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A mild and chemoselective CALB biocatalysed synthesis of sulfoxides exploiting the dual role of AcOEt as solvent and reagent.

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Supporting Information

General information

Reagents and solvents were used as supplied from the vendor without further purification. Thin layer chromatography plates (Merk, silica gel 60 F_{254}, aluminium backed) were viewed under UV light and stained using $KMnO_4$ developed using heat. $MgSO_4$ (Sigma Aldrich, anhydrous ≥ 98.0 %) was used as the drying agent. Dry loadings for column chromatography were done using Celite® (Acros Organics). Column chromatography was performed on silica gel for flash chromatography (Sigma Aldrich, 40-63 μm particle size, 60 Å pore size). Microwave irradiations were conducted using a CEM Discover Synthesis Unit. The machine consists of a continuous focused microwave power delivery system with operator, selectable power output from 0 to 300 W. The temperature of the contents of the vessels was monitored using a calibrated infrared temperature control mounted under the reaction vessel. All the experiments were performed using a stirring option whereby the contents of the vessel are stirred by means of rotating magnetic plate located below the floor of the microwave cavity and a Teflon® coated magnetic stirring bar in the vessel.

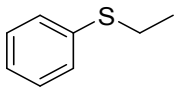
Products were characterised by ^{1}H NMR and ^{13}C NMR spectra where applicable obtained from either an Ascend400 Spectrometer (Bruker, Germany) in $CDCl_3$ (δ_H, 400 MHz), (δ_C, 101 MHz) at 300 K. Chemical shifts are reported in ppm relative to the reference peaks of the solvents: $CDCl_3$ (^{1}H NMR 7.26 and ^{13}C NMR 77.16) unless stated otherwise. Coupling constants (*J*) are reported in Hz, multiplicities are specified as singlet (s), doublet (d), triplet (t), doublet of doublet (dd), doublet of quartet (dq), doublet of doublet of triplet (ddt), pentet (p), heptept (h), multiplet (m).

HPLC and LC-MS analysis was carried out using an Agilent series 1100 LC/MSD system coupled with UV detector at l = 254 nm and an electrospray ionization source (ESI). The columns used were Chiralpak IC® (0.5μm, 4.6mm X 250mm), and Chiralpak IG® (5μm, 4.6mm X 250mm), supplied by Daicel. Hexane and isopropanol were used as an isocratic mobile phase system for the Chiralpak IC, while heptane and ethanol were used for the Chiralpak IG. Mass spectra were acquired in positive mode scanning over the mass range of 50 – 1500. The following ion source parameters were used: drying gas flow, 12 mL/min; nebulize pressure, 35 psi; and drying gas temperature, 350 ºC.

General procedure for the synthesis of sulfides (5a-r)

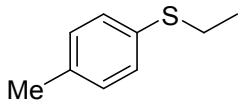
The appropriate thiophenol (1.36 mmol) and halo-alkane (2.04 mmol) were added to a microwave (MW) vial and dissolved in water (2 mL). K_2CO_3 (1.36 mmol) and NaI (0.13 mmol) were then added to the vial and the resulting reaction mixture was stirred at 140 ºC in intervals of 5 minutes until completion was observed on TLC under microwave irradiation. The reaction was then extracted in AcOEt (3 x 2mL) and the collected organic layers were washed with water (1 x 2mL), brine (2 x 2mL), dried on $MgSO_4$ and evaporated under vacuum. The desired sulfides **5** were obtained as pale yellow oils and proved to be pure enough to be used in the next step without any further purification.

Ethyl-phenyl sulfane (5c)[1]



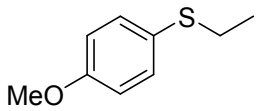
Yellow oil, >99 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.16 (m, 5H, *Ar*), 2.97 (q, *J* = 7.3 Hz, 2H), 1.35 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.7, 129.0 (2C), 128.9 (2C), 125.8, 27.7, 14.4 ppm.

Ethyl(4-methylphenyl)sulfane (5d)[2]



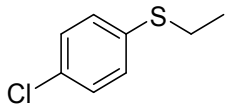
Oil, 64% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 (d, *J* = 8.2 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 2.96 (q, *J* = 7.3 Hz, 2H), 2.38 (s, 3H), 1.36 (t, *J* = 7.3 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.8, 132.8, 129.9, 129.6, 53.5, 28.3, 20.9, 14.5 ppm.

Ethyl(4-methoxyphenyl)sulfane (5e)[2]



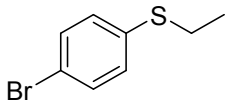
Yellow oil, 22 % yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 (d, *J* = 8.7 Hz, 2H, *Ar*), 6.85 (d, *J* = 8.8 Hz, 2H, *Ar*), 3.79 (s, 3H), 2.84 (q, *J* = 7.3 Hz, 2H), 1.25 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9, 133.3 (2C), 126.6, 114.6 (2C), 55.4, 29.9, 14.7 ppm.

Ethyl(4-chlorophenyl)sulfane (5f)[2]



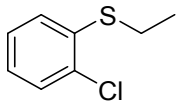
Colourless oil, 68 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (s, 4H, *Ar*), 2.93 (q, *J* = 7.4 Hz, 2H), 1.31 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.2, 131.7, 130.3 (2C), 129.0 (2C), 27.9, 14.3 ppm.

Ethyl(4-bromophenyl)sulfane (5g)[2]



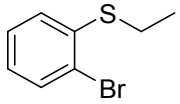
Oil, 68% yield. 1H NMR (400 MHz, Chloroform-d) δ 7.40 (d, J = 8.6 Hz, 2H), 7.19 (d, J = 8.6 Hz, 2H), 2.93 (q, J = 7.3 Hz, 2H), 1.32 (t, J = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.0, 131.9, 130.4, 119.5, 27.7, 14.3 ppm.

Ethyl(2-chlorophenyl)sulfane (5h)[3]



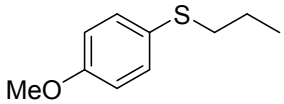
Pale yellow oil, 99 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (dd, *J* = 7.9, 1.5 Hz, 1H, *Ar*), 7.31 – 7.20 (m, 2H, *Ar*), 7.15 – 7.06 (m, 1H, *Ar*), 2.98 (q, *J* = 7.4 Hz, 2H), 1.38 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.3, 132.8, 129.5, 127.6, 127.0, 126.0, 26.3, 13.6 ppm.

Ethyl(2-bromophenyl)sulfane (5i)[4]



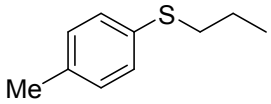
Pale yellow oil, 99 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 8.0, 1.4 Hz, 1H, *Ar*), 7.31 – 7.19 (m, 2H, *Ar*), 7.02 (ddd, *J* = 7.9, 7.0, 1.8 Hz, 1H, *Ar*), 2.97 (q, *J* = 7.4 Hz, 2H), 1.39 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.4, 132.9, 127.7, 127.4, 126.2, 123.0, 26.8, 13.7 ppm.

4-Methoxyphenyl(propyl)sulfide (5j)[2]



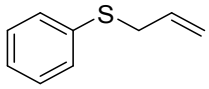
Pale yellow oil, 95 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.9 Hz, 2H, *Ar*), 6.89 (d, *J* = 8.9 Hz, 2H, *Ar*), 3.81 (s, 3H), 2.85 (t, *J* = 7.3 Hz, 2H), 1.67 (h, *J* = 7.3 Hz, 2H), 1.06 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.8, 133.0 (2C), 127.0, 114.5 (2C), 55.2, 37.8, 22.7, 13.3 ppm.

4-Methylphenyl(propyl)sulfide (5k)[5]



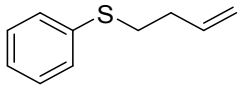
Pale yellow oil, 51 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 8.2 Hz, 2H, *Ar*), 7.15 (d, *J* = 8.3 Hz, 2H, *Ar*), 2.92 (t, *J* = 7.3 Hz, 2H), 2.38 (s, 3H), 1.72 (h, *J* = 7.3 Hz, 2H), 1.09 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.8, 133.2, 129.9 (2C), 129.6 (2C), 36.4, 22.7, 21.0, 13.4 ppm.

Allyl(phenyl)sulfane (5l)[1]



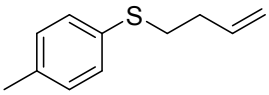
Pale yellow oil, 60 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.15 (m, 5H, *Ar*), 5.88 (ddt, *J* = 16.9, 10.0, 6.8 Hz, 1H, C*H*), 5.18 – 5.04 (m, 2H), 3.55 (d, *J* = 6.8 Hz, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.0, 131.2, 129.1 (2C), 125.3, 124.4 (2C), 124.0, 77.5, 77.2, 76.9, 61.0 ppm.

But-3-en-1-yl(phenyl)sulfane (5m)[6]



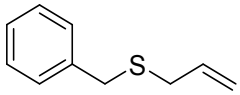
Oil, 65% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.33 (m, 2H, *Ar*), 7.32 – 7.25 (m, 2H, *Ar*), 7.21 – 7.16 (m, 1H, *Ar*), 5.86 (ddt, *J* = 16.9, 10.2, 6.6 Hz, 1H, C*H*), 5.13 – 5.04 (m, 2H), 2.99 (t, *J* = 7.5 Hz, 2H), 2.48 – 2.35 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.5, 129.4, 129.4, 129.0, 126.1, 116.4, 33.5, 33.2 ppm.

But-3-en-1-yl(p-tolyl)sulfane (5n)[7]



Pale yellow oil, 72 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.24 (m, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 5.90 – 5.78 (m, 1H), 5.11 – 5.01 (m, 2H), 2.94 (t, *J* = 7.4 Hz, 2H), 2.40 – 2.33 (m, 2H), 2.32 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.5, 132.6, 130.2, 129.7, 128.6, 116.1, 33.8, 33.5, 21.0 ppm.

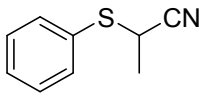
Allyl(benzyl)sulfane (5p)[8]



Yellow oil, 55 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.19 (m, 5H, *Ar*), 5.88 – 5.73 (m, 1H, C*H*), 5.18 – 5.03 (m, 2H), 3.67 (s, 2HS), 3.04 (d, *J* = 7.1 Hz, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.3, 134.2, 129.0, 128.5, 127.0, 117.3, 34.9, 34.1 ppm.

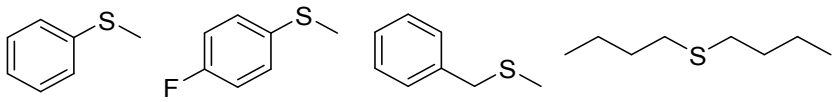
2-(Phenylthio)propanenitrile (5q)

The compound was synthesised according to previous literature.[9a]



Yellow oil, 76 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.60 (m, 2H, *Ar*), 7.42 – 7.37 (m, 3H, *Ar*), 3.80 (q, *J* = 7.3 Hz, 1H, C*H*), 1.61 (d, *J* = 7.3 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.8, 130.5, 129.7, 129.5, 119.9, 31.4, 18.8 ppm.

The compounds **5a**, **5b**, **5o** and **5r** were purchased and used without any purification.

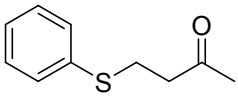


5a **5b** **5o** **5r**

General procedure for the synthesis of sulfides 12a-c

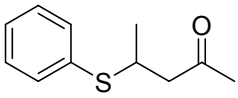
Thiophenol (14.3 mmol) was added to a solution of $NaHCO_3$ (14.3 mmol) in water at (8 mL) at RT, followed by the appropriate α,β-unsaturated ketone/aldehyde (7.14 mmol). The resulting mixture was stirred until the reaction was completed as observed on TLC. The reaction was then extracted in AcOEt (3x10 mL), the collected organic layers were washed with water (1x20 mL) and brine (2x20 mL), dried on $MgSO_4$ and evaporated under reduced pressure. The crude product was purified by column chromatography using a hexane/EtOAc (10:1) eluting system to afford the desired sulfides **12a-c**.

4-(Phenylthio)butan-2-one (12a)[9b]



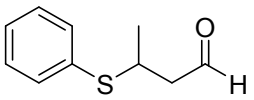
Yellow oil, 92 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.15 (m, 5H, *Ar*), 3.15 (t, *J* = 7.3 Hz, 2H), 2.77 (t, *J* = 7.3 Hz, 2H), 2.15 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 206.5, 135.7, 129.6 (2C), 129.0 (2C), 126.3, 43.1, 30.1, 27.5 ppm.

4-(Phenylthio)pentan-2-one (12b)[10]



Pale yellow oil, 82 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.0 Hz, 2H, *Ar*), 7.29 (dt, *J* = 14.7, 6.9 Hz, 3H, *Ar*), 3.70 (dq, *J* = 13.4, 6.6 Hz, 1H, C*H*), 2.76 (dd, *J* = 17.1, 5.1 Hz, 1H), 2.57 (dd, *J* = 17.1, 8.6 Hz, 1H), 2.14 (s, 3H), 1.30 (d, *J* = 6.7 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 206.6, 134.2, 132.4, 129.0 (2C), 127.3 (2C), 50.4, 38.2, 30.6, 21.0 ppm.

3-(Phenylthio)butanal (12c)[11]



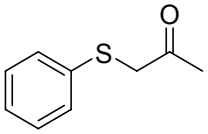
Colourless oil, 73 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.66 (d, *J* = 1.9 Hz, 1H, C*H*O), 7.34 (d, *J* = 6.4 Hz, 2H, *Ar*), 7.27 – 7.14 (m, 3H, *Ar*), 3.60 (h, *J* = 6.8 Hz, 1H, C*H*), 2.66 – 2.43 (m, 2H), 1.27 (d, *J* = 6.9 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.3, 133.6, 133.0 (2C), 129.1 (2C), 127.7, 50.1, 37.6, 21.2 ppm.

General procedure for the synthesis of sulfides 12d-f

Thiophenol (1.95 mmol) and the appropriate 1-bromo-ketone (1.50 mmol) were consecutively added to a solution of $NaHCO_3$ (3.45 mmol) previously dissolved in water (8 mL). The reaction mixture was stirred at RT until completion was observed on TLC. The reaction was extracted in ethyl acetate (3x4 mL), the collected organic layers were washed with water (1x10 mL) and brine (2x10 mL), dried on $MgSO_4$ and evaporated under

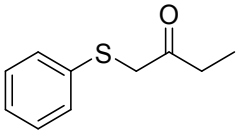
reduced pressure. The crude product was then purified by column chromatography using a hexane/EtOAc (10:1) eluting system to afford the desired sulfides **12d-f**.

3-(Phenylthio)-2-propanone (12d)[12]



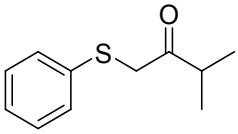
Yellow solid, 85 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.17 (m, 1H, *Ar*), 3.69 (s, 2H), 2.30 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 203.5, 134.7, 129.5 (2C), 129.2 (2C), 126.9, 44.7, 28.0 ppm.

1-(Phenylthio)-2-butanone (12e)[13]



Pale oil, 98 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.19 (m, 3H, *Ar*), 3.70 (s, 2H), 2.64 (q, J = 7.3 Hz, $2HCH_3$), 1.08 (t, J = 7.3 Hz, $3HCH_3$) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 206.2, 135.0, 129.5 (2C), 129.1 (2C), 126.8, 43.6, 33.9, 7.9 ppm.

1-(Phenylthio)-2-pentanone (12f)[14]

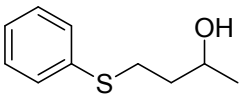


Colourless oil, 54 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.17 (m, 5H, *Ar*), 3.78 (s, 2H), 2.96 (p, J = 6.9 Hz, 1H, C*H*), 1.12 (d, J = 6.9 Hz, 6H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 208.9, 129.6 (2C), 129.1 (2C), 126.8, 42.5, 38.7, 18.4 ppm.

General procedure for the synthesis of sulfides 14a-b

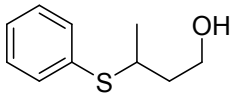
Ketones 12a or 12b (1.00 mmol) were reduced using $NaBH_4$ (1.50 mmol) previously dissolved in MeOH (20 mL). The resulting mixture was stirred until the reaction was completed as observed on TLC. Upon completion, MeOH was evaporated under reduced pressure and the residue dissolved in AcOEt (20 mL), washed with water (1x20 mL) and brine (2x 20 mL), dried on $MgSO_4$ and evaporated under reduced pressure. The crude product was purified by column chromatography to afford the desired sulfides **14a-b**.

4-(Phenylthio)butan-2-ol (14a)[15]



Oil, 67% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.33 (m, 2H, *Ar*), 7.34 – 7.24 (m, 2H, *Ar*), 7.23 – 7.15 (m, 1H, *Ar*), 3.98 (h, J = 6.2 Hz, 1H), 3.12 – 2.97 (m, 2H), 1.83 – 1.73 (m, 2H), 1.67 (s, 1H), 1.22 (d, J = 6.2 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 136.5, 129.3, 129.0, 126.1, 67.1, 38.2, 30.3, 23.8 ppm.

3-(Phenylthio)butan-1-ol (14b)[16]

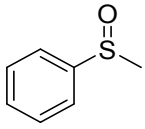


Oil, 74% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.40 (m, 2H, *Ar*), 7.35 – 7.28 (m, 2H, *Ar*), 7.28 – 7.21 (m, 1H, *Ar*), 3.89 – 3.71 (m, 2H), 3.41 (h, J = 6.8 Hz, 1H), 2.06 (s, 1H), 1.93 – 1.73 (m, 2H), 1.33 (d, J = 6.8 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.8, 132.3, 129.0, 127.0, 60.6, 40.4, 39.2, 21.6 ppm.

Biocatalytic oxidation of sulfides using CALB. General procedure.

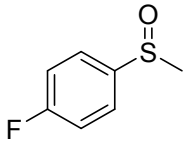
The appropriate sulfide (0.22 mmol), CALB (20 % w/w) and UHP or H_2O_2 (0.24 mmol) were added to a round bottom flask containing ethyl acetate (1 mL). The reaction was stirred for 2-24 h and monitored by TLC until completion. Upon completion, CALB was removed from the reaction mixture by filtration using a celite plug and then rinsed with ethyl acetate (3x2 mL) and the organic layer quenched with 10 mL 10% $Na_2S_2O_{3(aq)}$ followed by 10 mL of H_2O. The collected aqueous layer was then extracted in ethyl acetate (3x5 mL), the collected organic layers were washed with water (1x10 mL) and brine (2x10 mL), dried on $MgSO_4$ and evaporated under reduced pressure. The crude product was then purified by column chromatography using an appropriate hexane/EtOAc eluting system.

Methyl phenyl sulfoxide (6a)[17]



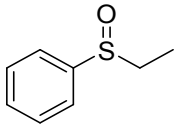
Oil, 89 % yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.59 (m, 2H, *Ar*), 7.57 – 7.45 (m, 3H, *Ar*), 2.71 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.9, 131.1, 129.5, 123.6, 44.1 ppm.

Methyl (4-fluoro)phenyl sulfoxide (6b)[17]



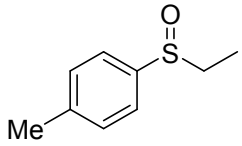
Pale yellow oil, 85% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 – 7.60 (m, 2H, *Ar*), 7.24 – 7.17 (m, 2H, *Ar*), 2.70 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.7, 163.2, 141.3, 141.2, 126.0, 125.9, 116.9, 116.7, 44.2, 44.2 ppm. ^{19}F NMR (376 MHz, $CDCl_3$) δ -108.61 ppm.

Ethyl phenyl sulfoxide (6c)[17]



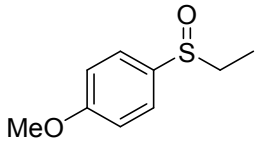
Pale yellow oil, 63 % yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 – 7.57 (m, 2H, *Ar*), 7.54 – 7.45 (m, 3H, *Ar*), 2.96 – 2.83 (m, 1H), 2.76 (dq, *J* = 13.2, 7.4 Hz, 1H), 1.19 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.5, 131.0, 129.3 (2C), 124.3 (2C), 50.4, 6.1 ppm.

Ethyl (4-methyl)phenyl sulfoxide (6d)[7]



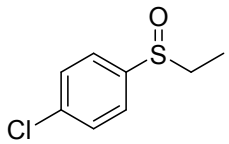
Yellow oil, 71% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 – 7.43 (m, 2H), 7.29 (d, *J* = 7.9 Hz, 2H), 2.84 (dq, *J* = 13.2, 7.4 Hz, 1H), 2.73 (dq, *J* = 13.2, 7.4 Hz, 1H), 2.39 (s, 3H), 1.16 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.4, 140.2, 129.9, 124.3, 50.4, 21.5, 6.1.

Ethyl (4-methoxy)phenyl sulfoxide (6e)[18]



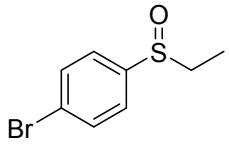
Yellow oil, 60% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 – 7.51 (m, 1H), 7.05 – 6.99 (m, 1H), 3.85 (s, 1H), 2.91 – 2.71 (m, 1H), 1.17 (t, *J* = 7.4 Hz, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.1, 134.4, 126.2, 114.8, 55.6, 50.6, 6.3 ppm.

