Electronic Supplementary Material (ESI) for Green Chemistry.

Supplementary Information for

Natural Gallic Acid Catalyzed Aerobic Oxidative Coupling in Assistance of $Mn(CO_3)_2$ for Synthesis of Disulfanes in Water

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Contents

(A) General Remarks

All starting materials and catalysts were purchased from commercial sources and used without further treatment unless noted. High Performance Liquid Chromatography was conducted using a WATERS 1525 LC system with UV detector and a Symmetry C18 5 μm column (4.8×250 mm). All products besides gram scale were purified by flash chromatography on silica gel. ^{1}H NMR and ^{13}C NMR spectra were recorded on 600 MHz Bruker spectrometers and 400 MHz Bruker spectrometers. The used abbreviations are as follows: *s* (singlet), *d* (doublet), *t* (triplet), *q* (quartet), *m* (multiplet), *br* (broad). High resolution mass spectra (HRMS) data were measured on a MALDI-FTMS by means of the ESI technique, with accurate masses reported for the molecular ion [M+H]+. The mass spectra were performed on the SHIMADZU GCMS-QP 2010 Plus mass spectrometer by means of EI technique. UV-Vis spectra were recorded on Agilent 8453 diode array UV-Visible spectroscopy equipped with 89054A thermostattable cell holder, 89090A Peltier temperature controller and 89055A stirring module. The melting points of these compounds were determined by an X-4 micro-melting point apparatus (Beijing, China).

(B) Typical experimental procedure

(a) General Typical Procedure for the Aerobic Oxidative Self-Coupling

The catalytic reactions were performed in a 25-mL Schlenk tube and the general procedure is described typically with self-coupling of 2-mercaptobenzothiazole (**1a**) as follows: **1a** (0.5 mmol), gallic acid (**GA**) (0.15 mol%), $MnCO_3$ (0.15 mol%), and H_2O (3 mL) was added into the reactor and adjusted pH to 9 by Na_2CO_3 solution under stirring. Subsequently, the reaction mixture was stirred under 0.3 MPa O_2 at 80 ^oC and monitored by thin layer chromatography (TLC). After cooling to room temperature, the end reaction mixture was added 10 mL water to and extracted with ethyl acetate (10 mL×3). The combined organic extract phase was dried over Na_2SO_4, and after filtration, the solvent was removed on rotovap under reduced pressure. The resulting residue was purified by flash chromatography on silica gel to give the desired product.

(b) General Typical Procedure for the Aerobic Oxidative Corss-Coupling

Typically, RSH (0.25 mmol), R_1SH (0.25 mmol), **GA** (0.15 mol%), $MnCO_3$ (0.15 mol%), Na_2CO_3 (1.0 mmol) and H_2O (3 mL) was added into a 25-mL Schlenk tube. other operations were in keeping with the above procedure of Self-Coupling (a).

(c) Gram Scale Procedure

The catalytic reactions were performed in a 100-mL autoclave and the general procedure is described typically with self-coupling of **1a** as follows: **1a** (3.34 g, 20 mmol), **GA** (0.15 mol%), $MnCO_3$ (0.15 mol%), and H_2O (50 mL) was added into autoclave and stirred for 0.5 h. The mixture was adjusted pH to 9 by Na_2CO_3 solution under stirring. After the reactor closed, the atmosphere over the mixture was changed with O2 for three times. The reactor was heated to 80 °C and kept the pressure of O_2 under 0.3 MPa for the desired reaction time. After the autoclave was cooled to room temperature, the reaction mixture was filtered and washed with water for three times. The filter cake was dried and analyzed by HPLC.

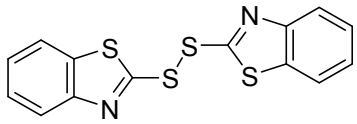
(d) In-situ UV invesitigation

In-situ UV invesitigation was conducted on Agilent 8453 diode array UV-Visible spectroscopy which equipped with 89054A thermostattable cell holder, 89090A Peltier temperature controller and 89055A stirring module. A CH_3CN solution of *p*-benzoquinone (10^{-7} mol/ml) and *t*-butylthiol (10^{-7} mol/ml) was removed O_2 with N_2, and then added into a covered quartz cell (optical path length 1 cm). The solution was heated to 70 ^oC under stirring, and then was recorded the UV spectra at desirable time.

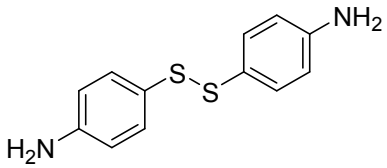
(e) HPLC tracing tests

Typically, to a 25 mL triangular flask 3 mL aqueous solution of GA (1.3×10^{-6} mol/ml) and 3 mL 4-methoxy-phenthiol (1.3×10^{-5} mol/ml) was added. The solution was adjusted pH to 9 by Na_2CO_3 solution under stirring, and then was sampled at desirable time and analyzed by HPLC. The flow phase was CH_3OH/H_2O (v:v = 9 : 1), and the detection wavelength was 254 nm.

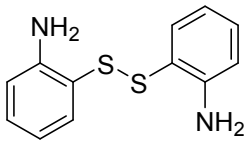
(C) Characterization Data of the Products



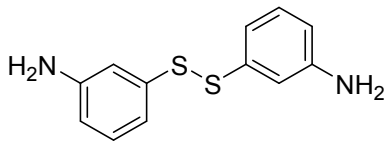
1,2-bis(benzo[*d*]thiazol-2-yl)disulfane (2a): White solid, isolated yield 98%; mp: 179-180 °C (lit[1] 179-180 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.94 (d, J = 8.2 Hz, 2H), 7.77 (d, J = 8.0 Hz, 2H), 7.49-7.43 (m, 2H), 7.39-7.32 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 167.87, 154.56, 136.16, 126.61, 125.32, 122.71, 121.33.



4,4'-disulfanediyldianiline (2b): Yellow solid, isolated yield 96%; mp: 76-77 °C (lit[1] 75-77 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.24 (d, J = 8.4 Hz, 4H), 6.56 (d, J = 8.4 Hz, 4H), 3.76 (br, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.17, 133.97, 125.67, 115.42. MS (EI) m/z calcd for $C_{12}H_{12}N_2S_2$ M^+: 248, found 248.

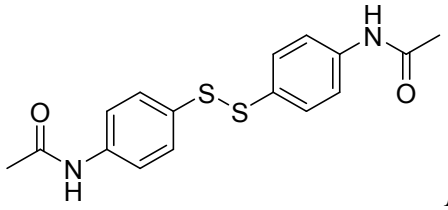


2,2'-disulfanediyldianiline (2c): Yellow solid, isolated yield 97%; mp: 90-91 °C (lit[3] 89-91 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.21-7.10 (m, 4H), 6.74-6.68 (m, 2H), 6.62-6.55 (m, 2H), 4.20 (s, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.65, 136.85, 131.63, 118.78, 118.27, 115.26. MS (EI) m/z calcd for $C_{12}H_{12}N_2S_2$ M^+: 248, found 248.

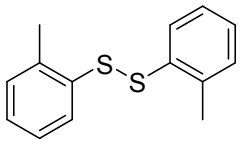


3,3'-disulfanediyldianiline (2d)[4]: Yellow liquid, isolated yield 98%; ^{1}H NMR (400

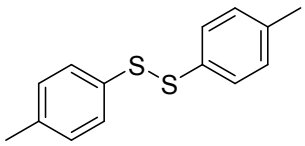
MHz, $CDCl_3$) δ: 7.08 (t, J = 7.9 Hz, 2H), 6.90-6.86 (m, 2H), 6.81 (t, J = 2.0 Hz, 2H), 6.53-6.47 (m, 2H), 3.56 (br, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.21, 138.06, 129.88, 117.07, 113.91, 112.99. MS (EI) m/z calcd for $C_{12}H_{12}N_2S_2$ M^+: 248, found 248.



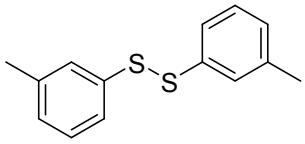
***N,N'*-(disulfanediylbis(4,1-phenylene))diacetamide (2e)**: White solid, isolated yield 97%; mp: 188-189 ^oC (lit[5] 181-182 ^oC); ^1H NMR (400 MHz, $(CD_3)_2SO$) δ: 10.08 (br, 2H), 7.71-7.25 (m, 8H), 2.04 (s, 6H); ^{13}C NMR (100 MHz, $(CD_3)_2SO$) δ: 168.98, 139.97, 130.61, 129.82, 120.14, 24.49.



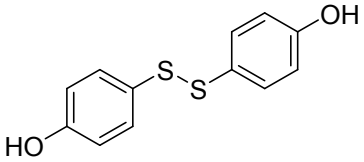
1,2-di-*o*-tolyldisulfane (2f): White solid, isolated yield 98%; mp: 38-39 ^oC (lit[1] 38-39 ^oC); ^1H NMR (400 MHz, $CDCl_3$) δ: 7.57-7.52 (m, 2H), 7.21-7.18 (m, 6H), 2.46 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 137.43, 135.46, 130.36, 128.69, 127.37, 126.74, 20.06. MS (EI) m/z calcd for $C_{14}H_{14}S_2$ M^+: 246, found 246.



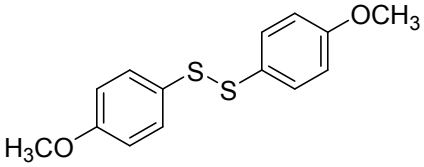
1,2-di-*p*-tolyldisulfane (2g): White solid, isolated yield 96%; mp: 48-49 ^oC (lit[1] 47-48 ^oC); ^1H NMR (400 MHz, $CDCl_3$) δ: 7.43 (d, J = 7.5 Hz, 4H), 7.14 (d, J = 8.3 Hz, 4H), 2.35 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 137.49, 133.98, 129.86, 128.60, 21.12. MS (EI) m/z calcd for $C_{14}H_{14}S_2$ M^+: 246, found 246.



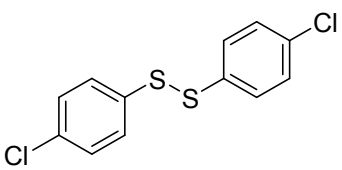
1,2-di-*m*-tolyldisulfane (2h)[1]: Light yellow liquid, isolated yield 99%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.35 (d, J = 6.1 Hz, 4H), 7.22 (t, J = 8.0 Hz, 2H), 7.06 (d, J = 7.4 Hz, 2H), 2.35 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 138.97, 136.98, 128.96, 128.07 (2C), 124.63, 21.43. MS (EI) m/z calcd for $C_{14}H_{14}S_2$ M^+: 246, found 246.



4,4'-disulfanediyldiphenol (2i): White solid, isolated yield 92%; mp: 148-149 ^{o}C (lit[1] 148-149 ^{o}C); ^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ: 9.83 (br, 2H), 7.27 (d, J = 8.6 Hz, 4H), 6.76 (d, J = 8.7 Hz, 4H); ^{13}C NMR (100 MHz, $(CD_3)_2SO$) δ: 158.74, 133.49, 125.59, 116.77. MS (EI) m/z calcd for $C_{12}H_{10}O_2S_2$ M^+: 250, found 250.

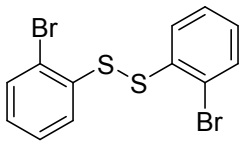


1,2-bis(4-methoxyphenyl)disulfane (2j)[1]: Light yellow liquid, isolated yield 96%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41 (d, J = 8.8 Hz, 4H), 6.84 (d, J = 8.8 Hz, 4H), 3.80 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.95, 132.68, 128.46, 114.66, 55.39. MS (EI) m/z calcd for $C_{14}H_{14}O_2S_2$ M^+: 278, found 278.

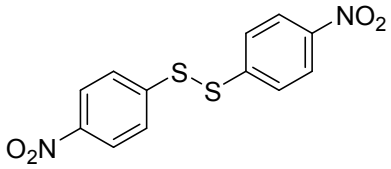


1,2-bis(4-chlorophenyl)disulfane (2k): White solid, isolated yield 94%; mp: 65-66 ^{o}C (lit[1] 63-64 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.39 (d, J = 8.6 Hz, 4H), 7.26 (d, J = 8.6 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 135.17, 133.67, 129.36, 129.34. MS

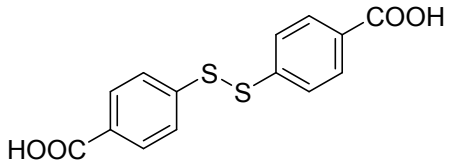
(EI) m/z calcd for $C_{12}H_8Cl_2S_2$ M^+: 286, found 286.



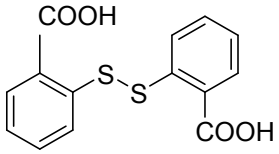
1,2-bis(2-bromophenyl)disulfane (2l): White solid, isolated yield 98%; mp: 96-97 ^oC (lit[6a] 97-98 ^oC); ^1H NMR (400 MHz, $CDCl_3$) δ: 7.56-7.50 (m, 4H), 7.29-7.23 (m, 2H), 7.11-7.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 136.18, 132.96, 128.25, 127.98, 126.98, 121.11. MS (EI) m/z calcd for $C_{12}H_8Br_2S_2$ M^+: 374, found 374.



1,2-bis(4-nitrophenyl)disulfane (2m): Yellow solid, isolated yield 96%; mp: 179-180 ^oC (lit[6b] 173-175 ^oC); ^1H NMR (400 MHz, $CDCl_3$) δ: 8.19 (d, J = 7.3 Hz, 4H), 7.62 (d, J = 7.3 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 146.98, 144.08, 126.39, 124.48.

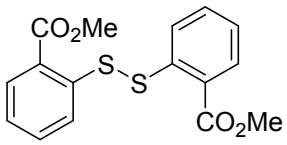


4,4'-disulfanediyldibenzoic acid (2n): White solid, isolated yield 98%; mp: ＞300 ^oC (lit[1] ＞300 ^oC); ^1H NMR (400 MHz, $(CD_3)_2SO$) δ: 7.92 (d, J = 8.6 Hz, 4H), 7.62 (d, J = 8.6 Hz, 4H); ^{13}C NMR (100 MHz, $(CD_3)_2SO$) δ: 167.09, 141.21, 130.80, 130.15, 126.54.

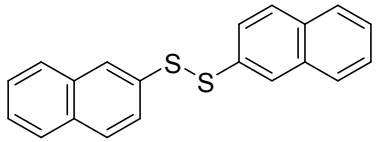


2,2'-disulfanediyldibenzoic acid (2o): White solid, isolated yield 97%; mp: 292-293

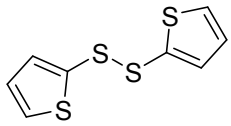
°C (lit[1] 291-293 °C); ^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ: 8.06-8.02 (m, 2H), 7.65-7.60 (m, 2H), 7.58-7.52 (m, 2H), 7.36-7.31 (m, 2H); ^{13}C NMR (100 MHz, $(CD_3)_2SO$) δ: 168.11, 139.39, 133.78, 132.08, 128.52, 126.48, 125.45.



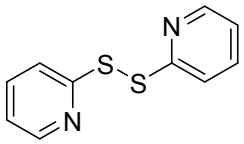
dimethyl 2,2'-disulfanediyldibenzoate (2p): White solid, isolated yield 97%; mp: 126-127 °C (lit[1] 126-128 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.98 (d, J = 6.4 Hz, 2H), 7.67 (d, J = 7.4 Hz, 2H), 7.36-7.29 (m, 2H), 7.18-7.11 (m, 2H), 3.90 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 166.93, 140.37, 133.11, 131.49, 127.30, 125.84, 125.51, 52.42. MS (EI) m/z calcd for $C_{16}H_{14}O_4S_2$ M^+: 334, found 334.



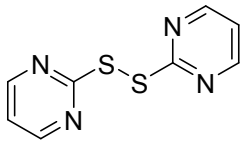
1,2-di(naphthalen-2-yl)disulfane (2q): White solid, isolated yield 99%; mp: 139-140 °C (lit[1] 139-141 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.99 (s, 2H), 7.82-7.77 (m, 4H), 7.76-7.71 (m , 2H), 7.66-7.60 (m, 2H), 7.50-7.42 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 134.29, 133.50, 132.53, 129.02, 127.80, 127.50, 126.78, 126.57, 126.28, 125.69.



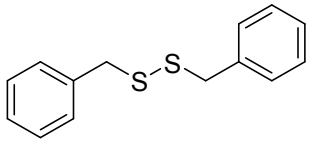
1,2-di(thiophen-2-yl)disulfane (2r): Yellow solid, isolated yield 81%; mp: 52-53 °C (lit[1] 52-53 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.50 (d, J = 5.6 Hz, 2H), 7.16 (d, J = 2.6 Hz, 2H), 7.04-7.01 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 135.74, 135.67, 132.31, 127.78. MS (EI) m/z calcd for $C_8H_6S_4$ M^+: 230, found 230.



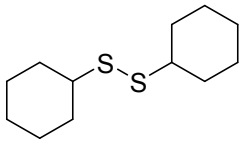
1,2-di(pyridin-2-yl)disulfane (2s): White solid, isolated yield 99%; mp: 50-51 ^{o}C (lit[1] 51-52 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.43 (d, J = 4.6 Hz, 2H), 7.60-7.54 (m, 4H), 7.07-7.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.91, 149.56, 137.41, 121.13, 119.68. MS (EI) m/z calcd for $C_{10}H_8N_2S_2$ M^+: 220, found 220.



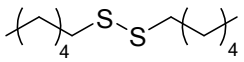
1,2-di(pyridin-2-yl)disulfane (2t): Yellow solid, isolated yield 77%; mp: 143-144 ^{o}C (lit[3] 143-145 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.55 (d, J = 4.8 Hz, 4H), 7.07 (t, J = 4.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 169.72, 157.92, 118.21.



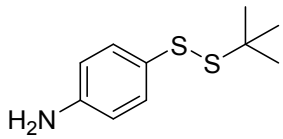
1,2-dibenzyldisulfane (2u): White solid, isolated yield 93%; mp: 71-72 ^{o}C (lit[3] 68-70 ^{o}C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.34-7.27 (m, 10H), 3.59 (s, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 137.39, 129.45, 128.51, 127.46, 43.30. MS (EI) m/z calcd for $C_{14}H_{14}S_2$ M^+: 246, found 246.



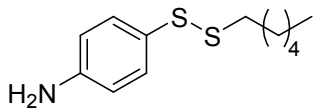
1,2-dicyclohexyldisulfane (2v)[1]: Colorless liquid, isolated yield 67%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.73-2.63 (m, 2H), 2.07-2.01 (m, 4H), 1.81-1.73 (m, 4H), 1.64-1.58 (m, 2H), 1.35-1.21 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 49.98, 32.87, 26.10, 25.72. MS (EI) m/z calcd for $C_{12}H_{22}S_2$ M^+: 230, found 230.



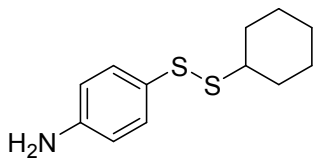
1,2-dipropyldisulfane (2w)[1]: Colorless liquid, isolated yield 71%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.68 (t, J = 7.4 Hz, 4H), 1.71-1.62 (m, 4H), 1.42-1.24 (m, 12H), 0.89 (t, J = 6.9 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 39.22, 31.46, 29.21, 28.23, 22.56, 14.04. MS (EI) m/z calcd for $C_{12}H_{26}S_2$ M^+: 234, found 234.



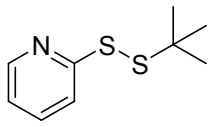
4-(*tert*-butyldisulfanyl)aniline (3a) (new compound based on SciFinder search) : Yellow liquid, isolated yield 93%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.37 (d, J = 8.6 Hz, 2H), 6.60 (d, J = 8.6 Hz, 2H), 3.60 (br, 2H), 1.30 (s, 9H); ^{13}C NMR (100MHz, $CDCl_3$) δ: 145.99, 131.39, 126.90, 115.52, 48.79, 30.01. HRMS m/z (ESI) calcd for $C_{10}H_{15}NS_2$ $[M+H]^+$: 214.0719, found 214.0720.



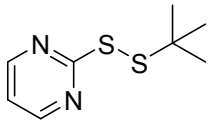
4-(propyldisulfanyl)aniline (3b)[1]: Yellow liquid, isolated yield 90%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.35 (d, J = 8.6 Hz, 2H), 6.62 (d, J = 8.6 Hz, 2H), 3.58 (br, 2H), 2.73(t, J = 7.4 Hz, 2H), 1.71-1.62 (m, 2H), 1.37-1.26 (m, 6H), 0.88 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 146.65, 132.84, 125.57, 115.55, 38.78, 31.41, 28.70, 28.22, 22.55, 14.07. MS (EI) m/z calcd for $C_{12}H_{19}NS_2$ M^+: 241, found 241.



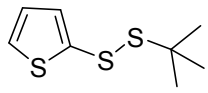
4-(cyclohexyldisulfanyl)aniline (3c)[1]: Yellow liquid, isolated yield 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.35 (d, J = 8.6 Hz, 2H), 6.62 (d, J = 8.6 Hz, 2H), 3.61 (br, 2H), 2.83-2.77 (m, 1H), 2.05-1.99 (m, 2H), 1.77-1.74 (m, 2H), 1.62-1.58 (m, 1H), 1.39-1.22 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 146.30, 131.97, 126.40, 115.56, 49.53, 32.61, 26.04, 25.73. MS (EI) m/z calcd for $C_{12}H_{17}NS_2$ M^+: 239, found 239.



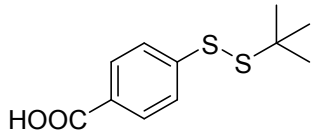
2-(*tert*-butyldisulfanyl)pyridine (3d)[2]: Colorless liquid, isolated yield 97%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.41-8.37 (m, 1H), 7.76 (d, J = 8.2 Hz, 1H), 7.62-7.55 (m, 1H), 7.04-6.98 (m, 1H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 161.65, 149.17, 136.79, 120.36, 119.61, 49.26, 29.78. MS (EI) m/z calcd for $C_9H_{13}NS_2$ M^+: 199, found 199.



2-(*tert*-butyldisulfanyl)pyrimidine (3e)[2]: Colorless liquid, isolated yield 96%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.56 (d, J = 4.8 Hz, 2H), 7.03 (t, J = 4.8 Hz, 1H), 1.32 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.24, 157.68, 117.86, 49.08, 29.72. MS (EI) m/z calcd for $C_8H_{12}N_2S_2$ M^+: 200, found 200.

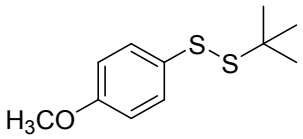


2-(*tert*-butyldisulfanyl)thiophene (3f)[7]: Yellow liquid, isolated yield 92%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.35-7.32 (m, 1H), 7.23-7.20 (m, 1H), 6.95-6.91 (m, 1H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 139.30, 132.57, 129.48, 127.35, 49.04, 30.02. MS (EI) m/z calcd for $C_8H_{12}S_3$ M^+: 204, found 204.

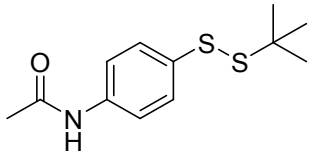


4-(*tert*-butyldisulfanyl)benzoic acid (3g) (new compound based on SciFinder search): White solid, isolated yield 93%; mp: 135-136 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.03 (d, J = 8.6 Hz, 2H), 7.65 (d, J = 8.6 Hz, 2H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 171.89, 146.58, 130.46, 126.84, 125.49, 49.79, 29.83. HRMS

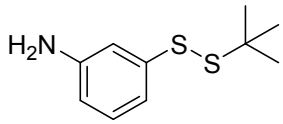
m/z (ESI) calcd for $C_{11}H_{14}O_2S_2$ $[M+H]^+$: 243.0508, found 243.0510.



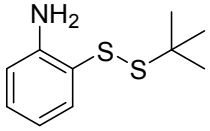
1-(*tert*-butyl)-2-(4-methoxyphenyl)disulfane (3h)[2]: Colorless liquid, isolated yield 78%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.49 (d, J = 8.9 Hz, 2H), 6.84 (d, J = 8.9 Hz, 2H), 3.79 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.93, 130.29, 129.77, 114.44, 55.37, 48.95, 29.93. MS (EI) m/z calcd for $C_{11}H_{16}OS_2$ M^+: 228, found 228.



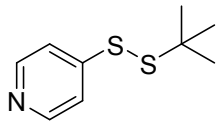
***N*-(4-(*tert*-butyldisulfanyl)phenyl)acetamide (3i) (new compound based on SciFinder search)**: White solid, isolated yield 90%; mp: 143-144 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.54-7.42 (m, 4H), 2.16 (s, 3H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.49, 136.55, 134.09, 128.24, 120.27, 49.25, 29.87, 24.56. HRMS m/z (ESI) calcd for $C_{12}H_{17}NOS_2$ $[M+H]^+$: 256.0824, found 256.0822.



