Supporting Information

Catalyst-free tandem reaction of 2,2′-diaminodiaryldisulfides, arylsulfinic acids and aromatic aldehydes: an approach to synthesize unsymmetric thiosulfonates and benzothiazoles

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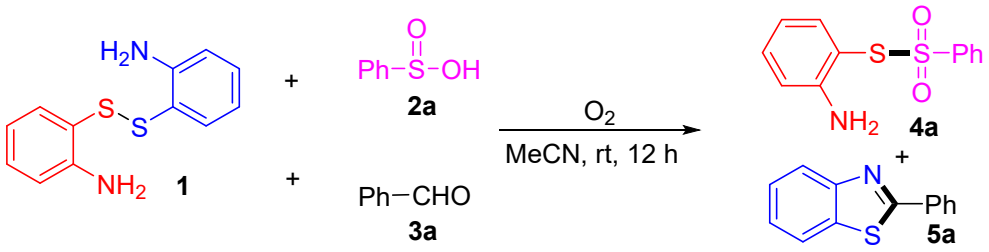
1. General remarks

All reactions were conduced in clean glassware with magnetic stirring. Chromatographic purification was performed on silica gel (400~500 mesh) and analytical thin layer chromatography (TLC) on silica gel HG/T2354-2010 GF254 (Qindao), which was detected by fluorescence. ^{1}H NMR and ^{13}C NMR spectra were measured on a Bruker Avance NMR spectrometer (600 MHz) in $CDCl_3$ as solvent, and tetramethylsilane (TMS; δ = 0.00 ppm) served as an internal standard for ^{1}H NMR. The corresponding residual non-deuterated solvent signal ($CDCl_3$; δ = 77.00 ppm) was used as internal standard for ^{13}C NMR. ^{1}H NMR data are reported as follows: δ, chemical shift; coupling constants (*J* are given in Hertz, Hz) and integration. Abbreviations to denote the multiplicity of a particular signal were s (singlet), d (doublet), t (triplet), q (quartet), and m (multiplet). High resolution mass spectra were obtained with Thermo Scientific LTQ Orbitrap XL mass spectrometer or Thermo Scientific Q Exactive mass spectrometer (ESI). Melting points were determined on a digital melting point apparatus and temperatures were uncorrected.

2. General procedure for the synthesis of unsymmetric thiosulfonates and benzothiazoles



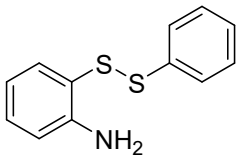
To a solution of 2,2'-diaminodiphenyl disulfides (0.25 mmol) in 2 mL of MeCN was added benzenesulfinic acid (0.2 mmol) and benzaldehyde (0.2 mmol) under oxygen atmosphere. The reaction mixture was stirred for 12 h at room temperature. The residue was then purified by column chromatography on silica gel (petroleum ether/EtOAc = 10:1) to give the pure products **4** and **5**.

Typical procedure for the synthesis of *S*-(2-aminophenyl) benzenesulfonothioate (4a) and 2-phenylbenzo[*d*]thiazole (5a) in 6.0 mmol scale

To a solution of 2,2'-diaminodiphenyl disulfides (1.86 g, 7.5 mmol) in 20 mL of MeCN was added benzenesulfinic acid (853 mg, 6 mmol) and benzaldehyde (637 mg, 6 mmol) under oxygen atmosphere. The reaction mixture was stirred for 24 h at room temperature. The residue was then purified by silica gel column chromatography (petroleum ether/EtOAc = 10:1) to give pure product compound **4a** (1.13 g, 71% yield) and **5a** (1.04 g, 82% yield).

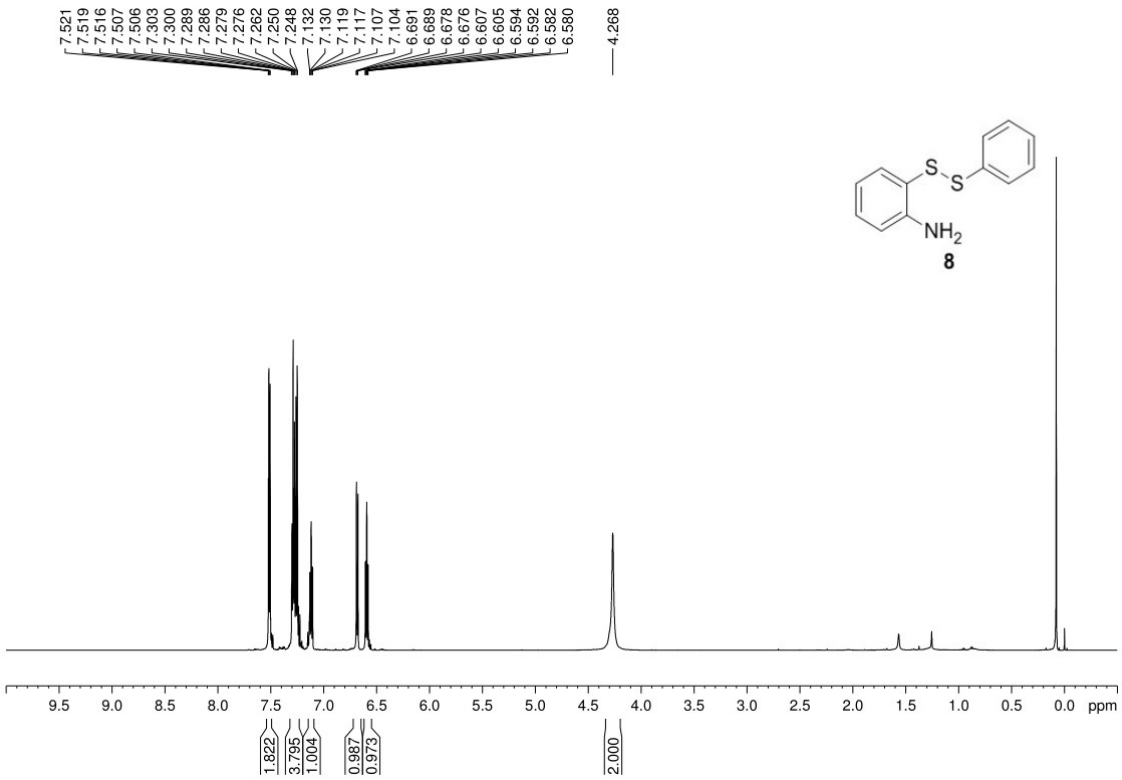
3. Characterization data and ^{1}H (^{13}C) NMR spectra of the products in Control experiments

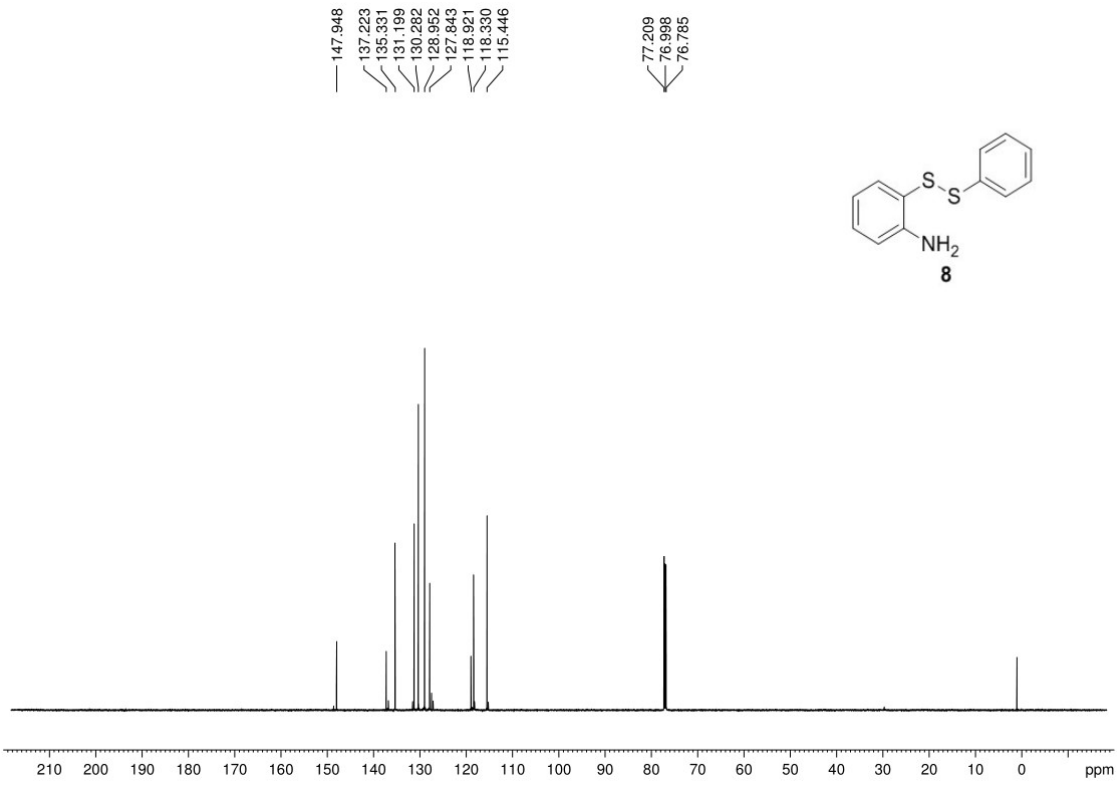
2-(Phenyldisulfanyl)aniline(8)[1]



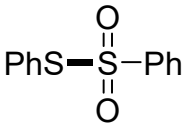
Pale yellow solid. Mp: 74–76 ℃ (lit.[1] 72–74 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): 7.52–7.51

(m, 2H), 7.30–7.25 (m, 4H), 7.13 (td, *J* = 7.5, 1.2 Hz, 1H), 6.69 (dd, *J* = 7.8, 1.2 Hz, 1H), 6.61 (td, *J* = 7.5, 1.2 Hz, 1H), 4.27 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 148.0, 137.2, 135.3, 131.2, 130.3, 129.0, 127.9, 118.9, 118.3, 115.4.

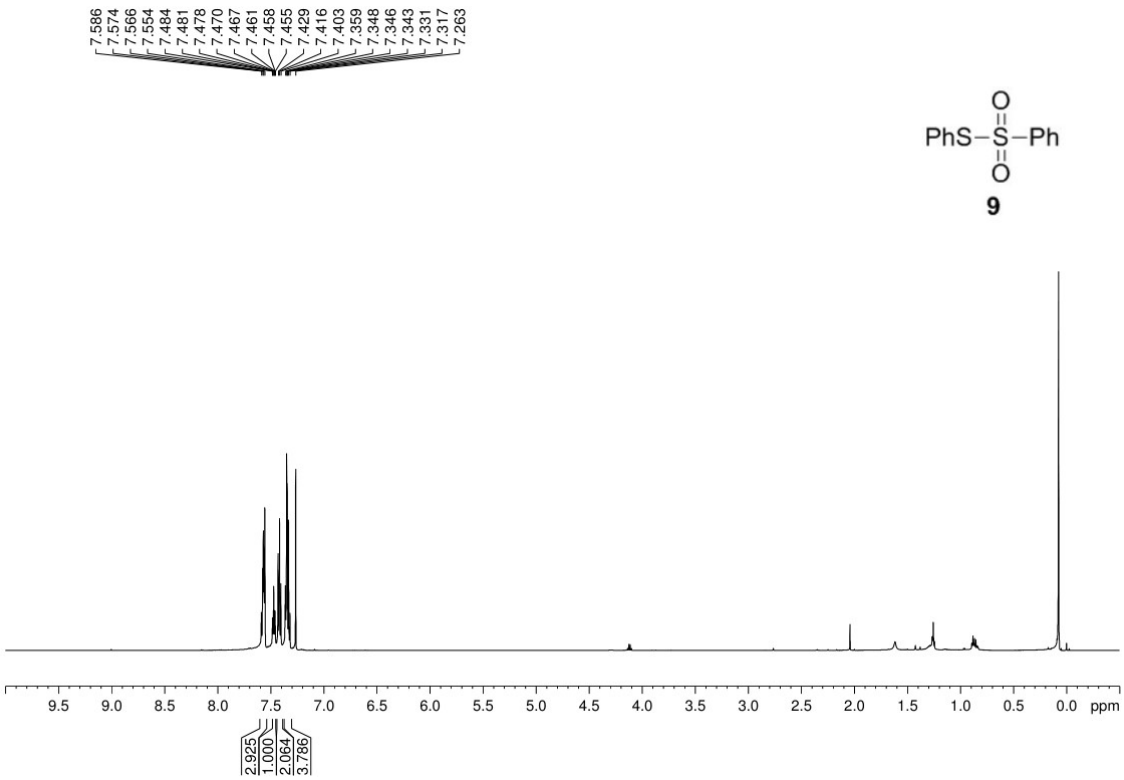


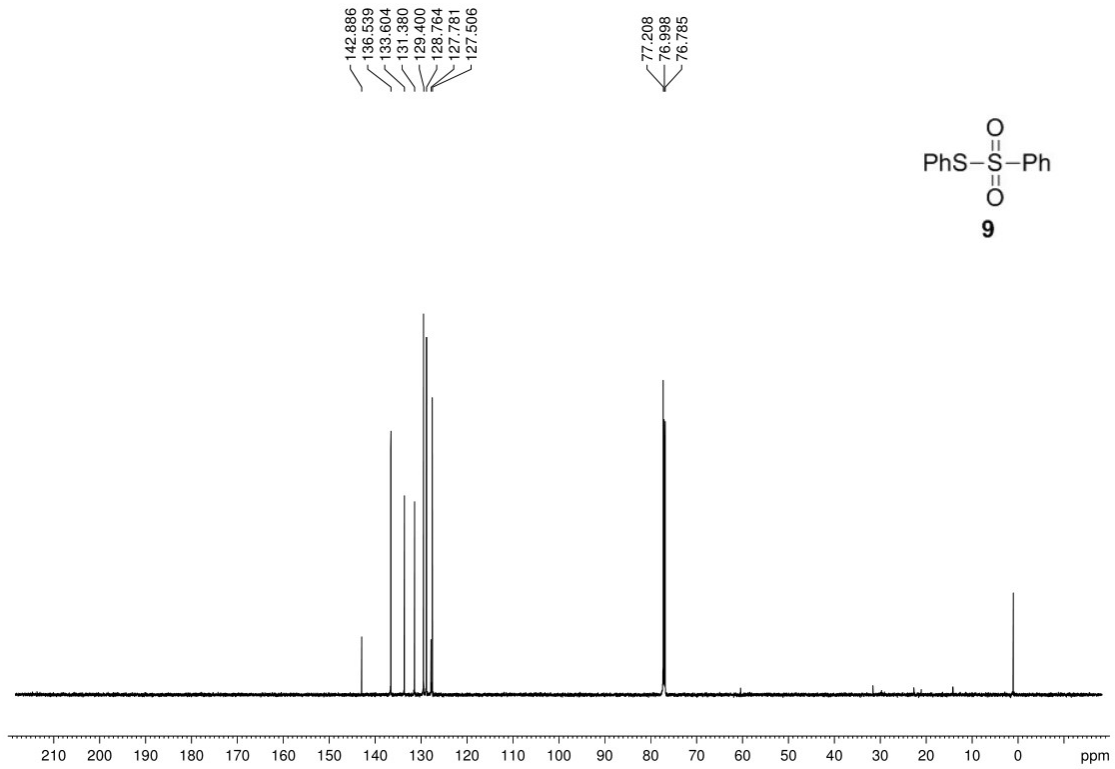


***S*-phenyl benzenesulfonothioate(9)**[2]

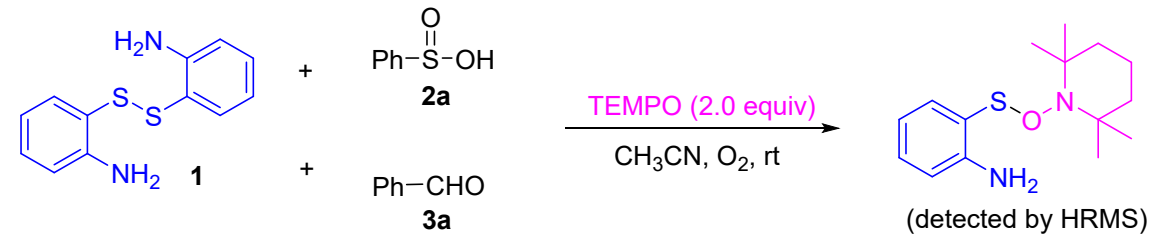


Yellow solid (33.9 mg, 68% yield). Mp: 41–43 ℃ (lit.[2] 45–47 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.59–7.55 (m, 3H), 7.48–7.46 (m, 1H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.36–7.32 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$):δ 142.9, 136.6, 133.6, 131.4, 129.4, 128.8, 127.8, 127.5.





4. Free radical capture experiment



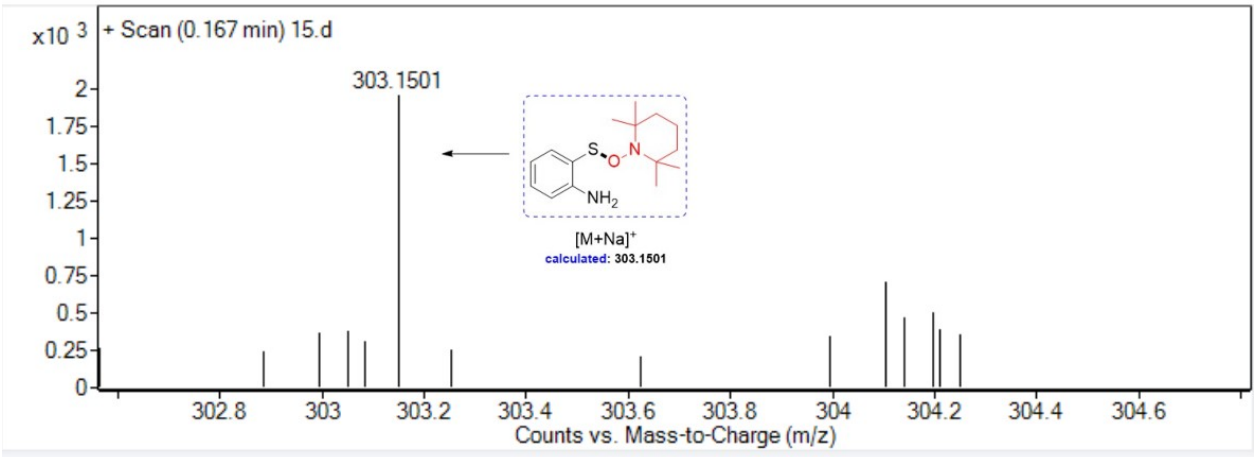
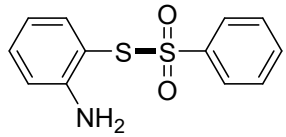


Figure S1. HRMS spectra of free radical capture experiment

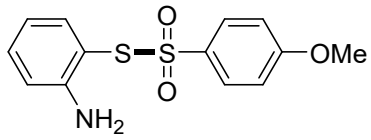
5. Characterization data for the products

S-(2-Aminophenyl) benzenesulfonothioate (4a)



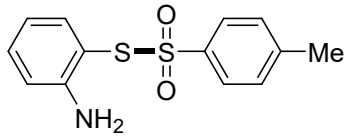
Yellow soild (47.8 mg, 90% yield). Mp: 81.7–83.7 ℃ (lit.[3] 83–83.5 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.64 (d, *J* = 7.8 Hz, 2H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.8Hz, 2H), 7.22 (t, *J* = 7.8 Hz, 1H), 6.90 (d, *J* = 7.8 Hz, 1H), 6.70 (d, *J* = 8.4 Hz, 1H), 6.56 (t, *J* = 7.8 Hz, 1H), 4.22 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.3, 142.7, 138.3, 133.7, 133.5, 128.8, 127.5, 118.4, 115.8, 109.6. HRMS (ESI) calcd for $C_{12}H_{12}NO_2S_2$ $(M+H)^+$: 266.0304; Found: 266.0307.

S-(2-Aminophenyl) 4-methoxybenzenesulfonothioate (4b)



Yellow solid (36.7 mg, 62% yield). Mp: 126–128 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.57 (d, *J* = 8.4 Hz, 2H), 7.23 (t, *J* = 7.8 Hz, 1H), 6.93 (d, *J* = 7.8 Hz, 1H), 6.89 (d, *J* = 9.0 Hz, 2H), 6.71 (d, *J* = 7.8 Hz, 1H), 6.59 (t, *J* = 7.2 Hz, 1H), 3.98 (s, 2H), 3.87 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.7, 150.3, 138.5, 134.7, 133.4, 129.9, 118.5, 115.9, 113.9, 110.3, 55.7. HRMS (ESI) calcd for $C_{13}H_{14}NO_3S_2$ $(M+H)^+$: 296.0410; Found: 296.0413.

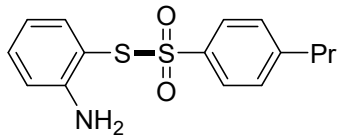
S-(2-Aminophenyl) 4-methylbenzenesulfonothioate (4c)



Yellow solid (50.5 mg, 90% yield). Mp:104–106 ℃ (lit.[4] 105-106 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.53 (d, *J* = 7.8 Hz, 2H), 7.23–7.20 (m, 3H), 6.91 (d, *J* = 7.8 Hz, 1H), 6.72 (d, *J* = 8.4 Hz, 1H), 6.58 (t, *J* = 7.2 Hz, 1H), 4.02 (s, 2H), 2.43 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.3, 144.8, 140.2, 138.4, 133.5, 129.5, 127.6, 118.6, 116.0, 110.2,

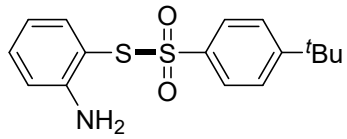
21.7. HRMS (ESI) calcd for $C_{13}H_{14}NO_2S_2$ $(M+H)^+$: 280.0460; Found: 280.0462.

_S_-(2-Aminophenyl) 4-propylbenzenesulfonothioate (4d)



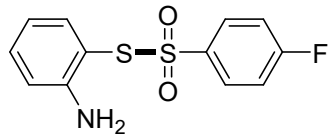
Yellow soild (39.9 mg, 65% yield). Mp: 148.4–150.4 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.54 (d, *J* = 8.4 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.20 (d, *J* = 7.8 Hz, 1H), 6.89 (d, *J* = 7.8 Hz, 1H), 6.70 (d, *J* = 7.8 Hz, 1H), 6.55 (t, *J* = 7.2 Hz, 1H), 4.25 (s, 2H), 2.65 (t, *J* = 7.8 Hz, 2H), 1.67–1.61 (m, 2H), 0.93 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.3, 149.4, 140.1, 138.3, 133.4, 128.8, 127.6, 118.4, 115.8, 109.9, 37.7, 24.0, 13.5. HRMS (ESI) calcd for $C_{15}H_{18}NO_2S_2$ $(M+H)^+$: 308.0773 ; Found: 308.0770.

_S_-(2-Aminophenyl) 4-(tert-butyl)benzenesulfonothioate (4e)



Yellow solid (50.7 mg, 79% yield). Mp: 72–75 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.57 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.21 (t, *J* = 7.8 Hz, 1H), 6.90 (d, *J* = 7.8 Hz, 1H), 6.71 (d, *J* = 8.4 Hz, 1H), 6.55 (t, *J* = 7.2 Hz, 1H), 4.14 (s, 2H), 1.33 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 157.8, 150.4, 139.8, 138.4, 133.4, 127.4, 125.8, 118.3, 115.8, 110.0, 35.2, 30.9. HRMS (ESI) calcd for $C_{16}H_{20}NO_2S_2$ $(M+H)^+$: 322.0930; Found: 322.0931.

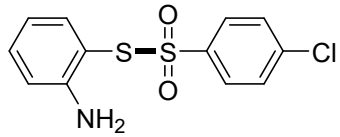
_S_-(2-Aminophenyl) 4-fluorobenzenesulfonothioate (4f)



Yellow soild (34.7 mg, 61% yield). Mp: 105.1–107.1 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.66–7.64 (m, 2H), 7.25–7.22 (m, 1H), 7.13 (d, *J* = 8.4 Hz, 2H), 6.91 (dd, *J* = 7.8, 1.2 Hz, 1H), 6.72 (d, *J* = 7.8 Hz, 1H), 6.59 (t, *J* = 7.2 Hz, 1H), 4.33 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.5 (d, *J* = 255.6 Hz), 150.4, 138.8 (d, *J* = 2.9 Hz), 138.4, 133.8, 130.6 (d, *J* =

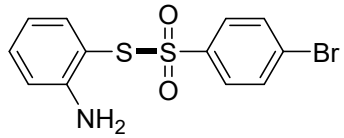
9.6 Hz), 118.6, 116.2 (d, J = 22.7 Hz), 116.0, 109.6. HRMS (ESI) calcd for $C_{12}H_{11}FNO_2S_2$ $(M+H)^+$: 284.0210; Found: 284.0206.

_S_-(2-Aminophenyl) 4-chlorobenzenesulfonothioate (4g)



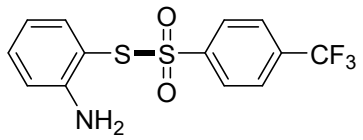
Yellow soild (31.7mg, 53% yield). Mp: 100.3–102.3 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.58 (d, J = 9.0 Hz, 2H), 7.42 (d, J =8.4 Hz, 2H), 7.26–7.23 (m, 1H), 6.92 (d, J = 7.8 Hz, 1H), 6.72 (d, J =8.4 Hz, 1H), 6.61 (t, J =7.8 Hz, 1H) , 4.33 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.4, 141.3, 140.4, 138.3, 133.8, 129.1, 129.0, 118.7, 116.0, 109.4. HRMS (ESI) calcd for $C_{12}H_{11}ClNO_2S_2$ $(M+H)^+$: 299.9914; Found: 299.9911.

_S_-(2-Aminophenyl) 4-bromobenzenesulfonothioate (4h)



Yellow brown soild (47 mg, 67% yield). Mp: 113–115 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.58 (d, J = 8.4 Hz, 2H), 7.49 (d, J = 8.4 Hz, 2H), 7.24 (t, J = 7.8 Hz, 1H), 6.92 (d, J = 7.8 Hz, 1H), 6.72 (d, J = 7.8 Hz, 1H), 6.60 (t, J = 7.8 Hz, 1H), 4.38 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.4, 141.8, 138.3, 133.8, 132.1, 129.0, 129.0, 118.6, 116.0, 109.3. HRMS (ESI) calcd for $C_{12}H_{11}BrNO_2S_2$ $(M+H)^+$: 343.9409; Found: 343.9408.

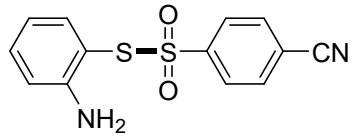
_S_-(2-Aminophenyl) 4-(trifluoromethyl)benzenesulfonothioate (4i)



Yellow solid (51 mg, 76% yield). Mp: 98.9–100.9 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.80 (d, J = 7.8 Hz, 2H), 7.75 (d, J = 7.8 Hz, 2H), 7.29 (d, J = 7.8 Hz, 1H), 6.92 (d, J = 8.4 Hz, 1H), 6.76 (d, J = 7.8 Hz, 1H), 6.62 (t, J = 7.2 Hz, 1H), 3.73 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.4, 146.0, 138.3, 135.6 (q, J = 33 Hz), 134.0, 128.2, 126.1 (q, J = 3.6 Hz),

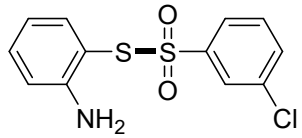
125.8 (q, J = 271.5 Hz), 118.8, 116.1, 109.0. HRMS (ESI) calcd for $C_{13}H_{10}F_3NNaO_2S_2$ $(M+Na)^+$: 355.9997; Found:355.9996.

_S_-(2-Aminophenyl) 4-cyanobenzenesulfonothioate (4j)



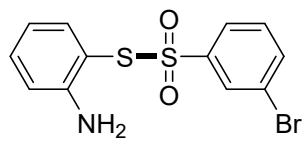
Yellow soild (41.3 mg, 71% yield). Mp: 147.2–149.2 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): 7.66 (s, 4H), 7.25–7.22 (m, 1H), 6.89 (t, J = 8.4, 1.2Hz, 1H), 6.71–6.70 (m, 1H), 6.59–6.57 (m, 1H), 4.28 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): 150.4, 146.3, 138.1, 134.1, 132.6, 128.1, 118.6, 117.1, 117.0, 116.0, 108.4. HRMS (ESI) calcd for $C_{13}H_{10}N_2O_2S_2$ $(M+H)^+$: 291.0256; Found: 291.0251.

_S_-(2-Aminophenyl) 3-chlorobenzenesulfonothioate (4k)



Yellow soild (40.2 mg, 67% yield). Mp: 88–90 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.57 (d, J = 12 Hz, 2H), 7.53 (d, J = 7.8 Hz, 1H), 7.40 (t, J = 7.8 Hz, 1H), 7.26 (t, J = 7.8 Hz, 1H), 6.93 (d, J = 7.8 Hz, 1H), 6.72 (d, J = 8.4 Hz, 1H), 6.61 (t, J = 7.2 Hz, 1H), 4.20 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.3, 144.0, 138.3, 135.0, 133.9, 133.7, 130.1, 127.6, 125.5, 118.6, 116.0, 109.1. HRMS (ESI) calcd for $C_{12}H_{11}ClNO_2S_2$ $(M+H)^+$: 299.9914; Found: 299.9918.

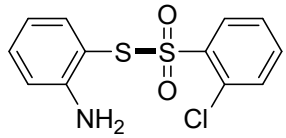
_S_-(2-Aminophenyl) 3-bromobenzenesulfonothioate (4l)



Yellow brown solid (45.4 mg, 66% yield). Mp: 104–106 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.71–7.69 (m, 2H), 7.57–7.56 (m, 1H), 7.33–7.30 (m, 1H), 7.25–7.23 (m, 1H), 6.93 (dd, J = 7.8, 1.8 Hz, 1H), 6.72 (dd, J = 8.4, 1.2 Hz, 1H), 6.61 (td, J = 7.8, 1.2 Hz, 1H), 4.24 (s,

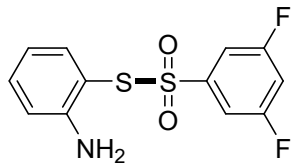
2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.3, 144.1, 138.3, 136.6, 133.9, 130.4, 130.3, 125.9, 122.7, 118.6, 116.0, 109.0. HRMS (ESI) calcd for $C_{12}H_{11}BrNO_2S_2$ $(M+H)^+$: 343.9409; Found: 343.9413.

_S_-(2-Aminophenyl) 2-chlorobenzenesulfonothioate (4m)



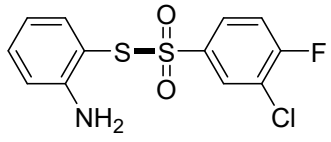
Yellow soild (31.8 mg, 53% yield). Mp: 99–101 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.64 (d, *J* = 7.8 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.53 (t, *J* = 7.8 Hz, 1H), 7.25 (t, *J* = 7.8 Hz, 1H), 7.19 (t, *J* = 7.8 Hz, 1H), 6.91 (d, *J* = 7.8 Hz, 1H), 6.67 (d, *J* = 8.4 Hz, 1H), 6.52 (t, *J* = 7.2 Hz, 1H), 3.96 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.4, 139.3, 138.3, 134.7, 133.7, 132.4, 132.2, 131.8, 126.6, 118.5, 115.8, 109.4. HRMS (ESI) calcd for $C_{12}H_{11}ClNO_2S_2$ $(M+H)^+$: 299.9914; Found: 299.9918.