Ethyl (4-chloro)phenyl sulfoxide (6f)[19]



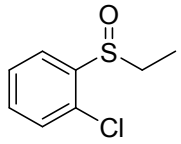
Oil, 67% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 (d, *J* = 8.6 Hz, 2H, *Ar*), 7.48 (d, *J* = 8.6 Hz, 2H, *Ar*), 2.94 – 2.80 (m, 1H), 2.80 – 2.66 (m, 1H), 1.17 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.0, 137.2, 129.5 (2C), 125.7 (2C), 50.4, 5.9 ppm.

Ethyl (4-bromo)phenyl sulfoxide (6g)[20]



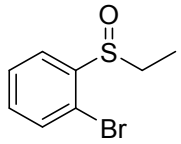
Yellow oil, 67% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 – 7.62 (m, 2H, *Ar*), 7.49 – 7.44 (m, 2H, *Ar*), 2.88 (dq, *J* = 13.3, 7.4 Hz, 1H), 2.72 (dq, *J* = 13.3, 7.4 Hz, 1H), 1.18 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.6, 132.5, 125.9, 125.5, 50.4, 5.9. MS (APCI): m/z = 232.1-234.1 $[M+H]^+$.

Ethyl (2-chloro)phenyl sulfoxide (6h)[3]



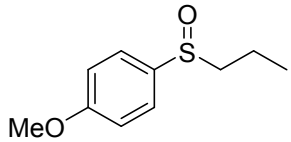
Yellow oil, 81 % yield: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (dd, *J* = 7.8, 1.7 Hz, 1H, *Ar*), 7.52 (td, *J* = 7.5, 1.5 Hz, 1H, *Ar*), 7.47 – 7.37 (m, 2H, *Ar*), 3.13 (dq, *J* = 14.8, 7.4 Hz, 1H), 2.86 (dq, *J* = 13.5, 7.4 Hz, 1H), 1.25 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.1, 131.8, 130.1, 129.8, 127.7, 126.6, 47.1, 5.6 ppm. MS (APCI): m/z = 189.1 $[M+H]^+$.

Ethyl (2-bromo)phenyl sulfoxide (6i)[21]



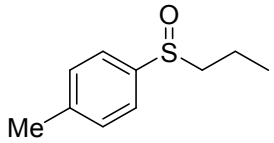
Pale yellow oil, 80 % yield: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 (dd, *J* = 8.0, 1.8 Hz, 1H, *Ar*), 7.62 – 7.50 (m, 2H, *Ar*), 7.40 – 7.32 (m, 1H, *Ar*), 3.13 (dq, *J* = 13.6, 7.4 Hz, 1H), 2.85 (dq, *J* = 13.5, 7.4 Hz, 1H), 1.25 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.0, 133.1, 132.4, 128.4, 127.1, 118.9, 47.5, 6.0 ppm. MS (APCI): m/z = 232.1-234.1 $[M+H]^+$.

(4-Methoxy)phenyl propyl sulfoxide (6j)[22]



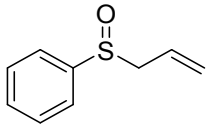
Yellow oil, 79 % yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 (d, *J* = 8.8 Hz, 2H, *Ar*), 6.97 (d, *J* = 8.8 Hz, 2H, *Ar*), 3.79 (s, 3H), 2.81 – 2.70 (m, 1H), 2.70 – 2.59 (m, 1H), 1.76 – 1.52 (m, 2H), 0.98 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.9, 134.9, 125.9, 114.7, 59.4, 55.5, 16.0, 13.3 ppm. MS (APCI): m/z = 199.1 $[M+H]^+$.

(4-Methyl)phenyl propyl sulfoxide (6k)



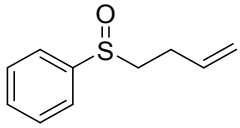
Yellow oil, 68 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.3 Hz, 2H, *Ar*), 7.31 (d, *J* = 7.9 Hz, 2H, *Ar*), 2.88 – 2.65 (m, 2H), 2.41 (s, 3H), 1.85 – 1.56 (m, 2H), 1.03 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.5, 141.0, 130.0, 124.2, 59.5, 21.5, 16.1, 13.4 ppm. HRMS (APCI) m/z calcd. for $C_{10}H_{15}OS^+$ $[M+H]^+$ 183.0838; found 183.0836.

Allyl phenyl sulfoxide (6l)[17]



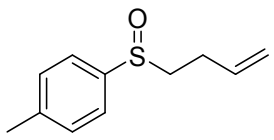
Yellow oil, 68 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.56 (m, 2H, *Ar*), 7.49 (m, 3H, *Ar*), 5.63 (m, 1H), 5.31 (dd, *J* = 10.2, 1.4 Hz, 1H), 5.17 (dd, *J* = 17.0, 1.3 Hz, 1H), 3.62 – 3.42 (m, 2H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.9, 131.1, 129.1 (2C), 125.3, 124.3 (2C), 123.9, 60.9 ppm.

(But-3-en-1-ylsulfinyl)benzene (6m)[23]



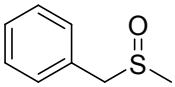
Yellow oil, 58 % yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.64 – 7.59 (m, 2H, *Ar*), 7.55 – 7.46 (m, 3H, *Ar*), 5.79 (ddt, *J* = 16.9, 10.2, 6.6 Hz, 1H, C*H*), 5.15 – 5.01 (m, 2H, *ene* CH_2), 2.94 – 2.76 (m, 2H), 2.60 – 2.45 (m, 1H), 2.39 – 2.24 (m, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.8, 135.0, 131.1, 129.4, 124.2, 117.2, 56.2, 26.3 ppm.

1-(but-3-en-1-ylsulfinyl)-4-methylbenzene (6n)[7]



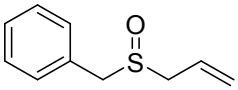
Pale yellow oil, 73 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.2 Hz, 2H, *Ar*), 7.33 (d, *J* = 8.0 Hz, 2H, *Ar*), 5.86 – 5.73 (m, 1H), 5.14 – 5.03 (m, 2H), 2.84 (t, *J* = 7.8 Hz, 2H), 2.57 – 2.45 (m, 1H), 2.42 (s, 3H), 2.39 – 2.27 (m, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.6, 140.7, 135.1, 130.1, 124.3, 117.1, 56.4, 26.4, 21.6 ppm.

Benzyl methyl sulfoxide (6o)[17]



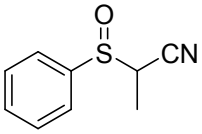
Yellow oil, 82% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.32 (m, 3H, *Ar*), 7.31 – 7.26 (m, 2H, *Ar*), 4.07 (d, *J* = 12.8 Hz, 1H), 3.93 (d, *J* = 12.8 Hz, 1H), 2.46 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 130.2, 129.8, 129.1, 128.6, 60.5, 37.4 ppm. MS (APCI): m/z = 155.1 $[M+H]^+$.

Allyl benzyl sulfoxide (6p)[24]



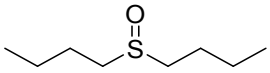
White crystal, 86% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.27 (m, 5H, *Ar*), 6.00 – 5.85 (m, 1H), 5.52 – 5.34 (m, 2H), 4.05 – 3.92 (m, 2H), 3.43 (ddt, *J* = 13.2, 7.1, 1.1 Hz, 1H), 3.27 (ddt, *J* = 13.1, 7.7, 1.0 Hz, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 130.1, 130.0, 129.0, 128.4, 125.8, 123.7, 56.9, 54.2 ppm.

2-(phenylsulfinyl)propanoic acid (6q)[25]



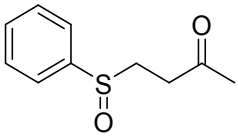
Colourless oil, 78 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 – 7.52 (m, 5H, *Ar*), 3.71 (q, *J* = 6.7, 6.2 Hz, *ent1* 1H), 3.63 (q, *J* = 7.3 Hz, *ent2* 1H), 1.58 (dd, *J* = 13.8, 7.3 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.3, 139.2, 132.9, 132.6, 129.5, 129.4, 125.0, 124.9, 115.6, 115.1, 51.3, 49.7, 12.2, 10.8 ppm.

1-(Butylsulfinyl)butane (6r)[26]



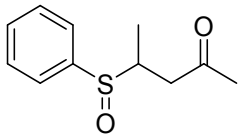
Oil, 89% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 2.72 – 2.53 (m, 2H), 1.80 – 1.63 (m, 2H), 1.57 – 1.35 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 52.3, 24.7, 22.2, 13.8 ppm.

4-(Phenylsulfinyl)butan-2-one (13a)[27]



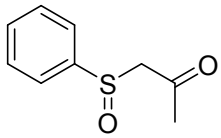
Oil, 71% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.39 (m, 5H, *Ar*), 3.16 (ddd, *J* = 13.5, 8.3, 6.3 Hz, 1H), 2.93 (ddd, *J* = 18.0, 8.1, 6.2 Hz, 1H), 2.82 (ddd, *J* = 13.4, 8.1, 5.2 Hz, 1H), 2.61 (ddd, *J* = 18.0, 8.2, 5.2 Hz, 1H), 2.09 (s, 3H, $COCH_3$) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 205.2, 143.3, 131.1, 129.3, 123.9, 50.0, 34.7, 30.0, 29.7 ppm.

4-(Phenylsulfinyl)pentan-2-one (13b)



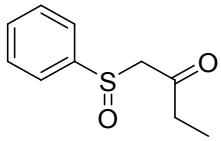
Mixture of diastereoisomers (1:0.5). Oil, 42 % yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.45 (m, 5H, *Ar*), 3.27 (dt, *J* = 13.5, 6.8 Hz, 1H), 3.18 (dd, *J* = 18.2, 6.1 Hz, 0.5H), 2.85 (dd, *J* = 18.1, 3.8 Hz, 0.5H), 2.49 (ddd, *J* = 18.1, 14.5, 8.1 Hz, 1H), 1.29 (d, *J* = 7.0 Hz, 1.5H), 0.99 (d, *J* = 6.9 Hz, 1.5H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 205.4, 205.2, 141.8, 141.2, 131.3, 130.9, 129.3, 129.1, 129.0, 124.9, 124.7, 54.8, 53.6, 43.7, 41.5, 30.5, 30.4, 29.7, 14.6, 10.3 ppm. HRMS (APCI) m/z calcd. for $C_{11}H_{15}O_2S^+$ $[M+H]^+$ 211.0787; found 211.0785.

1-(Phenylsulfinyl)propan-2-one (13d)[28]



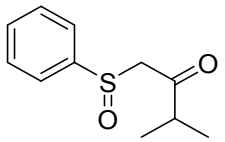
Oil, 67% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.63 (m, 2H, *Ar*), 7.55 (dd, *J* = 5.2, 2.2 Hz, 3H, *Ar*), 3.85 (q, *J* = 13.6 Hz, 2H), 2.25 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.5, 143.0, 131.7, 129.6, 124.1, 68.8, 32.1 ppm.

1-(phenylsulfinyl)butan-2-one (13e)[29]



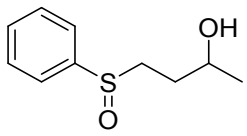
Oil, 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 – 7.59 (m, 2H, *Ar*), 7.51 (dd, *J* = 5.2, 2.0 Hz, 3H, *Ar*), 3.89 (d, *J* = 13.7 Hz, 1H), 3.76 (d, *J* = 13.7 Hz, 1H), 2.48 (dq, *J* = 12.1, 7.2 Hz, 2H), 0.99 (t, *J* = 7.2 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 202.1, 143.2, 131.7, 129.5, 124.1, 68.0, 38.5, 7.3.

3-Methyl-1-(phenylsulfinyl)butan-2-one (13f)



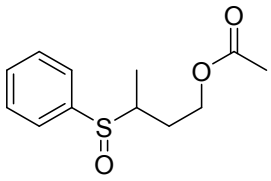
Oil, 68% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.61 (m, 2H, Ar), 7.52 (dd, *J* = 5.2, 2.0 Hz, 3H, Ar), 4.00 (d, *J* = 14.2 Hz, 1H), 3.81 (d, *J* = 14.2 Hz, 1H), 2.56 (hept, *J* = 7.0 Hz, 1H), 1.08 (d, *J* = 7.0 Hz, 3H), 0.99 (d, *J* = 6.9 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 205.6, 143.6, 131.7, 129.5, 124.2, 67.0, 42.3, 17.5, 17.4 ppm. HRMS (APCI) m/z calcd. for $C_{11}H_{15}O_2S^+$ $[M+H]^+$ 211.0787; found 211.0786.

4-(Phenylsulfinyl)butan-2-ol (15a)



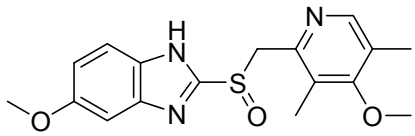
Mixture of diastereoisomers (1:0.5). Oil, 67% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 – 7.43 (m, 5H), 4.00 – 3.78 (m, 1H), 3.15 – 2.96 (m, 1H), 2.96 – 2.80 (m, 1H), 2.01 – 1.88 (m, 0.5H), 1.80 (p, *J* = 7.8, 7.4 Hz, 1H), 1.75 – 1.63 (m, 0.5H), 1.19 (d, *J* = 6.0 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4, 143.2, 131.1, 131.1, 129.4, 129.4, 124.3, 124.2, 66.6, 66.4, 53.8, 53.7, 32.1, 31.6, 23.6, 23.6 ppm. HRMS (APCI) m/z calcd. for $C_{10}H_{15}O_2S^+$ $[M+H]^+$ 199.0787; found 199.0784.

3-(Phenylsulfinyl)butyl acetate (15b)



Mixture of diastereoisomers (1:0.5). Oil, 74% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.64 – 7.43 (m, 4H), 4.30 (dt, *J* = 12.1, 6.2 Hz, 0.5H), 4.22 – 4.05 (m, 0.5H), 4.16 – 4.04 (m, 1H), 2.89 – 2.81 (m, 0.5H), 2.77 (dt, *J* = 7.9, 6.5 Hz, 0.5H), 2.32 – 2.23 (m, 0.5H), 2.05 (s, 1.5H), 2.00 (s, 1.5H), 1.74 – 1.62 (m, 0.5H), 1.21 (d, *J* = 7.0 Hz, 1.5H), 1.06 (d, *J* = 6.9 Hz, 1.5H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.0, 170.9, 141.4, 141.3, 131.4, 131.0, 129.1, 129.1, 125.3, 124.9, 61.6, 61.5, 56.4, 56.1, 29.7, 27.8, 21.1, 21.0, 13.0, 10.6 ppm. HRMS (APCI) m/z calcd. for $C_{12}H_{17}O_3S^+$ $[M+H]^+$ 241.0893; found 241.0886.

Omeprazole (1)[17]



Brown solid, 73% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 12.01 (br s, 1H), 8.20 (s, 1H), 7.63 (br s, 0.5H), 7.33 – 7.23 (br s, 0.5H), 6.94 (d, *J* = 9.0 Hz, 1H), 6.88 (s, 0.5H), 4.79 – 4.65 (m, 2H), 3.84 (s, 3H), 3.63 (s, 3H), 2.22 (s, 3H), 2.14 (s, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.6, 149.9, 148.9, 127.2, 126.5, 60.8, 60.0, 55.9, 13.5, 11.6 ppm. MS (APCI): m/z = 346.1 $[M+H]^+$.

CALB recycling experiments

The sulfide **5a** (20 mmol), CALB (20 % w/w) and UHP (22 mmol) were added to a round bottom flask containing AcOEt (50 mL) stirred at 37 ºC. The reaction was stirred for 24 h and monitored by TLC. Upon completion, CALB was removed through filtration on Buchner funnel and washed with CH_3CN/H_2O (9:1) (3x10 mL) to remove urea, followed by AcOEt (3x10 mL). The recovered CALB was air dried first and then

placed in a desiccator to ensure full dryness for the next cycle. The filtrate was instead cooled to 0ºC and quenched with 30mL 10% $Na_2S_2O_{3(aq)}$. The organic layer was washed with water (1x) and brine (2x), dried on $MgSO_4$ and evaporated under reduced pressure. The crude product analysed by NMR to determine conversion to sulfoxide. Quantities for the next reaction were calculated on the isolated dried CALB.

Peroxyacid 8a titration.

The concentration of the peroxyacid **8a** intermediate formed in the biocatalytic cycle was determined following the method described by Chavez et al..[30] 1 mL of the reaction mixture (1.0 mL of AcOEt, 6.0 mg of CALB and 25 mg of UHP) were incubated at 30 °C in 1.5 mL Eppendorf vials. At 0.5, 1, 2 and 4 h, 20 mg of catalase was added to the reaction vial and further incubated at room temperature for 5 min. Then, 65 mL of water, 2g of KI and 10 mL of 0.5 M sulfuric acid were added. This solution was titrated with 0.05 M $Na_2S_2O_3$ until the colour of the mixture changed to a very light yellow, after which drops of indicator (2% (w/v) starch solution) was added and the addition of thiosulfate was continued until the mixture was colourless. The concentration of the peroxyacid **8a** was determined at various times.

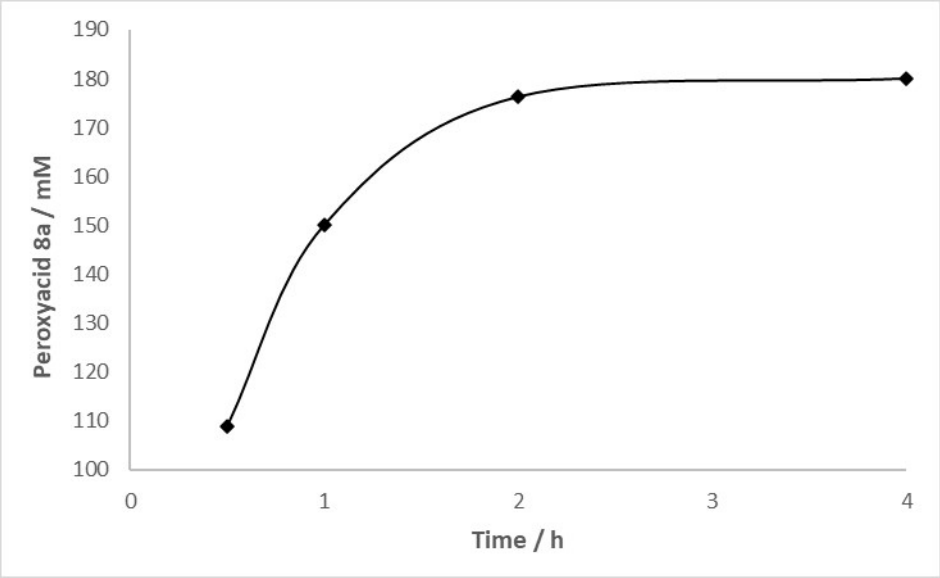


Figure S1. Concentration at different times of the peroxyacid **8a** formed from the reaction of AcOEt and UHP in presence of CALB

