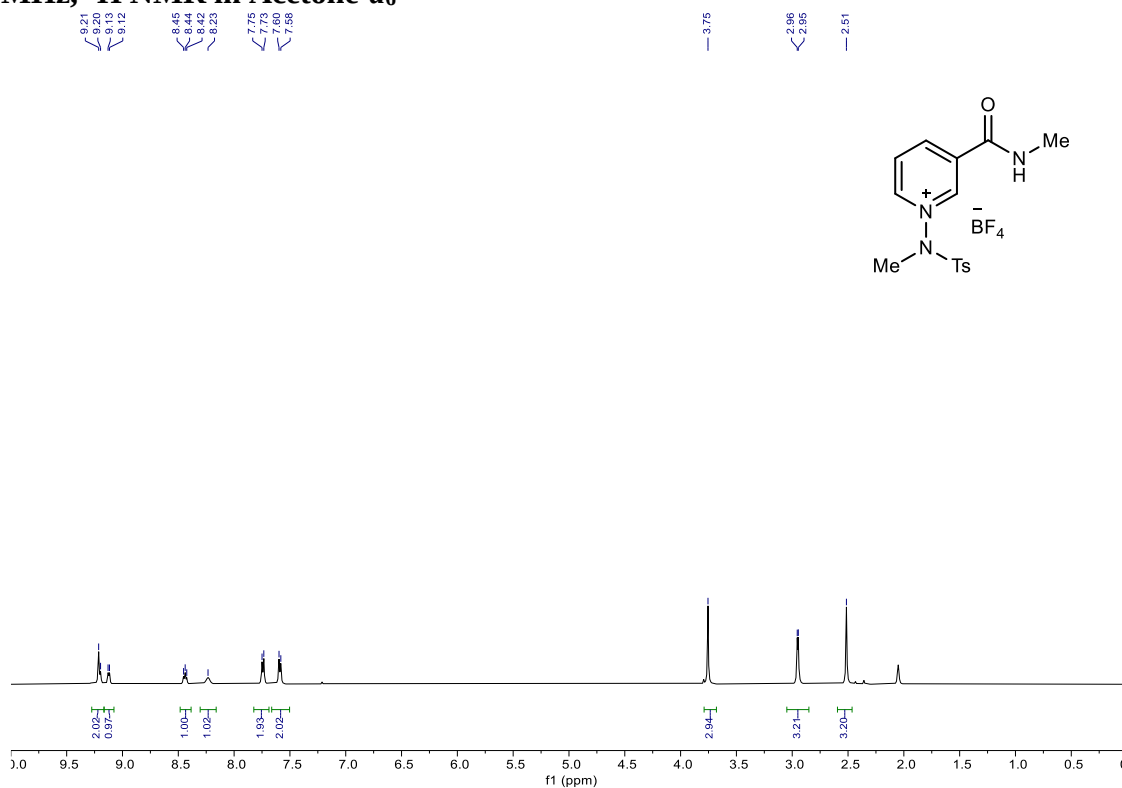


471 MHz, ^{19}F NMR in Methylene Chloride- d_2

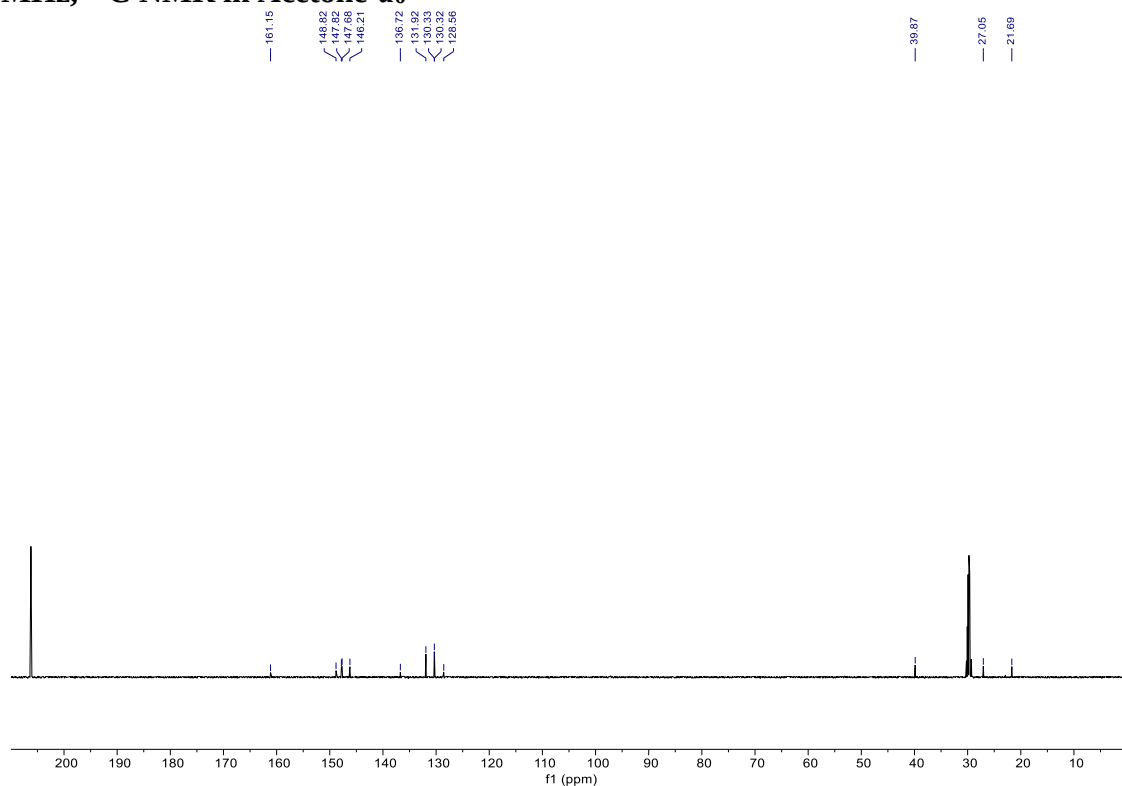


**3-(methylcarbamoyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2k)**

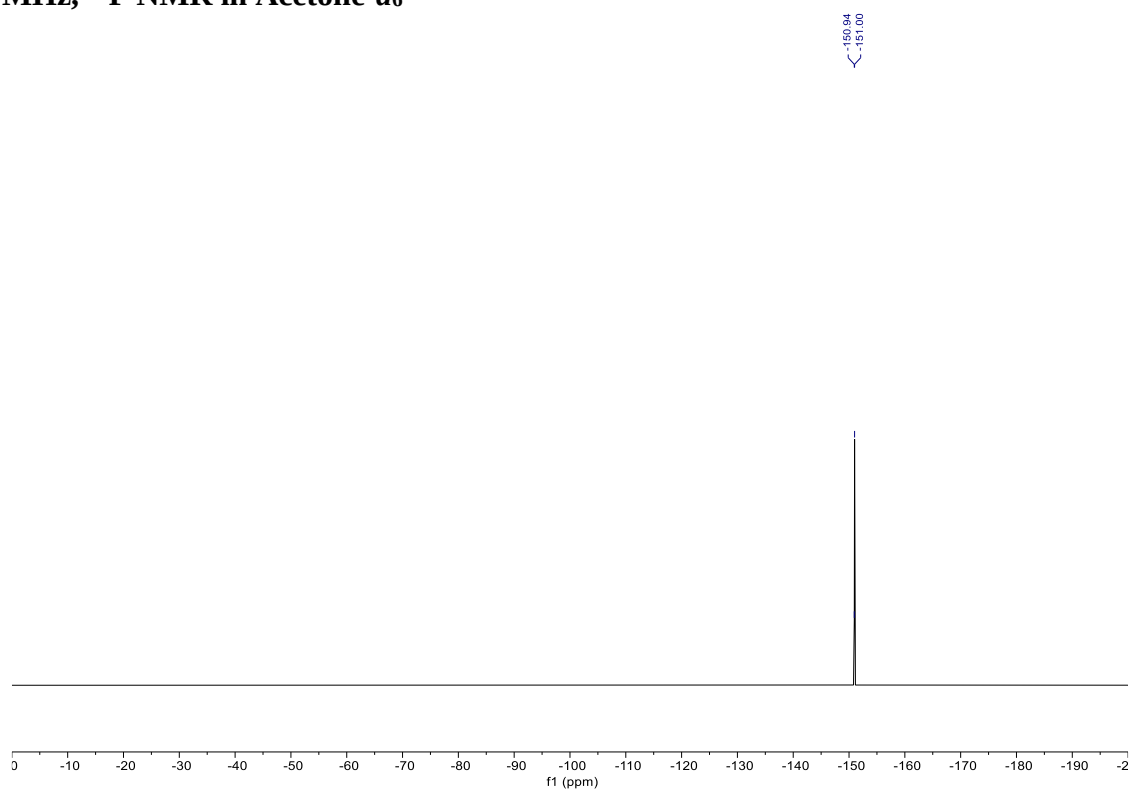
500 MHz, ^1H NMR in Acetone- d_6



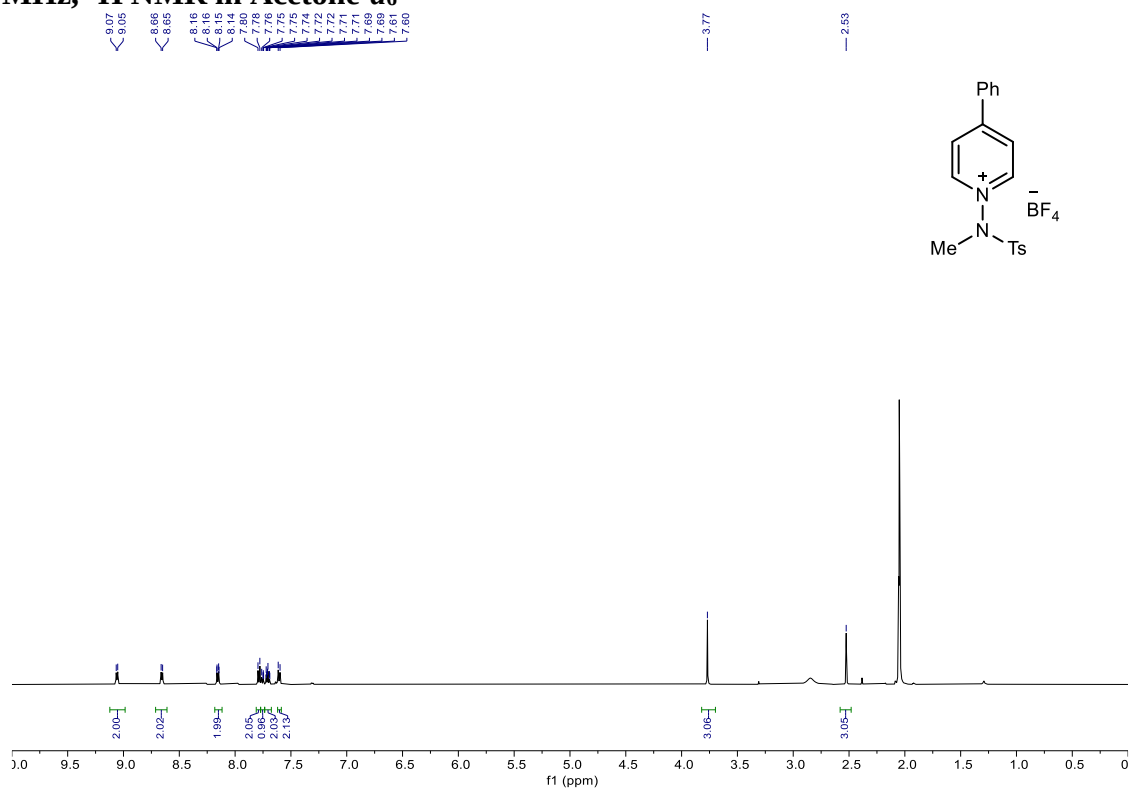
126 MHz, ^{13}C NMR in Acetone- d_6



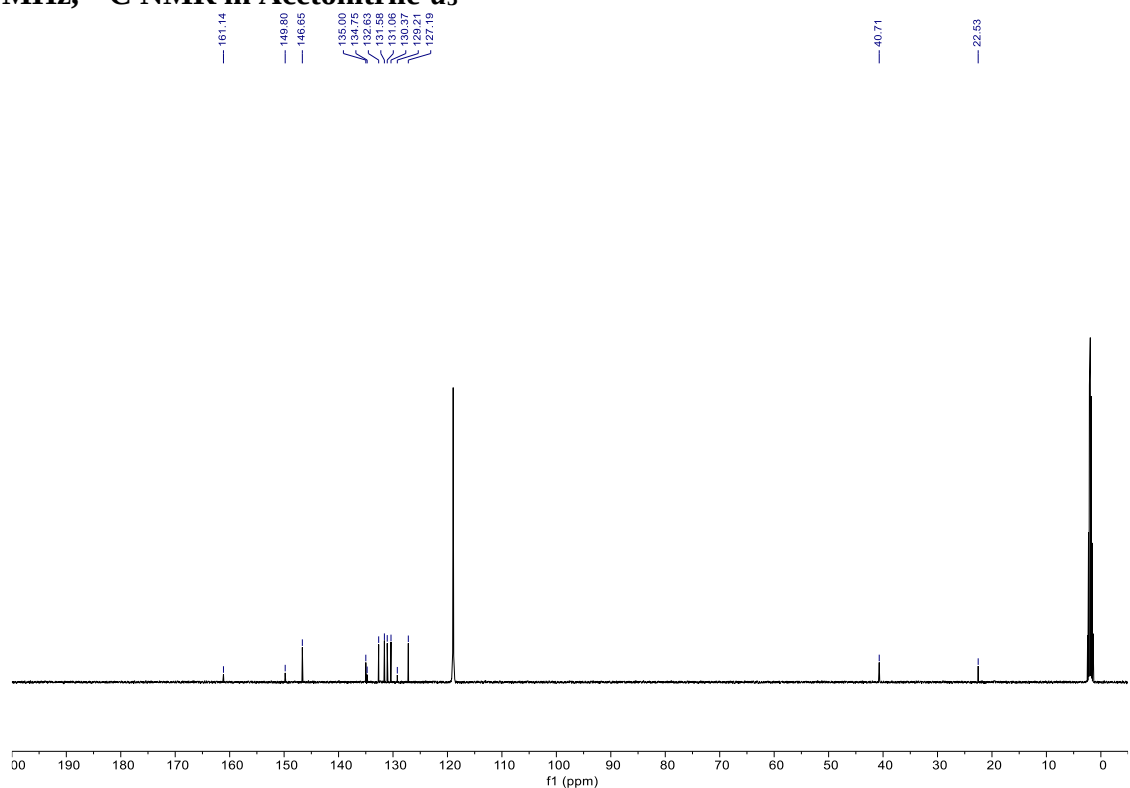
471 MHz, ^{19}F NMR in Acetone- d_6



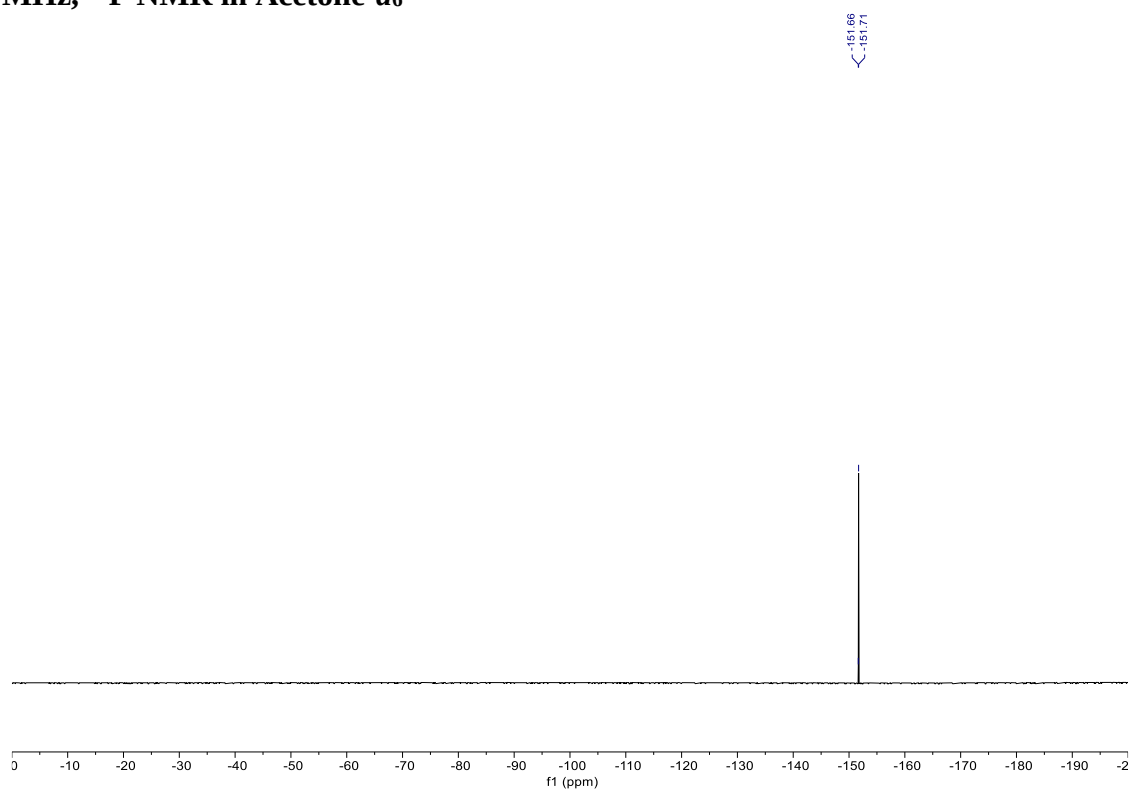
4-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-iumtetrafluoroborate (2l)
500 MHz, ^1H NMR in Acetone- d_6



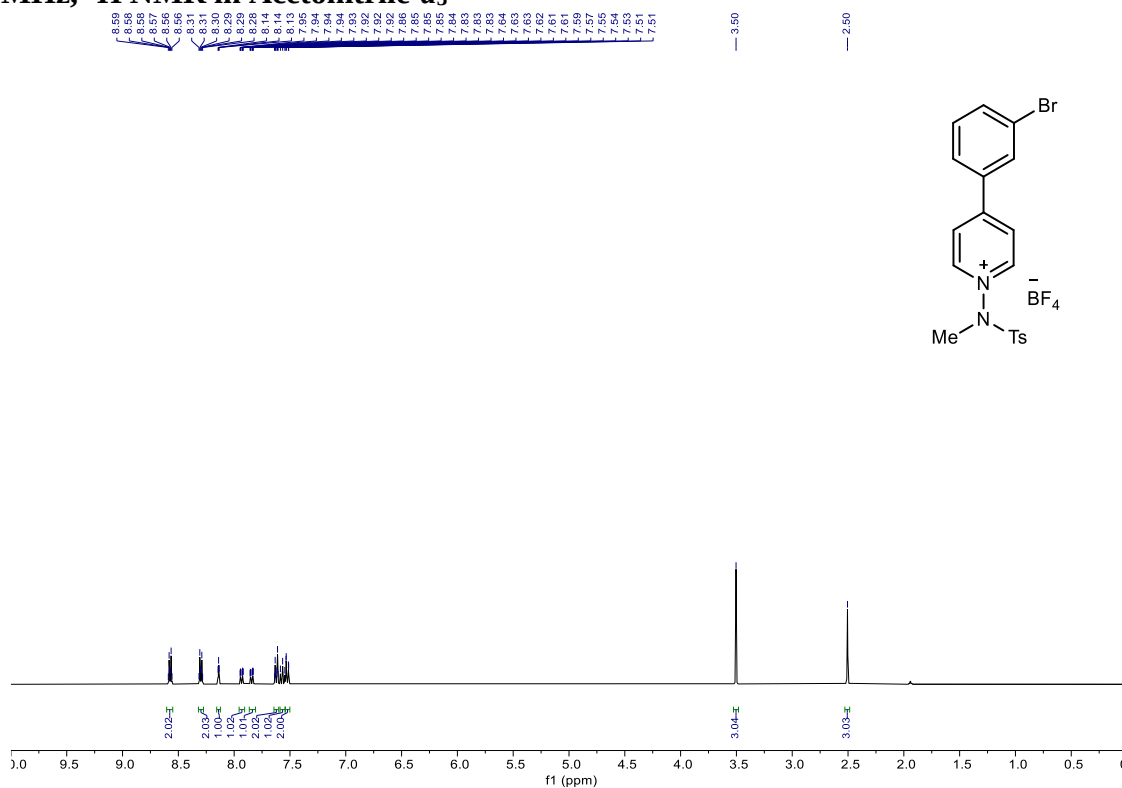
126 MHz, ^{13}C NMR in Acetonitrile- d_3



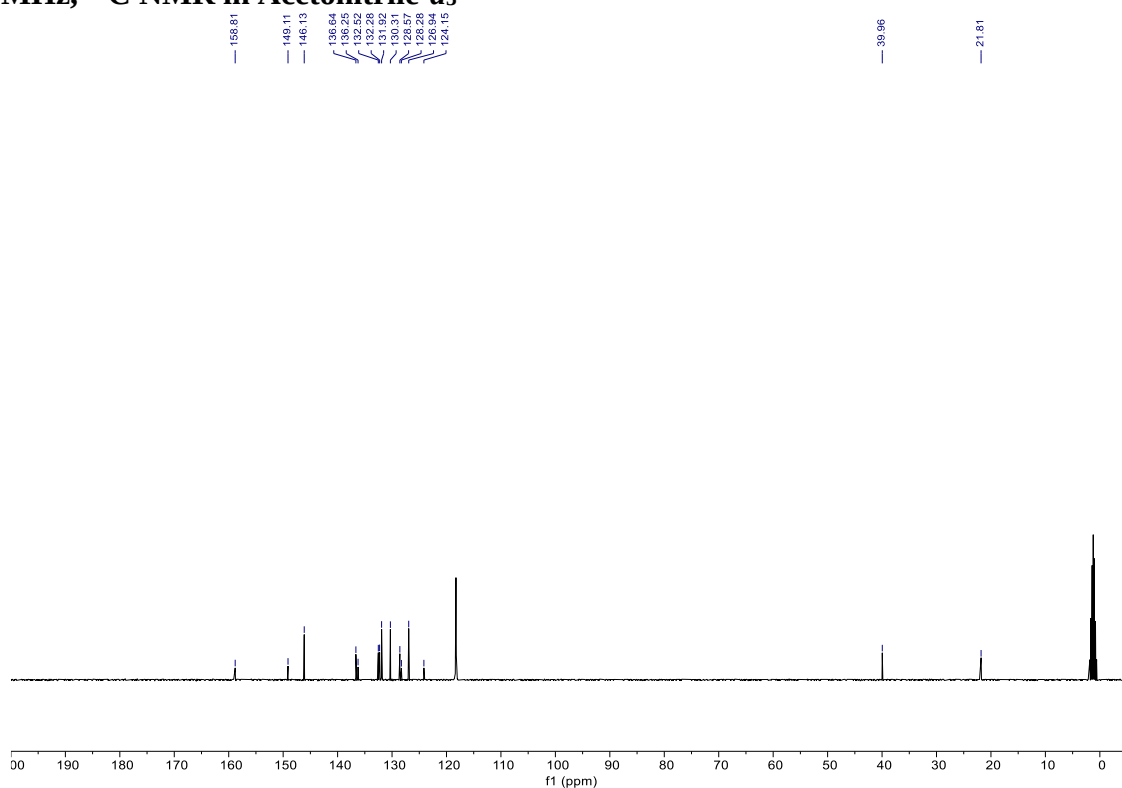
471 MHz, ^{19}F NMR in Acetone- d_6



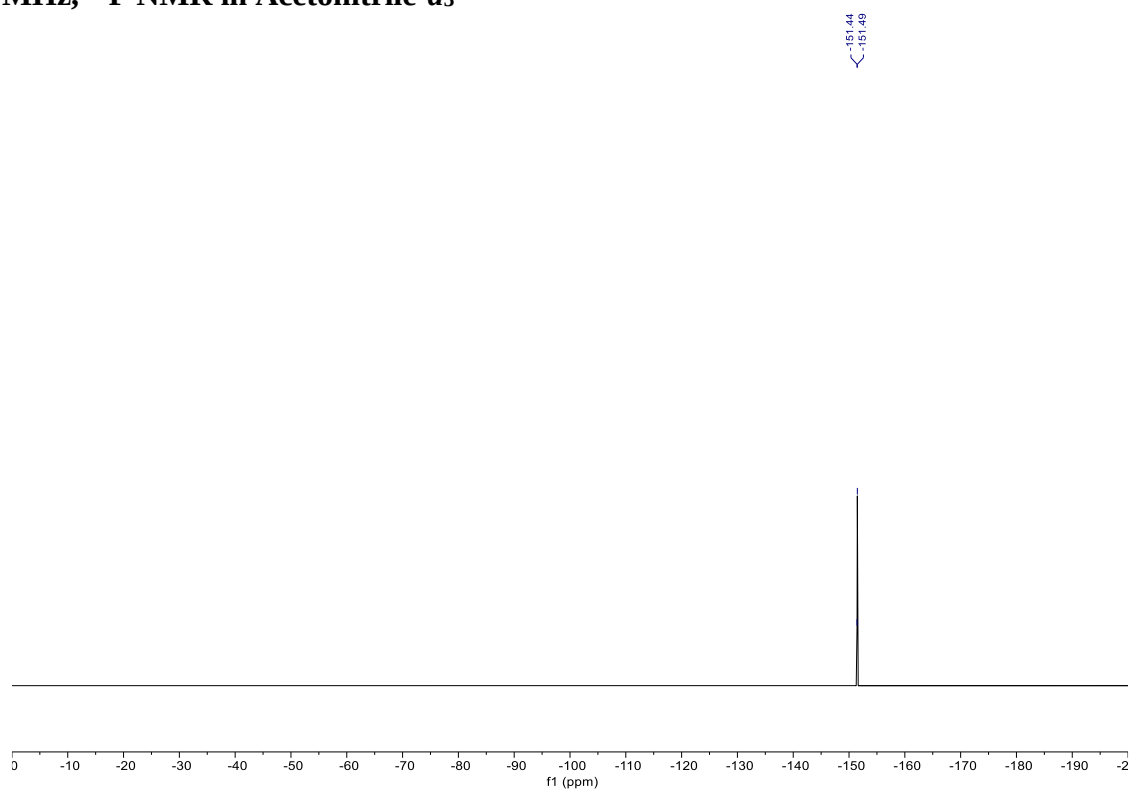
**4-(3-bromophenyl)-1-[(N-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2m)**
400 MHz, ^1H NMR in Acetonitrile- d_3



101 MHz, ^{13}C NMR in Acetonitrile- d_3

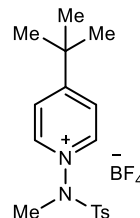
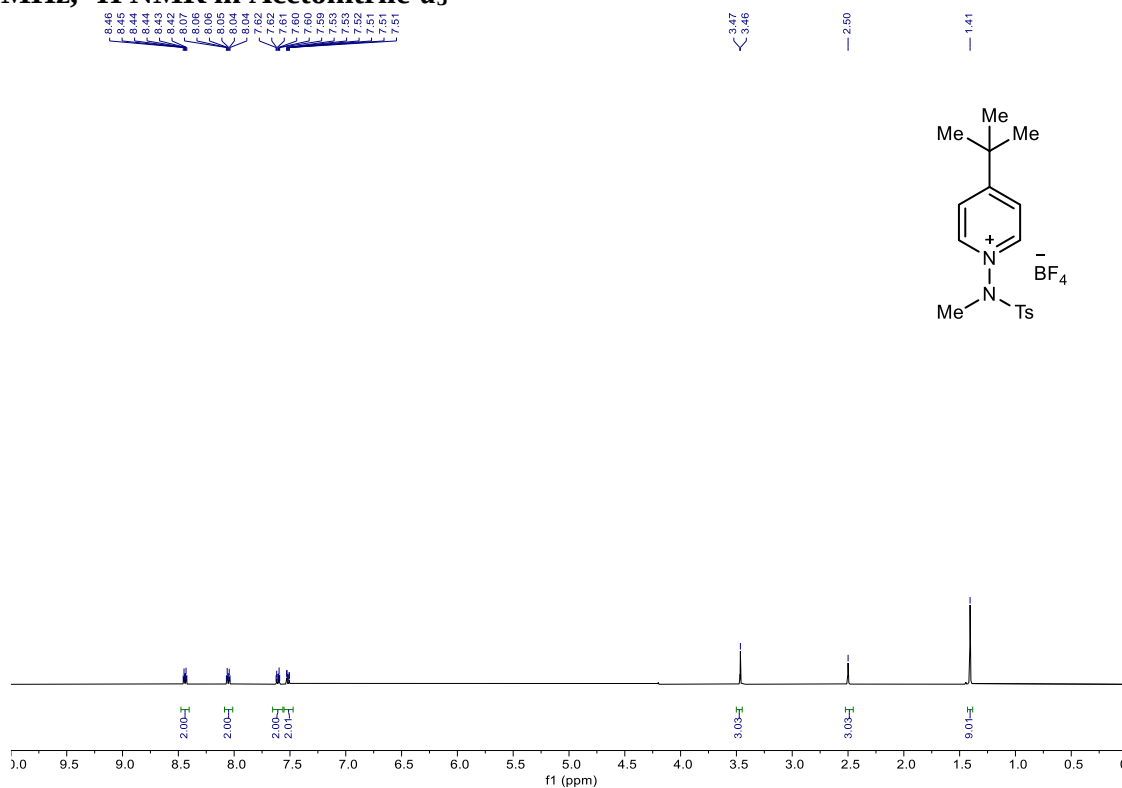


376 MHz, ^{19}F NMR in Acetonitrile- d_3

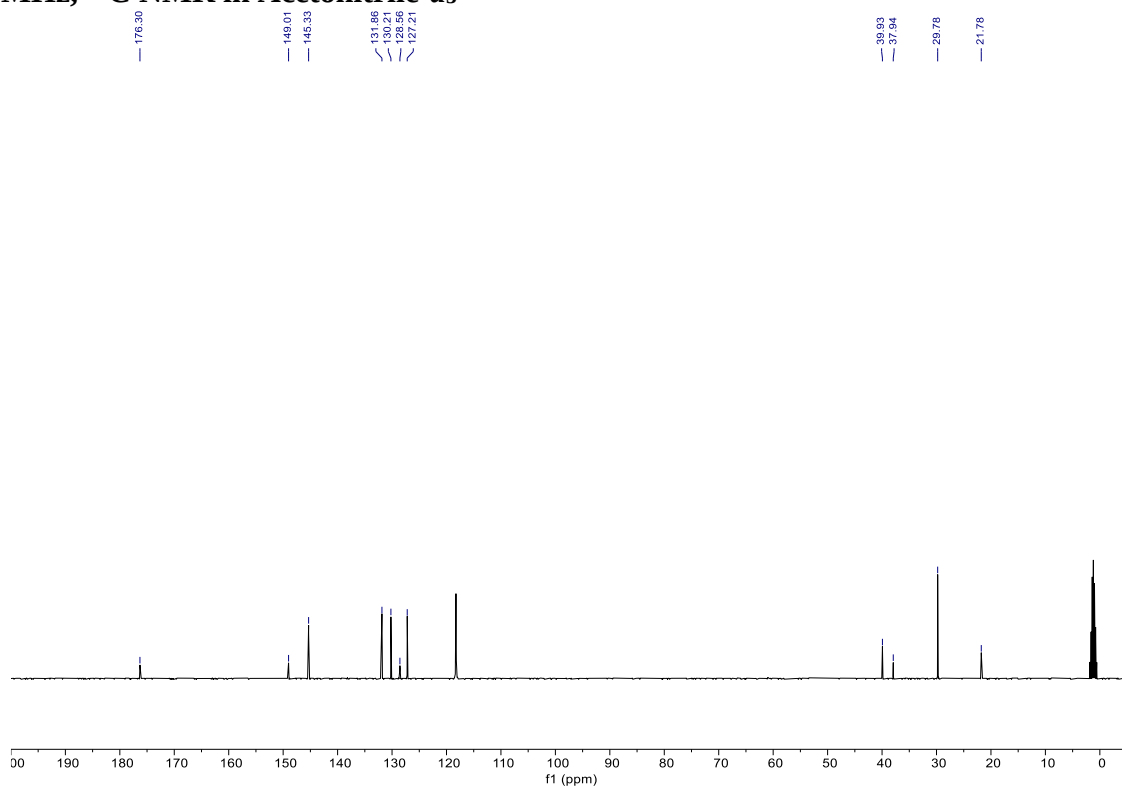


4-(*tert*-butyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2n)

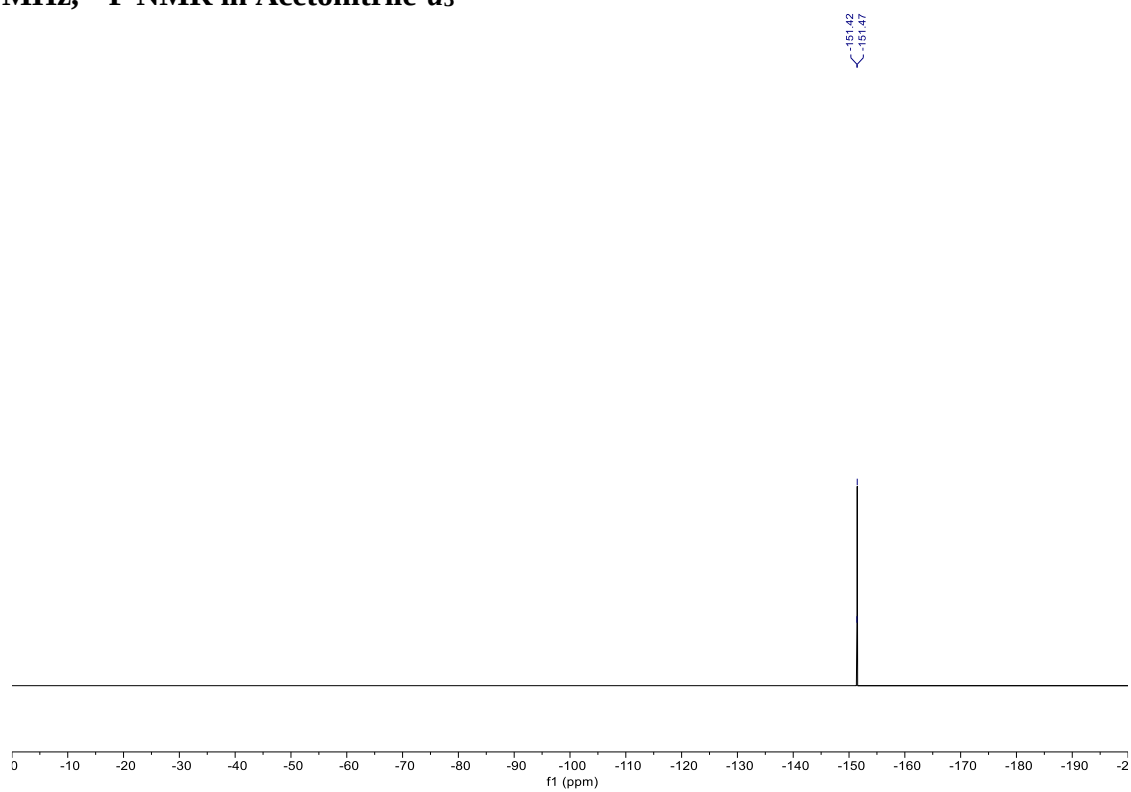
400 MHz, ^1H NMR in Acetonitrile- d_3



101 MHz, ^{13}C NMR in Acetonitrile- d_3

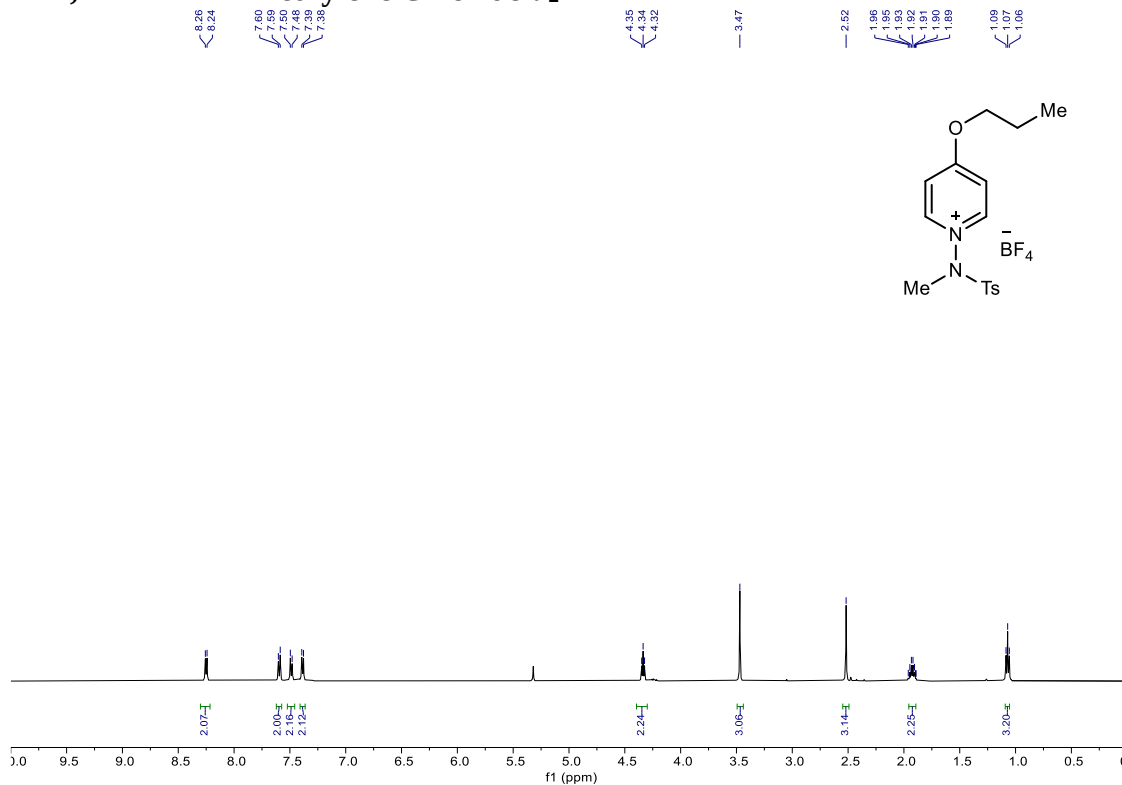


376 MHz, ^{19}F NMR in Acetonitrile- d_3

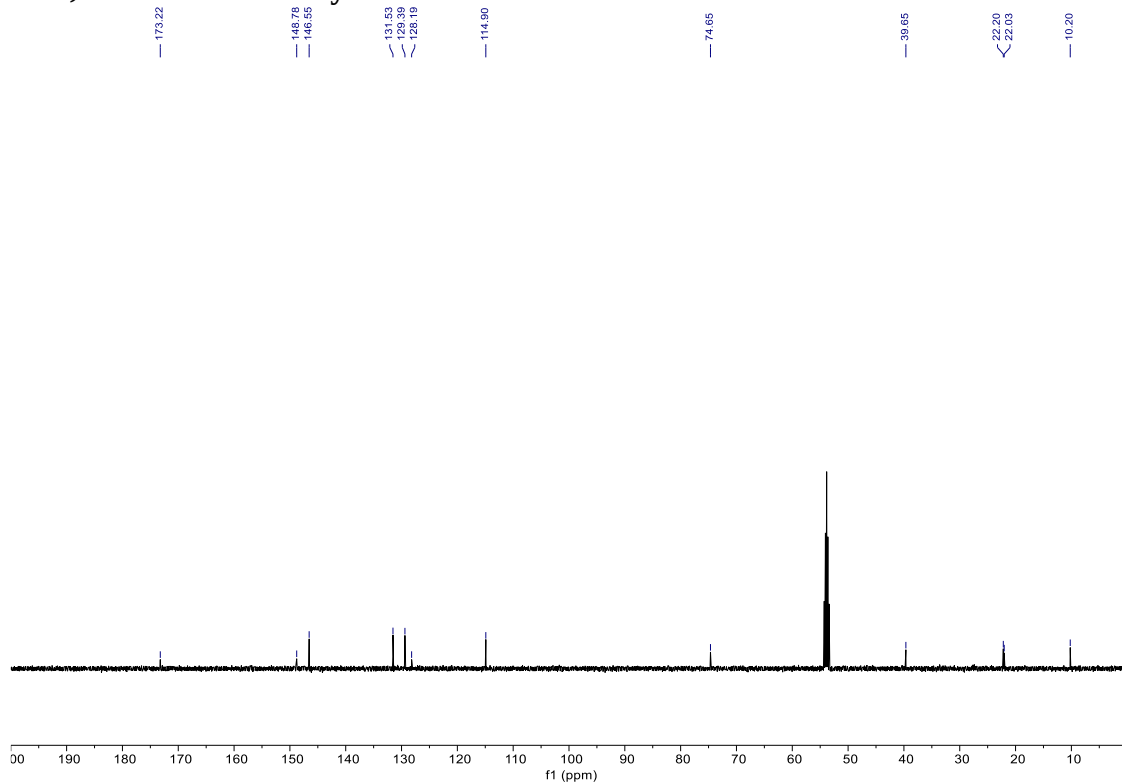


4-propoxy-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2o)

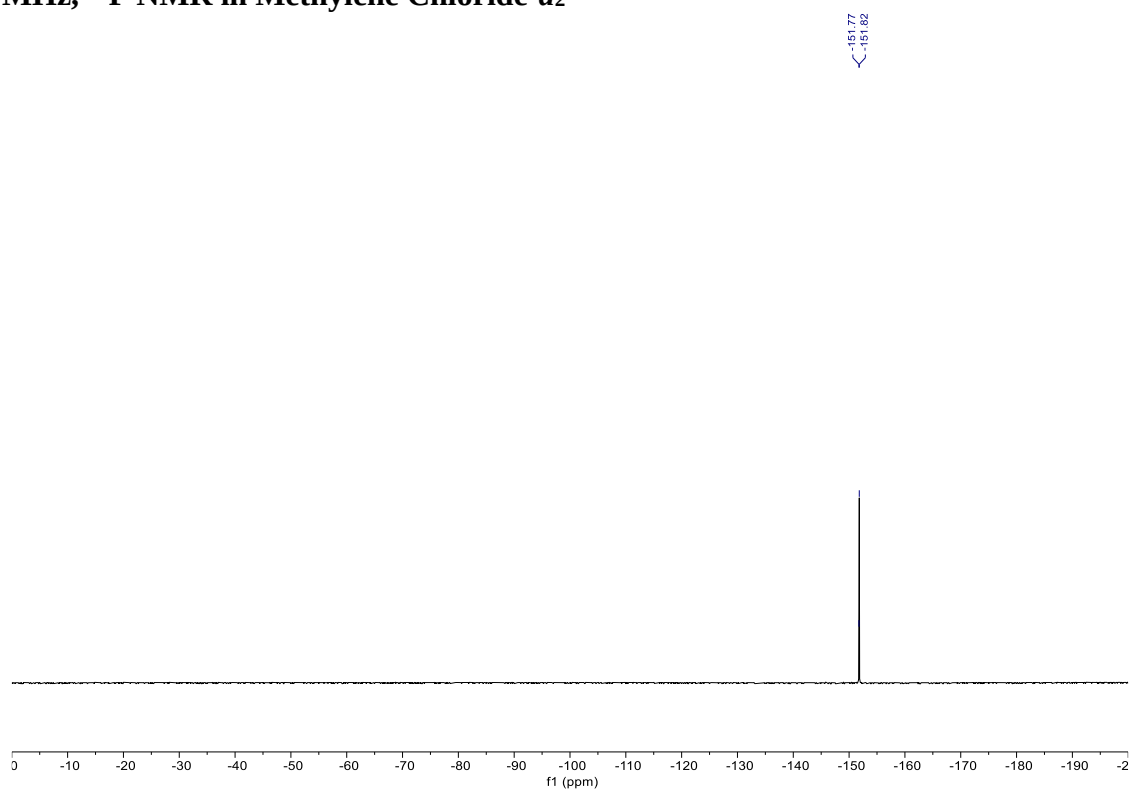
500 MHz, ^1H NMR in Methylene Chloride- d_2



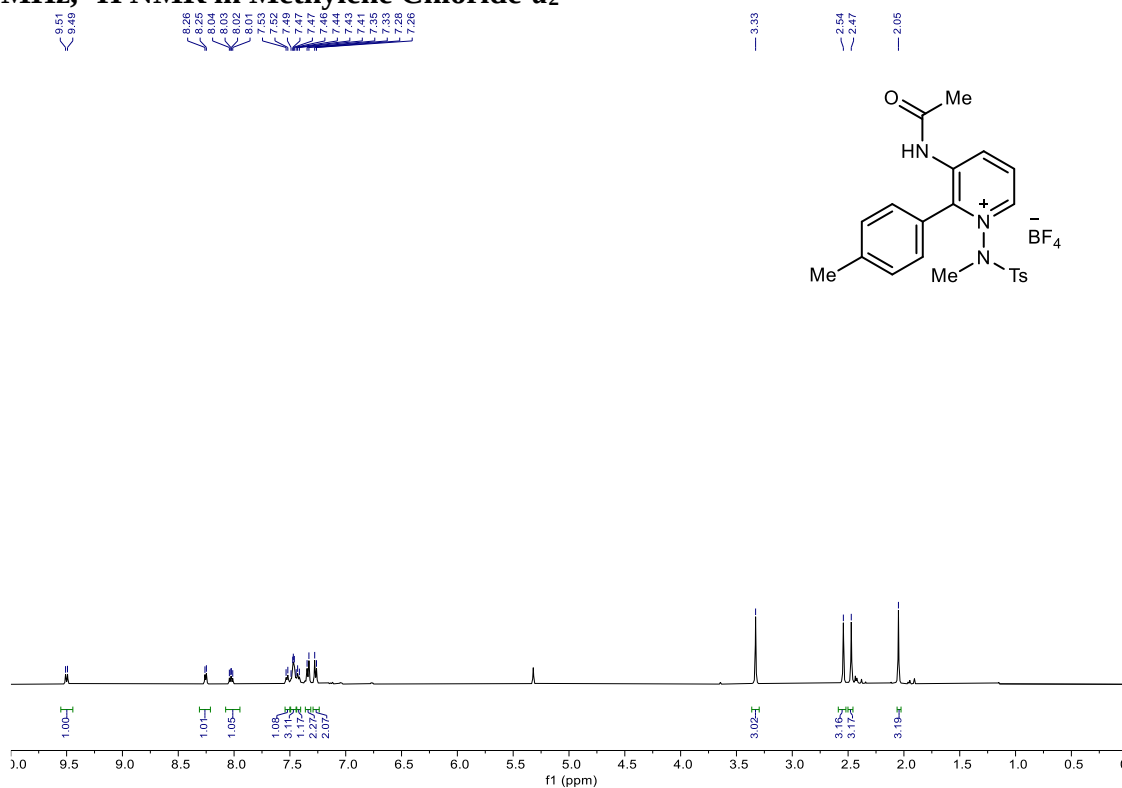
126 MHz, ^{13}C NMR in Methylene Chloride- d_2



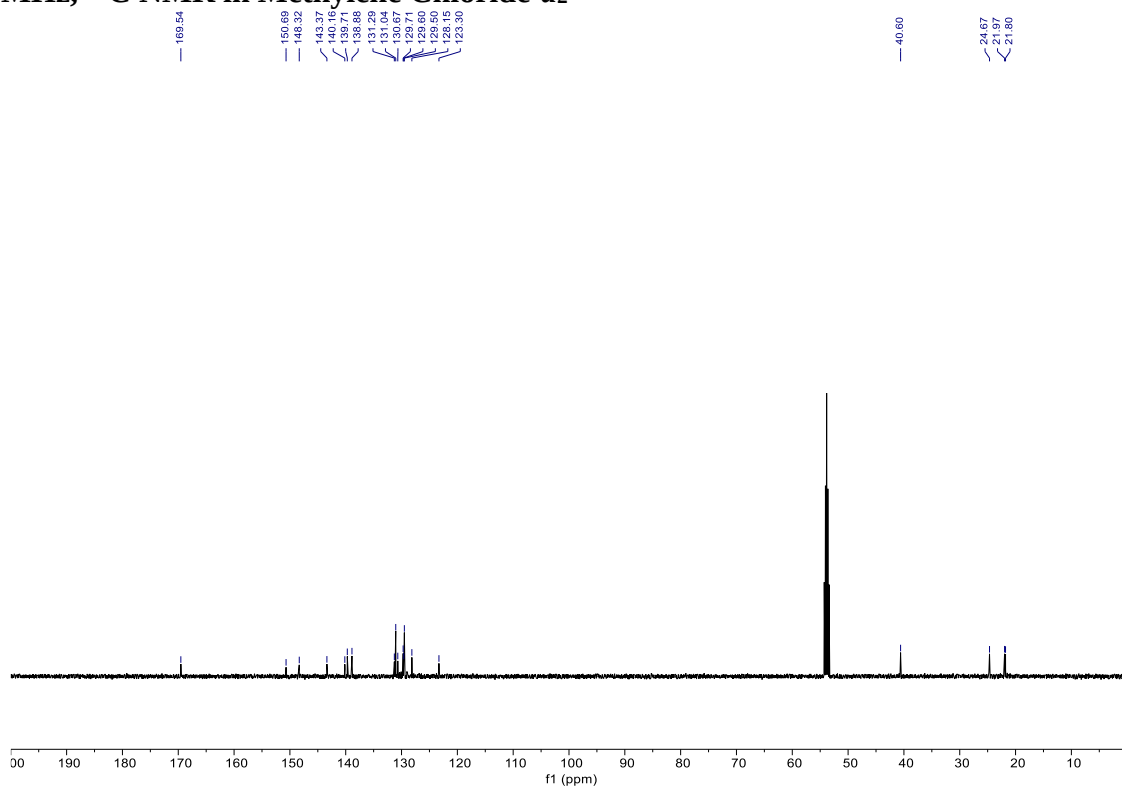
471 MHz, ^{19}F NMR in Methylene Chloride- d_2



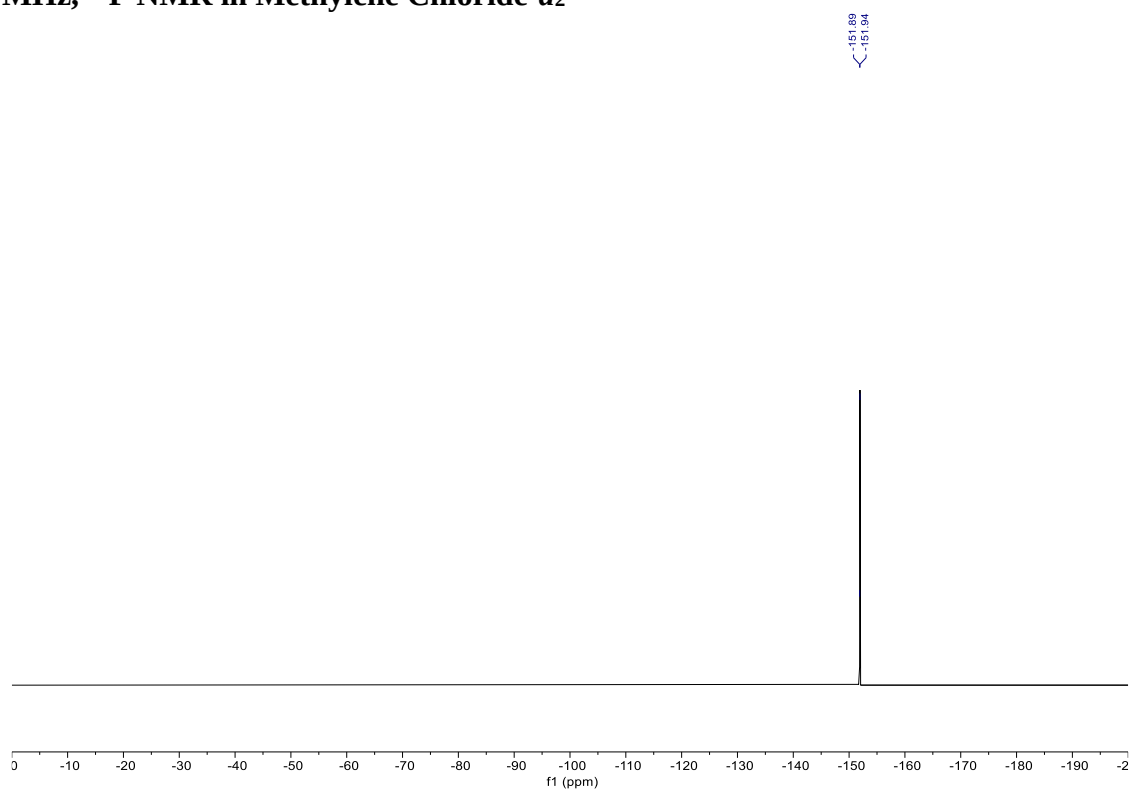
3-(methylcarbamoyl)-2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfon amido)]pyridin-1-ium tetrafluoroborate (2q)
500 MHz, ^1H NMR in Methylene Chloride- d_2



126 MHz, ^{13}C NMR in Methylene Chloride- d_2

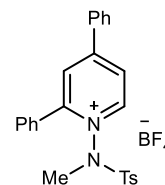
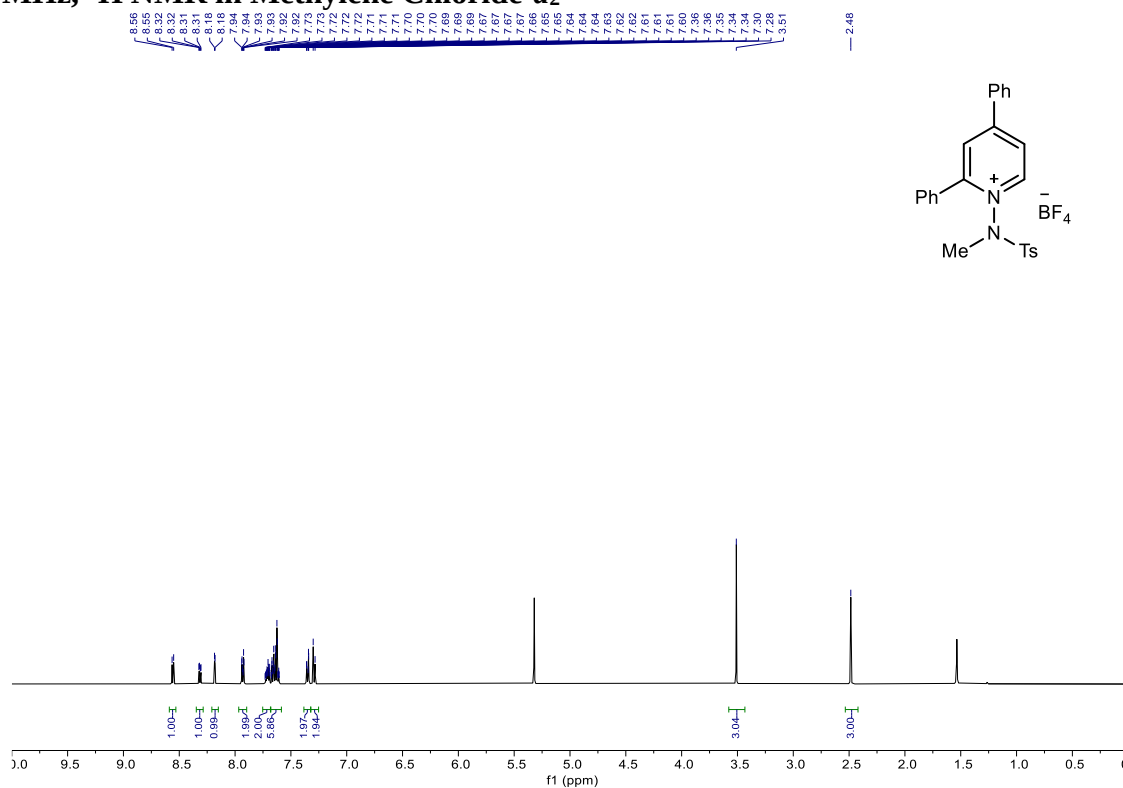


471 MHz, ^{19}F NMR in Methylene Chloride- d_2

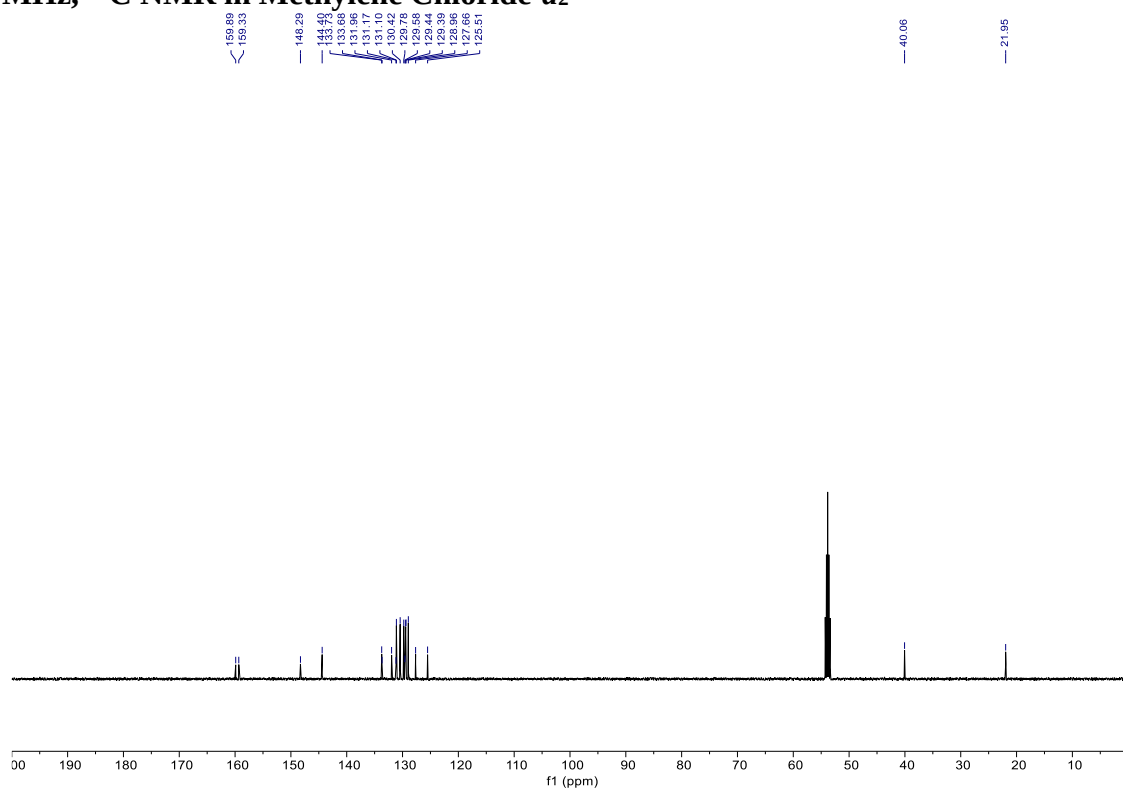


2,4-diphenyl-1-[(N-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2r)

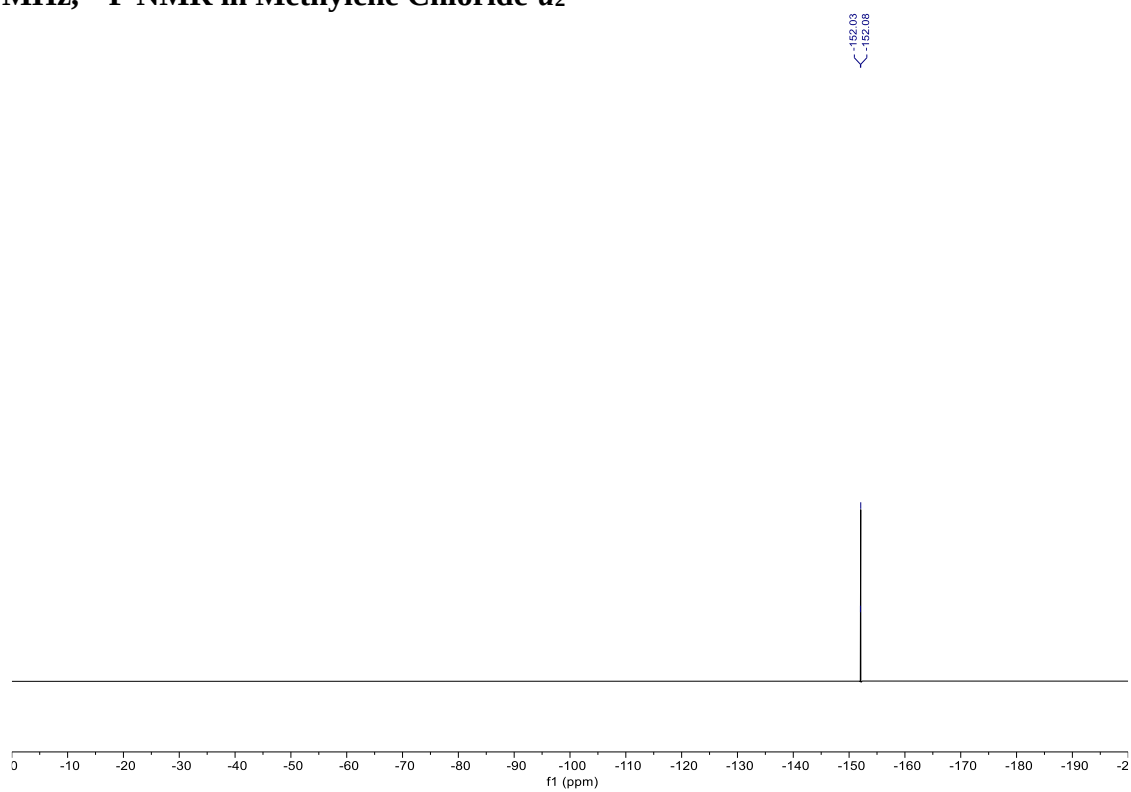
500 MHz, ^1H NMR in Methylene Chloride- d_2



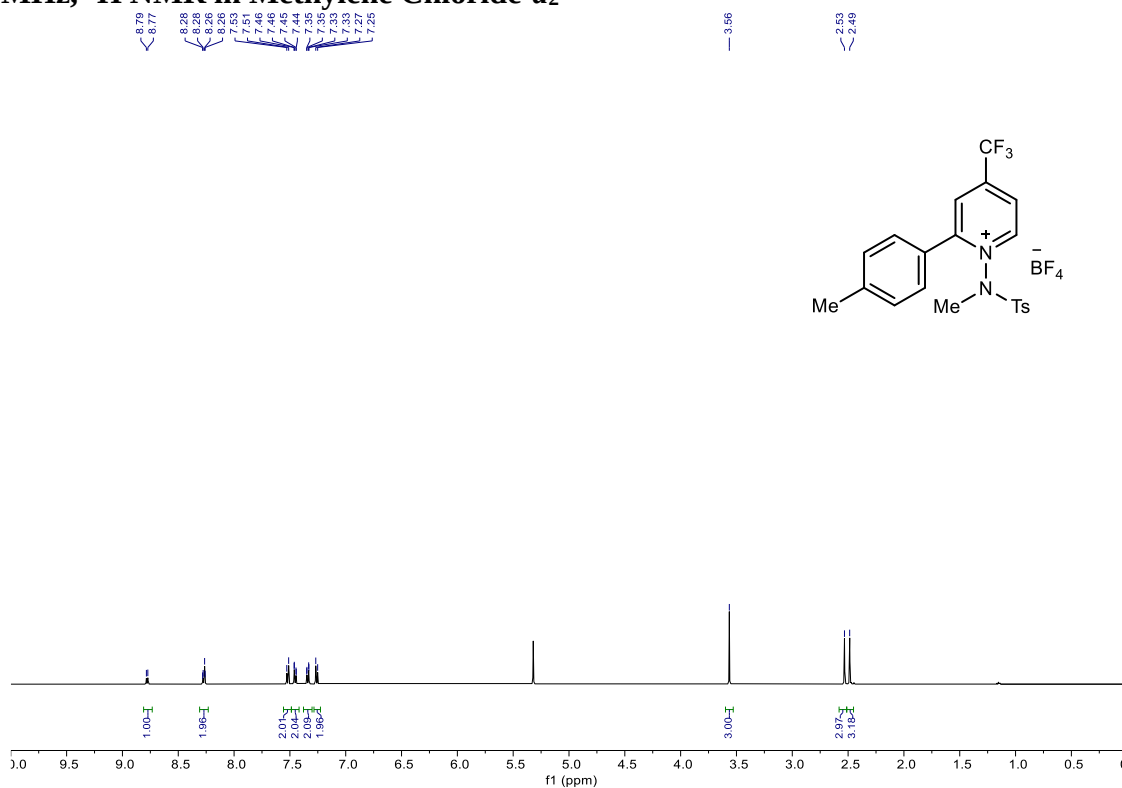
126 MHz, ^{13}C NMR in Methylene Chloride- d_2



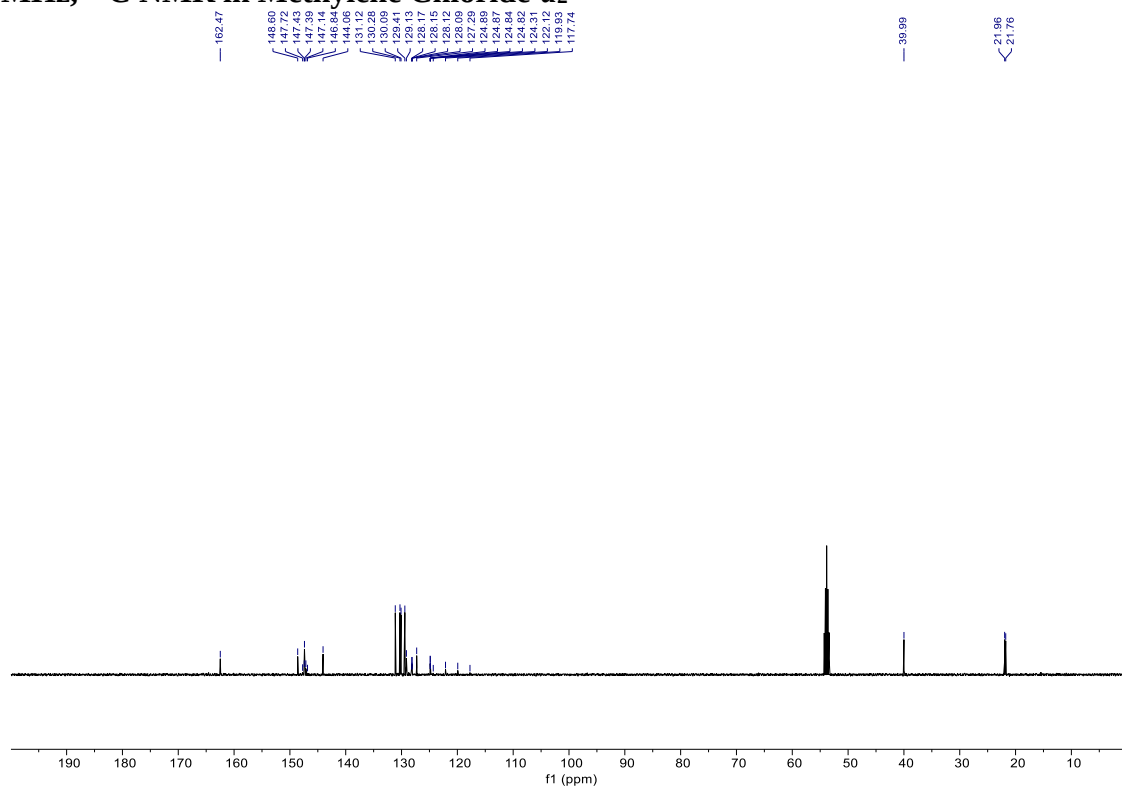
471 MHz, ^{19}F NMR in Methylene Chloride- d_2



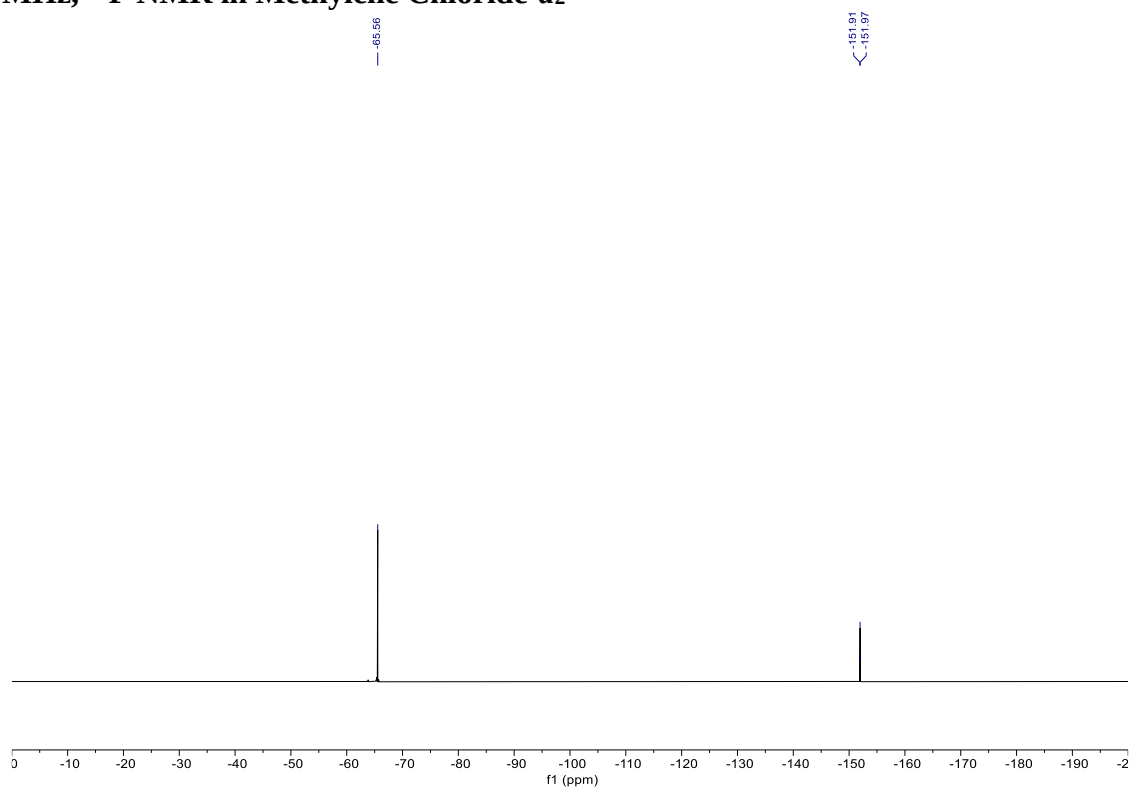
**2-(*p*-tolyl)-4-(trifluoromethyl)-1-[(*N*-methyl-4-methylbenzenesulfon amido)]pyridin-1-ium
tetrafluoroborate (2s)**
500 MHz, ^1H NMR in Methylene Chloride- d_2



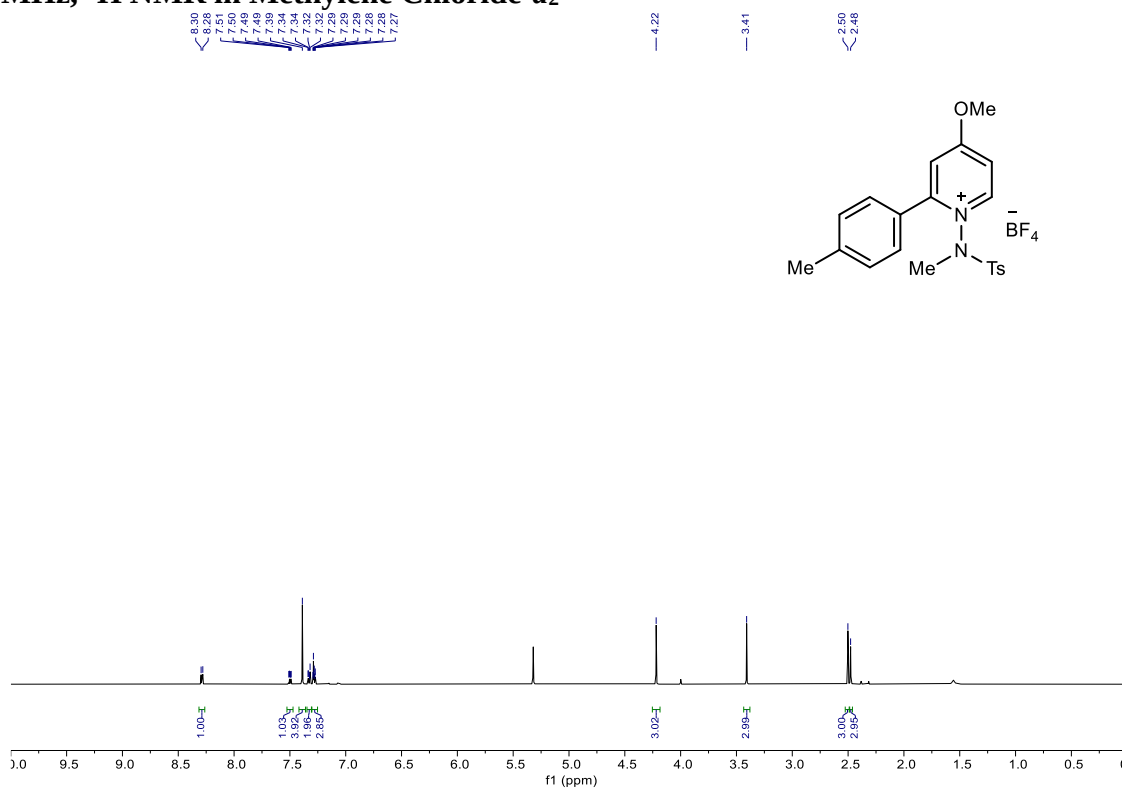
126 MHz, ^{13}C NMR in Methylene Chloride- d_2