_S_-(2-Aminophenyl) 3,5-difluorobenzenesulfonothioate (4n)



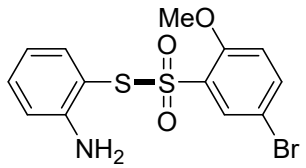
Yellow solid (36.3 mg, 60% yield). Mp: 135.6–137.6 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.28 (t, *J* = 7.8 Hz, 1H), 7.19–7.17 (m, 2H), 7.07–7.04 (m, 1H), 6.97 (d, *J* = 7.8 Hz, 1H), 6.74 (d, *J* = 8.4 Hz, 1H), 6.64 (t, *J* = 7.8 Hz, 1H), 4.33 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.2 (dd, *J* = 254.0, 11.1 Hz), 150.4, 145.4 (t, *J* = 8.4 Hz), 138.2, 134.2, 118.7, 116.1, 111.3 (dd, *J* = 22.4, 6.6 Hz), 109.4 (t, *J* = 24.9 Hz), 108.7. HRMS (ESI) calcd for $C_{12}H_9F_2NNaO_2S_2$ $(M+Na)^+$: 323.9935; Found: 323.9935.

_S_-(2-Aminophenyl) 3-chloro-4-fluorobenzenesulfonothioate (4o)



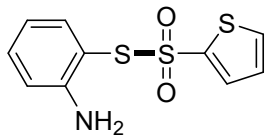
Yellow solid (36.2 mg, 57% yield). Mp: 96–98 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.65 (d, *J* = 6.6 Hz, 1H), 7.54–7.53 (m, 1H), 7.27 (t, *J* = 7.8 Hz, 1H), 7.21 (t, *J* = 8.4 Hz, 1H), 6.95 (d, *J* = 7.8 Hz, 1H), 6.73 (d, *J* = 7.8 Hz, 1H), 6.63 (t, *J* = 7.8 Hz, 1H), 4.21 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 162.0 (d, *J* = 257.6 Hz), 150.3, 139.4 (d, *J* = 3.8 Hz), 138.3, 134.0, 130.7, 128.1 (d, *J* = 8.7 Hz), 122.3 (d, *J* = 18.8 Hz), 118.7, 117.2 (d, *J* = 22.7 Hz), 116.0, 109.0. HRMS (ESI) calcd for $C_{12}H_{10}ClFNO_2S_2$ $(M+H)^+$: 317.9820; Found: 317.9817.

_S_-(2-Aminophenyl) 5-bromo-2-methoxybenzenesulfonothioate (4p)



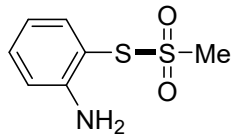
Yellow solid (56.1 mg, 75% yield). Mp: 124–126 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.65–7.63 (m, 2H), 7.22 (t, *J* = 7.8 Hz, 1H), 6.95–6.93 (m, 2H), 6.72 (d, *J* = 8.4 Hz, 1H), 6.58 (t, *J* = 7.8 Hz, 1H), 4.16 (s, 2H), 3.96 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$):δ 156.0, 150.5, 138.3, 138.1, 133.7, 133.0, 131.8, 118.4, 115.9, 114.4, 111.9, 109.9, 56.6. HRMS (ESI) calcd for $C_{13}H_{13}BrNO_3S_2$ $(M+H)^+$: 373.9515; Found:373.9515.

S-(2-Aminophenyl) thiophene-2-sulfonothioate (4q)



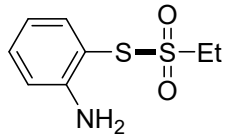
Yellow soild (35.8 mg, 66% yield). Mp: 118–120 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.67 (d, *J* = 4.8 Hz, 1H), 7.35 (d, *J* = 3.6 Hz, 1H), 7.25 (t, *J* = 7.8 Hz, 1H), 7.02–7.00 (m, 2H), 6.73 (d, *J* = 8.4 Hz, 1H), 6.62 (t, *J* = 7.8 Hz, 1H), 4.10 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.4, 143.1, 138.3, 134.2, 134.2, 133.8, 127.3, 118.6, 116.0, 110.0. HRMS (ESI) calcd for $C_{10}H_{10}NO_2S_3$ $(M+H)^+$: 271.9868; Found: 271.9866.

S-(2-Aminophenyl) methanesulfonothioate (4r)



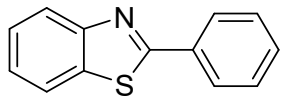
Yellow brown soild (36 mg, 87% yield). Mp: 103.4–105.4 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.46 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.32–7.29 (m, 1H), 6.81 (d, *J* = 8.4 Hz, 1H), 6.79 (t, *J* = 7.8 Hz, 1H), 4.57 (s, 2H), 3.23 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.1, 138.2, 133.9, 119.1, 116.3, 109.8, 47.7. HRMS (ESI) calcd for $C_7H_{10}NO_2S_2$ $(M+H)^+$: 204.0147; Found: 204.0150.

S-(2-Aminophenyl) ethanesulfonothioate (4s)



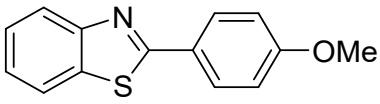
Yellow brown soild (32 mg, 74% yield). Mp: 83–85 ℃. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.42 (d, *J* = 7.8 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 1H), 6.79 (d, *J* = 8.4 Hz, 1H), 6.76 (t, *J* = 7.8 Hz, 1H), 4.43 (s, 2H), 3.30 (q, *J* = 7.2 Hz, 2H), 1.48 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 150.3, 138.1, 133.6, 118.9, 116.3, 109.7, 54.0, 8.1. HRMS (ESI) calcd for $C_8H_{12}NO_2S_2$ $(M+H)^+$: 218.0304; Found: 218.0303.

2-Phenylbenzo[d]thiazole (5a)



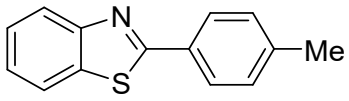
White solid (35.1 mg, 83% yield). Mp:115.1–117.1 ℃ (lit.[5] 112–114 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.11 (d, *J* = 7.2 Hz, 3H), 7.90 (d, *J* = 8.4 Hz, 1H), 7.51–7.49 (m, 4H), 7.40 (t, *J* = 7.8 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.0, 154.1, 135.0, 133.5, 130.9, 129.0, 127.5, 126.2, 125.1, 123.1, 121.5. HRMS (ESI) calcd for $C_{13}H_{10}NS$ $(M+H)^+$: 212.0528; Found: 212.0529.

2-(4-Methoxyphenyl)benzo[d]thiazole (5b)



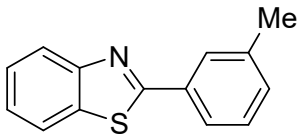
White solid (41 mg, 85% yield). Mp: 103–105 °C (lit.[6] 102 °C). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.05–8.02 (m, 3H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.48 (t, *J* = 7.2 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 1H), 6.99 (d, *J* = 8.4 Hz, 2H), 3.86 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 167.8, 161.8, 154.2, 134.8, 129.0, 126.3, 126.1, 124.7, 122.7, 121.4, 114.3, 55.4. HRMS (ESI) calcd for $C_{14}H_{11}NNaOS$ $(M+Na)^+$: 264.0454; Found: 264.0453.

2-(*p*-Tolyl)benzo[d]thiazole (5c)



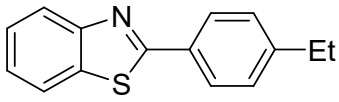
White solid (30.2 mg, 67% yield). Mp: 80–82 °C (lit.[7] 83-84 °C). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.08 (d, *J* = 7.8 Hz, 1H), 8.00 (d, *J* = 7.8 Hz, 2H), 7.90 (d, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.30 (d, *J* = 7.8 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.2, 154.1, 141.4, 134.9, 130.9, 129.7, 127.4, 126.2, 124.9, 123.0, 121.5, 21.5. HRMS (ESI) calcd for $C_{14}H_{12}NS$ $(M+H)^+$: 226.0685; Found: 226.0686.

2-(*m*-Tolyl)benzo[d]thiazole (5d)



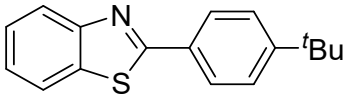
White solid (34.8 mg, 77% yield). Mp: 70–72 °C (lit.[8] 67-68 °C).^{1}H NMR (600 MHz, $CDCl_3$): δ 8.11 (d, *J* = 7.8 Hz, 1H), 7.96 (s, 1H), 7.90 (t, *J* = 7.8 Hz, 2H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 2H), 7.31 (d, *J* = 7.8 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.3, 154.0, 138.8, 134.9, 133.4, 131.7, 128.8, 127.9, 126.2, 125.0, 124.8, 123.1, 121.5, 21.30. HRMS (ESI) calcd for $C_{14}H_{11}NNaS$ $(M+Na)^+$: 248.0504; Found: 248.0505.

2-(4-Ethylphenyl)benzo[d]thiazole (5e)



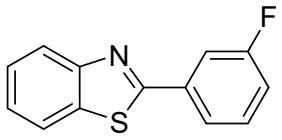
White solid (30 mg, 62% yield). Mp: 84–86 ℃ (lit.[8] 85–87 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.08 (d, *J* = 7.8 Hz, 1H), 8.03 (d, *J* = 7.8 Hz, 2H), 7.90 (d, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 1H), 7.33 (d, *J* = 7.8 Hz, 2H), 2.75 (q, *J* = 7.2 Hz, 2H), 1.31 (t, *J* = 7.8 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.2, 154.1, 147.7, 134.9, 131.1, 128.5, 127.6, 126.2, 125.0, 123.0, 121.5, 28.8, 15.3. HRMS (ESI) calcd for $C_{15}H_{14}NS$ $(M+H)^+$: 240.0841; Found: 240.0845.

2-(4-(*tert*-Butyl)phenyl)benzo[d]thiazole (5f)



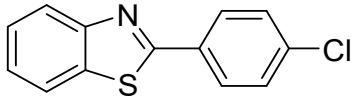
White solid (43 mg, 80% yield). Mp: 108–110 ℃ (lit.[8] 107–108 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.10 (d, *J* = 8.4 Hz, 1H), 8.05 (d, *J* = 7.8 Hz, 2H), 7.90 (d, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 2H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 1H), 1,39 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.1, 154.5, 154.2, 134.9, 130.9, 127.3, 126.2, 125.9, 124.9, 123.0, 121.5, 34.9, 31.1. HRMS (ESI) calcd for $C_{17}H_{18}NS$ $(M+H)^+$: 268.1154; Found: 268.1151.

2-(3-Fluorophenyl)benzo[d]thiazole (5g)



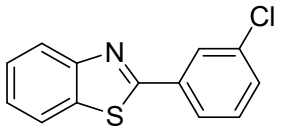
White solid (37.2 mg, 81% yield). Mp: 110–112 ℃ (lit.[9] 116–117 ℃).^{1}H NMR (600 MHz, $CDCl_3$): δ 8.09 (d, *J* = 7.8 Hz, 1H), 7.88 (d, *J* = 7.8 Hz, 1H), 7.84–7.82 (m, 2H), 7.51 (td, *J* = 7.8, 1.2 Hz, 1H), 7.44–7.37 (m, 2H), 7.19–7.15 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.3 (d, *J* = 2.9 Hz), 163.8 (d, *J* = 245.9 Hz), 153.9, 135.6 (d, *J* = 7.8 Hz), 135.0, 130.5 (d, *J* = 7.8 Hz), 126.4, 125.4, 123.4, 123.2 (d, *J* = 2.6 Hz), 121.6, 117.8 (d, *J* = 21.0 Hz), 114.3(d, *J* = 23.6 Hz). HRMS (ESI) calcd for $C_{13}H_9FNS$ $(M+H)^+$: 230.0434; Found: 230.0433.

2-(4-Chlorophenyl)benzo[d]thiazole (5h)



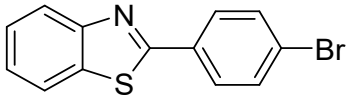
White solid (44 mg, 90% yield). Mp: 128–130 ℃ (lit.[5] 122–123 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.07 (d, *J* = 7.8 Hz, 1H), 7.99 (d, *J* = 7.8 Hz, 2H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 7.8 Hz, 2H), 7.38 (t, *J* = 7.8 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.5, 153.9, 136.9, 134.9, 132.0, 129.1, 128.6, 126.4, 125.3, 123.2, 121.5. HRMS (ESI) calcd for $C_{13}H_9ClNS$ $(M+H)^+$: 246.0139; Found: 246.0135.

2-(3-Chlorophenyl)benzo[d]thiazole (5i)



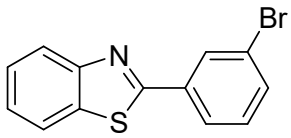
White solid (40.3 mg, 82% yield). Mp: 94–96 ℃ (lit.[8] 107–108 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.10 (s, 1H), 8.08 (d, *J* = 7.8 Hz, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.39–7.36 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.1, 153.8, 135.1, 135.0, 135.0, 130.7, 130.1, 127.2, 126.4, 125.6, 125.4, 123.3, 121.6. HRMS (ESI) calcd for $C_{13}H_9ClNS$ $(M+H)^+$: 246.0139; Found: 246.0141.

2-(4-Bromophenyl)benzo[d]thiazole (5j)



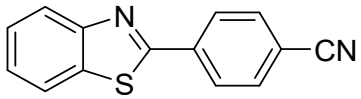
White solid (43.5 mg, 75% yield). Mp: 125.3–127.3 ℃ (lit.[7] 128–129 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.07 (d, *J* = 8.4 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.41 (t, *J* = 7.8 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.6, 154.0, 135.0, 132.5, 132.2, 128.8, 126.5, 125.4, 125.4, 123.3, 121.6. HRMS (ESI) calcd for $C_{13}H_9BrNS$ $(M+H)^+$: 289.9634; Found: 289.9630.

2-(3-Bromophenyl)benzo[d]thiazole (5k)



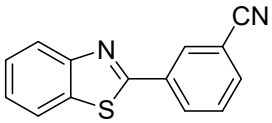
White solid (47.6 mg, 82% yield). Mp: 85–87 °C (lit.[10] 84–86 °C). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.25 (s, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 1H), 7.31 (t, *J* = 7.8 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.9, 153.8, 135.3, 134.9, 133.6, 130.3, 130.1, 126.4, 126.0, 125.4, 123.3, 123.1, 121.5. HRMS (ESI) calcd for $C_{13}H_9BrNS$ $(M+H)^+$: 289.9634; Found: 289.9636.

4-(Benzo[d]thiazol-2-yl)benzonitrile (5l)



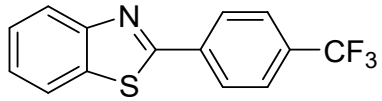
White solid (38.3 mg, 81% yield). Mp: 175–177 °C (lit.[5] 176 °C). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.16 (d, *J* = 7.8 Hz, 2H), 8.10 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 7.8 Hz, 2H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.2, 153.9, 137.3, 135.2, 132.7, 127.8, 126.8, 126.0, 123.7, 121.7, 118.2, 114.0. HRMS (ESI) calcd for $C_{14}H_9N_2S$ $(M+H)^+$: 237.0481; Found: 237.0483.

3-(Benzo[d]thiazol-2-yl)benzonitrile (5m)



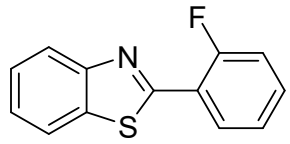
White solid (33 mg, 70% yield). Mp: 168–170 °C (lit.[8] 156–158 °C). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.38 (t, *J* = 1.2 Hz, 1H), 8.28–8.26 (m, 1H), 8.09 (d, *J* = 7.8 Hz, 1H), 7.93 (dd, *J* = 8.4, 0.6 Hz, 1H), 7.75–7.73 (m, 1H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.54–7.51 (m, 1H), 7.45 (td, *J* = 7.8, 1.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.0, 153.8, 135.0, 134.7, 133.8, 131.4, 130.8, 129.8, 126.7, 125.9, 123.6, 121.7, 118.0, 113.4. HRMS (ESI) calcd for $C_{14}H_9N_2S$ $(M+H)^+$: 237.0481; Found: 237.0485.

2-(4-(Trifluoromethyl)phenyl)benzo[d]thiazole (5n)



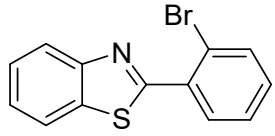
White solid (41 mg, 73% yield). Mp: 157.9–159.9 ℃ (lit.[8] 160–161 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): 8.20 (d, *J* = 7.8 Hz, 2H), 8.11 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 7.8 Hz, 2H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 166.0, 154.0, 136.7, 135.2, 132.7 (q, *J* = 32.6 Hz), 127.7, 126.6, 126.5 (q, *J* = 270.9 Hz), 126.0 (q, *J* = 3.6 Hz), 125.8, 123.6, 121.7. HRMS (ESI) calcd for $C_{14}H_9F_3NS$ $(M+H)^+$: 280.0402; Found: 280.0406.

2-(2-Fluorophenyl)benzo[d]thiazole (5o)



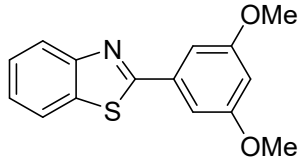
White solid (39 mg, 85% yield). Mp: 80–82 ℃ (lit.[11] 82 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.44 (t, *J* = 7.8 Hz, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.53 (t, *J* = 7.8 Hz, 1H), 7.46 (q, *J* = 7.2 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.31 (t, *J* = 7.2 Hz, 1H), 7.24–7.21 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.3 (d, *J* = 251.7 Hz), 161.0 (d, *J* = 5.9 Hz), 159.6, 152.4, 135.7 (d, *J* = 7.8 Hz), 132.1 (d, *J* = 8.6 Hz), 129.6 (d, *J* = 2.0 Hz), 126.2, 125.2, 124.6 (d, *J* = 3.3 Hz), 123.2, 121.4 (d, *J* = 12.3 Hz), 116.3 (d, *J* = 21.8 Hz). HRMS (ESI) calcd for $C_{13}H_9FNS$ $(M+H)^+$: 230.0434; Found: 230.0437.

2-(2-Bromophenyl)benzo[d]thiazole (5p)



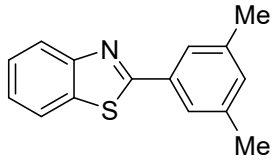
White solid (52 mg, 90% yield). Mp: 68–70 ℃ (lit.[12] 66–68 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.16 (d, *J* = 7.8 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.75 (t, *J* = 7.8 Hz, 1H), 7.55 (t, *J* = 7.8 Hz, 1H), 7.45–7.43 (m, 2H), 7.34 (t, *J* = 7.2 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.6, 152.7, 136.1, 134.4, 134.0, 132.1, 131.2, 127.5, 126.3, 125.4, 123.5, 122.0, 121.4. HRMS (ESI) calcd for $C_{13}H_9BrNS$ $(M+H)^+$: 289.9634; Found: 289.9632.

2-(3,5-dimethoxyphenyl)benzo[d]thiazole (5q)



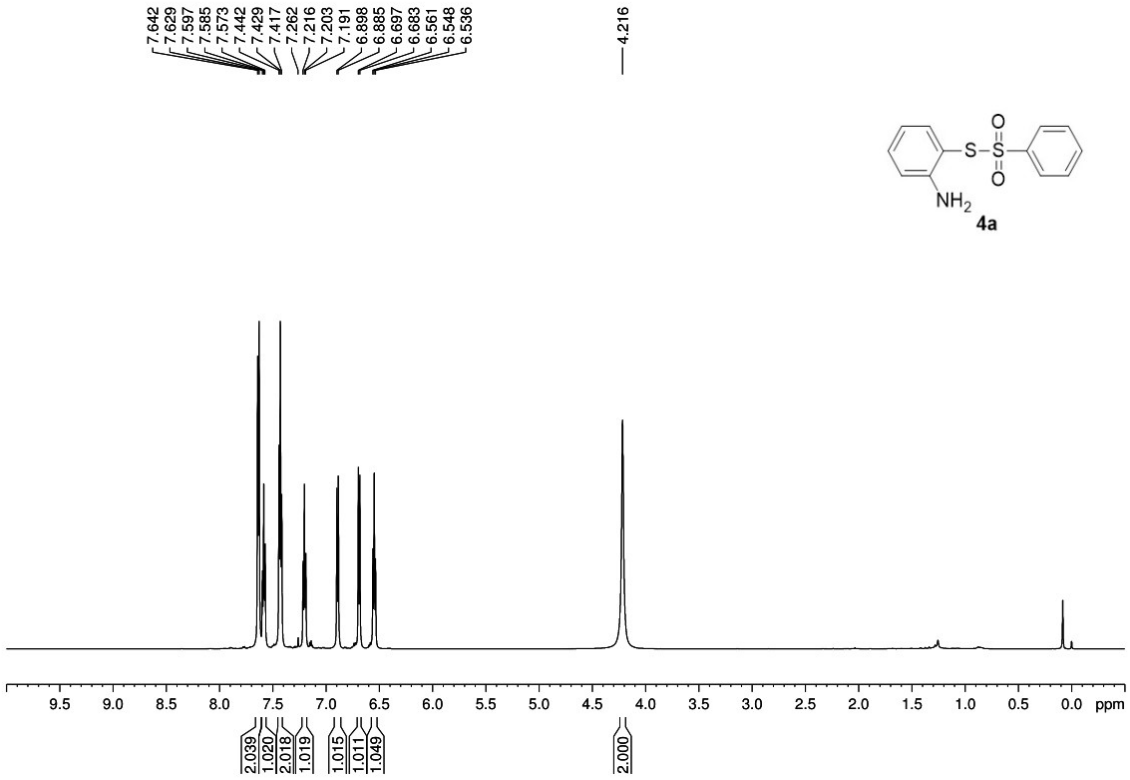
White solid (38 mg, 70% yield). Mp: 135–137 ℃ (lit.[13] 137–138 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.07 (d, *J* = 8.4 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.48 (td, *J* = 7.8, 1.2 Hz, 1H), 7.37–7.34 (m, 1H), 7.24 (d, *J* = 1.8 Hz, 2H), 6.58 (t, *J* = 2.4 Hz, 1H), 3.86 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 167.9, 161.0, 153.9, 135.3, 135.0, 126.2, 125.2, 123.2, 121.5, 105.4, 103.3, 55.5. HRMS (ESI) calcd for $C_{15}H_{14}NO_2S$ $(M+H)^+$: 272.0740; Found: 272.0744.

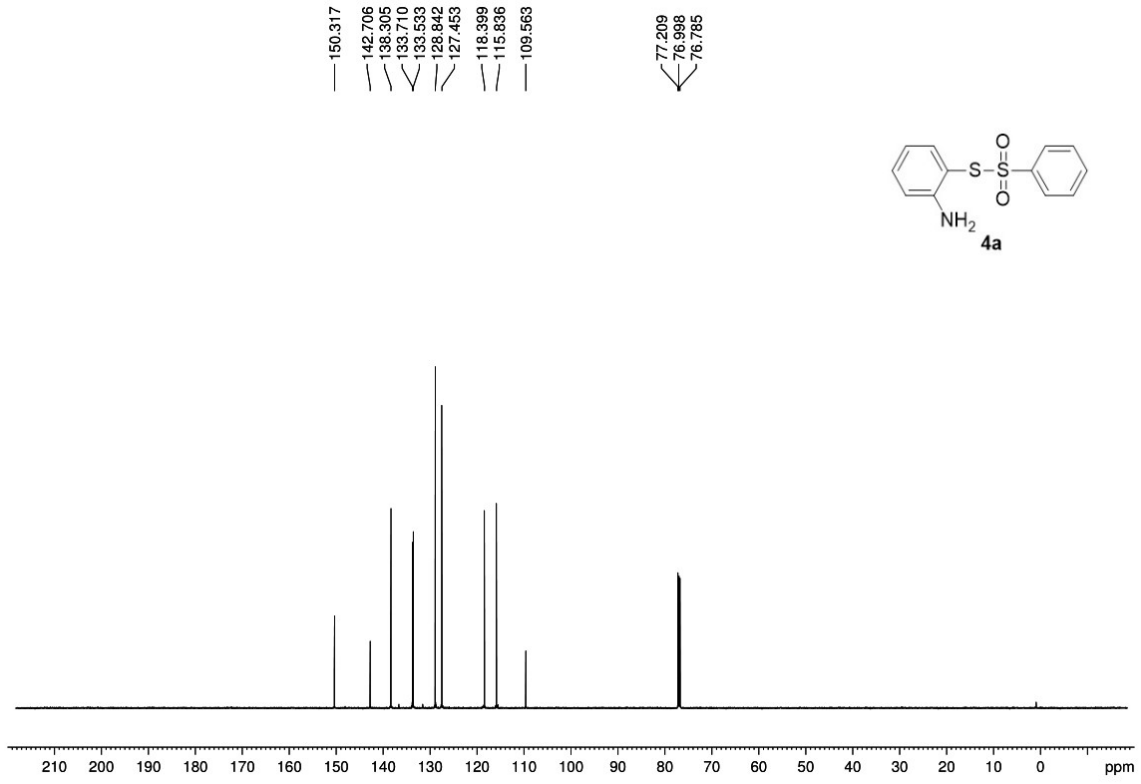
2-(3,5-Dimethylphenyl)benzo[d]thiazole (5r)

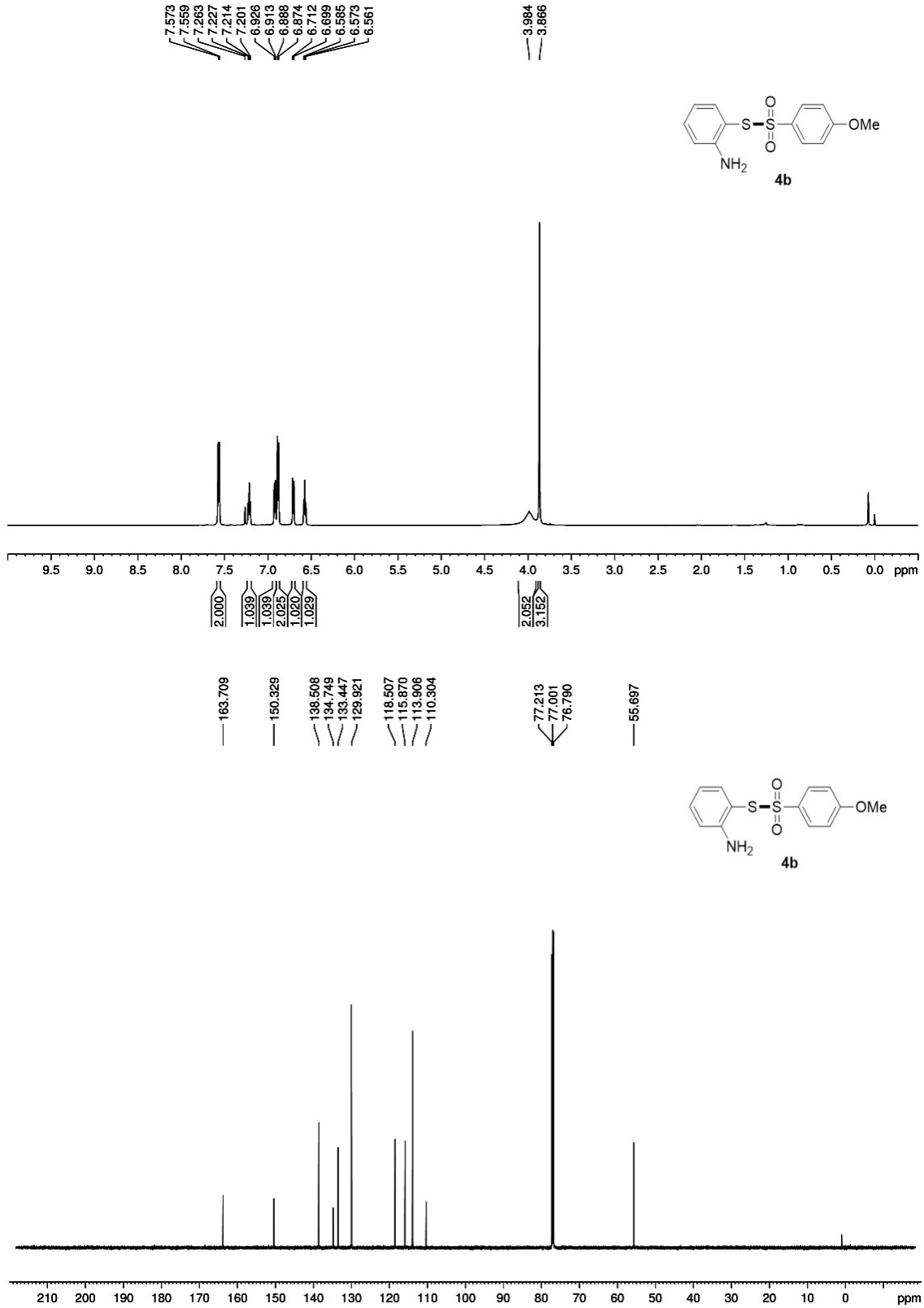


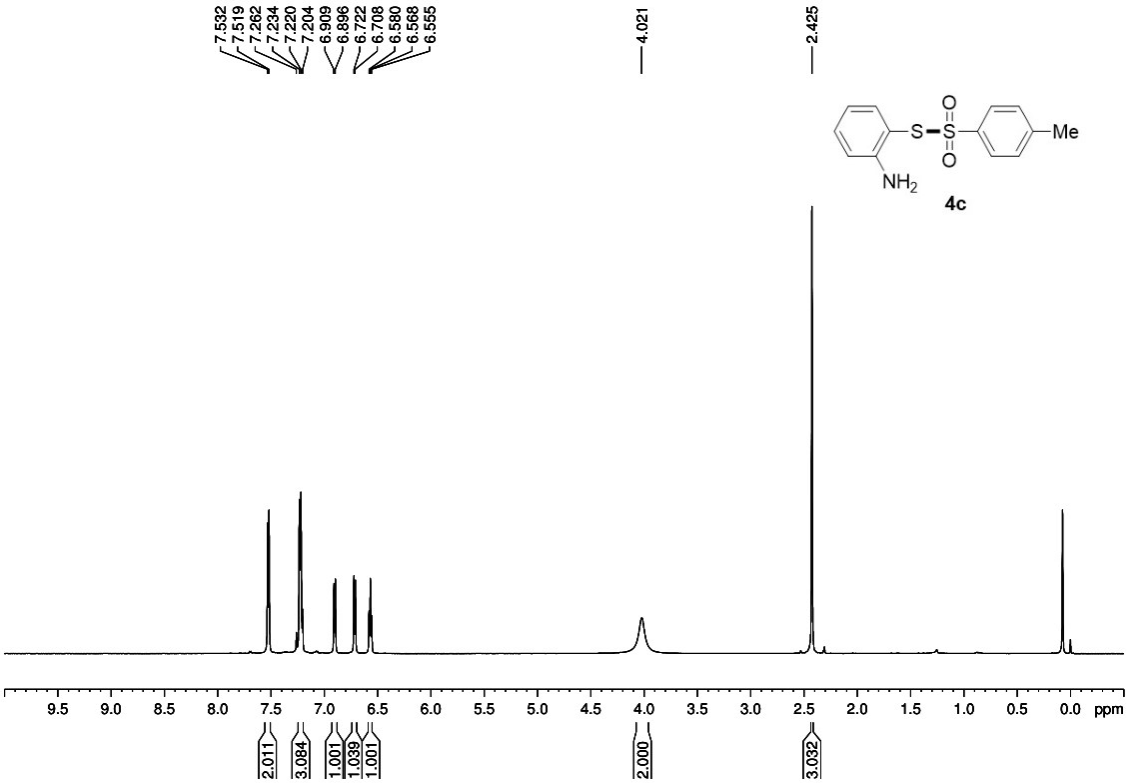
White solid (38 mg, 79% yield). Mp: 73–75 ℃ (lit.[7] 74–76 ℃). ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.08 (d, *J* = 8.4 Hz, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.72 (s, 2H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.40 (t, *J* = 7.8 Hz, 1H), 7.14 (s, 1H), 2.42 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.6, 154.1, 138.7, 135.0, 133.4, 132.8, 126.2, 125.3, 125.0, 123.1, 121.6, 21.2. HRMS (ESI) calcd for $C_{15}H_{14}NS$ $(M+H)^+$: 240.0841; Found: 240.0840.