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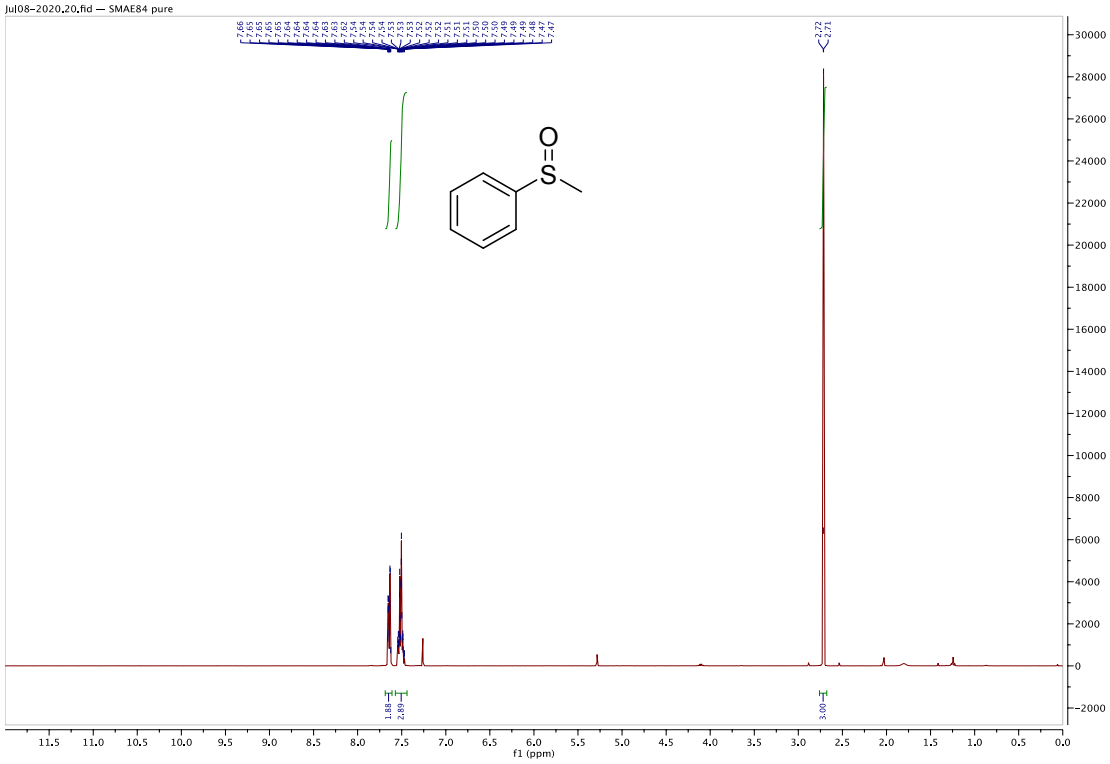
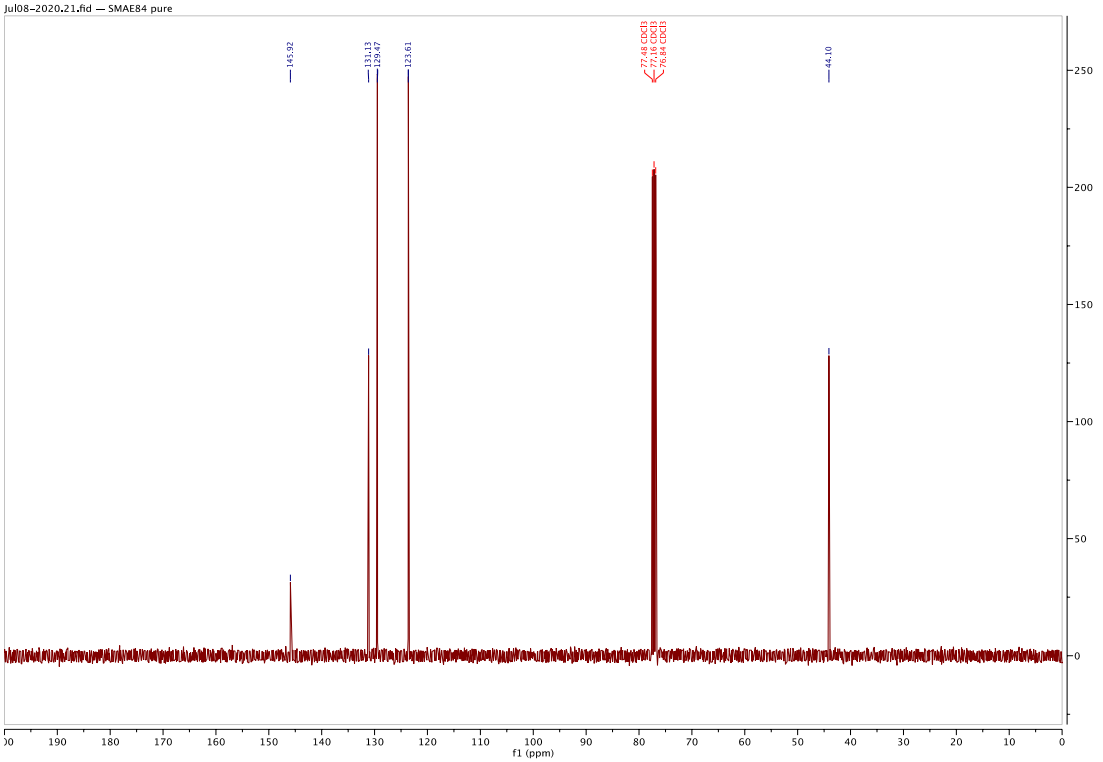
Copies of NMR spectra

Methyl phenyl sulfoxide 6a





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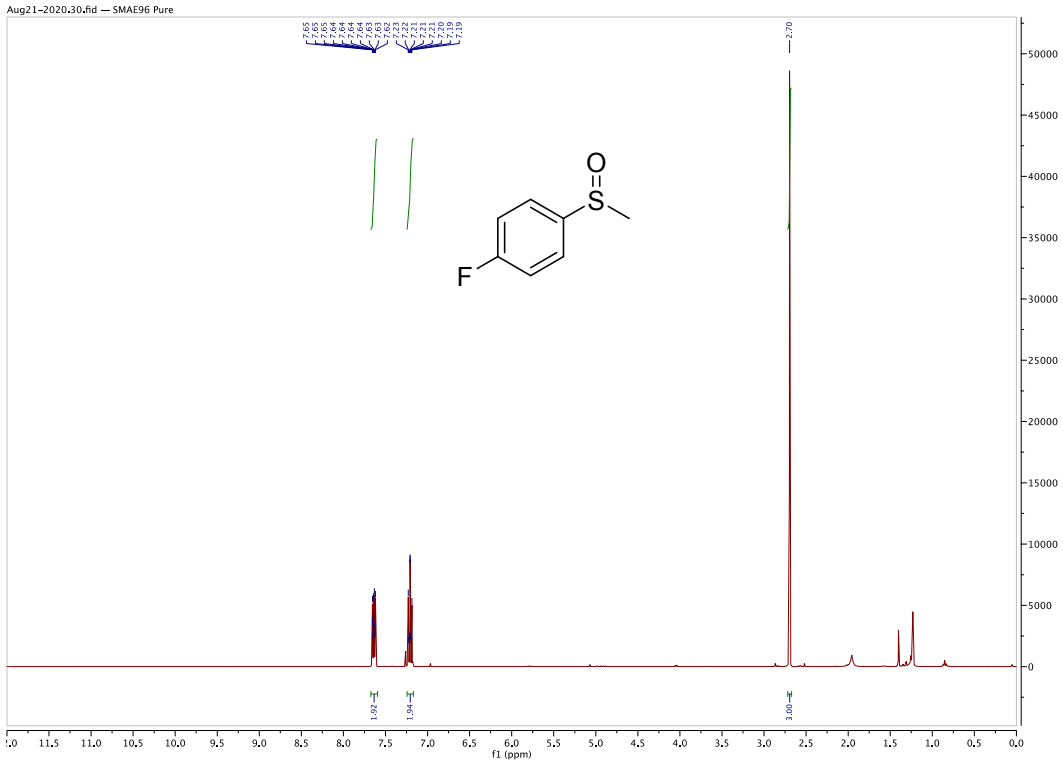

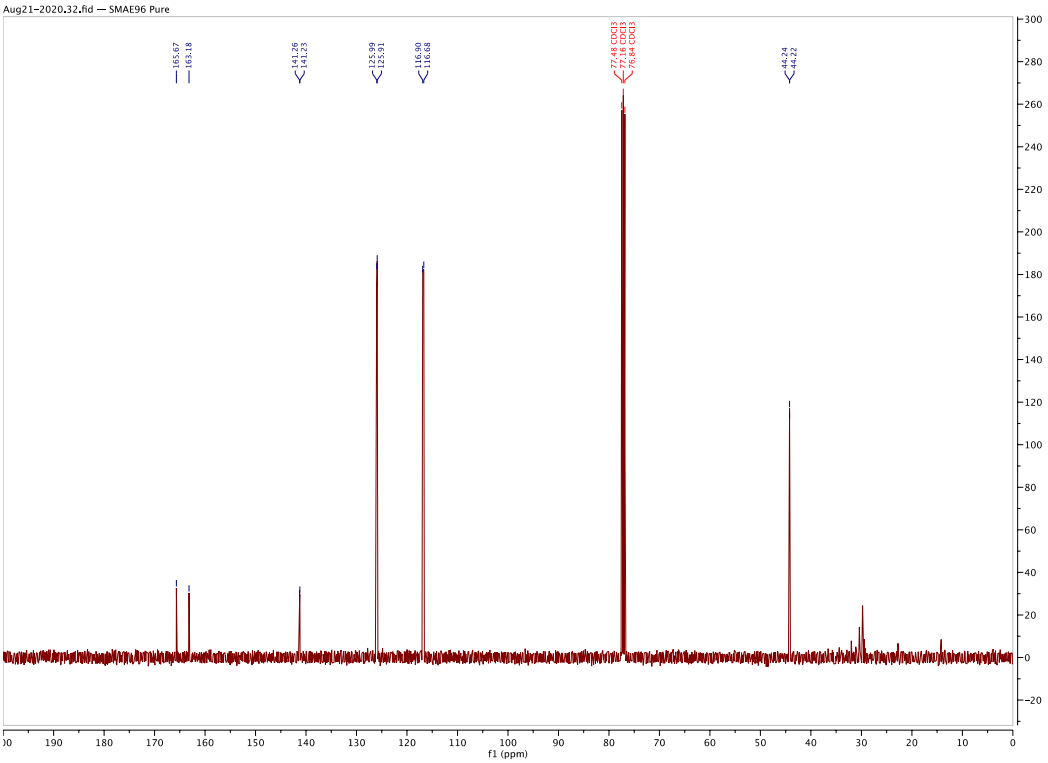

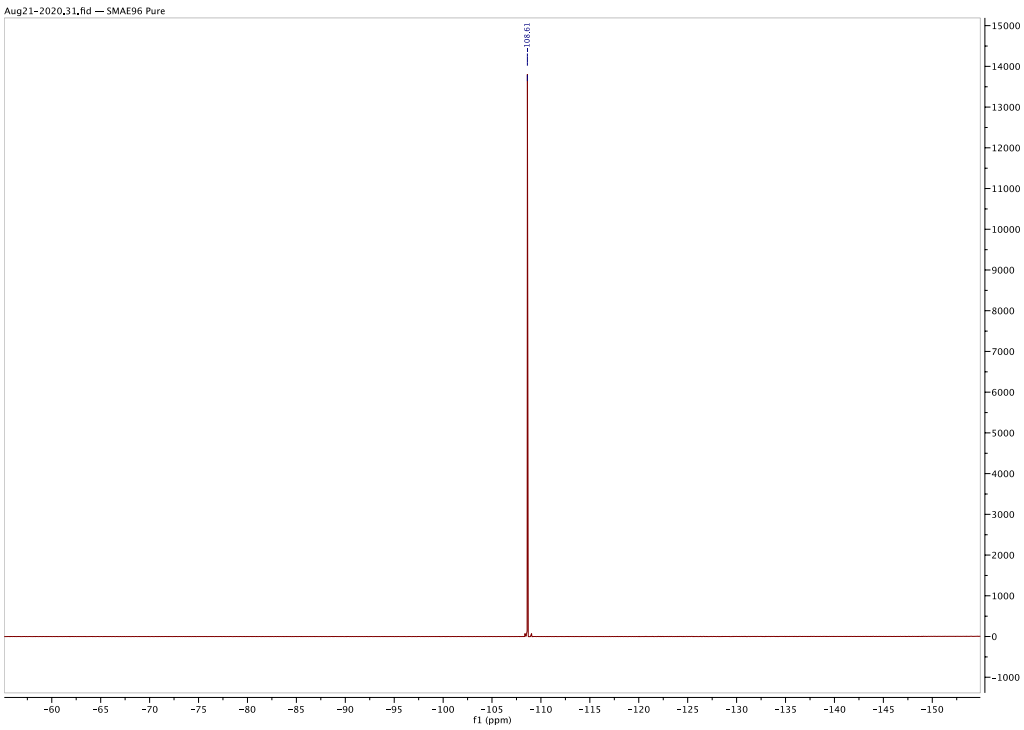
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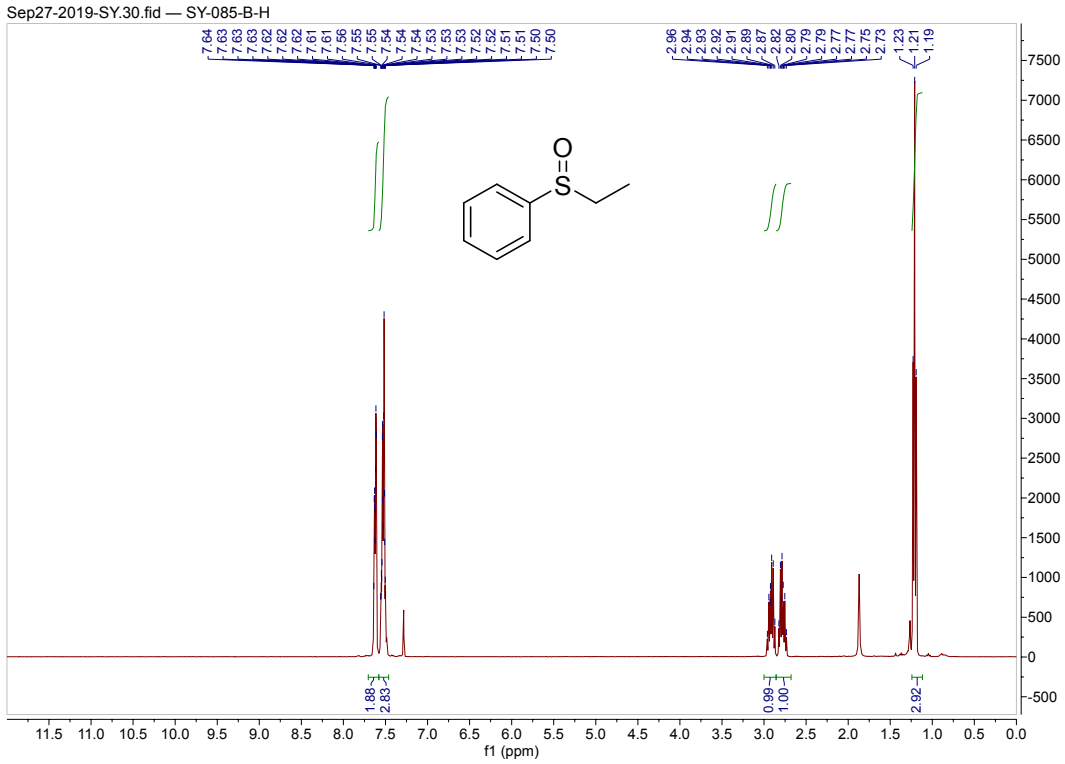
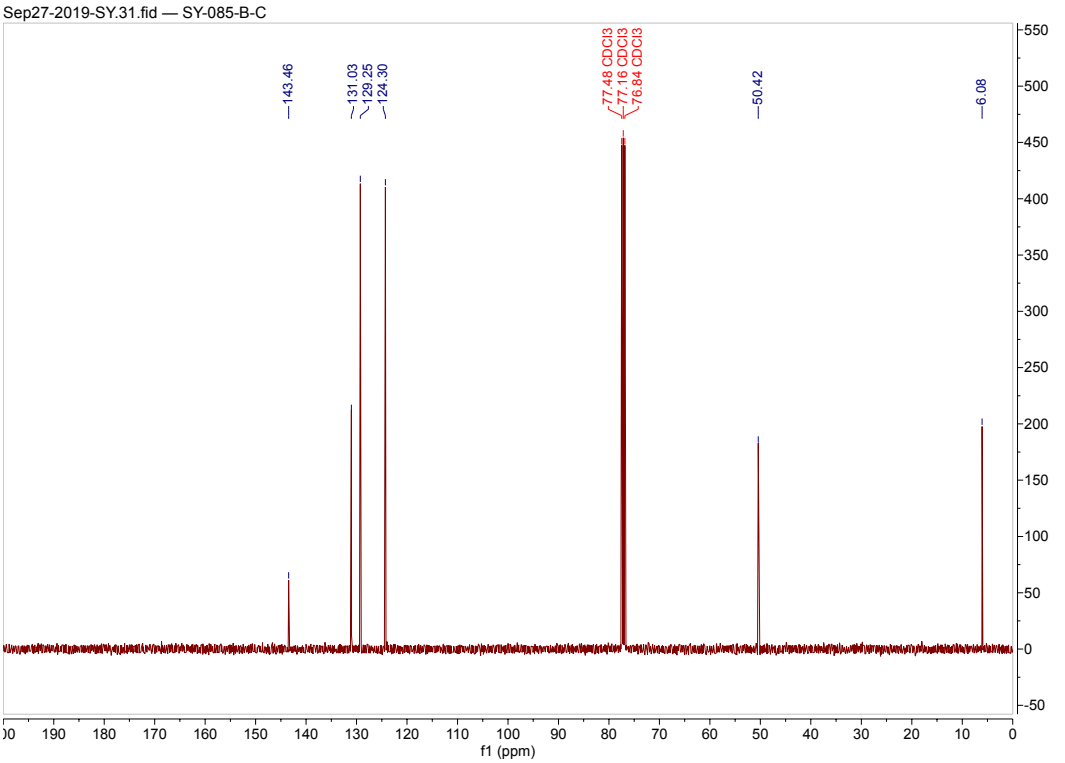
f1 (ppm)

Ethyl phenyl sulfoxide 6c





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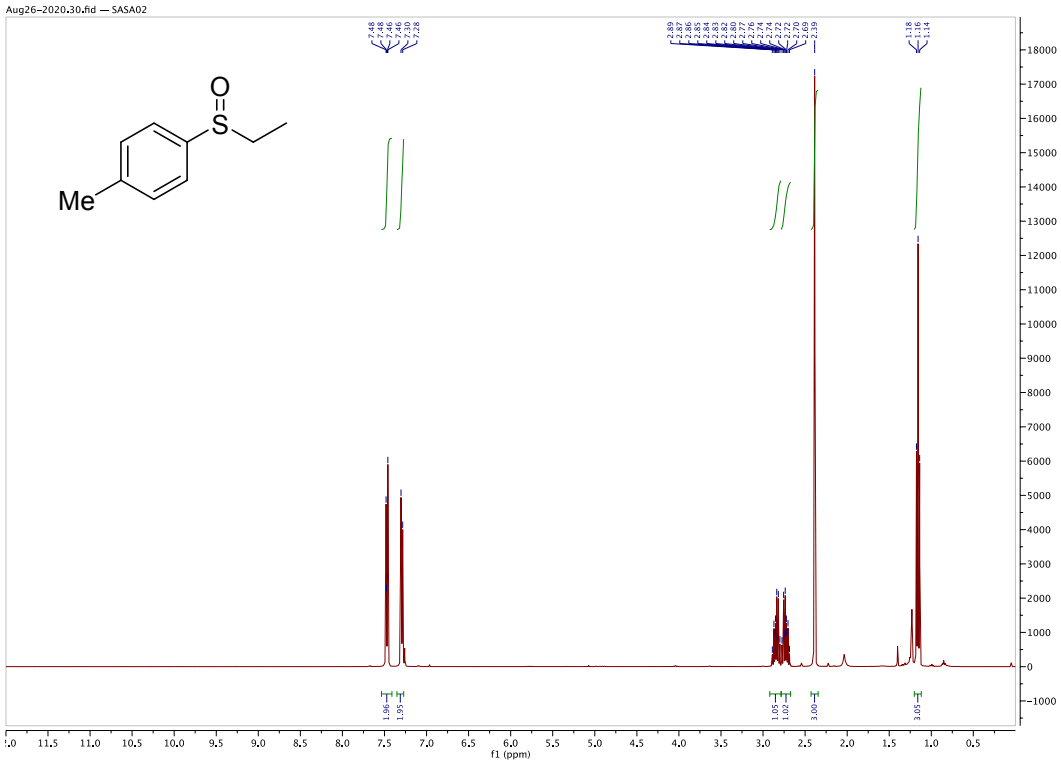

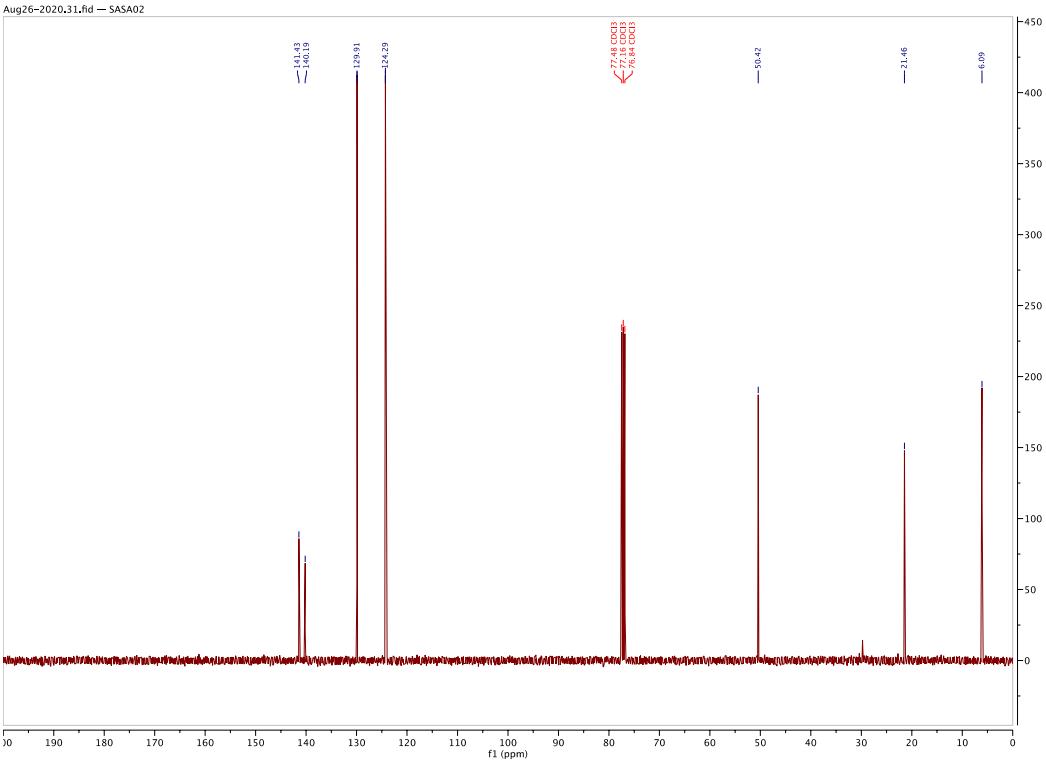

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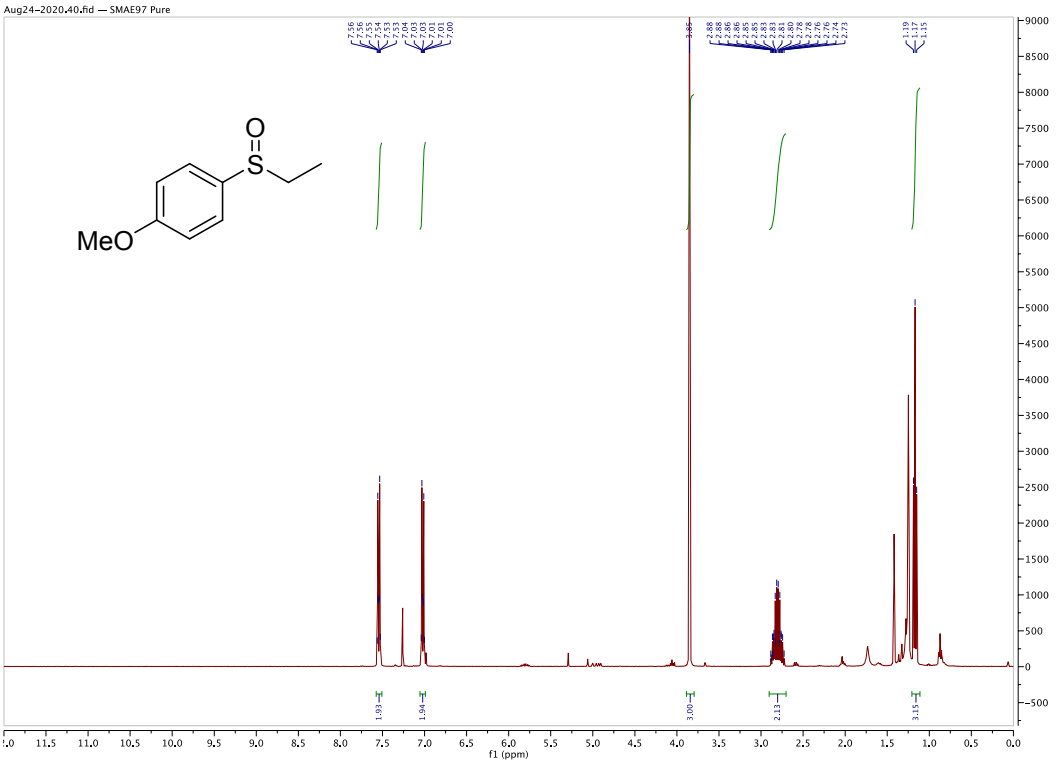

