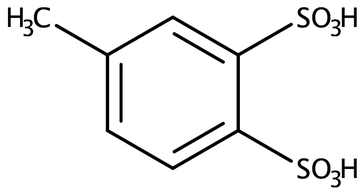
Electronic Supplementary Material (ESI) for New Journal of Chemistry.

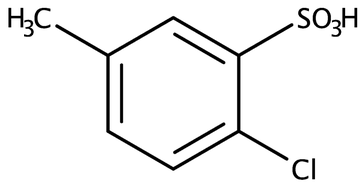
4-methyl-1,2-benzenedisulfonic acid (BMDSA)

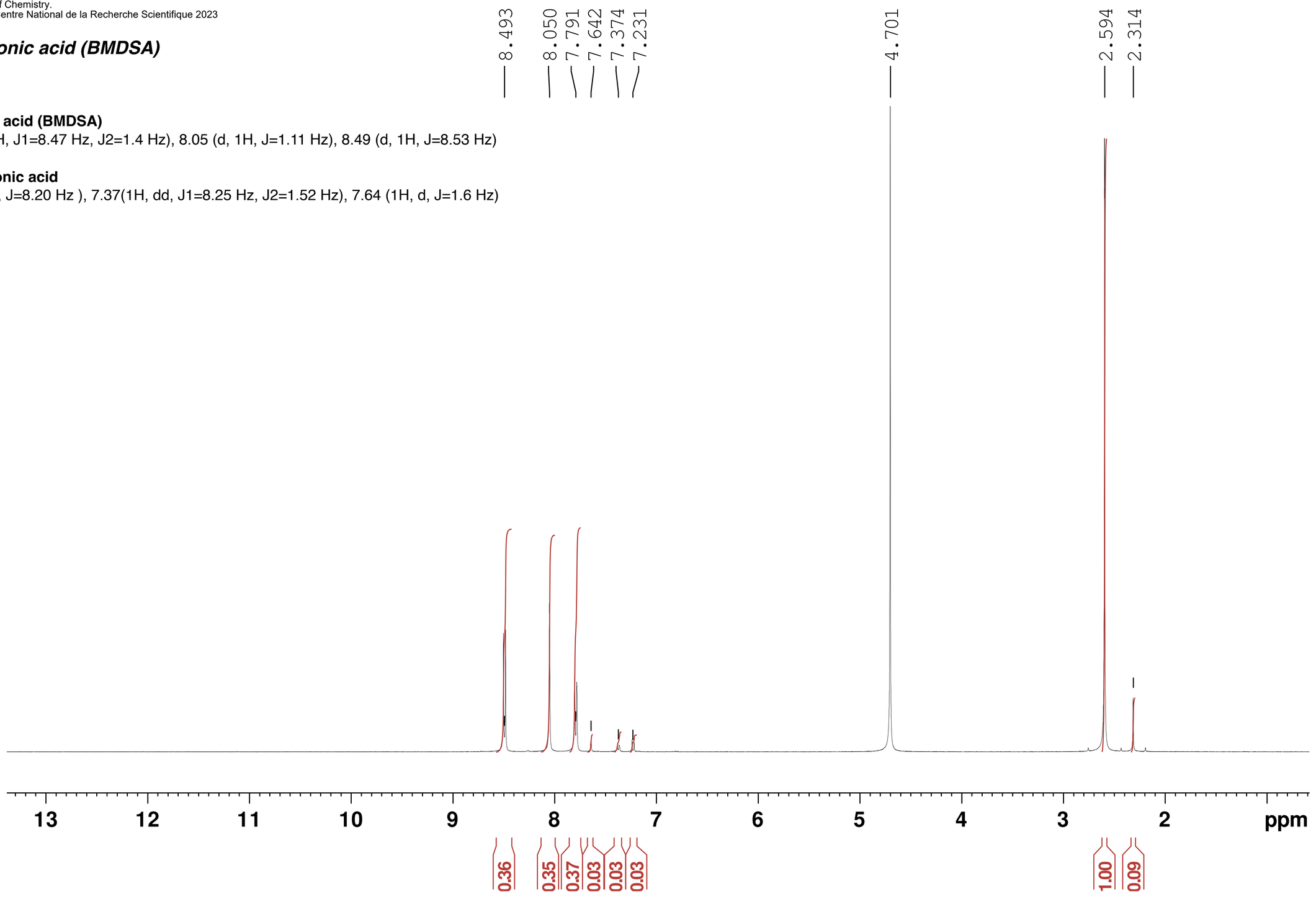
^{1}H NMR (400 MHz, D_2O):

4-methyl-1,2-benzenedisulfonic acid (BMDSA)
δ, ppm - 2.59 (s, 3H), 7.79 (dd, 1H, J1=8.47 Hz, J2=1.4 Hz), 8.05 (d, 1H, J=1.11 Hz), 8.49 (d, 1H, J=8.53 Hz)

2-chloro-5-methyl-benzenesulfonic acid
δ, ppm - 2.31 (3H, s), 7.23 (1H, d, J=8.20 Hz), 7.37(1H, dd, J1=8.25 Hz, J2=1.52 Hz), 7.64 (1H, d, J=1.6 Hz)





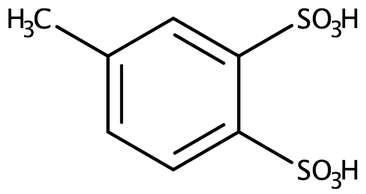


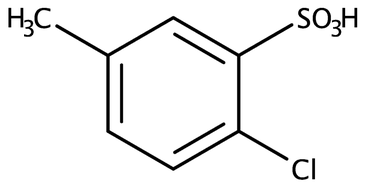
4-methyl-1,2-benzenedisulfonic acid (BMDSA)

