

SUPPORTING INFORMATION

Catalyst-free approach for solvent-depended selective oxidation of organic sulfides with oxone

Bing Yu, An-Hua Liu, Liang-Nian He,* Bin Li, Zhen-Feng Diao, Yu-Nong Li

*State Key Laboratory and Institute of Elemento-Organic Chemistry, Nankai University, Tianjin,
300071, People's Republic of China.*

E-mail: heln@nankai.edu.cn;

Table of Content

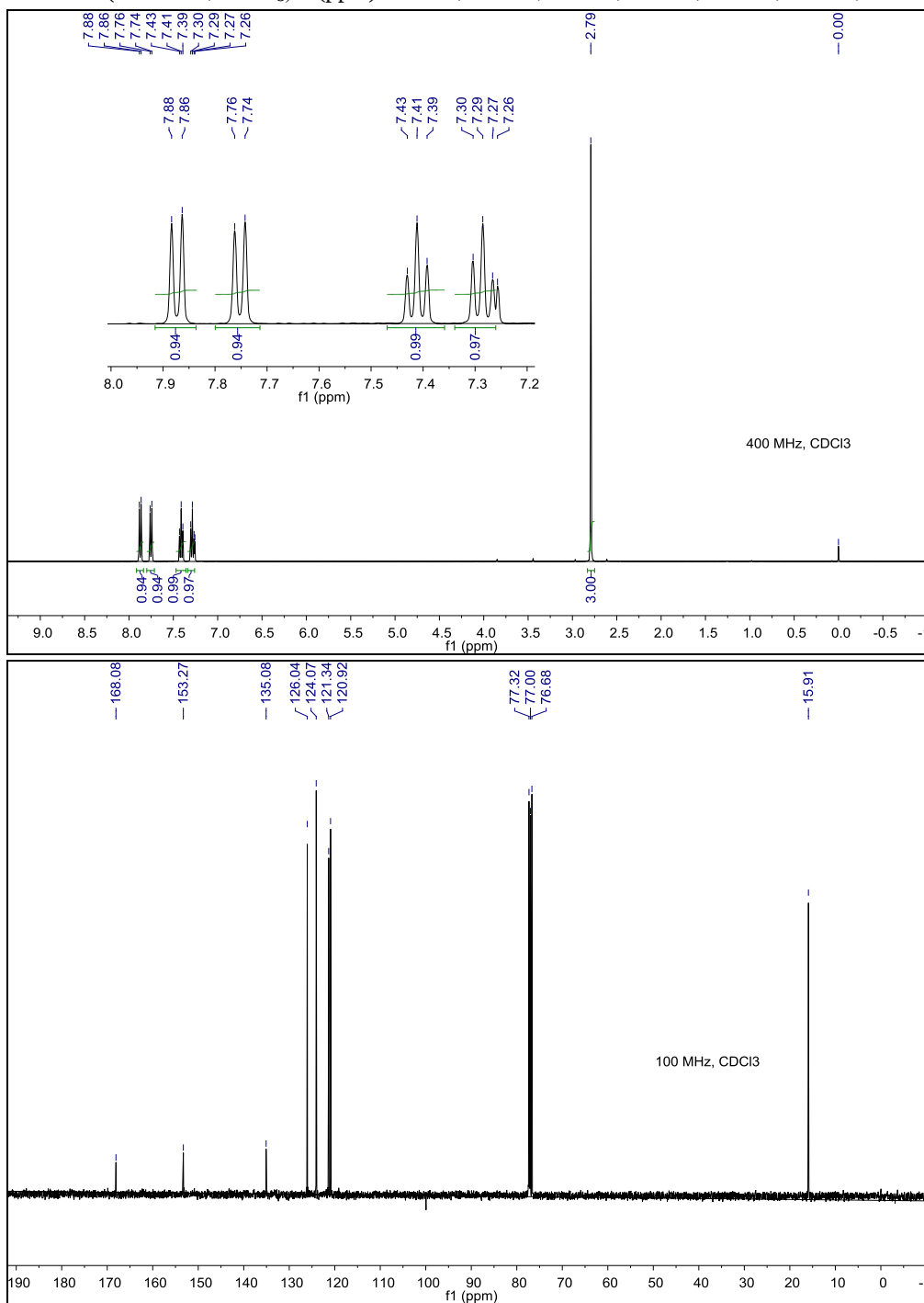
1. NMR Spectral Data of the Products	S2
2. GC-MS Spectral Data of the Products	S23

1. NMR Spectral Data of the Products

1j: 2-(Methylthio)benzothiazole

^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.87 (d, $J = 8.1$ Hz, 1H), 7.75 (d, $J = 8.0$ Hz, 1H), 7.41 (t, $J = 7.6$ Hz, 1H), 7.29 (t, $J = 7.5$ Hz, 1H), 2.79 (s, 3H).

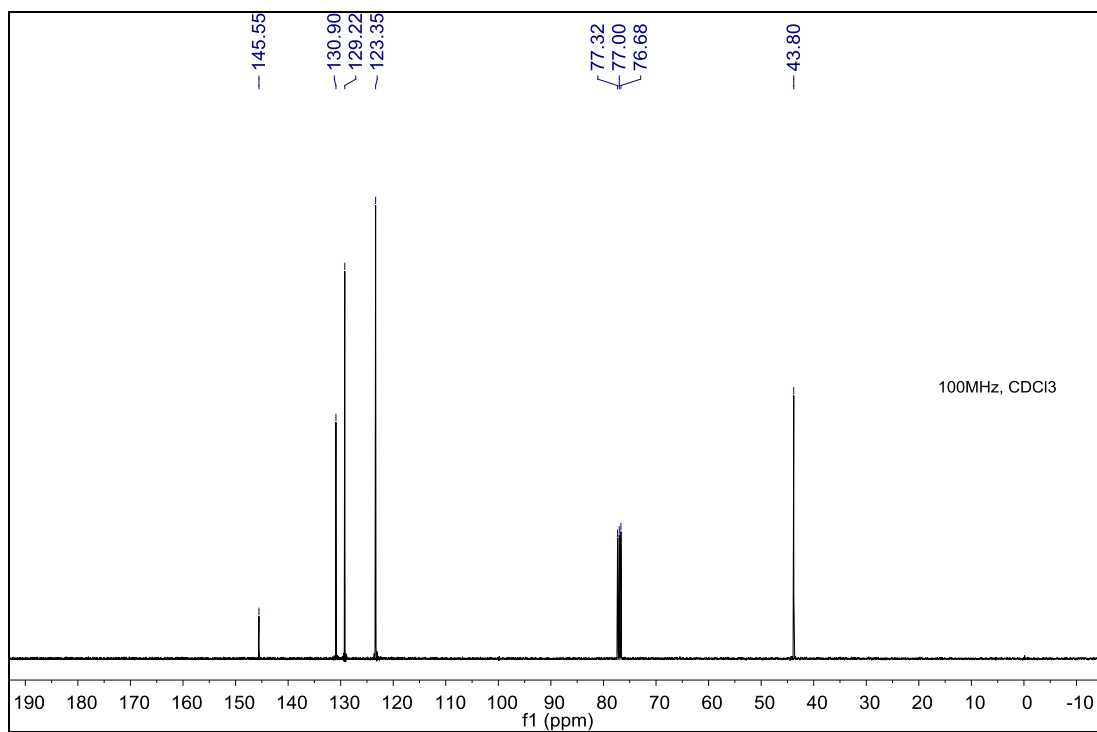
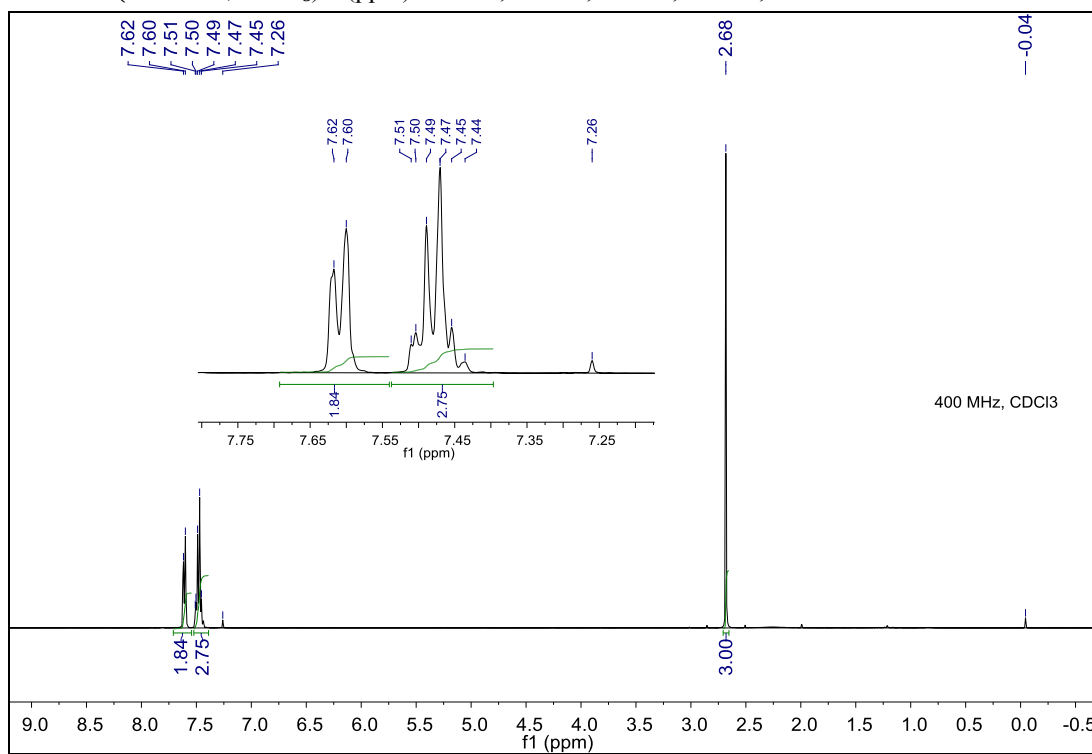
^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 168.08, 153.27, 135.08, 126.04, 124.07, 121.34, 120.92, 15.91.



2a: Phenyl methyl sulfoxide

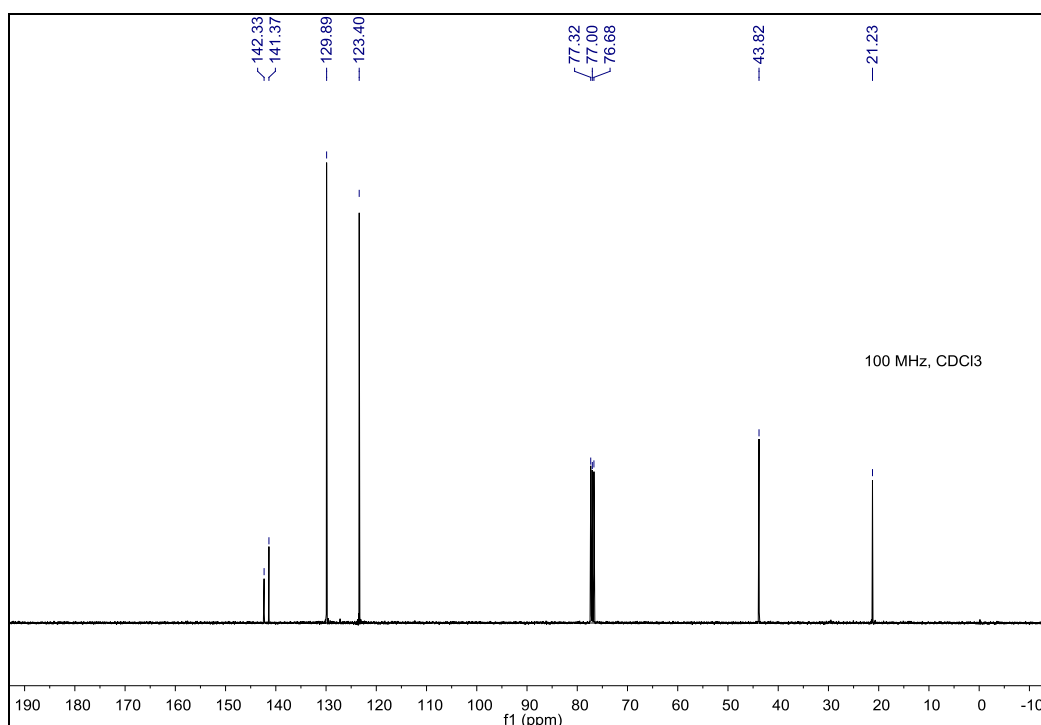
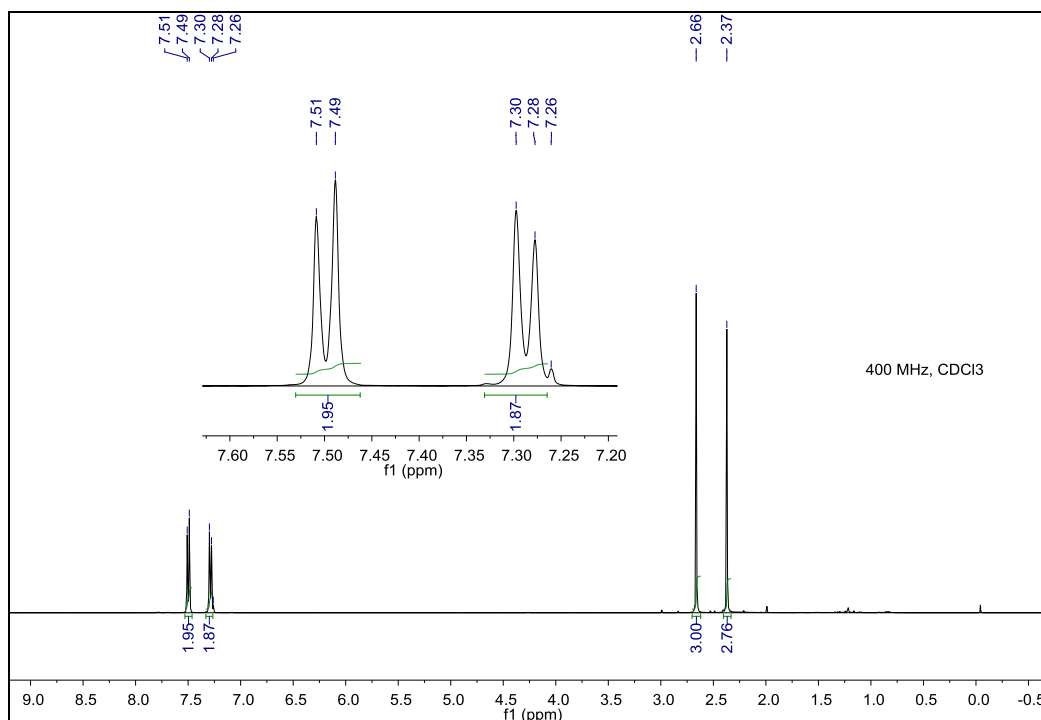
^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.62-7.60 (m, 2H), 7.51-7.44 (m, 3H), 2.68 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 145.55, 130.90, 129.22, 123.35, 43.80.



2b: *p*-Tolyl methyl sulfoxide

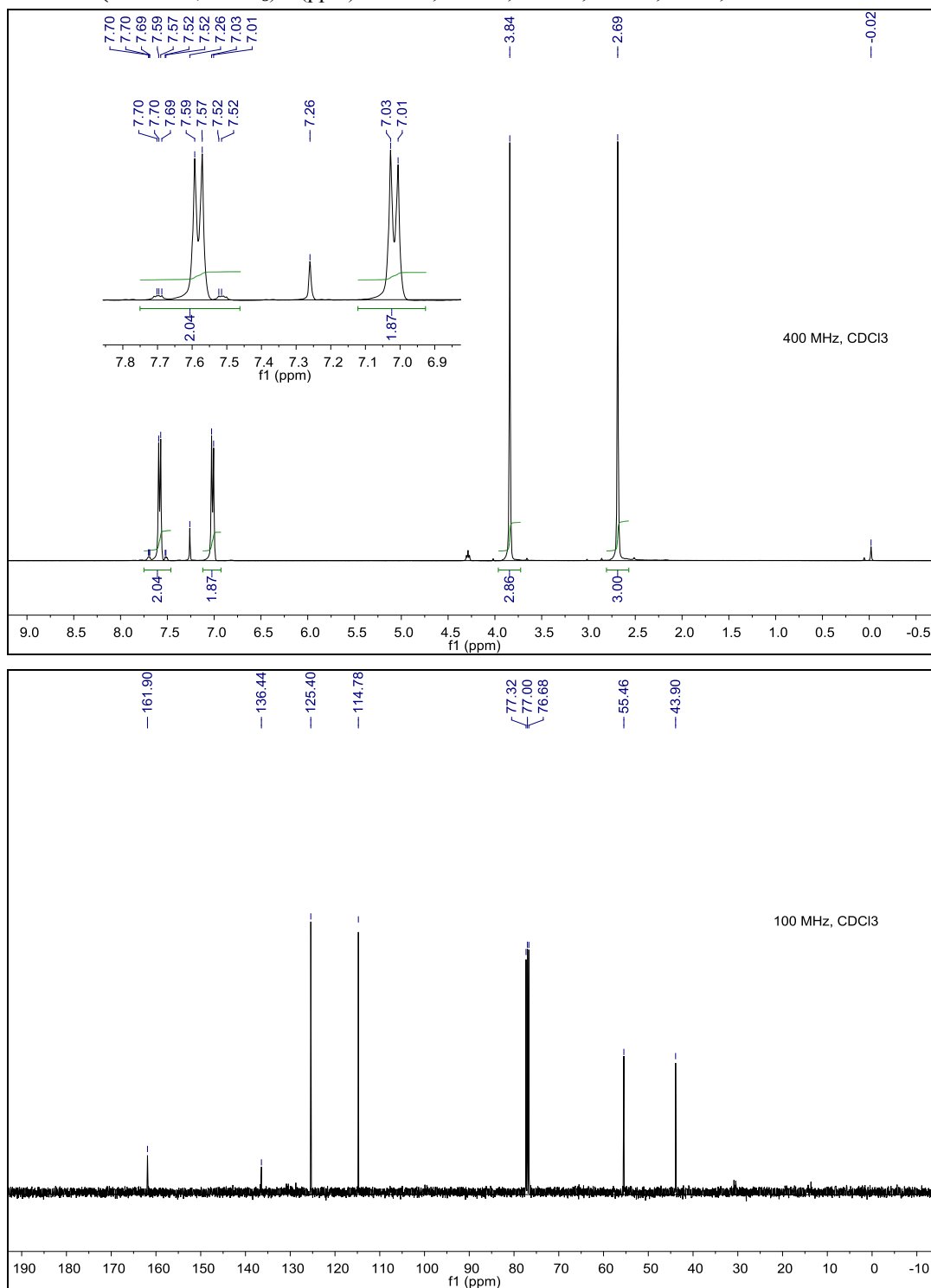
^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.50 (d, $J = 8.0$ Hz, 2H), 7.29 (d, $J = 8.0$ Hz, 2H), 2.66 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 142.33, 141.37, 129.89, 123.40, 43.82, 21.23.