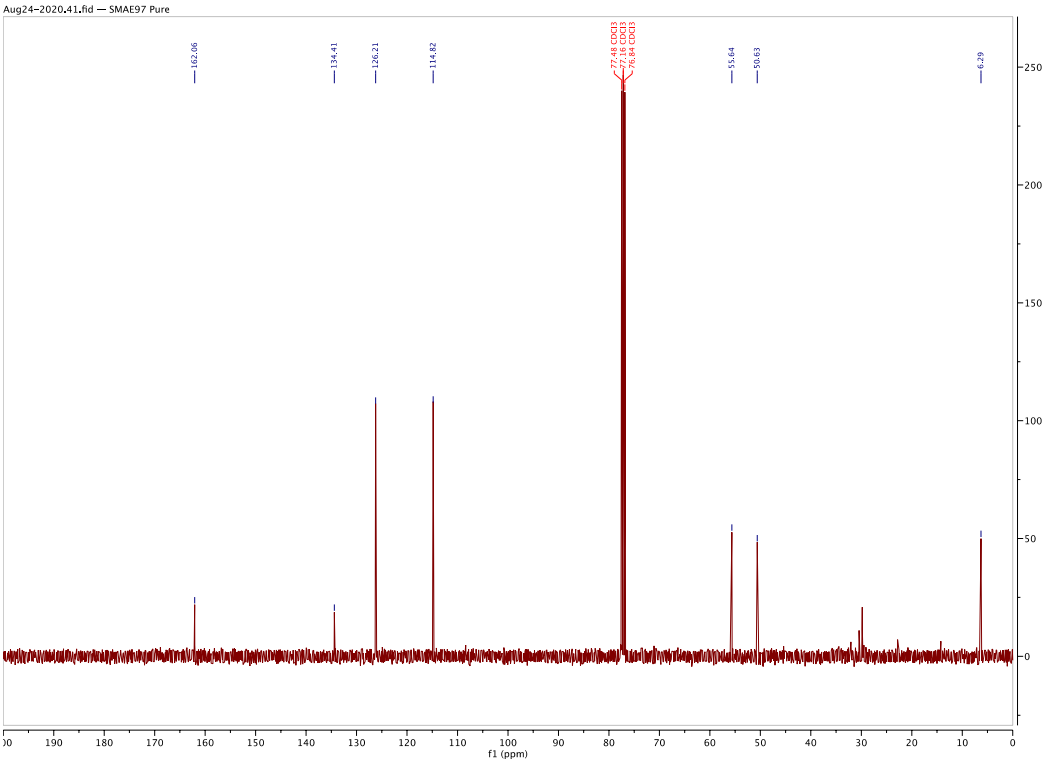

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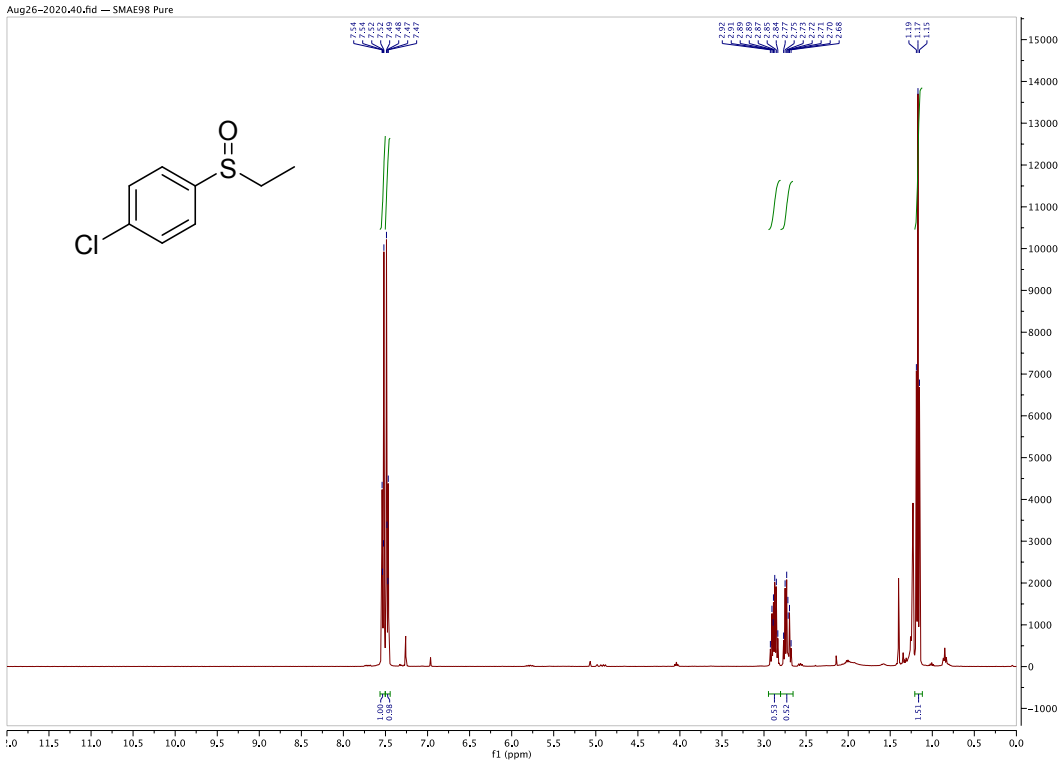

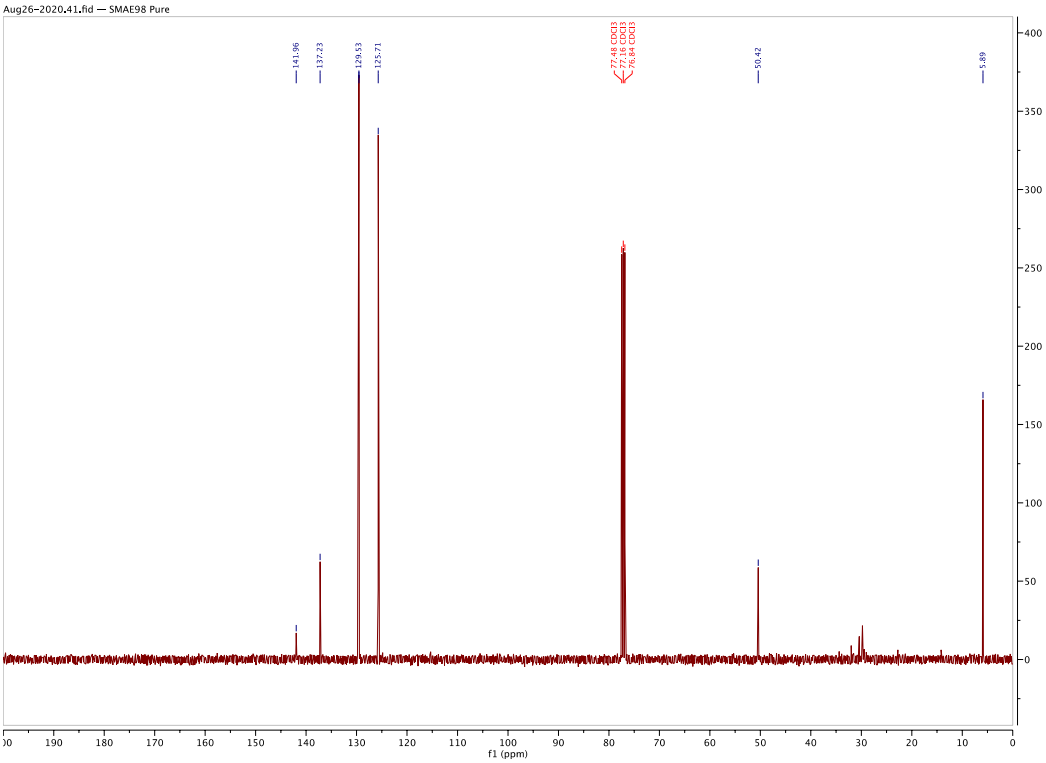

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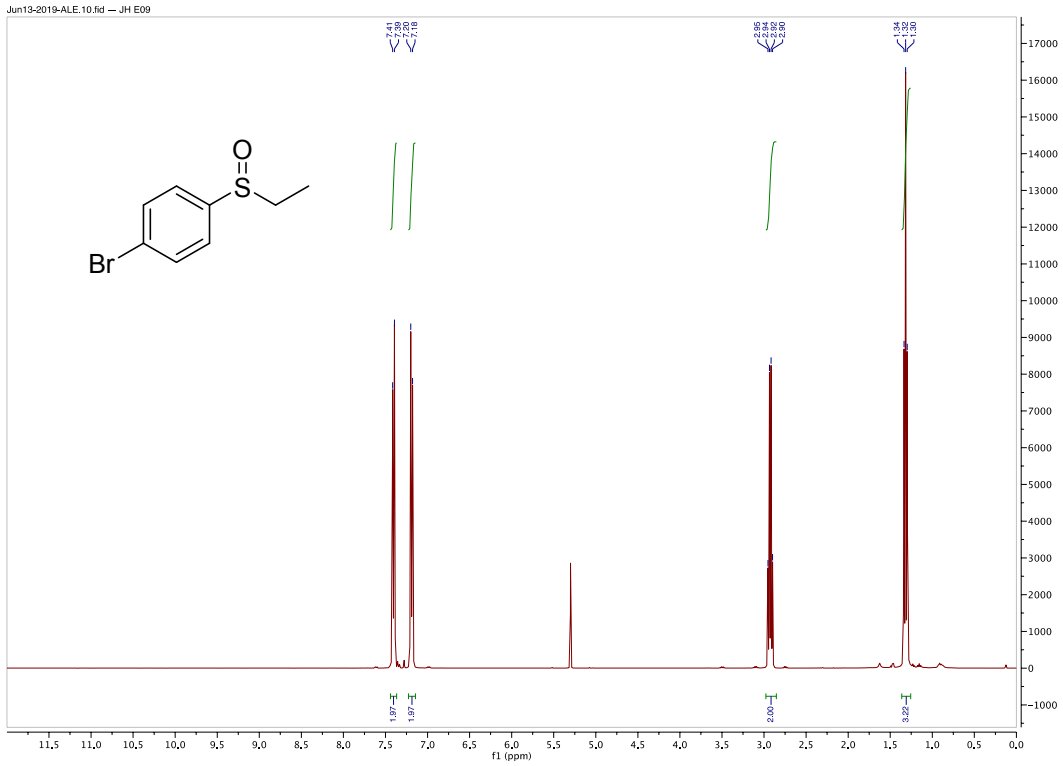

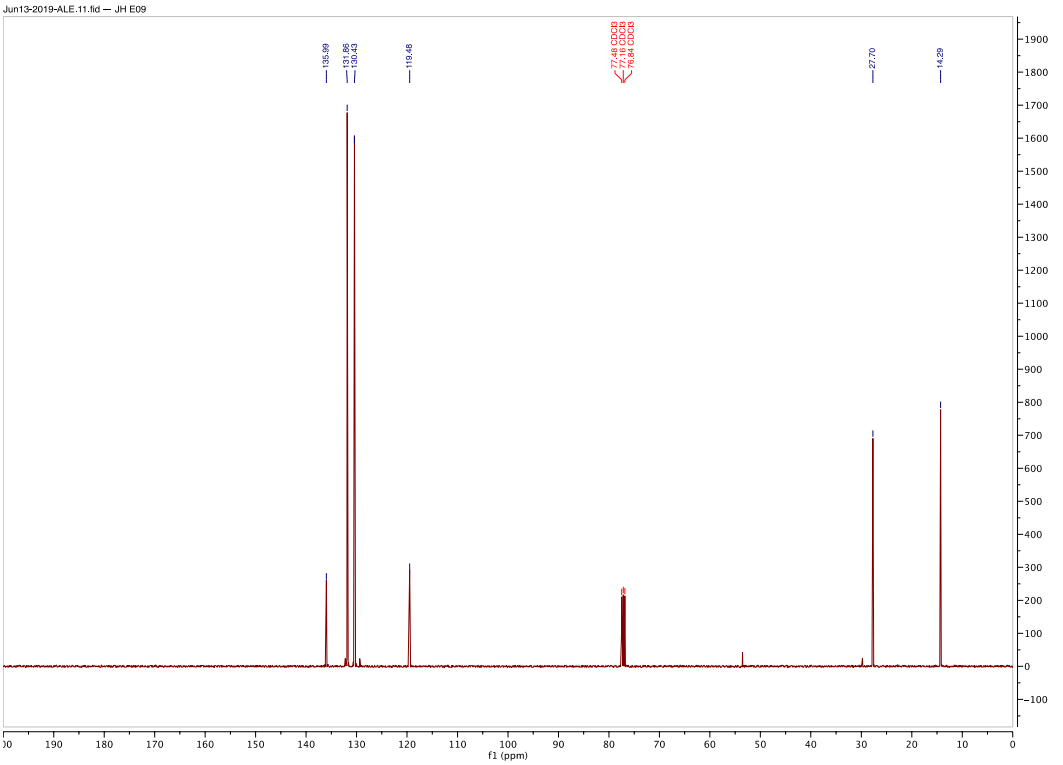

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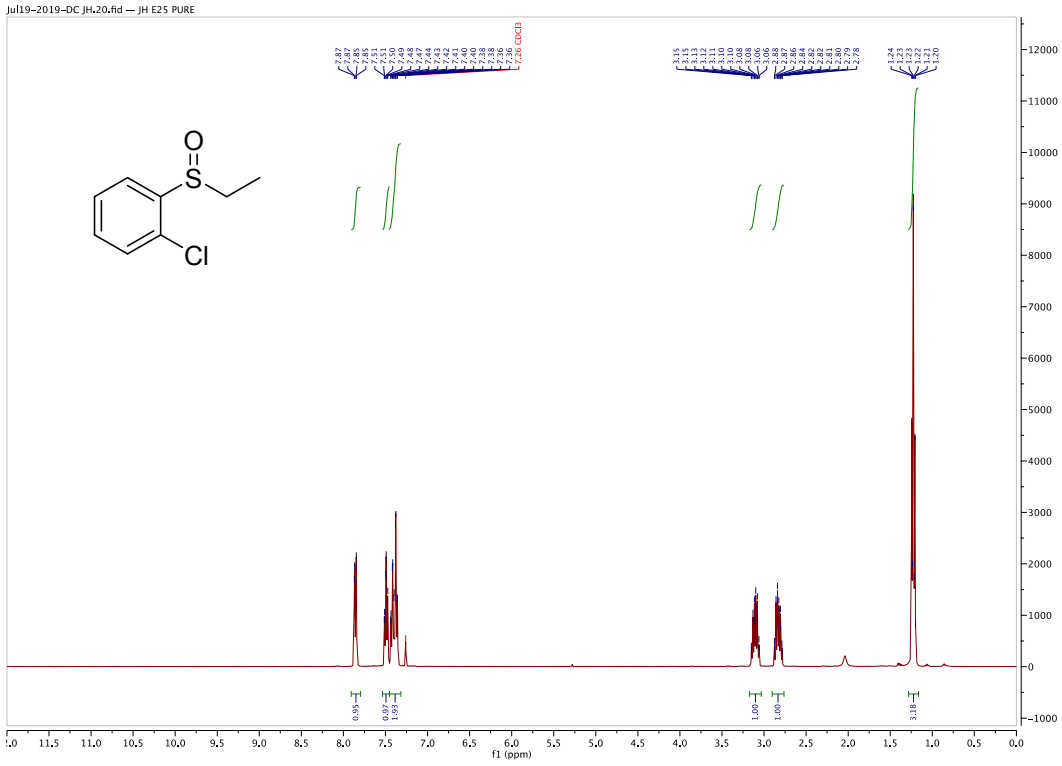