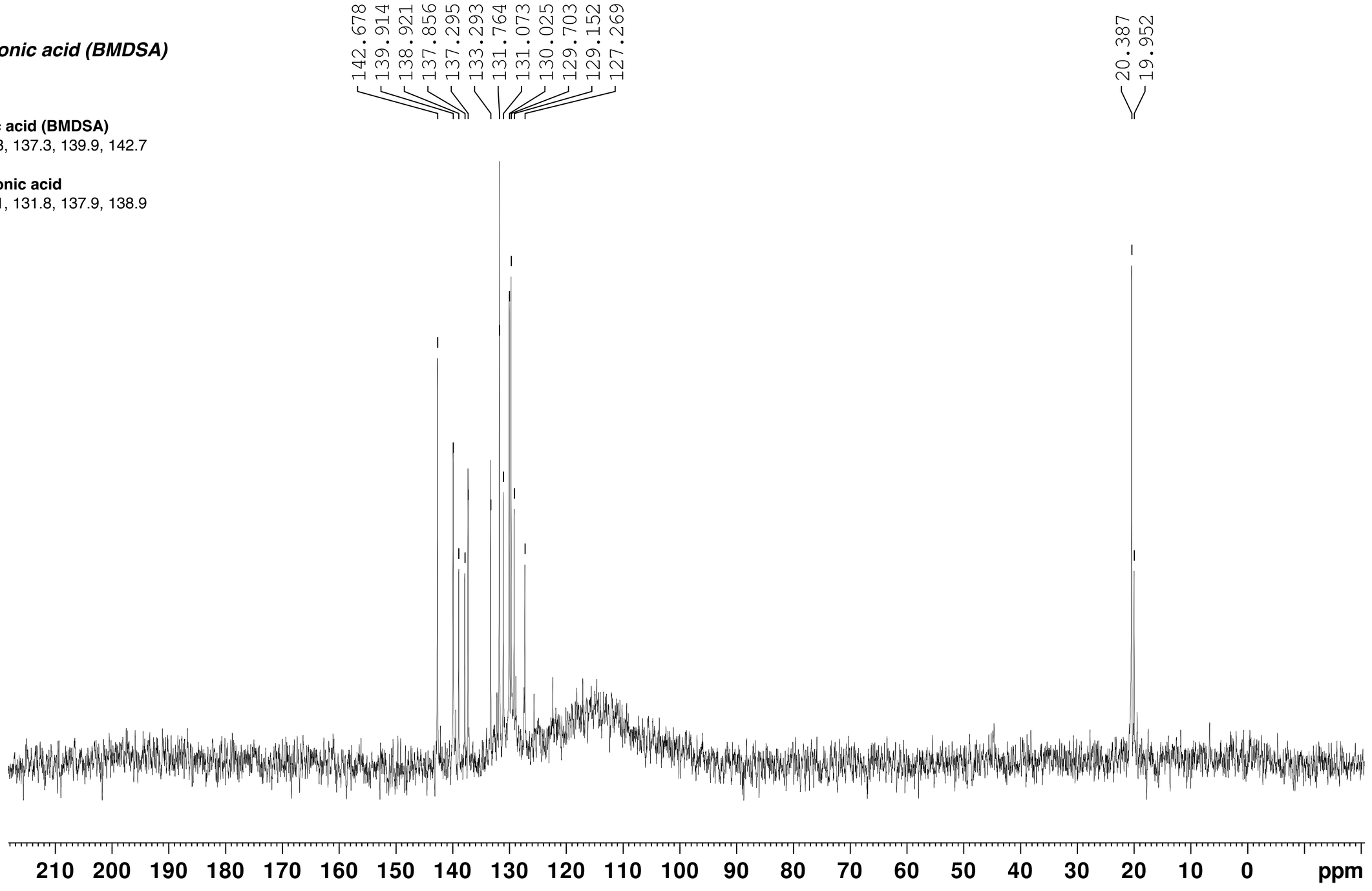
^{13}C NMR (100 MHz, D_2O):

4-methyl-1,2-benzenedisulfonic acid (BMDSA)
δ, ppm - 20.4, 129.7, 130.0, 133.3, 137.3, 139.9, 142.7

2-chloro-5-methyl-benzenesulfonic acid
δ, ppm - 20.0, 127.3, 129.1, 131.1, 131.8, 137.9, 138.9



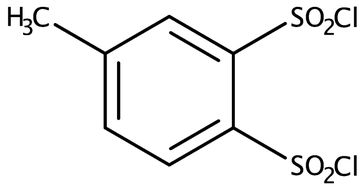


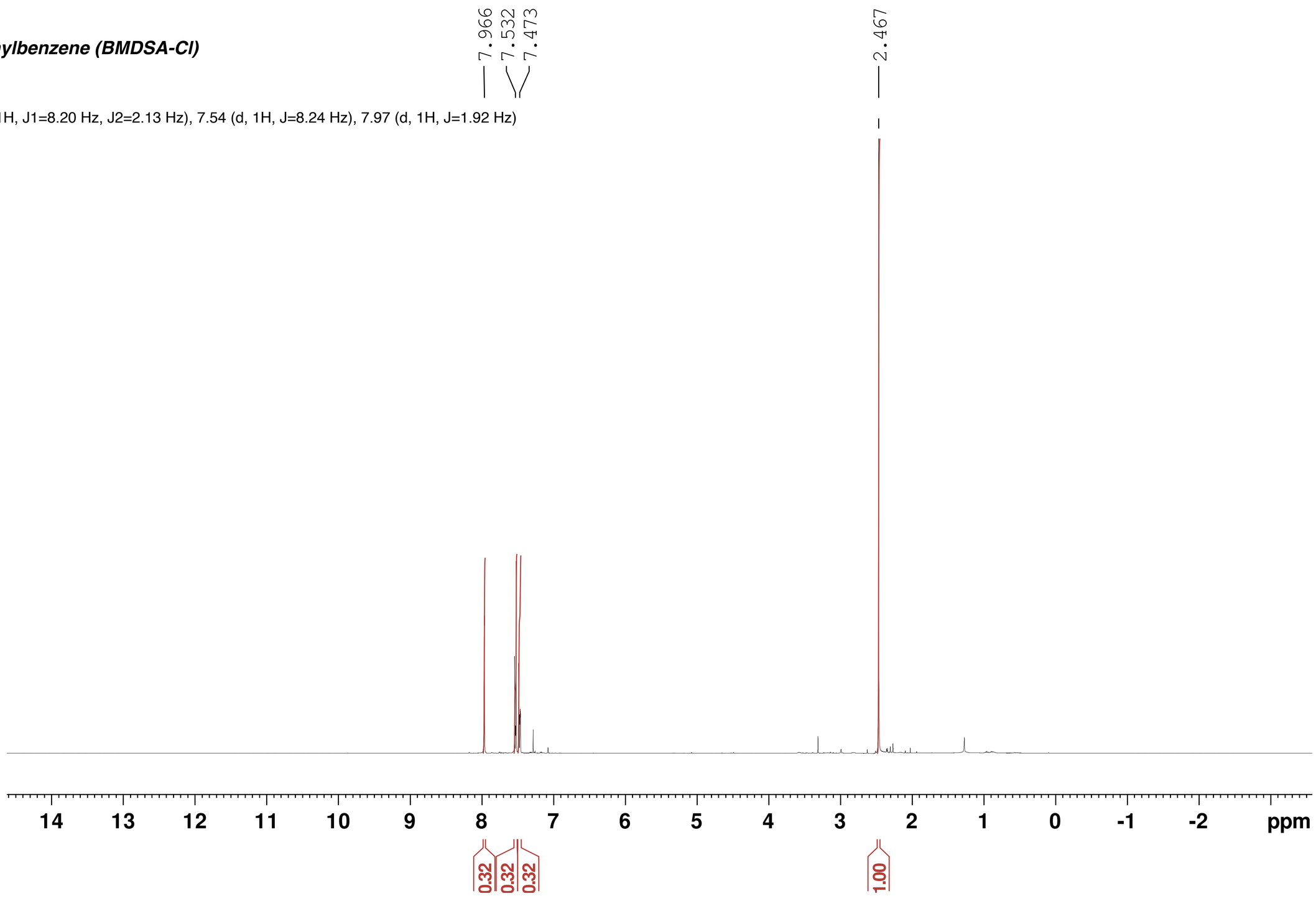


4-methyl-1,2-dichlorosulfonylbenzene (BMDSA-Cl)

