Supplementary Information

Organocatalytic Discrimination of Non-Directing Aryl and Heteroaryl Groups: Enantioselective Synthesis of Bioactive Indole-Containing Triarylmethanes

Qiaolin YAN[a†], Meng Duan[b,f†], Cien Chen[c,d], Zhiqing Deng[d,e], Mandi Wu[c,d], Peiyuan Yu[f], Ming-Liang He*[c,d], Guangyu Zhu*[d,e], K. N. Houk*[b] and Jianwei Sun*[a,g]

[a] *Department of Chemistry and the Hong Kong Branch of Chinese National Engineering Research Centre for Tissue Restoration & Reconstruction, The Hong Kong University of Science and Technology (HKUST), Clear Water Bay, Kowloon, Hong Kong SAR, China.*

[b] *Department of Chemistry and Biochemistry, University of California, Los Angeles, California 90095, USA.*

[c] *Department of Biomedical Sciences, City University of Hong Kong, Kowloon Tong, Hong Kong SAR, China.*

[d] *CityU Shenzhen Research Institute, Shenzhen, China.*

[e] *Department of Chemistry, City University of Hong Kong, Kowloon Tong, Hong Kong SAR, China.*

[f] *Department of Chemistry and Shenzhen Grubbs Institute, Guangdong Provincial Key Laboratory of Catalysis, Southern University of Science and Technology, Shenzhen, 518055, China.*

[g] *Shenzhen Research Institute, HKUST, No. 9 Yuexing 1st Rd, Shenzhen 518057, China*

[†] *These authors contributed equally to this work.*

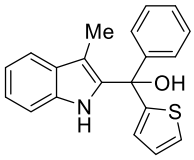
Table of Contents

I. General Information

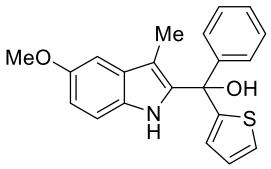
Flash column chromatography was performed over silica gel (200-300 mesh) purchased from Qindao Puke Co., China. All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using anhydrous solvents. Anhydrous dichloromethane, diethyl ether, and tetrahydrofuran were purified by the Innovative® solvent purification system or distilled under common conditions. ^{1}H, ^{13}C and ^{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: acetone-d_6 at 2.05 ppm; ^{13}C NMR: 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 = quartet; 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 5 mg/mL. The enantiomeric excess values were determined by chiral HPLC using an Agilent 1200 LC instrument with Daicel CHIRALCEL OD-H or Daicel CHIRALPAK AD-H columns.

II. Synthesis of the Tertiary Alcohol Substrates

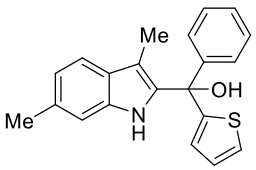
Substrates **1b**, **1i**, **1m** and **1n** were prepared according to General Procedure A. Substrates **1h**, **1o** and **1p** were prepared according to General Procedure B. Substrates **1a**, **1c**-**g** and **1j**-**l** are known compounds and were prepared according to the literature procedure.[1]



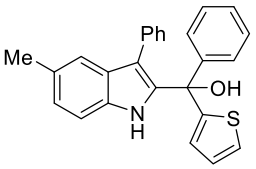
1a



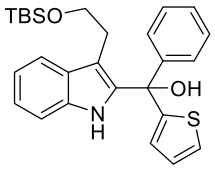
1b



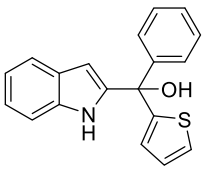
1c



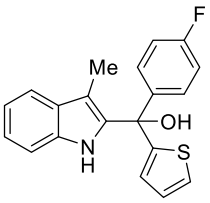
1d



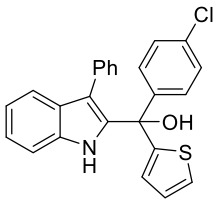
1e



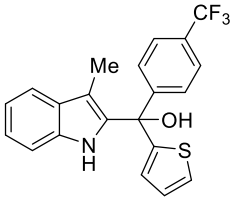
1f



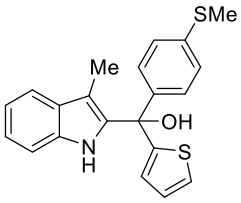
1g



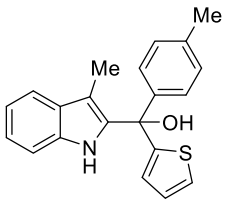
1h



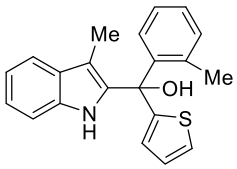
1i



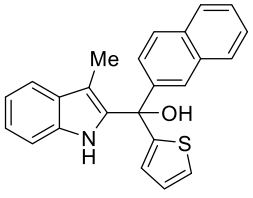
1j



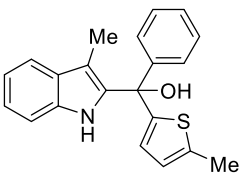
1k



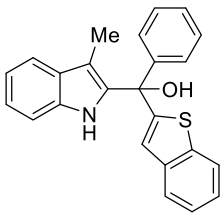
1l



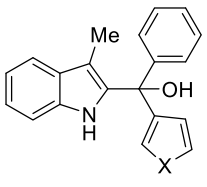
1m



1n



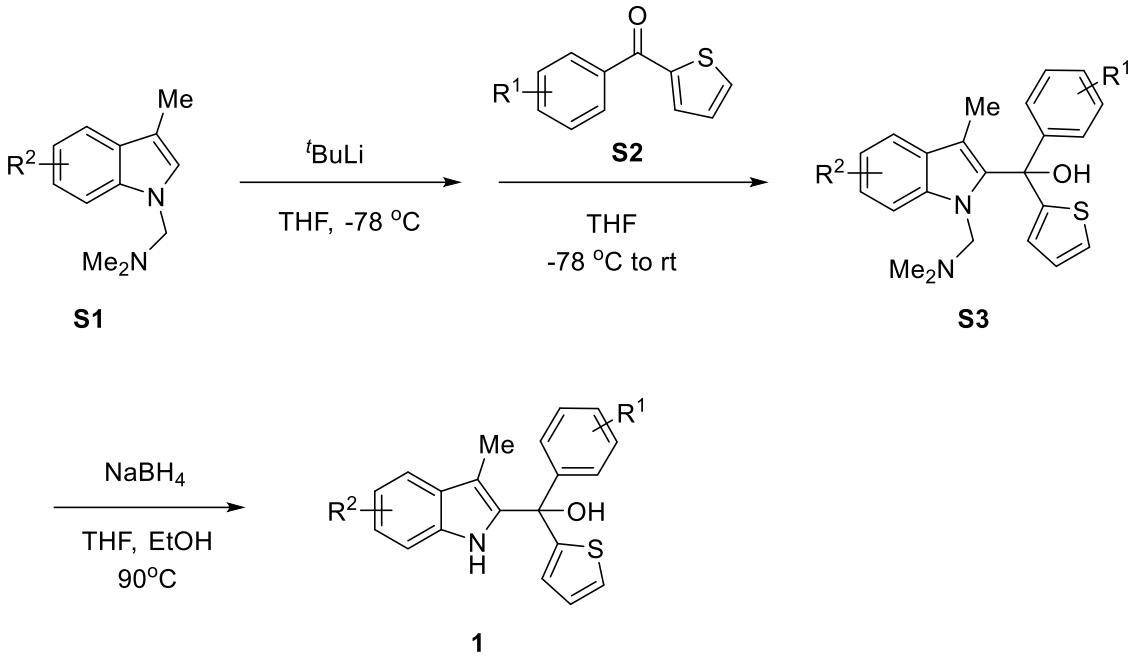
1o



1p (X = S)
1q (X = O)

1 X. Li, M. Duan, P. Yu, K. N. Houk and J. Sun. *Nat. Commun.* 2021, **12**, 4881.

General Procedure A.



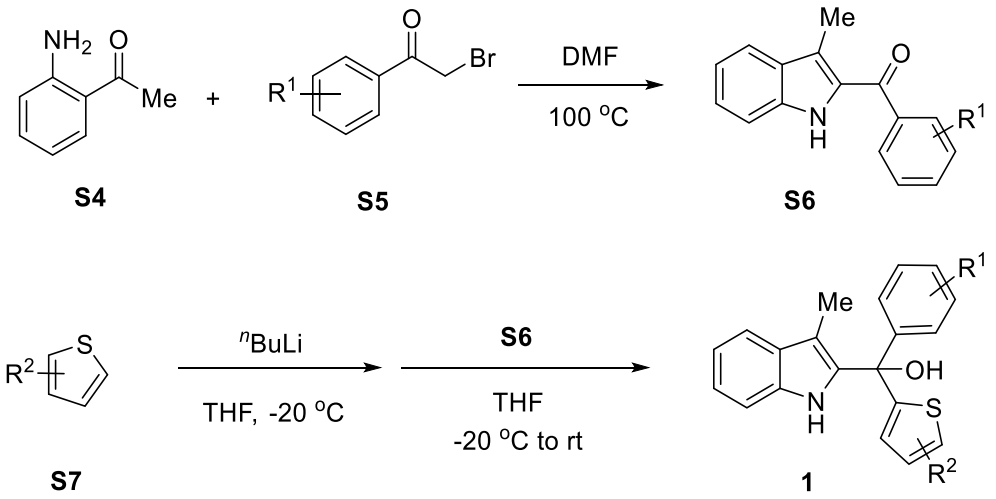
The starting indole **S1** was prepared according to the literature procedure.[2] At –78 °C under N_2, to a stirred solution of **S1** (2.0 mmol) in THF (15 mL) was slowly added *tert*-butyllithium (1.3 M in pentane, 1.6 mL, 2.1 mmol). The resulting mixture was kept stirring at –78 °C for 0.5 h. After that, a solution of ketone **S2** (2.0 mmol) in THF (10 mL) was slowly added. The mixture was allowed to warm to room temperature and stirred overnight. Then, a saturated aqueous NH_4Cl solution (30 mL) was slowly added to quench the reaction. The layers were separated, and the aqueous layer 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 pure tertiary alcohol **S3**.

To a solution of alcohol **S3** in THF (3 mL) and ethanol (3 mL) was added $NaBH_4$ (83.2 mg, 2.2 mmol). The reaction mixture was heated to reflux for 16 h before it was cooled to room temperature. A saturated aqueous solution of NH_4Cl (3 mL) was added to quench the reaction. Then, the mixture was concentrated under reduced pressure to remove most THF. The resulting mixture was extracted with EtOAc (3 ×

2 J. Yu, E. Lam, J. Sereda, N. Rampersad, A. Lough, C. Browning and D. Farrar, *Organometallics* 2005, **24**, 37−47.

20 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**.

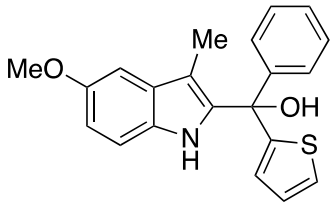
General Procedure B.



Under N_2 atmosphere, a suspension of *ortho*-aminoketone **S4** (1.08 g, 8 mmol), 2-bromo-1-phenylethan-1-one **S5** (8.1 mmol), and anhydrous DMF (15 mL) was stirred at 100 °C for 16 h. The mixture was cooled to room temperature before it was diluted with Et_2O (30 mL) and filtered through a pad of celite, which was wahsed with Et_2O (100 mL). The filtrate was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The crude product was purified by silica gel flash column chromatography to yield ketone **S6**.

At –20 °C, to a stirred solution of thiophene **S7** (9.0 mmol) in THF (15 mL) was slowly added *n*-butyllithium (2.4 M in hexane, 3.95 mL, 9.5 mmol). The resulting mixture was kept stirring at –20 °C for 1 h. After that, a solution of ketone **S6** (3.0 mmol) in THF (10 mL) was added at the same temperature and the reaction mixture was warmed up to room temperature and kept stirring overnight. A saturated aqueous NH_4Cl solution (20 mL) was added to quench the reaction. The layers were separated, and the aqueous layer 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 pure tertiary alcohol **1**.



1b

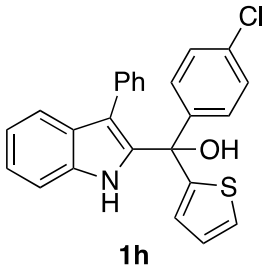
(5-Methoxy-3-methyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (1b) was prepared as white foam from phenyl(thiophen-2-yl)methanone (2.5 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 20:1 → 10:1) in 31% yield (2 steps, 0.27 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.53 (s, 1H), 7.49 – 7.47 (m, 2H), 7.41 – 7.40 (m, 1H), 7.36 – 7.30 (m, 3H), 7.27 – 7.25 (m, 1H), 6.98 – 6.95 (m, 2H), 6.87 – 6.86 (m, 1H), 6.75 – 6.72 (m, 1H), 5.73 (s, 1H), 3.79 (s, 3H), 1.83 (s, 3H).

^{13}C NMR (100 MHz, acetone-d6) δ 154.7, 152.6, 146.9, 140.2, 131.0, 130.7, 128.6, 128.3, 127.9, 127.1, 127.0, 126.4, 112.7, 112.5, 107.8, 100.8, 77.2, 55.8, 9.8.

IR (thin film) 3568, 3450, 3056, 2941, 1483, 1446, 1177, 735, 702 cm^{-1}.

HRMS (ES-) calcd for $C_{21}H_{18}NO_2S^-$ $[M–H]^-$: 348.1064, found: 348.1061.



1h

(4-Chlorophenyl)(3-phenyl-1*H*-indol-2-yl)(thiophen-2-yl)methanol (1h) was prepared as brown foam from (4-chlorophenyl)(3-phenyl-1*H*-indol-2-yl)methanone (3.0 mmol) according to the General Procedure B (eluent: hexanes/EtOAc = 10:1 → 5:1) in 84% yield (1.1 g).

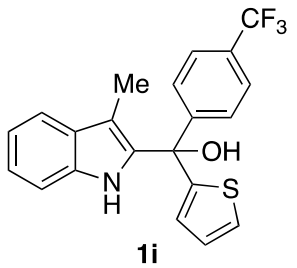
^{1}H NMR (400 MHz, acetone-d_6) δ 10.10 (s, 1H), 7.49 – 7.47 (m, 1H), 7.42 – 7.38 (m, 2H),

7.33 – 7.29 (m, 2H), 7.21 – 7.16 (m, 3H), 7.15 – 7.10 (m, 5H), 7.05 – 7.01 (m, 1H), 6.84 – 6.80 (m, 2H), 5.85 (s, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 151.8, 145.6, 138.6, 136.0, 135.6, 133.5, 131.3, 130.1, 129.9, 128.3, 128.1, 127.4, 127.1, 126.4, 126.3, 123.0, 120.3, 120.0, 116.0, 112.2, 77.2.

IR (thin film) 3542, 3440, 3055, 1488, 1450, 1263, 833, 735, 704 cm^{-1}.

HRMS (ES-) calcd for $C_{25}H_{17}ClNOS^-$ [M–H]$^-$: 414.0725, found: 414.0724.



1i

(3-Methyl-1*H*-indol-2-yl)(thiophen-2-yl)(4-(trifluoromethyl)phenyl)methanol (1i) was prepared as dark green foam from thiophen-2-yl(4-(trifluoromethyl)phenyl)methanone (3.0 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 70% yield (2 steps, 0.81 g).

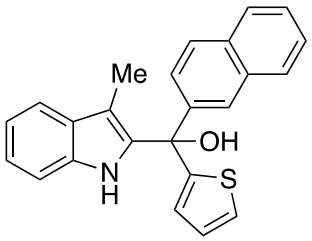
^{1}H NMR (400 MHz, acetone-d6) δ 9.80 (s, 1H), 7.78 – 7.72 (m, 4H), 7.51 – 7.49 (m, 1H), 7.45 – 7.44 (m, 1H), 7.40 – 7.37 (m, 1H), 7.13 – 7.09 (m, 1H), 7.05 – 7.00 (m, 2H), 6.94 – 6.93 (m, 1H), 6.08 (s, 1H), 1.91 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 151.7, 151.4, 138.6, 135.8, 130.6, 129.9 (q, J = 32 Hz), 128.6, 127.4, 127.3, 126.8, 125.7 (q, J = 4 Hz), 125.3 (q, J = 270 Hz), 122.5, 119.5, 119.2, 112.1, 108.5, 76.9, 9.7.

^{19}F NMR (376 MHz, acetone-d6) δ -62.7.

IR (thin film) 3580, 3451, 3057, 1620, 1456, 1413, 1323, 1265, 1124, 736 cm^{-1}.

HRMS (ES-) calcd for $C_{21}H_{15}F_3NOS^-$ [M–H]$^-$: 386.0832, found: 386.0832.



1m

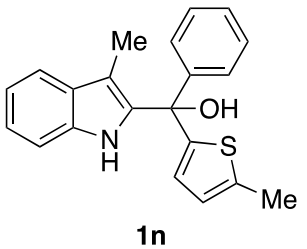
(3-Methyl-1*H*-indol-2-yl)(naphthalen-2-yl)(thiophen-2-yl)methanol (1m) was prepared as slightly yellow foam from naphthalen-2-yl(thiophen-2-yl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 77% yield (2 steps, 0.85 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.78 (s, 1H), 7.98 (s, 1H), 7.91 – 7.83 (m, 3H), 7.71 – 7.69 (m, 1H), 7.51 – 7.47 (m, 3H), 7.44 – 7.38 (m, 2H), 7.11 – 7.08 (m, 1H), 7.04 – 6.97 (m, 3H), 5.92 (s, 1H), 1.93 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 152.5, 144.4, 139.4, 135.8, 133.79, 133.76, 130.7, 129.2, 128.4, 128.3, 127.3, 127.1, 127.04, 126.99, 126.6, 126.44, 126.38, 122.3, 119.4, 119.1, 112.1, 108.2, 77.4, 9.8.

IR (thin film) 3567, 3449, 3055, 2984, 2924, 2865, 1601, 1457, 1264, 733 cm^{-1}.

HRMS (ES-) calcd for $C_{24}H_{18}NOS^-$ $[M–H]^-$: 368.1115, found: 368.1111.



1n

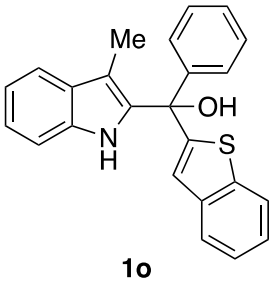
(3-Methyl-1*H*-indol-2-yl)(5-methylthiophen-2-yl)(phenyl)methanol (1n) was prepared as green foam from (5-methylthiophen-2-yl)(phenyl)methanone (3 mmol) according to the General Procedure A (eluent: hexanes/EtOAc = 10:1 → 5:1) in 75% yield (2 steps, 0.75 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.67 (s, 1H), 7.51 – 7.46 (m, 3H), 7.39 – 7.27 (m, 4H), 7.09 – 7.05 (m, 1H), 7.02 – 6.98 (m, 1H), 6.64 – 6.62 (m, 2H), 5.60 (s, 1H), 2.42 (s, 3H), 1.89 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 150.0, 146.9, 140.6, 139.6, 135.7, 130.8, 128.6, 128.3, 128.0, 127.0, 125.3, 122.2, 119.3, 119.0, 112.0, 107.9, 77.2, 15.2, 9.7.

IR (thin film) 3446, 3055, 2921, 1705, 1622, 1451, 1264, 732, 700 cm^{-1}.

HRMS (ES-) calcd for $C_{21}H_{18}NOS^-$ [M–H]$^-$: 332.1115, found: 332.1111.



1o

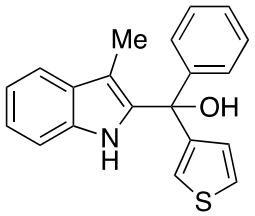
Benzo[*b*]thiophen-2-yl(3-methyl-1*H*-indol-2-yl)(phenyl)methanol (1o) was prepared as pale yellow foam from (3-methyl-1*H*-indol-2-yl)(phenyl)methanone (0.85 mmol) according to the General Procedure B (eluent: hexanes/EtOAc = 10:1 → 5:1) in 50% yield (0.15 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.84 (s, 1H), 7.87 – 7.85 (m, 1H), 7.77 – 7.74 (m, 1H), 7.60 – 7.57 (m, 2H), 7.51 – 7.49 (m, 1H), 7.40 – 7.29 (m, 6H), 7.16 (s, 1H), 7.12 – 7.08 (m, 1H), 7.05 – 7.01 (m, 1H), 5.97 (s, 1H), 1.95 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 153.5, 146.3, 141.0, 140.4, 138.8, 135.8, 130.7, 128.8, 128.5, 128.0, 125.1, 125.0, 124.6, 123.6, 123.0, 122.3, 119.5, 119.1, 112.1, 108.4, 77.6, 9.8.

IR (thin film) 3577, 3452, 3056, 2927, 2866, 1490, 998, 1264, 732 cm^{-1}.

HRMS (ES-) calcd for $C_{24}H_{18}NOS^-$ [M–H]$^-$: 368.1115, found: 368.1113.



1p

(3-Methyl-1*H*-indol-2-yl)(phenyl)(thiophen-3-yl)methanol (1p) was prepared as orange foam according to the General Procedure B. At –78 °C, to a stirred solution of

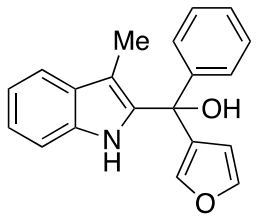
3-bromothiophene (6 mmol) in THF (10 mL) was slowly added *n*-butyllithium (2.4 M in hexane, 2.6 mL, 6.26 mmol). The resulting mixture was kept stirring at –78 °C for 30 min. After that, a solution of (3-methyl-1*H*-indol-2-yl)(phenyl)methanone (2 mmol) in THF (5 mL) was added at the same temperature and the reaction mixture was warmed up to room temperature and kept stirring overnight. A saturated aqueous NH_4Cl solution (20 mL) was added to quench the reaction. The layers were separated, and the aqueous layer 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 (eluent: hexanes/EtOAc = 10:1 → 8:1) to afford the pure tertiary alcohol **1p** in 86% yield (0.55 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.66 (s, 1H), 7.52 – 7.48 (m, 3H), 744 – 7.40 (m, 2H), 7.37 – 7.28 (m, 3H), 7.20 – 7.18 (m, 1H), 7.13 – 7.02 (m, 3H), 5.50 (s, 1H), 1.89 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 148.9, 146.9, 139.5, 135.6, 130.7, 128.8, 128.6, 128.04, 127.95, 126.4, 123.8, 122.0, 119.3, 118.9, 111.9, 107.5, 77.0, 9.5.

IR (thin film) 3440, 3057, 2975, 2866, 1591, 1488, 1453, 1327, 1142, 788, 743, 701 cm^{-1}.

HRMS (ES-) calcd for: $C_{20}H_{16}NOS^-$ $[M–H]^-$: 318.0958, found: 318.0957.



1q

Furan-3-yl(3-methyl-1*H*-indol-2-yl)(phenyl)methanol (1q) was prepared as orange foam according to the General Procedure B. At –78 °C, to a stirred solution of 3-bromofuran (2.25 mmol, 330.8 mg) in THF (5 mL) was slowly added *n*-butyllithium (2.4 M in hexane, 0.94 mL, 2.25 mmol). The resulting mixture was kept stirring at –78 °C for 30 min. After that, a solution of (3-methyl-1*H*-indol-2-yl)(phenyl)methanone (0.75 mmol, 176.3 mg) in THF (3 mL) was added at the same temperature and the reaction mixture was warmed up to room temperature and kept stirring overnight. A

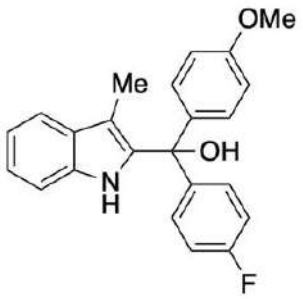
saturated aqueous NH_4Cl solution (10 mL) was added to quench the reaction. The layers were separated, and the aqueous layer was extracted with EtOAc (3 × 15 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered, and concentrated. The residue was purified by silica gel flash chromatography (eluent: hexanes/EtOAc = 10:1 → 8:1) to afford the pure tertiary alcohol **1p** in 46% yield (0.107 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.70 (s, 1H), 7.57 – 7.48 (m, 3H), 7.41– 7.39 (m, 2H), 7.36 – 7.27 (m, 3H), 7.190 – 7.189 (m, 1H), 7.12 – 7.08 (m, 1H), 7.05 – 7.01 (m, 1H), 6.559 – 6.555 (m, 1H), 5.39 (s, 1H), 1.96 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.6, 144.2, 141.7, 139.2, 135.6, 133.1, 130.8, 128.6, 128.1, 127.7, 122.0, 119.3, 118.9, 111.9, 111.5, 107.2, 74.4, 9.7.

IR (thin film) 3372, 2979, 2939, 2867, 1451, 1382, 1118, 1030, 740, 703 cm^{-1}.

HRMS (ES-) calcd for: $C_{20}H_{16}NO_2^-$ $[M–H]^-$: 302.1187, found: 302.1176.



1r

(4-Fluorophenyl)(4-methoxyphenyl)(3-methyl-1*H*-indol-2-yl)methanol (1r) was prepared as orange foam from (4-fluorophenyl)(3-methyl-1*H*-indol-2-yl)methanone according to General Procedure B (eluent: hexanes/EtOAc = 10:1 → 5:1) in 70% yield (0.10 g).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.62 (s, 1H), 7.48– 7.42 (m, 3H), 7.37 – 7.36 (m, 1H), 7.30 – 7.29 (m, 2H), 7.12 – 7.05 (m, 3H), 7.03 – 6.99 (m, 1H), 6.91 – 6.88 (m, 2H), 5.50 (br, 1H), 3.78 (s, 3H), 1.83 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 162.3 (d, J = 243 Hz), 159.4, 143.1 (d, J = 3 Hz), 139.4, 138.6, 135.3, 130.2, 130.1 (d, J = 8 Hz), 129.3, 121.6, 118.9, 118.4, 114.7 (d, J = 21 Hz), 113.5, 111.5, 107.5, 78.2, 55.0, 9.4.

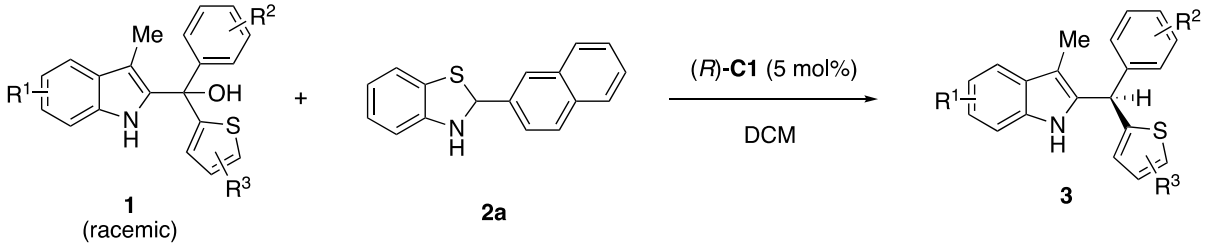
^{19}F NMR (376 MHz, acetone-d_6) δ -117.5.

IR (thin film) 3453, 3053, 2924, 2847, 1603, 1505, 1456, 1240, 1168, 1027, 832, 738 cm^{-1}.

HRMS (ES-) calcd for $C_{23}H_{19}FNO_2^-$ [M–H]$^-$: 360.1405, found: 360.1405.

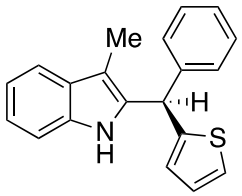
III. Catalytic Asymmetric Synthesis of Triarylmethanes

General Procedure C.



At 0 °C, to an oven-dried 30-mL vial were added the tertiary alcohol **1** (0.40 mmol), the hydride source **2a** (115.9 mg, 0.44 mmol), (*R*)-**C1** (15.04 mg, 0.02 mmol, 5.0 mol%) and DCM (8.0 mL). The mixture was stirred at the same temperature for 30 h and concentrated under reduced pressure. The residue was purified by silica gel flash chromatography to afford the desired product.

Unless noted otherwise, all the racemic products (used for HPLC reference in determining the ee value) were prepared from the same reaction using racemic 1,1'-binaphthyl-2,2'-diyl hydrogenphosphate as the catalyst.



3a

(*R*)-3-Methyl-2-(phenyl(thiophen-2-yl)methyl)-1*H*-indole (3a) was prepared as pale yellow foam from (3-methyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol **1a** (79.8 mg, 0.250 mmol) and **2a** (72.4 mg, 0.275 mmol) according to the General Procedure C (RT, 16 h, eluent: hexanes/dichloromethane = 3:2) in 87% yield (66.3 mg, 96% ee). $[\alpha]_D^{26}$: −10.8 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 8.4 min (major), 9.3 min (minor).

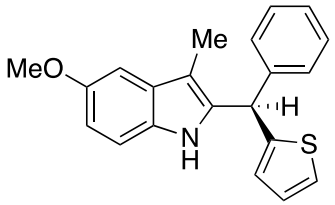
^{1}H NMR (400 MHz, acetone-d_6) δ 9.70 (s, 1H), 7.48 – 7.47 (m, 1H), 7.37 – 7.24 (m, 7H),

7.06 – 6.96 (m, 3H), 6.81 – 6.80 (m, 1H), 6.05 (s, 1H), 2.23 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.1, 143.5, 136.9, 136.5, 130.0, 129.3 (2C), 127.7, 127.5, 127.1, 125.6, 121.9, 119.5, 118.9, 111.8, 107.8, 44.7, 8.8.

IR (thin film) 3441, 3058, 2923, 2858, 1492, 1456, 742, 701 cm^{-1}.

HRMS (ES-) calcd for $C_{20}H_{16}NS^-$ [M–H]$^-$: 302.1009, found: 302.1001.



3b

(*R*)-5-Methoxy-3-methyl-2-(phenyl(thiophen-2-yl)methyl)-1*H*-indole (3b) was prepared as white foam from (5-methoxy-3-methyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol **1b** (139.8 mg, 0.400 mmol) and **2a** (106.4 mg, 0.404 mmol) according to the General Procedure C (0 °C, 30 h, eluent: hexanes/dichloromethane = 1:1) in 76% yield (90.7 mg, 96% ee).

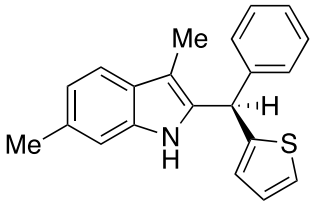
$[\alpha]_D^{26}$: –15.0 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 12.6 min (major), 15.1 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.50 (s, 1H), 7.37– 7.31 (m, 5H), 7.27 – 7.22 (m, 2H), 7.01 – 6.96 (m, 2H), 6.82 – 6.81 (m, 1H), 6.75 – 6.72 (m, 1H), 6.03 (s, 1H), 3.80 (s, 3H), 2.22 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 154.7, 147.1, 143.4, 137.2, 131.9, 130.4, 129.3, 129.3, 127.7, 127.5, 127.0, 125.6, 112.5, 112.0, 107.7, 100.9, 55.9, 44.8, 8.9.

IR (thin film) 3448, 3052, 2926, 1590, 1482, 1449, 1264, 1215, 1174, 1100, 1030, 735, 703 cm^{-1}.

HRMS (ES-) calcd for $C_{21}H_{18}NOS^-$ [M–H]$^-$: 332.1115, found: 332.1110.



3c

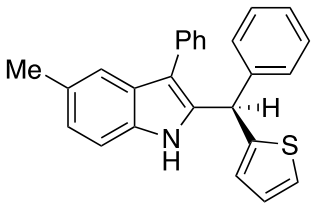
(*R*)-3,5-Dimethyl-2-(phenyl(thiophen-2-yl)methyl)-1*H*-indole (3c) was prepared as white foam from (3,5-dimethyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol (116.6 mg, 0.349 mmol) **1c** and **2a** (101.1 mg, 0.384 mmol) according to the General Procedure C (0°C, 30 h, eluent: hexanes/dichloromethane = 1:1) in 73% yield (80.0 mg, 94% ee). $[\alpha]_D^{26}$: –18.1 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 3% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 13.7 min (major), 17.1 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.52 (s, 1H), 7.37 – 7.30 (m, 6H), 7.26 – 7.23 (m, 1H), 7.11 (s, 1H), 6.98 – 6.95 (m, 1H), 6.86 – 6.84 (m, 1H), 6.80 – 6.79 (m, 1H), 6.02 (s, 1H), 2.37 (s, 3H), 2.21 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.2, 143.5, 137.3, 135.7, 131.2, 129.3 (2C), 128.0, 127.6, 127.5, 127.0, 125.5, 121.1, 118.7, 111.8, 107.6, 44.7, 21.8, 8.8

IR (thin film) 3449, 3033, 2922, 2860, 1455, 1332, 1264, 1226, 850, 804, 734, 701 cm^{-1}.

HRMS (ES-) calcd for $C_{21}H_{18}NS^-$ $[M–H]^-$: 316.1165, found: 316.1166.



3d

(*R*)-5-Methyl-3-phenyl-2-(phenyl(thiophen-2-yl)methyl)-1*H*-indole (3d) was prepared as bright orange foam from (5-methyl-3-phenyl-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol **1d** (158.2 mg, 0.400 mmol) and **2a** (115.9 mg, 0.440 mmol) according to the General Procedure C (0 °C, 30 h, eluent: hexanes/dichloromethane = 1:1) in 82% yield (123.6 mg, 92% ee).

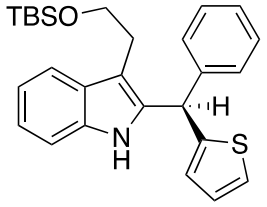
$[\alpha]_D^{26}$: +5.5 (c = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 3% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 9.4 min (major), 11.7 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.03 (s, 1H), 7.52 – 7.50 (m, 2H), 7.47 – 7.43 (m, 3H), 7.33 – 7.30 (m, 7H), 7.26 – 7.23 (m, 1H), 7.00 – 6.95 (m, 2H), 6.84 – 6.83 (m, 1H), 6.06 (s, 1H), 2.39 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.1, 143.5, 136.7, 136.2, 135.6, 130.4, 129.4, 129.4 (2C), 129.2, 128.5, 127.8, 127.6, 127.3, 127.0, 125.7, 124.2, 119.3, 115.2, 112.0, 44.5, 21.7.

IR (thin film) 3439, 3058, 3028, 2923, 2858, 1601, 1486, 1443, 1303, 1230, 738, 701 cm^{-1}.

HRMS (ES-) calcd for $C_{26}H_{20}NS^-$ $[M–H]^–$: 378.1322, found: 378.1317.



3e

(*R*)-3-(2-((*Tert*-butyldimethylsilyl)oxy)ethyl)-2-(phenyl(thiophen-2-yl)methyl)-1*H*-indole (3e) was prepared as yellow oil from (3-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)-1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol **1e** (123.0 mg, 0.265 mmol) and **2a** (76.2 mg, 0.289 mmol) according to the General Procedure C (0 ^oC, 72 h, eluent: hexanes/dichloromethane = 1:1) in 70% yield (79.5 mg, 90% ee).

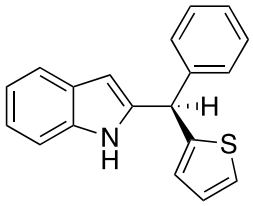
$[\alpha]_D^{26}$: –5.5 (c = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALCEL OD-H column; 2% *i*-PrOH in hexanes; 0.5 mL/min; retention times: 13.0 min (major), 14.3 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.76 (s, 1H), 7.57 – 7.55 (m, 1H), 7.38 – 7.31 (m, 6H), 7.28 – 7.24 (m, 1H), 7.07 – 6.96 (m, 3H), 6.83 – 6.81 (m, 1H), 6.12 (s, 1H), 3.77 – 3.67 (m, 2H), 3.05 – 3.01 (m, 2H), 0.88 (s, 9H), 0.00 (s. 6H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.0, 143.6, 137.2, 137.0, 129.5, 129.3, 129.3, 127.8, 127.5, 127.2, 125.6, 121.9, 119.6, 119.2, 112.0, 109.4, 64.5, 44.4, 29.0, 26.4, 18.9, -5.1.

IR (thin film) 3447, 3056, 2936, 2859, 1600, 1457, 1342, 1259, 1087, 837, 735, 701 cm^{-1}.

HRMS (ES+) calcd for $C_{27}H_{33}NONaSSi^+$ $[M+Na]^+$: 470.1944, found: 470.1949.



3f

(*R*)-2-(Phenyl(thiophen-2-yl)methyl)-1*H*-indole (3f) was prepared as white foam from (1*H*-indol-2-yl)(phenyl)(thiophen-2-yl)methanol **1f** (152.7 mg, 0.500 mmol) and **2a** (145.2 mg, 0.550 mmol) according to the General Procedure C (0 °C, 36 h, eluent: hexanes/ethyl acetate = 20:1) in 78% yield (112.0 mg, 89% ee).

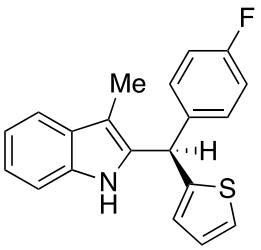
$[\alpha]_D^{26}$: –22.6 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 3% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 22.8 min (major), 24.6 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.13 (s, 1H), 7.50 – 7.48 (m, 1H), 7.38 – 7.33 (m, 6H), 7.29 – 7.25 (m, 1H), 7.08 – 7.04 (m, 1H), 7.01 – 6.97 (m, 2H), 6.89 – 6.88 (m, 1H), 6.182 – 6.178 (m, 1H), 5.93 (s, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.2, 143.7, 142.0, 137.8, 129.3, 129.3, 129.1, 127.8, 127.4, 126.9, 125.5, 122.0, 120.8, 120.0, 111.8, 102.1, 46.9.

IR (thin film) 3402, 3054, 2924, 2857, 1593, 1542, 1493, 1453, 1342, 1112, 737, 700 cm^{-1}.

HRMS (ES-) calcd for $C_{19}H_{14}NS^-$ $[M–H]^-$: 288.0852, found: 288.0851.



3g

(*R*)-2-((4-Fluorophenyl)(thiophen-2-yl)methyl)-3-methyl-1*H*-indole (3g) was

prepared as white foam from (4-fluorophenyl)(3-methyl-1*H*-indol-2-yl)(thiophen-2-yl)methanol **1g** (134.2 mg, 0.398 mmol) and **2a** (115.0 mg, 0.438 mmol) according to the General Procedure C (0°C, 48 h, eluent: hexanes/dichloromethane = 3:2) in 90% yield (112.4 mg, 89% ee).

$[\alpha]_D^{26}$: –19.6 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 3% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 12.5 min (major), 13.8 min (minor).

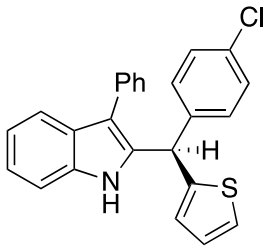
^{1}H NMR (400 MHz, acetone-d_6) δ 9.71 (s, 1H), 7.52– 7.50 (m, 1H), 7.40 – 7.31 (m, 4H), 7.13 – 6.97 (m, 5H), 6.83 – 6.82 (m, 1H), 6.09 (s, 1H), 2.25 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 162.6 (d, *J* = 242 Hz), 146.9, 139.51 (d, *J* = 3 Hz), 136.9, 136.2, 131.1 (d, *J* = 8 Hz), 130.0, 127.6, 127.1, 125.7, 122.0, 119.5, 119.0, 115.9 (d, *J* = 22 Hz), 111.8, 108.0, 43.9, 8.8.

^{19}F NMR (376 MHz, acetone-d_6) δ -117.3.

IR (thin film) 3449, 3054, 2923, 2858, 1602, 1505, 1457, 1308, 1264, 1225, 1157, 1100, 1014, 736, 700 cm^{-1}.

HRMS (ES-) calcd for $C_{20}H_{15}FNS^-$ $[M–H]^-$: 320.0915, found: 320.0910.



3h

(*R*)-2-((4-Chlorophenyl)(thiophen-2-yl)methyl)-3-phenyl-1*H*-indole (3h) was prepared as white foam from (4-chlorophenyl)(3-phenyl-1*H*-indol-2-yl)(thiophen-2-yl)methanol **1h** (141.1 mg, 0.339 mmol) and **2a** (98.3 mg, 0.373 mmol) according to the General Procedure C (–20°C, 48 h, eluent: hexanes/dichloromethane = 3:2) in 85% yield (115.4 mg, 93% ee).

$[\alpha]_D^{26}$: +15.1 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 5% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 8.2 min (major), 7.5

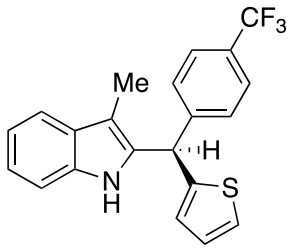
min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 10.20 (s, 1H), 7.60 – 7.58 (m, 1H), 7.49 – 7.40 (m, 5H), 7.38 – 7.29 (m, 6H), 7.16 – 7.12 (m, 1H), 7.08 – 7.05 (m, 1H), 7.00 – 6.98 (m, 1H), 6.86 – 6.85 (m, 1H), 6.07 (s, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.4, 142.3, 137.3, 136.1, 135.8, 133.2, 131.0, 130.4, 129.5, 129.4, 128.2, 127.8, 127.5, 127.2, 126.0, 122.8, 120.6, 119.7, 115.9, 112.3, 43.9.

IR (thin film) 3437, 3053, 2925, 2855, 1603, 1489, 1448, 1323, 1180, 1090, 1030, 736, 700 cm^{-1}.

HRMS (ES-) calcd for $C_{25}H_{17}ClNS^-$ [M–H]$^-$: 398.0776, found: 398.0772.



3i

(*R*)-3-Methyl-2-(thiophen-2-yl(4-(trifluoromethyl)phenyl)methyl)-1*H*-indole (3i) was prepared as pale blue foam from (3-methyl-1*H*-indol-2-yl)(thiophen-2-yl)(4-(trifluoromethyl)phenyl)methanol **1i** (68 mg, 0.175 mmol) and **2a** (50.7 mg, 0.193 mmol) according to the General Procedure C (0^{o}C, 72 h, eluent: hexanes/dichloromethane = 3:2) in 48% yield (31.0 mg, 91% ee).

$[\alpha]_D^{26}$: –23.7 (c = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALCEL OD-H column; 3% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 12.6 min (major), 14.5 min (minor).

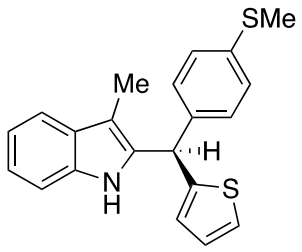
^{1}H NMR (400 MHz, acetone-d_6) δ 9.79 (s, 1H), 7.71– 7.69 (m, 2H), 7.58 – 7.56 (m, 2H), 7.51 – 7.49 (m, 1H), 7.40 – 7.39 (m, 1H), 7.31 – 7.29 (m, 1H), 7.08 – 7.00 (m, 3H), 6.87 – 6.86 (m, 1H), 6.21 (s, 1H), 2.25 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 148.1, 145.9, 137.0, 135.5, 130.1, 130.0, 129.4 (q, J = 32 Hz), 127.7, 126.3 (q, J = 4 Hz), 125.4 (q, J = 269 Hz), 126.0, 124.0, 122.2, 119.6, 119.1, 111.9, 108.4, 44.4, 8.7.

^{19}F NMR (376 MHz, acetone-d_6) δ −62.8.

IR (thin film) 3448, 3055, 2924, 2860, 1673, 1618, 1458, 1418, 1322, 1264, 1164, 1119, 1066, 1017, 738, 703 cm^{-1}.

HRMS (ES-) calcd for $C_{21}H_{15}F_3NS^-$ [M–H]$^-$: 370.0883, found: 370.0880.



3j

(*R*)-3-Methyl-2-((4-(methylthio)phenyl)(thiophen-2-yl)methyl)-1*H*-indole (3j) was prepared as white foam from (3-methyl-1*H*-indol-2-yl)(4-(methylthio)phenyl)(thiophen-2-yl)methanol **1j** (146.2 mg, 0.400 mmol) and **2a** (115.9 mg, 0.440 mmol) according to the General Procedure C (−30^{o}C, 144 h, eluent: hexanes/ethyl acetate = 20:1) in 77% yield (107.1 mg, 88% ee).

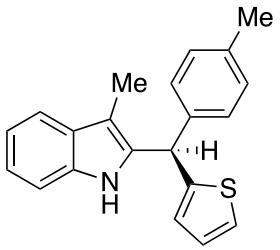
$[\alpha]_D^{26}$: –15.5 (c = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALCEL OD-H column; 10% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 8.5 min (major), 9.5 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.70 (s, 1H), 7.49 – 7.48 (m, 1H), 7.34 – 7.28 (m, 4H), 7.24 – 7.22 (m, 2H), 7.07 – 6.96 (m, 3H), 6.82 – 6.81 (m, 1H), 6.02 (s, 1H), 2.45 (s, 3H), 2.24 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.9, 140.1, 138.0, 136.9, 136.3, 130.0, 129.8, 127.5, 127.1, 127.0, 125.6, 121.9, 119.5, 118.9, 111.8, 107.8, 44.1, 15.4, 8.8.

IR (thin film) 3442, 3050, 2920, 2923, 2857, 1676, 1596, 1490, 1452, 1317, 1264, 1093, 962, 820, 735, 698 cm^{-1}.

HRMS (ES-) calcd for $C_{21}H_{18}NS_2^-$ [M–H]$^-$: 348.0886, found: 348.0878.



3k

(*R*)-3-Methyl-2-(thiophen-2-yl(*p*-tolyl)methyl)-1*H*-indole (3k) was prepared as white foam from (3-methyl-1*H*-indol-2-yl)(thiophen-2-yl)(*p*-tolyl)methanol **1k** (92.0 mg, 0.276 mmol) and **2a** (79.9 mg, 0.303 mmol) according to the General Procedure C (0 °C, 30 h, eluent: hexanes/dichloromethane = 3:2) in 89% yield (78.0 mg, 95% ee).

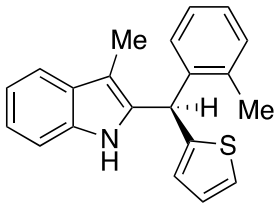
$[\alpha]_D^{26}$: –14.5 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 2% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 11.8 min (major), 10.8 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.64 (s, 1H), 7.51 – 7.49 (m, 1H), 7.33 – 7.31 (m, 2H), 7.27 – 7.25 (m, 2H), 7.16 – 7.14 (m, 2H), 7.08 – 7.00 (m, 2H), 6.97 – 6.95 (m, 1H), 6.82 – 6.81 (m, 1H), 6.02 (s, 1H), 2.31 (s, 3H), 2.25 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 147.3, 140.4, 137.1, 136.8, 136.6, 129.9, 129.2, 127.5, 127.3, 126.9, 125.5, 121.8, 119.4, 118.9, 111.8, 107.7, 44.3, 21.0, 8.8.

IR (thin film) 3449, 3051, 2924, 2862, 1510, 1601, 1458, 1335, 1104, 1033, 744, 704 cm^{-1}.

HRMS (ES-) calcd for $C_{21}H_{18}NS^-$ $[M–H]^-$: 316.1165, found: 316.1161.



3l

(*R*)-3-Methyl-2-(thiophen-2-yl(*o*-tolyl)methyl)-1*H*-indole (3l) was prepared as white foam from (3-methyl-1*H*-indol-2-yl)(thiophen-2-yl)(*o*-tolyl)methanol **1l** (133.4 mg, 0.400 mmol) and **2a** (115.9 mg, 0.440 mmol) according to the General Procedure C (–20 °C, 72 h, eluent: hexanes/dichloromethane = 3:2) in 83% yield (105.0 mg, 91% ee).

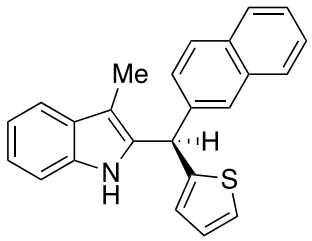
$[\alpha]_D^{26}$: –15.8 (c = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 1% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 10.1 min (major), 10.7 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.53 (s, 1H), 7.52 – 7.50 (m, 1H), 7.35 – 7.30 (m, 2H), 7.21 – 7.14 (m, 4H), 7.08 – 7.01 (m, 2H), 6.98 – 6.96 (m, 1H), 6.75 – 6.74 (m, 1H), 6.18 (s, 1H), 2.31 (s, 3H), 2.19 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.6, 141.7, 136.9, 136.7, 135.9, 131.2, 130.1, 128.9, 127.8, 127.5, 127.2, 126.9, 125.6, 121.8, 119.5, 118.8, 111.8, 107.8, 41.6, 19.5, 8.7.

IR (thin film) 3446, 3054, 2921, 2860, 1676, 1601, 1458, 1382, 1100, 1037, 737, 702 cm^{-1}.

HRMS (ES-) calcd for $C_{21}H_{18}NS^-$ $[M–H]^-$: 316.1165, found: 316.1166.



3m

(*R*)-3-Methyl-2-(naphthalen-2-yl(thiophen-2-yl)methyl)-1*H*-indole (3m) was prepared as white foam from (3-methyl-1*H*-indol-2-yl)(naphthalen-2-yl)(thiophen-2-yl)methanol **1m** (144.0 mg, 0.389 mmol) and **2a** (112.9 mg, 0.429 mmol) according to the General Procedure C (0 °C, 30 h, eluent: hexanes/dichloromethane = 3:2) in 76% yield (104.0 mg, 98% ee).

$[\alpha]_D^{26}$: –5.9 (c = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALCEL OD-H column; 3% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 14.8 min (major), 19.1 min (minor).

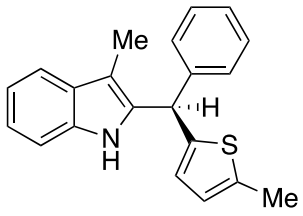
^{1}H NMR (400 MHz, acetone-d_6) δ 9.77 (s, 1H), 7.88 – 7.78 (m, 4H), 7.54 – 7.52 (m, 2H), 7.49 – 7.45 (m, 2H), 7.37 – 7.31 (m, 2H), 7.10 – 6.99 (m, 3H), 6.90 – 6.89 (m, 1H), 6.26 (s, 1H), 2.30 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.8, 141.0, 136.9, 136.3, 134.4, 133.4, 130.1, 129.0, 128.7, 128.4, 127.9, 127.61, 127.59, 127.2, 127.0, 126.7, 125.7, 121.9, 119.5, 119.0, 111.8,

108.0, 44.7, 8.8.

IR (thin film) 3445, 3053, 2922, 2858, 1457, 1310, 1264, 736, 703 cm^{-1}.

HRMS (ES-) calcd for $C_{24}H_{18}NS^-$ $[M–H]^-$: 352.1165, found: 352.1160.



3n

(*R*)-3-Methyl-2-((5-methylthiophen-2-yl)(phenyl)methyl)-1*H*-indole (3n) was prepared as yellow foam from (3-methyl-1*H*-indol-2-yl)(5-methylthiophen-2-yl)(phenyl)methanol **1n** (133.4 mg, 0.400 mmol) and **2a** (115.9 mg, 0.440 mmol) according to the General Procedure C (0 °C, 30 h, eluent: hexanes/dichloromethane = 3:2) in 82% yield (104.3 mg, 98% ee).

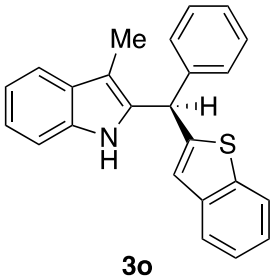
$[\alpha]_D^{26}$: –17.1 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 3% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 8.4 min (major), 8.9 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.70 (s, 1H), 7.49 – 7.48 (m, 1H), 7.34 – 7.28 (m, 4H), 7.24 – 7.22 (m, 2H), 7.07 – 6.96 (m, 3H), 6.82 – 6.81 (m, 1H), 6.02 (s, 1H), 2.45 (s, 3H), 2.24 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 146.9, 140.1, 138.0, 136.9, 136.3, 130.0, 129.8, 127.5, 127.1, 127.0, 125.6, 121.9, 119.5, 118.9, 111.8, 107.8, 44.1, 15.4, 8.8.

IR (thin film) 3447, 3054, 2922, 2862, 1676, 1599, 1455, 1330, 1264, 1163, 1032, 917, 802, 736 cm^{-1}.

HRMS (ES-) calcd for $C_{21}H_{18}NS^-$ $[M–H]^-$: 316.1165, found: 316.1159.



3o

(*R*)-2-(Benzo[*b*]thiophen-2-yl(phenyl)methyl)-3-methyl-1*H*-indole (3o) was prepared as white foam from benzo[*b*]thiophen-2-yl(3-methyl-1*H*-indol-2-yl)(phenyl)methanol **1o** (45.7 mg, 0.124 mmol) and **2a** (34.2 mg, 0.136 mmol) according to the General Procedure C (0 °C, 72 h, eluent: hexanes/dichloromethane = 1:1) in 63% yield (26.0 mg, 78% ee).

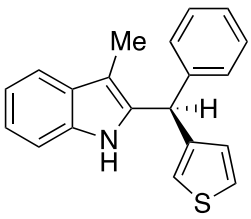
$[\alpha]_D^{26}$: –7.7 (*c* = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 3% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 17.1 min (major), 19.0 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.84 (s, 1H), 7.83 – 7.81 (m, 1H), 7.74 – 7.72 (m, 1H), 7.51 – 7.49 (m, 1H), 7.46 – 7.43 (m, 2H), 7.39 – 7.28 (m, 6H), 7.07 – 6.99 (m, 3H), 6.14 (s, 1H), 2.27 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 148.3, 142.7, 140.8, 140.8, 137.0, 135.8, 130.0, 129.5, 129.5, 128.0, 125.1, 124.9, 124.3, 123.9, 123.0, 122.0, 119.5, 119.0, 111.9, 108.2, 45.4, 8.8.

IR (thin film) 3443, 3056, 2921, 2860, 1595, 1456, 1380, 1183, 1077, 1017, 737, 667 cm^{-1}.

HRMS (ES-) calcd for $C_{24}H_{18}NS^-$ $[M–H]^-$: 352.1165, found: 352.1165.



3p

(*S*)-3-Methyl-2-(phenyl(thiophen-3-yl)methyl)-1*H*-indole (3p) was prepared as white foam from (3-methyl-1*H*-indol-2-yl)(phenyl)(thiophen-3-yl)methanol **1p** (132 mg, 0.41 mmol) and **2a** (119.2 mg, 0.45 mmol) according to the General Procedure C

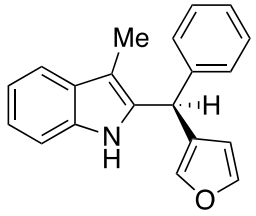
(0 °C, 41 h, eluent: hexanes/dichloromethane = 3:2) in 85% yield (107.0 mg, 92% ee). $[\alpha]_D^{26}$: +8.2 (c = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 3% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 11.5 min (major), 13.1 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.60 (s, 1H), 7.50 – 7.48 (m, 1H), 7.43 – 7.41 (m, 1H), 7.33 – 7.21 (m, 6H), 7.07 – 6.99 (m, 4H), 5.88 (s, 1H), 2.24 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 144.2, 143.6, 136.9, 136.7, 130.1, 129.34 (2C), 129.25, 127.4, 126.7, 123.4, 121.7, 119.4, 118.8, 111.7, 107.6, 45.1, 8.8.

IR (thin film) 3415, 3049, 2921, 2856, 1453, 1261, 1085, 1017, 794, 736, 701, 580 cm^{-1}.

HRMS (ES-) calcd for $C_{20}H_{16}NS^-$ $[M–H]^-$: 302.1009 found: 302.1011.



3q

(*S*)-2-(Furan-3-yl(phenyl)methyl)-3-methyl-1*H*-indole (3q) was prepared as yellow foam from furan-3-yl(3-methyl-1*H*-indol-2-yl)(phenyl)methanol **1q** (90.9 mg, 0.30 mmol) and **2a** (86.9 mg, 0.33 mmol) according to the General Procedure C (RT, 12 h, eluent: hexanes/dichloromethane = 3:2) in 44% yield (37.8 mg, 84% ee).

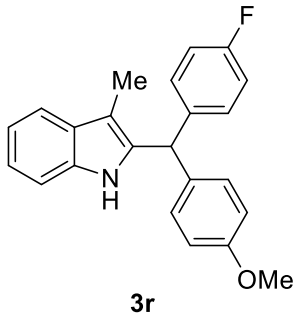
$[\alpha]_D^{26}$: –10.1 (c = 0.5, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 3% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 10.6 min (major), 12.0 min (minor).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.65 (s, 1H), 7.55 – 7.54 (m, 1H), 7.48 – 7.46 (m, 1H), 7.33 – 7.28 (m, 5H), 7.24 – 7.22 (m, 2H), 7.05 – 6.97 (m, 2H), 6.39 (m, 1H), 5.68 (s, 1H), 2.25 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 144.3, 143.3, 141.7, 136.8, 136.5, 130.1, 129.3, 129.1, 127.7, 127.4, 121.7, 119.4, 118.8, 112.1, 111.7, 107.3, 40.5, 8.7.

IR (thin film) 3332, 2976, 2930, 2864, 1455, 1381, 1120, 1074, 1028, 737, 563 cm^{-1}.

HRMS (ES-) calcd for $C_{20}H_{16}NO^-$ $[M–H]^-$: 286.1237 found: 286.1233.



3r

2-((4-Fluorophenyl)(4-methoxyphenyl)methyl)-3-methyl-1*H*-indole (3r) was prepared as light yellow foam from (4-fluorophenyl)(4-methoxyphenyl)(3-methyl-1*H*-indol-2-yl)methanol **1r** (65.2 mg, 0.180 mmol) and **2a** (49.7 mg, 0.189 mmol) according to the General Procedure C (0 °C, 30 h, eluent: hexanes/CH_2Cl_2 = 2:3) in 81% yield (50.3 mg, 44% ee).

$[\alpha]_D^{26}$: +7.3 (*c* = 1.0, CH_2Cl_2). HPLC analysis of the product: Daicel CHIRALPAK OD-H column; 12% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 8.48 min (minor), 8.96 min (major).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.50 (s, 1H), 7.48– 7.46 (m, 1H), 7.27 – 7.20 (m, 3H), 7.14 – 7.00 (m, 6H), 6.90 – 6.86 (m, 2H), 5.83 (s, 1H), 3.78 (s, 3H), 2.18 (s, 3H).

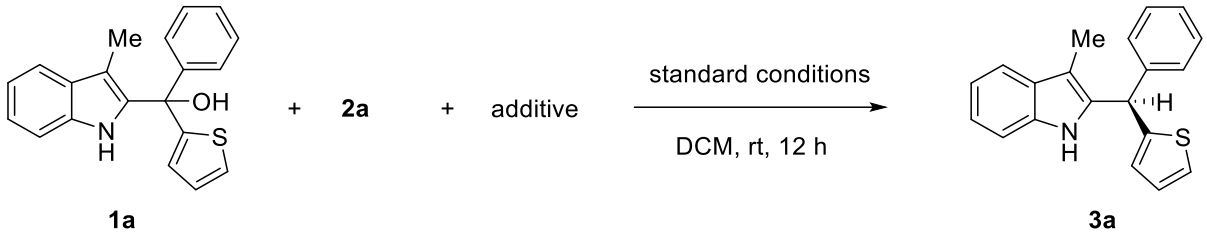
^{13}C NMR (100 MHz, acetone-d_6) δ 161.9 (d, *J* = 241 Hz), 158.9, 139.6 (d, *J* = 3 Hz), 136.5 (d, *J* = 7 Hz), 134.8, 131.1 (d, *J* = 8 Hz), 130.3, 129.7, 121.2, 119.0, 118.3, 115.5, 115.2, 114.3, 111.3, 107.3, 55.0, 47.3, 8.3.

^{19}F NMR (376 MHz, acetone-d_6) δ -118.4.

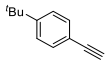
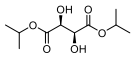
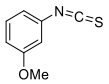
IR (thin film) 3453, 3052, 2924, 1605, 1506, 1254, 734 cm^{-1}.

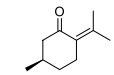
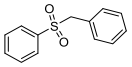
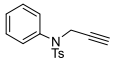
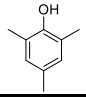
HRMS (ES-) calcd for $C_{23}H_{19}FNO^-$ $[M–H]^-$: 344.1456, found: 344.1455.

IV. Study on the Influence of Additives



At room temperature, to an oven-dried 4-mL vial were added the tertiary alcohol **1a** (25 μmol), the hydride source **2a** (7.3 mg, 27.5 μmol), the additive (25 μmol) and a solution of (*R*)-**C1** (0.94 mg, 1.25 μmol, 5.0 mol%) in DCM (0.5 mL). The mixture was stirred at room temperature for 12 h and then filtered through a silica gel pad and concentrated. The amount of each component (**1a**, **2a**, **3a**, and the additive) remaining in the mixture was determined by analysis of the ^{1}H NMR spectrum of this crude mixture with CH_2Br_2 as the internal standard. The ee value of **3a** was determined by HPLC analysis on a chiral stationary phase.

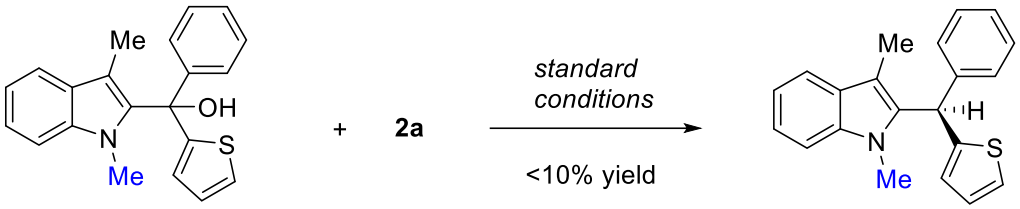
Entry	Additive	Additive recovery	Conversion **1a** (%)	Yield[a] **3a** (%)	Ee [a] **3a** (%)
1		90	100	95	91
2		82	70	49	94
3		95	100	88	96
4		85	100	99	94
5		95	100	87	94
6	Ph_3CSH	66	100	83	89
7		61	100	77	87
8		67	100	73	94
9		78	100	64	90
10		83	100	75	94
11	PPh_3	80	100	95	94

12		67	100	57	94
13		89	100	98	94
14		90	100	92	95
15		87	100	80	94

[a] Reaction scale: **1a** (25 μmol, **2a** (27.5 μmol), additive (25 μmol), (*R*)-**C1** (5 mol%), DCM (0.5 mL). Yield was determined by analysis of the ^{1}H NMR spectrum of the crude reaction mixture with CH_2Br_2 as internal standard. Ee was determined by HPLC analysis on a chiral stationary phase.

V. Mechanistic Experiments

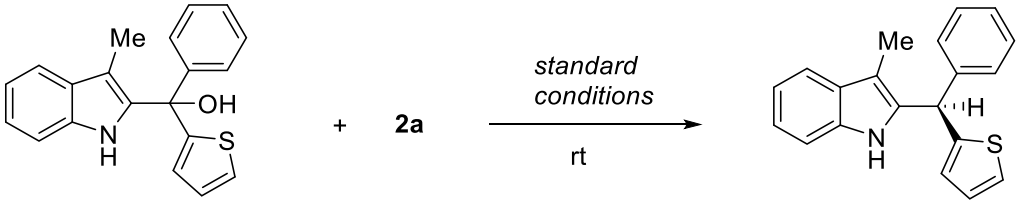
(1) Control experiment.



1a′ **3a′**

At room temperature, to an oven-dried 4-mL vial were added tertiary alcohol **1a′** (8.0 mg, 25 μmol) and **2a** (7.3 mg, 0.0275 mmol). A solution of the catalyst (*R*)-**C1** (0.94 mg, 1.25 μmol, 5.0 mol%) in DCM (0.5 mL) was added. The reaction mixture was stirred for 12 h at room temperature or for 48 h at 0 °C. After that, the reaction mixture was filtered through a short pad of silica gel and then concentrated. The crude mixture was examined by ^{1}H NMR and the ee value of the product was determined by HPLC. Reactions at both temperatures gave a messy mixture of essentially unidentifiable mixture. By comparison with the standard ^{1}H NMR spectra of **1a** and **3a′**, the reaction at room temperature showed 87% conversion and **3a′** was formed in only 9% yield. The reaction at 0 °C showed 70% conversion and **3a′** was formed in only 7% yield.

(2) Non-linear effects.