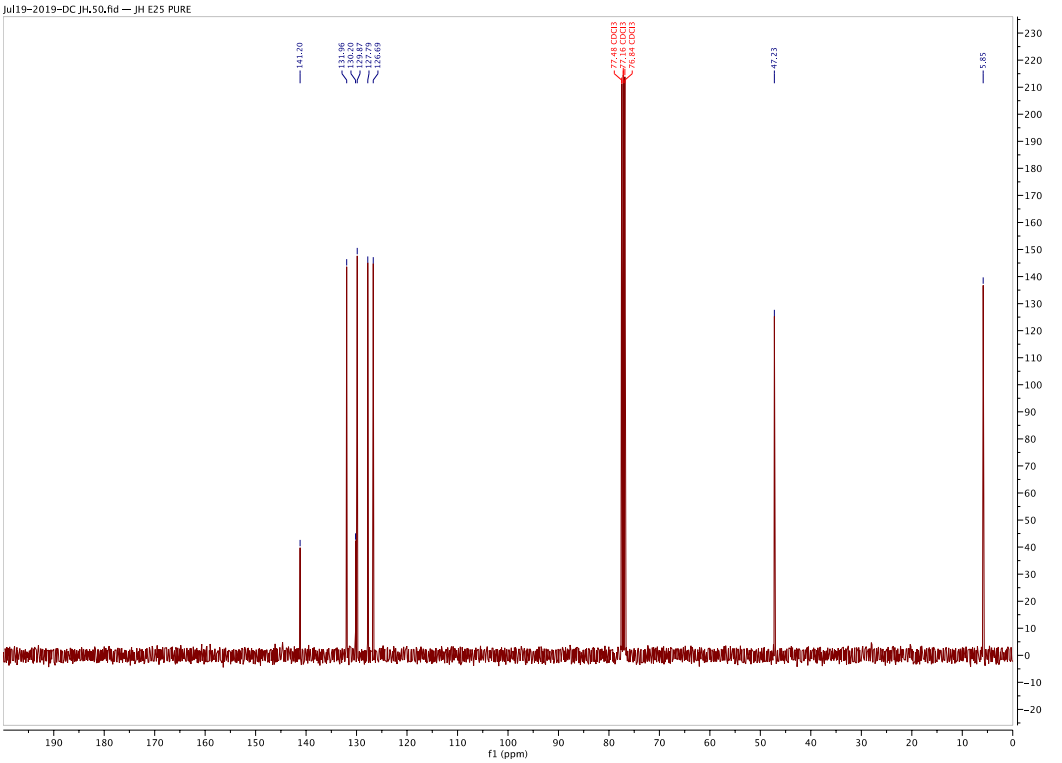

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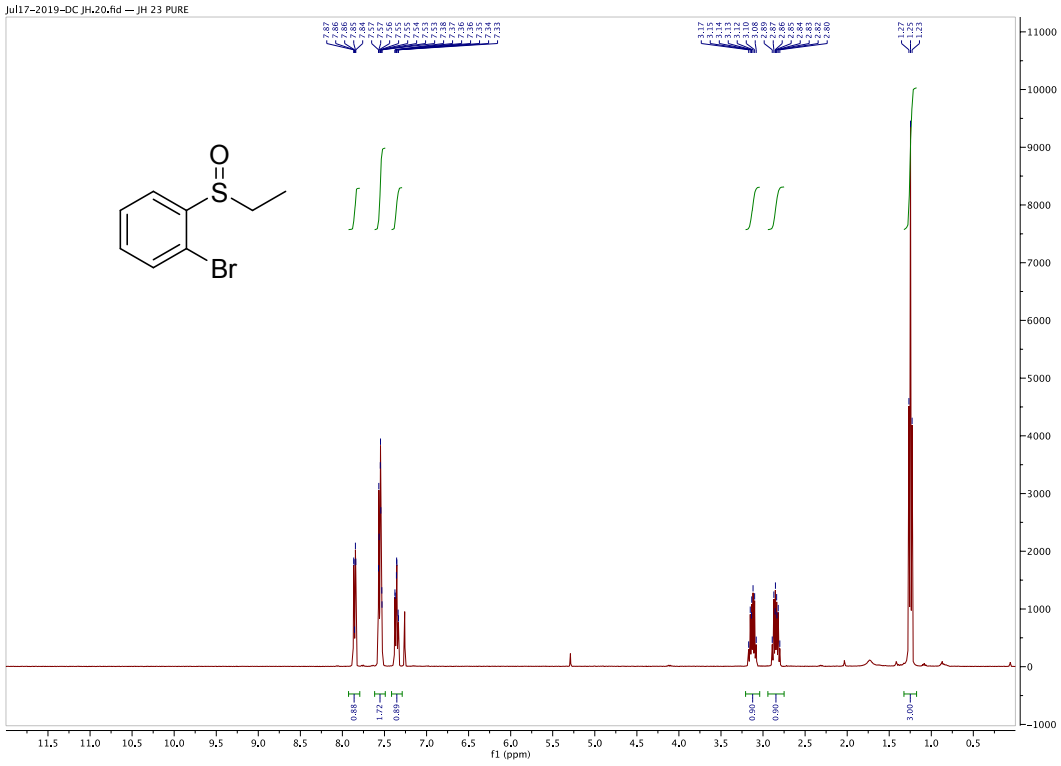
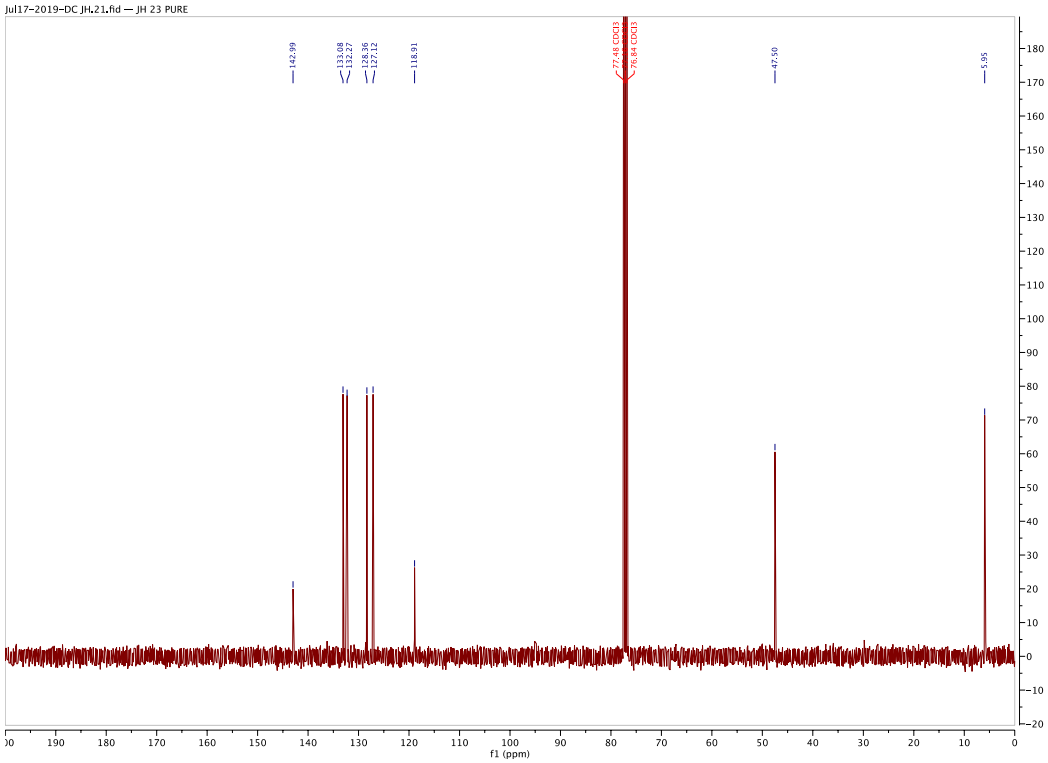
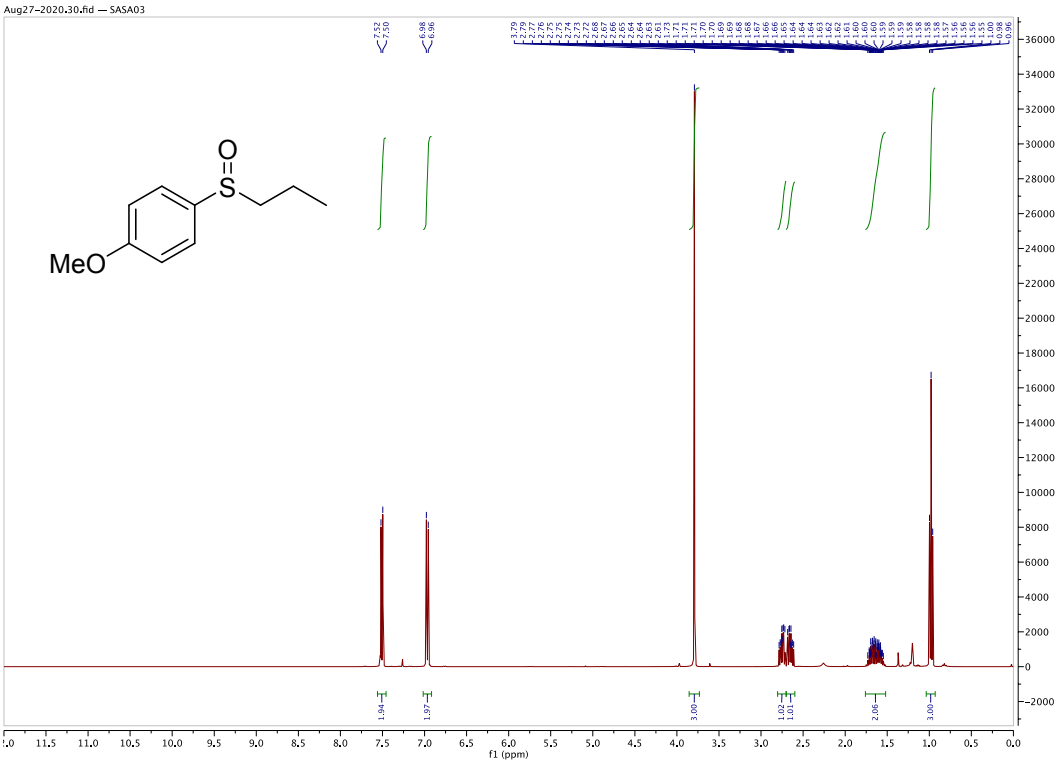
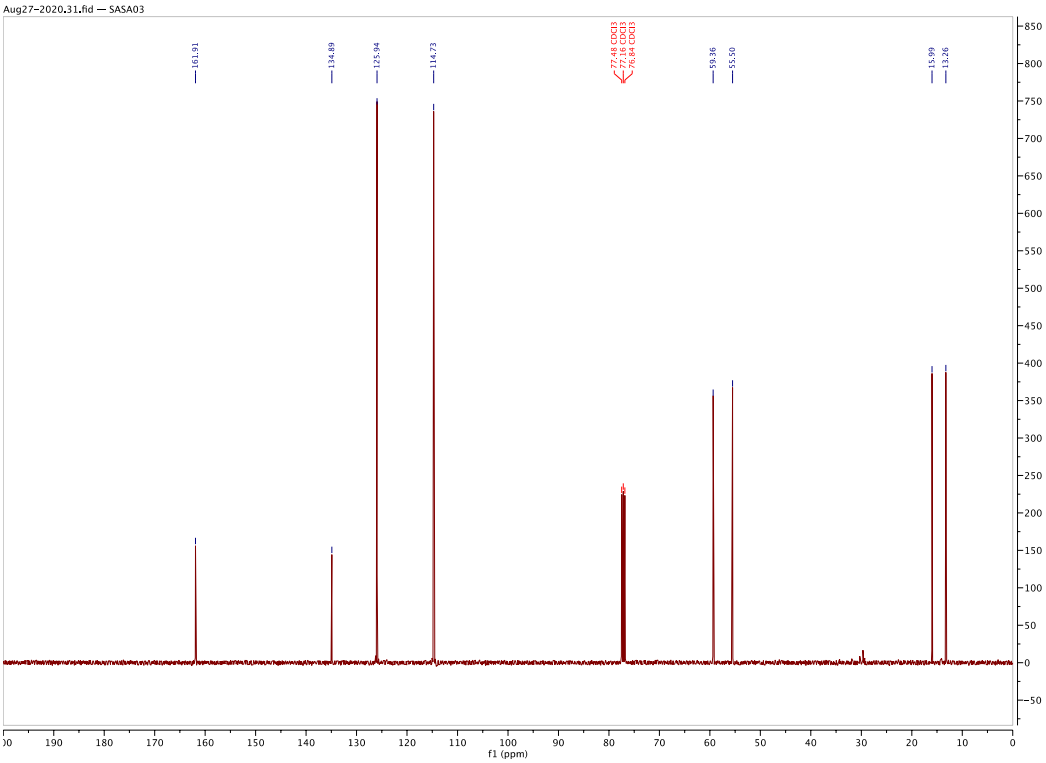




(4-Methoxy)phenyl propyl sulfoxide 6j





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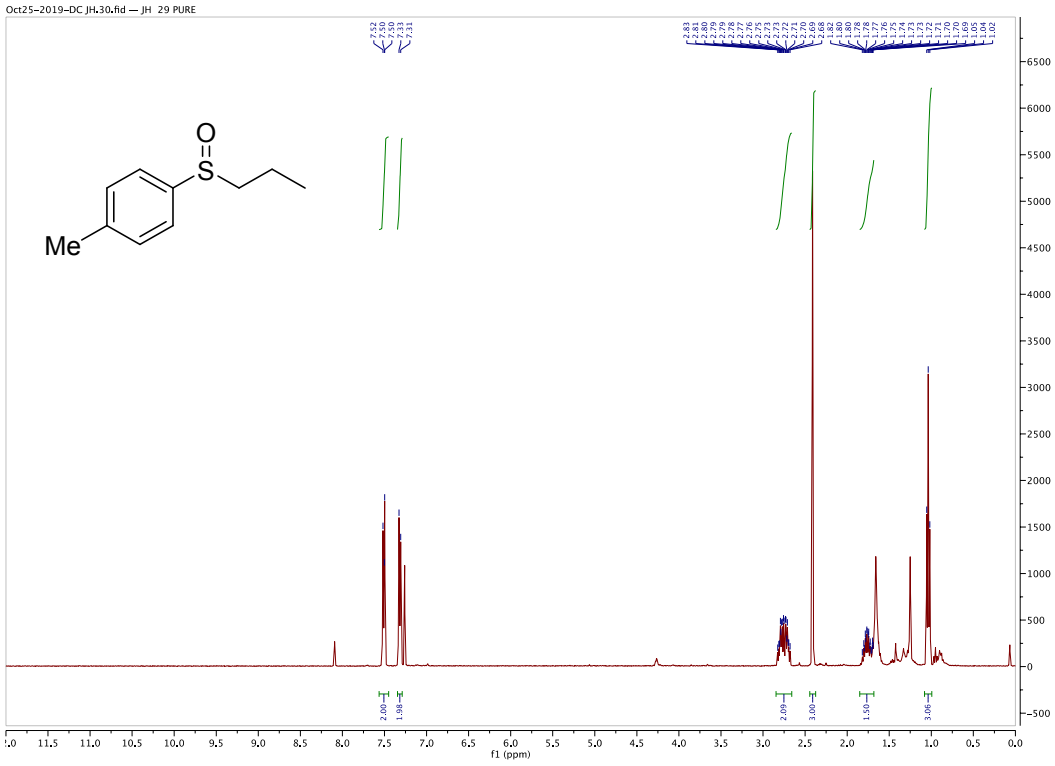
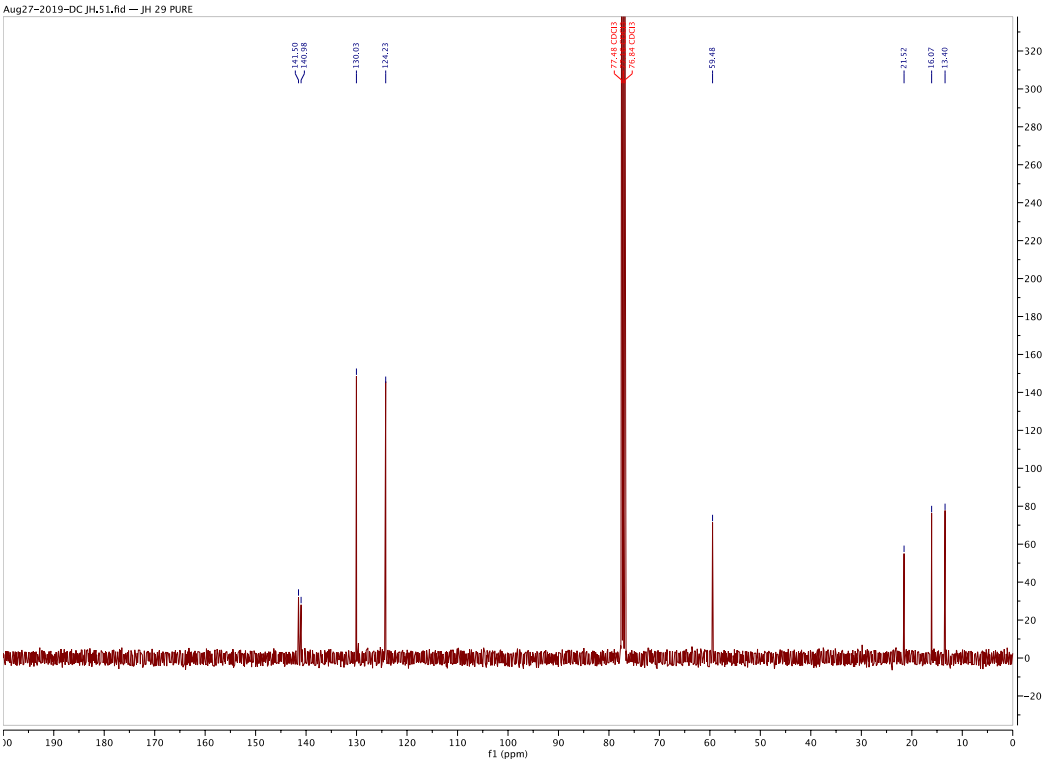
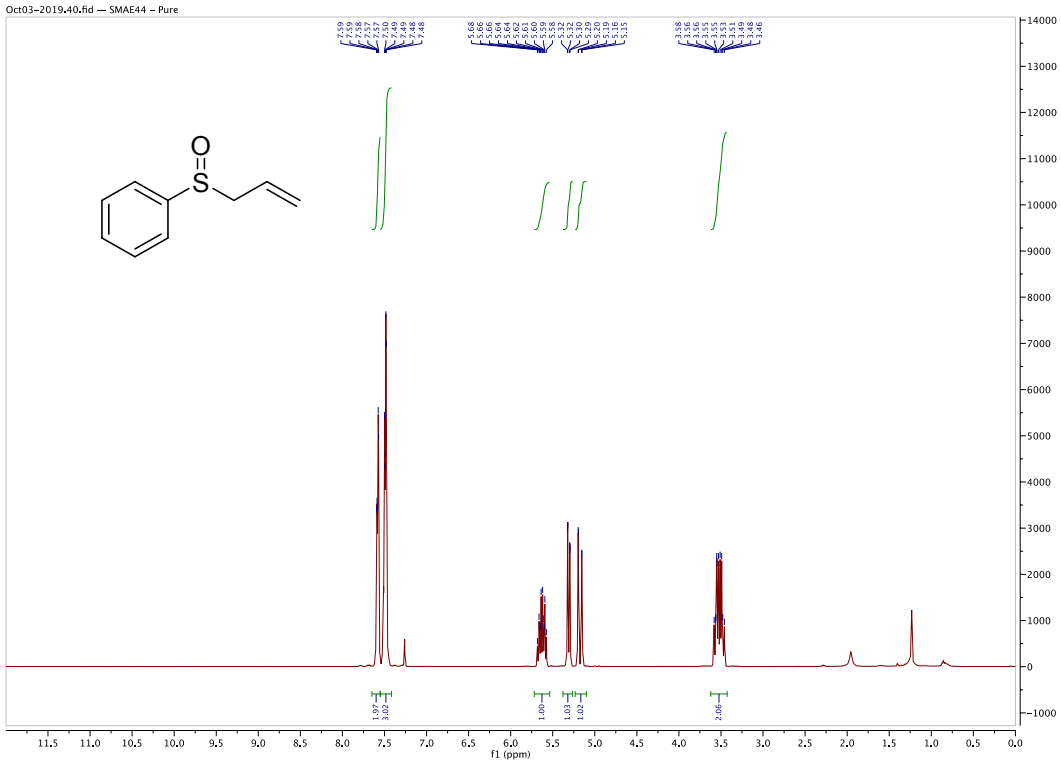
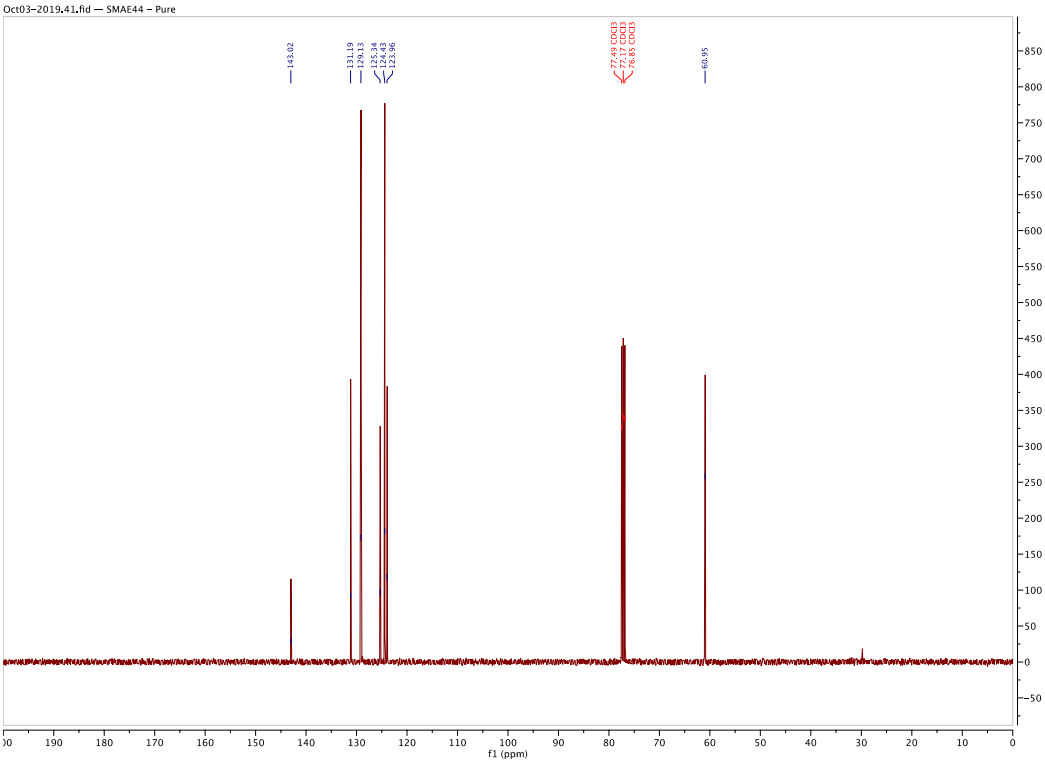


