Supporting Information

Metal- and Additive-Free Oxygen-Atom Transfer Reaction: An Efficient and Chemoselective Oxidation of Sulfides to Sulfoxides with Cyclic Diacyl Peroxides

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1. General Methods and Materials

All reactions were carried out directly under open air. Commercially available reagents, starting materials and solvents were used without further purification. The reaction solvent, CH_2Cl_2 and CH_3OH was used without purification. All reactions were monitored by TLC and visualized by UV lamp (254 nm)/or by staining with a solution of 10 g phosphomolybdic acid and 100 mL EtOH followed by heating. Flash column chromatography was performed using 200-300 mesh silica gel. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz or 150 MHz) spectra were obtained on Bruker 400M or 600M nuclear resonance spectrometers. HR-ESI-MS spectra were recorded on a Bruker Esquire LC mass spectrometer using electrospray ionization. Coupling constants are reported in Hertz (Hz). Data for ^{1}H-NMR spectra were reported as follows: chemical shift *(*ppm, referenced to protium; s = singlet, br s= broad singlet, d = doublet, t = triplet, dd = doublet of doublets, td = triplet of doublets, m = multiplet, coupling constant (Hz), and integration). Data for ^{1}H-NMR were reported in (ppm) relative to residual solvent peak ($CDCl_3$: 7.26 ppm and $(CD_3)_2SO$: 2.50 ppm). Data for ^{13}C-NMR were reported in (ppm) relative to residual solvent peak ($CDCl_3$: 77.16 ppm and $(CD_3)_2SO$: 39.52 ppm). Single crystal X-ray data were collected on an Agilent Technology SuperNova Eos Dual system with a (Mo-Kα, λ = 0.7107 Å) micro focus source and focusing multilayer mirror optics. The data were collected at a temperature of 293 K and processed using CrysAlisPro.[1] The structure of compound **2ai** was solved and refined using full-matrix least-squares based on F2 with program SHELXS-97 and SHELXL-97.[2] All non-hydrogen atoms were refined anisotropically, the hydrogen atoms of the organic ligands were localized in their calculated positions and refined using a riding model.

Caution[3, 4]: Peroxides are dangerous and the preparation and use of phthaloyl peroxide and cyclopentyl malonoyl peroxide should be conducted by experienced practitioners of organic synthesis using appropriate safety equipment. Thermogravimetric analysis (TGA) data has shown that phthaloyl peroxide is stable below 90 °C. Rapid loss of mass occurs at 110 °C, indicating an exothermic decomposition at that temperature. Differential scanning calorimetry (DSC) data for cyclopentyl malonoyl peroxide shows an onset temperature of 70 °C.

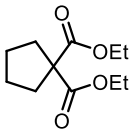
2. General procedure for the preparation of the phthaloyl peroxide

According to Siegel's method[5]: To a solution of phthaloyl chloride (0.40 g, 1.5 mmol, 1.0 equiv) in CH_2Cl_2 (25 mL), solid sodium percarbonate (Aldrich available H_2O_2: 20-30%) (0.34 g, 2.2 mmol, 1.5 equiv) was added in one portion. The heterogeneous reaction mixture was stirred vigorously for 3 hours (rapid stirring is required). The reaction mixture was filtered through celite and concentrated to provide the phthaloyl peroxide as white solid matching existing characterization data. Mp:118-119 °C, decomposition. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.29 (dd,

J= 5.8, 3.3 Hz), 8.03 (dd, *J* = 5.8, 3.3 Hz). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 162.1, 136.6, 130.3, 123.7.

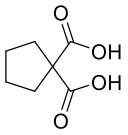
3. General procedure for the preparation of the cyclopentyl malonoyl peroxide[3]

Diethyl cyclopentane-1,1-dicarboxylate



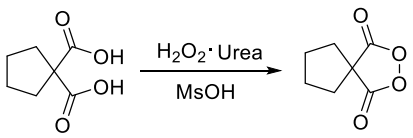
Sodium (200 mmol, 4.6 g) was added to absolute ethanol (175 mL) under argon at 25 ℃. Stirring was continued until the reaction mixture cooled to r.t. then, diethyl malonate (100 mmol, 15.2 mL) was added. The reaction mixture was stirred at 50 ℃ for 30 min and 1,4-dibromobutane (90 mmol, 10.7 mL) was added and stirring was continued at 50 ℃ for 60 h. The reaction mixture was cooled to r.t. and the solvent was removed under reduced pressure. Water (100 mL) was added and the aqueous layer was extracted with diethyl ether (100 mL). The aqueous layer was further extracted with diethyl ether (5 × 40 mL) and the combined organic layers dried over Na_2SO_4. The reaction mixture was reduced to dryness to give a yellow oil that was purified by distillation (80–88 ℃/ 10 torr [lit. b.p. 84–86 ℃/6 torr]) to afford the title compound as a pale yellow oil.

Cyclopentane-1,1-dicarboxylic acid



NaOH pellets (390 mmol, 15.6 g) were dissolved in water (78 mL) to make a 20% weight NaOH solution. Diethyl cyclopentane-1,1-dicarboxylate (65 mmol, 13.9 g) was added and the reaction mixture was stirred at 50 ℃ for 60 h. Residual diester was extracted with diethyl ether (2 x 20 mL). The aqueous layer was acidified to pH 1 with a 8 M HCl solution and then extracted with ethyl acetate (60 mL). The aqueous layer was further extracted with diethyl ether (3 x 30 mL) and the combined organic layers washed with brine (40 mL) and dried over Na_2SO_4. The solvents were removed under reduced pressure and the resulting slightly yellow solid was dissolved in the minimum of diethyl ether (10 mL) and petroleum ether (25 mL) was added. The resulting precipitate was filtered and washed with cold petroleum ether to afford the title compound as white solid.

cyclopentyl malonoyl peroxide

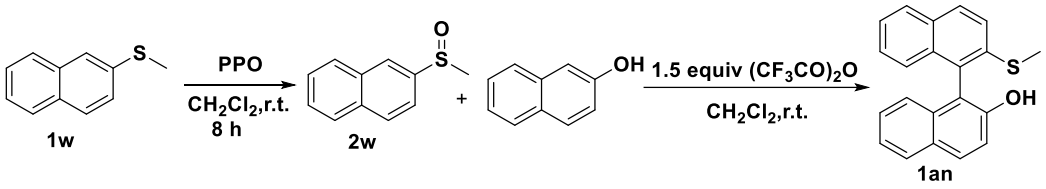


Methane sulfonic acid (30 mL) was placed in a round bottomed flask equipped with a large magnetic stirrer bar and immersed in a bath of water at 22 ℃. Urea hydrogen peroxide (9.82 g, 104 mmol) was added in a single portion and stirred for 30 seconds. Cyclopentane-1,1-dicarboxylic acid (35 mmol) was added in a single portion and the reaction stirred vigorously for 18 h. The reaction mixture was poured into a mixture of ice (80 g) and ethyl acetate (100 mL) and the layers separated. The aqueous layer was extracted with ethyl acetate (2 × 100 mL) and the combined organics were washed with $NaHCO_3$ (2 × 50 mL), brine (20 mL) and dried over $MgSO_4$. Removal of the solvent under reduced pressure gave the cyclopentyl malonoyl peroxide.

4. General procedure for the preparation of substrates.

2'-(methylthio)-[1,1'-binaphthalen]-2-ol[6]

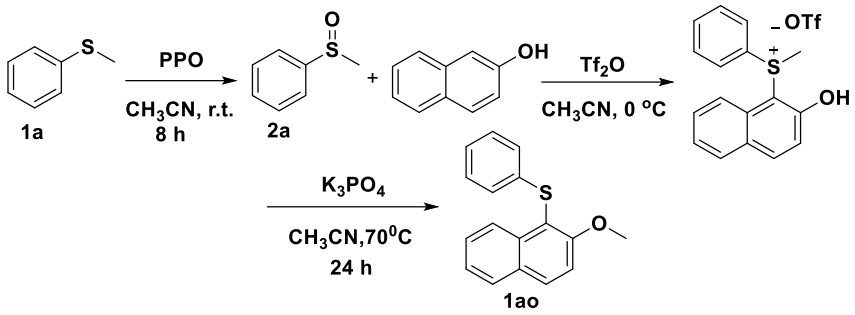
Methyl (naphthalen-2-yl) sulfane **1W** (174 mg, 1 mmol) was dissolved in CH_2Cl_2 (2 mL), phthaloyl peroxide (197 mg, 1.1 mmol) was added, and then the resulting solution was stirred at 25 ℃. After this period, naphthalen-2-ol (288 mg, 2 mmol) and trifluoroacetic anhydride (200 μL, 1.5 mmol) were added and the reaction mixture was stirred at 25 ℃ for 1 h. After the reaction period, saturated aqueous $NaHCO_3$ was added and the resulting biphasic solution was extracted with EtOAc. The combined organic layer was washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (eluent; petroleum ether/ethyl acetate = 10:1) to provide **1ao** (224 mg, 71 %).



1w 2w 1an

(2-methoxynaphthalen-1-yl)(phenyl)sulfane[7]

An oven-dried vial was charged with methyl(phenyl)sulfane **1a** (248 mg, 2 mmol) phthaloyl peroxide (394 mg, 2.2 mmol), and CH_3CN (4 mL), the resulting solution was stirred at 25 ℃. Then under argon Tf_2O (2.4 mmol, 1.2 eq) was then added to the resulting mixture at 0 ℃, followed by addition of phenol (2 mmol, 1 eq). The reaction mixture was stirred for several hours at 0 ℃. K_3PO_4 (8.8 mmol, 4.4 eq) was added to the residue, the mixture was stirred vigorously for 24 h at 70 ℃. After completion, the solution was allowed to cool to room temperature and extracted with EtOAc (1 mL x 3), dried over anhydrous Na_2SO_4, concentrated under reduced pressure. The crude mixture was purified by flash column chromatography (eluent; petroleum ether/ethyl acetate = 15:1) to afford desired products (303 mg, 57%).

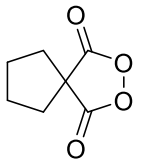


5. General experimental procedures for sulfoxides

A solution of an appropriate sulfide and PPO in CH_2Cl_2 was stirred in a standard schlenk tube at room temperature. The reaction was concentrated in vacuum and purified by column chromatography using petroleum ether/ethyl acetate to afford corresponding products, partially known compounds date are consistent with literature.

Physical data:

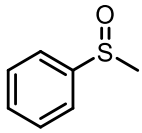
2,3-dioxaspiro[4.4]nonane-1,4-dione



White solid; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.38 – 2.20 (m, 4H), 2.10 – 1.93 (m, 4H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 175.8, 46.9, 37.7, 26.8.

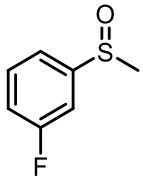
(methylsulfinyl)benzene (2a)[8]



Light yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 7.9, 1.8 Hz, 2H), 7.56 – 7.40 (m, 3H), 2.68 (s, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 145.3, 131.0, 129.3, 123.4, 43.7.

1-fluoro-3-(methylsulfinyl)benzene (2b)

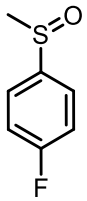


Light yellow oil ; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86 - 7.77 (m, 1H), 7.45 (td, *J* = 7.3, 1.3 Hz, 1H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.08 (t, *J* = 9.0 Hz, 1H), 2.79 (s, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 157.4 (d, J = 237.43 Hz), 132.7 (d, J = 8.82 Hz), 132.7 (d, J =18.14 Hz), 125.4 (dd, J =15.14 Hz), 115.7 (d, J =23.05 Hz), 42.1.

HRMS (ESI): $[M+H]^+$ calcd for $C_7H_8FOS^+$: 159.0274, found: 159.0281.

1-fluoro-4-(methylsulfinyl)benzene (2c)

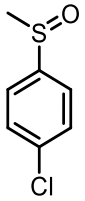


Light yellow oil ; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 6.7, 5.7 Hz, 2H), 7.24 (t, *J* = 8.0 Hz, 2H), 2.73 (s, 3H)

^{13}C NMR (150 MHz, $CDCl_3$) δ 164.5 (d, J = 253.35 Hz), 141.2 (d, J = 3.65 Hz), 126.0 (d, J = 10.66 Hz), 116.9 (d, J = 23.55 Hz). 44.2.

HRMS (ESI): $[M+H]^+$ calcd for $C_7H_8FOS^+$: 159.0274, found: 159.0282.

1-chloro-4-(methylsulfinyl)benzene (2d)

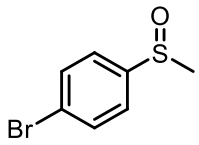


Light yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.61 – 7.56 (m, 2H), 7.52 – 7.48 (m, 2H), 2.71 (s, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 144.1, 137.4, 129.8, 125.1, 44.0.

HRMS (ESI): $[M+H]^+$ calcd for $C_7H_8ClOS^+$:174.9979, found: 174.9975.

1-bromo-4-(methylsulfinyl)benzene (2e)

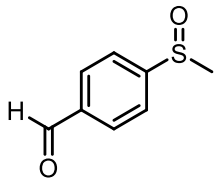


White solid ; m.p. 82-85 ℃ **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.68-7.63 (m, 2H), 7.53-7.48 (m, 2H), 2.70 (s, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 144.9, 132.7, 125.6, 125.2, 44.1.

HRMS (ESI): $[M+H]^+$ calcd for $C_7H_8BrOS^+$: 218.9474, found: 218.9479.

4-(methylsulfinyl)benzaldehyde (2f)

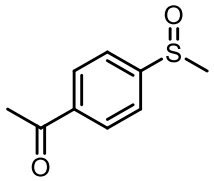


White solid; m.p. 84-87 ℃ **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.06 (s, 1H), 8.02 (d, *J* = 7.2 Hz, 2H), 7.83 – 7.78 (d, 2H), 2.76 (d, *J* = 2.0 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 191.2, 152.5, 138.2, 130.5, 124.3, 43.8.

HRMS (ESI): $[M+H]^+$ calcd for $C_8H_9O_2S^+$: 169.0318, found: 169.0325.

1-(4-(methylsulfinyl)phenyl)ethan-1-one (2g)

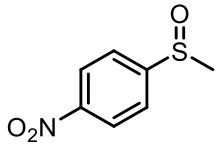


Brown solid; m.p. 128-130 ℃ **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.3 Hz, 2H), 7.74 (d, *J* = 8.3 Hz, 2H), 2.76 (s, 3H), 2.64 (s, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 197.2, 151.0, 139.2, 129.3, 123.9, 43.9, 26.9.

HRMS (ESI): $[M+H]^+$ calcd for $C_9H_{11}O_2S^+$: 183.0474, found: 183.0476.

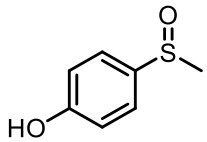
1-(methylsulfinyl)-4-nitrobenzene (2h)[8]



Yellow solid; m.p. 146-150 ℃ **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.7 Hz, 2H), 7.83 (d, *J* = 8.6 Hz, 2H), 2.78 (s, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 153.3, 149.5, 124.8, 124.6, 43.9.

4-(methylsulfinyl)phenol (2i)

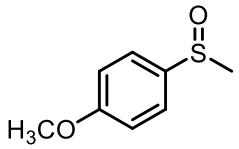


White solid; m.p. 106-109 ℃ **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.44 (s, 1H), 7.48 (d, *J* = 8.6 Hz, 2H), 6.96 (d, *J* = 8.6 Hz, 2H), 2.74 (s, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 160.8, 132.8, 126.2, 116.9, 43.1.

HRMS (ESI): $[M+H]^+$ calcd for $C_7H_9O_2S^+$: 157.0318, found: 157.0315.

1-methoxy-4-(methylsulfinyl)benzene (2j)

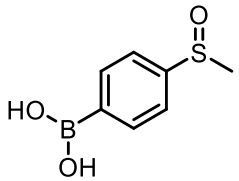


Brown solid; m.p. 43-47 ℃ **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.8 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 3.78 (s, 3H), 2.63 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.9, 136.5, 125.4, 114.8, 55.5, 43.9.

HRMS (ESI): $[M+H]^+$ calcd for $C_8H_{11}O_2S^+$: 171.0474, found: 171.0474.

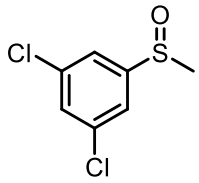
(4-(methylsulfinyl)phenyl)boronic acid (2k)[9]



White solid; m.p. 130-135 ℃ **^{1}H NMR** (400 MHz, DMSO) δ 8.25 (s, 2H), 7.95 (d, *J* = 7.6 Hz, 2H), 7.63 (d, *J* = 7.8 Hz, 2H), 2.73 (s, 3H).

^{13}C NMR (101 MHz, DMSO) δ 148.1, 134.7, 134.1, 122.4, 43.1.

1,3-dichloro-5-(methylsulfinyl)benzene (2l)

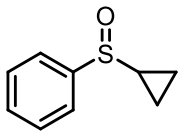


White solid; m.p. 63-67 ℃ **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 1.7 Hz, 2H), 7.47 (d, *J* = 1.7 Hz, 1H), 2.76 (s, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 149.4, 136.4, 131.2, 122.0, 44.1.

HRMS (ESI): $[M+H]^+$ calcd for $C_7H_7Cl_2OS^+$: 208.9589, found: 208.9588.

(cyclopropylsulfinyl)benzene (2m)

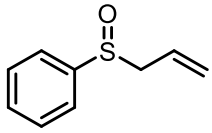


Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.5 Hz, 2H), 7.54 – 7.46 (m, 3H), 2.29 – 2.23 (m, 1H), 1.26 – 1.21 (m, 1H), 1.06 – 1.00 (m, 1H), 0.99 – 0.90 (m, 2H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 144.9, 131.0, 129.3, 124.1, 33.9, 3.5, 3.0.

HRMS (ESI): $[M+H]^+$ calcd for $C_9H_{11}OS^+$: 167.0525, found: 167.0535.

(allylsulfinyl)benzene (2n)

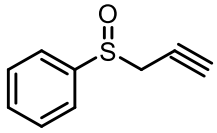


Light yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.52 – 7.40 (m, 2H), 7.35 (d, *J* = 6.9 Hz, 3H), 5.58 – 5.41 (m, 1H), 5.16 (d, *J* = 10.2 Hz, 1H), 5.04 (d, *J* = 17.0 Hz, 1H), 3.43 (dd, *J* = 12.8, 7.5 Hz, 1H), 3.34 (dd, *J* = 12.8, 7.5 Hz, 1H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 142.6, 130.8, 128.7, 124.9, 124.0, 123.5, 60.4.

HRMS (ESI): $[M+H]^+$ calcd for $C_9H_{11}OS^+$: 167.0525, found: 167.0527.

(prop-2-yn-1-ylsulfinyl)benzene (2o)

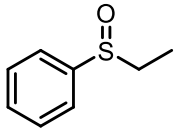


Light yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.74 – 7.66 (m, 2H), 7.56 – 7.50 (m, 3H), 3.69 – 3.57 (m, 2H), 2.33 (t, *J* = 2.7 Hz, 1H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 142.8, 131.8, 129.1, 124.5, 76.5, 72.8, 47.8.

HRMS (ESI): $[M+H]^+$ calcd for $C_9H_9OS^+$: 165.0369, found: 165.0370.

(ethylsulfinyl)benzene (2p)

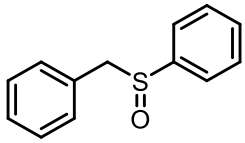


Light yellow oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.8 Hz, 2H), 7.55 – 7.45 (m, 3H), 2.90 (m, *J* = 14.4, 7.4 Hz, 1H), 2.76 (m, *J* = 14.4, 7.4 Hz, 1H), 1.19 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 143.3, 131.0, 129.2, 124.3, 50.4, 6.1.

HRMS (ESI): $[M+H]^+$ calcd for $C_8H_{11}OS^+$: 155.0525, found: 155.0527.

(benzylsulfinyl)benzene (2q)

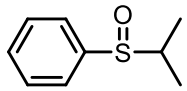


White solid: m.p. 128-130 ℃ **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.42 (m, *J* = 29.7, 18.2, 7.5 Hz, 5H), 7.26 (dt, *J* = 14.4, 7.5 Hz, 3H), 6.98 (d, *J* = 7.5 Hz, 2H), 4.09 (d, *J* = 12.7 Hz, 1H), 3.99 (d, *J* = 12.6 Hz, 1H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 142.8, 131.2, 130.4, 129.2, 128.9, 128.5, 128.3, 124.5, 63.6.

HRMS (ESI): $[M+H]^+$ calcd for $C_{13}H_{13}OS^+$: 217.0682, found: 217.0680.

(isopropylsulfinyl)benzene (2r)

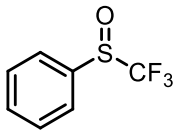


Light yellow oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.53 – 7.46 (m, 2H), 7.45 – 7.36 (m, 3H), 2.74 (m, *J* = 6.8 Hz, 1H), 1.13 (d, *J* = 6.9 Hz, 3H), 1.04 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 141.6, 130.9, 128.8, 124.8, 54.4, 15.8, 13.7.

HRMS (ESI): $[M+H]^+$ calcd for $C_9H_{13}OS^+$: 169.0682, 169.0685.

((trifluoromethyl)sulfinyl)benzene (2s)

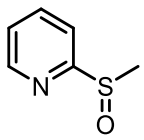


Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.6 Hz, 2H), 7.68 – 7.57 (m, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 135.70, 133.66, 133.66, 129.69, 126.01, 123.67.(q, *J*. = 336.5 Hz).

HRMS (ESI): $[M+H]^+$ calcd for $C_7H_6F_3OS^+$: 195.0086, found: 195.0083.

2-(methylsulfinyl)pyridine (2t)

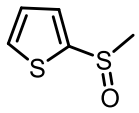


Colorless oil; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.62 – 8.57 (m, 1H), 7.99 (d, *J* = 7.9 Hz, 1H), 7.92 (td, *J* = 7.7, 1.7 Hz, 1H), 7.36 (m, *J* = 7.5, 4.7, 1.1 Hz, 1H), 2.83 (s, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 165.8, 149.6, 138.2, 124.7, 119.3, 41.3.

HRMS (ESI): $[M+H]^+$ calcd for $C_6H_8NOS^+$: 142.0321, found: 142.0327.

2-(methylsulfinyl)thiophene (2u)

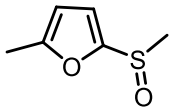


Light yellow oil; **^{1}H NMR** (600 MHz, CiDCl$_3$) δ 7.63 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.48 (dd, *J* = 3.6, 1.2 Hz, 1H), 7.10 (dd, *J* = 4.9, 3.7 Hz, 1H), 2.92 (s, 3H).

^{13}C NMR (150 MHz, CDCl$_3$) δ 147.2, 131.0, 129.5, 127.5, 44.4.

HRMS (ESI): [M+H]$^+$ calcd for $C_5H_7OS_2^+$: 146.9933, 146,9939.

2-methyl-5-(methylsulfinyl)furan (2v)

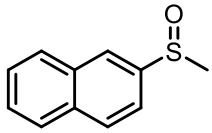


Light yellow oil: **^{1}H NMR** (400 MHz, CDCl$_3$) δ 6.75 (d, *J* = 3.2 Hz, 1H), 6.05 (d, *J* = 3.1 Hz, 1H), 2.86 (s, 3H), 2.31 (s, 3H).

^{13}C NMR (150 MHz, CDCl$_3$) δ 157.4, 150.0, 116.7, 107.5, 38.0, 13.5.

HRMS (ESI): [M+H]$^+$ calcd for $C_6H_9O_2S^+$: 145.0318, found: 145.0322.

2-(methylsulfinyl)naphthalene (2w)

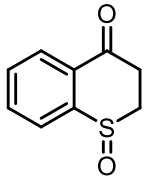


White solid; m.p. 92-99 ℃ **^{1}H NMR** (600 MHz, CDCl$_3$) δ 8.21 (s, 1H), 7.98 (d, *J* = 8.5 Hz, 1H), 7.96 – 7.86 (m, 2H), 7.59 (t, *J* = 7.9 Hz, 3H), 2.79 (s, 3H).

^{13}C NMR (150 MHz, CDCl3) δ 142.7, 134.5, 133.00 129.73 128.6, 128.12, 127.9, 127.45, 124.2, 119.5, 43.8.

HRMS (ESI): [M+H]$^+$ calcd for $C_{11}H_{11}OS^+$: 191.0525, found: 191.0535.

thiochroman-4-one 1-oxide (2x)

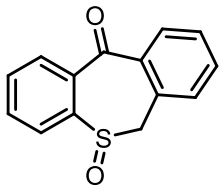


White solid; m.p. 47-51 ℃ **^{1}H NMR** (400 MHz, CDCl$_3$) δ 8.13 (d, *J* = 7.8 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.74 (td, *J* = 7.6, 1.0 Hz, 1H), 7.67 – 7.59 (m, 1H), 3.52 – 3.39 (m, 3H), 2.88 (m, *J* = 14.0, 10.5, 6.1 Hz, 1H).

^{13}C NMR (150 MHz, CDCl$_3$) δ 192.1, 145.5, 134.7, 132.2, 129.2, 129.0, 128.6, 46.7, 30.4.

HRMS (ESI): $[M+H]^+$ calcd for $C_9H_9O_2S^+$: 181.0318, found: 181.0313.

6,11-dihydrodibenzo[b,e]thiepine 5-oxide (2y)

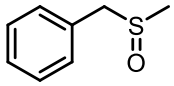


White solid; m.p. 93-96 ℃ **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.11 (t, *J* = 8.3 Hz, 2H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.76 – 7.67 (m, 1H), 7.61 – 7.50 (m, 2H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 7.5 Hz, 1H), 4.79 (d, *J* = 13.6 Hz, 1H), 4.24 (d, *J* = 13.6 Hz, 1H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 190.2, 146.8, 137.9, 134.1, 133.9, 133.3, 132.5, 131.9, 131.4, 130.7, 129.0, 127.9, 124.2, 60.9.

HRMS (ESI): $[M+H]^+$ calcd for $C_{14}H_{11}O_2S^+$: 243.0474, found: 243.0481.

((methylsulfinyl)methyl)benzene (2z)

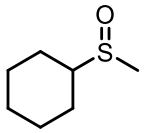


White solid; m.p. 53-59 ℃ **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 (m, *J* = 27.3, 10.8, 4.7 Hz, 5H), 4.06 (dd, *J* = 16.7, 12.9 Hz, 1H), 3.93 (dd, *J* = 12.6, 9.1 Hz, 1H), 2.46 (d, *J* = 11.5 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 130.0, 129.7, 129.0, 128.4, 60.3, 37.3.

HRMS (ESI): $[M+H]^+$ calcd for $C_8H_{11}OS^+$: 155.0525, found: 155.0527.

(methylsulfinyl)cyclohexane (2aa)

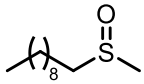


Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.44 – 2.33 (m, 4H), 2.00 (d, *J* = 13.0 Hz, 1H), 1.85 – 1.68 (m, 3H), 1.58 (d, *J* = 12.2 Hz, 1H), 1.37 – 1.05 (m, 5H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 60.5, 34.9, 25.8, 25.3, 25.1, 24.9, 24.5.

HRMS (ESI): $[M+H]^+$ calcd for $C_7H_{15}OS^+$: 147.0838, found: 147.0834.

1-(methylsulfinyl)propane (2ab)

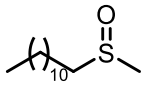


White solid; m.p. 45-50 ℃ **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.63 (m, *J* = 20.9, 13.2, 7.9 Hz, 2H), 2.50 (s, 3H), 1.80 – 1.60 (m, 2H), 1.50 – 1.10 (m, 14H), 0.81 (t, *J* = 6.5 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ54.7, 38.5, 31.8, 29.4, 29.3, 29.2, 29.2, 28.8, 22.6, 22.5, 14.1.

HRMS (ESI): $[M+H]^+$ calcd for $C_{11}H_{25}OS^+$: 205.1621, found: 205.1623.

1-(methylsulfinyl)propane (2ac)

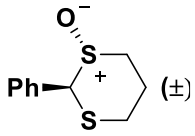


White solid; m.p. 62-68 ℃ **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.65 (m, *J* = 21.1, 13.1, 7.7 Hz, 2H), 2.51 (s, 3H), 1.79 – 1.62 (m, 2H), 1.52 – 1.10 (m, 18H), 0.83 (t, *J* = 6.6 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ54.8, 38.6, 31.9, 29.6 (2C), 29.5, 29.4, 29.3, 29.2, 28.8, 22.7, 22.6, 14.1.

HRMS (ESI): $[M+H]^+$ calcd for $C_{13}H_{29}OS^+$: 233.1934, found: 233.1939.

2-phenyl-1,3-dithiane 1-oxide (2ad)

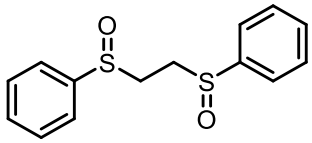


White solid; m.p. 140-146 ℃ **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.43 – 7.33 (m, 5H), 4.54 (s, 1H), 3.52 (d, *J* = 12.8 Hz, 1H), 2.88 – 2.78 (m, 1H), 2.72 (td, *J* = 13.1, 2.4 Hz, 1H), 2.66 – 2.58 (m, 1H), 2.46 (dd, *J* = 15.1, 3.4 Hz, 1H), 2.38 – 2.23 (m, 1H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 133.4, 129.5, 129.2, 128.8, 69.8, 54.9, 31.5, 29.6.

HRMS (ESI): $[M+H]^+$ calcd for $C_{10}H_{13}OS_2^+$: 213.0402, found: 213.0409.

1,2-bis(phenylsulfinyl)ethane (2ae)

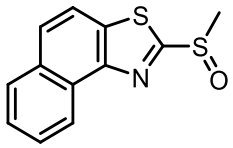


White solid; m.p. 115-120 ℃ **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.65 – 7.38 (m, 10H), 3.43 – 3.31 (m, 1H), 3.01 (d, *J* = 9.1 Hz, 2H), 2.77 – 2.66 (m, 1H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 142.3, 142.1, 131.4, 131.4, 129.5, 129.5, 124.0, 123.9, 47.7, 46.9.

HRMS (ESI): $[M+H]^+$ calcd for $C_{14}H_5O_2S_2^+$: 281.0607, found: 281.0610.

2-(methylsulfinyl)naphtho[1,2-d]thiazole (2af)

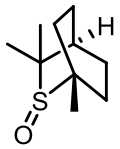


White solid; m.p. 100-104 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 8.2 Hz, 1H), 7.89 (dd, *J* = 15.7, 8.4 Hz, 2H), 7.80 (d, *J* = 8.8 Hz, 1H), 7.69 – 7.63 (m, 1H), 7.58 (m, *J* = 8.2, 7.0, 1.3 Hz, 1H), 3.10 (s, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 176.3, 150.3, 133.4, 131.9, 128.6, 128.2, 127.5, 127.2, 126.8, 123.5, 118.9, 43.5.

HRMS (ESI): $[M+H]^+$ calcd for $C_{12}H_{10}NOS_2^+$: 248.0198, found: 248.0189.

(1s,4s)-1,3,3,4-tetramethyl-2-thiabicyclo[2.2.2]octane (2ag)

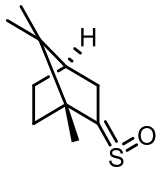


Colorless oil; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 2.90 (s, 1H), 2.33 (m, *J* = 13.7, 10.0, 4.9 Hz, 2H), 2.08 (s, 1H), 1.95 (d, *J* = 13.2 Hz, 1H), 1.57 – 1.37 (m, 5H), 1.32 – 1.22 (m, 5H), 1.01 (d, *J* = 7.1 Hz, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 70.4, 65.1, 48.1, 29.3, 29.2, 26.2, 22.6, 22.2, 20.8, 17.9.

HRMS (ESI): $[M+H]^+$ calcd for $C_{10}H_{19}OS^+$: 187.1151, found: 187.1155.

((1R,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-ylidene)-l4-sulfanone (2ah)

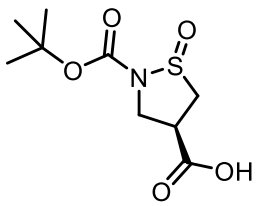


Red brown solid; m.p. 147-150 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.01 – 2.92 (m, 1H), 2.49 (d, *J* = 20.6 Hz, 1H), 2.02 (t, *J* = 4.0 Hz, 1H), 1.90 – 1.79 (m, 2H), 1.41 (t, *J* = 9.1 Hz, 1H), 1.22 (dd, *J* = 14.6, 5.1 Hz, 1H), 1.08 (s, 3H), 0.91 (s, 3H), 0.79 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 210.4, 56.2, 50.2, 44.3, 38.2, 35.6, 27.0, 19.3, 18.3, 12.2.

HRMS (ESI): $[M+H]^+$ calcd for $C_{10}H_{17}OS^+$: 185.0995, found: 185.0997.

(4R)-2-(tert-butoxycarbonyl)isothiazolidine-4-carboxylic acid 1-oxide (2ai)

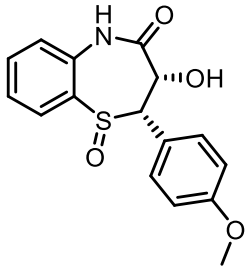


White solid; m.p. 162-166 ℃. **^{1}H NMR** (400 MHz, DMSO) δ 13.09 (s, 1H), 4.92 – 4.67 (m, 2H), 4.15 (t, *J* = 11.7 Hz, 1H), 3.53 (m, *J* = 24.0, 13.3, 5.9 Hz, 1H), 3.10 (m, *J* = 17.3, 13.9, 10.1 Hz, 1H), 1.41 (d, *J* = 11.1 Hz, 9H).

^{13}C NMR (151 MHz, DMSO) δ 172.1, 171.7, 154.1, 153.5, 80.7, 80.6, 68.8, 68.5, 58.1, 58.0, 53.2, 52.6, 27.9, 27.8(The carbamate C-N rotamer equilibrium was seen).

HRMS (ESI): $[M+H]^+$ calcd for $C_9H_{16}NO_5S^+$: 250.0744, found: 250.0735.

(2S,3S)-3-hydroxy-2-(4-methoxyphenyl)-2,3-dihydrobenzo[b][1,4]thiazepin-4(5H)-one 1-oxide (2aj)

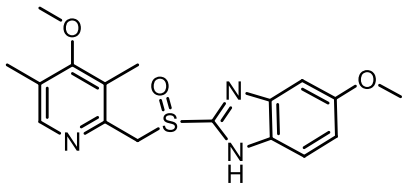


White solid; m.p. 194-198 ℃. **^{1}H NMR** (400 MHz, DMSO) δ 10.51 (s, 1H), 7.76 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.58 (m, *J* = 8.5, 7.5, 1.4 Hz, 2H), 7.34 (d, *J* = 8.7 Hz, 2H), 7.25 – 7.19 (m, 1H), 6.98 (d, *J* = 8.7 Hz, 2H), 5.05 (d, *J* = 5.5 Hz, 1H), 4.62 (d, *J* = 8.7 Hz, 1H), 4.44 (dd, *J* = 8.6, 5.4 Hz, 1H), 3.79 (s, 3H).

^{13}C NMR (100 MHz, DMSO) δ 171.4, 159.5, 135.0, 133.8, 131.8, 131.6, 126.8, 125.0, 124.3, 123.0, 113.9, 78.6, 64.6, 55.2.

HRMS (ESI): $[M+H]^+$ calcd for $C_{16}H_{16}NO_4S^+$:318.0795, found: 318.0799.

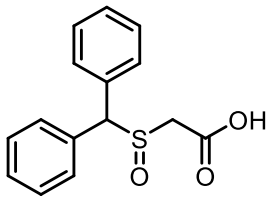
Omeprazole (2ak)[10]



White solid; m.p. 155-160 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 12.37 (s, 1H), 8.19 (s, 1H), 7.52 (d, *J* = 6.4 Hz, 1H), 6.92 (dd, *J* = 8.9, 2.0 Hz, 1H), 4.75 (s, 2H), 3.82 (s, 3H), 3.59 (s, 3H), 2.20 (s, 3H), 2.10 (s, 3H).

HRMS (ESI): $[M+H]^+$ calcd for $C_{17}H_{20}N_3O_3S^+$: 346.1220, found: 346.1214.

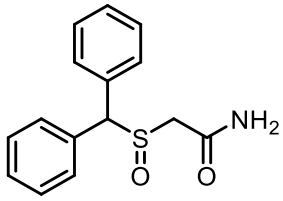
2-(benzhydrylsulfinyl) acetic acid (2al)[11]



White solid; m.p. 145-149 ℃. **^{1}H NMR** (400 MHz, DMSO) δ 13.14 (s, 1H), 7.52 (d, *J* = 7.2 Hz, 4H), 7.45 – 7.32 (m, 6H), 5.41 (s, 1H), 3.57 (d, *J* = 14.3 Hz, 1H), 3.33 (d, *J* = 14.2 Hz, 1H).

^{13}C NMR (150 MHz, DMSO) δ 167.4, 136.6, 134.9, 129.6, 129.2, 128.6, 128.5, 128.2, 128.1, 69.3, 55.4.

Modafinil (2am)

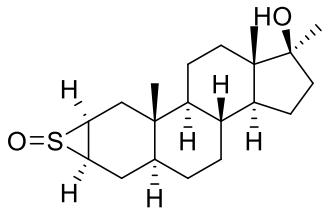


White solid; m.p. 159-164 ℃. **^{1}H NMR** (400 MHz, CDCl3) δ 7.53 – 7.32 (m, 10H), 7.05 (s, 1H), 5.61 (s, 1H), 5.20 (s, 1H), 3.52 – 3.47 (m, 1H), 3.10 (d, J = 14.4 Hz, 1H).

^{13}C NMR (150 MHz, CDCl3) δ 166.2, 134.4, 134.2, 129.6, 129.5, 129.1, 129.1, 128.9, 128.8, 71.7, 51.3.

