Electronic Supplementary Information (ESI) for

Selectivity switch in the aerobic oxygenation of sulfides photocatalysed by visible-light-responsive decavanadate

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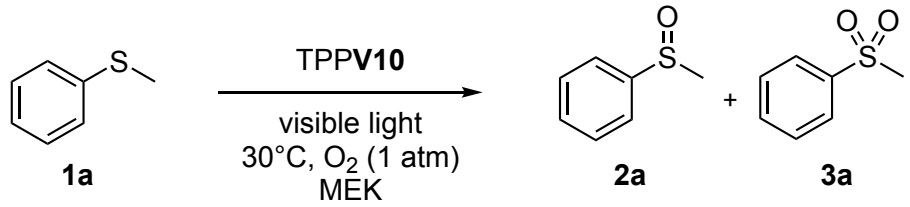
Table S1 Crystallographic data for TPP**V10**

Solvent	Acetonitrile/MEK
Formula	$C_{192}H_{160}O_{56}P_8V_{20}$
Fw (g mol^{-1})	4629.75
Crystal system	Monoclinic
Space group	$P2_1/n$ (No. 14)
a (Å)	12.2892(4)
b (Å)	20.1324(4)
c (Å)	18.9867(5)
α (deg)	90
β (deg)	102.411(3)
γ (deg)	120
V (Å^3)	4587.7(2)
Z	1
R_1[a] [$I>2\sigma(I)$]	0.0521
wR_2[a]	0.1285
GOF	1.017
ρ_{calcd} (g cm^{-3})	1. 676
Temp (K)	123

[a] $R_1 = \Sigma ||F_o|-|F_c||/\Sigma|F_o|$, $wR_2 = \{\Sigma[w(F_o^2-F_c^2)]/ \Sigma[w(F_o^2)^2]\}^{1/2}$.

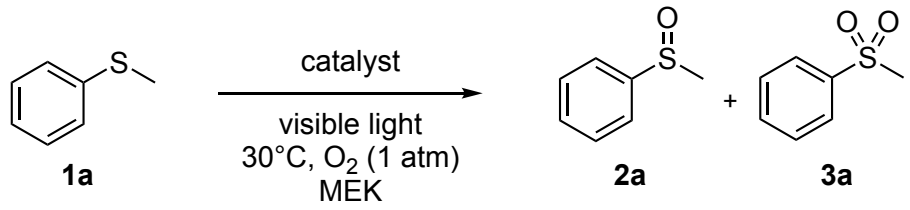
Table S2 Control experiments for the photocatalytic aerobic oxygenation of **1a** using TPP**V10**[a]



Entry	Catalyst	Conv. (%)	Yield (%)	
			2a	**3a**
1	TPP**V10**	98	<1	96
2	w/o	2	<1	<1
3[b]	TPP**V10**, dark	<1	<1	<1
4[c]	TPP**V10**, Ar	4	<1	<1
5[d]	TPP**V10**, Air	92	16	75
6[e]	TPP**V10**, O_2, LED	95	<1	94

[a]Reaction conditions: **1a** (0.2 mmol), **TPPV10** (0.4 mol%), MEK (4 mL), 30°C, visible light (λ > 400 nm), O_2 (1 atm), 8 h. Yields were determined by GC using dodecane as an internal standard. [b]Dark. [c]Ar (1 atm). [d]Air (1 atm), 24 h. [e]Blue LED (λ_{max} = 425 nm).

Table S3 Photocatalytic aerobic oxygenation of **1a** using various transition-metal complexes in MEK[a]

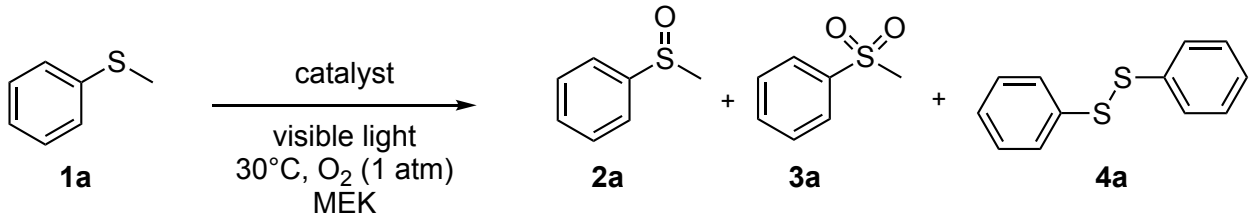


1a **2a** **3a**

Entry	Catalyst (mol%)	Conv. (%)	Yield (%)	
			2a	**3a**
1	TPP**V10** (0.4)	98	35	59
2	$VO(acac)_2$ (4)	53	44	4
3	V_2O_5 (2)	5	<1	<1
4	$NaVO_3$ (4)	3	<1	<1
5	$TiO(acac)_2$ (4)	<1	<1	<1
6	$Cr(acac)_3$ (4)	4	<1	<1
7	$Mn(acac)_3$ (4)	4	<1	<1
8	$Fe(acac)_3$ (4)	22	19	<1
9	$Co(acac)_2$ (4)	<1	<1	<1
10	$Ni(acac)_2$ (4)	2	<1	<1
11	$Cu(acac)_2$ (4)	2	<1	<1
12	$Ru(acac)_3$ (4)	2	<1	<1
13	$Pd(acac)_2$ (4)	1	<1	<1
14	Ag(OAc) (4)	3	<1	<1

[a]Reaction conditions: **1a** (0.2 mmol), solvent (4 mL), 30°C, xenon lamp (λ > 400 nm), O_2 (1 atm), 4 h. Yields were determined by GC using dodecane as an internal standard.

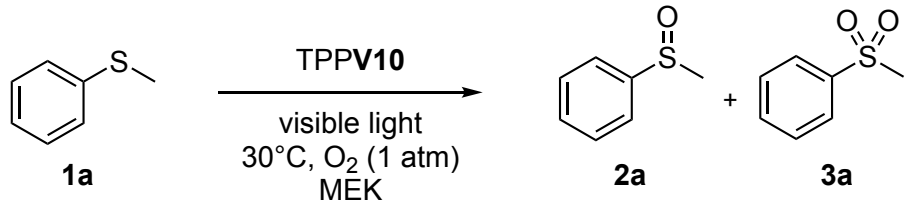
Table S4 Photocatalytic aerobic oxygenation of **1a** using various photocatalysts in MEK[a]



Entry	Catalyst (mol%)	Conv. (%)	Yield (%)		
			2a	**3a**	**4a**
1	TPP**V10** (0.4)	98	<1	96	<1
2	TBA**W10** (0.4)	95	67	25	<1
3	$Ru(bpy)_3Cl_2$ (1)	>99	59	6	14
4	Eosin Y (1)	47	24	0	2
5	Methylene blue (1)	64	34	3	11
6	Rose bengal (1)	67	32	2	9

[a]Reaction conditions: **1a** (0.2 mmol), MEK (4 mL), 30°C, xenon lamp (λ > 400 nm), O_2 (1 atm), 8 h. Yields were determined by GC using dodecane as an internal standard.

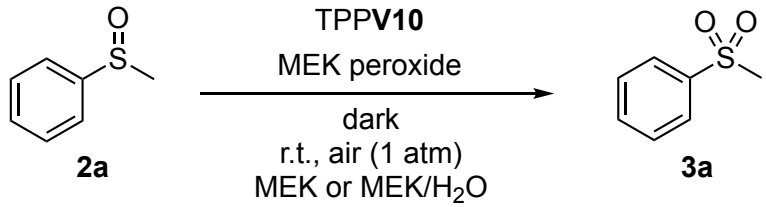
Table S5 Photocatalytic aerobic oxygenation of **1a** in the presence of various radical scavengers[a]



Entry	Radical scavenger	Inhibited species	Conv. (%)	Yield (%)	
				2a	**3a**
1	w/o	−	98	<1	96
2	TEMPO	Radicals	<1	<1	<1
3	1,4-Dimethoxybenzene	$R_2S^{+\bullet}$	32	30	1
4	Benzoquinone	Superoxide anion radical	39	31	6
5	Isopropanol	•OH	95	22	68

[a]Reaction conditions: **1a** (0.2 mmol), radical scavengers (0.2 mmol), TPP**V10** (0.35 mol%), MEK (4 mL), 30°C, xenon lamp (λ > 400 nm), O_2 (1 atm), 8 h. Yields were determined by GC using dodecane as an internal standard.

Table S6 Oxygenation of **2a** using MEK peroxide[a]



Entry	Solvent (v/v)	Conv. (%)	Yield (%)
1	MEK	74	74
2[b]	MEK	71	70
3	MEK/H_2O (92/8)	89	89
4[b]	MEK/H_2O (92/8)	84	81

[a]Reaction conditions: **2a** (0.2 mmol), TPP**V10** (0.4 mol%), MEK peroxide (0.6 mmol), solvent (4 mL), r.t., dark, air (1 atm), 4 h. [b]Without TPP**V10**.

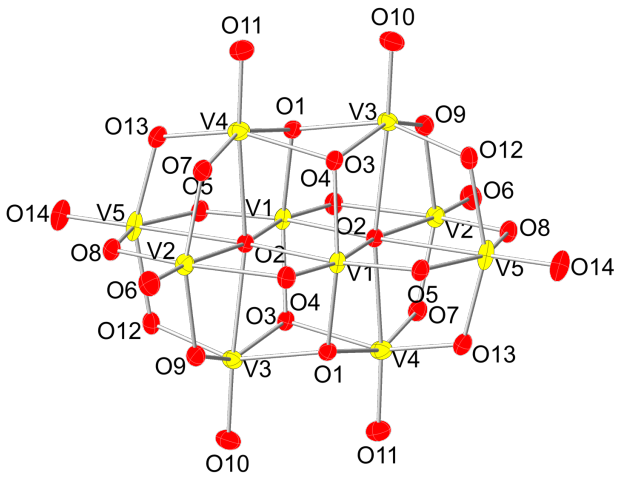


Fig. S1 Thermal ellipsoid plots representation (50% probability level) of the anion parts of TPP**V10**.

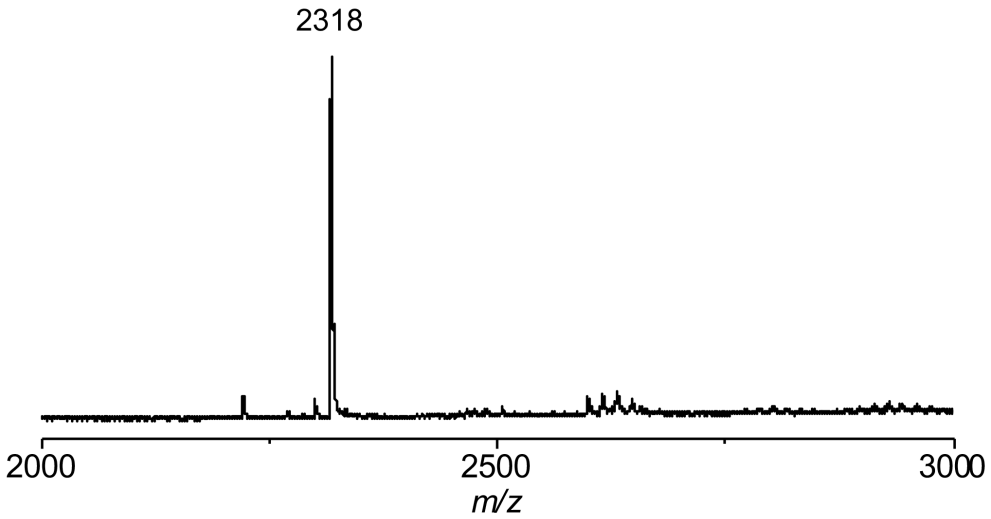


Fig. S2 Positive-ion CSI mass spectrum of TPP**V10** in acetonitrile. The set of signals at *m/z* 2318 was assignable to $[TPP_4H_3V_{10}O_{28}]^+$.

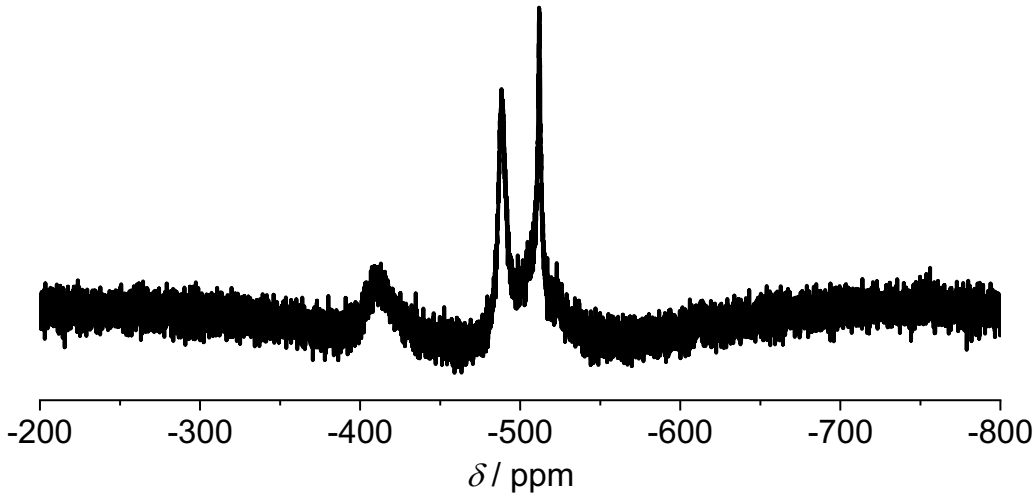


Fig. S3 ^{51}V NMR spectrum of TPP**V10** in acetonitrile-d_3.

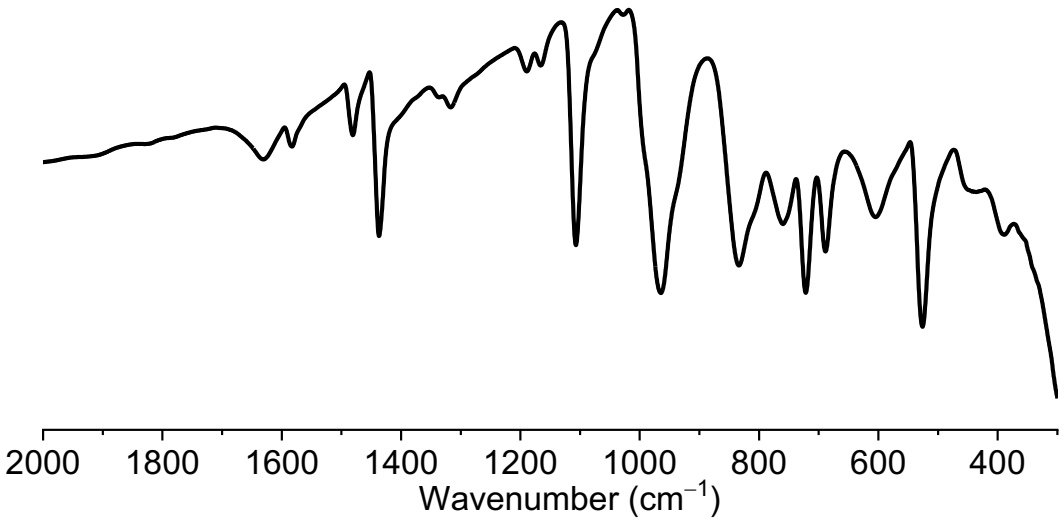


Fig. S4 IR spectrum of TPP**V10** (KCl disc).

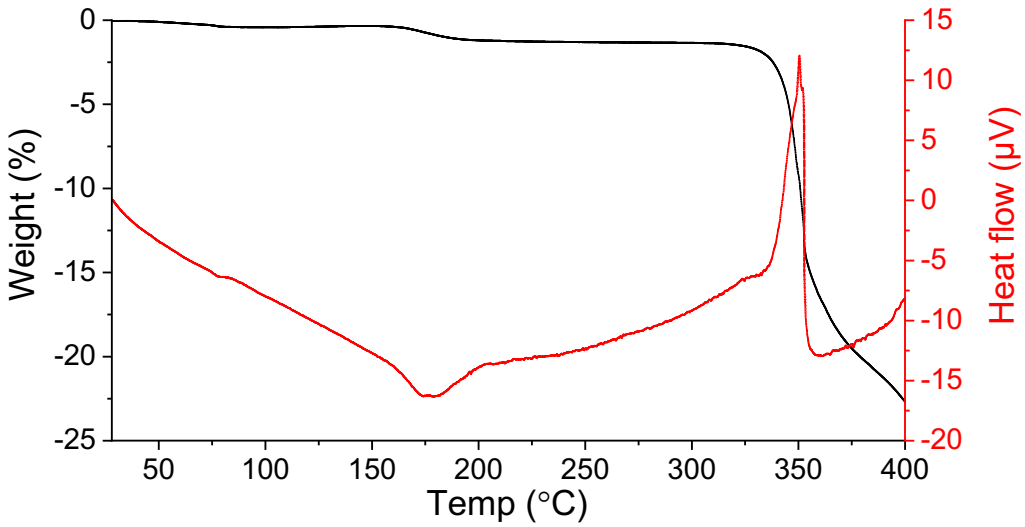


Fig. S5 TG–DTA curve of TPP**V10** under N_2 atmosphere.

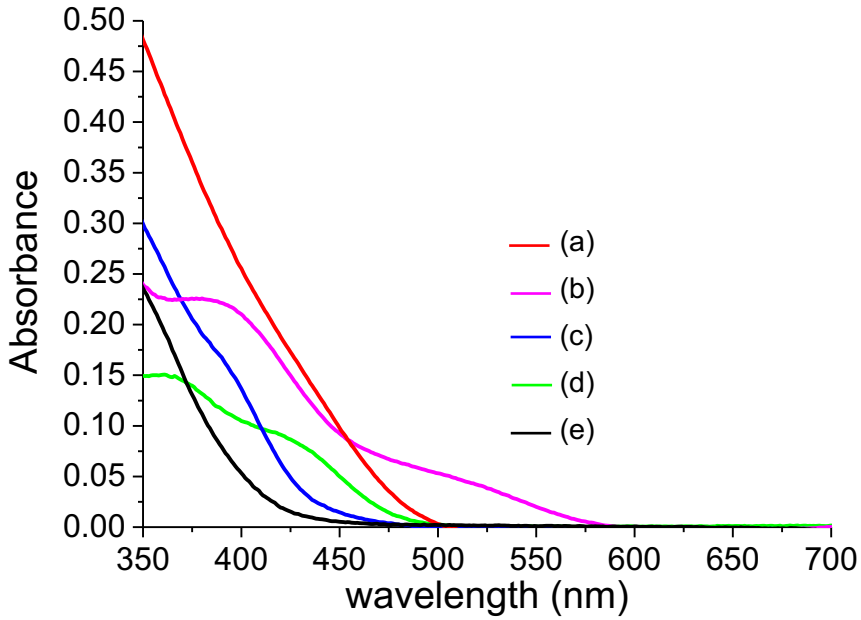


Fig. S6 UV-Vis spectra of (a) TBA**V10** (0.05 mM), (b) $TBA_6[\alpha\text{-}PV_3W_9O_{40}]$ (0.05 mM), (c) $TBA_4H[\gamma\text{-}PV_2W_{10}O_{40}]$ (0.05 mM), (d) $TBA_4[\alpha\text{-}PV_1W_{11}O_{40}]$ (0.05 mM), (e) $TBA_4H_2[\gamma\text{-}SiV_2W_{10}O_{40}]$ (0.05 mM) in acetonitrile (1 cm cell).