^{1}H NMR (400 MHz, $CDCl_3$):

δ, ppm - 2.47 (s, 3H), 7.47 (dd, 1H, J1=8.20 Hz, J2=2.13 Hz), 7.54 (d, 1H, J=8.24 Hz), 7.97 (d, 1H, J=1.92 Hz)

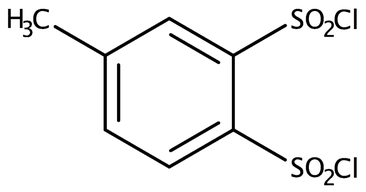


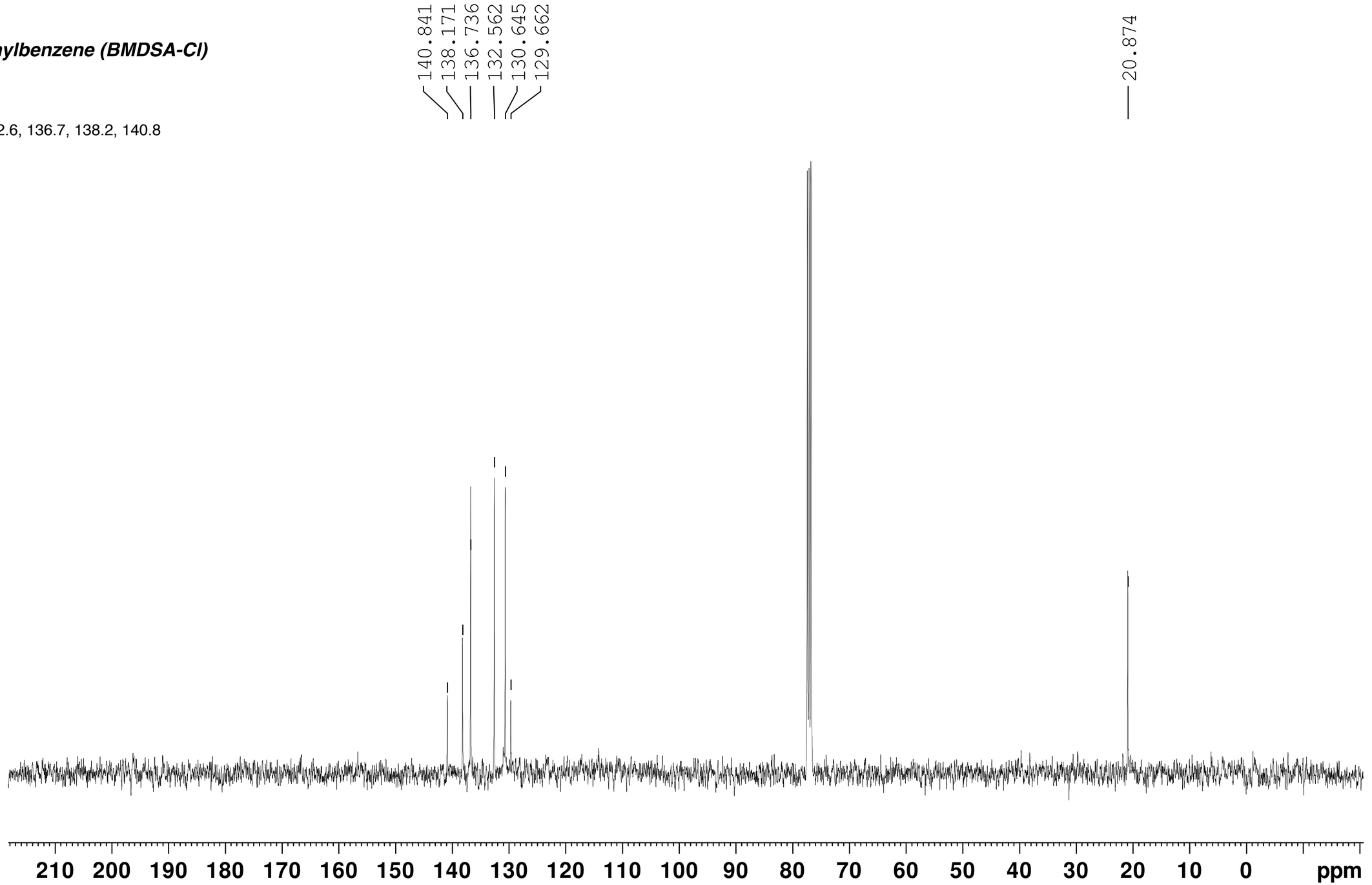


4-methyl-1,2-dichlorosulfonylbenzene (BMDSA-Cl)

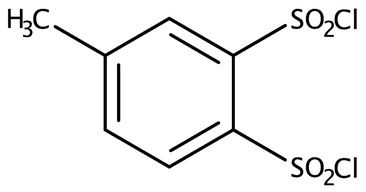
^{13}C NMR (100 MHz, $CDCl_3$):