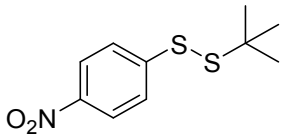
3-(*tert*-butyldisulfanyl)aniline (3j) (new compound based on SciFinder search): Yellow liquid, isolated yield 96%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.07 (t, J = 7.8 Hz, 1H), 6.96-6.88 (m, 2H), 6.51-6.46 (m, 1H), 3.57 (br, 2H), 1.32 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 146.87, 139.68, 129.55, 116.90, 113.31, 112.99, 49.16, 29.90. HRMS m/z (ESI) calcd for $C_{10}H_{15}NS_2$ $[M+H]^+$: 214.0719, found 214.0721.



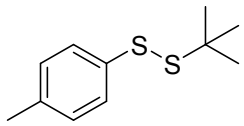
2-(*tert*-butyldisulfanyl)aniline (3k) (new compound based on SciFinder search): Yellow liquid, isolated yield 96%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.55-7.51 (m, 1H), 7.13-7.08 (m, 1H), 6.72-6.66 (m, 2H), 4.12 (br, 2H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.28, 134.09, 130.06, 120.63, 118.45, 115.61, 48.98, 30.07. HRMS m/z (ESI) calcd for $C_{10}H_{15}NS_2$ $[M+H]^+$: 214.0719, found 214.0720.



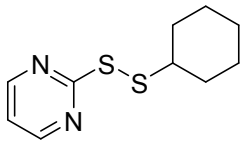
4-(*tert*-butyldisulfanyl)pyridine (3l)[8]: Colorless liquid, isolated yield 98%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.42 (d, J = 6.0 Hz, 2H), 7.46 (d, J = 6.2 Hz, 2H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.39, 149.23, 120.06, 49.88, 29.80. MS (EI) m/z calcd for $C_9H_{13}NS_2$ M^+: 199, found 199.



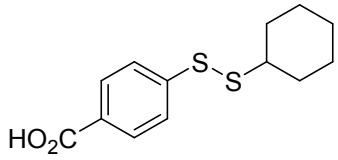
1-(*tert*-butyl)-2-(4-nitrophenyl)disulfane (3m)[2]: Yellow liquid, isolated yield 77%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.14 (d, J = 8.9 Hz, 2H), 7.69 (d, J = 8.9 Hz, 2H), 1.32 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.40, 146.00, 125.76, 123.85, 50.21, 29.80. MS (EI) m/z calcd for $C_{10}H_{13}NO_2S_2$ M^+: 243, found 243.



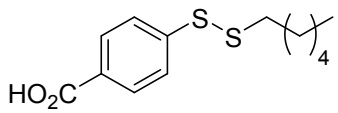
1-(*tert*-butyl)-2-(*p*-tolyl)disulfane (3n)[2]: Colorless liquid, isolated yield 88%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.45 (d, J = 8.2 Hz, 2H), 7.10 (d, J = 8.0 Hz, 2H), 2.32 (s, 3H), 1.30 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 136.32, 135.36, 129.52, 127.41, 49.08, 29.88, 21.00. MS (EI) m/z calcd for $C_{11}H_{16}S_2$ M^+: 212, found 212.



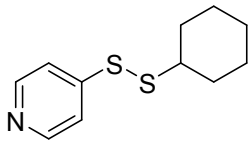
2-(cyclohexyldisulfanyl)pyrimidine (3o) (new compound based on SciFinder search): Colorless liquid, isolated yield 96%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.58 (d, J = 4.8 Hz, 2H), 7.05 (t, J = 4.8 Hz, 1H), 2.98-2.89 (m, 1H), 2.08-2.01 (m, 2H), 1.78-1.71 (m, 2H), 1.60-1.52 (m, 1H), 1.42-1.20 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.36, 157.75, 117.76, 49.38, 32.41, 26.00, 25.55. HRMS m/z (ESI) calcd for $C_{11}H_{15}N_2S_2$ $[M+H]^+$: 227.0671, found 227.0674.



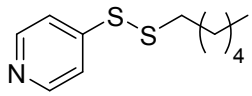
4-(cyclohexyldisulfanyl)benzoic acid (3p) (new compound based on SciFinder search): White solid, isolated yield 91%; mp: 126-127 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.04 (d, J = 8.6 Hz, 2H), 7.63 (d, J = 8.6 Hz, 2H), 2.87-2.79 (m, 1H), 2.08-1.96 (m, 2H), 1.85-1.74 (m, 2H), 1.64-1.54 (m, 1H), 1.40-1.24 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 171.89, 146.34, 130.54, 126.84, 125.35, 50.22, 32.69, 26.03, 25.48. HRMS m/z (ESI) calcd for $C_{13}H_{16}O_2S_2$ $[M+H]^+$: 269.0664, found 269.0665.



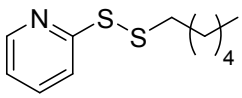
4-(propyldisulfanyl)benzoic acid (3q) (new compound based on SciFinder search): White solid, isolated yield 91%; mp: 70-71 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.06 (d, J = 8.6 Hz, 2H), 7.62 (d, J = 8.6 Hz, 2H), 2.76 (t, J = 8.0 Hz, 2H), 1.74-1.61 (m, 2H), 1.42- 1.22 (m, 6H), 0.88 (t, J = 7.0 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ: 171.89, 145.53, 130.64, 127.01, 125.58, 39.07, 31.34, 28.88, 28.14, 22.50, 14.00. HRMS m/z (ESI) calcd for $C_{13}H_{18}O_2S_2$ $[M+H]^+$: 271.0821, found 271.0825.



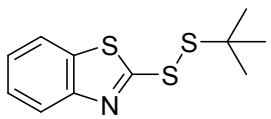
4-(cyclohexyldisulfanyl)pyridine (3r) (new compound based on SciFinder search): Colorless liquid, isolated yield 94%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.44 (s, 2H), 7.44 (d, J = 5.5 Hz, 2H), 2.88-2.72 (m, 1H), 2.03-1.89 (m, 2H), 1.82-1.73 (m, 2H), 1.68-1.53 (m, 1H), 1.45-1.14 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 150.08, 149.35, 119.93, 50.15, 32.68, 26.01, 25.41. HRMS m/z (ESI) calcd for $C_{11}H_{15}NS_2$ $[M+H]^+$: 226.0719, found 226.0724.



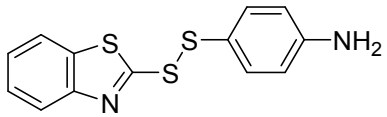
4-(propyldisulfanyl)pyridine (3s) (new compound based on SciFinder search): Yellow liquid, isolated yield 95%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.45 (d, J = 6.04 Hz, 2H), 7.43 (d, J = 6.2 Hz, 2H), 2.73 (t, J = 8.0 Hz, 2H), 1.68-1.61 (m, 2H), 1.45-1.03 (m, 6H), 0.86 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.47, 149.28, 119.95, 38.90, 31.32, 28.91, 28.12, 22.48, 14.00. HRMS m/z (ESI) calcd for $C_{11}H_{15}NS_2$ $[M+H]^+$: 228.0875, found 228.0877.



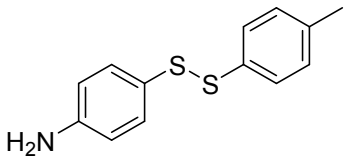
2-(propyldisulfanyl)pyridine (3t)[9]: Colorless liquid, isolated yield 94%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.46-8.43 (m, 1H), 7.72 (d, J = 7.3 Hz, 1H), 7.65-7.60 (m, 1H), 7.08-7.03 (m, 1H), 2.80 ((t, J = 7.5 Hz, 2H), 1.71-1.63 (m, 2H), 1.40-1.21 (m, 6H), 0.86 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 160.73, 149.55, 136.95, 120.46, 119.53, 39.05, 31.37, 28.90, 28.17, 22.51, 14.02. MS (EI) m/z calcd for $C_{11}H_{17}NS_2$ M^+: 227, found 227.



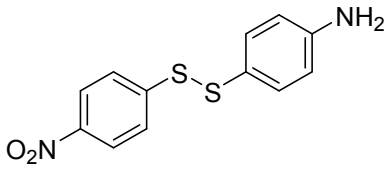
2-(*tert*-butyldisulfanyl)benzo[*d*]thiazole (3u): White solid, isolated yield 92%; mp: 78-79 °C (lit[7] 78-80 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.87-7.83 (m, 1H), 7.80-7.75 (m, 1H), 7.44-7.39 (m, 1H), 7.34-7.28 (m, 1H), 1.42 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 174.40, 154.89, 135.76, 126.18, 124.53, 122.07, 121.07, 50.29, 29.81. MS (EI) m/z calcd for $C_{11}H_{13}NS_3$ M^+: 225, found 225.



4-(benzo[*d*]thiazol-2-yldisulfanyl)aniline (3v)[10]: Yellow solid, isolated yield 85%; mp: 128-129 °C (lit[10] 128-130 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.86 (d, J = 8.2 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.50 (d, J = 8.6 Hz, 2H), 7.45-7.38 (m, 1H), 7.35-7.29 (m, 1H), 6.58 (d, J = 8.6 Hz, 2H), 3.89 (br, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.70, 155.00, 148.35, 135.87, 134.40, 126.22, 124.56, 122.30, 122.15, 121.17, 115.46.

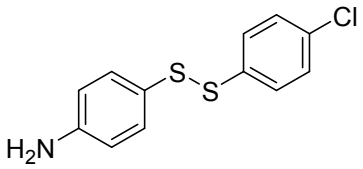


4-(*p*-tolyldisulfanyl)aniline (3w): Yellow solid, isolated yield 85%; mp: 42-43 °C (lit[1] 42-43 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.6 Hz, 2H), 7.12 (d, J = 7.9 Hz, 2H), 6.58 (d, J = 8.6 Hz, 2H), 3.76 (br, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.10, 137.55, 134.43, 133.12, 129.75, 129.49, 125.28, 115.48, 21.14. MS (EI) m/z calcd for $C_{13}H_{13}NS_2$ M^+: 247, found 247.

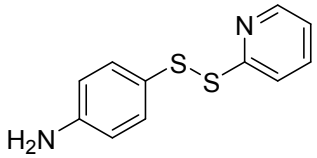


4-((4-nitrophenyl)disulfanyl)aniline (3x): Yellow solid, isolated yield 84%; mp: 116-118 °C (lit[11] 118 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.15 (d, J = 9.0 Hz, 2H), 7.67 (d, J = 9.0 Hz, 2H), 7.31 (d, J = 8.6 Hz, 2H), 6.58 (d, J = 8.6 Hz, 2H), 3.82 (br, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.85, 147.27, 146.23, 133.33, 126.49, 124.05,

122.98, 115.57.



4-((4-chlorophenyl)disulfanyl)aniline (3y)[12]: Yellow liquid, isolated yield 79%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.34 (d, J = 8.6 Hz, 2H), 7.21-14 (m, 4H), 6.48 (d, J = 8.6 Hz, 2H), 3.57 (br, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.40, 136.44, 133.32, 133.25, 130.09, 129.10, 124.44, 115.53. MS (EI) m/z calcd for $C_{12}H_{10}ClNS_2$ M^+: 267, found 267.



4-(pyridin-2-yldisulfanyl)aniline (3z)[13]: Yellow liquid, isolated yield 71%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.46 (d, J = 4.0 Hz, 1H), 7.76 (d, J = 8.1 Hz, 1H), 7.66-7.59 (m, 1H), 7.37 (d, J = 8.6 Hz, 2H), 7.10-7.03 (m, 1H), 6.58 (d, J = 8.6 Hz, 2H), 3.25 (br, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.48, 148.49, 146.08, 136.04, 131.41, 123.04, 119.58, 118.88, 114.51.

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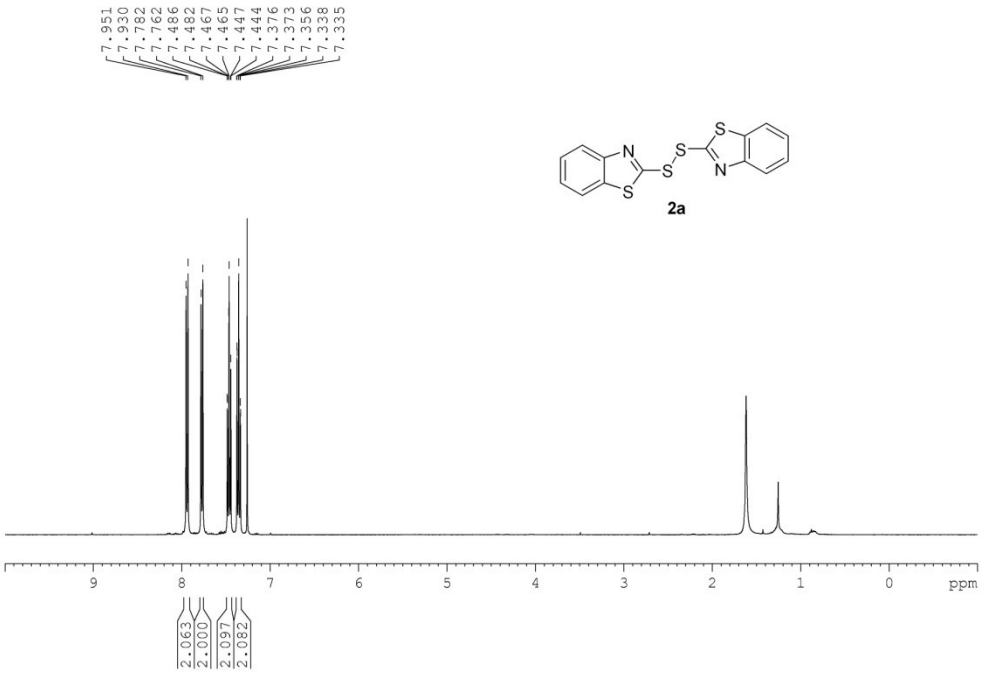
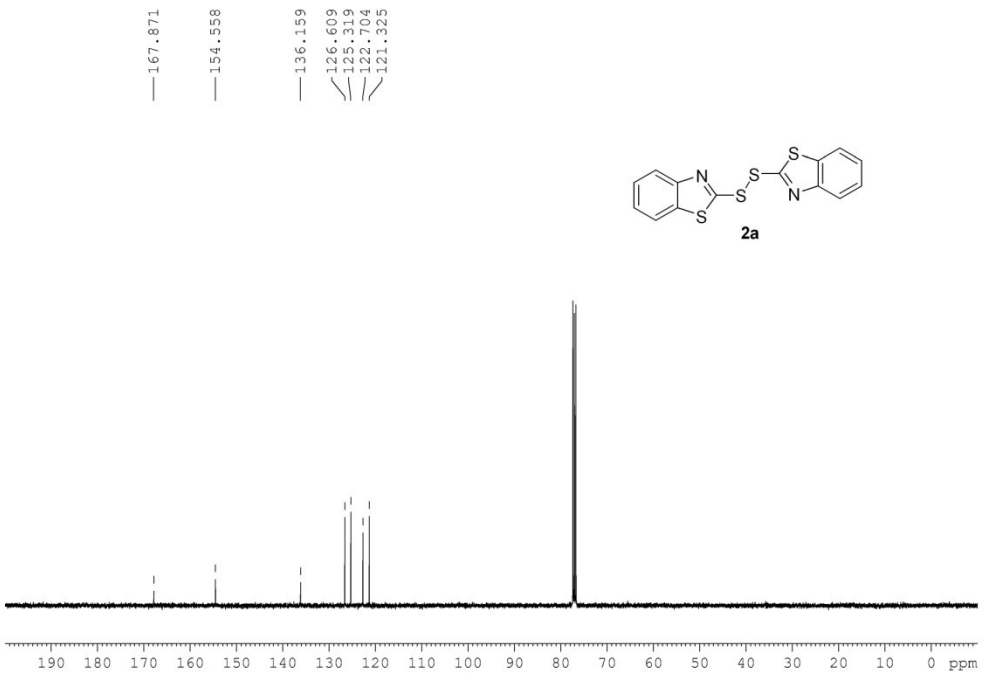
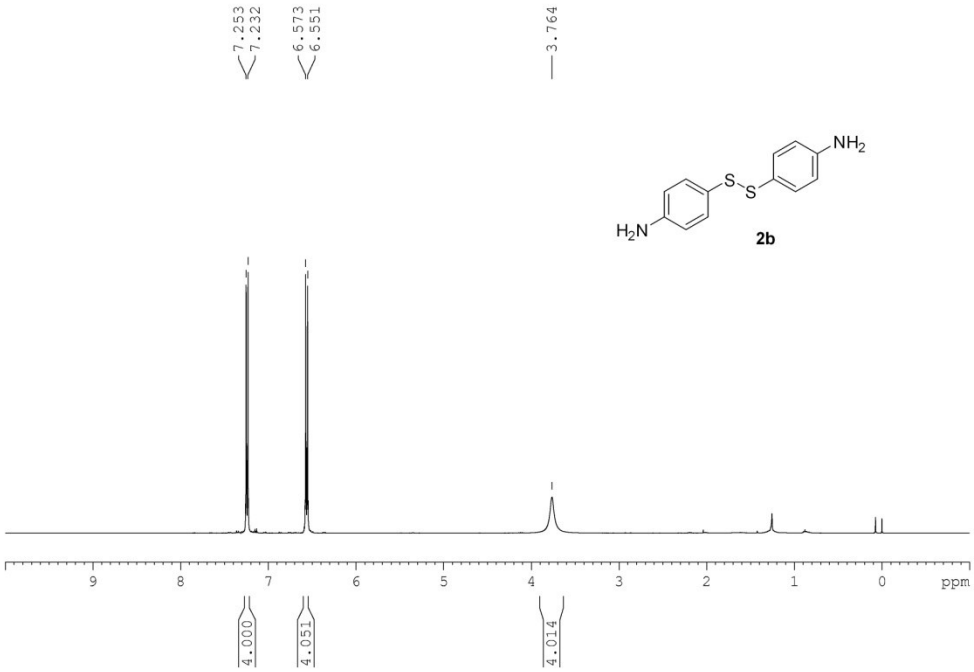
(D) Copies of all spectra