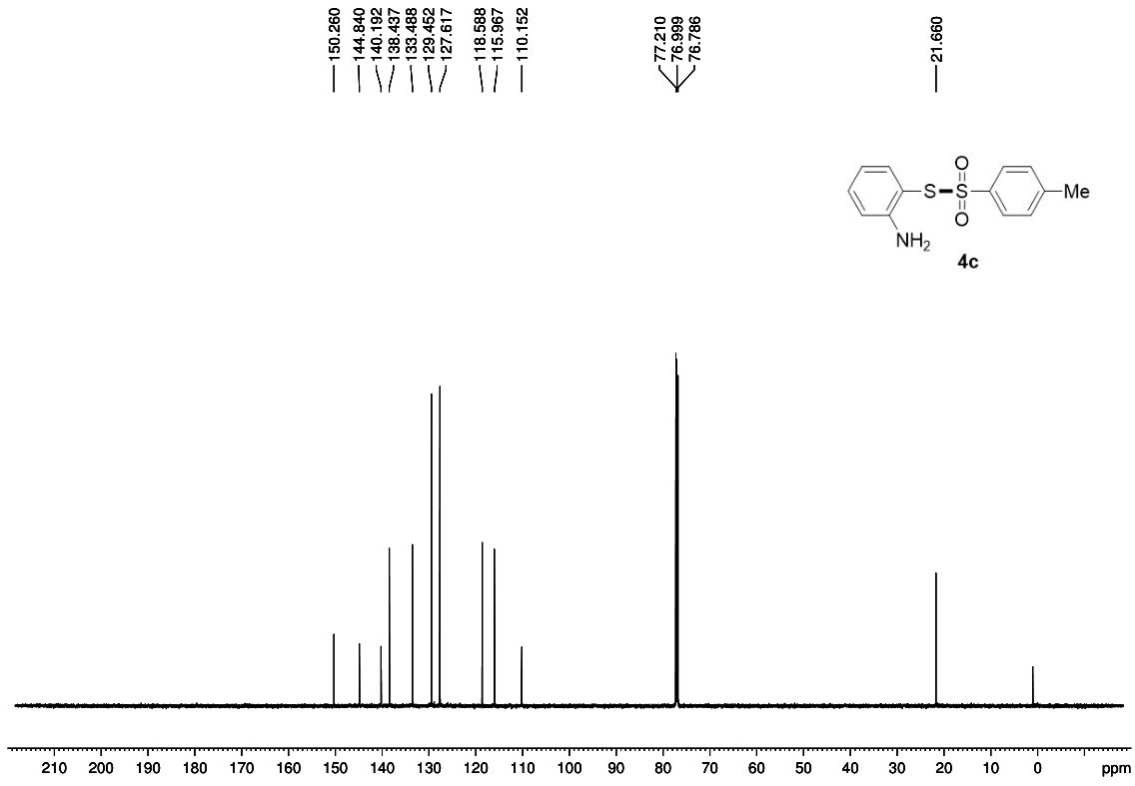
6. ^{1}H NMR and ^{13}C NMR spectra of products

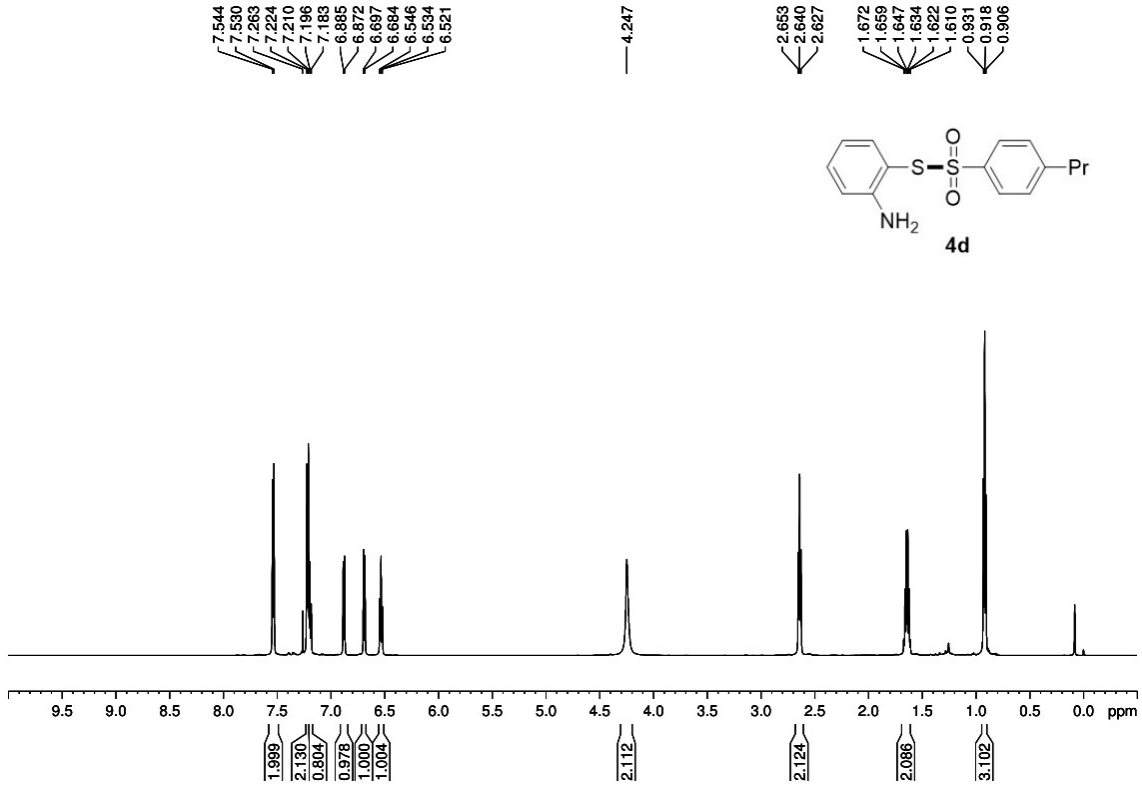


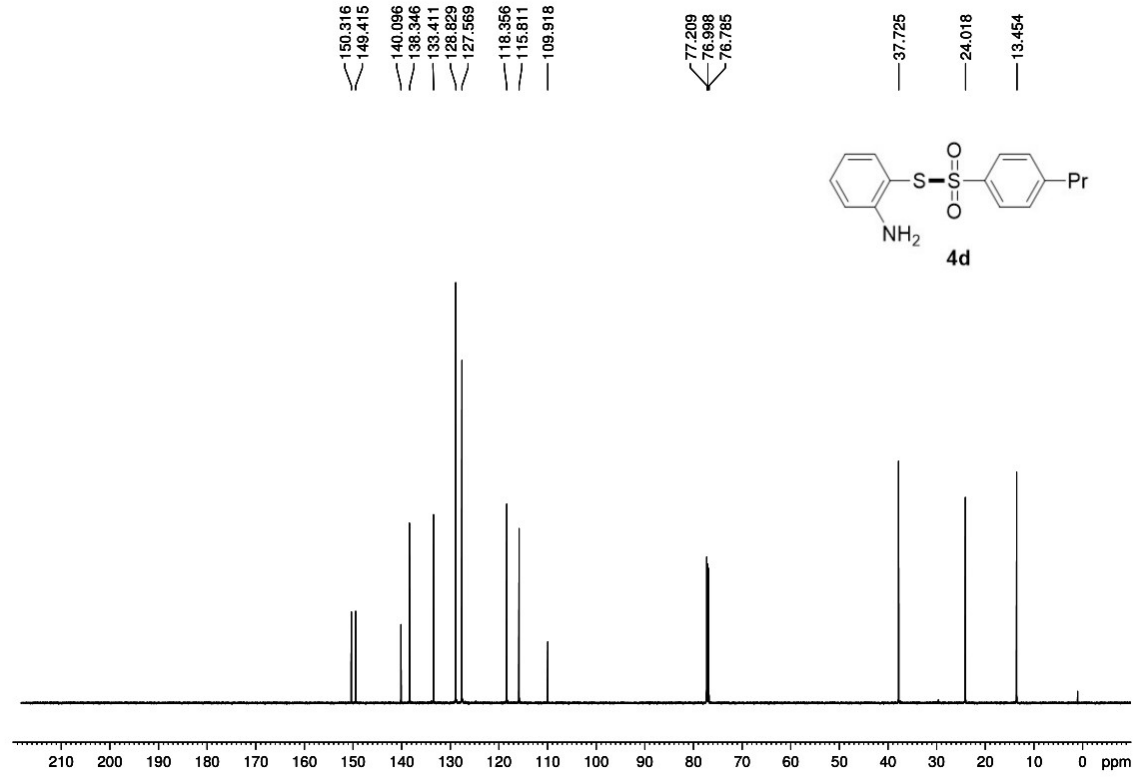


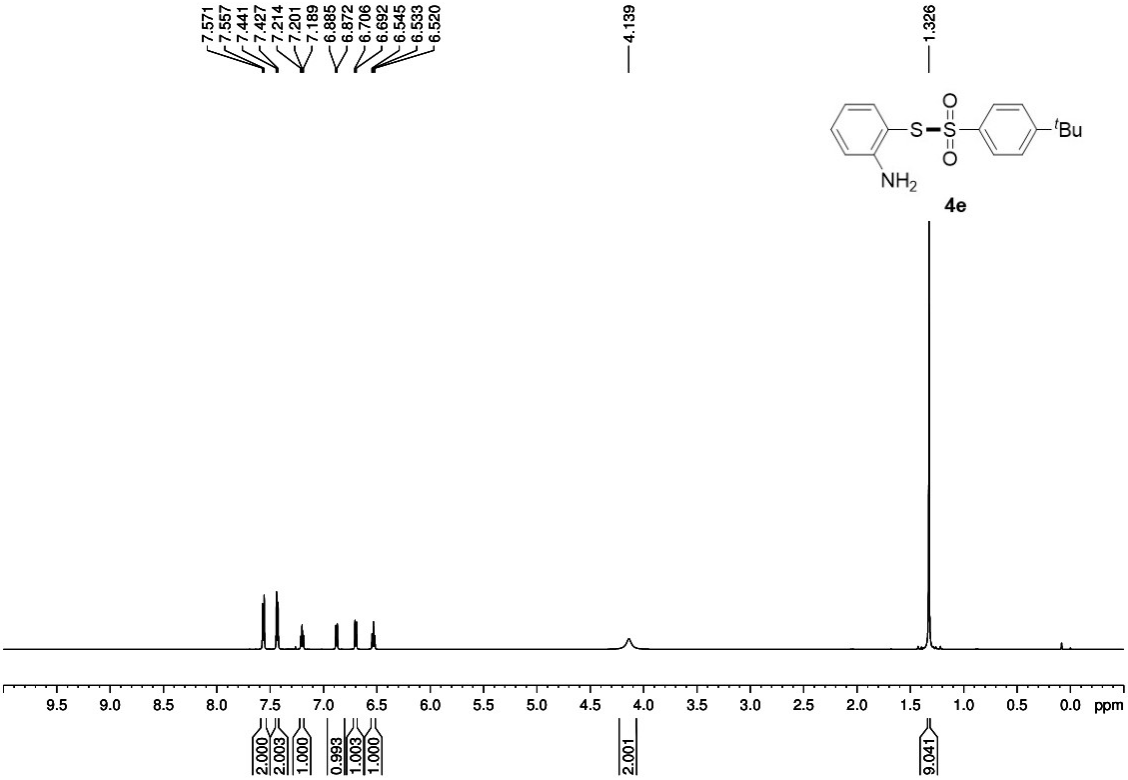

7.573
7.559
7.263
7.227
7.214
7.201
6.926
6.913
6.888
6.874
6.712
6.699
6.585
6.573
6.561
3.984
3.866
OMe
NH2
4b
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.000
1.039
1.039
2.025
1.020
1.029
2.052
3.152
163.709
150.329
138.508
134.749
133.447
129.921
118.507
115.870
113.906
110.304
77.213
77.001
76.790
55.697
OMe
NH2
4b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

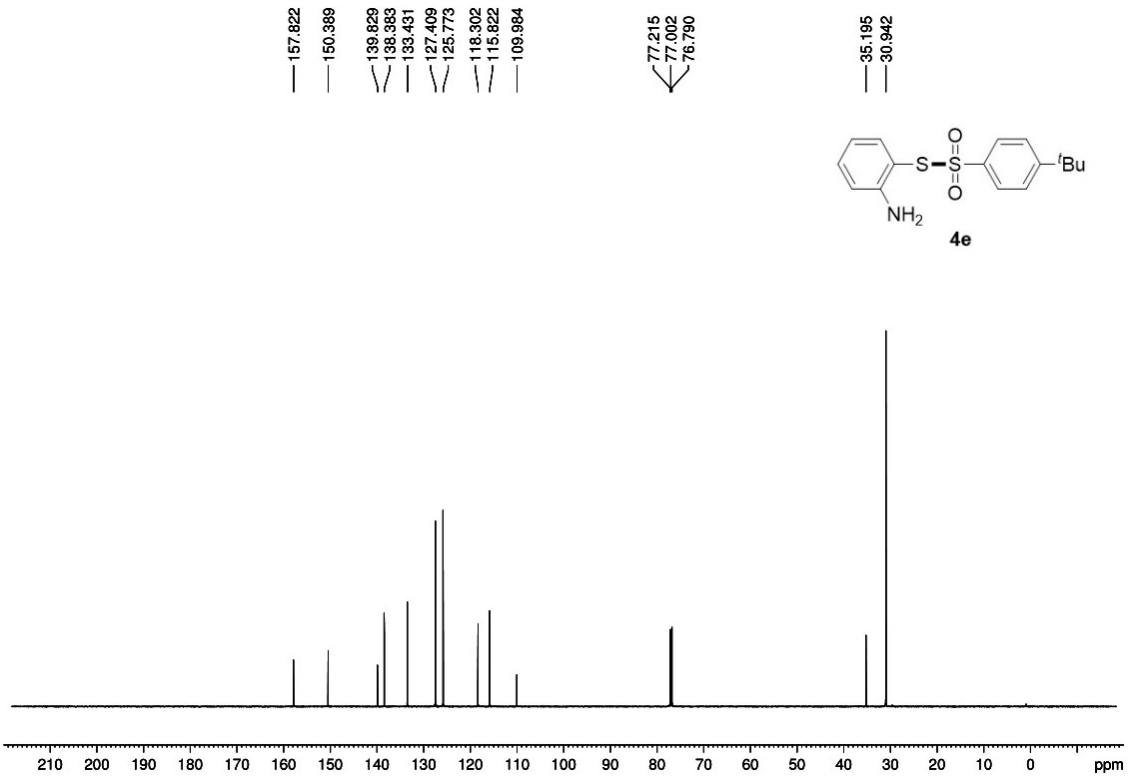

7.532
7.519
7.262
7.234
7.220
7.204
6.909
6.896
6.722
6.708
6.580
6.568
6.555
4.021
2.425
S
S
O
O
Me
NH2
4c
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.011
3.084
1.001
1.039
1.001
2.000
3.032

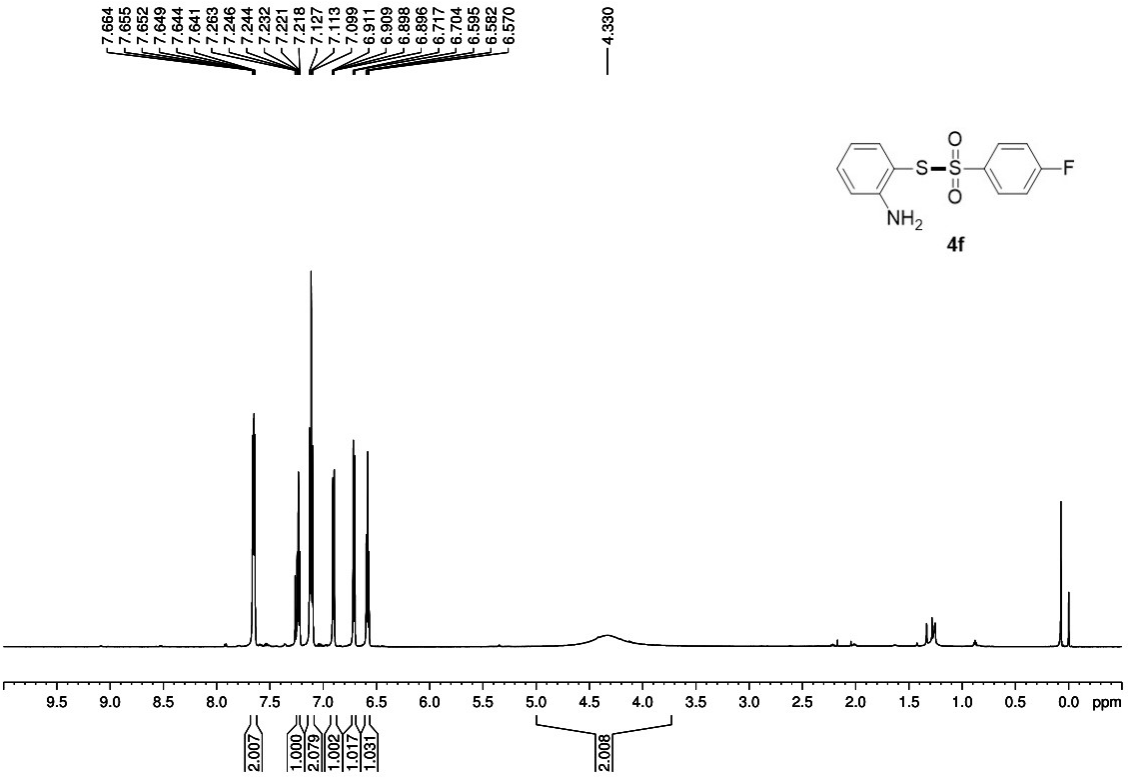

150.260
144.840
140.192
138.437
133.488
129.452
127.617
118.588
115.967
110.152
77.210
76.999
76.786
21.660
S
S
O
O
Me
NH2
4c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

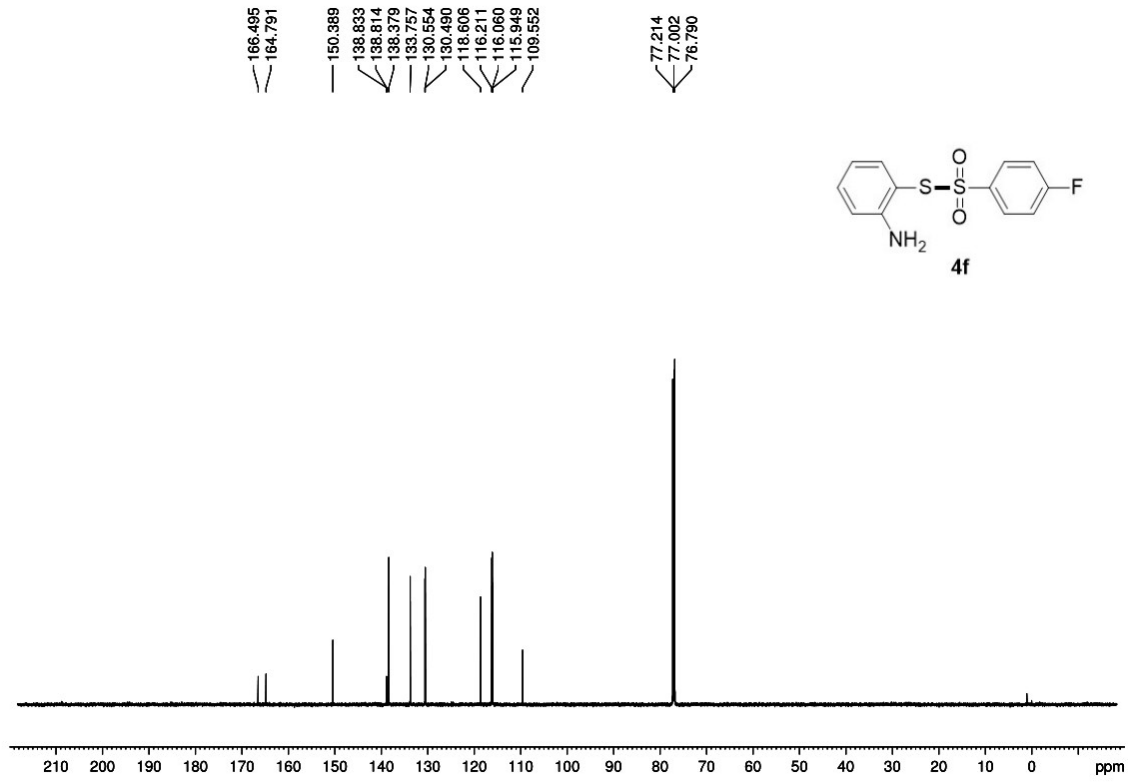

7.544
7.530
7.263
7.224
7.210
7.196
7.183
6.885
6.872
6.697
6.684
6.546
6.534
6.521
4.247
2.653
2.640
2.627
1.672
1.659
1.647
1.634
1.622
1.610
0.931
0.918
0.906
S
O
O
Pr
NH2
4d
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.999
2.130
0.804
0.978
1.000
1.004
2.112
2.124
2.086
3.102

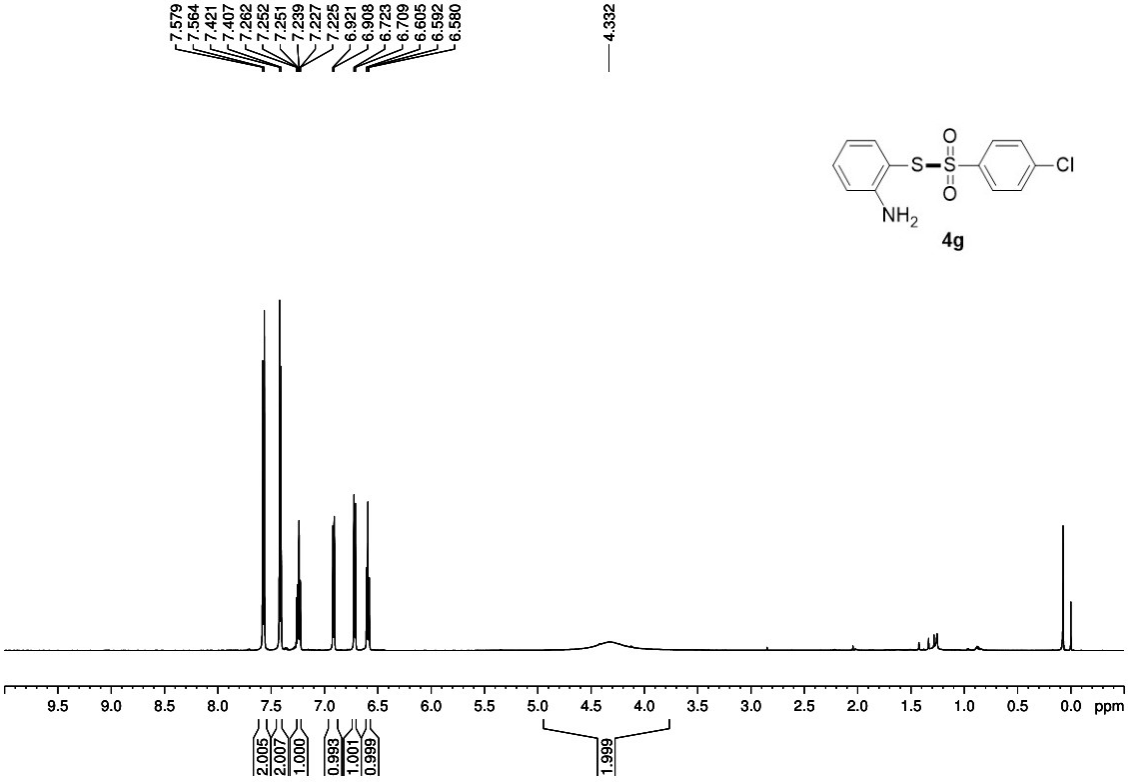

150.316
149.415
140.096
138.346
133.411
128.829
127.569
118.356
115.811
109.918
77.209
76.998
76.785
37.725
24.018
13.454
S
O
O
Pr
NH2
4d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

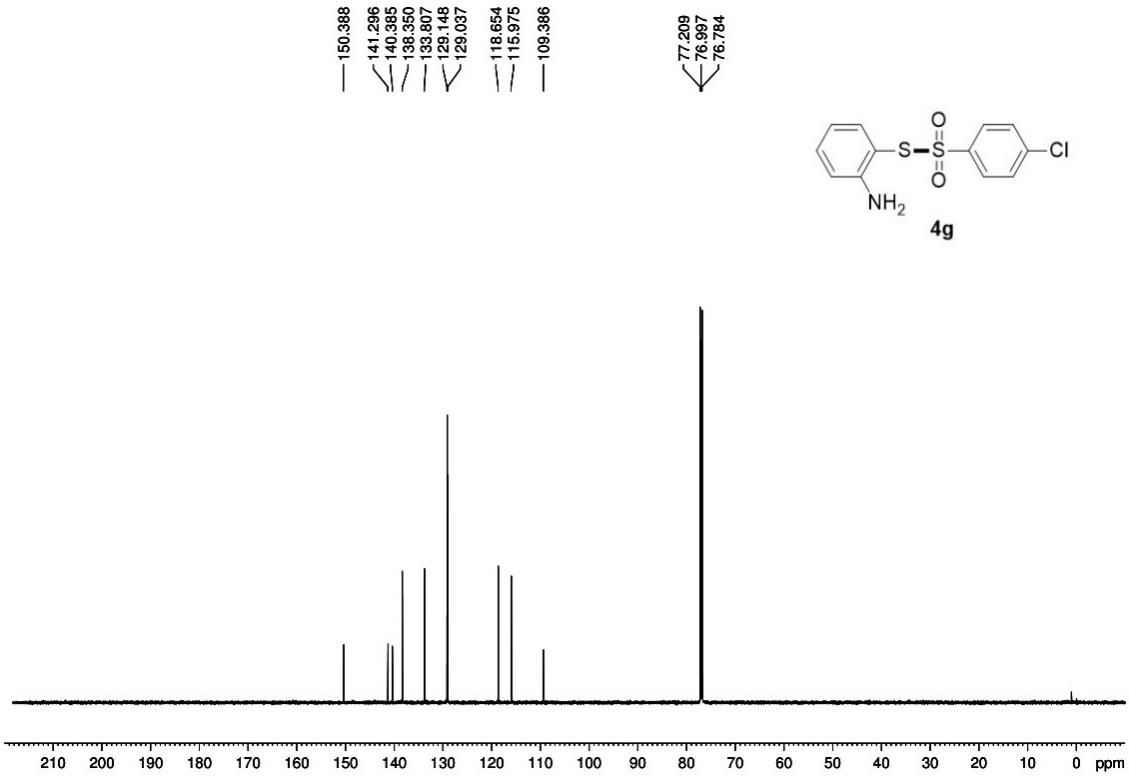

7.571
7.557
7.441
7.427
7.214
7.201
7.189
6.885
6.872
6.706
6.692
6.545
6.533
6.520
4.139
1.326
S
O
O
tBu
NH2
4e
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.000
2.003
1.000
0.993
1.003
1.000
2.001
9.041

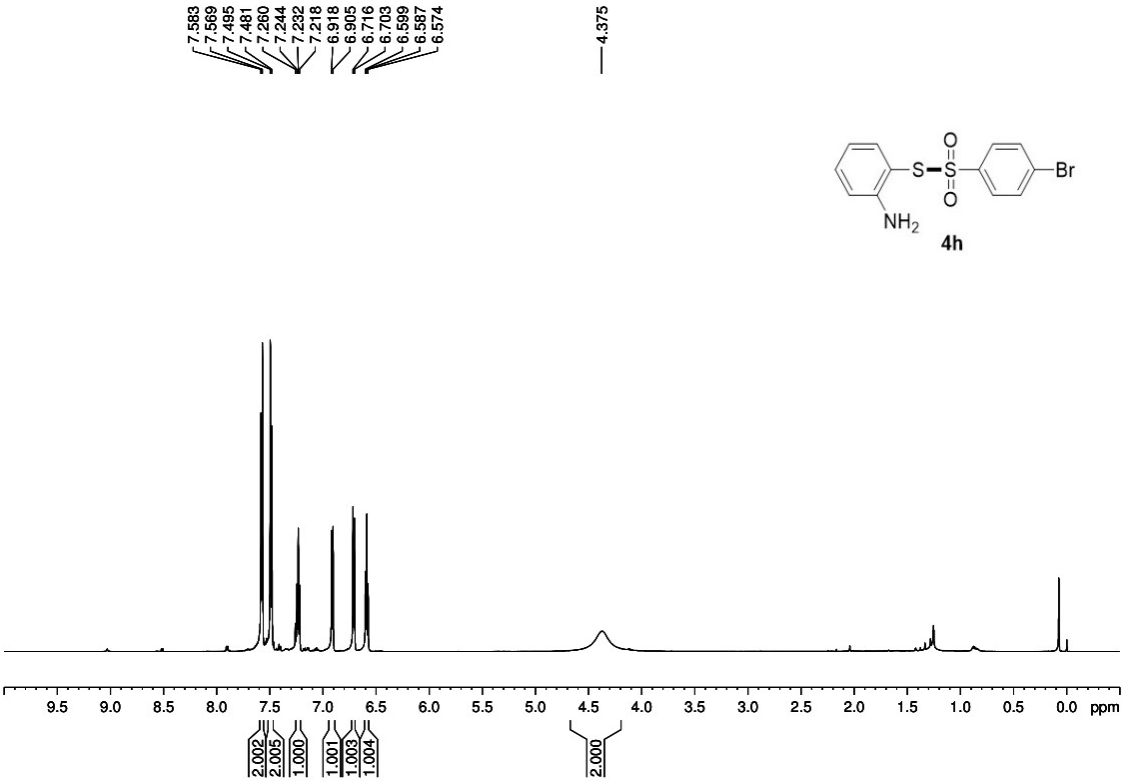

157.822
150.389
139.829
138.383
133.431
127.409
125.773
118.302
115.822
109.984
77.215
77.002
76.790
35.195
30.942
S
O
O
tBu
NH2
4e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