1a **3a**

At room temperature, to an oven-dried 4-mL vial were added tertiary alcohol **1a** (8.0 mg, 25 μmol) and **2a** (7.3 mg, 27.5 μmol). A solution of catalyst (*R*)-**C1** (0.94 mg, 5 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 DCM (0.5 mL) was added. The reaction mixture was stirred at room temperature 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% (**C1**)	0	20	40	60	80	100
ee% (**3a**)	– 4	16	35	55	75	96

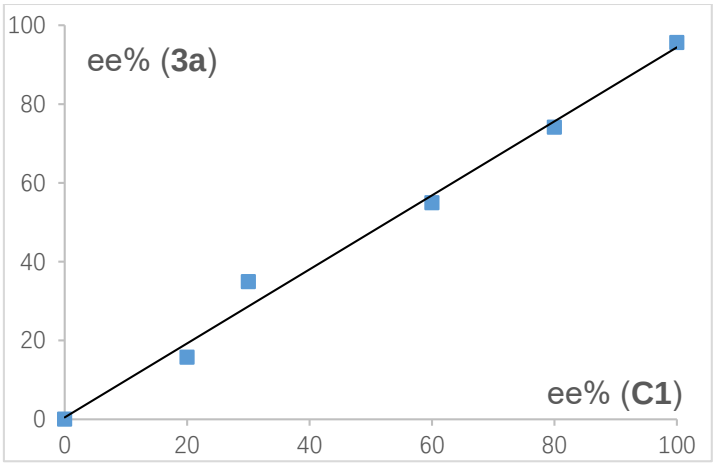
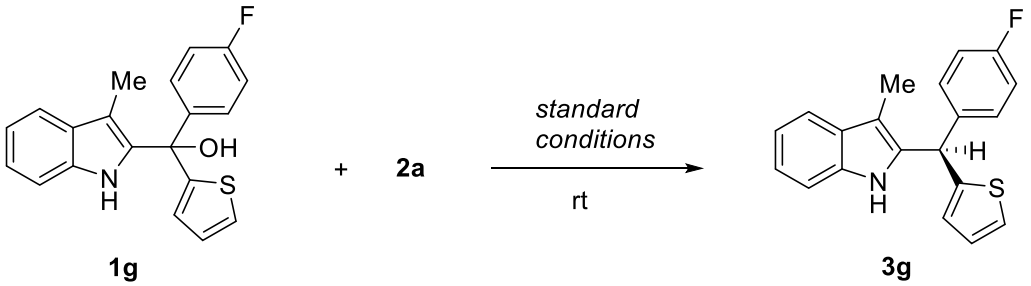


Figure S1. Linear relationship between the ee values of product 3a and catalyst C1.

(3) Kinetic study.



The reaction between substrate **1g** and reductant **2a** was used for kinetic study. To assess the order in species **X** (**X** = **2a** or catalyst **C1**), reactions of varying [**X**] were set up. For each reaction, to an oven-dried 4-mL vial were added **1g**, **2a**, and a solution of catalyst (*R*)-**C1** in DCM in the amounts illustrated in the tables below. The reaction mixture was quickly transferred into a 5-mm NMR tube, and the reaction progress was monitored by taking ^{19}F NMR spectra every 50 seconds. The yield of **3g** was determined by analysis of ^{19}F NMR spectra. A graph of [**3g**] vs. time was plotted for the three reactions with different [**X**]. A linear relationship within the first 10%

conversion was fitted to determine the initial rate.

(a) Reaction order in nucleophile 2a.

To an oven-dried 4-mL vial was added **1g** (8.4 mg, 25 μmol) and **2a** of different equivalents (1st run: 6.6 mg, 25 μmol, 1 equiv; 2nd run: 13.2 mg, 50 μmol, 2 equiv; 3rd run: 19.8 mg, 75 μmol, 3 equiv; 3rd run: 26.3 mg, 100 μmol, 4 equiv). A solution of (*R*)-**C1** (0.94 mg, 1.25 μmol, 5 mol%) in DCM (0.5 mL) was quickly added. The mixture was immediately transferred to a 5-mm NMR tube and the data were taken and analyzed according to the general procedure outlined above.

[**2a**] (M)	Initial rate (M/s)
0.050	2.32E-05
0.100	1.72E-05
0.150	2.22E-05
0.200	2.52E-05

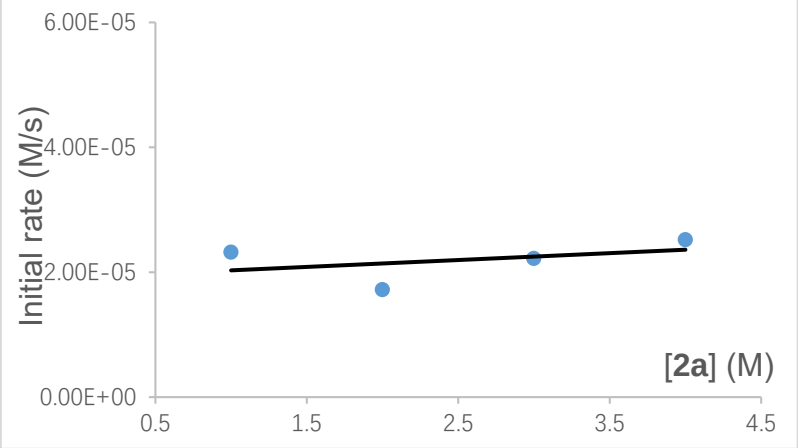


Figure S2. Original data and plot of initial rate vs [2a].

(b) Reaction order in catalyst C1.

To an oven-dried 4-mL vial were added **1g** (8.4 mg, 25 μmol) and **2a** (7.3 mg, 27.5 μmol, 1.1 equiv). A solution of catalyst (*R*)-**C1** of different loadings (1st run: 2 mol%; 2nd run: 4 mol%; 3rd run: 6 mol%) in DCM (0.5 mL) was quickly added. The mixture was

immediately transferred to a 5-mm NMR tube and the data were taken and analyzed according to the general procedure outlined above.

[(*R*)-**C1**] (M)	Initial rate (M/s)
0.001	2.38E-06
0.002	4.84E-06
0.003	7.55E-06

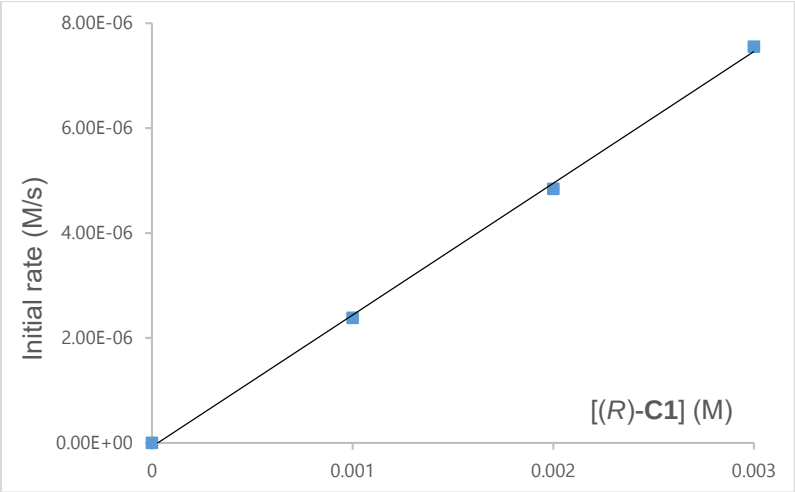


Figure S3. Original data and plot of initial rate vs [C1].

VI. Study of the Product Biological Activities

(1) Study of the Anticancer Activities

(a) Cell lines and cell culture

HeLa (ATCC® CCL-2™), MCF-7 (ATCC® HTB-22™), and A549 (ATCC® CCL-185™) cells were cultured in DMEM with 10% FBS and 50 U/mL penicillin and streptomycin. A2780 (ATCC) cells were cultured in RPMI 1640 with 10% FBS, 2 mM L-glutamine, and 50 U/mL penicillin and streptomycin. MRC-5 cells (human lung fibroblasts, ATCC® CCL-171) were maintained in MEM with 10% FBS, 1% L-glutamine, 1% NEAA, and 1% sodium pyruvate. HCT116 cells (ATCC® CCL-247™) were cultured in McCoy's 5A medium with 10% FBS and 50 U/mL penicillin and streptomycin.

(b) Cell viability test

Cancer cells (1.5×10^3 cells/well) or normal cells (2.5×10^3 cells/well) were cultured in 96-well plates for 48 h. Then, the culture medium was removed, and 200 μL fresh medium containing various concentrations of compounds was added into each well to incubate at 37 °C for 72 h. After incubation, the culture medium was replaced with serum-free medium containing 1 mg/mL MTT to incubate at 37 °C for 2 h. Subsequently, the medium was aspirated, and 150 μL DMSO was added to each well. The 96-well plates were placed on a shaker at 60 rpm for 15 min, then the absorption of 570 nm and 700 nm were measured by a microplate reader. The CC_{50} values were calculated by Origin 2019.

Study of the Antiviral Activities

(a) Viruses and cells[3]

Rhabdomyosarcoma (RD) cells (ATCC number CCL-136) and Vero E6 cells (ATCC number CRL-1586) were maintained in Dulbecco's modified Eagle's medium (DMEM) containing 10% fetal bovine serum (FBS) with 100 U/mL penicillin and 100 μg/mL streptomycin in a humidified 5% CO_2 incubator at 37 °C. RD cells were infected with EV-A71 (SHZH98 strain) at a MOI of 0.01. To test the antiviral effects, cells were incubated in DMEM with 2% FBS and different concentrations of chemicals for 2 h. Then viruses were added to the cells. Samples were collected at 48 h after infection.

(b) MTT assay

RD cells were seeded in 96-plates at 10,000 cells/well in DMEM with 2% FBS. The media were replaced with 100 μL/well of media containing various concentrations of chemicals after cells were attached. 48 h later, an MTT assay were performed as described.[3] The culture media were replaced with 100 μL/well containing MTT (5 mg/ml) in the serum-free DMEM. Then, cells were incubated for 4 h at 37 °C. Next, the medium was replaced with 100 μL/well of dimethyl sulfoxide. The absorbance was read at 590 nm with a microplate reader (BioTek SynergyTM).

(c) Cytopathic effects (CPE) assay[4,5]

RD cells were seeded in 24-well plates and incubated with 10%-FBS DMEM in the incubator for 24 h. After the culture media were removed, cells were infected with nil (mock) or EV-A71 at MOI of 0.01 and incubated in DMEM with 2% FBS for 36 h. The images of cell morphology were captured and recorded by a phase-contrast

3 J. Lu, L. Yi, J. Zhao, Y. Chen, M.C. Lin, H.-F. Kung and M.-L. He, *J. Virol.* 2012, **86**, 3767–3776.

4 Q. Dong, R. Men, X. Dan, Y. Chen, H. Li, G. Chen, B. Zee, M.H.T. Wang and M.-L.He, *Antiviral Res.* 2018, **150**, 39–46.

5 X. Dan, Q. Wan, L. Yi, J. Lu, Y. Jiao, H. Li, D. Song, Y. Chen, H. Xu and M.-L. He, *J. Virol.* 2019, **93**, e02322–18.

microscope associated with a CCD camera and computer.

(d) Viral RNA isolation, reverse transcription and quantitative real-time PCR[4,5]

To determine the EV-A71 viral RNA, the intracellular RNA were isolated with the TRIzol reagent (Ambion, Life Technologies) according to the manufacturer's protocol. Then, 2 μg of total RNA was used to synthesize cDNA by reverse transcription with PrimeScript RT reagent Kit (Takara). Viral DNA and cDNA are quantified by Real-time quantitative PCR (RT-qPCR) using SYBR Green Master Mix (Applied Biosystems, USA) on an applied Biosystems QuantStudio 3 real-time PCR system. The primers are as follows:

EV-71	Forward	5′-GCAGCCCAAAAGAACTTCAC-3′
	Reverse	5′-ATTTCAGCAGCTTGGAGTGC-3′
	Reverse	5′-GGCAAATCTGCCCAAGAATA-3′
GAPDH	Forward	5′-TGTGGGCATCAATGGATTTGG-3′
	Reverse	5′-ACACCATGTATTCCGGGTCAAT-3′

(e) Virus titration

To evaluate the extracellular virions, virus titers were determined by $TCID_{50}$ assay as reported previously.[6] Cells were cultured in 96-well plates for 24 h, then infected with 100 μL per well of serial 10-fold diluted supernatant. The 50% tissue culture-infected dose ($TCID_{50}$) was calculated by the Spearman-Karber method after 96 h of infection. The concentration required to reduce the cytopathic effect (CPE) by 50% (IC_{50}) was determined by using the linear regression analysis of GraphPad Prism 8.0. Data were shown as mean values with standard deviations from three independent assays. Selectivity index (SI) is calculated by the ratio of CC_{50} to IC_{50}.

6 F. Zhou, Q. Wan, J. Lu, Y. Chen., G. Lu and M.-L. He, *iScience* 2019, **19**, 715-727.

VII. DFT Studies

The rate-determining step of this reaction is the chiral phosphoric acid-catalyzed dehydration of tertiary alcohols **1a** to obtain the indolyl cation **IM**. However, the stereo-determining step for this reaction is the nucleophilic addition of the hydride **2a** on the indolyl cation **IM**. To evaluate the origins of stereoselectivity, density functional theory (DFT) calculations were performed. We first explored the stereo-determining transition structures. Geometry optimizations were conducted at B3LYP-D3(BJ) functional with the def2svp basis set in the Gaussian 16 package.[7] Single-point energies and solvent effects in dichloromethane were calculated with the CPCM solvation model at the M06-2X/def2tzvpp level of theory.[8] Conformational searches were conducted using the CREST conformer-rotamer ensemble sampling tool version 2.10.2 with xtb version 6.3.3.[9] Based on the results of conformational searches, the lowest energy conformers are depicted in Figure 2. The computed transition state **TS-*R*** delivering the preferred *R*-product is 3.6 kcal/mol lower than that of **TS-*S*** generating the *S*-product, in good accord with the 96% *ee* observed experimentally.

7 (a) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.* 2010, **132**, 154104; (b) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.* 2011, **32**, 1456-1465; (c) M. J. Frisch, et al. *Gaussian 16*, revision A.03, Gaussian, Inc., 2016.

8 (a) Y. Zhao and D. G. Truhlar, *Acc. Chem. Res.* 2008, **41**, 157-167; (b) Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.* 2008, **120**, 215-241; (c) M. Cossi, N. Rega, G. Scalmani and V. Barone, *J. Comput. Chem.* 2003, **24**, 669-681; (d) V. Barone and M. Cossi, *J. Phys. Chem.* 1998, **102**, 1995-2001.

9 (a) S. Grimme, C. Bannwarth, S. Dohm, A. Hansen, J. Pisarek, P. Pracht, J. Seibert and F. Neese, *Angew. Chem. Int. Ed.* 2017, **56**, 14763-14769; (b) S. Grimme, *J. Chem. Theory Comput.* 2019, **15**, 2847-2862; (c) S. Grimme, C. Bannwarth, P. Shushkov, *J. Chem. Theory Comput*. 2017, **13**,1989-2009; (d) C. Bannwarth, S. Ehlert, S. Grimme, *J. Chem. Theory Comput*. 2019, **15**, 1652-1671; (e) P. Pracht, E. Caldeweyher, S. Ehlert, S. Grimme, *ChemRxiv*, 2019, preprint. DOI:10.26434/chem-rxiv.8326202.v1.

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]
TS-*S*	-4949.506744	1.598913	1.394554	-4951.930591	-966.35
TS-*R*	-4949.511517	1.598817	1.394566	-4951.936287	-1224.67

[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 dichloromethane solvent. [5]The B3LYP-D3BJ calculated imaginary frequencies for the transition states.

B3LYP-D3BJ Geometries for All the Transition Stats

TS-*S*

C	-0.610023	-0.325775	2.954675
C	-0.893299	-1.398834	3.849397
C	-0.929470	-1.139986	5.239065
C	-0.677337	0.147953	5.683883
C	-0.393675	1.197492	4.771208
C	-0.354345	0.981325	3.401693
C	-0.927417	-2.179965	1.708011
C	-1.100976	-2.571770	3.059784
H	-0.696635	0.365045	6.754222
H	-0.199355	2.200226	5.157648
H	-0.141626	1.778341	2.692127
N	-0.652143	-0.815881	1.684697
H	-0.307087	-0.253331	0.888850
C	-1.528871	-3.880014	3.649150
H	-2.019959	-3.703724	4.617856
H	-0.678033	-4.556016	3.829995
H	-2.238766	-4.417579	3.008321
H	-1.144453	-1.941411	5.949304
C	-0.993357	-2.972597	0.486517
C	-1.517152	-2.434641	-0.799876
C	-1.943969	-1.103442	-0.970675
C	-1.479555	-3.269490	-1.942893
C	-2.263006	-0.608479	-2.233325
H	-2.045646	-0.439665	-0.119408
C	-1.821074	-2.781639	-3.196946
H	-1.129416	-4.295497	-1.848999
C	-2.190473	-1.440744	-3.349775
H	-2.530757	0.440913	-2.334205
H	-1.755607	-3.436743	-4.067648
H	-2.415975	-1.044130	-4.341240
C	-1.110732	-4.436991	0.681756
C	-0.185498	-5.303217	1.220168
S	-2.604428	-5.282443	0.320821
C	-0.665607	-6.638446	1.342773
H	0.800523	-4.974378	1.543511
C	-1.960831	-6.773882	0.905874
H	-0.076149	-7.464537	1.741937
H	-2.573097	-7.674404	0.889403
C	1.298936	-1.614511	-2.577909
C	1.605604	-2.927413	-2.999568
C	1.582372	-3.274053	-4.346554
C	1.244105	-2.283863	-5.278567
C	0.911944	-0.988516	-4.857836
C	0.921541	-0.635662	-3.507372
C	1.592425	-2.593675	-0.465826
H	1.228866	-2.531850	-6.341881
H	0.624875	-0.238057	-5.597102

H	0.623965	0.359824	-3.171372
N	1.401362	-1.447734	-1.220414
H	1.172585	-0.509928	-0.789044
H	1.821206	-4.289239	-4.668777
H	0.426310	-2.902901	0.015854
S	1.957984	-3.954620	-1.610920
C	2.339448	-2.537025	0.827750
C	2.336791	-1.377655	1.582035
C	2.945235	-3.712846	1.357152
C	2.868616	-1.361814	2.895794
H	1.916813	-0.453295	1.189531
C	3.488218	-3.717479	2.620934
H	3.000353	-4.615156	0.744979
C	3.446605	-2.554934	3.439347
C	2.825012	-0.186876	3.692509
H	3.962798	-4.621898	3.009353
C	3.961024	-2.527541	4.762148
C	3.322755	-0.194418	4.977302
H	2.382016	0.715606	3.275116
C	3.896496	-1.373055	5.515979
H	4.405391	-3.436543	5.175474
H	3.270714	0.711861	5.584619
H	4.289348	-1.365110	6.535525
P	-0.091275	2.010661	-0.666383
O	0.597072	0.767247	-0.099251
H	-1.234164	7.867840	0.241099
H	-1.706650	7.524643	1.911526
H	-3.845704	6.797268	-0.340376
C	-1.275366	7.071732	1.000874
C	-3.329904	5.865559	-0.094989
H	0.693599	6.987912	2.035669
C	0.101319	6.441894	1.286857
C	-2.096033	5.884084	0.551503
H	0.690900	6.396070	0.358181
C	-3.915941	4.635020	-0.401245
H	-4.912656	4.602743	-0.846253
H	-1.230253	5.803177	3.538606
H	1.144661	5.903201	4.181938
C	-1.431821	4.685032	0.858933
C	-0.218878	4.980762	1.731277
C	-0.601104	4.949798	3.247711
C	0.747437	4.890163	3.992156
C	-3.259292	3.418815	-0.143776
C	-1.974375	3.470235	0.436480
C	1.031322	4.119058	1.746620
C	1.628433	4.144295	3.016585
H	-1.176064	4.031230	3.442872
O	0.936782	3.293926	-0.479744
H	0.679260	4.391607	4.971969
C	1.628545	3.410073	0.708177
C	-4.065574	1.185606	0.638915
C	-3.959961	2.132606	-0.390890
C	2.854751	3.517118	3.224733
O	-1.218915	2.316137	0.529466
C	3.481455	2.494385	-1.532338
C	2.878079	2.769998	0.884822
H	3.333234	3.534639	4.207227
C	3.474633	2.861998	2.156584
C	-4.820560	0.018560	0.502010
C	-4.671596	1.907798	-1.567923
C	4.139870	1.864769	-2.597291
C	3.548538	2.033378	-0.216246
H	4.447483	2.392824	2.311224
C	-5.439999	-0.219340	-0.755588
C	-5.452844	0.758167	-1.776582
C	4.825681	0.661185	-2.308880
C	4.341619	0.906155	0.042193
C	5.002278	0.207565	-0.973421
O	-0.645262	2.057694	-2.046088
H	-4.608946	2.663373	-2.349404
H	-3.558543	1.398452	1.576099
H	2.908448	3.394898	-1.728274
H	4.432978	0.563954	1.068913
O	5.393181	-0.082717	-3.321298
O	-6.074271	-1.430620	-0.936139
C	4.496010	-0.893845	-4.060697

H	5.094357	-1.435675	-4.806636
H	3.982277	-1.620497	-3.414767
H	3.730014	-0.299633	-4.578888
C	-5.336492	-2.398558	-1.665252
H	-5.924819	-3.326925	-1.648743
H	-5.178694	-2.093870	-2.711321
H	-4.350997	-2.585518	-1.214385
C	-5.076023	-0.890611	1.728495
C	-4.363088	-0.349009	2.981040
C	-6.594420	-0.898425	2.013572
C	-4.591096	-2.340786	1.527721
H	-4.698850	0.665140	3.242924
H	-4.586219	-1.003026	3.837372
H	-3.271587	-0.329000	2.861830
H	-6.809686	-1.519269	2.899024
H	-6.956276	0.121645	2.217104
H	-7.153223	-1.304025	1.160128
H	-3.546983	-2.366690	1.193156
H	-4.640410	-2.882808	2.485537
H	-5.207734	-2.888362	0.808441
C	-6.272232	0.689075	-3.091211
C	-6.899369	2.078460	-3.366230
C	-5.339201	0.339646	-4.269406
C	-7.454680	-0.301531	-3.062586
H	-6.149535	2.858808	-3.552895
H	-7.538133	2.023887	-4.261346
H	-7.524012	2.401878	-2.519202
H	-4.895791	-0.658715	-4.148869
H	-5.898267	0.350615	-5.219472
H	-4.513169	1.063070	-4.350388
H	-8.078295	-0.158547	-2.168877
H	-8.082624	-0.123963	-3.950260
H	-7.143173	-1.350180	-3.088817
C	4.081778	2.588561	-3.968381
C	5.157708	2.148540	-4.981953
C	2.679845	2.406429	-4.587361
C	4.320114	4.103060	-3.742429
H	6.162506	2.162731	-4.536646
H	4.985955	1.148753	-5.392460
H	5.149124	2.852648	-5.829203
H	2.492067	1.354452	-4.841826
H	1.886342	2.725166	-3.893784
H	2.588941	2.999504	-5.512353
H	5.278835	4.278715	-3.230169
H	4.351255	4.618892	-4.714680
H	3.526255	4.577479	-3.150830
C	5.966401	-0.949934	-0.622731
C	7.380202	-0.595338	-1.134527
C	6.065203	-1.159538	0.899625
C	5.517242	-2.293752	-1.233872
H	7.383730	-0.453153	-2.222243
H	7.742095	0.330122	-0.659284
H	8.086510	-1.404240	-0.884070
H	6.797816	-1.954173	1.107322
H	6.404955	-0.252535	1.421566
H	5.108654	-1.471062	1.338402
H	4.459513	-2.496560	-1.016866
H	5.662438	-2.319976	-2.318667
H	6.108599	-3.116890	-0.801194

TS-*R*

C	-0.689780	-0.251970	3.001226
C	-0.968308	-1.320123	3.902401
C	-1.001633	-1.051404	5.289128
C	-0.751230	0.241232	5.725110
C	-0.470957	1.284954	4.806246
C	-0.434663	1.058313	3.437644
C	-0.999772	-2.116474	1.769927
C	-1.170486	-2.501754	3.117545
H	-0.769041	0.464594	6.794243
H	-0.277666	2.290913	5.185529
H	-0.223160	1.849360	2.720189
N	-0.731987	-0.751568	1.733511
H	-0.362196	-0.208050	0.937943
C	-1.575711	-3.817150	3.708714
H	-2.052846	-3.651719	4.686207

H	-0.713930	-4.484036	3.873098
H	-2.288047	-4.361763	3.076467
H	-1.212924	-1.847967	6.006088
C	-1.076877	-2.903035	0.539283
C	-1.263931	-4.384869	0.692403
C	-0.237966	-5.183658	1.217784
C	-2.485236	-4.991777	0.352801
C	-0.417542	-6.555616	1.387492
H	0.698347	-4.718791	1.521866
C	-2.669379	-6.363413	0.534313
H	-3.302668	-4.381684	-0.029134
C	-1.634953	-7.151340	1.046106
H	0.395284	-7.161114	1.795160
H	-3.629557	-6.816874	0.277930
H	-1.778994	-8.225604	1.182727
C	-1.606557	-2.301118	-0.683341
C	-1.931322	-0.980530	-0.970541
S	-1.662486	-3.264854	-2.162389
C	-2.178787	-0.738683	-2.341935
H	-2.020147	-0.205118	-0.218530
C	-2.055632	-1.877366	-3.104139
H	-2.396660	0.253653	-2.729164
H	-2.183669	-1.975384	-4.180616
C	1.262772	-1.662795	-2.528672
C	1.567819	-2.987265	-2.915758
C	1.559656	-3.364063	-4.255057
C	1.245960	-2.391878	-5.214224
C	0.918307	-1.084382	-4.828880
C	0.906684	-0.702627	-3.485826
C	1.524134	-2.595520	-0.392547
H	1.246716	-2.663655	-6.271883
H	0.652270	-0.347692	-5.589564
H	0.614392	0.302638	-3.175107
N	1.338841	-1.468655	-1.173363
H	1.127918	-0.517454	-0.759752
H	1.792483	-4.388669	-4.550318
H	0.328229	-2.874732	0.093142
S	1.883082	-3.985841	-1.500642
C	2.268611	-2.511314	0.901365
C	2.265495	-1.336704	1.632043
C	2.884524	-3.672383	1.452526
C	2.802222	-1.291482	2.943041
H	1.843073	-0.421058	1.222706
C	3.431413	-3.648704	2.714333
H	2.943563	-4.586919	0.859424
C	3.387005	-2.470359	3.509426
C	2.756838	-0.099842	3.714626
H	3.912272	-4.542751	3.118653
C	3.906239	-2.412974	4.829420
C	3.259541	-0.078130	4.997273
H	2.308272	0.791656	3.279781
C	3.839953	-1.242928	5.558666
H	4.355755	-3.311254	5.260266
H	3.205985	0.840549	5.585526
H	4.236509	-1.211728	6.576343
P	-0.081113	2.003837	-0.687445
O	0.596325	0.776383	-0.075600
H	-1.175999	7.902353	0.058764
H	-1.674239	7.596917	1.729139
H	-3.778852	6.831065	-0.553351
C	-1.232965	7.122604	0.834283
C	-3.275331	5.902688	-0.272408
H	0.721427	7.050059	1.897568
C	0.135873	6.490797	1.153248
C	-2.054908	5.930348	0.399382
H	0.737449	6.421381	0.233756
C	-3.863365	4.668217	-0.561030
H	-4.848906	4.629902	-1.030126
H	-1.211323	5.906984	3.411192
H	1.159560	5.995563	4.070040
C	-1.405055	4.735600	0.750203
C	-0.198159	5.041240	1.625803
C	-0.588918	5.042147	3.140033
C	0.754787	4.983110	3.893497
C	-3.221290	3.456239	-0.254445
C	-1.951061	3.514689	0.353975

C	1.044669	4.168971	1.663538
C	1.635375	4.213618	2.936007
H	-1.173898	4.132999	3.349213
O	0.951104	3.287834	-0.544396
H	0.675894	4.499744	4.880075
C	1.640890	3.432546	0.643519
C	-4.080170	1.272046	0.592866
C	-3.919006	2.164157	-0.476946
C	2.855250	3.580472	3.163303
O	-1.208647	2.357151	0.495083
C	3.498810	2.454530	-1.567102
C	2.883829	2.786156	0.839754
H	3.327864	3.612542	4.148253
C	3.475390	2.899112	2.111983
C	-4.835813	0.102943	0.479768
C	-4.567979	1.881778	-1.676866
C	4.153914	1.793931	-2.615210
C	3.550784	2.018560	-0.241908
H	4.442696	2.423567	2.281264
C	-5.403691	-0.190327	-0.790489
C	-5.351542	0.729615	-1.863083
C	4.821037	0.586937	-2.298225
C	4.324404	0.884762	0.044157
C	4.982066	0.157202	-0.952916
O	-0.640393	1.997220	-2.066573
H	-4.456892	2.595471	-2.491396
H	-3.615436	1.529661	1.540661
H	2.940256	3.359312	-1.784156
H	4.401749	0.560836	1.077935
O	5.385607	-0.184599	-3.291484
O	-6.054820	-1.399138	-0.932363
C	4.483949	-1.000179	-4.020216
H	5.082783	-1.576328	-4.739596
H	3.945538	-1.696517	-3.361194
H	3.738608	-0.407188	-4.569135
C	-5.308639	-2.417420	-1.574862
H	-5.864833	-3.356954	-1.444559
H	-5.187950	-2.224401	-2.652378
H	-4.306130	-2.521964	-1.136266
C	-5.143101	-0.745358	1.737681
C	-4.464147	-0.155728	2.987959
C	-6.669857	-0.725999	1.971783
C	-4.664341	-2.206705	1.619389
H	-4.796510	0.872194	3.194473
H	-4.723107	-0.768898	3.864164
H	-3.368750	-0.153225	2.903378
H	-6.921458	-1.305272	2.875611
H	-7.026621	0.305514	2.118702
H	-7.205130	-1.162468	1.118389
H	-3.609287	-2.252478	1.323388
H	-4.751990	-2.703925	2.598496
H	-5.263576	-2.780369	0.905179
C	-6.107504	0.595100	-3.210787
C	-6.669470	1.979937	-3.617513
C	-5.132905	0.132575	-4.314420
C	-7.327128	-0.349432	-3.168448
H	-5.883652	2.717800	-3.827250
H	-7.269074	1.878398	-4.535232
H	-7.318939	2.388363	-2.827866
H	-4.711211	-0.858084	-4.093742
H	-5.651516	0.074838	-5.285494
H	-4.291916	0.835373	-4.418771
H	-7.983351	-0.119172	-2.317130
H	-7.908470	-0.214749	-4.094477
H	-7.057081	-1.407746	-3.104592
C	4.111688	2.488133	-4.001972
C	5.192622	2.018089	-4.996660
C	2.713009	2.301930	-4.627219
C	4.358505	4.005774	-3.808855
H	6.193699	2.035396	-4.543063
H	5.017632	1.010480	-5.385960
H	5.196278	2.703155	-5.859412
H	2.518227	1.245639	-4.857414
H	1.917715	2.643812	-3.946799
H	2.633249	2.873309	-5.566804
H	5.313558	4.186906	-3.291715

H	4.402350	4.498560	-4.792488
H	3.562463	4.499418	-3.236205
C	5.926073	-1.007393	-0.572320
C	7.348264	-0.686257	-1.082910
C	6.012809	-1.185519	0.954706
C	5.458589	-2.356650	-1.157132
H	7.360662	-0.567466	-2.173343
H	7.722106	0.243299	-0.625217
H	8.040008	-1.500680	-0.810678
H	6.731176	-1.987178	1.184026
H	6.364157	-0.272890	1.458872
H	5.048975	-1.472076	1.394249
H	4.396863	-2.538311	-0.940965
H	5.608503	-2.408630	-2.240377
H	6.034705	-3.179580	-0.703995

VIII. Determination of the Absolute Stereochemistry

The structure and absolute stereochemistry of products **3a** and **3p** were determined by X-ray diffraction. The X-ray data have been deposited at the Cambridge Crystallographic Data Center (CCDC 2108959 for **3a**, CCDC2116827 for **3p**). The stereochemistry of other products was assumed by analogy.

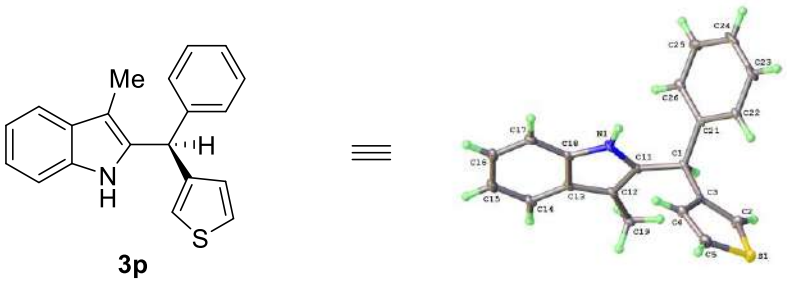


Table S1. Crystal data and structure refinement for 3a

Identification code	**3a**
Empirical formula	$C_{20}H_{17}NS$
Formula weight	303.40
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P1
a/Å	8.3698(2)
b/Å	8.6024(2)

c/Å	11.6963(2)
α/°	103.438(2)
β/°	103.111(2)
γ/°	102.977(2)
Volume/Å^3	762.79(3)
Z	2
ϱ_{calc}g/cm^3	1.321
μ/mm^{-1}	1.823
F(000)	320.0
Crystal size/mm^3	0.16 × 0.15 × 0.13
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.132 to 153.656
Index ranges	-10 ≤ h ≤ 10, -10 ≤ k ≤ 10, -11 ≤ l ≤ 14
Reflections collected	12888
Independent reflections	5874 [R_{int} = 0.0204, R_{sigma} = 0.0248]
Data/restraints/parameters	5874/183/435
Goodness-of-fit on F^2	1.056
Final R indexes [I>=2σ (I)]	R_1 = 0.0380, wR_2 = 0.1012
Final R indexes [all data]	R_1 = 0.0389, wR_2 = 0.1022
Largest diff. peak/hole / e Å^{-3}	0.71/-0.41
Flack parameter	0.011(6)

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 3a. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**

S(1)	4066.0(10)	4632.0(10)	6213.1(8)	22.5(2)
S(1B)	4983(16)	2676(14)	4252(11)	23(3)
N(1)	7305(3)	5356(3)	8717(2)	15.5(5)
C(1)	5355(4)	3485(3)	5758(3)	16.5(5)
C(2)	4864(7)	2816(6)	4463(5)	24.4(14)
C(2B)	4079(18)	4280(20)	5850(30)	22(2)
C(3)	3401(4)	3306(4)	3910(3)	26.8(7)
C(4)	2867(4)	4257(4)	4752(3)	22.1(6)
C(5)	6174(4)	1764(3)	7180(3)	14.3(6)
C(6)	4637(4)	507(4)	6546(3)	18.2(6)
C(7)	4153(4)	-853(4)	6968(3)	23.7(7)
C(8)	5195(4)	-979(4)	8031(3)	23.3(7)
C(9)	6743(4)	252(4)	8662(3)	20.5(6)
C(10)	7220(4)	1613(4)	8235(3)	17.8(6)
C(11)	6779(3)	3214(3)	6678(3)	14.2(6)
C(12)	7792(3)	4825(3)	7673(3)	13.8(5)
C(13)	9203(4)	6015(4)	7686(3)	14.7(6)
C(14)	9617(4)	7358(4)	8804(3)	14.8(6)
C(15)	10914(4)	8891(4)	9337(3)	18.7(6)
C(16)	10990(4)	9885(4)	10480(3)	20.5(6)
C(17)	9828(4)	9370(4)	11108(3)	20.5(6)
C(18)	8529(4)	7859(4)	10602(3)	18.6(6)
C(19)	8427(4)	6892(3)	9442(3)	15.0(6)
C(20)	10185(4)	5926(4)	6766(3)	20.2(6)
S(1A)	98(3)	4328(3)	1820(2)	32.8(6)
S(1C)	1006(3)	7528(3)	3531.4(18)	20.3(5)
N(1A)	5095(3)	7496(3)	3899(2)	18.1(5)

C(1A)	1475(4)	6218(4)	2372(3)	20.2(6)
C(2A)	1027(14)	7231(15)	3348(9)	24.8(18)
C(2C)	251(13)	4671(15)	2018(10)	37(2)
C(3A)	-611(5)	6156(5)	3516(4)	36.8(8)
C(4A)	-1019(5)	4631(5)	2717(4)	35.7(8)
C(5A)	3185(4)	5404(4)	928(3)	17.5(6)
C(6A)	2070(4)	4770(4)	-272(3)	26.7(8)
C(7A)	2264(5)	3494(4)	-1120(3)	29.0(8)
C(8A)	3601(4)	2839(4)	-808(3)	25.7(7)
C(9A)	4724(4)	3446(4)	348(4)	25.3(7)
C(10A)	4561(4)	4675(4)	1228(3)	19.4(6)
C(11A)	2902(4)	6833(4)	1843(3)	17.5(6)
C(12A)	4551(4)	7876(4)	2818(3)	17.6(6)
C(13A)	5780(4)	9183(4)	2760(3)	16.8(6)
C(14A)	7175(4)	9640(4)	3873(3)	16.2(6)
C(15A)	8797(4)	10844(4)	4341(3)	19.6(6)
C(16A)	9858(4)	10935(4)	5464(3)	21.4(7)
C(17A)	9336(4)	9871(4)	6142(3)	21.5(7)
C(18A)	7740(4)	8673(4)	5705(3)	18.9(6)
C(19A)	6697(4)	8572(4)	4571(3)	17.6(6)
C(20A)	5695(4)	9987(4)	1750(3)	21.5(6)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3a. 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}
S(1)	23.5(4)	26.1(4)	19.6(5)	5.8(3)	5.2(3)	12.5(3)

S(1B)	29(4)	26(5)	16(2)	7(2)	4.2(19)	17(4)
N(1)	16.2(11)	14.4(11)	16.4(13)	4.4(10)	7.1(10)	3.5(9)
C(1)	17.2(12)	15.0(12)	17.7(13)	6.6(10)	4.4(9)	4.8(10)
C(2)	30(2)	27(3)	20.4(18)	8.1(15)	3.9(13)	19(2)
C(2B)	22(3)	21(4)	22(2)	6.8(17)	4.9(15)	8(3)
C(3)	31.0(14)	26.3(15)	20.9(13)	6.3(11)	1.4(11)	11.6(12)
C(4)	21.4(13)	21.4(14)	25.0(13)	10.3(11)	4.8(10)	7.8(11)
C(5)	16.1(13)	12.6(12)	16.0(15)	3.5(11)	7.2(11)	5.6(10)
C(6)	18.3(14)	15.9(14)	18.1(16)	2.7(12)	3.5(12)	4.9(11)
C(7)	22.9(15)	18.5(14)	26.9(18)	4.7(13)	8.4(13)	1.8(12)
C(8)	33.8(17)	14.3(14)	27.2(18)	9.8(12)	13.6(14)	8.9(12)
C(9)	25.9(15)	20.3(15)	18.1(16)	7.8(12)	6.9(12)	9.8(12)
C(10)	18.7(14)	16.2(13)	18.3(16)	4.1(11)	4.6(12)	6.6(11)
C(11)	14.3(12)	14.9(13)	13.5(14)	3.9(11)	4.2(11)	4.7(10)
C(12)	15.6(12)	14.5(13)	12.0(14)	5.1(11)	2.8(11)	6.0(10)
C(13)	15.3(12)	16.3(13)	14.1(15)	6.4(11)	3.4(11)	6.4(10)
C(14)	17.0(13)	15.8(13)	13.7(15)	7.1(11)	3.6(11)	7.1(11)
C(15)	16.8(13)	16.9(14)	22.1(17)	7.1(12)	4.0(12)	4.6(11)
C(16)	18.8(14)	14.8(13)	23.8(17)	4.7(12)	1.2(12)	3.3(11)
C(17)	25.5(15)	17.8(15)	16.2(16)	2.0(12)	1.6(12)	10.1(12)
C(18)	22.2(14)	19.7(14)	18.5(16)	8.4(12)	7.5(12)	10.7(12)
C(19)	14.8(13)	13.1(13)	17.1(15)	5.6(11)	2.9(11)	5.1(10)
C(20)	23.1(14)	17.5(14)	21.8(17)	6.0(12)	10.7(13)	5.3(12)
S(1A)	32.8(9)	32.6(11)	33.3(11)	9.1(9)	9.1(8)	11.4(8)
S(1C)	23.6(8)	21.4(10)	16.4(9)	1.8(7)	4.4(7)	13.1(6)
N(1A)	19.0(12)	17.7(12)	17.1(13)	6.6(10)	2.5(10)	5.7(10)
C(1A)	21.3(12)	23.8(12)	17.1(13)	5.7(10)	2.1(10)	13.4(10)

C(2A)	26(2)	27(2)	24(3)	8.6(16)	2.2(19)	16.4(15)
C(2C)	37(3)	33(2)	37(3)	8.1(16)	9(2)	8.8(16)
C(3A)	33.4(13)	50.5(15)	34.0(15)	16.0(11)	9.7(11)	23.1(11)
C(4A)	28.8(13)	44.0(14)	34.4(15)	19.4(11)	2.3(11)	9.8(11)
C(5A)	18.1(13)	16.1(14)	17.0(16)	4.6(12)	3.4(12)	4.5(11)
C(6A)	25.7(16)	19.6(15)	27.8(19)	7.2(14)	-5.4(13)	6.4(13)
C(7A)	33.8(18)	27.5(17)	19.0(17)	3.1(14)	4.4(14)	3.6(14)
C(8A)	31.2(17)	18.7(14)	27.1(18)	2.6(13)	17.8(14)	2.2(13)
C(9A)	24.7(16)	25.7(16)	35(2)	15.2(15)	15.0(14)	12.5(13)
C(10A)	14.1(13)	30.6(16)	6.1(14)	4.2(12)	0.4(11)	-3.6(12)
C(11A)	18.1(13)	15.2(13)	17.2(15)	4.6(12)	0.8(11)	5.5(11)
C(12A)	19.3(14)	16.2(13)	17.2(16)	4.3(11)	3.1(12)	8.0(11)
C(13A)	17.2(13)	16.5(13)	15.7(15)	1.6(11)	4.0(11)	7.0(11)
C(14A)	18.9(13)	16.2(13)	14.5(15)	2.5(11)	5.1(11)	9.3(11)
C(15A)	21.7(15)	17.2(14)	20.9(17)	3.8(12)	7.7(12)	8.2(12)
C(16A)	19.0(14)	19.4(14)	20.7(17)	-0.4(12)	3.2(12)	5.0(11)
C(17A)	20.9(15)	24.2(16)	18.6(16)	3.5(13)	3.7(12)	10.2(12)
C(18A)	23.8(15)	18.2(14)	17.1(15)	5.6(12)	7.0(12)	9.9(12)
C(19A)	18.4(13)	17.0(13)	18.1(16)	3.3(12)	5.9(11)	7.9(11)
C(20A)	22.4(15)	21.2(15)	21.0(17)	6.9(13)	5.4(13)	7.2(12)

Table S4. Bond Lengths for 3a

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S(1)	C(1)	1.708(3)	S(1A)	C(1A)	1.650(4)
S(1)	C(4)	1.689(3)	S(1A)	C(4A)	1.572(5)
S(1B)	C(1)	1.664(12)	S(1C)	C(1A)	1.730(4)

S(1B)	C(3)	1.546(13)	S(1C)	C(3A)	1.577(5)
N(1)	C(12)	1.384(4)	N(1A)	C(12A)	1.382(4)
N(1)	C(19)	1.381(4)	N(1A)	C(19A)	1.378(4)
C(1)	C(2)	1.414(6)	C(1A)	C(2A)	1.443(11)
C(1)	C(2B)	1.40(2)	C(1A)	C(2C)	1.389(11)
C(1)	C(11)	1.514(4)	C(1A)	C(11A)	1.515(4)
C(2)	C(3)	1.447(6)	C(2A)	C(3A)	1.553(12)
C(2B)	C(4)	1.44(2)	C(2C)	C(4A)	1.481(13)
C(3)	C(4)	1.353(5)	C(3A)	C(4A)	1.340(6)
C(5)	C(6)	1.394(4)	C(5A)	C(6A)	1.399(4)
C(5)	C(10)	1.393(4)	C(5A)	C(10A)	1.445(4)
C(5)	C(11)	1.532(4)	C(5A)	C(11A)	1.532(4)
C(6)	C(7)	1.386(4)	C(6A)	C(7A)	1.364(5)
C(7)	C(8)	1.390(5)	C(7A)	C(8A)	1.377(5)
C(8)	C(9)	1.389(5)	C(8A)	C(9A)	1.363(5)
C(9)	C(10)	1.390(4)	C(9A)	C(10A)	1.348(5)
C(11)	C(12)	1.507(4)	C(11A)	C(12A)	1.505(4)
C(12)	C(13)	1.373(4)	C(12A)	C(13A)	1.369(4)
C(13)	C(14)	1.441(4)	C(13A)	C(14A)	1.441(4)
C(13)	C(20)	1.493(4)	C(13A)	C(20A)	1.499(4)
C(14)	C(15)	1.405(4)	C(14A)	C(15A)	1.408(4)
C(14)	C(19)	1.416(4)	C(14A)	C(19A)	1.416(4)
C(15)	C(16)	1.389(5)	C(15A)	C(16A)	1.382(5)
C(16)	C(17)	1.401(5)	C(16A)	C(17A)	1.405(5)
C(17)	C(18)	1.392(4)	C(17A)	C(18A)	1.391(5)
C(18)	C(19)	1.390(4)	C(18A)	C(19A)	1.385(5)

Table S5. Bond Angles for 3a

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C(4)	S(1)	C(1)	92.66(16)	C(4A)	S(1A)	C(1A)	96.1(2)
C(3)	S(1B)	C(1)	93.8(7)	C(3A)	S(1C)	C(1A)	94.4(2)
C(19)	N(1)	C(12)	109.4(2)	C(19A)	N(1A)	C(12A)	109.2(3)
C(2)	C(1)	S(1)	111.4(3)	C(2A)	C(1A)	S(1A)	110.4(6)
C(2)	C(1)	C(11)	126.8(3)	C(2A)	C(1A)	C(11A)	125.2(6)
C(2B)	C(1)	S(1B)	104.4(13)	C(2C)	C(1A)	S(1C)	107.2(6)
C(2B)	C(1)	C(11)	134.4(12)	C(2C)	C(1A)	C(11A)	130.4(6)
C(11)	C(1)	S(1)	121.8(2)	C(11A)	C(1A)	S(1A)	124.2(2)
C(11)	C(1)	S(1B)	121.2(5)	C(11A)	C(1A)	S(1C)	122.1(2)
C(1)	C(2)	C(3)	110.1(4)	C(1A)	C(2A)	C(3A)	108.2(8)
C(1)	C(2B)	C(4)	120(2)	C(1A)	C(2C)	C(4A)	113.2(9)
C(4)	C(3)	S(1B)	123.2(5)	C(4A)	C(3A)	S(1C)	117.8(3)
C(4)	C(3)	C(2)	112.7(3)	C(4A)	C(3A)	C(2A)	106.9(5)
C(3)	C(4)	S(1)	113.1(3)	C(3A)	C(4A)	S(1A)	118.4(3)
C(3)	C(4)	C(2B)	98.9(12)	C(3A)	C(4A)	C(2C)	107.4(6)
C(6)	C(5)	C(11)	121.0(3)	C(6A)	C(5A)	C(10A)	117.5(3)
C(10)	C(5)	C(6)	118.6(3)	C(6A)	C(5A)	C(11A)	118.9(3)
C(10)	C(5)	C(11)	120.2(3)	C(10A)	C(5A)	C(11A)	123.6(3)
C(7)	C(6)	C(5)	120.5(3)	C(7A)	C(6A)	C(5A)	121.1(3)
C(6)	C(7)	C(8)	120.3(3)	C(6A)	C(7A)	C(8A)	119.9(3)
C(9)	C(8)	C(7)	119.7(3)	C(9A)	C(8A)	C(7A)	120.4(3)
C(8)	C(9)	C(10)	119.7(3)	C(10A)	C(9A)	C(8A)	122.0(3)
C(9)	C(10)	C(5)	121.1(3)	C(9A)	C(10A)	C(5A)	119.1(3)
C(1)	C(11)	C(5)	113.8(2)	C(1A)	C(11A)	C(5A)	112.1(2)
C(12)	C(11)	C(1)	110.7(2)	C(12A)	C(11A)	C(1A)	112.9(3)

C(12)	C(11)	C(5)	113.2(2)	C(12A)	C(11A)	C(5A)	111.4(2)
N(1)	C(12)	C(11)	122.0(2)	N(1A)	C(12A)	C(11A)	121.8(3)
C(13)	C(12)	N(1)	109.7(3)	C(13A)	C(12A)	N(1A)	110.0(3)
C(13)	C(12)	C(11)	128.2(3)	C(13A)	C(12A)	C(11A)	127.9(3)
C(12)	C(13)	C(14)	106.4(3)	C(12A)	C(13A)	C(14A)	106.2(3)
C(12)	C(13)	C(20)	127.6(3)	C(12A)	C(13A)	C(20A)	127.1(3)
C(14)	C(13)	C(20)	126.0(3)	C(14A)	C(13A)	C(20A)	126.7(3)
C(15)	C(14)	C(13)	133.4(3)	C(15A)	C(14A)	C(13A)	133.8(3)
C(15)	C(14)	C(19)	119.1(3)	C(15A)	C(14A)	C(19A)	118.6(3)
C(19)	C(14)	C(13)	107.5(3)	C(19A)	C(14A)	C(13A)	107.6(3)
C(16)	C(15)	C(14)	118.5(3)	C(16A)	C(15A)	C(14A)	118.7(3)
C(15)	C(16)	C(17)	121.3(3)	C(15A)	C(16A)	C(17A)	121.2(3)
C(18)	C(17)	C(16)	121.5(3)	C(18A)	C(17A)	C(16A)	121.4(3)
C(19)	C(18)	C(17)	117.0(3)	C(19A)	C(18A)	C(17A)	117.0(3)
N(1)	C(19)	C(14)	106.9(3)	N(1A)	C(19A)	C(14A)	107.0(3)
N(1)	C(19)	C(18)	130.4(3)	N(1A)	C(19A)	C(18A)	130.0(3)
C(18)	C(19)	C(14)	122.6(3)	C(18A)	C(19A)	C(14A)	123.0(3)

Table S6. Torsion Angles for 3a

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S(1)	C(1)	C(2)	C(3)	-0.2(4)	S(1A)	C(1A)	C(2A)	C(3A)	-0.2(4)
S(1)	C(1)	C(11)	C(5)	83.9(3)	S(1A)	C(1A)	C(11A)	C(5A)	-12.9(4)
S(1)	C(1)	C(11)	C(12)	-45.0(3)	S(1A)	C(1A)	C(11A)	C(12A)	-139.6(3)
S(1B)	C(1)	C(2B)	C(4)	-0.9(5)	S(1C)	C(1A)	C(2C)	C(4A)	-0.1(4)
S(1B)	C(1)	C(11)	C(5)	-96.3(6)	S(1C)	C(1A)	C(11A)	C(5A)	174.0(2)
S(1B)	C(1)	C(11)	C(12)	134.8(5)	S(1C)	C(1A)	C(11A)	C(12A)	47.2(3)

S(1B)	C(3)	C(4)	C(2B)	-3.8(9)	S(1C)	C(3A)	C(4A)	C(2C)	-0.3(5)
N(1)	C(12)	C(13)	C(14)	0.1(3)	N(1A)	C(12A)	C(13A)	C(14A)	0.2(3)
N(1)	C(12)	C(13)	C(20)	177.5(3)	N(1A)	C(12A)	C(13A)	C(20A)	-179.6(3)
C(1)	S(1)	C(4)	C(3)	-0.7(3)	C(1A)	S(1A)	C(4A)	C(3A)	2.6(4)
C(1)	S(1B)	C(3)	C(4)	3.3(8)	C(1A)	S(1C)	C(3A)	C(4A)	0.3(3)
C(1)	C(2)	C(3)	C(4)	-0.4(5)	C(1A)	C(2A)	C(3A)	C(4A)	1.8(5)
C(1)	C(2B)	C(4)	C(3)	2.6(8)	C(1A)	C(2C)	C(4A)	C(3A)	0.2(5)
C(1)	C(11)	C(12)	N(1)	86.8(3)	C(1A)	C(11A)	C(12A)	N(1A)	38.2(4)
C(1)	C(11)	C(12)	C(13)	-88.9(3)	C(1A)	C(11A)	C(12A)	C(13A)	-148.1(3)
C(2)	C(1)	C(11)	C(5)	-93.6(4)	C(2A)	C(1A)	C(11A)	C(5A)	173.1(3)
C(2)	C(1)	C(11)	C(12)	137.5(3)	C(2A)	C(1A)	C(11A)	C(12A)	46.4(4)
C(2)	C(3)	C(4)	S(1)	0.7(4)	C(2A)	C(3A)	C(4A)	S(1A)	-2.9(5)
C(2B)	C(1)	C(11)	C(5)	80.5(6)	C(2C)	C(1A)	C(11A)	C(5A)	-11.9(5)
C(2B)	C(1)	C(11)	C(12)	-48.4(6)	C(2C)	C(1A)	C(11A)	C(12A)	-138.6(4)
C(3)	S(1B)	C(1)	C(2B)	-1.1(4)	C(3A)	S(1C)	C(1A)	C(2C)	-0.1(3)
C(3)	S(1B)	C(1)	C(11)	176.6(3)	C(3A)	S(1C)	C(1A)	C(11A)	175.2(3)
C(4)	S(1)	C(1)	C(2)	0.5(2)	C(4A)	S(1A)	C(1A)	C(2A)	-1.2(3)
C(4)	S(1)	C(1)	C(11)	-177.3(2)	C(4A)	S(1A)	C(1A)	C(11A)	-175.9(3)
C(5)	C(6)	C(7)	C(8)	0.1(5)	C(5A)	C(6A)	C(7A)	C(8A)	-1.6(5)
C(5)	C(11)	C(12)	N(1)	-42.4(4)	C(5A)	C(11A)	C(12A)	N(1A)	-89.0(3)
C(5)	C(11)	C(12)	C(13)	141.9(3)	C(5A)	C(11A)	C(12A)	C(13A)	84.7(4)
C(6)	C(5)	C(10)	C(9)	-0.7(4)	C(6A)	C(5A)	C(10A)	C(9A)	0.8(4)
C(6)	C(5)	C(11)	C(1)	20.6(4)	C(6A)	C(5A)	C(11A)	C(1A)	79.3(4)
C(6)	C(5)	C(11)	C(12)	148.2(3)	C(6A)	C(5A)	C(11A)	C(12A)	-153.2(3)
C(6)	C(7)	C(8)	C(9)	-1.0(5)	C(6A)	C(7A)	C(8A)	C(9A)	0.7(5)
C(7)	C(8)	C(9)	C(10)	1.1(5)	C(7A)	C(8A)	C(9A)	C(10A)	1.0(5)
C(8)	C(9)	C(10)	C(5)	-0.2(5)	C(8A)	C(9A)	C(10A)	C(5A)	-1.7(5)

C(10)	C(5)	C(6)	C(7)	0.8(4)	C(10A)	C(5A)	C(6A)	C(7A)	0.9(5)
C(10)	C(5)	C(11)	C(1)	-164.3(3)	C(10A)	C(5A)	C(11A)	C(1A)	-101.4(3)
C(10)	C(5)	C(11)	C(12)	-36.7(4)	C(10A)	C(5A)	C(11A)	C(12A)	26.1(4)
C(11)	C(1)	C(2)	C(3)	177.5(3)	C(11A)	C(1A)	C(2A)	C(3A)	174.5(3)
C(11)	C(1)	C(2B)	C(4)	-178.1(4)	C(11A)	C(1A)	C(2C)	C(4A)	-174.9(4)
C(11)	C(5)	C(6)	C(7)	176.0(3)	C(11A)	C(5A)	C(6A)	C(7A)	-179.8(3)
C(11)	C(5)	C(10)	C(9)	-176.0(3)	C(11A)	C(5A)	C(10A)	C(9A)	-178.5(3)
C(11)	C(12)	C(13)	C(14)	176.3(3)	C(11A)	C(12A)	C(13A)	C(14A)	-174.2(3)
C(11)	C(12)	C(13)	C(20)	-6.4(5)	C(11A)	C(12A)	C(13A)	C(20A)	6.1(5)
C(12)	N(1)	C(19)	C(14)	2.1(3)	C(12A)	N(1A)	C(19A)	C(14A)	-1.0(3)
C(12)	N(1)	C(19)	C(18)	-175.2(3)	C(12A)	N(1A)	C(19A)	C(18A)	179.7(3)
C(12)	C(13)	C(14)	C(15)	179.1(3)	C(12A)	C(13A)	C(14A)	C(15A)	178.5(3)
C(12)	C(13)	C(14)	C(19)	1.1(3)	C(12A)	C(13A)	C(14A)	C(19A)	-0.8(3)
C(13)	C(14)	C(15)	C(16)	-177.1(3)	C(13A)	C(14A)	C(15A)	C(16A)	-179.1(3)
C(13)	C(14)	C(19)	N(1)	-2.0(3)	C(13A)	C(14A)	C(19A)	N(1A)	1.1(3)
C(13)	C(14)	C(19)	C(18)	175.6(3)	C(13A)	C(14A)	C(19A)	C(18A)	-179.6(3)
C(14)	C(15)	C(16)	C(17)	1.2(4)	C(14A)	C(15A)	C(16A)	C(17A)	-0.9(4)
C(15)	C(14)	C(19)	N(1)	179.7(3)	C(15A)	C(14A)	C(19A)	N(1A)	-178.3(3)
C(15)	C(14)	C(19)	C(18)	-2.8(4)	C(15A)	C(14A)	C(19A)	C(18A)	1.0(4)
C(15)	C(16)	C(17)	C(18)	-1.3(5)	C(15A)	C(16A)	C(17A)	C(18A)	0.8(5)
C(16)	C(17)	C(18)	C(19)	-0.6(4)	C(16A)	C(17A)	C(18A)	C(19A)	0.3(5)
C(17)	C(18)	C(19)	N(1)	179.6(3)	C(17A)	C(18A)	C(19A)	N(1A)	178.0(3)
C(17)	C(18)	C(19)	C(14)	2.6(4)	C(17A)	C(18A)	C(19A)	C(14A)	-1.2(4)
C(19)	N(1)	C(12)	C(11)	-177.8(3)	C(19A)	N(1A)	C(12A)	C(11A)	175.3(3)
C(19)	N(1)	C(12)	C(13)	-1.4(3)	C(19A)	N(1A)	C(12A)	C(13A)	0.6(3)
C(19)	C(14)	C(15)	C(16)	0.7(4)	C(19A)	C(14A)	C(15A)	C(16A)	0.1(4)
C(20)	C(13)	C(14)	C(15)	1.7(5)	C(20A)	C(13A)	C(14A)	C(15A)	-1.7(5)

C(20)	C(13)	C(14)	C(19)	-176.3(3)	C(20A)	C(13A)	C(14A)	C(19A)	179.0(3)

Table S7. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 3a

Atom	*x*	*y*	*z*	U(eq)
H(1)	6419	4801	8891	19
H(2)	5414	2143	4021	29
H(2B)	4015	4830	6638	26
H(3A)	2873	2993	3048	32
H(3B)	2773	3010	3066	32
H(4A)	1914	4672	4543	26
H(4B)	1963	4760	4649	26
H(6)	3915	583	5819	22
H(7)	3103	-1702	6528	28
H(8)	4851	-1903	8326	28
H(9)	7471	164	9381	25
H(10)	8277	2455	8670	21
H(11)	7587	2894	6219	17
H(15)	11720	9239	8924	22
H(16)	11846	10935	10844	25
H(17)	9928	10068	11896	25
H(18)	7748	7505	11031	22
H(20A)	10191	6869	6429	30
H(20B)	9641	4874	6099	30
H(20C)	11367	5978	7167	30
H(1A)	4511	6693	4122	22

H(2A)	1630	8361	3808	30
H(2C)	232	3734	1390	44
H(3AA)	-1210	6512	4079	44
H(3AB)	-1275	6403	4057	44
H(4AA)	-1960	3756	2693	43
H(4AB)	-1952	3697	2618	43
H(6A)	1162	5235	-500	32
H(7A)	1478	3058	-1924	35
H(8A)	3743	1960	-1402	31
H(9A)	5648	2988	540	30
H(10A)	5341	5057	2033	23
H(11A)	2520	7580	1368	21
H(15A)	9155	11579	3895	23
H(16A)	10962	11732	5782	26
H(17A)	10088	9972	6915	26
H(18A)	7383	7956	6164	23
H(20D)	5304	10978	1965	32
H(20E)	4890	9192	983	32
H(20F)	6837	10318	1640	32

Table S8. Atomic Occupancy for 3a

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
S(1)	0.9	S(1B)	0.1	C(2)	0.9
H(2)	0.9	C(2B)	0.1	H(2B)	0.1
H(3A)	0.9	H(3B)	0.1	H(4A)	0.9
H(4B)	0.1	S(1A)	0.5	S(1C)	0.5

C(2A)	0.5	H(2A)	0.5	C(2C)	0.5		
H(2C)	0.5	H(3AA)	0.5	H(3AB)	0.5		
H(4AA)	0.5	H(4AB)	0.5				

Table S9. Crystal data and structure refinement for 3p.

