Supplementary Information

Organocatalytic Enantioselective Dearomatization of Thiophenes by 1,10-Conjugate Addition of Indole Imine Methides

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Table of Contents

Supplementary Methods S-3

I. General Information S-3

II. Synthesis of the Tertiary Alcohol Substrates S-4

III. Condition Optimization S-22

IV. Dearomatization of Thiophenes and Selenophenes S-33

V. Scale-up Reaction and Application S-60

VI. Mechanistic Experiments S-62

VII. DFTCalculations S-69

VIII. Determination of the Absolute Stereochemistry S-109

Supplementary References S-115

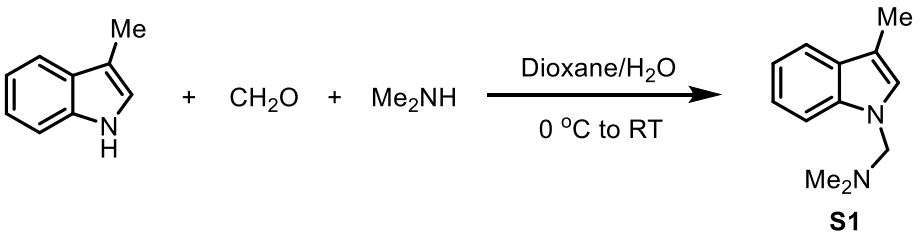
NMR Spectra and HPLC Traces

Supplementary Methods

I. General Information

Flash column chromatography was performed over silica gel (200-300 mesh) purchased from Qindao Puke Co., China. All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using anhydrous solvents. Anhydrous dichloromethane, toluene, diethyl ether, and tetrahydrofuran were purified by the Innovative® solvent purification system. Chemicals were purchased from commercial suppliers and used without further purification unless otherwise stated. ^{1}H, ^{13}C, ^{19}F NMR spectra were collected on a Bruker AV 400 MHz NMR spectrometer using residue solvent peaks as an internal standard (^{1}H NMR: $CDCl_3$ at 7.26 ppm, CD_2Cl_2 at 5.32 ppm, acetone-d_6 at 2.05 ppm; ^{13}C NMR: $CDCl_3$ at 77.16 ppm, CD_2Cl_2 at 53.84 ppm, acetone-d_6 at 29.84 ppm). Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet; d = doublet; t = triplet; q = quarter; p = pentet; sept = septet; m = multiplet; br = broad), coupling constant (Hz), integration. Mass spectra were collected on an Agilent GC/MS 5975C system, a MALDI Micro MX mass spectrometer, or an API QSTAR XL System. IR spectra were recorded on Bruker TENSOR 27 spectrometer and reported in terms of frequency of absorption (cm^{-1}). Optical rotations were measured on JASCO P-2000 polarimeter with $[\alpha]^{D}$ values reported in degrees; concentration (c) is in 10 mg/mL. The enantiomeric excess values were determined by chiral HPLC using an Agilent 1200 LC instrument with Daicel CHIRALPAK® AD-H, IC, AS-H, or CHIRALCEL® OD-H columns.

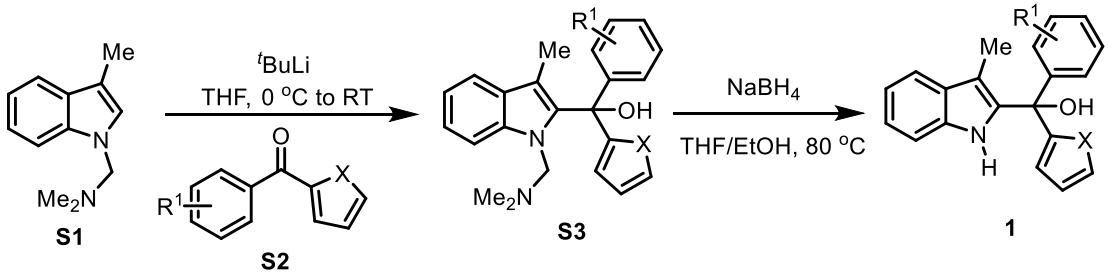
II. Synthesis of the Tertiary Alcohol Substrates



S1

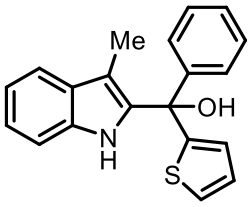
3-Methyl-1-[(*N*,*N*-dimethylamino)methyl]indole (S1). To a suspension of 3-methyl-indole (13.12 g, 100 mmol) in water/dioxane (1:1, 50 mL) was added formaldehyde (7.5 mL, 37% aqueous solution) and dimethylamine (15 mL, 33% aqueous solution) over 30 min at 0 °C. The mixture was stirred for 1 hour, then warmed to room temperature overnight. The solution was extracted twice with diethyl ether (2 x 30 mL), and the organic phases were combined and extracted with an aqueous HCl solution (2 N, 2 x 50 mL). The acid extracts were made alkaline with aqueous NaOH solution (40 wt%, 30 mL), then extracted with diethyl ether (2 x 50 mL), dried over Na_2SO_4, filtered, concentrated in vacuo to give **S1** as a light yellow oil (15.0 g, 80% yield) which was directly used in the next step. The NMR spectra are consistent with reported literature.[1]

General Procedure A.



At 0 °C, to a stirred solution of **S1** (0.56 g, 3 mmol) in THF (30 mL) was slowly added *tert*-butyllithium (1.6 M in pentane, 2.1 mL, 3.3 mmol). The resulting mixture was kept stirring at 0 °C for 30 min. Next, a solution of **S2**[2,3] (3 mmol) in THF (10 mL) was added and the reaction mixture was kept stirring overnight. A saturated aqueous solution of NH_4Cl was added to quench the reaction. The reaction mixture was extracted with EtOAc (3 × 30 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by silica gel flash chromatography to afford the crude tertiary alcohol **S3**.

To the solution of **S3** in the THF/EtOH (1:1, 2 mL/mmol), $NaBH_4$ (1.5 equiv.) was added. The resulting mixture was kept refluxing overnight for 12 h. After cooling to room temperature, saturated aqueous solution of NH_4Cl was slowly added to quench the reaction. The reaction mixture was extracted with EtOAc (2 × 30 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by silica gel flash chromatography to afford the pure tertiary alcohol **1**.



1a

(3-Methyl-*1H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (1a) was prepared as slightly yellow foam from phenyl(thiophen-2-yl)methanone (5 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 85% yield (2 steps, 1.36 g).

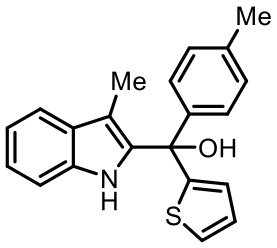
^{1}H NMR (400 MHz, acetone-d_6) δ 9.73 (s, 1H), 7.52-7.49 (m, 3H), 7.42-7.28 (m, 5H), 7.11-7.07 (m, 1H), 7.03-6.97 (m, 2H), 6.88 (dd, J_1 = 0.9 Hz, J_2 = 3.6 Hz, 1H), 5.78 (s,

1H), 1.88 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 152.6, 146.9, 139.5, 135.7, 130.7, 128.7, 128.4, 127.9, 127.2, 127.1, 126.4, 122.2, 119.4, 119.0, 112.0, 108.0, 77.2, 9.6.

IR (thin film) 3522, 3447, 3055, 1694, 1451, 1258, 1136, 733, 698 cm^{-1}.

HRMS (CI+) Calcd for $C_{20}H_{17}NOS$ (M^+): 319.1031, Found: 319.1038.



1b

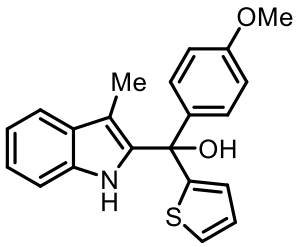
(3-Methyl-*1H*-indol-2-yl)(thiophen-2-yl)(*p*-tolyl)methanol (1b) was prepared as yellowish foam from (*p*-tolyl)(thiophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 32% yield (2 steps, 0.324 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.73 (s, 1H), 7.52 (d, J = 7.8 Hz, 1H), 7.43-7.38 (m, 4H), 7.18 (d, J = 8.2 Hz, 2H), 7.14-6.92 (m, 4H), 5.73 (s, 1H), 2.34 (s, 3H), 1.94 (s, 3H)

^{13}C NMR (100 MHz, acetone-d_6) δ 152.7, 143.9, 139.6, 137.8, 135.6, 130.7, 129.2, 127.9, 127.1, 126.9, 126.2, 122.1, 119.3, 119.0, 111.9, 107.8, 77.0, 21.1, 9.7.

IR (thin film) 3572, 3450, 3051, 1456, 1264, 1186, 995, 732, 704 cm^{-1}.

HRMS (CI+) Calcd for $C_{21}H_{19}NOS$ (M^+): 333.1187, Found: 333.1199.



1c

(4-Methoxyphenyl)(3-methyl-1*H*-indol-2-yl)(thiophen-2-yl)methanol (1c) was prepared as slightly green-yellow foam from (4-methoxyphenyl)

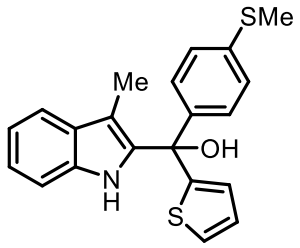
(thiophen-2-yl)methanone (2 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 46% yield (2 steps, 0.370 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.71 (s, 1H), 7.48 (d, J = 7.9 Hz, 1H), 7.40-7.37 (m, 4H), 7.11-7.06 (m, 1H), 7.03-6.96 (m, 2H), 6.91-6.88 (m, 3H), 5.66 (s, 1H), 3.79 (s, 3H), 1.89 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 160.0, 153.0, 139.8, 139.0, 135.6, 130.7, 129.3, 127.1, 126.9, 126.2, 122.1, 119.3, 119.0, 113.9, 111.9, 107.7, 76.9, 55.5, 9.7.

IR (thin film) 3510, 3446, 3052, 2999, 1695, 1607, 1507, 1246, 1174, 1123, 1028, 831, 733, 701 cm^{-1}.

HRMS (CI+) Calcd for $C_{21}H_{19}NO_2S$ (M^+): 349.1136, Found: 349.1144.



1d

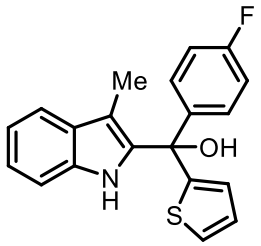
(3-Methyl-1*H*-indol-2-yl)(4-(methylthio)phenyl)(thiophen-2-yl)methanol (1d) was prepared as pale yellow foam from (4-(methylthio)phenyl)(thiophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 76% yield (2 steps, 0.830 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.72 (s, 1H), 7.49-7.37 (m, 5H), 7.24 (d, J = 8.4 Hz, 2H), 7.10-6.89 (m, 4H), 5.77 (s, 1H), 2.48 (s, 3H), 1.90 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 152.5, 143.6, 139.4, 138.9, 135.7, 130.7, 128.5, 127.2, 127.0, 126.4, 126.2, 122.2, 119.4, 119.0, 112.0, 108.0, 76.9, 15.3, 9.73.

IR (thin film) 3534, 3445, 3051, 2919, 1699, 1488, 1302, 1264, 994, 819, 732, 702 cm^{-1}.

HRMS (CI+) Calcd for $C_{21}H_{19}NOS_2$ (M^+): 365.0908, Found: 365.0901.



1e

(4-Fluorophenyl)(3-methyl-1*H*-indol-2-yl)(thiophen-2-yl)methanol (1e) was prepared as viscous yellow oil from (4-fluorophenyl)(thiophen-2-yl)methanone (2.5 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 41% yield (2 steps, 0.350 g).

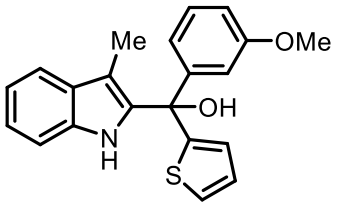
^{1}H NMR (400 MHz, acetone-d_6) δ 9.76 (s, 1H), 7.55-7.38 (m, 5H), 7.14-6.89 (m, 6H), 5.89 (s, 1H), 1.89 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 162.9 (d, J = 243.2 Hz), 152.4, 143.1 (d, J = 3.3 Hz), 139.3, 135.7, 130.6, 130.0 (d, J = 8.1 Hz), 127.3, 127.1, 126.5, 122.3, 119.4, 119.1, 115.2 (d, J = 21.3 Hz), 112.0, 108.0, 76.8, 9.6.

^{19}F NMR (376 MHz, acetone-d_6) δ -116.6.

IR (thin film) 3520, 3438, 3060, 2989, 1698, 1605, 1502, 1227, 1152, 999, 833, 746 cm^{-1}.

HRMS (CI+) Calcd for $C_{20}H_{16}FNOS$, (M^+): 337.0937, Found: 337.0939.



1f

(3-Methoxyphenyl)(3-methyl-1*H*-indol-2-yl)(thiophen-2-yl)methanol (1f) was prepared as slightly yellowish oil from (3-methoxyphenyl)(thiophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 81% yield (2 steps, 0.850 g).

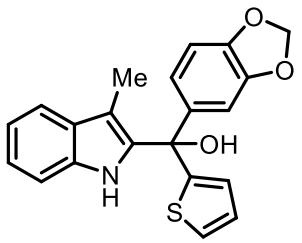
^{1}H NMR (400 MHz, acetone-d_6) δ 9.71 (s, 1H), 7.50-748 (m, 1H), 7.42-7.37 (m, 2H), 7.26 (t, J = 8.0 Hz, 1H), 7.15-6.91 (m, 5H), 6.92-6.86 (m, 2H), 5.78 (s, 1H), 3.73 (s, 3H), 1.92 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 160.3, 152.5, 148.5, 139.4, 135.7, 130.7, 129.7,

127.11, 127.07, 126.4, 122.2, 120.3, 119.4, 119.0, 114.0, 113.4, 112.0, 108.0, 77.1, 55.4, 9.7.

IR (thin film) 3363, 3056, 2998, 1701, 1590, 1441, 1243, 1143, 1036, 739 cm^{-1}.

HRMS (CI+) Calcd for $C_{21}H_{19}NO_2S$ (M^+): 349.1136, Found: 349.1131.



1g

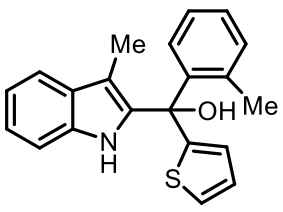
Benzo[*d*][1,3]dioxol-5-yl(3-methyl-1*H*-indol-2-yl)(thiophen-2-yl)methanol (1g) was prepared as slightly yellow gum-like liquid from benzo[*d*][1,3]dioxol-5-yl(thiophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 75% yield (2 steps, 0.820 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.70 (s, 1H), 7.52 (d, J = 7.9 Hz, 1H), 7.42-7.39 (m, 2H), 7.14-6.95 (m, 6H), 6.82 (d, J = 8.2 Hz, 1H), 5.98 (d, J = 0.9 Hz, 2H), 5.74 (s, 1H), 1.97 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 152.6, 148.3, 147.8, 141.0, 139.4, 135.6, 130.6, 127.1, 127.0, 126.3, 122.2, 121.5, 119.4, 119.0, 111.9, 108.6, 108.0, 107.9, 102.0, 77.0, 9.7.

IR (thin film) 3522, 3445, 3054, 2980, 1487, 1237, 1089, 932, 858, 731 cm^{-1}.

HRMS (CI+) Calcd for $C_{21}H_{17}NO_3S$ (M^+): 363.0929, Found: 363.0935.



1h

(3-Methyl-1*H*-indol-2-yl)(thiophen-2-yl)(*o*-tolyl)methanol (1h) was prepared as pale yellow foam from (*o*-tolyl)(thiophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 64% yield (2 steps,

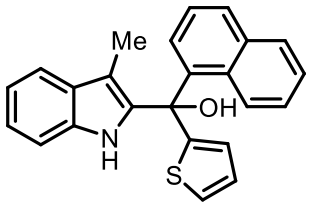
0.640 g).

^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.38 (s, 1H), 7.54 (d, J = 7.9 Hz, 1H), 7.38 (dd, J_1 = 5.1 Hz, J_2 = 1.2 Hz, 1H), 7.31-7.23 (m, 3H), 7.19-7.08 (m, 3H), 7.03-6.98 (m, 2H), 6.83 (dd, J_1 = 3.6 Hz, J_2 = 1.2 Hz, 1H), 3.38 (s, 1H), 2.20 (s, 3H), 1.86 (s, 3H).

^{13}C NMR (100 MHz, CD_2Cl_2) δ 150.9, 142.7, 138.2, 137.6, 134.6, 132.9, 130.2, 129.0, 128.8, 127.2, 126.7, 126.2, 125.8, 122.4, 119.5, 119.0, 111.2, 108.2, 78.5, 21.3, 9.0.

IR (thin film) 3531, 3448, 3054, 2919, 1455, 1265, 986, 838, 733, 702 cm^{-1}.

HRMS (CI+) Calcd for $C_{21}H_{19}NOS$ (M^+): 333.1187, Found: 333.1192.



1i

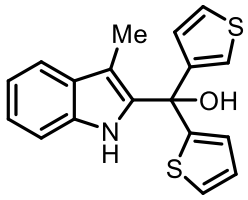
(3-Methyl-1*H*-indol-2-yl)(naphthalen-1-yl)(thiophen-2-yl)methanol (1i) was prepared as white solid from naphthalen-1-yl(thiophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 36% yield (2 steps, 0.398 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.98 (s, 1H), 8.43 (d, J = 8.8 Hz, 1H), 7.91 (d, J = 8.2 Hz, 2H), 7.48-7.36 (m, 5H), 7.24-7.20 (m, 2H), 7.15-7.11 (m, 1H), 7.06-7.02 (m, 3H), 6.13 (s, 1H), 1.68 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 153.1, 142.0, 139.7, 135.8, 135.6, 132.6, 130.7, 130.3, 129.2, 128.3, 127.5, 127.4, 126.7, 126.2, 126.1, 125.8, 125.2, 122.2, 119.4, 119.0, 112.0, 107.3, 78.6, 9.1.

IR (thin film) 3528, 3435, 3049, 2921, 1699, 1601, 1449, 1315, 1231, 1134, 980, 726 cm^{-1}.

HRMS (CI+) Calcd for $C_{24}H_{19}NOS$ (M^+): 369.1187, Found: 369.1172.



1j

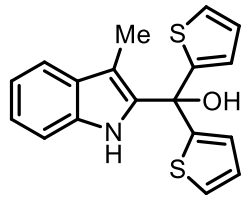
(3-Methyl-1*H*-indol-2-yl)(thiophen-2-yl)(thiophen-3-yl)methanol (1j) was prepared as slightly greenish gum-like liquid from thiophen-2-yl(thiophen-3-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 54% yield (2 steps, 0.530 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.78 (s, 1H), 7.50 (d, J = 7.9 Hz, 1H), 7.42-7.38 (m, 3H), 6.82 (dd, J_1 = 1.3 Hz, J_2 = 3.0 Hz, 1H), 7.19 (dd, J_1 = 1.3 Hz, J_2 = 5.1 Hz, 1H), 7.12-6.94 (m, 4H), 5.83 (s, 1H), 1.94 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 152.3, 148.6, 139.3, 135.5, 130.7, 128.4, 127.0, 126.5, 126.4, 126.2, 123.6, 122.2, 119.3, 119.0, 112.0, 107.3, 74.8, 9.4.

IR (thin film) 3438, 3101, 2976, 1699, 1514, 1415, 1228, 1128, 1003, 839, 732, 701 cm^{-1}.

HRMS (CI+) Calcd for $C_{18}H_{15}NOS_2$ (M^+): 325.0595, Found: 325.0609.



1k

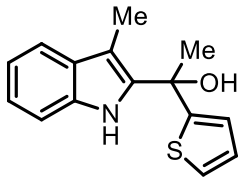
(3-Methyl-1*H*-indol-2-yl)di(thiophen-2-yl)methanol (1k) was prepared as slightly green foam from di(thiophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 32% yield (2 steps, 0.310 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.86 (s, 1H), 7.47 (d, J = 7.8 Hz, 1H), 7.42-7.39 (m, 3H), 7.08 (t, J = 7.1 Hz, 1H), 7.02-6.97 (m, 5H), 6.06 (s, 1H), 1.95 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 152.1, 139.4, 135.5, 130.7, 127.1, 126.8, 126.5, 122.4, 119.4, 119.1, 112.0, 107.7, 74.8, 9.7.

IR (thin film) 3528, 3443, 3096, 2918, 1691, 1456, 1324, 1301, 1233, 1115, 979, 838, 733, 700 cm^{-1}.

HRMS (CI+) Calcd for $C_{18}H_{15}NOS_2$ (M^+): 325.0595, Found: 325.0585.



1l

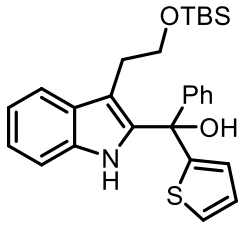
1-(3-Methyl-1*H*-indol-2-yl)-1-(thiophen-2-yl)ethan-1-ol (1l) was prepared as white solid from 1-(thiophen-2-yl)ethan-1-one (2 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 76% yield (2 steps, 0.392 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.88 (s, 1H), 7.48 (d, J = 7.8 Hz, 1H), 7.41 (d, J = 8.0 Hz, 1H), 7.33-7.31 (m, 1H), 7.10-7.06 (m, 3H), 6.93 (dd, J_1 = 3.6 Hz, J_2 = 5.0 Hz, 1H), 5.22 (s, 1H), 2.15 (s, 3H), 2.12 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 153.8, 140.5, 135.3, 130.9, 127.0, 125.6, 124.5, 121.7, 119.2, 118.7, 111.9, 105.6, 72.1, 31.1, 9.5.

IR (thin film) 3518, 3433, 3062, 2997, 1451, 1312, 1228, 901, 738, 698 cm^{-1}.

HRMS (CI+) Calcd for $C_{15}H_{15}NOS$ (M^+): 257.0874, Found: 257.0876.



1m

(3-(2-((*tert*-Butyldimethylsilyl)oxy)ethyl)-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (1m) was prepared as colorless oil from 1-(3-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-1*H*-indol-1-yl)-*N*,*N*-dimethylmethanamine (3 mmol) and phenyl(thiophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 66% yield (2 steps, 0.920 g).

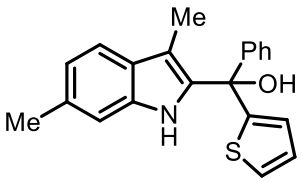
^{1}H NMR (400 MHz, acetone-d_6) δ 9.42 (s, 1H), 7.58-7.54 (m, 3H), 7.40-7.28 (m, 5H), 7.13-7.03 (m, 2H), 6.97 (dd, J_1 = 3.6 Hz, J_2 = 5.1 Hz, 1H), 6.86 (dd, J_1 = 1.2 Hz, J_2 = 3.6 Hz, 1H), 6.12 (s, 1H), 3.82 (t, J = 6.5 Hz, 2H), 2.97-2.78 (m, 2H), 0.86 (s, 9H), 0.01 (s, 6H).

^{13}C NMR (100 MHz, acetone-d_6) δ 152.9, 147.5, 141.2, 135.7, 129.7, 128.6, 128.2,

127.5, 127.2, 126.7, 126.2, 122.3, 119.7, 119.1, 112.3, 109.6, 77.0, 64.1, 28.5, 26.4, 19.0, -5.2.

IR (thin film) 3443, 3340, 3066, 1448, 1342, 1253, 1070, 898, 828, 732, 700 cm^{-1}.

HRMS (CI+) Calcd for $C_{27}H_{33}NO_2SSi$ (M^+): 463.2001, Found: 463.1992.



1n

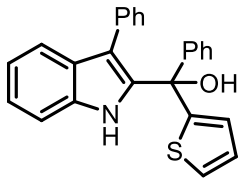
(3,6-Dimethyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (1n) was prepared as viscous brown oil from 1-(3,6-dimethyl-1*H*-indol-1-yl)- *N*,*N*-dimethylmethanamine (3 mmol) and phenyl(thiophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 39% yield (2 steps, 0.387 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.52 (s, 1H), 7.52-7.50 (m, 2H), 7.40-7.30 (m, 5H), 7.20 (s, 1H), 6.97 (dd, J_1 = 3.6 Hz, J_2 = 5.1 Hz, 1H), 6.89-6.87 (m, 2H), 5.73 (s, 1H), 2.41 (s, 3H), 1.86 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 152.7, 147.0, 138.8, 136.1, 131.5, 128.7, 128.6, 128.3, 127.9, 127.1, 127.0, 126.4, 121.3, 118.8, 111.9, 107.9, 77.2, 21.9, 9.7.

IR (thin film) 3521, 3439, 3026, 2919, 1625, 1450, 1323, 1230, 994, 749, 702 cm^{-1}.

HRMS (CI+) Calcd for $C_{21}H_{19}NOS$ (M^+): 333.1187, Found: 333.1175.



1o

Phenyl(3-phenyl-1*H*-indol-2-yl)(thiophen-2-yl)methanol (1o) was prepared as pale white solid from *N*,*N*-dimethyl-1-(3-phenyl-1*H*-indol-1-yl) methanamine (3 mmol) and phenyl(thiophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 54% yield (2 steps, 0.615 g).

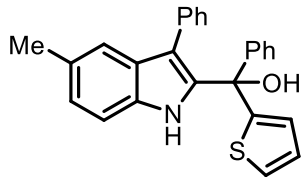
^{1}H NMR (400 MHz, acetone-d_6) δ 9.98 (s, 1H), 7.50-7.44 (m, 3H), 7.35 (d, J = 8.0

Hz, 1H), 7.28-7.10 (m, 10H), 7.05-7.02 (m, 1H), 6.81-6.79 (m, 1H), 6.76 (d, J = 3.5 Hz, 1H), 5.55 (s, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 152.1, 146.9, 139.1, 136.2, 135.6, 131.3, 130.3, 128.4, 128.3, 128.2, 128.1, 127.5, 126.9, 126.4, 126.1, 122.8, 120.2, 119.9, 115.7, 112.2, 77.8.

IR (thin film) 3517, 3430, 3044, 1599, 1481, 1328, 1241, 1025, 837, 936, 696 cm^{-1}.

HRMS (CI+) Calcd for $C_{25}H_{19}NOS$ (M^+): 381.1187, Found: 381.1176.



1p

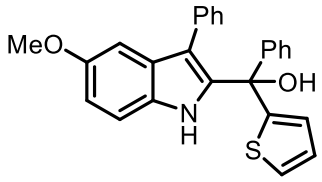
(5-Methyl-3-phenyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (1p) was prepared as pale white solid from *N*,*N*-dimethyl-1-(5-methyl-3-phenyl-1*H*-indol-1-yl)methanamine (3 mmol) and phenyl(thiophen-2-yl) methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 46% yield (2 steps, 0.513 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.88 (s, 1H), 7.42-7.39 (m, 2H), 7.35 (d, J = 8.3 Hz, 1H), 7.27 (dd, J_1 = 1.2 Hz, J_2 = 5.1 Hz, 1H), 7.24-7.19 (m, 3H), 7.13-7.06 (m, 6H), 6.98 (dd, J_1 = 1.3 Hz, J_2 = 8.3 Hz, 1H), 6.78 (dd, J_1 = 3.6 Hz, J_2 = 5.1 Hz, 1H), 6.71 (dd, J_1 = 1.2 Hz, J_2 = 3.6 Hz, 1H), 5.56 (s, 1H), 2.36 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 152.3, 147.0, 139.2, 136.5, 134.0, 131.4, 130.5, 129.1, 128.4, 128.3, 128.17, 128.16, 127.5, 126.9, 126.4, 126.1, 124.4, 119.4, 115.2, 112.0, 77.8, 21.6.

IR (thin film) 3515, 3434, 3045, 2920, 1600, 1480, 1270, 1027, 751, 699 cm^{-1}.

HRMS (CI+) Calcd for $C_{26}H_{21}NOS_2$ (M^+): 395.1344, Found: 395.1351.



1q

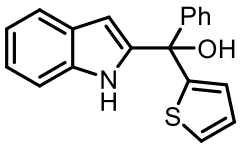
(5-Methoxy-3-phenyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (1q) was prepared as pale white solid from 1-(5-methoxy-3-phenyl-1*H*-indol-1-yl)-*N*,*N*-dimethylmethanamine (3 mmol) and phenyl(thiophen-2-yl) methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 20% yield (2 steps, 0.167 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.86 (s, 1H), 7.42-7.39 (m, 2H), 7.36 (dd, J_1 = 1.0 Hz, J_2 = 5.1 Hz, 1H), 7.28 (dd, J_1 = 1.2 Hz, J_2 = 5.1 Hz, 1H), 7.23-7.19 (m, 3H), 7.13-7.08 (m, 5H), 6.82-6.78 (m, 3H), 6.71 (dd, J_1 = 1.2 Hz, J_2 = 3.6 Hz, 1H), 5.55 (s, 1H), 3.69 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 155.3, 152.3, 147.0, 139.9, 136.4, 131.3, 130.7, 130.5, 129.5, 128.4, 128.3, 128.1, 127.5, 126.9, 126.4, 126.1, 115.5, 113.2, 113.0, 101.3, 77.8, 55.8.

IR (thin film) 3538, 3424, 3055, 2933, 1604, 1481, 1444, 1268, 1141, 836, 745, 698 cm^{-1}.

HRMS (CI+) Calcd for $C_{26}H_{21}NO_2S$ (M^+): 411.1293, Found: 411.1297.



1r

(1*H*-Indol-2-yl)(phenyl)(thiophen-2-yl)methanol (1r) At -78 °C, to a stirred solution of thiophene (0.277 g, 3.3 mmol) in THF (15 mL) was slowly added *n*-butyllithium (2.4 M in hexane, 1.4 mL, 3.3 mmol). The resulting mixture was then kept stirring at -20 °C for 1 h. Next, the mixture was slowly added to the solution of (1*H*-indol-2-yl)(phenyl)methanone (0.243 g, 1.1 mmol) in THF (10 mL) at -20 ºC. After that, the reaction mixture was warmed up and kept stirring overnight. A saturated aqueous solution of NH_4Cl was added to quench the reaction. The reaction mixture was extracted with EtOAc (3 × 30 mL). The combined organic layers were

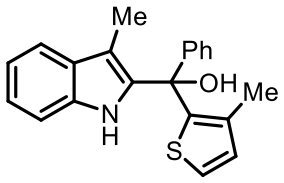
dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by silica gel flash chromatography to afford the product **1r** as yellow-green foam (eluent: hexanes/EtOAc = 10:1 → 5:1) in 95% yield (0.320 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.08 (s, 1H), 7.52-7.48 (m, 3H), 7.39 (d, J = 6.5 Hz, 2H), 7.35-7.27 (m, 3H), 7.10-7.06 (m, 1H), 7.00-6.96 (m, 2H), 6.88 (d, J = 3.4 Hz, 1H), 6.16 (s, 1H), 5.81 (s, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 152.7, 147.0, 144.8, 137.6, 128.5, 128.2, 127.6, 127.0, 126.8, 126.1, 122.4, 121.1, 120.0, 112.14, 112.09, 102.5, 77.0.

IR (thin film) 3520, 3410, 3051, 1442, 1282, 1133, 1133 1015, 733, 695 cm^{-1}.

HRMS (CI+) Calcd for $C_{19}H_{15}NOS$ (M^+): 305.0874, Found: 305.0881.



1s

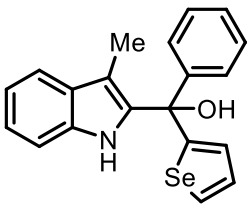
(3-Methyl-1*H*-indol-2-yl)(3-methylthiophen-2-yl)(phenyl)methanol (1s) was prepared as slightly yellowish foam from *N*,*N*-dimethyl-1-(3-methyl-1*H*-indol-1-yl)methanamine (3 mmol) and (3-methylthiophen-2-yl) (phenyl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 73% yield (2 steps, 0.730 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.70 (s, 1H), 7.57-7.50 (m, 3H), 7.40 (d, J = 8.0 Hz, 1H), 7.37-7.29 (m, 3H), 7.20 (d, J = 5.1 Hz, 1H), 7.12-7.01 (m, 2H), 6.89 (d, J = 5.1 Hz, 1H), 5.60 (s, 1H), 2.01 (s, 3H), 1.92 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.7, 144.1, 138.6, 136.7, 135.7, 132.5, 130.6, 128.5, 128.3, 128.0, 124.0, 122.1, 119.3, 119.0, 112.0, 107.9, 76.7, 15.3, 9.3.

IR (thin film) 3529, 3438, 3052, 2921, 1611, 1450, 1319, 1270, 981, 745 cm^{-1}.

HRMS (CI+) Calcd for $C_{21}H_{19}NOS$ (M^+): 333.1187, Found: 333.1189.



4a

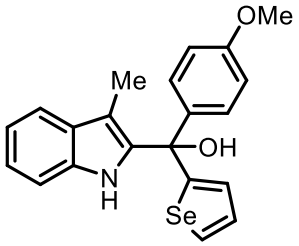
(3-Methyl-1*H*-indol-2-yl)(phenyl)(selenophen-2-yl)methanol (4a) was prepared as slightly yellow foam from phenyl(selenophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 81% yield (2 steps, 0.89 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.70 (s, 1H), 8.15-8.01 (m, 1H), 7.53-7.45 (m, 3H), 7.38-7.30 (m, 4H), 7.20 (dd, J_1 = 3.8 Hz, J_2 = 5.6 Hz, 1H), 7.09-7.05 (m, 1H), 7.01-6.98 (m, 2H), 5.82 (s, 1H), 1.89 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 160.3, 147.1, 139.6, 135.7, 131.8, 130.7, 129.8, 128.7, 128.7, 128.3, 127.9, 122.2, 119.4, 119.0, 112.0, 107.9, 78.7, 9.8.

IR (thin film) 3568, 3447, 3053, 1486, 1451, 1325, 1264, 1232, 994, 842, 731, 694 cm^{-1}.

HRMS (CI+) Calcd for $C_{20}H_{17}NOSe$ (M^+): 367.0475, Found: 367.0464.



4b

(4-Methoxyphenyl)(3-methyl-1*H*-indol-2-yl)(selenophen-2-yl)methanol (4b) was prepared as slightly yellow foam from (4-methoxyphenyl)(selenophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 68% yield (2 steps, 0.81 g).

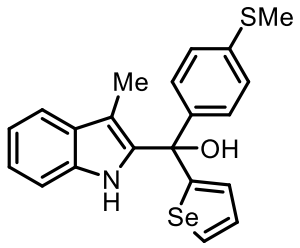
^{1}H NMR (400 MHz, acetone-d_6) δ 9.70 (s, 1H), 8.12-8.00 (m, 1H), 7.49-7.38 (m, 4H), 7.21-7.00 (m, 4H), 6.89 (d, J = 8.8 Hz, 2H), 5.74 (s, 1H), 3.78 (s, 3H), 1.93 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 160.7, 160.0, 139.8, 139.1, 135.6, 131.6, 130.7, 129.7, 129.3, 128.4, 122.1, 119.3, 119.0, 113.9, 112.0, 107.7, 78.4, 55.5, 9.9.

IR (thin film) 3446, 3051, 2921, 1607, 1506, 1454, 1300, 1251, 1175, 1028, 988, 831,

732, 694 cm^{-1}.

HRMS (CI+) Calcd for $C_{21}H_{19}NO_2Se$ (M^+): 397.0581, Found: 397.0578.



4c

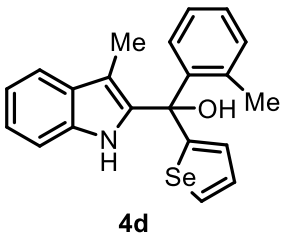
(3-Methyl-1*H*-indol-2-yl)(4-(methylthio)phenyl)(selenophen-2-yl)methanol (4c) was prepared as slightly yellow foam from (4-(methylthio)phenyl)(selenophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 67% yield (2 steps, 0.83 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.71 (s, 1H), 8.13-8.00 (m, 1H), 7.49-7.45 (m, 3H), 7.39 (d, J = 8.0 Hz, 1H), 7.25-7.19 (m, 3H), 7.11-7.00 (m, 3H), 5.83 (s, 1H), 2.48 (s, 3H), 1.95 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 160.2, 143.8, 139.4, 138.9, 135.6, 131.8, 130.7, 129.8, 128.6, 128.5, 126.2, 122.2, 119.4, 119.0, 112.0, 107.9, 78.4, 15.24, 9.9.

IR (thin film) 3514, 3441, 3050, 2918, 1693, 1487, 1450, 1325, 1260, 1121, 1001, 821, 732, 694 cm^{-1}.

HRMS (CI+) Calcd for $C_{21}H_{19}NOSSe$ (M^+): 413.0353, Found: 413.0363.



4d

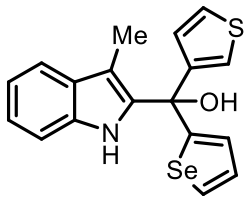
(3-Methyl-1*H*-indol-2-yl)(selenophen-2-yl)(*o*-tolyl)methanol (4d) was prepared as slightly yellow foam from (*o*-tolyl)(selenophen-2-yl)methanone (2.5 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 65% yield (2 steps, 0.62 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.79 (s, 1H), 8.09-8.07 (m, 1H), 7.47 (d, J = 7.8 Hz, 1H), 7.41 (d, J = 8.0 Hz, 1H), 7.25-7.18 (m, 3H), 7.12-7.00 (m, 5H), 5.75 (s, 1H), 2.20 (s, 3H), 1.81 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 160.7, 144.1, 139.6, 139.1, 135.6, 132.9, 131.6, 130.7, 130.0, 129.2, 128.9, 128.2, 125.8, 122.1, 119.4, 119.0, 112.0, 106.6, 79.6, 21.5, 9.3.

IR (thin film) 3528, 3442, 3053, 2972, 1453, 1323, 1300, 1265, 1137, 984, 842, 735, 693 cm^{-1}.

HRMS (CI+) Calcd for $C_{21}H_{19}NOSe$ (M^+): 381.0632, Found: 381.0631.



4e

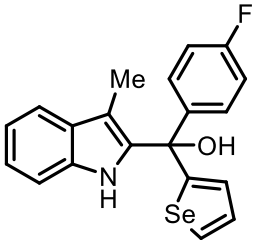
(3-Methyl-1*H*-indol-2-yl)(selenophen-2-yl)(thiophen-3-yl)methanol (4e) was prepared as slightly green liquid from selenophen-2-yl(thiophen-3-yl) methanone (2.5 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 60% yield (2 steps, 0.56 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.77 (s, 1H), 8.06-8.05 (m, 1H), 7.49 (d, J = 7.9 Hz, 1H), 7.42-7.37 (m, 2H), 7.27-7.00 (m, 6H), 5.87 (s, 1H), 1.96 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 159.9, 148.7, 139.4, 135.5, 131.6, 130.7, 129.6, 128.4, 128.1, 126.5, 123.7, 122.2, 119.3, 119.0, 112.0, 107.3, 76.2, 9.6.

IR (thin film) 3437, 3050, 2918, 1691, 1452, 1327, 1228, 1002, 840, 734, 691 cm^{-1}.

HRMS (CI+) Calcd for $C_{18}H_{15}NOSSe$ (M^+): 373.0040, Found: 373.0042.



4f

(4-Fluorophenyl)(3-methyl-1*H*-indol-2-yl)(selenophen-2-yl)methanol (4f) was prepared as slightly green viscous oil from (4-fluorophenyl)(selenophen-2-yl)methanone (2.5 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 48% yield (2 steps, 0.460 g).

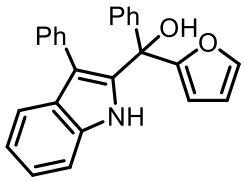
^{1}H NMR (400 MHz, acetone-d_6) δ 9.75 (s, 1H), 8.09-8.07 (m, 1H), 7.58-7.55 (m, 2H), 7.50 (d, J = 7.8 Hz, 1H), 7.39 (d, J = 8.0 Hz, 1H), 7.22-7.01 (m, 6H), 5.95 (s, 1H), 1.94 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 162.9 (d, J = 243.0 Hz), 160.1, 143.3 (d, J = 2.9 Hz), 139.3, 135.6, 131.9, 130.6, 130.0 (d, J = 8.3 Hz), 129.9, 128.7, 122.3, 119.4, 119.1, 115.3 (d, J = 21.3 Hz), 112.0, 108.0, 78.2, 9.9.

^{19}F NMR (376 MHz, acetone-d_6) δ -116.6.

IR (thin film) 3523, 3440, 3054, 2999, 1600, 1502, 1452, 1320, 1227, 996, 832, 751, 694 cm^{-1}.

HRMS (CI+) Calcd for $C_{20}H_{16}FNOSe$ (M^+): 385.0381, Found: 385.0392.



6

Furan-2-yl(phenyl)(3-phenyl-1*H*-indol-2-yl)methanol (6) At -78 °C, to a stirred solution of furan (0.204 g, 3 mmol) in THF (15 mL) was slowly added *tert*-butyllithium (1.3 M in pentane, 2.3 mL, 3 mmol). The resulting mixture was slowly warmed up to 0 °C and kept stirring at the same temperature for 1 h. Next, a solution of phenyl(3-phenyl-1*H*-indol-2-yl)methanone (0.357 g, 1.2 mmol) in THF (5 mL) was slowly added to the reaction mixture at 0 ºC. After that, the reaction mixture was warmed up to room temperature and kept stirring overnight. A saturated aqueous solution of NH_4Cl was added to quench the reaction. The reaction mixture was extracted with EtOAc (3 × 30 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by silica gel flash chromatography to afford the product as yellowish foam (eluent: hexanes/EtOAc = 30:1 → 20:1) in 94% yield (0.410 g).

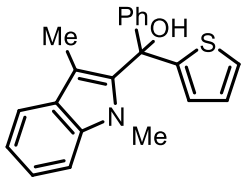
^{1}H NMR (400 MHz, acetone-d_6) δ 10.01 (s, 1H), 7.49 (d, J = 8.1 Hz, 1H), 7.43-7.40

(m, 2H), 7.32-7.21 (m, 5H), 7.17-7.10 (m, 6H), 7.03-6.99 (m, 1H), 6.16 (dd, J_1 = 1.8 Hz, J_2 = 3.2 Hz, 1H), 5.91 (d, J = 3.2 Hz, 1H), 5.61 (s, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 157.7, 145.0, 143.1, 137.8, 136.0, 135.8, 131.2, 130.2, 128.35, 128.30, 128.2, 128.0, 126.4, 122.7, 120.1, 119.8, 115.8, 112.1, 110.7, 110.1, 75.3.

IR (thin film) 3536, 3432, 3050, 1602, 1489, 1444, 1321, 1259, 1007, 741, 697 cm^{-1}.

HRMS (CI+) Calcd for $C_{25}H_{19}NO_2$ (M^+): 365.1416, Found: 365.1401.



1a'

(1,3-Dimethyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (1a') At -78 °C, to a stirred solution of 1,3-dimethyl-1*H*-indole (0.363 g, 2.5 mmol) in THF (20 mL) was slowly added *tert*-butyllithium (1.3 M in pentane, 1.9 mL, 2.5 mmol). The resulting mixture was slowly warmed up to 0 °C and kept stirring at the same temperature for 1 h. Next, a solution of phenyl(thiophen-2-yl)methanone (0.470 g, 2.5 mmol) in THF (5 mL) was slowly added to the reaction mixture at 0 ºC. After that, the reaction mixture was warmed up to room temperature and kept stirring overnight. A saturated aqueous solution of NH_4Cl was added to quench the reaction. The reaction mixture was extracted with EtOAc (3 × 30 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by silica gel flash chromatography to afford the product as slightly purple foam (eluent: hexanes/EtOAc = 40:1 → 20:1) in 41% yield (0.340 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.50 (d, J = 7.8 Hz, 1H), 7.46-7.44 (m, 3H), 7.40-7.33 (m, 3H), 7.28 (d, J = 8.3 Hz, 1H), 7.20-7.16 (m, 1H), 7.06-7.02 (m, 1H), 6.98 (dd, J_1 = 3.6 Hz, J_2 = 5.1 Hz, 1H), 6.78 (dd, J_1 = 1.2 Hz, J_2 = 3.6 Hz, 1H), 5.99 (s, 1H), 3.57 (s, 3H), 1.57 (s, 3H).

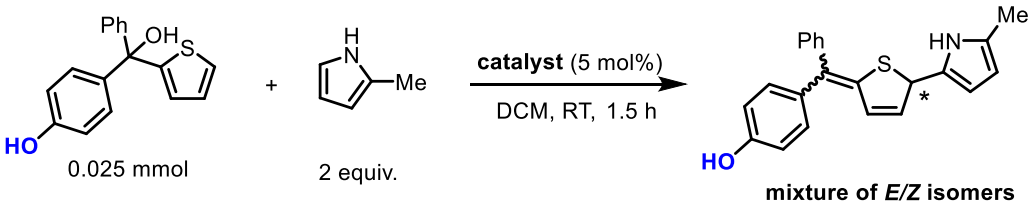
^{13}C NMR (100 MHz, acetone-d_6) δ 153.5, 147.2, 138.41, 138.38, 129.4, 128.9, 128.4, 127.6, 127.3, 127.2, 126.6, 122.9, 119.4, 119.3, 110.3, 109.6, 77.7, 32.8, 9.1.

IR (thin film) 3520, 3050, 1602, 1465, 1353, 1238, 1142, 996, 839, 733, 704 cm^{-1}.

HRMS (CI+) Calcd for $C_{21}H_{19}NOS$ (M^+): 333.1187, Found: 333.1187.

III. Condition Optimization

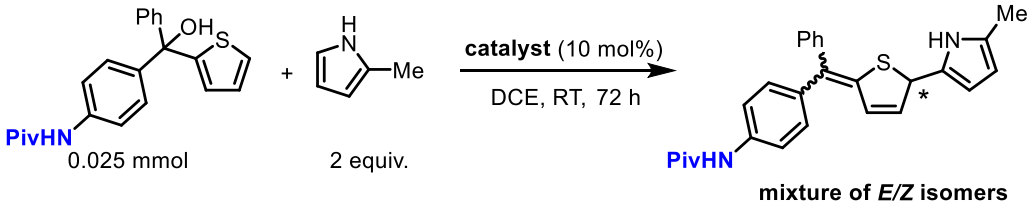
Supplementary Table 1. Initial condition study with *para*-quinone methide as intermediate[a]



Entry	Catalyst	Conv.(%)	Major		Minor		Ratio
			yield(%)	ee(%)	yield(%)	ee(%)	
1	(*R*)-BINOL-TRIP-OH	>95	47	7	23	22	2:1
2	(*R*)-8H-BINOL-TRIP-OH	94	46	10	25	23	1.8:1
3	(*R*)-SPINOL-TRIP-OH	39	12	7	9	11	1.3:1
4	(*R*)-BINOL-TRIP-NHTf	84	47	1	28	5	1.7:1
5	(*rac*-)-BINOL-H-OH	100	rt	-	-	-	-

[a] Reaction conditions: tertiary alcohol (0.025 mmol), 2-methylpyrrole (2 equiv.), catalyst (5 mol%), DCM (0.5 mL). Yield is based on analysis of the ^{1}H NMR spectrum of the crude reaction mixture using 1,3,5-triisopropylbenzene as an internal standard.

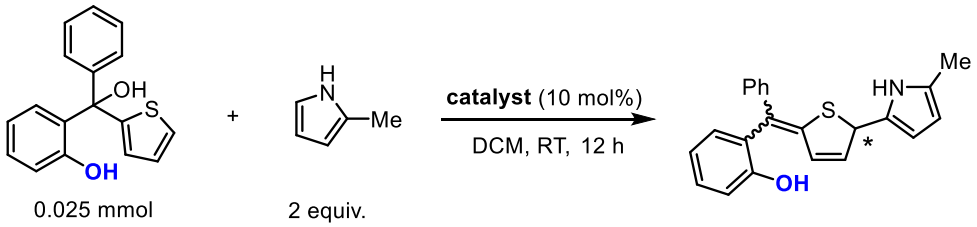
Supplementary Table 2. Initial condition study with aza-*para*-quinone methide as intermediate[a]



Entry	Catalyst	Conv.(%)	Major(%)	Minor(%)	Ratio
1	(*R*)-BINOL-TRIP-OH	>95	48	53	1.1:1
2	(*R*)-8H-BINOL-TRIP-OH	95	32	35	1.1:1
3	(*R*)-SPINOL-TRIP-OH	31	18	15	1.2:1
4	(*R*)-8H-BINOL-TRIP-NHTf	62	29	28	1:1

[a] Reaction conditions: tertiary alcohol (0.025 mmol), 2-methylpyrrole (2 equiv.), catalyst (5 mol%), DCE (0.5 mL). [b] Yield is based on analysis of the ^{1}H NMR spectrum of the crude reaction mixture using 1,3,5-triisopropylbenzene as an internal standard.

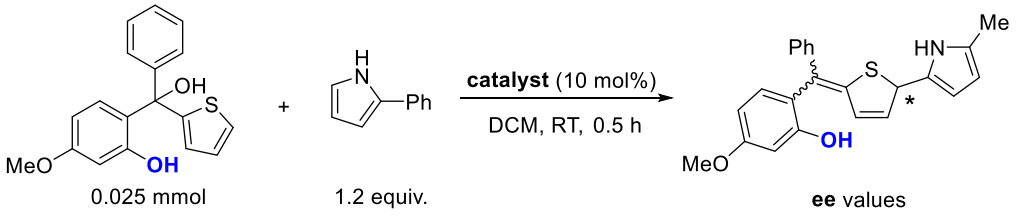
Supplementary Table 3. Initial condition study with *ortho*-quinone methide as intermediate[a]

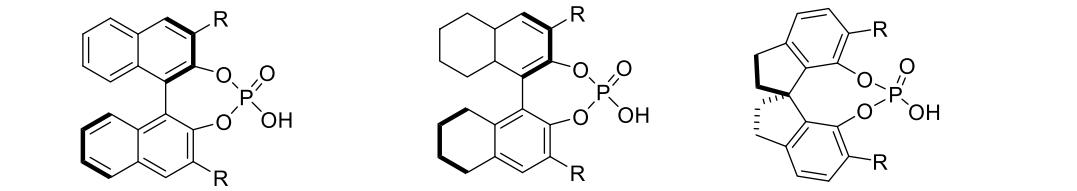


Entry	Catalyst	Conv.(%)	Yield	*E/Z (or Z/E)*	ee
1	(*R*)-BINOL-1-TRIP-OH	100	98	>20/1	28
2	(*R*)-BINOL-2,6-(^{i}Pr)$_2$-4-Ad-C$_6$H$_2$-OH	100	79	12.6/1	0
3	(*R*)-BINOL-2,4,6-Cy$_3$-C$_6$H$_2$-OH	91	96	>20/1	11
4	(*R*)-BINOL-SiPh$_3$-OH	93	95	>20/1	21
5	(*R*)-BINOL-2,6-Me$_2$-4-OMe-C$_6$H$_2$-OH	>95	90	12.6/1	-1
6	(*R*)-BINOL-C$_6$F$_5$-OH	100	69	4/1	7
7	(*S*)-BINOL-1-Nap-OH	100	76	7/1	-8
8	(*S*)-BINOL-9-Phen-OH	100	74	5.6/1	-5
9	(*R*)-BINOL-9-An-OH	100	82	12.71	-1
10	(*R*)-BINOL-1-Pyrene-OH	100	83	4.7/1	6

[a] Reaction conditions: tertiary alcohol (0.025 mmol), 2-methylpyrrole (2 equiv.), catalyst (10 mol%), DCM (0.5 mL). Yield is based on analysis of the ^{1}H NMR spectrum of the crude reaction mixture using 1,3,5-triisopropylbenzene as an internal standard.

Supplementary Table 4. Initial condition study with *ortho*-quinone methide as intermediate[a]





(*R*)-**A1**: R = 1-Ph, **-9%**
(*R*)-**A2**: R = 2,4,6-(*i*Pr)$_3$C$_6$H$_2$, **-32%**
(*S*)-**A3**: R = 1-Nap, **4%**
(*R*)-**A4**: R = 9-anthryl, **-41%**
(*S*)-**A5**: R = 9-phenanthryl, **22%**

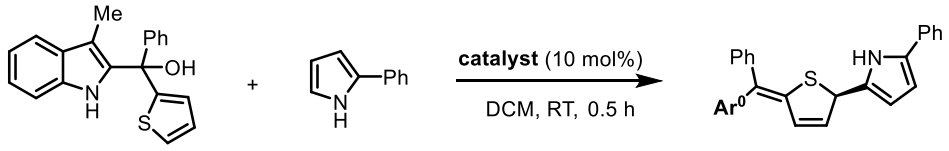
(*R*)-**B1**: R = 2,4,6-(*i*Pr)$_3$C$_6$H$_2$, **-54%**
(*R*)-**B3**: R = 1-Nap, **-6%**
(*R*)-**B4**: R = 9-anthryl, **-31%**
(*R*)-**B5**: R = 9-phenanthryl, **-27%**

(*R*)-**C1:** R = 2,4,6-(iP*r*)3C$_6$H$_2$, **-8%**
(*S*)-**C2:** R = 1-Nap, **-70%**
(*R*)-**C3:** R = 9-anthryl, **75%**
(*R*)-**C4:** R = 9-phenanthryl, **77%**

Entry	Catalyst	Conv.(%)	Yield (%)	*Z*/*E* (*E*/*Z*)	ee
1	(*R*)-BINOL-1-Ph-C$_6$H$_4$OH	63	39	6.3/1	-9
2	(*R*)-BINOL-TRIP-OH	100	79	8/1	-30
3	(*S*)-BINOL-1-Nap-OH	100	71	3.5/1	4
4	(*R*)-BINOL-9-An-OH	100	89	9.5/1	-41
5	(*S*)-BINOL-9-Phen-OH	100	70	3.5/1	22
6	(*R*)-8H-BINOL-TRIP-OH	50	46	9.5/1	-54
7	(*R*)-8H-BINOL-1-Nap-OH	100	86	3.5/1	-6
8	(*R*)-8H-BINOL-9-An-OH	100	96	10.8/1	-31
9	(*R*)-8H-BINOL-9-Phen-OH	100	92	9.2/1	-27
10	(*R*)-SPINOL-TRIP-OH	30	14	2.4/1	8
11	(*S*)-SPINOL-1-Nap-OH	82	68	11.2/1	-70
12	(*R*)-SPINOL-9-An-OH	100	74	11.8/1	75
13	(*R*)-SPINOL9-Phen-OH	100	91	11.8/1	77

[a] Reaction conditions: tertiary alcohol (0.025 mmol), 2-phenylpyrrole (1.2 equiv.), catalyst (10 mol%), DCM (0.5 mL). Yield is based on analysis of the ^{1}H NMR spectrum of the crude reaction mixture using 1,3,5-triisopropylbenzene as an internal standard.

Supplementary Table 5. Catalyst screening of the reaction of **1a** and **2a**[a]

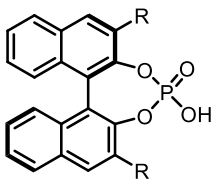


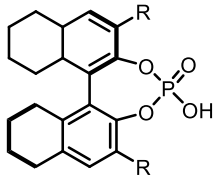
1a 0.025 mmol

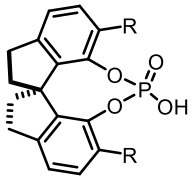
2a 1.2 equiv.

Ar^0 = 2-(3-methyl)indolyl

3a





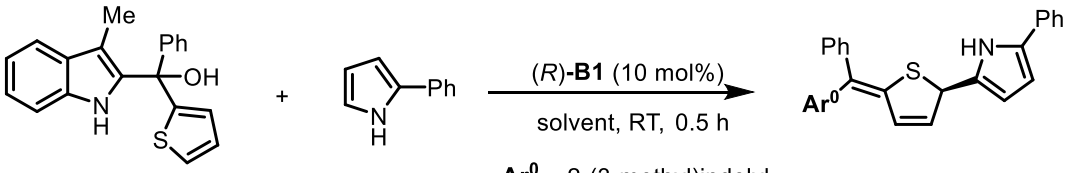


	(*ee*)				
(*R*)-**A1**: R = 2,4,6-(*i*Pr)$_3$C$_6$H$_2$,	**83%**	(*R*)-**B1**: R = 2,4,6-(*i*Pr)$_3$C$_6$H$_2$,	**84%**	(*R*)-**C1:** R = 2,4,6-(i**P***r*)$_3$C$_6$H$_2$,	**-77%**
(*R*)-**A2**: R = 2,6-(*i*Pr)$_2$-4-AdC$_6$H$_2$,	**80%**	(*R*)-**B2**: R = 2,4,6-Cy$_3$C$_6$H$_2$,	**85%**	(*S*)-**C2**: R = 2,4,6-Cy$_3$C$_6$H$_2$,	**44%**
(*R*)-**A3**: R = 2,4,6-Cy$_3$C$_6$H$_2$,	**79%**	(*R*)-**B3**: R = 1-Nap,	**33%**	(*R*)-**C3:** R = 1-Nap,	**-26%**
(*S*)-**A4**: R = 1-Nap,	**-11%**	(*R*)-**B4**: R = 9-anthryl,	**17%**	(*S*)-**C4:** R = 9-anthryl,	**72%**
(*R*)-**A5**: R = 9-anthryl,	**34%**	(*R*)-**B5**: R = 9-phenanthryl,	**22%**	(*S*)-**C5:** R = 9-phenanthryl,	**25%**
(*S*)-**A6**: R = 9-phenanthryl,	**-5%**			(*R*)-**C6:** R = SiPh$_3$	**-20%**
(*R*)-**A7:** R = SiPh$_3$	**58%**				

Entry	Catalyst	Conv.(%)	Yield (%)	*Z*/*E* (*E*/*Z*)	ee (%)
1	(*R*)-BINOL-TRIP-OH	100	85	20.3/1	83.2
2	(*R*)-BINOL-2,6-(i*Pr*)2_4-AdC$_6$H$_2$-OH	100	89	23.1/1	80.2
3	(*R*)-BINOL-2,4,6-Cy$_3$C$_6$H$_2$-OH,	100	92	25.2/1	78.5
4	(*S*)-BINOL-1-Nap-OH	98	88	6/1	-11.3
5	(*R*)-BINOL-9-An-OH	100	80	17.7/1	34.4
6	(*S*)-BINOL-9-Phen-OH	100	68	8.3/1	-4.6
7	(*R*)-BINOL-SiPh$_3$-OH	94	90	27.3/1	57.8
8	(*R*)-8H-BINOL-TRIP-OH	98	94	30/1	84.3
9	(*R*)-8H-BINOL-2,4,6-Cy$_3$C$_6$H$_2$-OH,	93	91	28.1/1	84.6
10	(*R*)-8H-BINOL-1-Nap-OH	100	86	6.3/1	32.6
11	(*R*)-8H-BINOL-9-An-OH	100	81	18.4/1	17.1
12	(*R*)-8H-BINOL-9-Phen-OH	95	85	23.4/1	21.5
13	(*R*)-SPINOL-TRIP-OH	37	32	6.3/1	-76.6
14	(*S*)-SPINOL-2,4,6-Cy$_3$C$_6$H$_2$-OH,	18	17	3.5/1	43.5
15	(*R*)-SPINOL-1-Nap-OH	100	82	20/1	-25.7
16	(*S*)-SPINOL-9-An-OH	100	82	17.7/1	72.4
17	(*S*)-SPINOL9-Phen-OH	100	62	14/1	24.6
18	(*R*)-SPINOL-SiPh$_3$-OH	36	36	8.4/1	-19.8

[a] Reaction conditions: tertiary alcohol (0.025 mmol), 2-phenylpyrrole (1.2 equiv.), catalyst (10 mol%), DCM (0.5 mL). Yield is based on analysis of the ^{1}H NMR spectrum of the crude reaction mixture using 1,3,5-triisopropylbenzene as an internal standard.

Supplementary Table 6. Solvent screening of the reaction of **1a** and **2a** by using (*R*)-8H-BINOL-TRIP-OH as the catalyst[a]



1a 0.025 mmol

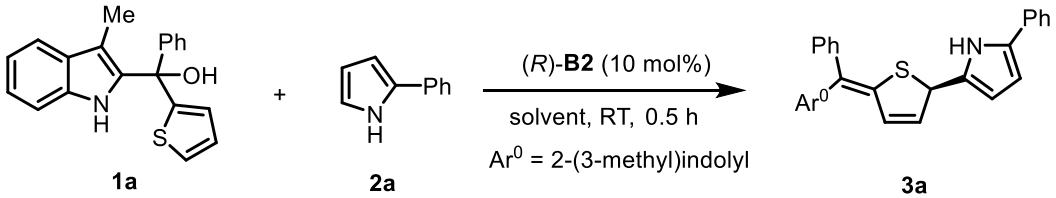
2a 1.2 equiv.

3a

Entry	Solvent	Conv.(%)	Yield (%)	*E*/*Z*	Ee (%)
1	DCM	100	91	>20/1	86
2	DCE	100	94	>20/1	77
3	$CHCl_3$	76	73	17.3/1	79
4	***toluene***	***91***	***87***	>20/1	***88***
5	$PhCF_3$	100	93	>20/1	83
6	PhF	100	87	18.4/1	86
7	CCl_4	100	>99	>20/1	81
8	Et_2O	100	91	9.6/1	(<80)
9	***PhCl***	***100***	***>99***	>20/1	***87***
10	EtOAc	100	90	13.1/1	74

[a] Reaction conditions: tertiary alcohol (0.025 mmol), 2-phenylpyrrole (1.2 equiv.), catalyst (10 mol%), solvent (0.5 mL). Yield is based on analysis of the ^{1}H NMR spectrum of the crude reaction mixture using 1,3,5-triisopropylbenzene as an internal standard.

Supplementary Table 7. Solvent screening of the reaction of **1a** and **2a** by using (*R*)-8H-BINOL-2,4,6-$Cy_3C_6H_2$-OH as the catalyst[a]

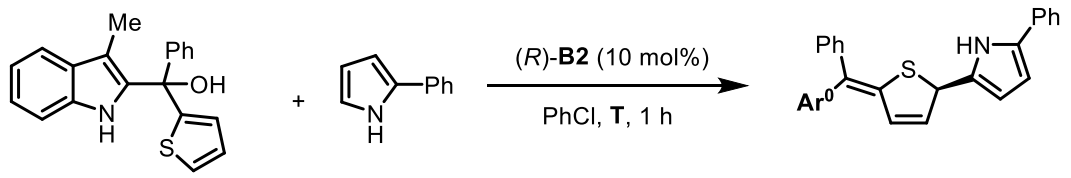


1a 0.025 mmol | **2a** 1.2 equiv. | **3a**

Entry	Solvent	Conv.(%)	Yield (%)	*E*/*Z*	Ee (%)
1	DCM	97	93	>20/1	84
2	DCE	87	88	>20/1	76
3	$CHCl_3$	85-90	83	20/1	85
4	toluene	98	95	>20/1	88
5	$PhCF_3$	100	91	>20/1	89 (88)
6	PhF	100	98	>20/1	88
7	CCl_4	100	96	>20/1	85
8	Et_2O	50-60	47	9.3/1	82
9	PhCl	100	>99	>20/1	>90 (89)
10	EtOAc	24	26	>20/1	86

[a]Reaction conditions: tertiary alcohol (0.025 mmol), 2-phenylpyrrole (1.2 equiv.), catalyst (10 mol%), solvent (0.5 mL). Yield is based on analysis of the ^{1}H NMR spectrum of the crude reaction mixture using 1,3,5-triisopropylbenzene as an internal standard.

Supplementary Table 8. Reaction temperature screening of the reaction of **1a** and **2a**[a]

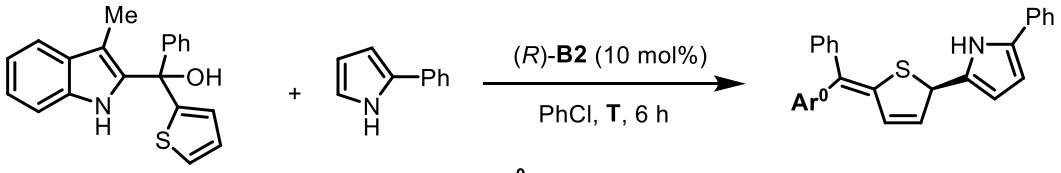


1a 0.025 mmol | **2a** 1.2 equiv. | **Ar^0** = 2-(3-methyl)indolyl | **3a**

Entry	T (°C)	Conv.(%)	Yield (%)	*E*/*Z*	Ee (%)
1	40	100	69	>20/1	81
2	rt	100	99	>20/1	88
3	0	97	96	>20/1	93
4	-20	79	88	>20/1	95

[a] Reaction conditions: tertiary alcohol (0.025 mmol), 2-phenylpyrrole (1.2 equiv.), catalyst (10 mol%), PhCl (0.5 mL). Yield is based on analysis of the ^{1}H NMR spectrum of the crude reaction mixture using 1,3,5-triisopropylbenzene as an internal standard.

Supplementary Table 9. Reaction temperature screening of the reaction of **1a** and **2a**[a]



1a 0.025 mmol

2a 1.2 equiv.

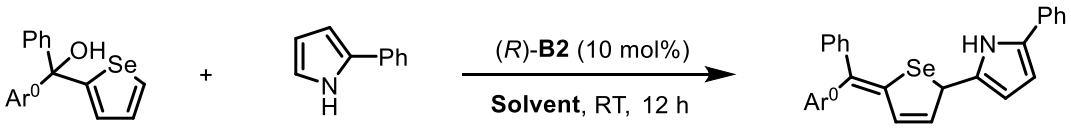
Ar^0 = 2-(3-methyl)indolyl

3a

Entry	T (°C)	Conv.(%)	Yield	*E/Z*	Ee (%)
1	0	100	98	>20/1	93
2	-20	100	>99	>20/1	95
3	***-40***	***100***	***>99***	***>20/1***	***96***

[a] Reaction conditions: tertiary alcohol (0.025 mmol), 2-phenylpyrrole (1.2 equiv.), catalyst (10 mol%), PhCl (0.5 mL). Yield is based on analysis of the ^{1}H NMR spectrum of the crude reaction mixture using 1,3,5-triisopropylbenzene as an internal standard.

Supplementary Table 10. Solvent screening of the reaction of **4a** and **2a**[a]



4a 0.025 mmol

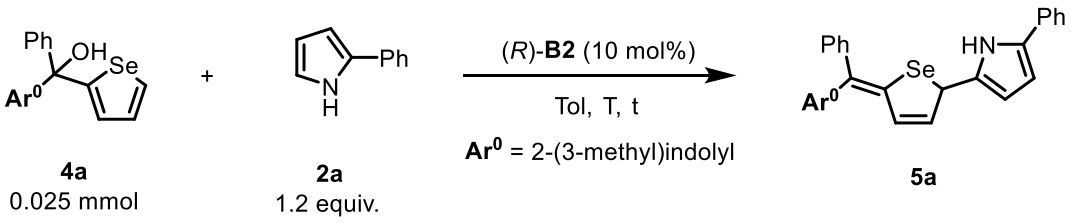
2a 1.2 equiv.

5a

Entry	Solvent	Conv.(%)	Yield (%)	*E/Z*	ee (%)
1	DCM	100	84	>20/1	80
2	DCE	100	96	>20/1	73
3	$CHCl_3$	100	91	>20/1	78
4	toluene	100	99	>20/1	90
5	$PhCF_3$	100	89	>20/1	89
6	PhF	100	90	>20/1	86
7	CCl_4	96	86	>20/1	90
8	Et_2O	44	44	>20/1	83
9	PhCl	100	97	>20/1	86
10	EtOAc	68	76	>20/1	76

[a] Reaction conditions: tertiary alcohol (0.025 mmol), 2-phenylpyrrole (1.2 equiv.), catalyst (10 mol%), solvent (0.5 mL). Yield is based on analysis of the ^{1}H NMR spectrum of the crude reaction mixture using 1,3,5-triisopropylbenzene as an internal standard.

Supplementary Table 11. Reaction temperature screening of the reaction of **4a** and **2a**[a]



4a 0.025 mmol

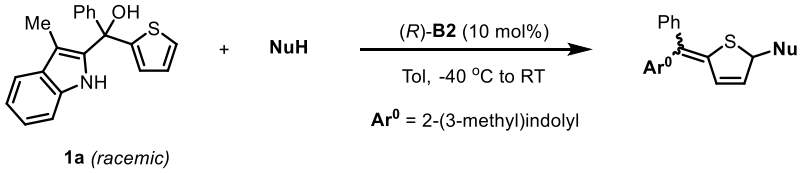
2a 1.2 equiv.

5a

Entry	T (°C)	t (h)	Conv.(%)	Yield (%)	*E*/*Z*	ee (%)
1	40	4	100	99	>20/1	86
2	rt	12	100	99	>20/1	90
3	0	48	100	97	>20/1	94
4	-20	48	100	98	>20/1	94
5	-40	48	72	70	>20/1	93

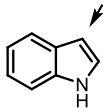
[a] Reaction conditions: tertiary alcohol (0.025 mmol), 2-phenylpyrrole (1.2 equiv.), catalyst (10 mol%), toluene (0.5 mL). Yield is based on analysis of the ^{1}H NMR spectrum of the crude reaction mixture using 1,3,5-triisopropylbenzene as an internal standard.

Supplementary Table 12. The reaction of **1a** and other nucleophiles[a]

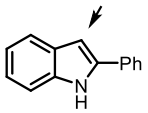


1a *(racemic)*

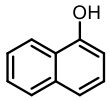
NuH:



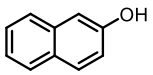
-20 °C, 12 h
90% yield,
E/*Z* or *Z*/*E*: 1.3/1
major: 42% ee
minor: 69% ee



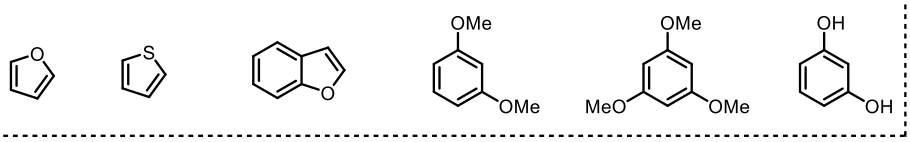
-40 °C, 12 h
90% yield,
E/*Z* or *Z*/*E*: 3/1
major: 28% ee
minor: uncertain



-20 °C, 24 h
messy



0 °C, 24 h
messy

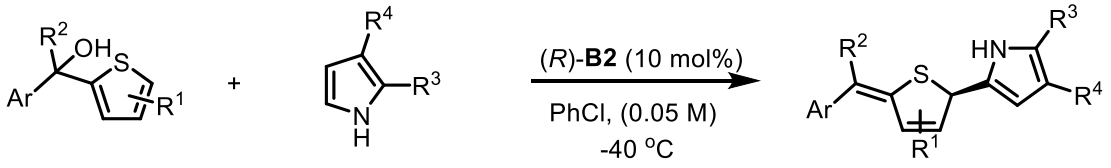


No desired product detected (-20 °C, NR; RT, substrate decomposed)

[a] Reaction conditions: **1a** (0.025 mmol), NuH (1.2 equiv.), (*R*)-**B2** (10 mol%), toluene (0.5 mL). Yield is based on analysis of the 1H NMR spectroscopy of the crude reaction mixture using 1,3,5-triisopropylbenzene as an internal standard.

IV. Dearomatization of Thiophenes and Selenophenes

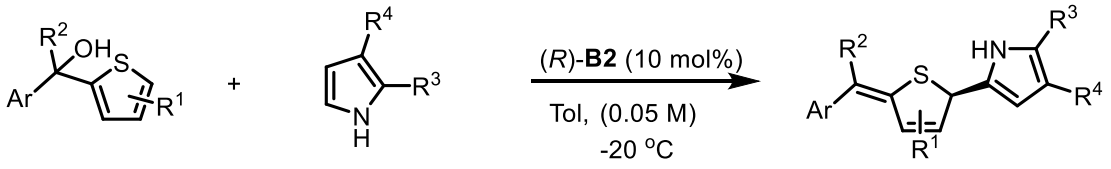
General Procedure B.



1 0.2 mmol + **2** 1.2 equiv. → **3**

At -40 °C, to an oven-dried 8-mL vial charged with a solution of the tertiary alcohol **1** (0.2 mmol) and pyrrole **2** (0.24 mmol) in PhCl (3.6 mL) was slowly added a solution of catalyst (*R*)-**B2** (20 mg, 0.015 mmol, 10 mol%) in PhCl (0.4 mL). The reaction mixture was stirred at the same temperature for 12 h. After that, triethylamine (2 drops) was added to quench the reaction. The mixture was concentrated under reduced pressure and purified by silica gel (deactivated by triethylamine) flash chromatography to afford the desired product **3**.

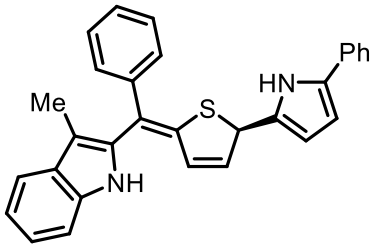
General Procedure C.



1 0.2 mmol + **2** 10 equiv. → **3**

At -20 °C, to an oven-dried 8-mL vial charged with a solution of the tertiary alcohol **1** (0.2 mmol) and pyrrole **2** (2.0 mmol) in toluene (3.6 mL) was slowly added a solution of catalyst (*R*)-**B2** (20 mg, 0.015 mmol, 10 mol%) in toluene (0.4 mL). The reaction mixture was stirred at the same temperature for 24 h. After that, triethylamine (2 drops) was added to quench the reaction. The mixture was concentrated under reduced pressure and purified by silica gel (deactivated by triethylamine) flash chromatography to afford the desired product **3**.

Unless noted otherwise, all the racemic products (used for HPLC reference in determining the ee value) were prepared from the same reaction using racemic BINOL-TRIP-OH as the catalyst.



3a

(*R*,*E*)-3-Methyl-2-(phenyl(5-(5-phenyl-1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene)methyl)-1*H*-indole (3a) was prepared as pale green foam from (3-methyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (63.9 mg, 0.2 mmol) and 2-phenylpyrrole (34.3 mg, 0.24 mmol) according to the General Procedure B (eluent: hexanes/EtOAc = 15:1 → 10:1) in 94% yield (83.7 mg, 95% ee, *E*/*Z* > 20:1).

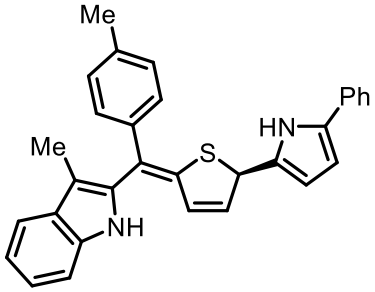
$[\alpha]_D^{26}$: +176.1 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 10% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 25.6 min (major), 34.9 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.48 (s, 1H), 9.82 (s, 1H), 7.62 (d, J = 7.6 Hz, 2H), 7.57 (d, J = 7.7 Hz, 1H), 7.39-7.28 (m, 7H), 7.21-7.05 (m, 4H), 6.52 (dd, J_1 = 2.1 Hz, J_2 = 6.2 Hz, 1H), 6.48 (t, J = 2.9 Hz, 1H), 6.40 (dd, J_1 = 3.0 Hz, J_2 = 6.2 Hz, 1H), 6.12 (t, J = 2.6 Hz, 1H), 5.94 (t, J = 2.5 Hz, 1H), 2.19 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.1, 141.9, 137.2, 135.3, 133.9, 133.4, 133.3, 132.5, 129.8, 129.5, 129.2, 128.9, 127.8, 126.5, 124.4(2C), 122.4, 121.4, 119.5, 119.2, 111.6, 110.7, 108.8, 106.9, 54.0, 9.8.

IR (thin film) 3408, 3051, 2915, 2859, 1690, 1598, 1484, 1253, 1139, 732, 690 cm^{-1}.

HRMS (CI+) Calcd for $C_{30}H_{24}N_2S$ (M^+): 444.1660, Found: 444.1668.



3b

(*R*,*E*)-3-Methyl-2-((5-(5-phenyl-1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(*p*-tolyl)methyl)-1*H*-indole (3b) was prepared as slightly green foam from

(3-methyl-1*H*-indol-2-yl)(thiophen-2-yl)(*p*-tolyl)methanol (66.7 mg, 0.2 mmol) and 2-phenylpyrrole (34.3 mg, 0.24 mmol) according to the General Procedure B (eluent: hexanes/EtOAc = 15:1 → 10:1) in 94% yield (86.0 mg, 92% ee, *E*/*Z* > 20:1).

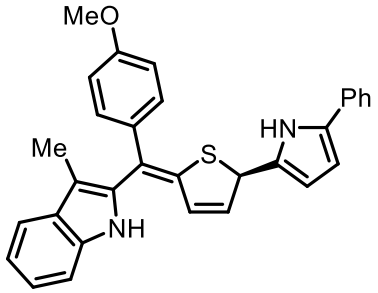
$[\alpha]_D^{26}$: +119.5 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 11.1 min (major), 13.8 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.47 (s, 1H), 9.79 (s, 1H), 7.62 (d, J = 7.4 Hz, 2H), 7.57 (d, J = 7.8 Hz, 1H), 7.35-7.26 (m, 5H), 7.17-7.04 (m, 5H), 6.50 (dd, J_1 = 2.2 Hz, J_2 = 6.2 Hz, 1H), 6.48 (t, J = 3.0 Hz, 1H), 6.37 (dd, J_1 = 3.0 Hz, J_2 = 6.2 Hz, 1H), 6.11 (t, J = 2.7 Hz, 1H), 5.94 (t, J = 2.5 Hz, 1H), 2.29 (s, 3H), 2.18 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.4, 139.0, 137.4, 137.2, 136.9, 135.5, 133.9, 133.4, 133.3, 132.6, 129.8, 129.6, 129.5, 129.2, 126.5, 124.4, 122.4, 121.4, 119.5, 119.2, 111.6, 110.6, 108.8, 106.9, 54.0, 21.2, 9.8.

IR (thin film) 3418, 3049, 2919, 1723, 1601, 1455, 1260, 1237, 1040, 731, 695 cm^{-1}.

HRMS (CI+) Calcd for $C_{31}H_{26}N_2S$ (M^+): 458.1817, Found: 458.1810.



3c

(*R*,*E*)-2-((4-Methoxyphenyl)(5-(5-phenyl-1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene) methyl)-3-methyl-1*H*-indole (3c) was prepared as slightly green foam from (4-methoxyphenyl)(3-methyl-1*H*-indol-2-yl)(thiophen-2-yl)methanol (69.9 mg, 0.2 mmol) and 2-phenylpyrrole (34.3 mg, 0.24 mmol) according to the General Procedure B (eluent: hexanes/EtOAc = 15:1 → 10:1) in 97% yield (92.1 mg, 95% ee, *E*/*Z* > 20:1).

$[\alpha]_D^{26}$: +132.1 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 16.4 min (major), 21.4 min (minor).

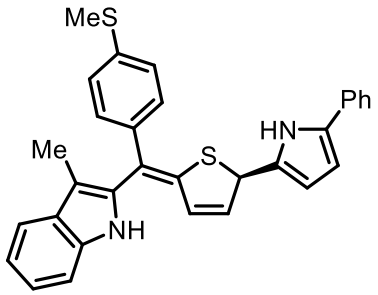
^{1}H NMR (400 MHz, acetone-d_6) δ 10.46 (s, 1H), 9.6 (s, 1H), 7.62 (d, J = 7.5 Hz, 2H),

7.57 (d, J = 7.7 Hz, 1H), 7.36-7.31 (m, 5H), 7.17-7.05 (m, 3H), 6.86 (d, J = 8.8 Hz, 2H), 6.51-6.48 (m, 2H), 6.34 (dd, J_1 = 3.0 Hz, J_2 = 6.1 Hz, 1H), 6.12 (t, J = 2.5 Hz, 1H), 5.92 (t, J = 2.6 Hz, 1H), 3.75 (s, 3H), 2.19 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 159.5, 145.5, 137.2, 136.4, 135.5, 134.2, 133.9, 133.4, 133.3, 132.7, 130.6, 129.8, 129.5, 126.5, 124.4, 122.4, 121.2, 119.5, 119.2, 114.2, 111.6, 110.5, 108.8, 106.9, 55.5, 53.9, 9.8.

IR (thin film) 3441, 3051, 2923, 1694, 1505, 1455, 1252, 1177, 1142, 1030, 730, 573 cm^{-1}.

HRMS (CI+) Calcd for $C_{31}H_{26}N_2OS$ (M^+): 474.1766, Found: 474.1772.



3d

(*R*,*E*)-3-Methyl-2-((4-(methylthio)phenyl)(5-(5-phenyl-1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene)methyl)-1*H*-indole (3d) was prepared as slightly green foam from (3-methyl-1*H*-indol-2-yl)(4-(methylthio)phenyl)(thiophen-2-yl)- methanol (73.1 mg, 0.2 mmol) and 2-phenylpyrrole (34.3 mg, 0.24 mmol) according to the General Procedure B (eluent: hexanes/EtOAc = 15:1 → 10:1) in 93% yield (91.3 mg, 99% ee, E/Z > 20:1).

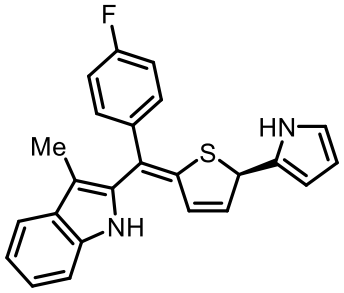
$[\alpha]_D^{26}$: +123.4 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 17.1 min (major), 21.5 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.47 (s, 1H), 9.80 (s, 1H), 7.61 (d, J = 7.3 Hz, 2H), 7.57 (d, J = 7.8 Hz, 1H), 7.35-7.30 (m, 5H), 7.20-7.05 (m, 5H), 6.50 (dd, J_1 = 2.2 Hz, J_2 = 6.2 Hz, 1H), 6.48 (t, J = 3.0 Hz, 1H), 6.38 (dd, J_1 = 3.0 Hz, J_2 = 6.2 Hz, 1H), 6.12 (t, J = 2.6 Hz, 1H), 5.95 (t, J = 2.5 Hz, 1H), 2.44 (s, 3H), 2.18 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.7, 138.4, 138.3, 137.2, 137.1, 135.2, 133.9 (2C), 133.5, 133.3, 132.5, 129.7, 129.5, 126.55, 126.49, 124.4, 122.5, 120.9, 119.5, 119.3, 111.6, 110.7, 108.9, 106.9, 54.1, 15.3, 9.8.

IR (thin film) 3404, 3050, 2918, 1693, 1595, 1484, 1254, 1191, 730, 694 cm^{-1}.

HRMS (CI+) Calcd for $C_{31}H_{26}N_2S_2$ (M^+): 490.1537, Found: 490.1553.



3e

(*R*,*E*)-2-((5-(1*H*-Pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(4-fluorophenyl)methyl)-3-methyl-1*H*-indole (3e) was prepared as slightly purple foam from (3-methyl-1*H*-indol-2-yl)(4-fluorophenyl)(thiophen-2-yl)-methanol (67.5 mg, 0.2 mmol) and pyrrole (134.0 mg, 2.0 mmol) according to the General Procedure C (eluent: hexanes/EtOAc = 40:1 → 20:1) in 92% yield (71.2 mg, 97% ee, *E*/*Z* >20:1). $[\alpha]_D^{26}$: +130.1 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 9.2 min (major), 18.5 min (minor).

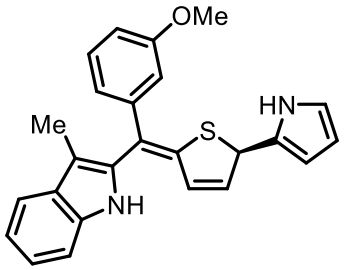
^{1}H NMR (400 MHz, acetone-d_6) δ 10.03 (s, 1H), 9.83 (s, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.41-7.38 (m, 2H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.14-7.04 (m, 4H), 6.78-6.76 (m, 1H), 6.50-6.47 (m, 1H), 6.34-6.32 (m, 1H), 6.06-6.02 (m, 2H), 5.93-5.90 (m, 1H), 2.17 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 162.2 (d, *J* = 244.0 Hz), 147.2, 138.3 (d, *J* = 3.1 Hz), 137.9, 137.2, 135.1, 132.9, 131.3 (d, *J* = 8.0 Hz), 130.2, 129.7, 122.5, 120.3, 119.6, 119.32, 119.27, 115.7 (d, *J* = 21.5 Hz), 111.6, 110.7, 108.7, 107.2, 54.1, 9.8.

^{19}F NMR (376 MHz, acetone-d_6) δ -115.4.

IR (thin film) 3417, 3050, 2965, 1597, 1441, 1307, 1084, 1017, 793, 730 cm^{-1}.

HRMS (CI+) Calcd for $C_{24}H_{19}FN_2S$ (M^+): 386.1253, Found: 386.1239.



3f

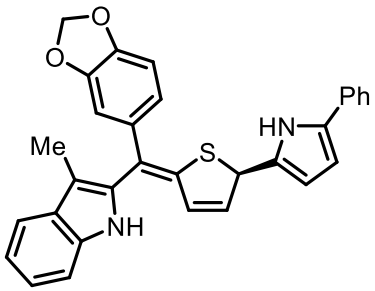
(*R*,*E*)-2-((5-(1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(3-methoxyphenyl)methyl)-3-methyl-1*H*-indole (3f) was prepared as slightly purple foam from (3-methyl-1*H*-indol-2-yl)(3-methoxyphenyl)(thiophen-2-yl)-methanol (69.9 mg, 0.2 mmol) and pyrrole (134.0 mg, 2.0 mmol) according to the General Procedure C (eluent: hexanes/EtOAc = 40:1 → 20:1) in 92% yield (73.2 mg, 97% ee, *E*/*Z* > 20:1). $[\alpha]_D^{26}$: -55.1 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 11.1 min (major), 21.2 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.02 (s, 1H), 9.82 (s, 1H), 7.55 (d, J = 7.8 Hz, 1H), 7.33 (d, J = 8.0 Hz, 1H), 7.22-7.15 (m, 4H), 6.90 (d, J = 7.8 Hz, 1H), 6.80-6.75 (m, 2H), 6.47 (dd, J_1 = 2.2 Hz, J_2 = 6.2 Hz, 1H), 6.47 (dd, J_1 = 3.0 Hz, J_2 = 6.2 Hz, 1H), 6.06-6.02 (m, 2H), 5.90 (t, J = 2.5 Hz, 1H), 3.71 (s, 3H), 2.78 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 160.4, 147.3, 143.2, 137.9, 137.2, 135.2, 133.0, 130.2, 130.0, 129.7, 122.4, 121.8, 121.3, 119.5, 119.3, 119.2, 114.9, 113.0, 111.6, 110.6, 108.7, 107.2, 55.4, 54.2, 9.8.

IR (thin film) 3395, 3049, 2925, 1584, 1448, 1259, 1135, 1030, 870, 792, 722 cm^{-1}.

HRMS (CI+) Calcd for $C_{25}H_{22}N_2OS$, (M^+): 398.1453, Found: 398.1442.



3g

(*R*,*E*)-2-(Benzo[*d*][1,3]dioxol-5-yl(5-(5-phenyl-1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene)methyl)-3-methyl-1*H*-indole (3g) was prepared as slightly green foam from

(3-methyl-1*H*-indol-2-yl)di(thiophen-2-yl)methanol (72.7 mg, 0.2 mmol) and 2-phenylpyrrole (34.3 mg, 0.24 mmol) according to the General Procedure B (eluent: hexanes/EtOAc = 15:1 → 10:1) in 93% yield (91.1 mg, 95% ee, *E*/*Z* > 20:1).

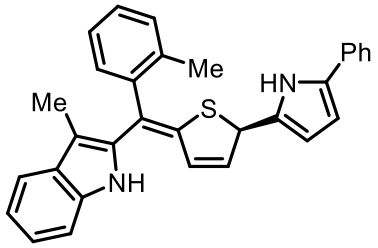
$[\alpha]_D^{26}$: +438.0 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 18.8 min (major), 31.5 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.46 (s, 1H), 9.79 (s, 1H), 7.62 (d, *J* = 7.4 Hz, 2H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.36-7.31 (m, 3H), 7.17-7.05 (m, 3H), 6.92 (d, *J* = 8.2 Hz, 1H), 6.87 (s, 1H), 6.79 (*J* = 8.2 Hz, 1H), 6.50-6.48 (m, 2H), 6.37 (dd, J_1 = 3.0 Hz, J_2 = 6.2 Hz, 1H), 6.12 (t, *J* = 2.6 Hz, 1H), 5.94 (s, 2H), 5.93 (t, *J* = 2.6 Hz, 1H), 2.20 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 148.4, 147.4, 146.1, 137.2, 136.9, 136.0, 135.3, 133.9, 133.31, 133.28, 132.6, 129.7, 129.5, 126.5, 1243, 123.3, 122.4, 121.1, 119.5, 119.2, 111.6, 110.6, 109.4, 108.8, 108.7, 106.9, 102.0, 53.9, 9.8.

IR (thin film) 3445, 3054, 2981, 2901, 1697, 1603, 1487, 1442, 1256, 1238, 1037, 730, 700 cm^{-1}.

HRMS (CI+) Calcd for $C_{31}H_{24}N_2O_2S$ (M^+): 488.1558, Found: 488.1569.



3h

(*R*,*E*)-3-Methyl-2-((5-(5-phenyl-1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(o-tolyl) methyl)-1*H*-indole (3h) was prepared as slightly green foam from (3-methyl-1*H*-indol-2-yl)(thiophen-2-yl)(*o*-tolyl)methanol (66.7 mg, 0.2 mmol) and 2-phenylpyrrole (34.3 mg, 0.24 mmol) according to the General Procedure B (eluent: hexanes/EtOAc = 15:1 → 10:1) in 87% yield (80.1 mg, 94% ee, *E*/*Z* > 20:1).

$[\alpha]_D^{26}$: +117.7 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 9.8 min (major), 16.2 min (minor).

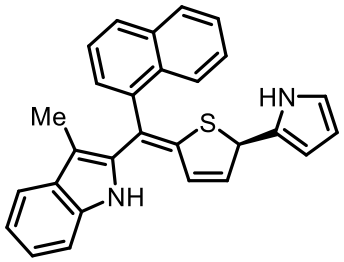
^{1}H NMR (400 MHz, acetone-d_6) δ 10.42 (s, 1H), 9.63 (s, 1H), 7.59 (d, *J* = 7.6 Hz,

2H), 7.57 (d, J = 7.7 Hz, 1H), 7.41-7.39 (m, 1H), 7.34-7.25 (m, 3H), 7.19-7.00 (m, 6H), 6.73 (dd, J_1 = 2.1 Hz, J_2 = 6.2 Hz, 1H), 6.48-6.46 (m, 2H), 6.09 (t, J = 2.5 Hz, 1H), 5.84 (t, J = 2.5 Hz, 1H), 2.23 (s, 3H), 2.11 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.7, 141.6, 138.2, 137.5, 137.3, 134.9, 133.9, 133.2, 132.9, 132.1, 131.3, 130.6, 130.1, 129.5, 128.6, 126.7, 126.5, 124.4, 122.4, 121.0, 119.5, 119.1, 111.5, 109.6, 108.6, 106.9, 53.2, 19.7, 10.3.

IR (thin film) 3448, 3051, 2960, 1605, 1456, 1332, 1133, 1116, 733, 702 cm^{-1}.

HRMS (CI+) Calcd for $C_{31}H_{26}N_2S$ (M^+): 458.1817, Found: 458.1821.



3i

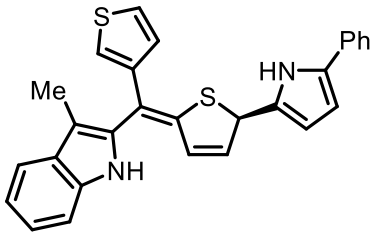
(*R*,*E*)-2-((5-(1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(naphthalen-1-yl)methyl)-3-methyl-1*H*-indole (3i) was prepared as slightly yellowish foam from (3-methyl-1*H*-indol-2-yl)(naphthalen-1-yl)(thiophen-2-yl)methanol (69.9 mg, 0.2 mmol) and pyrrole (134.0 mg, 2.0 mmol) according to the General Procedure C (30 h, eluent: hexanes/EtOAc = 40:1 → 20:1) in 94% yield (78.7 mg, 96% ee, *E*/*Z* > 20:1). $[\alpha]_D^{26}$: +74.3 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 7.8 min (major), 25.7 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.97 (s, 1H), 9.69 (s, 1H), 7.98 (d, J = 8.3 Hz, 1H), 7.89-7.85 (m, 2H), 7.66 (d, J = 7.0 Hz, 1H), 7.55-7.48 (m, 2H), 7.44-7.34 (m, 2H), 7.23 (d, J = 7.7 Hz, 1H), 7.09-7.01 (m, 2H), 6.83 (d, J = 6.2 Hz, 1H), 6.77-6.74 (m, 1H), 6.46-6.44 (m, 1H), 6.04-6.01 (m, 2H), 5.82-5.80 (m, 1H), 2.34 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 149.2, 139.8, 139.1, 137.2, 135.8, 135.0, 131.92, 131.86, 130.4, 130.2, 129.2, 129.0, 128.7, 126.8, 126.6, 126.42, 126.41, 122.4, 119.7, 119.5, 119.21, 119.19, 111.5, 109.4, 108.6, 107.1, 53.5, 10.5.

IR (thin film) 3403, 3048, 2917, 1574, 1455, 1331, 1260, 1139, 994, 785, 730 cm^{-1}.

HRMS (CI+) Calcd for $C_{28}H_{22}N_2S$ (M^+): 418.1504, Found: 418.1502.



3j

(*R*,*E*)-3-Methyl-2-((5-(5-phenyl-1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(thiophen-3-yl)methyl)-1*H*-indole (3j) was prepared as slightly green foam from (3-methyl-1*H*-indol-2-yl)di(thiophen-3-yl)methanol (63.8 mg, 0.2 mmol) and 2-phenylpyrrole (34.3 mg, 0.24 mmol) according to the General Procedure B (eluent: hexanes/EtOAc = 15:1 → 10:1) in 94% yield (84.5 mg, 98% ee, *E*/*Z* > 20:1).

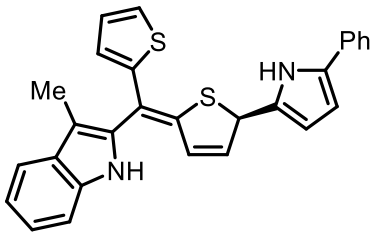
$[\alpha]_D^{26}$: +152.7 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 14.9 min (major), 18.4 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.49 (s, 1H), 9.87 (s, 1H), 7.62 (d, J = 7.4 Hz, 2H), 7.57 (d, J = 7.8 Hz, 1H), 7.39-7.31 (m, 5H), 7.17-7.10 (m, 4H), 6.49 (t, J = 3.0 Hz, 1H), 6.43 (dd, J_1 = 2.1 Hz, J_2 = 6.1 Hz, 1H), 6.35 (dd, J_1 = 3.0 Hz, J_2 = 6.1 Hz, 1H), 6.12 (t, J = 2.6 Hz, 1H), 5.94 (t, J = 2.4 Hz, 1H), 2.18 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.3, 142.6, 137.0, 136.8, 135.2, 133.8, 133.31, 133.27, 132.2, 129.7, 129.5, 129.0, 126.5, 125.7, 124.4, 124.0, 122.4, 119.5, 119.3, 116.7, 111.7, 110.1, 108.9, 107.0, 54.6, 9.6.

IR (thin film) 3403, 3050, 2914, 1690, 1598, 1506, 1137, 1080, 784, 735, 687 cm^{-1}.

HRMS (CI+) Calcd for $C_{28}H_{22}N_2S_2$ (M^+): 450.1224, Found: 450.1219.



3k

(*R*,*E*)-3-Methyl-2-((5-(5-phenyl-1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(thiophen-2-yl)methyl)-1*H*-indole (3k) was prepared as slightly green foam from

(3-methyl-1*H*-indol-2-yl)di(thiophen-2-yl)methanol (63.8 mg, 0.2 mmol) and 2-phenylpyrrole (34.3 mg, 0.24 mmol) according to the General Procedure B (eluent: hexanes/EtOAc = 15:1 → 10:1) in 88% yield (79.5 mg, 98% ee, *E*/*Z* > 20:1).

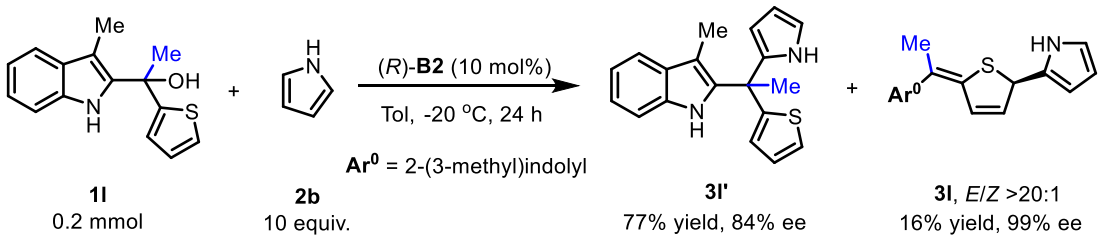
$[\alpha]_D^{26}$: +96.9 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 15.6 min (major), 20.3 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.54 (s, 1H), 10.02 (s, 1H), 7.63-7.59 (m, 3H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.37-7.31 (m, 3H), 7.17-7.10 (m, 3H), 7.01-6.96 (m, 2H), 6.49 (t, *J* = 3.0 Hz, 1H), 6.37-6.32 (m, 2H), 6.12 (t, *J* = 2.8 Hz, 1H), 6.03 (t, *J* = 2.0 Hz, 1H), 2.20 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 145.9, 145.4, 137.04, 136.98, 134.4, 133.8, 133.4, 133.3, 131.8, 129.5, 129.4, 127.9, 127.2, 126.6, 126.0, 124.4, 122.5, 119.6, 119.4, 115.5, 111.8, 110.4, 108.9, 107.0, 55.8, 9.5.

IR (thin film) 3410, 3051, 2996, 2858, 1694, 1604, 1455, 1262, 732, 692 cm^{-1}.

HRMS (CI+) Calcd for $C_{28}H_{22}N_2S_2$ (M^+): 450.1224, Found: 450.1234.

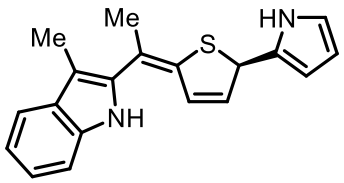


1l
0.2 mmol

2b
10 equiv.

3l'
77% yield, 84% ee

3l, *E*/*Z* >20:1
16% yield, 99% ee



3l

(*R*,*E*)-2-(1-(5-(1*H*-Pyrrol-2-yl)thiophen-2(5*H*)-ylidene)ethyl)-3-methyl-1*H*-indole (3l) was prepared as slightly green oil from 1-(3-methyl-1*H*-indol-2-yl)-1-(thiophen-2-yl)ethan-1-ol (51.5 mg, 0.2 mmol) and pyrrole (134.0 mg, 2.0 mmol) according to the General Procedure C (-40 °C, eluent: hexanes/EtOAc = 40:1 → 20:1) in 16% yield (10.7 mg, 99% ee, *E*/*Z* > 20:1).

Additionally, an undesired product chiral triarylethane **3l'** was isolated in 77% yield (50.2 mg, 84% ee).

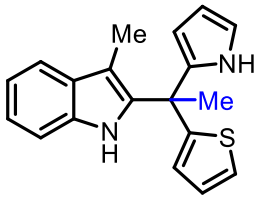
$[\alpha]_D^{26}$: -80.5 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 7.8 min (major), 19.4 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.99 (s, 1H), 9.89 (s, 1H), 7.48 (d, J = 7.7 Hz, 1H), 7.31 (d, J = 8.0 Hz, 1H), 7.10-6.99 (m, 2H), 6.76-6.73 (m, 1H), 6.41-6.39 (m, 1H), 6.19-6.17 (m, 1H), 6.02-6.00 (m, 2H), 5.85-5.83 (m, 1H), 2.20 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 145.1, 137.2, 136.8, 136.4, 131.5, 130.9, 130.1, 122.2, 119.5, 119.2, 119.1, 115.6, 111.5, 108.7, 108.2, 107.0, 53.7, 22.5, 10.1.

IR (thin film) 3395, 3050, 2960, 1607, 1453, 1255, 1088, 1021, 794, 731 cm^{-1}.

HRMS (CI+) Calcd for $C_{19}H_{18}N_2S$ (M^+): 306.1191, Found: 306.1176.



3l'

2-(1-(1*H*-Pyrrol-2-yl)-1-(thiophen-2-yl)ethyl)-3-methyl-1*H*-indole (3l').

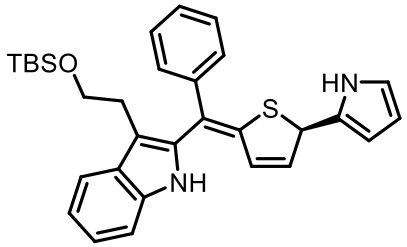
$[\alpha]_D^{26}$: -3.2 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 6.9 min (major), 13.5 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.75 (s, 1H), 9.42 (s, 1H), 7.45 (d, J = 7.7 Hz, 1H), 7.32-7.28 (m, 2H), 7.08-6.94 (m, 3H), 6.88-6.86 (m, 1H), 6.76-6.74 (m, 1H), 6.04-6.02 (m, 1H), 5.89-5.87 (m, 1H), 2.26 (s, 3H), 1.80 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 153.1, 140.0, 137.8, 135.8, 130.9, 127.2, 125.8, 125.1, 121.9, 119.3, 118.8, 118.3, 111.7, 108.0, 107.9, 106.9, 43.8, 30.1, 8.9.

IR (thin film) 3422, 3055, 2973, 2923, 1551, 1455, 1239, 1094, 1026, 801, 715 cm^{-1}.

HRMS (CI+) Calcd for $C_{19}H_{18}N_2S$ (M^+): 306.1191, Found: 306.1179.



3m

(*R*,*E*)-2-((5-(1*H*-Pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(phenyl)methyl)-3-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-1*H*-indole (3m) was prepared as slightly purple foam from (3-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (92.7 mg, 0.2 mmol) and pyrrole (134.0 mg, 2.0 mmol) according to the General Procedure C (RT, 48 h, eluent: hexanes/EtOAc = 40:1 → 20:1) in 52% yield (53.1 mg, 96% ee, *E*/*Z* > 20:1). In addition, 37.2 mg (40%) of starting material was recovered.

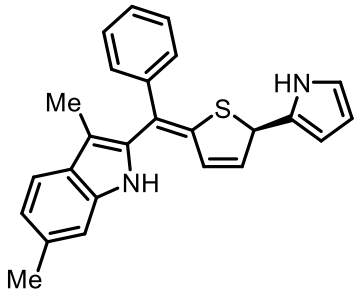
$[\alpha]_D^{26}$: +141.7 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 10% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 6.6 min (major), 9.9 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.00 (s, 2H), 7.62 (d, J = 7.8 Hz, 1H), 7.42-7.28 (m, 5H), 7.22-7.18 (m, 1H), 7.13-7.03 (m, 2H), 6.77-6.74 (m, 1H), 6.45 (dd, J_1 = 2.2 Hz, J_2 = 6.2 Hz, 1H), 6.33 (dd, J_1 = 3.0 Hz, J_2 = 6.2 Hz, 1H), 6.05-6.01 (m, 2H), 5.91 (t, J = 2.5 Hz, 1H), 3.76 (t, J = 7.8 Hz, 2H), 2.88-2.83 (m, 2H), 0.86 (s, 9H), 0.00 (s, 3H), -0.01 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.6, 141.9, 137.8, 137.2, 135.9, 133.1, 130.3, 129.4, 129.1, 128.9, 127.8, 122.4, 121.3, 119.68, 119.66, 119.2, 111.8, 111.7, 108.8, 107.2, 64.1, 54.3, 29.7, 26.4, 18.9, -5.0.

IR (thin film) 3408, 3049, 2947, 1587, 1441, 1256, 1080, 1020, 791, 720 cm^{-1}.

HRMS (CI+) Calcd for $C_{31}H_{36}N_2OSSi$ (M^+): 512.2318, Found: 512.2325.



3n

(*R*,*E*)-2-((5-(1*H*-Pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(phenyl)methyl)-3,6-dimethyl-1*H*-indole (3n) was prepared as slightly purple foam from (3,6-dimethyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (66.6 mg, 0.2 mmol) and pyrrole (134.0 mg, 2.0 mmol) according to the General Procedure C (eluent: hexanes/EtOAc = 40:1 → 20:1) in 89% yield (68.1 mg, 86% ee, *E*/*Z* > 20:1).

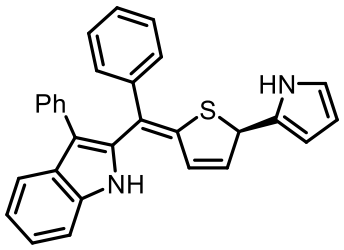
$[\alpha]_D^{26}$: +79.8 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 8.4 min (major), 19.9 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.02 (s, 1H), 9.65 (s, 1H), 7.43-7.17 (m, 6H), 7.13 (s, 1H), 6.90 (dd, J_1 = 0.8 Hz, J_2 = 8.0 Hz, 1H), 7.67-7.65 (m, 1H), 6.48 (dd, J_1 = 2.2 Hz, J_2 = 6.2 Hz, 1H), 6.31 (dd, J_1 = 3.0 Hz, J_2 = 6.2 Hz, 1H), 6.05-6.01 (m, 2H), 5.89 (t, J = 2.5 Hz, 1H), 2.41 (s, 3H), 2.14 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.9, 142.0, 137.7, 137.6, 134.7, 133.1, 131.8, 130.3, 129.3, 128.9, 127.75, 127.73, 121.6, 121.2, 119.3, 119.0, 111.6, 110.5, 108.7, 107.2, 54.1, 21.9, 9.8.

IR (thin film) 3391, 3039, 2916, 1577, 1446, 1324, 1258, 1087, 1020, 793, 724 cm^{-1}.

HRMS (CI+) Calcd for $C_{25}H_{22}N_2S$ (M^+): 382.1504, Found: 382.1516.



3o

(*R*,*E*)-((5-(1*H*-Pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(phenyl)methyl)-3-phenyl-1*H*-indole (3o) was prepared as yellowish foam from

phenyl(3-phenyl-1*H*-indol-2-yl)(thiophen-2-yl)methanol (76.3 mg, 0.2 mmol) and pyrrole (134.0 mg, 2.0 mmol) according to the General Procedure C (eluent: hexanes/EtOAc = 40:1 → 20:1) in 93% yield (80.3 mg, 86% ee, *E*/*Z* > 20:1).

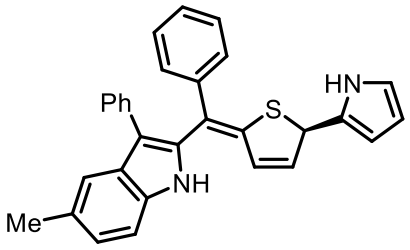
$[\alpha]_D^{26}$: -215.0 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 7.2 min (major), 18.6 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.27 (s, 1H), 9.28 (s, 1H), 7.80 (d, *J* = 7.9 Hz, 1H), 7.59 (d, *J* = 7.6 Hz, 2H), 7.48-737 (m, 5H), 7.32-7.13 (m, 6H), 6.73-6.71 (m, 1H), 6.37-6.34 (m, 1H), 6.01-5.97 (m, 2H), 5.90-5.87 (m, 1H), 5.71-5.69 (m, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 148.0, 141.7, 137.4, 137.3, 136.8, 135.4, 133.0, 129.8, 129.6, 129.3, 129.2, 129.0, 127.85, 127.84, 126.3, 123.0, 120.68, 120.65, 119.8, 119.1, 117.5, 112.1, 108.7, 107.2, 53.9.

IR (thin film) 3414, 3051, 2965, 1596, 1549, 1441, 1528, 1084, 1019, 792, 733, 699 cm^{-1}.

HRMS (CI+) Calcd for $C_{29}H_{22}N_2S$ (M^+): 430.1504, Found: 430.1499.



3p

(*R*,*E*)-2-((5-(1*H*-Pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(phenyl)methyl)-5-methyl-3-phenyl-1*H*-indole (3p) was prepared as slightly yellowish foam from (5-methyl-3-phenyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (79.1 mg, 0.2 mmol) and pyrrole (134.0 mg, 2.0 mmol) according to the General Procedure C (eluent: hexanes/EtOAc = 40:1 → 20:1) in 93% yield (82.6 mg, 83% ee, *E*/*Z* > 20:1).

$[\alpha]_D^{26}$: -240.9 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 6.5 min (major), 16.5 min (minor).

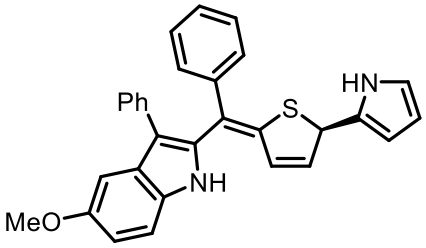
^{1}H NMR (400 MHz, acetone-d_6) δ 10.13 (s, 1H), 9.26 (s, 1H), 7.59-7.56 (m, 3H), 7.46-7.16 (m, 9H), 7.03 (dd, J_1 = 1.2 Hz, J_2 = 8.2 Hz, 1H), 6.72-6.70 (m, 1H), 6.35 (dd, J_1 = 2.1 Hz, J_2 = 6.2 Hz, 1H), 5.99-5.96 (m, 2H), 5.88-5.86 (m, 1H), 5.69 (t, *J* =

2.5 Hz, 1H), 2.44 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.8, 141.8, 137.1, 137.0, 135.8, 135.5, 133.0, 129.8, 129.7, 129.5, 129.3, 129.2, 129.0, 128.1, 127.8, 126.2, 124.6, 120.9, 119.4, 119.1, 117.1, 111.9, 108.7, 107.2, 53.9, 21.7.

IR (thin film) 3412, 3042, 2919, 1591, 1478, 1259, 1139, 1018, 721 cm^{-1}.

HRMS (CI+) Calcd for $C_{30}H_{24}N_2S$ (M^+): 444.1660, Found: 444.1654.



3q

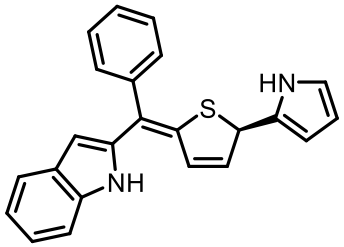
(*R*,*E*)-2-((5-(1*H*-Pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(phenyl)methyl)-5-methoxy-3-phenyl-1*H*-indole (3q) was prepared as slightly yellowish foam from (5-methoxy-3-phenyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (82.3 mg, 0.2 mmol) and pyrrole (134.0 mg, 2.0 mmol) according to the General Procedure C (eluent: hexanes/EtOAc = 40:1 → 20:1) in 95% yield (87.7 mg, 86% ee, *E*/*Z* > 20:1). $[\alpha]_D^{26}$: -214.4 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 7.6 min (major), 15.6 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.13 (s, 1H), 9.27 (s, 1H), 7.59-7.57 (m, 2H), 7.46-7.44 (m, 2H), 7.39-7.27 (m, 6H), 7.25-7.16 (m, 2H), 6.87 (dd, J_1 = 2.4 Hz, J_2 = 8.8 Hz, 1H), 6.72-6.70 (m, 1H), 6.35 (dd, J_1 = 2.1 Hz, J_2 = 6.1 Hz, 1H), 6.00-5.96 (m, 2H), 5.89-5.87 (m, 1H), 5.69 (t, J = 2.5 Hz, 1H), 3.81 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 155.6, 147.8, 141.8, 137.2, 137.0, 136.1, 133.0, 132.5, 129.8, 129.5, 129.3, 129.2, 129.0, 128.2, 127.8, 127.7, 126.3, 120.9, 119.1, 117.4, 113.2, 112.9, 108.7, 107.1, 55.9, 53.9.

IR (thin film) 3416, 3049, 1592, 1478, 1440, 1260, 1138, 1090, 1020, 793, 723 cm^{-1}.

HRMS (CI+) Calcd for $C_{30}H_{24}N_2OS$ (M^+): 460.1609, Found: 460.1620.



3r

(*R*,*E*)-2-((5-(1*H*-Pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(phenyl)methyl)-1*H*-indole (3r) was prepared as slightly yellowish foam from (1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (61.0 mg, 0.2 mmol) and pyrrole (134.0 mg, 2.0 mmol) according to the General Procedure C (eluent: hexanes/EtOAc = 40:1 → 20:1) in 62% yield (44.1 mg, 97% ee, *E*/*Z* > 20:1).

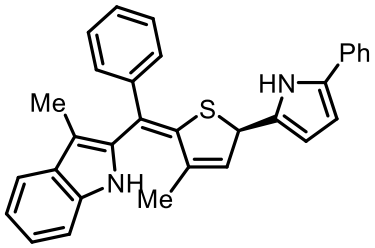
$[\alpha]_D^{26}$: +39.4 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 11.7 min (major), 19.7 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.04 (s, 1H), 9.93 (s, 1H), 7.56 (d, J = 7.7 Hz, 1H), 7.40-7.31 (m, 5H), 7.28-7.24 (m, 1H), 7.10-7.00 (m, 3H), 6.76-6.74 (m, 1H), 6.49-6.48 (m, 1H), 6.36 (dd, J_1 = 3.0 Hz, J_2 = 6.2 Hz, 1H), 6.04-5.99 (m, 2H), 5.85 (t, J = 2.6 Hz, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.0, 142.2, 138.7, 138.5, 138.5, 137.6, 132.0, 130.3, 129.9, 129.4, 129.1, 128.2, 122.4, 120.8, 120.3, 119.3, 111.9, 108.6, 107.2, 104.2, 53.5.

IR (thin film) 3396, 3050, 2962, 1575, 1445, 1259, 1086, 1015, 793, 721 cm^{-1}.

HRMS (CI+) Calcd for $C_{23}H_{18}N_2S$ (M^+): 354.1191, Found: 354.1181.



3s

(*R*,*E*)-3-Methyl-2-((3-methyl-5-(5-phenyl-1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(phenyl)methyl)-1*H*-indole (3s) was prepared as slightly yellowish foam from

(3-methyl-1*H*-indol-2-yl)(3-methylthiophen-2-yl)(phenyl)methanol (66.7 mg, 0.2 mmol) and 2-phenylpyrrole (34.3 mg, 0.24 mmol) according to the General Procedure B (-20 ºC, 48 h, eluent: hexanes/EtOAc = 40:1 → 20:1) in 81% yield (74.4 mg, 70% ee, *E*/*Z* = 8.6:1).

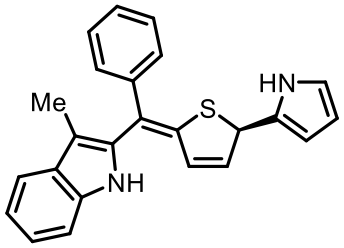
$[\alpha]_D^{26}$: +199.8 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 10% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 14.8 min (major), 24.1 min (minor).

^{1}H NMR (400 MHz, acetone-*d*$_6$) δ 10.43 (s, 1H), 9.98 (s, 1H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.39-7.25 (m, 7H), 7.29-7.03 (m, 4H), 6.49-6.46 (m, 1H), 6.26-6.24 (m, 1H), 6.12-6.10 (m, 1H), 5.62-5.58 (m, 1H), 2.21 (s, 3H), 1.51 (s, 3H).

^{13}C NMR (100 MHz, acetone-*d*$_6$) δ 148.3, 143.7, 140.9, 138.4, 136.9, 134.7, 134.0, 133.3, 133.1, 131.2, 129.5, 129.4, 129.3, 128.9, 128.5, 127.8, 126.5, 124.3, 122.3, 119.5, 119.2, 111.6, 108.5, 106.8, 48.9, 15.6, 9.3.

IR (thin film) 3407, 3049, 2966, 1599, 1256, 1015, 738, 693 cm^{-1}.

HRMS (CI+) Calcd for $C_{31}H_{26}N_2S$ (M^+): 458.1817, Found: 458.1813.



3t

(*R*,*E*)-2-((5-(1*H*-Pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(phenyl)methyl)-3-methyl-1*H*-indole (3t) was prepared as slightly purple foam from (3-methyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (127.6 mg, 0.4 mmol) and pyrrole (268 mg, 4.0 mmol) according to the General Procedure C (8 mL of toluene used, eluent: hexanes/EtOAc = 40:1 → 20:1) in 93% yield (136.5 mg, 96% ee, *E*/*Z* >20:1).

$[\alpha]_D^{26}$: 371.5 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 8.5 min (major), 17.0 min (minor).

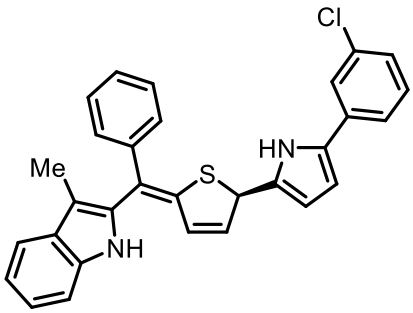
^{1}H NMR (400 MHz, acetone-*d*$_6$) δ 10.02 (s, 1H), 9.82 (s, 1H), 7.56 (d, *J* = 7.8 Hz,

1H), 7.39-7.21 (m, 5H), 7.22-7.17 (m, 1H), 7.14-7.04 (m, 2H), 6.77-6.75 (m, 1H), 6.49 (dd, J_1 = 2.2 Hz, J_2 = 6.2 Hz, 1H), 6.32 (dd, J_1 = 3.0 Hz, J_2 = 6.2 Hz, 1H), 6.05-6.02 (m, 2H), 5.90 (t, J = 2.6 Hz, 1H), 2.17 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.1, 141.9, 137.8, 137.2, 135.3, 133.0, 130.2, 129.7, 129.2, 128.9, 127.8, 122.4, 121.3, 119.5, 119.3, 119.2, 111.6, 110.6, 108.7, 107.2, 54.1, 9.8.

IR (thin film) 3398, 3050, 2977, 1564, 1446, 1306, 1254, 1137, 1086, 1137, 787, 725 cm^{-1}.

HRMS (CI+) Calcd for $C_{24}H_{20}N_2S$ (M^+): 368.1347, Found: 368.1337.



3u

(*R*,*E*)-3-Methyl-2-((5-(5-phenyl-1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(thiophen-2-yl)methyl)-1*H*-indole (3u) was prepared as slightly green foam from (3-methyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (63.8 mg, 0.2 mmol) and 2-(3-chlorophenyl)-1*H*-pyrrole (42.3 mg, 0.24 mmol) according to the General Procedure B (eluent: hexanes/EtOAc = 15:1 → 10:1) in 92% yield (94.6 mg, 91% ee, *E*/*Z* >20:1).

$[\alpha]_D^{26}$: +228.3 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 8.0 min (major), 11.2 min (minor).

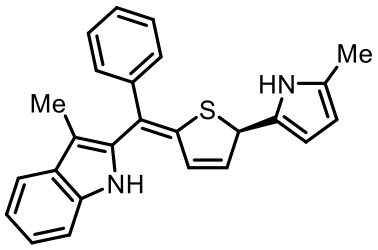
^{1}H NMR (400 MHz, acetone-d_6) δ 10.61 (s, 1H), 9.83 (s, 1H), 7.65 (t, J = 1.8 Hz, 1H), 7.56 (dd, J_1 = 0.7 Hz, J_2 = 7.8 Hz, 2H), 7.38-7.28 (m, 6H), 7.22-7.04 (m, 4H), 6.56 (dd, J_1 = 2.6 Hz, J_2 = 3.4 Hz, 1H), 6.53 (dd, J_1 = 2.6 Hz, J_2 = 6.6 Hz, 1H), 6.40 (dd, J_1 = 3.0 Hz, J_2 = 6.2 Hz, 1H), 6.14 (t, J = 2.3 Hz, 1H), 5.94 (t, J = 2.6 Hz, 1H), 2.18 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.0, 141.9, 137.2, 137.1, 135.9, 135.3, 135.1, 133.5, 133.5, 131.7, 131.2, 129.7, 129.3, 129.0, 127.8, 126.1, 123.9, 122.8, 122.5,

121.6, 119.5, 119.3, 111.6, 110.7, 109.1, 108.1, 53.8, 9.8.

IR (thin film) 3414, 3052, 2912, 2878, 1695, 1599, 1492, 1263, 1238, 1147, 1089, 770, 732, 696 cm^{-1}.

HRMS (LD+) Calcd for $C_{30}H_{22}ClN_2S$ $[(M-H)^+]$: 477.1187, Found: 477.1184.



3v

(*R*,*E*)-3-Methyl-2-((5-(5-methyl-1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(phenyl) methyl)-1*H*-indole (3v) was prepared as slightly purple foam from (3-methyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (63.8 mg, 0.2 mmol) and 2-methylpyrrole (32.4 mg, 0.40 mmol) according to the General Procedure C (48 h, eluent: hexanes/EtOAc = 40:1 → 20:1) in 72% yield (55.2 mg, 95% ee, *E*/*Z* = 14:1). In addition, 7.2 mg (11%) of starting material was recovered.

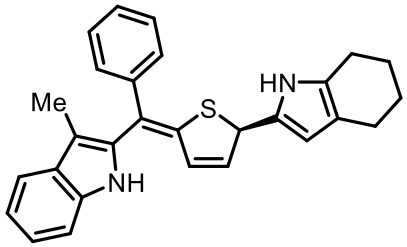
$[\alpha]_D^{26}$: +563.8 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 11.7 min (major), 19.7 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.80 (s, 1H), 9.72 (s, 1H), 7.55 (d, J = 7.8 Hz, 1H), 7.38-7.27 (m, 5H), 7.21-7.17 (m, 1H), 7.13-7.03 (m, 2H), 6.46 (dd, J_1 = 2.2 Hz, J_2 = 6.2 Hz, 1H), 6.30 (dd, J_1 = 3.0 Hz, J_2 = 6.2 Hz, 1H), 5.90-5.88 (m, 1H), 5.84 (t, J = 2.5 Hz, 1H), 5.70-5.68 (m, 1H), 2.20 (s, 3H), 2.16 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.4, 142.0, 138.0, 137.2, 135.4, 132.9, 129.8, 129.2, 129.1, 128.9, 128.6, 127.7, 122.4, 121.2, 119.5, 119.2, 111.6, 110.6, 107.5, 106.6, 54.5, 13.0, 9.8.

IR (thin film) 3393, 3048, 2959, 1586, 1444, 1260, 1130, 1023, 856, 779, 741 cm^{-1}.

HRMS (CI+) Calcd for $C_{25}H_{22}N_2S$ (M^+): 382.1504, Found: 382.1493.



3w

(*R*,*E*)-3-Methyl-2-(phenyl(5-(4,5,6,7-tetrahydro-1*H*-indol-2-yl)thiophen-2(5*H*)-ylidene)methyl)-1*H*-indole (3w) was prepared as slightly purple foam from (3-methyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (63.8 mg, 0.2 mmol) and 4,5,6,7-tetrahydro-1*H*-indole (48.4 mg, 0.40 mmol) according to the General Procedure C (48 h, eluent: hexanes/EtOAc = 40:1 → 20:1) in 57% yield (48.1 mg, 94% ee, *E*/*Z* >20:1). In addition, 13.1 mg (20%) of starting material was recovered.

$[\alpha]_D^{26}$: +146.4 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 12% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 12.8 min (major), 30.0 min (minor).

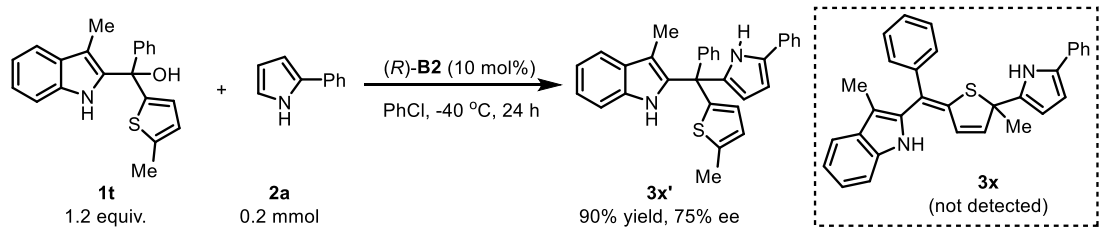
^{1}H NMR (400 MHz, acetone-d_6) δ 9.79 (s, 1H), 9.41 (s, 1H), 7.54 (d, J = 7.8 Hz, 1H), 7.37-7.27 (m, 5H), 7.21-7.17 (m, 1H), 7.12-7.02 (m, 2H), 6.44 (dd, J_1 = 2.2 Hz, J_2 = 6.2 Hz, 1H), 6.29 (dd, J_1 = 3.0 Hz, J_2 = 6.1 Hz, 1H), 5.82 (t, J = 2.5 Hz, 1H), 5.75-5.74 (m, 1H), 2.51 (t, J = 5.7 Hz, 2H), 2.51 (t, J = 6.0 Hz, 2H), 2.16 (s, 3H), 1.77-1.65 (m, 4H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.5, 142.0, 138.1, 137.2, 135.4, 132.8, 129.8, 129.3, 128.9, 128.3, 128.1, 127.7, 122.4, 121.1, 119.5, 119.2, 117.1, 111.6, 110.5, 106.5, 54.7, 24.7, 24.2, 23.7, 23.4, 9.8.

IR (thin film) 3395, 3052, 2923, 1591, 1443, 1257, 1083, 1015, 798, 730 cm^{-1}.

HRMS (CI+) Calcd for $C_{28}H_{26}N_2S$ (M^+): 422.1817, Found: 422.1810.

Note: With 5-methylthiophenyl-substituted alcohol (**1t**), the thiophene dearomatization product **3x** was not observed. Instead, the nucleophilic addition to the indole benzylic position by 1,6-addition to the indole imine methide was observed, leading to the enantioenriched tetraarylmethane **3x'**. The results are as shown below.



3-Methyl-2-((5-methylthiophen-2-yl)(phenyl)(5-phenyl-*1H*-pyrrol-2-yl)methyl)-1 H-indole (3x') was prepared as yellowish foam from (3-methyl-1*H*-indol-2-yl)(5-methylthiophen-2-yl)(phenyl)methanol **1t** (79.9 mg, 0.24 mmol) and 2-phenylpyrrole (28.6 mg, 0.2 mmol) according to the General Procedure B (eluent: hexanes/EtOAc = 15:1 → 10:1) for 24 h in 90% yield (82.6 mg, 75% ee). $[\alpha]_D^{26}$: +245.5 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 15% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 9.4 min (minor), 15.0 min (major).

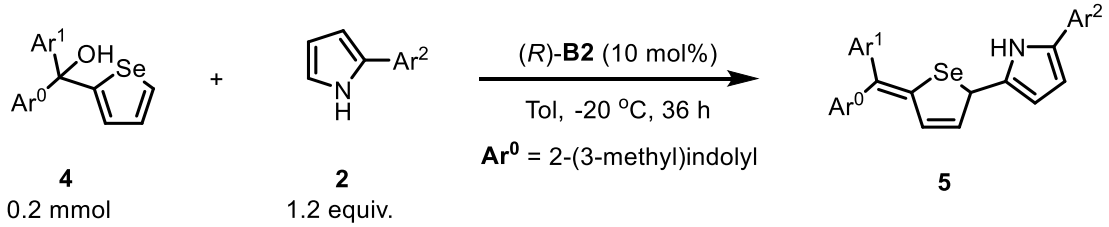
^{1}H NMR (400 MHz, acetone-d_6) δ 10.16 (s, 1H), 9.83 (s, 1H), 7.63 (d, *J* = 7.8 Hz, 2H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.38-7.21 (m, 7H), 7.21-7.07 (m, 4H), 6.46-6.37 (m, 3H), 6.16-6.14 (m, 1H), 2.21 (s, 3H), 2.03 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.2, 143.1, 141.8, 137.2, 136.8, 135.1, 133.9, 133.5, 130.8, 129.7, 129.4, 129.3, 128.9, 128.8, 126.5, 124.6, 122.4, 121.7, 119.5, 119.2, 111.6, 110.8, 107.6, 106.6, 63.3, 29.5, 9.8.

IR (thin film) 3418, 3046, 2967, 1593, 1447, 1245, 1096, 1032, 742, 692 cm^{-1}.

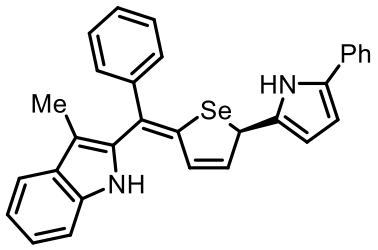
HRMS (CI+) Calcd for $C_{31}H_{26}N_2S$ (M^+): 458.1817, Found: 458.1808.

General Procedure D.



At -20 °C, to an oven-dried 8-mL vial charged with a solution of the tertiary alcohol **4** (0.2 mmol) and pyrrole **2** (0.24 mmol) in toluene (3.6 mL) was slowly added a solution of the catalyst (*R*)-**B2** (20 mg, 0.015 mmol, 10 mol%) in toluene (0.4 mL). The reaction mixture was stirred at the same temperature for 36 h. After that,

triethylamine (2 drops) was added to quench the reaction. The mixture was concentrated under reduced pressure and purified by silica gel (deactivated by triethylamine) flash chromatography to afford the desired product



5a

(*R*,*E*)-3-Methyl-2-(phenyl(5-(5-phenyl-1*H*-pyrrol-2-yl)selenophen-2(5*H*)-ylidene) methyl)-1*H*-indole (5a) was prepared as slightly yellow-brown foam from (3-methyl-1*H*-indol-2-yl)(phenyl)(selenophen-2-yl)methanol (73.2 mg, 0.2 mmol) and 2-phenylpyrrole (34.3 mg, 0.24 mmol) according to the General Procedure D (eluent: hexanes/EtOAc = 15:1 → 10:1) in 95% yield (93.5 mg, 94% ee, *E*/*Z* >20:1).

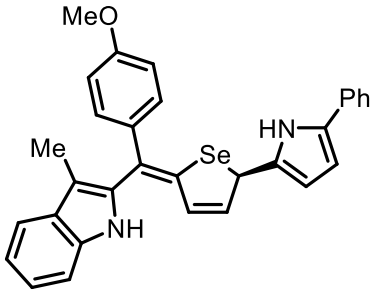
$[\alpha]_D^{26}$: +87.5 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 10% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 24.7 min (major), 34.8 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.48 (s, 1H), 9.85 (s, 1H), 7.61 (dd, J_1 = 1.2 Hz, J_2 = 8.5 Hz, 2H), 7.58 (d, J = 7.9 Hz, 1H), 7.39-7.05 (m, 11H), 6.63 (dd, J_1 = 2.2 Hz, J_2 = 6.6 Hz, 1H), 6.47 (t, J = 3.2 Hz, 1H), 6.30 (dd, J_1 = 3.1 Hz, J_2 = 6.6 Hz, 1H), 6.14 (t, J = 2.6 Hz, 1H), 6.10 (t, J = 2.8 Hz, 1H), 2.20 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 145.3, 143.3, 138.0, 137.2, 135.4, 135.3, 133.9, 133.9, 133.1, 129.7, 129.5, 129.1, 128.7, 128.1, 126.4, 126.3, 124.3, 122.5, 119.5, 119.2, 111.6, 110.7, 108.6, 107.0, 47.2, 9.9.

IR (thin film) 3418, 3076, 2920, 2854, 1682, 1548, 1505, 1296, 1264, 1187, 1122, 770, 733, 693 cm^{-1}.

HRMS (CI+) Calcd for $C_{30}H_{24}N_2Se$ (M^+): 492.1105, Found: 492.1121.



5b

(*R*,*E*)-2-((4-Methoxyphenyl)(5-(5-phenyl-1*H*-pyrrol-2-yl)selenophen-2(5*H*)-yliden e)methyl)-3-methyl-1*H*-indole (5b) was prepared as slightly yellow-brown foam from (4-methoxyphenyl)(3-methyl-1*H*-indol-2-yl)- (selenophen-2-yl)-methanol (78.9 mg, 0.2 mmol) and 2-phenylpyrrole (34.3 mg, 0.24 mmol) according to the General Procedure D (eluent: hexanes/EtOAc = 15:1 → 10:1) in 94% yield (97.2 mg, 98% ee, *E*/*Z* >20:1).

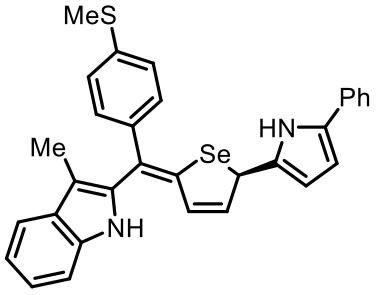
$[\alpha]_D^{26}$: +154.9 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 16.7 min (major), 21.2 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.45 (s, 1H), 9.79 (s, 1H), 7.63-7.57 (m, 3H), 7.36-7.29 (m, 5H), 7.16-7.06 (m, 3H), 6.86 (d, J = 8.9 Hz, 2H), 6.61 (dd, J_1 = 2.2 Hz, J_2 = 6.6 Hz, 1H), 6.48 (dd, J_1 = 2.8 Hz, J_2 = 3.3 Hz, 1H), 6.25 (dd, J_1 = 3.1 Hz, J_2 = 6.6 Hz, 1H), 6.13 (t, J = 2.5 Hz, 1H), 6.11 (t, J = 2.7 Hz, 1H), 3.75 (s, 3H), 2.20 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 159.7, 143.7, 137.2, 137.2, 135.6, 135.5, 135.4, 134.1, 133.9, 133.1, 130.1, 129.7, 129.5, 126.4, 126.0, 124.3, 122.4, 119.5, 119.2, 114.4, 111.6, 110.6, 108.6, 107.0, 55.5, 47.1, 9.9.

IR (thin film) 3441, 3049, 2930, 2814, 1604, 1506, 1243, 1175, 756, 733, 701 cm^{-1}.

HRMS (CI+) Calcd for $C_{31}H_{26}N_2OSe$ (M^+): 522.1210, Found: 522.1207.



5c

(*R*,*E*)-3-Methyl-2-((4-(methylthio)phenyl)(5-(5-phenyl-1*H*-pyrrol-2-yl)selenophen-2(5*H*)-ylidene)methyl)-1*H*-indole (5c) was prepared as slightly yellow-brown foam from (3-methyl-1*H*-indol-2-yl)(4-(methylthio)phenyl) (selenophen-2-yl)methanol (82.6 mg, 0.2 mmol) and 2-phenylpyrrole (34.3 mg, 0.24 mmol) according to the General Procedure D (eluent: hexanes/EtOAc = 15:1 → 10:1) in 90% yield (96.6 mg, 96% ee, *E*/*Z* >20:1).

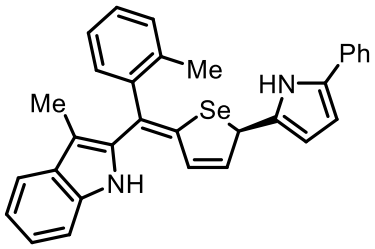
$[\alpha]_D^{26}$: +357.0 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 17.3 min (major), 21.2 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.45 (s, 1H), 9.83 (s, 1H), 7.61 (d, J = 7.4 Hz, 2H), 7.57 (d, J = 7.7 Hz, 1H), 7.34-7.28 (m, 5H), 7.20-7.05 (m, 5H), 6.61 (dd, J_1 = 2.2 Hz, J_2 = 6.6 Hz, 1H), 6.47 (t, J = 2.6 Hz, 1H), 6.29 (dd, J_1 = 3.1 Hz, J_2 = 6.6 Hz, 1H), 6.15 (t, J = 2.5 Hz, 1H), 6.10 (t, J = 2.2 Hz, 1H), 2.44 (s, 3H), 2.19 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 144.8, 139.7, 138.7, 137.9, 137.2, 135.5, 135.2, 133.9, 133.8, 133.1, 129.7, 129.5, 129.3, 126.5, 126.5, 125.7, 124.3, 122.5, 119.6, 119.3, 111.6, 110.8, 108.7, 107.0, 47.5, 15.1, 9.9.

IR (thin film) 3439, 3046, 2918, 2881, 1605, 1508, 1489, 1455, 1264, 1238, 1123, 756, 735, 695 cm^{-1}.

HRMS (LD+) Calcd for $C_{31}H_{25}N_2SSe$ [$(M-H)^+$]: 537.0898, Found: 537.0929.



5d

(*R*,*E*)-3-Methyl-2-((5-(5-phenyl-1H-pyrrol-2-yl)selenophen-2(5*H*)-ylidene)(*o*-tolyl)methyl)-1*H*-indole (5d) was prepared as slightly yellow-green foam from (3-methyl-1*H*-indol-2-yl)(selenophen-2-yl)(*o*-tolyl)methanol (76.0 mg, 0.2 mmol) and pyrrole (34.3 mg, 2.0 mmol) according to the General Procedure D (eluent: hexanes/EtOAc = 15:1 → 10:1) in 89% yield (90.1 mg, 97% ee, *E*/*Z* >20:1).

$[\alpha]_D^{26}$: +63.1 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 9.8 min (major),

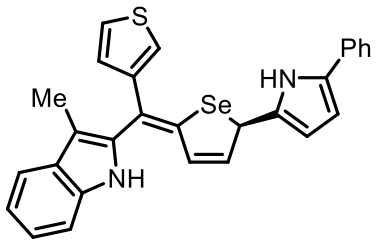
11.6 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.40 (s, 1H), 9.64 (s, 1H), 7.60-7.44 (m, 4H), 7.34-7.02 (m, 9H), 6.82-6.81 (m, 1H), 6.47 (t, J = 2.6 Hz, 1H), 6.37 (dd, J_1 = 3.0 Hz, J_2 = 6.4 Hz, 1H), 6.10-6.06 (m, 2H), 2.25 (s, 3H), 2.10 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.2, 143.1, 139.0, 137.3, 137.2, 134.7, 134.3, 134.1, 133.9, 133.0, 131.4, 130.1, 130.0, 129.5, 128.9, 126.8, 126.4, 125.7, 124.3, 122.5, 119.6, 119.2, 111.6, 109.7, 108.5 107.0, 46.6, 19.6, 10.4.

IR (thin film) 3438, 3054, 2916, 1605, 1508, 1455, 1298, 1264, 1123, 1040, 755, 734, 693 cm^{-1}.

HRMS (CI+) Calcd for $C_{31}H_{26}N_2Se$ (M^+): 506.1261, Found: 506.1277.



5e

(*R*,*E*)-3-Methyl-2-((5-(5-phenyl-1*H*-pyrrol-2-yl)selenophen-2(5*H*)-ylidene)(thiophen-3-yl)methyl)-1*H*-indole (5e) was prepared as slightly yellowish foam from (3-methyl-1*H*-indol-2-yl)(selenophen-2-yl)(thiophen-3-yl)methanol (74.4 mg, 0.2 mmol) and 2-phenylpyrrole (34.3 mg, 0.24 mmol) according to the General Procedure D (eluent: hexanes/EtOAc = 15:1 → 10:1) in 92% yield (91.6 mg, 98% ee, *E*/*Z* >20:1).

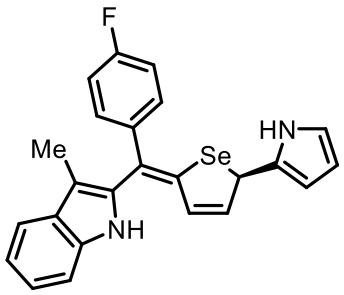
$[\alpha]_D^{26}$: +120.7 (c = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 14.7 min (major), 18.8 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.47 (s, 1H), 9.91 (s, 1H), 7.62-7.56 (m, 3H), 7.39-7.30 (m, 5H), 7.17-7.05 (m, 3H), 6.99 (dd, J_1 = 1.4 Hz, J_2 = 5.0 Hz, 1H), 6.55 (dd, J_1 = 2.2 Hz, J_2 = 6.6 Hz, 1H), 6.47 (t, J = 2.8 Hz, 1H), 6.27 (dd, J_1 = 3.1 Hz, J_2 = 6.6 Hz, 1H), 6.16 (t, J = 2.6 Hz, 1H), 6.09 (t, J = 2.6 Hz, 1H), 2.18 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 144.5, 144.0, 137.7, 137.0, 135.4, 135.2, 133.9, 133.7, 133.1, 129.7, 129.5, 128.6, 126.5, 126.1, 124.3, 124.0, 122.5, 121.4, 119.6, 119.3, 111.7, 110.1, 108.7, 107.0, 48.0, 9.7.

IR (thin film) 3404, 3049, 2912, 1694, 1603, 1507, 1455, 1263, 1122, 1039, 780, 731, 691 cm^{-1}.

HRMS (CI+) Calcd for $C_{28}H_{22}N_2SSe$ (M^+): 498.0669, Found: 498.0678.



5f

(*R*,*E*)-2-((5-(1*H*-pyrrol-2-yl)selenophen-2(5*H*)-ylidene)(4-fluorophenyl)methyl)-3-methyl-1*H*-indole (5f) was prepared as slightly yellow-brown foam from (4-fluorophenyl)(3-methyl-1*H*-indol-2-yl)(selenophen-2-yl)methanol (76.9 mg, 0.2 mmol) and pyrrole (134 mg, 2.0 mmol) according to the General Procedure D (24 h, eluent: hexanes/EtOAc = 30:1 → 20:1) in 57% yield (49.6 mg, 92% ee, *E*/*Z* >20:1). $[\alpha]_D^{26}$: +34.2 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 10.2 min (major), 21.1 min (minor).

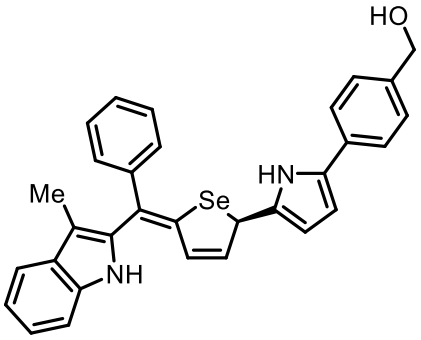
^{1}H NMR (400 MHz, acetone-d_6) δ 9.88 (s, 1H), 9.86 (s, 1H), 7.55 (d, J = 7.9 Hz, 1H), 7.40-7.36 (m, 2H), 7.31 (d, J = 8.0 Hz, 1H), 7.14-7.03 (m, 4H), 6.76-6.74 (m, 1H), 6.57 (dd, J_1 = 2.2 Hz, J_2 = 6.5 Hz, 1H), 6.25 (dd, J_1 = 3.1 Hz, J_2 = 6.6 Hz, 1H), 6.12 (t, J = 2.6 Hz, 1H), 6.03-5.99 (m, 2H), 2.16 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 162.5 (d, J = 241.9 Hz), 145.5, 139.7 (d, J = 3.5 Hz), 138.9, 137.3, 135.1, 134.9, 131.5, 130.9 (d, J = 8.0 Hz), 129.7, 125.2, 122.6, 119.6, 119.3, 119.2, 115.9 (d, J = 21.6 Hz), 111.7, 110.7, 108.8, 107.0, 47.7, 9.8.

^{19}F NMR (376 MHz, acetone-d_6) δ -114.9.

IR (thin film) 3393, 3049, 2963, 1595, 1501, 1258, 1226, 1087, 1019, 795, 729 cm^{-1}.

HRMS (LD+) Calcd for $C_{24}H_{19}FN_2Se$ [M^+]: 434.0697, Found: 434.0715.



5g

(*R*,*E*)-(4-(5-(5-((3-Methyl-1*H*-indol-2-yl)(phenyl)methylene)-2,5-dihydroselenophen-2-yl)-1*H*-pyrrol-2-yl)phenyl)methanol (5g) was prepared as slightly yellowish foam from (3-methyl-1*H*-indol-2-yl)(phenyl)(selenophen-2-yl) methanol (76.9 mg, 0.21 mmol) and (4-(1*H*-pyrrol-2-yl)phenyl)methanol (34.6 mg, 0.2 mmol) according to the General Procedure D (30 h, eluent: hexanes/EtOAc = 10:1 → 3:1) in 90% yield (93.9 mg, 95% ee, *E*/*Z* >20:1).

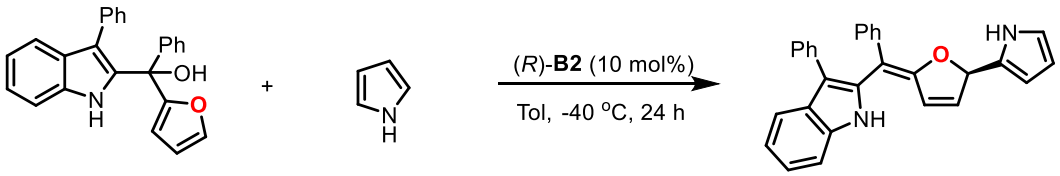
$[\alpha]_D^{26}$: +123.4 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 30% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 15.9 min (major), 20.8 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.44 (s, 1H), 9.87 (s, 1H), 7.58-7.56 (m, 3H), 7.37-7.20 (m, 8H), 7.14-7.04 (m, 2H), 6.62 (dd, J_1 = 2.2 Hz, J_2 = 6.6 Hz, 1H), 6.45 (t, J = 3.2 Hz, 1H), 6.31 (dd, J_1 = 3.1 Hz, J_2 = 6.5 Hz, 1H), 6.13 (t, J = 2.6 Hz, 1H), 6.08 (t, J = 2.9 Hz, 1H), 4.61 (s, 2H), 2.18 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 145.4, 143.4, 140.8, 138.1, 137.3, 135.4, 135.3, 133.7, 133.2, 132.6, 129.7, 129.1, 128.8, 128.2, 127.9, 126.3, 124.2, 122.5, 119.6, 119.3, 111.7, 110.7, 108.6, 106.8, 64.5, 47.3, 9.9.