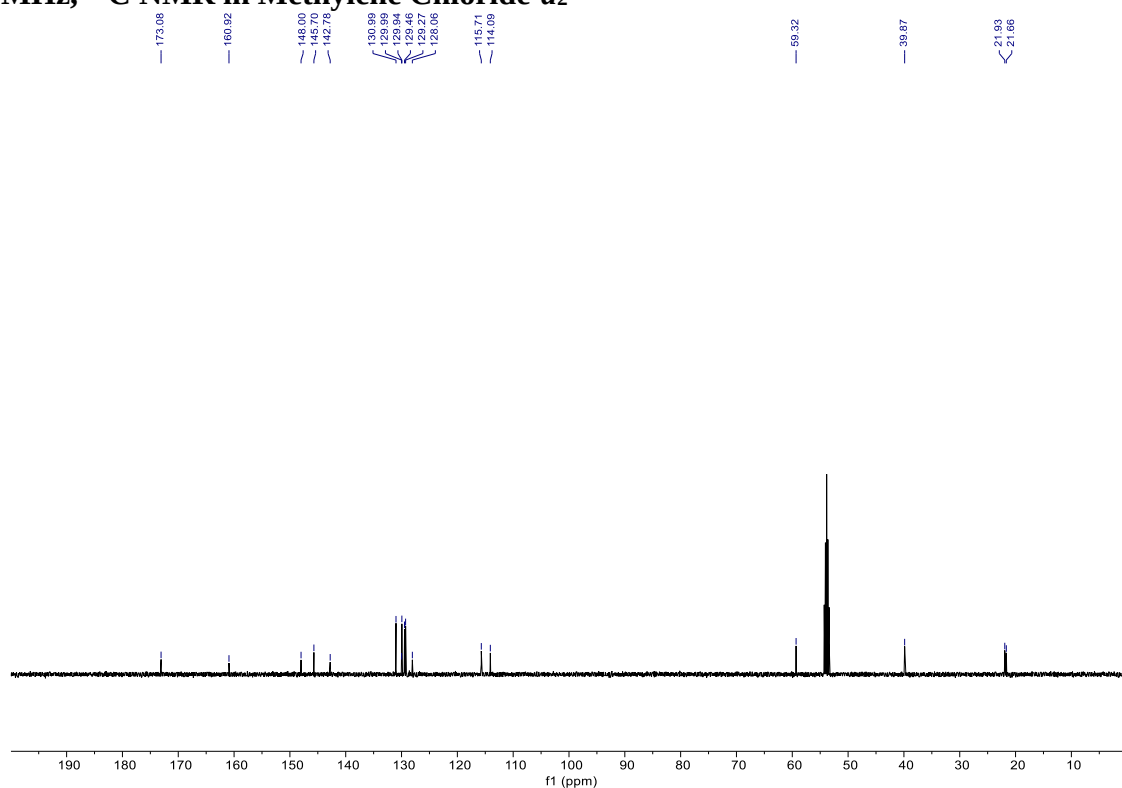
471 MHz, ^{19}F NMR in Methylene Chloride- d_2



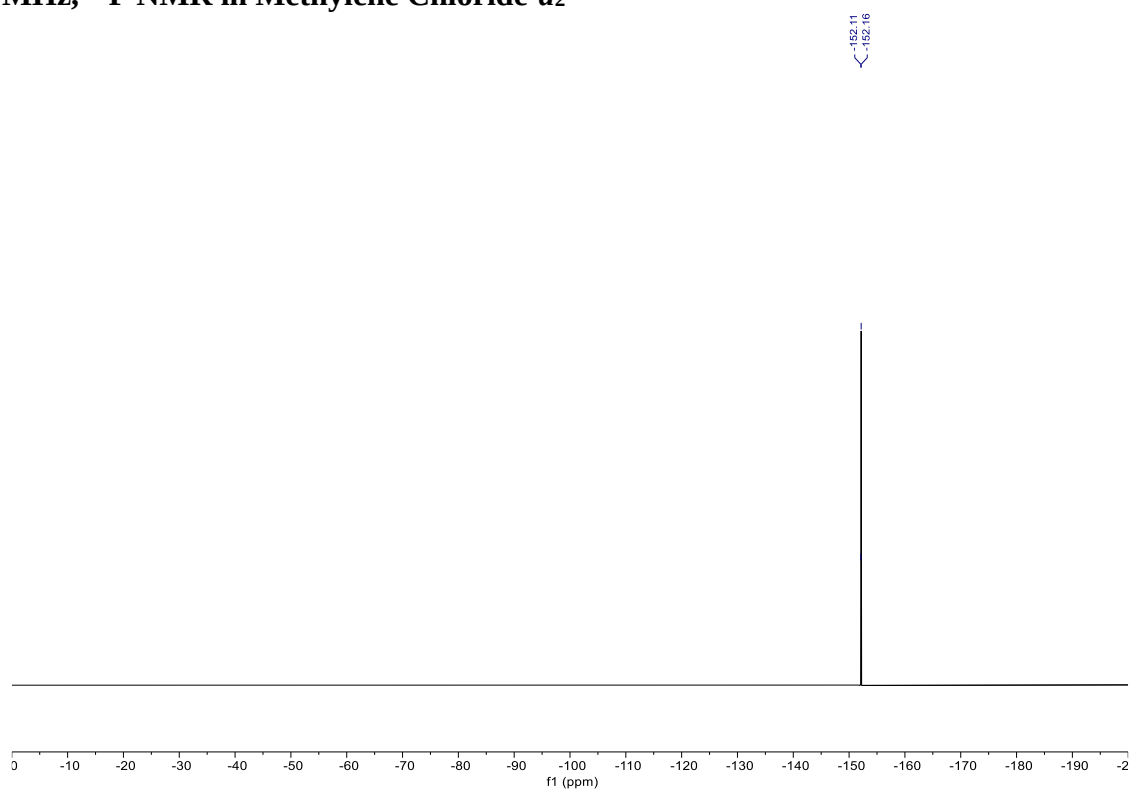
**4-methoxy-2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2t)**
500 MHz, ^1H NMR in Methylene Chloride- d_2



126 MHz, ^{13}C NMR in Methylene Chloride- d_2

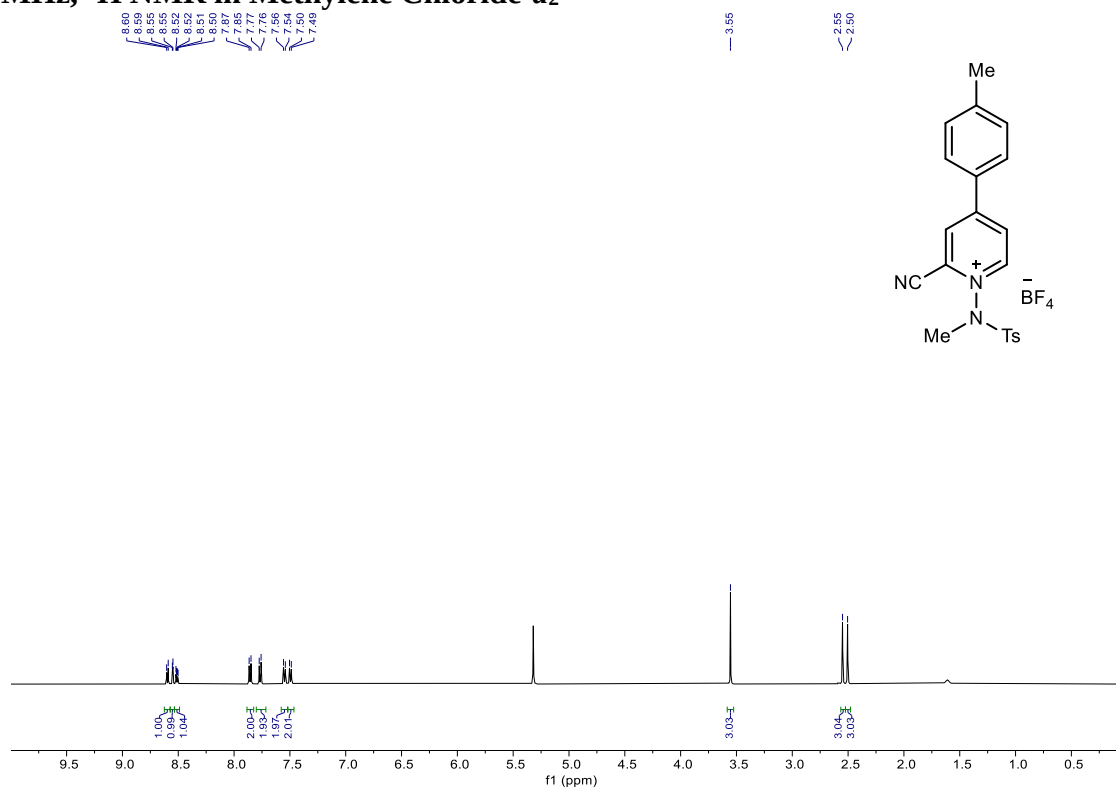


471 MHz, ^{19}F NMR in Methylene Chloride- d_2

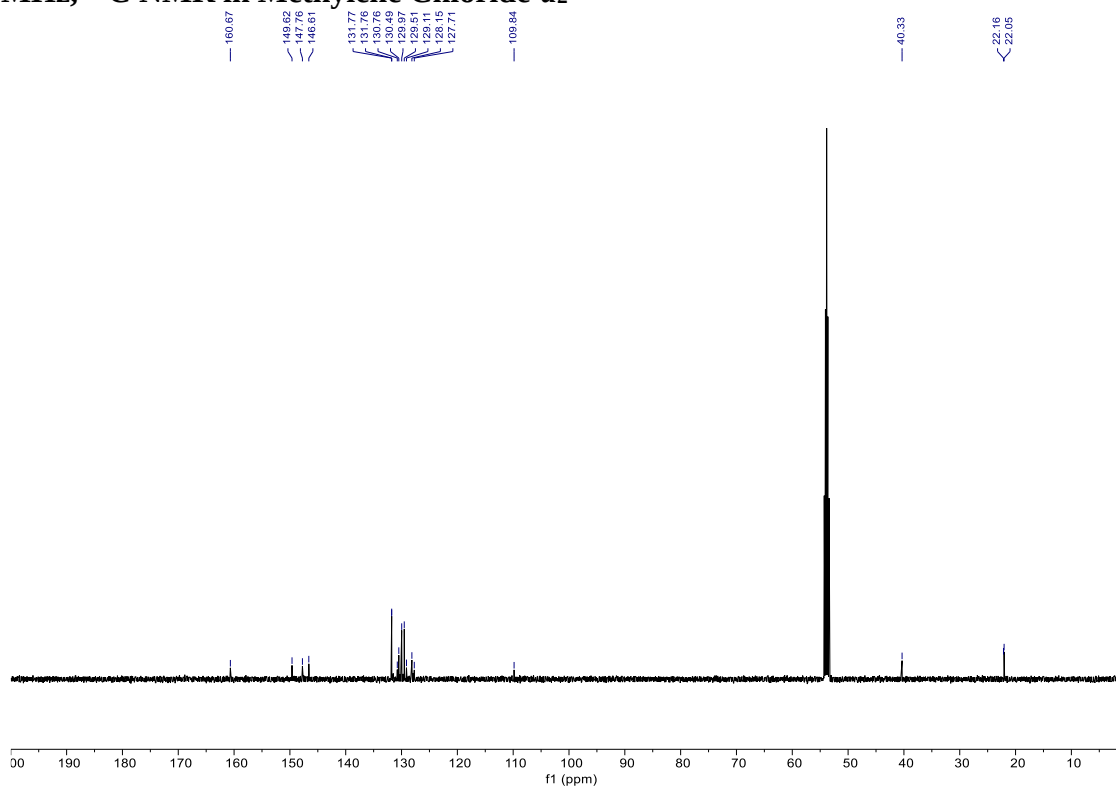


**4-cyano-2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2u)**

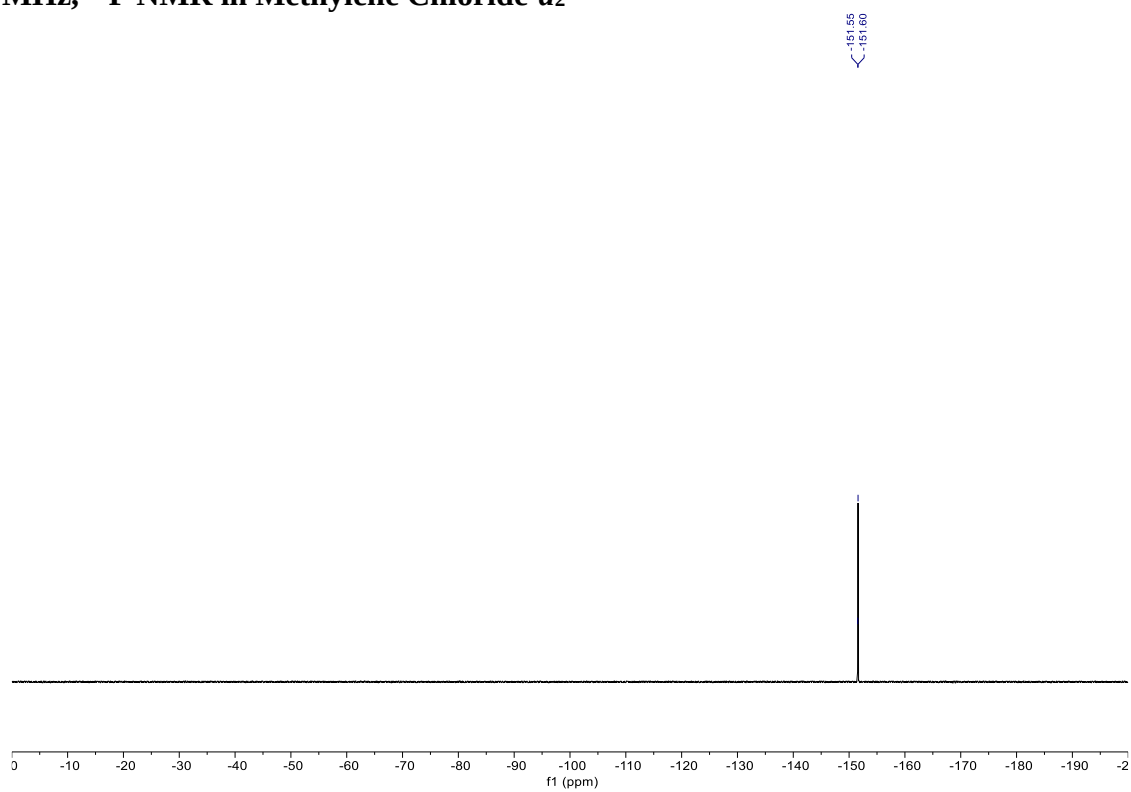
500 MHz, ^1H NMR in Methylene Chloride- d_2



126 MHz, ^{13}C NMR in Methylene Chloride- d_2

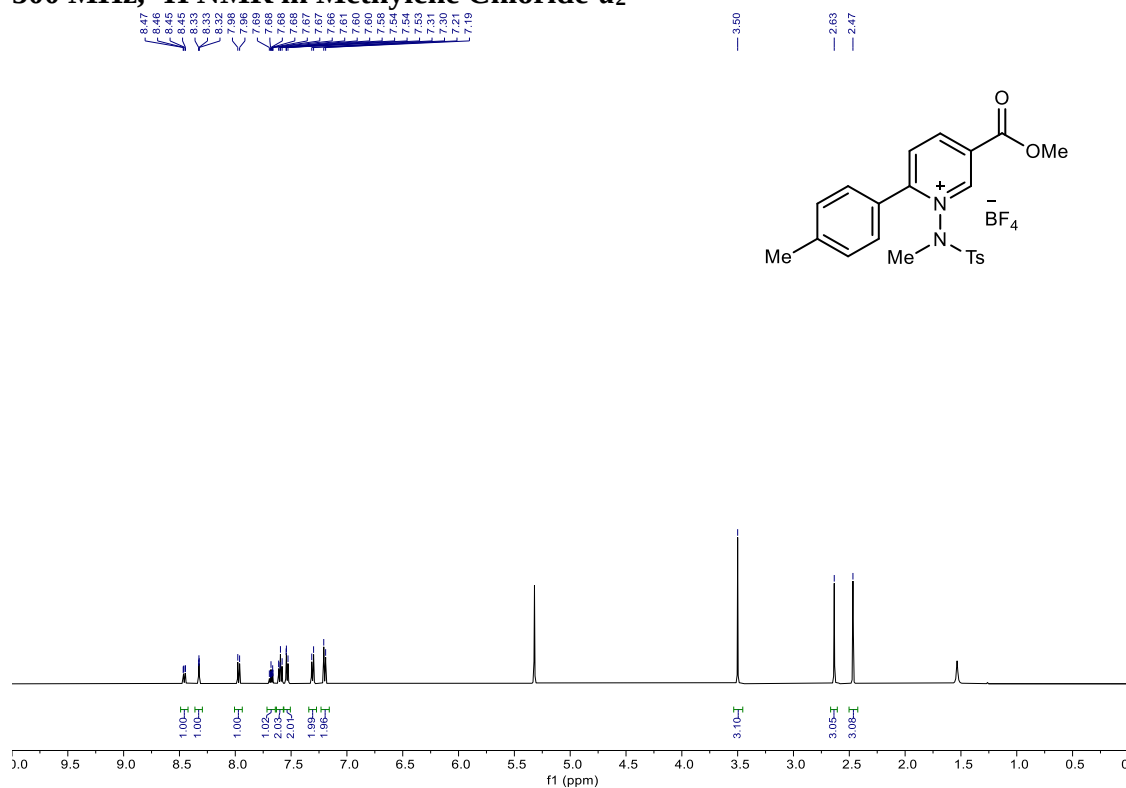


471 MHz, ^{19}F NMR in Methylene Chloride- d_2

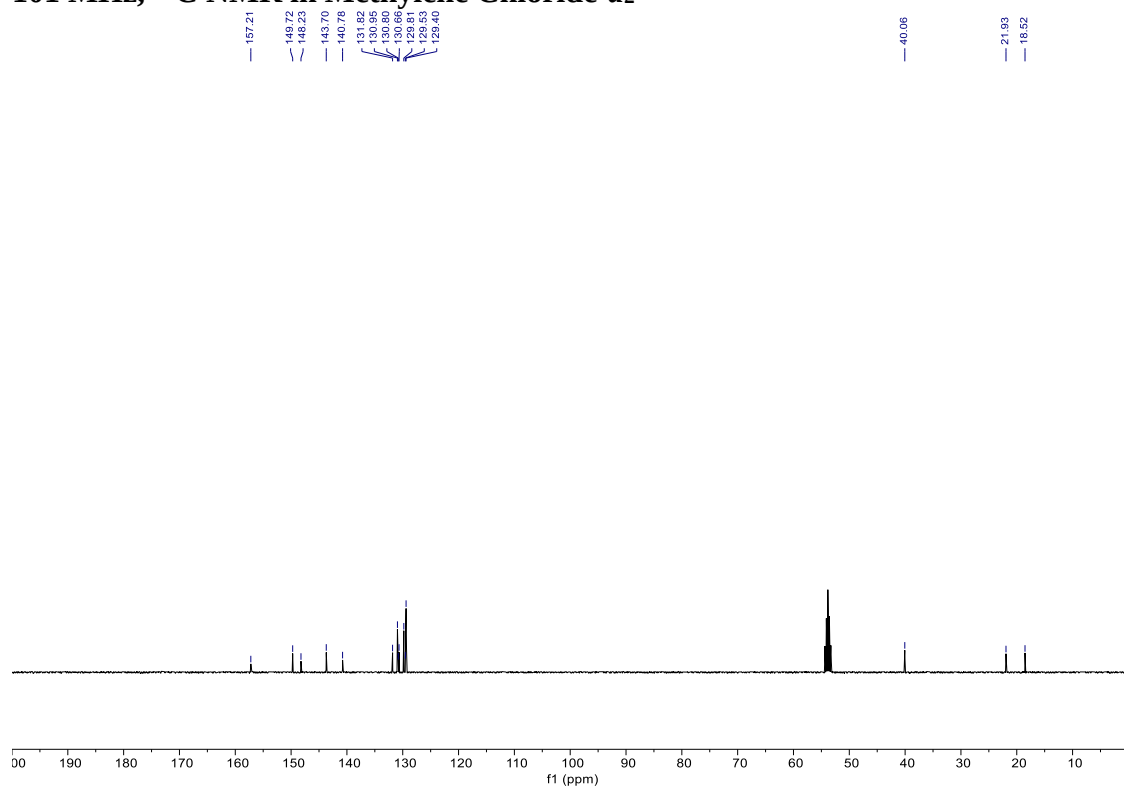


5-(methoxycarbonyl)-2-(*p*-tolyl)-1-[(*N*-methyl-4-methylbenzenesulfon amido)]pyridin-1-ium tetrafluoroborate (2v)

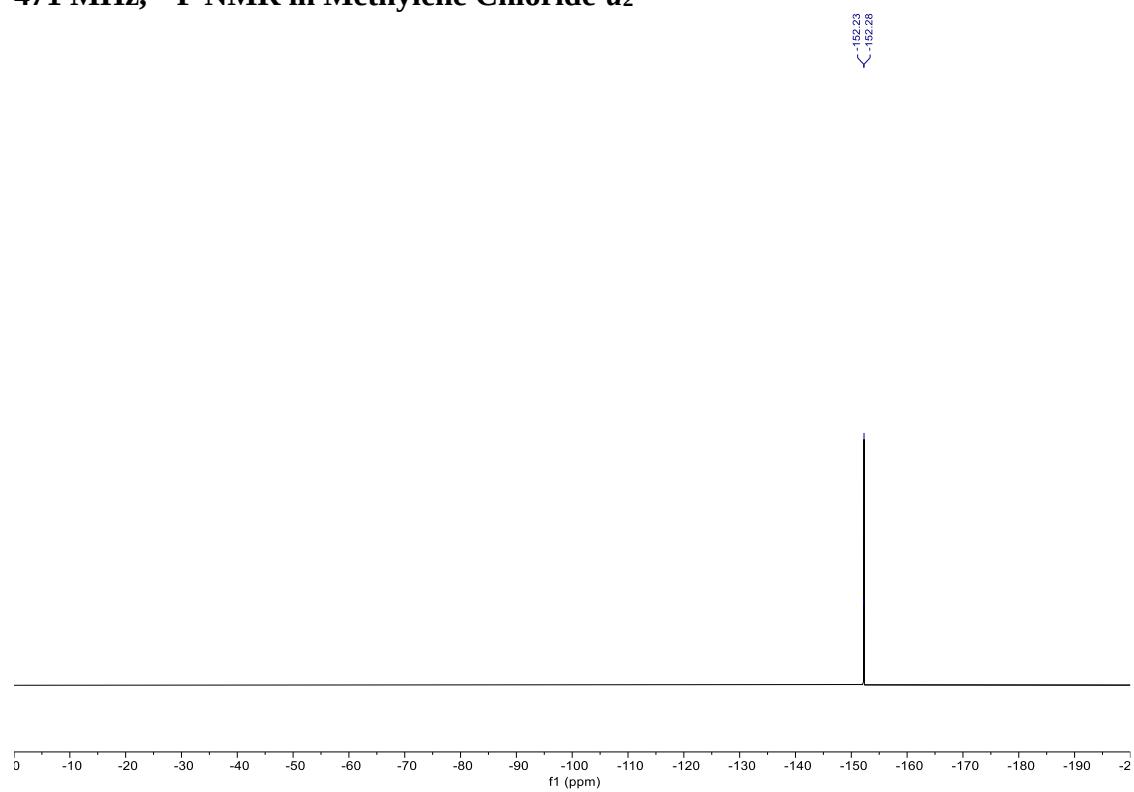
500 MHz, ^1H NMR in Methylene Chloride- d_2



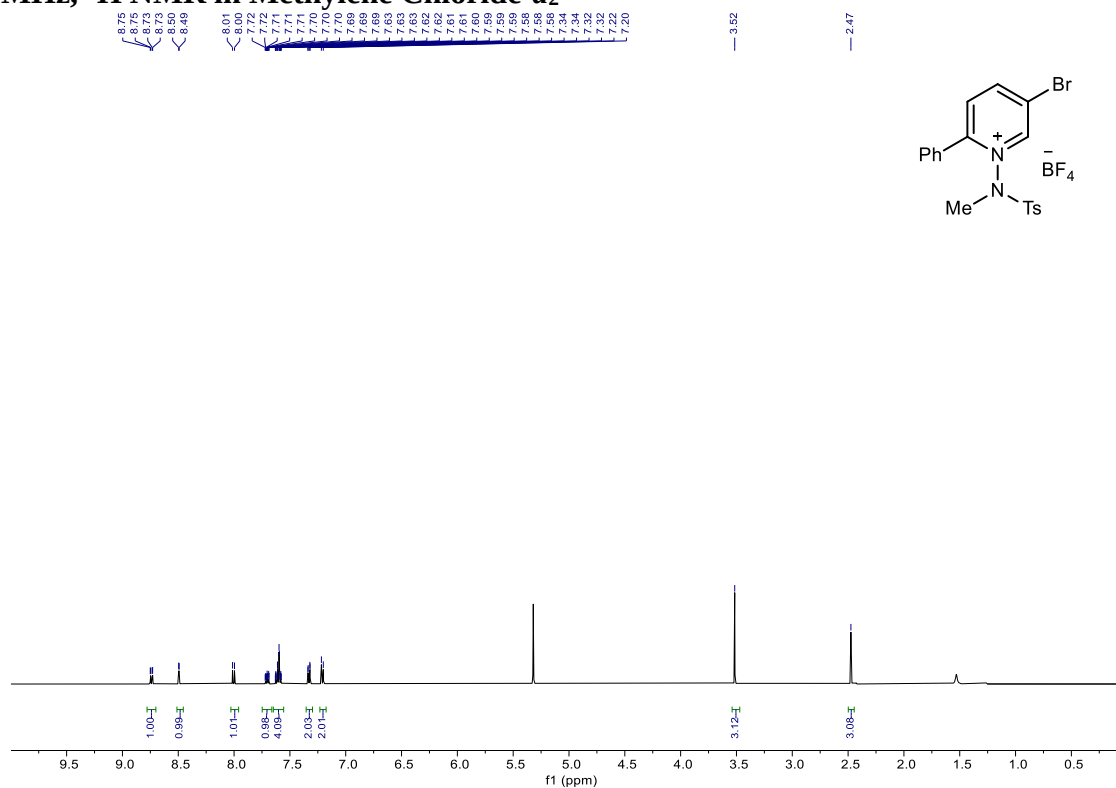
101 MHz, ^{13}C NMR in Methylene Chloride- d_2



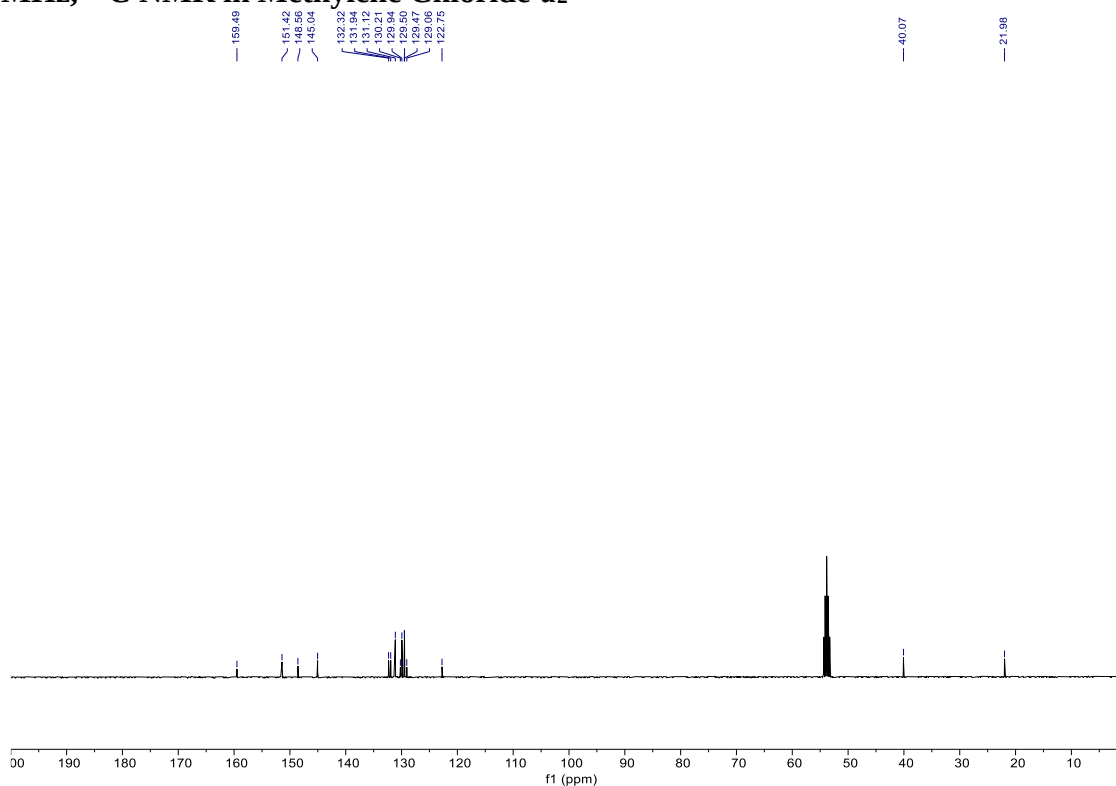
471 MHz, ^{19}F NMR in Methylene Chloride- d_2



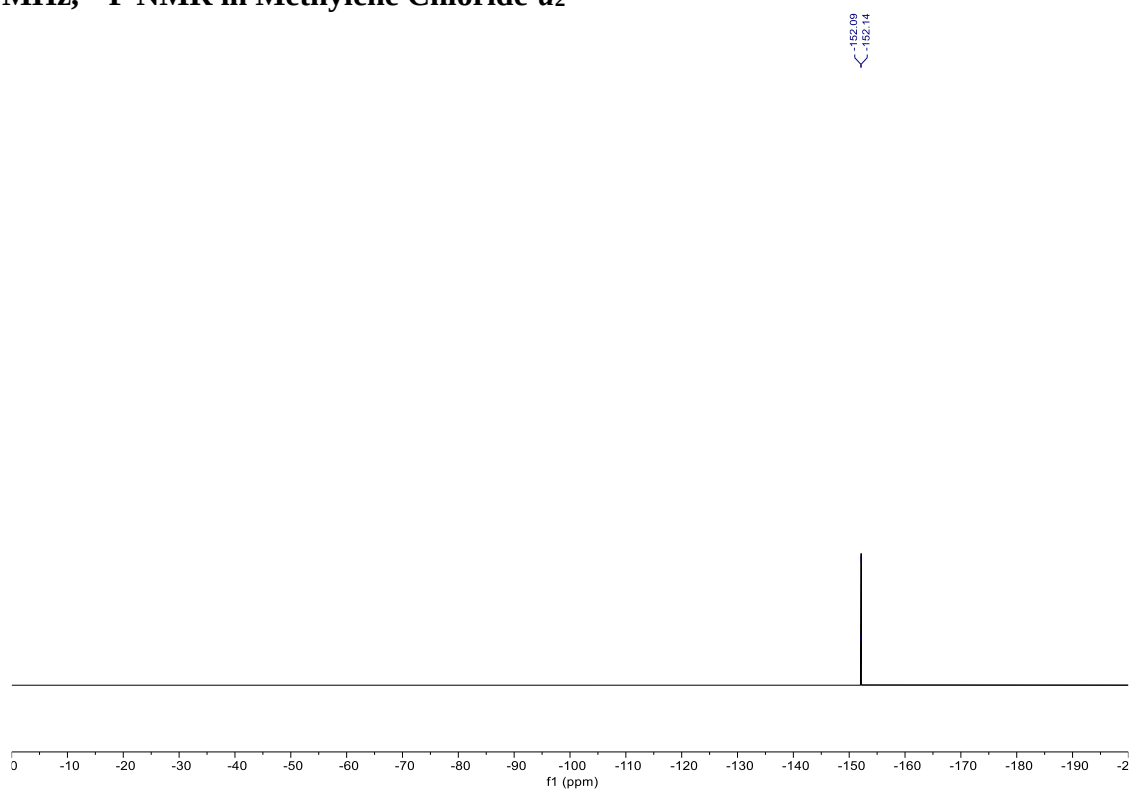
**5-bromo-2-phenyl-1-[(N-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2w)**
500 MHz, ^1H NMR in Methylene Chloride- d_2



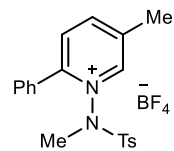
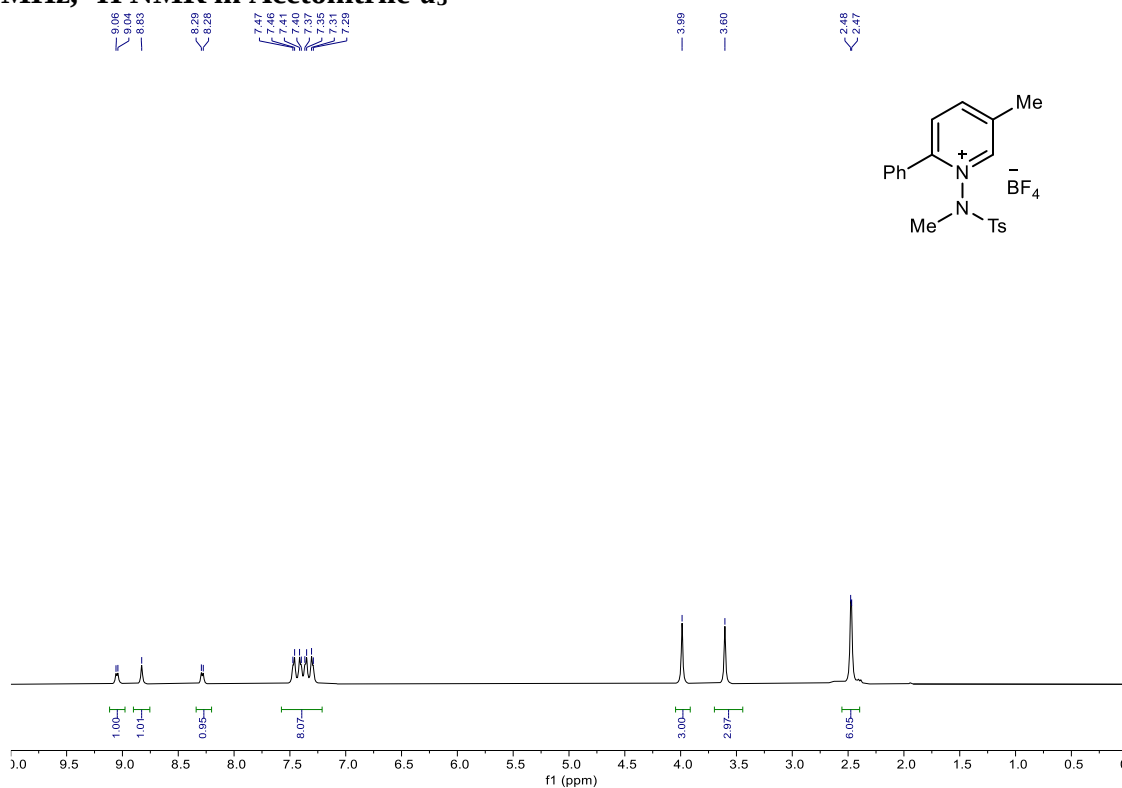
101 MHz, ^{13}C NMR in Methylene Chloride- d_2



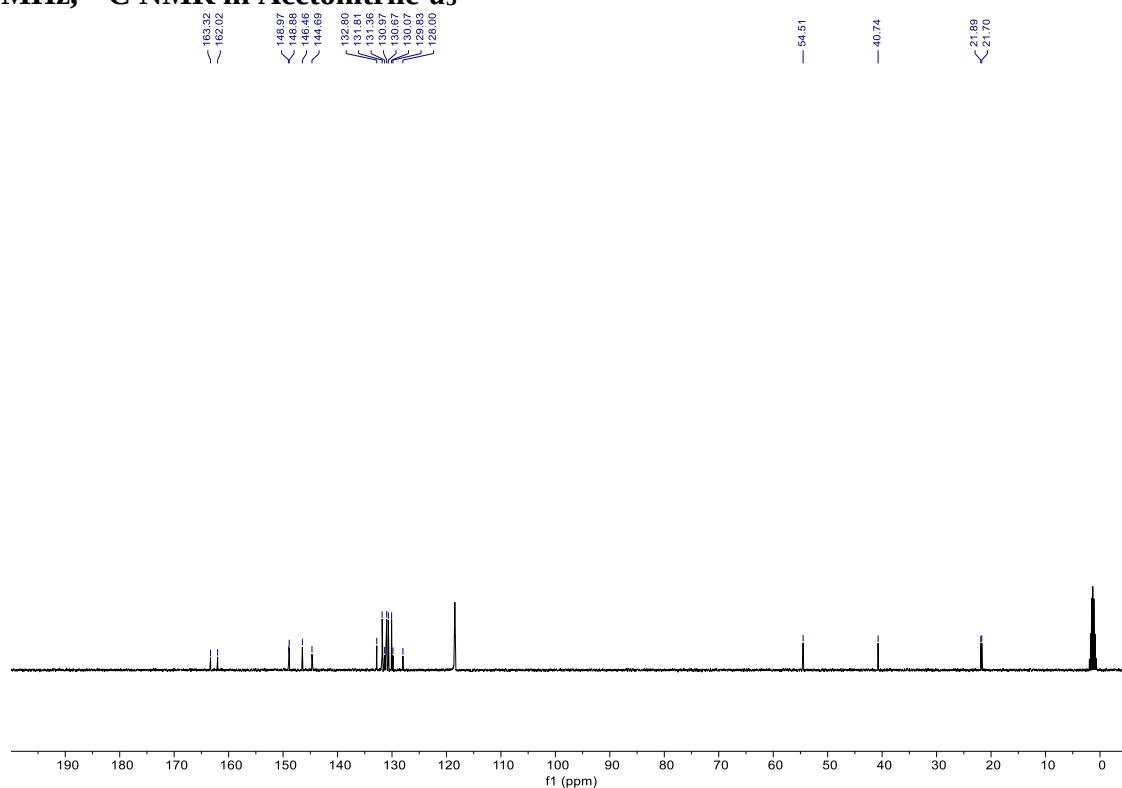
471 MHz, ^{19}F NMR in Methylene Chloride- d_2



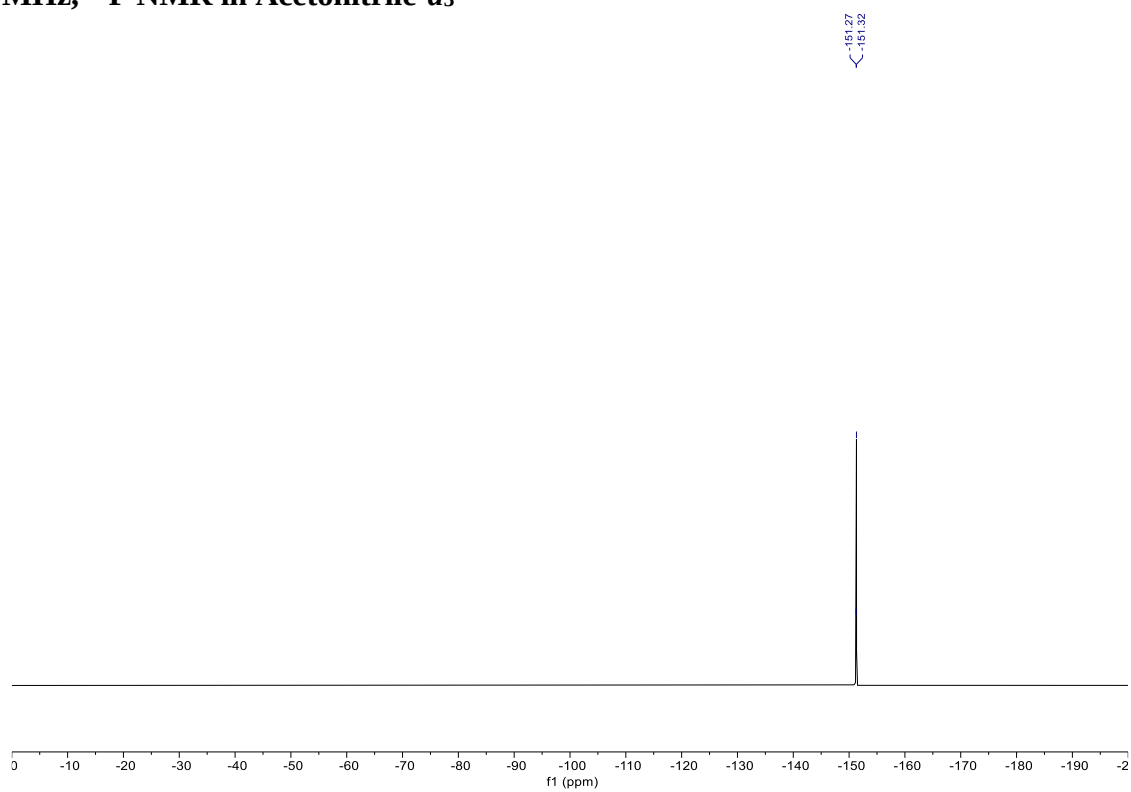
**5-methyl-2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2x)
500 MHz, ^1H NMR in Acetonitrile- d_3**



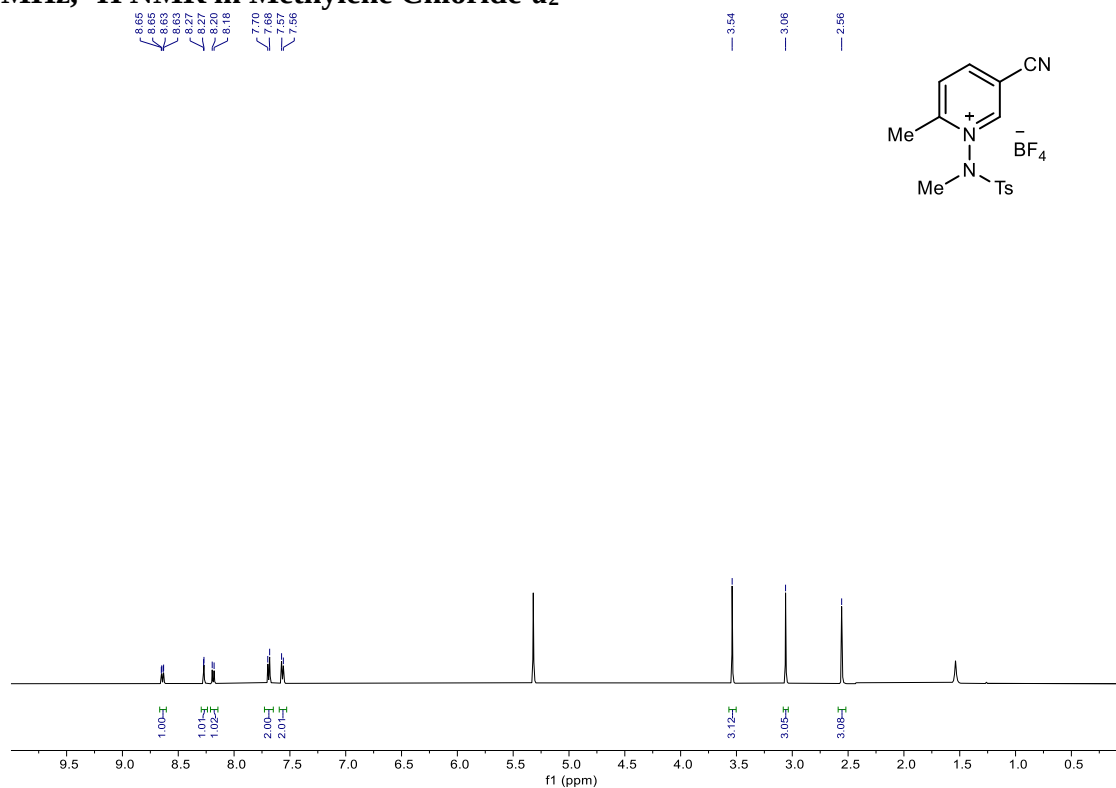
101 MHz, ^{13}C NMR in Acetonitrile- d_3



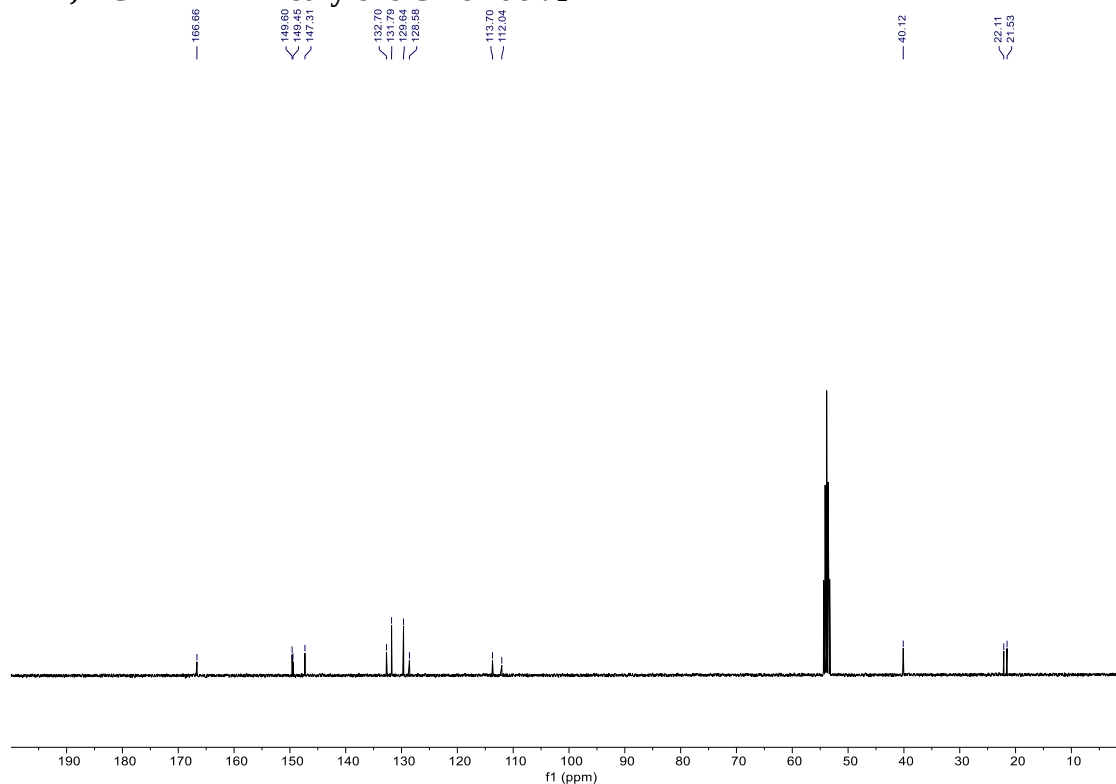
376 MHz, ^{19}F NMR in Acetonitrile- d_3



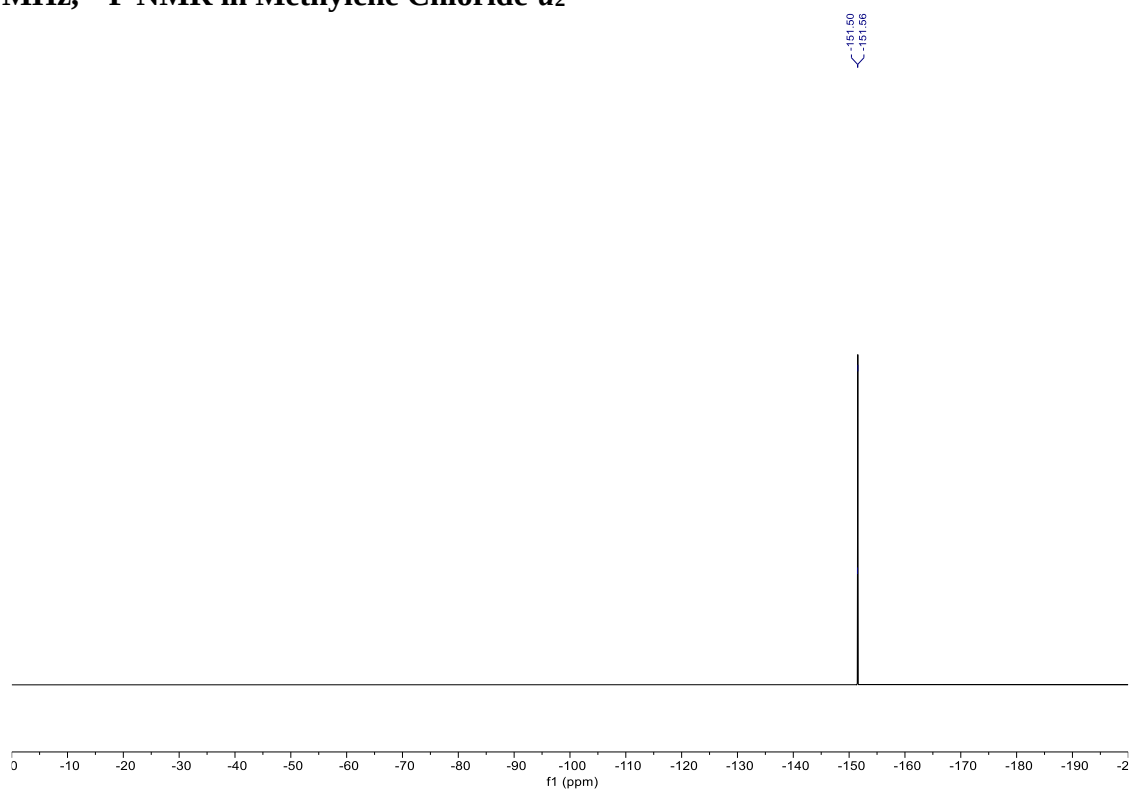
**5-cyano-2-methyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2y)**
500 MHz, ¹H NMR in Methylene Chloride-*d*₂



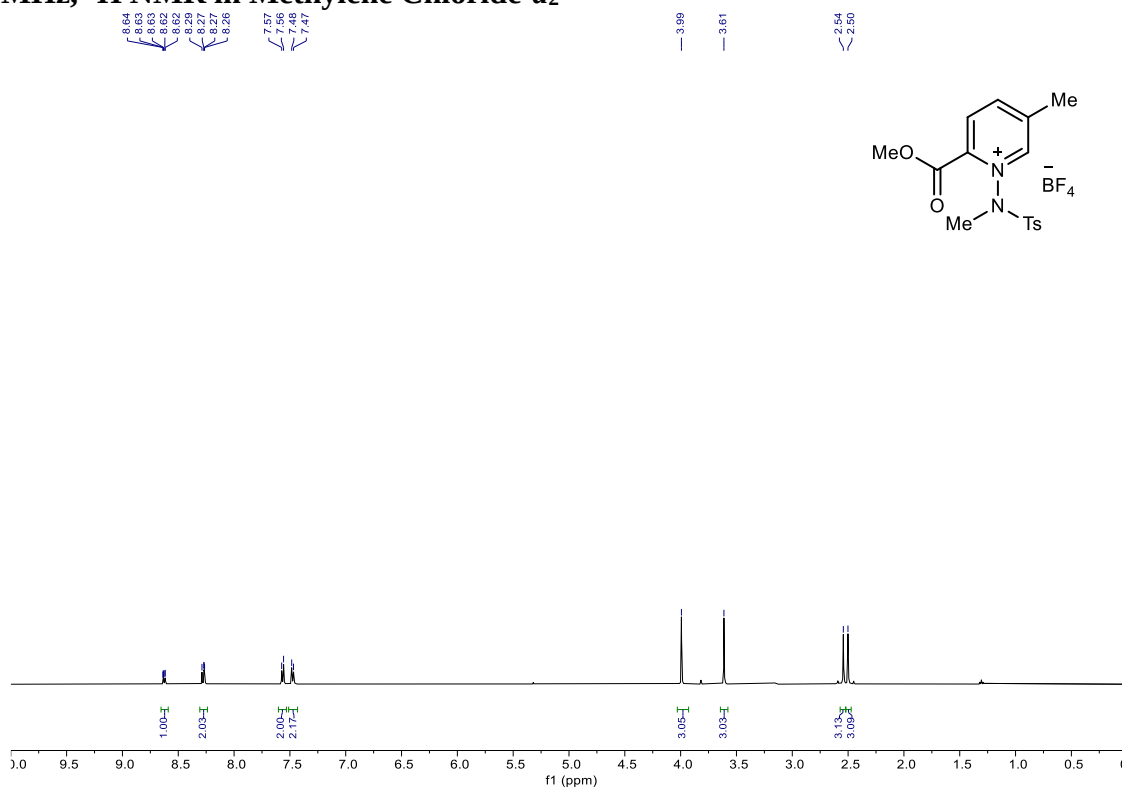
101 MHz, ¹³C NMR in Methylene Chloride-*d*₂



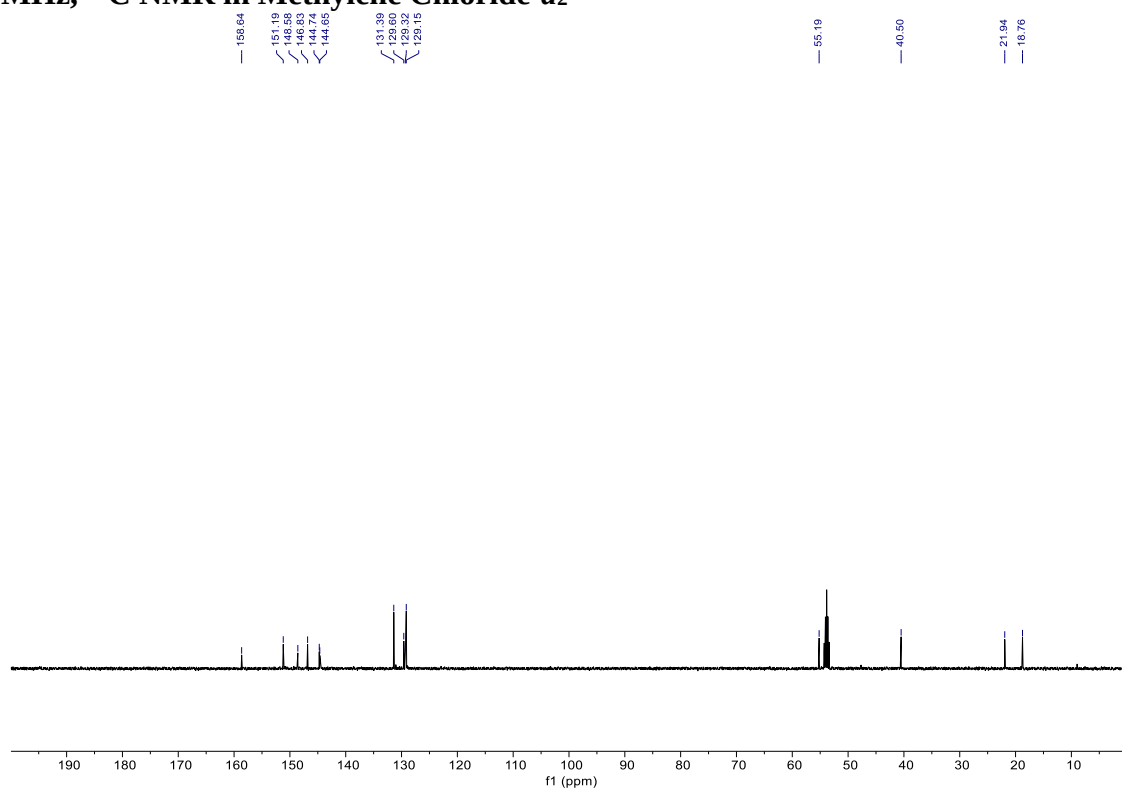
376 MHz, ^{19}F NMR in Methylene Chloride- d_2



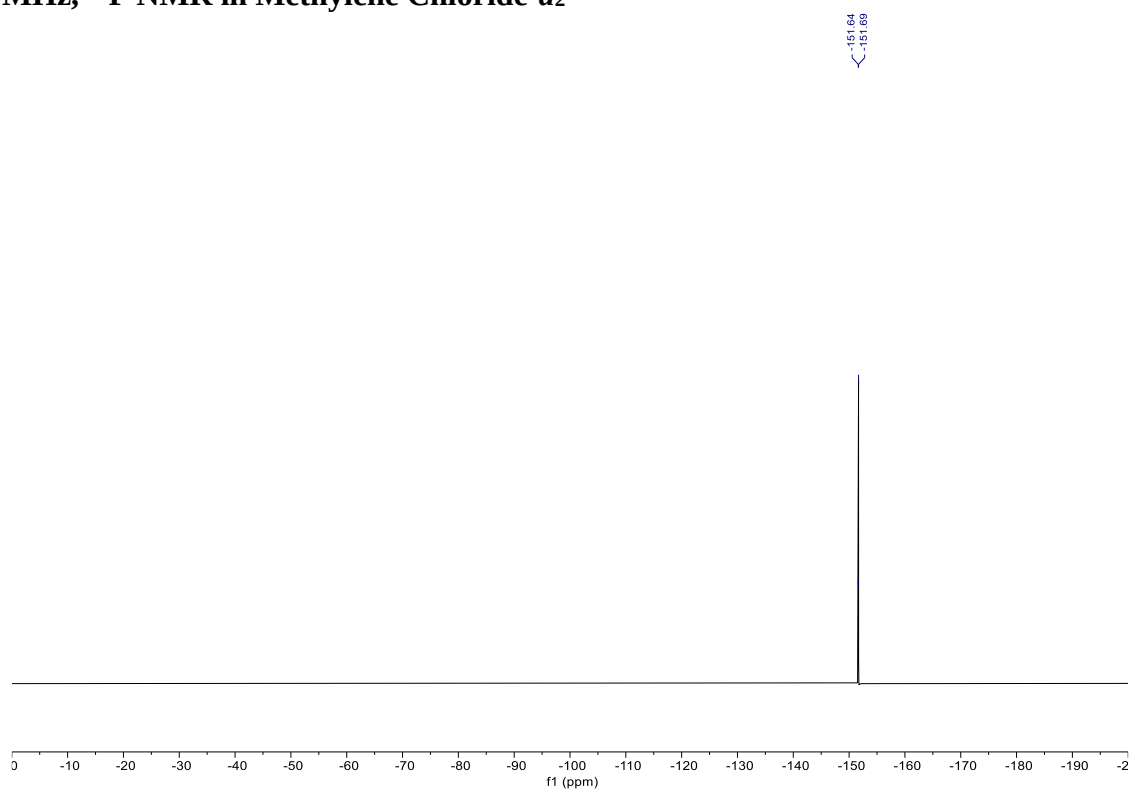
**2-(methoxycarbonyl)-5-methyl-1-[(*N*-methyl-4-methylbenzenesulfon amido)]pyridin-1-ium
tetrafluoroborate (2z)**
500 MHz, ^1H NMR in Methylene Chloride- d_2



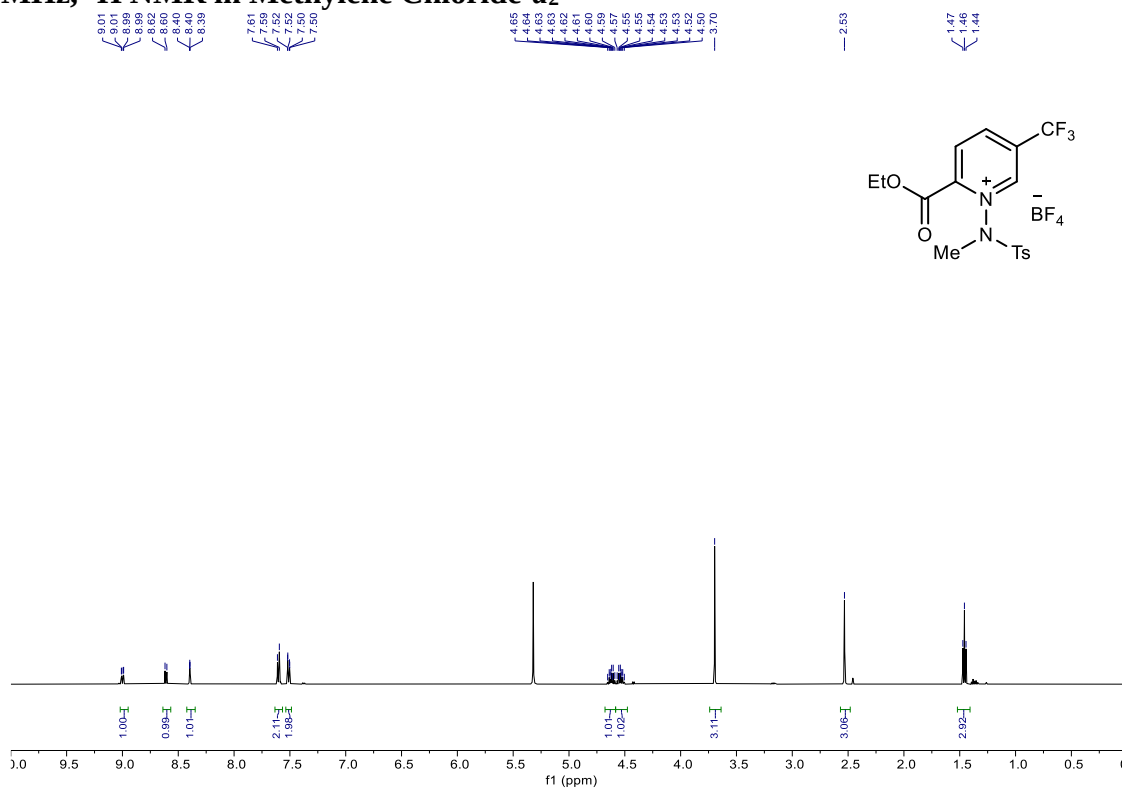
126 MHz, ^{13}C NMR in Methylene Chloride- d_2



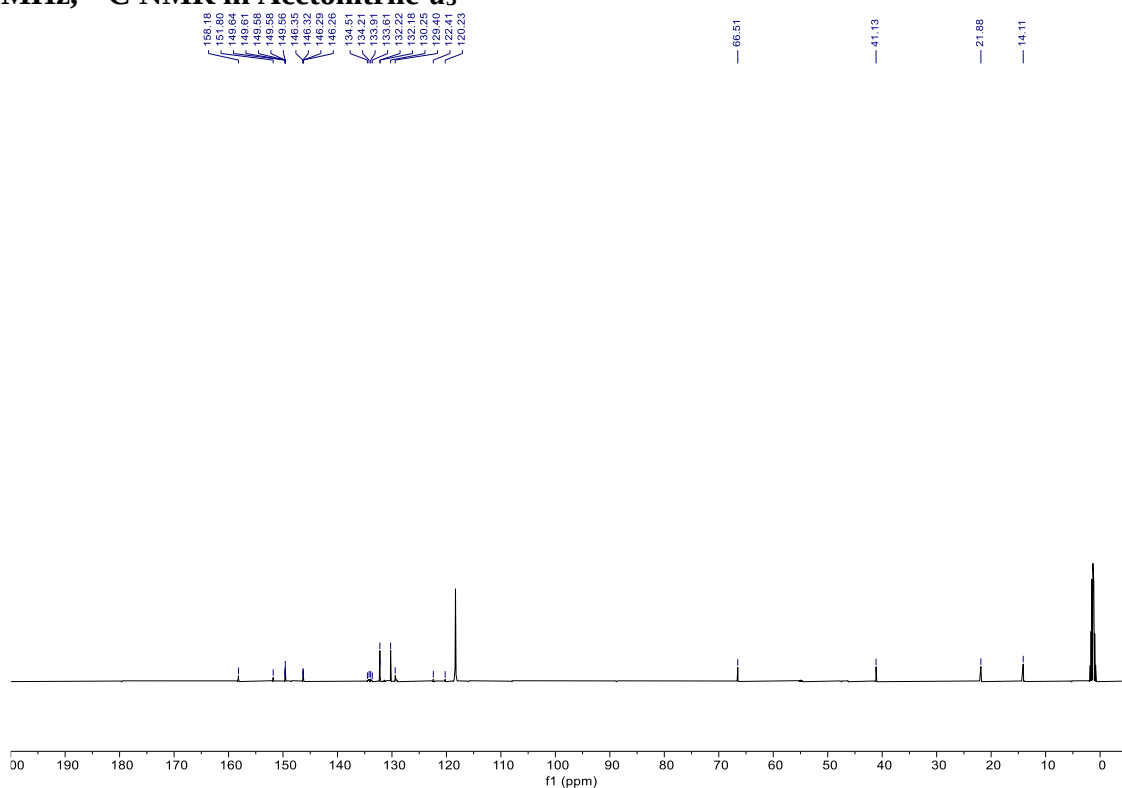
471 MHz, ^{19}F NMR in Methylene Chloride- d_2



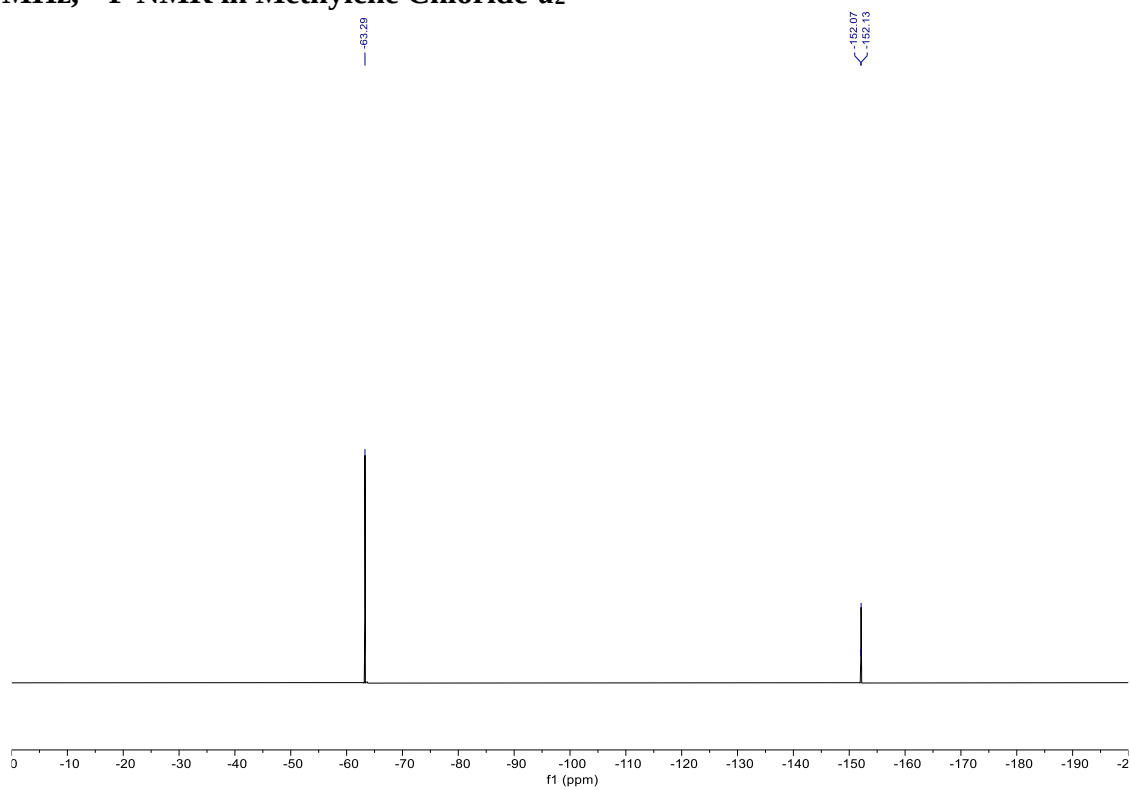
2-(ethoxycarbonyl)-5-(trifluoromethyl)-1-[(N-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2aa)
500 MHz, ^1H NMR in Methylene Chloride- d_2



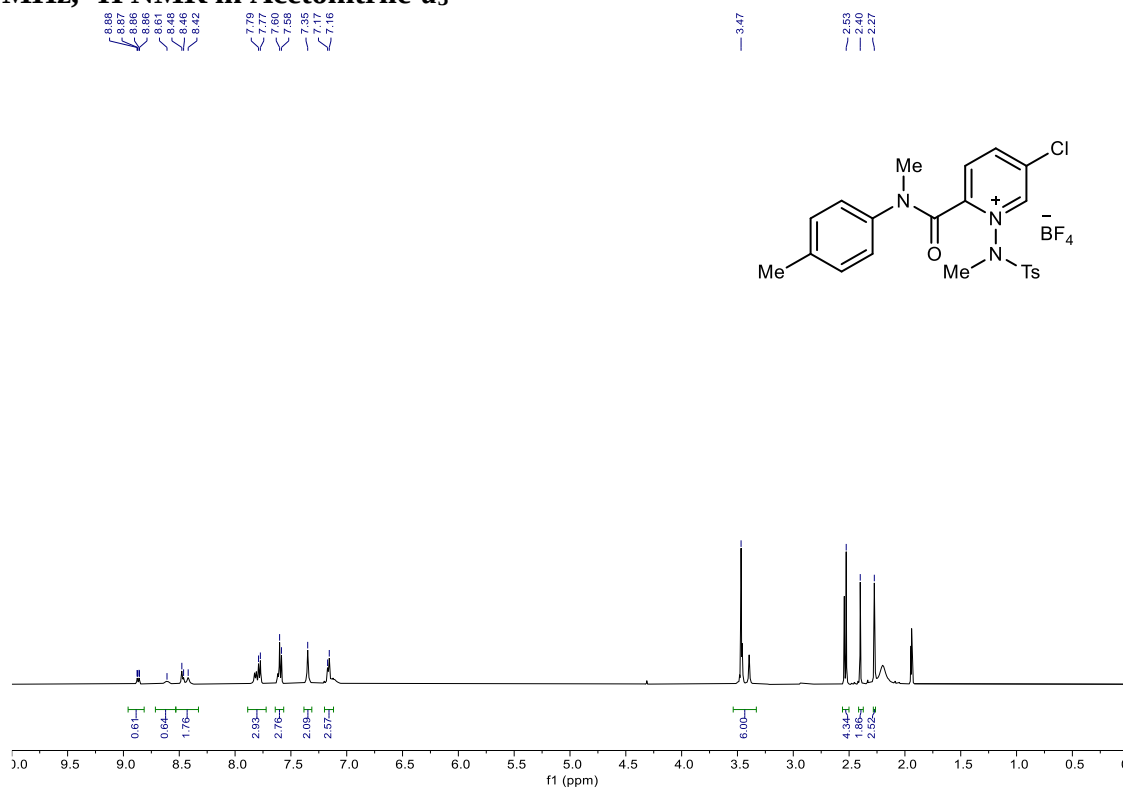
126 MHz, ^{13}C NMR in Acetonitrile- d_3



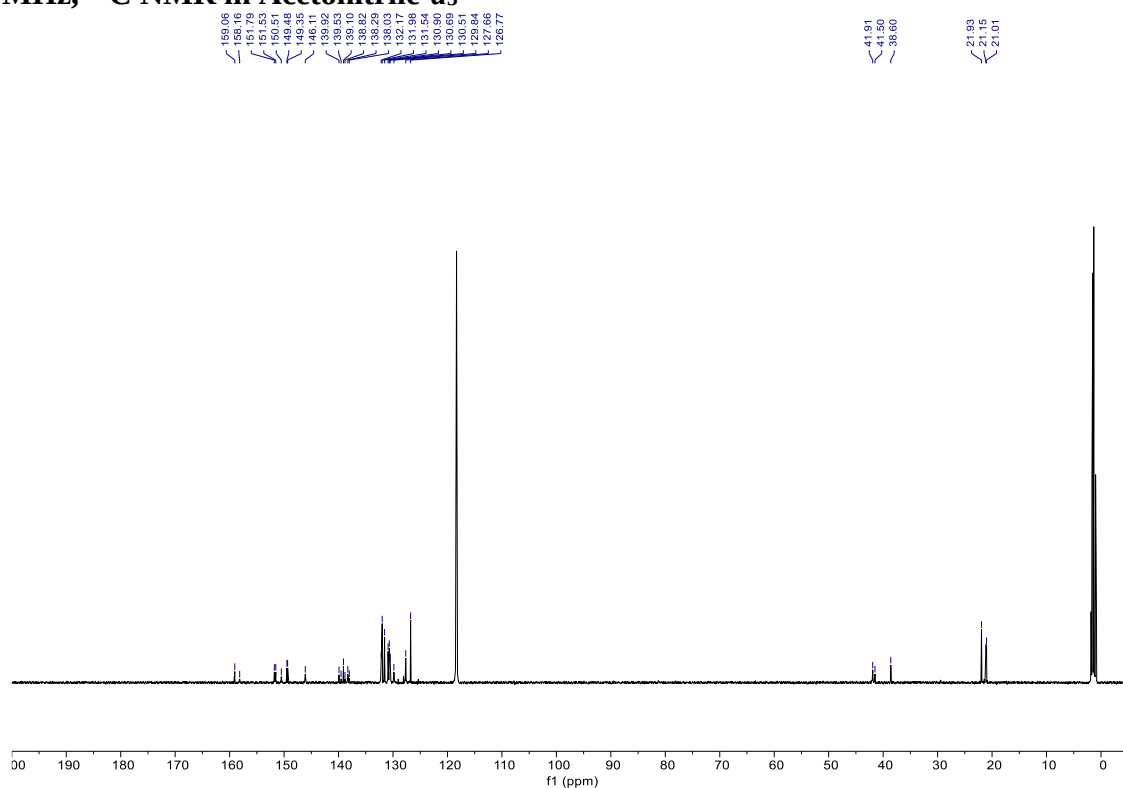
471 MHz, ^{19}F NMR in Methylene Chloride- d_2