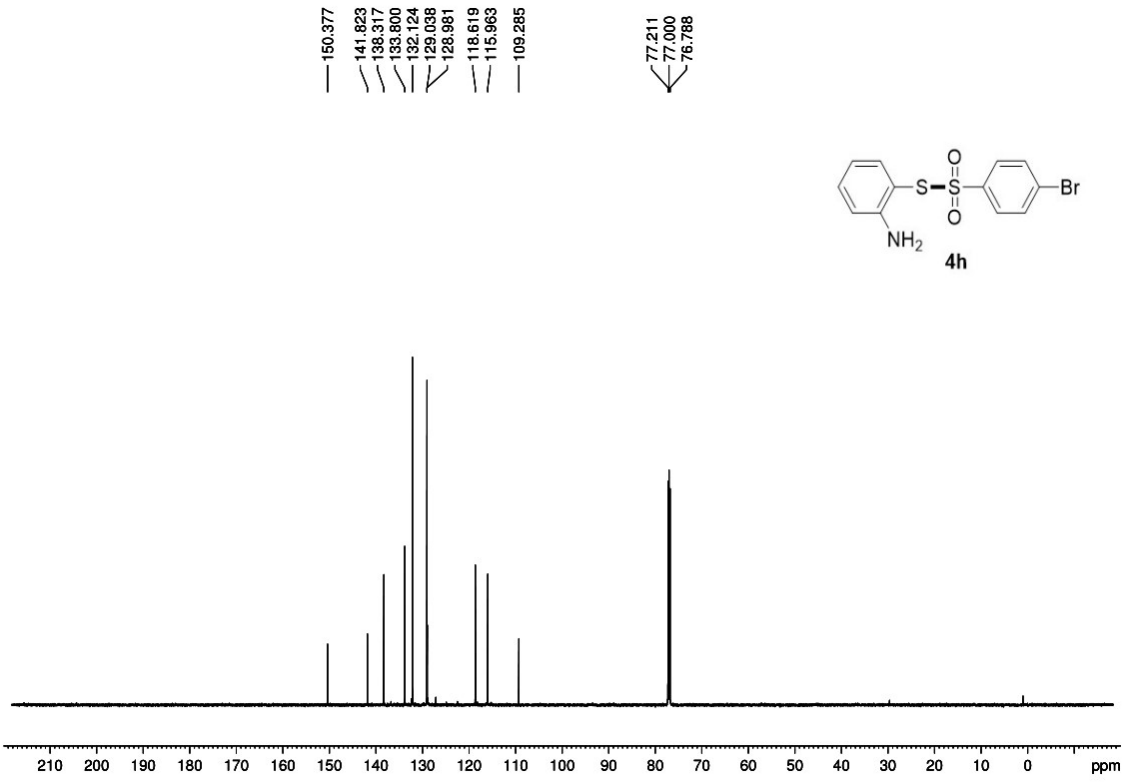

7.664
7.655
7.652
7.649
7.644
7.641
7.263
7.246
7.244
7.232
7.221
7.218
7.127
7.113
7.099
6.911
6.909
6.898
6.896
6.717
6.704
6.595
6.582
6.570
4.330
4f
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.007
1.000
2.079
1.002
1.017
1.031
2.008

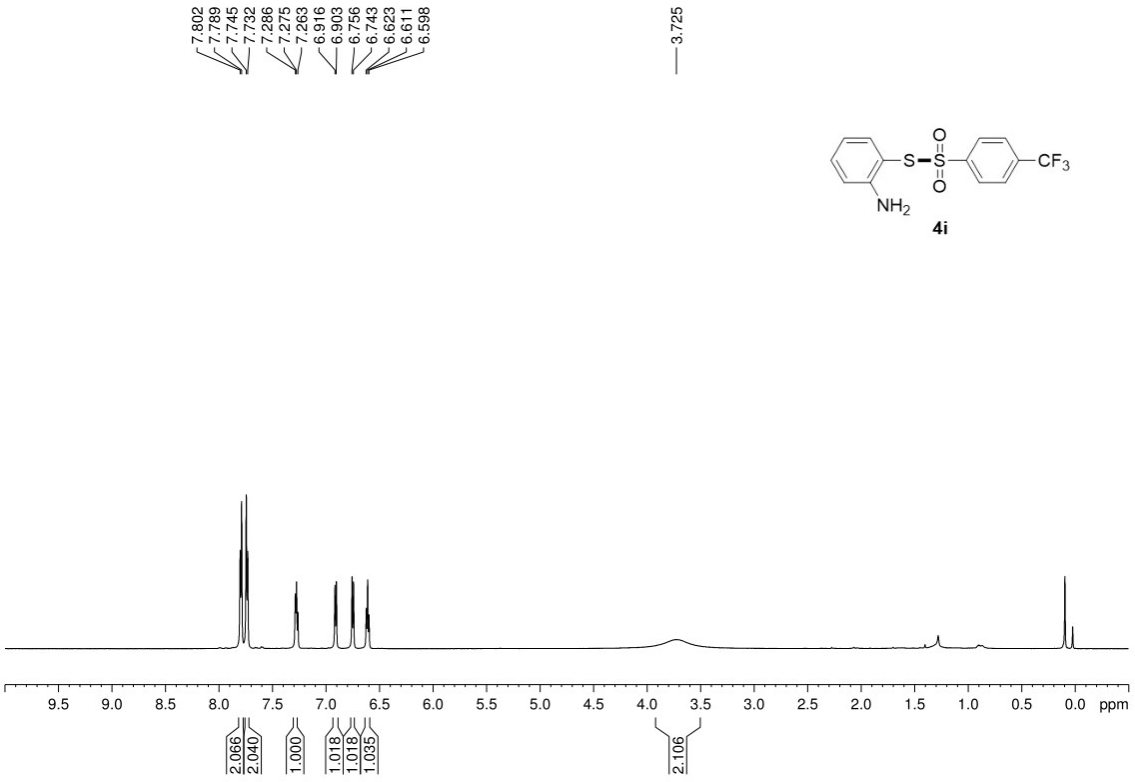

166.495
164.791
150.389
138.833
138.814
138.379
133.757
130.554
130.490
118.606
116.211
116.060
115.949
109.552
77.214
77.002
76.790
4f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

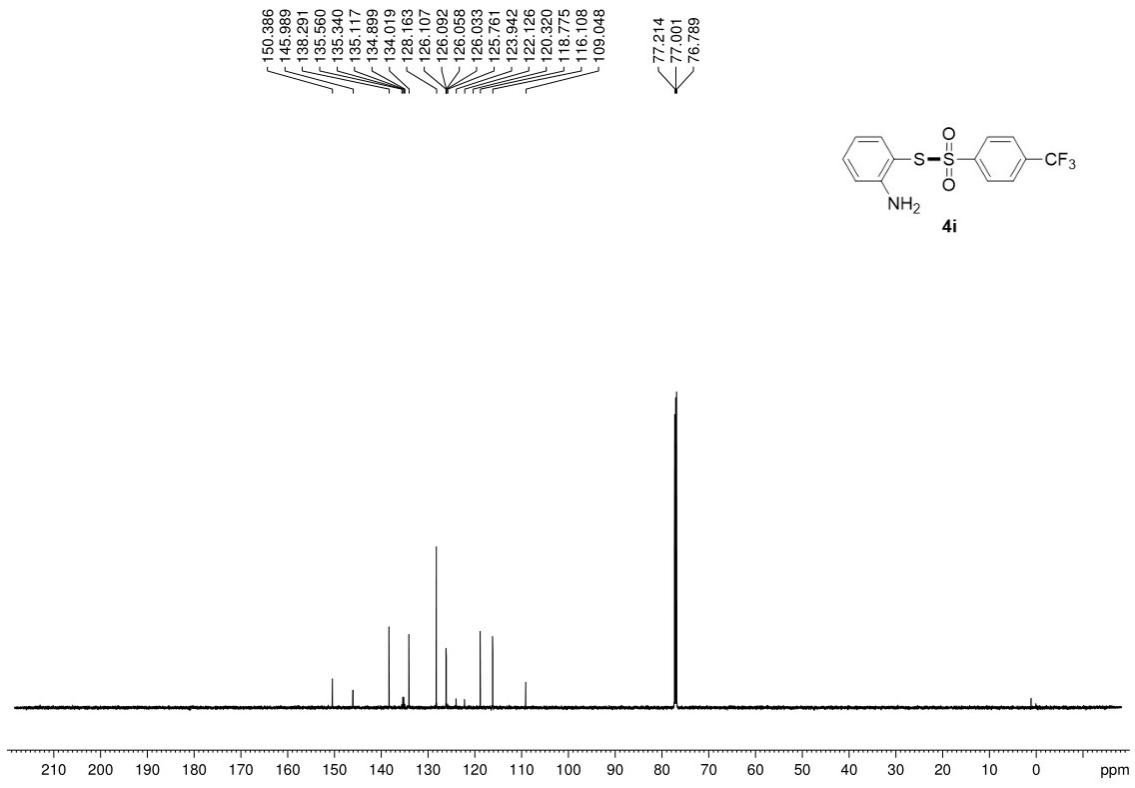

7.579
7.564
7.421
7.407
7.262
7.252
7.251
7.239
7.227
7.225
6.921
6.908
6.723
6.709
6.605
6.592
6.580
4.332
S
S
O
O
Cl
NH2
4g
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.005
2.007
1.000
0.993
1.001
0.999
1.999

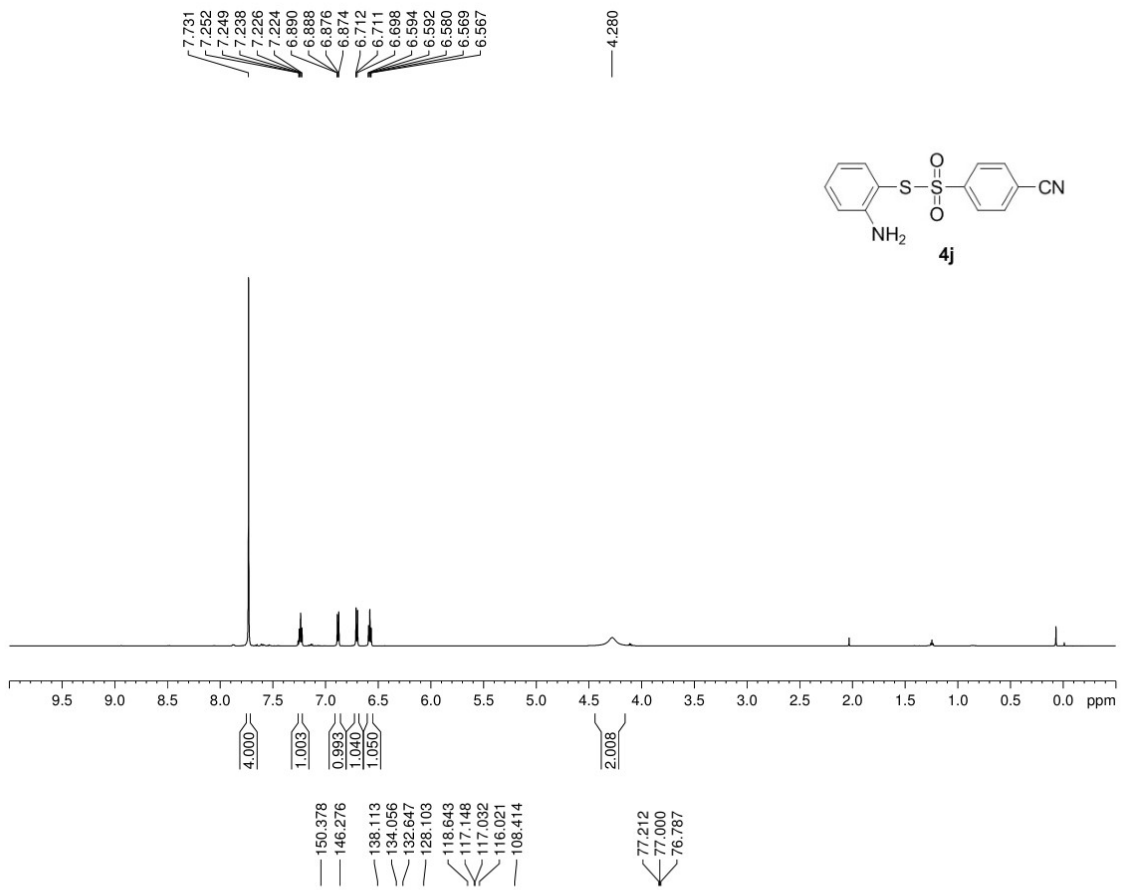

150.388
141.296
140.385
138.350
133.807
129.148
129.037
118.654
115.975
109.386
77.209
76.997
76.784
S
S
O
O
Cl
NH2
4g
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

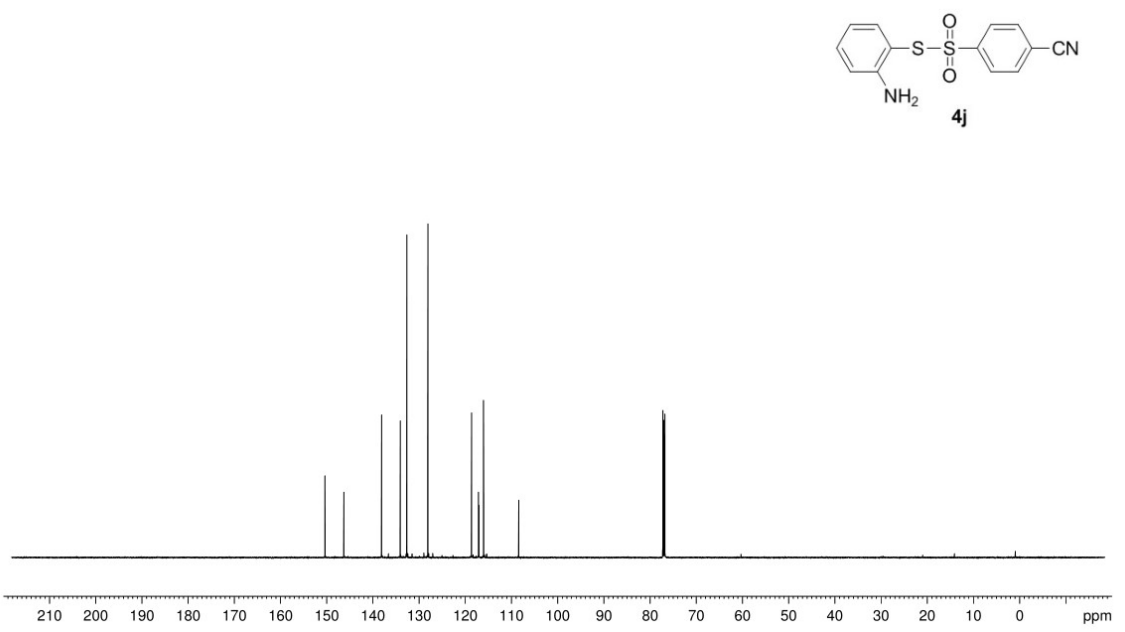

7.583
7.569
7.495
7.481
7.260
7.244
7.232
7.218
6.918
6.905
6.716
6.703
6.599
6.587
6.574
4.375
S
O
O
Br
NH2
4h
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.002
2.005
1.000
1.001
1.003
1.004
2.000

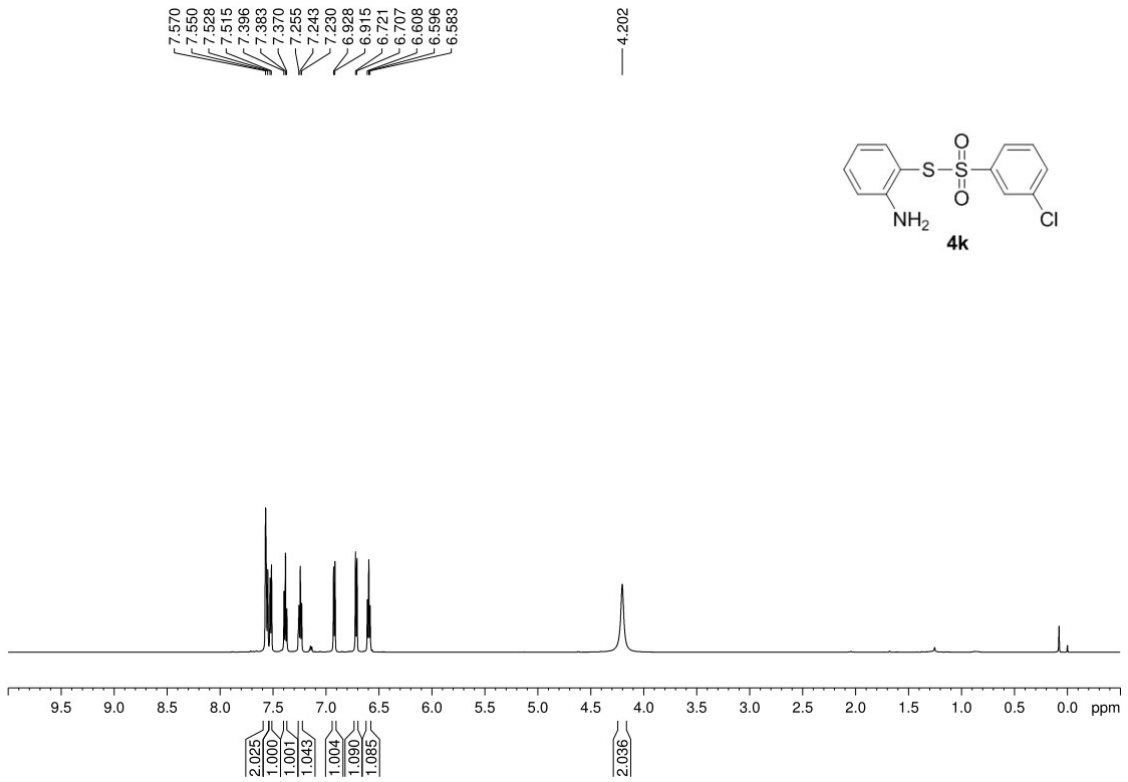

150.377
141.823
138.317
133.800
132.124
129.038
128.981
118.619
115.963
109.285
77.211
77.000
76.788
S
O
O
Br
NH2
4h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

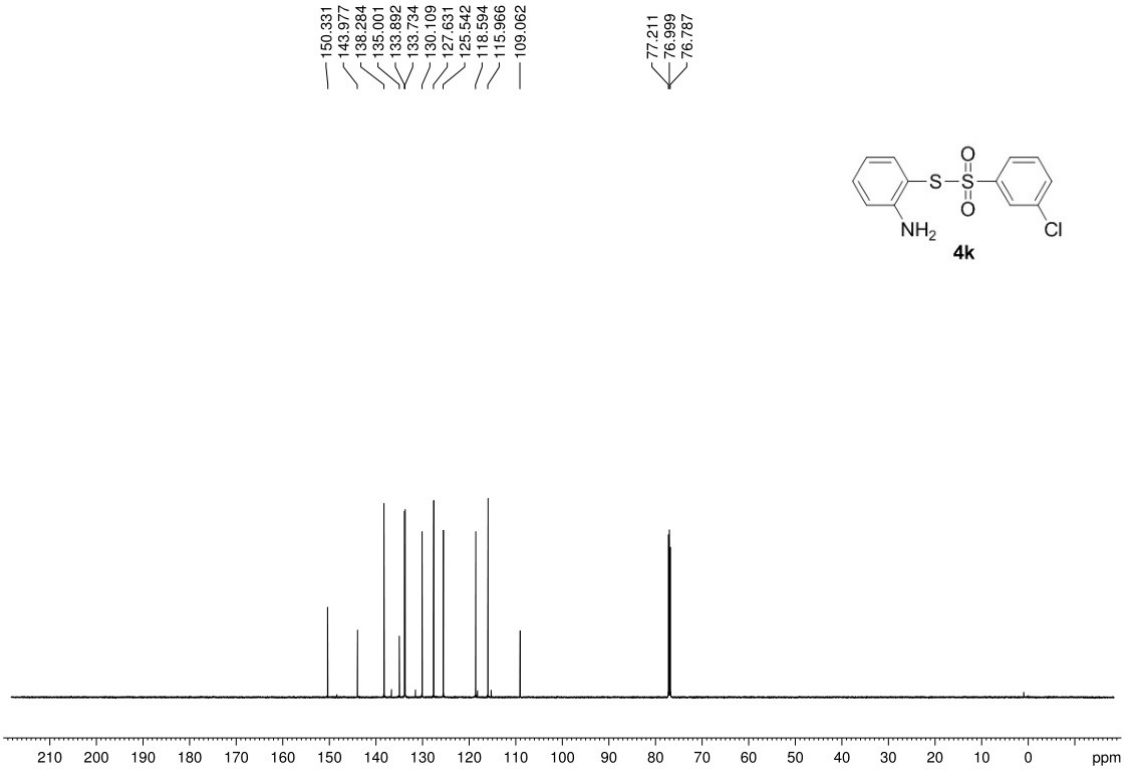

7.802
7.789
7.745
7.732
7.286
7.275
7.263
6.916
6.903
6.756
6.743
6.623
6.611
6.598
3.725
NH2
CF3
4i
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.066
2.040
1.000
1.018
1.018
1.035
2.106

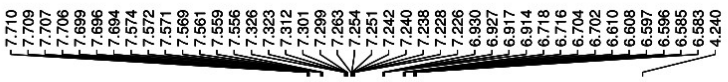

150.386
145.989
138.291
135.560
135.340
135.117
134.899
134.019
128.163
126.107
126.092
126.058
126.033
125.761
123.942
122.126
120.320
118.775
116.108
109.048
77.214
77.001
76.789
NH2
CF3
4i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

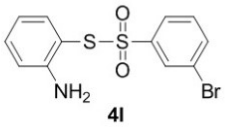

7.731
7.252
7.249
7.238
7.226
7.224
6.890
6.888
6.876
6.874
6.712
6.711
6.698
6.594
6.592
6.580
6.569
6.567
4.280
NH2
4j
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
4.000
1.003
0.993
1.040
1.050
2.008


150.378
146.276
138.113
134.056
132.647
128.103
118.643
117.148
117.032
116.021
108.414
77.212
77.000
76.787
NH2
4j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

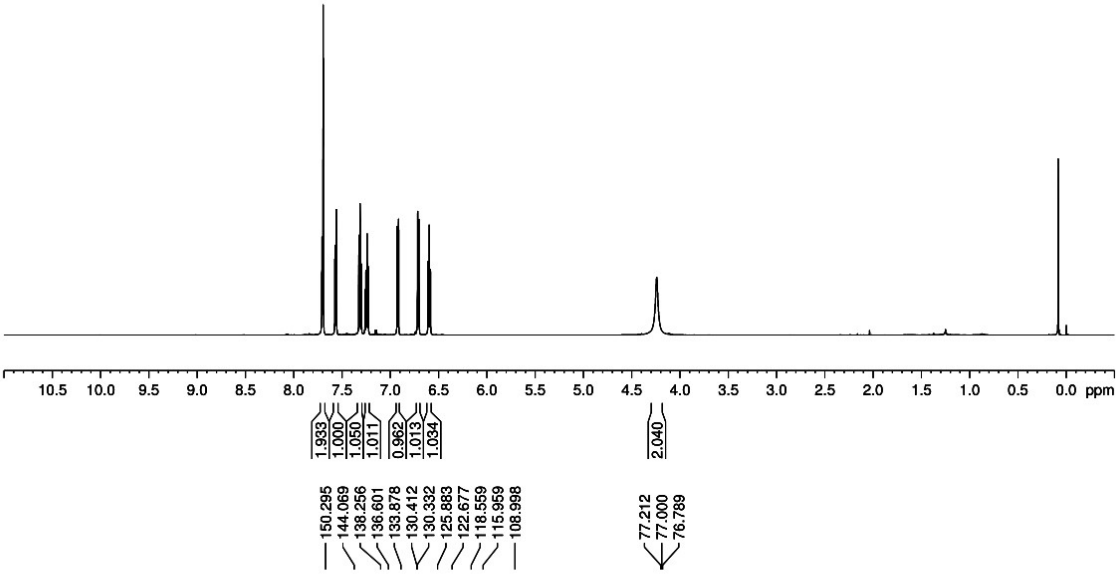

7.570
7.550
7.528
7.515
7.396
7.383
7.370
7.255
7.243
7.230
6.928
6.915
6.721
6.707
6.608
6.596
6.583
4.202
NH2
Cl
4k
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.025
1.000
1.001
1.043
1.004
1.090
1.085
2.036

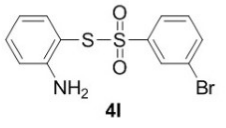

150.331
143.977
138.284
135.001
133.892
133.734
130.109
127.631
125.542
118.594
115.966
109.062
77.211
76.999
76.787
NH2
Cl
4k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.710
7.709
7.707
7.706
7.699
7.696
7.694
7.574
7.572
7.571
7.569
7.561
7.559
7.556
7.326
7.323
7.312
7.301
7.299
7.263
7.254
7.251
7.242
7.240
7.238
7.228
7.226
6.930
6.927
6.917
6.914
6.718
6.716
6.704
6.702
6.610
6.608
6.597
6.596
6.585
6.583
4.240

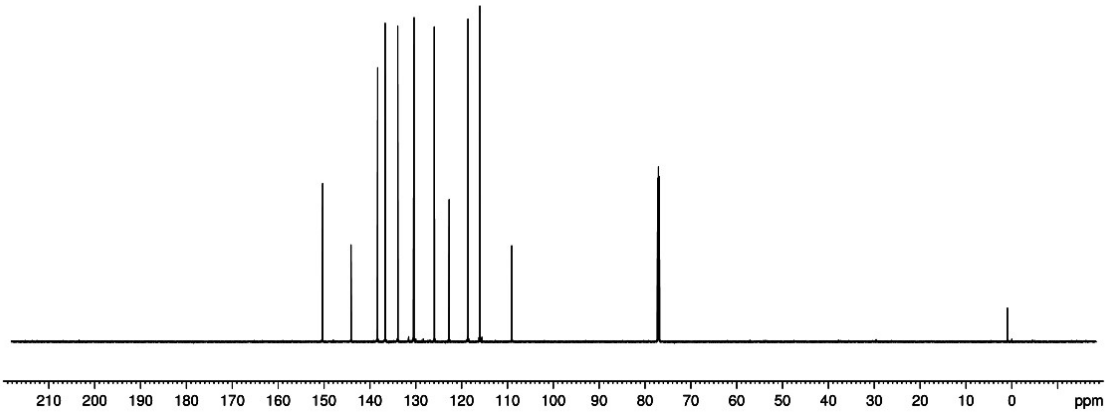

O
S
S
O
O
NH2
Br

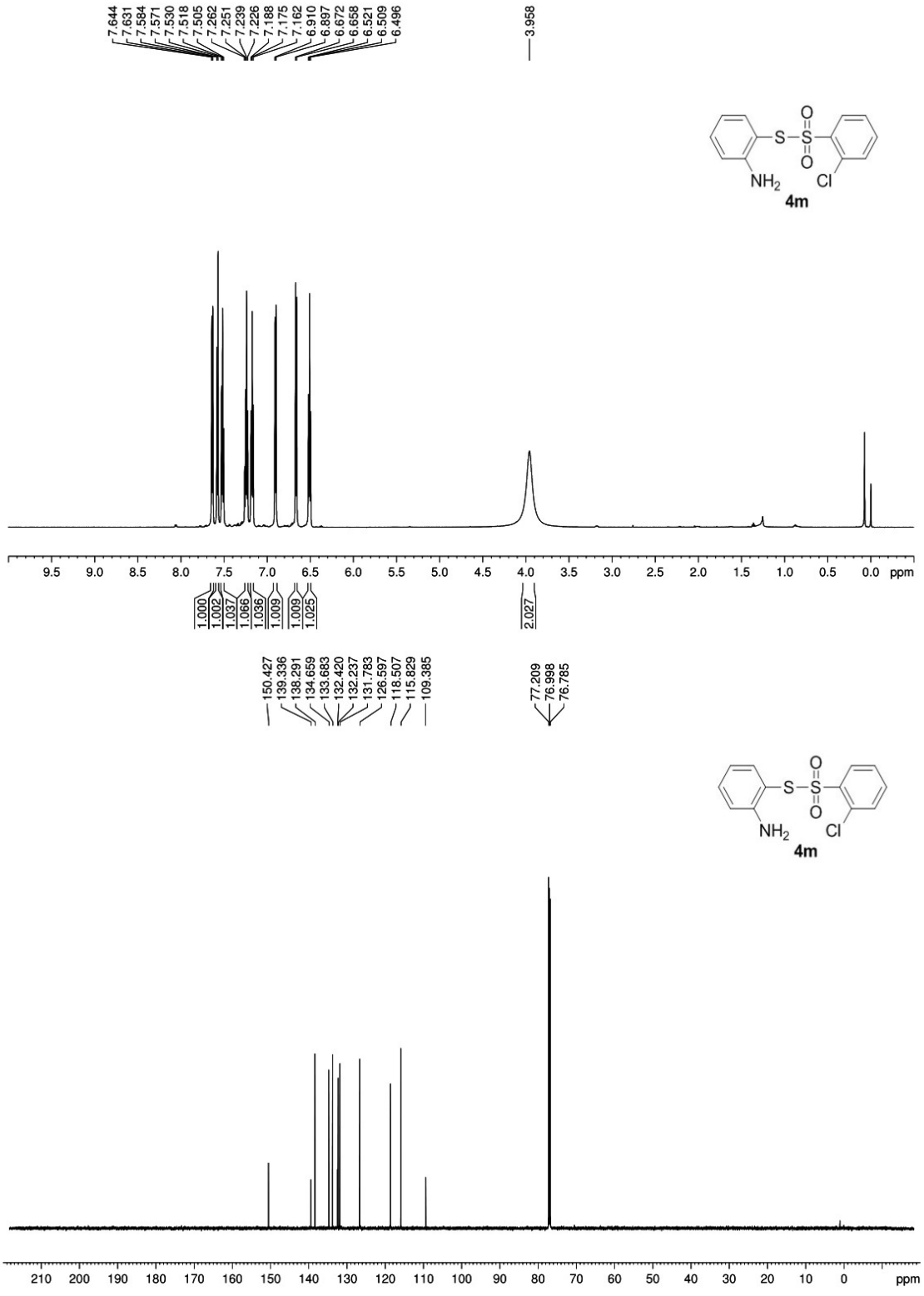
4l

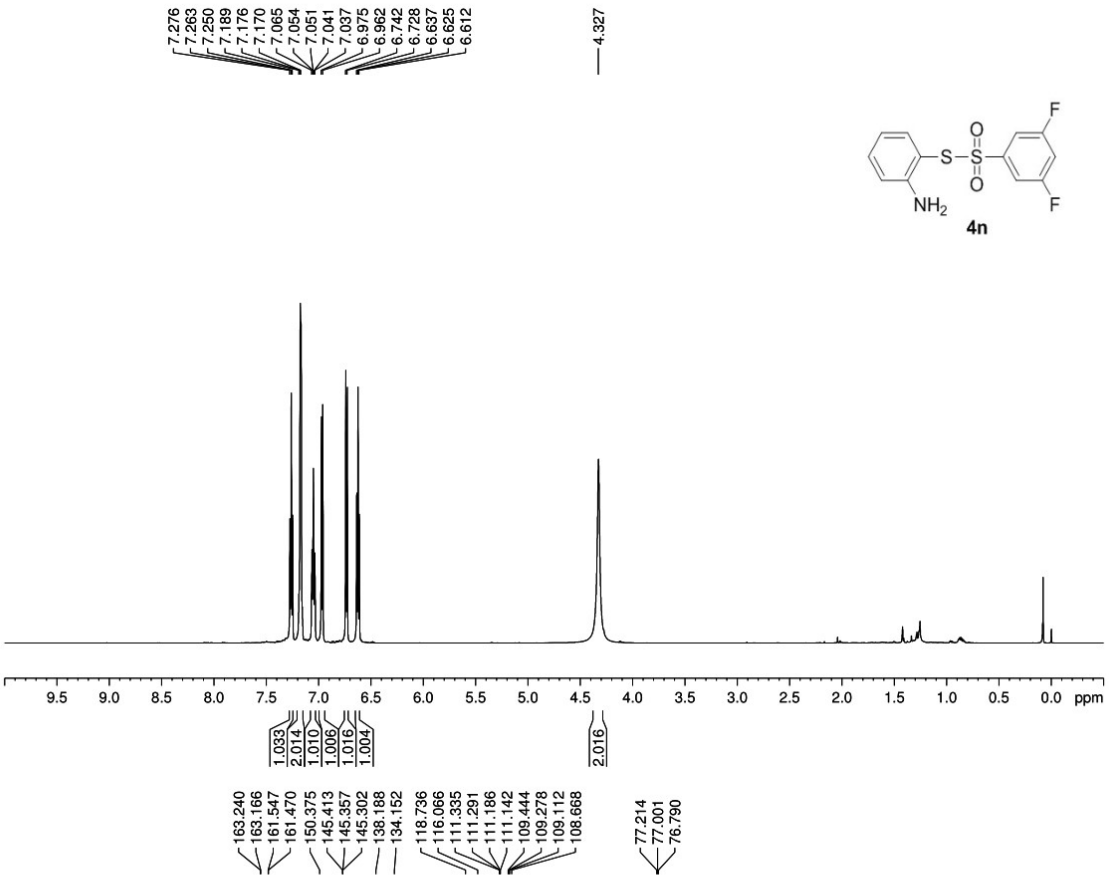

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.933
1.000
1.050
1.011
0.962
1.013
1.034
2.040
150.295
144.069
138.256
136.601
133.878
130.412
130.332
125.883
122.677
118.559
115.959
108.998
77.212
77.000
76.789