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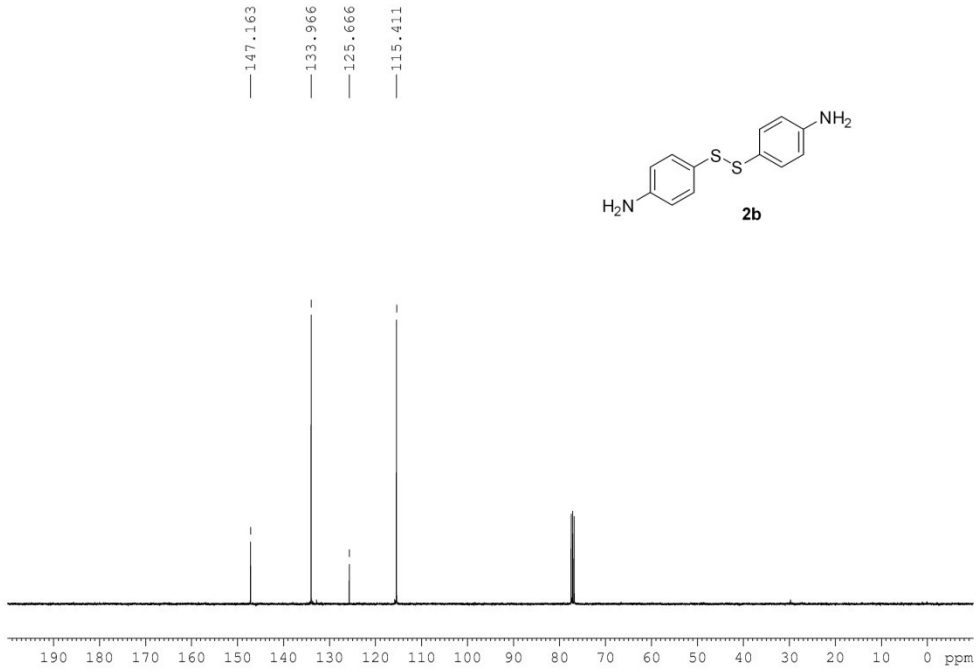
6.573
6.551
3.764
NH2
S
S
H2N
2b
9
8
7
6
5
4
3
2
1
0
ppm
4.000
4.051
4.014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NH2
S
S
H2N
2b
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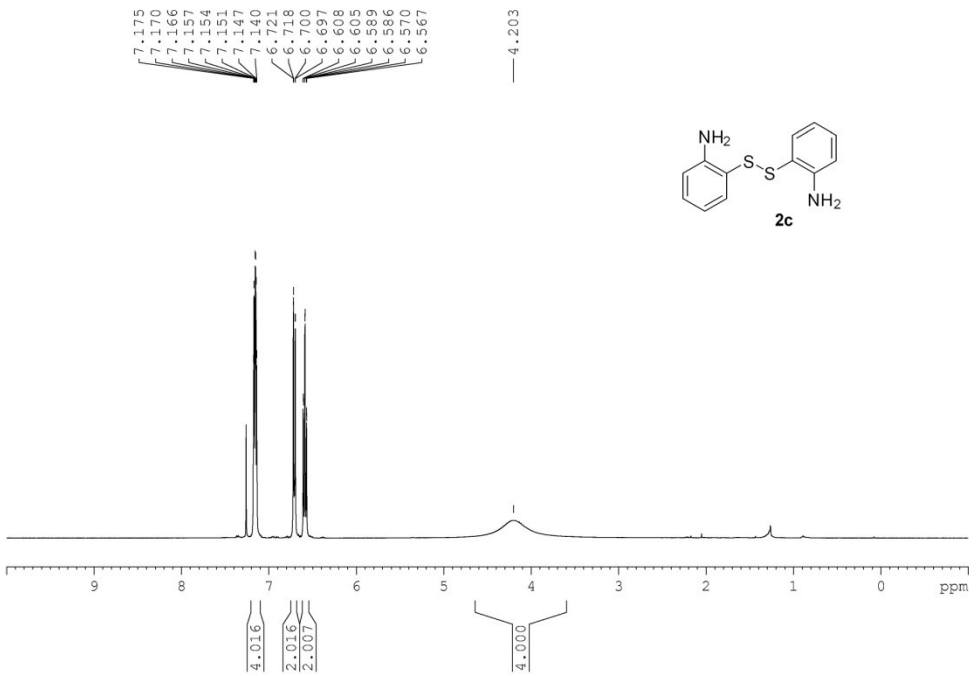
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7.170
7.166
7.157
7.154
7.151
7.147
7.140
6.721
6.718
6.700
6.697
6.608
6.605
6.589
6.586
6.570
6.567
4.203
NH2
S
S
NH2
2c
9
8
7
6
5
4
3
2
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0
ppm
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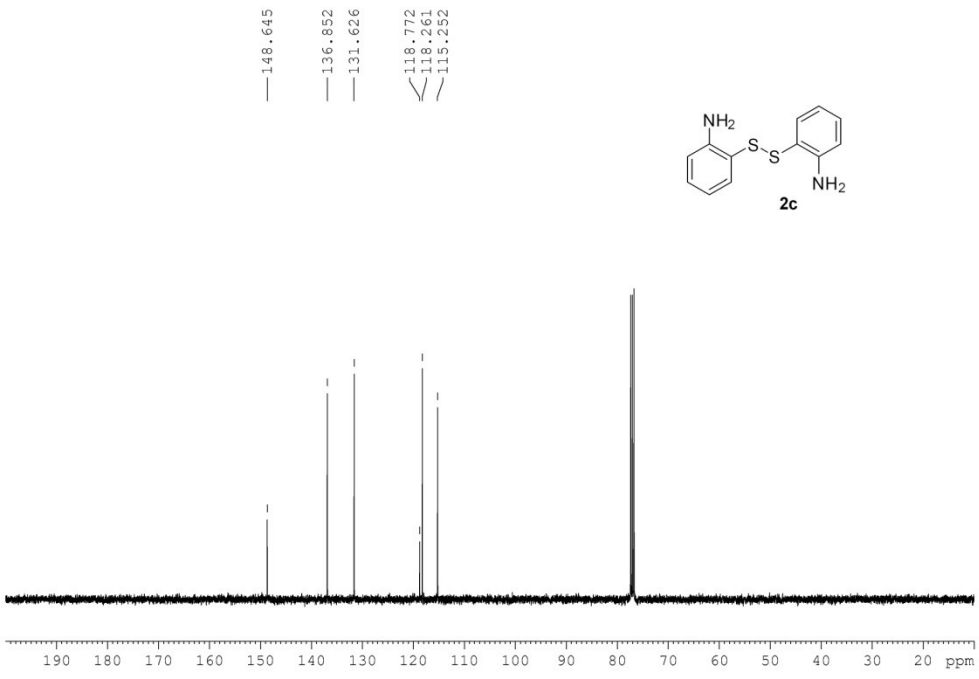
2.016
2.007
4.000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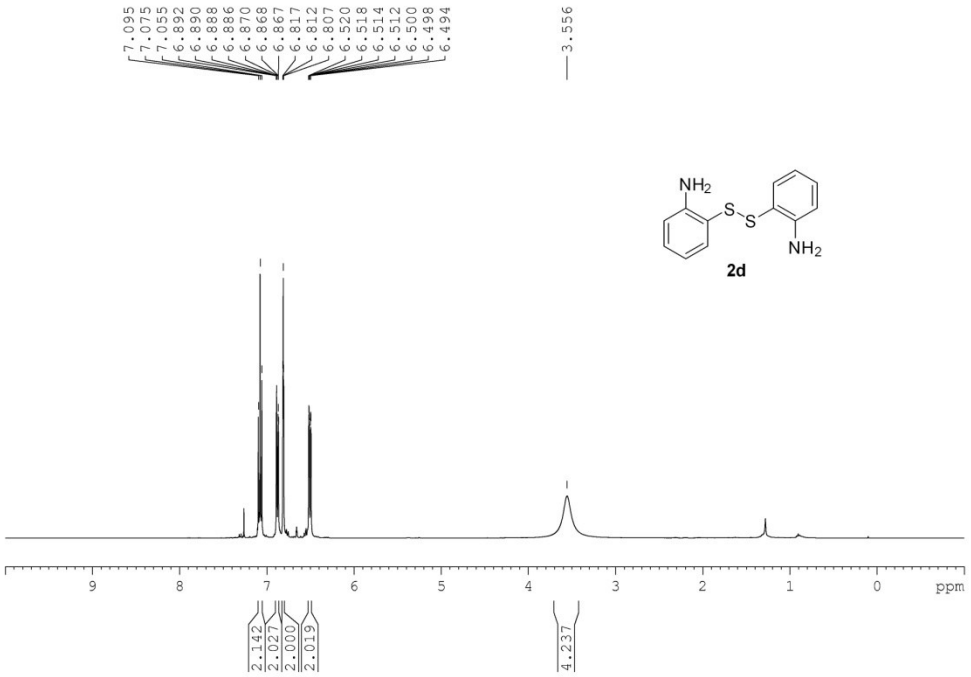
136.852
131.626
118.772
118.261
115.252
NH2
S
S
NH2
2c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm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7.075
7.055
6.892
6.890
6.888
6.886
6.870
6.868
6.867
6.817
6.812
6.807
6.520
6.518
6.514
6.512
6.500
6.498
6.494
3.556
NH2
S
S
NH2
2d
9
8
7
6
5
4
3
2
1
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ppm
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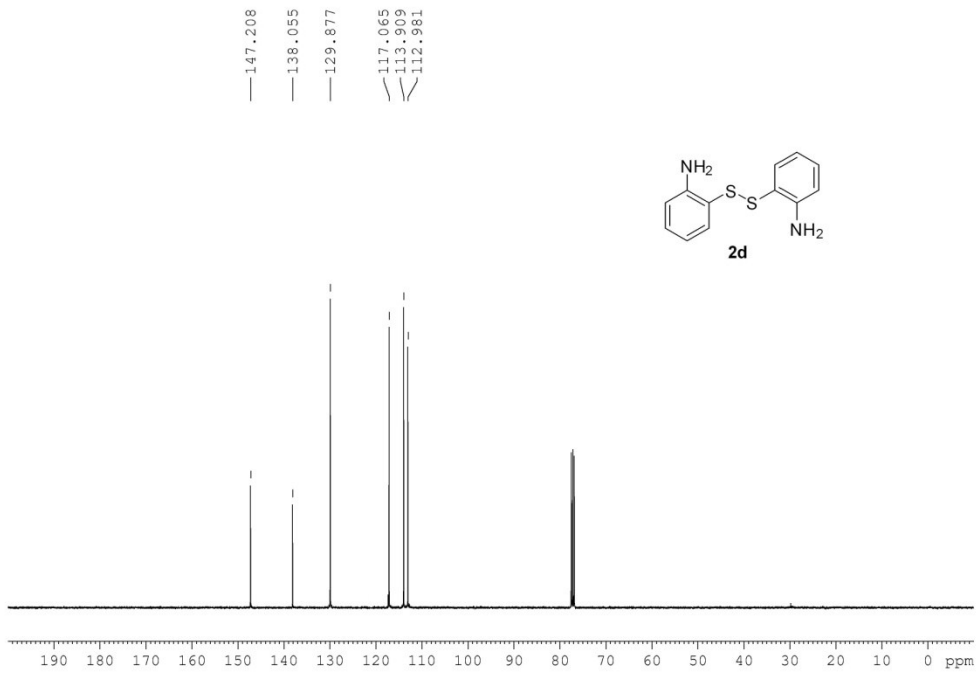
2.019
4.237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S
S
NH2
2d
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180
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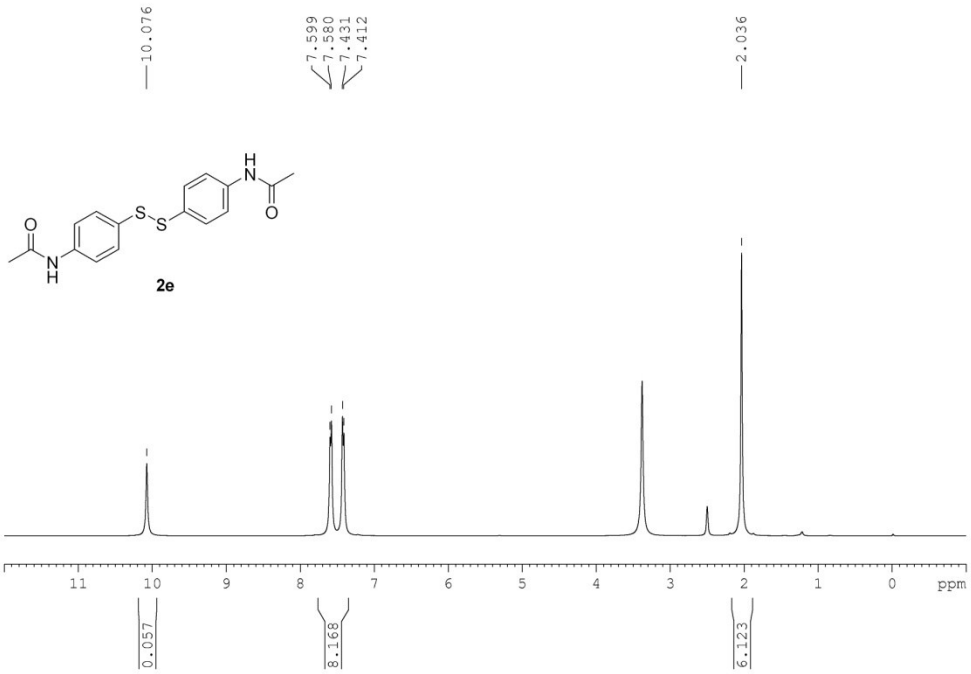
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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7.431
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2e
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.057
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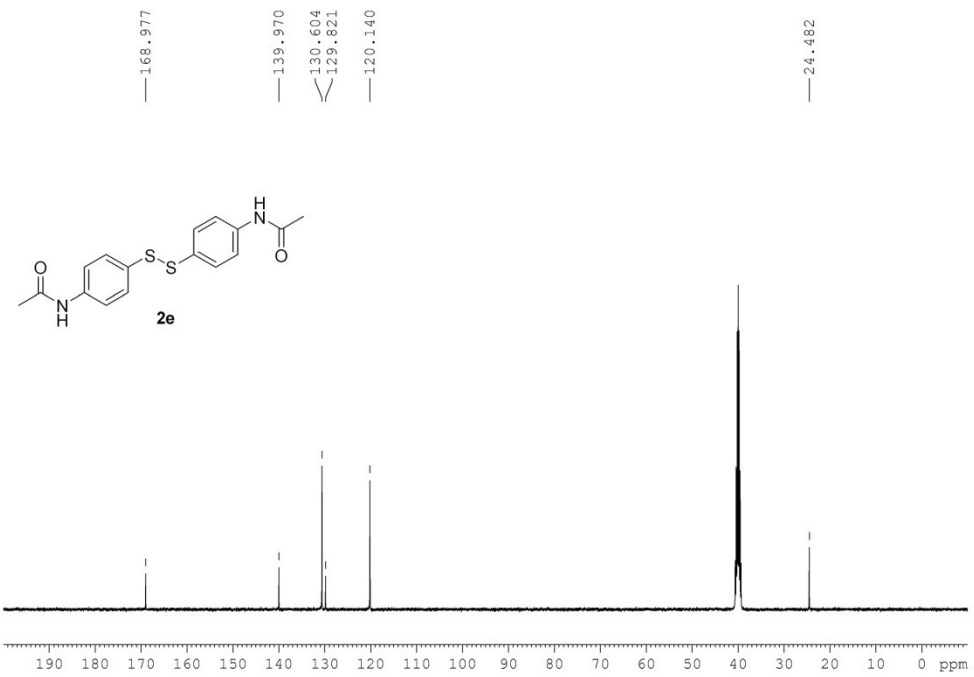
6.123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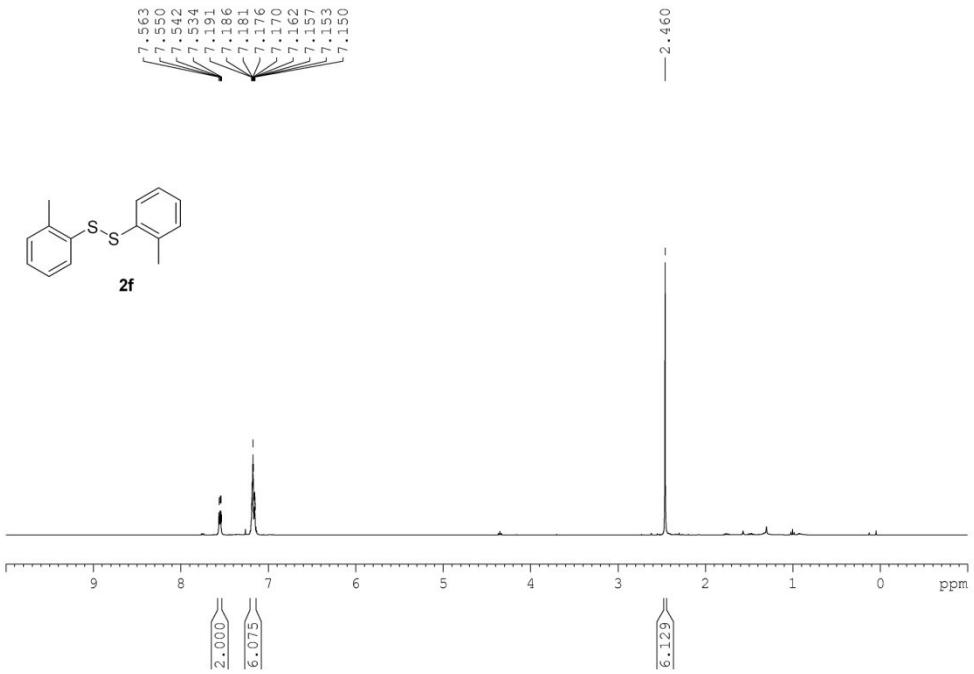
24.482
2e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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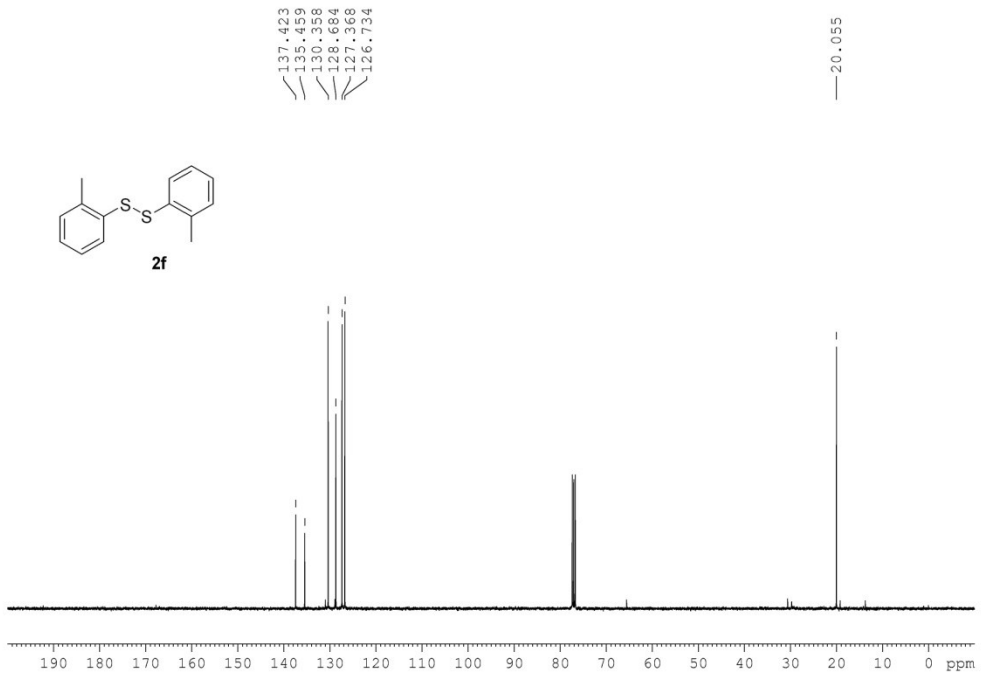
7.550
7.542
7.534
7.191
7.186
7.181
7.176
7.170
7.162
7.157
7.153
7.150
2.460
2f
9
8
7
6
5
4
3
2
1
0
ppm
2.000
6.075
6.129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20.055
2f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