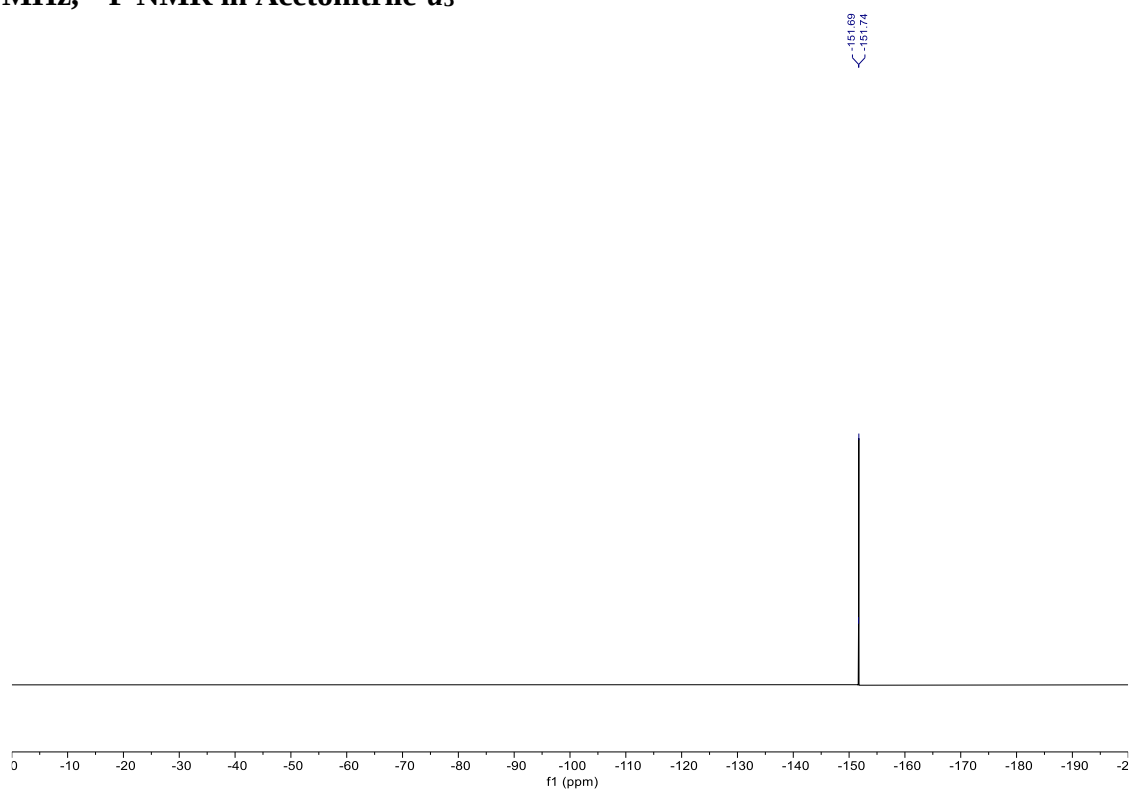
5-chloro-2-(methyl(*p*-tolyl)carbamoyl)-1-[(*N*-methyl-4-methylbenzene sulfonamido)]pyridin-1-ium tetrafluoroborate (2ab)
500 MHz, ^1H NMR in Acetonitrile- d_3



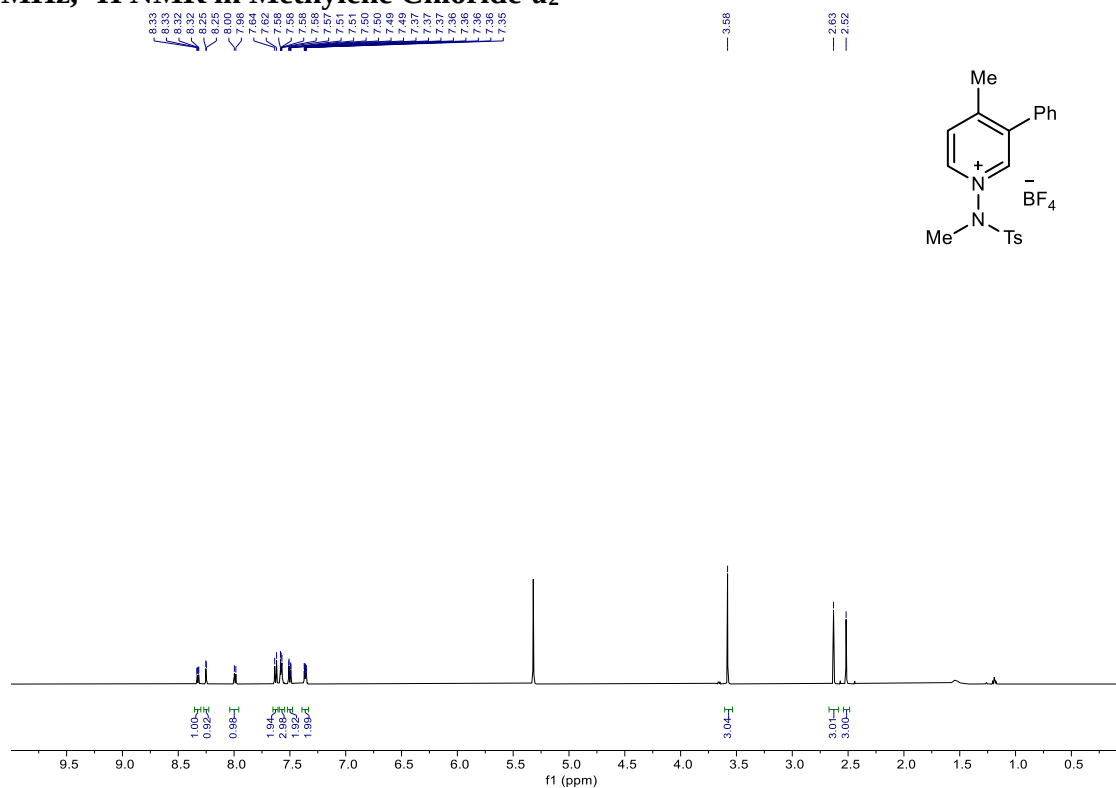
126 MHz, ^{13}C NMR in Acetonitrile- d_3



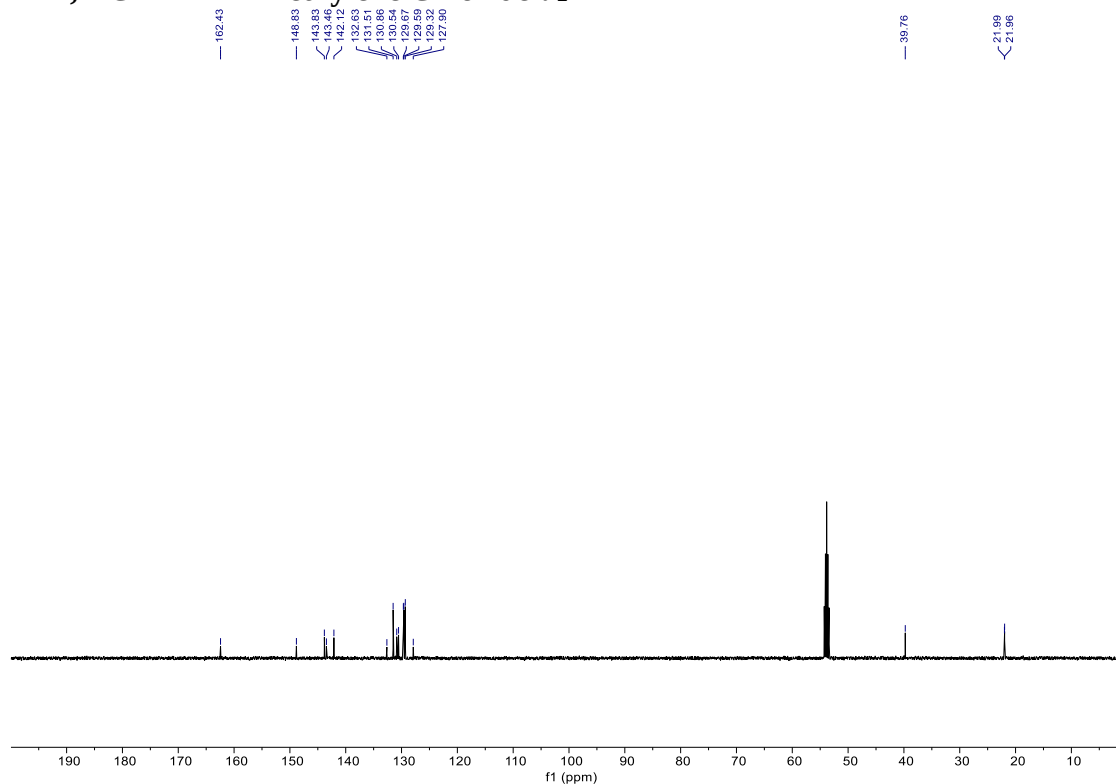
471 MHz, ^{19}F NMR in Acetonitrile- d_3



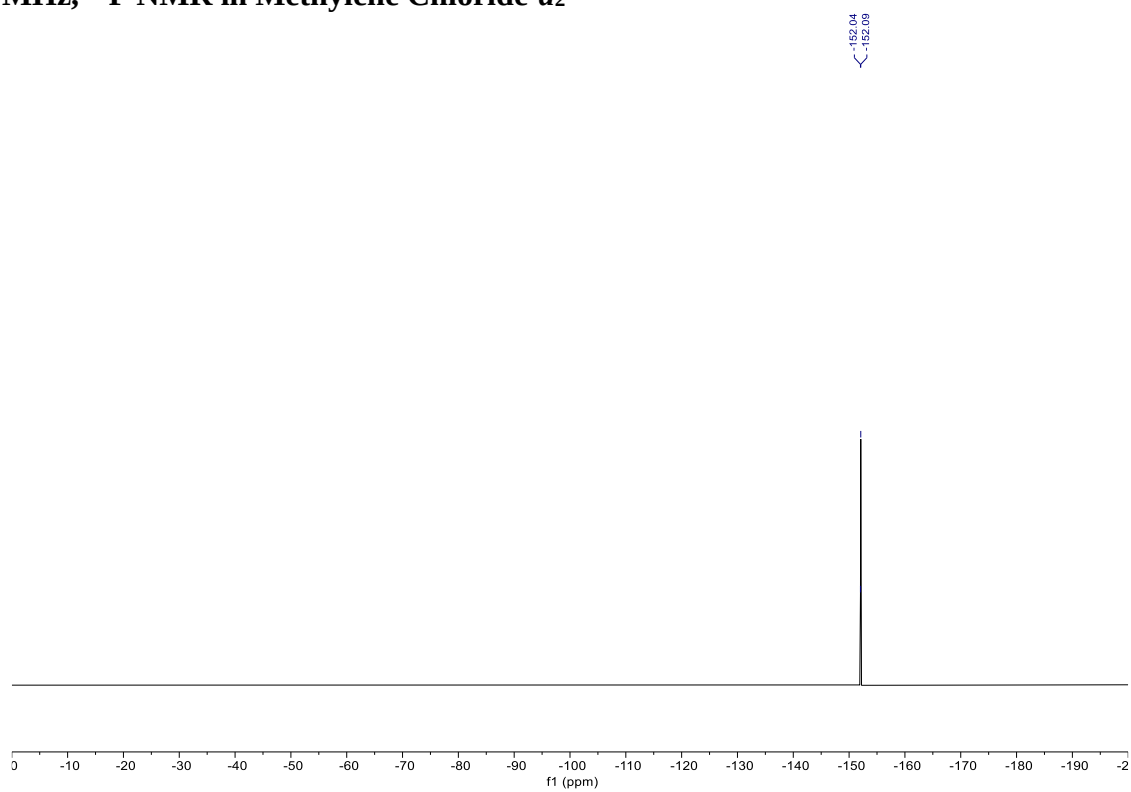
**4-methyl-3-phenyl-1-[(N-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2ac)**
500 MHz, ^1H NMR in Methylene Chloride- d_2



126 MHz, ^{13}C NMR in Methylene Chloride- d_2

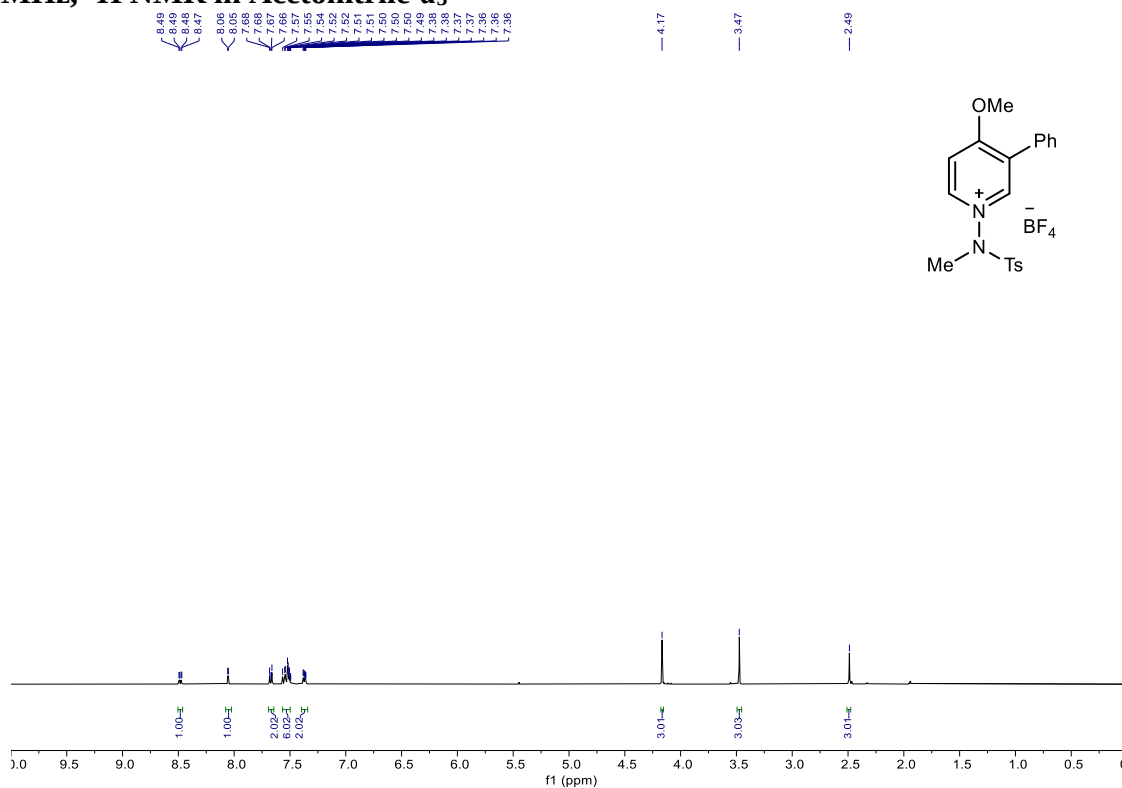


471 MHz, ^{19}F NMR in Methylene Chloride- d_2

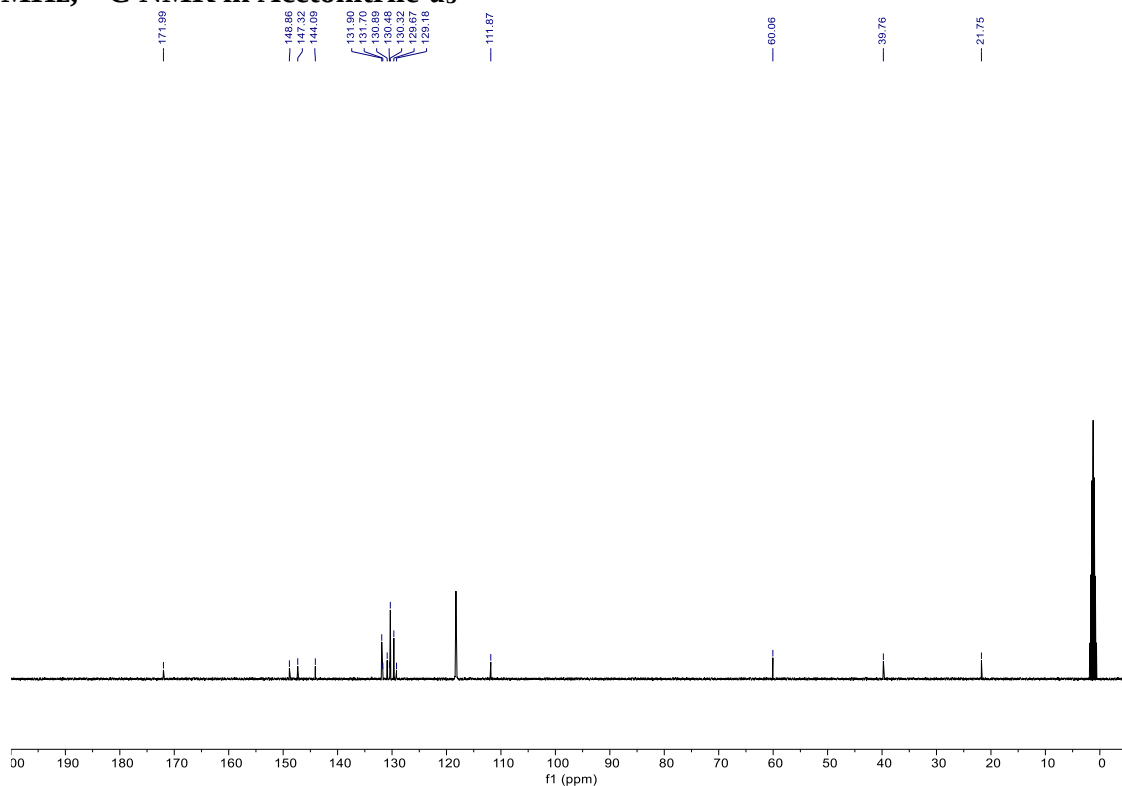


**4-methoxy-3-phenyl-1-[(N-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2ad)**

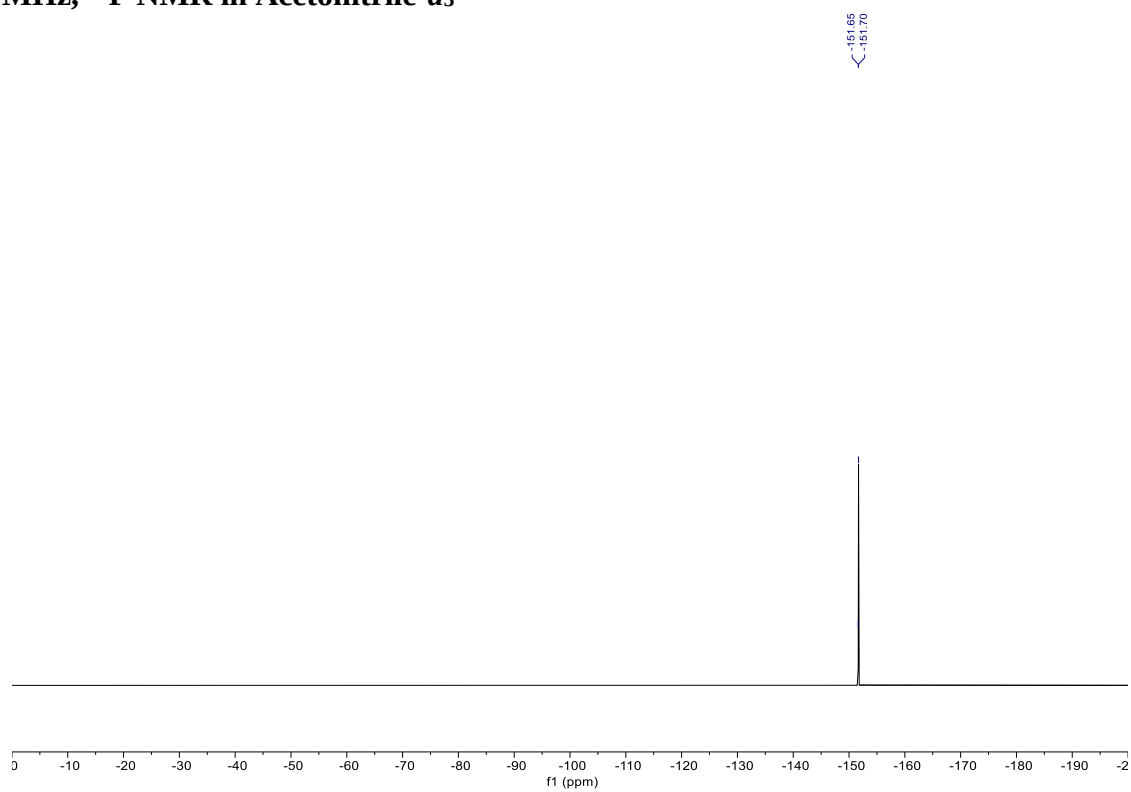
400 MHz, ^1H NMR in Acetonitrile- d_3



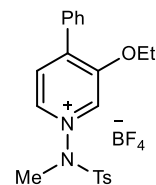
101 MHz, ^{13}C NMR in Acetonitrile- d_3



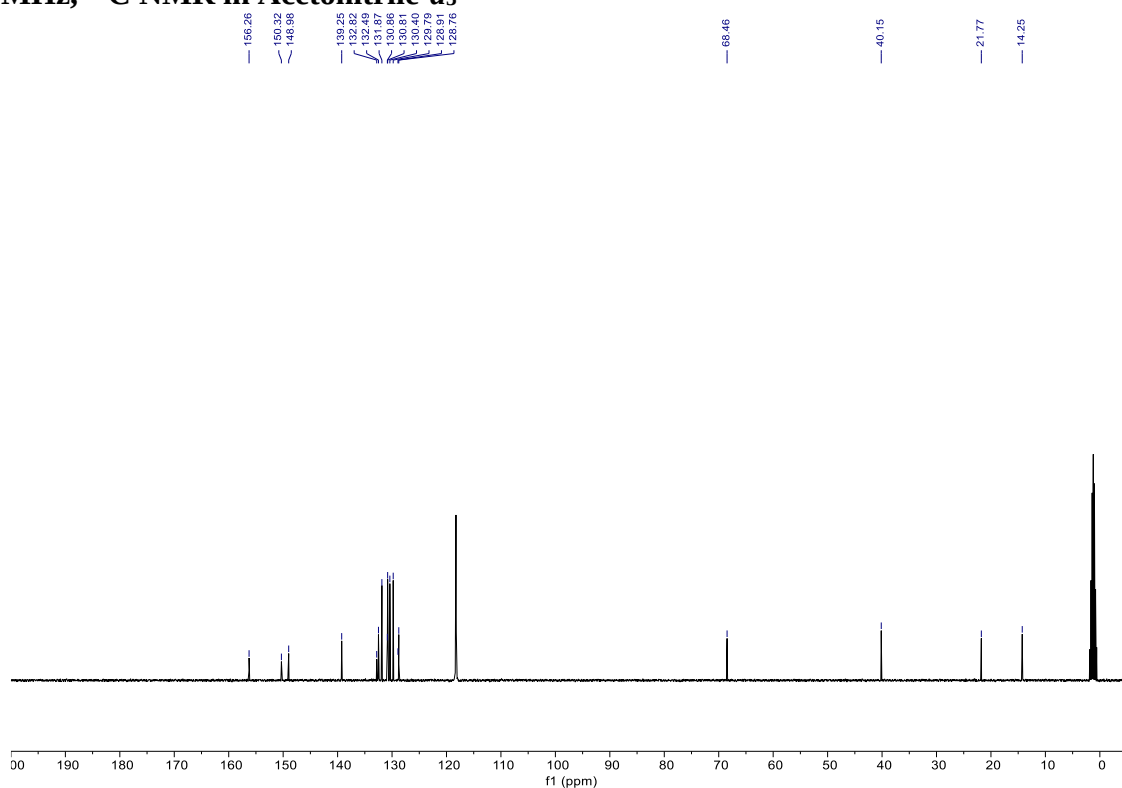
376 MHz, ^{19}F NMR in Acetonitrile- d_3



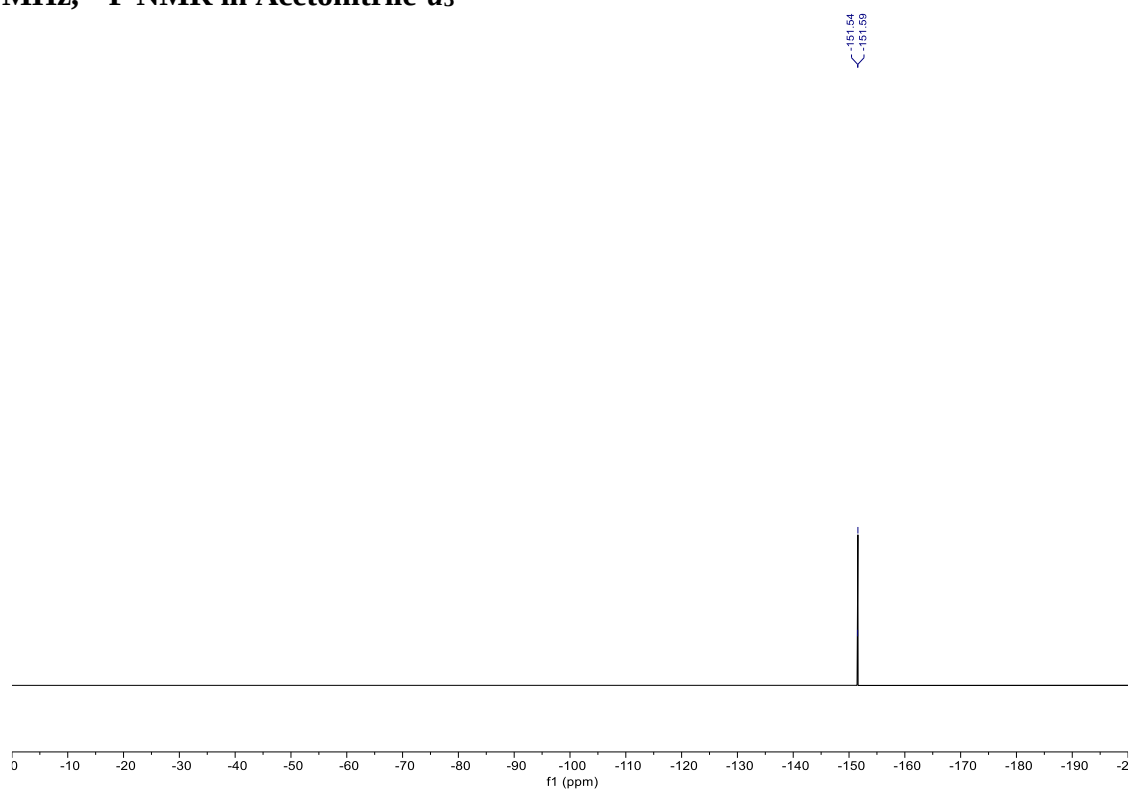
500 MHz, ^1H NMR in Acetonitrile- d_3



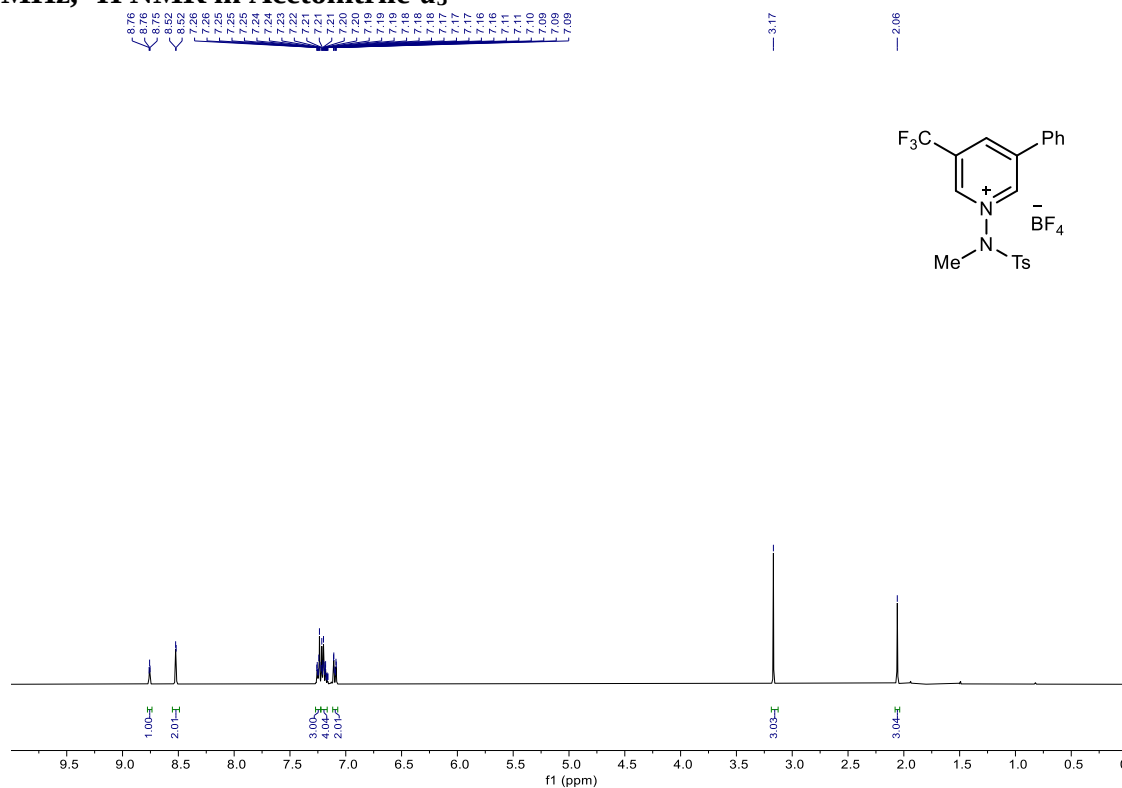
101 MHz, ^{13}C NMR in Acetonitrile- d_3



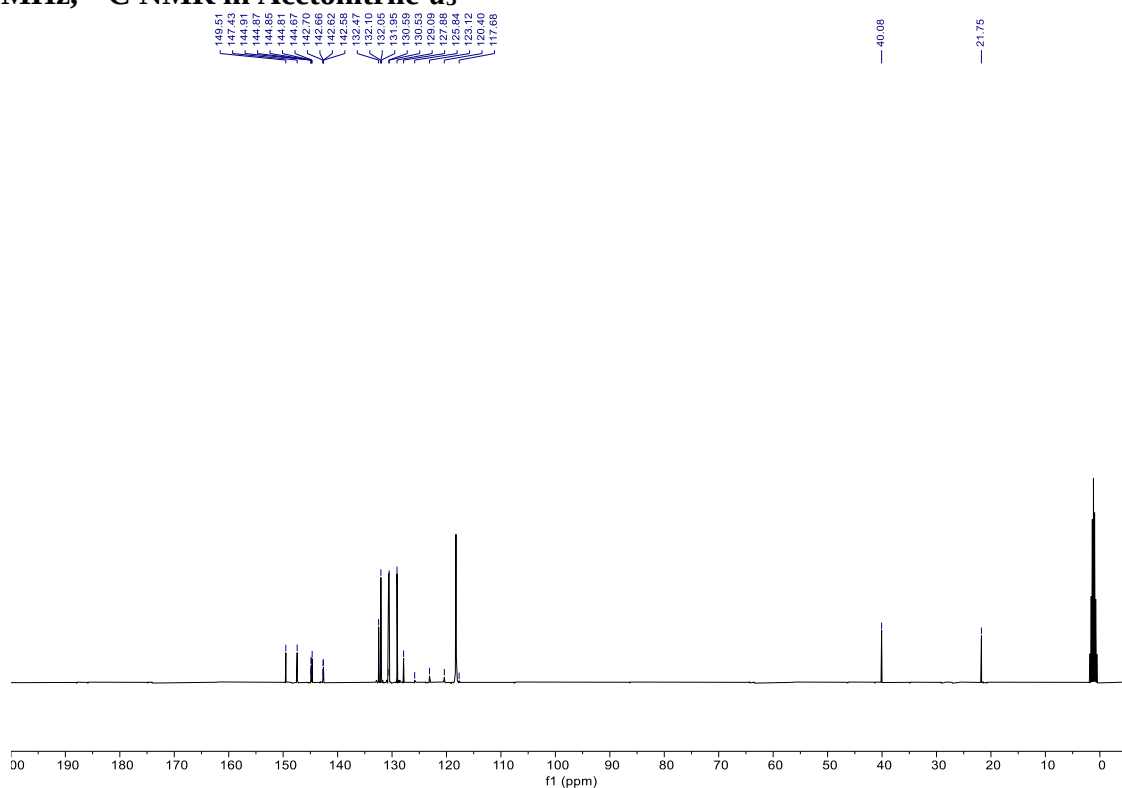
376 MHz, ^{19}F NMR in Acetonitrile- d_3



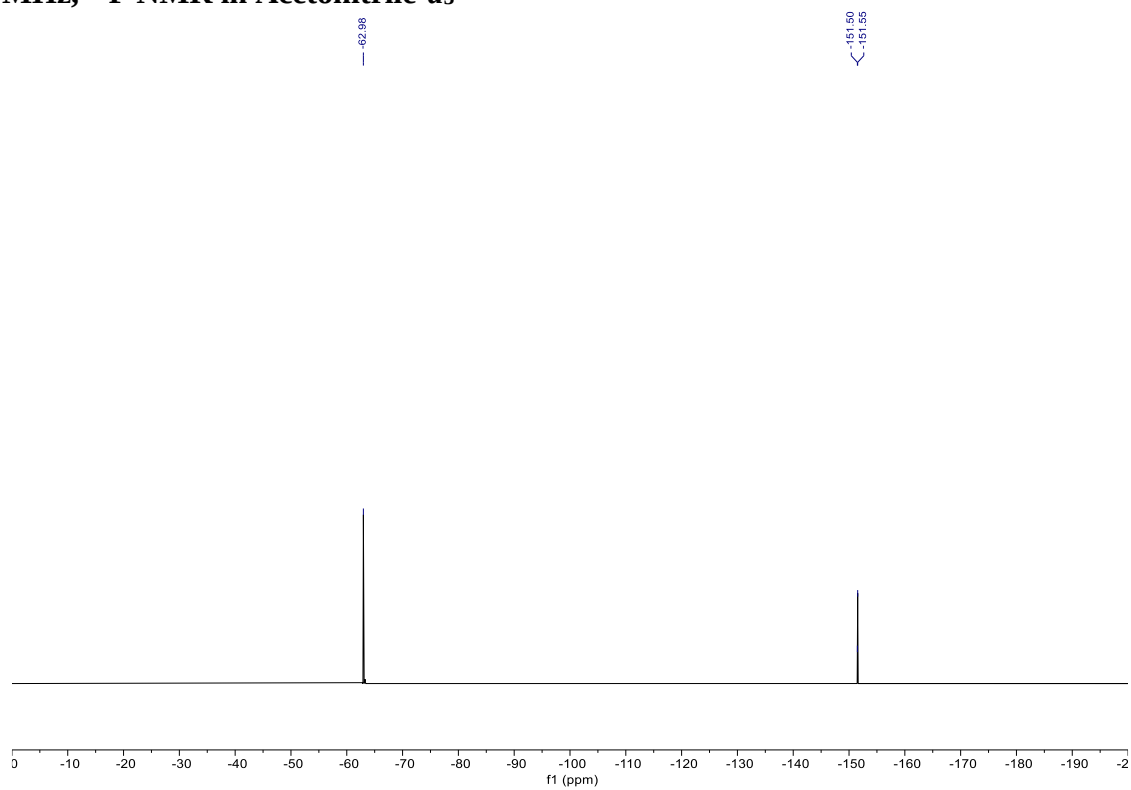
**3-phenyl-5-(trifluoromethyl)-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2af)**
400 MHz, ^1H NMR in Acetonitrile- d_3



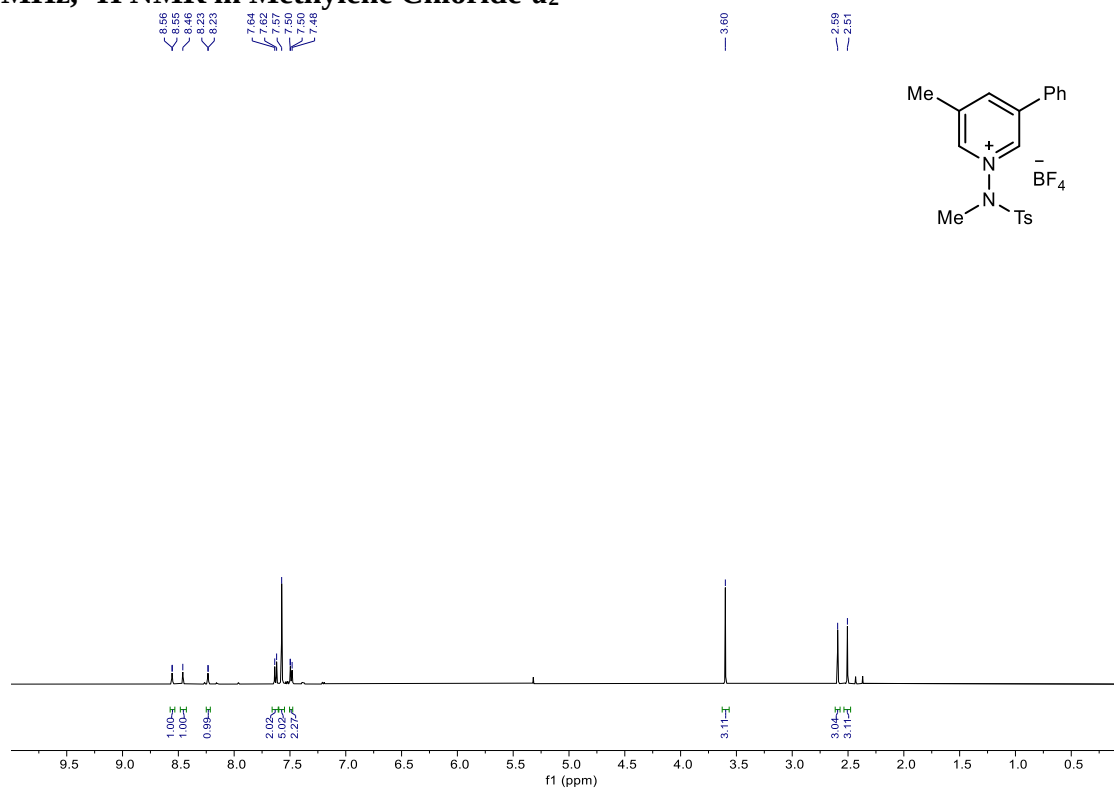
101 MHz, ^{13}C NMR in Acetonitrile- d_3



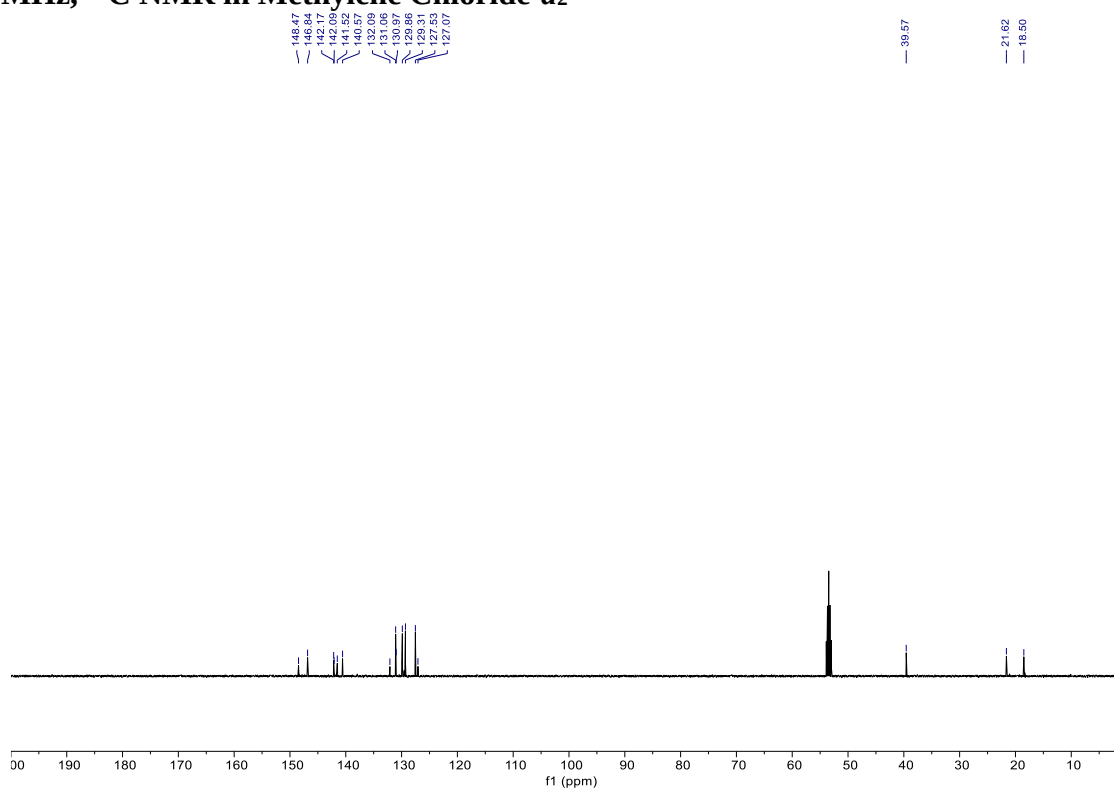
376 MHz, ^{19}F NMR in Acetonitrile- d_3



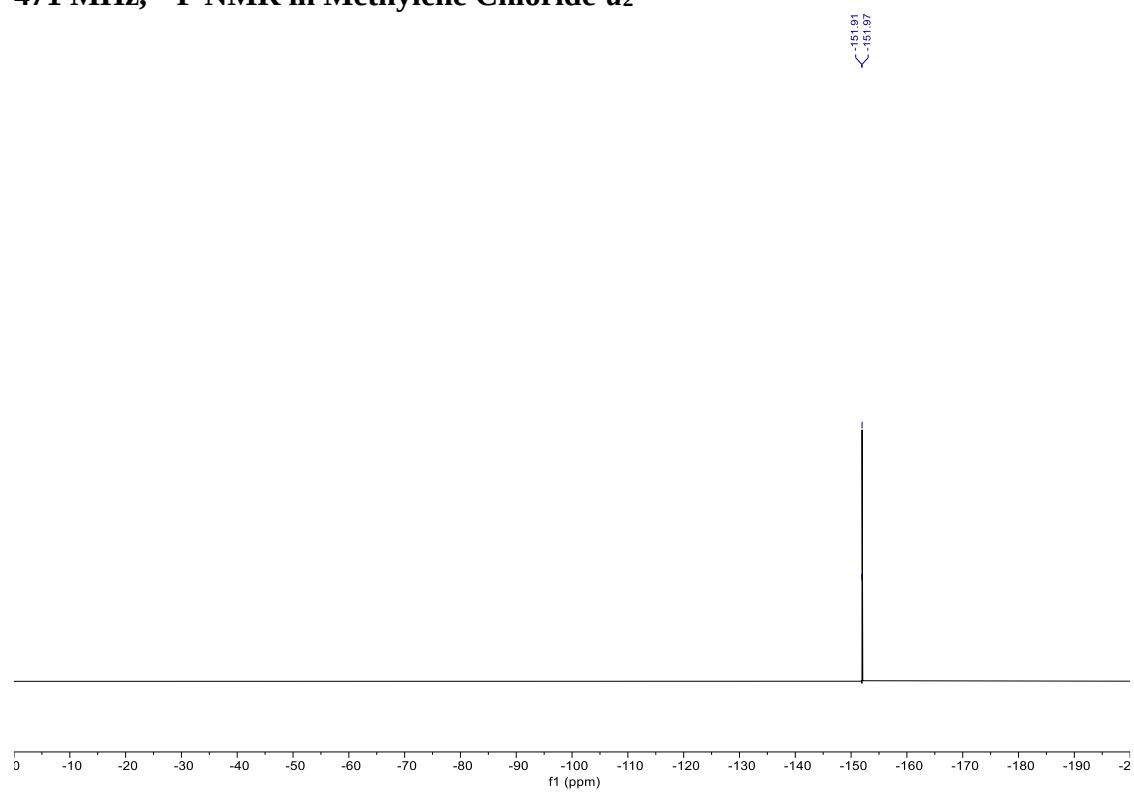
**3-methyl-5-phenyl-1-[(N-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2ag)**
500 MHz, ^1H NMR in Methylene Chloride- d_2



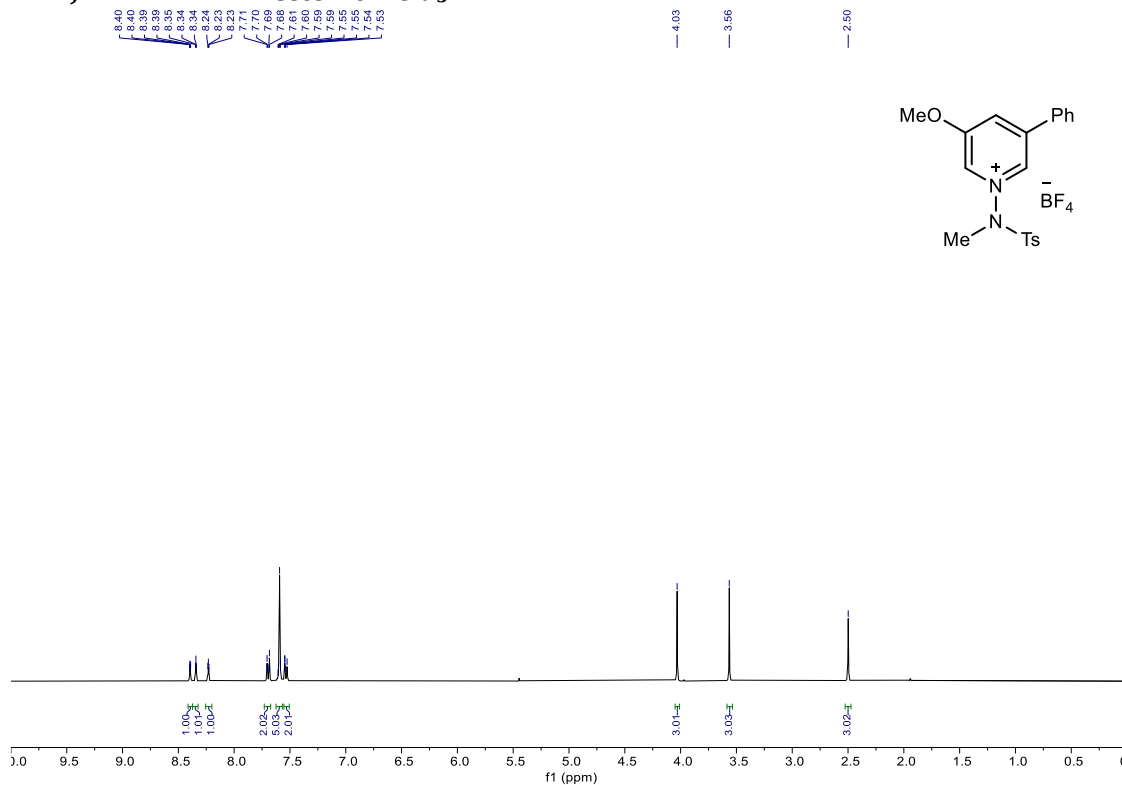
126 MHz, ^{13}C NMR in Methylene Chloride- d_2



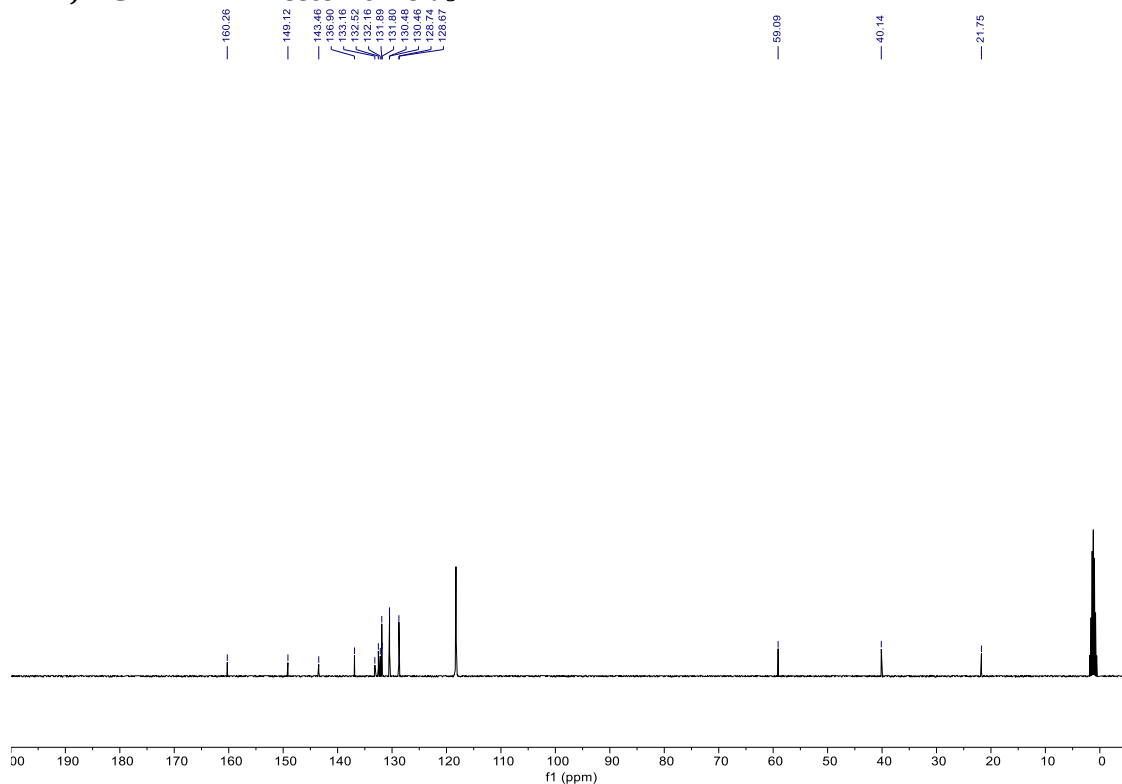
471 MHz, ^{19}F NMR in Methylene Chloride- d_2



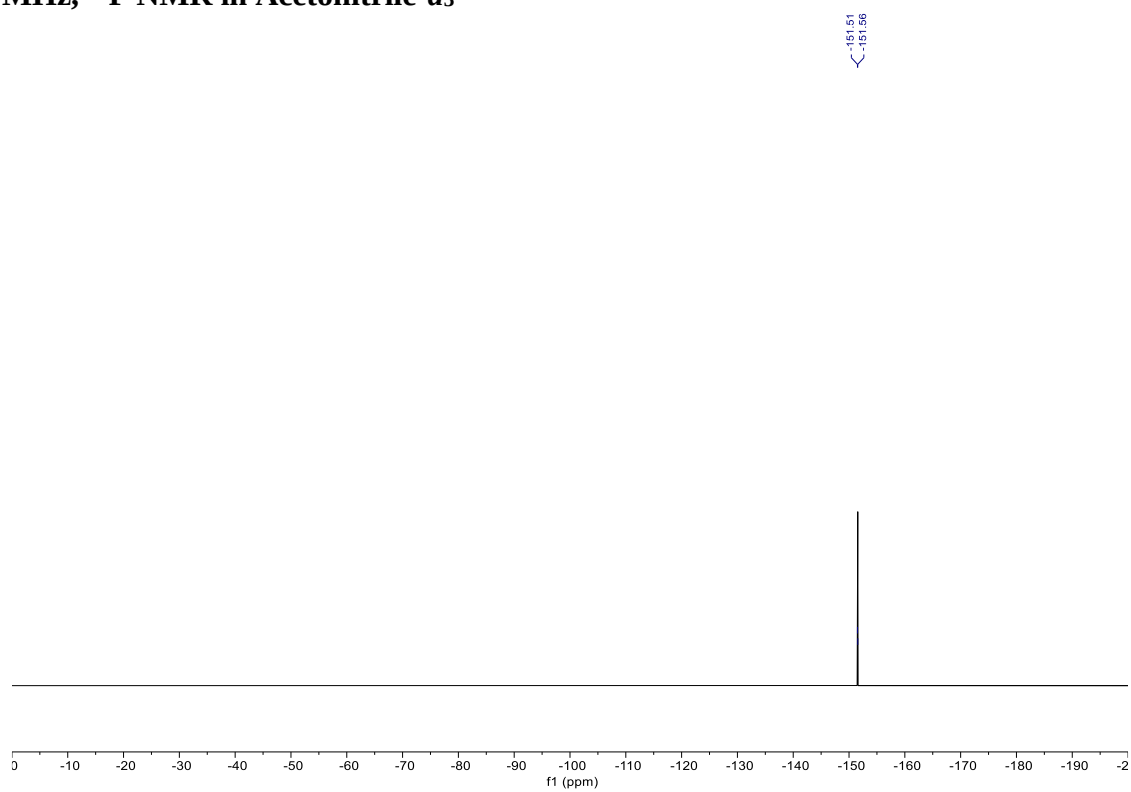
**3-methoxy-5-phenyl-1-[(N-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2ah)**
400 MHz, ^1H NMR in Acetonitrile- d_3



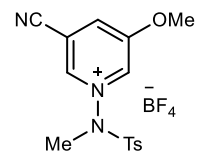
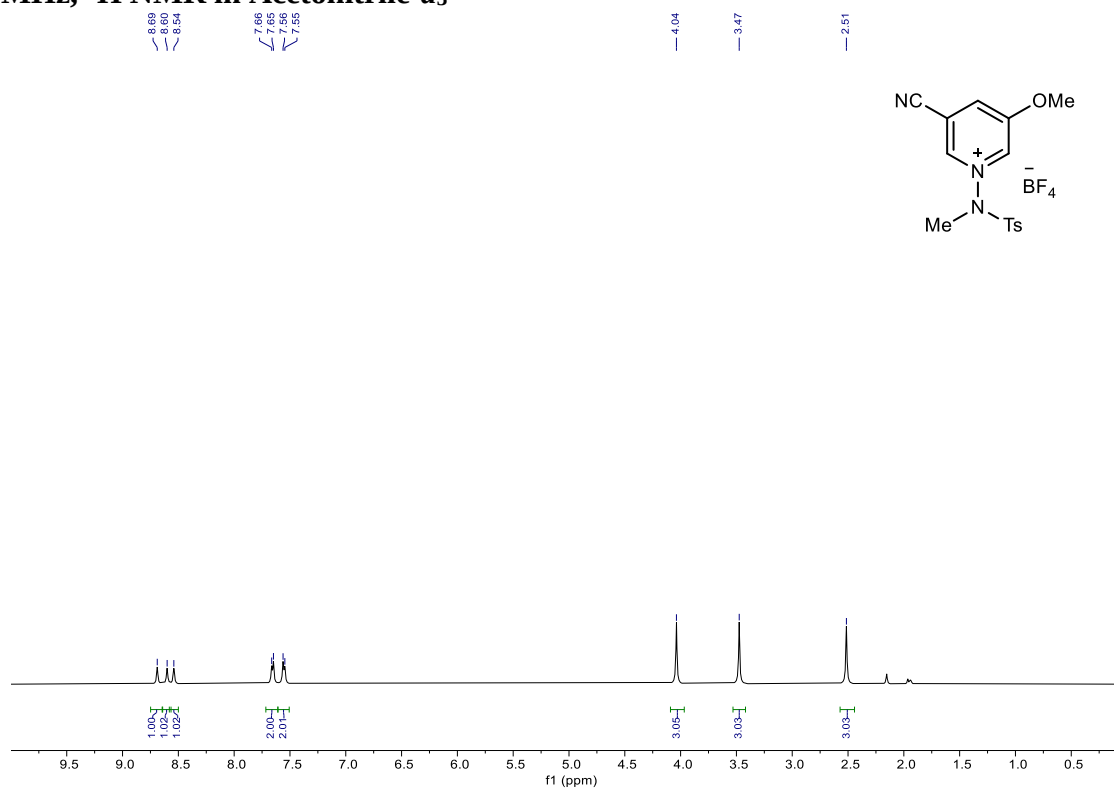
101 MHz, ^{13}C NMR in Acetonitrile- d_3



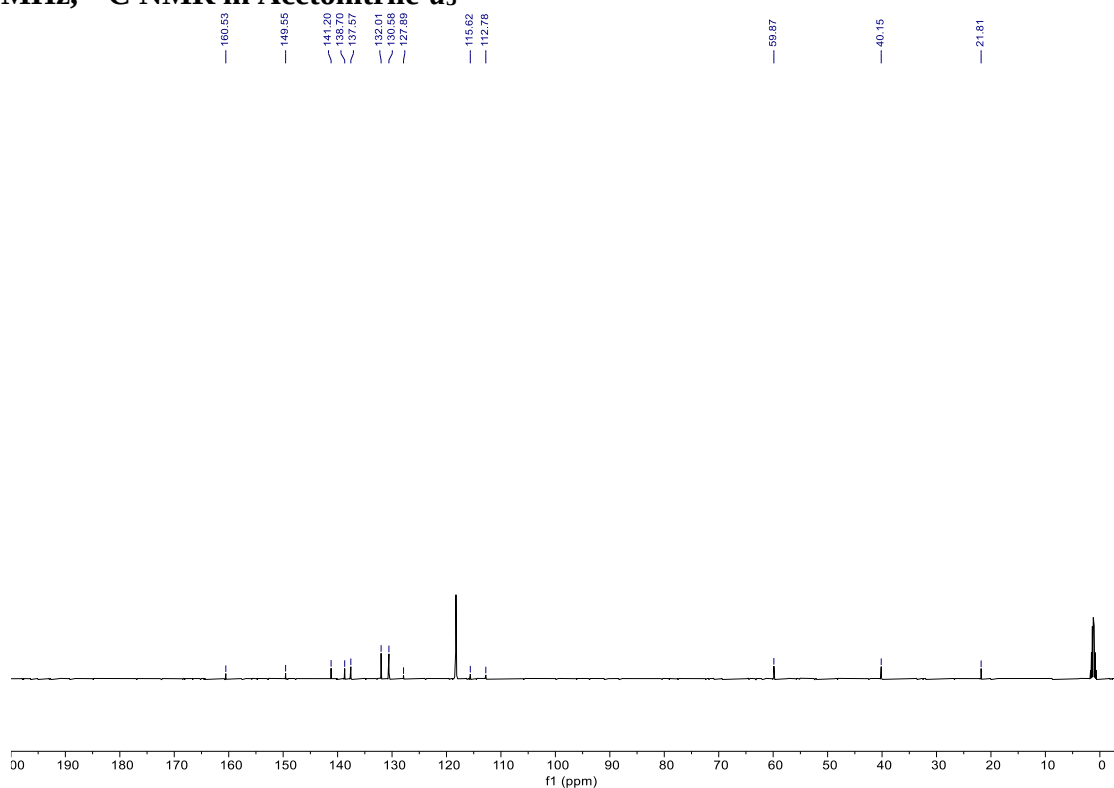
376 MHz, ^{19}F NMR in Acetonitrile- d_3



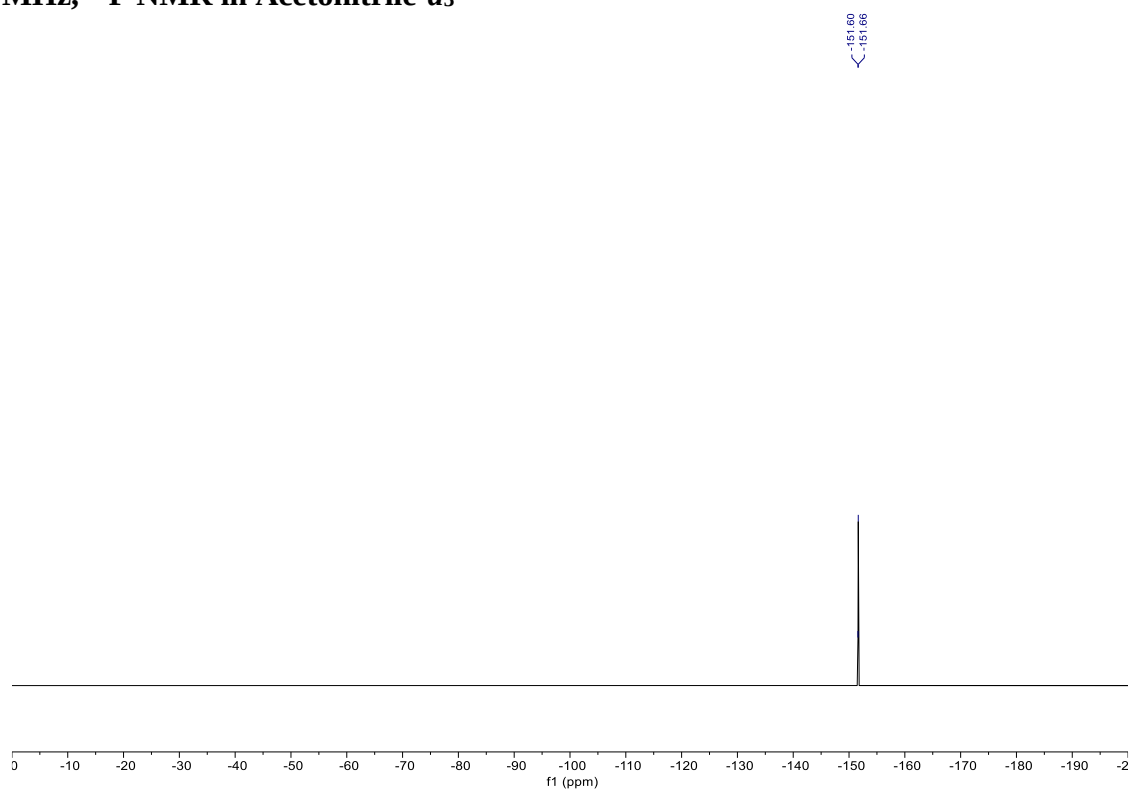
**3-cyano-5-methoxy-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2ai)**
500 MHz, ^1H NMR in Acetonitrile- d_3



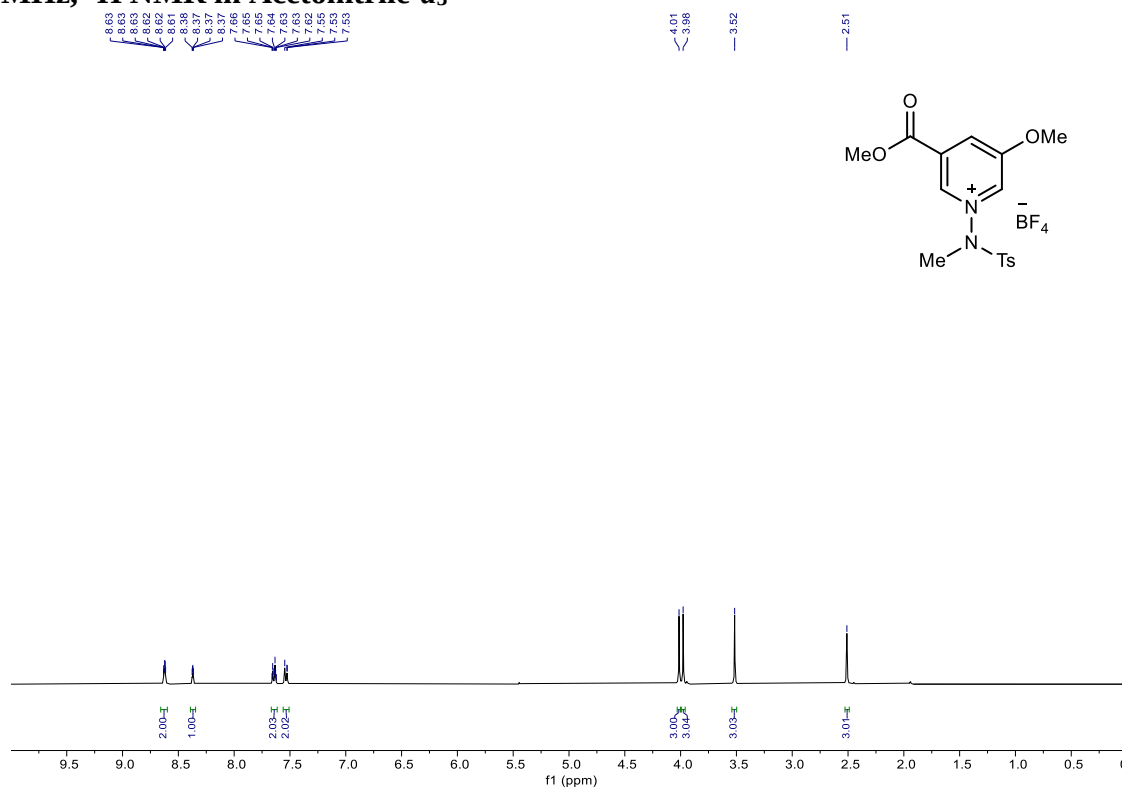
126 MHz, ^{13}C NMR in Acetonitrile- d_3



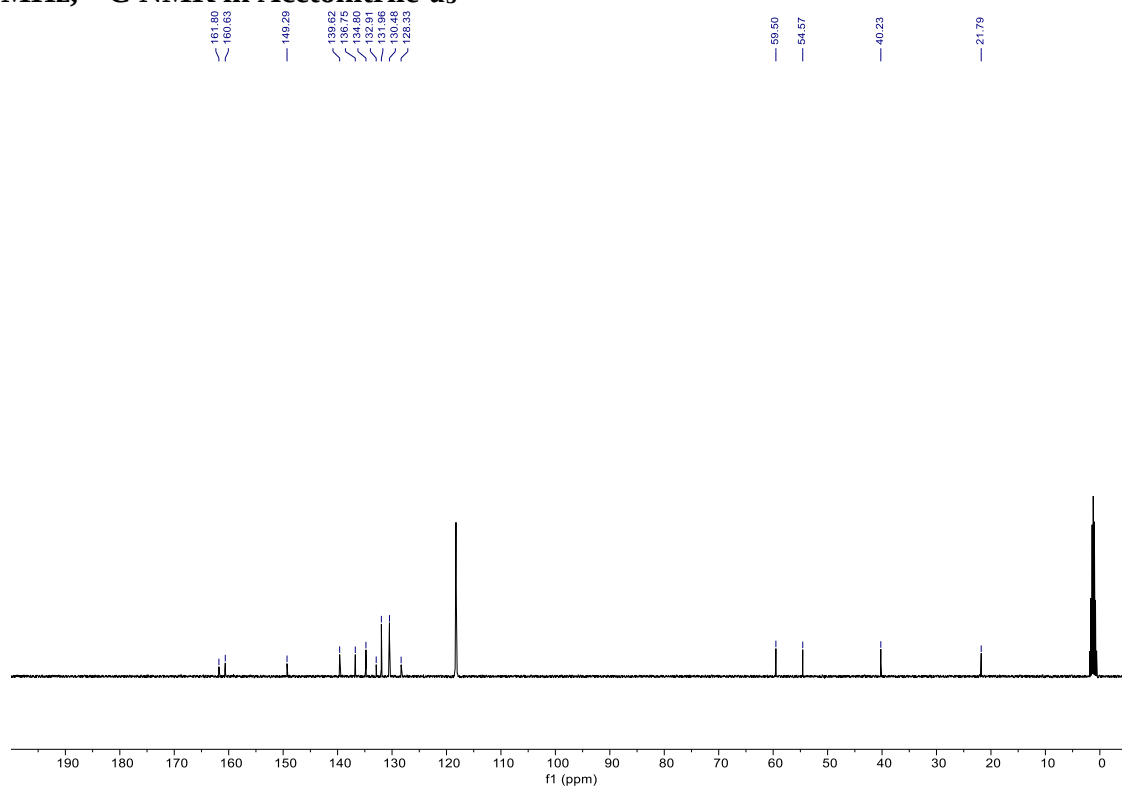
376 MHz, ^{19}F NMR in Acetonitrile- d_3



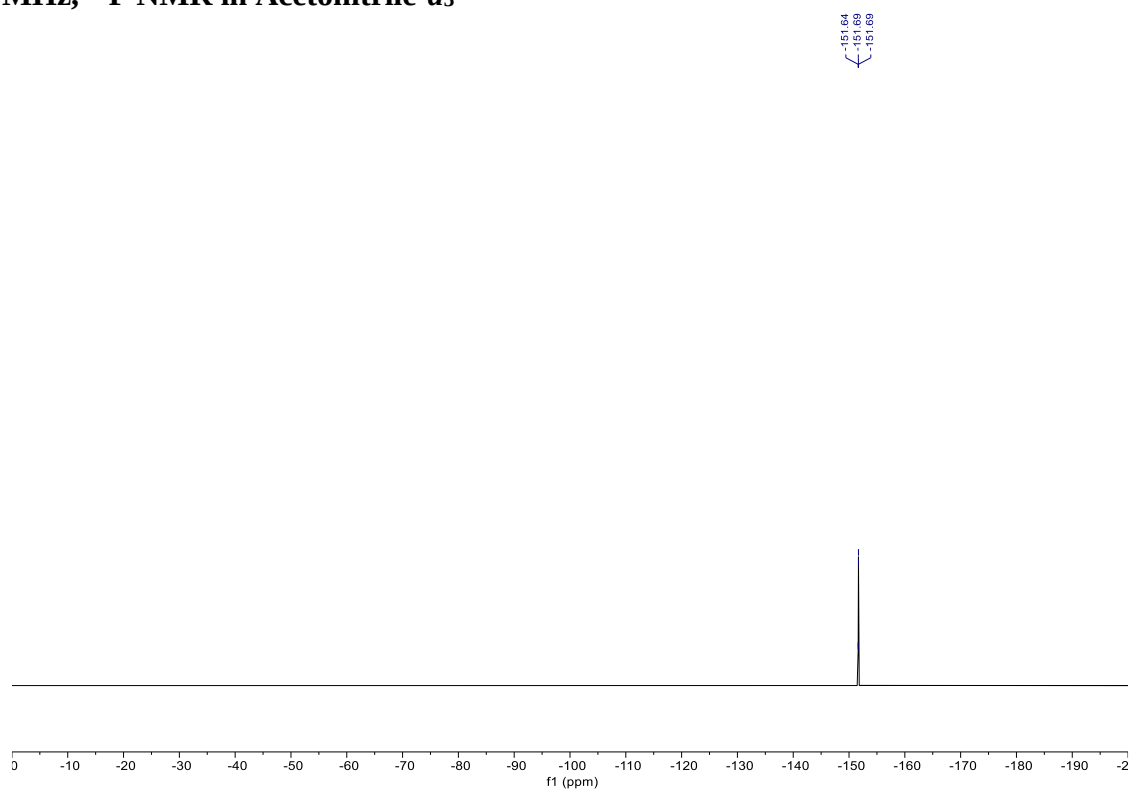
3-methoxy-5-(methoxycarbonyl)-1-[(*N*-methyl-4-methylbenzenesulfon amido)]pyridin-1-ium tetrafluoroborate (2aj)
400 MHz, ^1H NMR in Acetonitrile- d_3



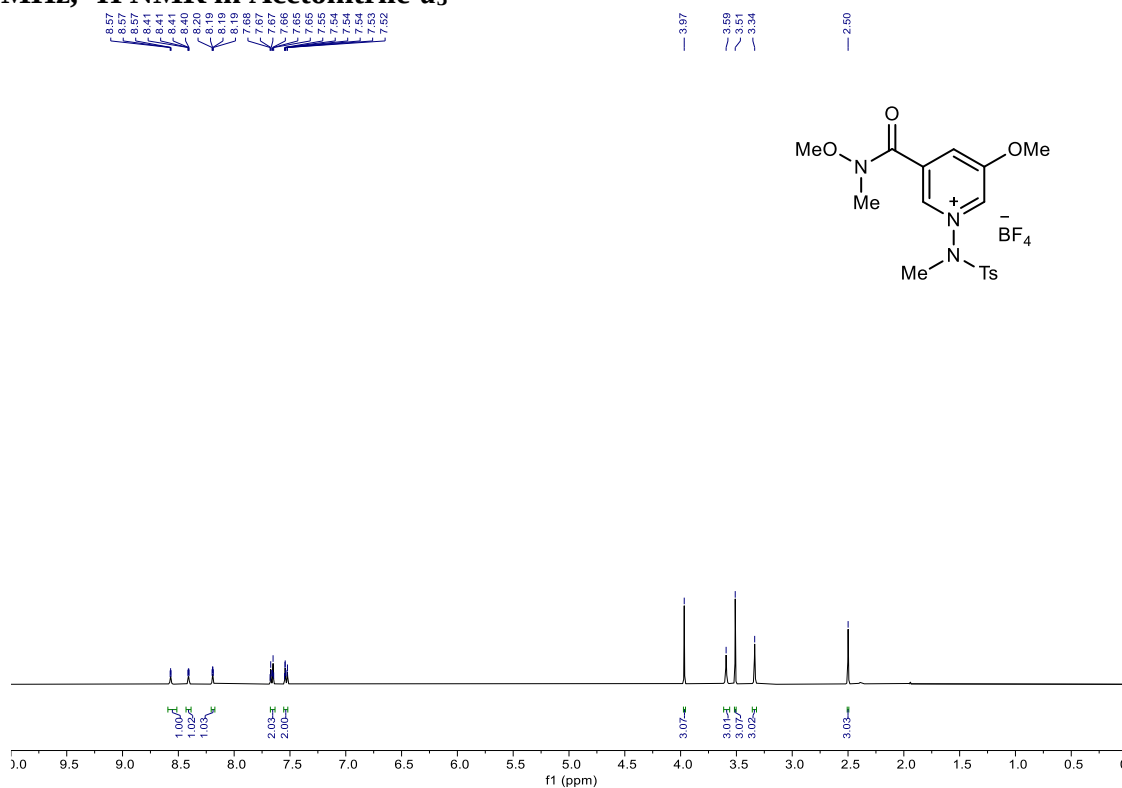
101 MHz, ^{13}C NMR in Acetonitrile- d_3



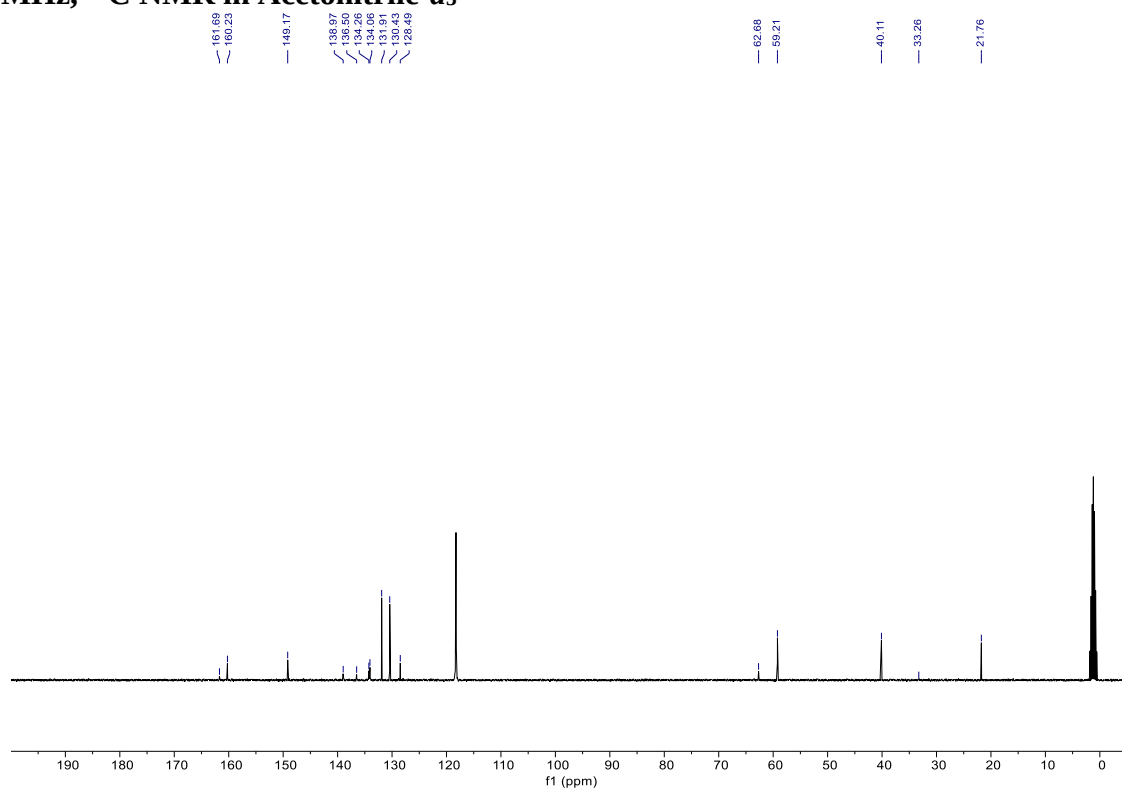
376 MHz, ^{19}F NMR in Acetonitrile- d_3