Identification code	**3p**
Empirical formula	$C_{20}H_{17}NS$
Formula weight	303.40
Temperature/K	100.01(10)
Crystal system	triclinic
Space group	P1
a/Å	8.4366(4)
b/Å	8.5299(4)
c/Å	11.8199(6)
α/°	103.482(4)
β/°	103.756(4)
γ/°	102.858(4)
Volume/Å^3	767.85(7)
Z	2
ϱ_{calc}g/cm^3	1.312
μ/mm^{-1}	1.811
F(000)	320.0
Crystal size/mm^3	0.4 × 0.35 × 0.15
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.078 to 152.404
Index ranges	-10 ≤ h ≤ 7, -9 ≤ k ≤ 10, -14 ≤ l ≤ 14

Reflections collected	4569
Independent reflections	3400 [R_{int} = 0.0274, R_{sigma} = 0.0261]
Data/restraints/parameters	3400/132/444
Goodness-of-fit on F^2	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0367, wR_2 = 0.0964
Final R indexes [all data]	R_1 = 0.0371, wR_2 = 0.0966
Largest diff. peak/hole / e $Å^{-3}$	0.48/-0.32
Flack parameter	0.016(17)

Table S10. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for 3p. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
S1	3205.1(16)	3129.4(15)	3705.3(9)	18.4(3)
S2	2837(8)	4550(8)	4881(5)	17.8(12)
N1	7275(3)	5330(3)	8740(2)	13.0(5)
C1	6715(3)	3159(3)	6709(2)	11.1(5)
C2	4898(9)	2672(11)	4531(6)	19.0(14)
C3	5290(20)	3410(20)	5765(9)	11.3(10)
C4	4270(20)	4480(30)	6030(9)	16.5(12)
C5	3055(11)	4422(11)	5015(7)	19.4(14)
C6	4260(80)	4490(100)	6100(30)	19(3)
C7	4650(30)	2490(40)	4580(20)	18(3)
C8	3410(30)	3100(30)	3997(19)	19(2)
C9	5260(80)	3440(90)	5810(30)	18(3)
C11	7724(3)	4794(3)	7692(2)	11.7(5)

C12	9109(3)	5999(3)	7699(3)	12.7(5)
C13	9547(3)	7361(3)	8808(3)	12.4(5)
C14	10847(4)	8905(3)	9340(3)	15.4(5)
C15	10961(4)	9913(4)	10479(3)	18.4(6)
C16	9837(4)	9386(4)	11115(3)	17.6(6)
C17	8537(4)	7860(4)	10612(3)	15.3(5)
C18	8407(3)	6880(3)	9452(3)	12.7(5)
C19	10041(4)	5892(4)	6764(3)	17.1(6)
C21	6099(3)	1711(3)	7213(2)	11.3(5)
C22	4543(4)	468(3)	6594(3)	15.1(5)
C23	4056(4)	-900(4)	7035(3)	21.6(6)
C24	5092(4)	-1024(4)	8069(3)	21.4(6)
C25	6668(4)	203(4)	8687(3)	18.0(6)
C26	7156(4)	1558(4)	8256(3)	15.5(5)
S1A	-980.3(9)	4655.7(10)	2845.9(7)	24.27(19)
N1A	5160(3)	7607(3)	3929(2)	13.3(5)
C1A	3006(3)	6945(3)	1872(2)	12.7(5)
C2A	506(4)	4761(4)	2061(3)	17.3(6)
C3A	1595(3)	6364(4)	2414(3)	12.9(5)
C4A	1200(4)	7494(4)	3330(3)	16.3(5)
C5A	-166(4)	6745(4)	3654(3)	20.3(6)
C11A	4660(3)	7984(3)	2849(2)	11.9(5)
C12A	5909(4)	9273(3)	2813(3)	12.7(5)
C13A	7283(4)	9732(3)	3920(3)	11.9(5)
C14A	8911(4)	10918(4)	4409(3)	15.8(6)
C15A	9943(4)	11027(3)	5536(3)	17.0(6)
C16A	9379(4)	9972(4)	6211(3)	15.9(5)

C17A	7782(4)	8786(4)	5757(3)	15.4(5)
C18A	6766(3)	8667(3)	4613(3)	12.2(5)
C19A	5835(4)	10106(4)	1816(3)	17.0(6)
C21A	3240(3)	5505(3)	954(3)	12.7(5)
C22A	4557(4)	4792(4)	1248(3)	14.9(5)
C23A	4718(4)	3465(4)	366(3)	18.5(6)
C24A	3585(4)	2876(4)	-796(3)	21.8(6)
C25A	2289(4)	3569(4)	-1094(3)	25.2(7)
C26A	2113(4)	4883(4)	-225(3)	21.0(6)

Table S11. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for 3p. 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}
S1	23.0(6)	15.2(4)	15.2(5)	3.4(4)	0.1(4)	9.3(4)
S2	16(2)	16.6(18)	21.3(17)	8.1(12)	5.7(13)	3.8(14)
N1	11.8(11)	7.9(10)	19.1(11)	2.7(9)	8.1(9)	0.5(8)
C1	10.0(12)	6.7(11)	17.7(12)	3.4(10)	6.2(10)	2.8(9)
C2	23(2)	19(3)	17.5(14)	5.3(12)	4.1(12)	12(2)
C3	9.9(15)	6.6(15)	17.0(14)	5.1(11)	4.5(11)	-0.4(12)
C4	16.7(16)	13.3(17)	20.9(15)	4.6(14)	6.8(13)	6.4(13)
C5	20(2)	16(2)	22.0(16)	4.3(13)	5.3(12)	7.1(16)
C6	19(4)	18(4)	21(2)	6.9(18)	5.9(17)	6(3)
C7	18(4)	16(4)	20(3)	7.3(19)	6.4(18)	4(3)
C8	19(3)	18(3)	22(3)	8.0(17)	6.3(18)	4(3)
C9	18(4)	17(4)	20(3)	6.9(19)	5.7(18)	5(3)
C11	10.5(12)	9.3(12)	16.4(12)	4.9(10)	4.5(10)	3.8(10)

C12	10.7(12)	8.6(12)	20.0(13)	5.6(10)	5.6(10)	2.9(10)
C13	9.9(12)	9.3(12)	18.7(13)	5.4(10)	3.6(10)	4.0(10)
C14	11.4(12)	10.5(13)	24.4(14)	7.0(11)	5.5(11)	1.4(10)
C15	16.0(13)	11.0(13)	23.5(14)	3.5(11)	0.3(11)	2.6(10)
C16	19.9(14)	11.7(13)	18.8(13)	2.5(10)	1.5(11)	6.6(11)
C17	17.3(14)	12.3(13)	19.0(13)	7.2(10)	7.0(11)	5.2(11)
C18	11.1(12)	8.2(12)	18.8(13)	6.0(10)	3.1(10)	2.7(10)
C19	16.6(14)	12.1(13)	24.3(14)	6.1(11)	11.3(11)	1.7(10)
C21	11.9(12)	5.8(11)	18.4(12)	2.1(9)	9.5(10)	3.5(9)
C22	12.8(13)	10.4(12)	20.6(13)	3.6(10)	5.3(11)	1.2(10)
C23	19.4(15)	9.0(13)	33.4(16)	4.1(12)	11.5(13)	-3.0(11)
C24	30.4(17)	8.2(12)	32.4(16)	8.2(11)	20.2(14)	5.0(12)
C25	23.9(15)	15.6(14)	19.9(13)	8.9(11)	8.3(12)	10.7(11)
C26	14.9(13)	10.8(12)	21.9(13)	3.5(10)	8.2(11)	4.4(10)
S1A	15.2(3)	24.7(4)	34.5(4)	12.5(3)	8.9(3)	3.9(3)
N1A	10.0(11)	11.6(10)	18.6(11)	5.6(9)	5.0(9)	2.0(8)
C1A	11.6(13)	9.1(12)	16.4(12)	2.7(10)	3.5(10)	3.2(10)
C2A	12.9(13)	14.9(13)	23.7(14)	7.4(11)	3.5(11)	4.0(11)
C3A	10.7(12)	13.2(12)	16.2(12)	5.0(10)	3.5(10)	6.2(10)
C4A	17.0(13)	15.8(13)	16.2(12)	4.0(11)	3.0(10)	8.2(11)
C5A	22.1(15)	27.0(16)	19.1(13)	8.2(12)	7.9(11)	18.0(13)
C11A	10.3(12)	9.1(12)	16.3(13)	1.4(10)	5.2(10)	4.4(10)
C12A	14.6(13)	7.8(11)	16.9(12)	2.2(9)	6.7(10)	5.1(10)
C13A	13.9(13)	7.1(12)	17.6(12)	3.5(10)	8.5(10)	5.2(10)
C14A	16.4(13)	9.2(12)	23.0(14)	3.6(10)	9.4(11)	3.5(10)
C15A	12.4(13)	10.0(12)	25.0(14)	0.9(11)	5.7(11)	0.8(10)
C16A	14.6(13)	14.3(13)	16.6(12)	2.3(10)	2.3(11)	5.1(10)

C17A	15.7(13)	12.7(13)	18.5(13)	3.3(10)	7.7(11)	4.0(11)
C18A	11.5(12)	7.5(12)	19.0(13)	2.3(10)	8.1(10)	3.4(10)
C19A	18.4(14)	14.4(13)	21.1(13)	9.3(11)	7.3(11)	4.9(11)
C21A	13.4(12)	7.8(12)	19.2(13)	4.2(10)	8.5(10)	3.6(10)
C22A	13.3(13)	14.7(13)	18.2(13)	5.4(10)	6.0(10)	4.9(10)
C23A	18.3(13)	14.0(13)	31.5(15)	10.3(11)	14.8(12)	9.6(11)
C24A	26.3(16)	11.8(13)	28.0(15)	0.8(11)	19.9(13)	0.0(12)
C25A	32.4(18)	17.2(14)	15.3(13)	0.5(11)	0.6(12)	-2.1(13)
C26A	22.8(15)	15.3(14)	22.5(14)	3.8(11)	2.0(12)	8.1(12)

Table S12. Bond Lengths for 3p.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	C2	1.705(6)	C23	C24	1.365(5)
S1	C5	1.729(8)	C24	C25	1.400(5)
S2	C6	1.66(3)	C25	C26	1.388(4)
S2	C8	1.66(2)	S1A	C2A	1.727(3)
N1	C11	1.387(4)	S1A	C5A	1.705(3)
N1	C18	1.380(3)	N1A	C11A	1.382(4)
C1	C3	1.526(6)	N1A	C18A	1.379(4)
C1	C9	1.526(18)	C1A	C3A	1.523(4)
C1	C11	1.505(4)	C1A	C11A	1.507(4)
C1	C21	1.535(3)	C1A	C21A	1.522(4)
C2	C3	1.373(9)	C2A	C3A	1.371(4)
C3	C4	1.417(9)	C3A	C4A	1.429(4)
C4	C5	1.364(10)	C4A	C5A	1.371(4)
C6	C9	1.40(3)	C11A	C12A	1.359(4)
C7	C8	1.39(3)	C12A	C13A	1.430(4)

C7	C9	1.39(3)	C12A	C19A	1.507(4)
C11	C12	1.371(4)	C13A	C14A	1.405(4)
C12	C13	1.440(4)	C13A	C18A	1.424(4)
C12	C19	1.499(4)	C14A	C15A	1.376(4)
C13	C14	1.406(4)	C15A	C16A	1.414(4)
C13	C18	1.412(4)	C16A	C17A	1.387(4)
C14	C15	1.388(4)	C17A	C18A	1.385(4)
C15	C16	1.405(4)	C21A	C22A	1.393(4)
C16	C17	1.394(4)	C21A	C26A	1.388(4)
C17	C18	1.395(4)	C22A	C23A	1.404(4)
C21	C22	1.394(4)	C23A	C24A	1.376(5)
C21	C26	1.392(4)	C24A	C25A	1.368(5)
C22	C23	1.405(4)	C25A	C26A	1.394(5)

Table S13. Bond Angles for 3p.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	S1	C5	91.3(4)	C24	C23	C22	120.6(3)
C8	S2	C6	90(2)	C23	C24	C25	119.9(3)
C18	N1	C11	109.0(2)	C26	C25	C24	119.8(3)
C3	C1	C21	113.5(9)	C25	C26	C21	120.8(3)
C9	C1	C21	113(4)	C5A	S1A	C2A	92.78(15)
C11	C1	C3	111.0(6)	C18A	N1A	C11A	109.1(2)
C11	C1	C9	110(2)	C11A	C1A	C3A	111.9(2)
C11	C1	C21	113.3(2)	C11A	C1A	C21A	112.1(2)
C3	C2	S1	112.5(5)	C21A	C1A	C3A	112.9(2)
C2	C3	C1	123.0(8)	C3A	C2A	S1A	111.1(2)

C2	C3	C4	111.7(6)	C2A	C3A	C1A	125.7(3)
C4	C3	C1	125.2(7)	C2A	C3A	C4A	111.7(3)
C5	C4	C3	112.8(8)	C4A	C3A	C1A	122.5(2)
C4	C5	S1	111.5(8)	C5A	C4A	C3A	113.6(3)
C9	C6	S2	113(2)	C4A	C5A	S1A	110.8(2)
C8	C7	C9	107(2)	N1A	C11A	C1A	121.1(2)
C7	C8	S2	116.7(17)	C12A	C11A	N1A	109.9(2)
C6	C9	C1	126(2)	C12A	C11A	C1A	128.8(3)
C7	C9	C1	122(3)	C11A	C12A	C13A	107.2(2)
C7	C9	C6	112(2)	C11A	C12A	C19A	126.5(3)
N1	C11	C1	122.2(2)	C13A	C12A	C19A	126.3(3)
C12	C11	N1	109.6(2)	C14A	C13A	C12A	134.8(3)
C12	C11	C1	128.1(3)	C14A	C13A	C18A	118.2(3)
C11	C12	C13	106.8(2)	C18A	C13A	C12A	107.0(2)
C11	C12	C19	126.8(3)	C15A	C14A	C13A	119.6(3)
C13	C12	C19	126.4(2)	C14A	C15A	C16A	120.8(3)
C14	C13	C12	133.7(3)	C17A	C16A	C15A	121.2(3)
C14	C13	C18	119.0(3)	C18A	C17A	C16A	117.5(3)
C18	C13	C12	107.2(2)	N1A	C18A	C13A	106.9(2)
C15	C14	C13	118.9(3)	N1A	C18A	C17A	130.4(2)
C14	C15	C16	120.9(3)	C17A	C18A	C13A	122.7(2)
C17	C16	C15	121.5(3)	C22A	C21A	C1A	122.4(2)
C16	C17	C18	117.0(3)	C26A	C21A	C1A	119.1(3)
N1	C18	C13	107.5(2)	C26A	C21A	C22A	118.5(3)
N1	C18	C17	129.9(3)	C21A	C22A	C23A	120.2(3)
C17	C18	C13	122.6(3)	C24A	C23A	C22A	120.1(3)
C22	C21	C1	121.1(2)	C25A	C24A	C23A	120.2(3)

C26	C21	C1	119.8(2)	C24A	C25A	C26A	120.2(3)		
C26	C21	C22	118.9(2)	C21A	C26A	C25A	120.8(3)		
C21	C22	C23	120.0(3)						

Table S14. Torsion Angles for 3p.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	C2	C3	C1	177.9(13)	C21	C1	C11	C12	143.6(3)
S1	C2	C3	C4	-5(2)	C21	C22	C23	C24	0.1(5)
S2	C6	C9	C1	178(6)	C22	C21	C26	C25	-0.8(4)
S2	C6	C9	C7	-9(9)	C22	C23	C24	C25	-1.1(5)
N1	C11	C12	C13	-0.1(3)	C23	C24	C25	C26	1.1(5)
N1	C11	C12	C19	177.3(3)	C24	C25	C26	C21	-0.2(4)
C1	C3	C4	C5	-177.8(17)	C26	C21	C22	C23	0.8(4)
C1	C11	C12	C13	176.7(3)	S1A	C2A	C3A	C1A	-176.7(2)
C1	C11	C12	C19	-5.8(5)	S1A	C2A	C3A	C4A	0.1(3)
C1	C21	C22	C23	176.1(3)	N1A	C11A	C12A	C13A	0.6(3)
C1	C21	C26	C25	-176.1(2)	N1A	C11A	C12A	C19A	-177.4(2)
C2	S1	C5	C4	0.1(14)	C1A	C3A	C4A	C5A	176.9(3)
C2	C3	C4	C5	5(3)	C1A	C11A	C12A	C13A	-174.5(3)
C3	C1	C11	N1	89.1(9)	C1A	C11A	C12A	C19A	7.5(5)
C3	C1	C11	C12	-87.4(9)	C1A	C21A	C22A	C23A	-179.9(2)
C3	C1	C21	C22	18.6(6)	C1A	C21A	C26A	C25A	179.7(3)
C3	C1	C21	C26	-166.2(5)	C2A	S1A	C5A	C4A	0.0(2)
C3	C4	C5	S1	-3(2)	C2A	C3A	C4A	C5A	-0.1(3)
C5	S1	C2	C3	2.6(12)	C3A	C1A	C11A	N1A	36.9(3)
C6	S2	C8	C7	2(4)	C3A	C1A	C11A	C12A	-148.5(3)

C8	S2	C6	C9	4(7)	C3A	C1A	C21A	C22A	-101.7(3)
C8	C7	C9	C1	-177(6)	C3A	C1A	C21A	C26A	78.9(3)
C8	C7	C9	C6	10(8)	C3A	C4A	C5A	S1A	0.0(3)
C9	C1	C11	N1	87(3)	C5A	S1A	C2A	C3A	-0.1(2)
C9	C1	C11	C12	-90(3)	C11A	N1A	C18A	C13A	-0.6(3)
C9	C1	C21	C22	20.9(17)	C11A	N1A	C18A	C17A	179.1(3)
C9	C1	C21	C26	-163.8(17)	C11A	C1A	C3A	C2A	-133.6(3)
C9	C7	C8	S2	-7(5)	C11A	C1A	C3A	C4A	49.8(3)
C11	N1	C18	C13	2.6(3)	C11A	C1A	C21A	C22A	25.9(4)
C11	N1	C18	C17	-175.5(3)	C11A	C1A	C21A	C26A	-153.5(3)
C11	C1	C3	C2	138.0(15)	C11A	C12A	C13A	C14A	178.5(3)
C11	C1	C3	C4	-39(2)	C11A	C12A	C13A	C18A	-1.0(3)
C11	C1	C9	C6	-38(9)	C12A	C13A	C14A	C15A	-179.9(3)
C11	C1	C9	C7	149(6)	C12A	C13A	C18A	N1A	0.9(3)
C11	C1	C21	C22	146.3(3)	C12A	C13A	C18A	C17A	-178.8(3)
C11	C1	C21	C26	-38.5(3)	C13A	C14A	C15A	C16A	-0.6(4)
C11	C12	C13	C14	178.1(3)	C14A	C13A	C18A	N1A	-178.6(2)
C11	C12	C13	C18	1.7(3)	C14A	C13A	C18A	C17A	1.7(4)
C12	C13	C14	C15	-176.5(3)	C14A	C15A	C16A	C17A	0.7(4)
C12	C13	C18	N1	-2.7(3)	C15A	C16A	C17A	C18A	0.4(4)
C12	C13	C18	C17	175.7(3)	C16A	C17A	C18A	N1A	178.8(3)
C13	C14	C15	C16	2.0(4)	C16A	C17A	C18A	C13A	-1.6(4)
C14	C13	C18	N1	-179.7(2)	C18A	N1A	C11A	C1A	175.5(2)
C14	C13	C18	C17	-1.4(4)	C18A	N1A	C11A	C12A	0.0(3)
C14	C15	C16	C17	-1.9(4)	C18A	C13A	C14A	C15A	-0.5(4)
C15	C16	C17	C18	0.2(4)	C19A	C12A	C13A	C14A	-3.5(5)
C16	C17	C18	N1	179.4(3)	C19A	C12A	C13A	C18A	177.0(3)

C16	C17	C18	C13	1.5(4)	C21A	C1A	C3A C2A -6.0(4)
C18	N1	C11	C1	-178.6(2)	C21A	C1A	C3A C4A 177.5(3)
C18	N1	C11	C12	-1.6(3)	C21A	C1A	C11A N1A -91.2(3)
C18	C13	C14	C15	-0.4(4)	C21A	C1A	C11A C12A 83.4(3)
C19	C12	C13	C14	0.7(5)	C21A	C22A	C23A C24A 0.6(4)
C19	C12	C13	C18	-175.8(3)	C22A	C21A	C26A C25A 0.3(4)
C21	C1	C3	C2	-93.1(18)	C22A	C23A	C24A C25A -0.5(4)
C21	C1	C3	C4	90(2)	C23A	C24A	C25A C26A 0.3(5)
C21	C1	C9	C6	89(8)	C24A	C25A	C26A C21A -0.2(5)
C21	C1	C9	C7	-84(7)	C26A	C21A	C22A C23A -0.5(4)
C21	C1	C11	N1	-39.9(3)			

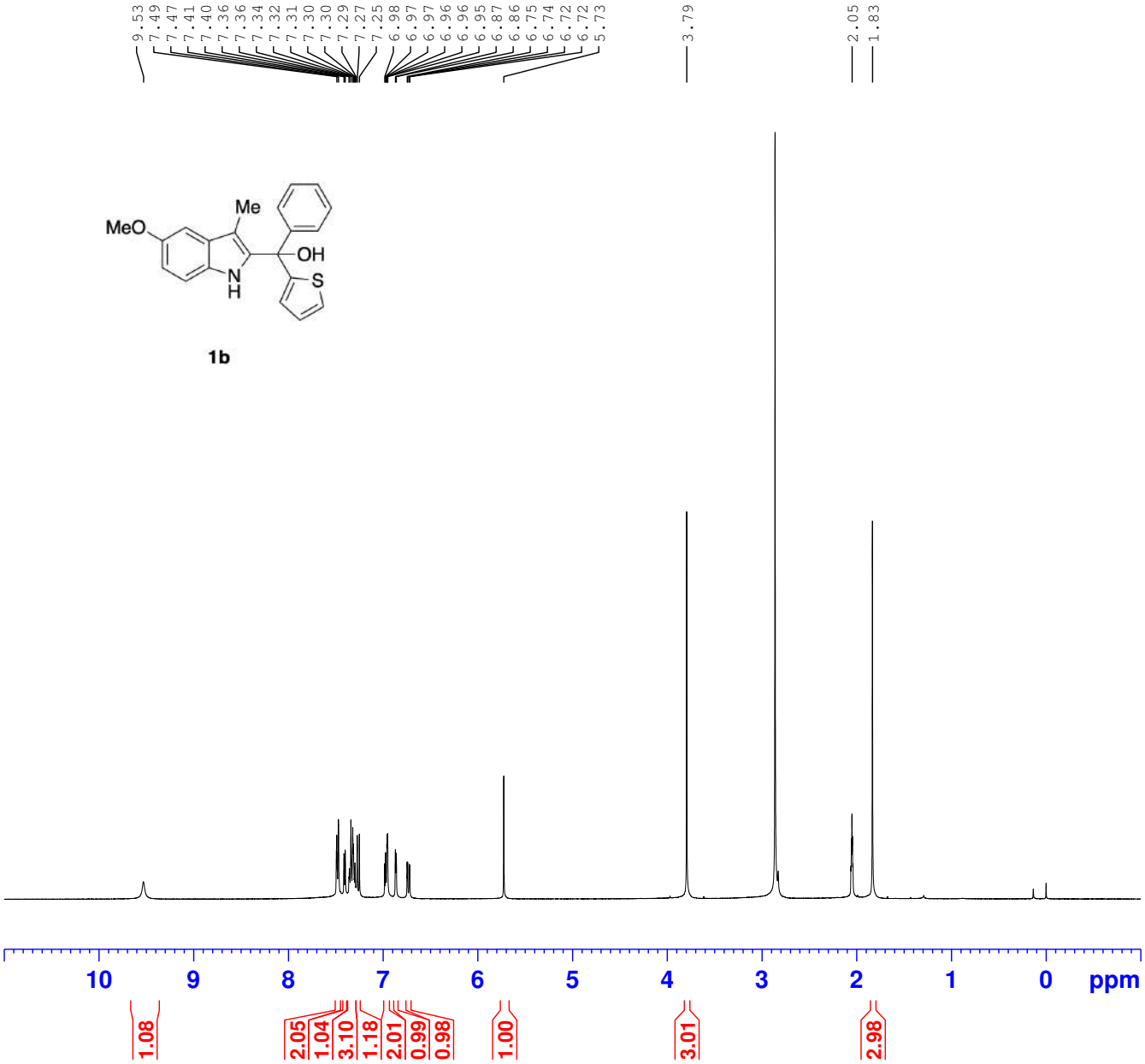
Table S15. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 3p.

Atom	*x*	*y*	*z*	U(eq)
H1	6409	4772	8922	16
H1A	7521	2823	6269	13
H1B	7500	2825	6247	13
H2	5502	1981	4176	23
H4	4420	5163	6830	20
H5	2229	5018	5027	23
H6	4388	5101	6916	23
H7	5026	1581	4208	21
H8	2913	2715	3134	23
H14	11635	9252	8926	19
H15	11812	10976	10835	22

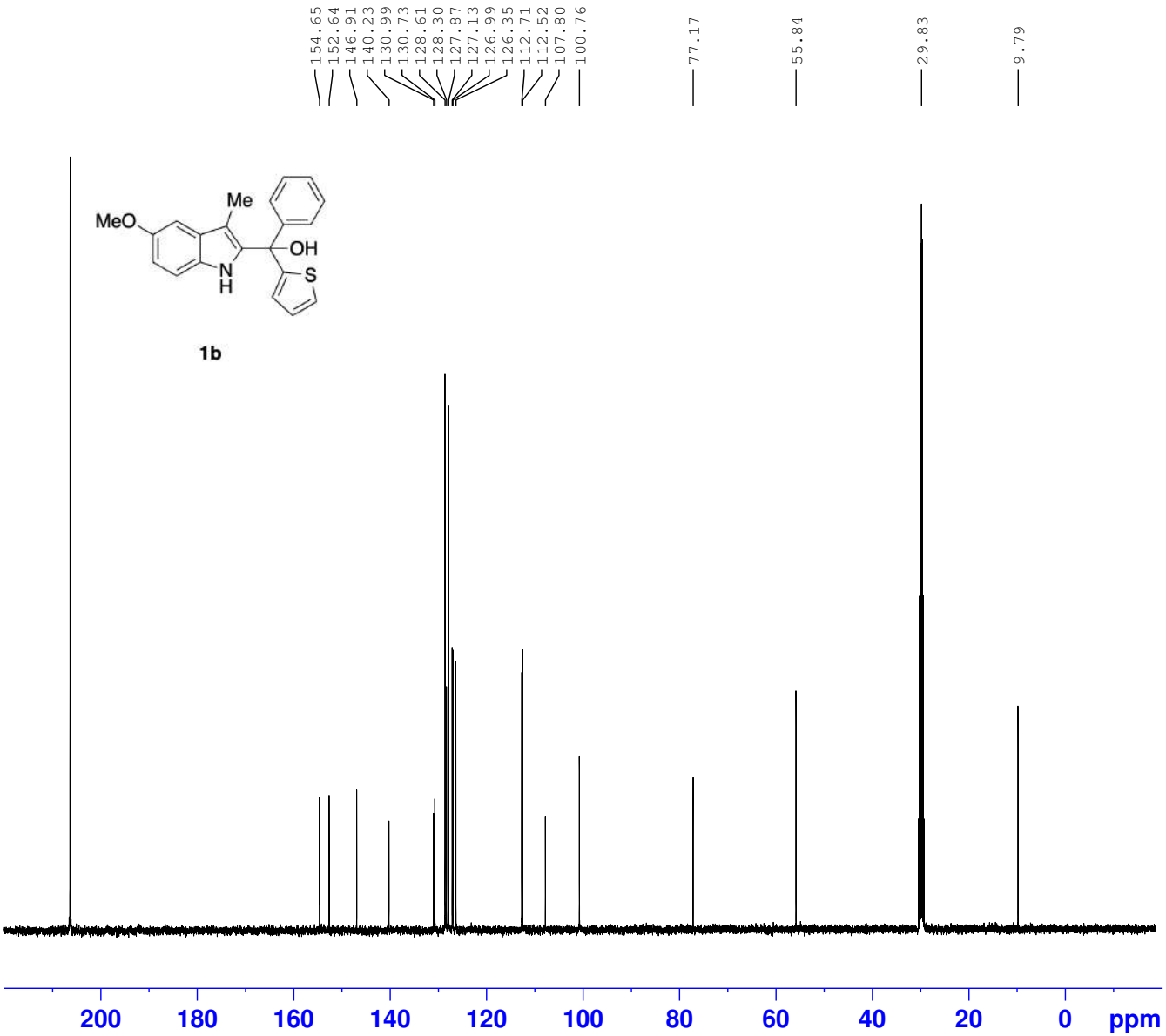
H16	9965	10084	11904	21
H17	7775	7505	11041	18
H19A	10053	6851	6440	26
H19B	9462	4838	6096	26
H19C	11216	5916	7144	26
H22	3813	547	5874	18
H23	2996	-1745	6609	26
H24	4743	-1943	8369	26
H25	7401	109	9398	22
H26	8225	2390	8678	19
H1AA	4550	6815	4146	16
H1AB	2635	7711	1409	15
H2A	561	3831	1463	21
H4A	1824	8655	3682	20
H5A	-600	7311	4248	24
H14A	9297	11639	3965	19
H15A	11048	11821	5863	20
H16A	10108	10077	6991	19
H17A	7399	8082	6212	19
H19D	5662	11212	2097	25
H19E	4886	9398	1089	25
H19F	6910	10249	1615	25
H22A	5348	5204	2047	18
H23A	5611	2974	572	22
H24A	3702	1984	-1393	26
H25A	1506	3154	-1897	30
H26A	1212	5359	-442	25

Table S16. Atomic Occupancy for 3p.

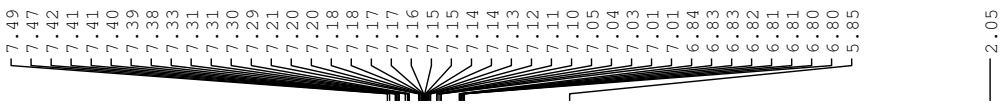
Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
S1	0.77	S2	0.23	H1A	0.77
H1B	0.23	C2	0.77	H2	0.77
C3	0.77	C4	0.77	H4	0.77
C5	0.77	H5	0.77	C6	0.23
H6	0.23	C7	0.23	H7	0.23
C8	0.23	H8	0.23	C9	0.23

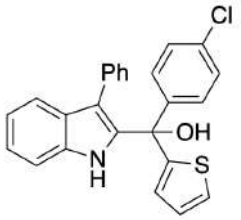



```
Current Data Parameters
NAME           YQL-2-3-S
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210806
Time               22.08
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                126.97
DW                62.400 usec
DE                 6.50 usec
TE                298.7 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300073 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

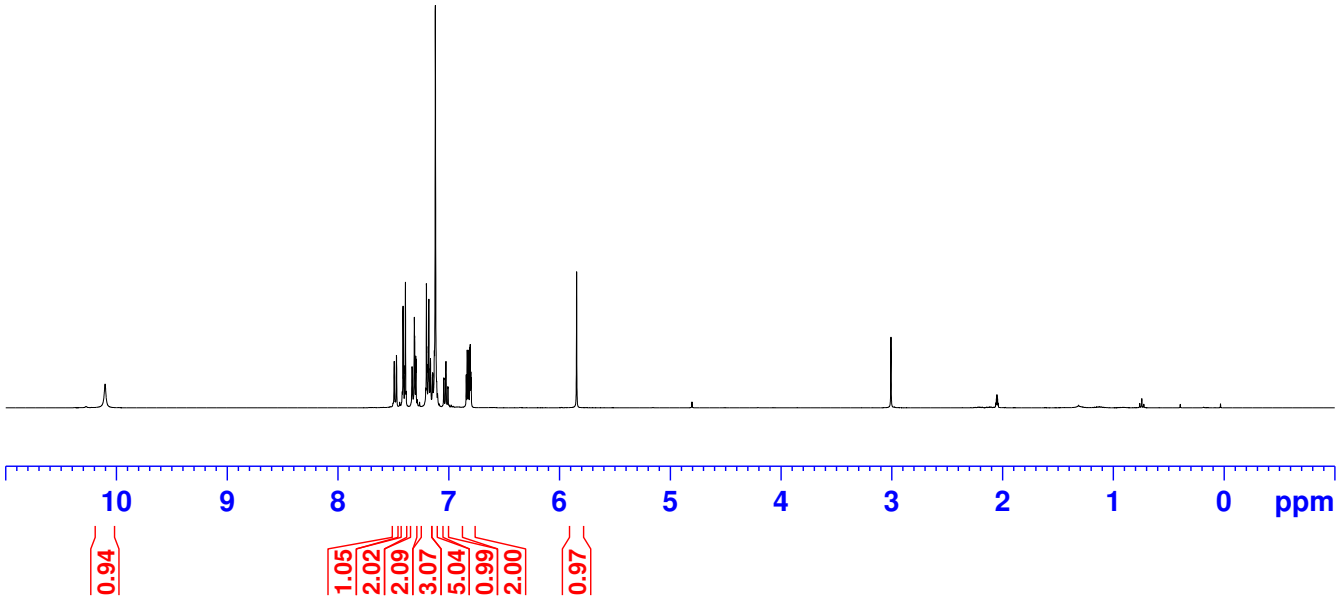



```
Current Data Parameters
NAME          YQL-1-182
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20210721
Time              22.42
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                   51
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 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
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                32768
SF           100.6126909 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

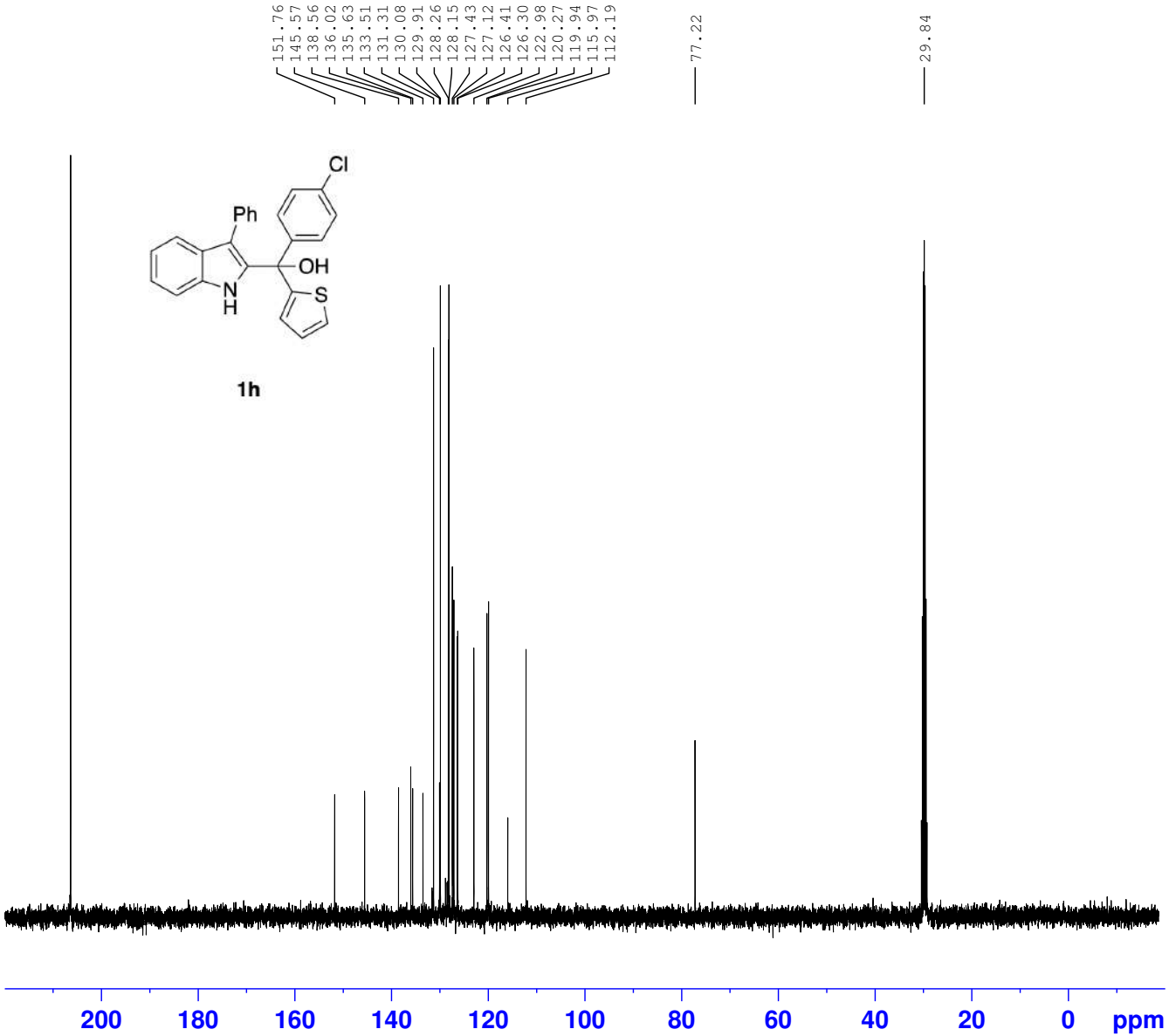




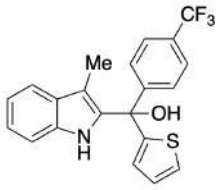
1h



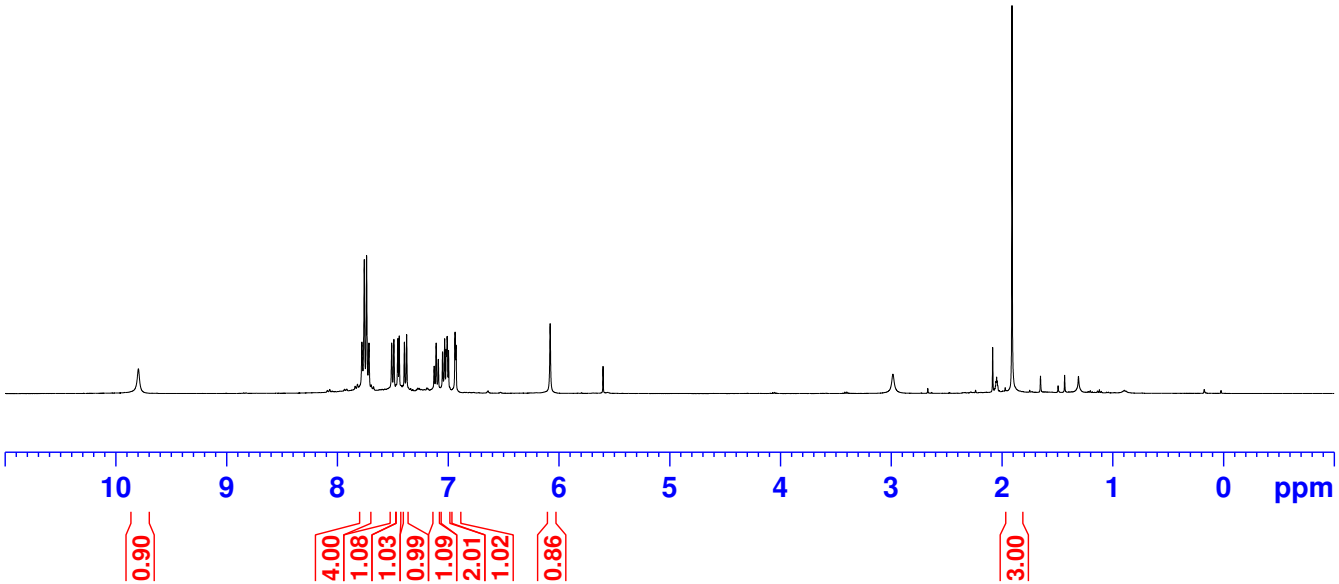

```
Current Data Parameters
NAME          YQL-1-167-
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210806
Time               14.40
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                   101
DW                60.800 usec
DE                 6.00 usec
TE                293.3 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.80 usec
PL1                -1.00 dB
PL1W        12.17476940 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300069 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



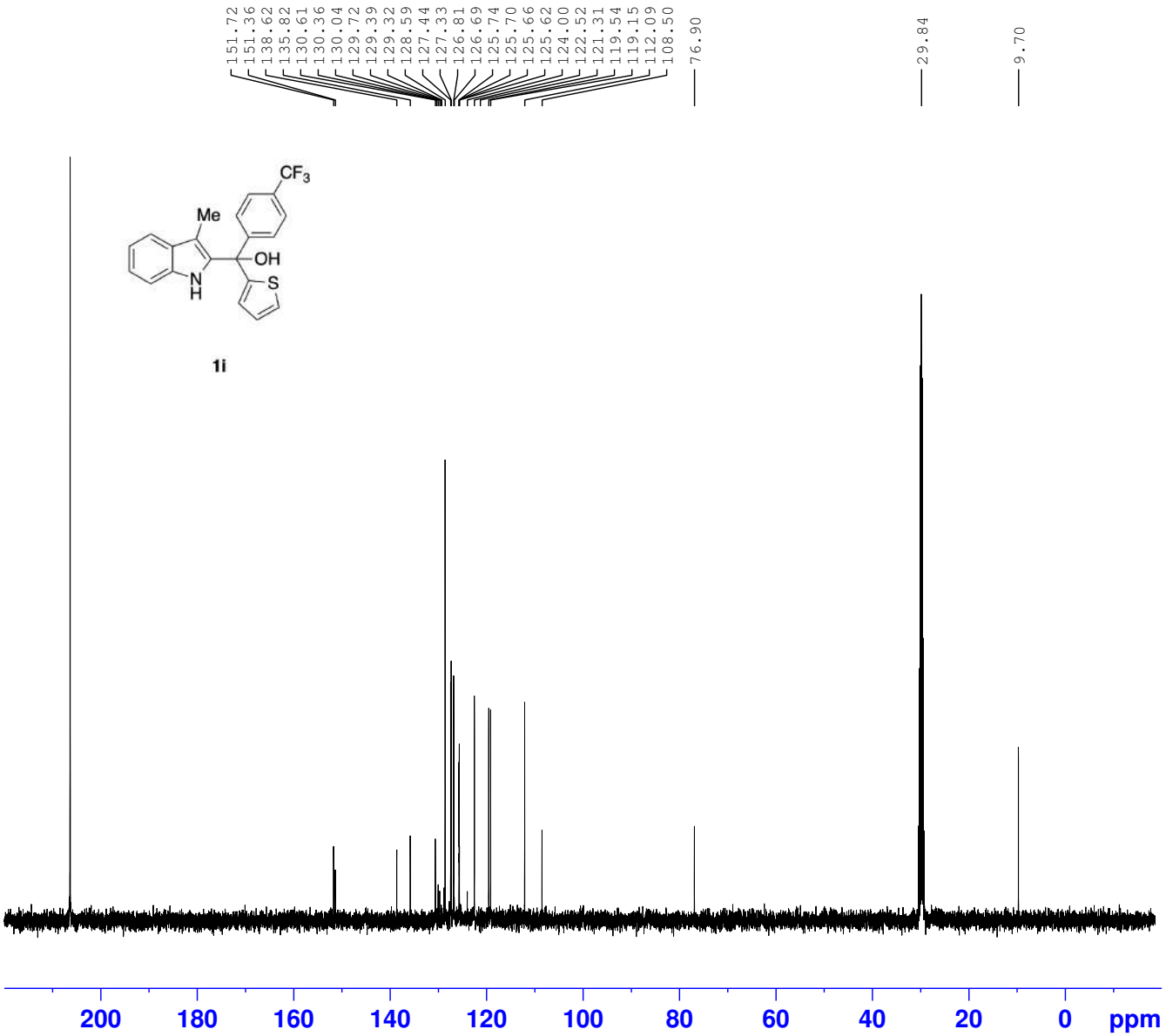

```
Current Data Parameters
NAME          YQL-1-167-
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210806
Time               14.44
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   62
DS                    1
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.00 usec
TE               293.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                40.00 usec
PL1               -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              14.39 dB
PL13              18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6126939 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



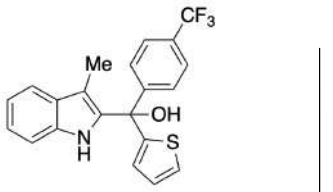
1i




```
Current Data Parameters
NAME         YQL-1-163-A
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210710
Time               22.10
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                 31.55
DW                62.400 usec
DE                 6.50 usec
TE                296.4 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                 65536
SF          400.1300076 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

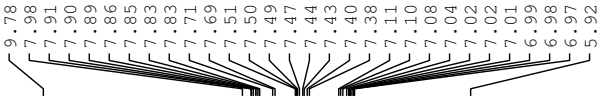


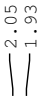

```
Current Data Parameters
NAME      YQL-1-163-A-13C
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210710
Time               22.40
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   80
DS                    1
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.00 usec
TE               295.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                40.00 usec
PL1               -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              14.39 dB
PL13              18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6126858 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

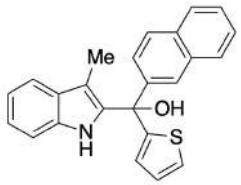


1i

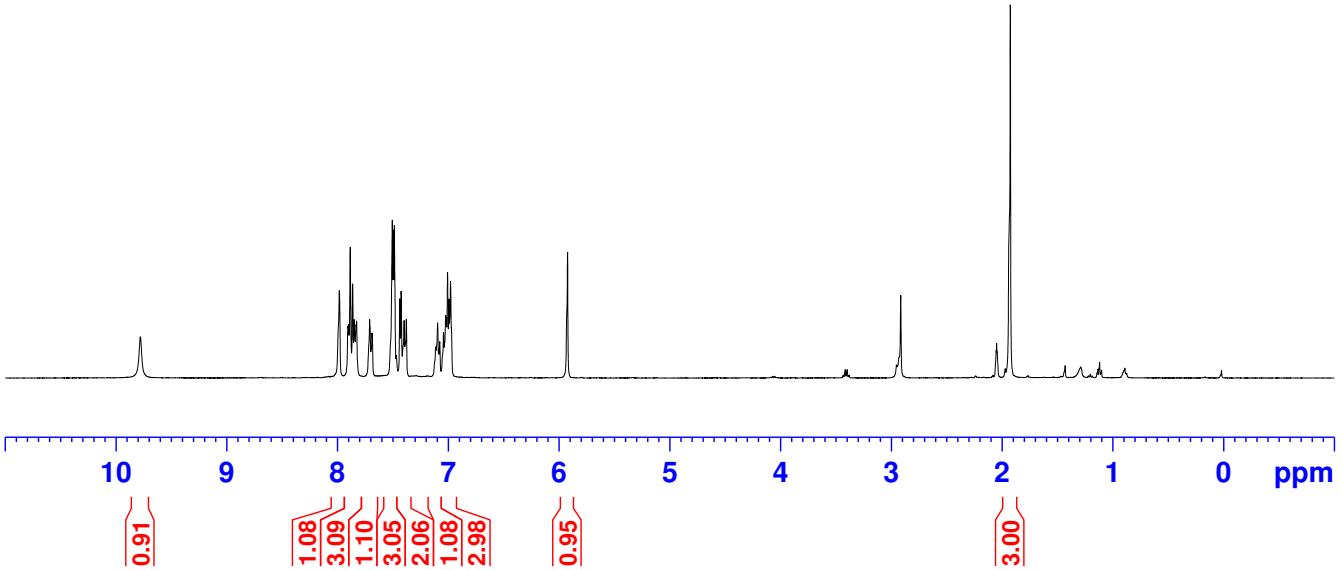

```
Current Data Parameters
NAME         YQL-1-163-A
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210710
Time               22.19
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD              131072
SOLVENT         Acetone
NS                  16
DS                   4
SWH          89285.711 Hz
FIDRES        0.681196 Hz
AQ           0.7340032 sec
RG              196.92
DW               5.600 usec
DE               6.50 usec
TE              296.6 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        376.4607164 MHz
NUC1               19F
P1               14.70 usec
PLW1        15.99600029 W

F2 - Processing parameters
SI                65536
SF          376.4983660 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



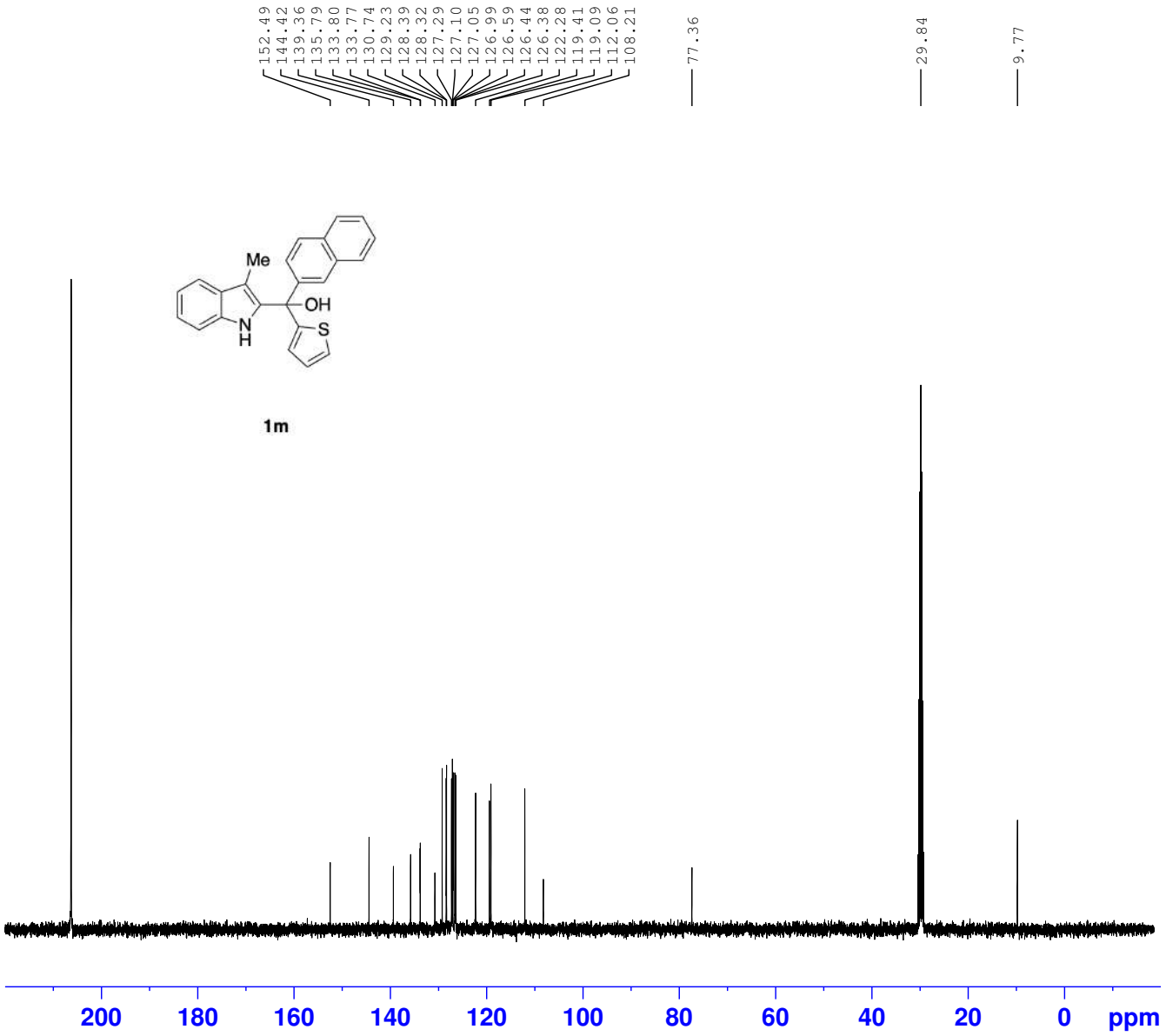




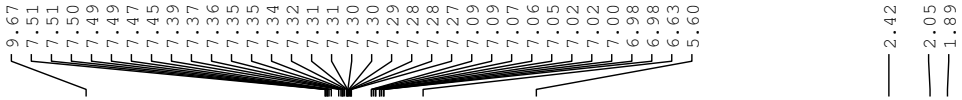
1m

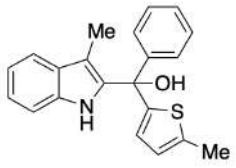



```
Current Data Parameters
NAME        YQL-1-151-Sm
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210710
Time               21.25
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                   181
DW                60.800 usec
DE                 6.00 usec
TE                295.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.80 usec
PL1               -1.00 dB
PL1W        12.17476940 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300074 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

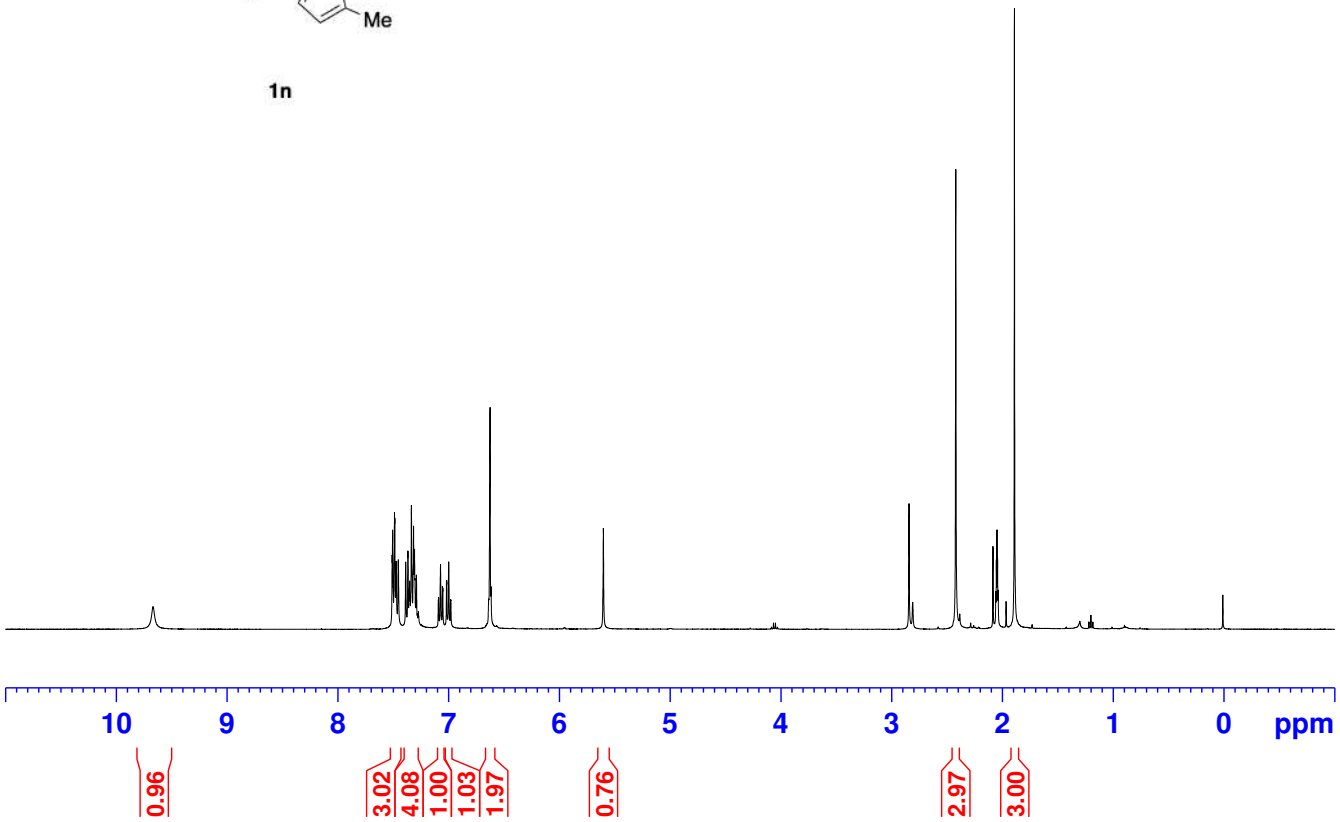



```
Current Data Parameters
NAME        YQL-1-151-Sm
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210710
Time               21.29
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT          Acetone
NS                   200
DS                     1
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                  2050
DW                20.800 usec
DE                 6.00 usec
TE                295.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 40.00 usec
PL1                -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               14.39 dB
PL13               18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF         100.6126851 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

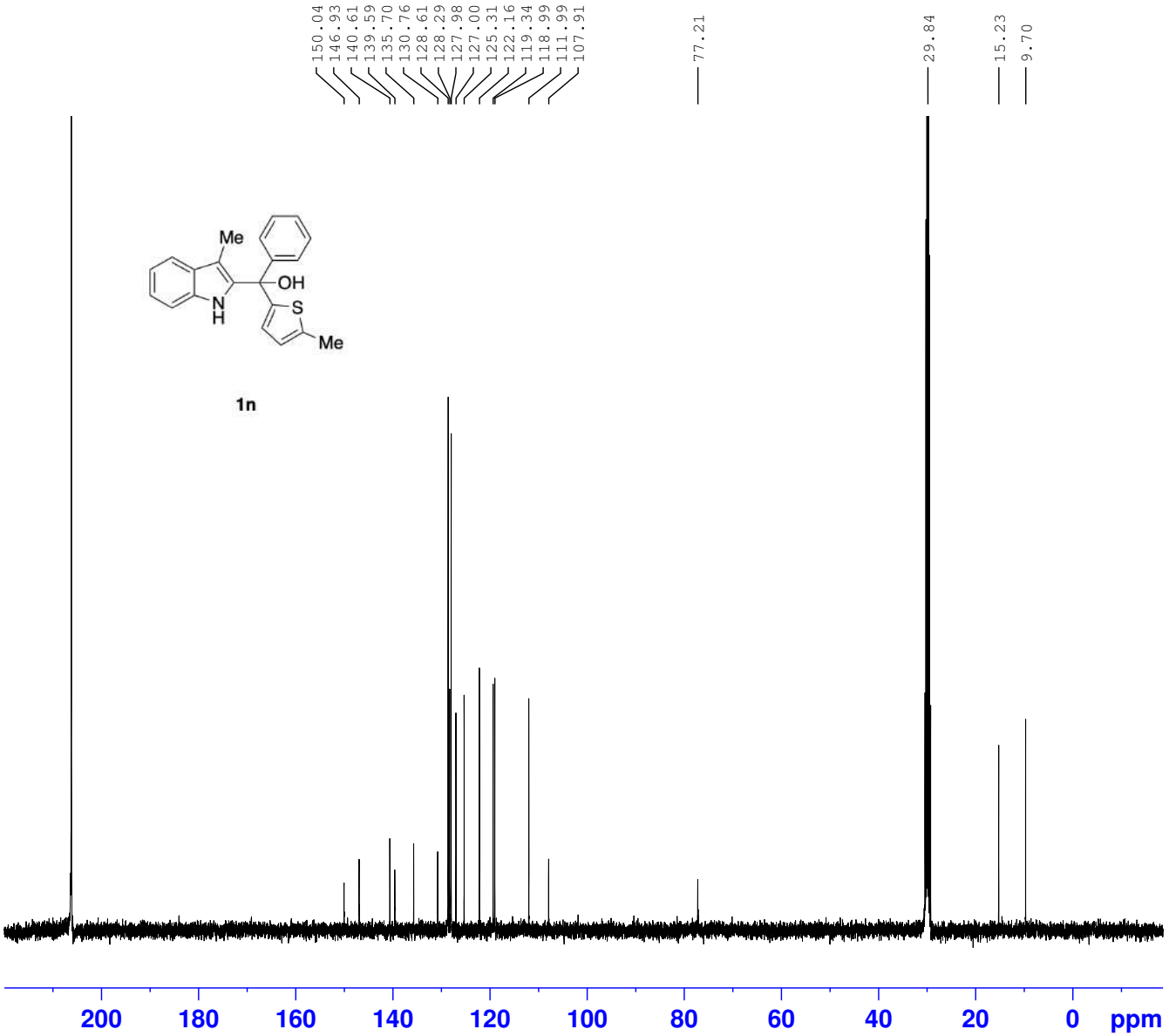




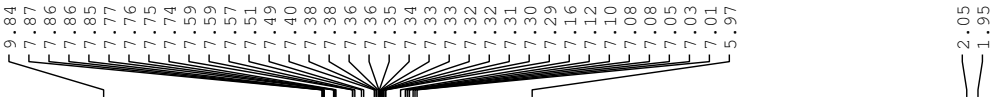
1n

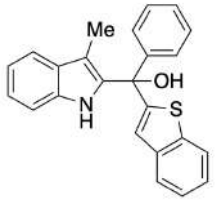



```
Current Data Parameters
NAME      CTAM-1013-re-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210628
Time              21.41
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32050
SOLVENT         Acetone
NS                    4
DS                    0
SWH            8012.820 Hz
FIDRES         0.250010 Hz
AQ            1.9999200 sec
RG                 62.3
DW               62.400 usec
DE                6.50 usec
TE               300.3 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                   1H
P1                  9.15 usec
PLW1        16.00000000 W

F2 - Processing parameters
SI                 65536
SF          400.1300068 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

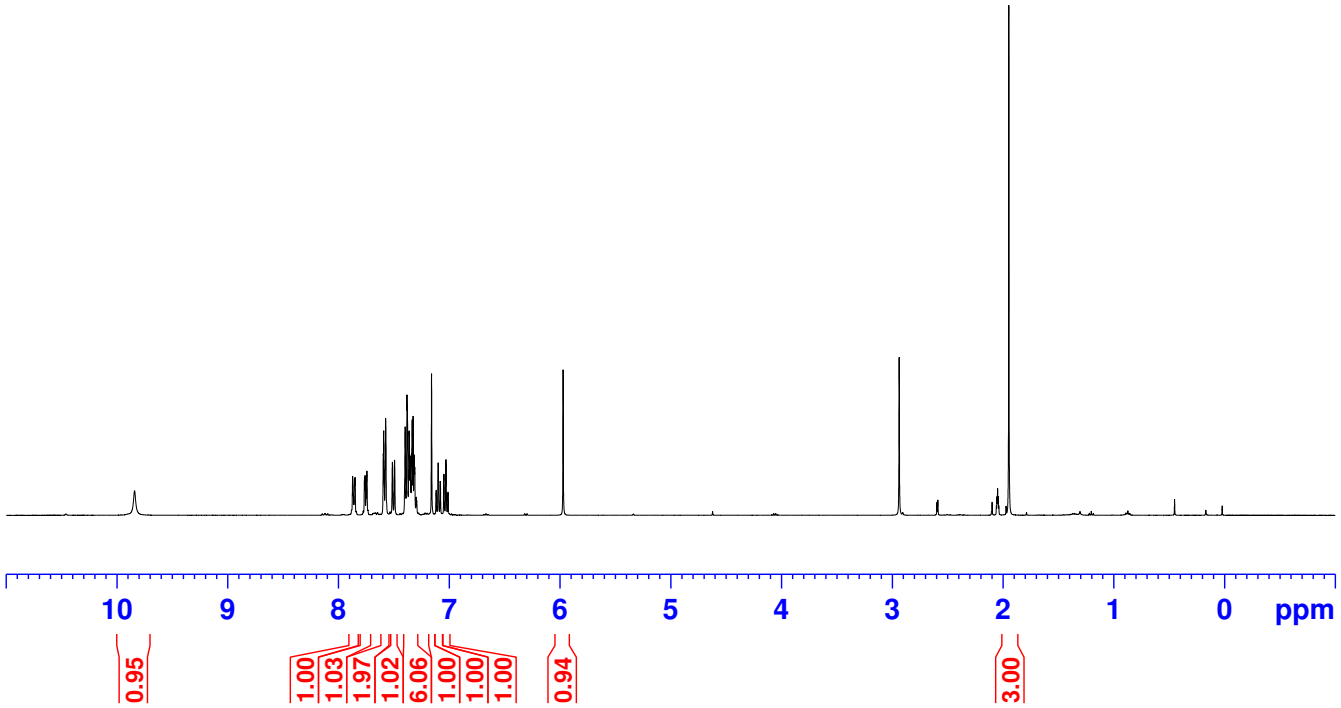



```
Current Data Parameters
NAME      CTAM-1013-re-2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210628
Time              21.34
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  100
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.42
DW               20.800 usec
DE                6.50 usec
TE               300.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                10.22 usec
PLW1        74.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        16.00000000 W
PLW12        0.16538000 W
PLW13        0.13395999 W

F2 - Processing parameters
SI                 32768
SF          100.6126803 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

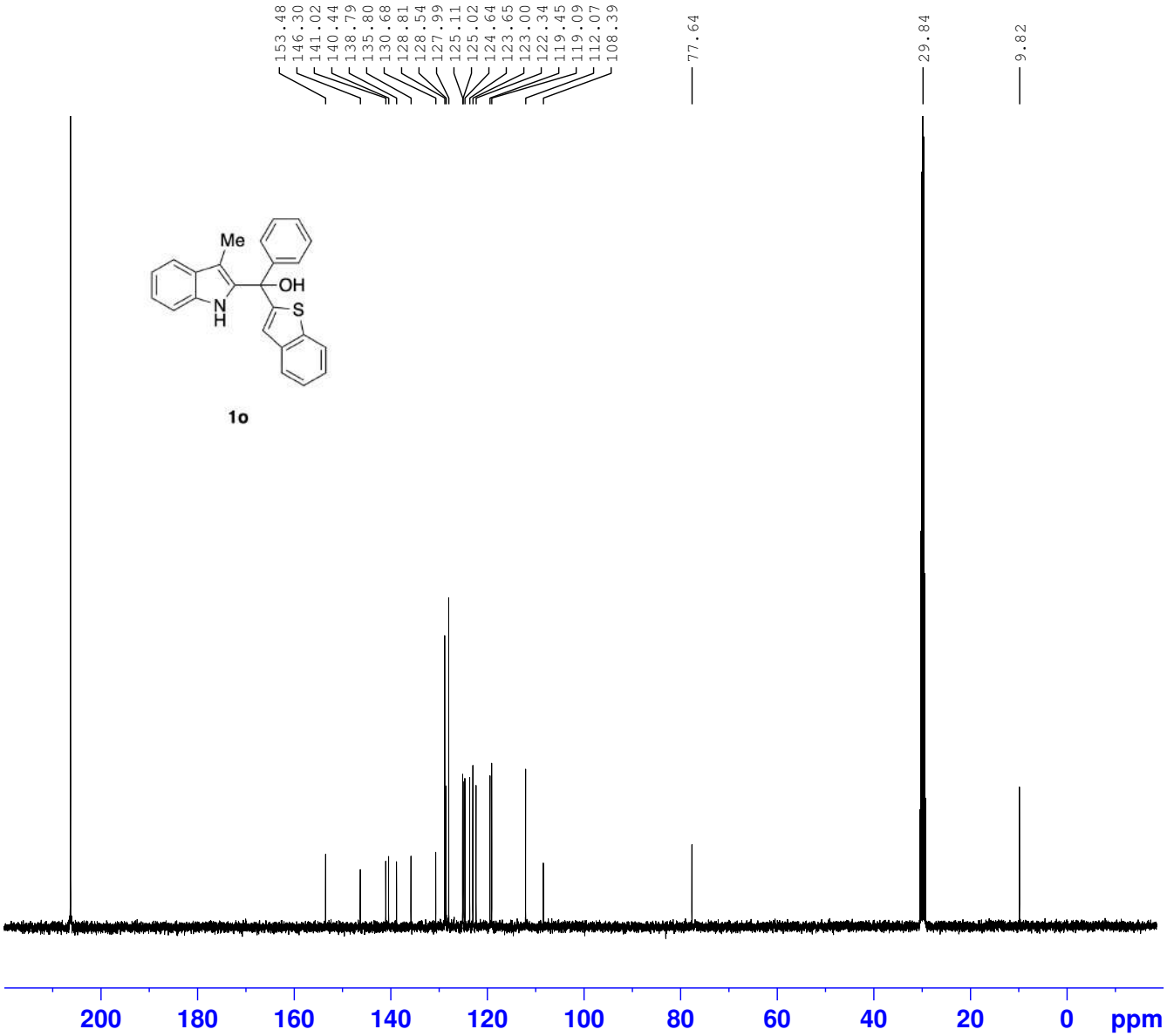




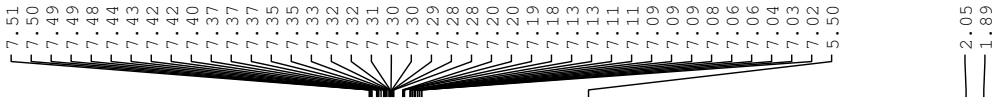
1o

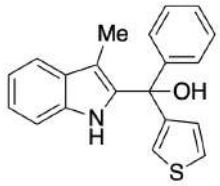