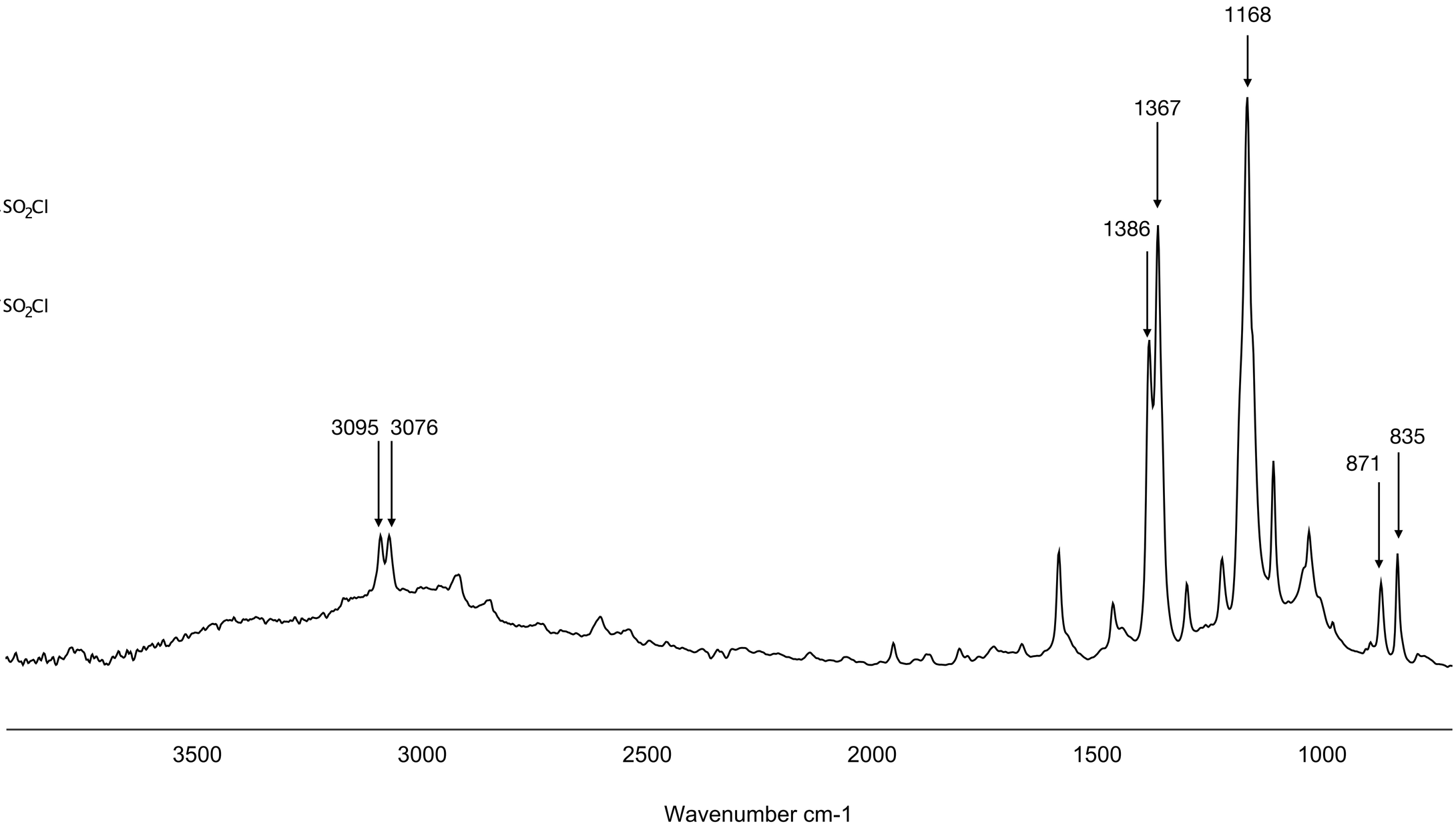
δ, ppm - 20.9, 129.7, 130.6, 132.6, 136.7, 138.2, 140.8





4-methyl-1,2-dichlorosulfonylbenzene (BMDSA-Cl)
FTIR





4-methyl-N-(p-methyl)-benzene-1,2-disulfonimide (DSI-Me)

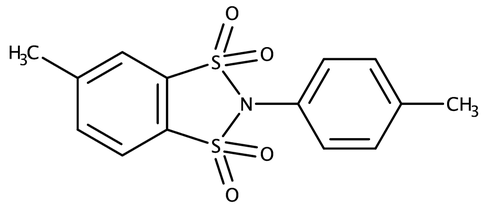
Melting point 198.6 °C

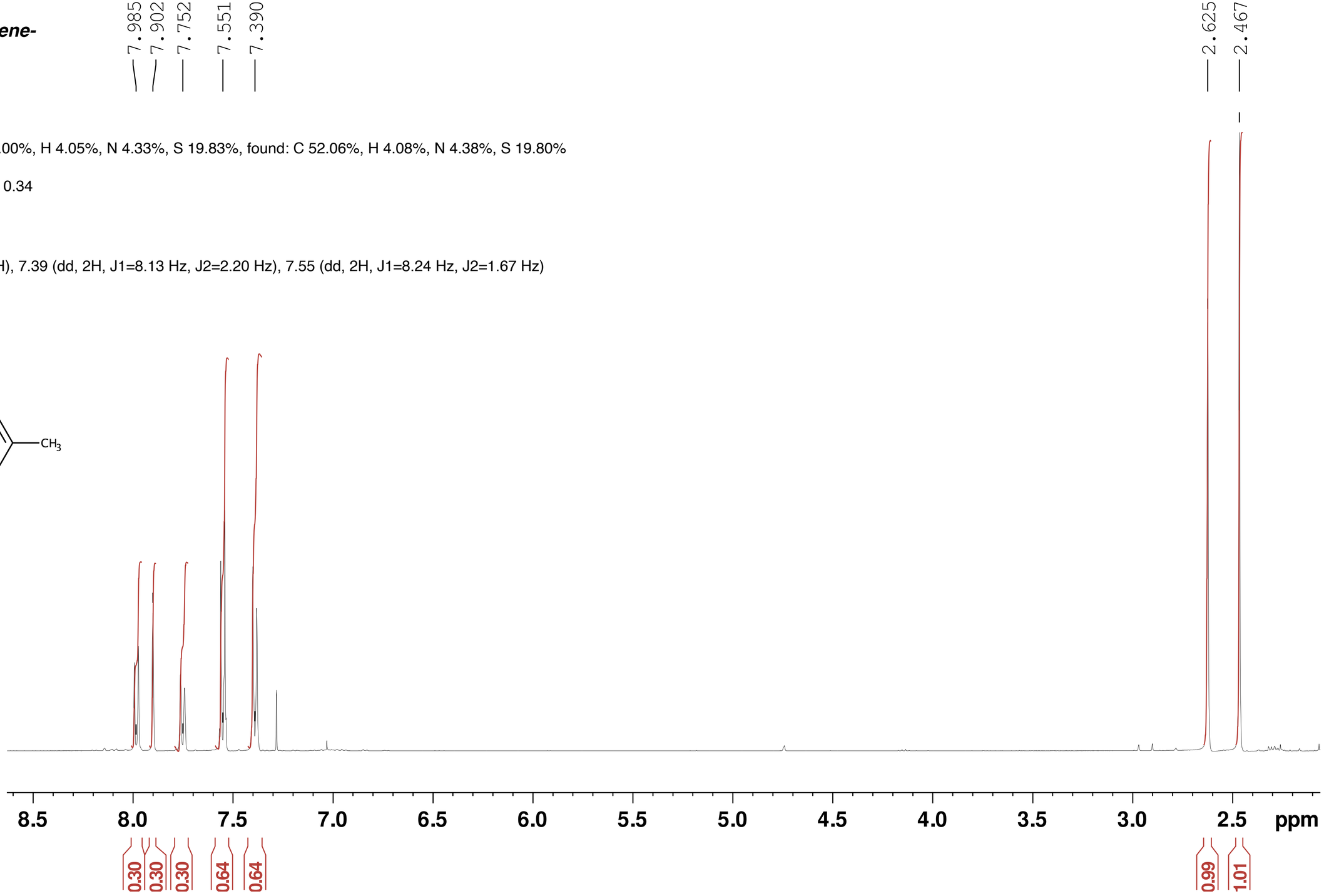
Elemental analysis:
calculated for C14H13NO4S2: C 52.00%, H 4.05%, N 4.33%, S 19.83%, found: C 52.06%, H 4.08%, N 4.38%, S 19.80%

TLC hexane : ethyl acetate 5:2, R_f = 0.34

^{1}H NMR (400 MHz, $CDCl_3$):