IR (thin film) 3540, 3413, 3329, 3031, 2915, 1613, 1457, 1263, 768, 732, 698 cm^{-1}.

HRMS (LD+) Calcd for $C_{31}H_{25}N_2OSe$ [$(M-H)^+$]: 521.1127, Found: 521.1109.



6 **2b** **7**

(*R*,*E*)-2-((5-(1*H*-pyrrol-2-yl)furan-2(5*H*)-ylidene)(phenyl)methyl)-3-phenyl-1*H*-indole (7) was prepared as pink foam from

furan-2-yl(phenyl)(3-phenyl-1*H*-indol-2-yl)methanol (73.0 mg, 0.2 mmol) and pyrrole (134.0 mg, 2.0 mmol) according to the General Procedure C (-40 °C, eluent: hexanes/EtOAc = 40:1 → 20:1) in 92% yield (76.5 mg, 92% ee, *E*/*Z* = 6.7:1).

$[\alpha]_D^{26}$: -7.1 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 6.1 min (major), 8.5 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.23 (s, 1H), 9.75 (s, 1H), 7.82 (d, J = 7.9 Hz, 1H), 7.61-7.53 (m, 4H), 7.46 (d, J = 7.9 Hz, 1H), 7.37-7.33 (m, 2H), 7.23-7.06 (m, 6H), 6.81-6.79 (m, 1H), 6.31-6.26 (m, 2H), 7.03 (dd, J_1 = 2.0 Hz, J_2 = 5.8 Hz, 1H), 6.07-6.05 (m, 1H), 6.03-6.01 (m, 1H).

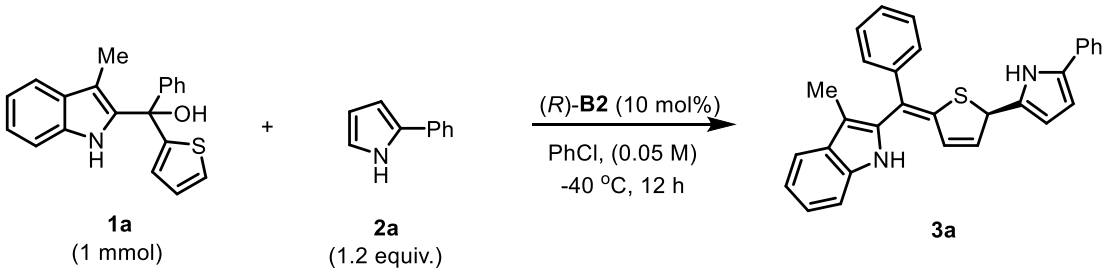
^{13}C NMR (100 MHz, acetone-d_6) δ 161.1, 139.3, 137.4, 137.0, 135.7, 134.8, 129.5, 129.2, 129.0, 128.6, 128.2, 128.0, 127.7, 126.3, 126.2, 122.7, 120.5, 119.9, 119.7, 117.3, 112.0, 108.9, 108.7, 102.2, 85.5.

IR (thin film) 3408, 3049, 2919, 1607, 1439, 1259, 1174, 1081, 1019, 913, 787, 727, 698 cm^{-1}.

HRMS (CI+) Calcd for $C_{29}H_{22}N_2O$ (M^+): 414.1732, Found: 414.1726.

V. Scale-up Reaction and Application

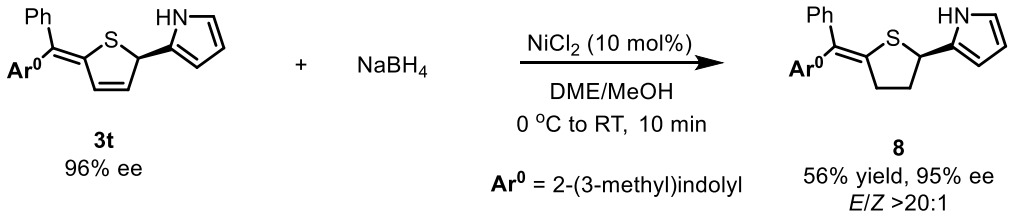
1-Mmol-scale synthesis



At -40 °C, to an oven-dried 50 mL flask charged with a solution of the tertiary alcohol **1a** (1 mmol, 319 mg) and 2-phenylpyrrole **2a** (0.24 mmol, 171.6 mg) in PhCl (9 mL) was slowly added a solution of catalyst (*R*)-**B2** (100 mg, 0.015 mmol, 10 mol%) in PhCl (1 mL). The reaction mixture was stirred at the same temperature for 12 h. After that, triethylamine (0.2 mL) was added to quench the reaction. The mixture was concentrated under reduced pressure and purified by silica gel (deactivated by triethylamine) flash chromatography to afford the desired product **3a** in 95% yield

(420 mg, 94% ee, *E*/*Z* >20:1) as pale green foam.

Regioselective reduction



At 0 °C, to an oven-dried 8-mL vial charged with a solution of **3t** (0.2 mmol, 73.6 mg) and $NiCl_2$ (0.02 mmol, 2.6 mg) in DME/MeOH (1 mL/1 mL) was slowly added $NaBH_4$ (76 mg, 2 mmol, 10 equiv.) in 3 portions over 5 min at room temperature with the formation of a black solid and evolution of hydrogen. After that, the reaction mixture was stirred at room temperature for 10 min. TLC showed the reaction was finished. Water (5 mL) was slowly added to quench the reaction and the final mixture was extracted with ethyl acetate (2 x 10 mL). The combined organic phase was dried, concentrated and then purified by silica gel (deactivated by triethylamine) flash chromatography (eluent: hexanes/EtOAc = 30:1 → 15:1) to afford the desired product **8** in 56% yield (41.1 mg, 95% ee, *E*/*Z* >20:1) as slightly purple foam.

$[\alpha]_D^{26}$: -98.6 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 8.1 min (major), 11.7 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.01 (s, 1H), 9.79 (s, 1H), 7.51 (d, J = 7.8 Hz, 1H), 7.35-7.25 (m, 5H), 7.18-7.14 (m, 1H), 7.10-6.99 (m, 2H), 6.74-6.72 (m, 1H), 6.10-6.08 (m, 1H), 6.02-5.99 (m, 1H), 4.95 (dd, J_1 = 5.3 Hz, J_2 = 9.7 Hz, 1H), 2.94-2.87 (m, 1H), 2.82-2.74 (m, 1H), 2.44-2.37 (m, 1H), 2.31-2.23 (m, 1H), 2.15 (s, 3H).

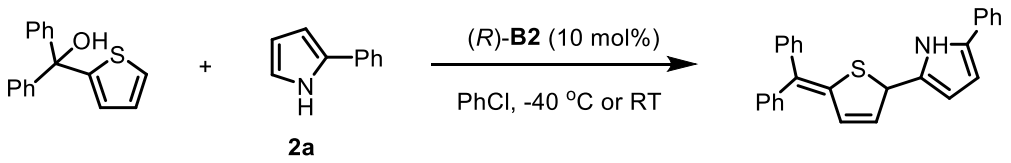
^{13}C NMR (100 MHz, acetone-d_6) δ 147.2, 142.4, 137.1, 136.2, 130.9, 129.8, 129.3, 128.8, 127.3, 122.0, 120.6, 119.3, 119.1, 118.7, 111.6, 109.1, 108.5, 106.8, 49.0, 37.8, 37.5, 9.6.

IR (thin film) 3398, 3048, 2924, 1590, 1447, 1311, 1247, 1088, 1024, 791, 724 cm^{-1}.

HRMS (CI+) Calcd for $C_{24}H_{22}N_2S$ (M^+): 370.1504, Found: 370.1500.

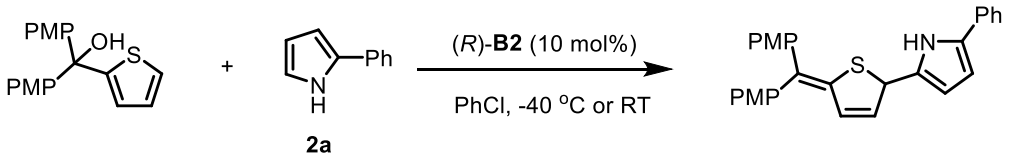
VI. Mechanistic Experiments

Control experiments.



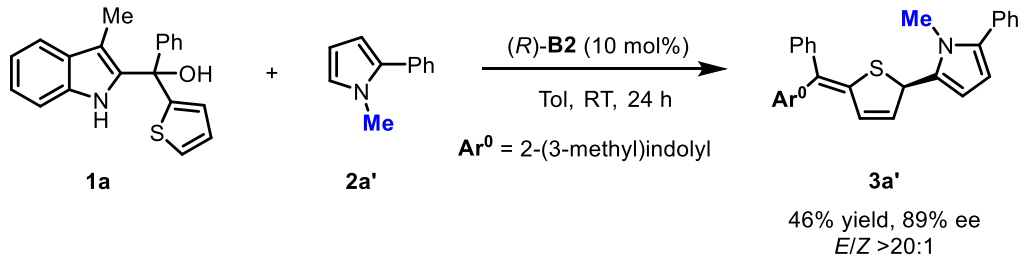
-40 °C, 72 h, NR
RT, 12 h, <5% Conv., trace pdt

At -40 °C or rt to an oven-dried 8-mL vial charged with a solution of diphenyl(thiophen-2-yl)methanol (6.7 mg, 0.025 mmol) and 2-phenylpyrrole **2a** (4.3 mg, 0.03 mmol) in PhCl (0.4 mL) was slowly added a solution of catalyst (*R*)-**B2** (2.5 mg, 0.015 mmol, 10 mol%) in PhCl (0.1 mL). The reaction mixture was stirred for 12 h at room temperature or for 72 h at -40 °C. After that, the reaction mixture was filtered through a short pad of silica gel and then concentrated. The crude mixture was examined by NMR and the ee value of the product was determined by HPLC. For the reaction at room temperature, crude NMR showed <5% conversion and <3% yield. For the reaction at -40 °C, crude ^{1}H NMR showed no reaction at all.



-40 °C, 72 h, 100% Conv., 75% yield, 16% ee
RT, 12 h, 100% Conv., 75% yield, 2% ee

At -40 °C or rt to an oven-dried 8-mL vial charged with a solution of bis(4-methoxyphenyl)(thiophen-2-yl)methanol (8.2 mg, 0.025 mmol) and 2-phenylpyrrole **2a** (4.3 mg, 0.03 mmol) in PhCl (0.4 mL) was slowly added a solution of catalyst (*R*)-**B2** (2.5 mg, 0.015 mmol, 10 mol%) in PhCl (0.1 mL). The reaction mixture was stirred at the same temperature for 12 h at room temperature or 72 h at -40 °C. After that, the reaction mixture was filtered through a short pad of silica gel and then concentrated. The crude mixture was examined by NMR and the ee value of the product was determined by HPLC. For the reaction at rt, crude ^{1}H NMR showed 100% conversion, 75% yield and 2% ee. For the reaction at -40 °C, crude NMR showed 75% yield and 2% ee



(*R*,*E*)-3-Methyl-2-((5-(1-methyl-5-phenyl-1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene) (phenyl)methyl)-1*H*-indole (3a'). At room temperature, to an oven-dried 8-mL vial charged with a solution of the tertiary alcohol **1a** (63.8 mg, 0.2 mmol) and pyrrole **2a'** (37.7 mg, 0.24 mmol) in toluene (3.6 mL) was added a solution of catalyst (*R*)-**B2** (20 mg, 0.015 mmol, 10 mol%) in toluene (0.4 mL). The reaction mixture was stirred at the same temperature for 24 h. After that, triethylamine (2 drops) was added to quench the reaction. The mixture was concentrated under reduced pressure and purified by silica gel (deactivated by triethylamine) flash chromatography to afford the desired product **3a'** in 46% yield (41.7 mg, 89% ee, *E*/*Z* >20:1) as slightly green foam.

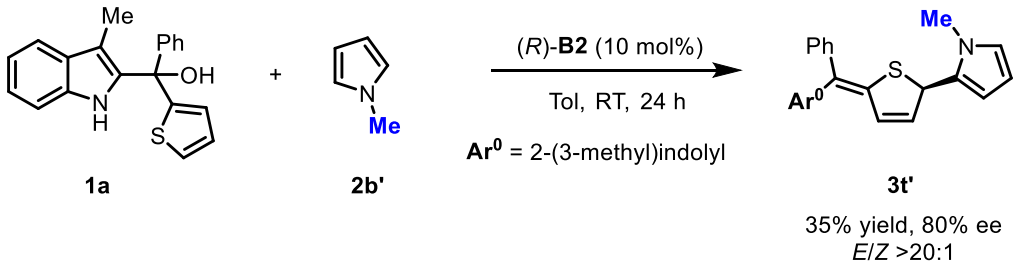
$[\alpha]_D^{26}$: -140.3 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 8.0 min (major), 27.4 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.76 (s, 1H), 7.56-7.21 (m, 12H), 7.12-7.09 (m, 1H), 6.06-6.03 (m, 1H), 6.58-6.55 (m, 1H), 6.47-6.44 (m, 1H), 6.08-6.05 (m, 3H), 3.65 (s, 3H), 2.18 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.0, 141.0, 136.3, 136.0, 134.4, 133.4, 132.9, 132.0, 131.6, 128.7, 128.5, 128.4, 128.1, 127.0, 126.8, 121.6, 118.7, 118.4, 111.5, 110.80, 110.75, 109.9, 107.7, 107.3, 52.7, 31.6, 8.8.

IR (thin film) 3409, 3050, 2920, 1595, 1452, 1258, 1219, 1139, 1080, 1014, 802, 793 cm^{-1}.

HRMS (LD+) Calcd for C31H26N2S (M^+):458.1817, Found: 458.1812.



(*R*,*E*)-3-Methyl-2-((5-(1-methyl-1*H*-pyrrol-2-yl)thiophen-2(5*H*)-ylidene)(phenyl) methyl)-1*H*-indole (3t'). At room temperature, to an oven-dried 8-mL vial charged with a solution of the tertiary alcohol **1a** (63.8 mg, 0.2 mmol) and pyrrole **2b'** (162 mg, 2.0 mmol) in toluene (3.6 mL) was added a solution of catalyst (*R*)-**B2** (20 mg, 0.015 mmol, 10 mol%) in toluene (0.4 mL). The reaction mixture was stirred at the same temperature for 24 h. After that, triethylamine (2 drops) was added to quench the reaction. The mixture was concentrated under reduced pressure and purified by silica gel (deactivated by triethylamine) flash chromatography to afford the desired product **3t'** in 35% yield (26.9 mg, 80% ee, *E*/*Z* >20:1) as slightly pink foam.

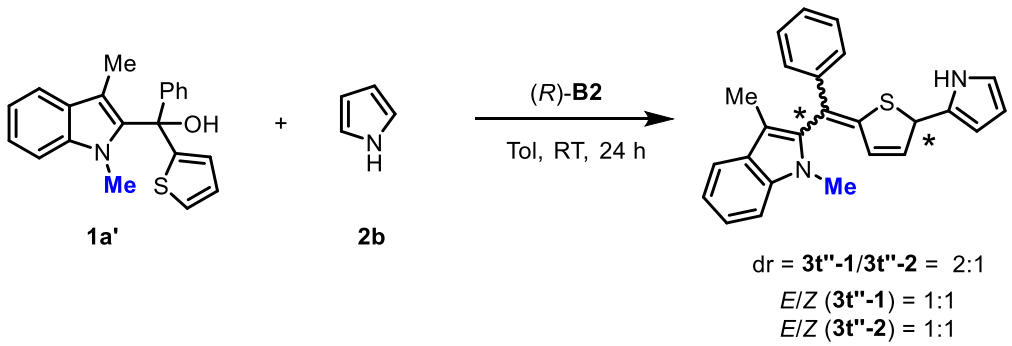
$[\alpha]_D^{26}$: -51.3 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 6.5 min (major), 20.3 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.85 (s, 1H), 7.54 (d, J = 7.8 Hz, 1H), 7.36-7.28 (m, 5H), 7.22-7.19 (m, 1H), 7.12-7.02 (m, 2H), 6.67-6.66 (m, 1H), 6.52 (dd, J_1 = 2.2 Hz, J_2 = 6.2 Hz, 1H), 6.37 (dd, J_1 = 3.0 Hz, J_2 = 6.2 Hz, 1H), 5.97-5.92 (m, 3H), 3.65 (s, 3H), 2.17 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.0, 141.9, 137.4, 137.3, 135.4, 133.6, 130.4, 129.8, 129.3, 129.0, 127.9, 124.4, 122.5, 121.6, 119.5, 119.3, 111.7, 110.7, 108.4, 107.5, 53.2, 34.2, 9.7.

IR (thin film) 3399, 3048, 2923, 1576, 1448, 1307, 1258, 1080, 1018, 797, 716 cm^{-1}.

HRMS (LD+) Calcd for $C_{25}H_{22}N_2S$ (M^+): 382.1504, Found: 382.1508.



At room temperature, to an oven-dried 8-mL vial charged with a solution of the tertiary alcohol **1a'** (66.6 mg, 0.2 mmol) and pyrrole **2b** (134 mg, 2.0 mmol) in toluene (3.6 mL) was added a solution of catalyst (*R*)-**B2** (20 mg, 0.015 mmol, 10 mol%) in toluene (0.4 mL). The reaction mixture was stirred at the same temperature for 24 h. After that, triethylamine (2 drops) was added to quench the reaction. The mixture was concentrated under reduced pressure and purified by silica gel (deactivated by triethylamine) flash chromatography to afford the desired product **3t"-1** in 55% yield (42.3 mg, *E*/*Z* = 1:1) as slightly green foam and product **3t"-2** in 26% yield (19.5 mg, *E*/*Z* = 1:1) as slightly green foam. Various HPLC conditions by using different chiral column were tried, however neither **3t"-1** nor **3t"-2** could be well separated to give their isomers. However, the mixture of isomers for **3t"-1** and **3t"-2** was reported as below.

For product **3t"-1**, *E*/*Z* = 1:1.

^{1}H NMR (400 MHz, acetone-d_6) δ 10.08 (s, 1H), 10.00 (s, 1H), 7.58-7.56 (m, 2H), 7.36-7.29 (m, 10H), 7.21-7.15 (m, 4H), 7.10-7.06 (m, 2H), 6.78-6.72 (m, 2H), 6.35-6.32 (m, 2H), 6.26 (dd, J_1 = 2.1Hz, J_1 = 6.2 Hz, 2H), 6.08-6.00 (m, 4H), 5.97 (t, J = 2.5 Hz, 1H), 5.95 (t, J = 2.5 Hz, 1H), 3.40 (s, 3H), 3.39 (s, 3H), 2.21 (s, 3H), 2.19 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 149.1, 148.9, 141.50, 141.49, 138.3, 138.2, 138.1, 138.0, 137.6, 137.5, 133.1, 133.0, 130.1, 130.0, 129.9, 129.22, 129.15, 129.1, 128.9, 128.7, 128.6, 127.8, 127.7, 127.6, 122.38, 122.36, 119.77, 119.76, 119.6, 119.4, 119.3, 119.2, 119.1, 110.55, 110.50, 109.99, 109.97, 108.8, 107.4, 107.2, 54.8, 54.5, 30.63, 30.56, 9.7, 9.6.

IR (thin film) 3438, 3050, 2922, 1568, 1465, 1358, 1256, 1140, 1016, 722 cm^{-1}.

HRMS (CI+) Calcd for $C_{25}H_{22}N_2S$ (M^+): 382.1504, Found: 382.1495.

For product **3t"-2**, *E*/*Z* = 1:1.

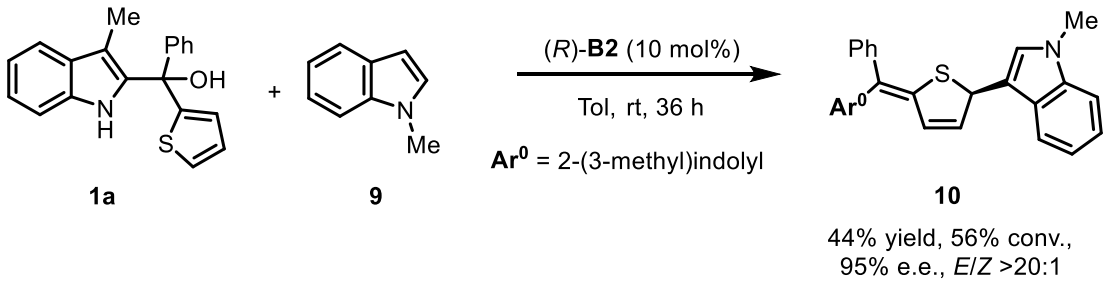
^{1}H NMR (400 MHz, acetone-d_6) δ 9.99 (s, 2H), 7.54-7.51 (m, 2H), 7.37-7.33 (m, 4H),

7.28-7.22 (m, 8H), 7.15-7.10 (m, 2H), 7.04-7.00 (m, 2H), 6.96-6.92 (m, 2H), 6.75-6.73 (m, 1H), 6.72-6.70 (m, 1H), 6.49-6.45 (m, 2H), 6.03-5.96 (m, 4H), 5.84 (t, *J* =2.6 Hz), 5.79 (t, *J* =2.6 Hz), 3.45 (s, 3H), 3.41 (s, 3H), 2.26 (s, 3H), 2.24 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 151.2, 151.1, 141.2, 141.10, 141.05, 141.0, 139.3, 139.1, 138.3, 138.2, 130.5, 130.3, 129.93, 129.92, 129.5, 129.4, 129.28, 129.25, 129.2, 127.70, 127.67, 122.4, 119.7, 119.62, 119.56, 119.45, 119.41 (2C), 119.3, 119.2, 119.14, 119.07, 110.0, 109.9, 109.7, 109.4, 108.7, 108.6, 107.3, 107.1, 53.2, 53.1, 30.7 (2C), 9.9, 9.8.

IR (thin film) 3397, 3047, 2919, 1584, 1464, 1359, 1254, 1137, 1090, 1047, 787, 728 cm^{-1}.

HRMS (CI+) Calcd for $C_{25}H_{22}N_2S$ (M^+): 382.1504, Found: 382.1496.



(*R*,*E*)-1-Methyl-3-(5-((3-methyl-1*H*-indol-2-yl)(phenyl)methylene)-2,5-dihydrothiophen-2-yl)-1*H*-indole (10). At room temperature, to an oven-dried 8-mL vial charged with a solution of the tertiary alcohol **1a** (63.8 mg, 0.2 mmol) and pyrrole **9** (32.8 mg, 0.25 mmol) in toluene (3.6 mL) was added a solution of catalyst (*R*)-**B2** (20 mg, 0.015 mmol, 10 mol%) in toluene (0.4 mL). The reaction mixture was stirred at the same temperature for 36 h. After that, triethylamine (2 drops) was added to quench the reaction. The mixture was concentrated under reduced pressure and purified by silica gel (deactivated by triethylamine) flash chromatography to afford the desired product **10** in 44% yield (37.9 mg, 95% e.e., *E*/*Z* >20:1) as slightly purple foam. Additionally, 28.0 mg (44%) of **1a** was recovered.

$[\alpha]_D^{26}$: +106.9 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 15% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 17.7 min (major), 29.1 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.88 (s, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.40-7.36 (m, 3H), 7.34-7.25 (m, 3H), 7.21-7.03 (m, 6H), 6.53-6.51 (m,

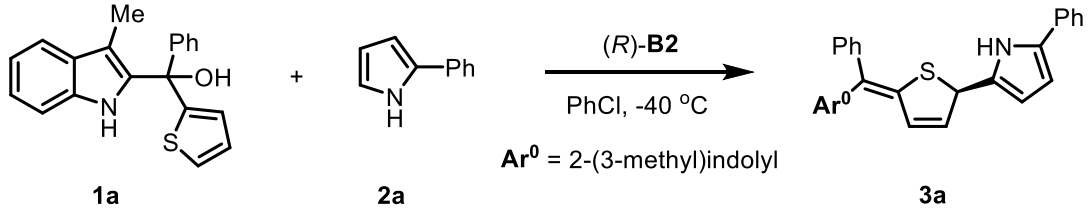
1H), 6.45-6.43 (m, 1H), 6.12-6.11 (m, 1H), 3.79 (s, 3H), 2.24 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 148.0, 142.1, 139.4, 138.6, 137.3, 135.6, 132.7, 129.8, 129.2, 128.9, 128.0, 127.7, 127.5, 122.6, 122.4, 120.8, 120.2, 119.8, 119.5, 119.2, 113.8, 111.7, 110.5 (2C), 53.7, 32.8, 9.8.

IR (thin film) 3402, 3051, 2919, 2861, 1724, 1591, 1459, 1330, 1253, 1139, 1084, 735, 695 cm^{-1}.

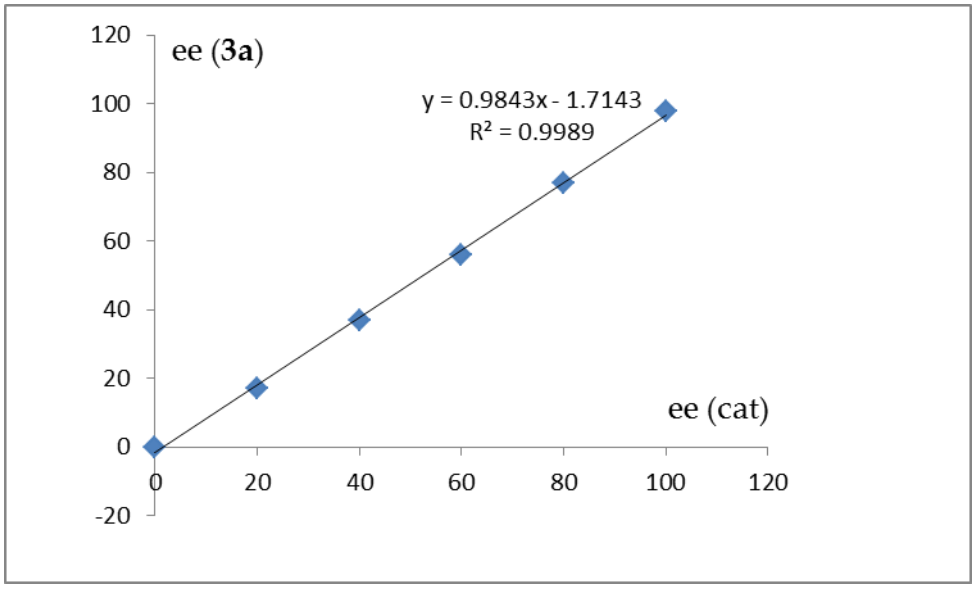
HRMS (ES-) Calcd for C29H23N2S (M-H)$^-$: 431.1587, Found: 431.1585.

Non-linear effects.



At -40 °C, to an oven-dried 4-mL vial charged with a solution of catalysts (*R*)-**B2** (2.5 mg, 10 mol%) with different enantiopurities (1st run: 0% ee, 2nd run: 20% ee; 3rd run: 40% ee; 4th run: 60% ee; 5th run: 80% ee; 6th run: 100% ee.) in PhCl (0.4 mL) was added a solution of **1a** (8.3 mg, 0.025 mmol,) and **2a** (4.3 mg, 0.03 mmol) in DCE (0.1 mL). The reaction mixture was stirred at 0 °C for 12 h. After that, the reaction mixture was filtered through a short pad of silica gel and then concentrated. The ee value of the product **3a** was determined by HPLC.

ee-(**B2**)	0	20	40	60	80	100
ee-(**3a**)	0	17	37	56	77	98



Linear relationship between product **3a** and catalyst's ee.

VII. DFTCalculations

Supplementary Table. 13. Absolute Calculation Energies, Enthalpies, and Free Energies

Geometry	$E_{(elec\text{-}B3LYP\text{-}D3BJ)}$[1]	$H_{(corr\text{-}B3LYP\text{-}D3BJ)}$[2]	$G_{(corr\text{-}B3LYP\text{-}D3BJ)}$[3]	$E_{(solv\text{-}M062X)}$[4]	IF[5]
(R)-B2	-3287.728073	1.518087	1.344659	-3286.830749	-
CP1	-722.762442	0.11661	0.072389	-722.7234764	-
CP2	-1300.614965	0.339407	0.268633	-1300.395637	-
CP3	-2023.417706	0.458625	0.365809	-2023.144971	-
CP4-E	-1946.962856	0.428696	0.339611	-1946.679999	-
CP4-Z	-1946.969004	0.428817	0.340623	-1946.684194	-
CP5	-441.266509	0.173545	0.13036	-441.1611084	-
CP6-E	-2388.28183	0.606584	0.498993	-2387.877831	-
CP6-Z	-2388.269229	0.606188	0.49552	-2387.870028	-
CP7-E	-1665.475587	0.487805	0.397048	-1665.138196	-
CP7-Z	-1665.478331	0.487886	0.398532	-1665.139526	-
H2O	-76.409528	0.024936	0.002835	-76.42737793	-
TS1-E	-2023.391742	0.453828	0.362046	-2023.11152	-269.93
TS1-Z	-2023.392778	0.453679	0.36266	-2023.112753	-382.17
TS2-E-E	-2388.257248	0.604358	0.49699	-2387.849406	-428.43
TS2-E-Z	-2388.261357	0.604354	0.498272	-2387.852443	-403.01
TS2-R-E	-4953.281913	2.008315	1.781288	-4951.995688	-432.32
TS2-S-E	-4953.271719	2.007285	1.778362	-4951.989286	-445.85
TS2-Z-E	-2388.274781	0.605123	0.498495	-2387.861903	-427.57
TS2-Z-Z	-2388.262244	0.604811	0.49653	-2387.851768	-431.2
TS3-E	-2388.258439	0.601328	0.491142	-2387.854771	-1328.87
TS3-Z	-2388.260518	0.601585	0.492136	-2387.857128	-956.97

[1]The electronic energy calculated by B3LYP-D3BJ in gas phase. [2]The thermal correction to enthalpy calculated by B3LYP-D3BJ in gas phase. [3] The thermal correction to Gibbs free energy calculated by B3LYP-D3BJ in gas phase. [4]The electronic energy calculated by M062X in chlorobenzene solvent. [5]The B3LYP-D3BJ calculated imaginary frequencies for the

transition states.

Supplementary Table. 14. B3LYP-D3BJ Geometries for All the Optimized Compounds and Transition States

CP1

P	-0.035562	0.461249	-0.108770
O	-0.009323	0.575770	1.516751
O	-0.619884	1.637011	-0.779919
O	1.462573	0.133399	-0.551583
O	-0.739491	-0.968005	-0.309915
C	-2.139685	-1.083243	0.000458
C	2.175026	-0.974661	0.026180
H	-0.068316	1.511549	1.770290
H	-2.715101	-0.345135	-0.565246
H	-2.437219	-2.091162	-0.291012
H	-2.300750	-0.942546	1.073645
H	1.701512	-1.917699	-0.258470
H	3.187543	-0.927123	-0.376366
H	2.202716	-0.884593	1.116211

CP2

C	-0.886709	0.038295	0.617371
C	4.079381	-1.166270	0.427788
C	2.793613	-0.609407	0.323507
C	5.144819	-0.516238	-0.180237
C	2.623478	0.601308	-0.405462
C	1.497613	-1.005041	0.812090
C	4.953484	0.685219	-0.894615
H	6.144024	-0.935884	-0.107176
C	3.694362	1.260059	-1.017510
C	0.606043	-0.043708	0.377472
H	5.807393	1.170814	-1.358174
H	3.547791	2.185223	-1.567910
H	0.835756	1.721973	-0.768620
H	4.234754	-2.091809	0.975456
N	1.284305	0.917077	-0.357269
C	1.189159	-2.254154	1.581771
H	1.297113	-3.145024	0.949598
H	1.872719	-2.376011	2.431239
H	0.166620	-2.246537	1.965810
C	-1.760747	1.629646	-1.264602
C	-2.201242	2.979280	-1.430194
H	-1.680657	0.909978	-2.071371
C	-2.232118	3.670058	-0.249556
H	-2.493786	3.405472	-2.383595

H	-2.548641	4.690698	-0.081620
C	-1.465096	1.319688	0.038349
S	-1.733751	2.683597	1.088672
C	-1.624893	-1.159157	0.010844
C	-2.813293	-1.604024	0.597729
C	-1.161513	-1.775634	-1.154360
C	-3.523837	-2.658956	0.028112
H	-3.166640	-1.126290	1.504410
C	-1.878181	-2.827112	-1.727977
H	-0.229905	-1.445340	-1.603475
C	-3.060369	-3.272618	-1.137603
H	-4.442069	-3.003086	0.496073
H	-1.504846	-3.302623	-2.630718
H	-3.615501	-4.095175	-1.579685
O	-1.131243	0.051374	2.040918
H	-0.268014	0.168144	2.467055

CP3

P	-3.093926	0.257509	-0.984802
O	-4.655659	0.375101	-1.307010
O	-2.975086	0.078356	0.611926
O	-2.324864	1.410029	-1.523781
O	-2.714628	-1.192527	-1.523466
C	0.866323	-0.948665	-0.286546
C	0.021056	-1.432925	0.894712
C	0.028254	-0.757131	2.116247
C	-0.765702	-2.582944	0.753864
C	-0.750693	-1.215900	3.179012
C	-1.551151	-3.033835	1.812007
C	-1.547882	-2.349985	3.028515
H	-0.767552	-3.118318	-0.189103
H	-0.735906	-0.680112	4.124194
H	-2.167765	-3.918865	1.684143
H	-2.160683	-2.701207	3.853919
H	-1.729076	-1.303511	-1.501452
O	-0.011848	-1.102056	-1.452662
H	0.463848	-0.782294	-2.237453
H	0.635580	0.134110	2.229353
C	2.073212	-1.836815	-0.492406
C	2.392161	-3.030307	0.099673
H	1.799408	-3.467503	0.893039
C	3.577846	-3.623428	-0.432224
C	4.139935	-2.878521	-1.431009
H	3.990701	-4.562682	-0.081498

H	5.036528	-3.085965	-1.999341
S	3.249137	-1.418645	-1.721115
C	0.247216	3.978008	-0.464781
C	0.812792	2.715609	-0.251251
C	0.958687	5.078011	-0.003707
C	2.062262	2.539352	0.403503
C	2.202363	4.928294	0.649040
H	0.550668	6.074724	-0.146710
C	2.759743	3.673600	0.854823
C	2.320443	1.122604	0.460316
C	1.245837	0.508783	-0.164035
H	2.729445	5.813663	0.993503
H	3.718747	3.569673	1.355549
C	3.514287	0.507195	1.128591
H	3.354692	-0.544787	1.373719
H	4.409903	0.563608	0.496587
H	3.741035	1.038945	2.060460
N	0.339426	1.470151	-0.582936
H	-0.562683	1.306405	-1.035252
H	-0.710179	4.078814	-0.967008
C	-2.797474	1.252356	1.426590
H	-3.649340	1.931383	1.318474
H	-2.732532	0.892943	2.453098
H	-1.875075	1.769565	1.153880
C	-5.554725	-0.661337	-0.874589
H	-5.470787	-0.815197	0.205430
H	-6.558987	-0.317480	-1.125310
H	-5.335353	-1.594620	-1.399930

CP4-E

P	-1.432228	-1.706537	-0.911940
O	-1.352721	-2.643504	-2.252923
O	-3.021991	-1.815276	-0.502494
O	-0.678946	-2.357419	0.231415
O	-1.097481	-0.300002	-1.340477
C	-0.052516	1.136782	0.562161
C	-1.012931	0.664028	1.554381
C	-0.575550	0.096603	2.767342
C	-2.396069	0.777123	1.308851
C	-1.498606	-0.334298	3.710932
C	-3.312513	0.330736	2.250032
C	-2.867336	-0.222183	3.453106
H	-2.724313	1.145733	0.345764
H	-1.153285	-0.763821	4.646284

H	-4.375123	0.386876	2.035870
H	-3.586750	-0.577627	4.185236
H	0.486764	0.012830	2.963856
C	-0.382946	2.301341	-0.209975
C	-1.101356	3.418888	0.203486
H	-1.480885	3.521088	1.212851
C	-1.226056	4.398629	-0.804538
C	-0.633609	4.005237	-1.987728
H	-1.736512	5.345621	-0.674354
H	-0.622756	4.547257	-2.924552
S	0.078006	2.445900	-1.889631
C	3.357132	-2.371538	0.517064
C	2.710751	-1.123611	0.475517
C	4.721914	-2.384481	0.300773
C	3.425680	0.082360	0.175700
C	5.456233	-1.193138	0.041766
H	5.255216	-3.330335	0.332147
C	4.826497	0.031662	-0.019676
C	2.479018	1.133724	0.131368
C	1.221617	0.537186	0.430124
H	6.528318	-1.260557	-0.116269
H	5.386641	0.937786	-0.231884
C	2.823508	2.582748	-0.022365
H	2.023962	3.234224	0.337024
H	3.011158	2.843598	-1.070456
H	3.735178	2.814176	0.540527
N	1.405703	-0.818032	0.687428
H	0.595604	-1.503541	0.599122
H	2.796458	-3.278906	0.715350
C	-3.958151	-1.231148	-1.402426
H	-3.721124	-0.177100	-1.586835
H	-4.945497	-1.314554	-0.939156
H	-3.963293	-1.759000	-2.364033
C	-1.532836	-4.048469	-2.078045
H	-0.804052	-4.447959	-1.365479
H	-1.389345	-4.512653	-3.057424
H	-2.543093	-4.272748	-1.713655

CP4-Z

P	-1.402559	-1.818821	0.892554
O	-1.601244	-2.966041	2.042932
O	-2.953755	-1.523196	0.421810
O	-0.672094	-2.507149	-0.251332
O	-0.878715	-0.536235	1.470871

C	0.064803	1.097541	-0.602447
C	3.216858	-2.652425	-0.653531
C	2.659823	-1.362838	-0.598620
C	4.575231	-2.763296	-0.427623
C	3.452965	-0.214312	-0.273054
C	5.389329	-1.629406	-0.144993
H	5.041430	-3.743663	-0.466725
C	4.846206	-0.365912	-0.065869
C	2.577901	0.892594	-0.200649
C	1.279171	0.388519	-0.517563
H	6.452830	-1.774151	0.018629
H	5.466892	0.494344	0.167039
C	3.011480	2.299125	0.071250
H	2.417147	3.029527	-0.482244
H	2.910366	2.551519	1.133060
H	4.062635	2.429097	-0.205055
N	1.375580	-0.973079	-0.802204
H	0.547192	-1.631798	-0.645714
H	2.592929	-3.515106	-0.861430
C	-3.639341	-2.574013	-0.252462
H	-3.782136	-3.437165	0.409033
H	-4.616063	-2.181442	-0.550644
H	-3.082940	-2.895408	-1.138797
C	-2.180002	-2.547169	3.278118
H	-3.209026	-2.196095	3.130251
H	-2.186070	-3.418191	3.938752
H	-1.592464	-1.740915	3.728783
C	-0.057264	2.354079	0.162978
C	0.123082	2.321471	1.555273
C	-0.341551	3.569406	-0.480234
C	0.037912	3.502392	2.286354
H	0.258377	1.356255	2.029746
C	-0.401352	4.749782	0.257945
H	-0.478006	3.587950	-1.556999
C	-0.210061	4.717033	1.640361
H	0.156834	3.475435	3.365532
H	-0.598637	5.691806	-0.244972
H	-0.265198	5.636703	2.215978
C	-1.036009	0.672100	-1.392752
C	-1.103253	-0.332423	-2.362628
H	-0.239696	-0.908838	-2.661401
C	-2.387786	-0.491193	-2.907045
C	-3.308281	0.373688	-2.346185
H	-2.636326	-1.216174	-3.672614

H	-4.363244	0.443545	-2.577176
S	-2.626263	1.393072	-1.154995

CP5

C	3.122894	-0.690235	-0.190222
C	3.211044	0.639799	0.167152
C	1.885057	1.132645	0.295555
C	1.009850	0.091099	0.018784
N	1.790585	-1.015268	-0.261970
H	1.426864	-1.891055	-0.604029
H	3.888160	-1.423856	-0.397056
H	4.125965	1.192965	0.328379
H	1.593322	2.128171	0.600067
C	-0.448704	0.038507	0.012787
C	-1.143331	-1.168373	0.208501
C	-1.199729	1.210219	-0.189671
C	-2.535859	-1.203771	0.190824
H	-0.591081	-2.082687	0.410496
C	-2.590535	1.174846	-0.192223
H	-0.679798	2.147134	-0.364795
C	-3.268087	-0.032833	-0.007661
H	-3.049961	-2.148321	0.346761
H	-3.149394	2.092950	-0.351957
H	-4.353779	-0.059851	-0.017025

CP6-E

P	-3.115576	-1.598666	0.276873
O	-4.253688	-1.611166	1.443134
O	-3.743443	-0.583322	-0.847150
O	-1.888846	-0.825505	0.785549
O	-2.938786	-2.991467	-0.236446
C	1.147514	0.760695	-1.333126
C	-2.904451	2.952407	0.488526
C	-1.647777	2.729131	-0.086366
C	-3.284632	4.270893	0.700163
C	-0.775380	3.797282	-0.445563
C	-2.439715	5.346850	0.344019
H	-4.254992	4.482155	1.141386
C	-1.195569	5.122803	-0.227498
C	0.414424	3.208687	-0.987580
C	0.230930	1.827466	-0.941783
H	-2.775607	6.364901	0.521013
H	-0.553014	5.956523	-0.498660
C	1.584620	3.970828	-1.530917

H	2.183744	3.365565	-2.215030
H	2.256702	4.315440	-0.733328
H	1.244428	4.859362	-2.076064
N	-1.027295	1.552327	-0.410565
H	-1.351274	0.634623	-0.080359
H	-3.552902	2.119134	0.738082
C	-4.889906	-1.038307	-1.570686
H	-4.682462	-1.993174	-2.064255
H	-5.118851	-0.273274	-2.315830
H	-5.747872	-1.165118	-0.900143
C	-4.545253	-0.385706	2.116243
H	-3.629928	0.078138	2.498020
H	-5.209963	-0.630448	2.947958
H	-5.051036	0.317586	1.443428
C	2.586867	0.966673	-1.042521
C	2.981440	1.481347	0.202615
C	3.579579	0.640252	-1.979371
C	4.328846	1.637388	0.511691
H	2.219767	1.741755	0.928106
C	4.929718	0.804950	-1.672228
H	3.288187	0.282674	-2.962326
C	5.309723	1.299379	-0.424158
H	4.613480	2.020512	1.487598
H	5.683930	0.555074	-2.413180
H	6.361695	1.428237	-0.185033
C	0.700318	-0.419518	-1.861443
C	-0.905107	-2.089904	-2.335135
C	0.260949	-2.968805	-1.987760
H	0.393611	-3.813922	-2.667507
C	0.070389	-3.587645	-0.512381
C	1.239785	-4.422651	-0.130678
C	1.961351	-3.768637	0.805115
C	1.244034	-2.542994	1.143516
N	0.126345	-2.513223	0.452284
H	-0.644254	-1.789639	0.531559
H	-0.919355	-4.056419	-0.488757
H	1.496619	-5.354672	-0.618039
H	2.897345	-4.077382	1.248049
C	1.655843	-1.490837	2.063332
C	0.762878	-0.467406	2.437451
C	2.975995	-1.468343	2.545103
C	1.194698	0.550089	3.280969
H	-0.261476	-0.471552	2.078939
C	3.400136	-0.441996	3.381434

H	3.679840	-2.235646	2.241609
C	2.509774	0.567389	3.753306
H	0.501793	1.336409	3.564008
H	4.425379	-0.425853	3.737673
H	2.841283	1.368858	4.407234
H	-1.882932	-2.525313	-2.493499
S	1.733343	-1.875371	-2.063674
C	-0.667273	-0.773995	-2.217368
H	-1.435475	-0.017261	-2.311204

CP6-Z

P	1.395925	-2.783182	-0.384552
O	2.077262	-3.855132	0.640277
O	-0.042542	-3.461123	-0.744499
O	1.004828	-1.526883	0.413200
O	2.282381	-2.660982	-1.584175
C	-1.671629	1.500422	-0.661344
C	-2.626539	-3.097039	0.966096
C	-2.752753	-1.769502	0.535239
C	-3.777555	-3.744552	1.394014
C	-4.007754	-1.094766	0.545685
C	-5.034153	-3.097883	1.396775
H	-3.712079	-4.776352	1.729542
C	-5.157902	-1.783010	0.975699
C	-3.778924	0.238826	0.080155
C	-2.414051	0.336401	-0.195434
H	-5.911714	-3.641828	1.735570
H	-6.124821	-1.286548	0.984772
C	-4.850336	1.270969	-0.104751
H	-4.583225	2.011930	-0.861136
H	-5.058434	1.820533	0.823051
H	-5.785672	0.792918	-0.418133
N	-1.808444	-0.892166	0.063576
H	-0.799762	-1.070403	0.096864
H	-1.664884	-3.593140	0.937551
C	-0.071088	-4.530937	-1.691607
H	0.361499	-4.210665	-2.643508
H	-1.121418	-4.798699	-1.824366
H	0.485767	-5.398034	-1.317129
C	1.419010	-4.113819	1.880414
H	1.213253	-3.181714	2.417032
H	2.090415	-4.741190	2.471611
H	0.474476	-4.646944	1.718427
C	-2.131431	2.817072	-0.141209

C	-2.349973	2.988942	1.234855
C	-2.391515	3.896533	-1.000186
C	-2.795831	4.208402	1.737827
H	-2.171921	2.151906	1.902566
C	-2.840386	5.116941	-0.497137
H	-2.266297	3.760952	-2.070257
C	-3.041850	5.278463	0.874112
H	-2.954270	4.324201	2.806529
H	-3.046799	5.937256	-1.179173
H	-3.397606	6.226985	1.266384
C	-0.599427	1.448198	-1.510100
C	1.501089	0.783659	-2.932406
C	1.344065	2.241709	-2.612889
H	2.108292	2.952557	-2.909453
C	2.722214	0.156821	-2.162460
C	4.004663	0.874996	-2.389722
C	4.470708	1.347845	-1.212908
C	3.545320	0.921547	-0.167246
N	2.555891	0.267088	-0.726732
H	1.833252	-0.339592	-0.228954
H	2.761738	-0.926234	-2.380586
H	4.454319	1.006196	-3.366187
H	5.380349	1.906545	-1.043870
C	3.673253	1.128846	1.270695
C	2.845426	0.433021	2.173655
C	4.630769	2.032952	1.762194
C	2.983819	0.650355	3.539917
H	2.115857	-0.285627	1.809288
C	4.755849	2.247687	3.130577
H	5.267513	2.580376	1.075177
C	3.933008	1.555722	4.021483
H	2.348064	0.107902	4.232823
H	5.493293	2.952681	3.501646
H	4.032615	1.720918	5.090350
S	-0.083554	-0.005187	-2.421920
C	0.294717	2.548768	-1.834101
H	0.117707	3.539097	-1.433357
H	1.666042	0.581719	-3.995774

CP7-E

C	1.741153	-0.928029	-0.242674
C	3.229739	3.818592	-0.354345
C	3.216510	2.422014	-0.315681
C	4.465601	4.450808	-0.269854

C	4.407356	1.654459	-0.186113
C	5.660140	3.710238	-0.156036
H	4.511069	5.535759	-0.295712
C	5.641679	2.322204	-0.115413
C	4.029681	0.267040	-0.158850
C	2.649855	0.221116	-0.272845
H	6.607695	4.238062	-0.097518
H	6.566258	1.758809	-0.023988
C	4.978897	-0.886804	-0.056683
H	4.509955	-1.824043	-0.363719
H	5.339128	-1.025564	0.971293
H	5.857891	-0.722581	-0.691435
N	2.168826	1.530602	-0.396412
H	1.194607	1.770465	-0.297785
H	2.310304	4.390058	-0.448692
C	2.039743	-1.973722	0.768005
C	2.427483	-1.604354	2.067112
C	1.976150	-3.340786	0.453504
C	2.720822	-2.570111	3.025695
H	2.499885	-0.550330	2.316067
C	2.274405	-4.307122	1.412597
H	1.715586	-3.644567	-0.554680
C	2.643996	-3.926810	2.702996
H	3.011046	-2.263676	4.026844
H	2.226862	-5.359316	1.146450
H	2.877409	-4.680472	3.449647
C	0.650676	-0.993596	-1.063936
C	-0.838601	-0.298350	-2.781760
C	-1.680230	-1.448662	-2.286858
H	-1.795149	-2.203813	-3.072443
C	-3.044232	-1.049013	-1.834840
C	-4.294450	-1.363327	-2.335857
C	-5.257963	-0.686161	-1.542535
C	-4.578885	0.030381	-0.565422
N	-3.231346	-0.185634	-0.779979
H	-2.501630	0.048909	-0.122661
H	-4.485726	-1.997266	-3.191307
H	-6.329215	-0.686881	-1.687567
C	-5.066526	0.887173	0.510240
C	-4.252993	1.882012	1.080506
C	-6.374339	0.734019	1.003205
C	-4.727124	2.687623	2.113046
H	-3.251657	2.047593	0.691628
C	-6.850208	1.549164	2.025285

H	-7.007749	-0.045060	0.590213
C	-6.028550	2.527585	2.590182
H	-4.081066	3.451053	2.537751
H	-7.863674	1.412071	2.392145
H	-6.399306	3.158207	3.392850
H	-1.211309	0.304517	-3.603888
S	-0.650486	-2.216291	-0.920398
C	0.327656	-0.082476	-2.156990
H	1.019570	0.703338	-2.436462

CP7-Z

C	1.853639	-0.941702	-0.259548
C	2.256950	4.004825	-0.052014
C	2.551812	2.638199	-0.071777
C	3.319194	4.886420	0.108899
C	3.879382	2.145636	0.069281
C	4.644680	4.421470	0.245028
H	3.125249	5.955075	0.127417
C	4.932576	3.063947	0.226218
C	3.819949	0.712463	0.005728
C	2.481432	0.370981	-0.164818
H	5.448961	5.141177	0.367765
H	5.955372	2.713950	0.335904
C	5.015653	-0.189008	0.070567
H	4.835886	-1.145744	-0.423562
H	5.308780	-0.411234	1.105039
H	5.873408	0.287619	-0.417697
N	1.730127	1.548119	-0.216706
H	0.725247	1.576992	-0.300643
H	1.237212	4.363327	-0.160729
C	2.501960	-2.042847	0.503070
C	2.835828	-1.863795	1.854900
C	2.820323	-3.265041	-0.109380
C	3.455143	-2.881415	2.575766
H	2.609404	-0.914990	2.331503
C	3.441300	-4.283991	0.612173
H	2.599023	-3.399918	-1.163850
C	3.759661	-4.096599	1.957626
H	3.701264	-2.726653	3.622640
H	3.687767	-5.219943	0.118513
H	4.248503	-4.887726	2.518923
C	0.708243	-1.187017	-0.966378
C	-1.522531	-1.175735	-2.448586
C	-1.189864	-2.431966	-1.683530

H	-1.876360	-3.271380	-1.732712
C	-2.836091	-0.587864	-2.067699
C	-3.874844	-0.088795	-2.833870
C	-4.888404	0.355663	-1.945781
C	-4.450204	0.126106	-0.646644
N	-3.196081	-0.440407	-0.748559
H	-2.656247	-0.803478	0.023123
H	-3.888643	-0.039263	-3.914373
H	-5.821862	0.828968	-2.216313
C	-5.080564	0.397124	0.641356
C	-4.318463	0.548457	1.813211
C	-6.478203	0.516805	0.736724
C	-4.933053	0.800531	3.037416
H	-3.233704	0.501164	1.762732
C	-7.088725	0.781846	1.958497
H	-7.083263	0.380792	-0.154451
C	-6.320983	0.920419	3.117272
H	-4.323599	0.916170	3.929415
H	-8.170545	0.869024	2.009202
H	-6.799627	1.120929	4.071270
S	-0.077000	-0.029164	-2.086836
C	-0.080989	-2.410976	-0.927538
H	0.226322	-3.238466	-0.299455
H	-1.523716	-1.348594	-3.530418

H2O

H	0.761649	-0.479066	0.000000
O	0.000000	0.119751	0.000000
H	-0.761649	-0.478941	0.000000

(R)-B2

P	0.298512	0.173692	-1.259675
O	0.945383	1.551179	-0.770047
O	-0.230616	0.148833	-2.631915
O	1.442496	-0.960782	-1.010586
O	-0.757337	-0.128268	-0.052081
C	-1.358519	-1.394931	-0.157268
C	-0.588173	-2.522331	0.141900
C	-2.699931	-1.471120	-0.530218
C	-1.100535	-3.798592	-0.176524
C	-3.212663	-2.750501	-0.742602
C	-2.423272	-3.902632	-0.638322
H	-4.256879	-2.846960	-1.027319
C	0.703888	-2.301217	0.850046

C	0.899753	-2.752264	2.178427
C	1.662669	-1.462780	0.277537
C	2.112563	-2.459982	2.826957
C	2.827743	-1.075829	0.942980
C	3.059530	-1.651811	2.190535
H	3.980899	-1.409283	2.711594
C	3.685583	0.016704	0.394335
C	3.546425	1.325561	0.932128
C	4.571144	-0.223408	-0.671976
C	4.317167	2.356059	0.384258
C	5.322066	0.843021	-1.178156
C	5.210699	2.136053	-0.669734
C	-3.553535	-0.249347	-0.590844
C	-3.989420	0.264872	-1.826269
C	-3.933992	0.372814	0.619732
C	-4.845694	1.371385	-1.824376
C	-4.778095	1.482660	0.568351
C	-5.253474	1.992101	-0.643730
C	-3.025790	-5.231835	-1.056258
H	-4.043851	-5.312668	-0.654964
H	-3.135205	-5.229180	-2.150757
C	-0.203781	-5.020693	-0.090949
H	0.815609	-4.739175	-0.377144
H	-0.136800	-5.372836	0.946255
C	-0.220888	-3.447273	2.932083
H	-0.267150	-4.507622	2.654550
H	-1.180671	-3.017407	2.626735
C	2.398700	-2.897701	4.253840
H	2.449741	-1.996423	4.882074
H	3.397133	-3.351066	4.300389
C	1.348900	-3.848212	4.834603
H	1.499545	-4.861973	4.438364
H	1.466249	-3.911210	5.922276
C	-2.186072	-6.444148	-0.645302
H	-2.546096	-7.339570	-1.164540
H	-2.301342	-6.631578	0.431537
C	-0.050652	-3.366692	4.451098
H	-0.824674	-3.970239	4.938555
H	-0.190357	-2.331168	4.790574
C	-0.710390	-6.181500	-0.951799
H	-0.103119	-7.073669	-0.760594
H	-0.595175	-5.936020	-2.016318
H	1.880972	1.459952	-0.491944
C	-6.168194	3.198619	-0.679154

C	-7.498144	2.946323	0.060487
C	-5.478283	4.462261	-0.124207
H	-6.413674	3.397919	-1.732807
C	-8.421052	4.170112	0.001871
H	-7.284462	2.703123	1.110785
H	-7.994126	2.066748	-0.367605
C	-6.402050	5.685278	-0.181828
H	-5.181083	4.279458	0.918055
H	-4.553281	4.648434	-0.682874
C	-7.724875	5.422731	0.549773
H	-9.345673	3.972186	0.558565
H	-8.716234	4.349636	-1.042378
H	-5.896157	6.560356	0.245058
H	-6.614013	5.927902	-1.233485
H	-8.386508	6.294104	0.467566
H	-7.521576	5.281566	1.621657
C	-3.426286	-0.119069	1.963477
C	-2.453189	0.886405	2.614605
C	-4.547690	-0.490779	2.951473
H	-2.857918	-1.038998	1.796842
C	-1.855626	0.310112	3.904180
H	-2.991512	1.818094	2.840034
H	-1.662539	1.138943	1.901694
C	-3.955623	-1.078505	4.240272
H	-5.143561	0.400031	3.194440
H	-5.232021	-1.207721	2.481536
C	-2.950333	-0.117992	4.890711
H	-1.188263	1.041811	4.376592
H	-1.231809	-0.558359	3.646206
H	-4.755931	-1.327083	4.948618
H	-3.446223	-2.023721	3.999061
H	-2.503626	-0.581236	5.779880
H	-3.485504	0.777662	5.238770
C	-3.534386	-0.350496	-3.135621
C	-4.633797	-1.214957	-3.786079
C	-3.014625	0.692103	-4.144101
H	-2.687409	-1.008529	-2.916543
C	-4.113927	-1.904047	-5.054341
H	-5.494576	-0.576654	-4.033471
H	-4.997757	-1.962244	-3.070086
C	-2.477031	0.001659	-5.402603
H	-3.825609	1.378176	-4.427227
H	-2.225850	1.284911	-3.674038
C	-3.544057	-0.888450	-6.053999

H	-4.913531	-2.493669	-5.521364
H	-3.322568	-2.613628	-4.771108
H	-2.120291	0.751407	-6.120152
H	-1.605169	-0.603863	-5.121081
H	-3.130231	-1.408407	-6.927578
H	-4.363652	-0.254818	-6.425075
C	2.586191	1.613509	2.080883
C	3.272541	1.484774	3.458459
C	1.886906	2.986433	2.006835
H	1.794519	0.855047	2.047231
C	2.242030	1.593825	4.589096
H	4.024575	2.281303	3.553047
H	3.812746	0.537113	3.530208
C	0.838919	3.114170	3.119468
H	2.627936	3.789119	2.123539
H	1.411992	3.125265	1.031322
C	1.457175	2.909913	4.508759
H	2.737676	1.504989	5.564071
H	1.543950	0.747158	4.510081
H	0.350366	4.094547	3.062834
H	0.054946	2.364887	2.951864
H	0.677111	2.935508	5.280117
H	2.139417	3.745197	4.724442
C	4.720215	-1.604369	-1.278388
C	4.297178	-1.638728	-2.761527
C	6.149590	-2.158308	-1.108151
H	4.051085	-2.284508	-0.739582
C	4.418184	-3.055049	-3.336979
H	4.936753	-0.956113	-3.338826
H	3.270154	-1.272069	-2.854804
C	6.270060	-3.573171	-1.688310
H	6.862148	-1.493987	-1.616870
H	6.421835	-2.153074	-0.045299
C	5.835598	-3.614875	-3.159348
H	4.136872	-3.054817	-4.397146
H	3.701161	-3.712090	-2.823208
H	7.299686	-3.937299	-1.582581
H	5.634242	-4.255179	-1.104888
H	5.892930	-4.640907	-3.543678
H	6.536861	-3.015124	-3.758228
C	6.016651	3.274719	-1.257918
C	5.111110	4.340199	-1.911132
C	6.951449	3.927789	-0.219130
H	6.652346	2.855279	-2.051459

C	5.932247	5.480999	-2.524804
H	4.432259	4.749202	-1.149731
H	4.477273	3.867045	-2.670605
C	7.771474	5.068233	-0.835484
H	6.347915	4.322934	0.610034
H	7.611602	3.165190	0.211694
C	6.865073	6.120133	-1.487997
H	5.262581	6.236099	-2.954301
H	6.533611	5.085748	-3.356484
H	8.405616	5.531408	-0.069441
H	8.449808	4.654397	-1.595892
H	7.469673	6.908317	-1.953279
H	6.259130	6.606332	-0.709317
H	-5.069142	1.963279	1.498457
H	-5.194996	1.771979	-2.772215
H	4.211950	3.358535	0.784841
H	6.005587	0.663156	-2.003975

TS1-E

P	-2.957300	0.567059	-0.790030
O	-4.085527	1.298583	-1.704451
O	-3.803441	0.043928	0.501498
O	-1.953679	1.618953	-0.401937
O	-2.483266	-0.704586	-1.491000
C	0.862556	-0.957817	0.048296
C	-0.278983	-1.201921	0.967407
C	-0.487495	-0.372921	2.080482
C	-1.120837	-2.309503	0.768543
C	-1.504206	-0.661036	2.986346
C	-2.144433	-2.582137	1.666258
C	-2.334095	-1.762663	2.780343
H	-0.984663	-2.929073	-0.110227
H	-1.649431	-0.020248	3.850782
H	-2.806619	-3.423141	1.487469
H	-3.136071	-1.977200	3.480834
H	-1.132531	-0.822719	-1.588952
O	-0.042833	-0.851277	-1.688951
H	0.159834	0.480213	2.243905
C	1.698474	-2.126851	-0.239167
C	1.905738	-3.221169	0.576553
H	1.403211	-3.340601	1.528102
C	2.863987	-4.130862	0.053982
C	3.355365	-3.730132	-1.163142
H	3.165275	-5.045013	0.552039

H	4.062913	-4.249910	-1.795494
S	2.664247	-2.238419	-1.689378
C	1.158868	3.955481	-0.023821
C	1.499083	2.596310	0.044374
C	2.186898	4.872393	0.122768
C	2.841208	2.159372	0.242773
C	3.527204	4.461228	0.329414
H	1.962007	5.934347	0.080702
C	3.862457	3.120064	0.391371
C	2.832086	0.728070	0.245056
C	1.494882	0.352398	0.056139
H	4.300283	5.216262	0.437825
H	4.893119	2.812021	0.543872
C	4.044239	-0.112729	0.510077
H	3.789300	-1.097746	0.905733
H	4.639707	-0.268068	-0.397627
H	4.688925	0.388247	1.240908
N	0.703762	1.491642	-0.051906
H	-0.333598	1.503227	-0.171751
H	0.129346	4.260923	-0.181032
C	-4.229830	1.027196	1.445089
H	-4.937790	1.728177	0.987350
H	-4.722970	0.489749	2.258663
H	-3.372574	1.584353	1.834110
C	-5.105748	0.480635	-2.283948
H	-5.709282	-0.000072	-1.505064
H	-5.738758	1.142394	-2.879488
H	-4.665139	-0.290504	-2.923166
H	0.186185	0.046456	-1.988090

TS1-Z

P	-3.079417	0.241237	0.586061
O	-4.151001	0.733464	1.707007
O	-4.023130	-0.334872	-0.608721
O	-2.301331	1.401260	0.026223
O	-2.339491	-0.925416	1.240042
C	1.025805	-0.775185	0.020812
H	-1.035761	-0.833172	1.458037
O	0.057089	-0.722228	1.657946
C	0.319560	4.088267	-0.399451
C	0.932910	2.829633	-0.311122
C	1.152185	5.189749	-0.505770
C	2.348040	2.669445	-0.314543
C	2.563015	5.055389	-0.522235

H	0.716077	6.181919	-0.580304
C	3.165439	3.813314	-0.428313
C	2.623815	1.270844	-0.179821
C	1.374608	0.635472	-0.118124
H	3.177120	5.947090	-0.607704
H	4.248018	3.722220	-0.434824
C	4.011351	0.699687	-0.169010
H	4.084554	-0.236820	-0.725576
H	4.365339	0.493671	0.847606
H	4.706287	1.413952	-0.621532
N	0.367172	1.592939	-0.206484
H	-0.658124	1.429361	-0.116929
H	-0.762052	4.176687	-0.385876
C	-4.737748	-1.548595	-0.362133
H	-4.042096	-2.370706	-0.171308
H	-5.324632	-1.755274	-1.260370
H	-5.410166	-1.438737	0.496206
C	-4.948404	1.879684	1.394349
H	-4.313329	2.744326	1.178535
H	-5.567373	2.080799	2.271461
H	-5.592275	1.681742	0.529432
C	2.149465	-1.693424	0.400932
C	2.720845	-1.664869	1.678698
C	2.710301	-2.522488	-0.581074
C	3.829349	-2.454563	1.969635
H	2.279090	-1.038395	2.442496
C	3.829802	-3.301665	-0.290563
H	2.285623	-2.534895	-1.578459
C	4.390674	-3.271257	0.985347
H	4.255763	-2.433319	2.968186
H	4.258950	-3.932882	-1.062946
H	5.258365	-3.883063	1.214417
C	0.002393	-1.332479	-0.863456
C	-0.735401	-0.703604	-1.848202
H	-0.594609	0.333150	-2.118983
C	-1.697604	-1.550656	-2.450971
C	-1.690422	-2.816256	-1.920277
H	-2.376423	-1.228371	-3.230496
H	-2.319990	-3.652523	-2.193784
S	-0.509427	-3.002302	-0.680631
H	0.156558	0.204635	1.939067

TS2-E-E

P	-1.968201	-0.854605	1.792433

O	-2.105255	-0.300341	3.332521
O	-3.265722	-1.835067	1.631453
O	-0.687399	-1.640567	1.762090
O	-2.234602	0.297548	0.843582
C	-0.044247	-0.695173	-1.651648
C	-0.966747	-1.845256	-1.696568
C	-0.427943	-3.105686	-2.027741
C	-2.343535	-1.751731	-1.427461
C	-1.242748	-4.227745	-2.113558
C	-3.151074	-2.883521	-1.497612
C	-2.610685	-4.120556	-1.848314
H	-2.758806	-0.822818	-1.062632
H	-0.810434	-5.188058	-2.379517
H	-4.203002	-2.796511	-1.244462
H	-3.246556	-5.000096	-1.900652
H	0.635289	-3.188880	-2.226352
C	-0.360748	0.592600	-2.018109
C	0.539299	1.717126	-2.012826
H	1.570619	1.598123	-1.713028
C	-0.016519	2.899940	-2.390022
C	-1.461807	2.842693	-2.479749
H	0.527429	3.832243	-2.456833
S	-1.954355	1.138902	-2.622704
C	3.392541	-2.180500	1.530667
C	2.770138	-1.702778	0.371063
C	4.780974	-2.162839	1.567196
C	3.518312	-1.205473	-0.737483
C	5.540855	-1.687762	0.473821
H	5.295490	-2.530051	2.451036
C	4.923473	-1.217221	-0.676405
C	2.571299	-0.752041	-1.717116
C	1.312479	-0.977770	-1.168370
H	6.625283	-1.694683	0.539370
H	5.515020	-0.849723	-1.511093
C	2.901677	-0.236985	-3.084394
H	2.000516	-0.101857	-3.689482
H	3.424307	0.729134	-3.048447
H	3.562541	-0.932987	-3.616172
N	1.441105	-1.588870	0.068281
H	0.647570	-1.682379	0.729947
H	2.803920	-2.548944	2.365452
C	-3.143899	-3.175996	2.109696
H	-2.937330	-3.194189	3.186237
H	-4.102473	-3.664506	1.916585

H	-2.344515	-3.702788	1.581389
C	-3.234721	0.514965	3.639856
H	-4.168247	-0.041496	3.495545
H	-3.142534	0.805795	4.689370
H	-3.255489	1.409524	3.007540
C	-2.103862	3.495127	-0.718834
C	-1.500683	4.808913	-0.641309
C	-0.343140	4.689134	0.084696
C	-0.277670	3.341636	0.577385
N	-1.395420	2.705368	0.195863
H	-1.643492	1.701746	0.425171
H	-3.167450	3.312302	-0.818418
H	-1.855732	5.683339	-1.170919
H	0.402503	5.449456	0.270869
C	0.814452	2.677012	1.278648
C	0.579603	1.533850	2.057384
C	2.136894	3.106767	1.068180
C	1.644865	0.804381	2.572105
H	-0.432975	1.215362	2.256684
C	3.199143	2.374269	1.588560
H	2.329822	3.979580	0.451164
C	2.956909	1.213774	2.329082
H	1.434431	-0.100597	3.131317
H	4.219309	2.692618	1.395785
H	3.787834	0.617494	2.691440
H	-2.013429	3.523458	-3.121215

TS2-E-Z

P	-2.174188	0.101330	1.741939
O	-2.072777	0.696524	3.274802
O	-3.752448	-0.327557	1.642253
O	-1.284077	-1.107755	1.713256
O	-2.022274	1.244879	0.756569
C	-0.467508	-0.693898	-1.813778
C	-1.666624	-1.558582	-1.718150
C	-1.533551	-2.917923	-2.057507
C	-2.916452	-1.088142	-1.285565
C	-2.629976	-3.771226	-2.006663
C	-4.008847	-1.950325	-1.222981
C	-3.874579	-3.288379	-1.592206
H	-3.006383	-0.075294	-0.914735
H	-2.513443	-4.815376	-2.282742
H	-4.957159	-1.573374	-0.852916
H	-4.728271	-3.958516	-1.539456

H	-0.562809	-3.291575	-2.367796
C	-0.525035	0.573829	-2.336108
C	-1.696900	1.292175	-2.773153
H	-2.645073	0.791794	-2.914567
C	-1.508670	2.625138	-2.934117
C	-0.159698	3.072905	-2.617382
H	-2.286816	3.326602	-3.213992
H	0.269630	3.889413	-3.186197
S	0.885814	1.671637	-2.404662
C	2.430269	-2.883713	1.485409
C	1.974615	-2.262637	0.317289
C	3.774142	-3.223959	1.548580
C	2.844375	-1.986434	-0.779171
C	4.654750	-2.957074	0.474341
H	4.159567	-3.710375	2.440693
C	4.200908	-2.350842	-0.687892
C	2.058275	-1.347102	-1.794091
C	0.767612	-1.248156	-1.275428
H	5.699768	-3.241050	0.562265
H	4.881889	-2.152655	-1.511647
C	2.532095	-1.005453	-3.173256
H	1.696208	-0.772943	-3.839173
H	3.206331	-0.138984	-3.177633
H	3.085715	-1.845814	-3.610368
N	0.719810	-1.834133	-0.018168
H	-0.055802	-1.656761	0.647095
H	1.751252	-3.080043	2.308904
C	-4.128445	-1.555972	2.268015
H	-3.907125	-1.534172	3.341672
H	-5.206620	-1.665165	2.123394
H	-3.603257	-2.398734	1.809944
C	-2.850713	1.852465	3.582235
H	-3.920605	1.643420	3.468445
H	-2.637861	2.113925	4.621986
H	-2.583826	2.689805	2.927596
C	-0.250330	3.983654	-0.806306
C	1.017510	4.671560	-0.860085
C	1.928151	3.916008	-0.167207
C	1.214163	2.834899	0.446384
N	-0.090872	2.965516	0.139068
H	-0.836075	2.254746	0.385464
H	-1.220986	4.457583	-0.883333
H	1.211392	5.562109	-1.443760
H	2.988451	4.092147	-0.055923

C	1.762261	1.803489	1.314015
C	0.988404	1.242109	2.338999
C	3.094266	1.381244	1.144580
C	1.534326	0.282731	3.184583
H	-0.032883	1.562274	2.488647
C	3.635248	0.423066	1.991514
H	3.684775	1.778946	0.324948
C	2.859195	-0.120067	3.019963
H	0.907160	-0.152012	3.955465
H	4.648603	0.069750	1.831716
H	3.284665	-0.876558	3.671014

TS2-R-E

C	0.791911	3.525099	1.721484
C	0.497638	-1.111622	3.406914
C	0.640513	0.280617	3.341449
C	0.562431	-1.693022	4.664099
C	0.851363	1.085079	4.501273
C	0.753535	-0.917122	5.832966
H	0.467520	-2.769541	4.751842
C	0.896358	0.459967	5.764185
C	0.964921	2.442811	4.062139
C	0.808749	2.423232	2.670407
H	0.791977	-1.415088	6.797548
H	1.047654	1.047137	6.665863
C	1.140688	3.628543	4.960796
H	0.810342	4.554767	4.485494
H	2.190565	3.770490	5.249505
H	0.564385	3.497103	5.884011
N	0.605899	1.109786	2.257990
H	0.623733	0.778386	1.280588
H	0.332513	-1.699882	2.512218
C	1.726843	4.646308	1.951893
C	3.043093	4.383552	2.365985
C	1.333991	5.982200	1.763256
C	3.949700	5.422069	2.548403
H	3.348265	3.355644	2.520437
C	2.240645	7.021846	1.957575
H	0.306337	6.204304	1.494489
C	3.553240	6.745405	2.343492
H	4.969946	5.197099	2.845295
H	1.918078	8.049447	1.816741
H	4.260377	7.556571	2.491659
C	-0.049228	3.492531	0.627590

C	-1.623221	2.599315	-0.880213
C	-0.973527	3.567759	-1.747125
H	-1.555268	4.078648	-2.506451
C	0.192816	2.462556	-2.945104
C	0.687495	3.461605	-3.857720
C	1.930254	3.848434	-3.423374
C	2.271529	3.029780	-2.296372
N	1.273852	2.145923	-2.119502
H	1.191007	1.416689	-1.382114
H	-0.491692	1.651551	-3.166151
H	0.116427	3.887494	-4.671979
H	2.547861	4.633816	-3.833186
C	3.454708	3.107969	-1.454187
C	3.686938	2.181374	-0.422392
C	4.383190	4.144874	-1.665157
C	4.824204	2.304926	0.370069
H	3.004042	1.355190	-0.252143
C	5.514872	4.258513	-0.868587
H	4.209826	4.873017	-2.449506
C	5.738339	3.336077	0.155222
H	4.992528	1.591406	1.165162
H	6.218121	5.067276	-1.042674
H	6.620789	3.419755	0.782972
H	-2.389942	1.934625	-1.244886
S	0.074393	4.608356	-0.772124
C	-1.096014	2.537800	0.364601
H	-1.421060	1.831818	1.112700
P	-0.361303	-0.666827	-0.914801
O	-0.962902	-0.244169	-2.213334
O	0.758780	0.154654	-0.291696
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C	0.363567	-3.027948	0.010979
C	-0.737861	-3.513172	0.718289
C	1.686922	-3.366347	0.338544
C	-0.531918	-4.283454	1.885976
C	1.844658	-4.253820	1.405334
C	0.775459	-4.686127	2.199441
H	2.844516	-4.588620	1.661078
C	-2.102424	-3.161095	0.240720
C	-3.018805	-4.165151	-0.149307
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C	-3.784445	-1.433638	-0.161814

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C	-4.914005	1.925370	-1.496067
C	-4.822766	2.048983	0.895134
C	-5.080135	2.672071	-0.325392
C	2.824363	-2.713326	-0.372368
C	3.754573	-1.927321	0.354420
C	2.918443	-2.778317	-1.783841
C	4.691089	-1.172942	-0.357883
C	3.869271	-1.995929	-2.442087
C	4.737534	-1.151403	-1.750922
C	1.075271	-5.546995	3.412691
H	1.820384	-6.305795	3.142364
H	1.550575	-4.923799	4.185685
C	-1.698606	-4.594947	2.809400
H	-2.292971	-3.682802	2.941908
H	-2.375233	-5.315456	2.337499
C	-2.541756	-5.594992	-0.349290
H	-2.445422	-6.115594	0.611638
H	-1.532703	-5.574754	-0.775732
C	-5.380732	-4.816454	-0.888666
H	-5.618991	-4.630417	-1.946426
H	-6.314206	-4.643942	-0.337516
C	-4.922341	-6.268350	-0.732641
H	-4.960901	-6.562153	0.325839
H	-5.603276	-6.935488	-1.273648
C	-0.174622	-6.204043	4.001956
H	0.066728	-6.681158	4.958882
H	-0.529075	-6.996916	3.328298
C	-3.485721	-6.409792	-1.238181
H	-3.169932	-7.459442	-1.244571
H	-3.426438	-6.050370	-2.274864
C	-1.274962	-5.155352	4.171832
H	-2.149635	-5.579990	4.677920
H	-0.906669	-4.344868	4.813289
C	5.700366	-0.228923	-2.466884
C	6.923758	-0.970279	-3.042174
C	5.017327	0.592643	-3.577102
H	6.075843	0.487852	-1.722081
C	7.910793	0.009028	-3.692340
H	6.579386	-1.702182	-3.786862

H	7.417328	-1.542184	-2.246902
C	5.994937	1.591579	-4.205051
H	4.645410	-0.085564	-4.357201
H	4.142250	1.107651	-3.170418
C	7.231645	0.873988	-4.763791
H	8.757805	-0.537509	-4.125927
H	8.326542	0.664582	-2.912881
H	5.495541	2.163173	-4.998041
H	6.304117	2.318717	-3.440207
H	7.945150	1.600366	-5.173223
H	6.922572	0.231003	-5.600970
C	2.060599	-3.718476	-2.612505
C	1.334303	-3.028990	-3.784609
C	2.889551	-4.912082	-3.134483
H	1.288939	-4.145730	-1.967200
C	0.426191	-4.024740	-4.515268
H	2.073174	-2.635039	-4.497065
H	0.752414	-2.180790	-3.417096
C	1.998643	-5.912175	-3.883982
H	3.679535	-4.542624	-3.803937
H	3.395989	-5.404950	-2.295104
C	1.219772	-5.236895	-5.021443
H	-0.085257	-3.528331	-5.349804
H	-0.359839	-4.361674	-3.823430
H	2.603232	-6.740854	-4.274677
H	1.284643	-6.353047	-3.172527
H	0.551647	-5.960946	-5.505427
H	1.930318	-4.901627	-5.791707
C	3.804145	-1.897107	1.875912
C	4.894356	-2.859000	2.401435
C	4.038392	-0.501443	2.483664
H	2.843150	-2.242806	2.265022
C	4.898723	-2.921214	3.933159
H	5.872884	-2.509070	2.041364
H	4.757105	-3.859173	1.974899
C	4.049160	-0.543029	4.016648
H	5.012067	-0.119799	2.150098
H	3.270490	0.192925	2.124728
C	5.099761	-1.527891	4.542721
H	5.678485	-3.609853	4.282870
H	3.936926	-3.330092	4.276942
H	4.232931	0.463331	4.414203
H	3.062749	-0.843782	4.379097
H	5.056194	-1.579667	5.637920

H	6.106577	-1.166967	4.283166
C	-4.192109	-0.143805	-2.765672
C	-5.460968	-0.787173	-3.362072
C	-3.504752	0.711101	-3.846396
H	-3.491182	-0.950252	-2.531420
C	-5.105174	-1.662579	-4.571157
H	-6.160286	0.007107	-3.662501
H	-5.975921	-1.386318	-2.604420
C	-3.112396	-0.161355	-5.043899
H	-4.179099	1.510420	-4.186632
H	-2.616181	1.182932	-3.421591
C	-4.336477	-0.871407	-5.638571
H	-6.013446	-2.101279	-5.004149
H	-4.483383	-2.500506	-4.223818
H	-2.620175	0.447895	-5.813455
H	-2.374128	-0.899410	-4.703847
H	-4.033288	-1.535610	-6.457883
H	-5.008910	-0.118768	-6.077155
C	-4.219897	0.061983	2.335106
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C	-5.463453	0.206740	3.235782
H	-4.074683	-1.011790	2.174171
C	-2.769793	-0.120342	4.417346
H	-3.038228	1.659742	3.210476
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C	-5.264348	-0.505308	4.579733
H	-5.665222	1.270562	3.421966
H	-6.342639	-0.190918	2.713638
C	-4.014030	0.011878	5.302247
H	-1.888302	0.284396	4.924781
H	-2.559185	-1.185293	4.243816
H	-6.154190	-0.377280	5.209293
H	-5.157100	-1.585693	4.402402
H	-3.868510	-0.526341	6.247499
H	-4.162393	1.070652	5.563016
C	-5.469527	4.134862	-0.377060
C	-4.335592	4.995405	-0.975569
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H	-5.620755	4.474543	0.658323
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H	-4.132816	4.646573	-1.999007
H	-3.414622	4.834561	-0.403703
C	-7.154769	5.871095	-1.162245
H	-6.684812	4.018634	-2.168607

H	-7.590923	3.792821	-0.678177
C	-6.021728	6.717376	-1.757685
H	-3.892590	7.062509	-1.467832
H	-4.804848	6.851304	0.023203
H	-8.081762	6.021099	-1.729579
H	-7.356883	6.210897	-0.135869
H	-6.288914	7.781311	-1.738125
H	-5.887756	6.445698	-2.815313
H	3.918696	-2.038076	-3.525678
H	5.398200	-0.555537	0.185801
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H	-4.948465	2.621505	1.810769

TS2-S-E

C	-3.250655	2.934387	0.416979
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H	-4.172397	5.186736	-0.814457
C	-7.334083	4.034159	-0.309171
H	-7.824212	2.179504	0.681192
H	-6.536078	5.808675	-1.239376
H	-8.369658	4.305002	-0.494582

C	-2.422148	2.778914	-0.677351
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C	-0.574897	2.224483	-2.031049
C	-1.626766	2.181965	-3.041352
H	0.456210	1.996359	-2.267440
H	-1.415201	2.533021	-4.047290
S	-3.115469	2.810746	-2.329637
C	-1.918795	0.282227	-3.493696
C	-3.147491	0.235288	-4.252598
C	-4.159956	-0.082051	-3.382173
C	-3.564371	-0.351809	-2.098782
N	-2.239906	-0.249916	-2.243348
H	-1.493237	-0.430599	-1.532360
H	-0.940699	0.043953	-3.895308
H	-3.246668	0.527283	-5.289491
H	-5.219794	-0.098726	-3.591159
C	-4.193920	-0.633853	-0.816471
C	-3.415981	-0.755032	0.350164
C	-5.591706	-0.753982	-0.720686
C	-4.026131	-0.978003	1.580423
H	-2.335535	-0.694083	0.299881
C	-6.195078	-0.996551	0.507857
H	-6.205399	-0.658145	-1.609805
C	-5.414286	-1.103535	1.663907
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H	-7.275012	-1.094468	0.566772
H	-5.887177	-1.281686	2.625230
P	0.778862	-0.434395	0.308802
O	-0.140686	-0.828086	-0.813527
O	0.394153	0.633164	1.291103
O	1.201469	-1.738306	1.221047
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C	3.319958	0.043343	0.413601
C	3.891808	-1.092583	1.001248
C	3.812601	1.336355	0.621366
C	4.899676	-0.916878	1.976238
C	4.888479	1.461717	1.499817
C	5.402457	0.373696	2.214196
H	5.308844	2.448832	1.671602
C	3.394475	-2.433551	0.570550
C	4.234992	-3.374855	-0.069484
C	2.022842	-2.702793	0.660395
C	3.694883	-4.609779	-0.470279

C	1.447648	-3.884348	0.179269
C	2.326154	-4.849285	-0.315094
H	1.912157	-5.786412	-0.679773
C	-0.030181	-4.012447	0.010018
C	-0.556332	-4.049095	-1.300724
C	-0.909762	-4.023456	1.114087
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C	-2.284154	-4.094371	0.885209
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C	3.190880	2.508866	-0.062703
C	2.551646	3.518875	0.690375
C	3.235549	2.609277	-1.473422
C	1.988952	4.609139	0.015761
C	2.652578	3.714868	-2.097675
C	2.024015	4.729950	-1.371893
C	6.454622	0.648691	3.275193
H	7.225579	1.311621	2.861715
H	5.980749	1.215258	4.090732
C	5.364109	-2.094410	2.814694
H	4.515258	-2.763071	2.994193
H	6.102090	-2.690144	2.263099
C	5.665528	-3.015324	-0.429913
H	6.331307	-3.168252	0.429023
H	5.719743	-1.946550	-0.663182
C	4.519861	-5.664755	-1.189887
H	4.121759	-5.771864	-2.209993
H	4.367004	-6.639241	-0.708126
C	6.013506	-5.338499	-1.273859
H	6.501061	-5.561047	-0.314428
H	6.491681	-5.974437	-2.027876
C	7.090134	-0.616498	3.857040
H	7.648212	-0.368717	4.767420
H	7.813619	-1.034668	3.143063
C	6.204107	-3.854689	-1.591107
H	7.261828	-3.619566	-1.757555
H	5.667839	-3.602138	-2.516845
C	6.006180	-1.659498	4.134824
H	6.422600	-2.534027	4.648221
H	5.244211	-1.228752	4.799017
C	1.388850	5.921310	-2.060521
C	2.383959	6.684575	-2.957693
C	0.134965	5.523653	-2.867382
H	1.058705	6.617358	-1.275051
C	1.728512	7.897549	-3.630004

H	2.765320	6.006033	-3.733371
H	3.251197	6.993723	-2.361926
C	-0.515563	6.733828	-3.547702
H	0.423725	4.785647	-3.630230
H	-0.580718	5.022193	-2.208396
C	0.485498	7.488808	-4.431171
H	2.452212	8.405219	-4.279895
H	1.436396	8.624590	-2.858070
H	-1.383164	6.411531	-4.137704
H	-0.899668	7.416207	-2.775149
H	0.011742	8.371430	-4.878850
H	0.792347	6.839247	-5.264453
C	3.937817	1.573869	-2.334305
C	2.997246	0.904507	-3.356750
C	5.174947	2.162705	-3.043018
H	4.308539	0.777502	-1.683783
C	3.736955	-0.168469	-4.165587
H	2.600322	1.665894	-4.044786
H	2.149178	0.459378	-2.827036
C	5.915915	1.085680	-3.845328
H	4.862994	2.973511	-3.716514
H	5.841417	2.614516	-2.298113
C	4.984776	0.400123	-4.853459
H	3.063791	-0.611996	-4.908729
H	4.031537	-0.982115	-3.486063
H	6.781030	1.522769	-4.359936
H	6.312068	0.330843	-3.149974
H	5.520324	-0.393853	-5.389264
H	4.673248	1.135228	-5.610647
C	0.316110	-3.970995	-2.543703
C	0.306022	-5.293251	-3.337275
C	-0.056087	-2.785903	-3.456010
H	1.348341	-3.792942	-2.233123
C	1.226340	-5.219746	-4.561851
H	-0.720618	-5.514364	-3.662382
H	0.606754	-6.120665	-2.682506
C	0.865894	-2.721517	-4.679126
H	-1.099413	-2.875095	-3.790277
H	0.021167	-1.871761	-2.863646
C	0.858247	-4.037051	-5.467211
H	1.185909	-6.160674	-5.125284
H	2.266093	-5.101177	-4.221051
H	0.576181	-1.885156	-5.330805
H	1.889920	-2.511996	-4.341205

H	1.547876	-3.978773	-6.318985
H	-0.146094	-4.203381	-5.884606
C	-0.402742	-3.985637	2.542526
C	-0.996959	-2.814821	3.348820
C	-0.652307	-5.320995	3.273778
H	0.680996	-3.837816	2.518903
C	-0.430888	-2.775840	4.772260
H	-2.089547	-2.923793	3.403987
H	-0.791350	-1.875983	2.826793
C	-0.088802	-5.286965	4.700248
H	-1.733041	-5.519988	3.308941
H	-0.202272	-6.141878	2.701705
C	-0.656883	-4.107298	5.500446
H	-0.887891	-1.952261	5.332453
H	0.647370	-2.564737	4.720957
H	-0.298934	-6.233896	5.213929
H	1.005920	-5.193202	4.649529
H	-0.210487	-4.076623	6.502616
H	-1.737557	-4.258052	5.642777
C	-4.332534	-4.258253	-0.567842
C	-4.836019	-4.021938	-2.000007
C	-4.860309	-5.616267	-0.053418
H	-4.779614	-3.480927	0.068125
C	-6.366633	-4.080281	-2.073815
H	-4.421504	-4.794100	-2.663621
H	-4.471670	-3.058925	-2.375244
C	-6.390555	-5.691218	-0.124596
H	-4.417998	-6.418042	-0.662110
H	-4.518597	-5.782591	0.974609
C	-6.900800	-5.417428	-1.545010
H	-6.700648	-3.918072	-3.106770
H	-6.786390	-3.261654	-1.472739
H	-6.738721	-6.671737	0.223749
H	-6.816544	-4.943721	0.561054
H	-7.997936	-5.427004	-1.566638
H	-6.565366	-6.226597	-2.210037
H	2.697386	3.786211	-3.181169
H	1.502396	5.390785	0.592909
H	-2.330845	-4.161280	-2.488684
H	-2.960719	-4.095436	1.736028
C	2.474492	3.479300	2.207065
C	3.444154	4.502056	2.838505
C	1.049763	3.696883	2.751619
H	2.780295	2.482388	2.538138

C	3.417907	4.433561	4.369954
H	3.158353	5.512104	2.510864
H	4.462140	4.336125	2.465530
C	1.023596	3.627373	4.283351
H	0.666308	4.676314	2.433395
H	0.391523	2.935838	2.330384
C	1.996316	4.632161	4.911147
H	4.100144	5.181831	4.793777
H	3.791581	3.449125	4.689421
H	0.003774	3.793675	4.649194
H	1.298012	2.612129	4.598307
H	1.987953	4.541145	6.004857
H	1.664096	5.655024	4.677883

TS2-Z-E

P	-3.281129	-1.361252	0.154126
O	-4.497939	-1.315061	1.239467
O	-3.741593	-0.249900	-0.966614
O	-2.033414	-0.716223	0.770091
O	-3.201619	-2.742491	-0.410975
C	1.228634	0.639360	-1.239187
C	-2.715395	3.061244	0.483278
C	-1.458494	2.763024	-0.059512
C	-3.018999	4.399056	0.684396
C	-0.513272	3.778726	-0.390898
C	-2.101328	5.425618	0.352669
H	-3.986506	4.669319	1.098525
C	-0.859340	5.129644	-0.183624
C	0.652636	3.124909	-0.895487
C	0.383397	1.748620	-0.858457
H	-2.382688	6.461025	0.522398
H	-0.160624	5.922964	-0.435353
C	1.869032	3.827720	-1.417584
H	2.419905	3.217831	-2.136736
H	2.570110	4.087406	-0.613658
H	1.582126	4.761357	-1.914815
N	-0.905966	1.552813	-0.368408
H	-1.305122	0.656687	-0.048795
H	-3.417626	2.267913	0.713384
C	-4.869239	-0.577069	-1.782235
H	-4.709078	-1.527957	-2.300467
H	-4.982227	0.231353	-2.508280
H	-5.778965	-0.653579	-1.175229
C	-4.712216	-0.106014	1.966681

H	-3.781085	0.246881	2.421784
H	-5.443297	-0.329030	2.747452
H	-5.113001	0.677261	1.310943
C	2.691164	0.790233	-1.054806
C	3.197302	1.297763	0.150797
C	3.591808	0.428071	-2.069791
C	4.569127	1.417987	0.346406
H	2.504880	1.573979	0.936262
C	4.965691	0.561218	-1.876671
H	3.208232	0.067327	-3.018952
C	5.458657	1.052272	-0.666724
H	4.943616	1.792638	1.294689
H	5.650242	0.288112	-2.674566
H	6.529721	1.153758	-0.516059
C	0.706098	-0.550538	-1.703407
C	-0.898587	-2.165728	-2.301186
C	0.217286	-3.035122	-1.955845
H	0.355594	-3.976527	-2.477301
C	-0.268462	-3.761572	-0.162032
C	0.860110	-4.602058	0.156144
C	1.701759	-3.884593	0.970138
C	1.060935	-2.633639	1.262810
N	-0.139752	-2.644611	0.664655
H	-0.855706	-1.882254	0.693200
H	-1.282267	-4.077194	-0.383007
H	1.042607	-5.578696	-0.272254
H	2.675175	-4.185033	1.329929
C	1.545805	-1.511040	2.056167
C	0.708792	-0.417519	2.352667
C	2.869544	-1.504313	2.530711
C	1.190992	0.644023	3.113193
H	-0.319195	-0.400939	2.007909
C	3.343520	-0.439860	3.288459
H	3.533892	-2.327686	2.290607
C	2.504867	0.637436	3.586375
H	0.534095	1.480377	3.332877
H	4.369571	-0.447885	3.643980
H	2.875446	1.468261	4.180060
H	-1.875272	-2.569338	-2.531016
S	1.674446	-2.055222	-1.767132
C	-0.646066	-0.848014	-2.098436
H	-1.394743	-0.073093	-2.194820

TS2-Z-Z

P	-3.267232	-1.260342	0.153086
O	-4.360304	-1.601879	1.315361
O	-3.852441	0.112690	-0.521490
O	-1.968088	-0.791727	0.824706
O	-3.246034	-2.392942	-0.823054
C	1.346903	0.864542	-1.050839
C	-2.856646	2.904559	0.589040
C	-1.556896	2.713080	0.098666
C	-3.246800	4.206900	0.860307
C	-0.658329	3.801754	-0.099457
C	-2.376849	5.305365	0.653278
H	-4.250065	4.392677	1.234398
C	-1.092590	5.115423	0.174896
C	0.575757	3.256715	-0.561612
C	0.394646	1.863090	-0.633478
H	-2.728215	6.309082	0.875227
H	-0.426061	5.960005	0.022488
C	1.764368	4.083881	-0.950670
H	2.349254	3.622275	-1.748671
H	2.448080	4.245229	-0.107518
H	1.435140	5.068529	-1.299943
N	-0.912433	1.558740	-0.258120
H	-1.267057	0.628601	0.010411
H	-3.522398	2.060196	0.716417
C	-4.953213	-0.007392	-1.424903
H	-4.703843	-0.687463	-2.244268
H	-5.150755	0.994492	-1.813032
H	-5.843646	-0.382163	-0.906305
C	-4.491994	-0.687916	2.404301
H	-3.524250	-0.511376	2.884295
H	-5.183630	-1.142218	3.117861
H	-4.902532	0.270576	2.063121
C	2.781708	1.182949	-0.813130
C	3.207600	1.536184	0.475075
C	3.724854	1.145029	-1.851465
C	4.546565	1.824118	0.724284
H	2.480534	1.567109	1.277647
C	5.063063	1.447295	-1.604270
H	3.395769	0.898395	-2.856405
C	5.478814	1.783850	-0.314793
H	4.862600	2.079020	1.731991
H	5.779691	1.426928	-2.420475
H	6.521931	2.018023	-0.122228
C	1.038590	-0.352622	-1.629330

C	-0.019477	-2.547784	-2.402564
C	1.429655	-2.554730	-2.377713
H	1.996659	-3.450165	-2.597696
C	-0.568443	-3.589872	-0.834369
C	0.368580	-4.688220	-0.727363
C	1.324753	-4.341179	0.194664
C	0.941730	-3.074146	0.759081
N	-0.223058	-2.725713	0.208571
H	-0.828442	-1.902985	0.452919
H	-1.633298	-3.653591	-1.045211
H	0.358280	-5.571441	-1.352576
H	2.210124	-4.900344	0.462946
C	1.632269	-2.225577	1.721538
C	0.998599	-1.087183	2.258478
C	2.958794	-2.507943	2.090148
C	1.683669	-0.266429	3.148955
H	-0.028540	-0.851650	1.997716
C	3.640045	-1.673958	2.970116
H	3.463029	-3.372333	1.669780
C	3.004141	-0.550938	3.504024
H	1.182010	0.603310	3.563247
H	4.668170	-1.898188	3.238167
H	3.535524	0.098478	4.193759
S	-0.571280	-0.862081	-2.212966
C	1.976137	-1.418967	-1.870018
H	3.027091	-1.309289	-1.638464
H	-0.568843	-3.110883	-3.151047

TS3-E

C	1.502281	-1.098256	-1.210623
C	2.887339	2.936030	1.323608
C	2.905596	1.721728	0.628315
C	4.090846	3.393659	1.844674
C	4.099168	0.962461	0.455643
C	5.288321	2.663463	1.676157
H	4.114134	4.333788	2.389138
C	5.303066	1.458003	0.987961
C	3.747820	-0.218270	-0.282115
C	2.383844	-0.139382	-0.533564
H	6.211089	3.055582	2.094854
H	6.229253	0.902410	0.865615
C	4.695878	-1.295408	-0.711253
H	4.259044	-1.933031	-1.483662
H	4.979133	-1.947575	0.126162

H	5.620956	-0.863831	-1.112817
N	1.887547	1.045072	0.008806
H	0.896744	1.278747	0.111257
H	1.963122	3.495045	1.439156
C	1.657968	-2.523782	-0.845326
C	1.925784	-2.877072	0.489876
C	1.525632	-3.551305	-1.792438
C	2.022507	-4.212571	0.868554
H	2.058011	-2.088756	1.224502
C	1.630017	-4.888882	-1.413426
H	1.373610	-3.298886	-2.837284
C	1.871991	-5.225777	-0.081686
H	2.218282	-4.464756	1.907216
H	1.530249	-5.668233	-2.163676
H	1.952353	-6.268233	0.212924
C	0.523004	-0.665664	-2.059614
C	-0.955488	0.986940	-2.882222
C	-1.912946	-0.176437	-2.826390
H	-2.532023	-0.253434	-3.724001
C	-2.841672	-0.140829	-1.595926
C	-4.102653	-0.829414	-1.571578
C	-4.261084	-1.451689	-0.349961
C	-3.072601	-1.220280	0.396027
N	-2.239446	-0.500432	-0.358552
H	-1.453999	0.044440	0.022931
H	-3.009772	1.195432	-1.319292
H	-4.797872	-0.850735	-2.401601
H	-5.106548	-2.032792	-0.009277
C	-2.705288	-1.650917	1.742883
C	-1.350948	-1.843866	2.065635
C	-3.687316	-1.898563	2.713370
C	-0.990238	-2.266023	3.340583
H	-0.588469	-1.700413	1.306772
C	-3.320115	-2.319925	3.988604
H	-4.733648	-1.738187	2.471446
C	-1.972219	-2.502489	4.305421
H	0.058239	-2.422033	3.576090
H	-4.085325	-2.501523	4.737491
H	-1.688597	-2.833319	5.300313
H	-1.314154	1.974889	-3.144064
S	-0.796645	-1.670456	-2.743330
C	0.282945	0.725214	-2.445972
H	1.050003	1.478380	-2.317295
P	-1.681966	2.755658	-0.074700

O	-2.893500	2.392918	-0.963086
O	-0.834341	1.651155	0.503029
O	-0.687183	3.729849	-0.903234
O	-2.312910	3.698979	1.075747
C	-1.442045	4.107159	2.142909
C	-1.247404	4.849872	-1.602969
H	-0.637084	4.745935	1.761896
H	-2.057388	4.672966	2.844207
H	-1.010430	3.233772	2.639391
H	-1.974628	4.512629	-2.347685
H	-1.738634	5.535891	-0.904985
H	-0.415005	5.356211	-2.094318

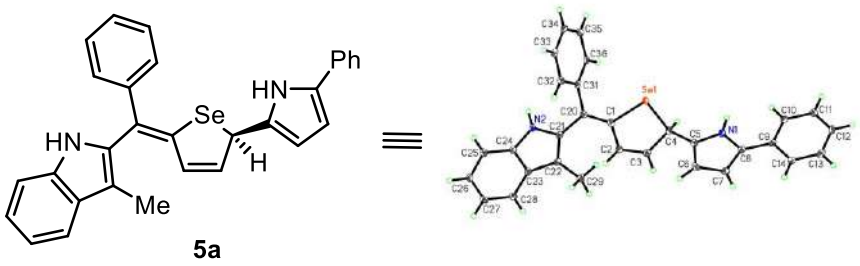
TS3-Z

P	-1.713041	2.193934	-0.700427
O	-2.813952	3.216610	-0.091830
O	-0.449607	3.125167	-1.078564
O	-1.223863	1.224162	0.353152
O	-2.371079	1.665297	-1.988027
C	2.208977	-1.292529	-0.438110
C	1.910526	3.429810	1.073168
C	2.391785	2.173882	0.683465
C	2.843180	4.376735	1.475526
C	3.781020	1.858662	0.704739
C	4.226366	4.089455	1.491948
H	2.502620	5.362656	1.781072
C	4.700845	2.842873	1.110663
C	3.916250	0.499795	0.269244
C	2.630420	0.035924	-0.000058
H	4.924870	4.858385	1.810616
H	5.765721	2.625855	1.130965
C	5.219081	-0.223314	0.108502
H	5.141557	-1.056103	-0.593788
H	5.580323	-0.637211	1.059592
H	5.990935	0.460773	-0.263586
N	1.719678	1.062984	0.244204
H	0.702593	0.989687	0.218843
H	0.849605	3.647162	1.042222
C	-0.513863	3.990225	-2.218873
H	-0.675738	3.407167	-3.129153
H	0.447826	4.503290	-2.265274
H	-1.321285	4.721995	-2.105578
C	-2.506335	3.863251	1.149682
H	-2.276874	3.125011	1.923982

H	-3.392279	4.435531	1.430763
H	-1.653822	4.541784	1.031899
C	2.956556	-2.445434	0.128142
C	3.232975	-2.499253	1.504103
C	3.432105	-3.482969	-0.689967
C	3.943823	-3.566442	2.046357
H	2.887223	-1.690965	2.140706
C	4.144547	-4.551303	-0.147008
H	3.262434	-3.429630	-1.761117
C	4.401274	-4.598739	1.223660
H	4.142646	-3.593062	3.114262
H	4.512194	-5.339507	-0.798415
H	4.962007	-5.427449	1.646690
C	1.168489	-1.507184	-1.298441
C	-1.029682	-1.318161	-2.739867
C	-0.586732	-2.704619	-2.351761
H	-1.215421	-3.554365	-2.599854
C	-2.346857	-0.940776	-2.046987
C	-3.609160	-1.491372	-2.468193
C	-4.377401	-1.758605	-1.357012
C	-3.600335	-1.422270	-0.210190
N	-2.387476	-1.044582	-0.625670
H	-1.732595	-0.487786	-0.058412
H	-2.436871	0.370266	-2.134567
H	-3.897253	-1.625880	-3.503302
H	-5.405528	-2.090956	-1.334055
C	-4.015523	-1.388901	1.192564
C	-3.372214	-0.549408	2.119308
C	-5.077199	-2.202378	1.620548
C	-3.787762	-0.538043	3.448007
H	-2.574857	0.113371	1.795318
C	-5.483406	-2.187044	2.951280
H	-5.569683	-2.862147	0.912756
C	-4.839177	-1.354695	3.868884
H	-3.290435	0.117473	4.156781
H	-6.300277	-2.826147	3.273068
H	-5.157450	-1.341328	4.907256
S	0.371561	-0.217478	-2.249071
C	0.509901	-2.774822	-1.581258
H	0.873535	-3.694903	-1.140216
H	-1.187348	-1.205140	-3.817914

VIII. Determination of the Absolute Stereochemistry

The structure and absolute stereochemistry of product **5a** were determined by X-ray diffraction. The X-ray data have been deposited at the Cambridge Crystallographic Data Center (CCDC 2022226). The stereochemistry of other products was assumed by analogy.



5a

Supplementary Table. 15. Crystal data and structure refinement for **5a.**

Identification code	**5a**
Empirical formula	$C_{30}H_{24}N_2Se$
Formula weight	491.47
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	14.3021(3)
b/Å	5.48120(8)
c/Å	15.6544(3)
α/°	90
β/°	113.745(2)
γ/°	90
Volume/Å^3	1123.30(4)
Z	2
ρ_{calc}g/cm^3	1.453
μ/mm^{-1}	2.414
F(000)	504.0
Crystal size/mm^3	0.08 × 0.02 × 0.02
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.078 to 134.828
Index ranges	-17 ≤ h ≤ 16, -5 ≤ k ≤ 6, -14 ≤ l ≤ 18
Reflections collected	6097
Independent reflections	3629 [R_{int} = 0.0358, R_{sigma} = 0.0518]
Data/restraints/parameters	3629/1/299
Goodness-of-fit on F^2	1.006
Final R indexes [I>=2σ (I)]	R_1 = 0.0268, wR_2 = 0.0576

Final R indexes [all data]	$R_1 = 0.0301$, $wR_2 = 0.0590$
Largest diff. peak/hole / e Å^{-3}	0.28/-0.30
Flack parameter	-0.023(16)

Supplementary Table. 16. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters (Å$^2\times 10^3$) for 5a. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Se1	5685.8(2)	4626.5(8)	2629.1(2)	18.20(10)
N1	7985(2)	5243(5)	4967.7(19)	14.4(7)
N2	1582.5(19)	4397(7)	1132.4(18)	15.1(6)
C1	4301(2)	4698(11)	2528(2)	15.2(6)
C2	4320(2)	4478(9)	3460(2)	14.4(6)
C3	5220(3)	4126(6)	4169(2)	16.1(9)
C4	6179(3)	4064(6)	4000(2)	15.7(8)
C5	6970(3)	5806(7)	4610(2)	14.5(7)
C6	6866(3)	7986(7)	4996(3)	16.6(8)
C7	7854(3)	8770(7)	5599(3)	16.8(8)
C8	8545(3)	7057(7)	5570(2)	14.0(7)
C9	9660(3)	7002(7)	6018(2)	13.9(7)
C10	10221(3)	5088(7)	5861(2)	15.8(9)
C11	11279(3)	5111(7)	6266(2)	16.7(9)
C12	11797(3)	7020(8)	6837(3)	19.0(8)
C13	11252(3)	8910(6)	7014(3)	18.4(8)
C14	10197(3)	8893(6)	6618(2)	16.0(8)
C20	3473(2)	4948(8)	1717(2)	12.6(7)
C21	2473(3)	5589(7)	1717(2)	14.7(7)
C22	2218(3)	7448(6)	2165(2)	13.4(7)
C23	1132(3)	7440(6)	1843(2)	14.0(7)
C24	752(3)	5488(6)	1207(2)	13.6(7)
C25	-288(2)	4976(8)	764(2)	15.9(8)
C26	-950(3)	6499(7)	964(3)	16.4(8)
C27	-589(3)	8498(7)	1579(3)	18.0(8)
C28	439(3)	8971(6)	2017(2)	15.7(8)
C29	2911(3)	9298(8)	2828(2)	19.1(8)
C31	3533(2)	4729(10)	792(2)	13.7(6)
C32	3083(3)	6519(7)	117(3)	17.0(8)
C33	3132(3)	6372(7)	-747(3)	17.8(8)
C34	3604(2)	4406(10)	-958(2)	18.9(8)
C35	4040(3)	2583(7)	-304(3)	19.0(8)
C36	4009(3)	2752(7)	574(2)	15.6(7)

Supplementary Table. 17. Anisotropic Displacement Parameters (Å$^2\times 10^3$) for 5a. The

Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Se1	9.64(15)	31.2(2)	12.74(15)	0.7(2)	3.50(11)	2.0(2)
N1	11.6(13)	15.3(19)	13.9(13)	-0.6(11)	2.7(11)	0.3(11)
N2	11.6(12)	17.2(16)	14.9(12)	-2.9(15)	3.5(10)	-1.0(15)
C1	11.3(13)	16.4(15)	17.8(15)	0(2)	5.7(11)	-1(2)
C2	12.9(14)	16.0(17)	15.0(14)	-0.3(19)	6.4(11)	-1.8(19)
C3	17.6(17)	16(2)	14.2(15)	0.9(14)	6.4(13)	-1.6(14)
C4	13.7(16)	19(2)	11.8(15)	2.5(13)	2.3(13)	2.3(13)
C5	15.1(18)	16.7(17)	11.1(17)	4.8(14)	4.7(14)	1.8(14)
C6	13.9(18)	18.8(19)	19.2(19)	3.0(15)	8.9(15)	1.8(14)
C7	19.6(19)	16.5(18)	15.0(17)	0.6(13)	8.0(15)	-0.4(13)
C8	15.2(17)	14.9(17)	12.0(16)	-0.2(13)	5.5(14)	-2.9(13)
C9	15.8(18)	16.8(18)	8.2(16)	1.0(13)	3.9(14)	-3.1(14)
C10	16.1(16)	19(2)	12.1(14)	-2.6(14)	5.6(12)	-3.2(14)
C11	17.2(16)	18(3)	15.3(15)	2.4(14)	7.3(13)	0.7(14)
C12	11.5(18)	29(2)	14.3(18)	2.6(15)	3.1(14)	-2.2(15)
C13	21.5(18)	19(2)	13.8(16)	-0.4(13)	6.2(14)	-7.1(13)
C14	17.9(18)	15.9(19)	14.9(17)	-1.3(13)	7.4(14)	-0.8(13)
C20	11.8(14)	11(2)	16.3(14)	-1.1(15)	6.7(12)	-3.0(15)
C21	15.4(18)	16.1(16)	11.5(16)	1.4(13)	4.4(14)	-0.7(13)
C22	15.2(18)	13.5(18)	10.4(16)	1.3(14)	4.0(14)	-0.4(14)
C23	14.4(18)	15.3(18)	11.5(16)	2.2(14)	4.4(14)	0.6(14)
C24	15.0(17)	13.7(17)	12.2(16)	3.0(13)	5.7(14)	0.8(13)
C25	13.3(15)	17(2)	16.3(14)	2.7(16)	5.0(12)	-0.6(16)
C26	10.4(17)	22(2)	15.3(18)	5.0(15)	3.8(14)	0.7(15)
C27	18.8(19)	18.5(18)	20.7(19)	5.5(15)	12.2(16)	8.0(15)
C28	17.7(17)	16(2)	14.7(16)	0.0(13)	8.3(14)	1.7(13)
C29	16.4(15)	18(2)	18.7(16)	-3.8(17)	3.3(13)	-0.4(17)
C31	7.9(13)	17.9(16)	13.6(13)	-3(2)	2.7(11)	-6(2)
C32	12.7(18)	19.0(19)	19.0(19)	-1.6(15)	5.9(15)	-0.3(14)
C33	16.9(19)	20(2)	12.5(18)	0.8(14)	1.5(15)	-0.8(15)
C34	16.0(15)	28(2)	11.7(14)	-5.7(19)	4.8(12)	-4(2)
C35	14.3(19)	22(2)	20.4(19)	-5.5(16)	6.4(16)	0.6(15)
C36	9.9(17)	18.5(19)	15.2(17)	-1.2(14)	1.6(14)	-1.0(14)

Supplementary Table. 18. Bond Lengths for **5a.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Se1	C1	1.923(3)	C12	C13	1.390(6)
Se1	C4	1.995(3)	C13	C14	1.382(5)
N1	C5	1.365(5)	C20	C21	1.472(5)
N1	C8	1.383(5)	C20	C31	1.490(4)

N2	C21	1.396(5)	C21	C22	1.367(5)
N2	C24	1.377(5)	C22	C23	1.427(5)
C1	C2	1.454(4)	C22	C29	1.503(5)
C1	C20	1.350(4)	C23	C24	1.413(5)
C2	C3	1.332(5)	C23	C28	1.406(5)
C3	C4	1.499(5)	C24	C25	1.393(5)
C4	C5	1.494(5)	C25	C26	1.390(5)
C5	C6	1.373(5)	C26	C27	1.412(6)
C6	C7	1.414(5)	C27	C28	1.373(5)
C7	C8	1.378(5)	C31	C32	1.395(6)
C8	C9	1.460(5)	C31	C36	1.393(6)
C9	C10	1.402(5)	C32	C33	1.385(5)
C9	C14	1.402(5)	C33	C34	1.380(6)
C10	C11	1.385(5)	C34	C35	1.387(6)
C11	C12	1.382(5)	C35	C36	1.396(5)

Supplementary Table. 19. Bond Angles for **5a.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	Se1	C4	89.87(14)	C1	C20	C21	120.6(3)
C5	N1	C8	110.2(3)	C1	C20	C31	122.3(3)
C24	N2	C21	109.4(3)	C21	C20	C31	117.1(3)
C2	C1	Se1	108.3(2)	N2	C21	C20	121.2(3)
C20	C1	Se1	124.4(2)	C22	C21	N2	108.9(3)
C20	C1	C2	127.4(3)	C22	C21	C20	129.6(3)
C3	C2	C1	118.0(3)	C21	C22	C23	107.1(3)
C2	C3	C4	120.1(3)	C21	C22	C29	128.3(3)
C3	C4	Se1	103.5(2)	C23	C22	C29	124.5(3)
C5	C4	Se1	115.9(2)	C24	C23	C22	107.8(3)
C5	C4	C3	112.6(3)	C28	C23	C22	133.0(3)
N1	C5	C4	121.6(3)	C28	C23	C24	119.2(3)
N1	C5	C6	107.6(3)	N2	C24	C23	106.8(3)
C6	C5	C4	130.4(3)	N2	C24	C25	130.9(3)
C5	C6	C7	107.6(3)	C25	C24	C23	122.3(4)
C8	C7	C6	108.0(3)	C26	C25	C24	117.0(4)
N1	C8	C9	122.2(3)	C25	C26	C27	121.6(3)
C7	C8	N1	106.6(3)	C28	C27	C26	120.8(3)
C7	C8	C9	131.1(3)	C27	C28	C23	119.1(3)
C10	C9	C8	121.5(3)	C32	C31	C20	119.4(4)
C14	C9	C8	120.3(3)	C36	C31	C20	121.7(4)
C14	C9	C10	118.2(3)	C36	C31	C32	118.9(3)
C11	C10	C9	120.7(3)	C33	C32	C31	120.7(4)
C12	C11	C10	120.4(3)	C34	C33	C32	120.1(4)
C11	C12	C13	119.7(3)	C33	C34	C35	120.2(3)

C14	C13	C12	120.3(3)	C34	C35	C36	119.8(3)
C13	C14	C9	120.7(3)	C31	C36	C35	120.4(3)

Supplementary Table. 20. Torsion Angles for **5a.**

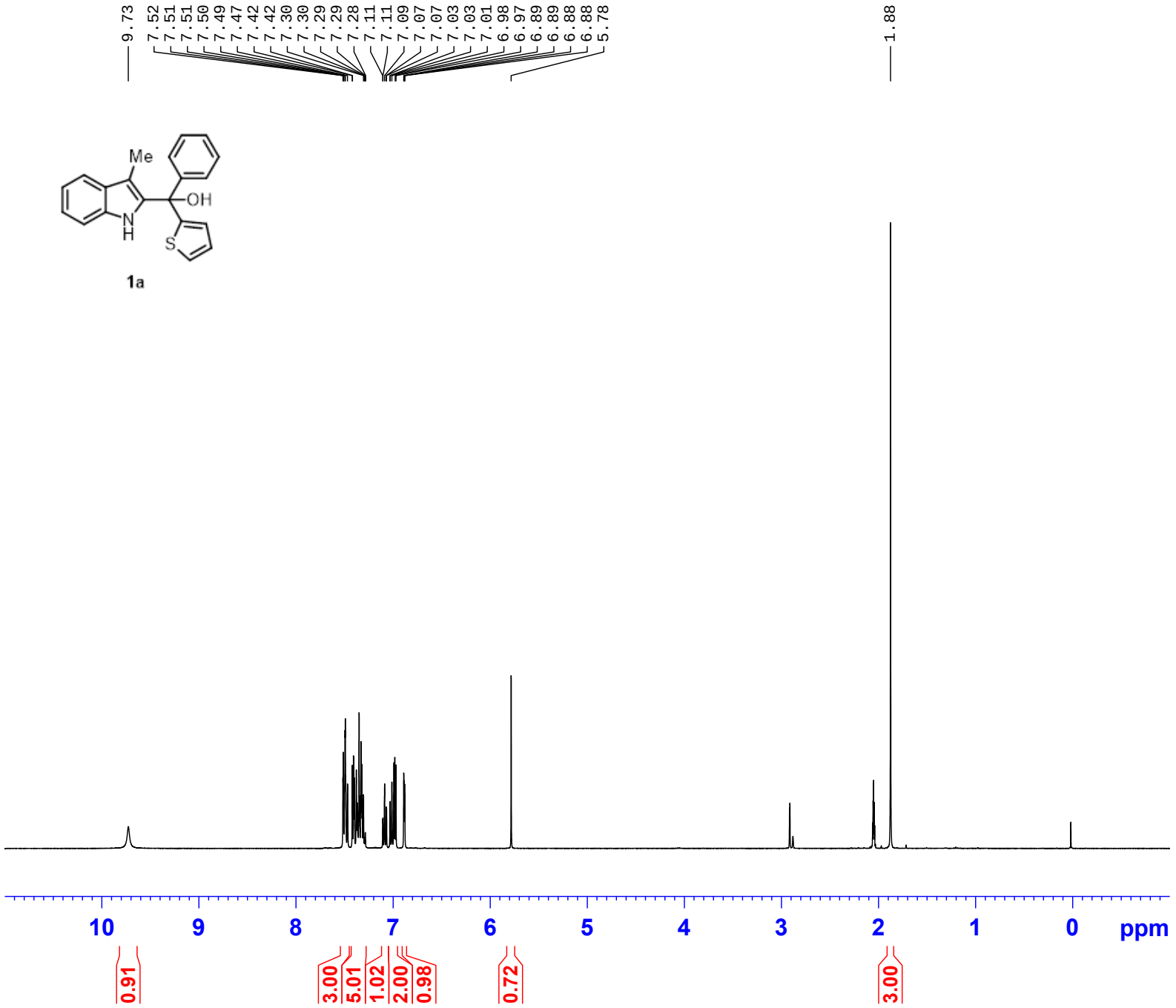
A	B	C	D	Angle/°	A	B	C	D	Angle/°
Se1	C1	C2	C3	-4.1(6)	C11	C12	C13	C14	-0.3(6)
Se1	C1	C20	C21	-164.8(3)	C12	C13	C14	C9	-1.3(6)
Se1	C1	C20	C31	11.8(8)	C14	C9	C10	C11	-1.9(5)
Se1	C4	C5	N1	-97.8(3)	C20	C1	C2	C3	176.8(5)
Se1	C4	C5	C6	90.1(4)	C20	C21	C22	C23	173.0(4)
N1	C5	C6	C7	0.6(4)	C20	C21	C22	C29	-3.5(6)
N1	C8	C9	C10	-0.2(5)	C20	C31	C32	C33	179.6(3)
N1	C8	C9	C14	179.4(3)	C20	C31	C36	C35	179.1(3)
N2	C21	C22	C23	-0.6(4)	C21	N2	C24	C23	1.0(4)
N2	C21	C22	C29	-177.1(3)	C21	N2	C24	C25	179.5(4)
N2	C24	C25	C26	-177.4(4)	C21	C20	C31	C32	45.6(5)
C1	C2	C3	C4	2.4(6)	C21	C20	C31	C36	-133.0(4)
C1	C20	C21	N2	-136.0(5)	C21	C22	C23	C24	1.2(4)
C1	C20	C21	C22	51.1(7)	C21	C22	C23	C28	-176.5(4)
C1	C20	C31	C32	-131.1(5)	C22	C23	C24	N2	-1.4(4)
C1	C20	C31	C36	50.3(7)	C22	C23	C24	C25	-180.0(3)
C2	C1	C20	C21	14.2(8)	C22	C23	C28	C27	178.8(4)
C2	C1	C20	C31	-169.2(5)	C23	C24	C25	C26	0.8(5)
C2	C3	C4	Se1	0.6(4)	C24	N2	C21	C20	-174.5(3)
C2	C3	C4	C5	126.6(4)	C24	N2	C21	C22	-0.3(4)
C3	C4	C5	N1	143.3(3)	C24	C23	C28	C27	1.3(5)
C3	C4	C5	C6	-28.9(5)	C24	C25	C26	C27	0.9(5)
C4	C5	C6	C7	173.6(4)	C25	C26	C27	C28	-1.5(6)
C5	N1	C8	C7	1.2(4)	C26	C27	C28	C23	0.4(5)
C5	N1	C8	C9	-176.7(3)	C28	C23	C24	N2	176.7(3)
C5	C6	C7	C8	0.1(4)	C28	C23	C24	C25	-1.9(5)
C6	C7	C8	N1	-0.8(4)	C29	C22	C23	C24	177.9(3)
C6	C7	C8	C9	176.9(4)	C29	C22	C23	C28	0.2(6)
C7	C8	C9	C10	-177.5(4)	C31	C20	C21	N2	47.3(6)
C7	C8	C9	C14	2.1(6)	C31	C20	C21	C22	-125.6(4)
C8	N1	C5	C4	-174.8(3)	C31	C32	C33	C34	1.8(6)
C8	N1	C5	C6	-1.1(4)	C32	C31	C36	C35	0.5(5)
C8	C9	C10	C11	177.7(3)	C32	C33	C34	C35	-0.6(6)
C8	C9	C14	C13	-177.2(3)	C33	C34	C35	C36	-0.6(6)
C9	C10	C11	C12	0.3(5)	C34	C35	C36	C31	0.7(5)
C10	C9	C14	C13	2.4(5)	C36	C31	C32	C33	-1.7(5)
C10	C11	C12	C13	0.8(6)					

Supplementary Table. 21. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **5a.**

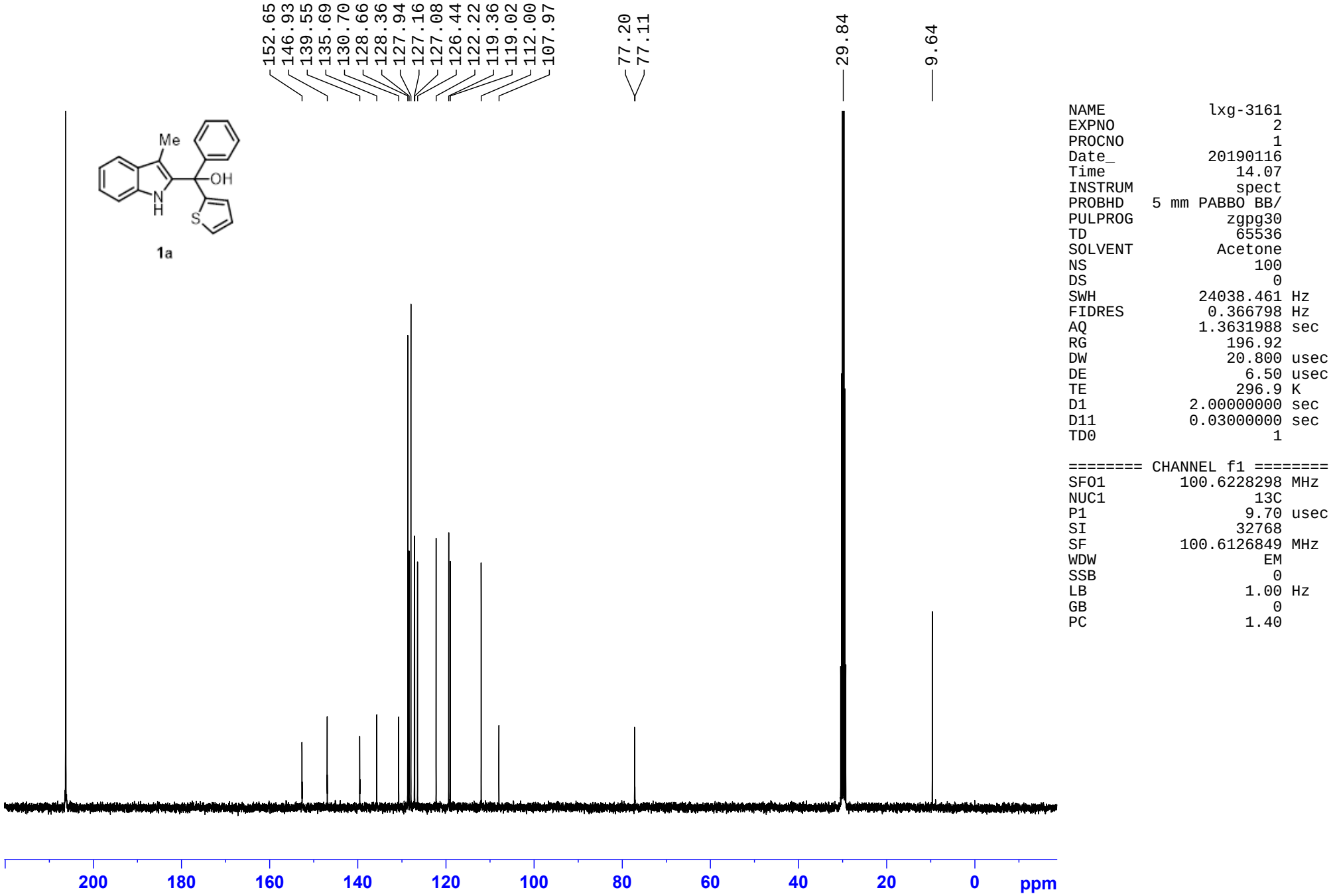
Atom	***x***	***y***	***z***	**U(eq)**
H1	8246	3916	4834	17
H2	1556	3143	772	18
H2A	3709	4581	3561	17
H3	5253	3914	4783	19
H4	6469	2378	4138	19
H6	6243	8815	4879	20
H7	8013	10222	5961	20
H10	9873	3762	5472	19
H11	11651	3807	6151	20
H12	12523	7039	7108	23
H13	11607	10221	7408	22
H14	9832	10177	6753	19
H25	-533	3646	343	19
H26	-1664	6187	681	20
H27	-1062	9529	1690	22
H28	679	10313	2433	19
H29A	2594	10916	2680	29
H29B	3567	9325	2768	29
H29C	3024	8861	3469	29
H32	2740	7853	251	20
H33	2840	7625	-1195	21
H34	3630	4302	-1554	23
H35	4358	1223	-452	23
H36	4314	1513	1025	19

Supplementary References

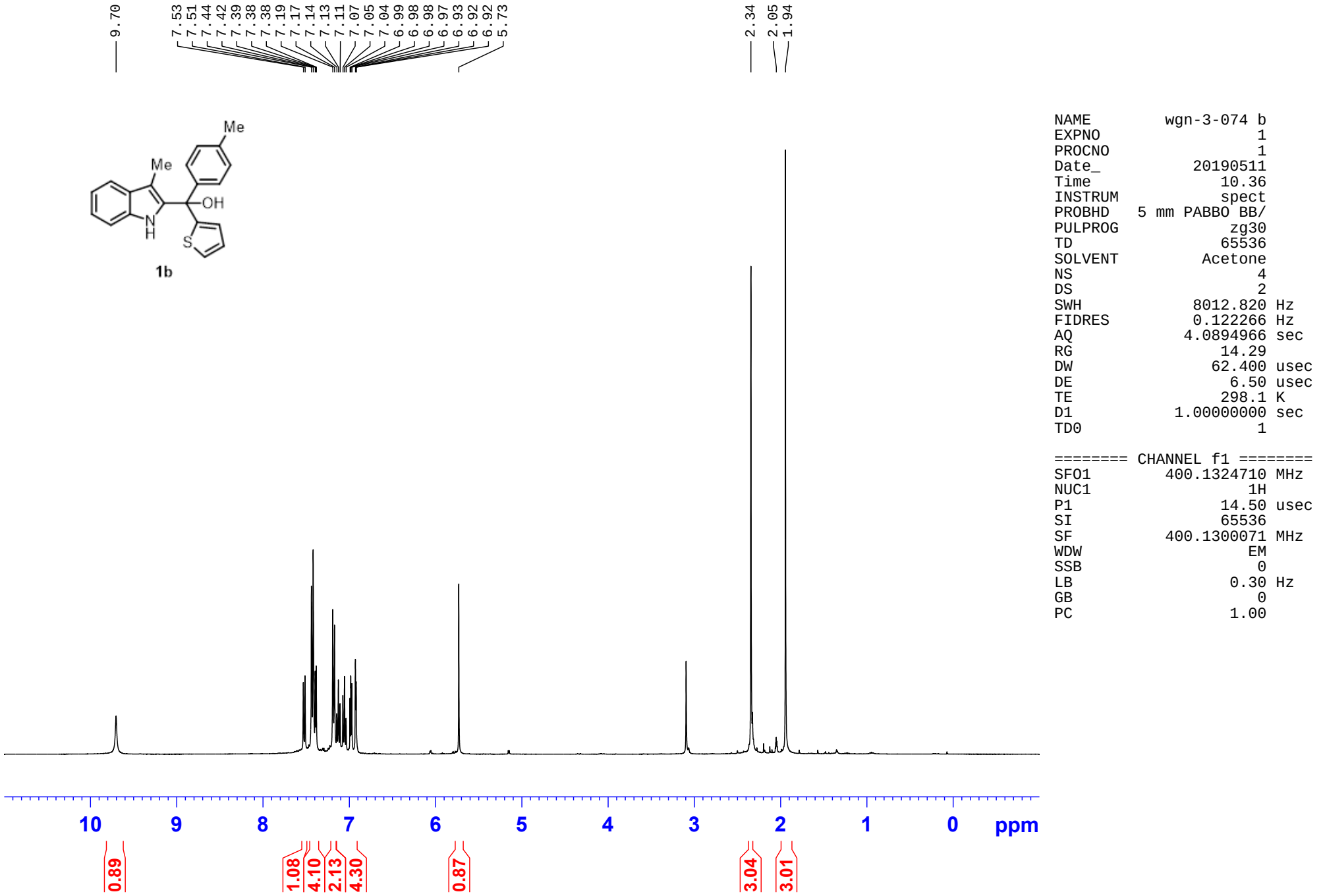
1. Yu, J. O. et al. 2-Indolylphosphines, a new class of tunable ligands: their synthesis, facile derivatization, and coordination to palladium(II). *Organometallics* **24**, 37−47 (2005).
2. Ip, H.-W., Ng, C.-F., Chow, H.-F. & Kuck, D. Three-fold scholl-type cycloheptatriene ring formation around a tribenzotriquinacene core: toward warped graphenes. *J. Am. Chem. Soc.* **138**, 13778−13781 (2016).
3. Ma, S. et al. Development of a general and practical iron nitrate/TEMPO-catalyzed aerobic oxidation of alcohols to aldehydes/ketones: catalysis with table salt. *Adv. Synth. Catal.* **353**, 1005−1017 (2011).