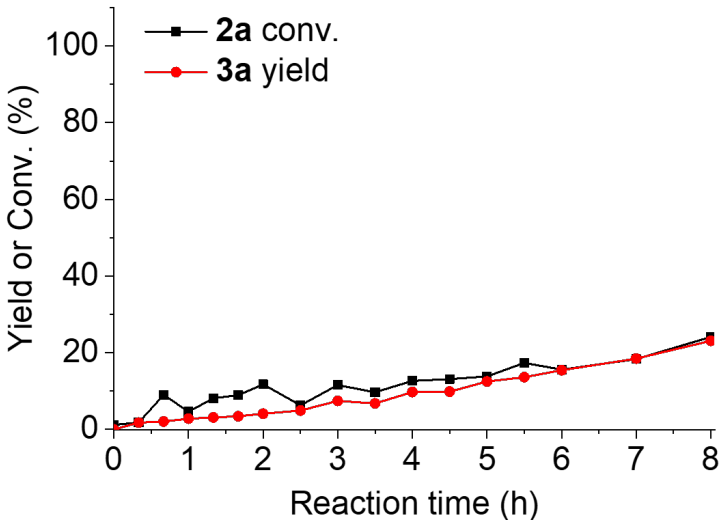
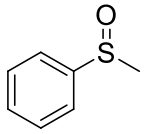


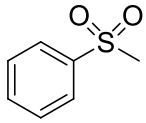
Fig. S7 A reaction profile of the photocatalytic aerobic oxygenation of **2a** using TPP**V10** as a catalyst in (a) MEK. Reaction conditions: **2a** (0.2 mmol), TPP**V10** (0.4 mol%), solvent (4 mL), 30°C, visible light (λ > 400 nm, xenon lamp), O_2 (1 atm).

Compound data

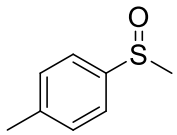
All compounds were analyzed by GC (TC-1 capillary column, 0.32 mm × 30 m, GL-science) and GC mass (InertCap-5 capillary column, 0.32 mm × 30 m, GL-science) with the following conditions: carrier gas inlet pressure (N_2, 150 kPa), initial column temperature (80℃), intermediate column temperature (150℃), progress rate (10℃ min^{-1}), final column temperature (280℃), progress rate (20℃ min^{-1}), injection temperature (280℃), detection temperature (280℃). Column chromatography was performed to isolate the products with silica gel and solvents were technical standard. NMR spectra were recorded on a JEOL ECA-500 spectrometer (^1H, 500.16 MHz; ^{13}C, 125.77 MHz) using 5 mm tubes. Chemical shifts (δ) are reported in ppm downfield from TMS for ^1H NMR spectra and ^{13}C NMR spectra.



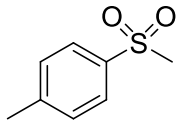
(Methylsulfinyl)benzene (**2a**) (CAS No. 1193-82-4) 93% GC yield, 76% isolated yield. Isolated as colorless liquid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate = 1/4, R_f = 0.26). ^1H NMR (500 MHz, $CDCl_3$, TMS): δ 7.67–7.64 (m, 2H, Ar), 7.56–7.49 (m, 3H, Ar), 2.73 (s, 3H, CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, TMS): δ 145.8, 131.2, 129.5, 123.6, 44.1. MS (EI) *m/z* (%): 50 (12), 51 (29), 63 (5), 65 (22), 69 (10), 77 (24), 78 (41), 79 (6), 91 (40), 97 (18), 108 (5), 109 (39), 123 (8), 124 (100), 125 (32), 126 (6), 140 (24) [M^+]. GC retention time (5.1 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.60 (calculated by calibration curve using a commercial substance). These NMR and MS spectral data accord with those previously reported.[1]



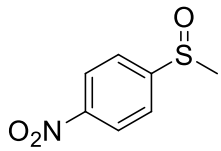
(Methylsulfonyl)benzene (3a): (CAS No. 3112-85-4) 96% GC yield, 63% isolated yield. Isolated as a colorless liquid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate = 1/1, R_f = 0.50). ^1H NMR (500 MHz, $CDCl_3$, TMS): δ 7.98–7.94 (m, 2H, Ar), 7.69–7.65 (m, 1H, Ar), 7.61–7.56 (m, 2H, Ar), 3.07 (s, 3H, CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, TMS): δ 140.7, 133.8, 129.5, 127.5, 44.6. MS (EI) *m/z* (%): 50 (13), 51 (35), 65 (10), 74 (4), 75 (3), 76 (4), 77 (100), 78 (7), 93 (6), 94 (37), 95 (3), 141 (25), 156 (24) [M^+]. GC retention time (5.6 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.62 (calculated by calibration curve using a commercial substance). These NMR and MS spectral data accord with those previously reported.[2]



1-Methyl-4-(methylsulfinyl)benzene (2b): (CAS No. 623-13-2) 91% GC yield, 63% isolated yield. Isolated as a colorless liquid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate = 1/3, R_f = 0.24). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.55 (d, J = 8.3 Hz, 2H, Ar), 7.34 (d, J = 8.3 Hz, 2H, Ar), 2.71 (s, 3H, CH_3), 2.42 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 142.5, 141.7, 130.2, 123.7, 40.1, 21.6. MS (EI) *m/z* (%): 50 (5), 51 (9), 62 (5), 63 (15), 65 (27), 67 (17), 77 (35), 78 (12), 79 (10), 89 (11), 90 (4), 91 (41), 92 (5), 107 (7), 108 (11), 111 (14), 121 (5), 123 (6), 138 (17), 139 (100), 140 (9), 141 (5), 154 (63) [M^+], 155 (6). GC retention time (6.5 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.67 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[4]

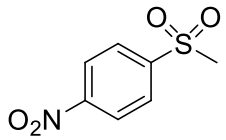


1-Methyl-4-(methylsulfonyl)benzene (3b): (CAS No. 3185-99-7) 95% GC yield, 63% isolated yield. Isolated as a colorless liquid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate = 1/3, R_f = 0.6). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.83 (d, J = 8.3 Hz, 2H, Ar), 7.37 (d, J = 8.3 Hz, 2H, Ar), 3.04 (s, 3H, CH_3), 2.46 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 144.8, 137.8, 130.1, 127.5, 44.7, 21.8. MS (EI) *m/z* (%):51 (5), 63 (9), 65 (26), 77 (10), 79 (6), 89 (8), 91 (100), 92 (8), 107 (31), 108 (5), 155 (32), 170 (30) [M^+], 171 (3). GC retention time (7.1 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.67 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[5]

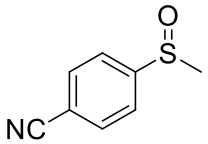


1-Nitro-4-(methylsulfinyl)benzene (2c): (CAS No. 940-12-5) 75% GC yield, 46% isolated yield. Isolated as a white solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate = 1/3, R_f = 0.30). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 8.40 (d, J = 8.9 Hz, 2H, Ar), 7.84 (d, J = 8.9 Hz, 2H, Ar), 2.80 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 153.4, 149.7, 124.8, 124.7, 44.0. MS (EI) *m/z* (%): 50 (31), 51 (8), 58 (6), 63 (22), 64 (10), 65 (6), 69 (11), 70 (13), 74 (14), 75 (22), 77

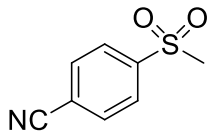
(13), 79 (8), 82 (11), 84 (16), 92 (12), 95 (8), 96 (14), 108 (11), 110 (5), 111 (10), 112 (18), 123 (6), 124 (16), 139 (15), 140 (27), 169 (17), 170 (42), 185 (100) [M^+], 186 (9), 187 (6). GC retention time (8.6 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.58 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[6]



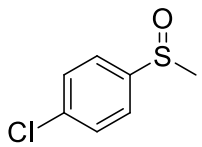
1-(Methylsulfonyl)-4-nitrobenzene (3c): (CAS No. 2976-30-9) 91% GC yield, 43% isolated yield. Isolated as a white solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate = 1/1, R_f = 0.56). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 8.44 (d, J = 8.9 Hz, 2H, Ar), 8.17 (d, J = 8.9 Hz, 2H, Ar), 3.13 (s, 3H, CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, TMS): δ 151.0, 146.1, 129.1, 124.8, 44.5. MS (EI) *m/z* (%):50 (33), 51 (7), 52 (4), 63 (33), 64 (16), 65 (17), 74 (12), 75 (30), 76 (29), 77 (7), 79 (9), 92 (32), 108 (9), 109 (14), 122 (52), 123 (9), 139 (100), 140 (8), 156 (11), 171 (9), 186 (25), 201 (20) [M^+]. GC retention time (9.0 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.58 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[5]



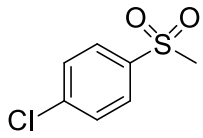
4-(Methylsulfinyl)benzonitrile (2d): (CAS No. 97474-48-1) 43% GC yield, 29% isolated yield. Isolated as white solid (silica gel column chromatography; eluent, ethyl acetate, R_f = 0.34). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.85 (d, J = 8.4 Hz, 2H, Ar), 7.78 (d, J = 8.6 Hz, 2H, Ar), 2.78 (s, 3H, CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, TMS): δ 151.6, 133.1, 124.4, 117.8, 114.9, 43.9. MS (EI) *m/z* (%): 50 (11), 51 (11), 63 (12), 64 (6), 69 (9), 74 (6), 75 (17), 76 (13), 90 (13), 102 (12), 103 (12), 104 (15), 107 (6), 116 (45), 117 (5), 119 (6), 122 (20), 133 (5), 134 (28), 148 (11), 149 (100), 150 (42), 151 (9), 165 (25) [M^+]. GC retention time (8.1 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.61 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[6]



4-(Methylsulfonyl)benzonitrile (3d): (CAS No. 22821-76-7) >99% GC yield, 89% isolated yield. Isolated as white solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate = 1/3, R_f = 0.50). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 8.10 (d, J = 8.0 Hz, 2H, Ar), 7.91 (d, J = 8.0 Hz, 2H, Ar), 3.11 (s, 3H, CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, TMS): δ 144.5, 133.3, 128.3, 117.7, 117.2, 44.3. MS (EI) m/z (%):50 (11), 51 (16), 52 (4), 63 (16), 74 (5), 75 (24), 76 (14), 90 (6), 102 (100), 103 (9), 119 (85), 120 (7), 166 (21), 181 (18) [M^+], 182 (2), 183 (1). GC retention time (8.4 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.61 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[7]

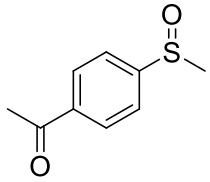


1-Chloro-4-(methylsulfinyl)benzene (2e): (CAS No. 934-73-6) 73% GC yield, 55% isolated yield. Isolated as colorless liquid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate = 1/9, R_f = 0.35). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.60 (d, J = 8.6 Hz, 2H, Ar), 7.52 (d, J = 8.6 Hz, 2H, Ar), 2.72 (s, 3H, CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, TMS): δ 144.4, 137.5, 129.8, 125.1, 44.2. MS (EI) *m/z* (%): 45 (32), 50 (24), 63 (11), 69 (14), 74 (17), 75 (35), 76 (11), 108 (32), 111 (22), 112 (15), 125 (12), 127 (12), 128 (18), 131 (36), 143 (39), 145 (12), 158 (54), 159 (100), 160 (28), 161 (34), 174 (48) [M^+], 175 (11), 176 (17). GC retention time (7.0 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.59 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[6]

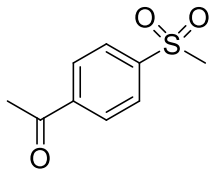


1-Chloro-4-(methylsulfonyl)benzene (3e): (CAS No. 98-57-7) 96% GC yield, 65% isolated yield. Isolated as white solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate = 2/1, R_f = 0.40). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.90 (d, J = 8.9 Hz, 2H, Ar), 7.56 (d, J = 8.9 Hz, 2H, Ar), 3.07 (s, 3H, CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, TMS): δ 140.6, 139.1, 129.8, 129.0, 44.6. MS (EI) *m/z* (%):49 (5), 50 (10), 51 (33), 77 (100), 78 (8), 125 (5), 141 (60), 142 (5), 190 (10) [M^+], 192 (4). GC retention time (7.4 min); relative sensitivity for quantification (vs dodecane, internal

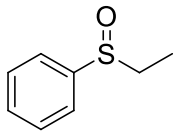
standard), 0.59 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[7]



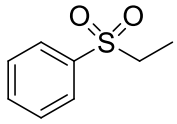
1-(4-(methylsulfinyl)phenyl)ethenone (2f): (CAS No. 32361-73-2) 81% GC yield, 65% isolated yield. Isolated as white solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =1/3, R_f = 0.28). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 8.12 (d, J = 8.3 Hz, 2H, Ar), 7.75 (d, J = 8.3 Hz, 2H, Ar), 2.77 (s, 3H, CH_3), 2.66 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 197.2, 151.0, 139.2, 129.3, 123.9, 43.9, 26.9. MS (EI) *m/z* (%):50 (15), 51 (9), 63 (9), 64 (2), 69 (10), 74 (6), 75 (6), 76 (12), 77 (15), 79 (15), 82 (5), 91 (5), 104 (6), 108 (13), 121 (12), 123 (20), 124 (9), 139 (13), 151 (100), 152 (52), 153 (9), 166 (52), 167 (60), 168 (8), 182 (35) [M^+], 183 (4), 184 (2). GC retention time (9.0 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.67 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[8]



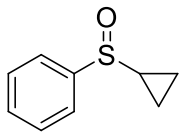
1-(4-(methylsulfonyl)phenyl)ethenone (3f): (CAS No. 10297-73-1) 91% GC yield, 82% isolated yield. Isolated as white solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =1/1, R_f = 0.32). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 8.14 (d, J = 8.5 Hz, 2H, Ar), 8.06 (d, J = 8.5 Hz, 2H, Ar), 3.10 (s, 3H, CH_3), 2.68 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 196.8, 144.3, 141.0, 129.3, 127.9, 44.4, 27.1. MS (EI) *m/z* (%): 50 (13), 51 (5), 63 (5), 64 (3), 65 (6), 75 (5), 76 (16), 77 (9), 91 (10), 93 (6), 104 (8), 119 (6), 121 (47), 183 (100), 184 (10), 185 (6), 198 (14) [M^+], 199 (2). GC retention time (9.4 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.67 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[8]



(Ethylsulfinyl)benzene (2g): (CAS No. 4170-80-3) 82% GC yield, 57% isolated yield. Isolated as colorless liquid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =1/4, R_f = 0.40). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.60–7.63 (m, 2H, Ar), 7.48–7.54 (m, 3H, Ar), 2.73–2.95 (m, 2H, CH_2), 1.20 (t, J = 7.5 Hz, 3H, CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 143.4, 131.0, 129.2, 124.3, 50.4, 6.1. MS (EI) *m/z* (%): 50 (8), 51 (23), 65 (9), 66 (6), 69 (5), 77 (25), 78 (100), 79 (10), 91 (8), 97 (13), 109 (7), 110 (12), 123 (10), 125 (15), 126 (58), 127 (5), 138 (15), 154 (19) [M^+]. GC retention time (6.0 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.67 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[4]

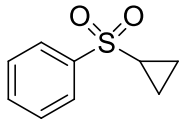


(Ethylsulfonyl)benzene (3g) : (CAS No. 599-70-2) 95% GC yield, 80% isolated yield. Isolated as colorless liquid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =1/1, R_f = 0.34). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.90–7.93 (m, 2H, Ar), 7.65–7.69 (m, 1H, Ar), 7.56–7.60 (m, 2H, Ar), 3.13 (q, J = 7.5 Hz, 2H, CH_2), 1.28 (t, J = 7.5 Hz, 3H, CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 138.6, 133.8, 129.4, 128.3, 50.7, 7.5. MS (EI) *m/z* (%): 50 (10), 51 (39), 65 (6), 77 (100), 78 (62), 79 (4), 91 (6), 94 (52), 125 (6), 141 (23), 142 (17), 170 (30) [M^+], 171 (3), 172 (2). GC retention time (6.6 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.67 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[9]

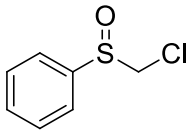


(Cyclopropylsulfinyl)benzene (2h): (CAS No. 50337-59-2) 89% GC yield, 62% isolated yield. Isolated as colorless liquid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =1/1, R_f = 0.24). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.65–7.69 (m, 2H, Ar), 7.48–7.55 (m, 3H, Ar), 2.27 (tt, J = 8.0, 4.9 Hz, 1H), 1.21–1.28 (m, 1H), 0.90–1.08 (m, 3H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 145.0, 131.0, 129.3, 124.1, 33.9, 3.5, 2.9. MS (EI) *m/z* (%):50 (15), 51 (44), 52 (5), 53 (6), 65 (22),

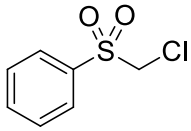
66 (10), 69 (11), 70 (2), 71 (6), 72 (8), 73 (7), 74 (7), 77 (42), 78 (30), 97 (33), 105 (13), 109 (20), 110 (9), 115 (18), 116 (10), 117 (90), 118 (23), 121 (8), 125 (100), 126 (10), 127 (5), 134 (7), 135 (37), 149 (24), 150 (35), 151 (5), 166 (26) [M^+]. GC retention time (7.3 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.75 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[6]



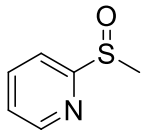
(Cyclopropylsulfonyl)benzene (3h): (CAS No. 17637-57-9) >99% GC yield, 69% isolated yield. Isolated as white solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =2/1, R_f = 0.24). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.89–7.93 (m, 2H, Ar), 7.62–7.67 (m, 1H, Ar), 7.54–7.59 (m, 2H, Ar), 2.47 (tt, J = 8.0, 4.9 Hz, 1H), 1.33–1.39 (m, 2H), 1.01–1.06 (m, 2H). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 140.8, 133.5, 129.4, 127.7, 33.0, 6.1. MS (EI) *m/z* (%):50 (10), 51 (38), 77 (100), 78 (17), 91 (8), 97 (5), 115 (6), 117 (25), 118 (13), 125 (7), 141 (53), 182 (26) [M^+]. GC retention time (7.9 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.75 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[8]



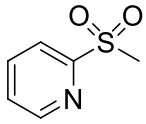
((Chloromethyl)sulfinyl)benzene (2i): (CAS No. 7205-94-9) 55% GC yield, 41% isolated yield. Isolated as pale-yellow liquid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =3/1, R_f = 0.60). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.70–7.73 (m, 2H, Ar), 7.55–7.60 (m, 3H, Ar), 4.40 (dd, J = 16.2, 10.8 Hz, 2H, Ar). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 141.0, 132.3, 129.5, 124.9, 61.4. MS (EI) *m/z* (%): 50 (10), 51 (28), 53 (6), 65 (7), 77 (32), 91 (12), 97 (28), 109 (7), 123 (22), 125 (100), 126 (9), 127 (6), 158(9), 174 (19), 175 (2) [M^+], 176 (7). GC retention time (8.4 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.58 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[9]



((Chloromethyl)sulfonyl)benzene (3i): (CAS No. 7205-98-3) 63% GC yield, 49% isolated yield. Isolated as pale-yellow solid (silica gel column chromatography; eluent, ethyl acetate/acetonitrile =2/1, R_f = 0.16). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.99 (d, J = 7.5 Hz, 2H, Ar), 7.74 (t, J = 7.5 Hz, 1H, Ar), 7.62 (t, J = 8.0 Hz, 2H, Ar), 4.54 (s, 2H, CH_2). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 135.8, 134.9, 129.5, 58.6. MS (EI) *m/z* (%): 50 (8), 51 (29), 77 (100), 78 (6), 125 (7), 141 (73), 142 (6), 143 (4), 190 (13), 191 (1) [M^+], 192 (5). GC retention time (8.7 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.58 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[9]

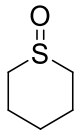


2-(Methylsulfinyl)pyridine (2j): (CAS No. 21948-75-4) 85% GC yield, 60% isolated yield. Isolated as pale-yellow solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =1/1, R_f = 0.18). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 8.63 (d, J = 4.9 Hz, 1H, Ar), 8.04 (d, J = 8.0 Hz, 1H, Ar), 7.96 (td, J = 7.7, 1.6 Hz, 1H, Ar), 7.37–7.41 (m, 1H, Ar), 2.86 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 166.1, 149.7, 138.3, 124.7, 119.4, 41.4. MS (EI) *m/z* (%): 55 (19), 57 (79), 58 (100), 59 (28), 67 (5), 71 (59), 72 (14), 85 (42), 86 (21), 99 (24), 100 (12), 113 (28), 127 (21), 128 (5), 141 (15) [M^+], 142 (5). GC retention time (4.8 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.42 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[10]

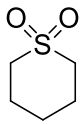


2-(Methylsulfonyl)pyridine (3j): (CAS No. 17075-14-8) 88% GC yield, 55% isolated yield. Isolated as pale-yellow solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =1/1, R_f = 0.34). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 8.75 (d, J = 4.6 Hz, 1H, Ar), 8.10 (d, J = 7.7 Hz, 1H, Ar), 7.99 (td, J = 7.7, 1.4 Hz, 1H, Ar), 7.58 (dd, J = 7.6, 4.8 Hz, 1H, Ar), 3.25 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 158.2, 150.2, 138.4, 127.6, 121.2, 40.1. MS (EI) *m/z* (%): 50 (10), 51 (50), 52 (15), 67 (1776 (3), 78 (100), 79 (10), 93 (33), 94 (3), 95 (28), 157 (1) [M^+]. GC retention time (6.0 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.42 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those

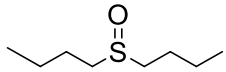
previously reported.[11]



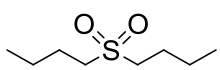
Pentamethylene sulfoxide (2k): (CAS No. 4988-34-5) 88% GC yield. Not isolated. MS (EI) *m/z* (%): 50 (4), 53 (10), 54 (4), 56 (21), 57 (4), 59 (12), 60 (5), 61 (8), 63 (73), 64 (8), 65 (6), 67 (28), 68 (28), 69 (100), 70 (7), 73 (6), 76 (5), 77 (4), 87 (10), 90 (18), 101 (23), 102 (10), 118 (66) [M^+], 119 (4). GC retention time (4.0 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.42 (estimated by the effective carbon number concept[3]).