```
Current Data Parameters
NAME            YQL-2-11
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210731
Time               18.29
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                 34.77
DW                62.400 usec
DE                 6.50 usec
TE                296.7 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300075 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

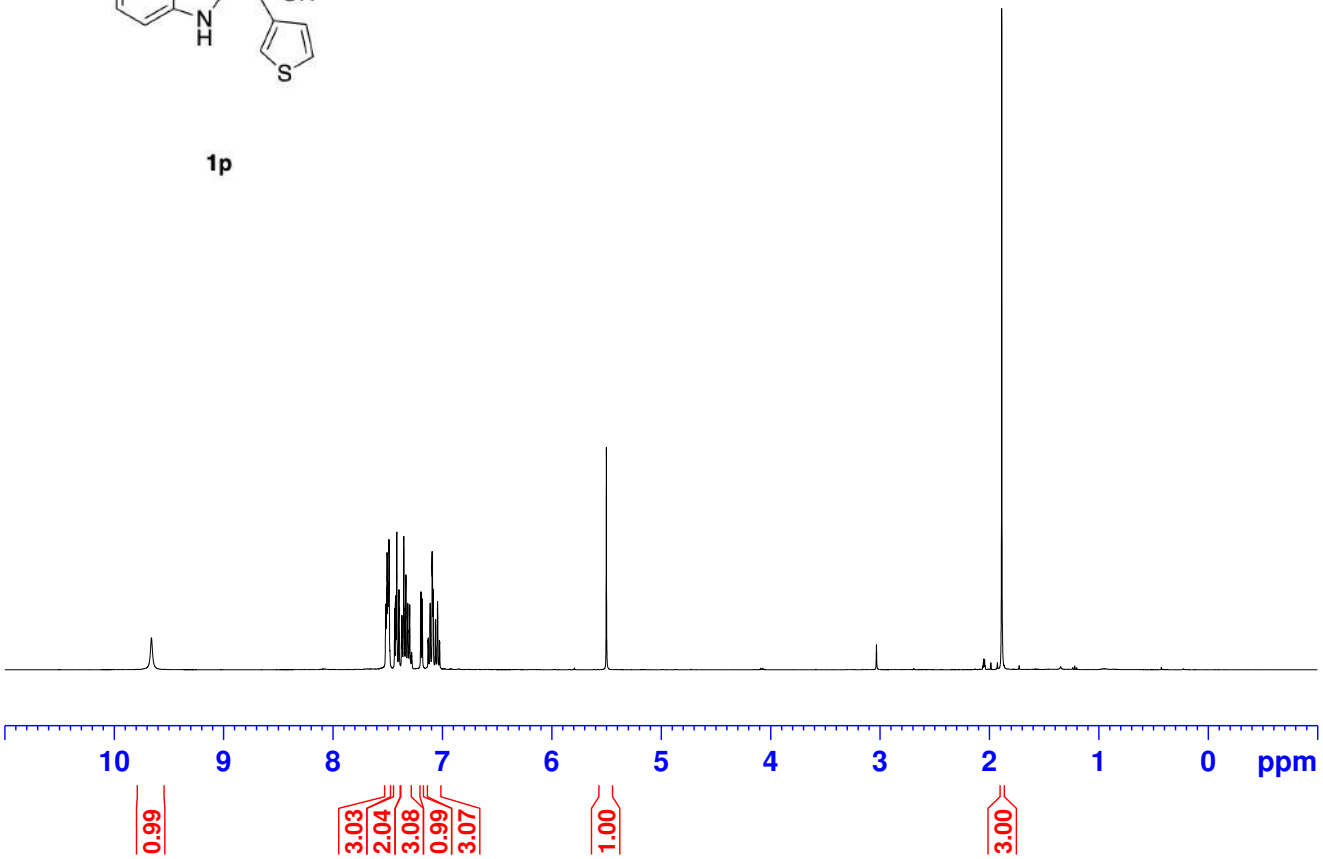



```
Current Data Parameters
NAME                  YQL-2-11
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20210731
Time                     18.32
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                Acetone
NS                            54
DS                             2
SWH                  24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631488 sec
RG                       196.92
DW                       20.800 usec
DE                        6.50 usec
TE                       297.3 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
SFO1               100.6228298 MHz
NUC1                       13C
P1                        9.70 usec
PLW1               46.98899841 W

======== CHANNEL f2 ========
SFO2               400.1316005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2               11.99499989 W
PLW12               0.34213999 W
PLW13               0.27713001 W

F2 - Processing parameters
SI                         32768
SF                 100.6126859 MHz
WDW                           EM
SSB                            0
LB                        1.00 Hz
GB                             0
PC                        1.40
```

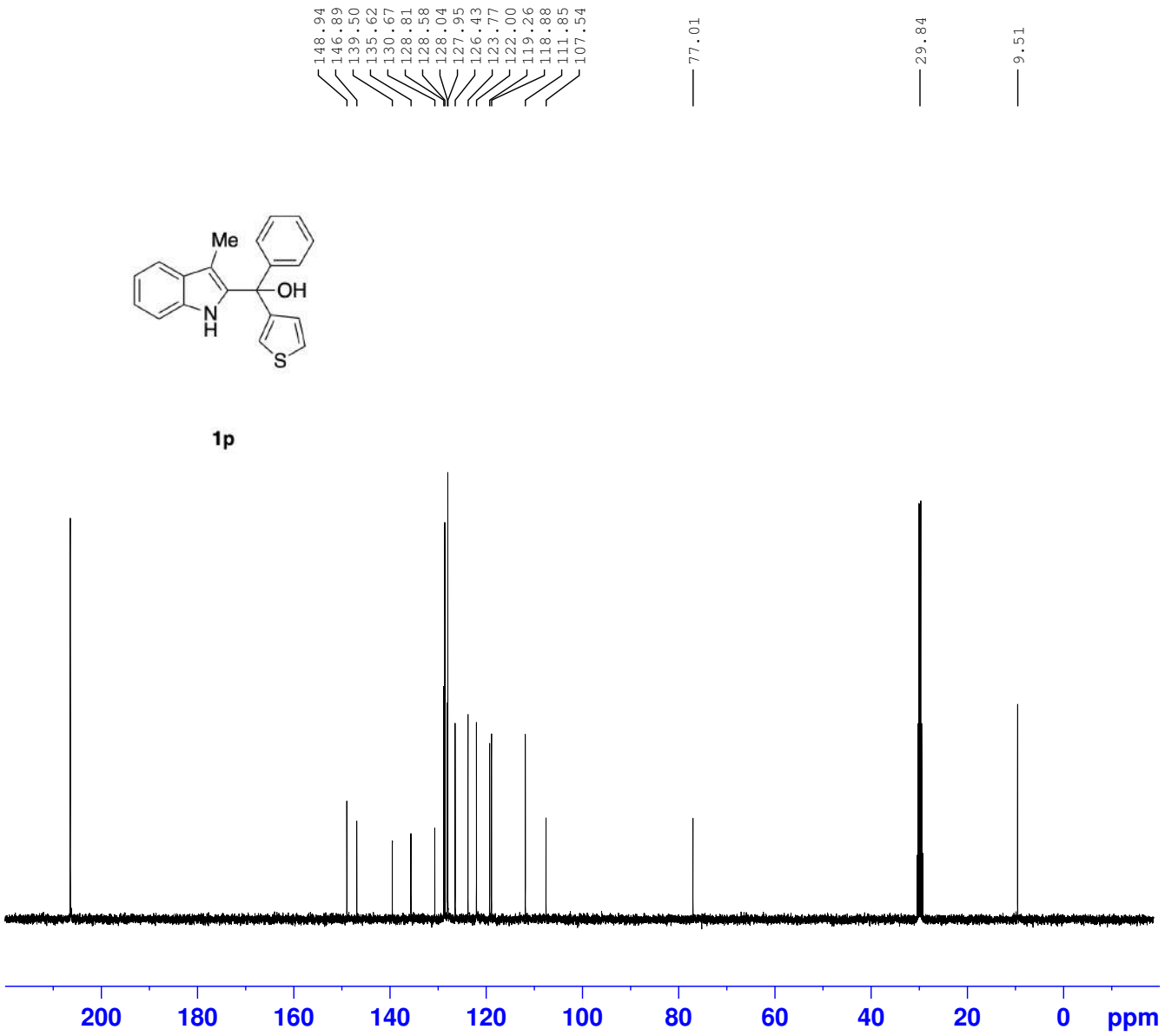




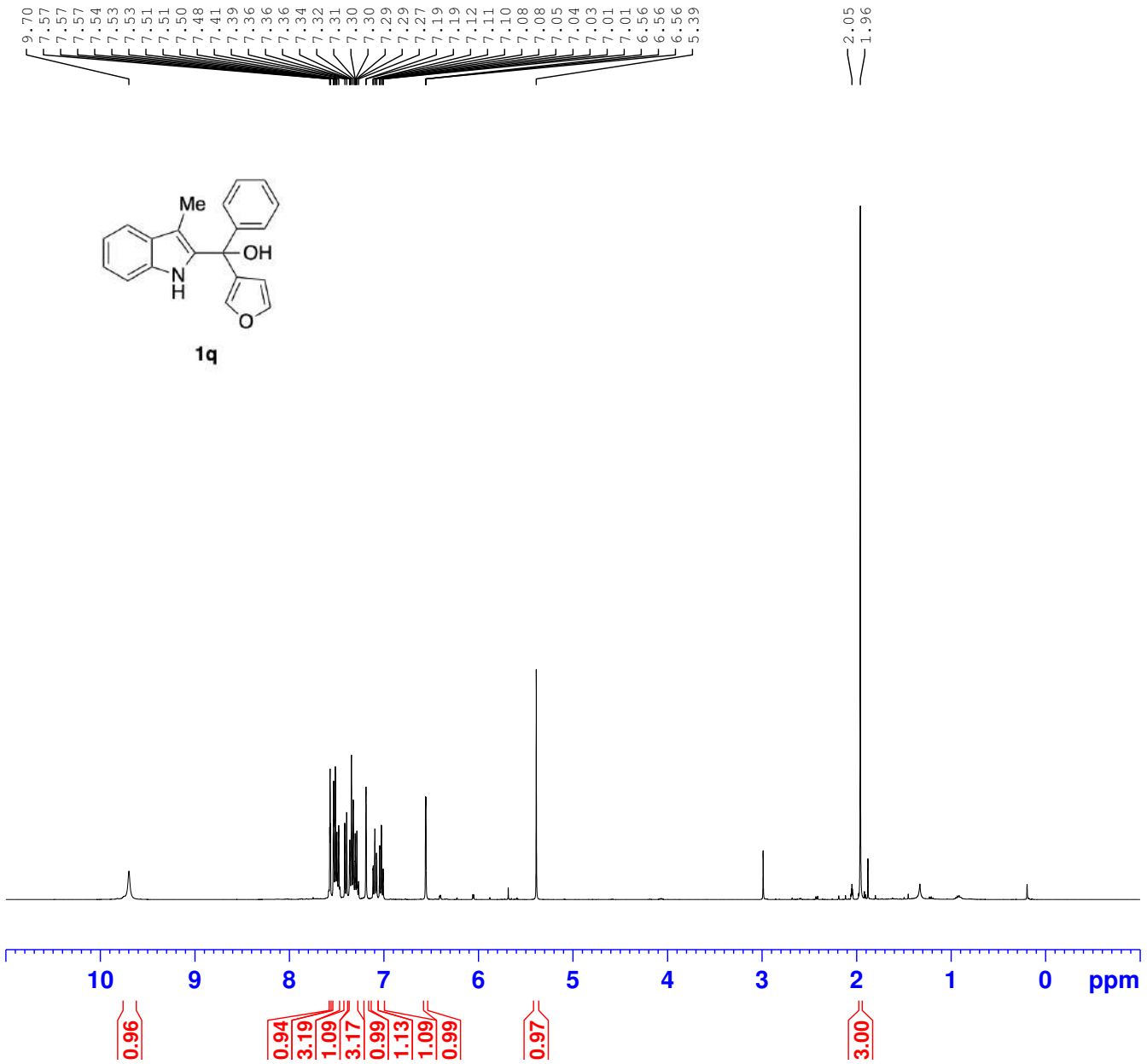
1p



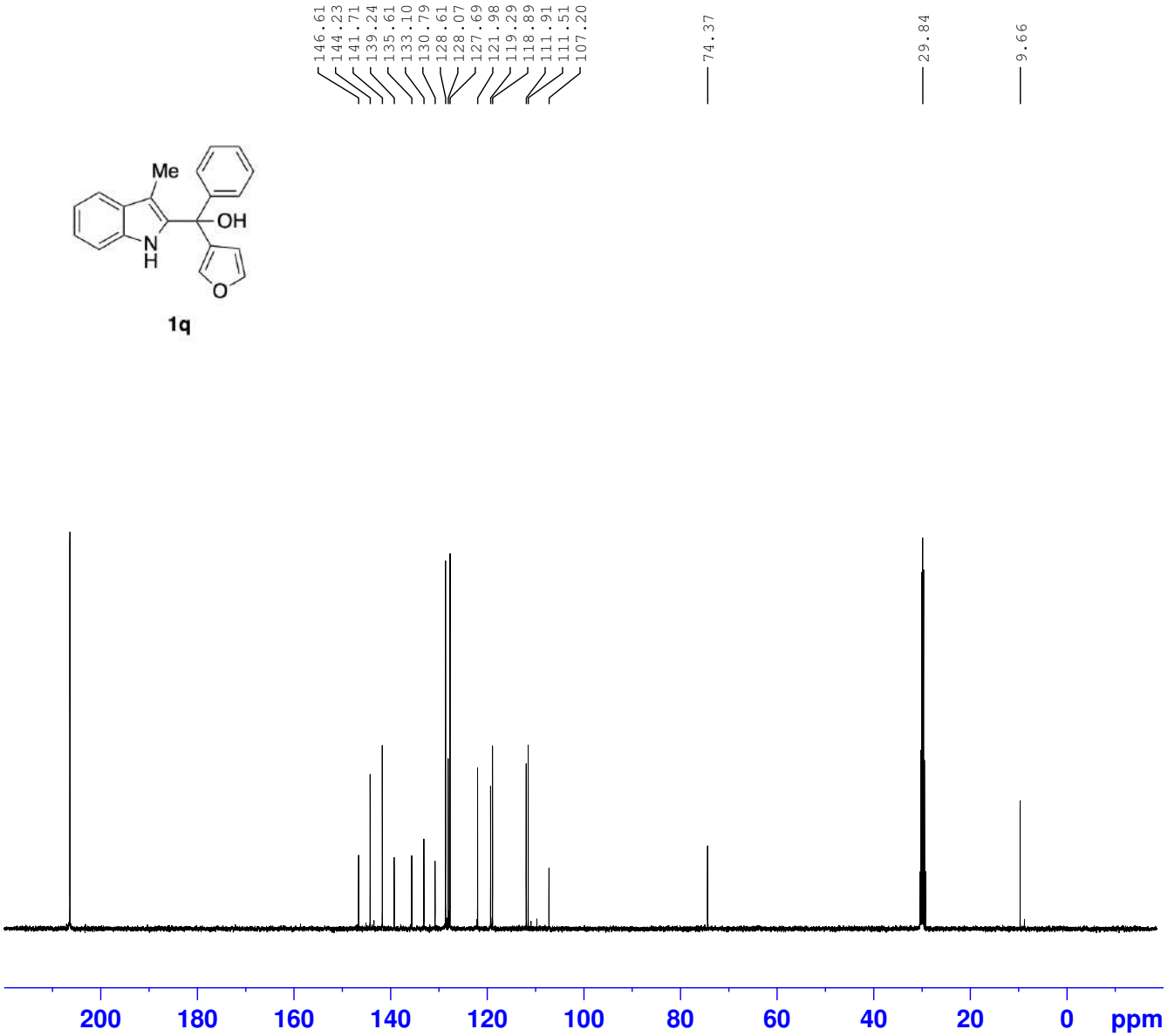

```
Current Data Parameters
NAME                  YQL-2-64
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20210918
Time                     10.54
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT               Acetone
NS                           8
DS                           0
SWH                 8012.820 Hz
FIDRES                0.122266 Hz
AQ                  4.0894465 sec
RG                       22.47
DW                     62.400 usec
DE                      6.50 usec
TE                     297.7 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1               11.99499989 W

F2 - Processing parameters
SI                      65536
SF                 400.1300072 MHz
WDW                        EM
SSB                          0
LB                      0.30 Hz
GB                           0
PC                      1.00
```



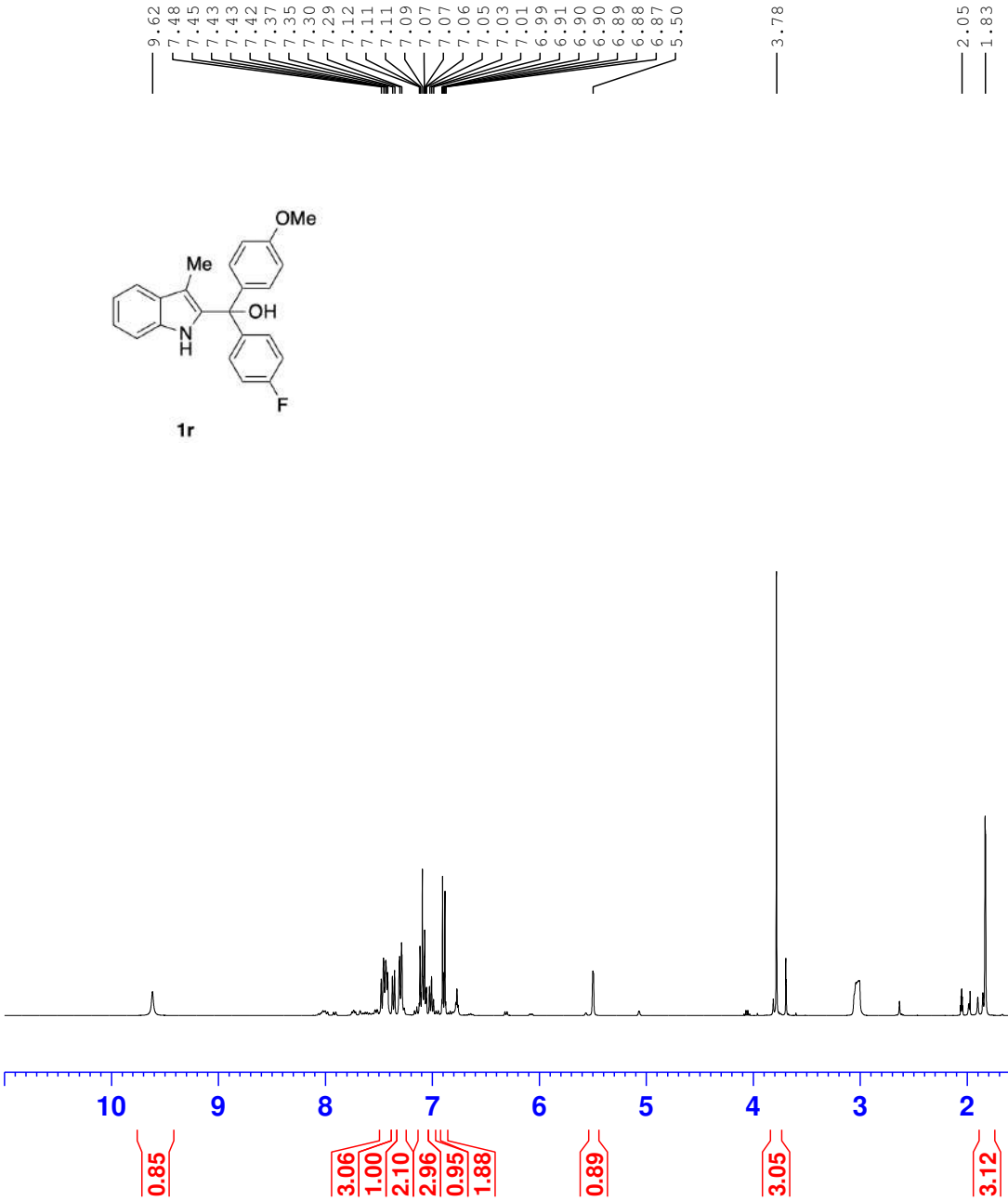

```
Current Data Parameters
NAME            YQL-2-64
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210918
Time               11.01
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                    22
DS                     2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                  9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6126986 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



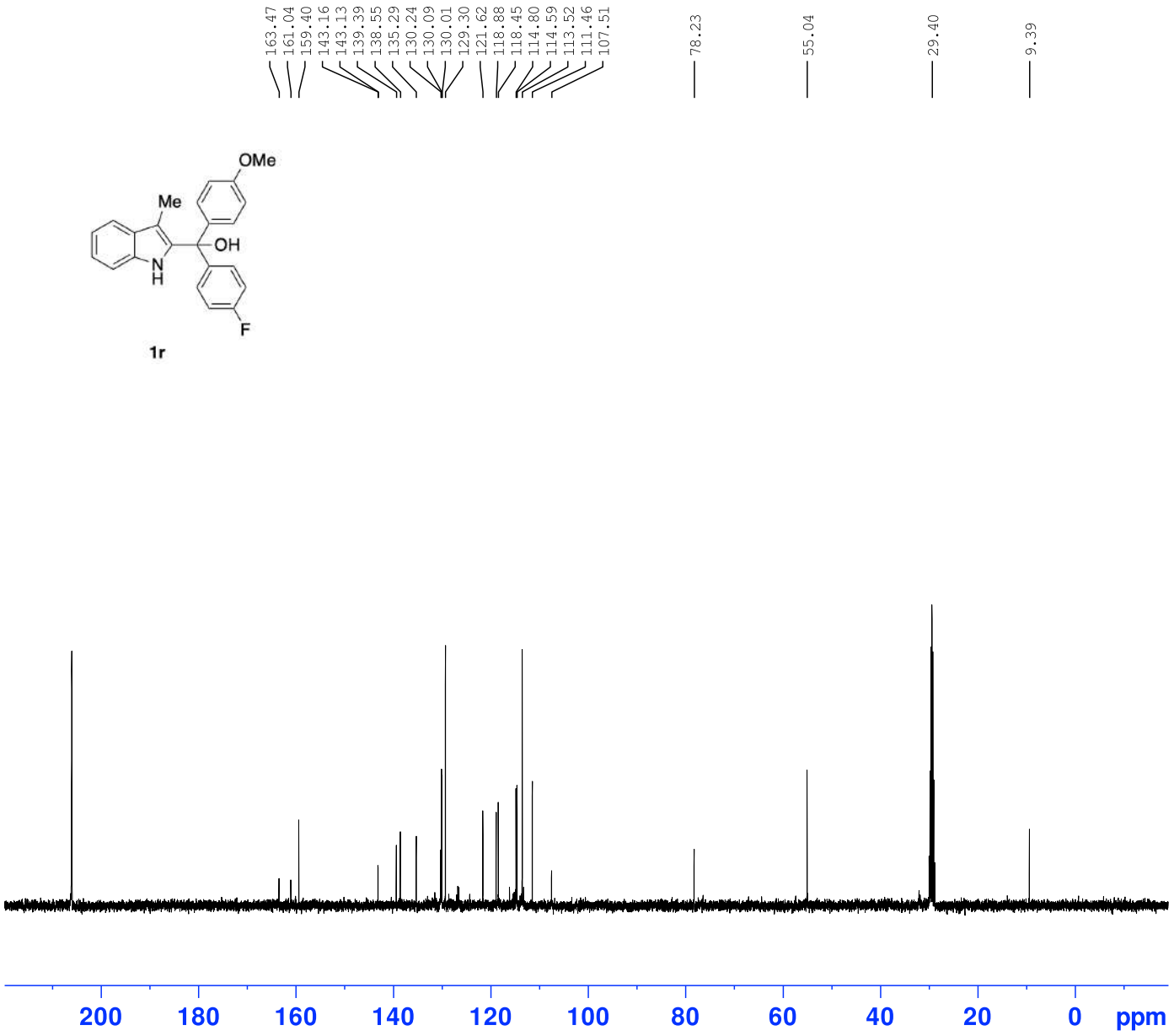

```
Current Data Parameters
NAME            YQL-2-77
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211007
Time                9.14
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ              4.0894465 sec
RG                 25.32
DW                62.400 usec
DE                 6.50 usec
TE                297.3 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300075 MHz
WDW                  EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```




```
Current Data Parameters
NAME            YQL-2-77
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211007
Time                9.17
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT          Acetone
NS                    56
DS                     2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 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
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6126902 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



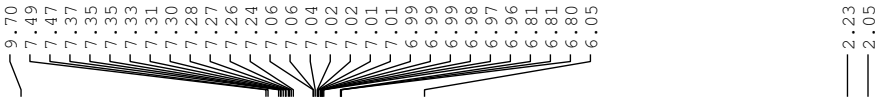

```
Current Data Parameters
NAME           YQL-2-183
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220302
Time               17.00
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9845889 sec
RG                   101
DW                60.800 usec
DE                 6.00 usec
TE                293.5 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.80 usec
PL1               -1.00 dB
PL1W        12.17476940 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300069 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```

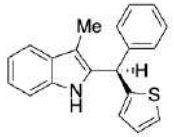



```
Current Data Parameters
NAME                  YQL-2-183
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20220302
Time                      17.08
INSTRUM                   spect
PROBHD    5 mm DUL 13C-1
PULPROG                  zgpg30
TD                        65536
SOLVENT                 Acetone
NS                             99
DS                              1
SWH                    24038.461 Hz
FIDRES                  0.366798 Hz
AQ                     1.3631488 sec
RG                           2050
DW                         20.800 usec
DE                          6.00 usec
TE                         293.6 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                          13C
P1                         40.00 usec
PL1                        -3.00 dB
PL1W                60.64365387 W
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                          1H
PCPD2                      80.00 usec
PL2                        -1.00 dB
PL12                       14.39 dB
PL13                       18.00 dB
PL2W                12.17476940 W
PL12W                0.35193357 W
PL13W                0.15327126 W
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                            32768
SF                 100.6127321 MHz
WDW                              EM
SSB                               0
LB                             1.00 Hz
GB                                0
PC                             1.40
```

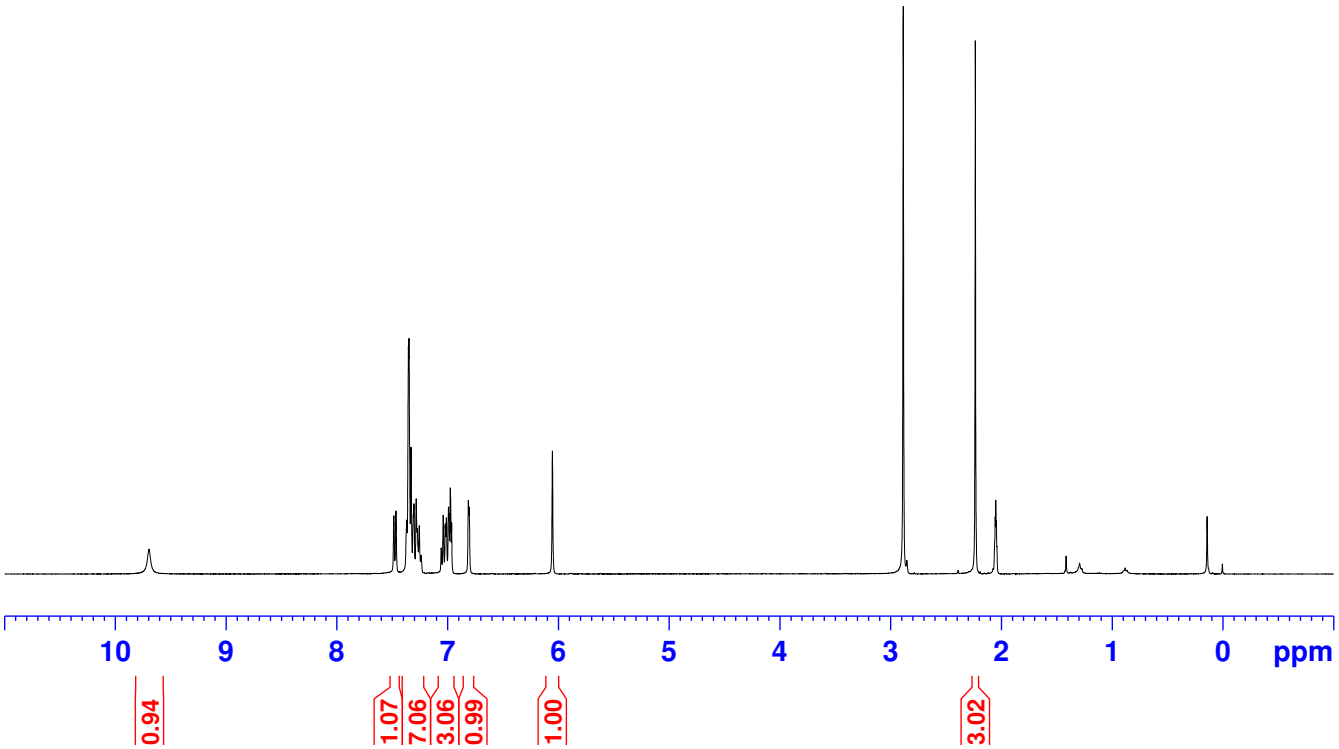
1r


```
Current Data Parameters
NAME         YQL-2-183-F
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220308
Time               16.20
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD               131072
SOLVENT         Acetone
NS                    16
DS                     4
SWH            89285.711 Hz
FIDRES         0.681196 Hz
AQ             0.7340032 sec
RG                196.92
DW                 5.600 usec
DE                 6.50 usec
TE                294.6 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         376.4607164 MHz
NUC1                19F
P1                 14.70 usec
PLW1         15.99600029 W

F2 - Processing parameters
SI                 65536
SF           376.4983660 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

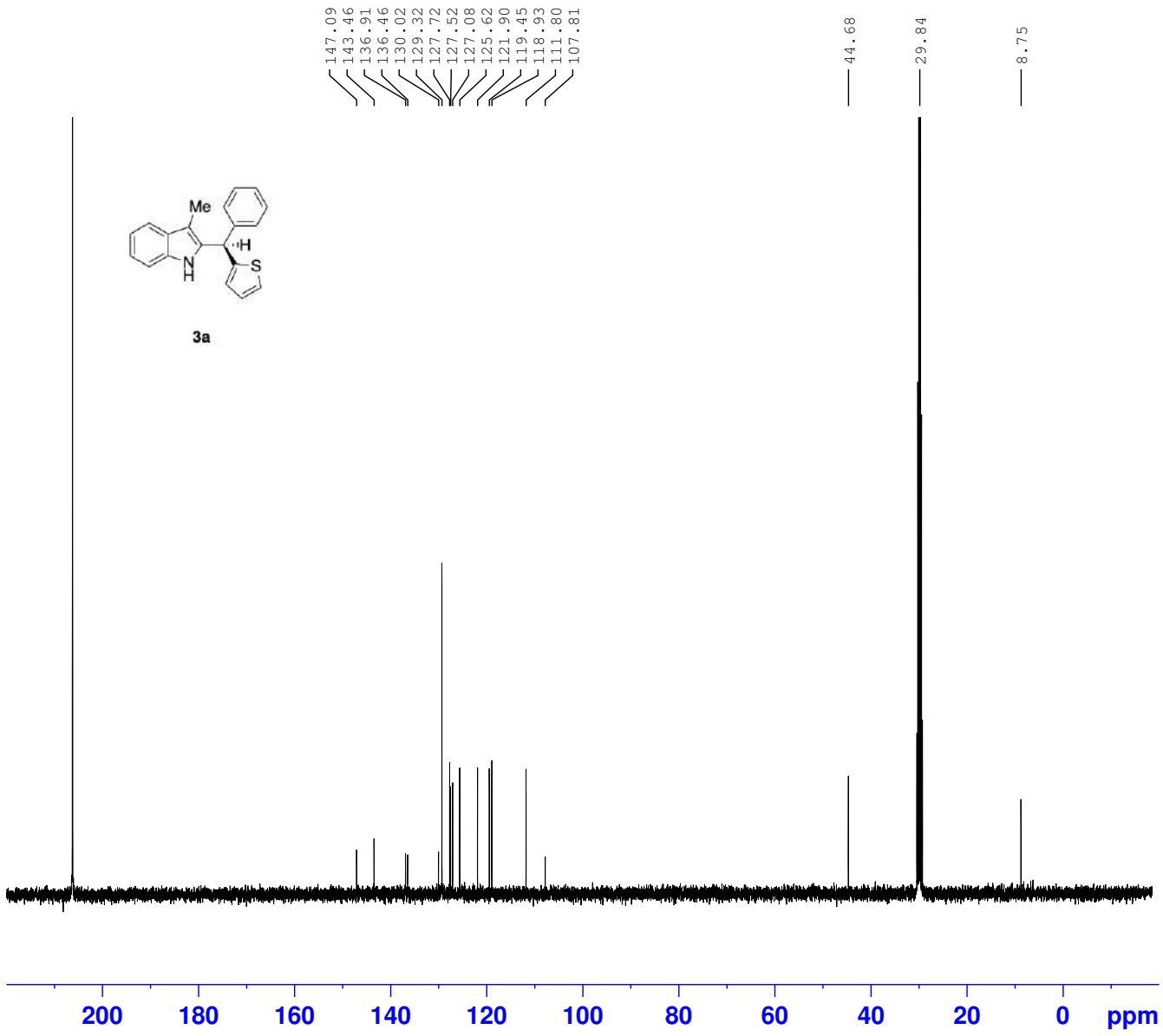




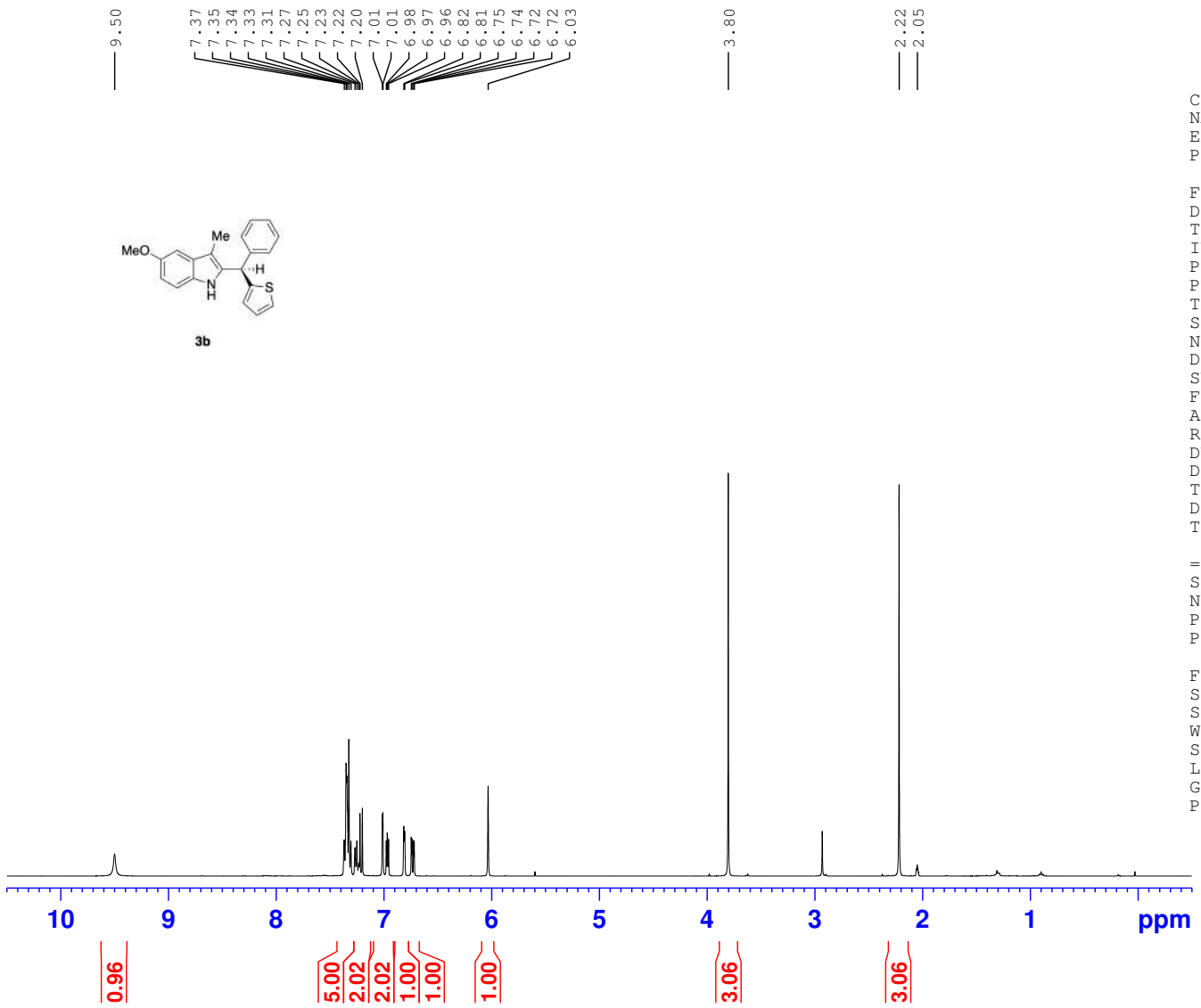
3a



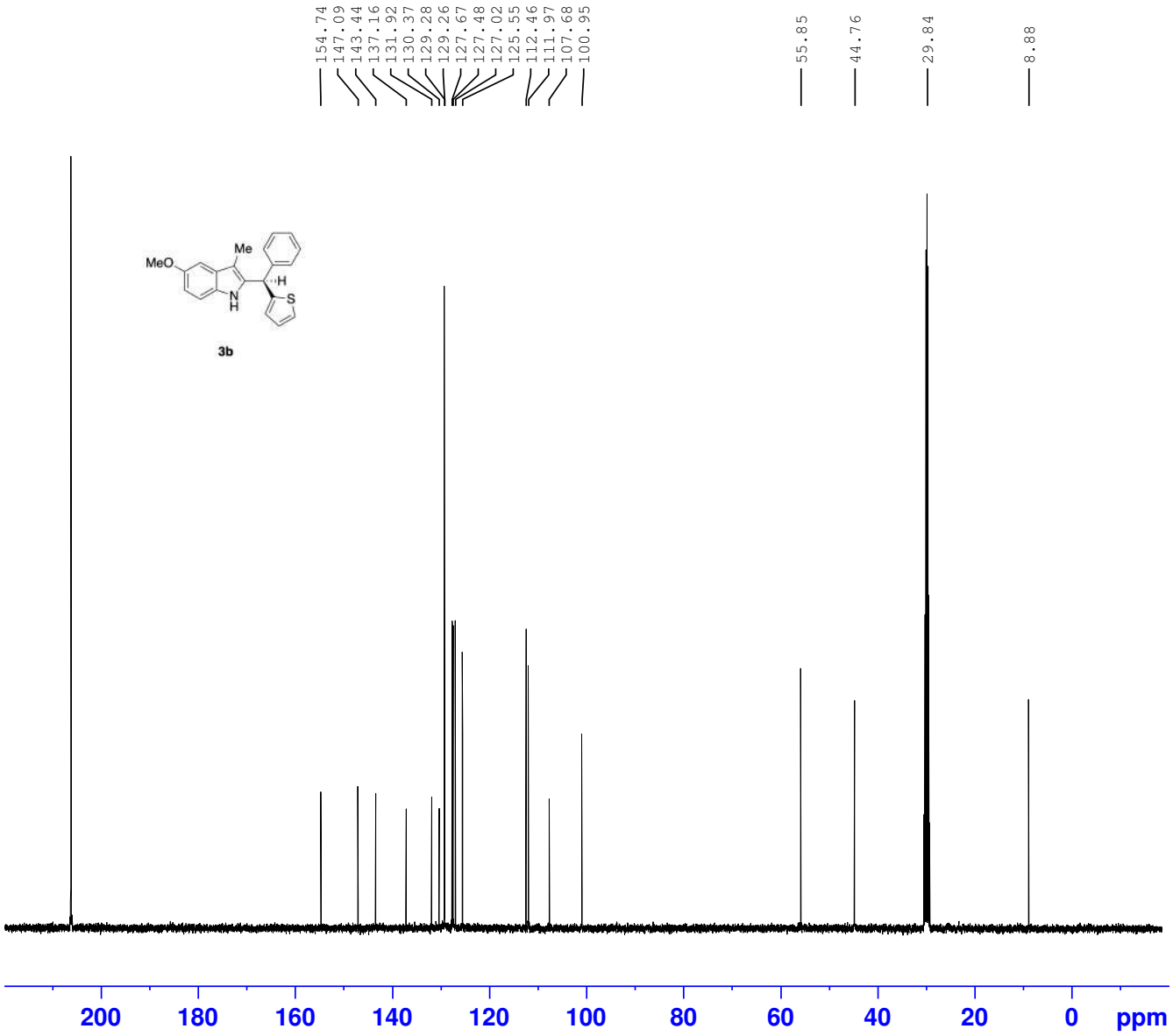

```
Current Data Parameters
NAME           YQL-1-146
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210701
Time               13.47
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9845889 sec
RG                   322
DW                60.800 usec
DE                 6.00 usec
TE                294.3 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.80 usec
PL1                -1.00 dB
PL1W        12.17476940 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300070 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



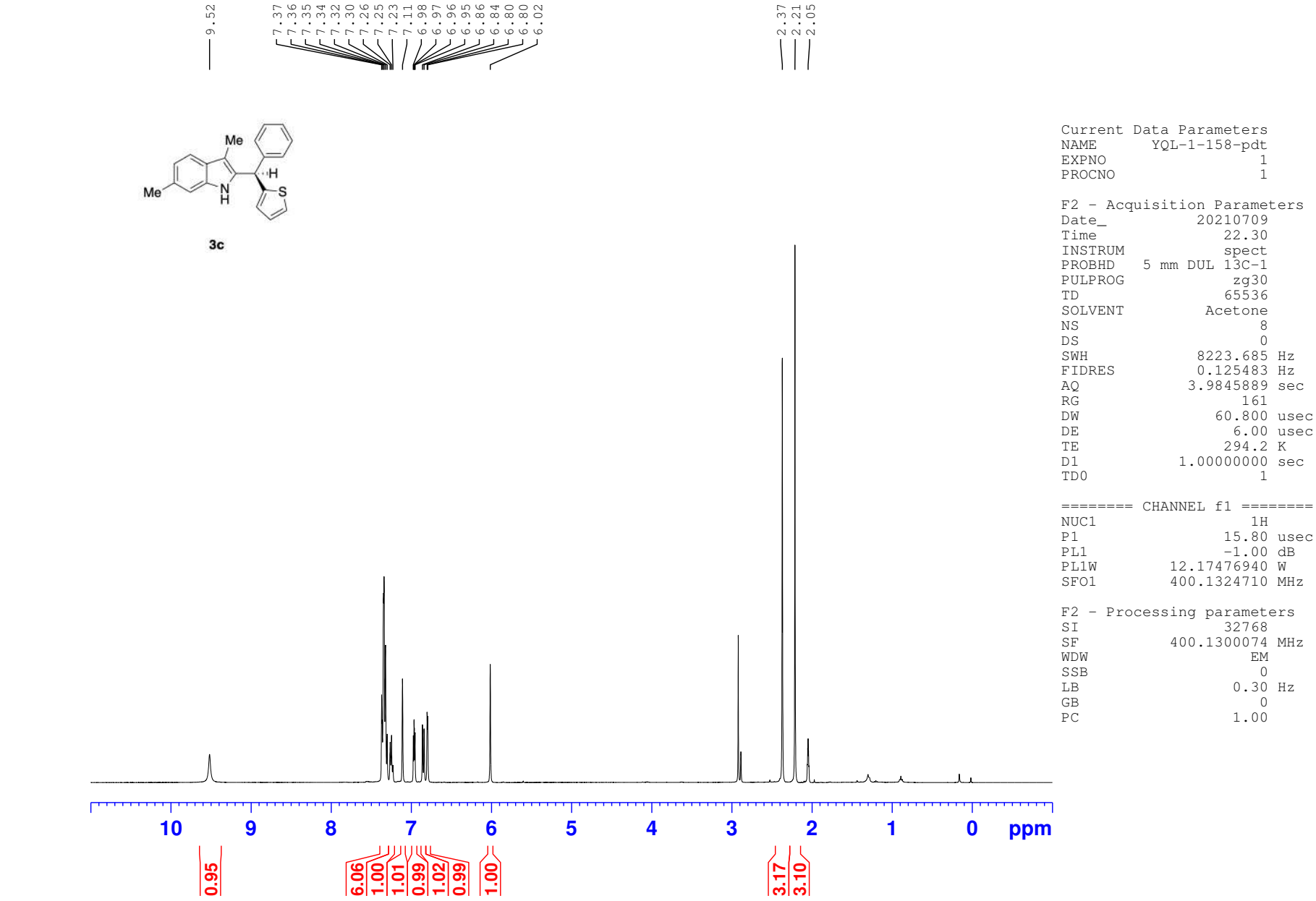

```
Current Data Parameters
NAME           YQL-1-146
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210701
Time               13.50
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT          Acetone
NS                   268
DS                     1
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                  2050
DW                20.800 usec
DE                 6.00 usec
TE                294.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 40.00 usec
PL1                -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               14.39 dB
PL13               18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF         100.6126815 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



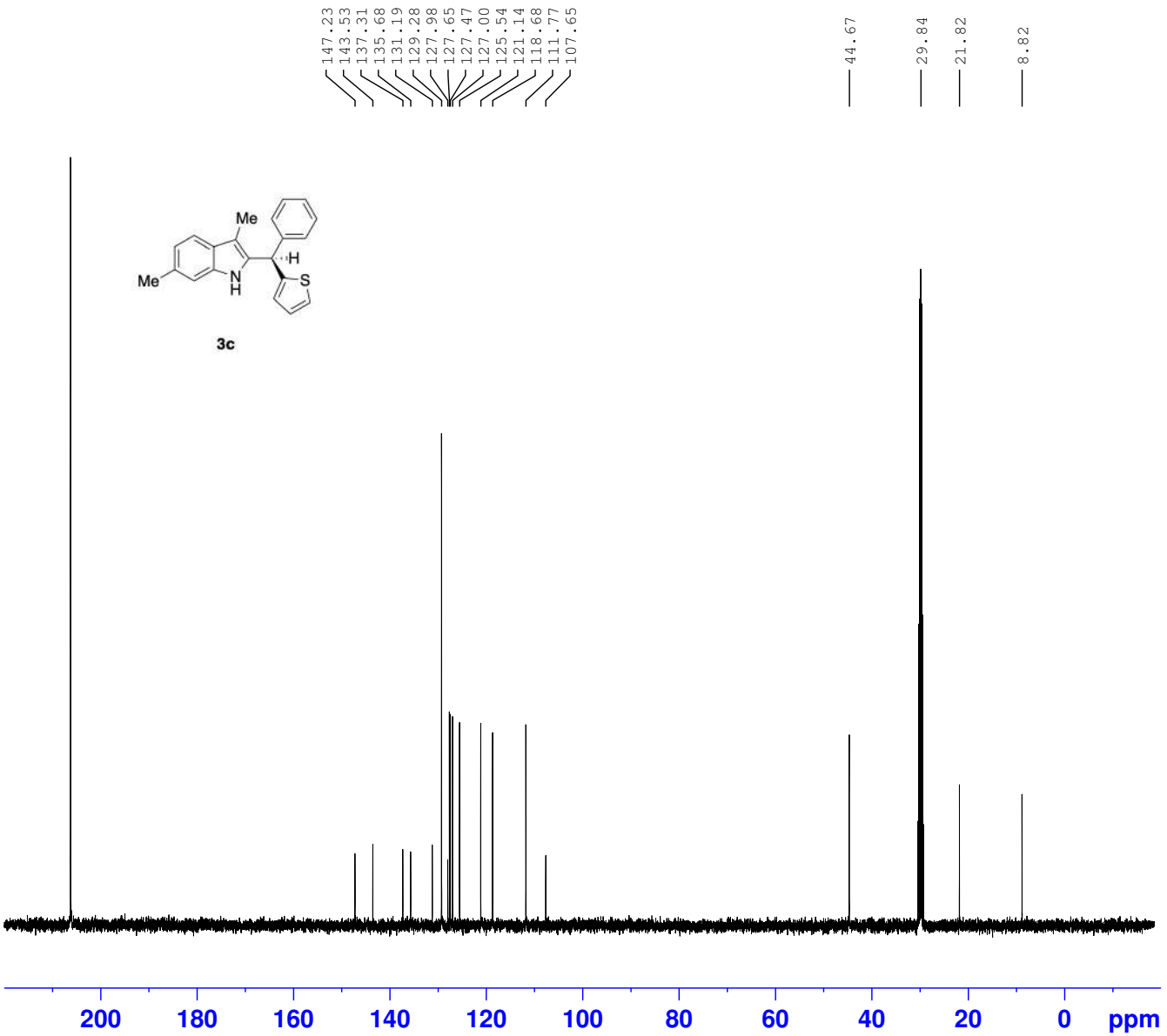

```
Current Data Parameters
NAME          YQL-2-3-p
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210725
Time              21.57
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                    8
DS                    0
SWH            8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                27.78
DW               62.400 usec
DE                6.50 usec
TE               296.5 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1                14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                65536
SF          400.1300077 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```



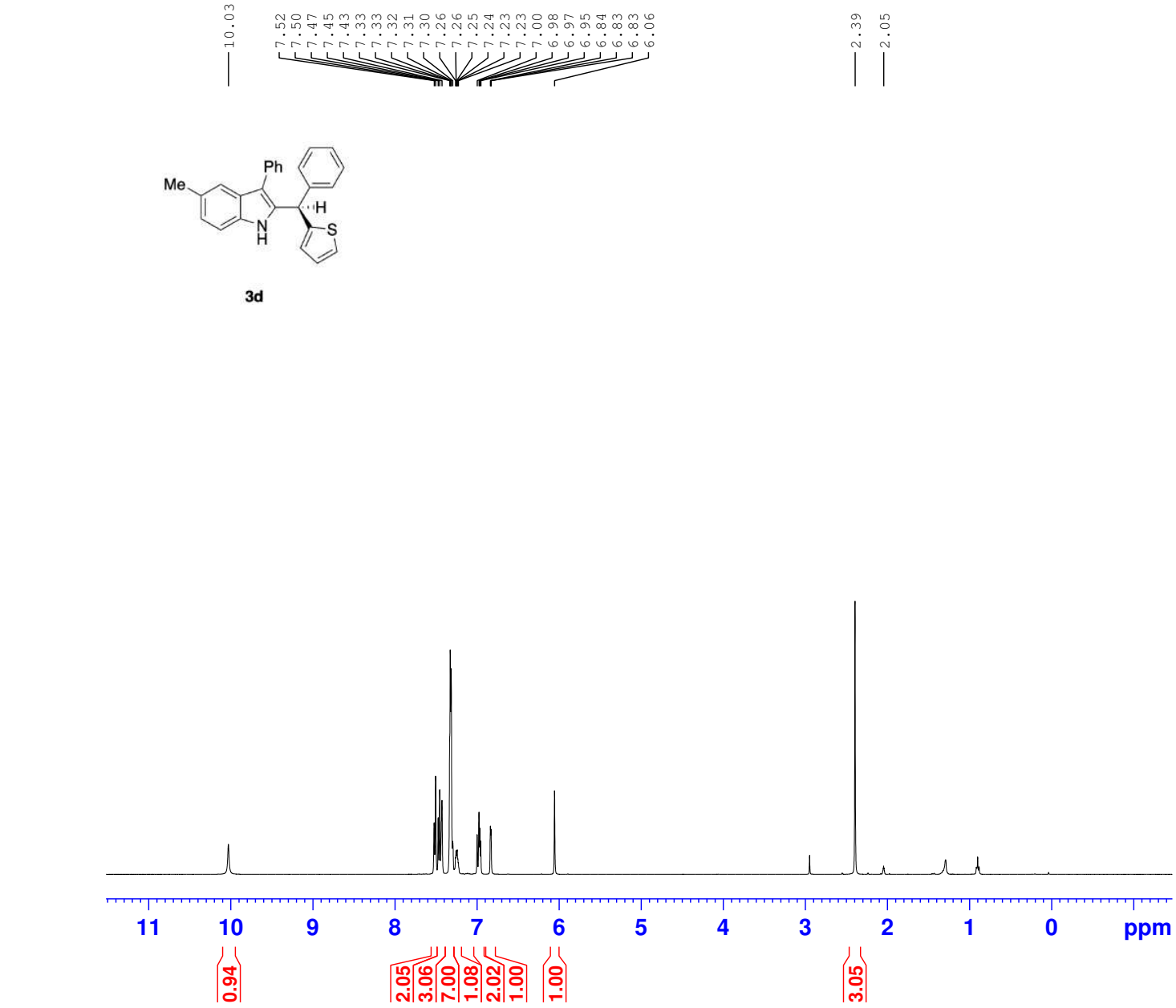

```
Current Data Parameters
NAME          YQL-2-3-p
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210725
Time              21.59
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                   67
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                296.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          100.6126886 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```



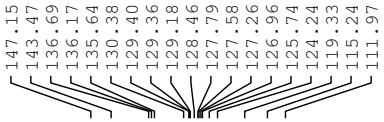

```
Current Data Parameters
NAME      YQL-1-158-pdt
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210709
Time              22.30
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                65536
SOLVENT         Acetone
NS                    8
DS                    0
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9845889 sec
RG                  161
DW               60.800 usec
DE                6.00 usec
TE                294.2 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.80 usec
PL1               -1.00 dB
PL1W        12.17476940 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300074 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

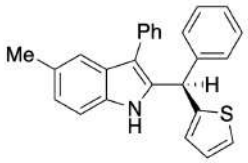



```
Current Data Parameters
NAME       YQL-1-158-pdt
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210709
Time               22.32
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  121
DS                    1
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.00 usec
TE                294.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 40.00 usec
PL1                -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               14.39 dB
PL13               18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF         100.6126856 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

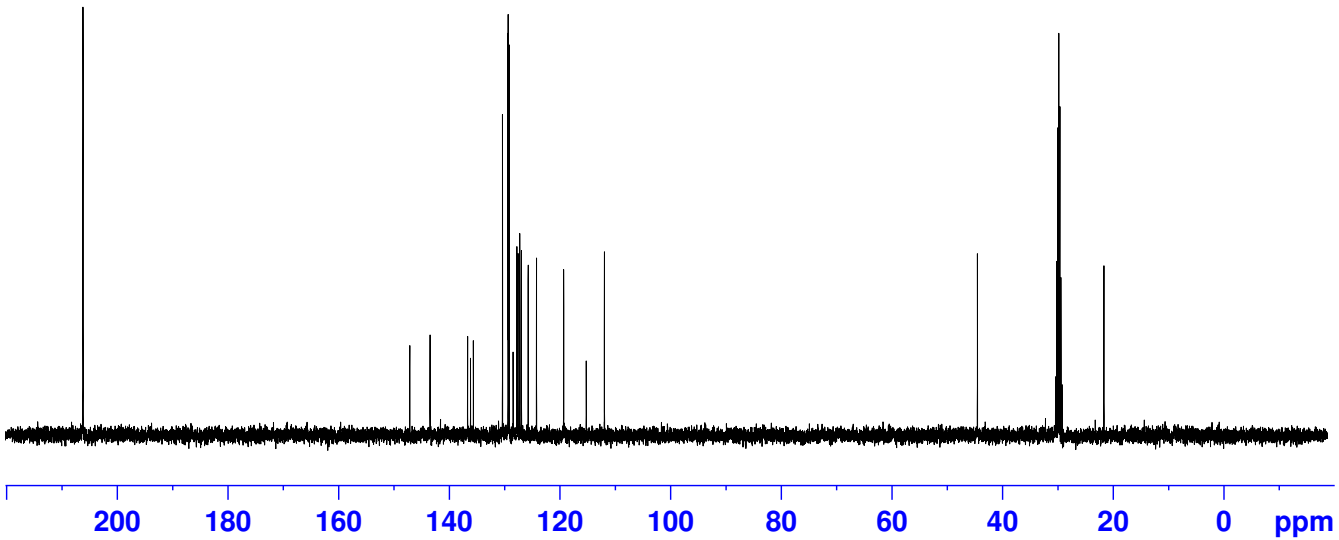



```
Current Data Parameters
NAME         YQL-1-155-P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210707
Time               23.05
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9845889 sec
RG                    64
DW                60.800 usec
DE                 6.00 usec
TE                293.9 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.80 usec
PL1               -1.00 dB
PL1W         12.17476940 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF           400.1300085 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

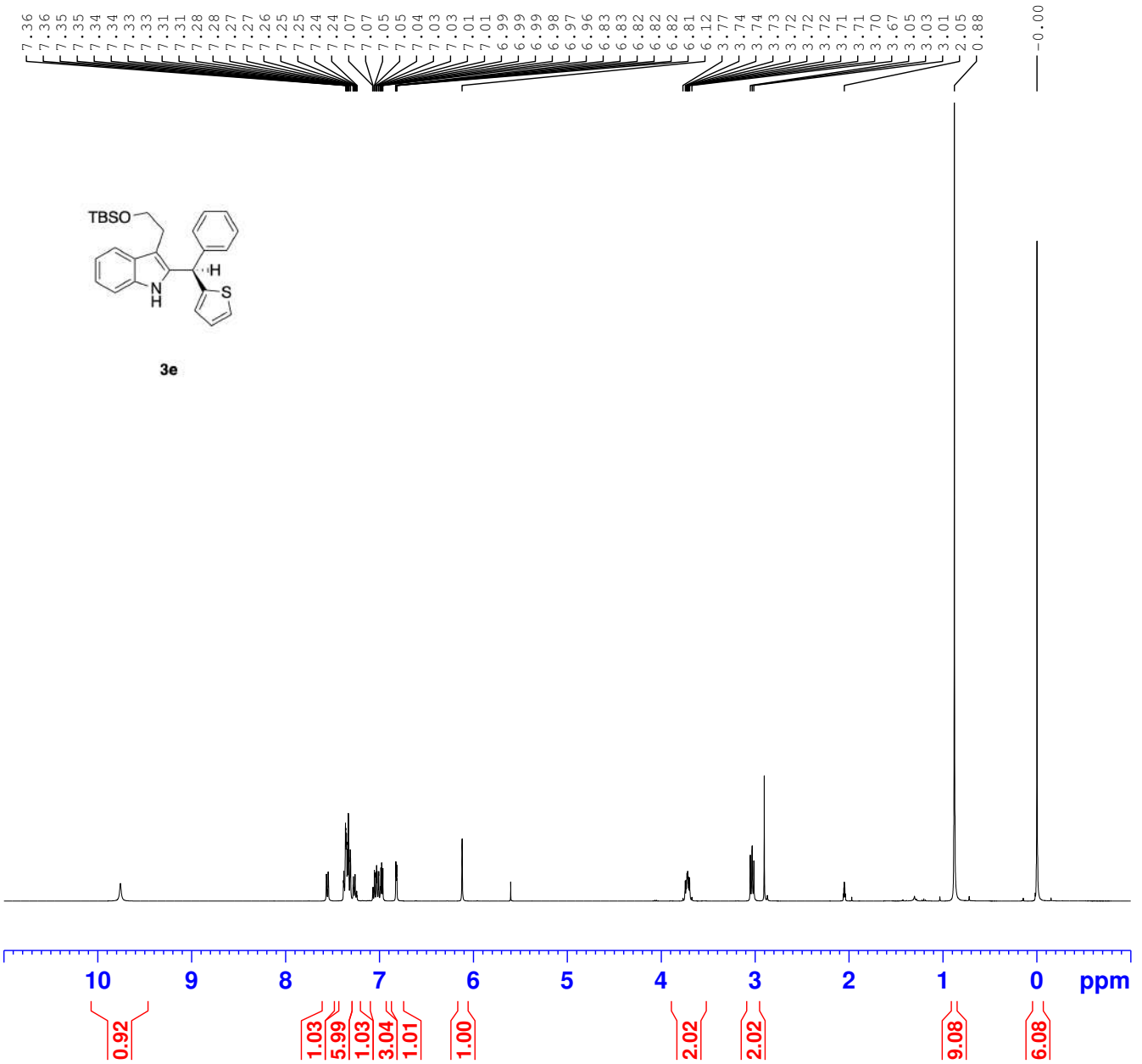




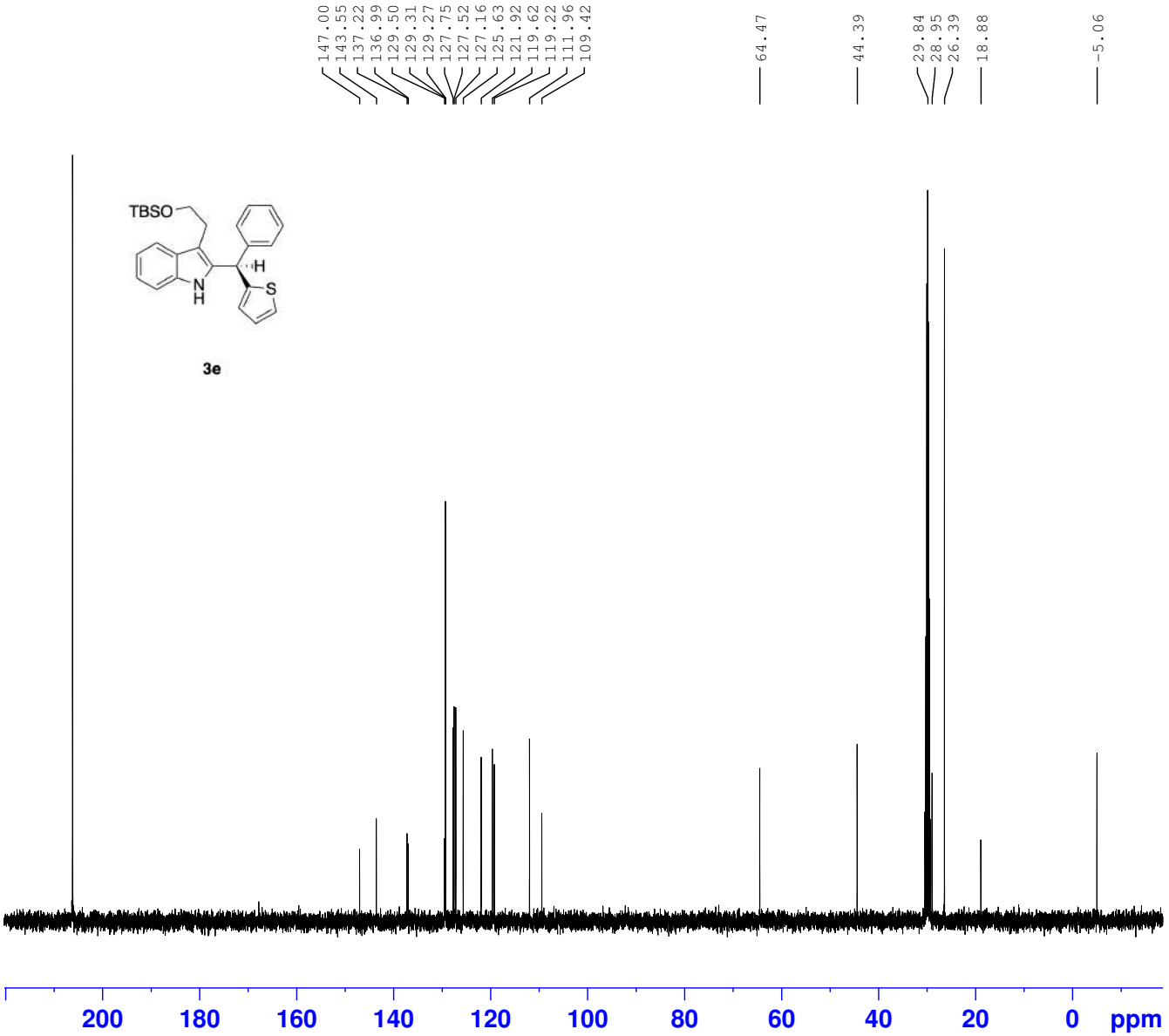
3d



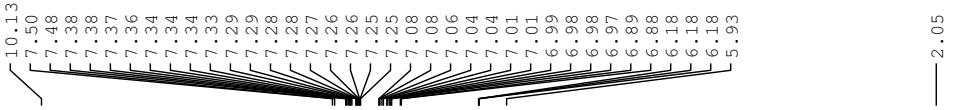

```
Current Data Parameters
NAME         YQL-1-155-P
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210707
Time               23.24
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   31
DS                    1
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                 2050
DW                20.800 usec
DE                 6.00 usec
TE                294.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                40.00 usec
PL1               -3.00 dB
PL1W        60.64365387 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              14.39 dB
PL13              18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126916 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

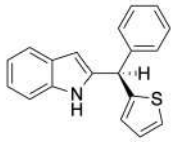