HRMS (ESI): $[M+H]^+$ calcd for $C_{15}H_{16}NO_2S^+$: 274.0896, found: 274.0890.

(1S,3aS,3bR,5aS,6aR,7aS,8aS,8bS,10aS)-1-hydroxy-1,8a,10a-trimethylhexadecahydro-1H-cyclopenta[7,8]phenanthro[2,3-b]thiirene 7-oxide (2an)

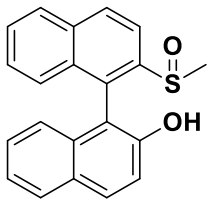


White solid; m.p. 142-146 ℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.24 (td, *J* = 10.5, 3.5 Hz, 1H), 3.10 (dd, *J* = 10.8, 5.7 Hz, 1H), 2.44 (dd, *J* = 15.9, 10.3 Hz, 1H), 2.18 (m, *J* = 15.7, 4.6, 1.1 Hz, 1H), 1.87 – 1.41 (m, 8H), 1.39 – 1.15 (m, 10H), 1.12 – 1.02 (m, 2H), 0.81 (s, 3H), 0.78 (d, *J* = 1.0 Hz, 3H), 0.42 (m, *J* = 28.8, 11.9, 9.4, 4.0 Hz, 2H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 81.69, 53.74, 53.50, 51.28, 50.53, 45.32, 40.59, 38.94, 36.53, 35.60, 33.23, 31.55, 31.08, 28.91, 25.90, 25.65, 23.30, 20.50, 13.98, 12.69.

HRMS (ESI): $[M+H]^+$ calcd for $C_{20}H_{33}O_2S^+$: 337.2196, found: 337.2197.

2'-(methylsulfinyl)-[1,1'-binaphthalen]-2-ol (2ao)

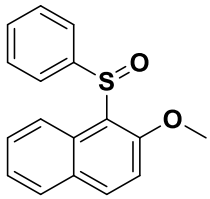


White solid; m.p. 248-255 ℃. **^{1}H NMR** (400 MHz, Chloroform-d) δ 8.23 – 8.13 (m, 2H), 7.96 (d, J = 8.3 Hz, 1H), 7.92 – 7.82 (m, 2H), 7.55 (m, J = 8.2, 6.0, 2.0 Hz, 1H), 7.40 (d, J = 8.9 Hz, 1H), 7.37 – 7.26 (m, 3H), 7.18 (m, J = 8.3, 6.8, 1.3 Hz, 1H), 6.74 (dd, J = 8.4, 1.1 Hz, 1H), 2.25 (s, 3H).

^{13}C NMR (150 MHz, CDCl3) δ 152.5, 141.9, 135.1, 134.0, 132.6, 132.2, 131.0, 130.5, 128.7, 128.6, 128.6, 128.0, 127.6, 127.1, 126.7, 123.8, 123.2, 119.2, 119.0, 113.4, 41.9.

HRMS (ESI): $[M+H]^+$ calcd for $C_{21}H_{17}O_2S^+$: 333.0944, found: 333.0943.

2-methoxy-1-(phenylsulfinyl)naphthalene (2ap)



White solid; m.p. 129-135 ℃ **^{1}H NMR** (400 MHz, Chloroform-d) δ 8.71 (d, J = 8.6 Hz, 1H), 7.95 (d, J = 9.0 Hz, 1H), 7.77 (d, J = 8.1 Hz, 1H), 7.68 – 7.62 (m, 2H), 7.46 (m, J = 8.5, 6.9, 1.4 Hz, 1H), 7.42 – 7.32 (m, 4H), 7.27 (d, J = 9.0 Hz, 1H), 3.95 (s, 3H).

^{13}C NMR (150 MHz, $CDCl_3$) δ 157.5, 145.2, 136.1, 135.0, 131.9, 129.6, 129.6, 128.8, 128.8, 128.2, 125.8, 124.6, 124.4, 123.6, 123.2, 113.2, 57.0.

HRMS (ESI):calcd for $C_{17}H_{15}O_2S^+$:283.0787, found: 283.0778.

5. References

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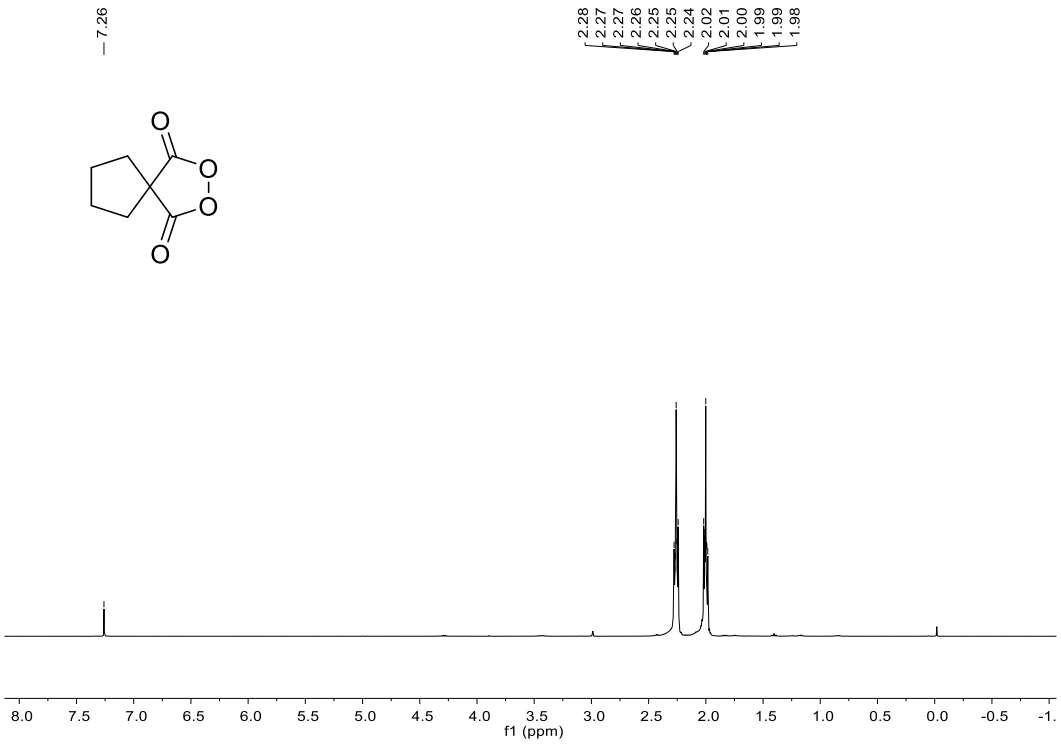
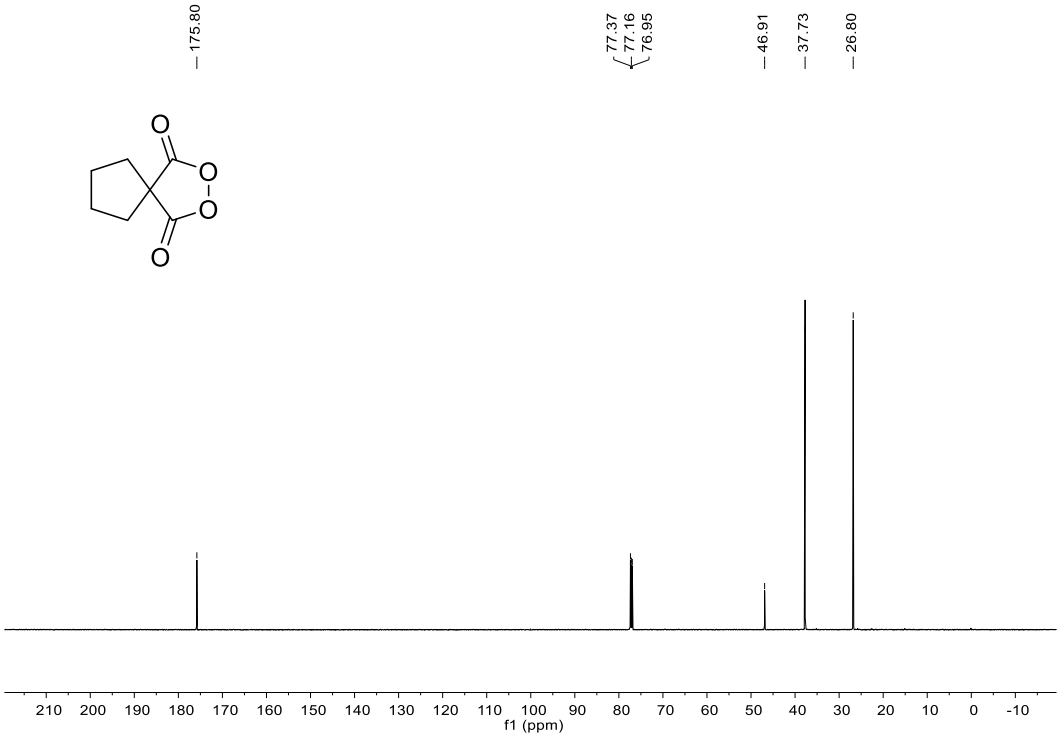
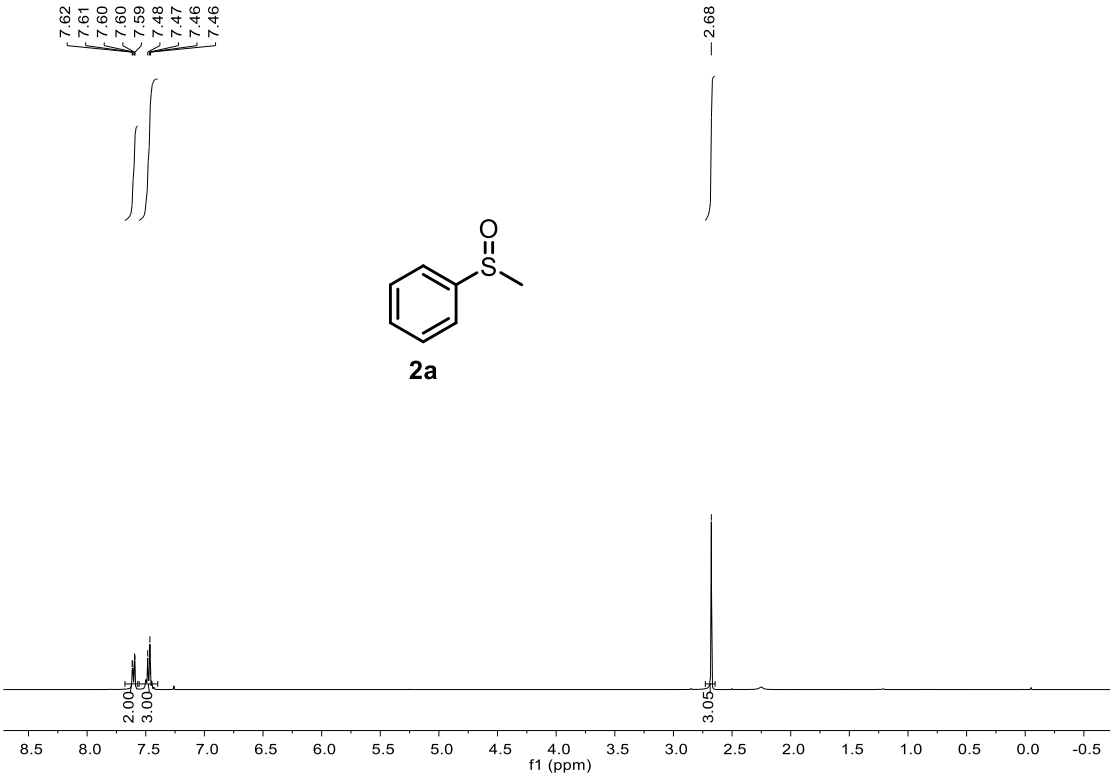
6. NMR Spectra for all the compounds



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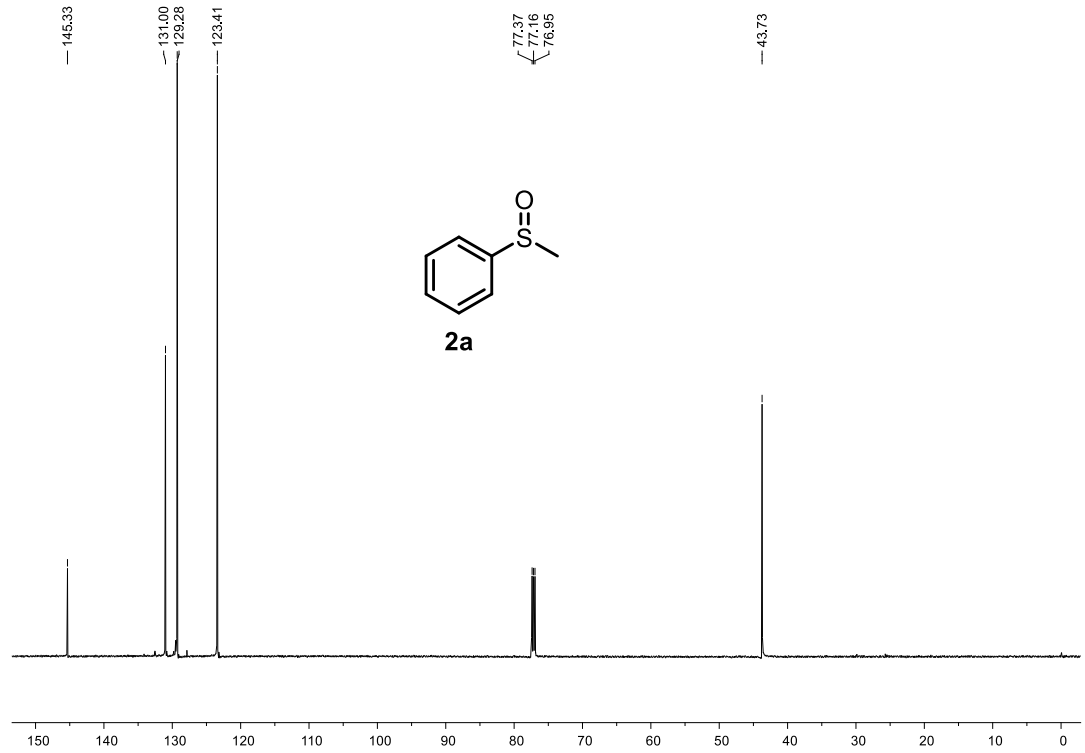
7.61
7.60
7.60
7.59
7.48
7.47
7.46
7.46
2.68
2a
2.00
3.00
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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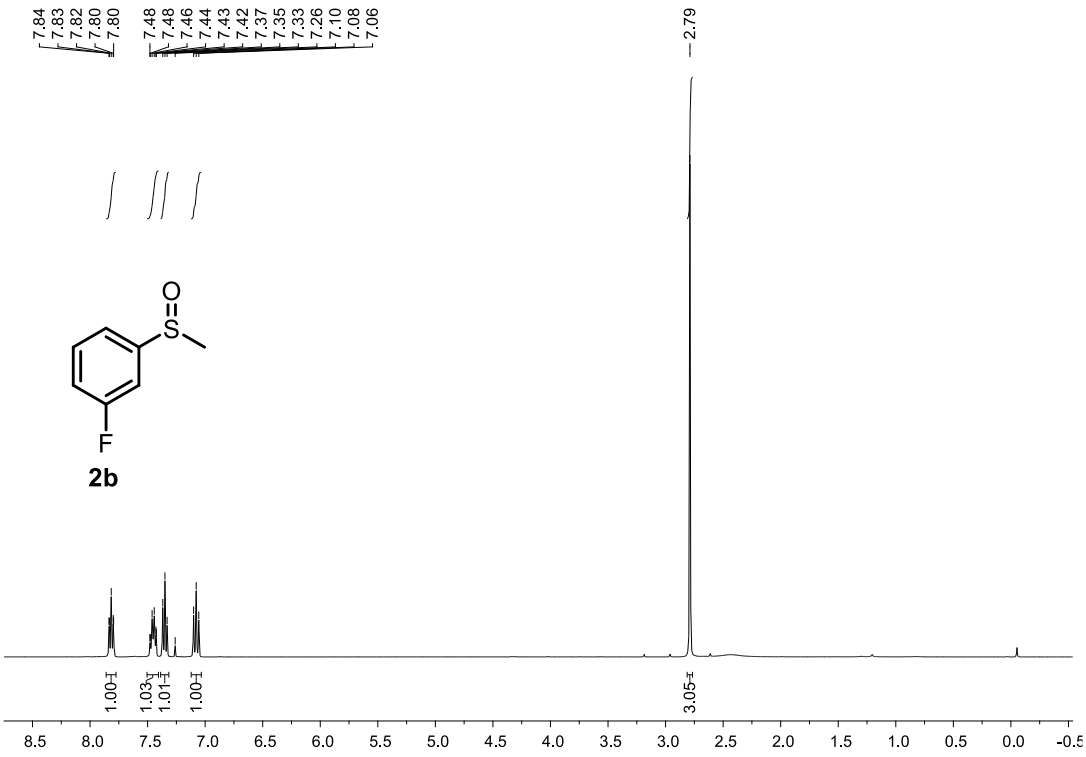
131.00
129.28
123.41
77.37
77.16
76.95
43.73
2a
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0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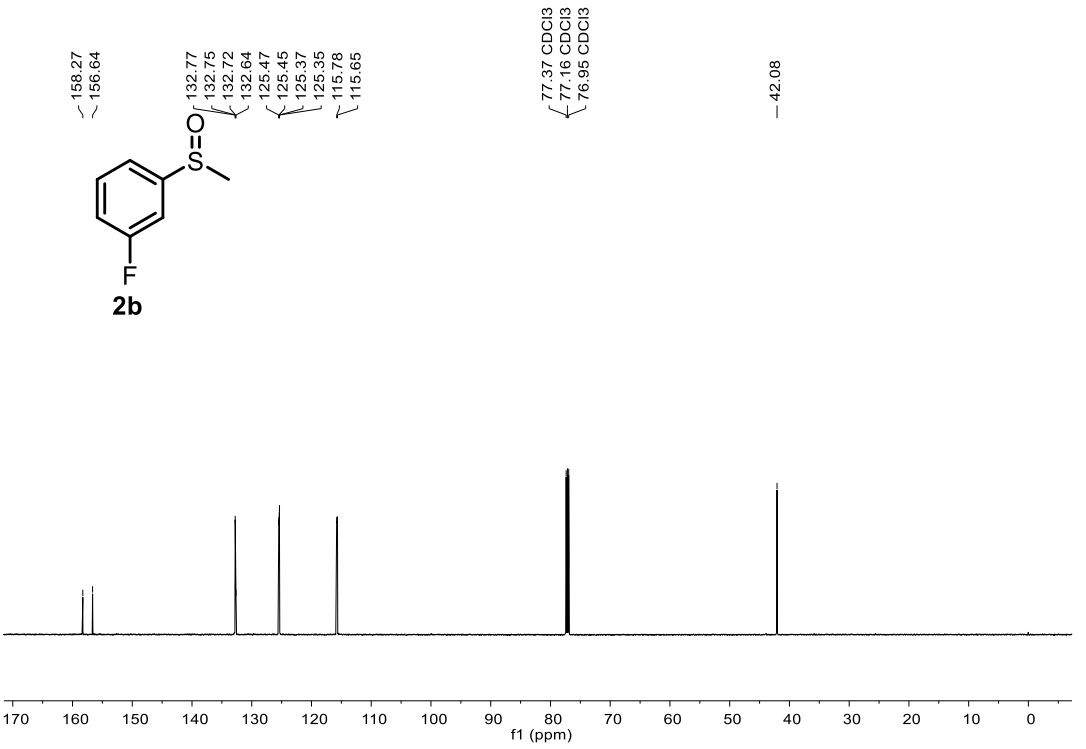
7.83
7.82
7.80
7.80
7.48
7.48
7.46
7.44
7.43
7.42
7.37
7.35
7.33
7.26
7.10
7.08
7.06
2.79
O
S
F
2b
1.00
1.03
1.01
1.00
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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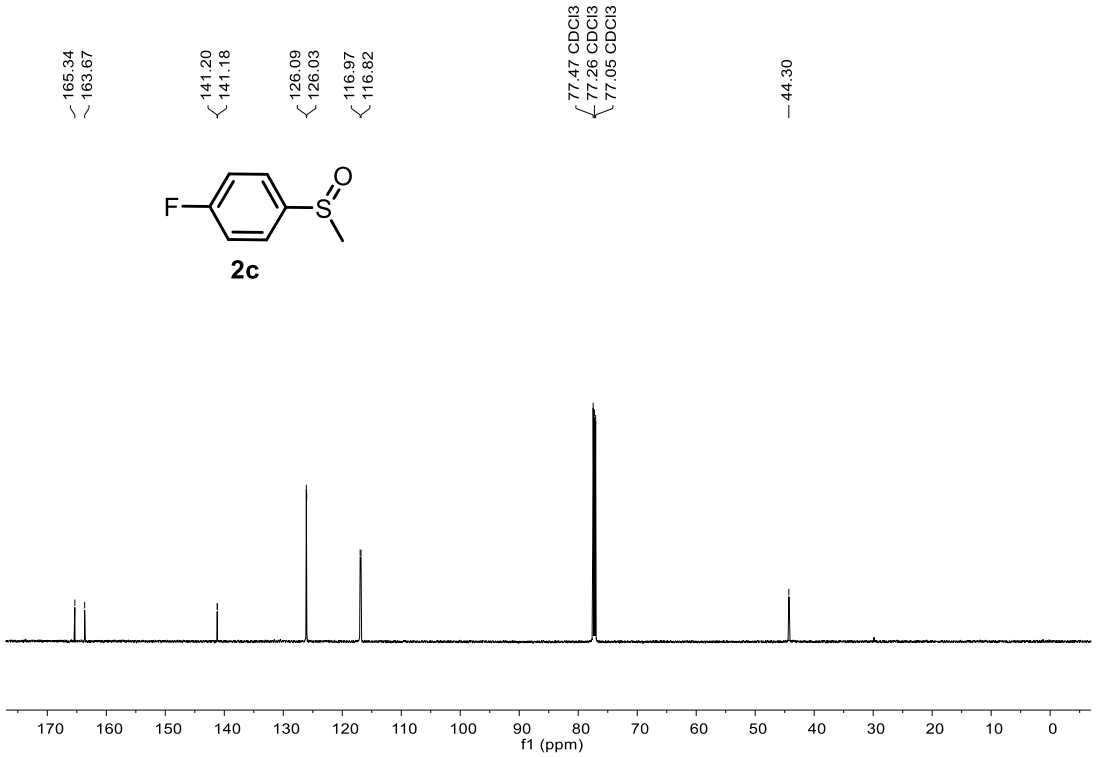
156.64
132.77
132.75
132.72
132.64
125.47
125.45
125.37
125.35
115.78
115.65
77.37 CDCl3
77.16 CDCl3
76.95 CDCl3
42.08
O
S
F
2b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.65
7.64
7.64
7.63
7.26
7.22
7.21
7.20
2.70
F
O
S
2c
2.03
1.99
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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163.67
141.20
141.18
126.09
126.03
116.97
116.82
77.47 CDCl3
77.26 CDCl3
77.05 CDCl3
44.30
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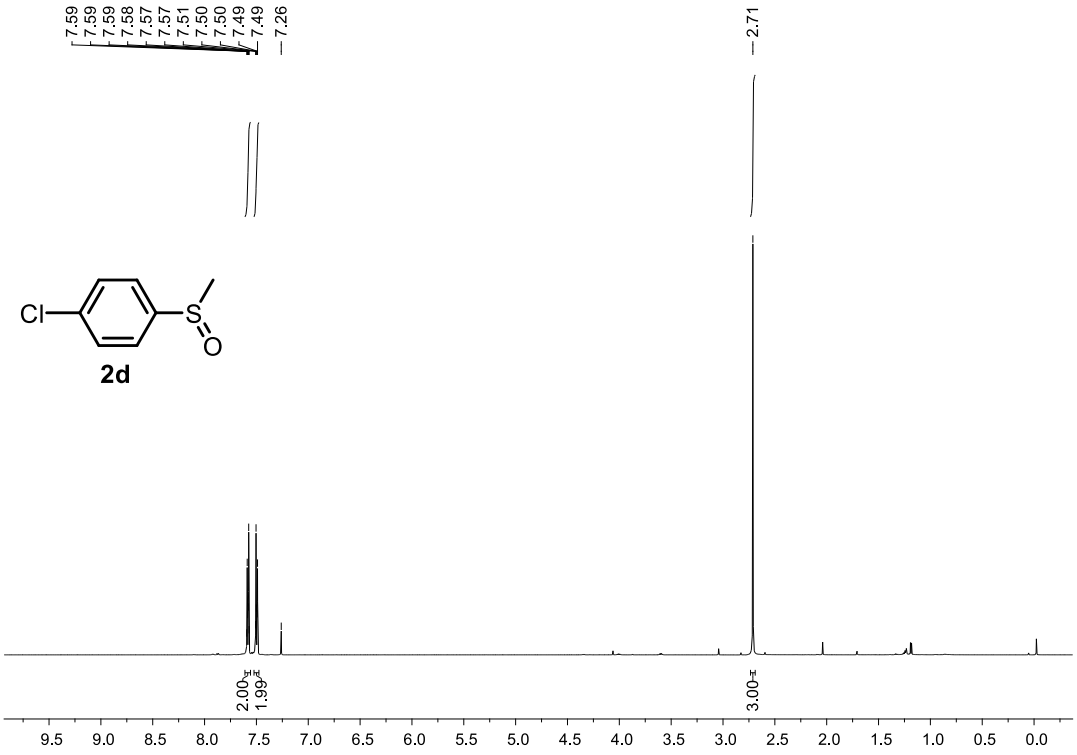
O
S
2c
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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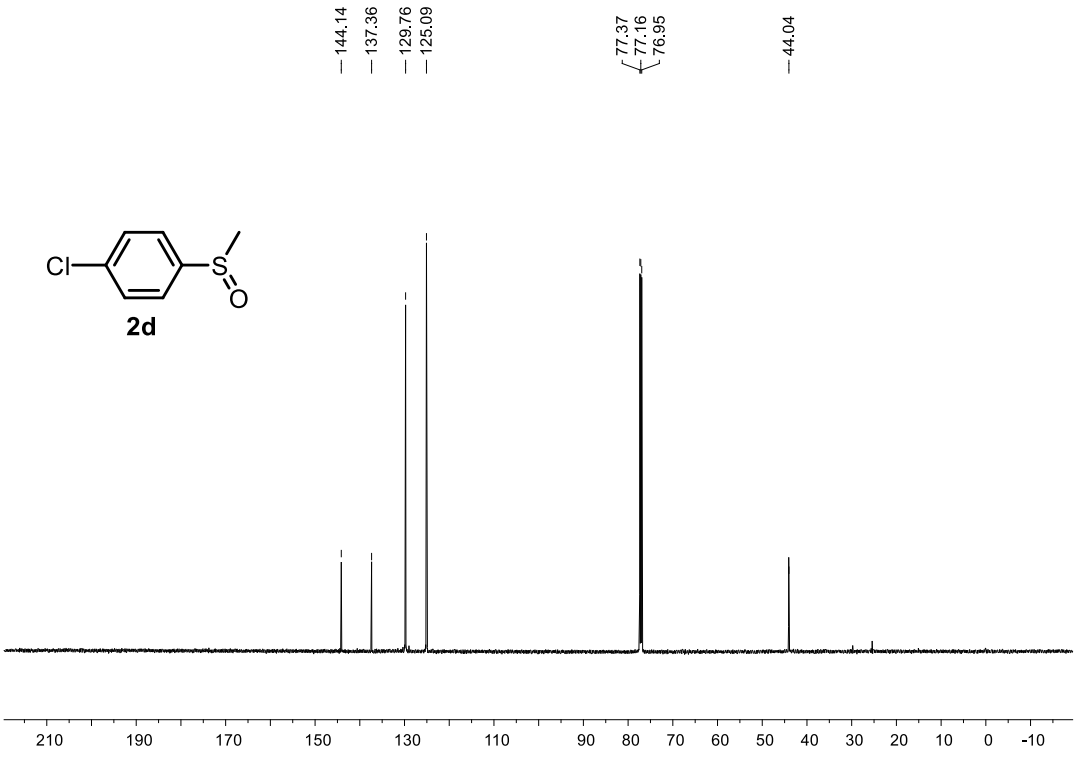
7.59
7.59
7.58
7.57
7.57
7.51
7.50
7.50
7.49
7.49
7.26
2.71
Cl
S
O
2d
2.00
1.99
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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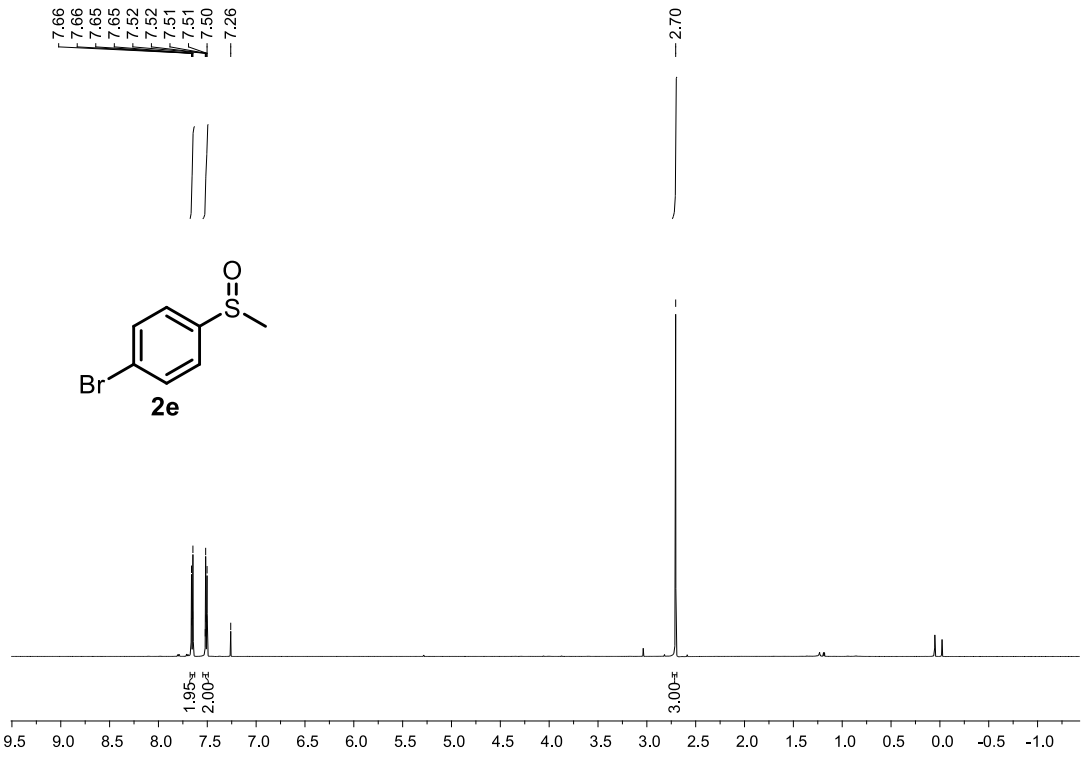
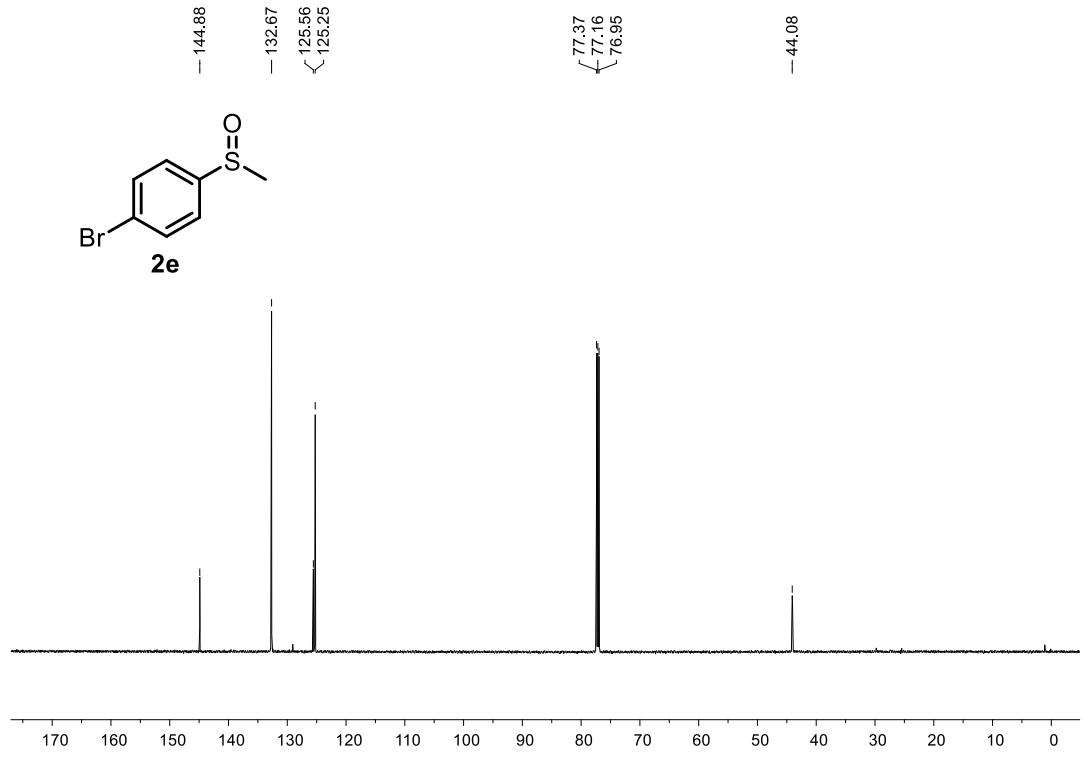
129.76
125.09
77.37
77.16
76.95
44.04
Cl
S
O
2d
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10