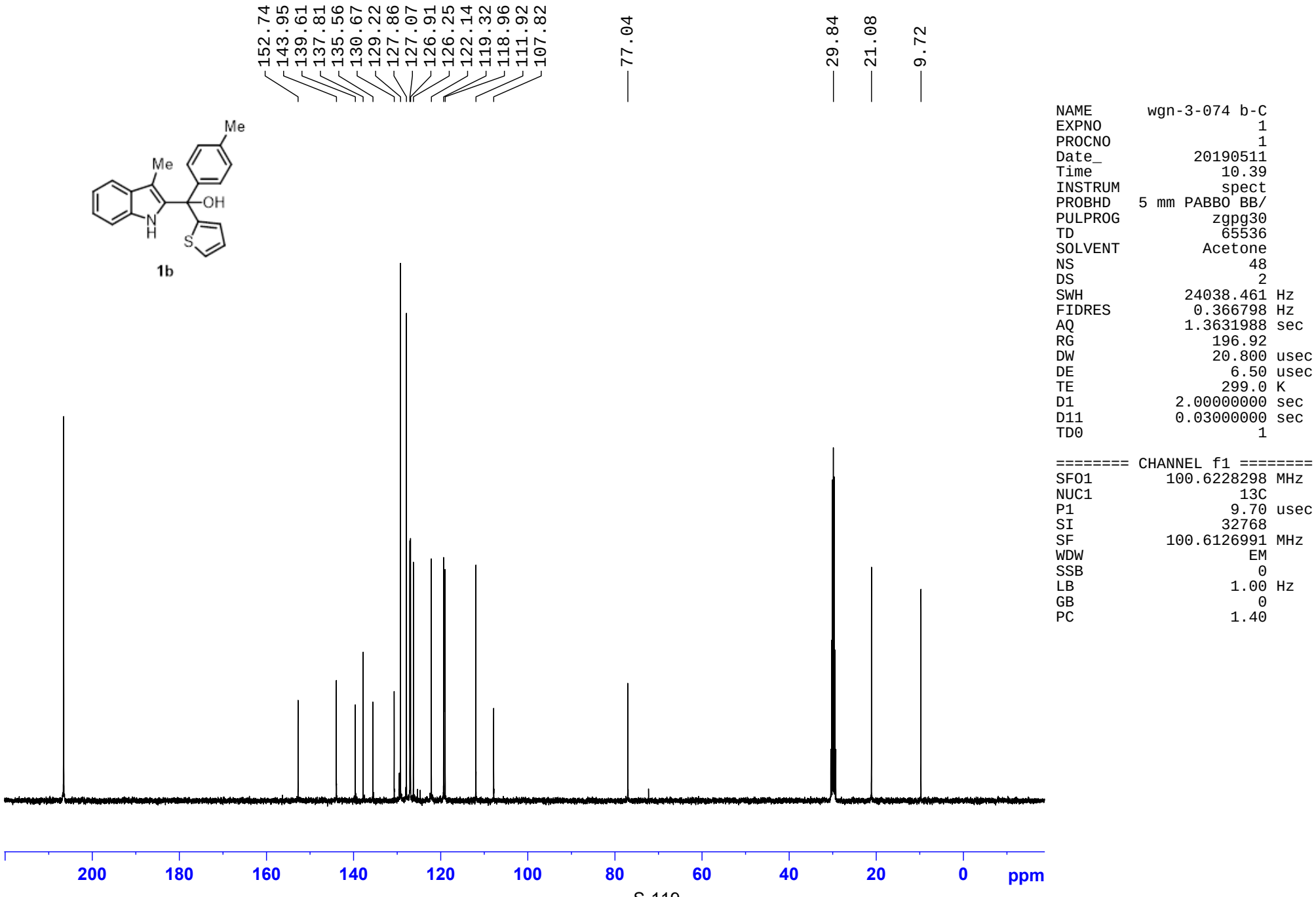
Supplementary Figure 1. ^{1}H NMR spectrum of **1a**



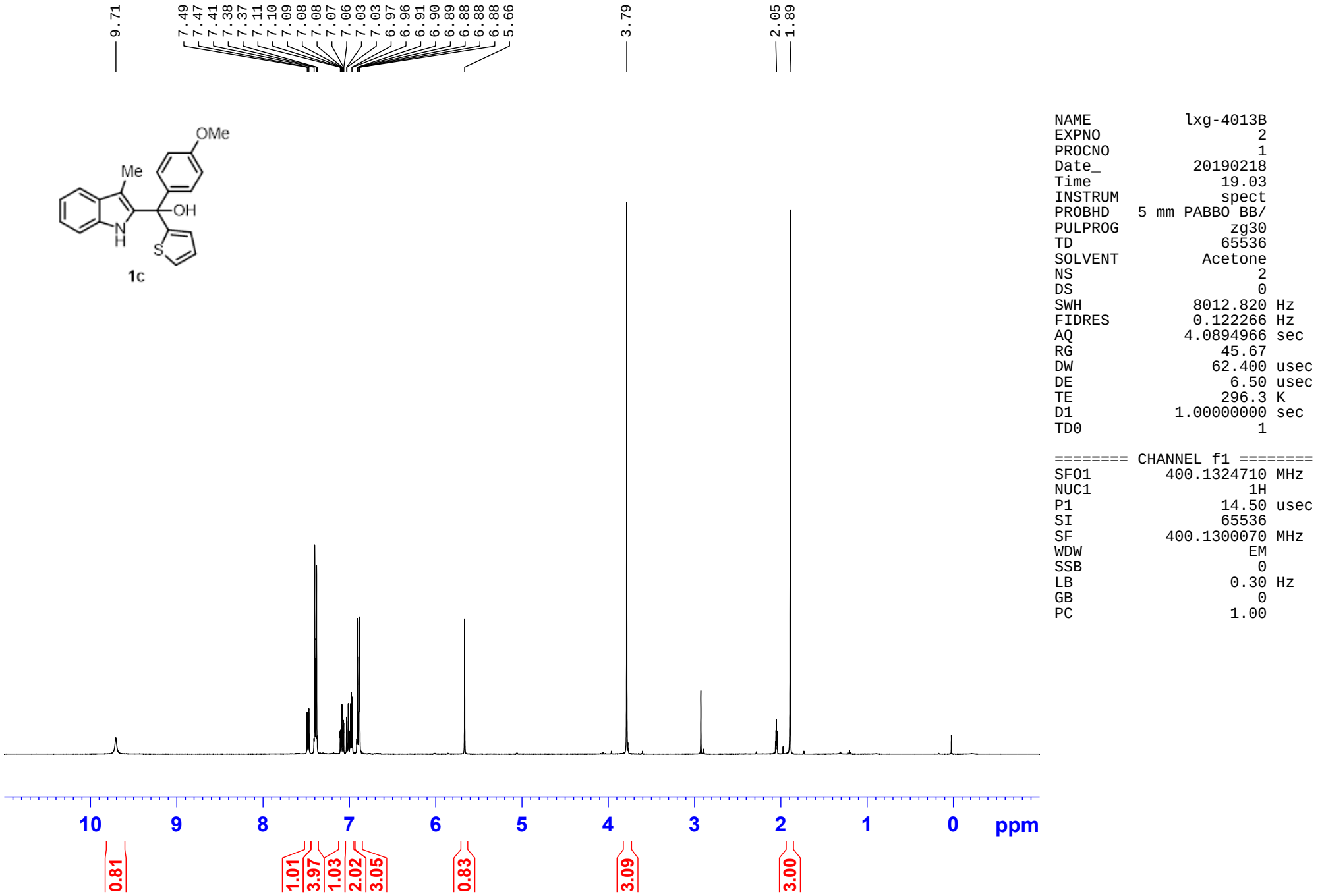
Supplementary Figure 2. ^{13}C NMR spectrum of **1a**



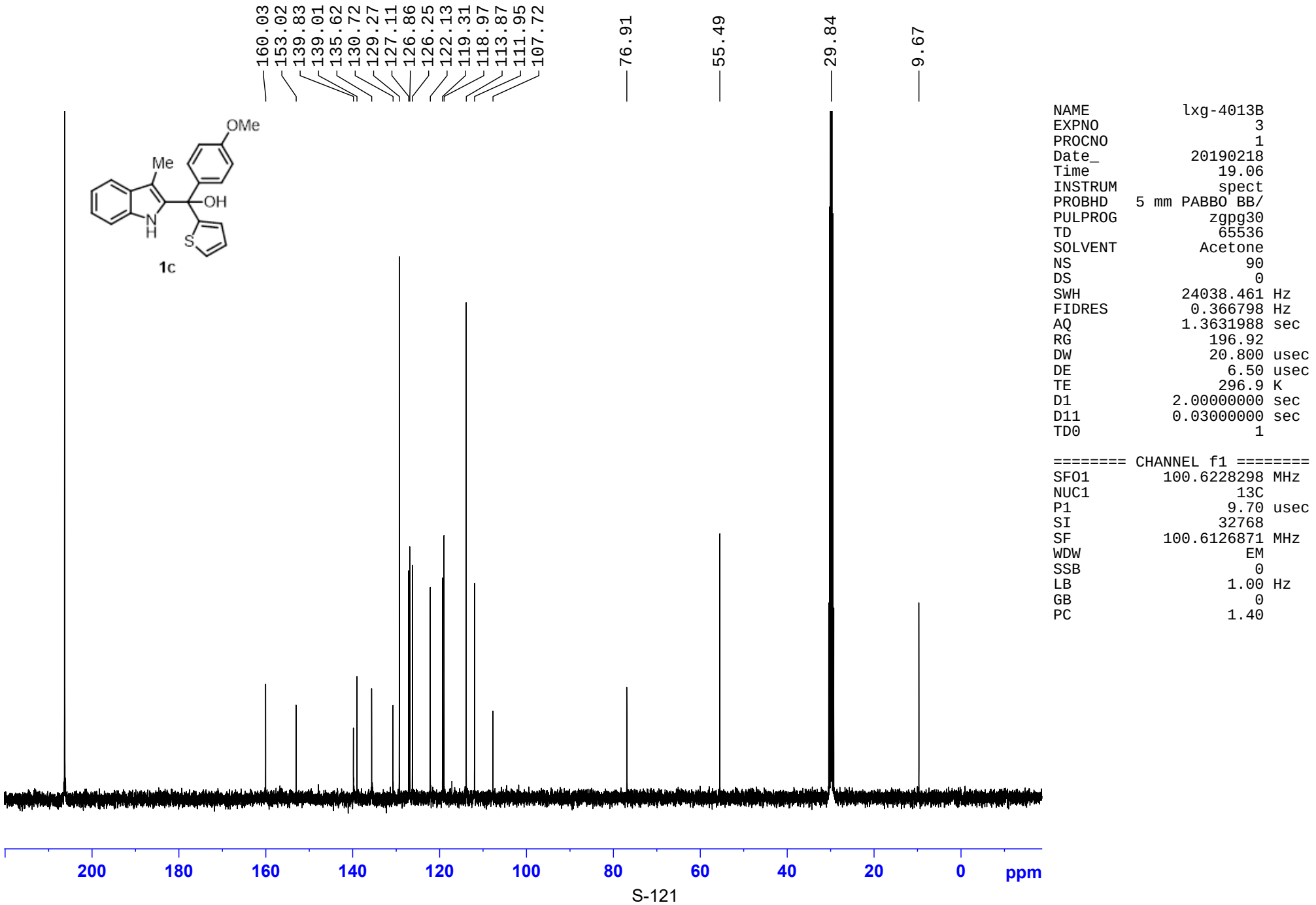
Supplementary Figure 3. ^{1}H NMR spectrum of **1b**



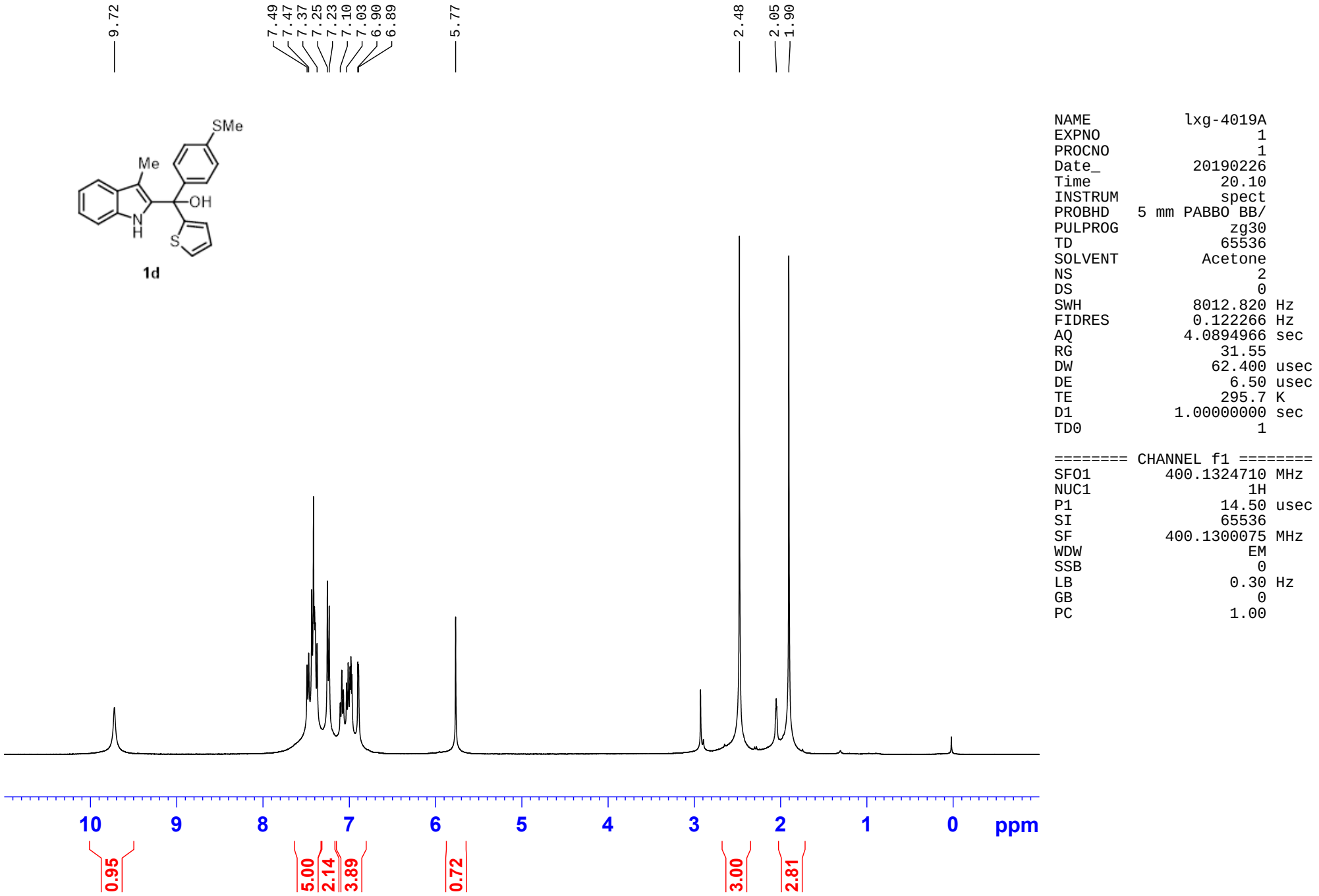
Supplementary Figure 4. ^{13}C NMR spectrum of **1b**



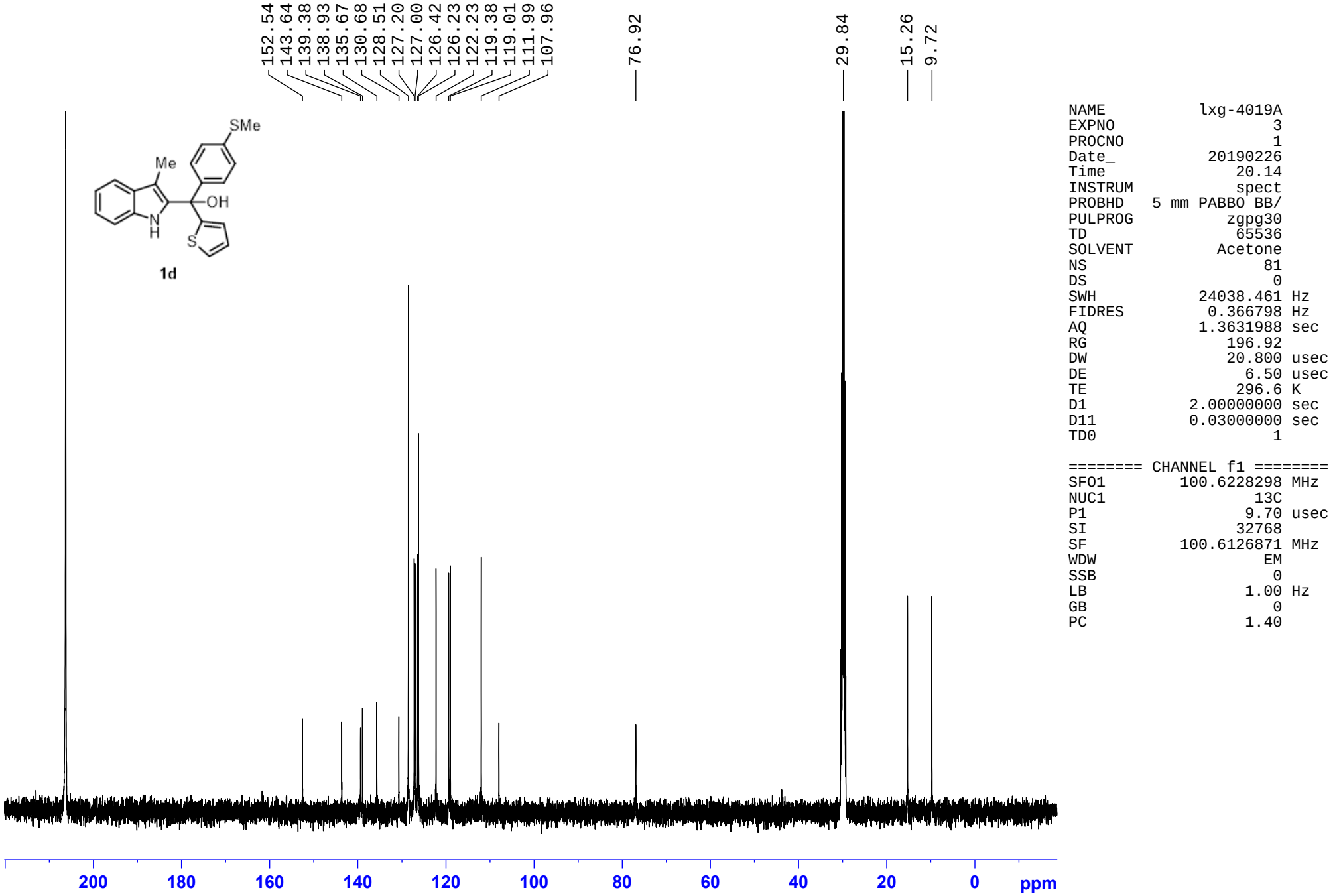
Supplementary Figure 5. ^{1}H NMR spectrum of **1c**



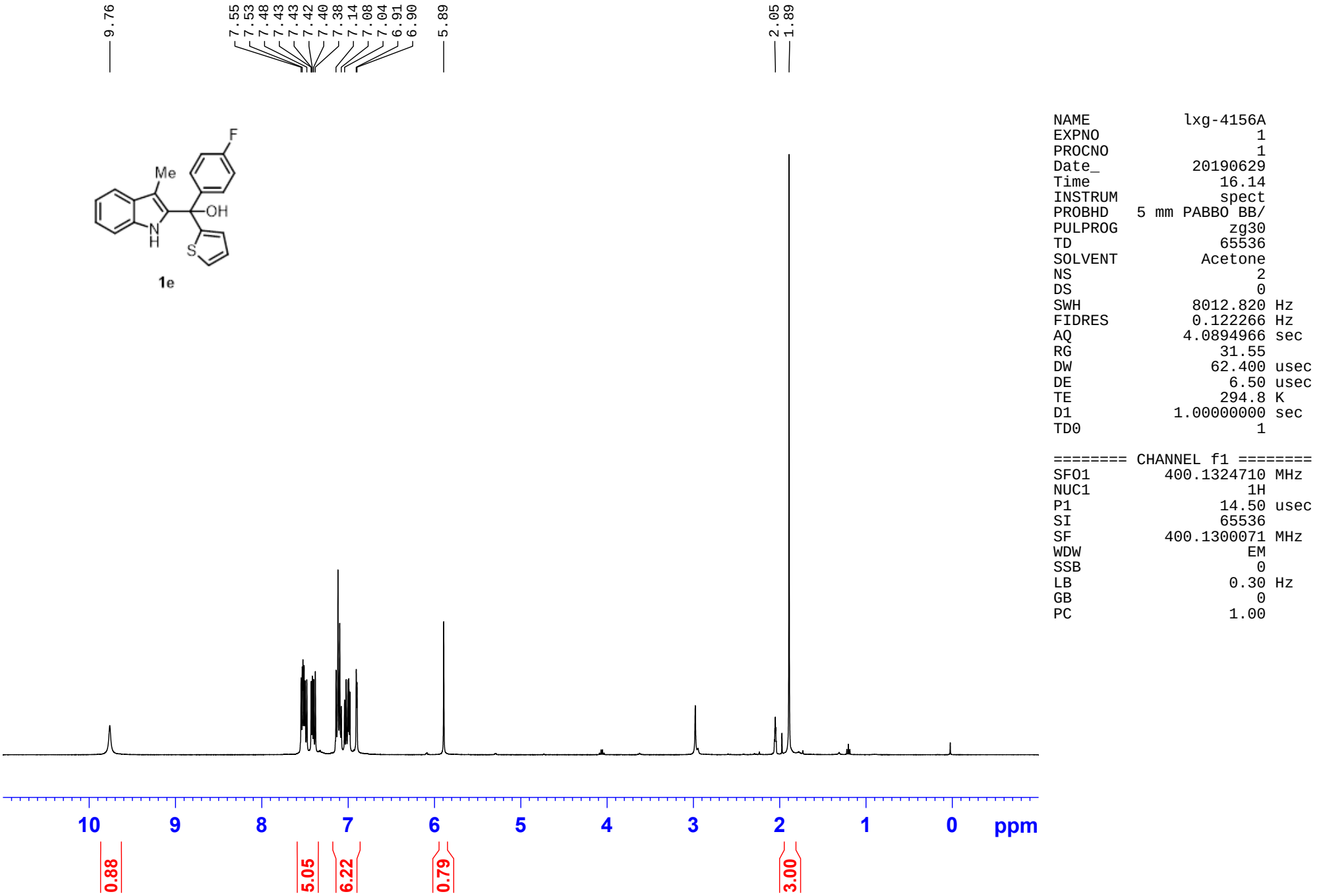
Supplementary Figure 6. ^{13}C NMR spectrum of **1c**



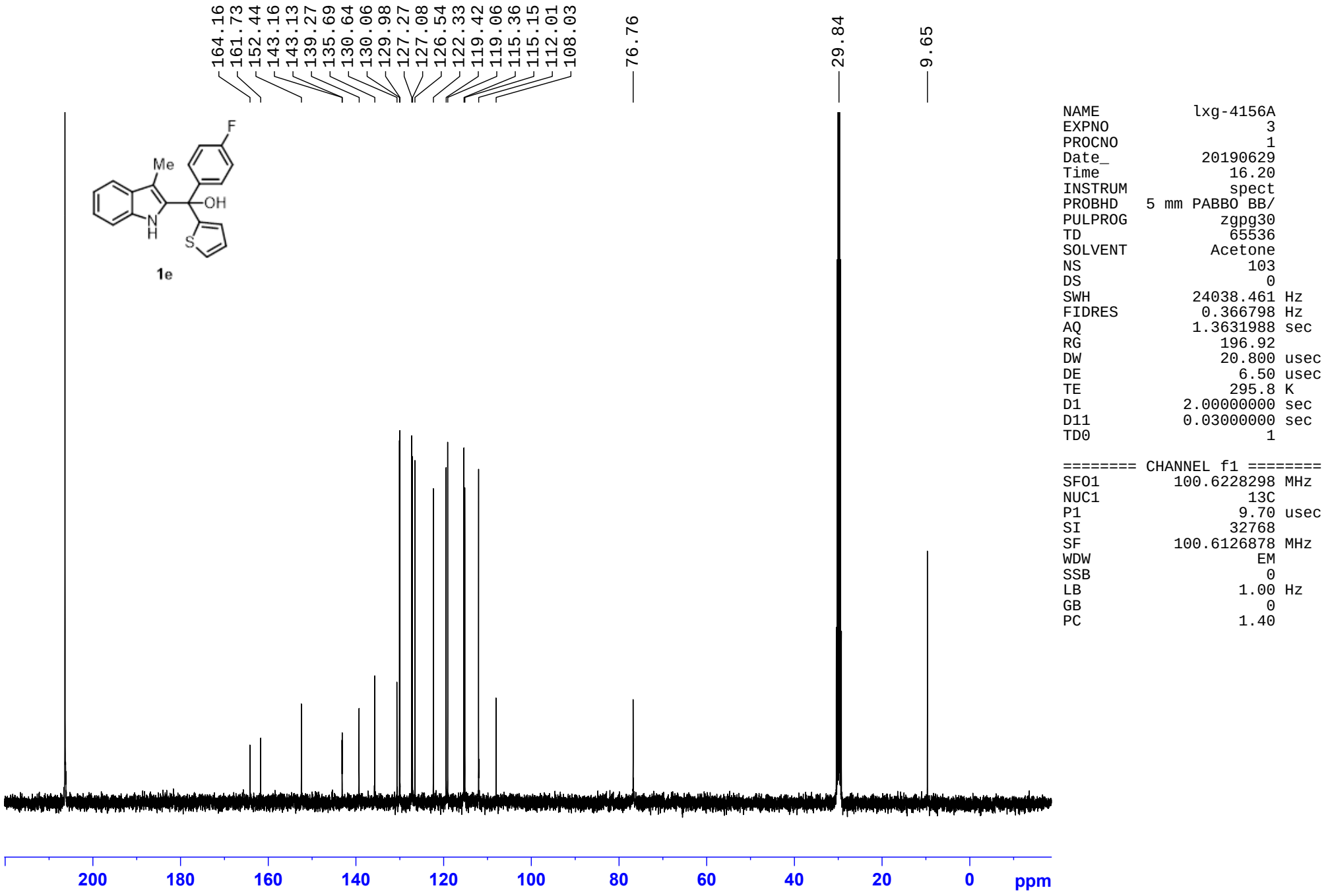
Supplementary Figure 7. ^{1}H NMR spectrum of **1d**



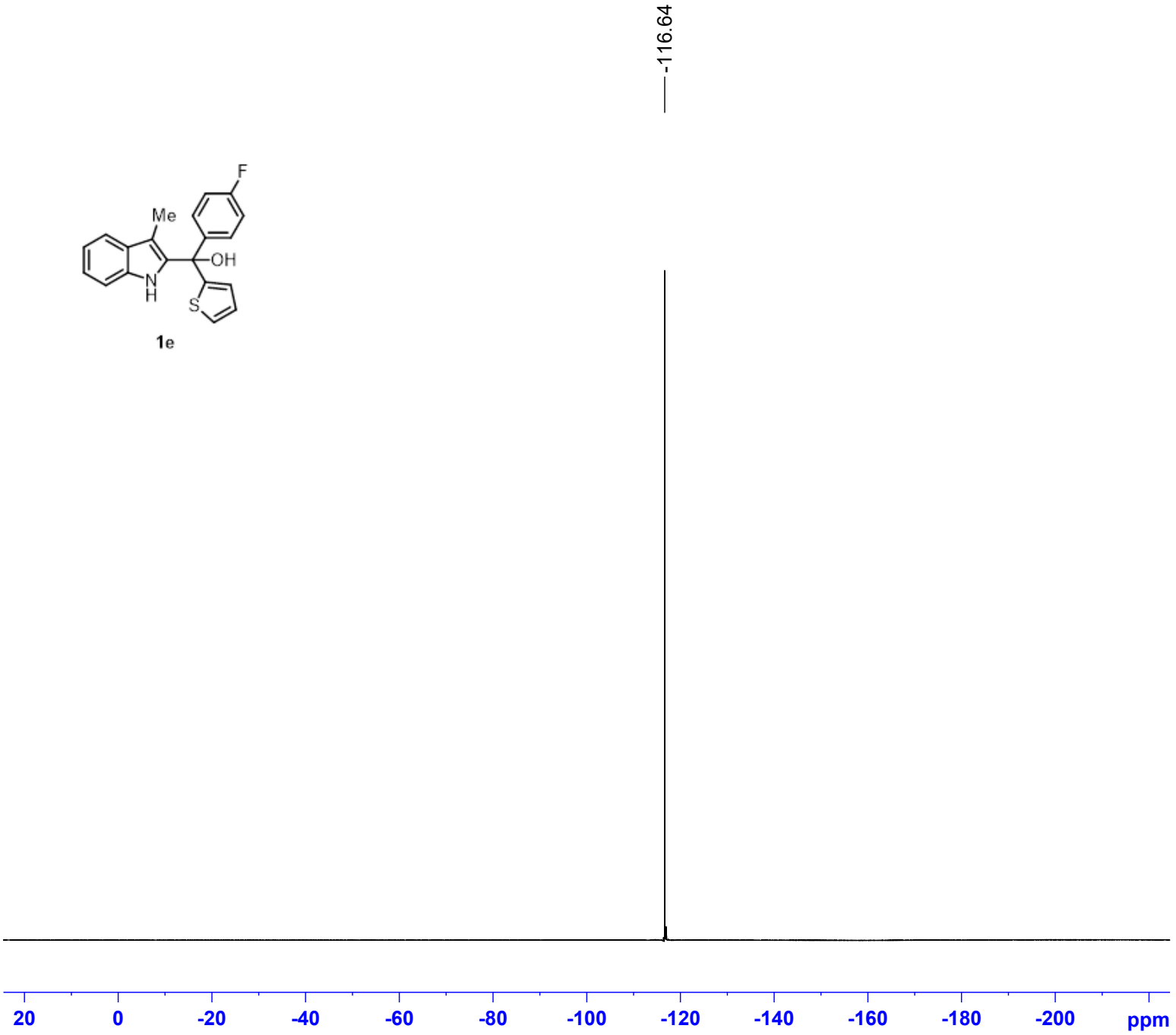
Supplementary Figure 8. ^{13}C NMR spectrum of **1d**



Supplementary Figure 9. ^{1}H NMR spectrum of **1e**



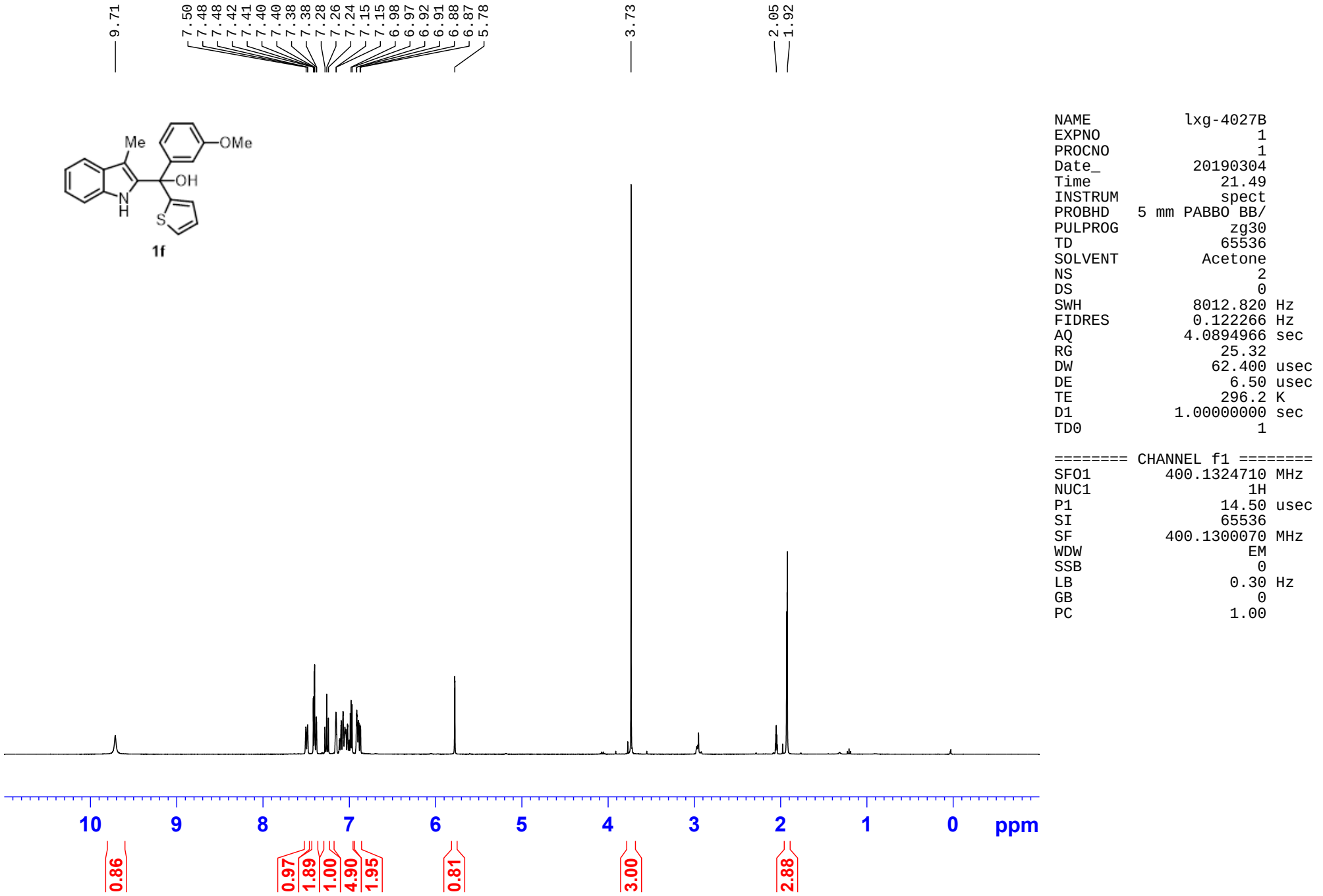
Supplementary Figure 10. ^{13}C NMR spectrum of **1e**



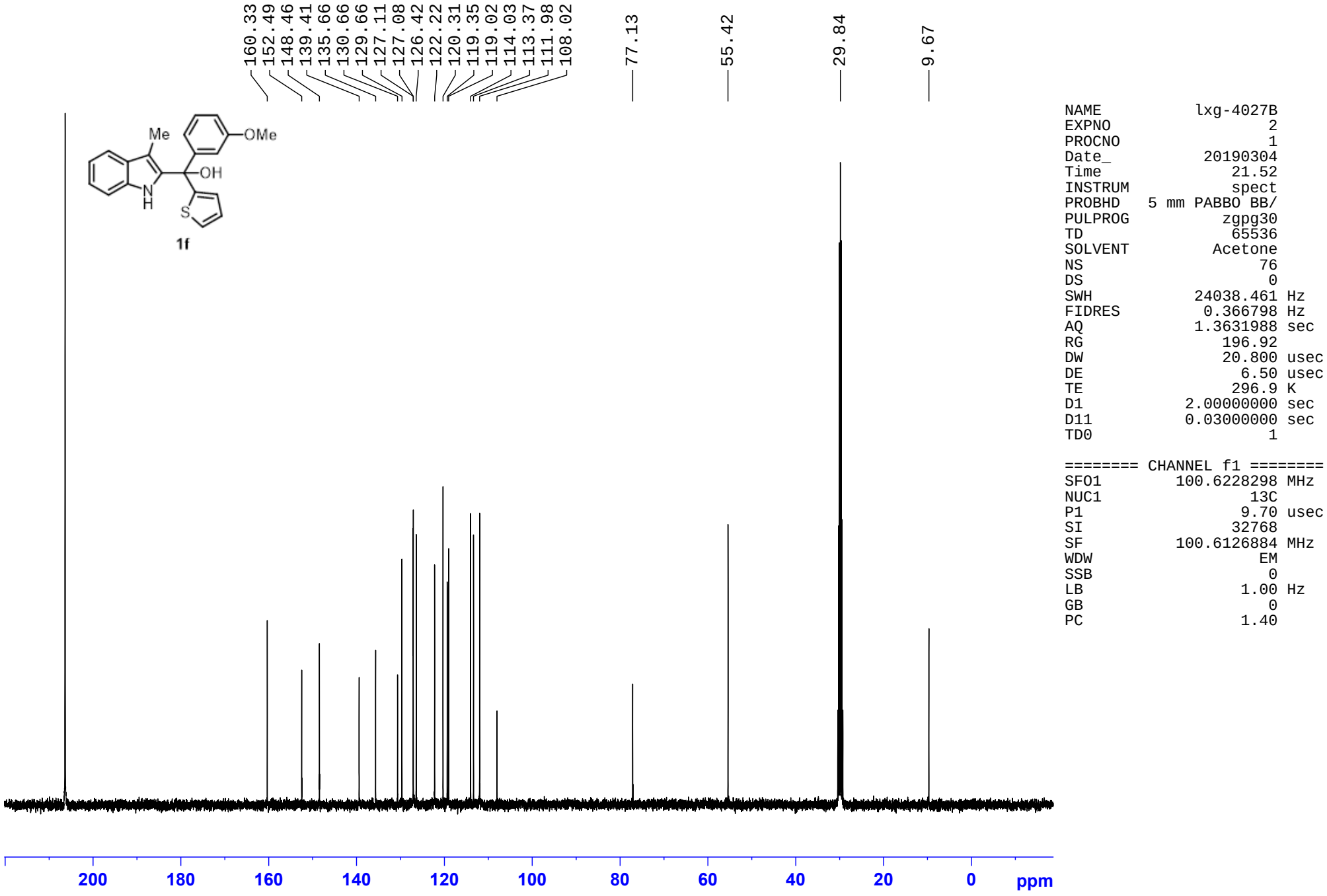

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PROCNO                 1
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RG                196.92
DW                5.333 usec
DE                6.50 usec
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D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
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PC                 1.40
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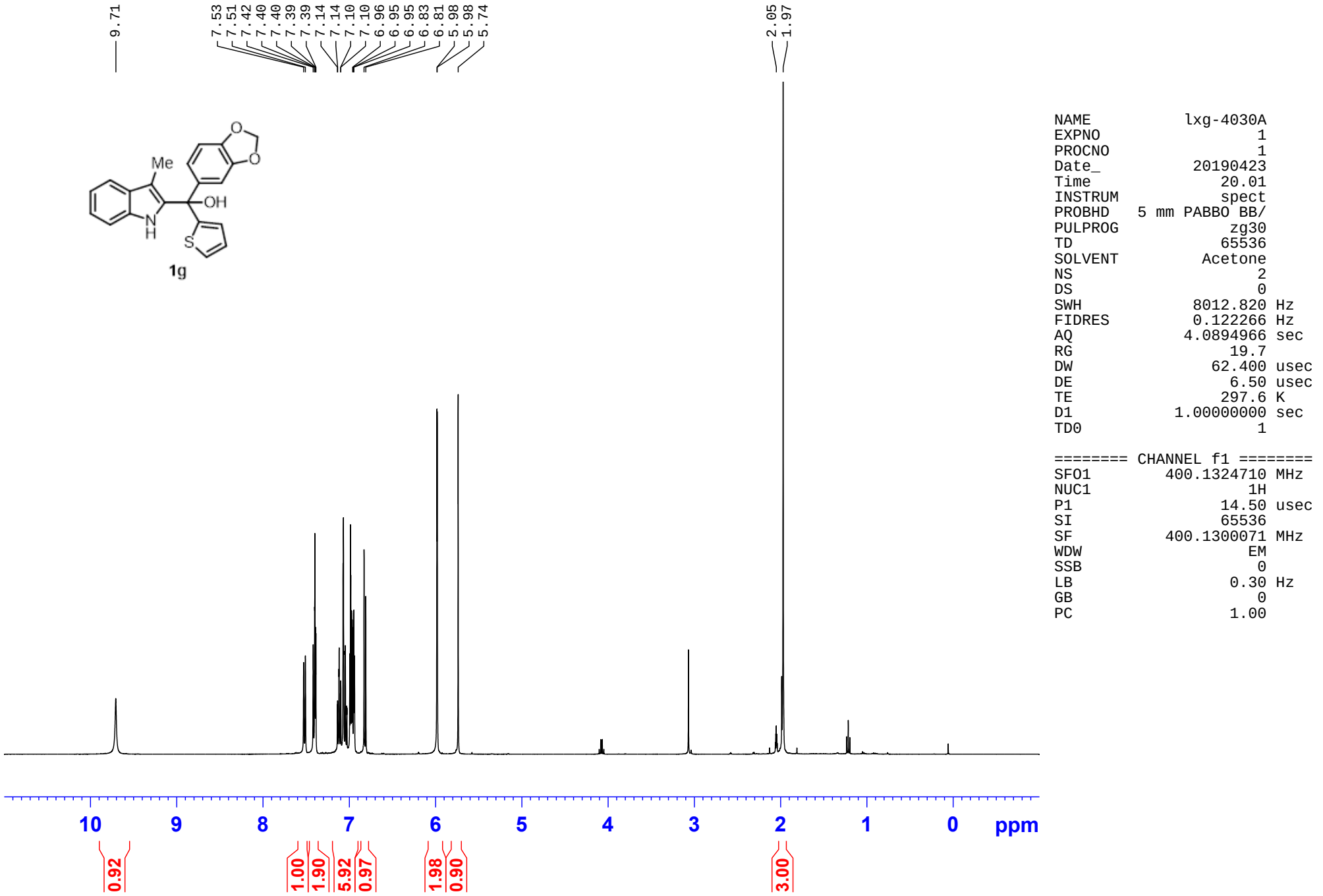
Supplementary Figure 11. ^{19}F NMR spectrum of **1e**



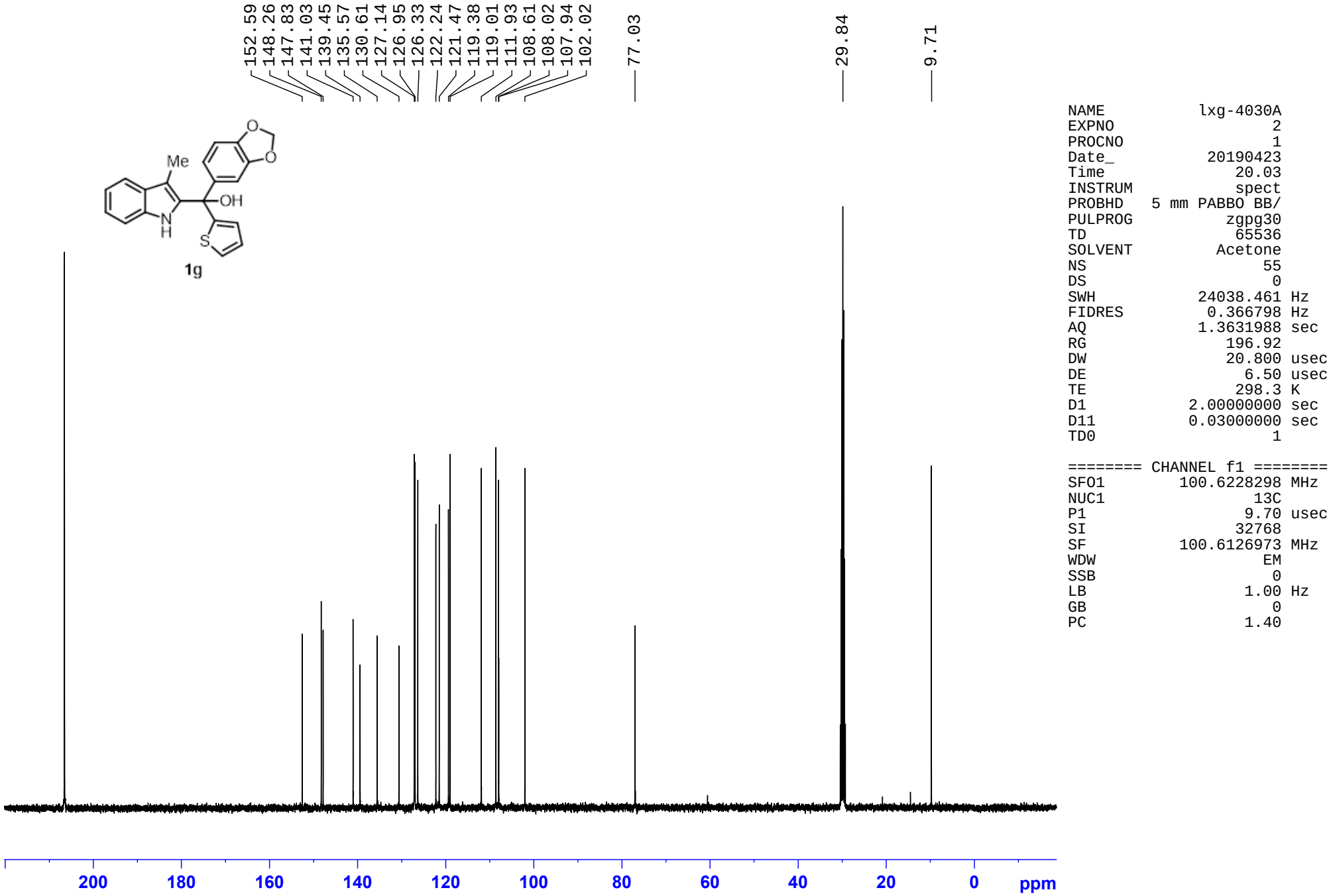
Supplementary Figure 12. ^{1}H NMR spectrum of **1f**



Supplementary Figure 13. ^{13}C NMR spectrum of **1f**



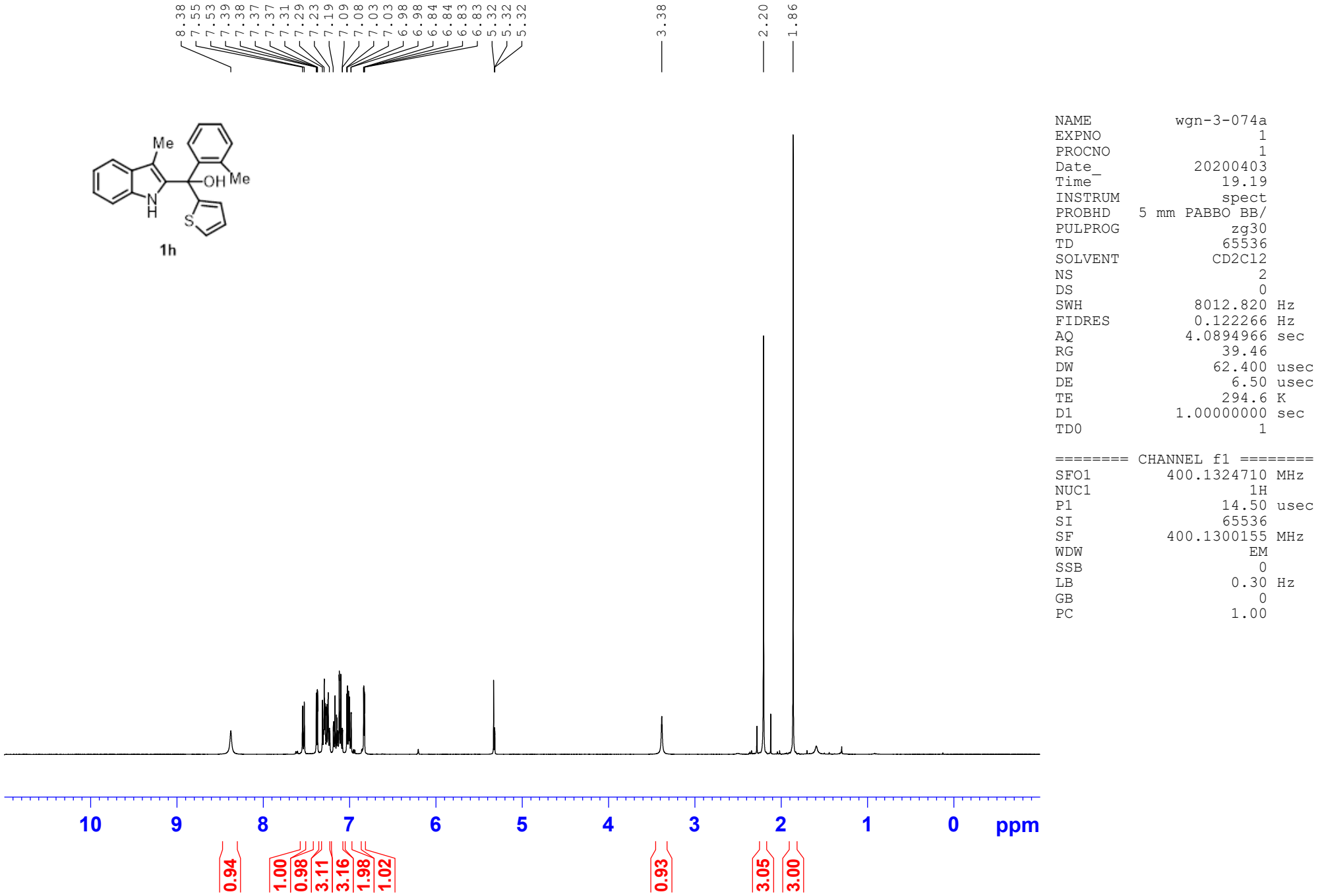
Supplementary Figure 14. ^{1}H NMR spectrum of **1g**



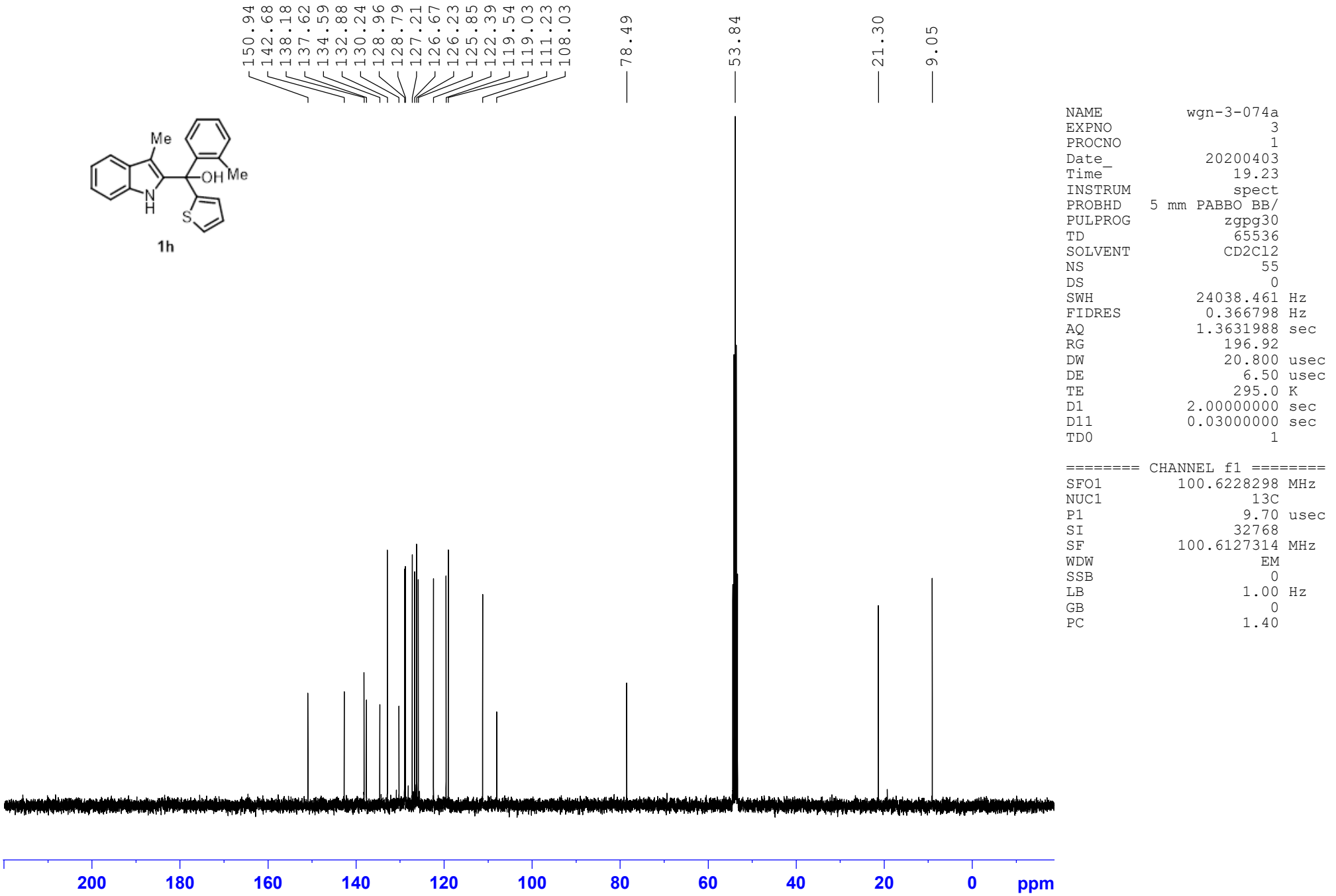

```
NAME            lxg-4030A
EXPNO                   2
PROCNO                  1
Date_            20190423
Time                20.03
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT           Acetone
NS                     55
DS                      0
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                 196.92
DW                 20.800 usec
DE                  6.50 usec
TE                 298.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                  13C
P1                  9.70 usec
SI                 32768
SF           100.6126973 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```


Supplementary Figure 15. ^{13}C NMR spectrum of **1g**



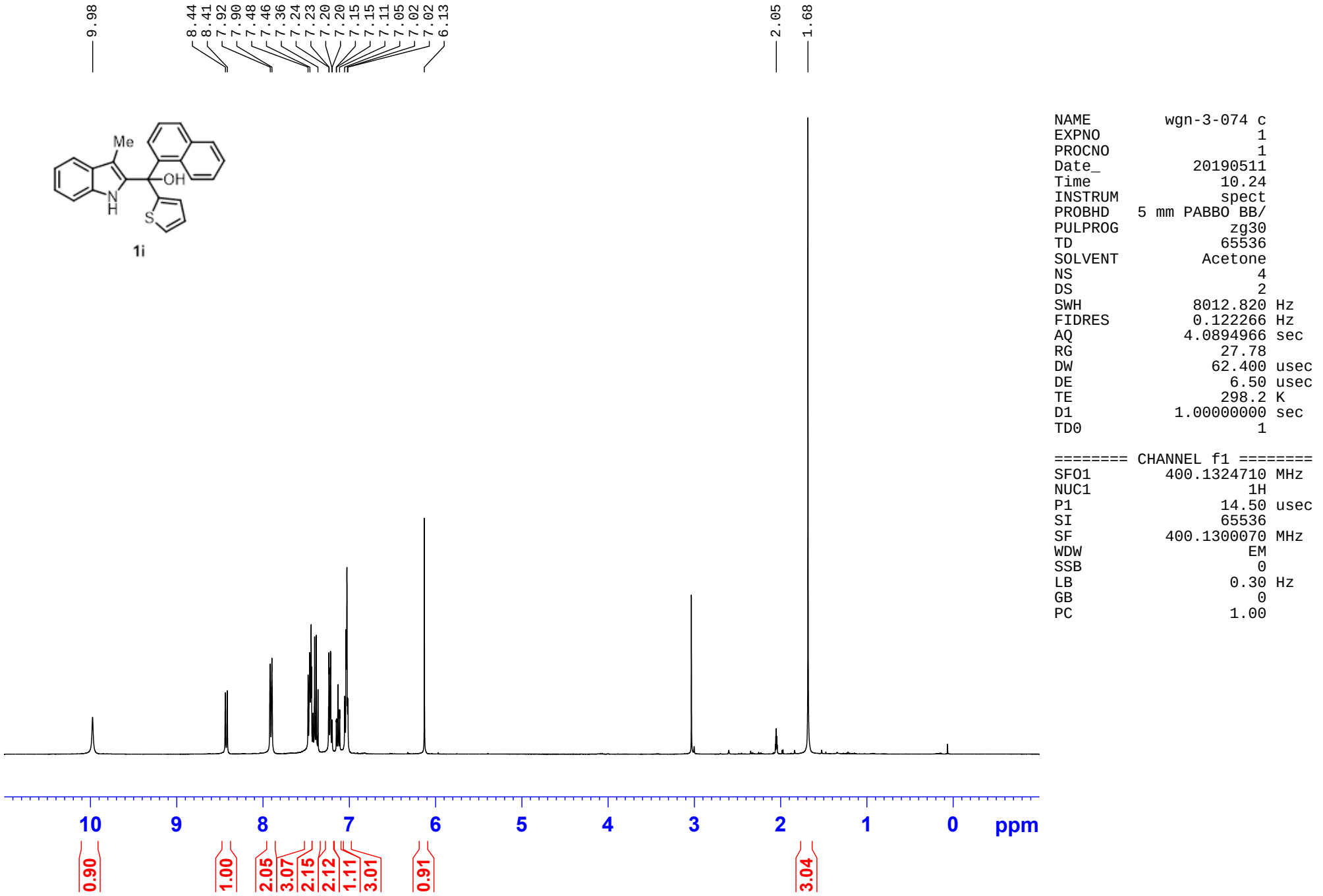
Supplementary Figure 16. ^{1}H NMR spectrum of **1h**



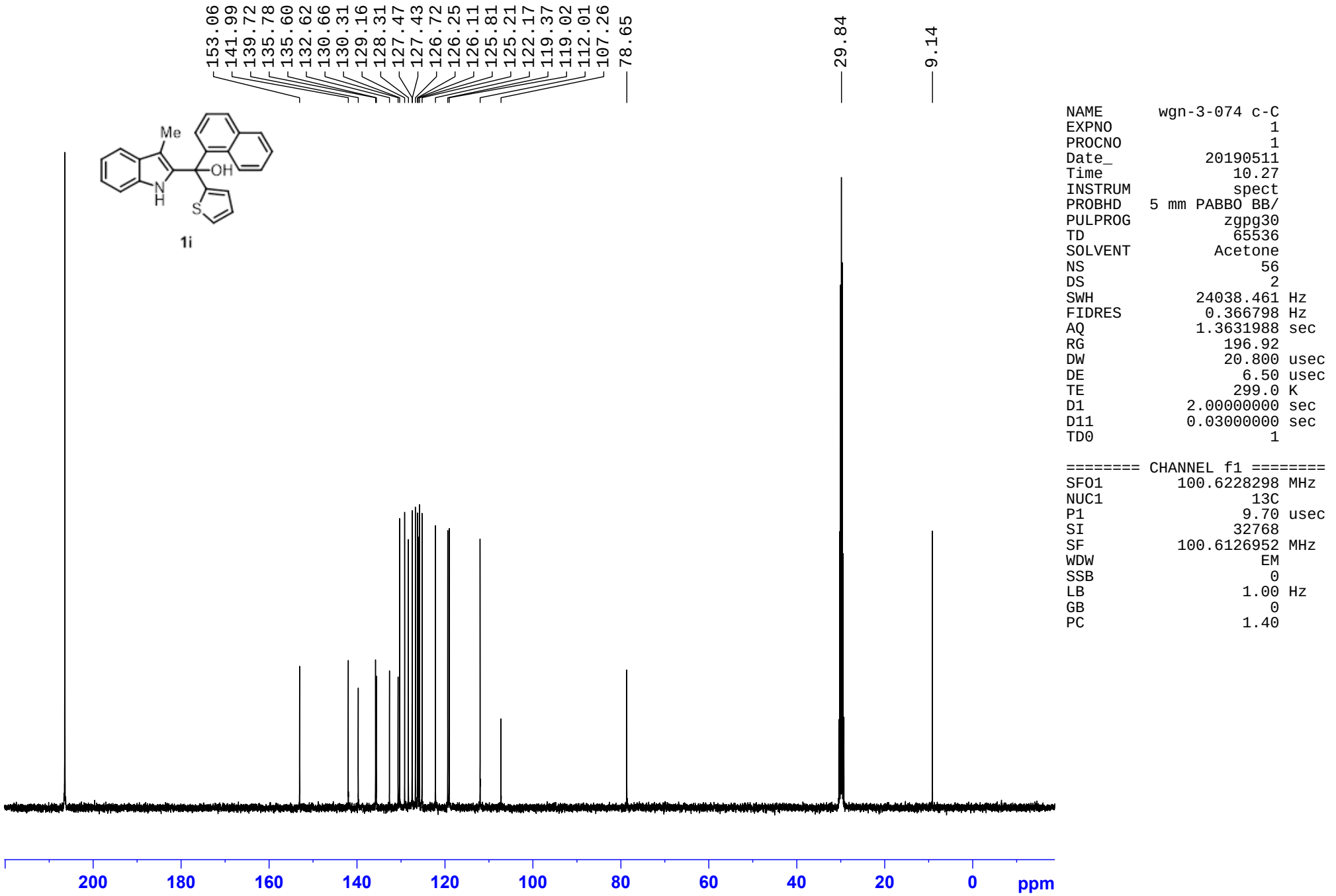

```
NAME          wgn-3-074a
EXPNO                  3
PROCNO                 1
Date_           20200403
Time               19.23
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          CD2Cl2
NS                    55
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                295.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
SI                32768
SF          100.6127314 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

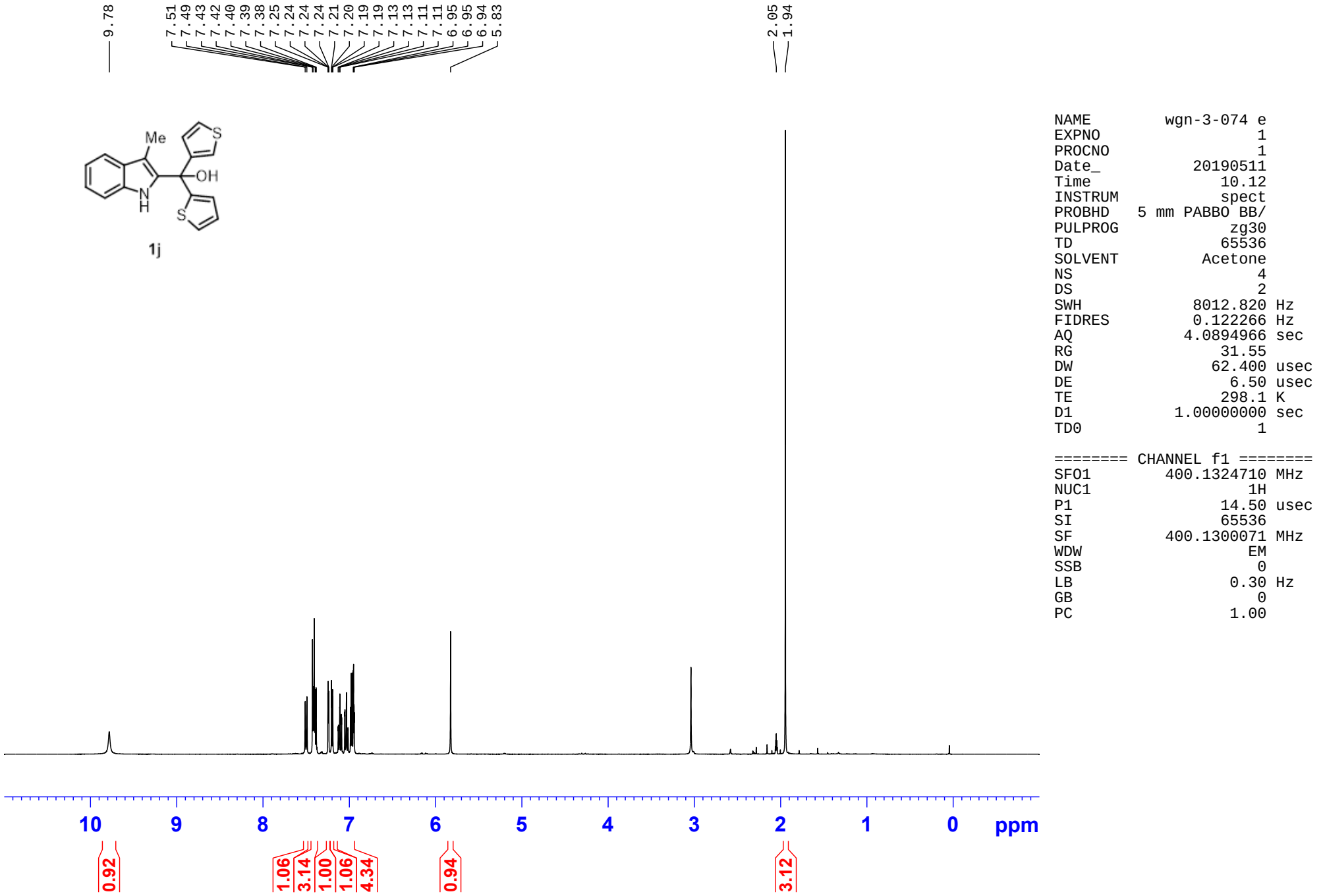

Supplementary Figure 17. ^{13}C NMR spectrum of **1h**



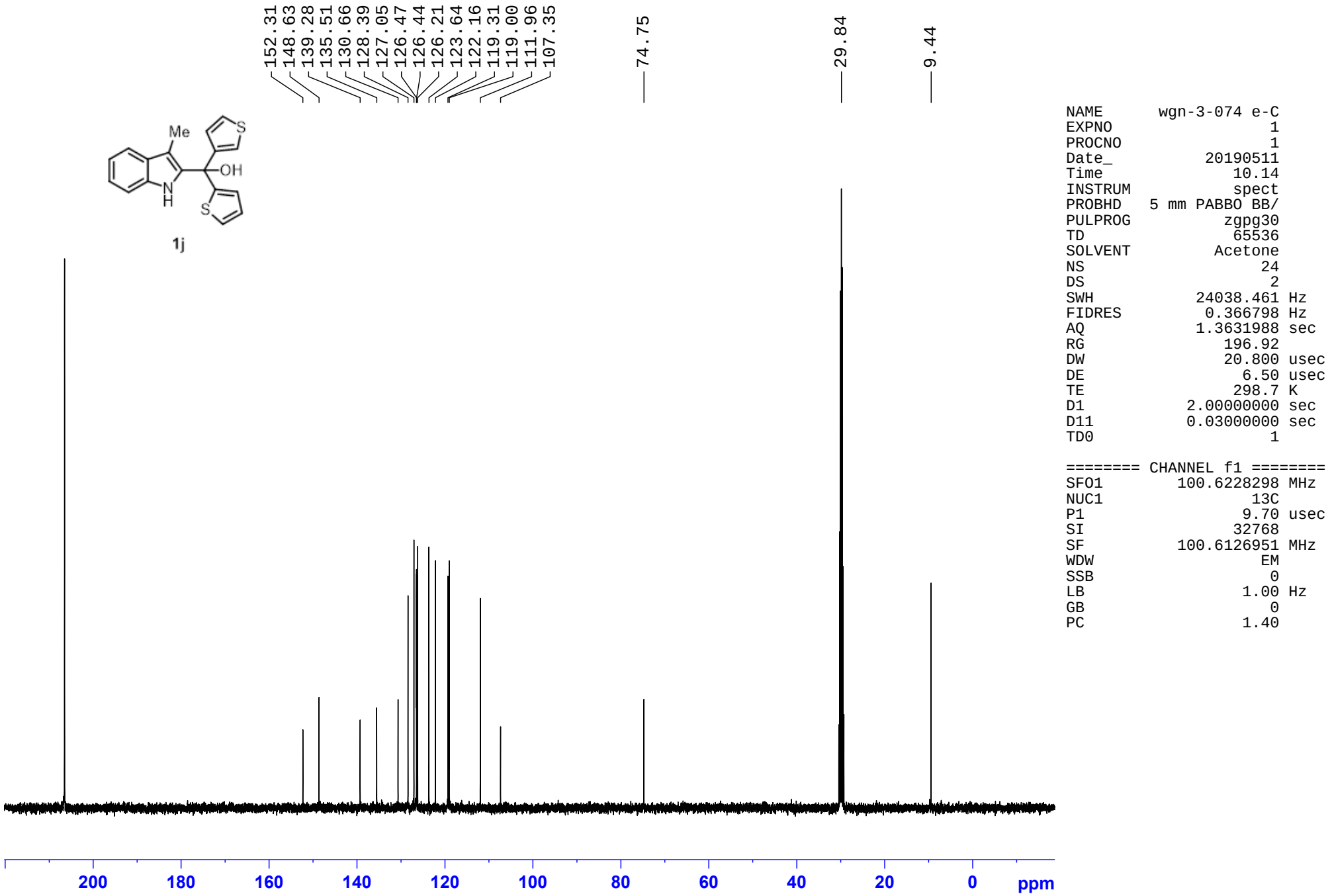
Supplementary Figure 18. ^{1}H NMR spectrum of **1i**



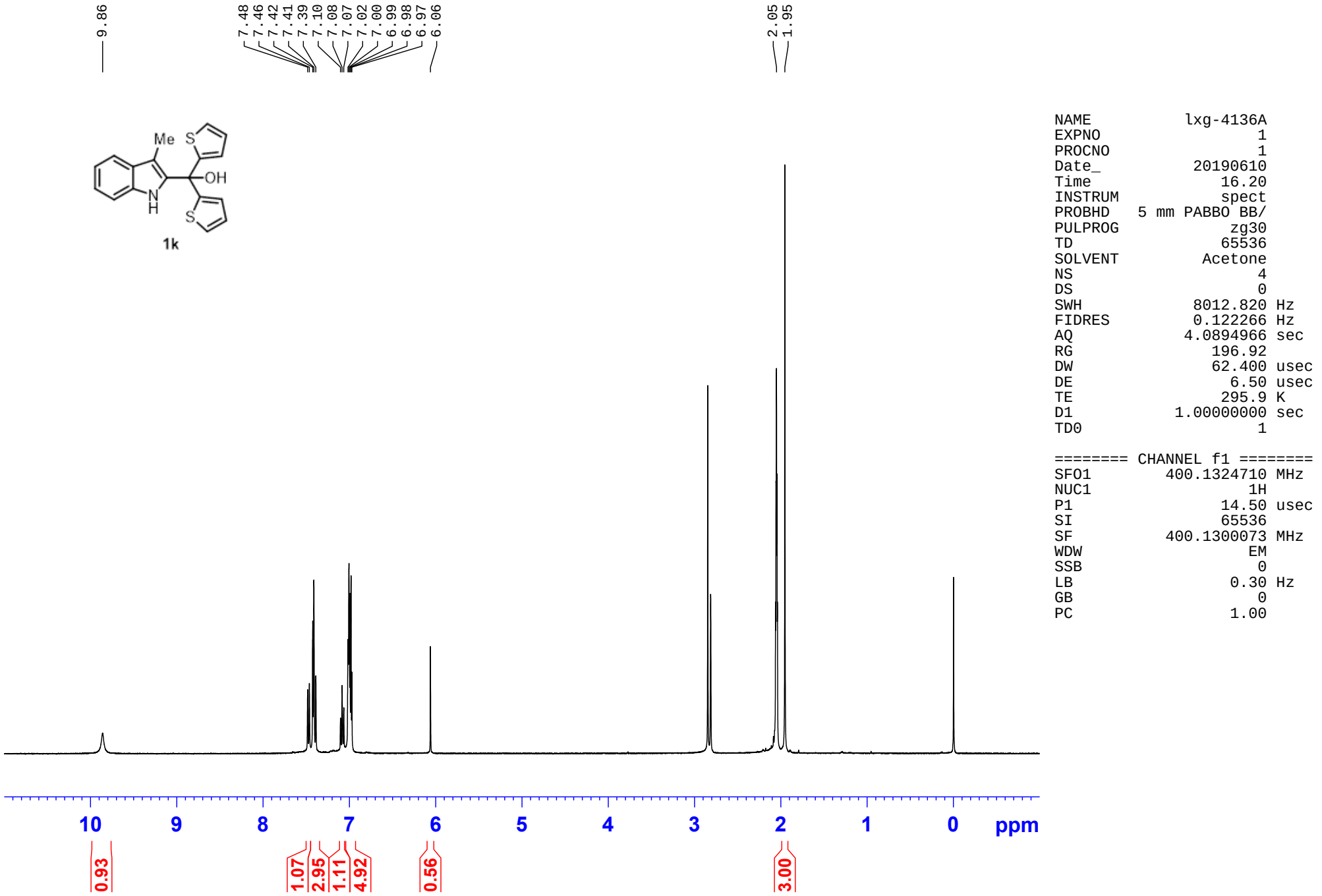
Supplementary Figure 19. ^{13}C NMR spectrum of **1i**



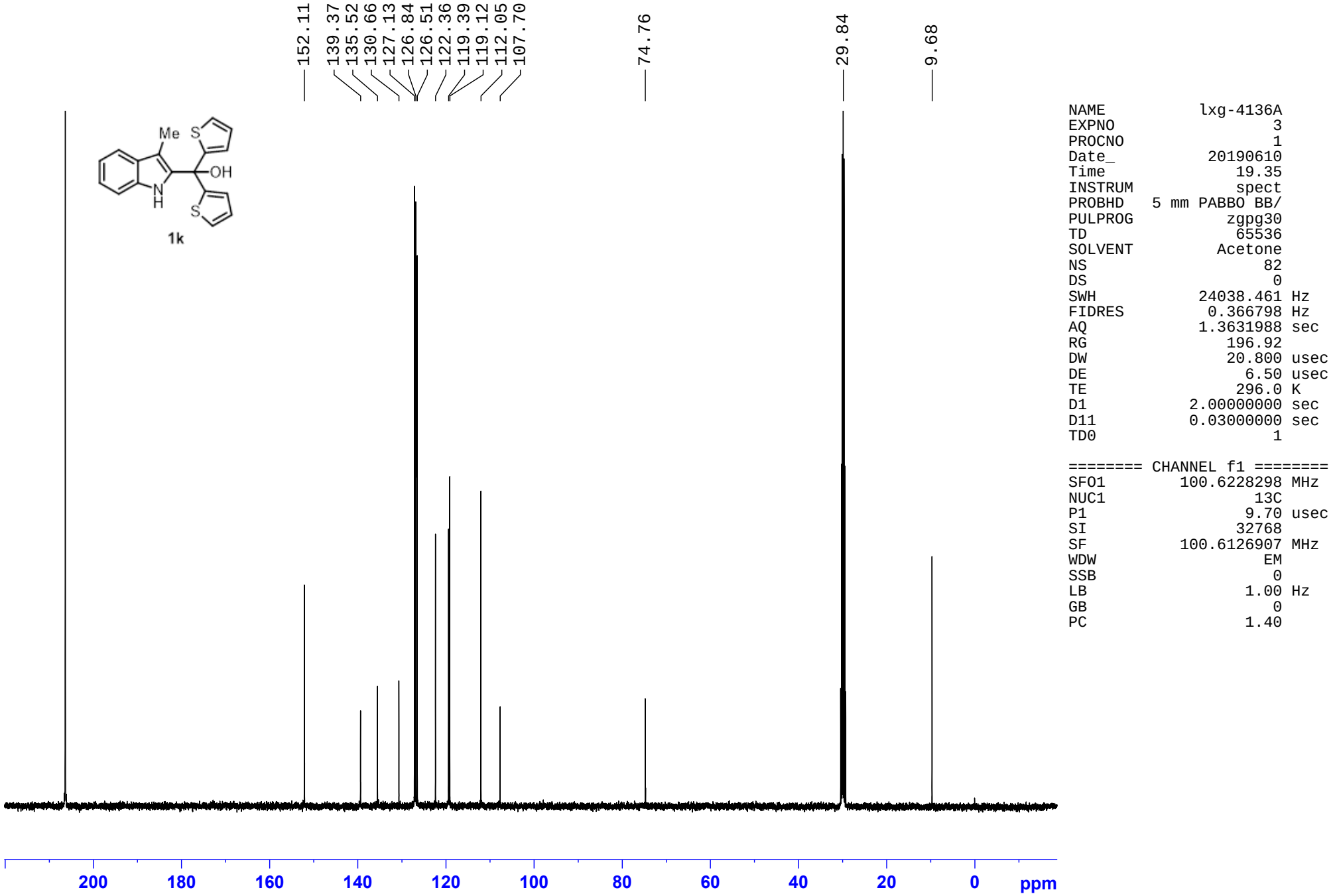
Supplementary Figure 20. ^{1}H NMR spectrum of **1j**



Supplementary Figure 21. ^{13}C NMR spectrum of **1j**



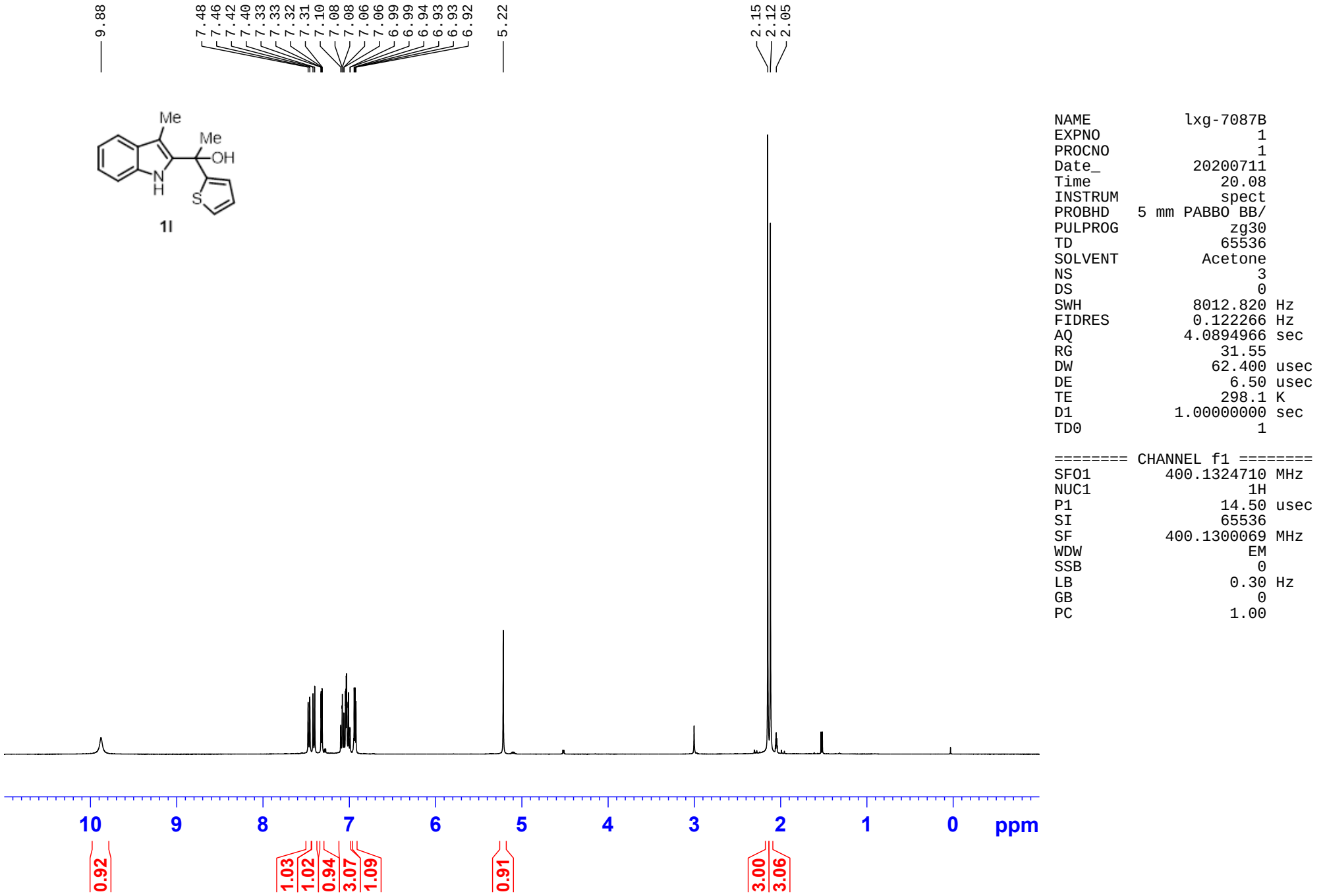
Supplementary Figure 22. ^{1}H NMR spectrum of **1k**



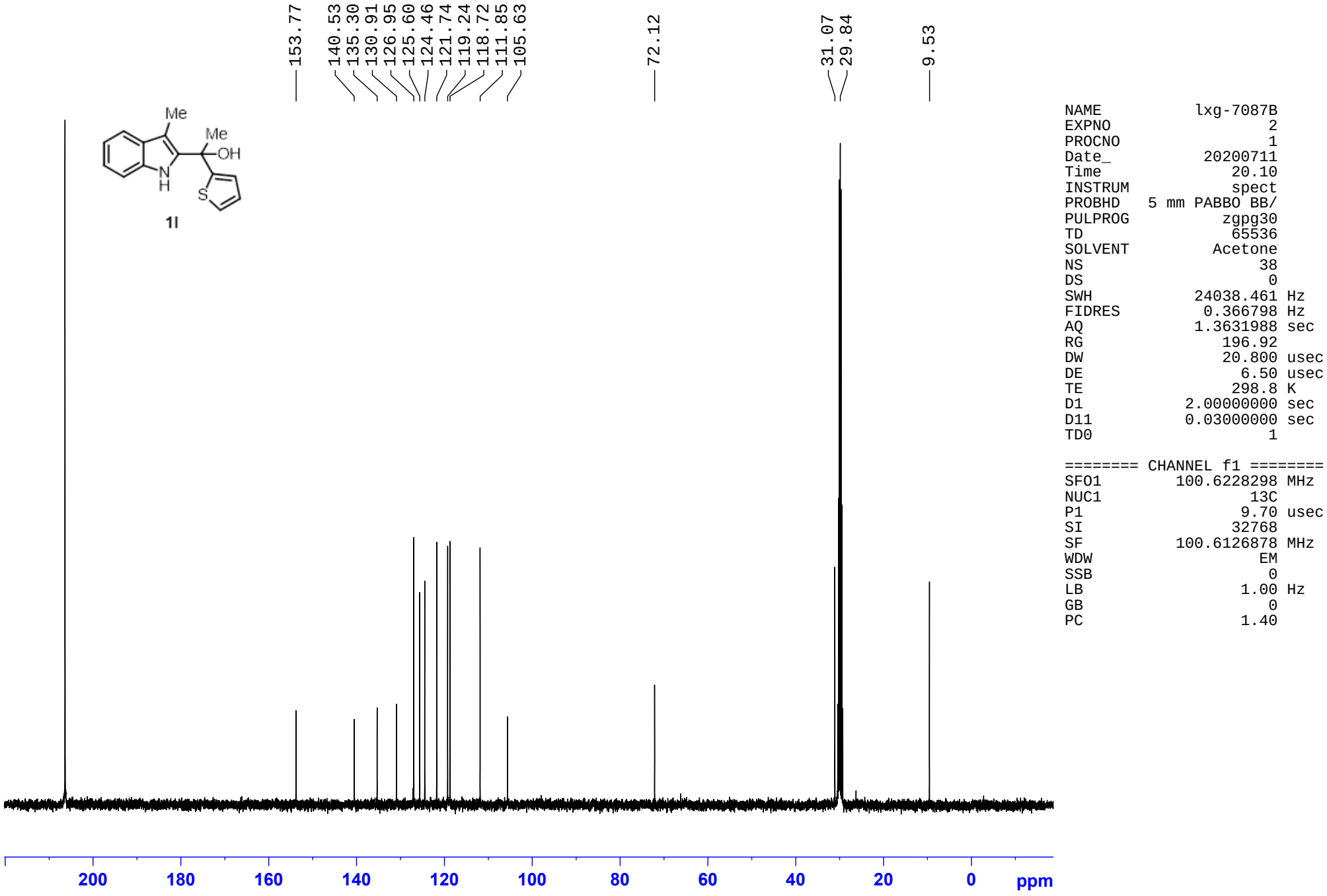

```
NAME           lxg-4136A
EXPNO                  3
PROCNO                 1
Date_           20190610
Time               19.35
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                    82
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
SI                32768
SF          100.6126907 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```

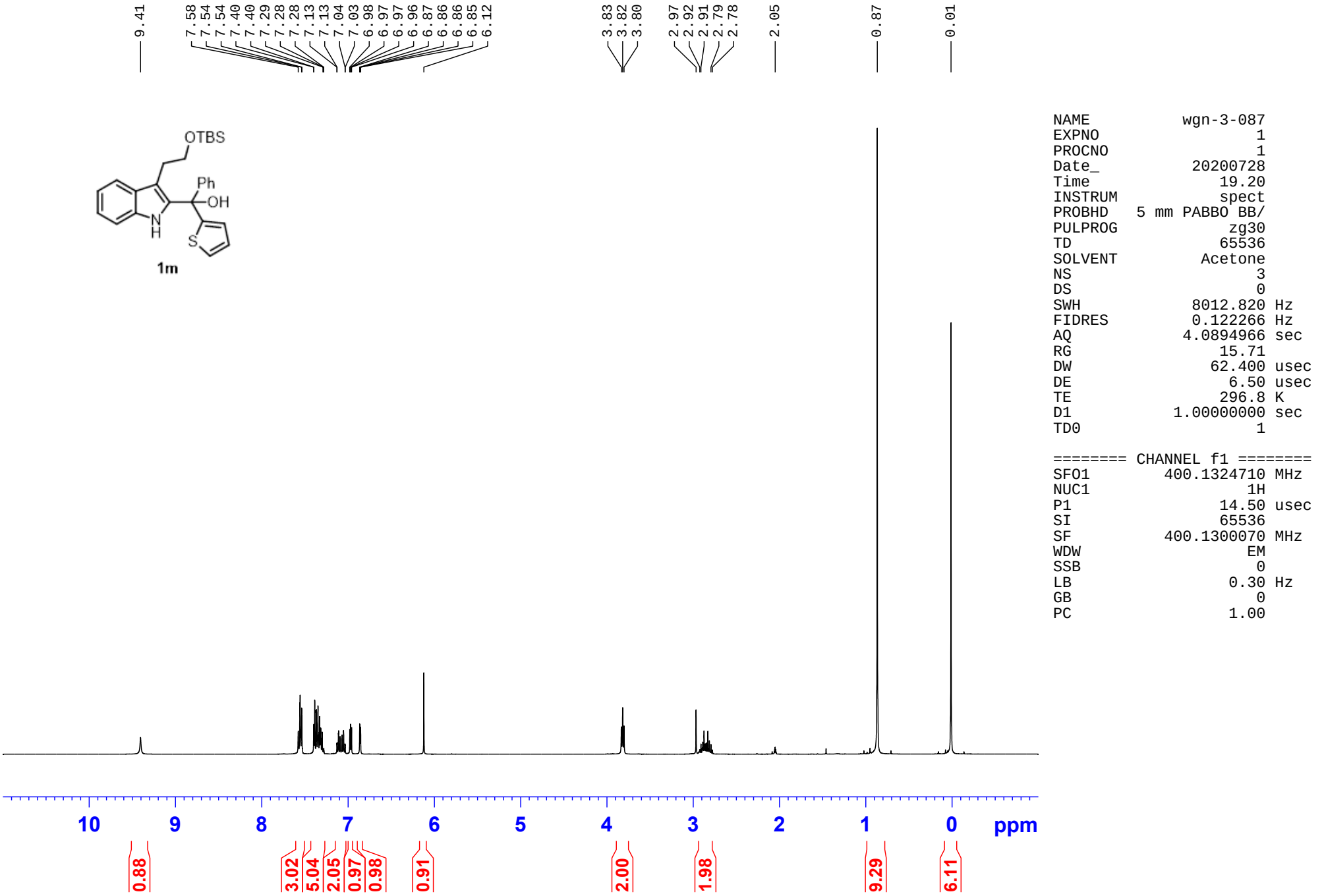

Supplementary Figure 23. ^{13}C NMR spectrum of **1k**



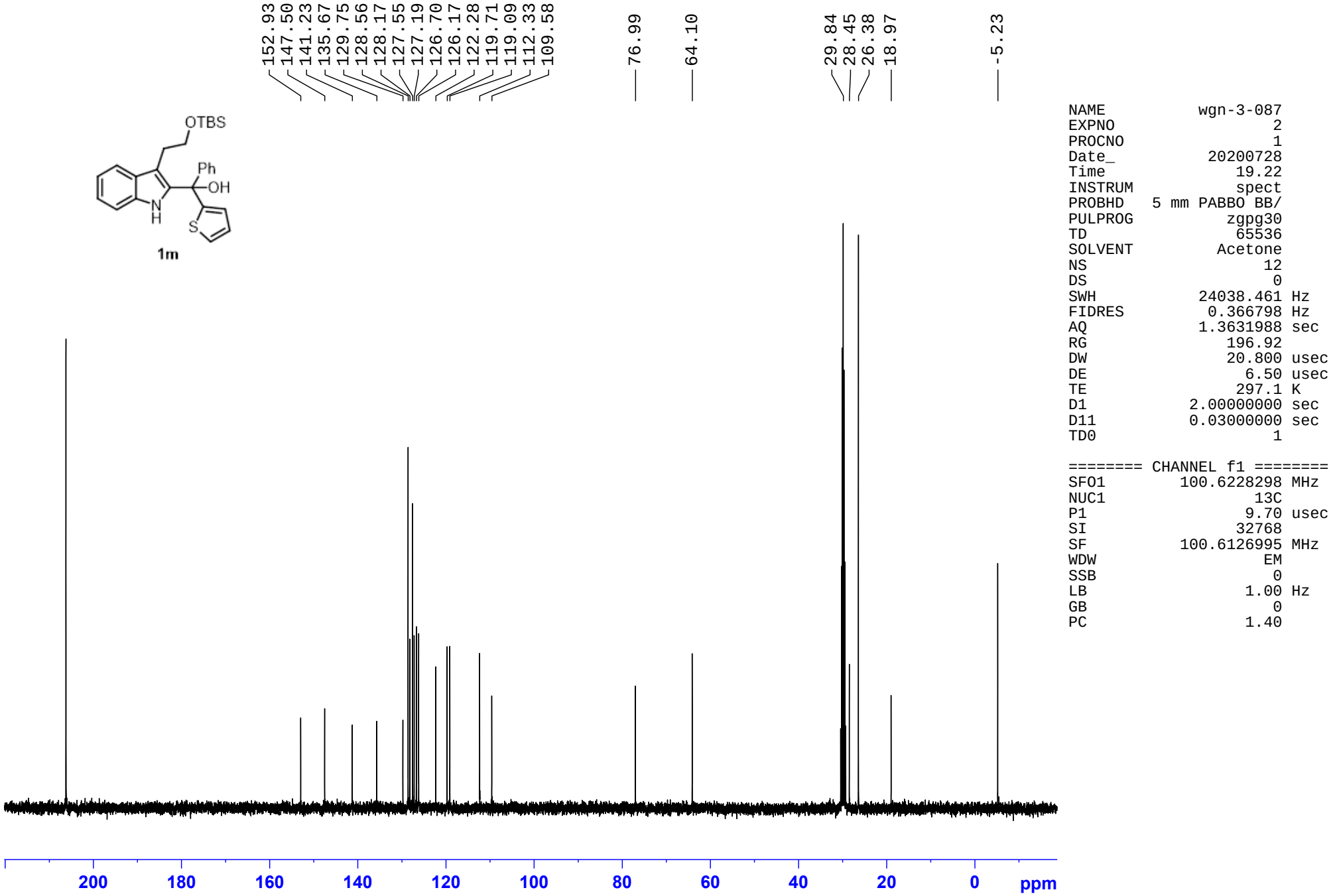
Supplementary Figure 24. ^{1}H NMR spectrum of **1l**



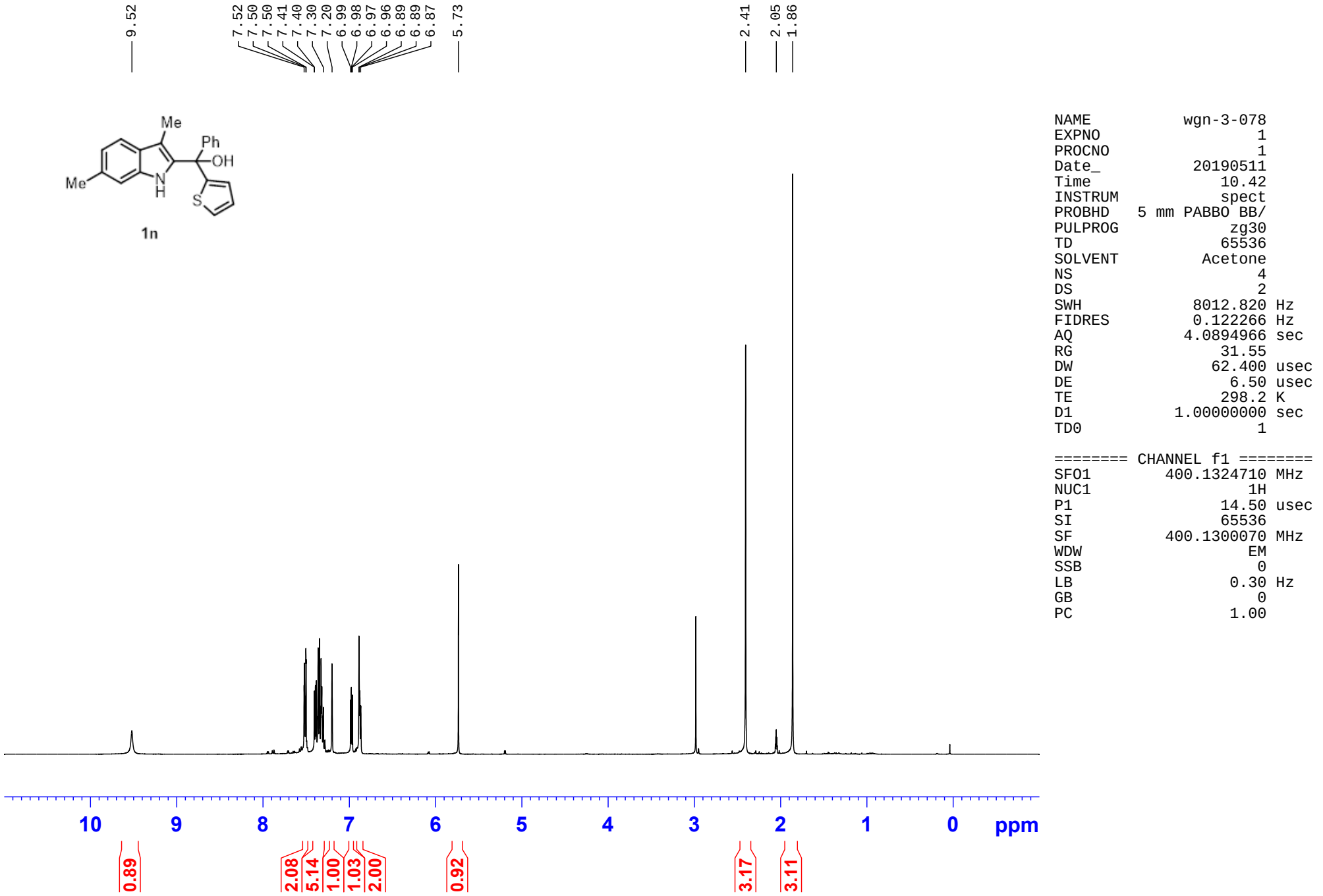
Supplementary Figure 25. ^{13}C NMR spectrum of **1l**



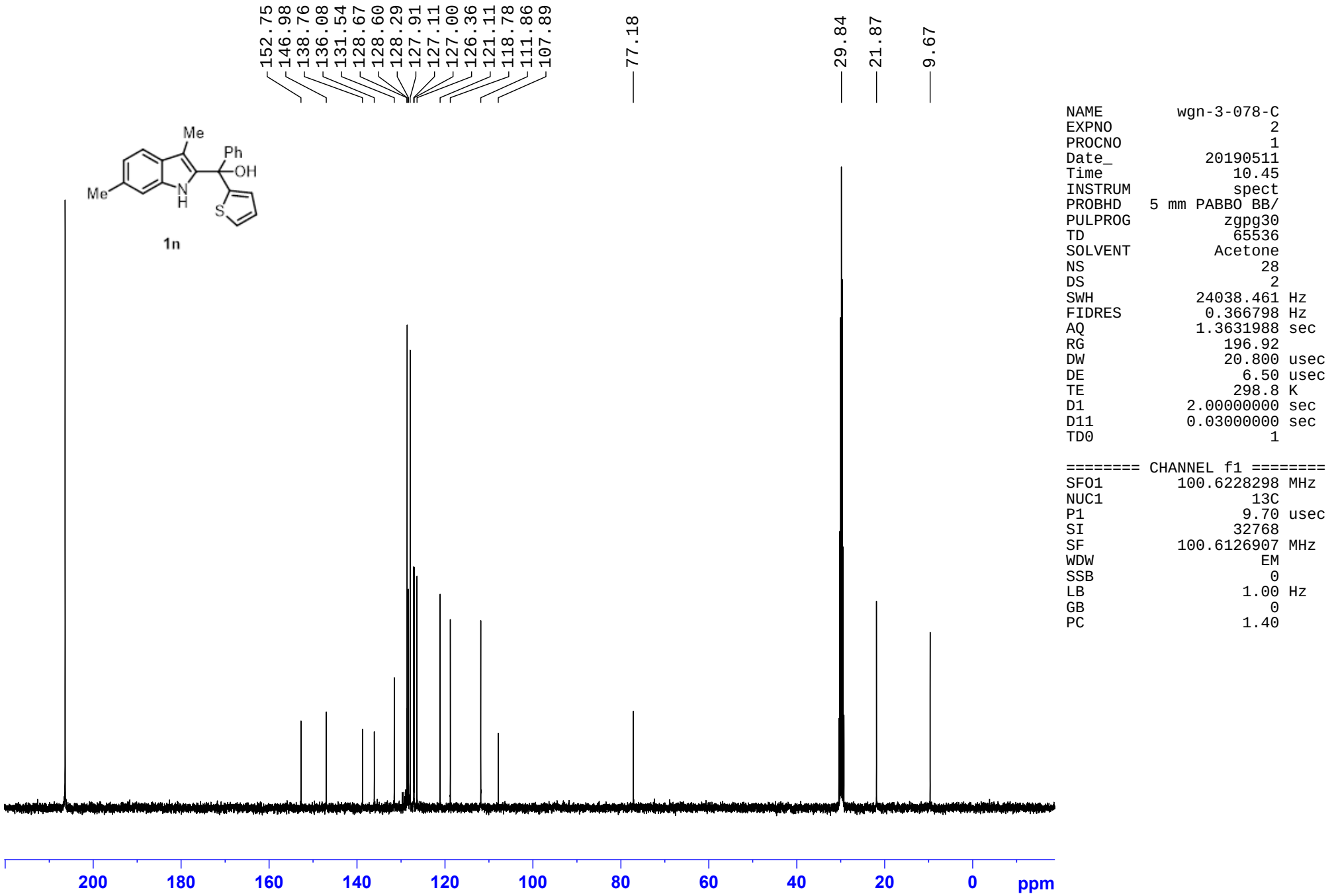
Supplementary Figure 26. ^{1}H NMR spectrum of **1m**



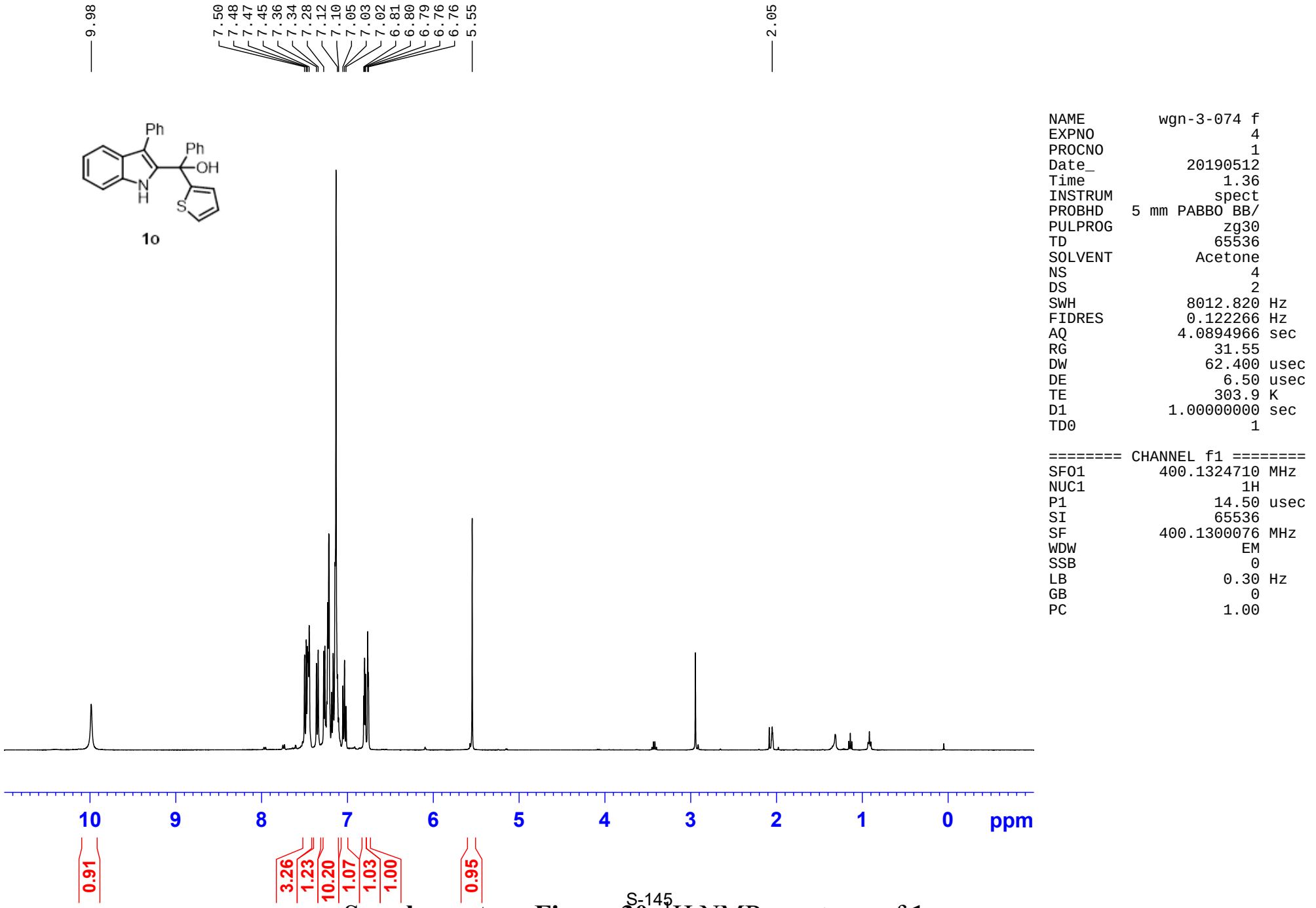
Supplementary Figure 27. ^{13}C NMR spectrum of **1m**



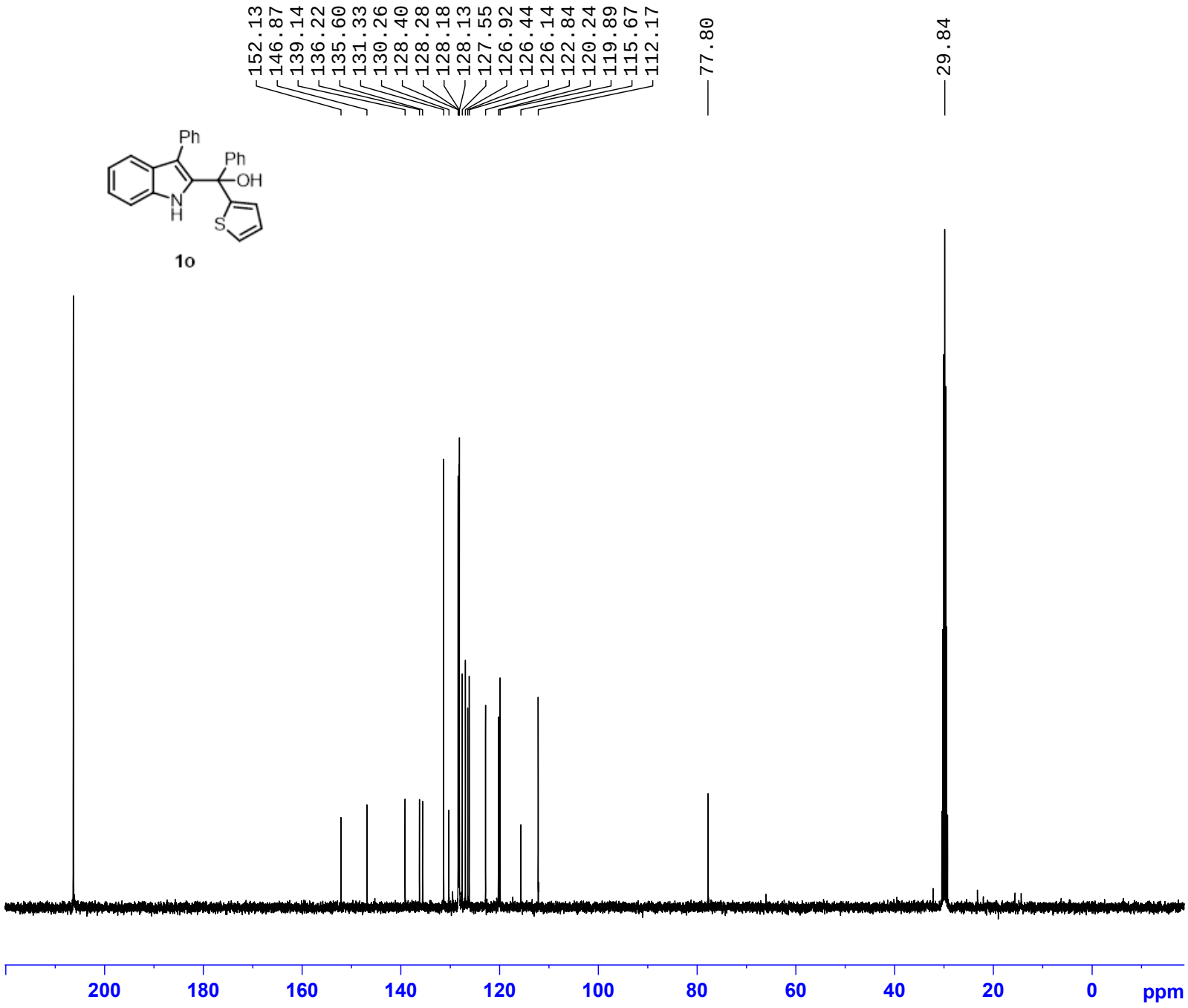
Supplementary Figure 28. ^{1}H NMR spectrum of **1n**



Supplementary Figure 29. ^{13}C NMR spectrum of **1n**

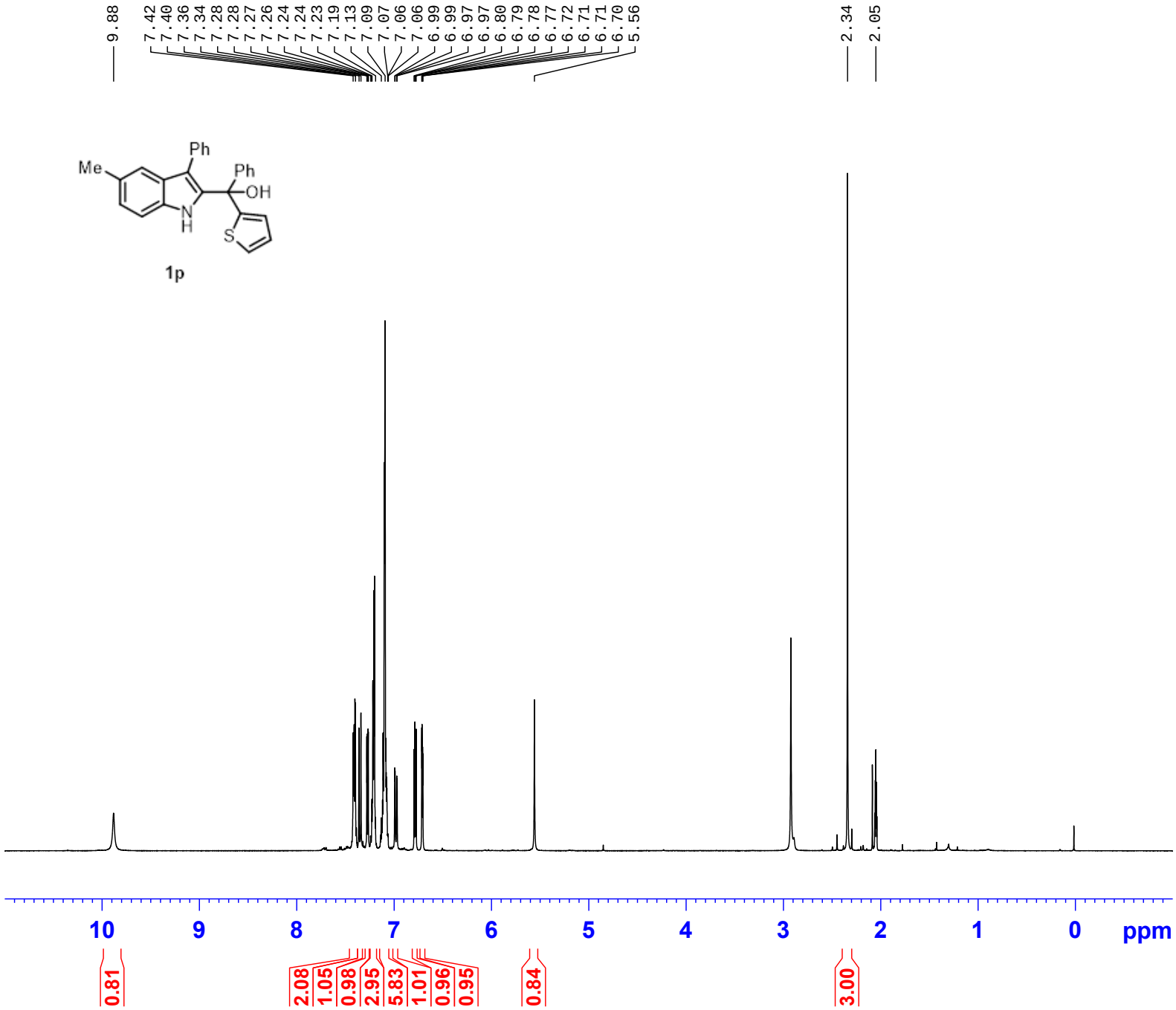


Supplementary Figure 30. ^{1}H NMR spectrum of **1o**

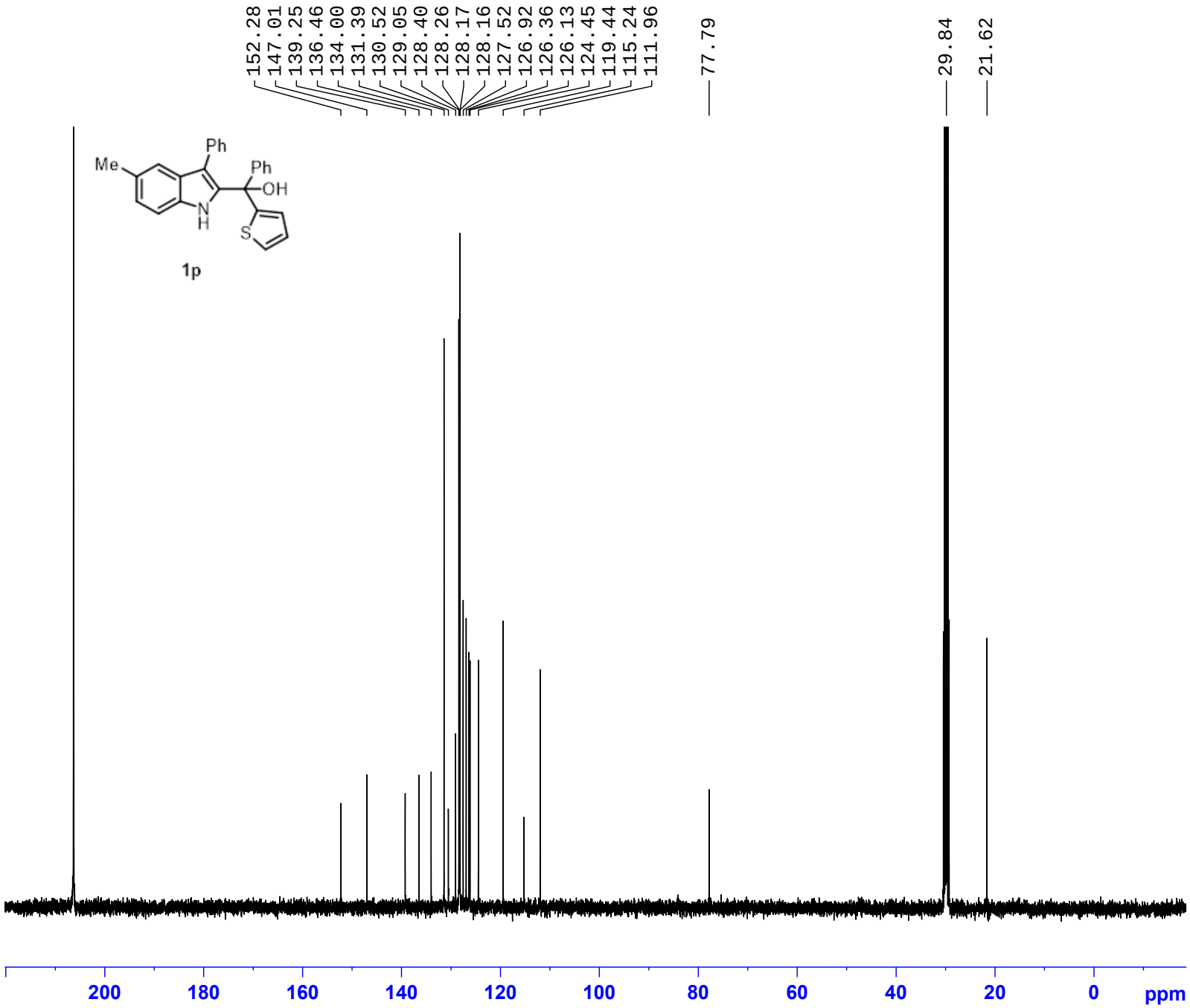


NAME	wgn-3-074 f-C
EXPNO	4
PROCNO	1
Date_	20190512
Time	1.38
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	31
DS	2
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	304.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6126929 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Supplementary Figure 31. ^{13}C NMR spectrum of **1o**



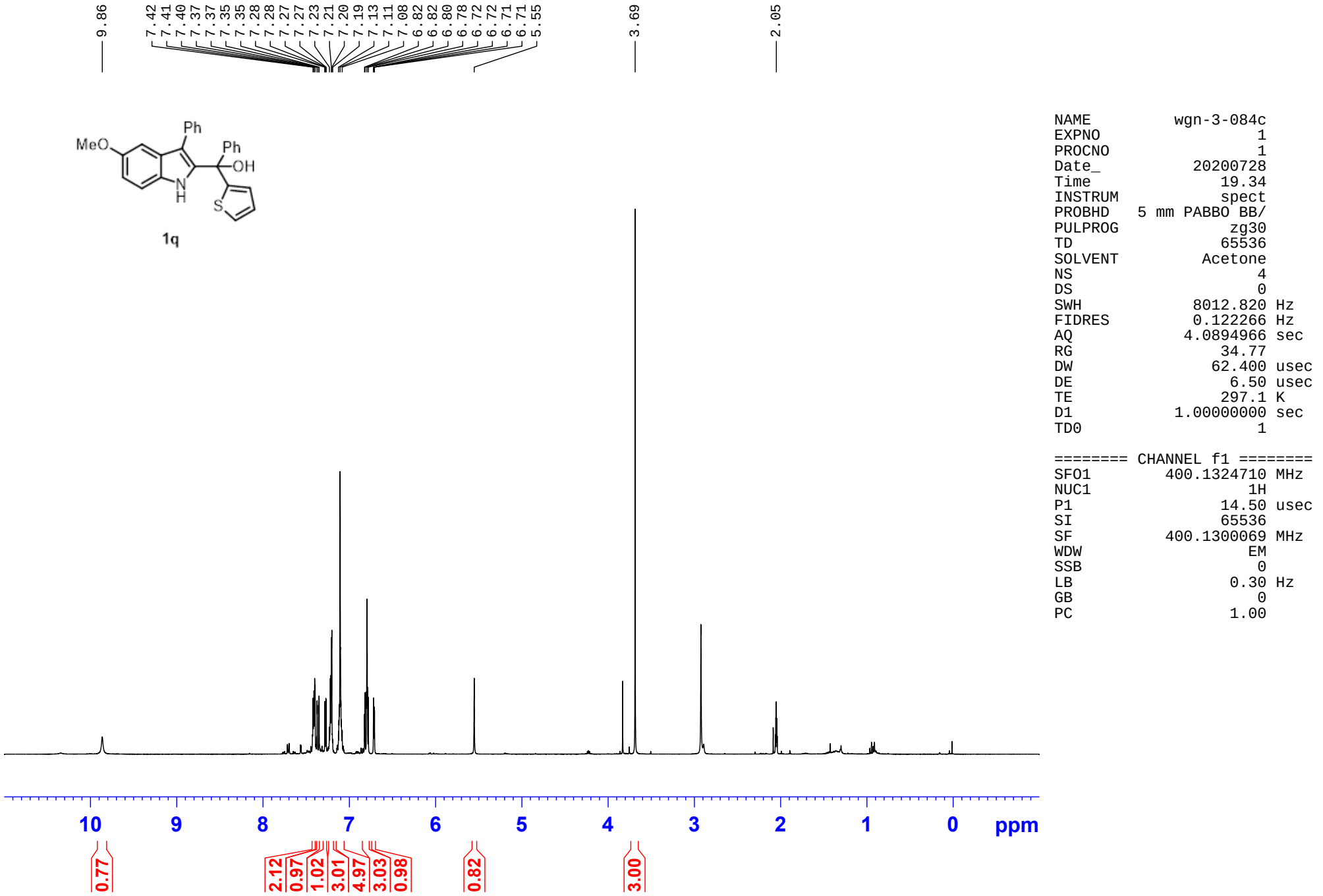
Supplementary Figure 32. ^{1}H NMR spectrum of **1p**



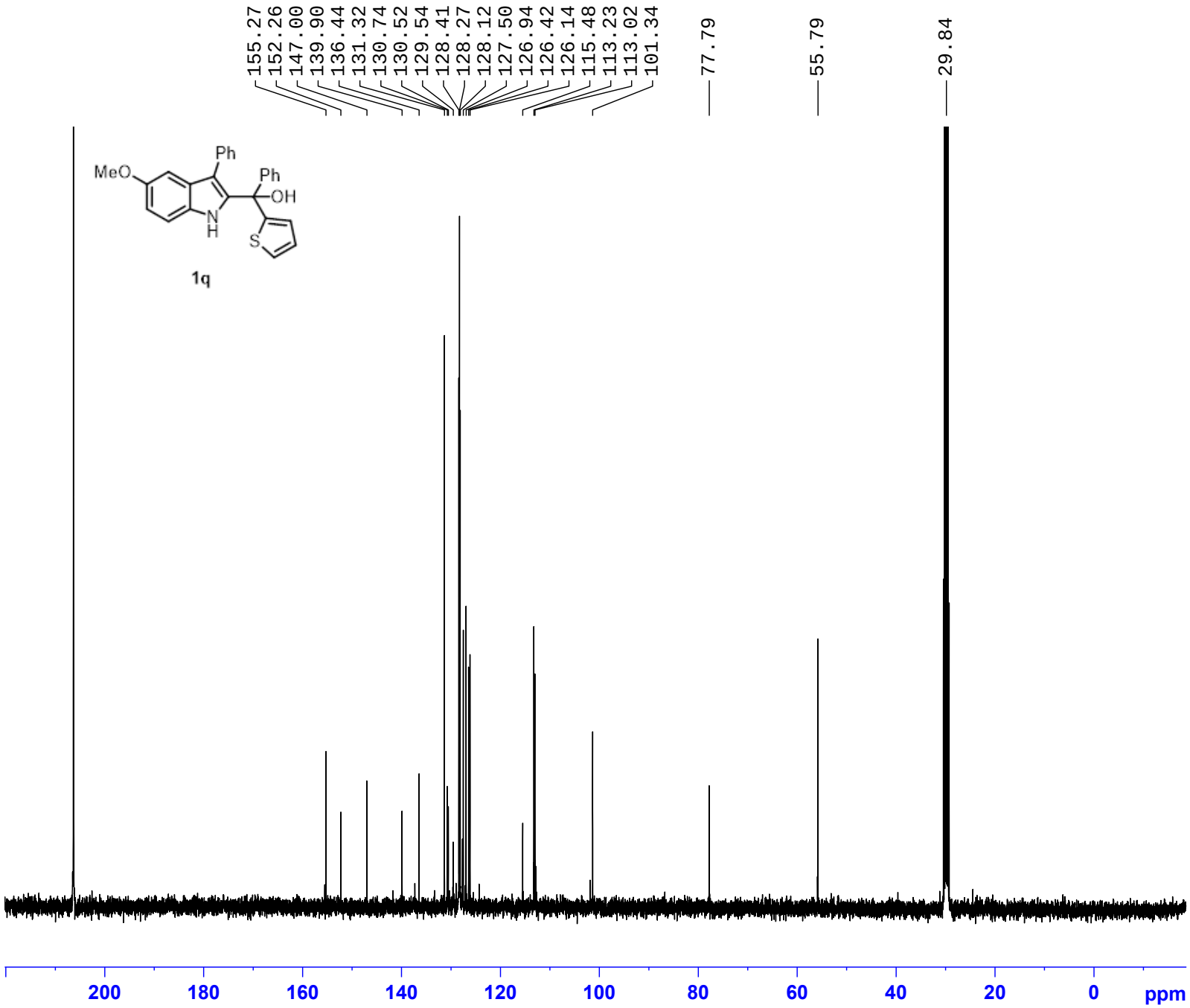

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NAME          wgn-3-084b
EXPNO                  2
PROCNO                 1
Date_           20200728
Time               19.31
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   103
DS                     0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ           1.3631988 sec
RG                196.92
DW              20.800 usec
DE               6.50 usec
TE               297.7 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                9.70 usec
SI                32768
SF          100.6126849 MHz
WDW                 EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

Supplementary Figure 33. ^{13}C NMR spectrum of **1p**

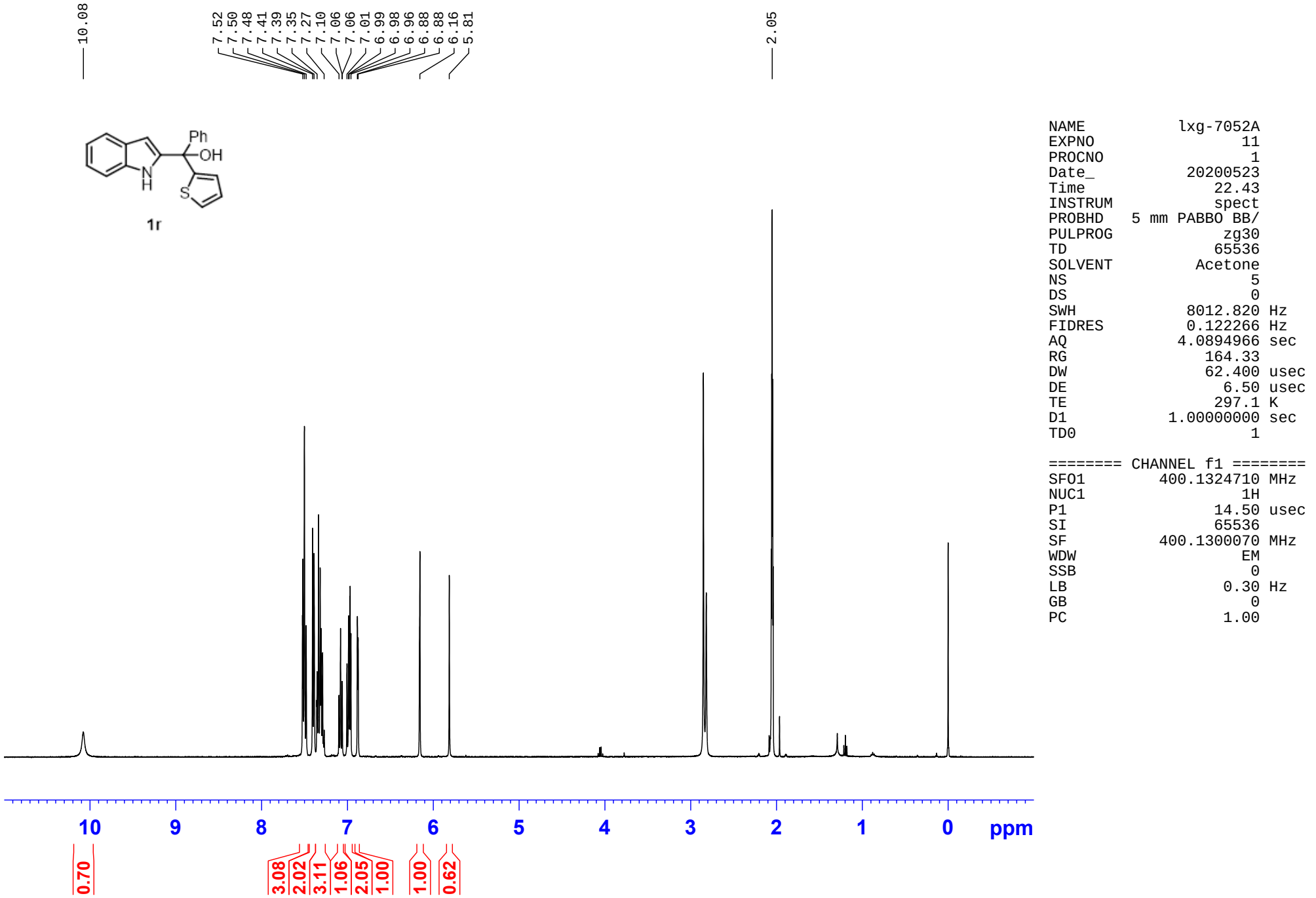


Supplementary Figure 34. ^{1}H NMR spectrum of **1q**

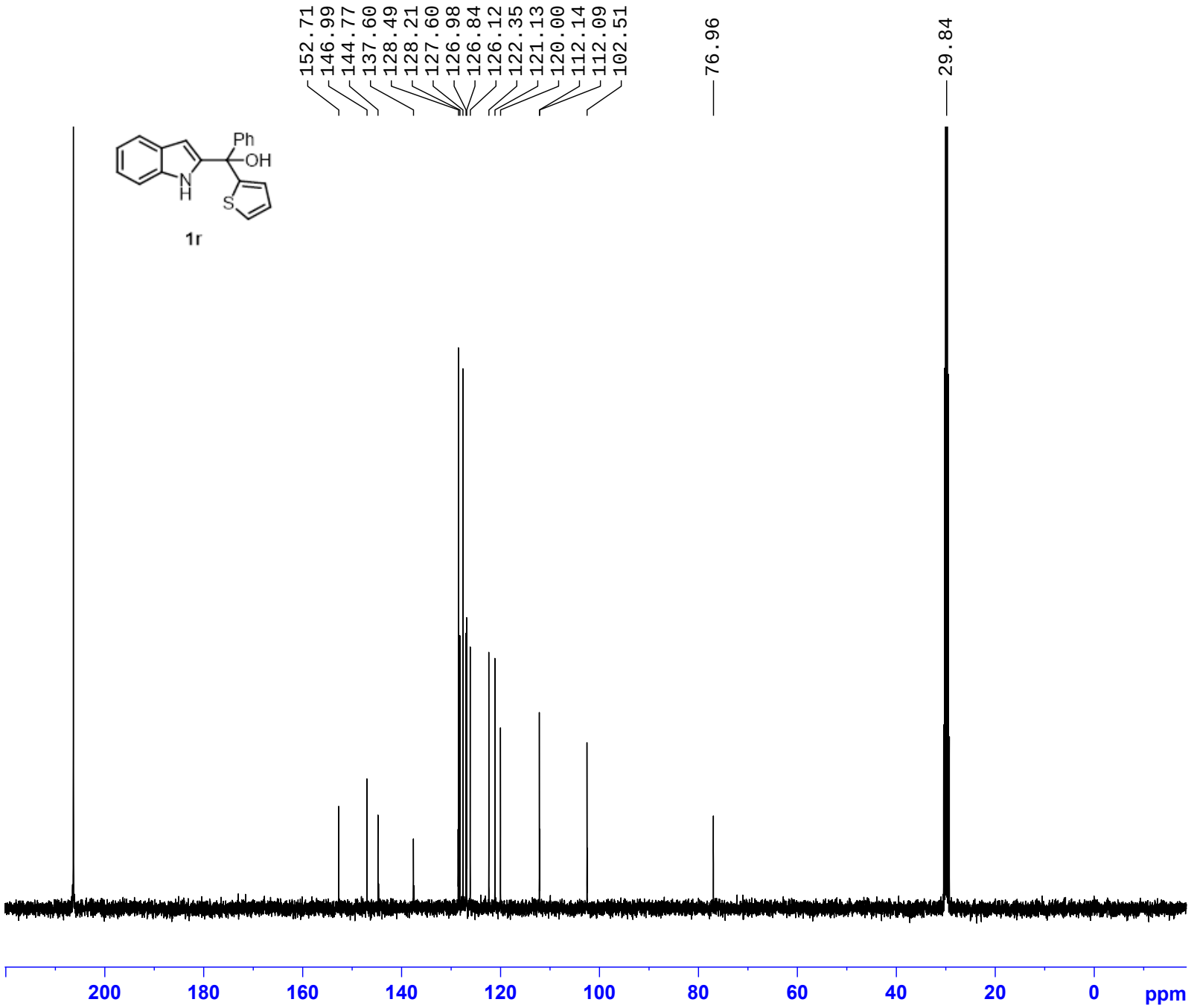


NAME	wgn-3-084c
EXPNO	2
PROCNO	1
Date_	20200728
Time	19.36
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	87
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	297.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6126849 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Supplementary Figure 35. ^{13}C NMR spectrum of **1q**



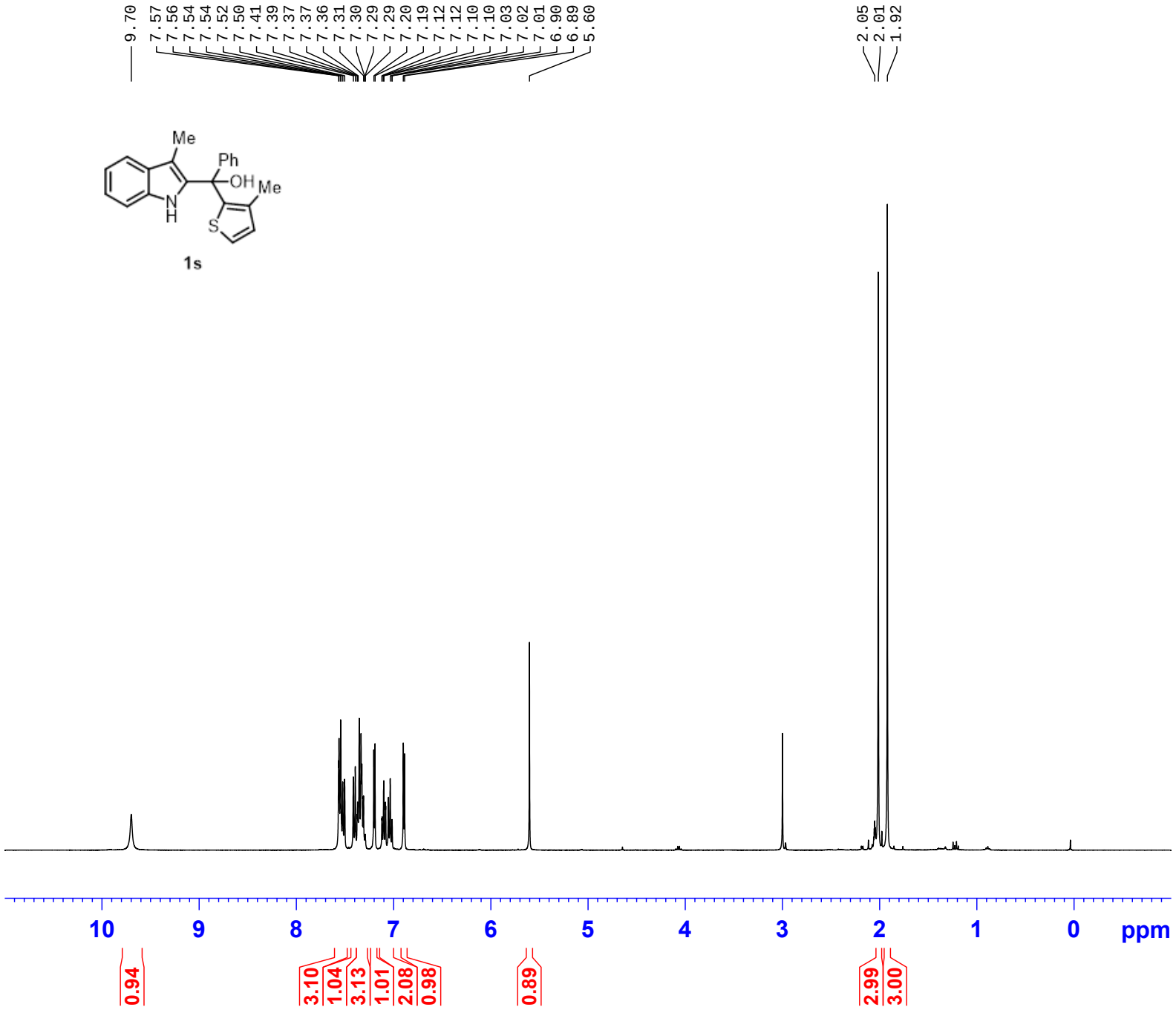
Supplementary Figure 36. ^{1}H NMR spectrum of **1r**



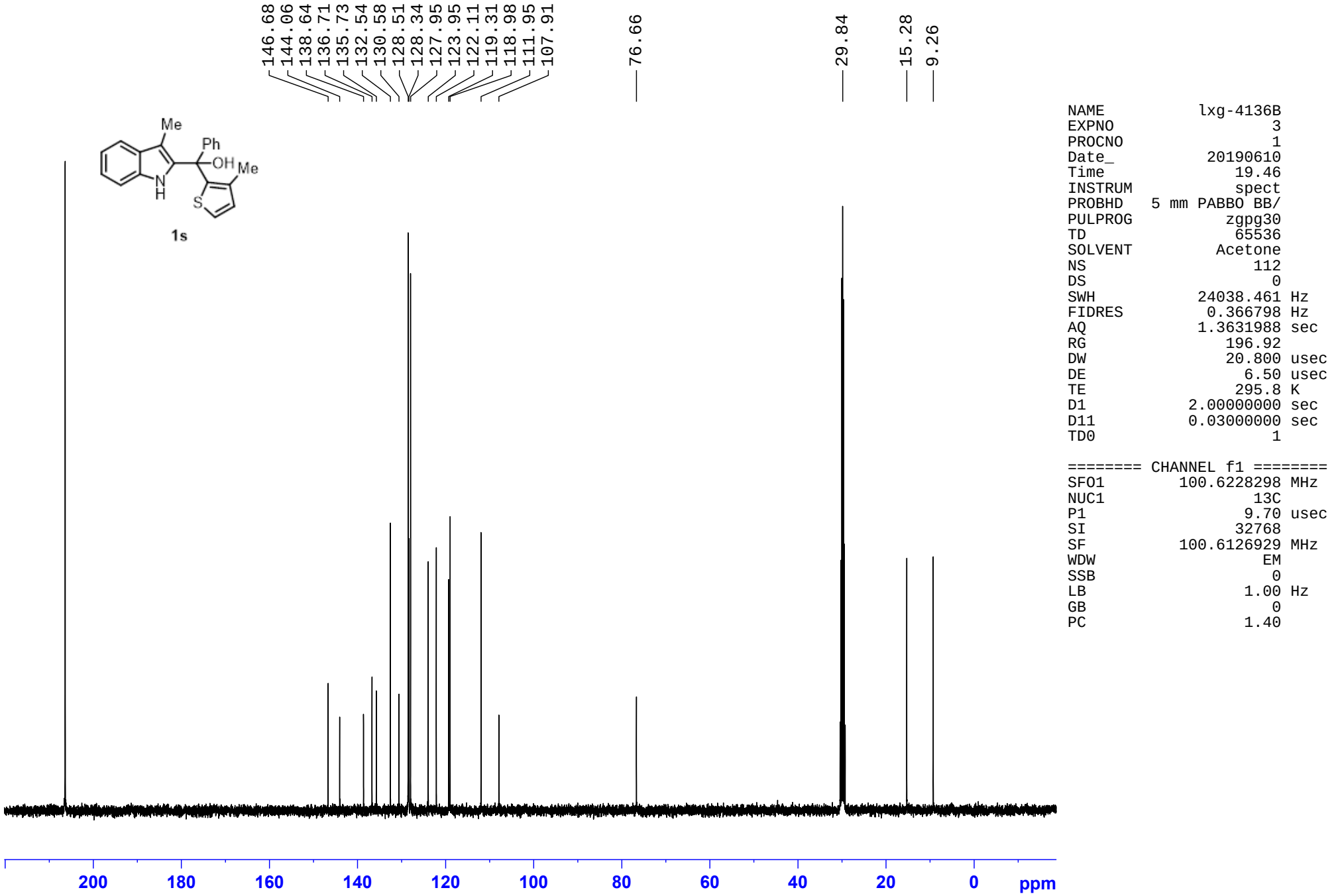

```
NAME           lxg-7052A
EXPNO                  2
PROCNO                 1
Date_           20200523
Time               10.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                    36
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                296.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
SI                32768
SF           100.6126878 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

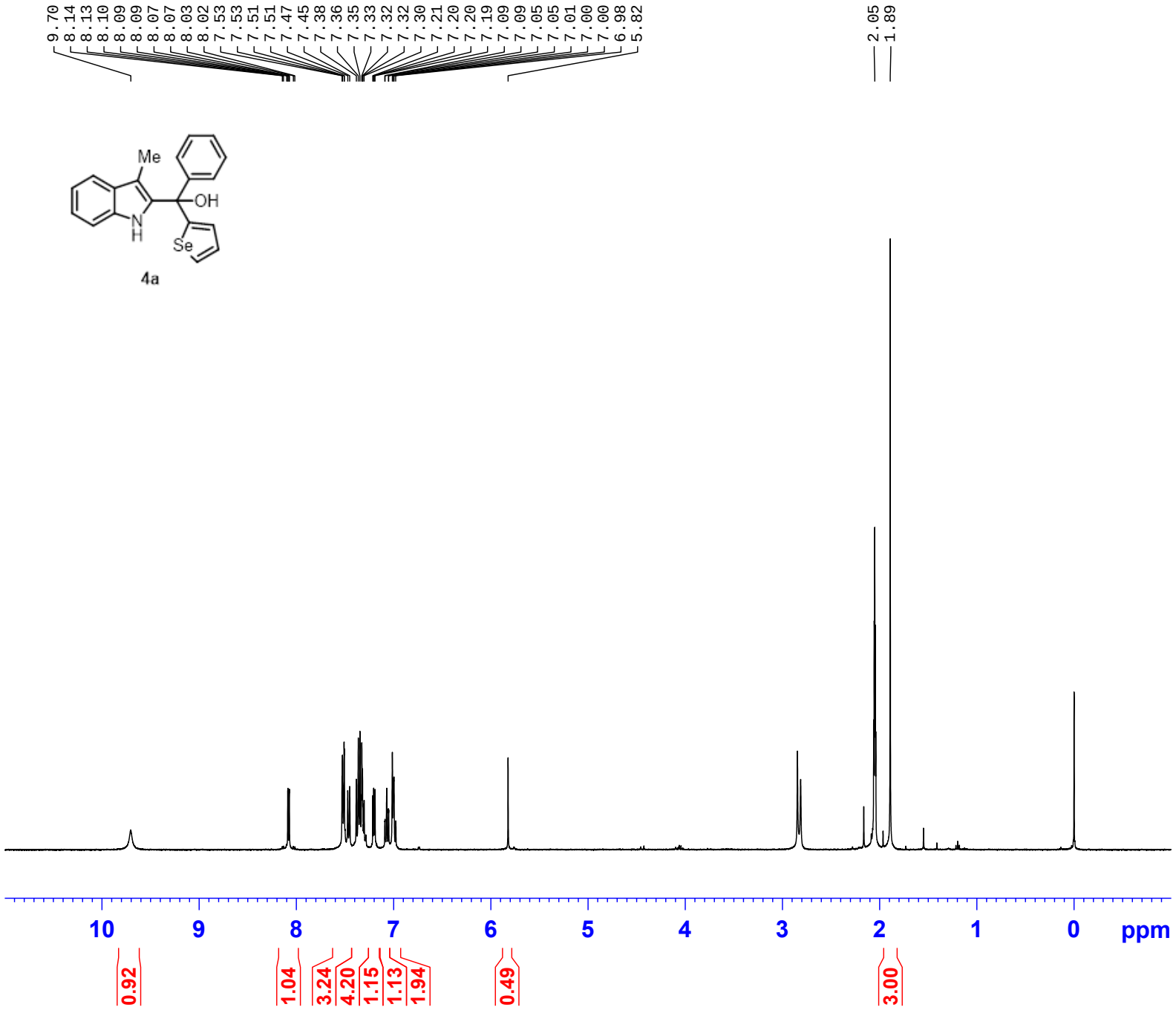

Supplementary Figure 37. ^{13}C NMR spectrum of **1r**



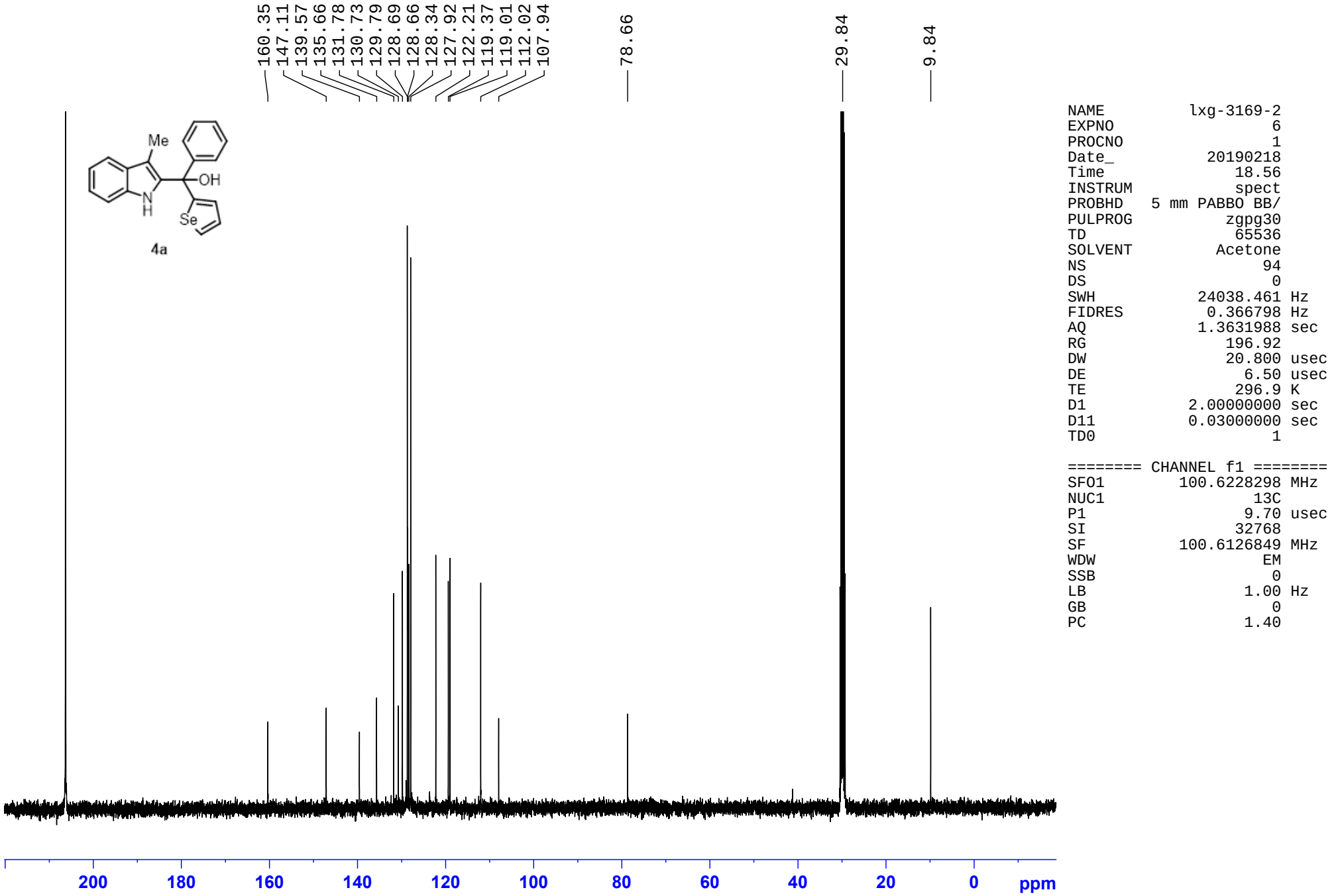
Supplementary Figure 38. ^{1}H NMR spectrum of **1s**



Supplementary Figure 39. ^{13}C NMR spectrum of **1s**



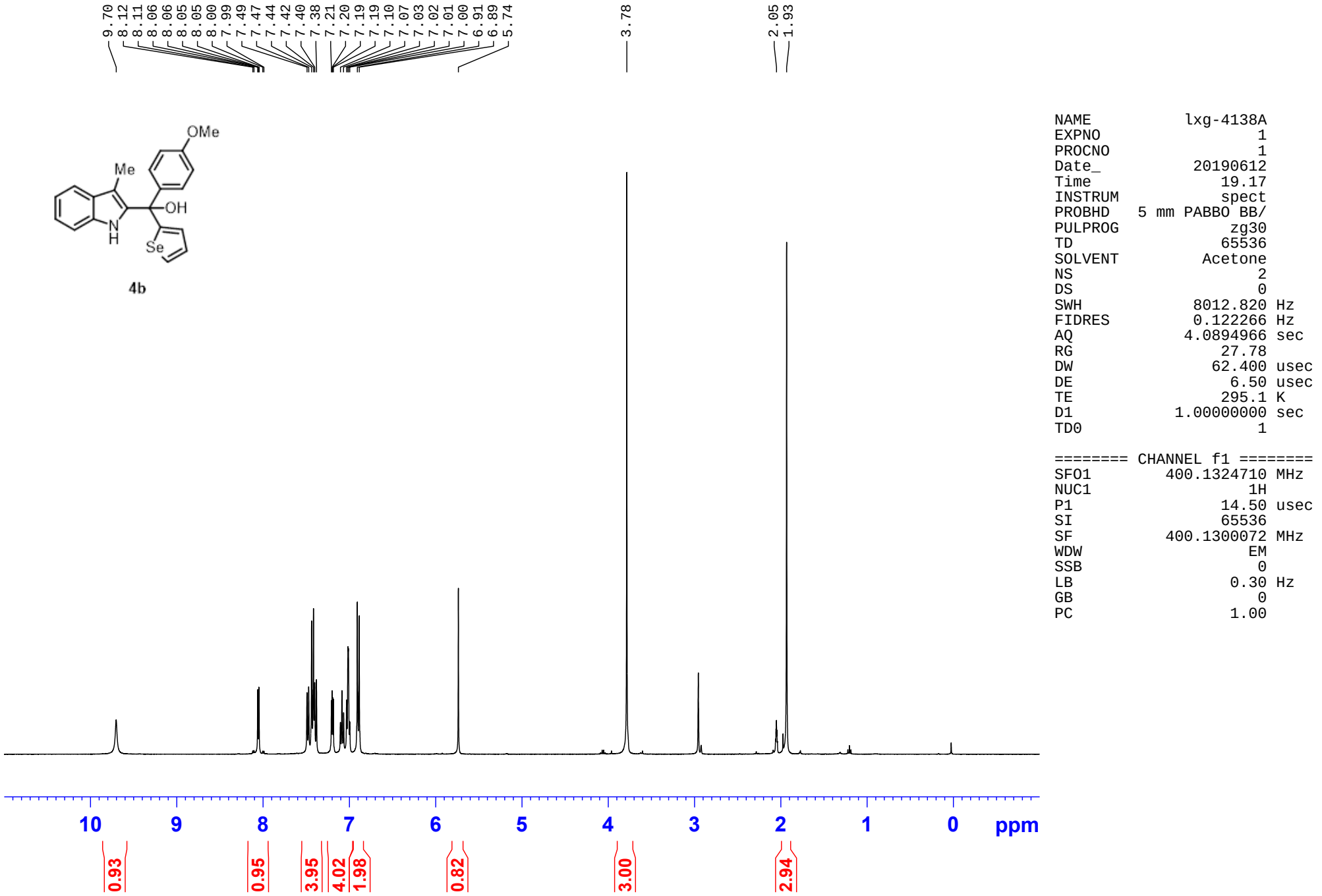
Supplementary Figure 40. ^{1}H NMR spectrum of **4a**



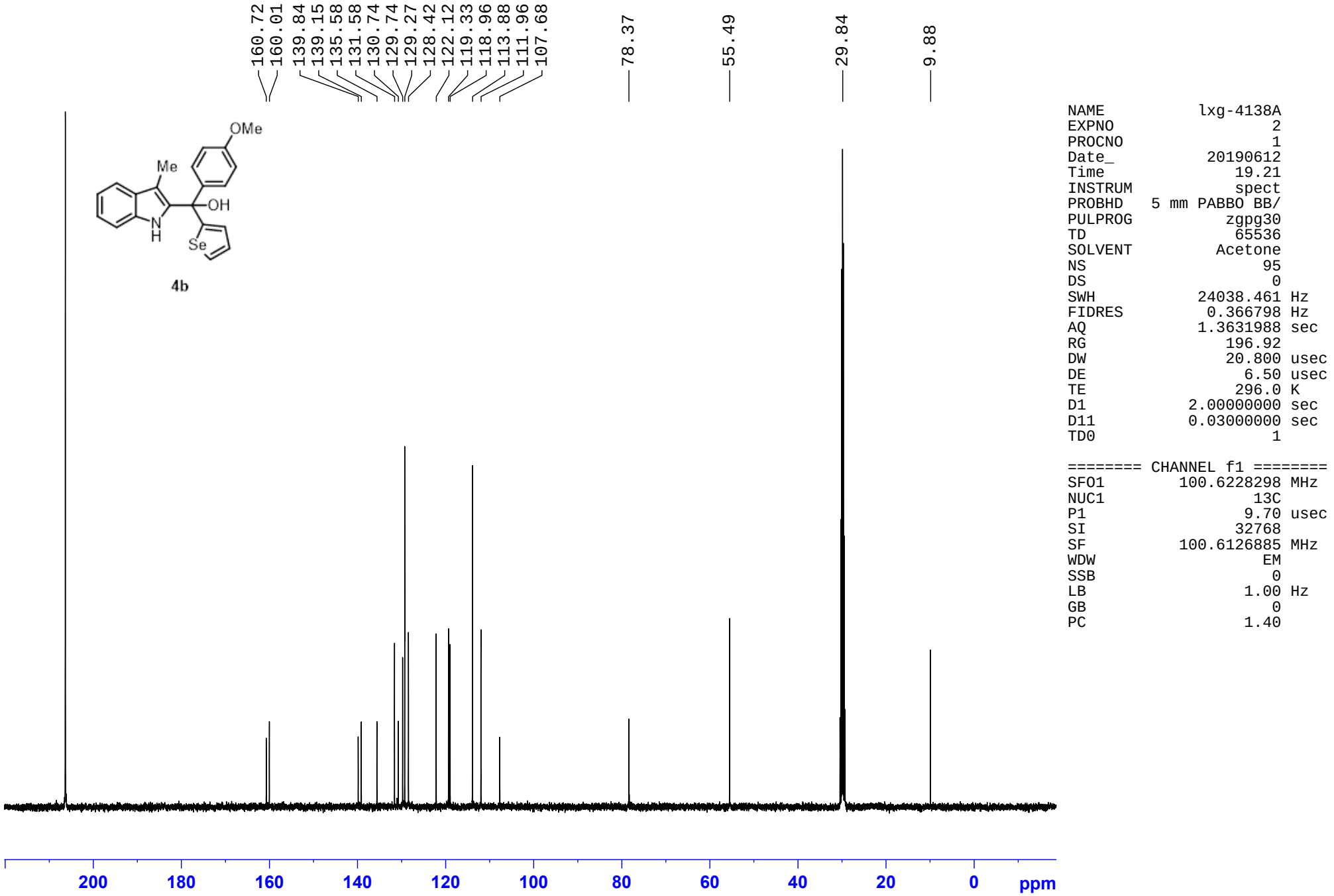

```
NAME          lxg-3169-2
EXPNO                  6
PROCNO                 1
Date_           20190218
Time               18.56
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                    94
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                296.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
SI                32768
SF          100.6126849 MHz
WDW                EM
SSB                 0
LB                 1.00 Hz
GB                  0
PC                 1.40
```

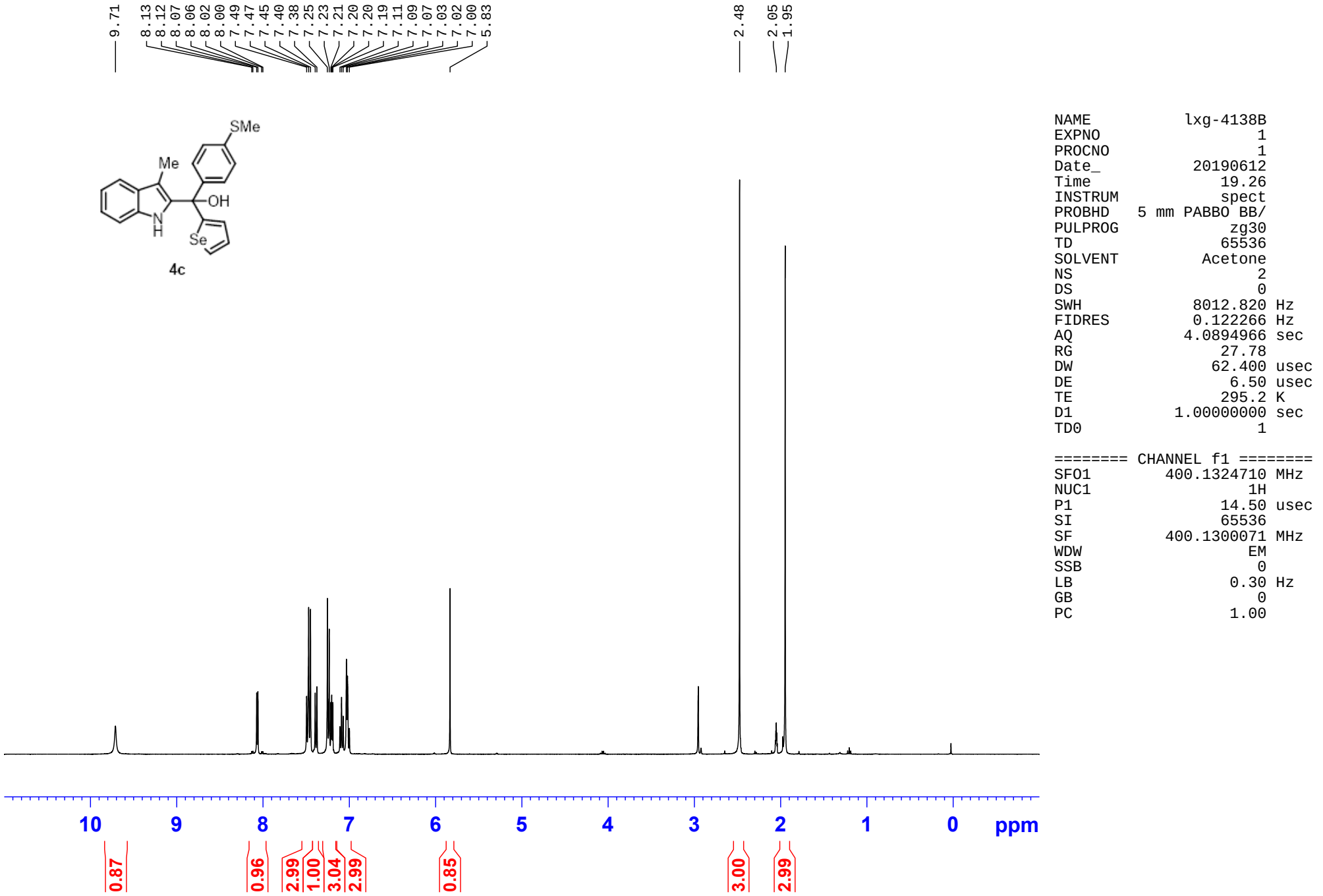
Supplementary Figure 41. ^{13}C NMR spectrum of **4a**



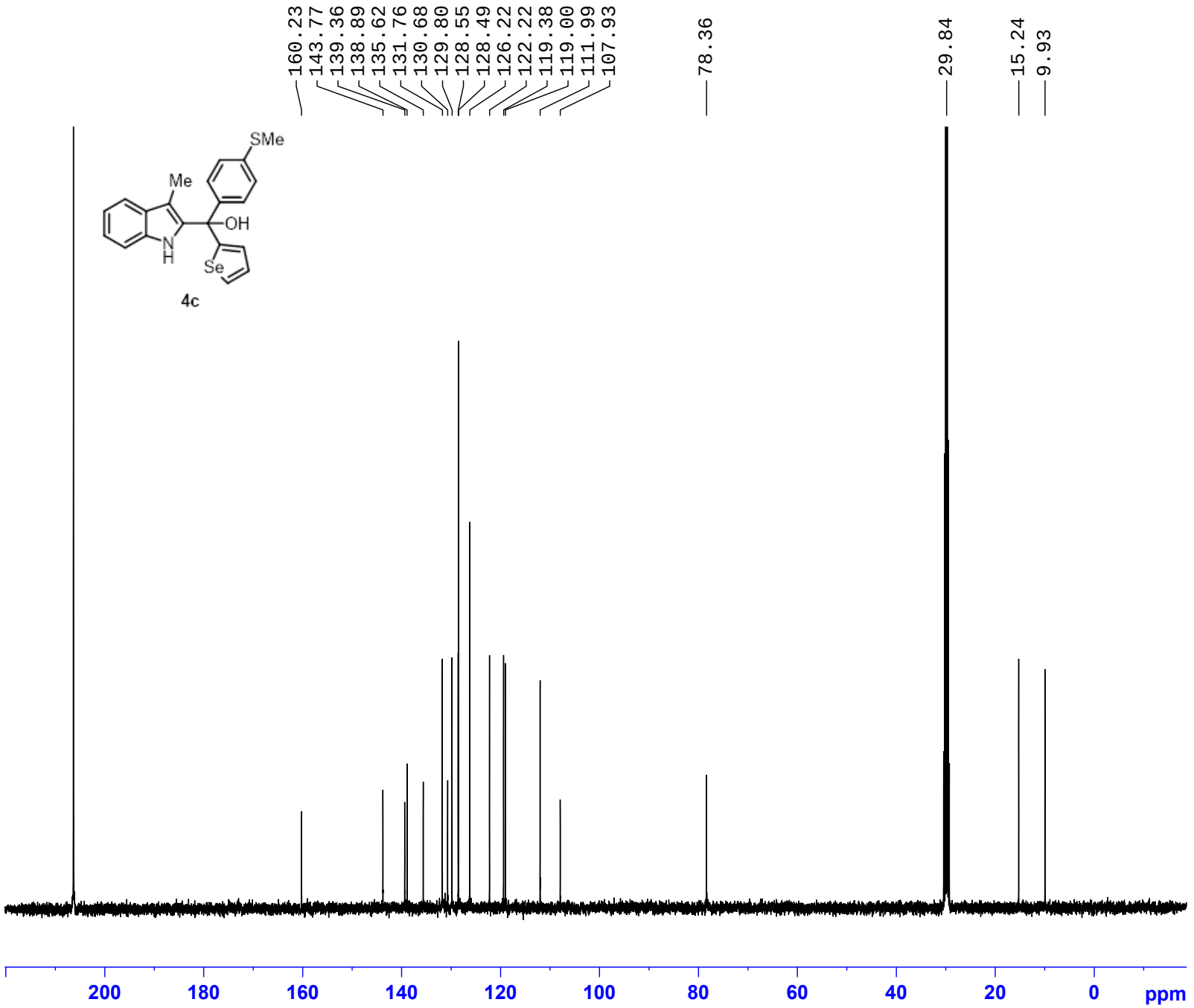
Supplementary Figure 42. ^{1}H NMR spectrum of **4b**