δ, ppm - 2.46 (s, 3H), 2.62 (s, 3H), 7.39 (dd, 2H, J1=8.13 Hz, J2=2.20 Hz), 7.55 (dd, 2H, J1=8.24 Hz, J2=1.67 Hz)

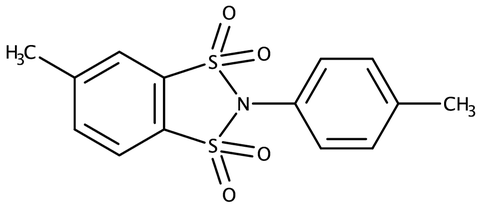


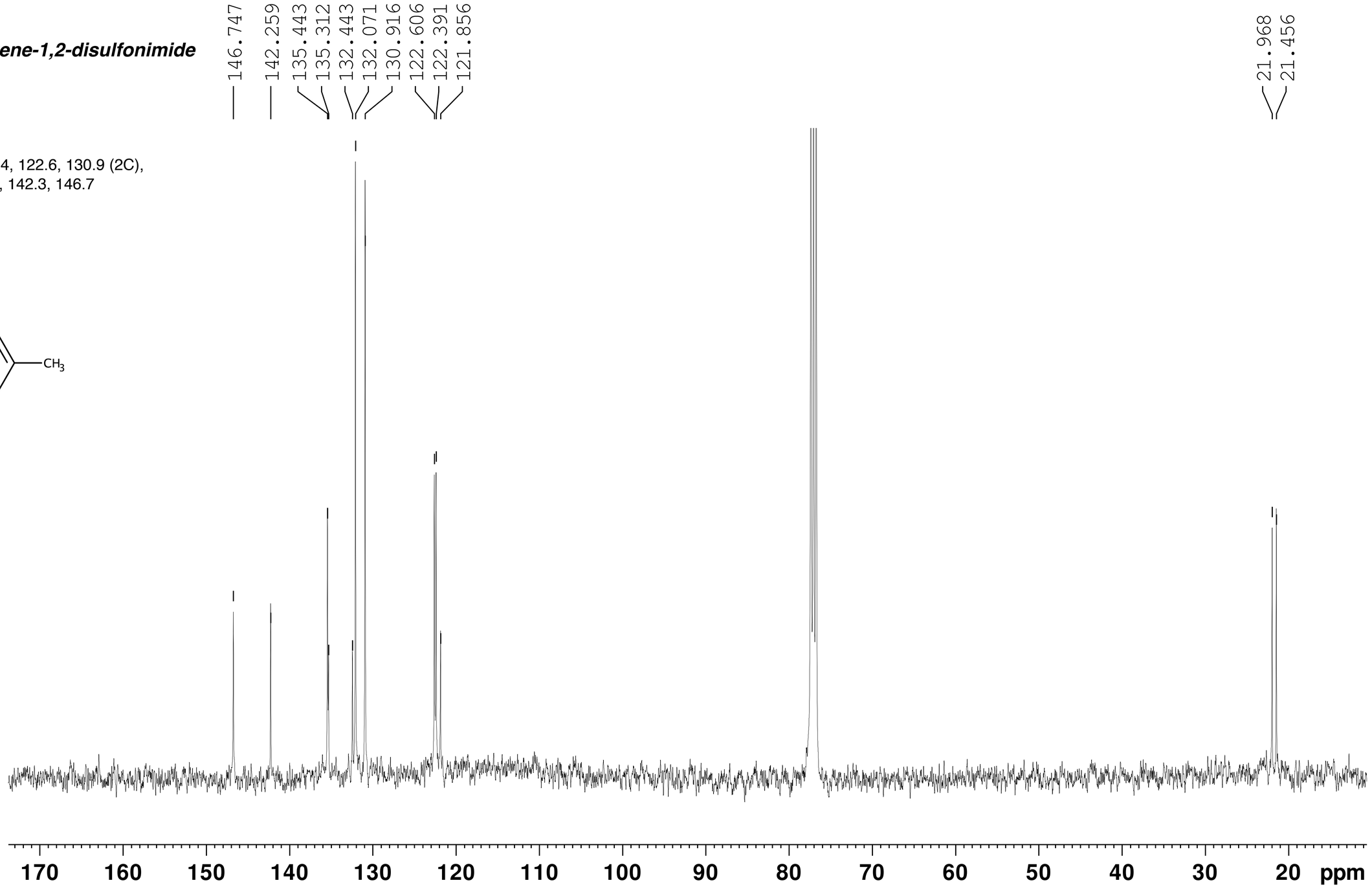


4-methyl-N-(p-methyl)-benzene-1,2-disulfonimide (DSI-Me)

^{13}C NMR (100 MHz, $CDCl_3$):

δ, ppm - 21.5, 22.0, 121.8, 122.4, 122.6, 130.9 (2C), 132.1 (2C), 132.4, 135.3, 135.4, 142.3, 146.7



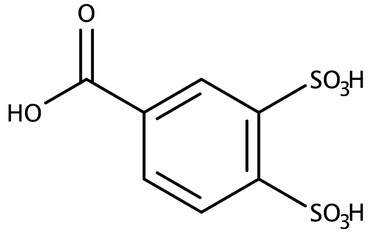


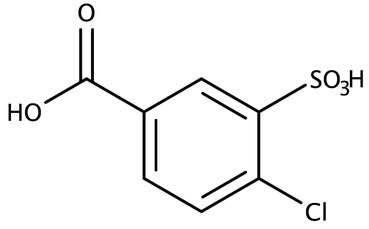
3,4-disulfobenzoic acid (DSBA)