7.436
7.417
7.146
7.126
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9
8
7
6
5
4
3
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1
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ppm
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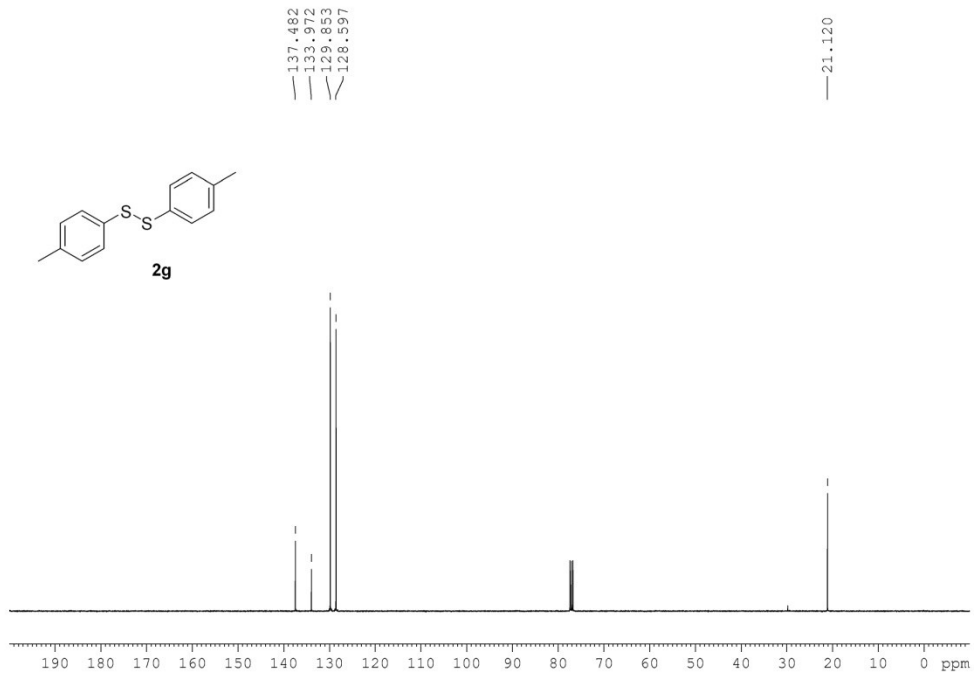
4.049
6.136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129.853
128.597
21.120
2g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.353
7.338
7.239
7.220
7.199
7.071
7.053
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2h
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8
7
6
5
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3
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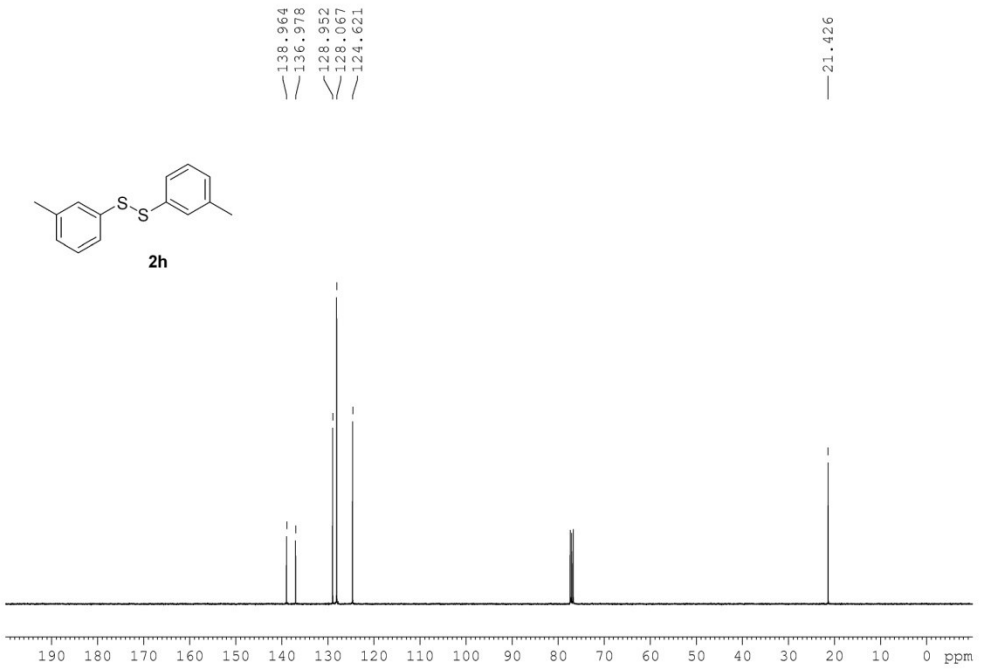
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2h
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150
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70
60
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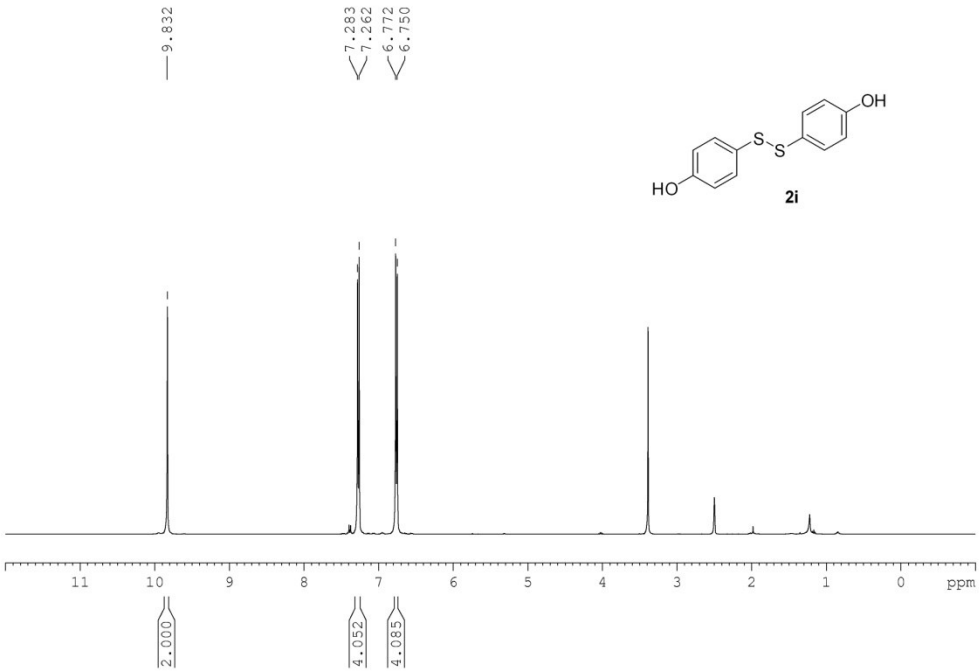
30
20
10
0 ppm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S
S
HO
2i
11
10
9
8
7
6
5
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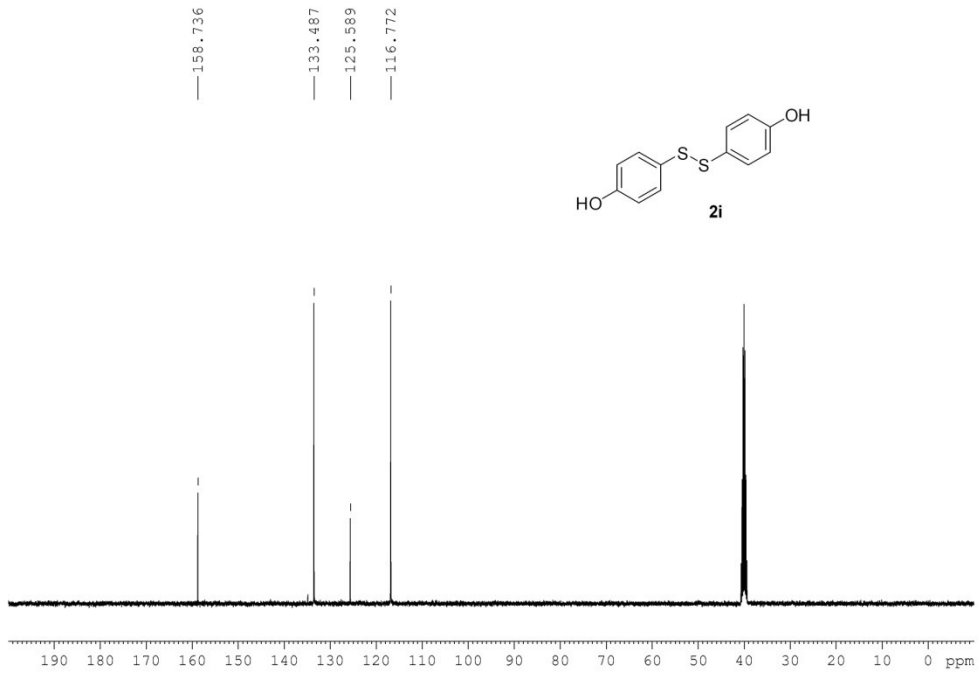
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S
HO
2i
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110
100
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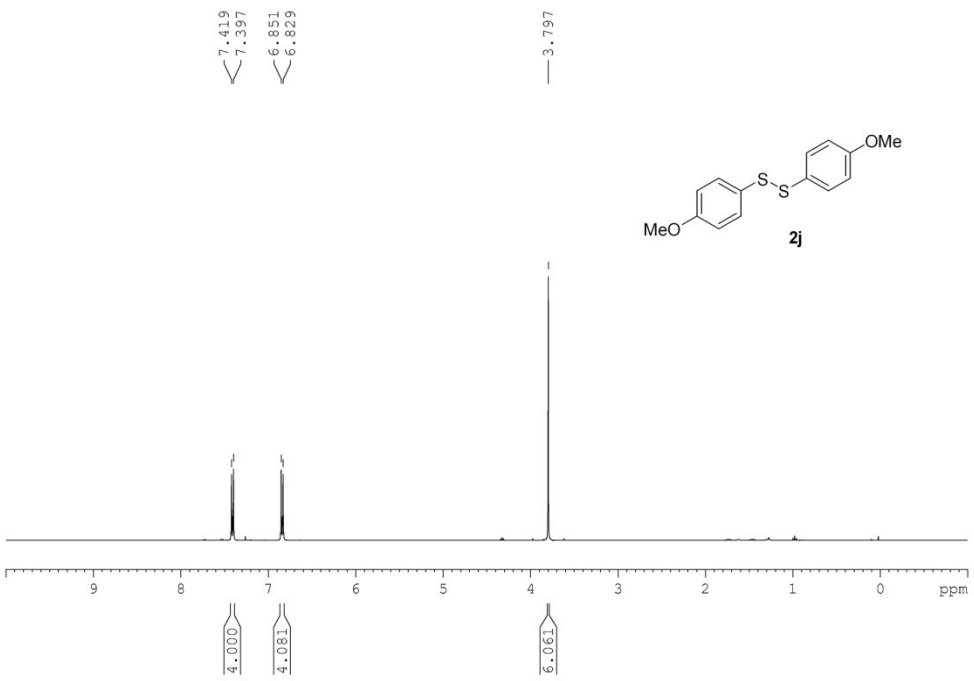
80
70
60
50
40
30
20
10
0
ppm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6.851
6.829
3.797
OMe
S
S
MeO
2j
9
8
7
6
5
4
3
2
1
0
ppm
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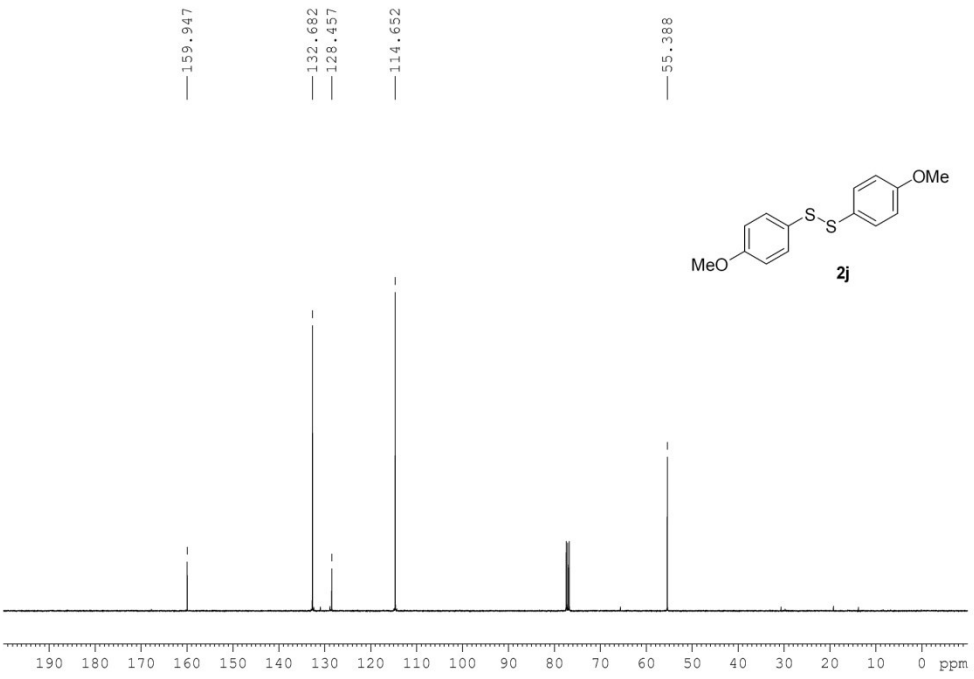
4.081
6.061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S
S
MeO
2j
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180
170
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140
130
120
110
100
90
80
70
60
50
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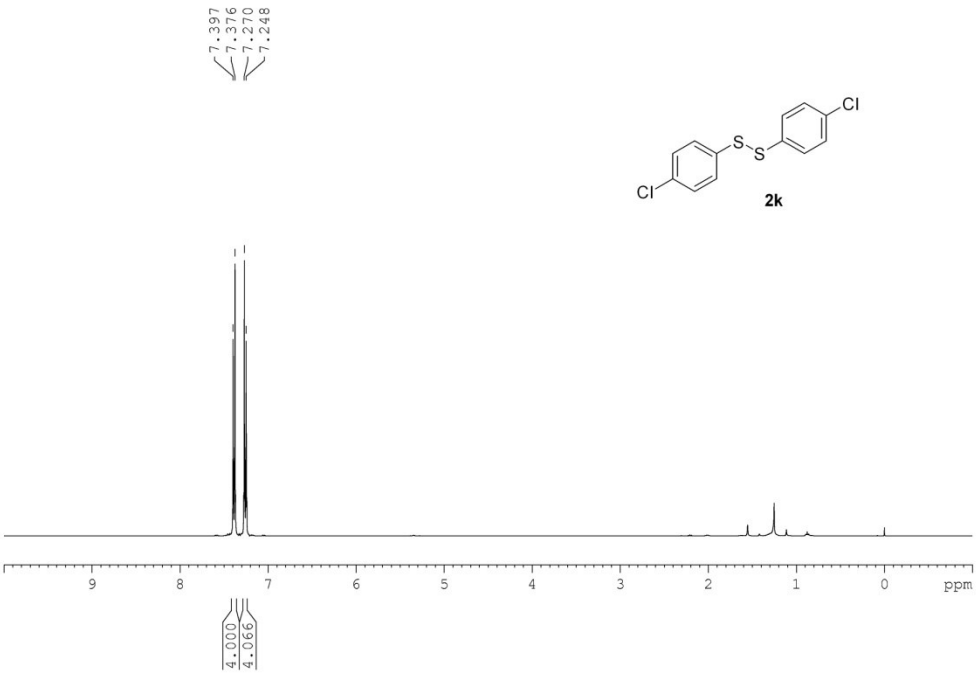
30
20
10
0
ppm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Cl
S
S
Cl
2k
9
8
7
6
5
4
3
2
1
0
ppm
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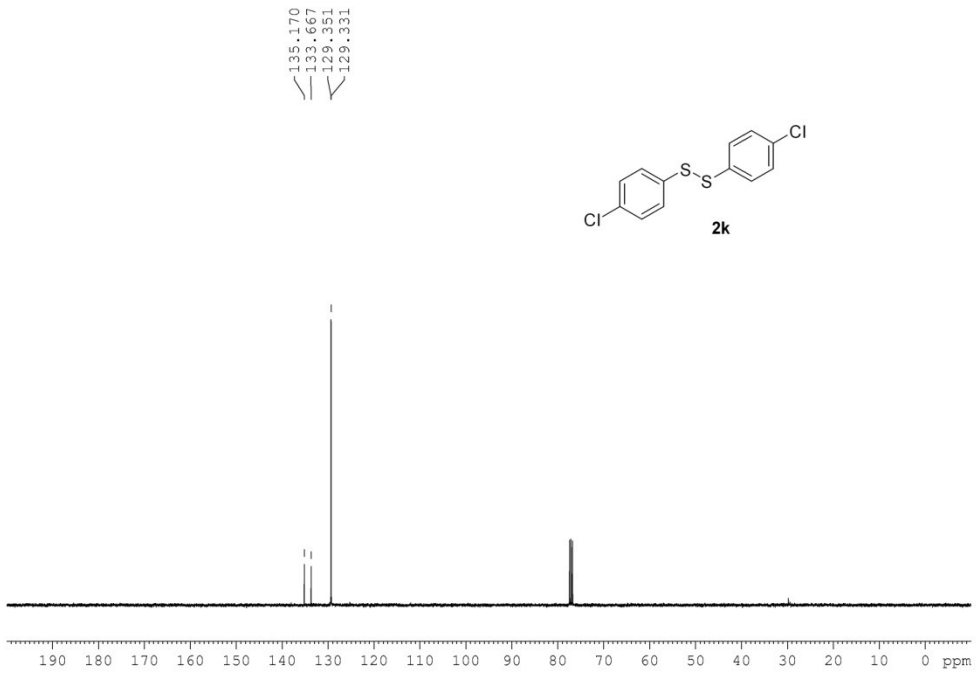
4.066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Cl
S
S
Cl
2k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
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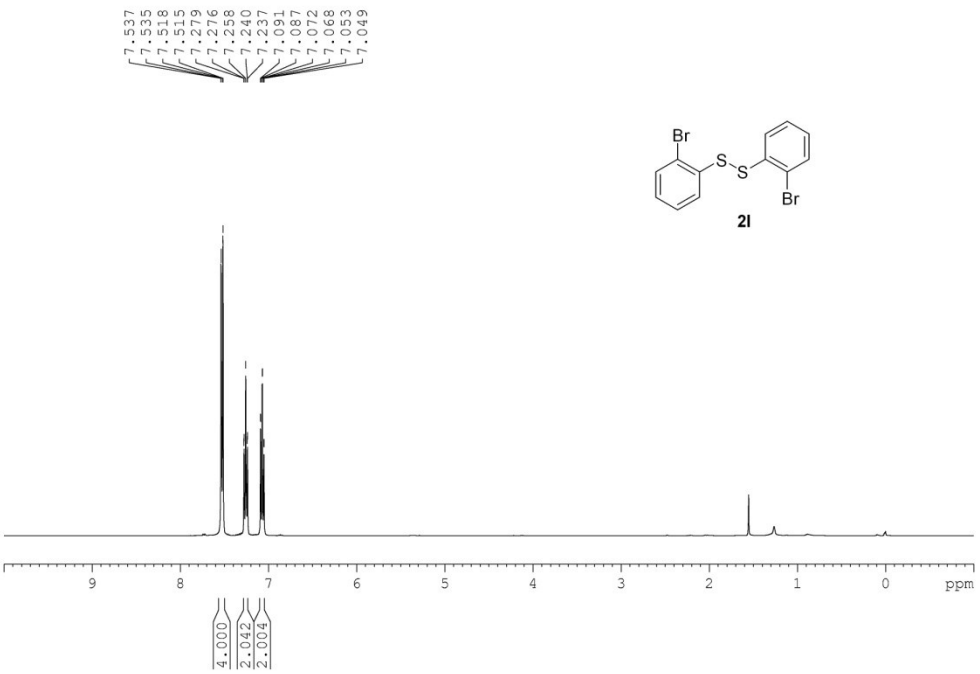
40
30
20
10
0 ppm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7.518
7.515
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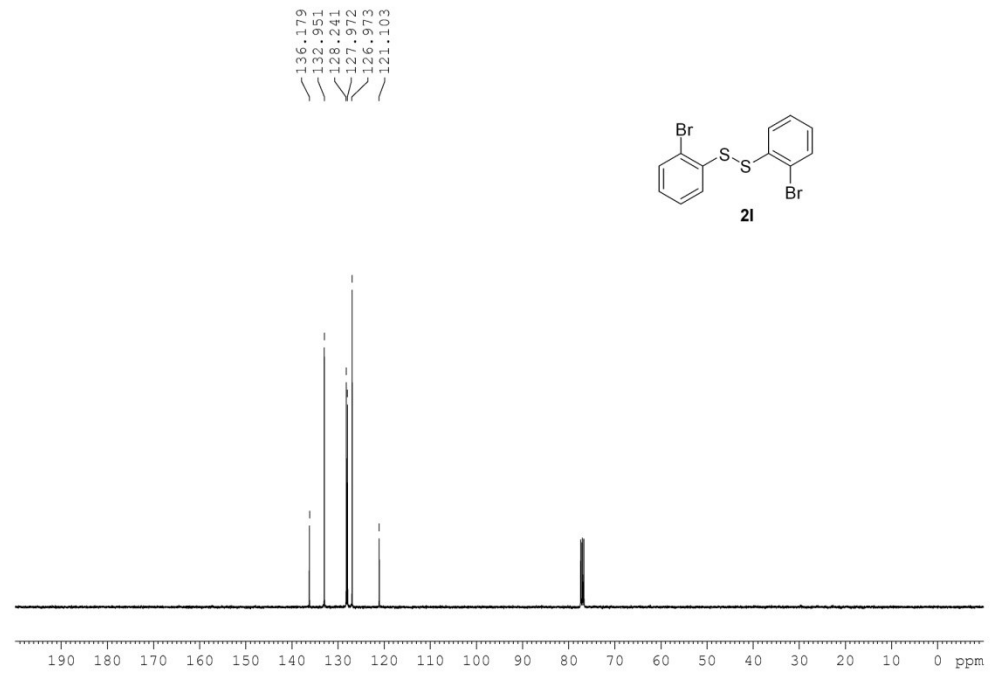
7.276
7.258
7.240
7.237
7.091
7.087
7.072
7.068
7.053
7.049
Br
S
S
Br
2l
9
8
7
6
5
4
3
2
1
0
ppm
4.000
2.042
2.004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127.972
126.973
121.103
Br
S
S
Br
2l
190
180
170
160
150
140
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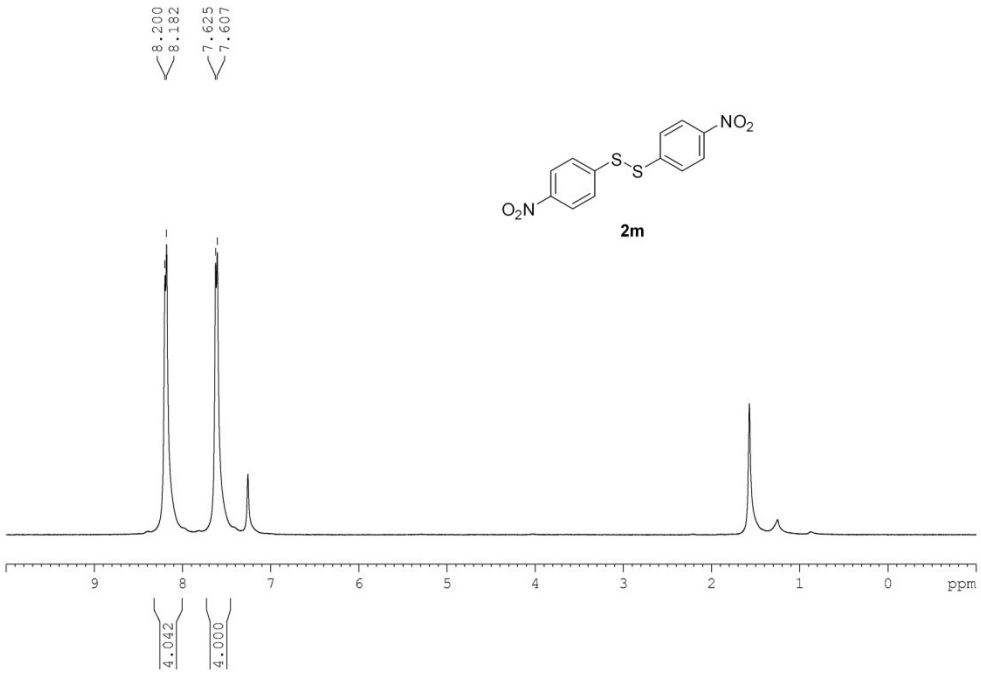
110
100
90
80
70
60
50
40
30
20
10
0 ppm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S
O2N
2m
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6
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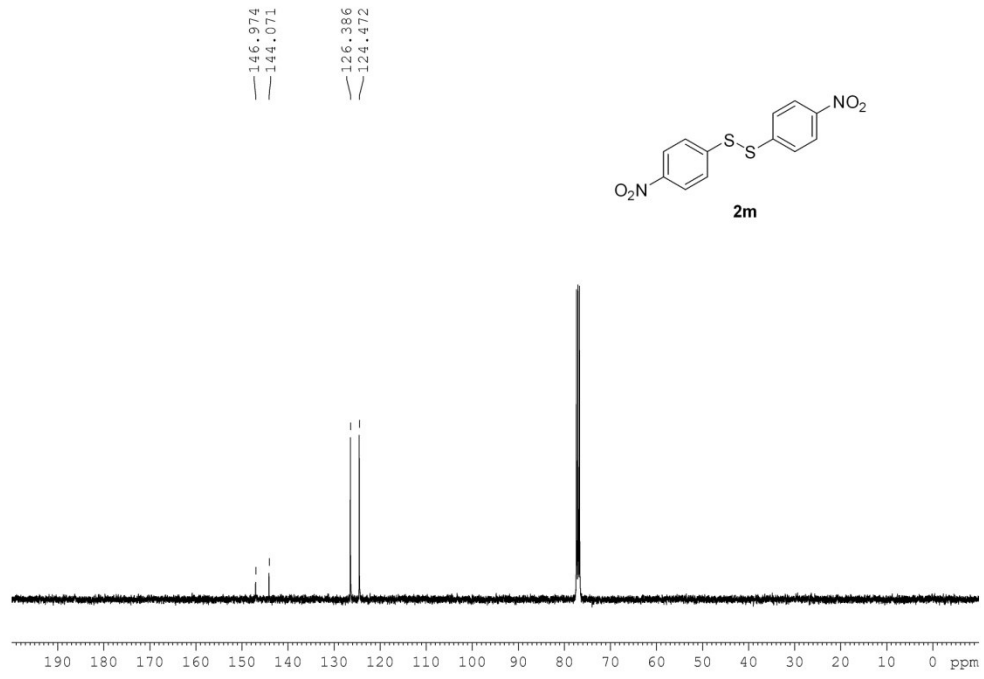
4.000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NO2
S
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O2N
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190
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100
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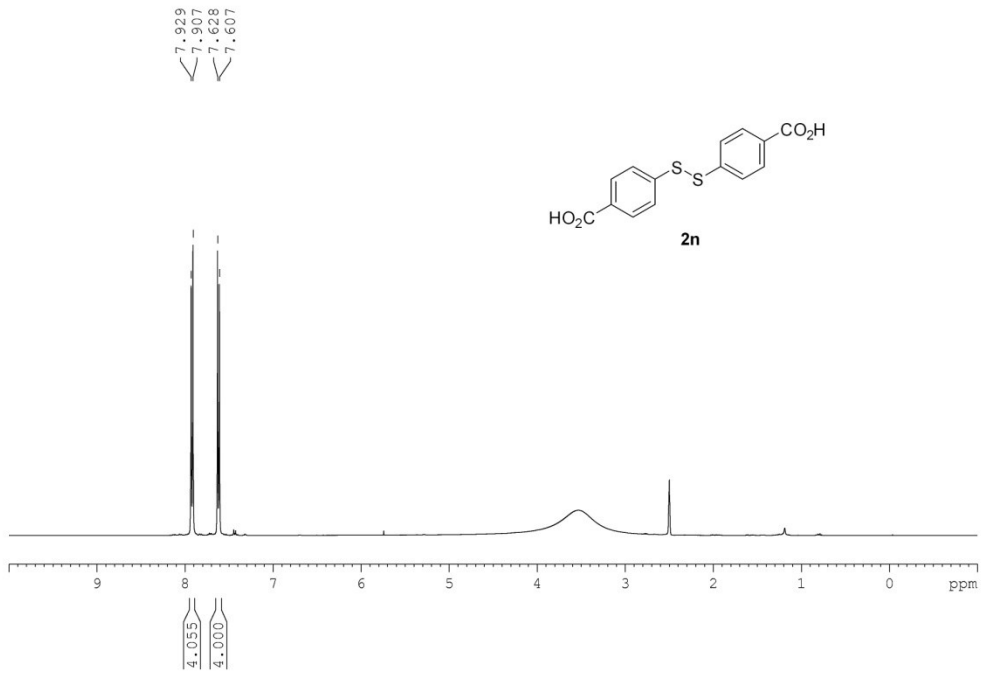
0
ppm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S
HO2C
2n
9
8
7
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5
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3
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ppm
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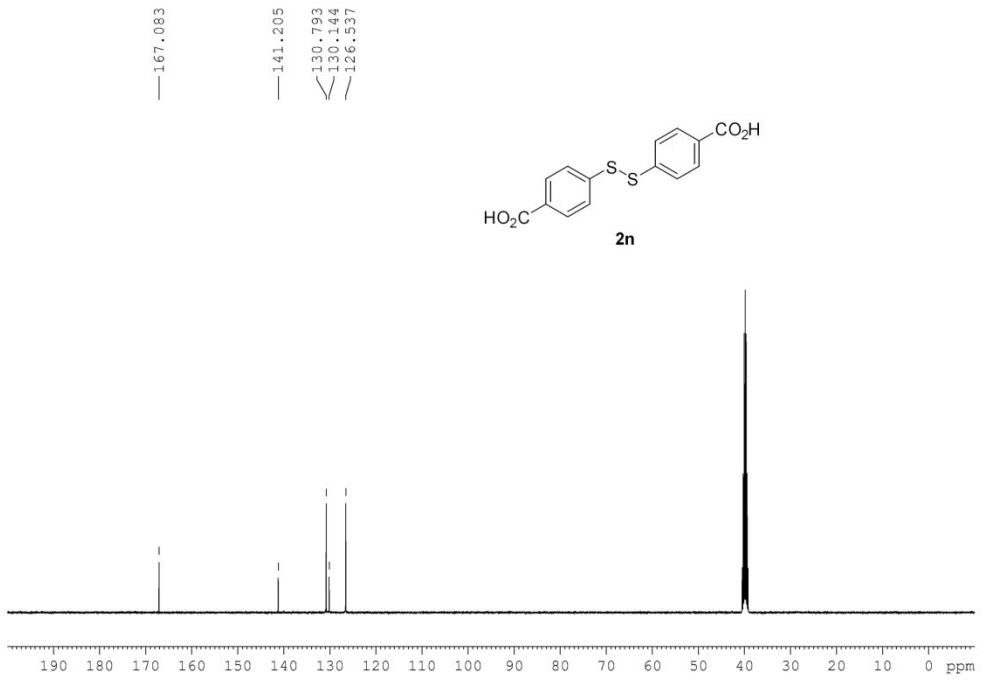
4.000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130.144
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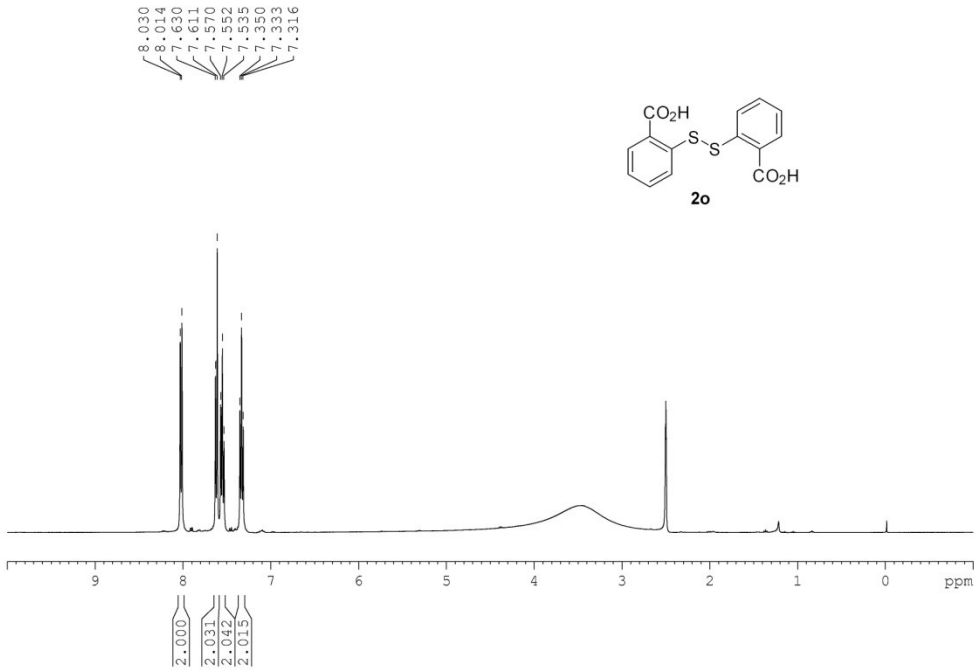
CO2H
S
S
HO2C
2n
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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8.014
7.630
7.611
7.570
7.552
7.535
7.350
7.333
7.316
CO2H
S
S
CO2H
2o
9
8
7
6
5
4
3
2
1
0
ppm
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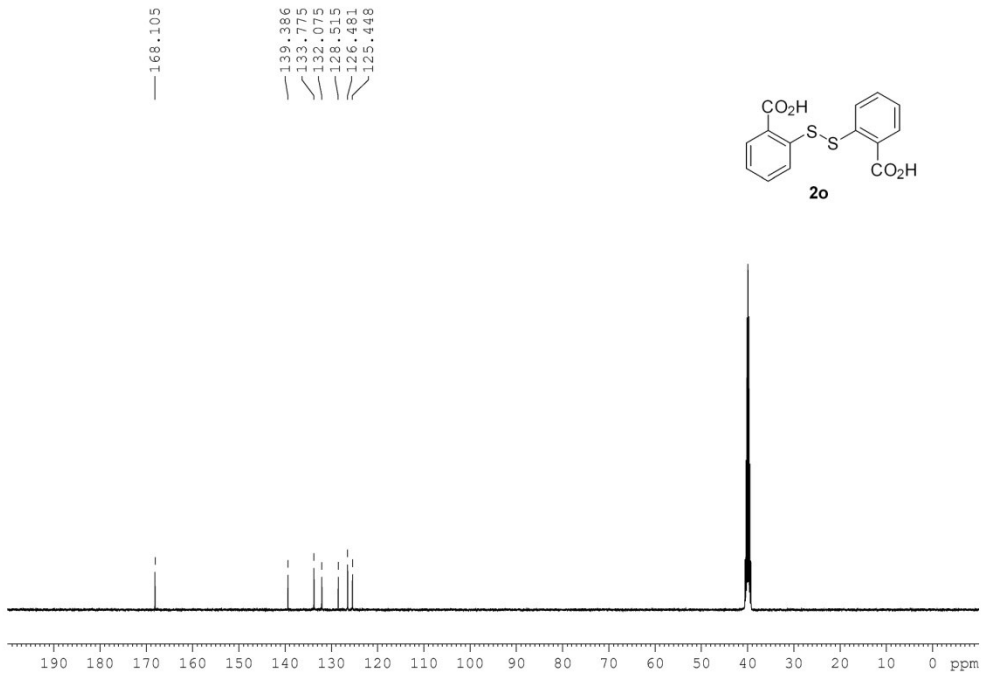
2.031
2.042
2.015