Supplementary Figure 43. ^{13}C NMR spectrum of **4b**



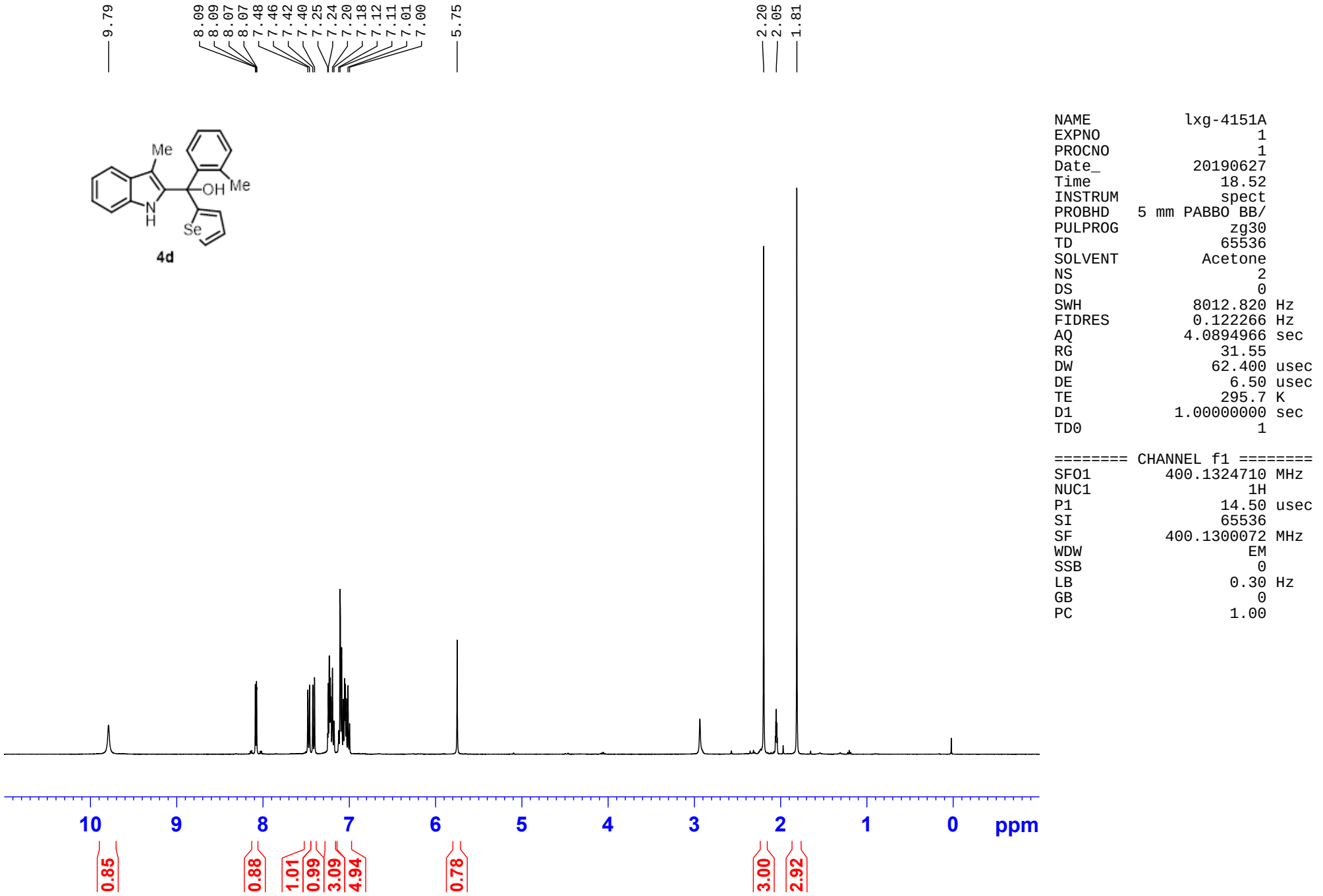
Supplementary Figure 44. ^{1}H NMR spectrum of **4c**



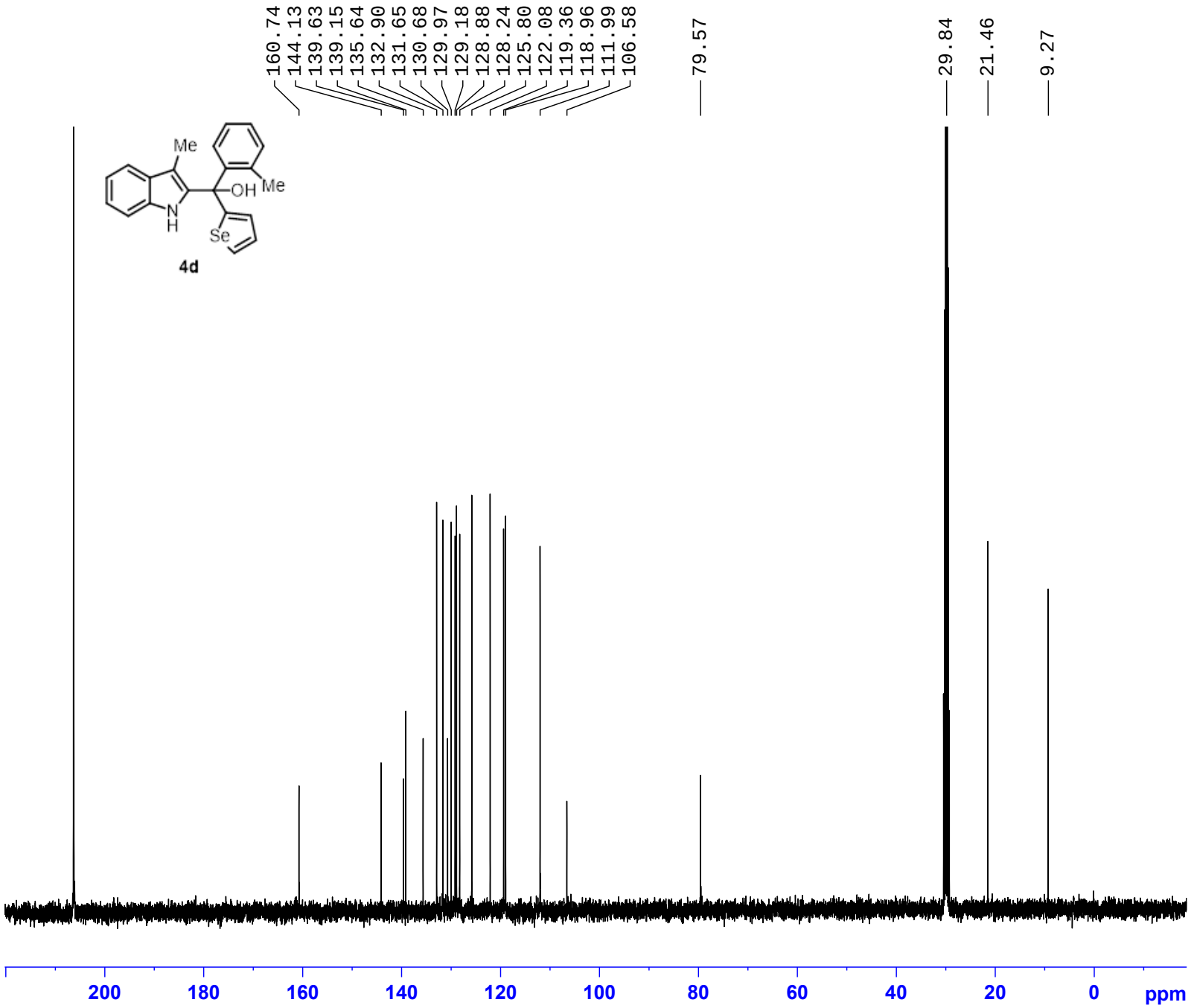

```
NAME           lxg-4138B
EXPNO                  2
PROCNO                 1
Date_           20190612
Time               19.31
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  104
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
SI                32768
SF          100.6126900 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```


Supplementary Figure 45. ^{13}C NMR spectrum of **4c**



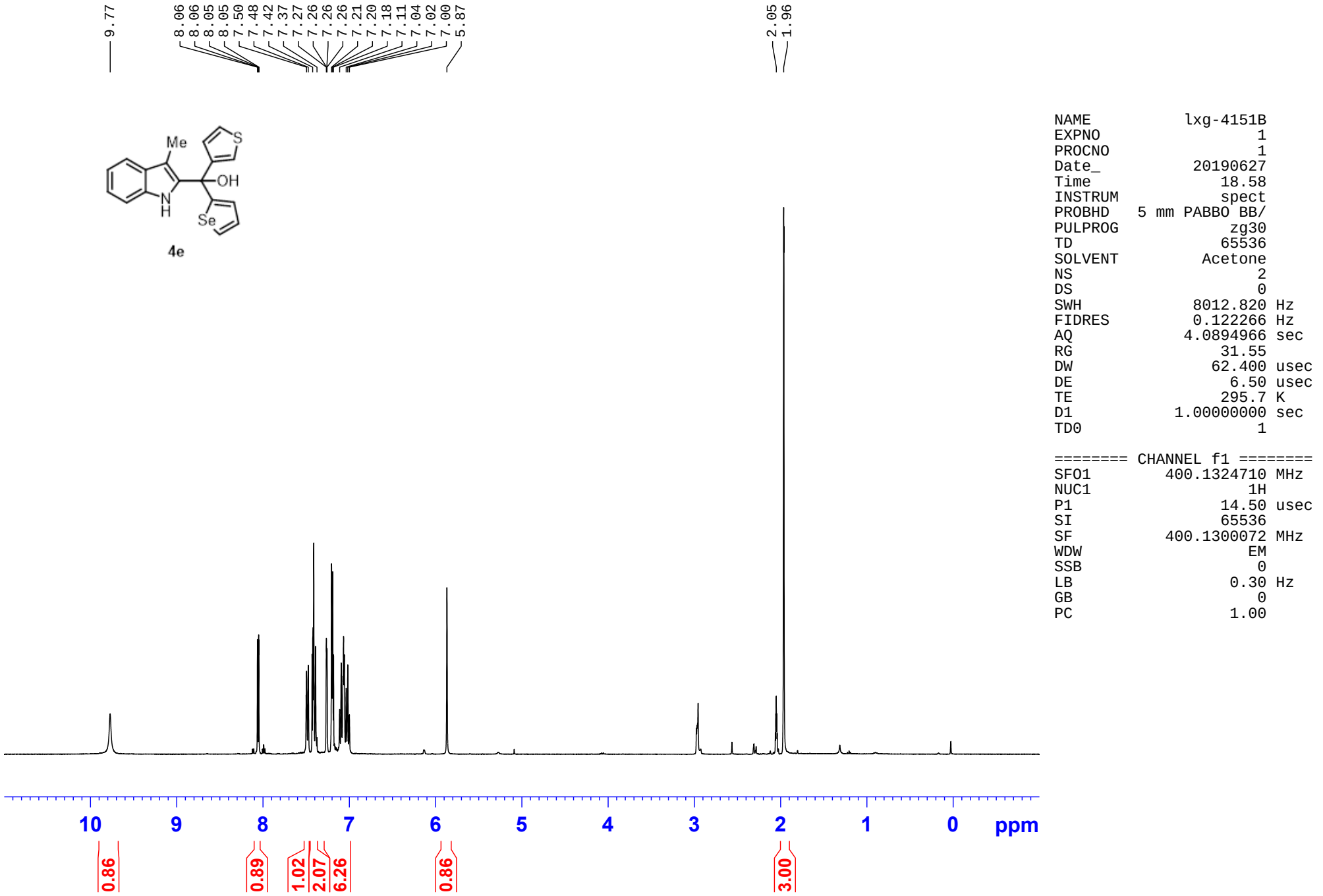
Supplementary Figure 46. ^{1}H NMR spectrum of **4d**



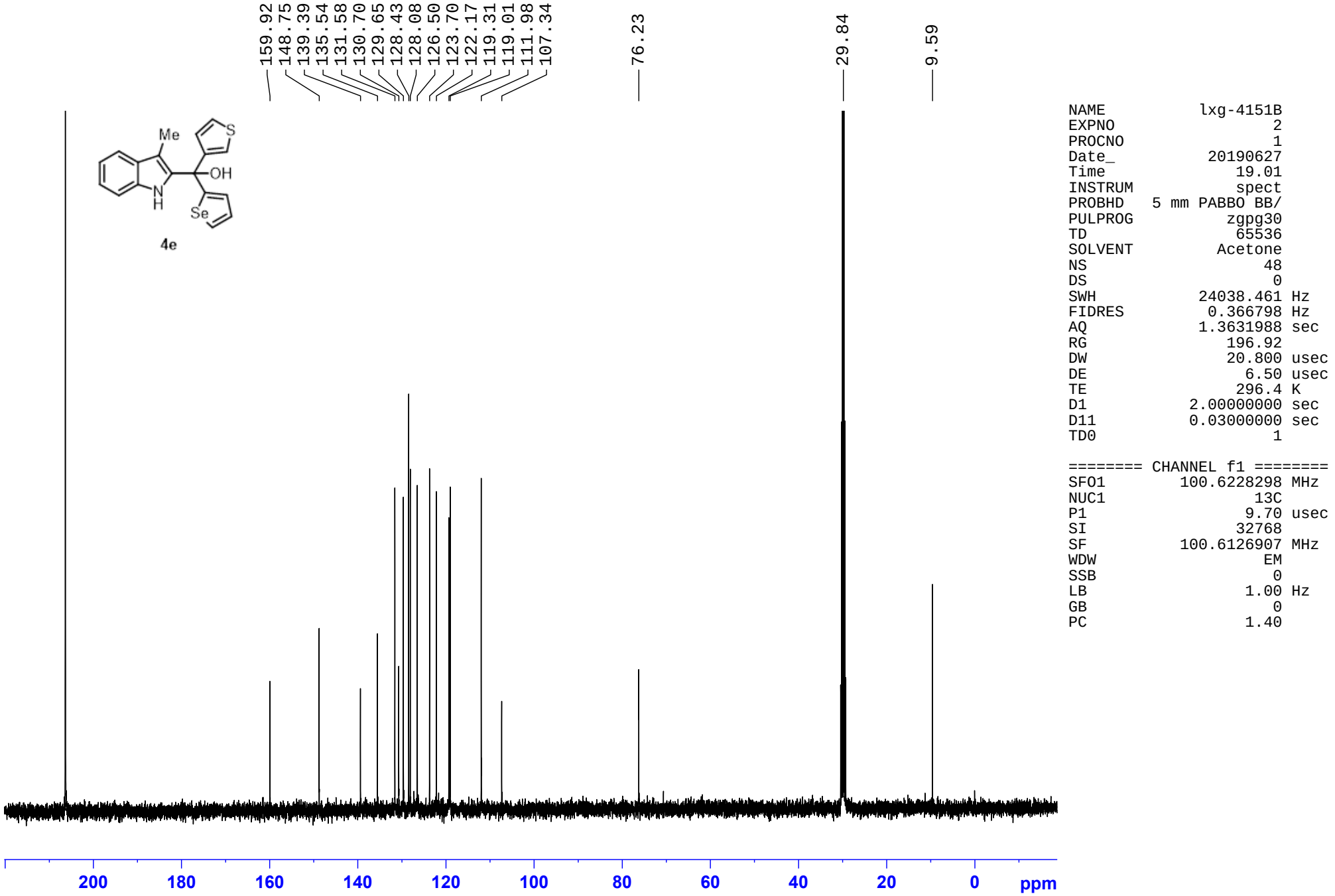

```
NAME            lxg-4151A
EXPNO                   2
PROCNO                  1
Date_            20190627
Time                18.55
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                      50
DS                       0
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                  196.92
DW                  20.800 usec
DE                   6.50 usec
TE                  296.4 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                   13C
P1                    9.70 usec
SI                   32768
SF            100.6126885 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```


Supplementary Figure 47. ^{13}C NMR spectrum of **4d**



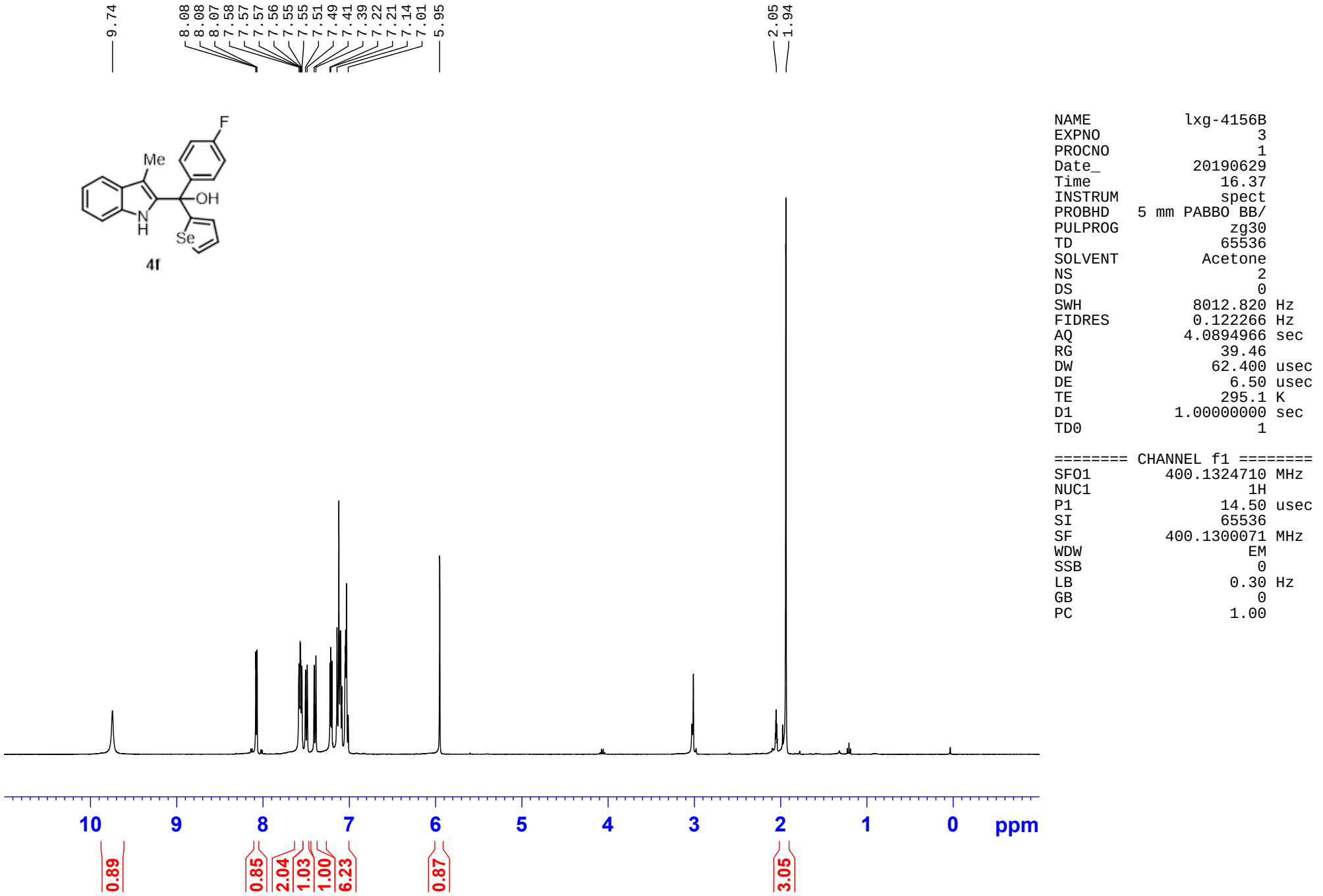
Supplementary Figure 48. ^{1}H NMR spectrum of **4e**



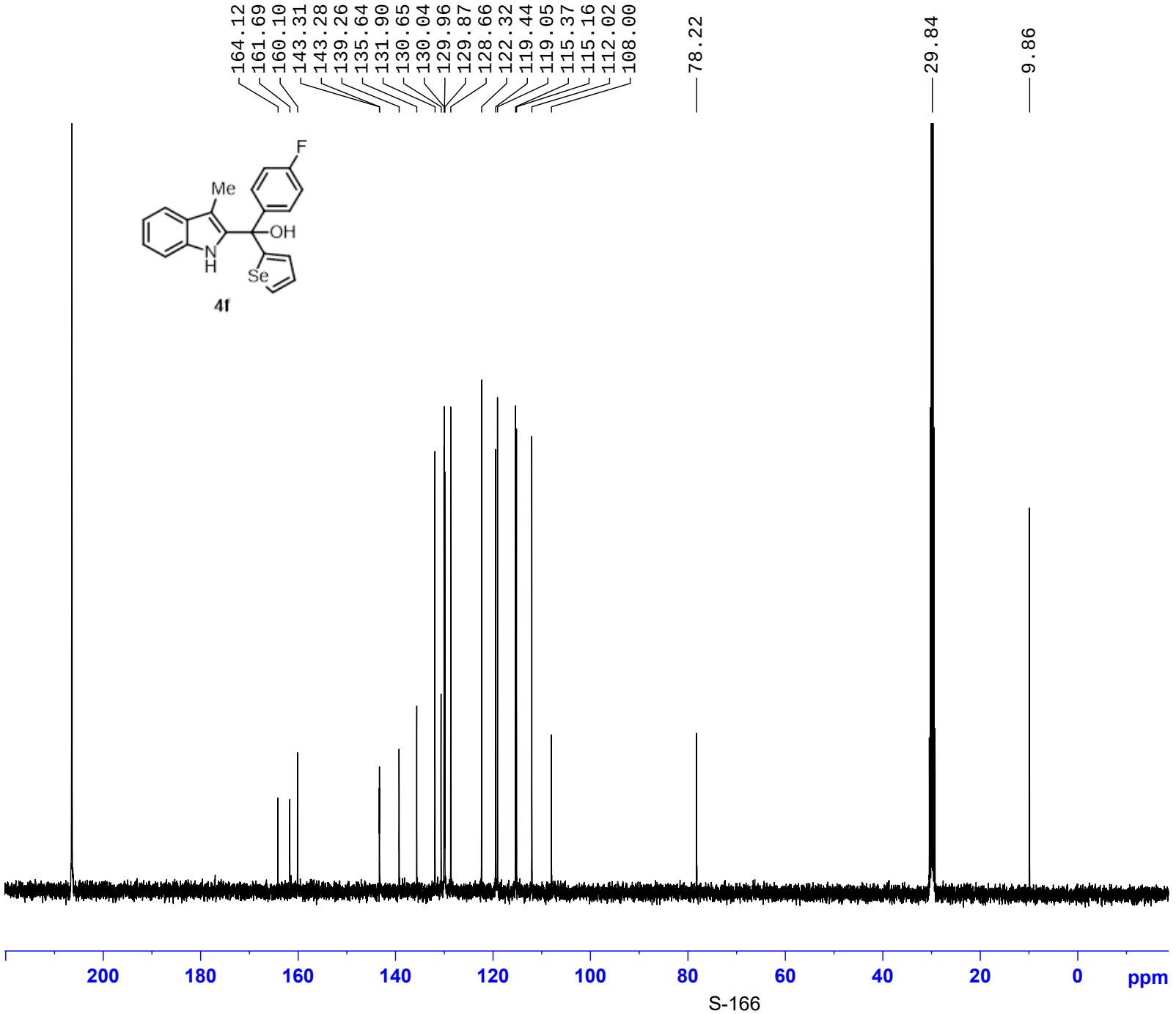

```
NAME           lxg-4151B
EXPNO                  2
PROCNO                 1
Date_           20190627
Time               19.01
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                    48
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                296.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                 9.70 usec
SI                32768
SF           100.6126907 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


Supplementary Figure 49. ^{13}C NMR spectrum of **4e**



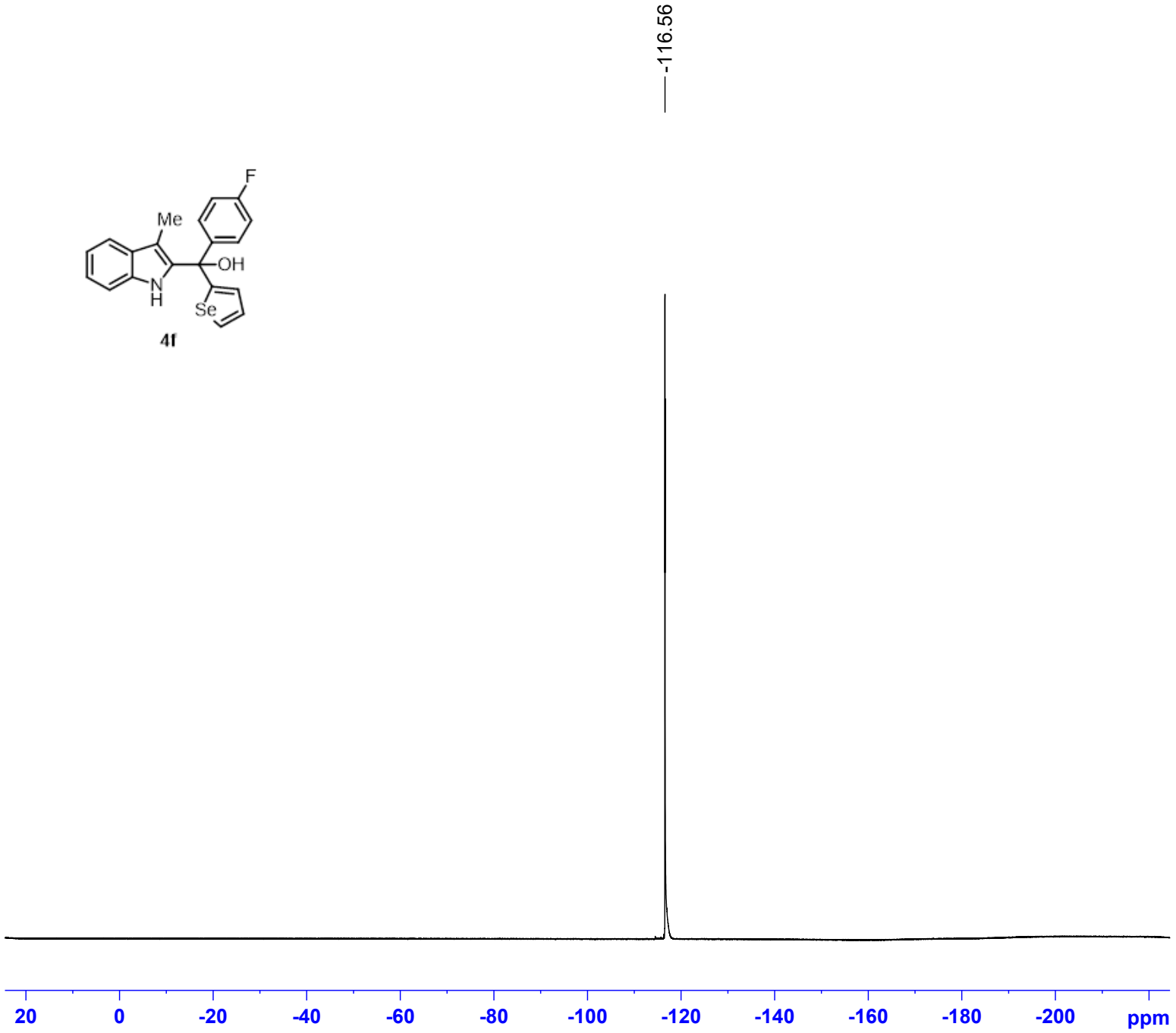
Supplementary Figure 50. ^{1}H NMR spectrum of **4f**




```
NAME           lxg-4156B
EXPNO                  5
PROCNO                 1
Date_           20190629
Time               16.40
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                    59
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                296.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                 9.70 usec
SI                32768
SF           100.6126907 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

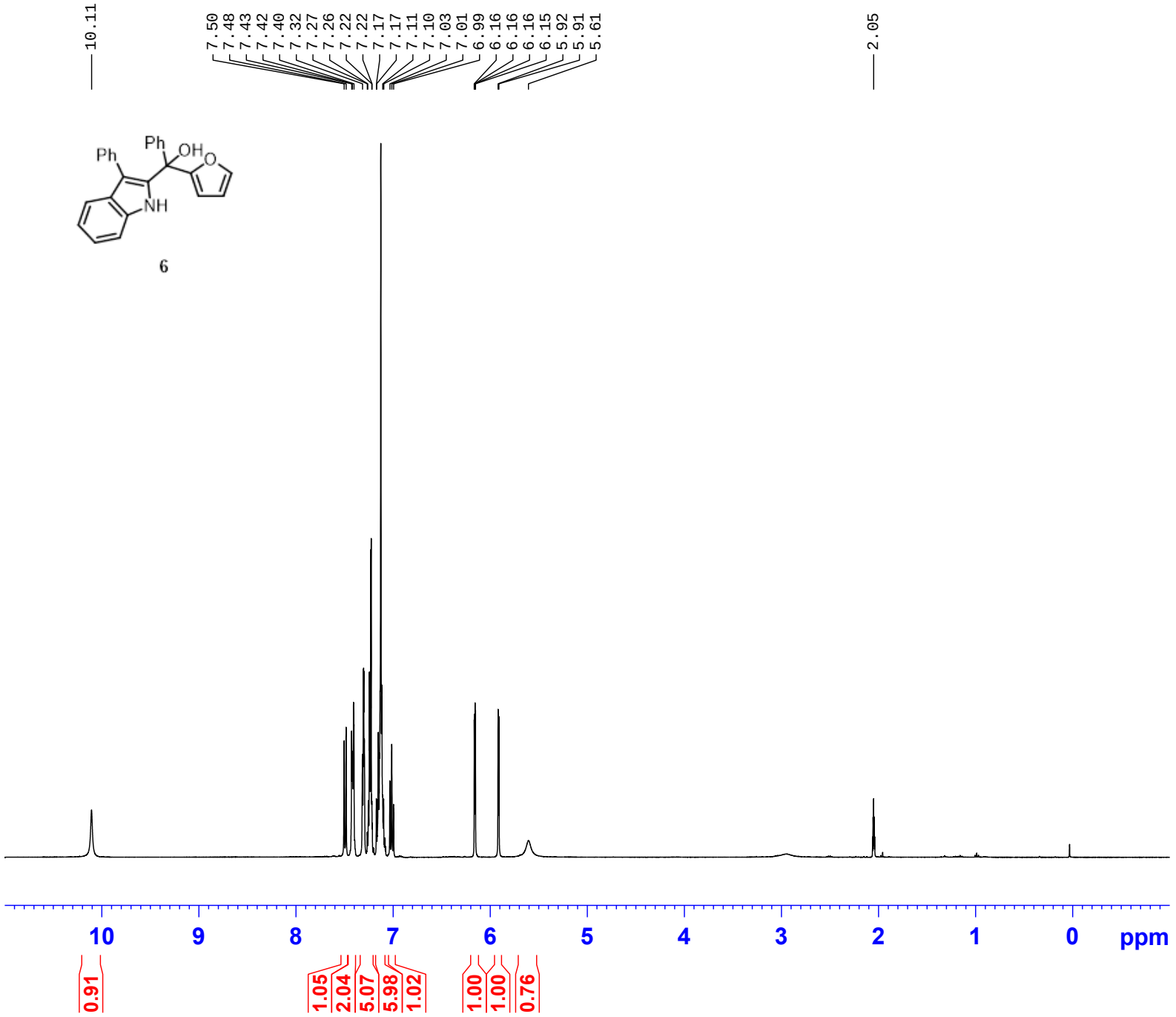

Supplementary Figure 51. ^{13}C NMR spectrum of **4f**



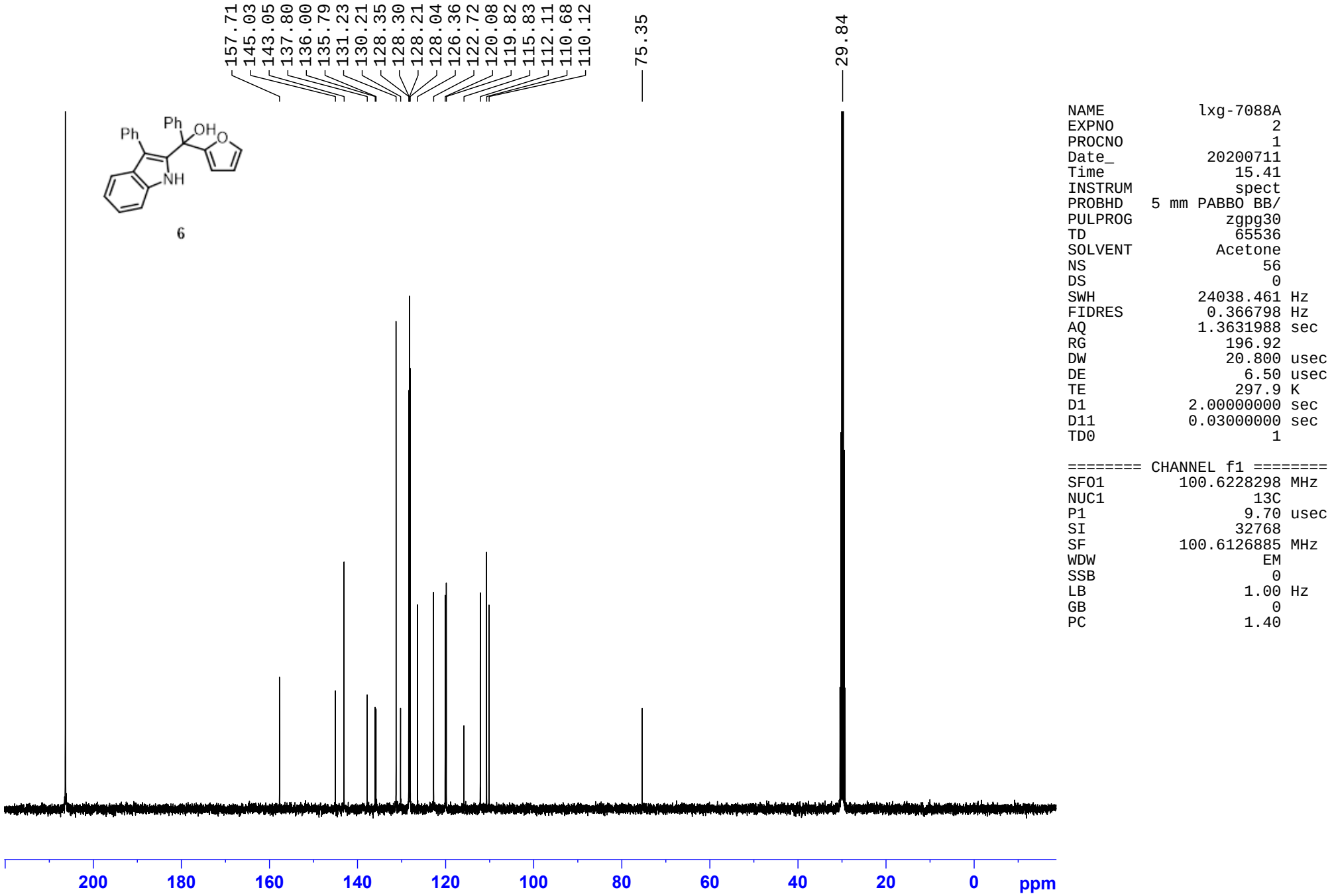

```
NAME           lxg-4156B
EXPNO                  4
PROCNO                 1
Date_           20190629
Time               16.28
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT          Acetone
NS                    20
DS                     0
SWH            93750.000 Hz
FIDRES          1.430511 Hz
AQ             0.3495753 sec
RG                196.92
DW                 5.333 usec
DE                 6.50 usec
TE                 295.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         376.4607162 MHz
NUC1                19F
P1                14.70 usec
SI                32768
SF           376.4983660 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

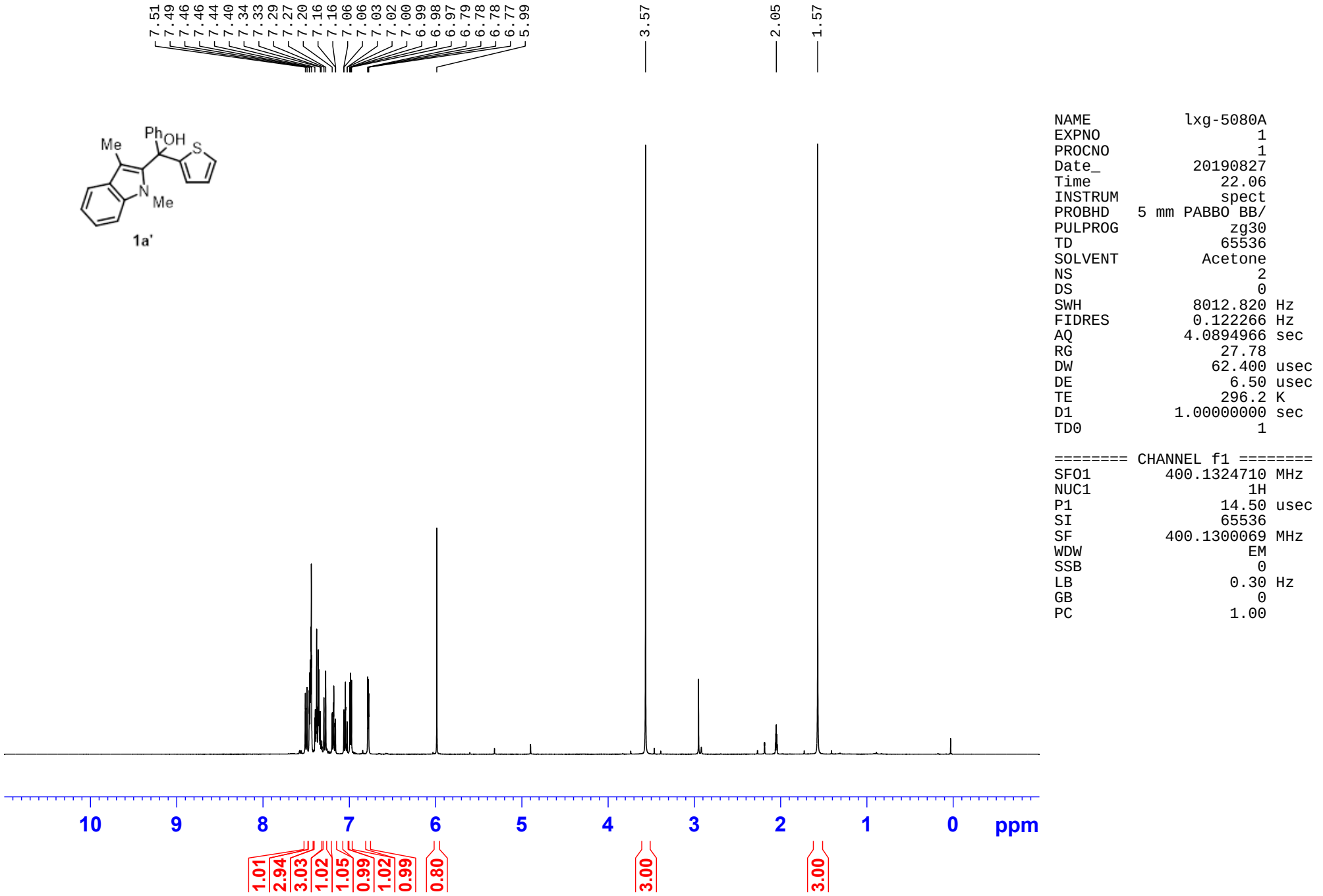
Supplementary Figure 52. ^{19}F NMR spectrum of **4f**



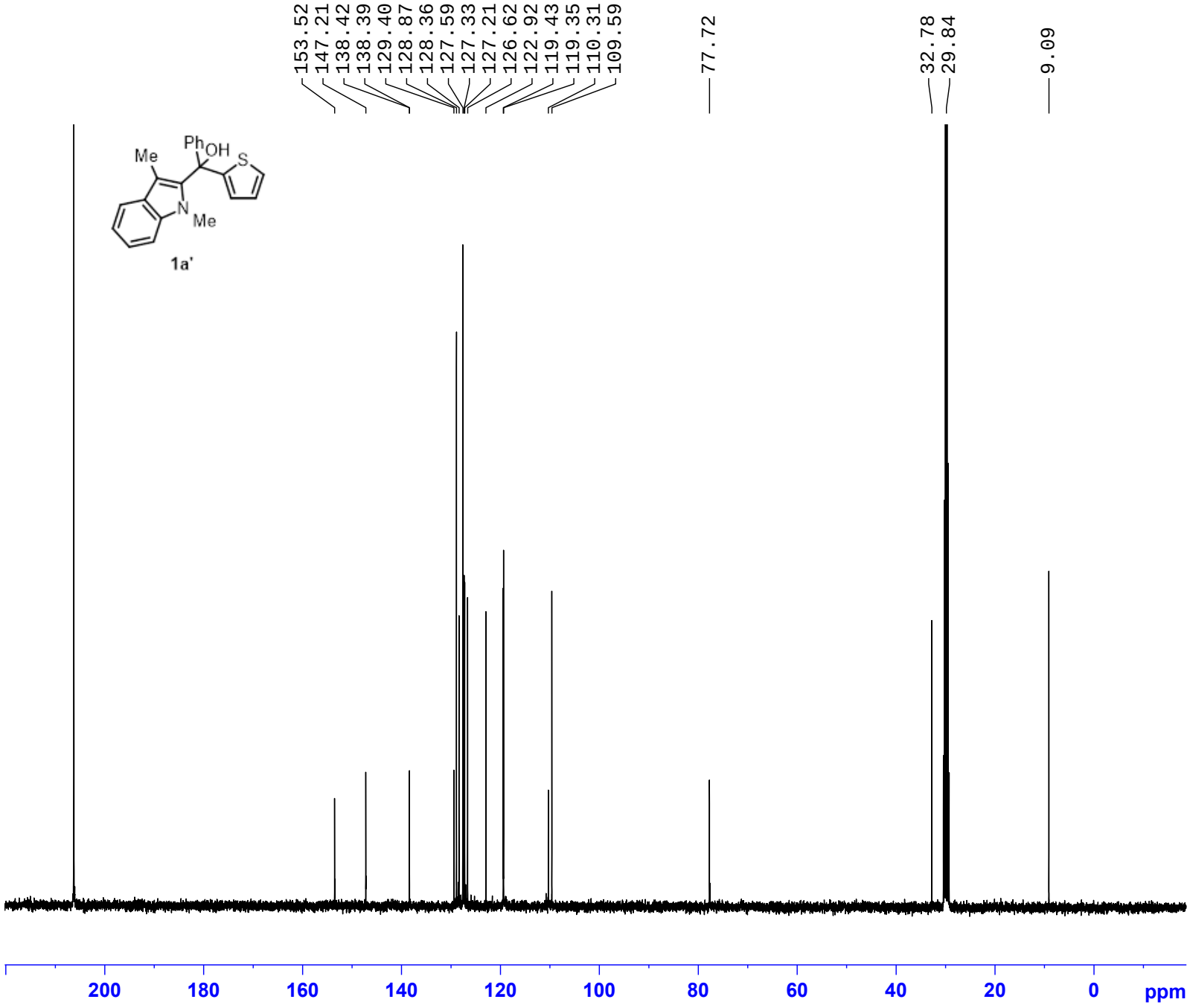
Supplementary Figure 53. ^{1}H NMR spectrum of **6**



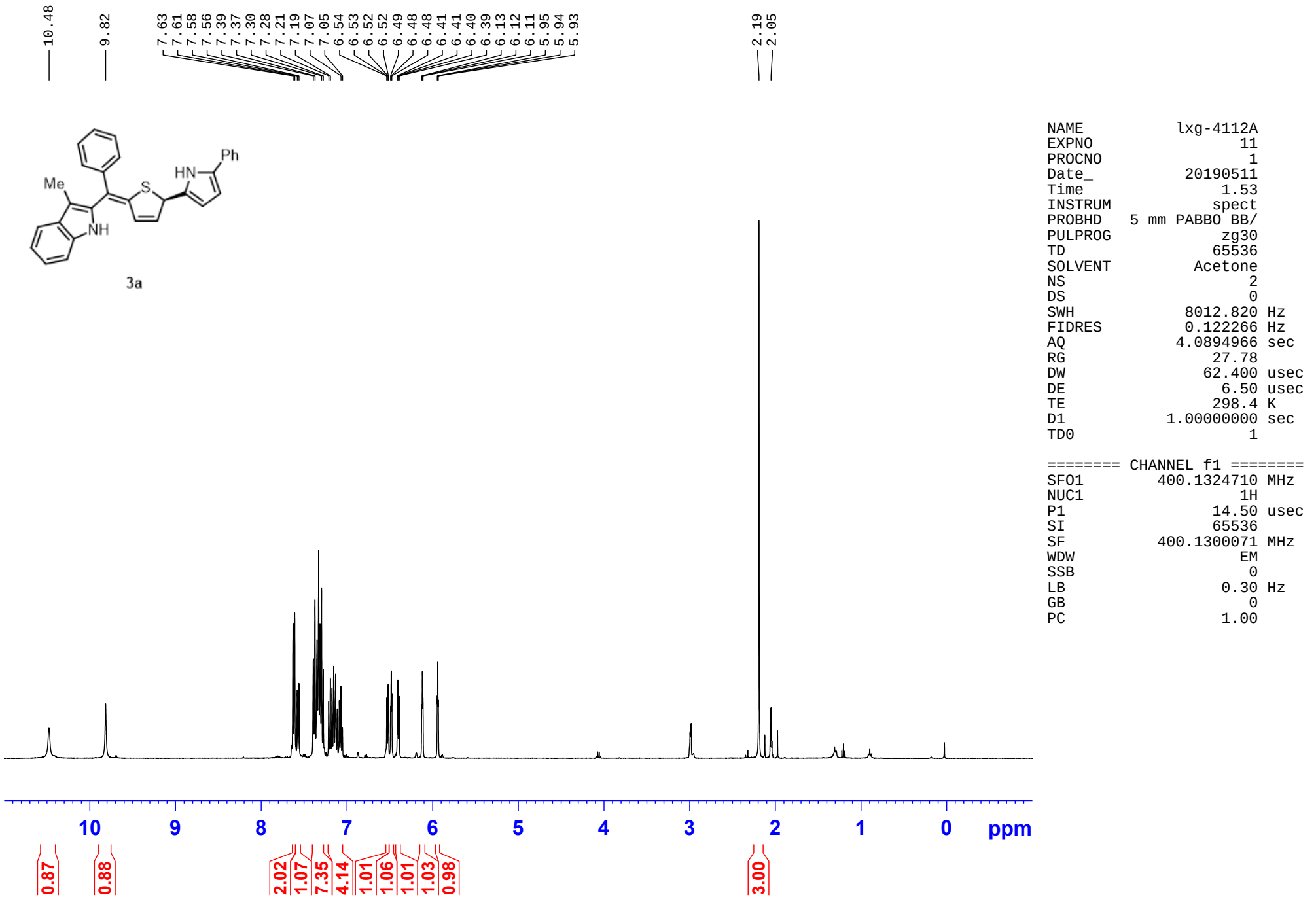
Supplementary Figure 54. ^{13}C NMR spectrum of **6**



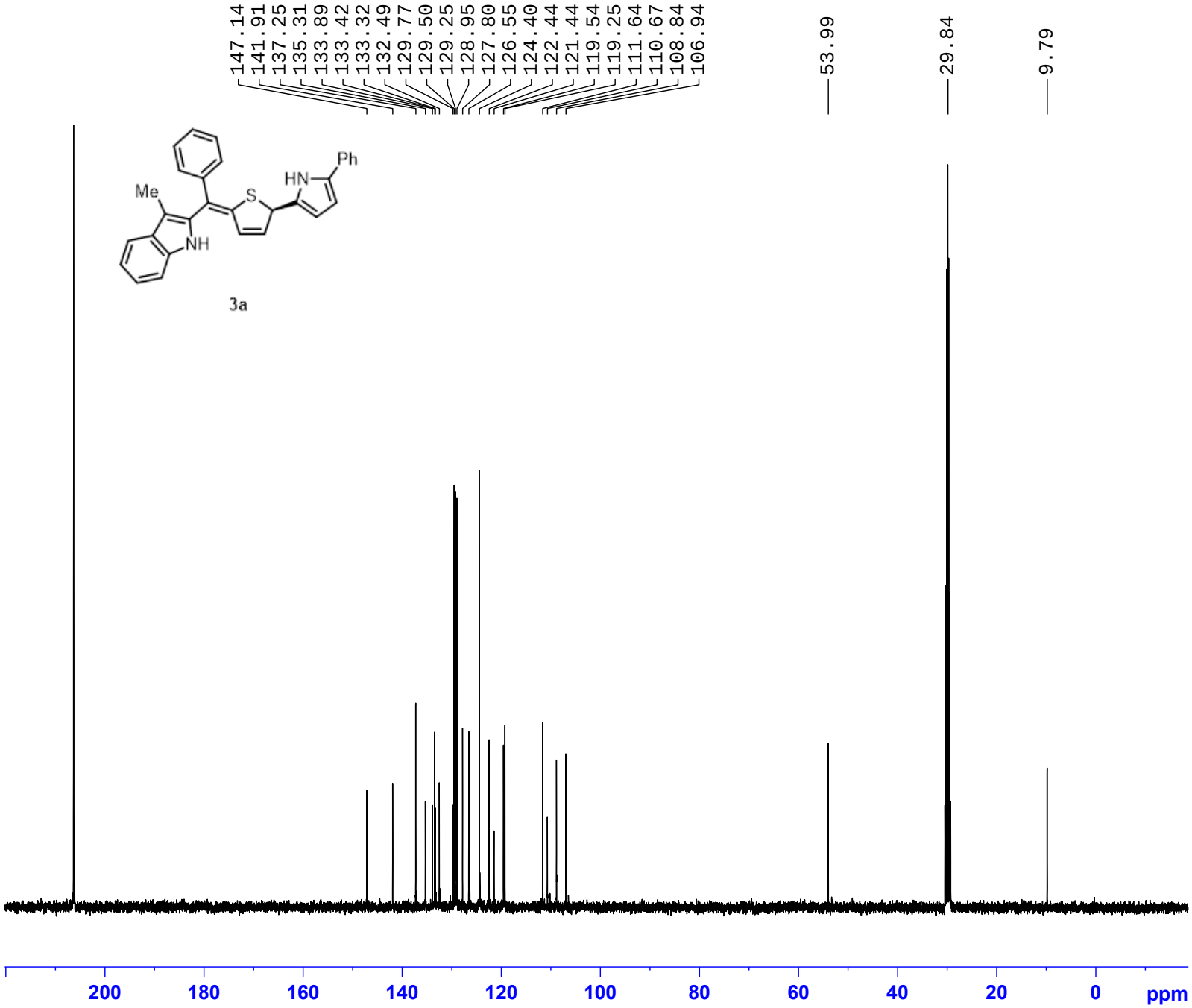
Supplementary Figure 55. ^{1}H NMR spectrum of **1a'**



Supplementary Figure 56. ^{13}C NMR spectrum of **1a'**

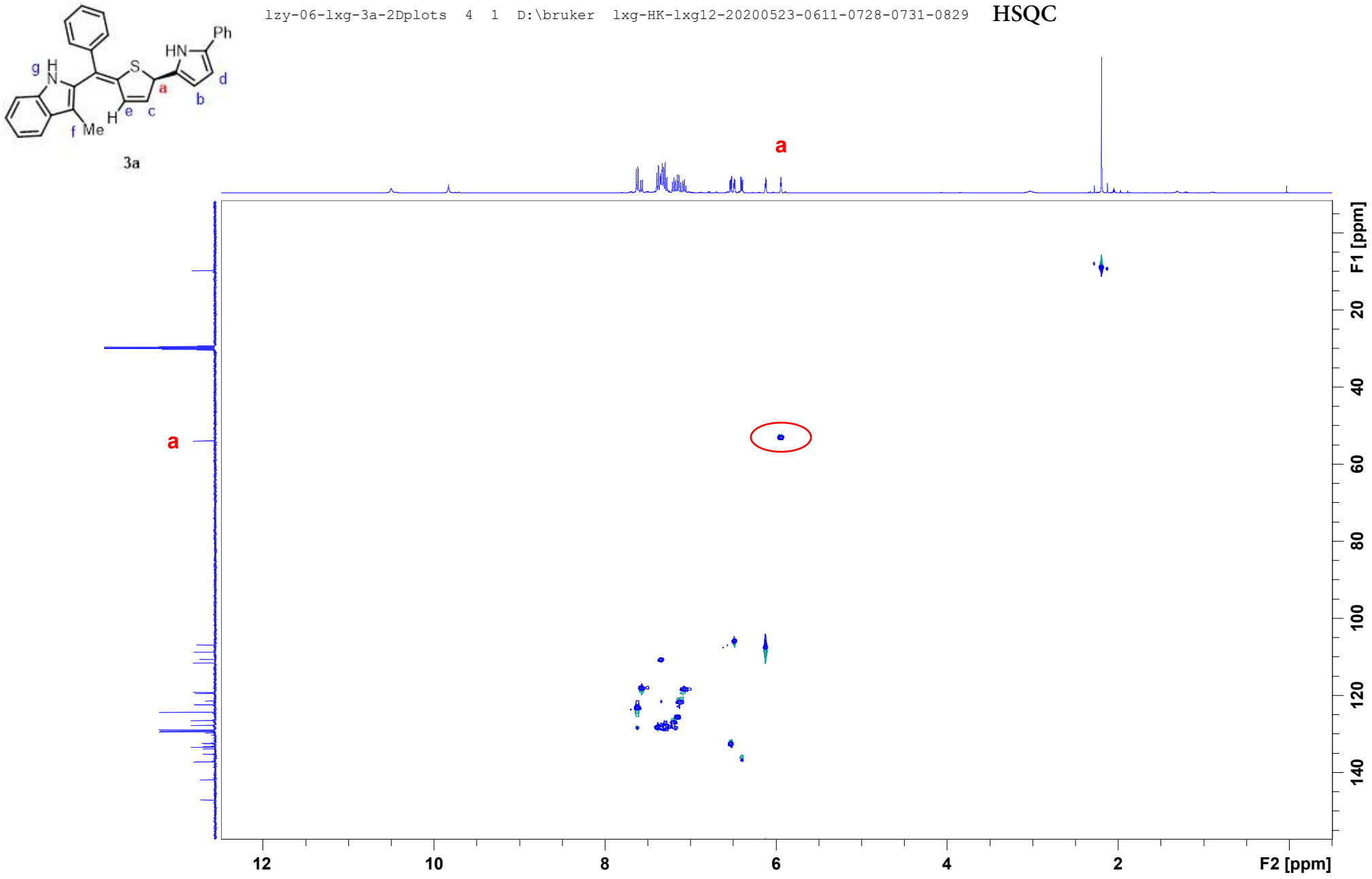


Supplementary Figure 57. ^{1}H NMR spectrum of **3a**

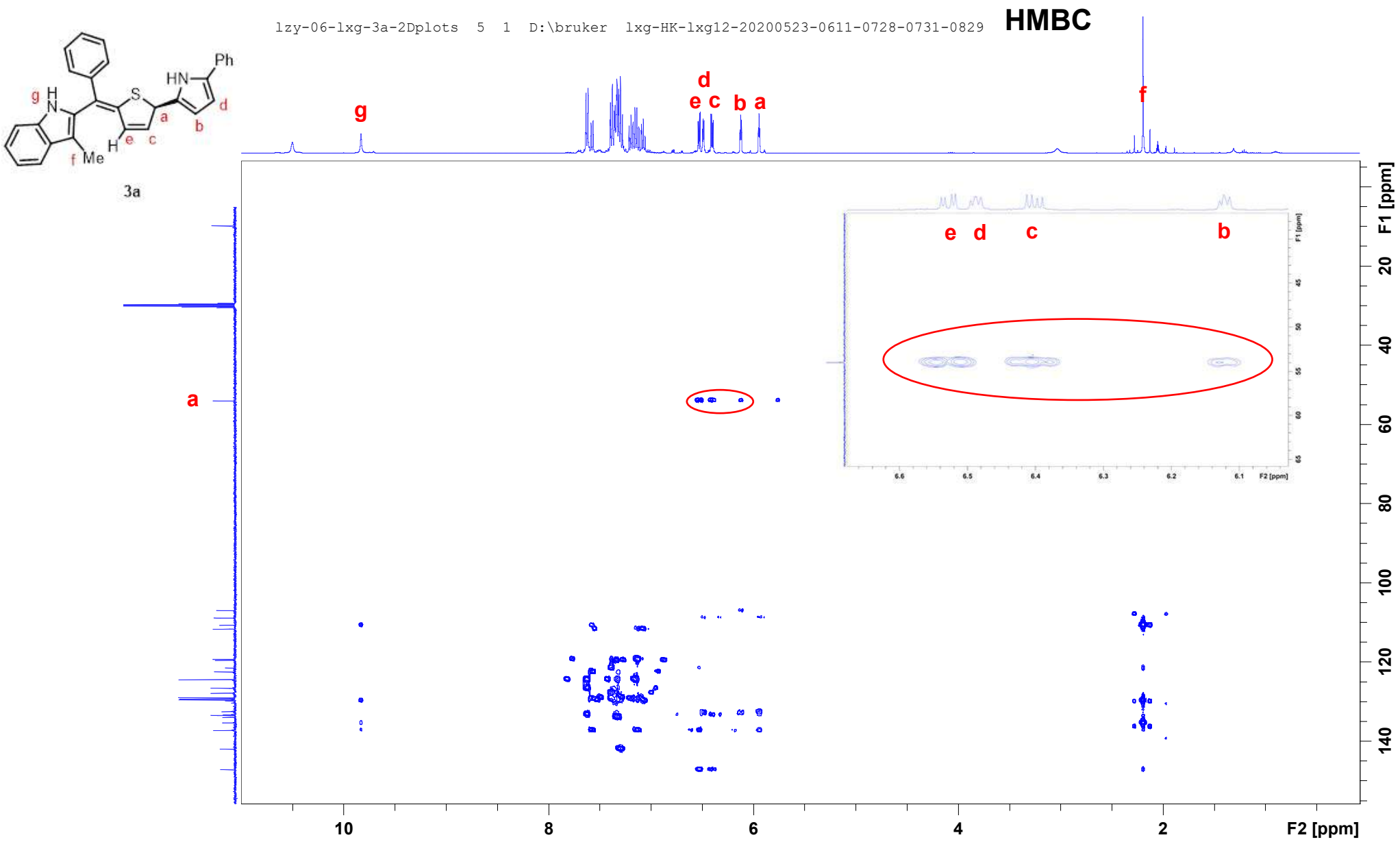


NAME	lxg-4112A
EXPNO	12
PROCNO	1
Date_	20190511
Time	1.58
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	57
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	299.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6126885 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

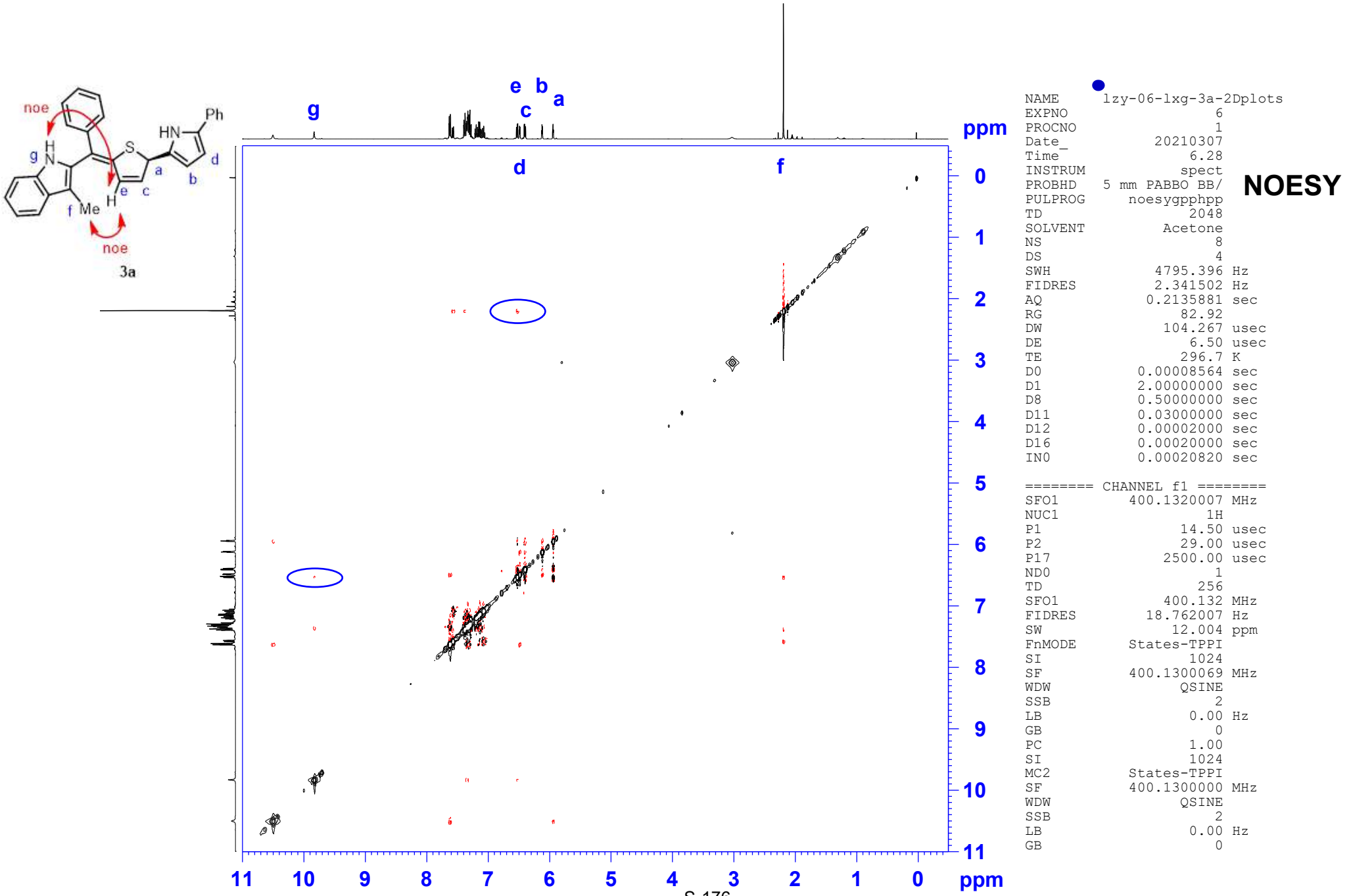
Supplementary Figure 58. ^{13}C NMR spectrum of **3a**



Supplementary Figure 59. ^{1}H-^{13}C HSQC spectrum of **3a**



Supplementary Figure 60. HMBC spectrum of **3a**

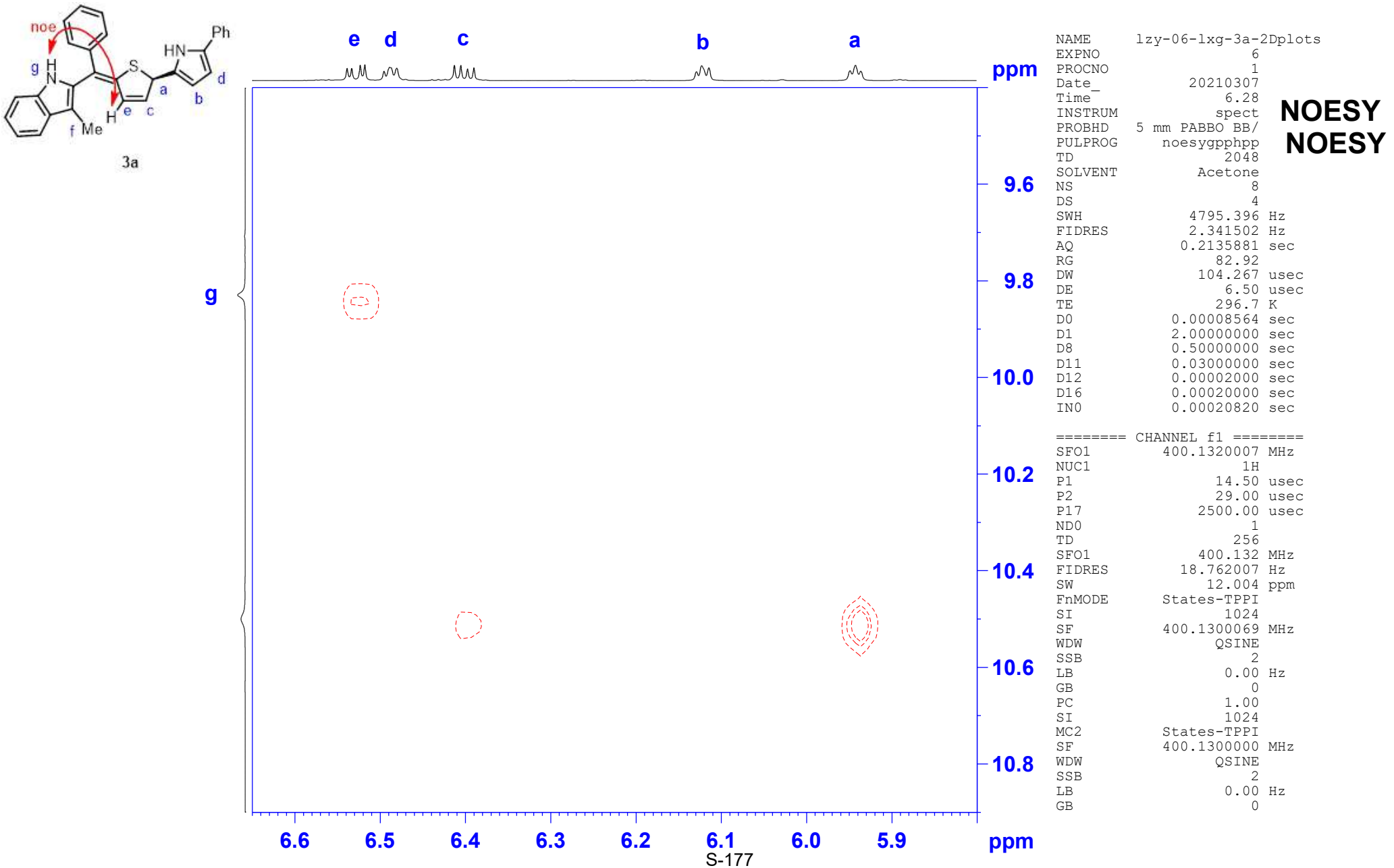


NOESY

```
NAME          lzy-06-lxg-3a-2Dplots
EXPNO                             6
PROCNO                            1
Date_                      20210307
Time                           6.28
INSTRUM                       spect
PROBHD    5 mm PABBO BB/
PULPROG              noesygpphpp
TD                             2048
SOLVENT                     Acetone
NS                                8
DS                                4
SWH                        4795.396 Hz
FIDRES                     2.341502 Hz
AQ                         0.2135881 sec
RG                             82.92
DW                           104.267 usec
DE                             6.50 usec
TE                            296.7 K
D0                       0.00008564 sec
D1                       2.00000000 sec
D8                       0.50000000 sec
D11                      0.03000000 sec
D12                      0.00002000 sec
D16                      0.00020000 sec
IN0                      0.00020820 sec

======== CHANNEL f1 ========
SFO1                  400.1320007 MHz
NUC1                          1H
P1                           14.50 usec
P2                           29.00 usec
P17                        2500.00 usec
ND0                               1
TD                              256
SFO1                      400.132 MHz
FIDRES                   18.762007 Hz
SW                           12.004 ppm
FnMODE                States-TPPI
SI                            1024
SF                    400.1300069 MHz
WDW                         QSINE
SSB                               2
LB                            0.00 Hz
GB                                0
PC                            1.00
SI                            1024
MC2                   States-TPPI
SF                    400.1300000 MHz
WDW                         QSINE
SSB                               2
LB                            0.00 Hz
GB                                0
```

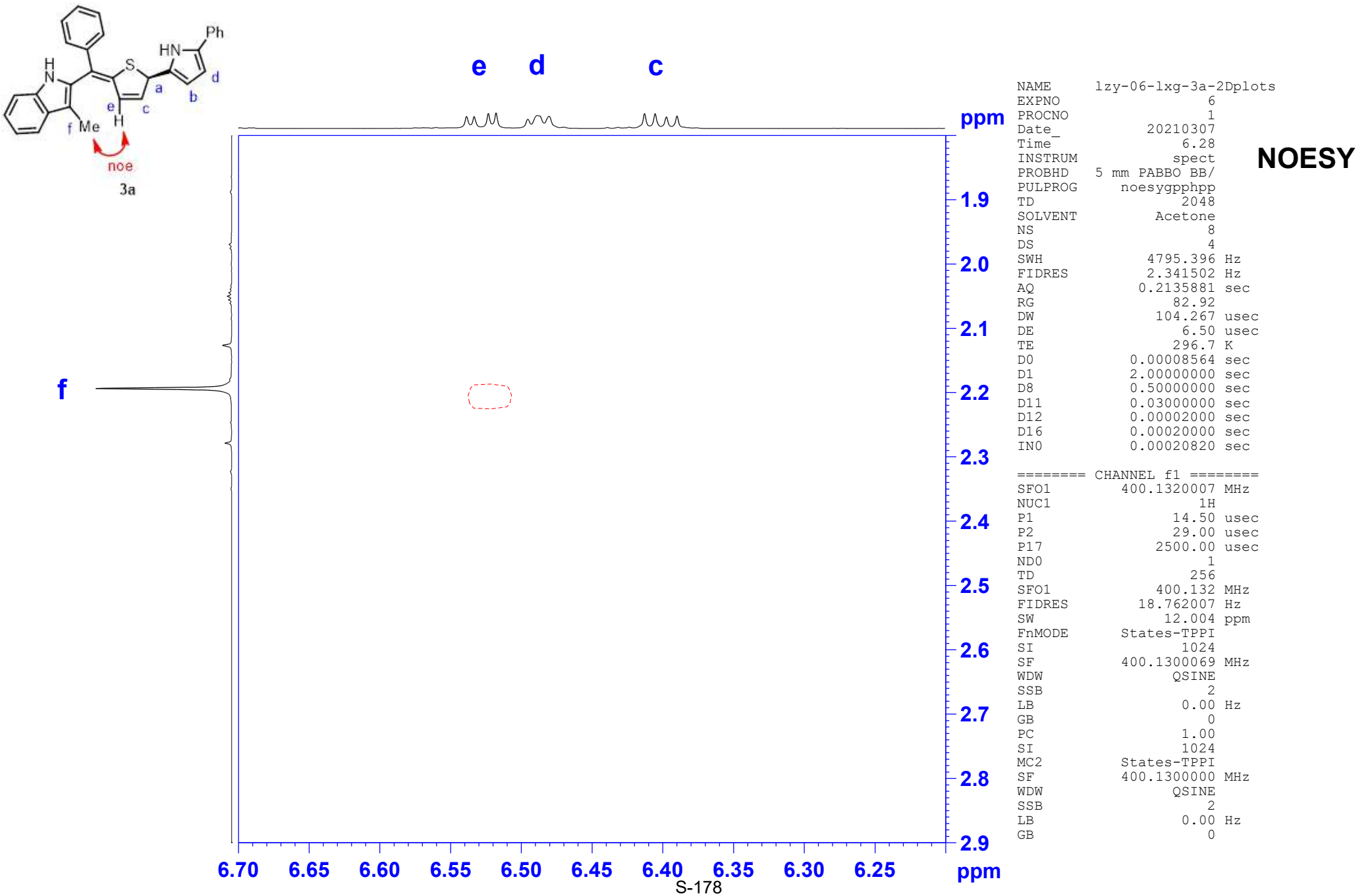

Supplementary Figure 61. NOESY spectrum of **3a**



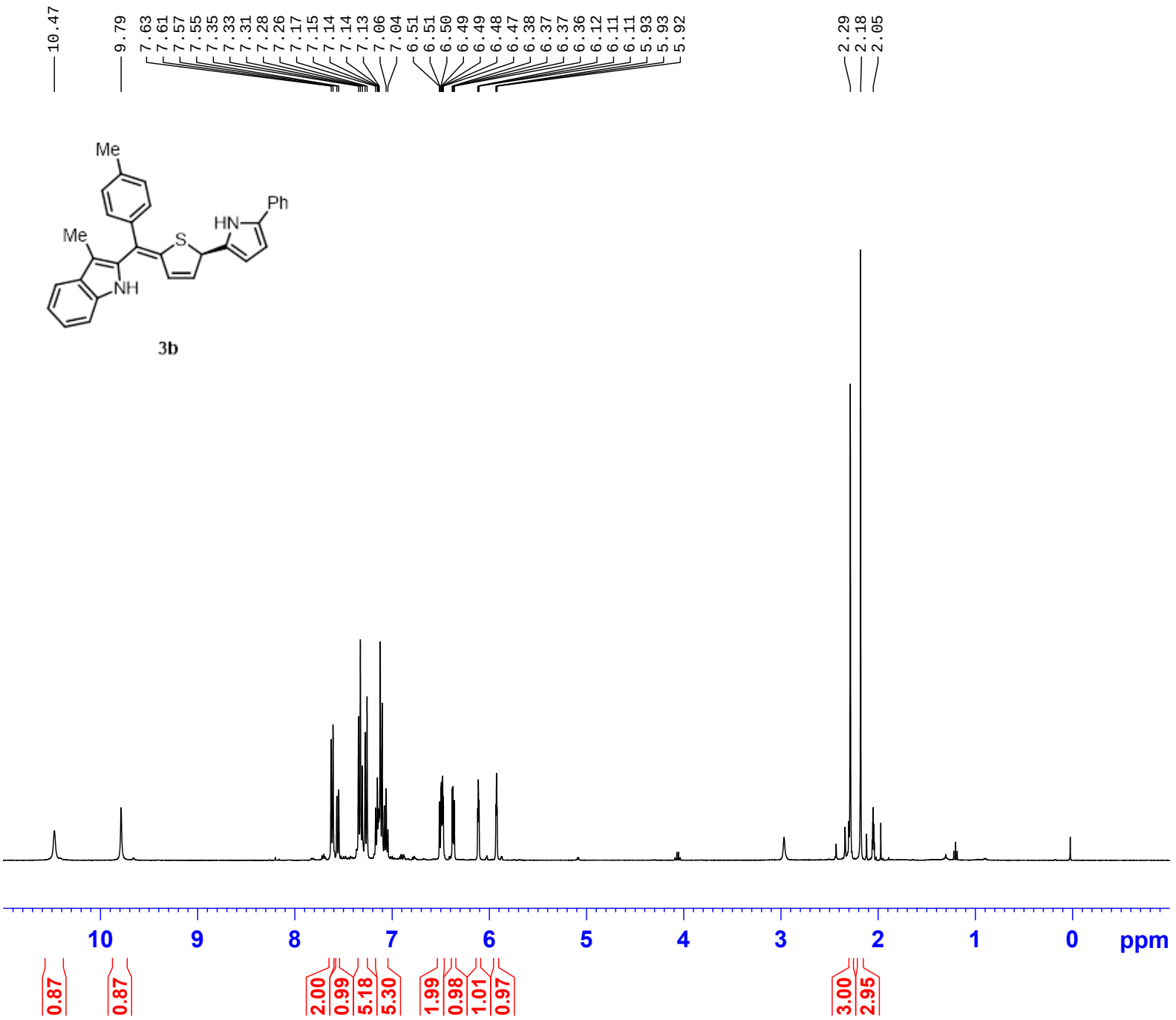

```
NAME      lzy-06-lxg-3a-2Dplots
EXPNO                         6
PROCNO                        1
Date_              20210307
Time                      6.28
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG       noesygpphpp
TD                         2048
SOLVENT             Acetone
NS                            8
DS                            4
SWH                4795.396 Hz
FIDRES             2.341502 Hz
AQ                 0.2135881 sec
RG                      82.92
DW                     104.267 usec
DE                        6.50 usec
TE                      296.7 K
D0                 0.00008564 sec
D1                 2.00000000 sec
D8                 0.50000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
D16                0.00020000 sec
IN0                0.00020820 sec

======== CHANNEL f1 ========
SFO1            400.1320007 MHz
NUC1                      1H
P1                     14.50 usec
P2                     29.00 usec
P17                  2500.00 usec
ND0                           1
TD                          256
SFO1                  400.132 MHz
FIDRES               18.762007 Hz
SW                       12.004 ppm
FnMODE            States-TPPI
SI                         1024
SF                400.1300069 MHz
WDW                       QSINE
SSB                           2
LB                         0.00 Hz
GB                            0
PC                         1.00
SI                         1024
MC2               States-TPPI
SF                400.1300000 MHz
WDW                       QSINE
SSB                           2
LB                         0.00 Hz
GB                            0
```

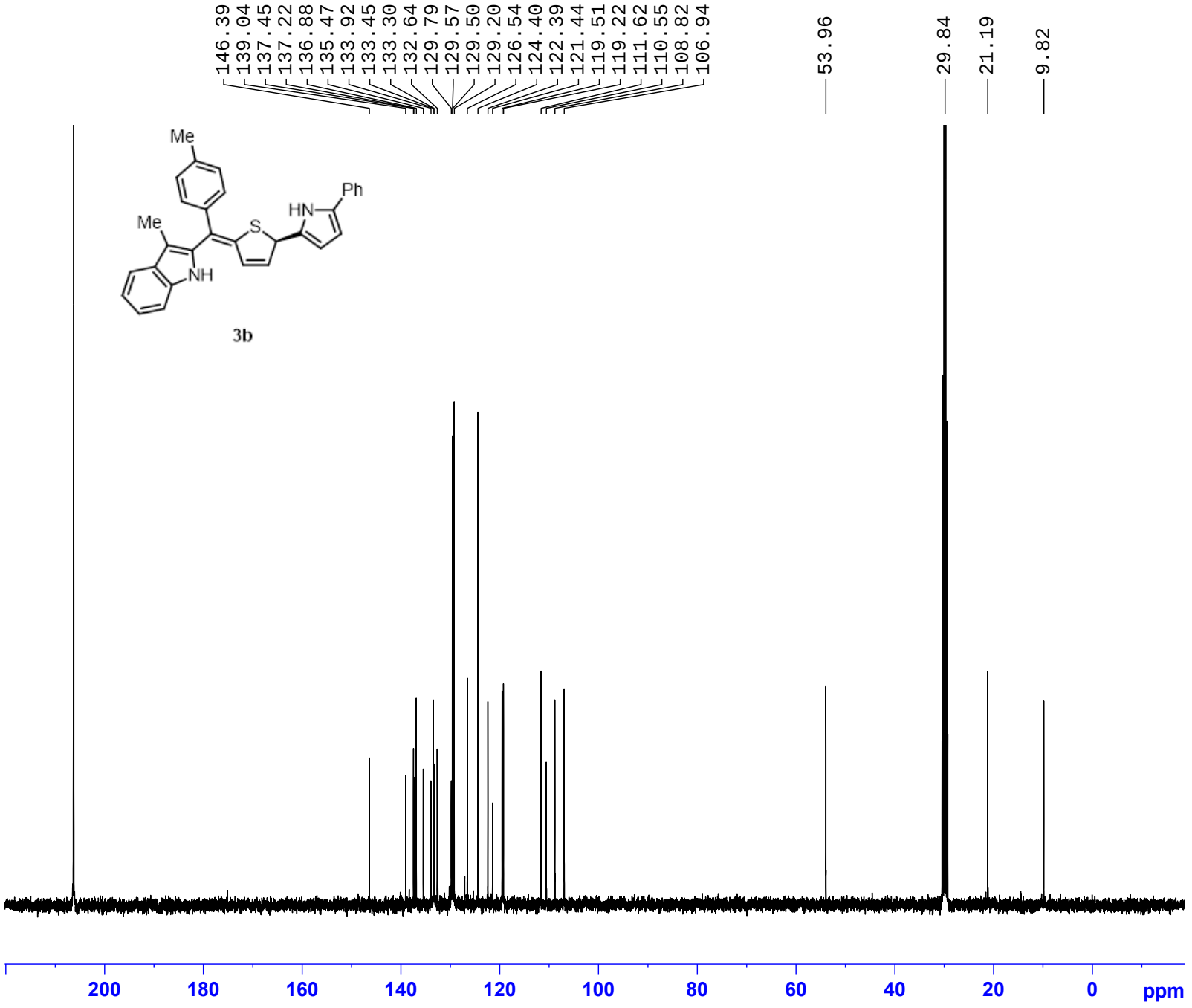

Supplementary Figure 62. NOESY spectrum (enlarged) of **3a**



Supplementary Figure 63. NOESY spectrum (enlarged) of **3a**



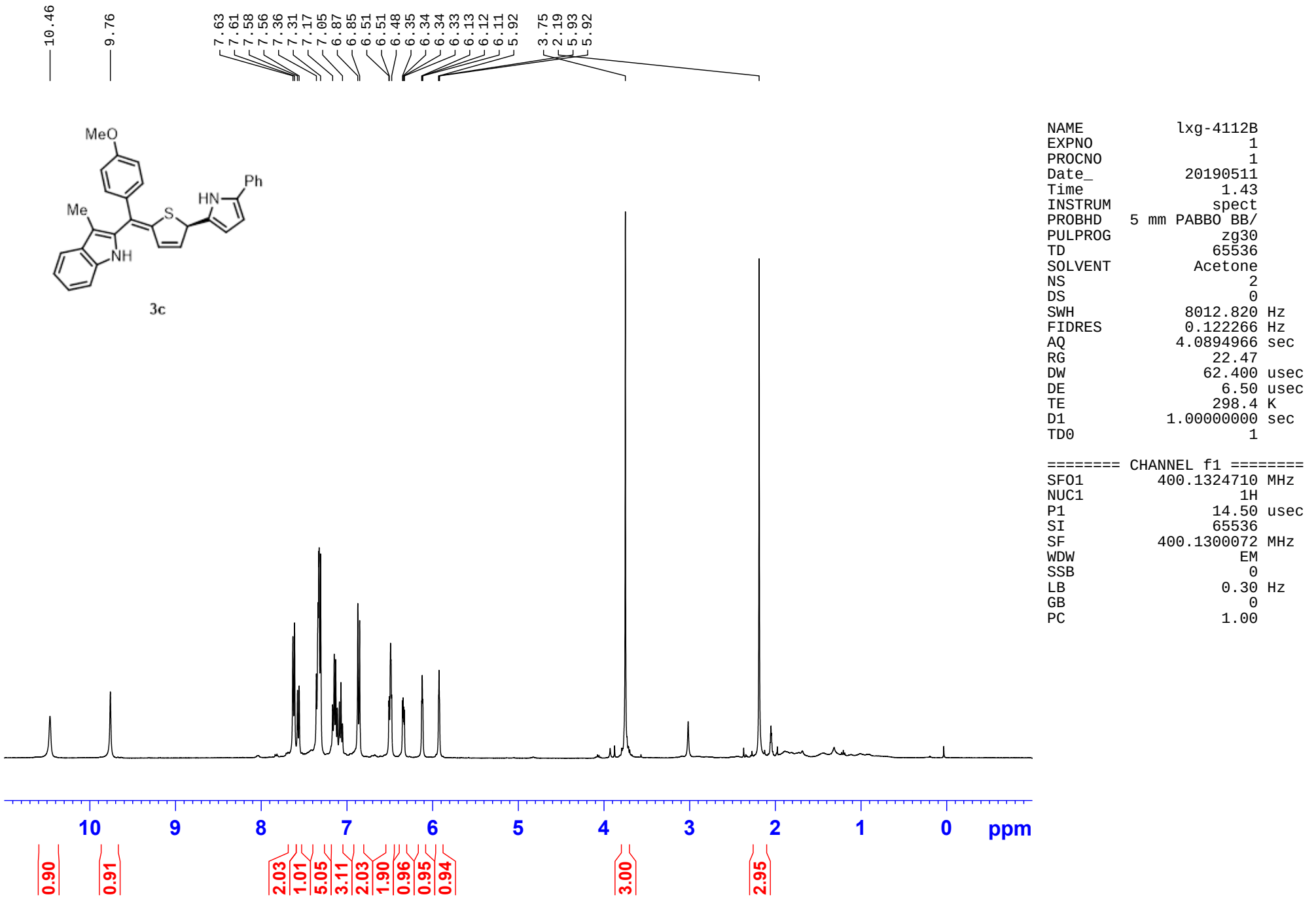
Supplementary Figure 64. ^{1}H NMR spectrum of **3b**



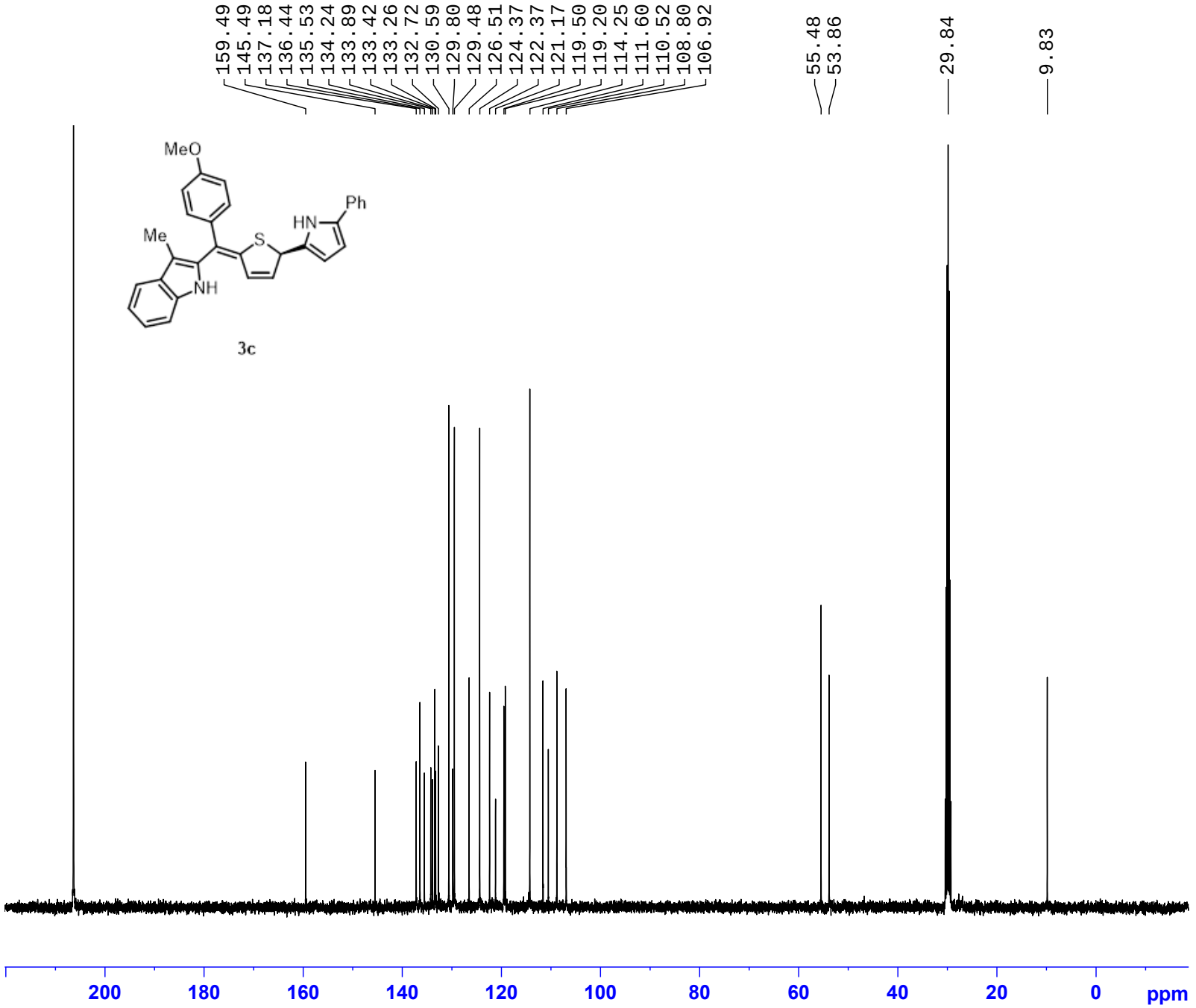

```
NAME            lxg-4116A
EXPNO                   2
PROCNO                  1
Date_            20190514
Time                18.33
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT          Acetone
NS                    93
DS                     0
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                298.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                 9.70 usec
SI                32768
SF           100.6126871 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


Supplementary Figure 65. ^{13}C NMR spectrum of **3b**



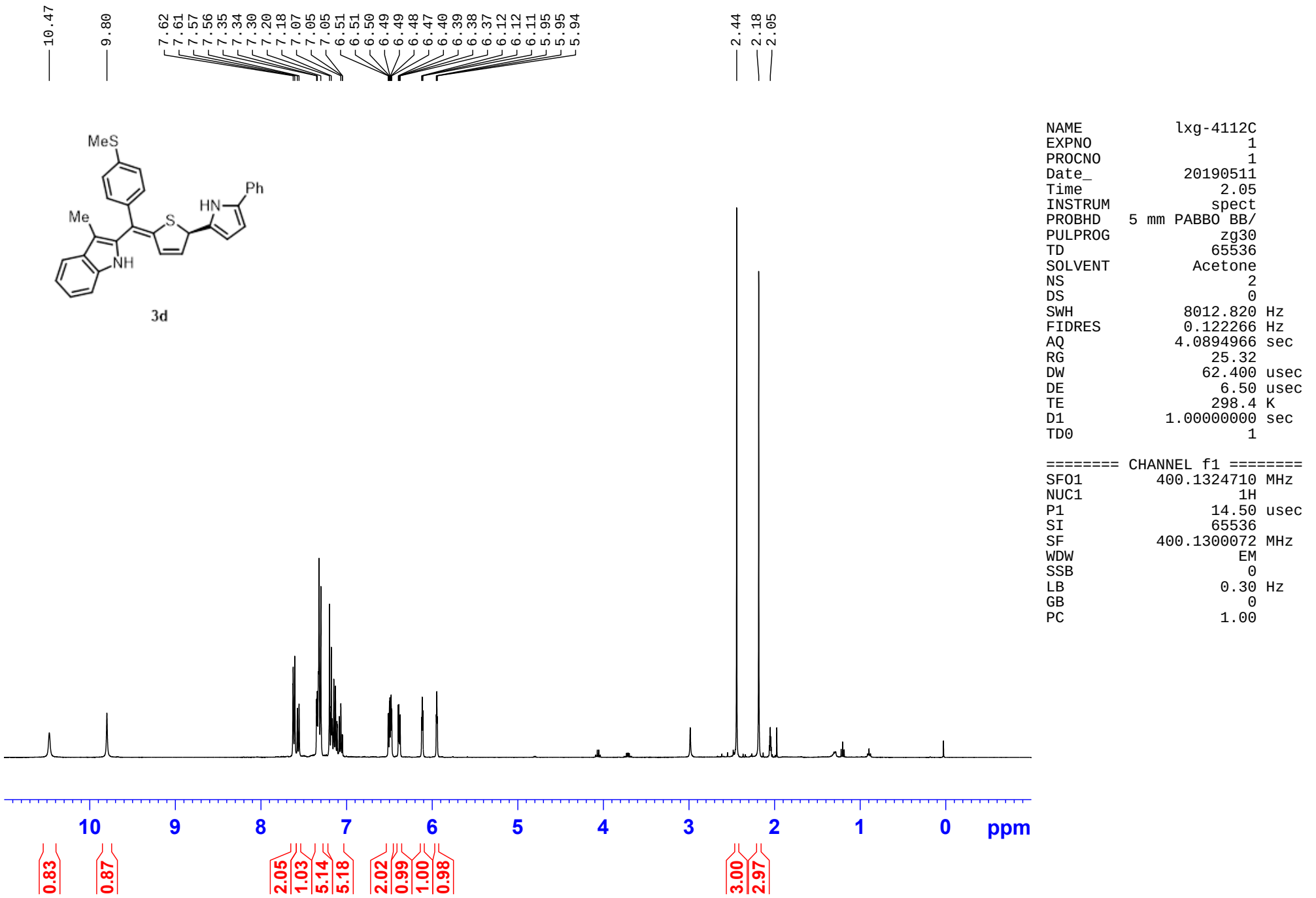
Supplementary Figure 66. ^{1}H NMR spectrum of **3c**



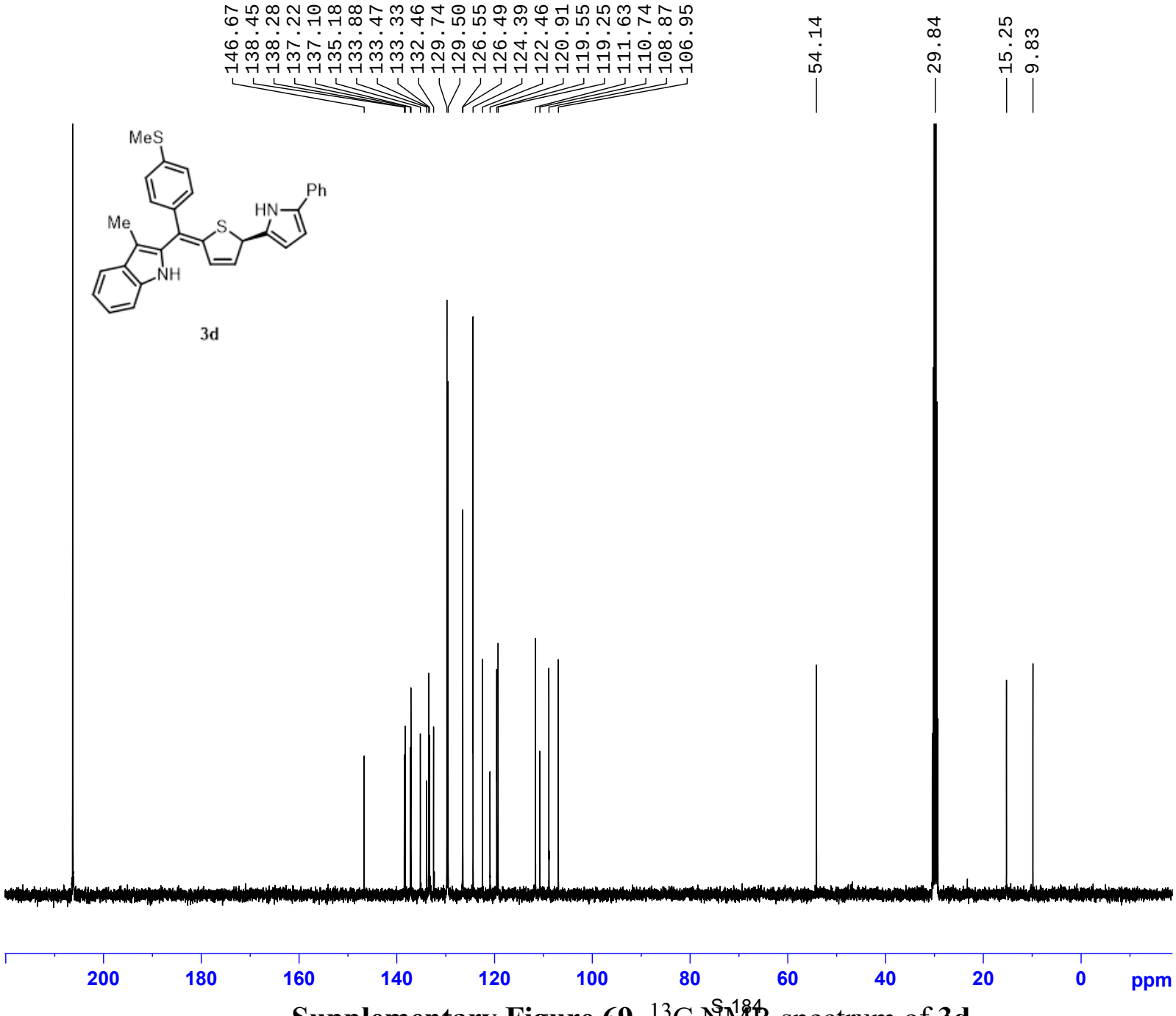

```
NAME            lxg-4112B
EXPNO                   2
PROCNO                  1
Date_            20190511
Time                1.47
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT          Acetone
NS                    73
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                299.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                 9.70 usec
SI                32768
SF           100.6126915 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Supplementary Figure 67. ^{13}C NMR spectrum of **3c**

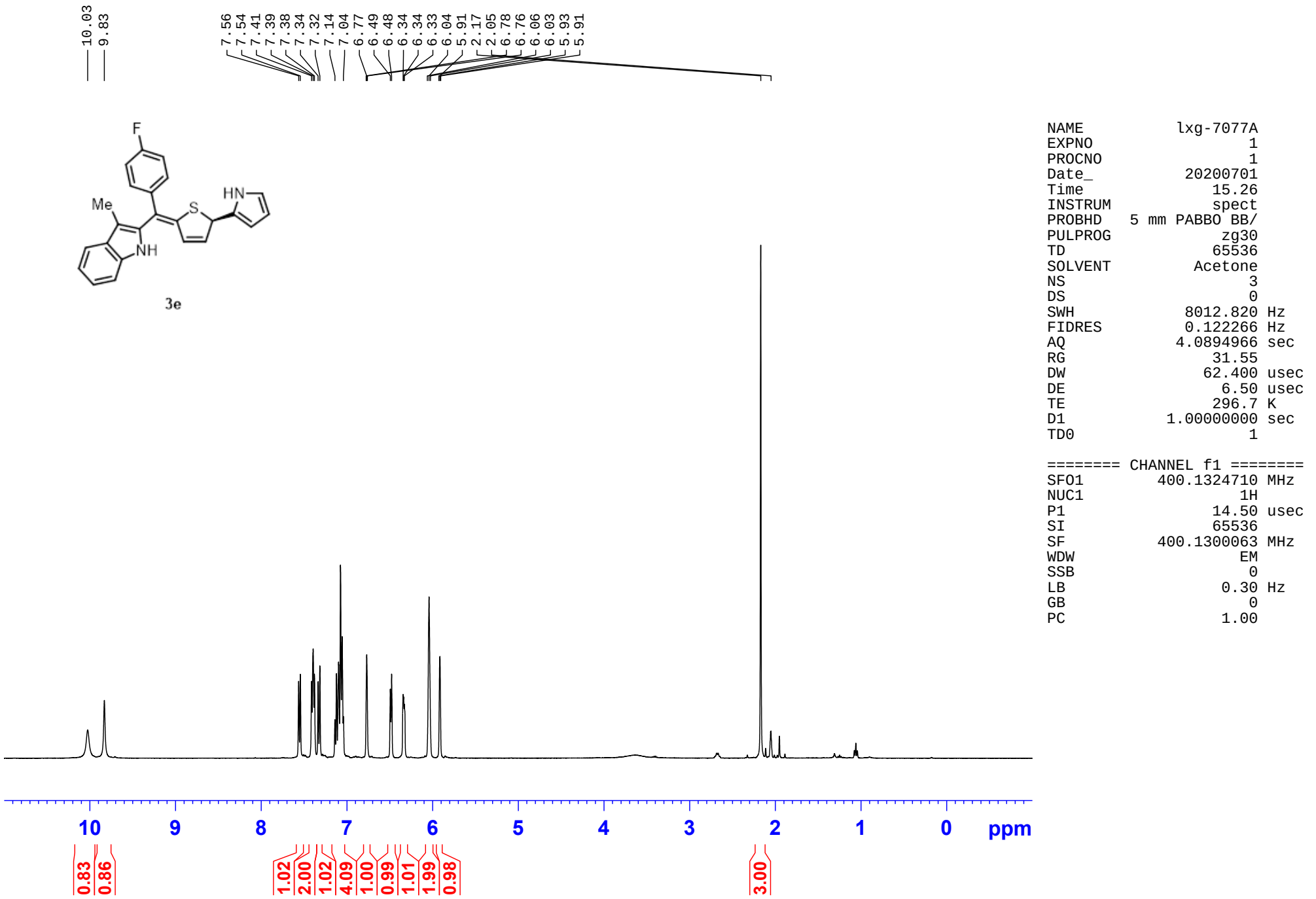


Supplementary Figure 68. ^{1}H NMR spectrum of **3d**

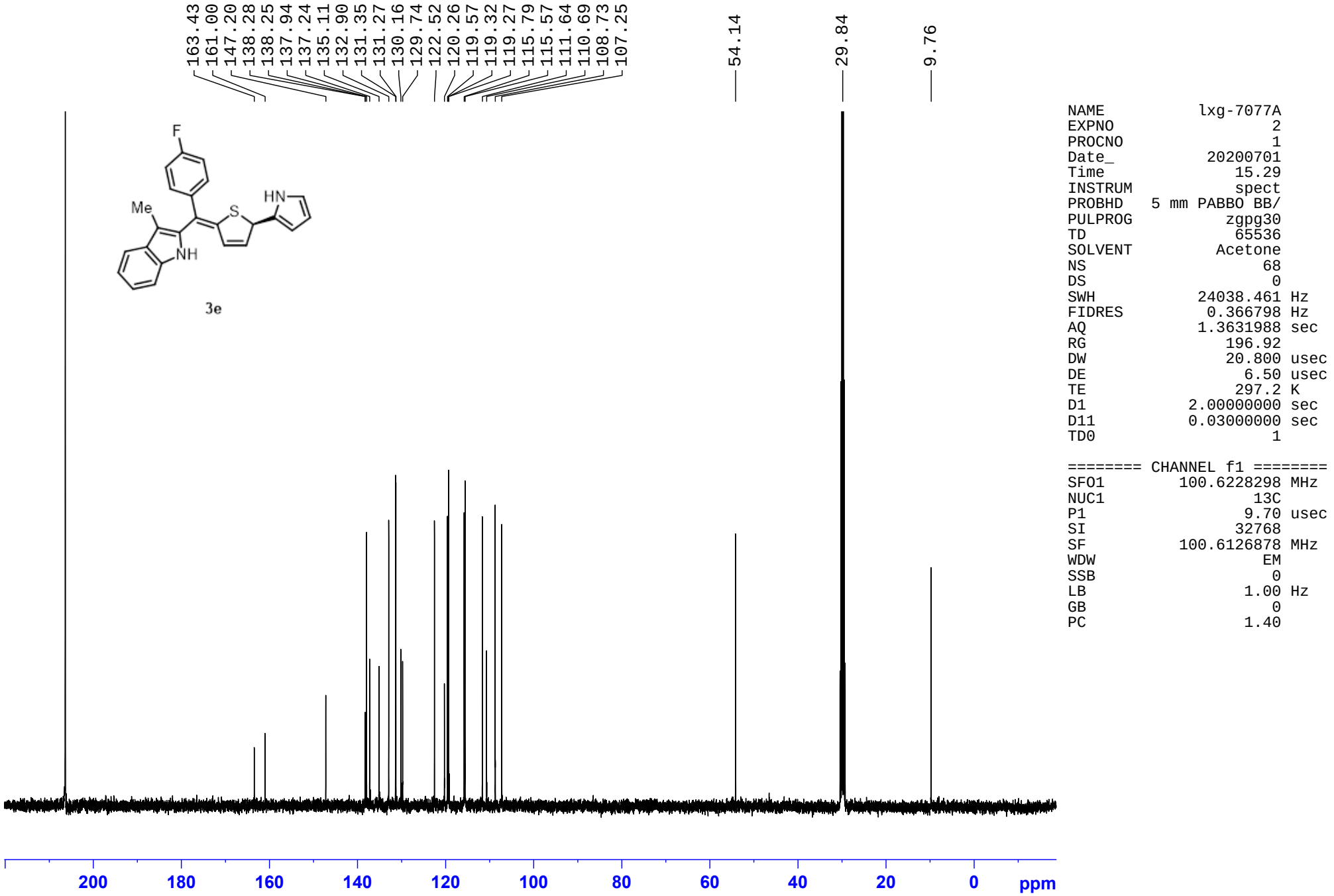


NAME	lxg-4112C
EXPNO	2
PROCNO	1
Date_	20190511
Time	2.09
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	56
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	299.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6126893 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

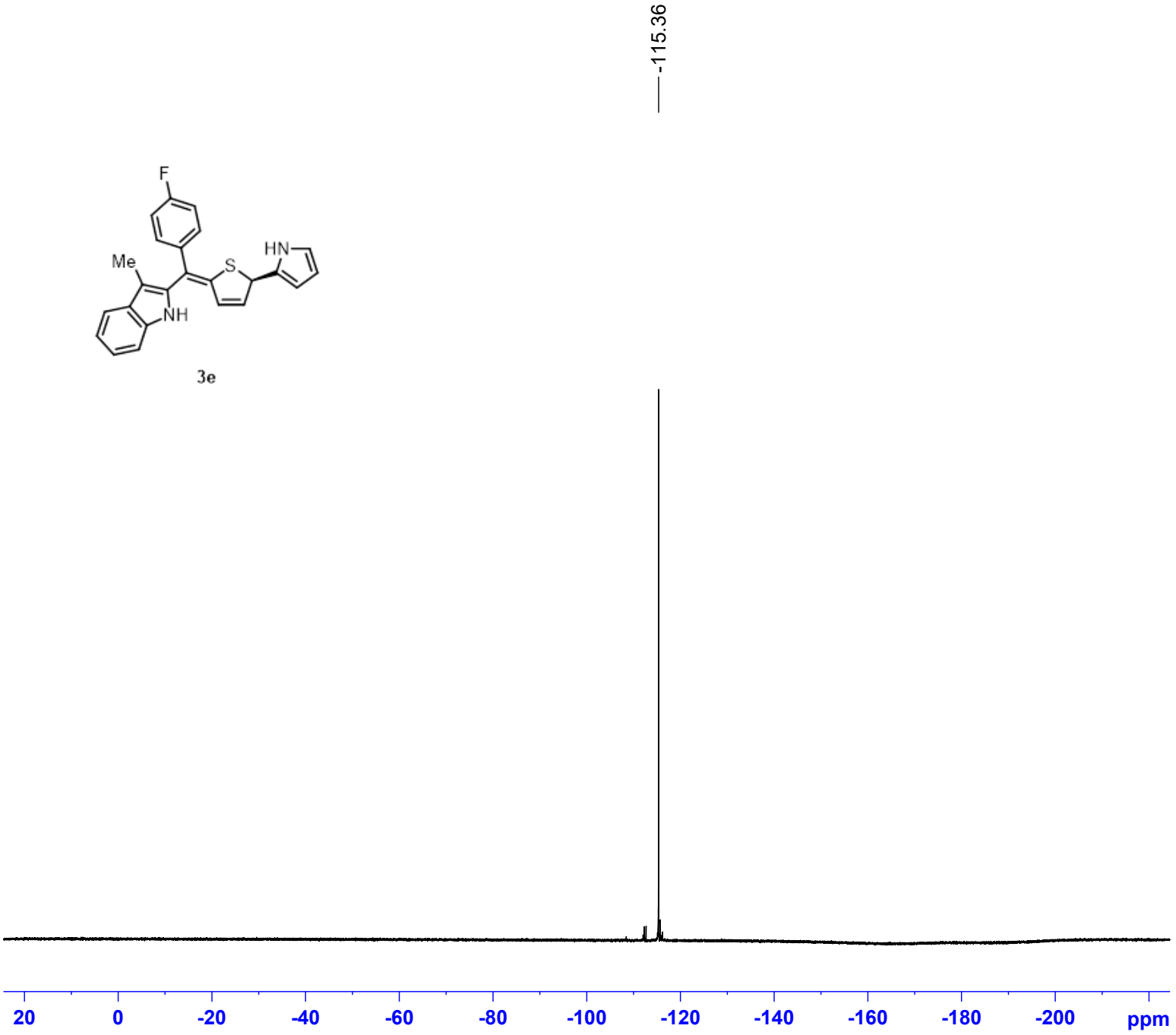
Supplementary Figure 69. ^{13}C NMR spectrum of **3d**



Supplementary Figure 70. ^{1}H NMR spectrum of **3e**



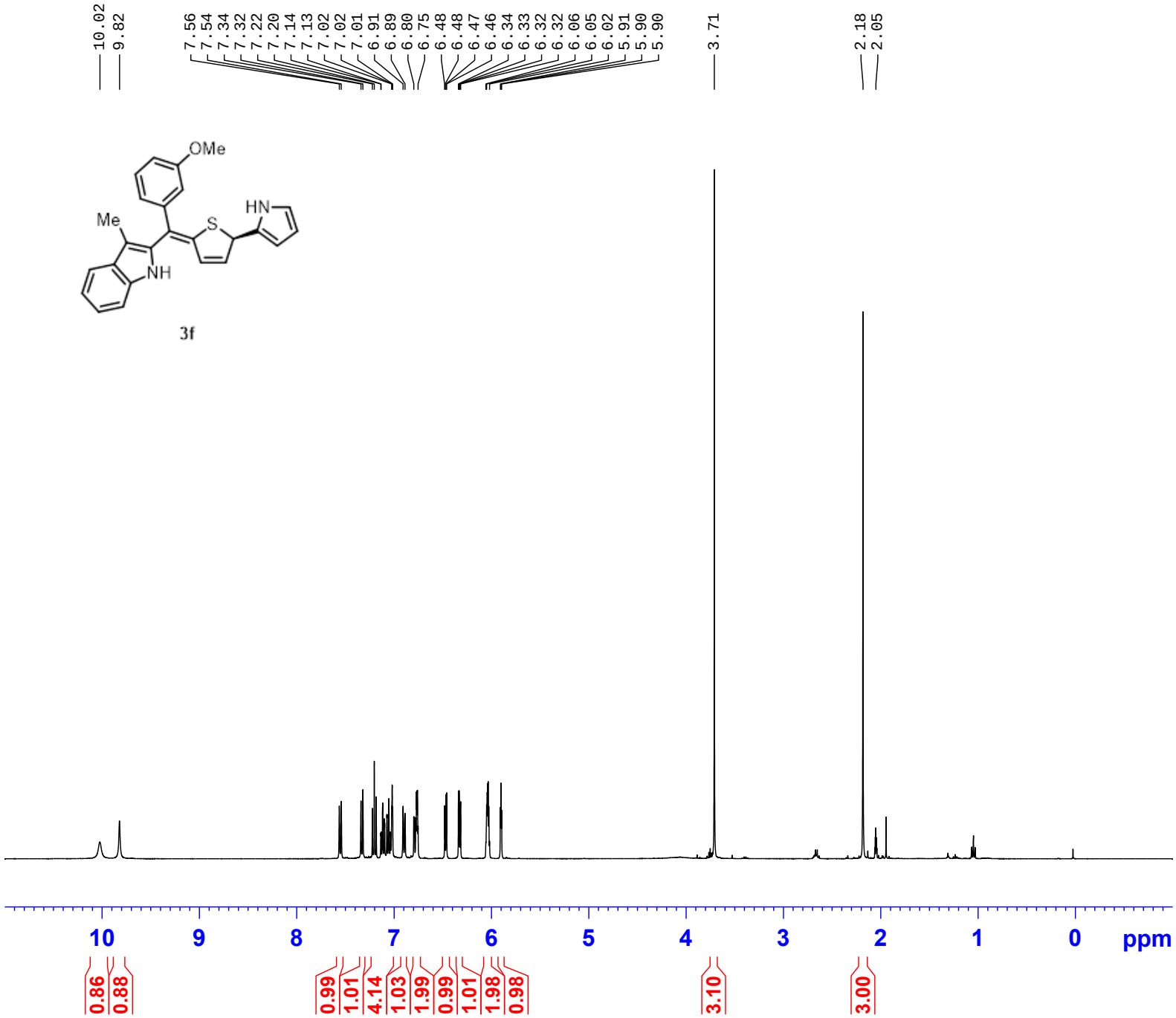
Supplementary Figure 71. ^{13}C NMR spectrum of **3e**



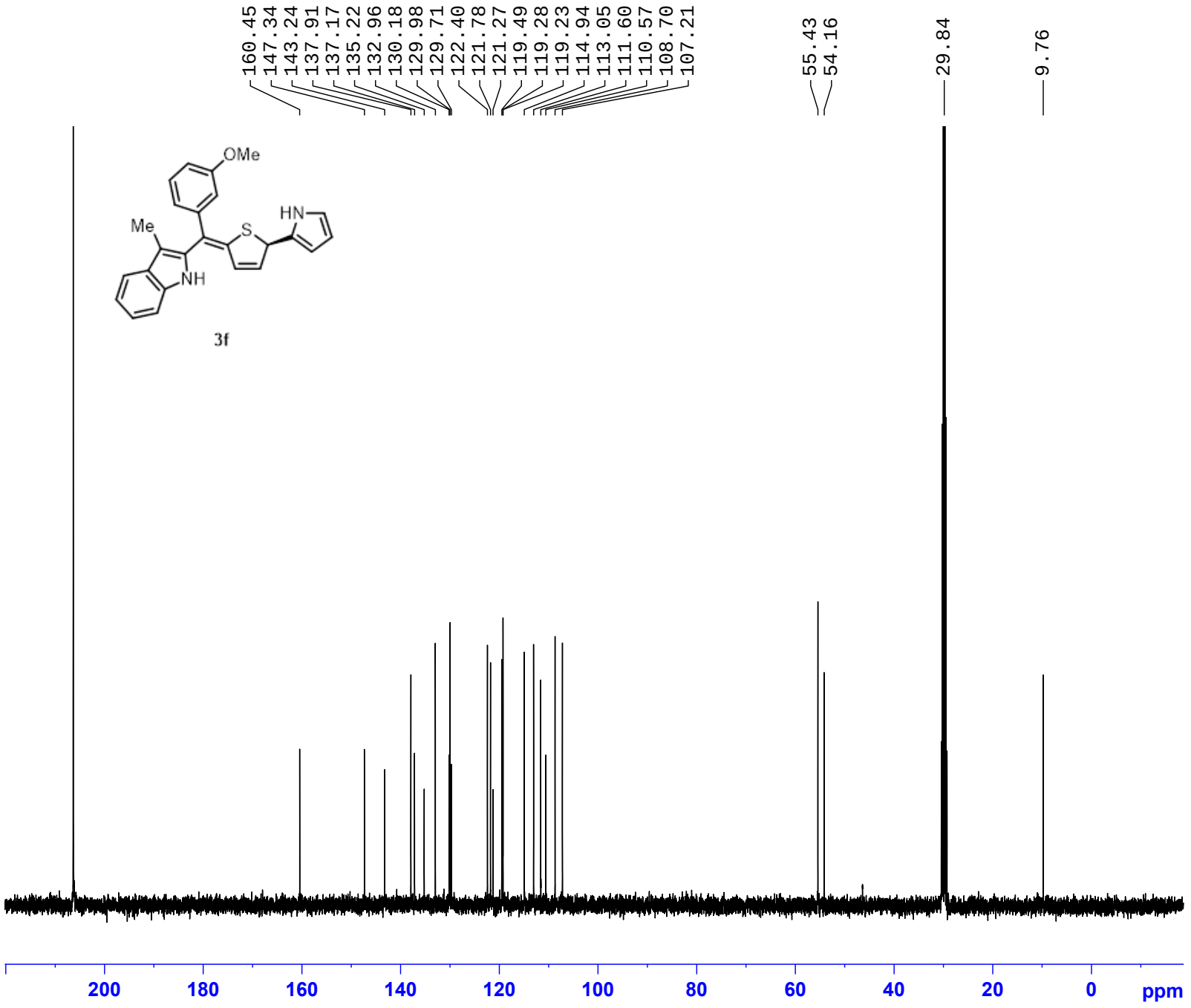

```
NAME           lxg-7077A
EXPNO                 11
PROCNO                 1
Date_           20200724
Time               15.02
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT          Acetone
NS                    13
DS                     0
SWH            93750.000 Hz
FIDRES          1.430511 Hz
AQ             0.3495753 sec
RG                196.92
DW                5.333 usec
DE                6.50 usec
TE                296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         376.4607162 MHz
NUC1                 19F
P1                14.70 usec
SI                32768
SF           376.4983660 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Supplementary Figure 72. ^{19}F NMR spectrum of **3e**



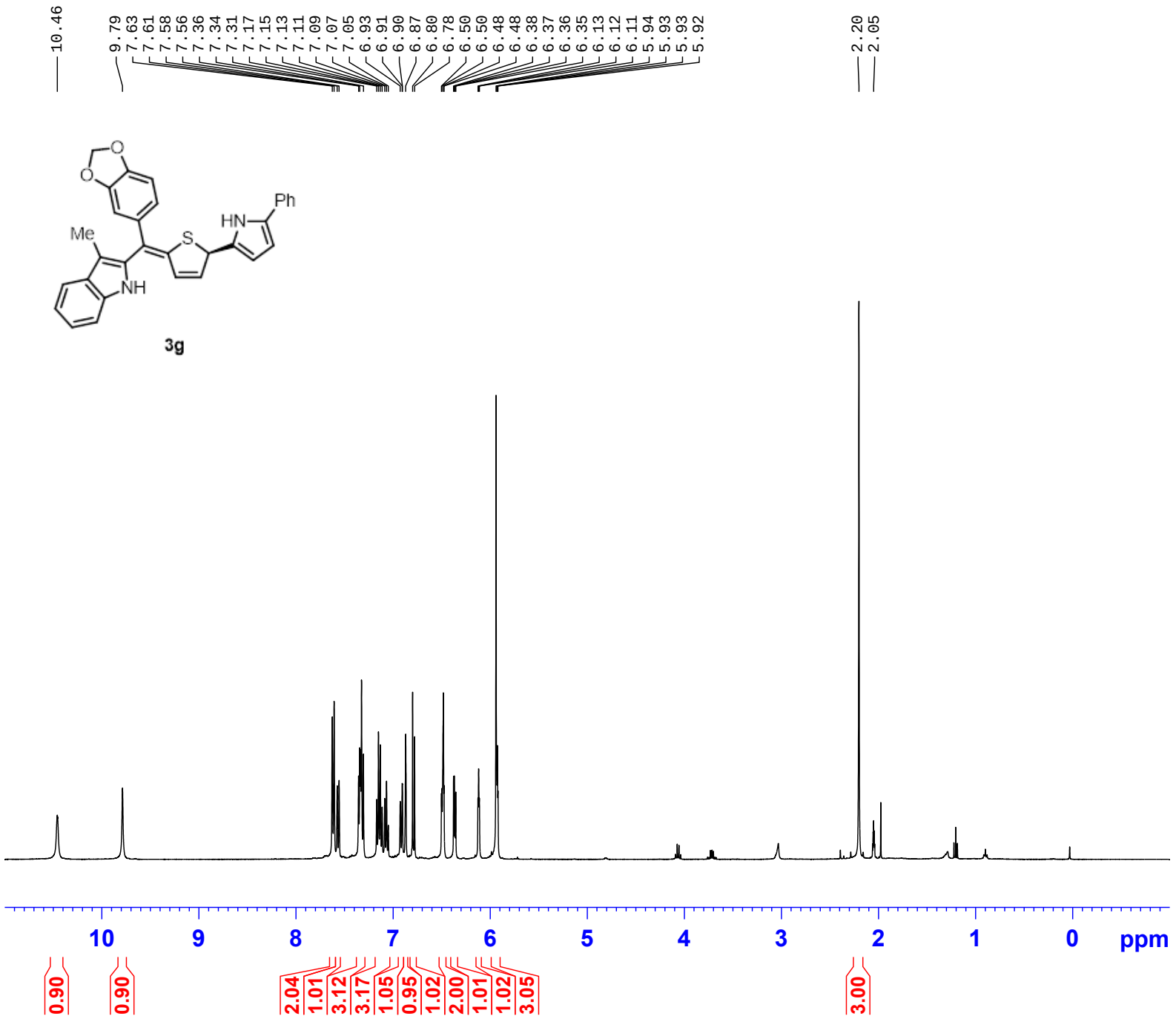
Supplementary Figure 73. ^{1}H NMR spectrum of **3f**