2c: 4-Methoxyphenyl methyl sulfoxide

^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.70-7.52 (m, 2H), 7.03-7.01 (m, 2H), 3.84 (s, 3H), 2.69 (s, 3H).

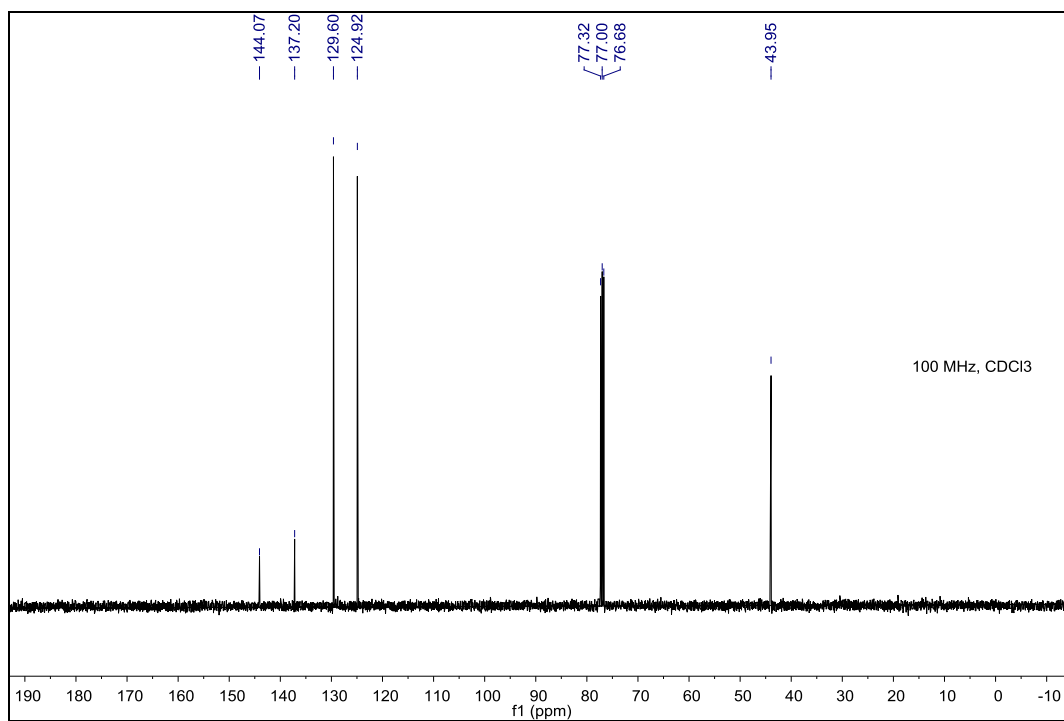
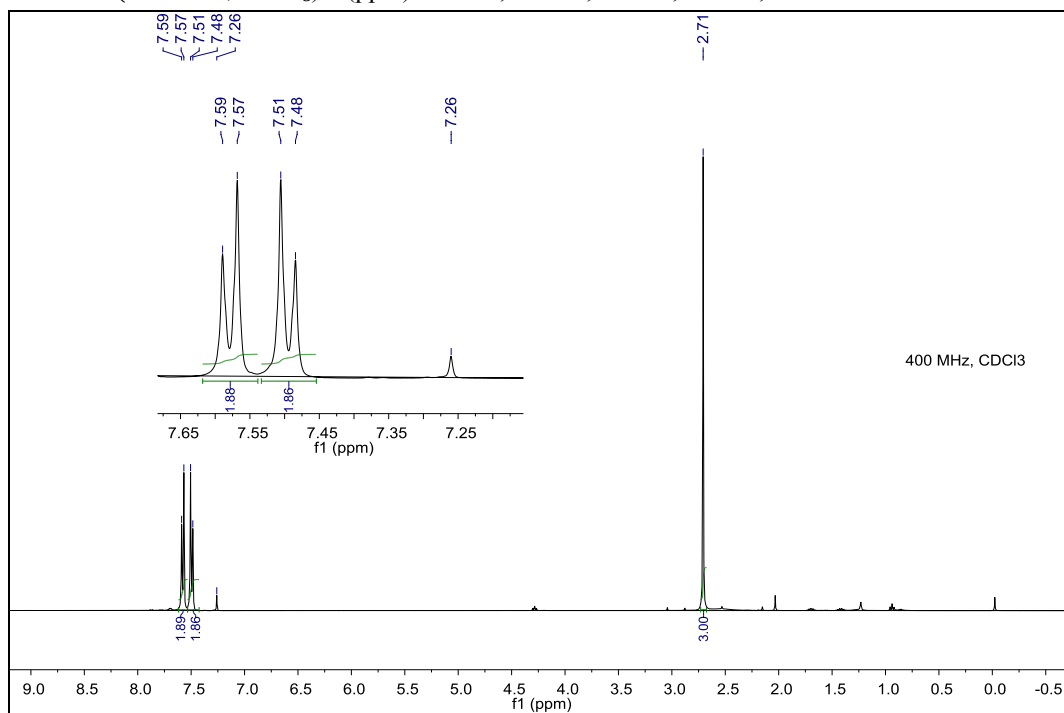
^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 161.90, 136.44, 125.40, 114.78, 55.46, 43.90.



2d: p-Chlorophenyl methyl sulfoxide

^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.58 (d, $J = 8.5$ Hz, 2H), 7.49 (d, $J = 8.5$ Hz, 2H), 2.71 (s, 3H).

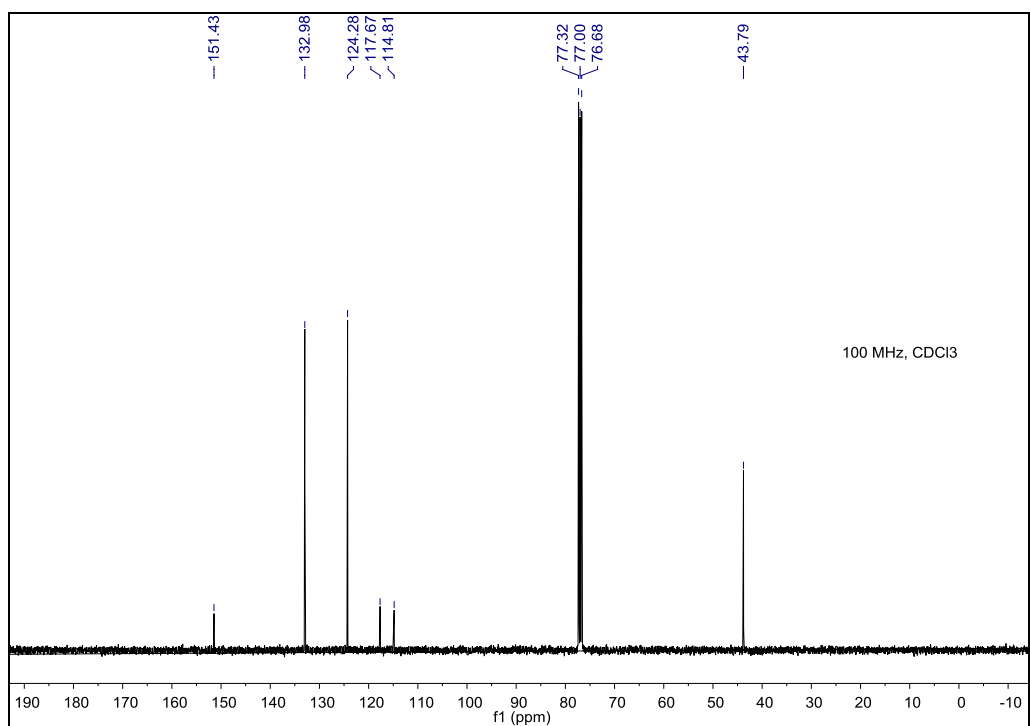
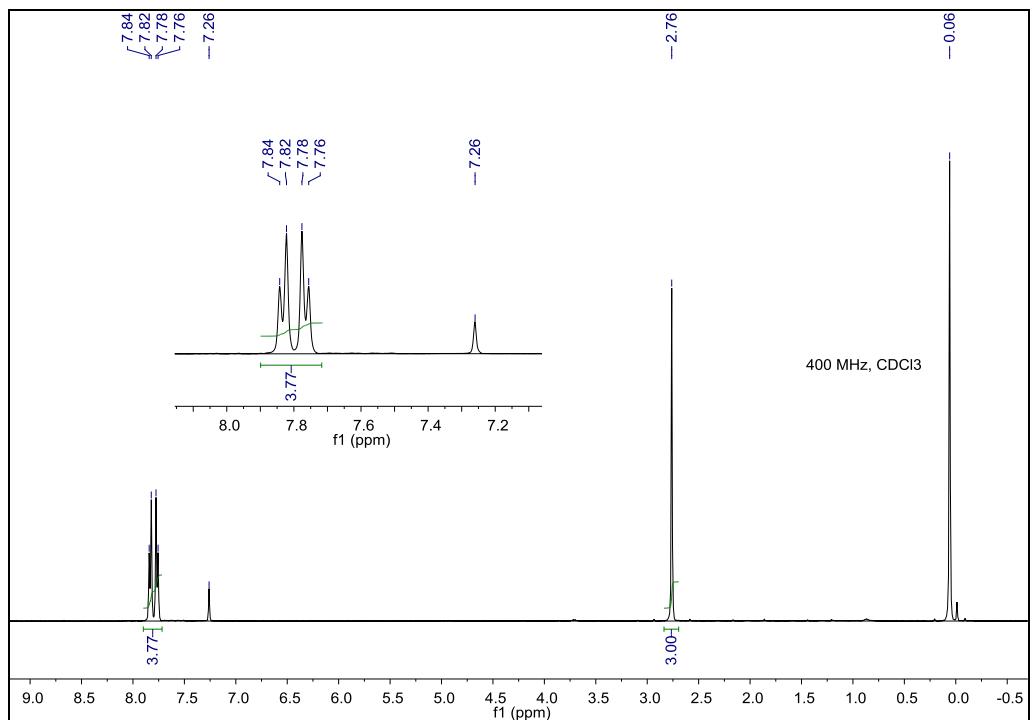
^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 144.07, 137.20, 129.60, 124.92, 43.95.



2e: 4-Cyanophenyl methyl sulfoxide

^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.83 (d, $J = 8.2$ Hz, 2H), 7.77 (d, $J = 8.1$ Hz, 2H), 2.76 (s, 3H).

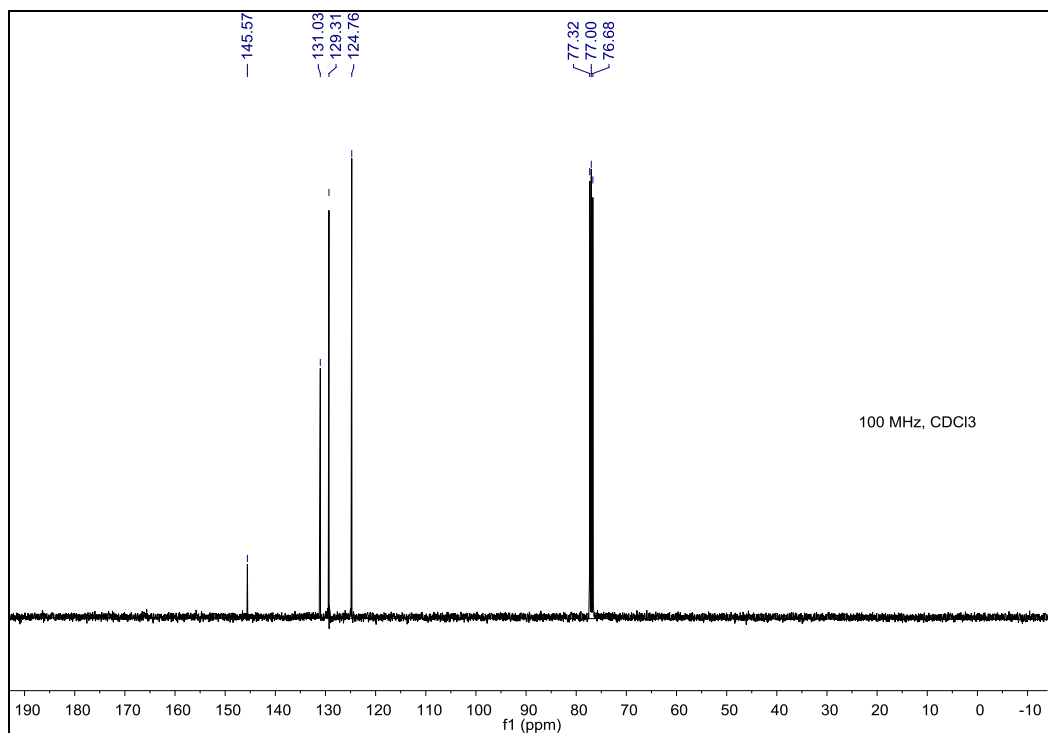
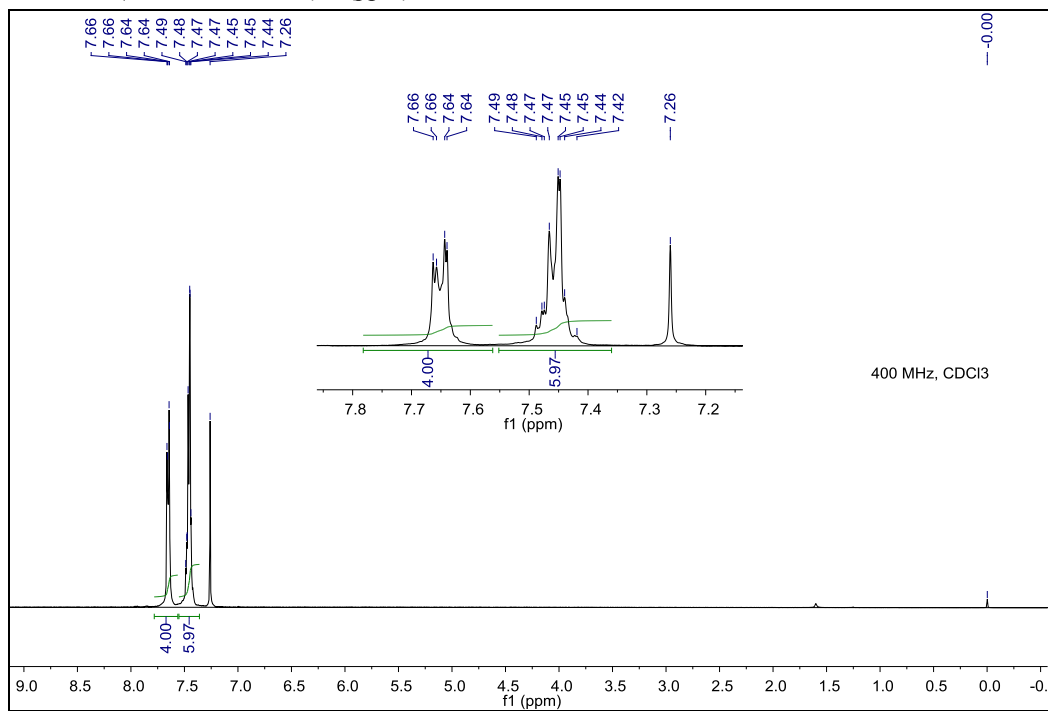
^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 151.43, 132.98, 124.28, 117.67, 114.81, 43.79.



2f: Diphenyl sulfoxide

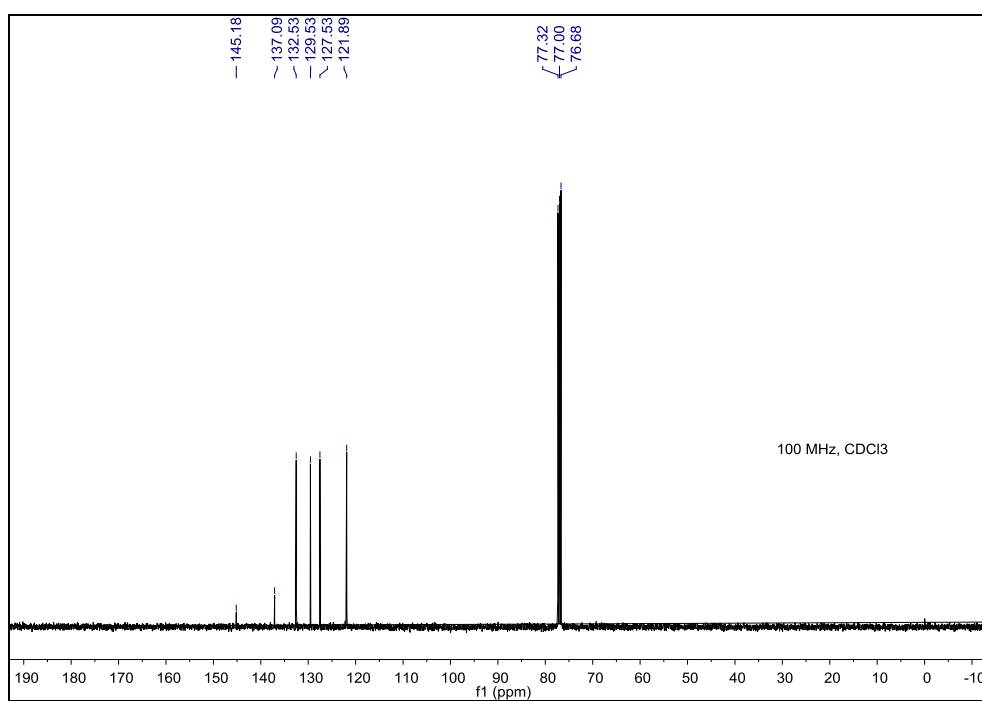
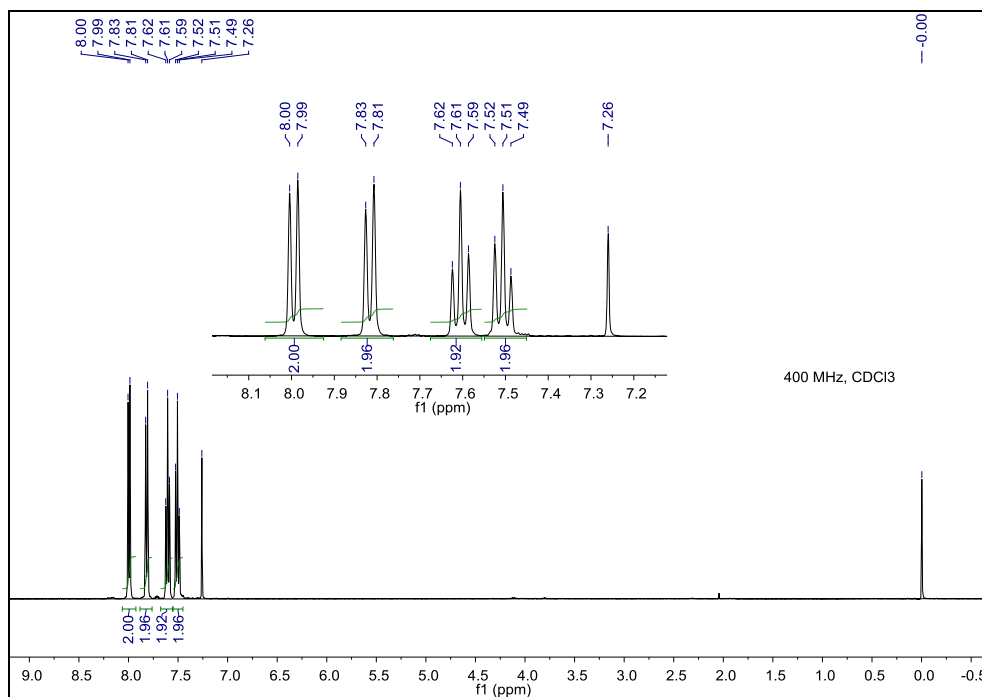
^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.66-7.64 (m, 4H), 7.49-7.42 (m, 6H).