7.66
7.66
7.65
7.65
7.52
7.52
7.51
7.51
7.50
7.26
2.70
O
S
Br
2e
1.95
2.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0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132.67
125.56
125.25
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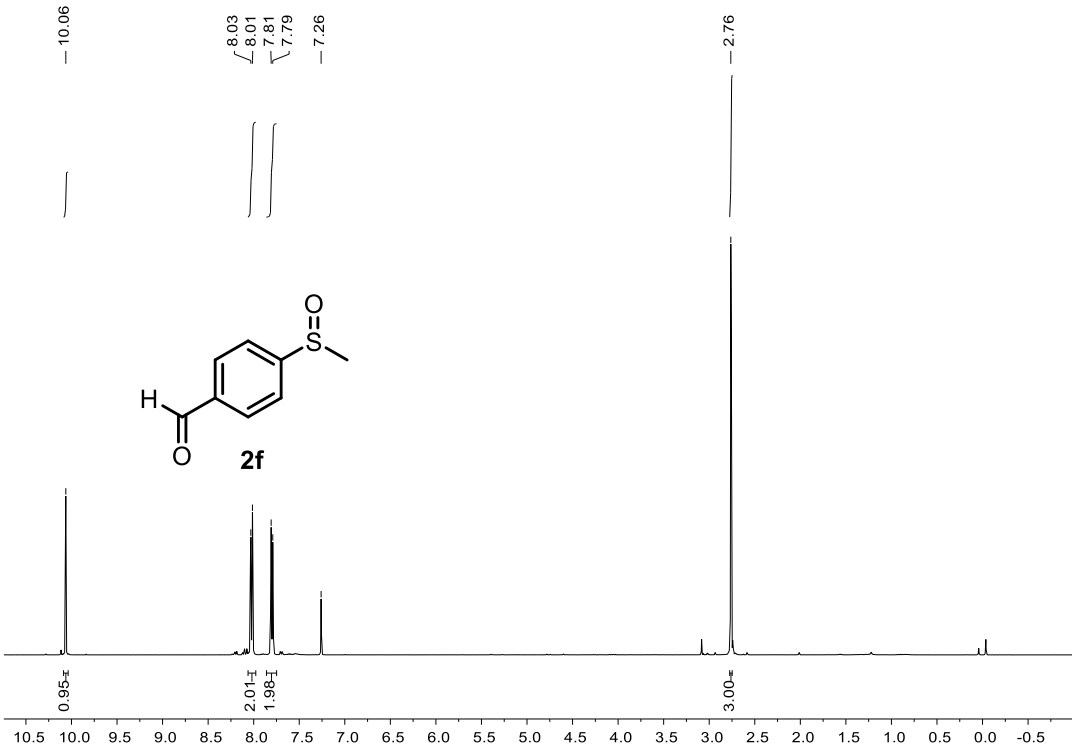
77.16
76.95
44.08
O
S
Br
2e
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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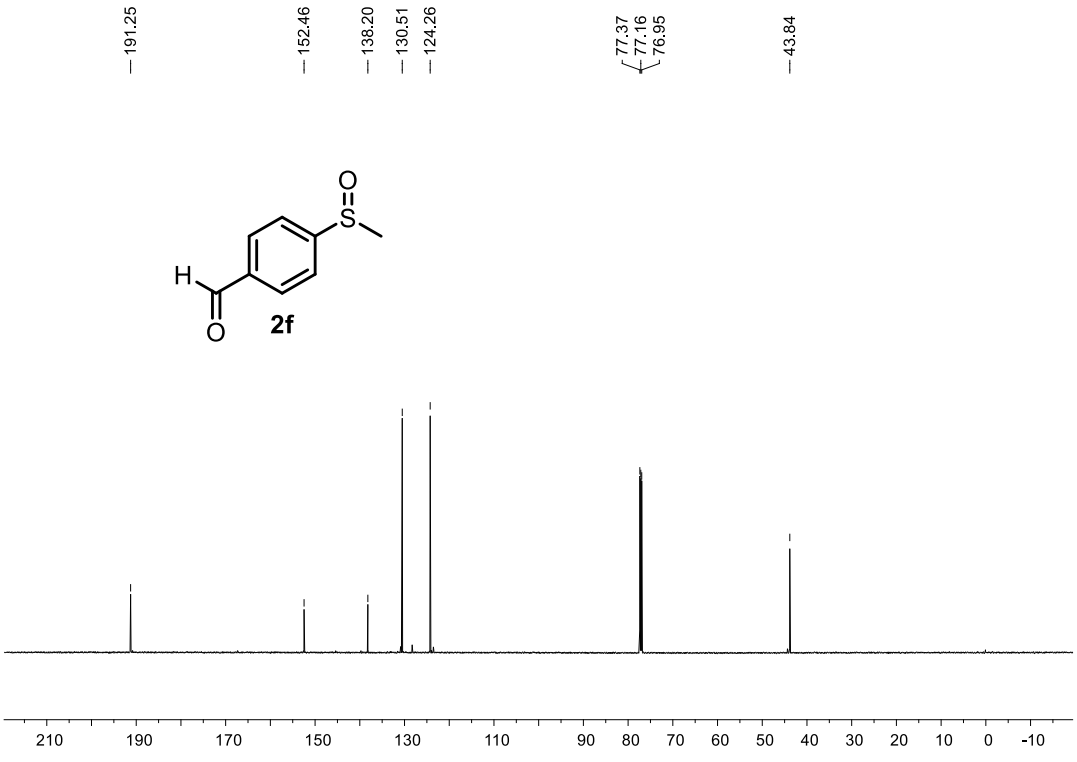
8.03
8.01
7.81
7.79
7.26
2.76
0.95
2.01
1.98
3.00
2f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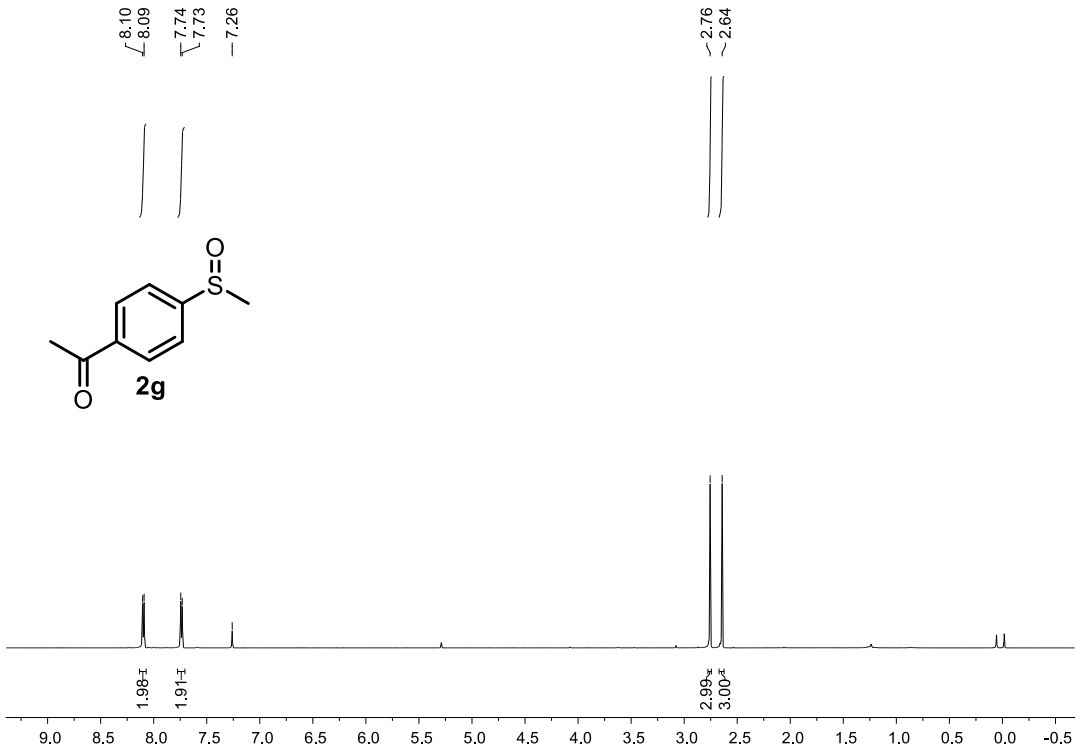
77.37
77.16
76.95
43.84
2f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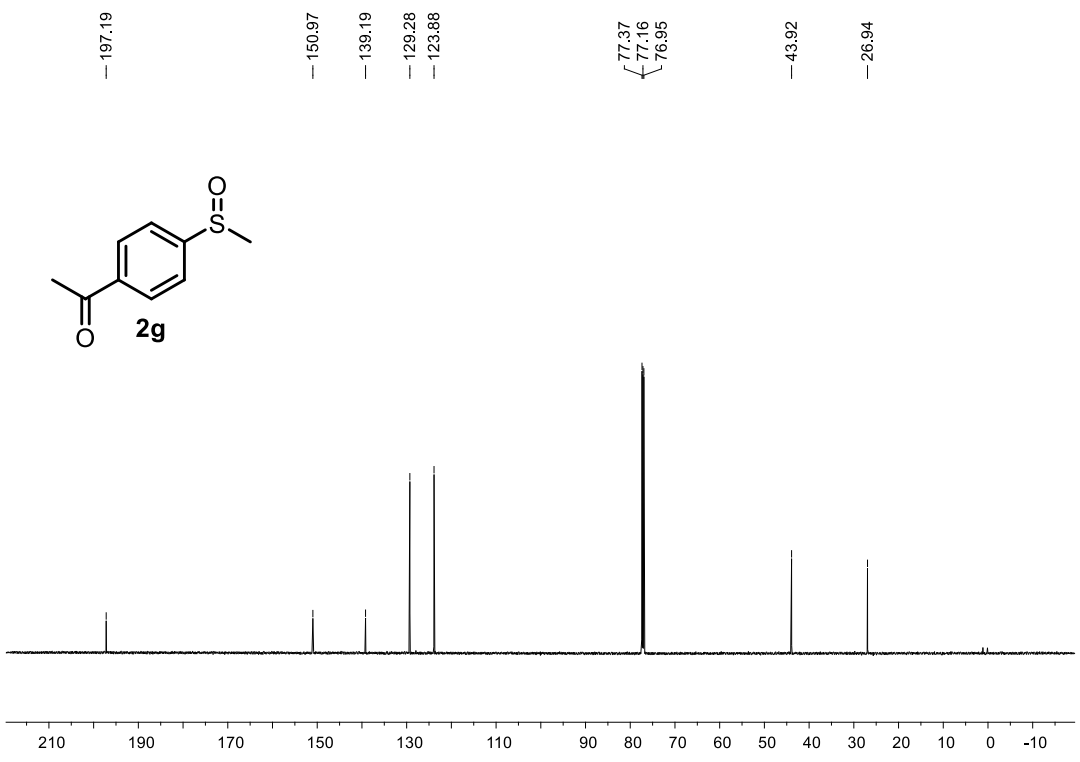
8.09
7.74
7.73
7.26
2.76
2.64
2g
1.98
1.91
2.99
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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77.16
76.95
43.92
26.94
2g
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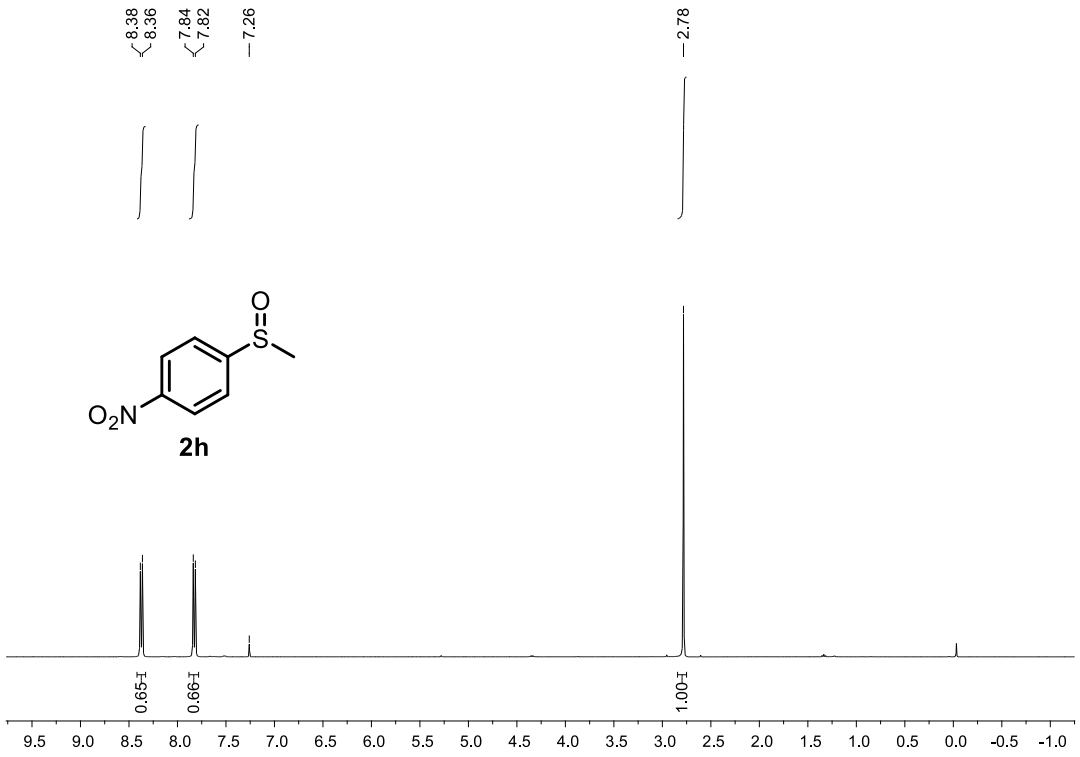
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7.82
7.26
2.78
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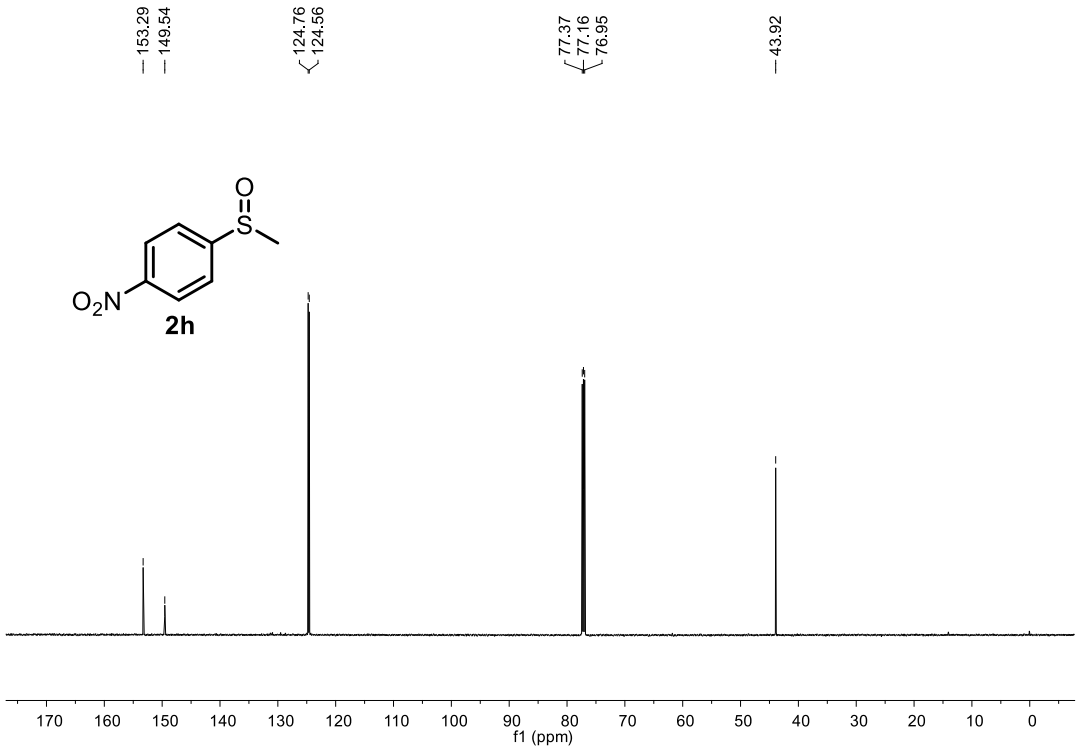
S
O2N
2h
0.65
0.66
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0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124.56
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43.92
O
S
O2N
2h
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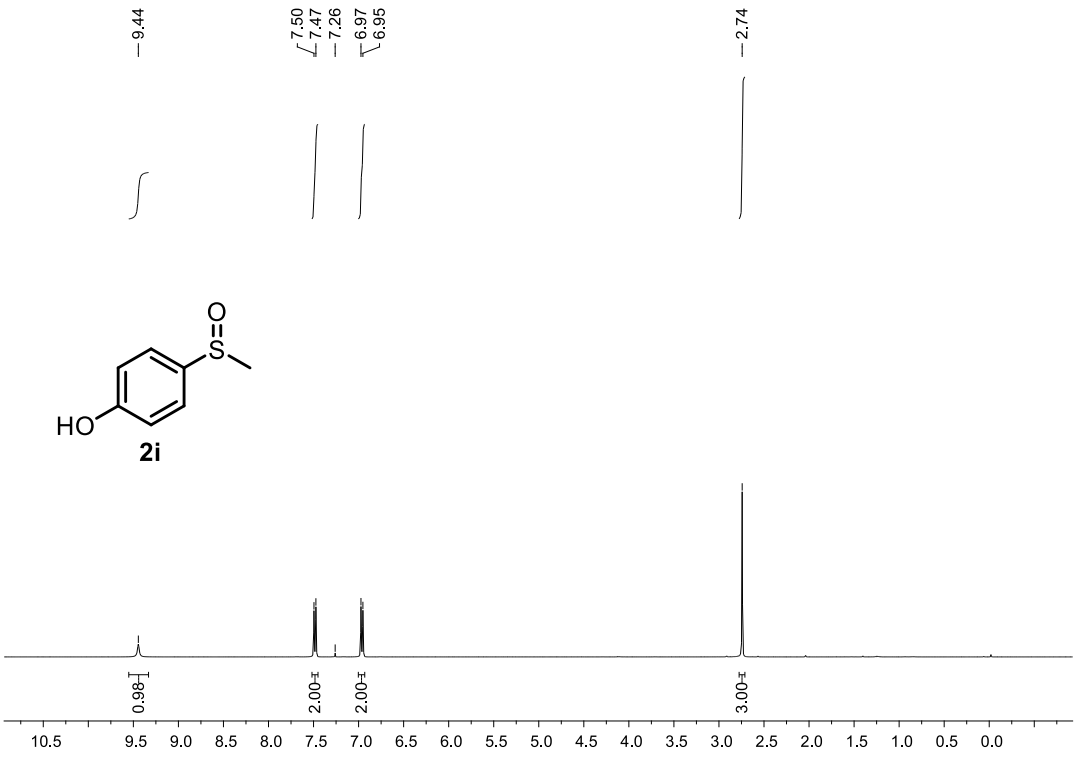
f1 (ppm)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6.95
2.74
HO
2i
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2.00
2.00
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.0
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3.0
2.5
2.0
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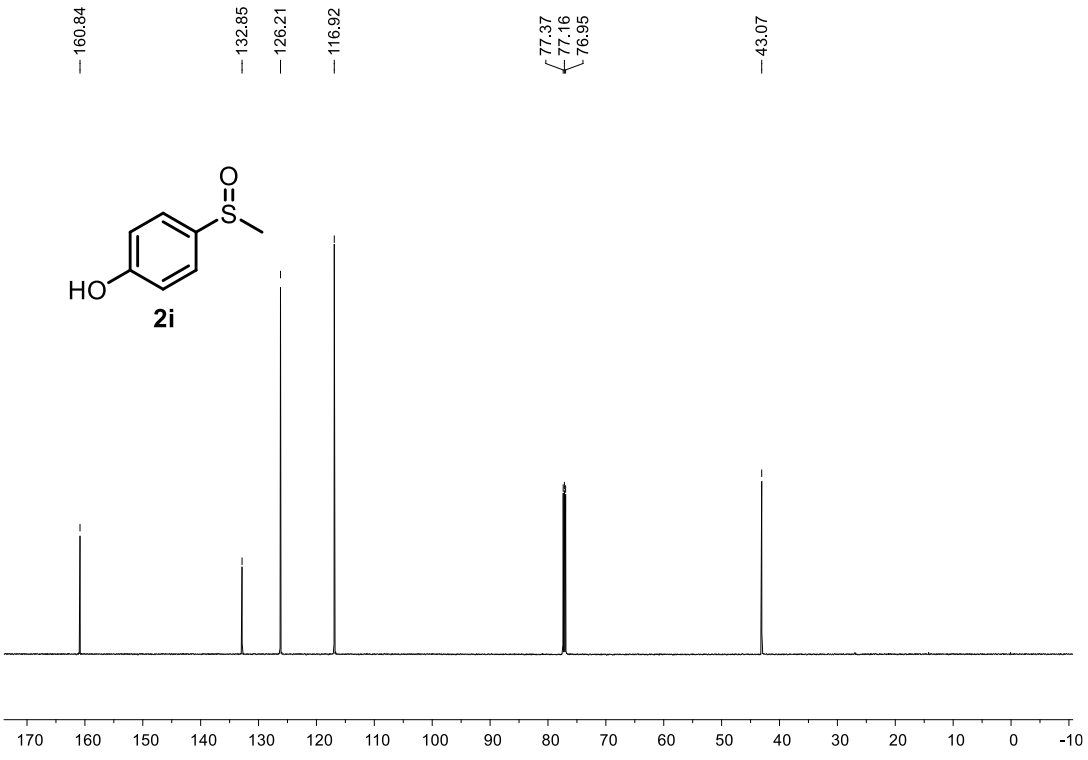
1.0
0.5
0.0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77.16
76.95
43.07
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2i
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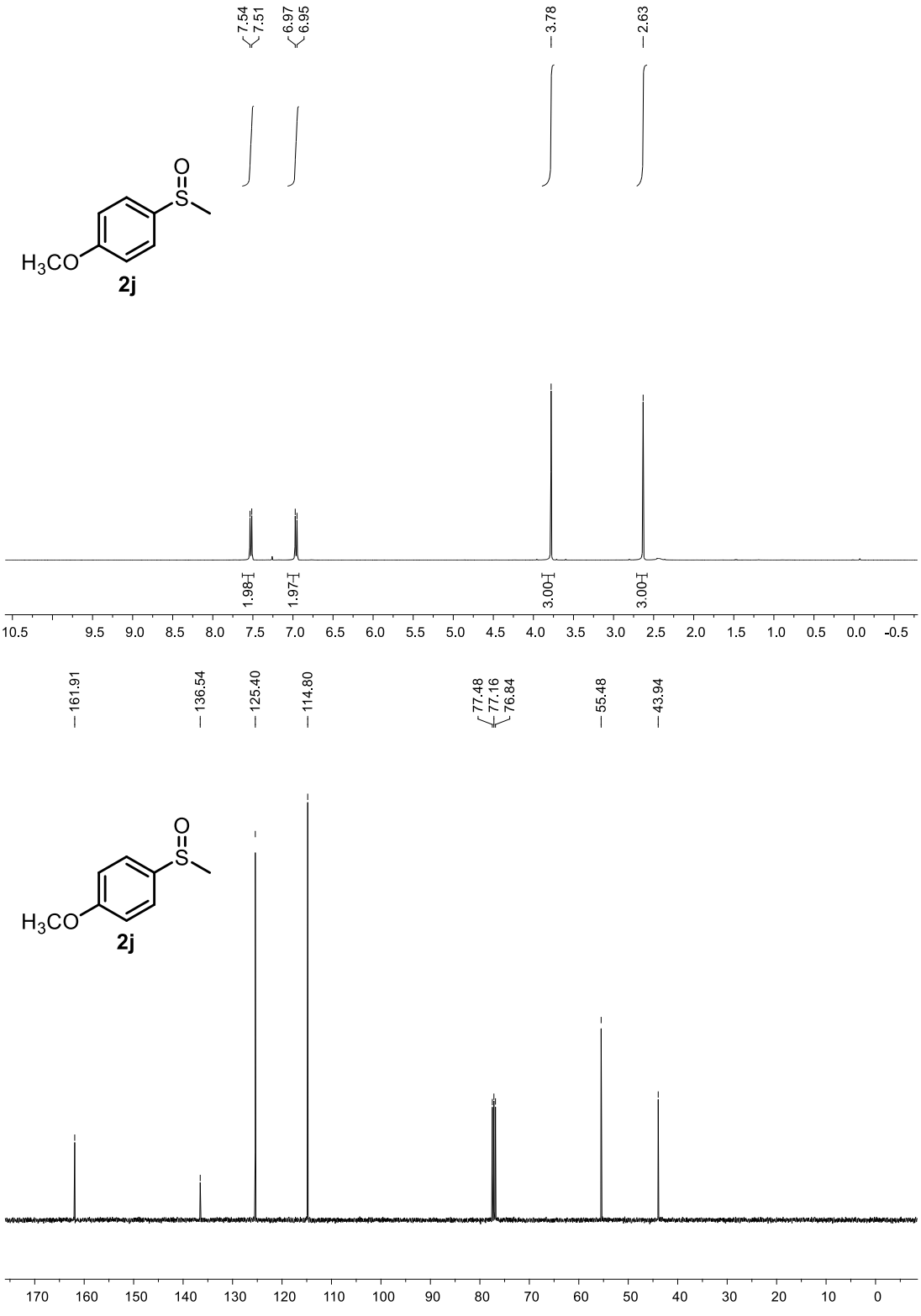
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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O
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H3CO
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1.97
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3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
161.91
136.54
125.40
114.80
77.48
77.16
76.84
55.48
43.94
O
S
H3CO
2j
170
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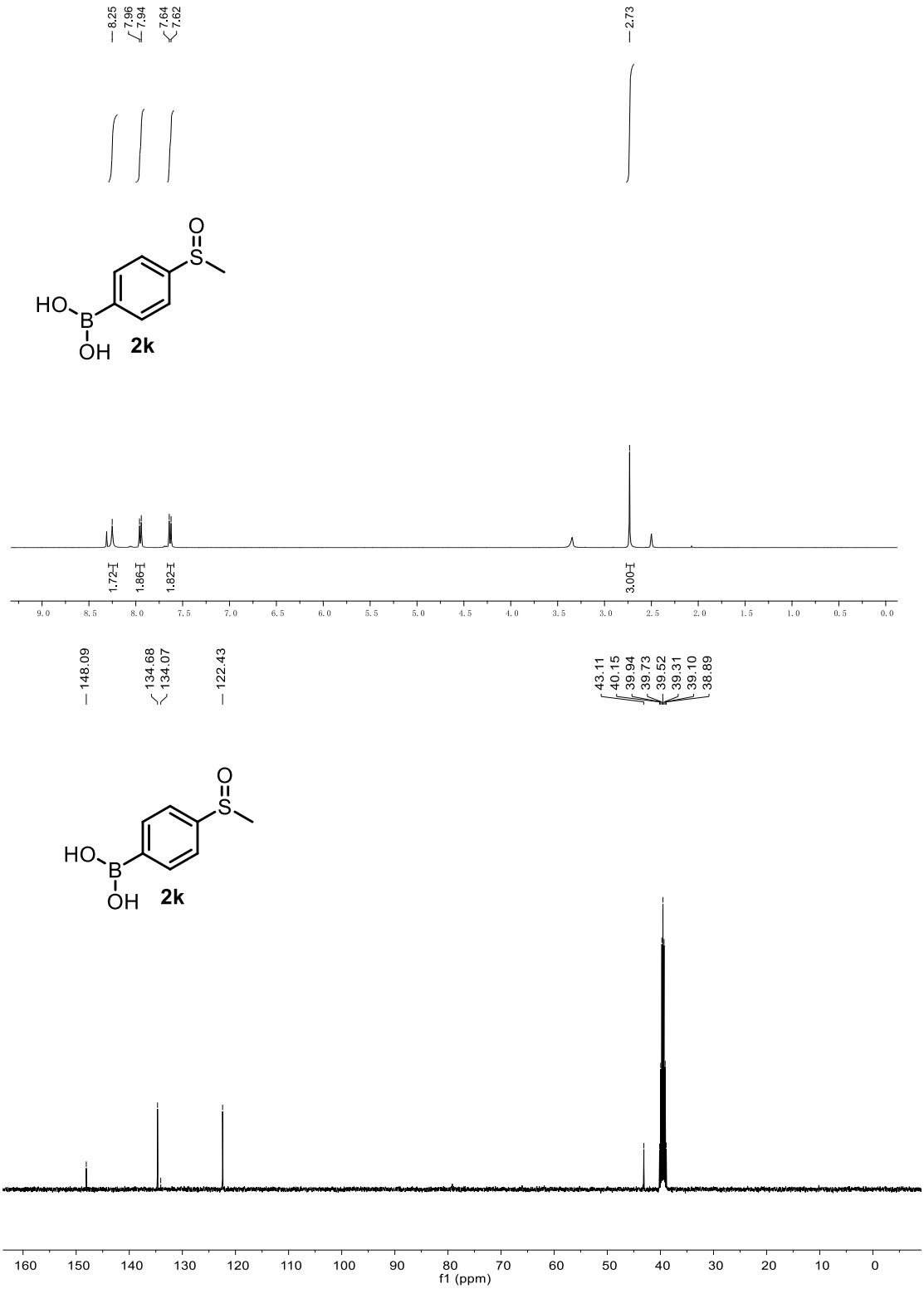
90
80
70
60
50
40
30
20
10
0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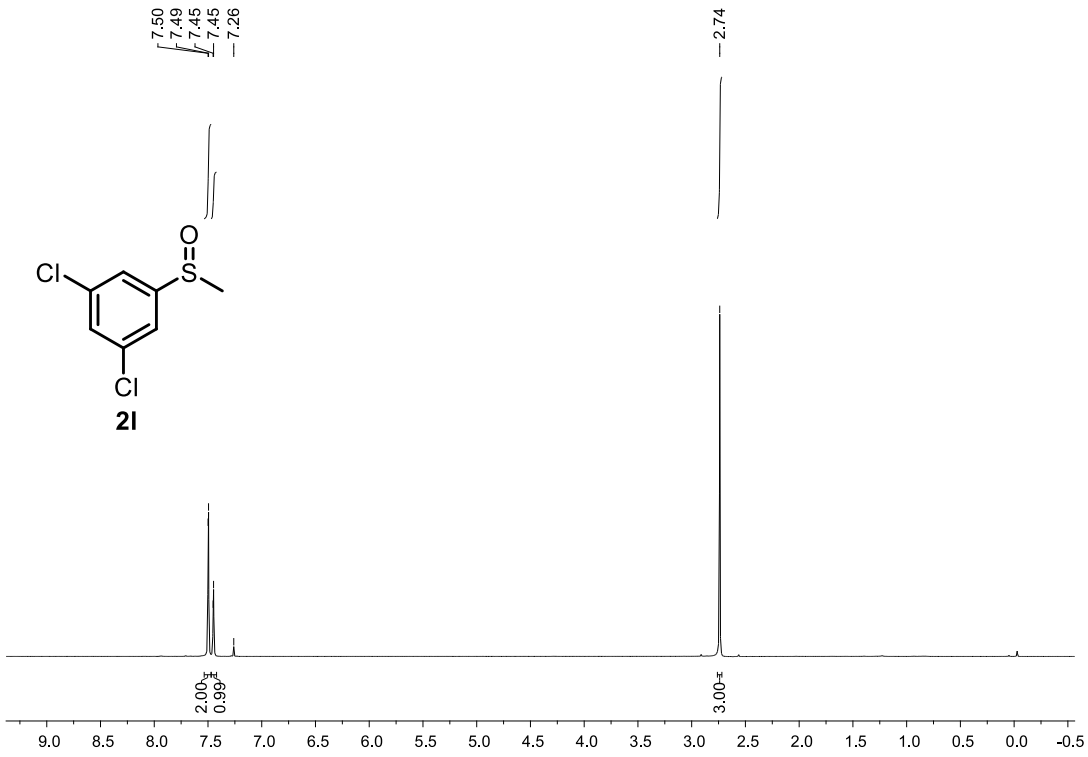
134.68
134.07
122.43
43.11
40.15
39.94
39.73
39.52
39.31
39.10
38.89
f1 (ppm)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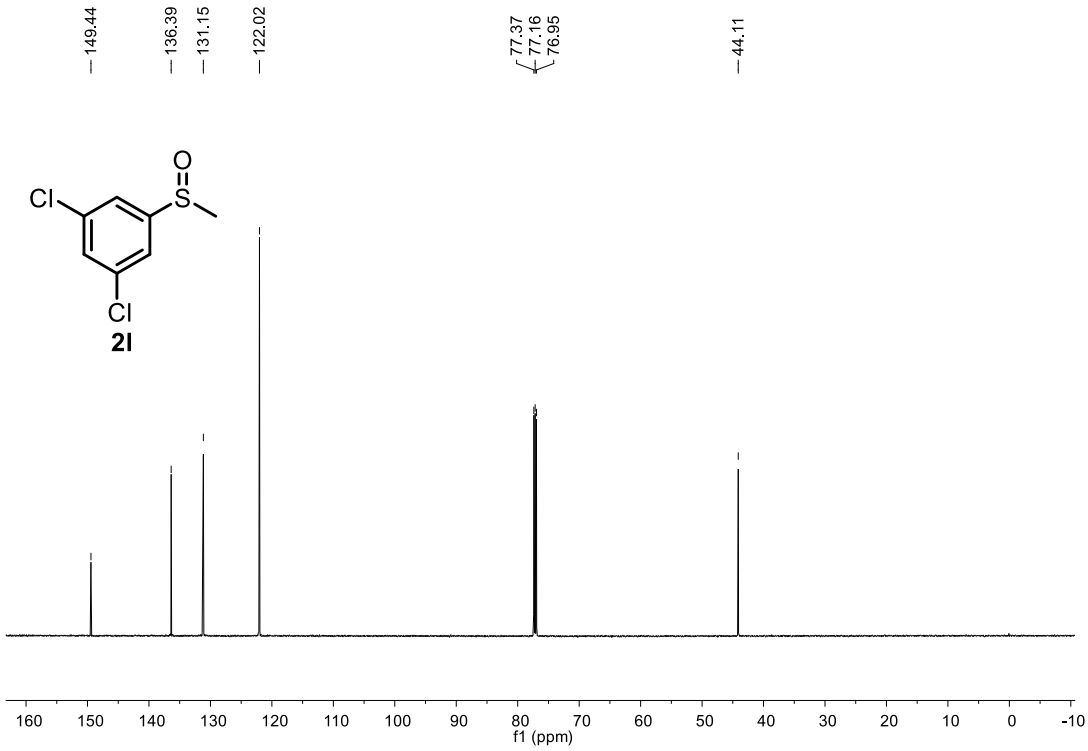
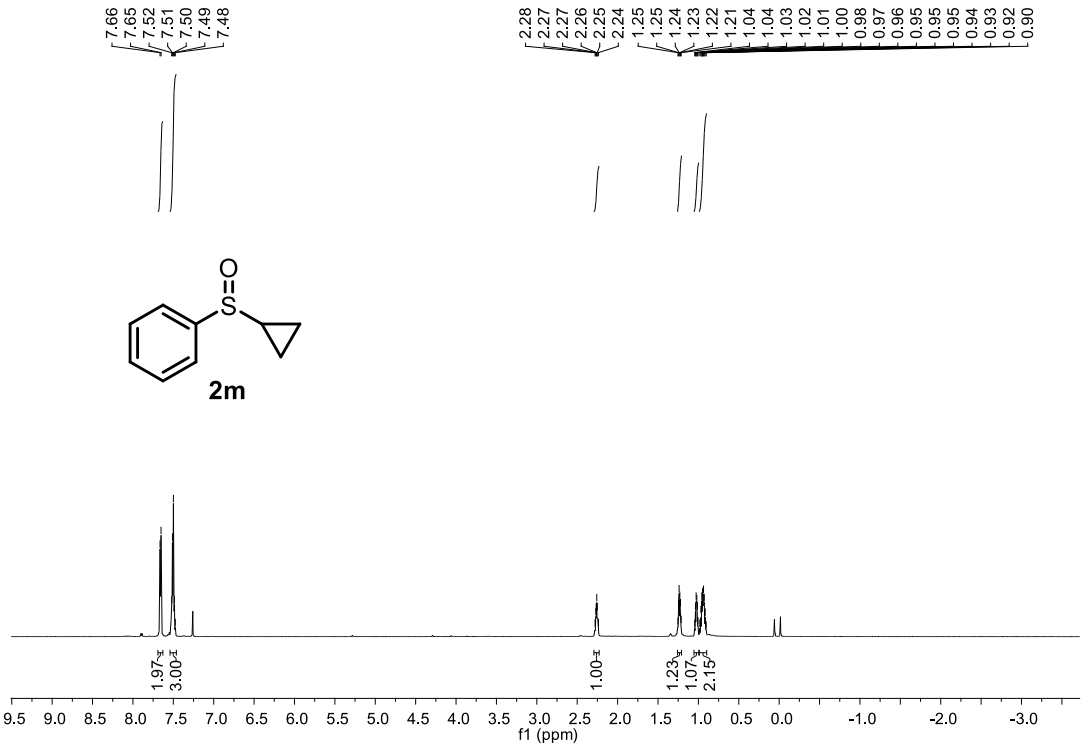
7.49
7.45
7.45
7.26
2.74
Cl
O
S
Cl
2l
2.00
0.99
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


149.44
136.39
131.15
122.02
77.37
77.16
76.95
44.11
Cl
O
S
Cl
2l
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.65
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7.51
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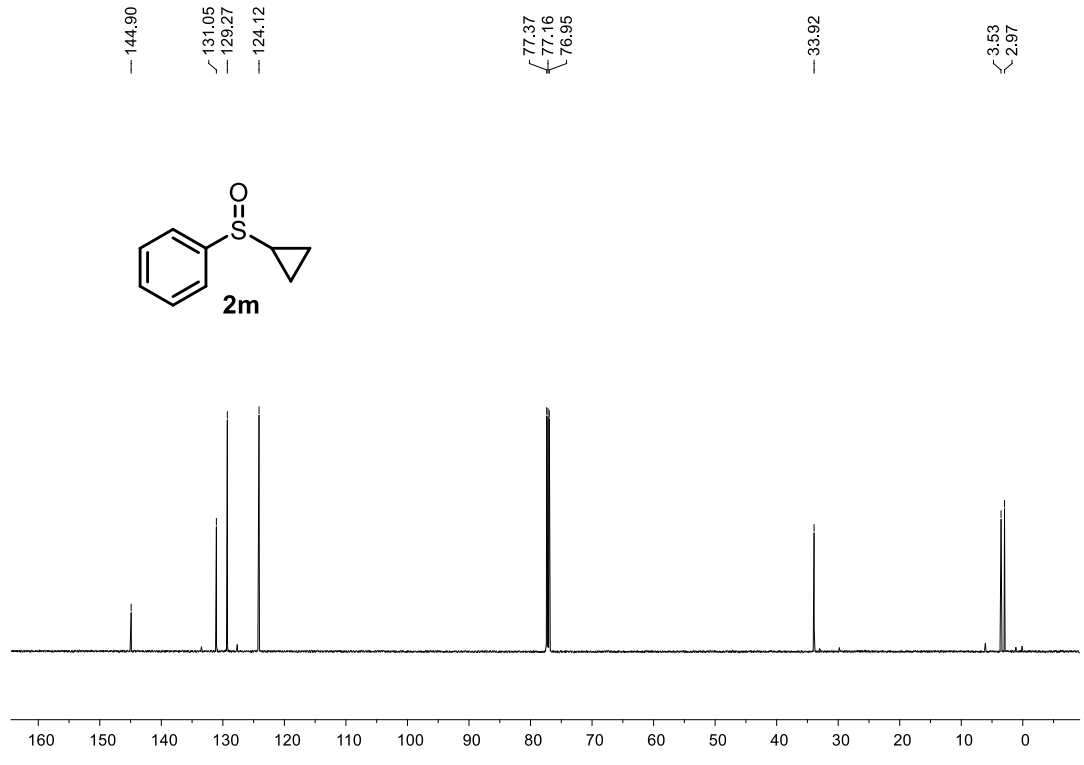
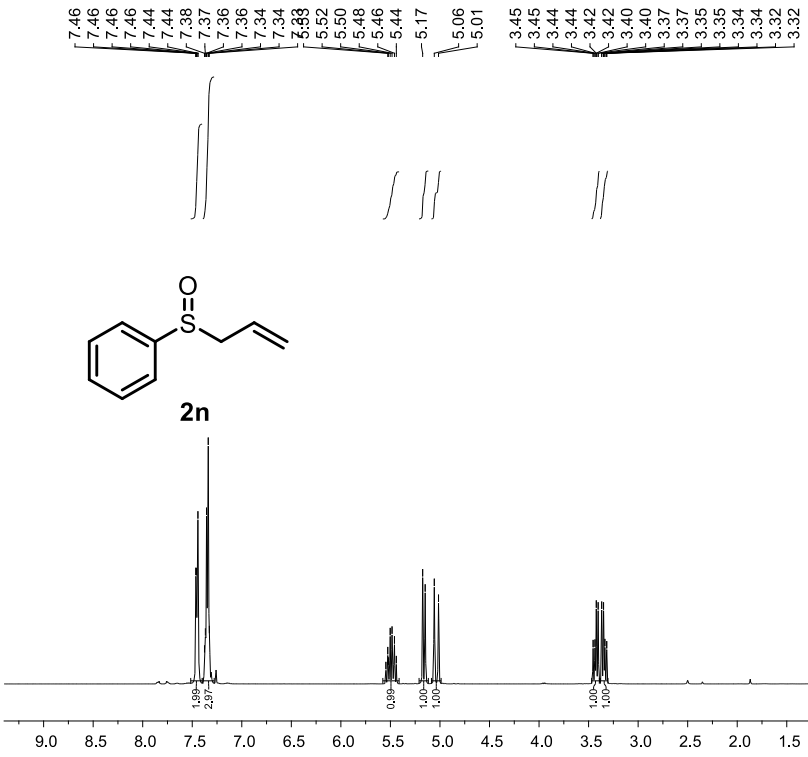
7.49
7.48
2.28
2.27
2.27
2.26
2.25
2.24
1.25
1.25
1.24
1.23
1.22
1.21
1.04
1.04
1.03
1.02
1.01
1.00
0.98
0.97
0.96
0.95
0.95
0.95
0.94
0.93
0.92
0.90
O
S
2m
1.97
3.00
1.00
1.23
1.07
2.15
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0 -2.0 -3.0
f1 (ppm)