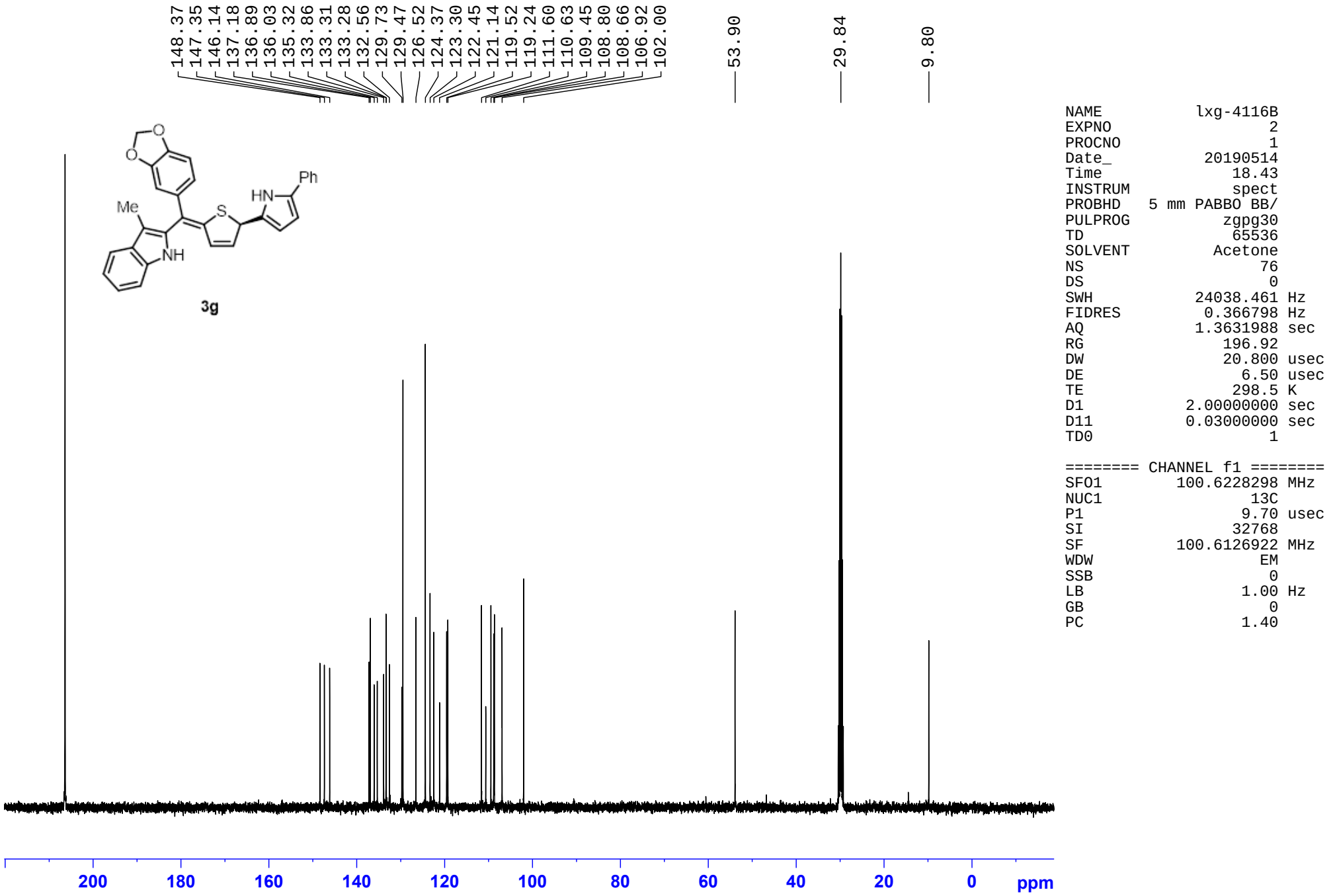

```
NAME            lxg-7079A
EXPNO                   2
PROCNO                  1
Date_            20200703
Time                20.05
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT           Acetone
NS                      23
DS                       0
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                  196.92
DW                  20.800 usec
DE                   6.50 usec
TE                  297.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                  13C
P1                   9.70 usec
SI                  32768
SF            100.6126893 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

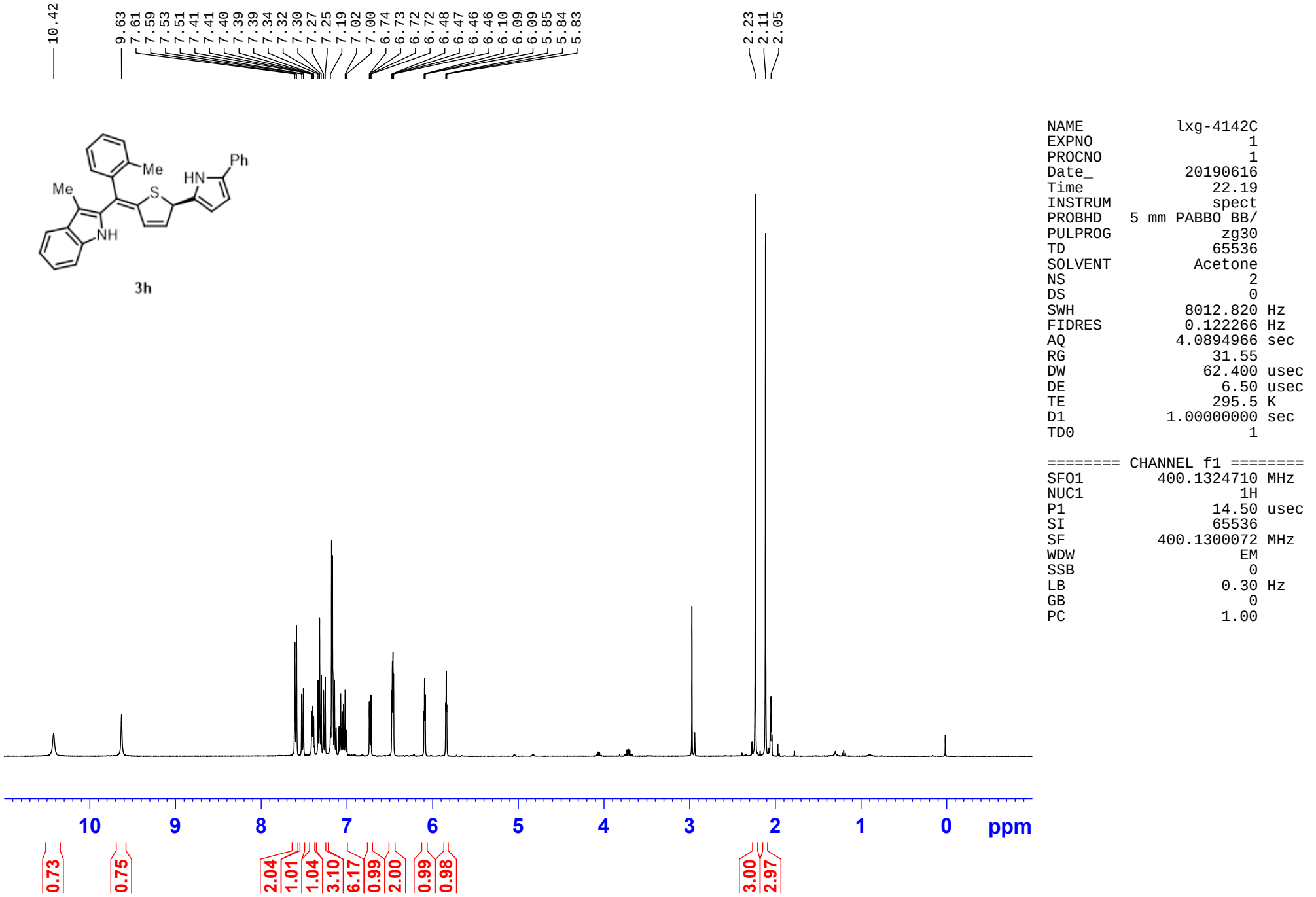

Supplementary Figure 74. ^{13}C NMR spectrum of **3f**



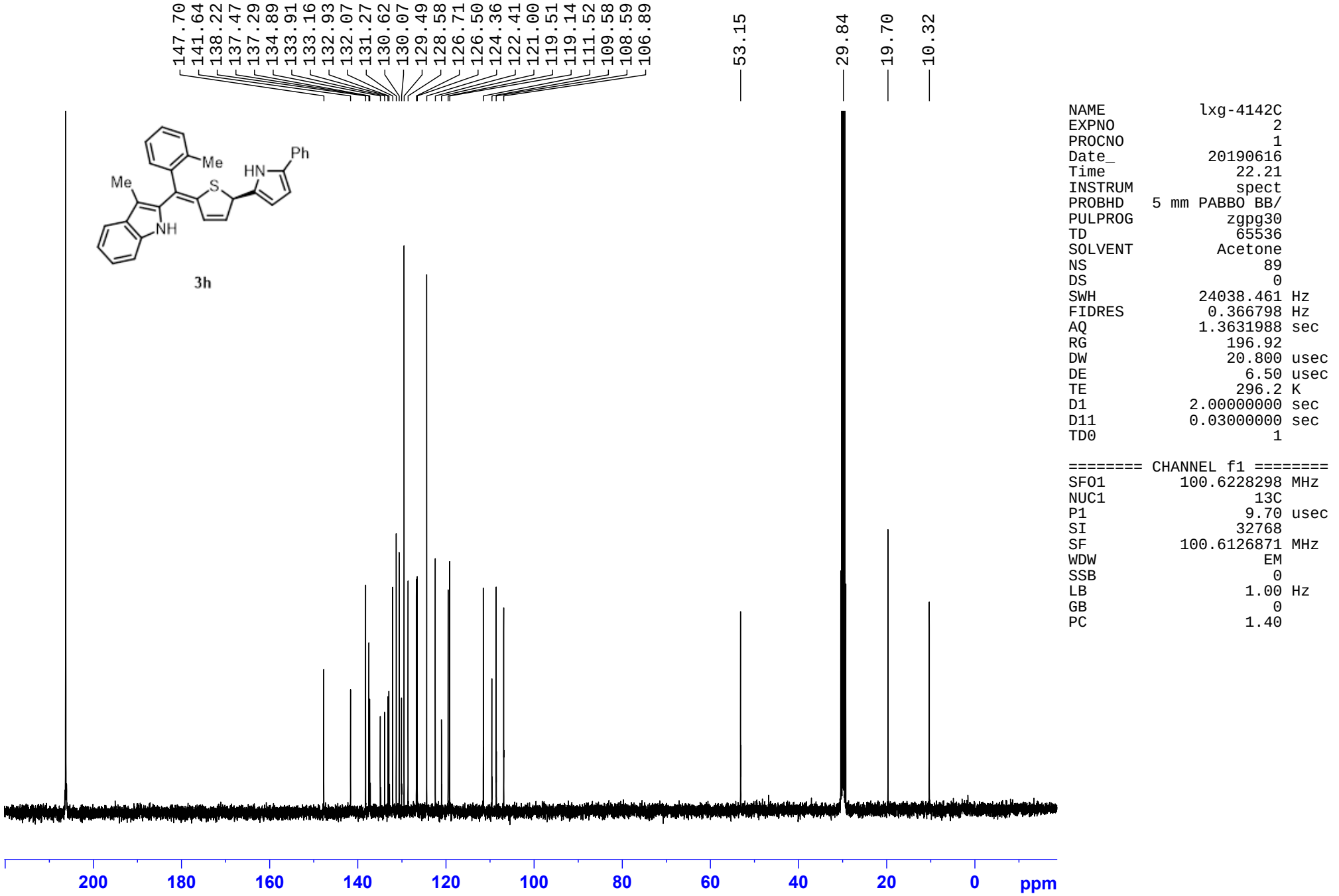
Supplementary Figure 75. ^{1}H NMR spectrum of **3g**



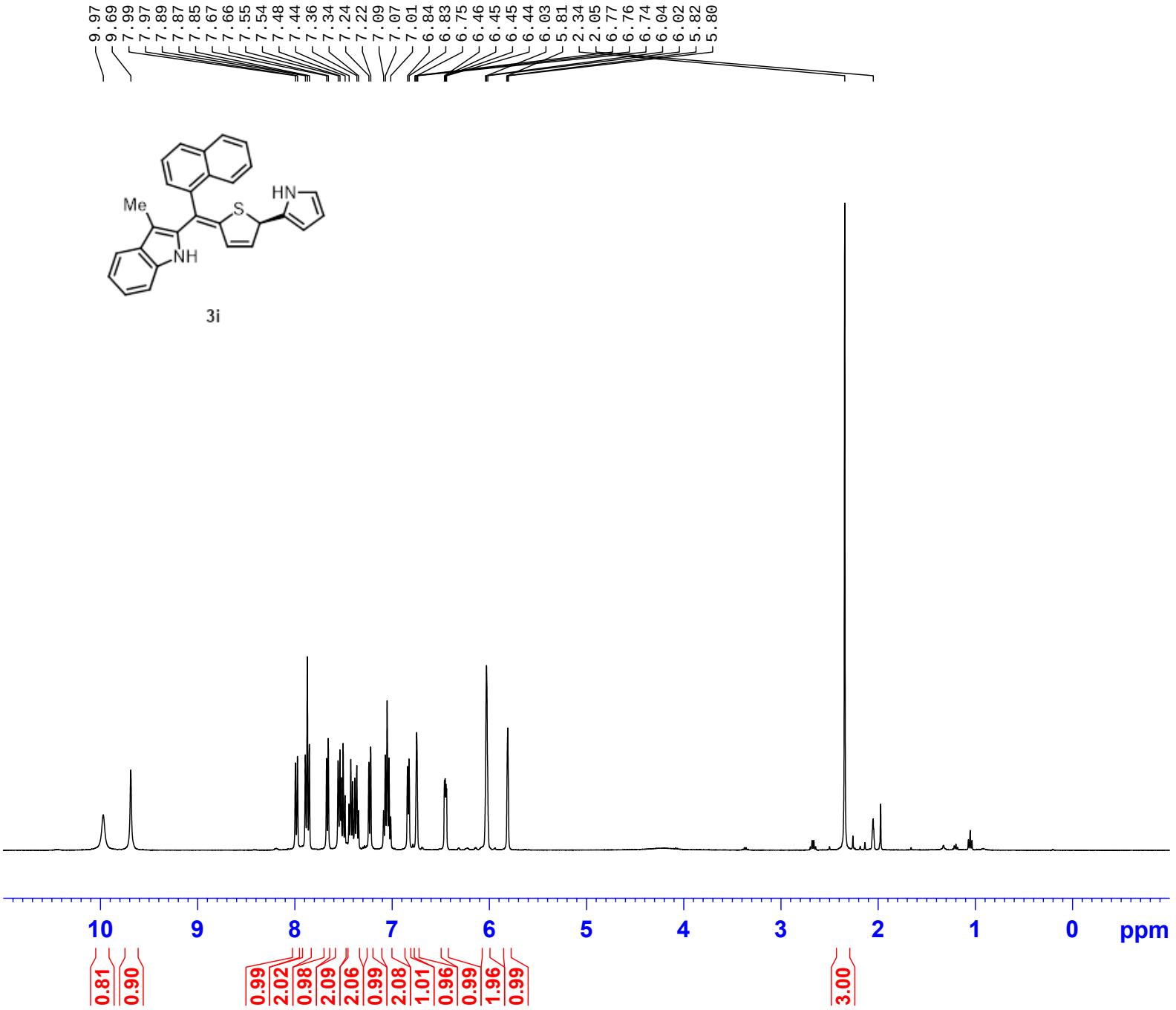
Supplementary Figure 76. ^{13}C NMR spectrum of **3g**



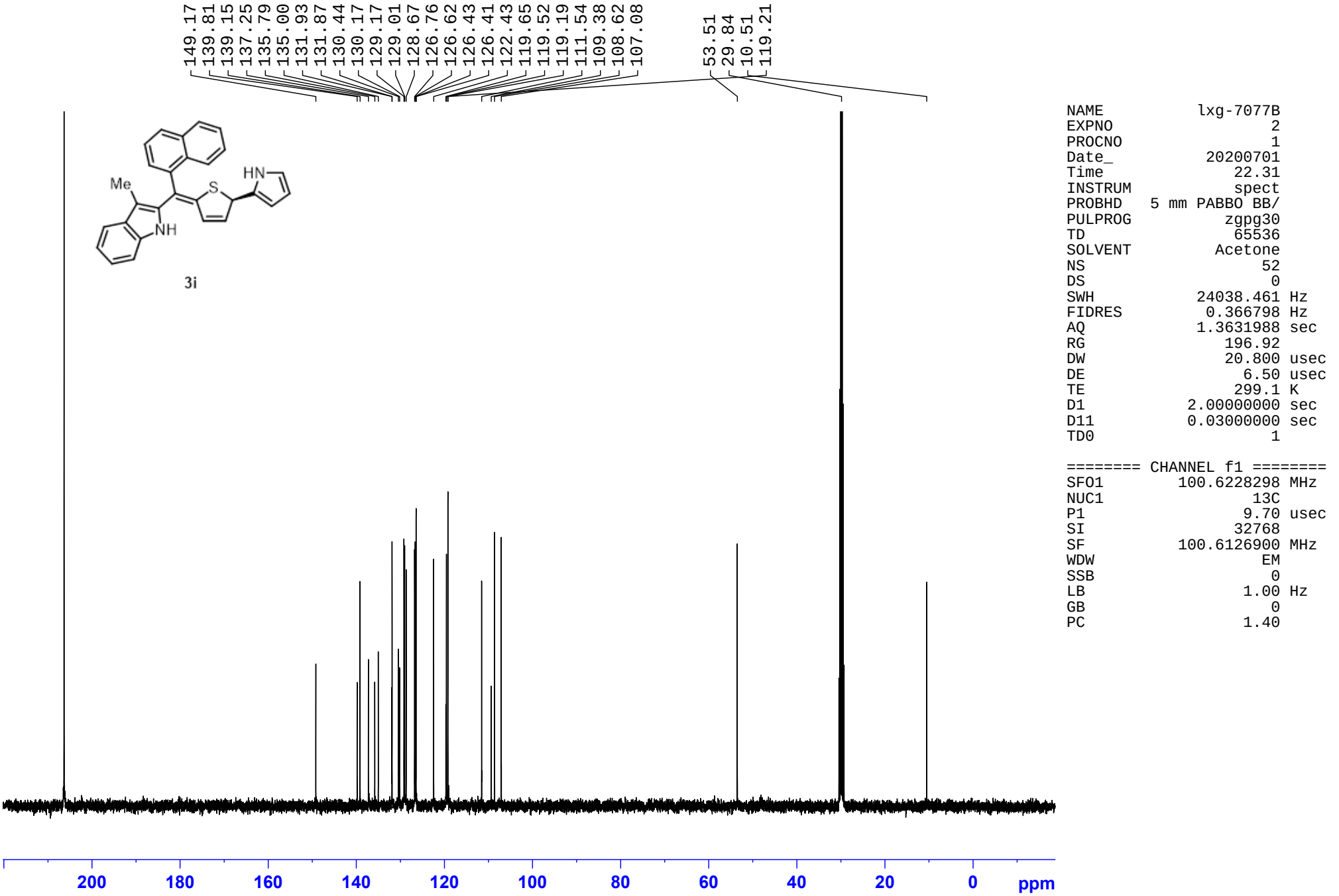
Supplementary Figure 77. ^{1}H NMR spectrum of **3h**



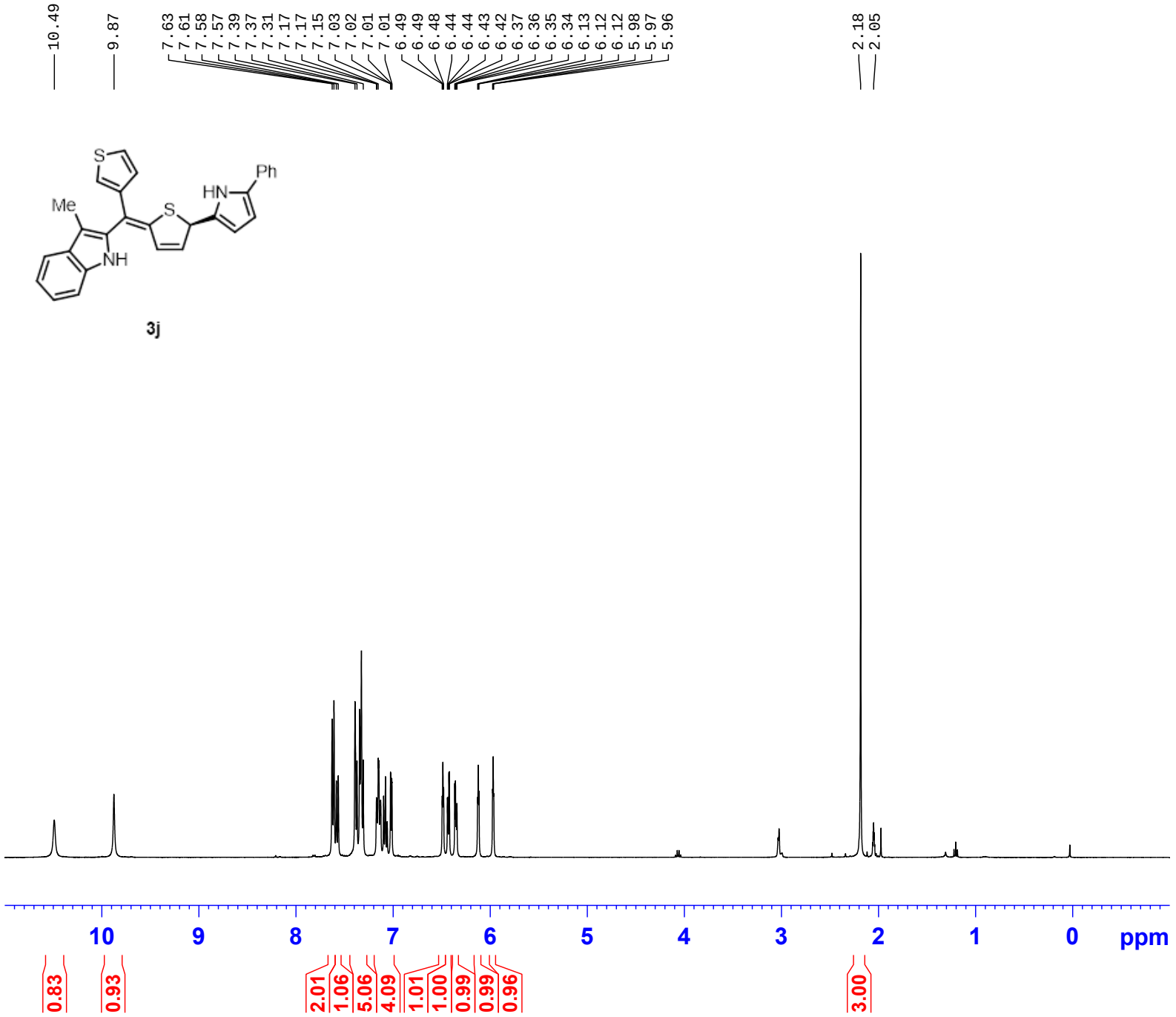
Supplementary Figure 78. ^{13}C NMR spectrum of **3h**



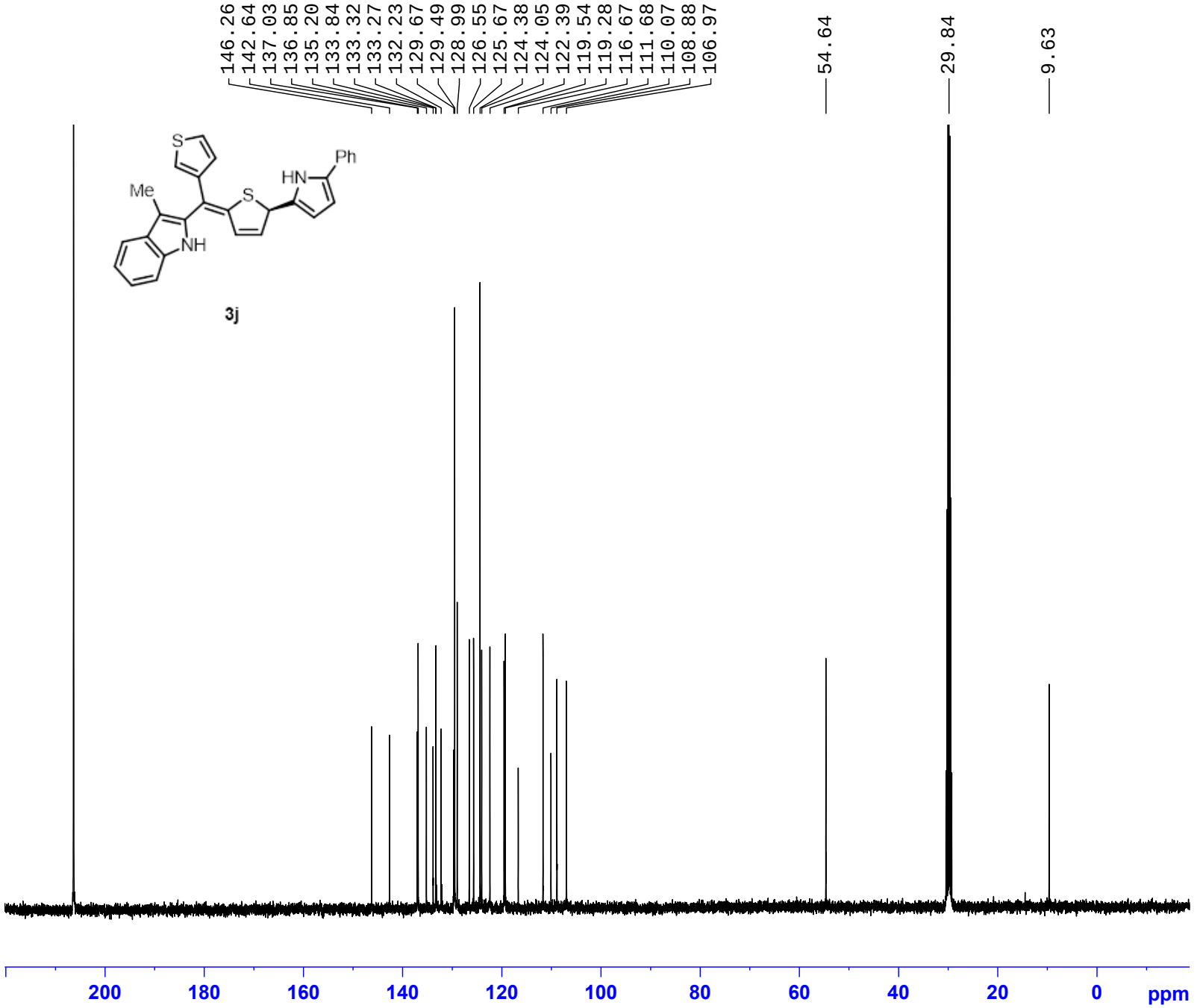
Supplementary Figure 79. ^{1}H NMR spectrum of **3l**



Supplementary Figure 80. ^{13}C NMR spectrum of **3l**

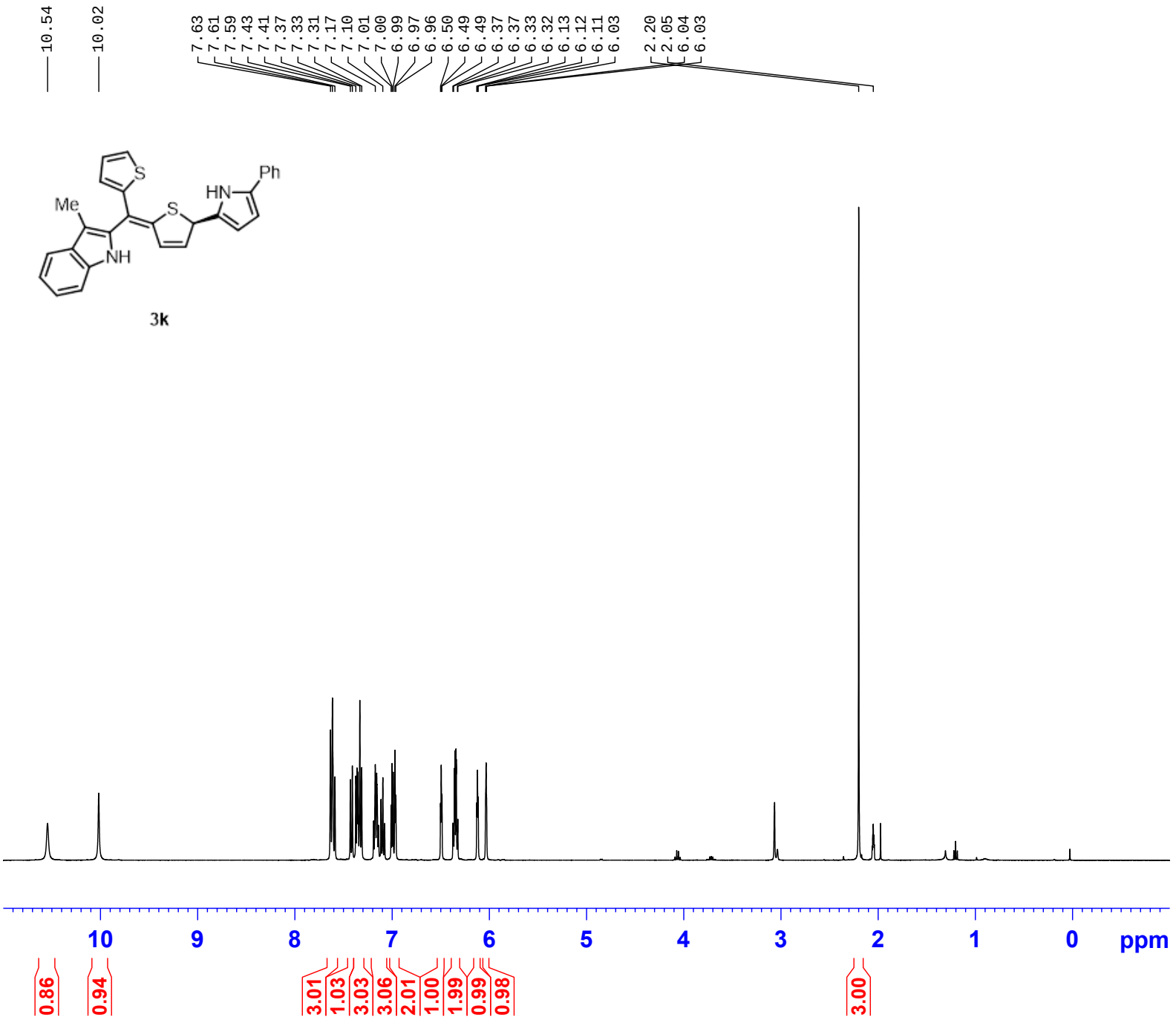


Supplementary Figure 81. ^{1}H NMR spectrum of **3j**

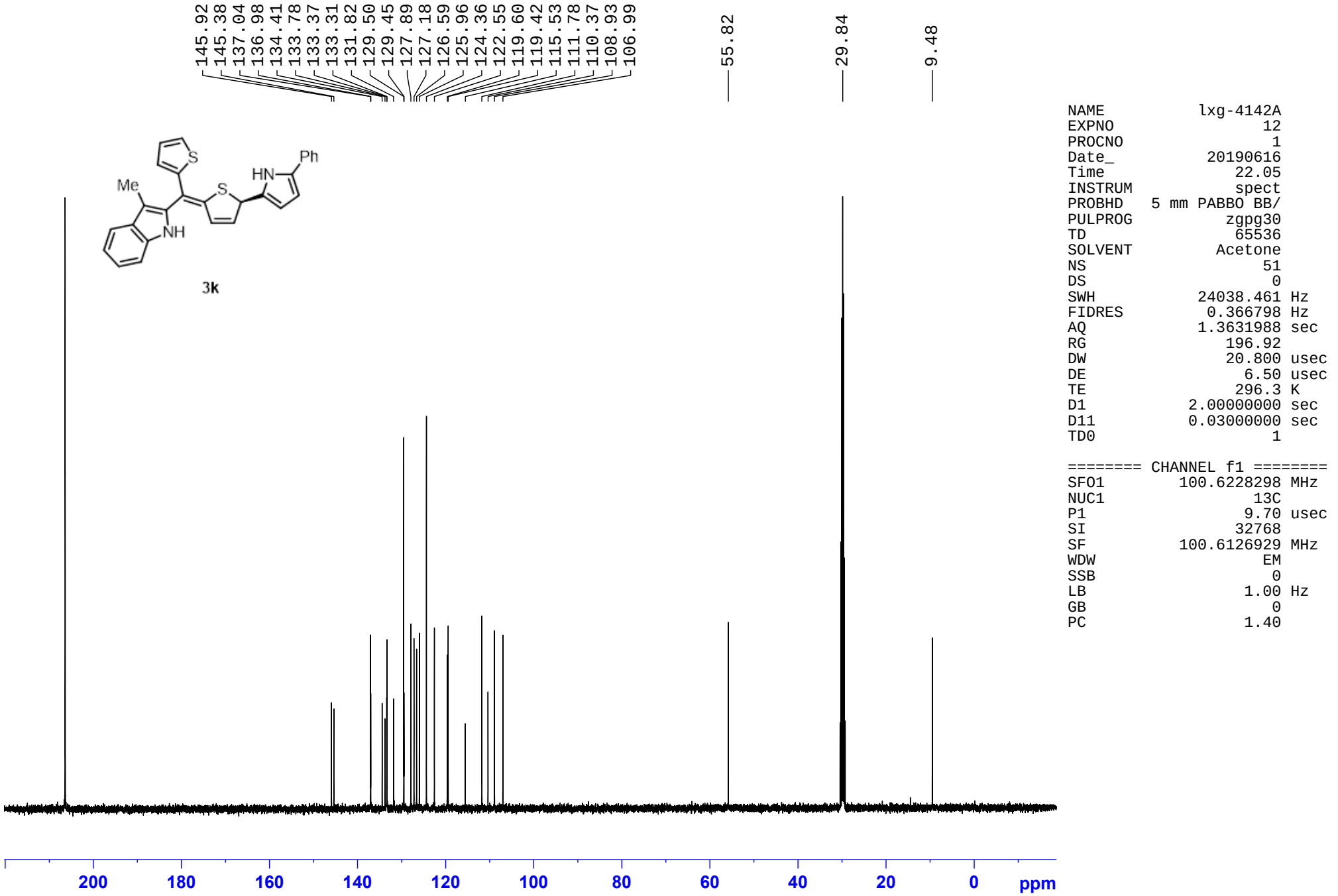


NAME	lxg-4116C
EXPNO	2
PROCNO	1
Date_	20190514
Time	18.52
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	107
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	298.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6126915 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

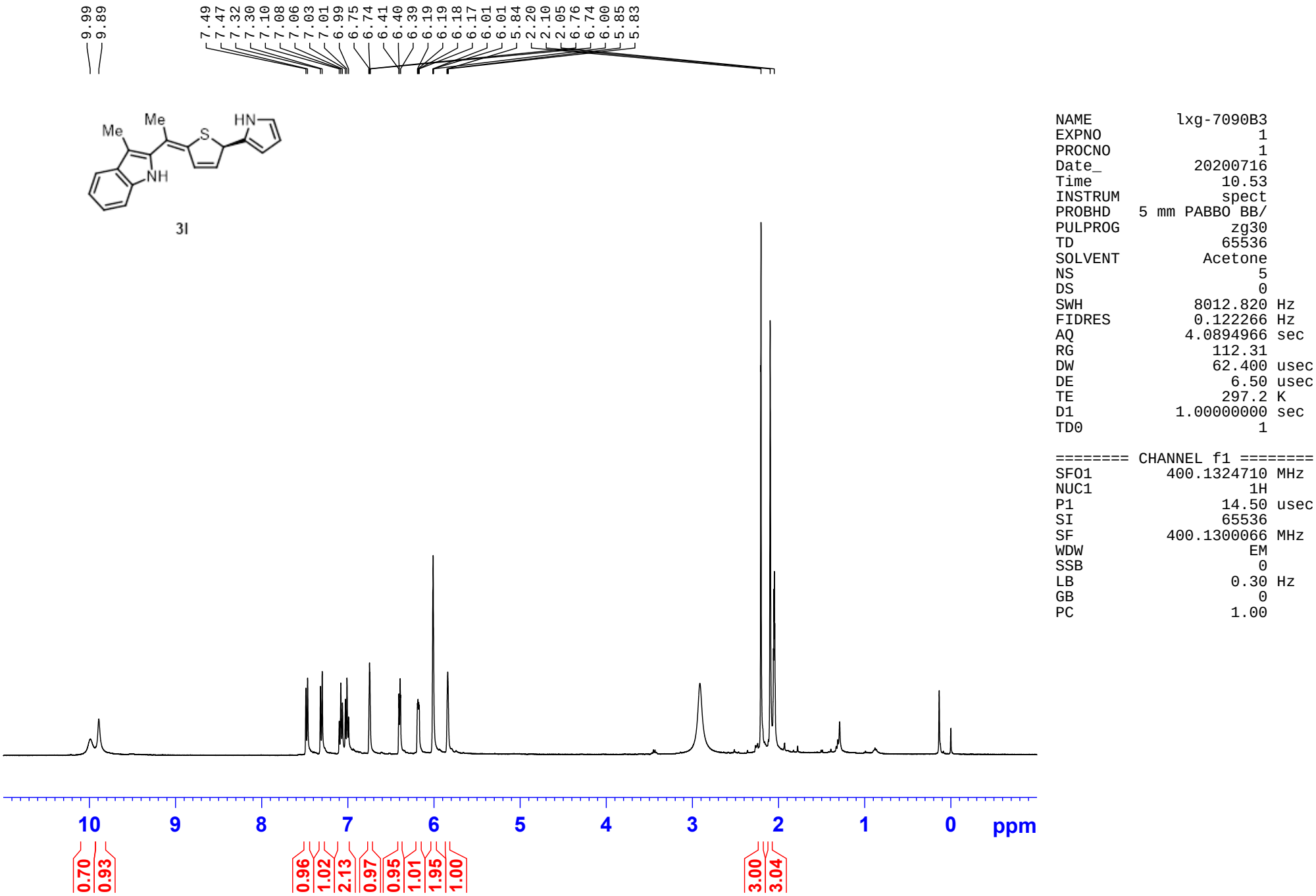
Supplementary Figure 82. ^{13}C NMR spectrum of **3j**



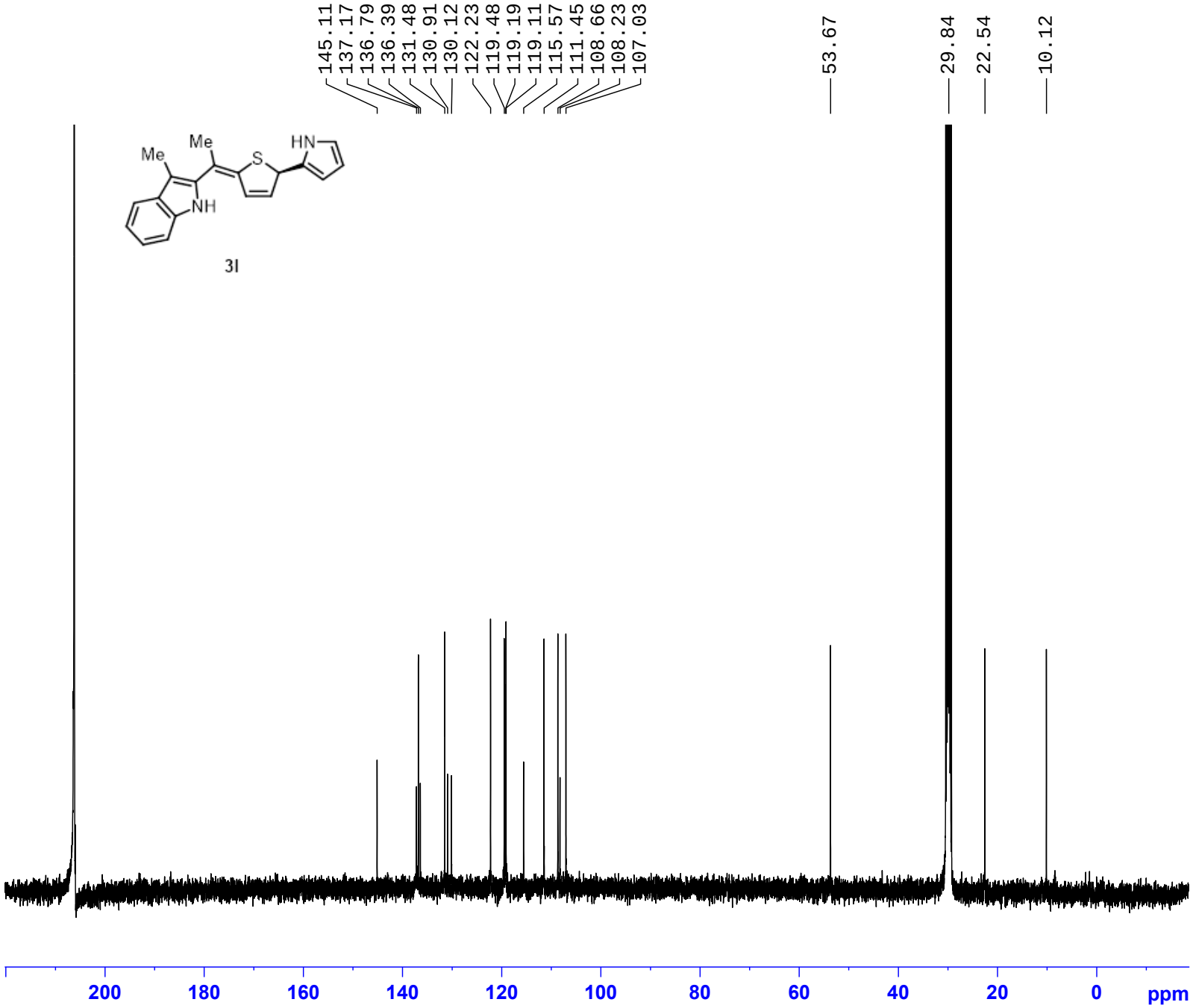
Supplementary Figure 83. ^{1}H NMR spectrum of **3k**



Supplementary Figure 84. ^{13}C NMR spectrum of **3k**



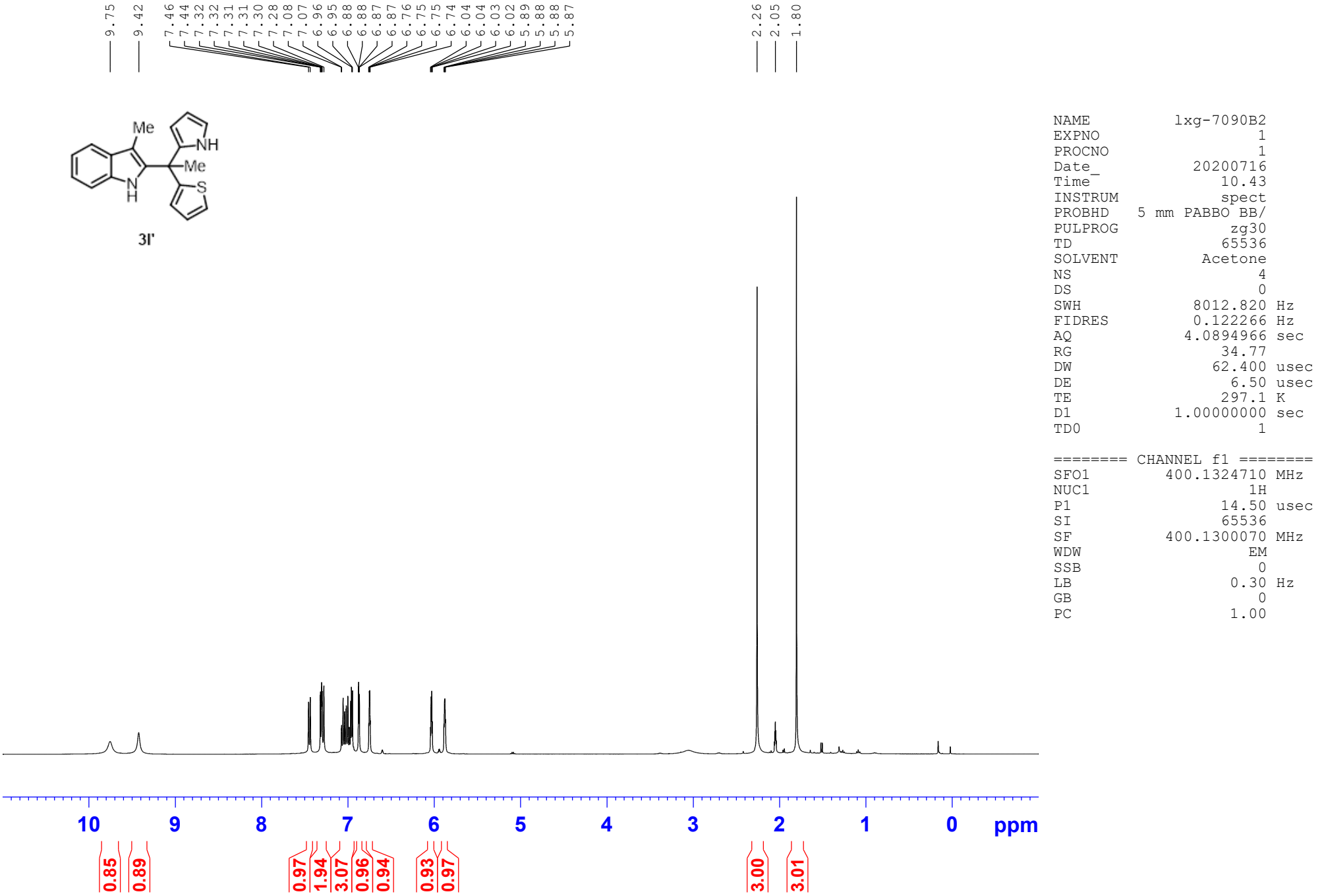
Supplementary Figure 85. ^{1}H NMR spectrum of **3l**



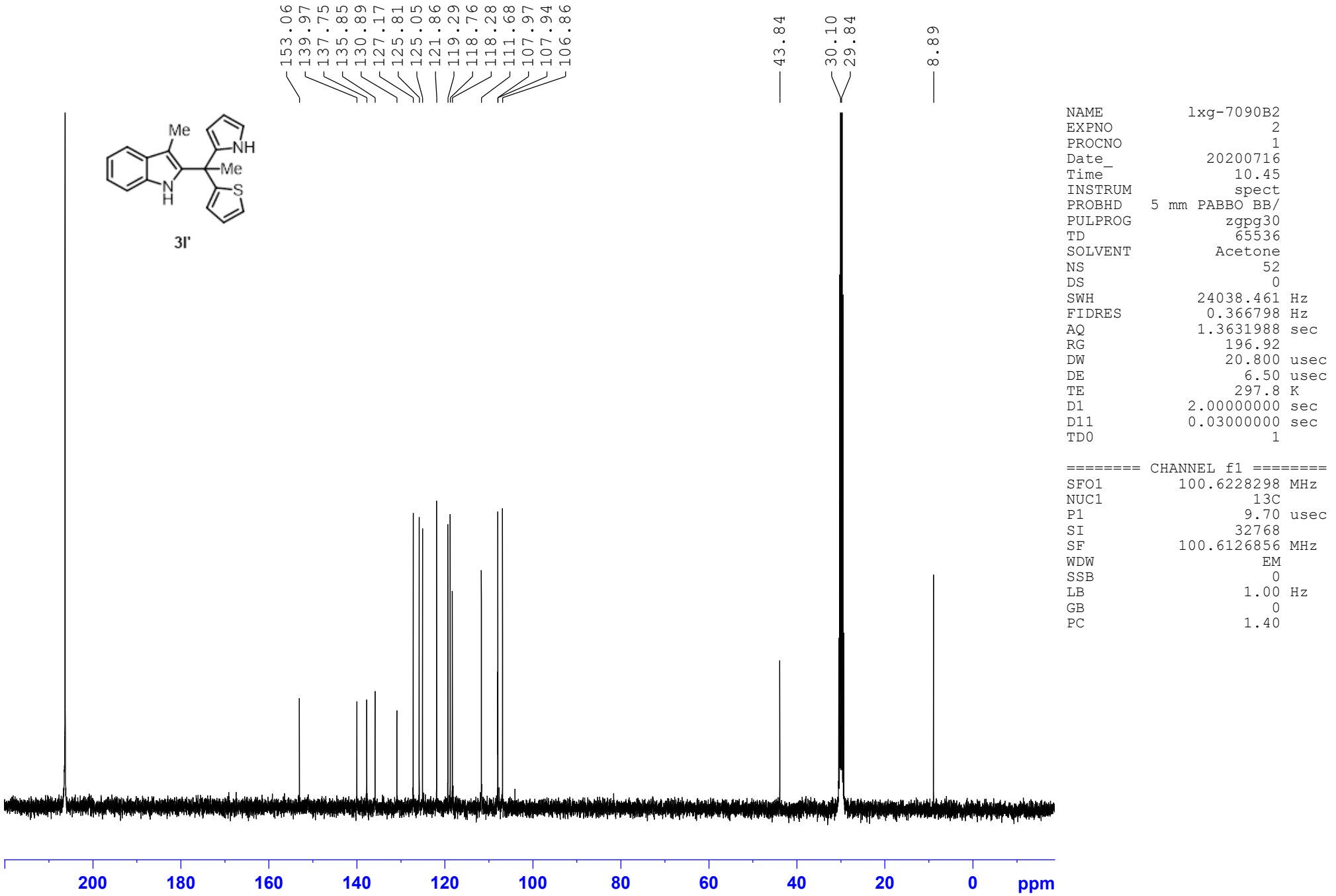
NAME lxg-7090B3
EXPNO 2
PROCNO 1
Date_ 20200716
Time 10.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 895
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 196.92
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 9.70 usec
SI 32768
SF 100.6126790 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Supplementary Figure 86. ^{13}C NMR spectrum of **3l**



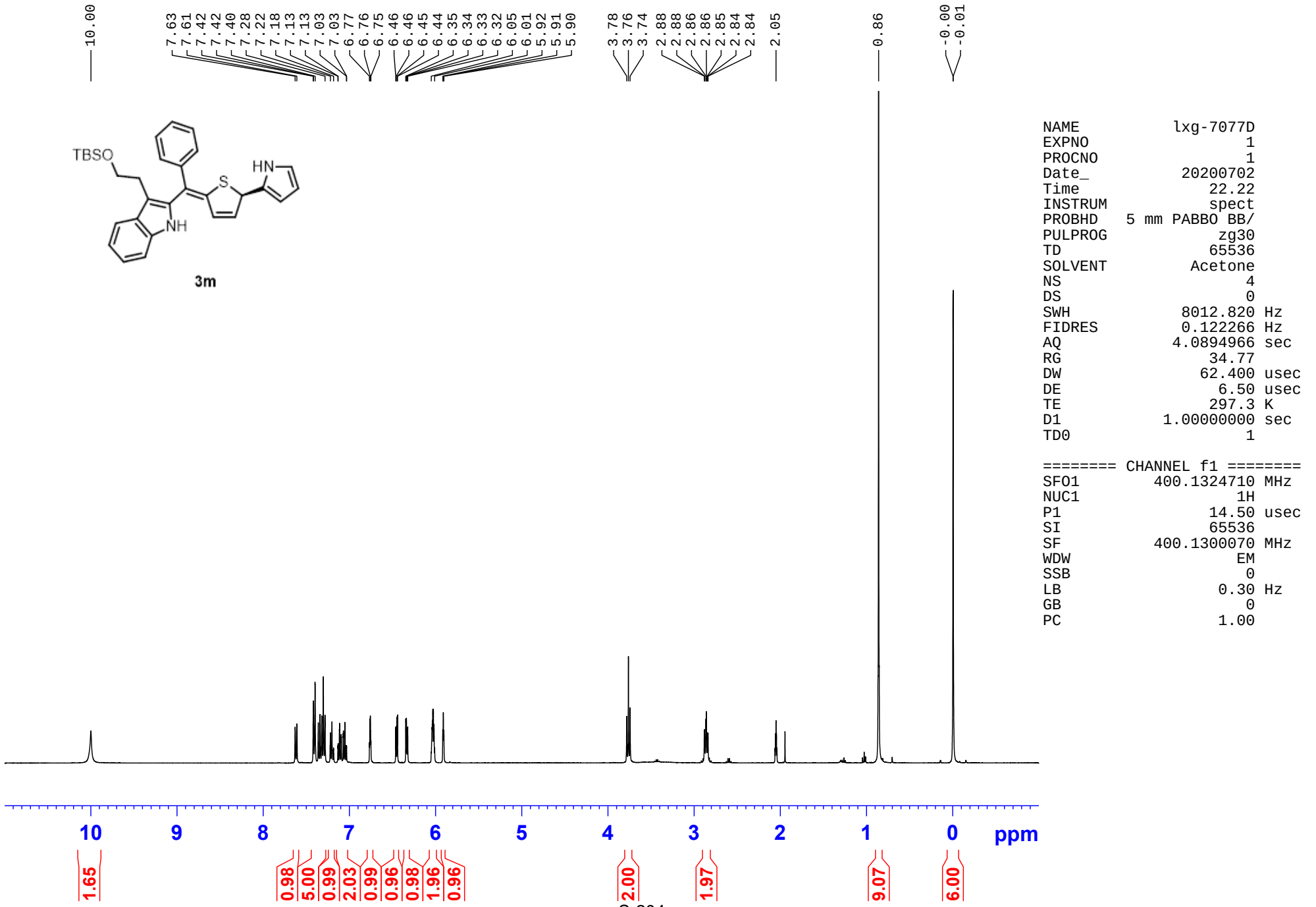
Supplementary Figure 87. ^{1}H NMR spectrum of **3l'**



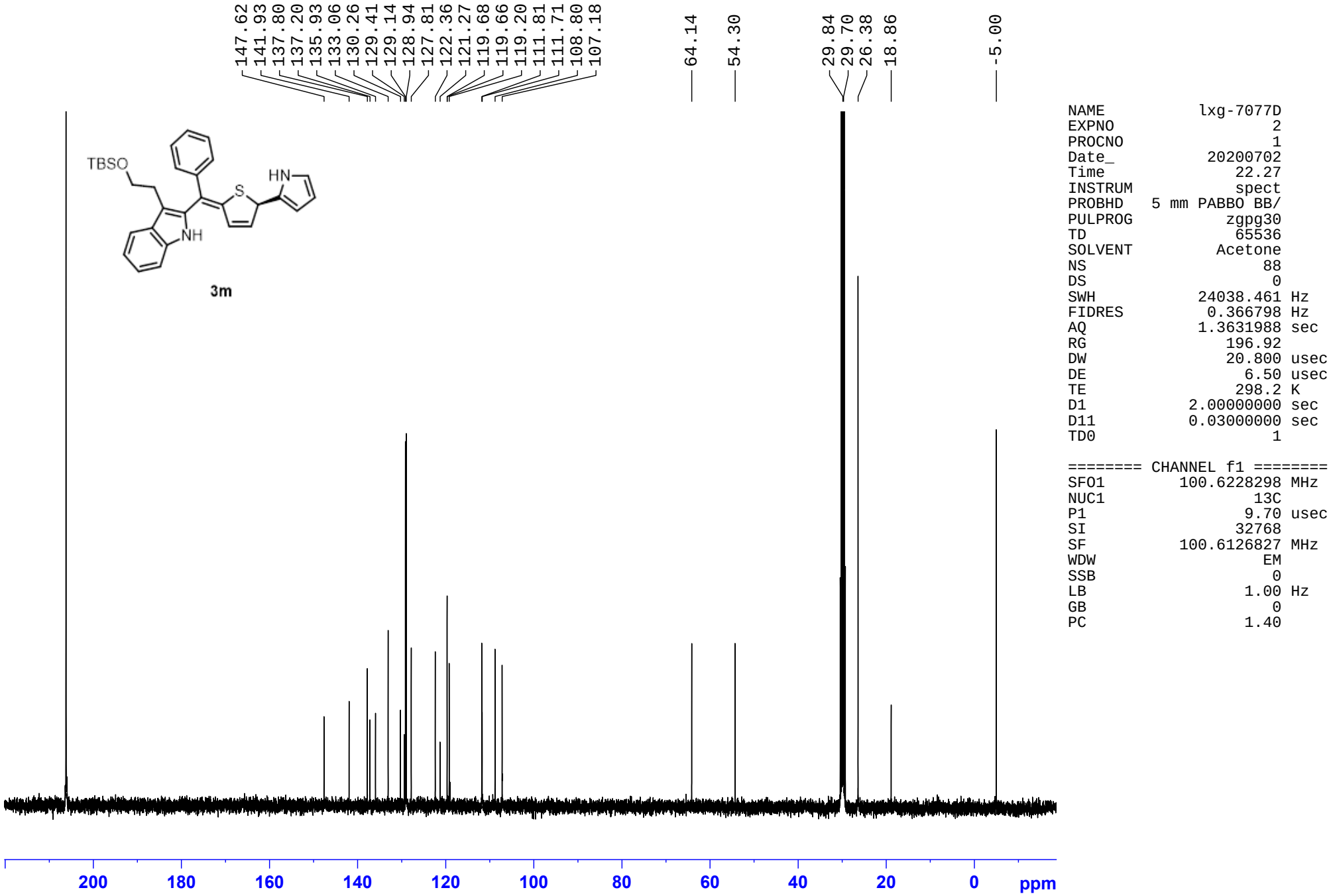

```
NAME          lxg-7090B2
EXPNO                  2
PROCNO                 1
Date_           20200716
Time               10.45
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                    52
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE                297.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                  13C
P1                 9.70 usec
SI                32768
SF          100.6126856 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

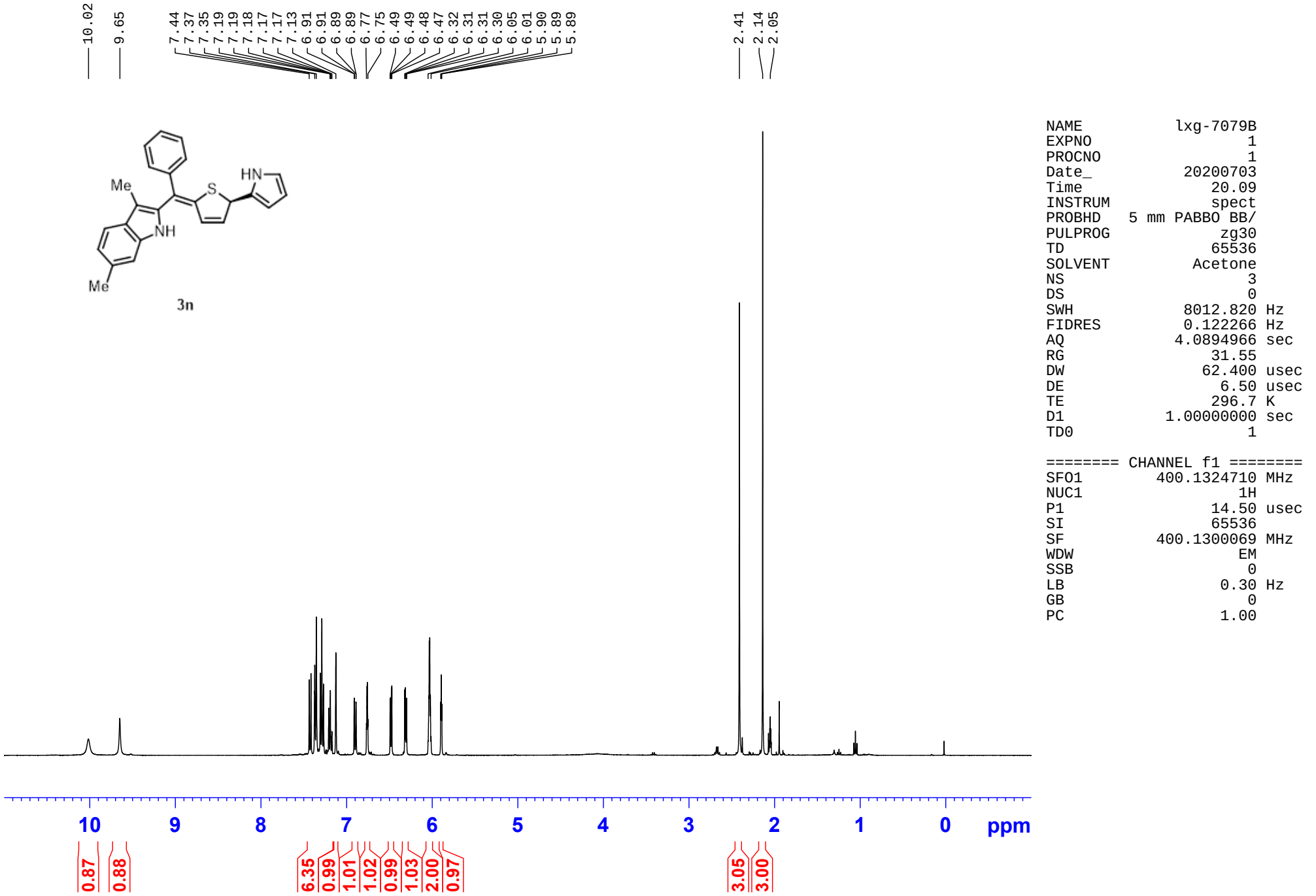

Supplementary Figure 88. ^{13}C NMR spectrum of **3l'**



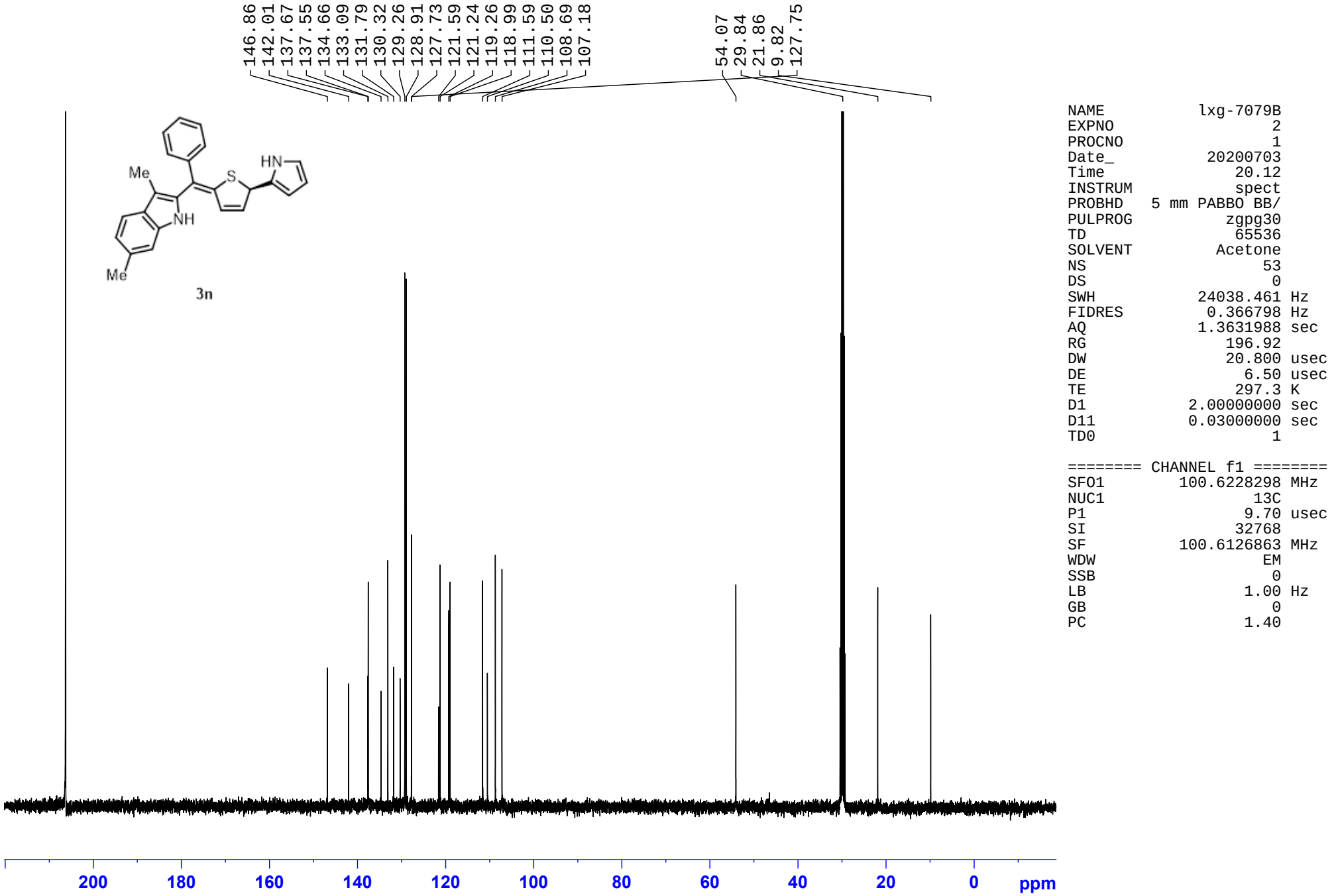
Supplementary Figure 89. ^{1}H NMR spectrum of **3m**



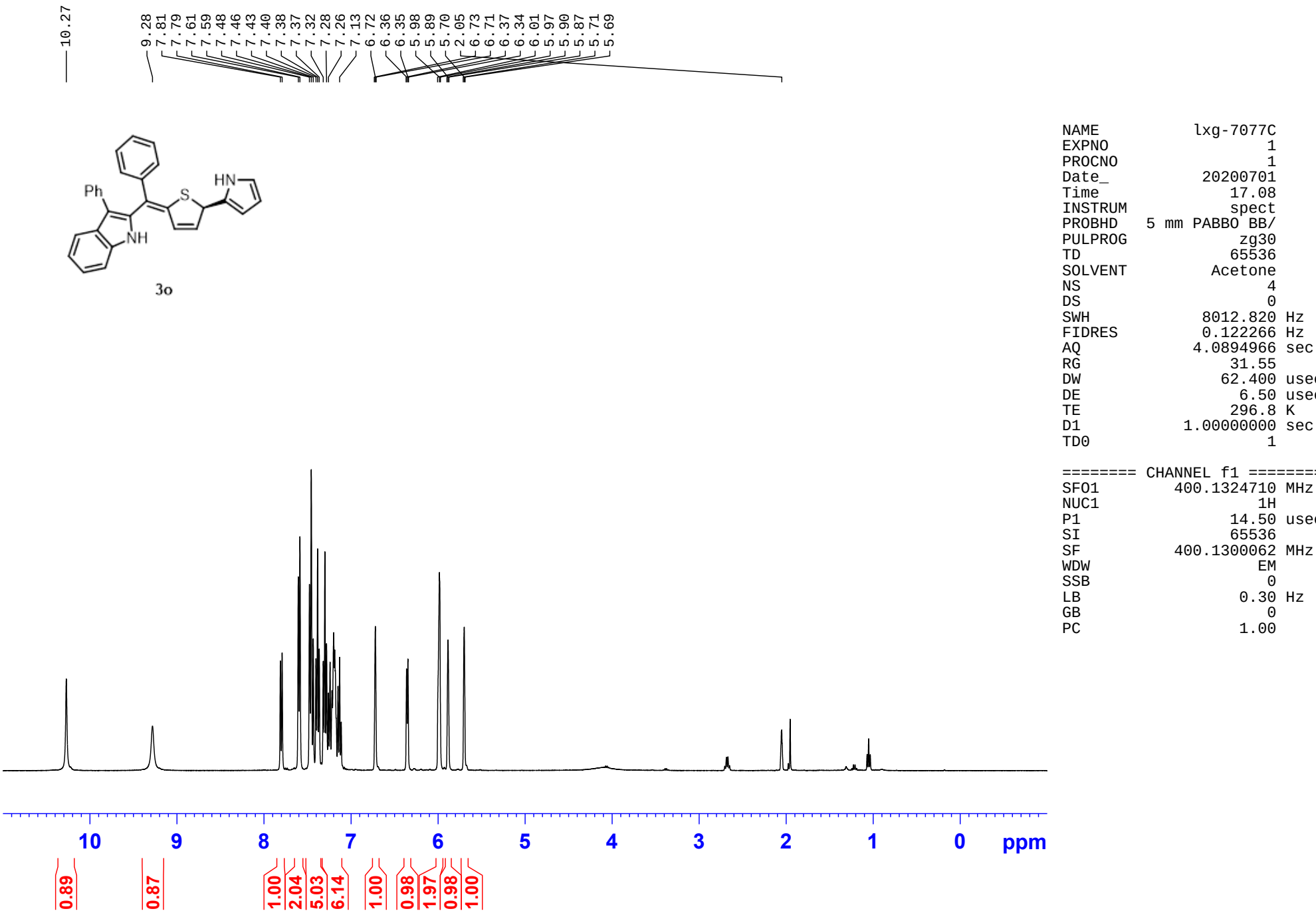
Supplementary Figure 90. ^{13}C NMR spectrum of **3m**



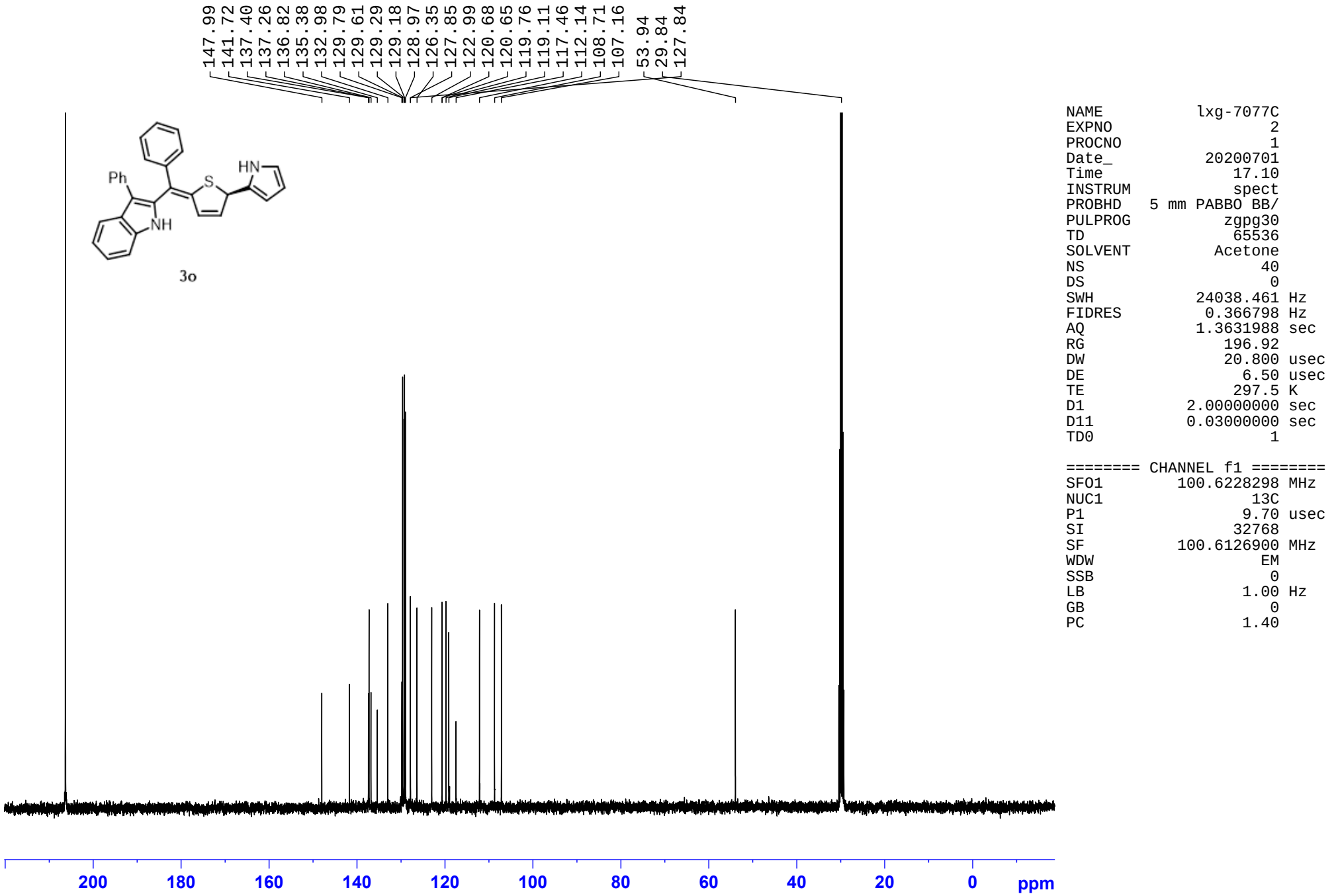
Supplementary Figure 91. ^{1}H NMR spectrum of **3n**



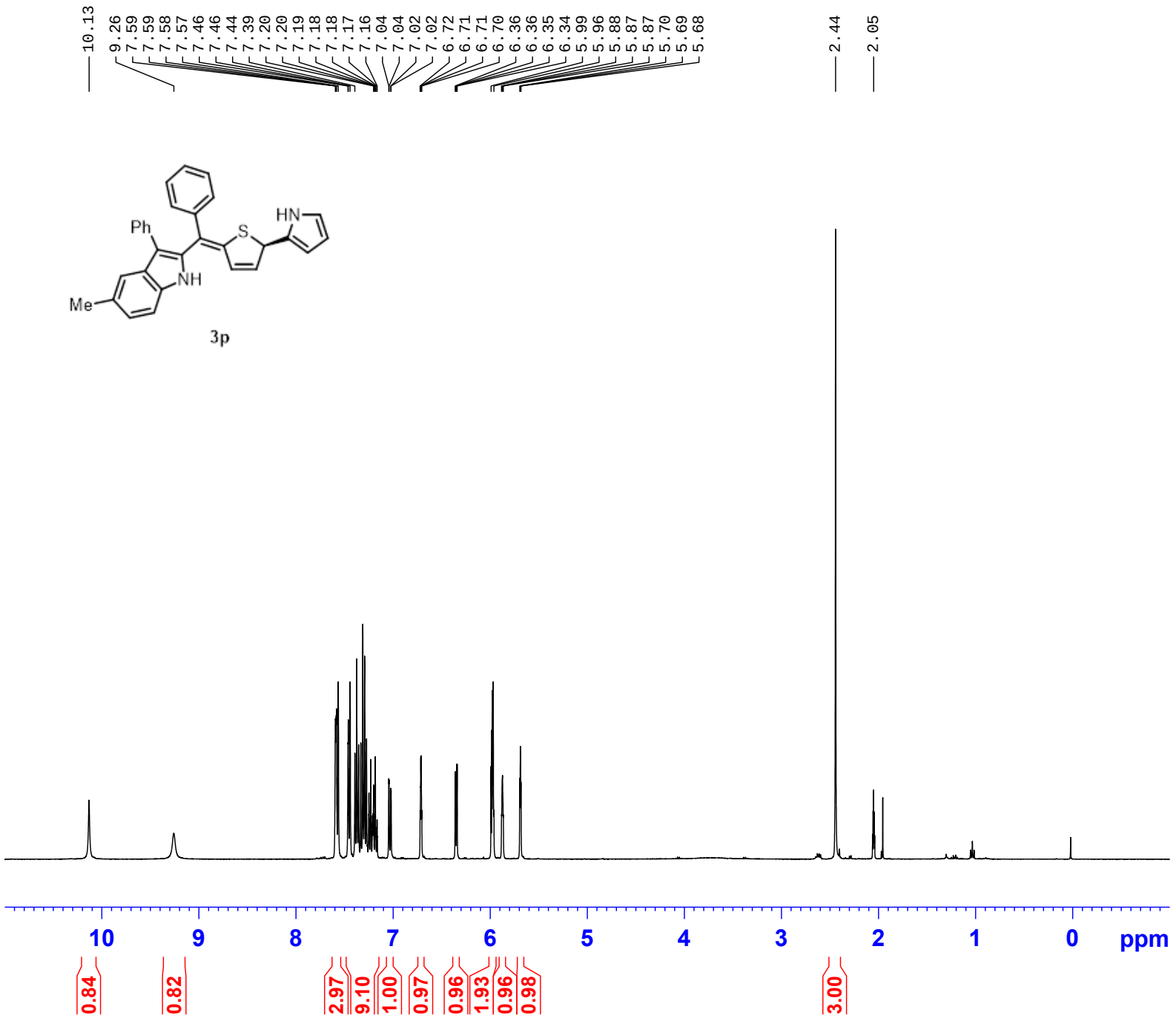
Supplementary Figure 92. ^{13}C NMR spectrum of **3n**



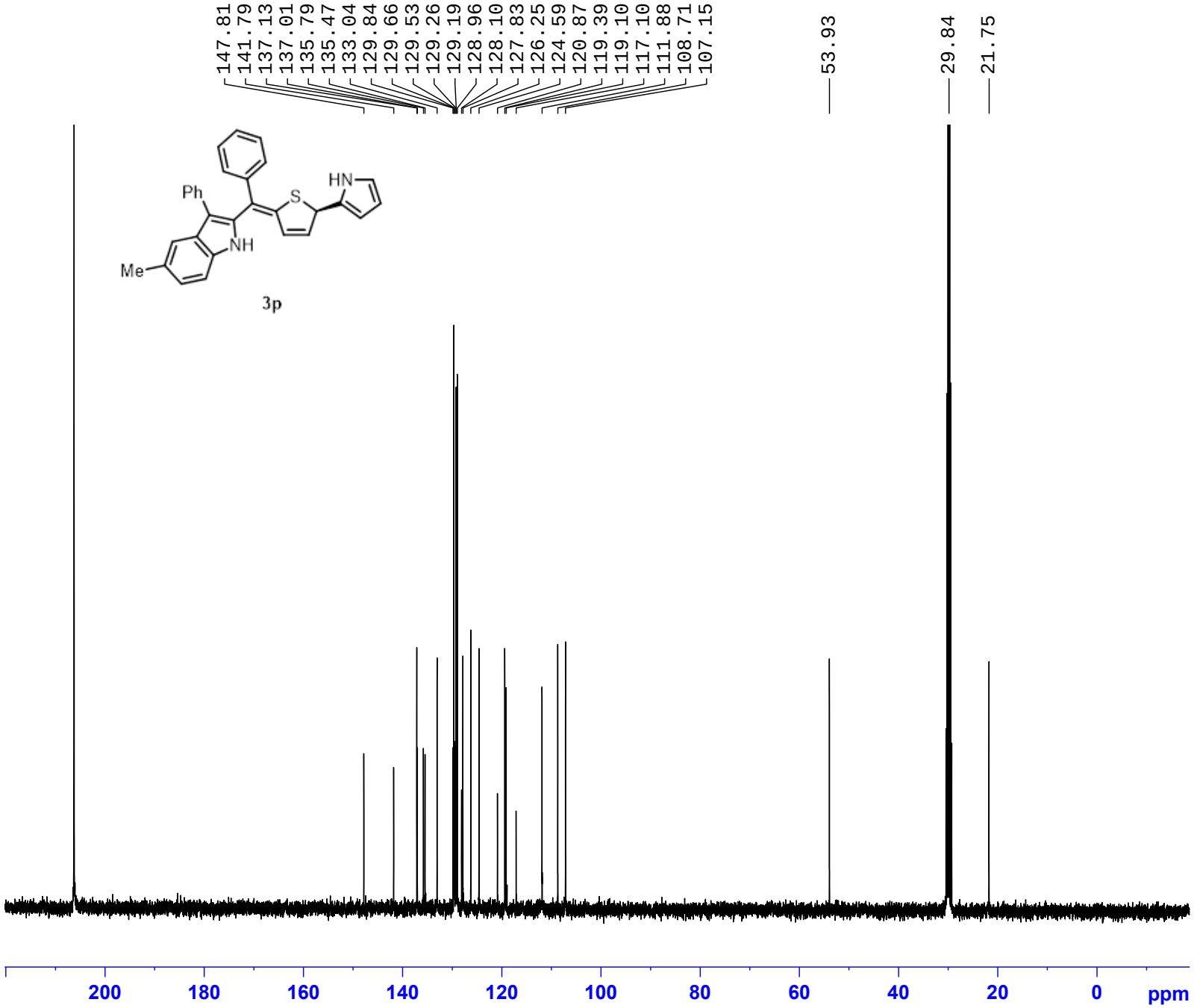
Supplementary Figure 93. ^{1}H NMR spectrum of **3o**



Supplementary Figure 94. ^{13}C NMR spectrum of **3o**



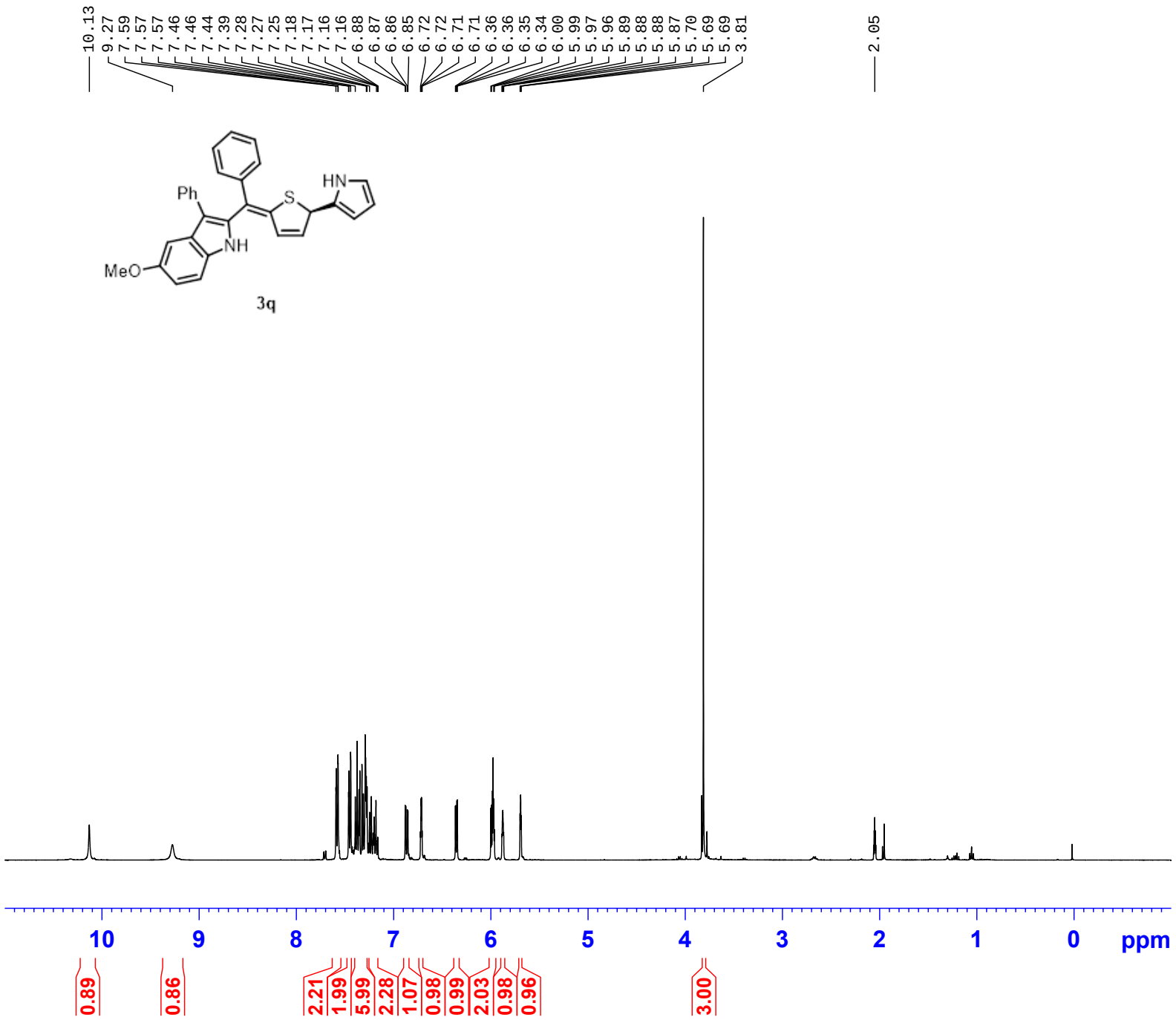
Supplementary Figure 95. ^{1}H NMR spectrum of **3p**



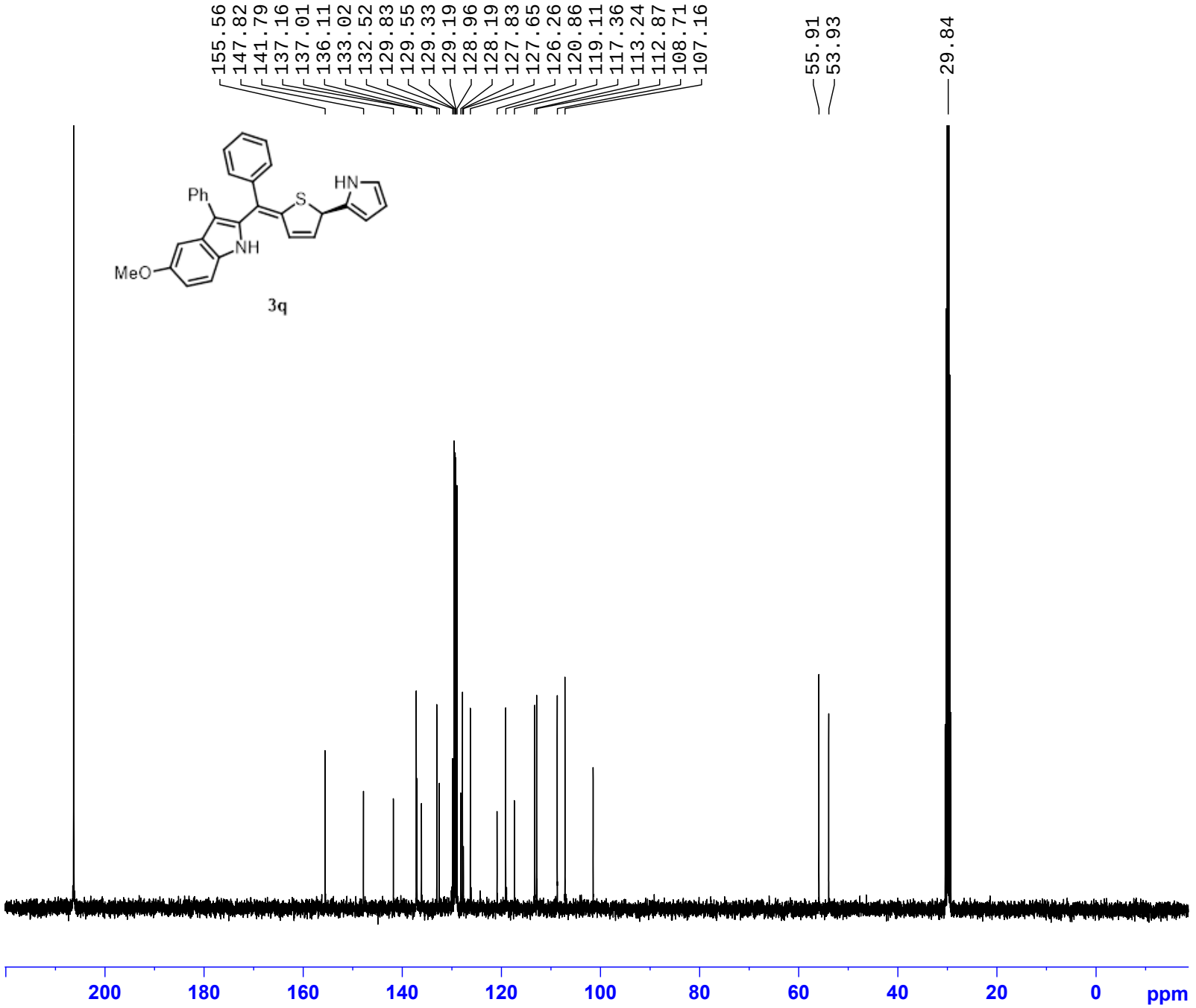

```
NAME           lxg-7079C
EXPNO                  2
PROCNO                 1
Date_           20200703
Time               20.22
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   58
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
SI                32768
SF          100.6126871 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```

Supplementary Figure 96. ^{13}C NMR spectrum of **3p**

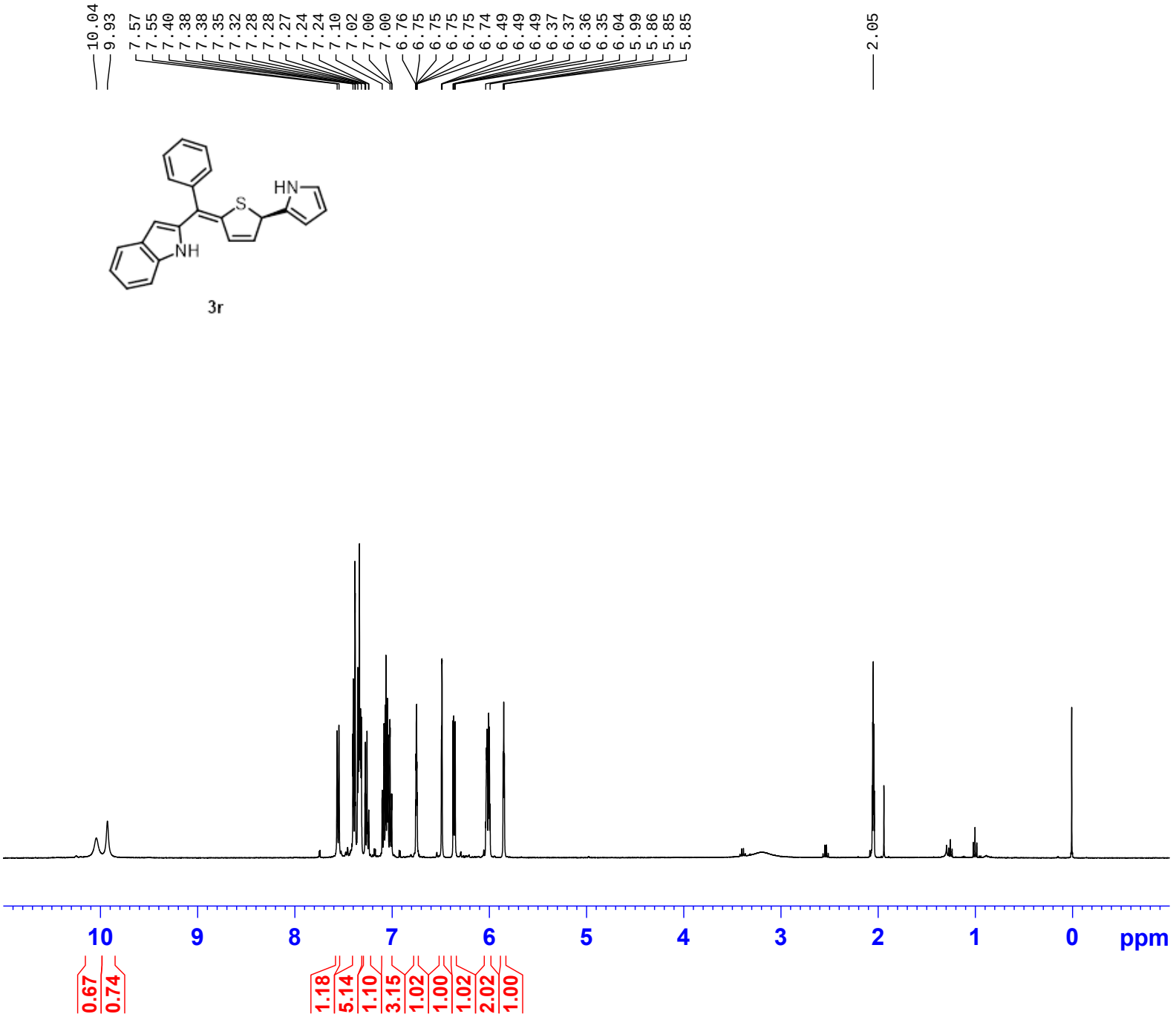


Supplementary Figure 97. ^{1}H NMR spectrum of **3q**

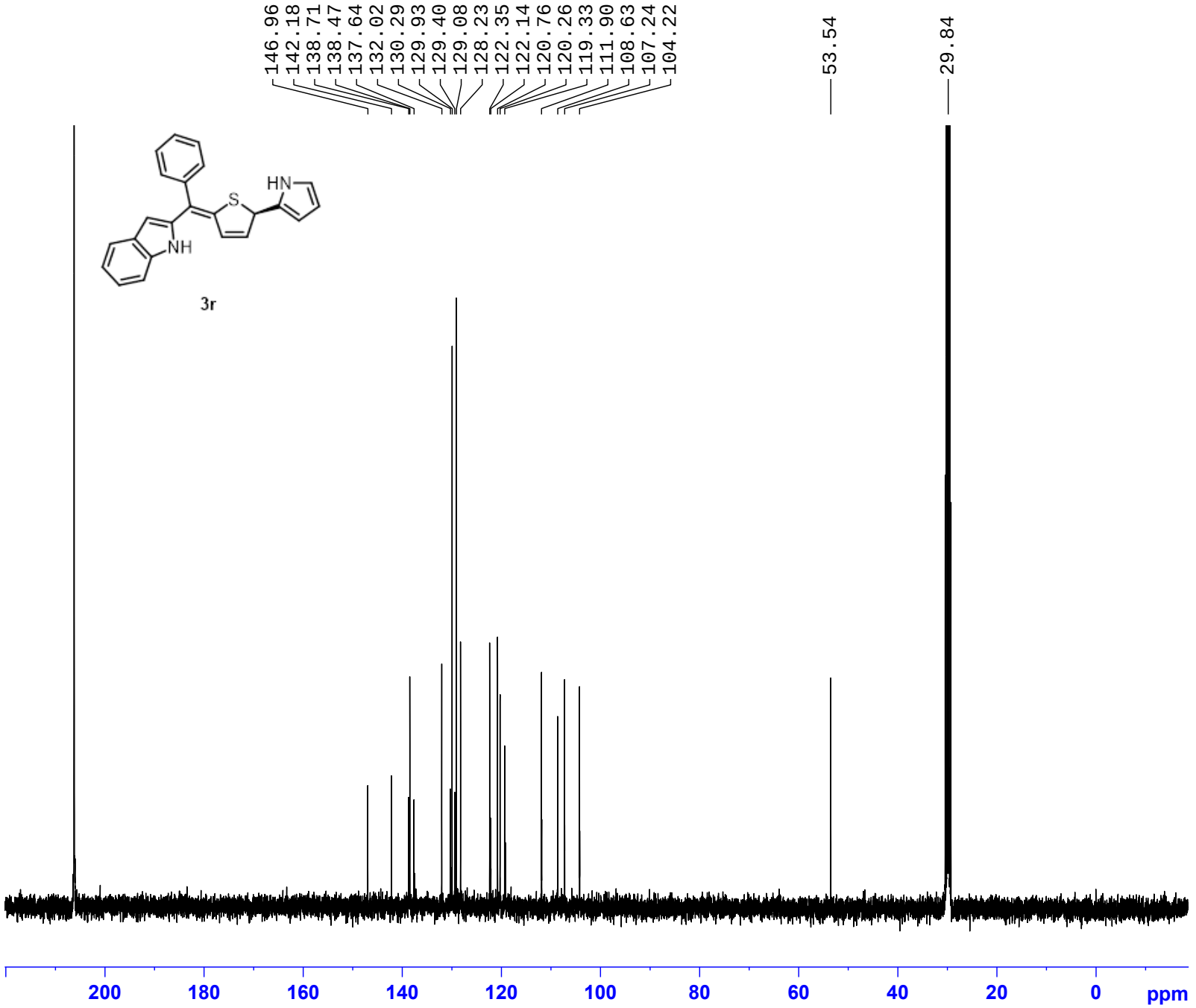


NAME	lxg-7079D
EXPNO	2
PROCNO	1
Date_	20200703
Time	22.44
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	39
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6126878 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Supplementary Figure 98. ^{13}C NMR spectrum of **3q**



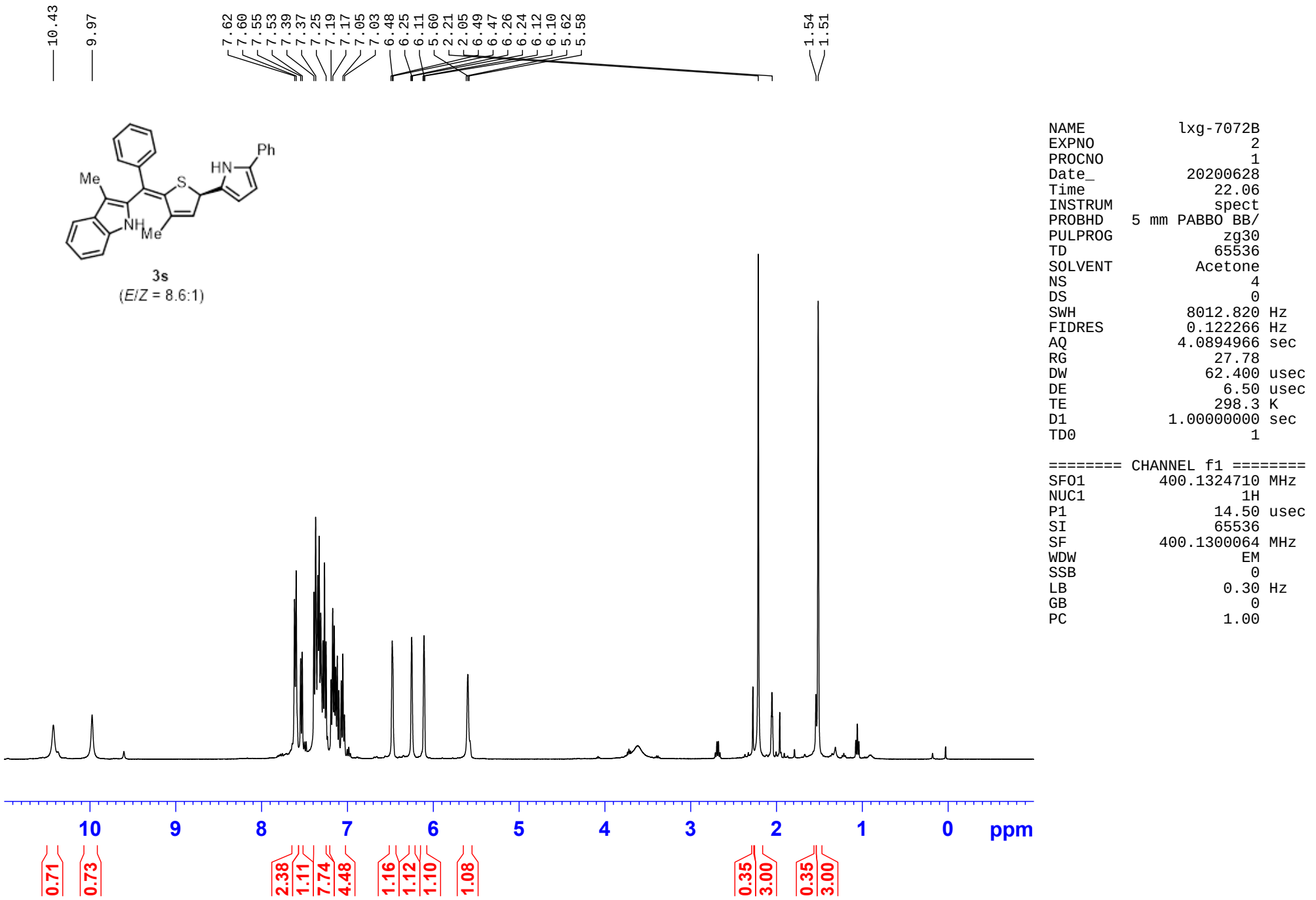
Supplementary Figure 99. ^{1}H NMR spectrum of **3r**



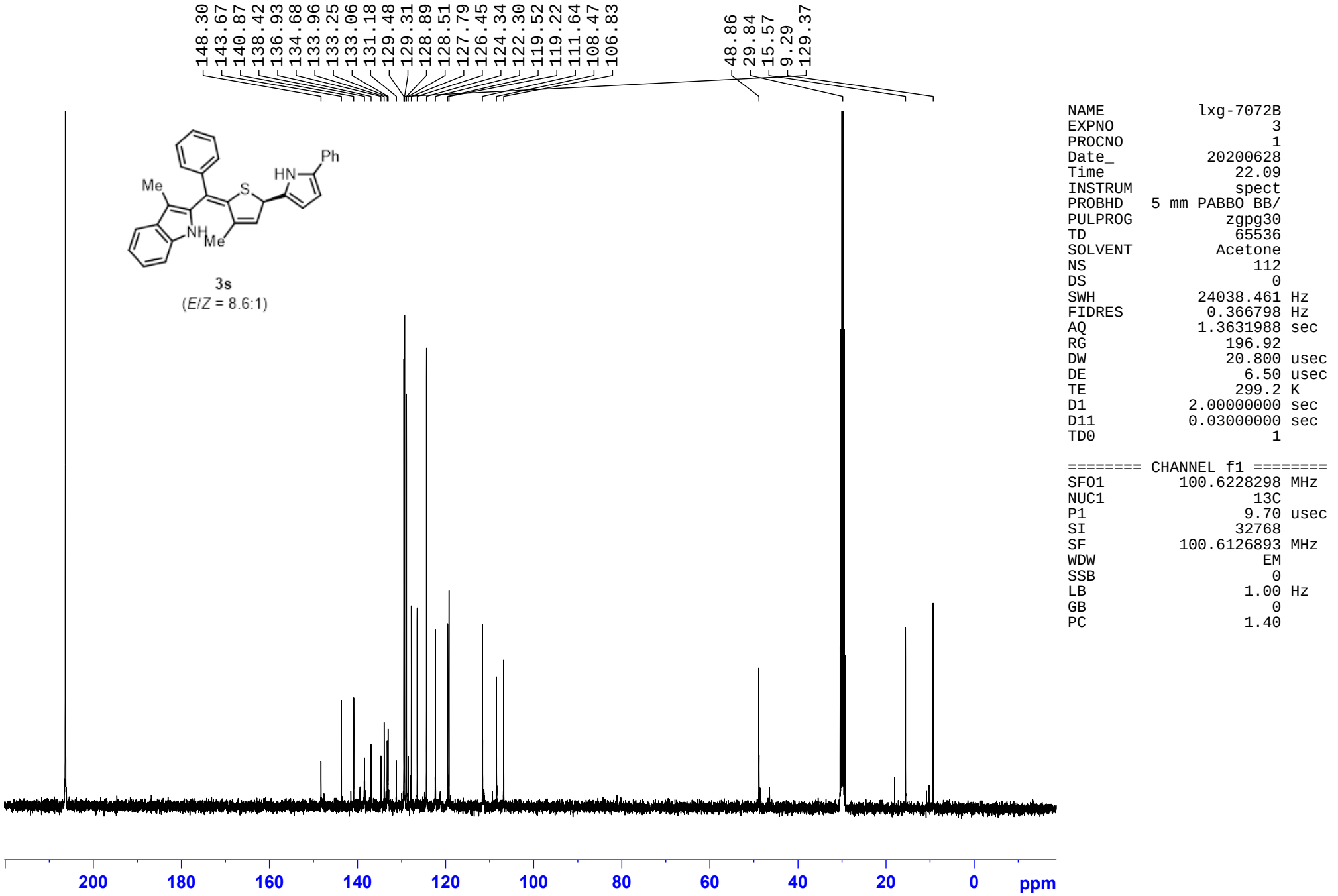

```
NAME           lxg-7096B
EXPNO                  2
PROCNO                 1
Date_           20200723
Time               22.50
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                    98
DS                     0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                298.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                 9.70 usec
SI                32768
SF           100.6126827 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


Supplementary Figure 100. ^{13}C NMR spectrum of **3r**



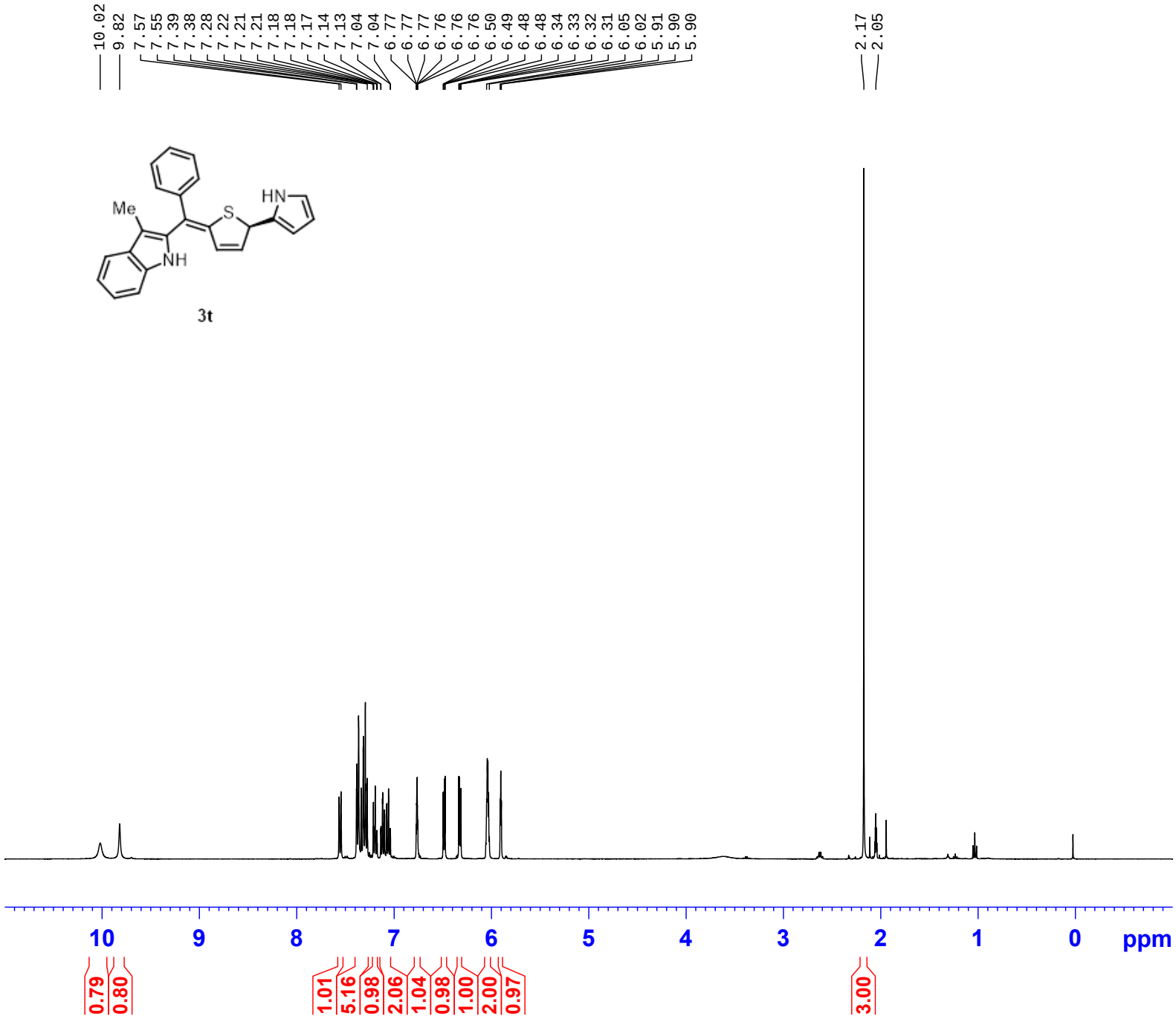
Supplementary Figure 101. ^{1}H NMR spectrum of **3s**



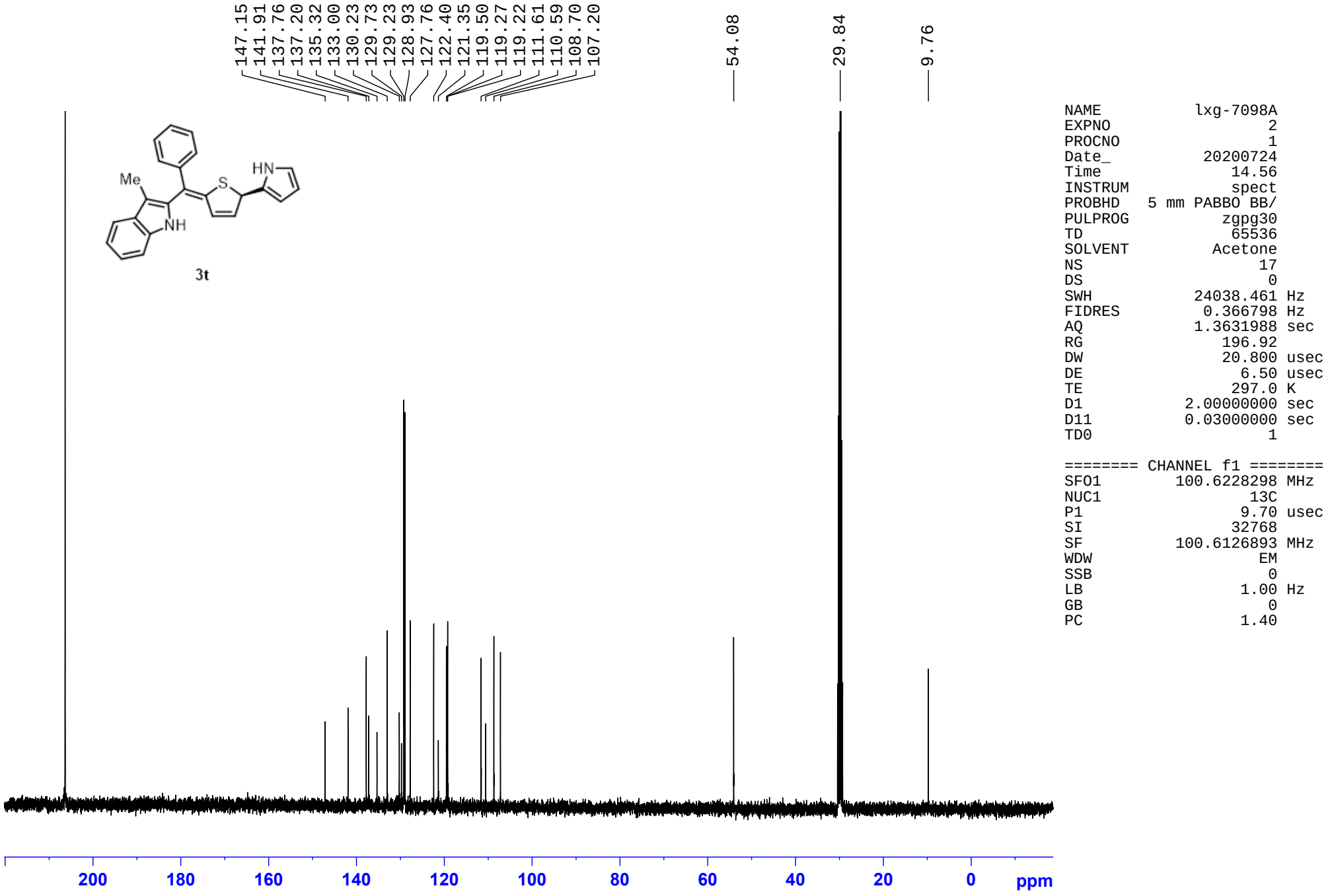

```
NAME            lxg-7072B
EXPNO                   3
PROCNO                  1
Date_            20200628
Time                22.09
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                     112
DS                       0
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                  196.92
DW                  20.800 usec
DE                   6.50 usec
TE                  299.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                  13C
P1                   9.70 usec
SI                  32768
SF           100.6126893 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

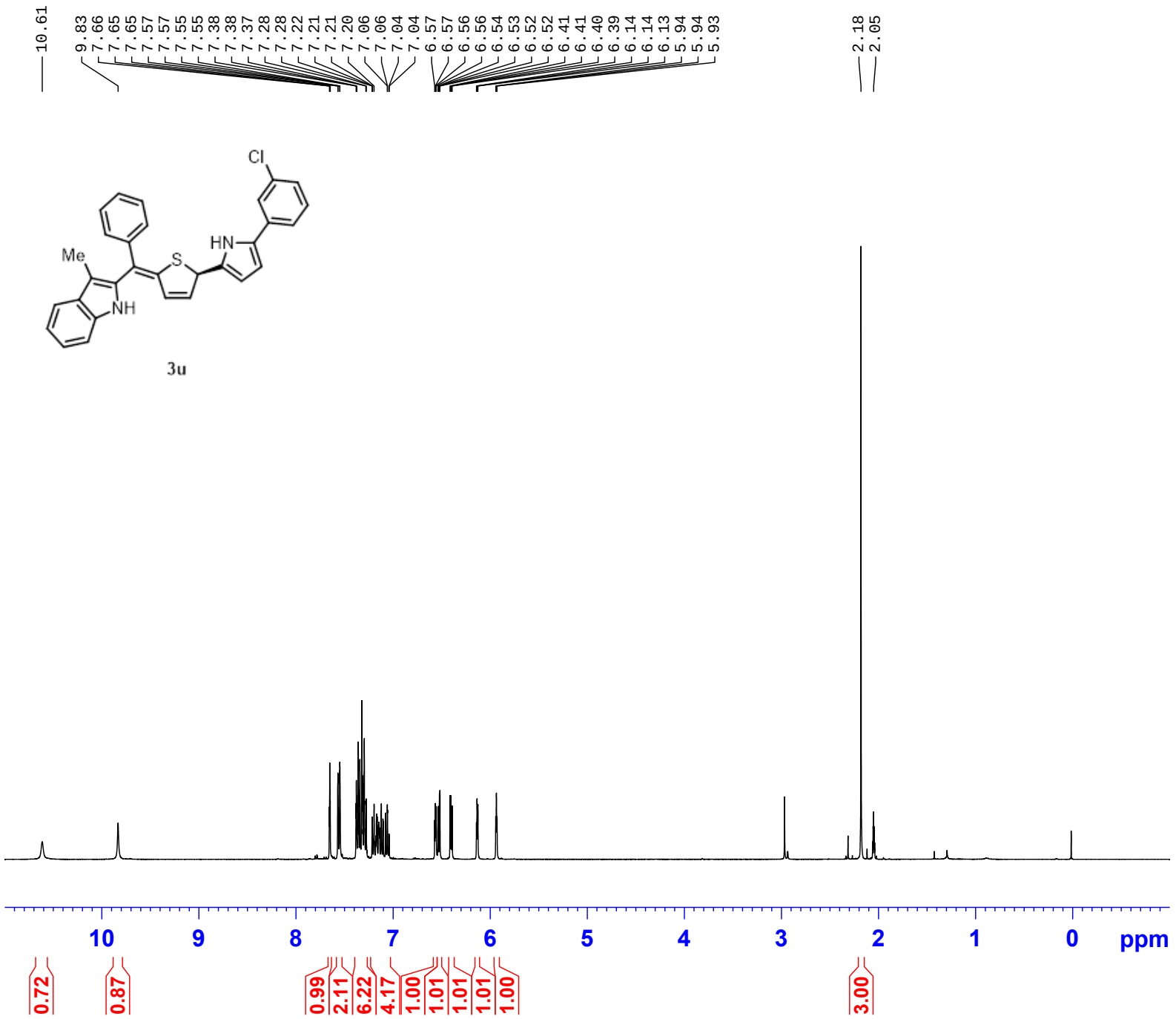
Supplementary Figure 102. ^{13}C NMR spectrum of **3s**



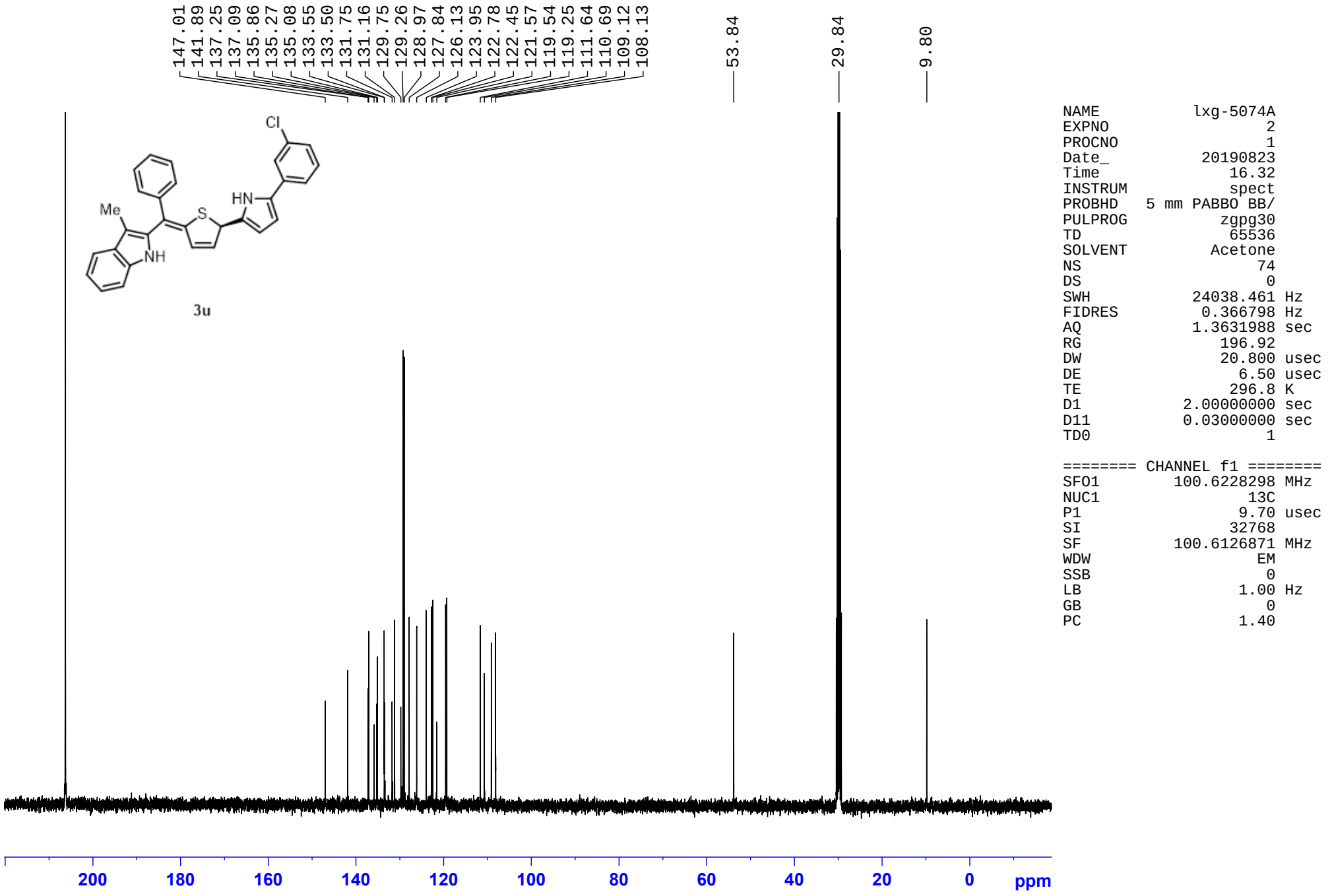
Supplementary Figure 103. ^{1}H NMR spectrum of **3t**



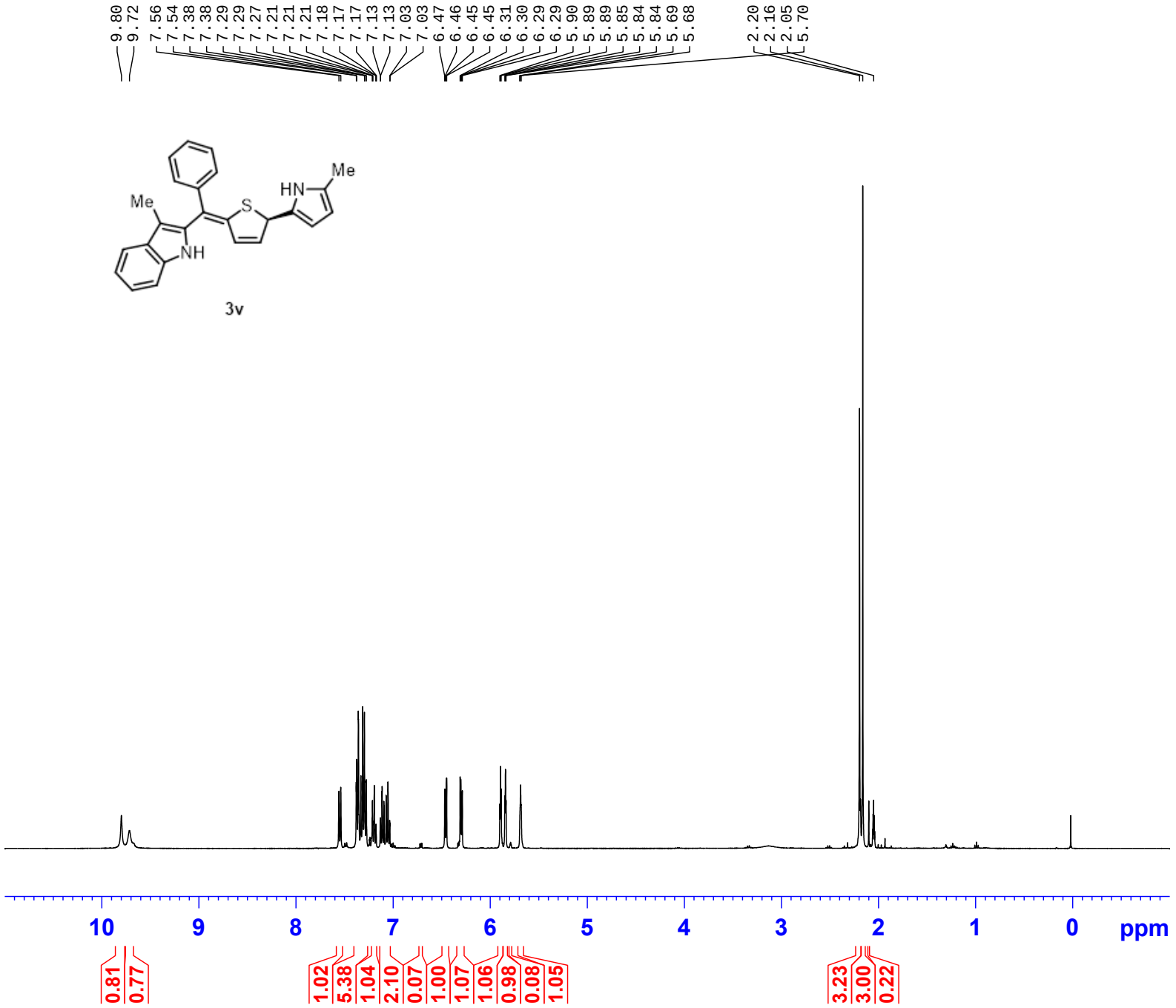
Supplementary Figure 104. ^{13}C NMR spectrum of **3t**



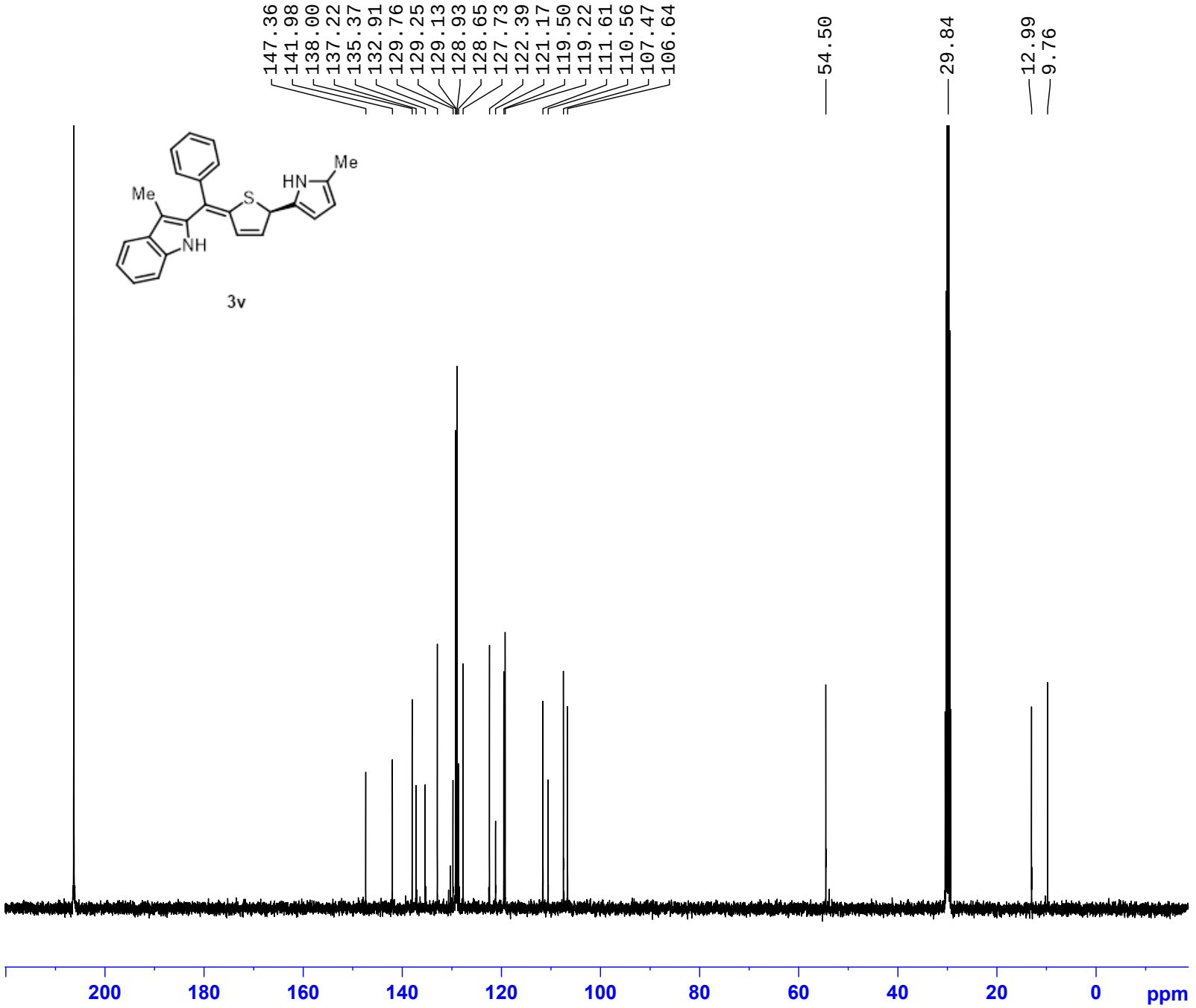
Supplementary Figure 105. ^{1}H NMR spectrum of **3u**



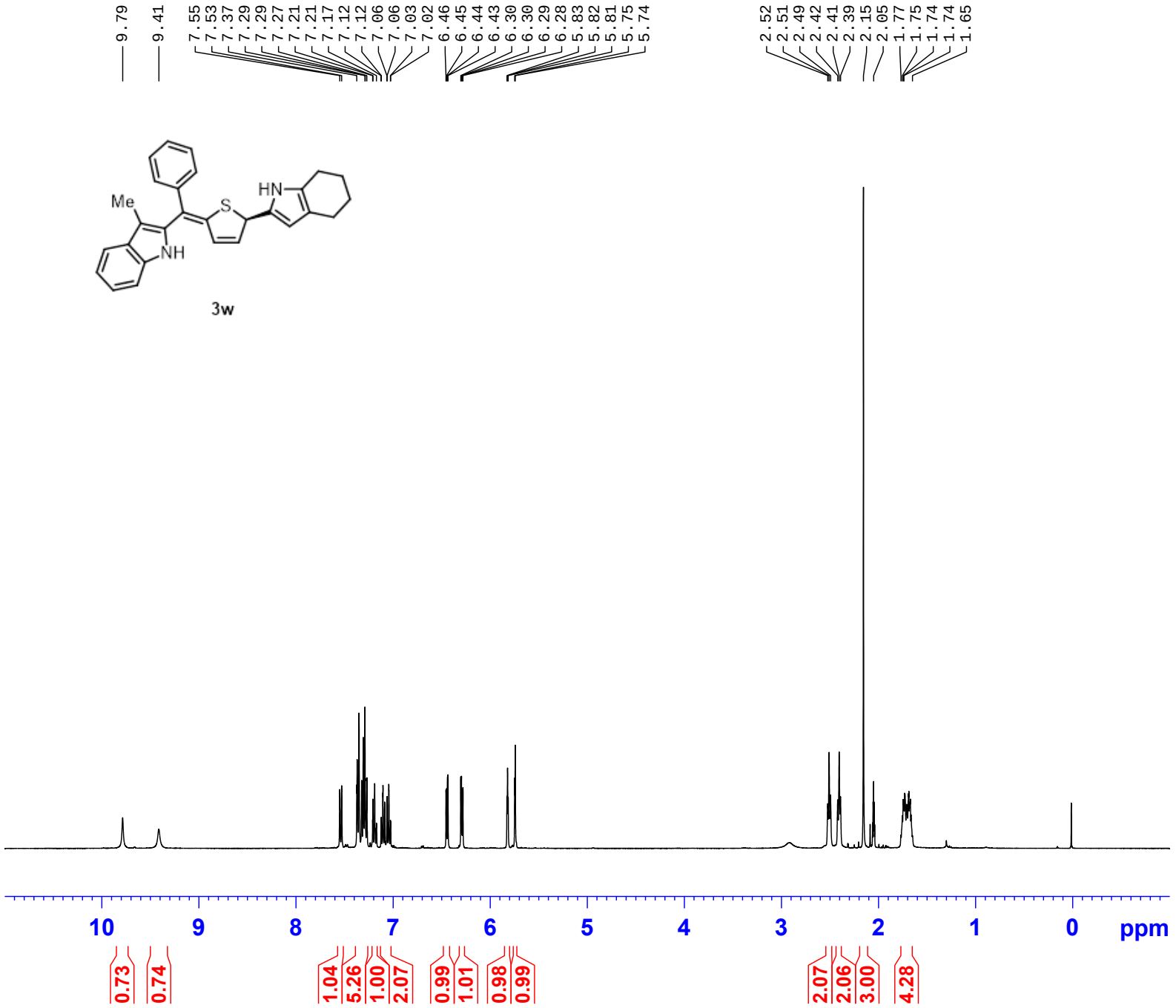
Supplementary Figure 106. ^{13}C NMR spectrum of **3u**



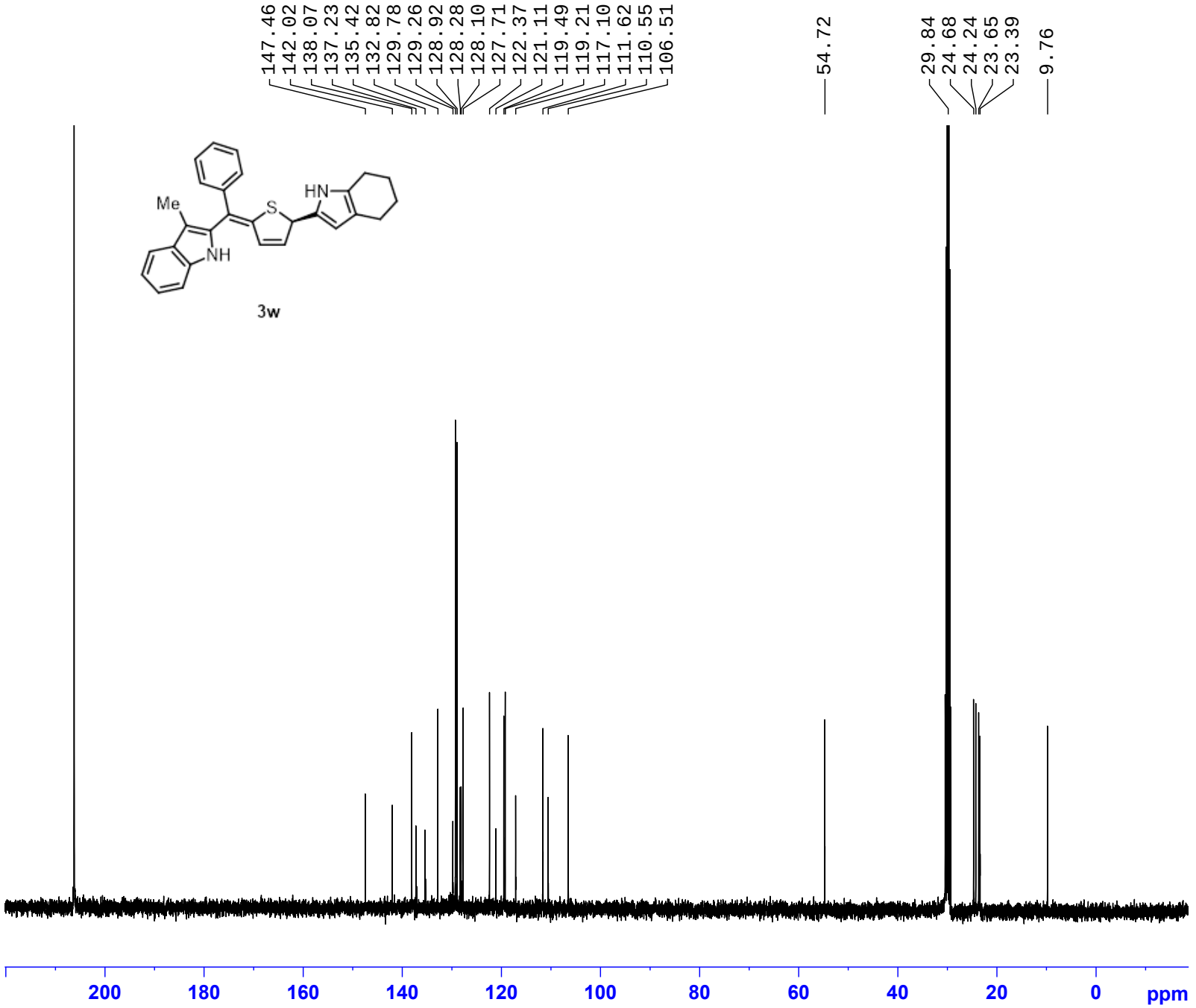
Supplementary Figure 107. ^{1}H NMR spectrum of **3v**



Supplementary Figure 108. ^{13}C NMR spectrum of **3v**

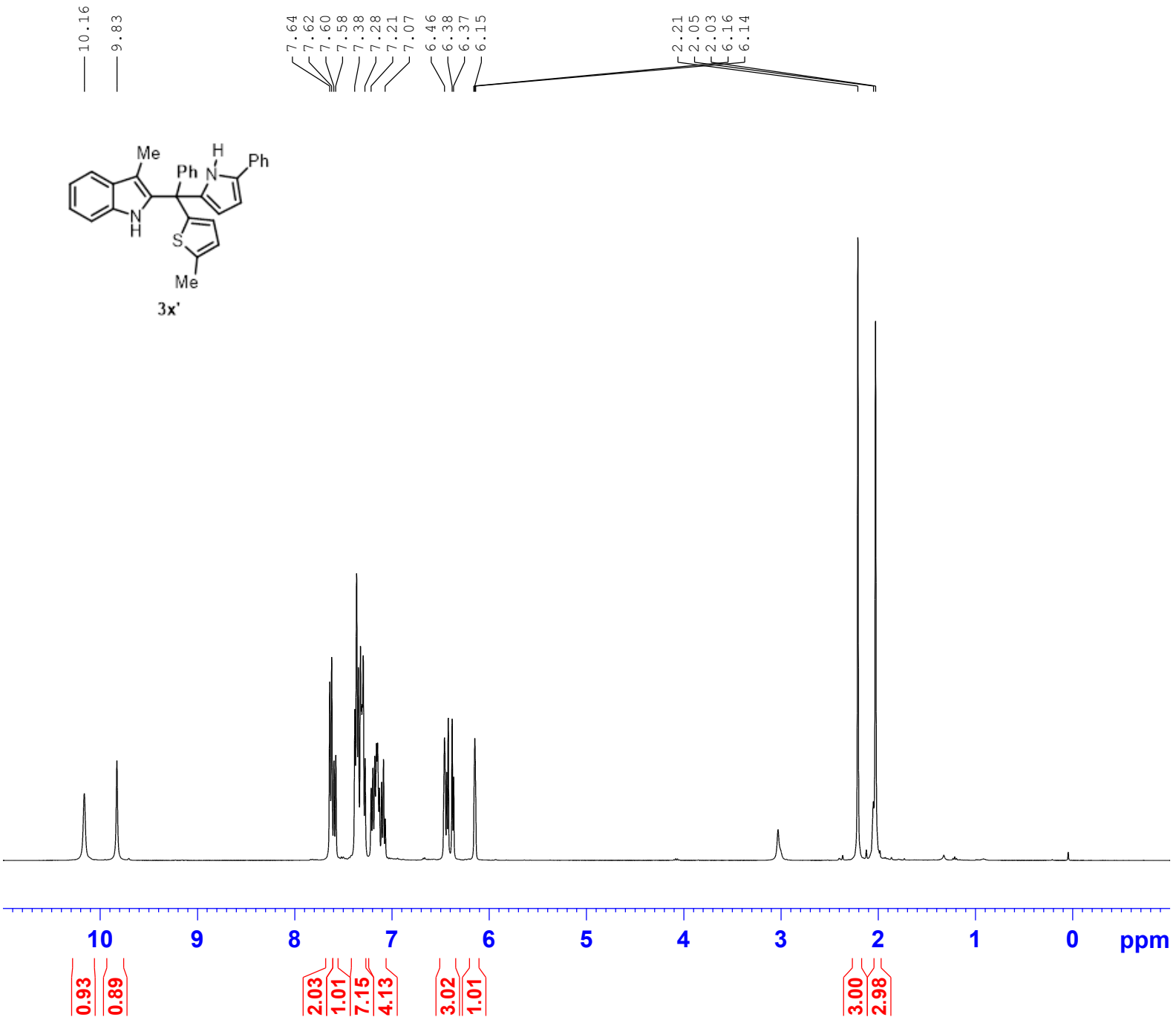


Supplementary Figure 109. ^{1}H NMR spectrum of **3w**

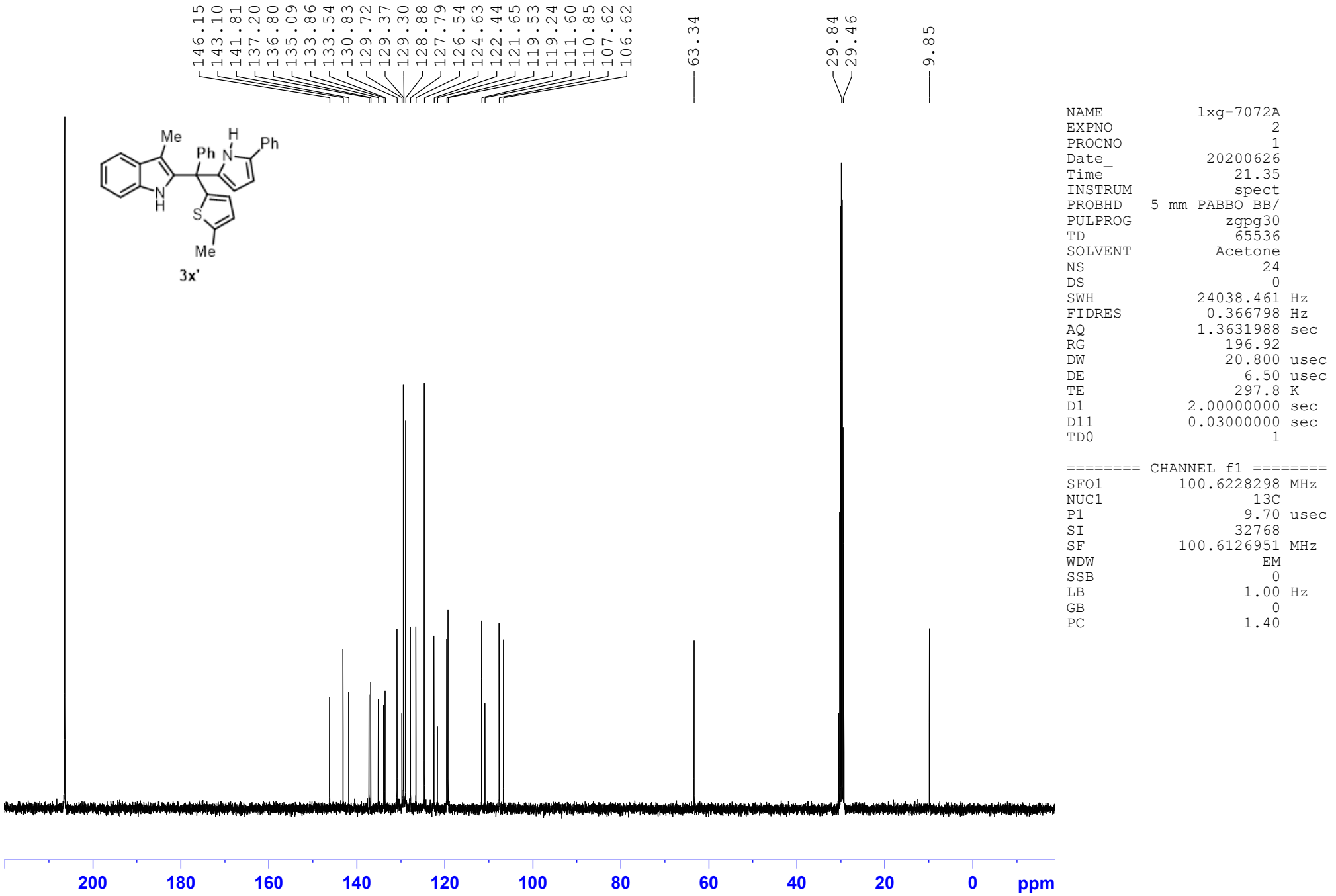


NAME	lxg-7094B
EXPNO	2
PROCNO	1
Date_	20200721
Time	22.47
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	71
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	298.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6126841 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

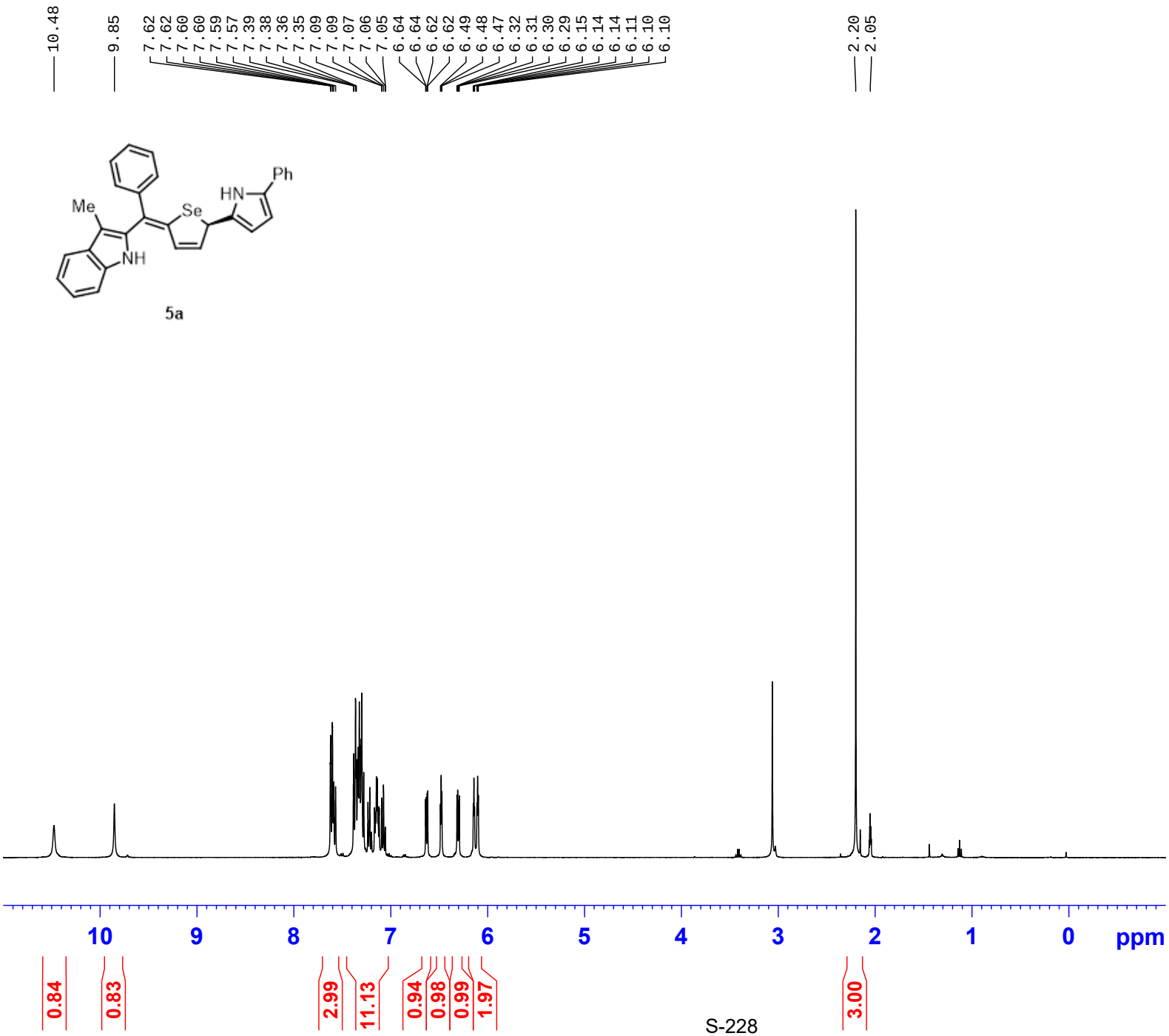
Supplementary Figure 110. ^{13}C NMR spectrum of **3w**



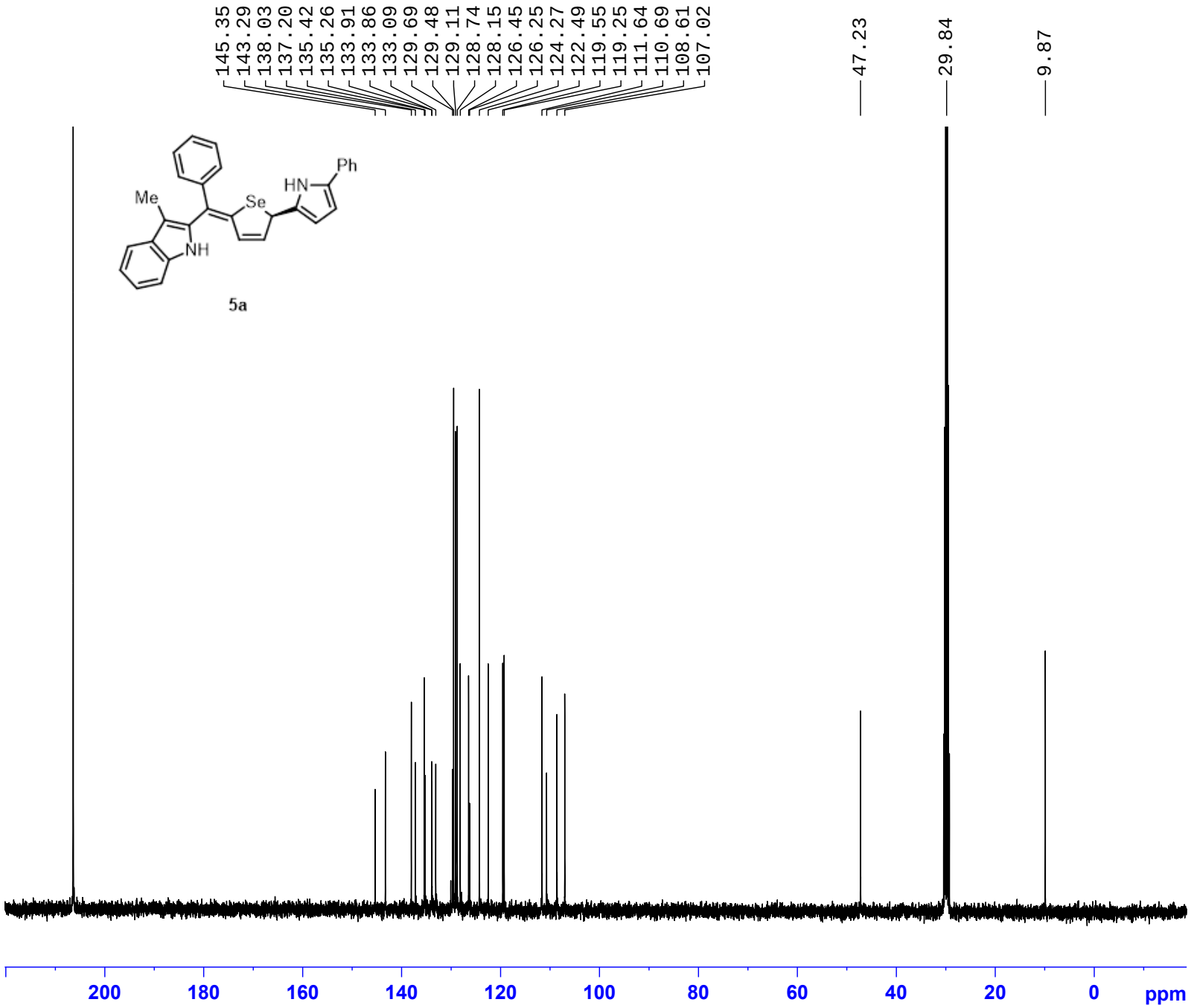
Supplementary Figure 111. ^{1}H NMR spectrum of **3x'**



Supplementary Figure 112. ^{13}C NMR spectrum of **3x'**



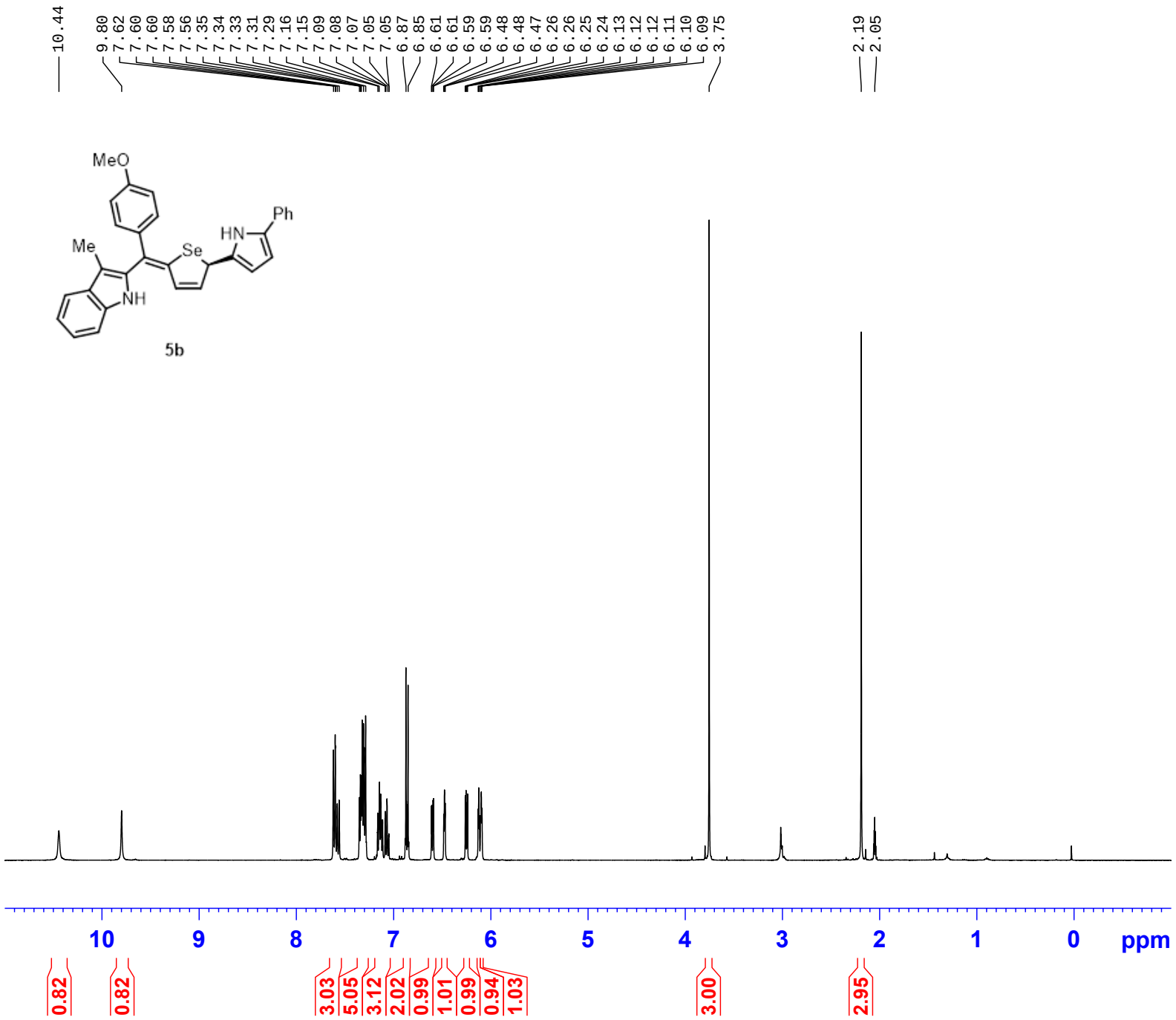
Supplementary Figure 113. ^{1}H NMR spectrum of **5a**



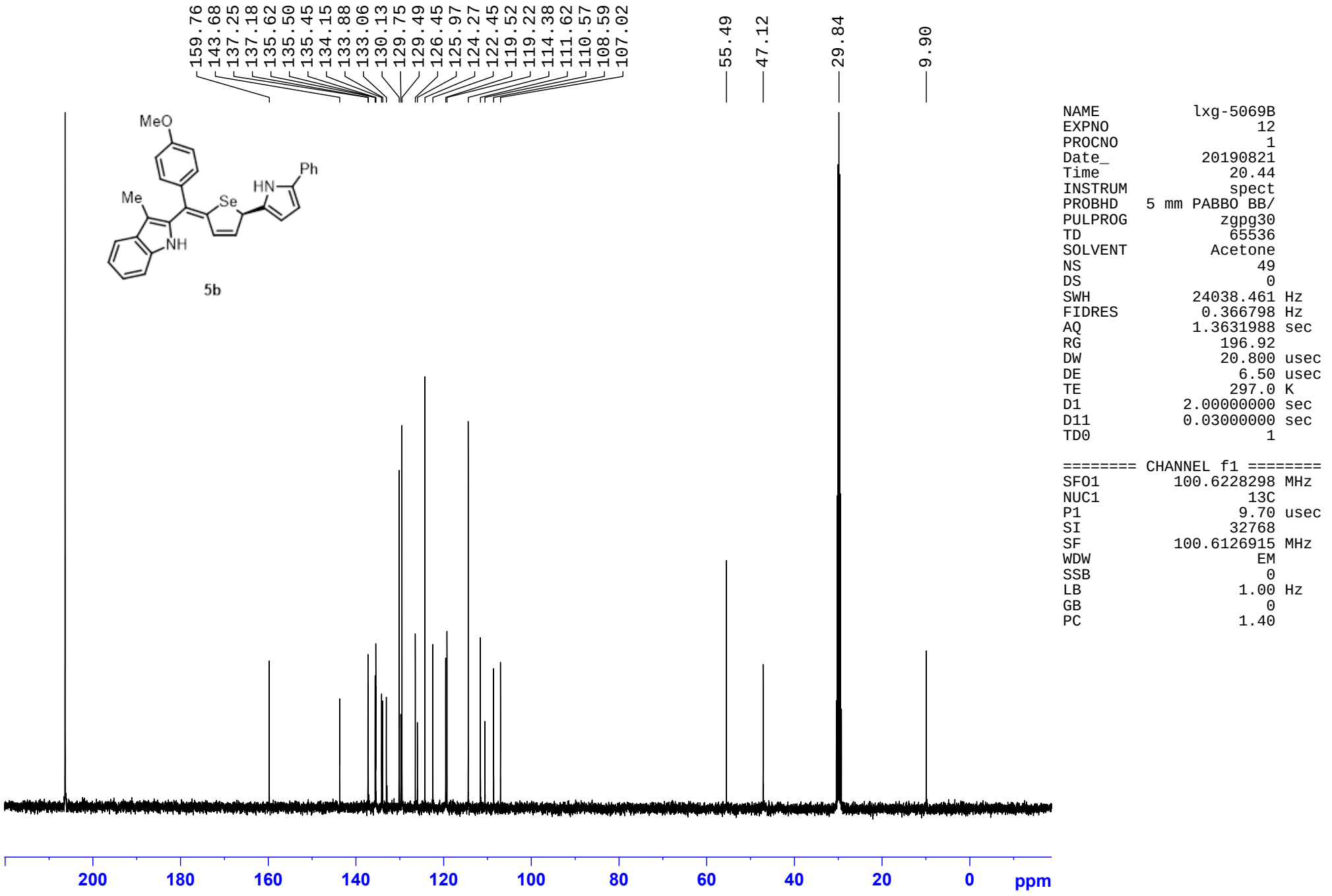