^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 145.57, 131.03, 129.31, 124.76.



2g: Dibenzothiophene sulfoxide

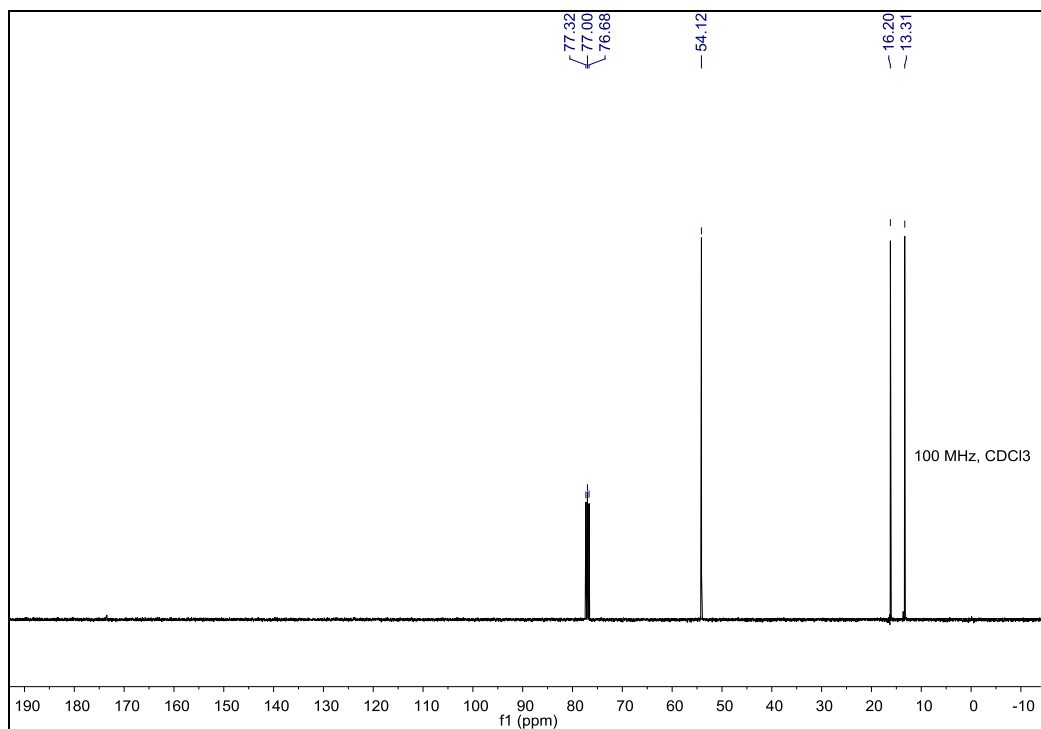
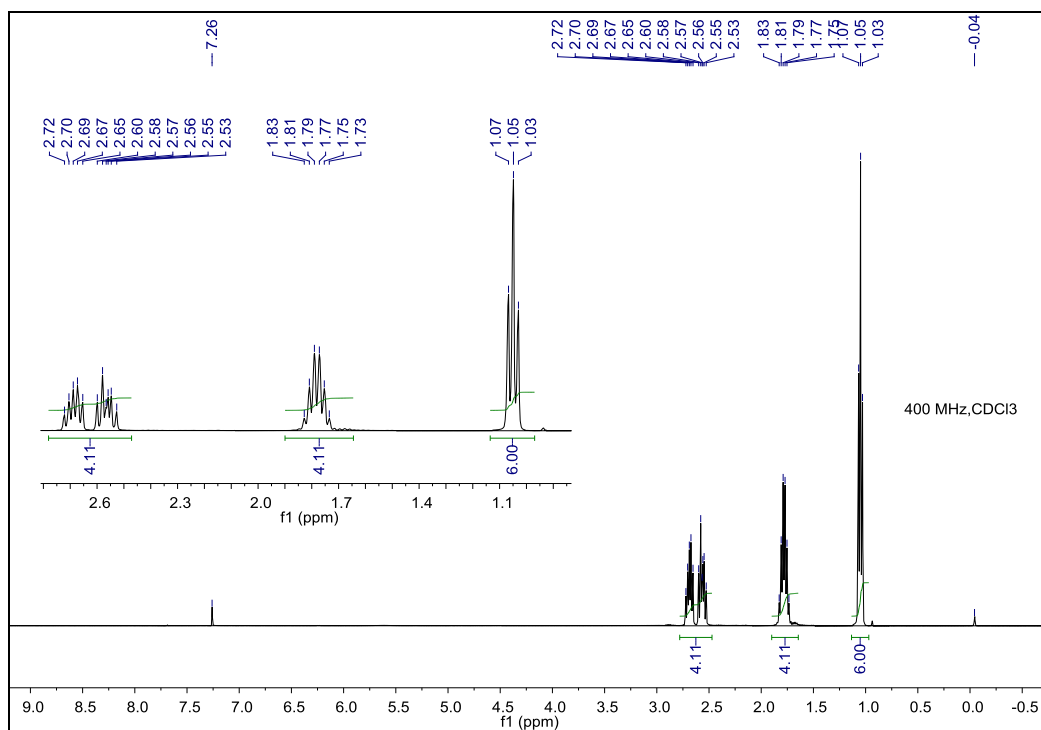
^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.99 (d, $J = 7.6$ Hz, 2H), 7.82 (d, $J = 7.7$ Hz, 2H), 7.61 (t, $J = 7.5$ Hz, 3H), 7.51 (t, $J = 7.5$ Hz, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 145.18, 137.09, 132.53, 129.53, 127.53, 121.89.



2h: Di(*n*-propyl) sulfoxide

^1H NMR (400 MHz, CDCl_3) δ (ppm): 2.72-2.53 (m, 4H), 1.83-1.73 (m, 4H), 1.05 (t, $J = 7.4$ Hz, 6H).

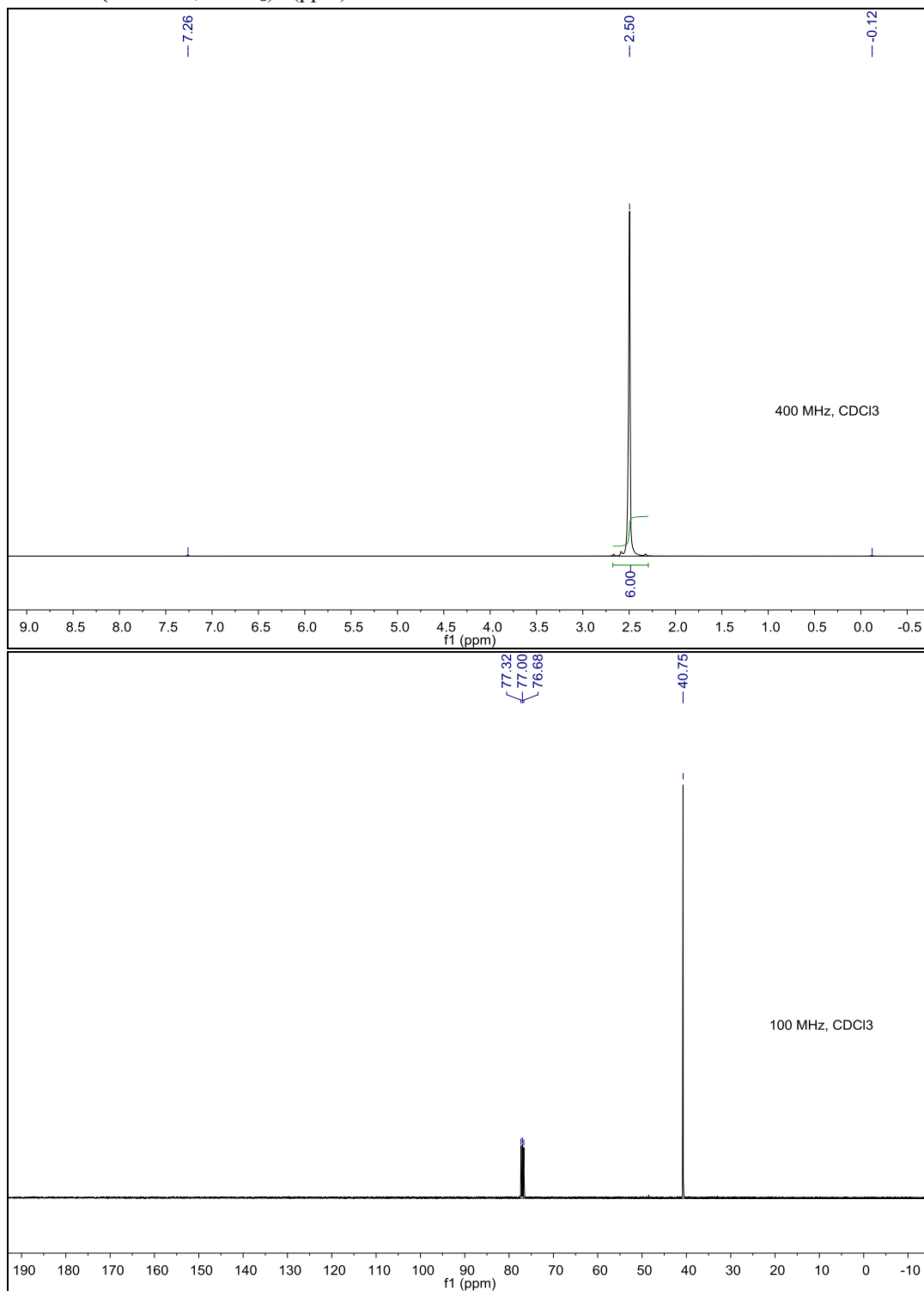
^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 54.12, 16.20, 13.31.



2i: Dimethyl sulfoxide

^1H NMR (400 MHz, CDCl_3) δ (ppm): 2.50 (s, 6H).

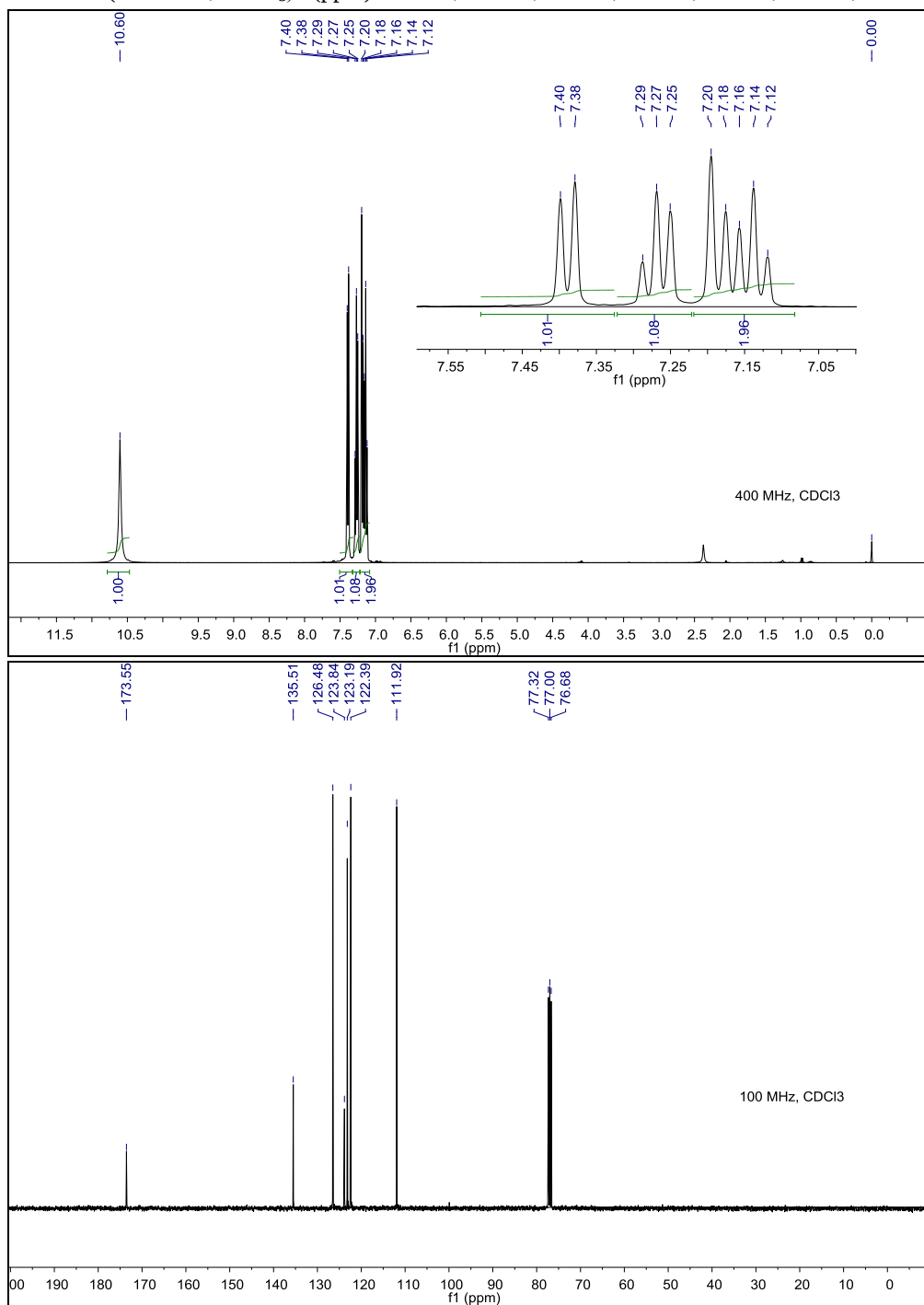
^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 40.75.



2j: 2-Benzothiazolone

^1H NMR (400 MHz, CDCl_3) δ (ppm): 10.60 (s, 1H), 7.39 (d, $J = 7.8$ Hz, 1H), 7.29-7.25 (m, 1H), 7.20-7.12 (m, 2H).

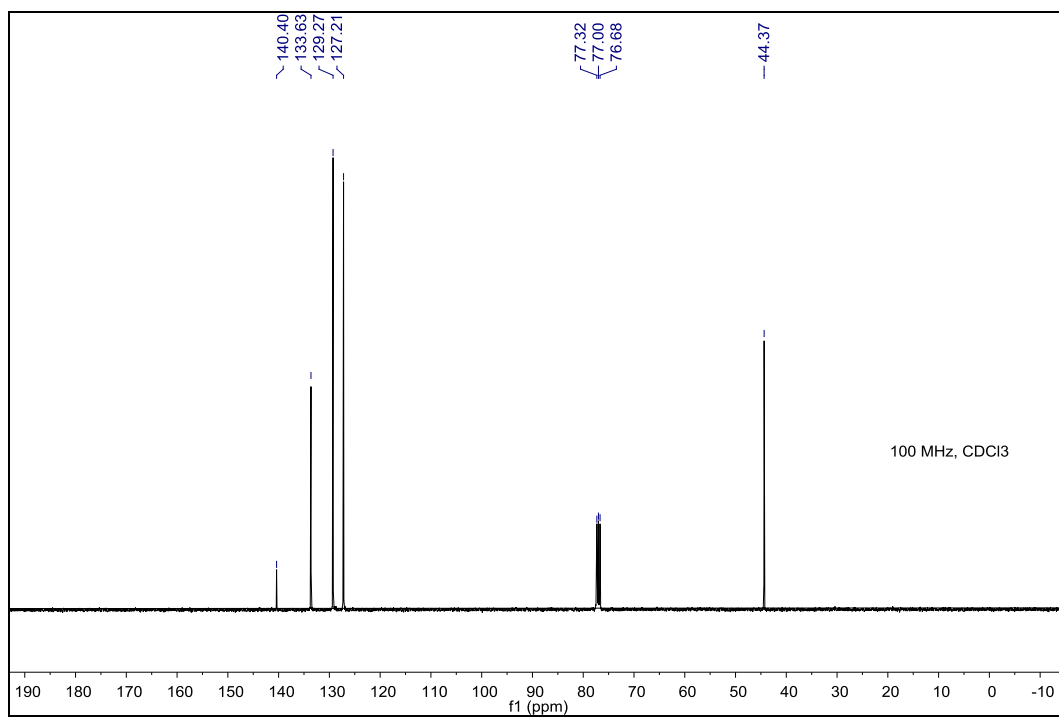
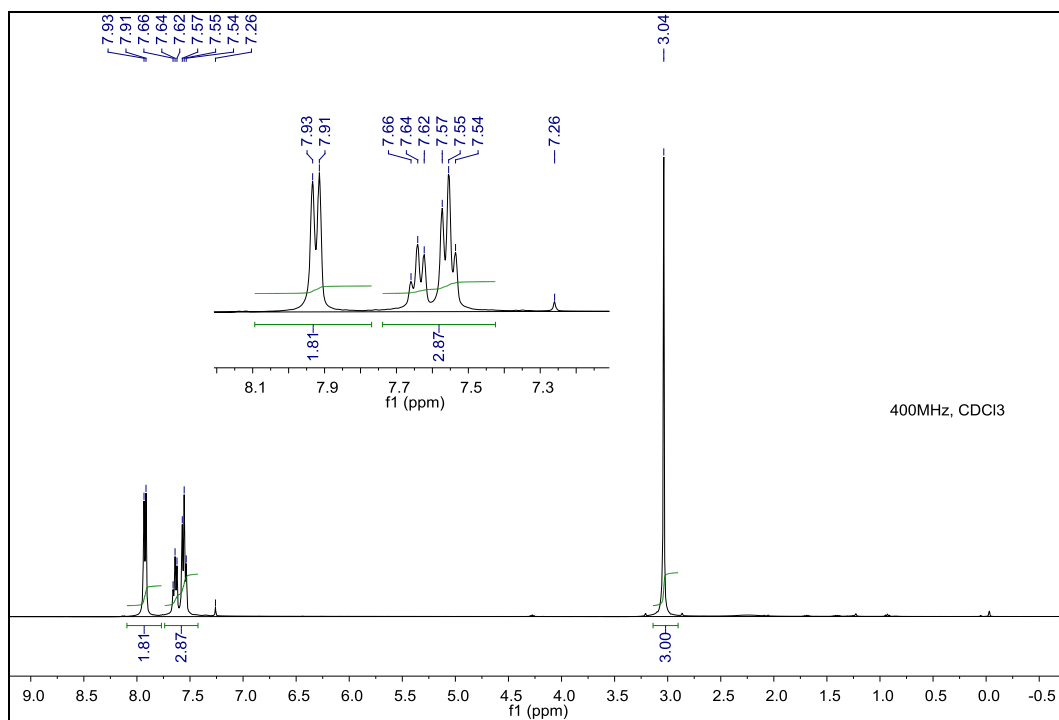
^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 173.55, 135.51, 126.48, 123.84, 123.19, 122.39, 111.92.