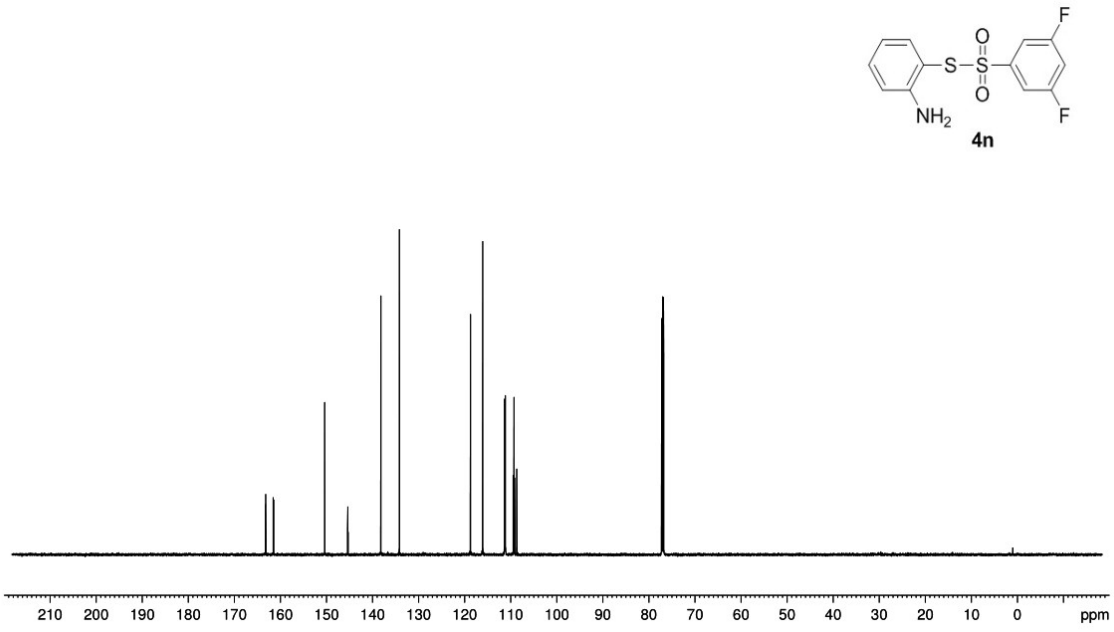

O
S
S
O
O
NH2
Br

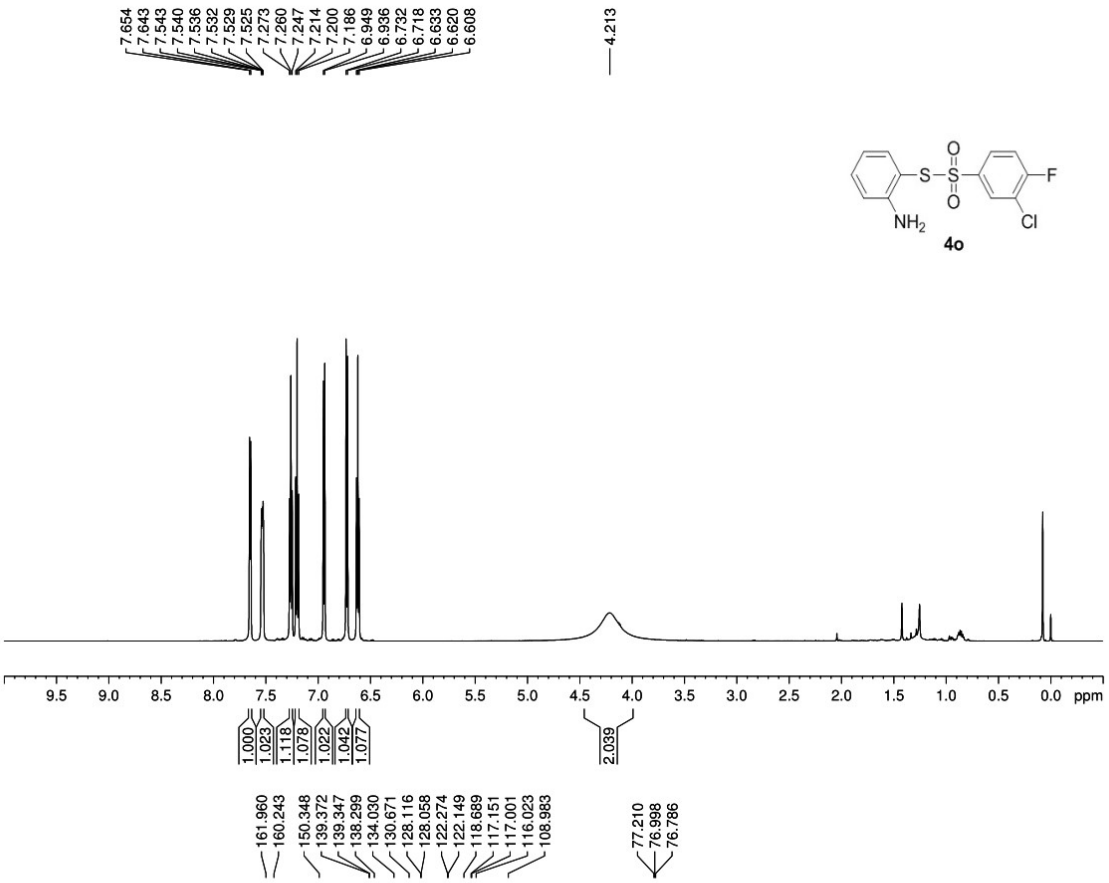
4l

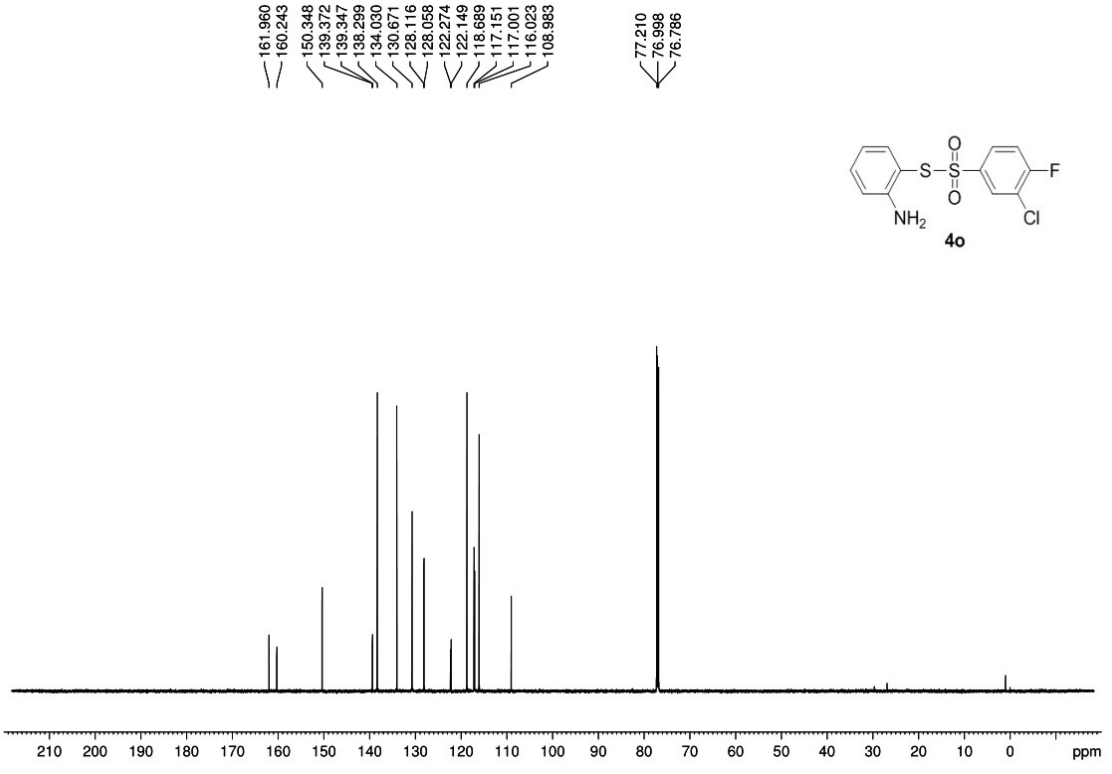

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

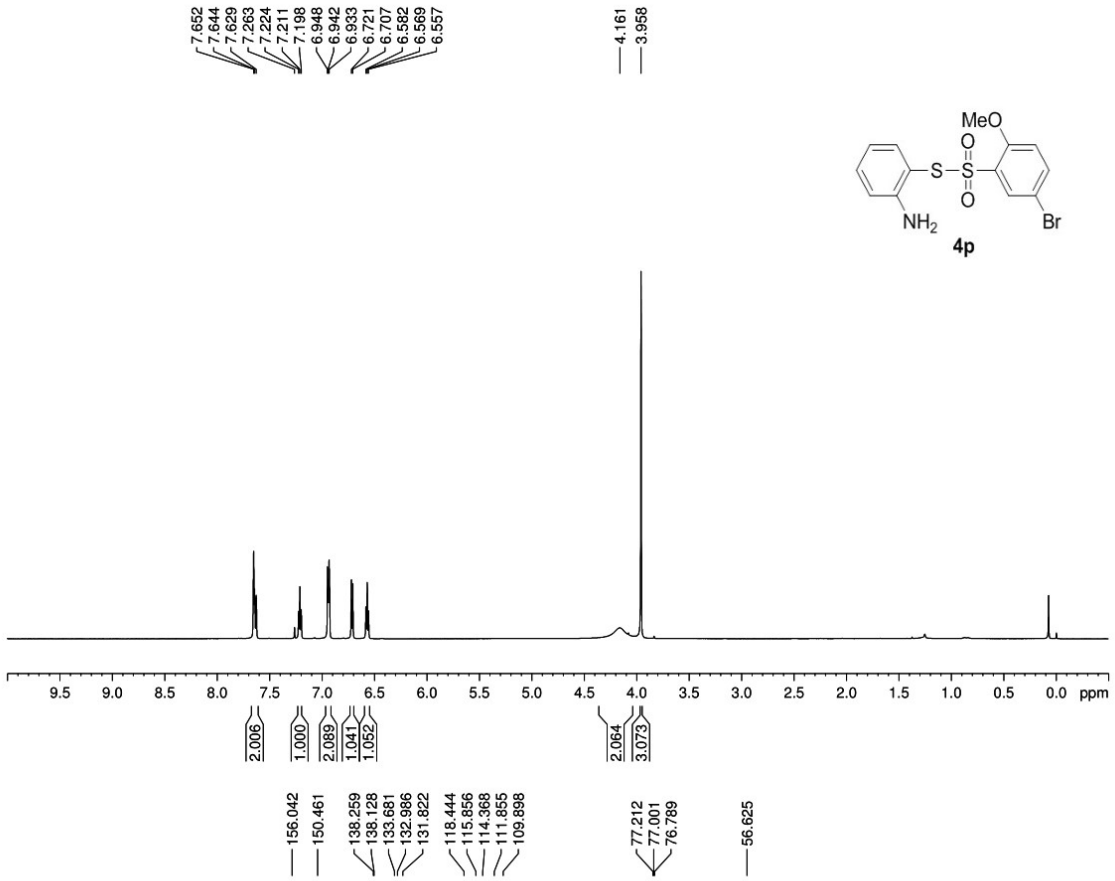

7.644
7.631
7.584
7.571
7.530
7.518
7.505
7.262
7.251
7.239
7.226
7.188
7.175
7.162
6.910
6.897
6.672
6.658
6.521
6.509
6.496
3.958
S
O
O
NH2
Cl
4m
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
1.002
1.037
1.066
1.036
1.009
1.009
1.025
2.027
150.427
139.336
138.291
134.659
133.683
132.420
132.237
131.783
126.597
118.507
115.829
109.385
77.209
76.998
76.785
S
O
O
NH2
Cl
4m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

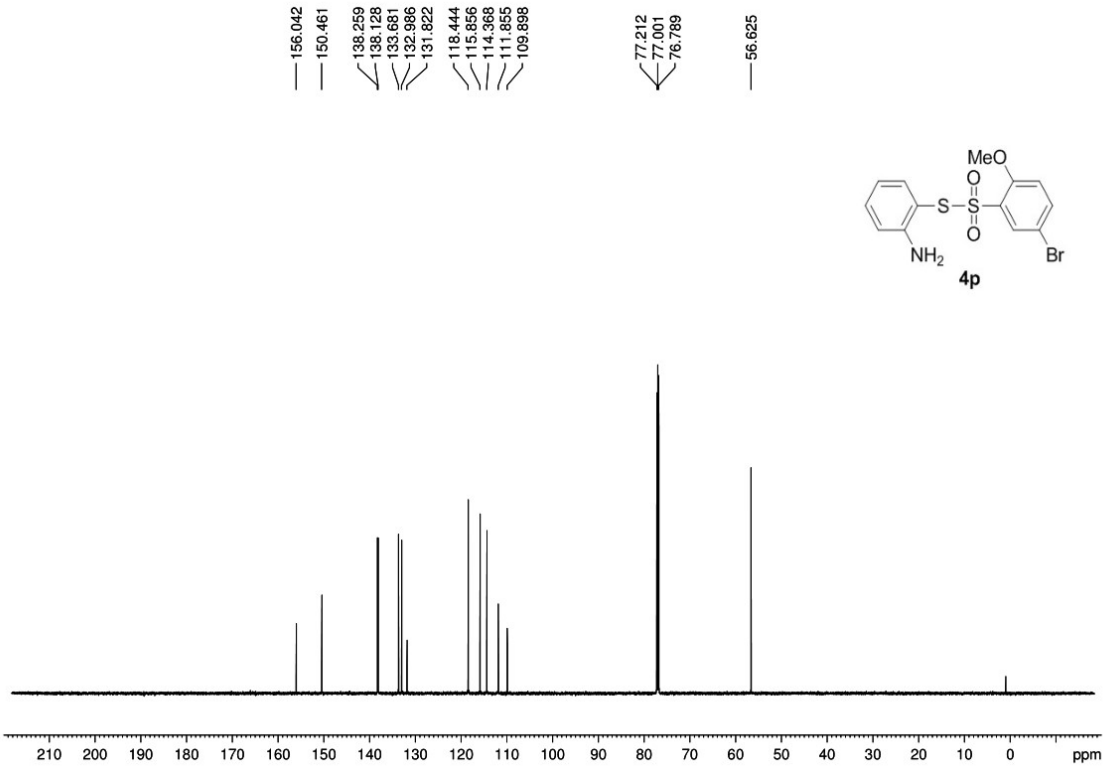

7.276
7.263
7.250
7.189
7.176
7.170
7.065
7.054
7.051
7.041
7.037
6.975
6.962
6.742
6.728
6.637
6.625
6.612
4.327
F
O
S
S
O
F
NH2
4n
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.033
2.014
1.010
1.006
1.016
1.004
2.016
163.240
163.166
161.547
161.470
150.375
145.413
145.357
145.302
138.188
134.152
118.736
116.066
111.335
111.291
111.186
111.142
109.444
109.278
109.112
108.668
77.214
77.001
76.790

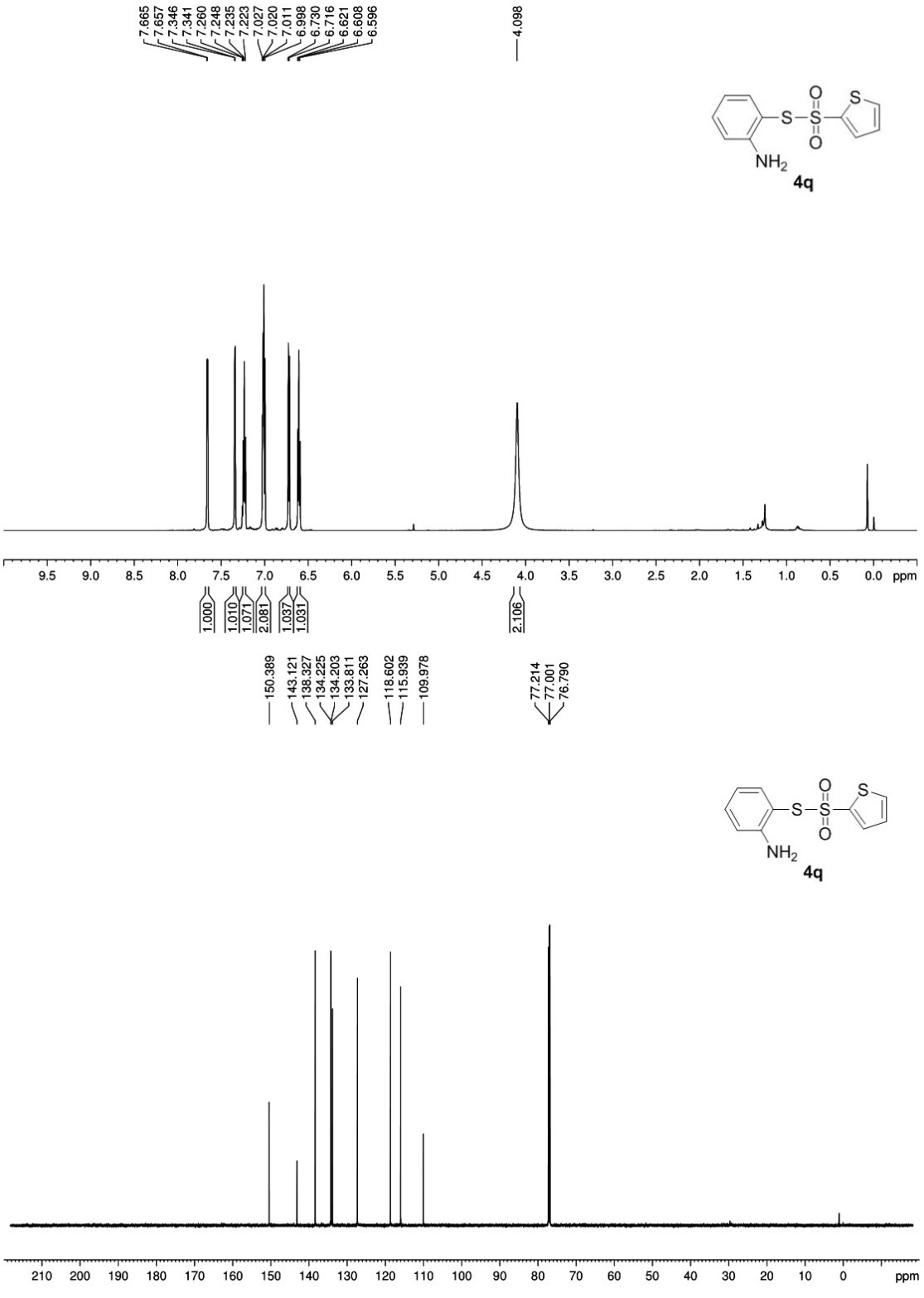

F
O
S
S
O
F
NH2
4n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

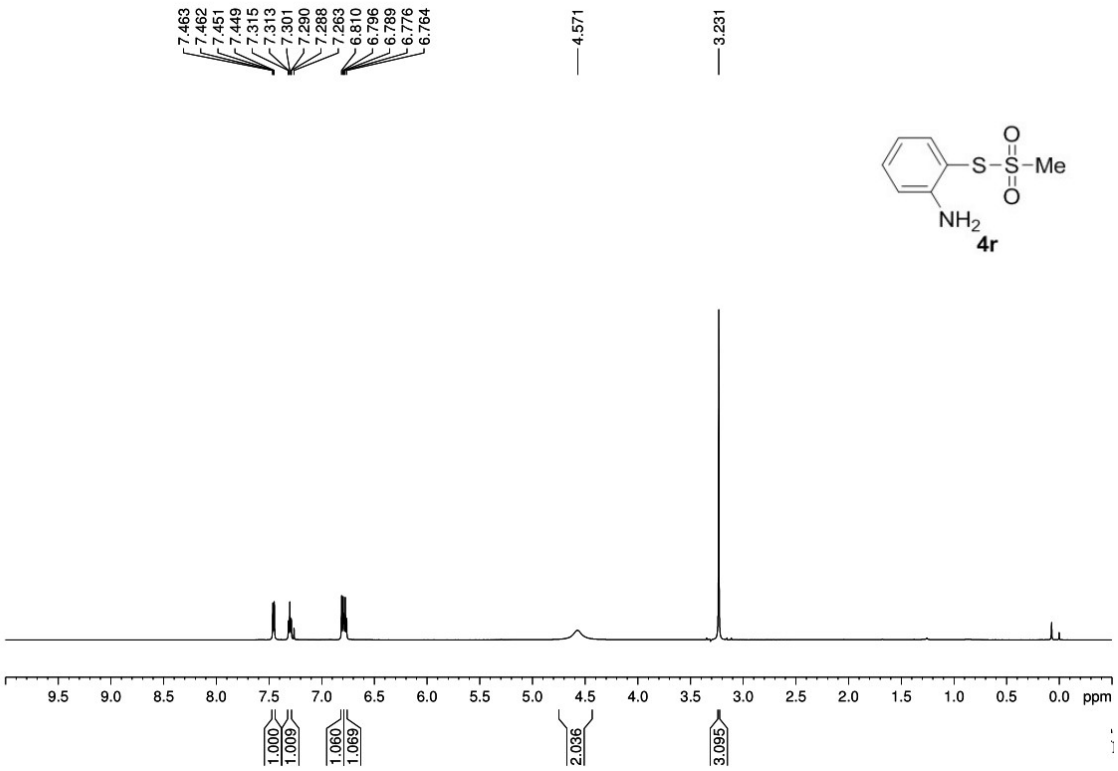

7.654
7.643
7.543
7.540
7.536
7.532
7.529
7.525
7.273
7.260
7.247
7.214
7.200
7.186
6.949
6.936
6.732
6.718
6.633
6.620
6.608
4.213
S
O
O
F
Cl
NH2
4o
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
1.023
1.118
1.078
1.022
1.042
1.077
2.039

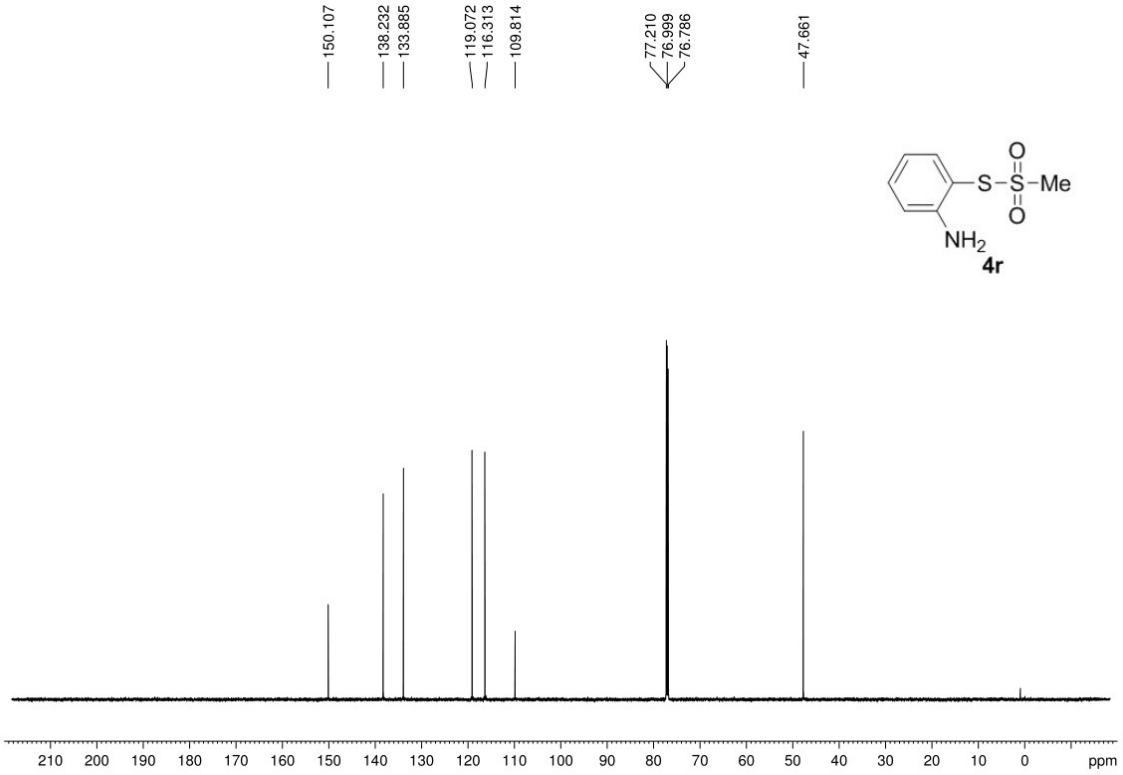

161.960
160.243
150.348
139.372
139.347
138.299
134.030
130.671
128.116
128.058
122.274
122.149
118.689
117.151
117.001
116.023
108.983
77.210
76.998
76.786
S
O
O
F
Cl
NH2
4o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

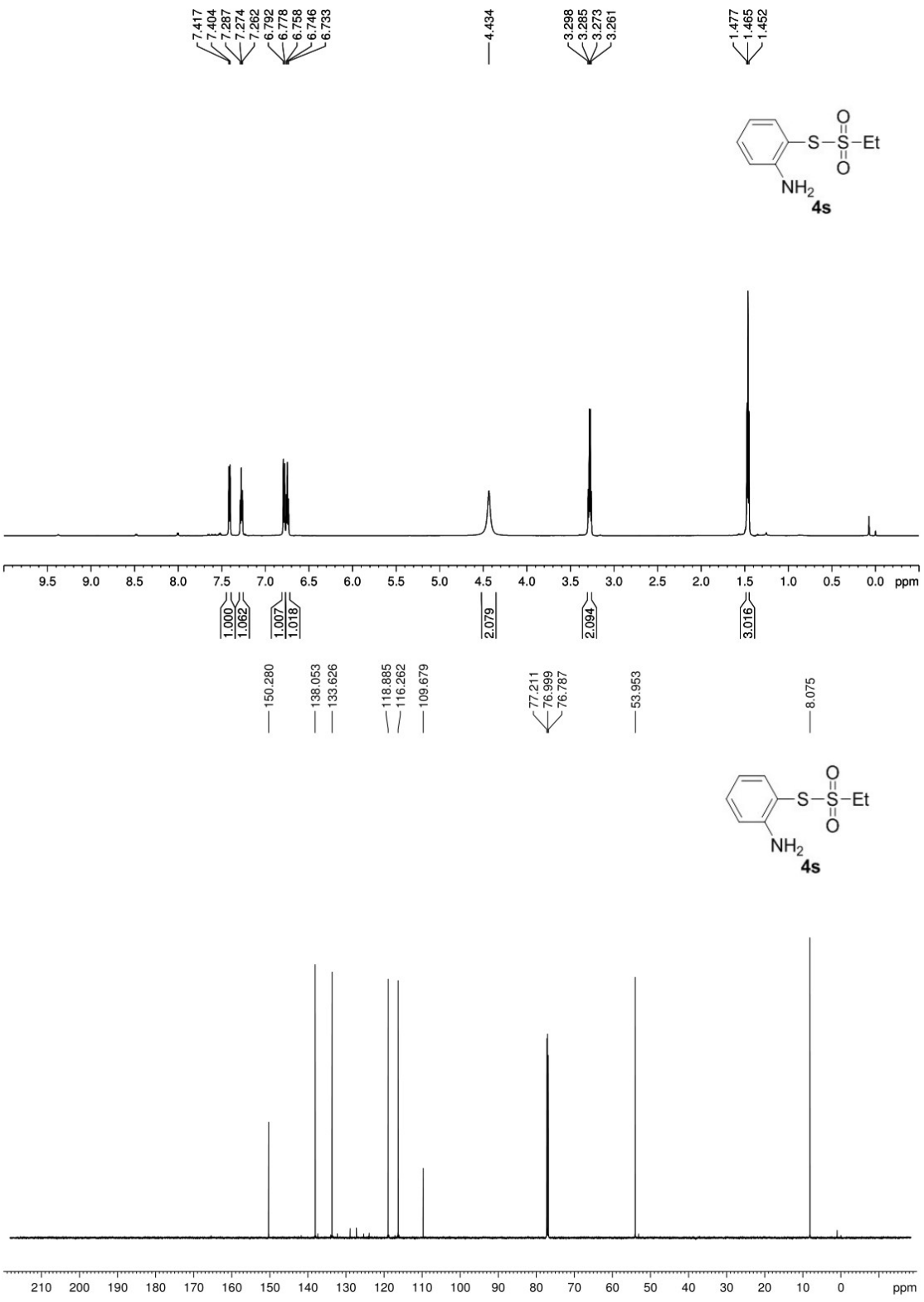

7.652
7.644
7.629
7.263
7.224
7.211
7.198
6.948
6.942
6.933
6.721
6.707
6.582
6.569
6.557
4.161
3.958
MeO
O
S
S
O
NH2
Br
4p
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.006
1.000
2.089
1.041
1.052
2.064
3.073

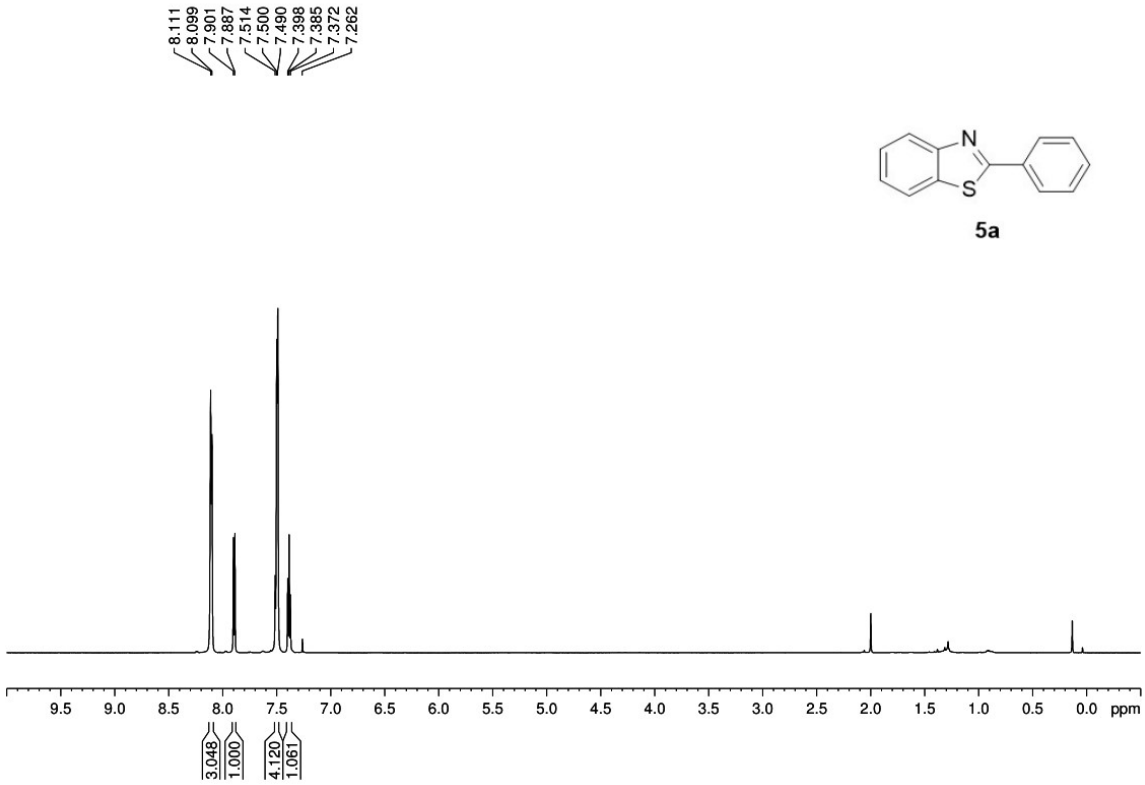

156.042
150.461
138.259
138.128
133.681
132.986
131.822
118.444
115.856
114.368
111.855
109.898
77.212
77.001
76.789
56.625
MeO
O
S
S
O
NH2
Br
4p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