Pentamethylene sulfone (3k): (CAS No. 4988-33-4) 97% GC yield. Not isolated. MS (EI) *m/z* (%): 53 (3), 55 (31), 56 (2), 63 (2), 67 (4), 68 (2), 69 (57), 70 (11), 106 (6), 117 (4), 134 (18) [M^+], 135 (1). GC retention time (4.8 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.42 (estimated by the effective carbon number concept[3]).

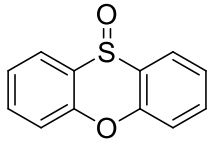


Dibutyl sulfoxide (2l): (CAS No. 2168-93-6) 83% GC yield, 54% isolated yield. Isolated as white solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =1/3, R_f = 0.27). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 2.60–2.73 (m, 4H, CH_2), 1.71–1.80 (m, 4H, CH_2), 1.41–1.57 (m, 4H, CH_2), 0.97 (t, J = 7.3 Hz, 6H, CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, TMS): δ 52.3, 24.7, 22.2, 13.8. MS (EI) *m/z* (%):55 (32), 56 (100), 57 (44), 57 (4), 60 (5), 61 (93), 62 (5), 63 (9), 75 (6), 88 (4), 89 (33), 90 (28), 91 (15), 103 (13), 106 (7), 117 (5), 145 (8), 146 (44), 147 (5), 154 (8), 162 (1) [M^+]. GC retention time (5.8 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.67 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[11]

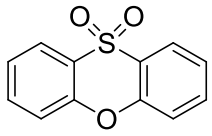


Dibutyl sulfone (3l): (CAS No. 598-04-9) 98% GC yield, 57% isolated yield. Isolated as white solid

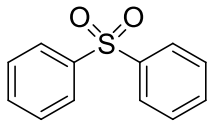
(silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =3/1, R_f = 0.30). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 2.93–2.98 (m, 4H, CH_2), 1.78–1.86 (m, 4H, CH_2), 1.44–1.53 (m, 4H, CH_2), 0.97 (t, J = 7.3 Hz, 6H, CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, TMS): δ 52.6, 24.0, 21.9, 13.7. MS (EI) *m/z* (%): 55 (8), 56 (16), 57 (100), 58 (4), 81 (4), 121 (8), 123 (36), 124 (2), 125 (2), 149 (2), 178 (1) [M^+]. GC retention time (6.4 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.67 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[12]



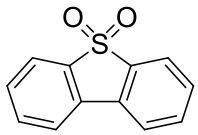
Phenoxathiine 10-oxide (2m): (CAS No. 948-44-7) 67% GC yield, 63% isolated yield. Isolated as white solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =1/3, R_f = 0.45). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.94 (dd, J = 7.7, 1.4 Hz, 2H, Ar), 7.63 (td, J = 7.9, 1.4 Hz, 2H, Ar), 7.44 (d, J = 8.3 Hz, 2H, Ar), 7.38 (t, J = 7.5 Hz, 2H, Ar). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, TMS): δ 149.6, 133.9, 131.2, 125.0, 123.8, 118.9. MS (EI) *m/z* (%): 50 (5), 51 (4), 63 (7), 69 (9), 85 (5), 100 (8), 127 (8), 128 (4), 139 (14), 168 (43), 169 (7), 171 (31), 172 (13), 187 (6), 200 (100), 201 (14), 202 (5), 216 (7) [M^+]. GC retention time (11.1 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.92 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[12]



Phenoxathiine 10,10-dioxide (3m): (CAS No. 950-47-0) 85% GC yield, 57% isolated yield. Isolated as white solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =3/1, R_f = 0.24). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 8.07 (dd, J = 7.9, 1.7 Hz, 2H, Ar), 7.65 (td, J = 8.0, 1.7 Hz, 2H, Ar), 7.38–7.43 (m, 4H, Ar). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$, TMS): δ 151.7, 134.3, 125.1, 125.0, 123.6, 119.0. MS (EI) *m/z* (%): 50 (11), 51 (7), 52 (18), 62 (5), 63 (21), 64 (10), 69 (7), 70 (9), 74 (6), 75 (5), 80 (30), 95 (5), 96 (68), 97 (5), 108 (14), 113 (5), 123 (8), 124 (25), 139 (23), 168 (14), 176 (5), 184 (5), 232 (100) [M^+], 233 (14), 234 (6). GC retention time (11.4 min); relative sensitivity for quantification (vs dodecane, internal standard), 0.92 (estimated by the effective carbon number concept[3]).

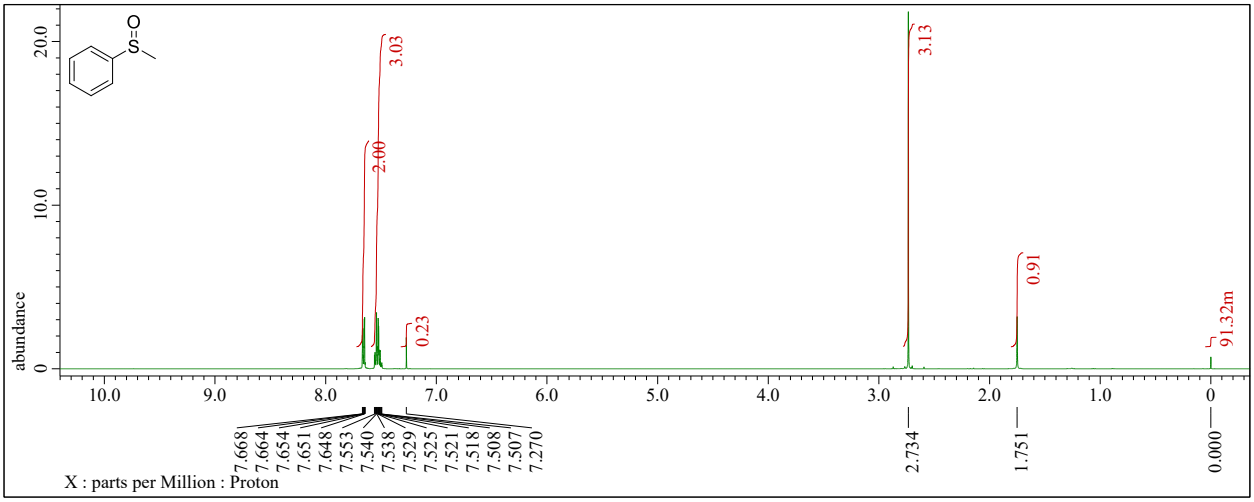


Sulfonyldibenzene (3n): (CAS No. 127-63-9) 88% GC yield, 73% isolated yield. Isolated as white solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =2/1, R_f = 0.44). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.95 (d, J = 7.5 Hz, 2H, Ar), 7.56 (t, J = 7.5 Hz, 1H, Ar), 7.50 (t, J = 7.5 Hz, 2H, Ar). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 141.7, 133.3, 129.4, 127.8. MS (EI) *m/z* (%): 50 (7), 51 (29), 65 (5), 77 (37), 97 (19), 125 (100), 126 (8), 127 (5), 152 (5), 218 (24) [M^+], 219 (3), 220 (1). GC retention time (10.3 min); relative sensitivity for quantification (vs dodecane, internal standard), 1.00 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[1]



Dibenzo[b,d]thiophene 5,5-dioxide (3o): (CAS No. 1016-05-3) 95% GC yield, 88% isolated yield. Isolated as white solid (silica gel column chromatography; eluent, *n*-hexane/ethyl acetate =2/1, R_f = 0.20). ^{1}H NMR (500 MHz, $CDCl_3$, TMS): δ 7.81 (dd, J = 14.9, 7.7 Hz, 4H, Ar), 7.64 (td, J = 7.6, 1.1 Hz, 2H, Ar), 7.53 (td, J = 7.6, 0.8 Hz, 2H, Ar). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$, TMS): δ 137.9, 134.0, 131.7, 130.5, 122.3, 121.7. MS (EI) *m/z* (%): 50 (7), 51 (9), 62 (5), 63 (17), 69 (6), 74 (9), 75 (13), 76 (11), 77 (5), 79 (18), 86 (5), 87 (6), 89 (6), 104 (16), 108 (7), 111 (6), 115 (20), 116 (8), 126 (7), 127 (6), 128 (8), 134 (10), 136 (32), 139 (30), 140 (5), 144 (17), 147 (7), 150 (16), 151 (10), 152 (5), 160 (26), 168 (29), 171 (12), 172 (5), 184 (6), 187 (36), 188 (10), 216 (100) [M^+], 217 (14), 218 (6). GC retention time (11.2 min); relative sensitivity for quantification (vs dodecane, internal standard), 1.00 (estimated by the effective carbon number concept[3]). These NMR and MS spectral data accord with those previously reported.[11]

NMR spectra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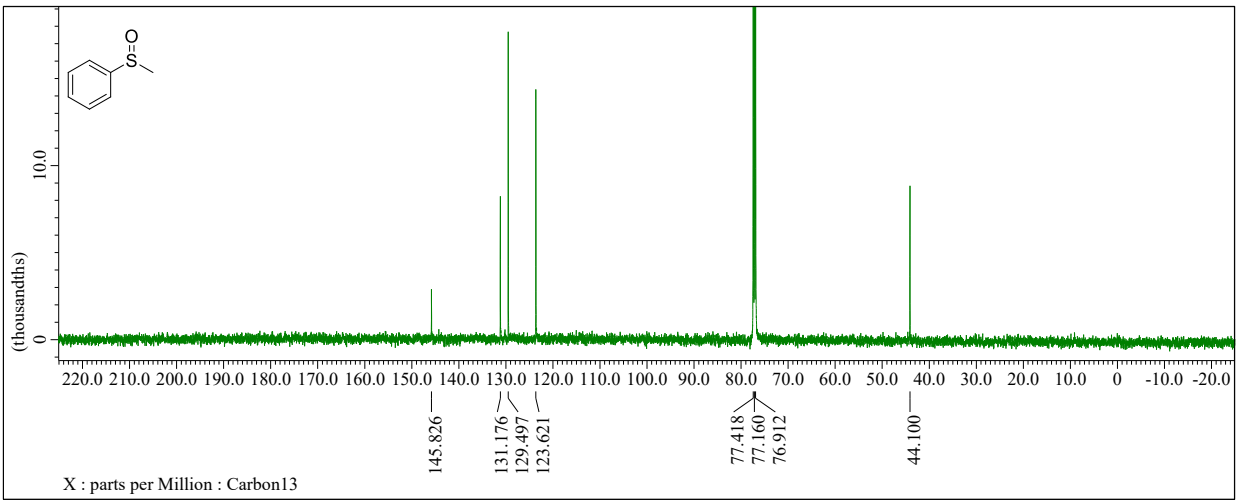
2.00
0.23
3.13
0.91
91.32m
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.668 7.664 7.654 7.651 7.648 7.553 7.540 7.538 7.529 7.525 7.521 7.518 7.508 7.507 7.270
2.734
1.751
0.000
X : parts per Million : Proton


(thousandths)
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0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
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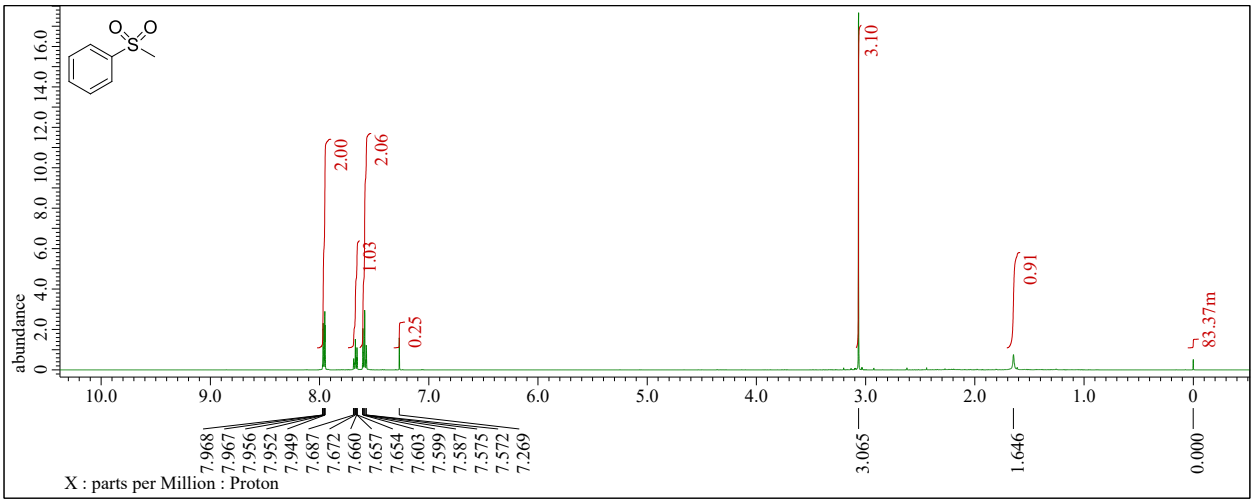
131.176
129.497
123.621
77.418
77.160
76.912
44.100
X : parts per Million : Carbon13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3.10
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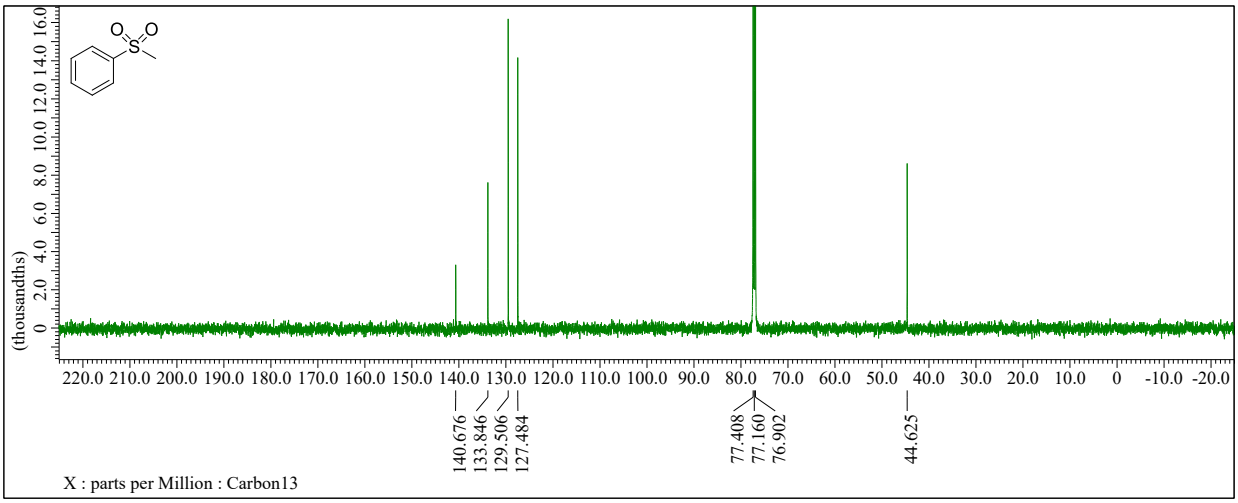
7.967
7.956
7.952
7.949
7.687
7.672
7.660
7.657
7.654
7.603
7.599
7.587
7.575
7.572
7.269
3.065
1.646
0.000
X : parts per Million : Proton


(thousandths)
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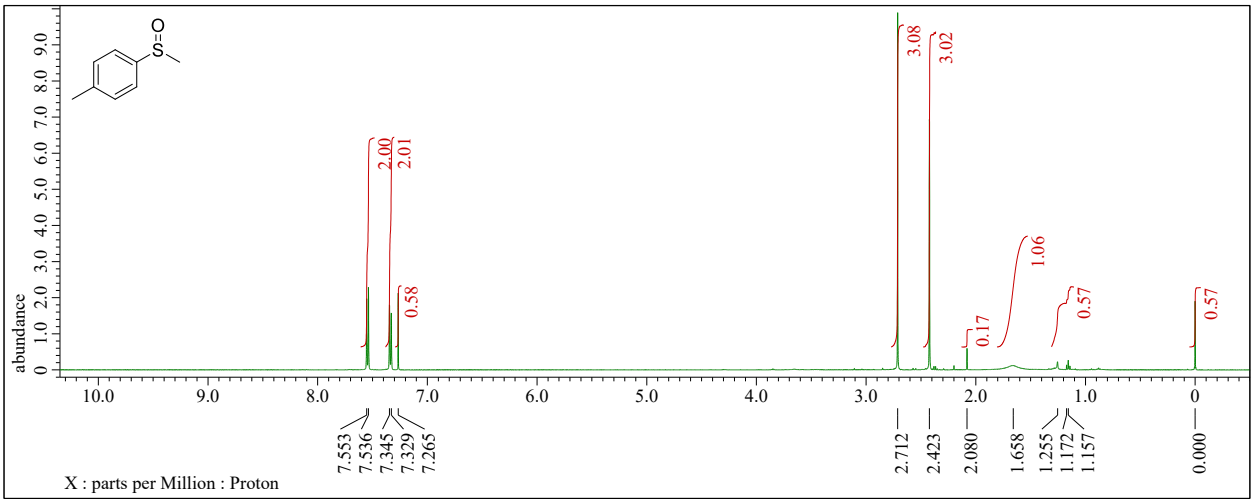
76.902
44.625
X : parts per Million : Carbon13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2.423
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1.172
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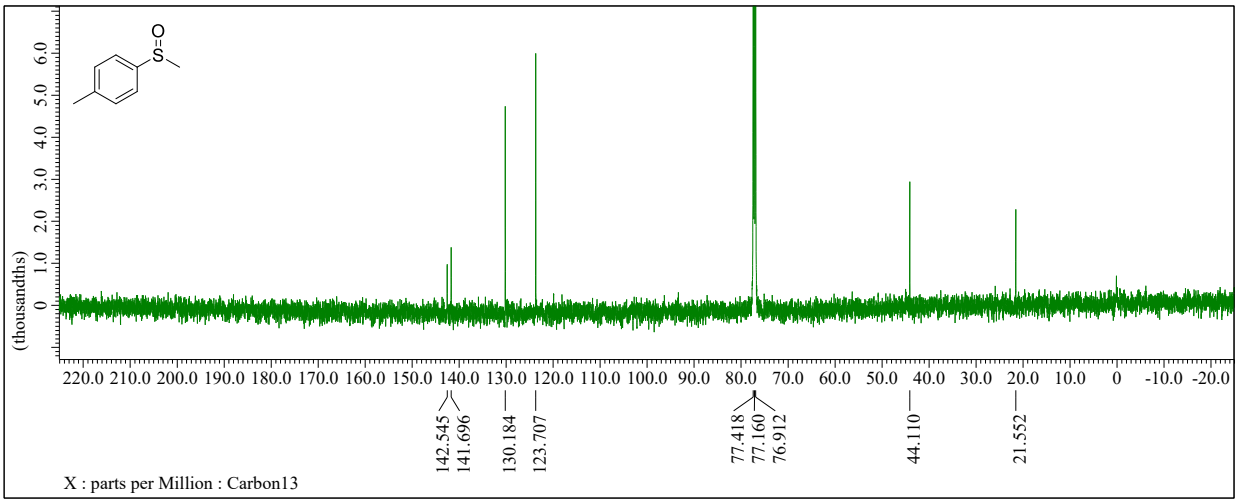
X : parts per Million : Proton