3a: Phenyl methyl sulfone

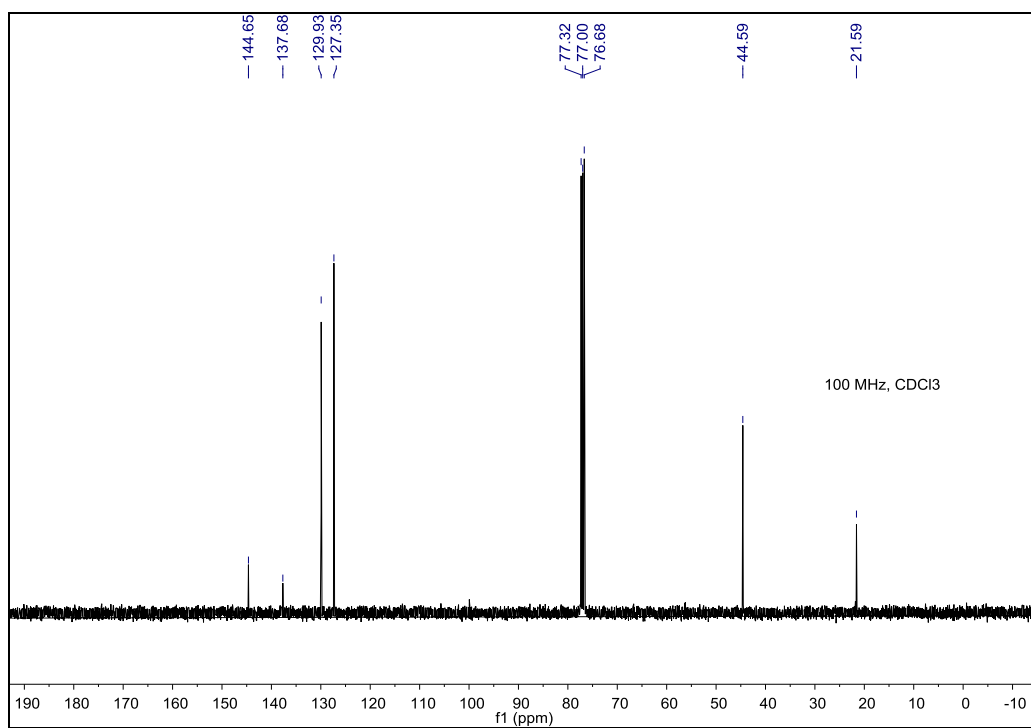
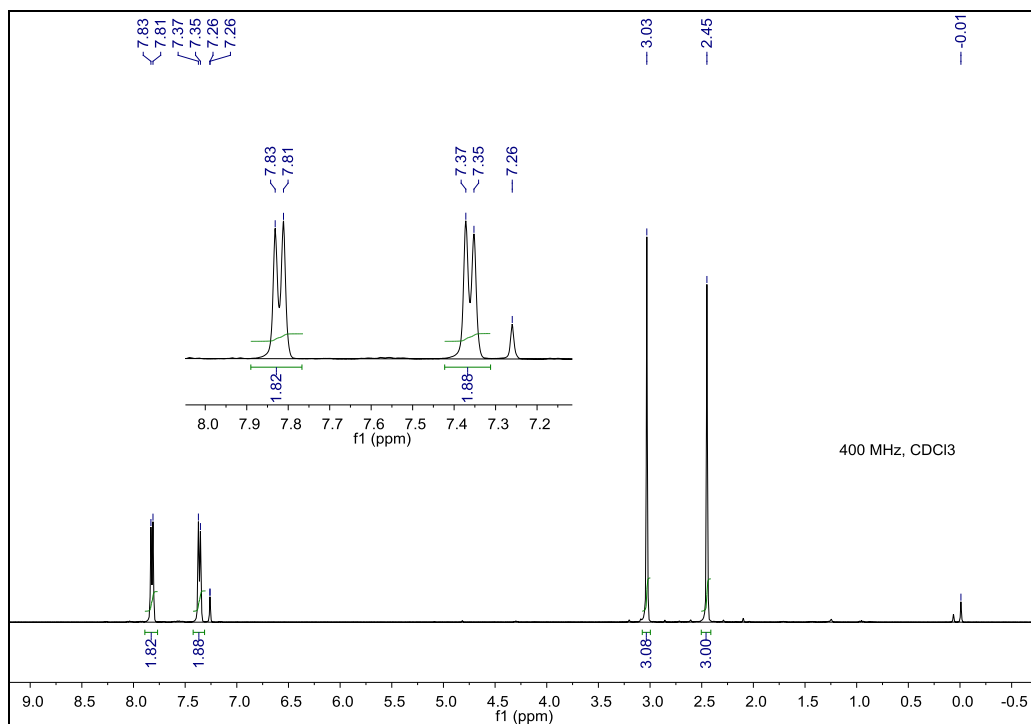
^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.92 (d, $J = 7.5$ Hz, 2H), 7.66-7.54 (m, 3H), 3.04 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 140.40, 133.63, 129.27, 127.21, 44.37.



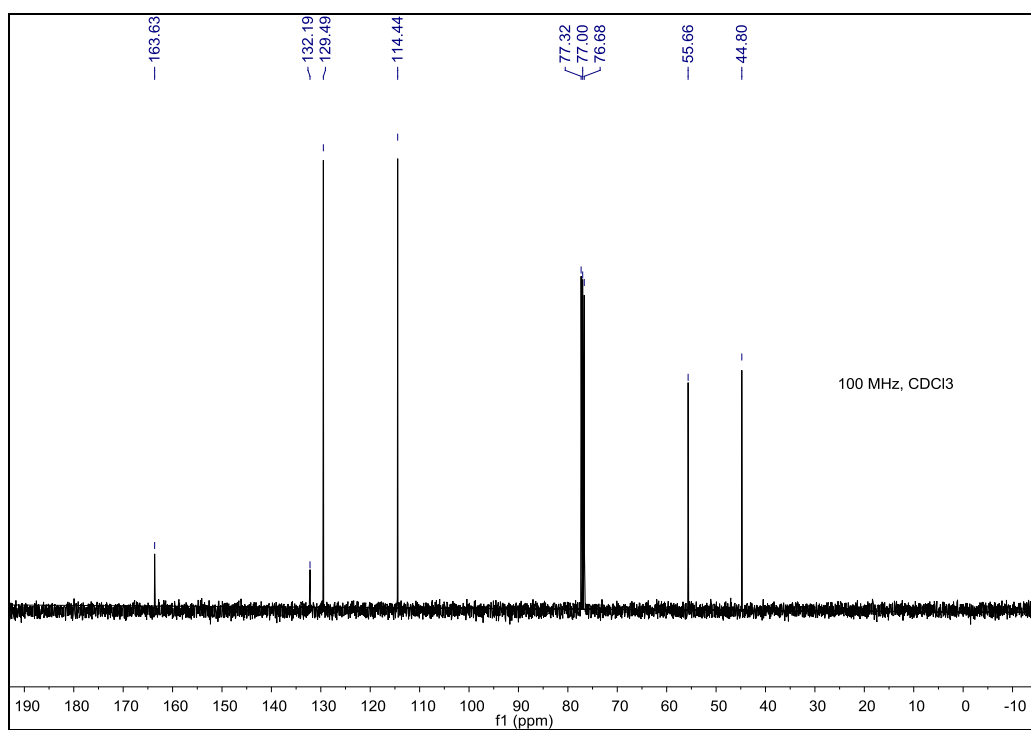
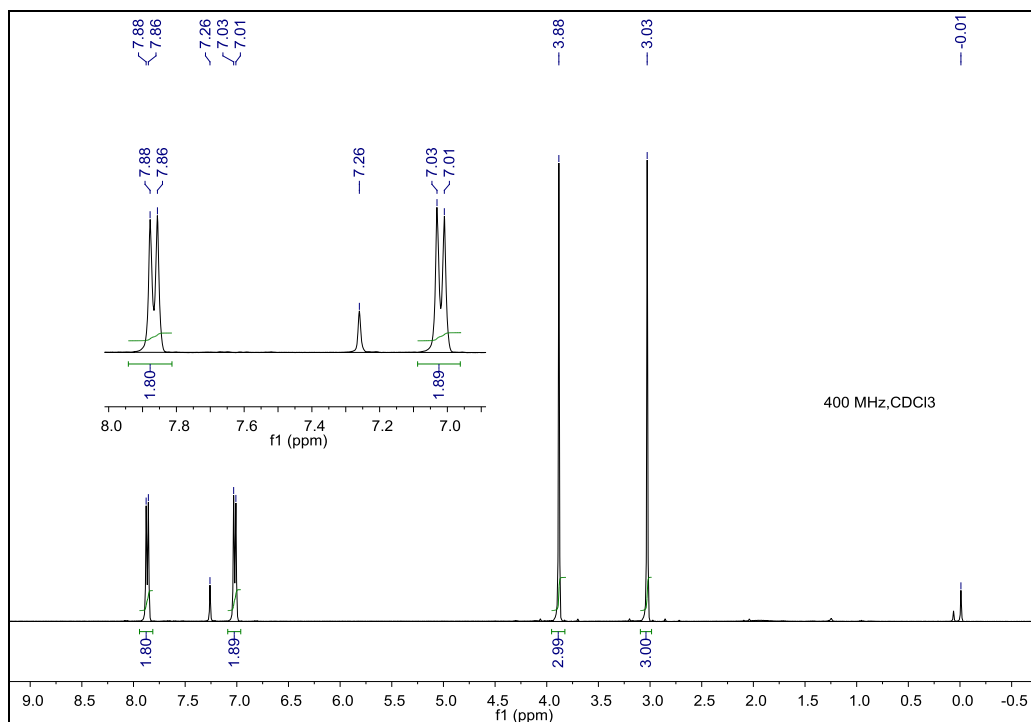
3b: p-Tolyl methyl sulfone

^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.82 (d, $J = 8.0$ Hz, 2H), 7.36 (d, $J = 7.9$ Hz, 2H), 3.03 (s, 3H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 144.65, 137.68, 129.93, 127.35, 44.59, 21.59.



3c: 4-Methoxyphenyl methyl sulfone

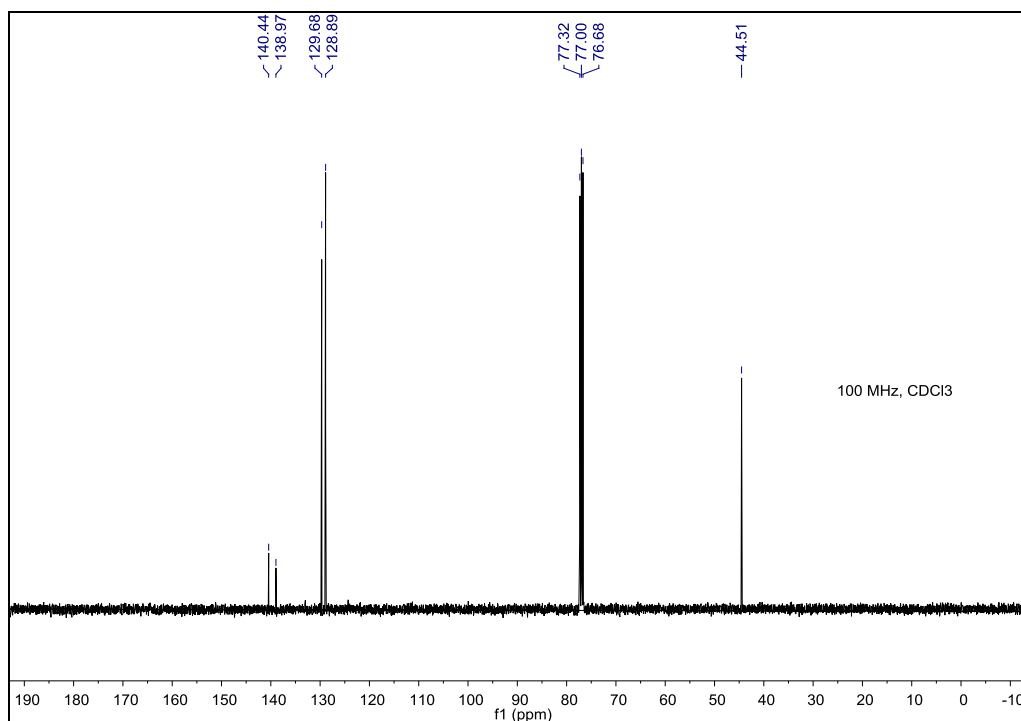
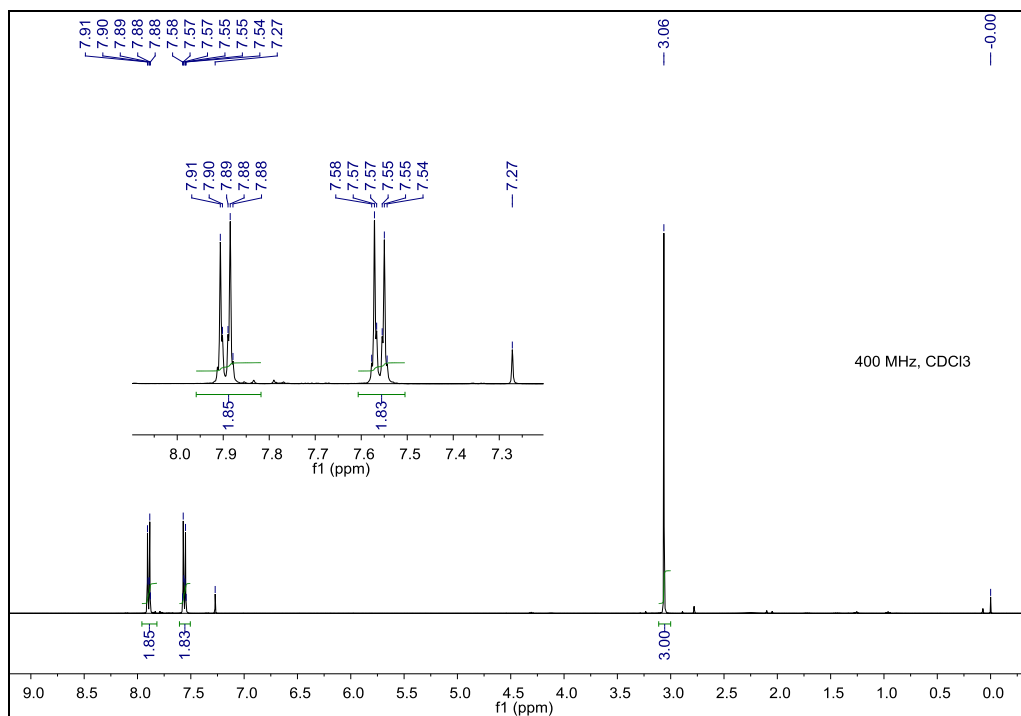
^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.87 (d, $J = 8.7$ Hz, 2H), 7.02 (d, $J = 8.7$ Hz, 2H), 3.88 (s, 3H), 3.03 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 163.63, 132.19, 129.49, 114.44, 55.66, 44.80.



3d: p-Chlorophenyl methyl sulfone

^1H NMR (400 MHz, CDCl_3) δ (ppm): 7.91-7.88 (m, 2H), 7.58-7.54 (m, 2H), 3.06 (s, 3H).

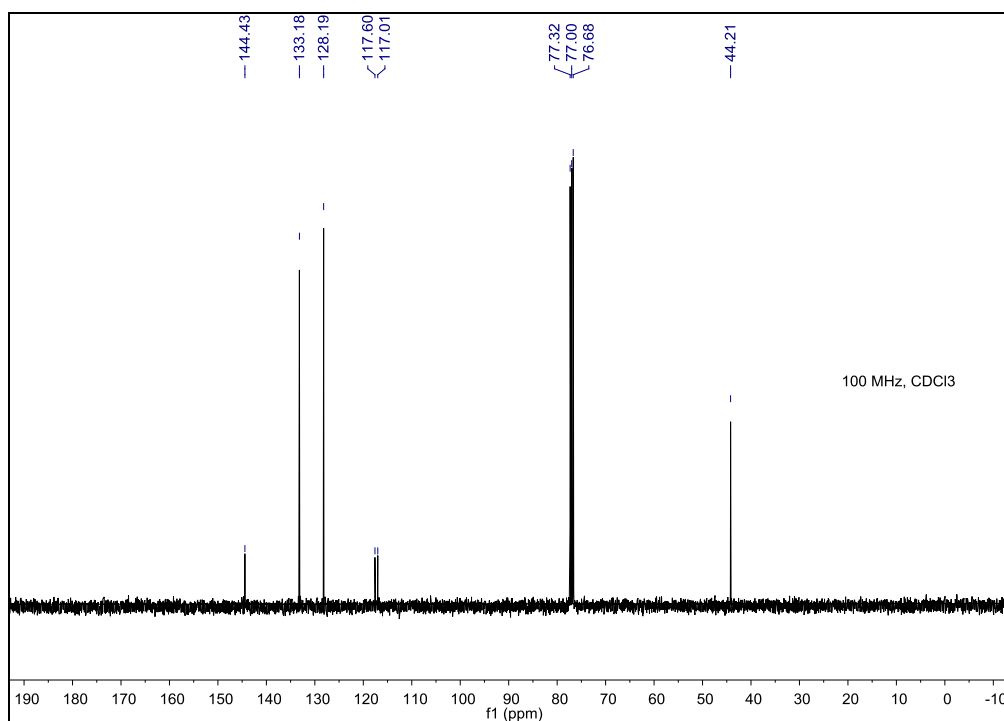
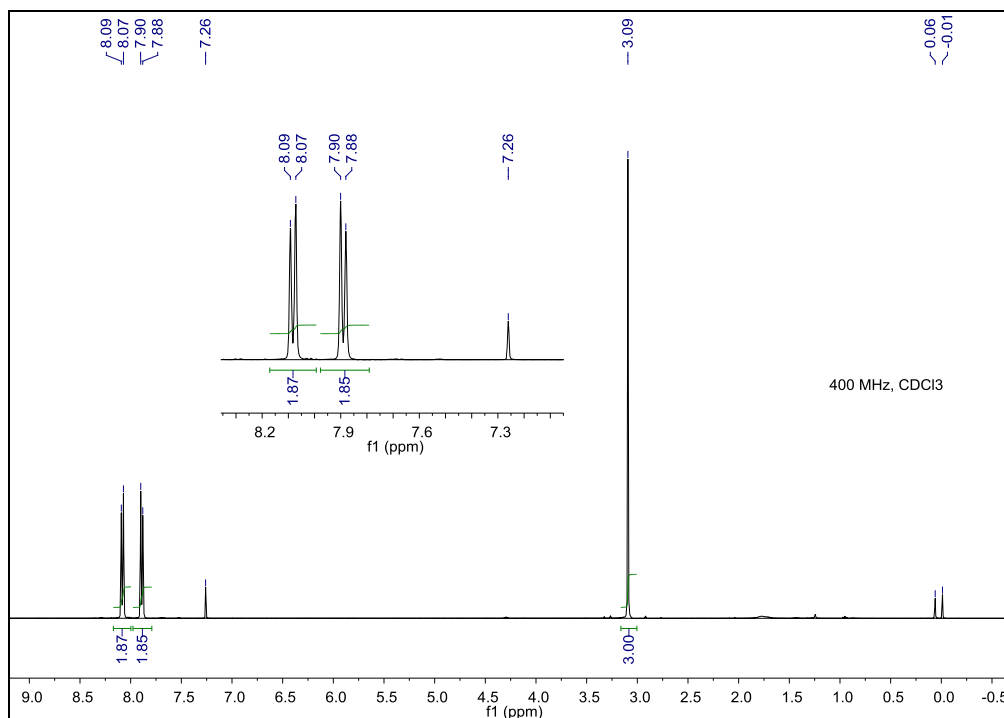
^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 140.44, 138.97, 129.68, 128.89, 44.51.