```
Current Data Parameters
NAME          YQL-2-37-P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210821
Time               10.01
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9845889 sec
RG                   101
DW                60.800 usec
DE                 6.00 usec
TE                300.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.80 usec
PL1                -1.00 dB
PL1W        12.17476940 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300069 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```

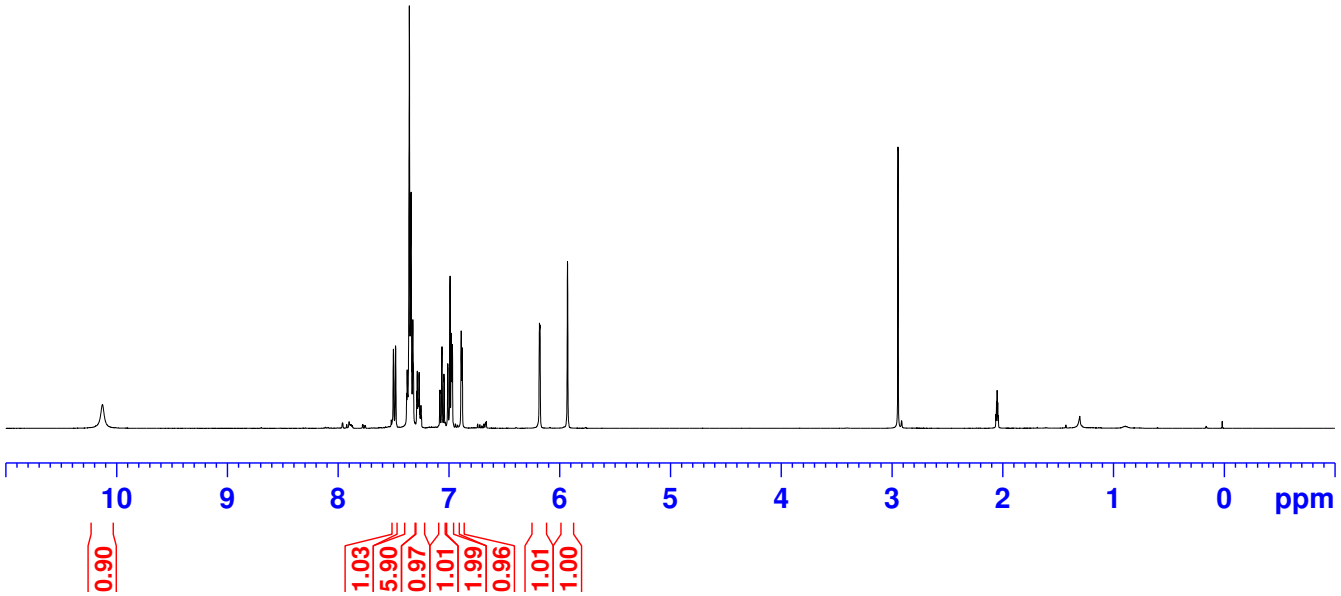



```
Current Data Parameters
NAME          YQL-2-37-P
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210821
Time               10.04
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT          Acetone
NS                   126
DS                     1
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                  2050
DW                20.800 usec
DE                 6.00 usec
TE                300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 40.00 usec
PL1                -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               14.39 dB
PL13               18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF         100.6126867 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.40
```

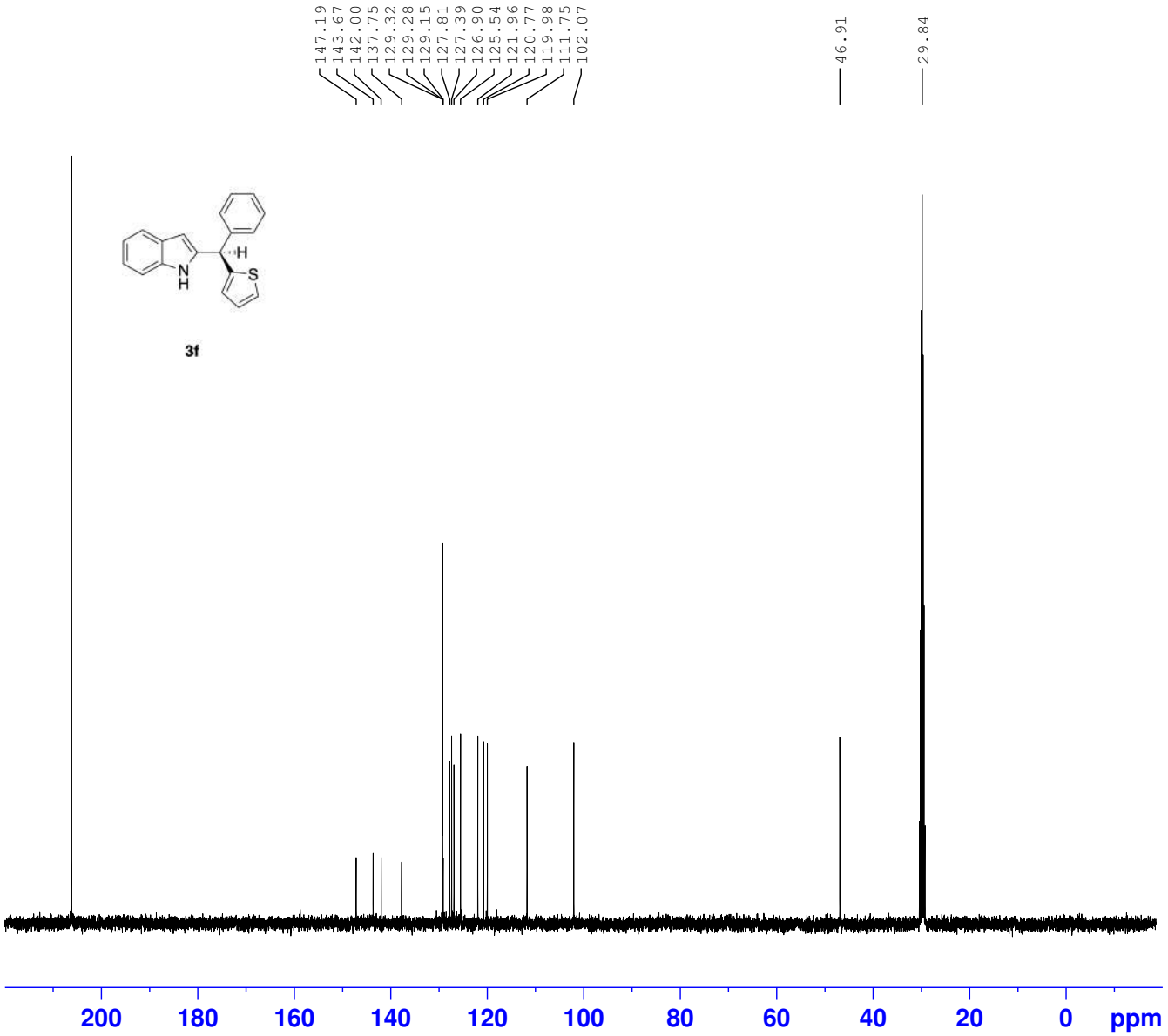




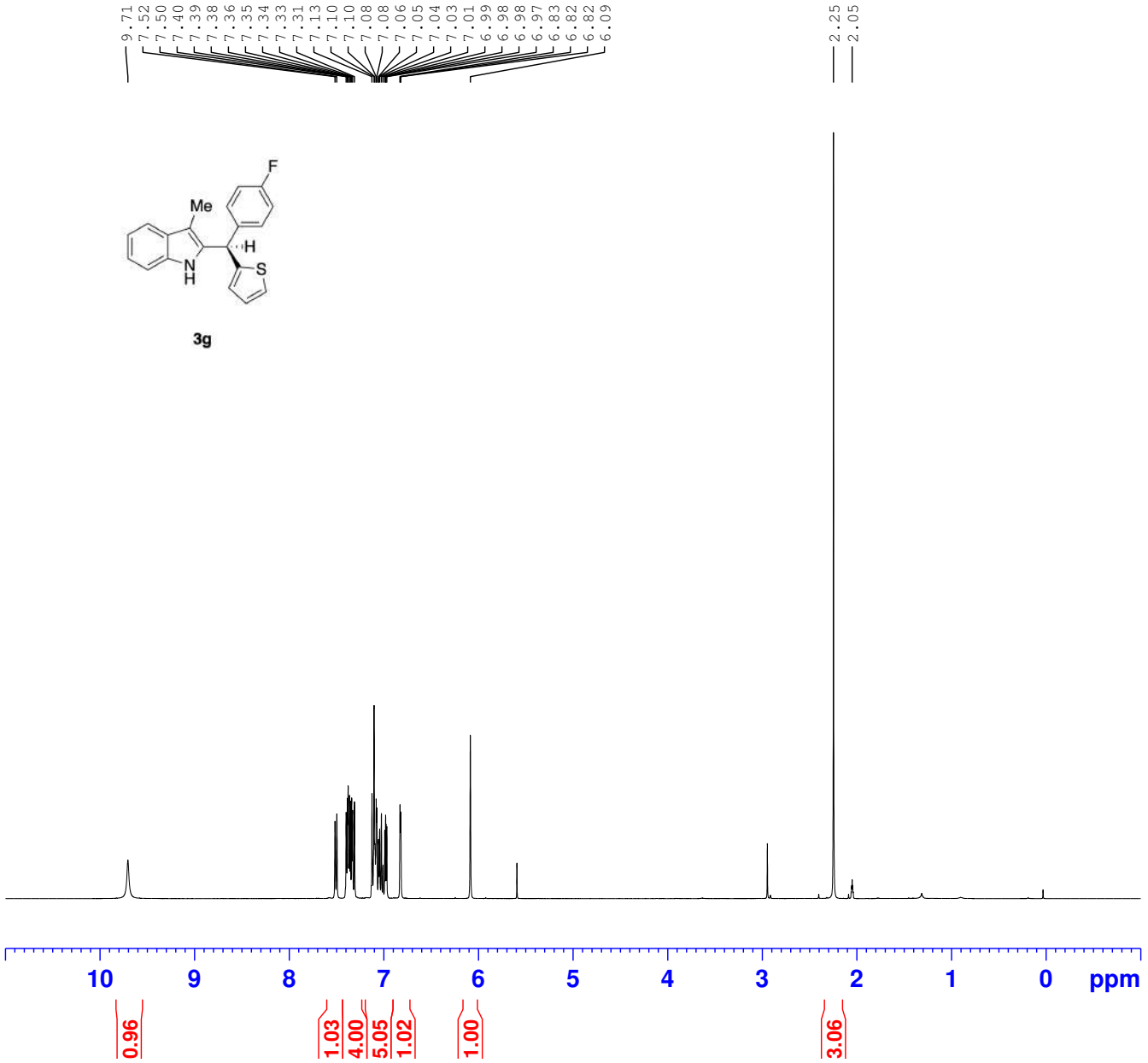
3f



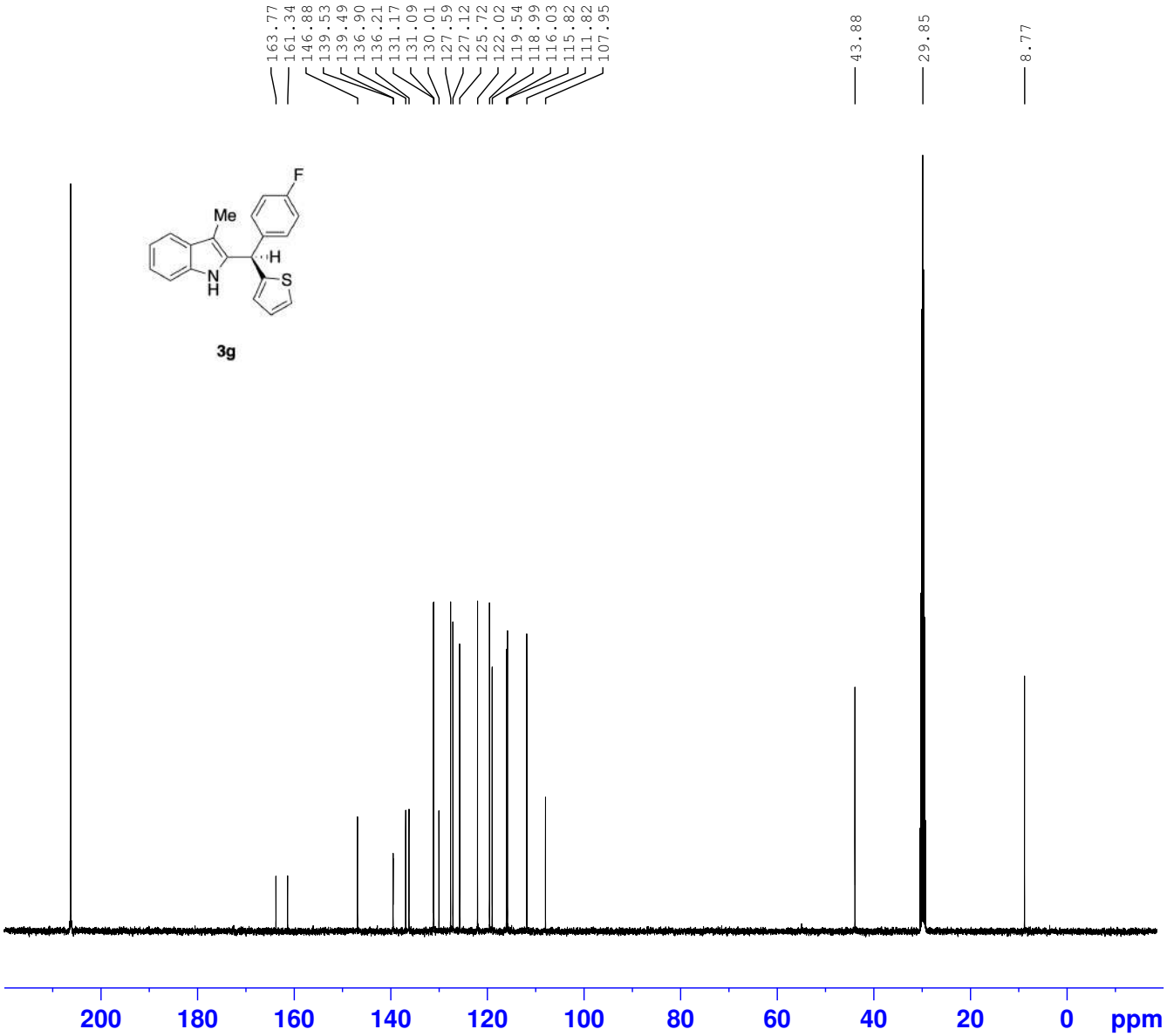

```
Current Data Parameters
NAME          YQL-1-156-
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210806
Time               14.48
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9845889 sec
RG                   161
DW                60.800 usec
DE                 6.00 usec
TE                293.4 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.80 usec
PL1               -1.00 dB
PL1W        12.17476940 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300069 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```




```
Current Data Parameters
NAME         YQL-1-156-P
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210707
Time               23.20
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT          Acetone
NS                    80
DS                     1
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                  2050
DW                20.800 usec
DE                 6.00 usec
TE                294.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                13C
P1                40.00 usec
PL1               -3.00 dB
PL1W        60.64365387 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              14.39 dB
PL13              18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6126859 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```



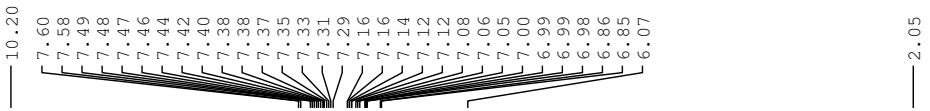

```
Current Data Parameters
NAME          YQL-2-1-p
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210725
Time              21.45
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                    8
DS                    0
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                27.78
DW               62.400 usec
DE                6.50 usec
TE                296.4 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                  1H
P1                14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                65536
SF          400.1300070 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

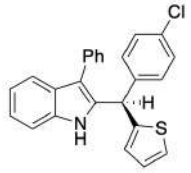



```
Current Data Parameters
NAME                YQL-2-1-p
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_                20210725
Time                    21.50
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT               Acetone
NS                          75
DS                           2
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631488 sec
RG                      196.92
DW                      20.800 usec
DE                       6.50 usec
TE                      296.6 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1               100.6228298 MHz
NUC1                       13C
P1                        9.70 usec
PLW1               46.98899841 W

======== CHANNEL f2 ========
SFO2               400.1316005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2               11.99499989 W
PLW12               0.34213999 W
PLW13               0.27713001 W

F2 - Processing parameters
SI                       32768
SF                 100.6126872 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

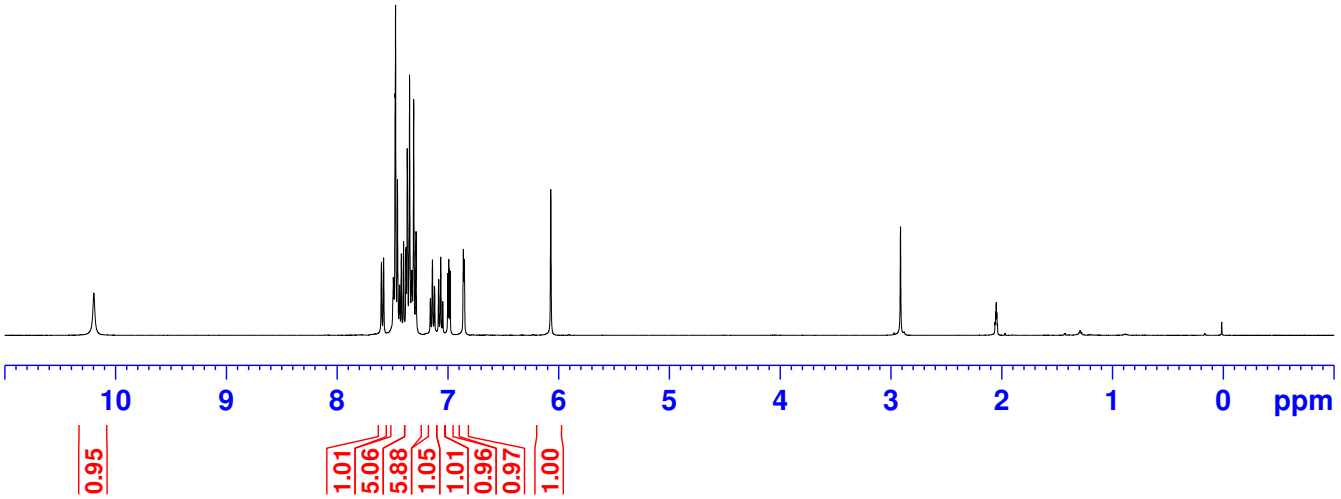
3g


```
Current Data Parameters
NAME          YQL-2-1-p
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210725
Time              21.48
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD               131072
SOLVENT         Acetone
NS                   16
DS                    4
SWH           89285.711 Hz
FIDRES         0.681196 Hz
AQ            0.7340032 sec
RG               196.92
DW                5.600 usec
DE                6.50 usec
TE               296.4 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        376.4607164 MHz
NUC1                19F
P1                14.70 usec
PLW1        15.99600029 W

F2 - Processing parameters
SI                65536
SF          376.4983660 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

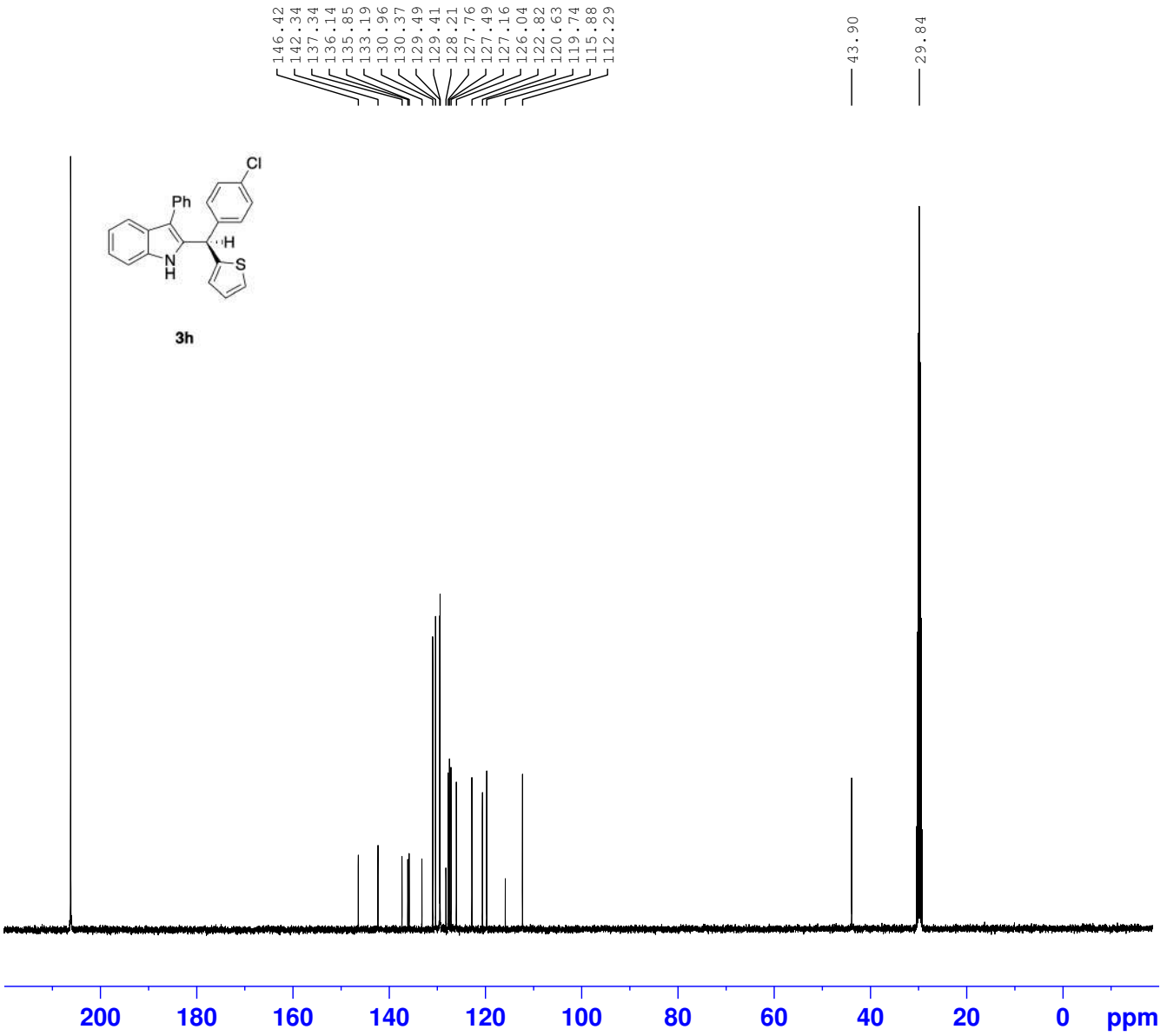




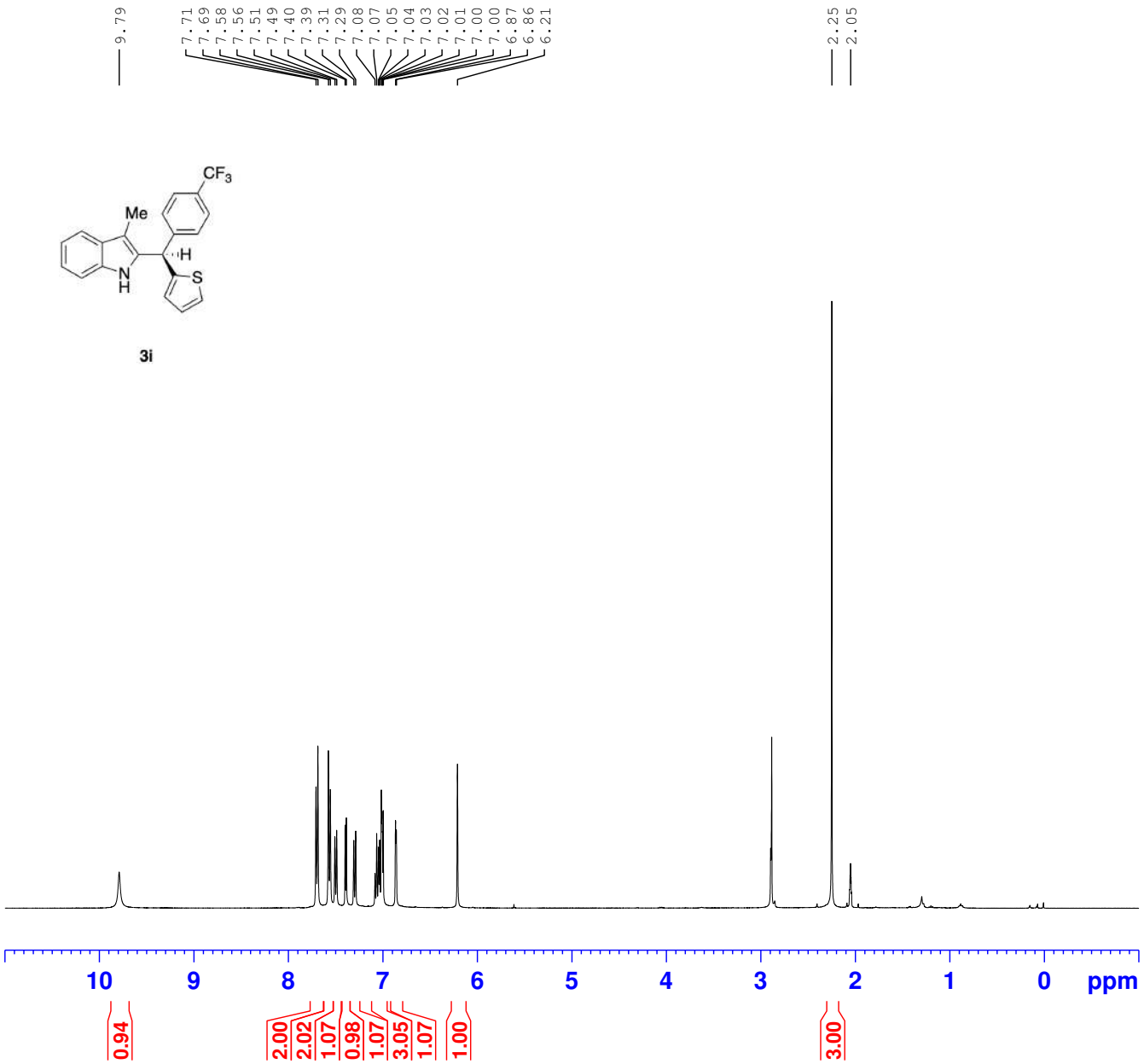
3h



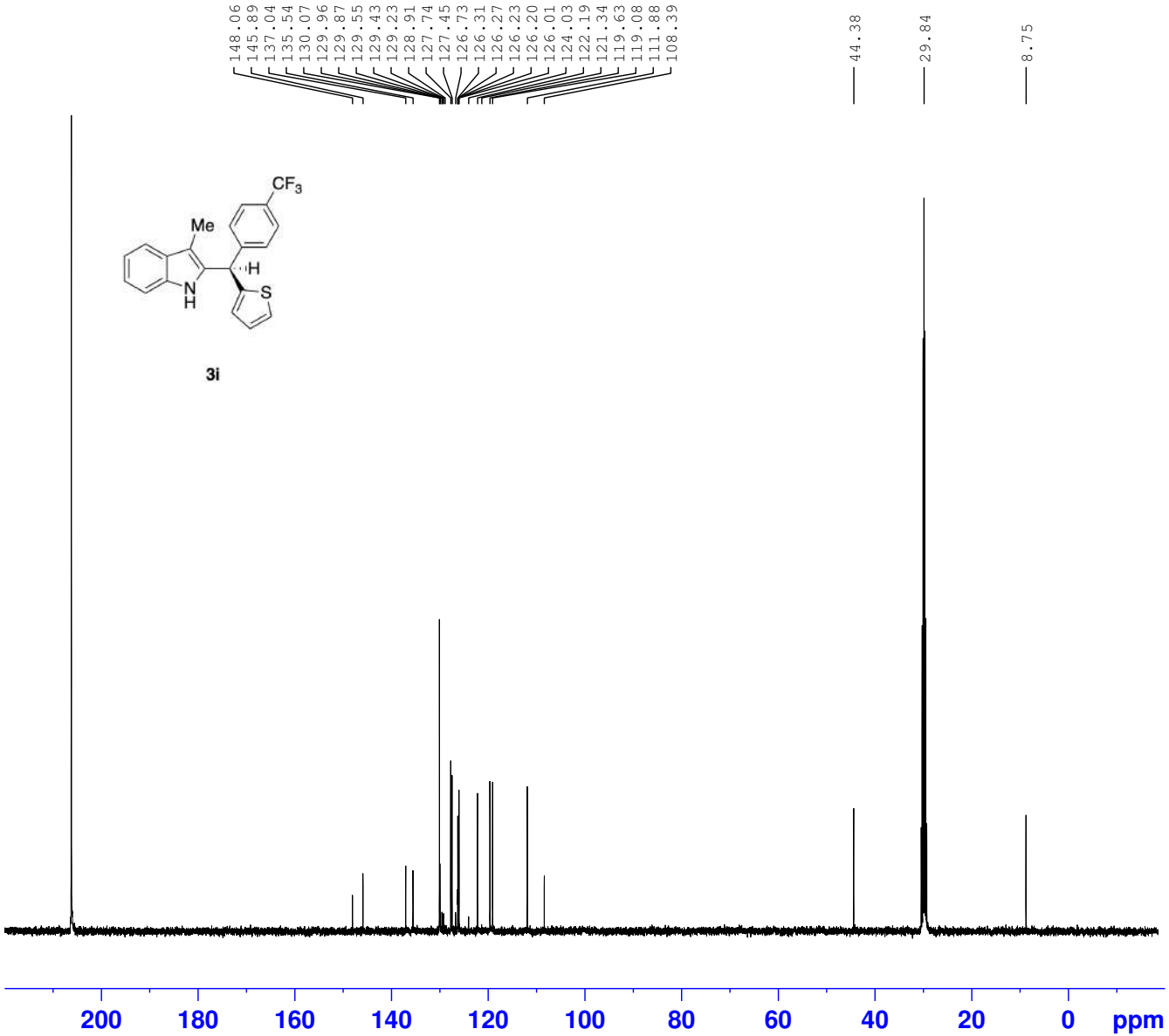

```
Current Data Parameters
NAME                  YQL-2-5
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20210731
Time                   18.20
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT              Acetone
NS                           8
DS                           0
SWH                 8012.820 Hz
FIDRES              0.122266 Hz
AQ                  4.0894465 sec
RG                      54.81
DW                     62.400 usec
DE                      6.50 usec
TE                     296.6 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1             400.1324710 MHz
NUC1                       1H
P1                      14.50 usec
PLW1             11.99499989 W

F2 - Processing parameters
SI                          65536
SF                400.1300073 MHz
WDW                           EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```



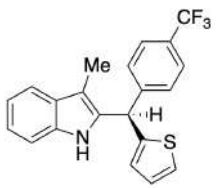

```
Current Data Parameters
NAME                  YQL-2-5
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20210731
Time                   18.23
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                     65536
SOLVENT              Acetone
NS                          88
DS                           2
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     196.92
DW                     20.800 usec
DE                      6.50 usec
TE                     297.3 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1             100.6228298 MHz
NUC1                     13C
P1                      9.70 usec
PLW1             46.98899841 W

======== CHANNEL f2 ========
SFO2             400.1316005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                   90.00 usec
PLW2             11.99499989 W
PLW12             0.34213999 W
PLW13             0.27713001 W

F2 - Processing parameters
SI                       32768
SF               100.6126858 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```




```
Current Data Parameters
NAME      YQL-1-179-pdt
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210721
Time              22.10
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                    8
DS                    0
SWH            8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                70.97
DW               62.400 usec
DE                6.50 usec
TE               296.8 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1                14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                65536
SF          400.1300069 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

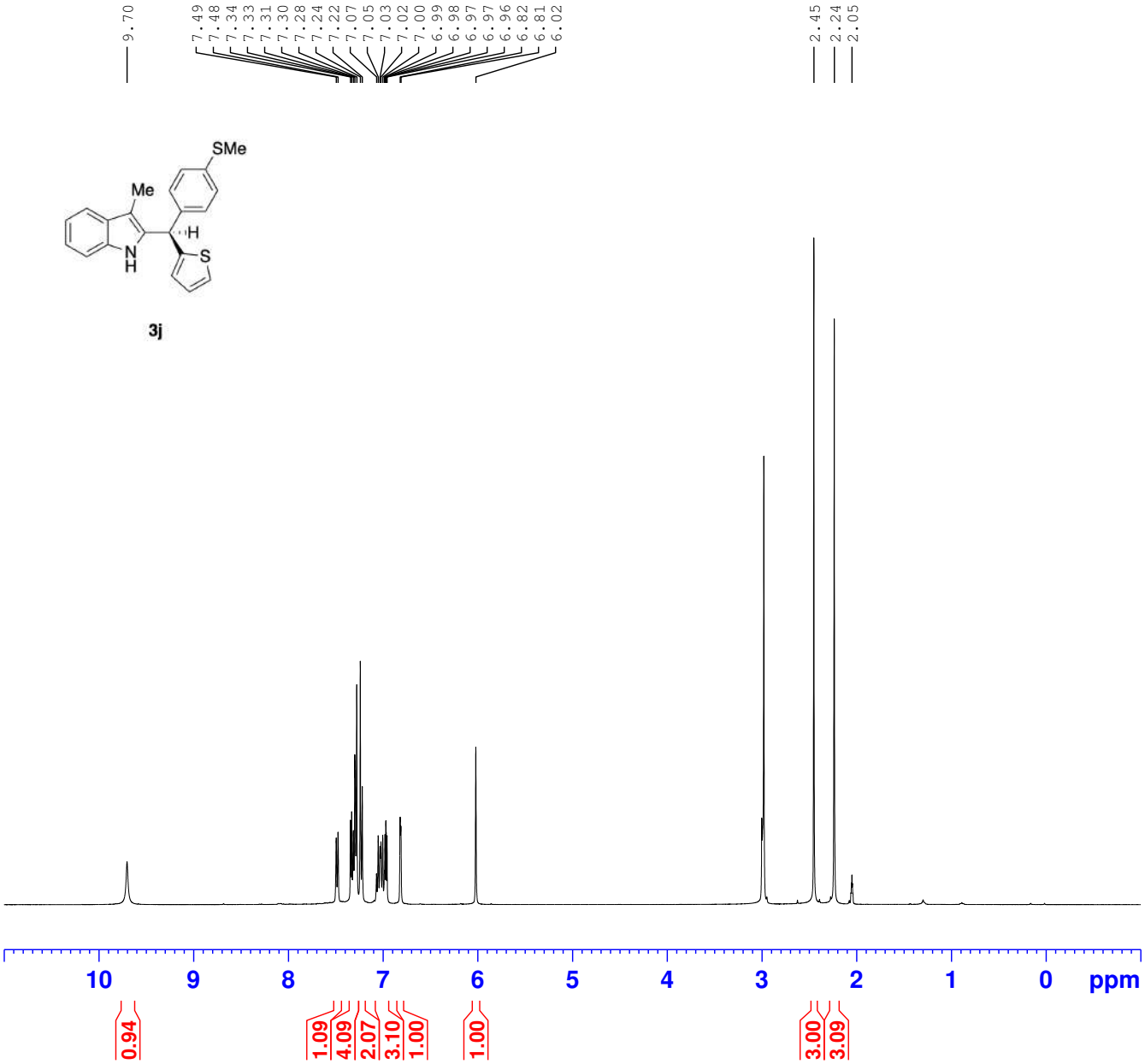



```
Current Data Parameters
NAME      YQL-1-179-pdt
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20210721
Time              22.14
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                  187
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 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
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                 32768
SF          100.6126806 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

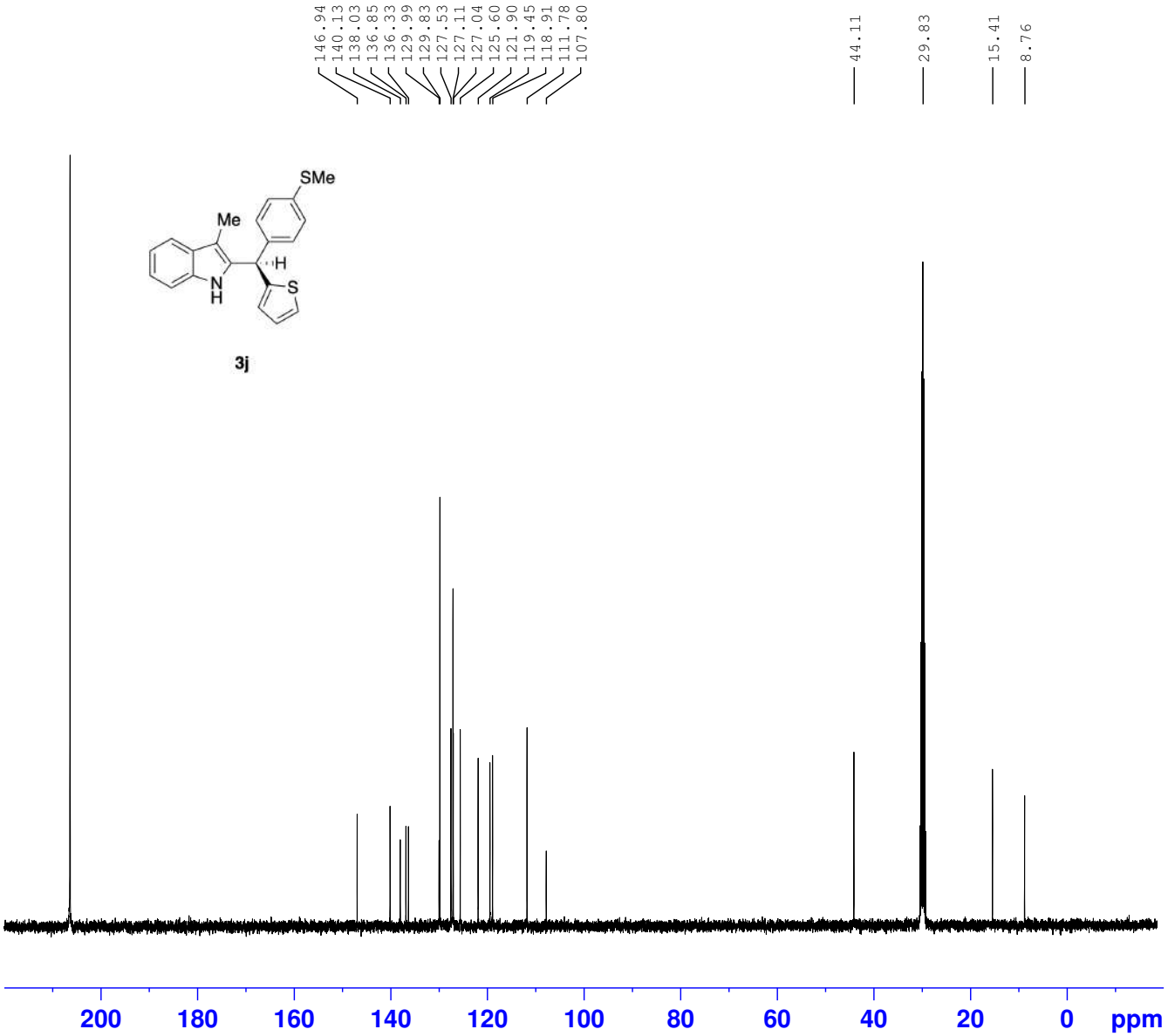


3i

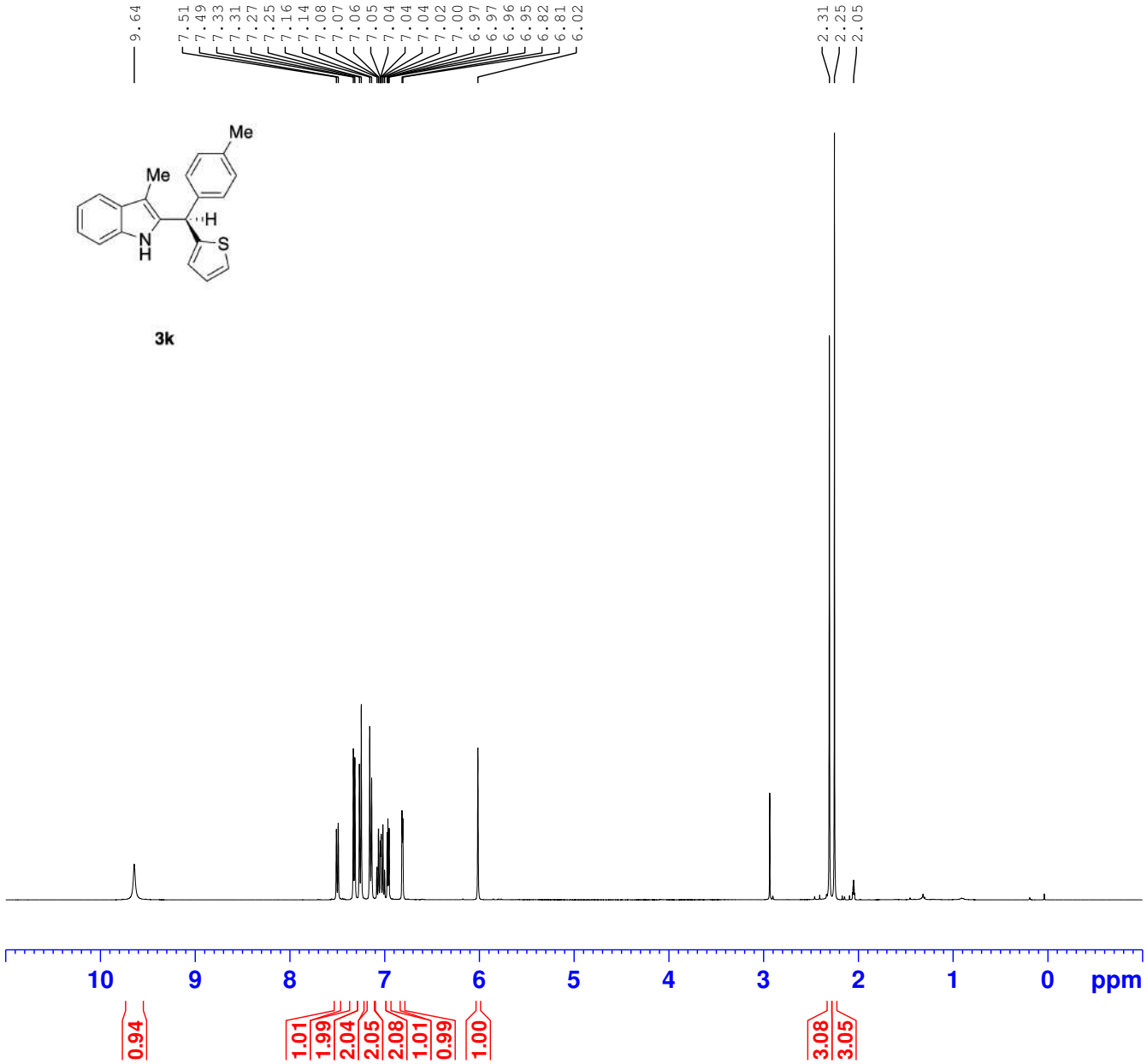

```
Current Data Parameters
NAME      YQL-1-179-pdt
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210721
Time              22.12
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgflqn
TD              131072
SOLVENT        Acetone
NS                   16
DS                    4
SWH           89285.711 Hz
FIDRES         0.681196 Hz
AQ            0.7340032 sec
RG               196.92
DW                5.600 usec
DE                6.50 usec
TE                296.8 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        376.4607164 MHz
NUC1                19F
P1                14.70 usec
PLW1        15.99600029 W

F2 - Processing parameters
SI                65536
SF          376.4983660 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



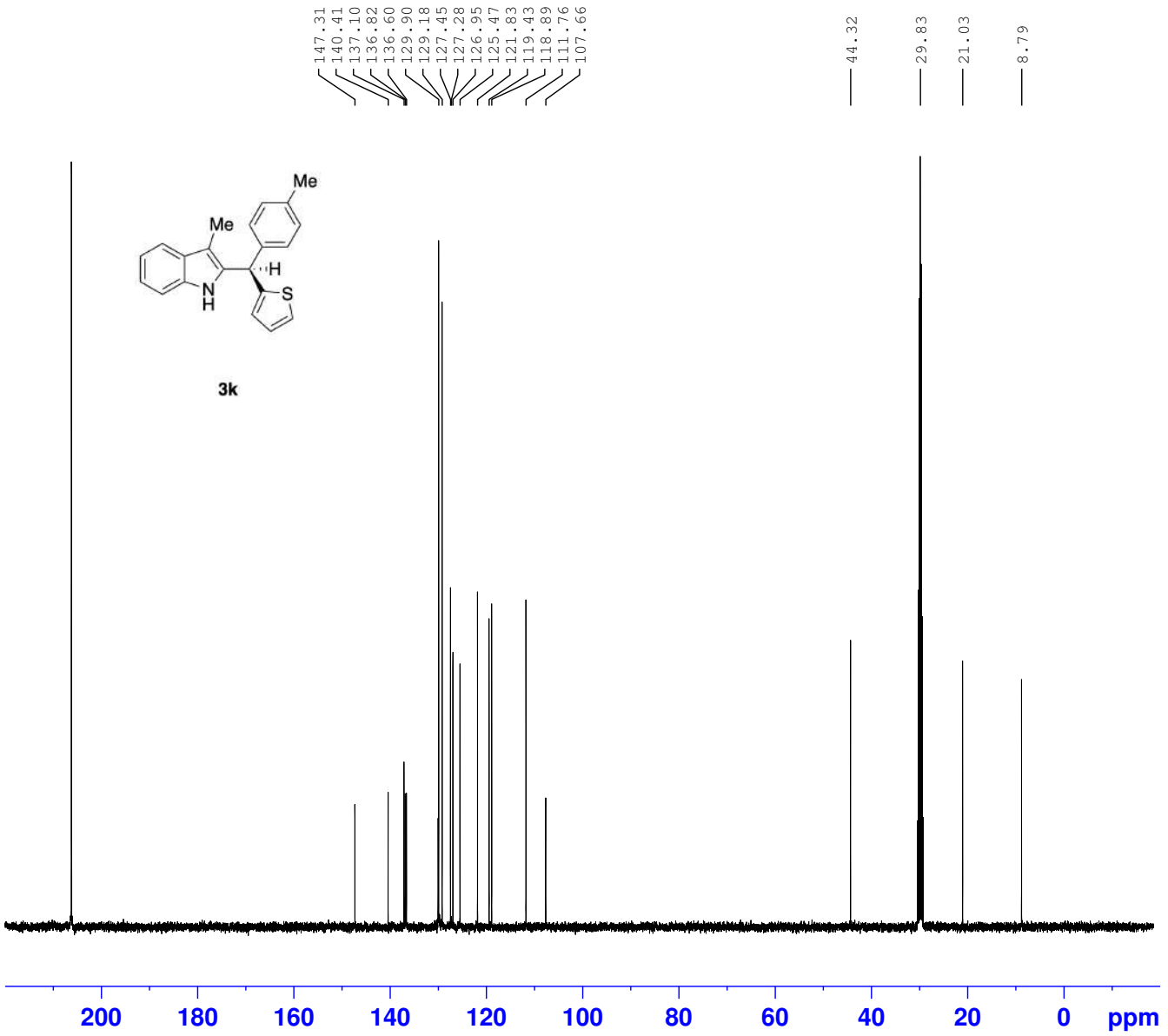

```
Current Data Parameters
NAME          YQL-1-168
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20210731
Time              18.10
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                    8
DS                    0
SWH            8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                31.55
DW               62.400 usec
DE                6.50 usec
TE               296.5 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                1H
P1                14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                65536
SF          400.1300071 MHz
WDW                 EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```



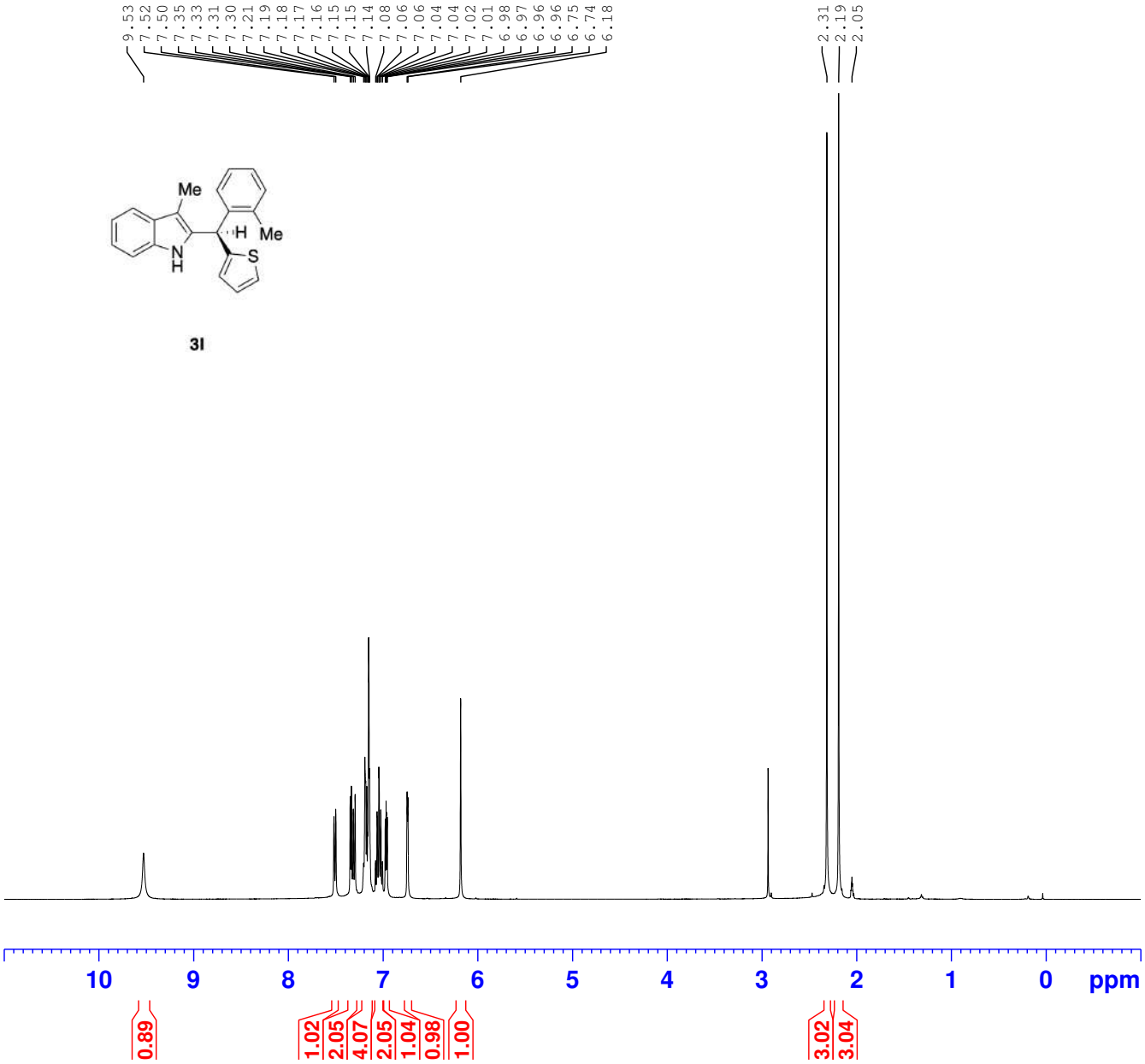

```
Current Data Parameters
NAME          YQL-1-168
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210731
Time              18.13
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                   66
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 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
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          100.6126878 MHz
WDW                EM
SSB                0
LB              1.00 Hz
GB                 0
PC              1.40
```



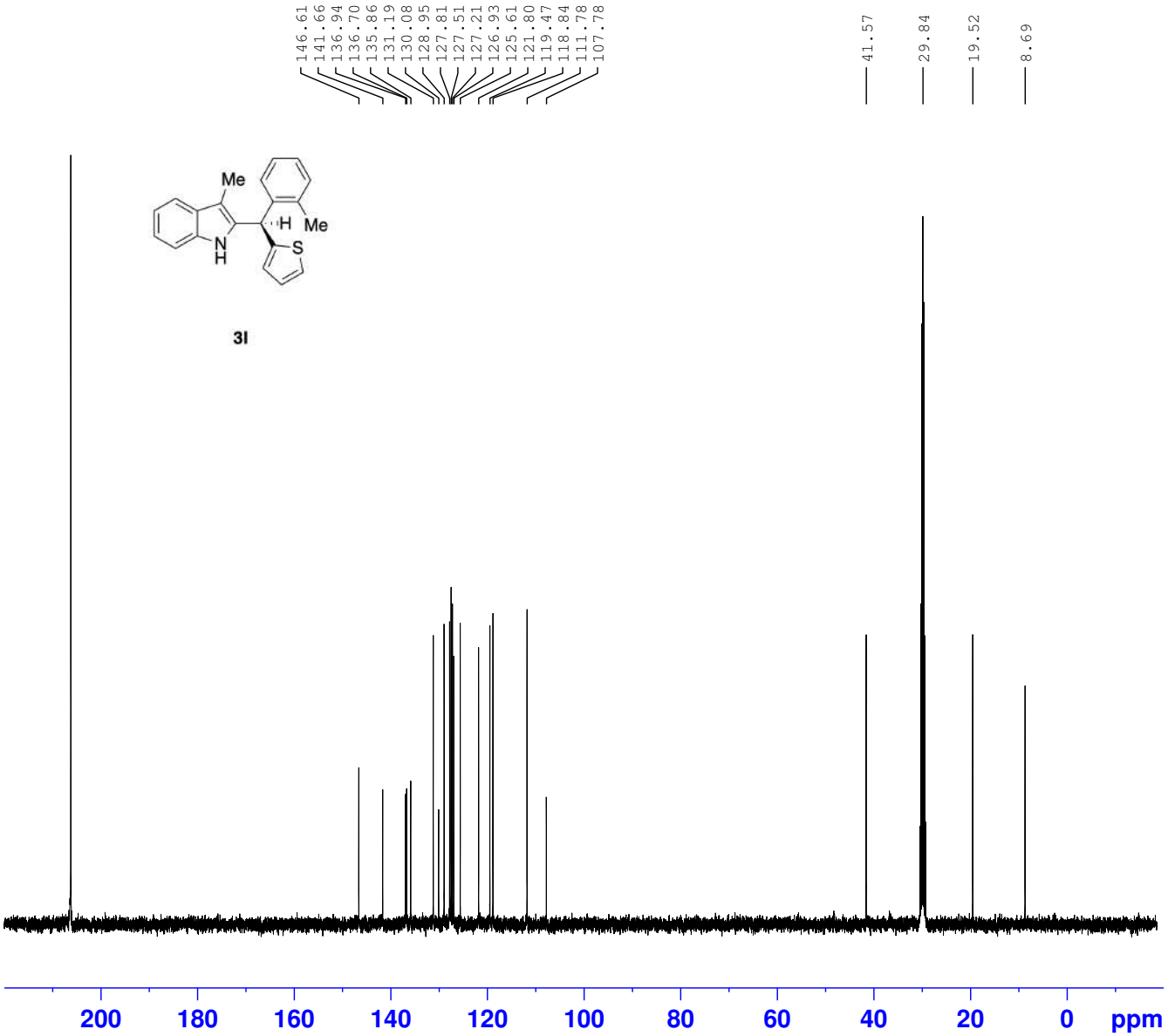

```
Current Data Parameters
NAME        YQL-2-19-PDT
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210801
Time               22.15
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 27.78
DW                62.400 usec
DE                 6.50 usec
TE                296.7 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300070 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```



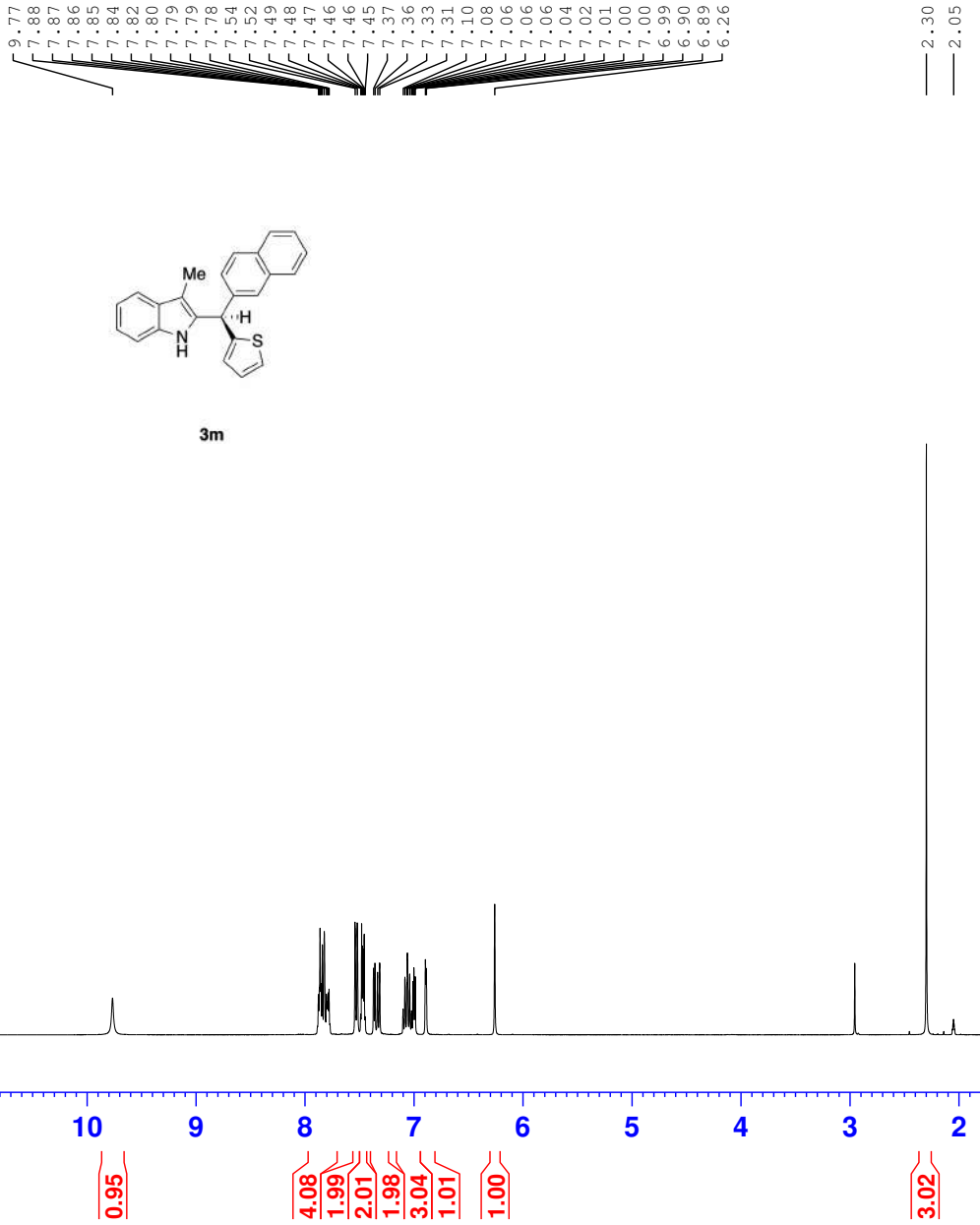

```
Current Data Parameters
NAME        YQL-2-19-PDT
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210801
Time               22.18
INSTRUM            spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   51
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                  13C
P1                   9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6126895 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



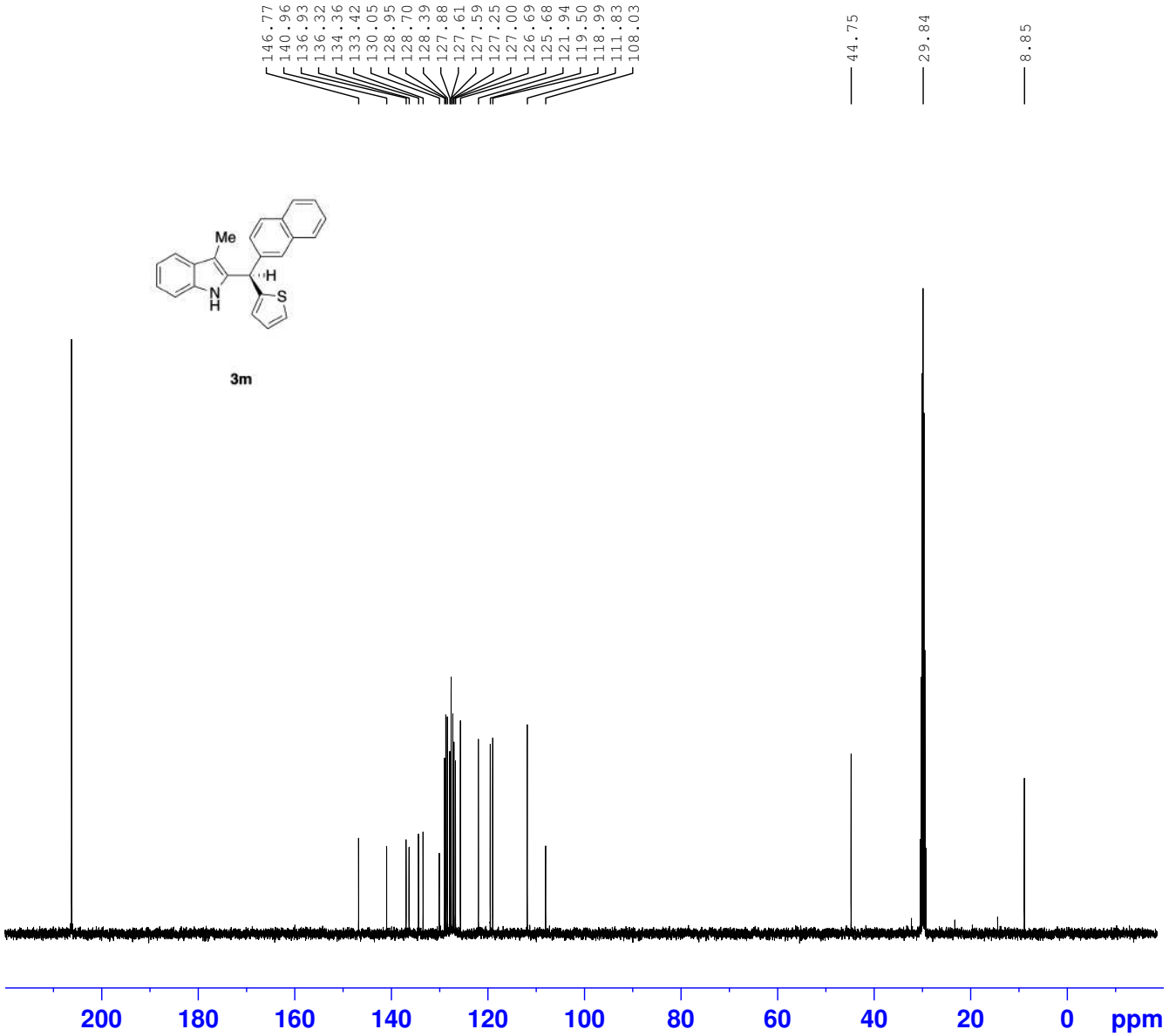

```
Current Data Parameters
NAME          YQL-2-18-P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210805
Time               22.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 27.78
DW                62.400 usec
DE                 6.50 usec
TE                296.5 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300071 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```