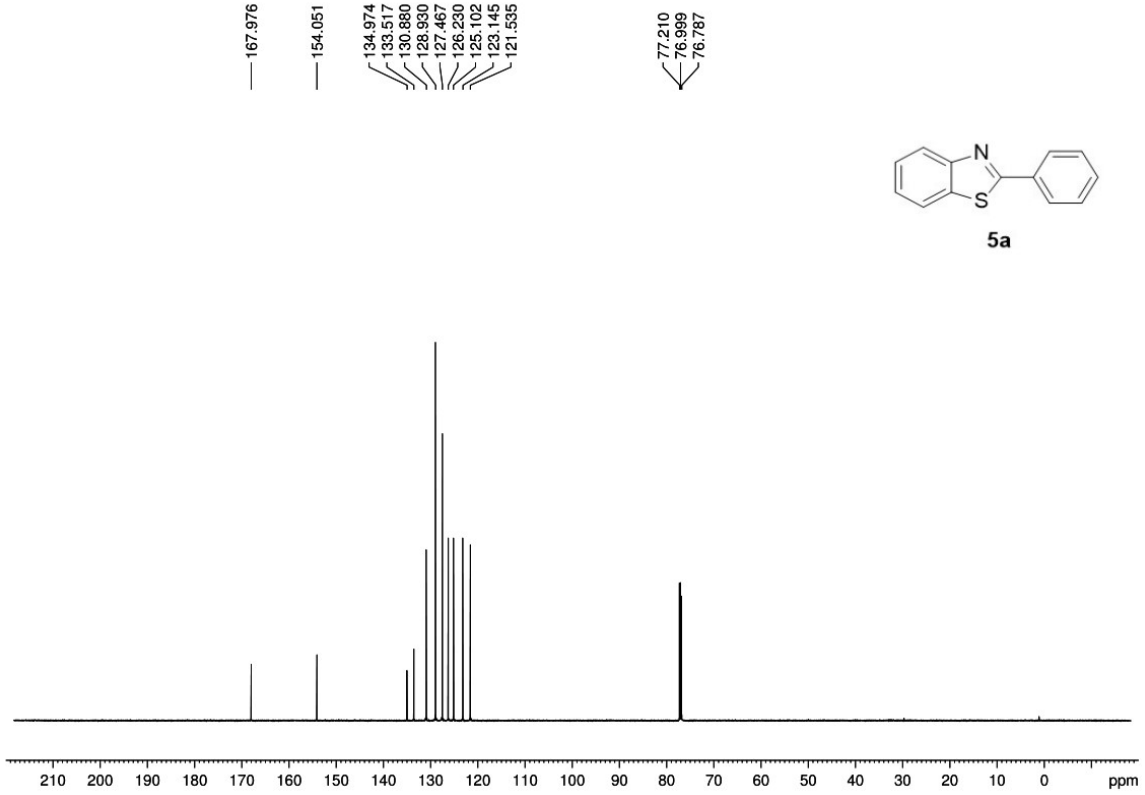

7.665
7.657
7.346
7.341
7.260
7.248
7.235
7.223
7.027
7.020
7.011
6.998
6.730
6.716
6.621
6.608
6.596
4.098
4q
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
1.010
1.071
2.081
1.037
1.031
2.106
150.389
143.121
138.327
134.225
134.203
133.811
127.263
118.602
115.939
109.978
77.214
77.001
76.790
4q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

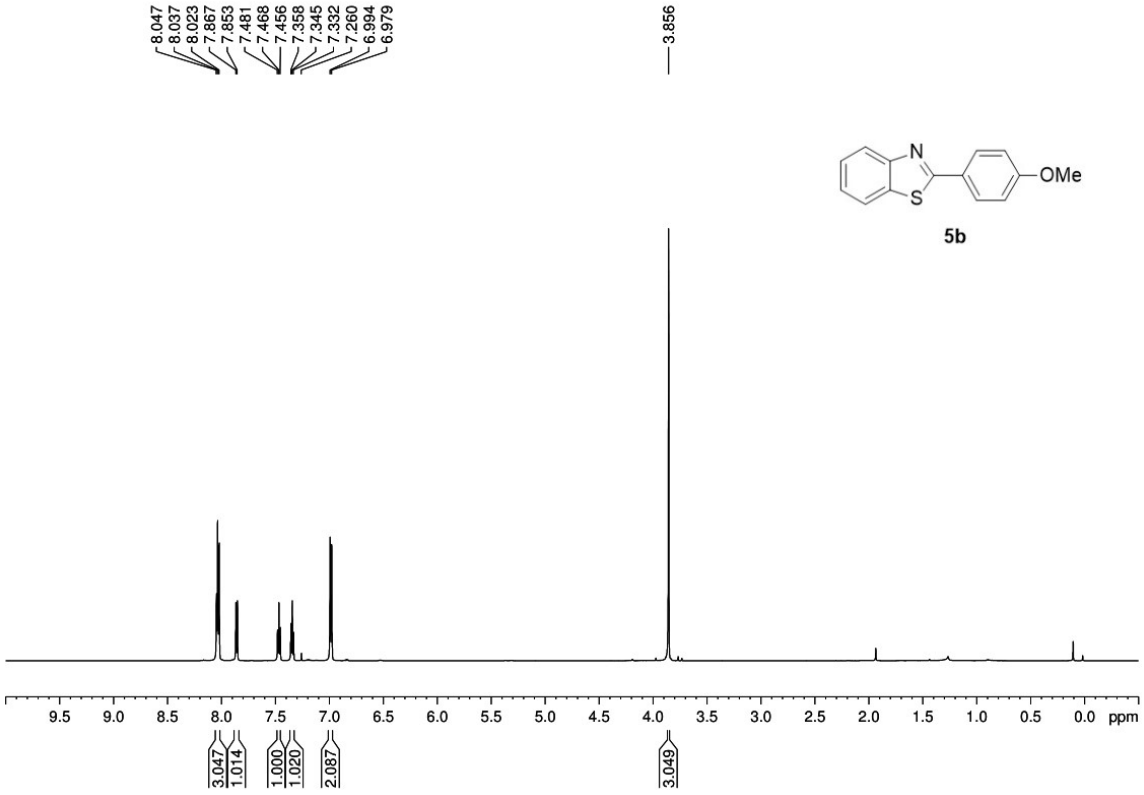

7.463
7.462
7.451
7.449
7.315
7.313
7.301
7.290
7.288
7.263
6.810
6.796
6.789
6.776
6.764
4.571
3.231
S
Me
NH2
4r
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
1.009
1.060
1.069
2.036
3.095

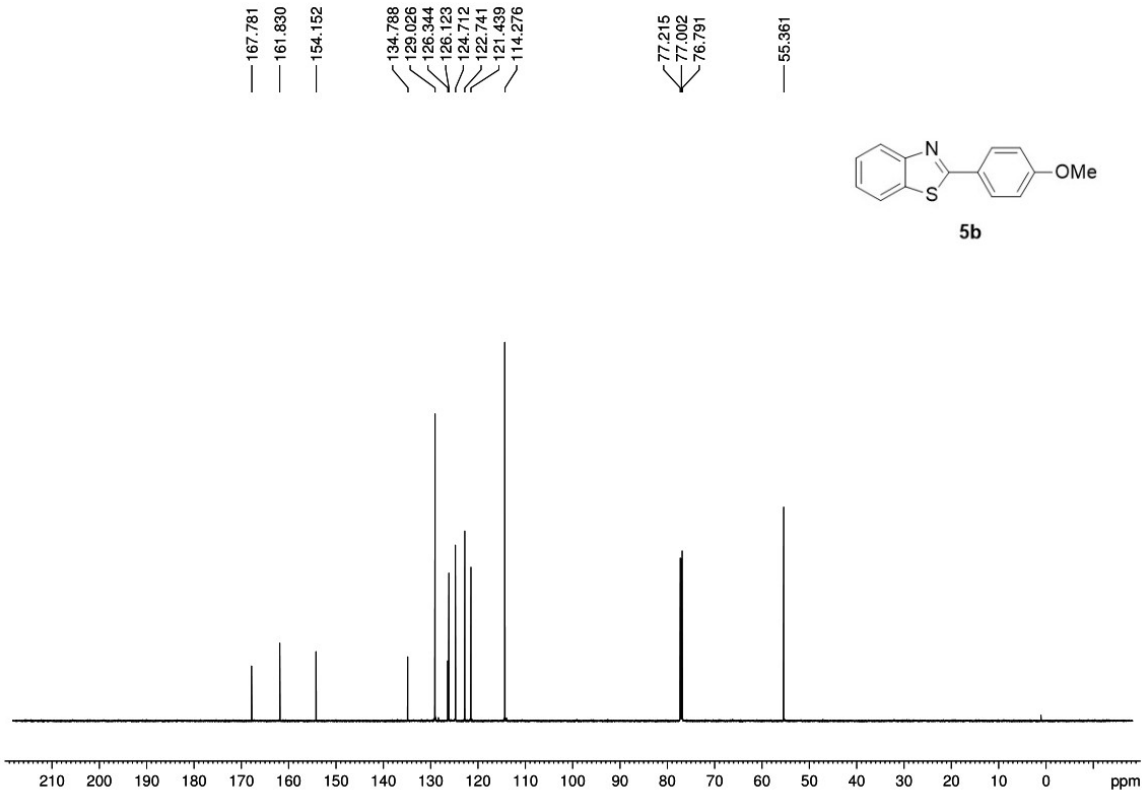

150.107
138.232
133.885
119.072
116.313
109.814
77.210
76.999
76.786
47.661
S
Me
NH2
4r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

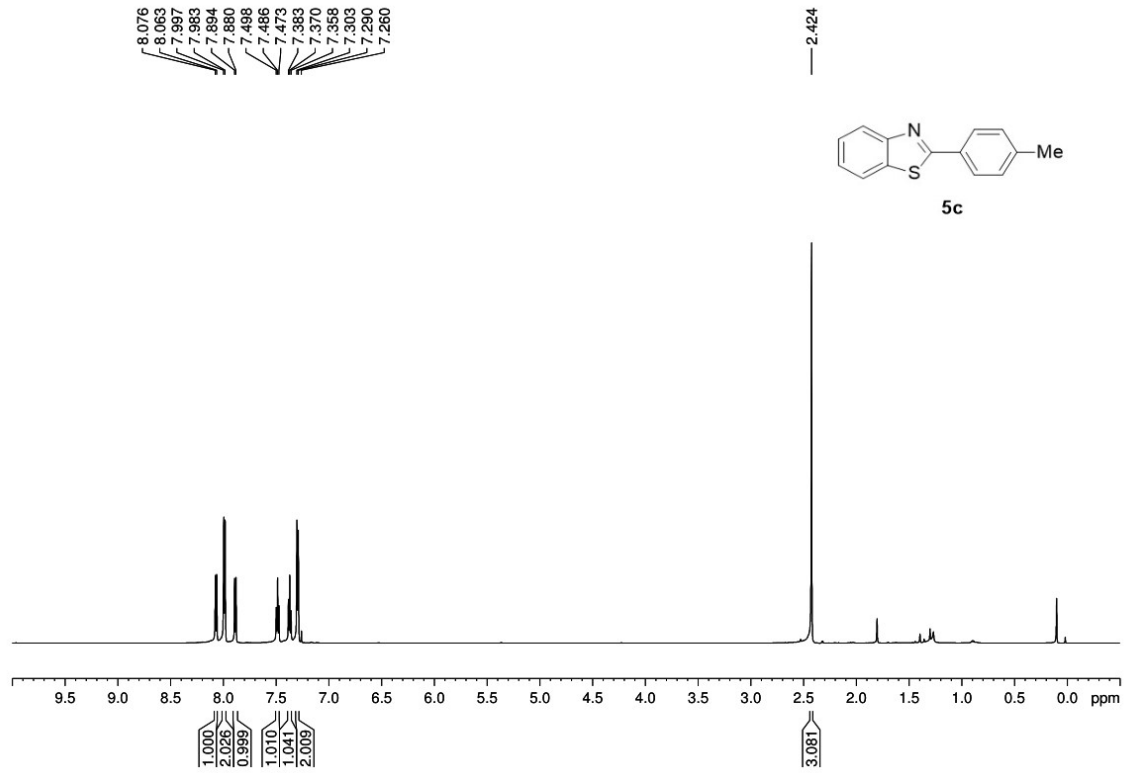

7.417
7.404
7.287
7.274
7.262
6.792
6.778
6.758
6.746
6.733
4.434
3.298
3.285
3.273
3.261
1.477
1.465
1.452
S
S
Et
O
O
NH2
4s
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
1.062
1.007
1.018
2.079
2.094
3.016
150.280
138.053
133.626
118.885
116.262
109.679
77.211
76.999
76.787
53.953
8.075
S
S
Et
O
O
NH2
4s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

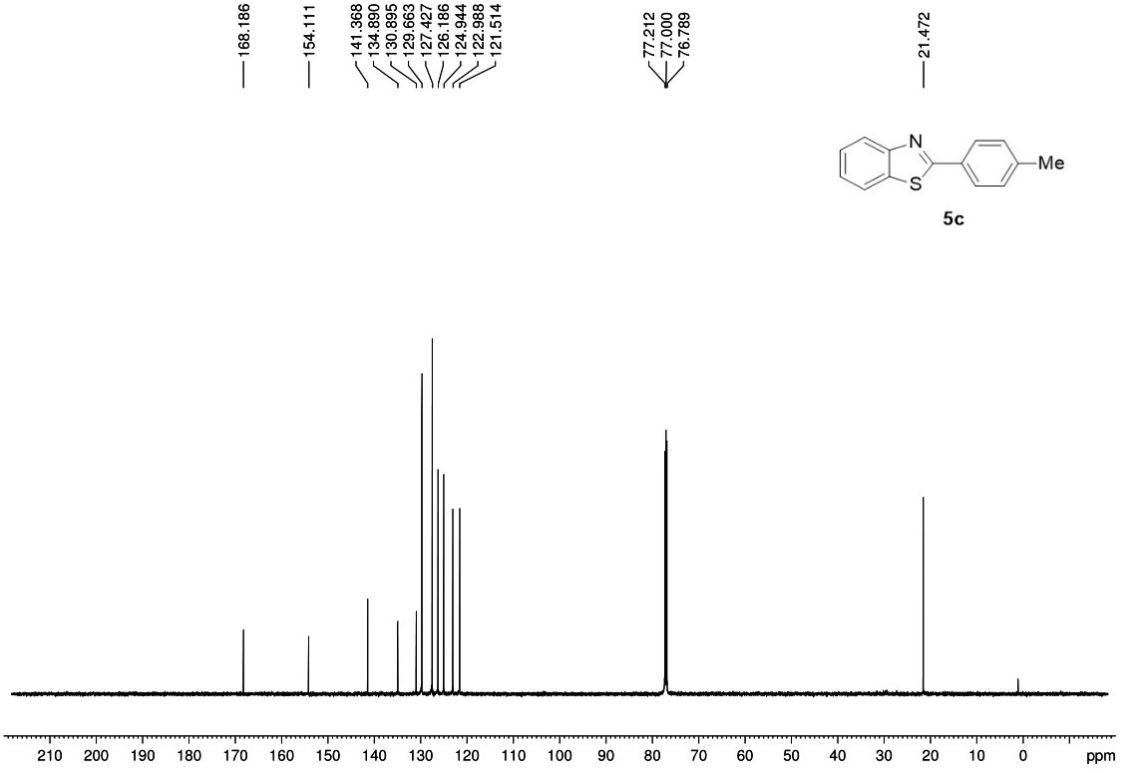

8.111
8.099
7.901
7.887
7.514
7.500
7.490
7.398
7.385
7.372
7.262
5a
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
3.048
1.000
4.120
1.061

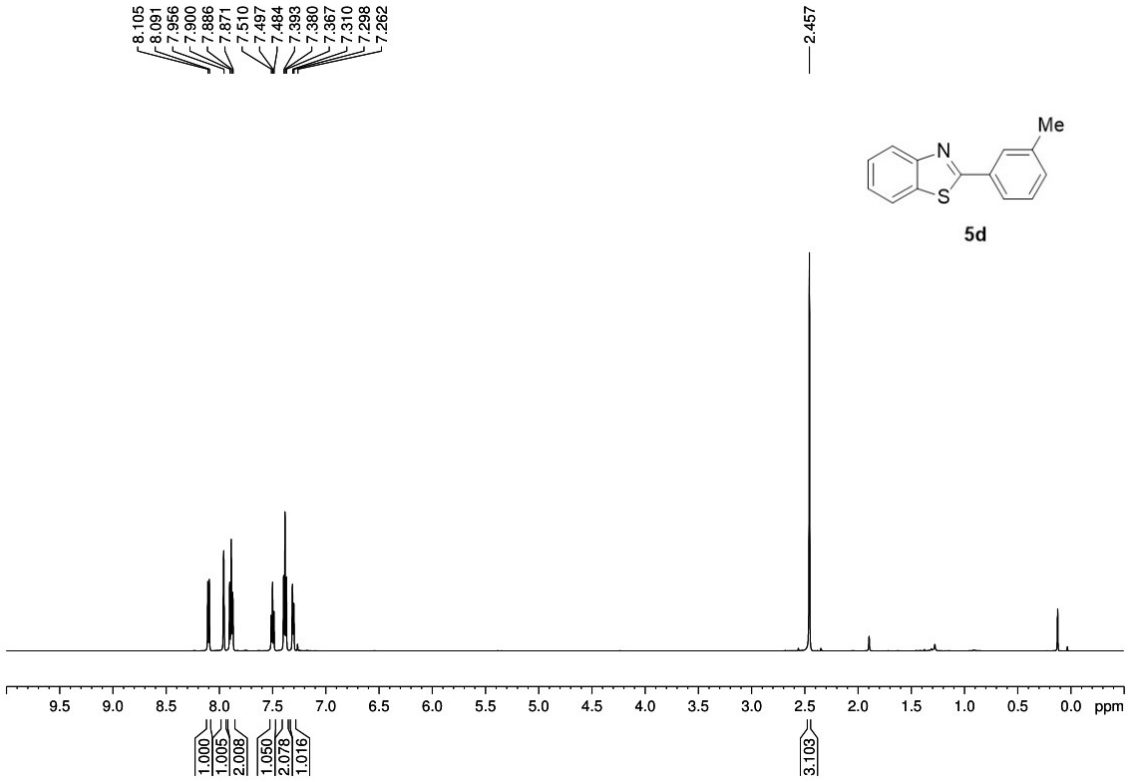

167.976
154.051
134.974
133.517
130.880
128.930
127.467
126.230
125.102
123.145
121.535
77.210
76.999
76.787
5a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

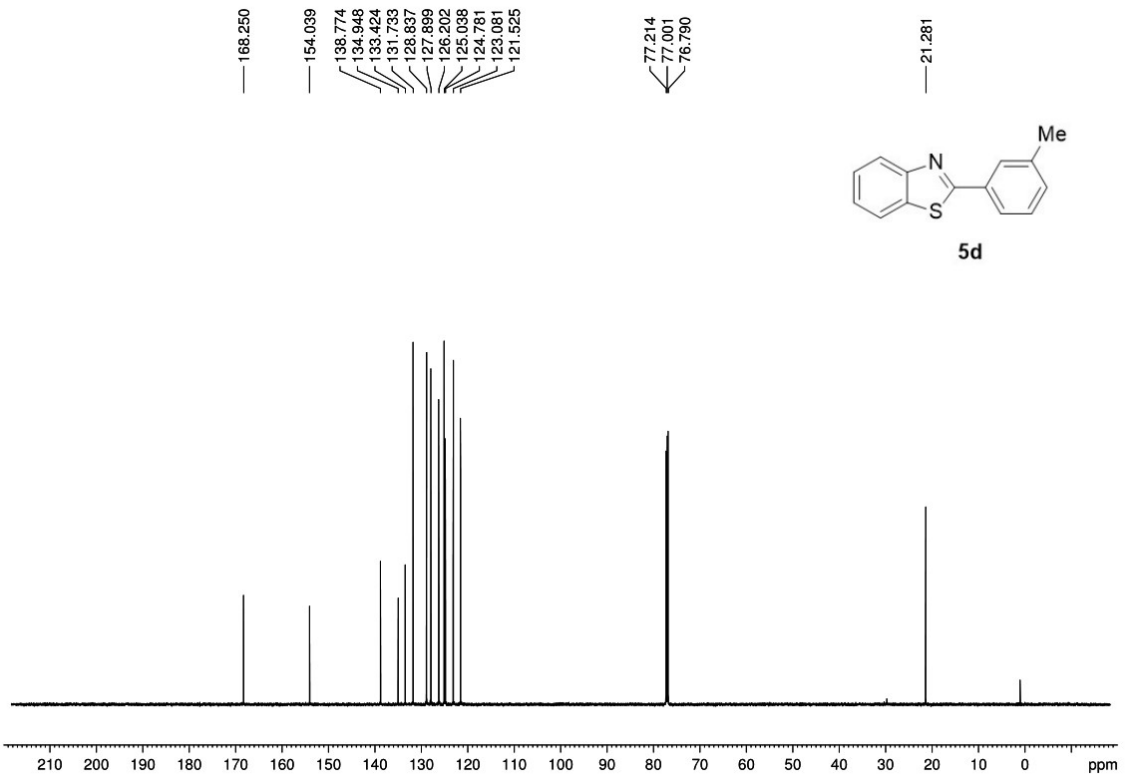

8.047
8.037
8.023
7.867
7.853
7.481
7.468
7.456
7.358
7.345
7.332
7.260
6.994
6.979
3.856
N
S
OMe
5b
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
3.047
1.014
1.000
1.020
2.087
3.049

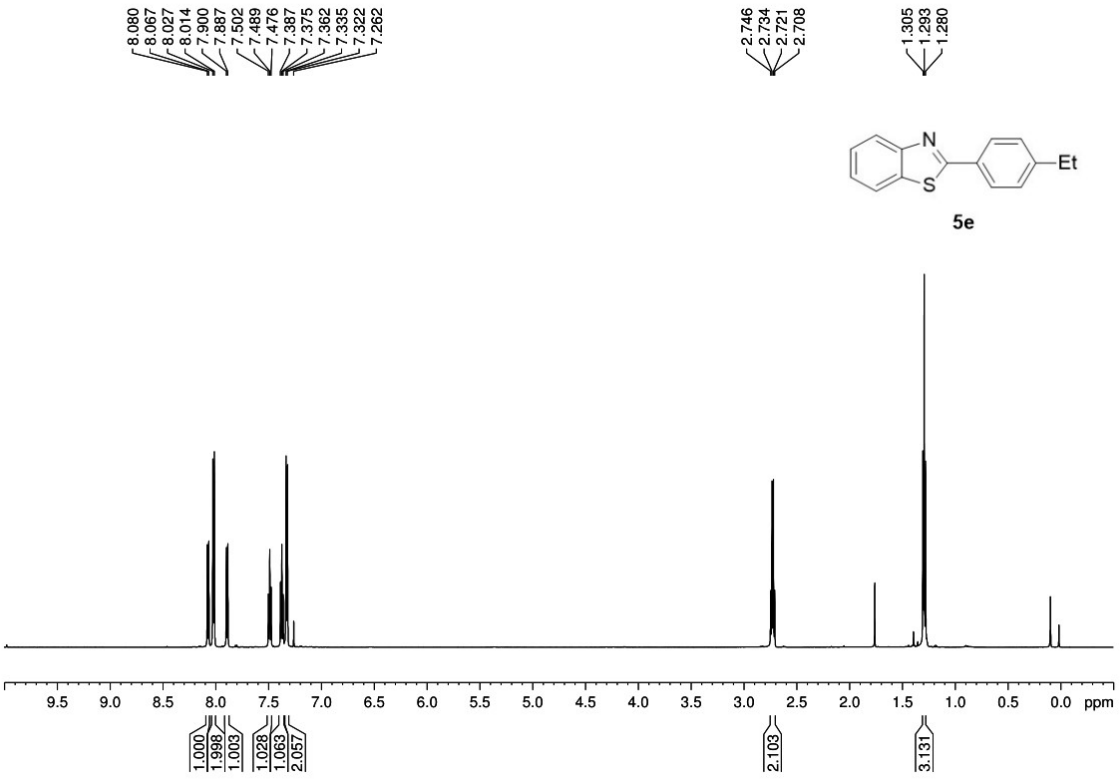

167.781
161.830
154.152
134.788
129.026
126.344
126.123
124.712
122.741
121.439
114.276
77.215
77.002
76.791
55.361
N
S
OMe
5b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

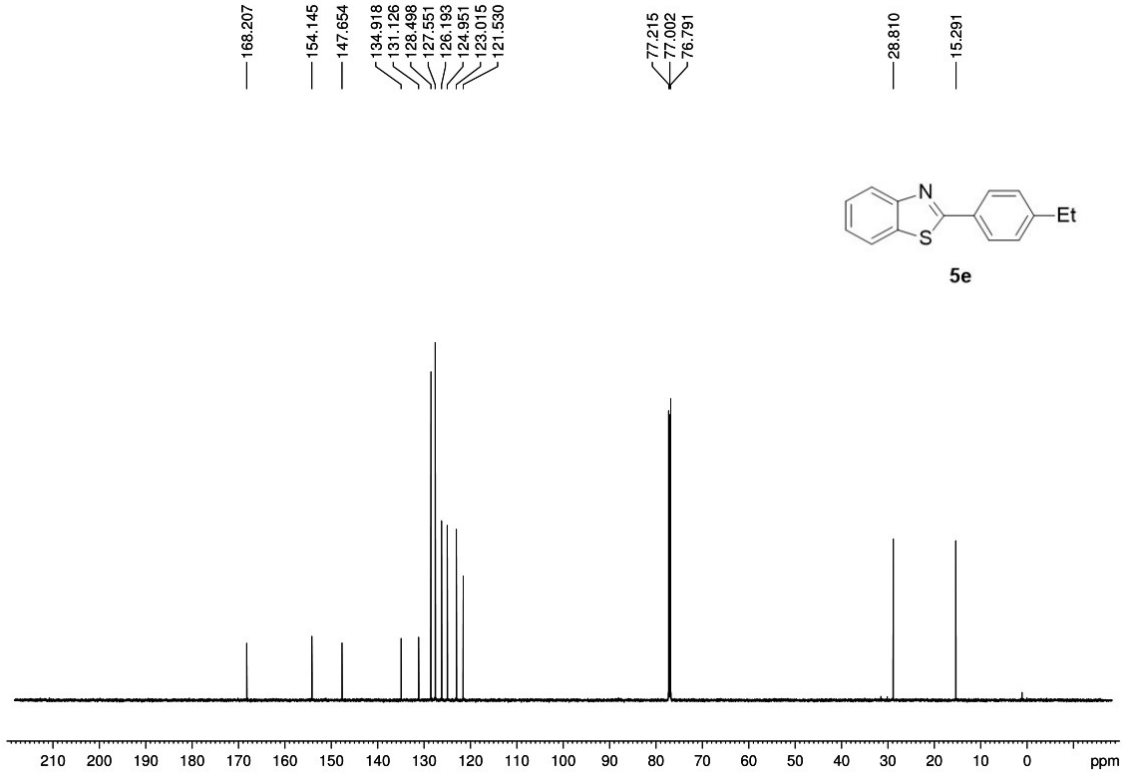

8.076
8.063
7.997
7.983
7.894
7.880
7.498
7.486
7.473
7.383
7.370
7.358
7.303
7.290
7.260
2.424
N
S
Me
5c
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
2.026
0.999
1.010
1.041
2.009
3.081

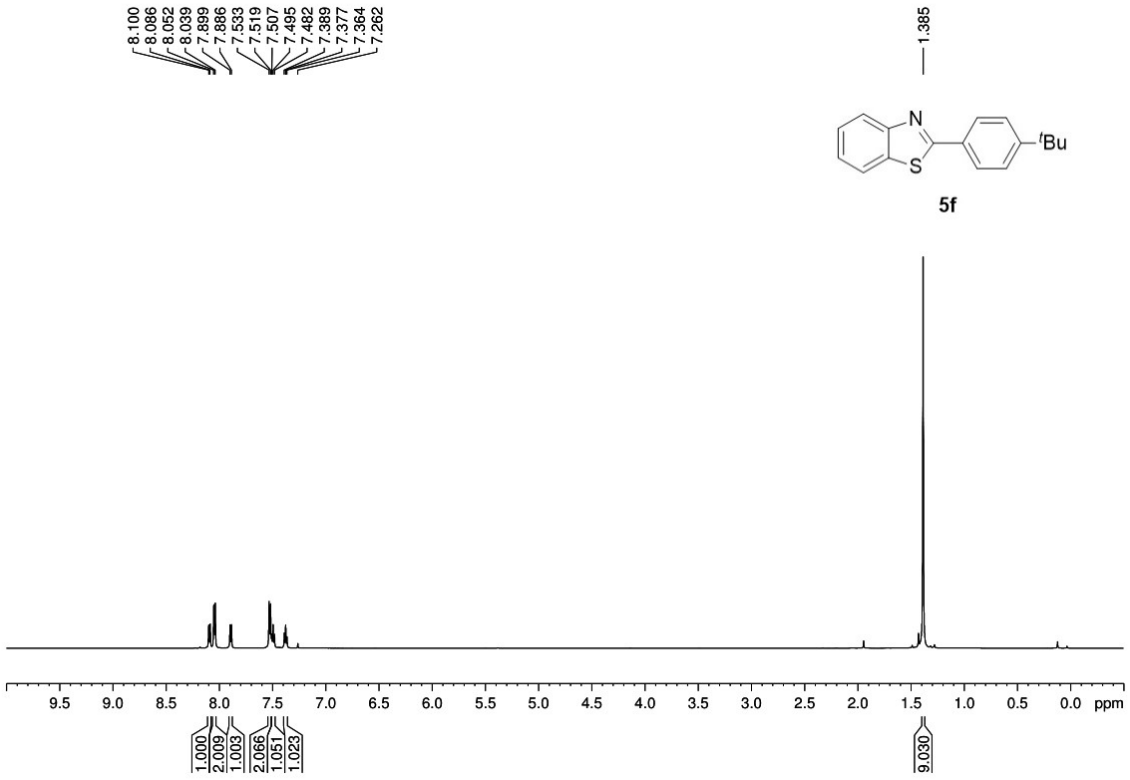

168.186
154.111
141.368
134.890
130.895
129.663
127.427
126.186
124.944
122.988
121.514
77.212
77.000
76.789
21.472
N
S
Me
5c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