168.105
139.386
133.775
132.075
128.515
126.481
125.448
CO2H
S
S
CO2H
2o
190
180
170
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150
140
130
120
110
100
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80
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60
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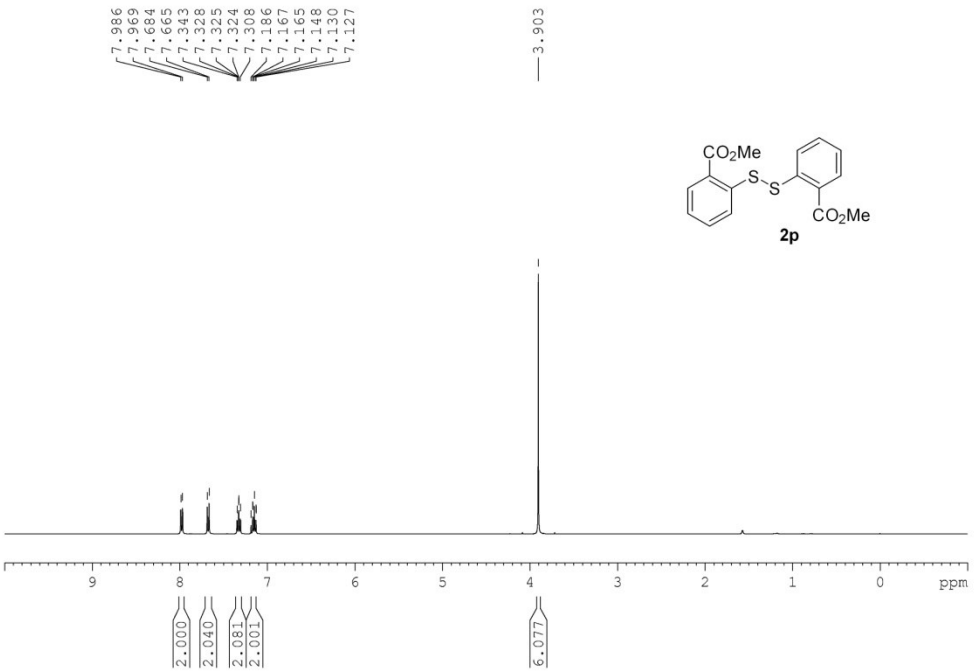
20
10
0
ppm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7.684
7.665
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7.325
7.324
7.308
7.186
7.167
7.165
7.148
7.130
7.127
3.903
CO2Me
S
S
CO2Me
2p
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8
7
6
5
4
3
2
1
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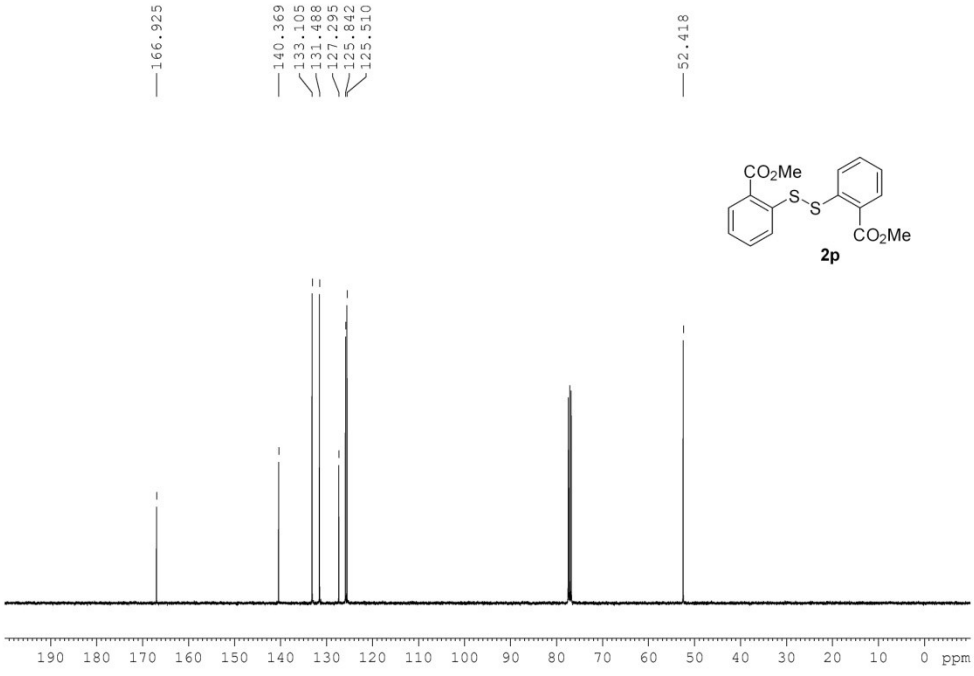
ppm
2.000
2.040
2.081
2.001
6.077


166.925
140.369
133.105
131.488
127.295
125.842
125.510
52.418
CO2Me
S
S
CO2Me
2p
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180
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140
130
120
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100
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60
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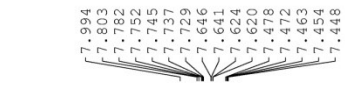
30
20
10
0
ppm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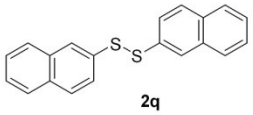
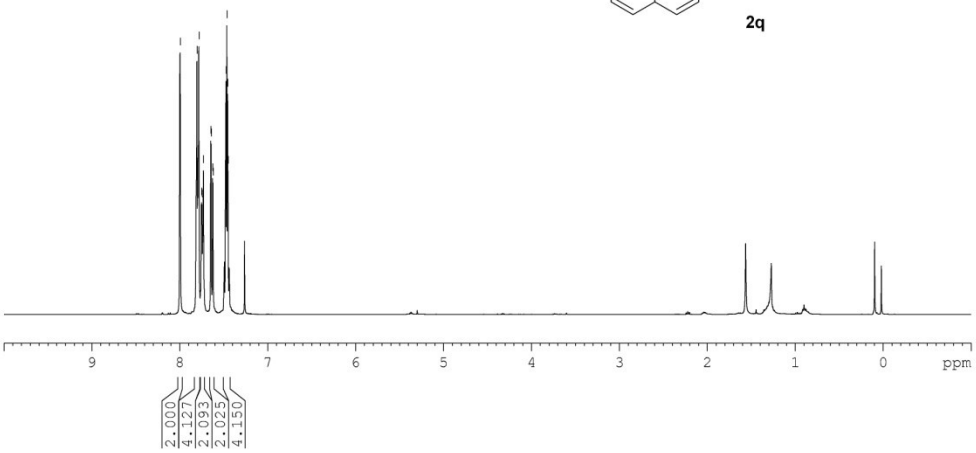
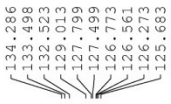
7.803
7.782
7.752
7.745
7.737
7.729
7.646
7.641
7.624
7.620
7.478
7.472
7.463
7.454
7.448


S
S

2q


9
8
7
6
5
4
3
2
1
0
ppm
2.000
4.127
2.093
2.025
4.150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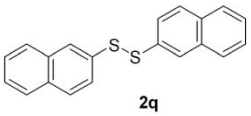
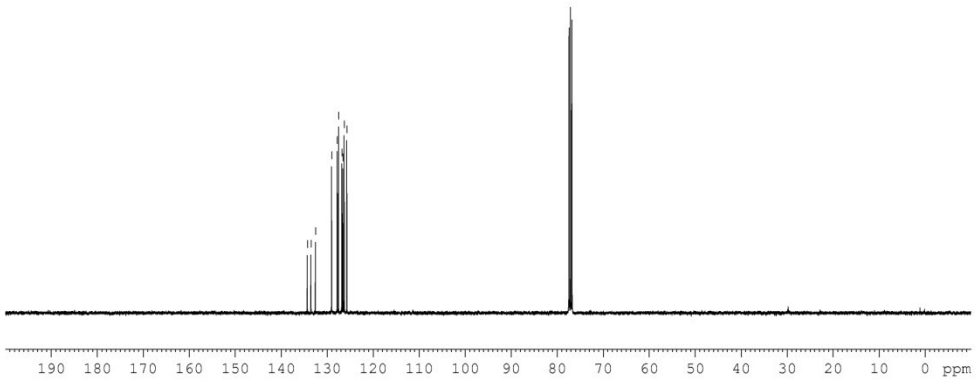
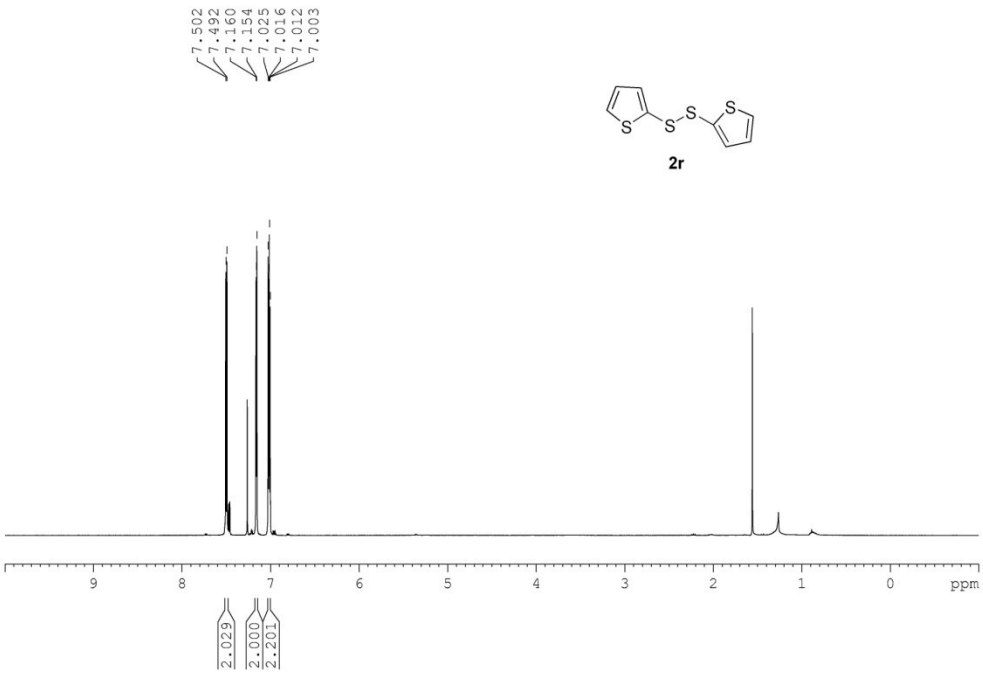
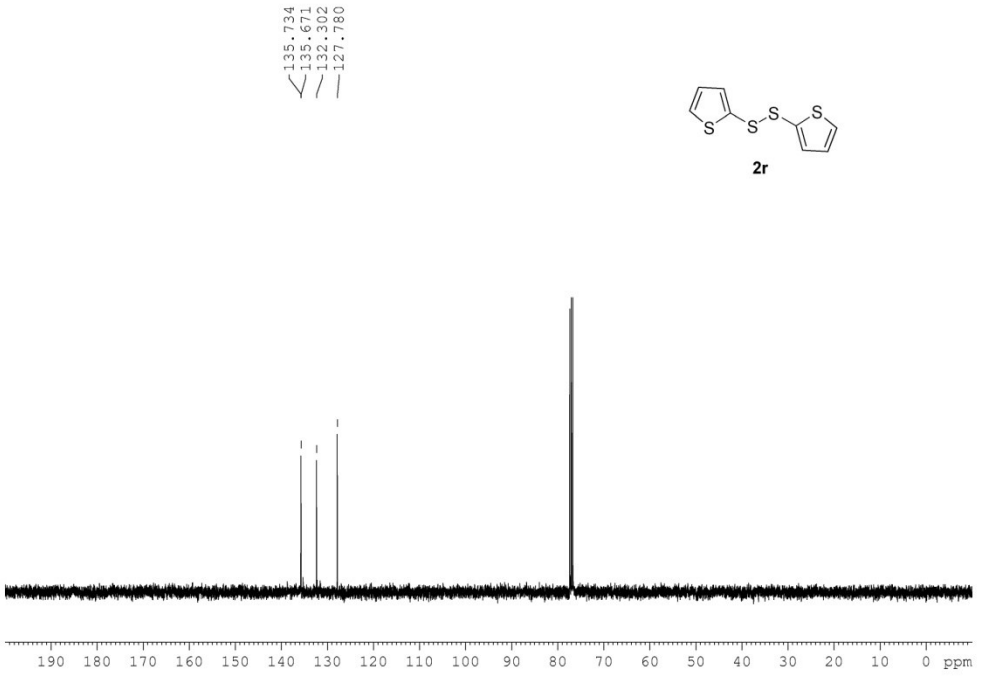
133.498
132.523
129.013
127.799
127.499
126.773
126.561
126.273
125.683

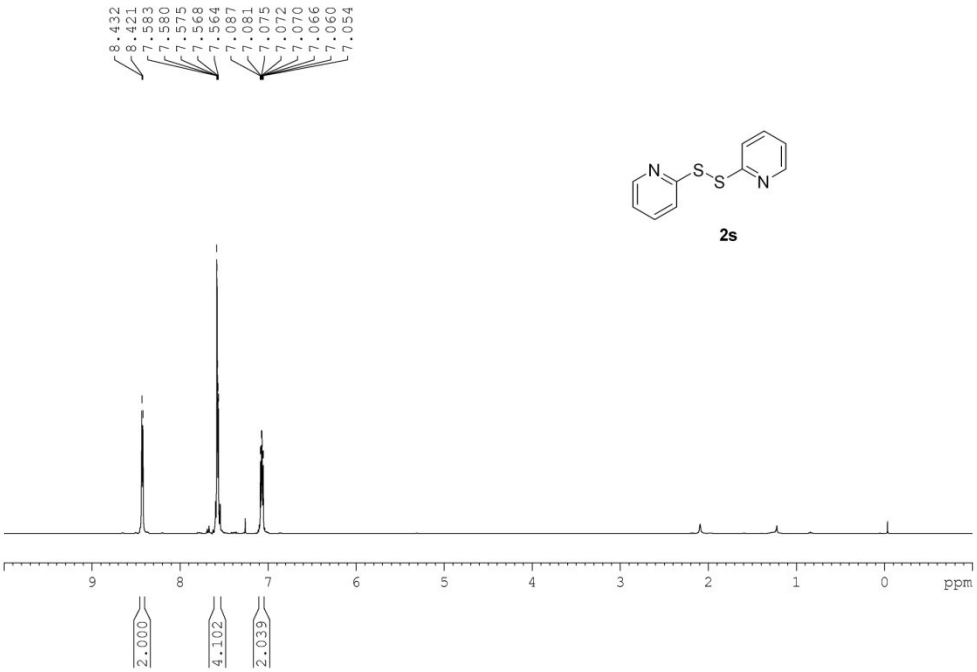

S
S

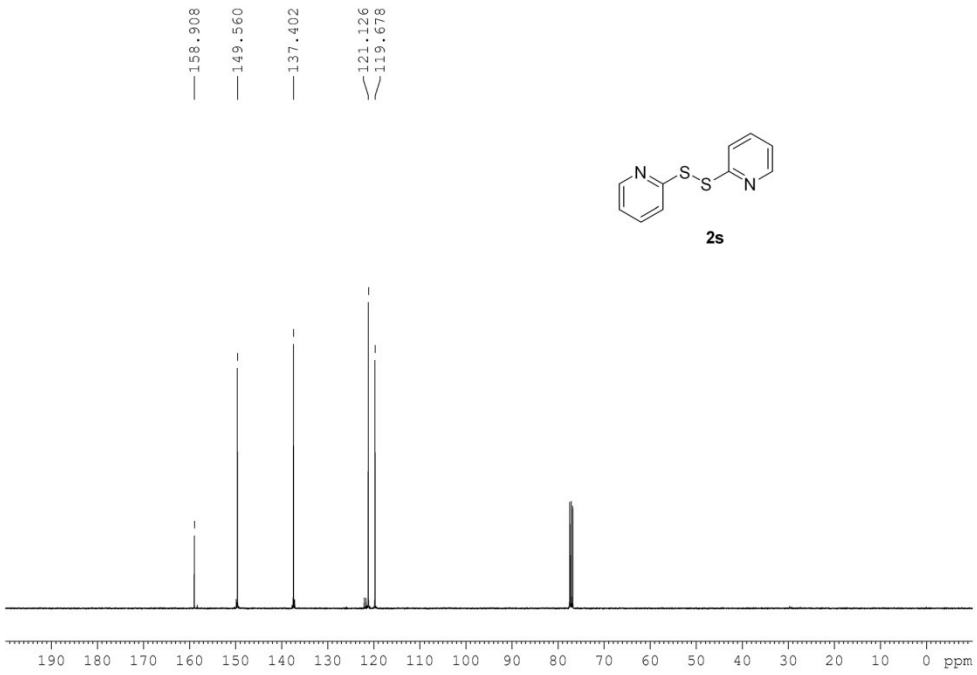
2q

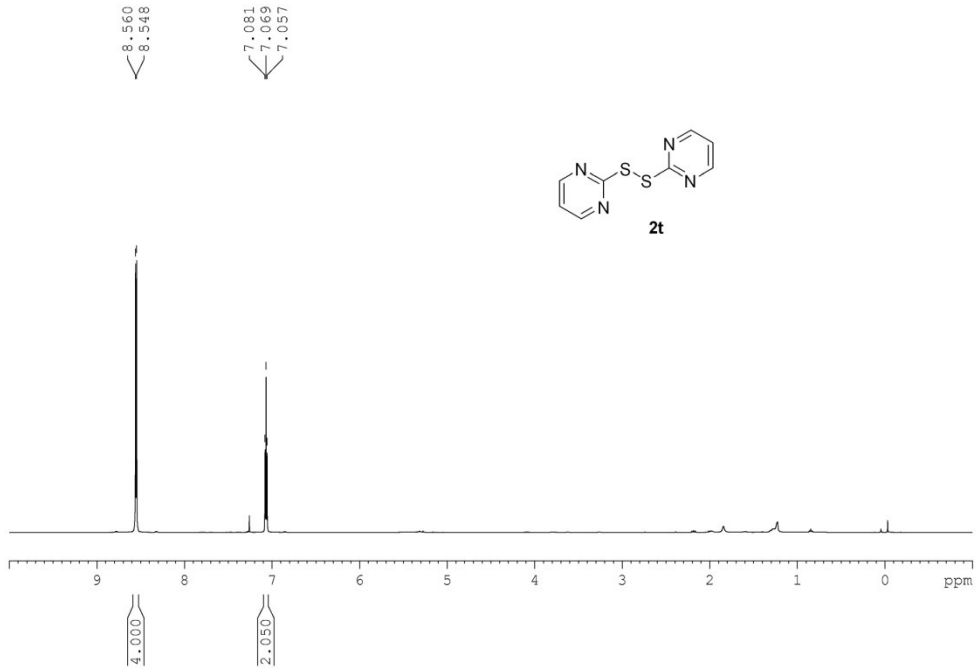

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

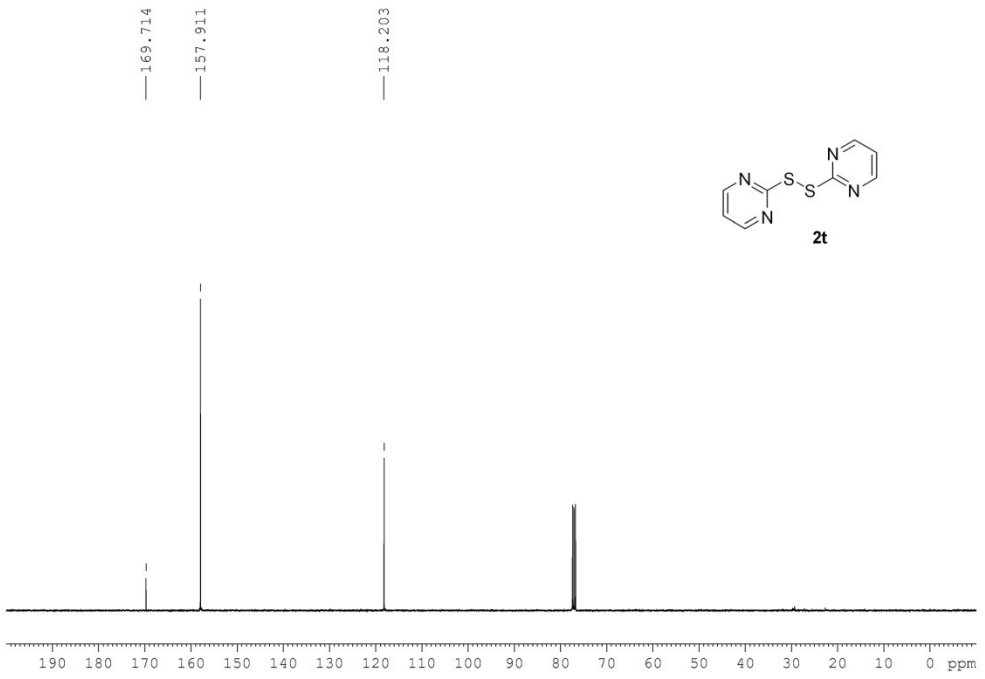

7.502
7.492
7.160
7.154
7.025
7.016
7.012
7.003
2r
9
8
7
6
5
4
3
2
1
0
ppm
2.029
2.000
2.201

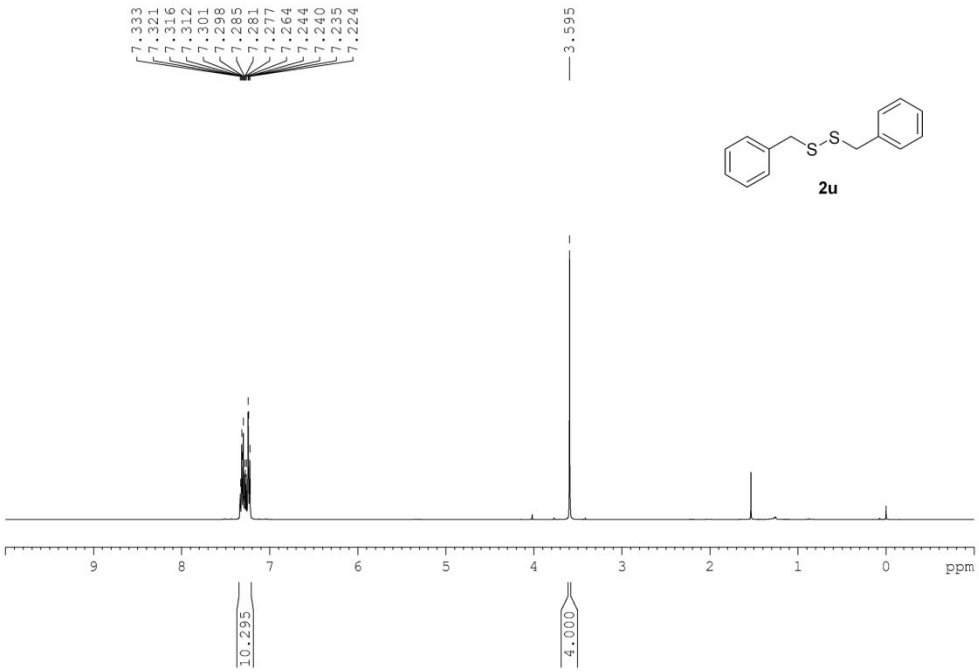

135.734
135.671
132.302
127.780
2r
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

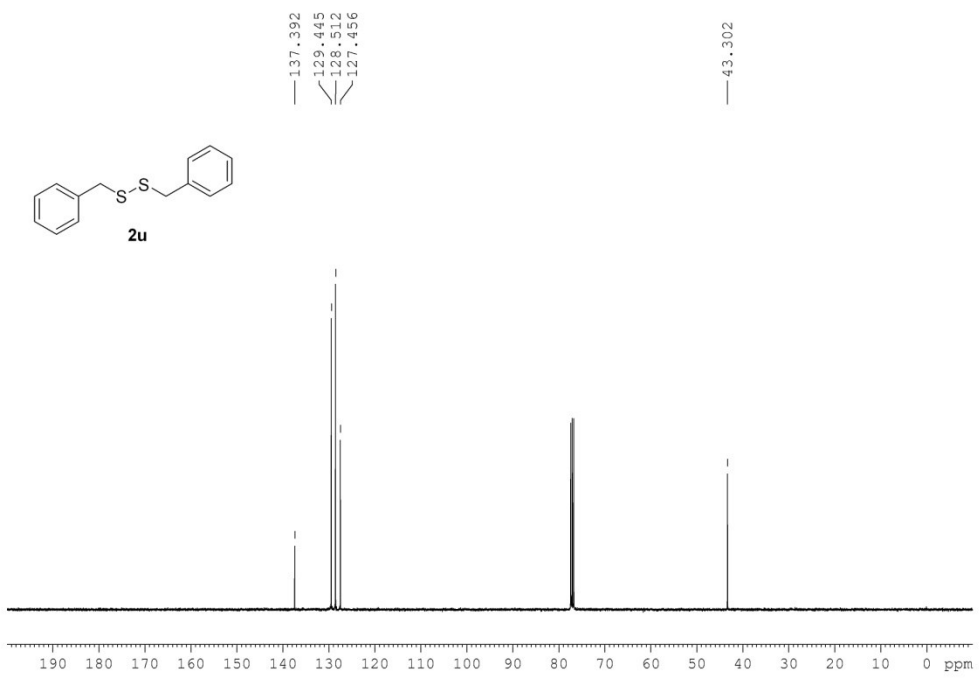

8.432
8.421
7.583
7.580
7.575
7.568
7.564
7.087
7.081
7.075
7.072
7.070
7.066
7.060
7.054
N
S
S
N
2s
9
8
7
6
5
4
3
2
1
0
ppm
2.000
4.102
2.039