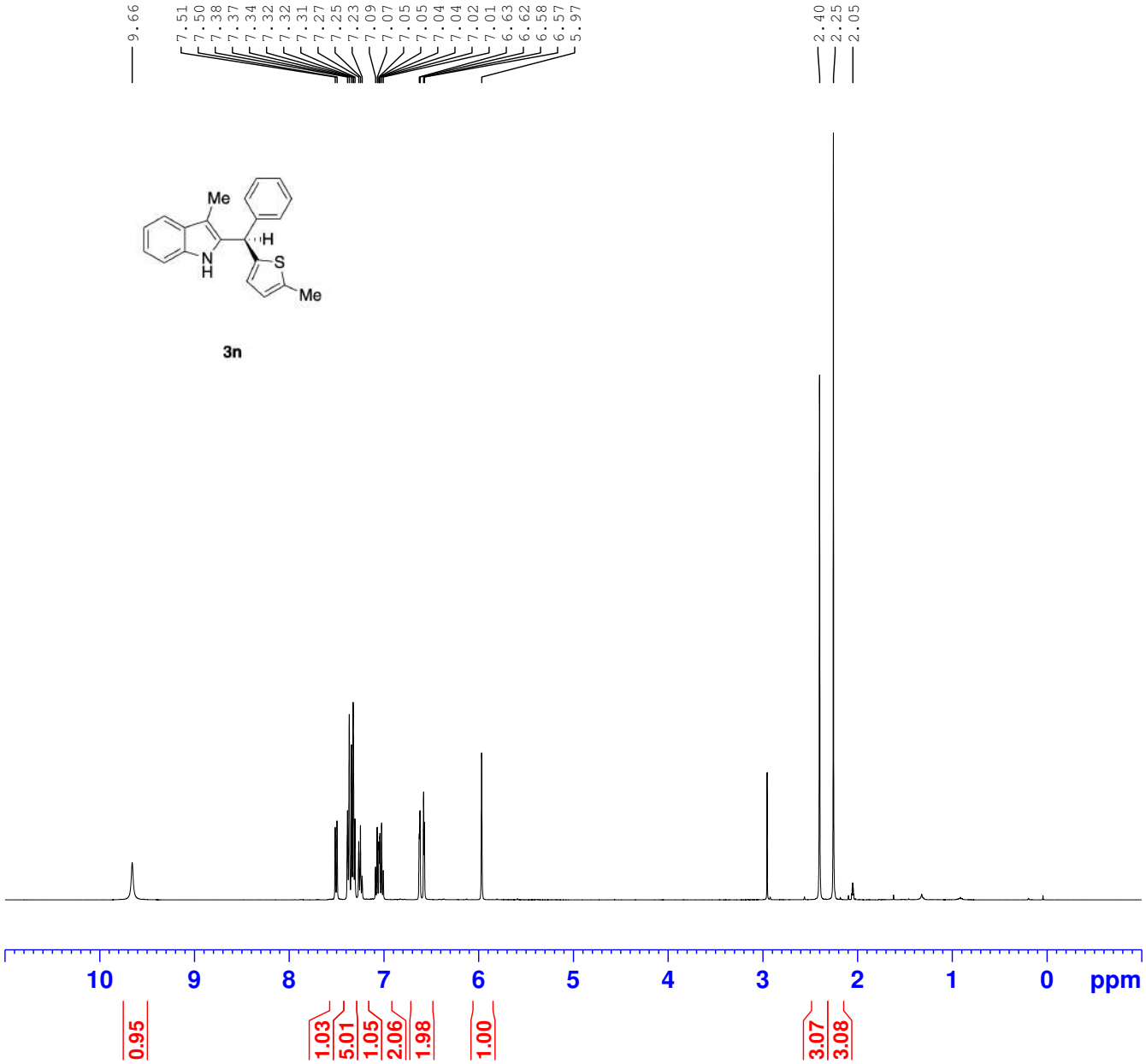

```
Current Data Parameters
NAME          YQL-2-18-P
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210805
Time               22.45
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   47
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                297.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                  9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6126899 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



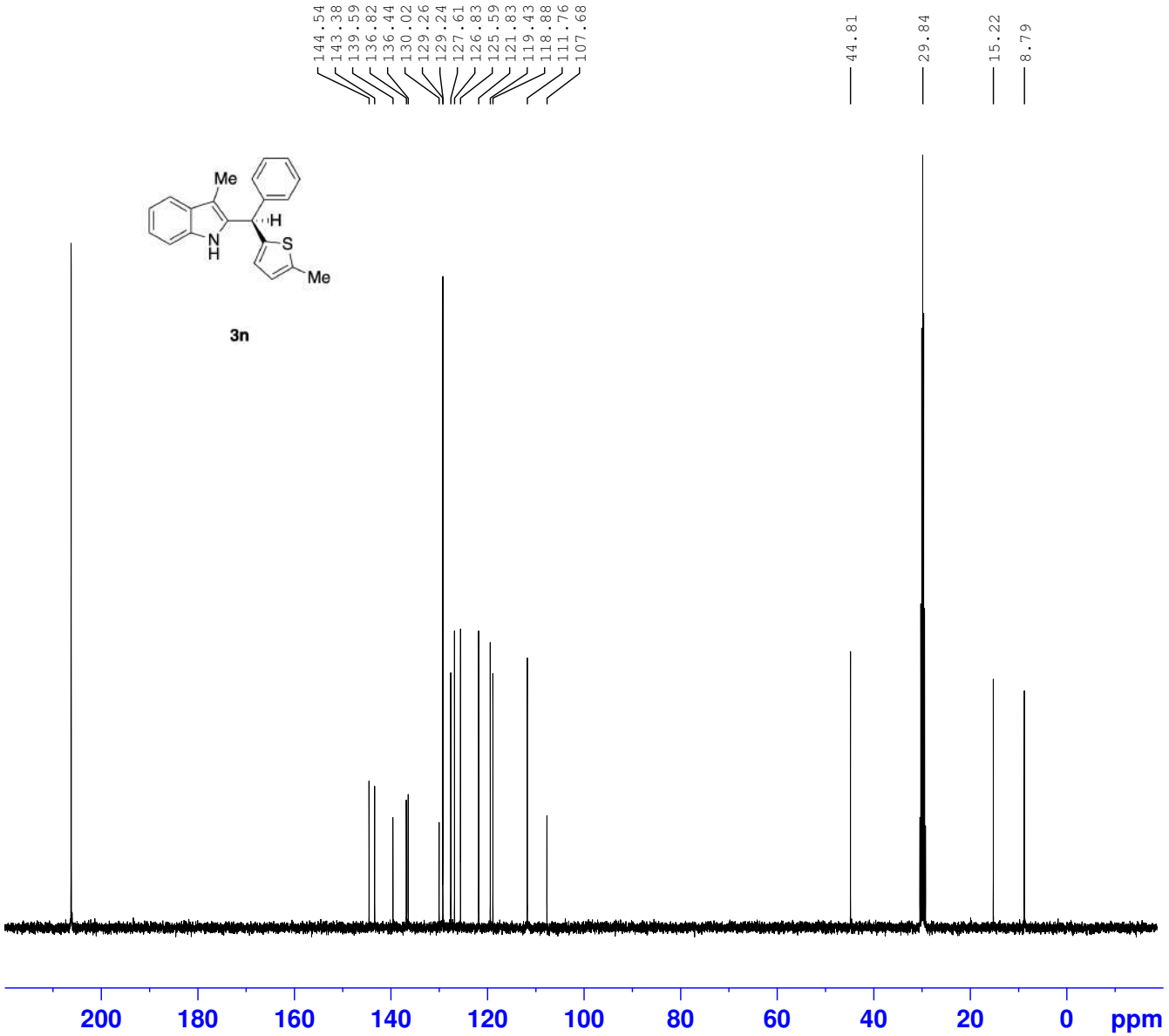

```
Current Data Parameters
NAME      YQL-1-151-product
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20210706
Time              10.15
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                65536
SOLVENT         Acetone
NS                    8
DS                    0
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ            4.0894465 sec
RG                27.78
DW               62.400 usec
DE                6.50 usec
TE               296.7 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                  1H
P1                14.50 usec
PLW1        11.99499989 W

F2 - Processing parameters
SI                65536
SF          400.1300073 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



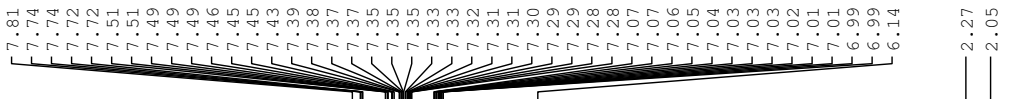

```
Current Data Parameters
NAME                  YQL-1-151
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210706
Time                      10.18
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                  zgpg30
TD                        65536
SOLVENT                 Acetone
NS                             17
DS                              2
SWH                    24038.461 Hz
FIDRES                  0.366798 Hz
AQ                     1.3631488 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
PLW1                46.98899841 W

======== CHANNEL f2 ========
SFO2                 400.1316005 MHz
NUC2                         1H
CPDPRG[2                 waltz16
PCPD2                     90.00 usec
PLW2                11.99499989 W
PLW12                0.34213999 W
PLW13                0.27713001 W

F2 - Processing parameters
SI                         32768
SF                   100.6126903 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40
```

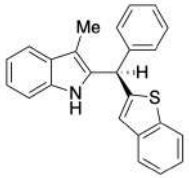



```
Current Data Parameters
NAME                  YQL-1-173
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20210717
Time                      21.22
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                    zg30
TD                        65536
SOLVENT                 Acetone
NS                              8
DS                              0
SWH                    8012.820 Hz
FIDRES                 0.122266 Hz
AQ                     4.0894465 sec
RG                        25.32
DW                        62.400 usec
DE                         6.50 usec
TE                        296.5 K
D1                   1.00000000 sec
TD0                             1

======== CHANNEL f1 ========
SFO1                 400.1324710 MHz
NUC1                         1H
P1                        14.50 usec
PLW1                 11.99499989 W

F2 - Processing parameters
SI                            65536
SF                   400.1300067 MHz
WDW                           EM
SSB                            0
LB                         0.30 Hz
GB                             0
PC                         1.00
```

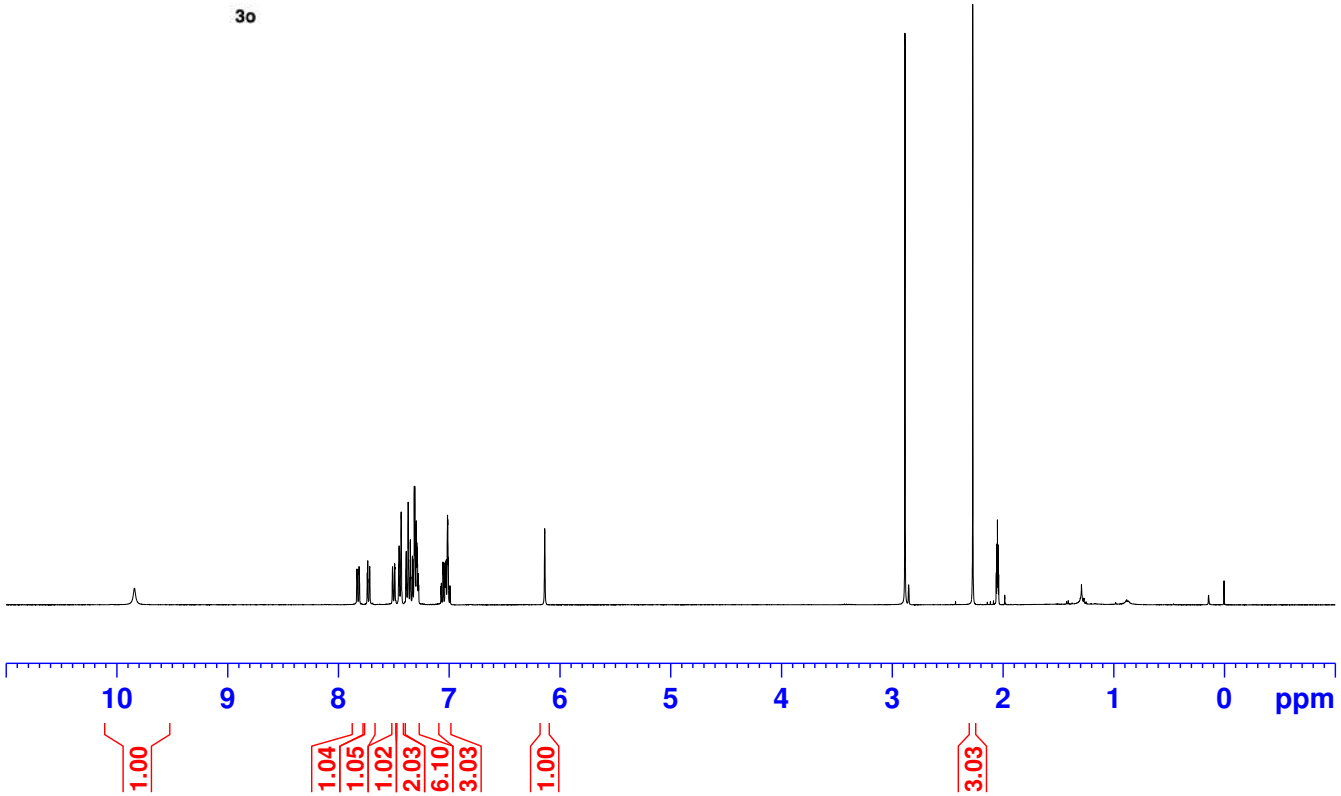



```
Current Data Parameters
NAME          YQL-1-173
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20210717
Time              21.25
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   36
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 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
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                32768
SF          100.6126902 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

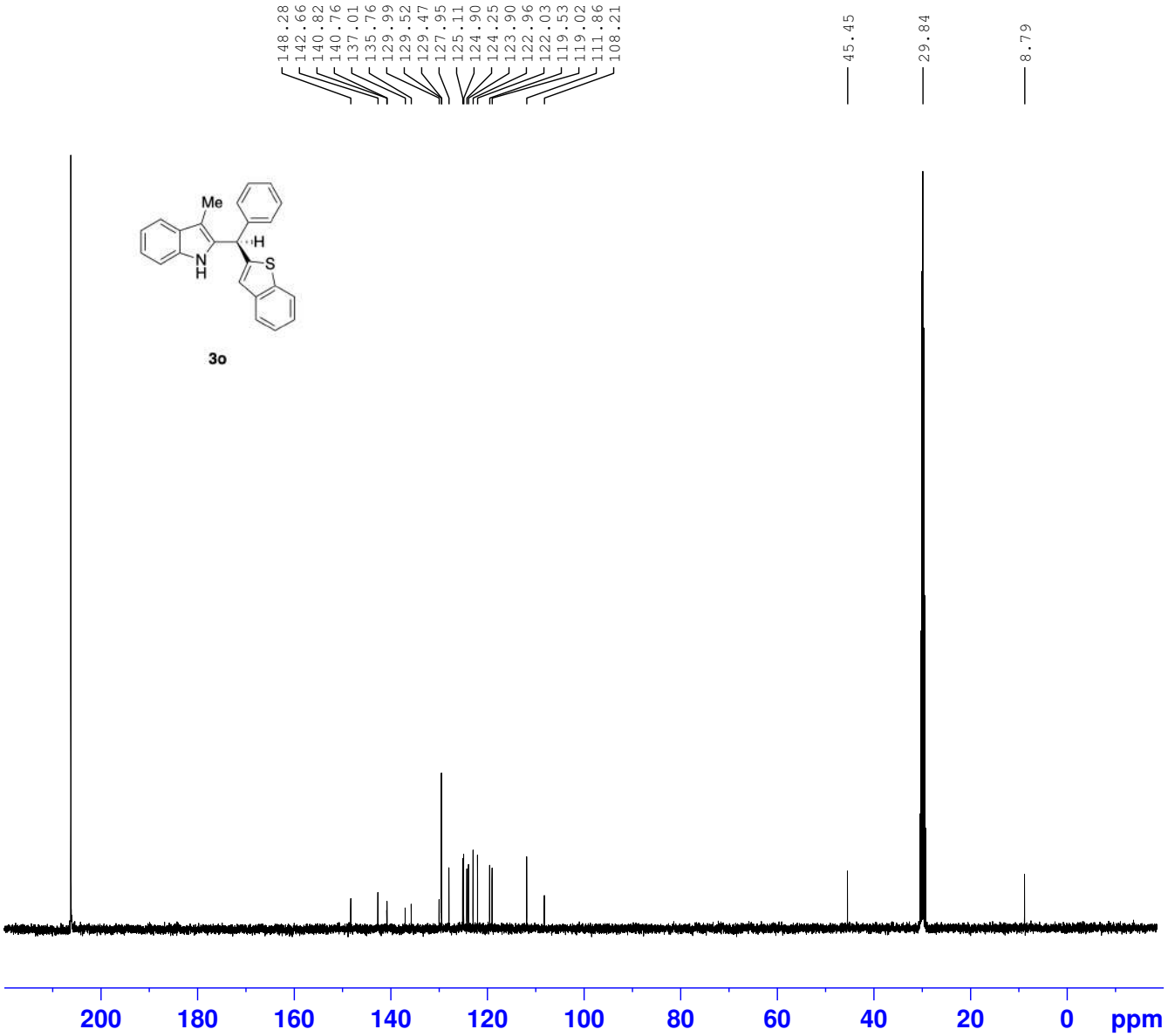




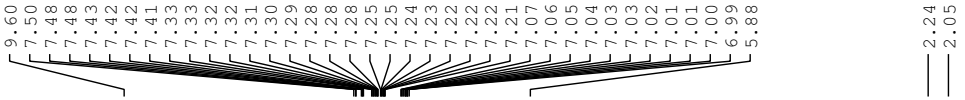
3o

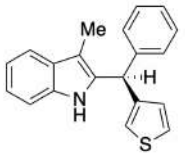



```
Current Data Parameters
NAME          YQL-2-36-P
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210821
Time               10.13
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9845889 sec
RG                   322
DW                60.800 usec
DE                 6.00 usec
TE                300.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.80 usec
PL1               -1.00 dB
PL1W        12.17476940 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300069 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                 1.00
```

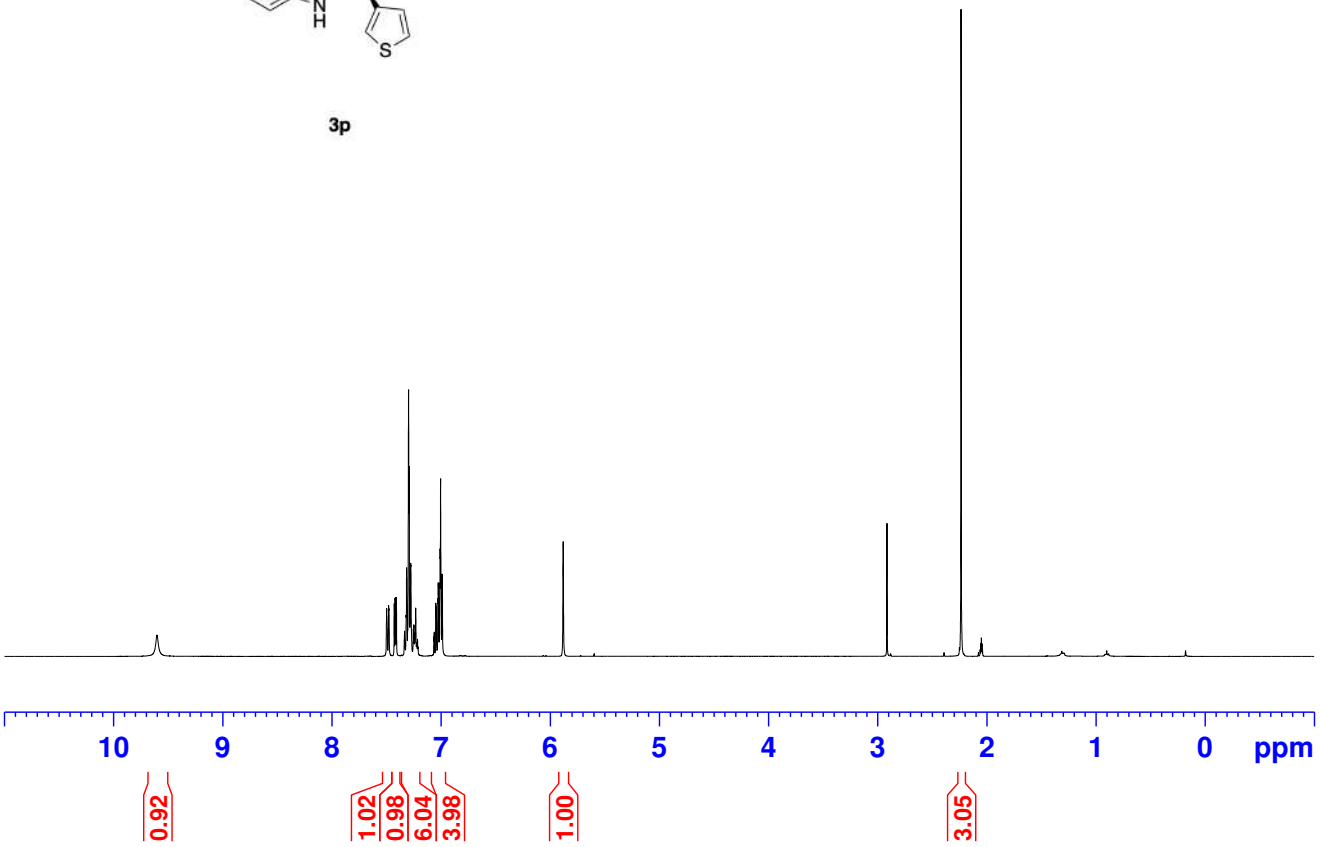



```
Current Data Parameters
NAME          YQL-2-36-P
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210821
Time               10.16
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  201
DS                    1
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.00 usec
TE               300.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                40.00 usec
PL1               -3.00 dB
PL1W        60.64365387 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              14.39 dB
PL13              18.00 dB
PL2W        12.17476940 W
PL12W        0.35193357 W
PL13W        0.15327126 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6126814 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```

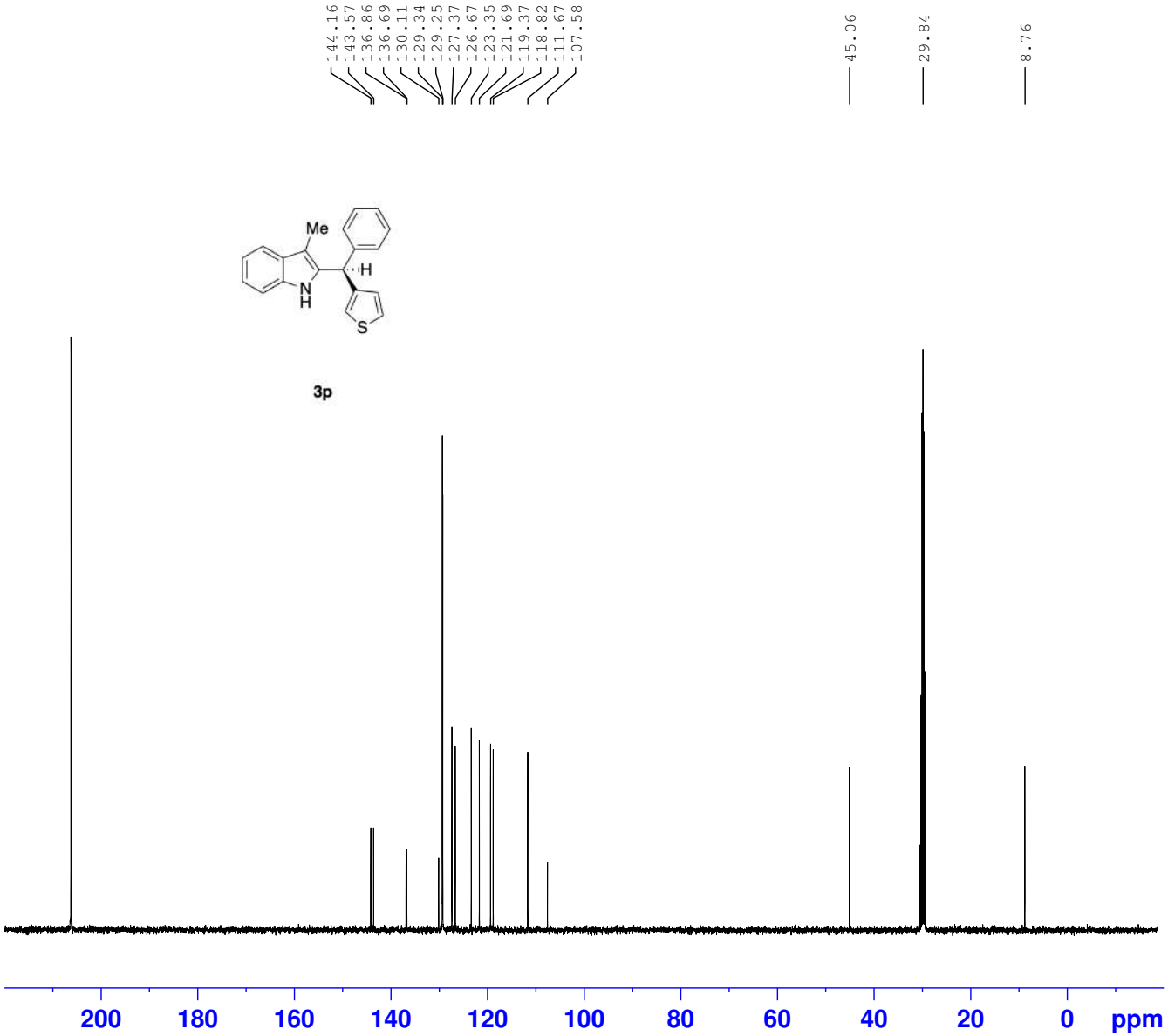




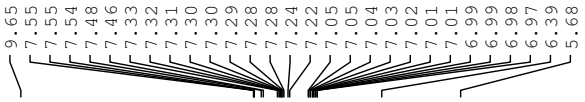
3p

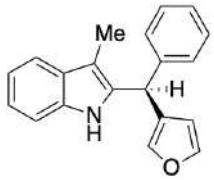



```
Current Data Parameters
NAME            YQL-2-67
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210921
Time                9.04
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 31.55
DW                62.400 usec
DE                 6.50 usec
TE                297.5 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF          400.1300070 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

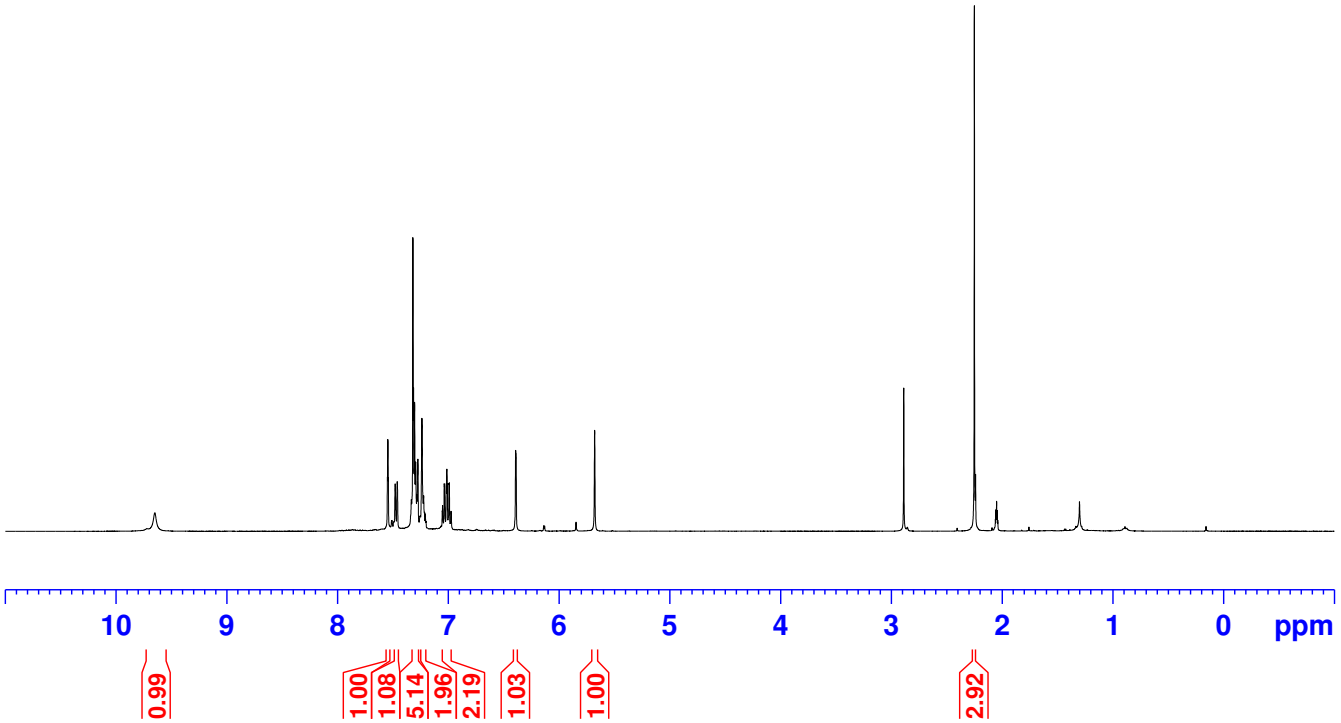



```
Current Data Parameters
NAME                  YQL-2-67
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20210921
Time                      9.07
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       65536
SOLVENT                Acetone
NS                           73
DS                            2
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631488 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
PLW1              46.98899841 W

======== CHANNEL f2 ========
SFO2              400.1316005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                    90.00 usec
PLW2              11.99499989 W
PLW12              0.34213999 W
PLW13              0.27713001 W

F2 - Processing parameters
SI                       32768
SF                100.6126867 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

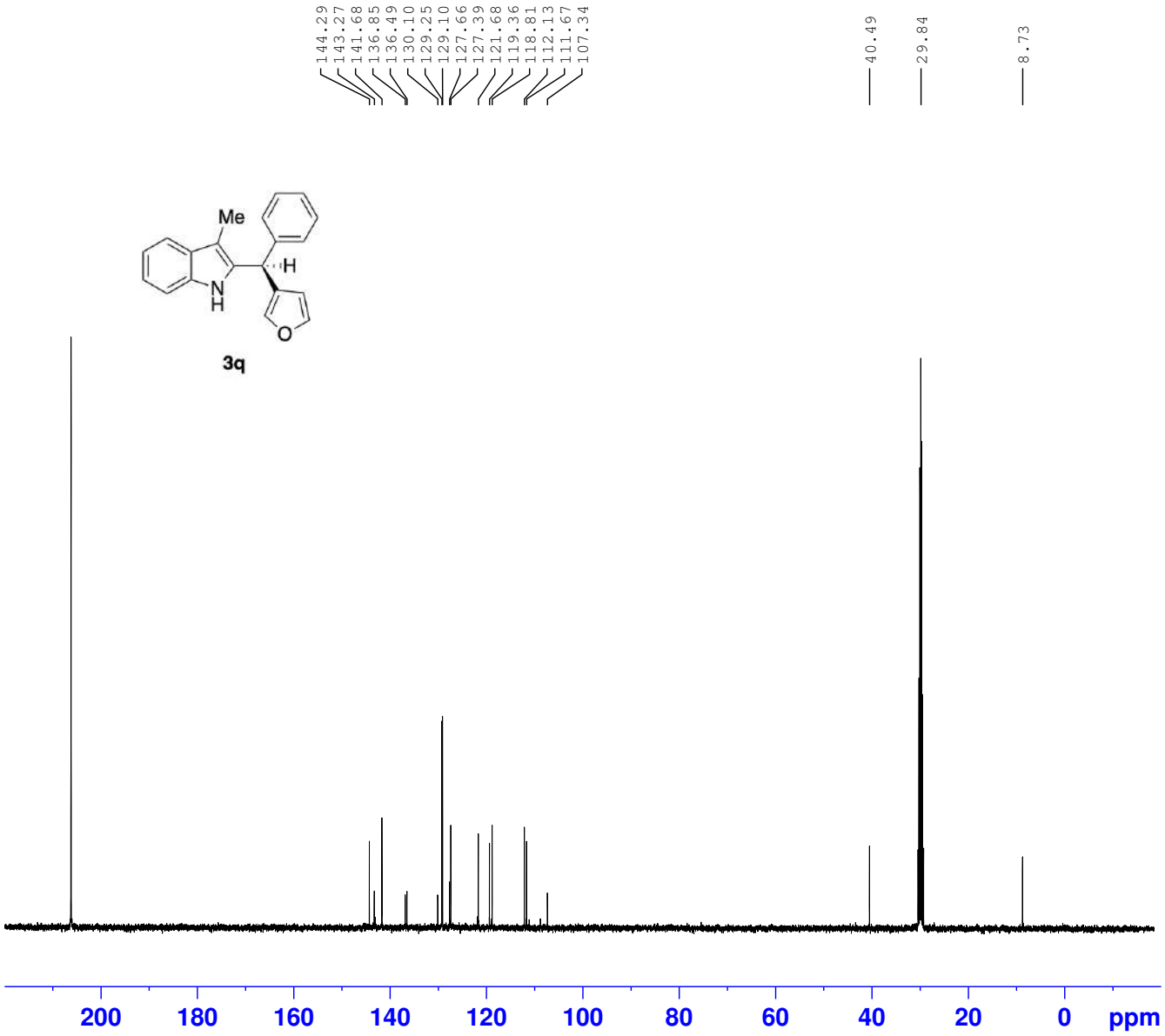




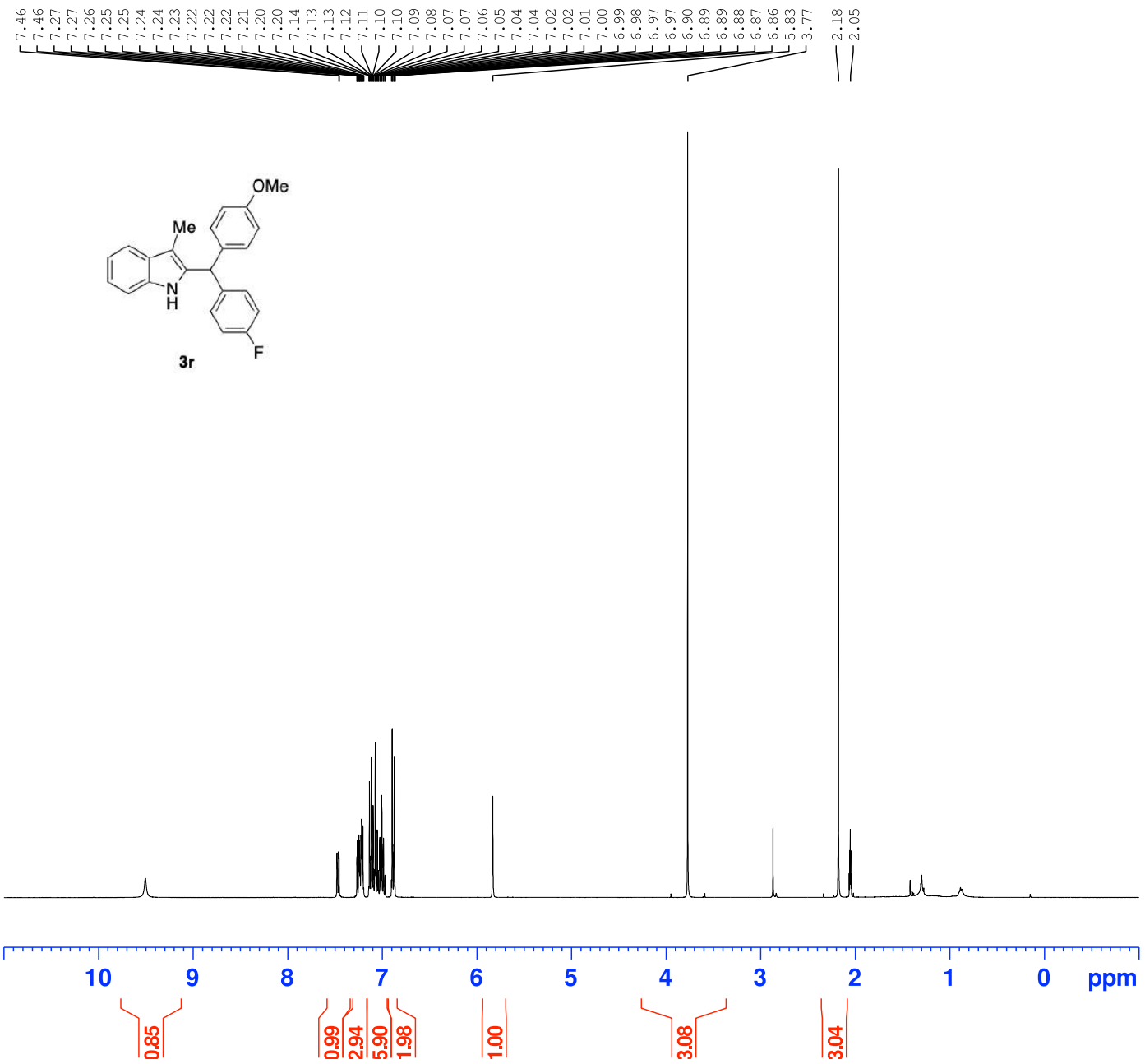
3q



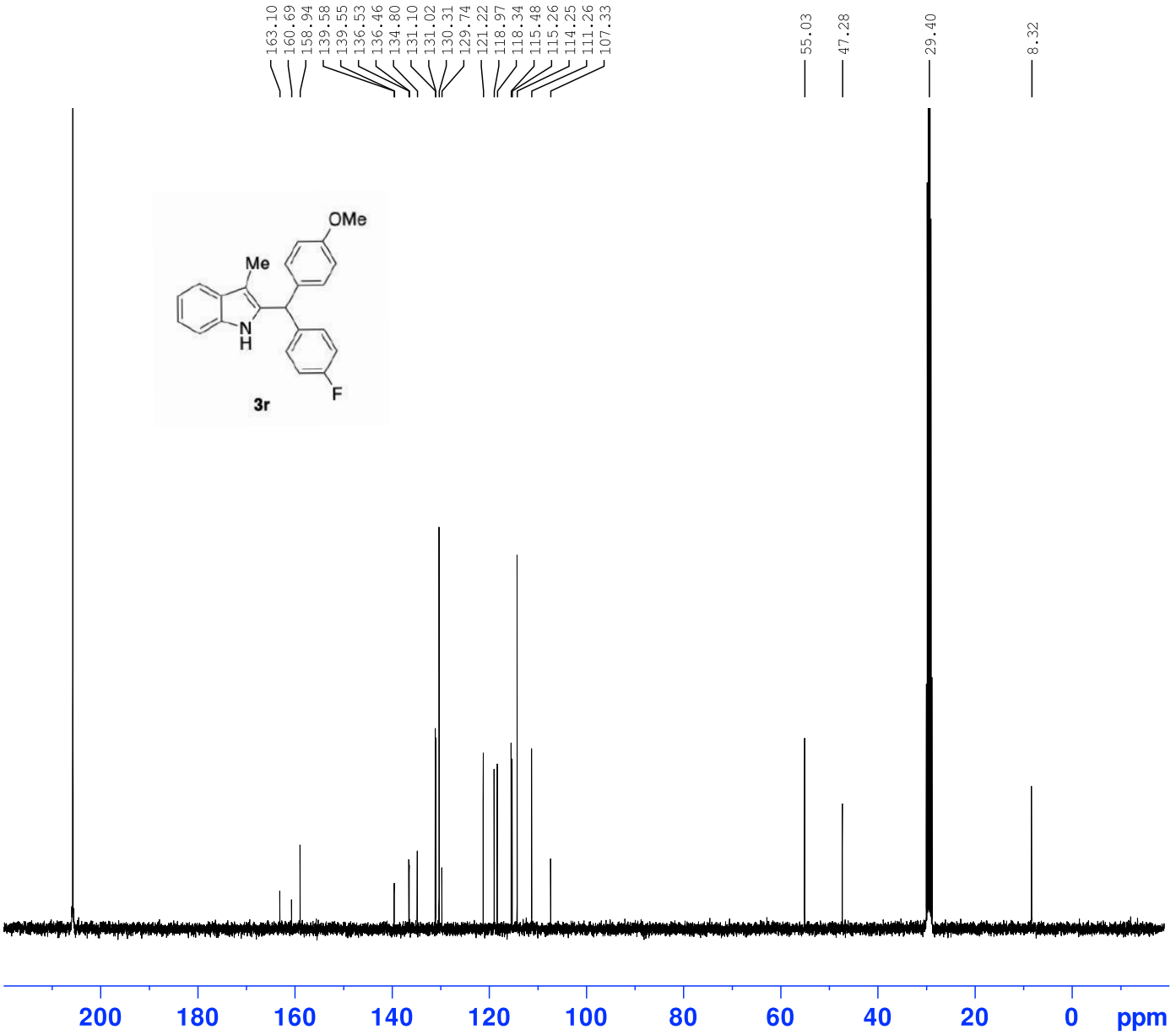

```
Current Data Parameters
NAME          YQL-2-91-P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211017
Time               20.18
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                 39.46
DW                62.400 usec
DE                 6.50 usec
TE                297.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300071 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```



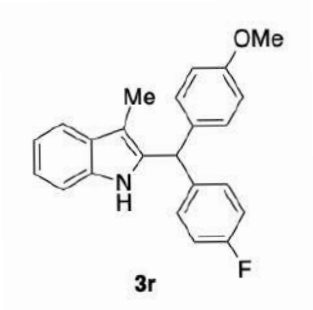

```
Current Data Parameters
NAME          YQL-2-91-P
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211017
Time               20.21
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   53
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               196.92
DW               20.800 usec
DE                6.50 usec
TE               297.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.70 usec
PLW1        46.98899841 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        11.99499989 W
PLW12        0.34213999 W
PLW13        0.27713001 W

F2 - Processing parameters
SI                 32768
SF          100.6126831 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```




```
Current Data Parameters
NAME         YQL-2-186-P
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220308
Time               14.04
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                     8
DS                     0
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                 70.97
DW                 62.400 usec
DE                  6.50 usec
TE                 294.7 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 14.50 usec
PLW1         11.99499989 W

F2 - Processing parameters
SI                 65536
SF           400.1300070 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



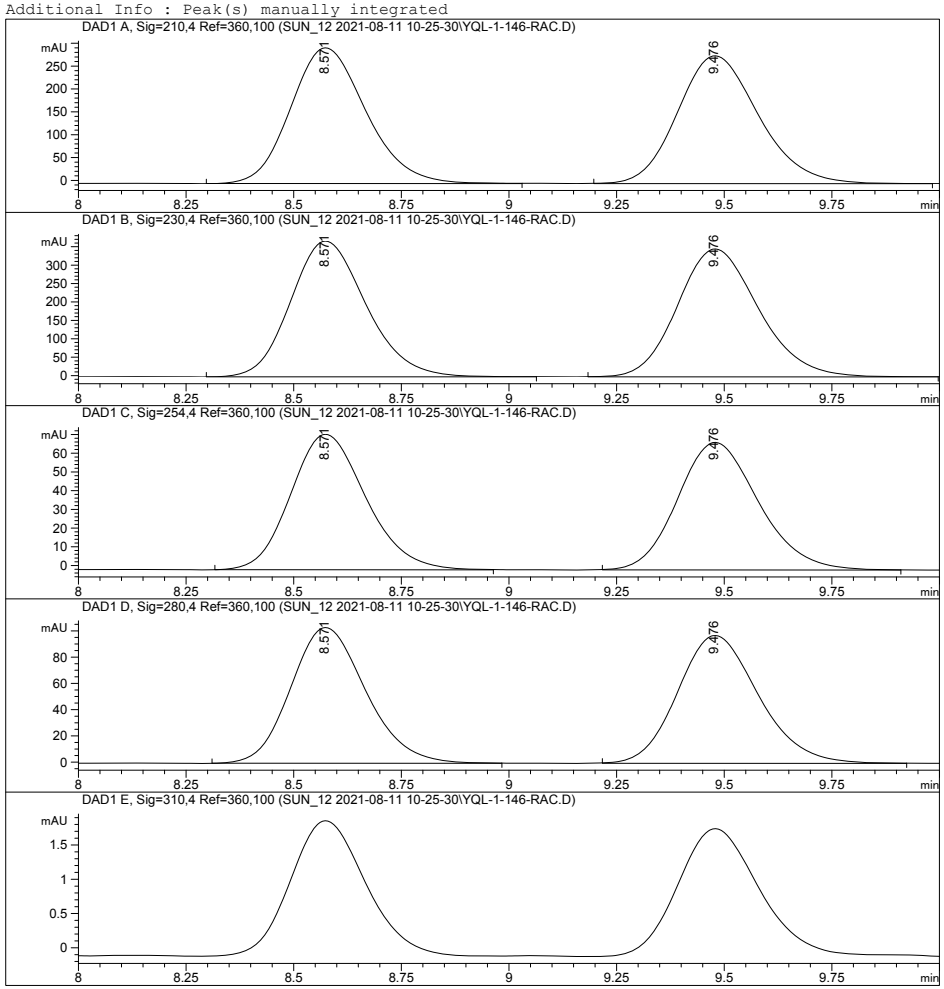

```
Current Data Parameters
NAME         YQL-2-186-P
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220308
Time               14.06
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT          Acetone
NS                    94
DS                     2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                196.92
DW                20.800 usec
DE                 6.50 usec
TE                295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                  13C
P1                  9.70 usec
PLW1         46.98899841 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2         11.99499989 W
PLW12         0.34213999 W
PLW13         0.27713001 W

F2 - Processing parameters
SI                 32768
SF           100.6127258 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```




```
Current Data Parameters
NAME         YQL-2-186-F
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220308
Time               16.16
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD               131072
SOLVENT         Acetone
NS                    16
DS                     4
SWH            89285.711 Hz
FIDRES          0.681196 Hz
AQ             0.7340032 sec
RG                196.92
DW                 5.600 usec
DE                 6.50 usec
TE                294.5 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         376.4607164 MHz
NUC1                19F
P1                14.70 usec
PLW1         15.99600029 W

F2 - Processing parameters
SI                 65536
SF           376.4983660 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

Data File C:\CHEM32\1\DATA\SUN_12 2021-08-11 10-25-30\YQL-1-146-RAC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location : Vial 51
Injection Date  : 8/11/2021 10:38:43 AM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 10.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-08-11 10-25-30\AD-05-15.M
Last changed    : 8/11/2021 10:37:49 AM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 3:46:19 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-08-11 10-25-30\YQL-1-146-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 [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.571	BB	0.1881	3613.95630	296.79227	49.6342
2	9.476	BB	0.2031	3667.21826	279.50912	50.3658
Totals :				7281.17456	576.30139	

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

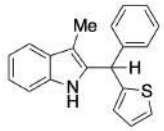
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.571	BB	0.1879	4483.67773	368.59171	49.5923
2	9.476	BB	0.2030	4557.39648	347.40057	50.4077
Totals :				9041.07422	715.99228	

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.571	BB	0.1875	877.68146	72.37300	49.5958
2	9.476	BB	0.2026	891.98700	68.17650	50.4042
Totals :				1769.66846	140.54950	

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.571	BB	0.1874	1252.94751	103.37744	49.5858
2	9.476	BB	0.2026	1273.88074	97.40432	50.4142
Totals :				2526.82825	200.78176	



3a

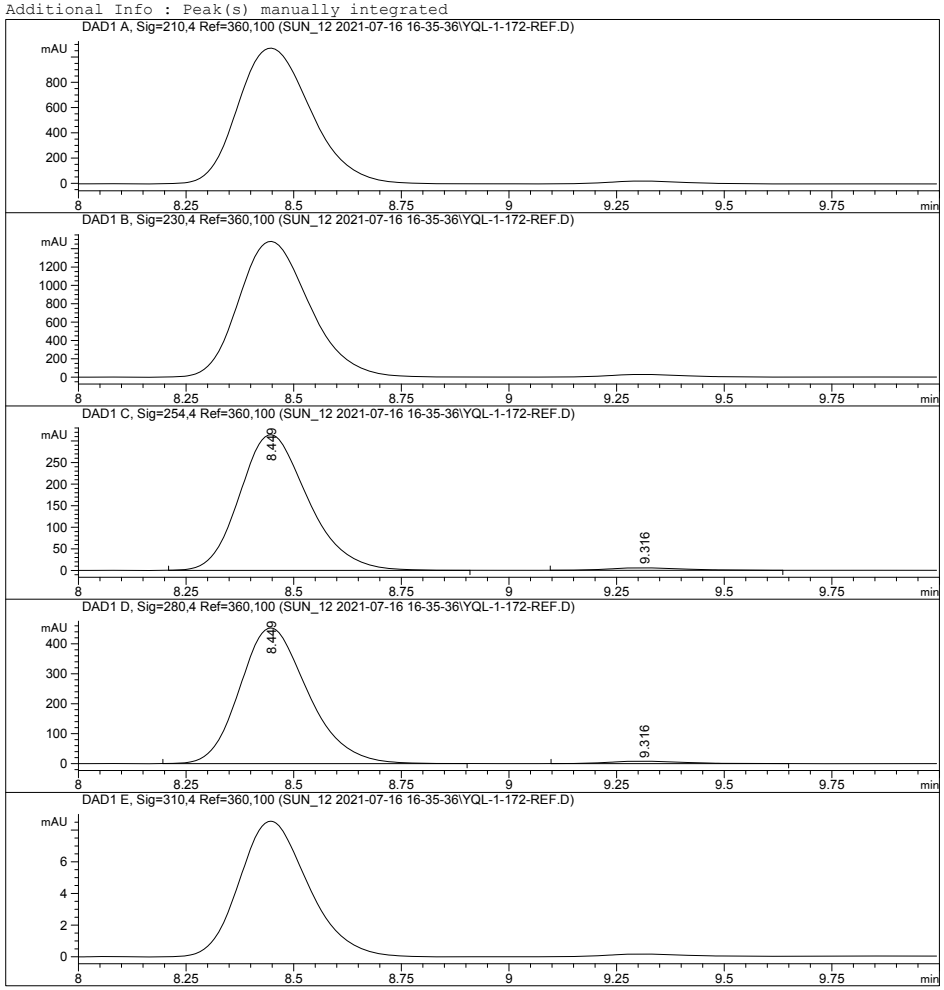
(racemic)

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

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

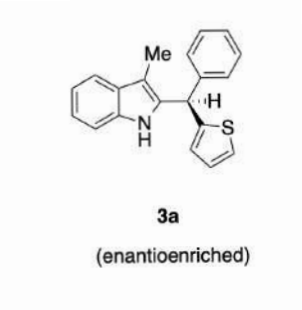
Data File C:\CHEM32\1\DATA\SUN_12 2021-07-16 16-35-36\YQL-1-172-REF.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location : Vial 53
Injection Date  : 7/16/2021 4:48:48 PM          Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-07-16 16-35-36\AD-05-10.M
Last changed    : 7/16/2021 4:36:08 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:26:07 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-16 16-35-36\YQL-1-172-REF.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


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


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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.449 BB    0.1709 3474.59839  314.54010  98.0495
   2   9.316 BB    0.1874   69.11983    5.70412   1.9505

Totals :                  3543.71822  320.24422



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.449 BB    0.1706 4996.17725  453.10181  98.1095
   2   9.316 BB    0.1830   96.27036    8.08061   1.8905

Totals :                  5092.44761  461.18242



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

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

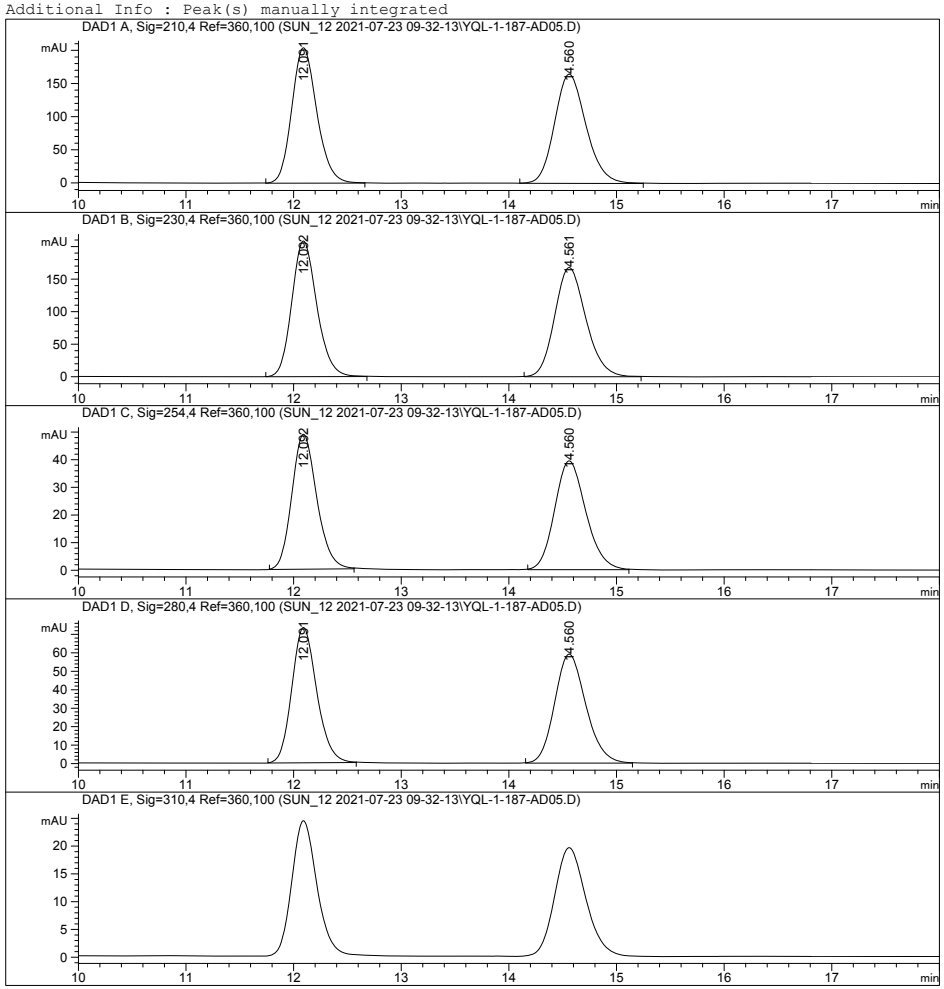


3a

(enantioenriched)

Data File C:\CHEM32\1\DATA\SUN_12 2021-07-23 09-32-13\YQL-1-187-AD05.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   8
Acq. Instrument : Instrument 1              Location : Vial 61
Injection Date  : 7/23/2021 1:17:46 PM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !   Actual Inj Volume : 10.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-07-23 09-32-13\AD-05-20.M
Last changed    : 7/23/2021 1:16:51 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 4:02:07 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-23 09-32-13\YQL-1-187-AD05.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 [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.091	BB	0.2486	3301.54468	204.24109	49.6654
2	14.560	BB	0.3130	3346.02930	164.74232	50.3346
Totals :				6647.57397	368.98341	

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

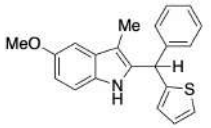
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.092	BB	0.2485	3366.98438	208.40799	49.8763
2	14.561	BB	0.3113	3383.68262	167.76050	50.1237
Totals :				6750.66699	376.16849	

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.092	BB	0.2480	786.85205	48.82372	49.8192
2	14.560	BB	0.3109	792.56238	39.35765	50.1808
Totals :				1579.41443	88.18137	

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.091	BB	0.2479	1181.10925	73.35355	49.8207
2	14.560	BB	0.3110	1189.61121	59.06180	50.1793
Totals :				2370.72046	132.41536	



3b

(racemic)

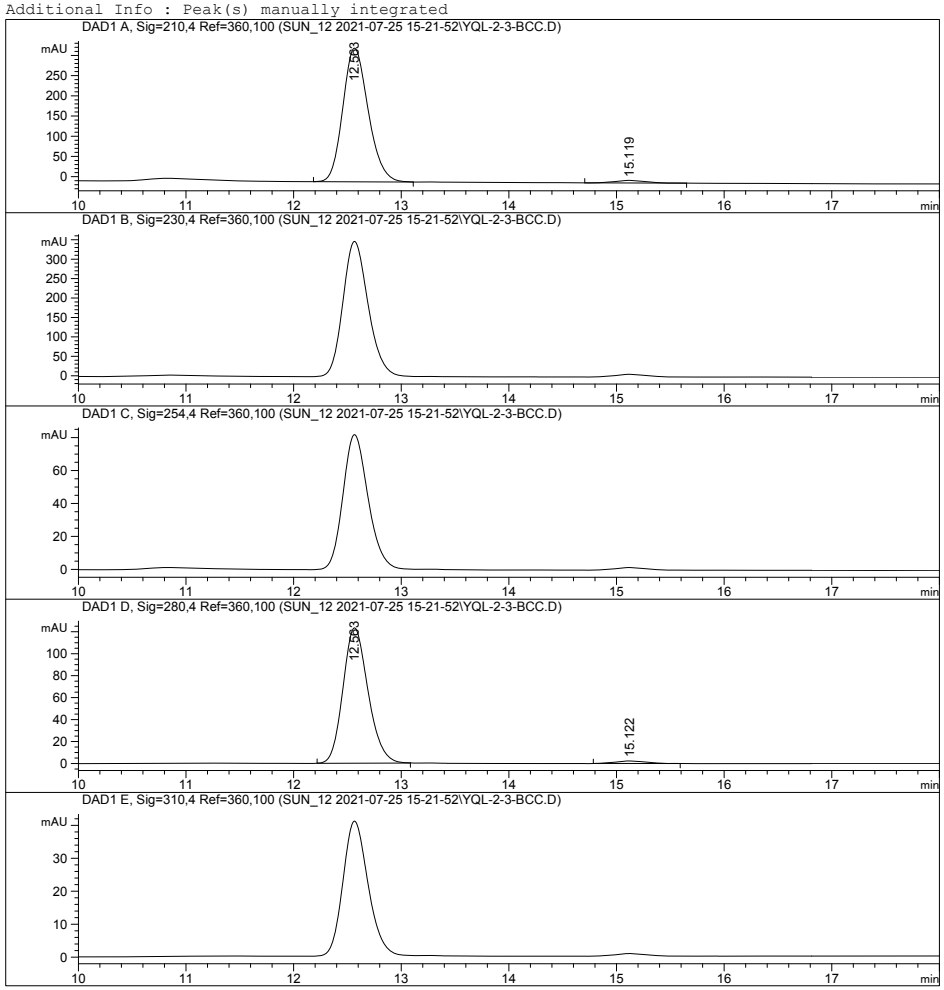
Signal 5: DAD1 E, Sig=310,4 Ref=360,100

==========

*** End of Report ***

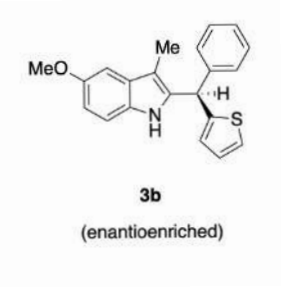
Data File C:\CHEM32\1\DATA\SUN_12 2021-07-25 15-21-52\YQL-2-3-BCC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location : Vial 62
Injection Date  : 7/25/2021 3:38:13 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-07-25 15-21-52\AD-05-20.M
Last changed    : 7/25/2021 3:37:20 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:49:34 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-25 15-21-52\YQL-2-3-BCC.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  12.563 BB    0.2532 5422.80713  330.83133  97.8119
   2  15.119 BB    0.2548  121.31109    6.46816   2.1881

Totals :                  5544.11822  337.29949



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.563 BB    0.2491 1998.53906  123.29641  97.7410
   2  15.122 BB    0.2928   46.19011    2.35510   2.2590

Totals :                  2044.72918  125.65150



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

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

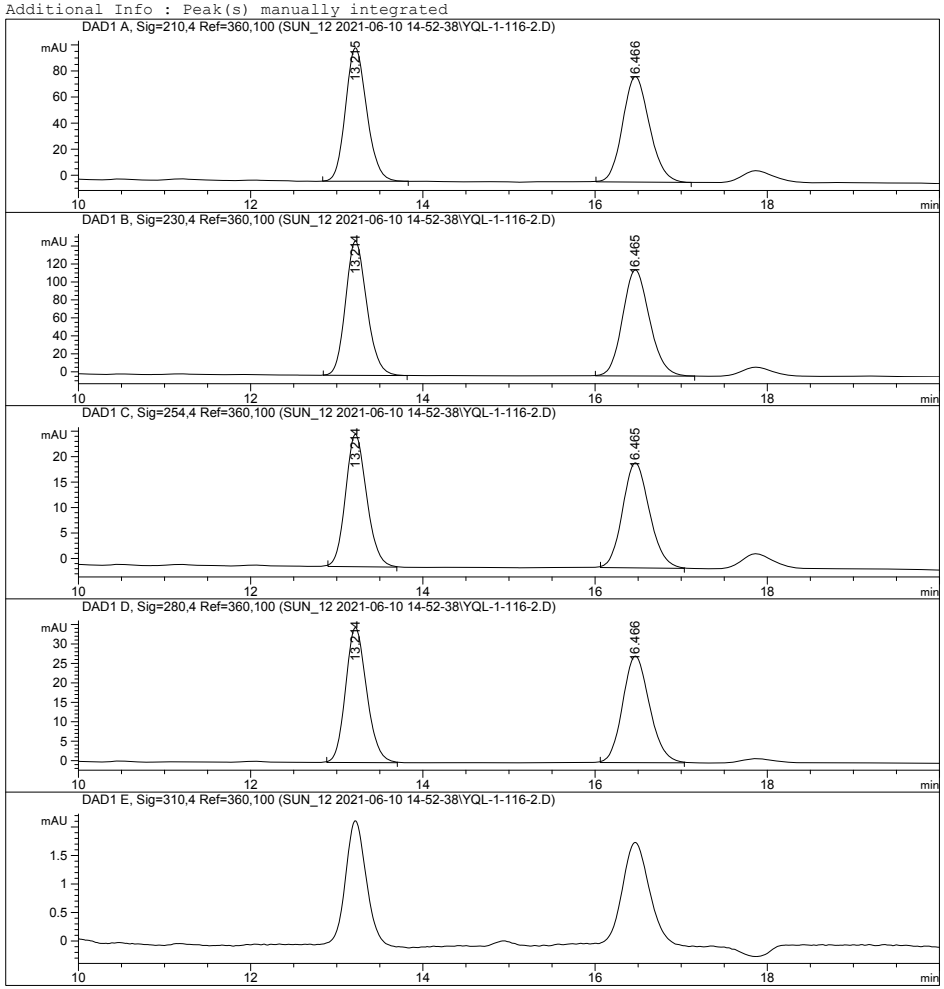


3b

(enantioenriched)

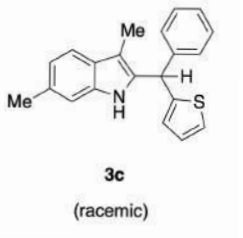
Data File C:\CHEM32\1\DATA\SUN_12 2021-06-10 14-52-38\YQL-1-116-2.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  21
Acq. Instrument : Instrument 1              Location : Vial 62
Injection Date  : 6/10/2021 8:53:19 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\SUN_12 2021-06-10 14-52-38\AD-03-30.M
Last changed    : 6/10/2021 8:52:26 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 3:52:45 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-06-10 14-52-38\YQL-1-116-2.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  13.215 BB    0.2637 1753.14038  102.41386  49.9503
   2  16.466 BB    0.3349 1756.63147   81.04115  50.0497

Totals :                  3509.77185  183.45502



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.214 BB    0.2635 2556.78418  149.50371  49.8842
   2  16.465 BB    0.3360 2568.64966  117.98009  50.1158

Totals :                  5125.43384  267.48380



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.214 BB    0.2628  443.21017   26.01645  49.7734
   2  16.465 BB    0.3330  447.24557   20.62712  50.2266

Totals :                   890.45575   46.64356



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.214 BB    0.2626  591.20020   34.72526  49.8822
   2  16.466 BB    0.3349  593.99365   27.40362  50.1178

Totals :                  1185.19385   62.12888
```