(thousandths)
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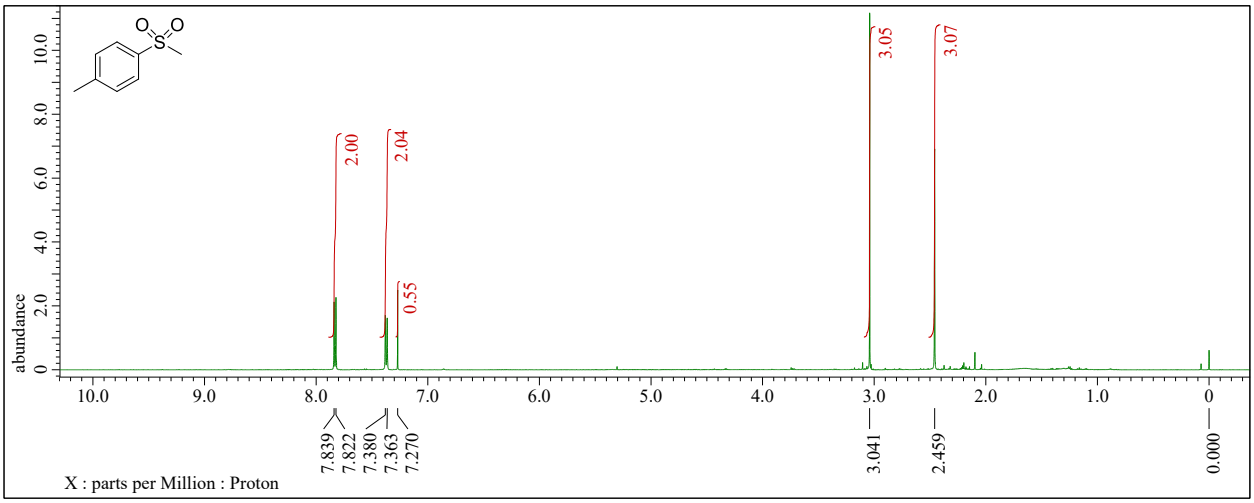
77.160
76.912
44.110
21.552
X : parts per Million : Carbon13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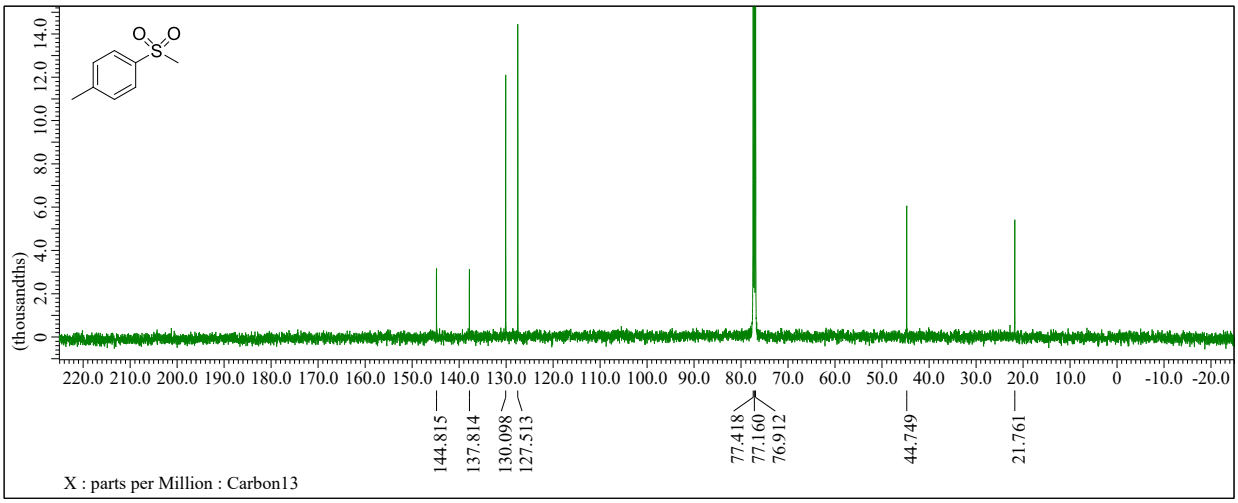
X : parts per Million : Proton


(thousandths)
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127.513
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76.912
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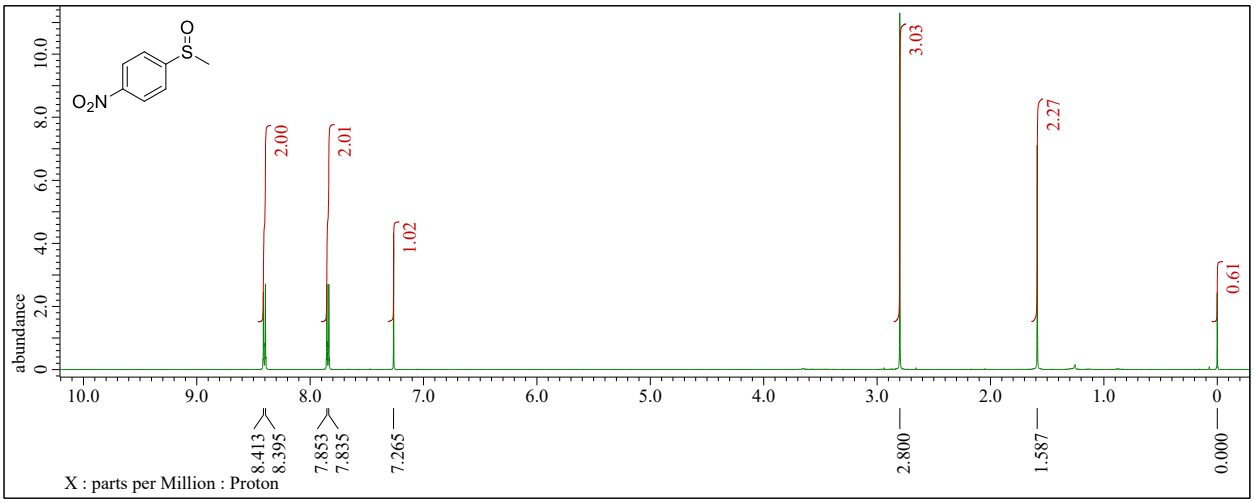
21.761
X : parts per Million : Carbon13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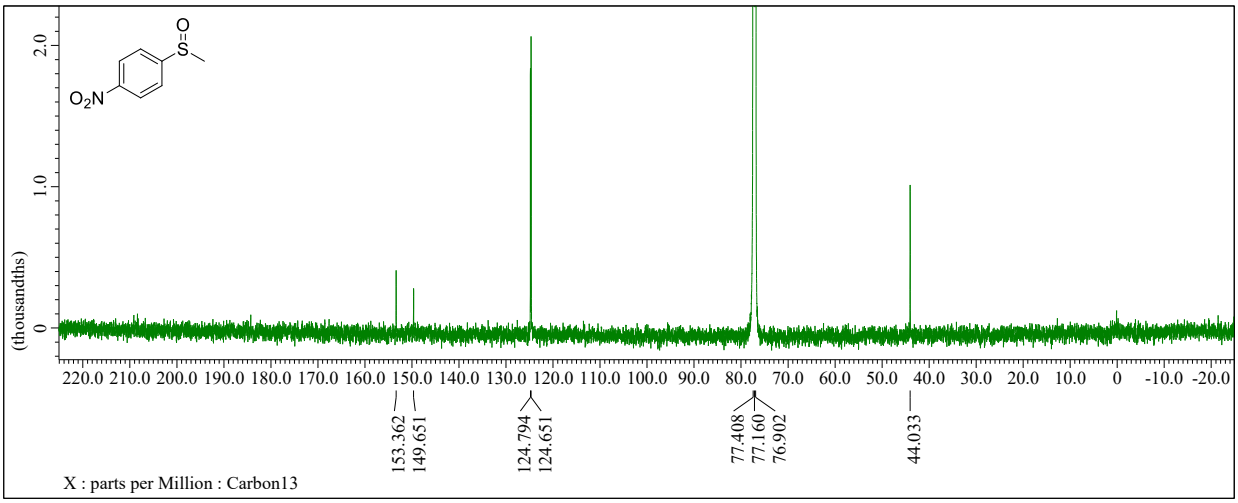
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124.651
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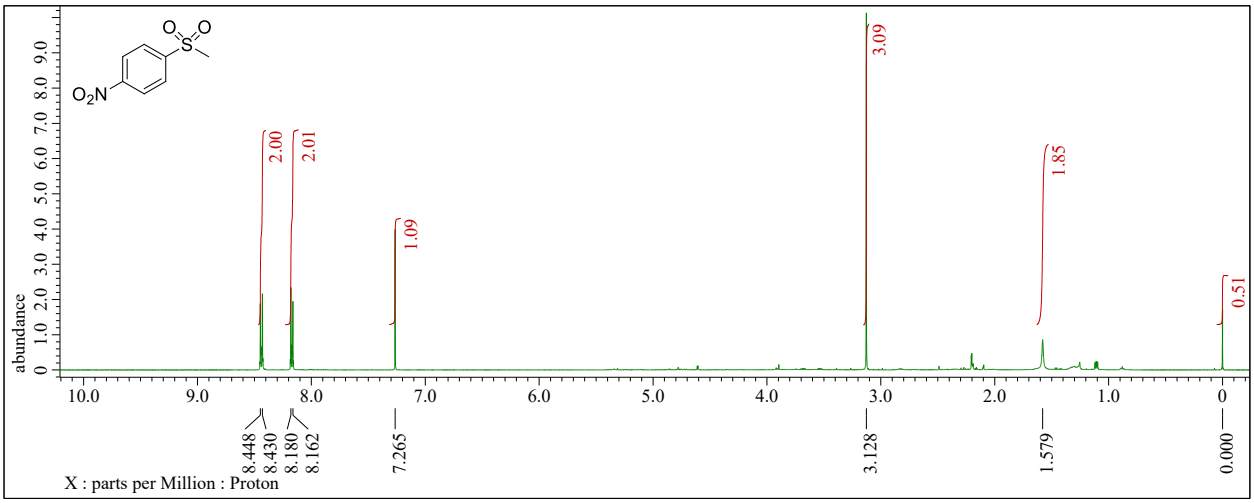
77.160
76.902
44.033
X : parts per Million : Carbon13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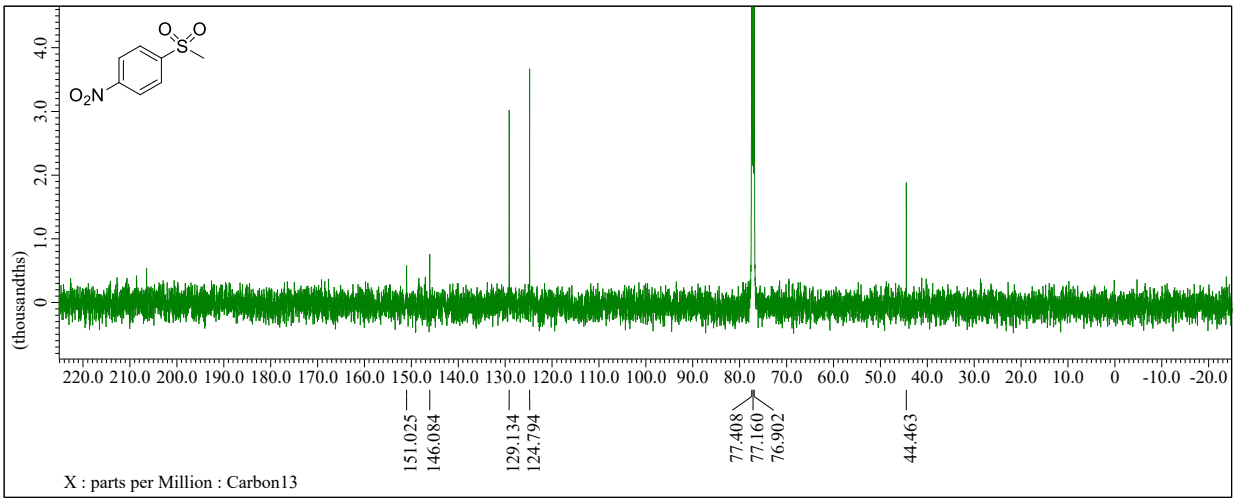
(thousandths)
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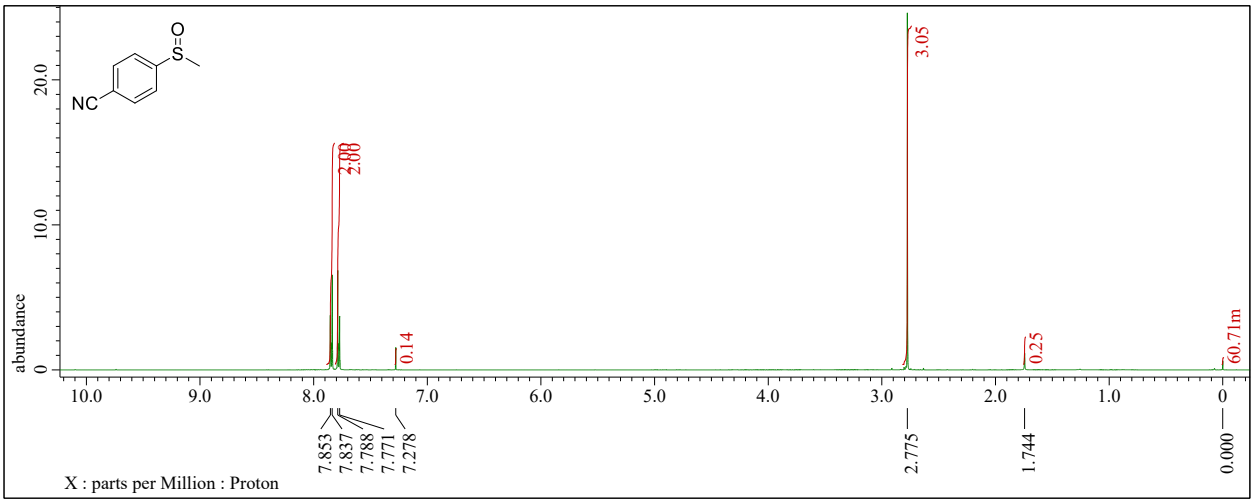
77.408
77.160
76.902
44.463
X : parts per Million : Carbon13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O
S
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9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
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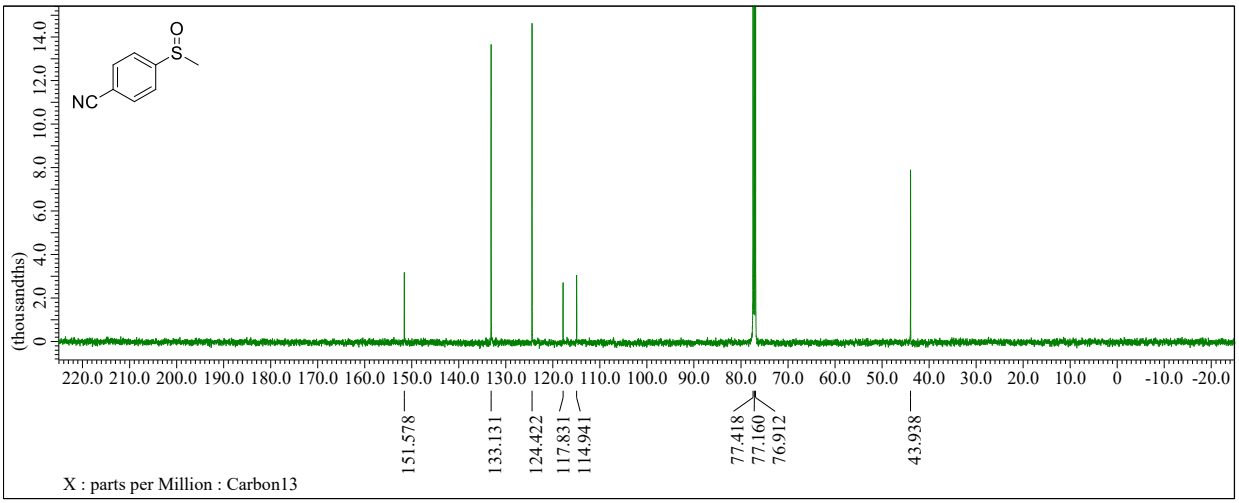
7.788
7.771
7.278
2.775
1.744
0.000
X : parts per Million : Proton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O
S
(thousandths)
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10.0
8.0
6.0
4.0
2.0
0
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124.422
117.831
114.941
77.418
77.160
76.912
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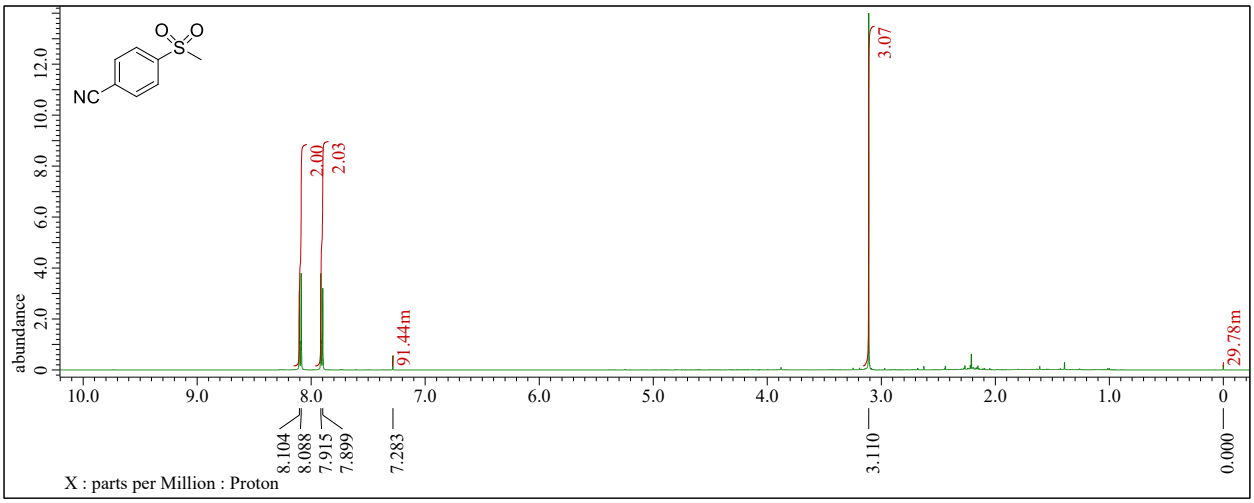
X : parts per Million : Carbon13