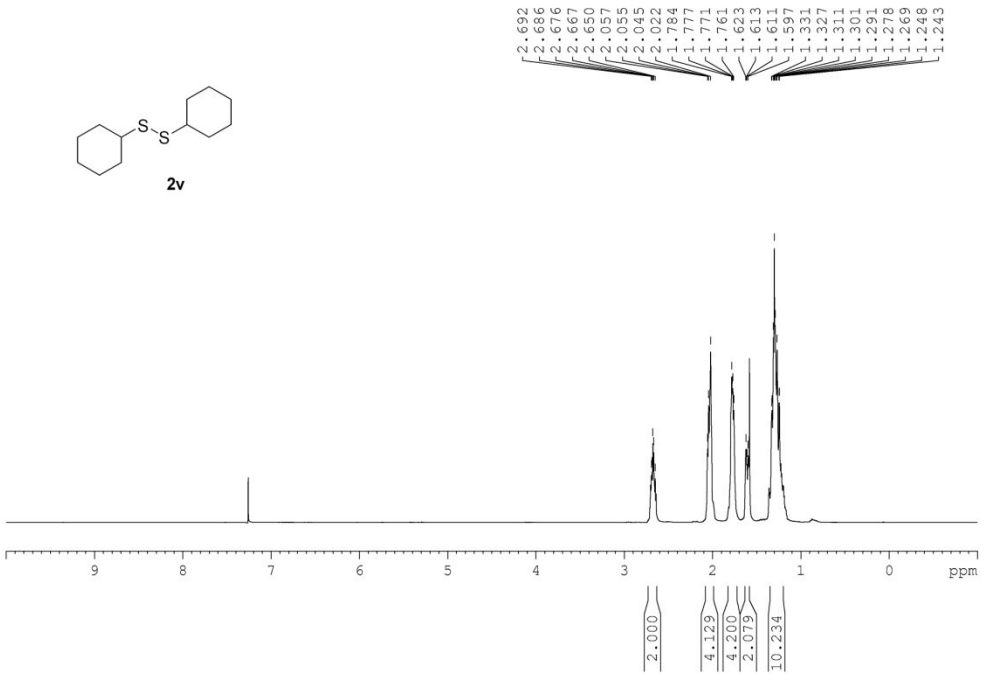

158.908
149.560
137.402
121.126
119.678
N
S
S
N
2s
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.560
8.548
7.081
7.069
7.057
2t
9
8
7
6
5
4
3
2
1
0
ppm
4.000
2.050


169.714
157.911
118.203
2t
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


7.333
7.321
7.316
7.312
7.301
7.298
7.285
7.281
7.277
7.264
7.244
7.240
7.235
7.224
3.595
S
S
2u
9
8
7
6
5
4
3
2
1
0
ppm
10.295
4.000


137.392
129.445
128.512
127.456
43.302
S
S
2u
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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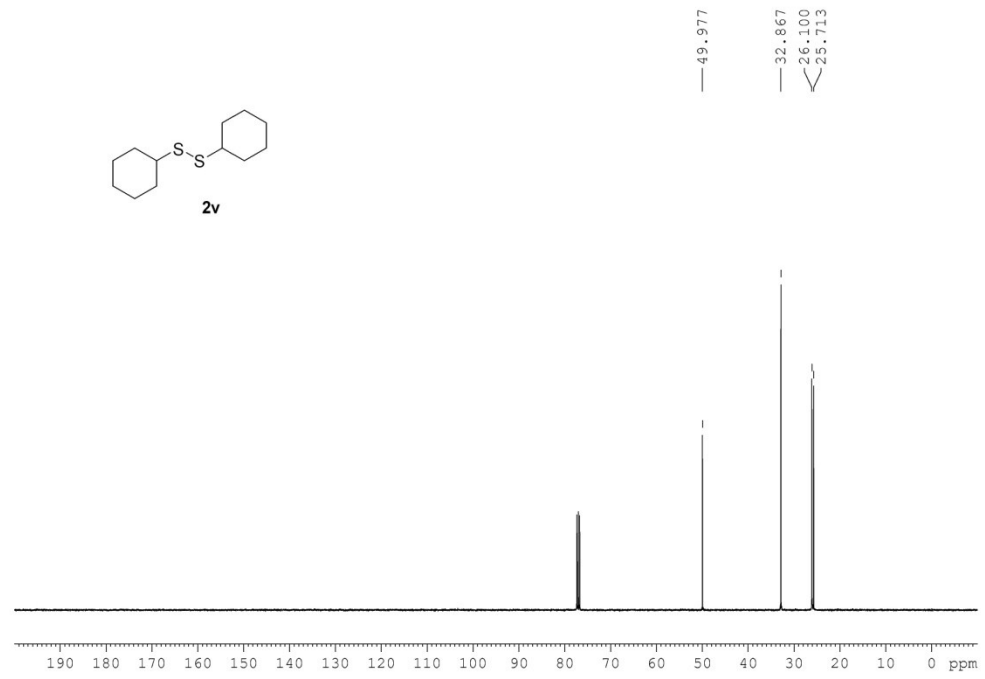
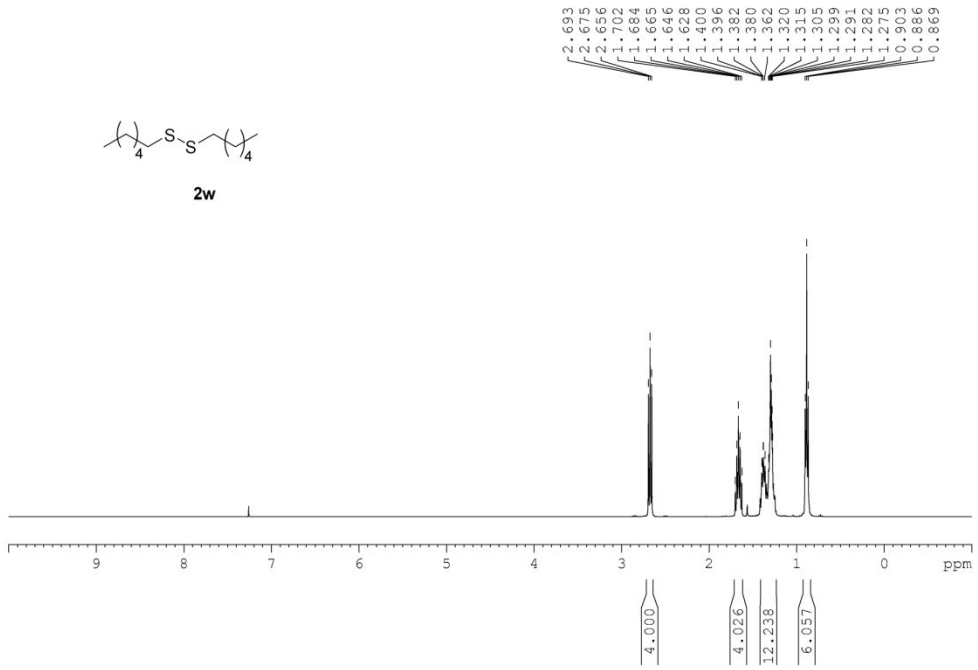
2.686
2.676
2.667
2.650
2.057
2.055
2.045
2.022
1.784
1.777
1.771
1.761
1.623
1.613
1.611
1.597
1.331
1.327
1.311
1.301
1.291
1.278
1.269
1.248
1.243
S
S
2v
9
8
7
6
5
4
3
2
1
0
ppm
2.000
4.129
4.200
2.079
10.234


49.977
32.867
26.100
25.713
S
S
2v
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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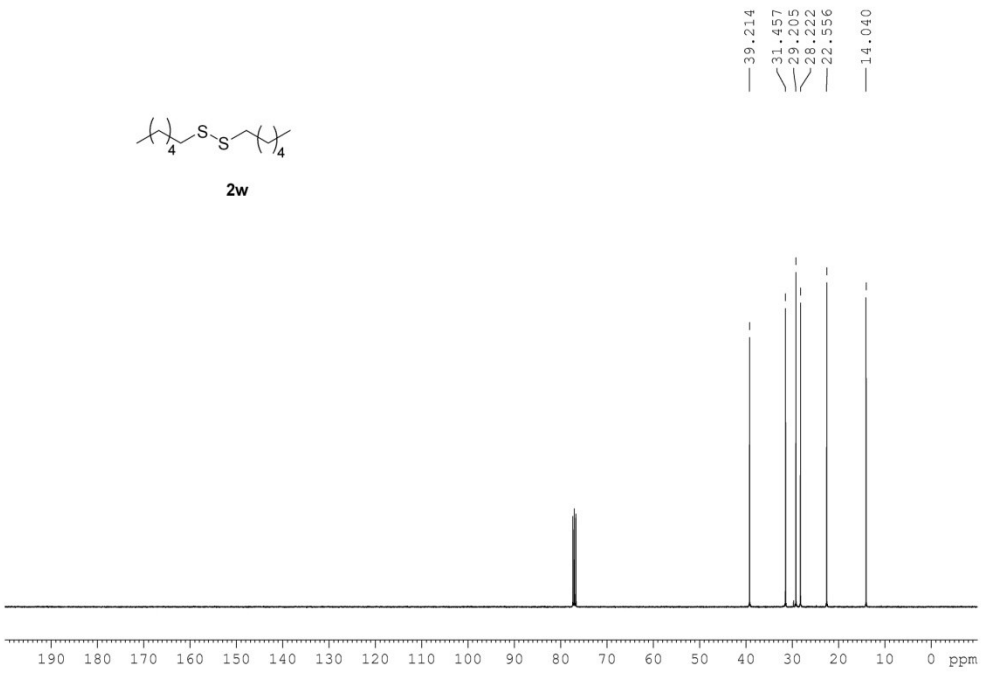
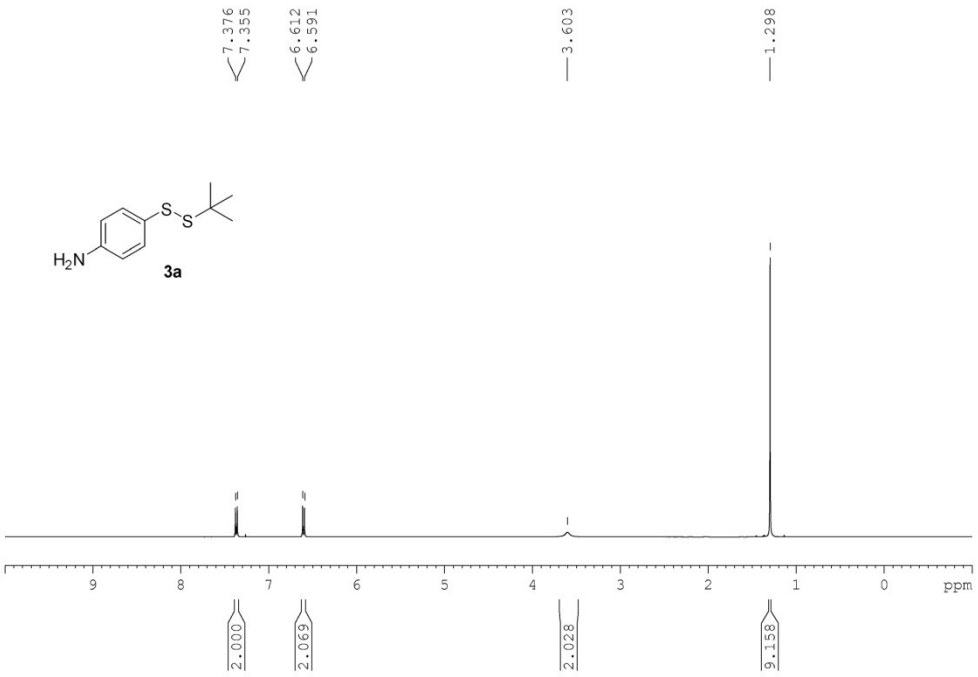
2.656
1.702
1.684
1.665
1.646
1.628
1.400
1.396
1.382
1.380
1.362
1.320
1.315
1.305
1.299
1.291
1.282
1.275
0.903
0.886
0.869
9
8
7
6
5
4
3
2
1
0
ppm
4.000
4.026
12.238
6.057

2w


39.214
31.457
29.205
28.222
22.556
14.040
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

2w


7.376
7.355
6.612
6.591
3.603
1.298
S
S
H2N
3a
9
8
7
6
5
4
3
2
1
0
ppm
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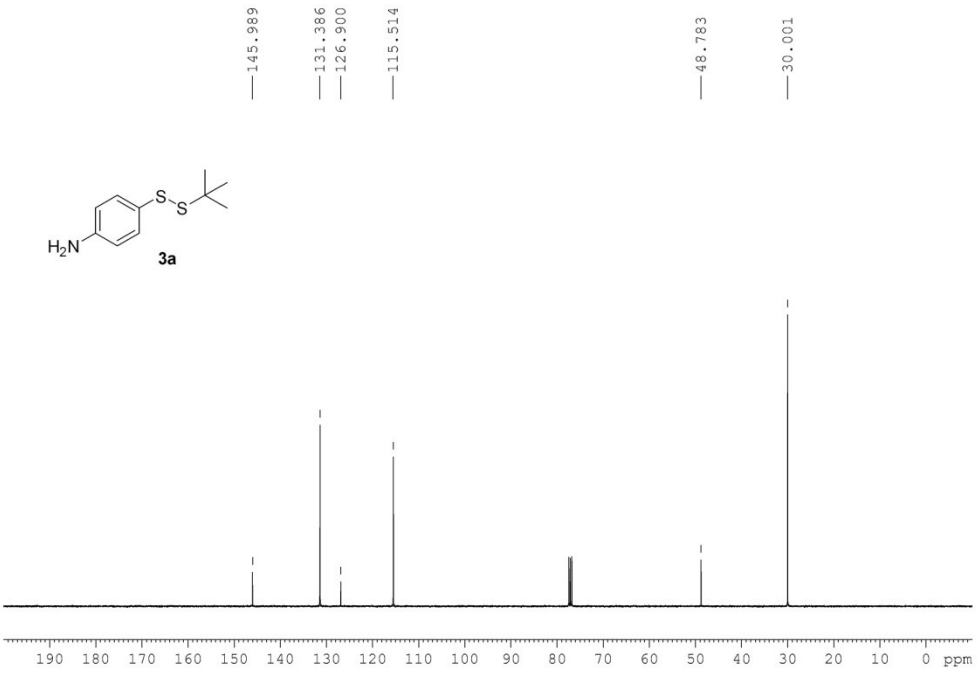
2.069
2.028
9.158


145.989
131.386
126.900
115.514
48.783
30.001
S
S
H2N
3a
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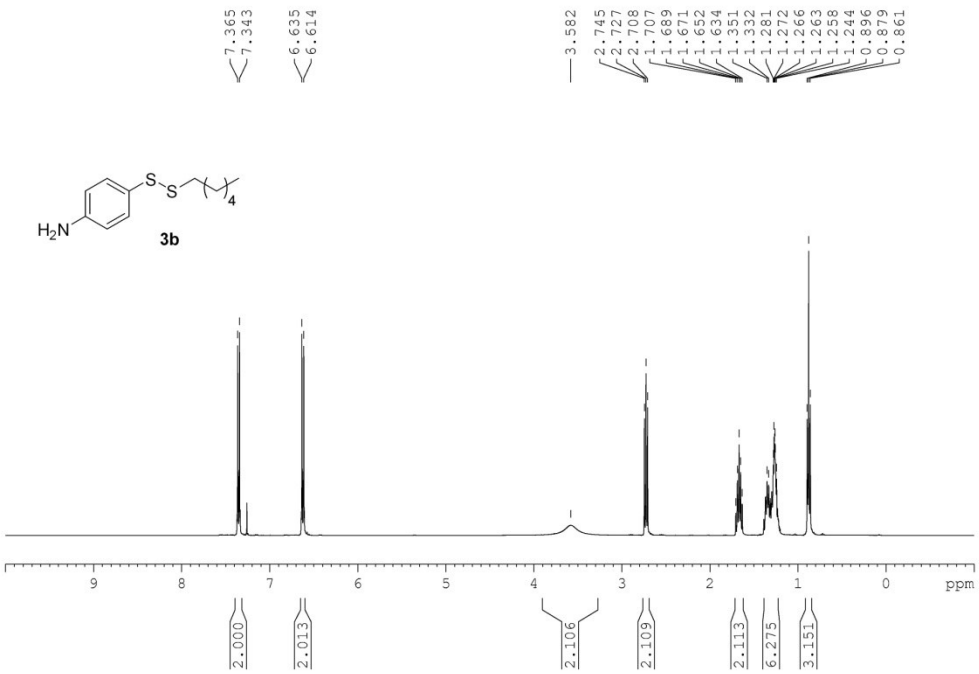
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.343
6.635
6.614
3.582
2.745
2.727
2.708
1.707
1.689
1.671
1.652
1.634
1.351
1.332
1.281
1.272
1.266
1.263
1.258
1.244
0.896
0.879
0.861
3b
9
8
7
6
5
4
3
2
1
0
ppm
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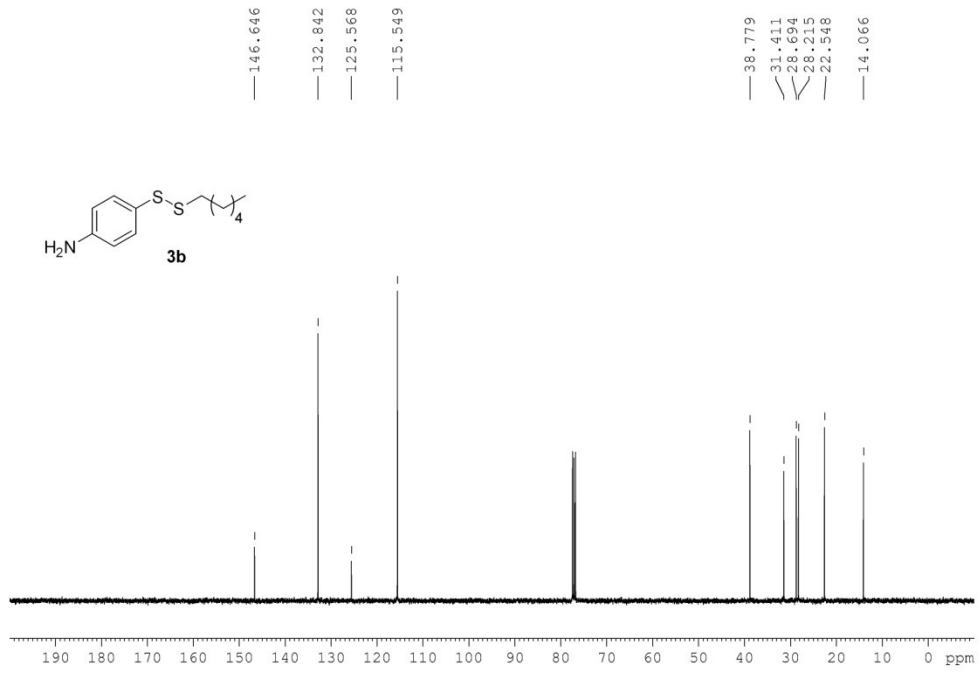
2.106
2.109
2.113
6.275
3.151


146.646
132.842
125.568
115.549
38.779
31.411
28.694
28.215
22.548
14.066
3b
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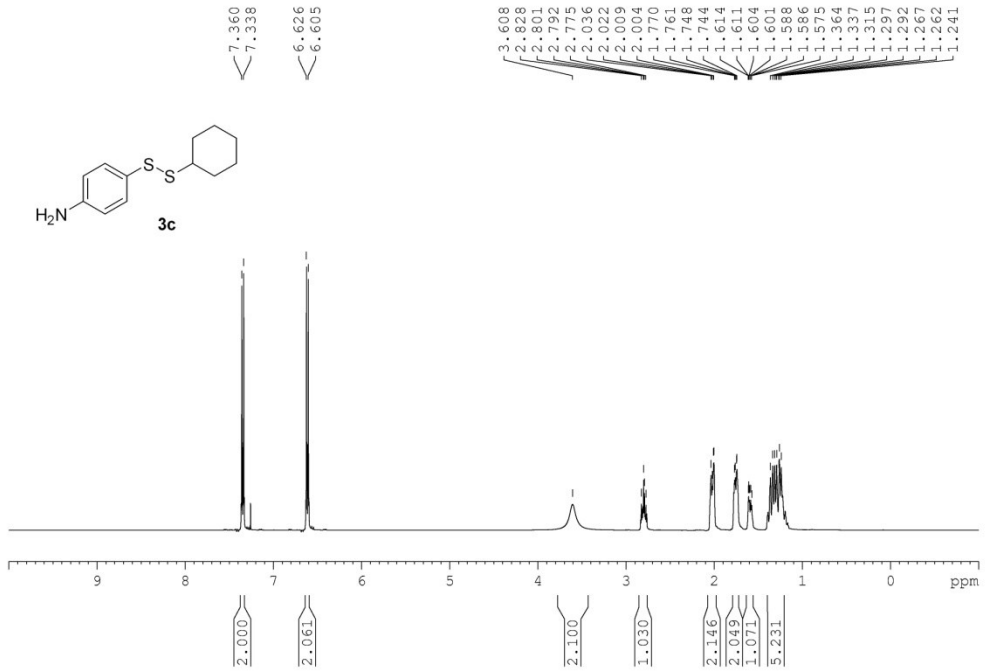
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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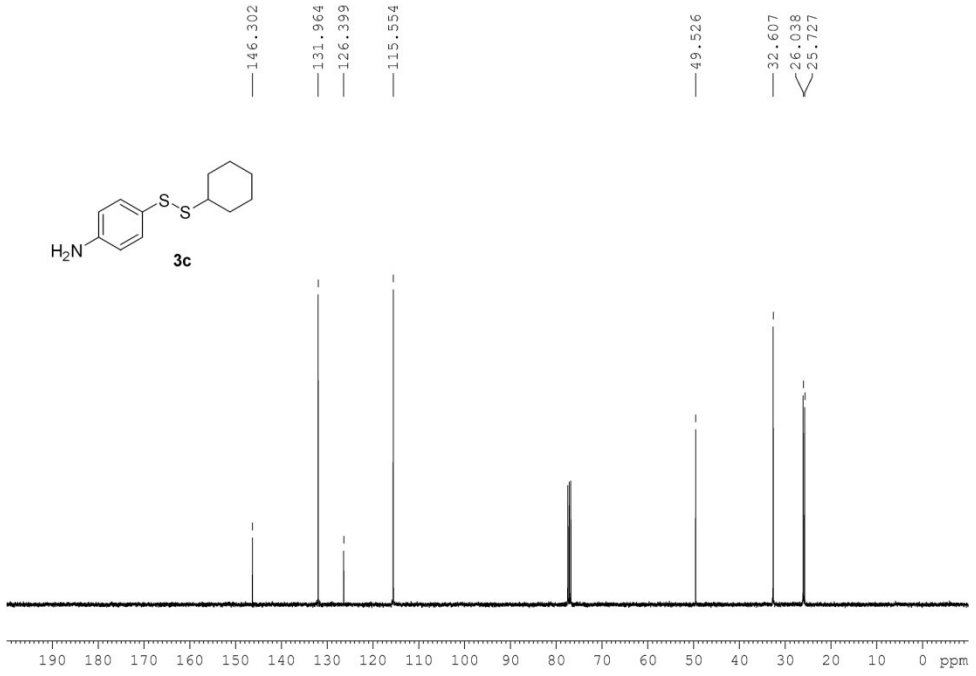
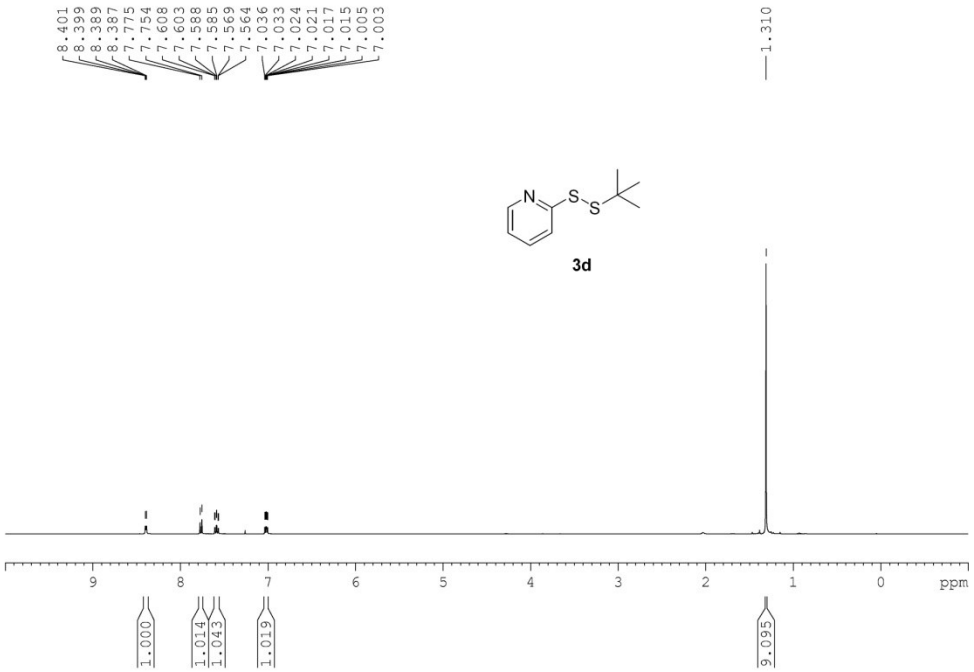
7.338
6.626
6.605
3.608
2.828
2.801
2.792
2.775
2.036
2.022
2.009
2.004
1.770
1.761
1.748
1.744
1.614
1.611
1.604
1.601
1.588
1.586
1.575
1.364
1.337
1.315
1.297
1.292
1.267
1.262
1.241
S
S
H2N
3c
9
8
7
6
5
4
3
2
1
0
ppm
2.000
2.061
2.100
1.030
2.146
2.049
1.071
5.231