3e: 4-Cyanophenyl methyl sulfone

^1H NMR (400 MHz, CDCl_3) δ (ppm): 8.08 (d, $J = 8.3$ Hz, 2H), 7.89 (d, $J = 8.0$ Hz, 2H), 3.09 (s, 3H).

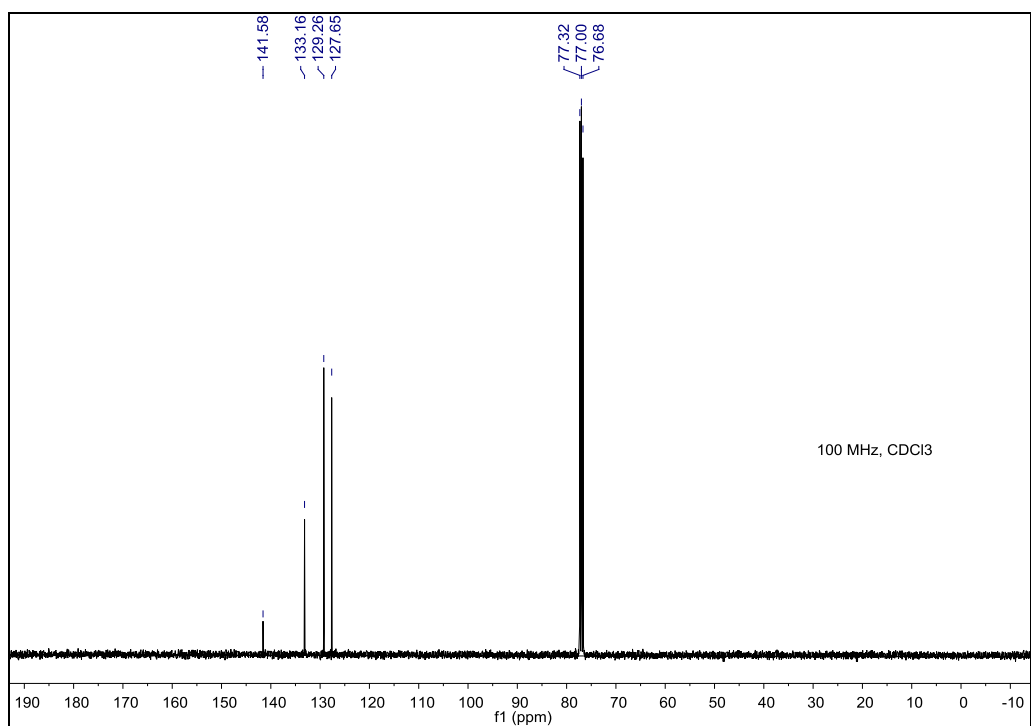
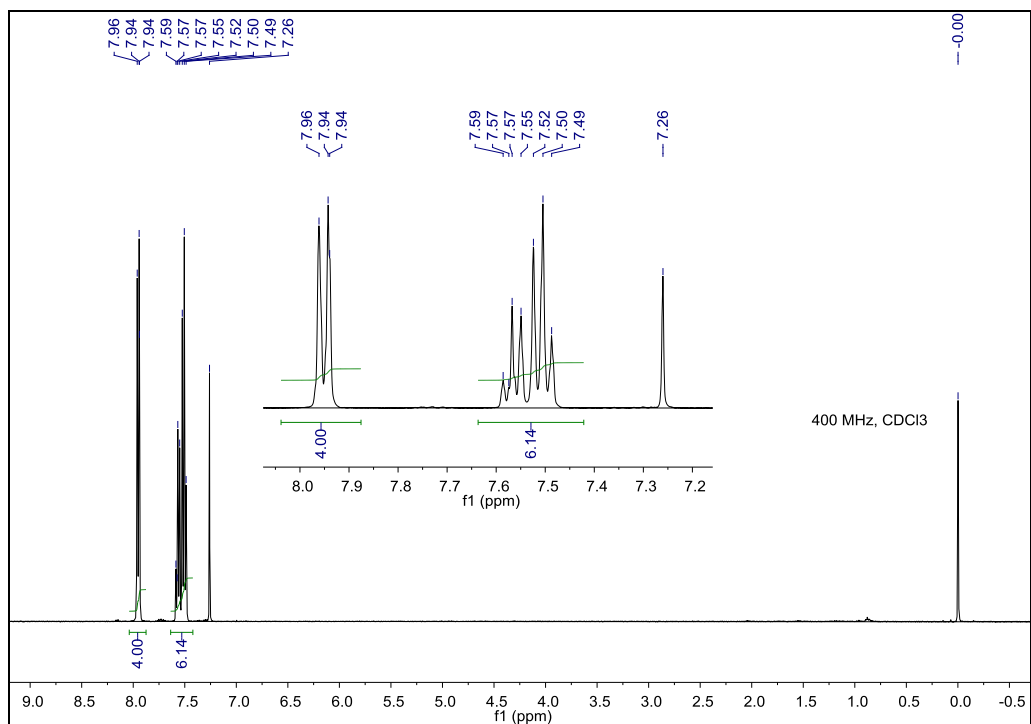
^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 144.43, 133.18, 128.19, 117.60, 117.01, 44.21.



3f: Diphenyl sulfone

^1H NMR (400 MHz,) δ (ppm): 7.96-7.94 (m, 4H), 7.59-7.49 (m, 6H).

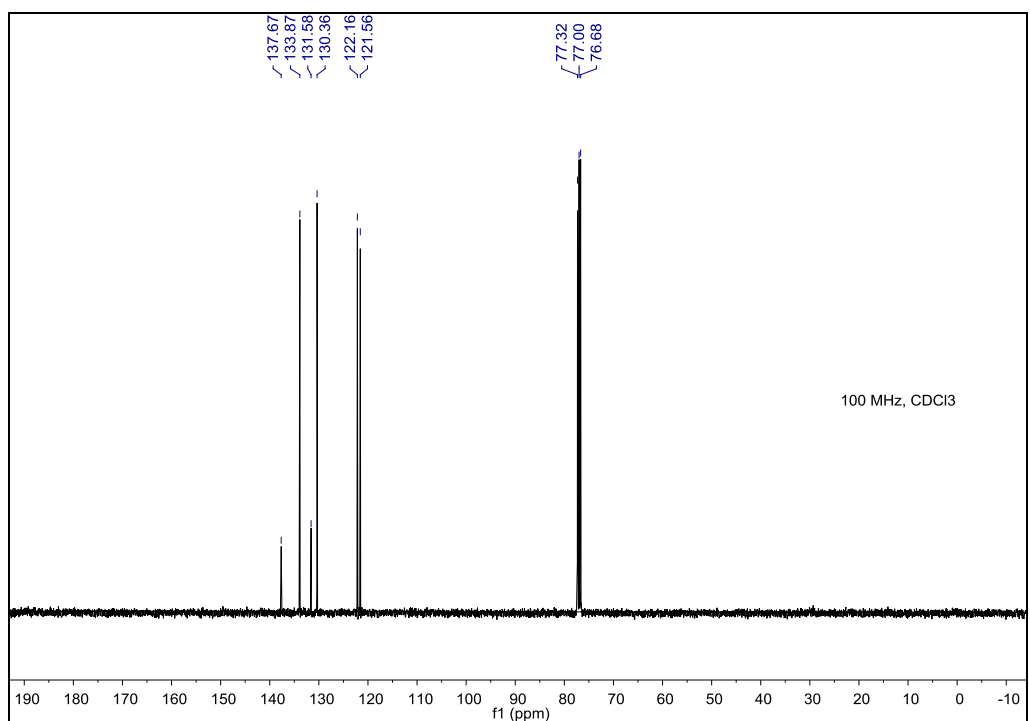
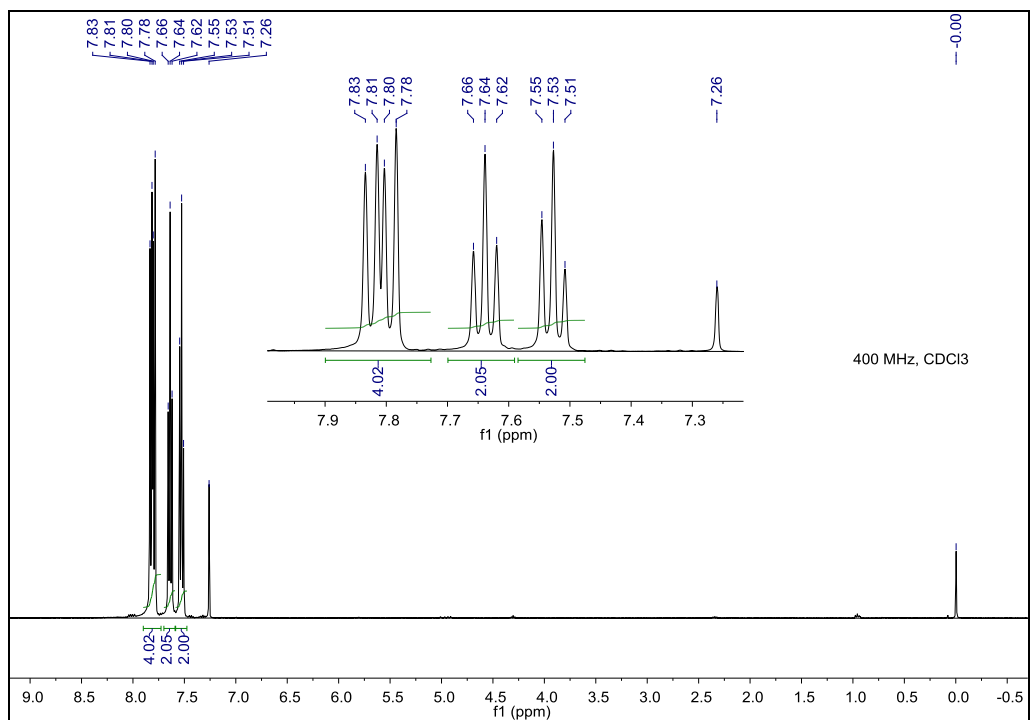
^{13}C NMR (100 MHz,) δ (ppm): 141.58, 133.16, 129.26, 127.65.



3g: Dibenzothiophene sulfone

^1H NMR (400 MHz,) δ (ppm): 7.83-7.78 (m, 4H), 7.66-7.62 (m, 2H), 7.55-7.51 (m, 2H)

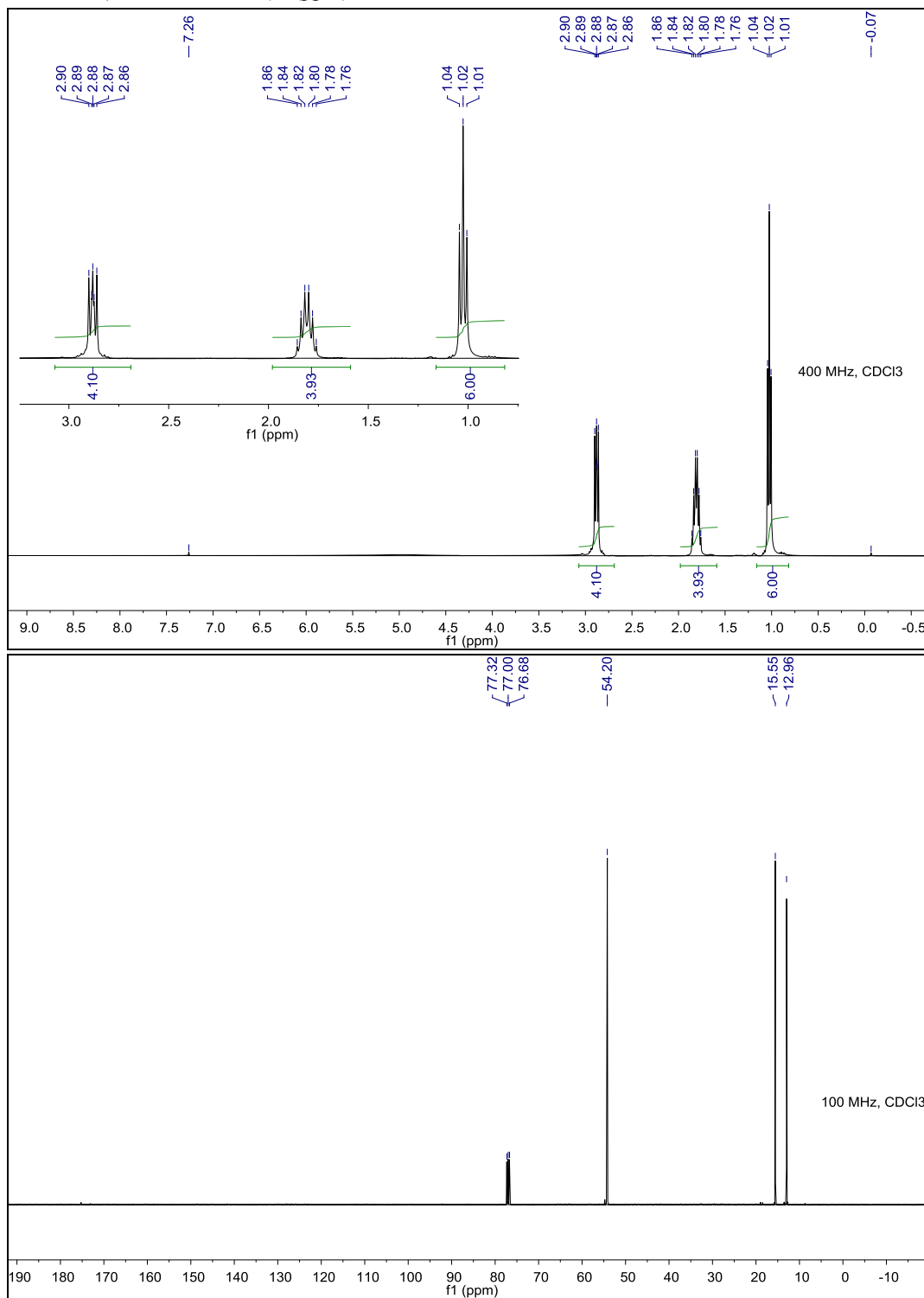
^{13}C NMR (100 MHz,) δ (ppm): 137.67, 133.87, 131.58, 130.36, 122.16, 121.56.



3h: Di(*n*-propyl) sulfone

^1H NMR (400 MHz, CDCl_3) δ (ppm): 2.90-2.86 (m, 4H), 1.86-1.76 (m, 4H), 1.02 (t, $J = 7.4$ Hz, 6H).

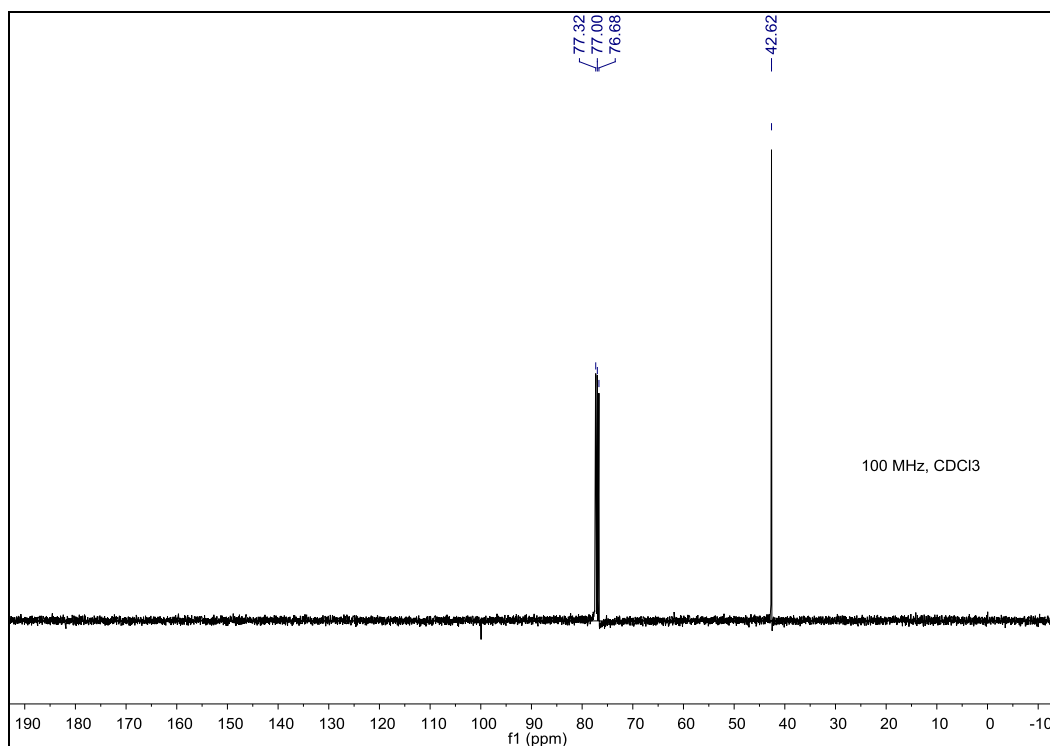
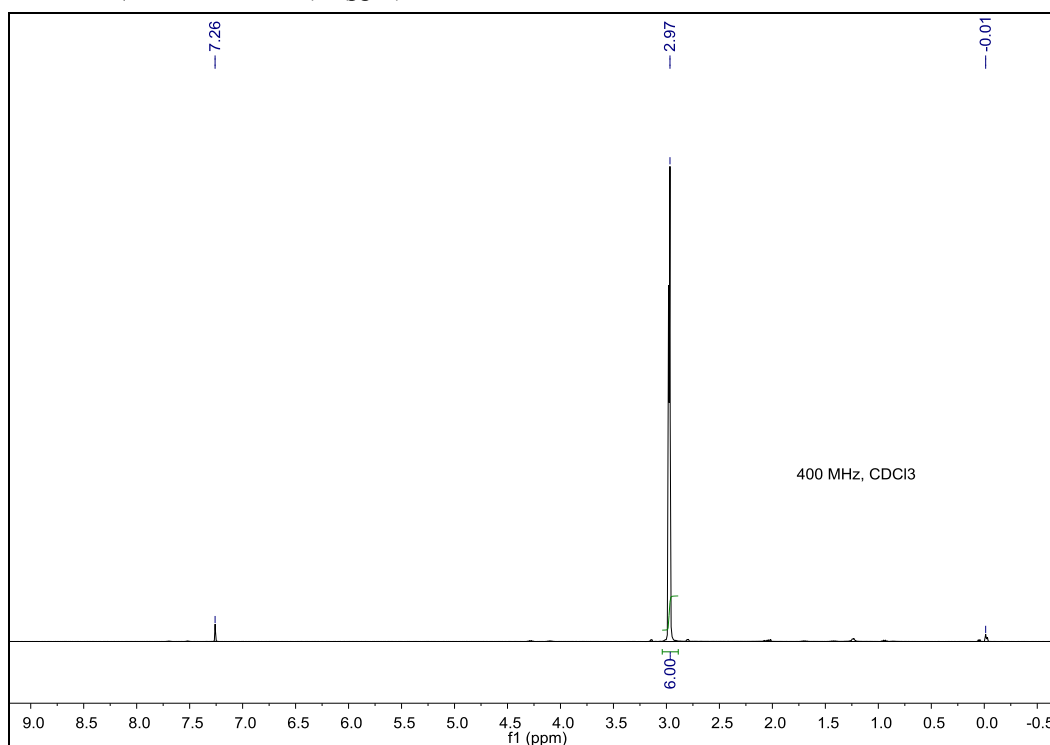
^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 54.20, 15.55, 12.96.