abundance
X : parts per Million : Proton
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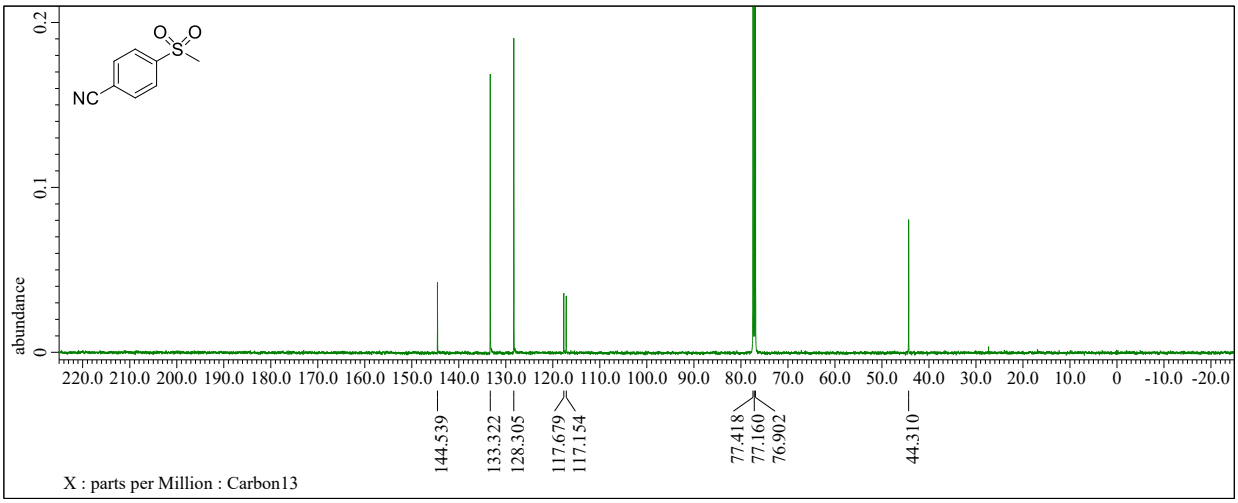
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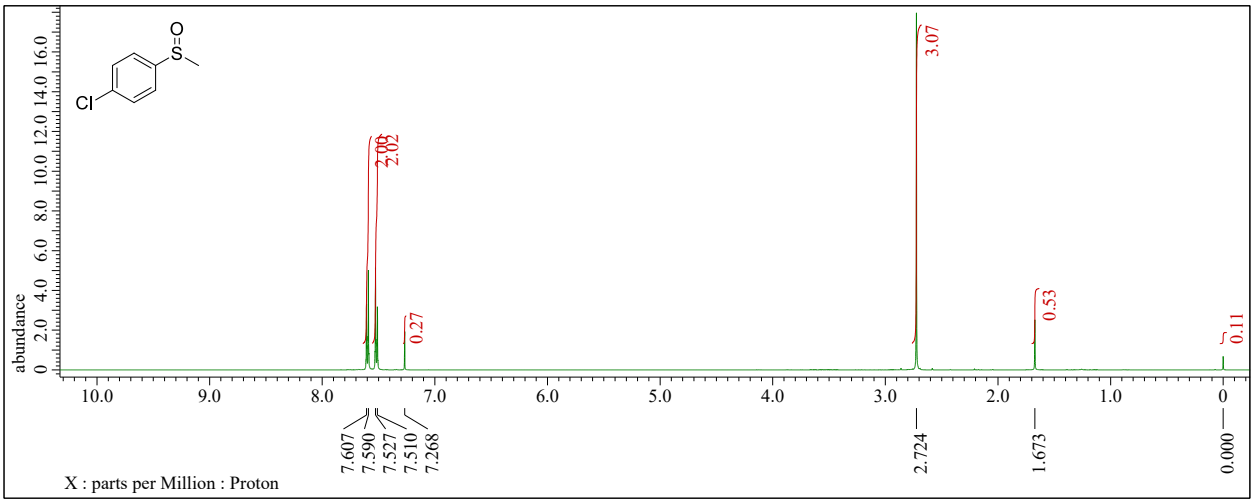
abundance
X : parts per Million : Proton
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1.673
0.000
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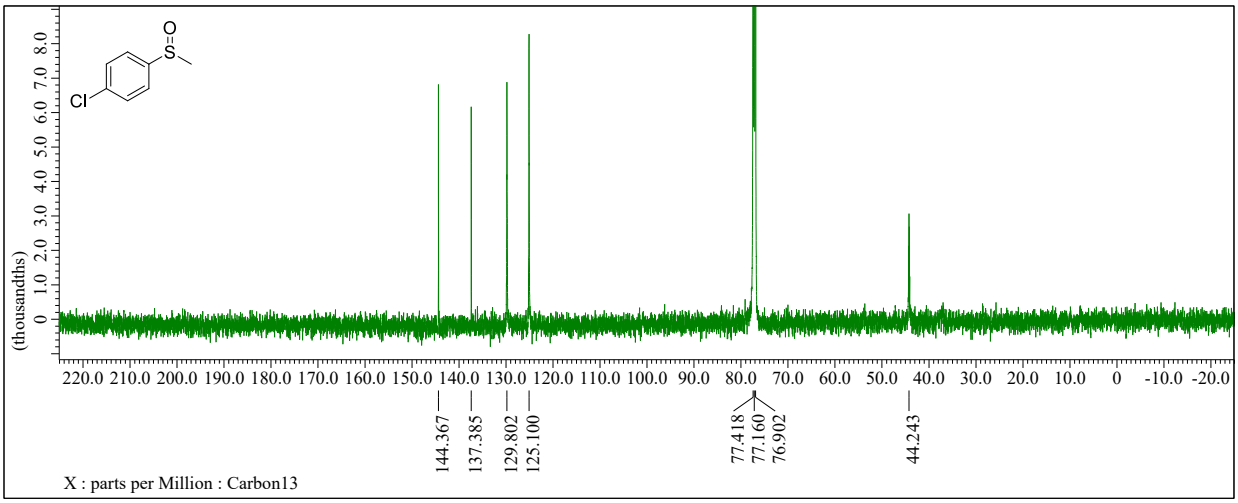
2.06
2.02
0.27
0.53
0.11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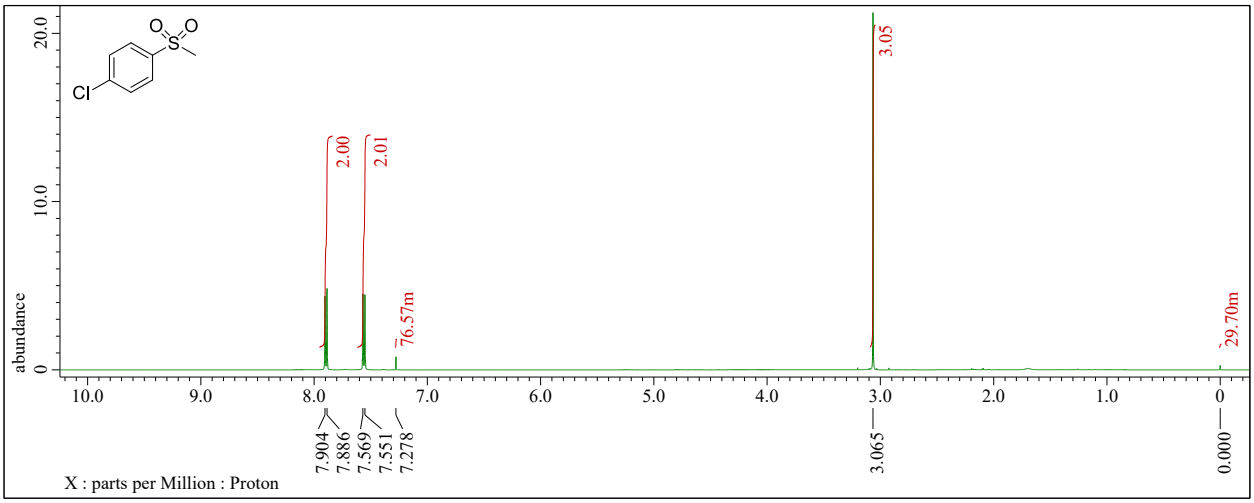
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2.01
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29.70m
10.0
9.0
8.0
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5.0
4.0
3.0
2.0
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0
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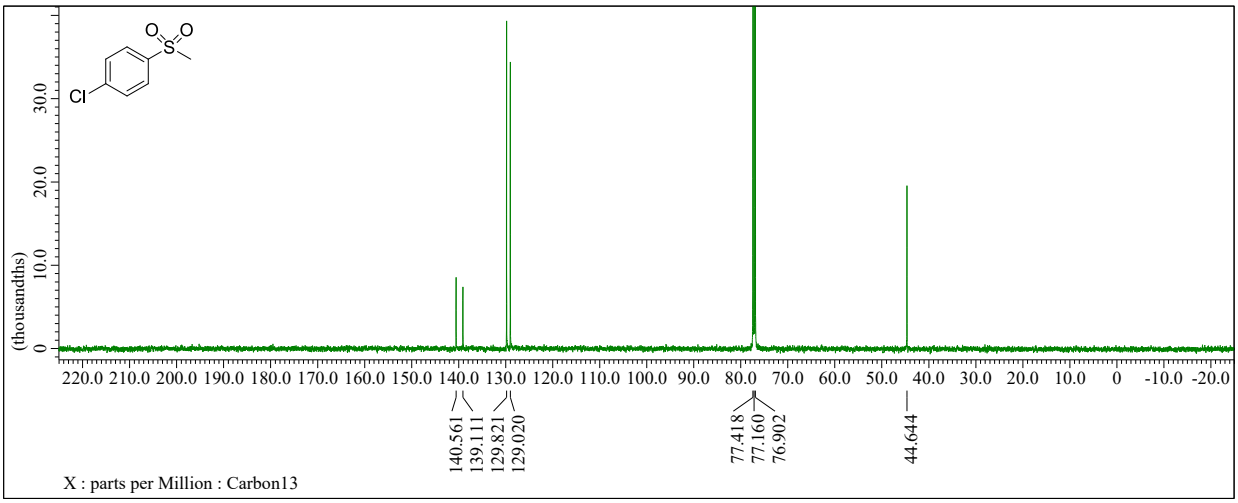
7.569
7.551
7.278
3.065
0.000
X : parts per Million : Proton


(thousandths)
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20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
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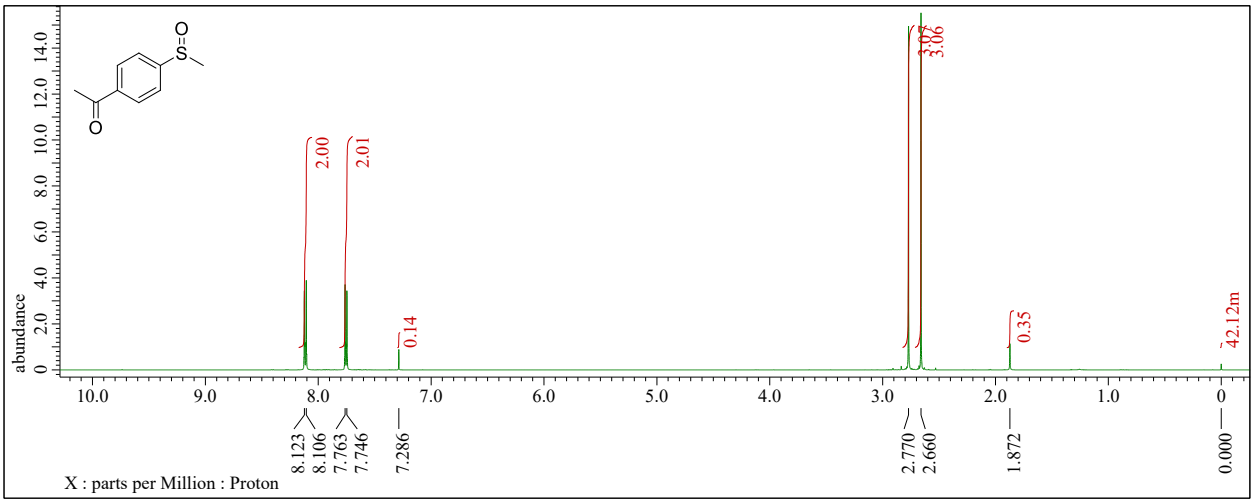
129.821
129.020
77.418
77.160
76.902
44.644
X : parts per Million : Carbon13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0.35
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2.660
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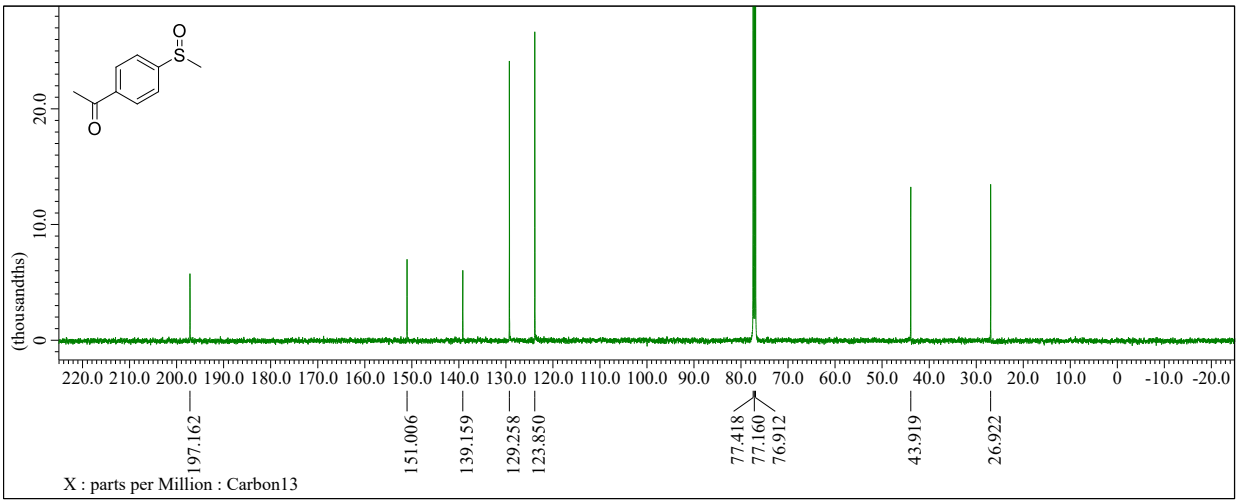
(thousandths)
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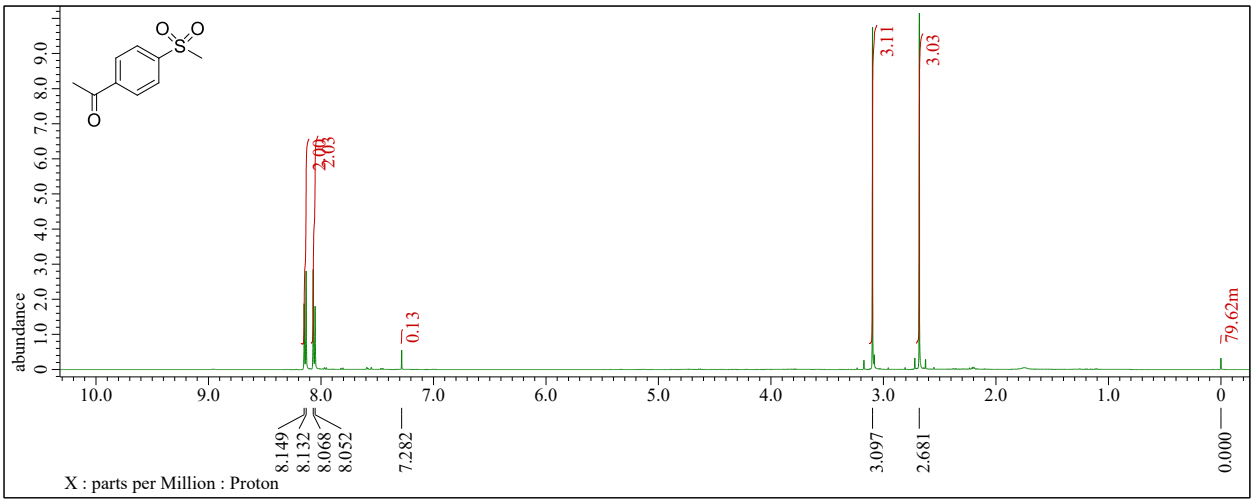
26.922
X : parts per Million : Carbon13


abundance
X : parts per Million : Proton
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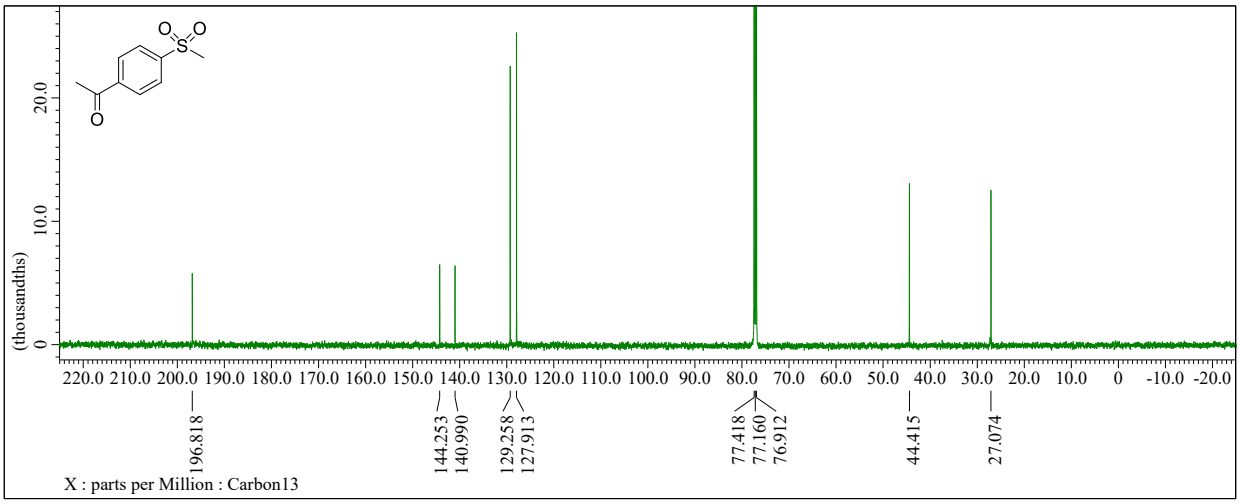
0.000
3.11
3.03
2.00
2.03
0.13
79.62m