144.90
131.05
129.27
124.12
77.37
77.16
76.95
33.92
3.53
2.97
O
S
2m
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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7.46
7.46
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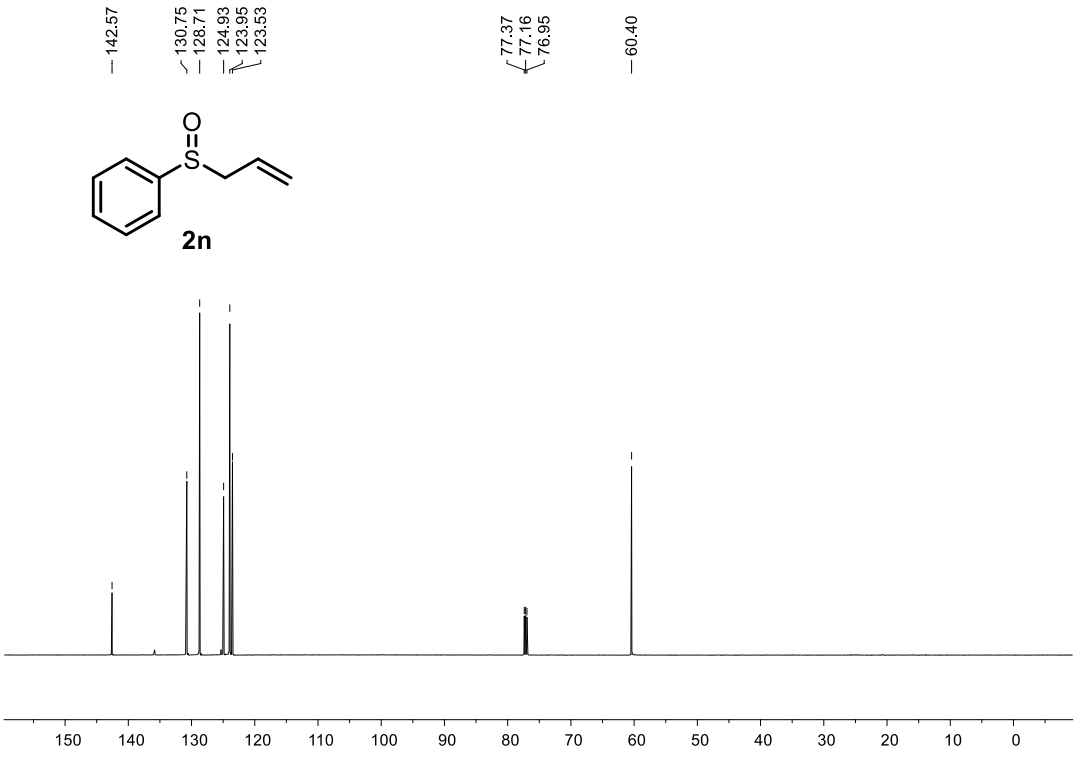
7.44
7.44
7.38
7.37
7.36
7.36
7.34
7.34
5.52
5.50
5.48
5.46
5.44
5.17
5.06
5.01
3.45
3.45
3.44
3.44
3.42
3.42
3.40
3.40
3.37
3.37
3.35
3.35
3.34
3.34
3.32
3.32
O
S
2n
1.99
2.97
0.99
1.00
1.00
1.00
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0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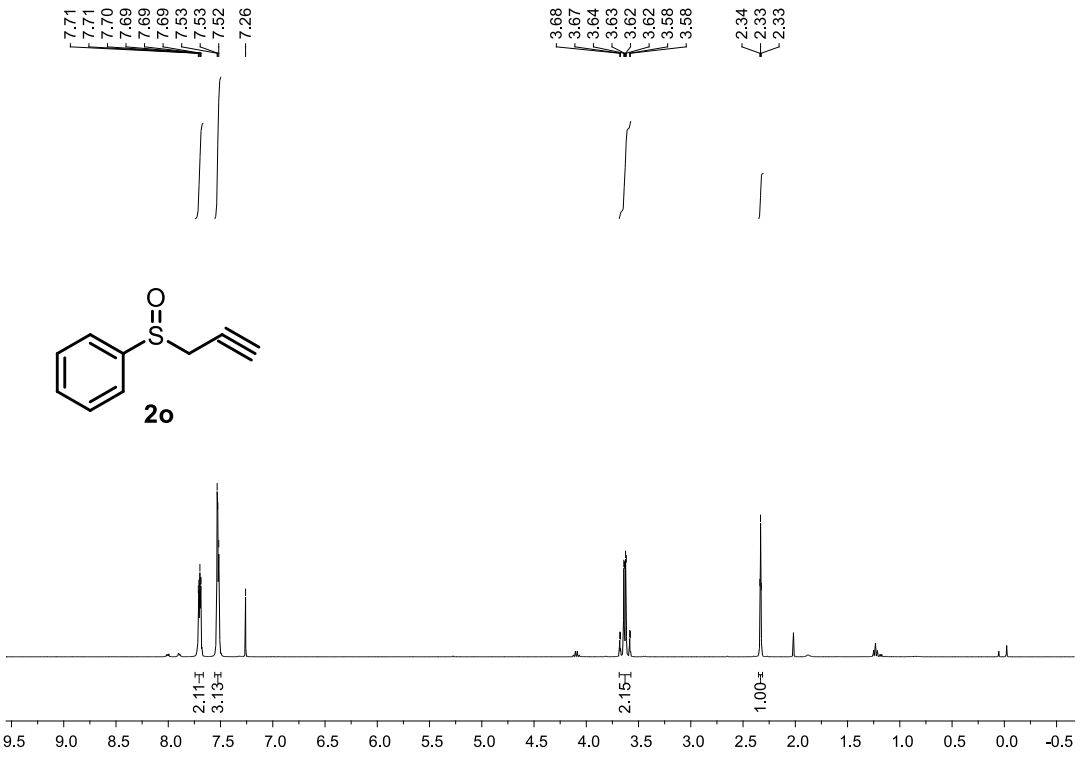
130.75
128.71
124.93
123.95
123.53
77.37
77.16
76.95
60.40
O
S
2n
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


7.71
7.71
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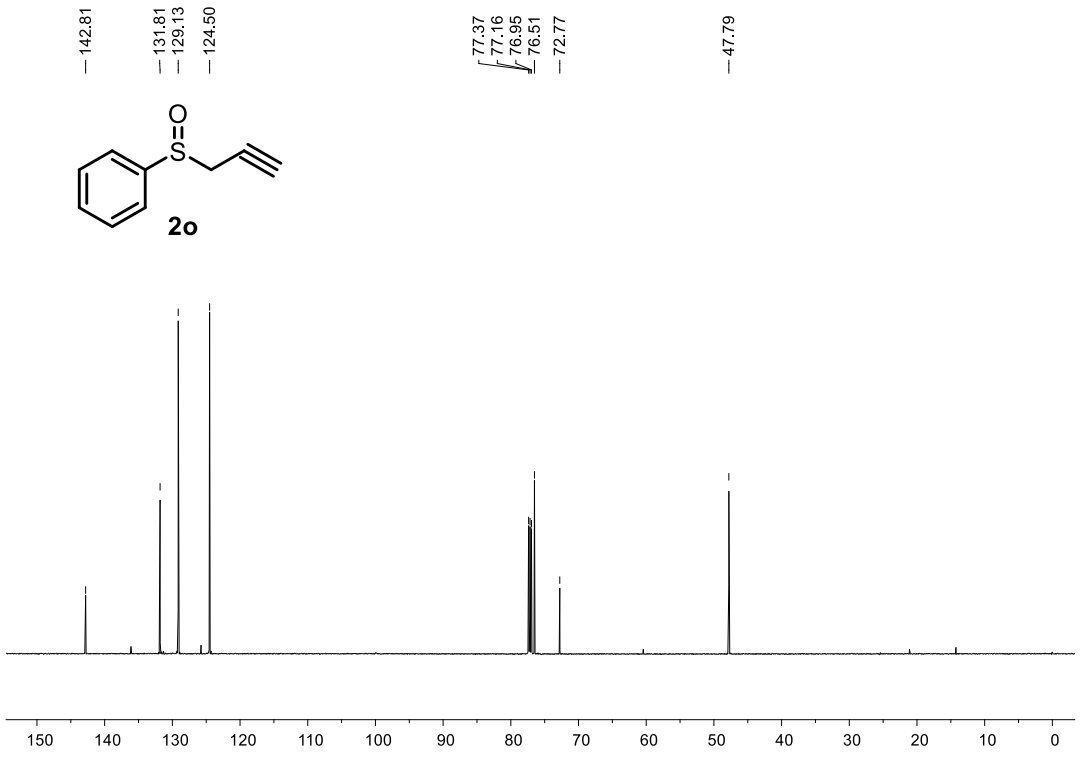
7.69
7.53
7.53
7.52
7.26
3.68
3.67
3.64
3.63
3.62
3.62
3.58
3.58
2.34
2.33
2.33
O
S
2o
2.11
3.13
2.15
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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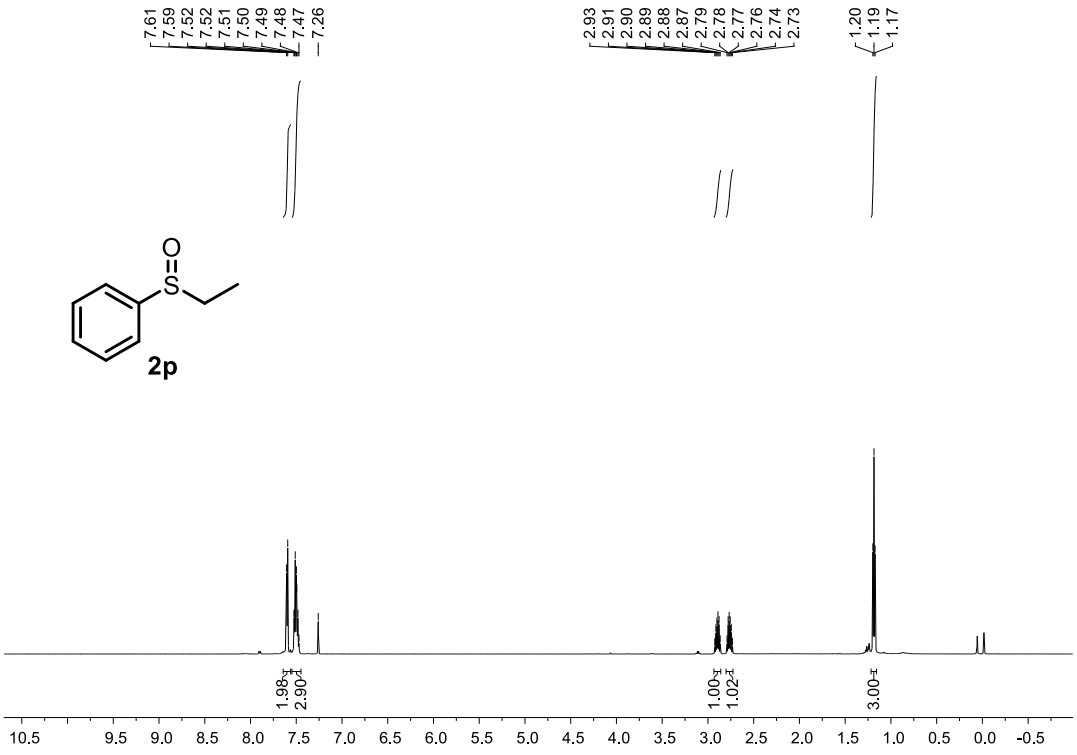
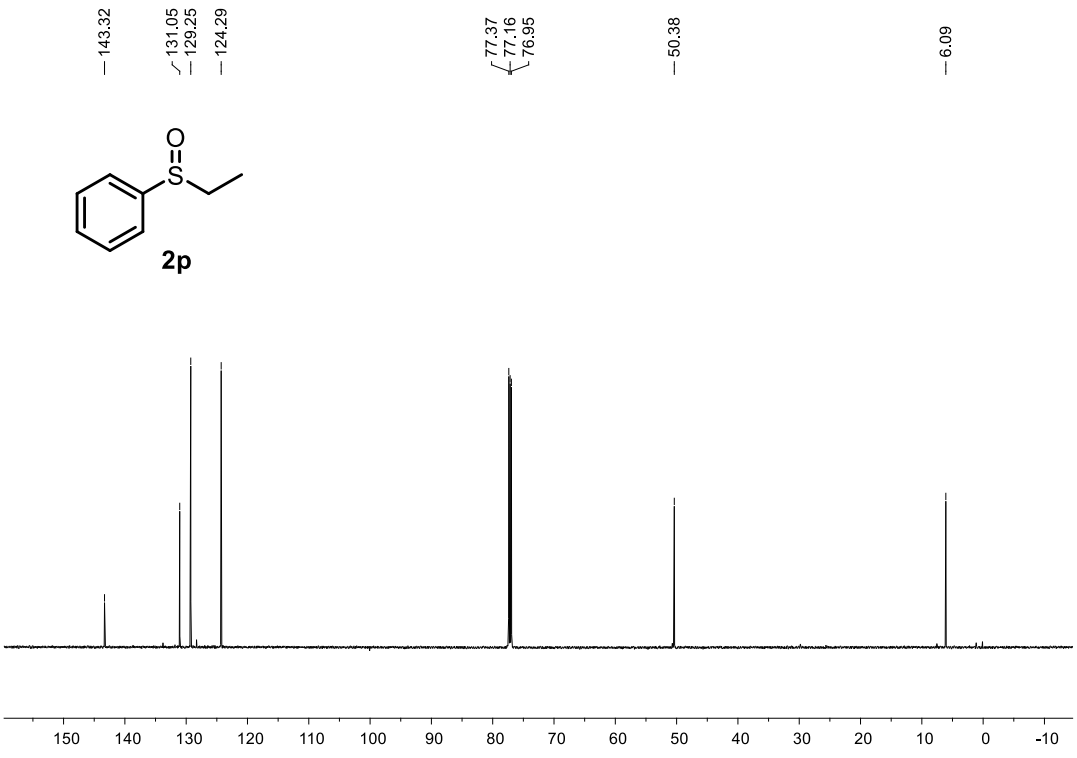
131.81
129.13
124.50
77.37
77.16
76.95
76.51
72.77
47.79
O
S
2o
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


7.61
7.59
7.52
7.52
7.51
7.50
7.49
7.48
7.47
7.26
2.93
2.91
2.90
2.89
2.88
2.87
2.79
2.78
2.77
2.76
2.74
2.73
1.20
1.19
1.17
O
S
2p
1.98
2.90
1.00
1.02
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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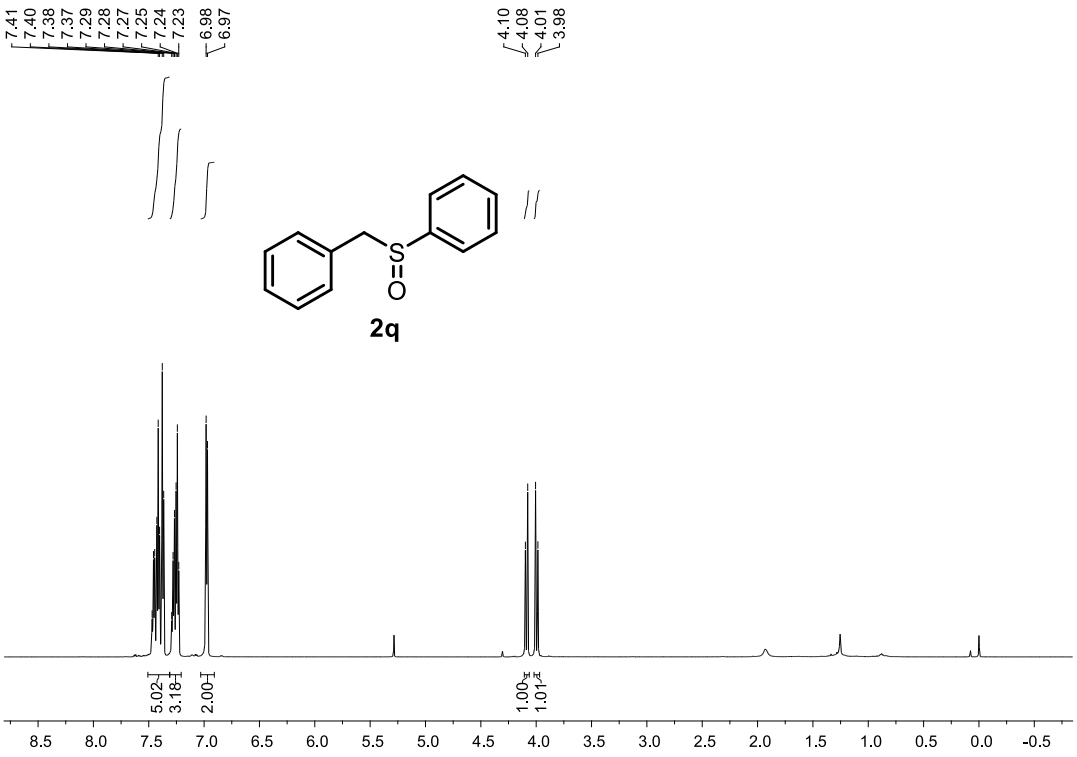
131.05
129.25
124.29
77.37
77.16
76.95
50.38
6.09
O
S
2p
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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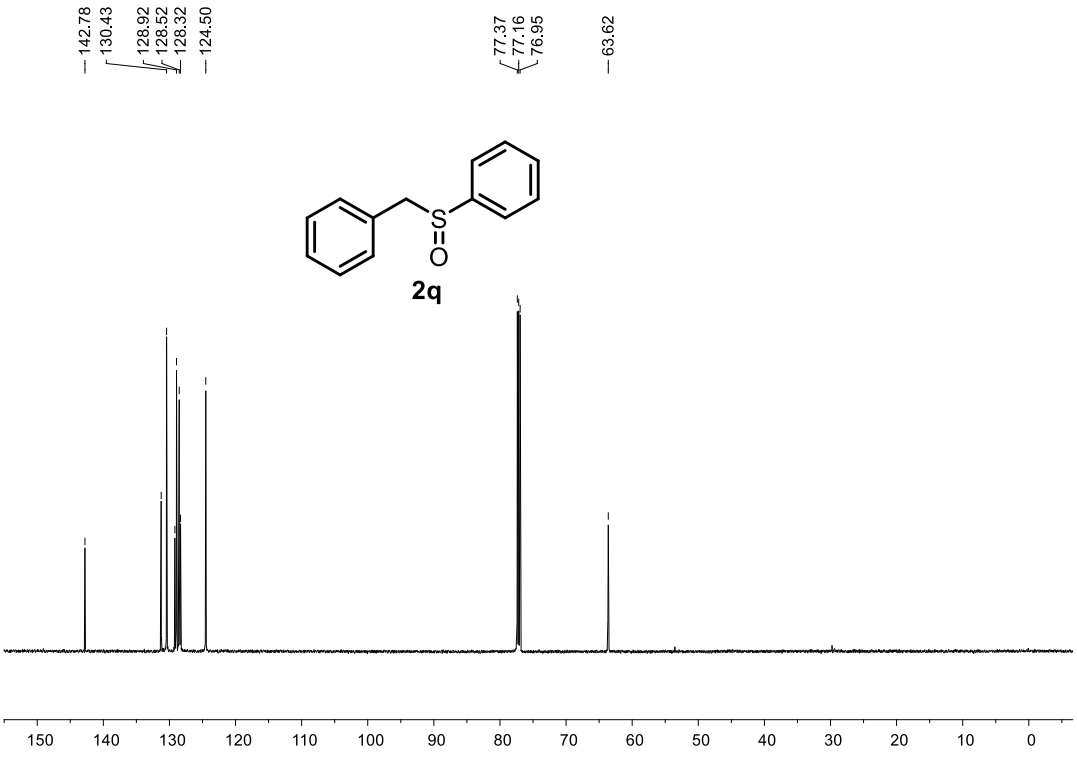
7.40
7.38
7.37
7.29
7.28
7.27
7.25
7.24
7.23
6.98
6.97
4.10
4.08
4.01
3.98
S
O
2q
5.02
3.18
2.00
1.00
1.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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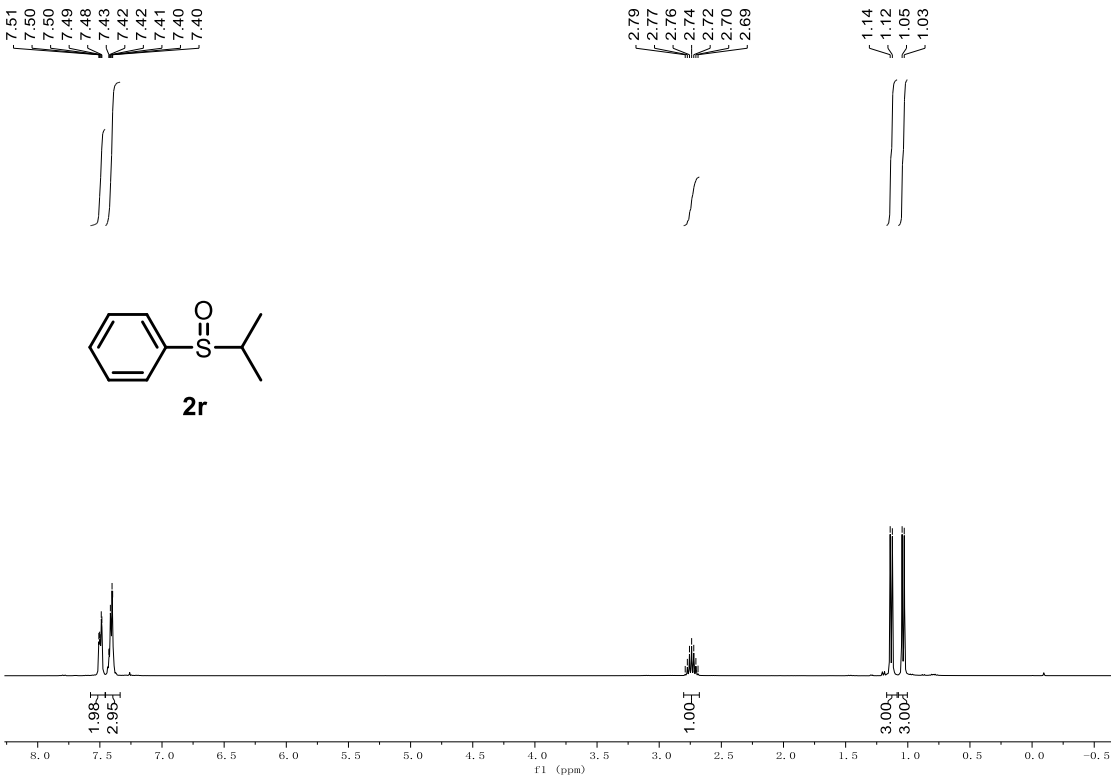
130.43
128.92
128.52
128.32
124.50
77.37
77.16
76.95
63.62
S
O
2q
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0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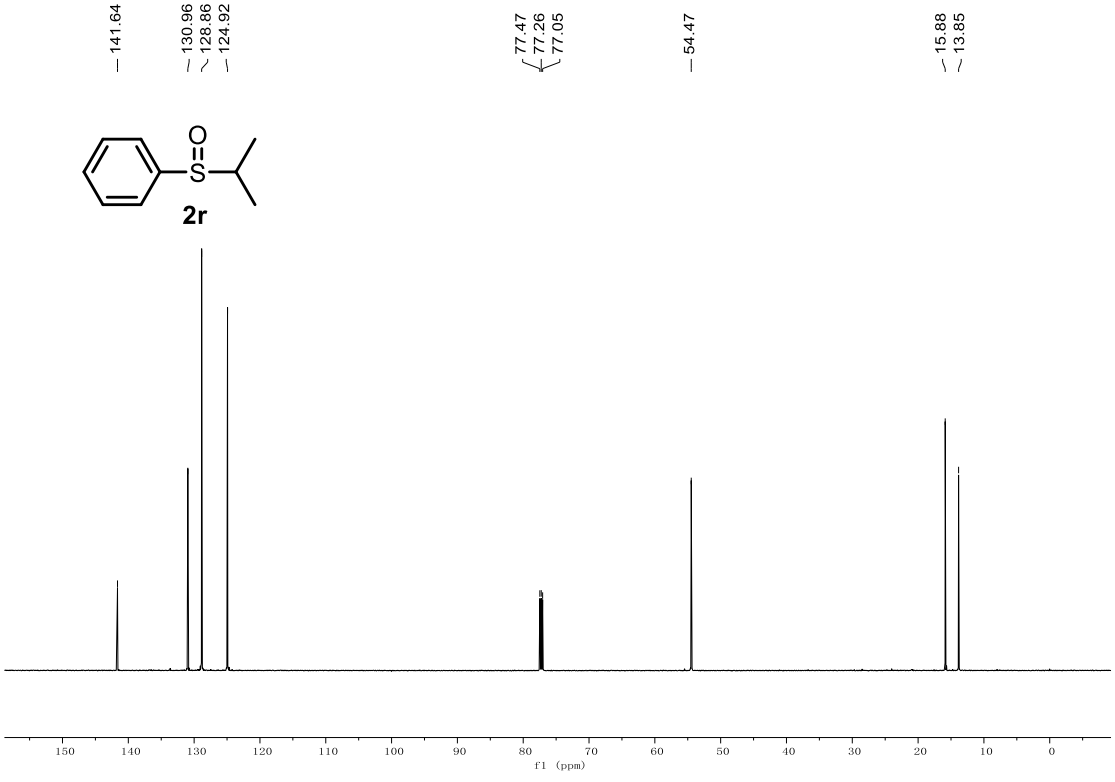
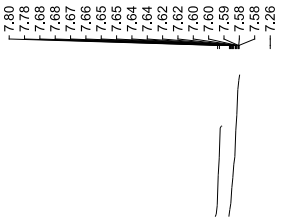
7.50
7.50
7.49
7.48
7.43
7.42
7.42
7.41
7.40
7.40
2.79
2.77
2.76
2.74
2.72
2.70
2.69
1.14
1.12
1.05
1.03
O
S
1.98
2.95
1.00
3.00
3.00
f1 (ppm)

2r


141.64
130.96
128.86
124.92
77.47
77.26
77.05
54.47
15.88
13.85
O
S
f1 (ppm)

2r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7.78
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7.68
7.67
7.66
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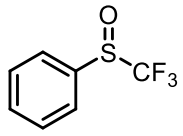
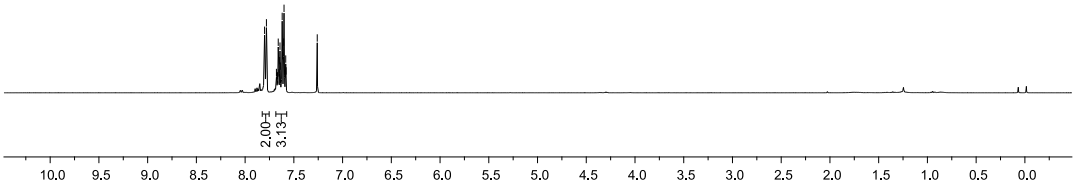
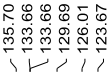
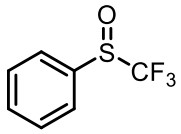
7.65
7.64
7.64
7.62
7.62
7.60
7.60
7.59
7.58
7.58
7.26


O
S
CF3

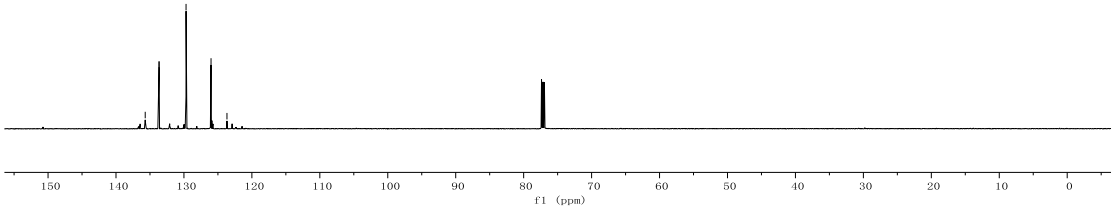
2s

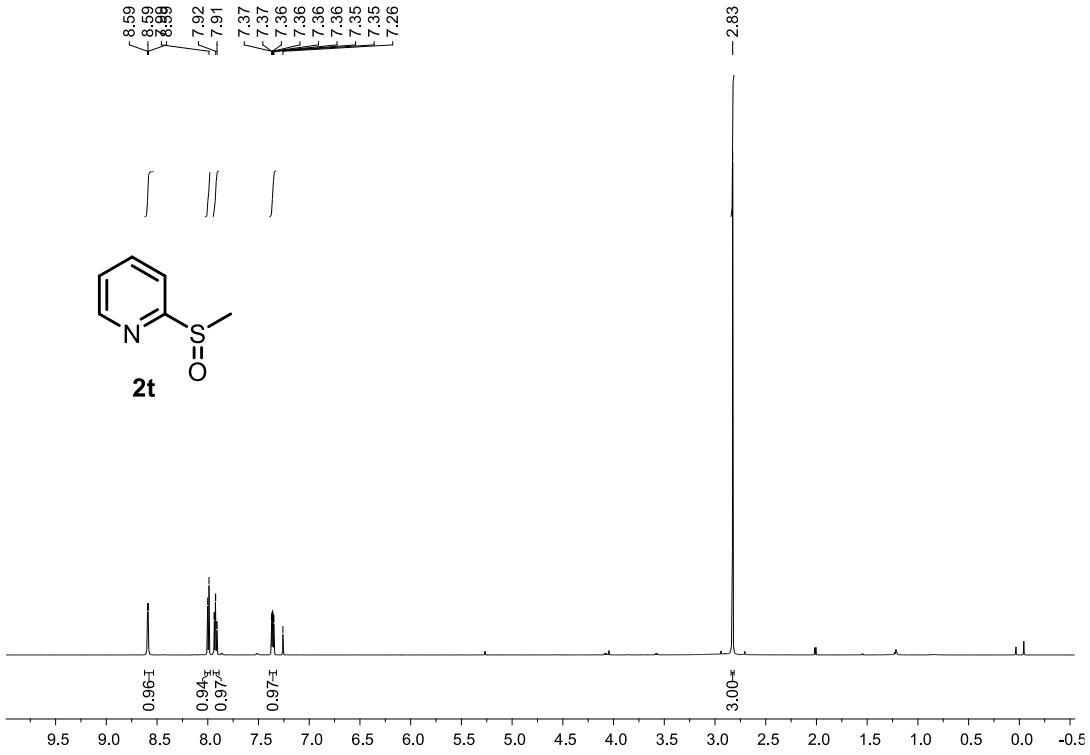

2.00
3.13
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


135.70
133.66
133.66
129.69
126.01
123.67

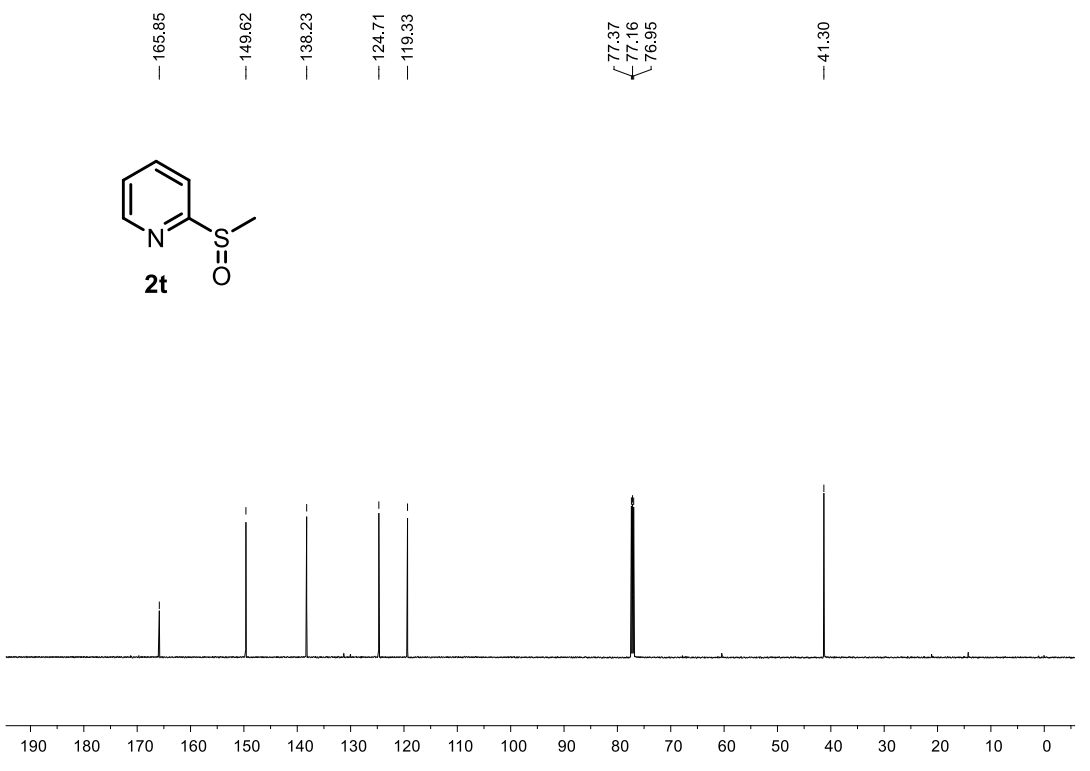

O
S
CF3

2s

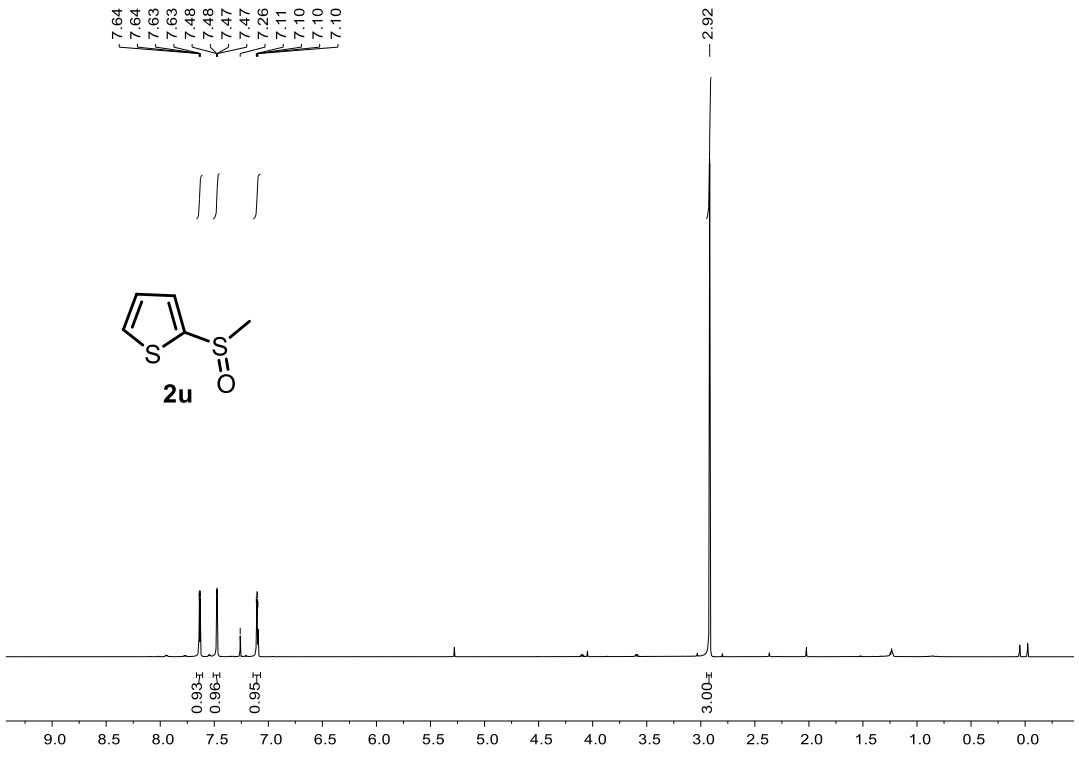

150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.59
8.59
7.92
7.91
7.37
7.37
7.36
7.36
7.36
7.36
7.35
7.35
7.26
2.83
0.96
0.94
0.97
0.97
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

2t


165.85
149.62
138.23
124.71
119.33
77.37
77.16
76.95
41.30
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