3i: Dimethyl sulfone

^1H NMR (400 MHz, CDCl_3) δ (ppm): 2.97 (s, 6H).

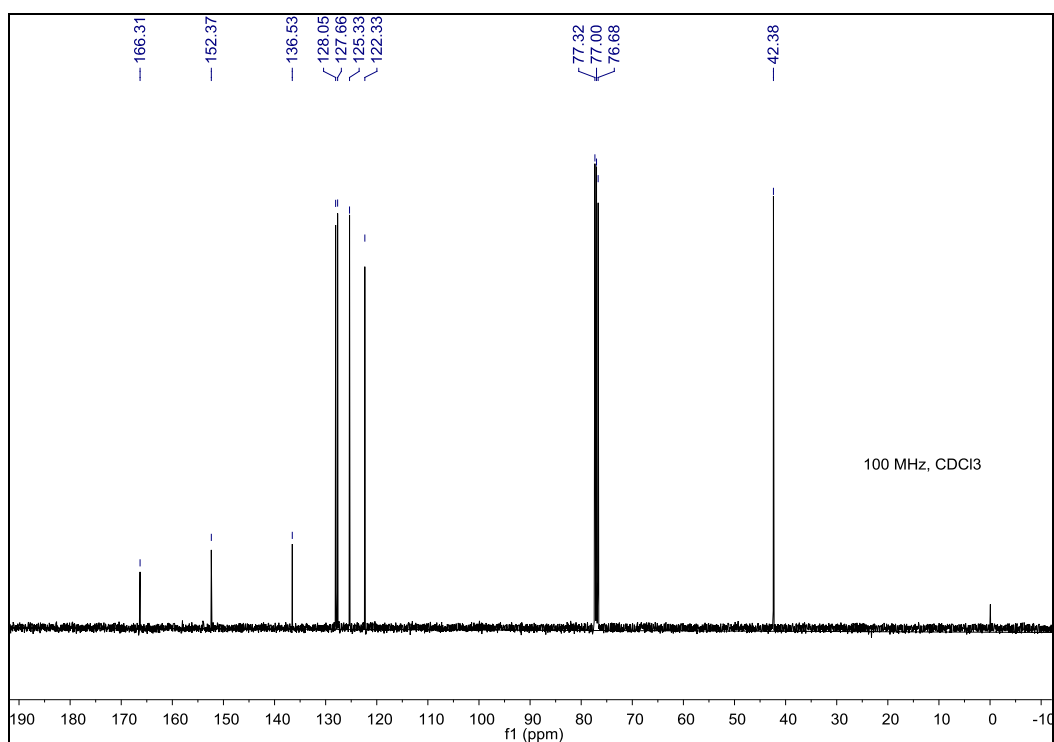
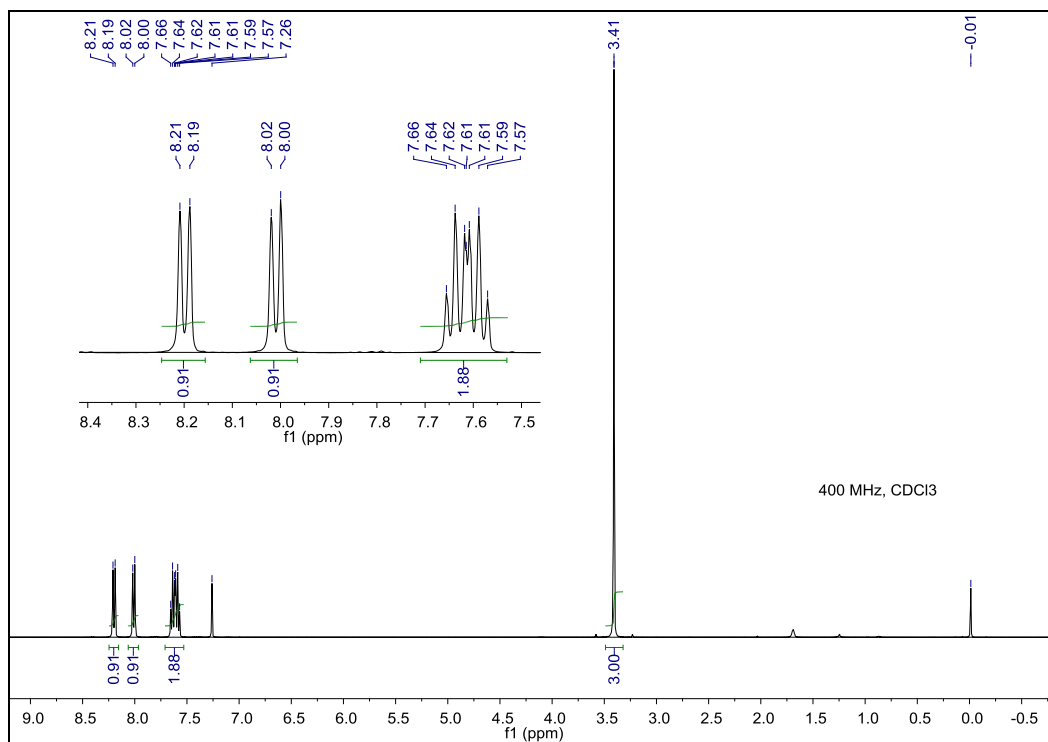
^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 42.62.



3j: 2-Methanesulfonylbenzothiazole

^1H NMR (400 MHz, CDCl_3) δ (ppm): 8.20 (d, $J = 8.3$ Hz, 1H), 8.01 (d, $J = 7.8$ Hz, 1H), 7.66-7.57 (m, 2H), 3.41 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ (ppm): 166.31, 152.37, 136.53, 128.05, 127.66, 125.33, 122.33, 42.38.

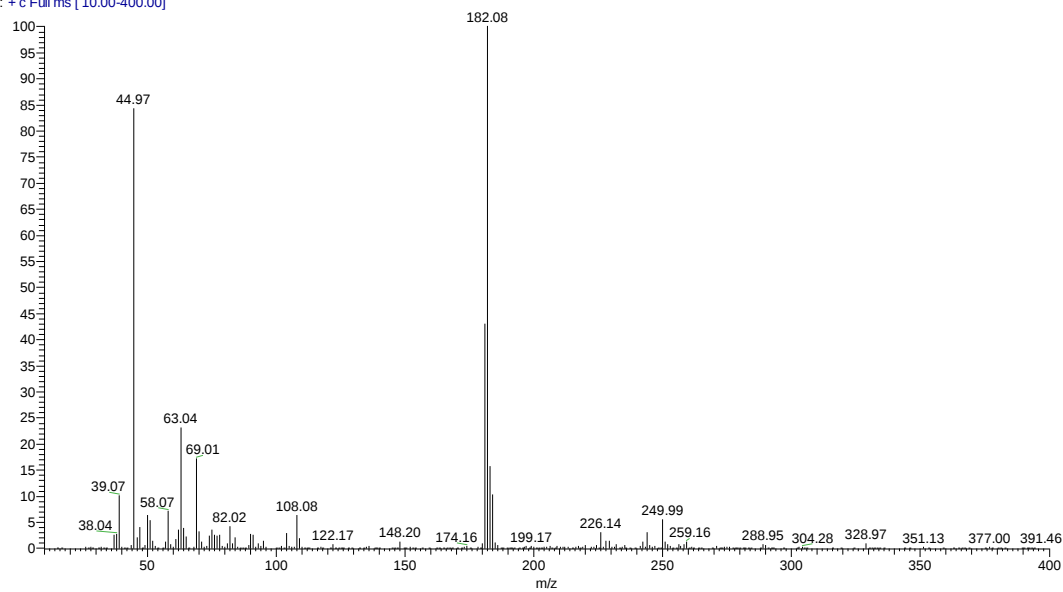


2. GC-MS Spectral Data of the Products

1j: 2-(Methylthio)benzothiazole

EI-MS, m/z (%): 182.08 (100) [M^+].

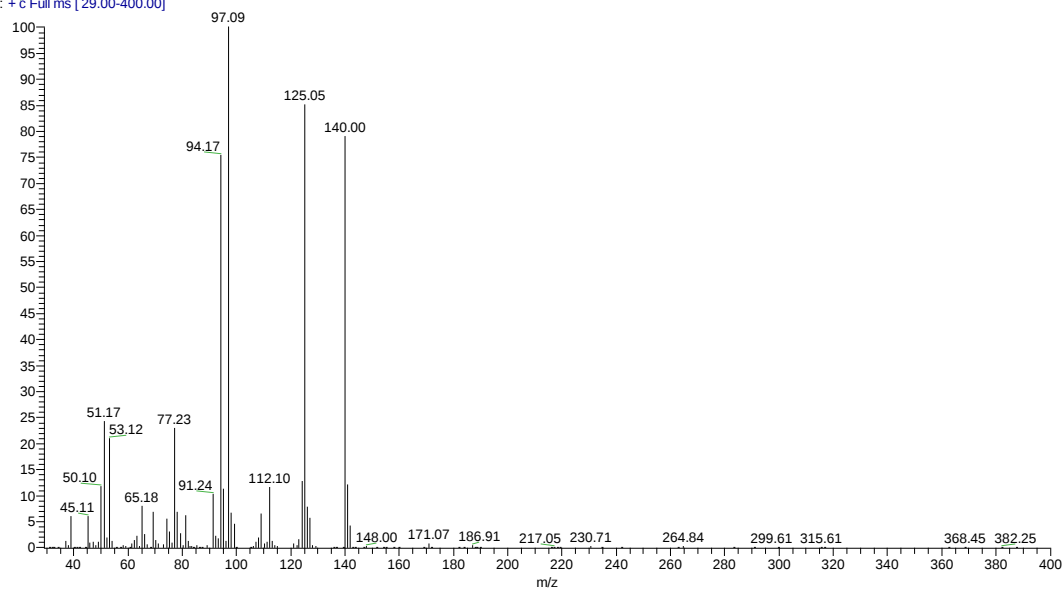
Benzo[1,2-b:4,5-b']diazole-S-Me #906 RT: 11.22 AV: 1 NL: 1.52E6
T: + c Full ms [10.00-400.00]



2a: Phenyl methyl sulfoxide

EI-MS, m/z (%): 140.00 (79) [M^+], 125.05 (85) [$M^+ - Me$].

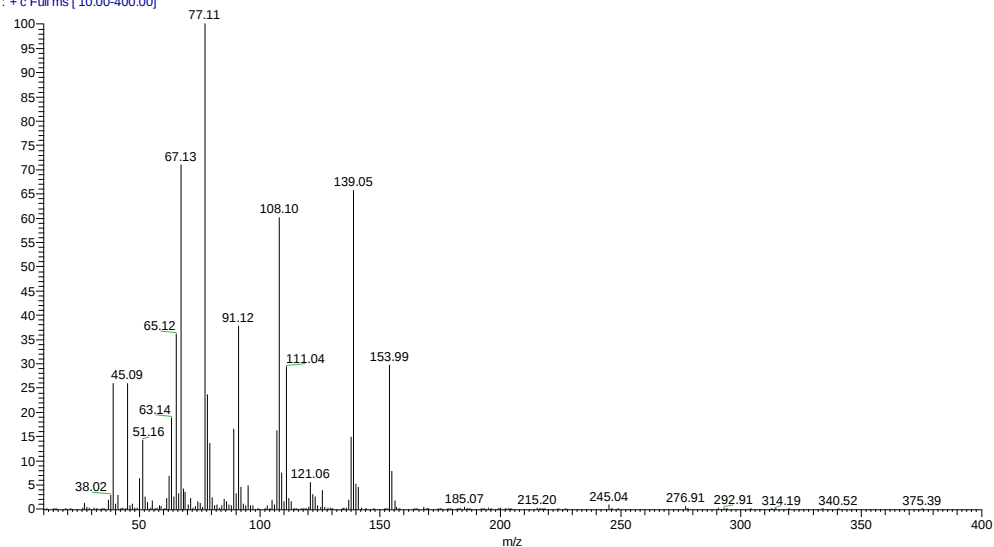
2a-Phenyl methyl sulfoxide #544 RT: 8.15 AV: 1 NL: 5.70E6
T: + c Full ms [29.00-400.00]



2b: p-Tolyl methyl sulfoxide

EI-MS, m/z (%): 153.99 (30) [M^+], 139.05 (66) [M^+-O], 108.10 (60) [$M^+-O-Me-Me$], 91.12 (37) [M^+-SOMe], 77.11 (100) [$M^+-SOMe-Me$].

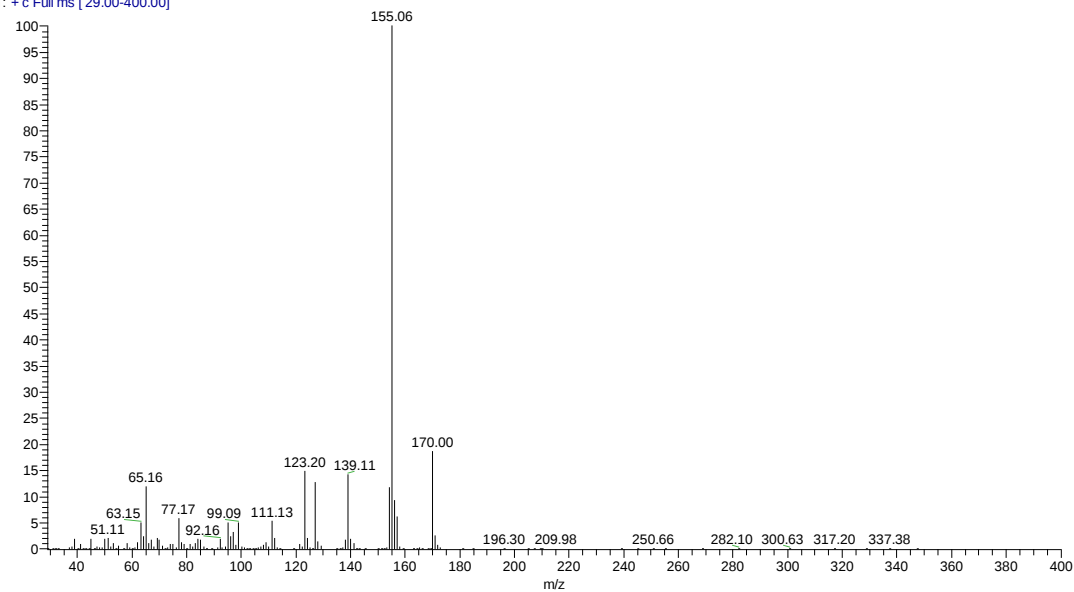
2b-p-Tolyl methyl sulfoxide #1084 RT: 12.93 AV: 1 NL: 8.97E5
T: + c Full ms [10.00-400.00]



2c: 4-Methoxyphenyl methyl sulfoxide

EI-MS, m/z (%): 170.00 (19) [M^+], 155.06 (100) [M^+-Me], 139.11 (14) [M^+-OMe], 123.20 (15) [M^+-SOMe].

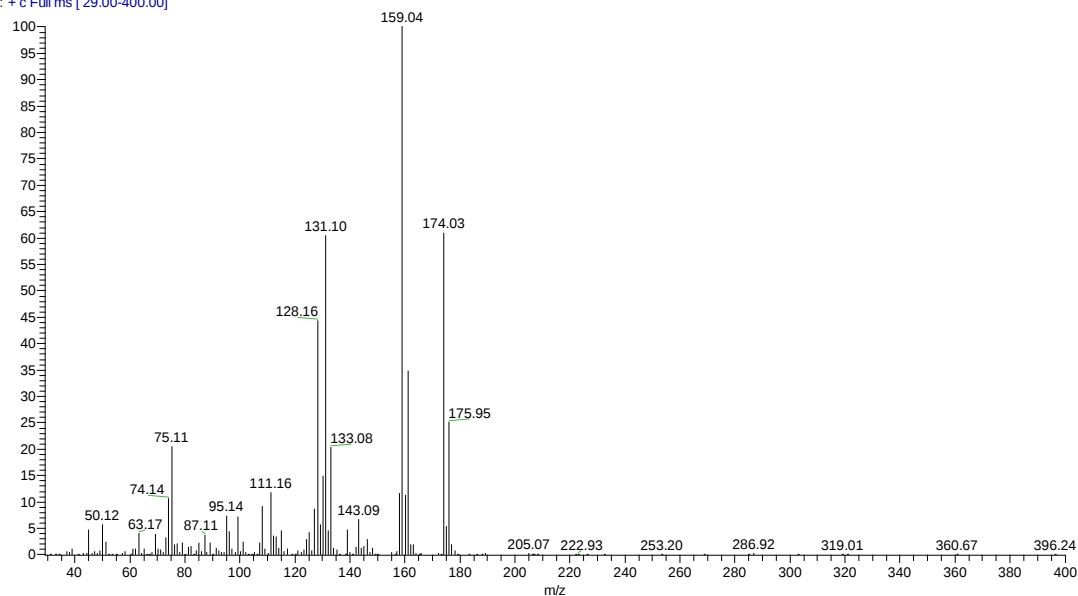
2c-4-Methoxyphenyl methyl sulfoxide #822 RT: 10.50 AV: 1 NL: 7.08E5
T: + c Full ms [29.00-400.00]



2d: *p*-Chlorophenyl methyl sulfoxide

EI-MS, m/z (%): 175.95 (25) [M^+], 174.03 (61) [M^+], 161.01 (35) [$M^+ - Me$], 159.04 (100) [$M^+ - Me$].