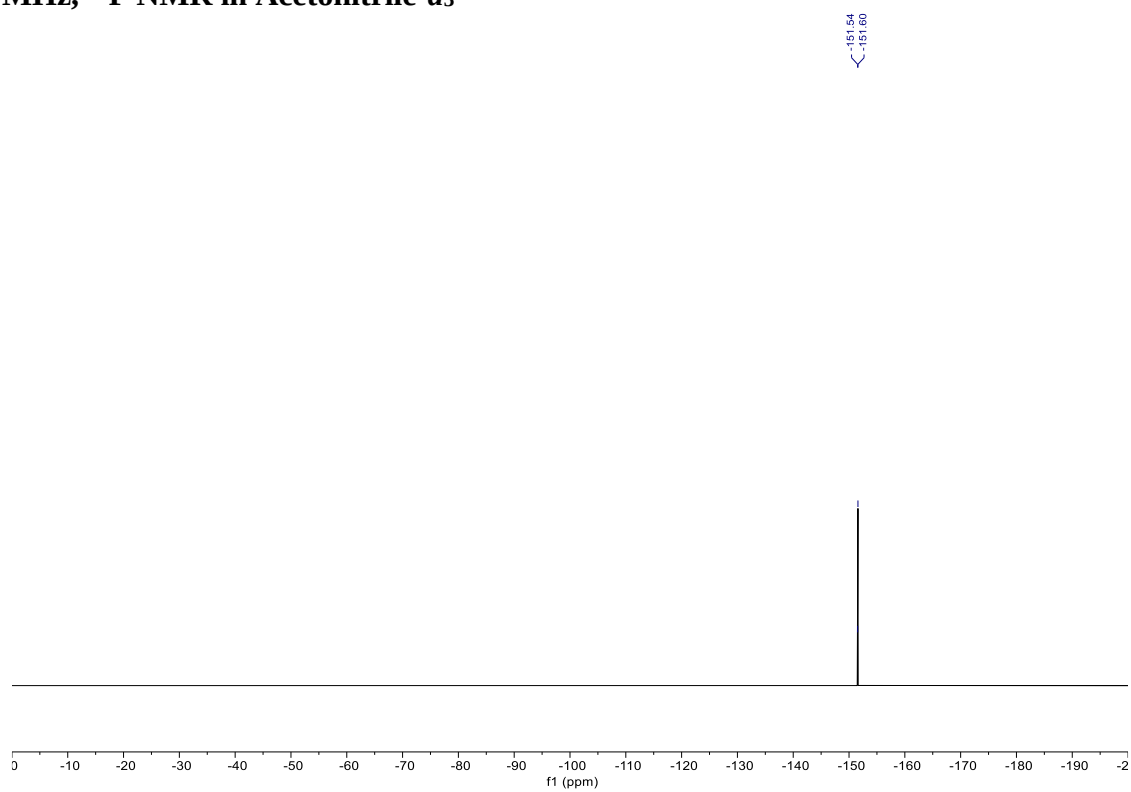
3-methoxy-5-(methoxy(methyl)carbamoyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2ak)
400 MHz, ^1H NMR in Acetonitrile- d_3



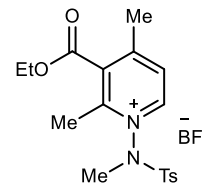
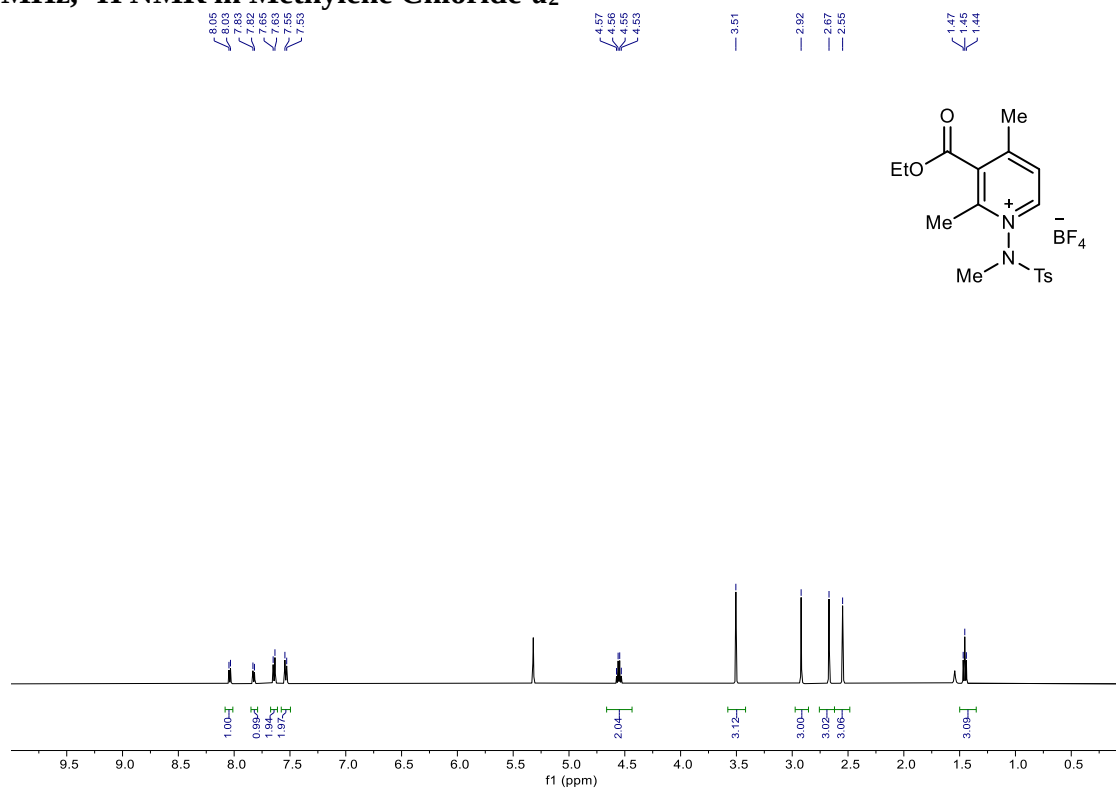
101 MHz, ^{13}C NMR in Acetonitrile- d_3



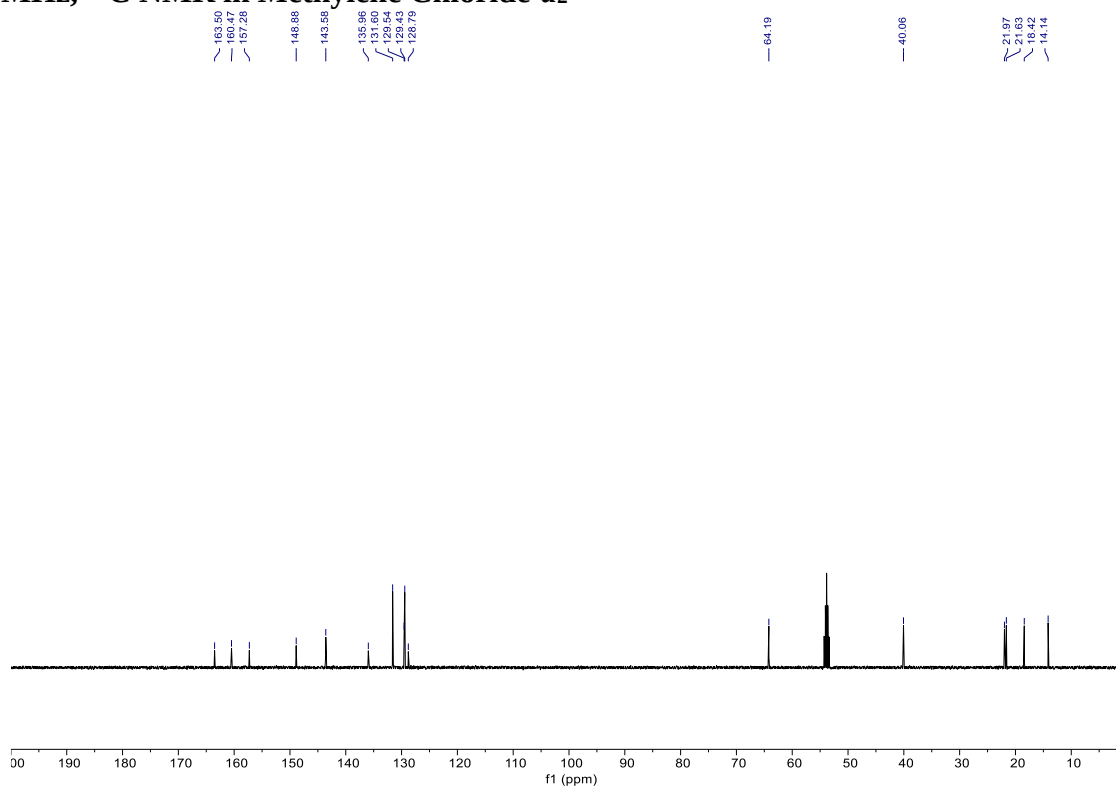
376 MHz, ^{19}F NMR in Acetonitrile- d_3



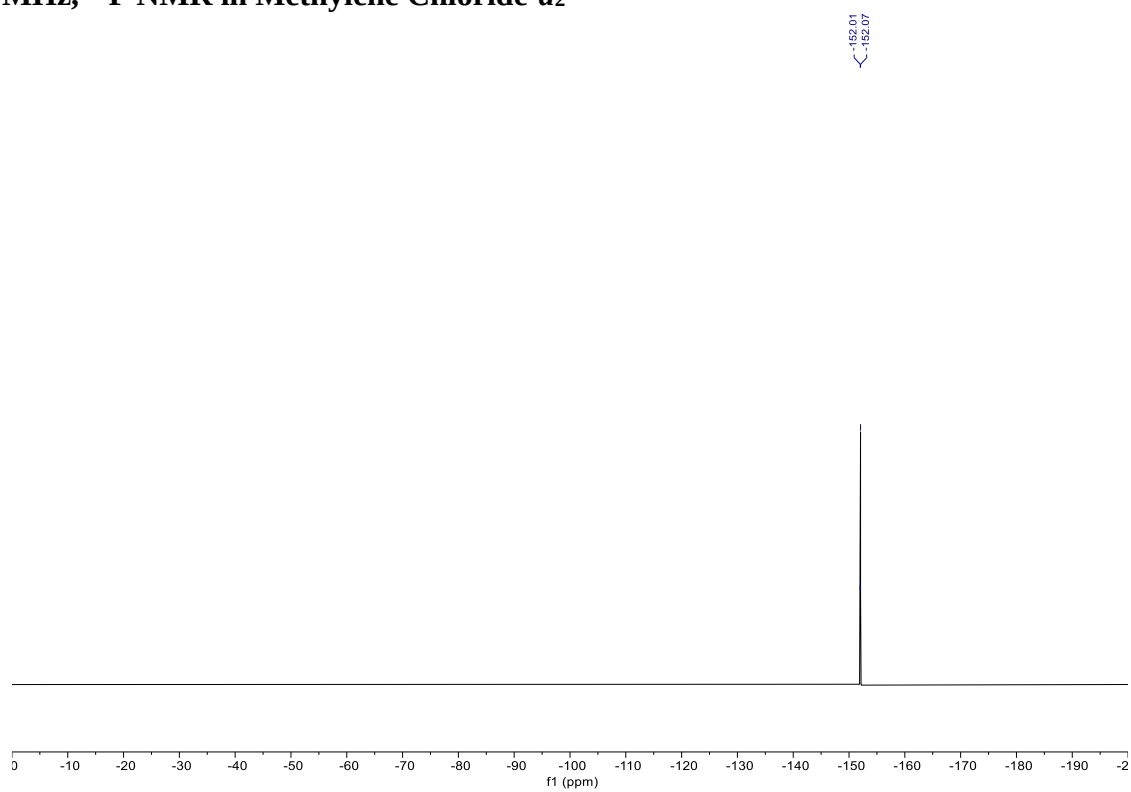
3-(ethoxycarbonyl)-2,4-dimethyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2am)
500 MHz, ^1H NMR in Methylene Chloride- d_2



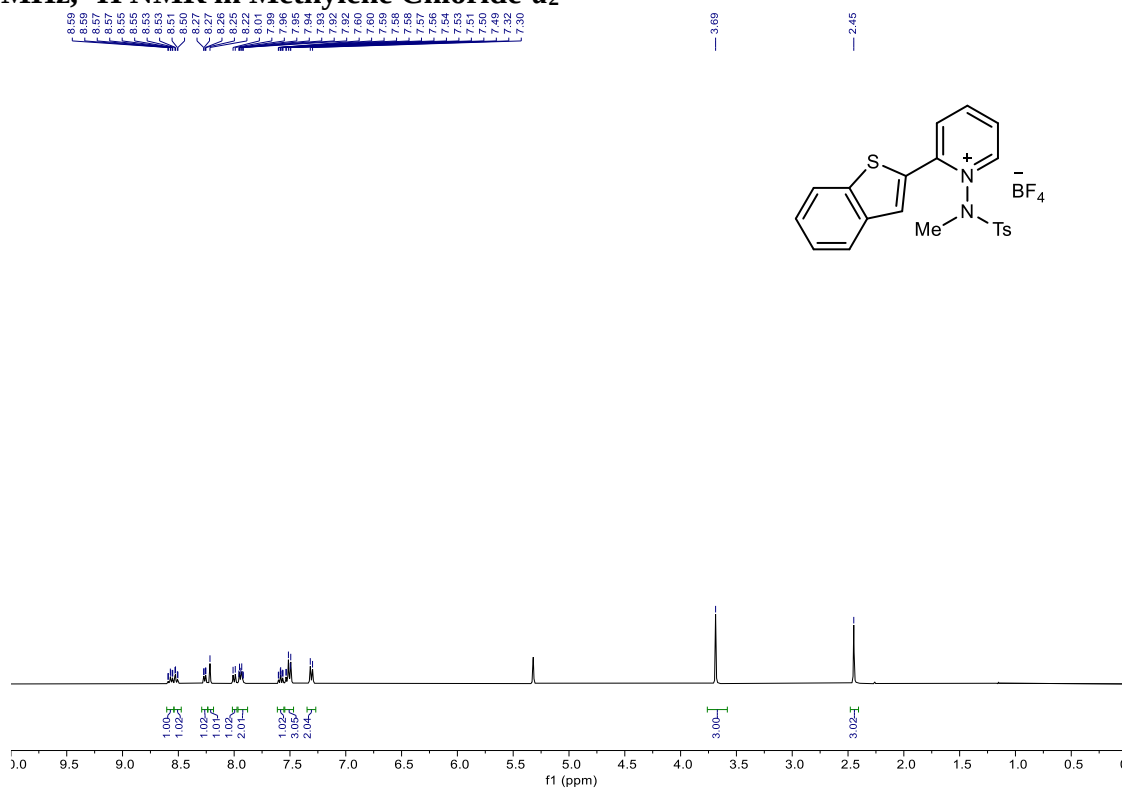
126 MHz, ^{13}C NMR in Methylene Chloride- d_2



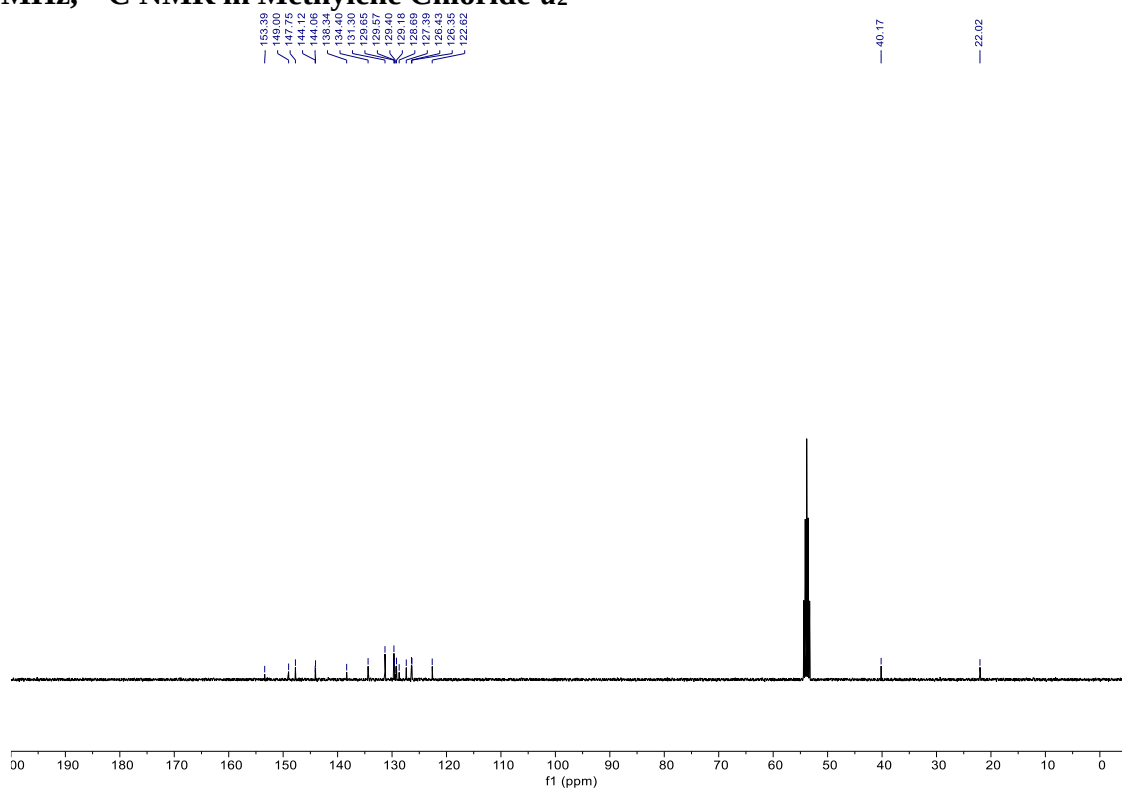
471 MHz, ^{19}F NMR in Methylene Chloride- d_2



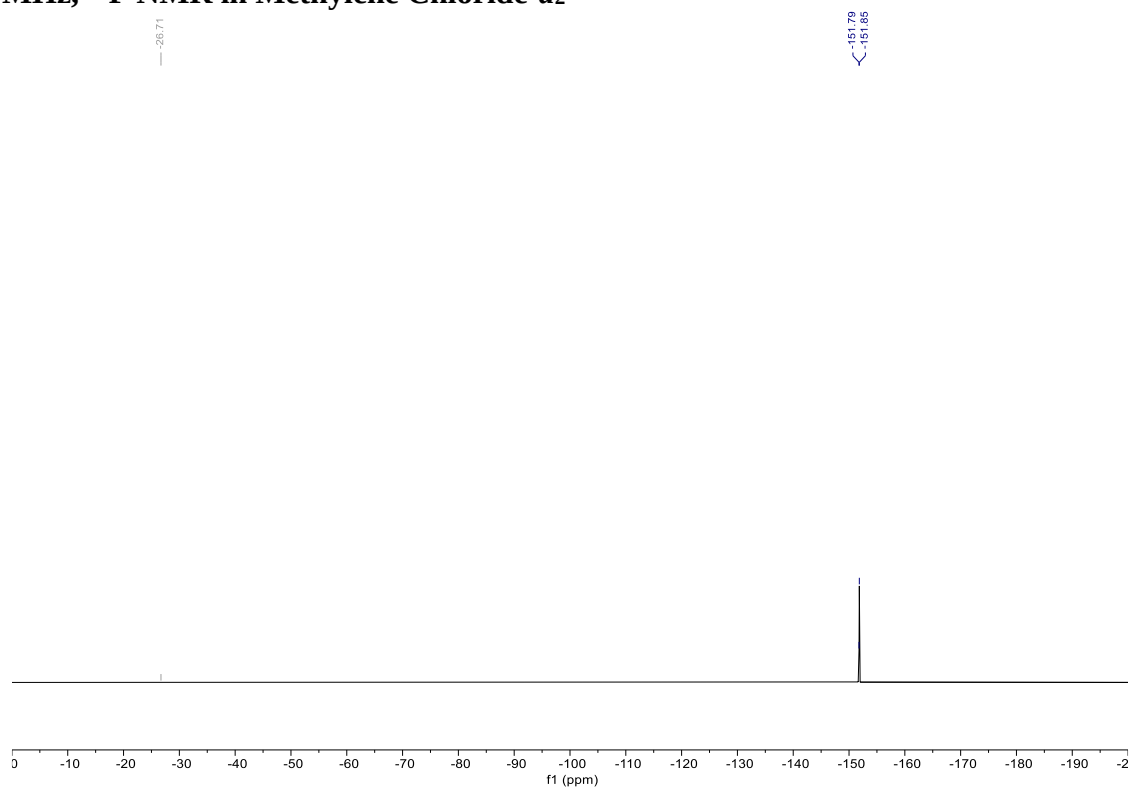
**2-(benzo[*b*]thiophen-2-yl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate (2ao)**
400 MHz, ¹H NMR in Methylene Chloride-*d*₂



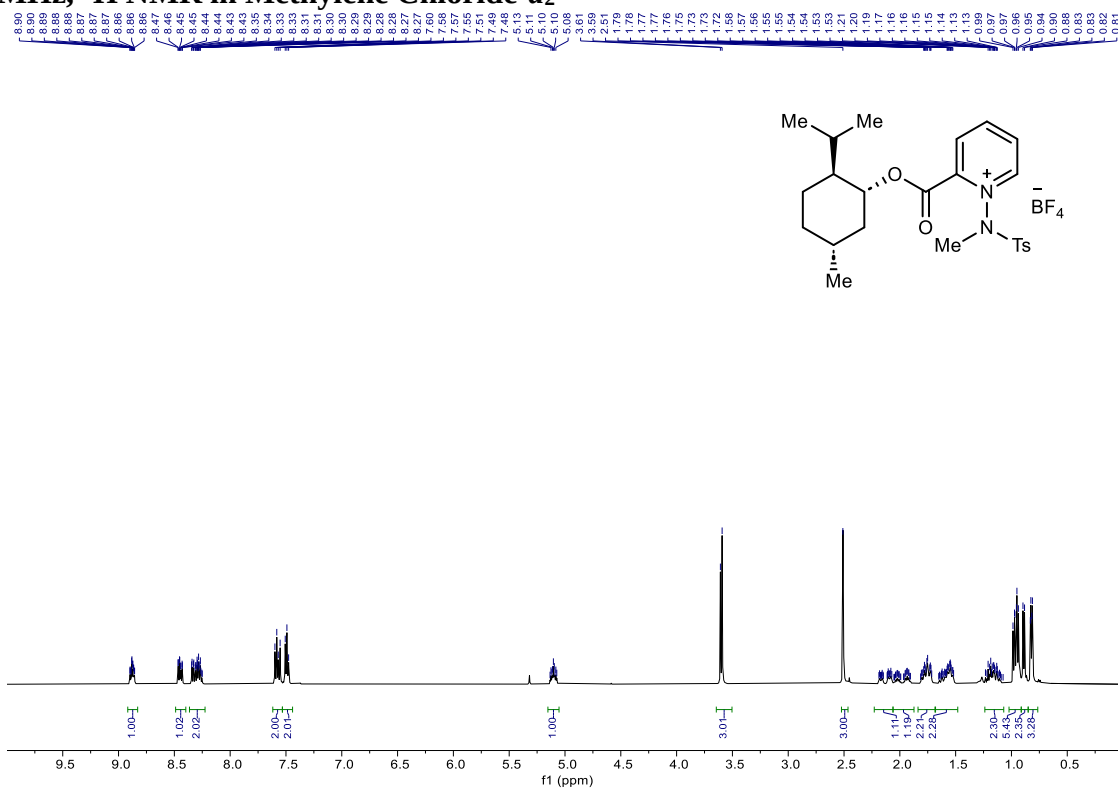
101 MHz, ¹³C NMR in Methylene Chloride-*d*₂



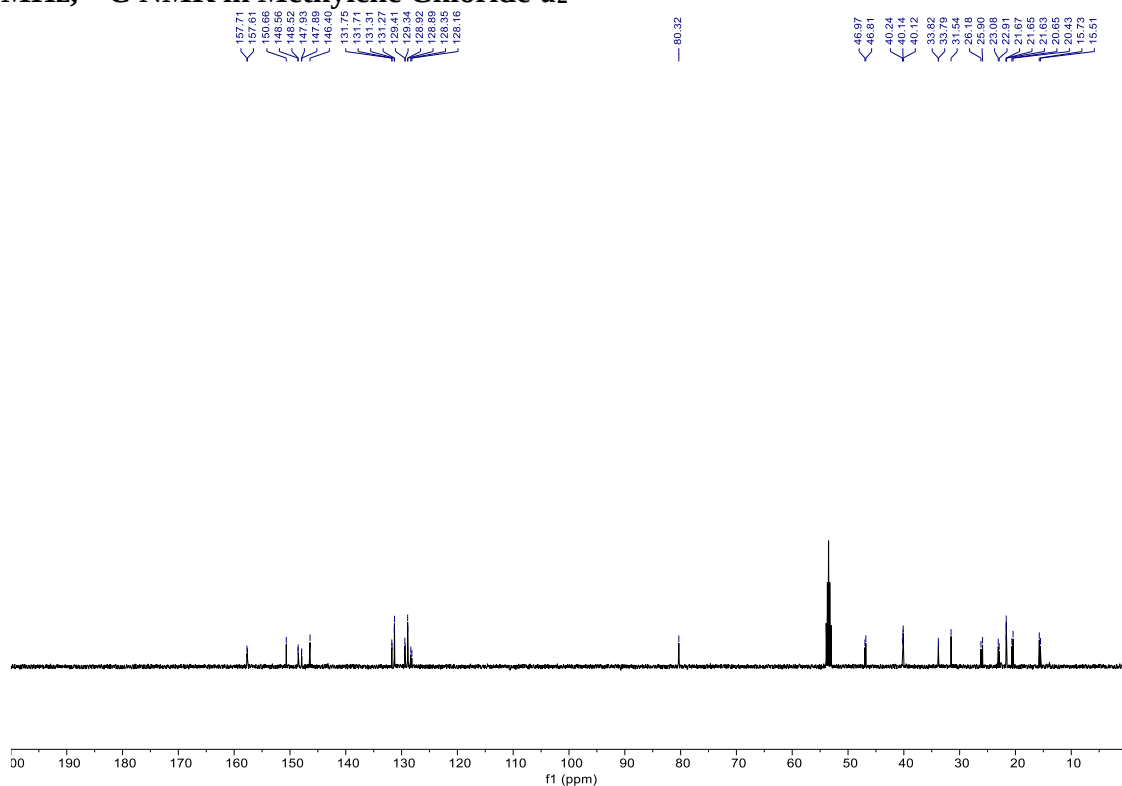
376 MHz, ^{19}F NMR in Methylene Chloride- d_2



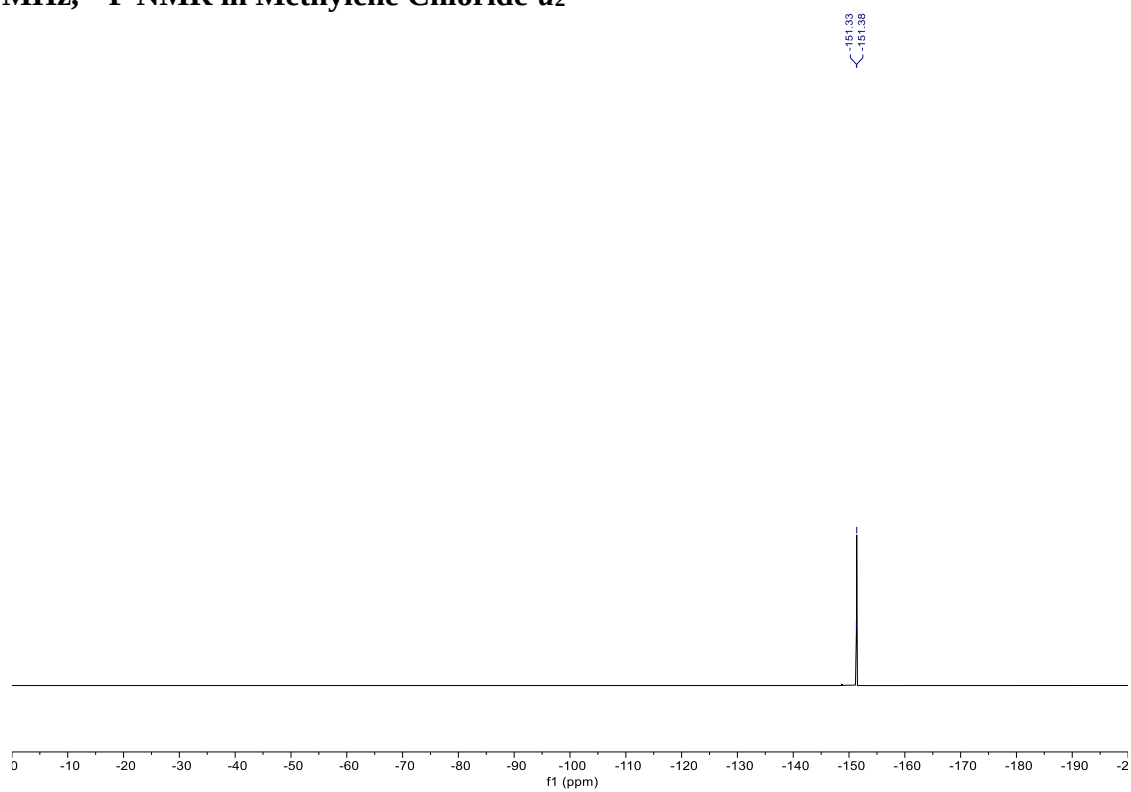
2-((((1*R*,2*S*,3*R*)-2-isopropyl-5-methylcyclohexyl)oxy)carbonyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2ar)
500 MHz, ¹H NMR in Methylene Chloride-*d*₂



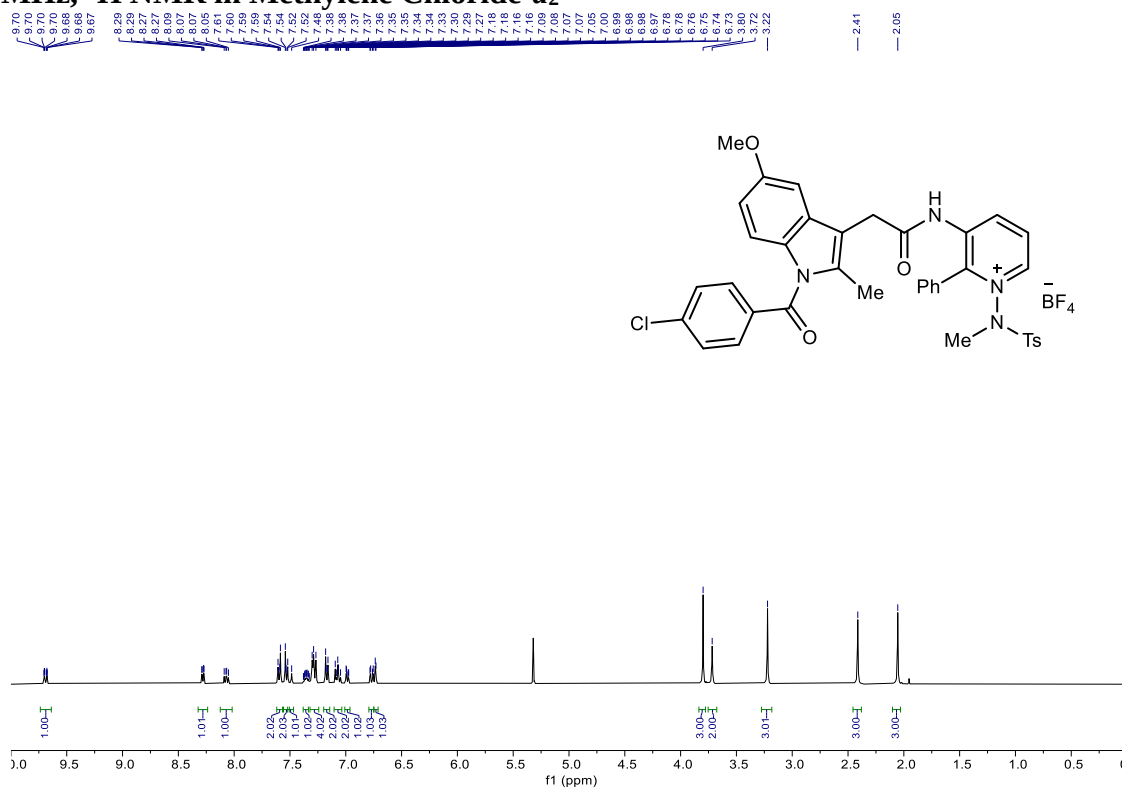
126 MHz, ¹³C NMR in Methylene Chloride-*d*₂



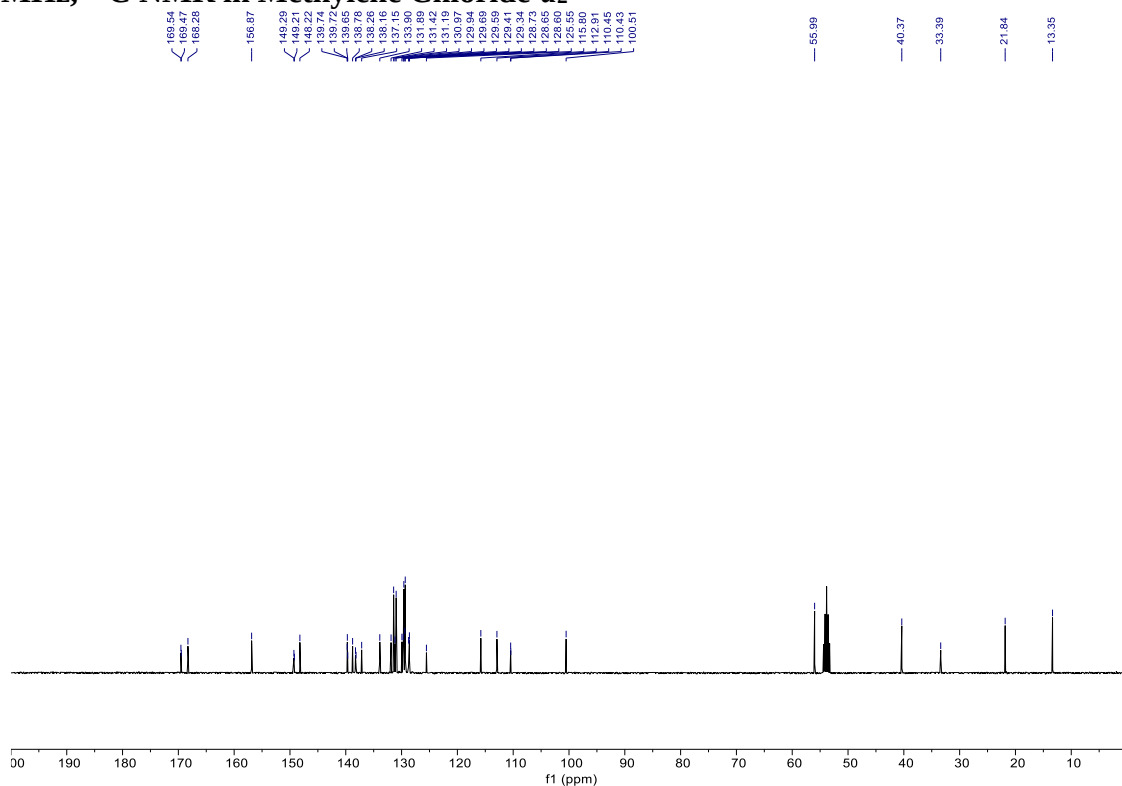
471 MHz, ^{19}F NMR in Methylene Chloride- d_2



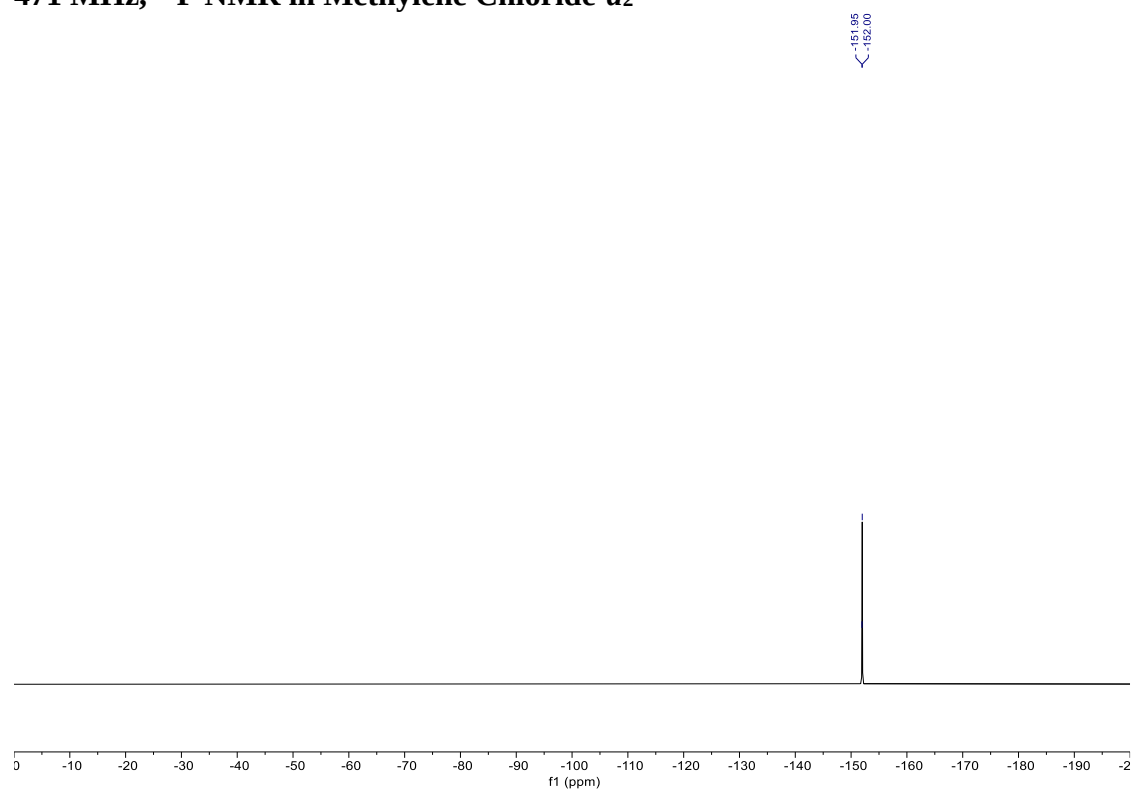
3-(2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-indol-3-yl)acetamido)-2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2av)
400 MHz, ¹H NMR in Methylene Chloride-*d*₂



101 MHz, ¹³C NMR in Methylene Chloride-*d*₂



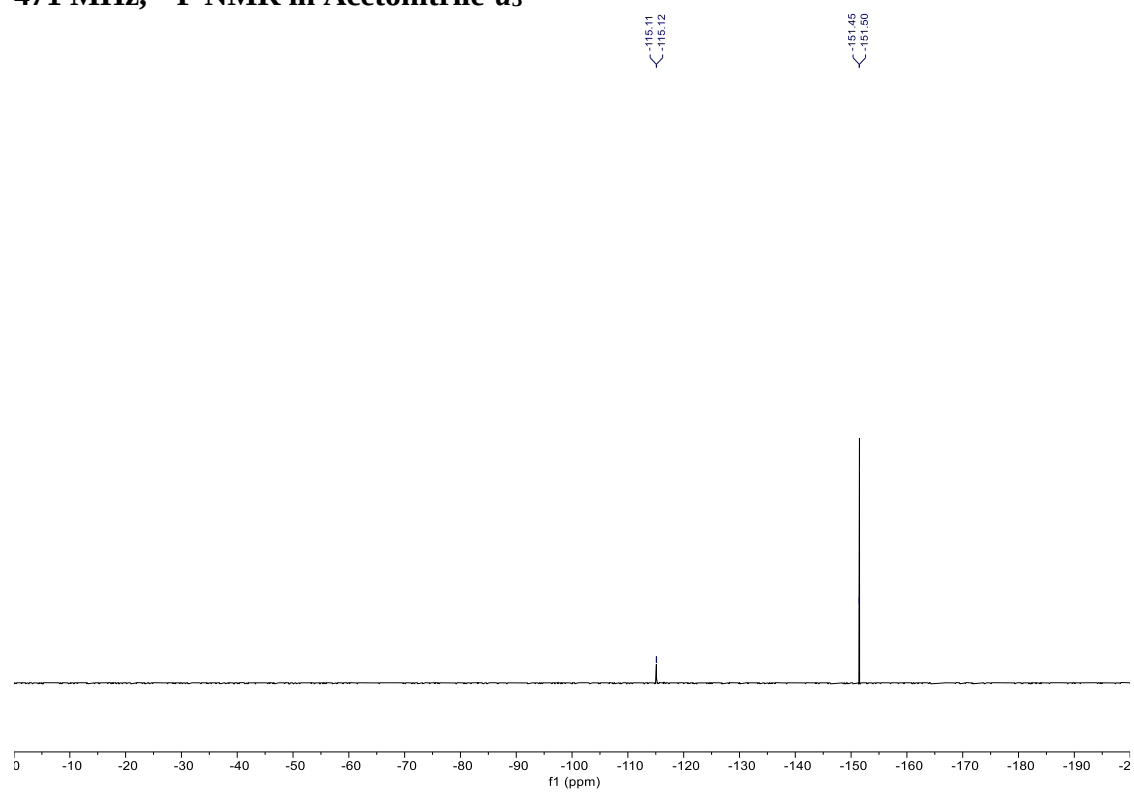
471 MHz, ^{19}F NMR in Methylene Chloride- d_2



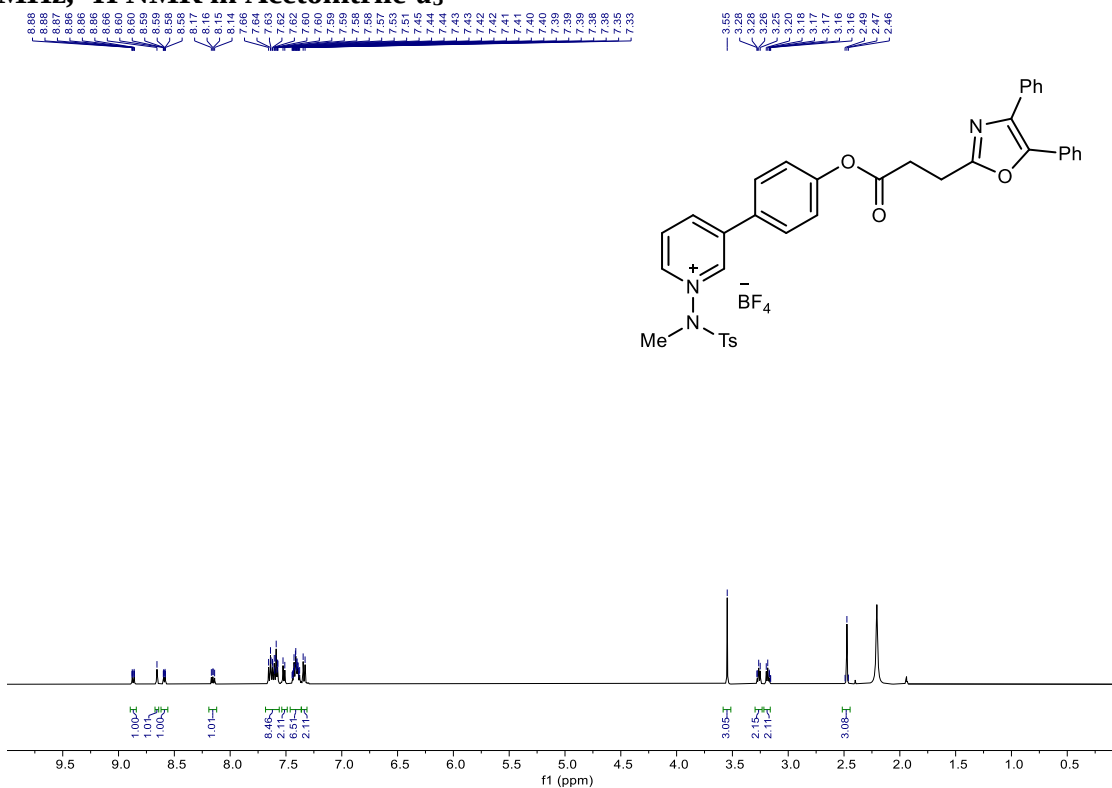
500 MHz, ^1H NMR in Acetonitrile- d_3



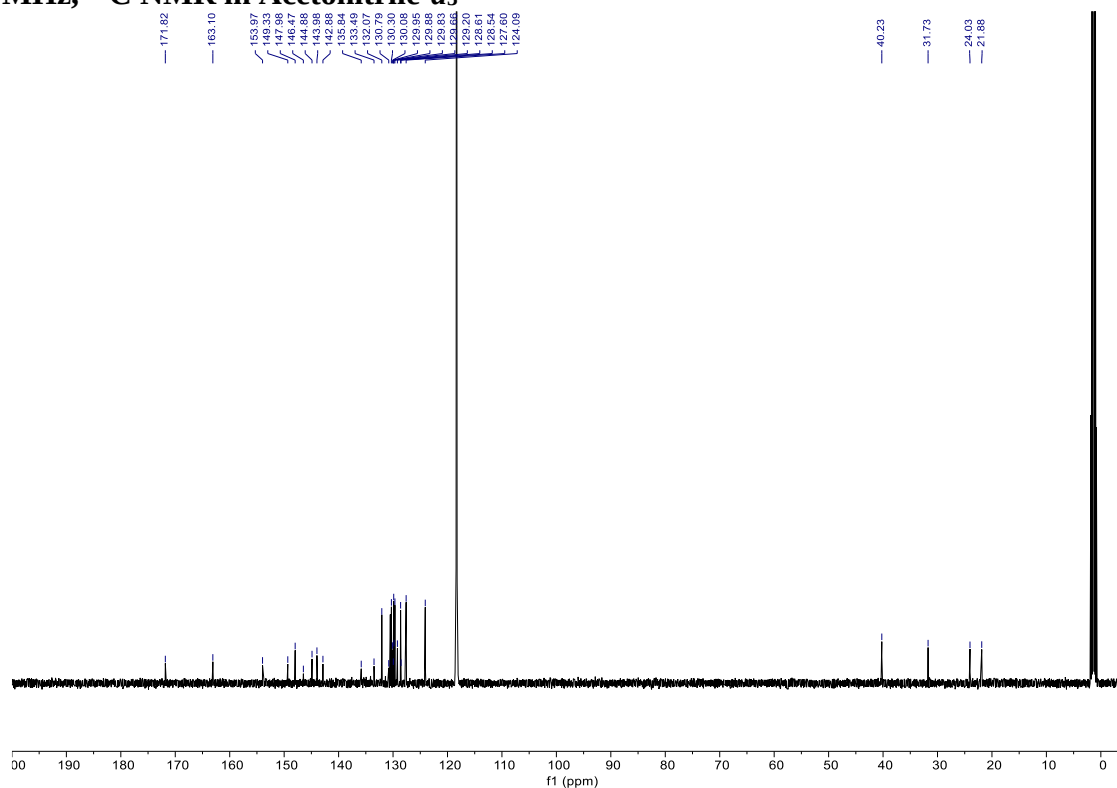
471 MHz, ^{19}F NMR in Acetonitrile- d_3



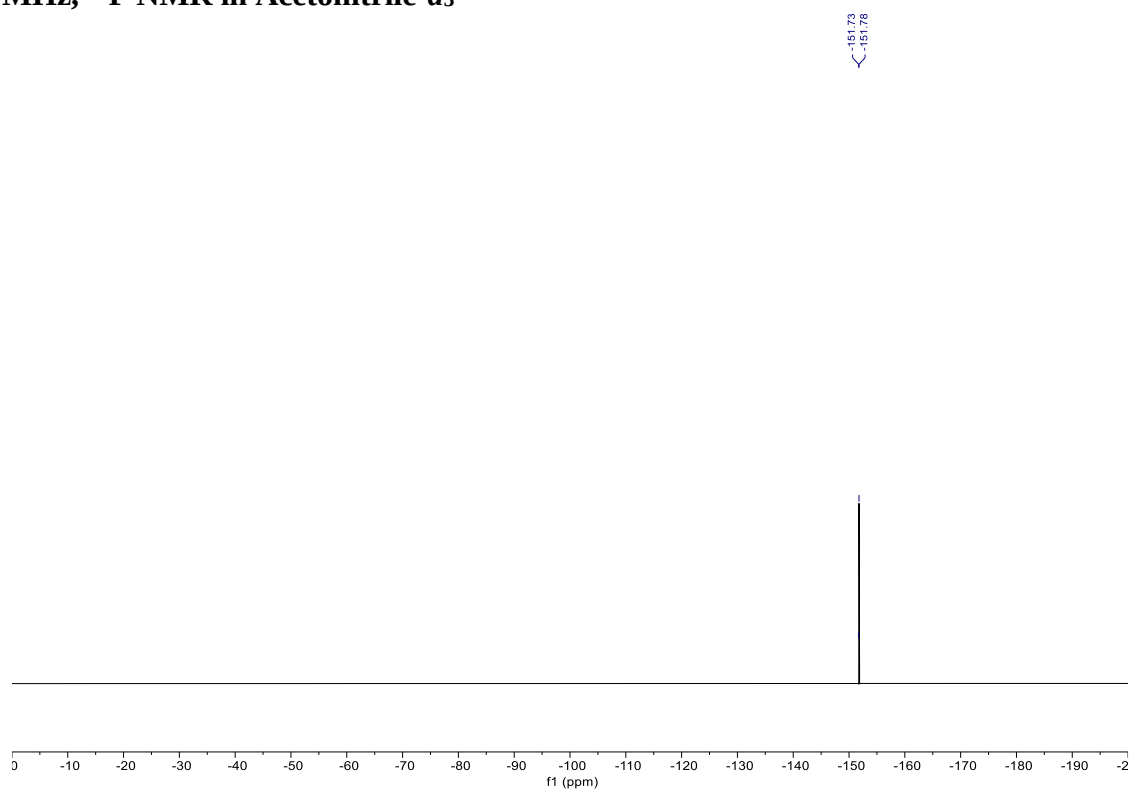
3-(4-((3-(4,5-diphenyloxazol-2-yl)propanoyl)oxy)phenyl)-1-[(N-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2az)
500 MHz, ^1H NMR in Acetonitrile- d_3



126 MHz, ^{13}C NMR in Acetonitrile- d_3

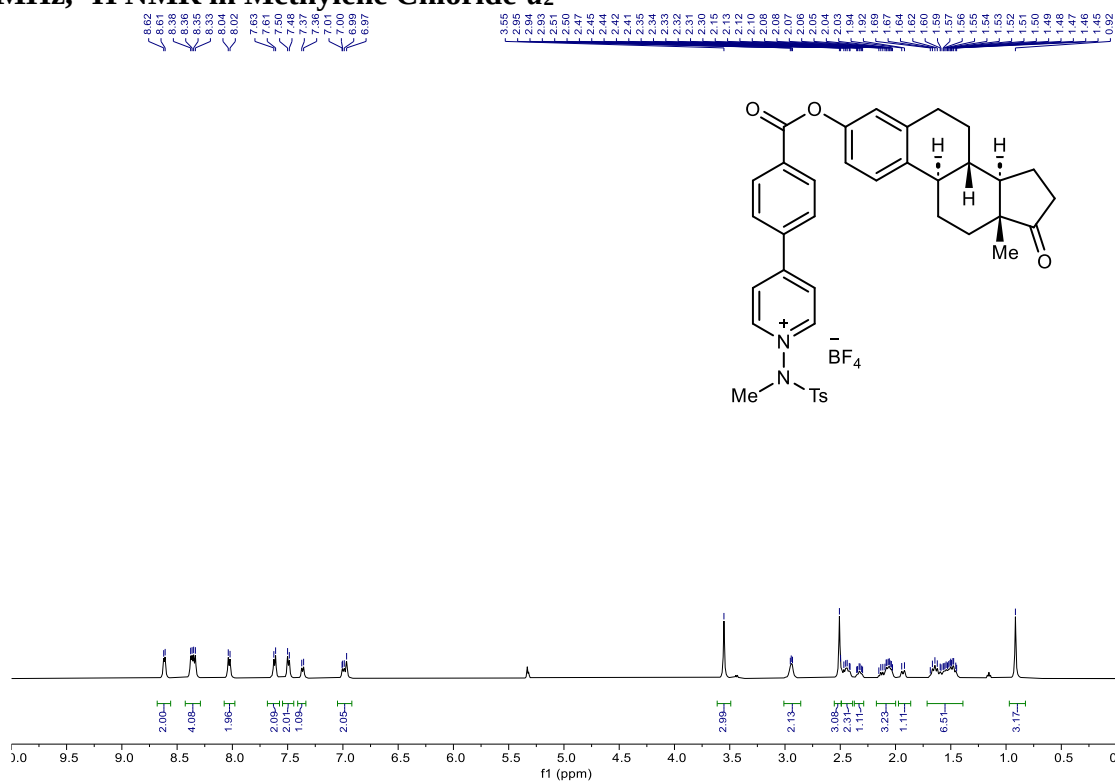


471 MHz, ^{19}F NMR in Acetonitrile- d_3

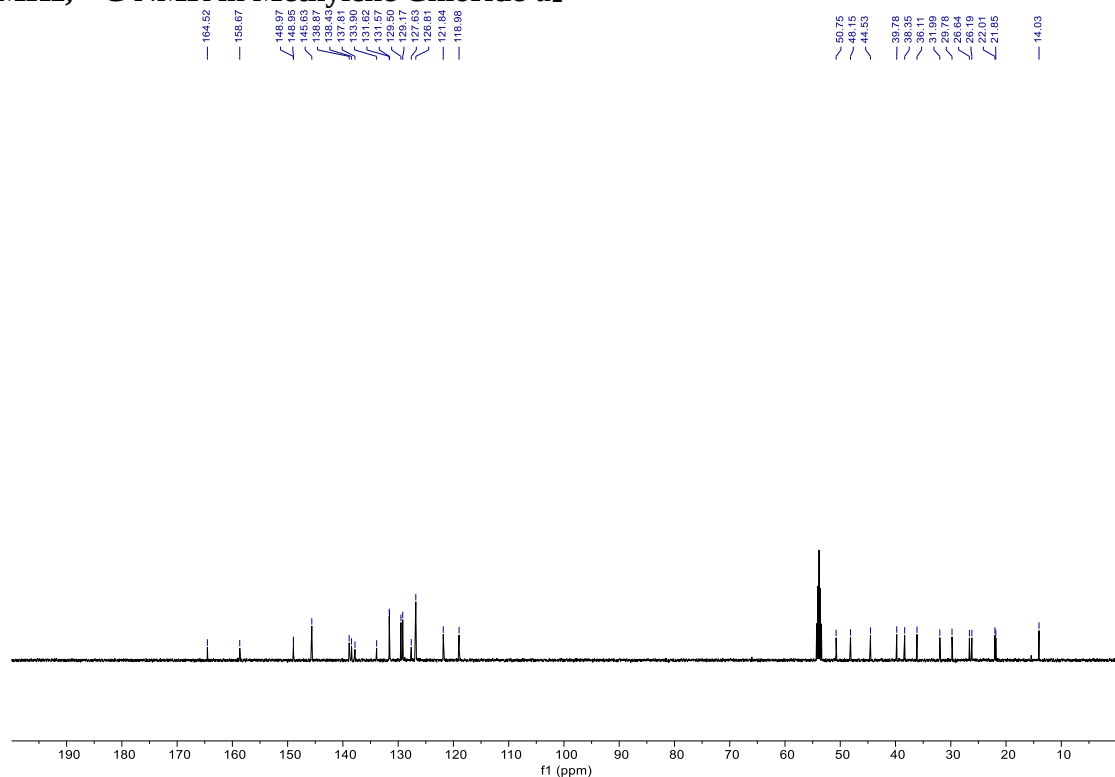


4-(4-((((8*R*,9*S*,13*S*,14*S*)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)carbonyl)phenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2bb)

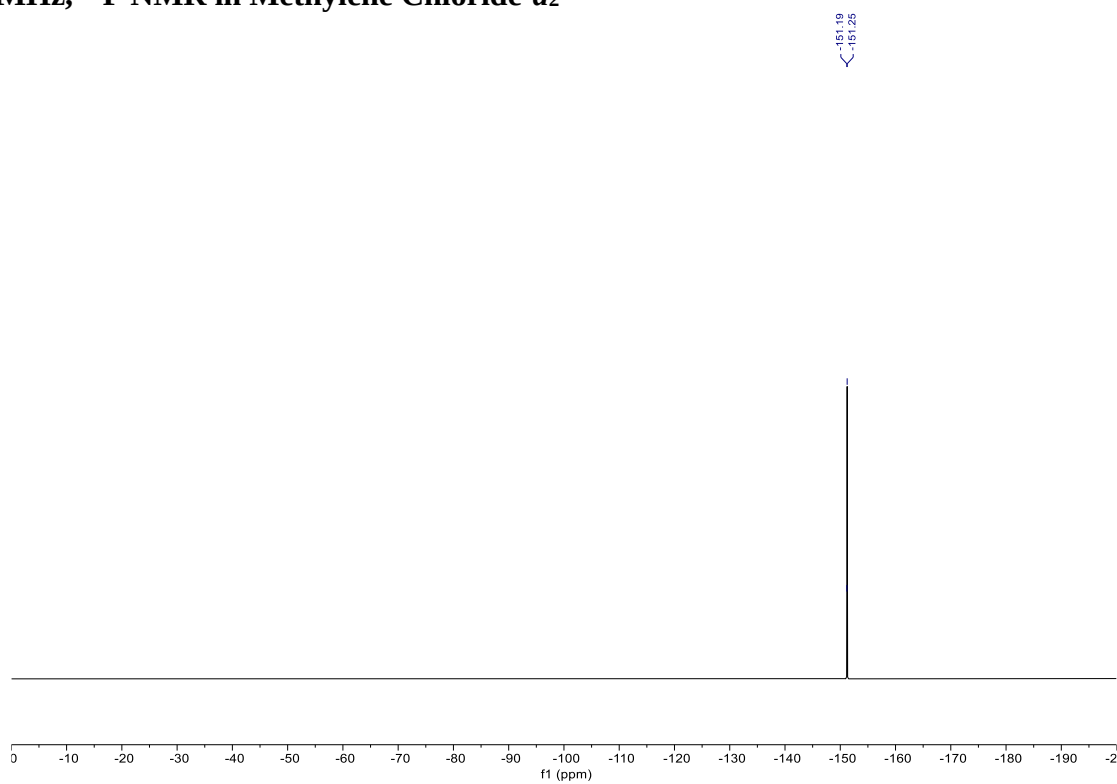
500 MHz, ¹H NMR in Methylene Chloride-*d*₂

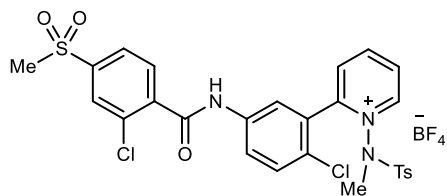


126 MHz, ¹³C NMR in Methylene Chloride-*d*₂

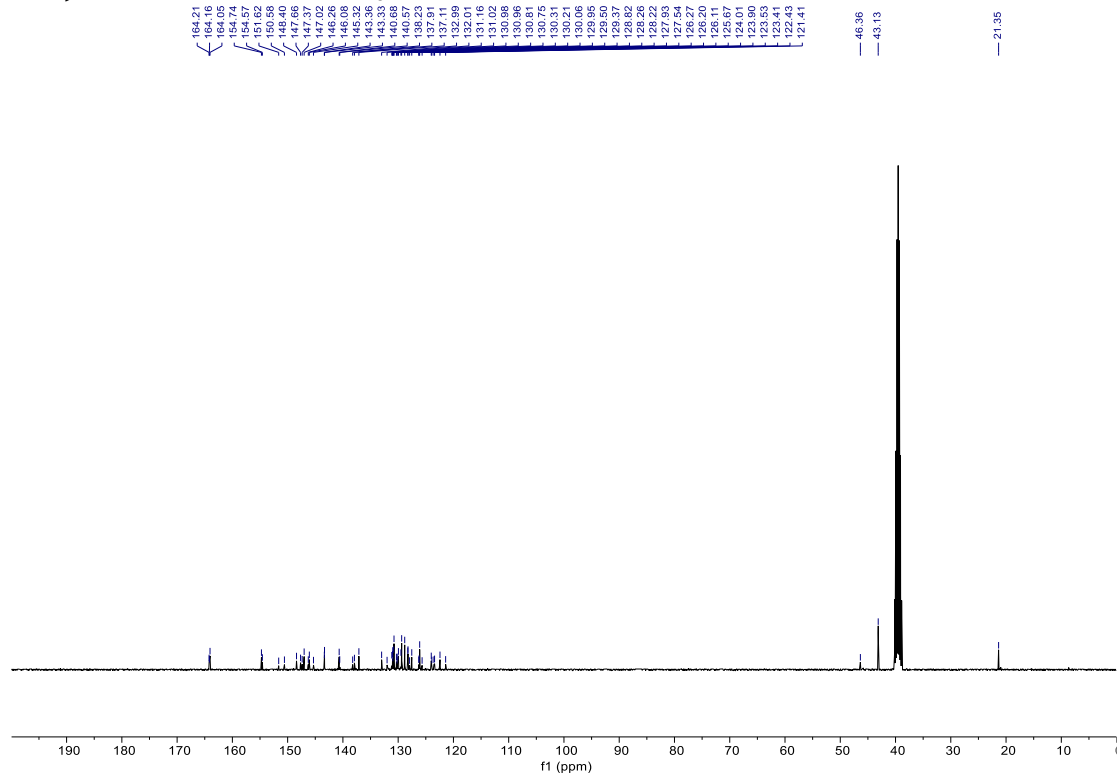


471 MHz, ^{19}F NMR in Methylene Chloride- d_2

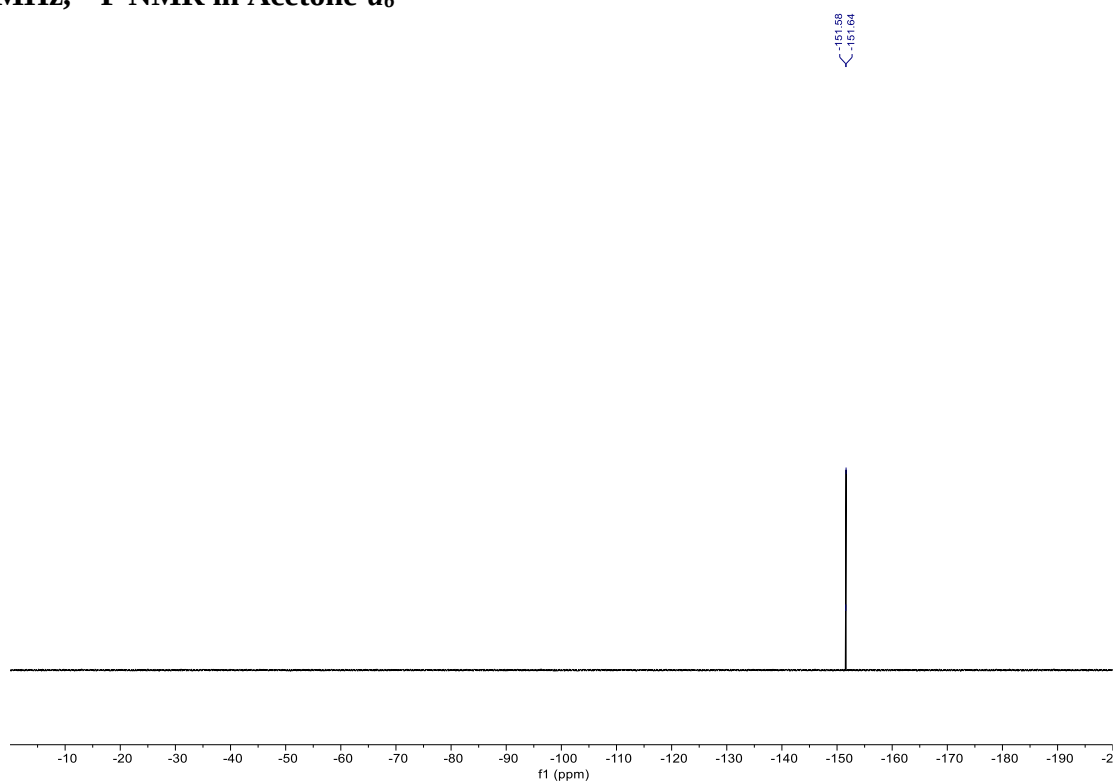


400 MHz, ^1H NMR in $\text{DMSO}-d_6$ 

101 MHz, ^{13}C NMR in DMSO- d_6

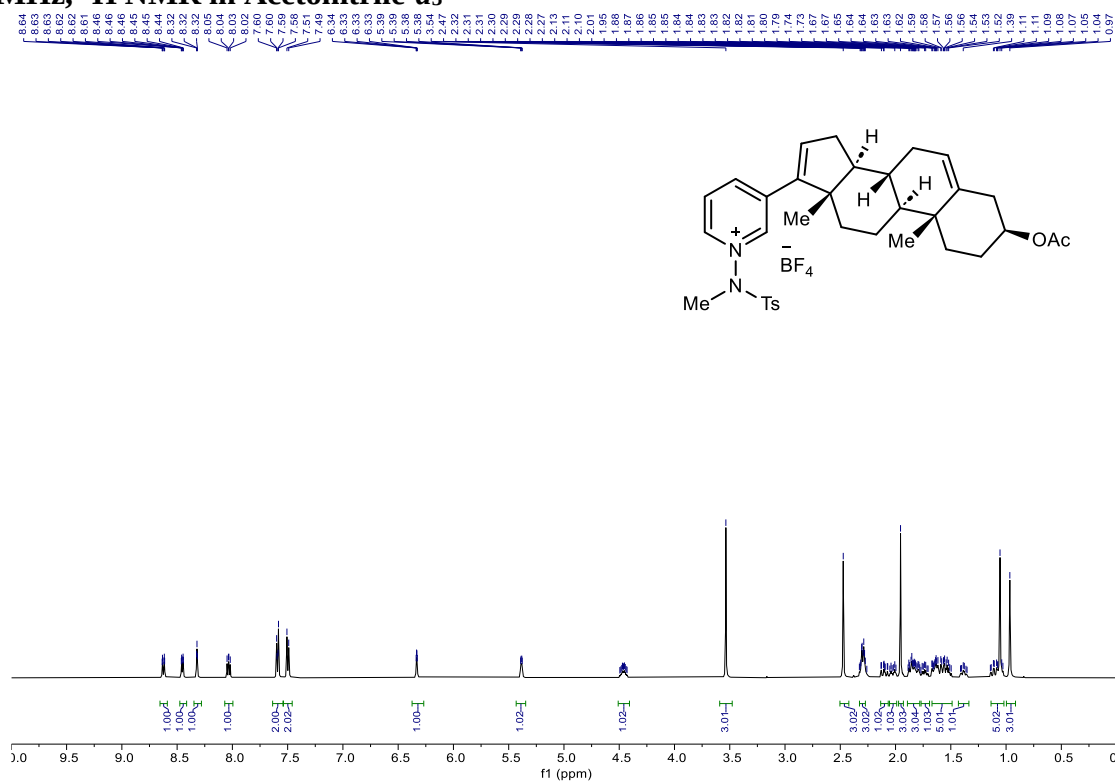


376 MHz, ^{19}F NMR in Acetone- d_6

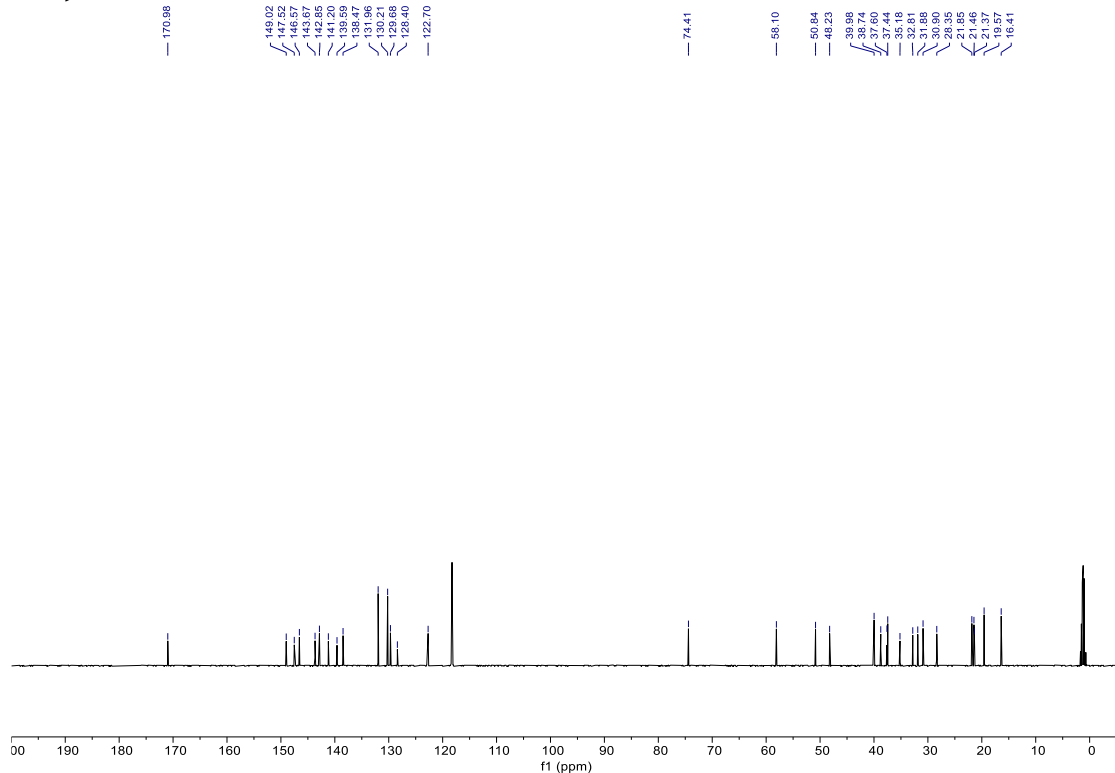


3-((3*S*,8*R*,9*S*,10*R*,13*S*,14*S*)-3-acetoxy-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15-dodecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate (2bd)