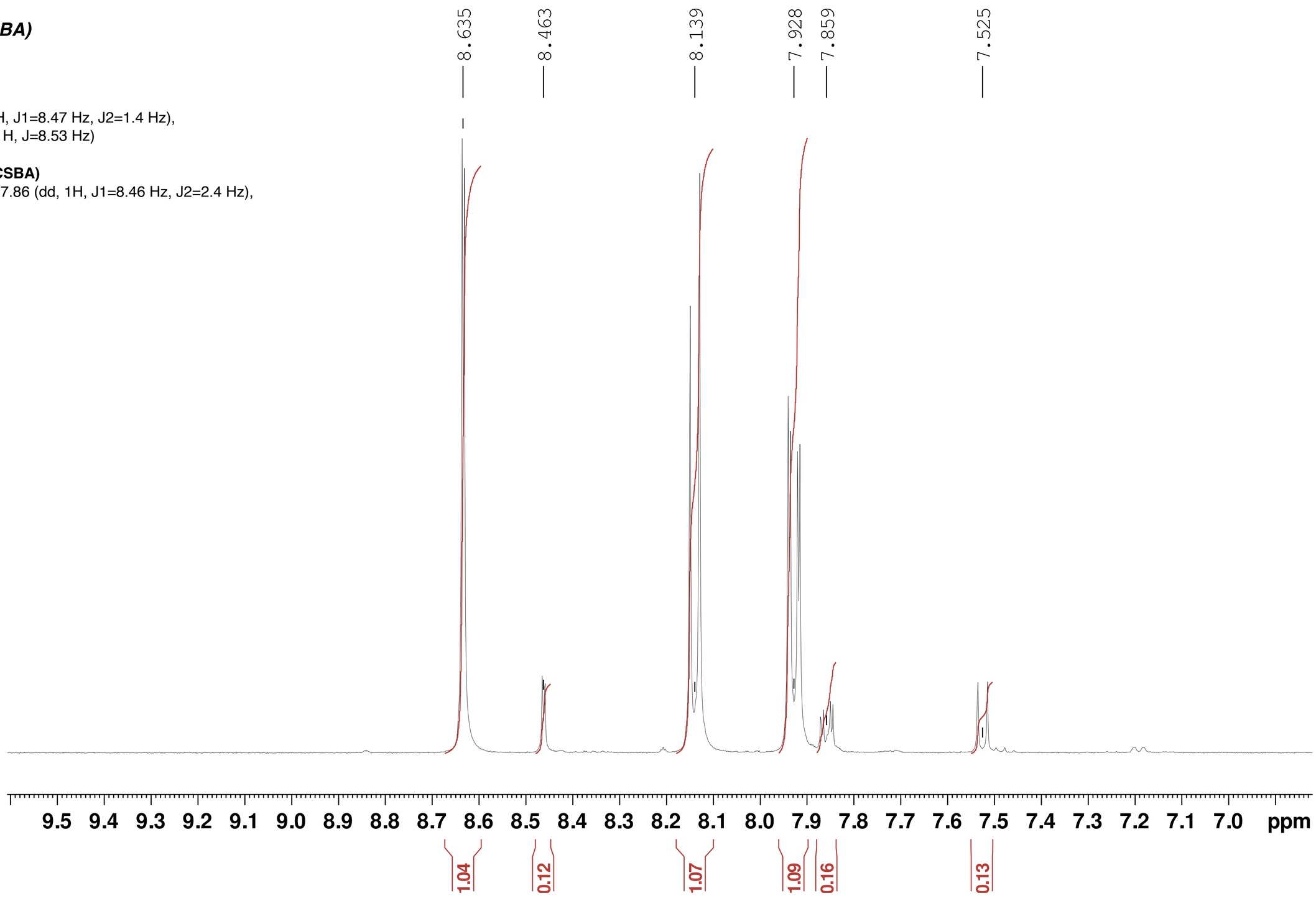
^{1}H NMR (400 MHz, DMSO d6):

3,4-disulfobenzoic acid (DSBA)
δ, ppm - 2.59 (s, 3H), 7.79 (dd, 1H, J1=8.47 Hz, J2=1.4 Hz),
8.05 (d, 1H, J=1.11 Hz), 8.49 (d, 1H, J=8.53 Hz)

4-chloro-3-sulfobenzoic acid (CSBA)
δ, ppm - 7.52 (d, 1H, J=8.48Hz), 7.86 (dd, 1H, J1=8.46 Hz, J2=2.4 Hz),
8.46 (d, 1H, J=2.50Hz)





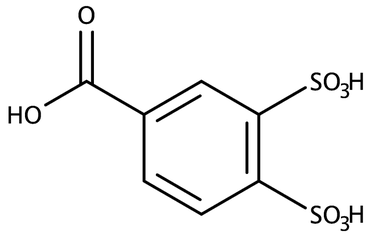


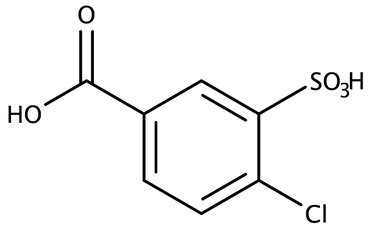
3,4-disulfobenzoic acid (DSBA)

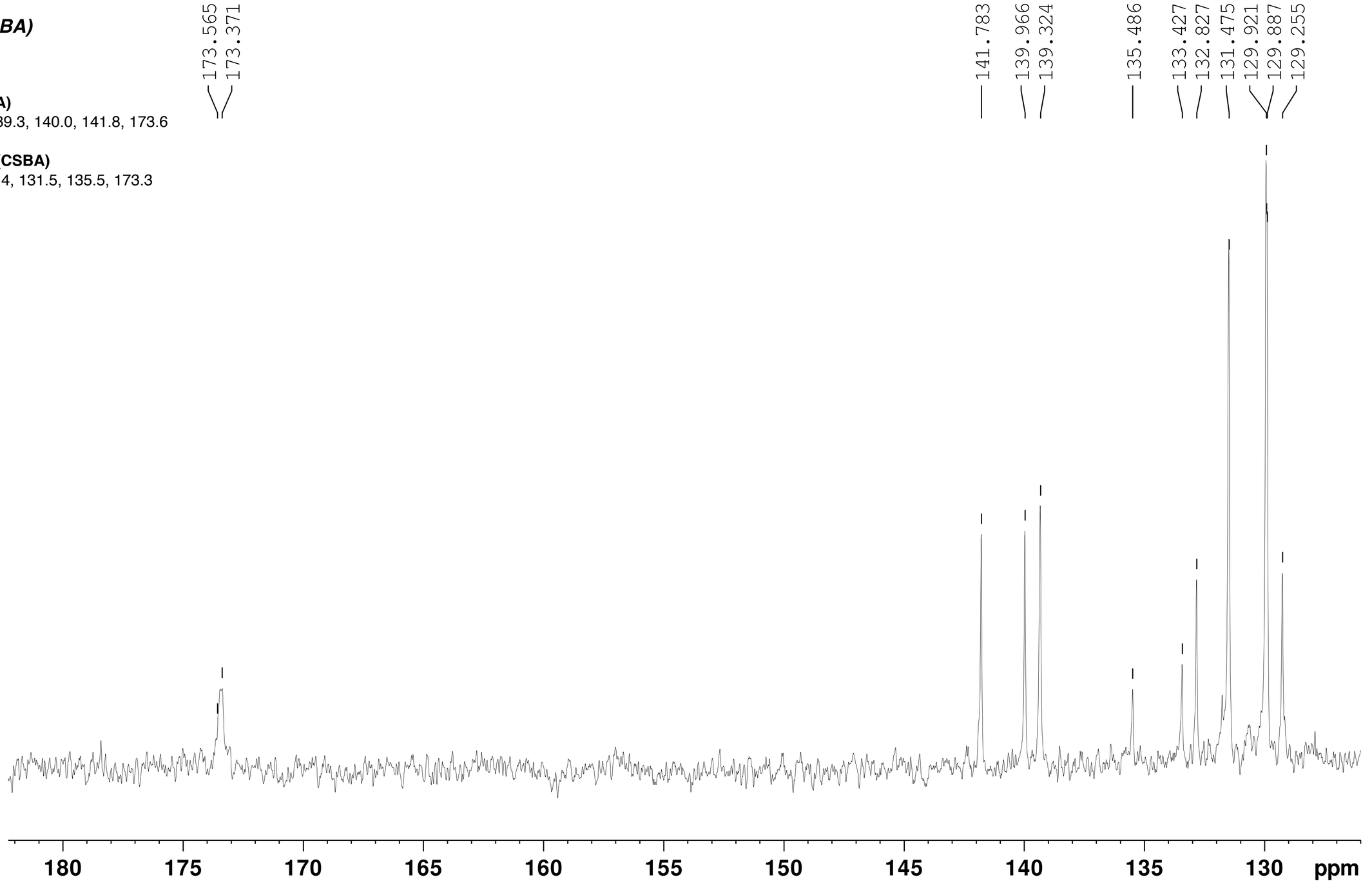
^{13}C NMR (100 MHz, D_2O):