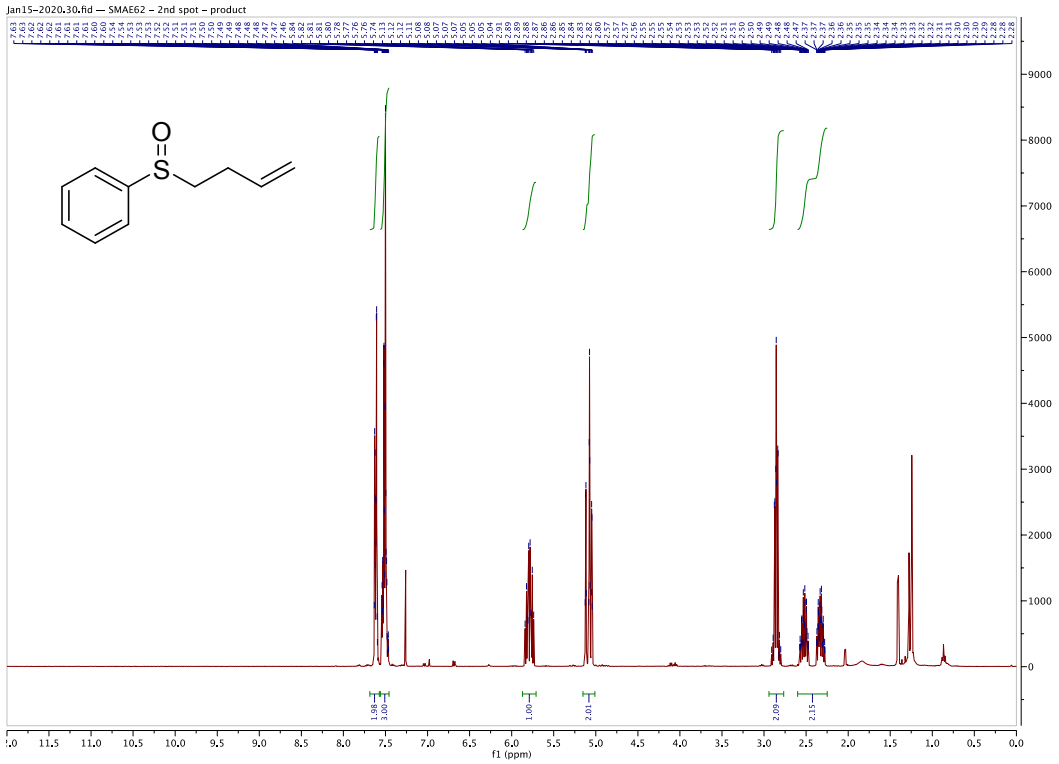


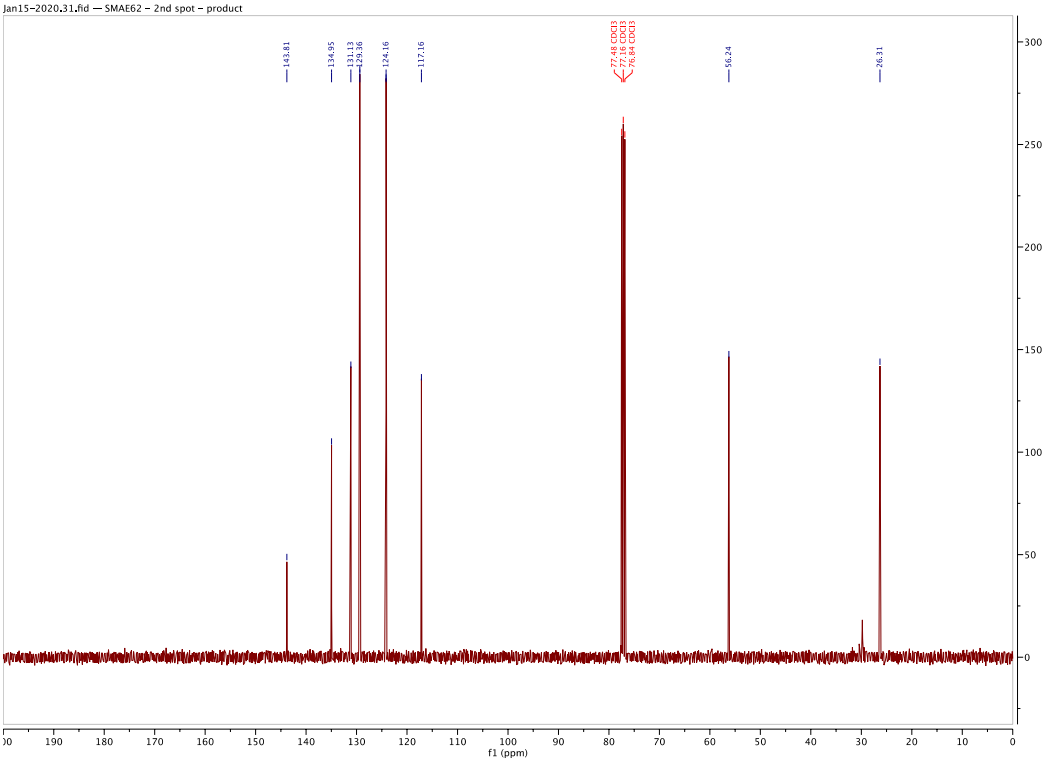
Allyl phenyl sulfoxide 6l



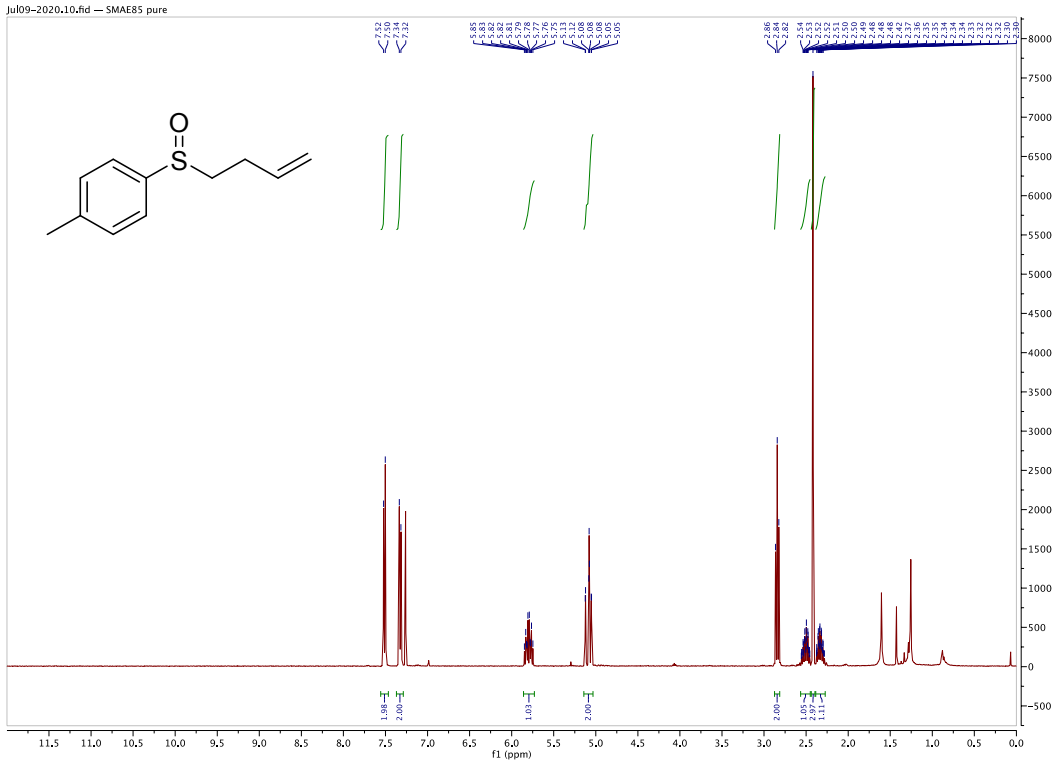


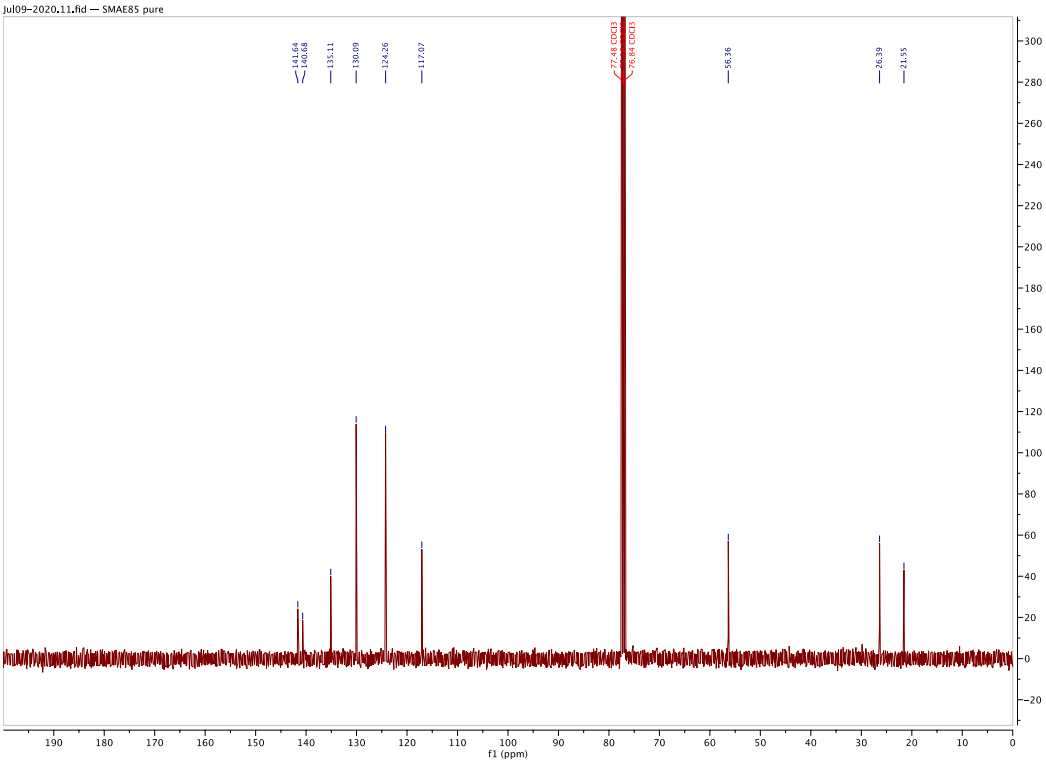
(But-3-en-1-ylsulfinyl)benzene 6m



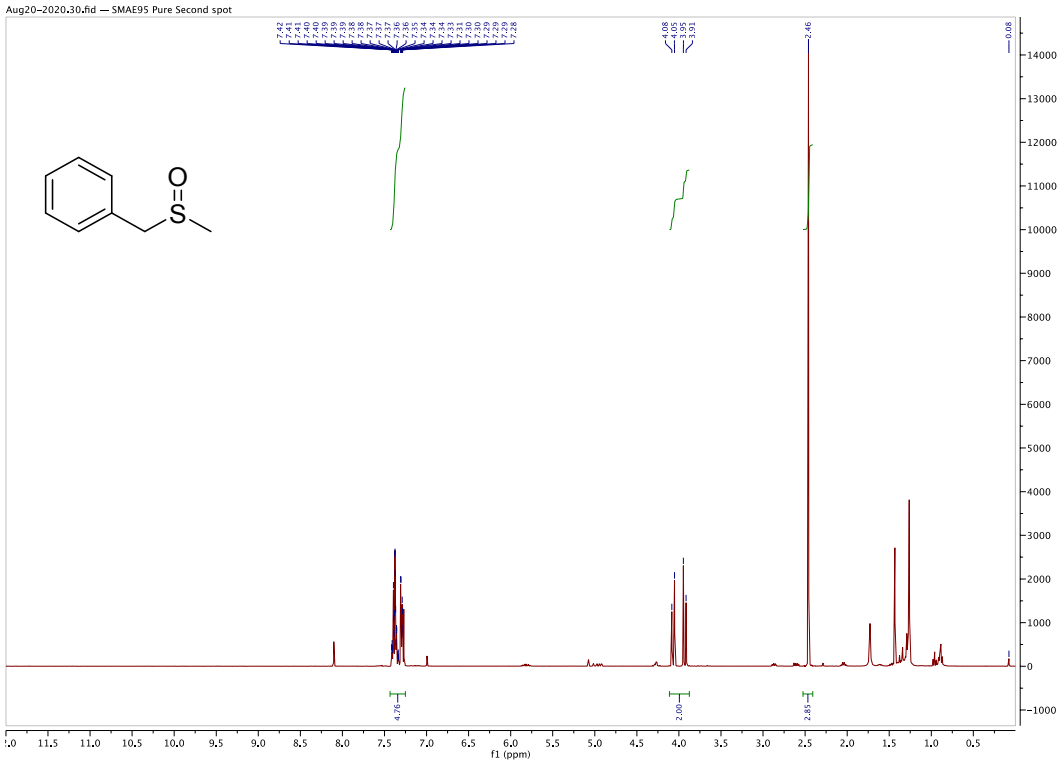


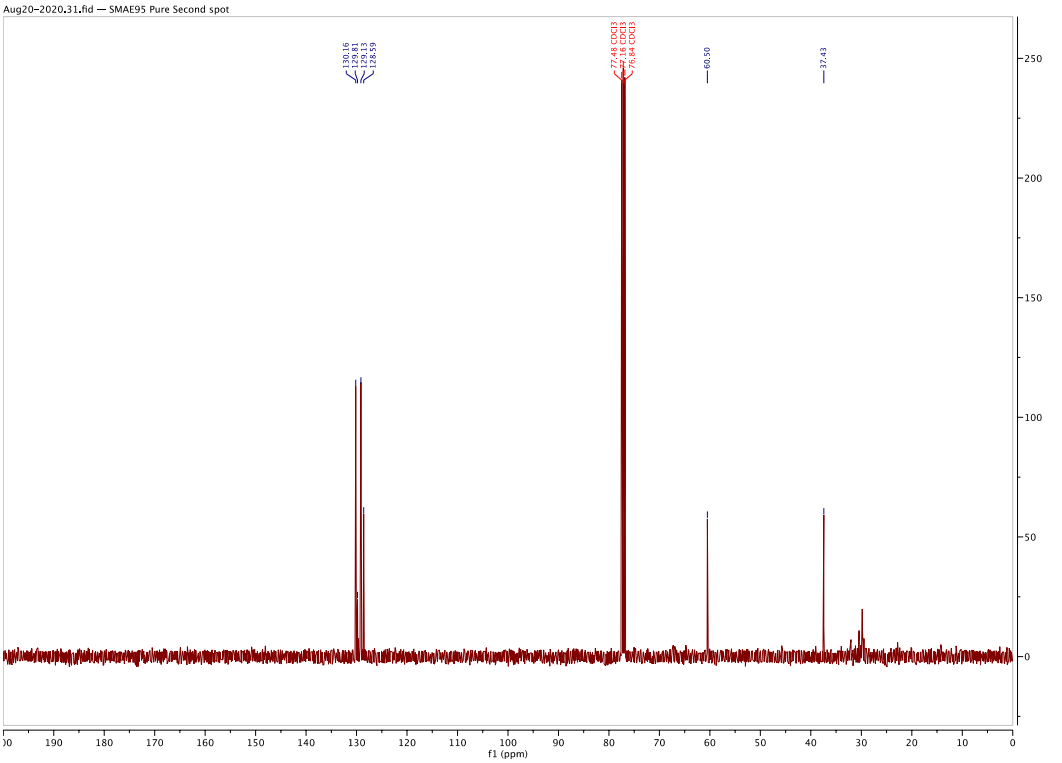
1-(but-3-en-1-ylsulfinyl)-4-methylbenzene 6n