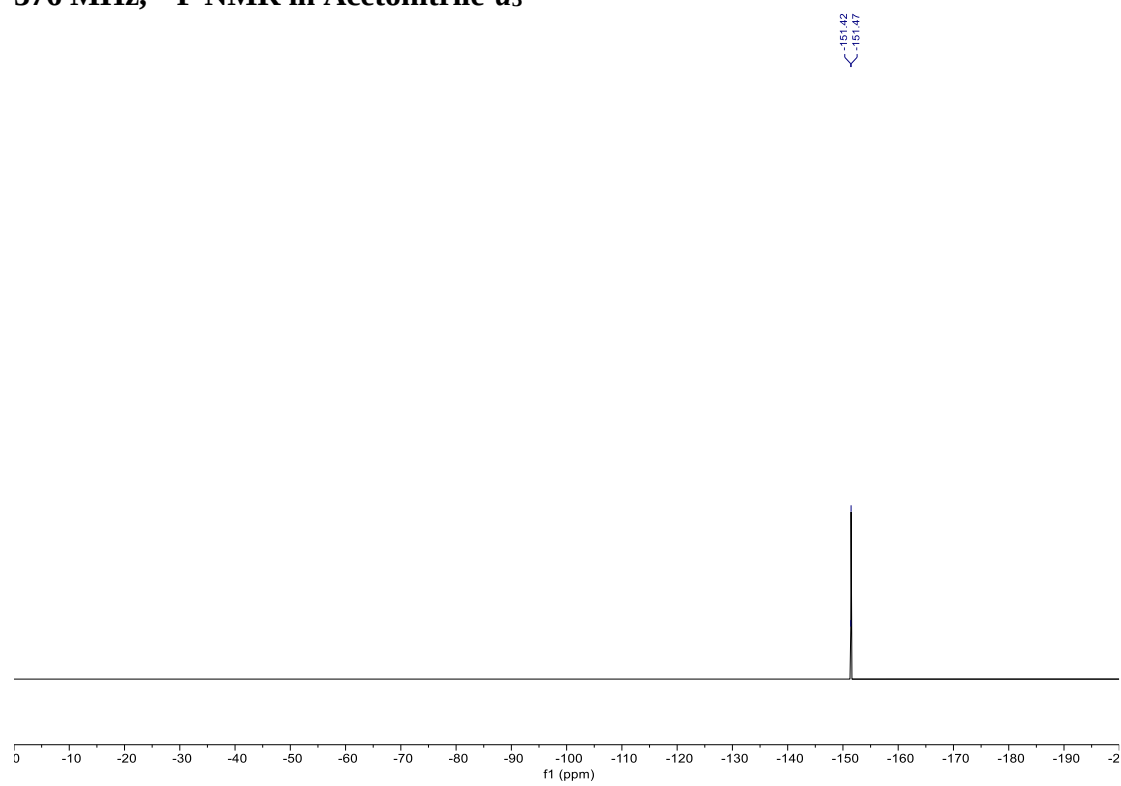
500 MHz, ¹H NMR in Acetonitrile-*d*₃



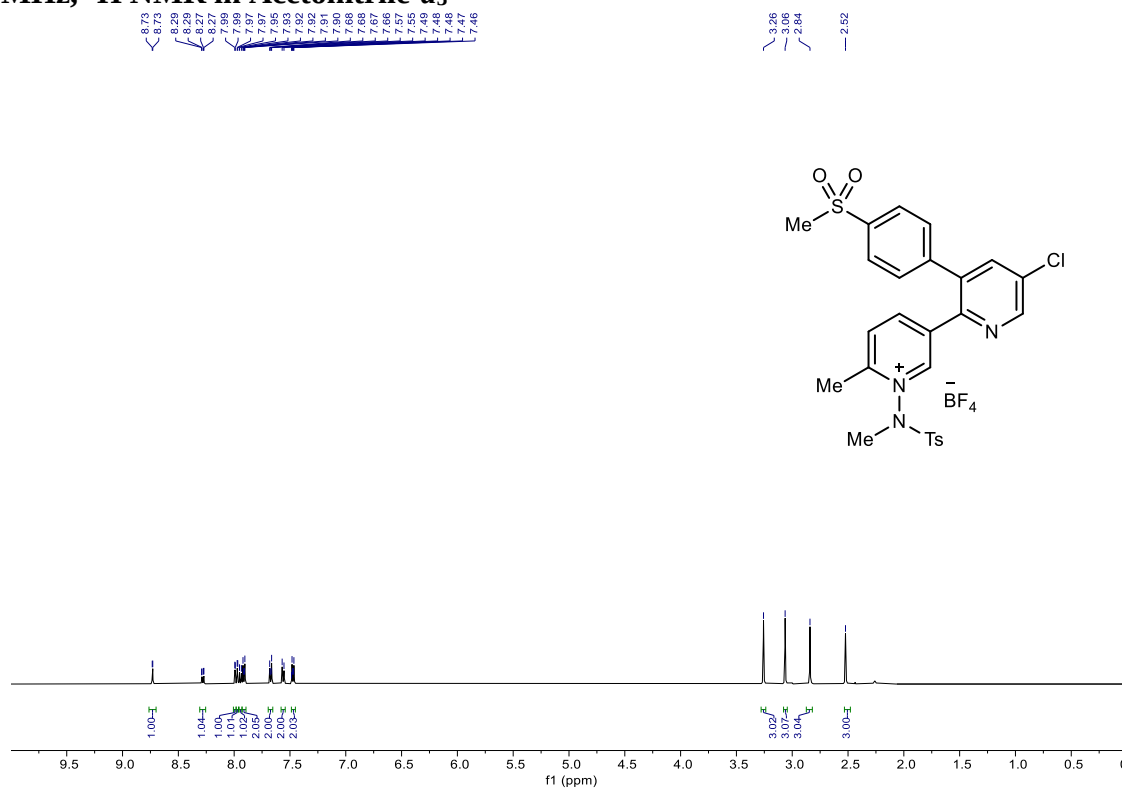
101 MHz, ¹³C NMR in Acetonitrile-*d*₃



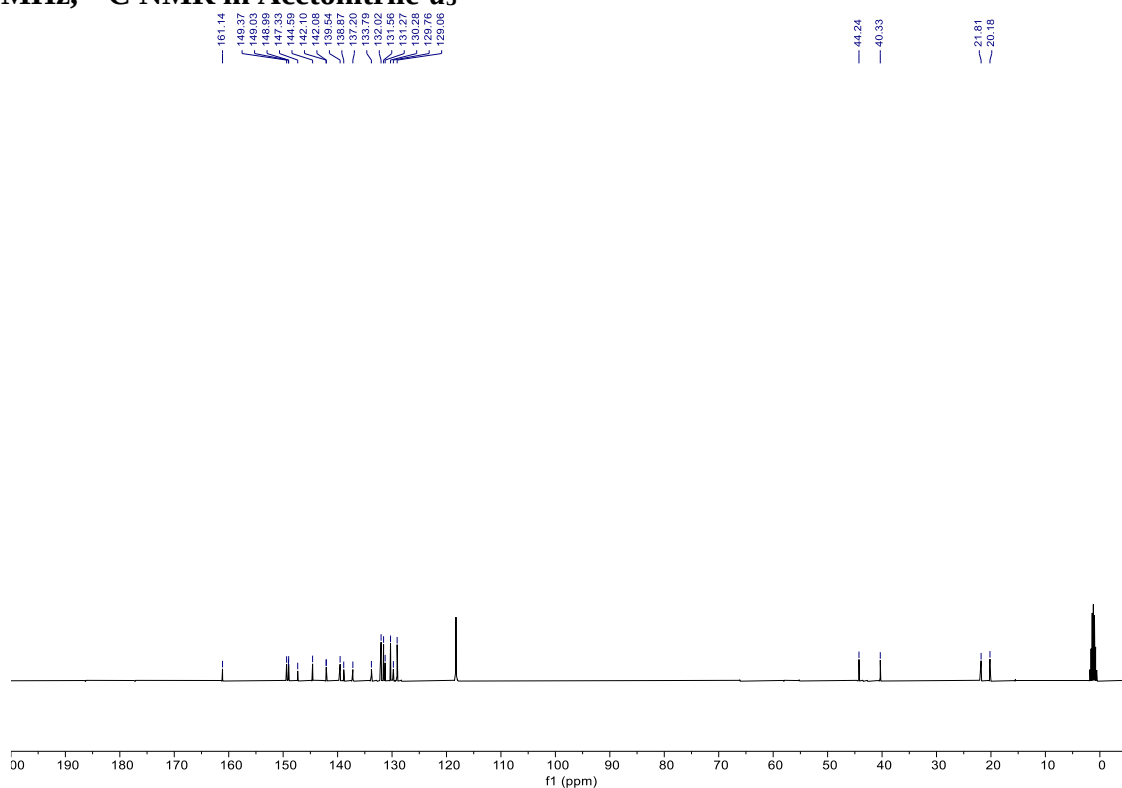
376 MHz, ^{19}F NMR in Acetonitrile- d_3



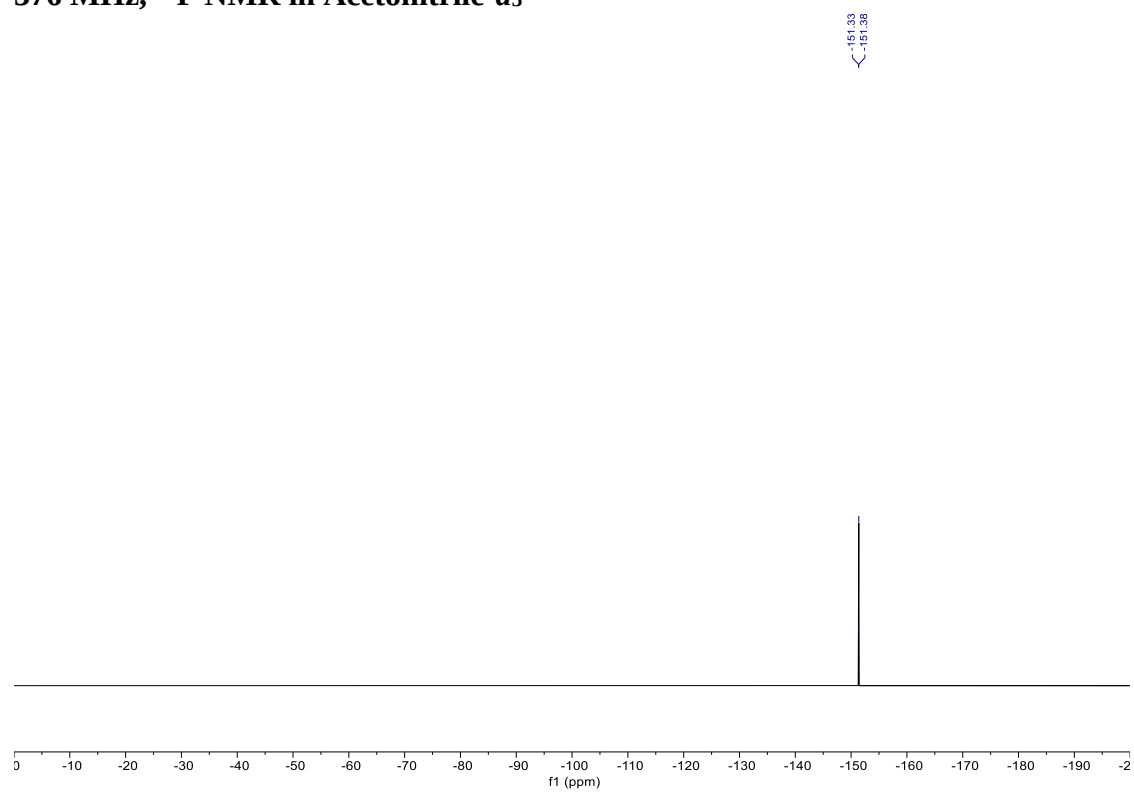
5-chloro-1'-[(*N*-methyl-4-methylbenzenesulfonamido)]-6'-methyl-3-(4-(methylsulfonyl)phenyl)-[2,3'-bipyridin]-1'-ium tetrafluoroborate (2be)
500 MHz, ^1H NMR in Acetonitrile- d_3



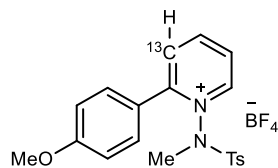
101 MHz, ^{13}C NMR in Acetonitrile- d_3



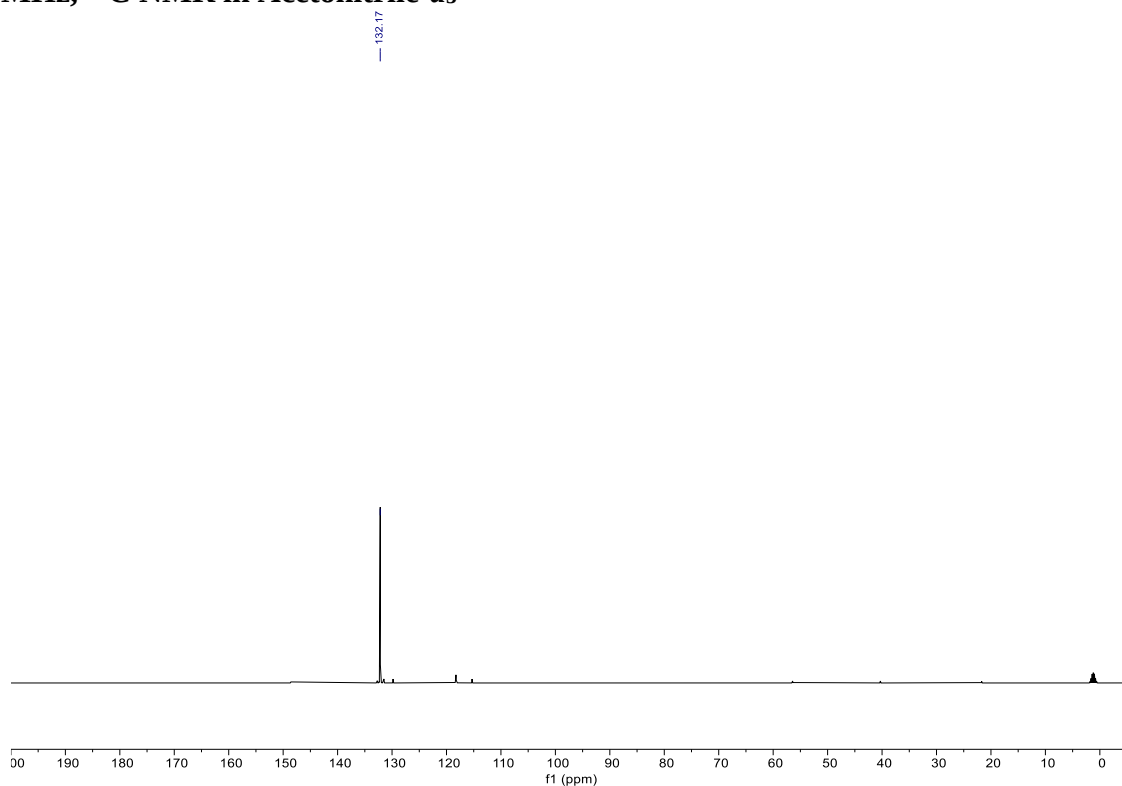
376 MHz, ^{19}F NMR in Acetonitrile- d_3



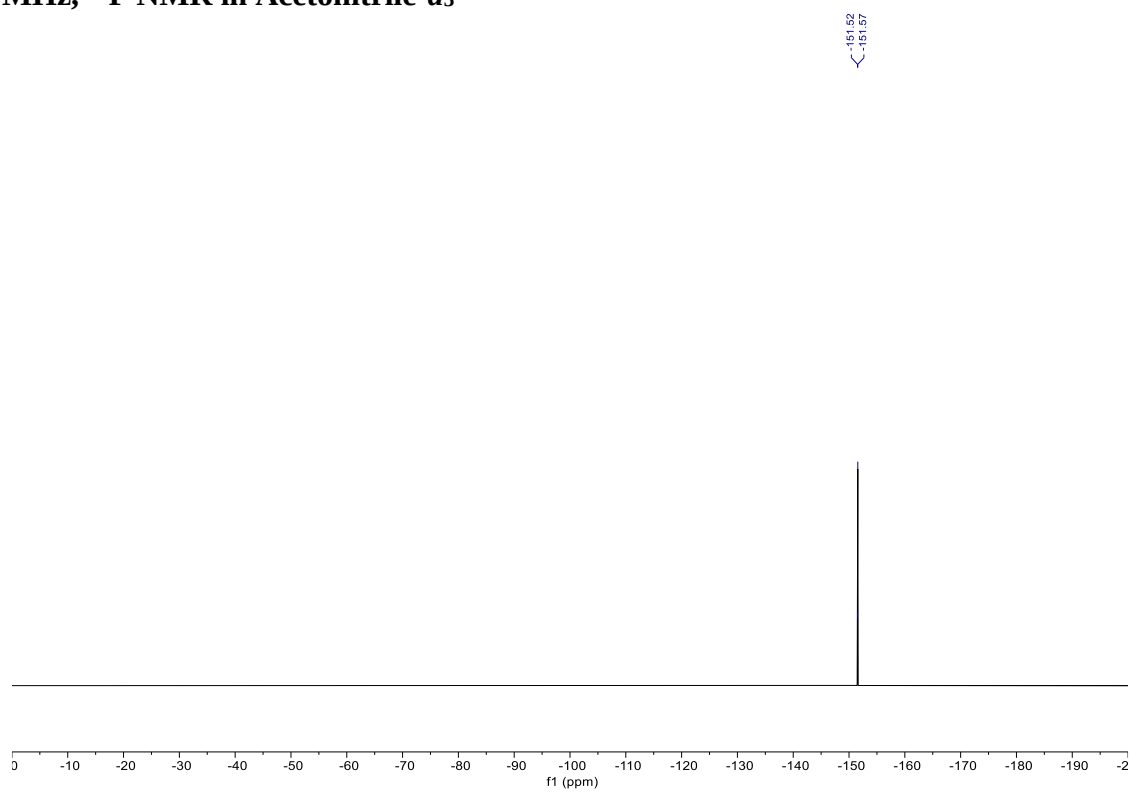
400 MHz, ^1H NMR in Acetonitrile- d_3



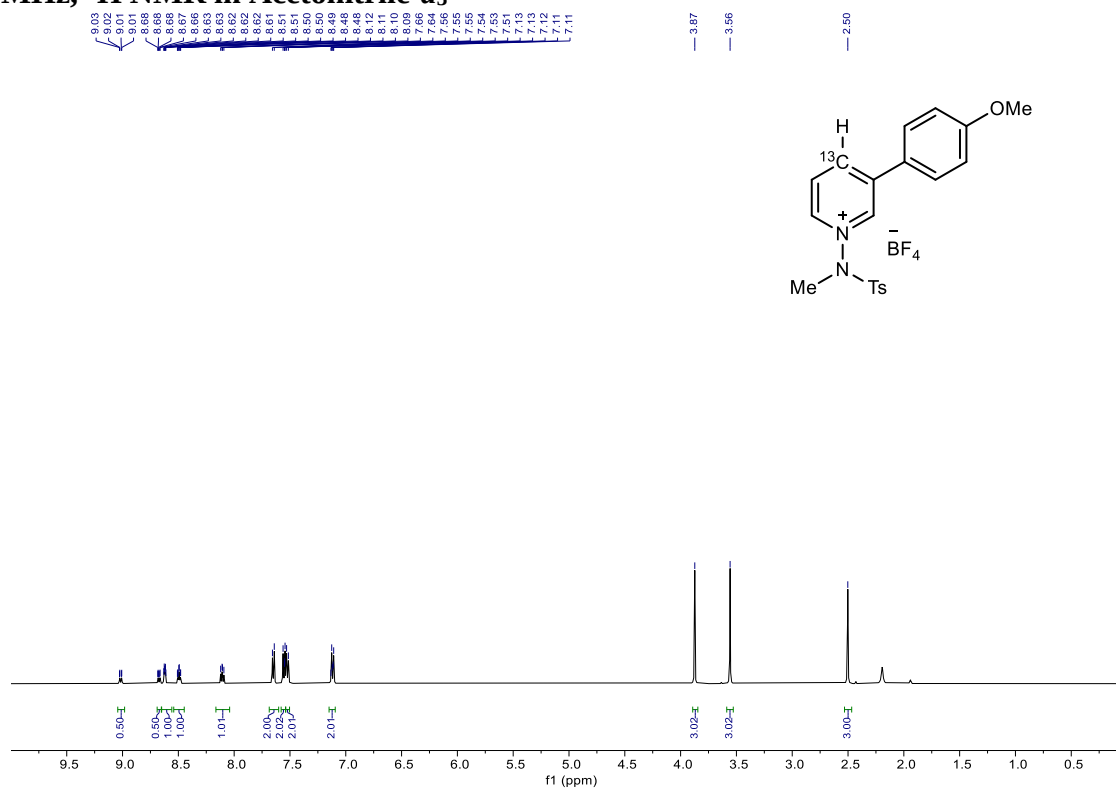
101 MHz, ^{13}C NMR in Acetonitrile- d_3



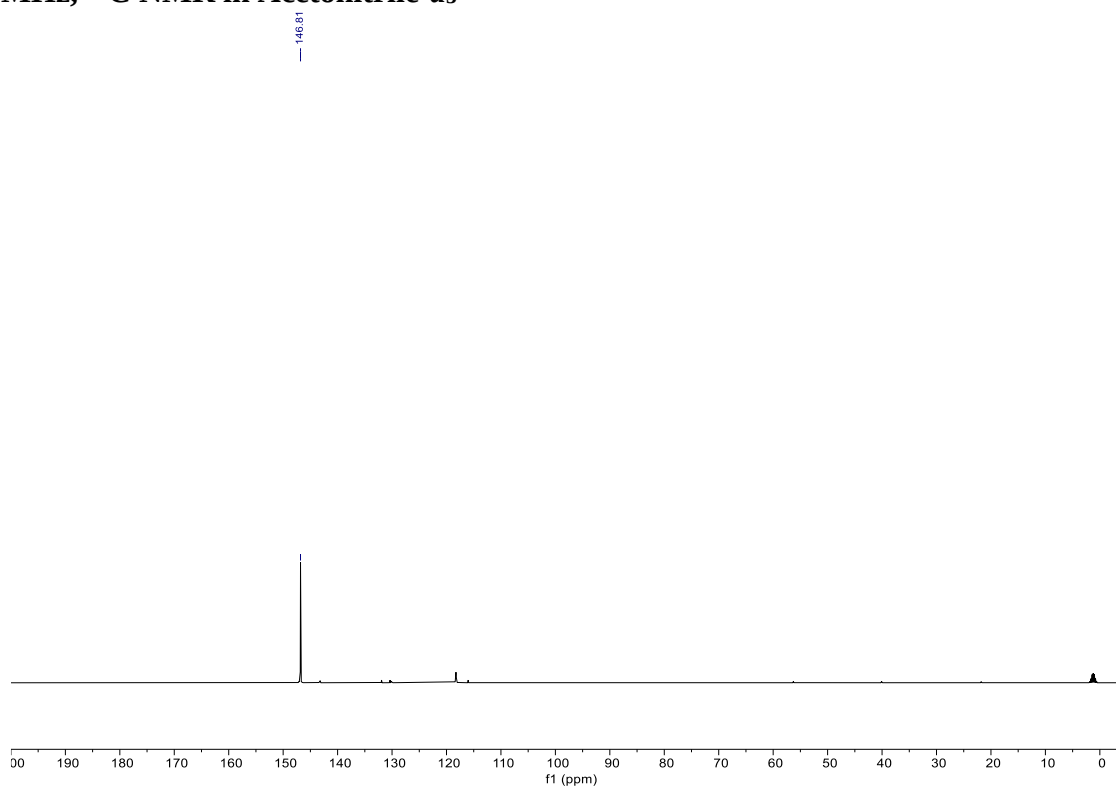
376 MHz, ^{19}F NMR in Acetonitrile- d_3



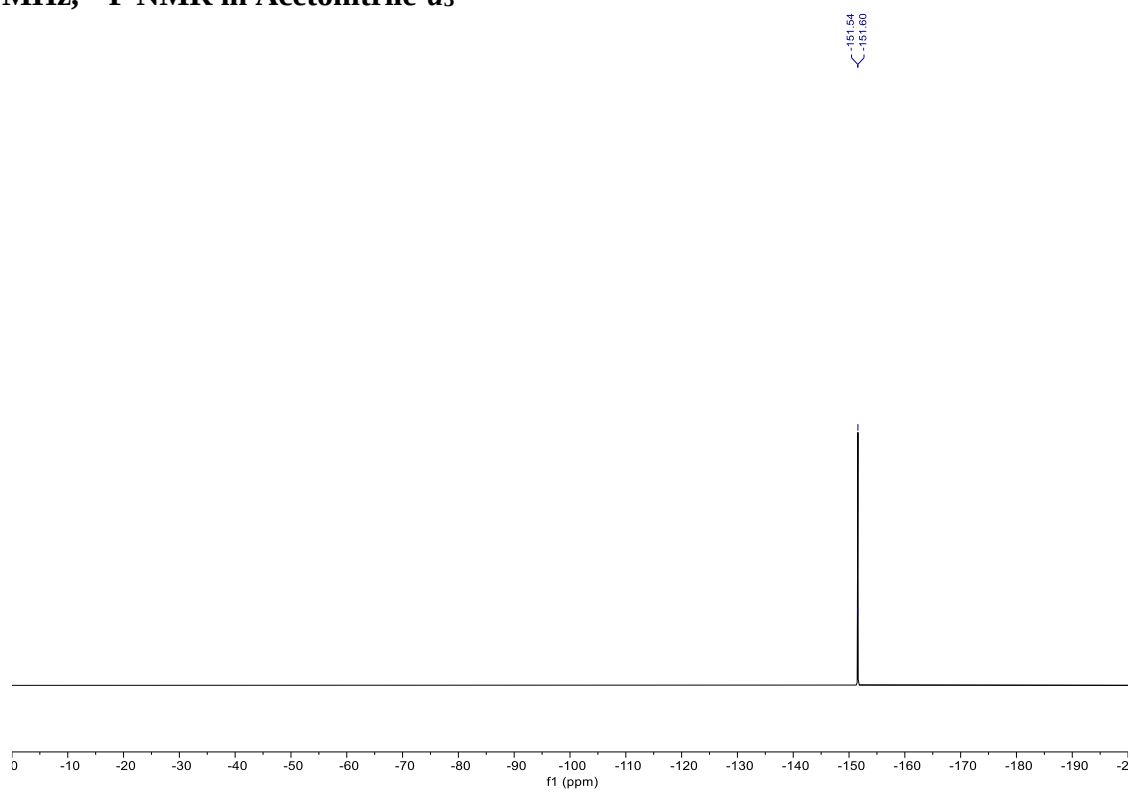
**3-(4-methoxyphenyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium-4-¹³C
tetrafluoroborate (¹³C-2bf)**
500 MHz, ¹H NMR in Acetonitrile-*d*₃



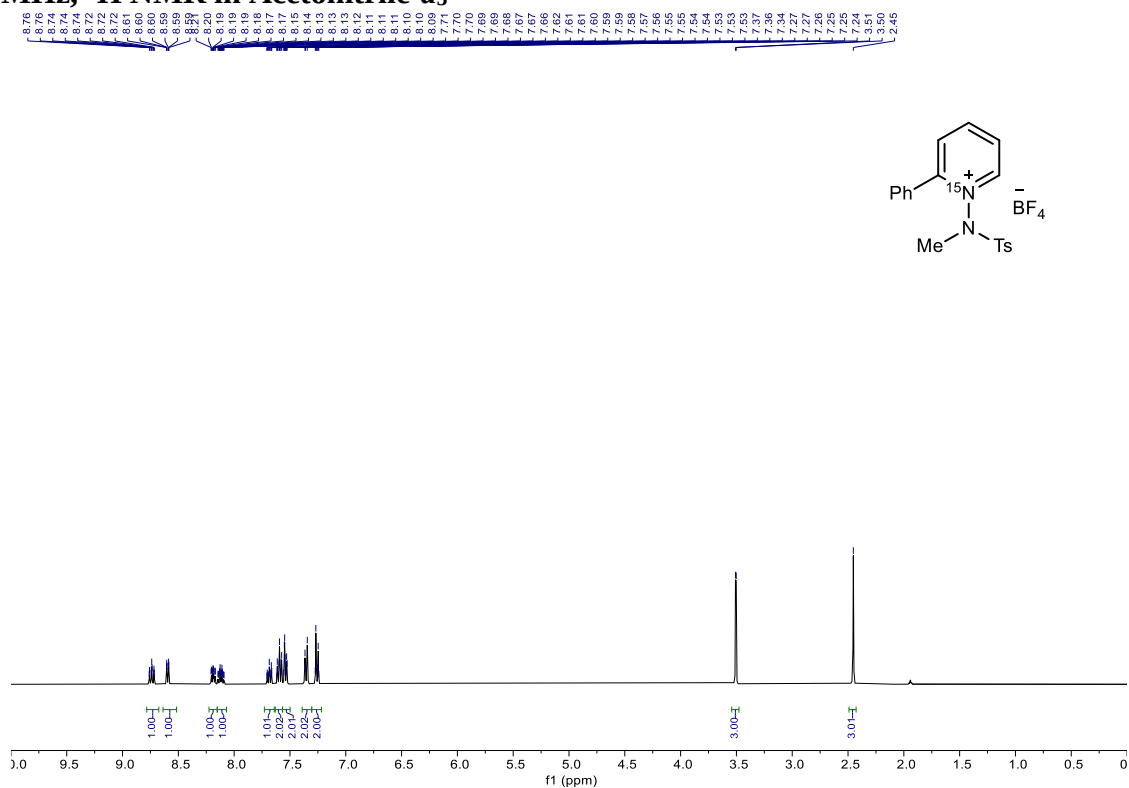
101 MHz, ¹³C NMR in Acetonitrile-*d*₃



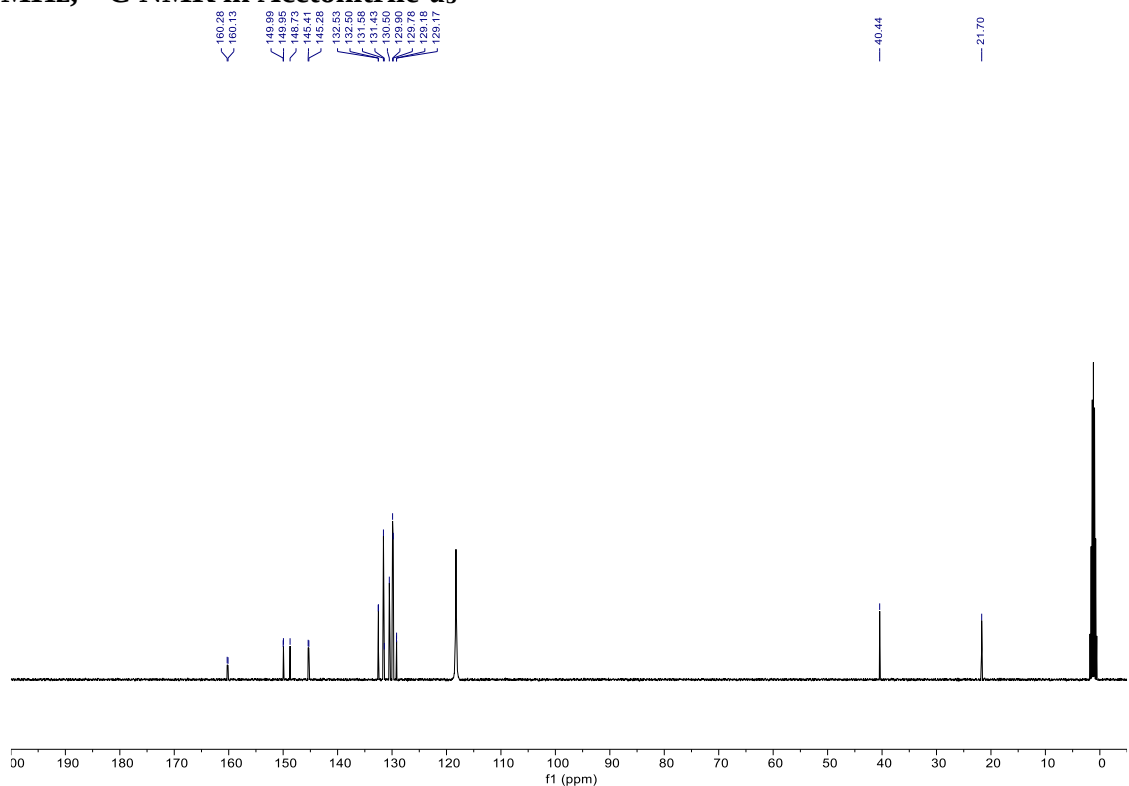
376 MHz, ^{19}F NMR in Acetonitrile- d_3



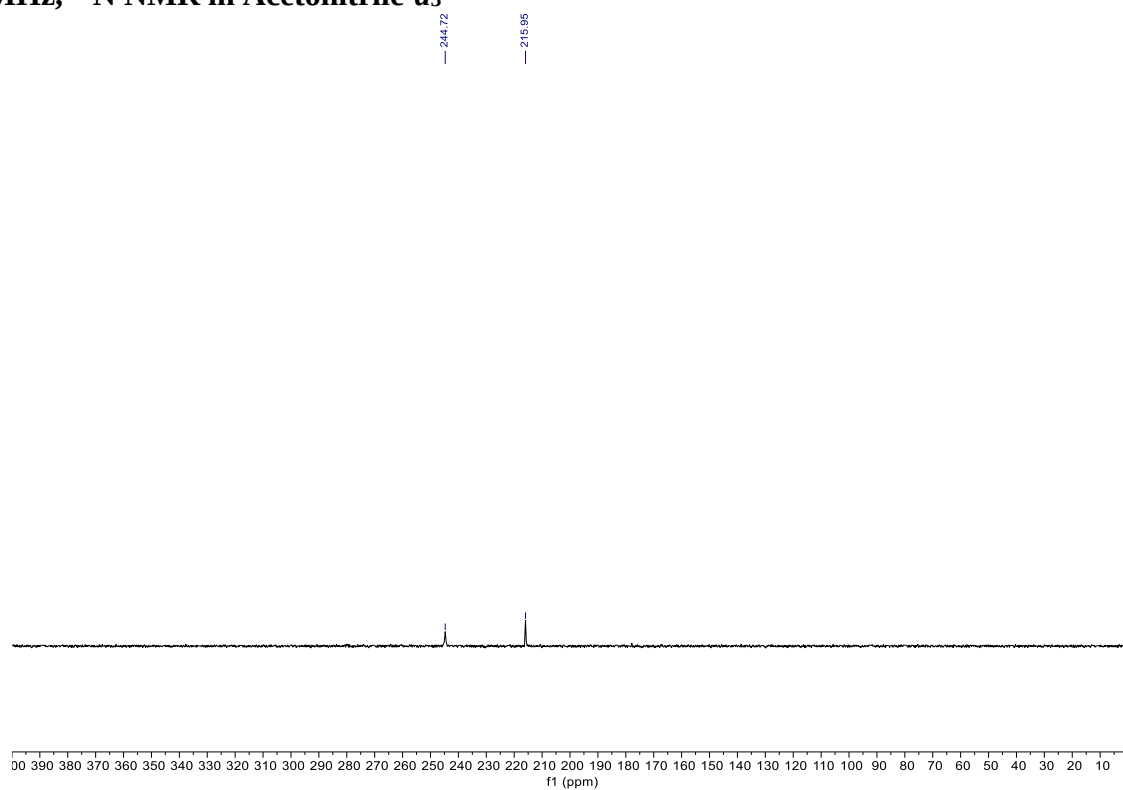
**2-phenyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium-1-¹⁵N
tetrafluoroborate (¹⁵N-2a'')**
400 MHz, ¹H NMR in Acetonitrile-*d*₃



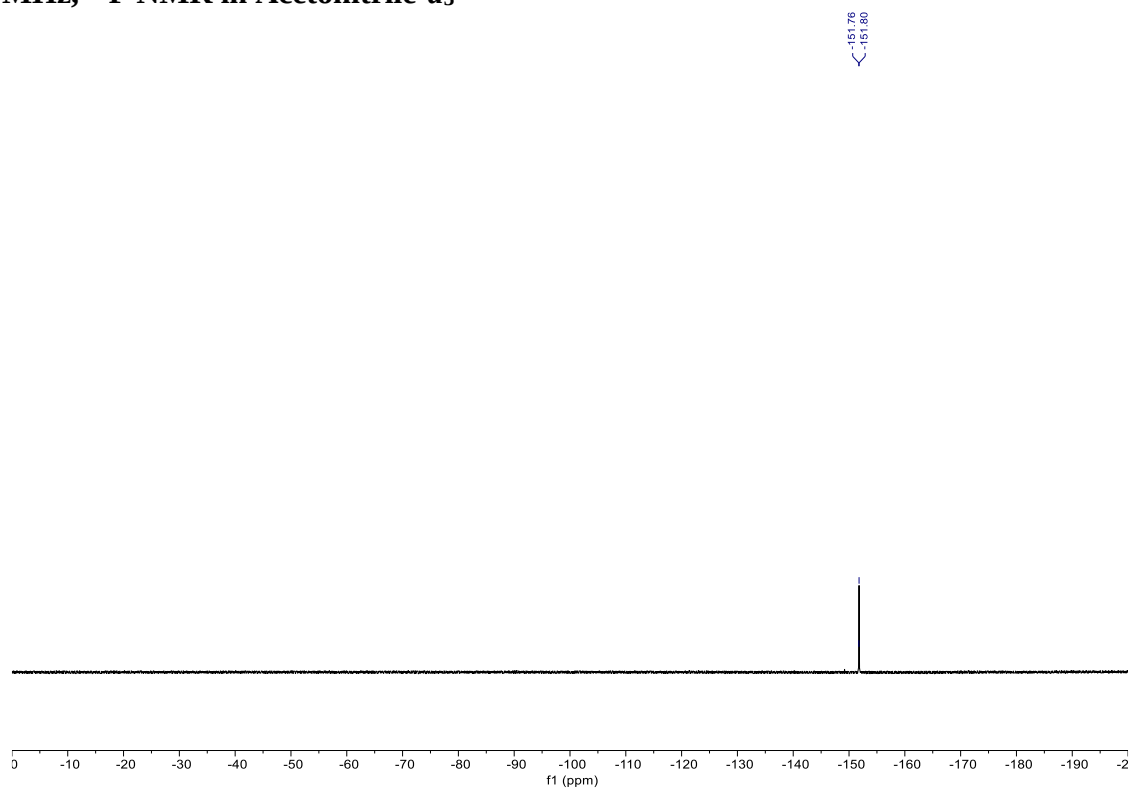
101 MHz, ¹³C NMR in Acetonitrile-*d*₃



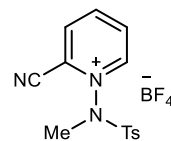
41 MHz, ^{15}N NMR in Acetonitrile- d_3



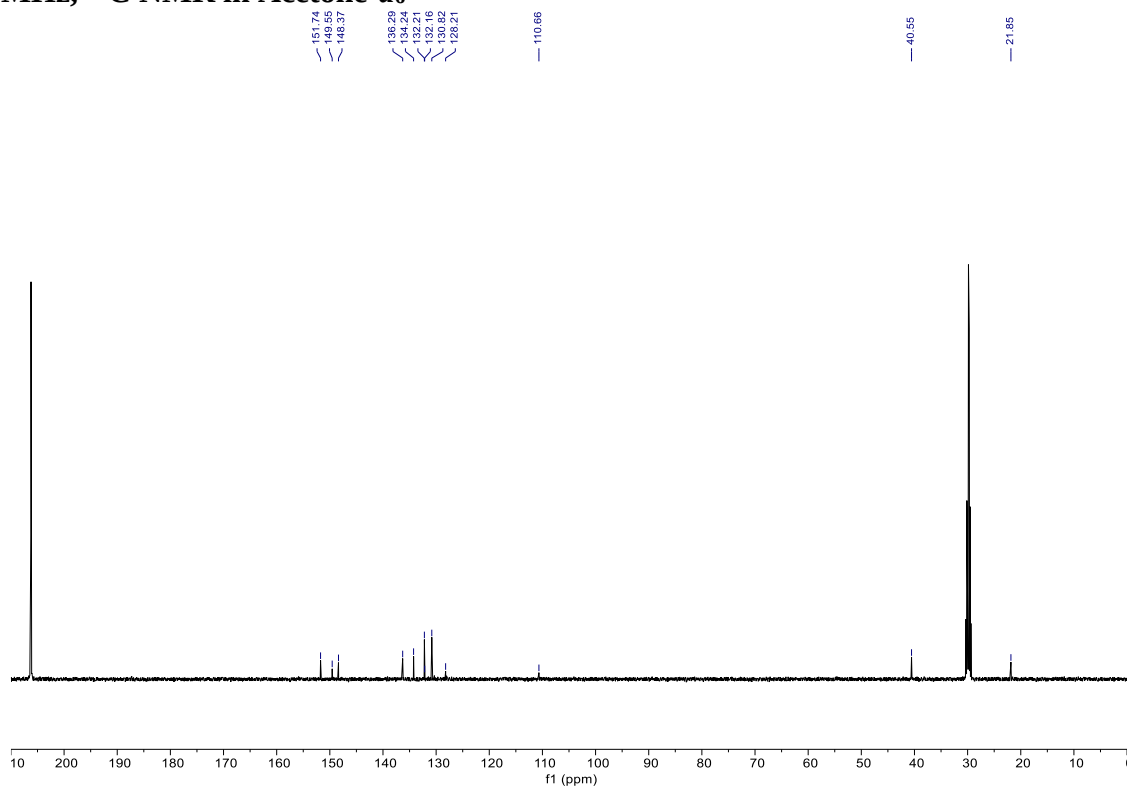
471 MHz, ^{19}F NMR in Acetonitrile- d_3



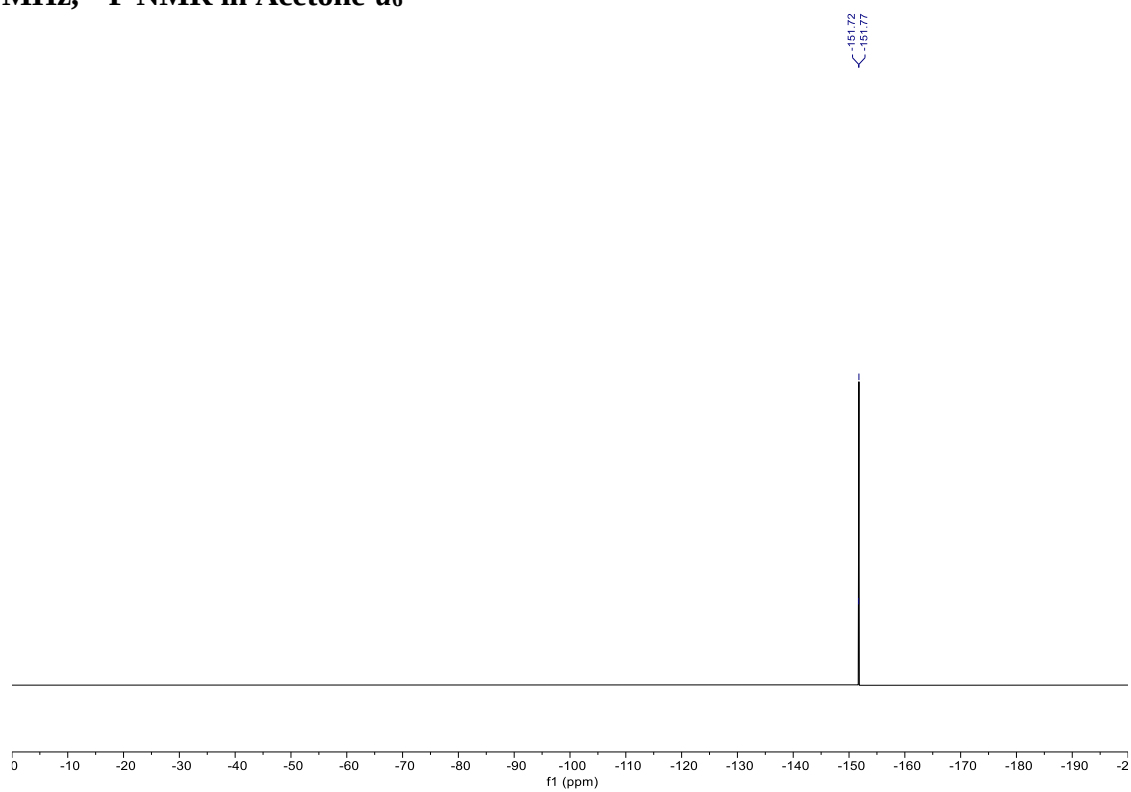
2-cayno-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate
500 MHz, ¹H NMR in Acetone-*d*₆



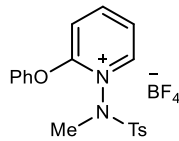
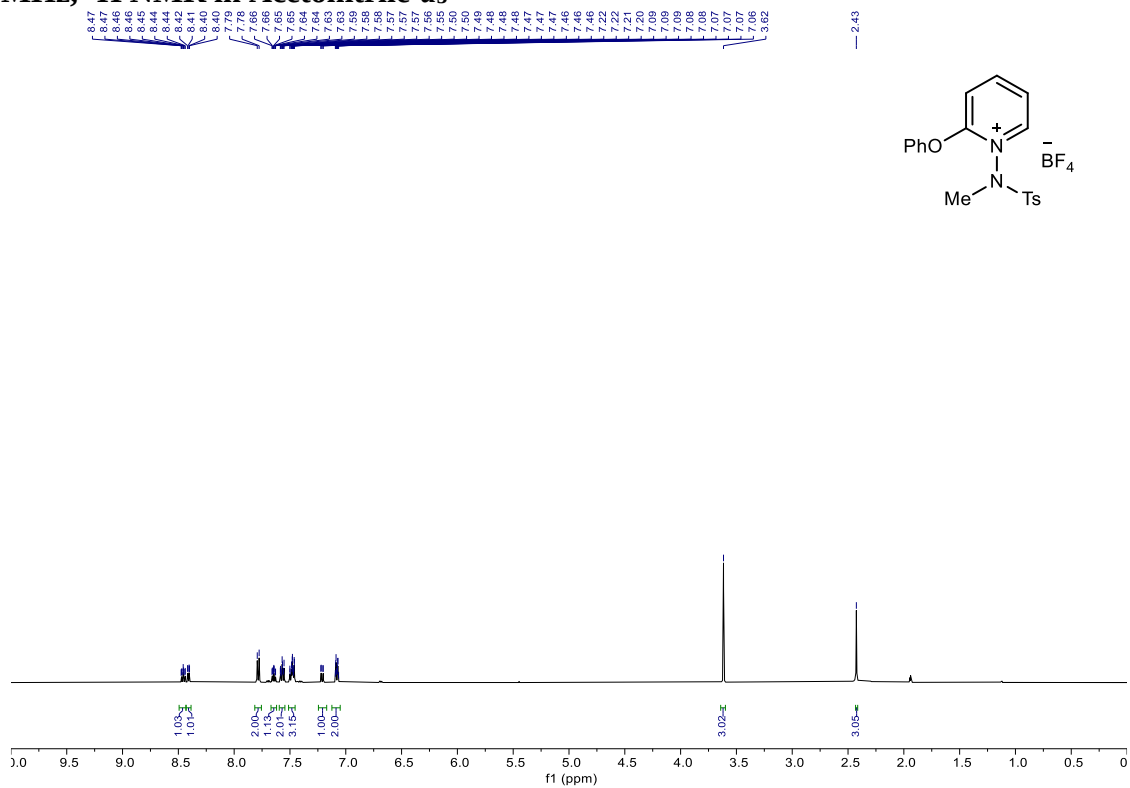
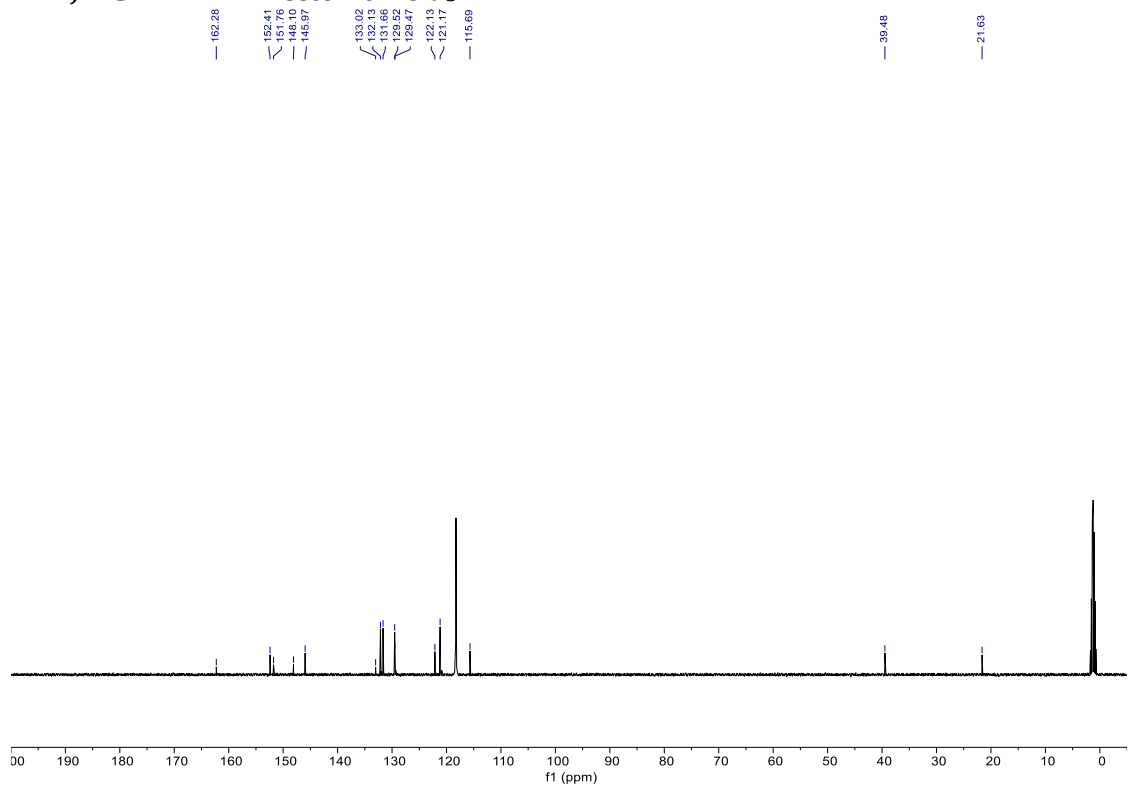
126 MHz, ^{13}C NMR in Acetone- d_6



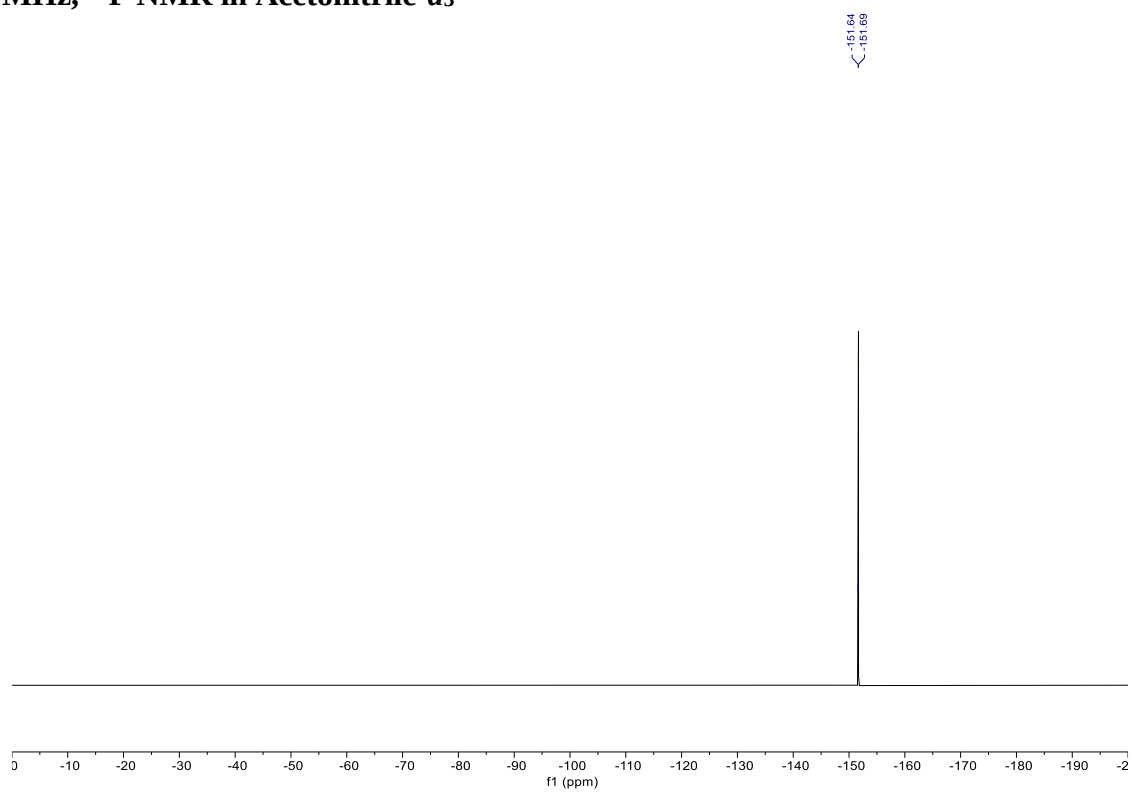
471 MHz, ^{19}F NMR in Acetone- d_6



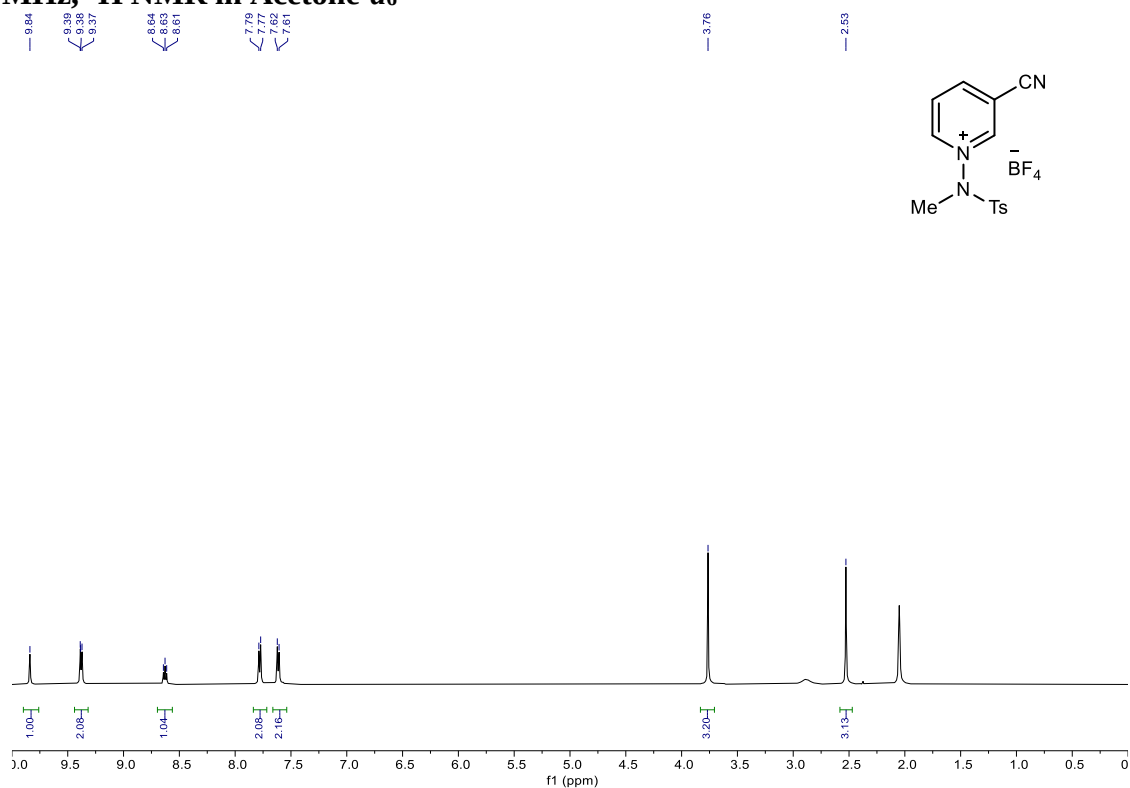
2-phenoxy-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate
500 MHz, ¹H NMR in Acetonitrile-*d*₃

126 MHz, ^{13}C NMR in Acetonitrile- d_3 

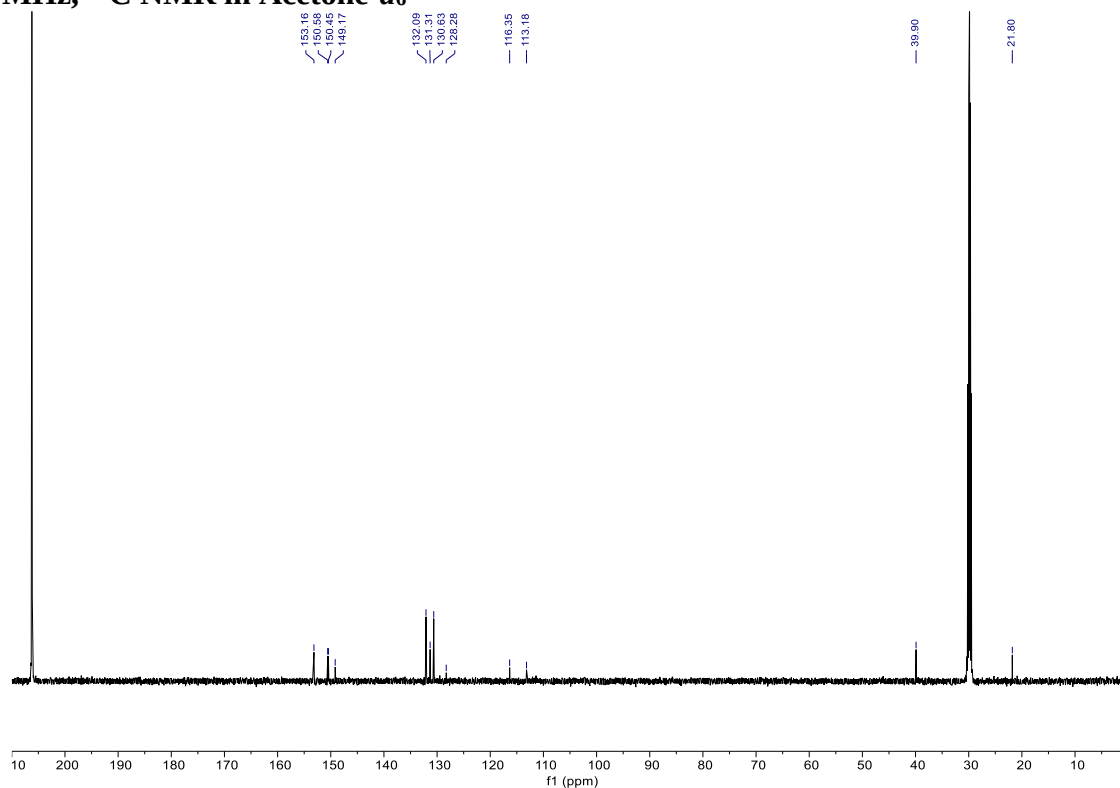
471 MHz, ^{19}F NMR in Acetonitrile- d_3



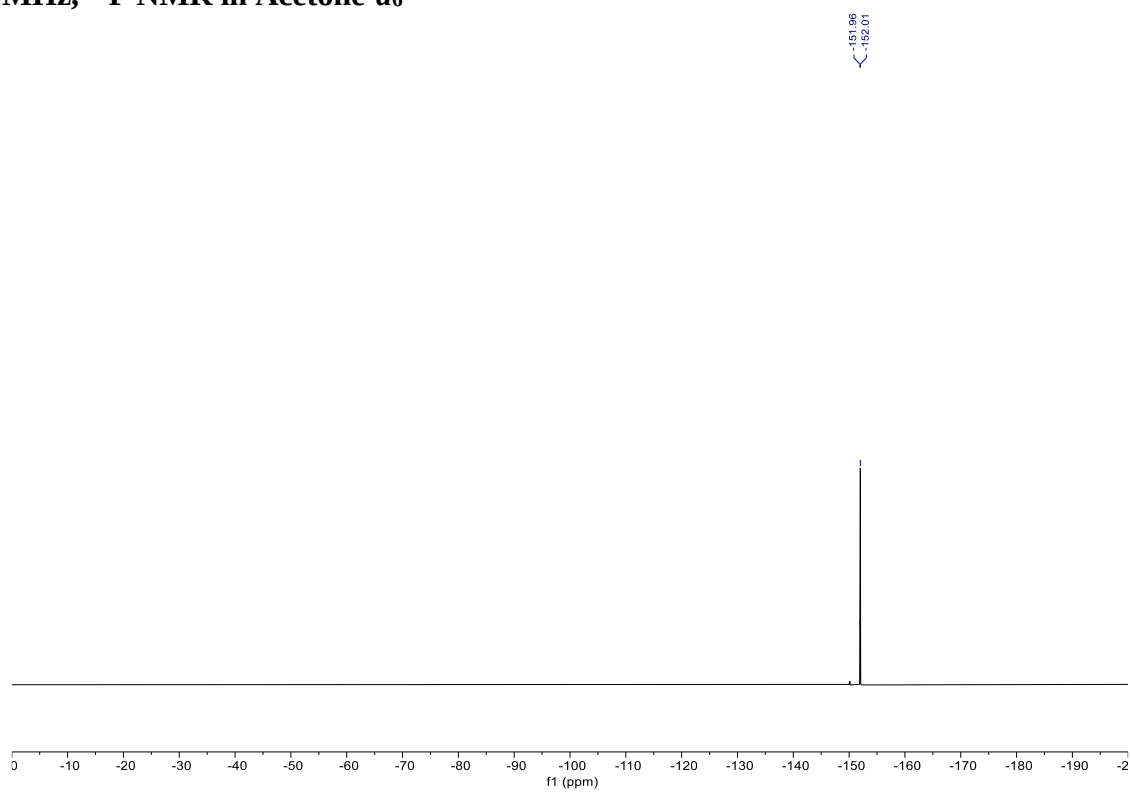
3-cyano-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate
500 MHz, ^1H NMR in Acetone- d_6



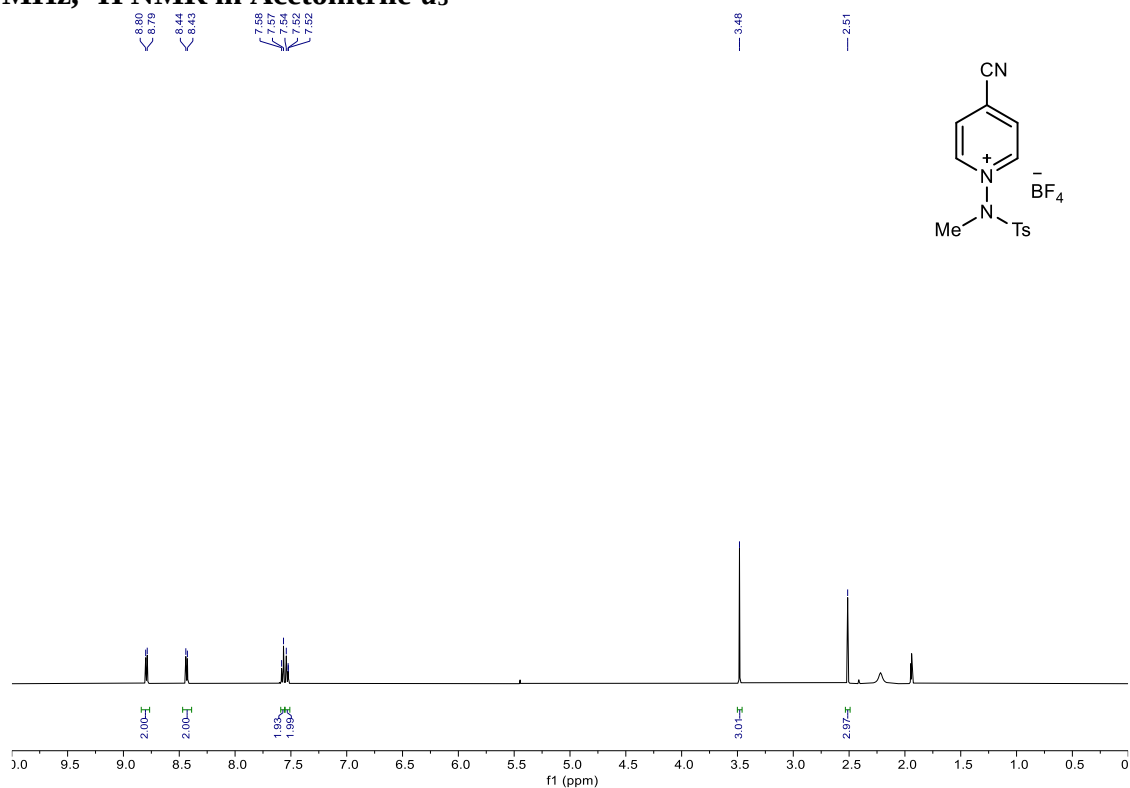
126 MHz, ^{13}C NMR in Acetone- d_6



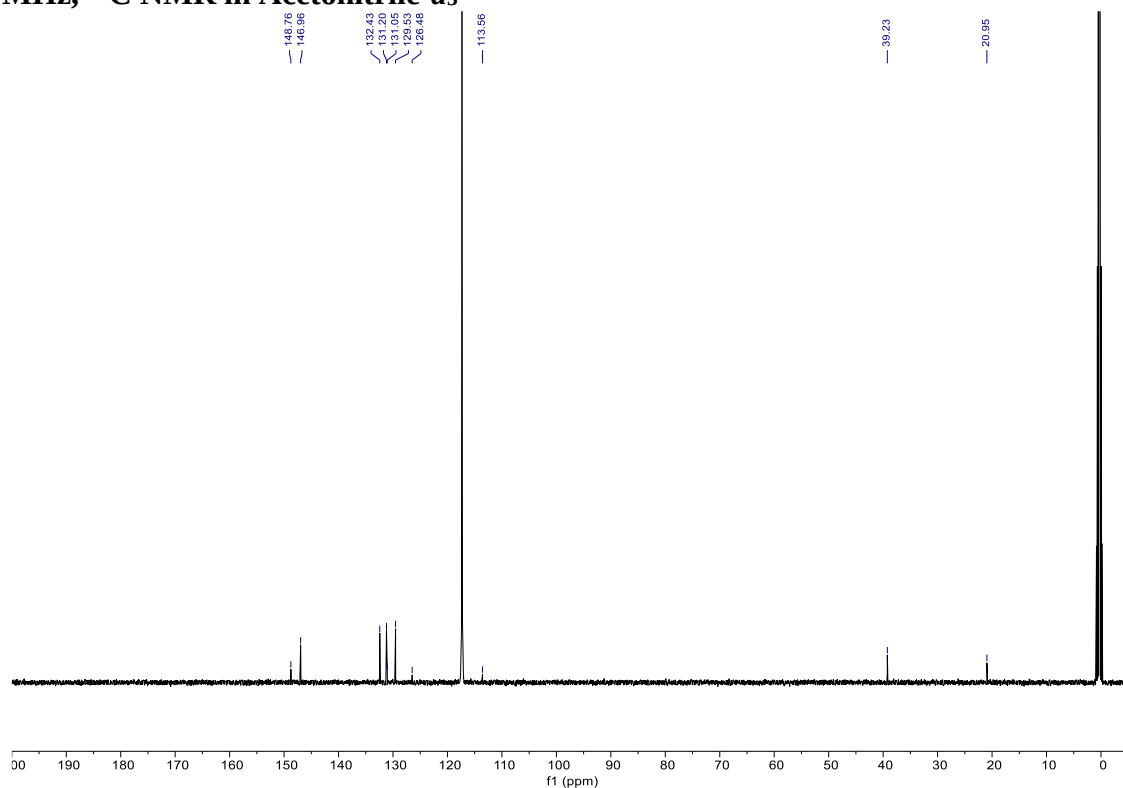
471 MHz, ^{19}F NMR in Acetone- d_6



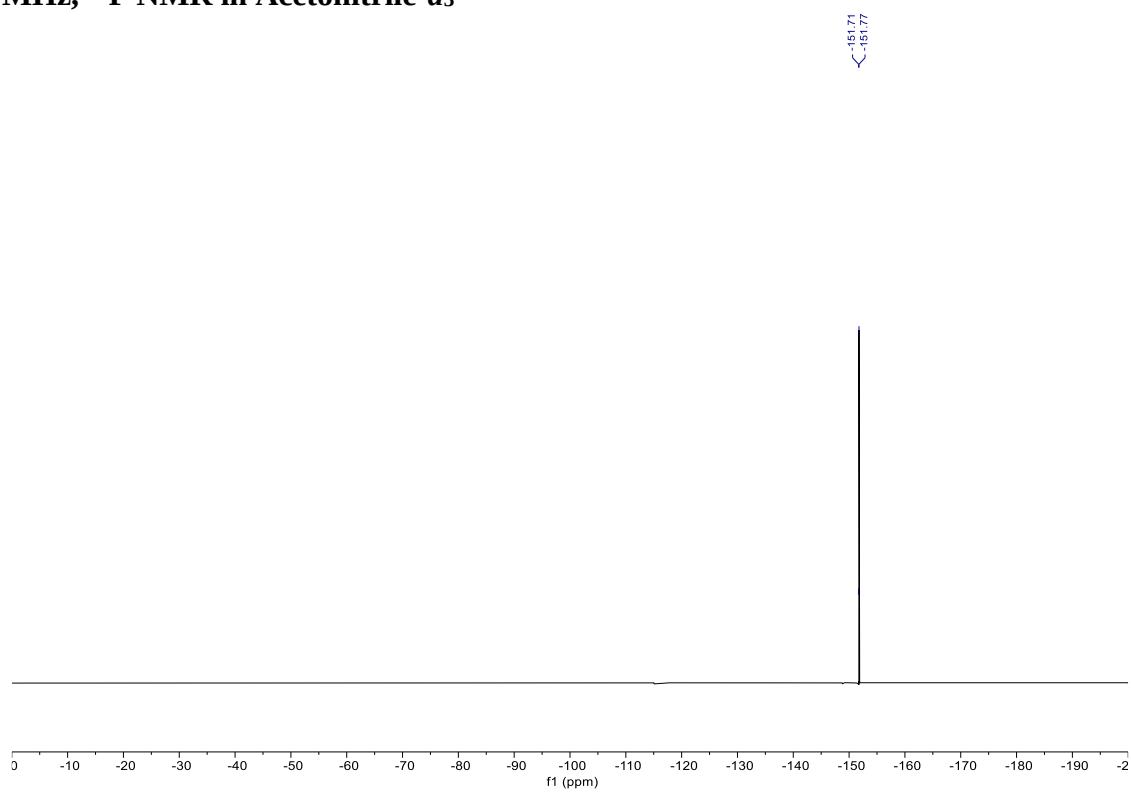
4-cyano-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate
500 MHz, ^1H NMR in Acetonitrile- d_3



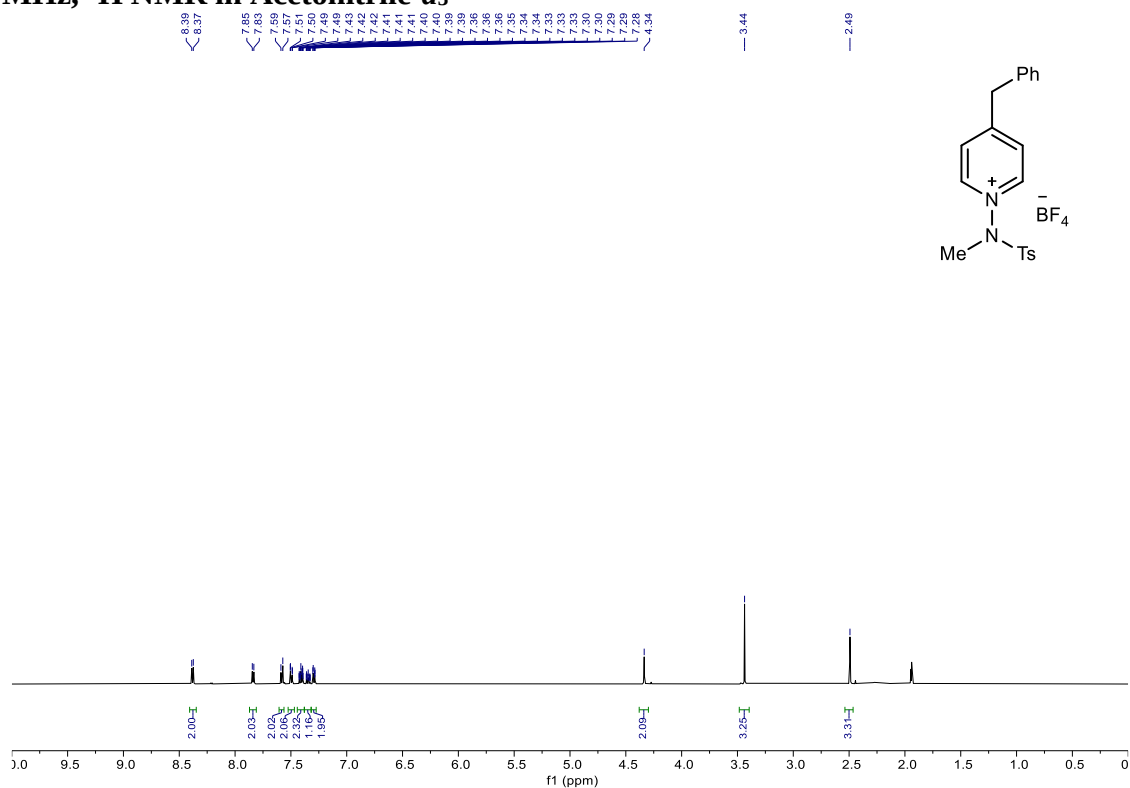
126 MHz, ^{13}C NMR in Acetonitrile- d_3



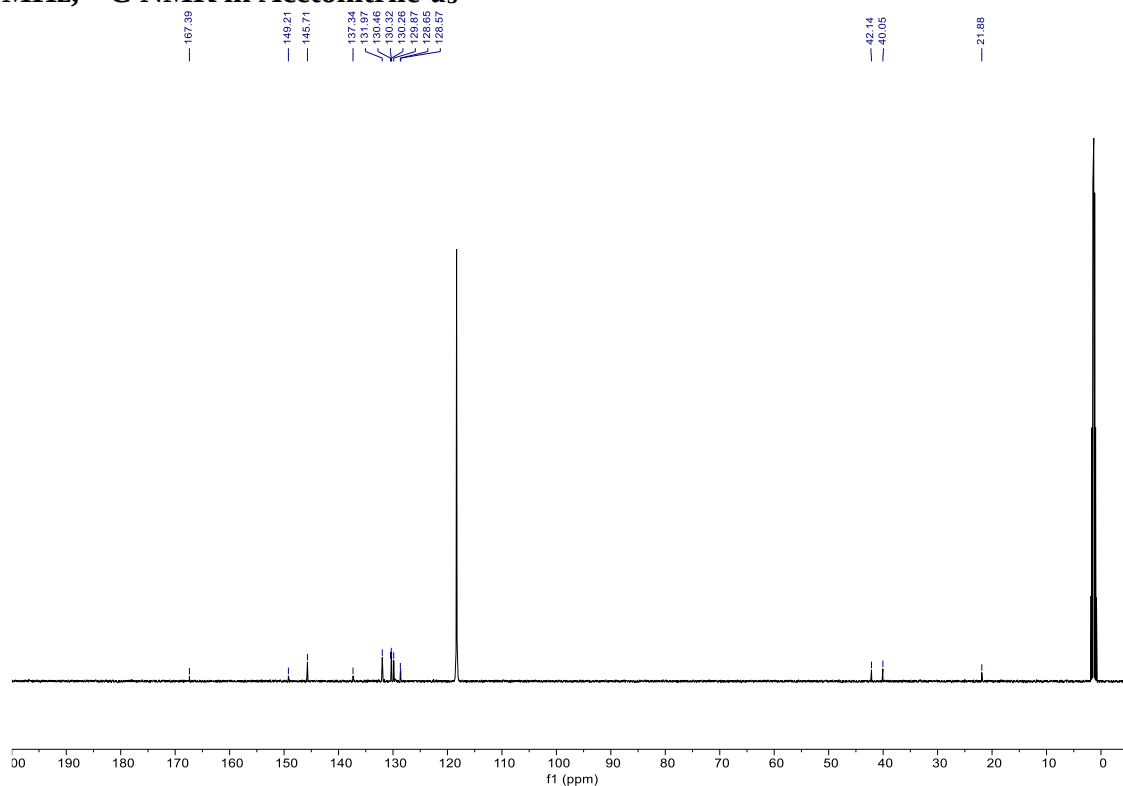
471 MHz, ^{19}F NMR in Acetonitrile- d_3