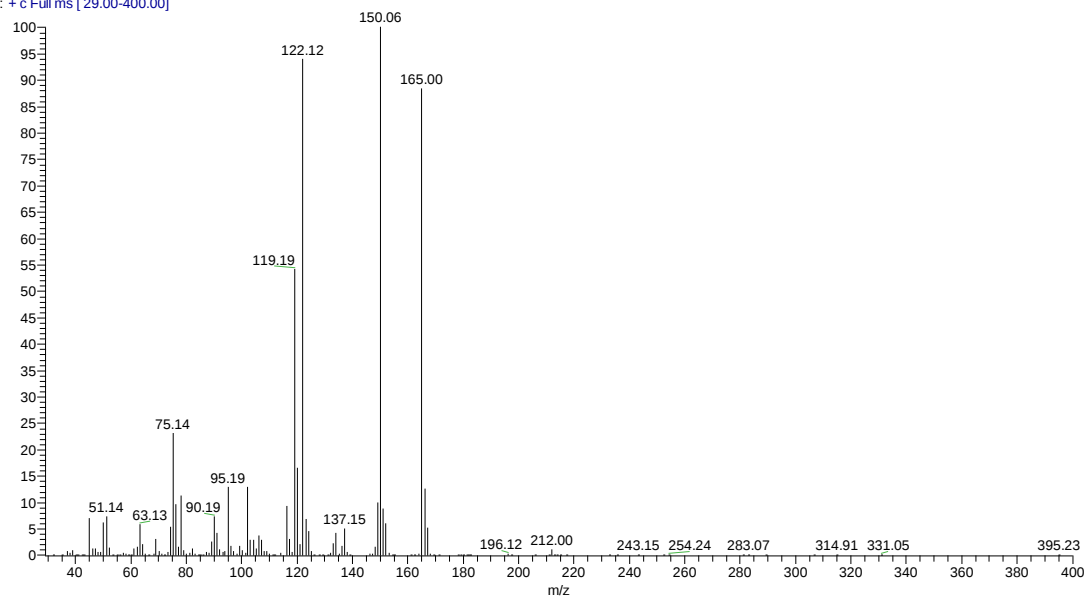
2d-*p*-Chlorophenyl methyl sulfoxide #634 RT: 9.00 AV: 1 NL: 1.42E6
T: + c Full ms [29.00-400.00]



2e: 4-Cyanophenyl methyl sulfoxide

EI-MS, m/z (%): 165.00 (88) [M^+], 150.06 (100) [$M^+ - Me$].

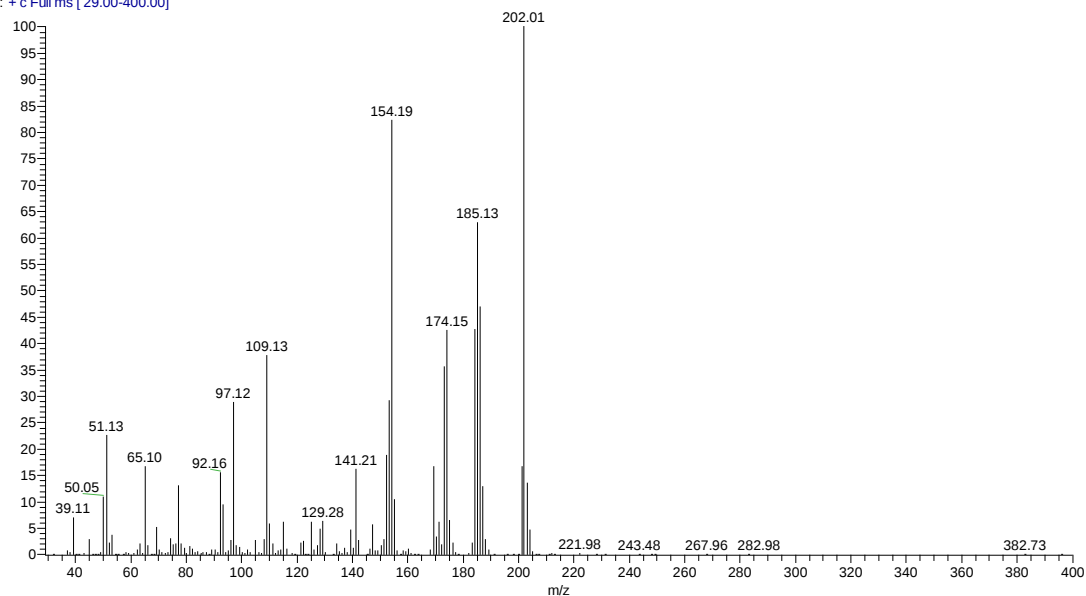
2e-4-Cyanophenyl methyl sulfoxide #799 RT: 10.12 AV: 1 NL: 3.02E6
T: + c Full ms [29.00-400.00]



2f: Diphenyl sulfoxide

EI-MS, m/z (%): 202.01 (100) [M^+], 185.13 (63) [$M^+ - O$].

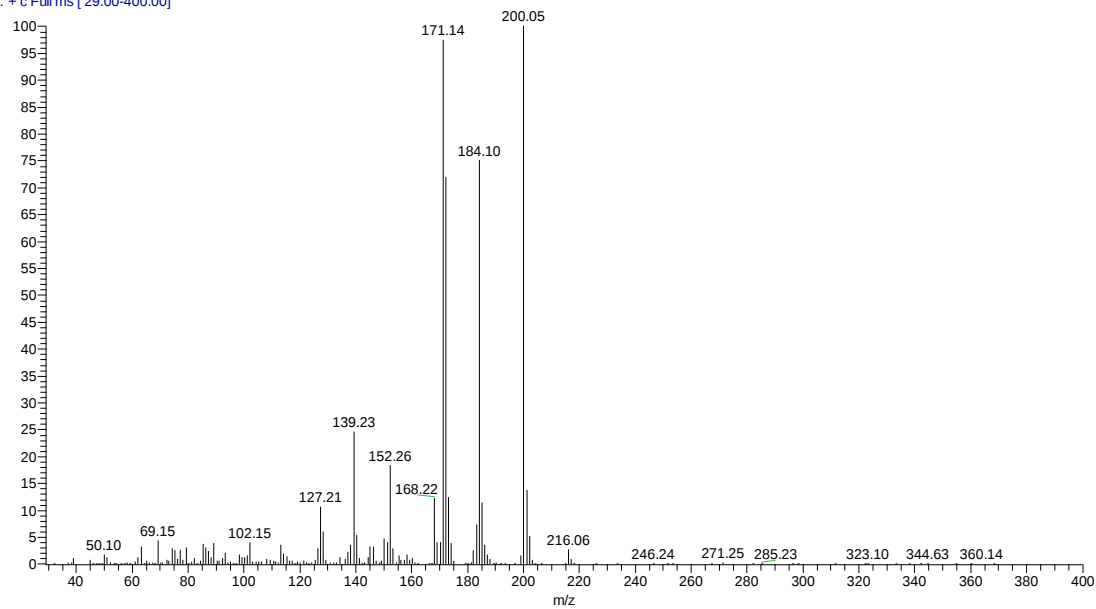
2f-Diphenyl sulfoxide #982 RT: 11.85 AV: 1 NL: 4.36E5
T: + c Full ms [29.00-400.00]



2g: Dibenzothiophene sulfoxide

EI-MS, m/z (%): 200.05 (100) [M^+], 184.10 (75) [$M^+ - O$].

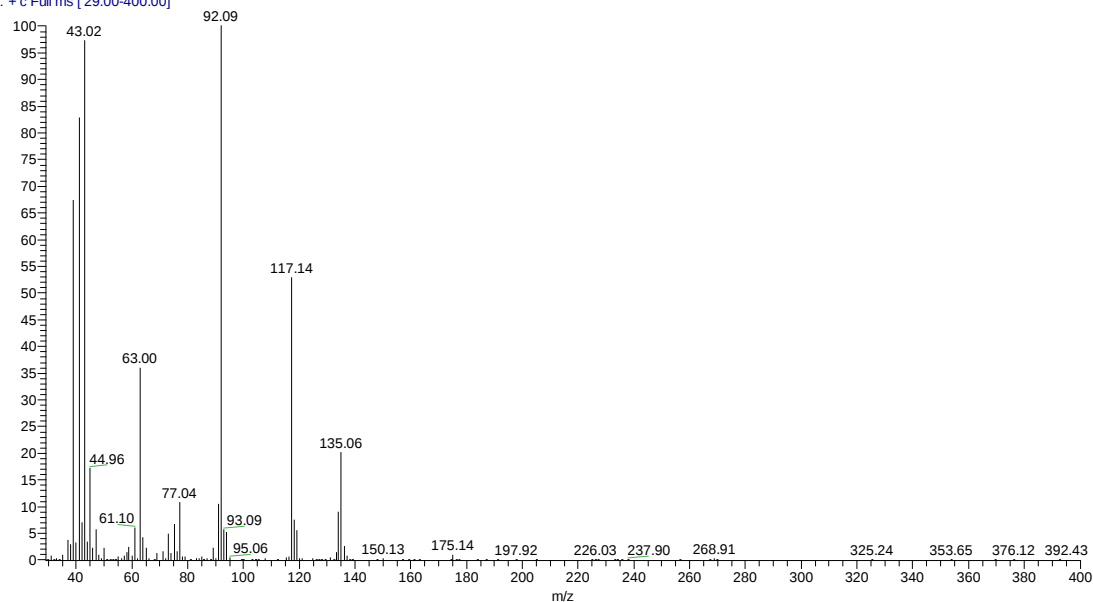
2g-Dibenzothiophene sulfoxide #1149 RT: 12.90 AV: 1 NL: 1.63E6
T: + c Full ms [29.00-400.00]



2h: Di(*n*-propyl) sulfoxide

EI-MS, *m/z* (%): 135.06 (20) [M^+], 117.14 (53) [$M^+ - O$], 92.09 (100) [$M^+ - CH_2CH_2CH_3$].

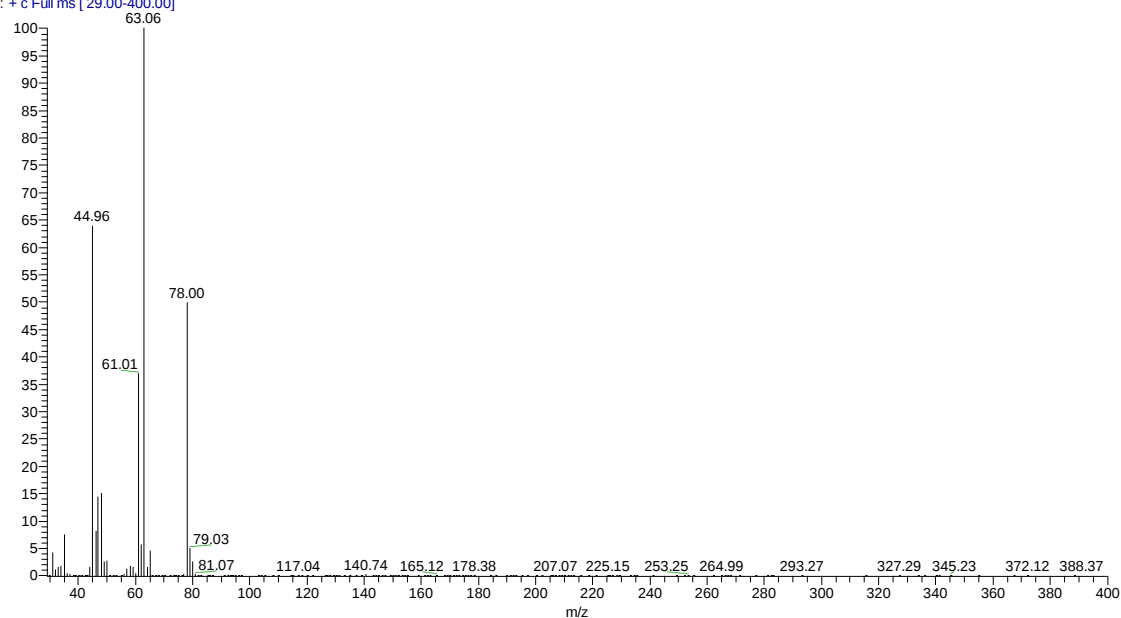
2h-Di(*n*-propyl) sulfoxide #404 RT: 6.78 AV: 1 NL: 3.37E6
T: + c Full ms [29.00-400.00]



2i: Dimethyl sulfoxide

EI-MS, *m/z* (%): 78.00 (50) [M^+], 63.06 (100) [$M^+ - Me$].

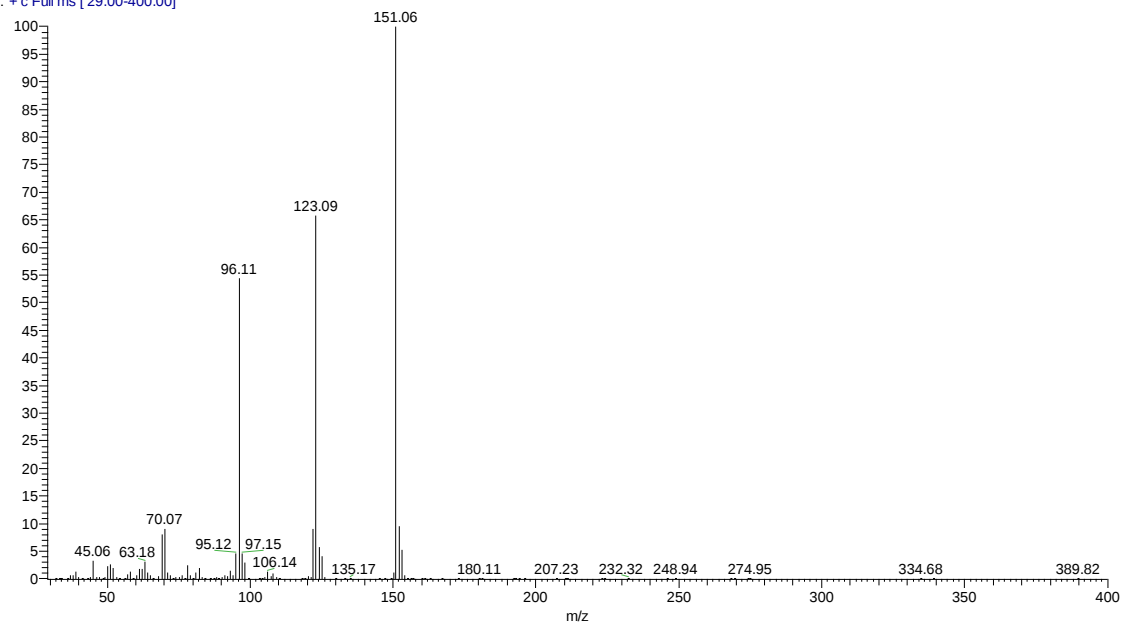
2i-Dimethyl sulfoxide #539 RT: 4.27 AV: 1 NL: 6.45E5
T: + c Full ms [29.00-400.00]



2j: 2-Benzothiazolone

EI-MS, m/z (%): 151.06 (100) [M^+], 123.09 (66) [$M^+ - CO$].

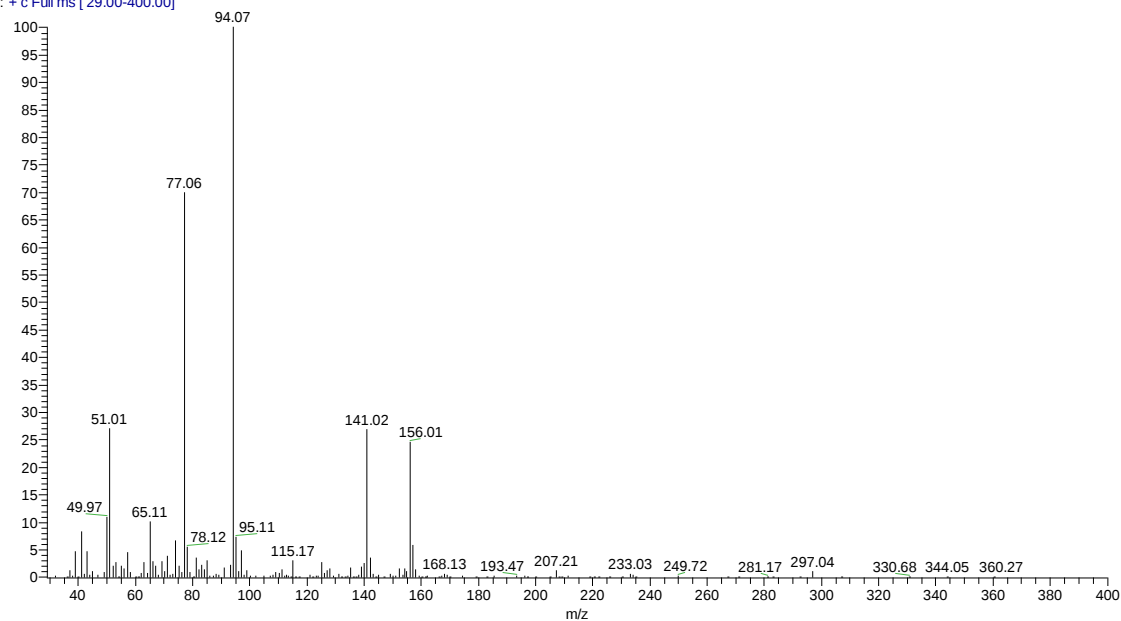
2j-2-Benzothiazolone #852 RT: 10.49 AV: 1 NL: 7.39E6
T: + c Full ms [29.00-400.00]



3a: Phenyl methyl sulfone

EI-MS, m/z (%): 156.01 (25) [M^+], 141.02 (27) [$M^+ - Me$].

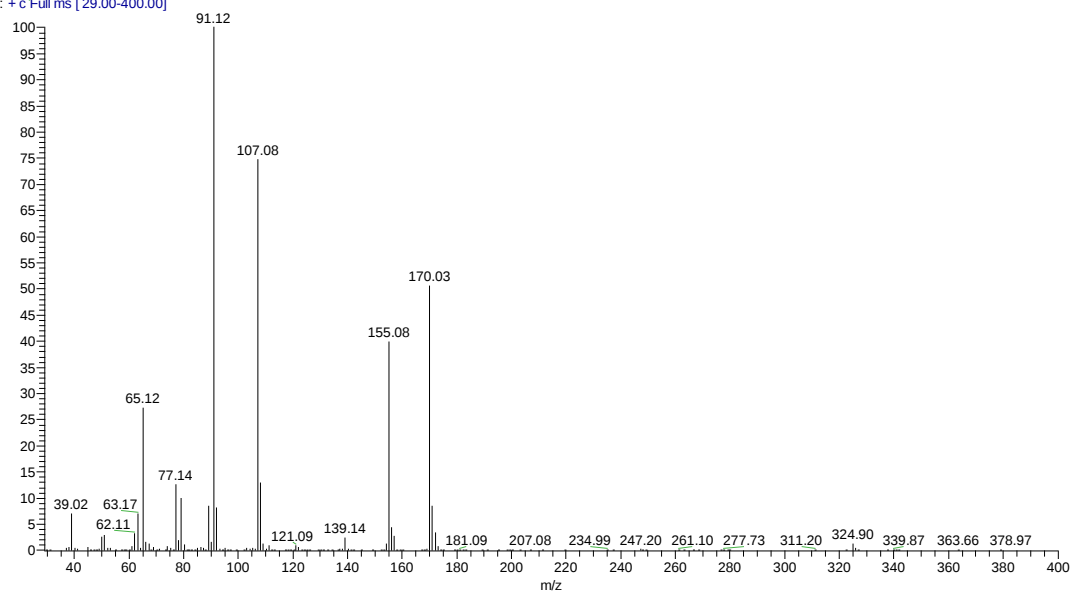
3a-Phenyl methyl sulfone #689 RT: 8.70 AV: 1 NL: 8.58E5
T: + c Full ms [29.00-400.00]



3b: *p*-Tolyl methyl sulfone

EI-MS, m/z (%): 170.03 (51) [M^+], 155.08 (40) [$M^+ - Me$], 91.12 (100) [$M^+ - SO_2Me$].