2t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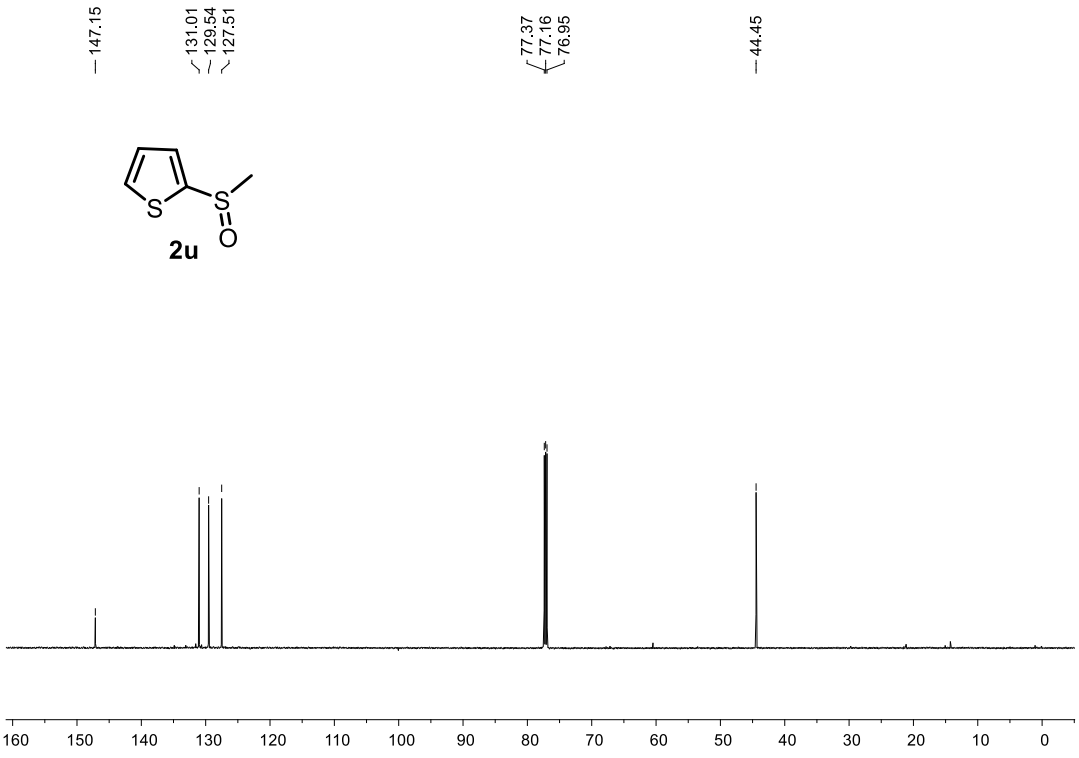
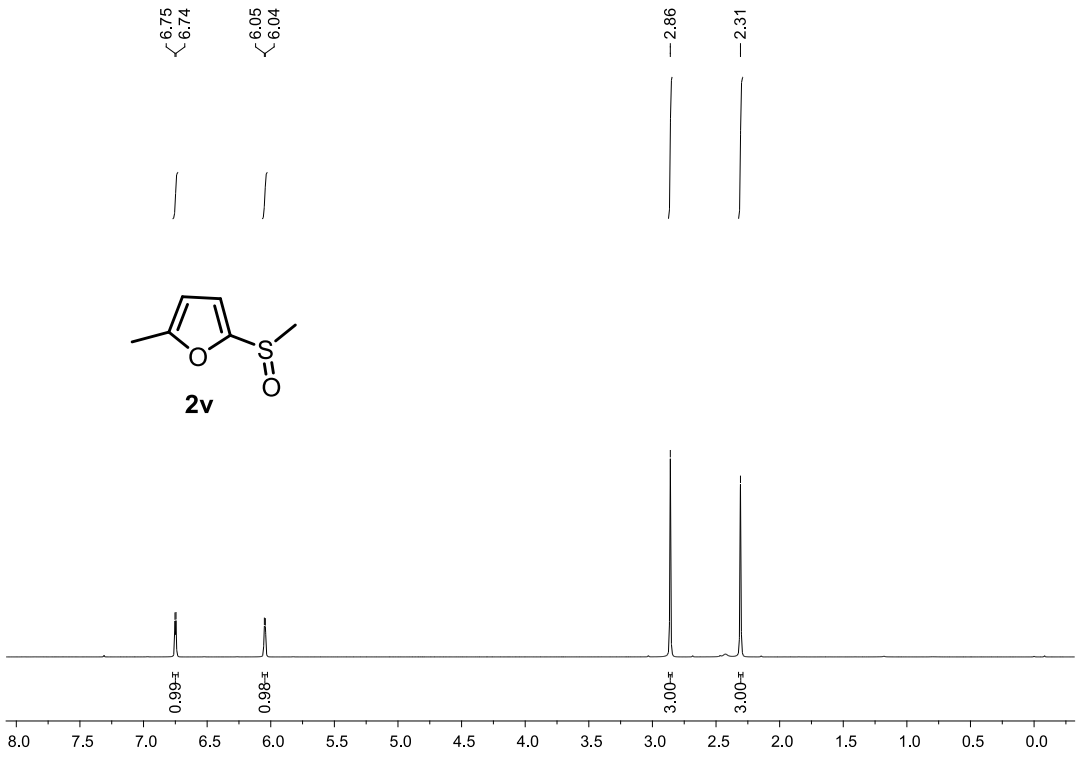
7.64
7.63
7.63
7.48
7.48
7.47
7.47
7.26
7.11
7.10
7.10
7.10
2.92
0.93
0.96
0.95
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

2u


147.15
131.01
129.54
127.51
77.37
77.16
76.95
44.45
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

2u


6.75
6.74
6.05
6.04
2.86
2.31
2v
0.99
0.98
3.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
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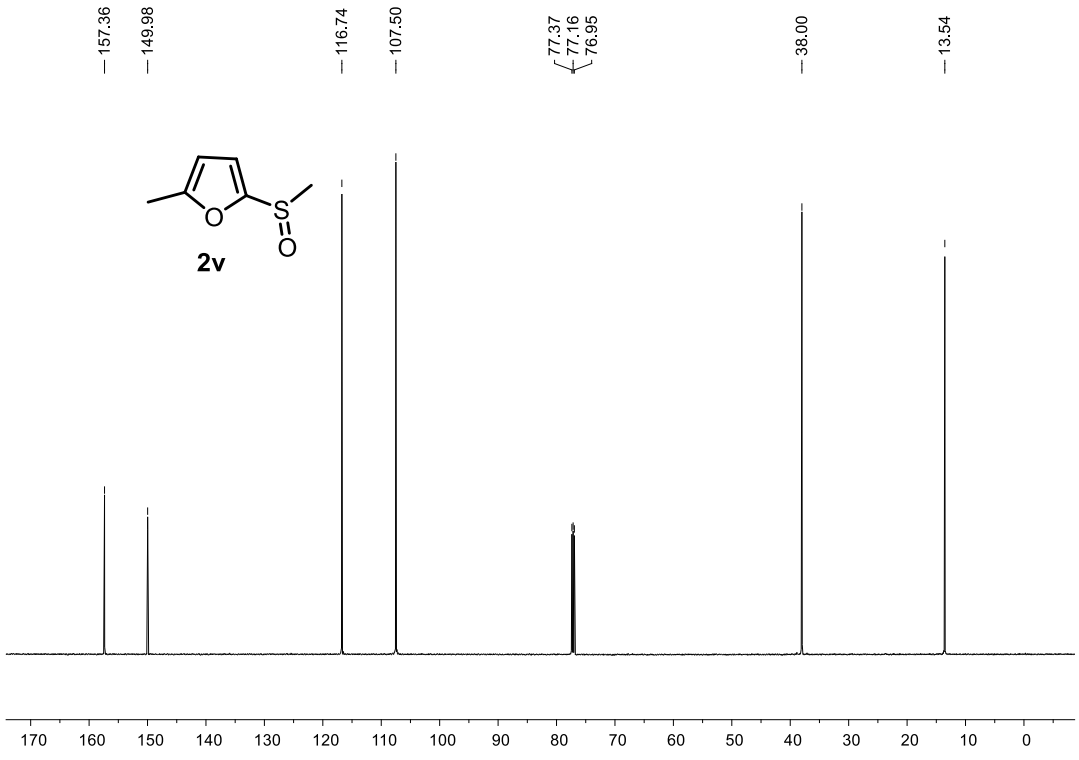
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


157.36
149.98
116.74
107.50
77.37
77.16
76.95
38.00
13.54
2v
170
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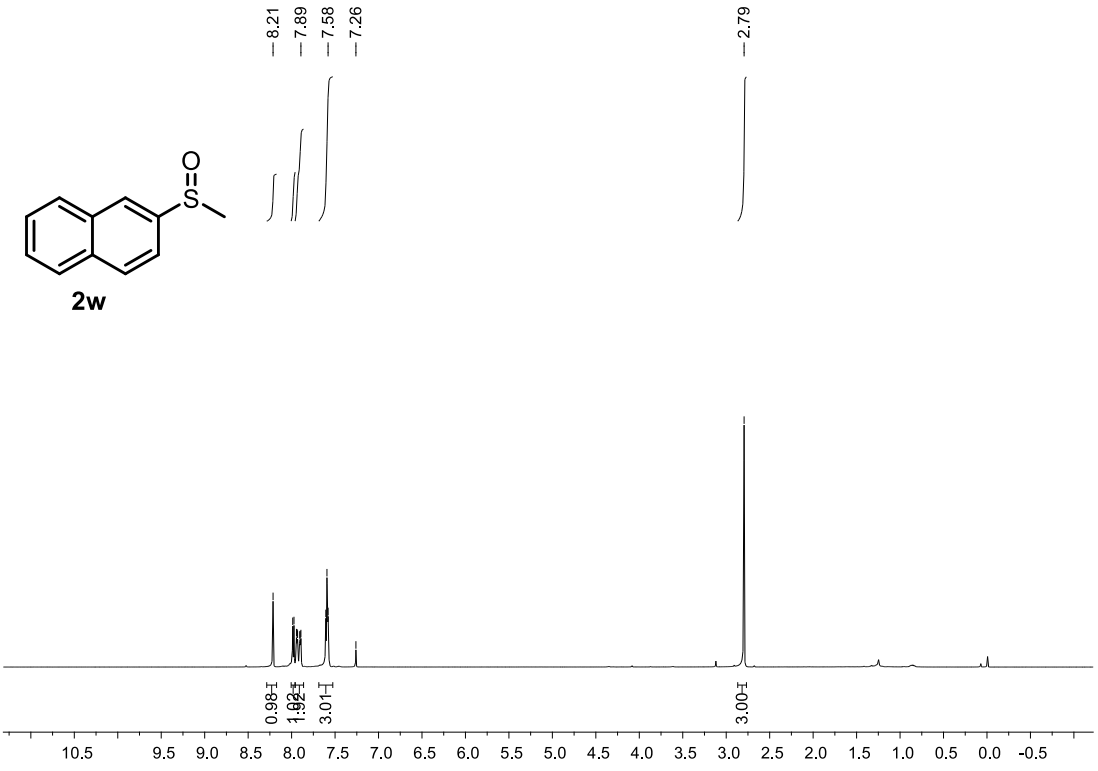
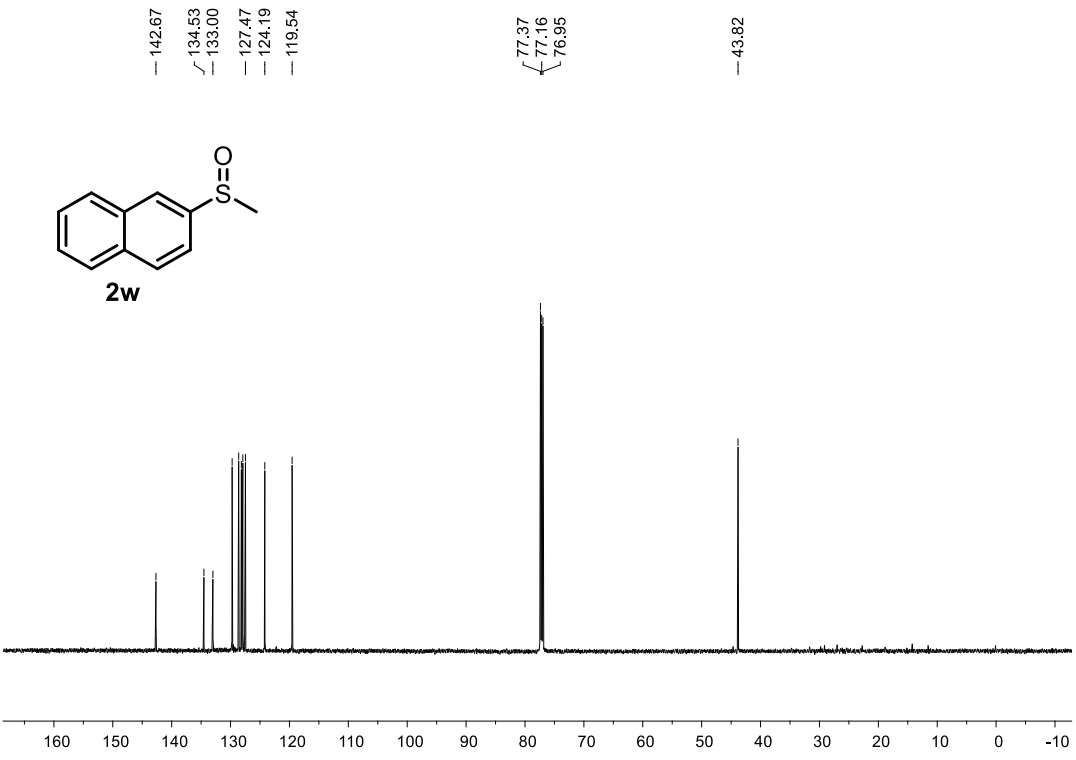
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


8.21
7.89
7.58
7.26
2.79
O
S
2w
0.98
1.92
1.92
3.01
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5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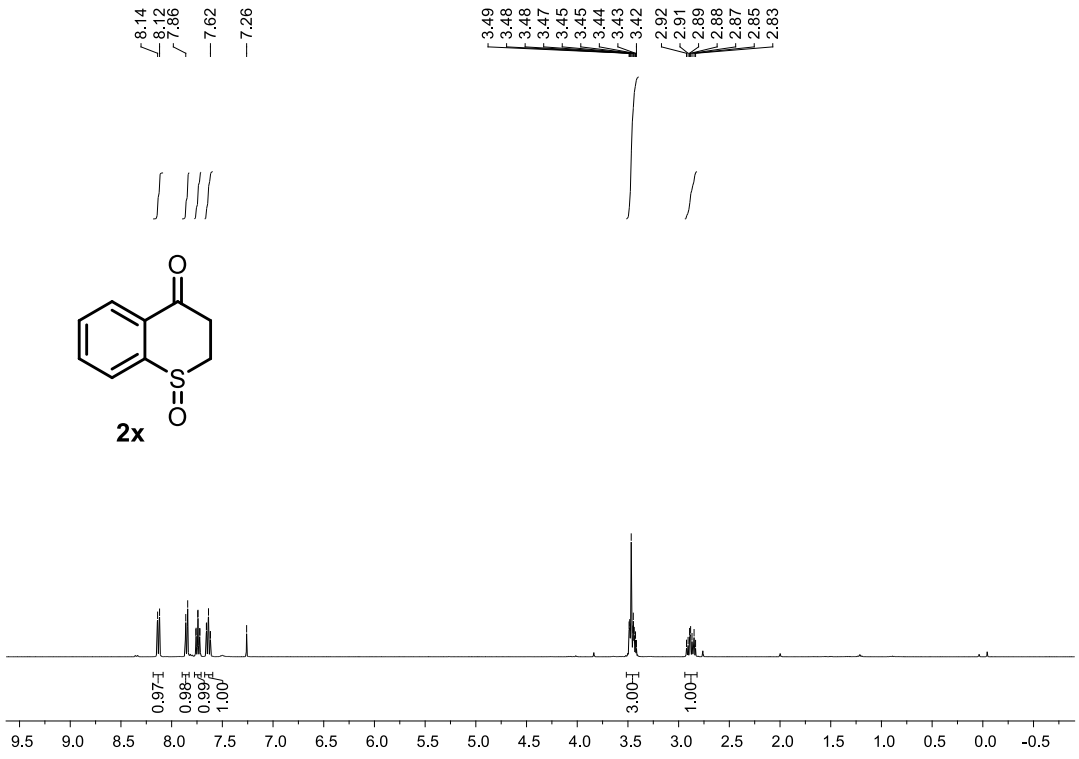
133.00
127.47
124.19
119.54
77.37
77.16
76.95
43.82
O
S
2w
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10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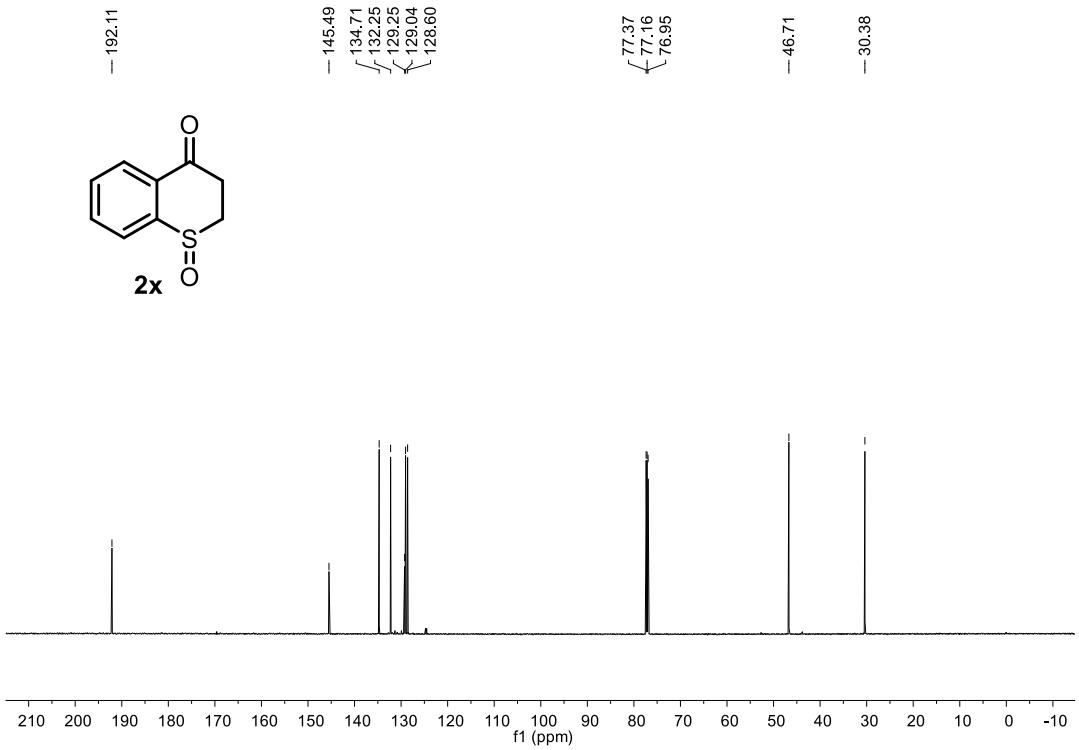
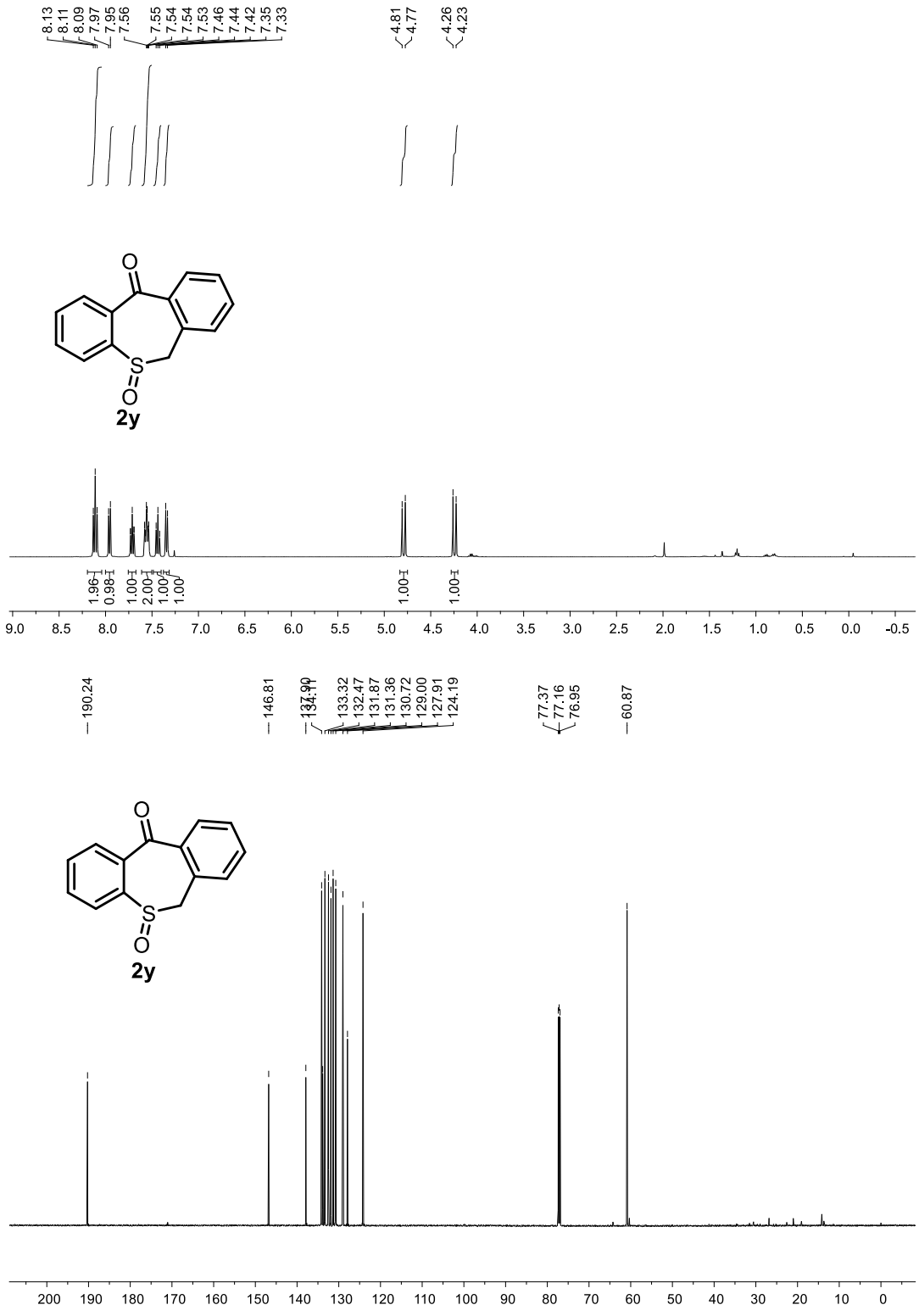
8.12
7.86
7.62
7.26
3.49
3.48
3.48
3.47
3.45
3.45
3.44
3.43
3.42
2.92
2.91
2.89
2.88
2.87
2.85
2.83
O
S
O
2x
0.97
0.98
0.99
1.00
3.00
1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


192.11
145.49
134.71
132.25
129.25
129.04
128.60
77.37
77.16
76.95
46.71
30.38
O
S
O
2x
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.13
8.11
8.09
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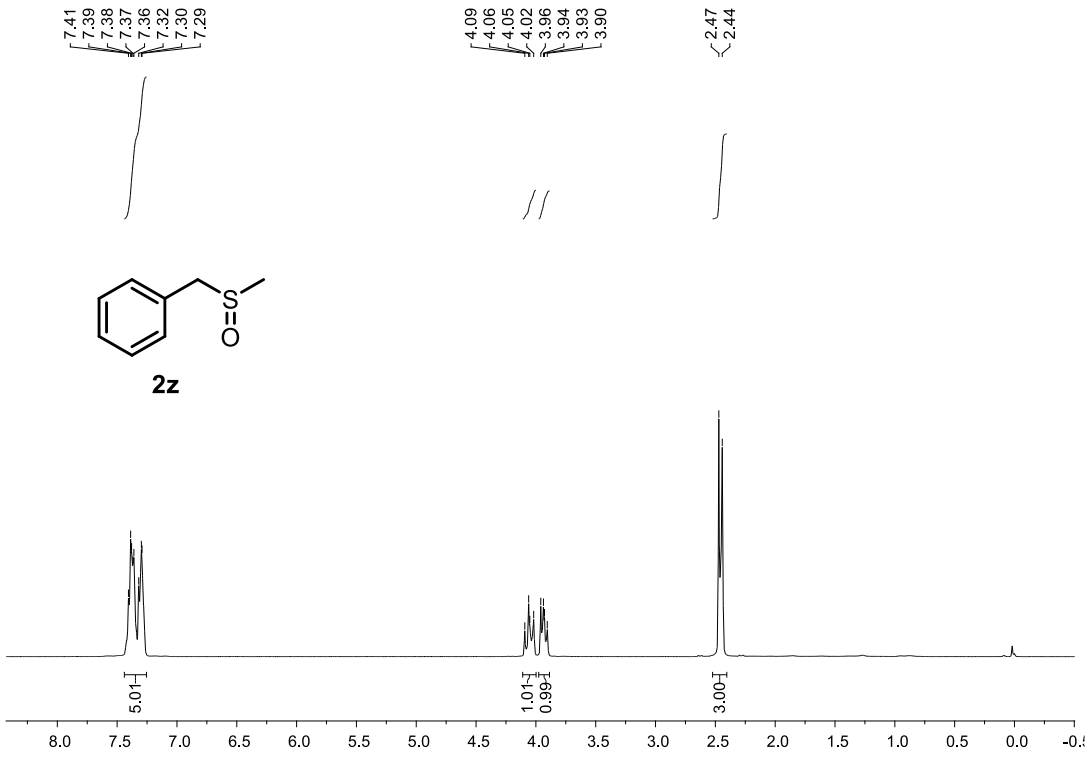
7.95
7.56
7.55
7.54
7.54
7.53
7.46
7.44
7.42
7.35
7.33
4.81
4.77
4.26
4.23
2y
1.96
0.98
1.00
2.00
1.00
1.00
1.00
1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
190.24
146.81
137.90
134.11
133.32
132.47
131.87
131.36
130.72
129.00
127.91
124.19
77.37
77.16
76.95
60.87
2y
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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7.39
7.38
7.37
7.36
7.32
7.30
7.29
4.09
4.06
4.05
4.02
3.96
3.94
3.93
3.90
2.47
2.44
S
O
5.01
1.01
0.99
3.00
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
4.0
3.5
3.0
2.5
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1.5
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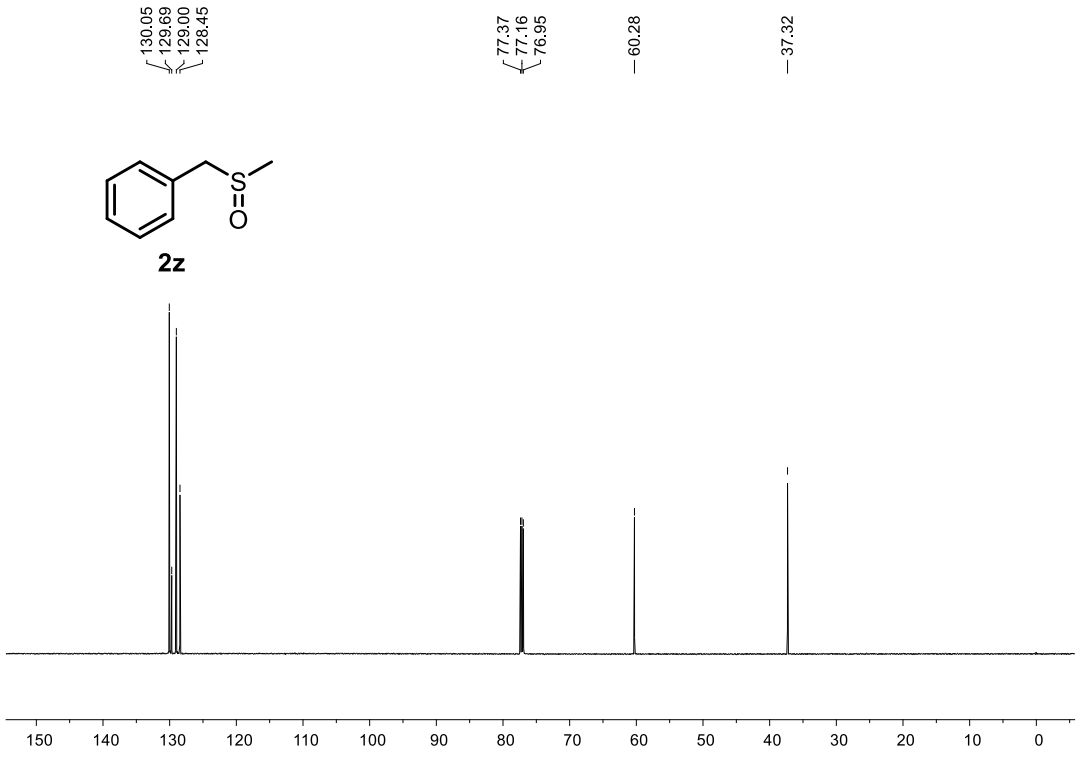
0.5
0.0

2z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128.45
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77.16
76.95
60.28
37.32
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O
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140
130
120
110
100
90
80
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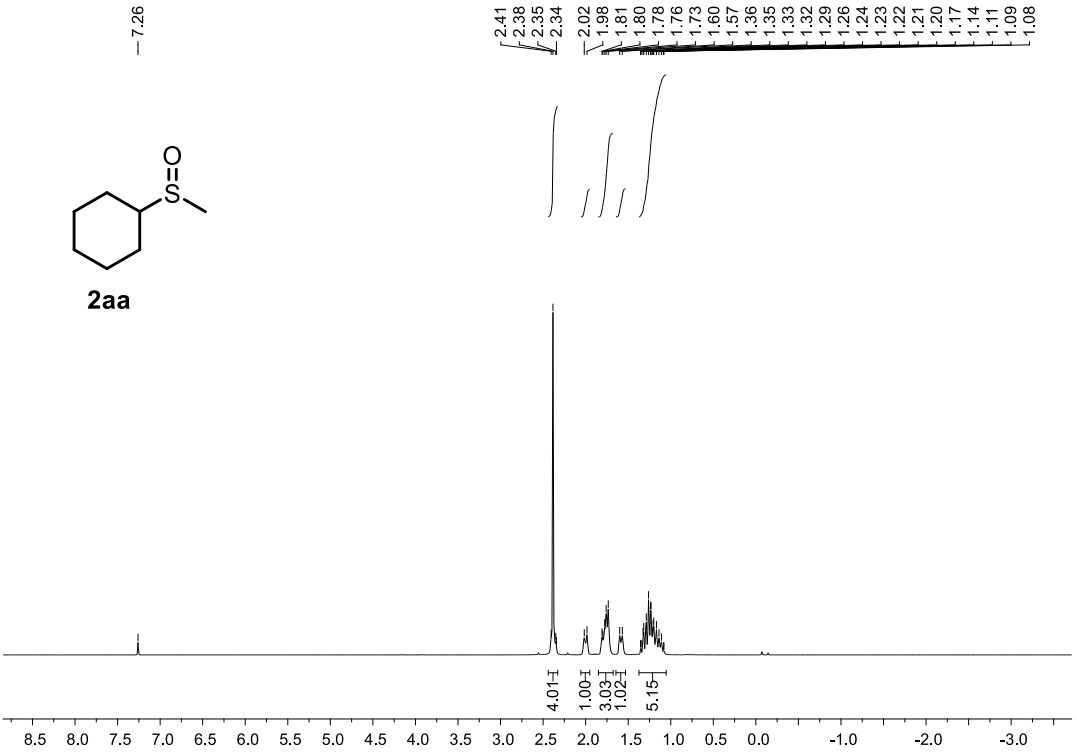
20
10
0

2z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2.38
2.35
2.34
2.02
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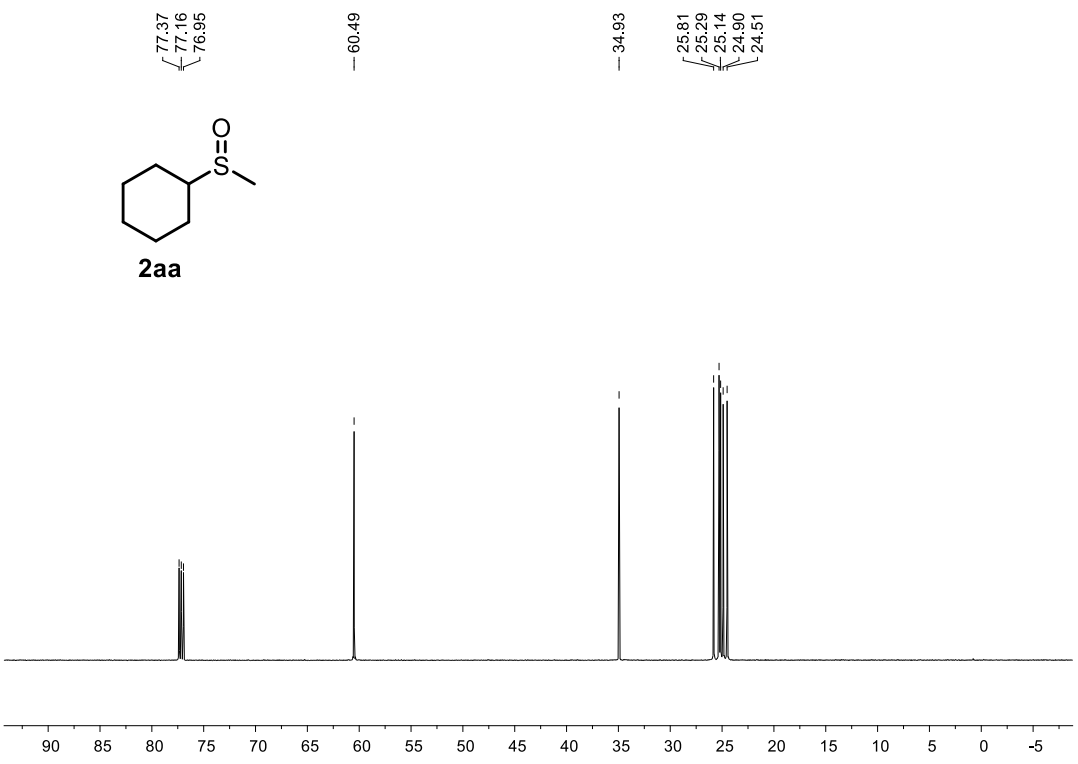
1.81
1.80
1.78
1.76
1.73
1.60
1.57
1.36
1.35
1.33
1.32
1.29
1.26
1.24
1.23
1.22
1.21
1.20
1.17
1.14
1.11
1.09
1.08
4.01
1.00
3.03
1.02
5.15
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0 -2.0 -3.0

2aa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77.16
76.95
60.49
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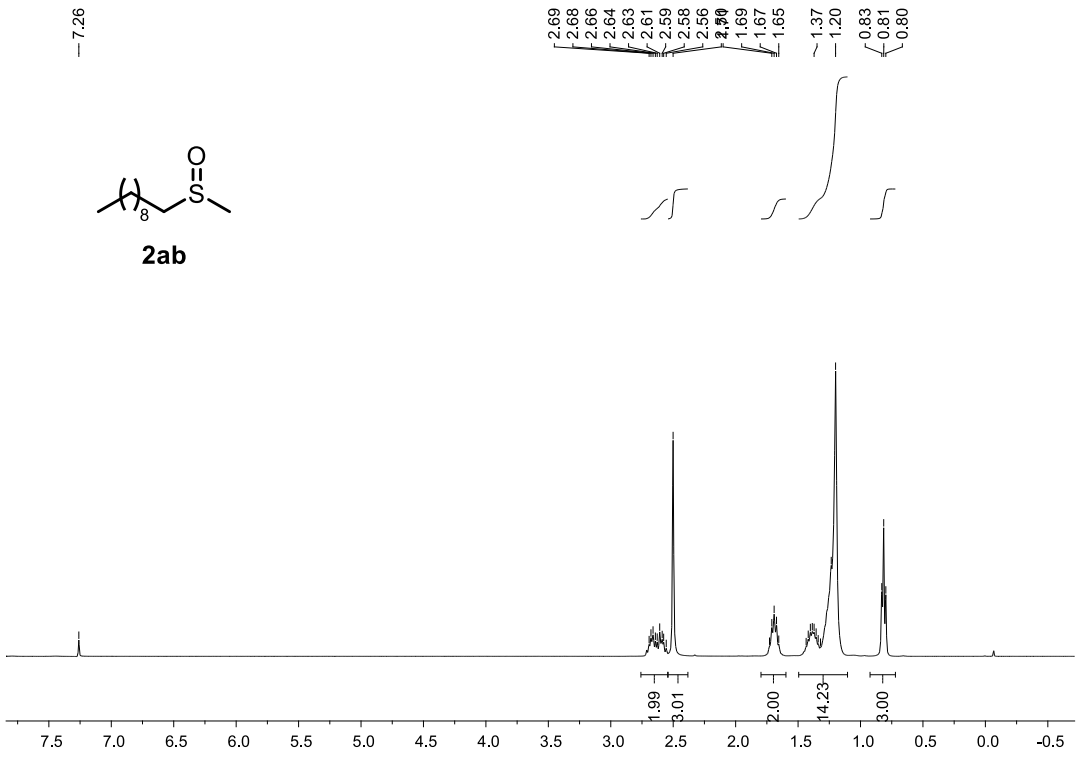
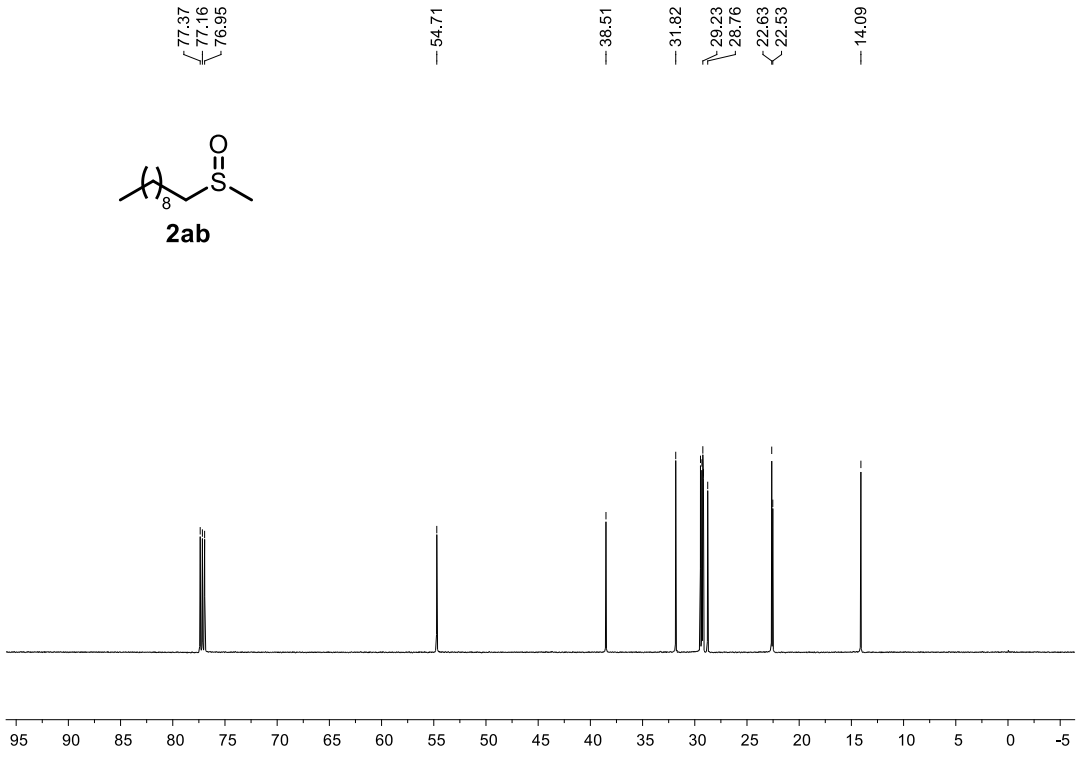
25.29
25.14
24.90
24.51
90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5