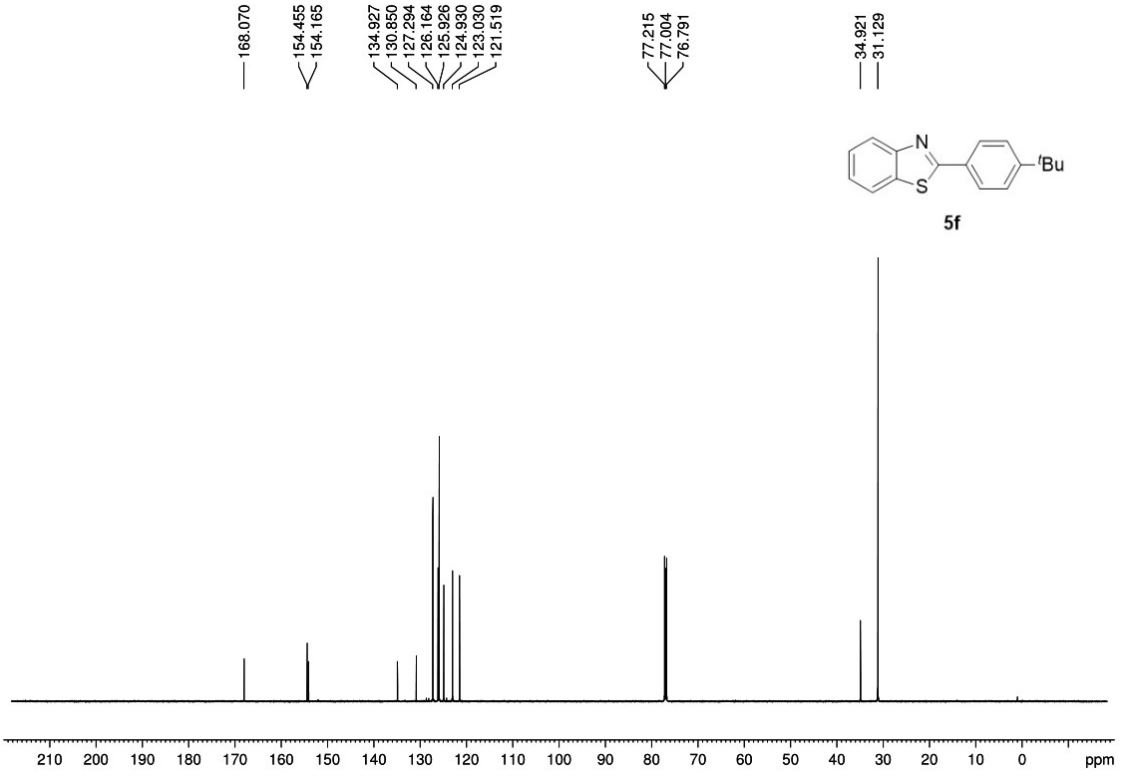

8.105
8.091
7.956
7.900
7.886
7.871
7.510
7.497
7.484
7.393
7.380
7.367
7.310
7.298
7.262
2.457
Me
N
S
5d
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
1.005
2.008
1.050
2.078
1.016
3.103


168.250
154.039
138.774
134.948
133.424
131.733
128.837
127.899
126.202
125.038
124.781
123.081
121.525
77.214
77.001
76.790
21.281
Me
N
S
5d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

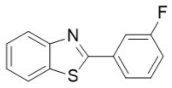

8.080
8.067
8.027
8.014
7.900
7.887
7.502
7.489
7.476
7.387
7.375
7.362
7.335
7.322
7.262
2.746
2.734
2.721
2.708
1.305
1.293
1.280
N
S
Et
5e
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
1.998
1.003
1.028
1.063
2.057
2.103
3.131


168.207
154.145
147.654
134.918
131.126
128.498
127.551
126.193
124.951
123.015
121.530
77.215
77.002
76.791
28.810
15.291
N
S
Et
5e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

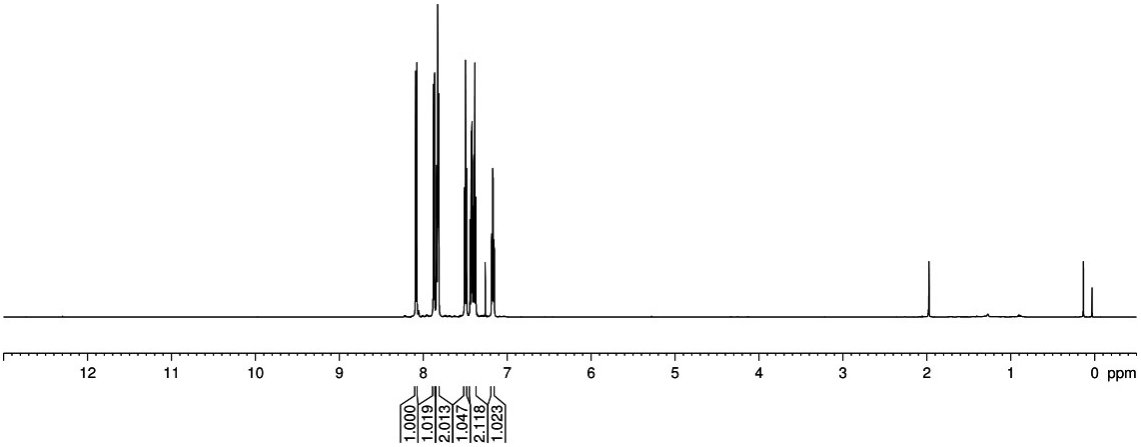

8.100
8.086
8.052
8.039
7.899
7.886
7.533
7.519
7.507
7.495
7.482
7.389
7.377
7.364
7.262
1.385
N
S
tBu
5f
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
2.009
1.003
2.066
1.051
1.023
9.030

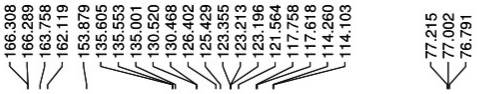

168.070
154.455
154.165
134.927
130.850
127.294
126.164
125.926
124.930
123.030
121.519
77.215
77.004
76.791
34.921
31.129
N
S
tBu
5f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

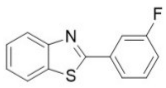

8.092
8.079
7.880
7.867
7.844
7.841
7.837
7.828
7.826
7.824
7.821
7.818
7.816
7.511
7.509
7.499
7.497
7.485
7.484
7.444
7.434
7.430
7.421
7.417
7.407
7.401
7.399
7.387
7.375
7.373
7.263
7.187
7.186
7.183
7.182
7.174
7.172
7.170
7.168
7.160
7.159
7.156
7.154


F
N
S

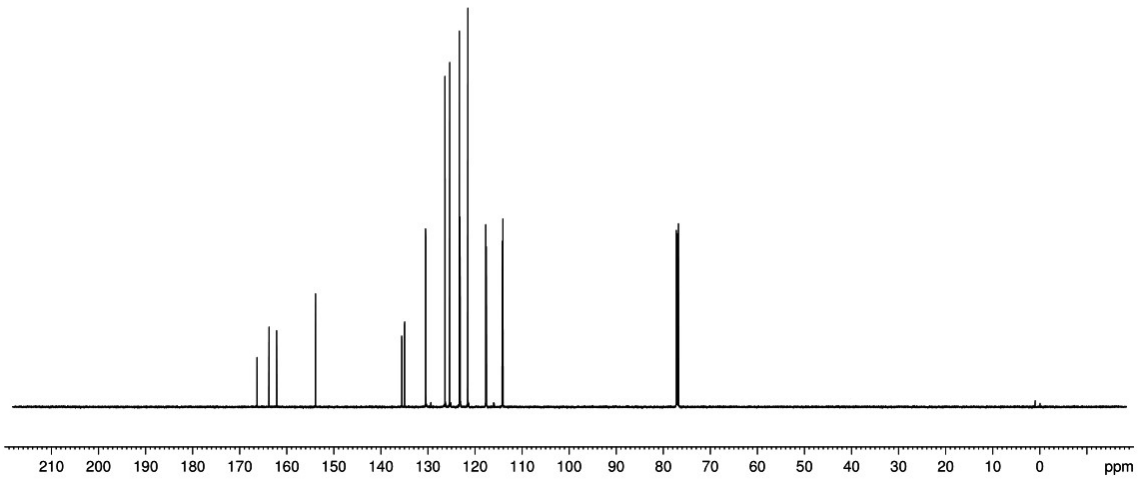
5g

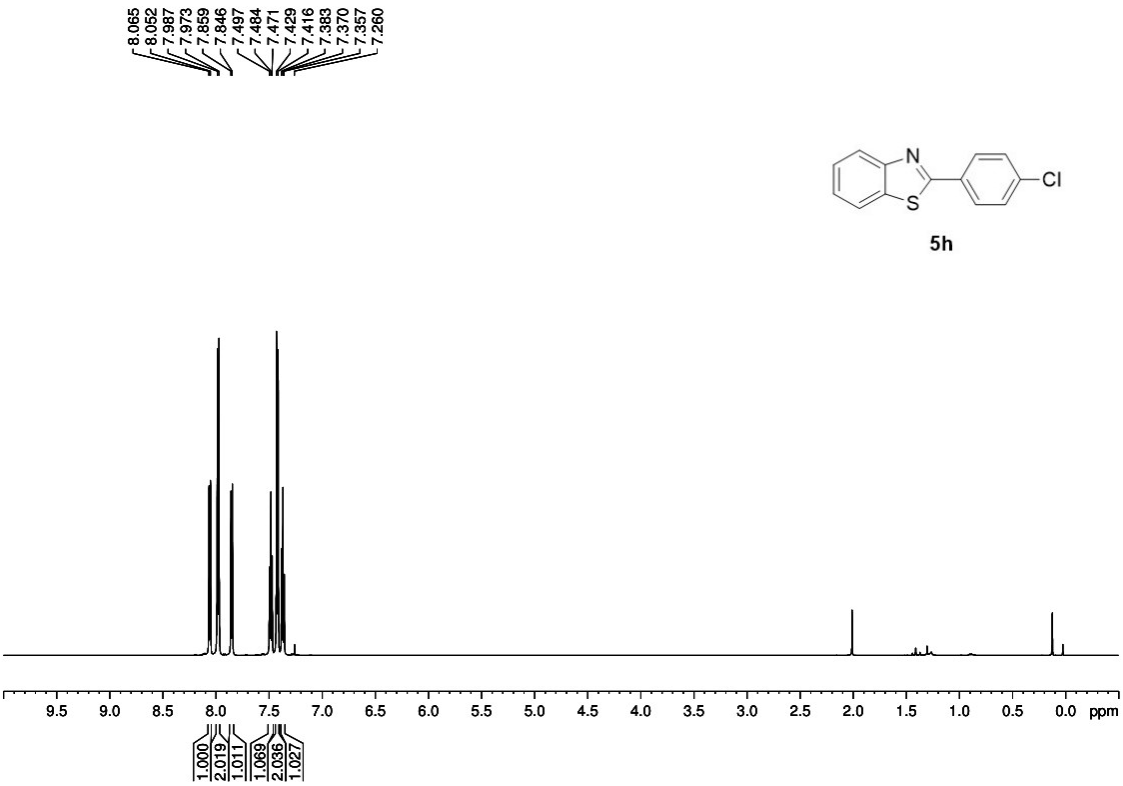

12
11
10
9
8
7
6
5
4
3
2
1
0 ppm
1.000
1.019
2.013
1.047
2.118
1.023

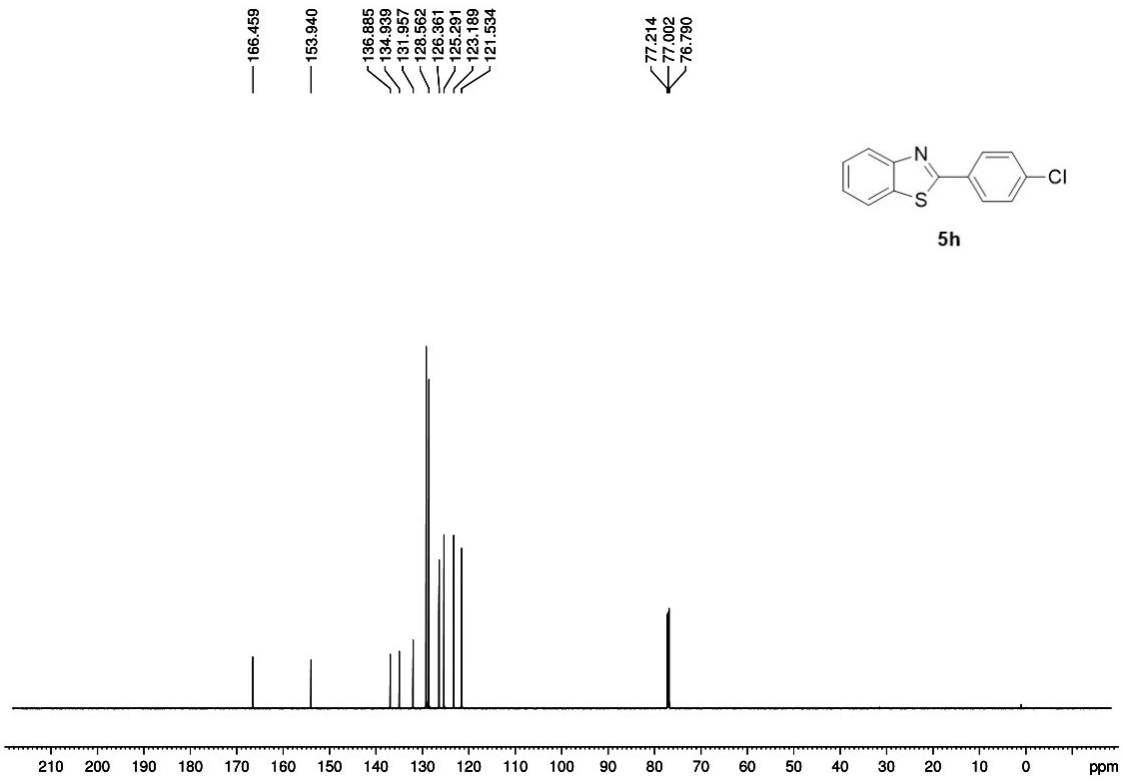

166.308
166.289
163.758
162.119
153.879
135.605
135.553
135.001
130.520
130.468
126.402
125.429
123.355
123.213
123.196
121.564
117.758
117.618
114.260
114.103
77.215
77.002
76.791

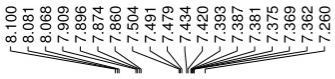

F
N
S

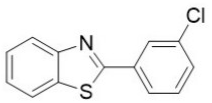
5g


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

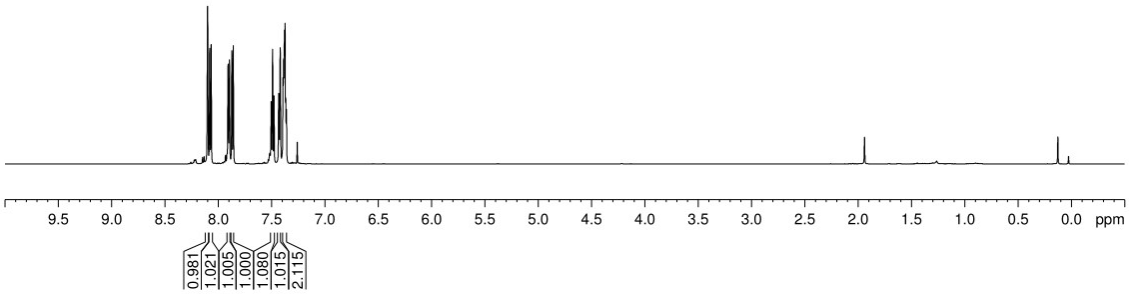

8.065
8.052
7.987
7.973
7.859
7.846
7.497
7.484
7.471
7.429
7.416
7.383
7.370
7.357
7.260
N
S
Cl
5h
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
2.019
1.011
1.069
2.036
1.027

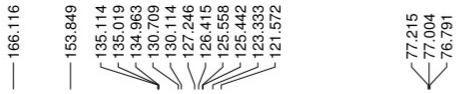

166.459
153.940
136.885
134.939
131.957
128.562
126.361
125.291
123.189
121.534
77.214
77.002
76.790
N
S
Cl
5h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

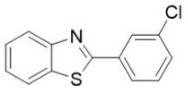

8.100
8.081
8.068
7.909
7.896
7.874
7.860
7.504
7.491
7.479
7.434
7.420
7.393
7.387
7.381
7.375
7.369
7.362
7.260


Cl
N
S

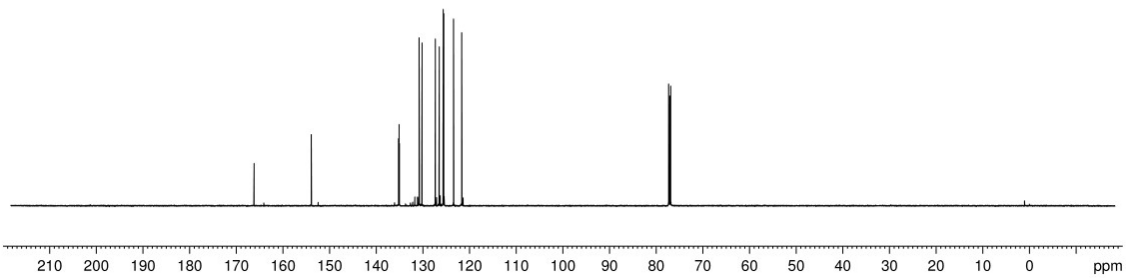
5i

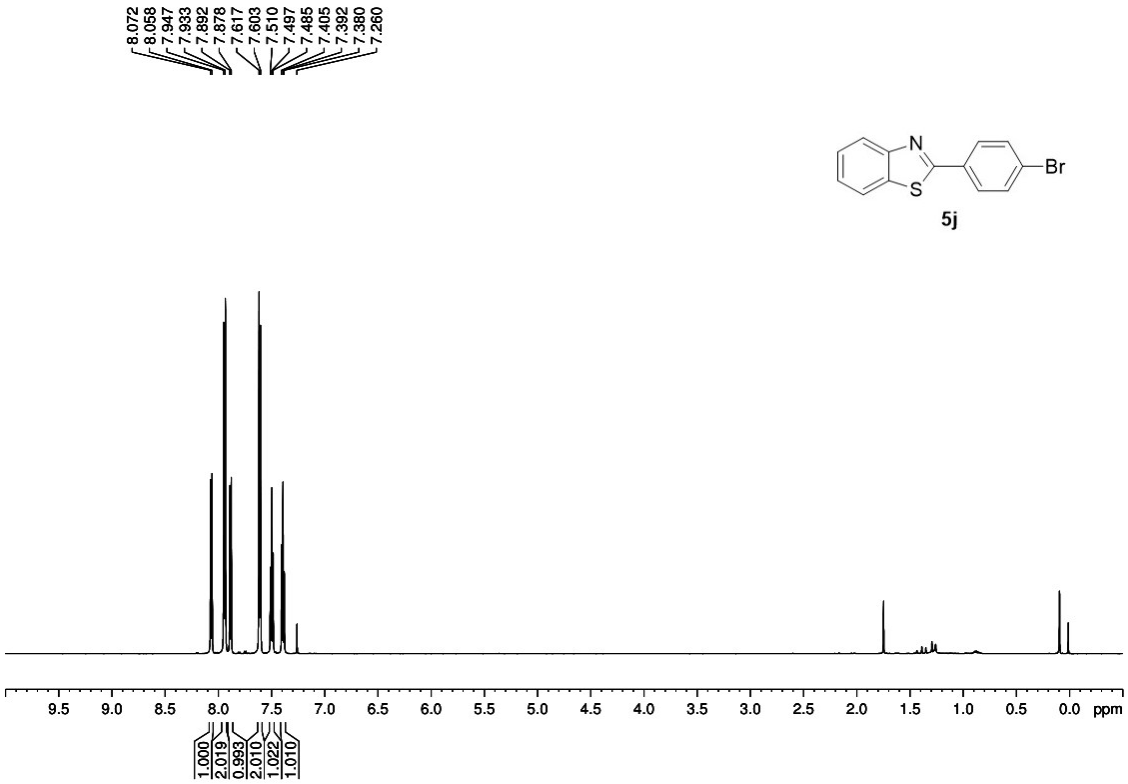

9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.981
1.021
1.005
1.000
1.080
1.015
2.115

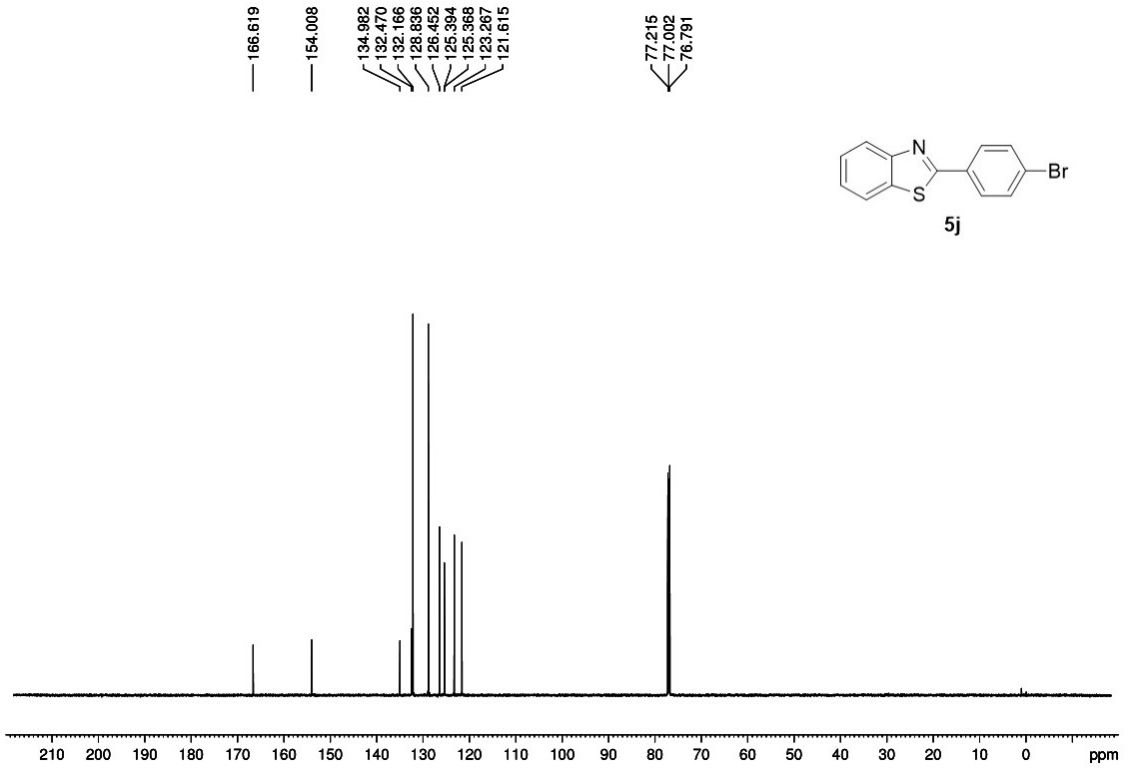

166.116
153.849
135.114
135.019
134.963
130.709
130.114
127.246
126.415
125.558
125.442
123.333
121.572
77.215
77.004
76.791


Cl
N
S

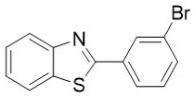
5i


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

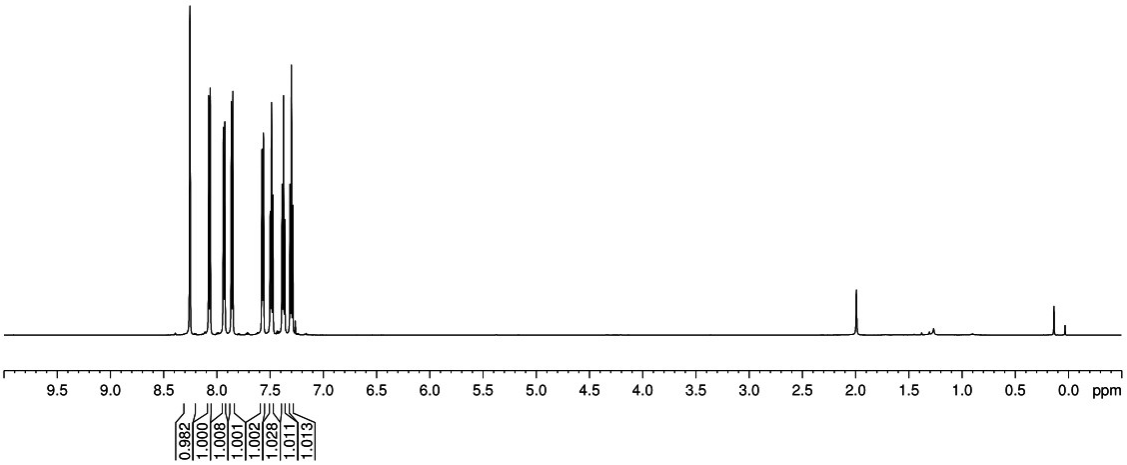

8.072
8.058
7.947
7.933
7.892
7.878
7.617
7.603
7.510
7.497
7.485
7.405
7.392
7.380
7.260
N
S
Br
5j
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
2.019
0.993
2.010
1.022
1.010

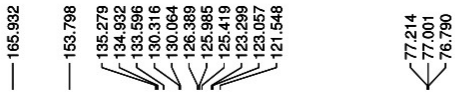

166.619
154.008
134.982
132.470
132.166
128.836
126.452
125.394
125.368
123.267
121.615
77.215
77.002
76.791
N
S
Br
5j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

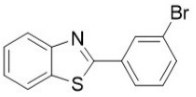

8.254
8.076
8.062
7.938
7.925
7.864
7.851
7.576
7.563
7.499
7.486
7.473
7.387
7.374
7.362
7.312
7.299
7.286
7.263


Br
N
S

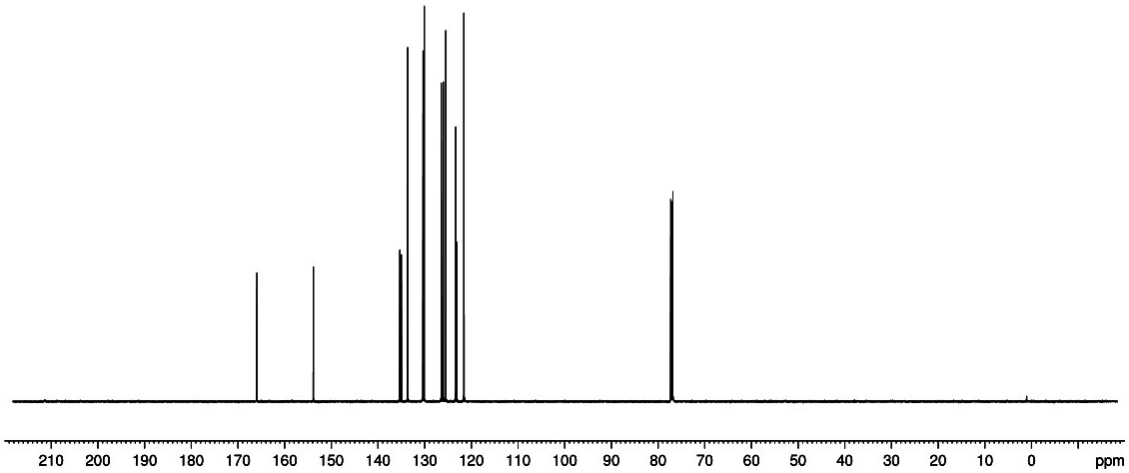
5k

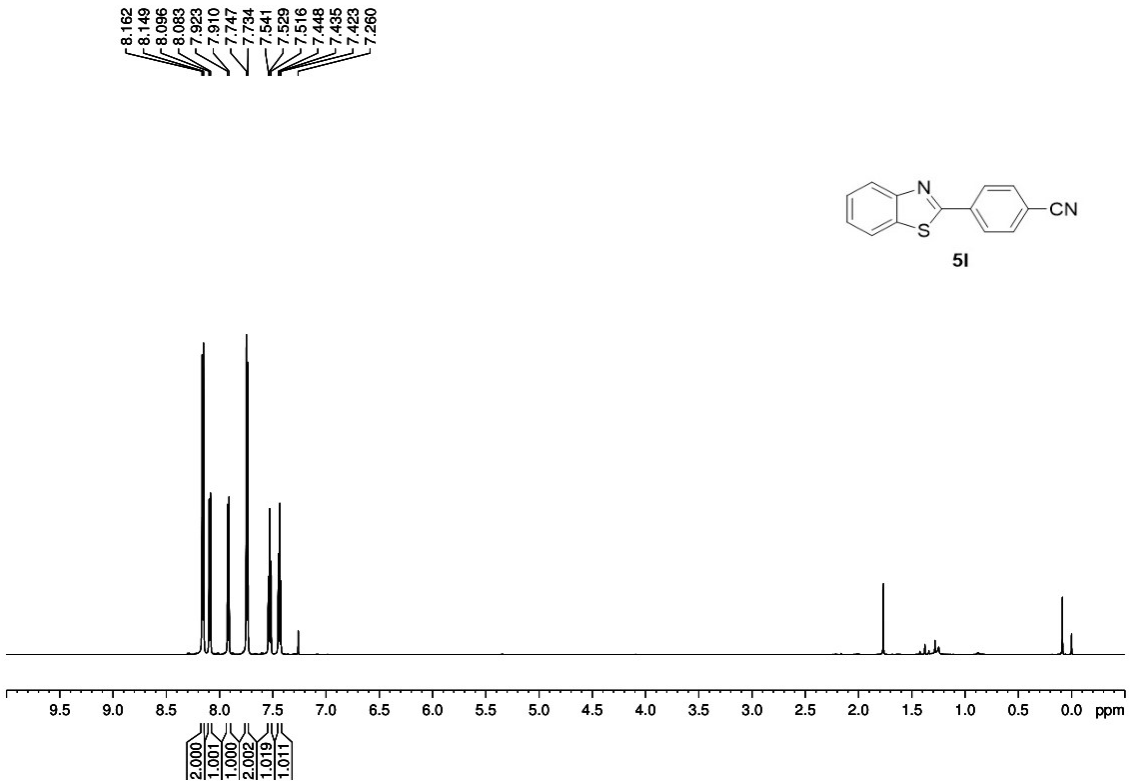

9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.982
1.000
1.008
1.001
1.002
1.028
1.011
1.013

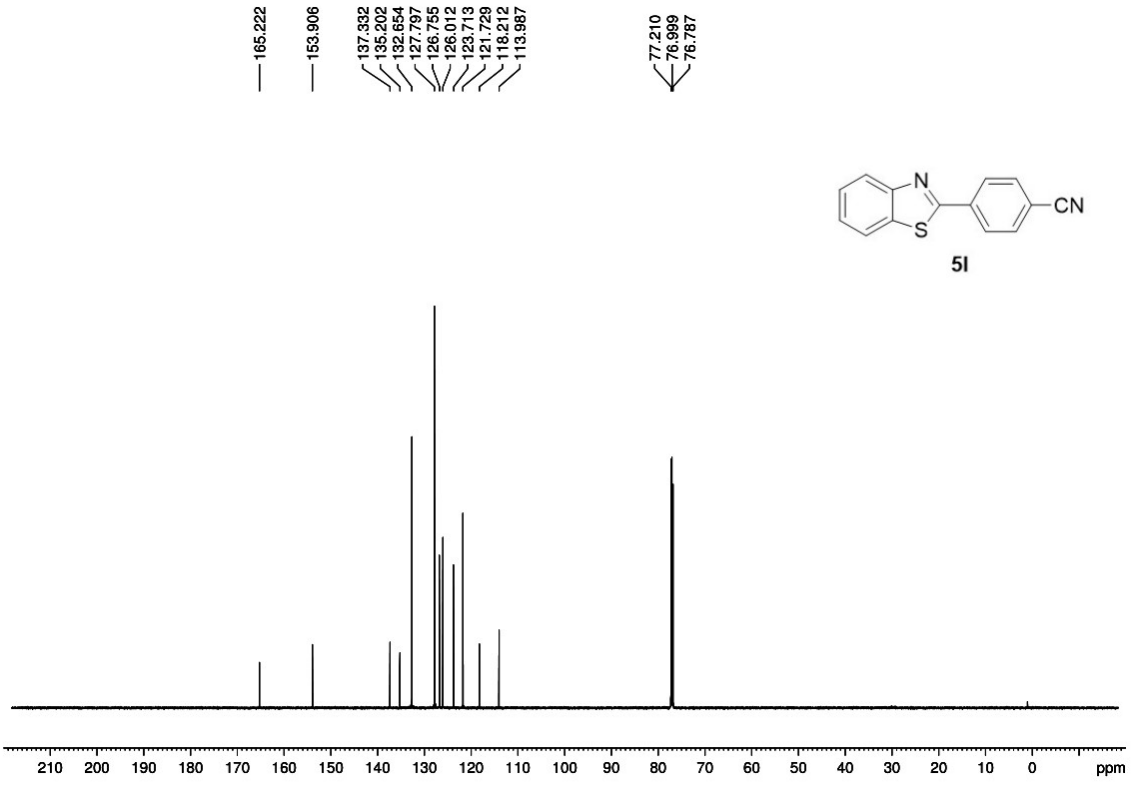

165.932
153.798
135.279
134.932
133.596
130.316
130.064
126.389
125.985
125.419
123.299
123.057
121.548
77.214
77.001
76.790