```
NAME            lxg-5069A
EXPNO                   2
PROCNO                  1
Date_            20190821
Time                19.30
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                      60
DS                       0
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                  196.92
DW                  20.800 usec
DE                   6.50 usec
TE                  297.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                  13C
P1                   9.70 usec
SI                  32768
SF            100.6126929 MHz
WDW                   EM
SSB                      0
LB                   1.00 Hz
GB                       0
PC                   1.40
```

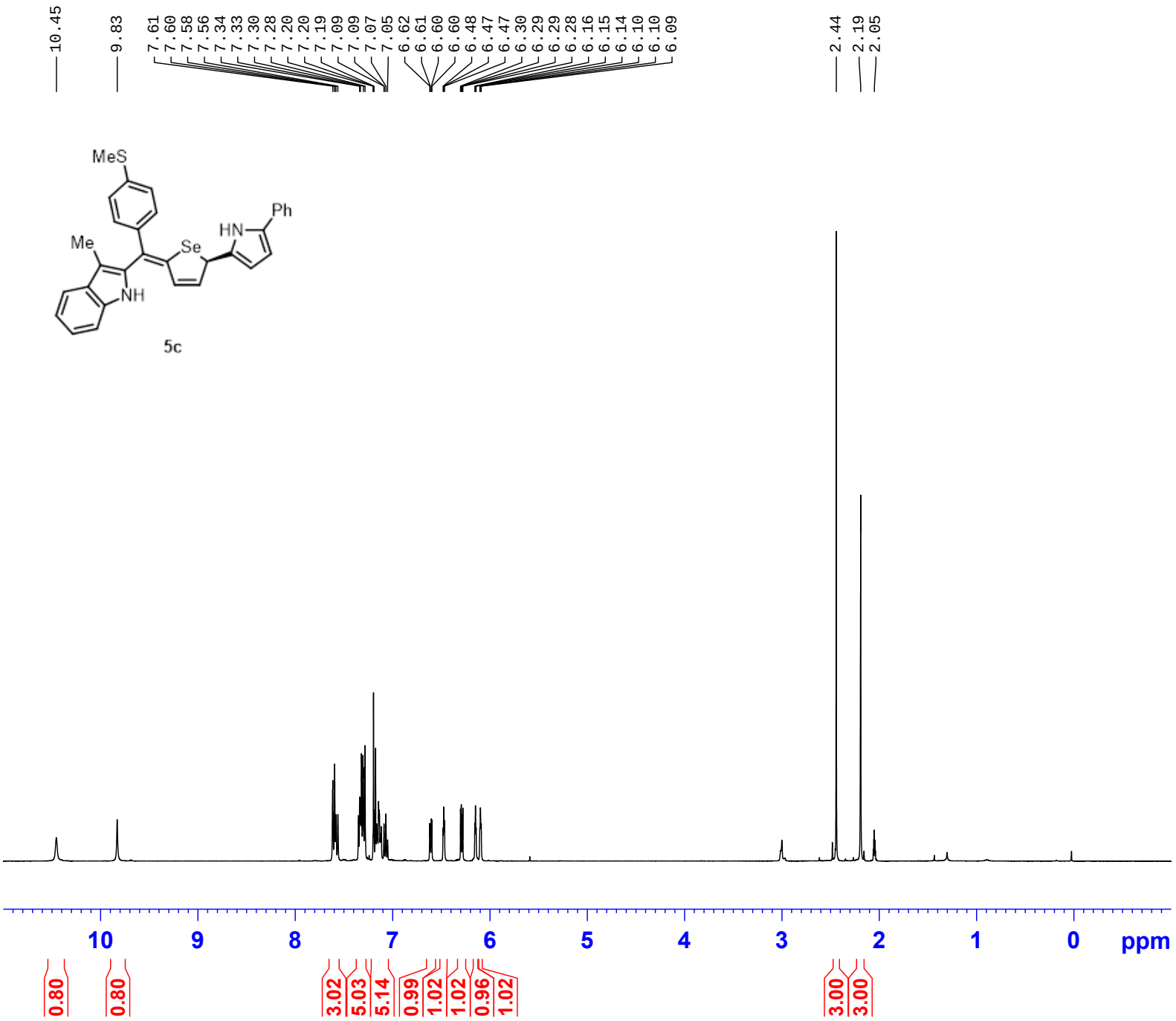

Supplementary Figure 114. ^{13}C NMR spectrum of **5a**



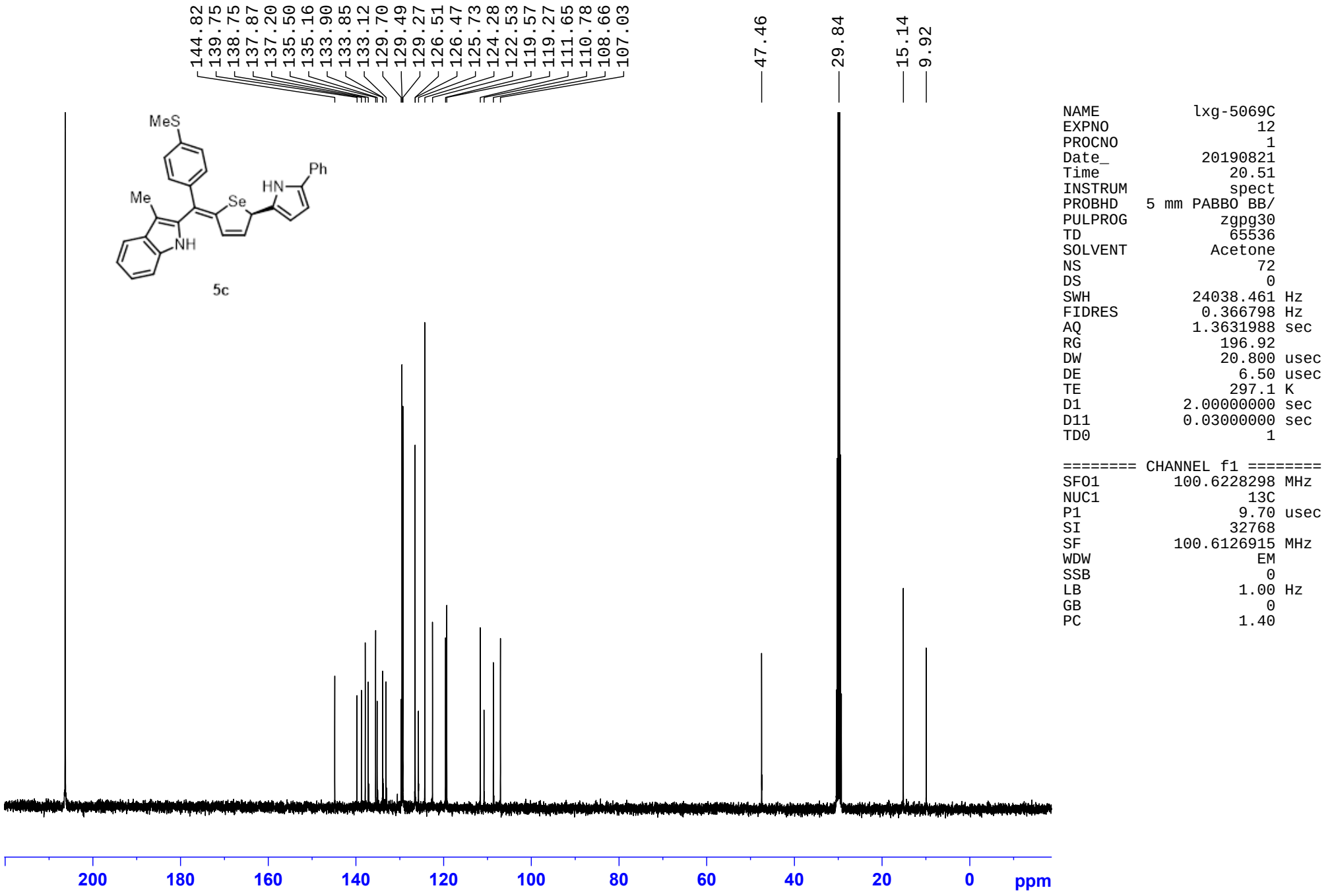
Supplementary Figure 115. ^{1}H NMR spectrum of **5b**



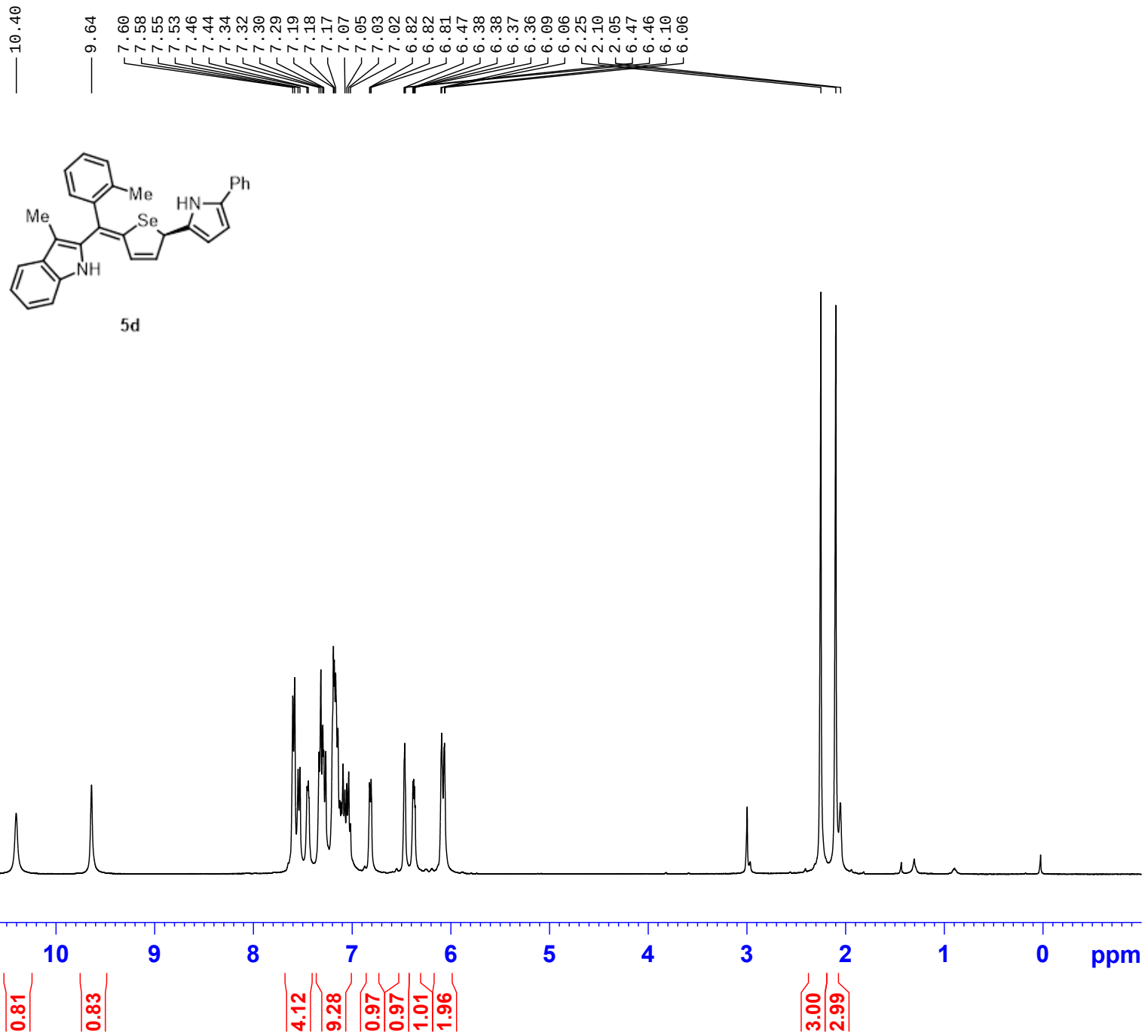
Supplementary Figure 116. ^{1}H NMR spectrum of **5b**



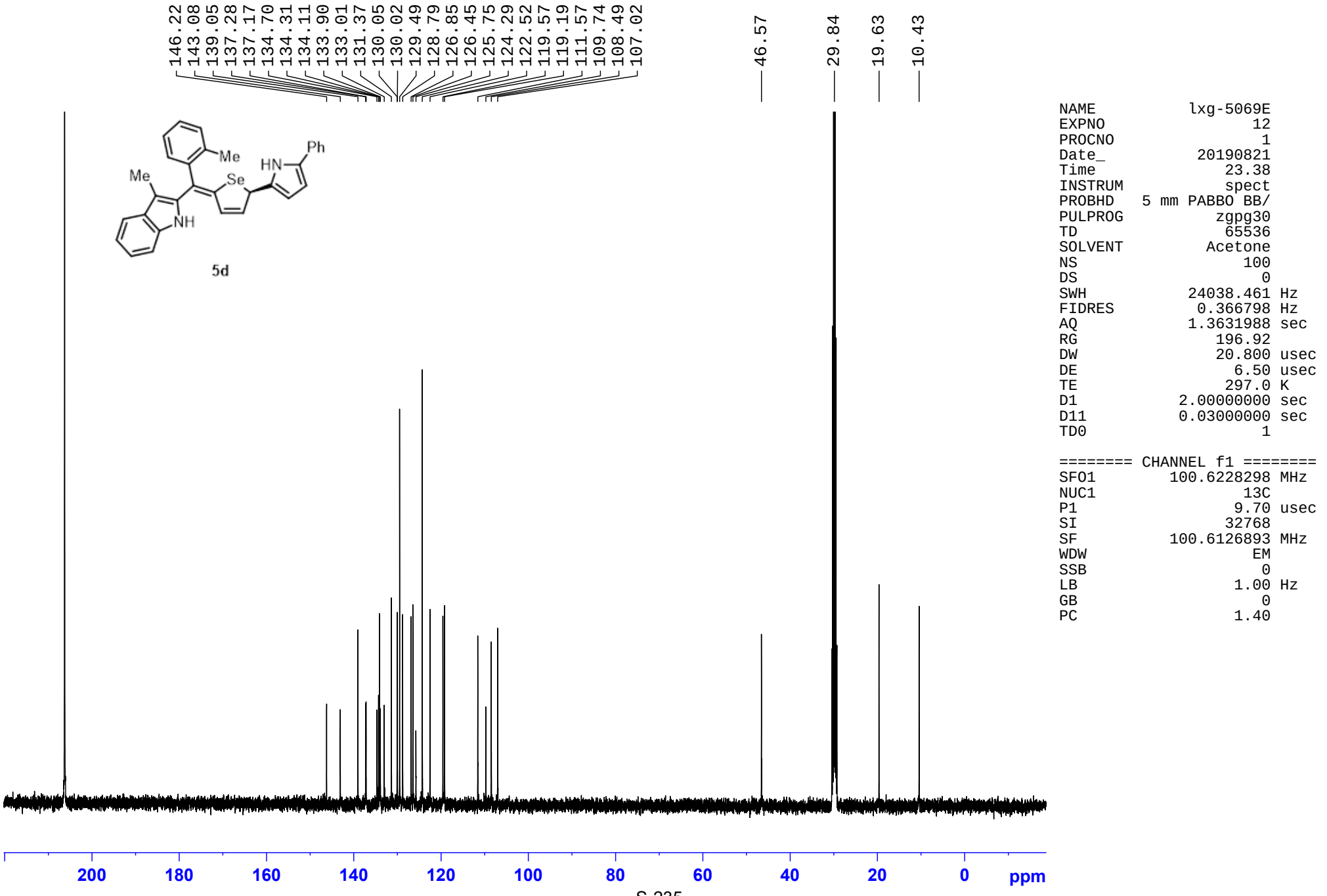
Supplementary Figure 117. ^{1}H NMR spectrum of **5c**



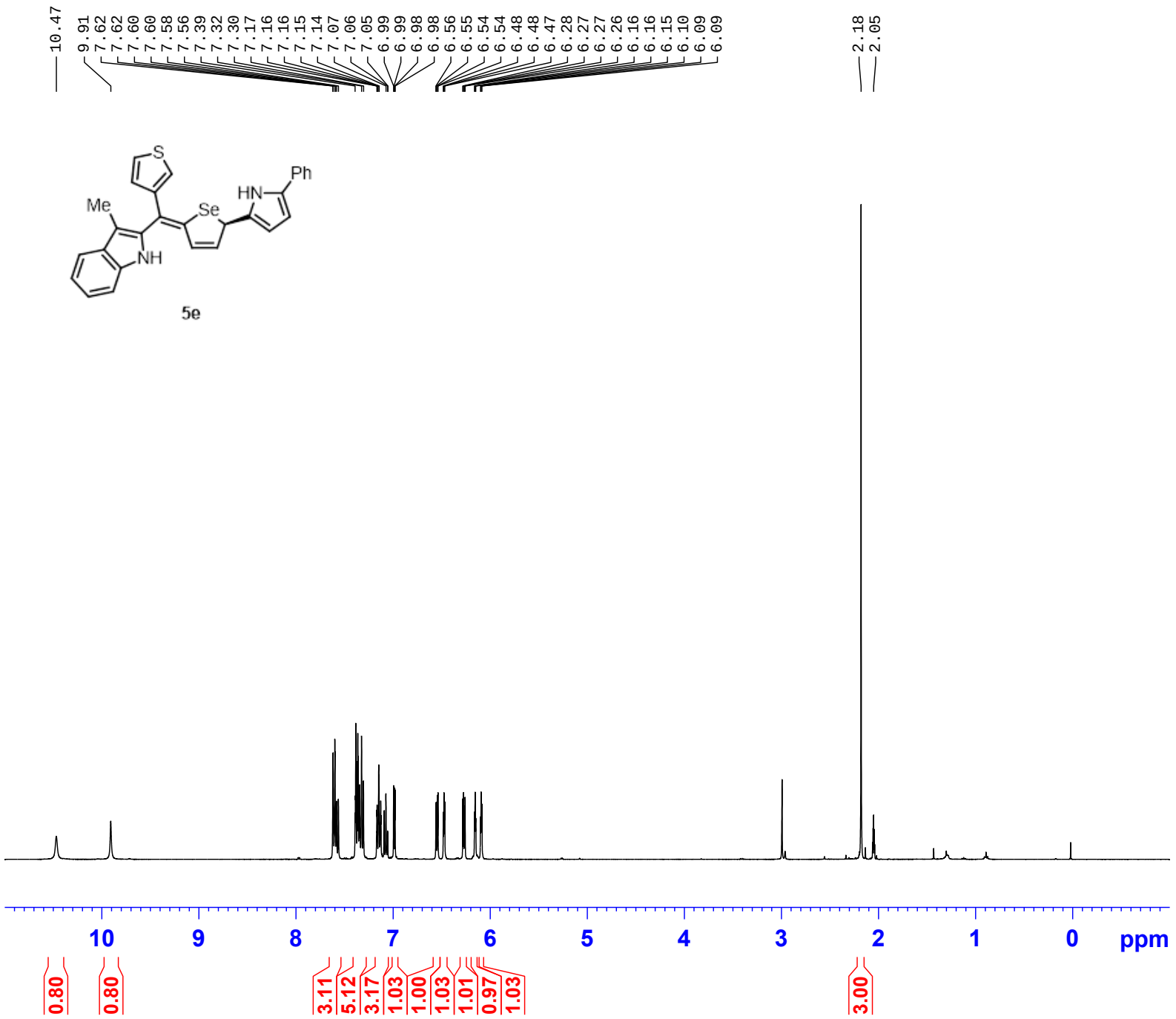
Supplementary Figure 118. ^{13}C NMR spectrum of **5c**



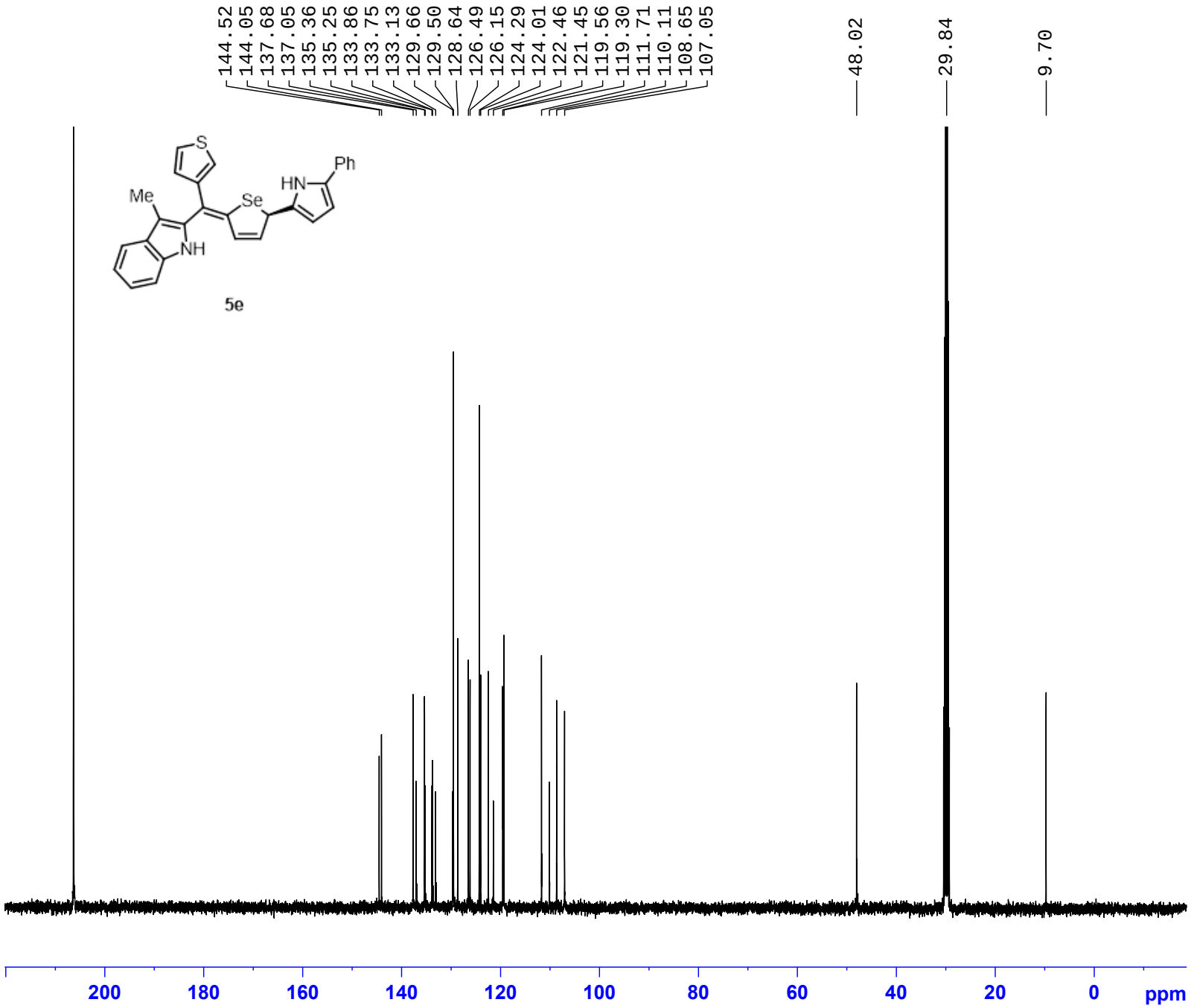
Supplementary Figure 119. ^{1}H NMR spectrum of **3d**



Supplementary Figure 119. ^{13}C NMR spectrum of **5d**

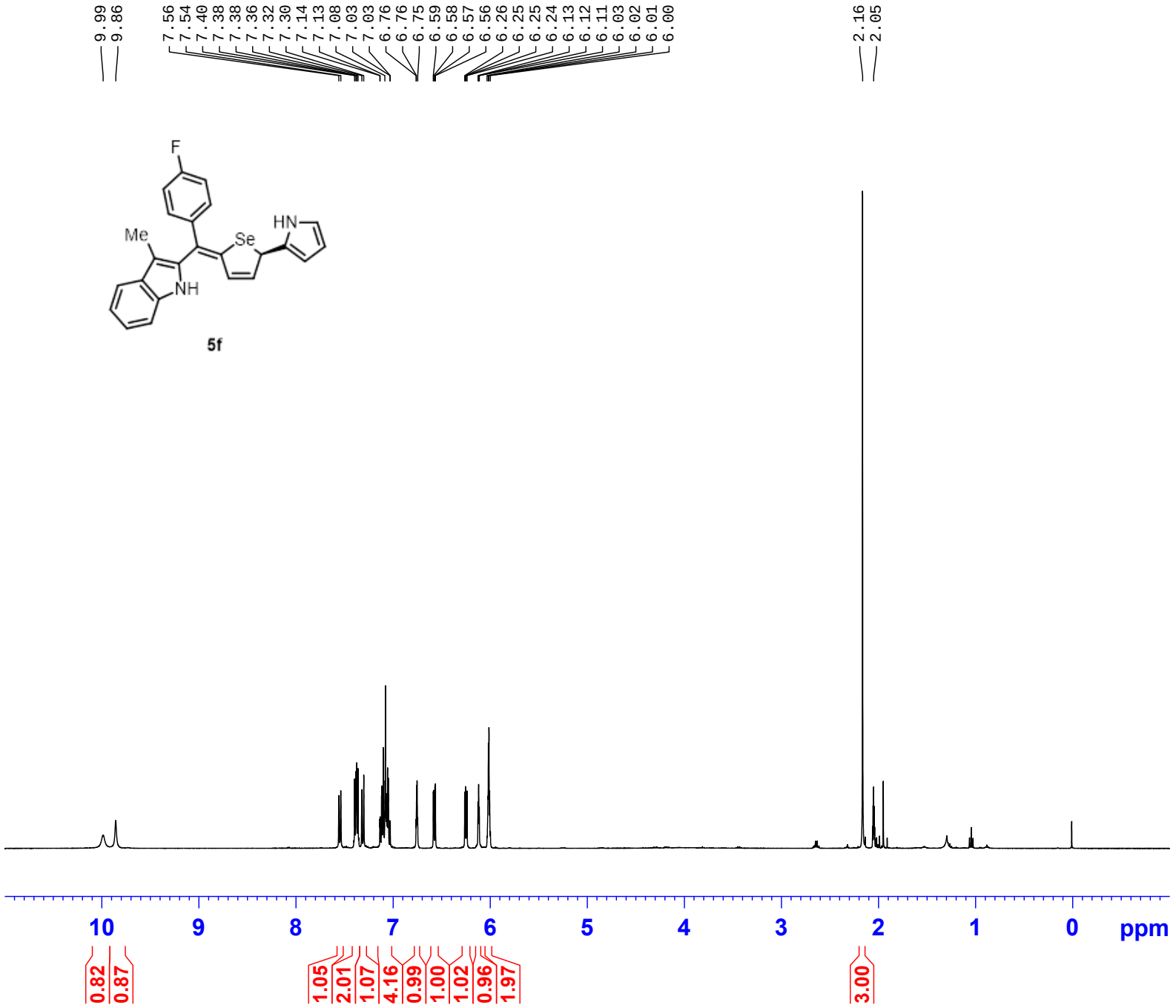


Supplementary Figure 121. ^{1}H NMR spectrum of **5e**

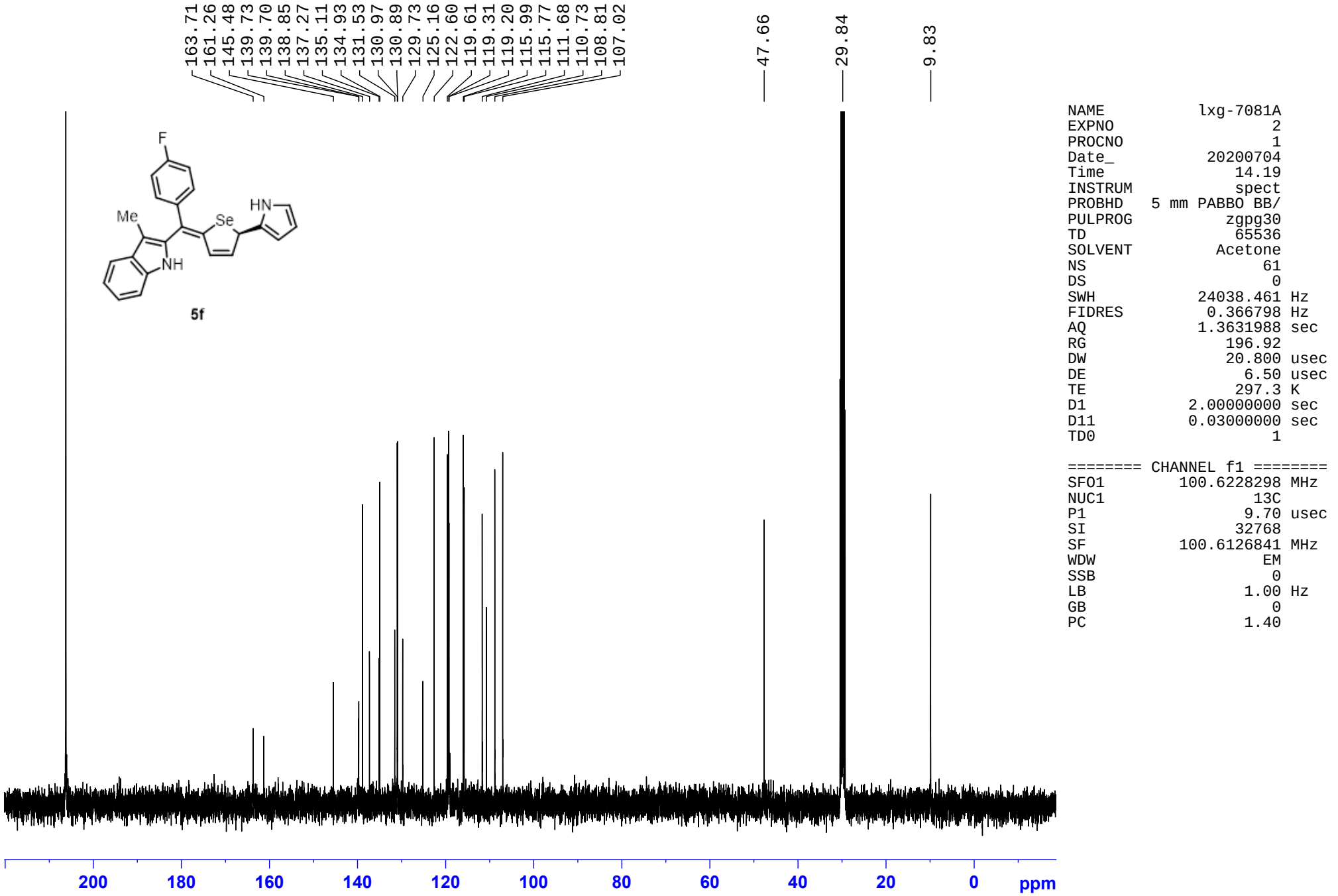


NAME	lxg-5069D
EXPNO	12
PROCNO	1
Date_	20190821
Time	21.00
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	87
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	297.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6126900 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

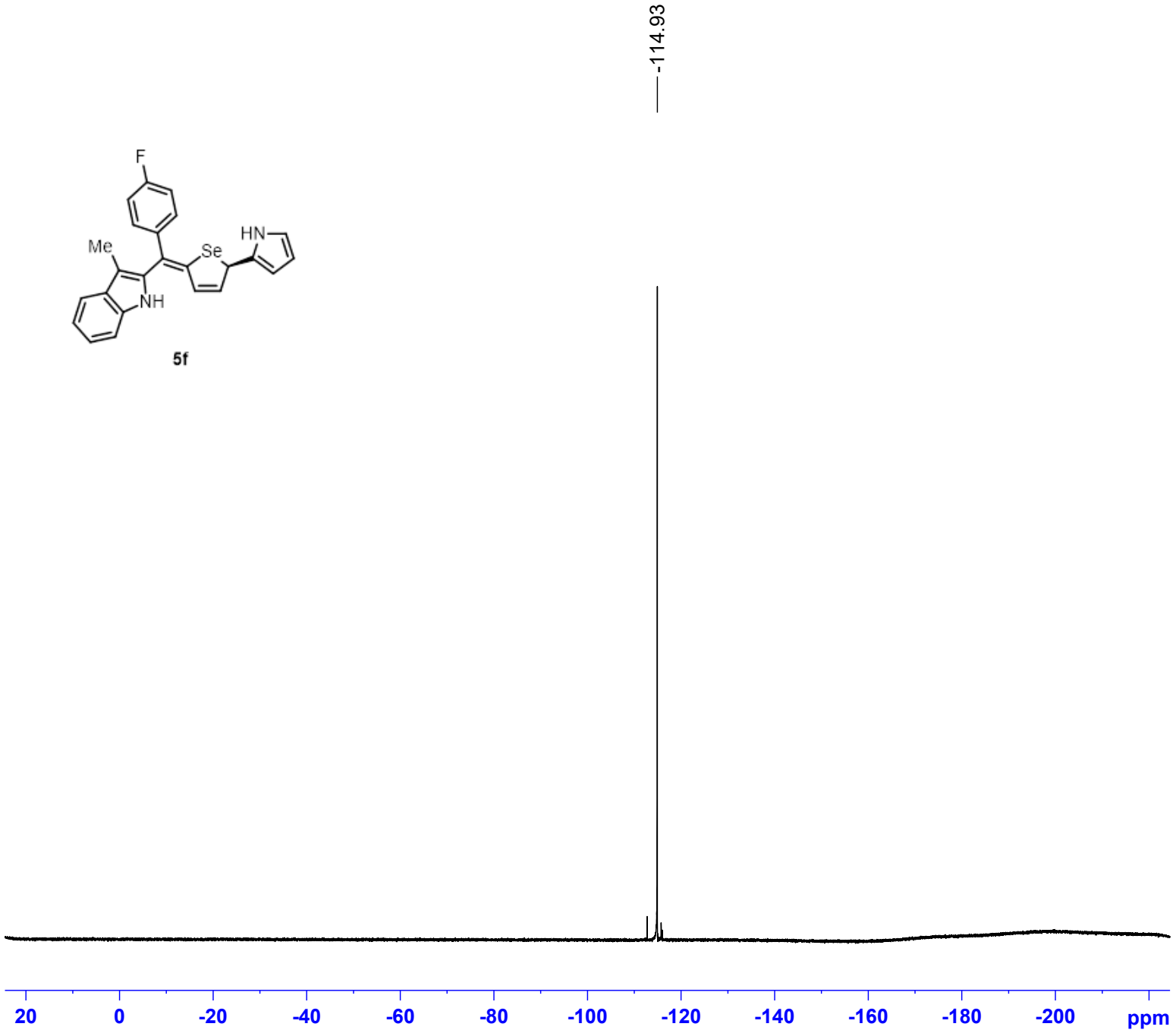
Supplementary Figure 122. ^{13}C NMR spectrum of **5e**



Supplementary Figure 123. ^{1}H NMR spectrum of **5f**



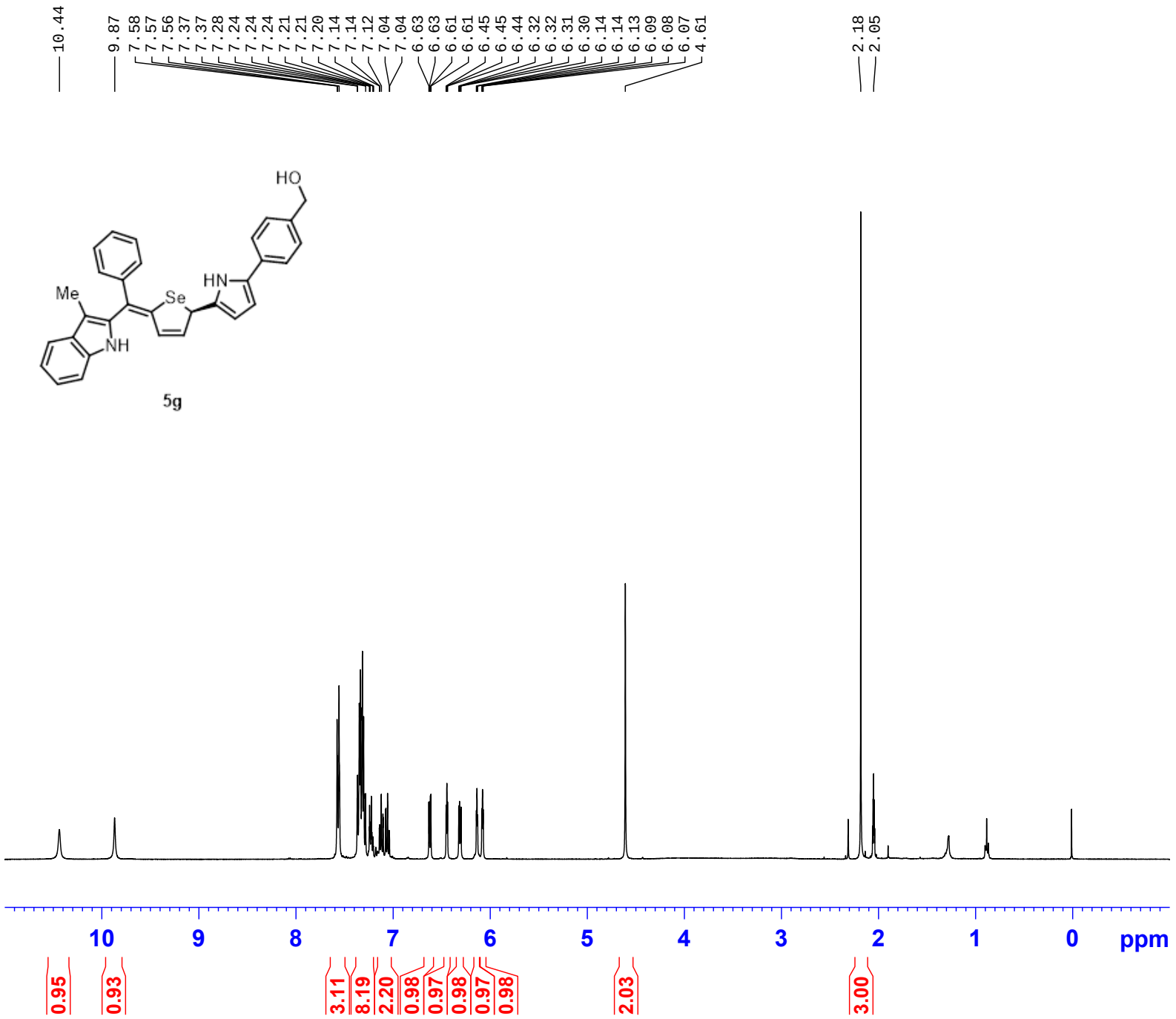
Supplementary Figure 124. ^{13}C NMR spectrum of **5f**



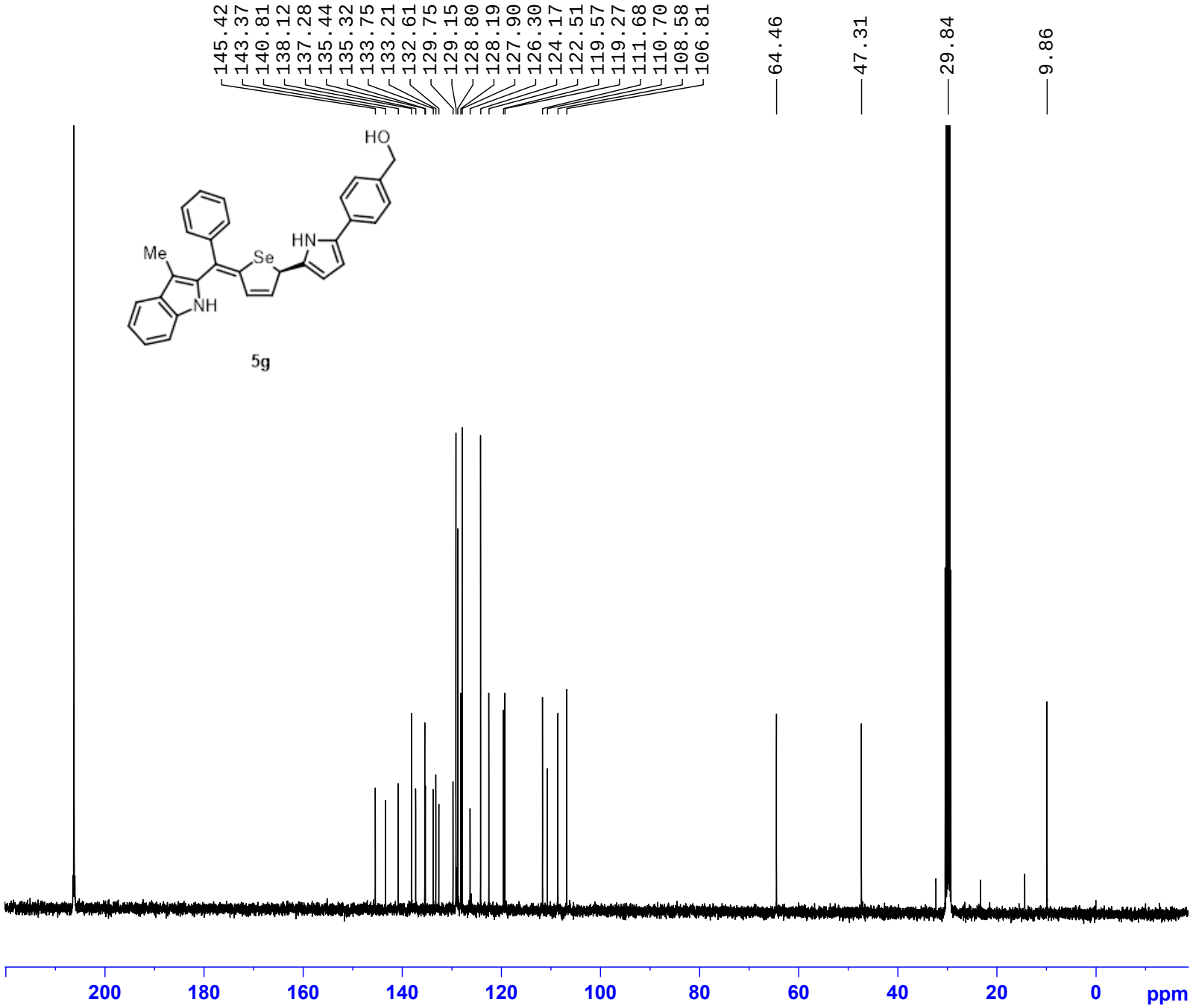

```
NAME           lxg-7081A
EXPNO                 11
PROCNO                 1
Date_           20200724
Time               15.04
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT          Acetone
NS                    16
DS                     0
SWH            93750.000 Hz
FIDRES          1.430511 Hz
AQ             0.3495753 sec
RG                196.92
DW                5.333 usec
DE                6.50 usec
TE                297.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         376.4607162 MHz
NUC1                 19F
P1                14.70 usec
SI                32768
SF           376.4983660 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Supplementary Figure 125. ^{19}F NMR spectrum of **5f**



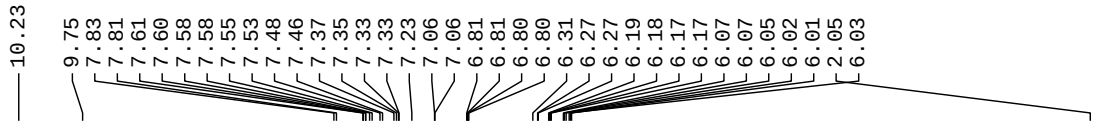
Supplementary Figure 126. ^{1}H NMR spectrum of **5g**

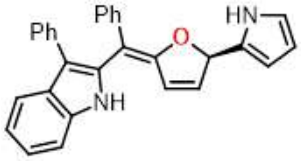



```
NAME          lxg-5074B-
EXPNO                  3
PROCNO                 1
Date_           20190824
Time               14.15
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   224
DS                     0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ           1.3631988 sec
RG                196.92
DW             20.800 usec
DE              6.50 usec
TE                297.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                  13C
P1                 9.70 usec
SI                 32768
SF          100.6126841 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```


Supplementary Figure 127. ^{13}C NMR spectrum of **5g**

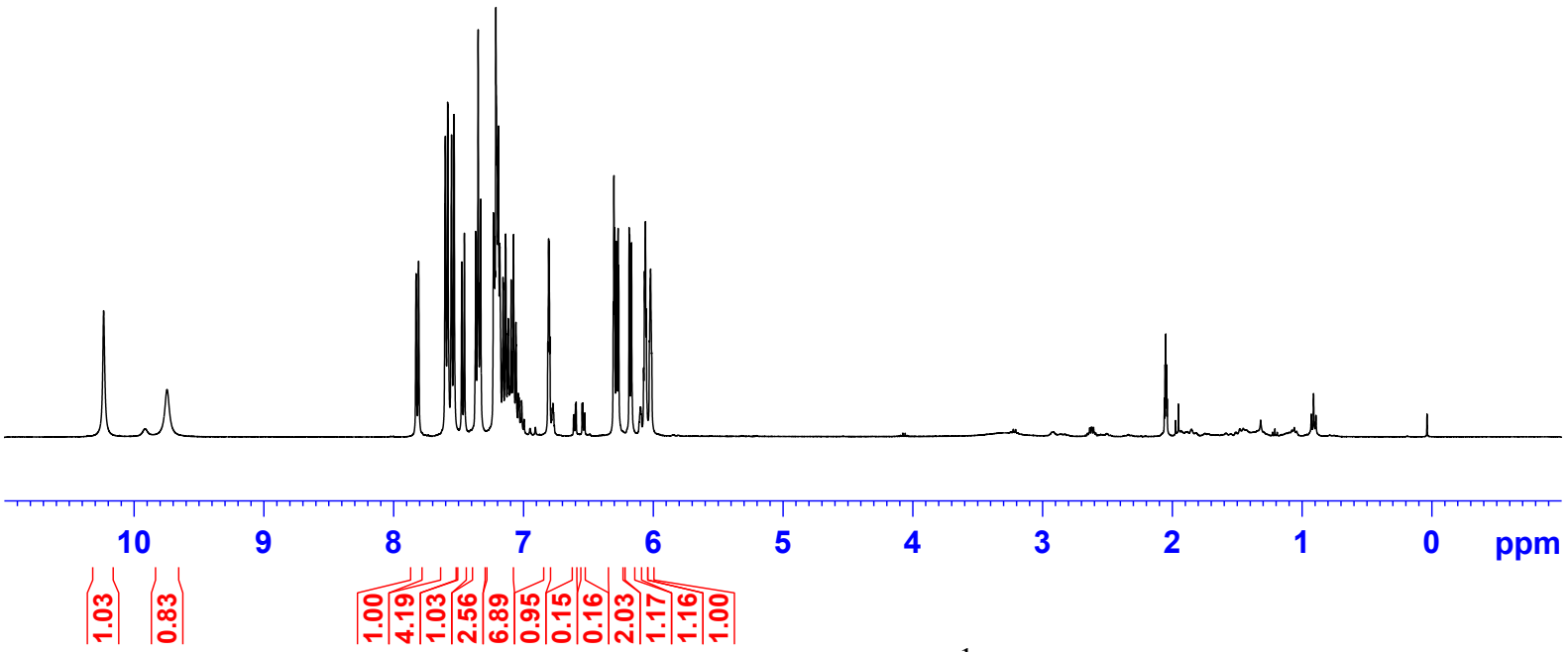




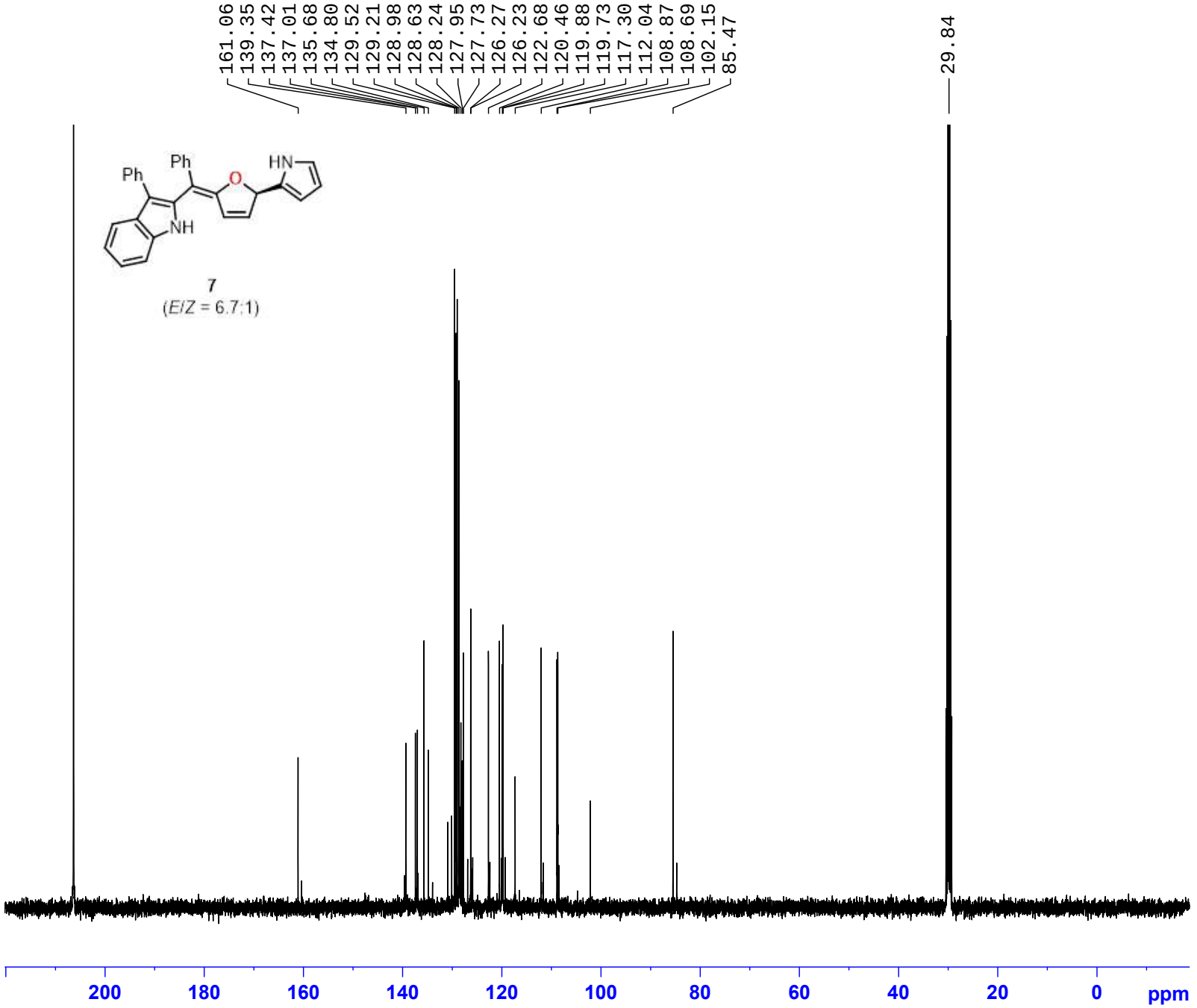
7
(*E*/*Z* = 6.7:1)

```
NAME           lxg-7090C
EXPNO                  1
PROCNO                 1
Date_           20200715
Time               19.56
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     4
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894966 sec
RG                 27.78
DW                62.400 usec
DE                 6.50 usec
TE                297.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                  1H
P1                 14.50 usec
SI                 65536
SF           400.1300069 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



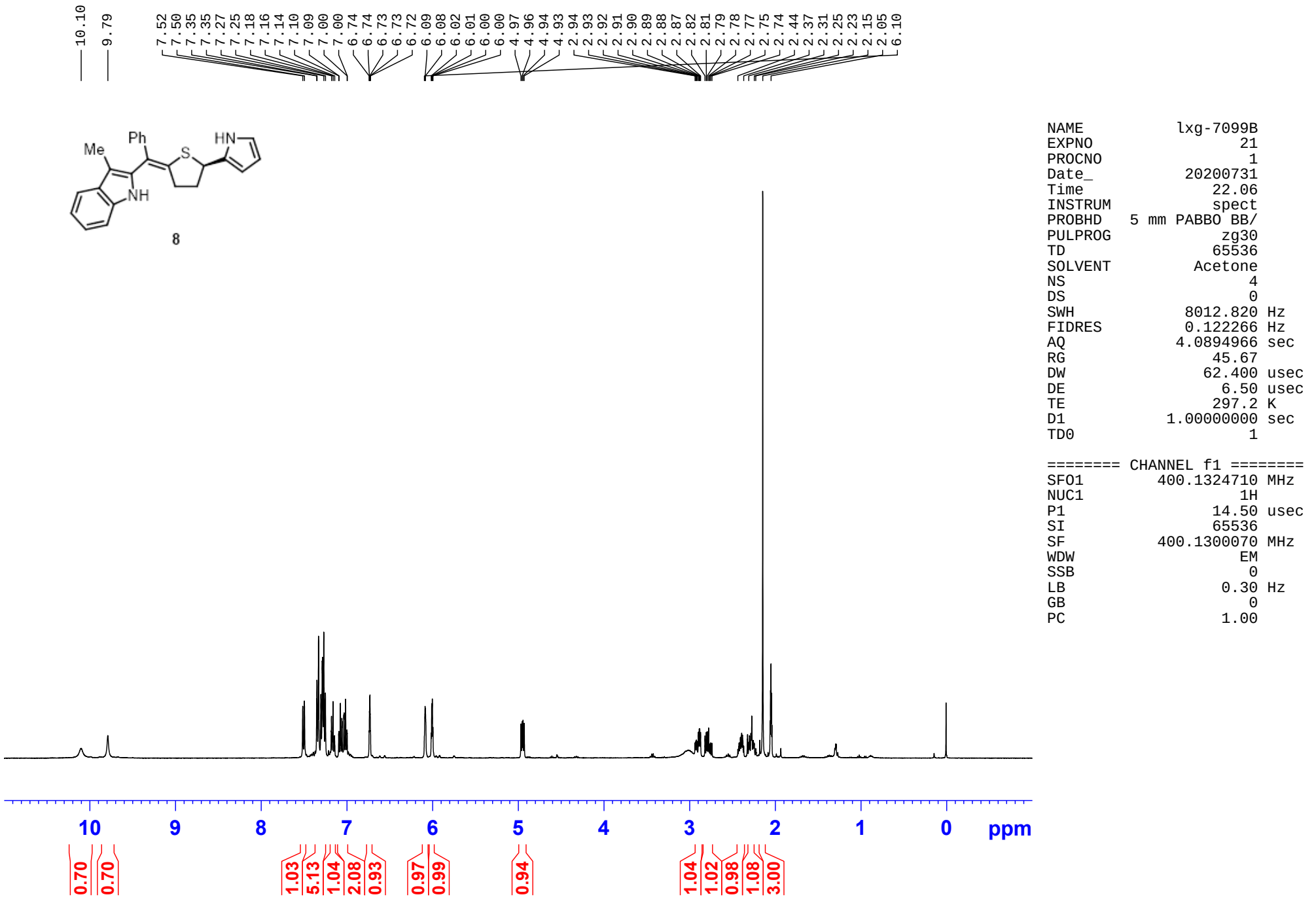
Supplementary Figure 128. ^{1}H NMR spectrum of **7**



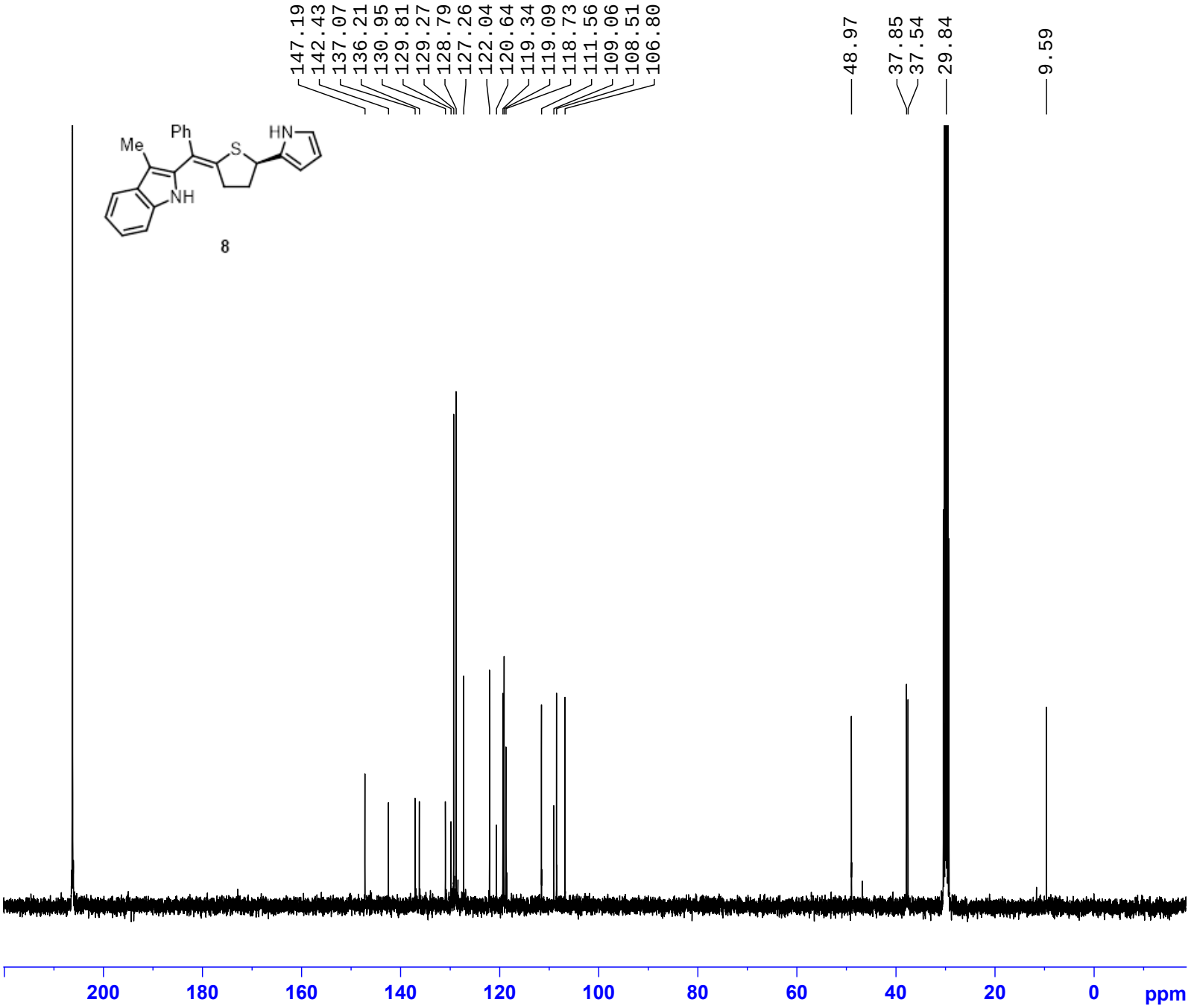

```
NAME            lxg-7090C
EXPNO                   2
PROCNO                  1
Date_            20200715
Time                20.00
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT           Acetone
NS                    101
DS                      0
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                 196.92
DW                 20.800 usec
DE                  6.50 usec
TE                 298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                 9.70 usec
SI                32768
SF           100.6126900 MHz
WDW                EM
SSB                 0
LB                 1.00 Hz
GB                  0
PC                 1.40
```

Supplementary Figure 129. ^{13}C NMR spectrum of **7**



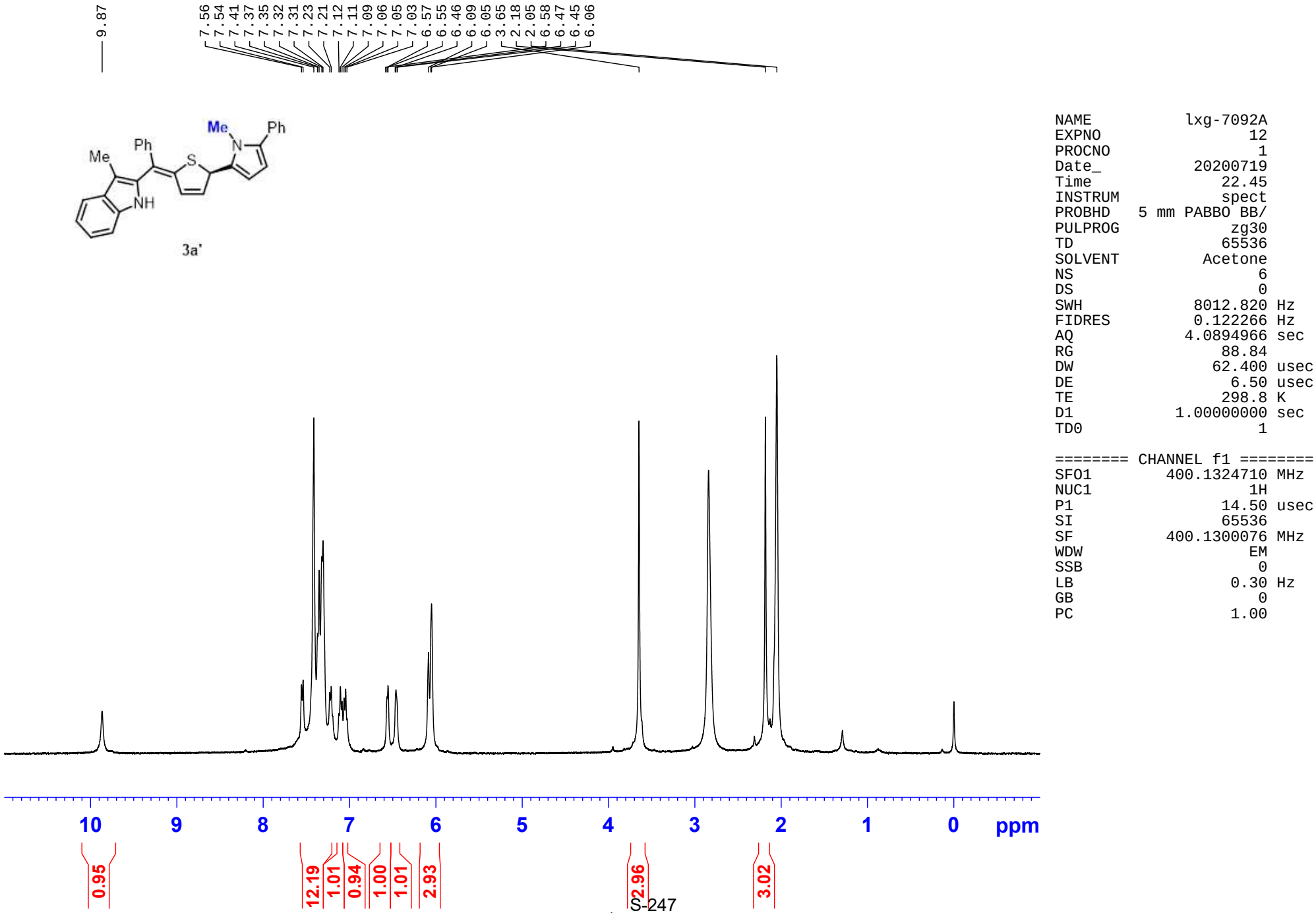
Supplementary Figure 13. ^{1}H NMR spectrum of **8**



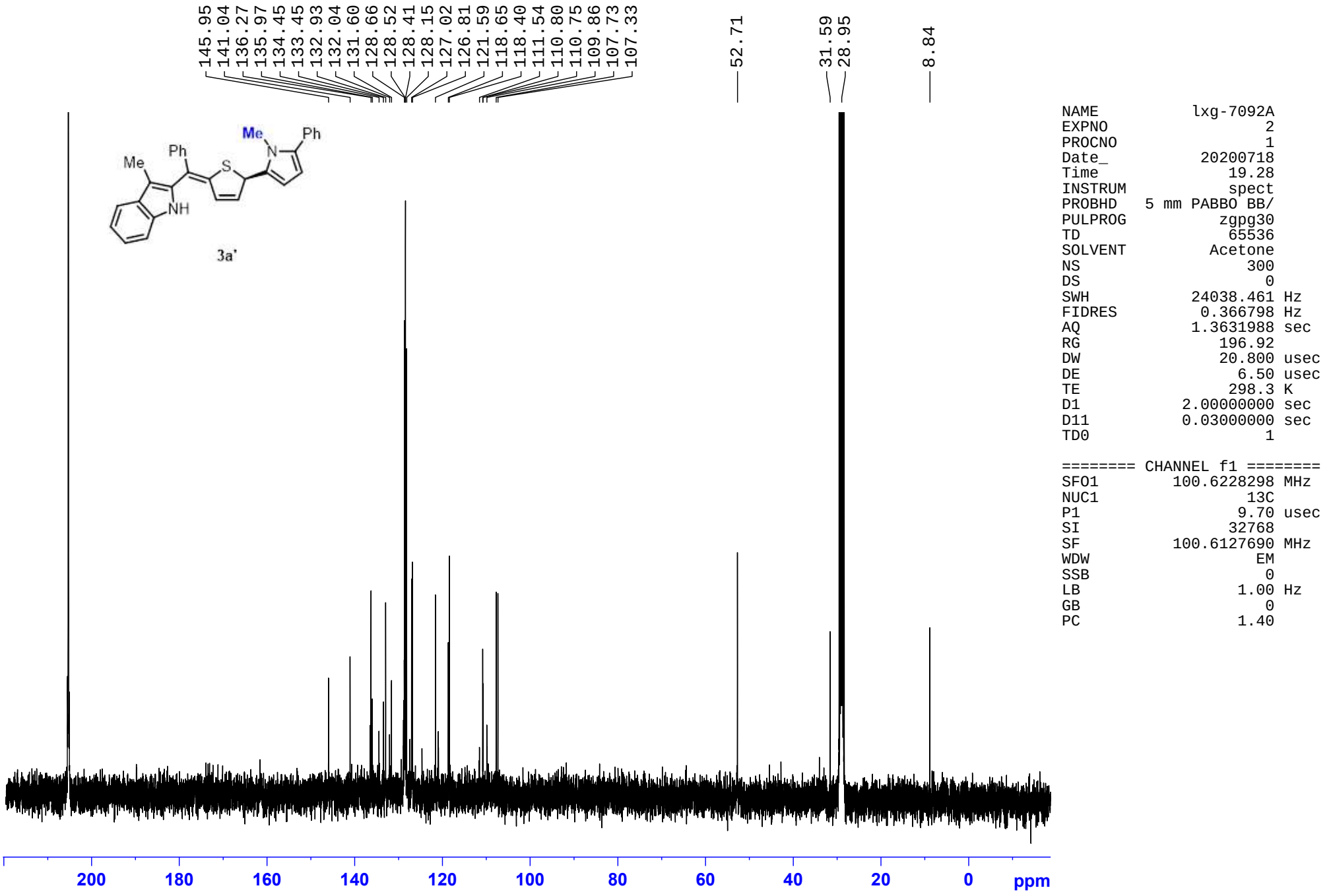

```
NAME           lxg-7099B
EXPNO                 12
PROCNO                 1
Date_           20200731
Time               19.19
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  154
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               297.5 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
SI                32768
SF          100.6126827 MHz
WDW                 EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

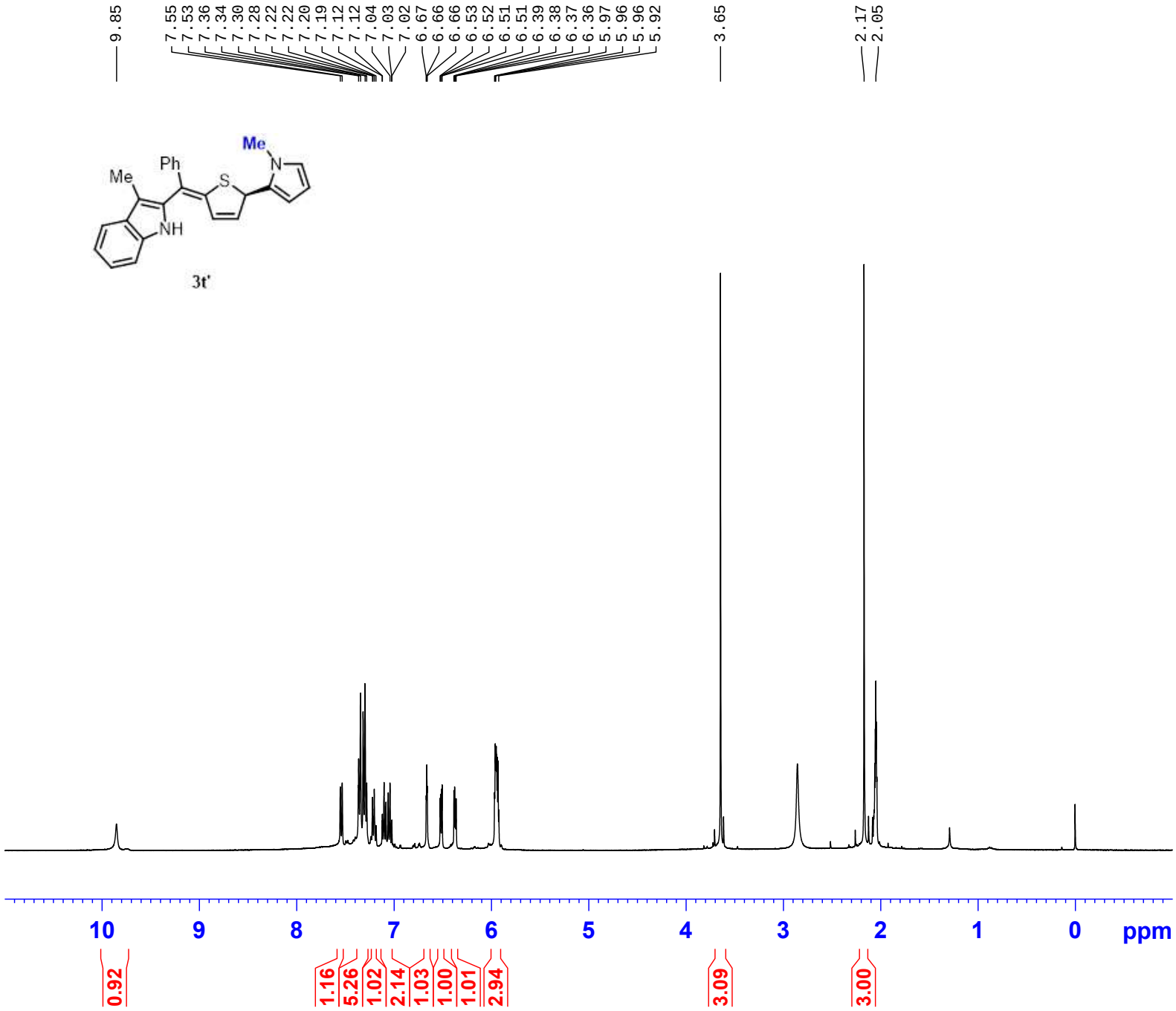

Supplementary Figure 131. ^{13}C NMR spectrum of **8**



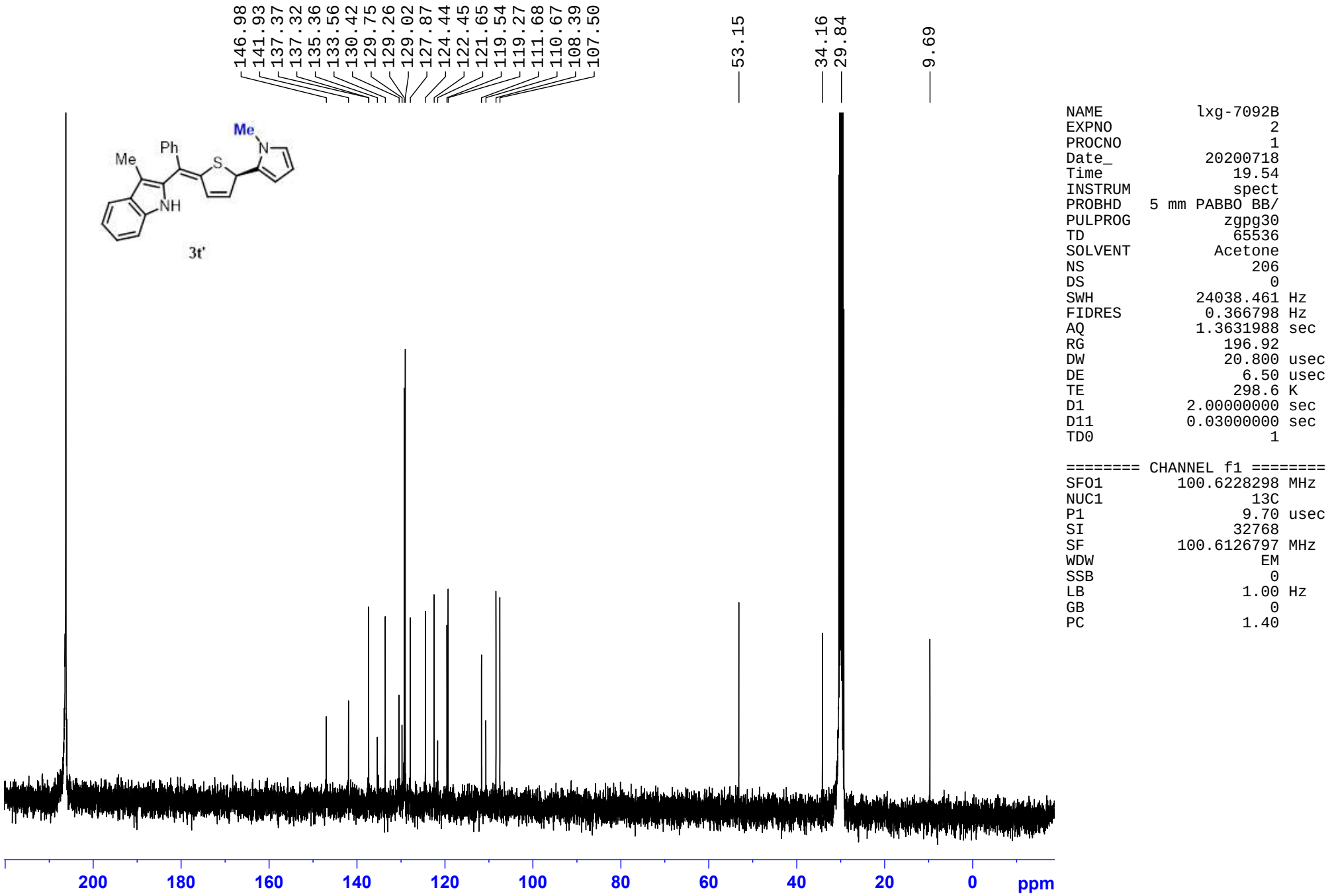
Supplementary Figure 132. ^{1}H NMR spectrum of **3a'**



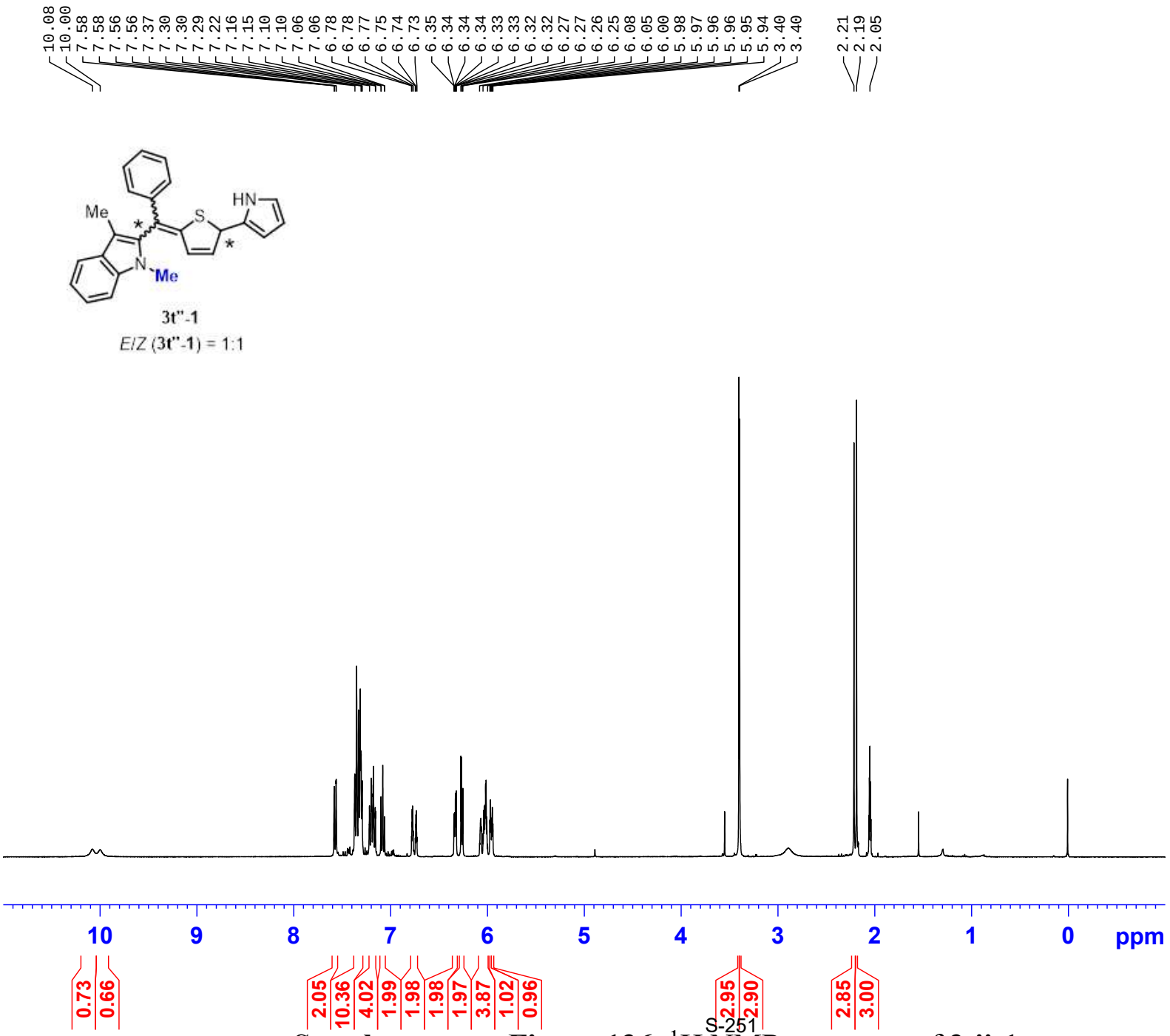
Supplementary Figure 133. ^{13}C NMR spectrum of **3a'**



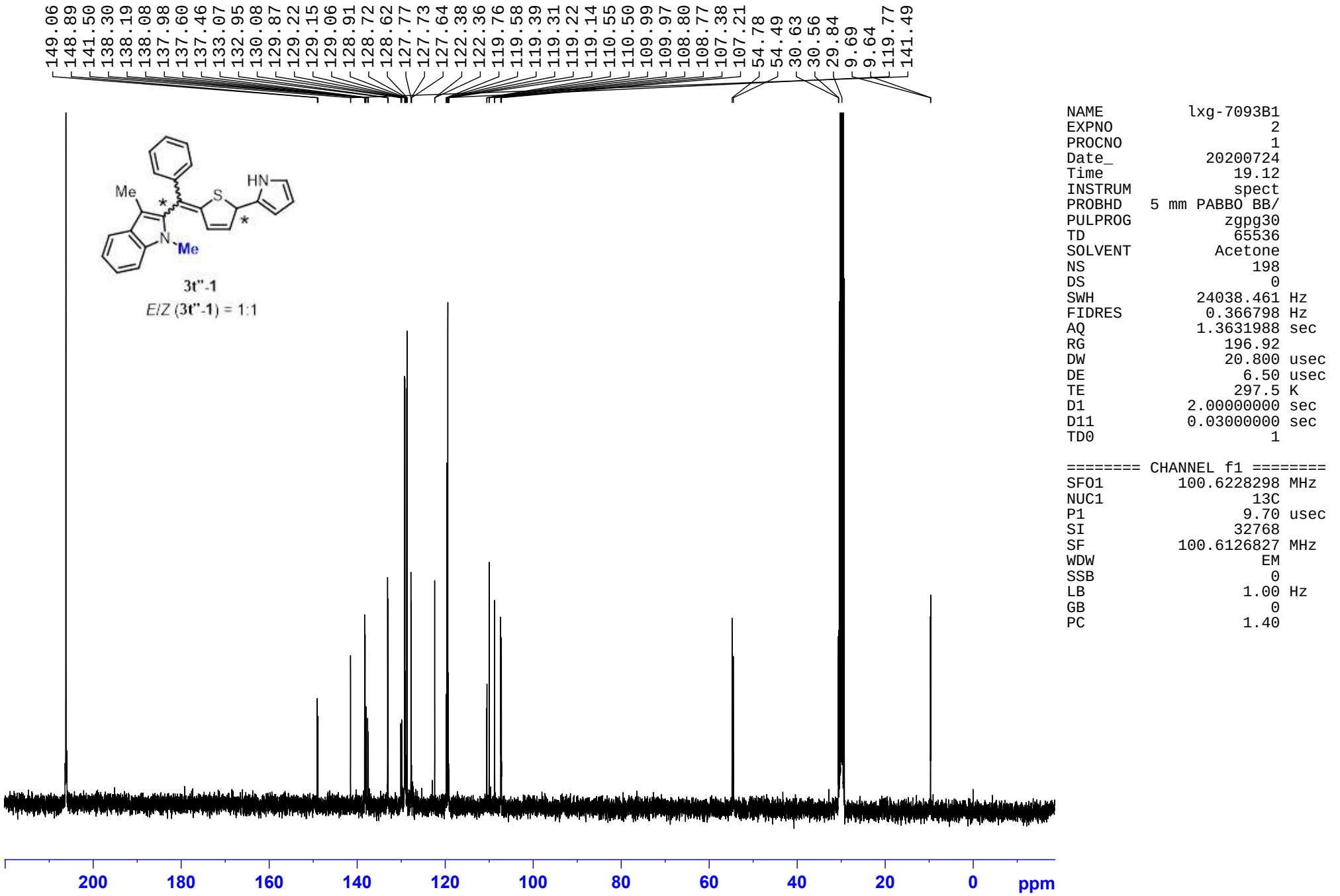
Supplementary Figure 134. ^{1}H NMR spectrum of **3t'**



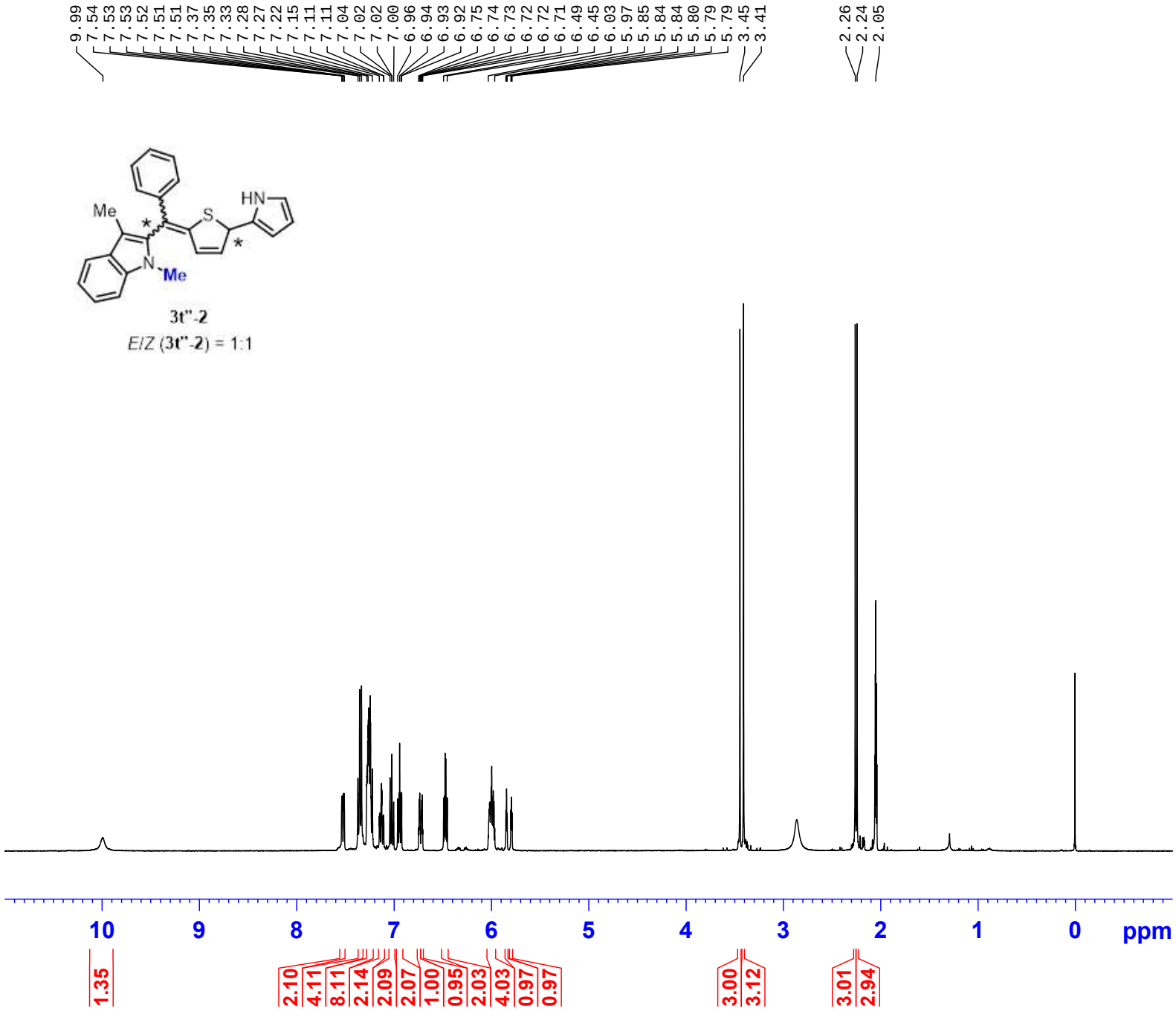
Supplementary Figure 135. ^{13}C NMR spectrum of **3t'**



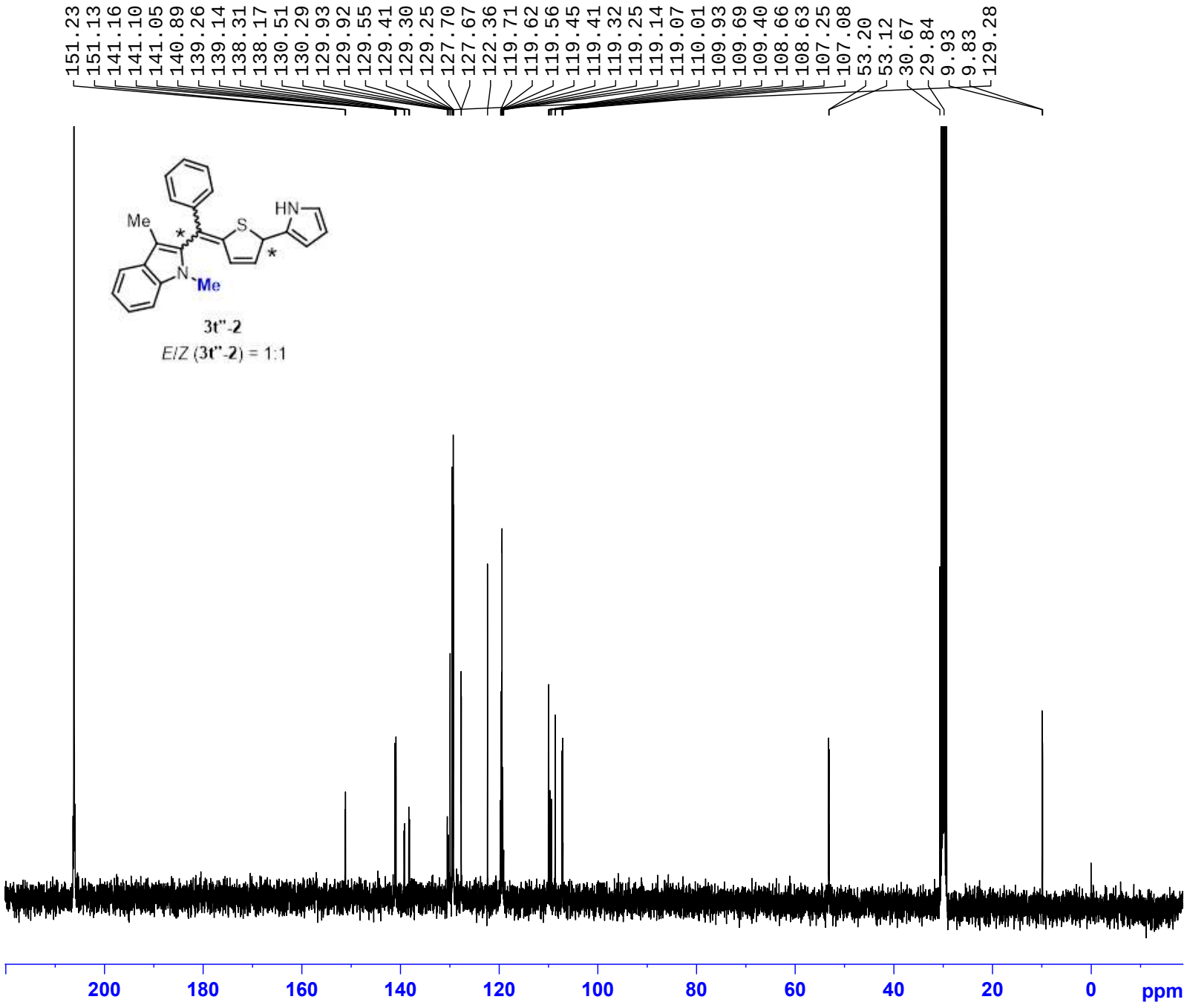
Supplementary Figure 136. ^{1}H NMR spectrum of **3t''-1**



Supplementary Figure 137. ^{13}C NMR spectrum of **3t''-1**



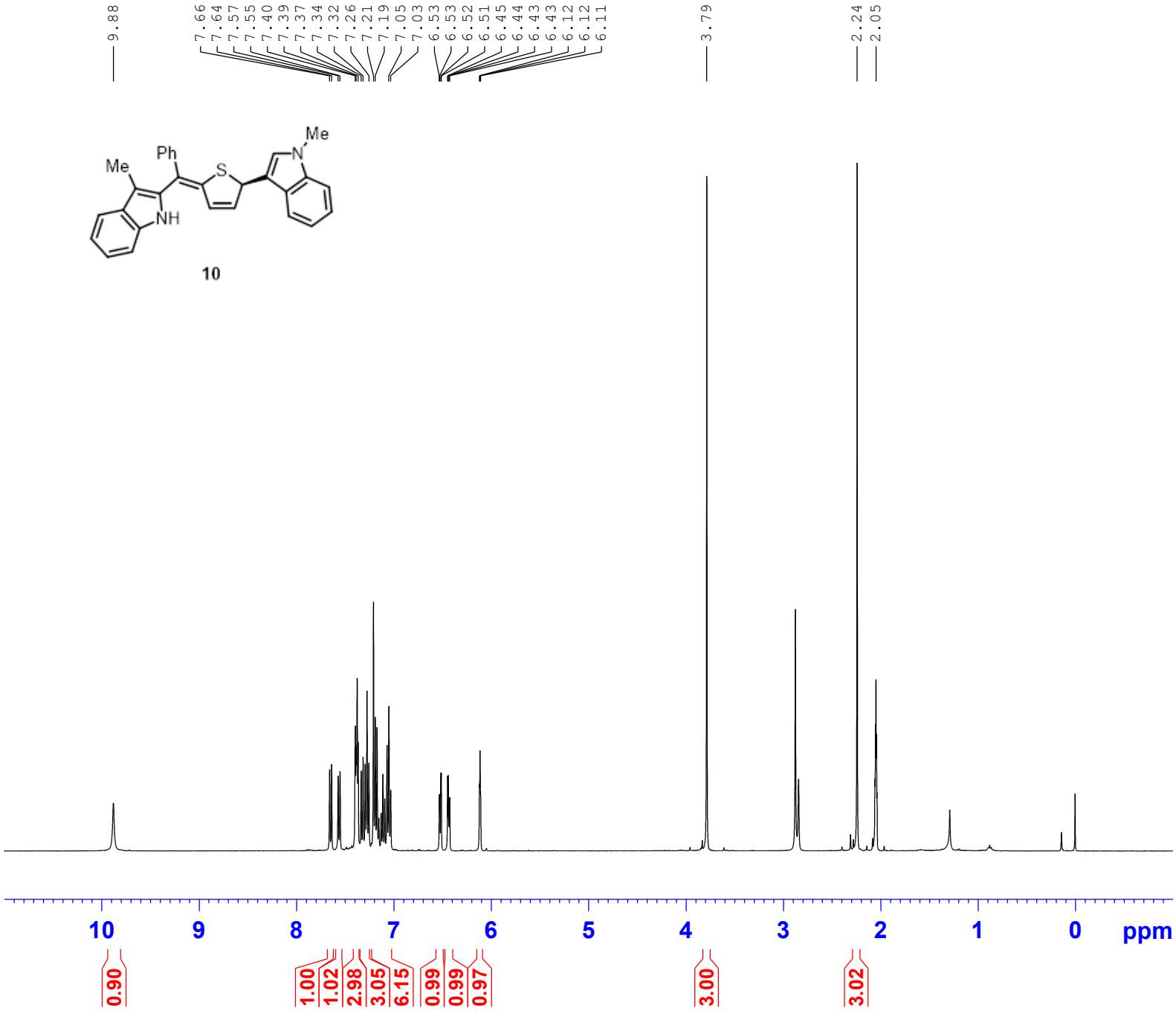
Supplementary Figure 138. ^{1}H NMR spectrum of **3t''-2**



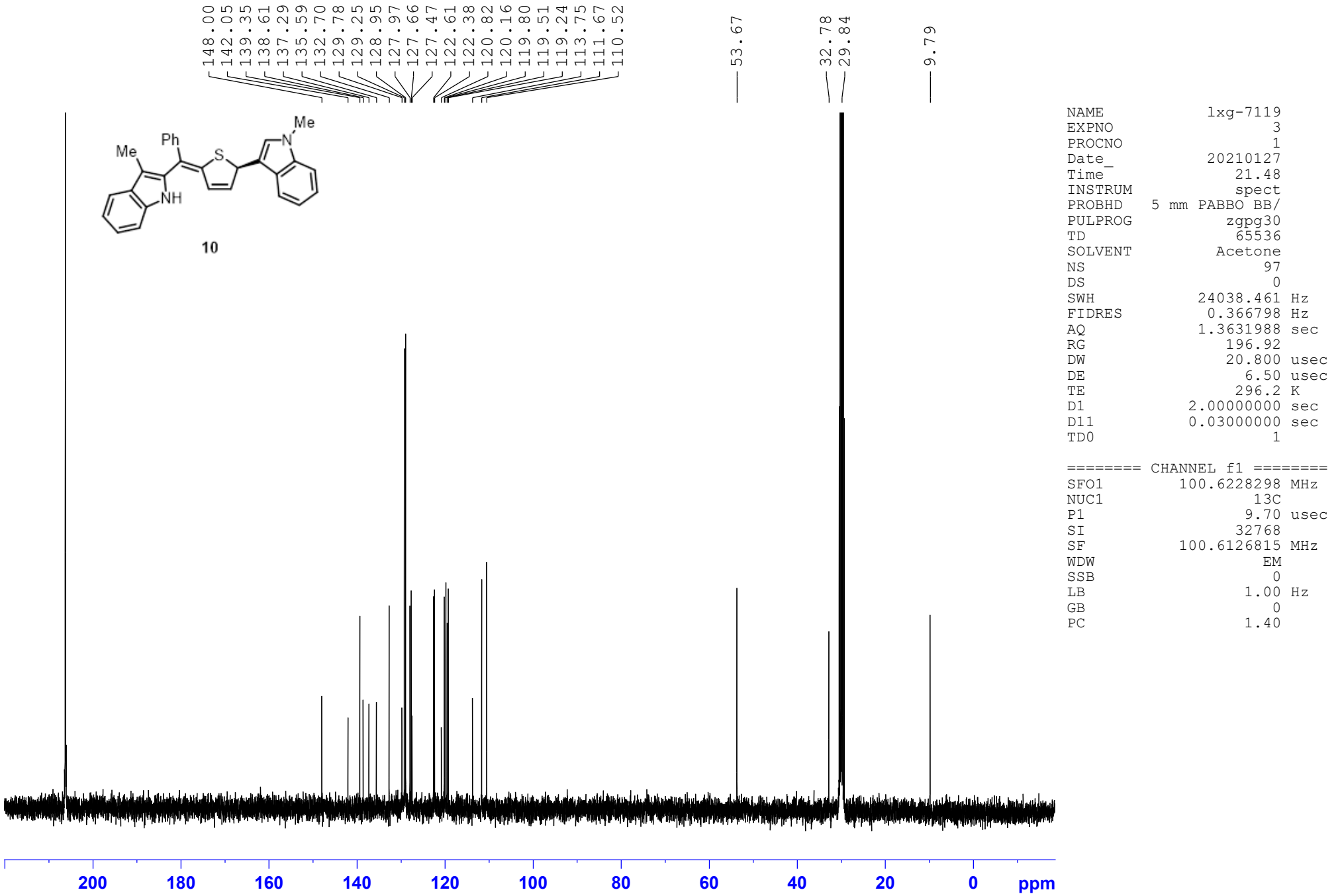

```
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EXPNO                  2
PROCNO                 1
Date_           20200724
Time               19.33
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  250
DS                    0
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                 9.70 usec
SI                32768
SF           100.6126805 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```


Supplementary Figure 139. ^{13}C NMR spectrum of **3t''-2**



Supplementary Figure 140. ^{1}H NMR spectrum of **10**

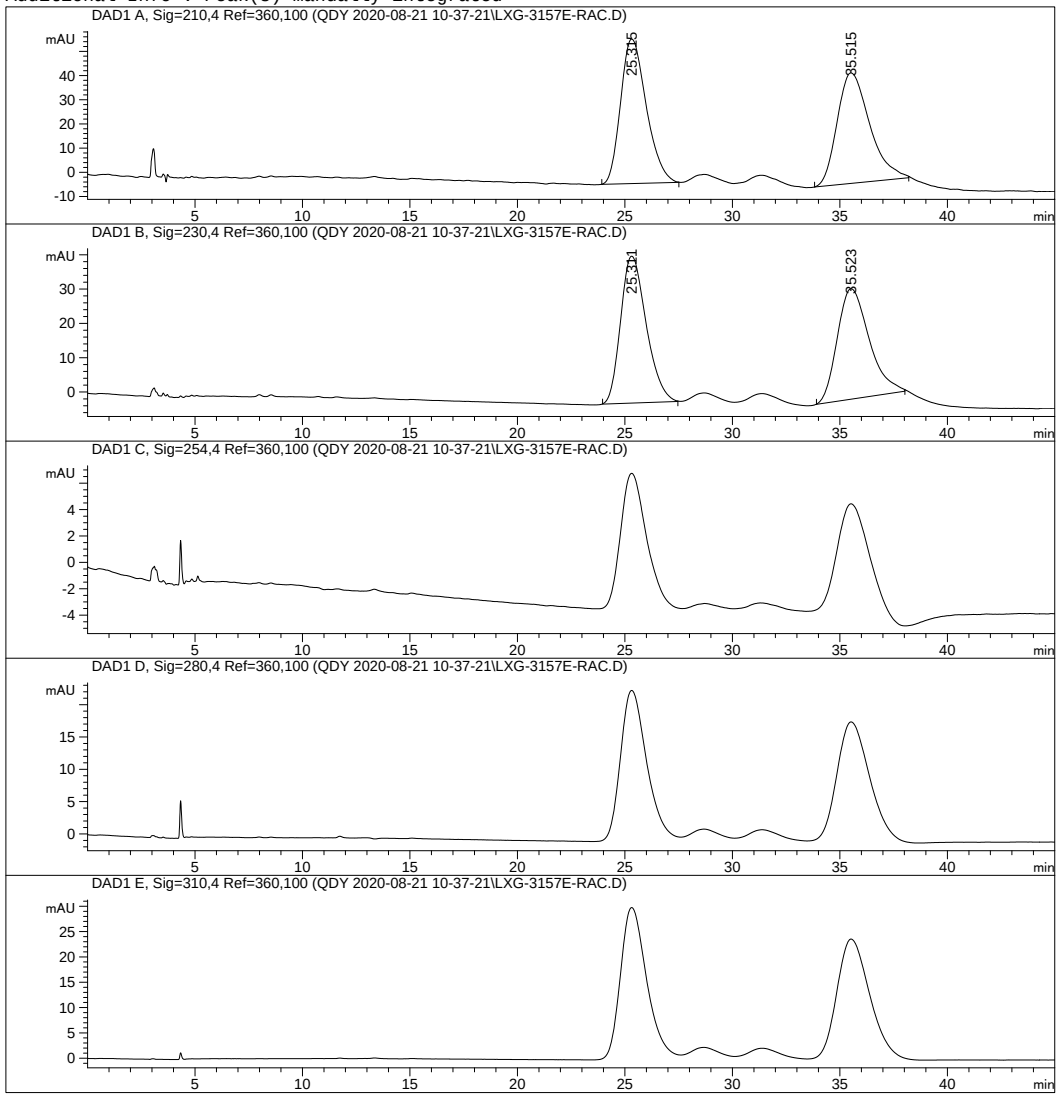


NAME	lxg-7119
EXPNO	3
PROCNO	1
Date_	20210127
Time	21.48
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	65536
SOLVENT	Acetone
NS	97
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	196.92
DW	20.800 usec
DE	6.50 usec
TE	296.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	100.6228298 MHz
NUC1	13C
P1	9.70 usec
SI	32768
SF	100.6126815 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Supplementary Figure 141. ^{13}C NMR spectrum of **10**

Data File C:\CHEM32\1\DATA\QDY 2020-08-21 10-37-21\LXG-3157E-RAC.D
Sample Name:

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Acq. Operator   :                                Seq. Line :   2
Acq. Instrument : Instrument 1                    Location : Vial 62
Injection Date  : 8/21/2020 10:50:24 AM              Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-08-21 10-37-21\OD-10-45.M
Last changed    : 1/4/2019 2:01:36 PM
Analysis Method : C:\CHEM32\1\METHODS\OD-01-45-0.5.M
Last changed    : 8/20/2020 10:26:25 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-08-21 10-37-21\LXG-3157E-RAC.D
Sample Name:

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                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  25.315 BB    1.1874 4961.68115   59.71409  50.7872
   2  35.515 BB    1.3096 4807.87109   45.69316  49.2128

Totals :                  9769.55225  105.40725



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  25.311 BB    1.2761 3536.50269   42.79575  51.6442
   2  35.523 BB    1.5276 3311.31250   32.20456  48.3558

Totals :                  6847.81519   75.00031

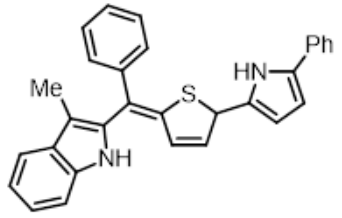


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



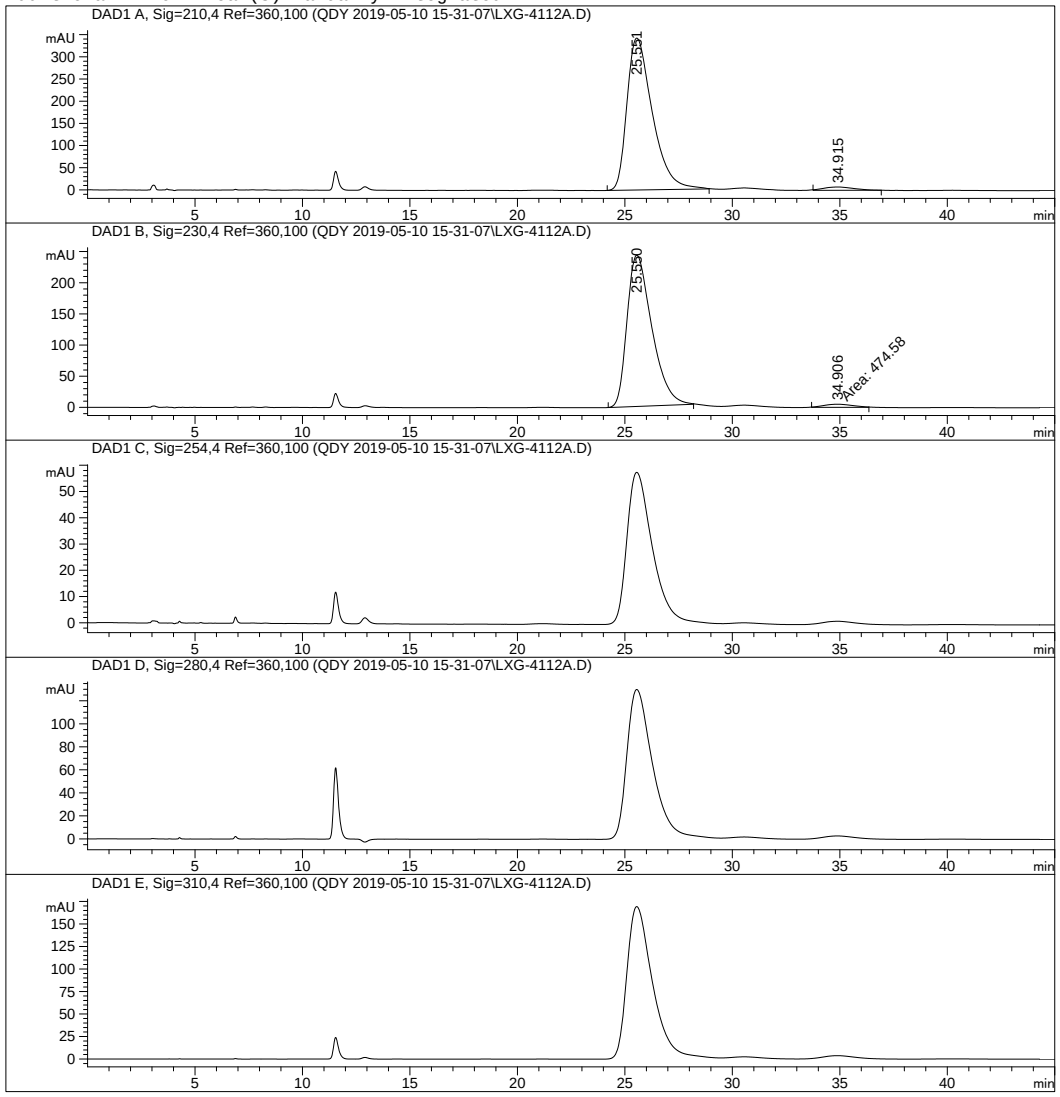
3a
(racemic)

Supplementary Figure 142. HPLC spectrum of **3a** (racemic)

Instrument 1 8/21/2020 7:51:44 PM

Data File C:\CHEM32\1\DATA\QDY 2019-05-10 15-31-07\LXG-4112A.D
Sample Name:

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Acq. Operator   :                                Seq. Line :  23
Acq. Instrument : Instrument 1                    Location : Vial 78
Injection Date  : 5/11/2019 1:03:51 AM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-05-10 15-31-07\OD-10-45.M
Last changed    : 1/4/2019 2:01:36 PM
Analysis Method : C:\CHEM32\1\METHODS\AD-07-60.M
Last changed    : 5/10/2019 8:11:55 PM
Additional Info : Peak(s) manually integrated
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Data File C:\CHEM32\1\DATA\QDY 2019-05-10 15-31-07\LXG-4112A.D
Sample Name:

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==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  25.551 BB    1.2333 2.80972e4   342.43576  97.5087
   2  34.915 BB    1.1400  717.87836    7.38589   2.4913

Totals :                  2.88150e4   349.82165



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  25.550 BB    1.2127 1.94362e4   242.58496  97.6165
   2  34.906 MM    1.5723  474.58044    5.03063   2.3835

Totals :                  1.99108e4   247.61560

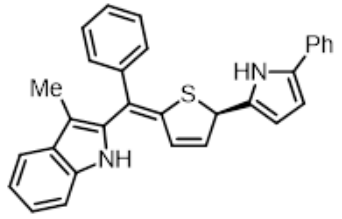


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

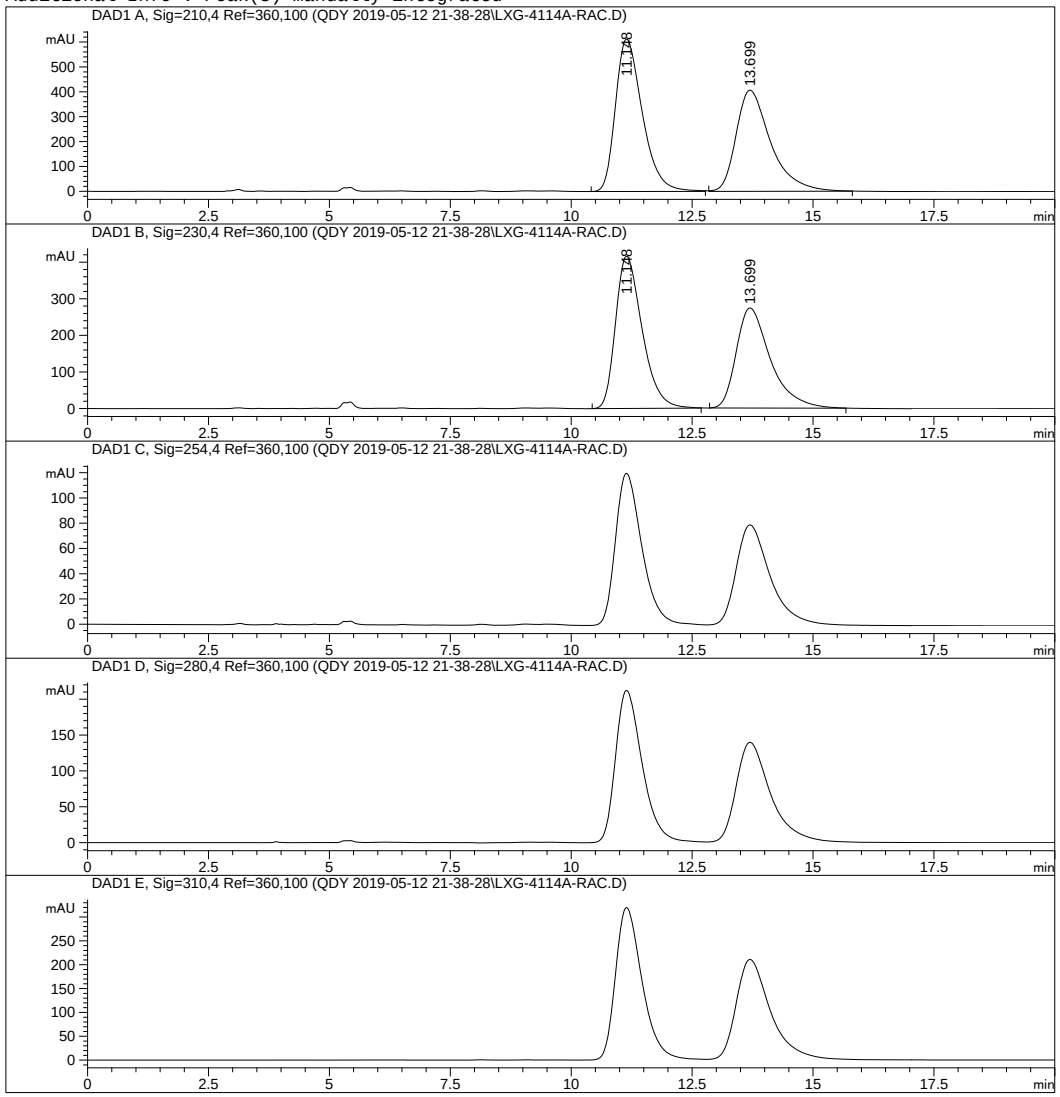


3a
(enantioenriched)

Supplementary Figure 143. HPLC spectrum of **3a** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2019-05-12 21-38-28\LXG-4114A-RAC.D
Sample Name:

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Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location : Vial 74
Injection Date  : 5/12/2019 9:51:36 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-05-12 21-38-28\OD-20-40.M
Last changed    : 5/12/2019 9:50:42 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-07-60.M
Last changed    : 5/14/2019 9:50:00 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-05-12 21-38-28\LXG-4114A-RAC.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.148 BB    0.5940 2.36213e4   612.36841  53.9615
   2  13.699 BB    0.7485 2.01531e4   406.44949  46.0385

Totals :                  4.37744e4  1018.81790



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.148 BB    0.5876 1.58890e4   415.99933  54.1782
   2  13.699 BB    0.7412 1.34383e4   273.52963  45.8218

Totals :                  2.93273e4   689.52896

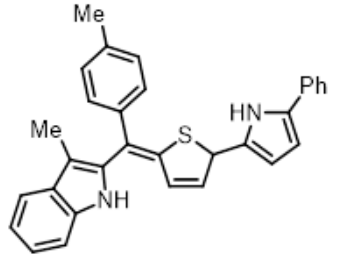


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```

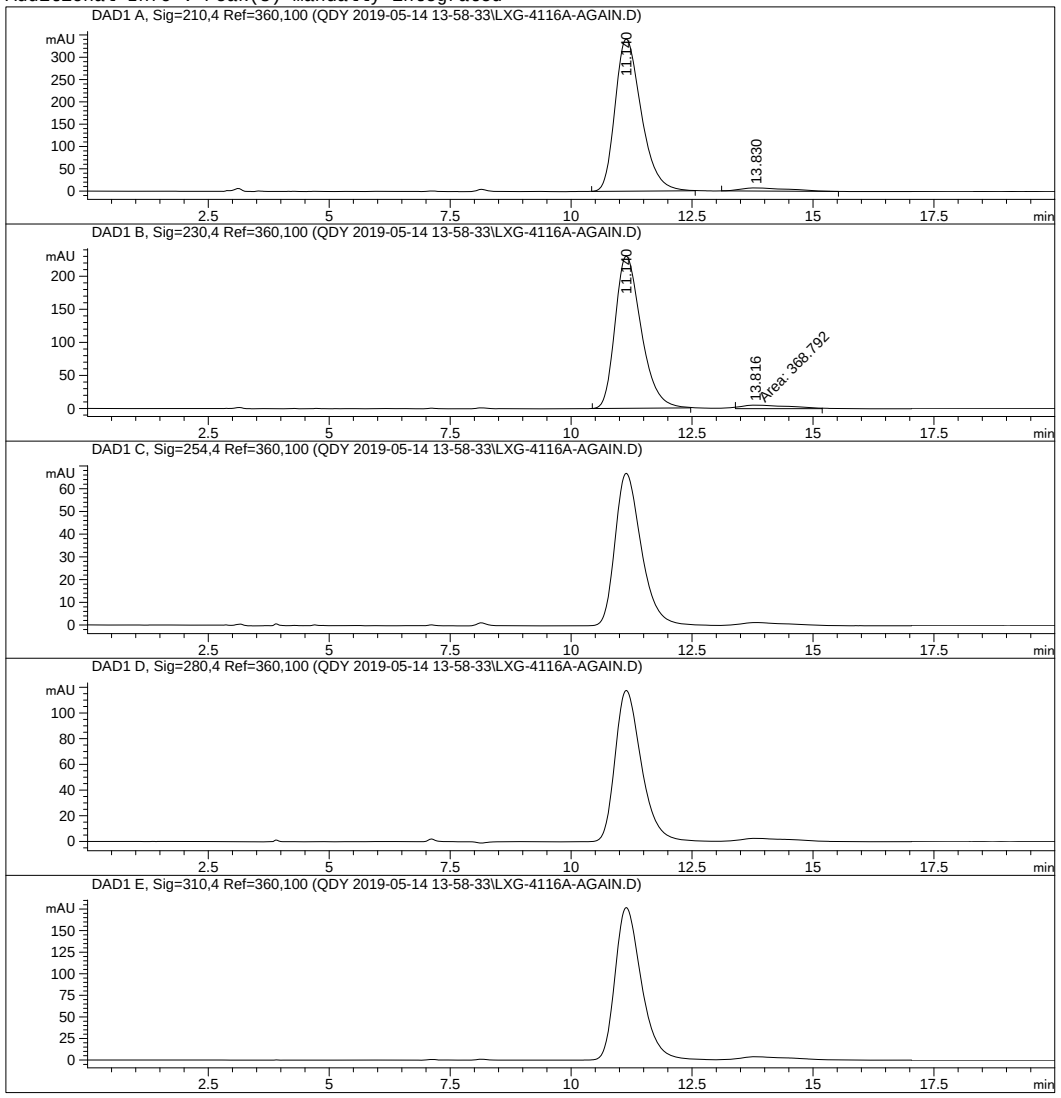


3b
(racemic)

Supplementary Figure 144. HPLC spectrum of **3b** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2019-05-14 13-58-33\LXG-4116A-AGAIN.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :  11
Acq. Instrument : Instrument 1                  Location : Vial 71
Injection Date  : 5/14/2019 5:03:43 PM               Inj :   1
                                               Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-05-14 13-58-33\OD-20-20.M
Last changed    : 1/7/2016 10:22:18 AM
Analysis Method : C:\CHEM32\1\METHODS\AD-07-60.M
Last changed    : 5/11/2019 10:45:40 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-05-14 13-58-33\LXG-4116A-AGAIN.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.140 BB    0.5783 1.28095e4   340.94614  96.2167
   2  13.830 BB    0.8642  503.67200    7.18166   3.7833

Totals :                  1.33132e4   348.12780



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.140 BB    0.5749 8615.99609  230.06705  95.8954
   2  13.816 MM    1.1363  368.79227    5.40923   4.1046

Totals :                  8984.78836  235.47627

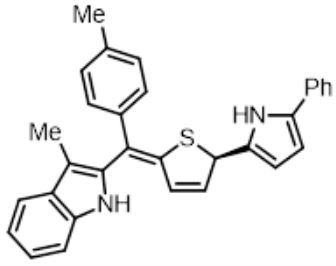


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

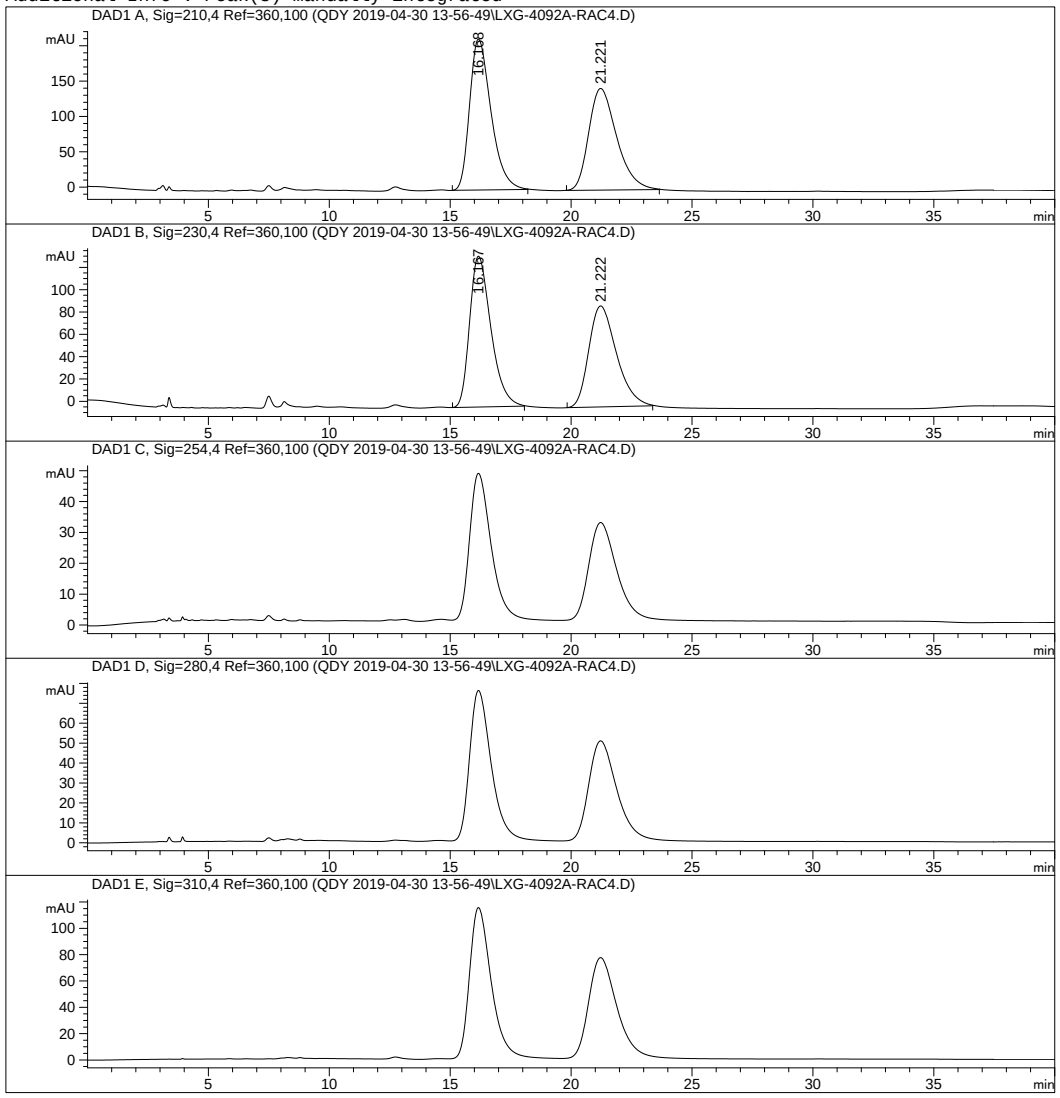


3b
(enantioenriched)

Supplementary Figure 145. HPLC spectrum of **3b** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2019-04-30 13-56-49\LXG-4092A-RAC4.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  20
Acq. Instrument : Instrument 1              Location : Vial 64
Injection Date  : 4/30/2019 10:13:48 PM          Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-04-30 13-56-49\OD-20-40.M
Last changed    : 4/30/2019 10:12:53 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-07-60.M
Last changed    : 5/10/2019 8:11:55 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-04-30 13-56-49\LXG-4092A-RAC4.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.168 BB    0.9450 1.31236e4   213.53802  53.1241
   2  21.221 BB    1.2213 1.15801e4   143.82903  46.8759

Totals :                  2.47036e4   357.36705



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.167 BB    0.9437 8262.72656  135.06790  53.4149
   2  21.222 BB    1.2216 7206.22119   90.43851  46.5851

Totals :                  1.54689e4   225.50641

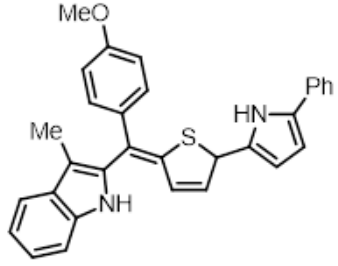


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```



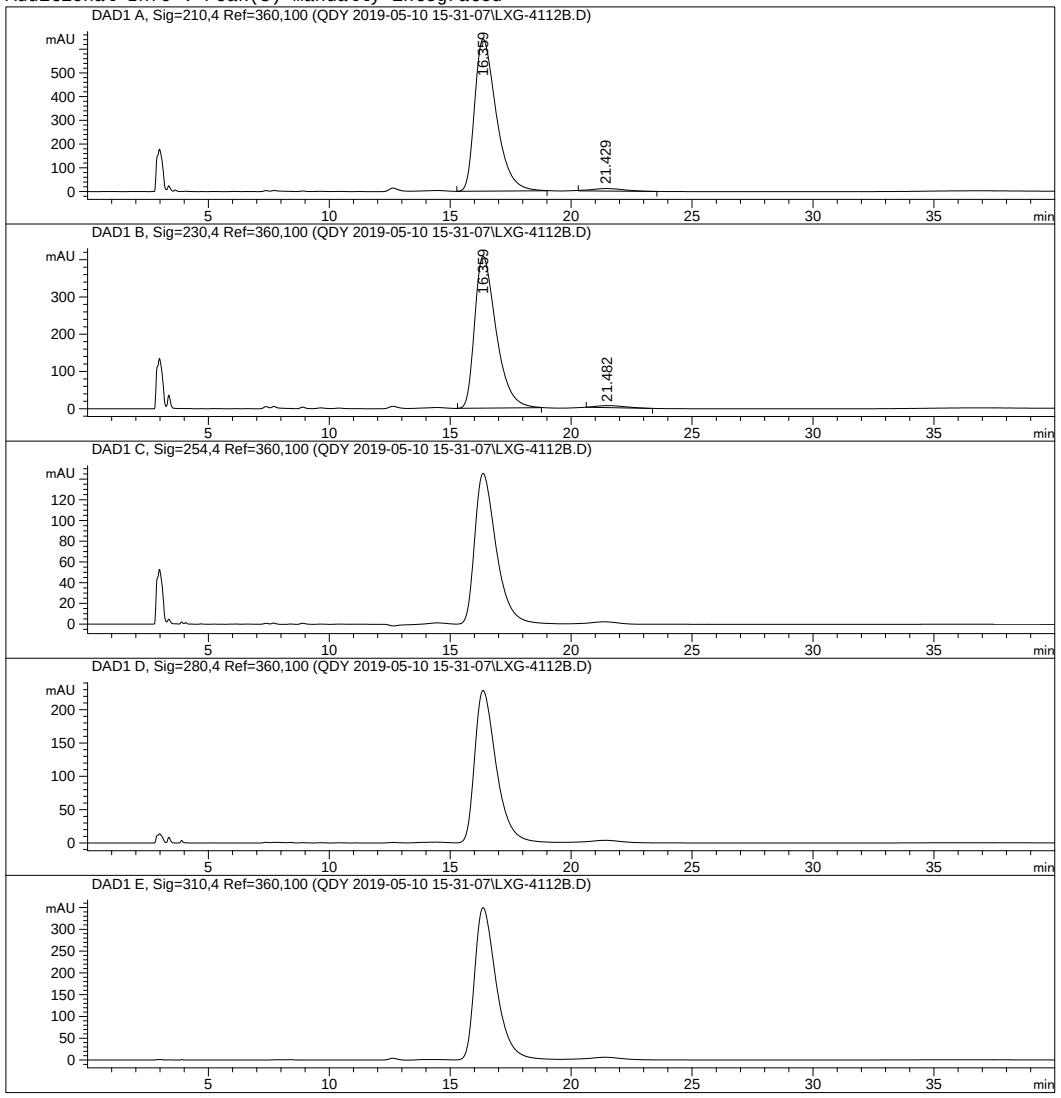
3c
(racemic)

Supplementary Figure 146. HPLC spectrum of **3c** (racemic)

Instrument 1 5/11/2019 10:32:51 AM

Data File C:\CHEM32\1\DATA\QDY 2019-05-10 15-31-07\LXG-4112B.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  25
Acq. Instrument : Instrument 1              Location : Vial 79
Injection Date  : 5/11/2019 2:01:39 AM           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-05-10 15-31-07\OD-20-40.M
Last changed    : 5/11/2019 2:00:46 AM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-07-60.M
Last changed    : 5/10/2019 8:11:55 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-05-10 15-31-07\LXG-4112B.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.359 BB    0.9547 3.96769e4   640.54059  97.5310
   2  21.429 BB    1.1596 1004.41107   10.73484   2.4690

Totals :                  4.06813e4   651.27542



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.359 BB    0.9498 2.50930e4   407.84644  98.2266
   2  21.482 BB    1.0759  453.02261    5.37173   1.7734

Totals :                  2.55460e4   413.21817

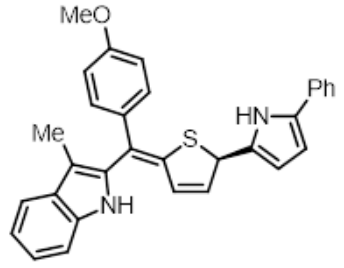


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```

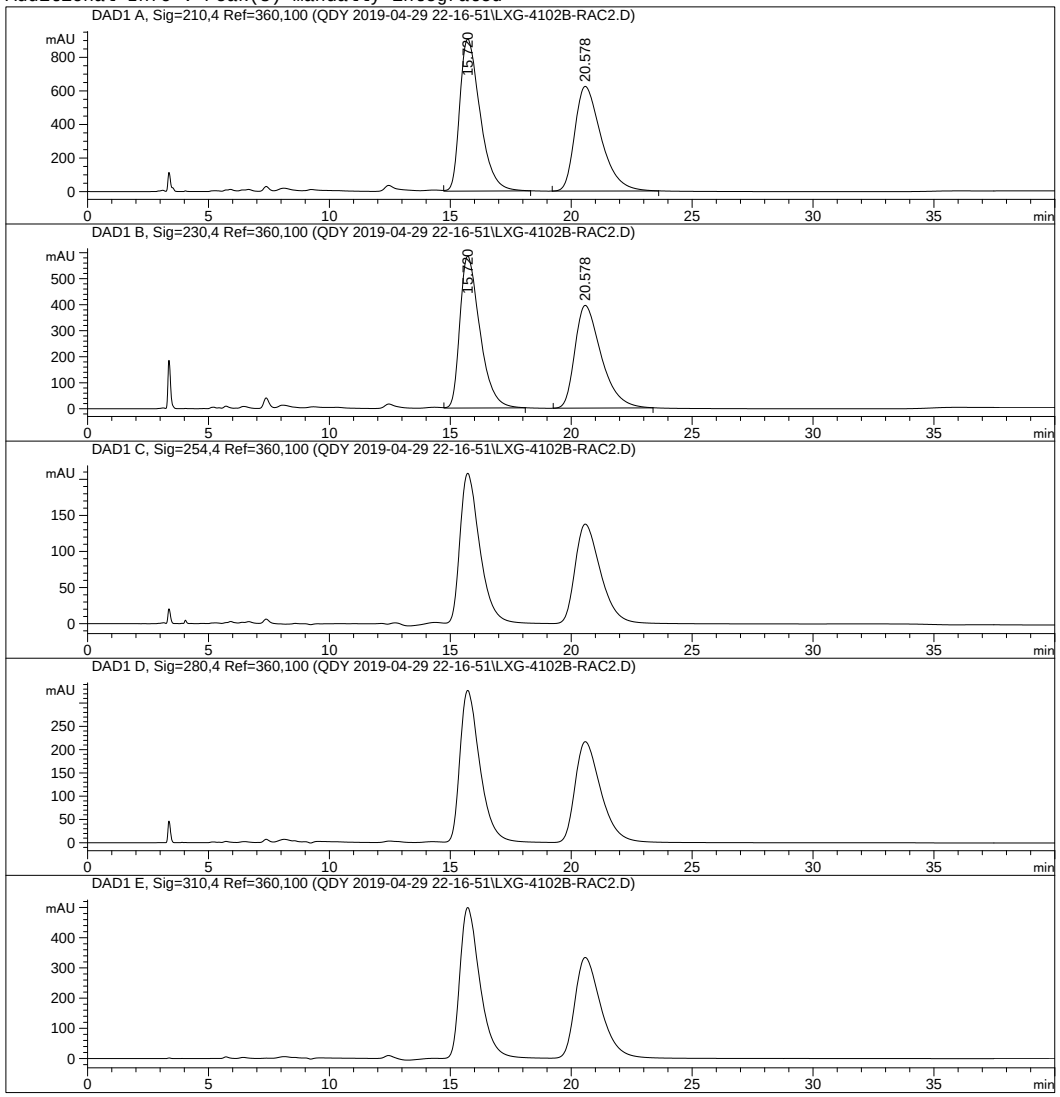


3c
(enantioenriched)

Supplementary Figure 147. HPLC spectrum of **3c** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2019-04-29 22-16-51\LXG-4102B-RAC2.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  11
Acq. Instrument : Instrument 1              Location : Vial 62
Injection Date  : 4/30/2019 3:22:49 AM           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-04-29 22-16-51\OD-20-60.M
Last changed    : 4/30/2019 2:20:20 AM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-07-60.M
Last changed    : 5/11/2019 10:41:57 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-04-29 22-16-51\LXG-4102B-RAC2.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.720 VB    0.8926 5.27028e4   906.06335  52.6512
   2  20.578 BB    1.1581 4.73952e4   623.99194  47.3488

Totals :                  1.00098e5  1530.05530



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.720 VB    0.8745 3.34375e4   583.57526  52.7437
   2  20.578 BB    1.1531 2.99586e4   394.87662  47.2563

Totals :                  6.33961e4   978.45187

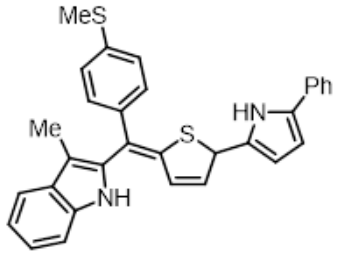


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```



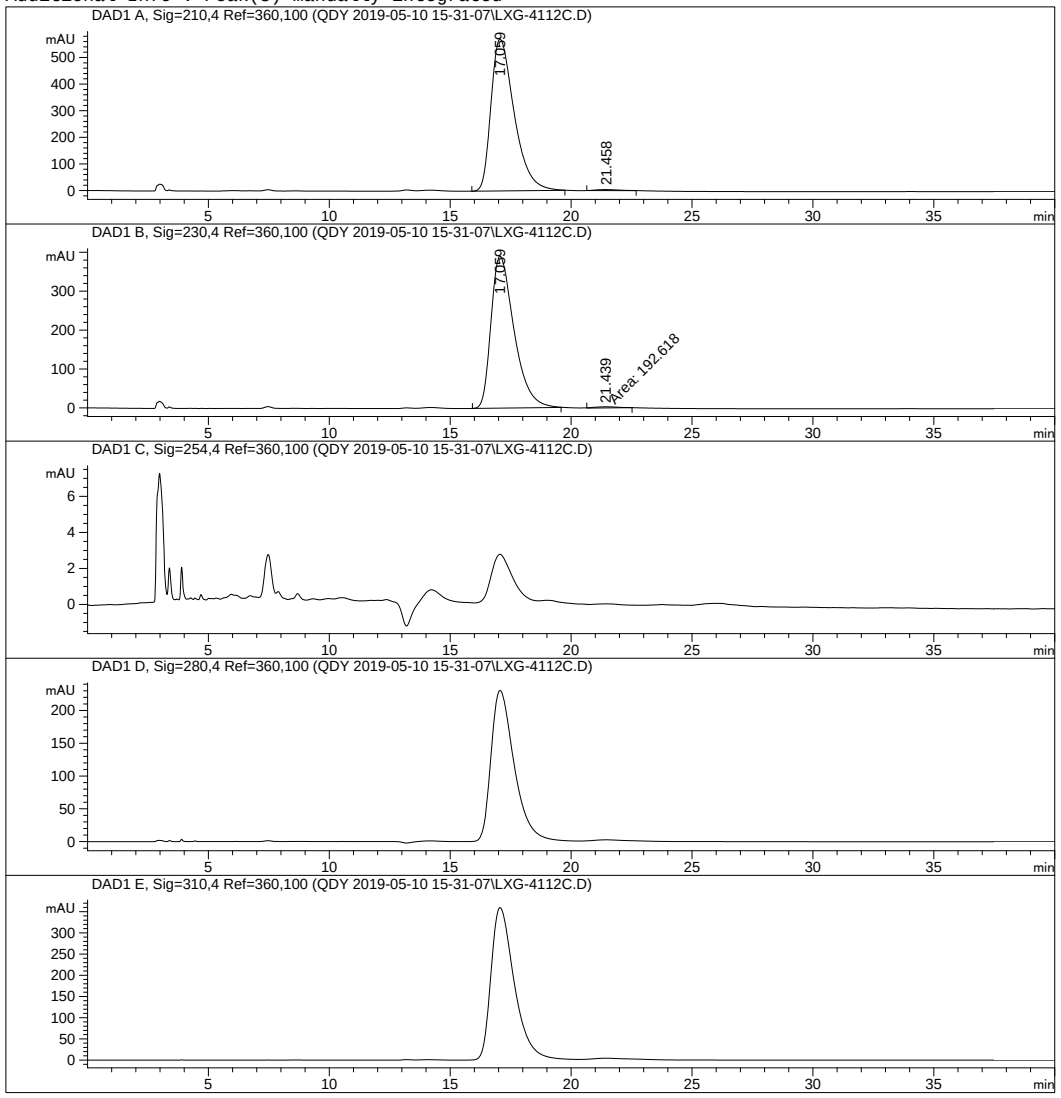
3d
(racemic)

Supplementary Figure 148. HPLC spectrum of **3d** (racemic)

Instrument 1 5/11/2019 10:42:05 AM

Data File C:\CHEM32\1\DATA\QDY 2019-05-10 15-31-07\LXG-4112C.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :  26
Acq. Instrument : Instrument 1                    Location : Vial 80
Injection Date  : 5/11/2019 2:42:47 AM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-05-10 15-31-07\OD-20-40.M
Last changed    : 5/11/2019 2:00:46 AM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-07-60.M
Last changed    : 5/10/2019 8:11:55 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-05-10 15-31-07\LXG-4112C.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.059 BB    1.0195 3.80362e4   570.76141  99.3399
   2  21.458 BB    0.7876  252.76334    3.81169   0.6601

Totals :                  3.82890e4   574.57310



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.059 BB    1.0122 2.58474e4   390.51089  99.2603
   2  21.439 MM    1.1052  192.61755    2.90478   0.7397

Totals :                  2.60401e4   393.41568

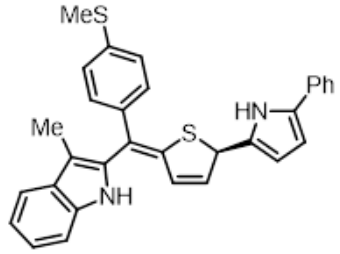


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

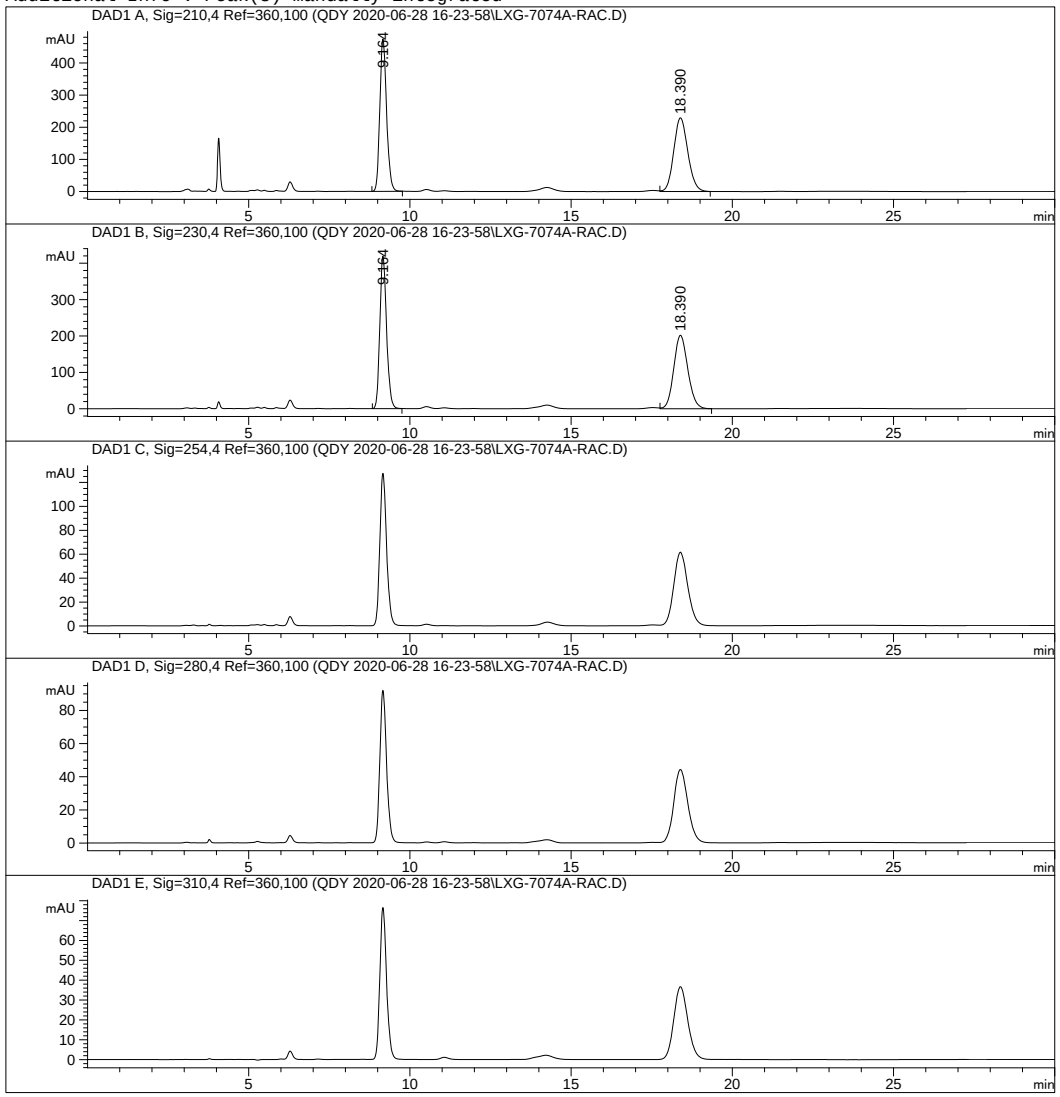


3d
(enantioenriched)

Supplementary Figure 149. HPLC spectrum of **3d** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\LXG-7074A-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   5
Acq. Instrument : Instrument 1                    Location : Vial 64
Injection Date  : 6/28/2020 6:09:56 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 3:07:23 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\LXG-7074A-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.164 BB    0.2239 6896.58789  473.69022  49.8099
   2  18.390 VB    0.4676 6949.21729  229.29904  50.1901

Totals :                  1.38458e4   702.98926



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.164 BB    0.2233 6077.68115  418.79807  49.8301
   2  18.390 VB    0.4696 6119.12939  201.88904  50.1699

Totals :                  1.21968e4   620.68710

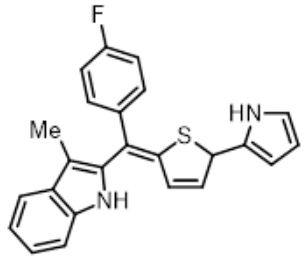


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

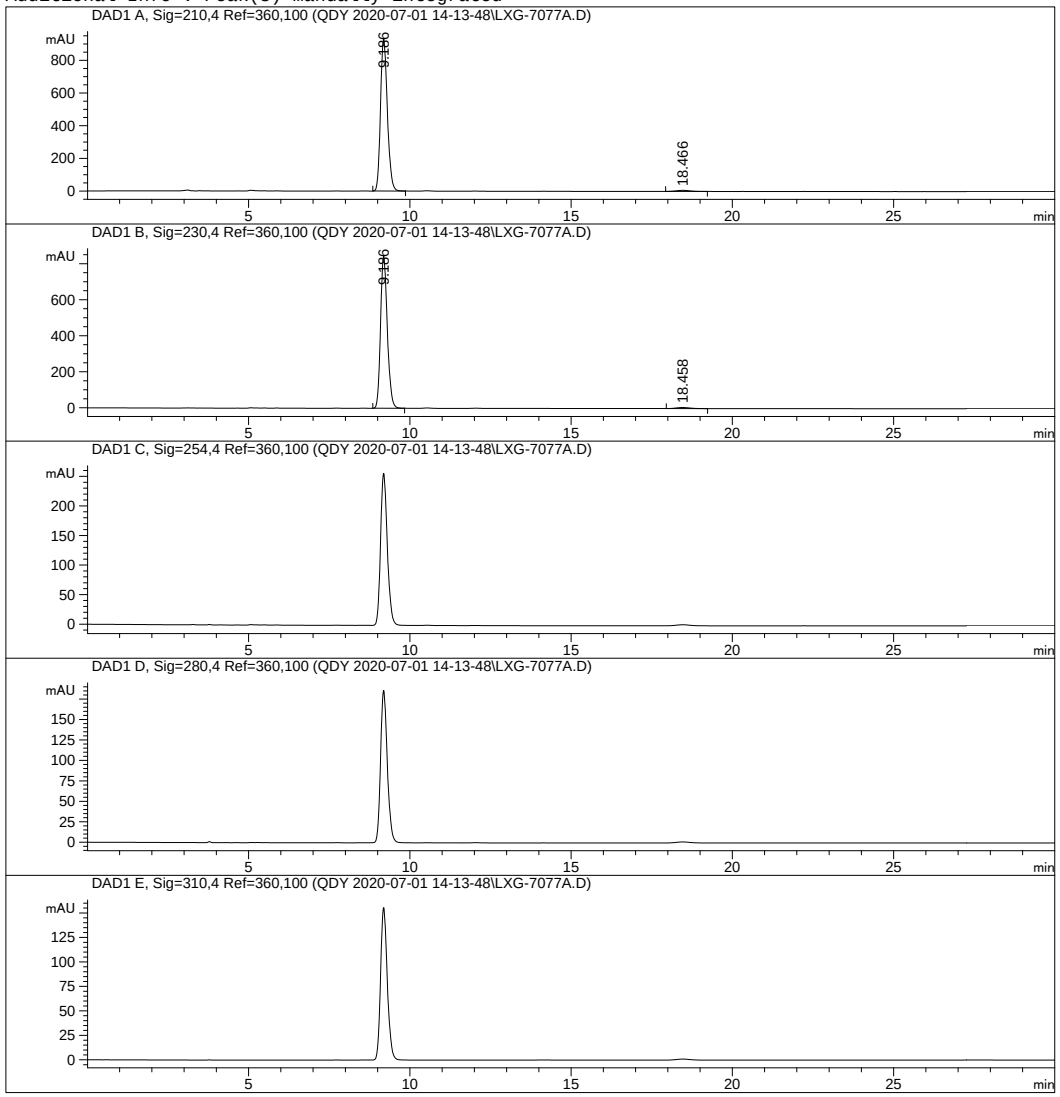


3e
(racemic)

Supplementary Figure 150. HPLC spectrum of **3e** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-01 14-13-48\LXG-7077A.D
Sample Name:

```
======================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location : Vial 65
Injection Date  : 7/1/2020 2:26:44 PM            Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-01 14-13-48\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 12:06:36 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-01 14-13-48\LXG-7077A.D
Sample Name:

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.186 BB    0.2279 1.37054e4   930.15314  98.6113
   2  18.466 BB    0.4517  193.00525    6.55141   1.3887

Totals :                  1.38984e4   936.70454



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.186 BB    0.2234 1.22628e4   844.31873  98.6389
   2  18.458 BB    0.4592  169.20894    5.75184   1.3611

Totals :                  1.24320e4   850.07057

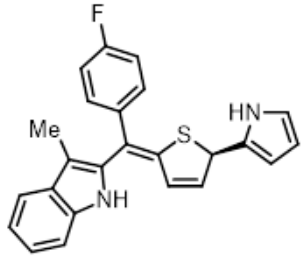


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

======================================================================
                        *** End of Report ***
```

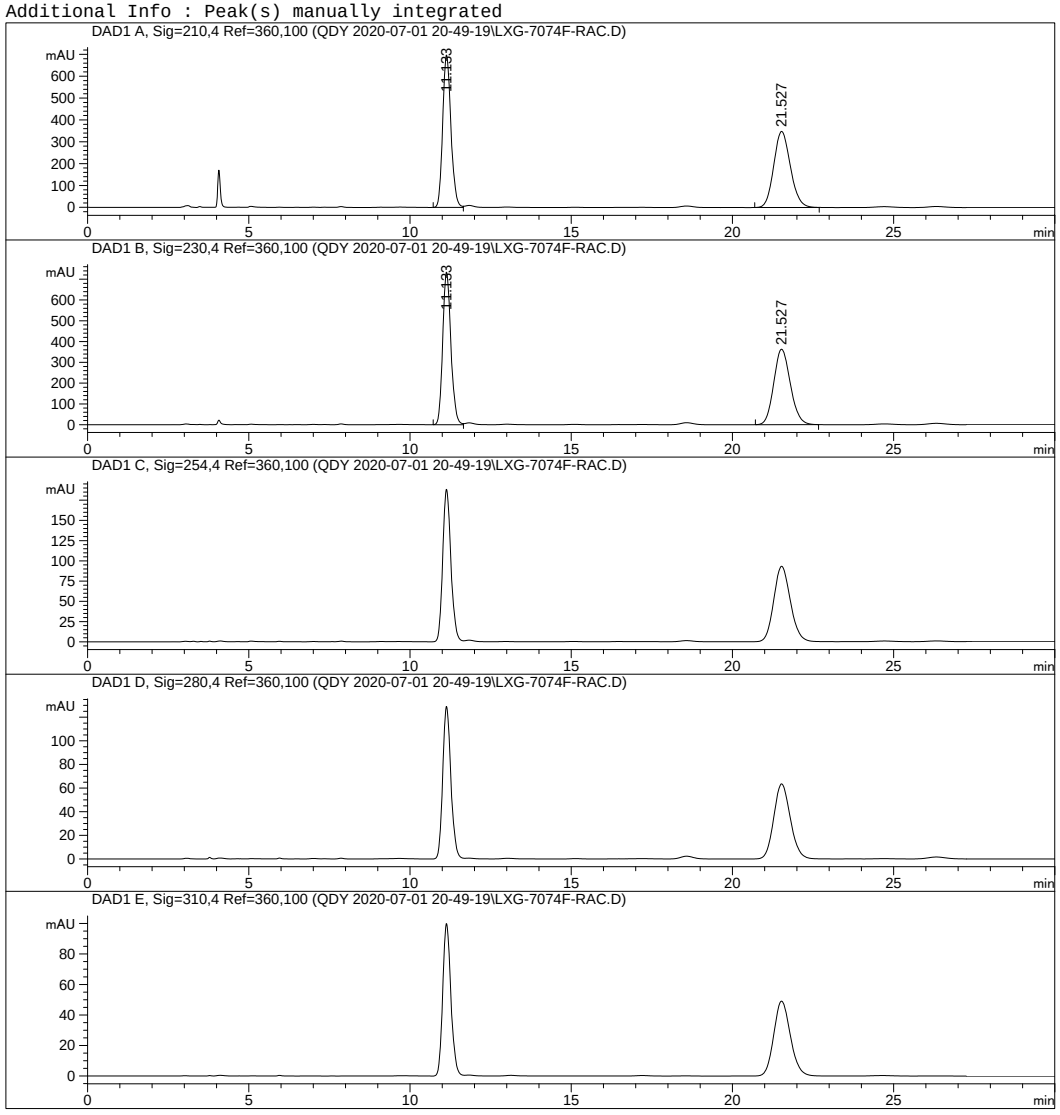


3e
(enantioenriched)

Supplementary Figure 151. HPLC spectrum of **3e** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-07-01 20-49-19\LXG-7074F-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :   9
Acq. Instrument : Instrument 1                  Location : Vial 68
Injection Date  : 7/1/2020 11:50:21 PM               Inj :   1
                                              Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-01 20-49-19\AD-20-40.M
Last changed    : 7/1/2020 11:49:28 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 3:25:56 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-01 20-49-19\LXG-7074F-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.133 BV    0.2727 1.23559e4   697.36481  49.7126
   2  21.527 BB    0.5565 1.24988e4   348.41791  50.2874

Totals :                  2.48547e4  1045.78271



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.133 BV    0.2717 1.29368e4   733.56958  49.8737
   2  21.527 BB    0.5534 1.30024e4   363.40698  50.1263

Totals :                  2.59392e4  1096.97656

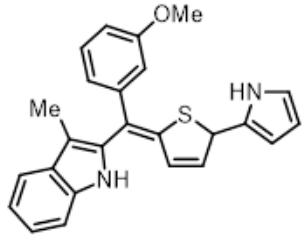


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

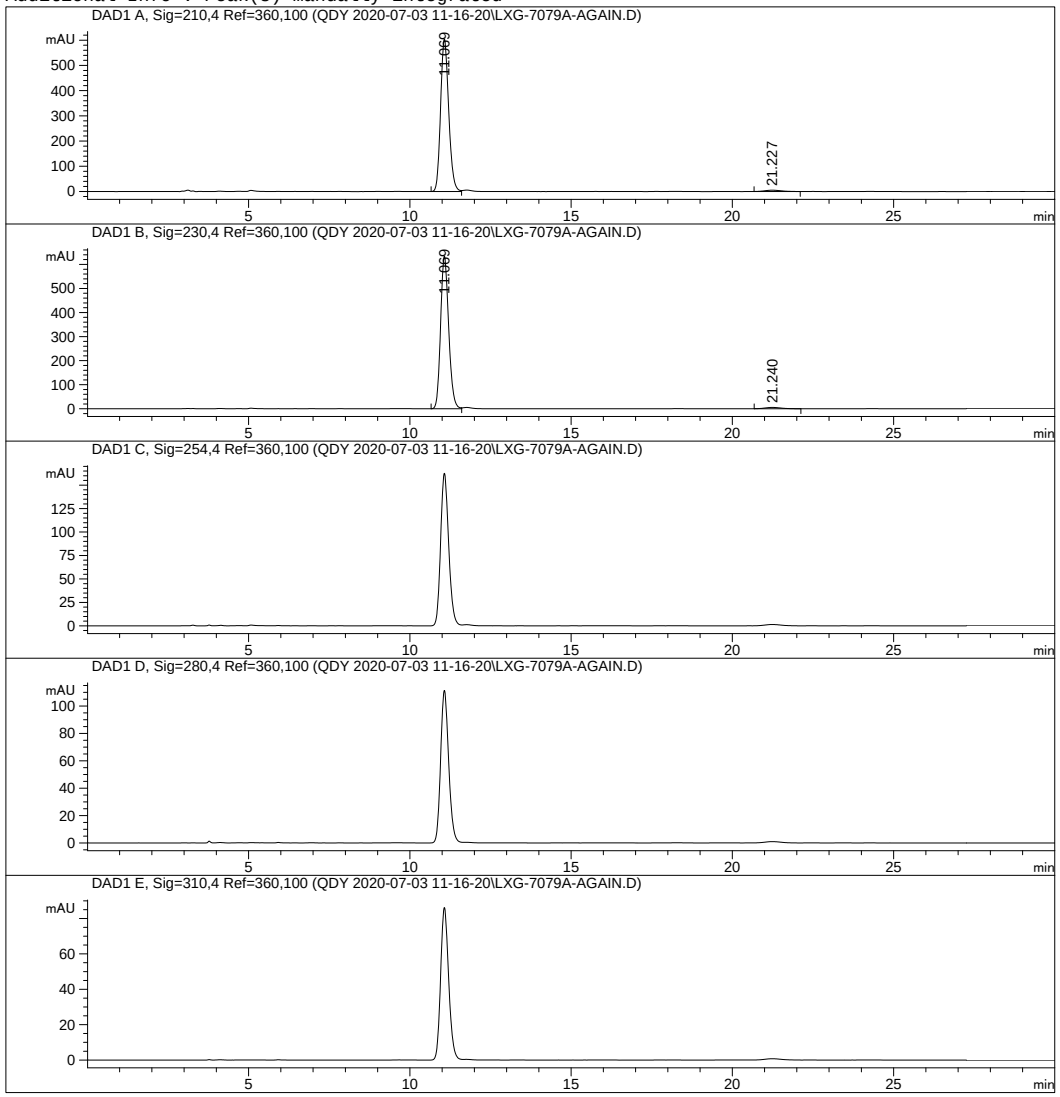


3f
(racemic)

Supplementary Figure 152. HPLC spectrum of **3f** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\LXG-7079A-AGAIN.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :  23
Acq. Instrument : Instrument 1                  Location : Vial 64
Injection Date  : 7/3/2020 7:12:32 PM               Inj :   1
                                               Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 3:16:15 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\LXG-7079A-AGAIN.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.069 BV    0.2696 1.05527e4   604.80225  98.2917
   2  21.227 BB    0.4792  183.40189    5.17820   1.7083

Totals :                  1.07361e4   609.98045



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.069 BV    0.2668 1.10218e4   634.18201  98.3362
   2  21.240 BB    0.5339  186.48531    5.41394   1.6638

Totals :                  1.12082e4   639.59595

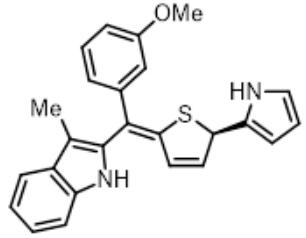


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



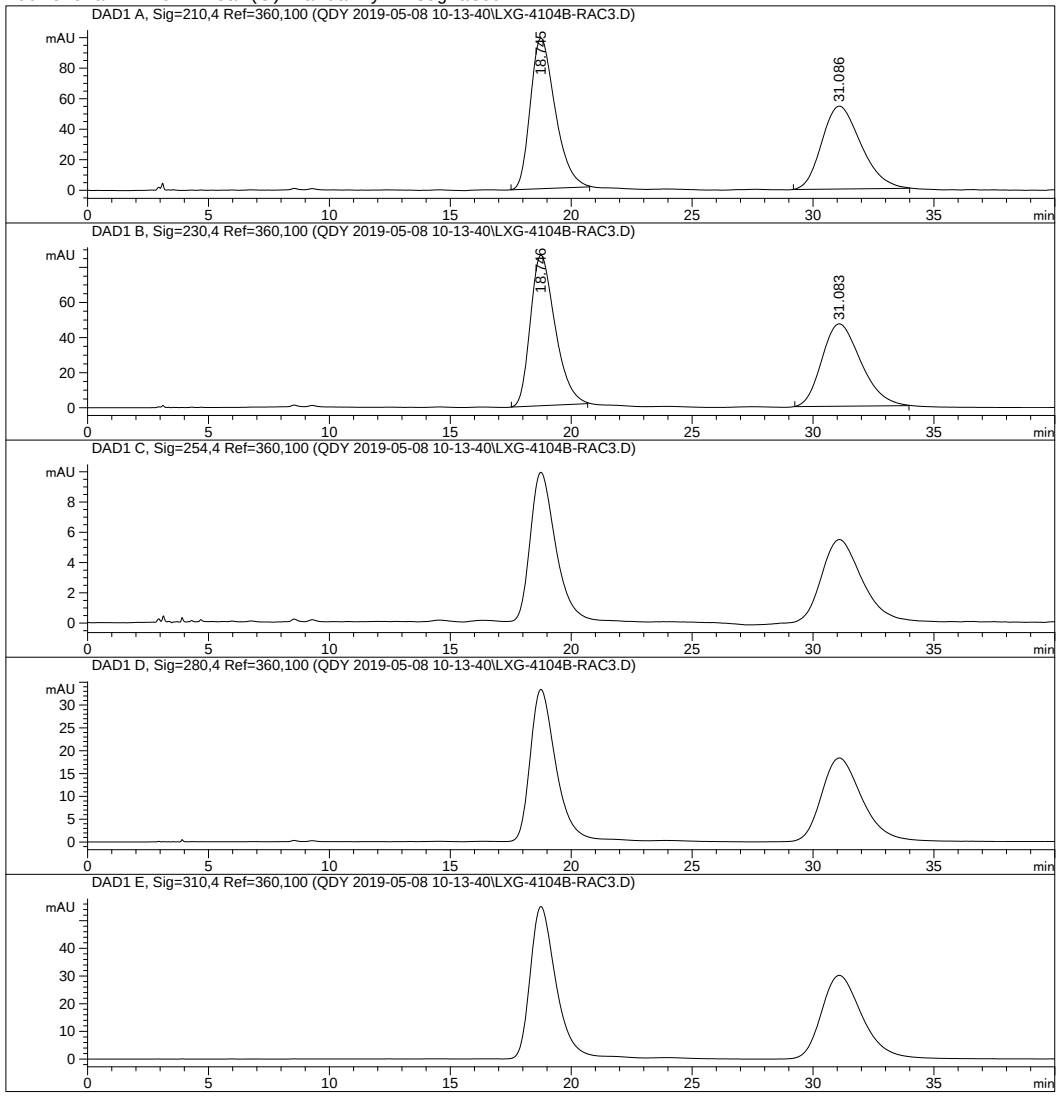
3f
(enantioenriched)

Supplementary Figure 153. HPLC spectrum of **3f** (enantioenriched)

Instrument 1 7/4/2020 3:18:55 PM

Data File C:\CHEM32\1\DATA\QDY 2019-05-08 10-13-40\LXG-4104B-RAC3.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   7
Acq. Instrument : Instrument 1              Location : Vial 72
Injection Date  : 5/8/2019 1:23:46 PM            Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-05-08 10-13-40\OD-20-60.M
Last changed    : 5/8/2019 1:22:54 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-07-60.M
Last changed    : 5/14/2019 9:51:54 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-05-08 10-13-40\LXG-4104B-RAC3.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  18.745 BB    1.0800 7038.53906   98.69179  53.4883
   2  31.086 BB    1.5403 6120.47754   54.32919  46.5117

Totals :                  1.31590e4   153.02098



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  18.746 BB    1.0908 6096.00684   85.81546  53.6420
   2  31.083 BB    1.6792 5268.23389   46.94790  46.3580