(thousandths)
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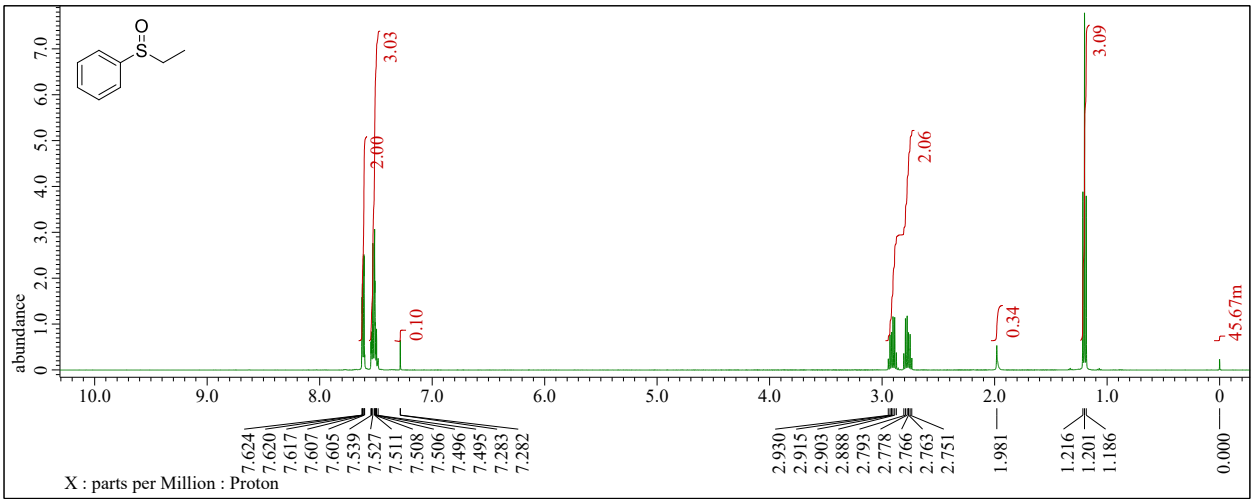
27.074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7.617
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2.915
2.903
2.888
2.793
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2.763
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1.981
1.216
1.201
1.186
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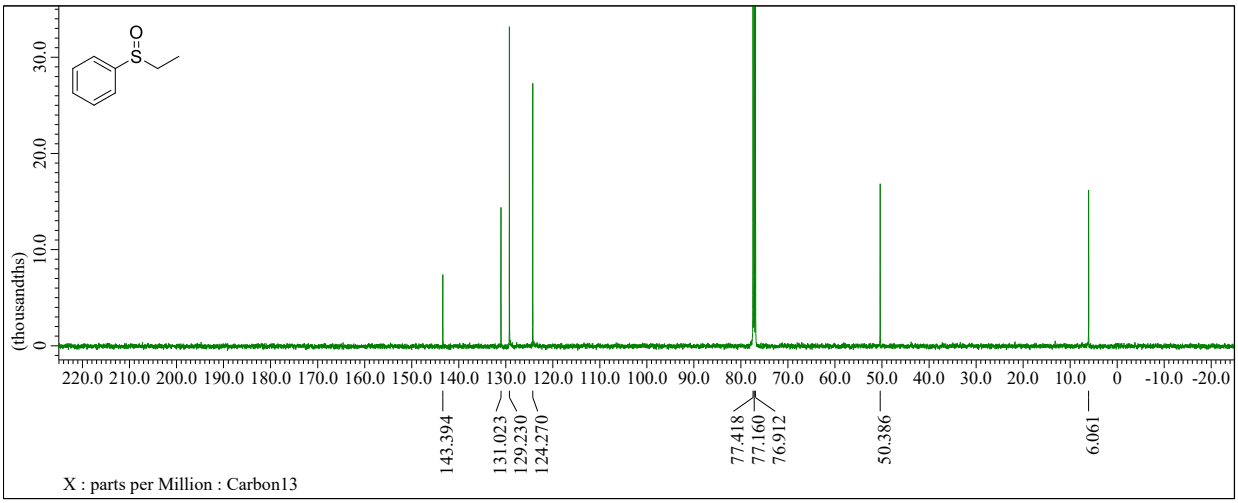
X : parts per Million : Proton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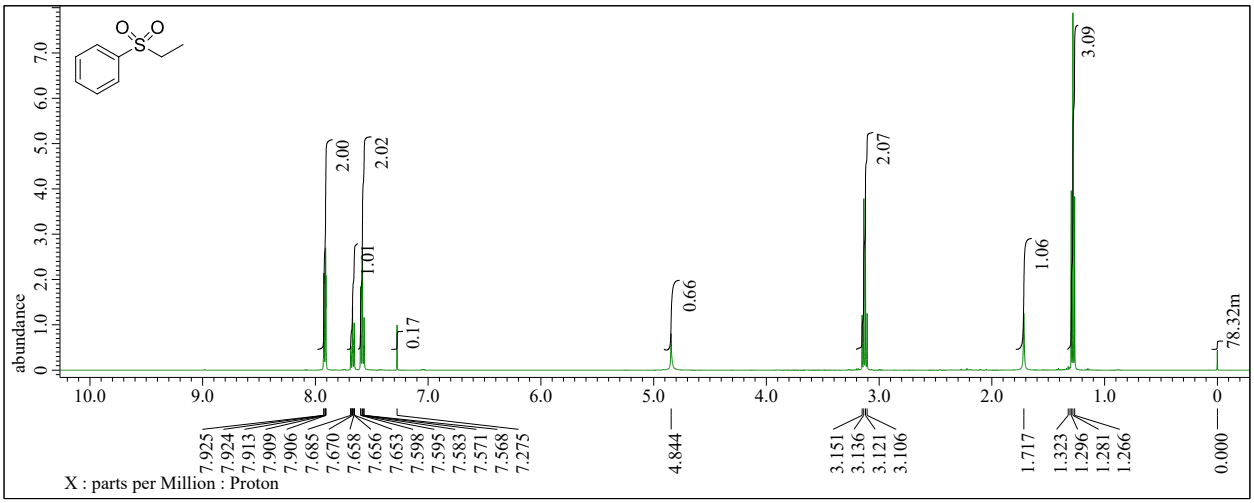
abundance
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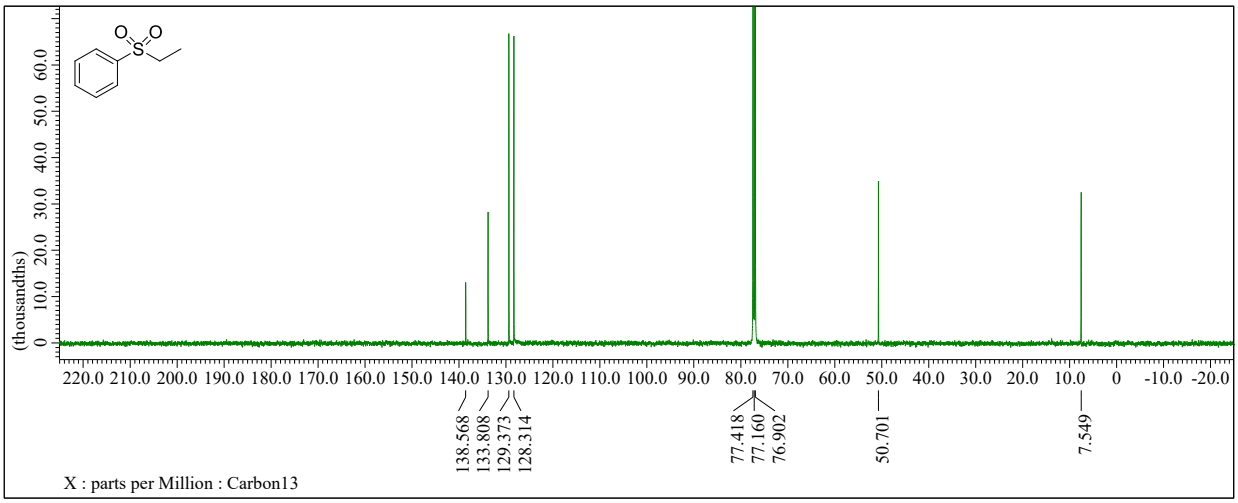
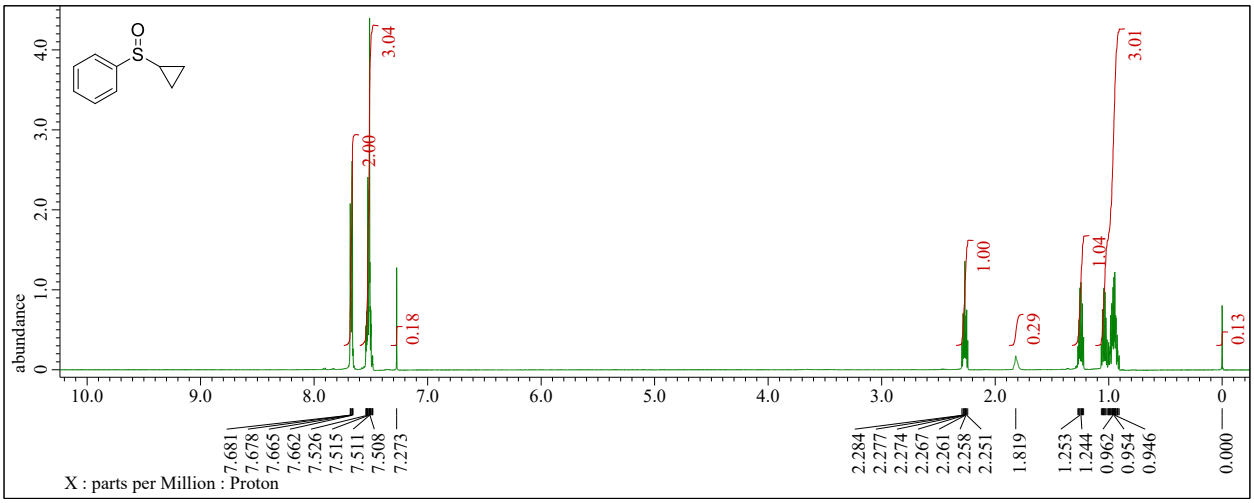
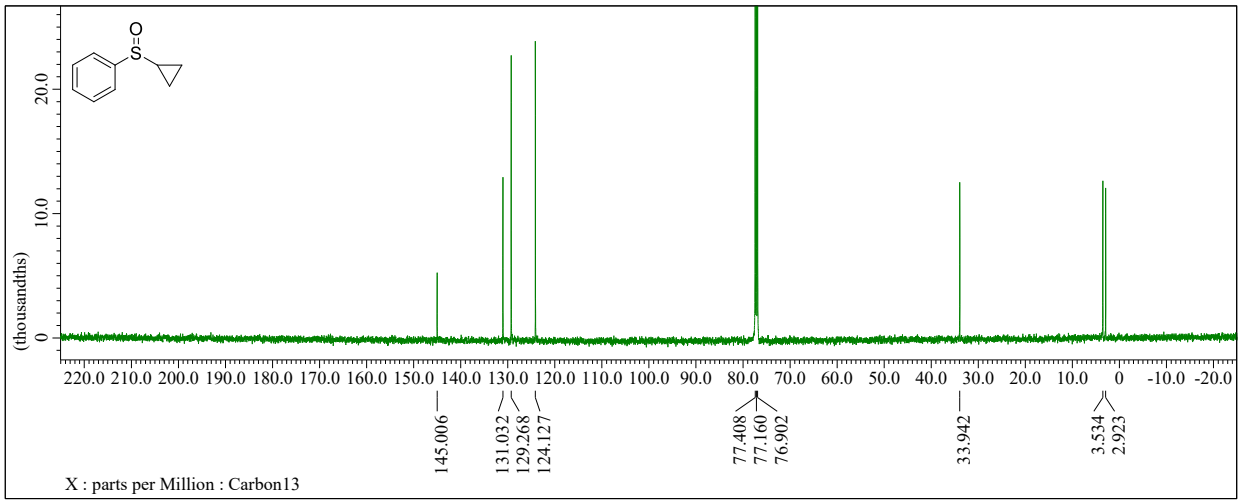
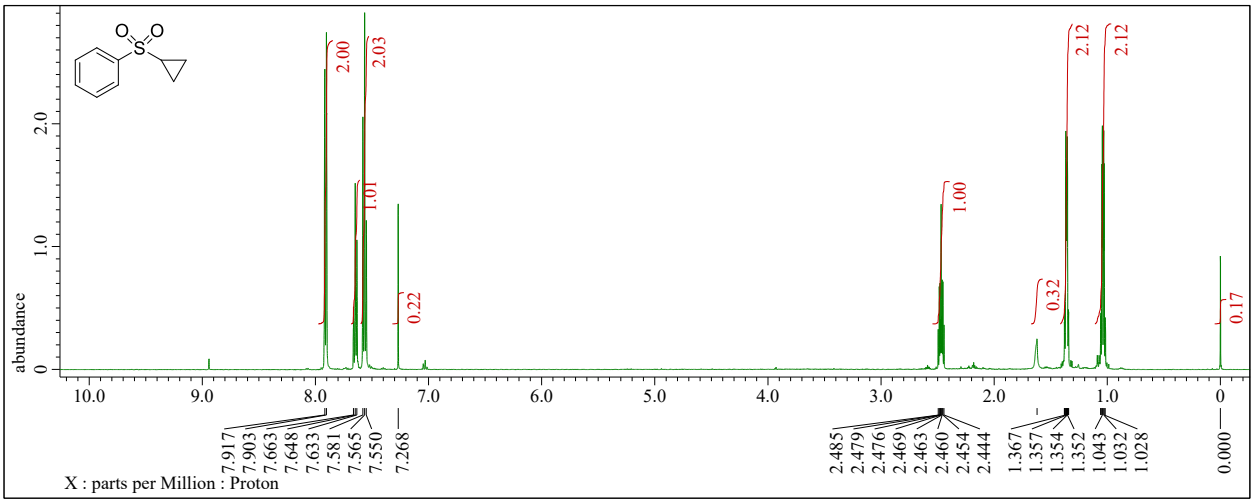
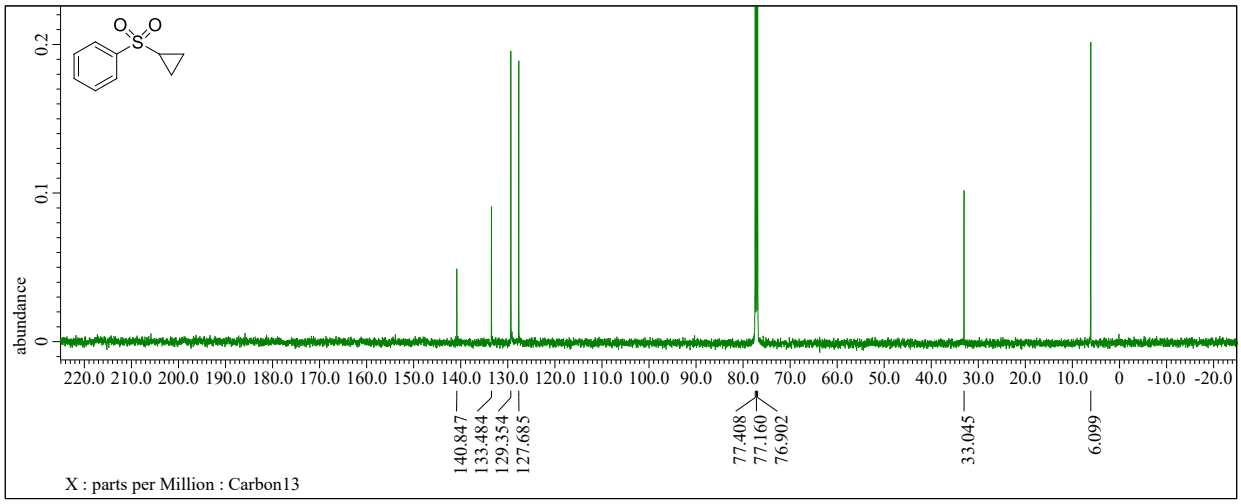
2.02
1.01
0.17
0.66
2.07
1.06
3.09
78.32m
7.925
7.924
7.913
7.909
7.906
7.685
7.670
7.658
7.656
7.653
7.598
7.595
7.583
7.571
7.568
7.275
4.844
3.151
3.136
3.121
3.106
1.717
1.323
1.296
1.281
1.266
0.000
X : parts per Million : Proton

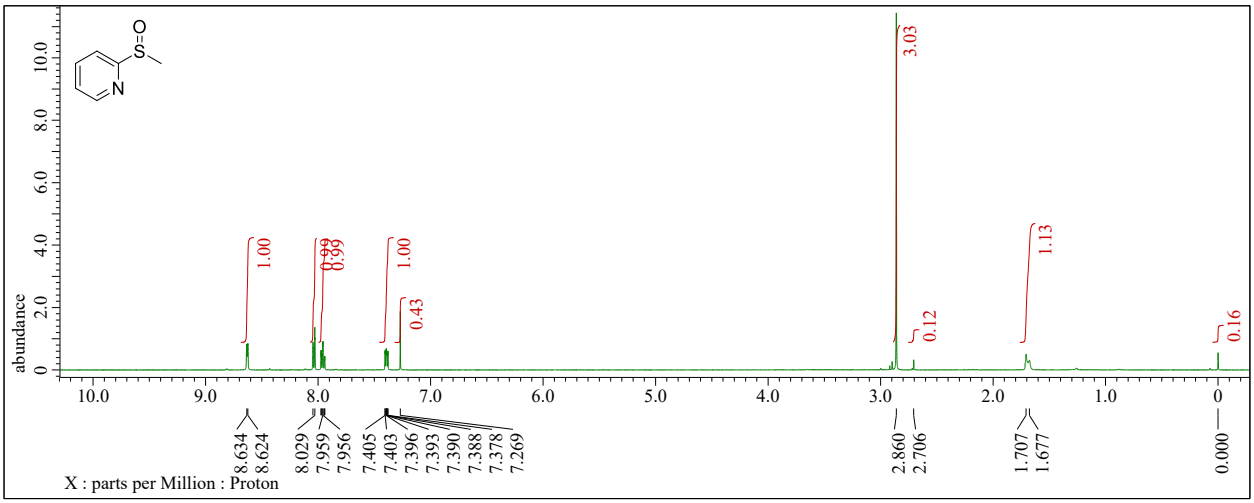

(thousandths)
138.568
133.808
129.373
128.314
77.418
77.160
76.902
50.701
7.549
X : parts per Million : Carbon13

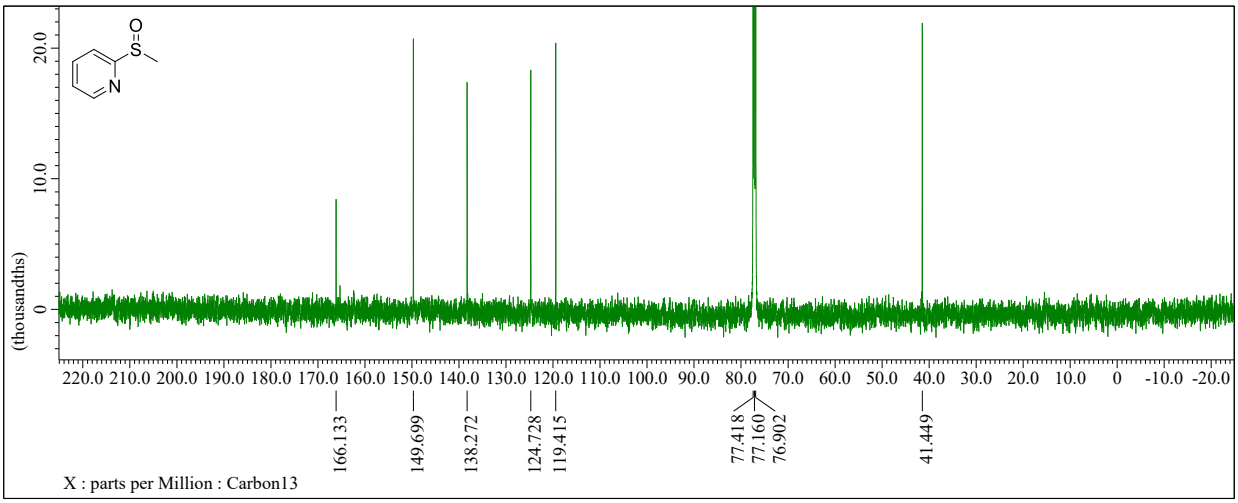

abundance
3.04
2.00
0.18
1.00
0.29
1.04
3.01
0.13
7.681
7.678
7.665
7.662
7.526
7.515
7.511
7.508
7.273
2.284
2.277
2.274
2.267
2.261
2.258
2.251
1.819
1.253
1.244
0.962
0.954
0.946
0.000
X : parts per Million : Proton