146.302
131.964
126.399
115.554
49.526
32.607
26.038
25.727
S
S
H2N
3c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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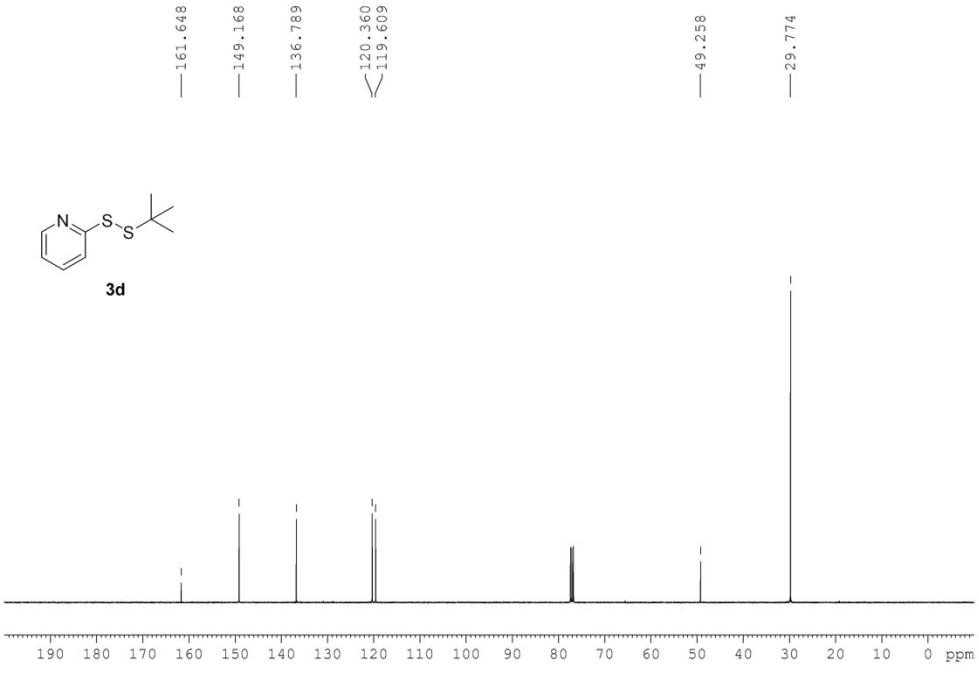
8.399
8.389
8.387
7.775
7.754
7.608
7.603
7.588
7.585
7.569
7.564
7.036
7.033
7.024
7.021
7.017
7.015
7.005
7.003
1.310
3d
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.014
1.043
1.019
9.095


161.648
149.168
136.789
120.360
119.609
49.258
29.774
3d
190
180
170
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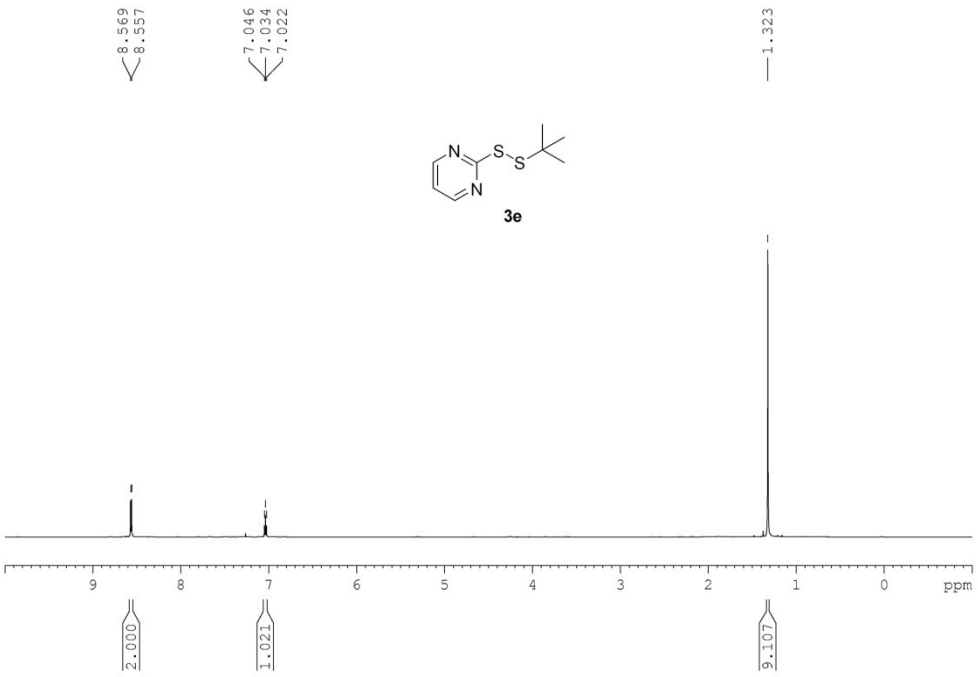
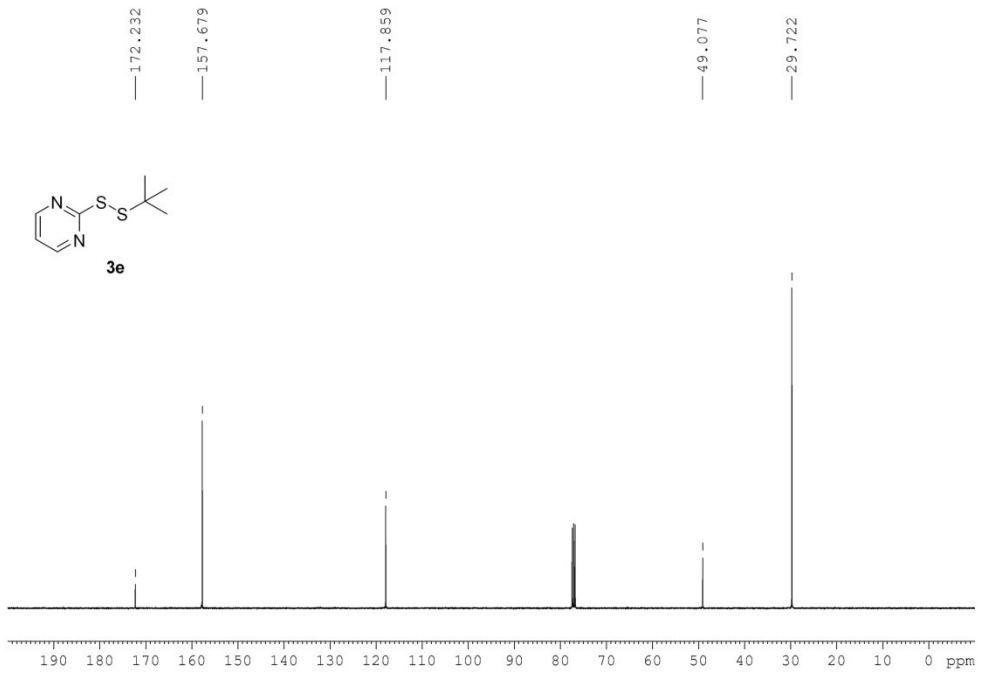
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


8.569
8.557
7.046
7.034
7.022
1.323
3e
9
8
7
6
5
4
3
2
1
0
ppm
2.000
1.021
9.107


172.232
157.679
117.859
49.077
29.722
3e
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180
170
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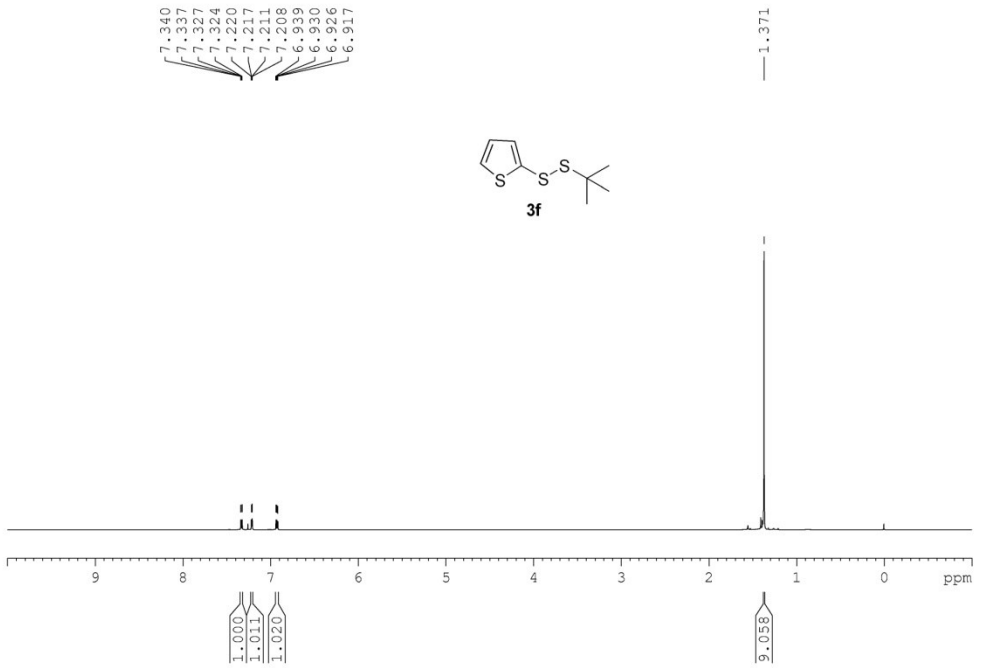
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.340
7.337
7.327
7.324
7.220
7.217
7.211
7.208
6.939
6.930
6.926
6.917
1.371
3f
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8
7
6
5
4
3
2
1
0
ppm
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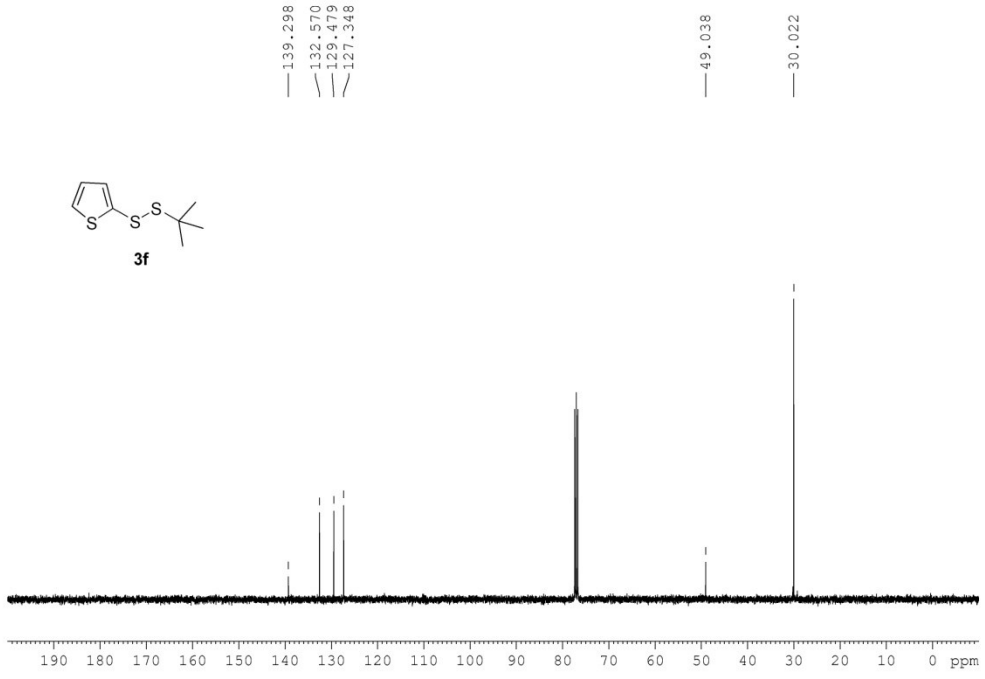
1.011
1.020
9.058


139.298
132.570
129.479
127.348
49.038
30.022
3f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
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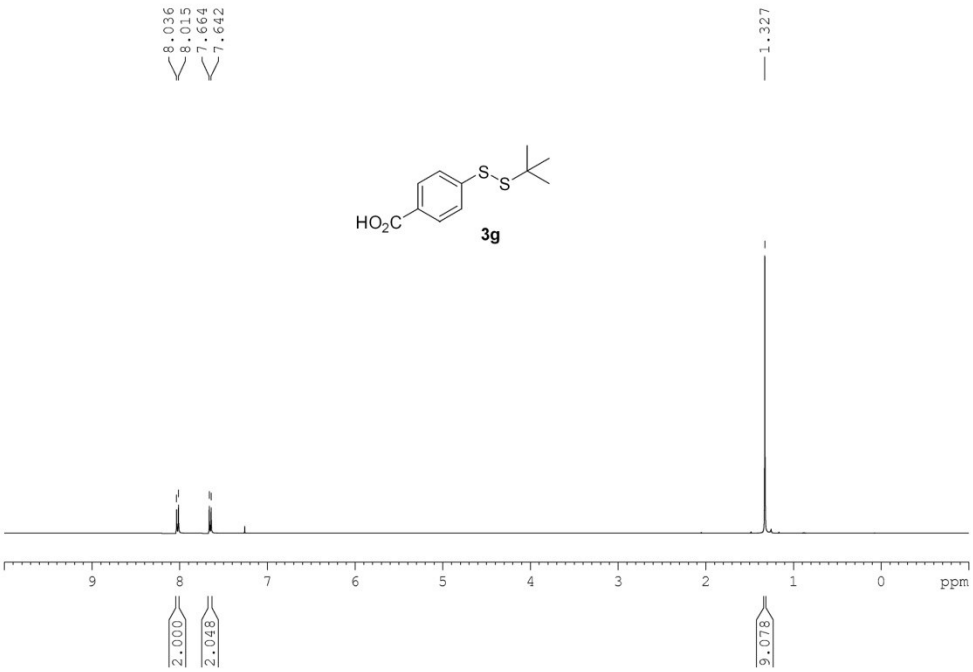
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8.015
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7.642
1.327
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S
3g
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8
7
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1
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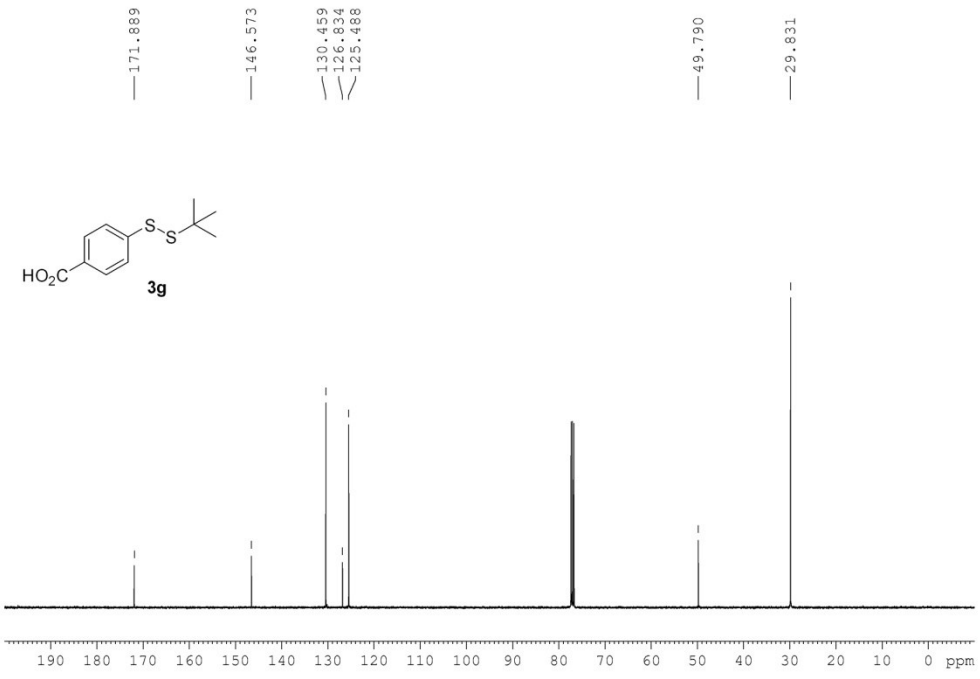
2.048
9.078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146.573
130.459
126.834
125.488
49.790
29.831
HO2C
S
S
3g
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120
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60
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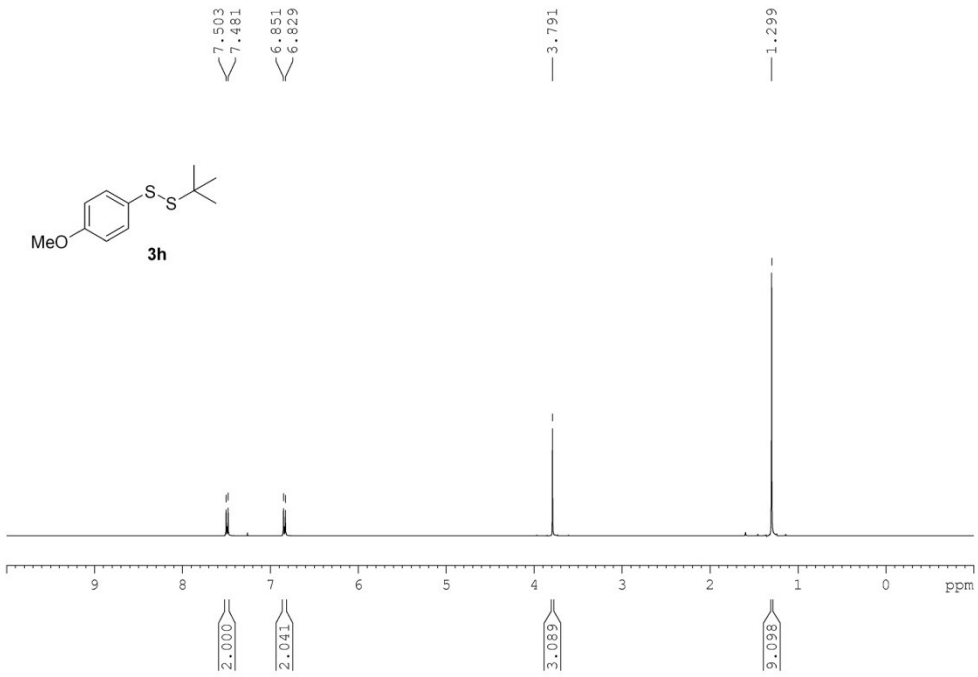
0
ppm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7.481
6.851
6.829
3.791
1.299
MeO
3h
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8
7
6
5
4
3
2
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0
ppm
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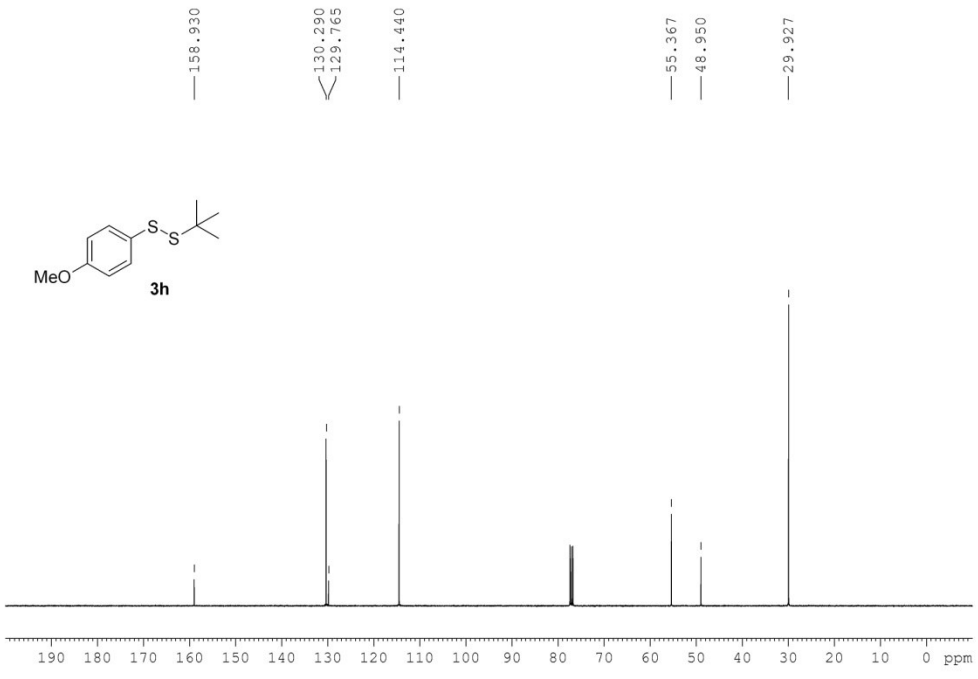
2.041
3.089
9.098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130.290
129.765
114.440
55.367
48.950
29.927
MeO
3h
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180
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140
130
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110
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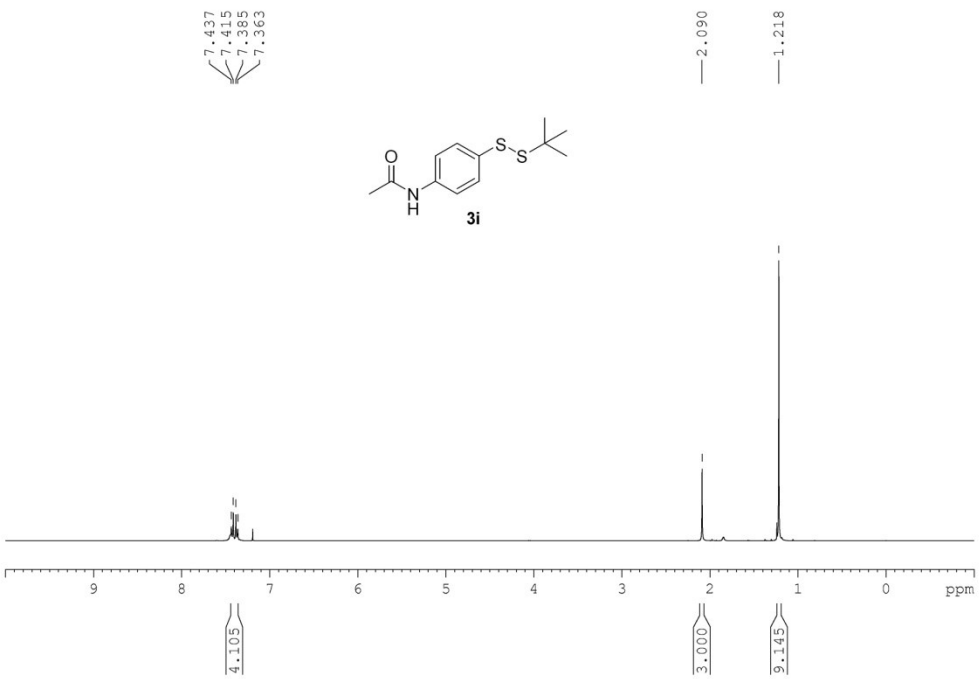
20
10
0 ppm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7.415
7.385
7.363
2.090
1.218
3i
9
8
7
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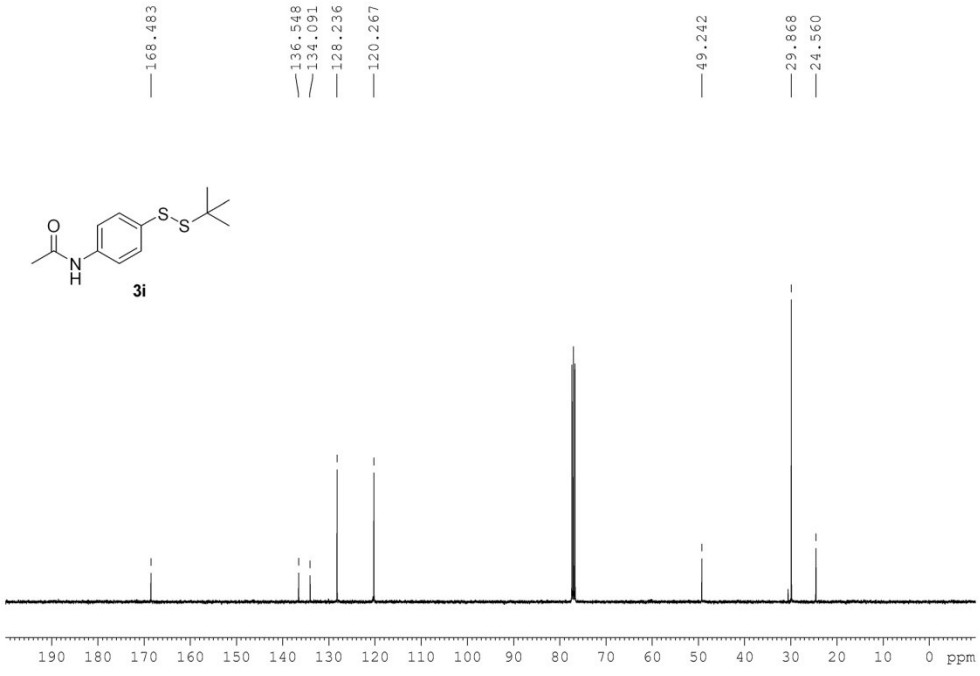
5
4
3
2
1
0
ppm
4.105
3.000
9.145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136.548
134.091
128.236
120.267
49.242
29.868
24.560
3i
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170
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140
130
120
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100
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80
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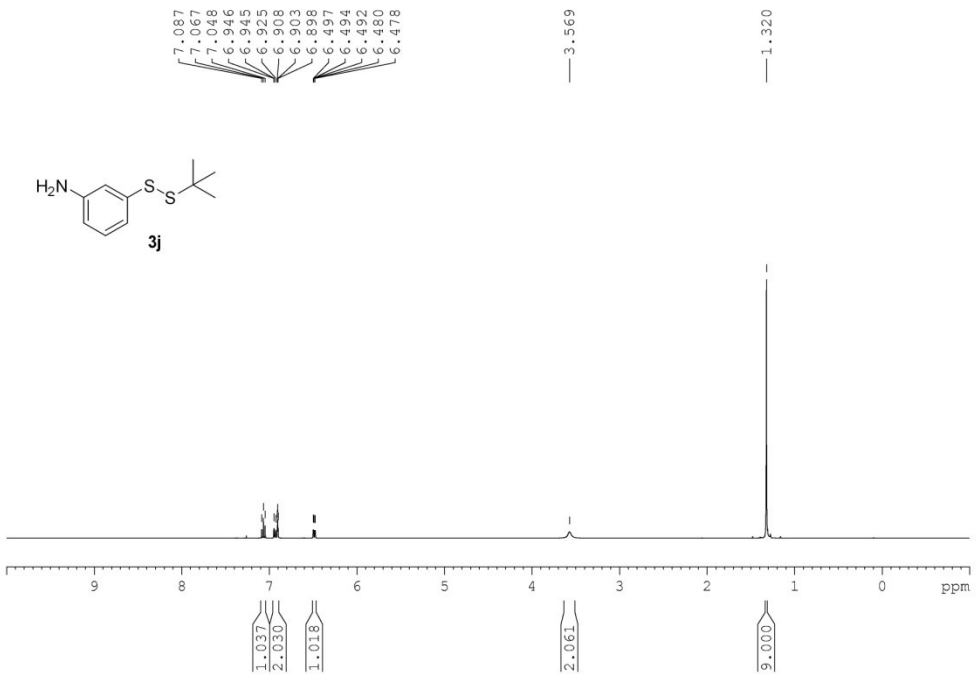
60
50
40
30
20
10
0
ppm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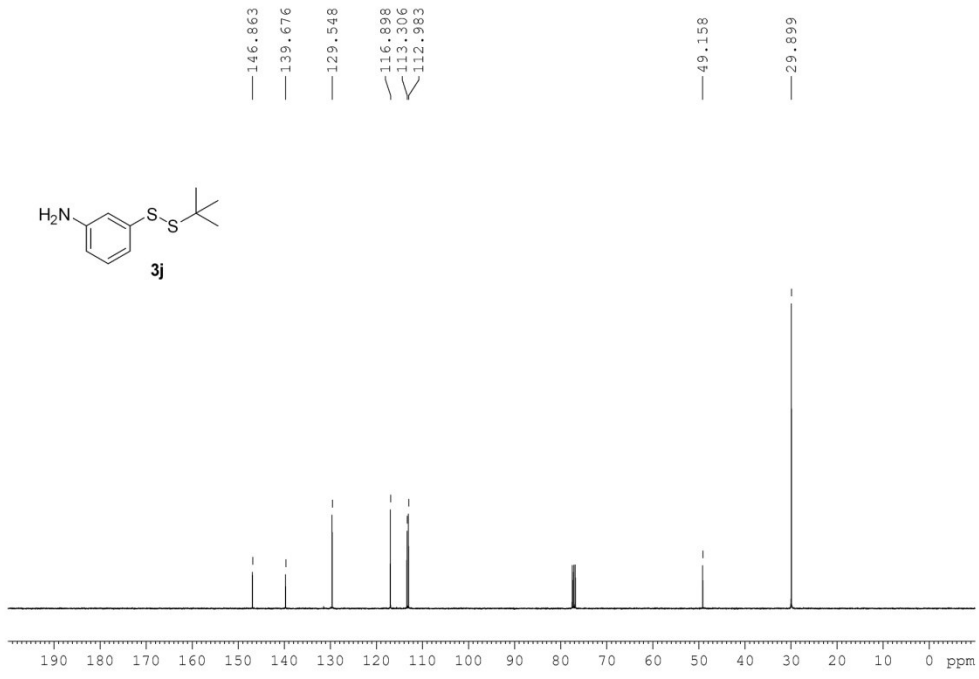
7.067
7.048
6.946
6.945
6.925
6.908
6.903
6.898
6.497
6.494
6.492
6.480
6.478
3.569
1.320
H_2N
S
S
3j
9
8
7
6
5
4
3
2
1
0
ppm
1.037
2.030
1.018
2.061
9.000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139.676
129.548
116.898
113.306
112.983
49.158
29.899
H_2N
S
S
3j
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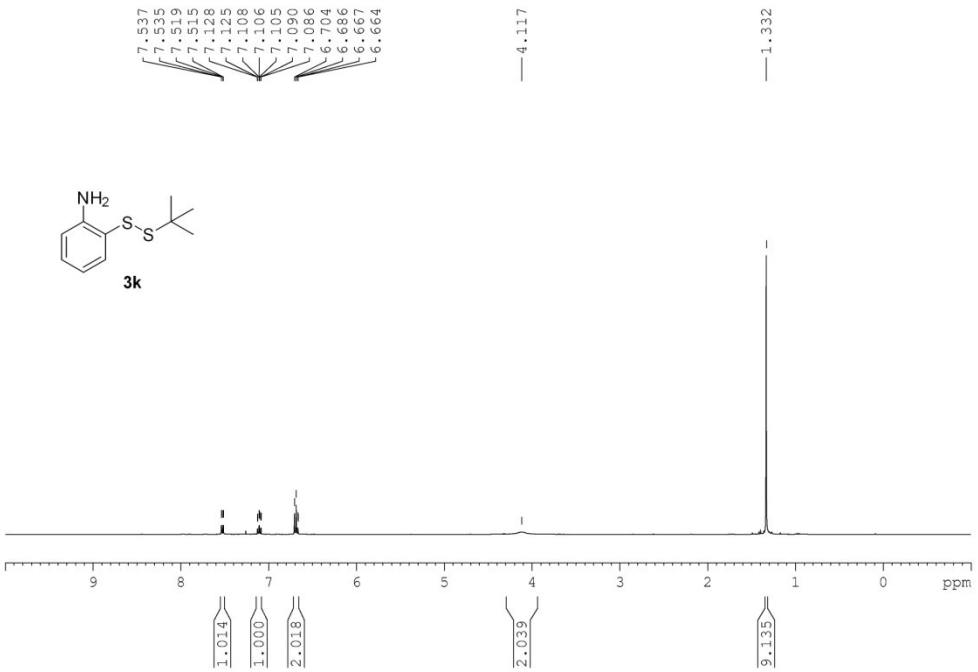
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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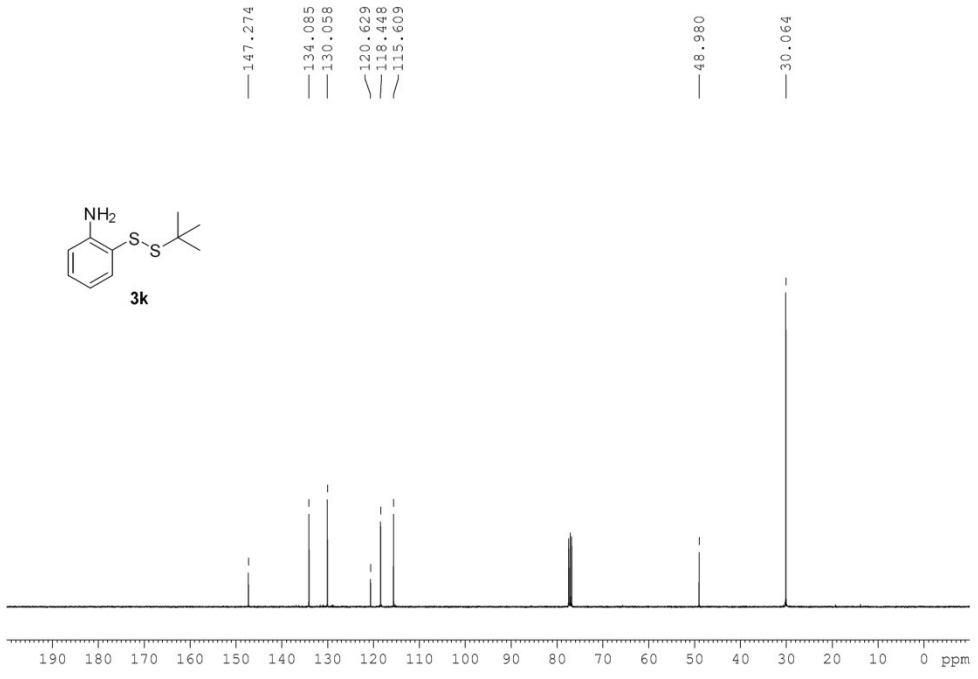
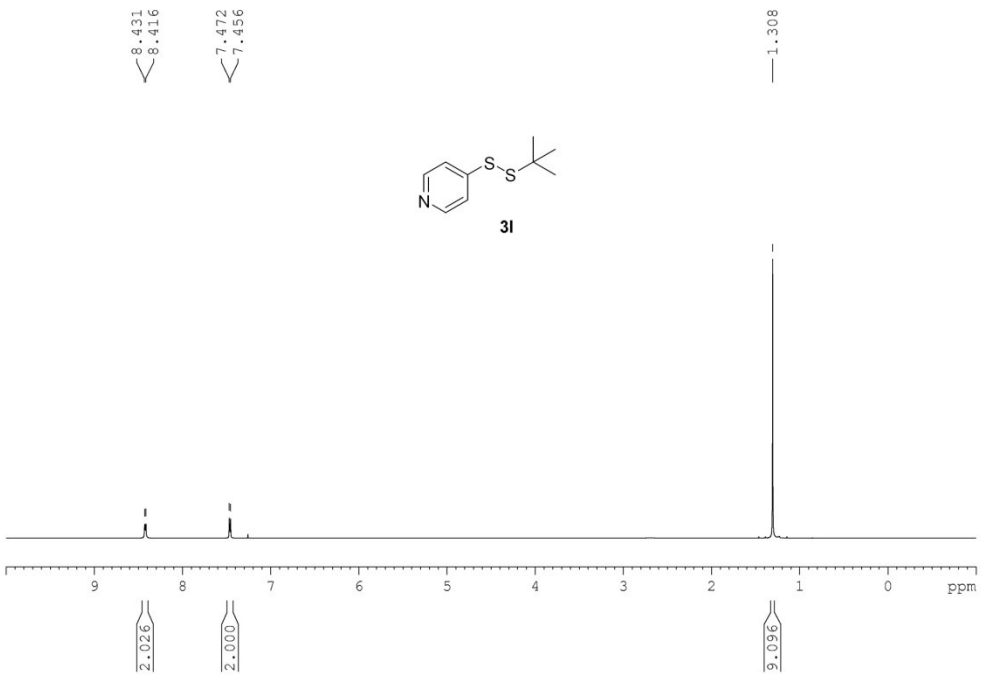
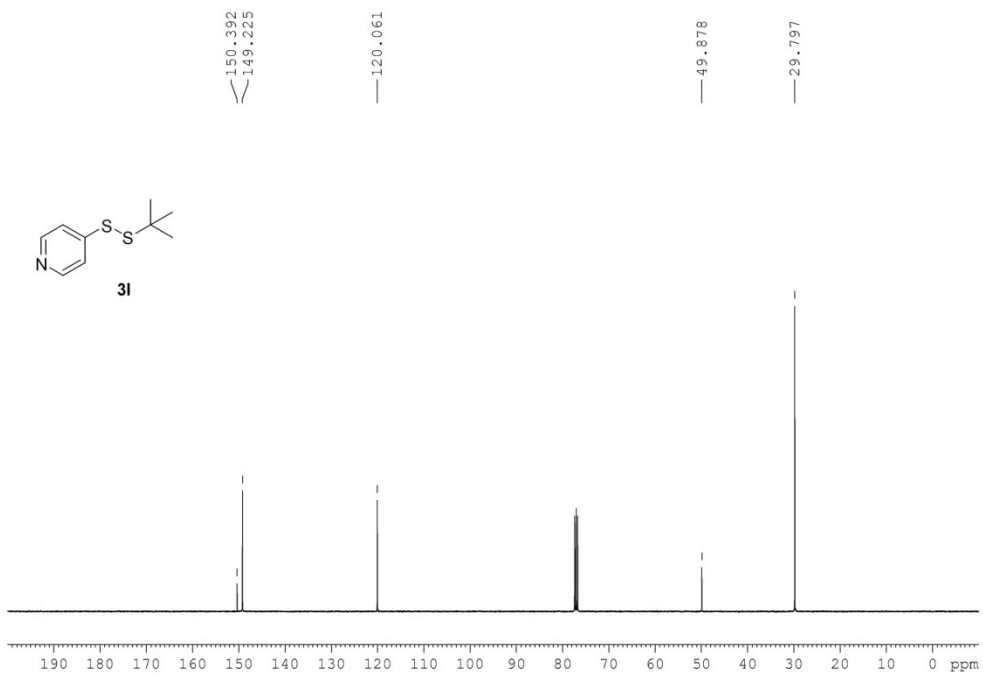
7.535
7.519
7.515
7.128
7.125
7.108
7.106
7.105
7.090
7.086
6.704
6.686
6.667
6.664
4.117
1.332
NH2
S
S
3k
9
8
7
6
5
4
3
2
1
0
ppm
1.014
1.000
2.018
2.039
9.135