2aa


7.26
2.69
2.68
2.66
2.64
2.63
2.61
2.59
2.58
2.56
1.69
1.67
1.65
1.37
1.20
0.83
0.81
0.80
1.99
3.01
2.00
14.23
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

2ab


77.37
77.16
76.95
54.71
38.51
31.82
29.23
28.76
22.63
22.53
14.09
95
90
85
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60
55
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45
40
35
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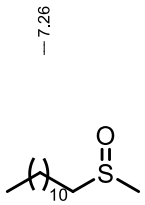
25
20
15
10
5
0
-5

2ab



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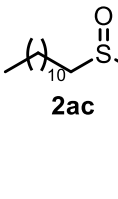

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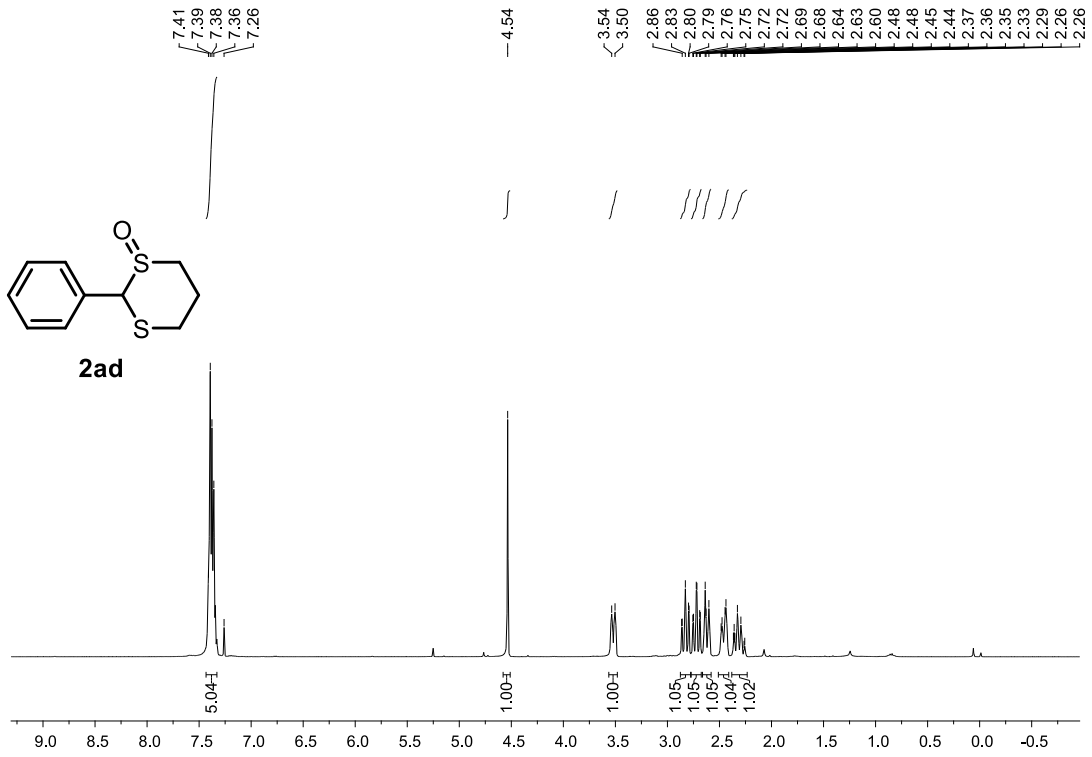
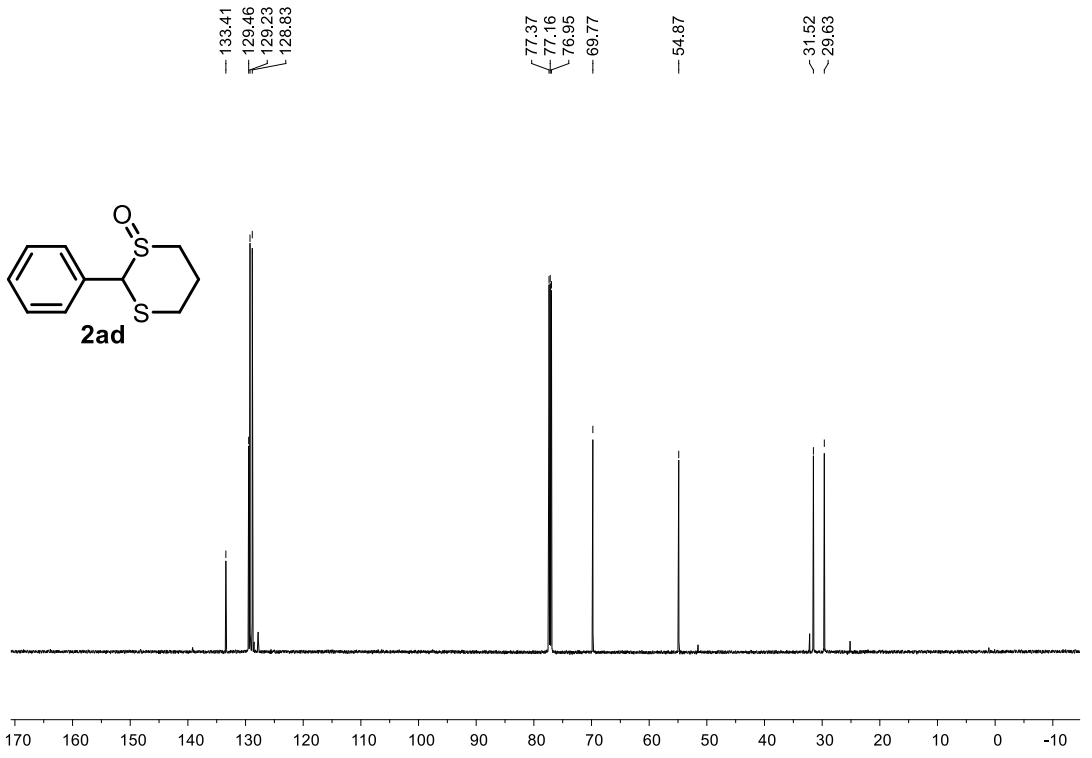

7.41
7.39
7.38
7.36
7.26
4.54
3.54
3.50
2.86
2.83
2.80
2.79
2.76
2.75
2.72
2.72
2.69
2.68
2.64
2.63
2.60
2.48
2.45
2.44
2.37
2.36
2.35
2.33
2.29
2.26
2.26
O
S
S
2ad
5.04
1.00
1.00
1.05
1.05
1.05
1.04
1.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


133.41
129.46
129.23
128.83
77.37
77.16
76.95
69.77
54.87
31.52
29.63
O
S
S
2ad
170
160
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140
130
120
110
100
90
80
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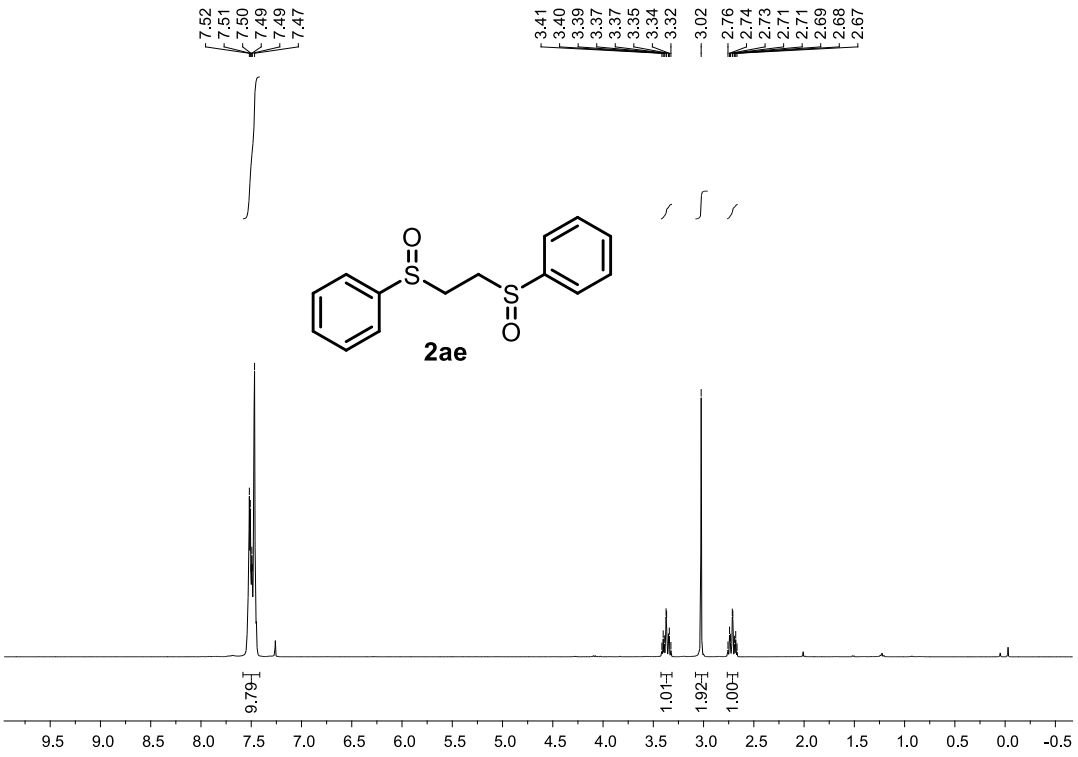
60
50
40
30
20
10
0
-10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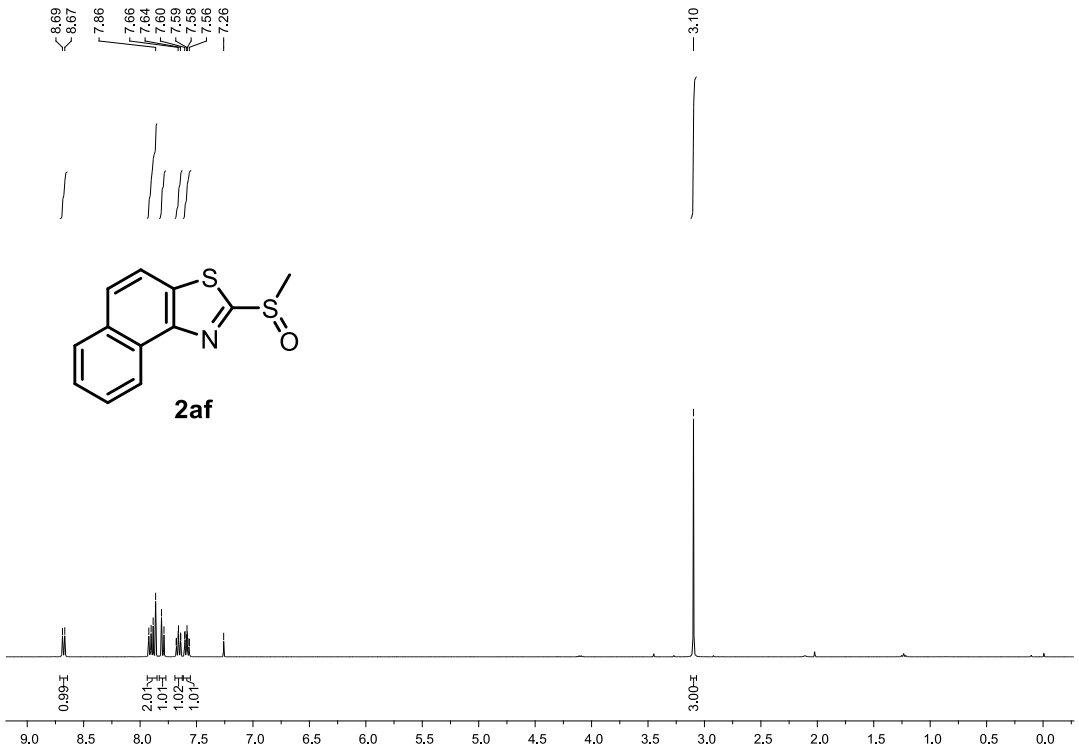
7.50
7.49
7.49
7.47
3.41
3.40
3.39
3.37
3.37
3.35
3.34
3.32
3.02
2.76
2.74
2.73
2.71
2.71
2.69
2.68
2.67
2ae
9.79
1.01
1.92
1.00


142.32
142.12
131.37
129.51
129.47
123.98
123.90
77.37
77.16
76.95
47.69
46.92
2ae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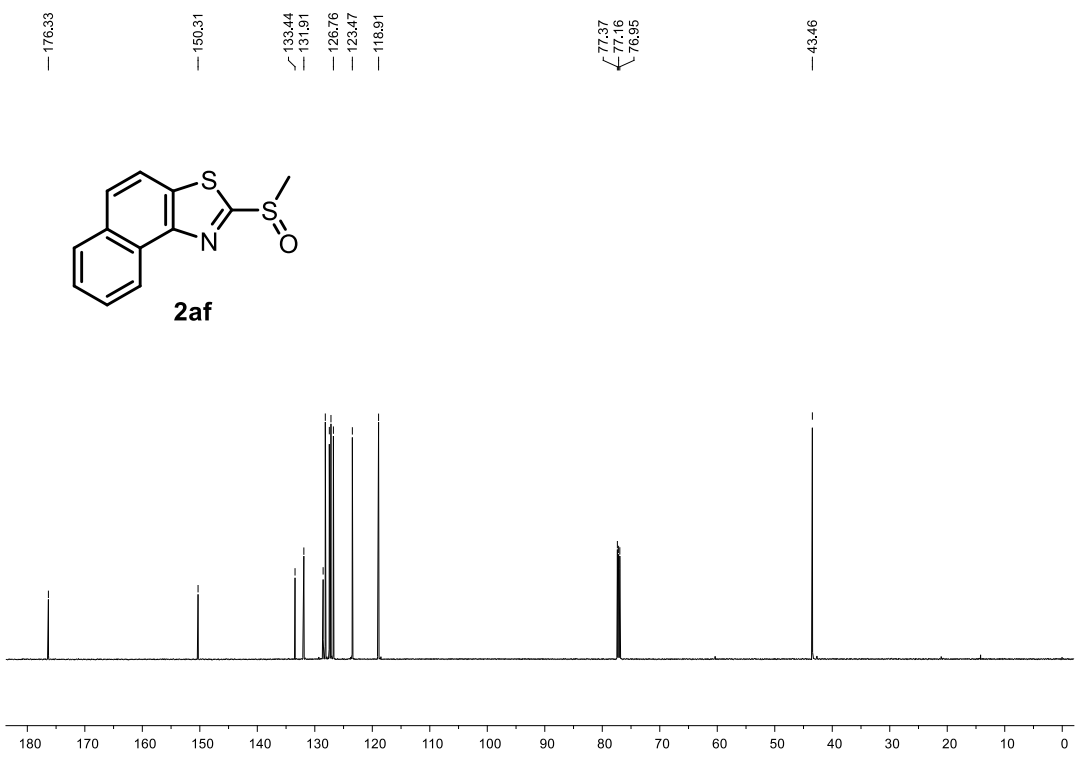
8.67
7.86
7.66
7.64
7.60
7.59
7.58
7.56
7.26
3.10
S
S
O
N
0.99
2.01
1.01
1.02
1.01
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

2af


176.33
150.31
133.44
131.91
126.76
123.47
118.91
77.37
77.16
76.95
43.46
S
S
O
N
180
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140
130
120
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100
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80
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60
50
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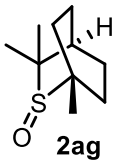
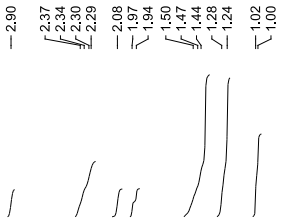
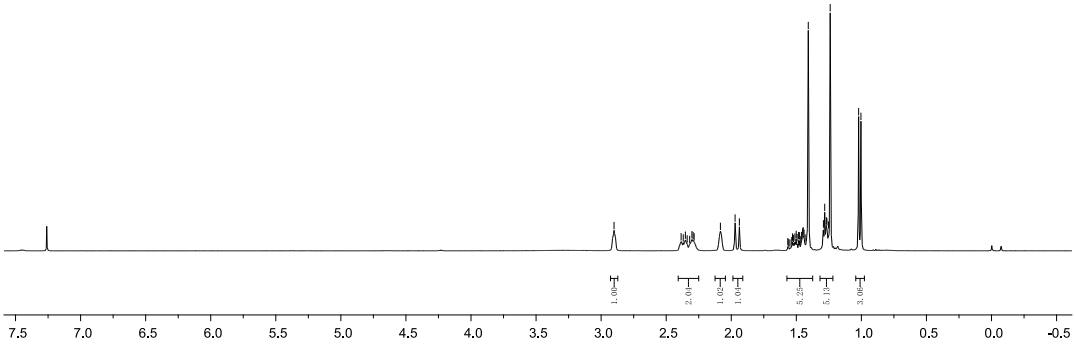
20
10
0

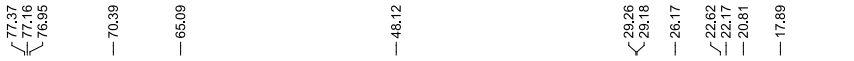
2af


H
S
O

2ag


2.90
2.37
2.34
2.30
2.29
2.08
1.97
1.94
1.50
1.47
1.44
1.28
1.24
1.02
1.00


1.00
2.01
1.02
1.01
5.25
5.10
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


77.37
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65.09
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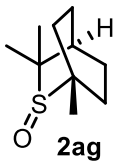
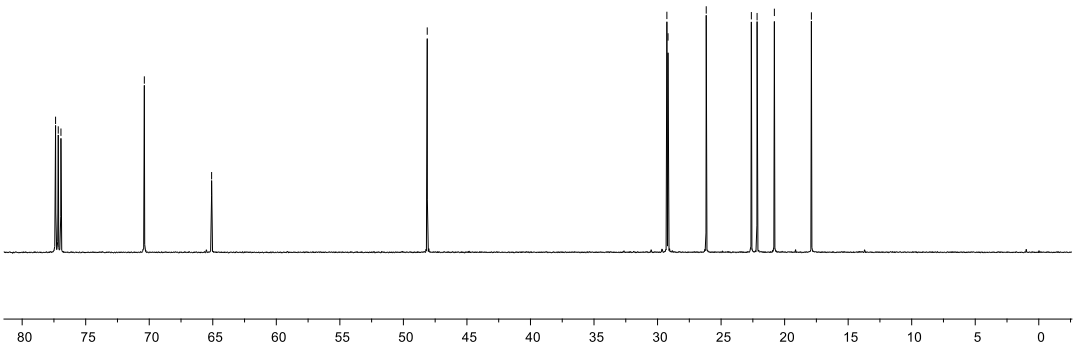
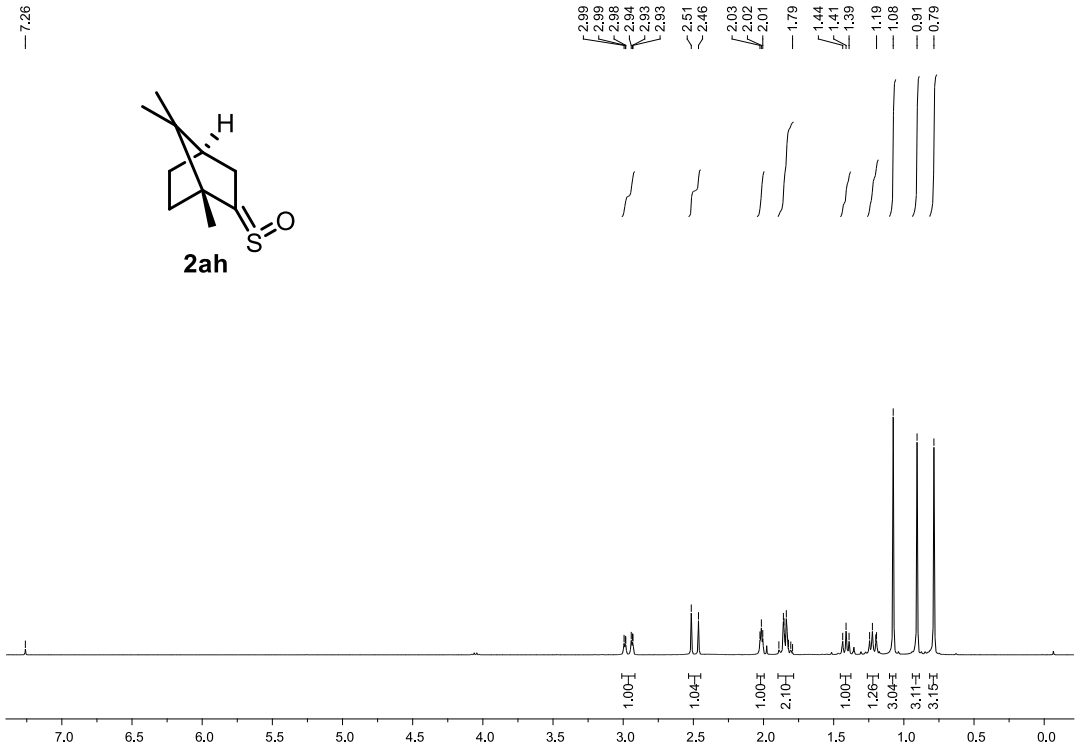
29.26
29.18
26.17
22.62
22.17
20.81
17.89


H
S
O

2ag


80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0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2.99
2.99
2.98
2.94
2.93
2.93
2.51
2.46
2.03
2.02
2.01
1.79
1.44
1.41
1.39
1.19
1.08
0.91
0.79
H
S
O
2ah
1.00
1.04
1.00
2.10
1.00
1.26
3.04
3.11
3.15
7.0
6.5
6.0
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4.0
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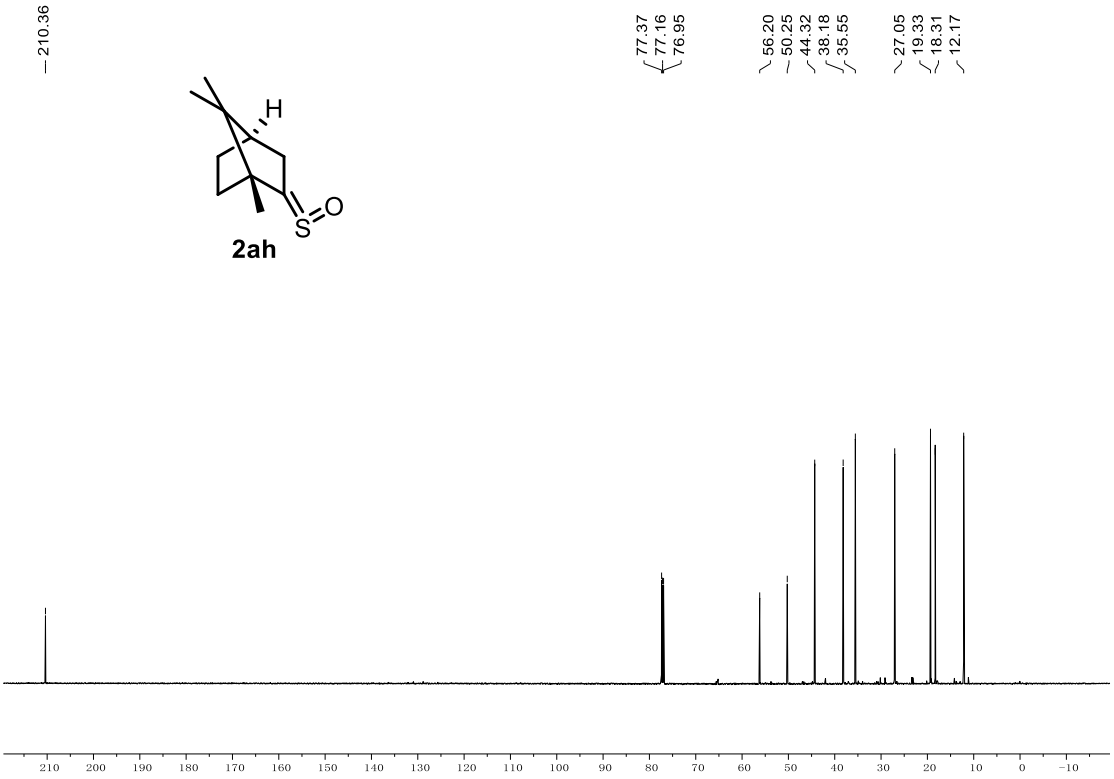
3.0
2.5
2.0
1.5
1.0
0.5
0.0


210.36
77.37
77.16
76.95
56.20
50.25
44.32
38.18
35.55
27.05
19.33
18.31
12.17
H
S
O
2ah
210
200
190
180
170
160
150
140
130
120
110
100
90
80
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60
50
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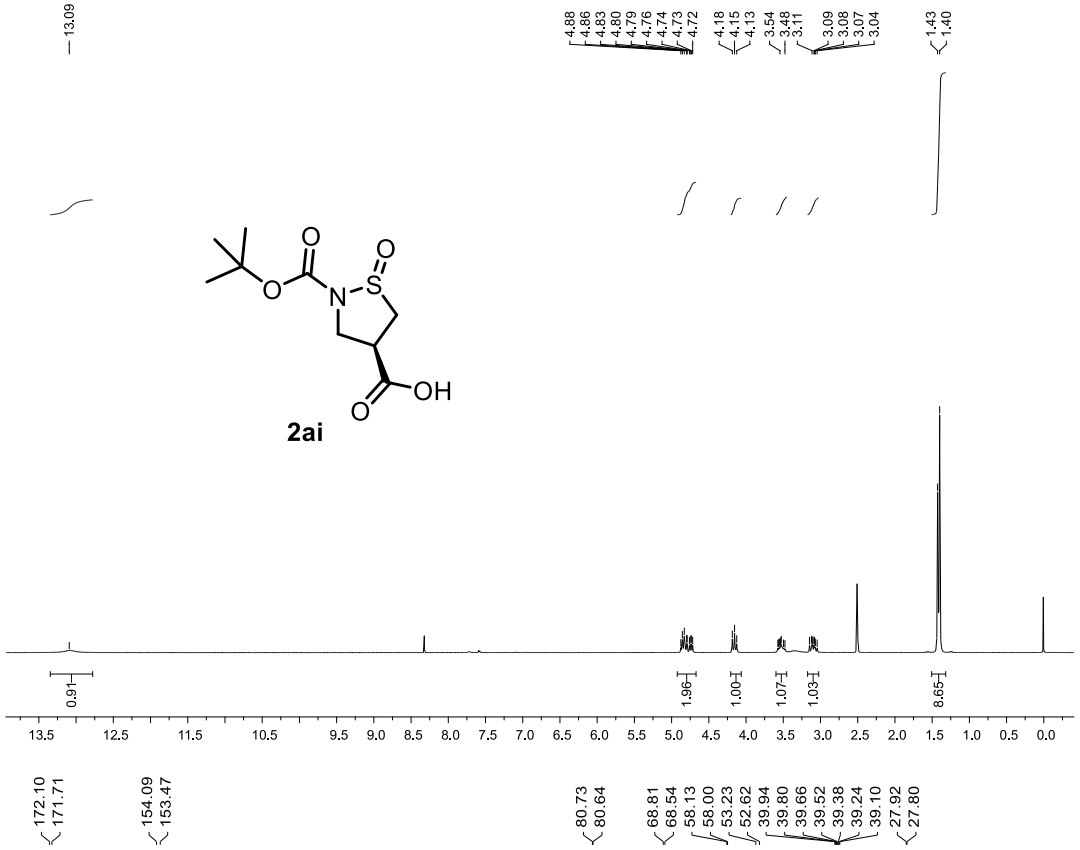
30
20
10
0
−10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4.79
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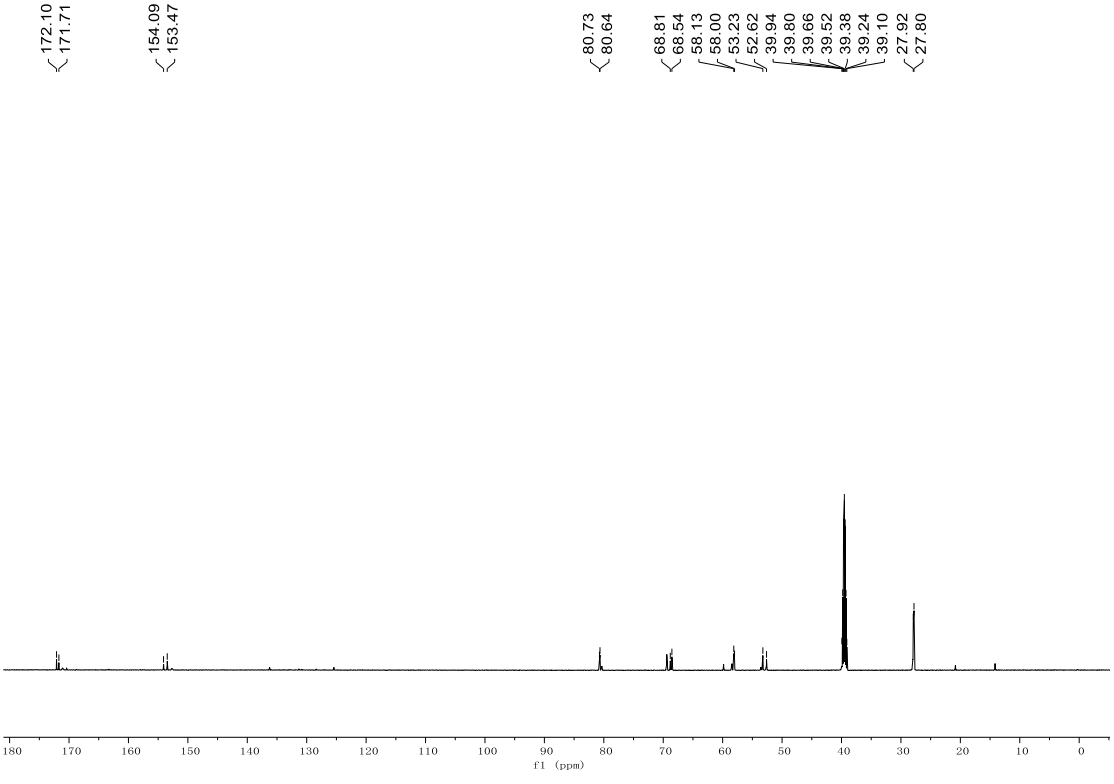
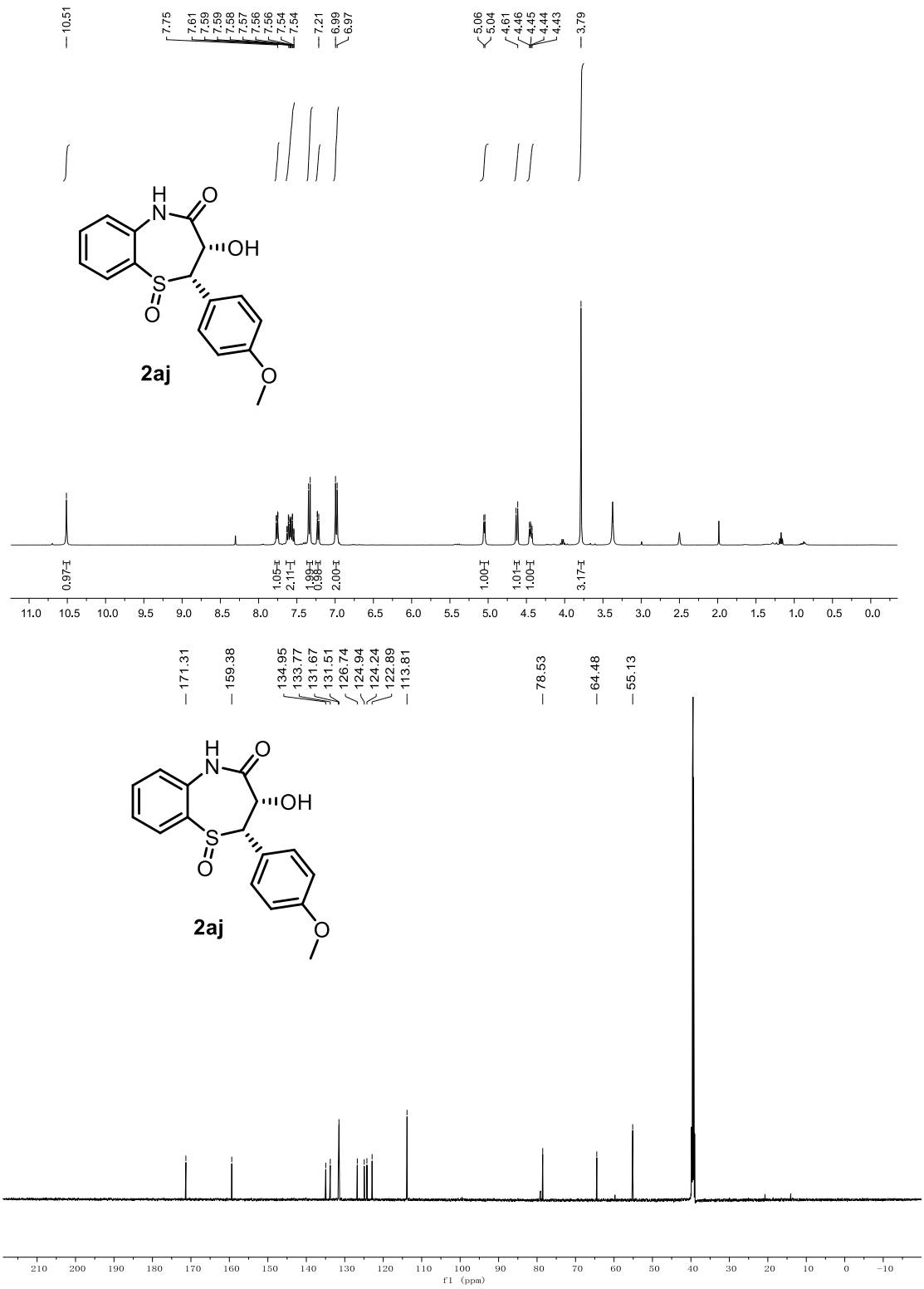
4.74
4.73
4.72
4.18
4.15
4.13
3.54
3.48
3.11
3.09
3.08
3.07
3.04
1.43
1.40
O
O
O
N
S
O
OH
O
2ai
0.91
1.96
1.00
1.07
1.03
8.65
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


172.10
171.71
154.09
153.47
80.73
80.64
68.81
68.54
58.13
58.00
53.23
52.62
39.94
39.80
39.66
39.52
39.38
39.24
39.10
27.92
27.80
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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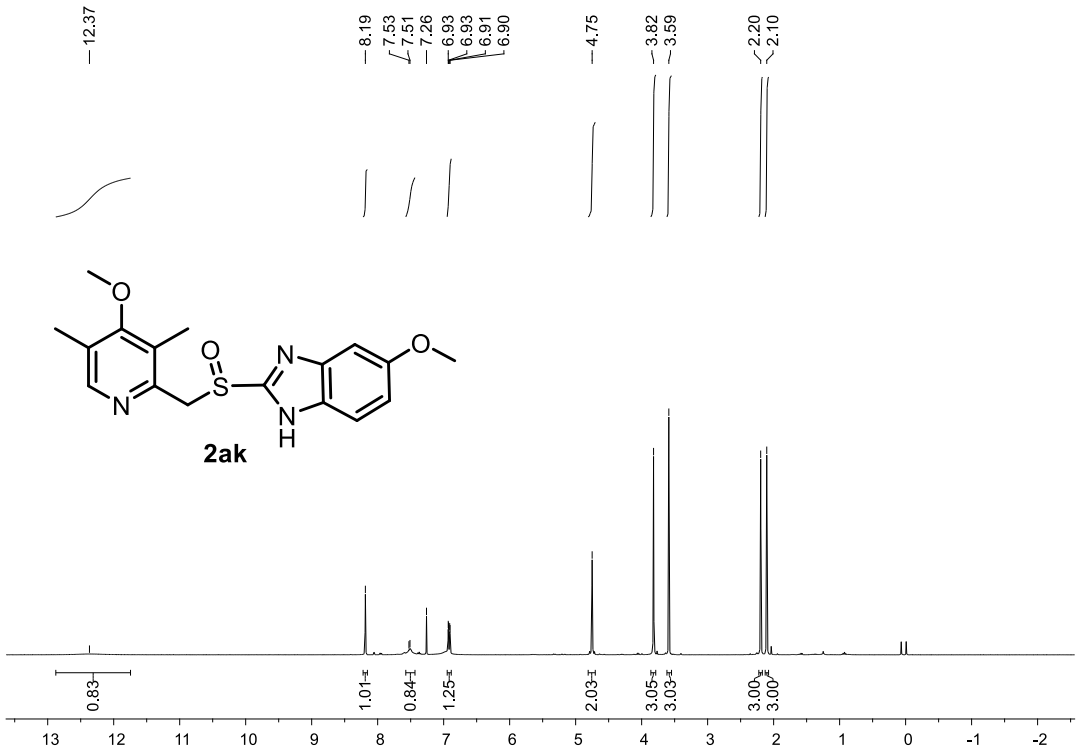
7.56
7.56
7.54
7.54
7.21
6.99
6.97
5.06
5.04
4.61
4.46
4.45
4.44
4.43
3.79
2aj
0.97
1.05
2.11
1.99
0.98
2.00
1.00
1.01
1.00
3.17
171.31
159.38
134.95
133.77
131.67
131.51
126.74
124.94
124.24
122.89
113.81
78.53
64.48
55.13
2aj
f1 (ppm)