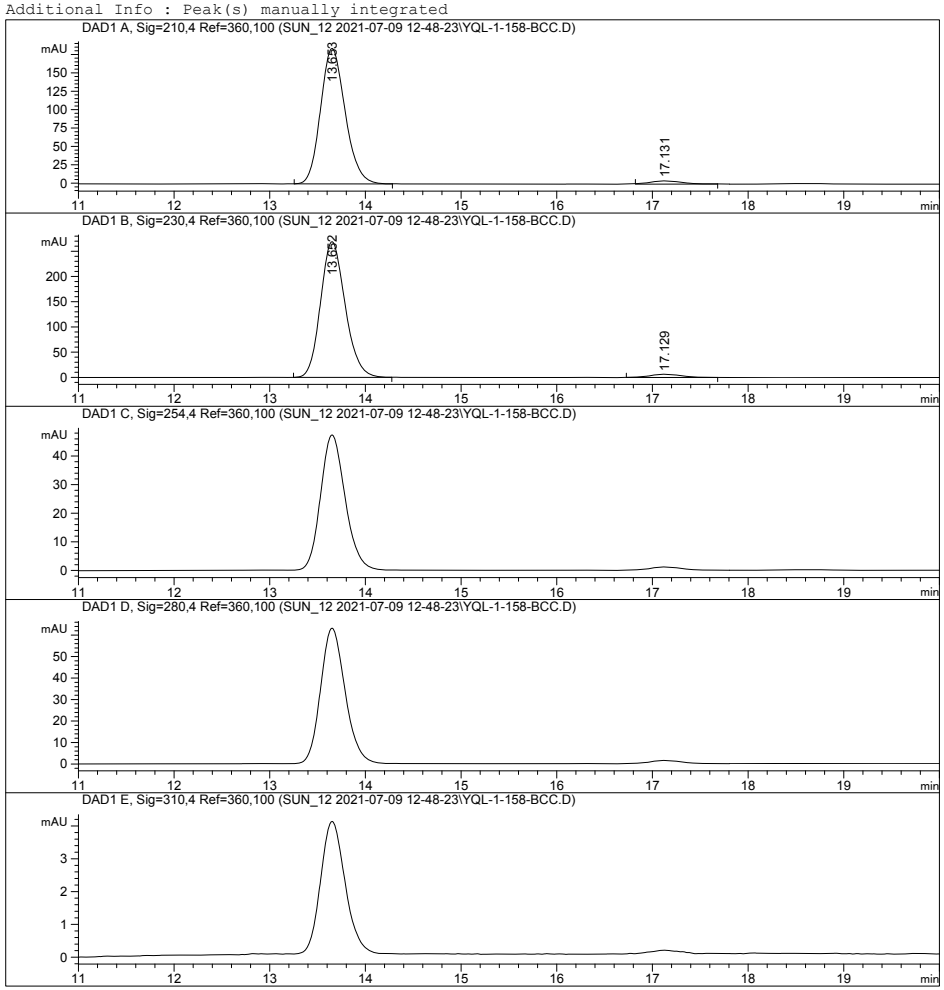
3c

(racemic)

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

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

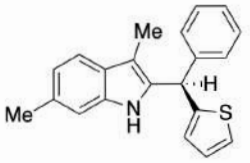
Data File C:\CHEM32\1\DATA\SUN_12 2021-07-09 12-48-23\YQL-1-158-BCC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  14
Acq. Instrument : Instrument 1              Location : Vial 62
Injection Date  : 7/9/2021 4:08:22 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-07-09 12-48-23\AD-03-20.M
Last changed    : 7/2/2016 3:26:02 PM
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:39:11 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-09 12-48-23\YQL-1-158-BCC.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  13.653 BB    0.2760 3283.48560  184.13354  97.0568
   2  17.131 BB    0.2769   99.57059    4.45330   2.9432

Totals :                  3383.05619  188.58685



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.652 BB    0.2761 4800.07617  269.08270  97.1286
   2  17.129 BB    0.3333  141.90361    6.48364   2.8714

Totals :                  4941.97978  275.56635



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 ***
```

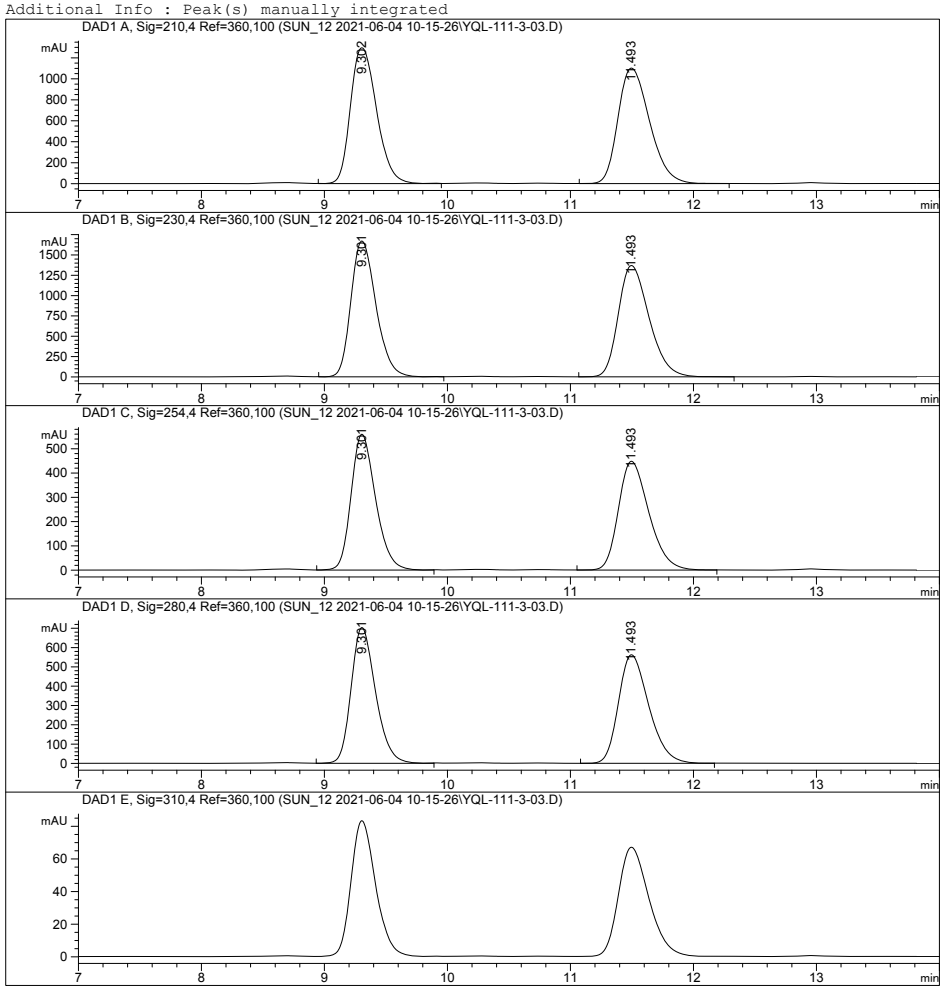


3c

(enantioenriched)

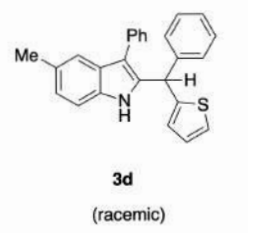
Data File C:\CHEM32\1\DATA\SUN_12 2021-06-04 10-15-26\YQL-111-3-03.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  12
Acq. Instrument : Instrument 1              Location : Vial 53
Injection Date  : 6/4/2021 2:08:56 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\SUN_12 2021-06-04 10-15-26\AD-03-30.M
Last changed    : 6/4/2021 1:05:36 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 3:50:28 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-06-04 10-15-26\YQL-111-3-03.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   9.302 VB    0.2321 1.91029e4  1295.24731  49.3089
   2  11.493 VB    0.2781 1.96384e4  1101.18909  50.6911

Totals :                  3.87413e4  2396.43640



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.301 VB    0.2187 2.35930e4  1671.41931  49.7826
   2  11.493 VB    0.2687 2.37991e4  1369.79346  50.2174

Totals :                  4.73921e4  3041.21277



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.301 VB    0.2132 7726.67627  559.19073  50.0923
   2  11.493 VB    0.2666 7698.19336  447.75427  49.9077

Totals :                  1.54249e4  1006.94501



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.301 VB    0.2130 9714.44727  703.87689  50.2187
   2  11.493 VB    0.2658 9629.84570  562.32385  49.7813

Totals :                  1.93443e4  1266.20074
```



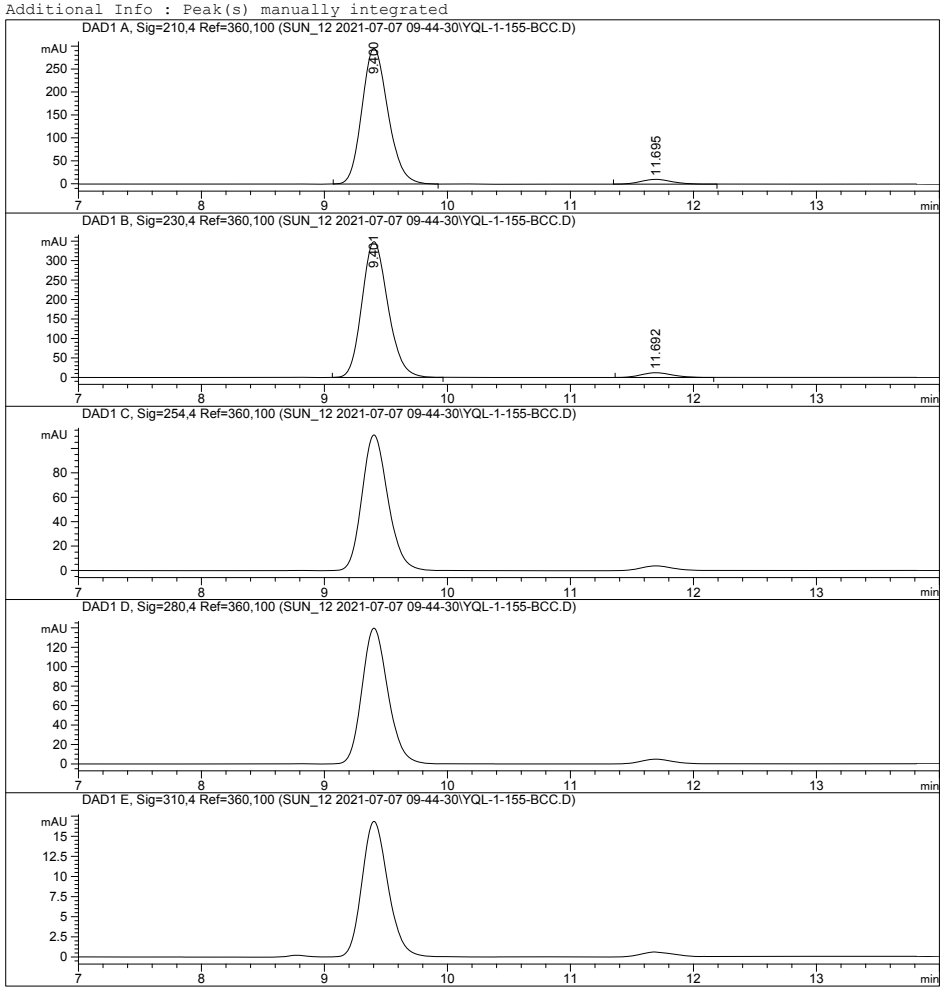
3d

(racemic)

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

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

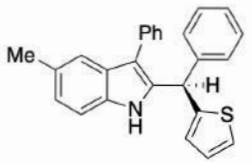
Data File C:\CHEM32\1\DATA\SUN_12 2021-07-07 09-44-30\YQL-1-155-BCC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  40
Acq. Instrument : Instrument 1              Location : Vial 62
Injection Date  : 7/7/2021 11:18:50 PM          Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-07-07 09-44-30\AD-03-20.M
Last changed    : 7/2/2016 3:26:02 PM
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:36:01 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-07 09-44-30\YQL-1-155-BCC.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   9.400 BB    0.2275 4346.56299  295.60614  95.9380
   2  11.695 BB    0.2624  184.03313   10.40223   4.0620

Totals :                  4530.59612  306.00837



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.401 BB    0.2270 5111.56934  348.71329  95.9421
   2  11.692 BB    0.2715  216.19398   12.15722   4.0579

Totals :                  5327.76332  360.87051



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 ***
```

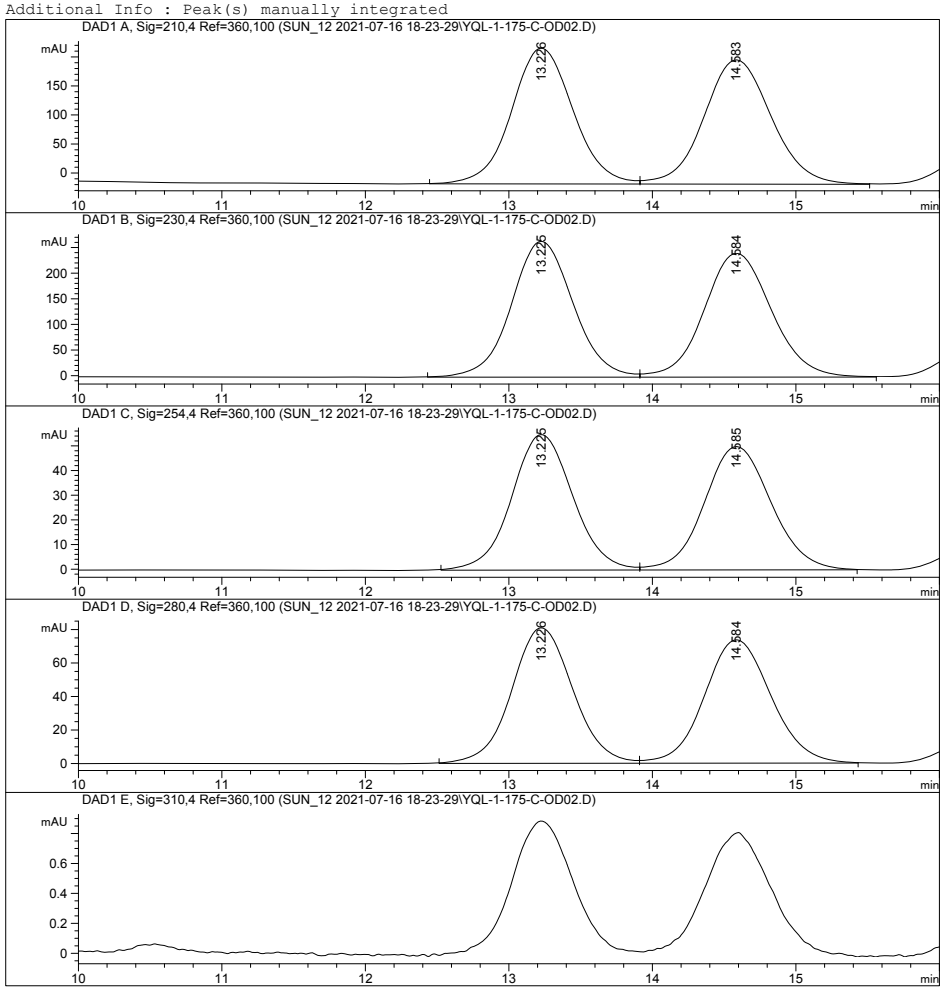


3d

(enantioenriched)

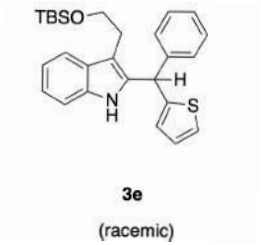
Data File C:\CHEM32\1\DATA\SUN_12 2021-07-16 18-23-29\YQL-1-175-C-OD02.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  31
Acq. Instrument : Instrument 1              Location : Vial 53
Injection Date  : 7/17/2021 5:24:22 AM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !   Actual Inj Volume : 8.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-07-16 18-23-29\OD-02-40-0.5.M
Last changed    : 7/14/2021 9:24:08 AM
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/21/2021 2:07:02 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-16 18-23-29\YQL-1-175-C-OD02.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  13.226 BV    0.4665 6990.55762  234.03725  49.9823
   2  14.583 VB    0.5069 6995.49854  214.28387  50.0177

Totals :                  1.39861e4   448.32112



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.225 BV    0.4648 7916.18555  264.80038  50.1033
   2  14.584 VB    0.5087 7883.55859  241.60342  49.8967

Totals :                  1.57997e4   506.40381



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.225 BV    0.4629 1633.32446   54.93291  50.1670
   2  14.585 VB    0.5022 1622.45325   50.05202  49.8330

Totals :                  3255.77771  104.98492



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.226 BV    0.4627 2404.30981   80.89833  50.2340
   2  14.584 VB    0.5033 2381.90845   73.64767  49.7660

Totals :                  4786.21826  154.54600



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

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

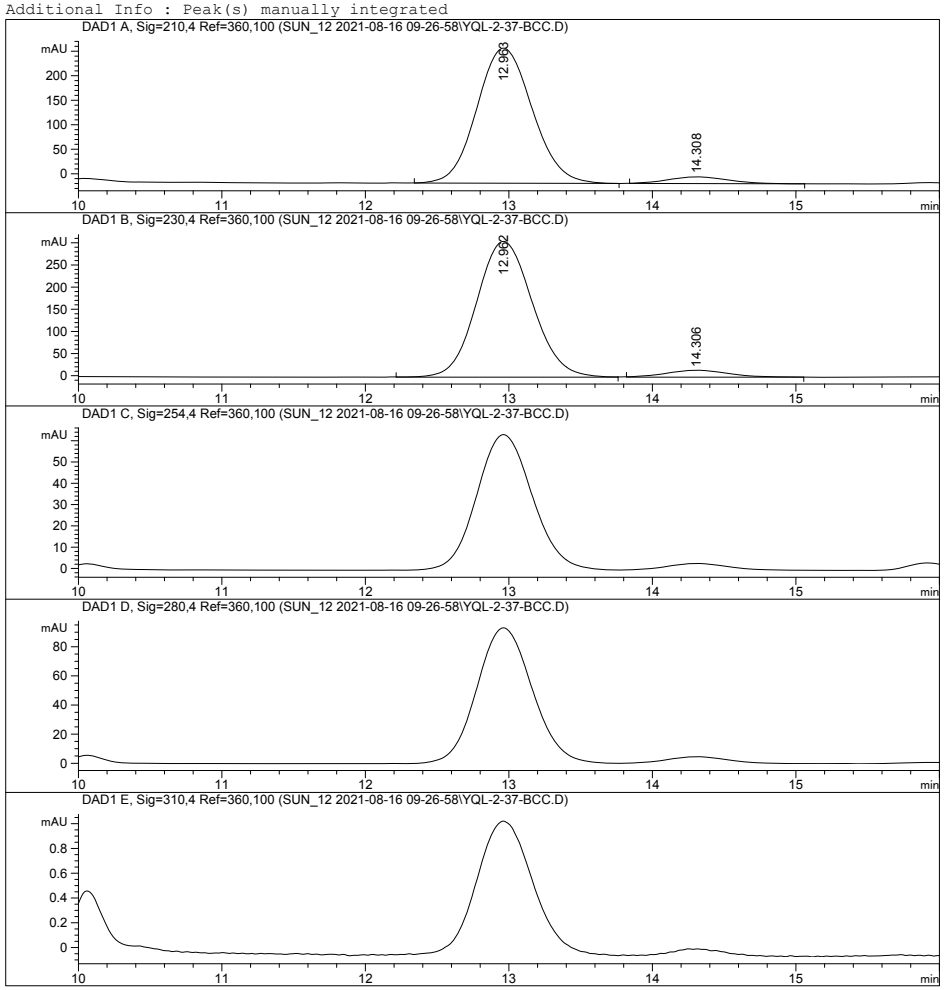


3e

(racemic)

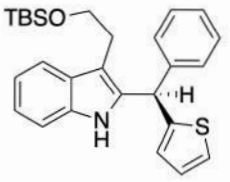
Data File C:\CHEM32\1\DATA\SUN_12 2021-08-16 09-26-58\YQL-2-37-BCC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  11
Acq. Instrument : Instrument 1              Location : Vial 63
Injection Date  : 8/16/2021 11:43:34 AM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 7.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-08-16 09-26-58\OD-02-40-0.5.M
Last changed    : 7/14/2021 9:24:08 AM
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 11:00:21 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-08-16 09-26-58\YQL-2-37-BCC.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  12.963 BB    0.4209 7394.72754  275.67648  94.8736
   2  14.308 BB    0.4312  399.57043   13.74294   5.1264

Totals :                  7794.29797  289.41942



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.962 BB    0.4229 8273.05273  306.50214  94.7027
   2  14.306 BB    0.4417  462.76218   15.61651   5.2973

Totals :                  8735.81491  322.11865



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 ***
```

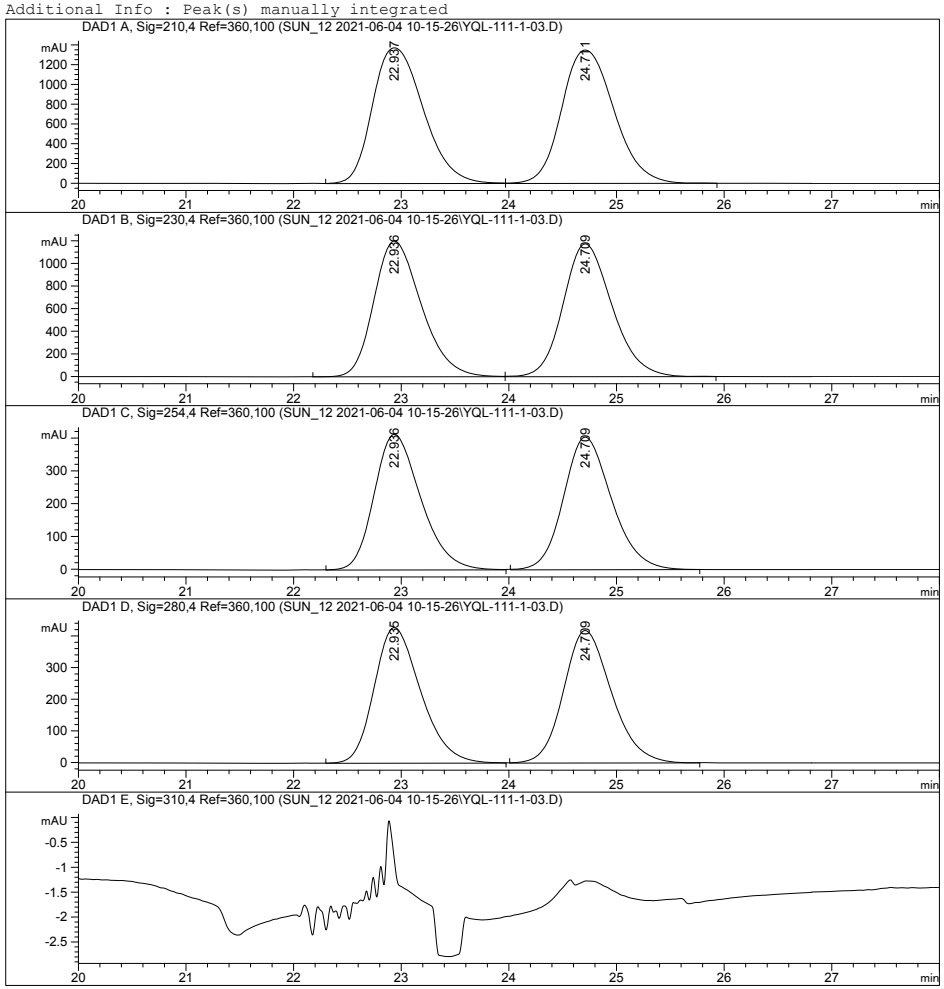


3e

(enantioenriched)

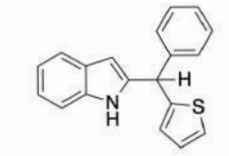
Data File C:\CHEM32\1\DATA\SUN_12 2021-06-04 10-15-26\YQL-111-1-03.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  10
Acq. Instrument : Instrument 1              Location : Vial 51
Injection Date  : 6/4/2021 1:06:27 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\SUN_12 2021-06-04 10-15-26\AD-03-30.M
Last changed    : 6/4/2021 1:05:36 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AS-20-60-0.5.M
Last changed    : 8/9/2021 10:31:08 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-06-04 10-15-26\YQL-111-1-03.D
Sample Name:

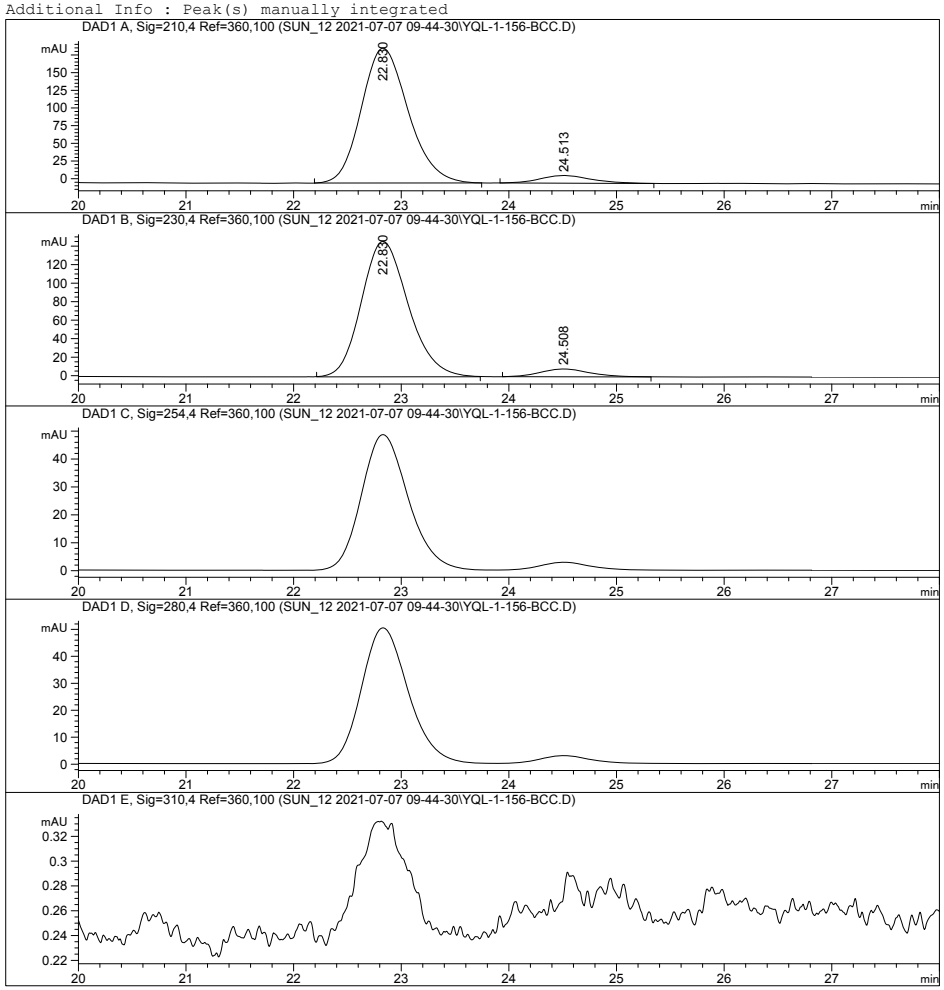
```
==================================================================
                        Area Percent Report
==================================================================

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  22.937 VV    0.5148 4.50575e4  1373.16296  49.6864
   2  24.711 VB    0.5349 4.56263e4  1347.91992  50.3136

Totals :                  9.06838e4  2721.08289



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  22.936 VV    0.4750 3.67318e4  1200.29749  49.7432
   2  24.709 VB    0.4888 3.71111e4  1173.88464  50.2568

Totals :                  7.38429e4  2374.18213



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  22.936 VB    0.4672 1.24562e4   413.83664  49.7823
   2  24.709 BB    0.4766 1.25651e4   404.31332  50.2177

Totals :                  2.50213e4   818.14996



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  22.935 VB    0.4667 1.28895e4   428.77884  49.7751
   2  24.709 BB    0.4765 1.30060e4   418.53918  50.2249

Totals :                  2.58954e4   847.31802



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

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



3f
(racemic)

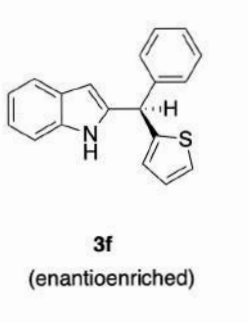
Data File C:\CHEM32\1\DATA\SUN_12 2021-07-07 09-44-30\YQL-1-156-BCC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   5
Acq. Instrument : Instrument 1              Location : Vial 61
Injection Date  : 7/7/2021 10:42:26 AM           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-07-07 09-44-30\AD-03-30.M
Last changed    : 7/7/2021 10:41:33 AM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:37:37 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-07 09-44-30\YQL-1-156-BCC.D
Sample Name:

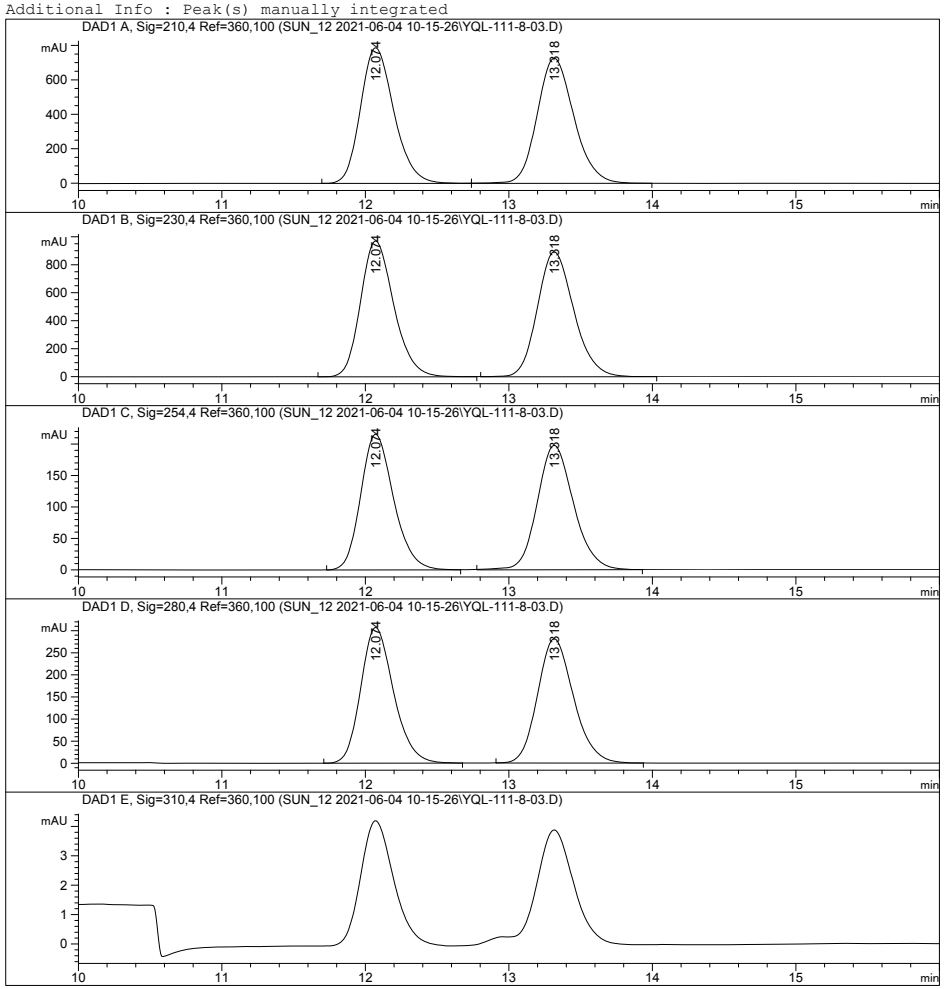
```
==================================================================
                        Area Percent Report
==================================================================

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  22.830 BB    0.4632 5776.67627  190.82646  94.1092
   2  24.513 BB    0.4089  361.59180   10.90215   5.8908

Totals :                  6138.26807  201.72861



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  22.830 BB    0.4667 4425.43994  146.38750  94.2613
   2  24.508 BB    0.4657  269.42255    8.45734   5.7387

Totals :                  4694.86249  154.84484



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)

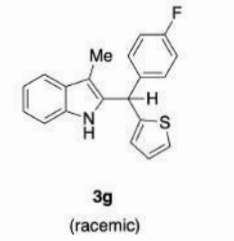
Data File C:\CHEM32\1\DATA\SUN_12 2021-06-04 10-15-26\YQL-111-8-03.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  17
Acq. Instrument : Instrument 1              Location : Vial 58
Injection Date  : 6/4/2021 4:44:55 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\SUN_12 2021-06-04 10-15-26\AD-03-30.M
Last changed    : 6/4/2021 1:05:36 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 3:59:31 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-06-04 10-15-26\YQL-111-8-03.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  12.074 BV    0.2510 1.27555e4   787.55853  49.6683
   2  13.318 VB    0.2736 1.29259e4   726.42029  50.3317

Totals :                  2.56814e4  1513.97882



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.074 BB    0.2479 1.56325e4   970.68988  49.8004
   2  13.318 BB    0.2719 1.57578e4   893.00250  50.1996

Totals :                  3.13902e4  1863.69238



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.074 BB    0.2457 3432.69995  215.64636  49.6389
   2  13.318 BB    0.2715 3482.63989  197.73688  50.3611

Totals :                  6915.33984  413.38324



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.074 BB    0.2453 4877.90283  307.04034  49.8985
   2  13.318 BB    0.2691 4897.74219  281.27936  50.1015

Totals :                  9775.64502  588.31970
```

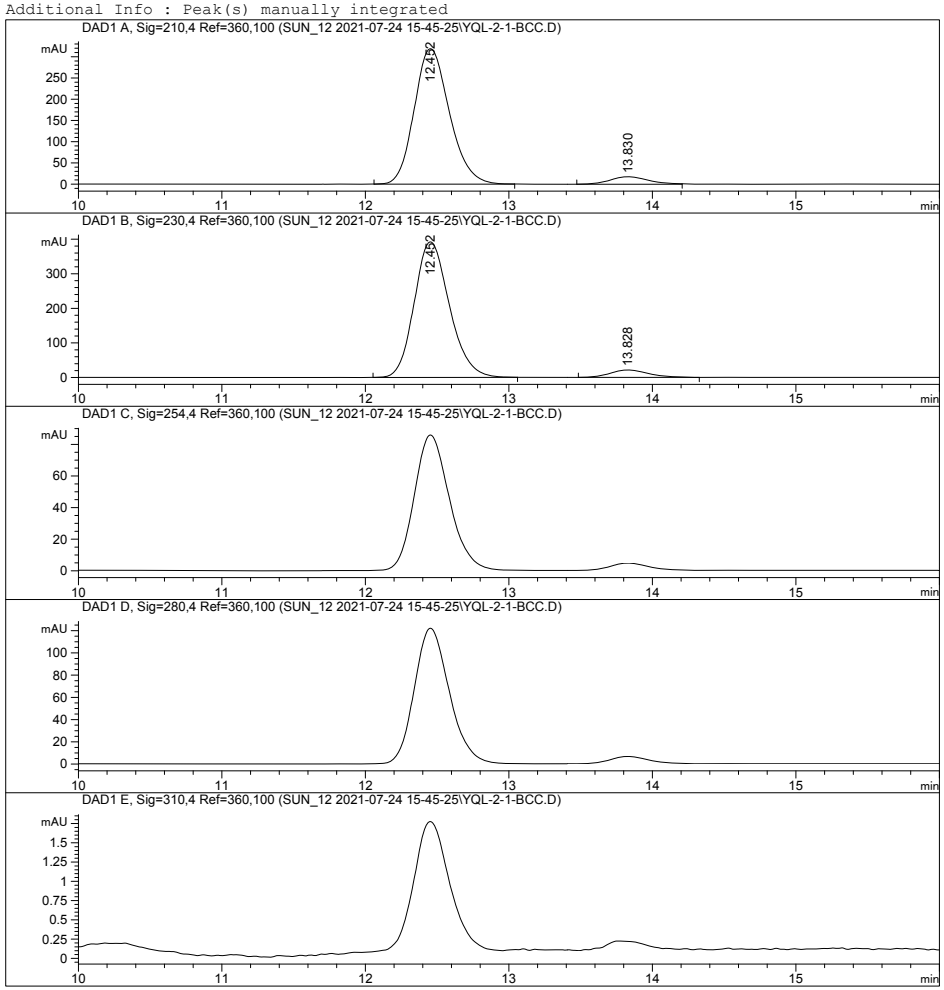


3g
(racemic)

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

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

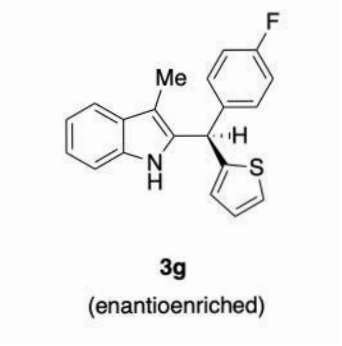
Data File C:\CHEM32\1\DATA\SUN_12 2021-07-24 15-45-25\YQL-2-1-BCC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  22
Acq. Instrument : Instrument 1              Location : Vial 62
Injection Date  : 7/25/2021 12:41:44 AM          Inj :  1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-07-24 15-45-25\AD-03-20.M
Last changed    : 7/2/2016 3:26:02 PM
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:47:33 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-24 15-45-25\YQL-2-1-BCC.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  12.452 BB    0.2625 5436.47119  319.52325  94.3130
   2  13.830 BV    0.2811  327.81601   17.77982   5.6870

Totals :                  5764.28720  337.30308



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.452 BB    0.2623 6670.25586  392.36011  94.3855
   2  13.828 BB    0.2852  396.77756   21.51443   5.6145

Totals :                  7067.03342  413.87454



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 ***
```

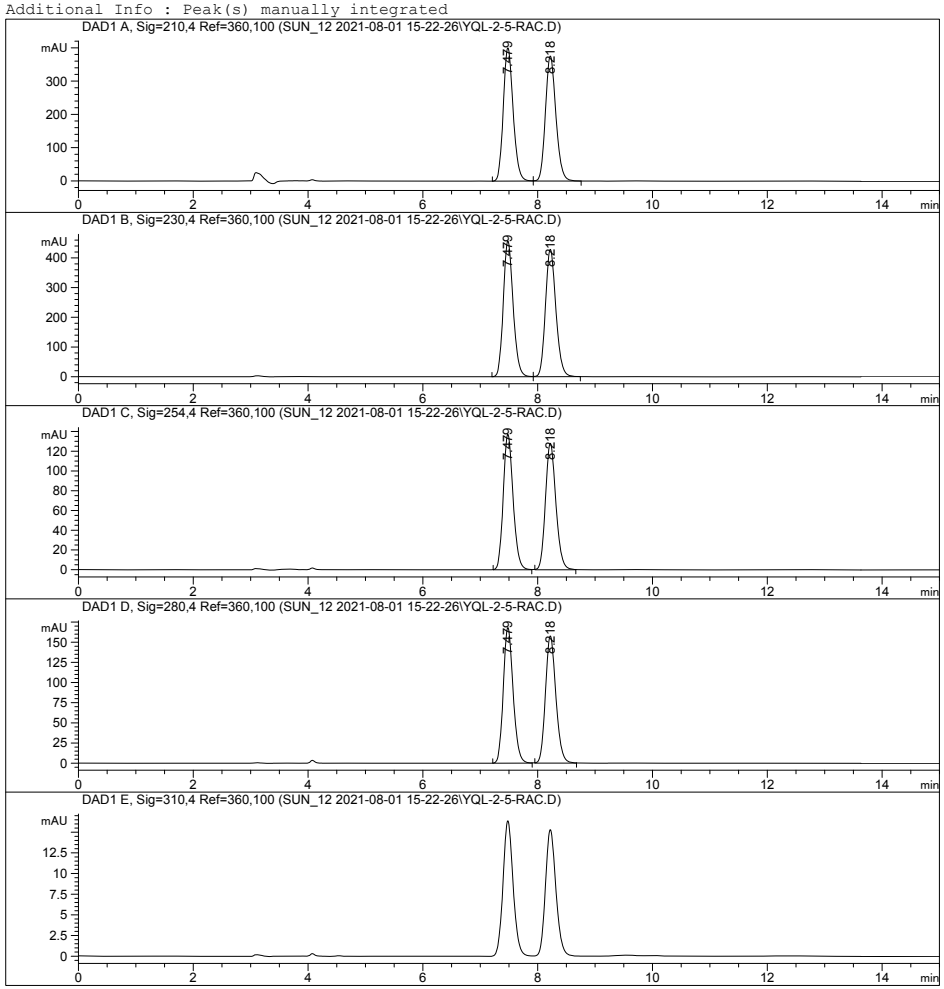


3g

(enantioenriched)

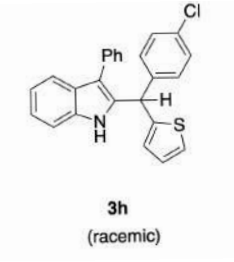
Data File C:\CHEM32\1\DATA\SUN_12 2021-08-01 15-22-26\YQL-2-5-RAC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   3
Acq. Instrument : Instrument 1              Location : Vial 62
Injection Date  : 8/1/2021 3:51:05 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\SUN_12 2021-08-01 15-22-26\AD-05-15.M
Last changed    : 8/1/2021 3:33:50 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 4:04:23 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-08-01 15-22-26\YQL-2-5-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   7.479 BV    0.1849 4769.45459  400.68921  50.0452
   2   8.218 VB    0.1978 4760.84424  375.85959  49.9548

Totals :                  9530.29883  776.54880



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.479 BV    0.1847 5432.73389  456.98373  50.0353
   2   8.218 VB    0.1976 5425.07910  428.92029  49.9647

Totals :                  1.08578e4   885.90402



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.479 BB    0.1849 1633.47925  137.17763  50.2564
   2   8.218 BB    0.1973 1616.80884  128.06210  49.7436

Totals :                  3250.28809  265.23973



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.479 BB    0.1845 1996.62109  168.17789  50.0971
   2   8.218 BB    0.1972 1988.87903  157.65567  49.9029

Totals :                  3985.50012  325.83356
```

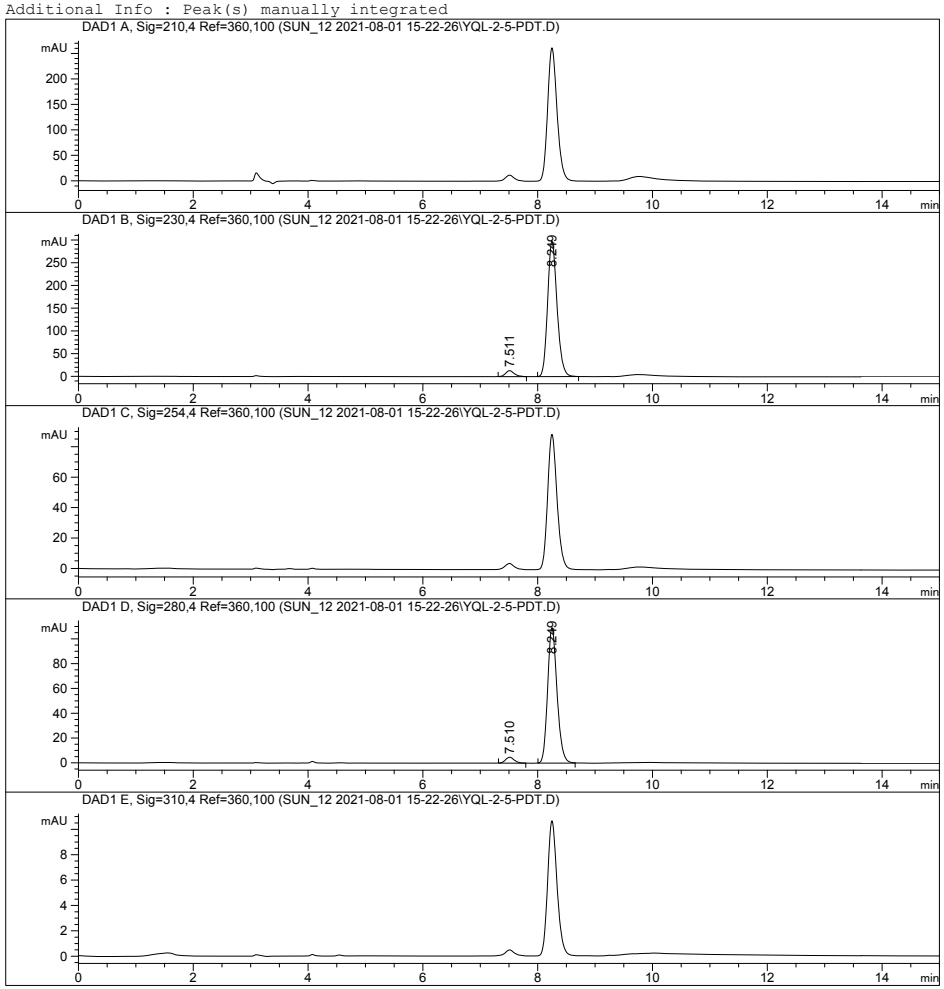


3h
(racemic)

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

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

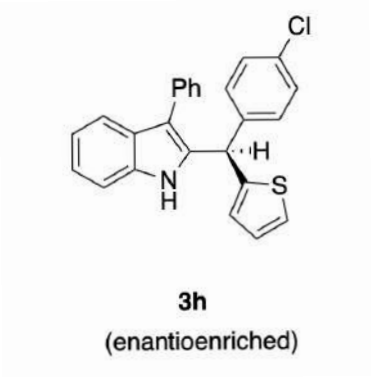
Data File C:\CHEM32\1\DATA\SUN_12 2021-08-01 15-22-26\YQL-2-5-PDT.D
Sample Name:

```
==========================================================================
Acq. Operator   :                              Seq. Line :   2
Acq. Instrument : Instrument 1                  Location : Vial 61
Injection Date  : 8/1/2021 3:34:41 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\SUN_12 2021-08-01 15-22-26\AD-05-15.M
Last changed    : 8/1/2021 3:33:50 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:53:10 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-08-01 15-22-26\YQL-2-5-PDT.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


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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.511 BB    0.1603  137.50772   13.11988   3.8821
   2   8.249 BB    0.1751 3404.54810  298.36481  96.1179

Totals :                   3542.05582  311.48468


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


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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.510 BB    0.1613   50.85761    4.81265   3.9190
   2   8.249 BB    0.1749 1246.85681  109.47958  96.0810

Totals :                   1297.71442  114.29224


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

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

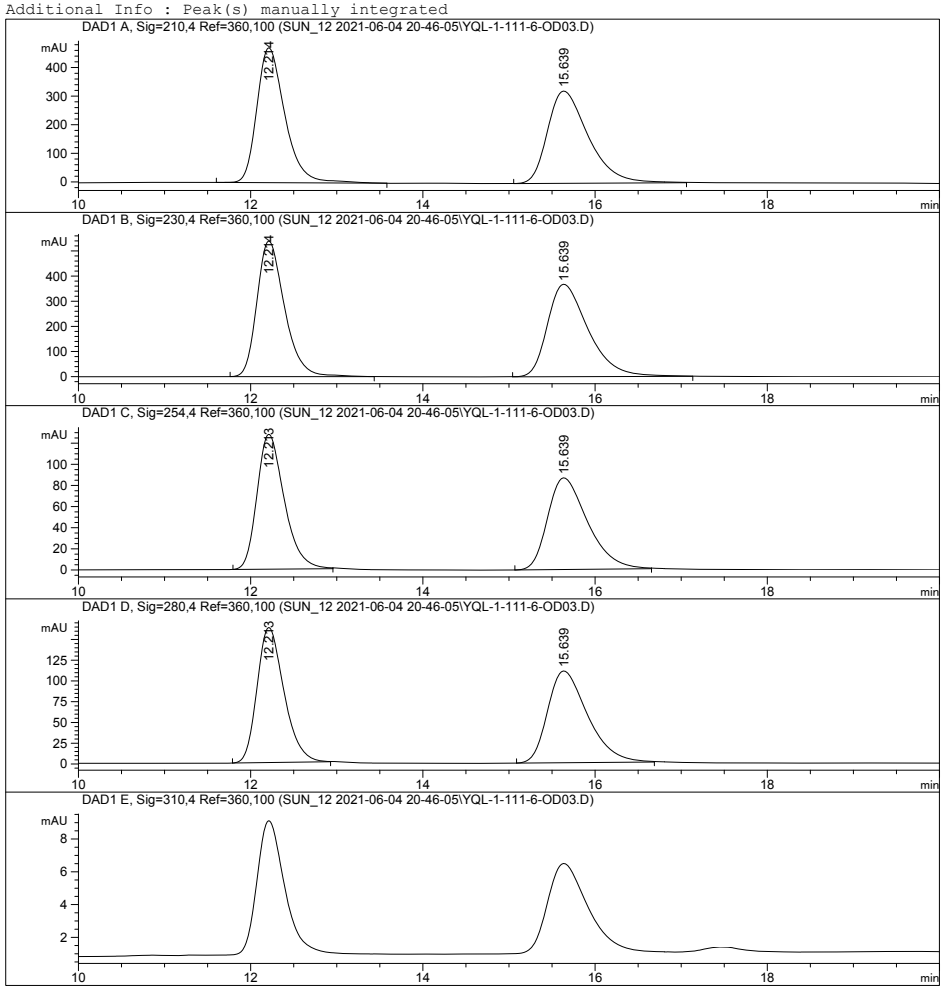


3h

(enantioenriched)

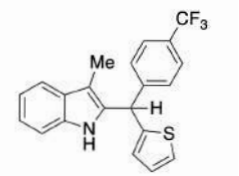
Data File C:\CHEM32\1\DATA\SUN_12 2021-06-04 20-46-05\YQL-1-111-6-OD03.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   5
Acq. Instrument : Instrument 1              Location : Vial 56
Injection Date  : 6/4/2021 9:51:53 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\SUN_12 2021-06-04 20-46-05\OD-03-30.M
Last changed    : 6/4/2021 9:51:03 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 3:58:15 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-06-04 20-46-05\YQL-1-111-6-OD03.D
Sample Name:

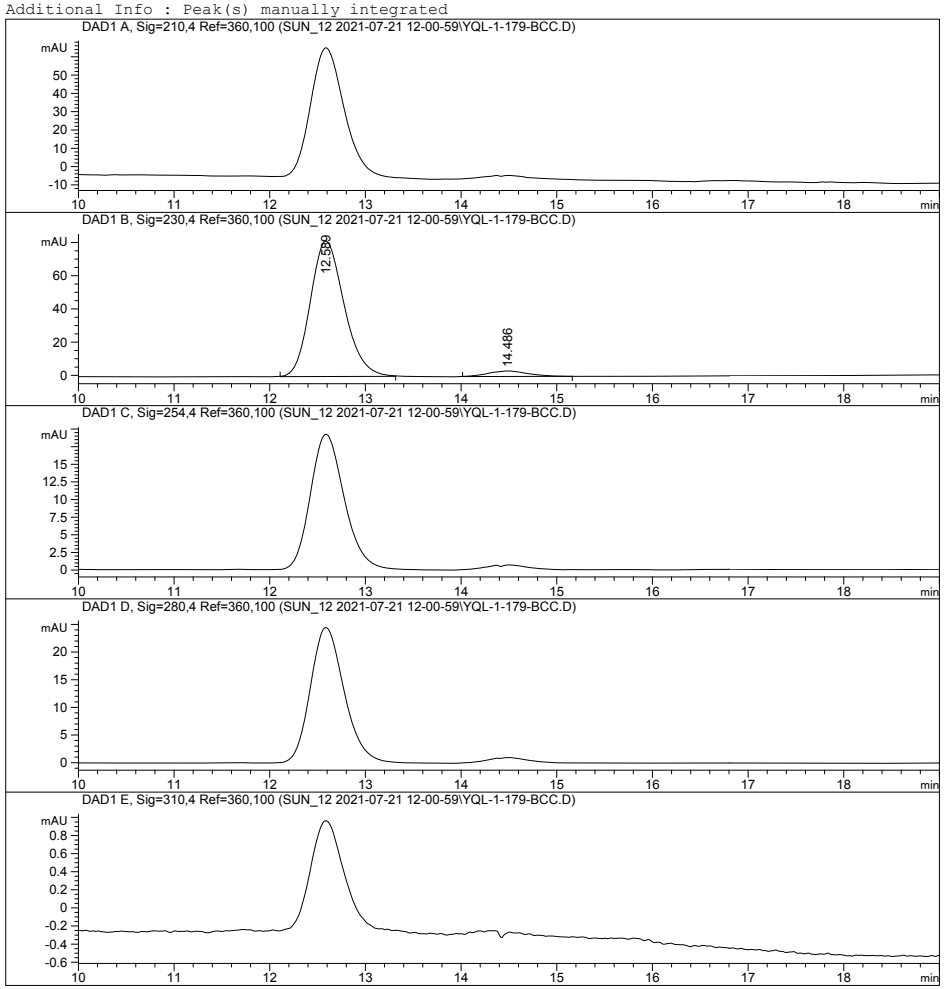
```
==================================================================
                        Area Percent Report
==================================================================

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  12.214 BB    0.3462 1.06843e4   471.83389  50.1255
   2  15.639 BB    0.5004 1.06308e4   322.63391  49.8745

Totals :                  2.13151e4   794.46780



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.214 BB    0.3419 1.20139e4   539.29846  49.8834
   2  15.639 BB    0.5012 1.20701e4   367.46014  50.1166

Totals :                  2.40840e4   906.75861



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.213 BB    0.3356 2797.30591  127.66143  50.0365
   2  15.639 BB    0.4937 2793.22607   86.72826  49.9635

Totals :                  5590.53198  214.38969



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.213 BB    0.3331 3530.92358  162.74519  49.7441
   2  15.639 BB    0.4943 3567.25269  110.59557  50.2559

Totals :                  7098.17627  273.34076



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

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



3l
(racemic)

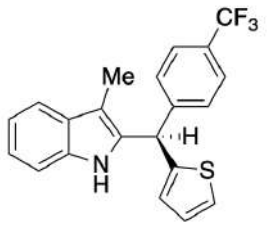
Data File C:\CHEM32\1\DATA\SUN_12 2021-07-21 12-00-59\YQL-1-179-BCC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location : Vial 51
Injection Date  : 7/21/2021 12:14:36 PM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 8.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-07-21 12-00-59\OD-03-20.M
Last changed    : 7/21/2021 12:13:44 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:45:44 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-21 12-00-59\YQL-1-179-BCC.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


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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.589 BB    0.3779 1999.08301   81.56667  95.5344
   2  14.486 BB    0.3752   93.44401    3.31168   4.4656

Totals :                  2092.52702   84.87834


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 ***
```

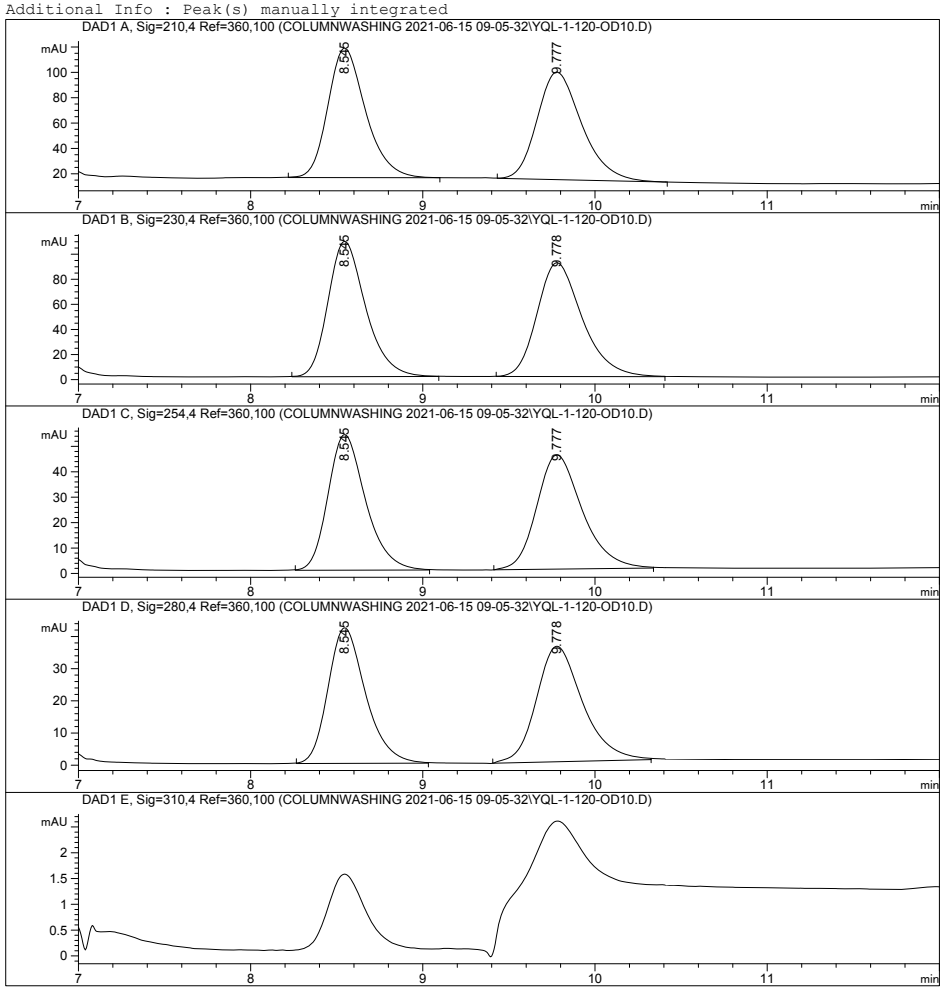


3i

(enantioenriched)

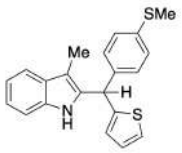
Data File C:\CHEM32\1\DATA\COLUMNWASHING 2021-06-15 09-05-32\YQL-1-120-OD10.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   7
Acq. Instrument : Instrument 1              Location : Vial 52
Injection Date  : 6/15/2021 11:02:26 AM          Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\COLUMNWASHING 2021-06-15 09-05-32\OD-10-30.M
Last changed    : 6/15/2021 11:01:35 AM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 3:55:03 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\COLUMNWASHING 2021-06-15 09-05-32\YQL-1-120-OD10.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   8.545 BB    0.2316 1554.74780  102.16038  50.3645
   2   9.777 BB    0.2748 1532.24512   84.78561  49.6355

Totals :                  3086.99292  186.94599



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.545 BB    0.2314 1641.40845  107.91986  49.7606
   2   9.778 BB    0.2770 1657.20349   90.76108  50.2394

Totals :                  3298.61194  198.68094



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.545 BB    0.2310  809.22986   53.33179  49.4336
   2   9.777 BB    0.2790  827.77338   44.91850  50.5664

Totals :                  1637.00323   98.25029



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.545 BB    0.2310  638.96191   42.11697  48.7686
   2   9.778 BB    0.2822  671.22949   35.89653  51.2314

Totals :                  1310.19141   78.01350
```

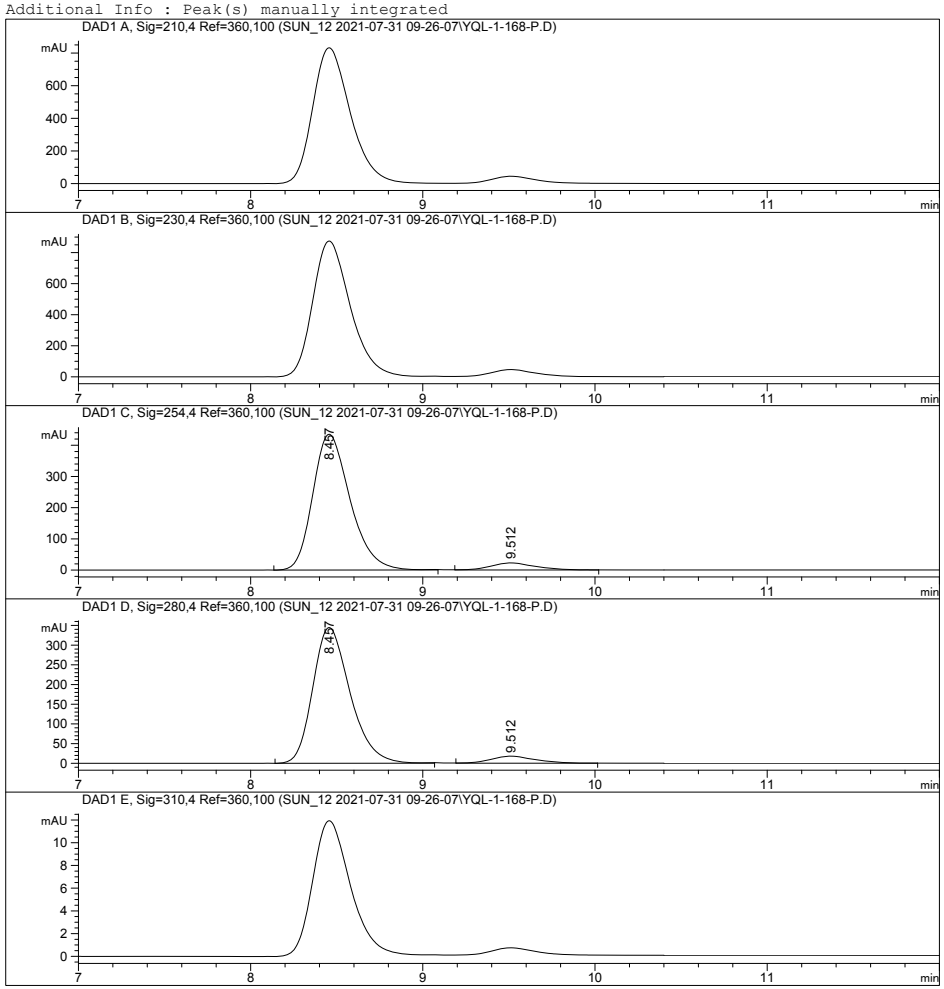


3j
(racemic)

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

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

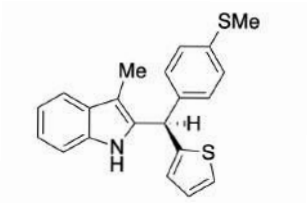
Data File C:\CHEM32\1\DATA\SUN_12 2021-07-31 09-26-07\YQL-1-168-P.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  34
Acq. Instrument : Instrument 1              Location : Vial 51
Injection Date  : 7/31/2021 8:57:38 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\SUN_12 2021-07-31 09-26-07\OD-10-15.M
Last changed    : 7/31/2021 8:40:42 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:40:50 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-31 09-26-07\YQL-1-168-P.D
Sample Name:

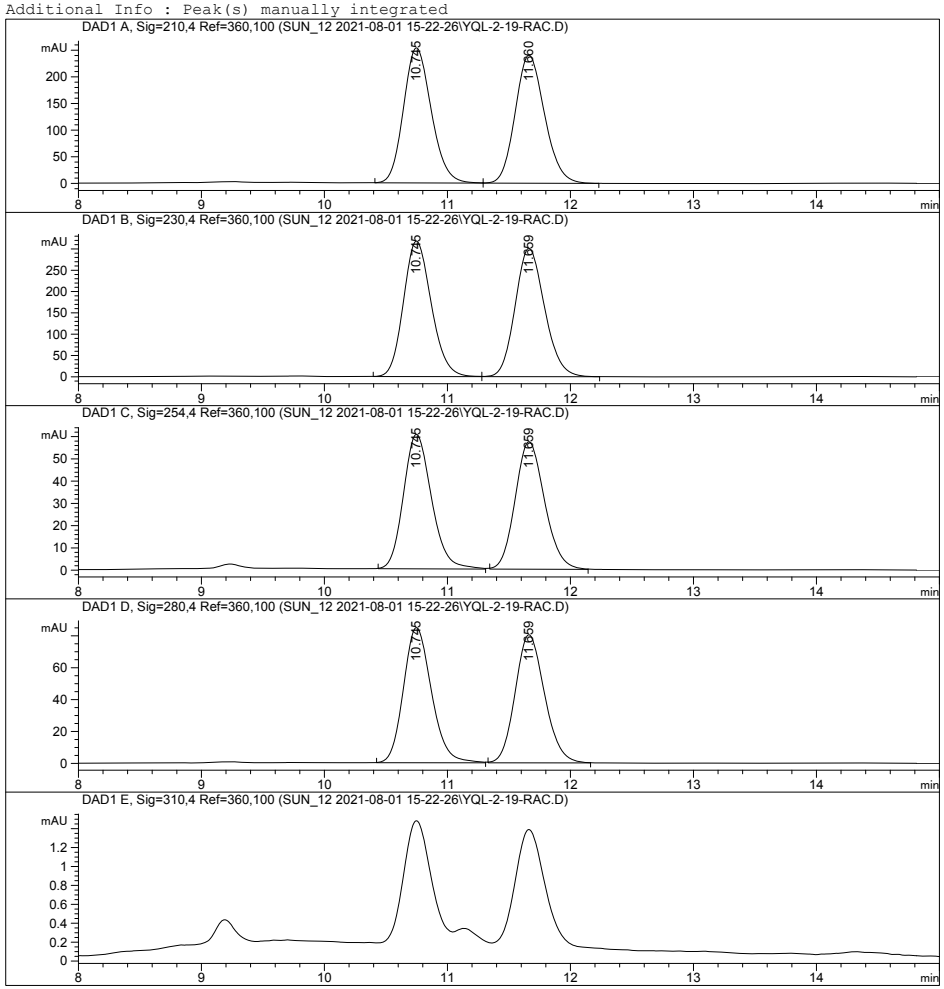
```
==================================================================
                        Area Percent Report
==================================================================