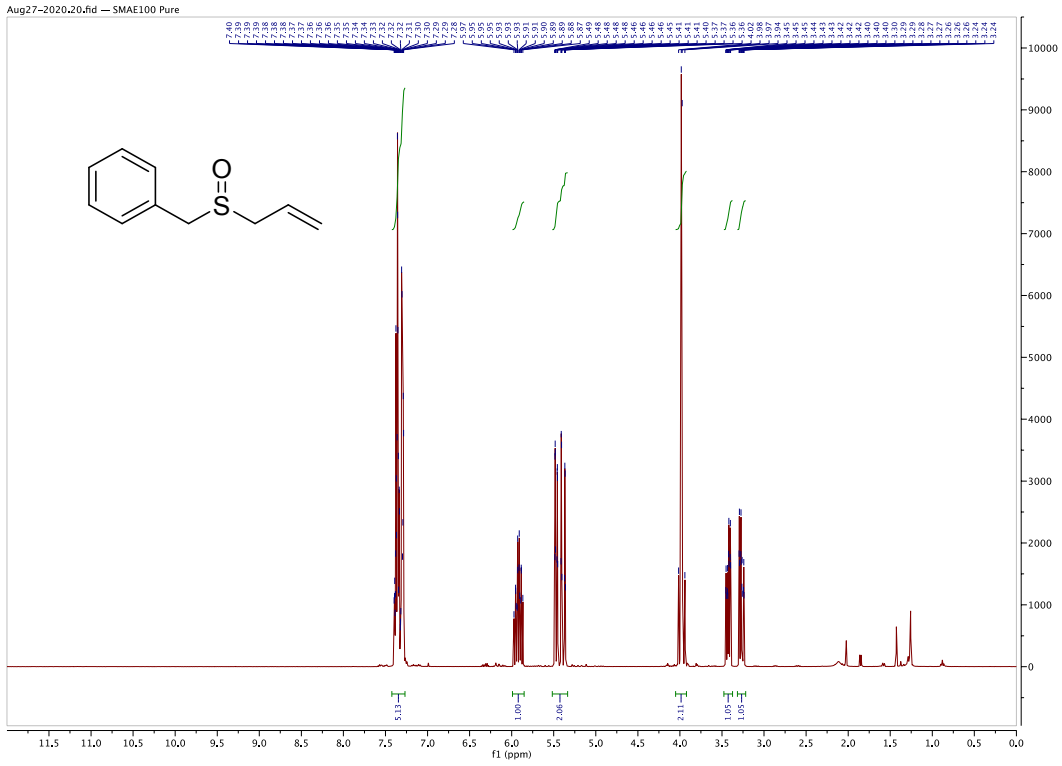


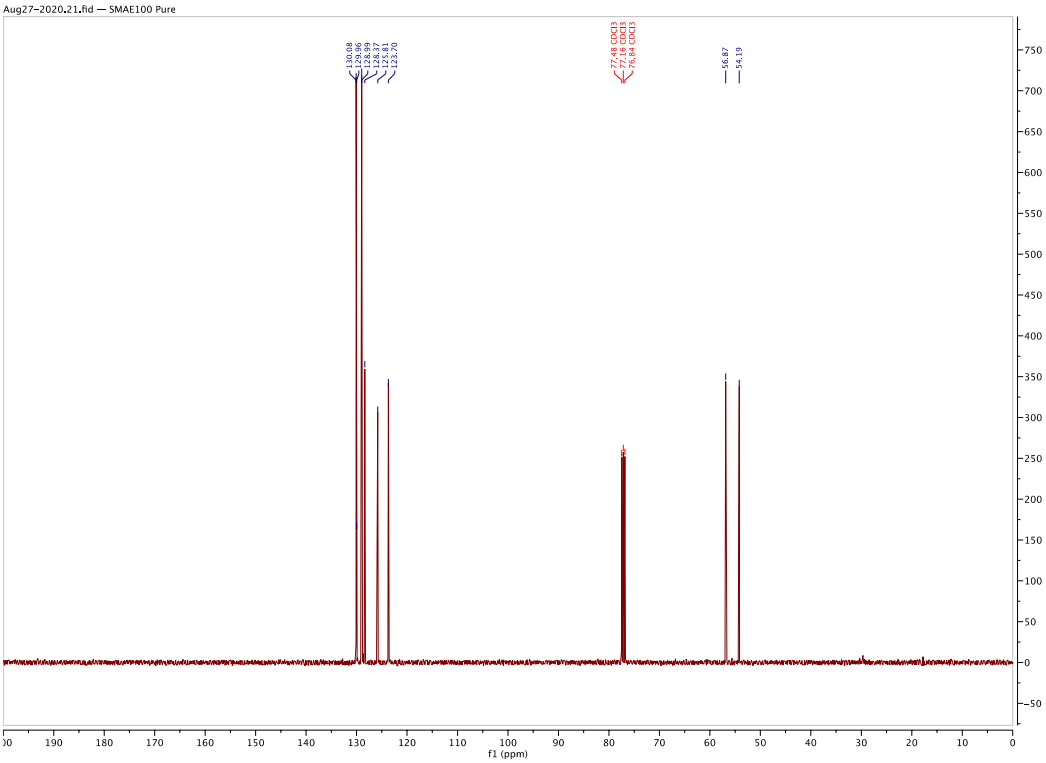
Benzyl methyl sulfoxide 6o



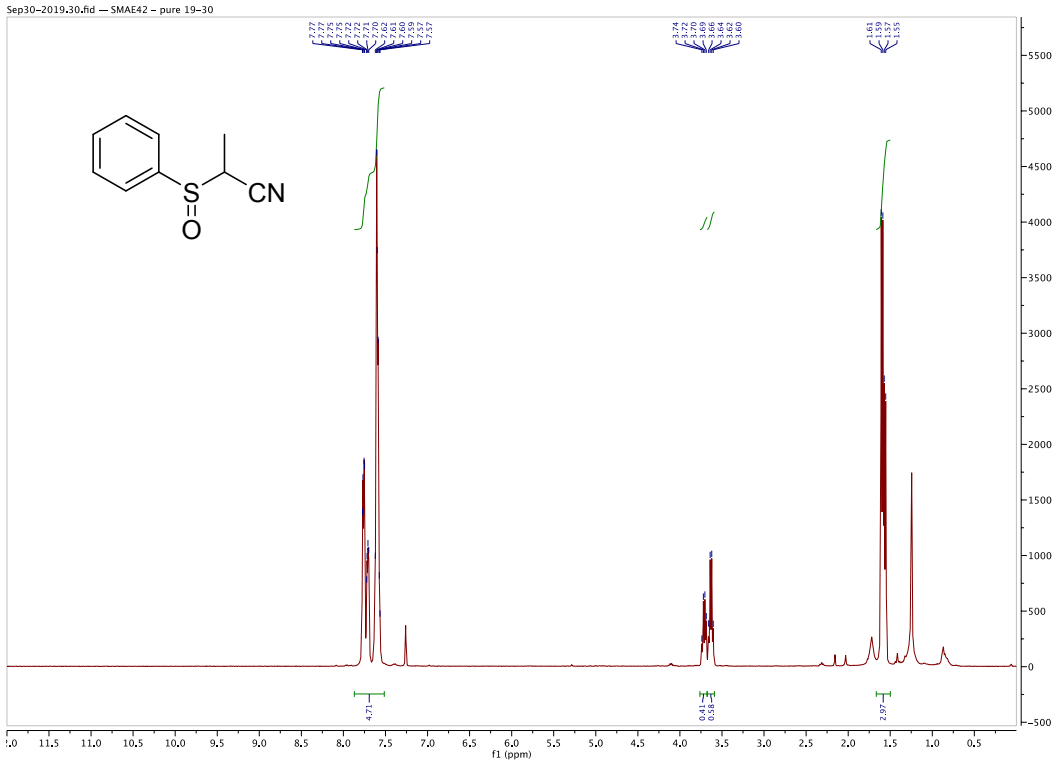


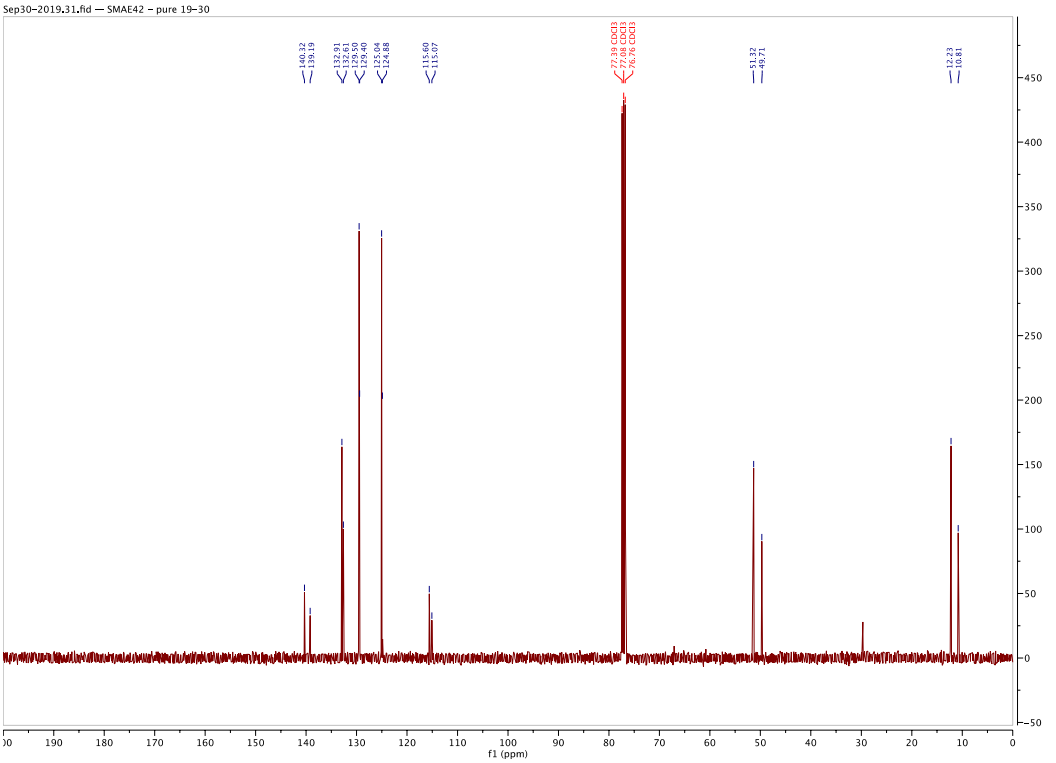
Allyl benzyl sulfoxide 6p



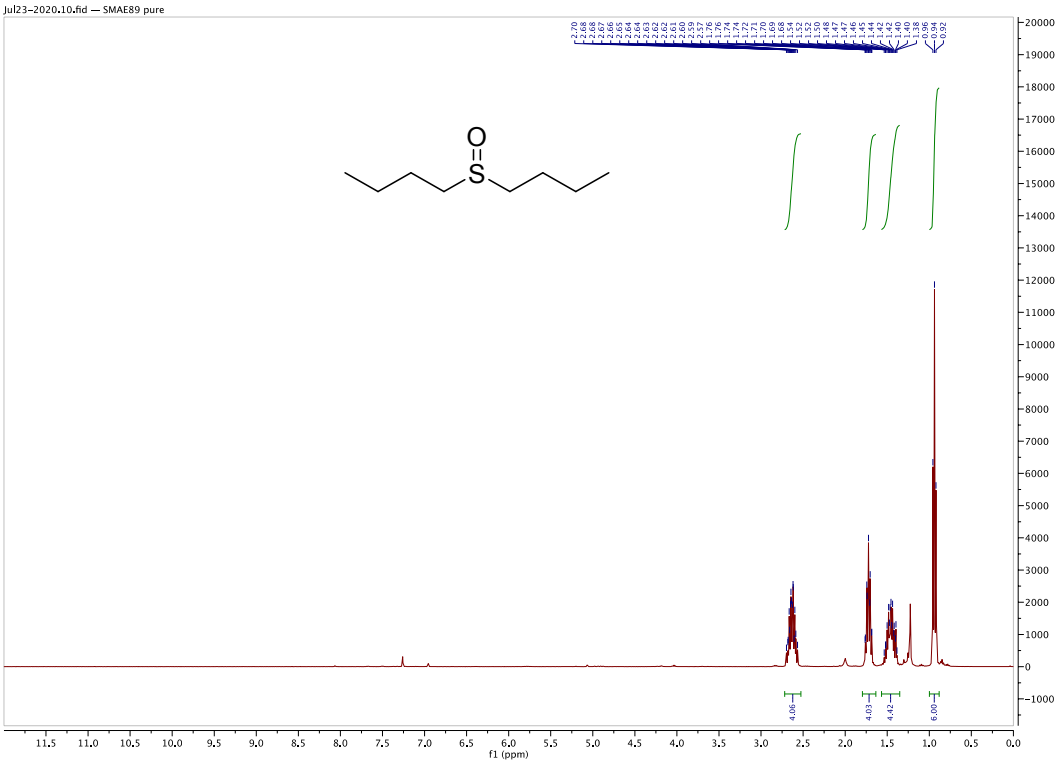


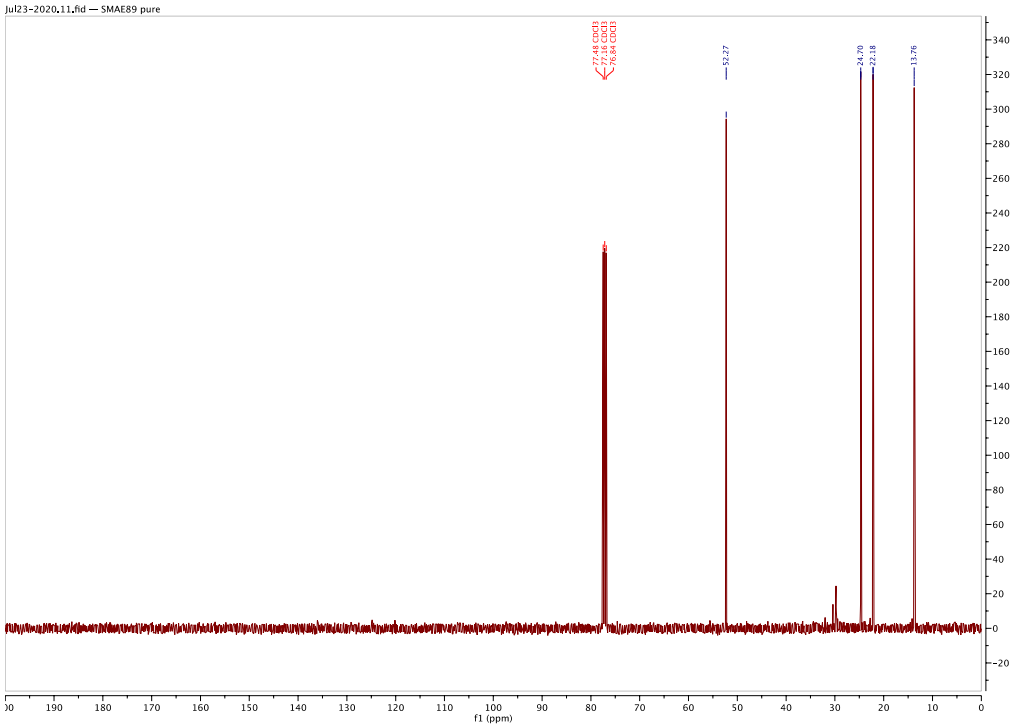
2-(Phenylsulfinyl)propanenitrile 6q



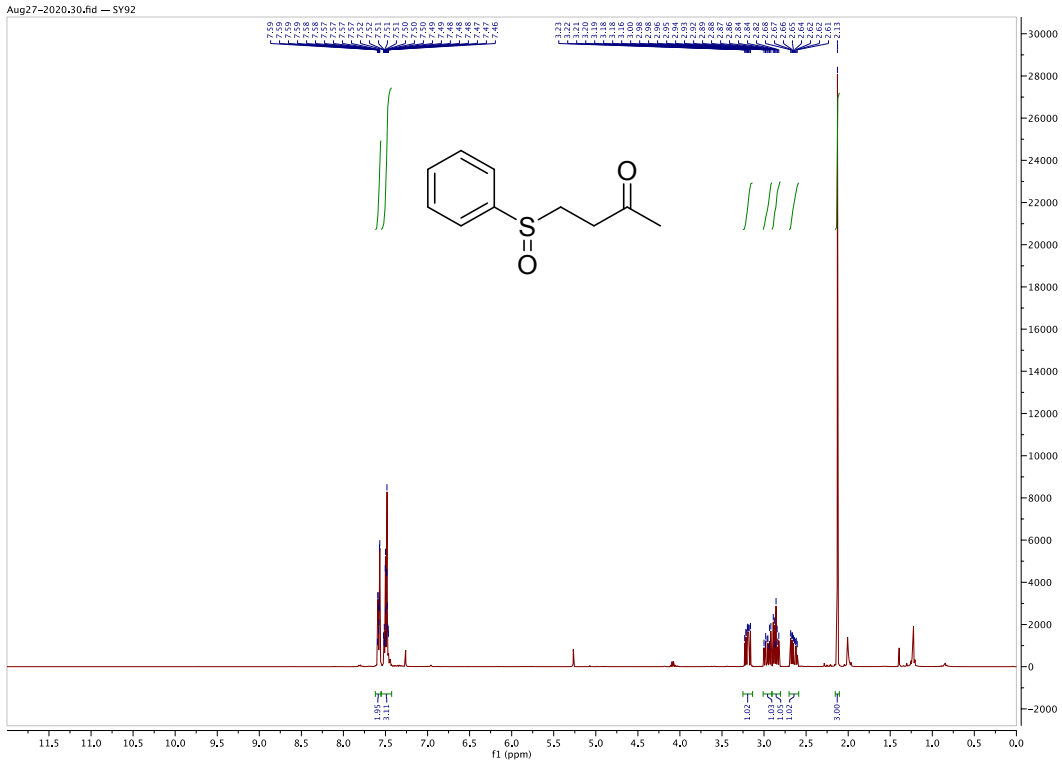


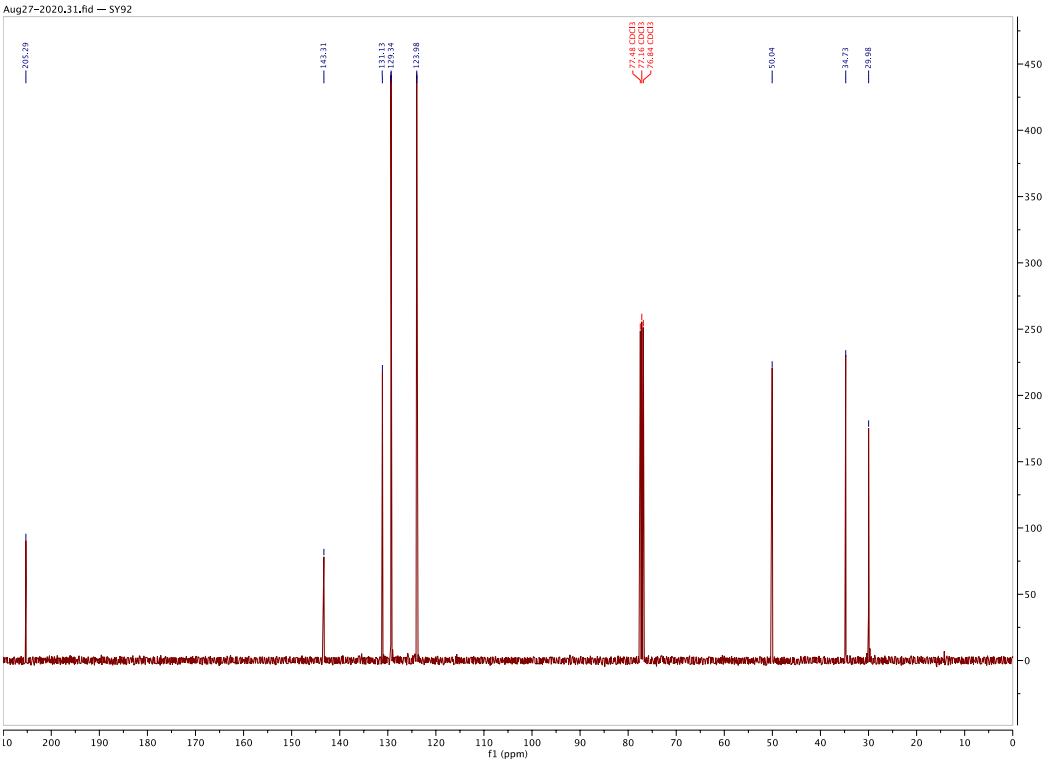
1-(Butylsulfinyl)butane 6r



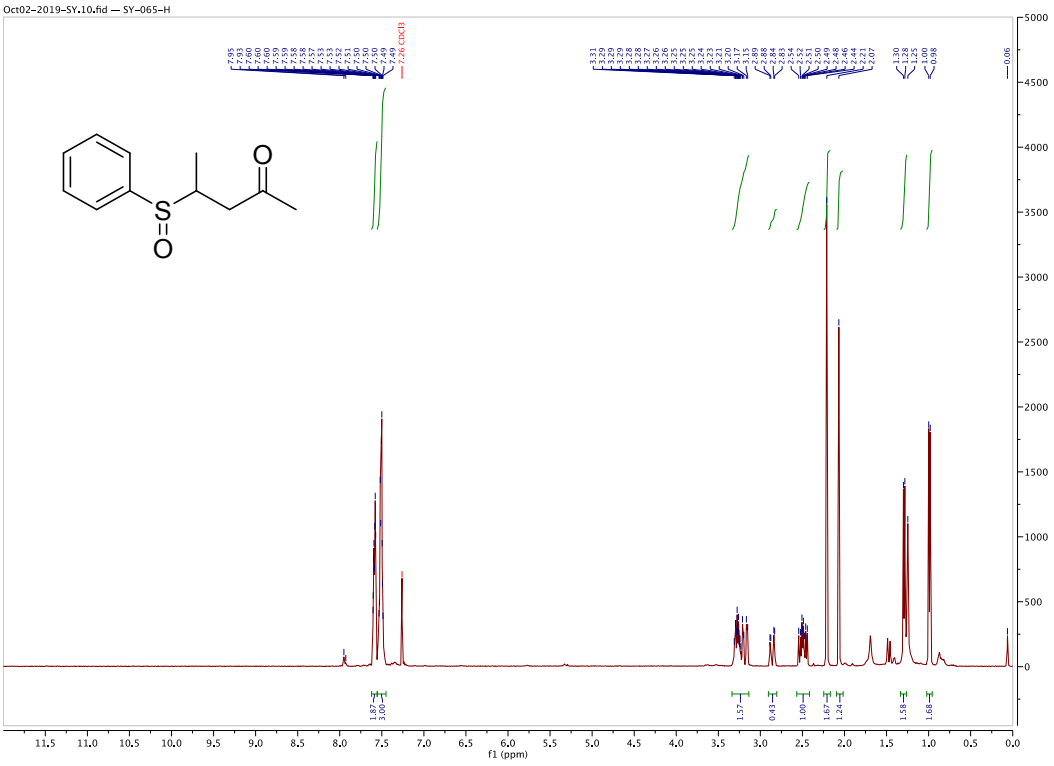


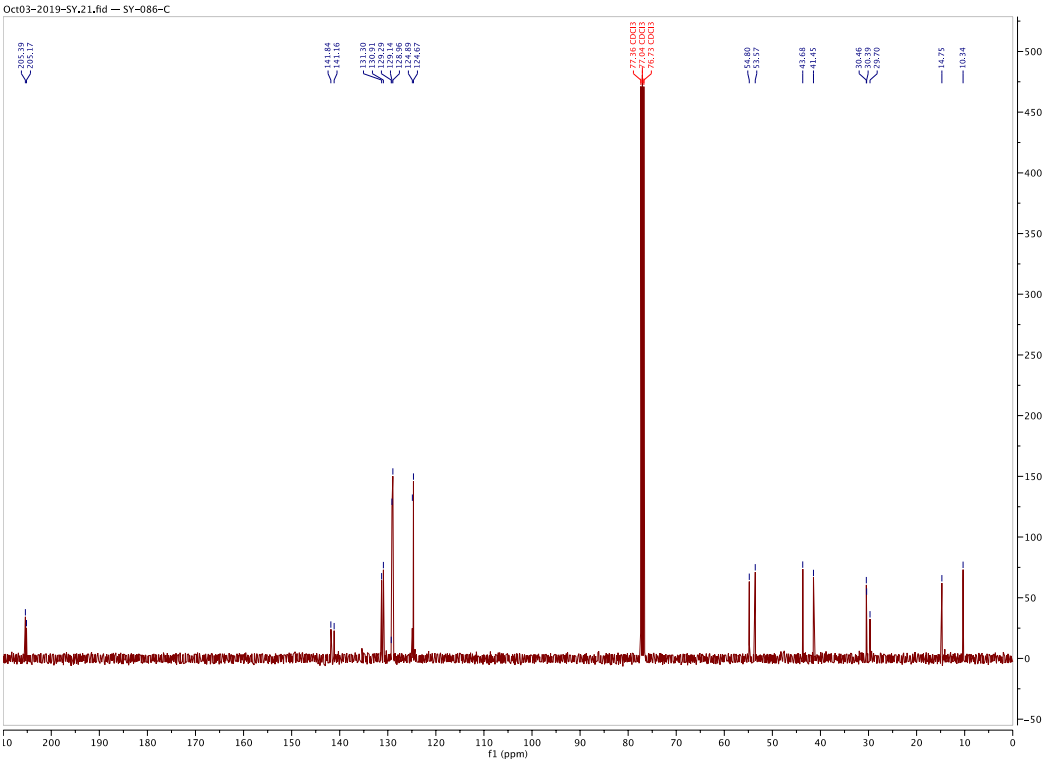
4-(Phenylsulfinyl)butan-2-one 13a