3,4-disulfobenzoic acid (DSBA)
δ, ppm - 129.9, 131.5, 132.8, 139.3, 140.0, 141.8, 173.6

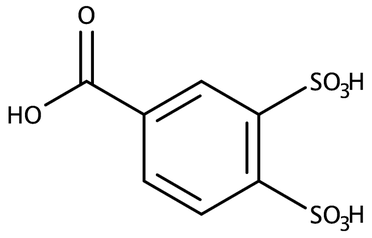
4-chloro-3-sulfobenzoic acid (CSBA)
δ, ppm - 129.2, 129.9 (2C), 133.4, 131.5, 135.5, 173.3

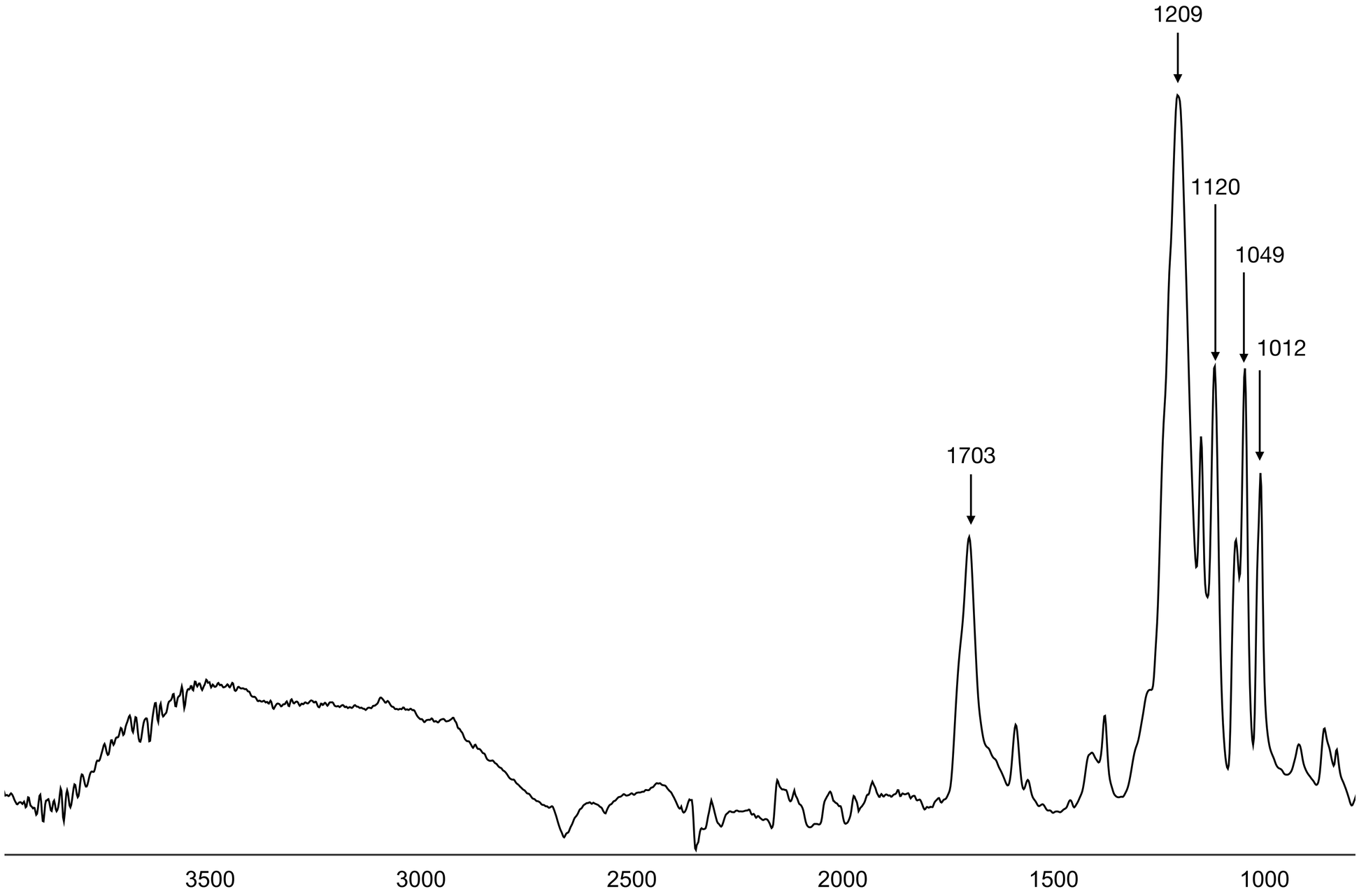






3,4-disulfobenzoic acid (DSBA)
FTIR

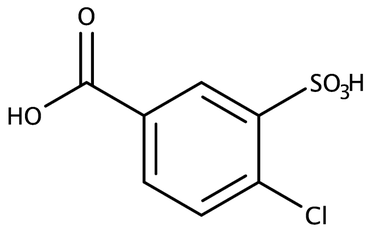


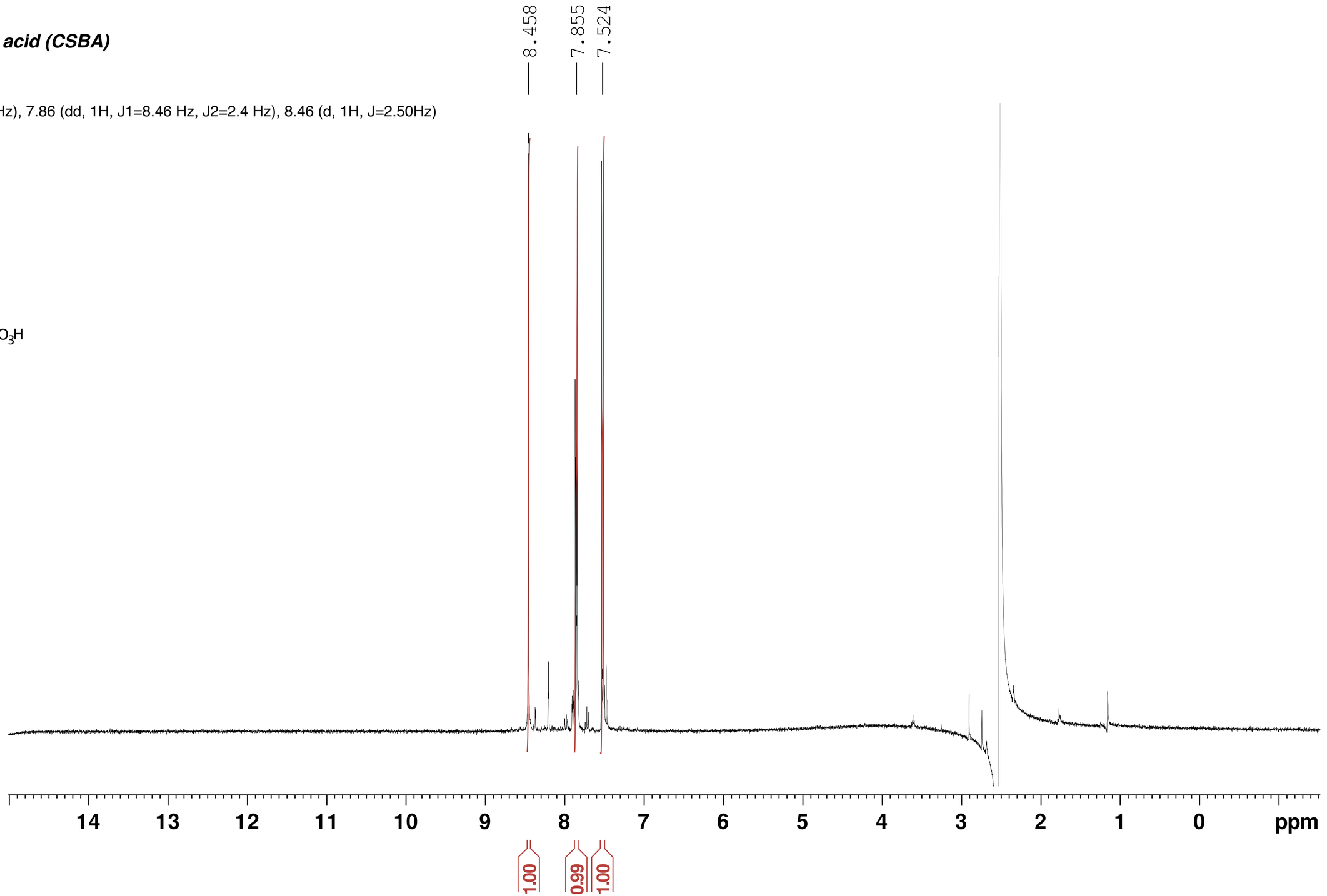