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


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


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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.457 BB    0.2317 6552.91553  435.21640  94.1902
   2   9.512 BB    0.2732  404.19287   22.53686   5.8098

Totals :                  6957.10840  457.75326


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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.457 BB    0.2316 5189.23193  344.71332  94.1993
   2   9.512 BB    0.2732  319.54523   17.82043   5.8007

Totals :                  5508.77716  362.53374


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

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



3j
(enantioenriched)

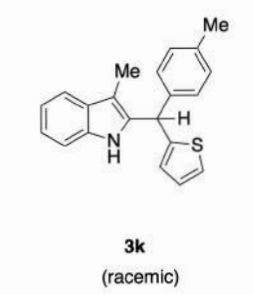
Data File C:\CHEM32\1\DATA\SUN_12 2021-08-01 15-22-26\YQL-2-19-RAC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  21
Acq. Instrument : Instrument 1              Location : Vial 52
Injection Date  : 8/1/2021 9:12:29 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 8.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-08-01 15-22-26\AD-02-30.M
Last changed    : 8/1/2021 8:40:34 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 4:05:22 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-08-01 15-22-26\YQL-2-19-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  10.745 BV    0.2429 3975.63159  253.58324  49.9317
   2  11.660 VB    0.2575 3986.50488  240.33554  50.0683

Totals :                  7962.13647  493.91878



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.745 BV    0.2431 4988.18896  317.92114  49.9227
   2  11.659 VB    0.2578 5003.62646  301.20465  50.0773

Totals :                  9991.81543  619.12579



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.745 BB    0.2447  957.09467   60.44659  50.2162
   2  11.659 BB    0.2573  948.85181   57.26980  49.7838

Totals :                  1905.94647  117.71639



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.745 BB    0.2445 1341.49451   84.82977  50.1741
   2  11.659 BB    0.2574 1332.18311   80.34924  49.8259

Totals :                  2673.67761  165.17901
```

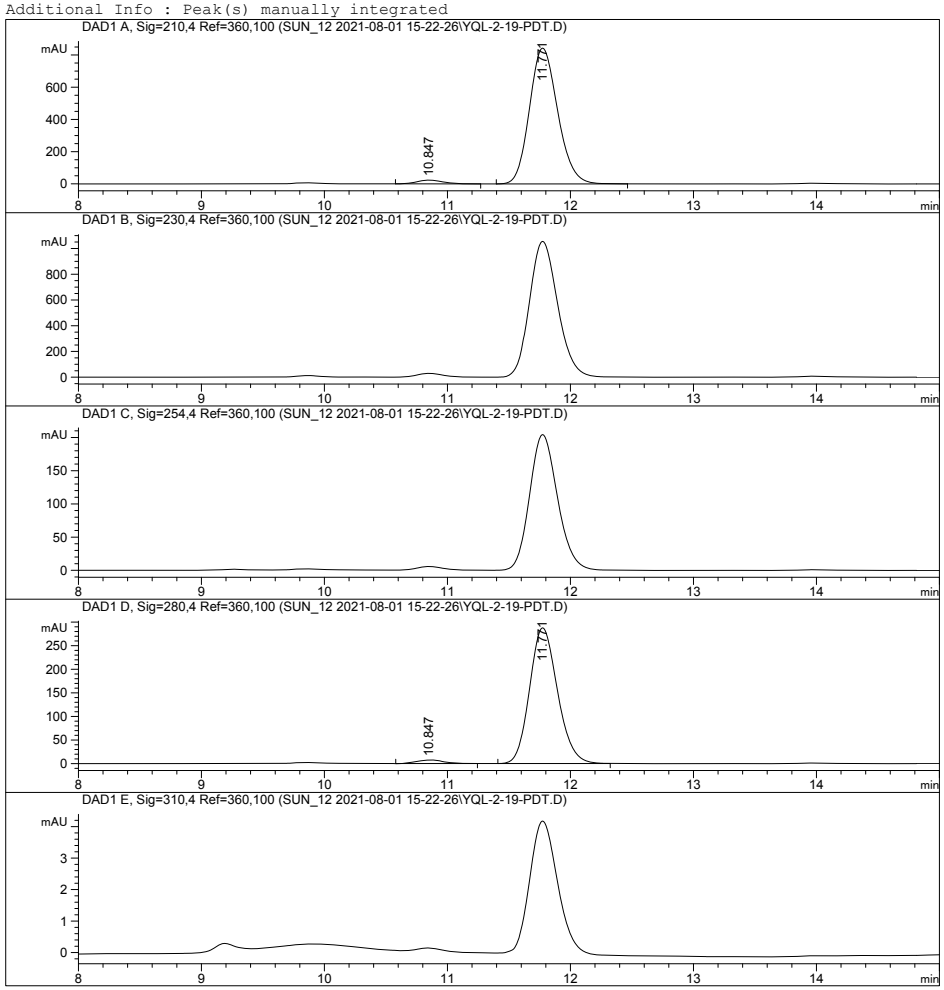


3k
(racemic)

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

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

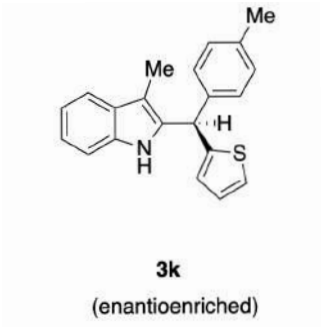
Data File C:\CHEM32\1\DATA\SUN_12 2021-08-01 15-22-26\YQL-2-19-PDT.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  20
Acq. Instrument : Instrument 1              Location : Vial 51
Injection Date  : 8/1/2021 8:41:26 PM            Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-08-01 15-22-26\AD-02-30.M
Last changed    : 8/1/2021 8:40:34 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:57:54 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-08-01 15-22-26\YQL-2-19-PDT.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  10.847 BB    0.2260  339.89786   23.33245   2.4679
   2  11.771 BB    0.2479 1.34329e4   842.92230  97.5321

Totals :                  1.37728e4   866.25475



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.847 BB    0.2226  111.17725    7.69383   2.3950
   2  11.771 BB    0.2438 4530.93994  287.64584  97.6050

Totals :                  4642.11719  295.33967



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

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

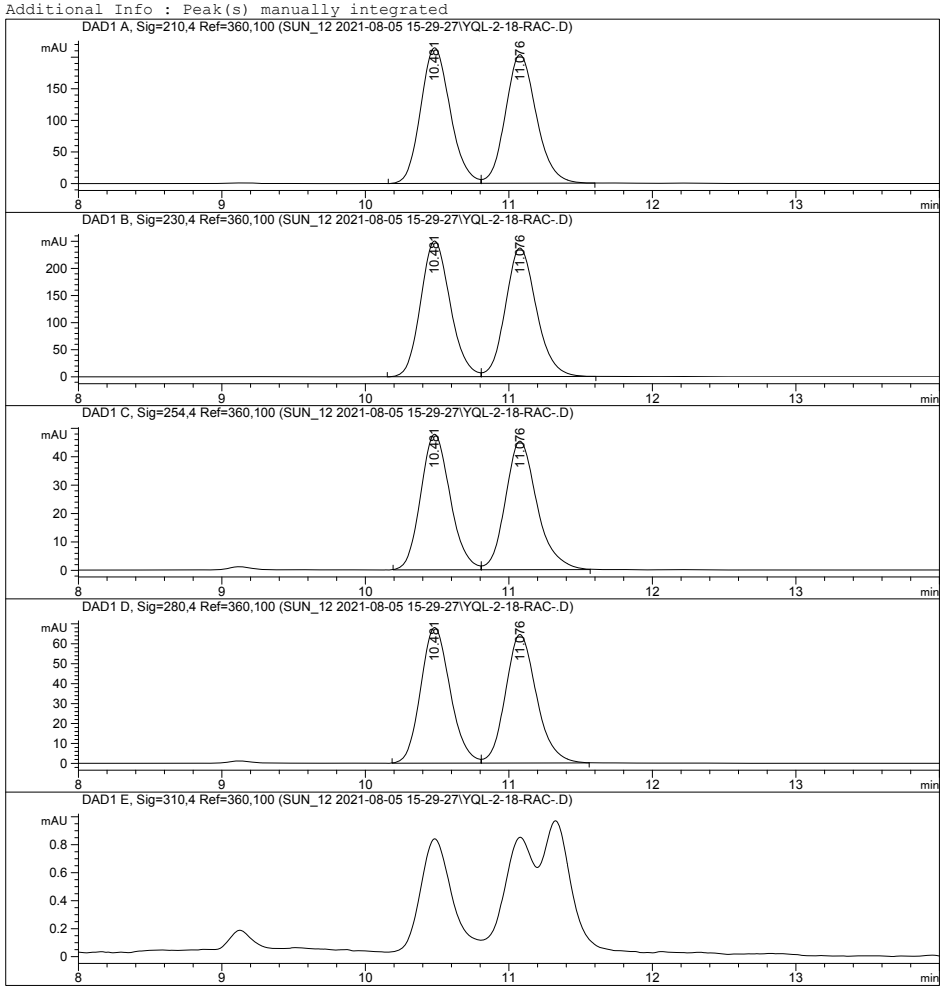


3k

(enantioenriched)

Data File C:\CHEM32\1\DATA\SUN_12 2021-08-05 15-29-27\YQL-2-18-RAC-.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   9
Acq. Instrument : Instrument 1              Location : Vial 62
Injection Date  : 8/5/2021 7:00:28 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\SUN_12 2021-08-05 15-29-27\AD-01-30.M
Last changed    : 8/5/2021 6:28:33 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AS-20-60-0.5.M
Last changed    : 8/5/2021 8:27:16 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-08-05 15-29-27\YQL-2-18-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 [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.481	BV	0.2203	3058.82690	214.55069	50.2156
2	11.076	VB	0.2299	3032.55640	203.45877	49.7844
Totals :				6091.38330	418.00946	

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

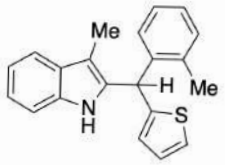
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.481	BV	0.2204	3569.91211	250.25285	50.2169
2	11.076	VB	0.2301	3539.07373	237.21893	49.7831
Totals :				7108.98584	487.47179	

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.481	BV	0.2202	679.87537	47.71381	49.5947
2	11.076	VB	0.2341	690.98895	45.25302	50.4053
Totals :				1370.86432	92.96682	

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

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.481	BV	0.2201	968.39294	68.03474	50.0410
2	11.076	VB	0.2309	966.80481	64.48117	49.9590
Totals :				1935.19775	132.51591	



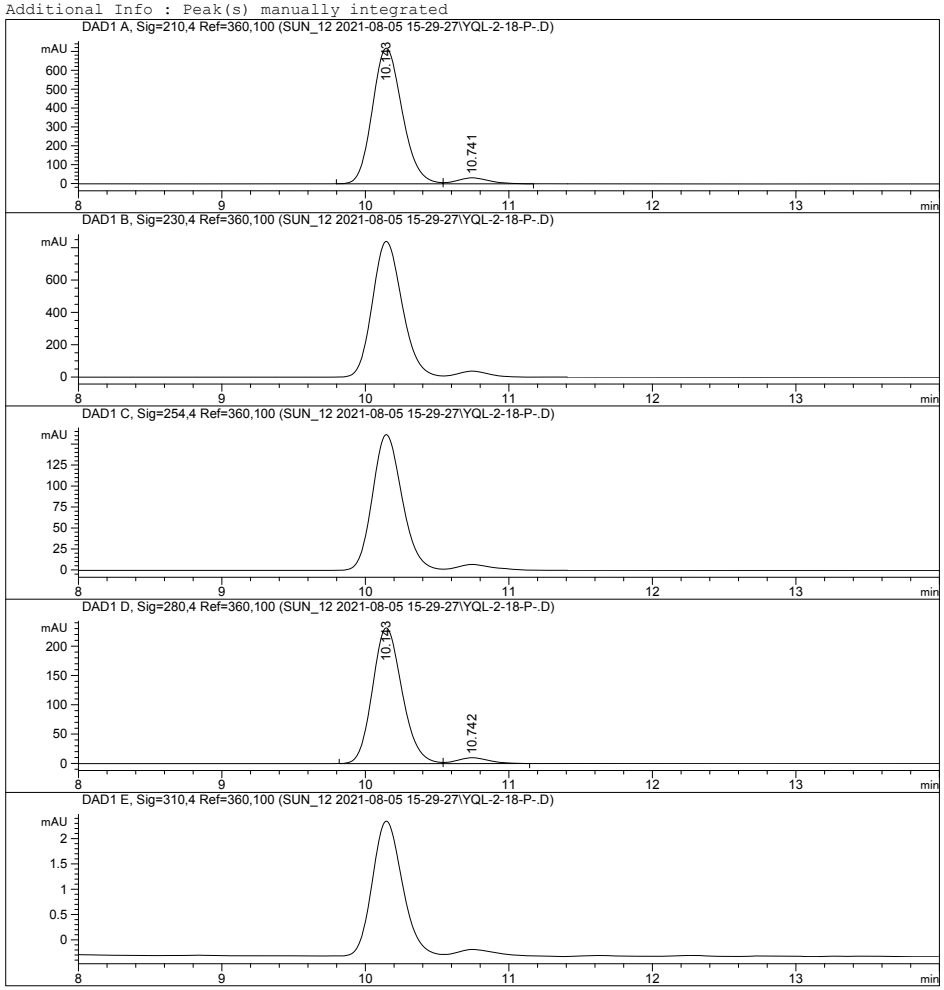
3l
(racemic)

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

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

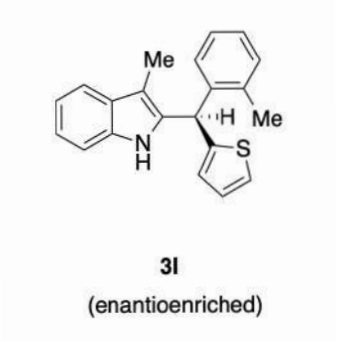
Data File C:\CHEM32\1\DATA\SUN_12 2021-08-05 15-29-27\YQL-2-18-P-.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   8
Acq. Instrument : Instrument 1              Location : Vial 61
Injection Date  : 8/5/2021 6:29:25 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-08-05 15-29-27\AD-01-30.M
Last changed    : 8/5/2021 6:28:33 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:55:09 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-08-05 15-29-27\YQL-2-18-P-.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  10.143 BV    0.2241 1.03618e4   719.05554  95.5579
   2  10.741 VB    0.2314  481.67227   31.67855   4.4421

Totals :                  1.08434e4   750.73409



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.143 BV    0.2209 3315.61475  231.72086  95.5891
   2  10.742 VB    0.2339  152.99873   10.03352   4.4109

Totals :                  3468.61348  241.75438



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

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

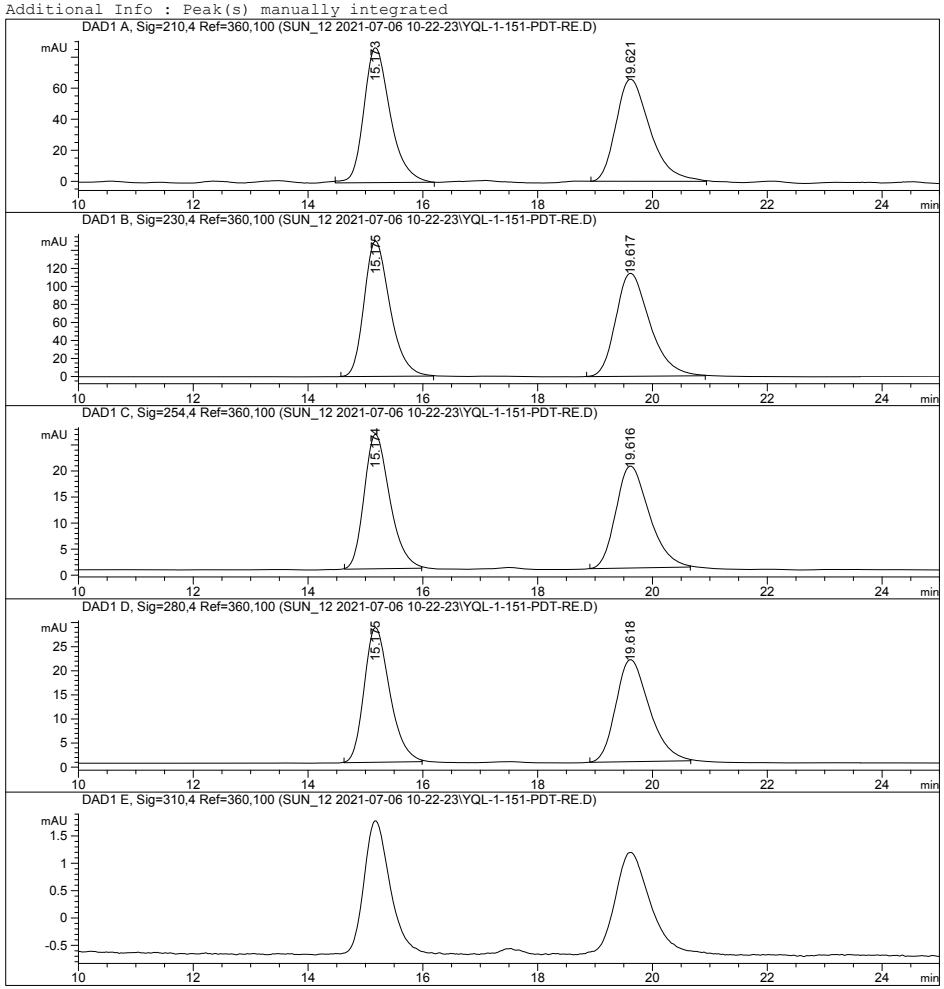


3l

(enantioenriched)

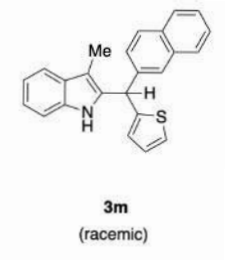
Data File C:\CHEM32\1\DATA\SUN_12 2021-07-06 10-22-23\YQL-1-151-PDT-RE.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  29
Acq. Instrument : Instrument 1              Location : Vial 61
Injection Date  : 7/6/2021 8:02:38 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 8.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-07-06 10-22-23\OD-03-30.M
Last changed    : 7/6/2021 8:01:46 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 3:48:08 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-06 10-22-23\YQL-1-151-PDT-RE.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  15.173 BB    0.4862 2771.65674   86.88142  50.5265
   2  19.621 BB    0.5942 2713.89063   65.93614  49.4735

Totals :                  5485.54736  152.81757



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.175 BB    0.4785 4695.36816  150.27930  49.8358
   2  19.617 BB    0.6293 4726.31592  114.55789  50.1642

Totals :                  9421.68408  264.83719



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.174 BB    0.4744  797.37183   25.81054  50.2317
   2  19.616 BB    0.6166  790.01532   19.58684  49.7683

Totals :                  1587.38715   45.39738



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.175 BB    0.4766  864.51868   27.96685  50.1680
   2  19.618 BB    0.6105  858.72845   21.20452  49.8320

Totals :                  1723.24713   49.17137
```



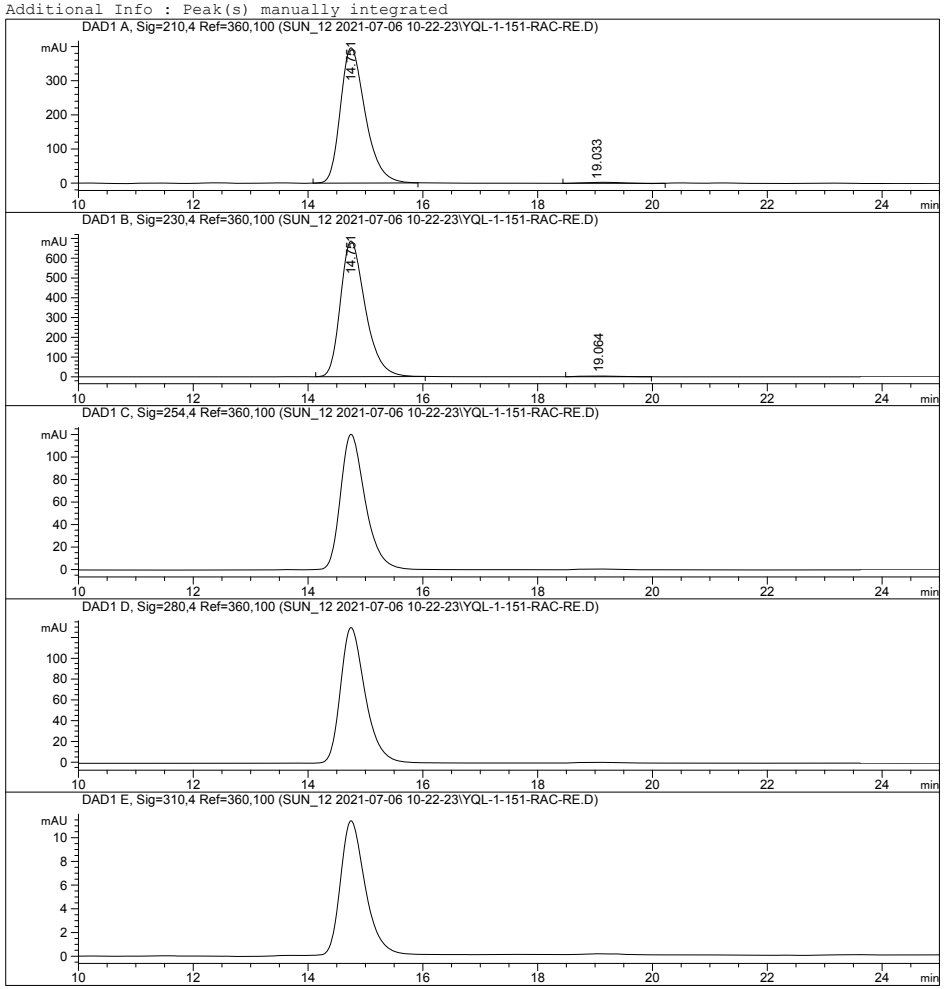
3m
(racemic)

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

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

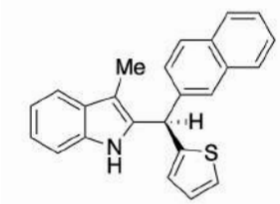
Data File C:\CHEM32\1\DATA\SUN_12 2021-07-06 10-22-23\YQL-1-151-RAC-RE.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  30
Acq. Instrument : Instrument 1              Location : Vial 62
Injection Date  : 7/6/2021 8:34:09 PM           Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 8.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-07-06 10-22-23\OD-03-30.M
Last changed    : 7/6/2021 8:01:46 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:34:02 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-06 10-22-23\YQL-1-151-RAC-RE.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  14.751 BB    0.4566 1.19124e4   396.36139  99.0691
   2  19.033 BB    0.4546  111.93133    2.92384   0.9309

Totals :                  1.20244e4   399.28523



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.751 BB    0.4581 2.05951e4   686.31970  99.1742
   2  19.064 BB    0.5181  171.49834    4.29237   0.8258

Totals :                  2.07666e4   690.61207



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 ***
```

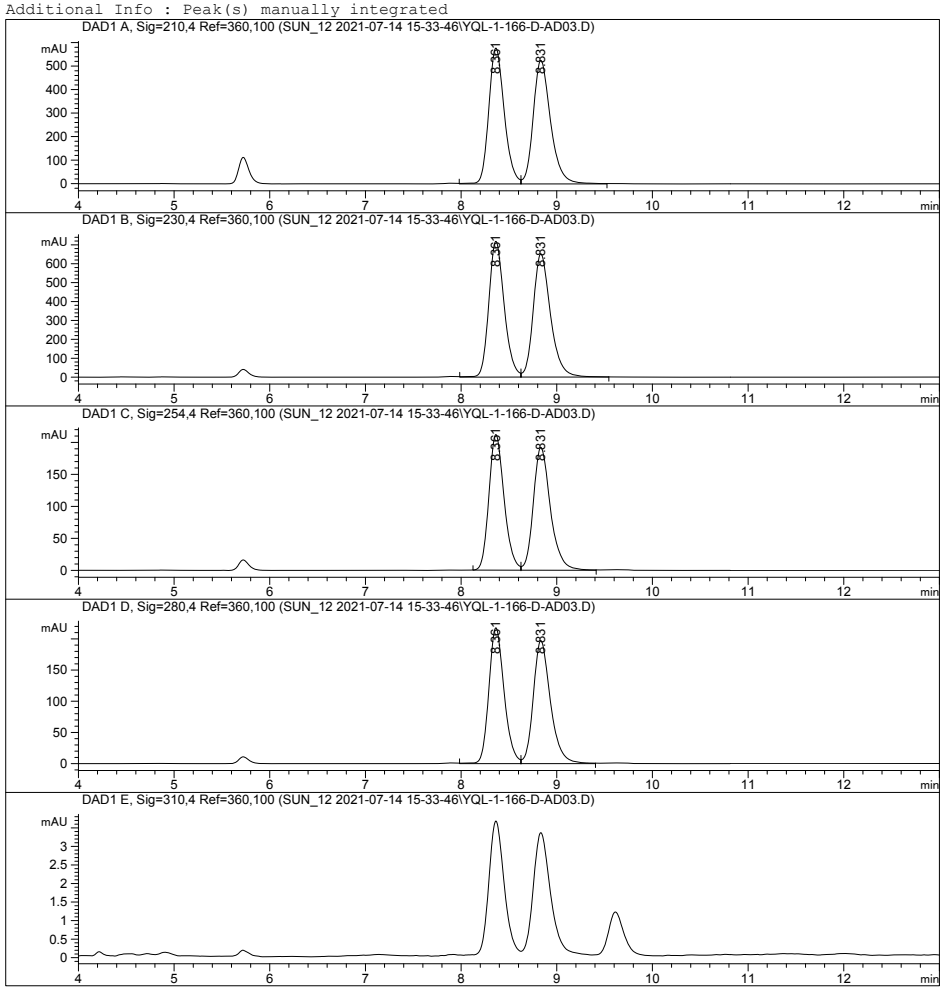


3m

(enantioenriched)

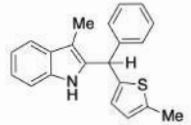
Data File C:\CHEM32\1\DATA\SUN_12 2021-07-14 15-33-46\YQL-1-166-D-AD03.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   4
Acq. Instrument : Instrument 1              Location : Vial 53
Injection Date  : 7/14/2021 4:49:12 PM          Inj :   1
                                          Inj Volume : 1.000 µl
Different Inj Volume from Sequence !   Actual Inj Volume : 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-07-14 15-33-46\AD-03-25-1.0.M
Last changed    : 9/5/2019 8:00:44 PM
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 3:56:51 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-14 15-33-46\YQL-1-166-D-AD03.D
Sample Name:

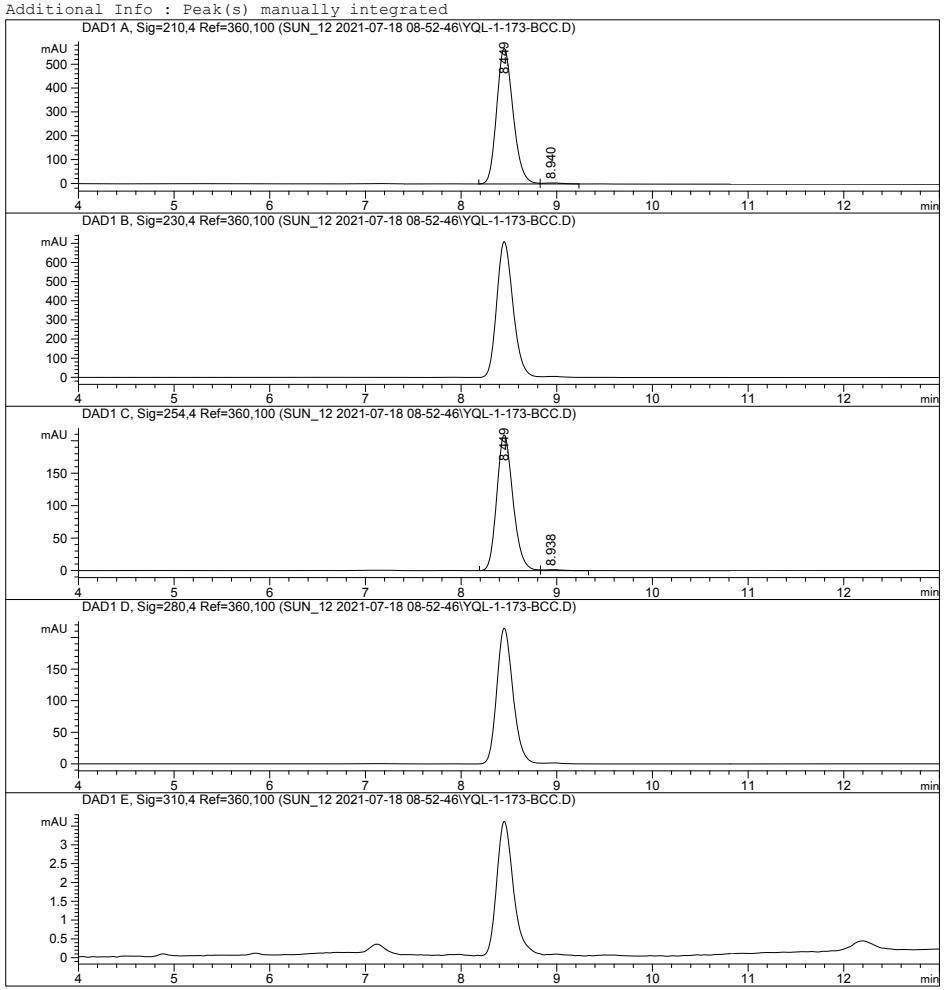
```
==================================================================
                        Area Percent Report
==================================================================

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   8.361 VV    0.1731 6496.25879  578.26459  49.4503
   2   8.831 VB    0.1934 6640.67822  525.74817  50.5497

Totals :                  1.31369e4  1104.01276



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.361 VV    0.1722 8022.81543  718.81738  49.5349
   2   8.831 VB    0.1902 8173.48926  652.34888  50.4651

Totals :                  1.61963e4  1371.16626



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.361 BV    0.1685 2335.00879  212.03368  49.4463
   2   8.831 VB    0.1890 2387.29956  192.02716  50.5537

Totals :                  4722.30835  404.06084



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.361 VV    0.1693 2415.45068  217.87877  49.5721
   2   8.831 VB    0.1894 2457.15381  197.21736  50.4279

Totals :                  4872.60449  415.09613



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

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



3n
(racemic)

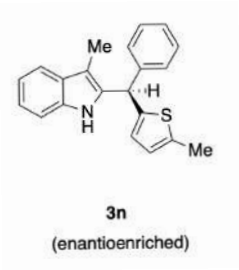
Data File C:\CHEM32\1\DATA\SUN_12 2021-07-18 08-52-46\YQL-1-173-BCC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   6
Acq. Instrument : Instrument 1              Location : Vial 51
Injection Date  : 7/18/2021 10:41:51 AM          Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-07-18 08-52-46\AD-03-20.M
Last changed    : 7/2/2016 3:26:02 PM
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:43:14 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-07-18 08-52-46\YQL-1-173-BCC.D
Sample Name:

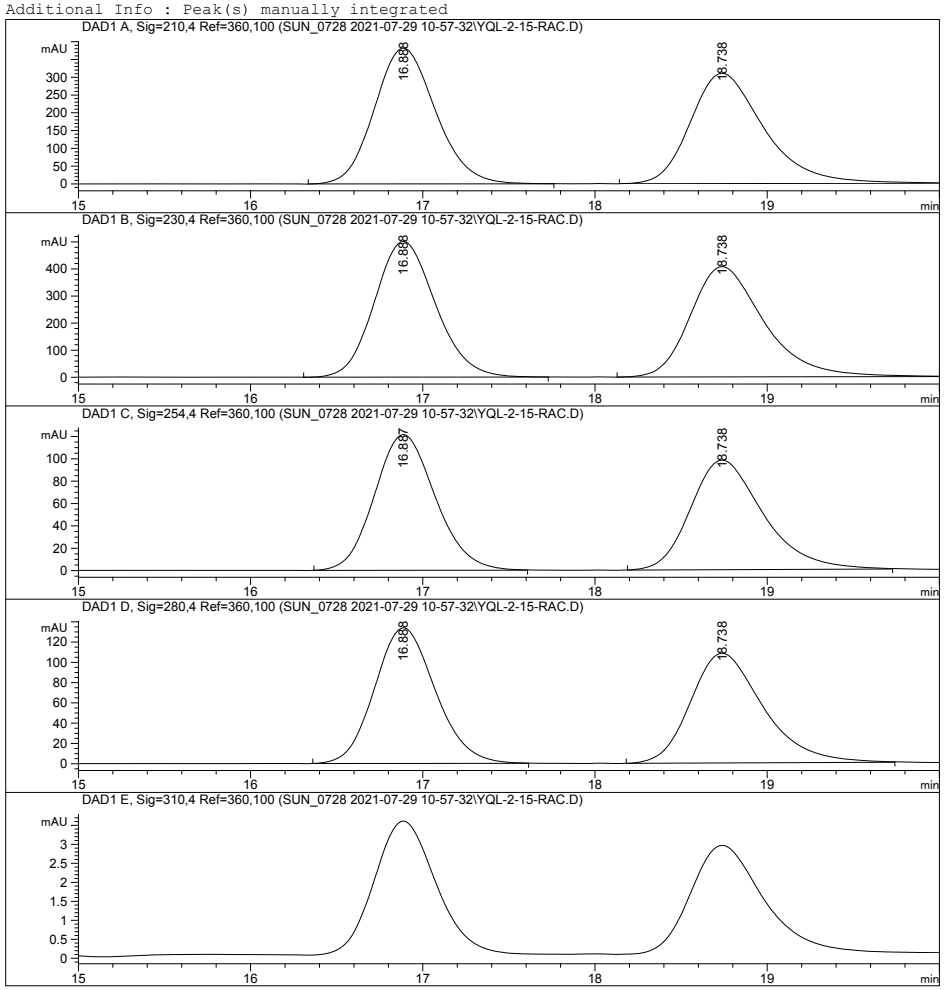
```
==================================================================
                        Area Percent Report
==================================================================

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   8.449 BV    0.1824 6746.79590  568.71948  99.1410
   2   8.940 VB    0.1847   58.45686    4.35330   0.8590

Totals :                  6805.25276  573.07278



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


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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.449 BV    0.1806 2453.16284  209.45598  99.1783
   2   8.938 VB    0.1958   20.32515    1.52165   0.8217

Totals :                  2473.48799  210.97762



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)

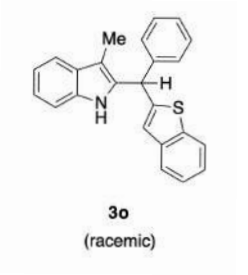
Data File C:\CHEM32\1\DATA\SUN_0728 2021-07-29 10-57-32\YQL-2-15-RAC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line : 110
Acq. Instrument : Instrument 1              Location : Vial 61
Injection Date  : 7/31/2021 12:54:11 AM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 10.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_0728 2021-07-29 10-57-32\AD-03-30.M
Last changed    : 1/30/2015 10:17:06 AM
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 4:07:18 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_0728 2021-07-29 10-57-32\YQL-2-15-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  16.888 BB    0.3818 9414.76855  381.70731  50.4797
   2  18.738 BB    0.4516 9235.84375  310.01077  49.5203

Totals :                  1.86506e4   691.71808



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.888 BB    0.3813 1.23456e4   501.41306  50.4719
   2  18.738 BB    0.4512 1.21148e4   407.12515  49.5281

Totals :                  2.44604e4   908.53821



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.887 BB    0.3807 2982.97070  121.39145  50.8971
   2  18.738 BB    0.4463 2877.81348   98.08718  49.1029

Totals :                  5860.78418  219.47863



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.888 BB    0.3804 3283.82007  133.78252  50.8602
   2  18.738 BB    0.4462 3172.73779  108.16469  49.1398

Totals :                  6456.55786  241.94720
```

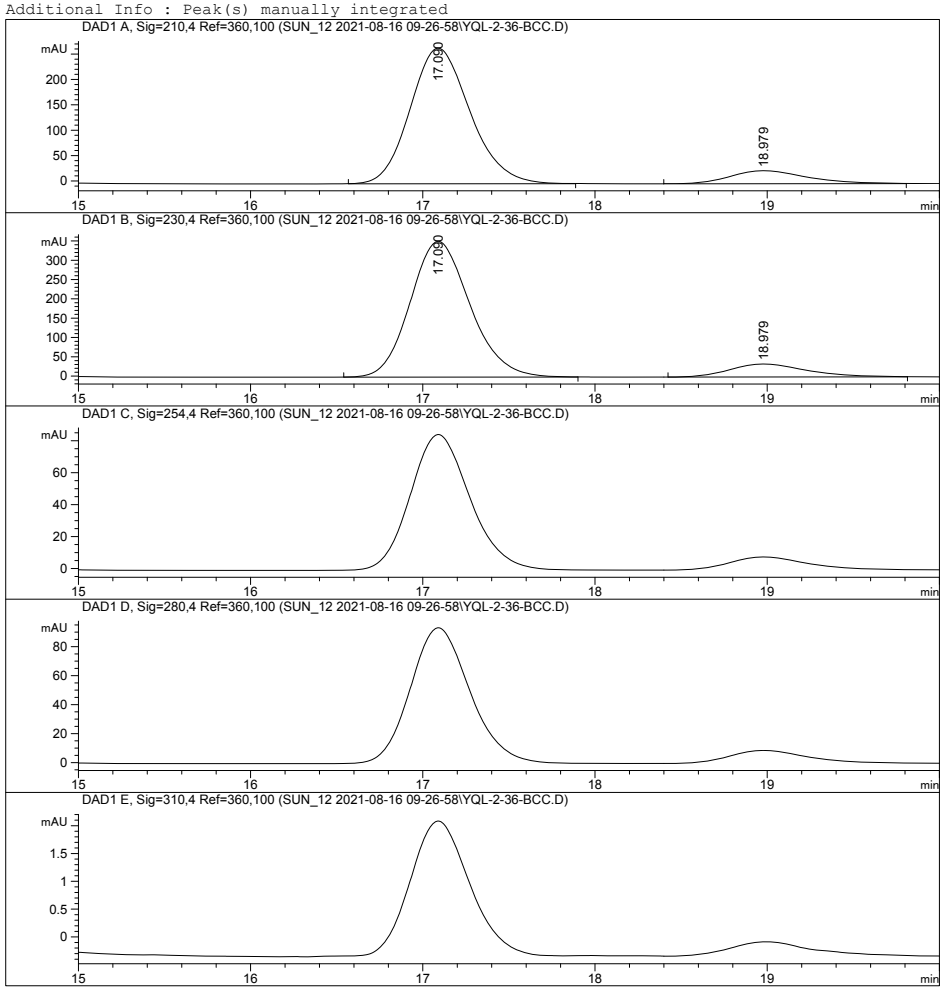


3o
(racemic)

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

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

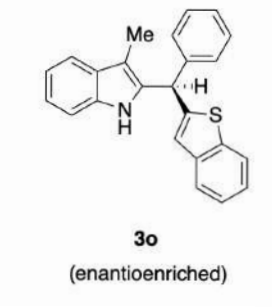
Data File C:\CHEM32\1\DATA\SUN_12 2021-08-16 09-26-58\YQL-2-36-BCC.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   8
Acq. Instrument : Instrument 1              Location : Vial 62
Injection Date  : 8/16/2021 11:00:09 AM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 7.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-08-16 09-26-58\AD-03-20.M
Last changed    : 7/2/2016 3:26:02 PM
Analysis Method : C:\CHEM32\1\METHODS\IC-07-60-0.5ML.M
Last changed    : 8/27/2021 10:59:27 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-08-16 09-26-58\YQL-2-36-BCC.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  17.090 BB    0.3717 6453.51807  267.27225  89.0859
   2  18.979 BB    0.4710  790.63757   25.69721  10.9141

Totals :                  7244.15564  292.96946



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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.090 BB    0.3716 8486.82813  351.58978  89.0295
   2  18.979 BB    0.4702 1045.77271   33.68077  10.9705

Totals :                  9532.60083  385.27055



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 ***
```

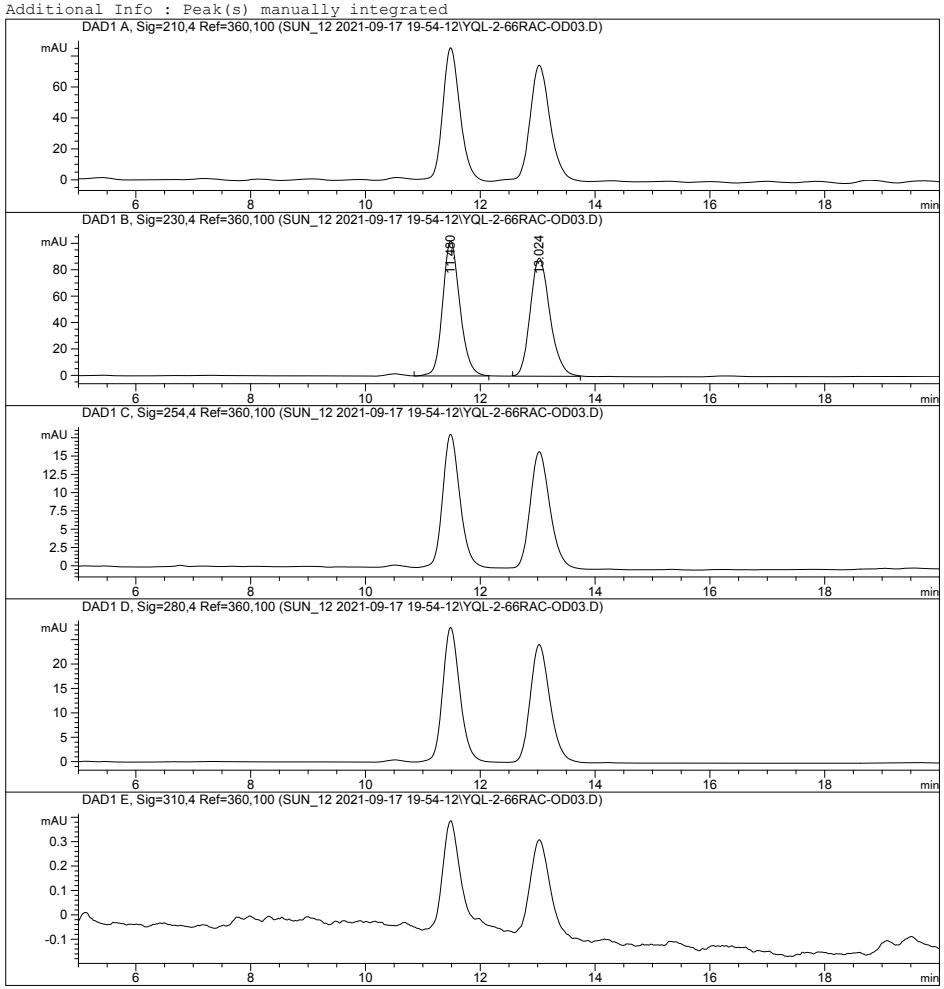


3o

(enantioenriched)

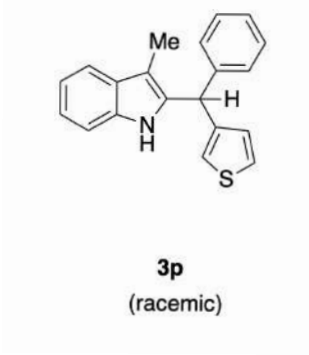
Data File C:\CHEM32\1\DATA\SUN_12 2021-09-17 19-54-12\YQL-2-66RAC-OD03.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  11
Acq. Instrument : Instrument 1              Location : Vial 51
Injection Date  : 9/17/2021 10:32:37 PM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 10.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-09-17 19-54-12\OD-03-30.M
Last changed    : 9/17/2021 10:31:43 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\IC-10-45.M
Last changed    : 9/18/2021 4:24:08 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-09-17 19-54-12\YQL-2-66RAC-OD03.D
Sample Name:

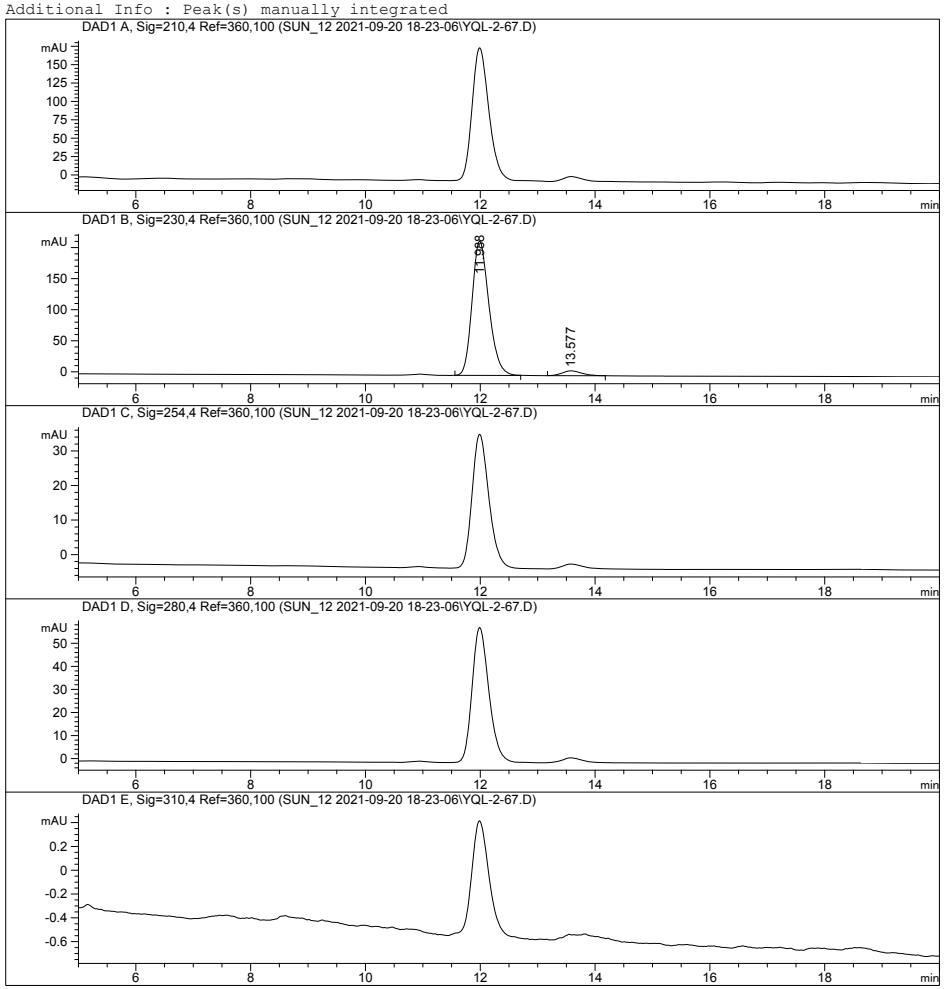
```
==================================================================
                        Area Percent Report
==================================================================

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


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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.480 VB    0.3190 2129.92676  102.27116  50.0385
   2  13.024 BB    0.3673 2126.64722   89.48769  49.9615

Totals :                  4256.57397  191.75885


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)

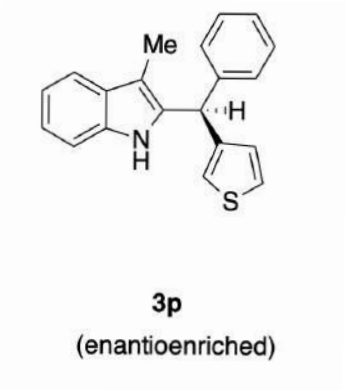
Data File C:\CHEM32\1\DATA\SUN_12 2021-09-20 18-23-06\YQL-2-67.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location : Vial 61
Injection Date  : 9/20/2021 6:36:17 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\SUN_12 2021-09-20 18-23-06\OD-03-20.M
Last changed    : 9/20/2021 6:35:25 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\DATA\SUN_12 2021-09-14 22-04-02\AD-20-30.M
Last changed    : 9/20/2021 7:03:35 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-09-20 18-23-06\YQL-2-67.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


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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.988 BB    0.3139 4412.83838  216.37926  96.0070
   2  13.577 BB    0.3498  183.53291    7.82150   3.9930

Totals :                  4596.37129  224.20075


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 ***
```

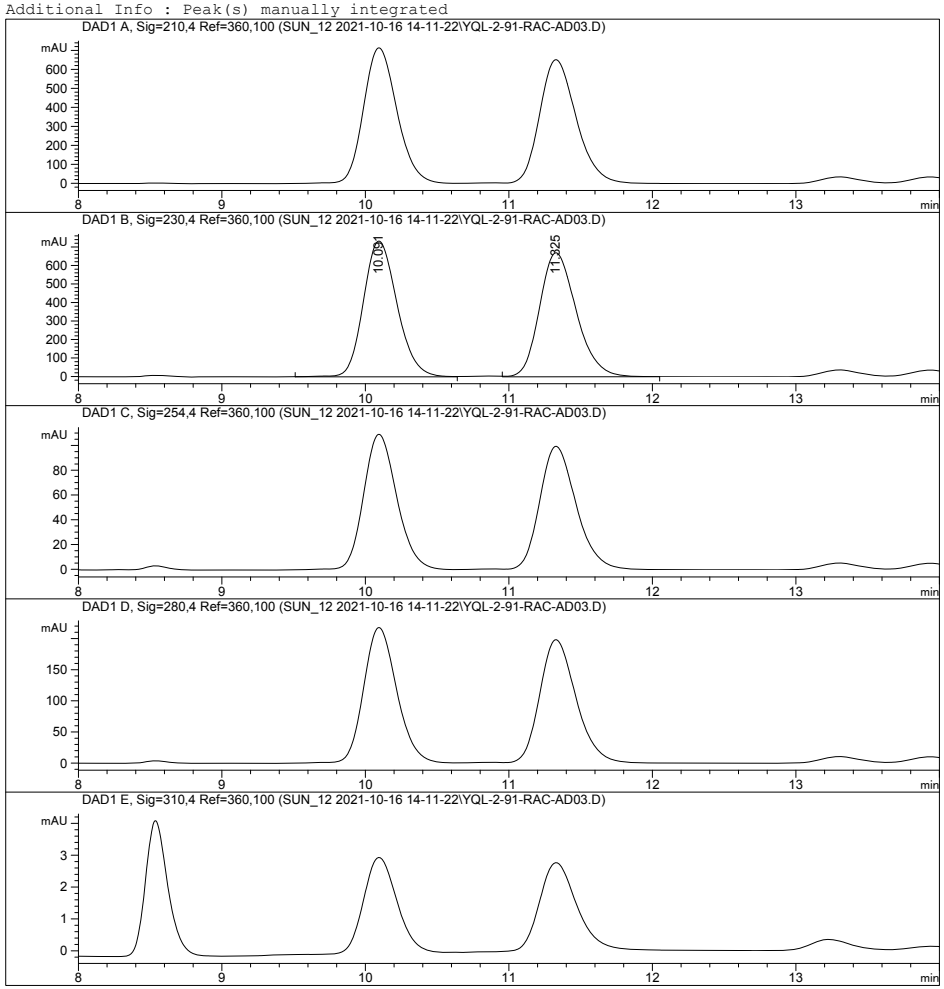


3p

(enantioenriched)

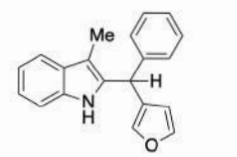
Data File C:\CHEM32\1\DATA\SUN_12 2021-10-16 14-11-22\YQL-2-91-RAC-AD03.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :  17
Acq. Instrument : Instrument 1              Location : Vial 51
Injection Date  : 10/16/2021 7:31:14 PM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 10.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-10-16 14-11-22\AD-03-30.M
Last changed    : 10/16/2021 7:30:20 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\AD-02-30-0.5.M
Last changed    : 10/17/2021 9:25:08 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-10-16 14-11-22\YQL-2-91-RAC-AD03.D
Sample Name:

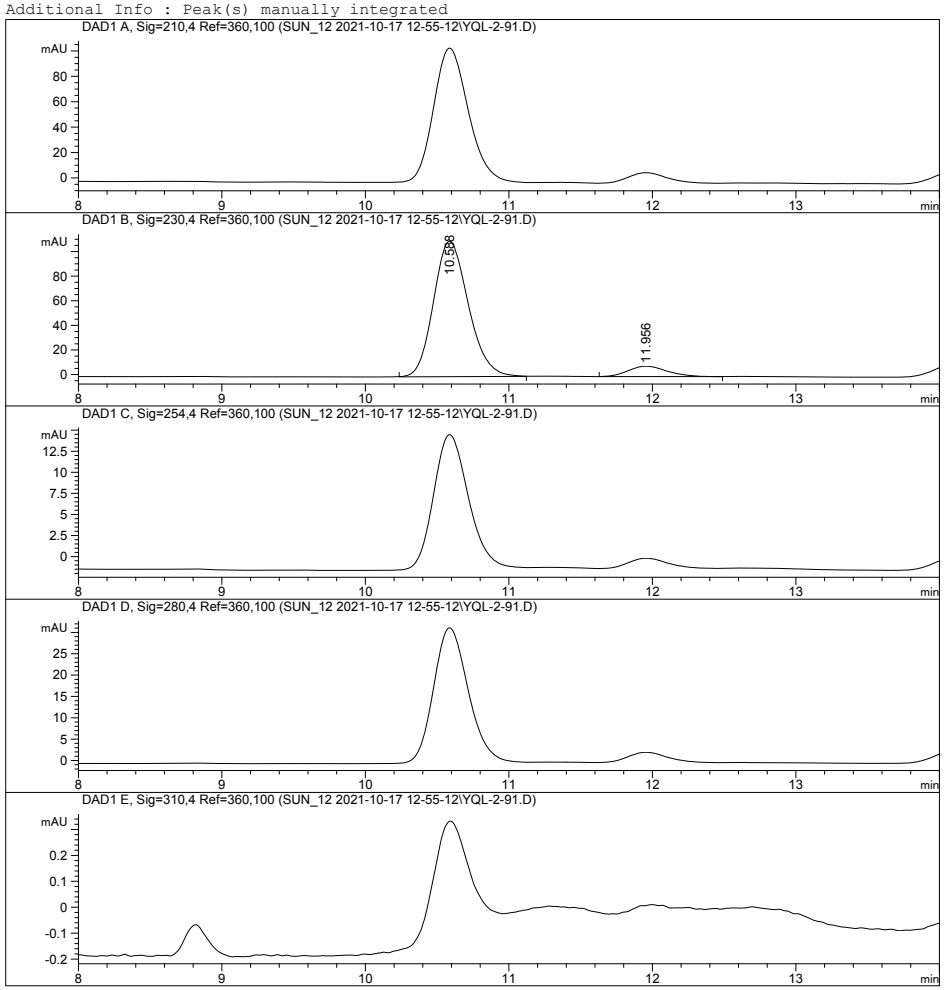
```
==================================================================
                        Area Percent Report
==================================================================

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


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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.091 BV    0.2539 1.19447e4   733.64148  50.0944
   2  11.325 VB    0.2752 1.18997e4   670.18823  49.9056

Totals :                  2.38444e4  1403.82971


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)

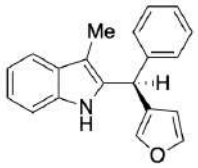
Data File C:\CHEM32\1\DATA\SUN_12 2021-10-17 12-55-12\YQL-2-91.D
Sample Name:

```
==================================================================
Acq. Operator   :                          Seq. Line :   2
Acq. Instrument : Instrument 1              Location : Vial 52
Injection Date  : 10/17/2021 1:08:01 PM          Inj :   1
                                          Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 10.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2021-10-17 12-55-12\AD-03-20.M
Last changed    : 7/2/2016 3:26:02 PM
Analysis Method : C:\CHEM32\1\METHODS\AD-02-30-0.5.M
Last changed    : 10/17/2021 9:25:08 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2021-10-17 12-55-12\YQL-2-91.D
Sample Name:

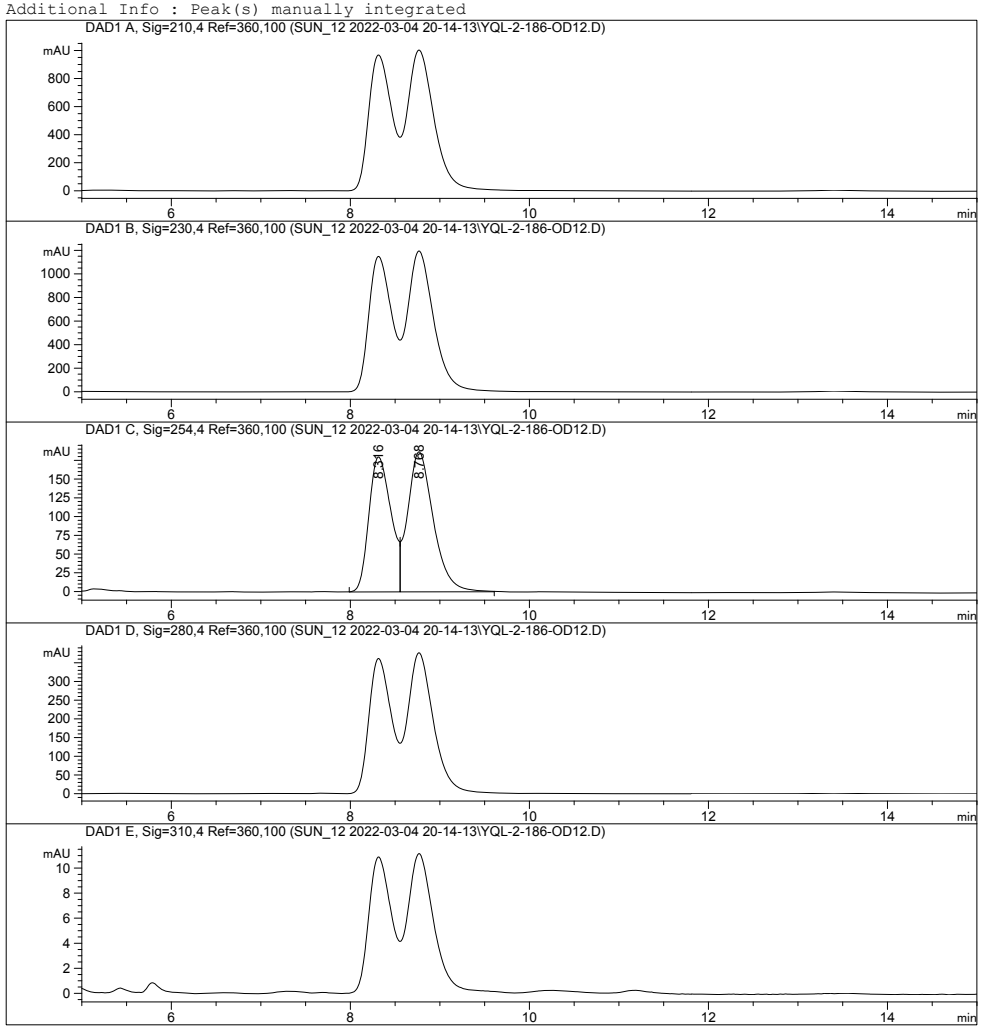
```
==================================================================
                        Area Percent Report
==================================================================

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


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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.588 BB    0.2623 1850.40784  109.97727  92.1284
   2  11.956 BB    0.2877  158.10217    8.47325   7.8716

Totals :                  2008.51001  118.45052


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)

Data File C:\CHEM32\1\DATA\SUN_12 2022-03-04 20-14-13\YQL-2-186-OD12.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :   2
Acq. Instrument : Instrument 1                    Location : Vial 51
Injection Date  : 3/4/2022 8:27:04 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 10.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2022-03-04 20-14-13\OD-12-25.M
Last changed    : 7/25/2016 11:18:52 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-03-60-0.6.M
Last changed    : 3/14/2022 9:24:14 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



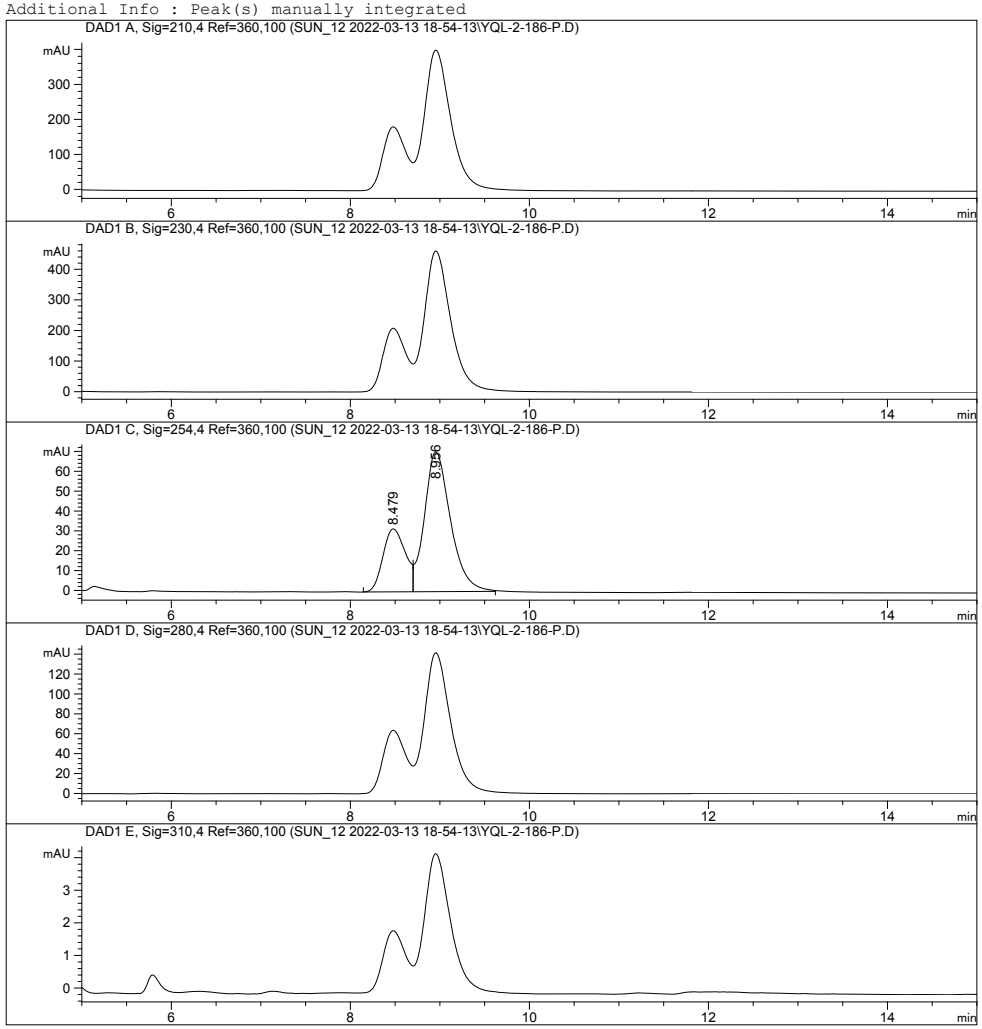
Data File C:\CHEM32\1\DATA\SUN_12 2022-03-04 20-14-13\YQL-2-186-OD12.D
Sample Name:

```
==========================================================================
                          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


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


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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.316 BV    0.2657 3081.24341  180.02193  45.2915
   2   8.768 VB    0.2984 3721.89697  186.80836  54.7085

Totals :                  6803.14038  366.83029


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

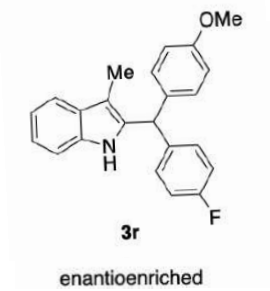
Data File C:\CHEM32\1\DATA\SUN_12 2022-03-13 18-54-13\YQL-2-186-P.D
Sample Name:

```
==========================================================================
Acq. Operator   :                                Seq. Line :  13
Acq. Instrument : Instrument 1                    Location : Vial 53
Injection Date  : 3/13/2022 9:56:59 PM                 Inj :  1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 10.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SUN_12 2022-03-13 18-54-13\OD-12-25.M
Last changed    : 7/25/2016 11:18:52 AM
Analysis Method : C:\CHEM32\1\METHODS\OD-03-60-0.6.M
Last changed    : 3/14/2022 9:24:14 AM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



Data File C:\CHEM32\1\DATA\SUN_12 2022-03-13 18-54-13\YQL-2-186-P.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


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


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

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.479 BV    0.2707  550.52435   31.69091  27.9239
   2   8.956 VB    0.3035 1420.99011   70.38960  72.0761

Totals :                   1971.51447  102.08051


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