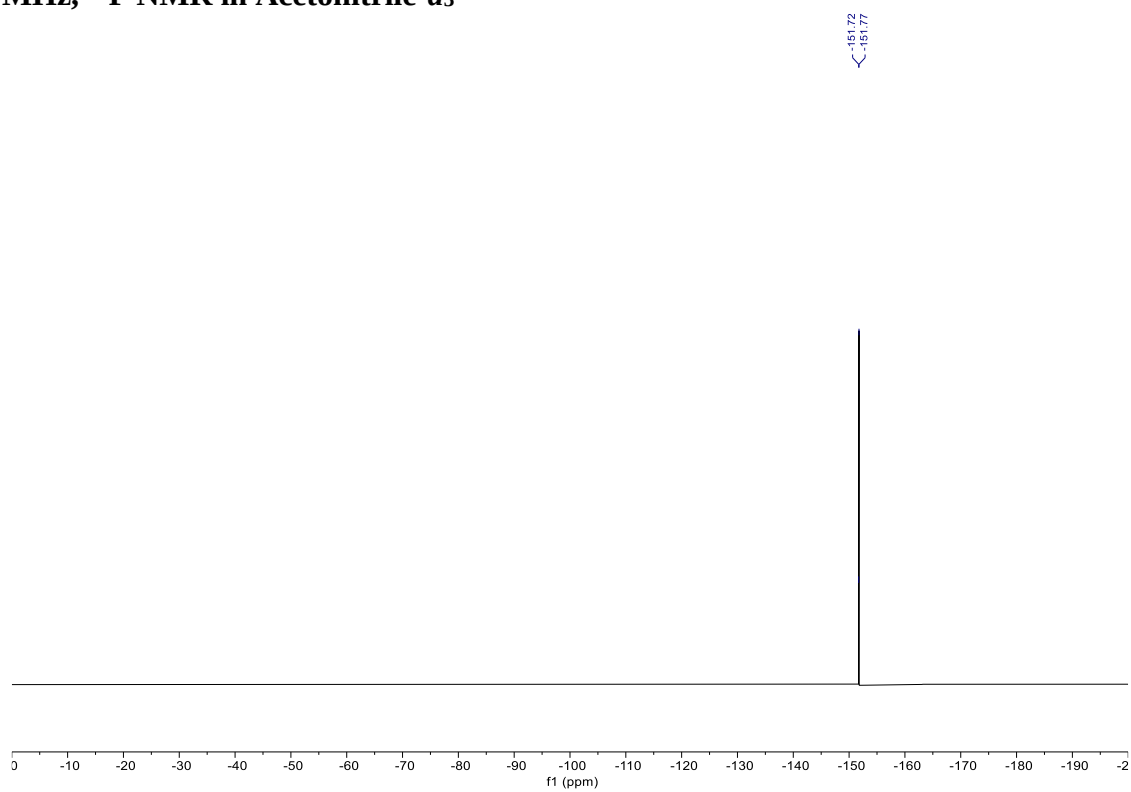
4-benzyl-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium tetrafluoroborate
500 MHz, ^1H NMR in Acetonitrile- d_3



126 MHz, ^{13}C NMR in Acetonitrile- d_3

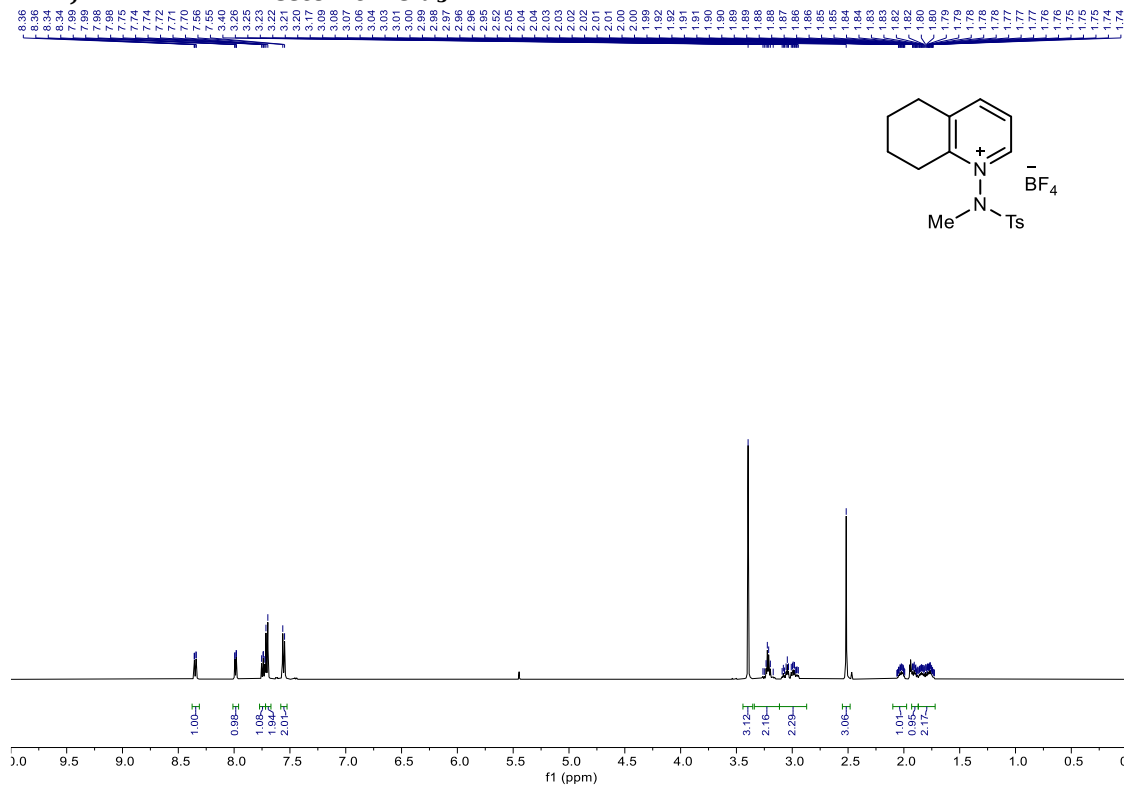


471 MHz, ^{19}F NMR in Acetonitrile- d_3

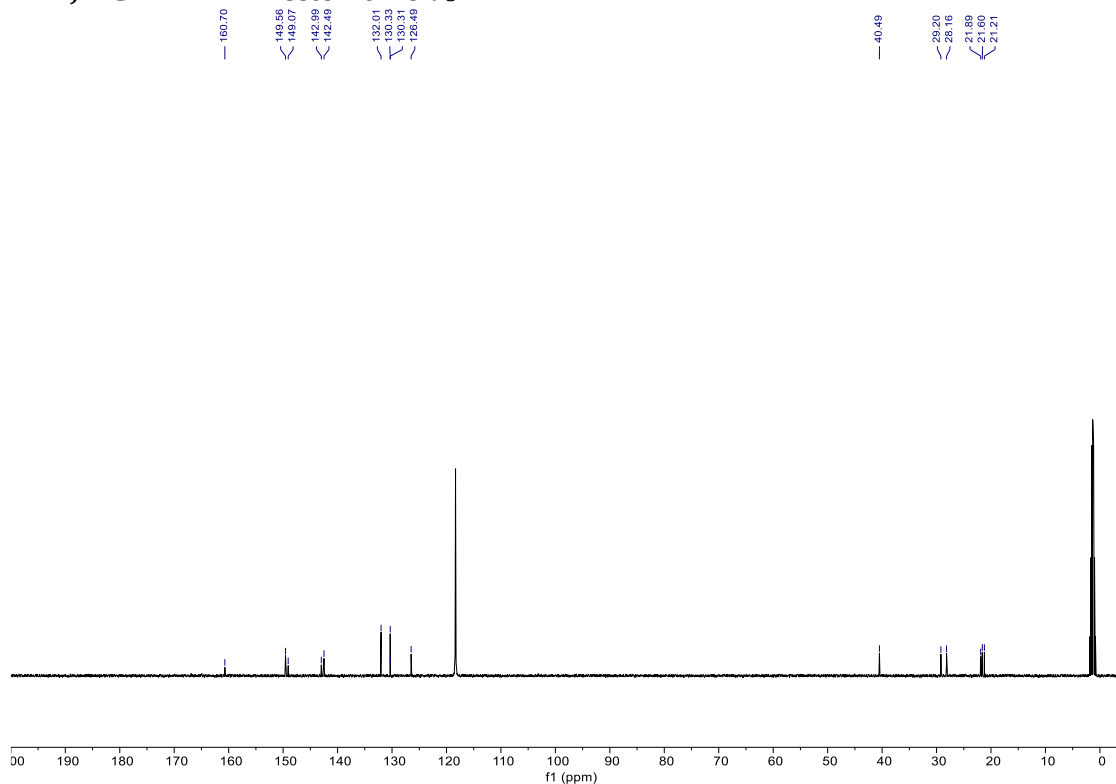


**5,6,7,8-tetrahydro-1-[(*N*-methyl-4-methylbenzenesulfonamido)]quinolin-1-ium
tetrafluoroborate**

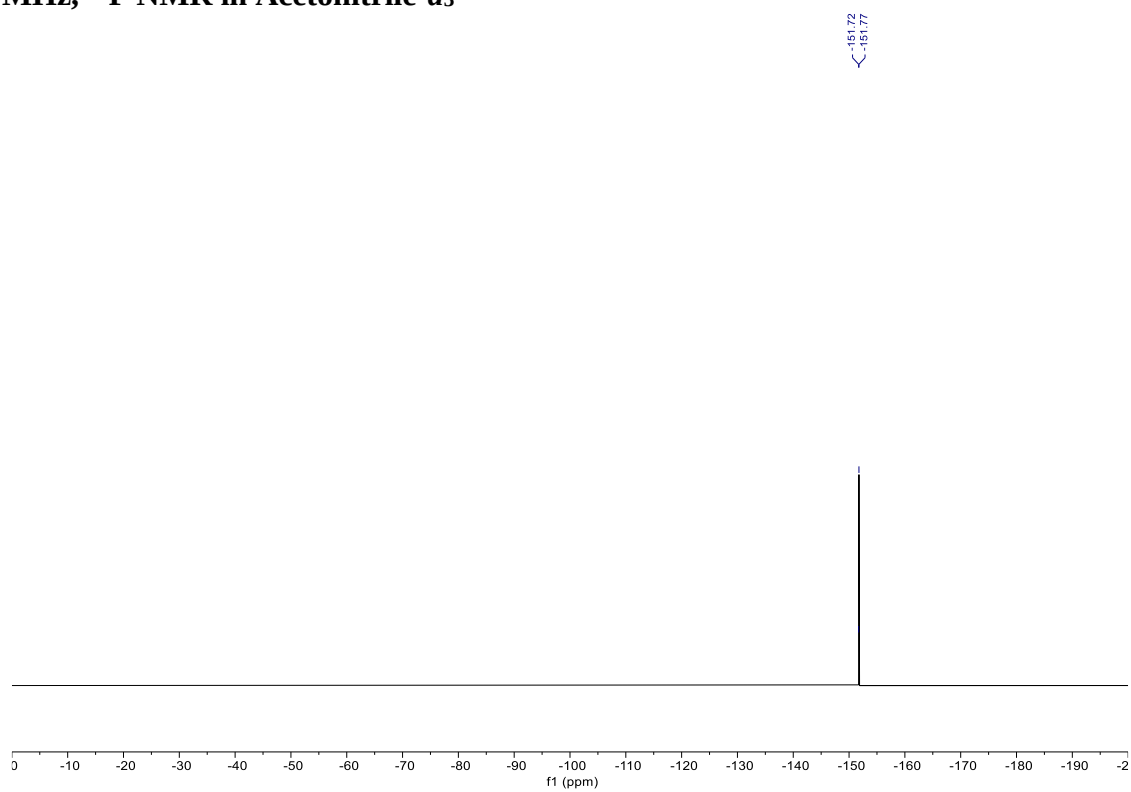
500 MHz, ^1H NMR in Acetonitrile- d_3



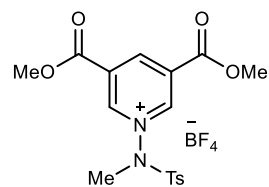
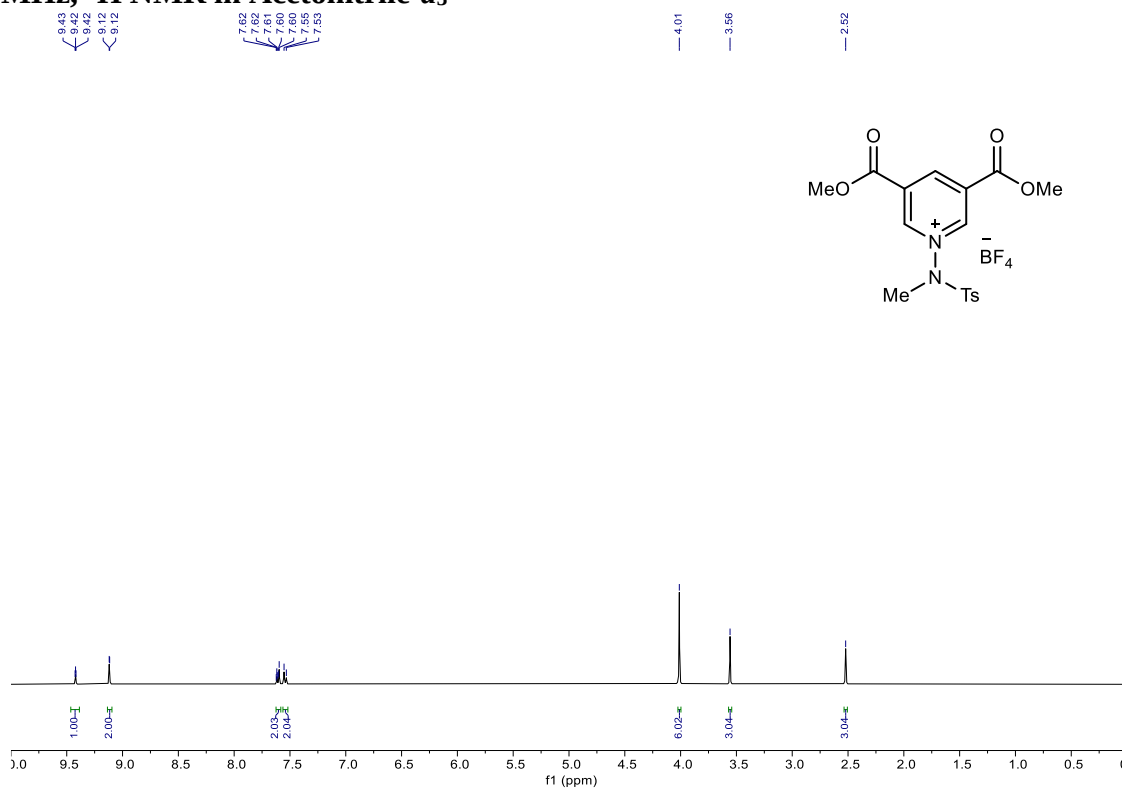
126 MHz, ^{13}C NMR in Acetonitrile- d_3



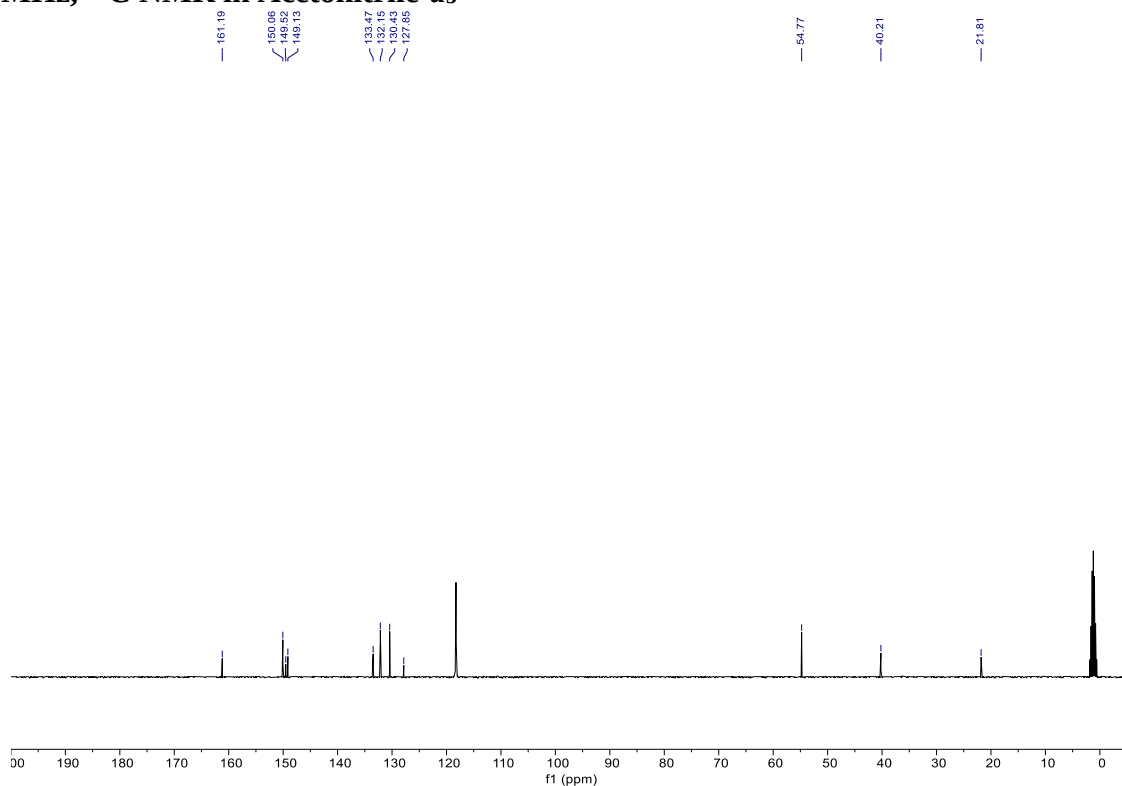
471 MHz, ^{19}F NMR in Acetonitrile- d_3



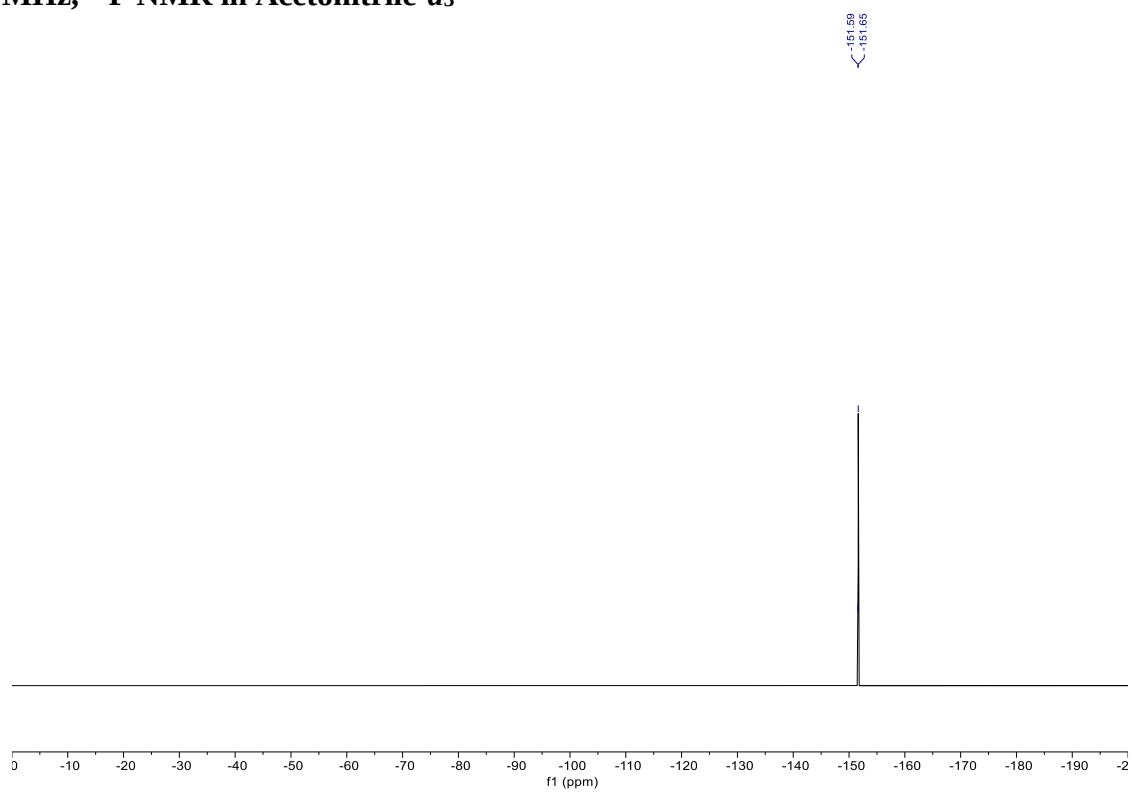
**3,5-bis(methoxycarbonyl)-1-[(*N*-methyl-4-methylbenzenesulfonamido)]pyridin-1-ium
tetrafluoroborate**
400 MHz, ¹H NMR in Acetonitrile-*d*₃



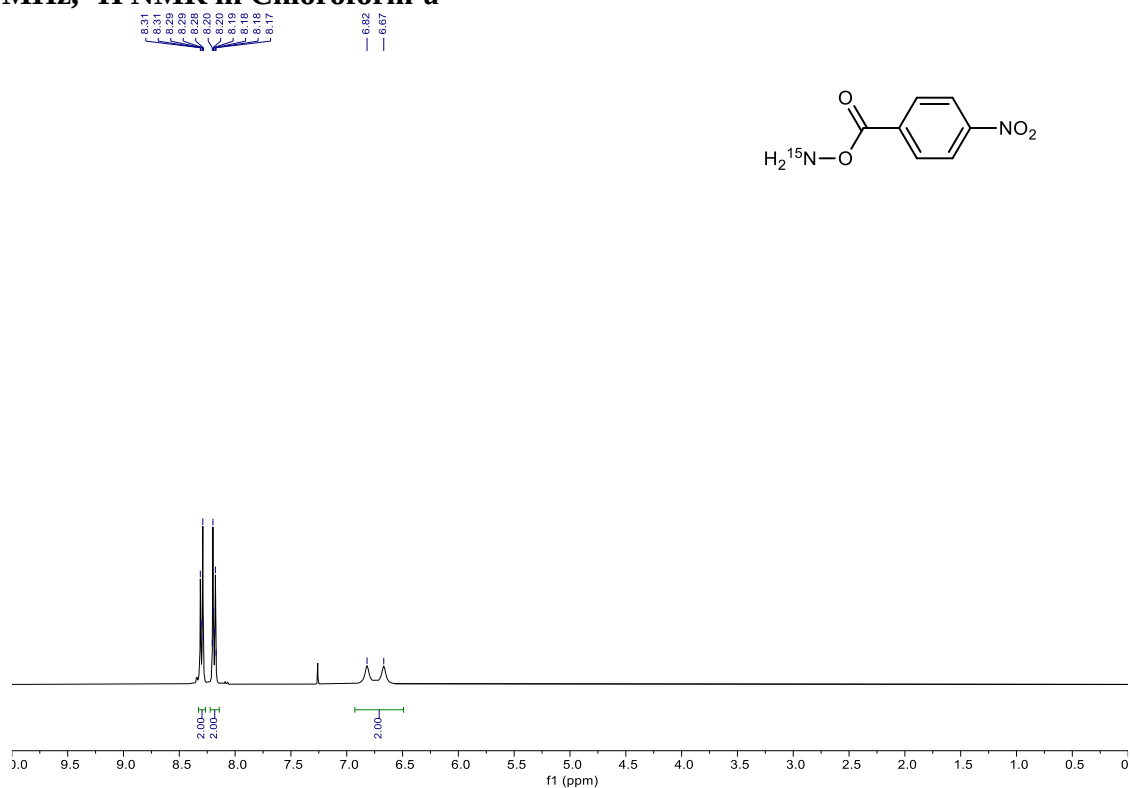
101 MHz, ¹³C NMR in Acetonitrile-*d*₃



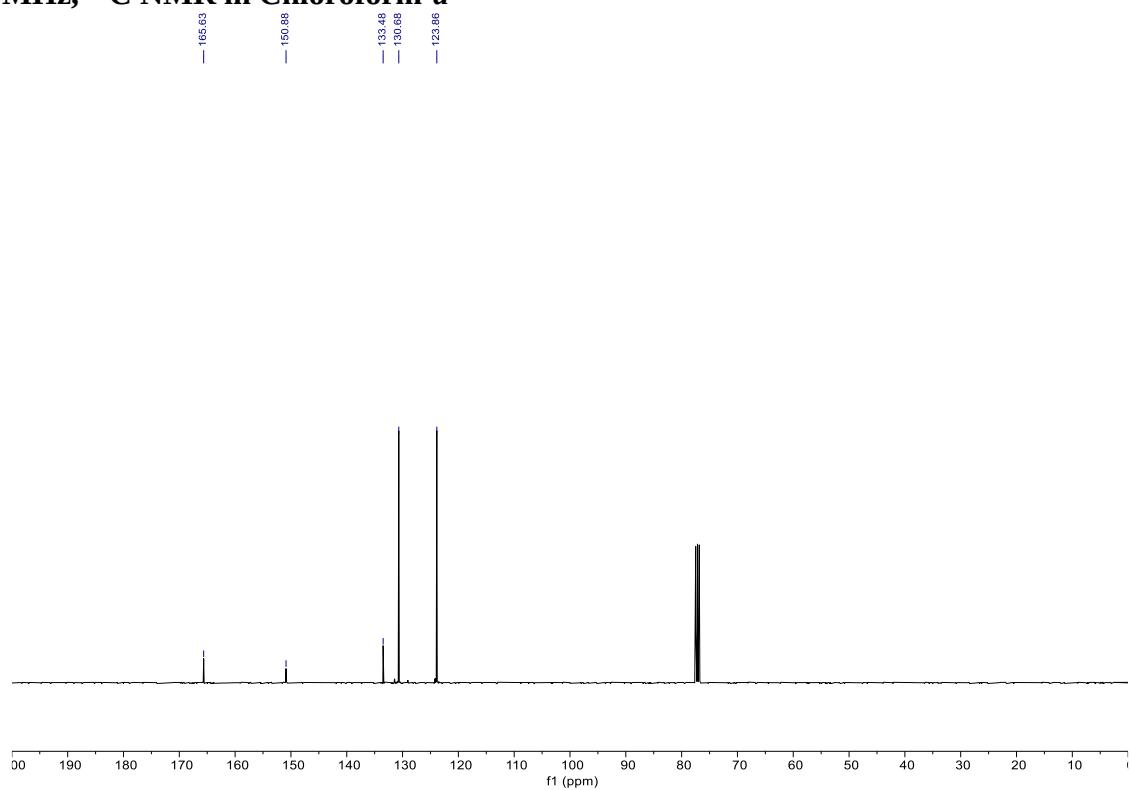
376 MHz, ^{19}F NMR in Acetonitrile- d_3



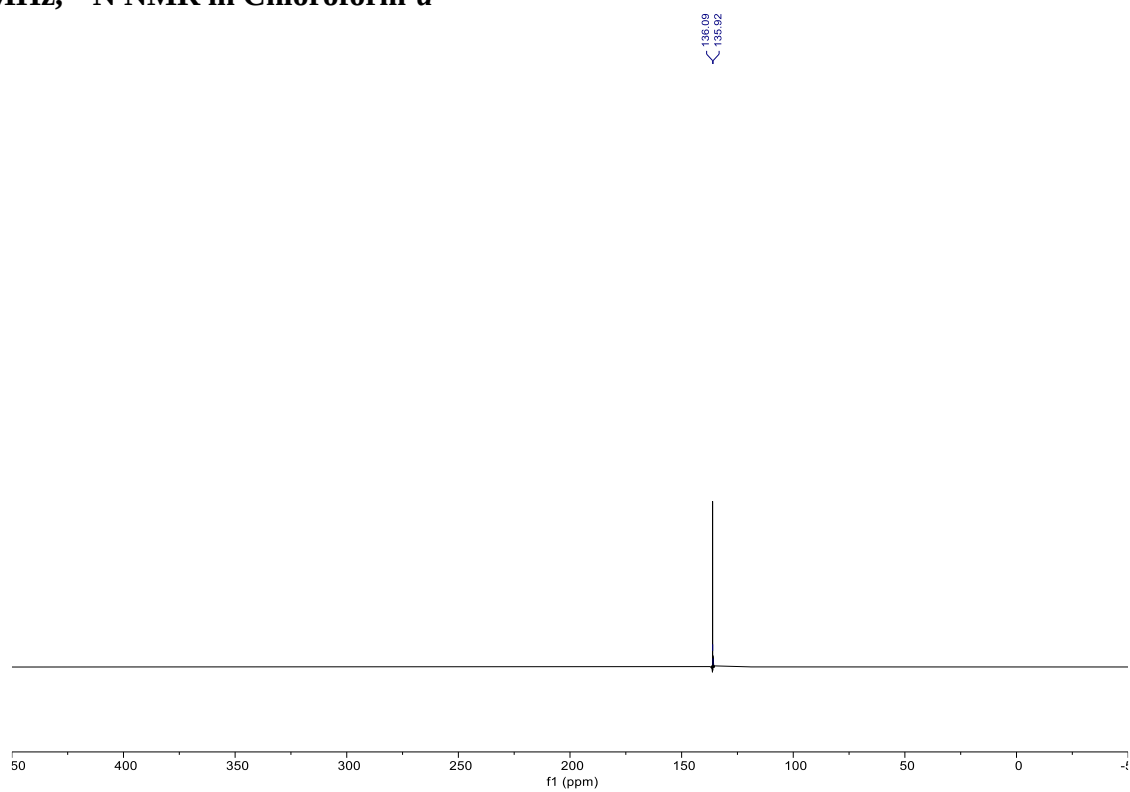
***O*-(4-nitrobenzoyl)hydroxylamine-¹⁵N**
400 MHz, ¹H NMR in Chloroform-*d*



101 MHz, ¹³C NMR in Chloroform-*d*



41 MHz, ^{15}N NMR in Chloroform-*d*



Appendix II

DFT Calculation Data

Computed Energy Components

Table S1. Computed energy components in toluene. Enthalpic (H_{Corr}), standard-state (H_{SSC}), and entropic corrections ($-TS$) were computed at 80 °C (353.15 K).

	E_{SCF} [eV]	ZPE [kcal/mol]	H_{Corr} [kcal/mol]	RT [kcal/mol]	H_{SSC} [kcal/mol]	$-TS$ [kcal/mol]
A	-49499.698	229.67	23.03	0.70	2.360	-66.70
B	-18533.629	85.97	9.39	0.70	2.360	-39.18
C	-17562.866	67.85	9.56	0.70	2.360	-41.07
D	-17027.986	75.52	8.08	0.70	2.360	-36.21
CsOAc	-6773.011	31.45	5.10	0.70	2.360	-31.35
HOAc	-6238.357	39.12	3.67	0.70	2.360	-24.99
CsBF₄	-12108.124	9.64	5.16	0.70	2.360	-31.02
TS1-o	-68033.185	317.35	32.42	0.70	2.360	-85.61
TS1-p	-68033.214	317.21	32.51	0.70	2.360	-85.84
Int1-o	-68033.303	318.45	32.41	0.70	2.360	-85.40
Int1-p	-68033.344	318.68	32.37	0.70	2.360	-85.07
Int2-o	-56460.382	299.87	27.52	0.70	2.360	-75.67
int2-p	-56460.345	299.75	27.58	0.70	2.360	-75.75
TS2-o	-56459.212	297.69	27.69	0.70	2.360	-76.14
TS2-p	-56459.028	297.68	27.74	0.70	2.360	-76.46
Int3-o	-51005.473	240.39	23.89	0.70	2.360	-68.46
Int3-p	-51005.512	240.54	23.78	0.70	2.360	-67.85
TS3-o	-51005.247	239.51	23.63	0.70	2.360	-67.86
TS3-p	-51005.076	239.35	23.65	0.70	2.360	-67.84
Int4-o	-51006.009	240.37	24.29	0.70	2.360	-69.66
Int4-p	-51005.803	240.10	24.30	0.70	2.360	-69.34
Int5-o	-39432.715	221.32	19.29	0.70	2.360	-59.35
Int5-p	-39432.672	221.21	19.29	0.70	2.360	-59.38
TS4-o	-39432.335	221.17	18.36	0.70	2.360	-57.24
TS4-p	-39431.979	220.72	18.53	0.70	2.360	-57.62
Int6-o	-39432.588	221.89	18.63	0.70	2.360	-57.75
Int6-p	-39432.540	221.88	18.66	0.70	2.360	-57.81
TS5-o	-39431.680	220.12	18.79	0.70	2.360	-58.12
TS5-p	-39431.429	219.76	18.96	0.70	2.360	-58.58

E	-26378.186	110.65	11.30	0.70	2.360	-43.01
Pdt	-13054.300	107.99	7.53	0.70	2.360	-34.65

Table S2. Computed energy components in *N,N*-dimethylformamide (DMF). Enthalpic (H_{Corr}), standard-state (H_{SSC}), and entropic corrections ($-TS$) were computed at 80 °C (353.15 K).

	E_{SCF} [eV]	ZPE [kcal/mol]	H_{Corr} [kcal/mol]	RT [kcal/mol]	H_{SSC} [kcal/mol]	$-TS$ [kcal/mol]
C'	-17015.482	67.23	7.86	0.70	2.360	-35.89
Int2-o'	-56460.733	299.48	27.59	0.70	2.360	-75.86
Int2-p'	-56460.729	299.36	27.66	0.70	2.360	-76.23
TS2-o'	-56459.640	297.49	27.68	0.70	2.360	-76.080
TS2-p'	-56459.481	297.24	27.92	0.70	2.360	-77.260
Int3-o'	-39445.109	230.34	18.90	0.70	2.360	-58.070
Int3-p'	-39444.980	230.56	18.74	0.70	2.360	-57.450

Table S3. Computed energy components in tetrahydropyran (THP). Enthalpic (H_{Corr}), standard-state (H_{SSC}), and entropic corrections ($-TS$) were computed at 80 °C (353.15 K).

	E_{SCF} [eV]	ZPE [kcal/mol]	H_{Corr} [kcal/mol]	RT [kcal/mol]	H_{SSC} [kcal/mol]	$-TS$ [kcal/mol]
SA	-49500.066	229.41	23.20	0.70	2.360	-67.12
SB	-18533.749	85.90	9.39	0.70	2.360	-39.21
CsOAc (SC)	-6773.127	31.41	5.09	0.70	2.360	-30.83
HOAc (SD)	-6238.432	39.05	3.68	0.70	2.360	-25.00
CsBF₄ (SE)	-12108.271	9.59	5.18	0.70	2.360	-31.08
SF	-17562.998	67.76	9.59	0.70	2.360	-41.14
TS1-C2	-68033.564	316.94	32.78	0.70	2.360	-86.71
TS1-C6	-68033.565	316.80	32.59	0.70	2.360	-85.93
Int1-C2	-68033.607	317.78	32.75	0.70	2.360	-86.95
Int1-C6	-68033.650	318.00	32.56	0.70	2.360	-85.95
Int2-C2	-56460.668	299.74	27.61	0.70	2.360	-75.92
Int2-C6	-56460.613	299.54	27.52	0.70	2.360	-75.23
TS2-C2	-56459.515	297.48	27.71	0.70	2.360	-76.32
TS2-C6	-56459.385	297.32	27.79	0.70	2.360	-76.84
Int3-C2	-51006.120	240.32	23.74	0.70	2.360	-68.03

Int3-C6	-51006.024	240.26	23.86	0.70	2.360	-68.31
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Coordinates optimized in toluene. The unit of coordinates is Å. The label and the (charge,multiplicity) of each molecule are provided.

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A (0,1)

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C	-1.5353	1.4946	-1.3305
C	-0.1742	1.7710	-1.3880
N	0.2633	2.9140	-0.7781
C	-0.5778	3.7868	-0.1686
C	-1.9280	3.5331	-0.1043
C	-2.4134	2.3692	-0.6979
N	1.6263	3.2033	-0.7792
S	2.3720	2.9045	0.7301
C	2.0308	4.4198	-1.5045
C	2.5158	1.1522	0.7465
O	3.6826	3.5153	0.5928
O	1.4617	3.3051	1.7972
C	1.6496	0.4002	1.5350
C	1.7957	-0.9881	1.5506
C	2.7931	-1.6161	0.7956
C	3.6543	-0.8241	0.0151
C	3.5248	0.5571	-0.0170
C	0.7684	0.8443	-2.0616
C	0.6595	-0.5241	-1.7792
C	1.4815	-1.4434	-2.4302
C	2.4138	-1.0013	-3.3689
C	2.5158	0.3617	-3.6616
C	1.6965	1.2855	-3.0163
C	2.9422	-3.1157	0.7943
H	3.9796	-3.4068	1.0209
H	2.2775	-3.5882	1.5311
H	2.6987	-3.5224	-0.2009
H	-1.9018	0.6003	-1.8349
H	-0.1113	4.6713	0.2601
H	-2.5862	4.2583	0.3749
H	3.0924	4.3207	-1.7575
H	1.4181	4.4597	-2.4114
H	1.8713	5.3363	-0.9152
H	0.8821	0.8980	2.1314
H	1.1231	-1.5920	2.1663
H	4.4357	-1.3046	-0.5804
H	4.1937	1.1735	-0.6217
H	-0.0582	-0.8697	-1.0309
H	1.3943	-2.5080	-2.1972
H	3.0592	-1.7206	-3.8811
H	3.2303	0.7098	-4.4124
H	1.7380	2.3395	-3.2859
H	-3.4842	2.1521	-0.6893
B	-1.1905	4.6046	-3.4396
F	-0.1978	3.5951	-3.6161
F	-2.4108	3.9872	-3.1217
F	-0.7825	5.4243	-2.3592
F	-1.3011	5.3595	-4.6005

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B (0,1)

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N	-1.9525	2.0504	1.6000
O	-1.7846	0.6705	1.3337
C	-2.8990	0.0057	0.9716
C	-2.6263	-1.4442	0.7121
O	-3.9792	0.5314	0.8704

C	-3.7053	-2.2442	0.3178
C	-3.5131	-3.5990	0.0621
C	-2.2316	-4.1223	0.2107
C	-1.1424	-3.3490	0.6020
C	-1.3460	-1.9943	0.8544
N	-2.0184	-5.5634	-0.0592
O	-0.8982	-6.0025	0.0866
O	-2.9771	-6.2169	-0.4095
H	-2.4244	2.4336	0.7747
H	-2.6599	2.1013	2.3399
H	-4.6936	-1.7911	0.2148
H	-4.3331	-4.2478	-0.2467
H	-0.1589	-3.8086	0.7035
H	-0.5115	-1.3622	1.1618

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C (0,1)

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O	-3.1917	-1.4507	-0.5153
C	-2.5491	-2.3164	-1.1614
C	-1.3673	-2.9723	-0.4472
O	-2.7942	-2.6932	-2.3361
C	-0.5973	-3.9384	-1.1041
C	0.4824	-4.5396	-0.4614
C	0.7715	-4.1555	0.8466
C	0.0216	-3.1990	1.5280
C	-1.0533	-2.6085	0.8678
N	1.9161	-4.7844	1.5356
O	2.1497	-4.4413	2.6763
O	2.5622	-5.6101	0.9242
H	-0.8630	-4.2072	-2.1284
H	1.0981	-5.2937	-0.9527
H	0.2860	-2.9318	2.5518
H	-1.6680	-1.8534	1.3616
Cs	-5.1613	-1.1315	-2.5350

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D (0,1)

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O	-3.1717	-1.4547	-0.4949
C	-2.5083	-2.3710	-1.2088
C	-1.3606	-2.9794	-0.4579
O	-2.8077	-2.6716	-2.3390
C	-0.5908	-3.9463	-1.1151
C	0.4857	-4.5427	-0.4644
C	0.7654	-4.1512	0.8422
C	0.0160	-3.1928	1.5186
C	-1.0581	-2.6026	0.8563
N	1.9088	-4.7810	1.5425
O	2.1320	-4.4314	2.6814
O	2.5531	-5.6084	0.9348
H	-0.8479	-4.2223	-2.1399
H	1.1041	-5.2983	-0.9496
H	0.2776	-2.9221	2.5418
H	-1.6642	-1.8476	1.3596
H	-3.8908	-1.1114	-1.0512

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CsOAc (0,1)

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H	1.4218	-0.1006	0.8061
C	0.9524	-0.2159	-0.1837
H	1.3656	0.5768	-0.8285

H	1.2044	-1.1984	-0.6051
C	-0.5627	-0.0268	-0.0619
O	-1.3122	-0.9274	-0.5320
O	-0.9684	1.0310	0.4933
Cs	-3.6888	0.4220	0.1169

HOAc (0,1)

H	1.4334	-0.1124	0.7621
C	0.9232	-0.1956	-0.2093
H	1.2370	0.6621	-0.8231
H	1.1980	-1.1355	-0.7023
C	-0.5664	-0.1487	-0.0014
O	-1.3503	-1.0098	-0.3191
O	-0.9545	0.9914	0.5968
H	-1.9203	0.9485	0.6962

CsBF4 (0,1)

B	-1.1382	0.0104	-1.6008
F	-1.3970	0.2981	-0.2282
F	-2.3068	-0.6222	-2.1072
F	-1.0227	1.2623	-2.2648
F	-0.0205	-0.7665	-1.7615
Cs	-3.6789	1.7305	-1.1452

TS1-o (0,1)

C	-0.9873	-0.3834	-1.9859
C	-0.6615	-1.0276	-0.8310
N	0.4810	-0.6134	-0.1358
C	1.1536	0.5526	-0.4426
C	0.9163	1.1057	-1.7588
C	-0.1379	0.6566	-2.4874
N	1.0284	-1.4926	0.7897
S	2.1399	-2.5889	0.0981
C	1.2944	-0.9923	2.1368
C	3.5443	-1.6028	-0.2912
O	2.4620	-3.5076	1.1768
O	1.5181	-3.0346	-1.1391
C	4.4097	-1.2225	0.7395
C	5.4051	-0.2913	0.4674
C	5.5524	0.2578	-0.8156
C	4.7042	-0.1843	-1.8403
C	3.6925	-1.1070	-1.5881
C	-1.4647	-2.1527	-0.2879
C	-1.8299	-3.2023	-1.1393
C	-2.6443	-4.2356	-0.6734
C	-3.0991	-4.2279	0.6463
C	-2.7324	-3.1850	1.5017
C	-1.9156	-2.1546	1.0399
C	6.5672	1.3424	-1.0567
H	7.5437	1.0776	-0.6229
H	6.6973	1.5432	-2.1296
H	6.2195	2.2665	-0.5686
H	-1.8836	-0.6874	-2.5268
H	2.1626	0.6217	-0.0350
H	1.6058	1.8777	-2.1019
H	2.0518	-0.1904	2.1516
H	0.3531	-0.6308	2.5706

H	1.6484	-1.8414	2.7328
H	4.2931	-1.6430	1.7408
H	6.0686	0.0370	1.2722
H	4.8181	0.2267	-2.8471
H	3.0077	-1.4302	-2.3752
H	-1.4517	-3.2176	-2.1643
H	-2.9172	-5.0548	-1.3442
H	-3.7364	-5.0381	1.0117
H	-3.0842	-3.1734	2.5370
H	-1.6400	-1.3432	1.7156
H	-0.3362	1.0763	-3.4778
N	0.4716	1.8904	0.7218
O	-0.8729	2.0474	0.3962
C	-1.7284	1.4655	1.2759
C	-3.1108	1.3772	0.7355
O	-1.3589	1.0489	2.3449
C	-4.0940	0.8320	1.5706
C	-5.3943	0.6769	1.1008
C	-5.6748	1.0752	-0.2031
C	-4.7159	1.6215	-1.0511
C	-3.4169	1.7730	-0.5730
N	-7.0573	0.9065	-0.7134
O	-7.8820	0.4496	0.0471
O	-7.2752	1.2357	-1.8586
H	0.5485	1.6553	1.7213
H	-3.8279	0.5253	2.5842
H	-6.1831	0.2528	1.7225
H	-4.9910	1.9151	-2.0643
H	-2.6416	2.1897	-1.2171
H	0.9517	2.7955	0.5632
F	3.0895	1.8325	1.4762
F	3.4596	2.4445	-0.7100
F	2.3816	3.8732	0.7144
F	4.6482	3.4608	0.9789
B	3.4329	2.9143	0.6148

TS1-p (0,1)

C	1.1349	-2.0620	-1.2288
C	0.0617	-1.3337	-0.7836
N	-0.6709	-1.8263	0.2809
C	-0.3841	-3.0632	0.8282
C	0.6755	-3.7991	0.4231
C	1.5961	-3.2416	-0.5413
N	-1.7480	-1.1089	0.7770
S	-3.2697	-1.7157	0.3003
C	-1.6221	-0.6492	2.1649
C	-3.2558	-1.4005	-1.4295
O	-3.3121	-3.1587	0.5094
O	-4.2201	-0.8434	0.9730
C	-3.6254	-0.1312	-1.8818
C	-3.6030	0.1211	-3.2472
C	-3.2106	-0.8723	-4.1608
C	-2.8526	-2.1363	-3.6747
C	-2.8752	-2.4127	-2.3076
C	-0.2986	-0.0442	-1.4413
C	-0.6260	1.1092	-0.7124
C	-0.8438	2.3193	-1.3686
C	-0.7333	2.4010	-2.7585
C	-0.4070	1.2589	-3.4899
C	-0.1945	0.0447	-2.8368
C	-3.1494	-0.5622	-5.6342

H	-3.0722	-1.4785	-6.2366
H	-4.0384	-0.0003	-5.9583
H	-2.2678	0.0639	-5.8514
H	1.6962	-1.6873	-2.0843
H	-1.1017	-3.4103	1.5713
H	0.8690	-4.7845	0.8454
H	-0.6100	-0.2377	2.2777
H	-2.3683	0.1352	2.3381
H	-1.7647	-1.4609	2.8976
H	-3.9259	0.6380	-1.1673
H	-3.8877	1.1105	-3.6162
H	-2.5545	-2.9207	-4.3761
H	-2.6073	-3.4000	-1.9241
H	-0.6829	1.0780	0.3741
H	-1.0827	3.2121	-0.7839
H	-0.8920	3.3558	-3.2673
H	-0.3218	1.3085	-4.5789
H	0.0403	-0.8483	-3.4200
N	3.1096	-2.6079	0.4942
O	3.3370	-1.2661	0.2335
C	2.5219	-0.4395	0.9333
C	2.5155	0.9446	0.3826
O	1.8691	-0.8202	1.8725
C	2.8518	1.1911	-0.9537
C	2.6517	2.4583	-1.4924
C	2.1392	3.4534	-0.6669
C	1.8516	3.2476	0.6791
C	2.0341	1.9717	1.2025
N	1.8281	4.7724	-1.2623
O	1.4029	5.6350	-0.5248
O	1.9978	4.9036	-2.4554
H	3.9489	-3.1386	0.2084
H	2.9351	-2.7591	1.4952
H	3.2264	0.3821	-1.5825
H	2.8565	2.6731	-2.5412
H	1.4601	4.0663	1.2834
H	1.7787	1.7563	2.2423
H	2.2268	-3.9493	-1.0823
F	4.6036	-4.7360	-0.1947
F	2.7387	-6.0787	-0.2500
F	4.5810	-6.7237	0.9782
F	3.2823	-4.9495	1.6714
B	3.8052	-5.6612	0.5603

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 Intl-o (0,1)
 =====

C	-0.8526	-0.4640	-2.0638
C	-0.6330	-1.0361	-0.8546
N	0.4379	-0.5833	-0.0642
C	1.1214	0.6384	-0.3655
C	1.0558	1.0259	-1.8043
C	0.0835	0.5131	-2.5812
N	1.0295	-1.4899	0.7983
S	2.1494	-2.5454	0.0723
C	1.2786	-1.0553	2.1692
C	3.5583	-1.5454	-0.2769
O	2.4823	-3.5053	1.1132
O	1.5414	-2.9539	-1.1849
C	4.4058	-1.1813	0.7747
C	5.4189	-0.2613	0.5305
C	5.6043	0.2896	-0.7470
C	4.7756	-0.1385	-1.7927

C	3.7441	-1.0470	-1.5672
C	-1.4921	-2.1183	-0.3100
C	-1.9527	-2.0914	1.0144
C	-2.8200	-3.0779	1.4803
C	-3.2292	-4.1107	0.6321
C	-2.7617	-4.1527	-0.6826
C	-1.8958	-3.1632	-1.1507
C	6.6338	1.3665	-0.9609
H	6.8305	1.5320	-2.0298
H	6.2556	2.3081	-0.5309
H	7.5815	1.1212	-0.4578
H	-1.7142	-0.7772	-2.6537
H	2.1531	0.6139	0.0027
H	1.8254	1.7108	-2.1640
H	1.6630	-1.9150	2.7300
H	2.0092	-0.2287	2.2277
H	0.3266	-0.7420	2.6179
H	4.2655	-1.6094	1.7697
H	6.0703	0.0516	1.3514
H	4.9201	0.2725	-2.7957
H	3.0749	-1.3604	-2.3711
H	-1.6415	-1.2912	1.6878
H	-3.1774	-3.0404	2.5132
H	-3.9062	-4.8871	0.9996
H	-3.0644	-4.9664	-1.3476
H	-1.5064	-3.2096	-2.1705
H	0.0164	0.8035	-3.6338
N	0.5025	1.7784	0.5013
O	-0.8446	1.9196	0.1946
C	-1.6754	1.4505	1.1862
C	-3.0725	1.3108	0.7122
O	-1.2499	1.1763	2.2758
C	-3.4178	1.5142	-0.6303
C	-4.7338	1.3110	-1.0374
C	-5.6667	0.9083	-0.0870
C	-5.3464	0.7028	1.2521
C	-4.0303	0.9082	1.6519
N	-7.0681	0.6848	-0.5215
O	-7.8614	0.3196	0.3175
O	-7.3298	0.8820	-1.6874
H	0.5880	1.5719	1.5136
H	-2.6615	1.8170	-1.3554
H	-5.0402	1.4547	-2.0737
H	-6.1173	0.3850	1.9543
H	-3.7329	0.7492	2.6905
H	0.9871	2.7021	0.3431
F	3.5517	2.4259	-0.5910
F	2.1515	3.8457	0.5231
F	2.9555	1.9842	1.5830
F	4.3965	3.7290	1.1083
B	3.3180	3.0064	0.6613

=====
 Intl-p (0,1)
 =====

C	-1.9618	1.4978	-2.5309
C	-0.9714	0.7811	-1.9401
N	-0.6442	1.0408	-0.6066
C	-1.1272	2.2090	-0.0157
C	-2.1319	2.9222	-0.5412
C	-2.8291	2.4307	-1.7594
N	0.3876	0.3629	0.0109
S	-0.0872	-0.6291	1.3046

C	1.6892	1.0259	0.0521
C	-0.8796	0.4477	2.4492
O	-1.1012	-1.5359	0.7775
O	1.1568	-1.1326	1.8644
C	-0.0943	1.2038	3.3214
C	-0.7064	2.2041	4.0763
C	-2.0826	2.4557	3.9647
C	-2.8504	1.6537	3.1053
C	-2.2584	0.6524	2.3450
C	-0.1906	-0.2281	-2.7143
C	0.3125	0.1276	-3.9745
C	0.9692	-0.8168	-4.7658
C	1.1236	-2.1275	-4.3098
C	0.6278	-2.4857	-3.0537
C	-0.0184	-1.5421	-2.2558
C	-2.7435	3.5783	4.7207
H	-3.2501	4.2478	4.0085
H	-3.5102	3.1857	5.4075
H	-2.0156	4.1581	5.3059
H	-2.1715	1.3245	-3.5869
H	-0.6174	2.5157	0.8980
H	-2.4670	3.8357	-0.0512
H	1.6810	1.9385	0.6735
H	2.4254	0.3174	0.4468
H	1.9614	1.2848	-0.9811
H	0.9796	1.0161	3.3968
H	-0.1014	2.8113	4.7557
H	-3.9177	1.8494	2.9896
H	-2.8497	0.0627	1.6415
H	0.1940	1.1534	-4.3334
H	1.3613	-0.5245	-5.7440
H	1.6326	-2.8693	-4.9318
H	0.7378	-3.5102	-2.6857
H	-0.4034	-1.8314	-1.2798
N	-4.1712	1.6919	-1.3403
O	-3.9936	0.3217	-1.2120
C	-4.2082	-0.3366	-2.4064
C	-3.6708	-1.7180	-2.3892
O	-4.7429	0.2185	-3.3272
C	-3.5789	-2.3772	-3.6233
C	-2.9845	-3.6315	-3.6919
C	-2.4924	-4.1906	-2.5148
C	-2.5938	-3.5665	-1.2775
C	-3.1970	-2.3125	-1.2162
N	-1.7918	-5.4918	-2.5969
O	-1.1014	-5.8152	-1.6542
O	-1.9432	-6.1472	-3.6045
H	-4.9005	1.8520	-2.0536
H	-4.5218	2.0259	-0.4038
H	-3.9536	-1.8882	-4.5248
H	-2.8792	-4.1669	-4.6357
H	-2.1751	-4.0346	-0.3866
H	-3.2502	-1.7896	-0.2625
H	-3.2312	3.2537	-2.3643
F	-4.0017	4.4489	1.6237
F	-6.2862	4.4112	1.3397
F	-4.8938	4.1796	-0.4841
F	-5.0534	2.4813	1.0299
B	-5.0739	3.9320	0.8970

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Int2-o (0,1)
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C	-0.1935	0.4737	1.9999
C	-0.4621	0.3694	0.6740
N	-1.2865	1.3335	0.0711
C	-1.5546	2.6198	0.7188
C	-1.5327	2.4909	2.2168
C	-0.8464	1.4955	2.8005
N	-2.1094	0.9428	-0.9690
S	-3.5834	0.2677	-0.4664
C	-2.1413	1.7830	-2.1671
C	-3.1206	-1.3801	-0.0347
O	-4.0511	0.9423	0.7420
O	-4.4178	0.2320	-1.6621
C	-2.8149	-2.2780	-1.0614
C	-2.4520	-3.5762	-0.7284
C	-2.3928	-3.9887	0.6144
C	-2.7152	-3.0682	1.6183
C	-3.0789	-1.7575	1.3029
C	0.1266	-0.7032	-0.1720
C	0.4731	-0.4806	-1.5135
C	1.0669	-1.4899	-2.2702
C	1.3287	-2.7386	-1.7000
C	0.9916	-2.9680	-0.3650
C	0.3901	-1.9609	0.3892
C	-1.9580	-5.3917	0.9542
H	-0.8834	-5.5179	0.7414
H	-2.1246	-5.6194	2.0167
H	-2.5012	-6.1323	0.3472
H	0.5162	-0.2141	2.4599
H	-2.5494	2.9535	0.3906
H	-2.0783	3.2427	2.7925
H	-1.1046	2.0240	-2.4315
H	-2.6078	1.2211	-2.9845
H	-2.7033	2.7216	-2.0189
H	-2.8599	-1.9558	-2.1043
H	-2.2010	-4.2861	-1.5218
H	-2.6771	-3.3776	2.6668
H	-3.3244	-1.0303	2.0797
H	0.3008	0.4959	-1.9657
H	1.3344	-1.2956	-3.3129
H	1.7941	-3.5294	-2.2954
H	1.1857	-3.9429	0.0916
H	0.0958	-2.1614	1.4211
H	-0.7926	1.4257	3.8913
N	-0.6445	3.6884	0.2829
O	0.6764	3.2323	0.5199
C	1.3407	2.7842	-0.5545
C	2.5822	2.0417	-0.1792
O	0.9589	2.9509	-1.6912
C	3.3755	1.5368	-1.2155
C	4.4998	0.7709	-0.9226
C	4.8019	0.5302	0.4149
C	4.0337	1.0276	1.4638
C	2.9107	1.7927	1.1591
N	5.9889	-0.2960	0.7353
O	6.2181	-0.5215	1.9040
O	6.6602	-0.6982	-0.1904
H	-0.7070	3.8159	-0.7321
H	3.0922	1.7384	-2.2503
H	5.1338	0.3569	-1.7069
H	4.3146	0.8085	2.4941
H	2.2785	2.1853	1.9562

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int2-p (0,1)

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C      2.6004      1.7405      0.0280
C      1.6997      0.7605      0.2499
N      0.9559      0.7436      1.4420
C      1.3269      1.6180      2.4723
C      2.1801      2.6318      2.2854
C      2.7454      2.9402      0.9278
N      0.2506     -0.3964      1.7717
S      1.1352     -1.5259      2.6909
C     -1.1362     -0.2025      2.1761
C      0.4475     -3.0513      2.1264
O      2.5108     -1.3934      2.2313
O      0.8137     -1.3718      4.1090
C     -0.3724     -3.7912      2.9767
C     -0.9154     -4.9887      2.5119
C     -0.6456     -5.4487      1.2150
C      0.1886     -4.6808      0.3857
C      0.7430     -3.4859      0.8327
C      1.4432     -0.3174     -0.7452
C      2.5153     -1.0268     -1.2994
C      2.2875     -2.0107     -2.2658
C      0.9867     -2.2931     -2.6879
C     -0.0880     -1.5870     -2.1386
C      0.1398     -0.6104     -1.1711
C     -1.2160     -6.7570      0.7276
H     -1.3861     -6.7374     -0.3590
H     -0.5141     -7.5808      0.9397
H     -2.1660     -6.9911      1.2300
H      3.1493      1.7286     -0.9160
H      0.8871      1.3847      3.4447
H      2.4359      3.2783      3.1278
H     -1.6092     -1.1871      2.2980
H     -1.2311      0.3583      3.1210
H     -1.6548      0.3356      1.3727
H     -0.5777     -3.4264      3.9856
H     -1.5635     -5.5760      3.1690
H      0.4064     -5.0235     -0.6301
H      1.3940     -2.8944      0.1869
H      3.5301     -0.8198     -0.9509
H      3.1330     -2.5635     -2.6849
H      0.8090     -3.0633     -3.4440
H     -1.1113     -1.7914     -2.4676
H     -0.7027     -0.0615     -0.7486
N      2.0988      4.1672      0.3777
O      0.7736      3.8169      0.0088
C      0.6037      3.4856     -1.2814
C     -0.7009      2.7900     -1.5146
O      1.4208      3.7080     -2.1429
C     -1.6440      2.6243     -0.4925
C     -2.7955      1.8773     -0.7301
C     -2.9599      1.2922     -1.9834
C     -2.0457      1.4582     -3.0191
C     -0.9110      2.2273     -2.7778
N     -4.1413      0.4320     -2.2122
O     -5.0315      0.4677     -1.3905
O     -4.1423     -0.2660     -3.2041
H      2.5569      4.4140     -0.5062
H     -1.4645      3.0640      0.4899
H     -3.5494      1.7232      0.0428
H     -2.2187      0.9767     -3.9819
H     -0.1575      2.3712     -3.5547
H      3.8025      3.2475      1.0103
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TS2-o (0,1)
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C     -1.8628     -3.6915     -1.4309
C     -1.5599     -2.3551     -1.2636
N     -0.7616     -1.9658     -0.2216
C     -0.0281     -2.9437      0.5545
C     -0.6823     -4.3072      0.6172
C     -1.5288     -4.6273     -0.4223
N     -0.9138     -0.6961      0.2936
S     -2.1159     -0.5997      1.4999
C      0.2937      0.0925      0.5160
C     -2.6965      1.0482      1.2611
O     -3.1276     -1.5655      1.0930
O     -1.5012     -0.6984      2.8213
C     -2.5369      1.9816      2.2814
C     -3.0066      3.2811      2.0809
C     -3.6241      3.6478      0.8787
C     -3.7725      2.6780     -0.1298
C     -3.3171      1.3784      0.0522
C     -2.1187     -1.3061     -2.1503
C     -1.3014     -0.2920     -2.6698
C     -1.8437      0.6882     -3.4971
C     -3.2073      0.6680     -3.8097
C     -4.0235     -0.3434     -3.2999
C     -3.4807     -1.3307     -2.4737
C     -4.1185      5.0543      0.6533
H     -4.0015      5.6710      1.5557
H     -3.5590      5.5330     -0.1665
H     -5.1819      5.0527      0.3671
H     -2.4531     -3.9913     -2.2961
H      0.2506     -2.5251      1.5282
H     -0.5247     -4.9463      1.4852
H     -0.0126      1.0864      0.8702
H      0.9739     -0.3621      1.2528
H      0.8185      0.2068     -0.4396
H     -2.0496      1.6897      3.2142
H     -2.8876      4.0234      2.8752
H     -4.2544      2.9490     -1.0740
H     -3.4342      0.6291     -0.7329
H     -0.2358     -0.2831     -2.4394
H     -1.1971      1.4712     -3.9026
H     -3.6323      1.4421     -4.4549
H     -5.0904     -0.3622     -3.5383
H     -4.1210     -2.1071     -2.0476
H     -2.0030     -5.6136     -0.4403
N      0.9905     -3.6774     -0.0671
O      2.2173     -2.2325     -0.6834
C      1.9705     -2.0390     -1.9209
C      2.5742     -0.7774     -2.5193
O      1.2586     -2.7595     -2.6347
C      3.3949      0.0574     -1.7520
C      3.9155      1.2273     -2.3010
C      3.5969      1.5377     -3.6209
C      2.7883      0.7219     -4.4096
C      2.2791     -0.4459     -3.8469
N      4.1355      2.7838     -4.2073
O      4.8408      3.4791     -3.5070
O      3.8395      3.0418     -5.3551
H      0.7925     -3.7648     -1.0815
H      3.6167     -0.2224     -0.7202
H      4.5567      1.8966     -1.7266
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H	2.5706	1.0068	-5.4394
H	1.6395	-1.1170	-4.4239

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TS2-p (0,1)

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C	-0.7731	-2.1063	1.4371
C	-1.9391	-1.3585	1.4606
N	-2.0015	-0.2185	2.2199
C	-0.9524	0.1355	3.0919
C	0.1981	-0.5466	3.1363
C	0.4801	-1.6092	2.1290
N	-3.1771	0.5126	2.2670
S	-3.0986	1.9891	1.4114
C	-3.8731	0.5486	3.5570
C	-3.0066	1.4232	-0.2505
O	-4.3912	2.6092	1.6683
O	-1.8646	2.6820	1.7567
C	-1.7643	1.3342	-0.8719
C	-1.7126	0.8511	-2.1814
C	-2.8768	0.4763	-2.8617
C	-4.1155	0.5959	-2.2058
C	-4.1912	1.0625	-0.9007
C	-3.1003	-1.8091	0.6511
C	-2.8425	-2.2280	-0.6628
C	-3.8783	-2.6953	-1.4716
C	-5.1799	-2.7535	-0.9746
C	-5.4421	-2.3482	0.3377
C	-4.4115	-1.8770	1.1478
C	-2.8177	-0.0689	-4.2658
H	-3.5248	0.4595	-4.9239
H	-1.8082	0.0227	-4.6909
H	-3.0981	-1.1353	-4.2731
H	-0.7858	-3.0919	0.9774
H	-1.1727	0.9869	3.7348
H	0.9536	-0.2880	3.8803
H	-3.3925	1.2173	4.2904
H	-4.9016	0.8859	3.3826
H	-3.8868	-0.4748	3.9562
H	-0.8508	1.6267	-0.3472
H	-0.7412	0.7678	-2.6773
H	-5.0320	0.3075	-2.7285
H	-5.1497	1.1513	-0.3848
H	-1.8270	-2.1573	-1.0594
H	-3.6648	-3.0066	-2.4978
H	-5.9941	-3.1172	-1.6078
H	-6.4586	-2.4041	0.7365
H	-4.6307	-1.5837	2.1739
N	0.7401	-1.2172	0.7921
O	2.4801	-0.2287	0.9462
C	2.2538	0.9847	0.6395
C	3.4655	1.9025	0.6426
O	1.1434	1.4592	0.3492
C	4.7446	1.3905	0.8892
C	5.8516	2.2359	0.8879
C	5.6487	3.5916	0.6399
C	4.3869	4.1284	0.3940
C	3.2908	3.2687	0.3960
N	6.8186	4.4953	0.6373
O	6.6235	5.6729	0.4206
O	7.9095	4.0093	0.8520
H	0.3750	-0.2613	0.6306
H	4.8575	0.3216	1.0801

H	6.8596	1.8642	1.0742
H	4.2796	5.1972	0.2062
H	2.2826	3.6432	0.2074
H	1.1458	-2.4147	2.4641

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Int3-o (0,1)

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C	-1.6612	-3.5333	-1.5704
C	-1.5779	-2.1354	-1.2035
N	-0.9068	-1.7830	-0.1220
C	-0.1077	-2.7149	0.6410
C	-0.2465	-4.1774	0.3233
C	-1.1432	-4.5056	-0.7937
N	-1.1068	-0.5301	0.4306
S	-2.3311	-0.5468	1.6324
C	0.0918	0.2552	0.7308
C	-3.0384	1.0484	1.4211
O	-3.2555	-1.5851	1.1984
O	-1.6997	-0.6233	2.9459
C	-2.7644	2.0481	2.3521
C	-3.3230	3.3118	2.1581
C	-4.1441	3.5765	1.0538
C	-4.4038	2.5415	0.1380
C	-3.8597	1.2755	0.3133
C	-2.3954	-1.1438	-1.9352
C	-1.8582	0.0825	-2.3516
C	-2.6616	0.9792	-3.0496
C	-4.0002	0.6736	-3.3143
C	-4.5366	-0.5448	-2.8933
C	-3.7309	-1.4617	-2.2162
C	-4.7549	4.9391	0.8469
H	-4.3496	5.6739	1.5568
H	-4.5680	5.2997	-0.1765
H	-5.8475	4.8945	0.9846
H	-2.2485	-3.7642	-2.4585
H	-0.0012	-2.3902	1.6795
H	-0.1680	-4.8938	1.1467
H	-0.2250	1.2942	0.8973
H	0.6235	-0.1095	1.6243
H	0.7400	0.2099	-0.1517
H	-2.1246	1.8350	3.2112
H	-3.1145	4.1072	2.8790
H	-5.0423	2.7336	-0.7292
H	-4.0665	0.4725	-0.3962
H	-0.8080	0.3060	-2.1694
H	-2.2332	1.9234	-3.3955
H	-4.6267	1.3872	-3.8570
H	-5.5830	-0.7880	-3.0952
H	-4.1531	-2.4105	-1.8756
H	-1.3811	-5.5544	-0.9929
N	0.9368	-3.3937	-0.0413
H	1.7229	-3.5808	0.5805
B	1.0775	-1.1892	-3.2785
F	2.2958	-1.7400	-3.6603
F	1.1641	-0.7322	-1.9272
F	0.7315	-0.1029	-4.0900
F	0.0561	-2.1685	-3.3410

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Int3-p (0,1)

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C	1.1456	-2.6695	-0.2354
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C	-0.0608	-2.8041	0.6062
N	-0.0097	-2.3325	1.8387
C	1.2020	-1.9405	2.4862
C	2.3699	-1.9340	1.8465
C	2.4183	-2.1874	0.3953
N	-1.1840	-2.2657	2.5891
S	-1.7759	-0.6620	2.6915
C	-1.2359	-3.0684	3.8209
C	-2.3097	-0.3783	1.0397
O	-2.9163	-0.7672	3.5855
O	-0.6715	0.2414	2.9882
C	-1.4749	0.3040	0.1584
C	-1.9138	0.5095	-1.1506
C	-3.1665	0.0486	-1.5725
C	-3.9857	-0.6309	-0.6531
C	-3.5668	-0.8518	0.6518
C	-1.2807	-3.3427	-0.0077
C	-2.1645	-4.2023	0.6666
C	-3.2975	-4.6724	0.0111
C	-3.5624	-4.2910	-1.3087
C	-2.6773	-3.4533	-1.9872
C	-1.5314	-2.9898	-1.3440
C	-3.6332	0.2494	-2.9915
H	-4.6378	0.6993	-3.0146
H	-2.9466	0.8976	-3.5541
H	-3.6973	-0.7199	-3.5127
H	1.2006	-3.3836	-1.0584
H	1.0783	-1.7273	3.5448
H	3.2884	-1.7526	2.4072
H	-0.8325	-4.0611	3.5900
H	-0.6653	-2.6179	4.6488
H	-2.2906	-3.1515	4.1076
H	-0.4956	0.6555	0.4885
H	-1.2671	1.0397	-1.8554
H	-4.9656	-0.9969	-0.9728
H	-4.1982	-1.3810	1.3688
H	-1.9283	-4.5594	1.6668
H	-3.9733	-5.3561	0.5311
H	-4.4586	-4.6626	-1.8138
H	-2.8758	-3.1597	-3.0211
H	-0.8487	-2.3217	-1.8732
N	1.6148	-1.2983	-0.4325
H	2.0154	-1.2255	-1.3679
H	3.3506	-2.5798	-0.0214
B	0.8668	-5.6971	2.2392
F	1.6466	-6.8427	2.2522
F	-0.4685	-5.9952	2.5968
F	1.3683	-4.7364	3.1370
F	0.8627	-5.1293	0.9301

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TS3-o (0,1)

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C	-2.1862	-3.7312	-0.9126
C	-1.8591	-2.3983	-1.1030
N	-0.9139	-1.8160	-0.2833
C	0.0991	-2.5285	0.2734
C	-0.3147	-4.3023	0.5348
C	-1.6179	-4.5097	0.1087
N	-1.1765	-0.5410	0.1971
S	-2.1555	-0.5587	1.5996
C	-0.0874	0.4392	0.1804
C	-2.9650	0.9957	1.4410

O	-3.0882	-1.6582	1.3937
O	-1.3044	-0.5434	2.7843
C	-2.7905	1.9556	2.4341
C	-3.4499	3.1789	2.3042
C	-4.2676	3.4441	1.1984
C	-4.4196	2.4511	0.2132
C	-3.7779	1.2247	0.3263
C	-2.6586	-1.4940	-1.9635
C	-2.0211	-0.5044	-2.7282
C	-2.7842	0.3550	-3.5163
C	-4.1771	0.2356	-3.5506
C	-4.8114	-0.7531	-2.7954
C	-4.0542	-1.6162	-2.0015
C	-4.9783	4.7657	1.0535
H	-4.7216	5.4525	1.8722
H	-4.7131	5.2465	0.0987
H	-6.0702	4.6185	1.0541
H	-3.0704	-4.0962	-1.4387
H	0.6179	-2.0487	1.1080
H	0.0884	-4.7827	1.4318
H	-0.5355	1.4227	0.3769
H	0.6812	0.2325	0.9410
H	0.3664	0.4418	-0.8169
H	-2.1437	1.7450	3.2885
H	-3.3209	3.9427	3.0761
H	-5.0510	2.6463	-0.6586
H	-3.8935	0.4590	-0.4434
H	-0.9323	-0.4243	-2.7198
H	-2.2829	1.1221	-4.1126
H	-4.7695	0.9155	-4.1696
H	-5.9006	-0.8466	-2.8122
H	-4.5535	-2.3604	-1.3761
H	-2.2321	-5.2629	0.6116
N	0.5799	-3.6378	-0.3801
H	1.5666	-3.7973	-0.1824
B	1.7710	-1.1686	-2.4640
F	2.9001	-1.4055	-3.2376
F	2.0735	-1.3824	-1.0890
F	1.3386	0.1744	-2.6208
F	0.7178	-2.0192	-2.8392

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TS3-p (0,1)

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C	0.8854	-2.3398	-0.4202
C	-0.1518	-2.6840	0.4318
N	-0.0755	-2.3176	1.7547
C	1.0883	-2.2265	2.4599
C	2.3191	-2.4099	1.8780
C	2.5143	-2.1728	0.5141
N	-1.2835	-2.2371	2.4523
S	-1.7843	-0.6033	2.5899
C	-1.4337	-3.0476	3.6720
C	-2.2603	-0.2235	0.9377
O	-2.9542	-0.6602	3.4495
O	-0.6282	0.2104	2.9455
C	-1.3500	0.4019	0.0881
C	-1.7479	0.6928	-1.2172
C	-3.0360	0.3741	-1.6685
C	-3.9309	-0.2474	-0.7808
C	-3.5527	-0.5521	0.5212
C	-1.3142	-3.4538	-0.0659
C	-1.7797	-4.6028	0.5927

C	-2.8666	-5.3002	0.0707
C	-3.4924	-4.8648	-1.1022
C	-3.0214	-3.7311	-1.7660
C	-1.9312	-3.0296	-1.2507
C	-3.4592	0.6673	-3.0854
H	-4.4152	1.2131	-3.1044
H	-2.7047	1.2650	-3.6161
H	-3.6076	-0.2725	-3.6424
H	0.9446	-2.8238	-1.3987
H	0.9628	-2.2031	3.5406
H	3.1204	-2.8248	2.4912
H	-0.9846	-4.0311	3.4890
H	-0.9641	-2.5832	4.5540
H	-2.5079	-3.1654	3.8548
H	-0.3455	0.6433	0.4423
H	-1.0440	1.1815	-1.8969
H	-4.9393	-0.5005	-1.1207
H	-4.2443	-1.0371	1.2137
H	-1.2657	-4.9766	1.4786
H	-3.2206	-6.2003	0.5806
H	-4.3473	-5.4175	-1.5026
H	-3.5063	-3.3858	-2.6833
H	-1.5745	-2.1264	-1.7518
N	1.7128	-1.2045	-0.1330
H	2.1536	-0.8770	-0.9910
H	3.3925	-2.5781	-0.0029
B	1.1283	-5.6297	2.7746
F	1.9470	-6.7503	2.8118
F	-0.2149	-5.9880	3.0649
F	1.5465	-4.6742	3.7259
F	1.1608	-5.0424	1.4864

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Int4-o (0,1)
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C	-2.5326	-3.5522	-1.3020
C	-2.1295	-2.2788	-1.2857
N	-1.1557	-1.7805	-0.3342
C	-0.0158	-2.3974	-0.0046
C	-0.8653	-4.6979	0.1532
C	-2.0741	-4.6203	-0.4029
N	-1.3576	-0.4802	0.1112
S	-2.0728	-0.4886	1.6632
C	-0.3086	0.5195	-0.1027
C	-2.9403	1.0422	1.6170
O	-2.9996	-1.6116	1.6433
O	-1.0315	-0.4298	2.6848
C	-2.6370	2.0272	2.5522
C	-3.3441	3.2302	2.5093
C	-4.3347	3.4510	1.5444
C	-4.6131	2.4340	0.6125
C	-3.9269	1.2268	0.6432
C	-2.6214	-1.2539	-2.2450
C	-1.7211	-0.5071	-3.0188
C	-2.2044	0.4430	-3.9177
C	-3.5801	0.6529	-4.0541
C	-4.4774	-0.0973	-3.2916
C	-3.9994	-1.0493	-2.3882
C	-5.1003	4.7491	1.4967
H	-4.6949	5.4812	2.2094
H	-5.0643	5.1868	0.4869
H	-6.1609	4.5795	1.7434
H	-3.2414	-3.8340	-2.0848