Br
N
S

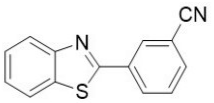
5k


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

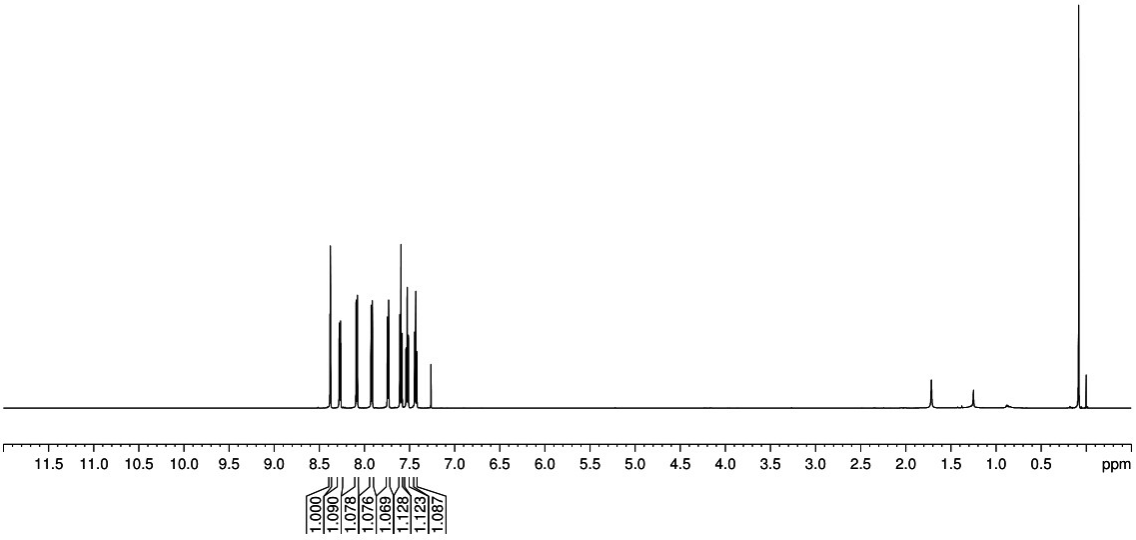

8.162
8.149
8.096
8.083
7.923
7.910
7.747
7.734
7.541
7.529
7.516
7.448
7.435
7.423
7.260
N
S
CN
5l
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.000
1.001
1.000
2.002
1.019
1.011


165.222
153.906
137.332
135.202
132.654
127.797
126.755
126.012
123.713
121.729
118.212
113.987
77.210
76.999
76.787
N
S
CN
5l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

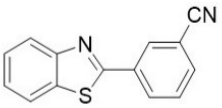

8.380
8.378
8.375
8.280
8.278
8.278
8.275
8.267
8.265
8.264
8.262
8.092
8.079
7.927
7.926
7.913
7.913
7.747
7.745
7.742
7.734
7.732
7.730
7.609
7.595
7.582
7.540
7.538
7.528
7.526
7.524
7.514
7.512
7.445
7.443
7.432
7.430
7.420
7.418
7.263


CN
N
S

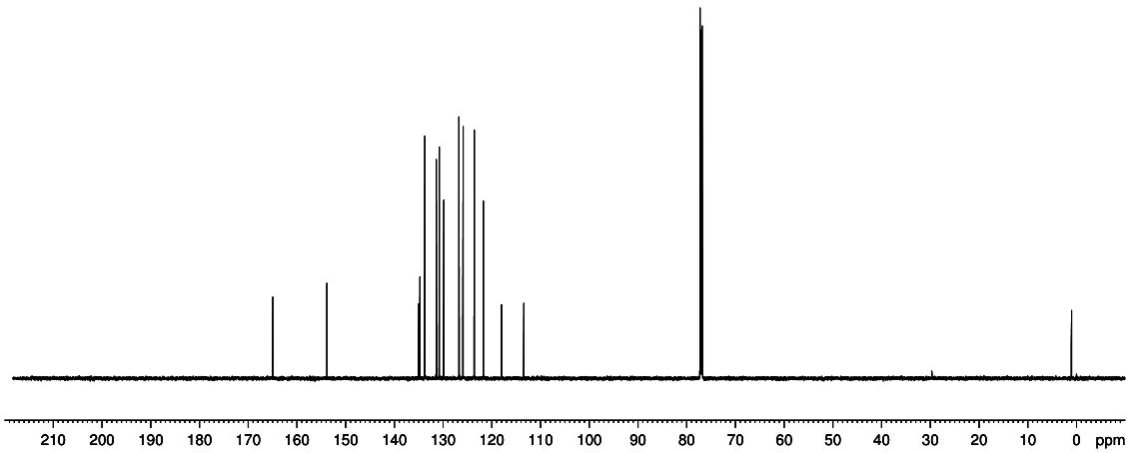
5m


11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.000
1.090
1.078
1.076
1.069
1.128
1.123
1.087

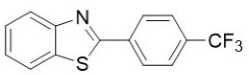

164.957
153.841
135.011
134.738
133.756
131.378
130.779
129.845
126.721
125.890
123.600
121.740
117.976
113.413
77.209
76.998
76.785


CN
N
S

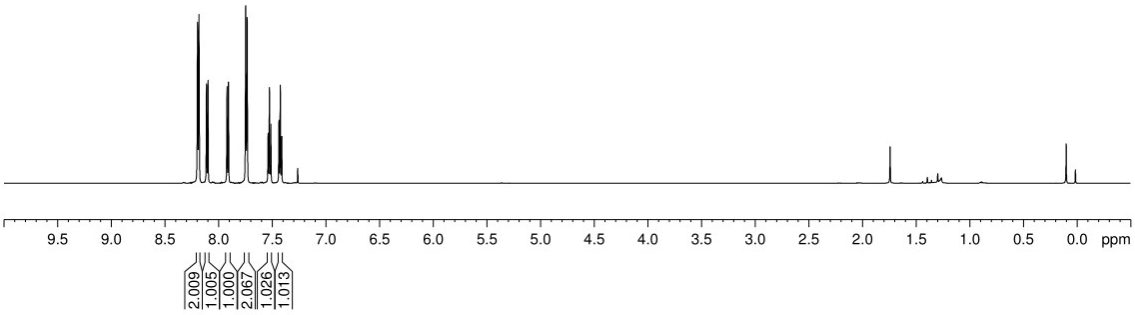
5m

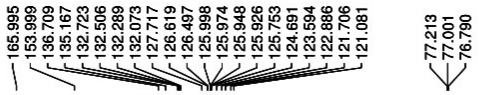

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

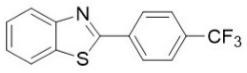

8.196
8.183
8.113
8.099
7.921
7.908
7.747
7.734
7.538
7.526
7.513
7.437
7.425
7.412
7.262


N
S
CF3

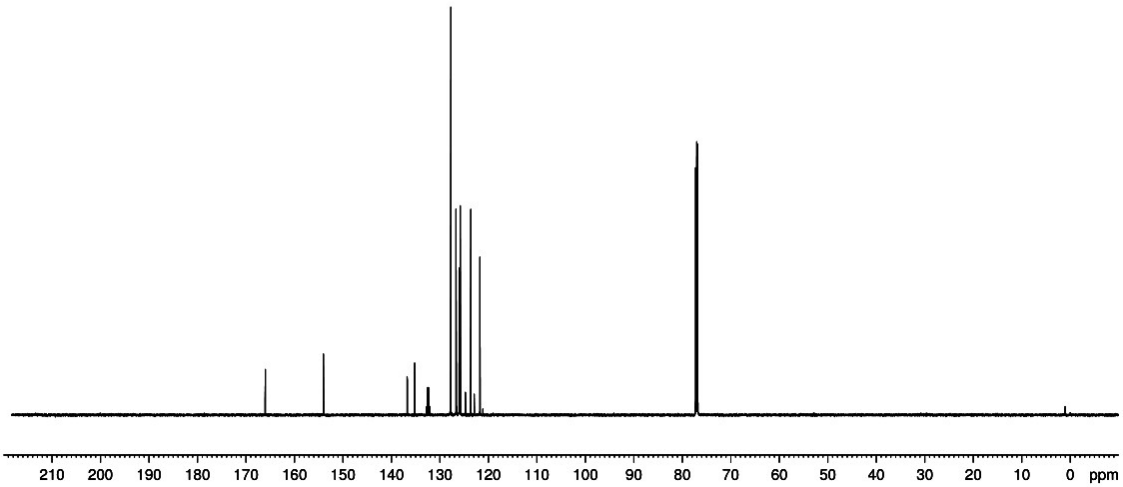
5n


9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.009
1.005
1.000
2.067
1.026
1.013

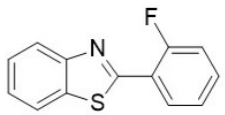

165.995
153.999
136.709
135.167
132.723
132.506
132.289
132.073
127.717
126.619
126.497
125.998
125.974
125.948
125.926
125.753
124.691
123.594
122.886
121.706
121.081
77.213
77.001
76.790


N
S
CF3

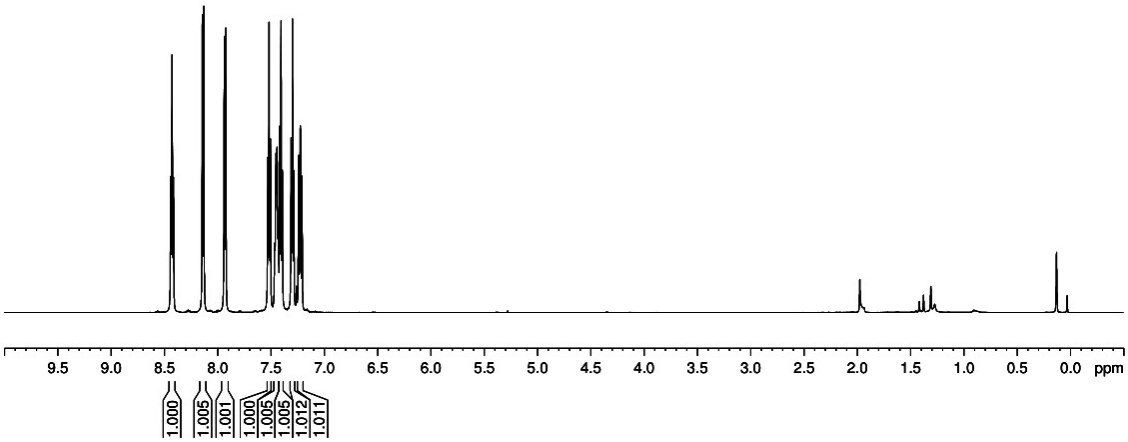
5n


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

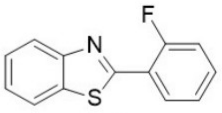

8.440
8.427
8.415
8.143
8.129
7.937
7.924
7.529
7.517
7.504
7.465
7.453
7.442
7.431
7.418
7.405
7.393
7.310
7.298
7.285
7.260
7.240
7.223
7.208


F
N
S

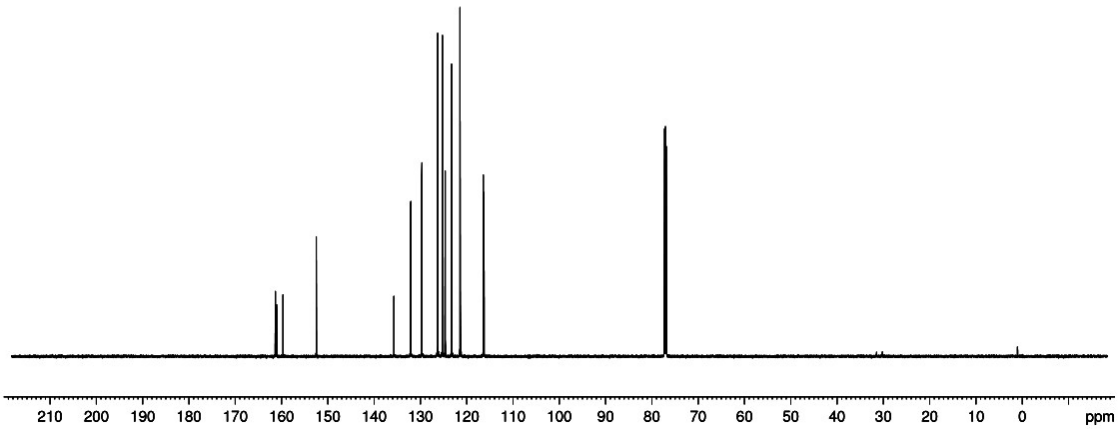
5o


9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
1.005
1.001
1.000
1.005
1.005
1.012
1.011

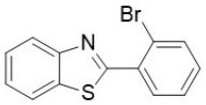

161.289
160.970
160.931
159.611
152.449
135.670
135.618
132.055
131.998
129.646
129.633
126.210
125.199
124.596
124.574
123.190
121.374
121.292
116.348
116.203
77.210
76.999
76.787


F
N
S

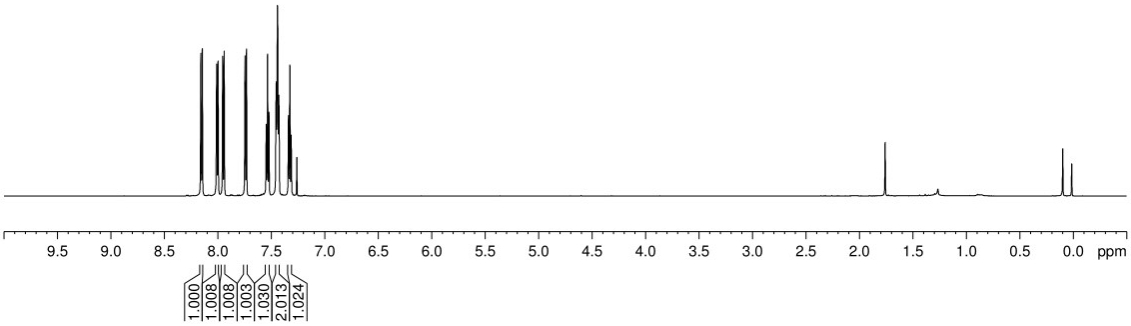
5o

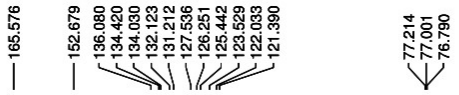

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

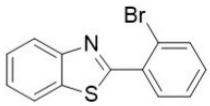

8.160
8.146
8.012
7.999
7.955
7.942
7.747
7.734
7.548
7.536
7.523
7.454
7.444
7.431
7.340
7.327
7.315
7.262


Br
N
S

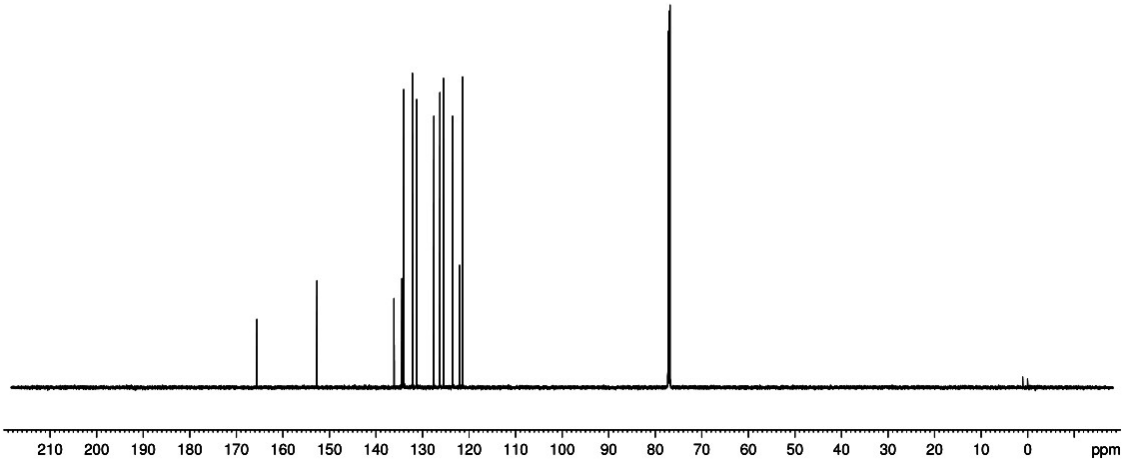
5p


9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.000
1.008
1.008
1.003
1.030
2.013
1.024


165.576
152.679
136.080
134.420
134.030
132.123
131.212
127.536
126.251
125.442
123.529
122.033
121.390
77.214
77.001
76.790


Br
N
S

5p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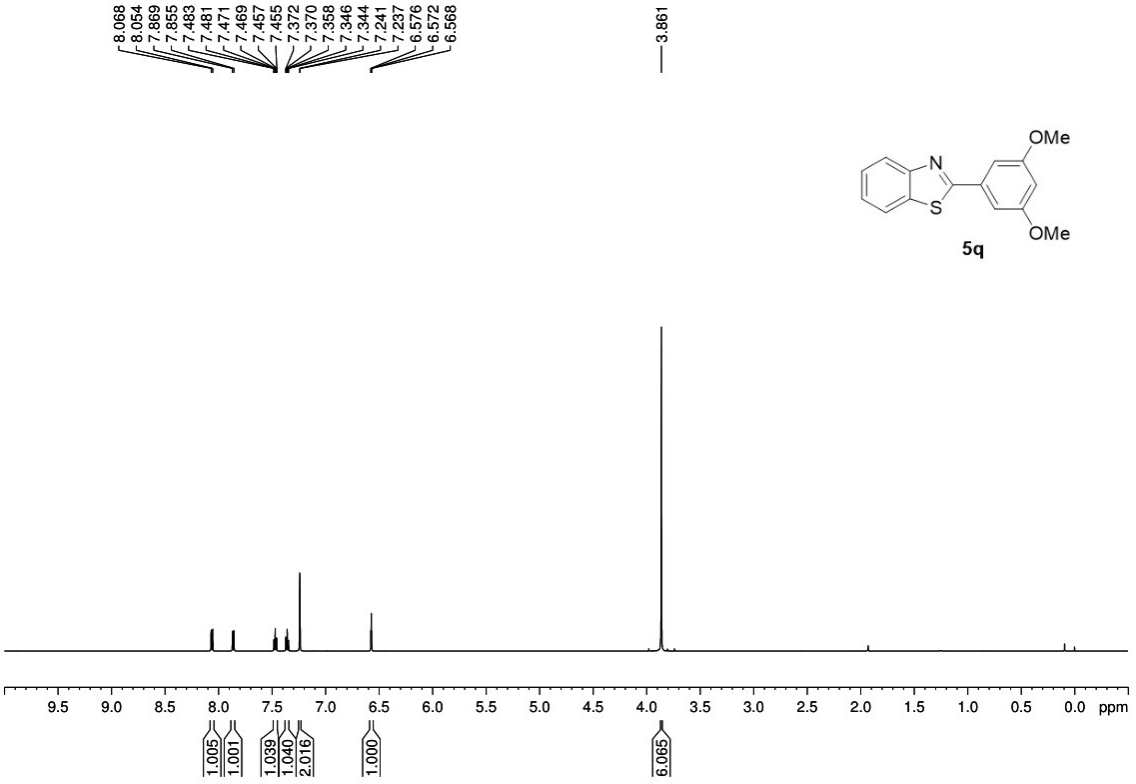
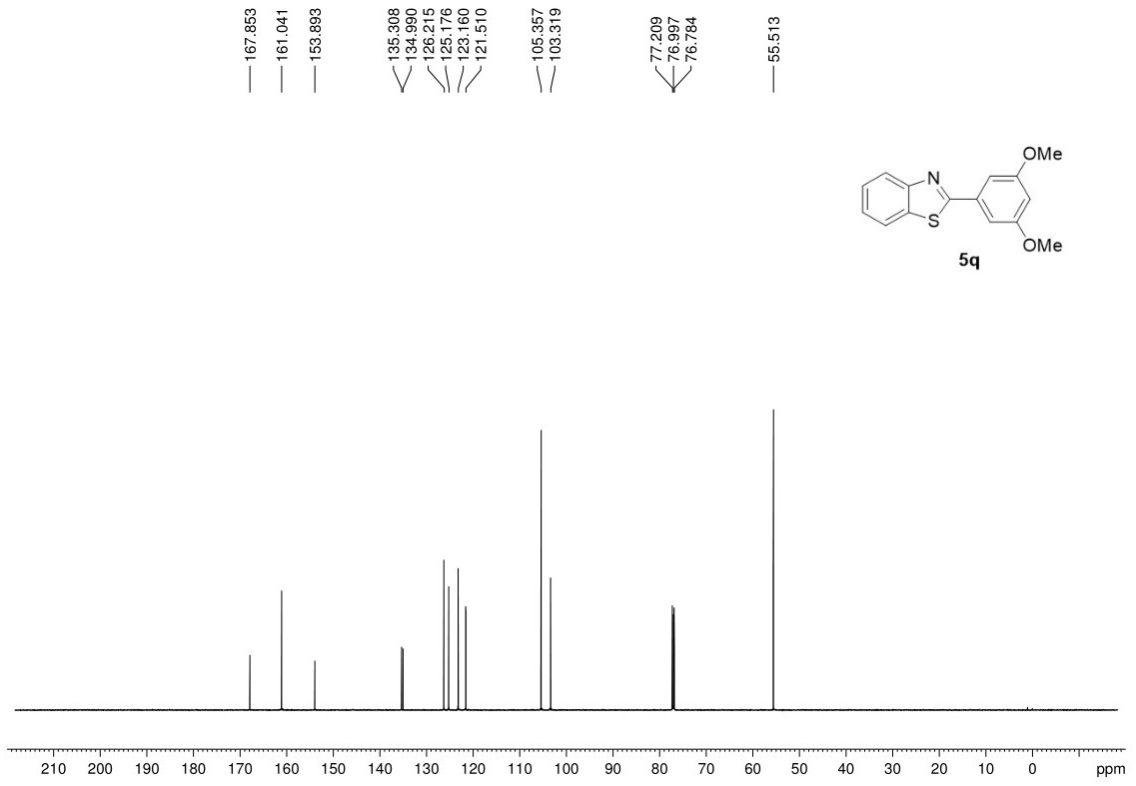
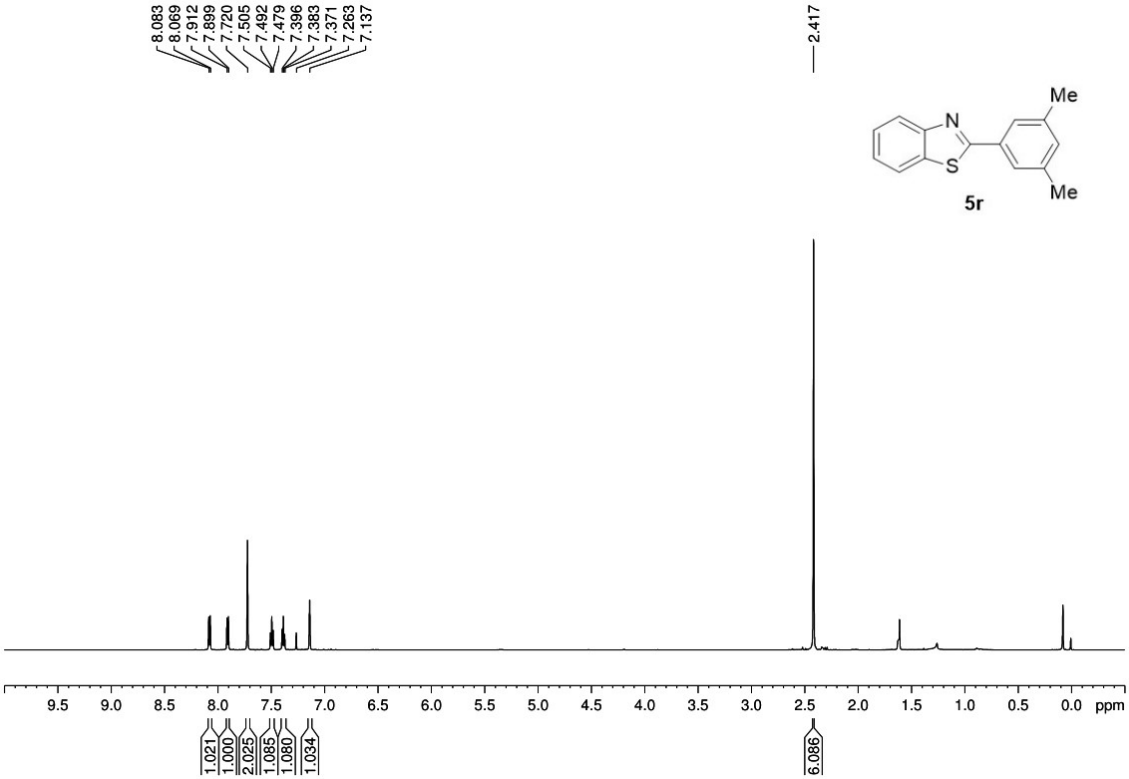
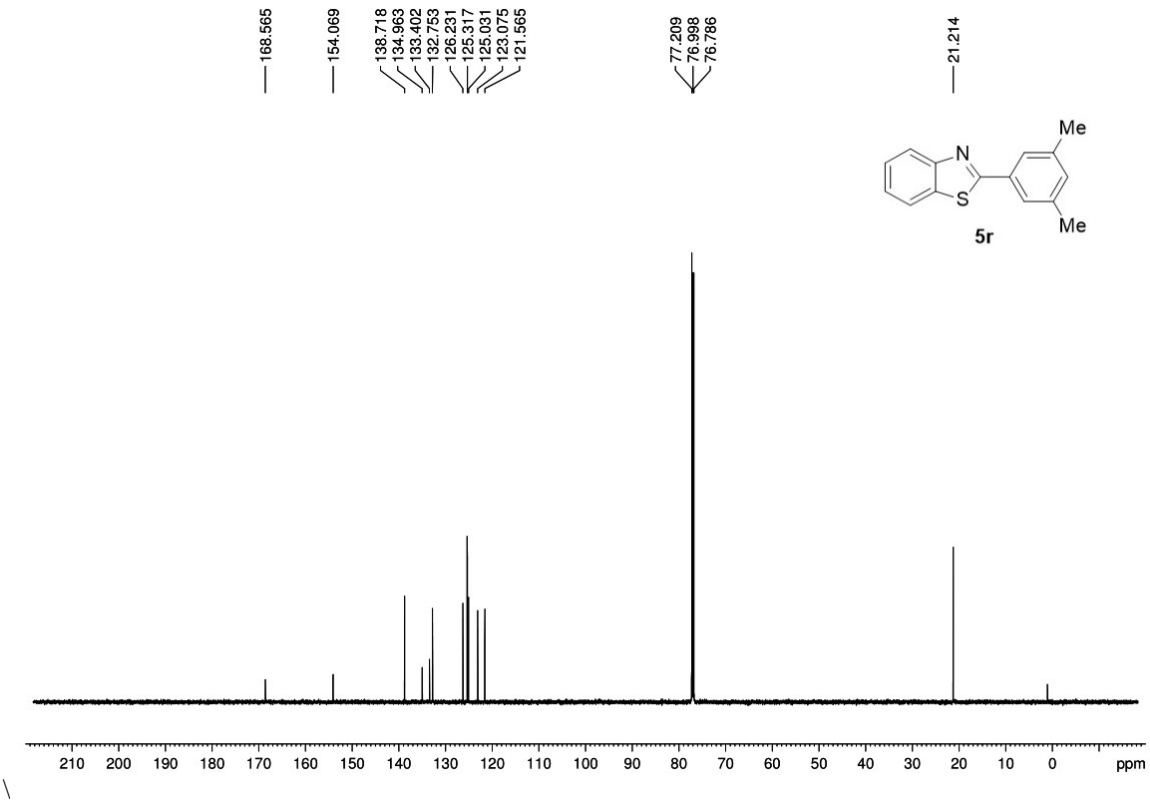

8.068
8.054
7.869
7.855
7.483
7.481
7.471
7.469
7.457
7.455
7.372
7.370
7.358
7.346
7.344
7.241
7.237
6.576
6.572
6.568
3.861
OMe
N
S
OMe
5q
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.005
1.001
1.039
1.040
2.016
1.000
6.065


167.853
161.041
153.893
135.308
134.990
126.215
125.176
123.160
121.510
105.357
103.319
77.209
76.997
76.784
55.513
OMe
N
S
OMe
5q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.083
8.069
7.912
7.899
7.720
7.505
7.492
7.479
7.396
7.383
7.371
7.263
7.137
2.417
Me
N
S
Me
5r
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.021
1.000
2.025
1.085
1.080
1.034
6.086


168.565
154.069
138.718
134.963
133.402
132.753
126.231
125.317
125.031
123.075
121.565
77.209
76.998
76.786
21.214
Me
N
S
Me
5r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

7. References:

1. R. Ye, H. Ruan, H. Xu, Zi. Li, L.-G. Meng, *Org. Chem. Front.,* 2021, **8**, 5345–5351.

2. P. Mampuys, Y. Zhu, S. Sergeyev, E. Ruijter, R. V. A. Orru, S. V. Doorslaer, B. U. W. Maes, *Org. Lett.,* 2016, **18**, 2808–2811.

3. C. G. Overberger, M. P. Mazzeo, J. J. Godfrey, *J. Org. Chem.,* 1959, **24**, 1407–1409.

4. K. Kanemoto, Y. Sakata, T. Hosoya, S. Yoshida, *Chem. Lett.,* 2020, **49**, 593–596.

5. Y. Kawashita, J. Yanagi, T. Fujii, M. Hayashi, *Bull. Chem. Soc. Jpn.,* 2009, **82**, 482–488.

6. E. A. El Rady, *Synth. Commun.,* 2006, **36**, 37–49.

7. S. Rezazadeh, B. Akhlaghinia, N. Razavi, *Aust. J. Chem.,* 2015, **68**, 145–155.

8. Y. Gao, Q. Song, G. Cheng, X. Cui, *Org. Biomol. Chem.,* 2014, **12**, 1044–1047.

9. Y. Tong, Q. Pan, Z. Jiang, D. Miao, X. Shi, S. Han, *Tetrahedron Lett.,* 2014, **55**, 5499–5503.

10. D. Azarifar, B. Maleki, M. Setayeshnazar, *Phosphorus, Sulfur Silicon. Relat. Elem.,* 2009, **184**, 2097–2102.

11. L. Ye, J. Chen, P. Mao, Z. Mao, X. Zhang, M. Yan, *Tetrahedron Lett.,* 2017, **58**, 874–876.

12. N. Mishra, A. S. Singh, A. K. Agrahari, S. K. Singh, M. Singh, V. K. Tiwari, *ACS Comb. Sci.,* 2019, **21**, 389–399.

13. A. Shaikh, O. Ravi, S. P. Ragini, N. Sadhana, S. R. Bathula, *Tetrahedron Lett.,* 2020, **61**, 151356.