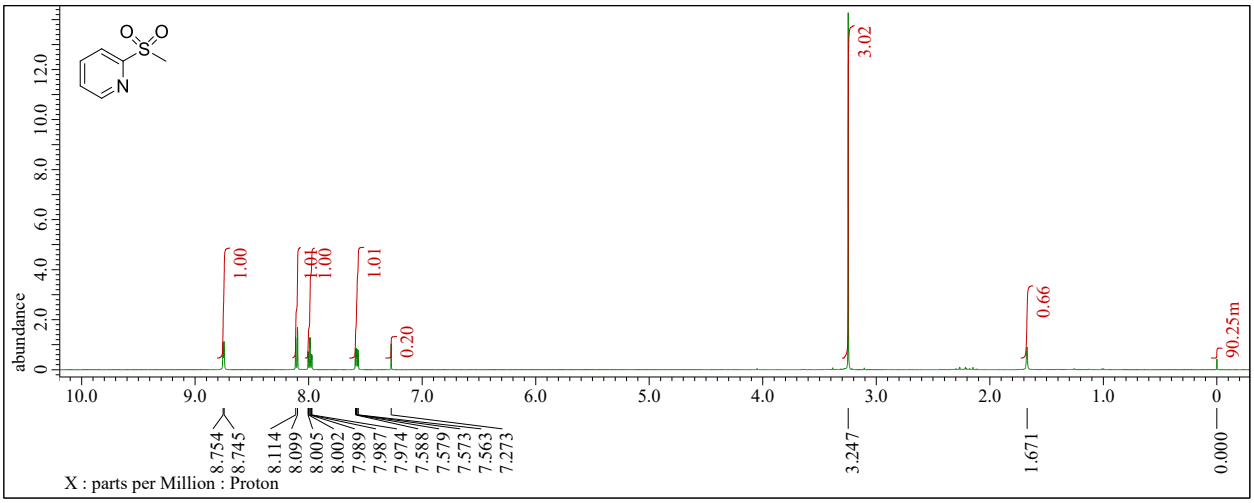

(thousandths)
145.006
131.032
129.268
124.127
77.408
77.160
76.902
33.942
3.534
2.923
X : parts per Million : Carbon13

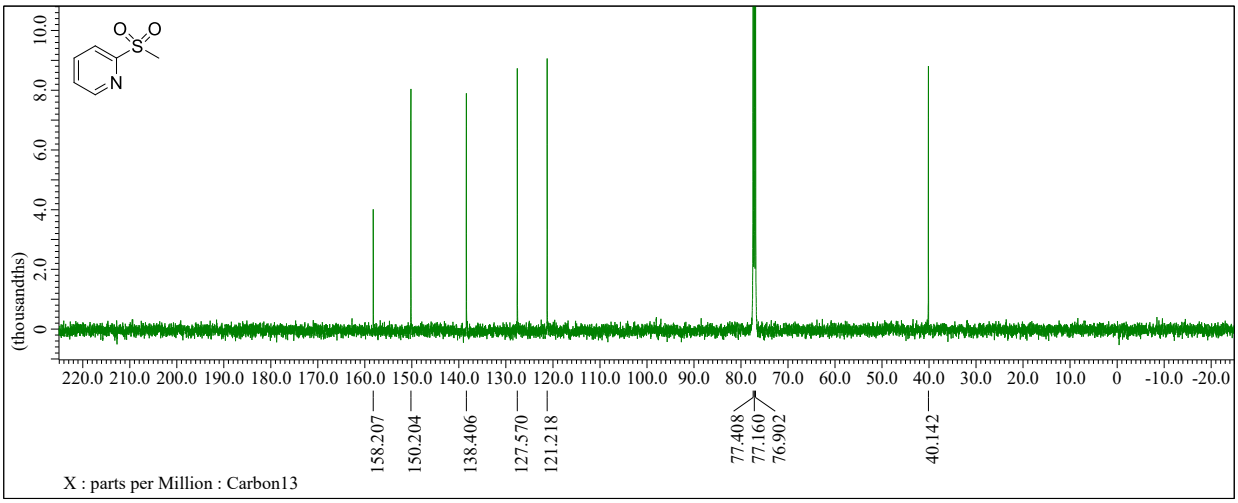

abundance
2.00
2.03
1.01
0.22
1.00
0.32
2.12
2.12
0.17
7.917
7.903
7.663
7.648
7.633
7.581
7.565
7.550
7.268
2.485
2.479
2.476
2.469
2.463
2.460
2.454
2.444
1.367
1.357
1.354
1.352
1.043
1.032
1.028
0.000
X : parts per Million : Proton

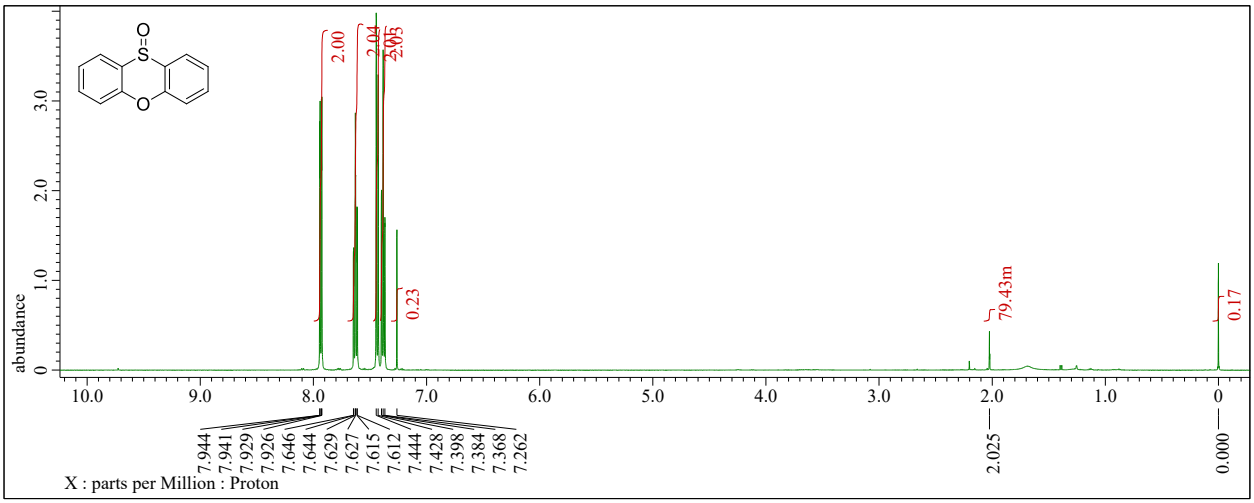

abundance
140.847
133.484
129.354
127.685
77.408
77.160
76.902
33.045
6.099
X : parts per Million : Carbon13

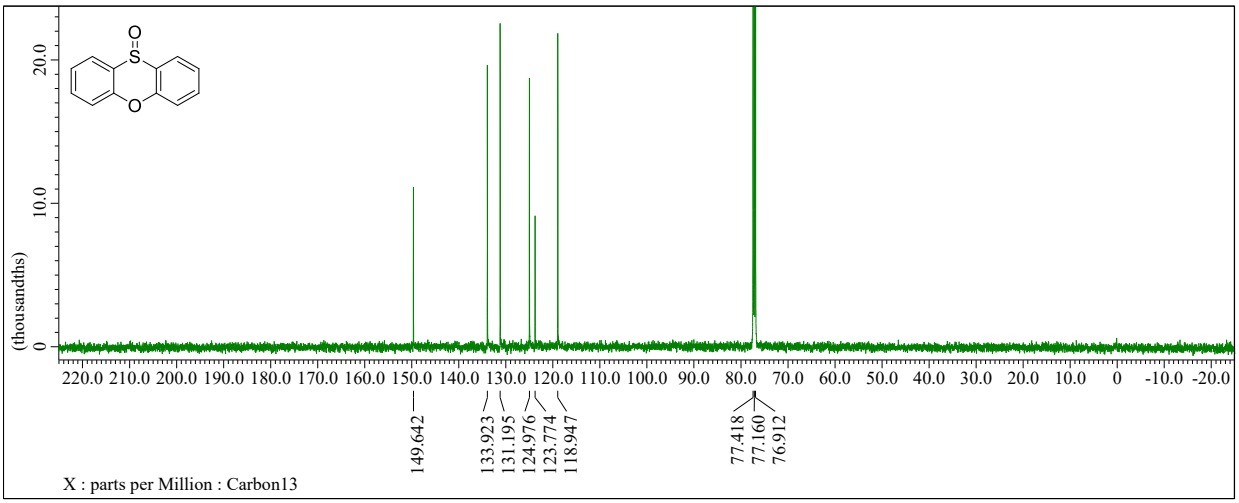

abundance
X : parts per Million : Proton
8.634
8.624
8.029
7.959
7.956
7.405
7.403
7.396
7.393
7.390
7.388
7.378
7.269
2.860
2.706
1.707
1.677
0.000
1.00
1.00
0.43
3.03
0.12
1.13
0.16

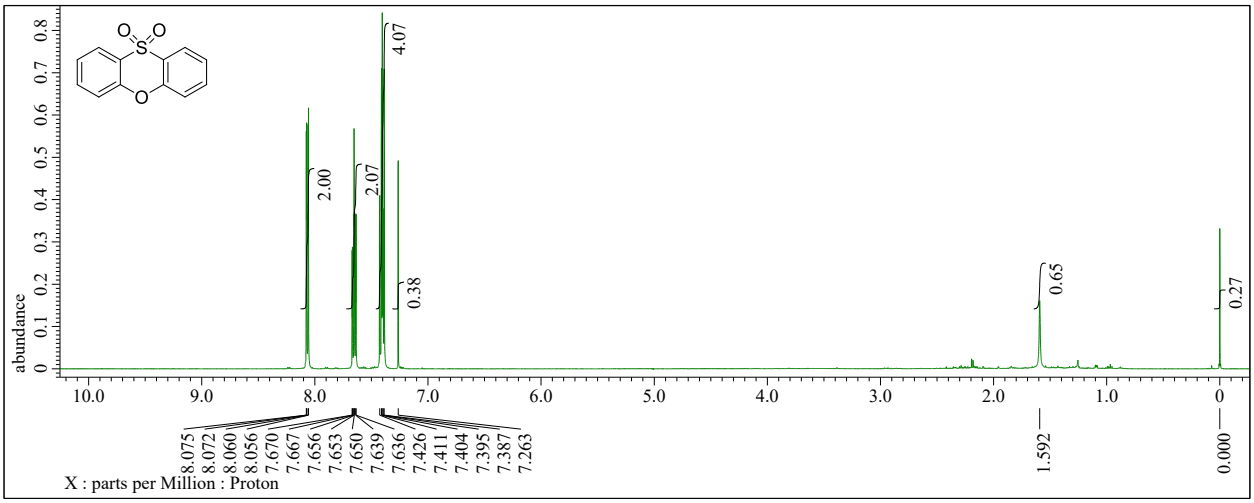

(thousandths)
X : parts per Million : Carbon13
166.133
149.699
138.272
124.728
119.415
77.418
77.160
76.902
41.449

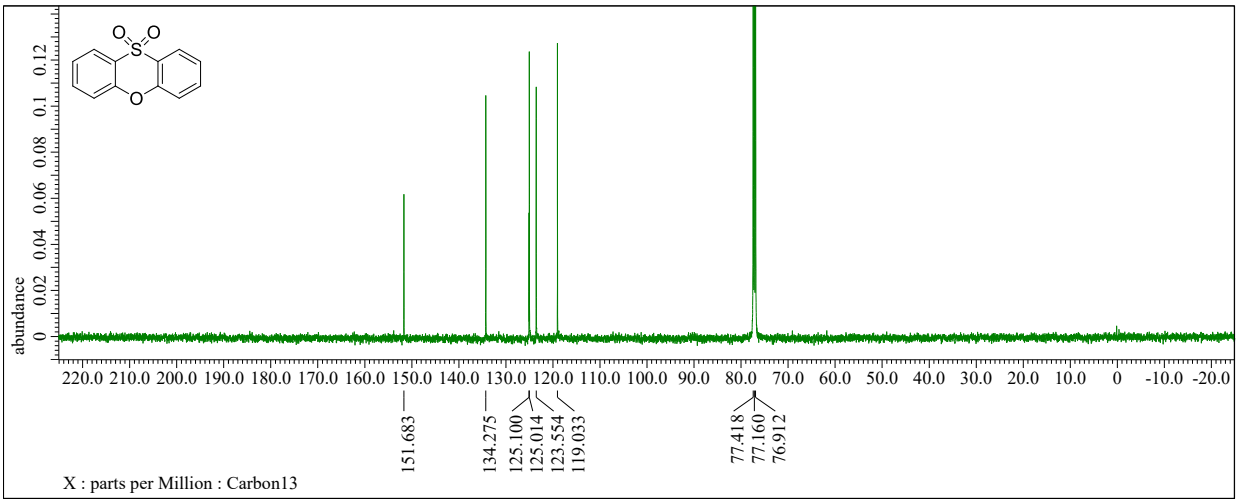

abundance
1.00
1.00
1.00
1.01
0.20
3.02
0.66
90.25m
8.754
8.745
8.114
8.099
8.005
8.002
7.989
7.987
7.974
7.588
7.579
7.573
7.563
7.273
3.247
1.671
0.000
X : parts per Million : Proton

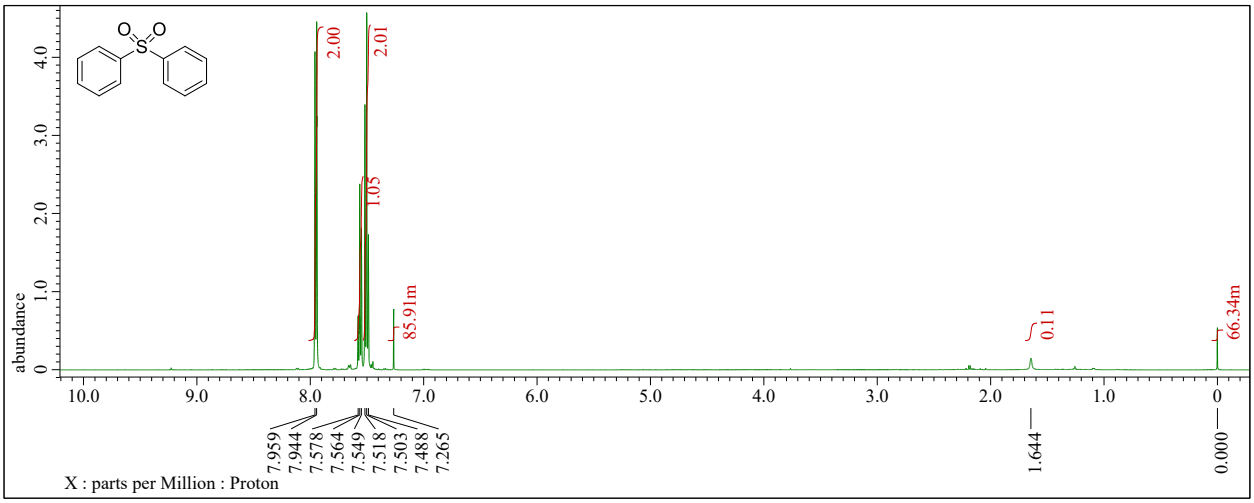

(thousandths)
158.207
150.204
138.406
127.570
121.218
77.408
77.160
76.902
40.142
X : parts per Million : Carbon13

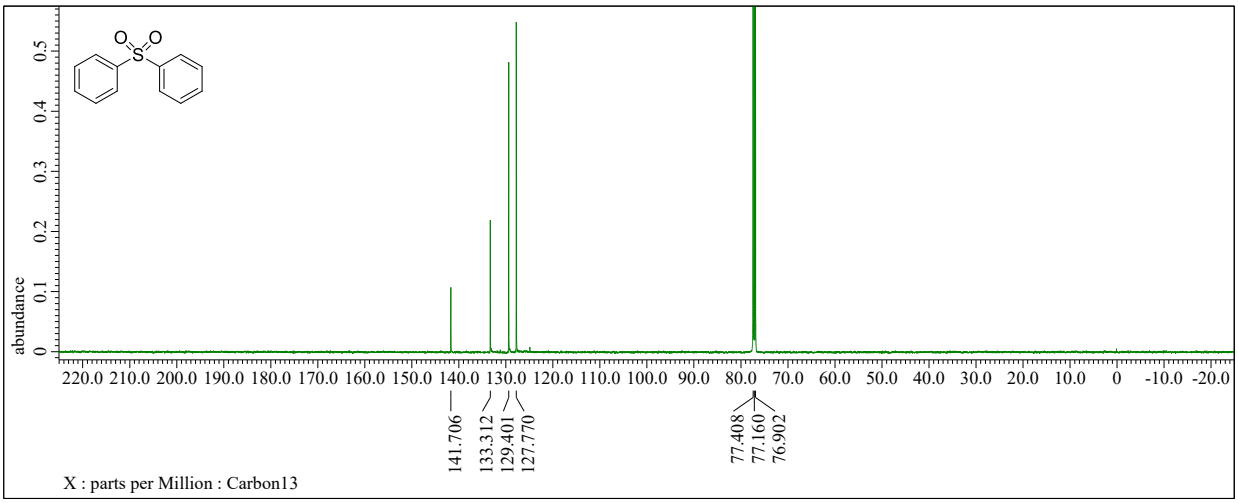

abundance
2.00
2.04
2.05
0.23
79.43m
0.17
7.944
7.941
7.929
7.926
7.646
7.644
7.629
7.627
7.615
7.612
7.444
7.428
7.398
7.384
7.368
7.262
2.025
0.000
X : parts per Million : Proton

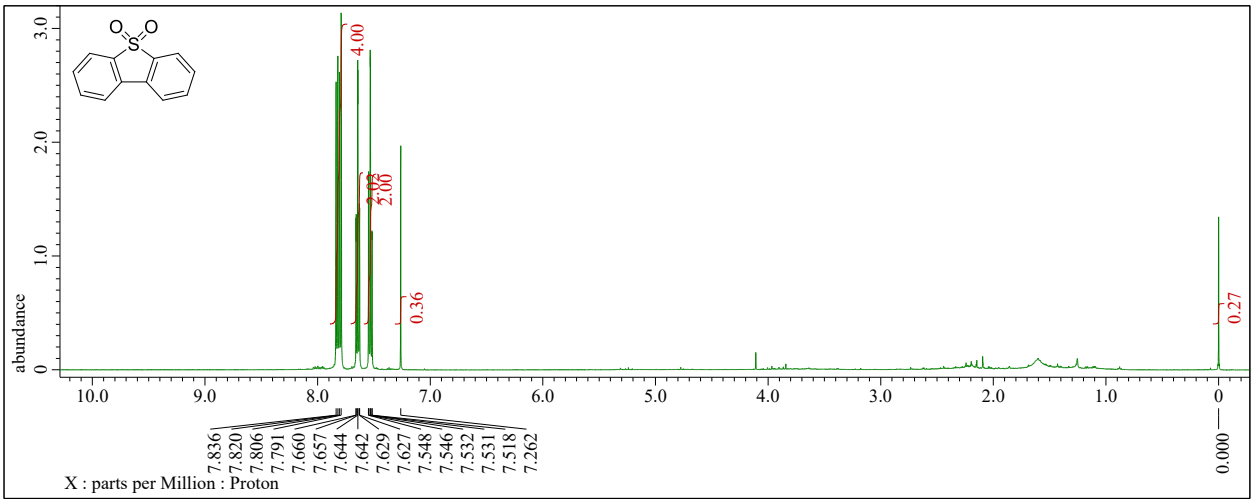

(thousandths)
149.642
133.923
131.195
124.976
123.774
118.947
77.418
77.160
76.912
X : parts per Million : Carbon13