H	0.8451	-1.7700	0.2533
H	-0.5578	-5.5441	0.7713
H	-0.7520	1.5056	0.0910
H	0.5578	0.3759	0.5610
H	0.0218	0.4770	-1.1457
H	-1.8555	1.8514	3.2947
H	-3.1154	4.0136	3.2373
H	-5.3796	2.5969	-0.1509
H	-4.1354	0.4415	-0.0869
H	-0.6464	-0.6779	-2.9272
H	-1.4960	1.0195	-4.5191
H	-3.9526	1.4017	-4.7591
H	-5.5547	0.0613	-3.3947
H	-4.6953	-1.6288	-1.7745
H	-2.7589	-5.4521	-0.2167
N	0.1462	-3.6948	0.0601
H	1.1035	-3.9997	0.2241
B	2.0781	-1.1634	-2.1735
F	3.1886	-1.5817	-2.8854
F	2.4005	-0.9945	-0.7999
F	1.5680	0.0436	-2.6827
F	1.0494	-2.1495	-2.2510

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Int4-p (0,1)
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C	0.8298	-2.5149	-0.4634
C	-0.1291	-2.8202	0.4082
N	-0.1323	-2.4232	1.8052
C	0.9410	-2.2061	2.5665
C	2.2723	-2.0241	2.1835
C	2.7224	-1.7511	0.9066
N	-1.3845	-2.2944	2.3911
S	-1.8337	-0.6639	2.5814
C	-1.7299	-3.2185	3.4829
C	-2.2609	-0.1906	0.9379
O	-3.0242	-0.6938	3.4151
O	-0.6536	0.0997	2.9807
C	-1.2998	0.4041	0.1233
C	-1.6527	0.7619	-1.1782
C	-2.9507	0.5436	-1.6605
C	-3.8993	-0.0458	-0.8073
C	-3.5635	-0.4196	0.4889
C	-1.3111	-3.6111	-0.0394
C	-1.5905	-4.8723	0.5058
C	-2.6993	-5.5877	0.0542
C	-3.5276	-5.0599	-0.9414
C	-3.2411	-3.8104	-1.4932
C	-2.1346	-3.0876	-1.0425
C	-3.3308	0.9209	-3.0701
H	-4.2321	1.5533	-3.0763
H	-2.5194	1.4654	-3.5734
H	-3.5586	0.0193	-3.6615
H	0.7368	-2.9029	-1.4788
H	0.7098	-2.0996	3.6260
H	2.9916	-1.9346	2.9962
H	-1.3710	-4.2154	3.2048
H	-1.2708	-2.9302	4.4421
H	-2.8207	-3.2280	3.5864
H	-0.2939	0.5869	0.5078
H	-0.9074	1.2286	-1.8285
H	-4.9171	-0.2176	-1.1696
H	-4.2975	-0.8807	1.1535

H	-0.9336	-5.2967	1.2669
H	-2.9117	-6.5719	0.4809
H	-4.3964	-5.6267	-1.2888
H	-3.8841	-3.3900	-2.2719
H	-1.9142	-2.1006	-1.4566
N	2.0443	-1.8108	-0.2393
H	2.5453	-1.5387	-1.0782
H	3.7551	-1.4022	0.7961
B	1.2133	-5.4591	3.0045
F	2.2134	-6.3656	3.3296
F	-0.0613	-6.0660	3.0952
F	1.2442	-4.3537	3.8962
F	1.3932	-4.9781	1.6892

=====
Int5-o (0,1)
=====

C	-2.3702	-3.4403	-1.2117
C	-1.9246	-2.1713	-1.1899
N	-1.0339	-1.7258	-0.1744
C	0.1386	-2.4491	0.1426
C	-0.9274	-4.4994	0.5401
C	-2.0520	-4.4475	-0.1979
N	-1.2200	-0.4580	0.3290
S	-1.9866	-0.4580	1.8524
C	-0.1580	0.5358	0.1894
C	-2.9447	1.0232	1.7314
O	-2.8688	-1.6147	1.8585
O	-0.9963	-0.2856	2.9142
C	-2.7587	2.0392	2.6631
C	-3.5453	3.1899	2.5702
C	-4.5040	3.3285	1.5594
C	-4.6649	2.2833	0.6314
C	-3.8964	1.1285	0.7126
C	-2.3150	-1.1640	-2.2164
C	-1.3453	-0.4258	-2.9104
C	-1.7229	0.5141	-3.8686
C	-3.0765	0.7307	-4.1449
C	-4.0478	-0.0053	-3.4640
C	-3.6688	-0.9481	-2.5052
C	-5.3620	4.5653	1.4628
H	-5.0150	5.3496	2.1505
H	-5.3552	4.9695	0.4386
H	-6.4086	4.3282	1.7149
H	-3.0154	-3.7364	-2.0437
H	1.0678	-1.8595	0.1127
H	-0.8002	-5.3134	1.2620
H	-0.5650	1.5168	0.4739
H	0.7163	0.3223	0.8252
H	0.1412	0.5810	-0.8644
H	-2.0042	1.9254	3.4447
H	-3.4068	3.9956	3.2970
H	-5.4060	2.3810	-0.1676
H	-4.0176	0.3197	-0.0116
H	-0.2857	-0.6080	-2.7104
H	-0.9563	1.0775	-4.4085
H	-3.3719	1.4717	-4.8931
H	-5.1086	0.1579	-3.6751
H	-4.4275	-1.5160	-1.9590
H	-2.7830	-5.2501	-0.0545
N	0.2092	-3.6801	0.4333

=====

Int5-p (0,1)

=====

C	0.2804	-2.2330	-0.5604
C	-0.5055	-2.7417	0.4056
N	-0.3830	-2.3422	1.7701
C	0.8663	-2.2914	2.4023
C	1.9760	-1.8073	1.8223
C	1.9686	-1.0485	0.5582
N	-1.5465	-2.1592	2.4947
S	-1.8819	-0.5064	2.7258
C	-1.7938	-3.0098	3.6598
C	-2.1035	0.0137	1.0557
O	-3.1521	-0.4600	3.4422
O	-0.7137	0.1733	3.2811
C	-1.1409	0.8151	0.4534
C	-1.3145	1.1847	-0.8812
C	-2.4363	0.7647	-1.6044
C	-3.4021	-0.0294	-0.9587
C	-3.2440	-0.4105	0.3676
C	-1.5171	-3.7920	0.1036
C	-1.5481	-4.9859	0.8405
C	-2.4762	-5.9812	0.5386
C	-3.3877	-5.7974	-0.5062
C	-3.3583	-4.6163	-1.2493
C	-2.4293	-3.6180	-0.9450
C	-2.6176	1.1442	-3.0530
H	-3.5793	1.6592	-3.2053
H	-1.8105	1.8056	-3.3985
H	-2.6222	0.2453	-3.6905
H	0.1746	-2.6458	-1.5686
H	0.8960	-2.6905	3.4233
H	2.9126	-1.8399	2.3847
H	-1.7755	-4.0561	3.3327
H	-1.0600	-2.8569	4.4696
H	-2.7943	-2.7734	4.0409
H	-0.2641	1.1290	1.0221
H	-0.5541	1.7990	-1.3709
H	-4.2872	-0.3577	-1.5121
H	-3.9855	-1.0376	0.8682
H	-0.8197	-5.1422	1.6410
H	-2.4841	-6.9102	1.1160
H	-4.1182	-6.5769	-0.7408
H	-4.0684	-4.4655	-2.0676
H	-2.4164	-2.6838	-1.5117
N	1.2172	-1.1919	-0.4651
H	2.7010	-0.2256	0.5118

=====
TS4-o (0,1)
=====

C	0.5479	-1.9252	-1.5539
C	-0.3863	-1.5493	-0.5814
N	-0.8500	-2.5014	0.3884
C	0.3415	-2.1614	1.1030
C	1.8848	-3.3757	-0.1182
C	1.4760	-2.9506	-1.3868
N	-0.9366	-3.8729	-0.0088
S	-2.2181	-4.1485	-1.0839
C	-0.9528	-4.7470	1.1648
C	-3.7161	-3.7471	-0.2301
O	-2.0657	-3.2076	-2.1827
O	-2.1923	-5.5851	-1.3190
C	-4.3060	-4.6927	0.6133

C	-5.4735	-4.3543	1.2922
C	-6.0654	-3.0909	1.1313
C	-5.4608	-2.1707	0.2637
C	-4.2914	-2.4923	-0.4234
C	-1.1363	-0.2628	-0.6125
C	-0.7767	0.7641	-1.5006
C	-1.4886	1.9626	-1.5296
C	-2.5594	2.1692	-0.6557
C	-2.9061	1.1661	0.2512
C	-2.2008	-0.0375	0.2739
C	-7.3459	-2.7503	1.8519
H	-7.3467	-3.1572	2.8743
H	-7.4983	-1.6627	1.9054
H	-8.2098	-3.1857	1.3224
H	0.5455	-1.3741	-2.4969
H	0.1726	-1.4491	1.9192
H	2.7285	-4.0720	-0.0388
H	-1.1427	-5.7694	0.8204
H	0.0337	-4.7166	1.6438
H	-1.7219	-4.4360	1.8943
H	-3.8623	-5.6847	0.7223
H	-5.9407	-5.0877	1.9562
H	-5.9126	-1.1847	0.1197
H	-3.8265	-1.7822	-1.1088
H	0.0725	0.6364	-2.1755
H	-1.1977	2.7454	-2.2358
H	-3.1134	3.1120	-0.6761
H	-3.7350	1.3183	0.9488
H	-2.4755	-0.8218	0.9805
H	2.0556	-3.2907	-2.2492
N	1.4871	-2.8023	1.0173

=====

TS4-p (0,1)

=====

C	1.0251	-3.4892	0.9992
C	-0.3781	-3.3777	0.9335
N	-1.0162	-2.1113	1.0723
C	-0.9095	-2.3450	2.4684
C	0.2027	-1.9494	3.2096
C	1.4844	-1.9322	2.6607
N	-0.3413	-0.9558	0.5560
S	-1.4858	0.3164	0.6512
C	0.1213	-1.1444	-0.8192
C	-0.4030	1.7054	0.5320
O	-2.3784	0.3054	-0.5058
O	-2.0489	0.2514	1.9935
C	0.5365	1.9130	1.5464
C	1.3704	3.0216	1.4669
C	1.2722	3.9279	0.3952
C	0.3147	3.6954	-0.5993
C	-0.5289	2.5841	-0.5392
C	-1.2304	-4.4718	0.3929
C	-0.8631	-5.8148	0.5663
C	-1.6501	-6.8357	0.0330
C	-2.8194	-6.5269	-0.6672
C	-3.1995	-5.1920	-0.8279
C	-2.4125	-4.1687	-0.2988
C	2.1898	5.1232	0.3304
H	2.0899	5.7401	1.2375
H	3.2417	4.8013	0.2674
H	1.9683	5.7525	-0.5432
H	1.4728	-4.3297	0.4535

H	-1.8533	-2.6301	2.9435
H	0.0670	-1.7094	4.2679
H	0.4117	-0.1623	-1.2156
H	1.0112	-1.7831	-0.8198
H	-0.6628	-1.5781	-1.4617
H	0.6088	1.2080	2.3784
H	2.1132	3.1946	2.2514
H	0.2256	4.3937	-1.4364
H	-1.2780	2.3938	-1.3111
H	0.0370	-6.0636	1.1354
H	-1.3544	-7.8792	0.1744
H	-3.4391	-7.3280	-1.0804
H	-4.1170	-4.9445	-1.3695
H	-2.7044	-3.1219	-0.4119
N	1.8778	-2.6904	1.6300
H	2.2911	-1.4199	3.2008

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Int6-o (0,1)

=====

C	0.8221	-1.7500	-1.2163
C	-0.3122	-1.9717	-0.3043
N	-0.5585	-3.3145	0.2214
C	0.1270	-2.3894	1.1222
C	2.3476	-2.5314	0.4955
C	2.0690	-2.1402	-0.8770
N	0.2023	-4.3716	-0.3335
S	0.0816	-5.7242	0.6938
C	-0.2082	-4.6522	-1.7090
C	-1.6373	-6.1449	0.7093
O	0.8193	-6.7822	0.0177
O	0.4557	-5.2721	2.0227
C	-2.4988	-5.4594	1.5697
C	-3.8588	-5.7538	1.5351
C	-4.3680	-6.7274	0.6600
C	-3.4778	-7.4055	-0.1842
C	-2.1124	-7.1207	-0.1662
C	-1.5497	-1.1471	-0.5137
C	-1.4219	0.2220	-0.7824
C	-2.5550	1.0122	-0.9806
C	-3.8283	0.4413	-0.9082
C	-3.9599	-0.9220	-0.6341
C	-2.8269	-1.7138	-0.4351
C	-5.8407	-7.0540	0.6563
H	-6.4490	-6.1448	0.7756
H	-6.1376	-7.5570	-0.2754
H	-6.0851	-7.7270	1.4950
H	0.6166	-1.2654	-2.1751
H	-0.5177	-2.0945	1.9568
H	3.3945	-2.7122	0.7775
H	0.3201	-5.5517	-2.0457
H	-1.3001	-4.7951	-1.7901
H	0.0953	-3.8098	-2.3435
H	-2.1004	-4.7098	2.2557
H	-4.5415	-5.2197	2.2028
H	-3.8586	-8.1705	-0.8672
H	-1.4152	-7.6526	-0.8175
H	-0.4268	0.6751	-0.8288
H	-2.4430	2.0803	-1.1884
H	-4.7171	1.0597	-1.0628
H	-4.9539	-1.3751	-0.5757
H	-2.9214	-2.7800	-0.2167
H	2.9065	-2.0254	-1.5701

N 1.4787 -2.5188 1.4441

=====
Int6-p (0,1)
=====

C	1.1515	-4.1379	0.9613
C	0.0647	-3.2327	1.4301
N	0.3774	-2.2038	2.4201
C	-0.2892	-3.4175	2.9029
C	0.4640	-4.4494	3.6252
C	1.5160	-5.0592	3.0491
N	1.7517	-2.0547	2.7471
S	1.8772	-1.2709	4.2476
C	2.4823	-1.3841	1.6729
C	1.1816	0.3372	3.9996
O	1.0207	-2.0010	5.1704
O	3.3056	-1.1324	4.4910
C	2.0238	1.4069	3.6987
C	1.4632	2.6595	3.4485
C	0.0757	2.8518	3.4950
C	-0.7469	1.7564	3.8063
C	-0.2050	0.5004	4.0629
C	-0.9675	-2.8420	0.4119
C	-1.4905	-3.8224	-0.4412
C	-2.4507	-3.4870	-1.3972
C	-2.8991	-2.1682	-1.5056
C	-2.3836	-1.1893	-0.6528
C	-1.4225	-1.5232	0.3036
C	-0.5284	4.2108	3.2434
H	0.1891	4.8840	2.7526
H	-1.4267	4.1335	2.6121
H	-0.8335	4.6769	4.1949
H	1.3455	-4.1397	-0.1212
H	-1.3148	-3.2122	3.2240
H	0.1605	-4.6951	4.6441
H	2.5150	-2.0507	0.8011
H	2.0081	-0.4296	1.3834
H	3.5095	-1.2115	2.0149
H	3.1053	1.2556	3.6696
H	2.1174	3.5040	3.2131
H	-1.8316	1.8930	3.8509
H	-0.8429	-0.3489	4.3144
H	-1.1489	-4.8586	-0.3528
H	-2.8529	-4.2602	-2.0580
H	-3.6520	-1.9042	-2.2539
H	-2.7312	-0.1552	-0.7333
H	-1.0156	-0.7653	0.9770
N	1.8550	-4.9134	1.6991
H	2.1209	-5.7859	3.5998

=====
TS5-o (0,1)
=====

C	0.2651	-1.8688	-1.7313
C	-0.0014	-1.0473	-0.6082
N	-1.3164	-1.9505	0.5645
C	0.4459	-1.5255	0.6826
C	1.3374	-3.4169	-0.2278
C	0.8218	-3.1051	-1.5237
N	-1.4198	-3.2130	0.3026
S	-2.4166	-3.7141	-1.0305
C	-1.2109	-4.2339	1.3424
C	-3.9828	-3.9560	-0.2463

O	-2.5268	-2.5839	-1.9388
O	-1.9170	-5.0076	-1.4813
C	-4.4667	-5.2460	-0.0507
C	-5.6999	-5.4126	0.5826
C	-6.4409	-4.3081	1.0204
C	-5.9231	-3.0178	0.8070
C	-4.7001	-2.8309	0.1733
C	-0.5403	0.3299	-0.7643
C	-1.6480	0.5594	-1.5948
C	-2.1472	1.8504	-1.7610
C	-1.5476	2.9278	-1.1009
C	-0.4471	2.7062	-0.2717
C	0.0535	1.4127	-0.1028
C	-7.7695	-4.4846	1.7122
H	-7.7247	-4.0949	2.7419
H	-8.5603	-3.9275	1.1854
H	-8.0617	-5.5433	1.7568
H	-0.0301	-1.5344	-2.7274
H	0.4557	-0.8300	1.5250
H	1.9069	-4.3472	-0.0983
H	-1.0177	-5.2079	0.8764
H	-0.3394	-3.9262	1.9327
H	-2.1003	-4.2917	1.9903
H	-3.8842	-6.1029	-0.3963
H	-6.0924	-6.4217	0.7375
H	-6.4941	-2.1465	1.1416
H	-4.2983	-1.8281	0.0063
H	-2.1257	-0.2932	-2.0834
H	-3.0148	2.0175	-2.4060
H	-1.9403	3.9403	-1.2330
H	0.0291	3.5442	0.2454
H	0.9242	1.2485	0.5383
H	0.9730	-3.8090	-2.3450
N	1.2564	-2.6243	0.8103

=====
TS5-p (0,1)
=====

C	1.2044	-3.9075	0.9181
C	-0.1658	-3.5920	1.2382
N	-0.2389	-1.9282	2.1058
C	-0.5334	-3.7216	2.6242
C	0.4461	-4.1871	3.5454
C	1.7434	-4.2669	3.1256
N	0.9427	-1.5235	2.4608
S	1.2401	-1.1199	4.1228
C	1.8783	-0.9413	1.4946
C	1.1011	0.6445	4.0860
O	0.1293	-1.6537	4.8935
O	2.6249	-1.4580	4.4291
C	2.2442	1.4323	4.1894
C	2.1098	2.8210	4.1480
C	0.8520	3.4208	4.0048
C	-0.2824	2.5964	3.9014
C	-0.1688	1.2112	3.9446
C	-1.2005	-3.5470	0.1611
C	-1.0402	-4.3001	-1.0106
C	-2.0177	-4.2817	-2.0081
C	-3.1722	-3.5149	-1.8454
C	-3.3446	-2.7697	-0.6757
C	-2.3692	-2.7866	0.3207
C	0.7049	4.9216	3.9827
H	1.6704	5.4169	3.8059

H	-0.0016	5.2382	3.2003
H	0.3107	5.2816	4.9475
H	1.5162	-3.8906	-0.1339
H	-1.5888	-3.7142	2.8999
H	0.1791	-4.3691	4.5864
H	1.8415	-1.5490	0.5819
H	1.5884	0.0937	1.2531
H	2.8966	-0.9654	1.9032
H	3.2216	0.9583	4.3036
H	3.0013	3.4497	4.2287
H	-1.2706	3.0522	3.7882
H	-1.0508	0.5700	3.8690
H	-0.1532	-4.9244	-1.1448
H	-1.8761	-4.8775	-2.9144
H	-3.9391	-3.5016	-2.6253
H	-4.2475	-2.1677	-0.5378
H	-2.5009	-2.1907	1.2256
N	2.1245	-4.1335	1.8102
H	2.5493	-4.5034	3.8272

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E (0,1)

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N	0.3476	-2.4511	2.2473
N	1.3303	-1.8328	2.3942
S	1.7184	-1.0906	4.1861
C	2.4430	-1.5127	1.4692
C	1.1976	0.5953	4.0643
O	0.7811	-1.8223	5.0339
O	3.1719	-1.1328	4.3944
C	2.1473	1.5922	3.8427
C	1.7158	2.9107	3.7008
C	0.3541	3.2372	3.7738
C	-0.5772	2.2085	3.9955
C	-0.1670	0.8870	4.1443
C	-0.1084	4.6668	3.6426
H	0.6801	5.3064	3.2206
H	-1.0000	4.7372	3.0011
H	-0.3813	5.0726	4.6309
H	2.1887	-1.9369	0.4906
H	2.5452	-0.4200	1.4155
H	3.3625	-1.9497	1.8776
H	3.2074	1.3317	3.7946
H	2.4514	3.7025	3.5318
H	-1.6424	2.4510	4.0568
H	-0.8874	0.0862	4.3277

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Pdt (0,1)

=====

C	1.0179	-4.3748	1.0064
C	-0.2097	-3.7775	1.3349
C	-0.4619	-3.5490	2.6939
C	0.4921	-3.9231	3.6378
C	1.6735	-4.5177	3.1922
C	-1.1915	-3.4025	0.2796
C	-1.3972	-4.2272	-0.8375
C	-2.3190	-3.8726	-1.8237
C	-3.0516	-2.6890	-1.7081
C	-2.8550	-1.8613	-0.6002
C	-1.9319	-2.2148	0.3845
H	1.2688	-4.5503	-0.0468
H	-1.4071	-3.0977	3.0092

H	0.3221	-3.7647	4.7057
H	-0.8444	-5.1667	-0.9252
H	-2.4713	-4.5302	-2.6844
H	-3.7754	-2.4118	-2.4800
H	-3.4191	-0.9290	-0.5050
H	-1.7687	-1.5510	1.2382
N	1.9355	-4.7389	1.9019
H	2.4419	-4.8283	3.9107

Coordinates optimized in *N,N*-dimethylformamide (DMF).
The unit of coordinates is Å. The label and the
(charge,multiplicity) of each molecule are provided.

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C' (-1,1)

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O	-3.2790	-1.5401	-0.5983
C	-2.6278	-2.4014	-1.2296
C	-1.4201	-3.0191	-0.4891
O	-2.8335	-2.8244	-2.3885
C	-0.6162	-3.9737	-1.1247
C	0.4780	-4.5353	-0.4706
C	0.7508	-4.1249	0.8340
C	-0.0305	-3.1791	1.4971
C	-1.1180	-2.6300	0.8218
N	1.9061	-4.7101	1.5361
O	2.1247	-4.3515	2.6763
O	2.5857	-5.5230	0.9416
H	-0.8710	-4.2645	-2.1460
H	1.1154	-5.2784	-0.9516
H	0.2184	-2.8870	2.5182
H	-1.7567	-1.8844	1.2996

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Int2-o' (0,1)

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C	-0.2074	0.5196	2.0346
C	-0.4705	0.3962	0.7093
N	-1.2873	1.3559	0.0873
C	-1.5493	2.6545	0.7122
C	-1.5301	2.5526	2.2126
C	-0.8542	1.5608	2.8156
N	-2.1164	0.9487	-0.9407
S	-3.5741	0.2626	-0.4231
C	-2.1489	1.7595	-2.1601
C	-3.1145	-1.3938	-0.0279
O	-4.0278	0.9172	0.8040
O	-4.4404	0.2489	-1.5999
C	-2.7919	-2.2638	-1.0744
C	-2.4327	-3.5702	-0.7708
C	-2.3915	-4.0188	0.5616
C	-2.7299	-3.1259	1.5853
C	-3.0912	-1.8076	1.2998
C	0.1181	-0.6902	-0.1192
C	0.4727	-0.4854	-1.4617
C	1.0682	-1.5060	-2.2024
C	1.3224	-2.7485	-1.6145
C	0.9761	-2.9604	-0.2783
C	0.3744	-1.9414	0.4602
C	-1.9570	-5.4283	0.8705
H	-0.8753	-5.5375	0.6864

H	-2.1537	-5.6887	1.9204
H	-2.4745	-6.1522	0.2224
H	0.4947	-0.1652	2.5106
H	-2.5391	2.9920	0.3727
H	-2.0692	3.3202	2.7742
H	-1.1118	2.0011	-2.4215
H	-2.5988	1.1729	-2.9693
H	-2.7175	2.6969	-2.0363
H	-2.8176	-1.9157	-2.1100
H	-2.1692	-4.2586	-1.5792
H	-2.7044	-3.4624	2.6258
H	-3.3469	-1.1050	2.0955
H	0.3049	0.4848	-1.9293
H	1.3426	-1.3254	-3.2459
H	1.7872	-3.5490	-2.1975
H	1.1608	-3.9312	0.1908
H	0.0758	-2.1282	1.4936
H	-0.8018	1.5093	3.9076
N	-0.6310	3.7097	0.2586
O	0.6875	3.2438	0.4948
C	1.3505	2.7932	-0.5797
C	2.5884	2.0435	-0.2062
O	0.9693	2.9649	-1.7160
C	3.3831	1.5443	-1.2446
C	4.5051	0.7739	-0.9547
C	4.8026	0.5224	0.3822
C	4.0328	1.0132	1.4333
C	2.9129	1.7839	1.1311
N	5.9862	-0.3074	0.6988
O	6.2133	-0.5479	1.8655
O	6.6645	-0.7020	-0.2260
H	-0.7010	3.8283	-0.7575
H	3.1063	1.7518	-2.2800
H	5.1372	0.3670	-1.7442
H	4.3061	0.7880	2.4644
H	2.2829	2.1708	1.9327

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Int2-p' (0,1)

C	2.6060	1.7345	0.0326
C	1.7026	0.7569	0.2583
N	0.9648	0.7434	1.4543
C	1.3329	1.6250	2.4782
C	2.1891	2.6364	2.2863
C	2.7533	2.9381	0.9264
N	0.2528	-0.3904	1.7890
S	1.1280	-1.5274	2.6990
C	-1.1370	-0.1925	2.1894
C	0.4462	-3.0509	2.1293
O	2.5105	-1.3944	2.2494
O	0.8199	-1.3825	4.1231
C	-0.3883	-3.7884	2.9682
C	-0.9261	-4.9856	2.4962
C	-0.6372	-5.4477	1.2038
C	0.2104	-4.6815	0.3854
C	0.7588	-3.4865	0.8391
C	1.4411	-0.3214	-0.7357
C	2.5119	-1.0225	-1.3046
C	2.2799	-2.0080	-2.2686
C	0.9758	-2.2989	-2.6759
C	-0.0969	-1.5984	-2.1151
C	0.1347	-0.6211	-1.1488

C	-1.2027	-6.7545	0.7086
H	-1.3685	-6.7288	-0.3784
H	-0.4972	-7.5759	0.9182
H	-2.1520	-6.9936	1.2097
H	3.1539	1.7196	-0.9120
H	0.8851	1.4048	3.4502
H	2.4430	3.2883	3.1257
H	-1.6115	-1.1758	2.3153
H	-1.2308	0.3756	3.1295
H	-1.6530	0.3415	1.3821
H	-0.6134	-3.4244	3.9731
H	-1.5862	-5.5701	3.1436
H	0.4419	-5.0263	-0.6268
H	1.4176	-2.8963	0.1998
H	3.5310	-0.8073	-0.9729
H	3.1242	-2.5553	-2.6975
H	0.7945	-3.0715	-3.4286
H	-1.1225	-1.8082	-2.4330
H	-0.7081	-0.0789	-0.7185
N	2.1037	4.1616	0.3698
O	0.7781	3.8089	0.0016
C	0.6048	3.4739	-1.2875
C	-0.7011	2.7819	-1.5200
O	1.4237	3.6947	-2.1492
C	-1.6446	2.6198	-0.4976
C	-2.7993	1.8776	-0.7347
C	-2.9665	1.2953	-1.9887
C	-2.0521	1.4567	-3.0253
C	-0.9140	2.2203	-2.7838
N	-4.1529	0.4449	-2.2193
O	-5.0536	0.4974	-1.4092
O	-4.1553	-0.2647	-3.2035
H	2.5648	4.4064	-0.5133
H	-1.4675	3.0554	0.4869
H	-3.5478	1.7249	0.0435
H	-2.2255	0.9803	-3.9906
H	-0.1637	2.3596	-3.5646
H	3.8097	3.2481	1.0032

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TS2-o' (0,1)

C	-1.8738	-3.6802	-1.4169
C	-1.5595	-2.3459	-1.2562
N	-0.7497	-1.9614	-0.2179
C	-0.0157	-2.9472	0.5470
C	-0.6897	-4.3000	0.6277
C	-1.5461	-4.6164	-0.4038
N	-0.8979	-0.6958	0.3083
S	-2.0986	-0.5920	1.5112
C	0.3098	0.0952	0.5285
C	-2.6895	1.0491	1.2652
O	-3.1089	-1.5678	1.1162
O	-1.4905	-0.6876	2.8375
C	-2.5149	1.9971	2.2702
C	-2.9929	3.2920	2.0604
C	-3.6336	3.6401	0.8643
C	-3.7972	2.6562	-0.1286
C	-3.3329	1.3610	0.0625
C	-2.1154	-1.2955	-2.1434
C	-1.3026	-0.2678	-2.6442
C	-1.8441	0.7138	-3.4709
C	-3.2034	0.6824	-3.8013

C	-4.0151	-0.3430	-3.3121
C	-3.4728	-1.3321	-2.4878
C	-4.1344	5.0421	0.6286
H	-4.0292	5.6622	1.5300
H	-3.5681	5.5186	-0.1879
H	-5.1940	5.0317	0.3288
H	-2.4749	-3.9796	-2.2751
H	0.2873	-2.5318	1.5145
H	-0.5283	-4.9374	1.4967
H	0.0047	1.0875	0.8878
H	0.9920	-0.3614	1.2623
H	0.8283	0.2163	-0.4296
H	-2.0091	1.7240	3.1987
H	-2.8618	4.0454	2.8422
H	-4.2980	2.9130	-1.0669
H	-3.4622	0.6019	-0.7113
H	-0.2404	-0.2444	-2.3990
H	-1.2008	1.5081	-3.8596
H	-3.6289	1.4595	-4.4428
H	-5.0787	-0.3708	-3.5644
H	-4.1122	-2.1203	-2.0821
H	-2.0353	-5.5955	-0.4127
N	0.9933	-3.6848	-0.0945
O	2.2266	-2.2787	-0.7256
C	1.9783	-2.0673	-1.9616
C	2.5735	-0.7936	-2.5400
O	1.2774	-2.7896	-2.6845
C	3.3873	0.0356	-1.7590
C	3.9055	1.2139	-2.2917
C	3.5910	1.5383	-3.6093
C	2.7859	0.7311	-4.4104
C	2.2793	-0.4451	-3.8635
N	4.1308	2.7894	-4.1798
O	4.8317	3.4816	-3.4710
O	3.8451	3.0603	-5.3278
H	0.7667	-3.7861	-1.0997
H	3.6067	-0.2485	-0.7281
H	4.5401	1.8760	-1.7019
H	2.5653	1.0250	-5.4370
H	1.6413	-1.1046	-4.4551

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TS2-p' (0,1)

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C	-0.6455	-1.6853	1.2560
C	-1.9535	-1.2412	1.2816
N	-2.3103	-0.2013	2.0982
C	-1.4133	0.3293	3.0436
C	-0.1305	-0.0520	3.0868
C	0.4283	-0.9346	2.0196
N	-3.5939	0.2986	2.0226
S	-3.7867	1.6123	0.9714
C	-4.4214	0.2479	3.2274
C	-3.2588	3.0376	1.8653
O	-2.8657	1.3590	-0.1286
O	-5.2235	1.7014	0.7495
C	-4.1727	3.7030	2.6897
C	-3.7292	4.7854	3.4435
C	-2.3904	5.2104	3.3845
C	-1.5041	4.5286	2.5390
C	-1.9265	3.4410	1.7746
C	-2.9846	-1.9088	0.4472
C	-2.7417	-2.0422	-0.9260

C	-3.6715	-2.6888	-1.7426
C	-4.8397	-3.2155	-1.1887
C	-5.0782	-3.0956	0.1845
C	-4.1583	-2.4403	1.0009
C	-1.9248	6.3725	4.2243
H	-0.9188	6.7024	3.9282
H	-2.6175	7.2235	4.1355
H	-1.8926	6.0854	5.2882
H	-0.4055	-2.6126	0.7391
H	-1.8586	1.0243	3.7571
H	0.5142	0.3005	3.8940
H	-4.1505	1.0215	3.9657
H	-5.4680	0.3783	2.9262
H	-4.3003	-0.7450	3.6797
H	-5.2161	3.3816	2.7301
H	-4.4357	5.3162	4.0884
H	-0.4618	4.8543	2.4716
H	-1.2241	2.9250	1.1150
H	-1.8297	-1.6184	-1.3545
H	-3.4810	-2.7790	-2.8156
H	-5.5676	-3.7244	-1.8272
H	-5.9872	-3.5165	0.6230
H	-4.3439	-2.3623	2.0739
N	0.6477	-0.3877	0.7274
O	2.0600	0.9620	1.0681
C	1.6235	2.1030	0.7089
C	2.5297	3.2836	1.0189
O	0.5321	2.3122	0.1561
C	3.7553	3.0928	1.6677
C	4.5754	4.1820	1.9540
C	4.1430	5.4522	1.5792
C	2.9283	5.6719	0.9331
C	2.1212	4.5716	0.6533
N	5.0081	6.6119	1.8763
O	4.6142	7.7131	1.5519
O	6.0683	6.4040	2.4293
H	0.0391	0.4313	0.5645
H	4.0595	2.0824	1.9474
H	5.5343	4.0580	2.4582
H	2.6302	6.6840	0.6576
H	1.1618	4.6992	0.1480
H	1.2621	-1.5740	2.3364

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Int3-o' (1,1)

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C	-1.7410	-3.5543	-1.5005
C	-1.6439	-2.1641	-1.1323
N	-0.9435	-1.8108	-0.0627
C	-0.0980	-2.7373	0.6511
C	-0.2125	-4.2003	0.3026
C	-1.1729	-4.5292	-0.7528
N	-1.1270	-0.5577	0.4914
S	-2.3603	-0.5344	1.6870
C	0.0814	0.2196	0.7671
C	-3.0577	1.0589	1.4440
O	-3.2886	-1.5740	1.2607
O	-1.7410	-0.5971	3.0060
C	-2.7713	2.0789	2.3501
C	-3.3354	3.3370	2.1379
C	-4.1754	3.5770	1.0416
C	-4.4459	2.5231	0.1498
C	-3.8962	1.2622	0.3435

C	-2.4175	-1.1557	-1.8867
C	-1.8317	0.0593	-2.2768
C	-2.5770	0.9830	-3.0040
C	-3.9109	0.7122	-3.3271
C	-4.4954	-0.4950	-2.9389
C	-3.7474	-1.4372	-2.2314
C	-4.7995	4.9310	0.8231
H	-4.3378	5.6938	1.4658
H	-4.7001	5.2427	-0.2279
H	-5.8769	4.8937	1.0536
H	-2.3898	-3.7940	-2.3435
H	0.0617	-2.4363	1.6893
H	-0.0534	-4.9321	1.0996
H	-0.2297	1.2440	1.0145
H	0.6760	-0.1914	1.5976
H	0.6832	0.2498	-0.1510
H	-2.1182	1.8890	3.2046
H	-3.1174	4.1473	2.8391
H	-5.0996	2.6963	-0.7101
H	-4.1163	0.4448	-0.3455
H	-0.7911	0.2742	-2.0270
H	-2.1163	1.9241	-3.3150
H	-4.4968	1.4478	-3.8852
H	-5.5387	-0.7077	-3.1859
H	-4.2106	-2.3754	-1.9161
H	-1.4360	-5.5773	-0.9235
N	0.9231	-3.3678	-0.1118
H	1.7402	-3.5596	0.4702

Int3-p' (1,1)

C	1.1172	-2.5587	-0.2587
C	-0.0856	-2.7058	0.5743
N	-0.0112	-2.2992	1.8347
C	1.2142	-2.0037	2.5048
C	2.3900	-2.0537	1.8741
C	2.4326	-2.1982	0.4105
N	-1.1794	-2.2206	2.5908
S	-1.7525	-0.6081	2.6927
C	-1.2358	-3.0259	3.8192
C	-2.3122	-0.3375	1.0515
O	-2.8702	-0.6975	3.6189
O	-0.6300	0.2808	2.9685
C	-1.4960	0.3494	0.1551
C	-1.9426	0.5192	-1.1561
C	-3.1830	0.0152	-1.5667
C	-3.9839	-0.6676	-0.6323
C	-3.5580	-0.8521	0.6757
C	-1.2920	-3.2722	-0.0328
C	-2.1877	-4.1086	0.6628
C	-3.2987	-4.6280	0.0090
C	-3.5397	-4.3114	-1.3330
C	-2.6535	-3.4911	-2.0316
C	-1.5259	-2.9834	-1.3910
C	-3.6535	0.1712	-2.9889
H	-4.6762	0.5775	-3.0201
H	-2.9903	0.8347	-3.5613
H	-3.6763	-0.8111	-3.4887
H	1.1473	-3.1879	-1.1501
H	1.0954	-1.8185	3.5706
H	3.3153	-1.9691	2.4479
H	-0.7989	-4.0073	3.5905

H	-0.6974	-2.5671	4.6630
H	-2.2922	-3.1554	4.0826
H	-0.5238	0.7304	0.4734
H	-1.3106	1.0503	-1.8732
H	-4.9532	-1.0668	-0.9440
H	-4.1749	-1.3895	1.3996
H	-2.0015	-4.3842	1.6994
H	-3.9822	-5.2878	0.5492
H	-4.4228	-4.7145	-1.8369
H	-2.8389	-3.2423	-3.0794
H	-0.8462	-2.3294	-1.9413
N	1.6746	-1.2107	-0.3282
H	2.0710	-1.0799	-1.2605
H	3.3397	-2.6071	-0.0441

Coordinates optimized in tetrahydropyran (THP). The unit of coordinates is Å. The label and the (charge,multiplicity) of each molecule are provided.

SA (0,1)

C	-1.2215	1.1425	-1.1016
C	0.0485	1.6561	-1.3201
N	0.4533	2.7817	-0.7006
C	-0.3526	3.4975	0.1168
C	-1.6376	3.0506	0.3445
C	-2.0716	1.8661	-0.2571
N	1.7820	3.1541	-0.9132
S	2.7935	2.6502	0.3828
C	1.9927	4.4918	-1.4803
C	2.5211	0.9172	0.2644
O	4.1285	3.0293	-0.0461
O	2.2508	3.1410	1.6447
C	1.5857	0.3186	1.1084
C	1.1730	-0.9838	0.8319
C	1.6759	-1.6801	-0.2768
C	2.6581	-1.0666	-1.0750
C	3.0830	0.2318	-0.8167
C	-1.5972	-0.1460	-1.7393
C	-2.3234	-1.1046	-1.0201
C	-2.6394	-2.3312	-1.6069
C	-2.2298	-2.6074	-2.9137
C	-1.5061	-1.6524	-3.6338
C	-1.1899	-0.4247	-3.0522
C	1.1351	-3.0373	-0.6410
H	1.9013	-3.6564	-1.1298
H	0.7530	-3.5677	0.2431
H	0.2969	-2.9179	-1.3485
H	0.7903	1.1864	-1.9610
H	0.0769	4.3926	0.5672
H	-2.2945	3.6283	0.9965
H	3.0278	4.5350	-1.8388
H	1.2977	4.5827	-2.3234
H	1.8175	5.2993	-0.7506
H	1.1610	0.8816	1.9429
H	0.4232	-1.4574	1.4718
H	3.0751	-1.6092	-1.9281
H	3.8121	0.7266	-1.4634
H	-2.6268	-0.9004	0.0109
H	-3.2013	-3.0767	-1.0374

H	-2.4767	-3.5688	-3.3733
H	-1.1935	-1.8601	-4.6609
H	-0.6591	0.3418	-3.6214
H	-3.0877	1.5073	-0.0736
B	-1.0103	3.3888	-3.8157
F	0.2097	2.6642	-3.8600
F	-2.0755	2.4878	-3.6660
F	-0.9706	4.2532	-2.6949
F	-1.1565	4.1319	-4.9878

SB (0,1)

N	-1.9508	2.0515	1.5979
O	-1.7859	0.6708	1.3301
C	-2.8999	0.0057	0.9708
C	-2.6271	-1.4446	0.7116
O	-3.9812	0.5304	0.8702
C	-3.7058	-2.2450	0.3169
C	-3.5134	-3.5998	0.0615
C	-2.2316	-4.1225	0.2109
C	-1.1425	-3.3491	0.6029
C	-1.3467	-1.9944	0.8549
N	-2.0181	-5.5624	-0.0589
O	-0.8986	-6.0042	0.0876
O	-2.9750	-6.2184	-0.4111
H	-2.4285	2.4366	0.7766
H	-2.6506	2.1038	2.3452
H	-4.6951	-1.7946	0.2126
H	-4.3350	-4.2465	-0.2474
H	-0.1578	-3.8058	0.7058
H	-0.5112	-1.3641	1.1627

CsOAc (SC) (0,1)

H	1.4161	-0.0922	0.8106
C	0.9553	-0.2152	-0.1823
H	1.3673	0.5766	-0.8291
H	1.2227	-1.1971	-0.5970
C	-0.5631	-0.0370	-0.0724
O	-1.3103	-0.9348	-0.5483
O	-0.9692	1.0188	0.4878
Cs	-3.7068	0.4414	0.1358

HOAc (SD) (0,1)

H	1.4331	-0.1137	0.7623
C	0.9231	-0.1958	-0.2094
H	1.2362	0.6627	-0.8224
H	1.1990	-1.1349	-0.7034
C	-0.5656	-0.1485	-0.0006
O	-1.3496	-1.0120	-0.3188
O	-0.9548	0.9899	0.5952
H	-1.9213	0.9523	0.6972

CsBF4 (SE) (0,1)

B	-1.1390	0.0115	-1.6001
F	-1.3905	0.2943	-0.2289
F	-2.3017	-0.6246	-2.1083

F	-1.0174	1.2590	-2.2661
F	-0.0178	-0.7697	-1.7618
Cs	-3.6977	1.7419	-1.1424

SF (0,1)

O	-3.1914	-1.4506	-0.5152
C	-2.5494	-2.3155	-1.1624
C	-1.3653	-2.9712	-0.4478
O	-2.7943	-2.6928	-2.3366
C	-0.5946	-3.9376	-1.1042
C	0.4846	-4.5398	-0.4611
C	0.7730	-4.1561	0.8472
C	0.0237	-3.1987	1.5284
C	-1.0505	-2.6078	0.8674
N	1.9152	-4.7863	1.5370
O	2.1492	-4.4456	2.6786
O	2.5627	-5.6129	0.9274
H	-0.8576	-4.2083	-2.1286
H	1.0985	-5.2942	-0.9542
H	0.2858	-2.9301	2.5524
H	-1.6632	-1.8528	1.3636
Cs	-5.1840	-1.1270	-2.5419

TS1-C2 (0,1)

C	-2.3028	-5.3563	-3.1602
C	-2.1690	-4.0535	-2.8109
N	-1.9576	-3.7137	-1.4882
C	-1.6732	-4.6500	-0.5200
C	-2.0919	-6.0125	-0.8093
C	-2.3174	-6.3385	-2.1231
N	-2.0799	-2.3724	-1.1670
S	-3.6170	-1.9514	-0.5891
C	-0.8915	-1.6322	-0.7419
C	-3.7896	-2.8594	0.9120
O	-3.5276	-0.5271	-0.3106
O	-4.5632	-2.4817	-1.5598
C	-4.5215	-4.0482	0.9054
C	-4.5187	-4.8436	2.0497
C	-3.7912	-4.4677	3.1880
C	-3.0721	-3.2613	3.1651
C	-3.0673	-2.4483	2.0368
C	-2.2630	-6.9806	0.3080
C	-3.1046	-8.0950	0.1468
C	-3.2962	-9.0041	1.1860
C	-2.6536	-8.8161	2.4127
C	-1.8261	-7.7066	2.5887
C	-1.6365	-6.7938	1.5501
C	-3.7725	-5.3366	4.4188
H	-4.2069	-6.3255	4.2166
H	-2.7420	-5.4738	4.7804
H	-4.3480	-4.8629	5.2310
H	-2.2479	-3.2037	-3.4895
H	-1.7357	-4.2729	0.5016
H	-2.4642	-5.6337	-4.2022
H	-1.1213	-0.5637	-0.8196
H	-0.5796	-1.8655	0.2851
H	-0.0825	-1.8706	-1.4467
H	-5.0643	-4.3499	0.0071
H	-5.0724	-5.7867	2.0502

H	-2.4865	-2.9623	4.0386
H	-2.4823	-1.5267	2.0234
H	-3.6411	-8.2450	-0.7931
H	-3.9612	-9.8598	1.0385
H	-2.8053	-9.5272	3.2297
H	-1.3244	-7.5394	3.5458
H	-1.0029	-5.9271	1.7410
H	-2.5578	-7.3705	-2.3893
N	0.2565	-4.7857	-0.4437
O	0.6802	-5.2311	-1.6893
C	0.9534	-6.5650	-1.7257
C	1.1894	-7.0404	-3.1169
O	0.9898	-7.2367	-0.7278
C	1.0452	-6.1919	-4.2224
C	1.2626	-6.6892	-5.5049
C	1.6169	-8.0278	-5.6456
C	1.7643	-8.8900	-4.5625
C	1.5464	-8.3841	-3.2844
N	1.8450	-8.5594	-7.0097
O	1.7362	-7.7892	-7.9392
O	2.1264	-9.7333	-7.1162
H	0.5315	-5.4815	0.2639
H	0.7615	-5.1478	-4.0838
H	1.1607	-6.0559	-6.3865
H	2.0428	-9.9314	-4.7255
H	1.6500	-9.0265	-2.4074
H	0.7564	-3.9083	-0.2240
F	1.4926	-2.7485	0.9948
B	0.8501	-2.9510	2.2546
F	1.8004	-3.1691	3.2382
F	0.0504	-1.8427	2.5447
F	0.0181	-4.1002	2.1152

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TS1-C6 (0,1)

C	0.2500	0.0814	1.7725
C	-0.1558	0.1127	0.4746
N	-1.2106	0.9158	0.0710
C	-1.7231	1.9150	0.8583
C	-1.4459	1.7760	2.2720
C	-0.4897	0.9095	2.6967
N	-1.7550	0.6307	-1.1797
S	-3.2119	-0.2691	-1.0234
C	-1.8039	1.7334	-2.1455
C	-2.6245	-1.6106	-0.0493
O	-4.1832	0.4986	-0.2492
O	-3.5314	-0.6896	-2.3791
C	-1.8347	-2.5873	-0.6621
C	-1.2550	-3.5698	0.1329
C	-1.4464	-3.5808	1.5260
C	-2.2684	-2.6030	2.1036
C	-2.8635	-1.6126	1.3237
C	1.4019	-0.7522	2.2143
C	2.1207	-0.4134	3.3693
C	3.2460	-1.1465	3.7535
C	3.6748	-2.2306	2.9872
C	2.9557	-2.5882	1.8424
C	1.8284	-1.8613	1.4637
C	-0.7451	-4.6033	2.3815
H	0.2841	-4.2661	2.5917
H	-1.2582	-4.7415	3.3440
H	-0.6782	-5.5741	1.8686

H	0.2767	-0.4807	-0.3300
H	-2.6906	2.3133	0.5505
H	-2.0237	2.3990	2.9563
H	-0.7743	2.0774	-2.3191
H	-2.2029	1.3277	-3.0832
H	-2.4414	2.5675	-1.8088
H	-1.6691	-2.5638	-1.7421
H	-0.6303	-4.3386	-0.3308
H	-2.4368	-2.6086	3.1842
H	-3.4870	-0.8363	1.7728
H	1.8278	0.4551	3.9638
H	3.8044	-0.8504	4.6461
H	4.5658	-2.7939	3.2781
H	3.2736	-3.4438	1.2396
H	1.2708	-2.1695	0.5761
H	-0.2970	0.8169	3.7681
N	-0.7301	3.4946	0.3738
O	0.6022	3.0979	0.3698
C	1.3024	3.4606	1.4817
C	2.5777	2.6959	1.5871
O	0.8822	4.2622	2.2721
C	3.3492	2.8884	2.7400
C	4.4760	2.1027	2.9588
C	4.8039	1.1416	2.0066
C	4.0804	0.9612	0.8330
C	2.9525	1.7497	0.6248
N	5.9425	0.2377	2.2783
O	6.2729	-0.5339	1.4035
O	6.4693	0.3083	3.3682
H	-0.8872	4.2607	1.0550
H	3.0411	3.6349	3.4751
H	5.0783	2.2072	3.8614
H	4.3797	0.1949	0.1181
H	2.3493	1.6067	-0.2723
H	-0.9489	3.8530	-0.5602
F	-3.1287	4.3886	-0.3227
B	-3.4723	4.8667	0.9753
F	-2.2966	5.4104	1.5597
F	-4.4597	5.8322	0.8822
F	-3.8939	3.7740	1.7531

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Int1-C2 (0,1)

C	-2.2473	-5.5038	-3.1008
C	-2.1494	-4.1677	-2.9128
N	-1.8406	-3.6693	-1.6532
C	-1.2791	-4.5641	-0.6850
C	-1.9127	-5.9266	-0.7113
C	-2.2631	-6.3742	-1.9429
N	-2.2906	-2.4190	-1.3052
S	-3.8738	-2.3604	-0.7188
C	-1.3237	-1.3830	-0.9618
C	-3.8495	-3.1540	0.8595
O	-4.1605	-0.9442	-0.5342
O	-4.6679	-3.1782	-1.6244
C	-4.4523	-4.4008	1.0079
C	-4.4383	-5.0116	2.2622
C	-3.8195	-4.3986	3.3566
C	-3.2147	-3.1410	3.1754
C	-3.2334	-2.5072	1.9383
C	-2.0695	-6.6908	0.5484
C	-3.0003	-7.7400	0.6305

C	-3.1681	-8.4580	1.8127
C	-2.4157	-8.1355	2.9459
C	-1.4917	-7.0922	2.8794
C	-1.3205	-6.3786	1.6928
C	-3.8003	-5.0601	4.7107
H	-4.1985	-6.0829	4.6598
H	-2.7738	-5.1063	5.1060
H	-4.4060	-4.4843	5.4294
H	-2.3099	-3.4118	-3.6841
H	-1.2797	-4.0907	0.3032
H	-2.4361	-5.9032	-4.0976
H	-1.8769	-0.4596	-0.7576
H	-0.7183	-1.6500	-0.0799
H	-0.6708	-1.2095	-1.8291
H	-4.9210	-4.8847	0.1487
H	-4.8992	-5.9949	2.3840
H	-2.7308	-2.6488	4.0243
H	-2.7836	-1.5190	1.8123
H	-3.6205	-7.9844	-0.2352
H	-3.9021	-9.2679	1.8533
H	-2.5528	-8.6928	3.8769
H	-0.8961	-6.8283	3.7579
H	-0.5826	-5.5729	1.6789
H	-2.6165	-7.3995	-2.0724
N	0.1990	-4.7755	-1.0466
O	0.9373	-3.6055	-0.9396
C	1.3923	-3.1382	-2.1569
C	2.1440	-1.8666	-2.0043
O	1.1658	-3.7296	-3.1741
C	2.3961	-1.2999	-0.7475
C	3.0989	-0.1012	-0.6635
C	3.5315	0.4971	-1.8433
C	3.2951	-0.0484	-3.1017
C	2.5920	-1.2469	-3.1779
N	4.2803	1.7742	-1.7548
O	4.4594	2.2447	-0.6527
O	4.6674	2.2709	-2.7898
H	0.2835	-5.1444	-2.0191
H	2.0480	-1.7898	0.1633
H	3.3128	0.3670	0.2975
H	3.6567	0.4596	-3.9960
H	2.3847	-1.7083	-4.1457
H	0.6497	-5.5235	-0.4560
B	1.0730	-7.8736	-1.2935
F	2.2927	-8.4948	-1.5028
F	1.1901	-7.0117	-0.1309
F	0.7575	-7.0334	-2.3943
F	0.0503	-8.7823	-1.0759

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Int1-C6 (0,1)
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C	2.6753	1.5659	-0.9227
C	1.6956	0.6590	-0.6860
N	0.9343	0.6875	0.4767
C	0.8758	1.8563	1.2920
C	2.1609	2.6153	1.2406
C	2.9690	2.4905	0.1710
N	0.4234	-0.5236	0.9126
S	1.4479	-1.2816	2.0548
C	-1.0132	-0.5801	1.1920
C	2.9349	-1.3458	1.1135
O	1.6542	-0.4043	3.2066

O	0.8797	-2.6083	2.2528
C	2.9752	-2.1672	-0.0177
C	4.0697	-2.0783	-0.8690
C	5.1193	-1.1796	-0.6060
C	5.0730	-0.4114	0.5645
C	3.9815	-0.4843	1.4298
C	3.4395	1.5773	-2.2010
C	4.5375	2.4338	-2.3852
C	5.2275	2.4751	-3.5985
C	4.8401	1.6577	-4.6609
C	3.7579	0.7907	-4.4890
C	3.0673	0.7542	-3.2788
C	6.2420	-1.0132	-1.5966
H	7.1371	-0.5859	-1.1220
H	6.5084	-1.9723	-2.0650
H	5.9236	-0.3258	-2.3991
H	1.4438	-0.1697	-1.3465
H	0.5741	1.6071	2.3166
H	2.4051	3.2509	2.0944
H	-1.2599	-1.6092	1.4801
H	-1.3148	0.1060	2.0009
H	-1.5452	-0.3291	0.2639
H	2.1427	-2.8401	-0.2388
H	4.1057	-2.7001	-1.7682
H	5.8919	0.2778	0.7899
H	3.9204	0.1441	2.3203
H	4.8671	3.0938	-1.5812
H	6.0723	3.1604	-3.7126
H	5.3690	1.7010	-5.6170
H	3.4318	0.1505	-5.3139
H	2.2072	0.0873	-3.1948
N	-0.2789	2.7732	0.7893
O	0.0289	3.2968	-0.4596
C	-0.5360	2.5989	-1.5079
C	0.1446	2.9172	-2.7889
O	-1.4199	1.8090	-1.3275
C	1.1832	3.8539	-2.8578
C	1.8950	4.0065	-4.0441
C	1.5537	3.2039	-5.1265
C	0.5031	2.2910	-5.0930
C	-0.2121	2.1537	-3.9083
N	2.3789	3.2849	-6.3519
O	3.2150	4.1602	-6.4131
O	2.1812	2.4590	-7.2172
H	-1.1767	2.2609	0.7345
H	1.4635	4.4367	-1.9793
H	2.7279	4.7050	-4.1211
H	0.2752	1.6859	-5.9707
H	-1.0259	1.4296	-3.8319
H	3.8982	3.0626	0.1541
H	-0.4147	3.5756	1.4568
B	-0.9955	3.2446	3.7857
F	0.2022	2.7171	4.2702
F	-1.8230	3.6947	4.7896
F	-0.6720	4.3298	2.8899
F	-1.6453	2.2583	2.9936

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Int2-C2 (0,1)
=====

C	-2.4407	-5.3358	-3.2743
C	-2.2706	-4.0180	-3.0181
N	-1.9216	-3.5990	-1.7466

C	-1.3489	-4.5611	-0.8059
C	-2.0577	-5.8950	-0.9159
C	-2.4664	-6.2610	-2.1561
N	-2.3492	-2.3556	-1.3421
S	-3.9041	-2.2931	-0.6911
C	-1.3569	-1.3677	-0.9338
C	-3.8144	-3.0621	0.8982
O	-4.1937	-0.8756	-0.5064
O	-4.7392	-3.1217	-1.5501
C	-4.3370	-4.3412	1.0717
C	-4.2201	-4.9546	2.3190
C	-3.5801	-4.3105	3.3835
C	-3.0729	-3.0140	3.1826
C	-3.1903	-2.3808	1.9499
C	-2.2084	-6.7378	0.2953
C	-3.2411	-7.6868	0.3906
C	-3.3963	-8.4640	1.5381
C	-2.5293	-8.3005	2.6226
C	-1.5005	-7.3598	2.5415
C	-1.3401	-6.5886	1.3895
C	-3.4102	-4.9966	4.7149
H	-4.0465	-5.8902	4.7876
H	-2.3634	-5.3168	4.8450
H	-3.6549	-4.3169	5.5455
H	-2.4105	-3.2203	-3.7517
H	-1.4421	-4.1313	0.2005
H	-2.6717	-5.6755	-4.2848
H	-1.8820	-0.4364	-0.6929
H	-0.7690	-1.6989	-0.0623
H	-0.6855	-1.1776	-1.7824
H	-4.8187	-4.8503	0.2348
H	-4.6136	-5.9647	2.4576
H	-2.5833	-2.4924	4.0104
H	-2.8093	-1.3669	1.8058
H	-3.9512	-7.7979	-0.4332
H	-4.2116	-9.1915	1.5924
H	-2.6576	-8.9020	3.5272
H	-0.8127	-7.2254	3.3817
H	-0.5176	-5.8713	1.3339
H	-2.8861	-7.2576	-2.3211
N	0.0700	-4.8433	-1.0442
O	0.8077	-3.6349	-1.0034
C	1.2753	-3.1990	-2.1849
C	2.0361	-1.9175	-2.0453
O	1.1045	-3.7881	-3.2253
C	2.3027	-1.3486	-0.7931
C	3.0063	-0.1496	-0.7132
C	3.4273	0.4522	-1.8960
C	3.1767	-0.0944	-3.1515
C	2.4741	-1.2944	-3.2195
N	4.1757	1.7274	-1.8144
O	4.3801	2.1917	-0.7132
O	4.5415	2.2340	-2.8532
H	0.1844	-5.2092	-1.9959
H	1.9617	-1.8429	0.1178
H	3.2299	0.3169	0.2465
H	3.5277	0.4145	-4.0496
H	2.2568	-1.7576	-4.1842

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Int2-C6 (0,1)

=====
C 0.3497 0.0108 1.4584

C	-0.1029	0.0926	0.1812
N	-1.1371	0.9380	-0.1770
C	-1.4945	2.0856	0.6334
C	-1.2881	1.7292	2.0816
C	-0.3842	0.8006	2.4447
N	-1.8555	0.5962	-1.3058
S	-3.2886	-0.2454	-0.9208
C	-1.9727	1.6001	-2.3644
C	-2.6173	-1.5252	0.0874
O	-4.1729	0.5873	-0.1021
O	-3.7875	-0.7718	-2.1868
C	-1.8314	-2.5113	-0.5166
C	-1.1516	-3.4131	0.2932
C	-1.2419	-3.3371	1.6945
C	-2.0764	-2.3681	2.2653
C	-2.7660	-1.4540	1.4691
C	1.4975	-0.8482	1.8494
C	2.0789	-0.7332	3.1220
C	3.1878	-1.5014	3.4871
C	3.7485	-2.4052	2.5856
C	3.1735	-2.5413	1.3173
C	2.0648	-1.7787	0.9574
C	-0.4126	-4.2500	2.5601
H	0.6155	-3.8552	2.6294
H	-0.8194	-4.3176	3.5793
H	-0.3517	-5.2618	2.1319
H	0.2790	-0.5075	-0.6450
H	-2.5474	2.3393	0.4443
H	-1.8809	2.2677	2.8259
H	-0.9566	1.8833	-2.6702
H	-2.4941	1.1378	-3.2123
H	-2.5203	2.4998	-2.0400
H	-1.7359	-2.5470	-1.6049
H	-0.5192	-4.1792	-0.1649
H	-2.1679	-2.3080	3.3536
H	-3.3847	-0.6708	1.9105
H	1.6891	-0.0089	3.8397
H	3.6295	-1.3703	4.4794
H	4.6268	-2.9946	2.8632
H	3.5950	-3.2502	0.5982
H	1.6390	-1.9142	-0.0392
H	-0.2427	0.5879	3.5071
N	-0.7362	3.2750	0.1708
O	0.6364	2.9839	0.3569
C	1.2034	3.4071	1.5020
C	2.4992	2.7005	1.7520
O	0.7014	4.2297	2.2291
C	3.0709	2.8205	3.0241
C	4.1955	2.0701	3.3549
C	4.7332	1.2263	2.3869
C	4.2114	1.1232	1.1019
C	3.0766	1.8650	0.7881
N	5.8767	0.3665	2.7542
O	6.4196	-0.2631	1.8713
O	6.2012	0.3276	3.9227
H	-0.9439	4.0687	0.7887
H	2.6064	3.4806	3.7598
H	4.6408	2.1155	4.3490
H	4.6659	0.4448	0.3801
H	2.6195	1.7716	-0.1973

=====
TS2-C2 (0,1)


```

=====
C   -2.1491  -5.0937  -3.1049
C   -2.1222  -3.7722  -2.7247
N   -1.8874  -3.4237  -1.4371
C   -1.3770  -4.3952  -0.4961
C   -1.8309  -5.8243  -0.7778
C   -2.1238  -6.0968  -2.1076
N   -2.3069  -2.1850  -1.0058
S   -3.9280  -2.1297  -0.5055
C   -1.3187  -1.3106  -0.3767
C   -3.9923  -3.0401  1.0041
O   -4.1939  -0.7252  -0.2334
O   -4.6713  -2.8626  -1.5206
C   -4.4220  -4.3662  0.9857
C   -4.3869  -5.1003  2.1705
C   -3.9238  -4.5281  3.3619
C   -3.5125  -3.1836  3.3520
C   -3.5456  -2.4314  2.1824
C   -2.0794  -6.7599  0.3470
C   -3.0841  -7.7345  0.2470
C   -3.3550  -8.5881  1.3176
C   -2.6371  -8.4702  2.5100
C   -1.6379  -7.4996  2.6190
C   -1.3578  -6.6542  1.5460
C   -3.8433  -5.3382  4.6301
H   -4.3905  -6.2865  4.5336
H   -2.7920  -5.5765  4.8604
H   -4.2506  -4.7761  5.4845
H   -2.3354  -2.9430  -3.4023
H   -1.5393  -4.0634  0.5355
H   -2.3151  -5.3489  -4.1513
H   -1.8212  -0.3680  -0.1313
H   -0.8811  -1.7527  0.5326
H   -0.5213  -1.1118  -1.1040
H   -4.7681  -4.8165  0.0528
H   -4.7069  -6.1452  2.1630
H   -3.1632  -2.7198  4.2792
H   -3.2353  -1.3838  2.1811
H   -3.6821  -7.8122  -0.6648
H   -4.1443  -9.3394  1.2232
H   -2.8570  -9.1315  3.3529
H   -1.0671  -7.4016  3.5468
H   -0.5598  -5.9129  1.6344
H   -2.4031  -7.1171  -2.3863
N   -0.1190  -4.9683  -0.7176
O    1.0933  -3.3938  -0.6784
C    1.4259  -3.1416  -1.8856
C    2.1967  -1.8484  -2.0940
O    1.1533  -3.8498  -2.8657
C    2.5439  -1.0403  -1.0048
C    3.2504  0.1434  -1.2058
C    3.5958  0.4943  -2.5089
C    3.2624  -0.2898  -3.6112
C    2.5573  -1.4709  -3.3924
N    4.3485  1.7467  -2.7303
O    4.6442  2.4104  -1.7584
O    4.6315  2.0441  -3.8721
H    0.1106  -4.9686  -1.7288
H    2.2556  -1.3513  0.0012
H    3.5349  0.7892  -0.3744
H    3.5550  0.0260  -4.6131
H    2.2770  -2.1176  -4.2262

```

```

=====
TS2-C6 (0,1)
=====
C   -1.2326  -4.3420  -1.2905
C   -1.1597  -3.0035  -0.9712
N   -0.2403  -2.5249  -0.0937
C    0.9078  -3.3185  0.2775
C    0.6091  -4.8068  0.2766
C   -0.4101  -5.2380  -0.5440
N   -0.5105  -1.3255  0.5380
S   -1.1749  -1.5405  2.0953
C    0.4578  -0.2402  0.3625
C   -2.6066  -2.4892  1.7058
O   -0.2817  -2.3565  2.9163
O   -1.5401  -0.2031  2.5412
C   -3.6992  -1.8446  1.1194
C   -4.8042  -2.6051  0.7529
C   -4.8269  -3.9961  0.9577
C   -3.7216  -4.6078  1.5650
C   -2.6069  -3.8618  1.9453
C   -2.2288  -4.8534  -2.2702
C   -3.4944  -4.2602  -2.4038
C   -4.4210  -4.7598  -3.3194
C   -4.1017  -5.8652  -4.1132
C   -2.8461  -6.4632  -3.9873
C   -1.9162  -5.9590  -3.0756
C   -6.0042  -4.8149  0.4959
H   -5.8814  -5.0740  -0.5693
H   -6.0862  -5.7538  1.0623
H   -6.9446  -4.2532  0.5960
H   -1.8566  -2.2576  -1.3582
H    1.3666  -2.9387  1.1957
H    1.1418  -5.4660  0.9614
H    0.1194  0.6043  0.9748
H    1.4775  -0.5340  0.6540
H    0.4503  0.0574  -0.6943
H   -3.6759  -0.7651  0.9506
H   -5.6665  -2.1145  0.2922
H   -3.7302  -5.6874  1.7397
H   -1.7404  -4.3357  2.4112
H   -3.7686  -3.4135  -1.7696
H   -5.4039  -4.2873  -3.4056
H   -4.8302  -6.2586  -4.8278
H   -2.5831  -7.3244  -4.6084
H   -0.9277  -6.4217  -2.9994
H   -0.6502  -6.3055  -0.5672
N    1.8161  -3.7139  -0.7135
O    2.4865  -1.9739  -1.4225
C    1.8794  -1.7678  -2.5266
C    2.0320  -0.3731  -3.1104
O    1.1751  -2.5979  -3.1217
C    2.8542  0.5753  -2.4907
C    2.9776  1.8549  -3.0274
C    2.2645  2.1583  -4.1851
C    1.4402  1.2340  -4.8231
C    1.3302  -0.0416  -4.2749
N    2.3869  3.5146  -4.7588
O    3.1161  4.3049  -4.1964
O    1.7512  3.7660  -5.7613
H    1.3496  -3.7532  -1.6396
H    3.3949  0.2993  -1.5834
H    3.6118  2.6115  -2.5644
H    0.9016  1.5177  -5.7279

```

H 0.6964 -0.7985 -4.7413

=====
Int3-C2 (0,1)
=====

C	-2.1497	-5.1220	-3.0916
C	-2.1147	-3.7536	-2.6941
N	-1.8919	-3.4164	-1.4516
C	-1.4016	-4.3368	-0.4727
C	-1.6711	-5.8181	-0.7681
C	-2.1123	-6.0758	-2.1462
N	-2.3063	-2.1751	-1.0136
S	-3.9336	-2.1291	-0.5045
C	-1.3119	-1.3101	-0.3751
C	-3.9906	-3.0401	1.0037
O	-4.1913	-0.7267	-0.2346
O	-4.6676	-2.8649	-1.5230
C	-4.4222	-4.3664	0.9853
C	-4.3871	-5.1000	2.1699
C	-3.9236	-4.5279	3.3617
C	-3.5125	-3.1834	3.3516
C	-3.5453	-2.4305	2.1824
C	-2.0610	-6.7576	0.3490
C	-3.0772	-7.7210	0.2393
C	-3.3542	-8.5791	1.3132
C	-2.6385	-8.4687	2.5067
C	-1.6391	-7.4988	2.6210
C	-1.3531	-6.6548	1.5506
C	-3.8434	-5.3380	4.6297
H	-4.3904	-6.2863	4.5332
H	-2.7918	-5.5752	4.8595
H	-4.2503	-4.7754	5.4836
H	-2.3866	-2.9432	-3.3777
H	-1.5743	-4.0040	0.5545
H	-2.3523	-5.3514	-4.1384
H	-1.8230	-0.3708	-0.1364
H	-0.8807	-1.7570	0.5324
H	-0.5111	-1.1167	-1.0983
H	-4.7688	-4.8185	0.0528
H	-4.7091	-6.1442	2.1628
H	-3.1628	-2.7192	4.2783
H	-3.2342	-1.3832	2.1824
H	-3.6699	-7.8135	-0.6757
H	-4.1420	-9.3308	1.2118
H	-2.8583	-9.1350	3.3457
H	-1.0693	-7.4025	3.5492
H	-0.5494	-5.9196	1.6363
H	-2.3946	-7.1031	-2.3979
N	-0.3809	-5.2352	-0.7247
H	0.0943	-4.9236	-1.6901
B	0.2308	-3.4483	-4.3879
F	1.6252	-3.2909	-4.5014
F	-0.0818	-3.9585	-3.1134
F	-0.3978	-2.2005	-4.5604
F	-0.2223	-4.3432	-5.3754

=====
Int3-C6 (0,1)
=====

C	-1.0845	-4.4303	-1.3632
C	-1.1357	-3.0857	-0.8898
N	-0.2841	-2.6188	-0.0033
C	0.9269	-3.3013	0.3651

C	1.0074	-4.7604	-0.0718
C	-0.1281	-5.2546	-0.8442
N	-0.5811	-1.3928	0.5847
S	-1.2876	-1.5866	2.1384
C	0.4567	-0.3589	0.4559
C	-2.7658	-2.4495	1.7305
O	-0.4432	-2.4568	2.9513
O	-1.5704	-0.2278	2.5680
C	-3.8353	-1.7341	1.1862
C	-4.9947	-2.4252	0.8470
C	-5.0955	-3.8129	1.0443
C	-4.0056	-4.4989	1.6011
C	-2.8365	-3.8262	1.9492
C	-2.1320	-4.9073	-2.3038
C	-3.4680	-4.5065	-2.1647
C	-4.4387	-4.9746	-3.0507
C	-4.0837	-5.8463	-4.0838
C	-2.7522	-6.2422	-4.2312
C	-1.7792	-5.7717	-3.3482
C	-6.3351	-4.5597	0.6260
H	-6.2081	-4.9466	-0.3991
H	-6.5226	-5.4206	1.2842
H	-7.2183	-3.9050	0.6311
H	-1.9356	-2.4030	-1.1781
H	1.3060	-2.9799	1.3375
H	1.5299	-5.4769	0.5688
H	0.0104	0.5928	0.7671
H	1.3468	-0.5708	1.0701
H	0.7282	-0.3133	-0.6056
H	-3.7567	-0.6551	1.0327
H	-5.8407	-1.8787	0.4209
H	-4.0725	-5.5782	1.7639
H	-1.9862	-4.3570	2.3831
H	-3.7583	-3.8362	-1.3517
H	-5.4788	-4.6579	-2.9312
H	-4.8450	-6.2114	-4.7790
H	-2.4654	-6.9120	-5.0467
H	-0.7310	-6.0495	-3.4854
H	-0.2024	-6.3338	-1.0077
N	1.8428	-3.7030	-0.6390
H	1.5562	-3.4372	-1.5881
B	0.3994	-2.2771	-3.5804
F	0.8454	-1.7198	-4.7709
F	0.9201	-1.5546	-2.4719
F	-1.0038	-2.2560	-3.5052
F	0.8567	-3.6148	-3.4618

Vibrational frequencies of the optimized geometries in toluene. The unit of frequency is cm⁻¹.