4-chloro-3-sulfobenzoic acid (CSBA)

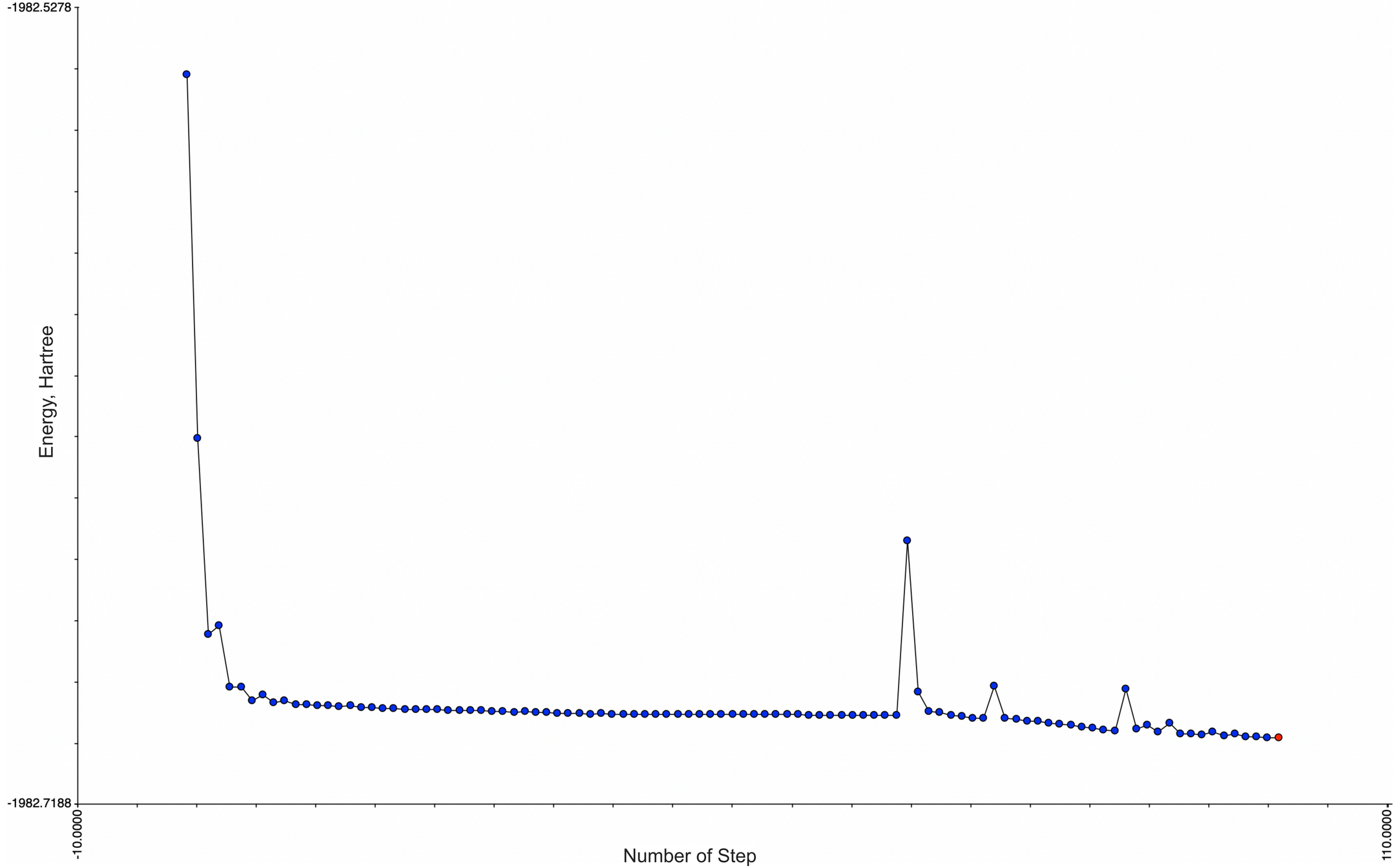
^{1}H NMR (400 MHz, DMSO d6):

δ, ppm - 7.52 (d, 1H, J=8.48Hz), 7.86 (dd, 1H, J1=8.46 Hz, J2=2.4 Hz), 8.46 (d, 1H, J=2.50Hz)





Energy plot for a 100-step geometry optimisation run for DSI-DA-CI (N31 basis, GAMESS)



Energy plot for a 100-step geometry optimisation run for CFPI (N31 basis, GAMESS)