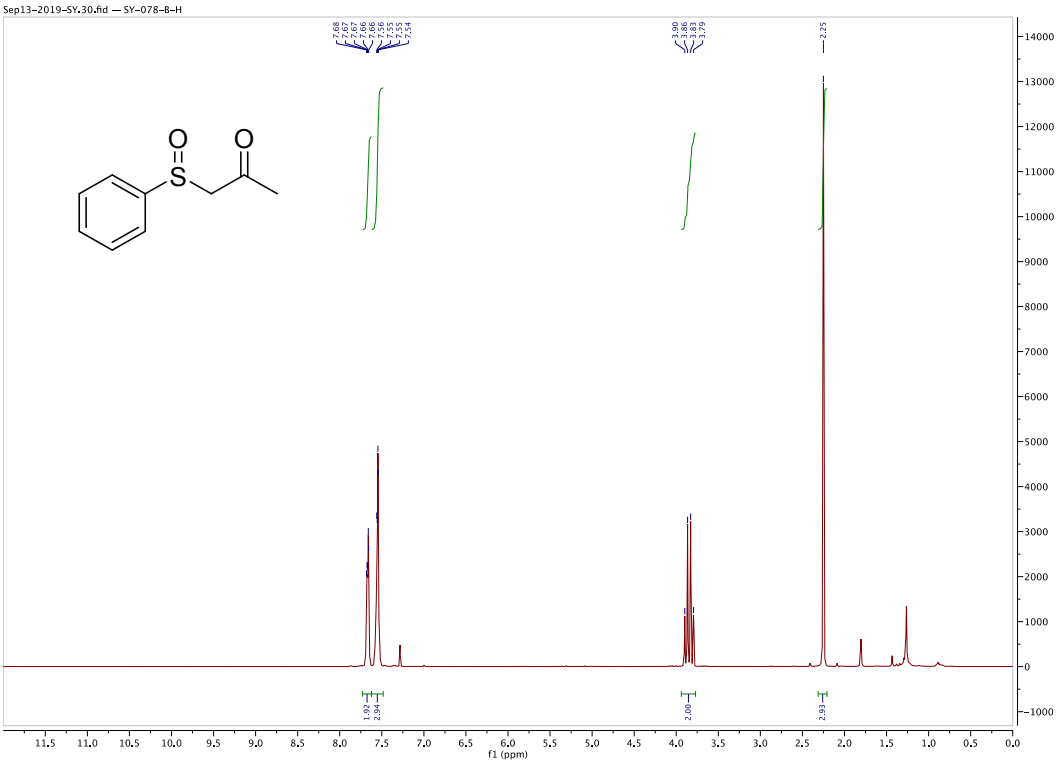


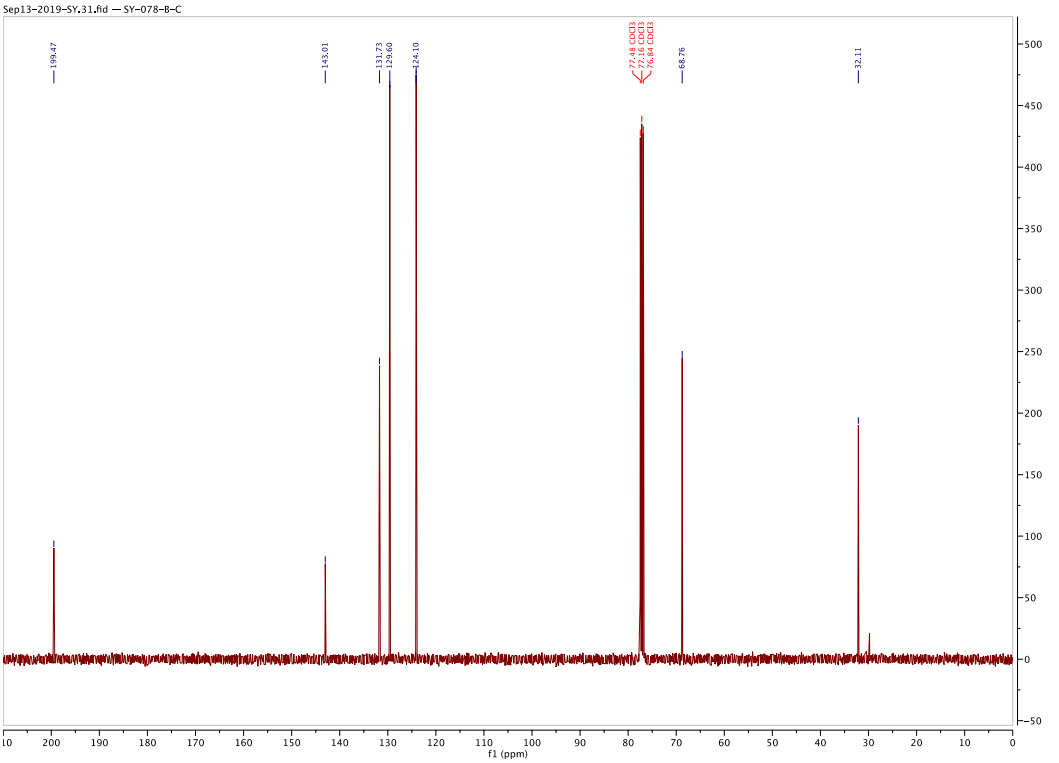
4-(Phenylsulfinyl)pentan-2-one 13b



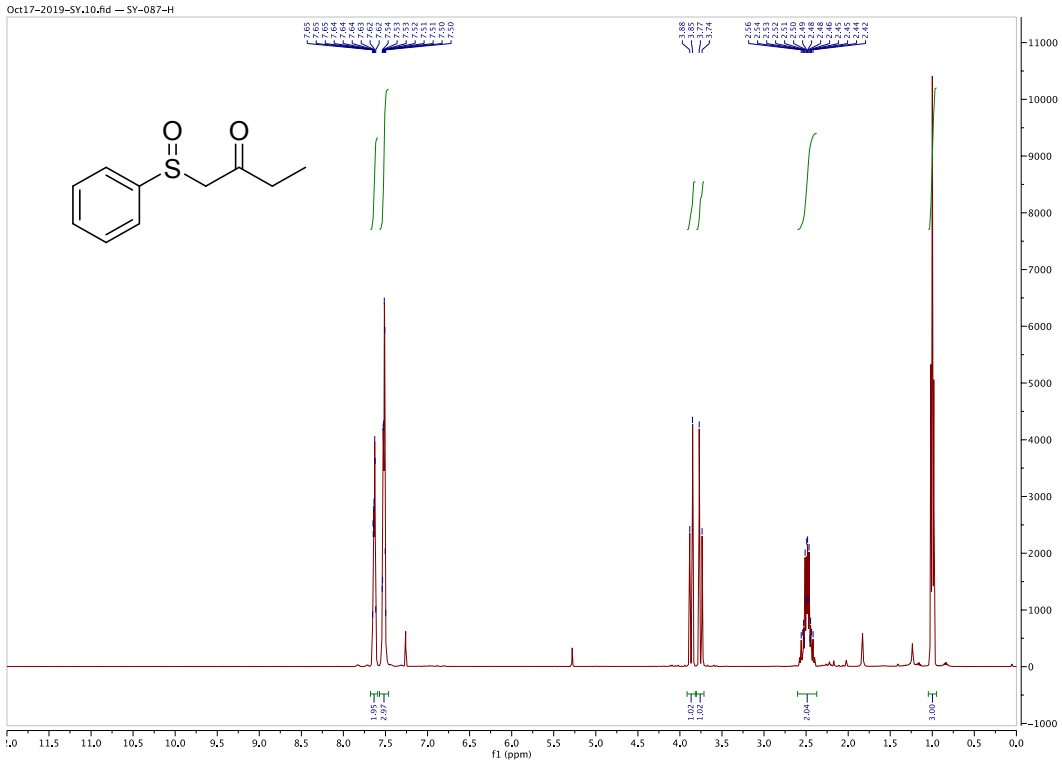


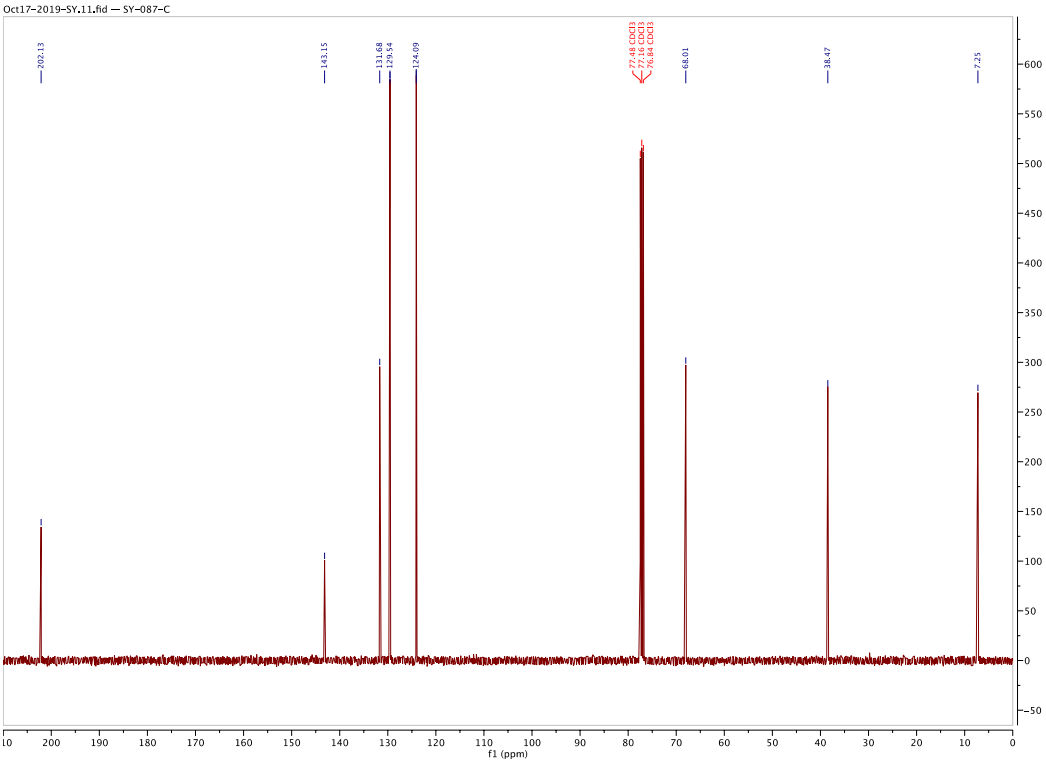
1-(Phenylsulfinyl)propan-2-one 13d



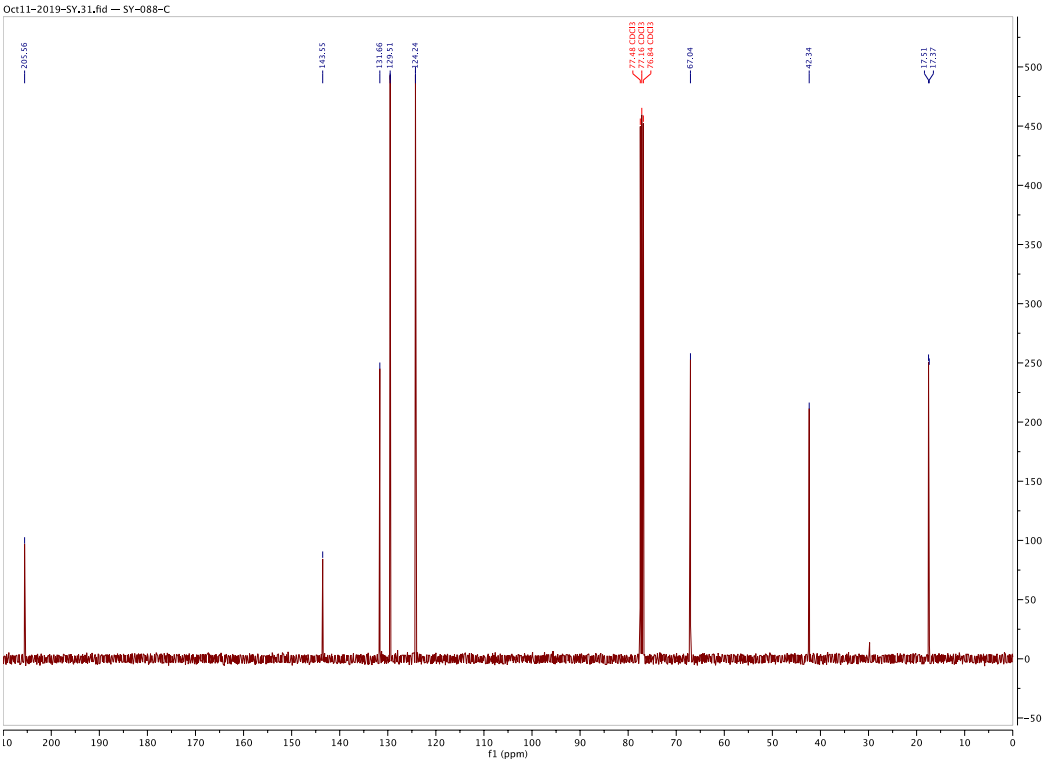


1-(phenylsulfinyl)butan-2-one 13e

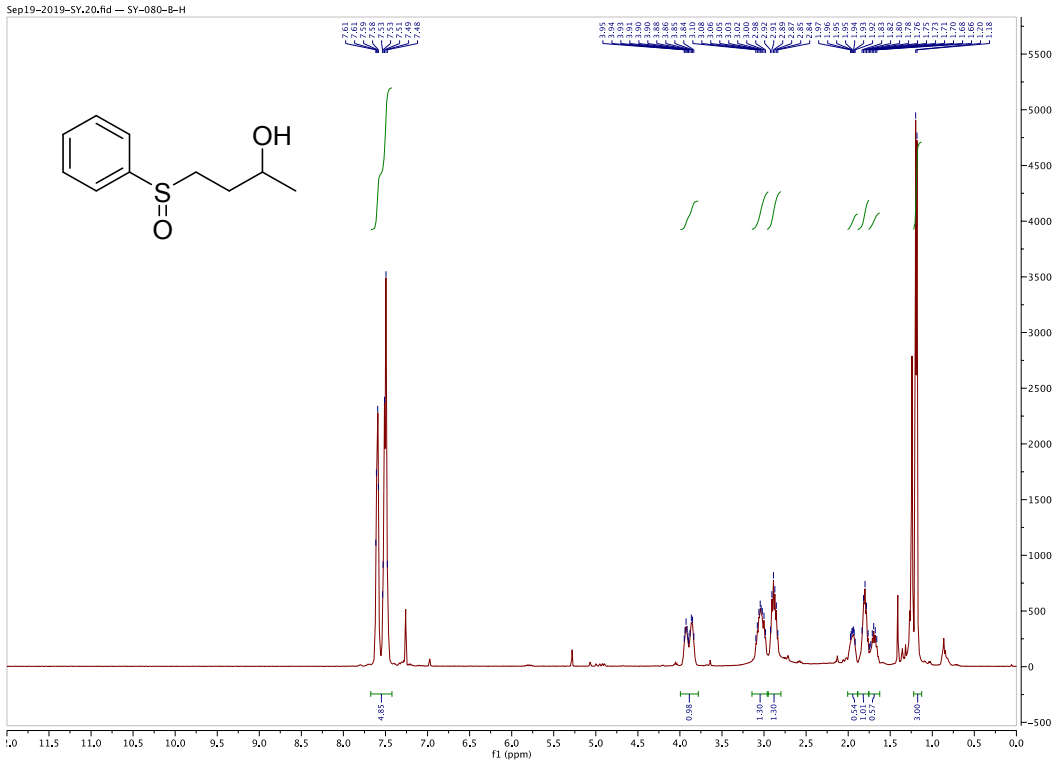


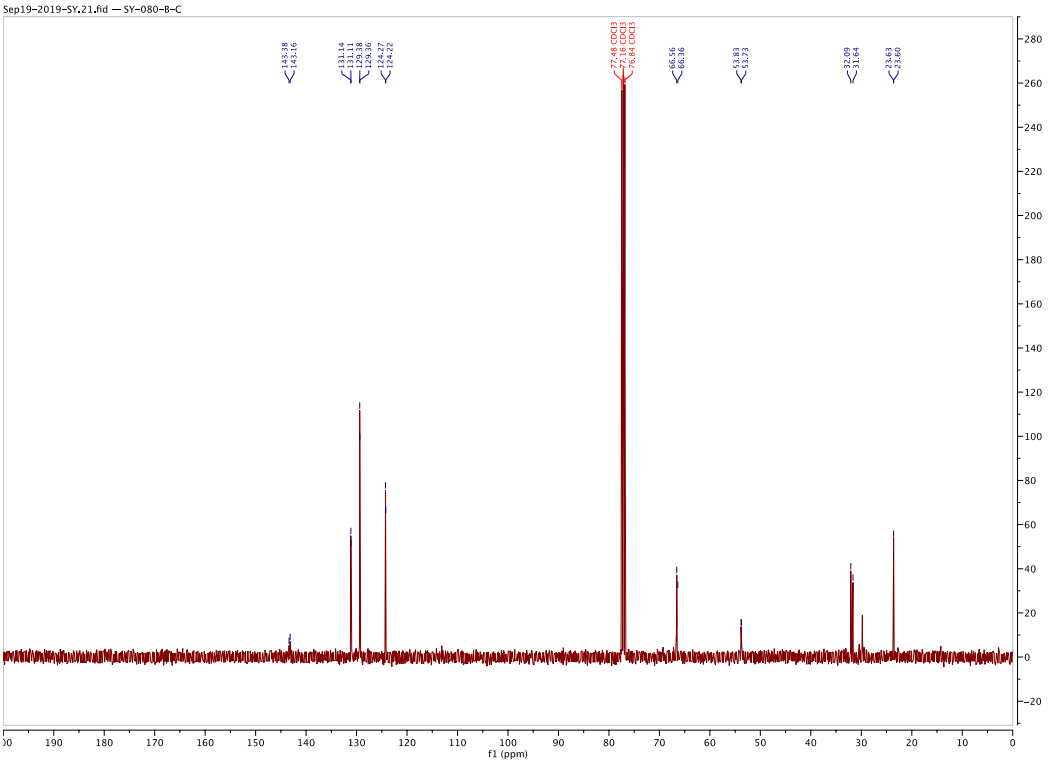


3-Methyl-1-(phenylsulfinyl)butan-2-one 13f

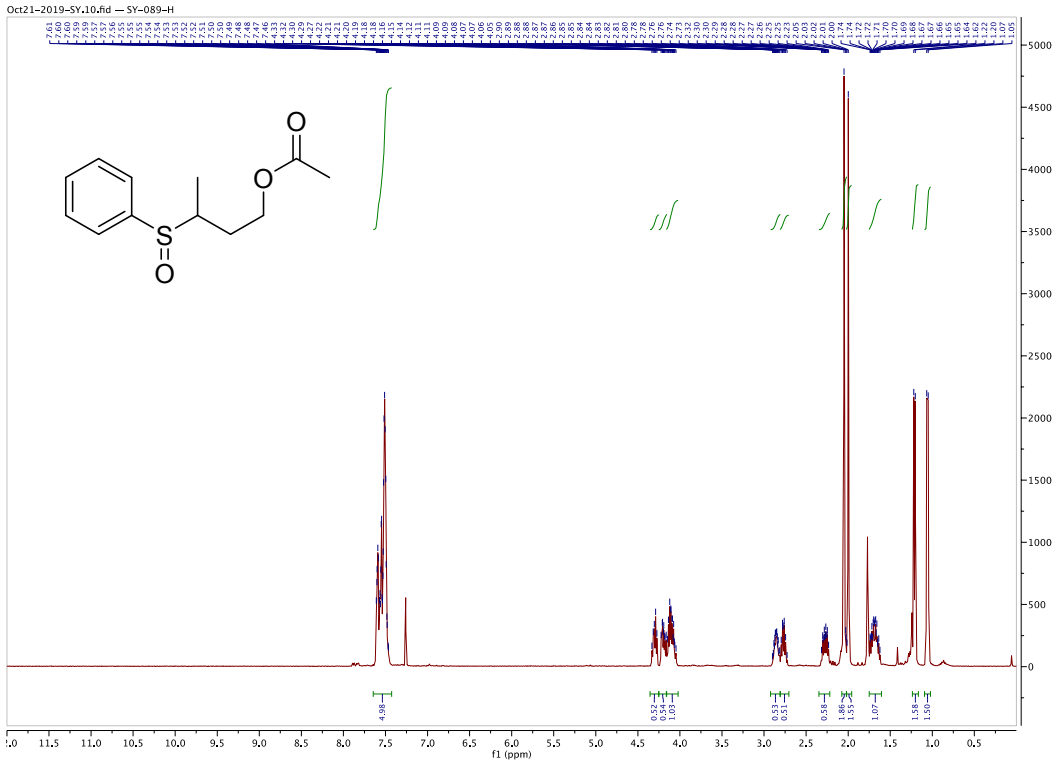


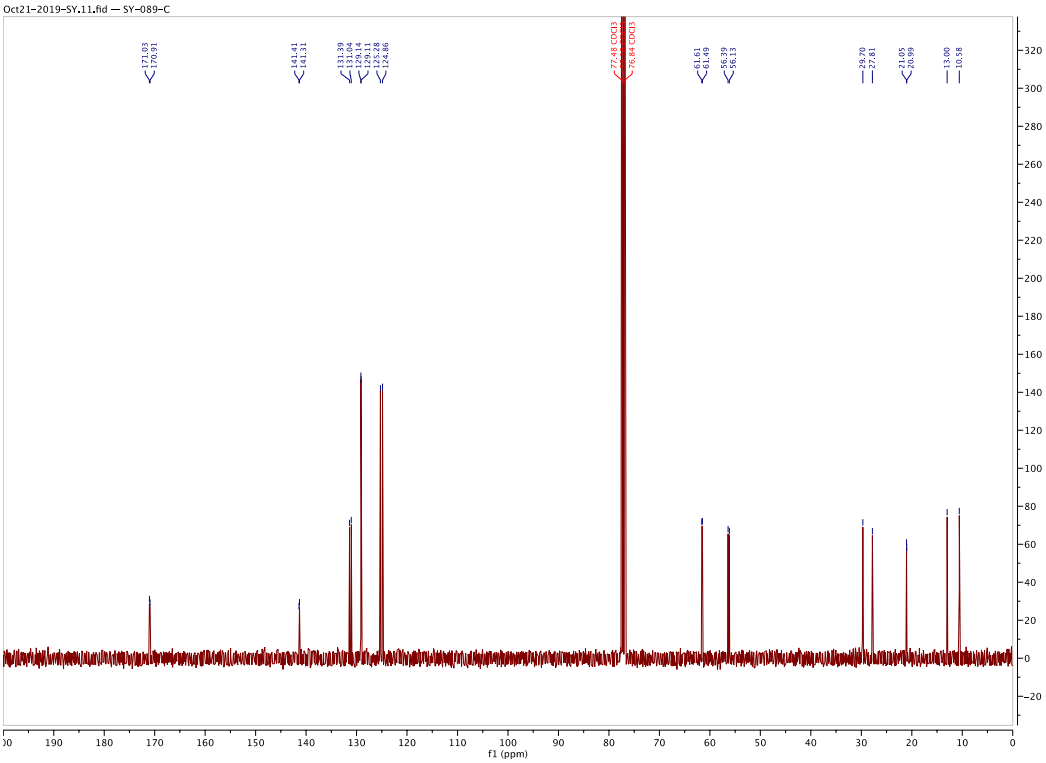
4-(Phenylsulfinyl)butan-2-ol 15a





3-(Phenylsulfinyl)butyl acetate 15b





Omeprazole 1