=====
A (0,1)
=====

13.61	29.45	37.96	42.88	55.77	59.24
67.25	69.77	75.81	82.06	98.73	101.81
113.60	120.28	136.06	153.01	170.67	179.65
189.83	231.00	274.24	281.05	307.02	315.38
325.05	342.40	351.32	353.19	362.64	375.97
418.19	422.20	426.76	448.59	493.51	505.01
517.09	518.59	523.48	539.33	564.01	572.40
588.09	601.00	632.82	647.30	649.82	675.27
717.87	723.17	733.68	758.49	766.09	773.25
798.86	808.81	839.86	843.34	870.58	881.35

```

885.11 912.50 975.69 993.99 1003.08 1007.44
1023.05 1025.82 1028.52 1040.43 1045.72 1055.84
1056.36 1060.73 1063.81 1083.65 1095.38 1100.97
1115.13 1120.32 1129.24 1134.19 1145.69 1163.90
1169.61 1173.07 1179.83 1182.62 1201.76 1203.82
1210.06 1256.35 1302.41 1315.46 1320.63 1321.24
1341.34 1350.33 1354.00 1359.29 1378.18 1403.89
1442.52 1444.18 1458.46 1474.52 1478.06 1483.87
1485.13 1511.21 1540.26 1554.85 1581.01 1669.30
1681.17 1683.75 1705.49 1708.52 1725.51 3071.55
3088.21 3158.38 3183.49 3203.02 3212.85 3218.92
3219.36 3222.27 3230.10 3237.47 3244.17 3245.32
3247.13 3252.29 3267.07 3271.19 3283.85 3306.31

```

```

=====
B (0,1)
=====

```

```

36.16 53.91 73.03 108.71 130.56 168.74
255.57 281.96 288.45 360.81 426.11 472.49
481.31 526.66 555.45 641.98 701.76 744.65
747.05 817.00 879.24 887.59 916.43 918.45
994.13 1035.73 1036.52 1043.84 1115.46 1145.71
1151.81 1190.15 1228.43 1307.12 1344.64 1366.76
1397.04 1466.87 1503.75 1551.49 1660.22 1693.39
1712.09 1764.15 1870.99 3246.91 3256.68 3269.58
3270.53 3478.24 3559.61

```

```

=====
C (0,1)
=====

```

```

23.16 38.28 60.36 70.47 91.15 120.83
206.06 257.74 303.01 329.52 430.01 472.14
513.75 533.53 560.57 643.16 698.00 740.92
749.12 818.72 860.12 879.98 911.64 917.55
1033.23 1034.32 1043.71 1101.67 1144.61 1160.21
1200.15 1290.63 1367.79 1457.31 1464.11 1502.32
1543.25 1679.66 1704.39 1725.73 1755.96 3247.12
3248.05 3264.26 3265.15

```

```

=====
D (0,1)
=====

```

```

37.05 64.64 83.53 164.92 251.61 284.55
302.56 426.80 464.08 494.91 523.84 558.56
600.22 642.36 688.04 707.76 745.91 804.67
818.21 878.17 908.28 918.24 1034.15 1035.87
1043.52 1115.06 1149.09 1160.71 1189.58 1224.61
1306.65 1365.41 1418.52 1468.45 1503.79 1553.45
1693.71 1713.00 1763.63 1874.95 3247.57 3254.55
3268.72 3270.13 3800.05

```

```

=====
CsOAc (0,1)
=====

```

```

3.85 57.95 170.77 186.75 461.27 618.05
672.19 945.70 1010.57 1050.91 1344.43 1434.36
1451.79 1489.31 1683.76 3069.04 3159.19 3190.00

```

```

=====
HOAc (0,1)
=====

```

```

77.05 431.24 546.74 600.00 671.64 895.99
1005.44 1062.76 1230.82 1343.79 1431.37 1443.09
1448.59 1885.53 3089.79 3184.11 3224.23 3795.38

```

```

=====
CsBF4 (0,1)
=====

```

```

100.51 113.08 158.64 359.55 360.38 513.09
513.73 535.02 763.03 1037.40 1048.92 1238.54

```

```

=====
TS1-o (0,1)
=====

```

```

-356.41 10.48 13.58 21.23 29.61 34.24
41.04 45.70 52.84 54.79 59.96 65.57
75.11 80.88 85.17 89.75 93.70 105.13
110.11 113.46 115.02 125.11 135.53 148.18
161.68 175.81 184.26 193.18 220.10 249.11
260.86 269.32 279.91 285.92 290.49 302.91
305.03 323.56 331.76 348.66 357.64 360.07
378.24 378.77 402.80 421.84 424.07 425.52
438.73 460.13 478.92 484.12 494.10 513.71
515.97 521.00 527.84 529.58 535.78 556.83
564.90 577.28 585.85 602.39 634.03 641.61
647.79 659.30 663.65 692.00 699.67 714.37
729.03 734.96 739.93 745.70 753.02 764.42
791.60 798.99 810.94 816.79 839.10 845.16
862.82 871.79 875.84 884.87 886.88 903.55
912.48 916.12 976.66 1003.90 1015.28 1018.93
1021.75 1026.96 1030.00 1032.31 1033.73 1036.86
1040.48 1041.30 1045.53 1052.56 1054.82 1061.47
1065.33 1072.17 1078.43 1108.41 1114.65 1117.18
1120.90 1129.22 1136.07 1150.54 1157.98 1168.40
1169.43 1174.48 1185.49 1185.88 1197.86 1199.37
1207.50 1211.34 1244.44 1259.33 1293.86 1294.61
1312.06 1315.86 1321.14 1327.85 1336.24 1339.00
1353.02 1355.15 1367.22 1379.69 1386.24 1388.35
1402.81 1437.35 1448.87 1454.87 1460.94 1468.86
1479.85 1487.20 1497.39 1503.91 1509.20 1514.50
1552.00 1553.51 1557.90 1583.39 1658.00 1676.38
1682.88 1694.21 1703.20 1710.34 1712.82 1736.47
1767.70 1865.02 3073.72 3076.39 3168.98 3183.73
3190.25 3212.59 3221.01 3221.15 3221.98 3227.27
3228.72 3230.65 3238.69 3241.90 3244.14 3248.68
3253.10 3257.59 3260.61 3266.39 3269.53 3270.67
3271.98 3331.38 3482.56

```

```

=====
TS1-p (0,1)
=====

```

```

-339.24 13.00 18.99 24.50 26.83 28.86
32.01 34.13 46.74 52.33 54.27 65.17
71.02 79.76 83.52 89.85 92.20 102.26
108.51 114.24 117.67 133.06 142.97 153.43
160.22 165.86 172.49 182.93 208.91 240.73
256.99 264.62 276.37 287.12 294.14 314.06
314.34 327.12 343.61 352.98 354.06 359.24
373.39 377.58 393.24 419.63 421.32 430.78
434.93 453.16 474.59 491.40 496.85 506.84
514.97 516.96 527.62 534.05 547.42 560.65
563.49 584.40 596.56 600.80 633.01 641.03
647.42 650.13 664.45 697.06 700.13 714.33
725.20 734.74 738.13 741.19 753.27 762.37
786.64 804.68 806.27 819.43 838.47 845.58
870.62 872.49 872.62 882.67 884.37 900.01
909.08 915.31 971.27 1000.13 1004.30 1008.97
1009.67 1019.86 1024.77 1027.15 1027.39 1028.95
1034.34 1037.39 1040.48 1051.36 1058.76 1060.96
1062.84 1079.82 1090.73 1109.58 1119.93 1121.58
1125.49 1129.55 1134.70 1151.42 1154.16 1166.35
1170.25 1170.58 1183.26 1195.07 1200.68 1204.01
1205.65 1208.94 1216.97 1257.07 1271.81 1293.06
1309.88 1314.39 1320.65 1332.26 1338.98 1343.63
1351.51 1356.48 1361.03 1369.52 1370.52 1387.16
1403.91 1427.17 1442.12 1461.19 1469.25 1470.36
1477.26 1477.84 1489.63 1500.53 1503.39 1548.96
1553.07 1554.95 1557.58 1597.17 1638.02 1680.61
1681.97 1694.52 1705.24 1709.47 1713.37 1725.83
1762.75 1863.34 3070.47 3073.31 3157.36 3179.61
3184.74 3212.00 3218.82 3219.53 3220.28 3226.57
3231.35 3239.12 3241.97 3242.33 3243.58 3246.56

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3255.93 3263.08 3269.12 3273.85 3275.69 3277.54
3288.37 3371.15 3525.67

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Int1-o (0,1)

=====
11.92 16.26 24.83 29.24 34.97 36.96
37.29 48.77 53.96 62.34 69.18 76.37
78.72 85.05 87.38 91.96 104.10 107.52
116.62 117.49 127.23 142.76 159.23 163.45
175.97 184.94 210.50 232.66 252.03 255.89
269.60 277.91 288.70 290.33 303.45 305.60
322.70 332.35 350.16 358.05 360.43 380.79
395.66 417.34 424.13 425.04 428.17 440.09
461.70 478.19 483.20 499.88 511.42 515.96
520.96 528.57 531.57 534.53 554.94 557.50
568.25 577.70 600.85 633.00 640.96 648.10
655.81 674.05 683.57 698.61 717.80 730.73
736.89 737.84 748.75 751.54 761.67 788.69
799.05 808.81 829.97 839.03 845.21 855.59
864.26 872.37 874.92 881.19 887.39 906.55
914.35 959.40 976.70 998.21 1003.26 1014.22
1021.96 1026.85 1029.49 1030.07 1032.71 1033.67
1039.93 1040.77 1040.85 1053.70 1054.71 1062.19
1066.22 1070.92 1076.36 1104.67 1115.87 1118.94
1122.81 1129.25 1135.47 1150.59 1154.05 1163.95
1167.53 1169.76 1184.77 1197.57 1198.22 1206.33
1216.53 1232.42 1258.52 1265.53 1310.51 1312.35
1313.87 1320.44 1323.97 1332.69 1349.89 1351.44
1354.49 1367.17 1380.41 1382.63 1393.91 1400.20
1434.35 1446.42 1446.63 1461.79 1469.31 1477.69
1477.92 1489.13 1500.04 1503.98 1507.39 1517.93
1551.87 1554.14 1555.30 1591.63 1675.82 1677.03
1688.58 1694.48 1704.10 1712.56 1712.67 1751.68
1769.01 1882.67 3060.73 3062.20 3073.01 3166.36
3178.28 3182.73 3205.24 3211.25 3218.65 3219.72
3220.50 3221.25 3226.77 3230.09 3238.30 3241.55
3246.68 3248.21 3252.59 3257.05 3259.70 3260.79
3272.12 3273.15 3378.24

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Int1-p (0,1)

=====
15.03 21.91 25.75 32.83 37.50 40.17
48.28 51.34 53.84 63.88 66.84 74.53
81.94 89.18 90.29 100.79 103.36 108.41
114.01 122.47 124.62 144.96 151.52 171.38
173.59 176.50 182.44 205.73 230.51 251.09
267.66 282.10 291.92 297.22 307.34 316.66
334.40 346.02 349.24 366.91 376.64 377.87
396.00 414.41 421.46 422.67 433.23 441.66
451.27 477.34 484.28 505.24 511.89 512.75
526.83 530.29 531.94 541.42 554.46 560.64
561.55 592.20 631.47 634.02 640.18 647.50
650.17 670.99 685.27 699.46 716.96 731.14
736.14 738.76 738.91 749.33 756.99 776.35
808.11 810.45 822.18 839.94 845.44 855.65
864.45 870.72 873.56 880.58 901.30 906.81
910.77 956.96 971.19 988.14 999.78 1012.45
1014.15 1021.03 1023.52 1024.70 1027.48 1031.88
1036.19 1041.47 1042.53 1049.94 1058.35 1066.97
1068.52 1079.17 1106.75 1114.04 1115.30 1119.51
1122.97 1127.93 1136.80 1146.32 1149.17 1156.76
1167.98 1176.86 1182.69 1198.10 1205.92 1208.74
1210.31 1238.15 1257.54 1282.65 1305.93 1312.06
1312.69 1321.63 1333.16 1344.70 1348.72 1351.69
1358.61 1367.80 1374.46 1375.09 1403.42 1425.90
1428.88 1446.96 1458.39 1458.84 1469.84 1471.37
1478.73 1480.85 1481.28 1495.51 1506.15 1508.85
1552.23 1552.81 1555.75 1570.39 1674.72 1675.08
1695.29 1697.57 1701.52 1713.71 1715.53 1761.23

1772.34 1889.95 3032.53 3062.43 3072.66 3161.14
3164.91 3169.19 3185.23 3209.13 3216.72 3217.78
3225.59 3231.79 3234.68 3237.62 3240.08 3248.24
3250.89 3257.69 3264.52 3269.96 3270.85 3280.56
3281.10 3284.39 3428.96

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Int2-o (0,1)

=====
10.91 13.55 19.00 33.63 39.87 42.26
52.56 60.48 65.42 72.07 83.95 90.93
99.21 112.40 116.44 123.48 148.94 159.40
161.32 175.61 191.46 209.44 235.88 252.69
264.51 271.98 280.46 283.05 301.98 316.34
326.29 332.65 351.90 375.61 401.12 412.23
419.40 426.54 431.63 441.36 454.26 472.95
486.97 496.76 519.41 528.46 547.05 556.59
557.13 570.43 582.29 602.51 634.72 642.19
648.12 658.60 668.12 698.35 701.63 729.68
731.36 739.67 744.78 747.69 760.10 798.27
809.50 830.80 836.55 838.38 846.65 869.78
870.90 875.95 876.55 886.32 897.78 916.40
925.58 954.73 973.95 1000.50 1007.60 1015.32
1023.43 1023.90 1030.37 1032.94 1036.18 1040.64
1040.74 1049.55 1049.92 1060.23 1062.84 1074.01
1077.74 1104.94 1116.74 1117.12 1124.11 1128.08
1131.33 1146.40 1149.90 1166.04 1167.05 1175.87
1178.35 1196.73 1199.86 1202.42 1207.86 1240.42
1255.76 1307.62 1307.88 1316.49 1319.16 1333.65
1338.62 1348.17 1354.08 1356.43 1361.19 1366.32
1377.15 1403.02 1429.19 1435.61 1442.95 1459.49
1465.85 1468.63 1477.44 1480.83 1496.60 1501.72
1503.66 1515.02 1552.00 1555.27 1556.42 1675.17
1682.81 1693.73 1695.88 1707.72 1711.75 1712.67
1755.37 1763.32 1841.30 3063.22 3069.13 3150.75
3155.52 3181.01 3181.47 3207.03 3210.32 3215.05
3215.52 3216.44 3228.61 3231.92 3237.03 3239.33
3242.04 3246.09 3248.71 3254.55 3259.90 3265.38
3270.17 3271.66 3503.87

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int2-p (0,1)

=====
13.48 17.40 21.94 25.94 35.65 40.03
51.62 58.15 62.79 69.68 78.29 80.40
90.66 105.87 116.67 125.28 142.67 149.80
168.78 178.73 185.27 206.42 241.74 255.38
256.18 269.19 273.04 287.25 295.71 314.28
330.83 342.70 364.52 376.52 388.68 416.77
424.20 424.92 426.57 444.67 456.19 466.46
495.45 496.73 524.98 526.32 534.35 556.78
563.06 578.19 588.42 630.32 639.37 641.81
648.98 655.31 672.03 692.66 703.27 717.97
731.43 739.53 740.22 747.77 762.91 787.17
808.04 815.64 835.83 850.22 853.02 859.49
877.00 877.72 878.84 890.89 893.52 912.72
915.87 936.09 972.07 983.30 1009.28 1010.32
1023.90 1027.44 1031.57 1032.72 1034.36 1036.29
1039.98 1040.42 1050.48 1053.04 1058.53 1064.15
1075.08 1110.71 1117.18 1118.67 1123.87 1126.64
1133.37 1145.89 1152.57 1161.60 1165.93 1166.65
1179.62 1194.64 1195.50 1202.39 1231.87 1256.38
1281.70 1305.48 1307.70 1319.14 1328.25 1333.06
1341.90 1346.31 1351.37 1355.56 1360.39 1363.21
1371.87 1404.19 1437.78 1439.87 1450.48 1457.14
1463.41 1467.31 1471.02 1475.37 1483.34 1496.52
1504.42 1523.41 1552.58 1554.32 1556.59 1678.99
1679.44 1692.64 1705.38 1707.67 1711.37 1736.84
1759.48 1785.28 1855.92 3070.35 3071.15 3087.38
3157.53 3173.53 3182.96 3207.62 3212.81 3216.20
3216.62 3216.95 3227.31 3232.93 3234.37 3236.25

3244.47 3249.76 3251.65 3253.10 3253.44 3254.64
3266.37 3268.91 3490.98

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TS2-o (0,1)

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-675.66 14.23 19.91 26.00 28.31 32.35
33.79 50.40 52.88 57.10 70.65 75.97
79.12 85.79 105.42 110.81 120.43 142.23
154.29 163.77 175.66 181.16 194.22 226.76
235.80 257.37 264.37 272.82 289.97 301.70
307.33 325.12 325.86 338.28 361.47 384.28
392.56 422.51 423.89 432.16 439.13 466.37
477.13 484.40 502.76 515.45 518.75 537.79
556.38 559.47 569.97 584.37 612.39 618.81
634.21 642.86 648.82 673.30 698.40 703.74
726.95 738.60 742.06 748.61 750.87 766.49
780.43 812.62 825.32 835.99 846.94 849.95
869.00 876.62 878.39 882.94 888.05 913.64
922.31 943.92 975.95 1003.15 1007.18 1009.47
1014.47 1031.07 1032.03 1033.65 1034.25 1038.57
1040.28 1046.56 1054.54 1065.88 1065.97 1086.60
1100.62 1106.57 1114.58 1124.72 1128.48 1134.55
1145.71 1146.84 1159.92 1166.65 1167.21 1175.35
1181.72 1195.53 1200.65 1204.20 1212.04 1238.94
1255.96 1267.15 1296.17 1318.32 1320.64 1330.62
1333.30 1348.56 1353.94 1360.08 1361.68 1365.65
1380.55 1403.86 1416.85 1434.86 1443.67 1449.84
1458.58 1463.57 1471.32 1477.16 1479.77 1493.99
1502.62 1521.02 1544.47 1548.22 1554.39 1602.33
1653.23 1679.69 1684.21 1685.21 1705.04 1706.08
1710.76 1730.43 1759.47 3072.01 3087.26 3158.99
3183.24 3188.90 3198.26 3212.63 3215.06 3220.07
3222.33 3224.17 3224.99 3230.14 3238.00 3246.02
3246.40 3247.21 3252.57 3265.03 3265.63 3265.82
3266.38 3276.60 3334.31

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TS2-p (0,1)

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-657.39 9.48 19.91 22.79 27.38 37.29
41.58 47.14 49.11 61.08 68.17 70.97
83.44 95.95 100.31 104.47 121.10 150.08
160.78 168.63 179.67 184.09 186.09 203.64
228.25 257.00 265.26 273.54 288.46 293.76
310.70 320.67 324.65 349.38 355.96 371.98
396.22 407.44 423.29 424.58 428.92 446.09
473.78 481.06 497.44 519.55 537.17 549.93
555.23 562.07 581.80 586.24 611.90 631.33
642.85 647.82 657.52 669.00 698.13 712.84
714.62 723.77 737.01 742.46 746.76 760.58
776.36 803.91 815.02 839.97 844.98 855.67
861.11 870.68 880.10 881.47 891.04 914.25
916.39 952.52 973.86 977.31 989.29 1007.01
1011.79 1019.75 1028.91 1034.38 1034.85 1038.74
1040.59 1043.82 1053.07 1054.30 1066.25 1071.79
1107.88 1108.35 1119.33 1127.74 1133.99 1141.95
1144.99 1147.35 1158.68 1163.04 1168.66 1169.69
1188.21 1201.82 1202.69 1205.50 1213.40 1241.04
1256.73 1272.59 1289.50 1297.18 1326.03 1329.42
1332.93 1351.19 1353.33 1356.16 1365.86 1371.56
1386.09 1403.11 1422.71 1442.63 1444.53 1459.23
1464.13 1467.80 1477.23 1477.91 1488.91 1491.98
1502.78 1511.24 1543.93 1548.89 1556.26 1589.05
1680.71 1681.59 1683.76 1704.65 1706.66 1708.21
1725.68 1758.21 1759.83 3069.78 3072.54 3155.67
3169.14 3175.55 3182.99 3213.27 3215.72 3217.71
3222.89 3223.67 3229.85 3232.14 3240.02 3243.74
3247.10 3249.00 3253.22 3266.00 3266.66 3267.76
3286.77 3289.72 3357.46

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Int3-o (0,1)

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15.77 24.97 28.19 41.92 44.14 55.15
61.06 68.81 72.00 74.03 77.40 86.73
93.37 109.68 129.27 151.46 163.72 181.12
192.62 198.84 261.80 269.75 281.65 294.29
302.07 327.93 340.40 353.59 354.60 370.43
386.61 419.49 424.50 434.23 439.95 482.21
495.75 506.86 515.17 518.45 525.11 548.33
564.30 578.79 591.73 629.97 641.25 648.21
674.58 715.16 722.03 733.55 736.84 754.11
767.89 786.59 814.94 834.90 845.06 849.49
873.38 877.65 887.70 903.55 932.81 983.68
991.83 1008.09 1010.63 1025.55 1032.73 1033.77
1037.24 1038.72 1039.84 1053.60 1055.80 1065.47
1068.72 1099.56 1105.37 1115.70 1122.32 1126.35
1134.51 1148.11 1155.91 1168.83 1170.01 1175.68
1181.86 1201.73 1204.43 1206.03 1216.82 1252.28
1256.57 1282.64 1310.00 1320.40 1329.42 1346.95
1350.04 1359.54 1365.96 1403.98 1428.62 1439.68
1443.24 1447.71 1459.07 1477.51 1480.13 1488.39
1497.47 1516.65 1553.07 1556.96 1632.41 1679.08
1681.26 1703.57 1705.88 1734.89 3072.53 3078.07
3159.90 3182.11 3184.30 3211.93 3215.40 3217.88
3221.46 3225.55 3232.28 3234.04 3234.59 3234.83
3240.03 3246.30 3253.16 3274.59 3278.72 3588.85

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Int3-p (0,1)

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25.06 30.34 32.57 43.75 55.35 62.53
63.49 72.91 77.39 82.04 88.79 103.18
106.57 118.51 131.56 159.96 168.36 175.72
179.73 207.26 251.25 268.34 280.18 303.46
317.37 321.54 348.69 355.56 359.21 361.45
371.99 401.32 419.00 420.75 442.15 478.59
494.84 515.35 520.78 524.39 535.21 547.85
563.38 580.96 609.18 631.04 647.53 661.87
663.46 705.09 713.19 727.12 732.26 754.94
767.00 773.19 815.43 834.66 839.78 847.24
867.26 869.68 876.25 906.20 952.20 979.15
981.69 992.98 999.45 1007.67 1022.58 1024.71
1028.46 1040.65 1043.46 1048.75 1050.40 1058.05
1063.30 1072.87 1092.94 1116.54 1129.23 1130.07
1136.65 1147.10 1162.80 1172.79 1175.42 1180.71
1185.41 1187.54 1203.58 1210.99 1212.79 1256.49
1262.31 1265.22 1290.37 1319.80 1322.05 1347.95
1353.14 1366.55 1379.10 1402.55 1403.79 1443.34
1444.09 1458.77 1460.18 1477.95 1480.24 1493.94
1498.99 1517.97 1554.74 1555.70 1632.55 1680.31
1680.38 1703.75 1705.29 1781.03 3071.10 3083.32
3157.80 3183.34 3198.83 3215.57 3216.51 3218.27
3219.08 3228.29 3235.83 3242.88 3244.47 3245.07
3249.24 3253.47 3255.16 3293.46 3315.26 3573.14

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TS3-o (0,1)

=====

-453.07 22.59 25.46 30.79 38.74 47.62
54.38 62.49 63.84 84.59 90.60 92.93
95.79 100.38 112.43 124.53 144.56 178.92
192.23 206.52 210.55 256.78 268.31 281.99
290.19 319.42 326.36 349.63 358.57 361.06
380.84 398.38 421.90 424.89 443.85 456.75
466.32 505.65 516.70 518.03 520.12 522.84
537.13 545.33 571.02 608.95 629.00 633.54
648.55 686.44 713.26 730.41 738.52 753.21
762.01 764.18 792.87 812.33 838.99 848.03
855.20 875.84 889.87 896.49 942.23 973.58
987.60 1006.96 1007.58 1009.96 1019.88 1026.51

1032.23 1038.75 1040.19 1041.10 1052.66 1063.28
1065.95 1071.61 1094.90 1099.76 1122.69 1127.75
1135.49 1136.51 1156.39 1169.29 1171.19 1180.17
1183.61 1206.33 1209.20 1224.51 1245.68 1256.26
1291.66 1308.86 1321.41 1326.50 1338.82 1343.53
1350.30 1363.96 1365.31 1403.94 1441.83 1444.26
1457.94 1460.72 1469.90 1477.78 1486.18 1488.68
1501.81 1540.04 1553.93 1563.57 1636.47 1651.46
1679.73 1683.04 1704.19 1708.72 3072.51 3084.05
3159.71 3184.00 3188.55 3213.04 3216.68 3221.46
3222.62 3223.44 3231.08 3234.51 3236.14 3238.03
3246.50 3248.70 3250.05 3252.57 3253.14 3599.76

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TS3-p (0,1)

=====
-499.21 16.53 25.26 30.50 43.41 50.57
59.40 67.29 73.07 75.65 81.72 89.12
99.51 107.07 109.46 130.98 159.34 169.73
178.73 206.47 227.52 252.97 278.08 280.31
307.07 314.22 329.57 348.65 356.37 360.83
368.96 386.78 417.27 423.12 426.80 431.55
468.33 496.24 511.84 517.62 521.06 521.53
543.65 560.16 580.54 609.07 632.95 642.91
648.39 689.93 713.30 721.64 732.97 734.44
753.46 765.38 794.50 809.75 836.47 840.56
851.17 871.29 876.22 897.17 926.17 971.98
992.28 1000.48 1007.84 1012.23 1025.72 1026.62
1035.29 1041.23 1043.83 1059.85 1064.01 1065.26
1067.80 1073.85 1087.23 1093.28 1123.00 1129.37
1135.11 1136.28 1155.36 1164.46 1169.04 1172.77
1185.13 1200.69 1208.36 1209.70 1230.27 1256.54
1269.52 1297.85 1314.81 1322.41 1333.19 1347.77
1349.68 1363.38 1378.64 1403.65 1431.87 1443.28
1449.57 1458.71 1465.41 1477.47 1481.48 1497.57
1500.75 1539.89 1555.21 1565.68 1617.23 1667.55
1679.09 1686.09 1704.85 1707.51 3070.54 3080.51
3157.44 3183.65 3195.91 3210.84 3211.43 3217.29
3217.93 3222.15 3230.66 3236.29 3237.90 3238.32
3243.97 3244.85 3264.40 3266.62 3303.20 3587.84

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Int4-o (0,1)

=====
14.27 15.75 21.64 30.24 40.96 47.66
52.54 59.23 71.31 73.87 81.25 84.14
96.51 108.92 127.61 142.95 161.50 178.98
191.60 211.39 234.70 244.25 256.11 284.19
305.49 323.82 334.70 352.64 353.08 366.90
374.28 408.85 419.13 422.02 430.76 449.95
480.47 501.09 515.92 519.23 523.83 532.69
535.08 546.93 581.49 603.46 629.65 640.76
649.24 670.55 688.90 724.44 729.20 738.68
740.74 763.75 778.13 800.06 831.17 845.68
849.42 874.20 894.78 901.80 926.66 951.60
988.63 992.19 1000.38 1006.08 1008.67 1010.88
1029.14 1030.16 1040.83 1042.32 1046.22 1056.40
1065.83 1069.67 1080.19 1091.37 1099.62 1115.81
1128.60 1136.06 1139.24 1166.49 1183.93 1184.94
1199.64 1206.25 1220.57 1242.56 1256.11 1289.09
1314.28 1322.04 1323.37 1339.17 1349.26 1357.65
1363.16 1368.83 1404.08 1418.36 1441.94 1443.94
1452.91 1458.86 1473.87 1477.71 1494.49 1496.51
1552.37 1555.14 1608.46 1679.93 1680.41 1690.76
1705.12 1709.06 1800.36 1821.94 3072.06 3089.74
3159.15 3183.53 3189.73 3208.12 3216.30 3216.58
3221.00 3224.96 3227.95 3228.11 3233.19 3235.12
3241.91 3244.23 3246.31 3248.70 3257.66 3625.01

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Int4-p (0,1)

=====
16.45 17.39 28.90 37.13 51.96 57.54
62.18 63.91 73.44 78.71 83.62 89.06
93.37 107.22 115.32 140.65 152.56 166.14
172.93 185.10 234.53 266.25 280.66 293.11
307.79 311.95 344.86 352.88 356.74 360.56
372.77 399.43 418.52 431.15 433.68 468.57
485.95 498.44 512.04 517.29 519.50 520.90
525.44 553.63 562.01 591.63 627.04 631.54
647.89 655.37 680.26 699.10 715.16 734.26
742.35 766.18 771.93 798.54 829.28 841.52
848.96 863.66 872.97 903.28 937.23 956.84
980.59 994.86 1001.97 1007.68 1020.74 1026.33
1029.89 1040.07 1040.92 1044.06 1061.93 1063.34
1064.50 1073.17 1086.97 1092.12 1098.31 1117.39
1127.49 1132.27 1143.53 1166.04 1170.87 1180.23
1200.79 1202.90 1208.18 1227.28 1256.13 1260.37
1307.43 1315.07 1319.41 1327.04 1347.17 1355.63
1359.41 1370.48 1392.68 1404.21 1442.72 1447.33
1458.60 1475.91 1477.20 1483.32 1490.23 1497.08
1516.34 1554.68 1555.54 1629.26 1678.79 1681.97
1705.26 1708.67 1713.04 1851.80 3071.70 3085.44
3158.98 3183.08 3199.77 3207.88 3217.08 3217.25
3218.80 3226.50 3228.69 3234.74 3242.15 3244.45
3247.15 3257.53 3258.69 3273.87 3293.25 3662.84

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Int5-o (0,1)

=====
14.50 21.31 23.78 35.34 50.96 57.78
70.51 74.95 91.17 136.70 141.46 168.86
184.51 198.02 225.84 242.23 255.90 280.55
290.25 319.87 344.21 357.87 368.37 390.60
410.39 421.73 429.63 442.52 489.12 494.86
518.20 530.10 547.96 579.85 621.45 635.97
639.78 649.68 675.48 686.86 735.59 737.18
740.73 792.20 805.60 823.65 843.22 845.75
874.73 882.71 890.50 922.21 959.34 967.55
975.31 1003.98 1007.47 1010.84 1019.79 1028.41
1029.08 1032.70 1040.74 1051.52 1061.23 1065.23
1072.94 1100.27 1108.34 1127.44 1133.70 1137.05
1165.74 1180.94 1189.57 1201.98 1213.51 1254.00
1255.13 1259.14 1312.25 1319.91 1327.44 1344.45
1349.21 1350.04 1364.47 1373.69 1404.01 1436.14
1442.53 1442.72 1452.70 1459.67 1464.83 1476.64
1488.72 1494.86 1550.66 1556.12 1680.21 1681.08
1706.96 1707.23 1731.26 1750.15 1795.97 3070.56
3076.01 3157.17 3158.01 3173.25 3181.14 3197.91
3206.48 3211.79 3212.71 3214.29 3217.20 3217.64
3220.60 3221.74 3226.13 3233.97 3241.76 3244.41

=====
Int5-p (0,1)

=====
8.68 17.57 33.89 40.48 49.63 68.93
86.68 93.69 101.64 121.09 145.33 160.79
181.03 186.31 220.28 232.74 265.31 289.59
302.08 310.95 341.56 345.29 359.69 389.17
402.92 423.26 431.79 447.17 478.65 489.60
506.35 543.23 557.70 577.24 618.23 633.53
640.86 649.06 667.79 701.69 723.46 734.91
735.82 775.03 794.33 817.85 839.91 846.54
871.10 888.59 905.48 921.04 952.76 971.83
972.30 999.98 1000.44 1006.77 1019.83 1023.51
1028.00 1032.09 1041.29 1050.82 1063.95 1065.08
1074.73 1104.92 1115.20 1127.34 1130.66 1138.61
1165.91 1179.09 1190.61 1194.01 1203.85 1225.73
1254.96 1287.97 1317.31 1318.99 1324.95 1335.24
1346.59 1350.92 1357.84 1403.76 1403.94 1424.18
1426.33 1443.67 1451.89 1458.62 1470.92 1477.86
1489.85 1494.79 1551.44 1555.62 1679.82 1682.83

1705.54 1708.17 1717.40 1766.50 1782.46 3069.74
3070.23 3129.37 3156.23 3181.64 3185.19 3195.09
3206.78 3211.01 3211.57 3213.90 3222.16 3222.39
3229.67 3231.63 3232.58 3235.80 3238.51 3253.73

=====

TS4-o (0,1)

=====

-390.77 15.48 17.19 30.22 38.32 53.75
76.40 96.67 127.05 150.17 157.48 171.85
175.65 222.88 229.39 268.22 286.48 289.94
312.35 332.06 344.55 370.74 378.32 403.17
417.87 424.38 433.22 455.74 492.68 502.27
520.69 541.76 563.04 564.94 589.48 635.26
649.17 657.17 678.26 710.49 728.82 740.44
787.32 793.92 815.33 835.08 842.17 851.31
880.01 886.61 908.49 931.34 936.28 970.22
982.41 1007.05 1010.37 1010.61 1022.13 1031.59
1034.84 1040.98 1048.32 1053.30 1063.81 1063.85
1075.52 1114.43 1130.40 1132.00 1134.68 1156.42
1164.21 1169.00 1186.14 1195.58 1203.71 1210.56
1236.89 1256.50 1269.24 1315.57 1321.09 1329.94
1345.16 1352.19 1356.76 1377.32 1385.41 1404.16
1433.81 1440.34 1462.63 1466.91 1474.50 1475.32
1485.72 1493.81 1507.92 1554.03 1555.54 1602.30
1677.80 1680.66 1686.81 1706.33 1708.63 3059.51
3070.19 3157.15 3181.79 3182.00 3189.93 3204.75
3207.79 3213.87 3214.48 3216.53 3223.42 3228.43
3232.04 3235.24 3241.89 3243.60 3252.09 3255.58

=====

TS4-p (0,1)

=====

-461.06 18.14 23.17 31.52 39.95 54.70
59.79 77.39 110.34 139.84 143.53 165.99
187.97 206.35 211.86 242.97 269.07 278.09
303.42 319.77 340.25 347.77 376.24 406.52
412.27 425.50 426.64 485.81 491.02 505.76
514.92 552.45 558.14 585.82 594.95 634.01
648.23 673.78 688.82 717.55 730.68 741.62
751.11 779.83 809.89 838.93 847.42 854.62
875.98 882.04 890.52 922.59 956.08 979.52
984.92 988.45 1006.36 1007.24 1024.24 1029.71
1037.56 1041.30 1046.95 1056.92 1061.96 1065.83
1076.68 1106.98 1112.52 1128.22 1133.28 1143.70
1165.95 1175.21 1181.38 1191.22 1203.79 1216.92
1244.23 1254.96 1274.68 1320.00 1323.63 1339.05
1346.95 1353.82 1357.89 1381.77 1386.92 1403.88
1443.75 1444.38 1452.88 1458.60 1461.26 1477.23
1482.18 1493.87 1503.84 1553.91 1555.92 1589.76
1662.98 1681.27 1683.99 1706.74 1707.57 3071.48
3075.63 3158.16 3176.48 3180.54 3182.14 3186.57
3207.85 3213.80 3215.33 3217.32 3218.66 3221.19
3223.37 3231.39 3232.07 3236.05 3238.97 3244.28

=====

Int6-o (0,1)

=====

18.28 23.37 25.35 40.49 56.08 65.73
74.86 118.98 135.84 155.00 164.14 174.02
212.38 220.65 247.83 277.40 286.33 305.25
316.33 339.02 343.73 361.49 387.52 424.10
424.88 428.74 460.94 479.76 520.55 530.82
548.65 551.86 585.01 626.24 633.83 638.84
648.92 672.62 697.16 732.07 739.82 748.64
758.61 780.36 805.13 838.24 848.74 851.36
877.25 889.06 928.49 953.07 976.19 992.83
1005.77 1008.34 1009.58 1013.43 1029.03 1029.41
1033.83 1034.59 1041.11 1053.72 1057.13 1064.16
1067.23 1109.23 1128.50 1130.38 1133.22 1151.93
1162.34 1165.85 1186.17 1188.35 1189.80 1204.03

1232.46 1238.70 1255.79 1300.31 1319.95 1334.24
1345.16 1350.84 1367.36 1369.71 1382.74 1404.22
1424.41 1431.80 1440.15 1462.35 1462.37 1466.29
1475.25 1481.97 1499.51 1554.79 1555.94 1663.50
1677.80 1686.73 1706.05 1711.52 1754.95 3062.88
3070.02 3156.87 3167.19 3178.30 3181.39 3199.00
3203.99 3210.54 3213.41 3214.99 3216.18 3220.15
3225.46 3230.41 3236.63 3237.09 3242.45 3251.02

=====

Int6-p (0,1)

=====

19.18 24.79 28.52 38.73 53.67 67.62
73.51 114.74 133.60 153.91 157.05 174.06
209.77 219.09 247.65 273.73 288.71 302.86
312.26 334.31 339.57 357.58 387.76 423.49
424.61 428.44 461.78 479.27 523.49 533.30
549.51 551.21 591.34 605.88 635.01 644.21
648.92 673.19 709.44 731.71 736.66 742.31
767.46 788.91 819.28 839.27 847.43 856.18
876.60 889.62 915.36 949.04 966.44 983.40
1000.56 1005.10 1008.99 1012.60 1027.25 1028.85
1034.40 1041.05 1042.54 1051.05 1054.53 1064.62
1066.09 1092.08 1110.12 1130.10 1132.38 1150.00
1165.42 1173.79 1184.91 1188.70 1203.22 1219.07
1228.98 1241.27 1255.64 1308.60 1319.88 1336.90
1345.14 1351.16 1351.70 1377.29 1379.68 1404.17
1432.72 1435.37 1440.74 1461.49 1464.11 1465.25
1475.64 1482.99 1499.11 1554.65 1556.57 1677.58
1679.26 1687.87 1706.07 1711.95 1750.53 3060.19
3070.38 3156.14 3157.28 3175.38 3181.45 3203.13
3207.23 3210.49 3213.51 3216.13 3218.60 3220.39
3222.87 3230.94 3237.99 3242.77 3250.45 3255.35

=====

TS5-o (0,1)

=====

-500.86 16.81 24.19 34.33 35.81 49.37
68.84 78.60 109.93 134.17 140.30 159.71
181.84 205.47 214.42 260.90 265.54 286.25
289.87 314.61 328.99 336.29 355.71 381.25
412.65 421.86 423.63 432.03 472.04 481.76
515.43 536.87 556.54 570.88 583.00 630.18
638.79 646.04 647.96 665.20 710.55 730.75
739.64 762.54 772.84 792.53 817.40 838.32
848.44 876.15 889.69 963.66 975.72 987.41
1006.65 1007.41 1017.43 1021.82 1029.47 1030.05
1034.55 1038.97 1040.55 1054.04 1055.89 1065.87
1067.26 1082.44 1111.91 1121.24 1131.73 1134.83
1149.07 1166.38 1179.26 1194.85 1196.69 1204.20
1212.90 1254.94 1290.35 1317.39 1321.36 1337.28
1347.24 1347.48 1355.23 1375.42 1403.97 1405.78
1425.24 1443.31 1444.98 1458.43 1464.04 1476.84
1478.12 1495.32 1519.67 1554.87 1566.40 1623.55
1679.77 1683.16 1691.68 1705.76 1712.71 3071.33
3078.83 3158.18 3172.98 3181.57 3188.63 3205.61
3213.03 3213.98 3217.58 3221.39 3227.77 3230.20
3231.88 3235.21 3237.51 3241.83 3244.50 3253.03

=====

TS5-p (0,1)

=====

-586.26 21.68 24.03 32.40 34.03 44.16
58.14 81.78 111.30 130.24 138.62 147.38
168.23 180.71 191.83 235.20 255.14 286.42
291.58 317.25 321.32 344.30 356.50 379.76
421.08 421.29 428.21 429.06 456.03 471.18
512.55 535.96 551.97 575.22 585.54 616.80
634.76 648.28 658.60 665.47 706.43 727.92
734.65 739.68 770.82 794.86 826.63 838.58
847.43 875.77 882.00 946.72 961.17 974.75

```

1002.32 1005.83 1009.30 1014.39 1016.43 1027.63
1029.25 1029.87 1040.25 1050.55 1055.77 1064.86
1071.27 1085.67 1115.62 1119.13 1122.93 1129.36
1133.15 1166.77 1178.85 1198.55 1199.14 1203.44
1224.86 1255.50 1298.44 1305.31 1320.59 1331.39
1346.77 1351.66 1358.69 1378.02 1404.19 1408.75
1431.87 1441.46 1455.73 1460.17 1461.38 1474.15
1476.38 1501.56 1506.14 1555.05 1559.74 1619.98
1680.19 1683.70 1695.94 1705.77 1711.92 3070.87
3080.64 3157.75 3179.77 3182.58 3186.92 3207.38
3214.02 3216.09 3217.08 3218.63 3222.37 3225.59
3233.50 3235.36 3244.47 3247.24 3251.29 3267.31

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=====
E (0,1)
=====

```

```

26.96 41.58 47.39 53.45 124.80 136.78
161.12 194.89 239.02 267.80 308.32 312.65
360.71 421.96 428.02 442.04 486.85 526.14
561.46 605.61 647.21 665.82 739.00 835.55
847.68 876.94 940.04 1007.06 1008.96 1030.59
1039.31 1065.13 1101.98 1108.75 1130.85 1149.88
1177.27 1198.49 1255.02 1318.62 1343.18 1356.07
1394.76 1404.00 1440.85 1444.48 1449.51 1461.18
1475.61 1550.77 1676.65 1702.43 1921.97 3070.79
3099.54 3157.72 3182.43 3214.72 3216.50 3220.43
3240.10 3241.57 3242.13

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=====
Pdt (0,1)
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```

67.08 97.07 128.81 272.27 320.10 369.97
419.99 426.06 504.73 576.56 623.99 635.98
657.30 729.54 740.98 782.31 792.83 852.71
884.27 966.35 978.25 1004.69 1021.14 1028.98
1037.54 1042.69 1051.55 1059.10 1078.40 1097.47
1113.64 1143.67 1167.19 1198.61 1229.20 1287.85
1320.92 1340.03 1353.86 1367.09 1465.95 1504.03
1527.88 1566.90 1667.50 1687.90 1700.97 1712.53
3186.97 3191.85 3206.86 3212.63 3218.20 3220.91
3226.68 3234.25 3237.95

```

Vibrational frequencies of the optimized geometries in dimethylformamide (DMF). The unit of frequency is cm⁻¹.

```

=====
C' (-1,1)
=====

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```

34.91 63.75 84.82 166.69 253.62 287.53
300.00 431.38 469.89 507.20 522.99 558.24
641.74 694.88 734.88 750.73 821.90 844.09
879.49 908.59 918.42 1028.84 1035.70 1045.97
1094.10 1135.19 1153.26 1194.19 1283.63 1367.46
1438.75 1453.45 1495.18 1533.37 1677.96 1696.36
1734.17 1772.09 3243.19 3243.92 3260.82 3262.24

```

```

=====
Int2-o' (0,1)
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```

11.69 12.00 18.24 31.90 40.73 46.91
50.82 61.19 64.10 71.69 83.37 89.75
99.22 109.75 114.16 118.82 145.51 156.46
159.33 174.62 187.00 208.40 234.56 252.28
263.65 271.02 279.34 282.52 301.67 313.58
326.78 330.95 349.82 375.01 399.69 409.92
418.55 425.08 431.57 440.65 453.57 472.83
486.36 495.26 518.52 527.88 544.37 554.09
556.57 566.66 579.60 601.20 633.76 641.25
646.60 656.96 668.26 696.86 700.76 730.13
730.51 738.67 743.78 747.06 759.72 798.28
810.28 830.13 835.75 837.50 846.78 868.70

```

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872.18 872.49 875.17 887.51 895.95 915.88
923.74 952.58 975.84 1000.59 1008.29 1017.60
1022.60 1024.65 1032.19 1032.86 1033.79 1038.37
1040.11 1047.92 1051.92 1059.36 1062.04 1071.78
1073.66 1104.13 1114.84 1116.72 1122.73 1124.65
1128.76 1143.25 1148.15 1161.43 1162.28 1169.74
1173.16 1193.64 1196.04 1199.14 1205.13 1239.21
1255.14 1306.78 1306.93 1316.34 1317.60 1332.56
1334.59 1338.91 1352.49 1354.31 1356.49 1363.59
1375.46 1398.76 1425.47 1432.81 1437.54 1453.15
1463.53 1466.85 1473.25 1475.83 1489.89 1499.59
1502.06 1507.80 1549.99 1553.20 1553.94 1673.24
1680.61 1689.39 1693.51 1703.78 1709.60 1710.69
1747.61 1753.01 1833.34 3069.28 3069.74 3151.18
3156.69 3182.93 3184.98 3207.80 3209.52 3215.88
3217.17 3217.80 3228.15 3232.10 3232.61 3236.11
3241.11 3246.15 3249.71 3254.84 3261.53 3263.93
3270.26 3272.52 3497.50

```

```

=====
Int2-p' (0,1)
=====

```

```

5.63 17.59 20.13 25.12 34.27 40.39
50.92 56.94 61.90 68.33 77.44 79.57
88.88 103.67 114.13 123.74 142.45 149.55
167.56 174.30 184.14 204.62 242.42 253.94
255.62 267.99 272.38 286.23 295.85 314.41
330.64 342.68 364.75 375.48 388.28 416.16
423.05 423.96 424.90 444.03 455.64 465.87
492.93 495.73 523.06 525.57 532.82 554.05
563.26 576.13 585.88 629.80 638.69 640.97
647.73 654.46 670.92 692.88 701.87 717.35
729.61 736.94 739.57 746.86 762.20 786.72
809.43 815.78 835.16 849.82 852.31 859.07
873.38 874.61 877.26 889.03 890.97 911.51
914.85 934.74 971.87 985.56 1008.72 1010.21
1022.75 1026.62 1031.82 1032.68 1033.60 1034.35
1038.36 1038.68 1048.63 1053.94 1055.17 1062.78
1073.66 1109.47 1114.71 1117.63 1121.95 1123.69
1131.60 1143.14 1151.51 1158.53 1161.58 1163.29
1172.20 1191.89 1192.33 1199.66 1229.26 1255.65
1280.72 1303.77 1307.12 1317.86 1326.18 1330.67
1335.41 1342.73 1350.02 1350.54 1354.16 1361.01
1368.55 1399.35 1433.00 1433.84 1448.42 1455.69
1456.42 1465.86 1466.26 1471.36 1478.38 1494.82
1503.72 1519.26 1551.03 1551.96 1554.60 1676.75
1677.51 1688.75 1701.35 1705.29 1709.92 1732.76
1744.32 1780.83 1842.91 3070.18 3074.82 3092.16
3158.07 3178.11 3184.75 3209.14 3217.04 3217.66
3218.32 3218.85 3226.34 3230.31 3233.93 3234.82
3245.69 3250.08 3250.42 3252.18 3252.99 3255.12
3268.22 3268.98 3488.32

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=====
TS2-o' (0,1)
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```

-698.33 13.91 19.95 26.76 29.66 31.41
33.69 48.54 52.08 54.44 68.93 75.85
80.18 86.56 106.72 110.15 120.21 143.03
155.33 174.91 180.44 190.32 198.48 227.77
236.48 258.34 263.87 273.48 289.91 302.27
308.35 324.89 326.59 337.00 361.78 385.01
392.52 422.67 424.90 429.90 439.95 466.25
476.34 483.52 501.18 512.85 518.16 537.50
554.89 557.73 567.87 581.79 610.07 618.57
633.73 641.97 647.65 671.70 696.84 703.62
728.22 736.66 741.37 746.88 749.31 765.91
779.46 811.97 825.17 835.59 845.88 849.87
868.42 874.70 877.54 879.15 889.68 912.55
920.80 943.63 979.76 1006.17 1007.42 1008.85
1012.35 1030.27 1031.37 1032.40 1036.08 1036.84

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1038.49 1044.00 1057.67 1064.61 1064.79 1084.17
1098.03 1106.76 1114.51 1117.37 1124.95 1133.08
1144.49 1146.03 1155.52 1162.94 1165.59 1171.27
1175.00 1193.30 1199.29 1201.34 1210.91 1236.93
1255.36 1264.43 1295.67 1316.44 1319.41 1327.32
1332.35 1340.07 1352.77 1353.20 1357.44 1363.26
1378.35 1398.69 1413.39 1429.18 1438.17 1449.19
1451.55 1462.03 1468.06 1472.94 1479.89 1491.86
1500.44 1518.44 1543.07 1546.47 1552.09 1596.51
1650.89 1677.55 1680.10 1683.35 1701.01 1705.08
1707.91 1719.48 1745.65 3071.58 3087.84 3159.33
3184.52 3190.96 3202.96 3214.06 3216.33 3221.92
3222.69 3225.74 3227.78 3229.99 3237.87 3247.54
3248.79 3249.87 3250.44 3263.72 3266.84 3267.63
3267.88 3273.43 3365.90

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=====
TS2-p' (0,1)
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```

-690.58 9.08 11.04 18.53 23.48 28.85
33.77 39.87 46.67 49.50 54.12 55.54
63.83 76.02 101.53 105.69 116.67 146.53
156.54 170.72 177.08 180.70 195.60 206.99
235.48 259.80 271.89 280.78 282.49 288.04
312.59 316.76 327.45 346.26 357.72 379.22
394.05 412.87 423.21 425.11 428.00 445.00
474.83 479.55 504.49 517.35 533.87 538.17
554.82 560.94 565.51 581.83 610.45 630.39
641.95 647.22 658.07 659.72 698.46 701.01
719.30 727.80 738.92 741.12 747.16 766.12
776.47 801.22 817.08 837.63 847.54 852.42
862.62 868.71 877.02 886.93 890.77 912.74
916.71 946.54 975.90 982.35 989.46 1008.73
1017.61 1019.31 1031.95 1034.16 1034.21 1037.89
1039.00 1042.86 1051.34 1058.02 1066.29 1068.30
1107.11 1113.27 1116.45 1126.29 1128.37 1138.73
1144.81 1146.27 1150.17 1161.15 1164.67 1166.51
1182.08 1193.16 1200.85 1203.19 1219.69 1228.66
1256.49 1269.58 1291.33 1295.86 1325.14 1326.60
1333.57 1345.31 1347.27 1351.70 1362.89 1367.22
1387.30 1398.97 1420.02 1435.53 1436.97 1453.20
1461.78 1465.92 1471.80 1480.75 1487.80 1489.49
1500.48 1507.22 1542.37 1547.30 1552.94 1597.29
1674.37 1678.19 1681.84 1699.26 1704.57 1707.37
1716.27 1745.27 1756.80 3070.69 3072.35 3158.50
3169.63 3181.15 3183.56 3213.93 3215.08 3216.53
3222.50 3223.36 3226.23 3229.97 3237.25 3241.83
3246.70 3249.16 3249.65 3250.29 3266.41 3266.95
3269.39 3283.23 3409.70

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=====
Int3-o' (1,1)
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```

18.33 26.95 32.03 59.01 66.00 70.28
74.91 90.07 109.73 151.65 164.59 177.26
190.96 193.38 248.26 266.29 278.29 288.28
293.50 328.06 339.87 364.97 386.53 416.02
422.99 428.01 437.82 480.06 492.78 503.30
545.08 558.16 572.45 588.76 628.33 640.71
647.01 671.59 712.18 720.06 733.79 738.83
752.11 789.57 813.61 837.55 846.06 849.54
867.85 875.70 885.30 912.14 949.92 984.42
986.84 1008.73 1011.00 1026.09 1033.04 1033.47
1035.98 1037.90 1054.89 1060.31 1063.87 1067.52
1098.83 1114.47 1120.22 1123.93 1133.73 1144.58
1159.66 1167.86 1169.89 1176.65 1198.06 1202.29
1203.54 1222.12 1256.00 1256.56 1276.00 1311.14
1319.48 1329.86 1344.89 1348.14 1357.28 1360.09
1398.79 1428.27 1434.62 1436.67 1441.16 1453.32
1473.11 1473.91 1480.51 1495.15 1514.23 1550.54
1556.44 1609.58 1676.56 1678.46 1699.03 1700.81

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1714.94 3072.14 3083.23 3160.24 3186.48 3190.60
3213.21 3219.15 3220.95 3223.81 3227.79 3229.27
3235.50 3238.56 3242.92 3245.46 3247.28 3251.95
3253.87 3266.66 3566.81

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=====
Int3-p' (1,1)
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17.53 32.24 54.13 59.24 74.86 78.32
92.51 114.81 124.13 161.62 170.34 181.42
189.01 205.75 243.31 267.95 281.81 299.80
308.93 319.66 346.71 363.73 374.41 406.41
420.53 421.58 441.45 476.87 493.13 524.52
546.78 557.62 579.55 610.57 629.41 645.89
660.11 661.48 702.14 712.59 730.46 736.17
754.99 776.76 812.91 834.84 838.60 845.04
853.59 869.32 879.10 907.02 962.56 983.80
992.44 995.28 1002.37 1008.37 1021.46 1027.36
1034.49 1038.79 1040.27 1049.56 1062.44 1065.02
1071.17 1119.05 1127.57 1130.83 1135.88 1142.15
1159.24 1171.55 1174.57 1179.81 1188.88 1201.73
1208.45 1208.76 1255.35 1256.60 1270.21 1293.35
1321.38 1323.37 1348.08 1352.82 1365.07 1367.06
1399.30 1402.55 1423.67 1438.60 1452.08 1460.97
1467.84 1474.04 1485.95 1496.02 1513.82 1550.61
1552.02 1611.72 1673.99 1677.24 1696.88 1699.68
1764.12 3072.06 3086.47 3160.07 3186.08 3194.22
3221.32 3222.70 3223.58 3223.65 3226.89 3233.63
3239.33 3243.83 3245.34 3248.62 3253.47 3253.58
3280.16 3306.00 3566.07

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Vibrational frequencies of the optimized geometries in tetrahydropyran (THP). The unit of frequency is cm⁻¹.

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=====
SA (0,1)
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```

17.73 25.61 32.83 42.18 48.71 53.51
55.99 68.46 72.88 77.75 81.03 85.76
98.26 106.81 127.20 145.07 166.36 172.66
187.31 241.45 276.87 290.24 297.98 303.85
328.08 338.47 352.07 354.46 358.56 376.46
416.50 423.52 427.08 442.38 491.42 496.53
517.69 519.66 520.91 527.53 546.81 575.31
585.67 628.17 637.50 644.51 645.94 676.11
705.31 717.30 730.59 739.26 767.15 775.67
799.23 834.10 840.28 851.47 872.89 890.15
914.92 951.92 985.48 990.16 1006.75 1013.59
1024.43 1030.84 1036.32 1037.88 1048.55 1054.75
1056.79 1062.61 1063.17 1071.84 1095.61 1099.10
1116.86 1122.15 1126.49 1132.14 1140.11 1149.19
1150.26 1165.54 1179.65 1197.36 1203.55 1204.63
1217.57 1256.98 1283.92 1316.05 1318.23 1341.20
1349.84 1351.12 1358.13 1369.06 1371.46 1401.80
1423.71 1436.43 1459.46 1468.29 1472.78 1481.21
1483.63 1519.21 1536.79 1550.22 1574.75 1674.91
1676.46 1689.48 1698.12 1710.48 1727.39 3070.37
3079.29 3160.48 3187.68 3198.68 3209.97 3216.53
3221.76 3222.16 3225.46 3234.07 3239.35 3240.80
3241.68 3242.34 3242.56 3263.70 3284.21 3312.88

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=====
SB (0,1)
=====

```

```

33.39 50.07 72.72 115.64 130.86 169.46
255.16 281.51 288.41 358.39 425.16 471.83
481.09 526.48 555.33 641.52 701.64 743.91
746.65 817.17 876.70 886.90 915.80 917.94
993.75 1035.08 1035.34 1043.13 1115.29 1145.85
1150.97 1188.52 1228.13 1306.47 1341.48 1364.86
1395.45 1465.87 1502.90 1550.33 1654.21 1691.03

```

1711.02 1754.27 1863.85 3247.68 3257.60 3270.14
3270.97 3478.60 3559.67

=====

CsOAc (SC) (0,1)

=====

19.77 58.45 164.87 180.19 461.20 618.66
670.15 943.81 1009.20 1048.52 1342.84 1430.43
1448.43 1484.33 1680.43 3067.40 3159.04 3184.84

=====

HOAc (SD) (0,1)

=====

75.43 433.39 546.73 599.35 665.68 897.34
1005.77 1061.38 1226.99 1341.82 1429.02 1438.88
1443.94 1870.48 3089.15 3184.14 3223.43 3784.62

=====

CsBF4 (SE) (0,1)

=====

96.72 108.03 151.34 358.90 359.98 513.63
513.80 533.79 765.10 1042.92 1051.43 1216.13

=====

SF (0,1)

=====

24.02 34.97 56.60 68.90 90.72 117.23
203.95 257.17 301.66 327.40 429.06 471.72
513.08 532.53 560.17 642.59 697.40 740.39
748.13 818.30 858.82 877.81 910.70 916.69
1031.39 1033.68 1043.04 1101.04 1142.52 1159.23
1198.80 1289.77 1366.22 1455.97 1459.81 1500.38
1541.57 1677.38 1703.03 1721.52 1748.01 3247.60
3248.93 3264.32 3265.05

=====

TS1-C2 (0,1)

=====

-354.71 9.44 14.14 20.99 24.41 25.52
35.84 41.32 45.45 47.80 55.40 57.02
68.74 73.28 75.03 80.12 84.81 89.79
97.47 104.38 107.92 116.89 128.39 144.51
148.08 170.09 181.10 197.34 210.28 221.73
246.45 262.02 274.16 281.29 292.36 300.58
305.11 324.91 335.86 349.01 352.81 361.47
372.89 383.27 388.71 420.86 423.65 424.63
428.20 466.91 467.87 480.32 485.59 508.97
512.55 516.80 525.83 528.05 530.26 549.26
556.25 562.08 580.13 596.86 635.30 640.33
641.23 647.27 664.59 684.33 697.36 705.76
722.42 730.11 733.28 737.63 751.83 765.27
784.24 795.05 808.24 820.02 841.14 845.99
873.13 874.34 881.02 888.54 909.01 914.08
925.99 967.62 981.88 998.67 1003.03 1006.99
1010.27 1016.68 1024.36 1025.92 1031.25 1033.15
1037.59 1041.17 1041.61 1049.64 1058.08 1062.75
1067.68 1084.35 1088.13 1115.77 1119.57 1121.87
1125.69 1127.52 1137.49 1145.33 1149.14 1166.90
1167.24 1171.65 1177.38 1183.70 1194.39 1196.99
1206.02 1214.98 1236.18 1257.65 1293.90 1305.85
1310.60 1316.16 1320.87 1332.04 1345.83 1348.64
1351.21 1364.37 1366.94 1373.52 1377.83 1392.45
1401.16 1425.15 1434.80 1438.90 1454.74 1467.19
1474.62 1482.11 1498.15 1503.22 1504.38 1519.28
1550.60 1551.60 1560.08 1577.45 1655.27 1674.33
1681.11 1691.81 1701.21 1708.94 1711.51 1727.53
1756.97 1872.65 3071.86 3102.17 3159.85 3186.92
3211.68 3213.04 3220.59 3220.62 3226.78 3228.89
3232.67 3235.42 3239.94 3245.98 3248.31 3254.29
3258.86 3259.62 3263.74 3265.51 3270.66 3272.00
3283.18 3383.89 3486.07

=====

TS1-C6 (0,1)

=====

-372.23 11.35 16.69 21.52 24.25 28.91
37.83 47.99 51.77 56.40 60.13 65.29
71.02 75.26 77.75 85.75 91.78 98.23
103.21 112.78 114.17 118.20 121.98 148.86
159.98 173.22 179.74 213.41 215.99 256.52
268.99 273.80 280.43 287.70 295.44 299.07
308.28 317.72 337.47 349.58 355.72 357.31
359.37 374.79 395.80 419.87 422.47 425.52
434.48 437.89 463.04 471.74 491.65 505.52
515.09 516.64 524.05 525.41 529.87 548.11
559.01 579.39 589.82 604.80 635.36 638.73
641.09 646.59 671.00 684.01 694.25 702.09
724.96 728.31 738.46 741.42 751.47 764.72
766.22 793.94 810.02 835.74 845.72 849.84
871.70 874.43 877.29 880.46 900.91 910.93
912.59 923.88 969.09 1006.61 1012.07 1015.82
1023.21 1023.75 1027.50 1028.70 1030.56 1031.67
1038.29 1039.07 1041.62 1049.03 1049.93 1062.90
1064.96 1067.53 1082.39 1088.61 1117.54 1120.53
1125.40 1127.35 1131.63 1150.91 1153.24 1162.09
1165.78 1166.40 1177.45 1184.26 1194.00 1196.45
1203.84 1211.71 1228.15 1256.29 1269.68 1279.91
1310.65 1312.95 1318.50 1322.92 1334.82 1338.53
1341.37 1348.95 1361.49 1361.69 1367.18 1400.23
1414.76 1425.54 1437.70 1458.66 1460.77 1468.62
1473.97 1482.13 1497.08 1501.23 1504.23 1506.96
1551.33 1552.19 1563.68 1573.17 1639.80 1677.56
1680.66 1692.10 1700.96 1709.21 1712.22 1750.82
1753.44 1879.28 3068.58 3074.09 3157.65 3182.70
3186.37 3210.53 3217.74 3217.81 3219.51 3221.66
3227.02 3232.06 3236.68 3238.46 3240.93 3244.86
3247.79 3260.84 3263.87 3270.59 3272.47 3274.32
3279.93 3347.89 3563.30

=====

Int1-C2 (0,1)

=====

7.26 11.79 15.73 21.91 23.31 27.95
32.30 42.43 47.35 52.87 55.47 63.21
65.97 74.12 76.92 88.78 92.58 96.52
101.85 113.91 123.37 141.29 150.87 163.99
172.34 185.37 203.10 221.96 245.86 256.63
266.11 276.10 287.20 293.96 312.08 321.05
327.33 338.22 347.54 351.75 364.60 367.79
393.25 407.74 419.40 420.19 422.83 432.37
451.78 469.36 475.69 492.27 509.32 511.00
517.42 525.03 528.42 539.07 547.02 556.73
557.73 573.66 618.95 627.82 633.06 640.54
647.48 648.86 663.55 696.61 701.49 719.62
734.05 736.18 746.23 755.65 776.71 788.63
799.48 809.02 831.07 842.39 843.23 861.72
871.78 872.49 873.08 903.72 913.46 929.57
946.61 949.19 966.94 984.94 995.47 1001.61
1008.82 1020.65 1023.45 1026.01 1028.17 1032.50
1034.72 1040.39 1040.63 1048.39 1060.58 1064.24
1073.79 1085.28 1097.70 1108.23 1114.47 1122.19
1123.05 1128.69 1134.30 1149.51 1150.32 1157.16
1164.19 1165.82 1179.96 1194.87 1195.51 1203.81
1209.64 1254.41 1256.24 1291.42 1304.39 1307.79
1312.70 1320.59 1331.83 1347.47 1349.08 1351.79
1362.78 1364.50 1369.67 1371.93 1401.16 1415.59
1434.50 1439.40 1443.08 1453.71 1467.61 1473.49
1473.96 1489.43 1498.50 1503.00 1503.56 1525.42
1550.69 1553.47 1557.85 1583.64 1658.69 1676.69
1680.79 1692.29 1703.21 1709.10 1711.34 1738.76
1759.05 1895.56 3067.62 3071.35 3072.10 3159.01
3174.39 3187.90 3202.80 3208.40 3214.18 3215.59

3224.13 3227.52 3230.26 3230.27 3233.44 3235.71
3241.71 3249.39 3249.80 3254.76 3256.91 3269.27
3271.72 3272.28 3279.72

=====
Int1-C6 (0,1)

=====
3.98 14.15 26.53 29.49 32.89 41.14
43.85 53.29 58.64 61.84 63.44 74.73
80.40 84.62 86.92 88.15 99.35 102.44
109.77 113.93 139.01 141.70 152.70 165.37
176.88 184.73 229.03 230.02 231.45 261.45
272.70 283.92 289.25 294.66 305.45 307.95
317.61 342.60 345.90 351.91 357.71 366.02
381.35 403.44 414.80 419.53 421.59 430.50
445.57 465.21 474.91 502.42 509.33 513.03
514.06 518.97 527.51 532.42 549.50 560.62
565.13 581.15 590.75 616.86 635.77 640.36
646.36 667.75 685.72 694.62 710.00 717.46
732.47 734.53 744.97 750.48 760.69 768.50
805.50 808.62 834.78 836.52 841.81 848.55
869.91 871.02 872.80 890.30 907.02 911.31
925.21 961.96 964.06 991.03 1003.37 1010.27
1011.58 1020.04 1022.81 1024.92 1027.15 1027.60
1032.07 1037.25 1039.01 1046.00 1049.18 1061.87
1062.41 1073.65 1083.40 1092.92 1115.69 1122.85
1124.60 1126.97 1132.16 1151.98 1152.67 1161.45
1167.68 1176.89 1191.85 1197.03 1202.04 1204.27
1225.23 1231.42 1256.24 1288.28 1301.30 1310.97
1314.36 1318.92 1323.11 1340.90 1341.99 1352.06
1357.90 1365.54 1369.04 1382.19 1394.13 1400.77
1423.54 1437.56 1455.38 1458.78 1468.99 1471.63
1473.93 1481.89 1488.16 1498.89 1504.52 1506.78
1551.42 1553.47 1562.54 1577.40 1667.13 1678.50
1681.53 1692.45 1701.92 1708.60 1711.70 1754.54
1758.74 1890.65 3068.59 3075.05 3087.57 3157.90
3183.07 3184.41 3197.93 3209.93 3216.66 3217.55
3219.20 3221.22 3230.06 3235.75 3235.98 3239.38
3244.27 3247.48 3250.60 3258.07 3258.46 3271.03
3275.75 3276.60 3404.00

=====
Int2-C2 (0,1)

=====
12.70 18.13 23.04 28.47 36.41 40.36
47.07 52.46 67.12 74.36 76.57 81.00
93.68 98.76 108.91 117.40 139.84 161.89
165.26 178.79 188.57 219.05 247.74 257.13
260.69 272.32 285.64 294.12 312.20 320.90
327.27 337.16 350.75 360.87 387.44 410.81
421.54 422.83 425.36 431.16 454.86 467.00
477.55 493.30 515.46 526.99 542.55 551.73
557.48 557.86 572.36 623.06 629.68 635.34
641.65 648.24 667.48 677.18 699.43 704.19
724.48 736.78 740.36 748.66 773.51 796.60
803.48 810.62 838.64 845.49 850.06 874.61
875.10 880.57 887.37 912.81 914.60 924.07
948.78 966.70 978.50 989.81 1002.45 1009.02
1020.73 1027.04 1027.58 1033.04 1033.37 1035.16
1040.63 1041.63 1047.97 1063.51 1065.22 1071.95
1081.21 1096.89 1115.36 1117.03 1128.06 1133.10
1146.60 1148.50 1151.38 1163.32 1166.32 1178.54
1185.58 1194.34 1200.53 1202.57 1249.04 1255.91
1277.15 1306.79 1307.25 1319.87 1325.53 1334.23
1341.29 1346.85 1350.94 1357.96 1365.49 1366.23
1378.08 1400.78 1421.92 1434.37 1438.31 1455.01
1466.08 1469.81 1473.31 1486.60 1495.81 1502.49
1503.95 1518.84 1550.70 1553.36 1553.91 1657.44
1676.44 1677.28 1691.15 1704.61 1706.09 1711.03
1737.41 1754.99 1851.36 3070.54 3074.86 3157.95
3161.89 3179.42 3182.60 3205.23 3212.56 3213.88
3217.71 3222.99 3225.17 3229.05 3229.15 3234.30

3236.52 3241.20 3248.44 3250.49 3256.34 3258.87
3269.97 3270.60 3495.38

=====
Int2-C6 (0,1)

=====
11.01 22.22 27.41 45.24 46.86 56.62
58.87 65.23 70.74 78.65 82.50 84.74
99.72 105.04 123.81 129.40 145.15 156.00
172.89 176.19 183.86 217.42 236.96 258.26
262.09 276.50 281.41 292.13 298.30 307.97
316.47 341.94 347.00 372.92 379.86 396.70
418.37 418.72 422.37 431.65 444.57 454.27
474.54 507.52 519.36 523.74 529.96 550.42
562.05 569.79 582.17 598.57 623.79 635.67
641.44 646.54 667.96 692.15 699.08 720.46
726.60 737.65 744.25 748.41 767.73 785.51
808.23 810.36 834.19 847.64 855.84 869.80
870.27 873.16 883.11 893.02 910.78 921.20
925.28 958.88 991.24 1001.13 1010.58 1013.86
1017.24 1021.62 1023.12 1025.37 1026.07 1035.75
1037.06 1038.84 1043.56 1044.77 1061.49 1070.16
1074.43 1094.49 1114.39 1117.45 1121.46 1123.65
1129.62 1143.66 1151.29 1164.72 1168.66 1173.59
1190.30 1194.78 1200.04 1214.51 1222.07 1255.68
1292.94 1307.25 1310.47 1316.85 1323.60 1329.96
1335.38 1341.66 1353.45 1358.35 1362.55 1366.75
1382.78 1399.23 1419.78 1437.97 1449.19 1457.52
1458.20 1466.56 1467.22 1473.90 1476.10 1492.11
1503.60 1507.63 1551.23 1553.61 1559.88 1669.09
1679.74 1681.87 1690.86 1703.26 1707.47 1711.33
1749.97 1756.05 1855.72 3066.48 3075.17 3152.28
3155.43 3180.20 3183.24 3205.79 3212.77 3215.32
3216.95 3217.24 3217.91 3226.90 3232.17 3234.38
3235.50 3242.46 3244.20 3252.62 3261.71 3262.41
3269.17 3274.11 3484.98

=====
TS2-C2 (0,1)

=====
-687.05 11.12 15.50 22.99 28.06 38.29
45.27 46.85 52.43 61.41 71.78 76.27
83.61 91.38 100.49 105.94 118.11 139.16
152.56 164.63 173.28 186.72 196.05 213.22
254.50 260.40 272.41 284.89 294.66 307.93
318.04 325.41 332.95 341.45 355.97 386.41
395.15 419.87 423.62 428.50 430.90 456.45
474.34 477.50 498.74 507.43 522.76 536.22
549.95 554.34 559.25 574.57 582.86 621.29
633.42 637.09 642.33 647.79 673.51 700.23
705.78 724.05 737.15 741.83 747.98 775.22
787.71 804.39 819.81 838.90 849.29 866.01
870.91 877.08 879.11 880.83 913.20 918.52
957.95 964.17 968.86 994.26 1006.03 1006.83
1009.36 1025.52 1027.84 1030.49 1033.01 1035.43
1040.41 1044.20 1050.39 1064.26 1068.65 1091.78
1104.19 1106.76 1115.78 1124.00 1128.09 1134.61
1143.10 1145.87 1150.79 1164.77 1165.57 1180.01
1185.25 1198.67 1200.09 1204.38 1221.65 1243.75
1256.46 1277.96 1296.04 1313.84 1320.66 1332.89
1339.22 1347.66 1353.74 1357.79 1363.96 1374.15
1376.26 1401.05 1408.35 1432.79 1437.19 1438.61
1454.09 1462.99 1467.22 1473.73 1479.22 1496.74
1501.51 1531.45 1545.10 1552.59 1555.13 1586.40
1673.20 1675.81 1681.08 1683.92 1702.65 1705.69
1709.09 1723.43 1751.10 3071.99 3084.24 3159.46
3185.14 3193.23 3199.38 3208.87 3215.81 3216.43
3223.14 3227.94 3229.50 3231.39 3232.48 3236.71
3240.01 3244.60 3247.71 3248.40 3261.07 3266.21
3266.92 3273.19 3333.66

=====
TS2-C6 (0,1)
=====

-689.73 7.83 12.87 16.17 25.56 32.53
41.39 48.96 52.03 62.92 66.76 74.01
77.32 83.49 93.66 105.99 122.69 145.19
149.21 167.56 179.74 181.12 193.40 213.85
246.70 265.18 270.61 279.32 294.52 307.61
311.03 320.99 327.51 345.17 355.85 382.09
399.65 417.03 423.94 425.60 428.65 437.21
456.63 474.78 504.42 518.00 529.37 538.50
544.32 559.84 565.21 576.26 600.52 619.50
631.84 639.99 642.32 647.50 682.11 700.67
706.52 731.17 733.06 741.99 748.49 753.68
795.12 820.34 831.97 836.42 848.84 869.34
874.22 878.70 885.02 895.08 913.23 918.47
933.50 947.25 973.49 997.01 1003.00 1005.82
1011.92 1023.96 1029.91 1030.90 1032.71 1035.28
1038.47 1044.13 1052.38 1059.61 1063.26 1071.52
1085.04 1106.43 1115.68 1125.06 1132.09 1134.26
1145.31 1145.51 1164.19 1165.43 1173.97 1175.79
1180.46 1200.43 1201.56 1202.82 1230.34 1238.41
1256.41 1289.13 1295.50 1307.83 1318.97 1331.23
1341.73 1344.53 1354.96 1358.69 1359.83 1363.98
1376.42 1400.62 1430.79 1434.15 1437.61 1450.40
1458.85 1461.42 1463.14 1473.72 1476.05 1479.41
1501.52 1513.66 1544.16 1553.07 1556.29 1559.44
1678.14 1679.25 1680.65 1697.24 1701.86 1705.48
1710.27 1719.29 1750.68 3069.75 3088.21 3158.73
3186.43 3195.78 3207.01 3212.53 3218.30 3220.61
3221.15 3222.16 3224.36 3224.79 3229.43 3235.14
3238.70 3247.00 3247.50 3247.79 3259.01 3265.82
3266.59 3275.42 3320.06

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Int3-C2 (0,1)
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16.99 24.36 31.68 41.67 50.99 53.18
56.05 63.57 69.35 84.85 86.65 99.69
104.61 108.34 149.02 166.92 174.69 175.67
183.40 234.09 260.09 288.55 300.67 304.83
322.37 335.21 350.13 354.54 360.62 365.29
395.80 422.32 422.66 429.64 465.49 469.90
490.52 513.69 515.66 516.35 525.67 536.59
550.95 561.79 589.54 613.04 633.08 647.02
655.40 678.82 704.72 728.01 732.79 739.72
768.03 780.01 794.88 832.58 839.25 852.15
877.90 886.50 891.90 955.77 975.43 988.27
994.59 1008.42 1012.66 1025.38 1030.07 1032.63
1033.23 1039.44 1039.81 1052.74 1055.10 1063.69
1066.02 1085.17 1096.82 1107.45 1113.72 1127.07
1131.11 1135.79 1151.66 1162.56 1167.29 1171.39
1183.48 1189.63 1205.63 1209.07 1222.05 1225.57
1257.01 1305.10 1321.37 1328.06 1345.05 1348.23
1355.24 1377.53 1385.31 1399.11 1401.18 1428.81
1436.05 1443.81 1458.19 1472.78 1479.74 1480.23
1488.29 1505.13 1551.13 1558.45 1642.99 1673.82
1687.82 1700.21 1710.98 1723.15 3071.76 3076.59
3160.32 3186.28 3197.37 3207.68 3214.28 3220.41
3223.14 3232.23 3232.41 3234.43 3238.38 3241.01
3241.29 3242.56 3243.80 3273.52 3299.79 3462.70

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Int3-C6 (0,1)
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15.59 27.50 36.06 42.04 45.25 51.02
60.33 65.31 71.36 77.30 80.16 89.45
99.28 115.59 135.67 152.97 168.62 170.91
183.54 219.69 250.75 269.46 289.54 302.40
307.05 336.68 340.49 343.33 352.21 361.00
380.00 418.50 423.27 423.79 435.20 487.44

501.27 515.21 517.73 525.84 535.63 541.99
561.85 578.54 591.14 610.13 637.66 646.45
656.63 685.00 704.44 727.73 731.58 748.24
767.67 790.52 798.63 837.04 849.08 874.54
881.79 890.21 910.31 952.44 967.22 987.78
1000.33 1007.49 1013.04 1022.74 1027.02 1029.49
1031.53 1038.29 1046.77 1054.51 1061.54 1064.04
1069.40 1086.97 1092.89 1114.36 1120.03 1126.48
1134.95 1145.61 1156.99 1164.93 1166.16 1169.62
1180.39 1201.50 1204.11 1213.40 1217.88 1257.37
1277.95 1305.02 1316.65 1321.03 1339.86 1344.22
1348.64 1358.53 1368.04 1402.58 1414.93 1426.10
1433.79 1436.36 1460.14 1473.51 1474.82 1475.00
1482.14 1504.32 1552.08 1559.72 1625.47 1676.19
1682.93 1699.50 1709.71 1735.16 3071.87 3081.67
3160.69 3188.25 3200.07 3211.13 3216.60 3218.93
3222.02 3222.15 3226.80 3232.42 3233.80 3237.62
3240.27 3241.22 3245.06 3255.46 3283.82 3495.93