12.37
8.19
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7.51
7.26
6.93
6.93
6.91
6.90
4.75
3.82
3.59
2.20
2.10
O
O
S
N
N
H
N
O
2ak
0.83
1.01
0.84
1.25
2.03
3.05
3.03
3.00
3.00
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12
11
10
9
8
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6
5
4
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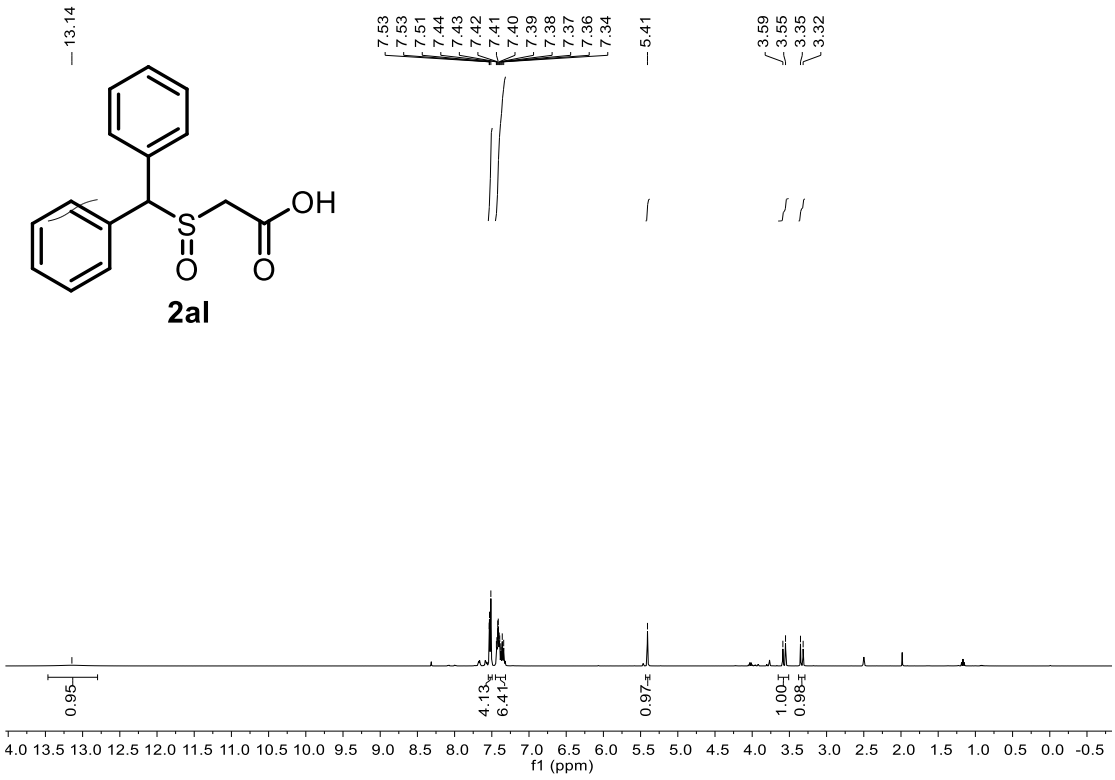
1
0
-1
-2


13.14
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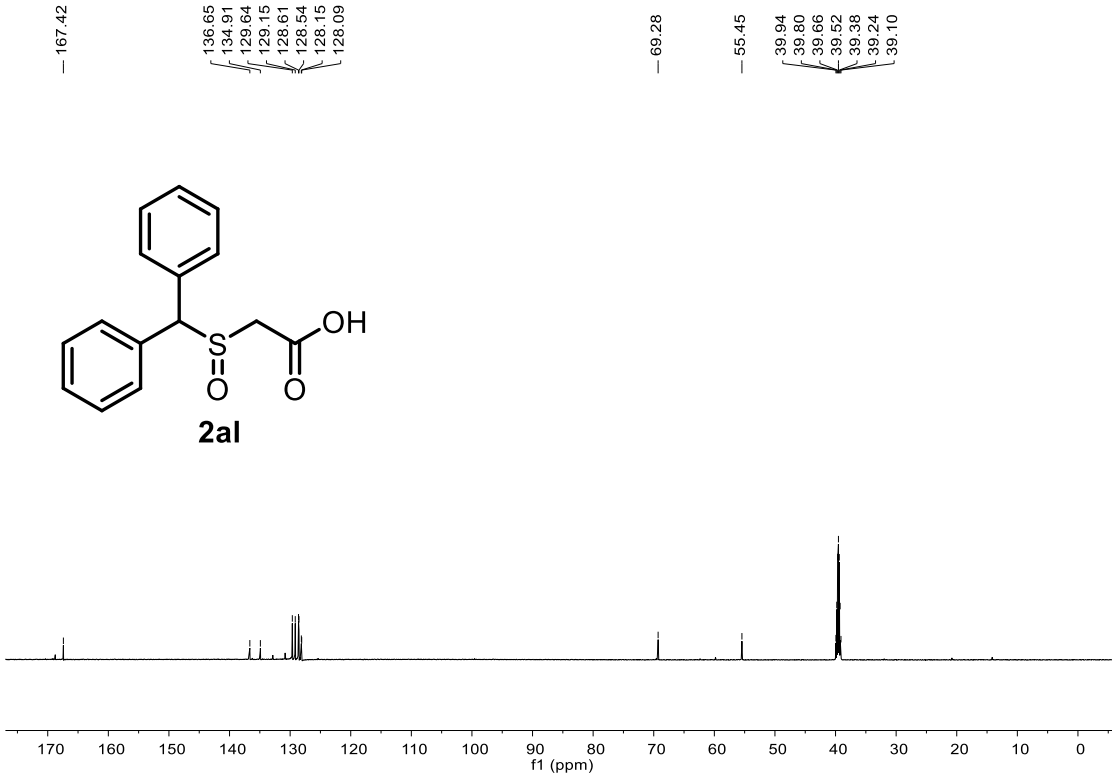
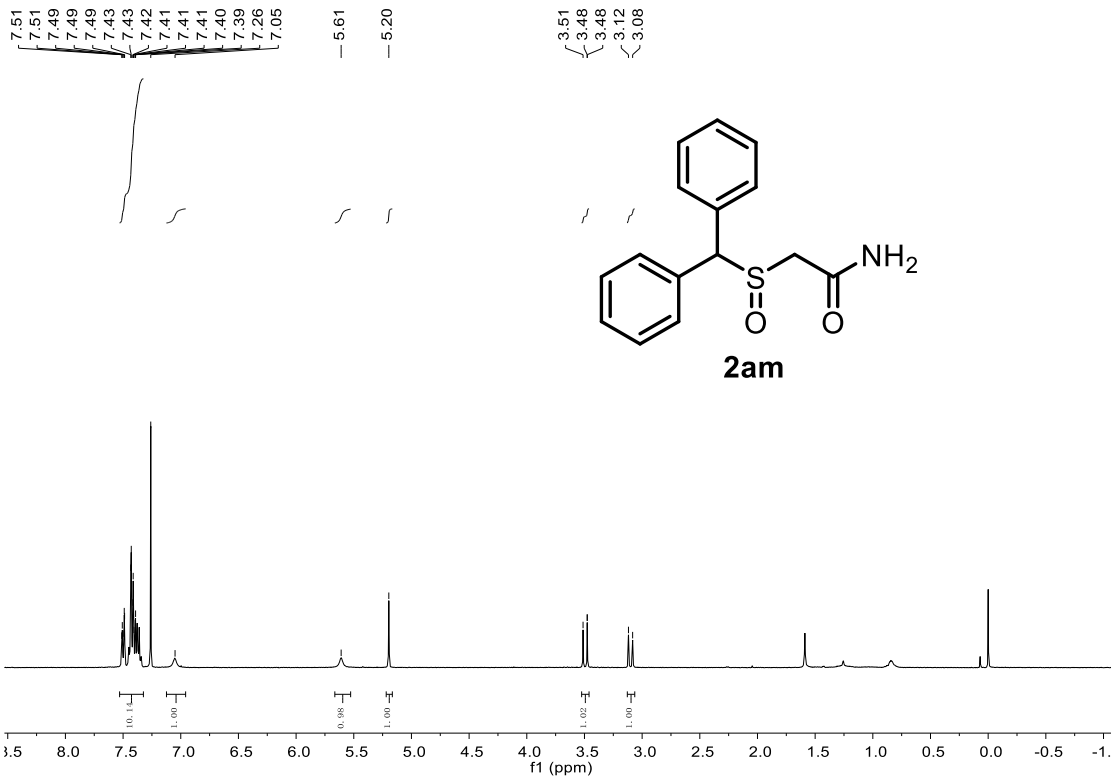
7.43
7.42
7.41
7.40
7.39
7.38
7.37
7.36
7.34
5.41
3.59
3.55
3.35
3.32
OH
S
O
O
2al
0.95
4.13
6.41
0.97
1.00
0.98
f1 (ppm)


167.42
136.65
134.91
129.64
129.15
128.61
128.54
128.15
128.09
69.28
55.45
39.94
39.80
39.66
39.52
39.38
39.24
39.10
OH
S
O
O
2al
f1 (ppm)


7.51
7.51
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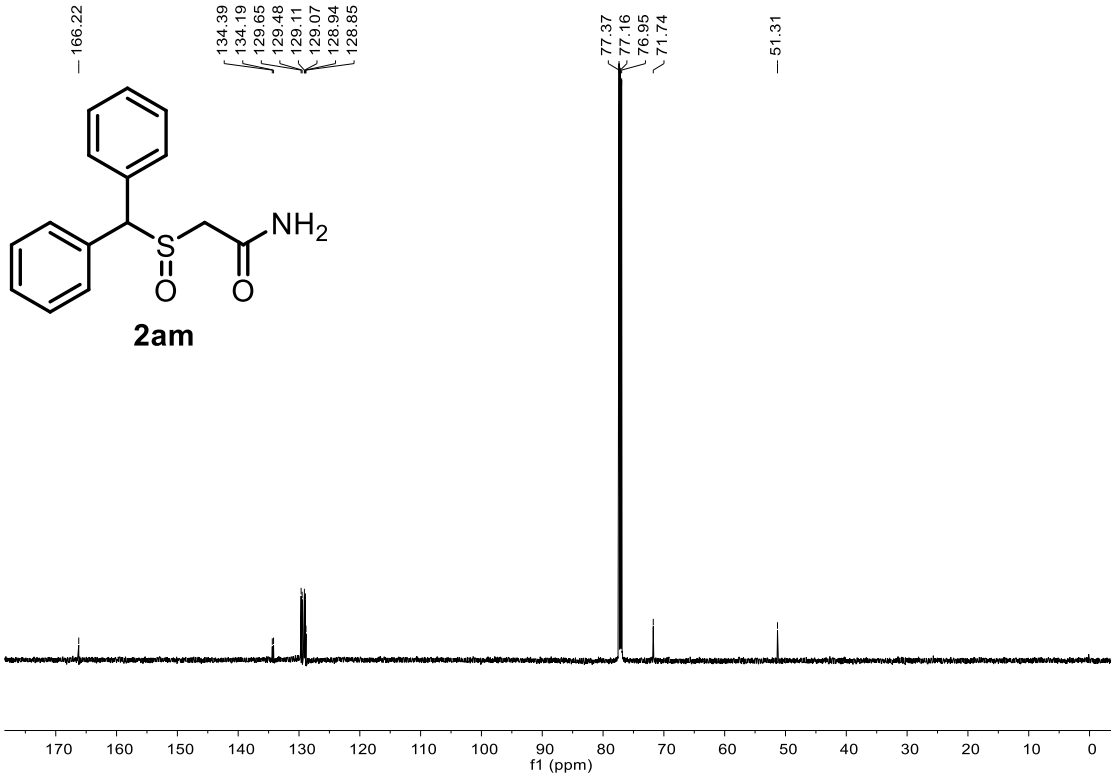
7.49
7.49
7.43
7.43
7.42
7.41
7.41
7.41
7.40
7.39
7.26
7.05
5.61
5.20
3.51
3.48
3.48
3.12
3.08
NH2
S
O
O
2am
f1 (ppm)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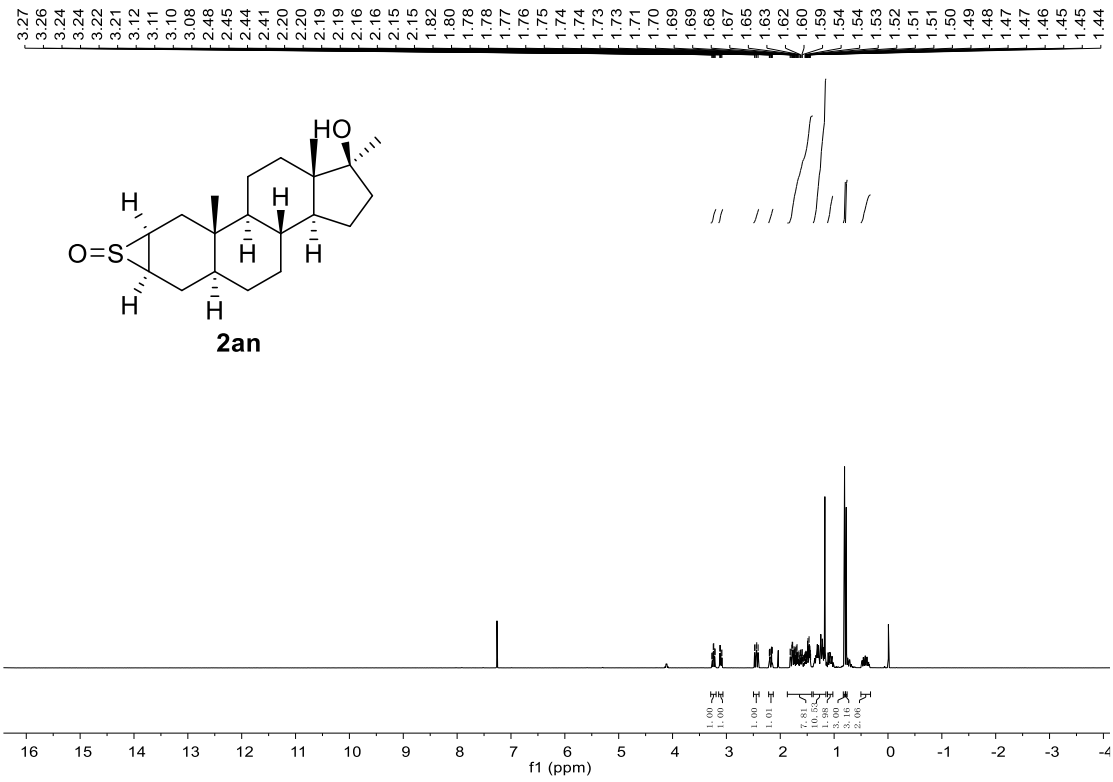
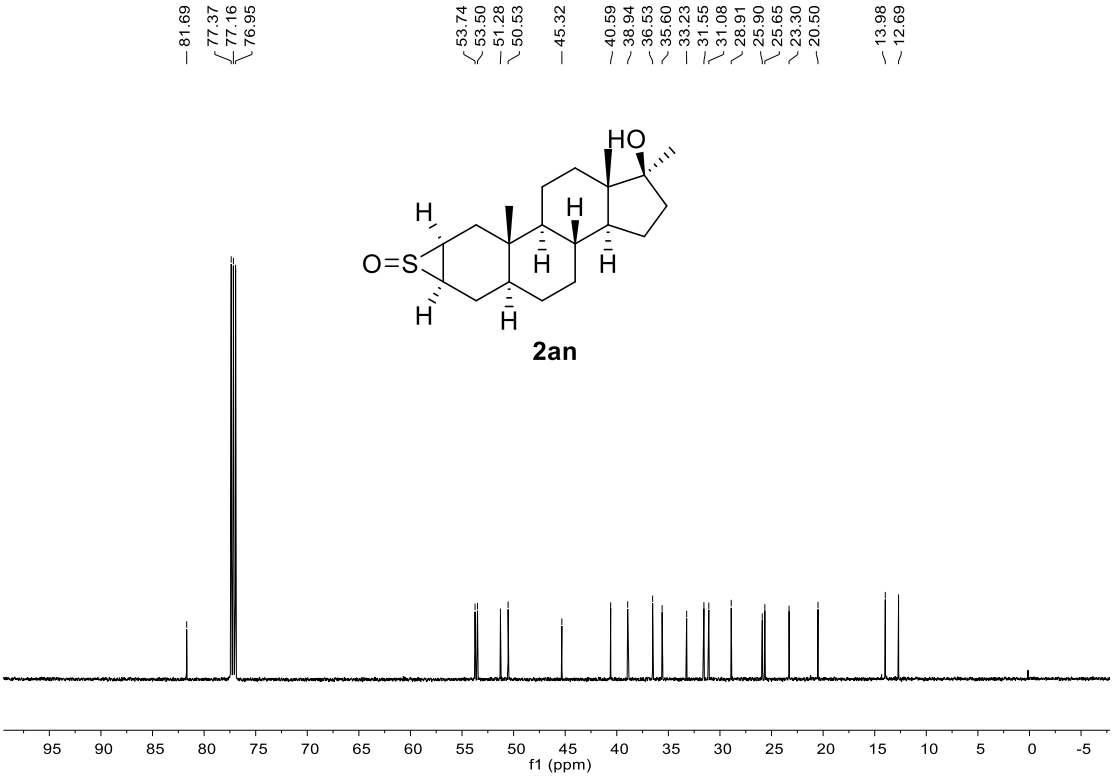
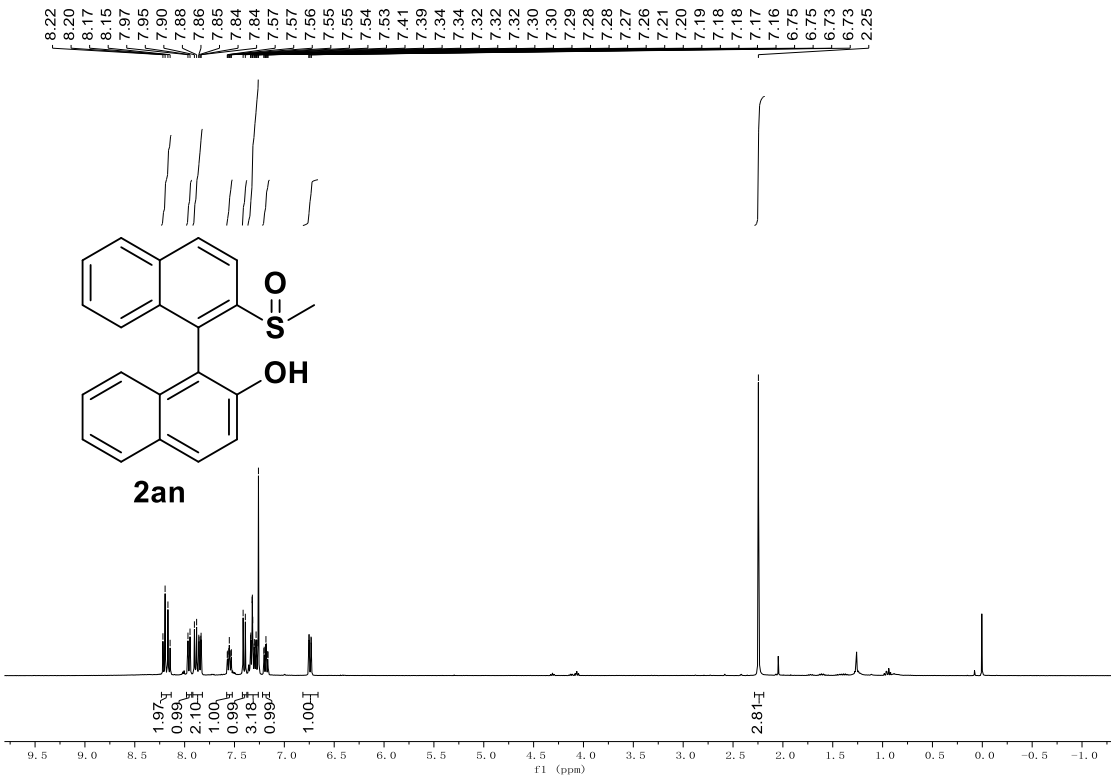
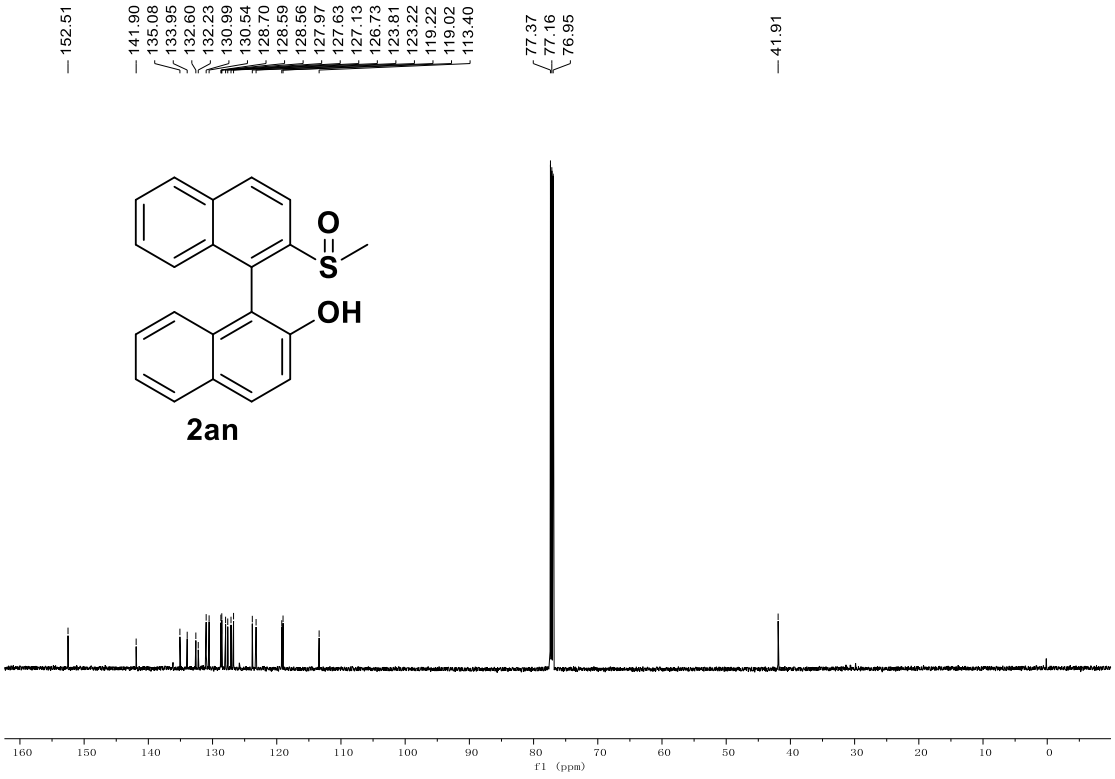
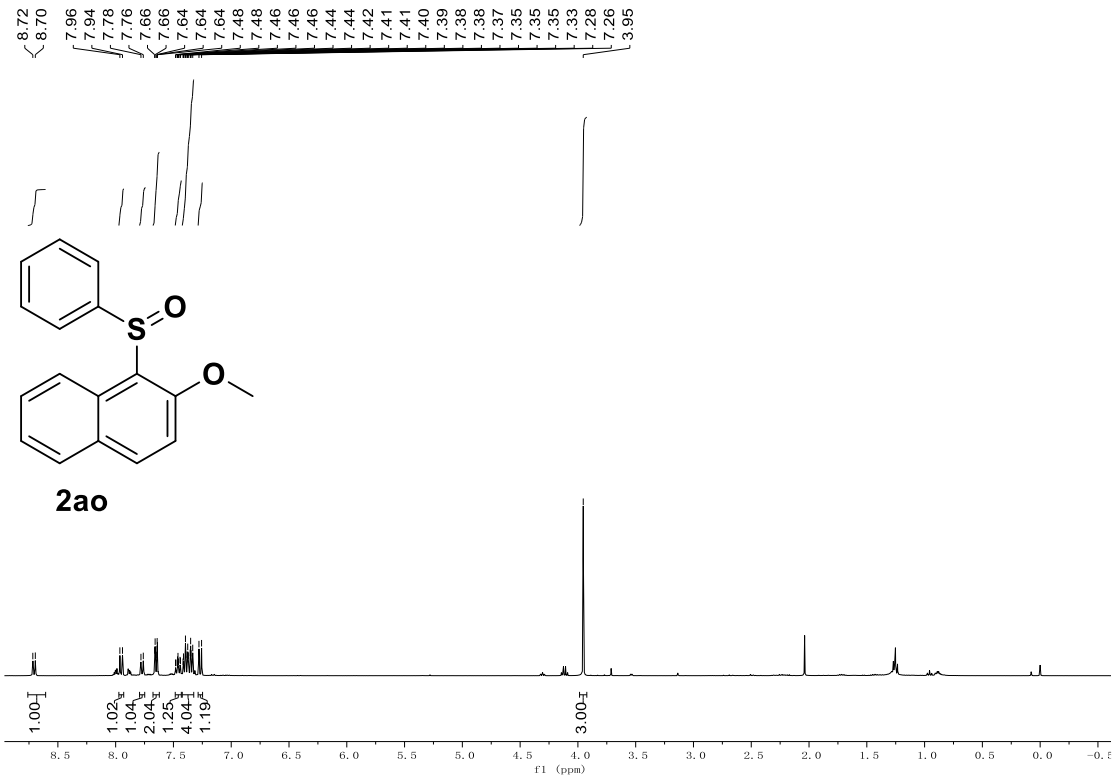
129.11
129.07
128.94
128.85
77.37
77.16
76.95
71.74
51.31
NH2
S
O
O
2am
f1 (ppm)


3.27 3.26 3.24 3.24 3.22 3.21 3.12 3.11 3.10 3.08 2.48 2.45 2.44 2.41 2.20 2.20 2.19 2.19 2.16 2.16 2.15 2.15 1.82 1.80 1.78 1.78 1.77 1.76 1.75 1.74 1.74 1.73 1.73 1.71 1.70 1.69 1.69 1.68 1.67 1.65 1.63 1.62 1.60 1.59 1.54 1.54 1.53 1.52 1.51 1.51 1.50 1.49 1.48 1.47 1.47 1.46 1.45 1.45 1.44
HO
H
H
O=S
H
H
H
H
2an
1.00
1.00
1.00
1.01
7.81
10.58
1.98
3.00
3.16
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4
f1 (ppm)

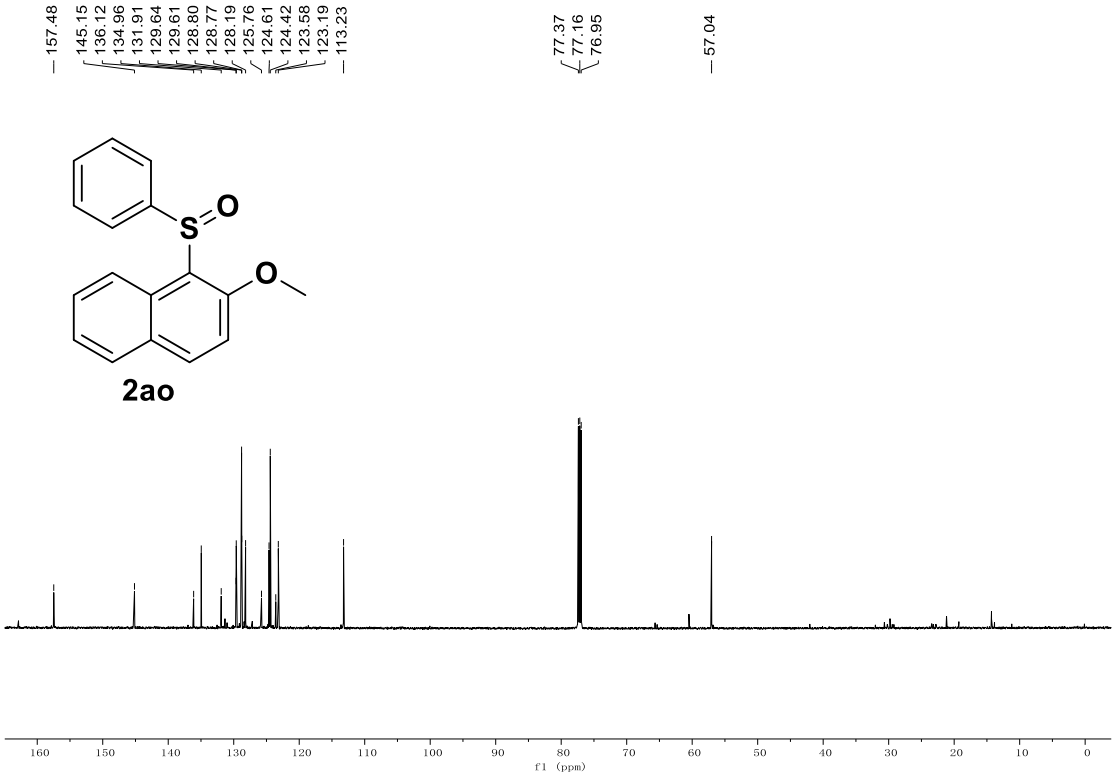

81.69
77.37
77.16
76.95
53.74
53.50
51.28
50.53
45.32
40.59
38.94
36.53
35.60
33.23
31.55
31.08
28.91
25.90
25.65
23.30
20.50
13.98
12.69
HO
H
H
O=S
H
H
H
H
2an
95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5
f1 (ppm)


8.22
8.20
8.17
8.15
7.97
7.95
7.90
7.88
7.86
7.85
7.84
7.84
7.57
7.57
7.56
7.55
7.55
7.54
7.53
7.41
7.39
7.34
7.34
7.32
7.32
7.30
7.30
7.29
7.28
7.28
7.27
7.26
7.21
7.20
7.19
7.18
7.18
7.17
7.16
6.75
6.75
6.73
6.73
2.25
O
S
OH
2an
1.97
0.99
2.10
1.00
0.99
3.18
0.99
1.00
2.81
f1 (ppm)


152.51
141.90
135.08
133.95
132.60
132.23
130.99
130.54
128.70
128.59
128.56
127.97
127.63
127.13
126.73
123.81
123.22
119.22
119.02
113.40
77.37
77.16
76.95
41.91
O
S
OH
2an
f1 (ppm)


8.72
8.70
7.96
7.94
7.78
7.76
7.66
7.66
7.64
7.64
7.64
7.48
7.48
7.46
7.46
7.46
7.44
7.44
7.42
7.41
7.41
7.40
7.39
7.38
7.38
7.37
7.35
7.35
7.33
7.28
7.26
3.95
O
S
O
1.00
1.02
1.04
2.04
1.25
4.04
1.19
3.00
f1 (ppm)

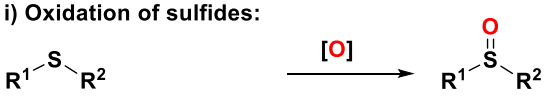
2ao


157.48
145.15
136.12
134.96
131.91
129.64
129.61
128.80
128.77
128.19
125.76
124.61
124.42
123.58
123.19
113.23
77.37
77.16
76.95
57.04
O
S
O
f1 (ppm)

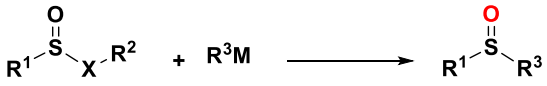
2ao

Scheme S-1 Four Synthetic Approaches to Sulfoxides

i) Oxidation of sulfides:

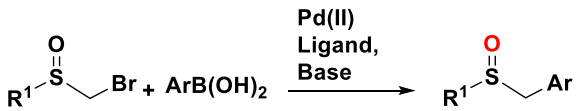


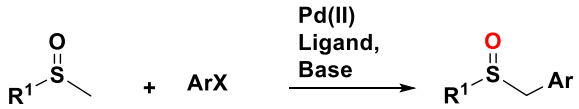
ii) Nucleophilic substitution:



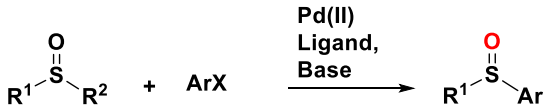
R^1, R^2, R^3 = alkyl, aryl
X = heteratom, such as O, N
M = Li, Mg

iii) Palladium-catalyzed Suzuki coupling or alpha-arylation:

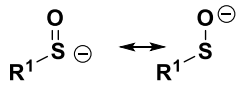




iv) Palladium-catalyzed arylation of sulfenate anions:

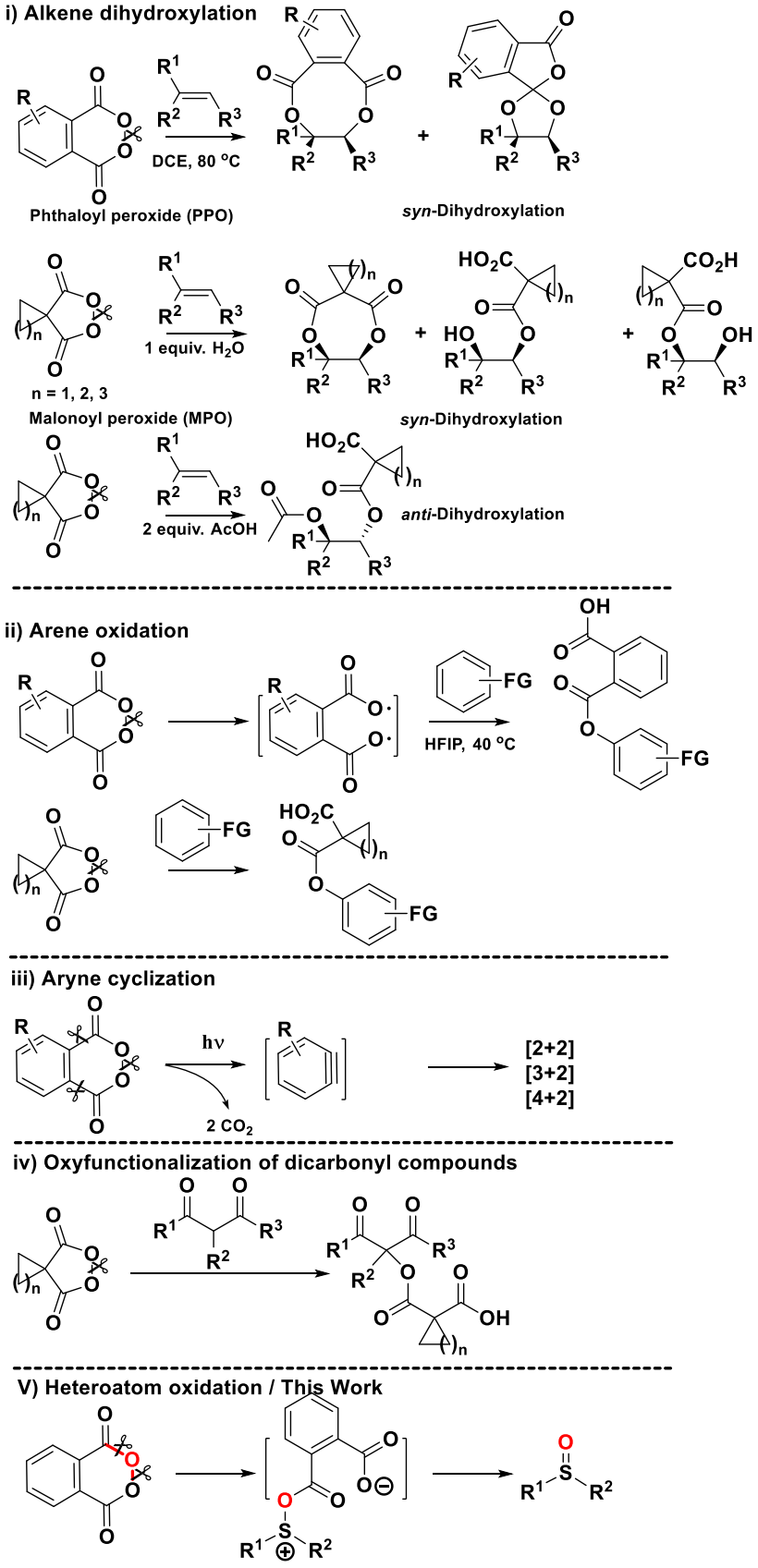


R^2 = $(CH_2)_2CO_2Me$, $(CH_2)_2TMS$, $CH_2CH{=}CH_2$, t-Bu, Me, Bn,



sulfenate anion

Scheme S-2 Cyclic Diacyl Peroxides as Versatile Reagents



7. DFT Calculation Details and Results

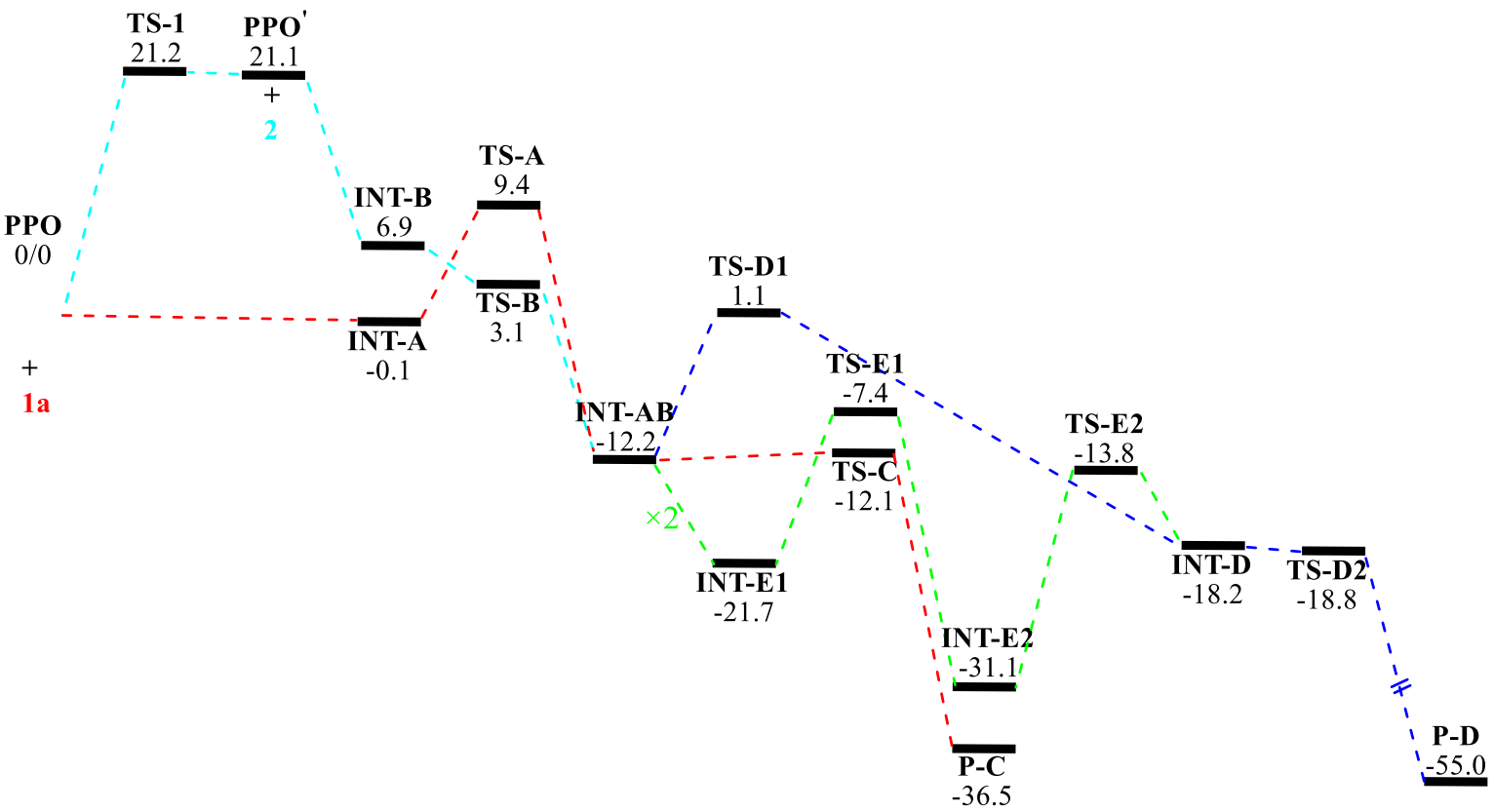


Fig. S-1 Schematic diagram of energy barrier

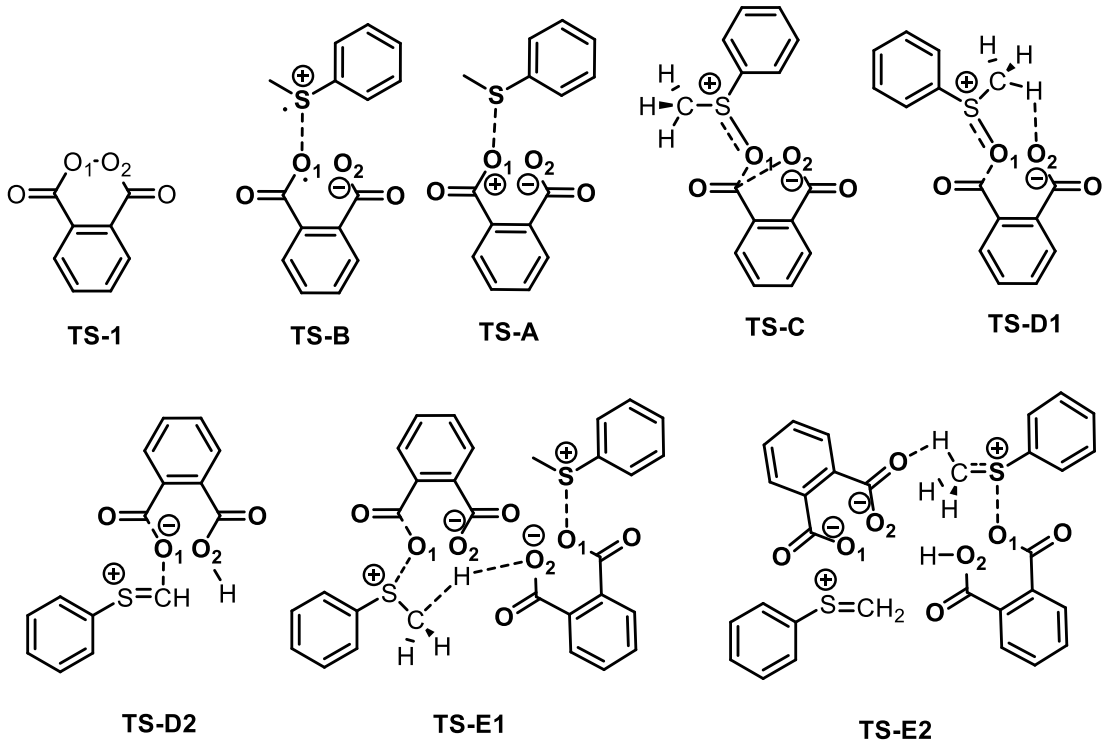


Fig. S - 2 Transition state structure

Coordinates of the stationary points

1

HF=-608.1015544

6	-2.699194	0.701030	0.000062
6	-2.699183	-0.701058	-0.000004
6	-1.496655	-1.405297	0.000074
6	-0.286770	-0.700930	0.000131
6	-0.286785	0.700933	-0.000159

6	-1.496675	1.405287	-0.000069
6	0.981658	1.448976	-0.000197
8	2.161653	0.741738	0.001563
8	1.103430	2.651337	-0.000384
6	0.981684	-1.448964	0.000130
8	2.161668	-0.741722	-0.001378
8	1.103449	-2.651330	0.000212
1	-3.640708	1.242753	0.000256
1	-3.640688	-1.242795	-0.000158
1	-1.474327	-2.490172	0.000061
1	-1.474363	2.490162	-0.000069

TS-1

HF=-608.0639588 <S2>=1.005444

6	-2.654528	0.697842	0.000151
6	-2.654510	-0.697905	-0.000147
6	-1.444501	-1.394831	0.006376
6	-0.224671	-0.706595	0.006667
6	-0.224688	0.706591	-0.006666
6	-1.444534	1.394799	-0.006375
6	0.999942	1.543414	-0.093184
8	1.044002	2.729993	0.337213
8	2.077155	1.204737	-0.658805
6	0.999980	-1.543390	0.093183
8	2.077175	-1.204700	0.658826
8	1.044073	-2.729960	-0.337238
1	-3.592204	1.246022	-0.001561

1	-3.592175	-1.246109	0.001566
1	-1.434871	-2.480226	0.028059
1	-1.434931	2.480194	-0.028058

1'

HF=-608.063996 <S2>=1.010512

6	-2.657358	0.697781	0.001091
6	-2.657159	-0.698428	-0.001019
6	-1.447639	-1.396718	0.005814
6	-0.229326	-0.706223	0.007911
6	-0.229560	0.706346	-0.008038
6	-1.448047	1.396444	-0.005834
6	1.003181	1.527860	-0.111848
8	1.103278	2.674981	0.408315
8	2.024095	1.210681	-0.781139
6	1.003452	-1.527648	0.111765
8	2.023957	-1.210497	0.781689
8	1.103994	-2.674577	-0.408764
1	-3.595611	1.244968	0.000044
1	-3.595264	-1.245871	0.000178
1	-1.438127	-2.482149	0.028608
1	-1.438869	2.481876	-0.028688

2

HF=-669.7606308

6	0.334141	1.098547	-0.000191
6	1.705181	1.378952	-0.000119
6	2.644433	0.347169	0.000062
6	2.199968	-0.980107	0.000171
6	0.836774	-1.269377	0.000127
6	-0.111972	-0.230648	-0.000053
1	-0.371502	1.922411	-0.000382
1	2.033402	2.415671	-0.000215
1	3.707698	0.570935	0.000111
1	2.918128	-1.796399	0.000319
1	0.503130	-2.304490	0.000263
16	-1.827347	-0.721143	-0.000256
6	-2.730056	0.861454	0.000398
1	-2.517141	1.450755	-0.896452
1	-3.790155	0.593331	0.000485
1	-2.516829	1.450121	0.897592

INT-B

HF=-1277.8495636 <S2>=1.013373

6	4.702914	-0.896506	0.705100
6	4.183105	-1.933156	-0.076860
6	2.894492	-1.835835	-0.607359
6	2.106620	-0.706920	-0.368617
6	2.627057	0.332459	0.432472
6	3.926029	0.231781	0.961260
6	1.850596	1.541246	0.809293
8	2.273458	2.709219	0.576819

8	0.787521	1.518041	1.488945
6	0.738791	-0.634627	-1.032097
8	0.364451	0.587284	-1.254107
8	0.129872	-1.667580	-1.313457
1	5.705779	-0.968791	1.116754
1	4.782640	-2.817691	-0.275791
1	2.477612	-2.631482	-1.216643
1	4.312888	1.037974	1.577994
6	-3.121561	-1.386391	-0.370377
6	-3.720263	-2.027403	0.710433
6	-3.909247	-1.346040	1.918316
6	-3.486513	-0.019122	2.042844
6	-2.882630	0.635798	0.969371
6	-2.711769	-0.044849	-0.247162
1	-2.949049	-1.920518	-1.299862
1	-4.032215	-3.063404	0.611912
1	-4.374969	-1.849757	2.760922
1	-3.616639	0.509802	2.983022
1	-2.540607	1.656858	1.091881
16	-1.975720	0.662141	-1.687773
6	-1.771547	2.420696	-1.285240
1	-1.310789	2.870665	-2.167230
1	-2.744783	2.881542	-1.097415
1	-1.097217	2.538034	-0.435050

TS-B

HF=-1277.8467396 <S2>=0.658697

6	4.636929	-0.943462	0.721370
6	4.122229	-2.001459	-0.041076
6	2.836774	-1.918030	-0.574280
6	2.046038	-0.785288	-0.347174
6	2.561543	0.288145	0.419069
6	3.861975	0.189362	0.949039
6	1.785210	1.531146	0.734097
8	2.271894	2.646484	0.425509
8	0.684009	1.449752	1.349858
6	0.674116	-0.754176	-0.975279
8	0.372346	0.464239	-1.369504
8	-0.017174	-1.755219	-1.116095
1	5.639911	-1.006569	1.134900
1	4.721214	-2.892206	-0.211469
1	2.421745	-2.732397	-1.159990
1	4.252953	1.017195	1.532976
6	-3.466883	-1.022096	-0.581738
6	-4.203899	-1.667436	0.407033
6	-4.089022	-1.265097	1.742390
6	-3.225287	-0.219495	2.089619
6	-2.479625	0.437530	1.113292
6	-2.619417	0.046587	-0.229551
1	-3.541225	-1.338207	-1.618228
1	-4.862554	-2.487780	0.136589
1	-4.660977	-1.774225	2.513304
1	-3.116654	0.076357	3.129209
1	-1.770024	1.205684	1.398393
16	-1.744648	0.793572	-1.564839
6	-1.392307	2.480450	-0.995628

1	-0.867432	2.970290	-1.818266
1	-2.338407	2.987485	-0.789929
1	-0.743016	2.455079	-0.115315

INT-AB

HF=-1277.8684676

6	-3.897233	-2.075580	-0.167267
6	-4.389638	-1.101216	0.715126
6	-3.649319	0.045509	0.989479
6	-2.390356	0.263264	0.407811
6	-1.905189	-0.724545	-0.487459
6	-2.660654	-1.884916	-0.765080
6	-0.603015	-0.639567	-1.159617
8	-0.146644	0.696038	-1.160144
8	0.057104	-1.510874	-1.676739
6	-1.632540	1.543259	0.793505
8	-0.626471	1.382914	1.550687
8	-2.087578	2.599776	0.318679
1	-4.478166	-2.967495	-0.384510
1	-5.359692	-1.240315	1.186807
1	-4.042951	0.800177	1.664293
1	-2.257192	-2.618623	-1.456585
6	1.991474	-0.087451	1.203070
6	2.783421	-0.876451	2.038365
6	3.912175	-1.537290	1.539615
6	4.259267	-1.434117	0.188961
6	3.476262	-0.664451	-0.671478

6	2.365949	0.009627	-0.143719
1	1.085200	0.404737	1.564487
1	2.509904	-0.976034	3.084844
1	4.518659	-2.145579	2.205358
1	5.126247	-1.961268	-0.198184
1	3.718224	-0.597064	-1.728547
16	1.478782	1.022138	-1.317710
6	1.342154	2.635622	-0.490606
1	2.362017	2.990553	-0.320684
1	0.803121	3.293288	-1.175903
1	0.766279	2.490397	0.437880

INT-A

HF=-1277.8656768

6	1.820146	3.058105	-0.265137
6	2.464644	2.472275	-1.363616
6	2.669355	1.094425	-1.407860
6	2.225629	0.298347	-0.345916
6	1.580035	0.884198	0.751869
6	1.376095	2.268308	0.793481
6	1.091432	0.052013	1.862255
8	1.279069	-1.311191	1.792701
8	0.508179	0.436147	2.848674
6	2.463052	-1.153667	-0.387786
8	2.057561	-1.916488	0.685421
8	3.028669	-1.764792	-1.263235
1	1.662636	4.132599	-0.238710

1	2.807260	3.094314	-2.185729
1	3.166490	0.621411	-2.248462
1	0.867696	2.700265	1.649243
6	-2.733463	-0.433059	0.688427
6	-3.554382	0.607142	1.136577
6	-3.889837	1.665741	0.290857
6	-3.398713	1.675849	-1.019589
6	-2.587284	0.638786	-1.477984
6	-2.243846	-0.426007	-0.625551
1	-2.477595	-1.235106	1.372512
1	-3.923761	0.586201	2.158864
1	-4.528088	2.470825	0.644851
1	-3.657710	2.488770	-1.693765
1	-2.226084	0.645746	-2.503819
16	-1.166827	-1.679321	-1.304018
6	-1.297579	-3.057122	-0.114168
1	-2.339858	-3.359625	0.021607
1	-0.741324	-3.883862	-0.563894
1	-0.839948	-2.813827	0.847942

TS-A

HF=-1277.8416244

6	4.064732	-2.220712	0.062390
6	4.867195	-1.172055	-0.397495
6	4.308194	0.087638	-0.599744
6	2.951368	0.325417	-0.339888
6	2.143614	-0.727240	0.133272

6	2.714949	-1.998505	0.320850
6	0.685287	-0.635210	0.492969
8	0.119896	0.595814	0.573548
8	0.040755	-1.643906	0.755104
6	2.443855	1.711359	-0.635288
8	1.188680	1.944895	-0.427035
8	3.189911	2.587256	-1.085548
1	4.488171	-3.209144	0.220153
1	5.921591	-1.337119	-0.603648
1	4.903791	0.915113	-0.970731
1	2.078587	-2.800637	0.677273
6	-3.212536	0.839473	-0.755055
6	-4.049335	0.409167	-1.784810
6	-4.541351	-0.899799	-1.797740
6	-4.191864	-1.787913	-0.774850
6	-3.361026	-1.371175	0.262809
6	-2.878439	-0.050576	0.277688
1	-2.817348	1.849116	-0.771662
1	-4.307269	1.097807	-2.584579
1	-5.189529	-1.228238	-2.605462
1	-4.564315	-2.808375	-0.785407
1	-3.076505	-2.061410	1.051278
16	-1.811351	0.370772	1.622860
6	-1.830755	2.185849	1.666362
1	-2.860302	2.550649	1.685485
1	-1.319198	2.468684	2.589215
1	-1.273313	2.584416	0.814953

TS-C

HF=-1277.8662385

6	4.669498	-0.433421	-0.914320
6	4.460462	0.933367	-1.156418
6	3.233971	1.496369	-0.839234
6	2.207736	0.704586	-0.278230
6	2.404929	-0.682534	-0.038911
6	3.659033	-1.220316	-0.368298
6	1.330021	-1.635383	0.513962
8	1.293962	-1.772859	1.760180
8	0.593202	-2.154669	-0.363773
6	0.962588	1.418179	0.030821
8	0.080141	0.520714	0.680562
8	0.640912	2.564018	-0.170368
1	5.628805	-0.884346	-1.157871
1	5.249173	1.545543	-1.584510
1	3.044021	2.551620	-1.011051
1	3.830931	-2.278573	-0.192598
6	-3.649356	1.025731	-0.253540
6	-4.573116	0.510682	-1.164245
6	-4.335394	-0.726942	-1.770807
6	-3.177067	-1.455616	-1.476466
6	-2.242858	-0.973302	-0.557764
6	-2.510455	0.264595	0.042176
1	-3.807823	1.997942	0.205888
1	-5.464384	1.081267	-1.408351
1	-5.051666	-1.119858	-2.487472
1	-2.987287	-2.405878	-1.966967

1	-1.315909	-1.522810	-0.360167
16	-1.394288	0.963491	1.247167
6	-1.374557	-0.262397	2.599265
1	-0.915996	0.228591	3.460665
1	-2.410472	-0.538015	2.808959
1	-0.749118	-1.110544	2.278045

P-C

HF=-1277.9205663

6	-4.379225	0.895972	-1.182448
6	-4.585133	1.132150	0.186927
6	-3.778260	0.524589	1.156434
6	-2.771042	-0.319555	0.703899
6	-2.567340	-0.553871	-0.653089
6	-3.359834	0.044868	-1.625407
6	-1.421593	-1.484694	-0.779796
8	-0.889919	-1.947262	-1.754861
8	-1.003964	-1.809915	0.510384
6	-1.761859	-1.105441	1.453208
8	0.058787	1.049291	0.015115
8	-1.565995	-1.210714	2.633015
1	-5.023466	1.384261	-1.908652
1	-5.385215	1.799102	0.496583
1	-3.927246	0.703759	2.216857
1	-3.189837	-0.140696	-2.681557
6	3.959610	0.679168	0.717547
6	4.974389	-0.256310	0.500468

6	4.723850	-1.391583	-0.277787
6	3.458878	-1.594569	-0.837372
6	2.438303	-0.661350	-0.632168
6	2.706850	0.473398	0.132688
1	4.142954	1.550915	1.342746
1	5.952849	-0.105354	0.949029
1	5.511676	-2.123309	-0.436590
1	3.258170	-2.484136	-1.428290
1	1.446076	-0.818227	-1.043730
16	1.376487	1.685172	0.440708
6	1.817544	2.850268	-0.911971
1	1.078298	3.655652	-0.890321
1	2.820741	3.251120	-0.739456
1	1.769098	2.314712	-1.863957

TS-D1

HF=-1277.8517396

6	4.702132	-1.405914	-0.326922
6	3.803955	-2.474202	-0.224459
6	2.446578	-2.227061	-0.013201
6	1.993773	-0.907640	0.101605
6	2.895706	0.170520	0.021633
6	4.249037	-0.090337	-0.205950
6	2.388238	1.578056	0.234864
8	2.805799	2.524905	-0.421196
8	1.465281	1.616534	1.174350
6	0.535900	-0.651589	0.288560

8	0.078229	0.126355	-0.788661
8	-0.193005	-1.106335	1.130768
1	5.758096	-1.600505	-0.496197
1	4.159373	-3.497484	-0.310880
1	1.738621	-3.048102	0.059334
1	4.936507	0.747345	-0.278399
6	-3.505804	-0.180646	-1.348470
6	-4.669873	-0.912426	-1.100572
6	-5.011908	-1.252881	0.209406
6	-4.191054	-0.866329	1.276278
6	-3.025213	-0.139729	1.043789
6	-2.693737	0.200066	-0.272620
1	-3.234808	0.092229	-2.364740
1	-5.304679	-1.210374	-1.930078
1	-5.917574	-1.821220	0.402855
1	-4.453513	-1.141577	2.293772
1	-2.376218	0.128141	1.869102
16	-1.279787	1.208426	-0.729396
6	-0.919554	2.337281	0.525226
1	-0.984778	3.341094	0.104149
1	-1.487200	2.195590	1.442853
1	0.403270	2.125353	0.861485

INT-D

HF=-1277.8896175

6	-4.688940	1.459898	-0.538632
6	-3.851741	2.413756	0.045722

6	-2.552910	2.064399	0.416887
6	-2.070486	0.764368	0.219734
6	-2.927430	-0.202846	-0.342873
6	-4.225410	0.158448	-0.730802
6	-2.571536	-1.643270	-0.519219
8	-2.860637	-2.310427	-1.492894
8	-1.980999	-2.194969	0.574681
6	-0.613227	0.511161	0.540047
8	-0.012038	-0.285201	-0.293876
8	-0.077251	1.085466	1.498817
1	-5.698918	1.724687	-0.840146
1	-4.205610	3.429398	0.203800
1	-1.885257	2.796913	0.859889
1	-4.867814	-0.596171	-1.174625
6	3.778238	-0.753383	-0.970861
6	4.766417	0.098885	-1.471403
6	4.813613	1.432905	-1.059480
6	3.868043	1.922946	-0.152084
6	2.872066	1.086619	0.355717
6	2.852238	-0.249598	-0.053273
1	3.735423	-1.791296	-1.289869
1	5.493705	-0.282034	-2.182991
1	5.581151	2.094083	-1.452846
1	3.894161	2.965597	0.152935
1	2.097780	1.456966	1.022468
16	1.627204	-1.410467	0.567519
6	1.812842	-1.369987	2.182147
1	1.228299	-2.081331	2.757034
1	2.293921	-0.542750	2.691853

1	-1.825359	-3.131354	0.348589

TS-D2

HF=-1277.888656

6	4.898277	-1.097055	-0.494153
6	4.131043	-2.193292	-0.091310
6	2.771356	-2.029973	0.176905
6	2.154300	-0.778320	0.054506
6	2.938642	0.329812	-0.323473
6	4.301111	0.157998	-0.608741
6	2.430664	1.730840	-0.401413
8	2.742655	2.534124	-1.257767
8	1.653770	2.094720	0.659422
6	0.651138	-0.717821	0.234409
8	0.006331	0.037757	-0.574453
8	0.121137	-1.416938	1.133715
1	5.955772	-1.216032	-0.714738
1	4.587856	-3.175233	0.004133
1	2.160171	-2.875717	0.477276
1	4.885653	1.021874	-0.910805
6	-3.963314	1.005208	-0.488099
6	-5.046840	0.334587	-1.061311
6	-5.074188	-1.062317	-1.078441
6	-4.015186	-1.794816	-0.530869
6	-2.922318	-1.141951	0.041542
6	-2.922905	0.256174	0.069924
1	-3.936085	2.091603	-0.472755

1	-5.864085	0.905103	-1.493624
1	-5.916409	-1.581286	-1.528234
1	-4.029188	-2.880822	-0.563609
1	-2.066227	-1.687279	0.430958
16	-1.555045	1.169419	0.784811
6	-1.342967	0.515606	2.260045
1	-0.576706	0.953933	2.890459
1	-1.859652	-0.379425	2.582215
1	1.415592	3.027182	0.497298

P-D

HF=-1277.9572109

6	5.223644	-0.452034	0.010875
6	4.575453	-1.658462	-0.258798
6	3.185067	-1.690045	-0.376928
6	2.427287	-0.521500	-0.219459
6	3.082219	0.690813	0.082882
6	4.477342	0.715798	0.179241
6	2.371257	1.979204	0.369175
8	2.709348	3.057592	-0.073065
8	1.366239	1.828916	1.261017
6	0.962875	-0.543724	-0.514677
8	0.346859	0.384313	-0.997711
8	0.409252	-1.751753	-0.239877
1	6.306464	-0.417478	0.093746
1	5.148852	-2.572115	-0.389053
1	2.678526	-2.619713	-0.612534

1	4.969038	1.658600	0.398427
6	-4.597690	-0.695224	0.500799
6	-5.594693	0.186245	0.072562
6	-5.250026	1.373003	-0.578735
6	-3.902009	1.681282	-0.789260
6	-2.897986	0.819345	-0.341570
6	-3.246416	-0.380498	0.297374
1	-4.864727	-1.628748	0.988132
1	-6.639654	-0.064375	0.237236
1	-6.025484	2.053436	-0.920962
1	-3.626080	2.604419	-1.292987
1	-1.852809	1.069547	-0.493078
16	-2.015781	-1.507290	0.969169
6	-0.990547	-1.924367	-0.503796
1	-1.092987	-2.987662	-0.721021
1	-1.304734	-1.313894	-1.350992
1	0.947842	2.703057	1.375362

INT-E1

HF=-2555.7821006

6	5.052668	4.172314	-0.240190
6	5.850277	3.221150	-0.884863
6	5.300127	1.998145	-1.272655
6	3.950666	1.730396	-1.009190
6	3.140649	2.684028	-0.374417
6	3.705847	3.903196	0.009691
6	1.666589	2.389310	-0.152054

8	1.251450	1.313017	-0.694700
8	0.992358	3.187683	0.540192
6	3.404240	0.413752	-1.456103
8	3.290992	-0.483080	-0.370636
8	3.269240	0.010255	-2.585921
1	5.480486	5.125700	0.059529
1	6.896907	3.430167	-1.089630
1	5.912074	1.257441	-1.780724
1	3.063187	4.629112	0.498191
6	1.714813	-2.852267	1.611965
6	1.885573	-3.488905	2.844287
6	3.117316	-4.044804	3.198930
6	4.200967	-3.988444	2.314714
6	4.051207	-3.372006	1.074672
6	2.811161	-2.800164	0.743726
1	0.728458	-2.469671	1.351116
1	1.036775	-3.550354	3.519024
1	3.232518	-4.535092	4.161944
1	5.155693	-4.430320	2.584735
1	4.883189	-3.332256	0.376498
16	2.769913	-2.023789	-0.861555
6	1.024741	-1.754756	-1.303875
1	0.965845	-1.964569	-2.373484
1	0.353074	-2.393304	-0.715717
1	0.813543	-0.698421	-1.109391
6	-4.441052	-3.750367	-2.033816
6	-4.647751	-2.714608	-2.955479
6	-4.096113	-1.465093	-2.706160
6	-3.336141	-1.235726	-1.541312

6	-3.121759	-2.275809	-0.604058
6	-3.686661	-3.530467	-0.883458
6	-2.324679	-2.136957	0.701265
8	-1.169962	-2.651700	0.668103
8	-2.892342	-1.565560	1.660017
6	-2.824954	0.142265	-1.374109
8	-1.900938	0.201399	-0.342176
8	-3.133840	1.129276	-2.004582
1	-4.869629	-4.733144	-2.216693
1	-5.233103	-2.884007	-3.854998
1	-4.240129	-0.643225	-3.400857
1	-3.525089	-4.340664	-0.177646
6	-3.165013	3.725573	0.737636
6	-4.310344	4.303099	1.290619
6	-5.212812	3.512803	2.007292
6	-4.976905	2.143434	2.178985
6	-3.830168	1.548531	1.651005
6	-2.938102	2.360108	0.938239
1	-2.462002	4.323369	0.163887
1	-4.499782	5.363448	1.149826
1	-6.108686	3.962713	2.427272
1	-5.688375	1.530534	2.725448
1	-3.650559	0.478522	1.763549
16	-1.413680	1.718095	0.224232
6	-0.647584	0.995548	1.706003
1	0.296551	0.568879	1.373517
1	-0.469238	1.827224	2.388450
1	-1.327926	0.239022	2.107206

TS-E1

HF=-2555.7595398

6	4.537715	4.050049	-1.426327
6	5.251847	3.063953	-2.112338
6	4.779109	1.751449	-2.122862
6	3.595526	1.418229	-1.448784
6	2.856400	2.411354	-0.774626
6	3.351509	3.720984	-0.768623
6	1.503192	2.140391	-0.129094
8	0.895940	1.083052	-0.503571
8	1.063508	2.974295	0.700967
6	3.203910	-0.027203	-1.489739
8	3.206353	-0.572800	-0.231766
8	3.028953	-0.688700	-2.489788
1	4.899211	5.075405	-1.412433
1	6.170813	3.312407	-2.636937
1	5.325681	0.975477	-2.651954
1	2.774211	4.474247	-0.241833
6	1.444378	-2.294914	2.502956
6	1.629529	-2.330177	3.889570
6	2.907171	-2.219272	4.440352
6	4.019706	-2.079451	3.603171
6	3.854276	-2.050534	2.219742
6	2.563142	-2.144345	1.680906
1	0.447655	-2.403339	2.090800
1	0.763119	-2.450965	4.534142
1	3.039407	-2.248541	5.518593

1	5.017137	-1.995323	4.025477
1	4.715900	-1.936625	1.568902
16	2.452781	-2.184548	-0.117960
6	0.812106	-2.047255	-0.577037
1	0.772788	-2.310249	-1.635829
1	-0.243054	-2.722814	0.130087
1	0.470479	-1.022024	-0.411854
6	-2.804991	-3.751822	-3.230949
6	-2.895613	-2.583039	-3.992565
6	-2.756601	-1.347377	-3.369318
6	-2.533159	-1.263159	-1.983539
6	-2.454970	-2.440700	-1.207799
6	-2.581515	-3.676733	-1.855597
6	-2.335618	-2.480996	0.308645
8	-1.209539	-2.956101	0.783536
8	-3.294982	-2.158197	1.001488
6	-2.353753	0.110837	-1.454473
8	-1.841625	0.115810	-0.166940
8	-2.596967	1.143564	-2.034982
1	-2.906333	-4.723613	-3.707244
1	-3.064464	-2.634646	-5.064316
1	-2.803406	-0.426870	-3.941955
1	-2.514644	-4.586777	-1.266008
6	-3.383660	3.515616	0.932386
6	-4.616731	3.985818	1.392274
6	-5.555755	3.090210	1.909717
6	-5.269570	1.721182	1.971529
6	-4.037162	1.235578	1.532203
6	-3.105772	2.148418	1.022497

1	-2.653710	4.200107	0.507505
1	-4.844357	5.046320	1.332332
1	-6.518213	3.456681	2.256712
1	-6.008273	1.024790	2.358440
1	-3.824604	0.168875	1.555474
16	-1.462745	1.654607	0.436498
6	-0.780224	1.021770	1.991959
1	0.176747	0.568561	1.744303
1	-0.624848	1.900181	2.621123
1	-1.487499	0.317249	2.432906

INT-E2

HF=-2555.7986934

6	4.220644	4.313691	-0.053813
6	5.480765	3.759249	-0.291328
6	5.599603	2.397590	-0.573536
6	4.471284	1.570371	-0.619669
6	3.197253	2.133659	-0.400237
6	3.087822	3.502135	-0.109120
6	1.950253	1.319880	-0.567378
8	1.841367	0.382472	-1.345692
8	0.945421	1.744869	0.215330
6	4.713510	0.094177	-0.863388
8	4.181091	-0.686945	0.035276
8	5.410129	-0.271368	-1.813379
1	4.118313	5.373001	0.166757
1	6.369625	4.384226	-0.257071

1	6.573872	1.956729	-0.763037
1	2.104078	3.926320	0.061947
6	2.097817	-4.256336	0.204829
6	1.275778	-4.721370	1.234195
6	1.374682	-4.174579	2.515952
6	2.302253	-3.159916	2.769008
6	3.123694	-2.677088	1.747967
6	3.004946	-3.219425	0.461652
1	2.040534	-4.707592	-0.780124
1	0.566268	-5.519192	1.032442
1	0.735422	-4.541324	3.314416
1	2.386282	-2.733131	3.764880
1	3.822367	-1.870374	1.932921
16	4.152686	-2.682621	-0.825109
6	3.302343	-2.817126	-2.202638
1	3.862416	-2.659078	-3.117725
1	-3.254955	-2.795461	-0.724324
1	2.218693	-2.781489	-2.229189
6	-7.210574	-1.318309	-1.457666
6	-6.871863	-0.265590	-2.312480
6	-5.613528	0.325815	-2.217473
6	-4.672880	-0.128698	-1.283219
6	-5.014498	-1.194047	-0.426152
6	-6.287499	-1.775314	-0.515827
6	-4.097451	-1.741263	0.643340
8	-3.251513	-2.732737	0.246467
8	-4.158888	-1.437891	1.811220
6	-3.341899	0.581948	-1.222965
8	-2.484960	0.000627	-0.407970

8	-3.121596	1.600223	-1.869664
1	-8.192703	-1.779849	-1.517047
1	-7.588293	0.097014	-3.044690
1	-5.332161	1.156067	-2.857502
1	-6.555382	-2.582028	0.161590
6	-1.401888	3.478130	0.561159
6	-2.023391	4.434967	1.365187
6	-2.738085	4.042953	2.500507
6	-2.843130	2.688679	2.827781
6	-2.228689	1.719439	2.030861
6	-1.502517	2.130806	0.912596
1	-0.854733	3.776380	-0.326916
1	-1.952205	5.485517	1.097406
1	-3.222094	4.791040	3.122659
1	-3.413658	2.376099	3.697832
1	-2.352218	0.668436	2.267595
16	-0.715121	0.932180	-0.198019
6	-0.266996	-0.479860	0.877663
1	0.533287	-0.997122	0.347290
1	0.106222	-0.078009	1.819166
1	-1.134973	-1.120524	1.013217

TS-E2

HF=-2555.7685469

6	6.050178	-2.832445	-1.138725
6	6.514139	-2.045804	-0.079858
6	5.645871	-1.168621	0.571459
6	4.304164	-1.063665	0.182785

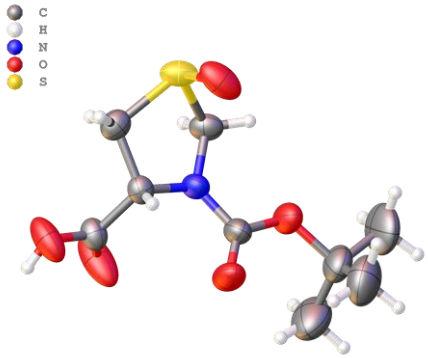
6	3.835826	-1.858601	-0.883061
6	4.717139	-2.736995	-1.532649
6	2.406976	-1.797603	-1.325203
8	1.620079	-0.982407	-0.785937
8	2.034813	-2.620281	-2.255676
6	3.431517	-0.091837	0.963370
8	3.493616	1.120048	0.502036
8	2.821613	-0.459354	1.974218
1	6.722256	-3.515706	-1.651394
1	7.551614	-2.113508	0.238723
1	6.008150	-0.558259	1.394764
1	4.334248	-3.341443	-2.348373
6	1.301561	4.692521	0.248283
6	1.517006	5.774154	-0.608313
6	2.719653	5.887800	-1.310007
6	3.710955	4.915478	-1.152962
6	3.509990	3.824078	-0.305027
6	2.295144	3.711970	0.382710
1	0.376479	4.624189	0.810853
1	0.743794	6.529884	-0.716310
1	2.884944	6.732949	-1.972921
1	4.647158	4.997137	-1.698503
1	4.263494	3.053647	-0.203506
16	2.052983	2.377865	1.578999
6	0.478778	2.009170	1.419706
1	0.068999	1.324173	2.153412
1	-3.276231	1.702346	0.986299
1	-0.093139	2.229765	0.525298
6	-7.530128	-0.170468	-0.534407

6	-6.816185	-1.337820	-0.803612
6	-5.427352	-1.321786	-0.719063
6	-4.723623	-0.164324	-0.336741
6	-5.447350	1.031368	-0.067420
6	-6.845950	0.993221	-0.191522
6	-4.927092	2.427604	0.282415
8	-3.766674	2.563761	0.926503
8	-5.601099	3.402767	0.015290
6	-3.234796	-0.311142	-0.226954
8	-2.735652	-1.254843	-1.019315
8	-2.520204	0.338446	0.540687
1	-8.614625	-0.158419	-0.600858
1	-7.331357	-2.252579	-1.083235
1	-4.864217	-2.219987	-0.943581
1	-7.387297	1.916593	-0.019287
6	0.094391	-2.213590	1.439344
6	0.162218	-3.091001	2.525540
6	-0.625242	-4.243273	2.556416
6	-1.488812	-4.534853	1.493950
6	-1.563457	-3.677153	0.397116
6	-0.764729	-2.526817	0.382417
1	0.740885	-1.343361	1.408101
1	0.847341	-2.863790	3.336859
1	-0.566665	-4.918924	3.405645
1	-2.104295	-5.430006	1.517143
1	-2.241785	-3.895707	-0.421313
16	-0.850738	-1.377554	-1.004914
6	-0.577396	-2.363427	-2.381060
1	0.788298	-2.514619	-2.350192

1	-1.041730	-3.348505	-2.338702
1	-0.804536	-1.802750	-3.290316

Table S - 1 Crystal data and structure refinement for SL-20160929.

Identification code	SL-20160929
Empirical formula	$C_9H_{15}NO_5S$
Formula weight	249.28
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	6.2179(3)
b/Å	10.0744(4)
c/Å	10.4155(5)
α /°	90
β /°	107.042(5)
γ /°	90
Volume/Å^3	623.80(5)
Z	2
ρ calcg/cm^3	1.327
μ /mm^{-1}	0.265
F(000)	264.0
Crystal size/mm^3	0.1 × 0.1 × 0.06
Radiation	MoKα (λ = 0.71073)
2$^\Theta$ range for data collection/°	6.854 to 50.676
Index ranges	-7 ⩽ h ⩽ 7, -12 ⩽ k ⩽ 12, -12 ⩽ l ⩽ 12
Reflections collected	5929
Independent reflections	2288 [R_{int} = 0.0261, R_{sigma} = 0.0277]
Data/restraints/parameters	2288/1/160
Goodness-of-fit on F^2	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0325, wR_2 = 0.0771
Final R indexes [all data]	R_1 = 0.0350, wR_2 = 0.0791
Largest diff. peak/hole / e Å^{-3}	0.17/-0.16



Flack parameter	-0.04(3)