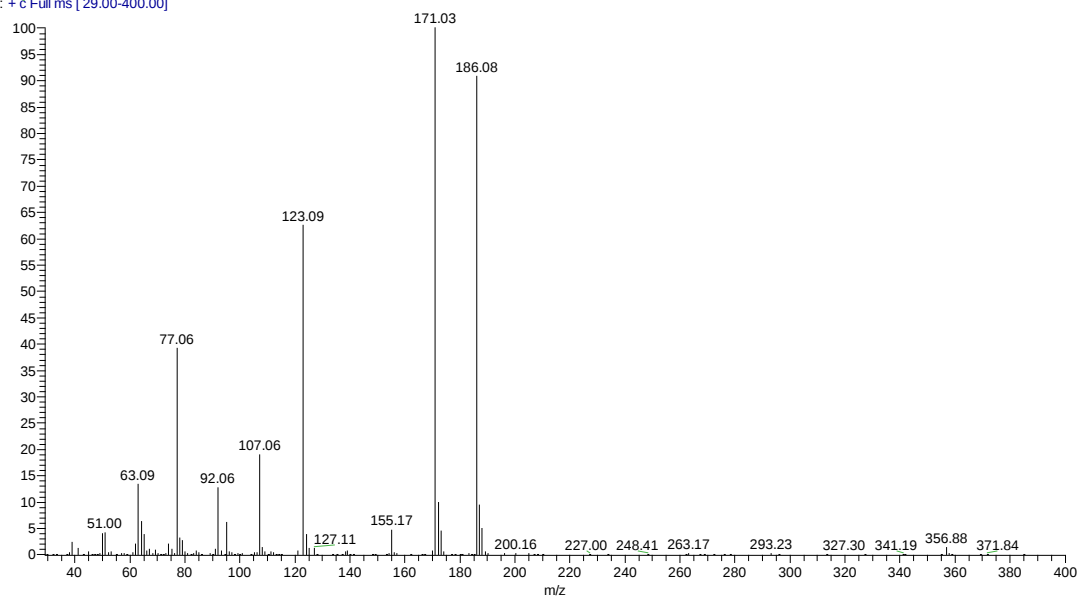
3b-*p*-Tolyl methyl sulfone #713 RT: 9.05 AV: 1 NL: 1.82E7
T: + c Full ms [29.00-400.00]



3c: 4-Methoxyphenyl methyl sulfone

EI-MS, m/z (%): 186.08 (91) [M^+], 171.03 (100) [$M^+ - OMe$], 155.17 (5) [$M^+ - Me$], 123.09 (63) [$M^+ - OMe - O - O$], 107.06 (19) [$M^+ - SO_2Me$].

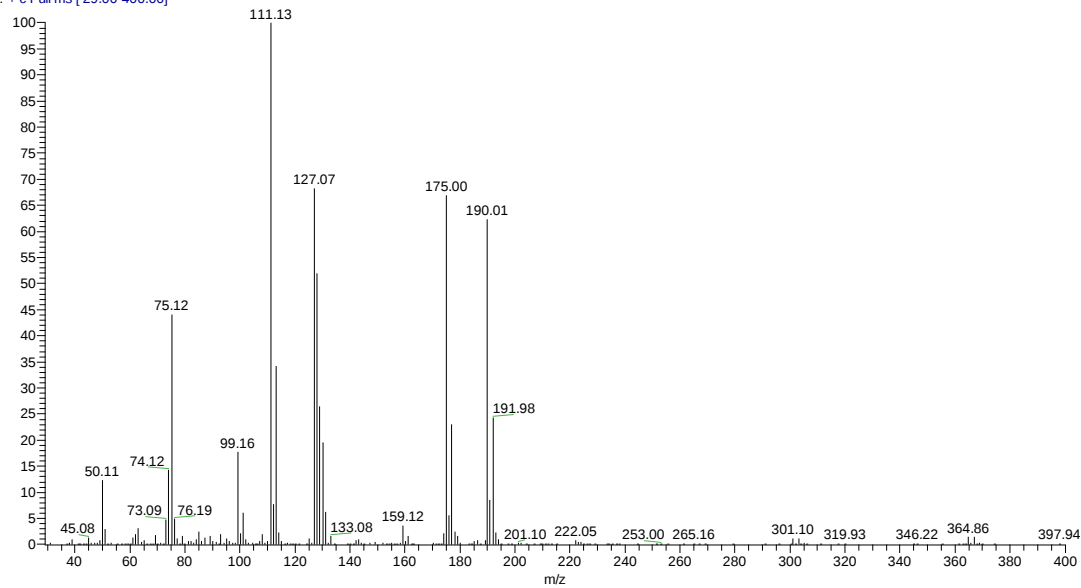
3c-4-Methoxyphenyl methyl sulfone #895 RT: 10.39 AV: 1 NL: 5.06E6
T: + c Full ms [29.00-400.00]



3d: *p*-Chlorophenyl methyl sulfone

EI-MS, m/z (%): 191.98 (24) [M^+], 190.01 (62) [M^+], 176.99 (23) [$M^+ - Me$], 175.00 (67) [$M^+ - Me$], 113.12 (34) [$M^+ - SO_2Me$], 111.13 (100) [$M^+ - SO_2Me$].

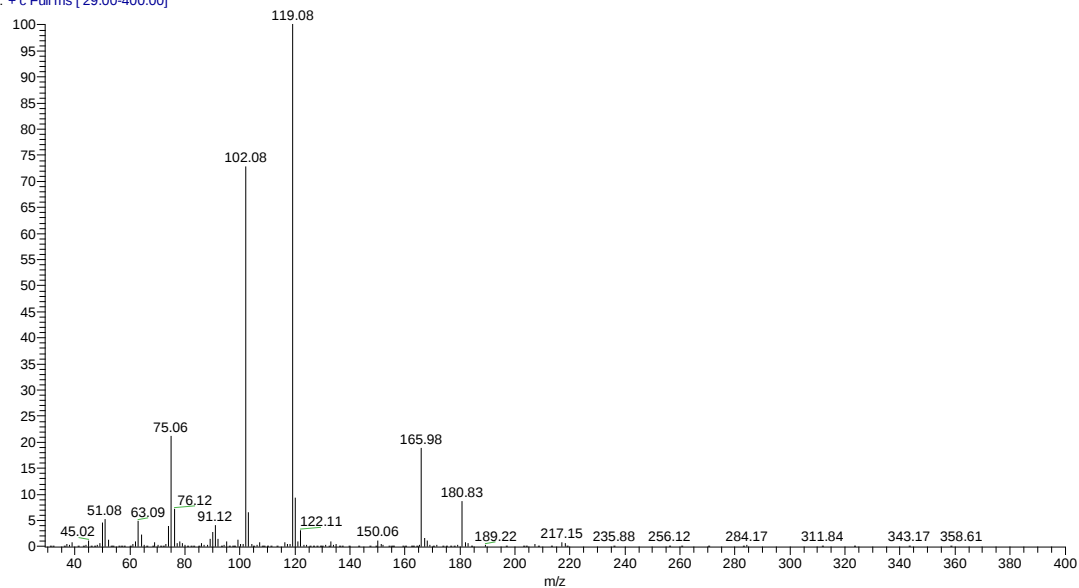
3d-*p*-Chlorophenyl methyl sulfone #766 RT: 9.34 AV: 1 NL: 1.34E7
T: + c Full ms [29.00-400.00]



3e: 4-Cyanophenyl methyl sulfone

EI-MS, m/z (%): 180.83 (9) [M^+], 165.98 (19) [$M^+ - Me$].

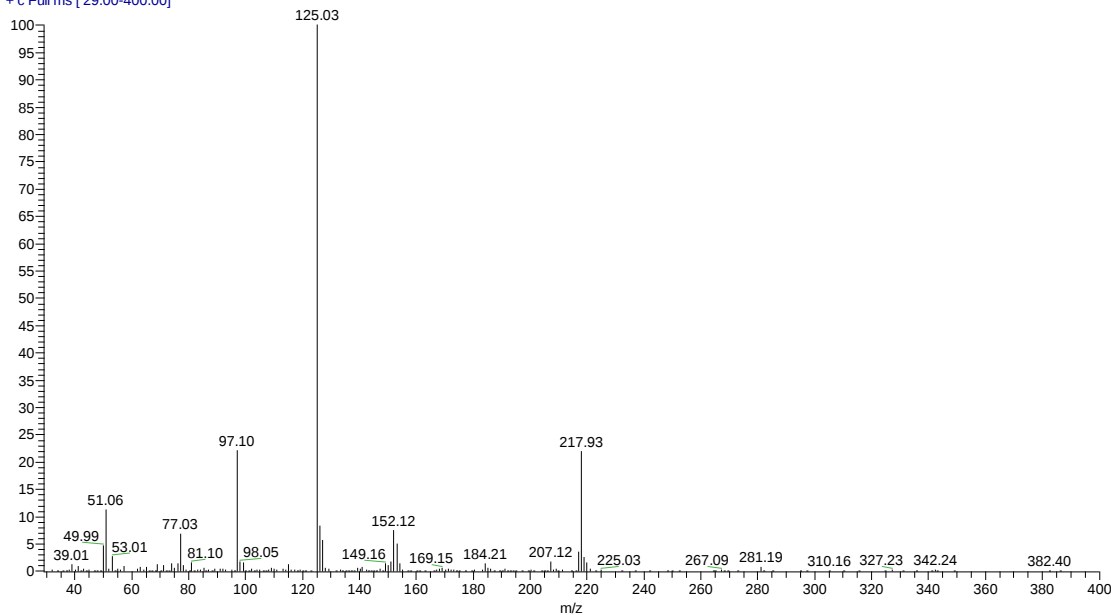
3e-4-Cyanophenyl methyl sulfone #765 RT: 9.52 AV: 1 NL: 3.28E6
T: + c Full ms [29.00-400.00]



3f: Diphenyl sulfone

EI-MS, *m/z* (%): 217.93 (20) [M^+].

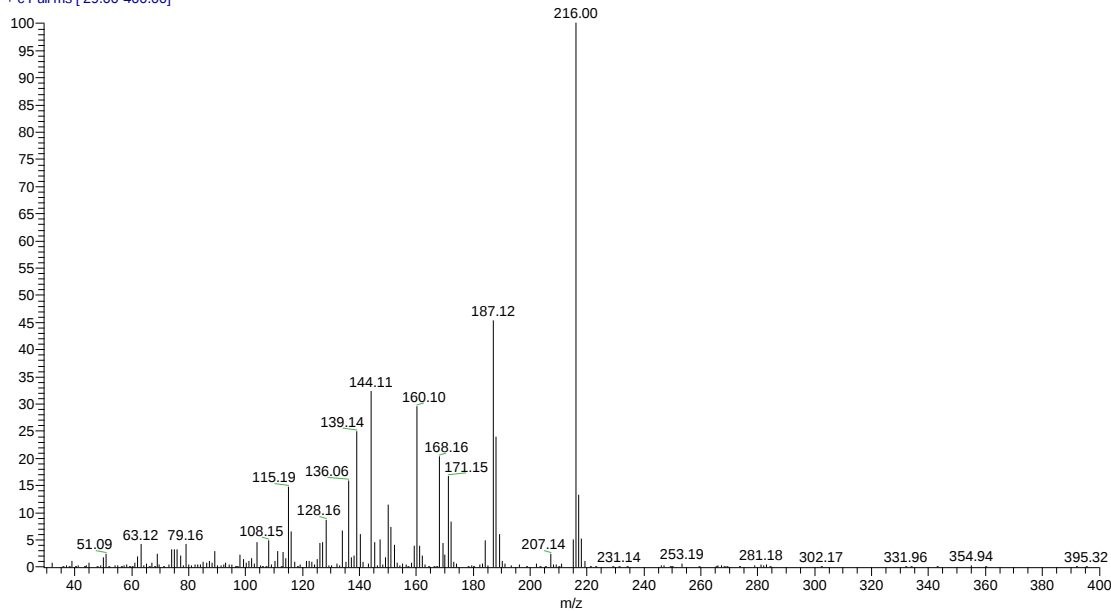
3f-Diphenyl sulfone #1079 RT: 11.65 AV: 1 NL: 6.91E5
T: + c Full ms [29.00-400.00]



3g: Dibenzothiophene sulfone

EI-MS, *m/z* (%): 216.00 (100) [M^+].

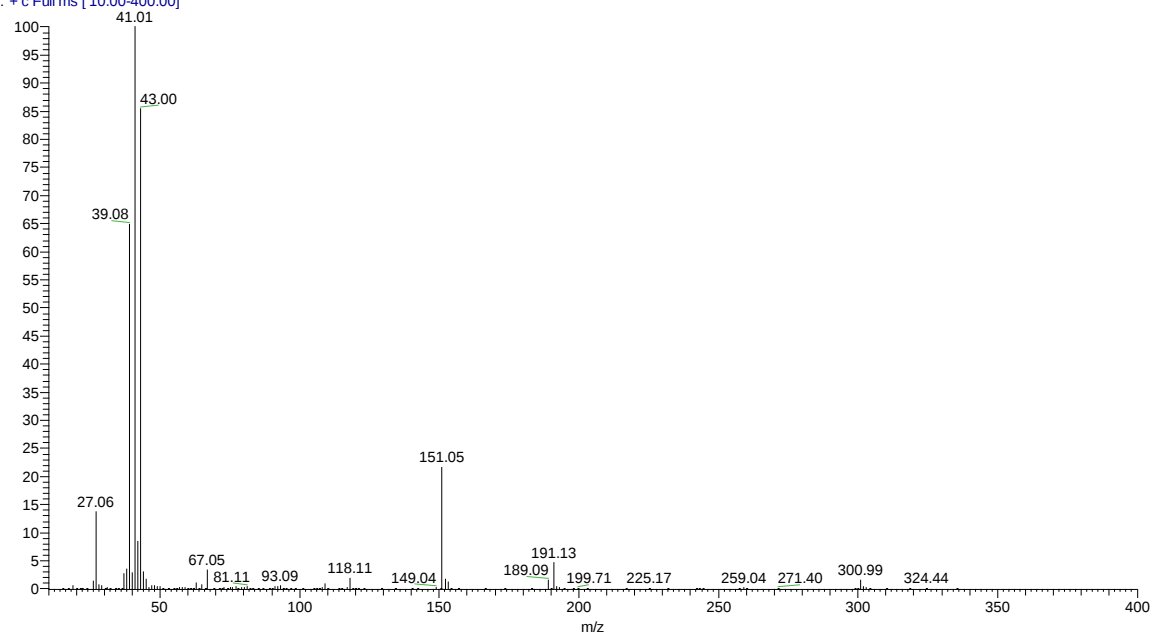
3g-Dibenzothiophene sulfone #1239 RT: 12.94 AV: 1 NL: 7.27E5
T: + c Full ms [29.00-400.00]



3h: Di(*n*-propyl) sulfone

EI-MS, *m/z* (%): 151.05 (22) [M^+], 43.00 (85) [$M^+ - SO_2CH_2CH_2CH_3$].

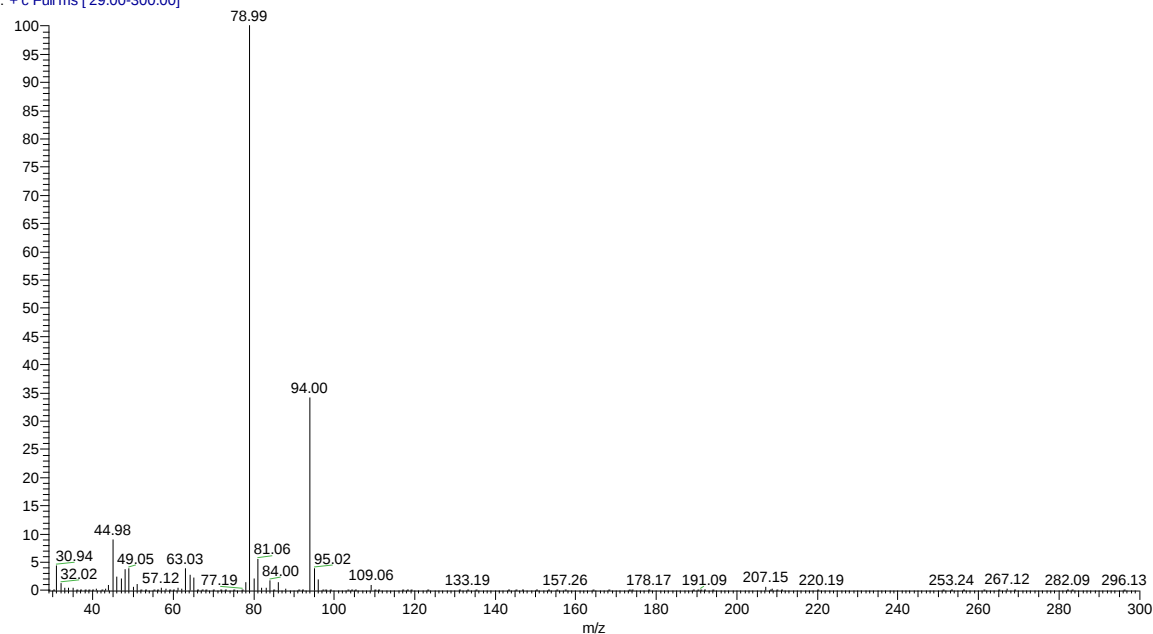
3h-Di(*n*-propyl) sulfone #519 RT: 7.98 AV: 1 NL: 3.72E6
T: + c Full ms [10.00-400.00]



3i: Dimethyl sulfone

EI-MS, *m/z* (%): 94.00 (34) [M^+], 78.99 (100) [$M^+ - Me$].

3i-Dimethyl sulfone #276 RT: 5.84 AV: 1 NL: 1.87E5
T: + c Full ms [29.00-300.00]



3j: 2-Methanesulfonylbenzothiazole
EI-MS, *m/z* (%): 212.98 (72) [M^+].

3j-2-methanesulfonylbenzothiazole #1050 RT: 11.93 AV: 1 NL: 6.45E5
T: + c Full ms [29.00-400.00]