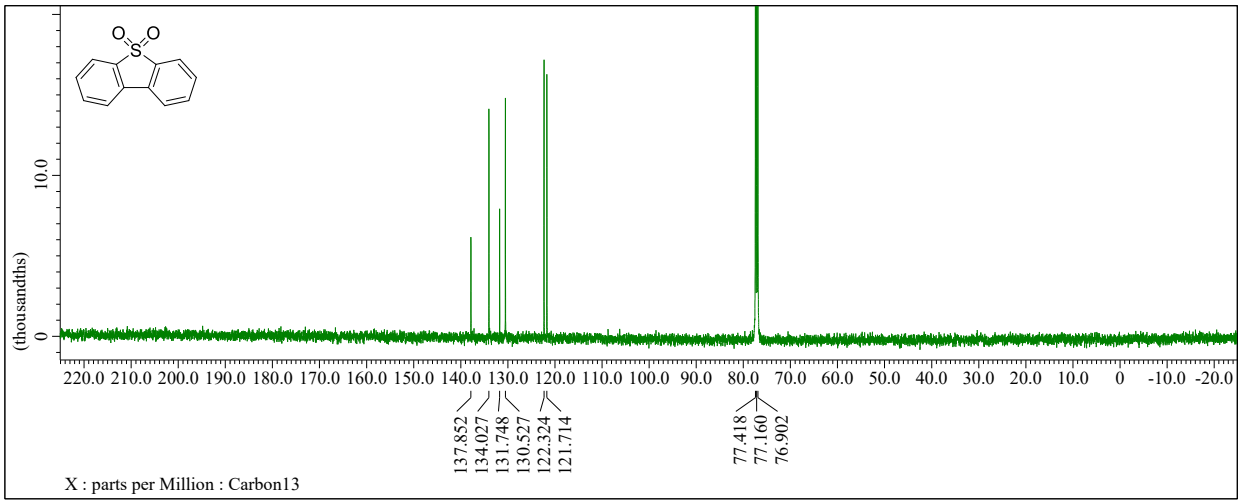

abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
2.00
2.07
4.07
0.38
0.65
0.27
8.075 8.072 8.060 8.056 7.670 7.667 7.656 7.653 7.650 7.639 7.636 7.426 7.411 7.404 7.395 7.387 7.263
1.592
0.000
X : parts per Million : Proton

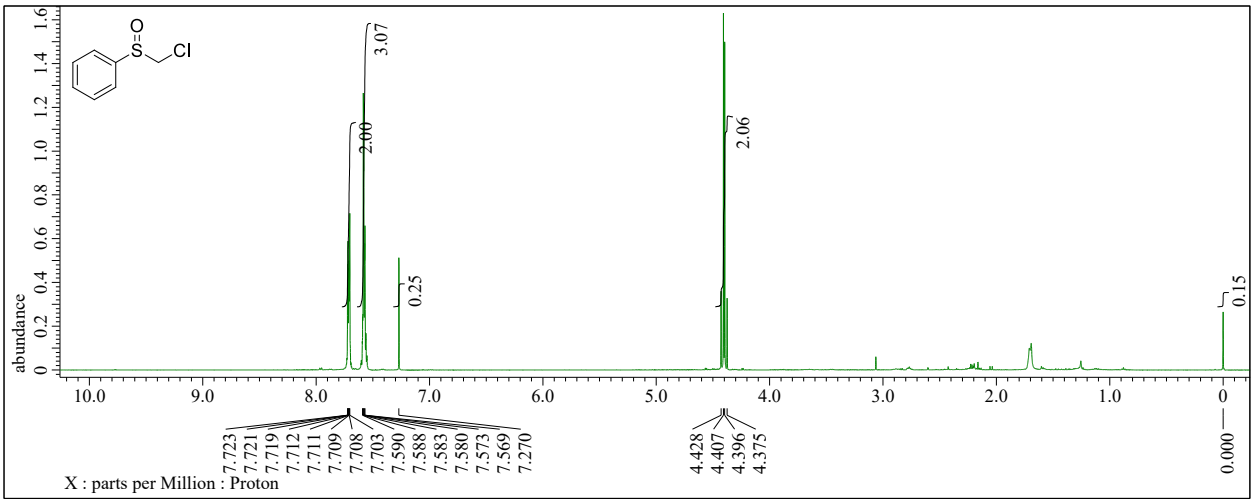

abundance
0 0.02 0.04 0.06 0.08 0.1 0.12
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
151.683
134.275
125.100
125.014
123.554
119.033
77.418
77.160
76.912
X : parts per Million : Carbon13

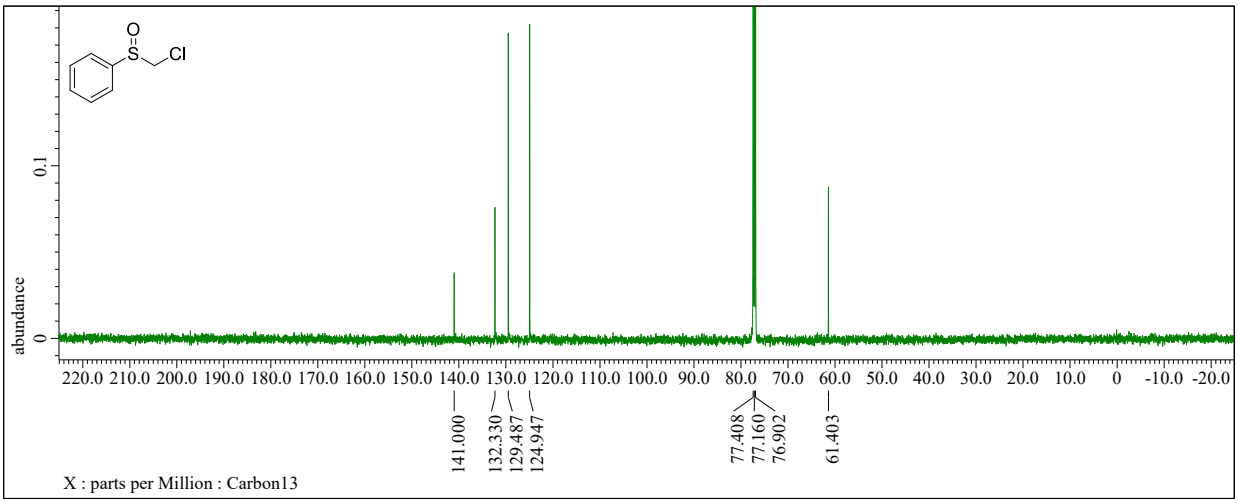

abundance
2.00
2.01
1.05
85.91m
0.11
66.34m
7.959
7.944
7.578
7.564
7.549
7.518
7.503
7.488
7.265
1.644
0.000
X : parts per Million : Proton

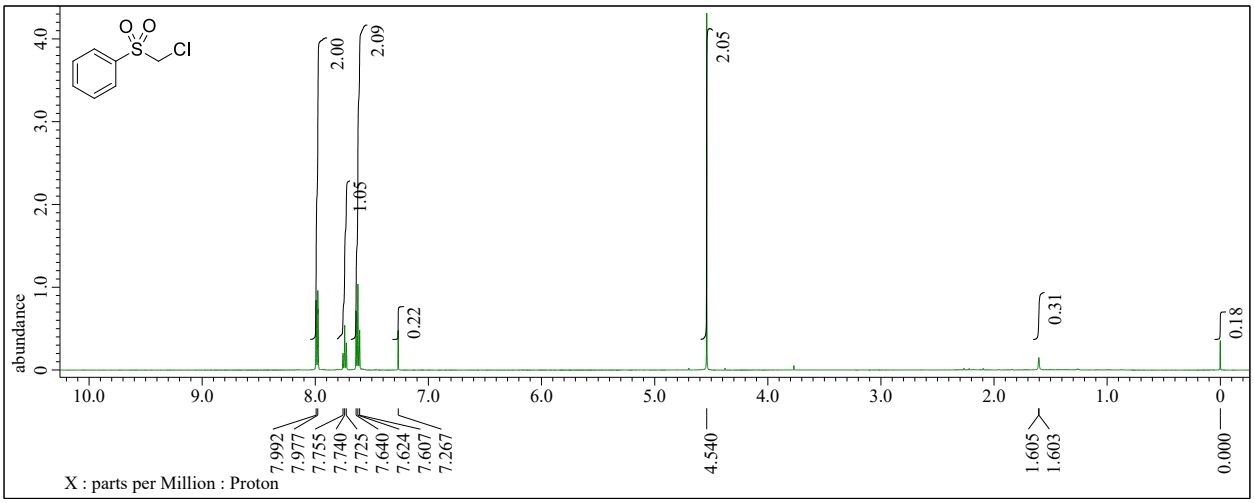

abundance
141.706
133.312
129.401
127.770
77.408
77.160
76.902
X : parts per Million : Carbon13

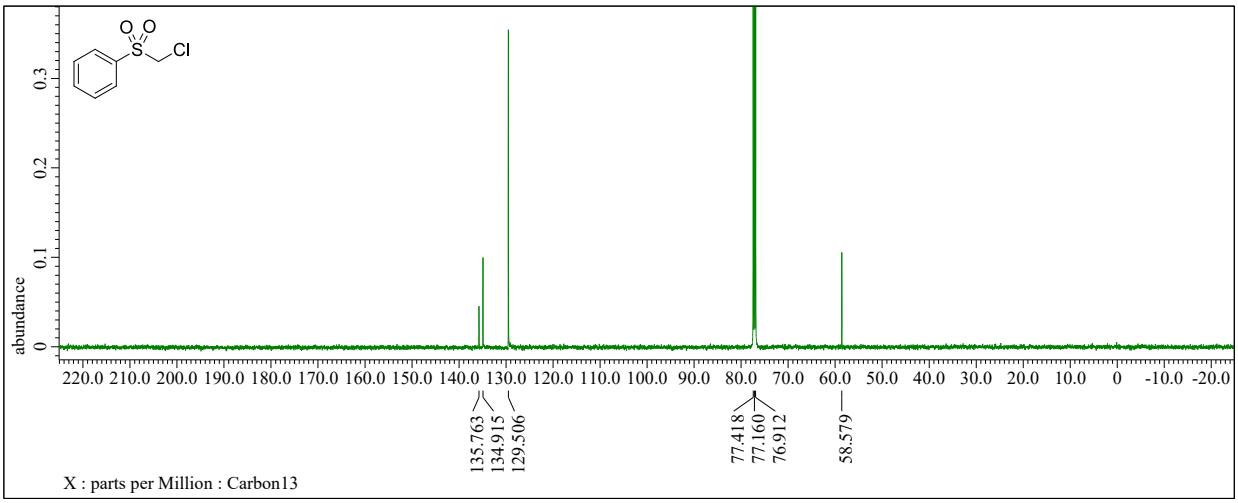

abundance
4.00
2.05
2.00
0.36
0.27
7.836
7.820
7.806
7.791
7.660
7.657
7.644
7.642
7.629
7.627
7.548
7.546
7.532
7.531
7.518
7.262
0.000
X : parts per Million : Proton

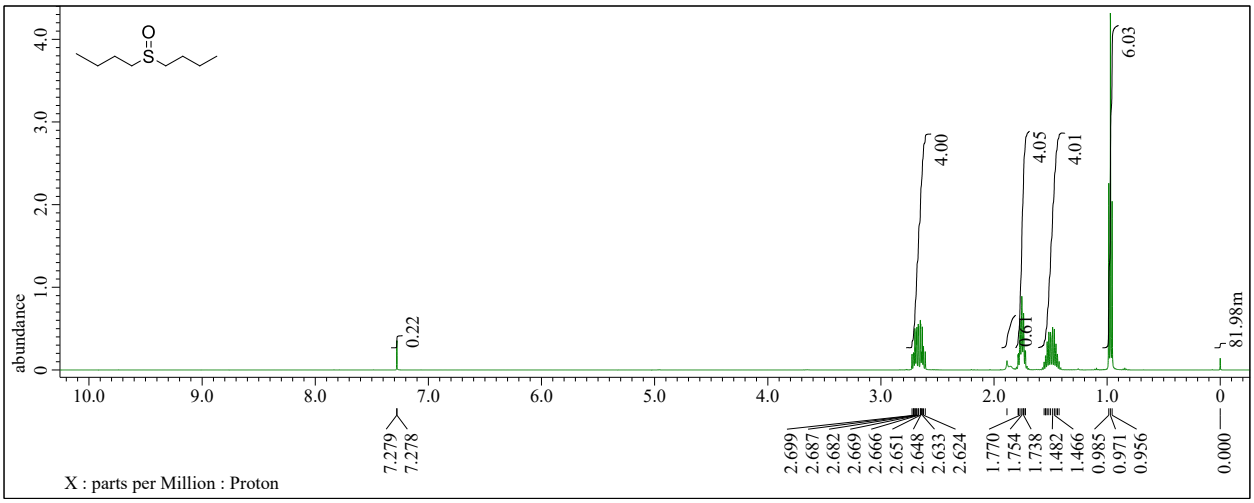

(thousandths)
137.852
134.027
131.748
130.527
122.324
121.714
77.418
77.160
76.902
X : parts per Million : Carbon13

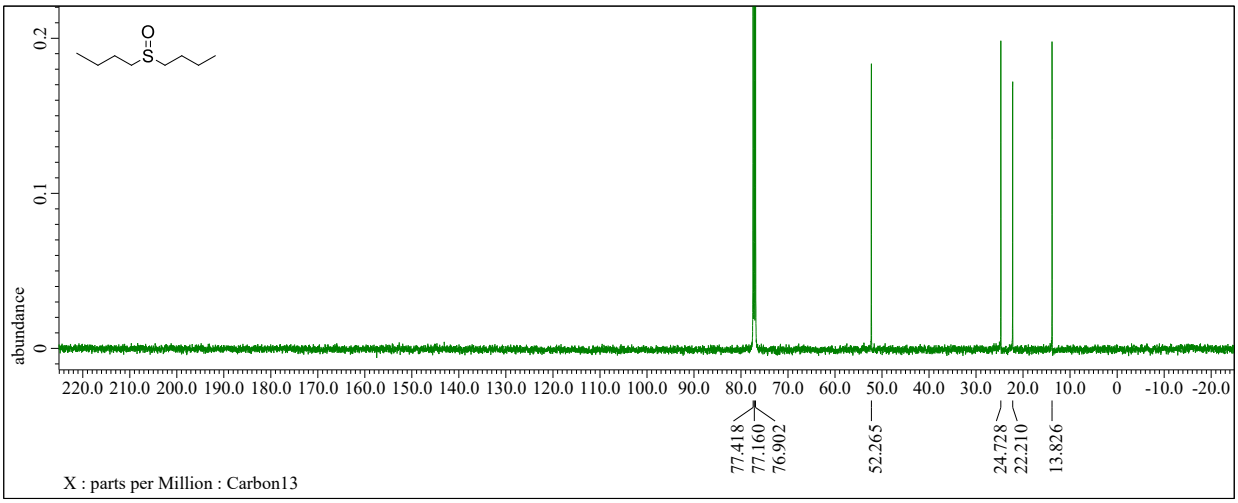

O
S
Cl
3.07
2.00
2.06
0.25
0.15
abundance
0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.723
7.721
7.719
7.712
7.711
7.709
7.708
7.703
7.590
7.588
7.583
7.580
7.573
7.569
7.270
4.428
4.407
4.396
4.375
0.000
X : parts per Million : Proton

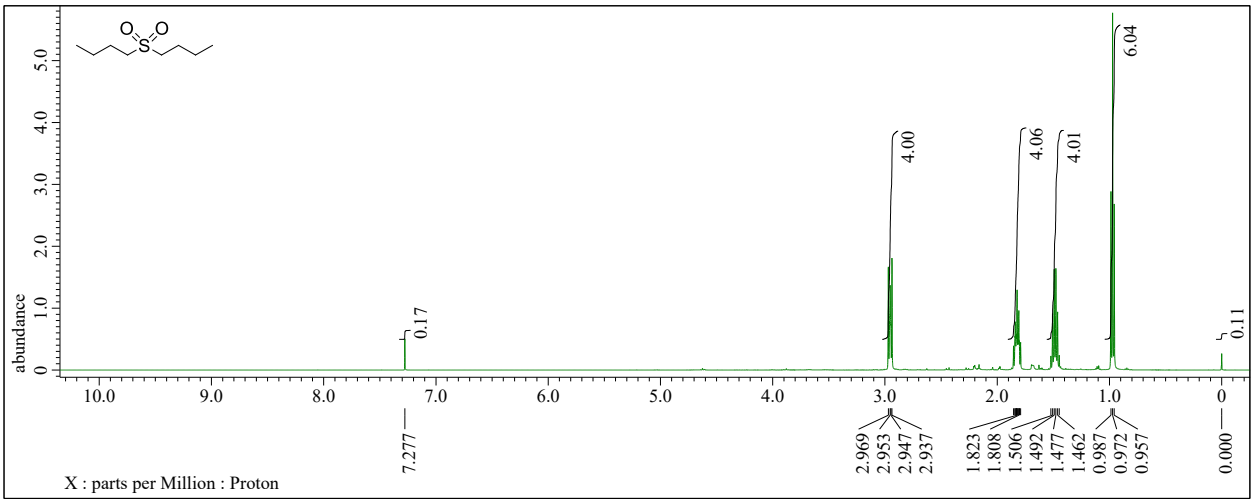

O
S
Cl
0.1
abundance
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
141.000
132.330
129.487
124.947
77.408
77.160
76.902
61.403
X : parts per Million : Carbon13

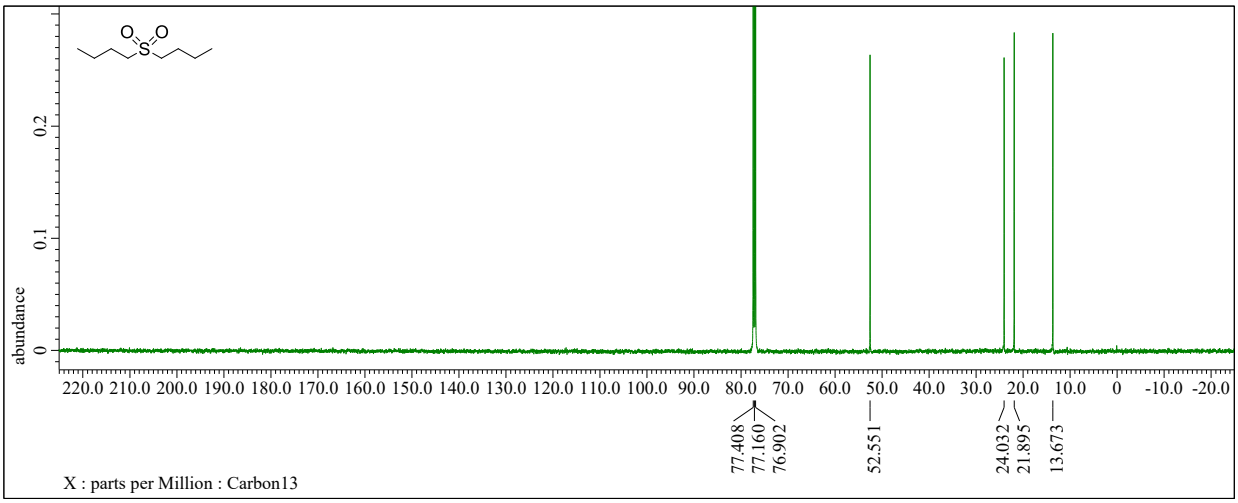

abundance
2.00
2.09
1.05
0.22
2.05
0.31
0.18
7.992
7.977
7.755
7.740
7.725
7.640
7.624
7.607
7.267
4.540
1.605
1.603
0.000
X : parts per Million : Proton


abundance
135.763
134.915
129.506
77.418
77.160
76.912
58.579
X : parts per Million : Carbon13


abundance
4.00
4.05
4.01
6.03
0.22
0.61
81.98m
7.279
7.278
2.699
2.687
2.682
2.669
2.666
2.651
2.648
2.633
2.624
1.770
1.754
1.738
1.482
1.466
0.985
0.971
0.956
0.000
X : parts per Million : Proton


abundance
77.418
77.160
76.902
52.265
24.728
22.210
13.826
X : parts per Million : Carbon13


abundance
0
1.0
2.0
3.0
4.0
5.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.17
4.00
4.06
4.01
6.04
0.11
7.277
2.969
2.953
2.947
2.937
1.823
1.808
1.506
1.492
1.477
1.462
0.987
0.972
0.957
0.000
X : parts per Million : Proton


abundance
0
0.1
0.2
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
77.408
77.160
76.902
52.551
24.032
21.895
13.673
X : parts per Million : Carbon13

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