Totals :                  1.13642e4   132.76336

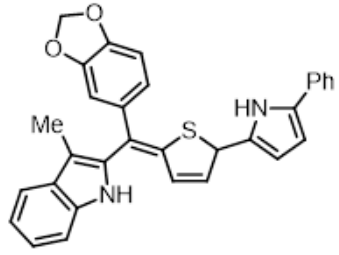


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```

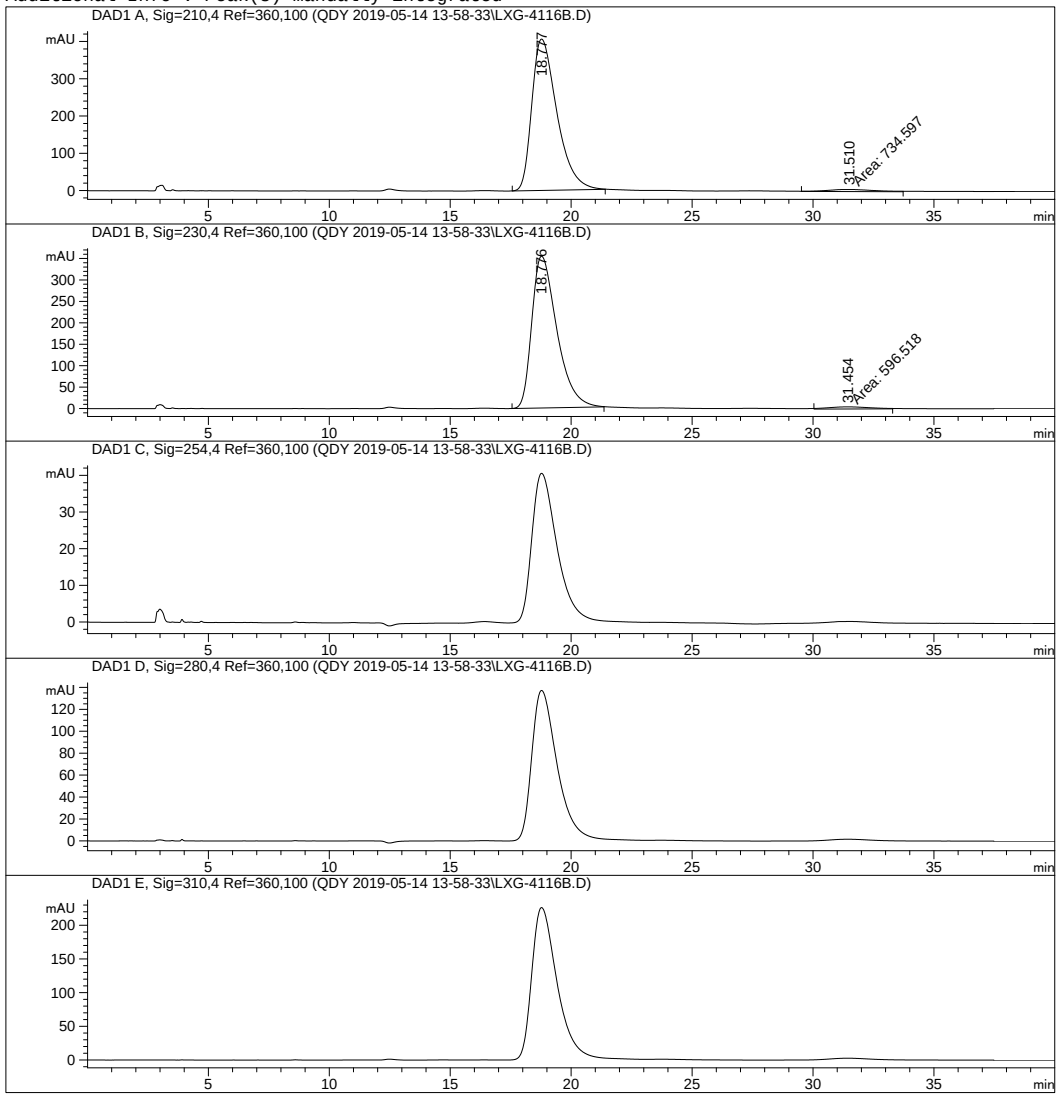


3g
(racemic)

Supplementary Figure 154. HPLC spectrum of **3g** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2019-05-14 13-58-33\LXG-4116B.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  12
Acq. Instrument : Instrument 1              Location : Vial 72
Injection Date  : 5/14/2019 5:24:48 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-05-14 13-58-33\OD-20-40.M
Last changed    : 5/14/2019 5:23:58 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-07-60.M
Last changed    : 5/11/2019 10:45:40 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-05-14 13-58-33\LXG-4116B.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  18.777 BB    1.0965 2.92674e4   406.26563  97.5515
   2  31.510 MM    2.2217  734.59674    5.51070   2.4485

Totals :                  3.00020e4   411.77632



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  18.776 BB    1.0948 2.54552e4   354.03140  97.7103
   2  31.454 MM    2.0271  596.51813    4.90447   2.2897

Totals :                  2.60517e4   358.93587

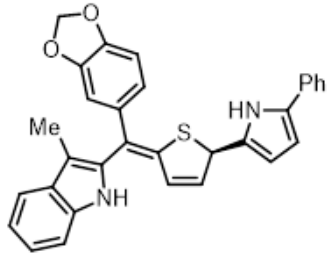


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```

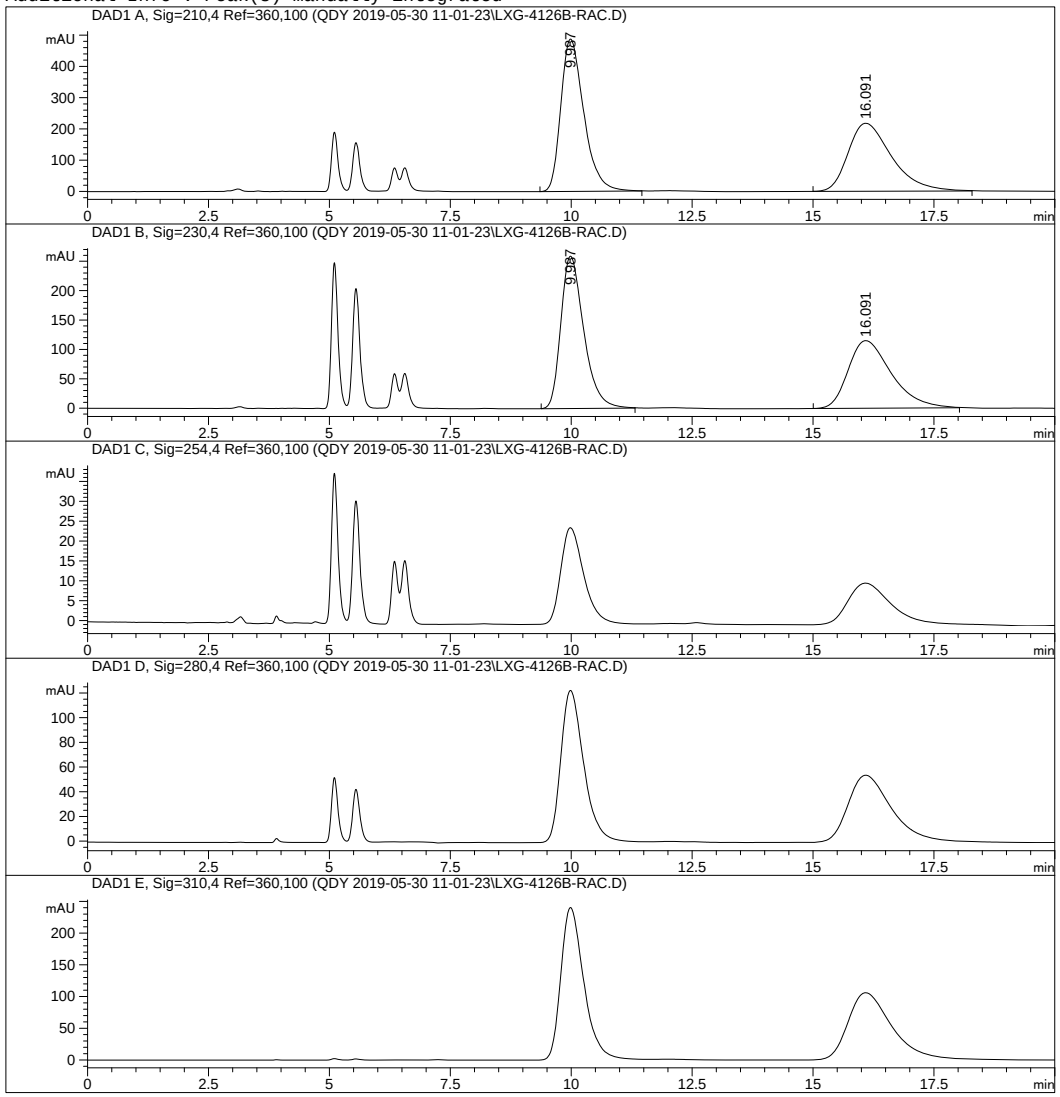


3g
(enantioenriched)

Supplementary Figure 155. HPLC spectrum of **3g** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2019-05-30 11-01-23\LXG-4126B-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   2
Acq. Instrument : Instrument 1                    Location : Vial 78
Injection Date  : 5/30/2019 11:15:01 AM               Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-05-30 11-01-23\OD-20-40.M
Last changed    : 5/30/2019 11:14:08 AM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\OD-01-45-0.5.M
Last changed    : 8/20/2020 7:42:57 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-05-30 11-01-23\LXG-4126B-RAC.D
Sample Name:

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.987 BB    0.5077 1.61082e4   487.29367  54.1869
   2  16.091 BB    0.9504 1.36189e4   217.53532  45.8131

Totals :                  2.97271e4   704.82899



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.987 BB    0.5033 8513.64551  259.14014  54.3847
   2  16.091 BB    0.9463 7140.83887  115.02266  45.6153

Totals :                  1.56545e4   374.16280

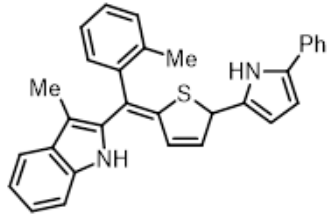


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                          *** End of Report ***
```

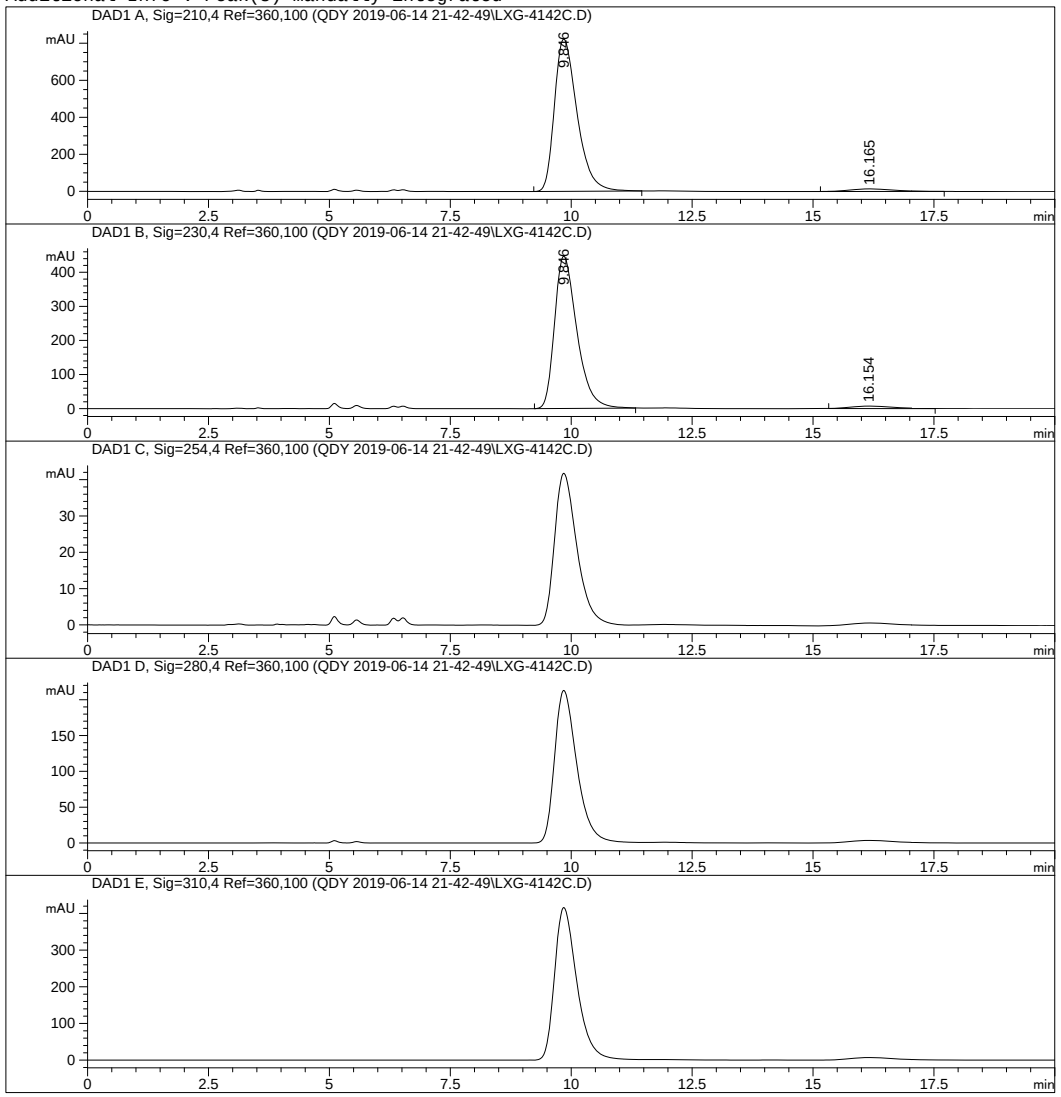


3h
(racemic)

Supplementary Figure 156. HPLC spectrum of **3h** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2019-06-14 21-42-49\LXG-4142C.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   4
Acq. Instrument : Instrument 1              Location : Vial 67
Injection Date  : 6/14/2019 10:58:30 PM          Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-06-14 21-42-49\OD-20-20.M
Last changed    : 6/14/2019 10:57:33 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\OD-01-45-0.5.M
Last changed    : 8/20/2020 6:53:30 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-06-14 21-42-49\LXG-4142C.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.846 BB    0.5020 2.67951e4   822.72748  96.8372
   2  16.165 BB    0.8935  875.14276   13.95693   3.1628

Totals :                  2.76703e4   836.68441



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.846 BB    0.4903 1.43359e4   446.82480  97.0729
   2  16.154 BB    0.8596  432.28616    7.16802   2.9271

Totals :                  1.47682e4   453.99282

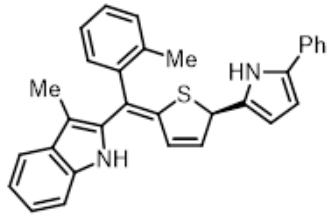


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```

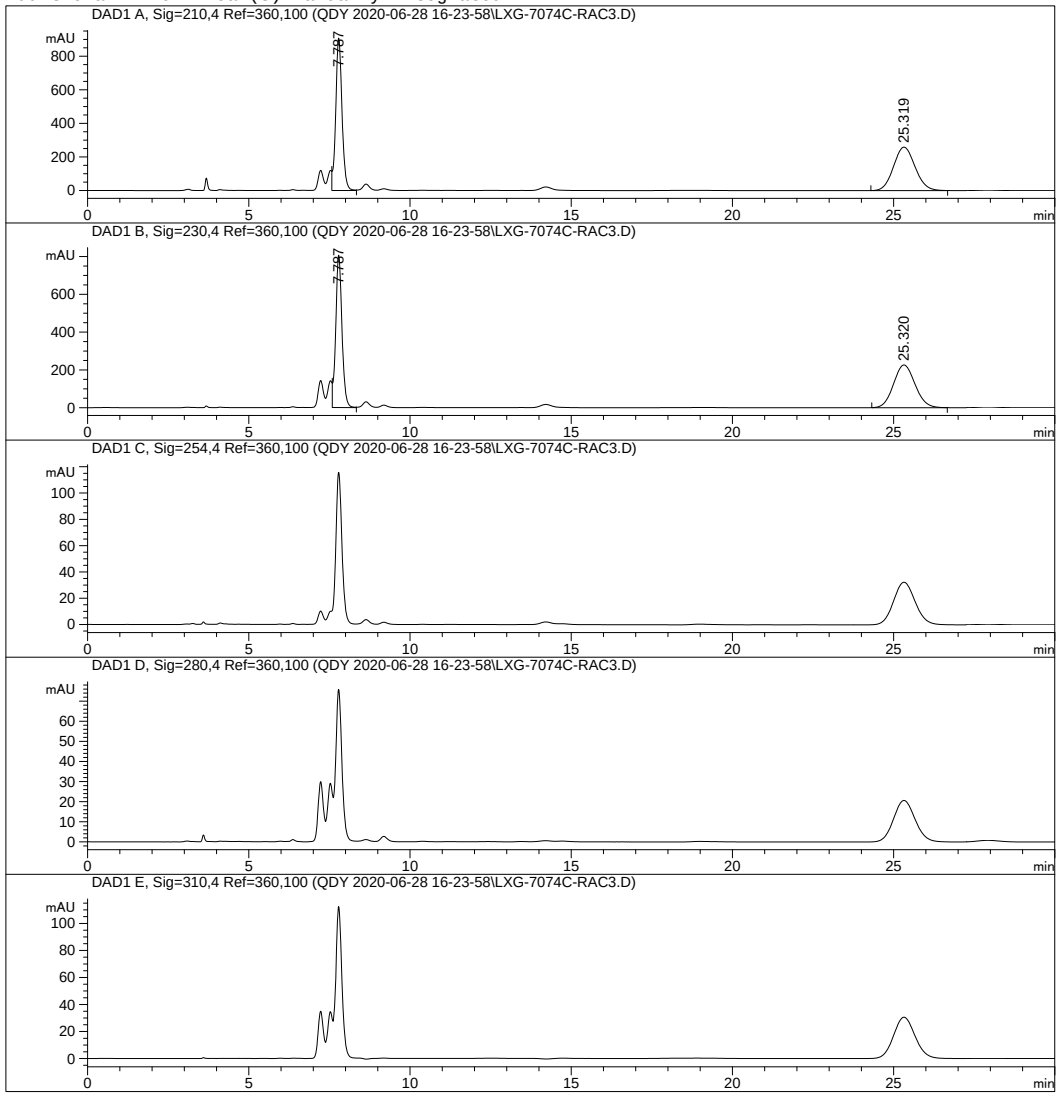


3h
(enantioenriched)

Supplementary Figure 157. HPLC spectrum of **3h** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\LXG-7074C-RAC3.D
Sample Name:

```
=====================================================================
Acq. Operator   :                          Seq. Line :  15
Acq. Instrument : Instrument 1              Location : Vial 65
Injection Date  : 6/28/2020 10:41:11 PM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\AD-30-40.M
Last changed    : 6/28/2020 10:40:18 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 3:11:19 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\LXG-7074C-RAC3.D
Sample Name:

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.787 VV    0.2058 1.22812e4   908.22375  50.5301
   2  25.319 BB    0.7240 1.20235e4   258.81998  49.4699

Totals :                  2.43047e4  1167.04373



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.787 VV    0.2047 1.08387e4   806.81927  50.7838
   2  25.320 BB    0.7236 1.05042e4   226.28265  49.2162

Totals :                  2.13429e4  1033.10193

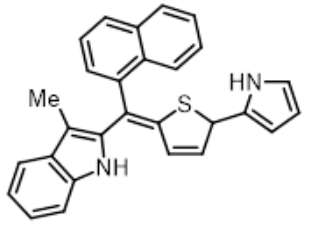


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

=====================================================================
                        *** End of Report ***
```

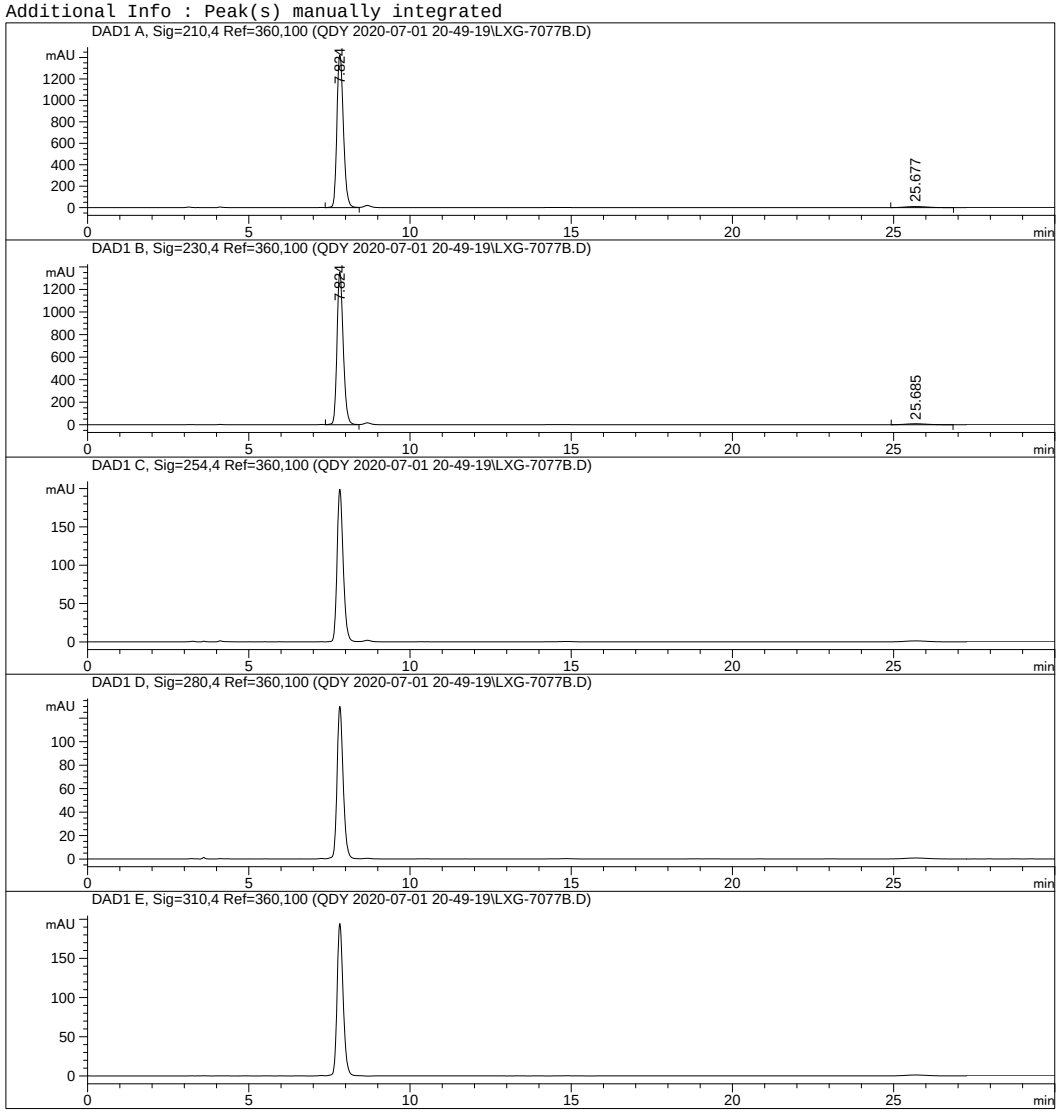


3i
(racemic)

Supplementary Figure 158. HPLC spectrum of **3i** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-01 20-49-19\LXG-7077B.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   7
Acq. Instrument : Instrument 1                    Location : Vial 67
Injection Date  : 7/1/2020 10:58:10 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-01 20-49-19\AD-30-40.M
Last changed    : 7/1/2020 10:57:18 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 3:05:35 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-01 20-49-19\LXG-7077B.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.824 VB    0.2172 1.99111e4  1422.99902  97.7720
   2  25.677 BB    0.6922  453.73734    9.65661   2.2280

Totals :                  2.03648e4  1432.65563



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.824 VB    0.2063 1.81337e4  1353.30127  97.8936
   2  25.685 BB    0.7127  390.19366    8.38851   2.1064

Totals :                  1.85239e4  1361.68978

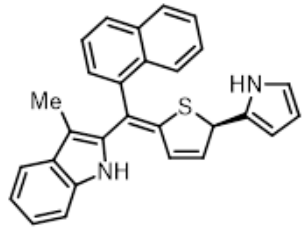


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



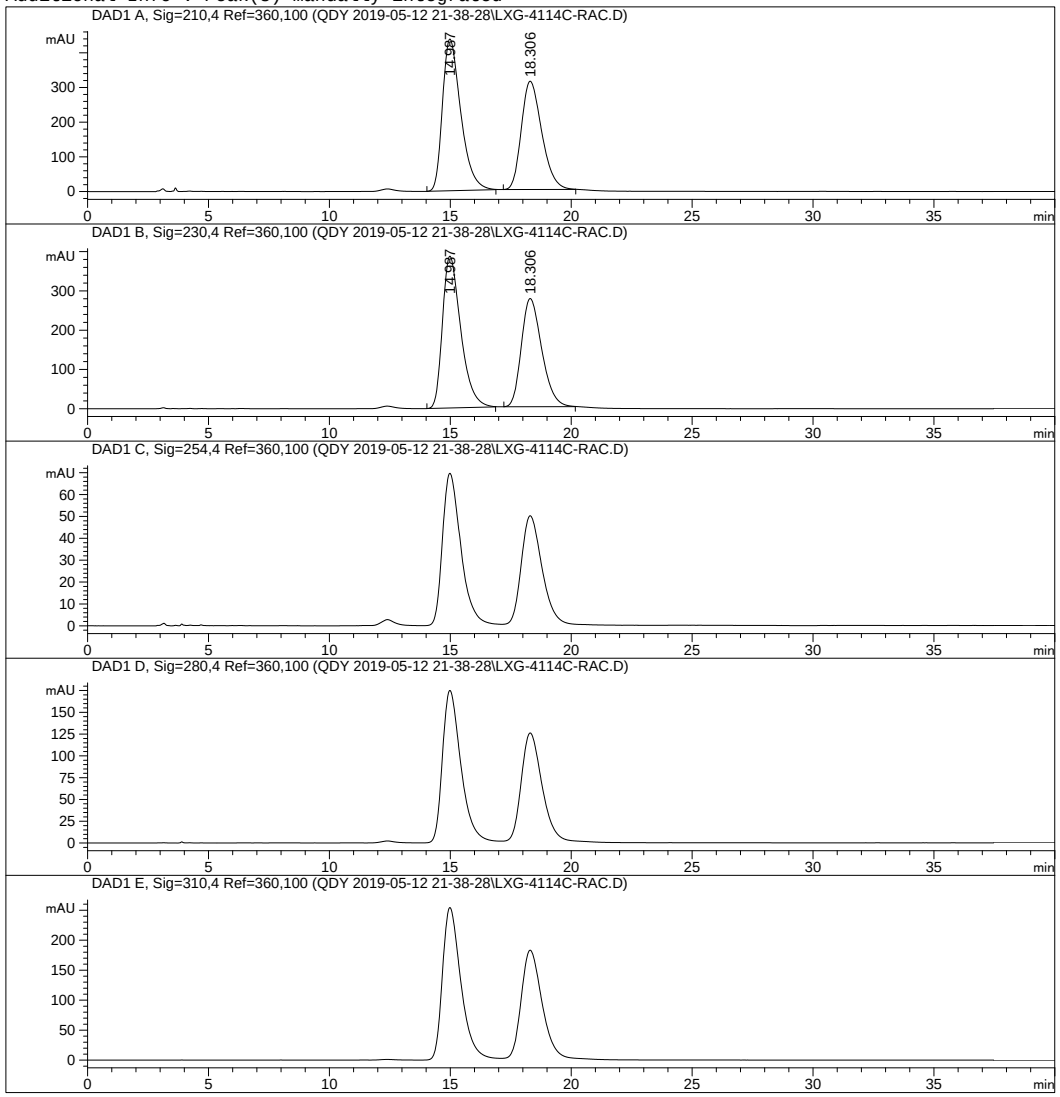
3i
(enantioenriched)

Supplementary Figure 159. HPLC spectrum of **3i** (enantioenriched)

Instrument 1 7/4/2020 3:05:48 PM

Data File C:\CHEM32\1\DATA\QDY 2019-05-12 21-38-28\LXG-4114C-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   3
Acq. Instrument : Instrument 1                    Location : Vial 75
Injection Date  : 5/12/2019 10:33:12 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-05-12 21-38-28\OD-20-40.M
Last changed    : 5/12/2019 9:50:42 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-07-60.M
Last changed    : 5/14/2019 9:51:54 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-05-12 21-38-28\LXG-4114C-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.987 BB    0.8076 2.29960e4   437.23770  55.6941
   2  18.306 BB    0.9118 1.82939e4   312.10123  44.3059

Totals :                  4.12899e4   749.33893



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.987 BB    0.8091 2.03070e4   386.39313  55.7363
   2  18.306 BB    0.9070 1.61271e4   275.48026  44.2637

Totals :                  3.64341e4   661.87338

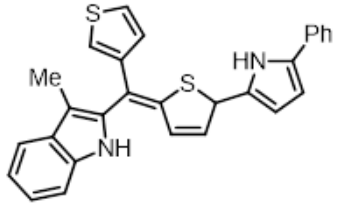


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



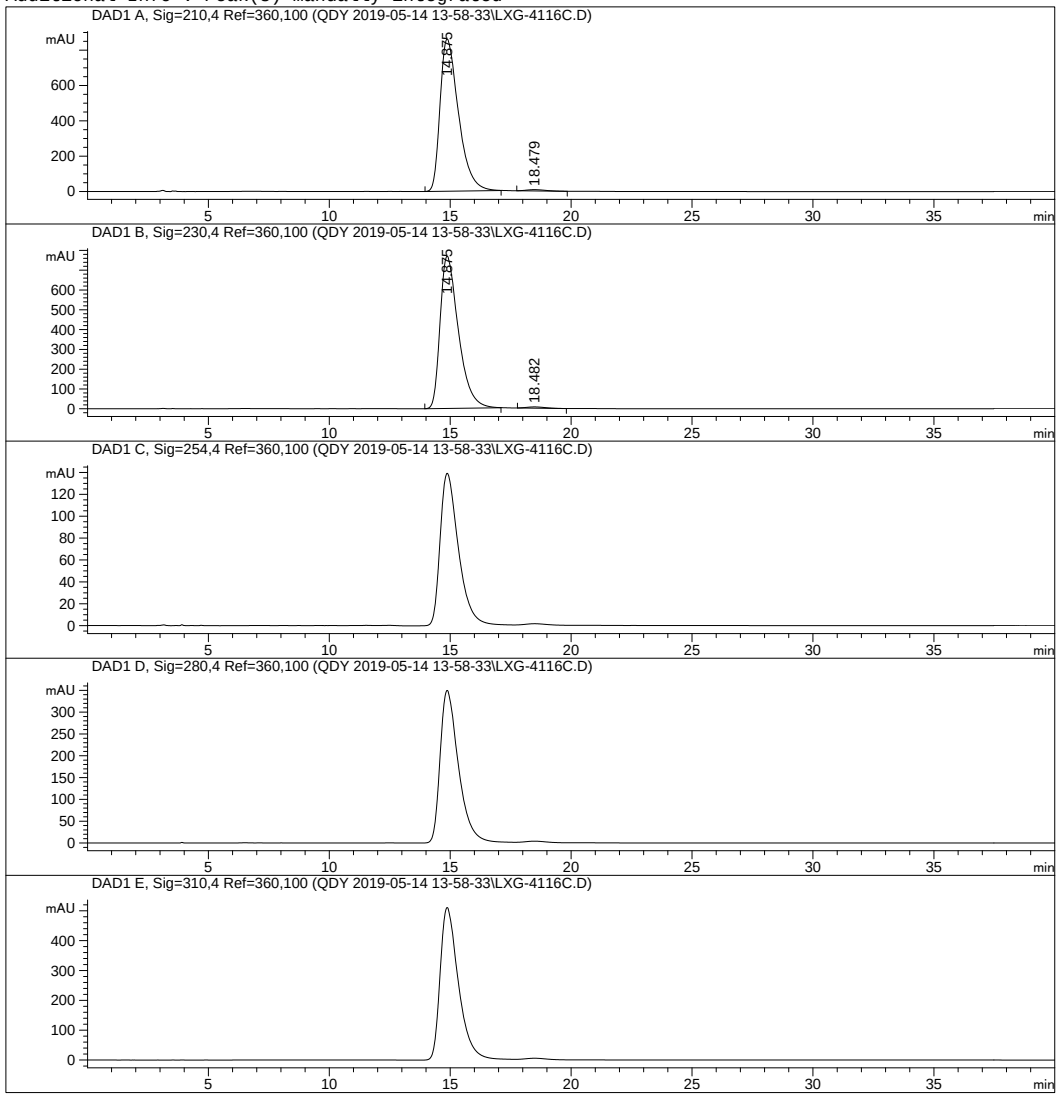
3J
(racemic)

Supplementary Figure 160. HPLC spectrum of **3l** (racemic)

Instrument 1 5/14/2019 9:53:51 PM Page 2 of 2

Data File C:\CHEM32\1\DATA\QDY 2019-05-14 13-58-33\LXG-4116C.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :  13
Acq. Instrument : Instrument 1                    Location : Vial 73
Injection Date  : 5/14/2019 6:06:42 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-05-14 13-58-33\OD-20-40.M
Last changed    : 5/14/2019 5:23:58 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-07-60.M
Last changed    : 5/11/2019 10:45:40 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-05-14 13-58-33\LXG-4116C.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.875 BB    0.8070 4.55299e4   860.87372  99.1609
   2  18.479 BB    0.7376  385.25839    7.25471   0.8391

Totals :                  4.59151e4   868.12842



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.875 BB    0.8032 4.04170e4   768.98621  99.1820
   2  18.482 BB    0.7998  333.31796    6.39790   0.8180

Totals :                  4.07503e4   775.38411

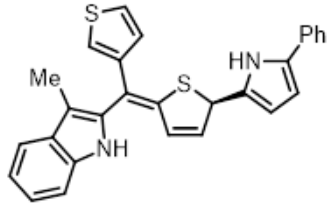


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

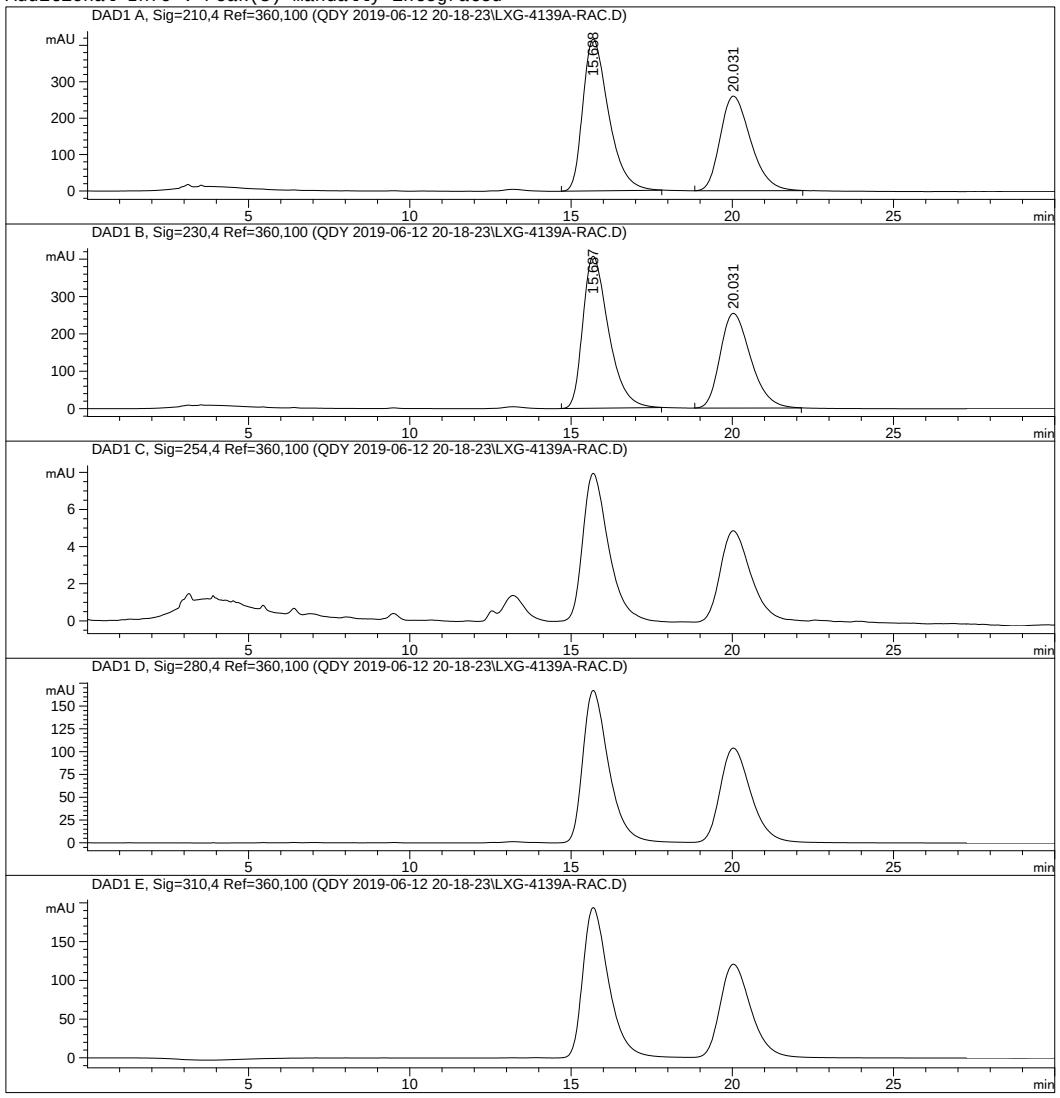


3j
(enantioenriched)

Supplementary Figure 161. HPLC spectrum of **3j** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2019-06-12 20-18-23\LXG-4139A-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   5
Acq. Instrument : Instrument 1                    Location : Vial 63
Injection Date  : 6/12/2019 10:05:17 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-06-12 20-18-23\OD-20-30.M
Last changed    : 5/3/2016 10:14:35 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-01-45-0.5.M
Last changed    : 8/20/2020 6:54:41 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-06-12 20-18-23\LXG-4139A-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.688 BB    0.8527 2.31229e4   417.12521  57.4932
   2  20.031 BB    1.0194 1.70956e4   259.88626  42.5068

Totals :                  4.02185e4   677.01147



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.687 BB    0.8498 2.25266e4   406.93353  57.5159
   2  20.031 BB    1.0204 1.66393e4   253.28590  42.4841

Totals :                  3.91658e4   660.21944

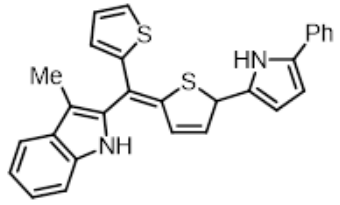


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

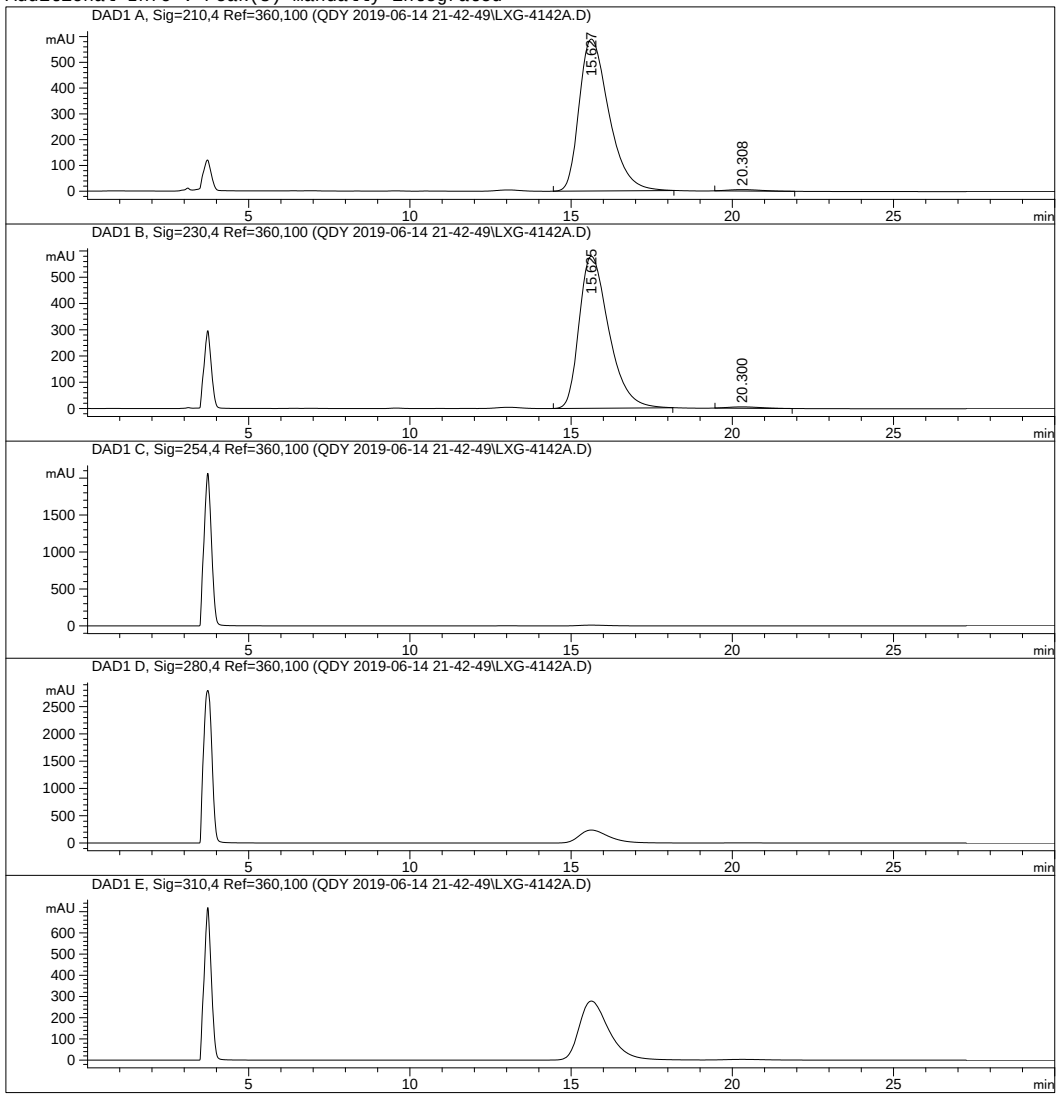


3k
(racemic)

Supplementary Figure 162. HPLC spectrum of **3k** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2019-06-14 21-42-49\LXG-4142A.D
Sample Name:

```
======================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location : Vial 65
Injection Date  : 6/14/2019 9:56:07 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-06-14 21-42-49\OD-20-30.M
Last changed    : 5/3/2016 10:14:35 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-01-45-0.5.M
Last changed    : 8/20/2020 6:54:41 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-06-14 21-42-49\LXG-4142A.D
Sample Name:

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.627 BB    0.9779 3.76749e4   589.29059  98.9965
   2  20.308 BB    0.8524  381.91217    5.43105   1.0035

Totals :                  3.80568e4   594.72163



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.625 BB    0.9774 3.69196e4   579.39685  99.0134
   2  20.300 BB    1.0100  367.89136    5.25984   0.9866

Totals :                  3.72875e4   584.65669

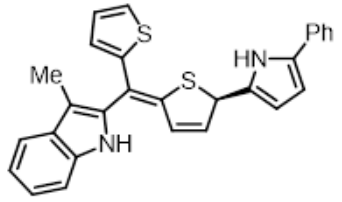


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

======================================================================
                        *** End of Report ***
```

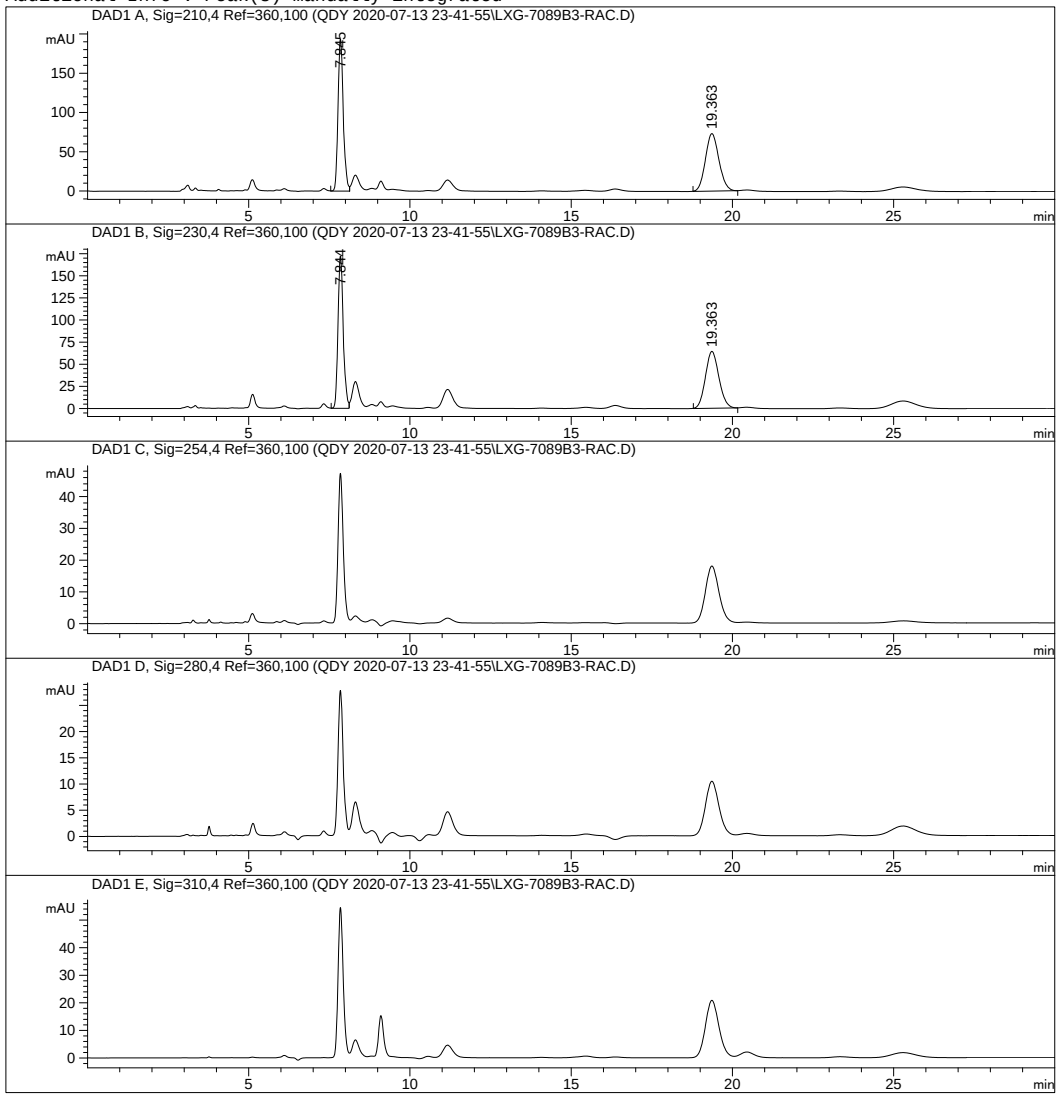


3k
(enantioenriched)

Supplementary Figure 163. HPLC spectrum of **3k** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-07-13 23-41-55\LXG-7089B3-RAC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   4
Acq. Instrument : Instrument 1              Location : Vial 63
Injection Date  : 7/14/2020 12:57:18 AM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-13 23-41-55\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/10/2020 9:21:13 AM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-13 23-41-55\LXG-7089B3-RAC.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.845 VV    0.1740 2189.89258  193.54507  50.7406
   2  19.363 BB    0.4509 2125.96704   73.18436  49.2594

Totals :                  4315.85962  266.72943



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.844 VV    0.1742 1949.09778  171.97502  51.0868
   2  19.363 BB    0.4507 1866.16663   64.28641  48.9132

Totals :                  3815.26440  236.26143

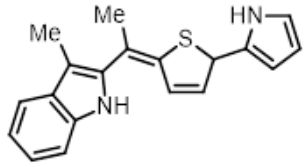


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```



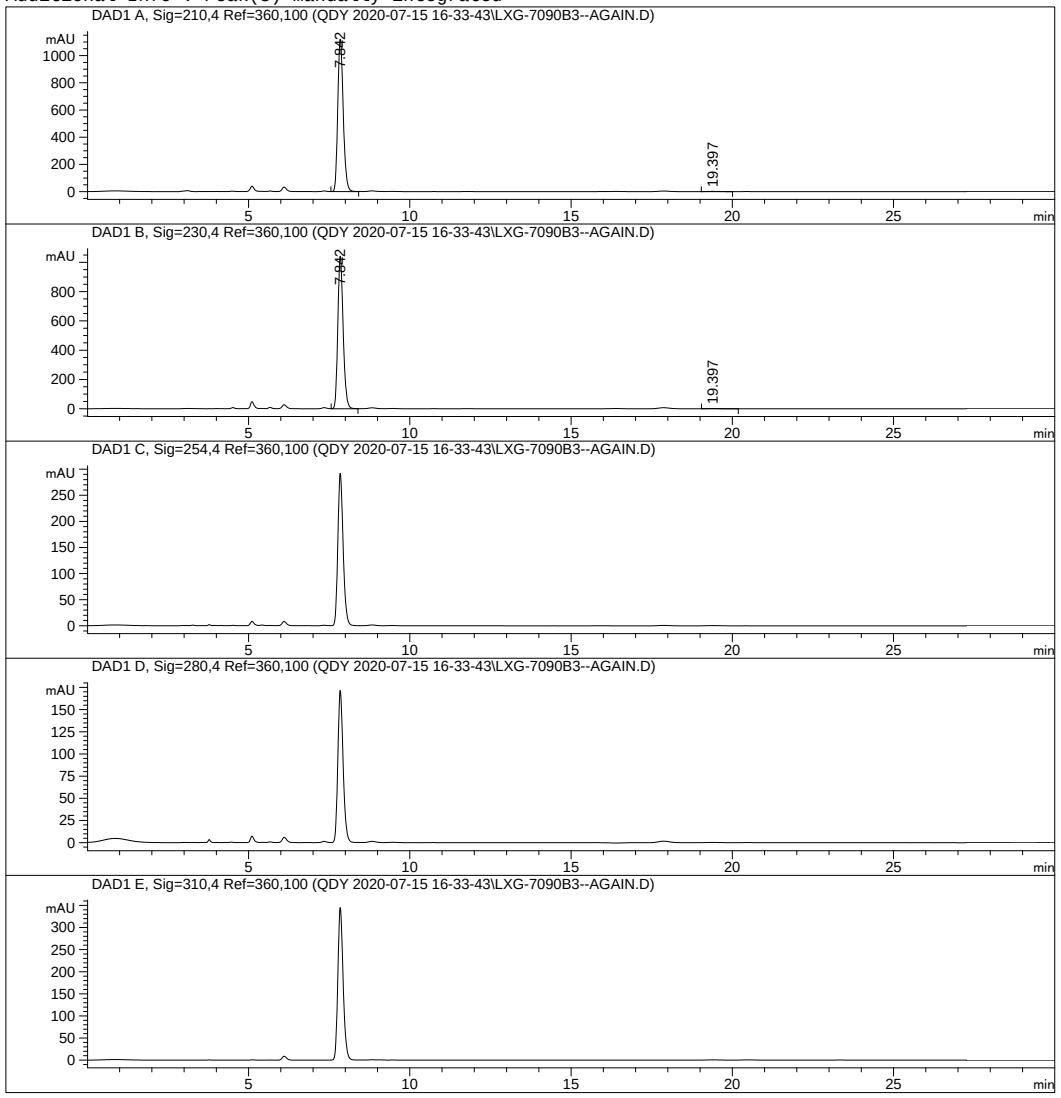
3l
(racemic)

Supplementary Figure 164. HPLC spectrum of **3l** (racemic)

Instrument 1 7/25/2020 7:01:13 PM

Data File C:\CHEM32\1\DATA\QDY 2020-07-15 16-33-43\LXG-7090B3--AGAIN.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :  24
Acq. Instrument : Instrument 1                    Location : Vial 62
Injection Date  : 7/16/2020 12:21:39 AM               Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-15 16-33-43\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/10/2020 9:21:13 AM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-15 16-33-43\LXG-7090B3--AGAIN.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.842 VB    0.1811 1.31779e4  1121.64160  99.5431
   2  19.397 BB    0.3991   60.47977    2.10594   0.4569

Totals :                  1.32384e4  1123.74754



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.842 VB    0.1757 1.19394e4  1042.07349  99.6063
   2  19.397 BB    0.4287   47.18557    1.77169   0.3937

Totals :                  1.19866e4  1043.84518

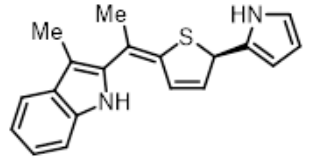


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



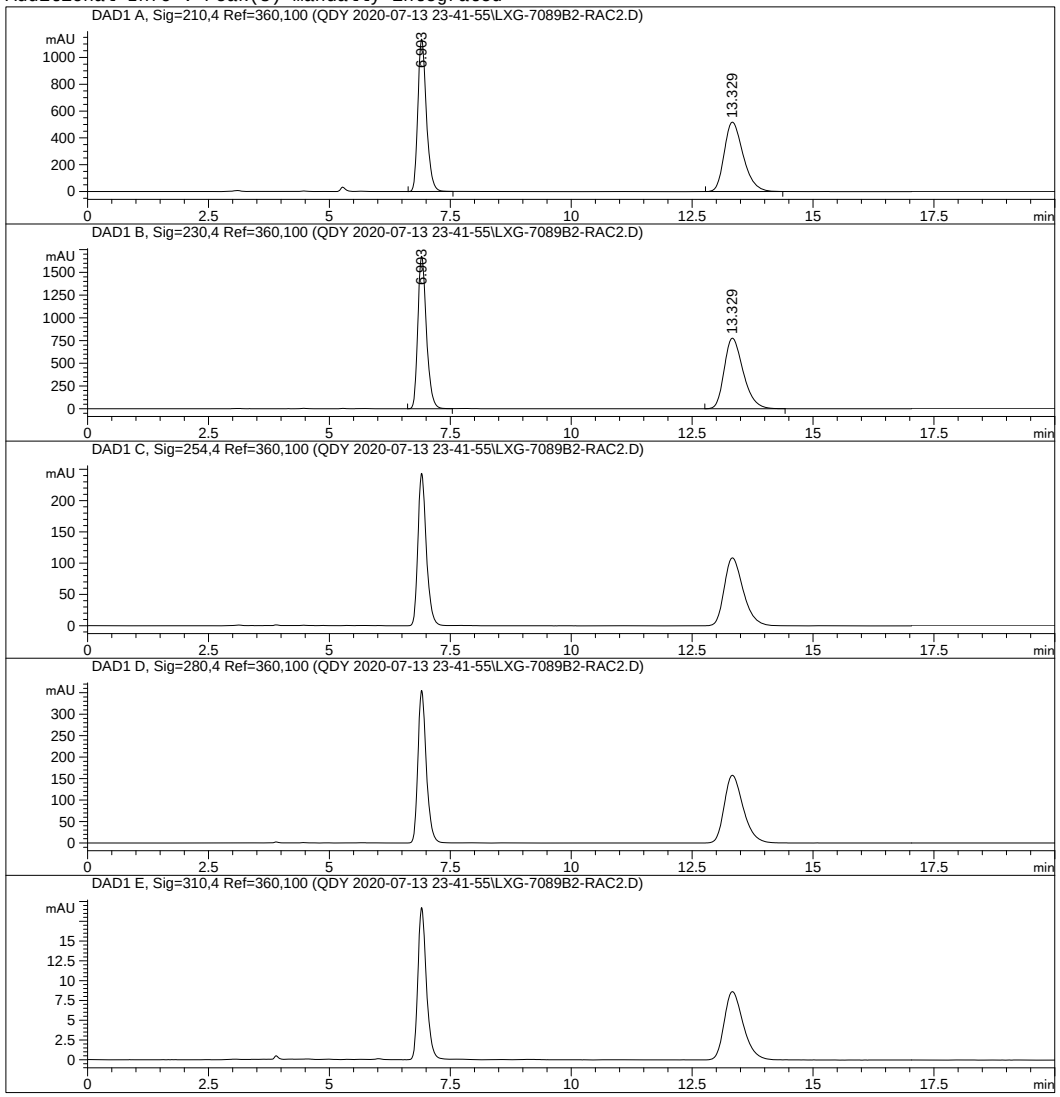
3l
(enantioenriched)

Supplementary Figure 165. HPLC spectrum of **3l** (enantioenriched)

Instrument 1 7/25/2020 6:52:15 PM

Data File C:\CHEM32\1\DATA\QDY 2020-07-13 23-41-55\LXG-7089B2-RAC2.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :  10
Acq. Instrument : Instrument 1                    Location : Vial 62
Injection Date  : 7/14/2020 3:23:45 AM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-13 23-41-55\OD-20-30.M
Last changed    : 5/3/2016 10:14:35 AM
Analysis Method : C:\CHEM32\1\DATA\QDY 2020-12-12 14-50-34\L1.D\DA.M
Last changed    : 1/23/2021 10:49:11 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-13 23-41-55\LXG-7089B2-RAC2.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.903 BB    0.1888 1.39130e4  1136.78003  49.6651
   2  13.329 BB    0.4197 1.41007e4   517.81897  50.3349

Totals :                  2.80138e4  1654.59900



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.903 BB    0.1902 2.07432e4  1677.82849  49.4895
   2  13.329 BB    0.4202 2.11712e4   776.22736  50.5105

Totals :                  4.19144e4  2454.05585

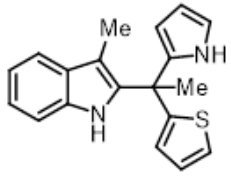


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

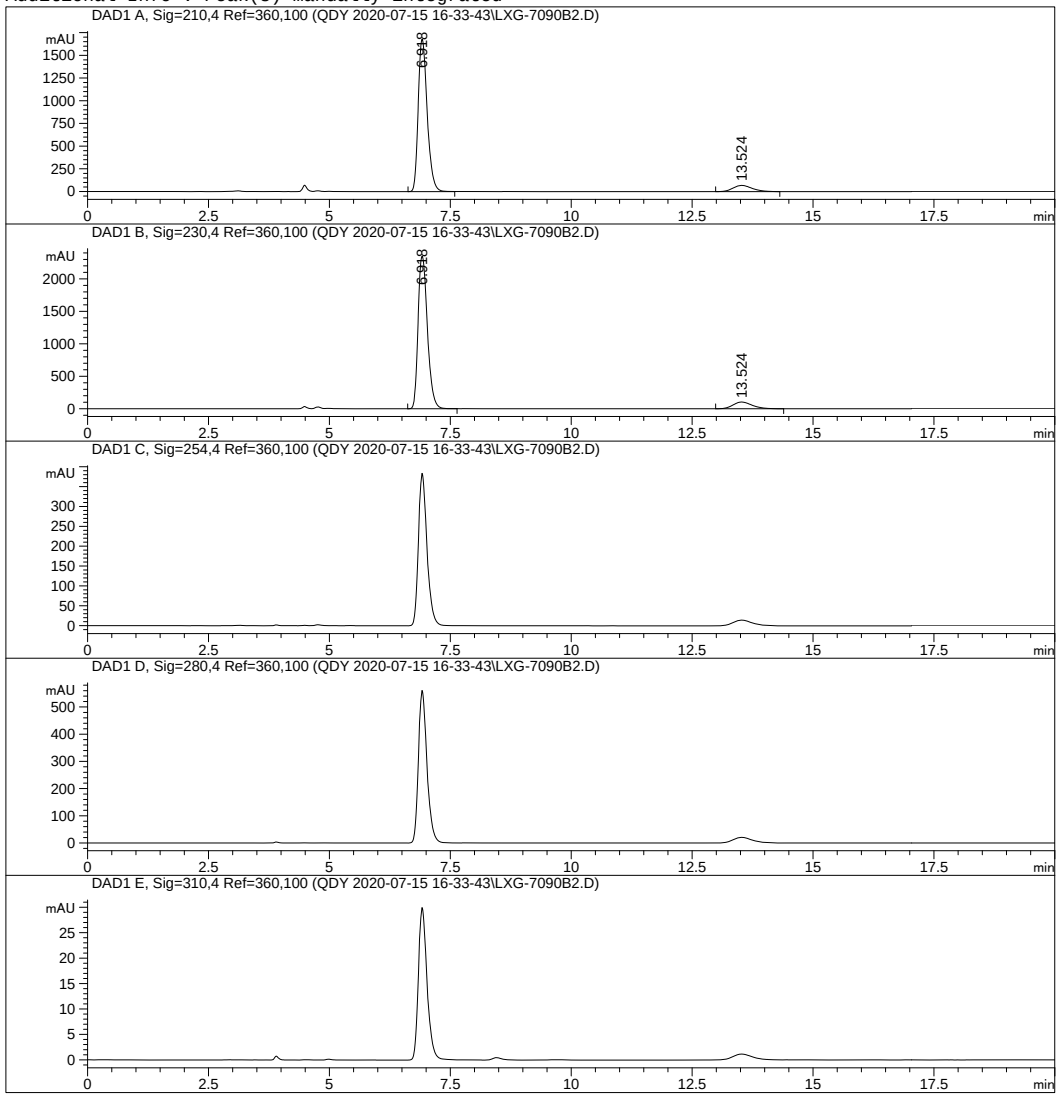


3l'
(racemic)

Supplementary Figure 166. HPLC spectrum of **3l'** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-15 16-33-43\LXG-7090B2.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :  20
Acq. Instrument : Instrument 1                    Location : Vial 61
Injection Date  : 7/15/2020 11:06:54 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-15 16-33-43\OD-20-20.M
Last changed    : 1/7/2016 10:22:18 AM
Analysis Method : C:\CHEM32\1\DATA\QDY 2020-12-12 14-50-34\L1.D\DA.M
Last changed    : 1/23/2021 10:49:11 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-15 16-33-43\LXG-7090B2.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.918 BB    0.2006 2.16919e4  1680.42749  91.9022
   2  13.524 BB    0.4260 1911.34253   68.81486   8.0978

Totals :                  2.36032e4  1749.24235



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.918 BB    0.2102 3.14638e4  2350.51831  91.5961
   2  13.524 BB    0.4286 2886.77588  103.76046   8.4039

Totals :                  3.43506e4  2454.27877

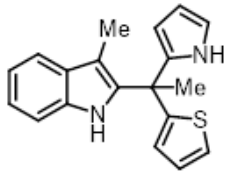


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

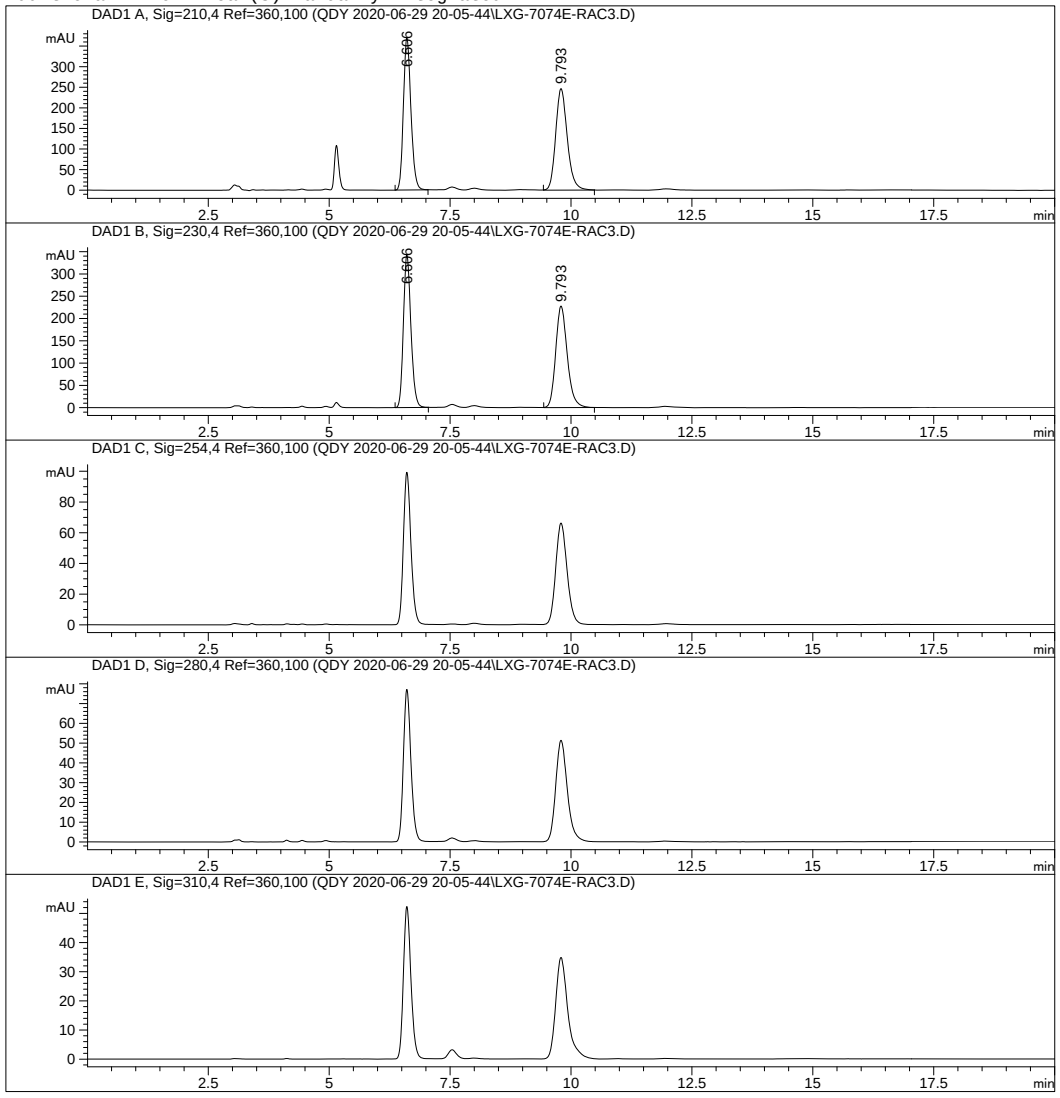


3l'
(enantioenriched)

Supplementary Figure 167. HPLC spectrum of **3l'** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-06-29 20-05-44\LXG-7074E-RAC3.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   4
Acq. Instrument : Instrument 1                    Location : Vial 61
Injection Date  : 6/29/2020 9:10:49 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-06-29 20-05-44\AD-10-20.M
Last changed    : 6/29/2020 9:09:59 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 3:16:15 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-06-29 20-05-44\LXG-7074E-RAC3.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.606 BB    0.1663 3998.21582  369.46530  49.3345
   2   9.793 BB    0.2563 4106.08936  246.48531  50.6655

Totals :                   8104.30518  615.95061



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.606 BB    0.1661 3697.47021  342.10355  49.3400
   2   9.793 BB    0.2564 3796.38501  227.85043  50.6600

Totals :                   7493.85522  569.95398

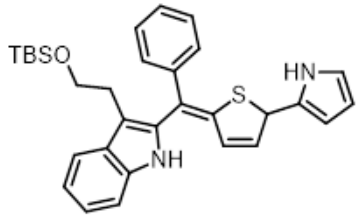


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

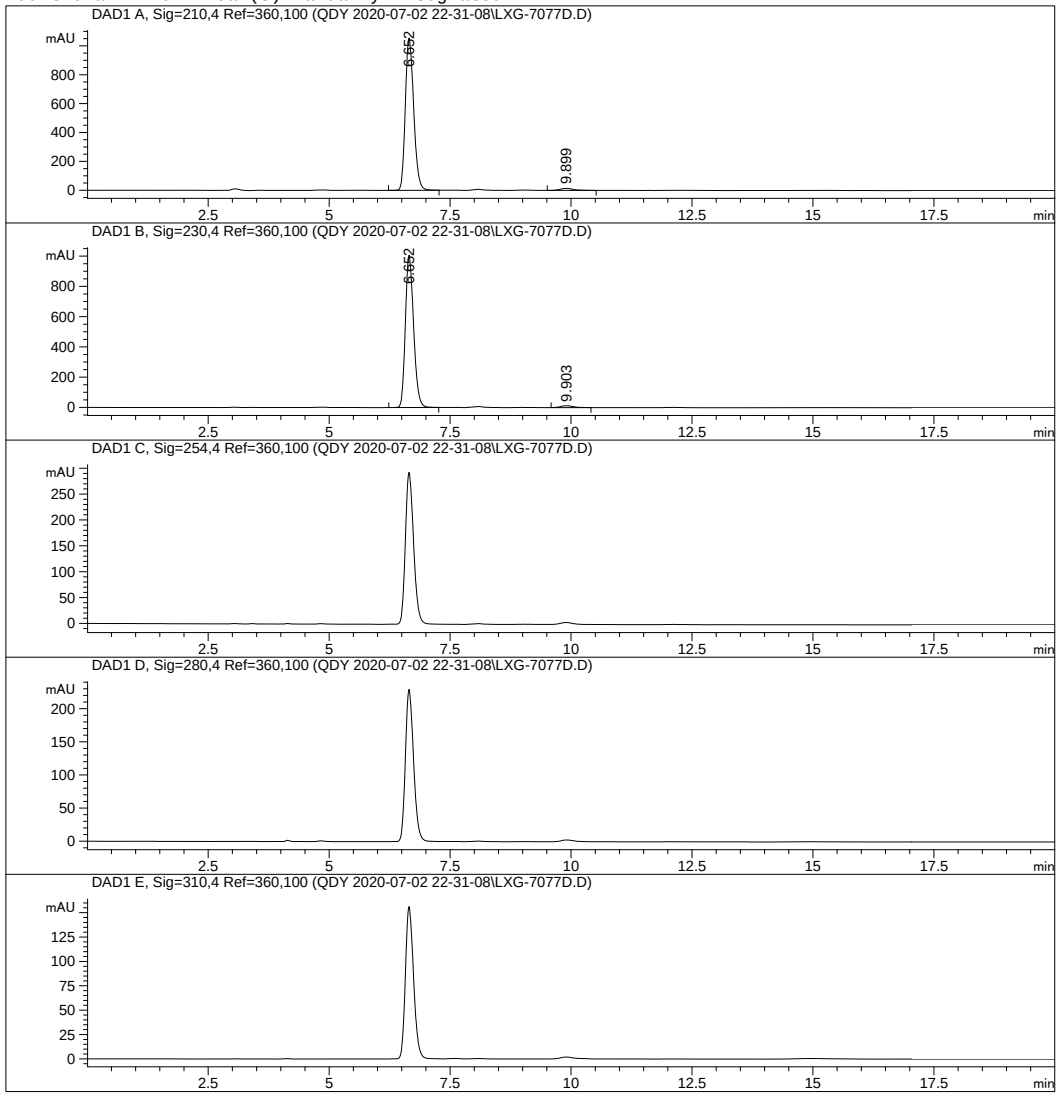


3m
(racemic)

Supplementary Figure 168. HPLC spectrum of **3m** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-02 22-31-08\LXG-7077D.D
Sample Name:

```
=====================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location : Vial 69
Injection Date  : 7/2/2020 10:44:01 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-02 22-31-08\AD-10-20.M
Last changed    : 7/2/2020 10:43:09 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 3:07:23 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-02 22-31-08\LXG-7077D.D
Sample Name:

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.652 BB    0.1882 1.26663e4  1054.37170  97.9792
   2   9.899 VB    0.2809  261.24567   14.18415   2.0208

Totals :                   1.29275e4  1068.55585



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.652 BB    0.1840 1.19065e4  1006.84686  98.1388
   2   9.903 BB    0.2729  225.81224   12.60866   1.8612

Totals :                   1.21323e4  1019.45552

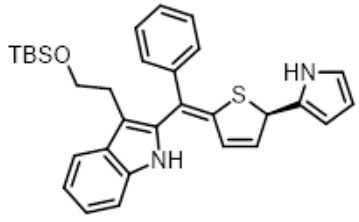


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

=====================================================================
                        *** End of Report ***
```

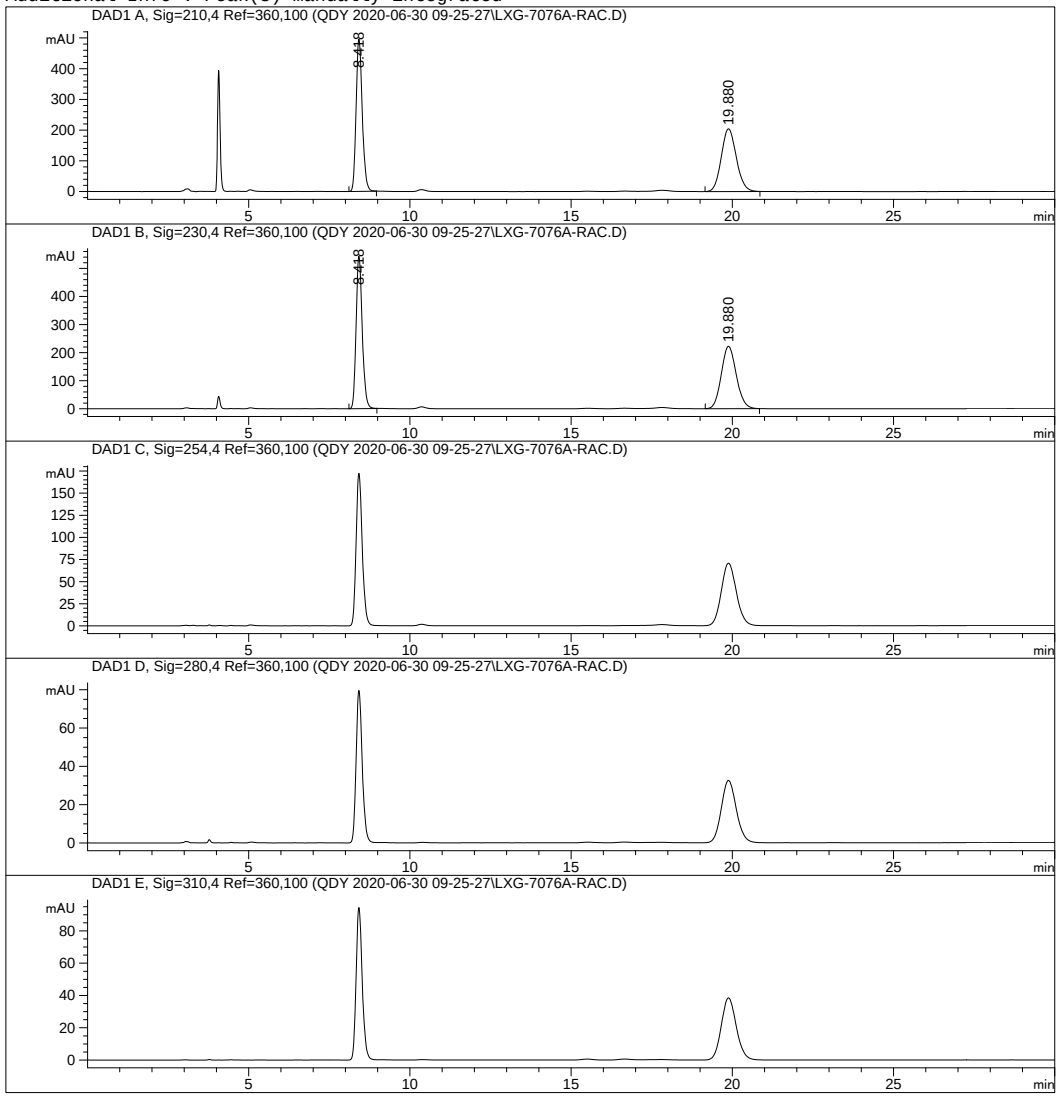


3m
(enantioenriched)

Supplementary Figure 169. HPLC spectrum of **3m** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-06-30 09-25-27\LXG-7076A-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :  12
Acq. Instrument : Instrument 1                    Location : Vial 62
Injection Date  : 6/30/2020 1:29:23 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-06-30 09-25-27\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 3:28:28 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-06-30 09-25-27\LXG-7076A-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.418 BB    0.2023 6566.19678  496.47937  49.7740
   2  19.880 BB    0.5021 6625.81348  204.46458  50.2260

Totals :                  1.31920e4   700.94395



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.418 BB    0.2018 7164.24072  543.28973  49.9198
   2  19.880 BB    0.5011 7187.27441  222.34601  50.0802

Totals :                  1.43515e4   765.63574

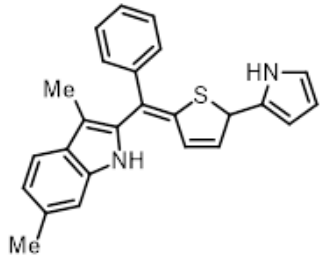


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

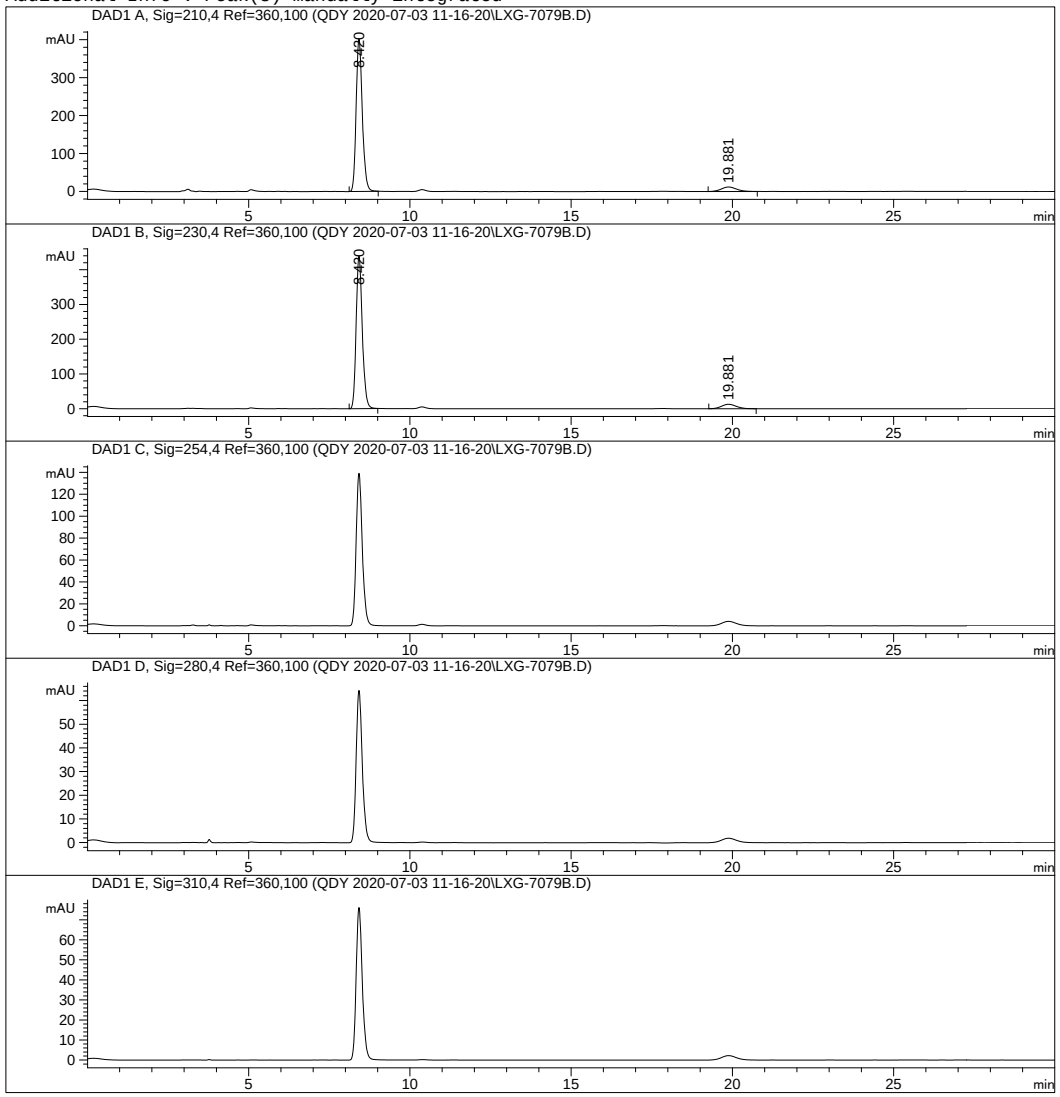


3n
(racemic)

Supplementary Figure 170. HPLC spectrum of **3n** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\LXG-7079B.D
Sample Name:

```
=====================================================================
Acq. Operator   :                          Seq. Line :  20
Acq. Instrument : Instrument 1              Location : Vial 65
Injection Date  : 7/3/2020 6:19:13 PM            Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 3:16:15 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\LXG-7079B.D
Sample Name:

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.420 BB    0.2025 5321.66992  401.91852  93.1099
   2  19.881 BB    0.4943  393.80081   11.89208   6.8901

Totals :                  5715.47073  413.81060



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.420 BB    0.2020 5795.16406  439.01126  93.3268
   2  19.881 BB    0.5043  414.37753   12.84661   6.6732

Totals :                  6209.54160  451.85787

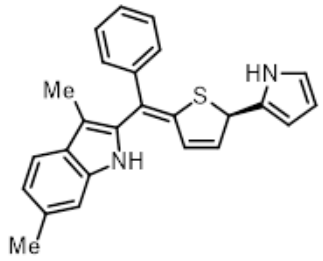


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

=====================================================================
                        *** End of Report ***
```

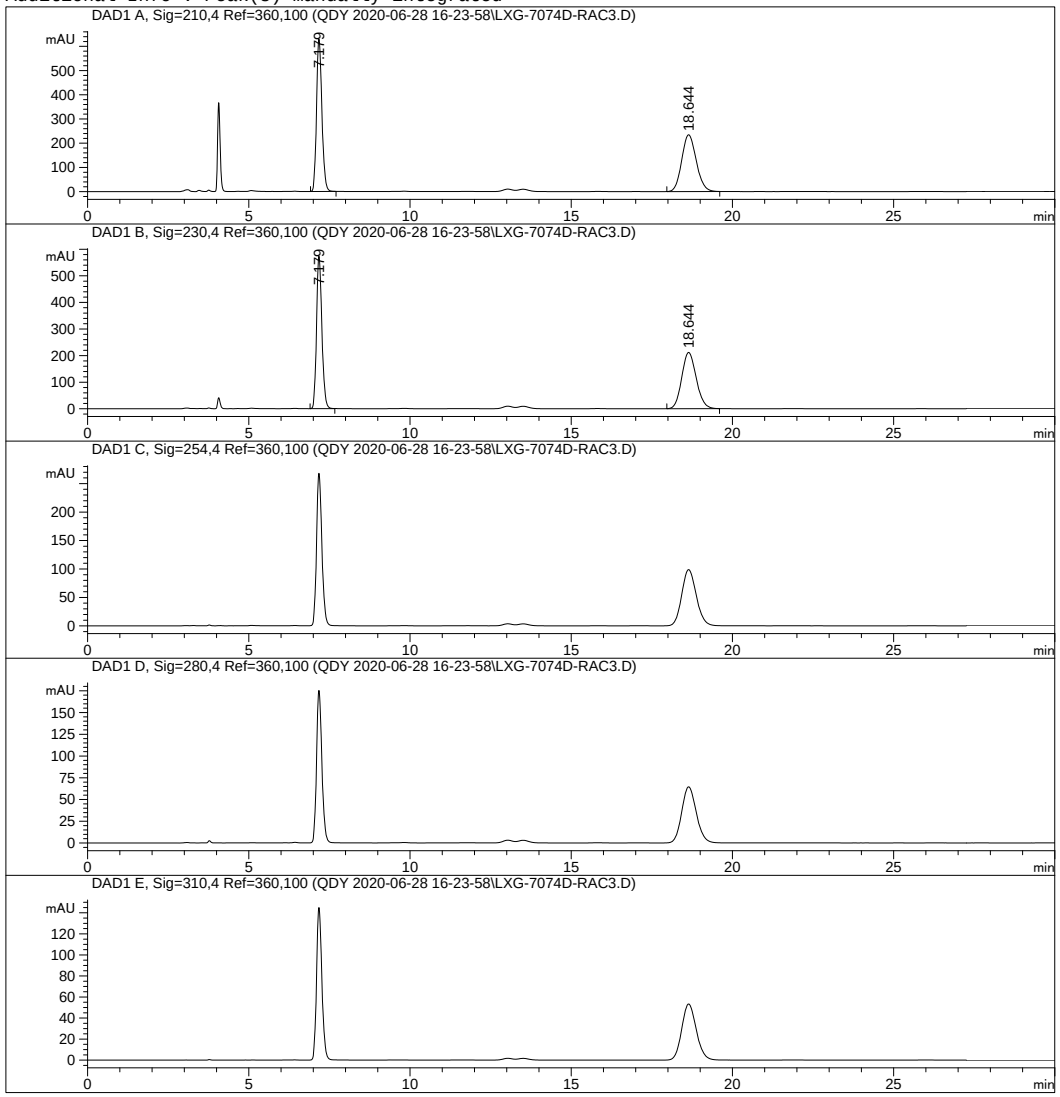


3n
(enantioenriched)

Supplementary Figure 171. HPLC spectrum of **3n** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\LXG-7074D-RAC3.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   8
Acq. Instrument : Instrument 1              Location : Vial 66
Injection Date  : 6/28/2020 7:43:09 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 3:11:19 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\LXG-7074D-RAC3.D
Sample Name:

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.179 BB    0.1786 7264.91260  629.84473  49.7575
   2  18.644 BB    0.4848 7335.71191  234.59599  50.2425

Totals :                  1.46006e4   864.44072



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.179 BB    0.1779 6584.26807  573.82117  49.9065
   2  18.644 BB    0.4823 6608.92773  211.65363  50.0935

Totals :                  1.31932e4   785.47479

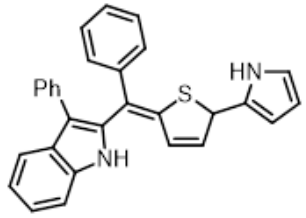


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

======================================================================
                        *** End of Report ***
```

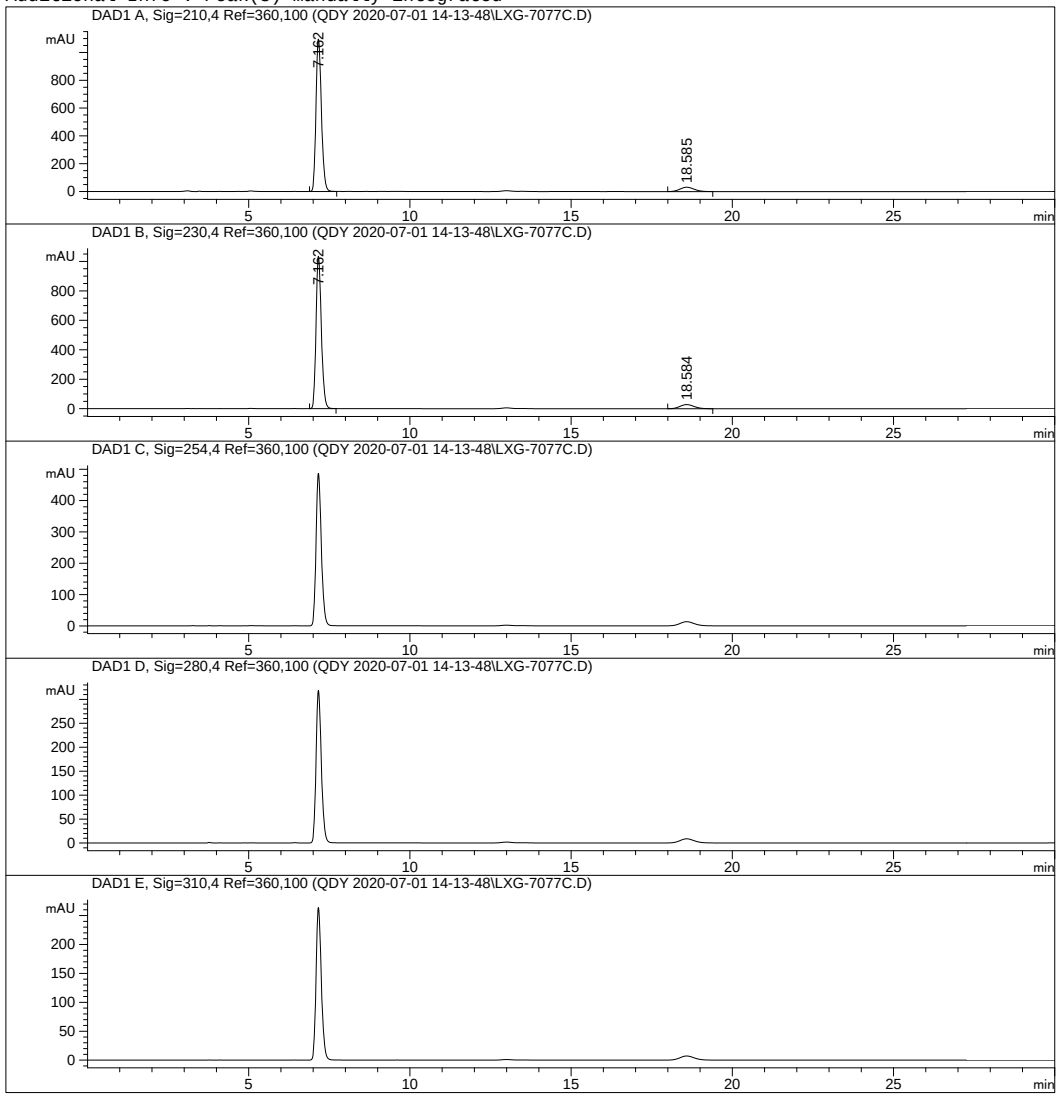


3o
(racemic)

Supplementary Figure 172. HPLC spectrum of **3o** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-01 14-13-48\LXG-7077C.D
Sample Name:

```
======================================================================
Acq. Operator   :                          Seq. Line :   5
Acq. Instrument : Instrument 1              Location : Vial 66
Injection Date  : 7/1/2020 3:20:51 PM            Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-01 14-13-48\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 12:06:36 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-01 14-13-48\LXG-7077C.D
Sample Name:

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.162 BB    0.1820 1.27756e4  1096.18677  92.9054
   2  18.585 BB    0.4792  975.58557   31.50851   7.0946

Totals :                  1.37512e4  1127.69527



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.162 BB    0.1750 1.18066e4  1035.32043  93.0994
   2  18.584 BB    0.4802  875.12103   28.34671   6.9006

Totals :                  1.26817e4  1063.66715

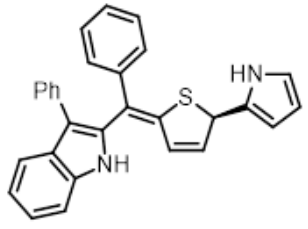


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

======================================================================
                        *** End of Report ***
```

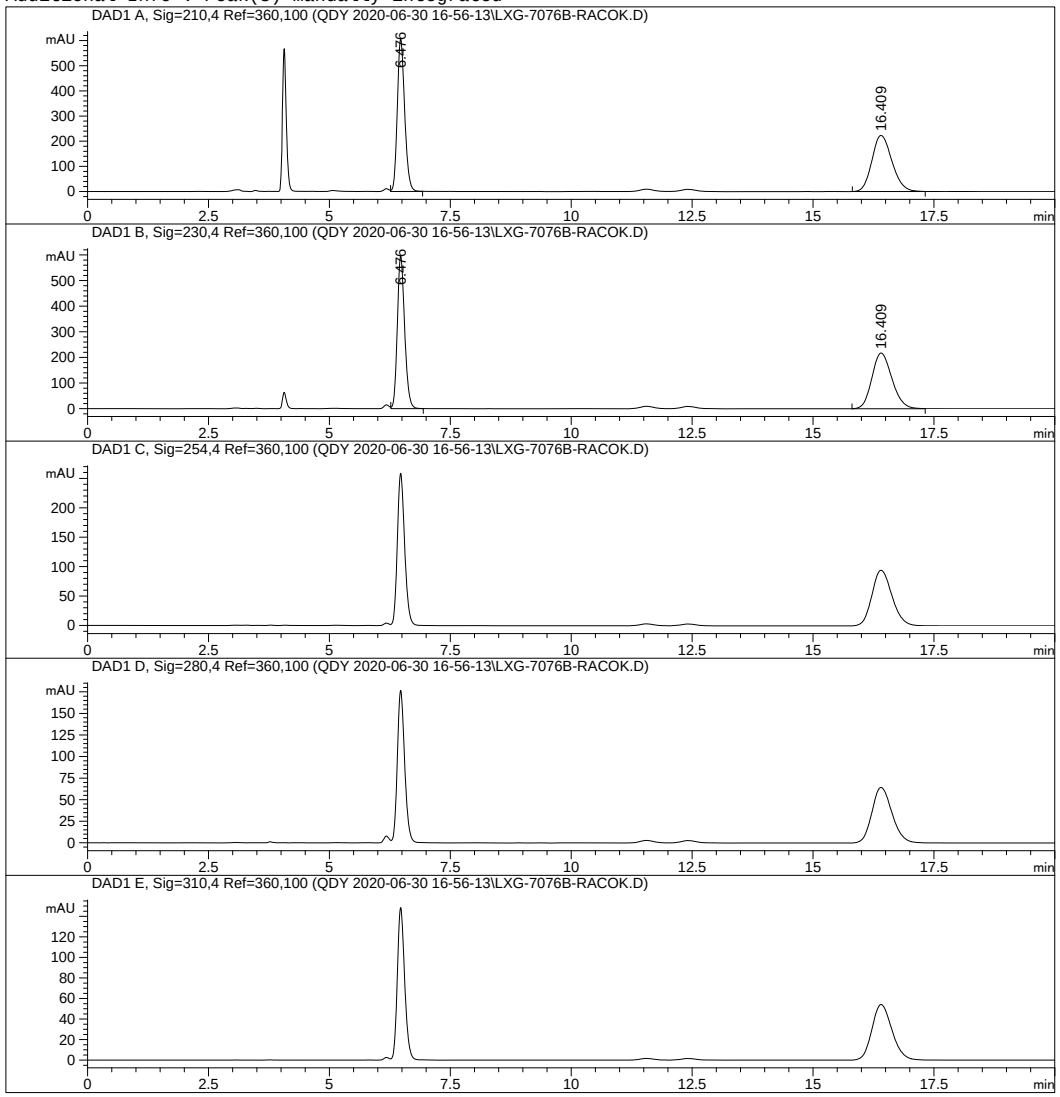


3o
(enantioenriched)

Supplementary Figure 173. HPLC spectrum of **3o** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-06-30 16-56-13\LXG-7076B-RACOK.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   3
Acq. Instrument : Instrument 1                    Location : Vial 64
Injection Date  : 6/30/2020 5:20:12 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-06-30 16-56-13\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-01-45-0.5.M
Last changed    : 8/22/2020 12:07:56 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-06-30 16-56-13\LXG-7076B-RACOK.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.476 VB    0.1633 6397.48779  605.55389  49.8967
   2  16.409 BB    0.4476 6423.98975  223.29907  50.1033

Totals :                  1.28215e4   828.85297



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.476 VB    0.1607 6258.13525  595.15112  50.0114
   2  16.409 BB    0.4474 6255.27832  217.57716  49.9886

Totals :                  1.25134e4   812.72829

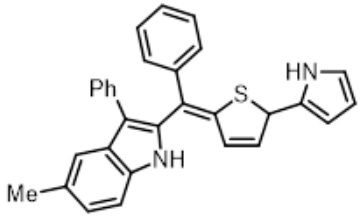


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

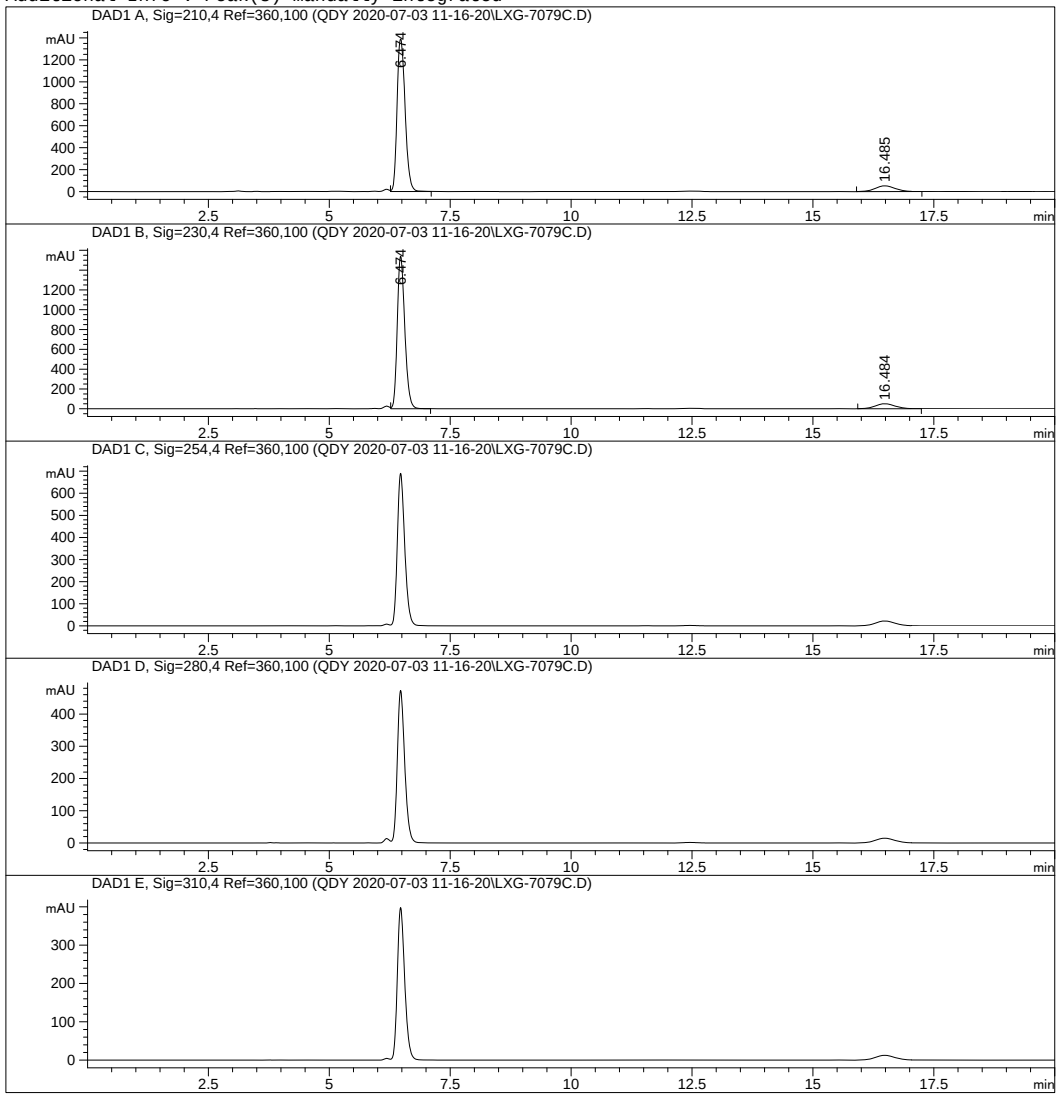


3p
(racemic)

Supplementary Figure 174. HPLC spectrum of **3p** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\LXG-7079C.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :  24
Acq. Instrument : Instrument 1                  Location : Vial 66
Injection Date  : 7/3/2020 7:43:37 PM               Inj :   1
                                               Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\AD-20-20.M
Last changed    : 7/4/2015 10:27:19 AM
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 3:16:15 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\LXG-7079C.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.474 VB    0.1827 1.60315e4  1388.66321  91.4658
   2  16.485 BB    0.4434 1495.81299   52.34620   8.5342

Totals :                  1.75273e4  1441.00940



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.474 VB    0.1682 1.66535e4  1540.03833  91.9762
   2  16.484 BB    0.4432 1452.81128   50.86245   8.0238

Totals :                  1.81064e4  1590.90078

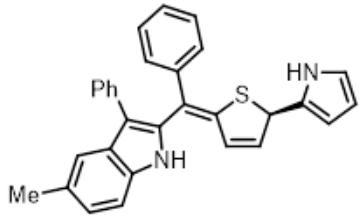


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

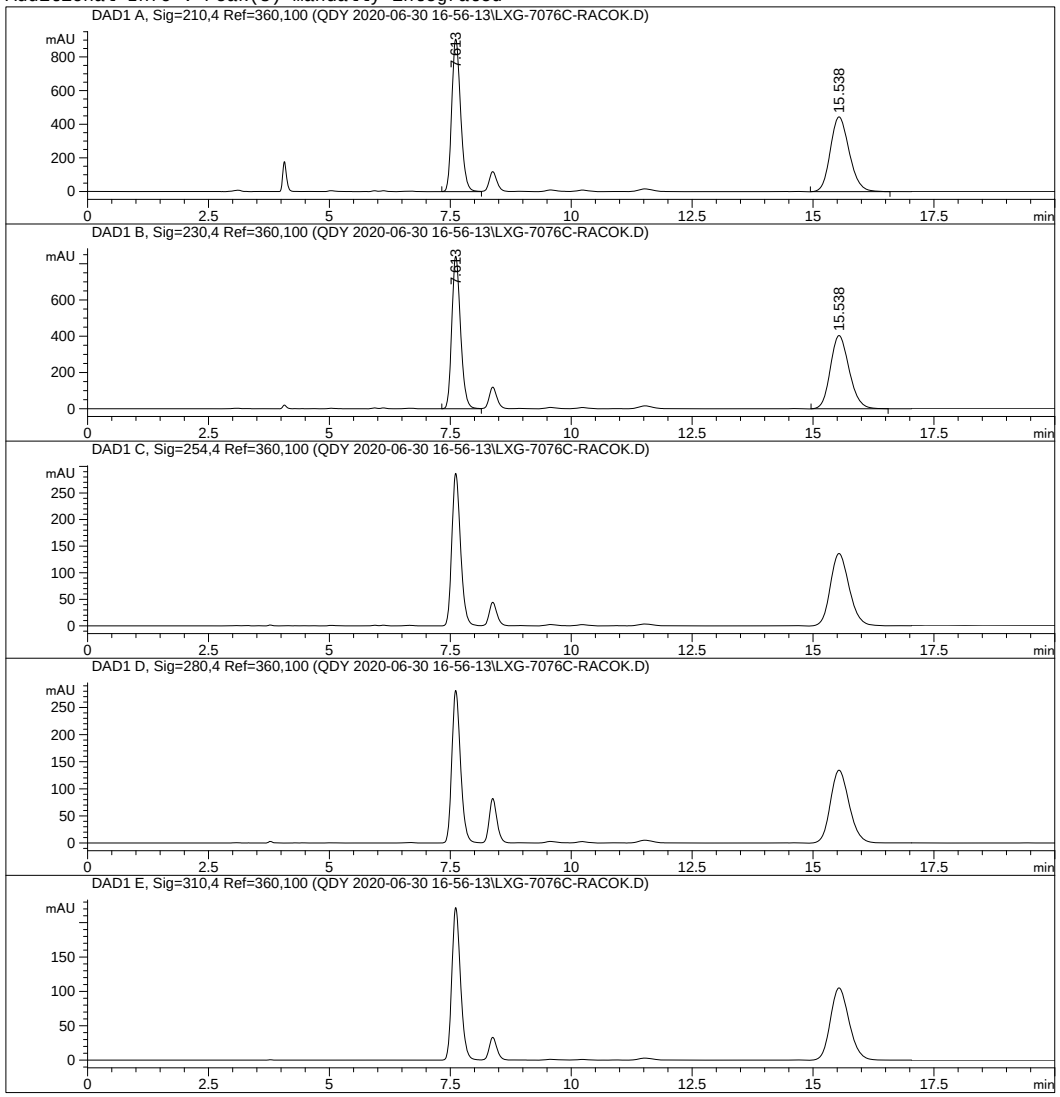


3p
(enantioenriched)

Supplementary Figure 175. HPLC spectrum of **3p** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-06-30 16-56-13\LXG-7076C-RACOK.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   4
Acq. Instrument : Instrument 1                    Location : Vial 63
Injection Date  : 6/30/2020 5:51:17 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-06-30 16-56-13\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 3:29:47 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-06-30 16-56-13\LXG-7076C-RACOK.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.613 BV    0.1960 1.15018e4   906.76239  48.8909
   2  15.538 BB    0.4197 1.20237e4   444.39545  51.1091

Totals :                  2.35255e4  1351.15784



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.613 BV    0.1921 1.05353e4   841.55798  49.1840
   2  15.538 BB    0.4165 1.08849e4   403.81821  50.8160

Totals :                  2.14202e4  1245.37619

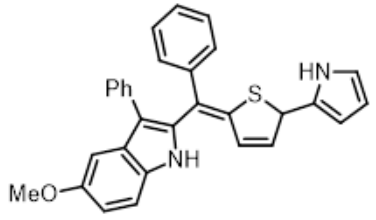


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

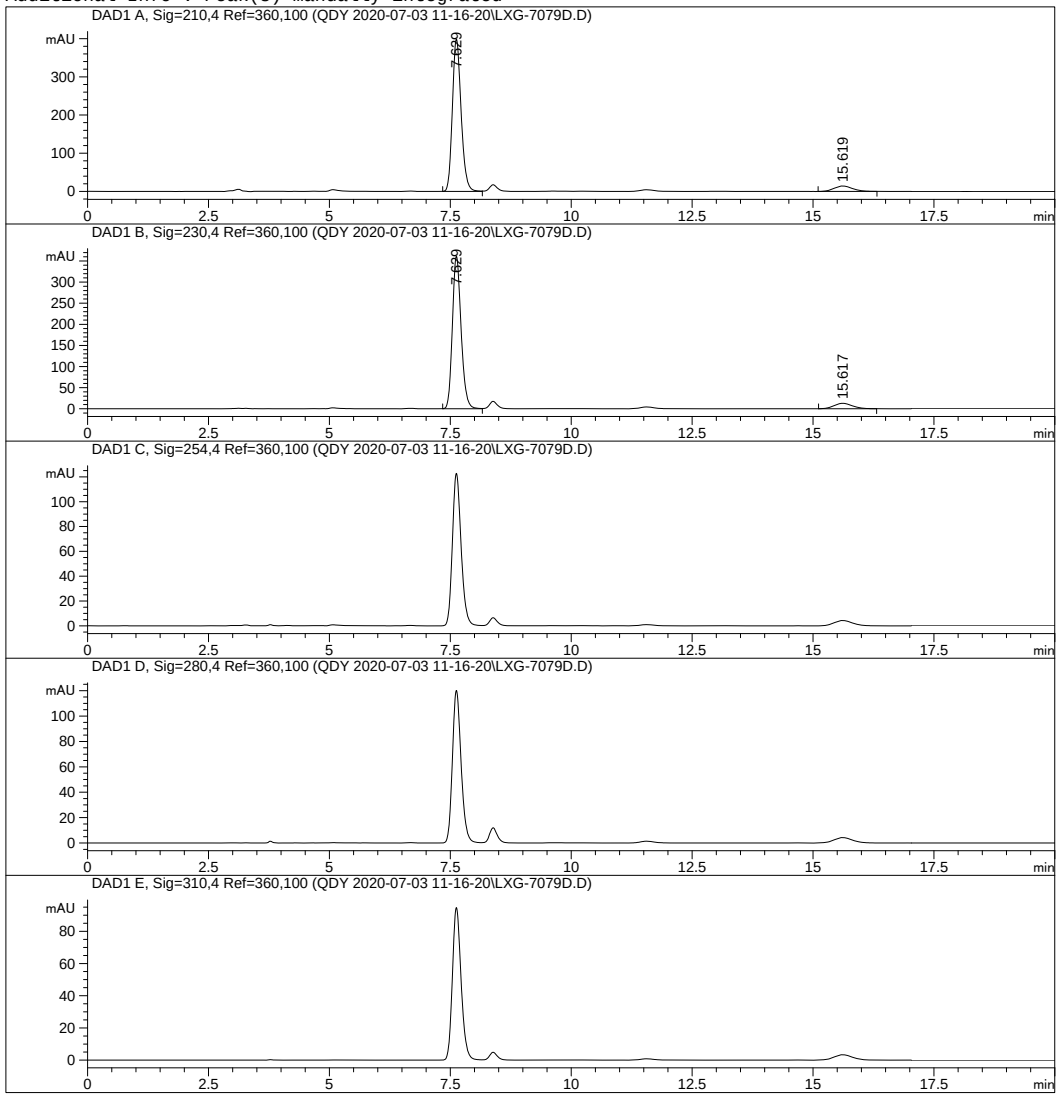


3q
(racemic)

Supplementary Figure 176. HPLC spectrum of **3q** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\LXG-7079D.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :  35
Acq. Instrument : Instrument 1                    Location : Vial 67
Injection Date  : 7/3/2020 11:45:25 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\AD-20-20.M
Last changed    : 7/4/2015 10:27:19 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-01-45-0.5.M
Last changed    : 8/20/2020 7:42:57 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\LXG-7079D.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.629 BB    0.1923 5002.79199  398.98288  92.9864
   2  15.619 BB    0.4132  377.34076   14.23963   7.0136

Totals :                  5380.13275  413.22251



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.629 BB    0.1919 4517.89209  361.29172  92.9591
   2  15.617 BB    0.4122  342.19412   12.86958   7.0409

Totals :                  4860.08621  374.16129

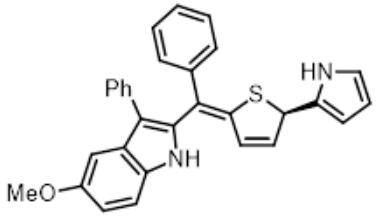


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

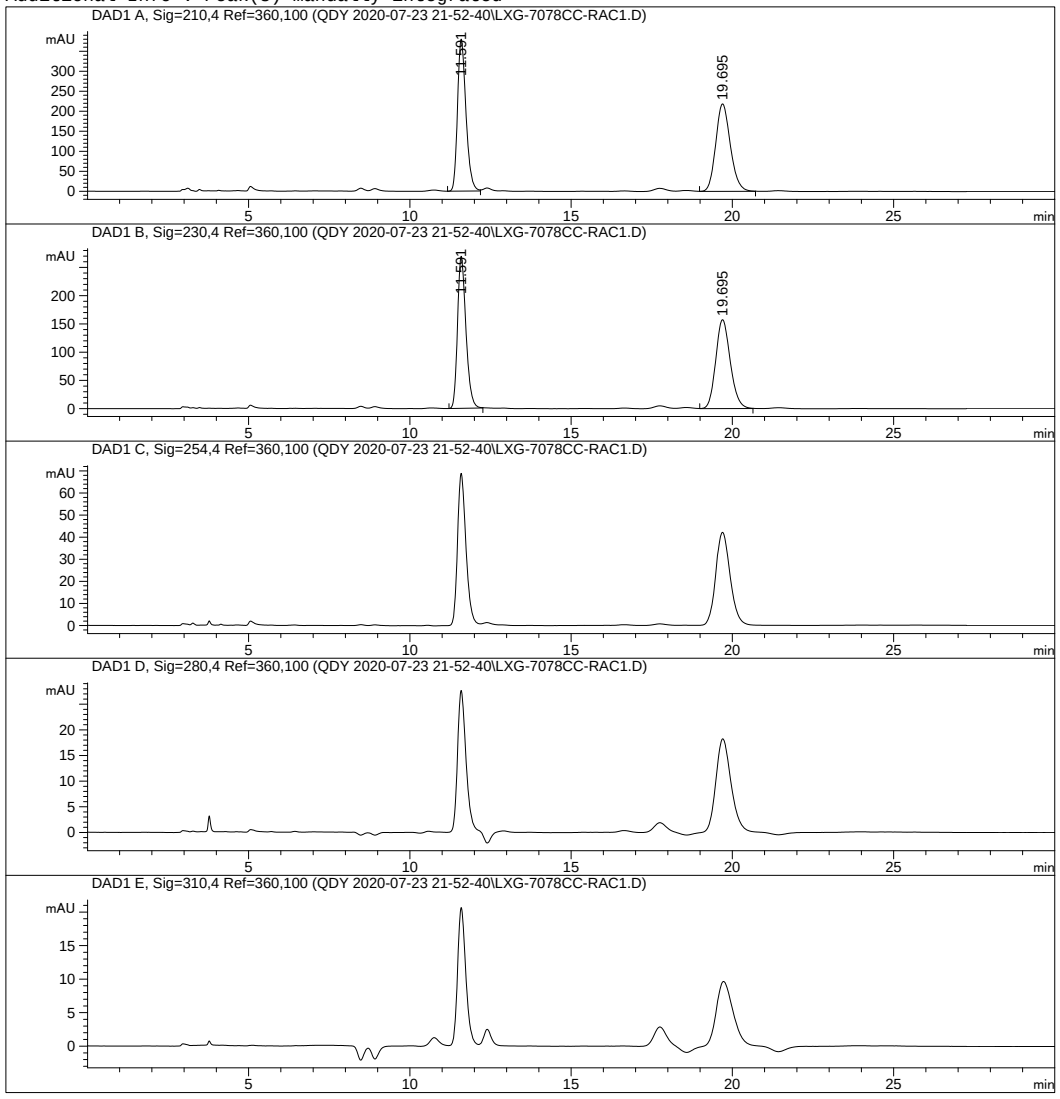


3q
(enantioenriched)

Supplementary Figure 177. HPLC spectrum of **3q** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-07-23 21-52-40\LXG-7078CC-RAC1.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location : Vial 61
Injection Date  : 7/23/2020 10:25:53 PM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-23 21-52-40\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/25/2020 7:11:23 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-23 21-52-40\LXG-7078CC-RAC1.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.591 VV    0.2783 6912.13135  379.90875  50.1463
   2  19.695 VB    0.4846 6871.79346  218.69592  49.8537

Totals :                  1.37839e4   598.60468



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.591 BB    0.2774 4877.55859  269.19696  49.7728
   2  19.695 VB    0.4827 4922.08057  157.45436  50.2272

Totals :                  9799.63916  426.65132

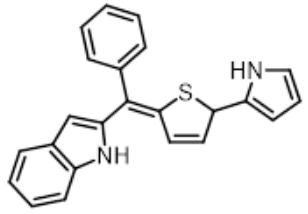


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```

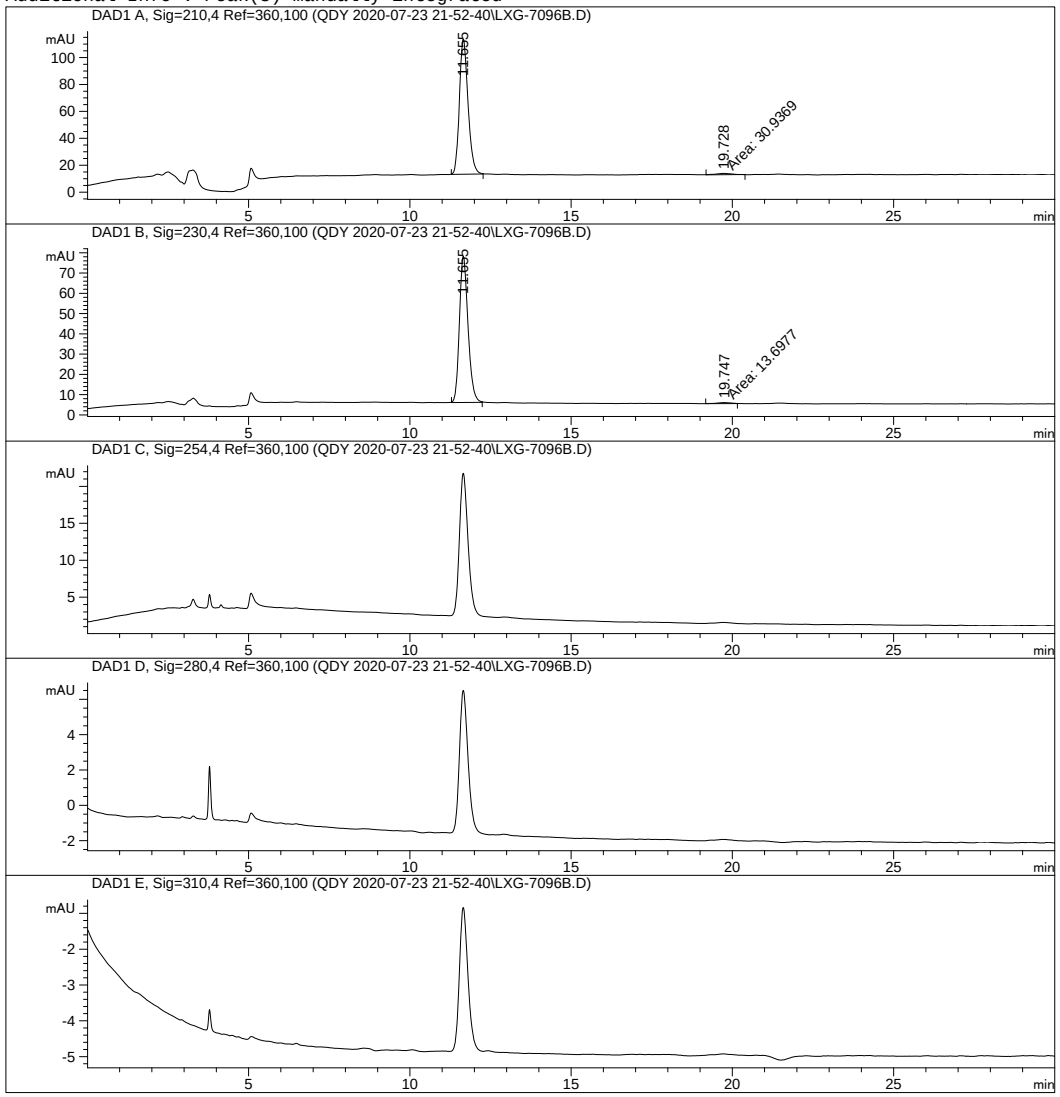


3r
(racemic)

Supplementary Figure 178. HPLC spectrum of **3r** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-23 21-52-40\LXG-7096B.D
Sample Name:

```
======================================================================
Acq. Operator   :                          Seq. Line :   1
Acq. Instrument : Instrument 1              Location : Vial 62
Injection Date  : 7/23/2020 9:54:29 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-23 21-52-40\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/25/2020 7:11:23 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-23 21-52-40\LXG-7096B.D
Sample Name:

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.655 BB    0.2849 1867.79529  100.47170  98.3707
   2  19.728 MM    0.5511   30.93695 9.35695e-1   1.6293

Totals :                  1898.73224  101.40740



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.655 BB    0.2847 1341.24048   72.21307  98.9891
   2  19.747 MM    0.4835   13.69767 4.72175e-1   1.0109

Totals :                  1354.93815   72.68524

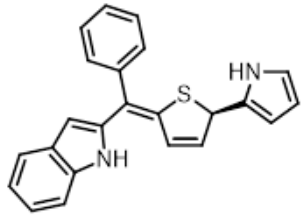


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

======================================================================
                        *** End of Report ***
```



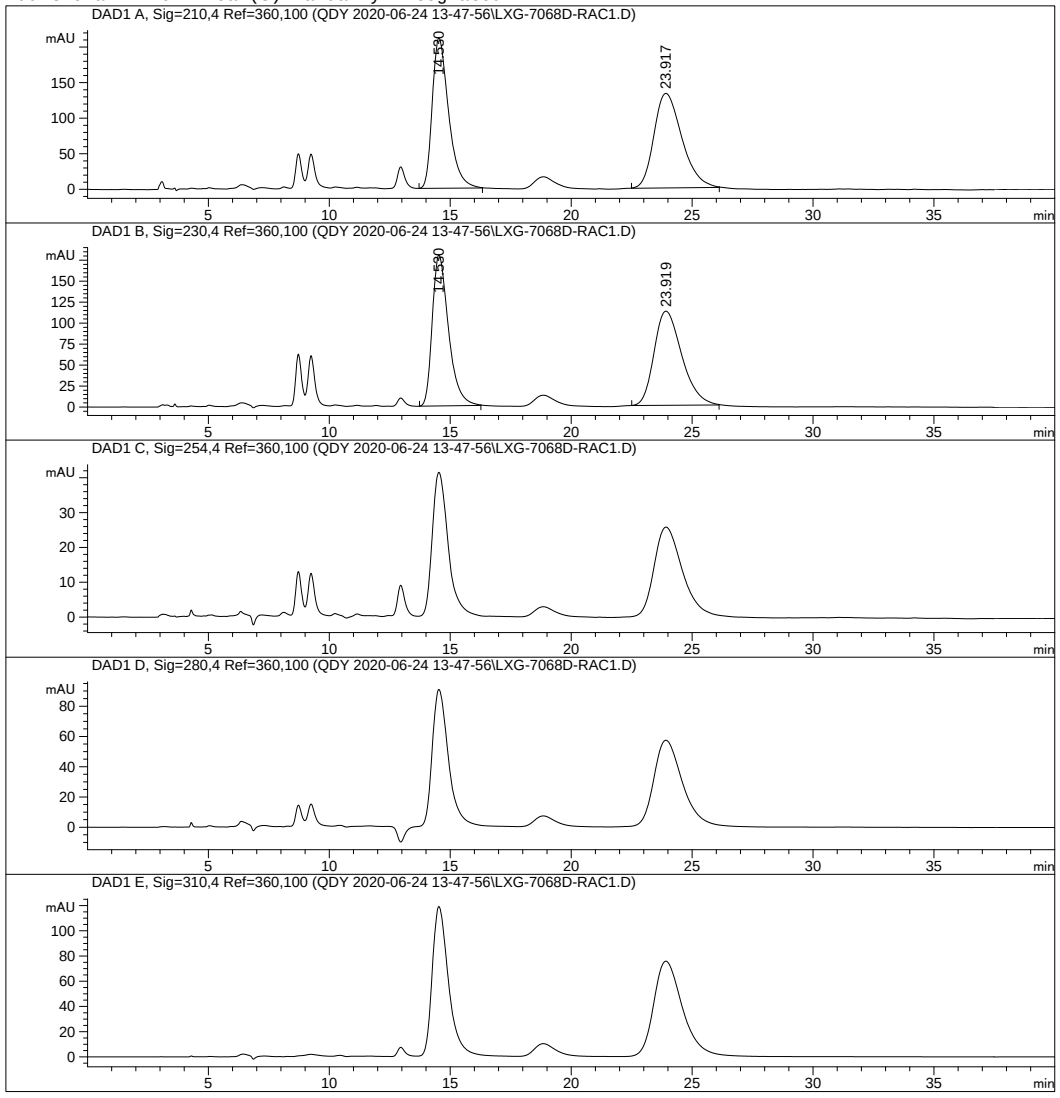
3r
(enantioenriched)

Supplementary Figure 179. HPLC spectrum of **3r** (enantioenriched)

Instrument 1 7/25/2020 7:21:13 PM

Data File C:\CHEM32\1\DATA\QDY 2020-06-24 13-47-56\LXG-7068D-RAC1.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   8
Acq. Instrument : Instrument 1                    Location : Vial 64
Injection Date  : 6/24/2020 4:52:15 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-06-24 13-47-56\OD-10-40.M
Last changed    : 6/24/2020 3:29:18 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 12:06:36 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-06-24 13-47-56\LXG-7068D-RAC1.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.530 BB    0.7216 9914.00586  211.21516  48.1994
   2  23.917 BB    1.2231 1.06547e4   132.93356  51.8006

Totals :                  2.05687e4   344.14873



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.530 BB    0.7203 8385.44629  179.72000  48.3618
   2  23.919 BB    1.2266 8953.55469  112.24313  51.6382

Totals :                  1.73390e4   291.96313

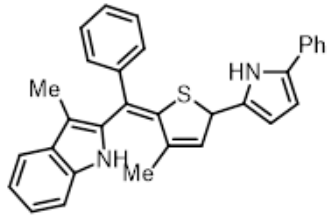


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

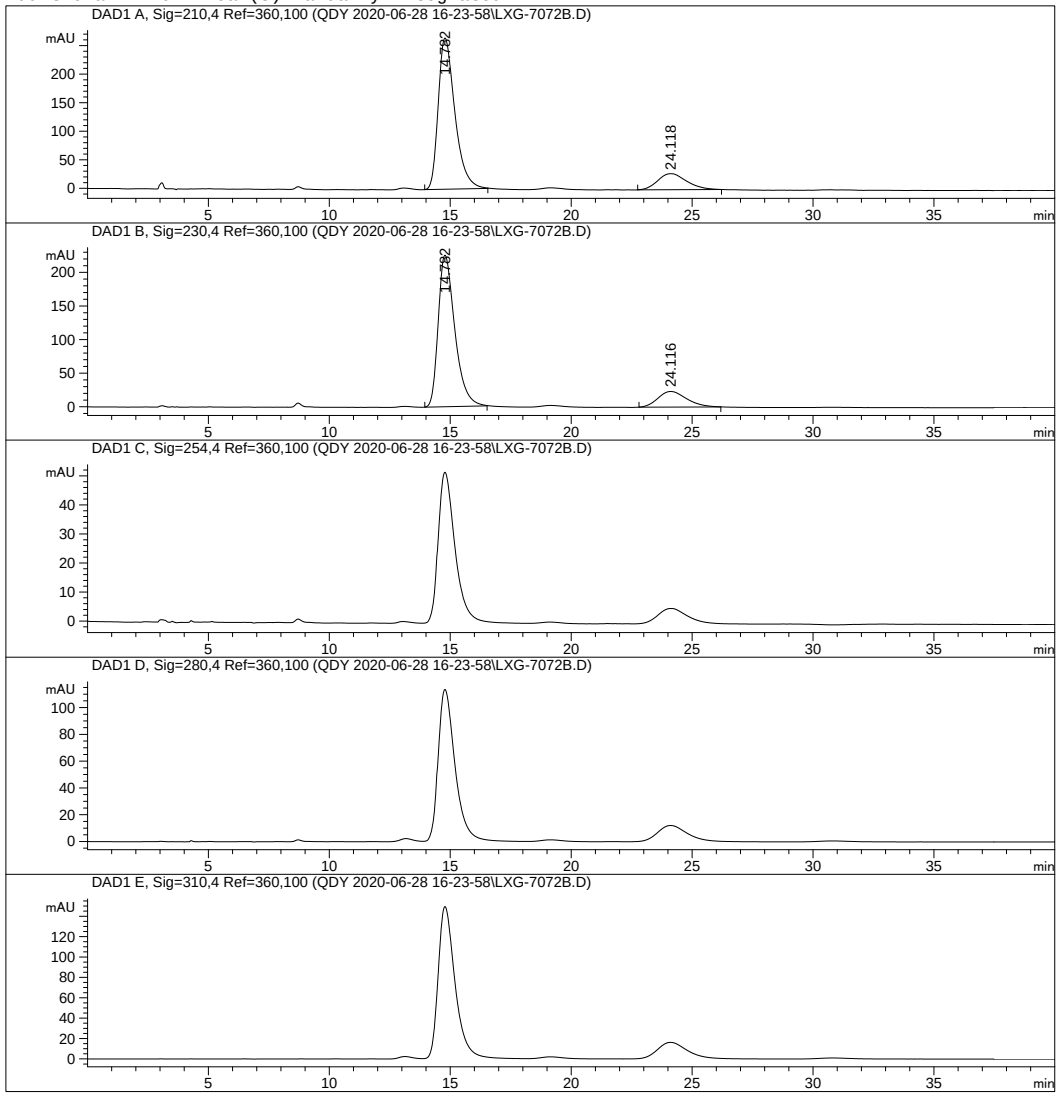


3s
(racemic)

Supplementary Figure 180. HPLC spectrum of **3s** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\LXG-7072B.D
Sample Name:

```
======================================================================
Acq. Operator   :                          Seq. Line :  11
Acq. Instrument : Instrument 1              Location : Vial 68
Injection Date  : 6/28/2020 8:56:48 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\OD-10-40.M
Last changed    : 6/28/2020 8:55:55 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 12:06:36 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\LXG-7072B.D
Sample Name:

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.782 BB    0.7299 1.26581e4   264.72620  84.3879
   2  24.118 BB    1.1321 2341.79321   28.10609  15.6121

Totals :                  1.49999e4   292.83229



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.782 BB    0.7264 1.07576e4   225.56746  84.8413
   2  24.116 BB    1.2257 1922.07410   23.22079  15.1587

Totals :                  1.26797e4   248.78825

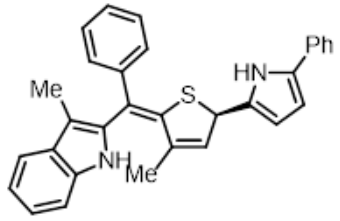


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

======================================================================
                        *** End of Report ***
```

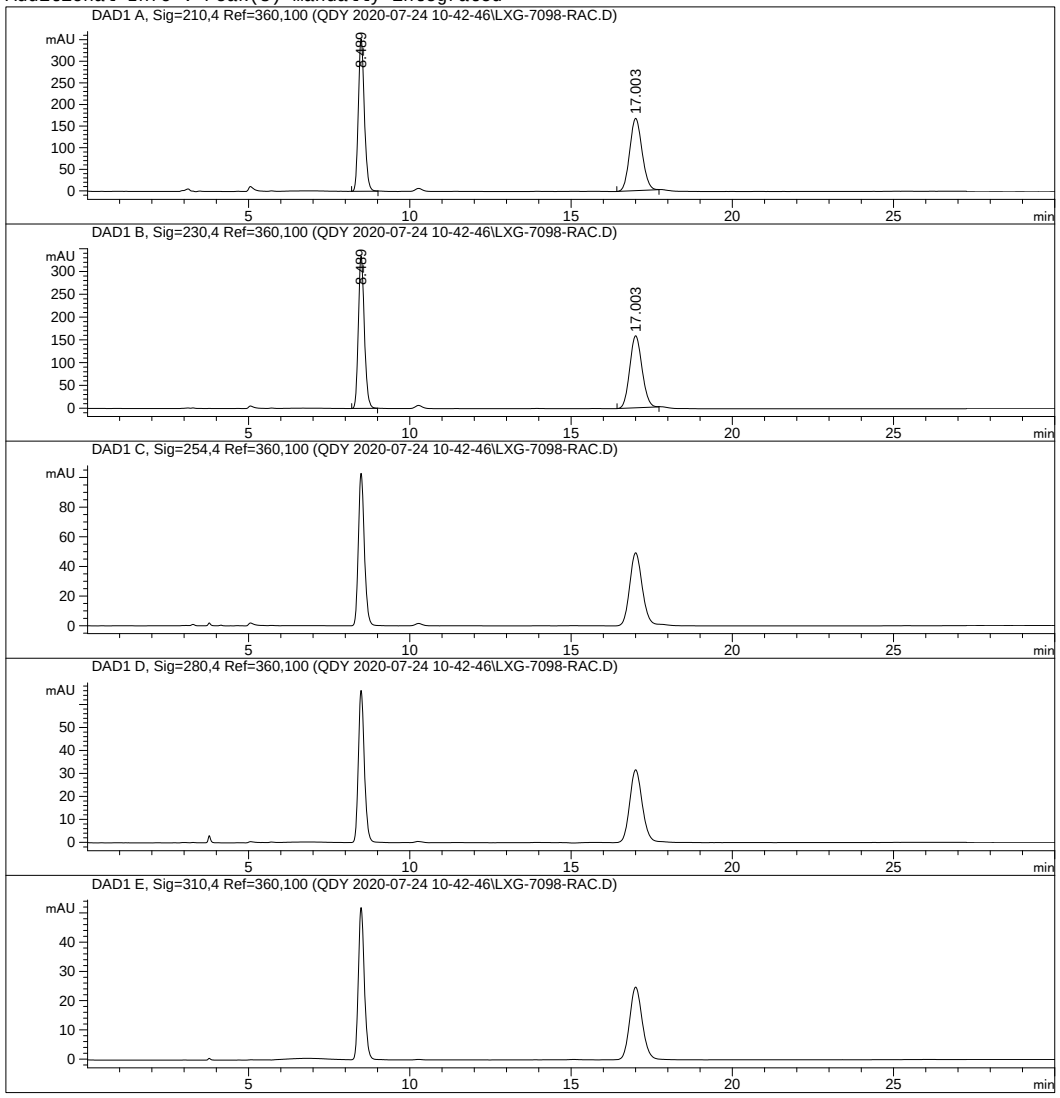


3s
(enantioenriched)

Supplementary Figure 181. HPLC spectrum of **3s** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-07-24 10-42-46\LXG-7098-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   6
Acq. Instrument : Instrument 1                    Location : Vial 63
Injection Date  : 7/24/2020 12:40:20 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-24 10-42-46\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/10/2020 9:21:13 AM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-24 10-42-46\LXG-7098-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.489 BB    0.1986 4548.04297  352.30460  50.6533
   2  17.003 BB    0.4129 4430.71875  167.31779  49.3467

Totals :                  8978.76172  519.62239



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.489 BB    0.1983 4307.11865  334.25439  50.7287
   2  17.003 BB    0.4106 4183.38037  158.15608  49.2713

Totals :                  8490.49902  492.41048

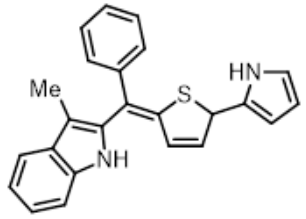


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

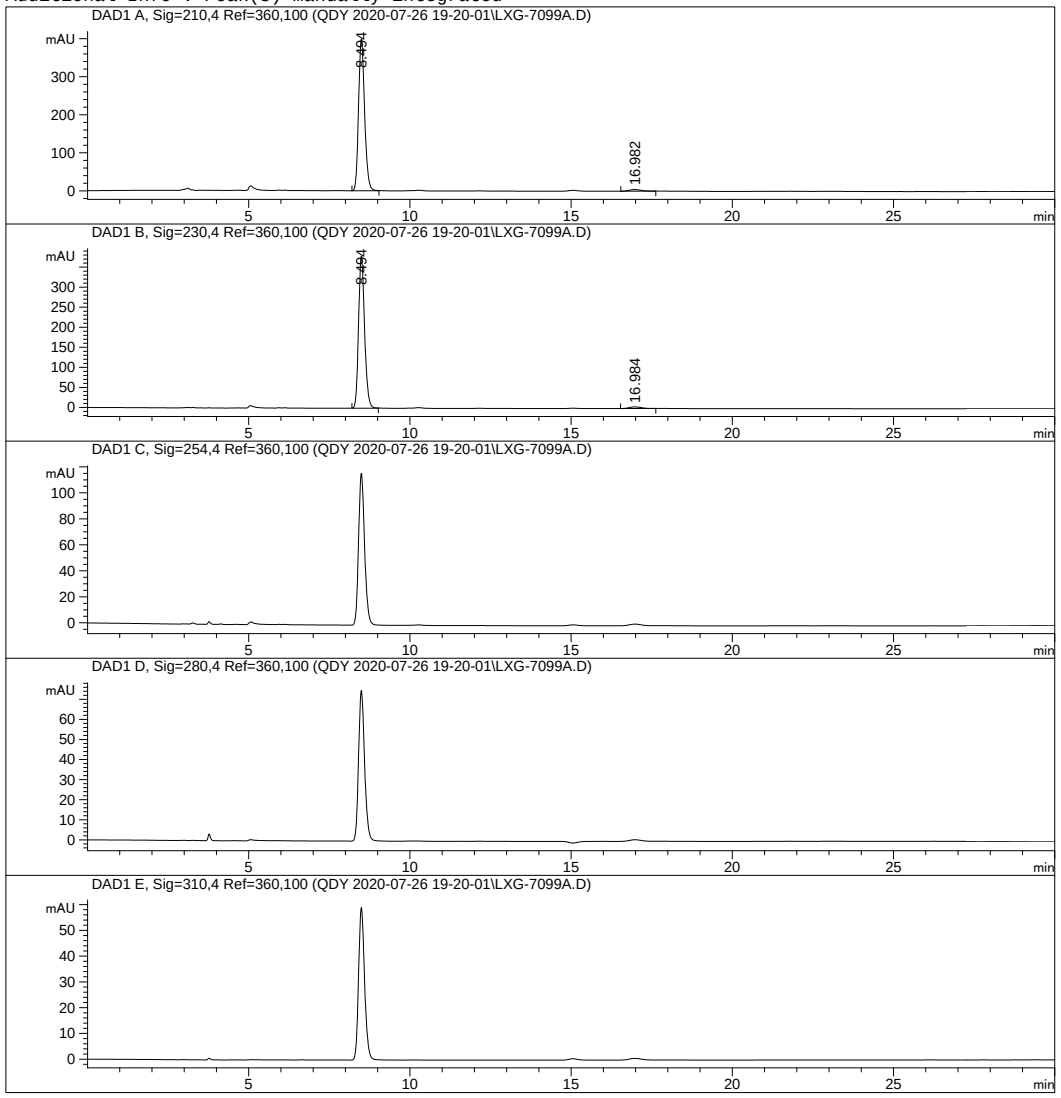


3t
(racemic)

Supplementary Figure 182. HPLC spectrum of **3t** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-26 19-20-01\LXG-7099A.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   2
Acq. Instrument : Instrument 1                    Location : Vial 68
Injection Date  : 7/26/2020 7:35:19 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-26 19-20-01\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/10/2020 9:21:13 AM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-26 19-20-01\LXG-7099A.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.494 BB    0.1991 5162.85303  398.64743  98.0465
   2  16.982 BB    0.3791  102.86679    4.20987   1.9535

Totals :                  5265.71982  402.85730



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.494 BB    0.1986 4893.23730  379.18848  97.9982
   2  16.984 BB    0.3858   99.95373    4.02419   2.0018

Totals :                  4993.19103  383.21267

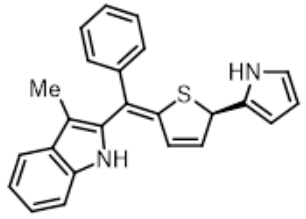


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

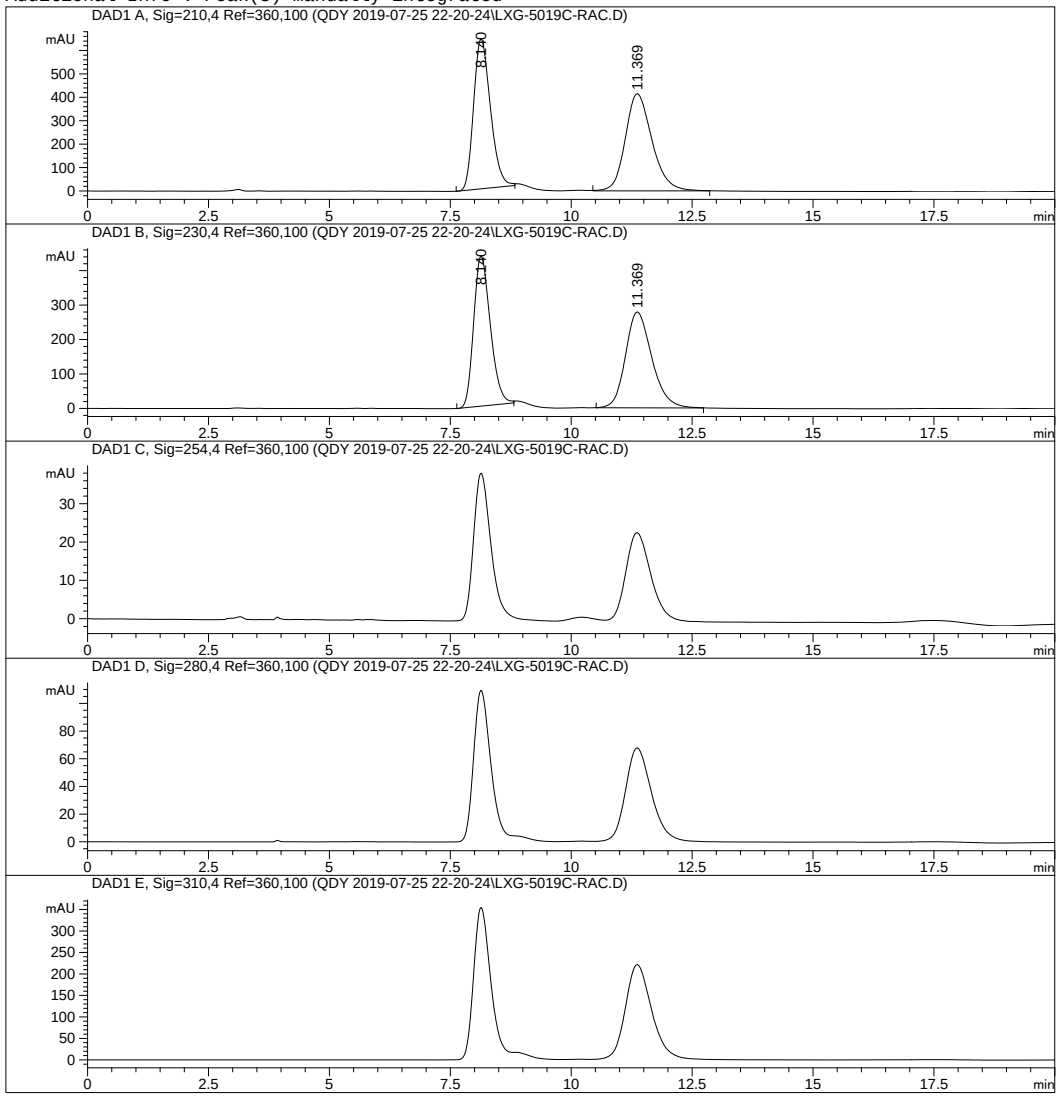


3t
(enantioenriched)

Supplementary Figure 183. HPLC spectrum of **3t** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2019-07-25 22-20-24\LXG-5019C-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   4
Acq. Instrument : Instrument 1                    Location : Vial 63
Injection Date  : 7/25/2019 11:56:33 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-07-25 22-20-24\OD-20-40.M
Last changed    : 7/25/2019 10:32:57 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\OD-001-10-0.7.M
Last changed    : 8/23/2019 7:32:17 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-07-25 22-20-24\LXG-5019C-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.140 BB    0.3739 1.54492e4   639.37677  49.3760
   2  11.369 VB    0.5859 1.58397e4   414.41437  50.6240

Totals :                  3.12888e4  1053.79114



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.140 BB    0.3713 1.04251e4   435.41559  49.7444
   2  11.369 BB    0.5796 1.05322e4   278.27737  50.2556

Totals :                  2.09573e4   713.69296

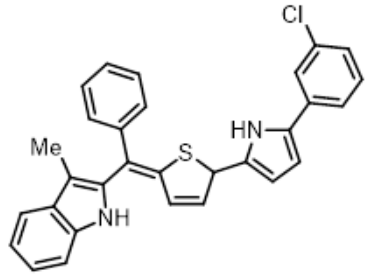


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

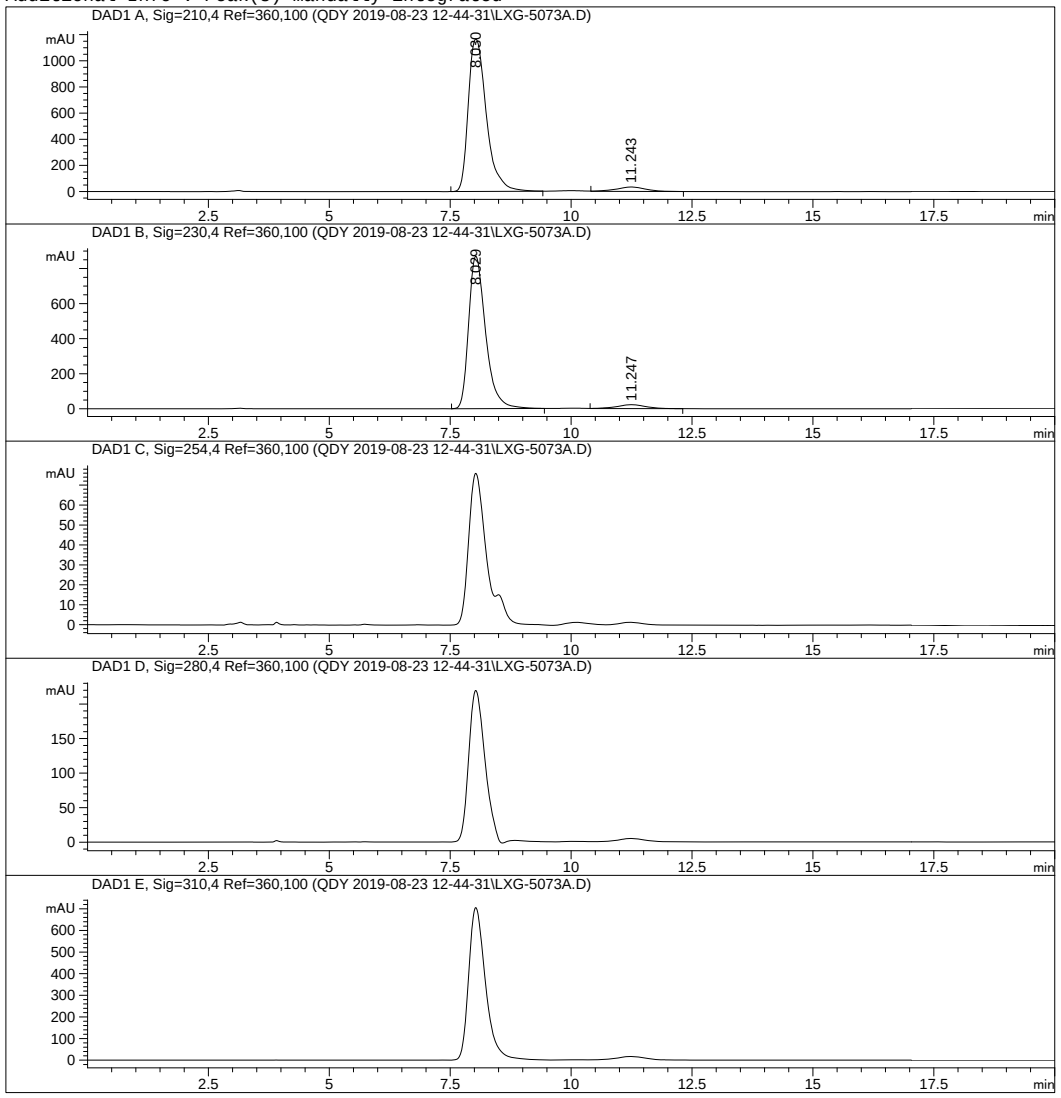


3u
(racemic)

Supplementary Figure 184. HPLC spectrum of **3u** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2019-08-23 12-44-31\LXG-5073A.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  11
Acq. Instrument : Instrument 1              Location : Vial 65
Injection Date  : 8/23/2019 4:59:31 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-08-23 12-44-31\OD-20-20.M
Last changed    : 8/23/2019 4:58:39 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\OD-001-10-0.7.M
Last changed    : 8/21/2019 8:26:51 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-08-23 12-44-31\LXG-5073A.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.030 BB    0.4014 3.03079e4  1165.40076  95.5616
   2  11.243 VB    0.6249 1407.65125   33.45370   4.4384

Totals :                  3.17156e4  1198.85445



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.029 BB    0.3727 2.12207e4   869.62476  95.7986
   2  11.247 VB    0.6219  930.66052   22.34653   4.2014

Totals :                  2.21514e4   891.97128

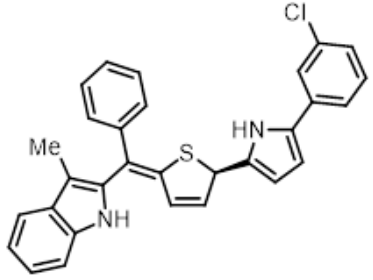


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```

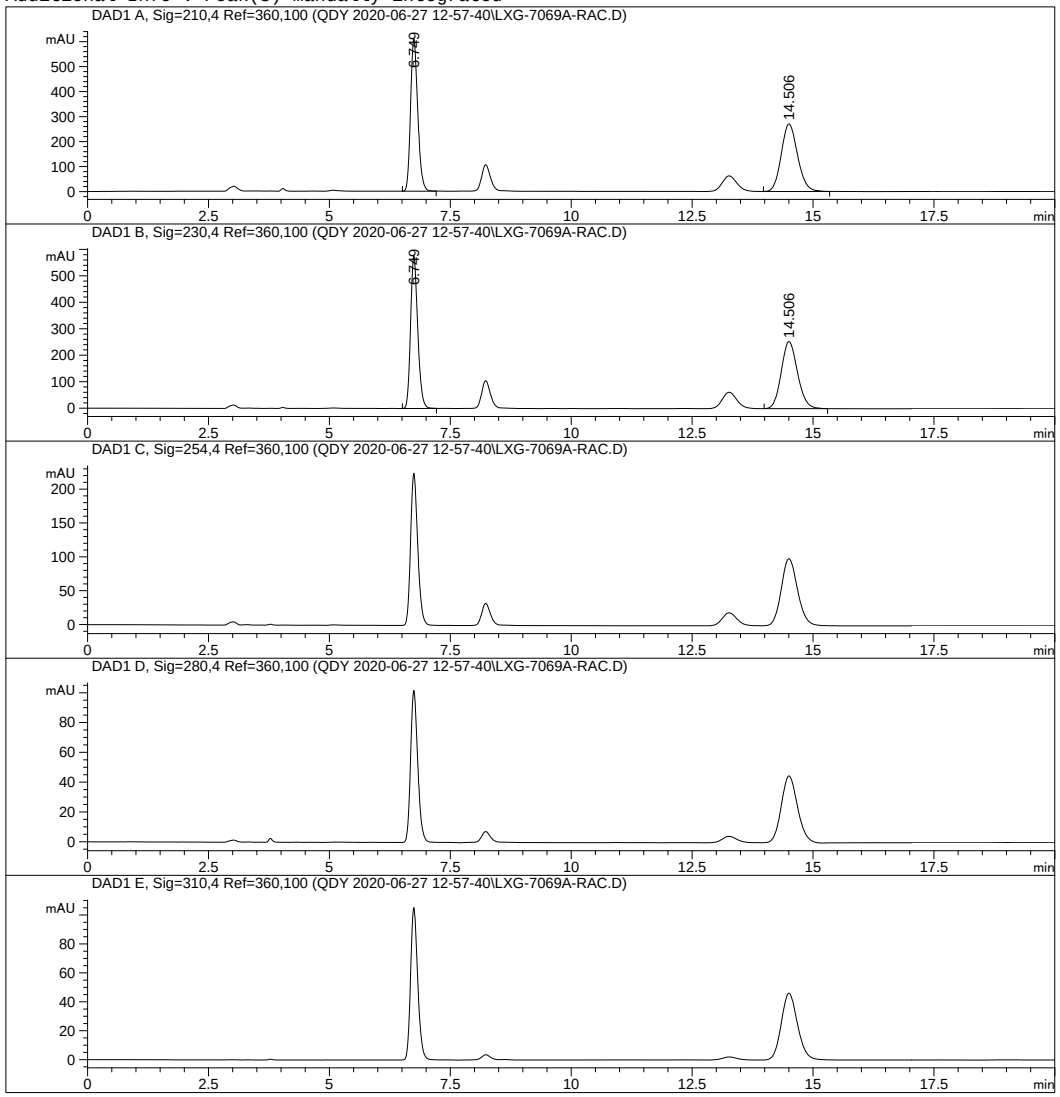


3u
(enantioenriched)

Supplementary Figure 185. HPLC spectrum of **3u** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-06-27 12-57-40\LXG-7069A-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   2
Acq. Instrument : Instrument 1                    Location : Vial 69
Injection Date  : 6/27/2020 1:10:37 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-06-27 12-57-40\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/25/2020 7:09:18 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-06-27 12-57-40\LXG-7069A-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.749 BB    0.1583 6273.87695  608.65845  49.7314
   2  14.506 BB    0.3617 6341.64795  270.30951  50.2686

Totals :                  1.26155e4   878.96796



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.749 BB    0.1577 5902.71289  575.31378  49.9236
   2  14.506 BB    0.3607 5920.78662  253.34920  50.0764

Totals :                  1.18235e4   828.66298

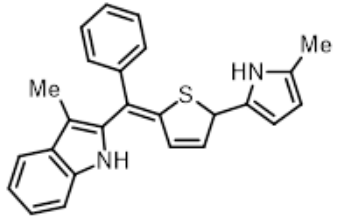


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

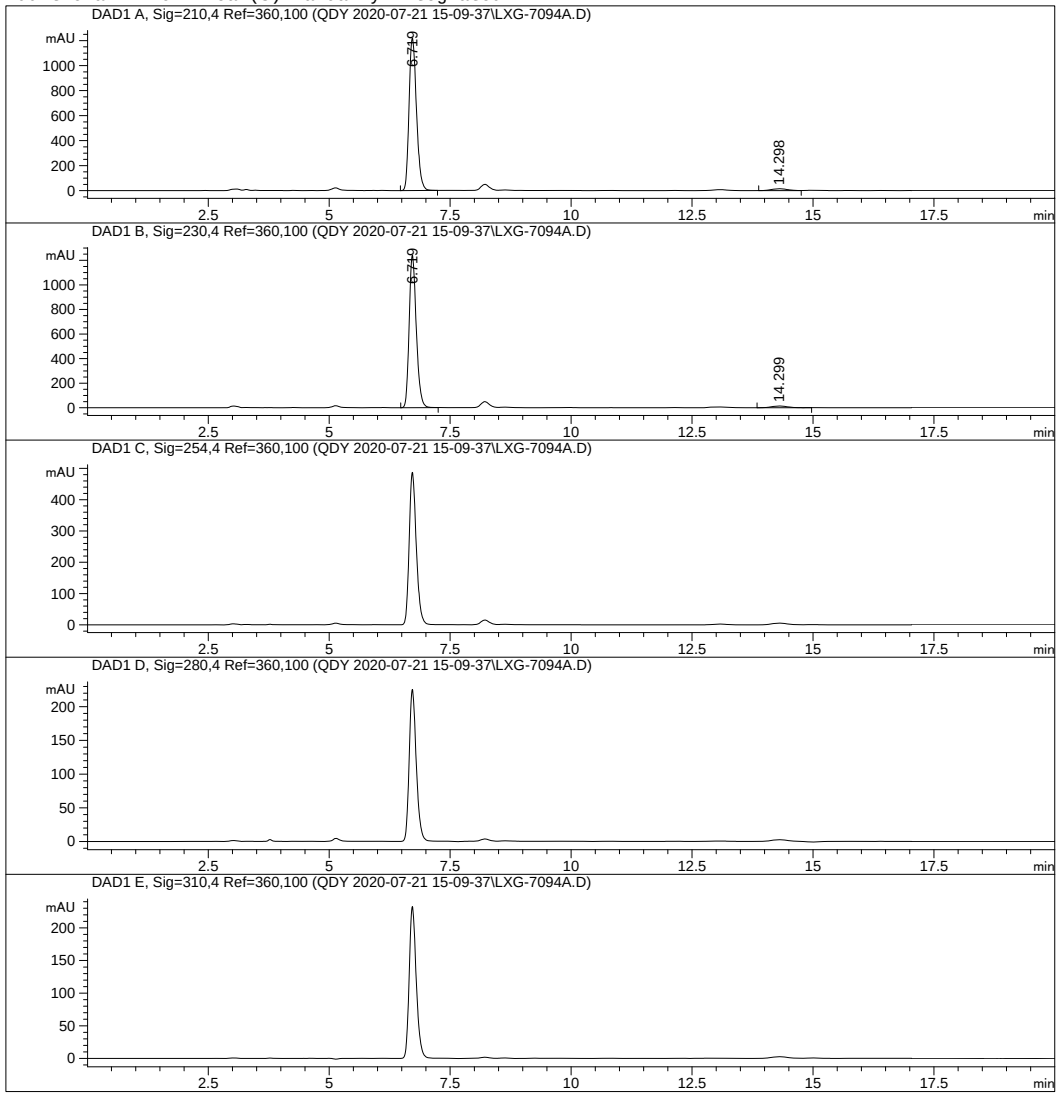


3v
(racemic)

Supplementary Figure 186. HPLC spectrum of **3v** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-21 15-09-37\LXG-7094A.D
Sample Name:

```
======================================================================
Acq. Operator   :                          Seq. Line :  10
Acq. Instrument : Instrument 1              Location : Vial 64
Injection Date  : 7/21/2020 8:02:04 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-21 15-09-37\AD-20-20.M
Last changed    : 7/21/2020 8:01:12 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/25/2020 7:05:21 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-21 15-09-37\LXG-7094A.D
Sample Name:

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.719 BB    0.1663 1.29935e4  1219.68762  97.4356
   2  14.298 BV    0.3488  341.97498   15.18033   2.5644

Totals :                  1.33354e4  1234.86795



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.719 BB    0.1574 1.27013e4  1241.25940  97.5656
   2  14.299 BB    0.3497  316.91843   14.02218   2.4344

Totals :                  1.30182e4  1255.28158

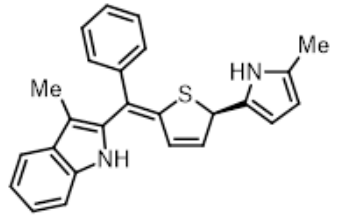


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

======================================================================
                        *** End of Report ***
```

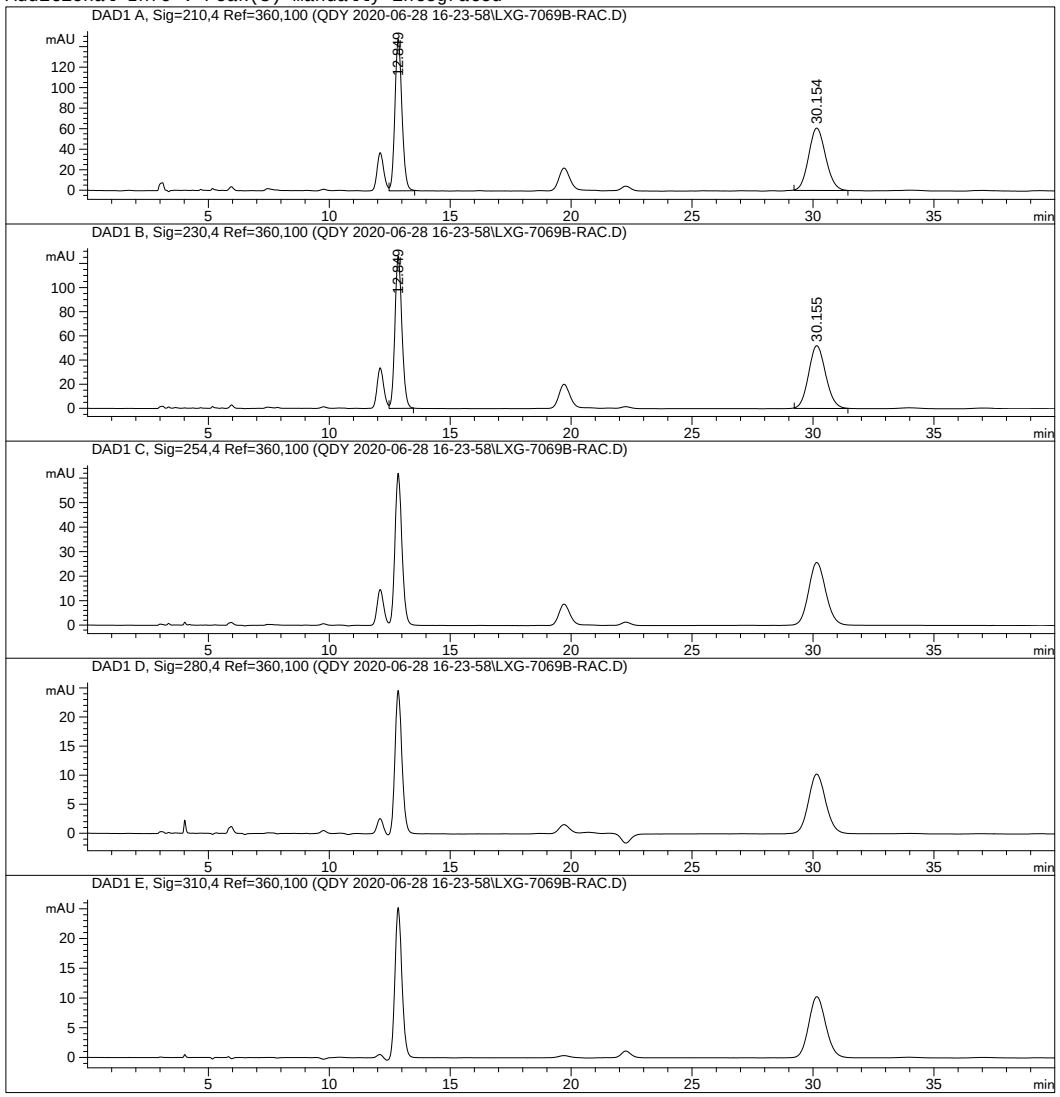


3v
(enantioenriched)

Supplementary Figure 187. HPLC spectrum of **3v** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\LXG-7069B-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :  13
Acq. Instrument : Instrument 1                    Location : Vial 70
Injection Date  : 6/28/2020 9:49:01 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\AD-12-40.M
Last changed    : 11/15/2017 2:34:57 PM
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/25/2020 7:11:23 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-06-28 16-23-58\LXG-7069B-RAC.D
Sample Name:

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.849 VB    0.3125 2997.79565  147.90913  50.1303
   2  30.154 BB    0.7560 2982.20581   60.82712  49.8697

Totals :                  5980.00146  208.73625



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.849 VB    0.3113 2541.47949  125.98605  49.9009
   2  30.155 BB    0.7592 2551.57446   51.93589  50.0991

Totals :                  5093.05396  177.92194

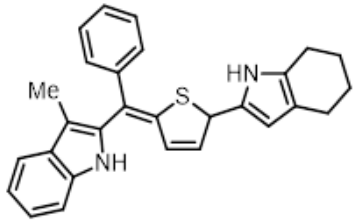


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

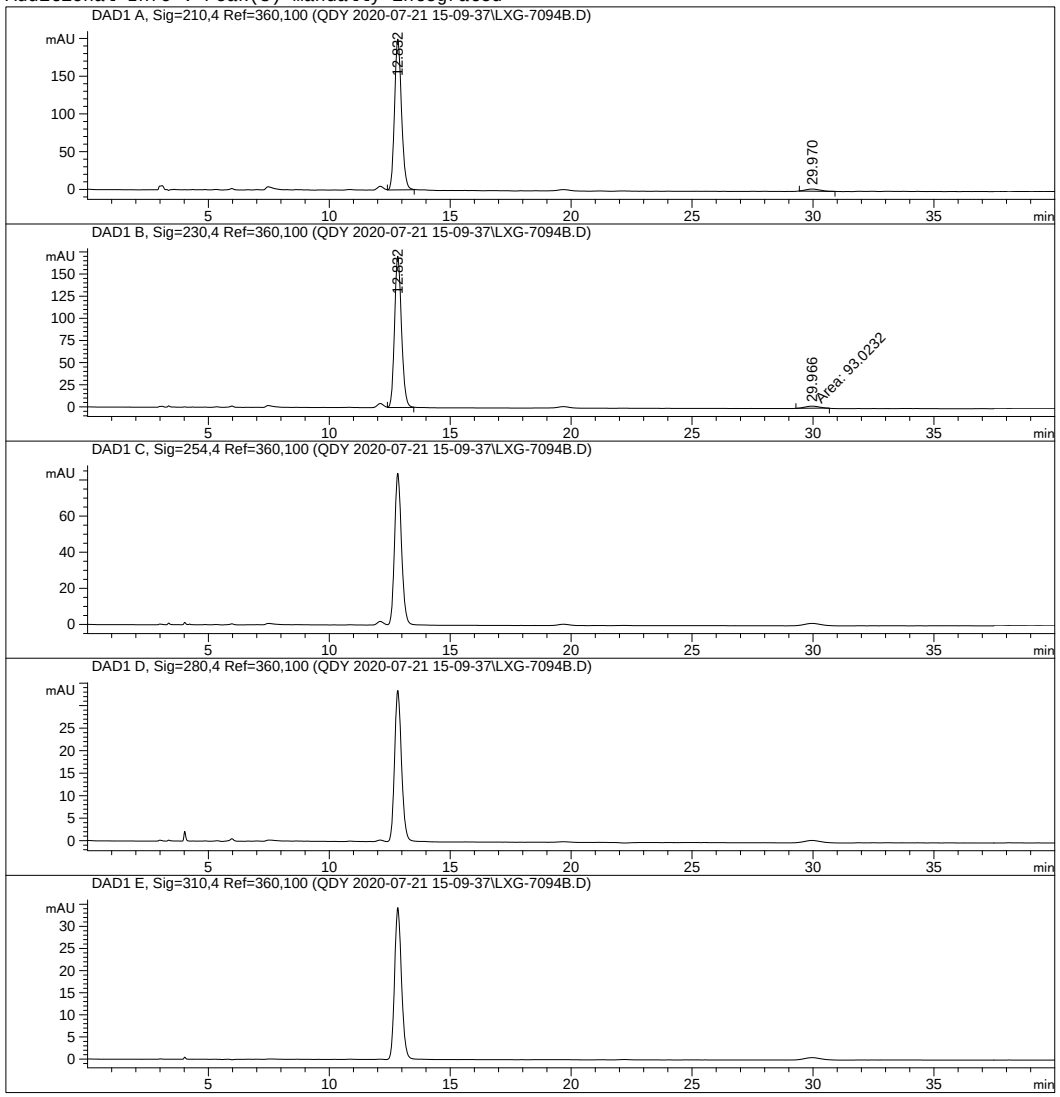


3w
(racemic)

Supplementary Figure 188. HPLC spectrum of **3w** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-21 15-09-37\LXG-7094B.D
Sample Name:

```
======================================================================
Acq. Operator   :                          Seq. Line :  19
Acq. Instrument : Instrument 1              Location : Vial 65
Injection Date  : 7/21/2020 11:02:44 PM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-21 15-09-37\AD-12-40.M
Last changed    : 11/15/2017 2:34:57 PM
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/25/2020 7:05:21 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-21 15-09-37\LXG-7094B.D
Sample Name:

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.832 VB    0.3085 3983.05957  199.86339  97.0836
   2  29.970 BB    0.4977  119.65260    2.91032   2.9164

Totals :                  4102.71217  202.77371



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.832 VB    0.3060 3396.93945  170.79012  97.3345
   2  29.966 MM    0.6613   93.02322    2.34452   2.6655

Totals :                  3489.96267  173.13463

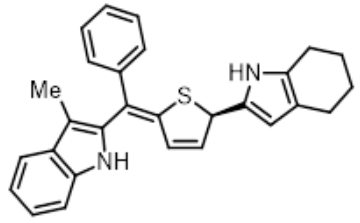


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

======================================================================
                        *** End of Report ***
```

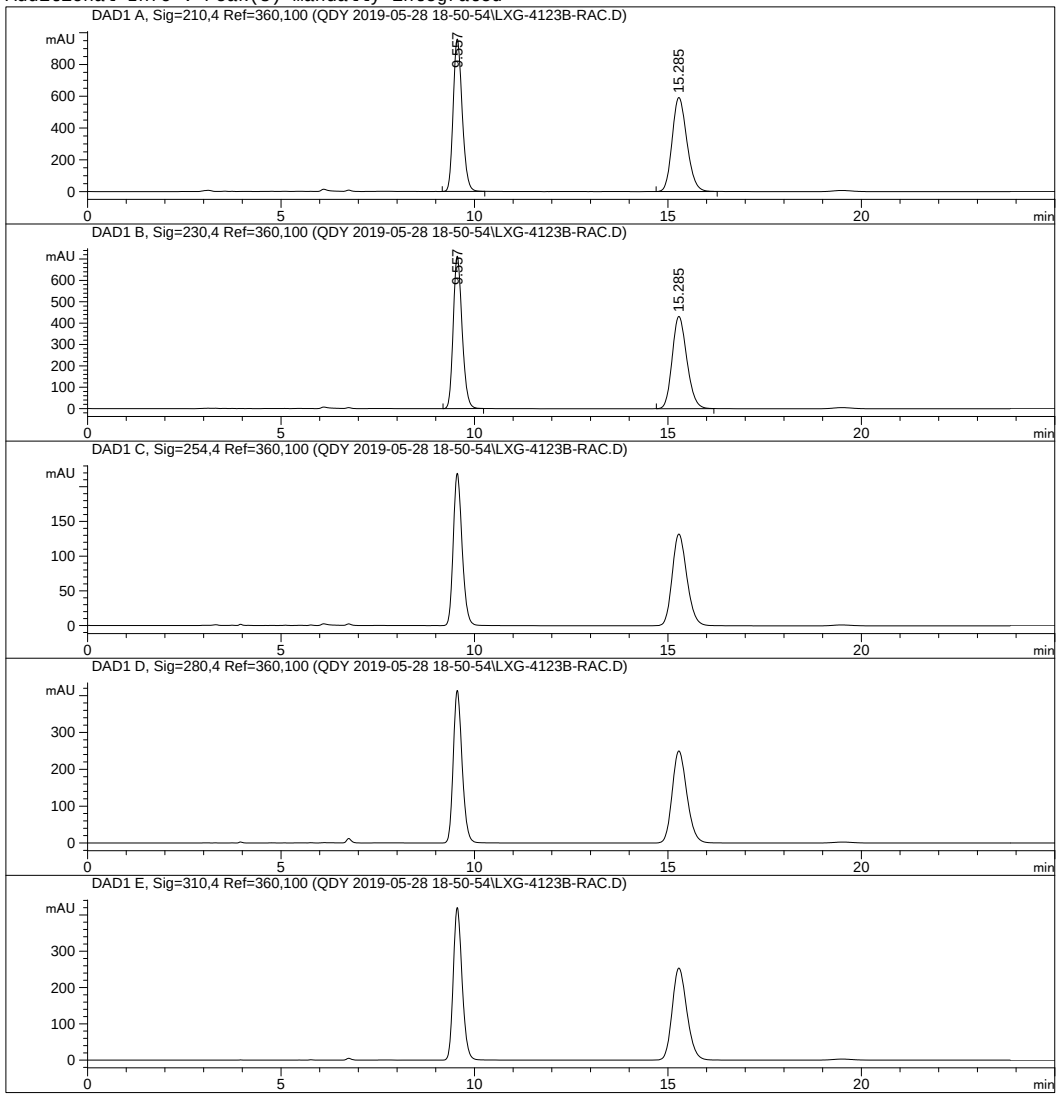


3w
(enantioenriched)

Supplementary Figure 189. HPLC spectrum of **3w** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2019-05-28 18-50-54\LXG-4123B-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   2
Acq. Instrument : Instrument 1                    Location : Vial 67
Injection Date  : 5/28/2019 7:33:31 PM                Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-05-28 18-50-54\AD-15-30.M
Last changed    : 5/28/2019 7:32:38 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\OD-01-45-0.5.M
Last changed    : 8/20/2020 6:37:54 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-05-28 18-50-54\LXG-4123B-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.557 BB    0.2482 1.54742e4   959.04773  49.7055
   2  15.285 BB    0.4108 1.56576e4   591.53687  50.2945

Totals :                  3.11318e4  1550.58459



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.557 BB    0.2456 1.13503e4   713.50891  49.9574
   2  15.285 BB    0.4093 1.13697e4   431.63516  50.0426

Totals :                  2.27199e4  1145.14407

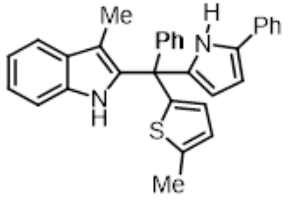


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

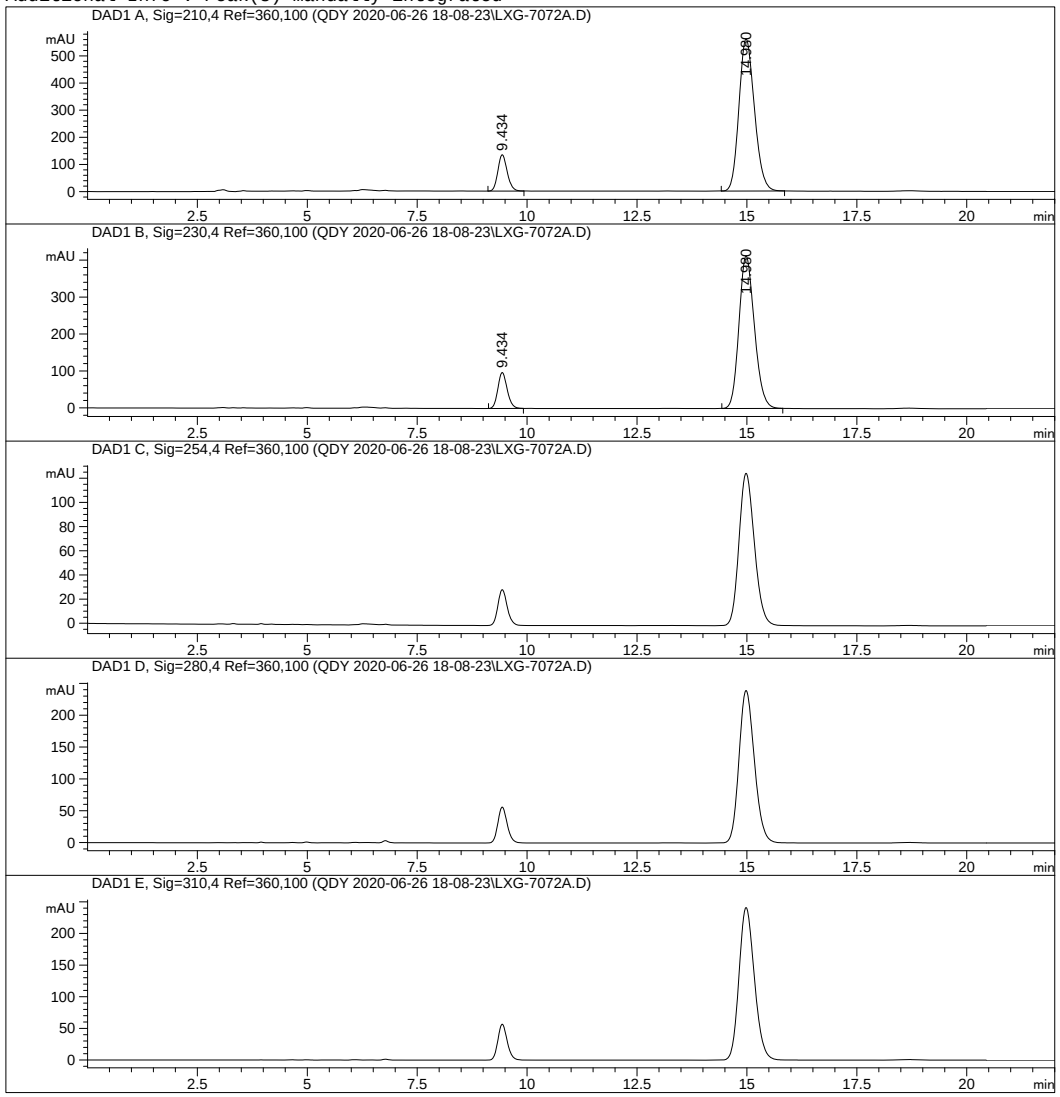


3x'
(racemic)

Supplementary Figure 190. HPLC spectrum of **3x'** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-06-26 18-08-23\LXG-7072A.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :   2
Acq. Instrument : Instrument 1                  Location : Vial 67
Injection Date  : 6/26/2020 6:21:17 PM               Inj :   1
                                              Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-06-26 18-08-23\AD-15-25.M
Last changed    : 12/10/2016 9:14:33 PM
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 12:06:36 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-06-26 18-08-23\LXG-7072A.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.434 BB    0.2286 1982.63293  134.04240  12.6282
   2  14.980 BB    0.3798 1.37174e4   559.99109  87.3718

Totals :                  1.57000e4   694.03349



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.434 BB    0.2283 1437.11633   97.32681  12.5179
   2  14.980 BB    0.3782 1.00434e4   412.26346  87.4821

Totals :                  1.14805e4   509.59027

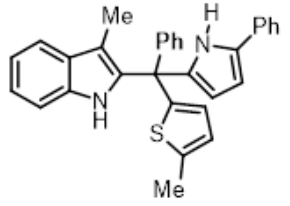


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

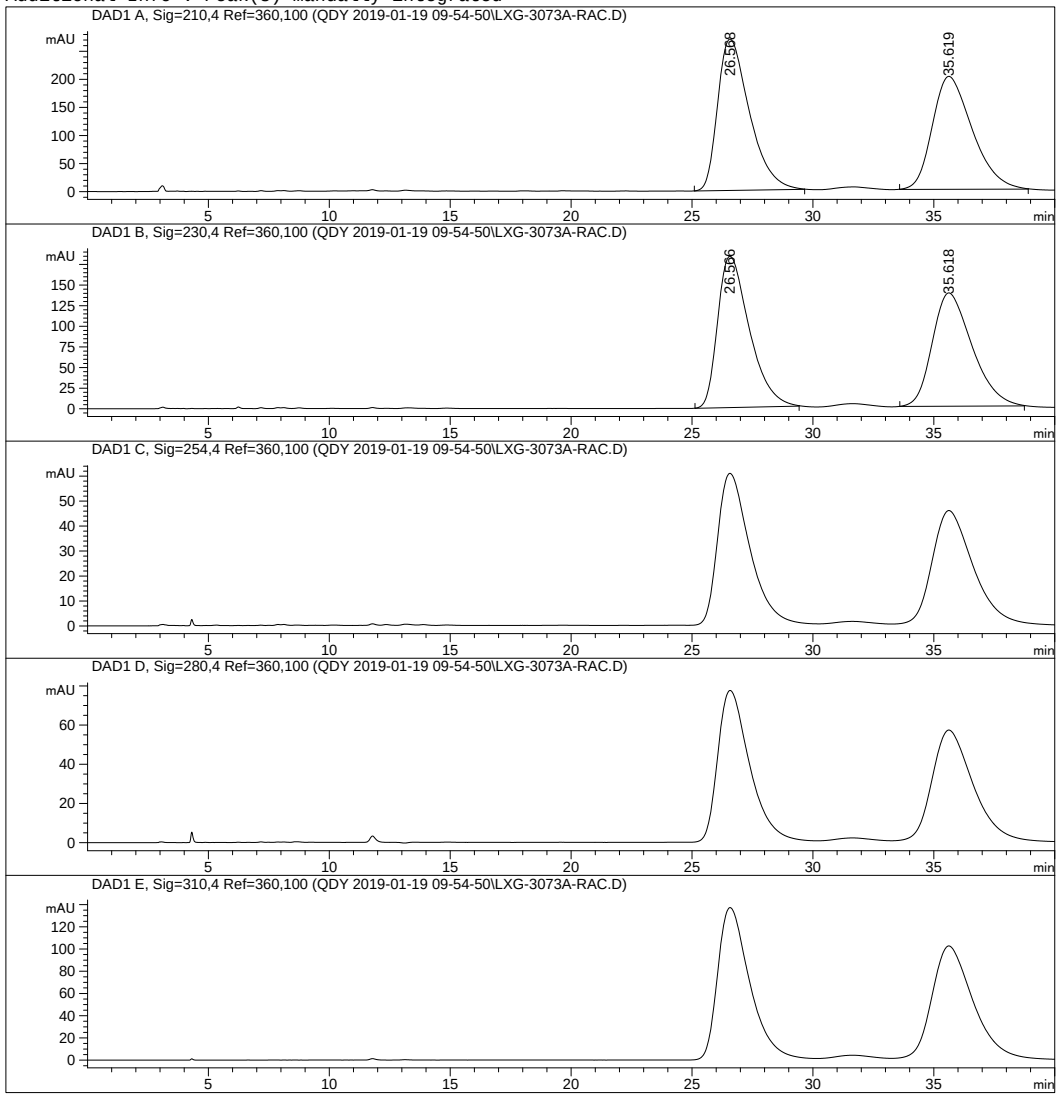


3x'
(enantioenriched)

Supplementary Figure 191. HPLC spectrum of **3x'** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2019-01-19 09-54-50\LXG-3073A-RAC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  21
Acq. Instrument : Instrument 1              Location : Vial 65
Injection Date  : 1/19/2019 7:32:31 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-01-19 09-54-50\OD-10-40.M
Last changed    : 1/19/2019 7:31:39 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\OD-001-10-0.7.M
Last changed    : 8/21/2019 8:26:51 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-01-19 09-54-50\LXG-3073A-RAC.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  26.568 BB    1.3730 2.46620e4   269.65048  51.6475
   2  35.619 BB    1.7563 2.30886e4   201.27979  48.3525

Totals :                  4.77506e4   470.93027



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  26.566 BB    1.3693 1.66925e4   183.50626  51.5215
   2  35.618 BB    1.7553 1.57066e4   137.43654  48.4785

Totals :                  3.23992e4   320.94279

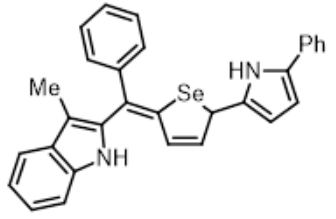


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```

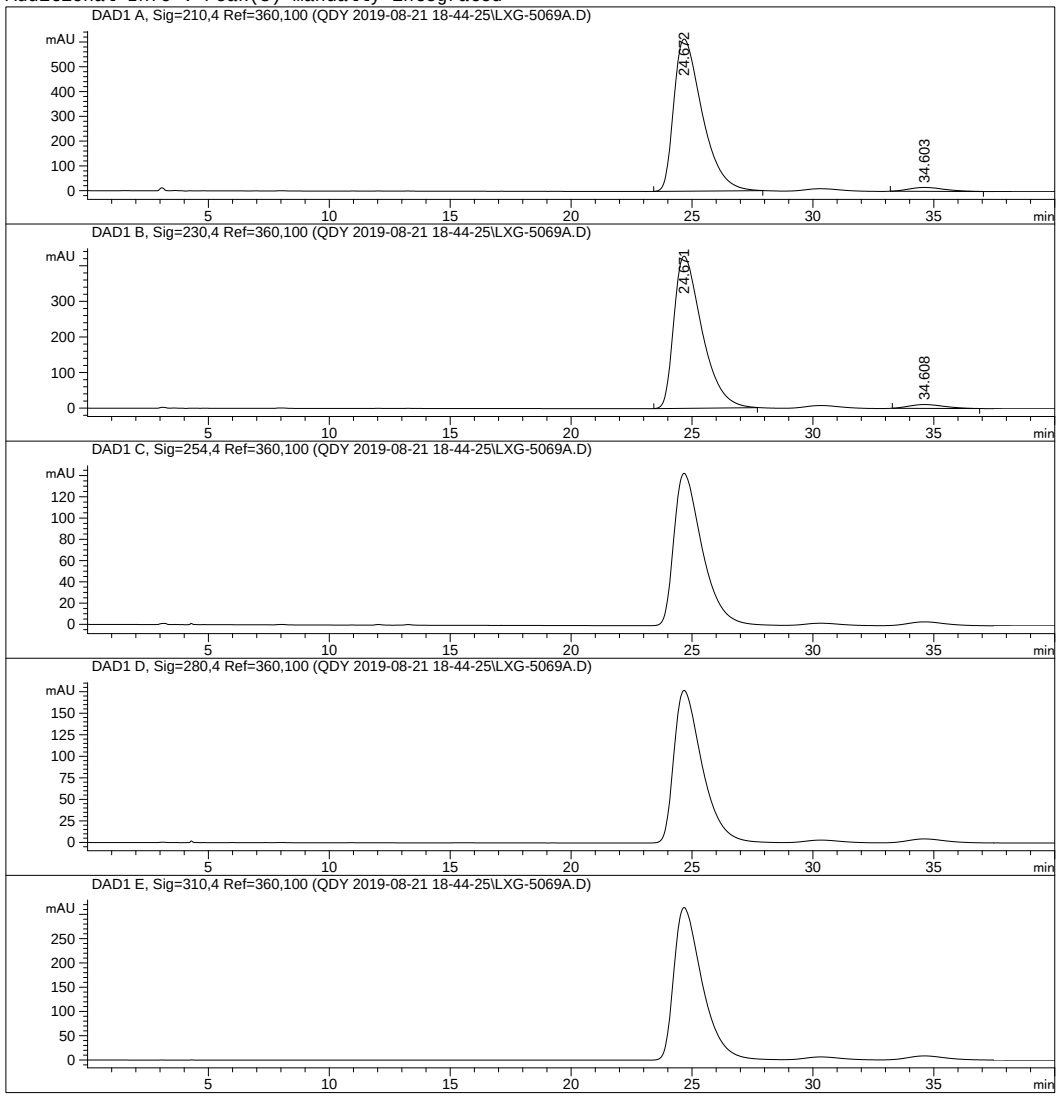


5a
(racemic)

Supplementary Figure 192. HPLC spectrum of **5a** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2019-08-21 18-44-25\LXG-5069A.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :   2
Acq. Instrument : Instrument 1                  Location : Vial 77
Injection Date  : 8/21/2019 6:58:04 PM               Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-08-21 18-44-25\OD-10-40.M
Last changed    : 8/21/2019 6:57:10 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\OD-001-10-0.7.M
Last changed    : 8/21/2019 8:26:51 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-08-21 18-44-25\LXG-5069A.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  24.672 BB    1.2346 5.00090e4   613.77332  96.9052
   2  34.603 BB    1.2039 1597.08594   15.63325   3.0948

Totals :                  5.16060e4   629.40657



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  24.671 BB    1.2190 3.44732e4   427.39185  96.9604
   2  34.608 BB    1.3018 1080.71167   10.76000   3.0396

Totals :                  3.55539e4   438.15184

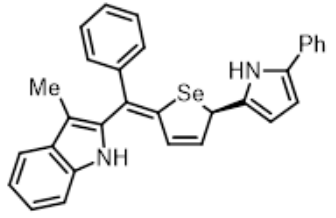


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

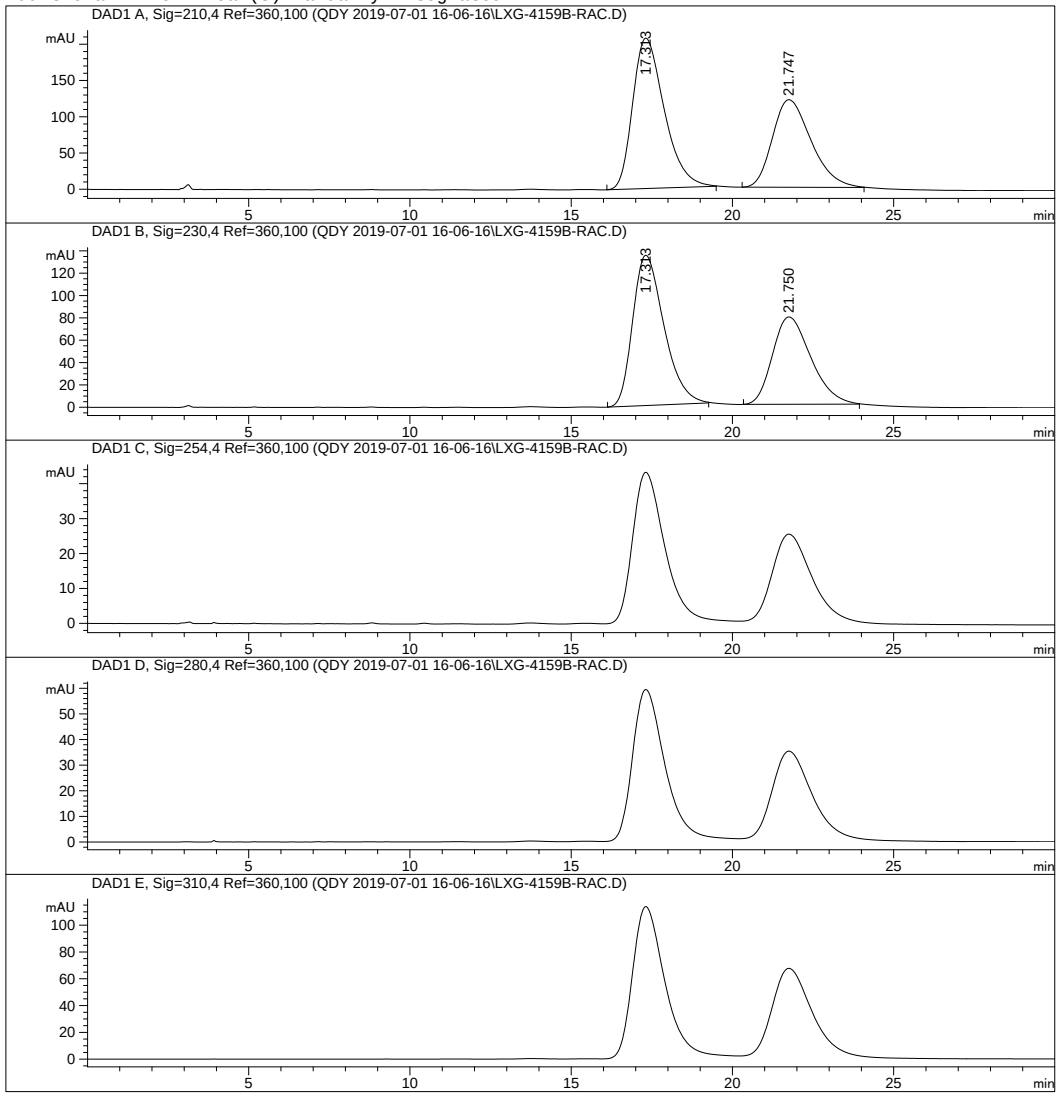


5a
(enantioenriched)

Supplementary Figure 193. HPLC spectrum of **5a** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2019-07-01 16-06-16\LXG-4159B-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :   6
Acq. Instrument : Instrument 1                  Location : Vial 62
Injection Date  : 7/1/2019 5:34:20 PM              Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-07-01 16-06-16\OD-20-30.M
Last changed    : 5/3/2016 10:14:35 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-001-10-0.7.M
Last changed    : 8/21/2019 8:26:51 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-07-01 16-06-16\LXG-4159B-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.313 BB    1.0336 1.41090e4   207.41411  58.3510
   2  21.747 BB    1.2449 1.00705e4   120.76174  41.6490

Totals :                  2.41795e4   328.17585



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.313 BB    1.0355 9056.10059  134.51042  58.3394
   2  21.750 BB    1.2714 6467.02539   78.15504  41.6606

Totals :                  1.55231e4   212.66546

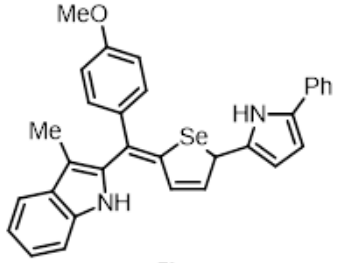


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

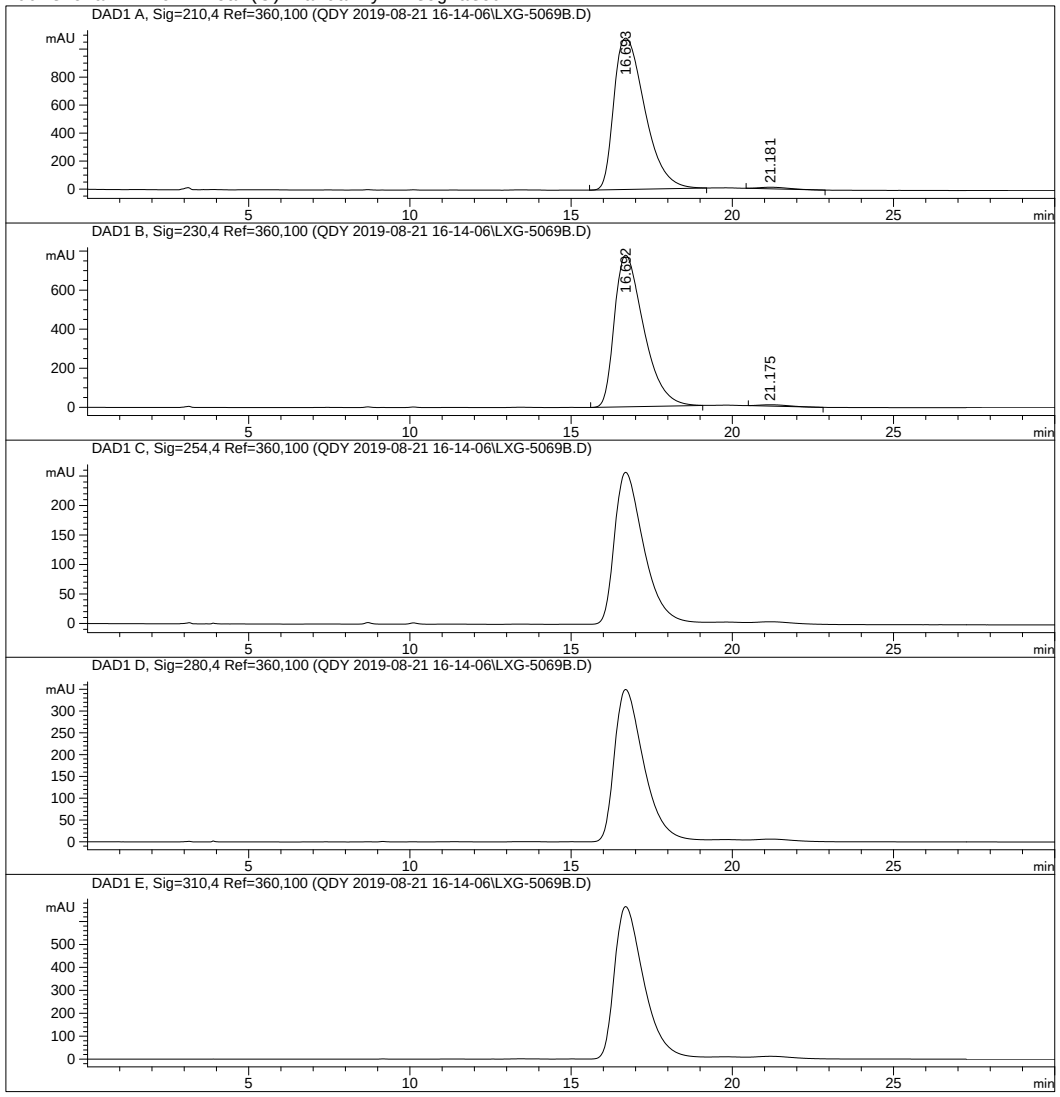


5b
(racemic)

Supplementary Figure 194. HPLC spectrum of **5b** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2019-08-21 16-14-06\LXG-5069B.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location : Vial 74
Injection Date  : 8/21/2019 4:27:17 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-08-21 16-14-06\OD-20-30.M
Last changed    : 5/3/2016 10:14:35 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-001-10-0.7.M
Last changed    : 8/21/2019 8:26:51 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-08-21 16-14-06\LXG-5069B.D
Sample Name:

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.693 BB    1.0374 7.20678e4  1081.57385  99.0203
   2  21.181 BB    0.7996  713.00836   11.33909   0.9797

Totals :                  7.27808e4  1092.91294



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.692 BB    0.9693 4.90714e4   776.52466  99.1475
   2  21.175 BB    0.8957  421.91968    6.91649   0.8525

Totals :                  4.94934e4   783.44115

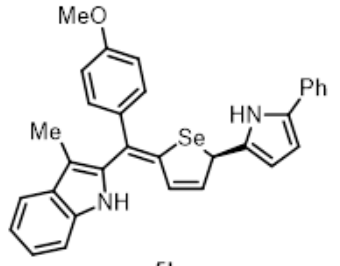


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

======================================================================
                        *** End of Report ***
```

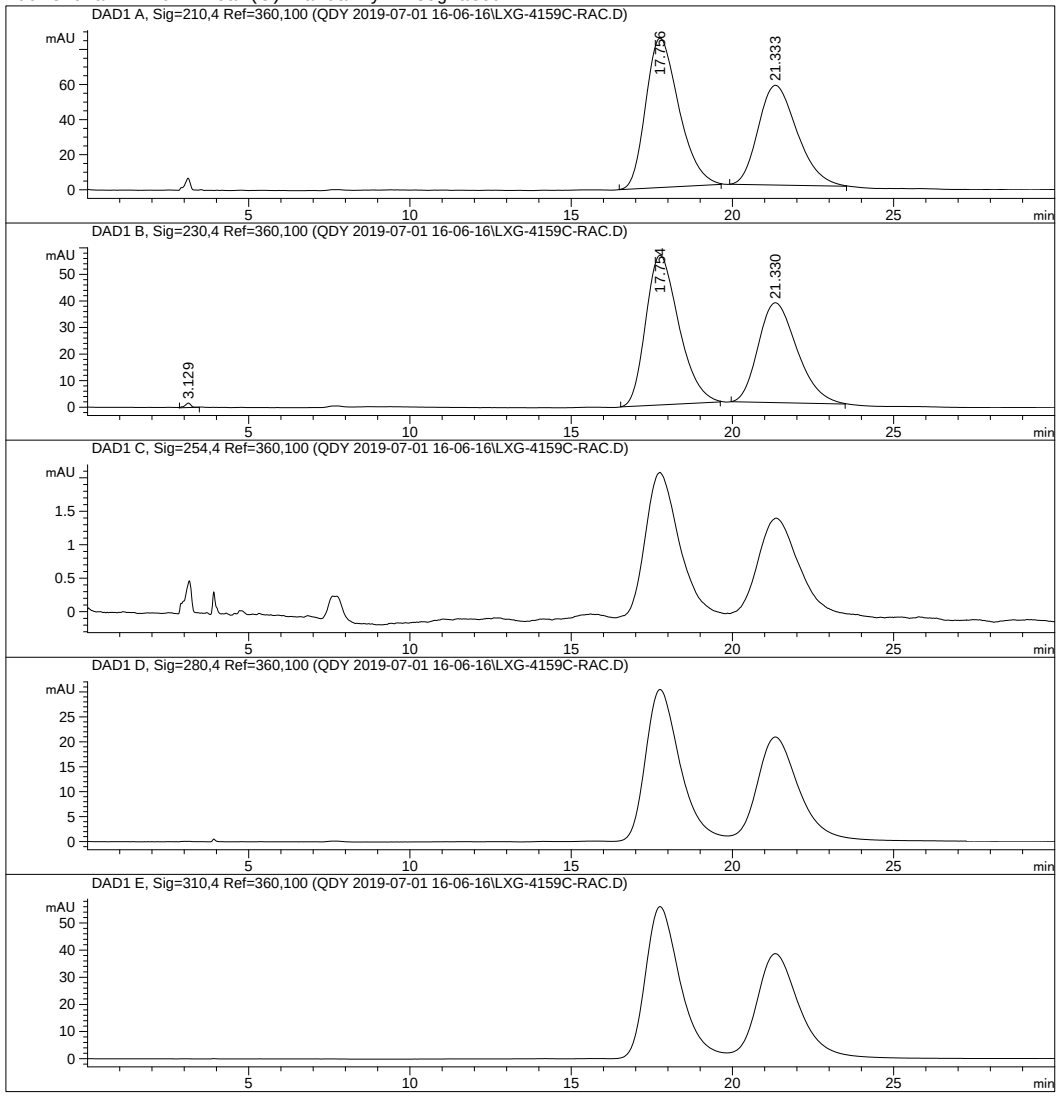


5b
(enantioenriched)

Supplementary Figure 195. HPLC spectrum of **5b** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2019-07-01 16-06-16\LXG-4159C-RAC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   7
Acq. Instrument : Instrument 1              Location : Vial 63
Injection Date  : 7/1/2019 6:05:27 PM            Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-07-01 16-06-16\OD-20-30.M
Last changed    : 5/3/2016 10:14:35 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-001-10-0.7.M
Last changed    : 8/21/2019 8:26:51 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-07-01 16-06-16\LXG-4159C-RAC.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.756 BB    1.0835 6086.35791   85.18929  56.0648
   2  21.333 BB    1.2569 4769.57471   56.84240  43.9352

Totals :                  1.08559e4   142.03168



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   3.129 BB    0.1905   21.22253    1.66784   0.2952
   2  17.754 BB    1.1010 4016.74316   56.39124  55.8705
   3  21.330 BB    1.2950 3151.41309   37.63034  43.8343

Totals :                  7189.37878   95.68942

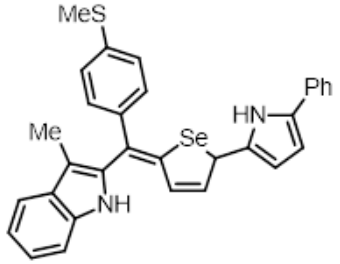


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```

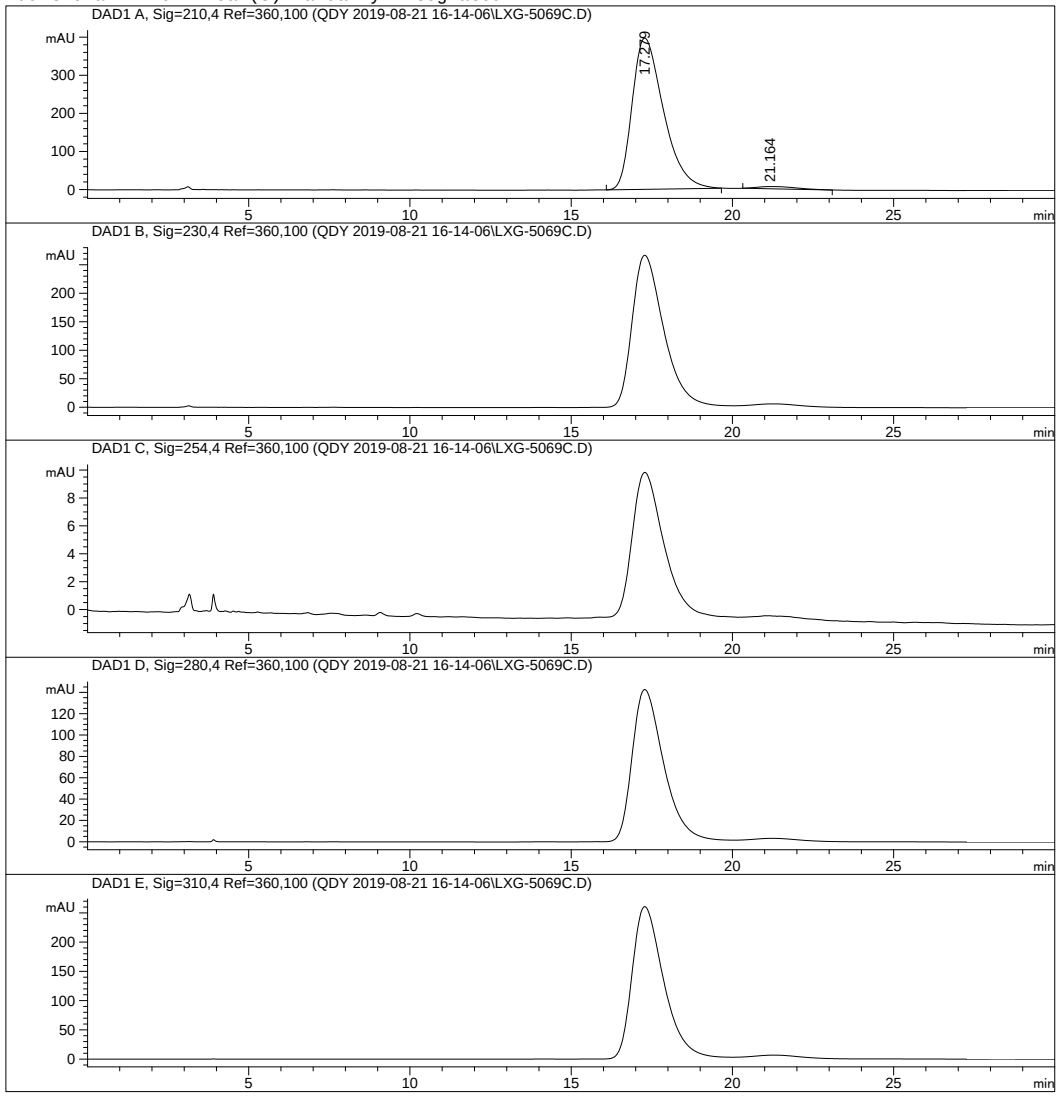


5c
(racemic)

Supplementary Figure 196. HPLC spectrum of **5c** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2019-08-21 16-14-06\LXG-5069C.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :   3
Acq. Instrument : Instrument 1                  Location : Vial 75
Injection Date  : 8/21/2019 4:58:24 PM             Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-08-21 16-14-06\OD-20-30.M
Last changed    : 5/3/2016 10:14:35 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-001-10-0.7.M
Last changed    : 8/21/2019 8:26:51 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-08-21 16-14-06\LXG-5069C.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.279 BB    1.0237 2.67879e4   396.73367  98.1361
   2  21.164 BB    1.0184  508.78308    5.92134   1.8639

Totals :                  2.72967e4   402.65501



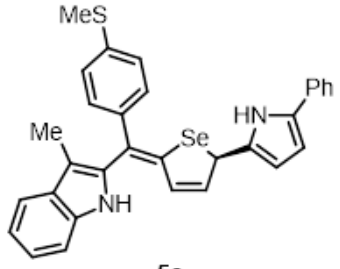
Signal 2: DAD1 B, Sig=230,4 Ref=360,100


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

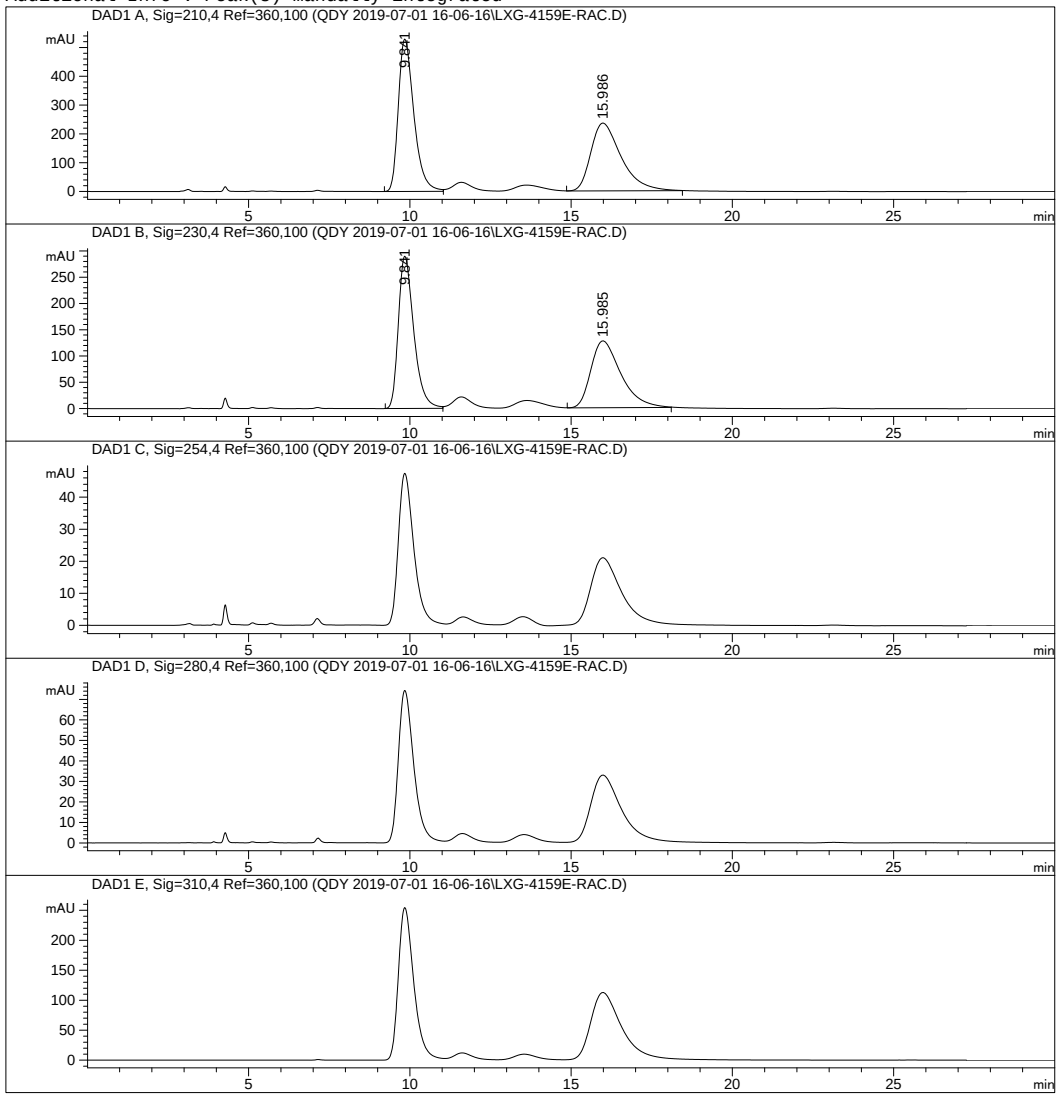


5c
(enantioenriched)

Supplementary Figure 197. HPLC spectrum of **5c** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2019-07-01 16-06-16\LXG-4159E-RAC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   9
Acq. Instrument : Instrument 1              Location : Vial 65
Injection Date  : 7/1/2019 7:07:50 PM            Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-07-01 16-06-16\OD-20-30.M
Last changed    : 5/3/2016 10:14:35 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-01-45-0.5.M
Last changed    : 8/22/2020 12:14:44 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-07-01 16-06-16\LXG-4159E-RAC.D
Sample Name:

```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.841 BV    0.5130 1.77344e4   529.16589  53.4554
   2  15.986 VB    0.9867 1.54416e4   235.59125  46.5446

Totals :                  3.31760e4   764.75714



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.841 BB    0.5083 9648.12891  289.88367  53.9886
   2  15.985 VB    0.9839 8222.54004  127.24164  46.0114

Totals :                  1.78707e4   417.12531

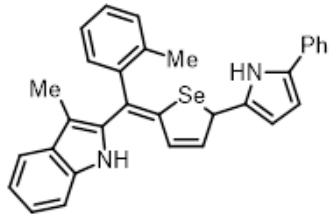


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                     *** End of Report ***
```

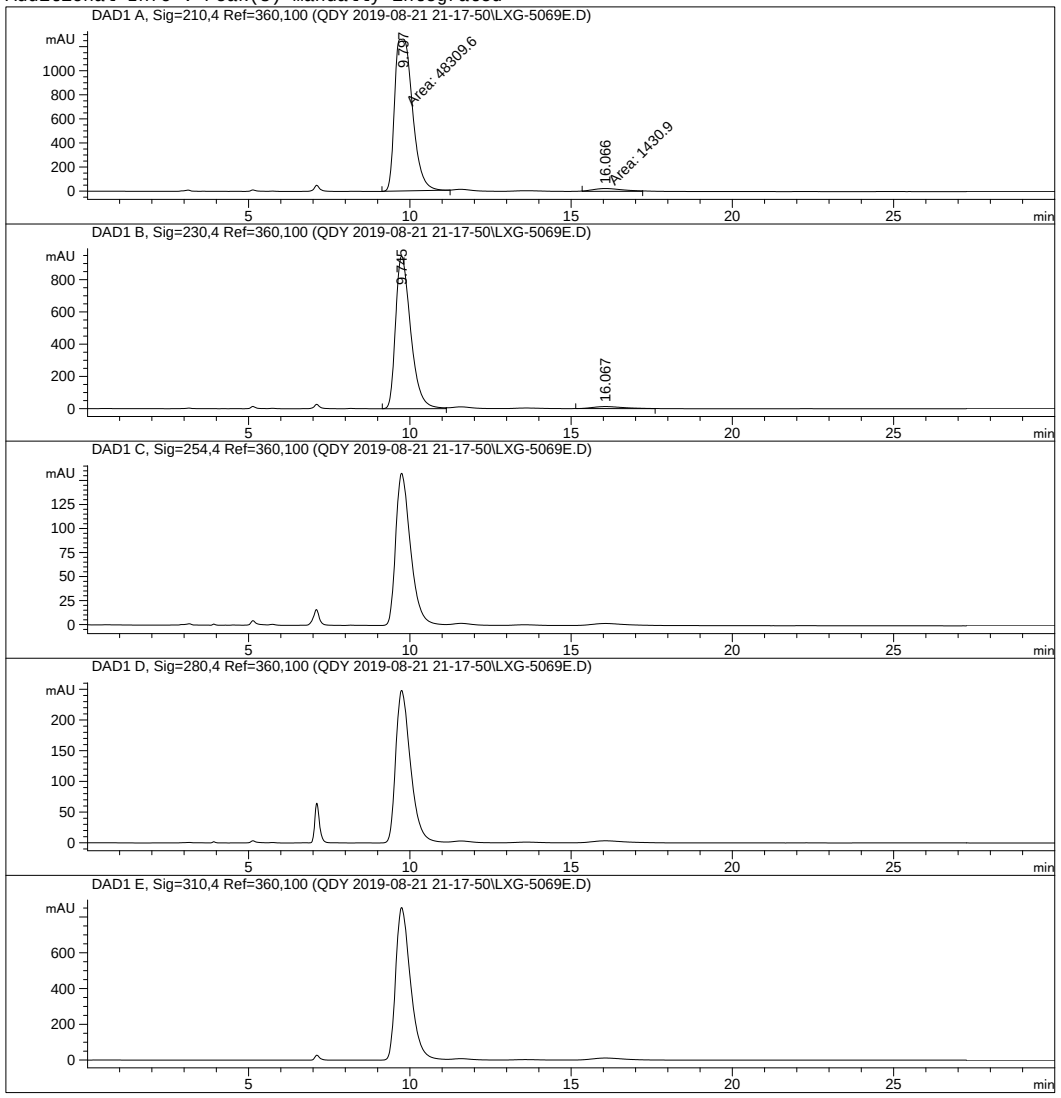


5d
(racemic)

Supplementary Figure 198. HPLC spectrum of **5d** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2019-08-21 21-17-50\LXG-5069E.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   5
Acq. Instrument : Instrument 1                    Location : Vial 78
Injection Date  : 8/22/2019 12:25:37 AM               Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-08-21 21-17-50\OD-20-30.M
Last changed    : 5/3/2016 10:14:35 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-01-45-0.5.M
Last changed    : 8/22/2020 12:14:44 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-08-21 21-17-50\LXG-5069E.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.797 MM    0.6383 4.83096e4  1261.36279  97.1233
   2  16.066 MM    1.0433 1430.90393   22.85865   2.8767

Totals :                  4.97405e4  1284.22144



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.745 BB    0.5004 3.06799e4   945.89362  97.3828
   2  16.067 BB    0.9766  824.52002   12.51598   2.6172

Totals :                  3.15044e4   958.40960

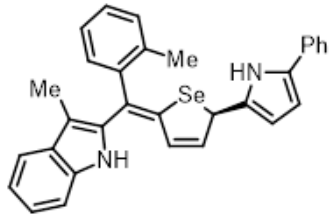


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

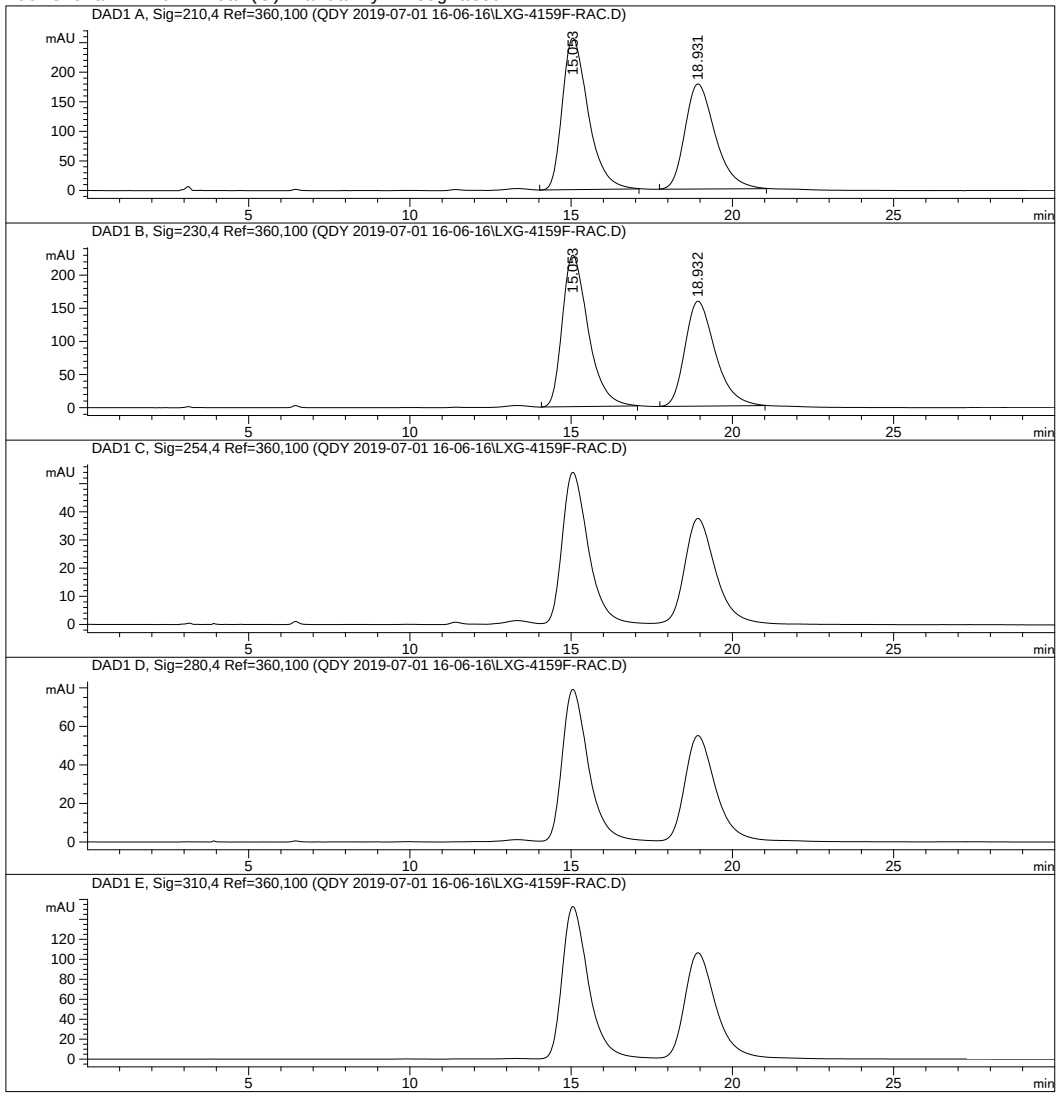


5d
(enantioenriched)

Supplementary Figure 199. HPLC spectrum of **5d** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2019-07-01 16-06-16\LXG-4159F-RAC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  10
Acq. Instrument : Instrument 1              Location : Vial 66
Injection Date  : 7/1/2019 7:39:26 PM            Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-07-01 16-06-16\OD-20-30.M
Last changed    : 5/3/2016 10:14:35 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-001-10-0.7.M
Last changed    : 8/21/2019 8:26:51 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-07-01 16-06-16\LXG-4159F-RAC.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.053 VB    0.8594 1.42659e4   256.28500  55.1132
   2  18.931 BB    0.9986 1.16188e4   177.75638  44.8868

Totals :                  2.58847e4   434.04138



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.053 BB    0.8566 1.27061e4   228.56815  55.1172
   2  18.932 BB    1.0018 1.03468e4   158.45694  44.8828

Totals :                  2.30529e4   387.02509

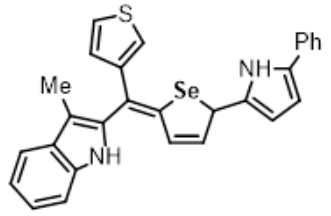


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```

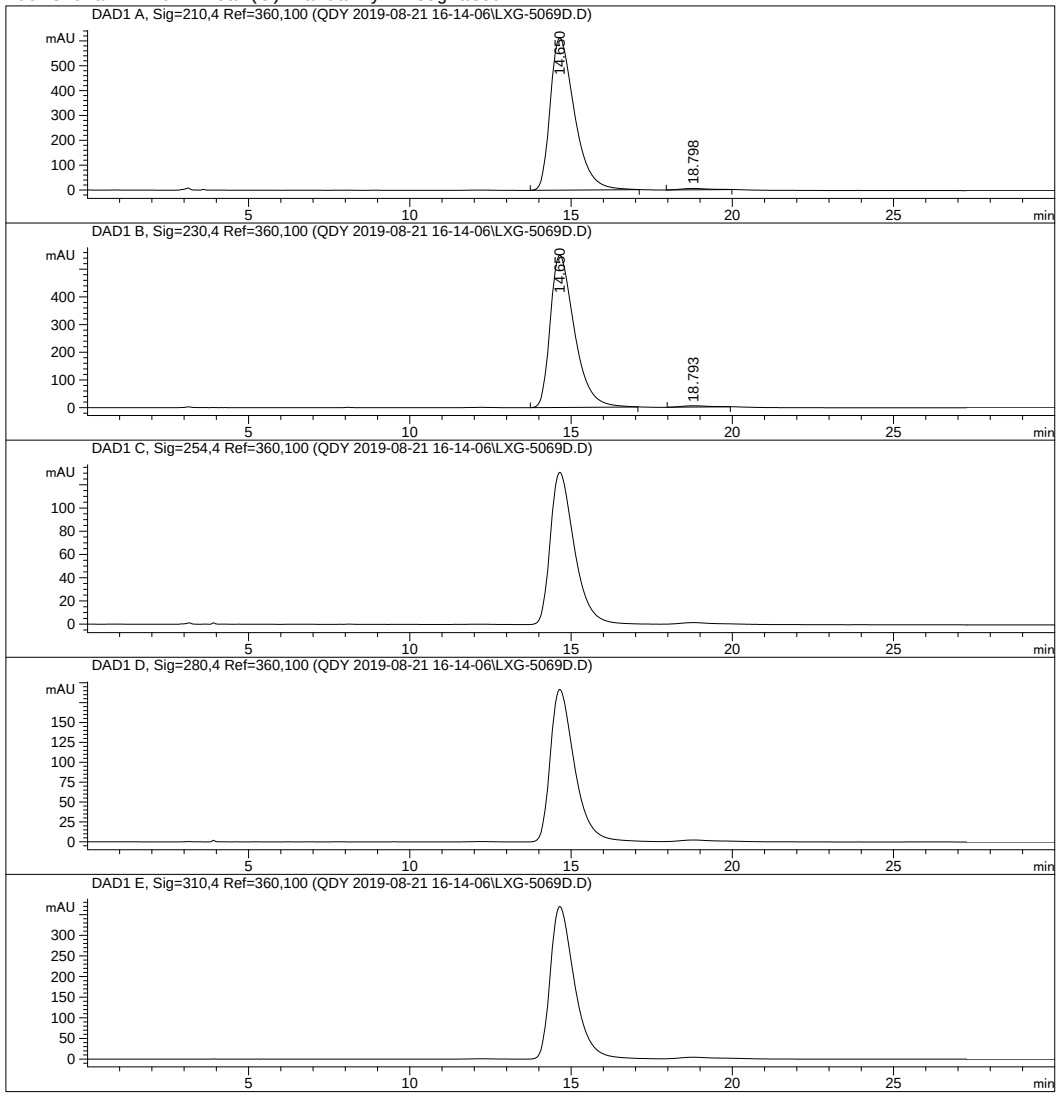


5e
(racemic)

Supplementary Figure 200. HPLC spectrum of **5e** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2019-08-21 16-14-06\LXG-5069D.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :   4
Acq. Instrument : Instrument 1                  Location : Vial 76
Injection Date  : 8/21/2019 5:29:53 PM               Inj :   1
                                            Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-08-21 16-14-06\OD-20-30.M
Last changed    : 5/3/2016 10:14:35 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-001-10-0.7.M
Last changed    : 8/21/2019 8:26:51 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-08-21 16-14-06\LXG-5069D.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.650 BB    0.8012 3.19468e4   611.85522  98.9937
   2  18.798 BB    0.7090  324.73480    5.56324   1.0063

Totals :                  3.22715e4   617.41846



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.650 BB    0.7961 2.85797e4   550.14484  99.0468
   2  18.793 BB    0.8295  275.05164    4.79296   0.9532

Totals :                  2.88548e4   554.93780

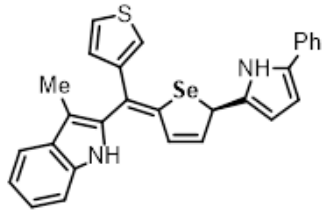


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



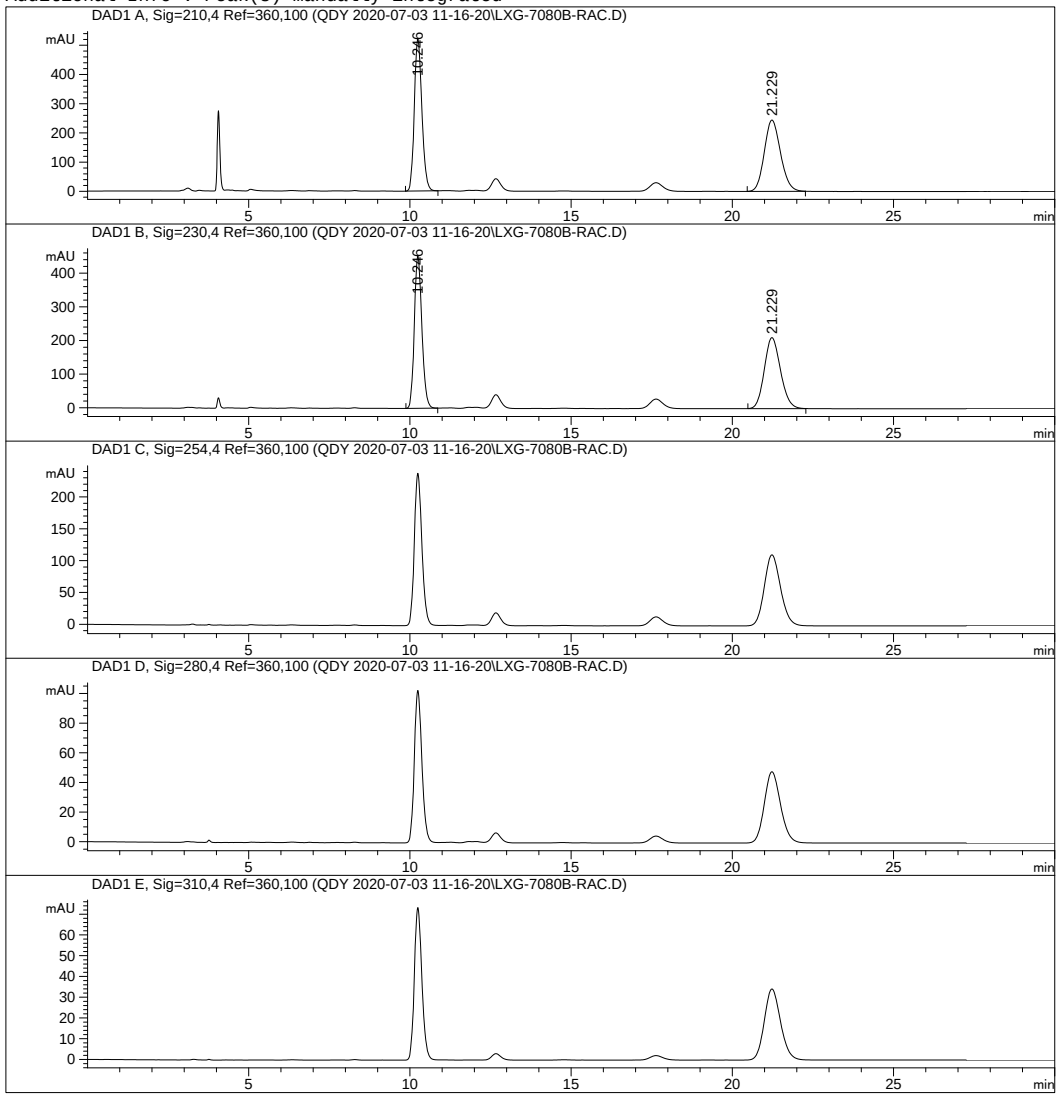
5e
(enantioenriched)

Supplementary Figure 201. HPLC spectrum of **5e** (enantioenriched)

Instrument 1 8/22/2019 10:57:47 AM

Data File C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\LXG-7080B-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :   2
Acq. Instrument : Instrument 1                  Location : Vial 61
Injection Date  : 7/3/2020 11:29:15 AM               Inj :   1
                                            Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/6/2020 6:52:33 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-03 11-16-20\LXG-7080B-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.246 BB    0.2524 8486.69434  520.03217  49.8361
   2  21.229 BB    0.5401 8542.52637  244.19833  50.1639

Totals :                  1.70292e4   764.23050



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.246 BB    0.2496 7347.05469  452.02606  49.9152
   2  21.229 BB    0.5414 7372.02881  211.10132  50.0848

Totals :                  1.47191e4   663.12738

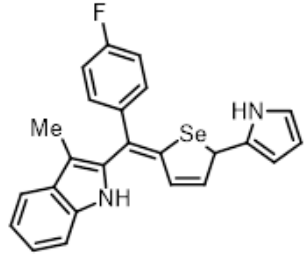


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

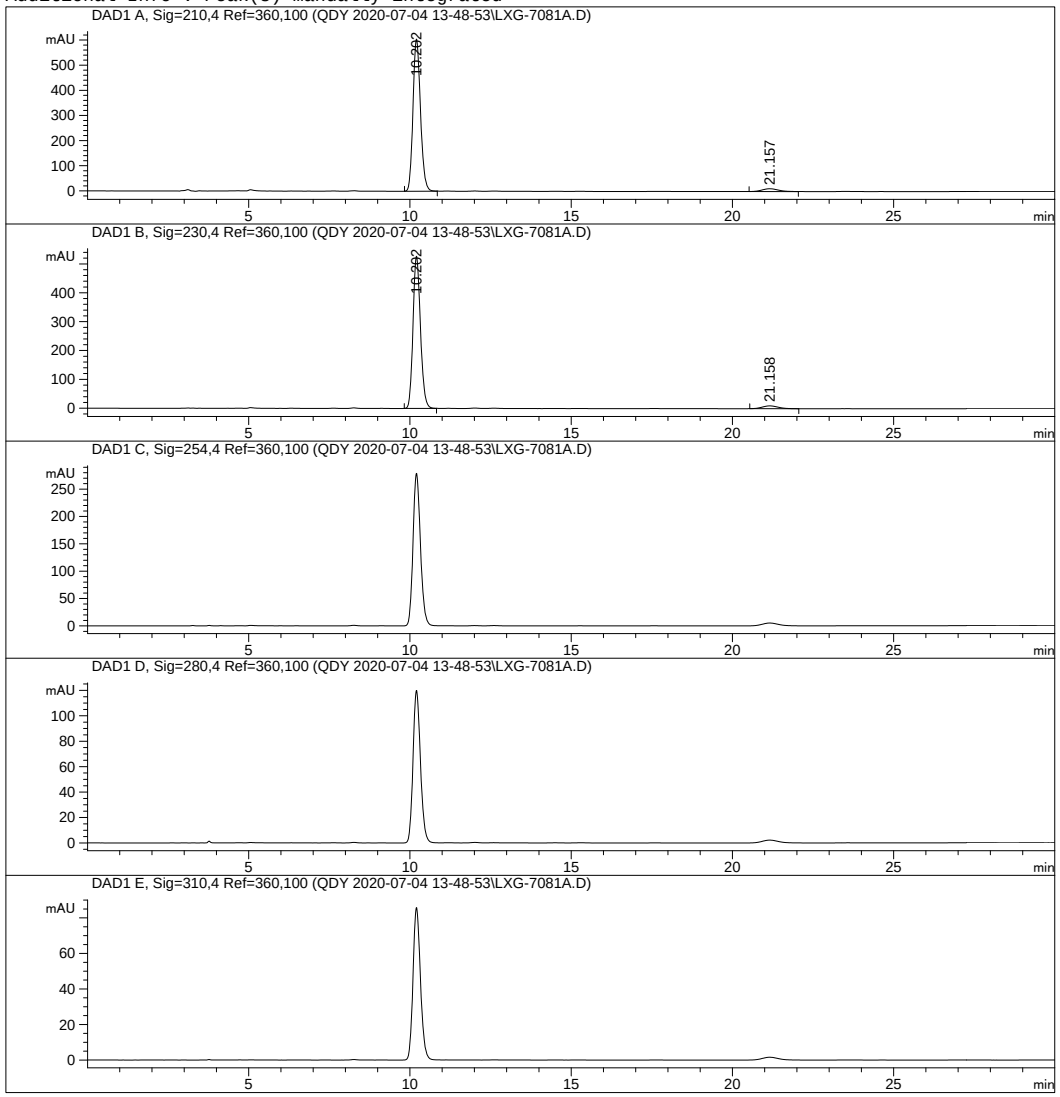


5f
(racemic)

Supplementary Figure 205. HPLC spectrum of **5f** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-04 13-48-53\LXG-7081A.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   3
Acq. Instrument : Instrument 1                    Location : Vial 68
Injection Date  : 7/4/2020 2:22:56 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-04 13-48-53\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\LXG-IC-10-10.M
Last changed    : 7/4/2020 3:31:39 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-04 13-48-53\LXG-7081A.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.202 BB    0.2490 9701.01563  605.15961  96.1062
   2  21.157 BB    0.5394  393.03787   11.25435   3.8938

Totals :                  1.00941e4   616.41396



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.202 BB    0.2462 8420.31055  527.64069  96.1535
   2  21.158 BB    0.5361  336.84317    9.77255   3.8465

Totals :                  8757.15372  537.41323

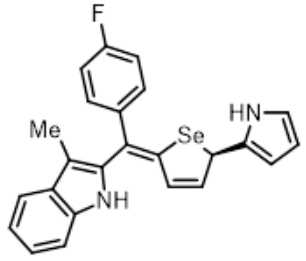


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

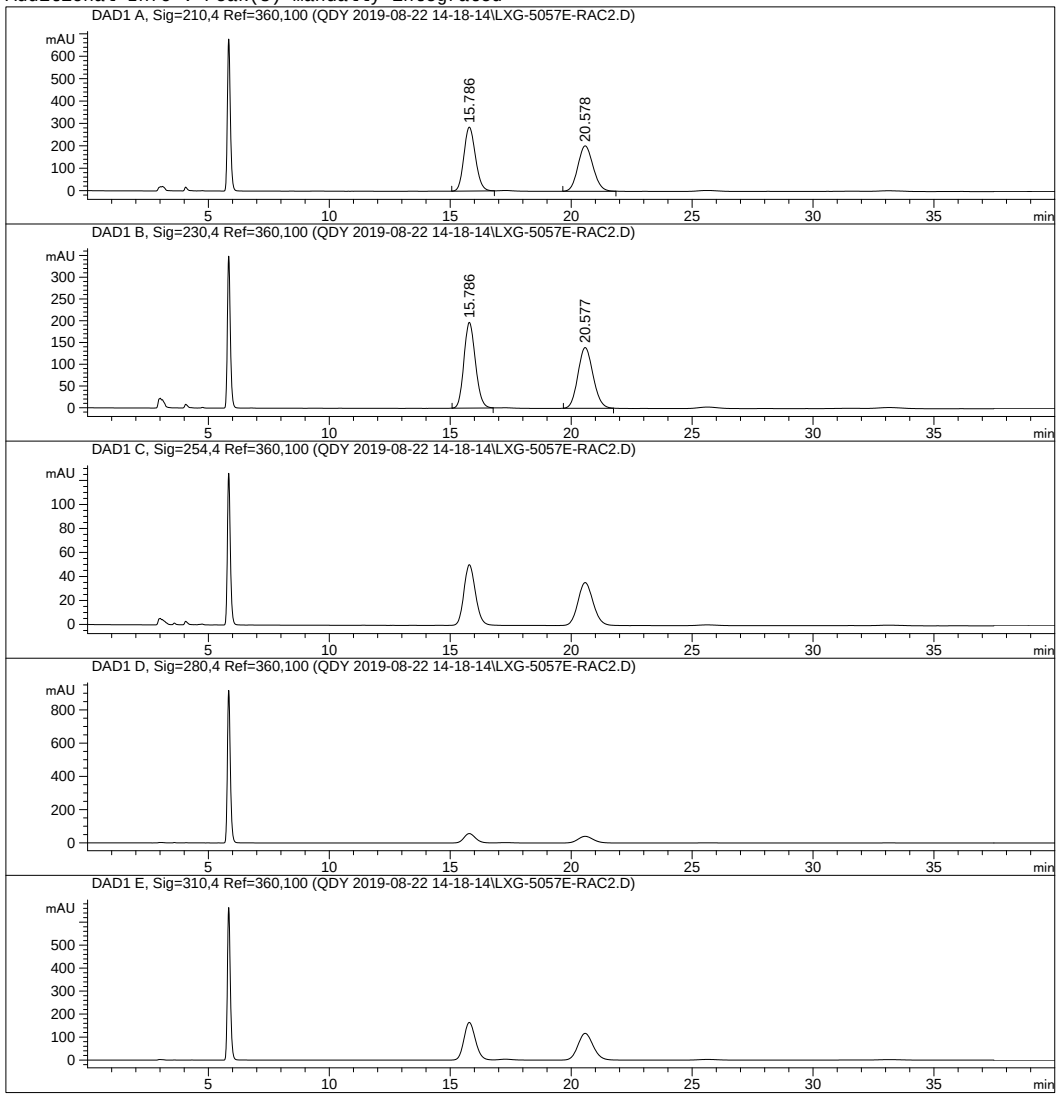


5f
(enantioenriched)

Supplementary Figure 203. HPLC spectrum of **5f** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2019-08-22 14-18-14\LXG-5057E-RAC2.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   5
Acq. Instrument : Instrument 1              Location : Vial 62
Injection Date  : 8/22/2019 3:35:40 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-08-22 14-18-14\AD-30-40.M
Last changed    : 8/22/2019 3:34:47 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\OD-001-10-0.7.M
Last changed    : 8/23/2019 7:50:41 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-08-22 14-18-14\LXG-5057E-RAC2.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.786 BB    0.5160 9434.80957  285.17068  51.6033
   2  20.578 BB    0.6792 8848.51953  202.74086  48.3967

Totals :                  1.82833e4   487.91154



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.786 BB    0.5137 6511.24707  196.96703  51.7182
   2  20.577 BB    0.6776 6078.59863  139.70050  48.2818

Totals :                  1.25898e4   336.66753

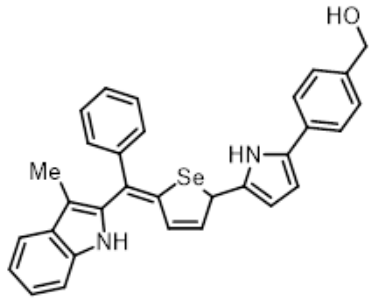


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```

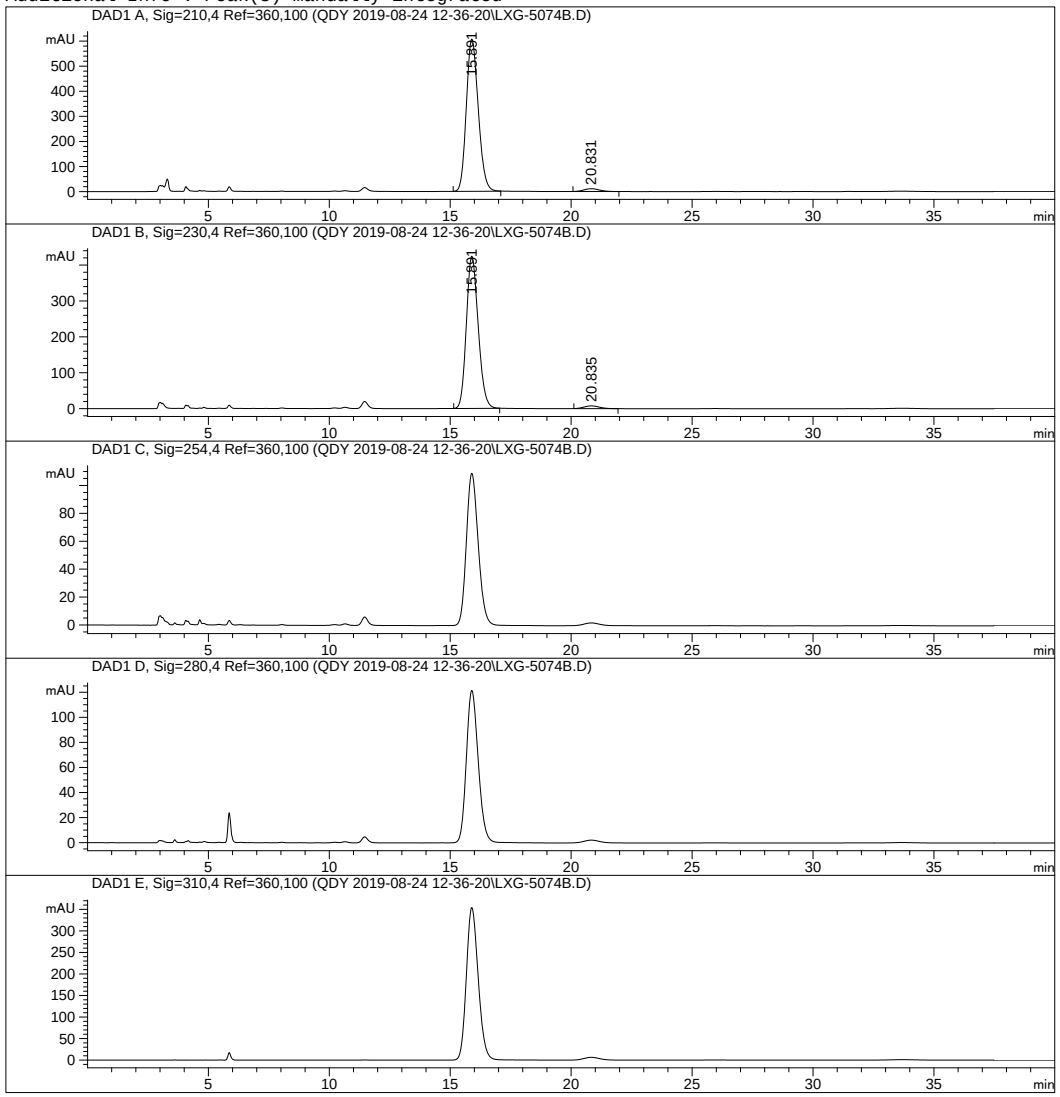


5g
(racemic)

Supplementary Figure 204. HPLC spectrum of **5g** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2019-08-24 12-36-20\LXG-5074B.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   2
Acq. Instrument : Instrument 1                    Location : Vial 66
Injection Date  : 8/24/2019 12:49:22 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2019-08-24 12-36-20\AD-30-40.M
Last changed    : 8/24/2019 12:48:29 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\OD-001-10-0.7.M
Last changed    : 8/23/2019 7:50:41 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2019-08-24 12-36-20\LXG-5074B.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.891 BB    0.5345 2.08257e4   606.72327  97.6474
   2  20.831 BB    0.6835  501.74051   11.22448   2.3526

Totals :                  2.13275e4   617.94774



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.891 BB    0.5294 1.44505e4   424.22931  97.6875
   2  20.835 BB    0.6690  342.07294    7.71936   2.3125

Totals :                  1.47926e4   431.94867

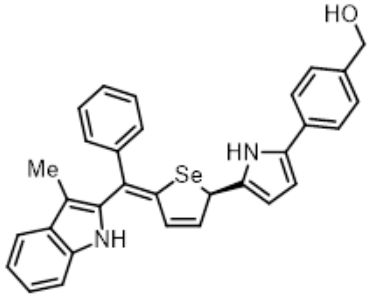


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

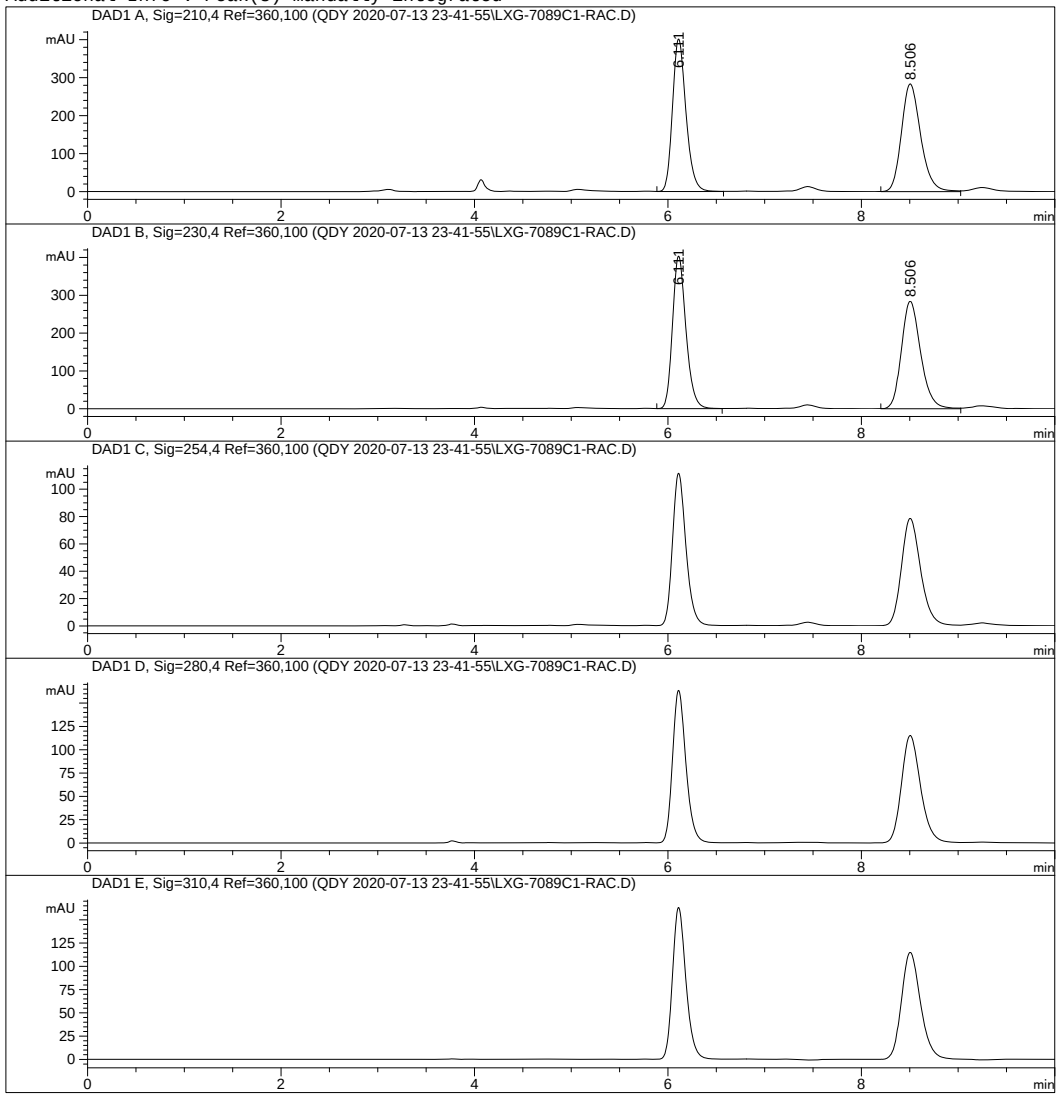


5g
(enantioenriched)

Supplementary Figure 205. HPLC spectrum of **5g** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-07-13 23-41-55\LXG-7089C1-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   5
Acq. Instrument : Instrument 1                    Location : Vial 64
Injection Date  : 7/14/2020 1:28:21 AM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-13 23-41-55\AD-20-30.M
Last changed    : 6/15/2018 10:29:43 AM
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/25/2020 7:02:41 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-13 23-41-55\LXG-7089C1-RAC.D
Sample Name:

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.111 VB    0.1490 3892.64526  401.89789  49.7598
   2   8.506 BV    0.2137 3930.22095  283.60449  50.2402

Totals :                   7822.86621  685.50238



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.111 VB    0.1487 3899.03467  403.65198  49.8315
   2   8.506 BV    0.2130 3925.40625  284.38757  50.1685

Totals :                   7824.44092  688.03955

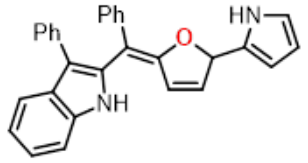


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                          *** End of Report ***
```

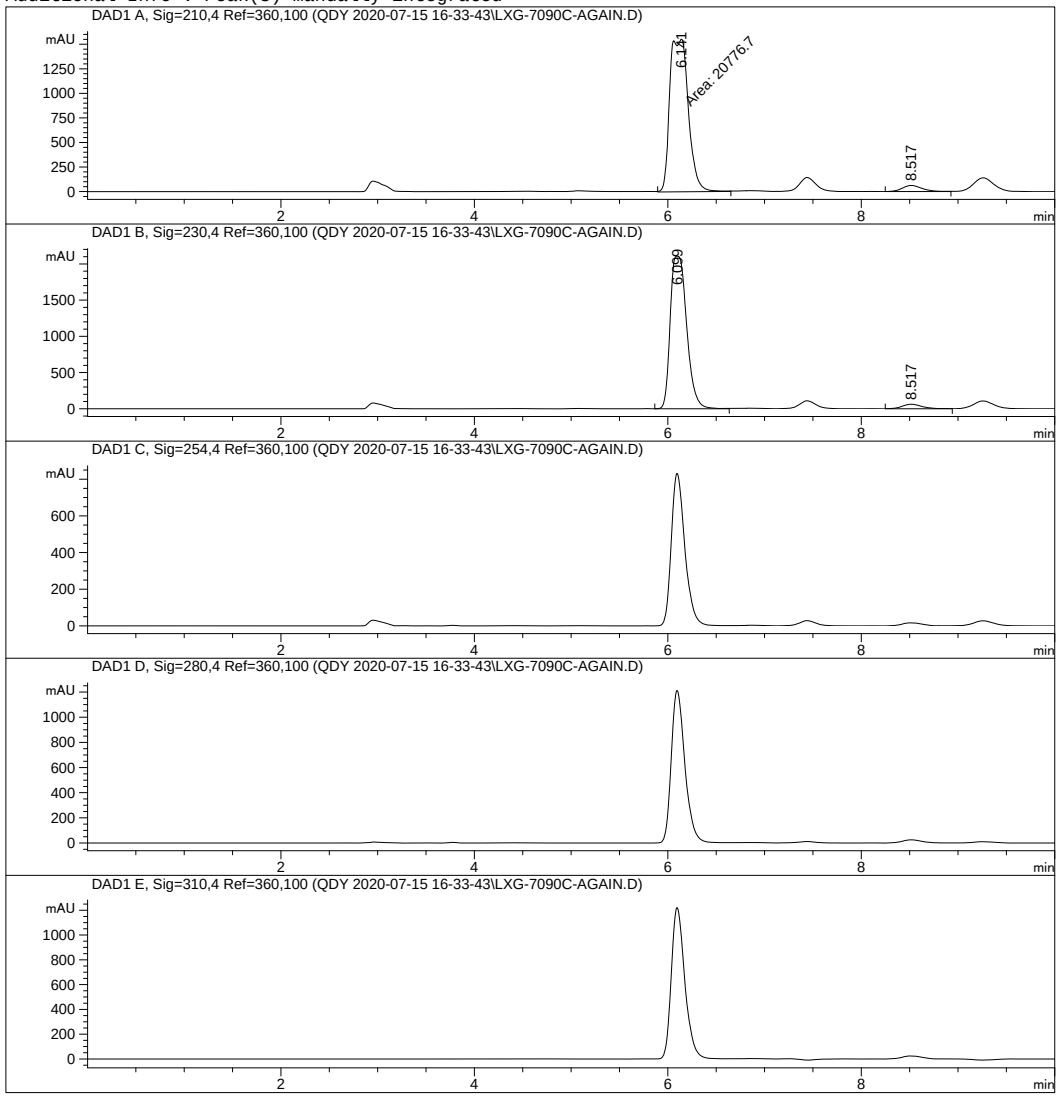


7
(racemic)

Supplementary Figure 206. HPLC spectrum of **7** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-15 16-33-43\LXG-7090C-AGAIN.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :  16
Acq. Instrument : Instrument 1                  Location : Vial 70
Injection Date  : 7/15/2020 9:22:33 PM               Inj :   1
                                              Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-15 16-33-43\AD-20-10.M
Last changed    : 2/7/2015 11:42:28 AM
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/10/2020 9:21:13 AM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-15 16-33-43\LXG-7090C-AGAIN.D
Sample Name:

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.141 MM    0.2226 2.07767e4  1555.80688  95.8682
   2   8.517 BB    0.2161  895.45807   62.89251   4.1318

Totals :                  2.16722e4  1618.69939



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.099 VV    0.1853 2.47872e4  2106.66748  96.5491
   2   8.517 BB    0.2148  885.95630   62.72213   3.4509

Totals :                  2.56731e4  2169.38961

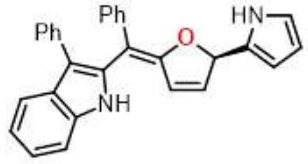


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                          *** End of Report ***
```

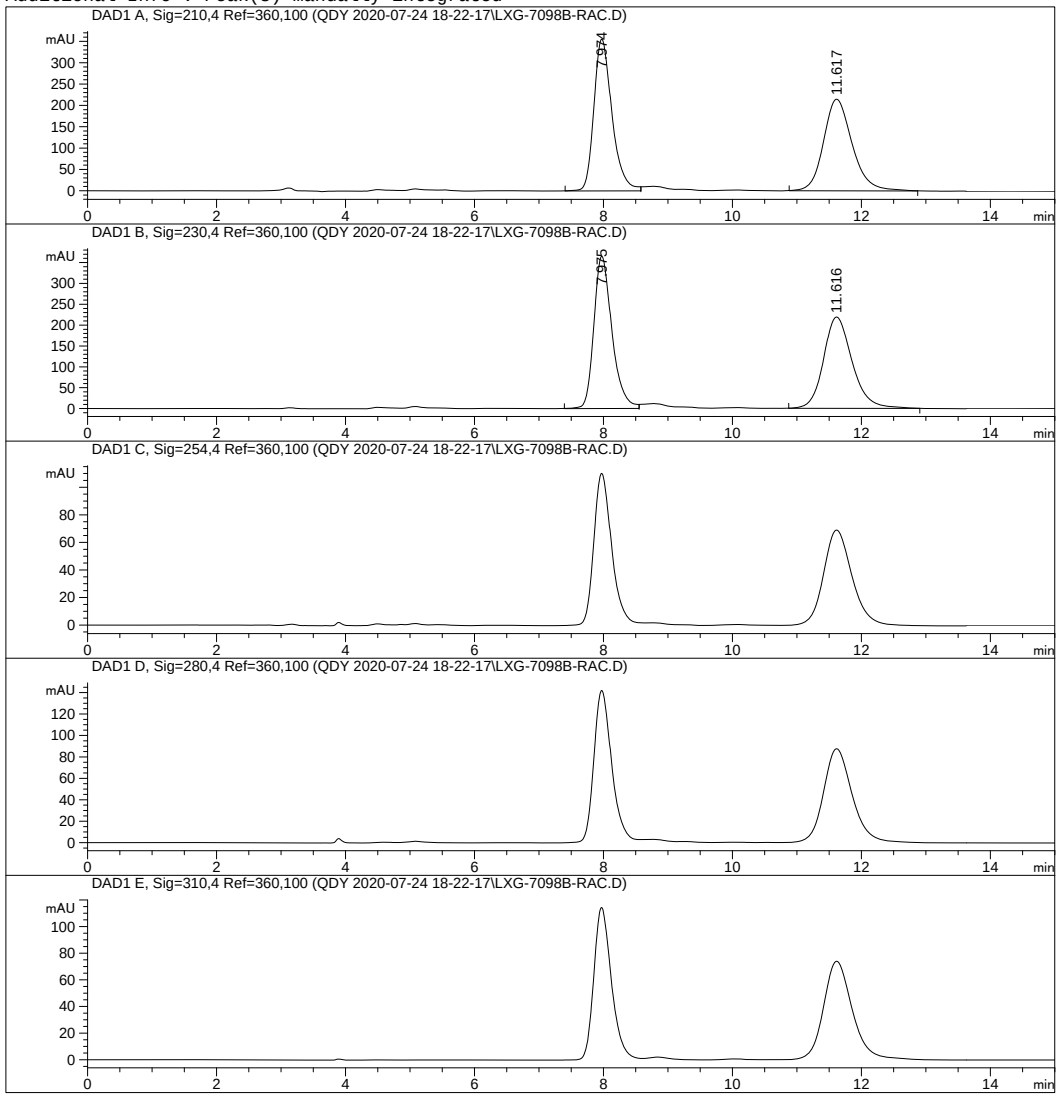


7
(enantioenriched)

Supplementary Figure 207. HPLC spectrum of **7** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-07-24 18-22-17\LXG-7098B-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :  57
Acq. Instrument : Instrument 1                  Location : Vial 67
Injection Date  : 7/25/2020 2:57:17 PM               Inj :   1
                                              Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-24 18-22-17\OD-20-40.M
Last changed    : 7/25/2020 2:56:25 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/31/2020 7:38:22 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-24 18-22-17\LXG-7098B-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.974 BB    0.2956 6940.48926  355.68835  51.1597
   2  11.617 BB    0.4701 6625.82324  214.68097  48.8403

Totals :                  1.35663e4   570.36932



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.975 BV    0.2952 7109.08398  365.05750  51.1949
   2  11.616 BB    0.4710 6777.24072  219.02634  48.8051

Totals :                  1.38863e4   584.08383

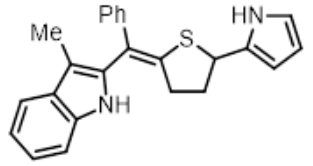


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

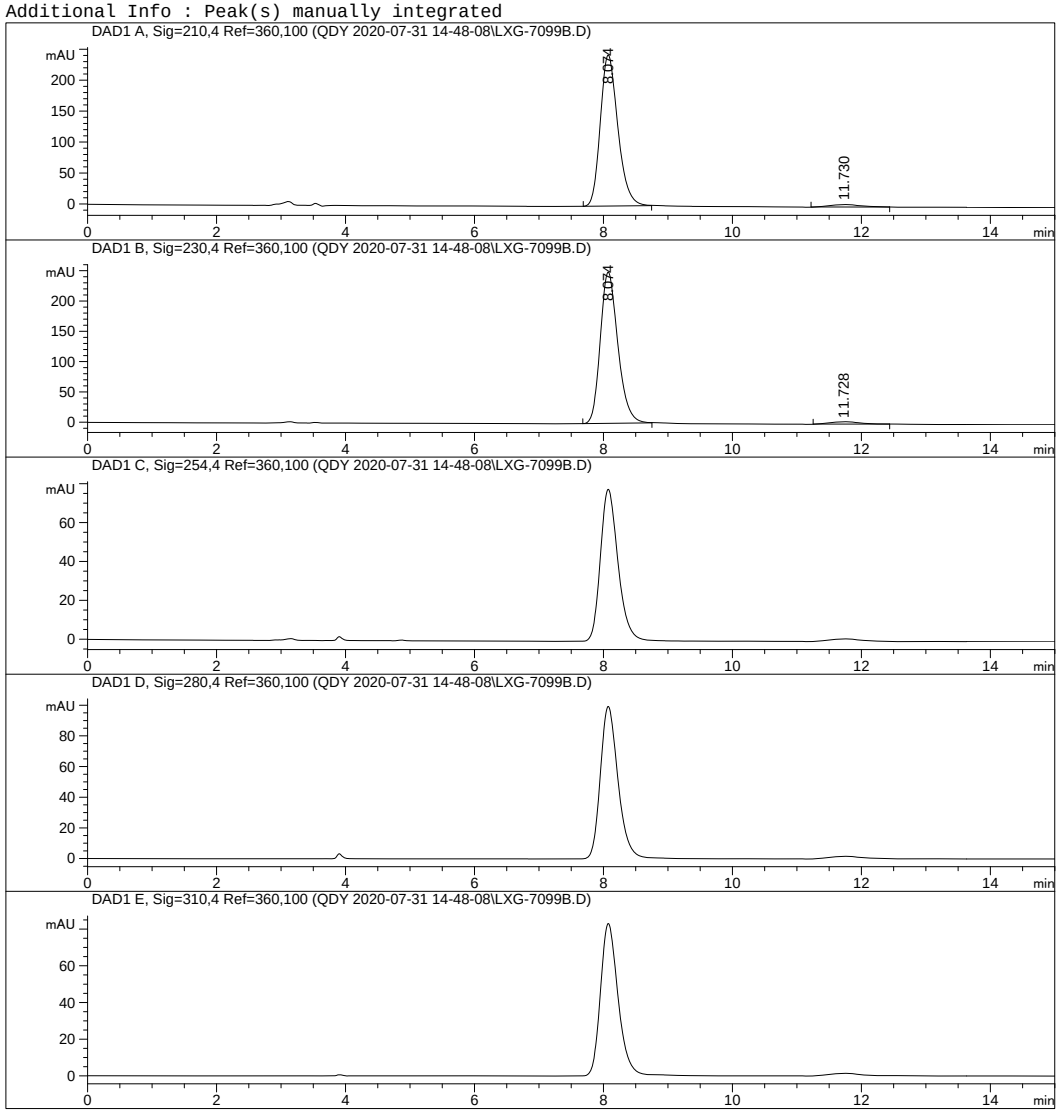


8
(racemic)

Supplementary Figure 208. HPLC spectrum of **8** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-31 14-48-08\LXG-7099B.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :  11
Acq. Instrument : Instrument 1                  Location : Vial 70
Injection Date  : 7/31/2020 6:11:50 PM               Inj :   1
                                              Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-31 14-48-08\OD-20-40.M
Last changed    : 7/31/2020 6:10:55 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/31/2020 7:38:22 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-31 14-48-08\LXG-7099B.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.074 BB    0.2905 4613.42578  244.08182  97.3442
   2  11.730 BB    0.4262  125.86478    4.19339   2.6558

Totals :                  4739.29057  248.27521



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.074 BB    0.2904 4712.54053  249.45163  94.9553
   2  11.728 BB    0.4470  120.56906    4.12544   2.4294
   3  18.823 BB    0.6525  129.79692    2.77089   2.6153

Totals :                  4962.90651  256.34796

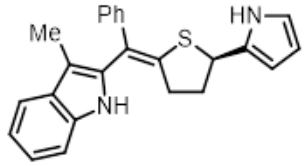


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

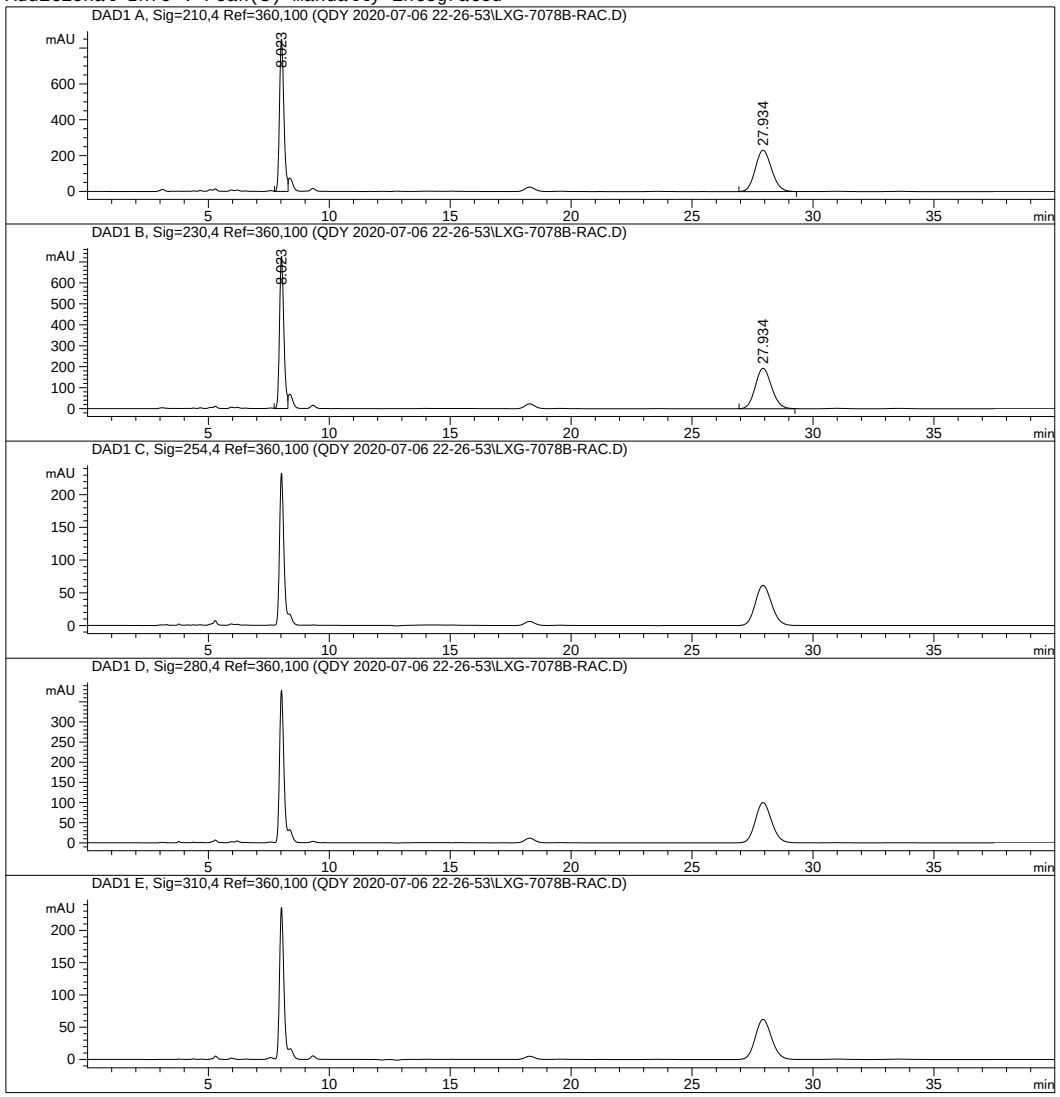


8
(enantioenriched)

Supplementary Figure 209. HPLC spectrum of **8** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-07-06 22-26-53\LXG-7078B-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   9
Acq. Instrument : Instrument 1                    Location : Vial 65
Injection Date  : 7/7/2020 1:12:53 AM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-06 22-26-53\AD-20-40.M
Last changed    : 7/7/2020 12:30:52 AM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/25/2020 7:11:23 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-06 22-26-53\LXG-7078B-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.023 VV    0.1926 1.06791e4   849.79663  49.6574
   2  27.934 BB    0.7291 1.08264e4   230.85995  50.3426

Totals :                  2.15055e4  1080.65659



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.023 VV    0.1908 9025.42285  727.09631  49.9839
   2  27.934 BB    0.7262 9031.23047  192.90782  50.0161

Totals :                  1.80567e4   920.00414

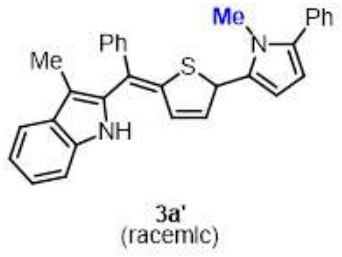


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

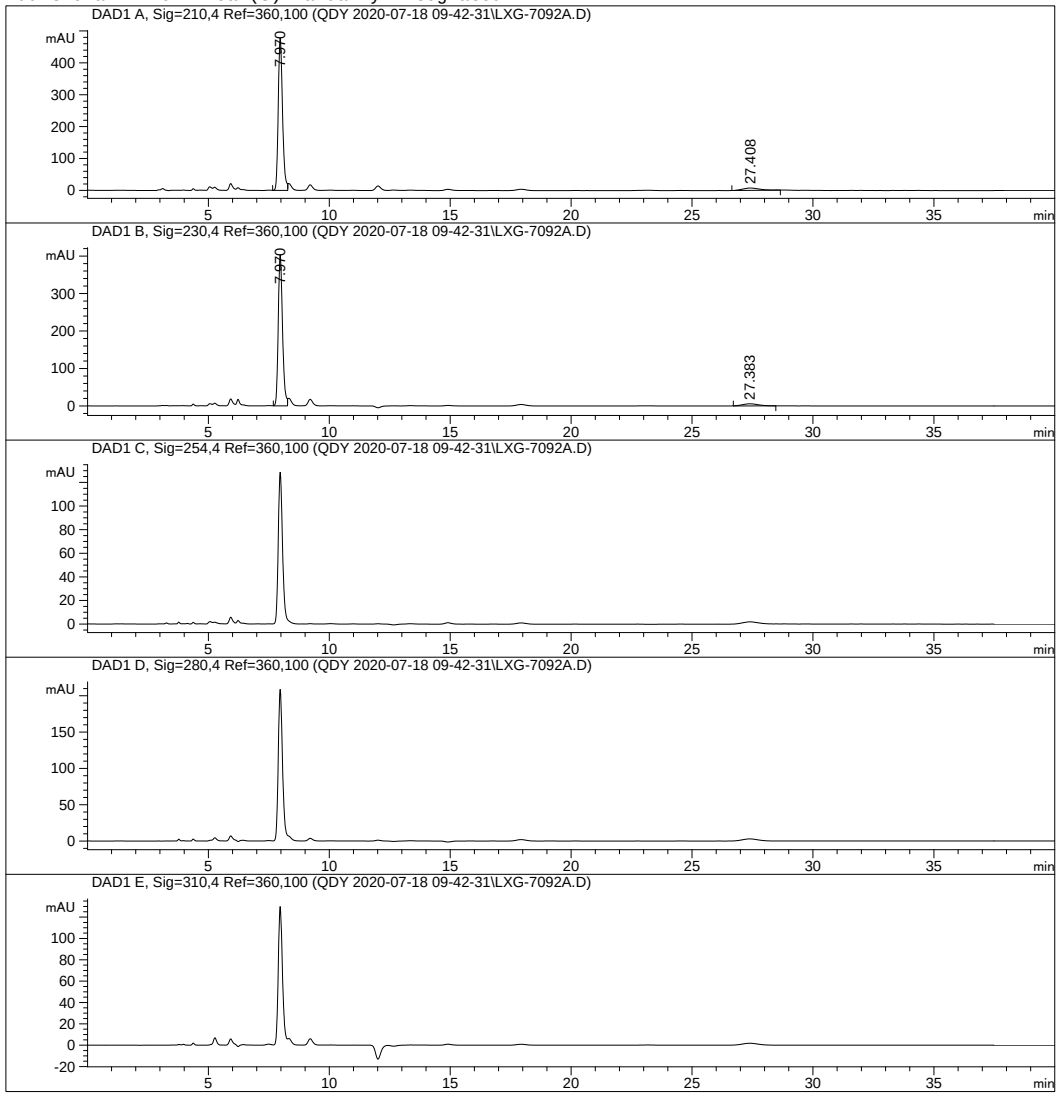


3a'
(racemic)

Supplementary Figure 210. HPLC spectrum of **3a'** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-18 09-42-31\LXG-7092A.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :  19
Acq. Instrument : Instrument 1                  Location : Vial 67
Injection Date  : 7/18/2020 3:00:13 PM               Inj :   1
                                              Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-18 09-42-31\AD-20-40.M
Last changed    : 7/18/2020 2:59:21 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/25/2020 7:11:23 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-18 09-42-31\LXG-7092A.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.970 VV    0.1897 5888.96143  478.02817  94.2839
   2  27.408 BB    0.7033  357.02933    7.29058   5.7161

Totals :                  6245.99075  485.31875



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.970 BV    0.1870 4930.58838  402.14981  95.1420
   2  27.383 BB    0.6629  251.76088    5.57428   4.8580

Totals :                  5182.34926  407.72410

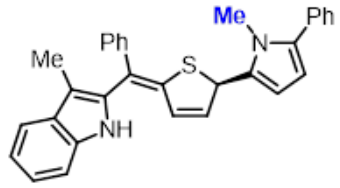


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```

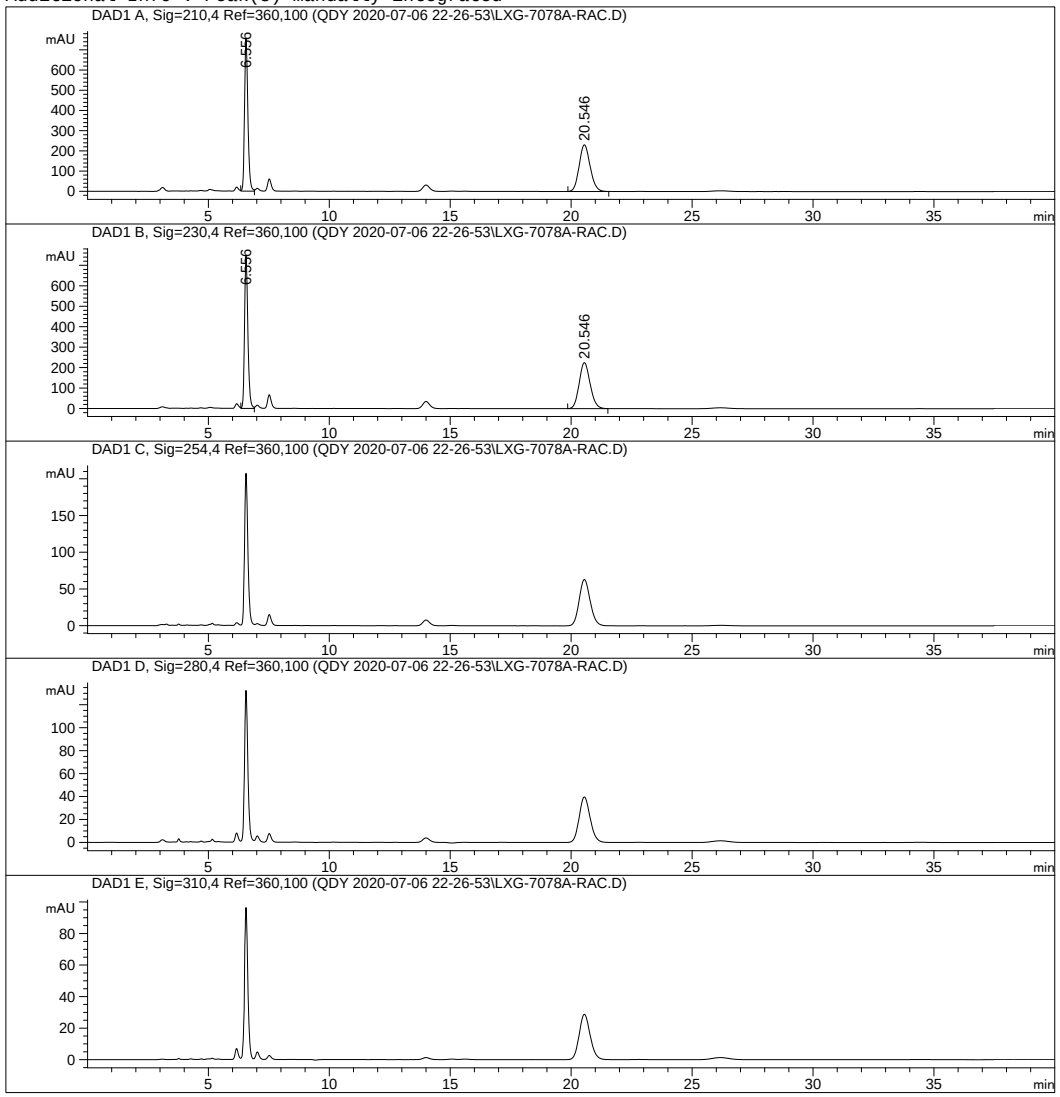


3a'
(enantioenriched)

Supplementary Figure 211. HPLC spectrum of **3a'** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2020-07-06 22-26-53\LXG-7078A-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   8
Acq. Instrument : Instrument 1                    Location : Vial 64
Injection Date  : 7/7/2020 12:31:45 AM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-06 22-26-53\AD-20-40.M
Last changed    : 7/7/2020 12:30:52 AM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/25/2020 7:11:23 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-06 22-26-53\LXG-7078A-RAC.D
Sample Name:

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.556 VV    0.1488 7279.98633  752.79919  49.9059
   2  20.546 BB    0.4911 7307.43311  230.95979  50.0941

Totals :                  1.45874e4   983.75899



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.556 VV    0.1460 7142.89111  744.14386  50.1425
   2  20.546 BB    0.4905 7102.28369  224.84528  49.8575

Totals :                  1.42452e4   968.98914

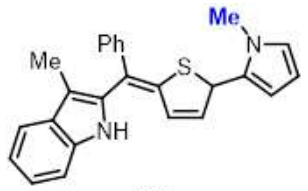


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                          *** End of Report ***
```

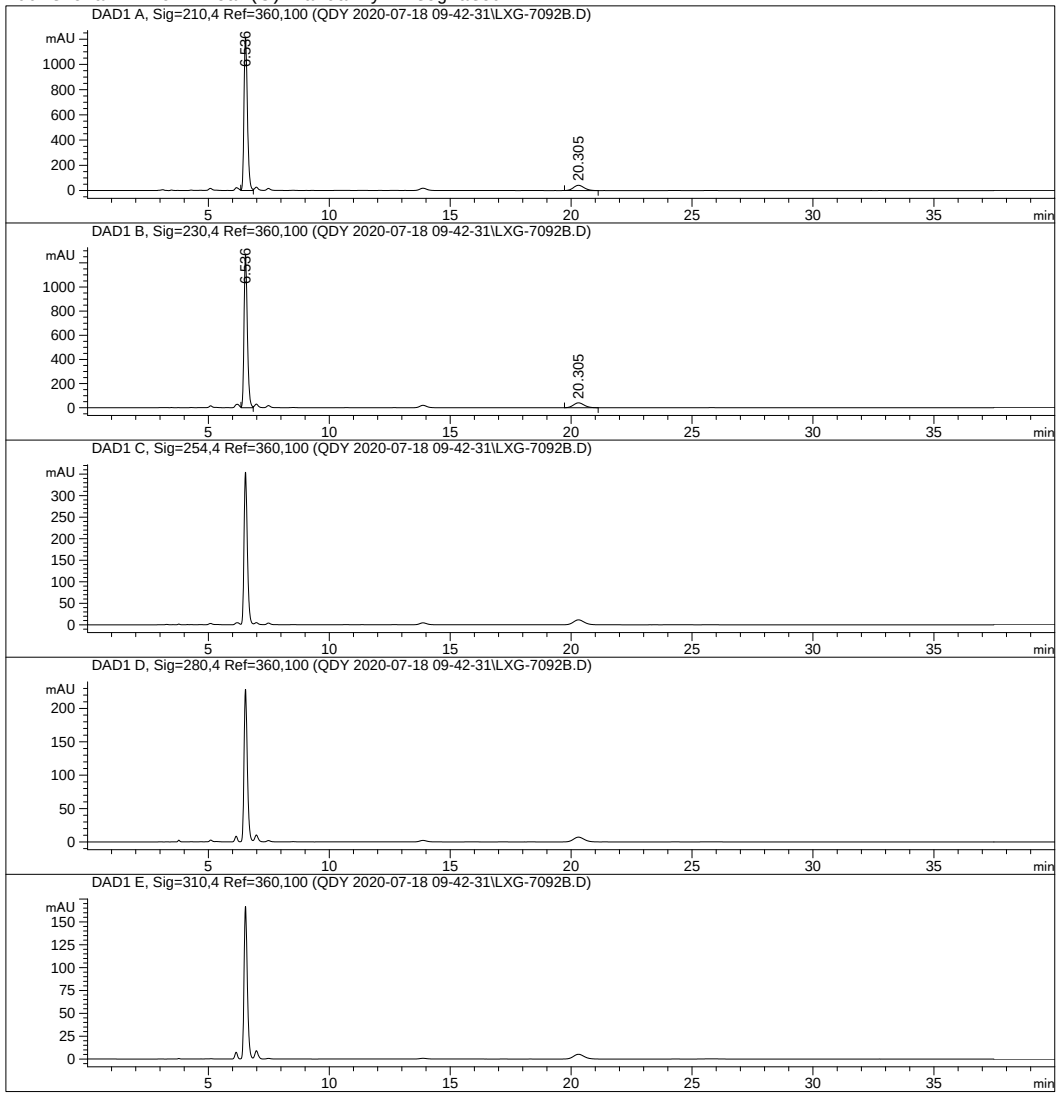


3t'
(racemic)

Supplementary Figure 212. HPLC spectrum of **3t'** (racemic)

Data File C:\CHEM32\1\DATA\QDY 2020-07-18 09-42-31\LXG-7092B.D
Sample Name:

```
=====================================================================
Acq. Operator   :                          Seq. Line :  20
Acq. Instrument : Instrument 1              Location : Vial 68
Injection Date  : 7/18/2020 3:41:19 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 4.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2020-07-18 09-42-31\AD-20-40.M
Last changed    : 7/18/2020 2:59:21 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-008-50.M
Last changed    : 7/25/2020 7:11:23 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2020-07-18 09-42-31\LXG-7092B.D
Sample Name:

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.536 VV    0.1523 1.18542e4  1209.83167  90.2199
   2  20.305 BB    0.4813 1285.03748   41.72567   9.7801

Totals :                  1.31393e4  1251.55733



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.536 VV    0.1464 1.19689e4  1264.49561  90.6123
   2  20.305 BB    0.4761 1240.01331   40.40369   9.3877

Totals :                  1.32089e4  1304.89930

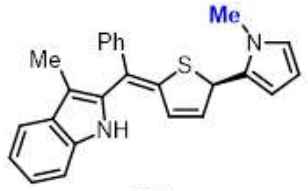


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

=====================================================================
                        *** End of Report ***
```

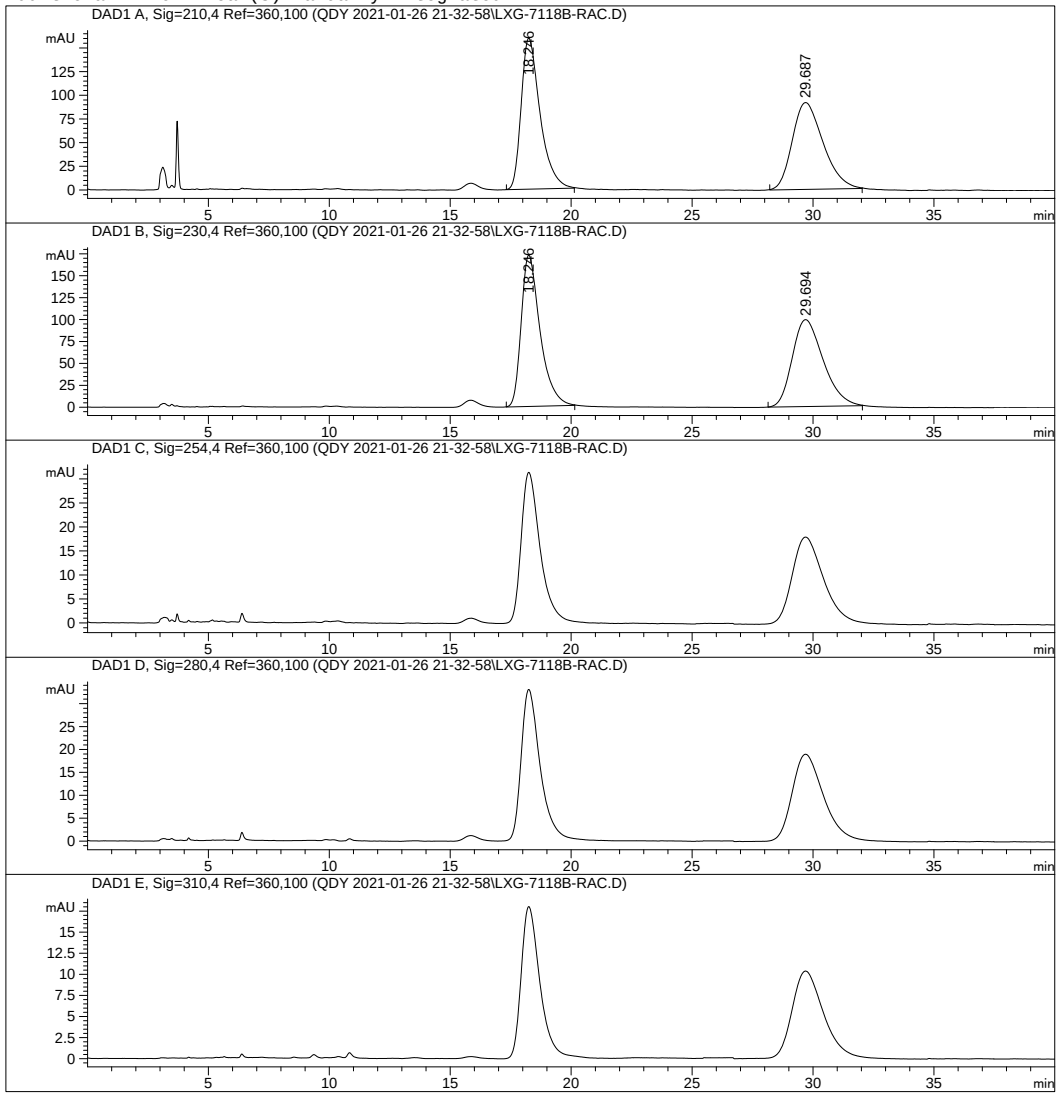


3t'
(enantioenriched)

Supplementary Figure 213. HPLC spectrum of **3t'** (enantioenriched)

Data File C:\CHEM32\1\DATA\QDY 2021-01-26 21-32-58\LXG-7118B-RAC.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                 Seq. Line :  12
Acq. Instrument : Instrument 1                     Location : Vial 32
Injection Date  : 1/27/2021 1:36:35 AM                 Inj :   1
                                                  Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2021-01-26 21-32-58\OD-15-40.M
Last changed    : 9/24/2015 2:07:59 PM
Analysis Method : C:\CHEM32\1\DATA\QDY 2021-01-24 19-32-15\OD-07-10.M
Last changed    : 1/9/2019 4:35:28 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2021-01-26 21-32-58\LXG-7118B-RAC.D
Sample Name:

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  18.246 BB    0.8204 8649.07520  159.56844  51.4866
   2  29.687 BB    1.2352 8149.62891   91.66927  48.5134

Totals :                  1.67987e4   251.23770



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  18.246 BB    0.8235 9369.46582  172.55296  51.5250
   2  29.694 BB    1.3633 8814.84668   99.14123  48.4750

Totals :                  1.81843e4   271.69419

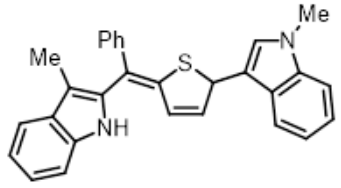


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========================================================================
                        *** End of Report ***
```



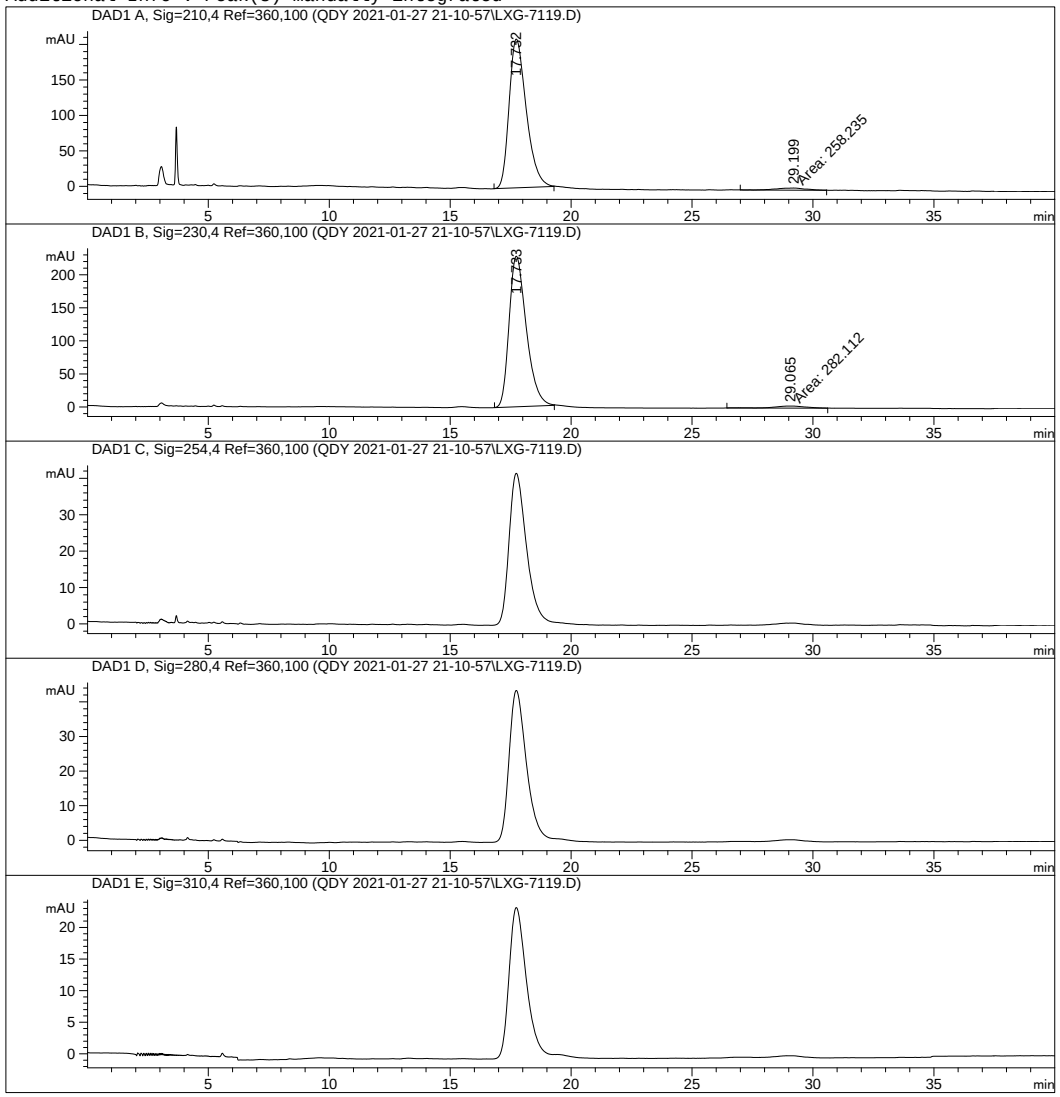
10
(racemic)

Supplementary Figure 214. HPLC spectrum of **10** (racemic)

Instrument 1 1/27/2021 1:37:09 PM Page 2 of 2

Data File C:\CHEM32\1\DATA\QDY 2021-01-27 21-10-57\LXG-7119.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location : Vial 33
Injection Date  : 1/27/2021 9:23:48 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 6.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2021-01-27 21-10-57\OD-15-40.M
Last changed    : 1/27/2021 9:22:55 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\DATA\QDY 2021-01-24 19-32-15\OD-07-10.M
Last changed    : 1/9/2019 4:35:28 PM
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\QDY 2021-01-27 21-10-57\LXG-7119.D
Sample Name:

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.732 BB    0.7599 1.03510e4   209.69389  97.5659
   2  29.199 MM    1.4392  258.23492    2.99052   2.4341

Totals :                  1.06093e4   212.68441



Signal 2: DAD1 B, Sig=230,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.733 BB    0.7647 1.12584e4   227.75662  97.5555
   2  29.065 MM    1.5051  282.11191    3.12401   2.4445

Totals :                  1.15405e4   230.88064

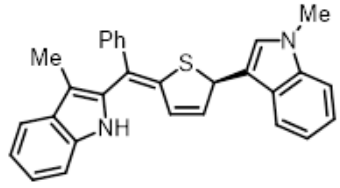


Signal 3: DAD1 C, Sig=254,4 Ref=360,100


Signal 4: DAD1 D, Sig=280,4 Ref=360,100


Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==================================================================
                        *** End of Report ***
```



10
(enantioenriched)

Supplementary Figure 215. HPLC spectrum of **10** (enantioenriched)