147.274
134.085
130.058
120.629
118.448
115.609
48.980
30.064
NH2
S
S
3k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.431
8.416
7.472
7.456
1.308
3l
9
8
7
6
5
4
3
2
1
0
ppm
2.026
2.000
9.096


150.392
149.225
120.061
49.878
29.797
3l
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180
170
160
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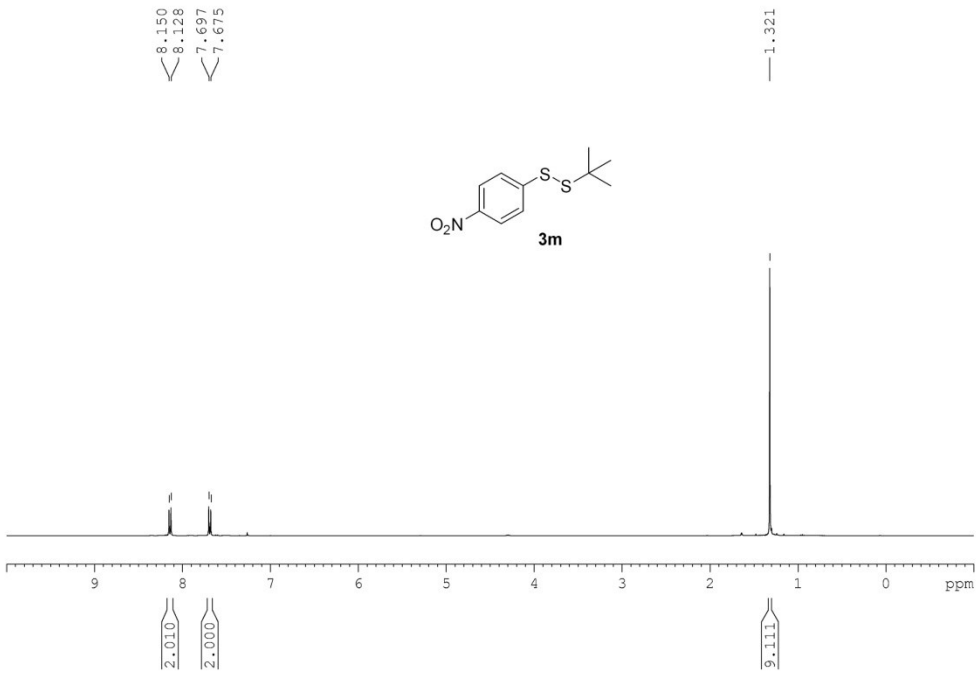
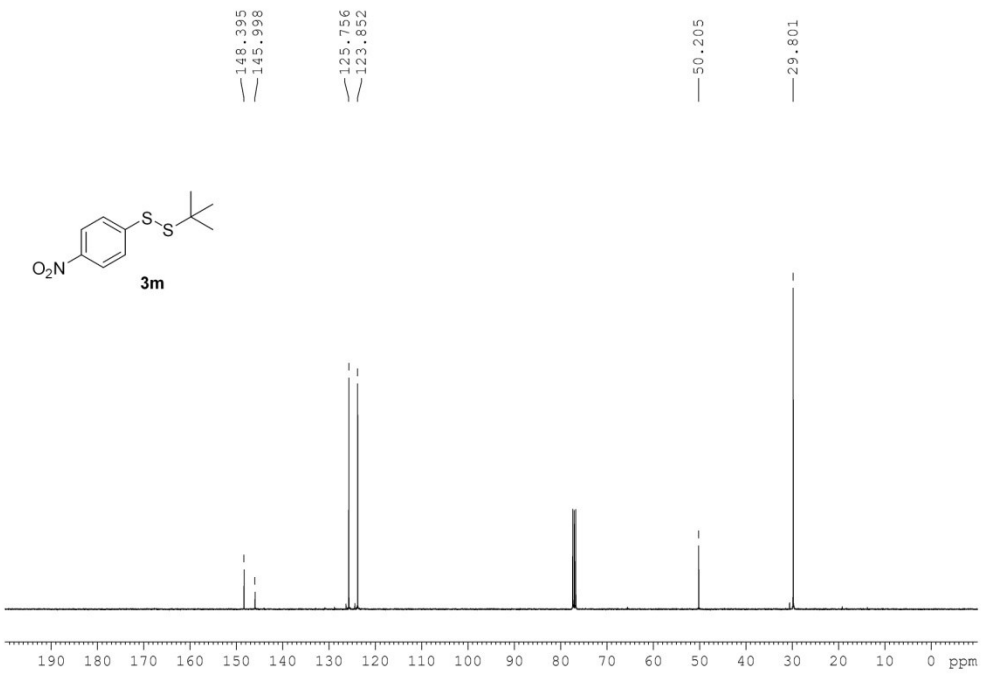
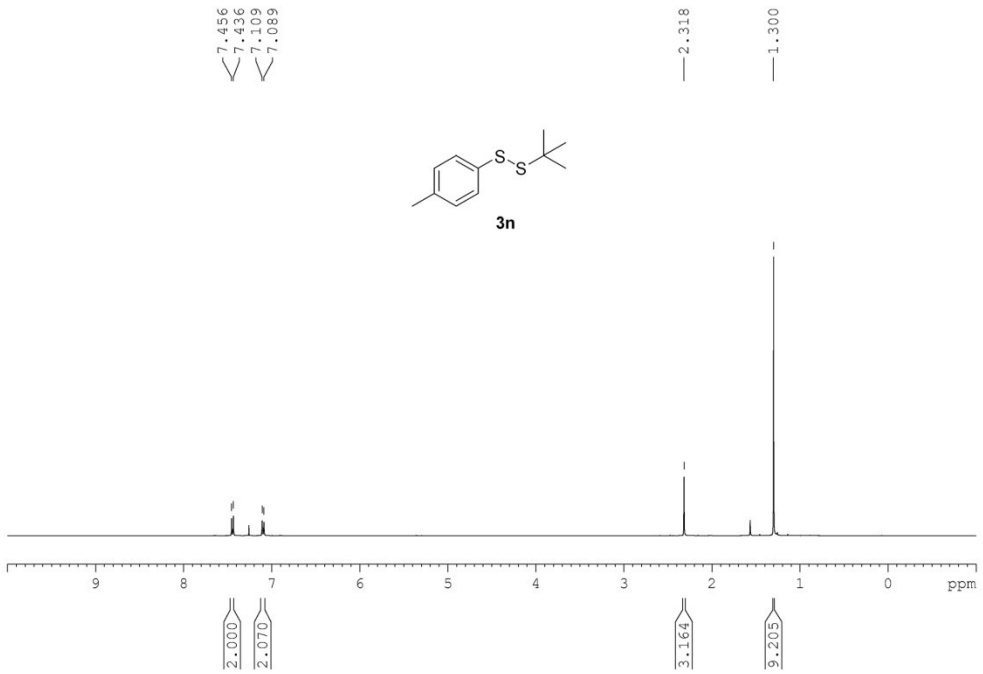
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.150
8.128
7.697
7.675
1.321
3m
9
8
7
6
5
4
3
2
1
0
ppm
2.010
2.000
9.111


148.395
145.998
125.756
123.852
50.205
29.801
3m
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.456
7.436
7.109
7.089
2.318
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3n
9
8
7
6
5
4
3
2
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ppm
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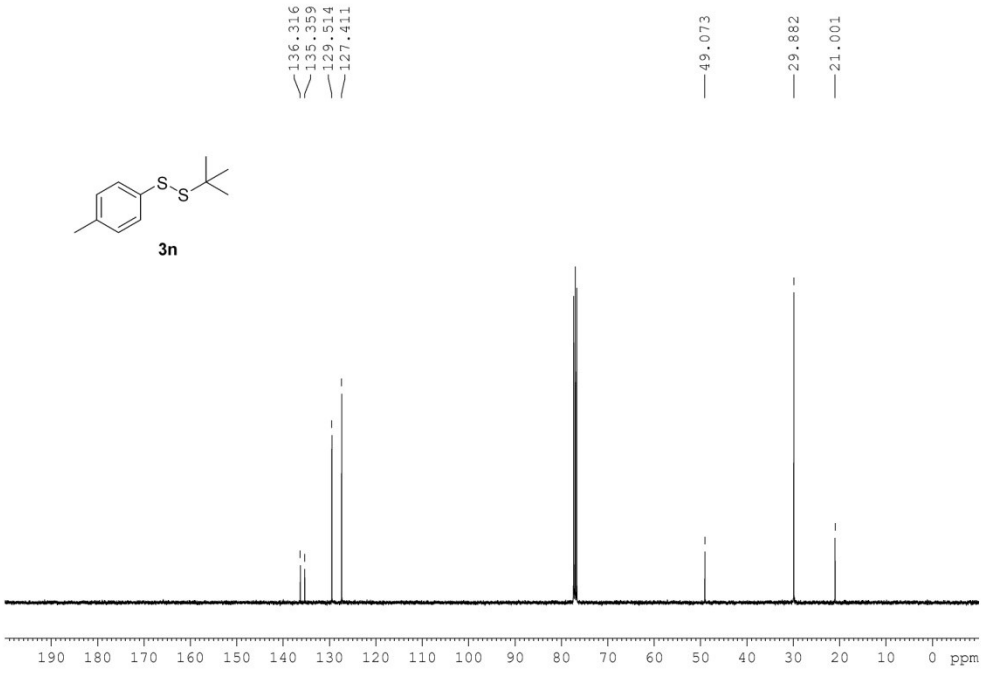
2.070
3.164
9.205


136.316
135.359
129.514
127.411
49.073
29.882
21.001
3n
190
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170
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150
140
130
120
110
100
90
80
70
60
50
40
30
20
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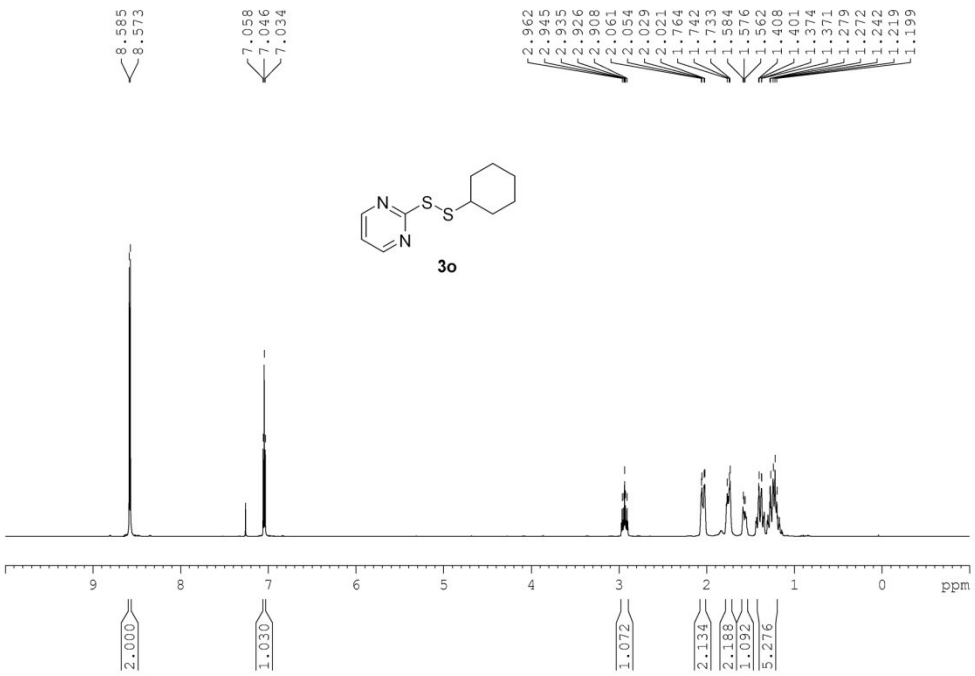
0
ppm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7.034
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2.945
2.935
2.926
2.908
2.061
2.054
2.029
2.021
1.764
1.742
1.733
1.584
1.576
1.562
1.408
1.401
1.374
1.371
1.279
1.272
1.242
1.219
1.199
3o
9
8
7
6
5
4
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2
1
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1.072
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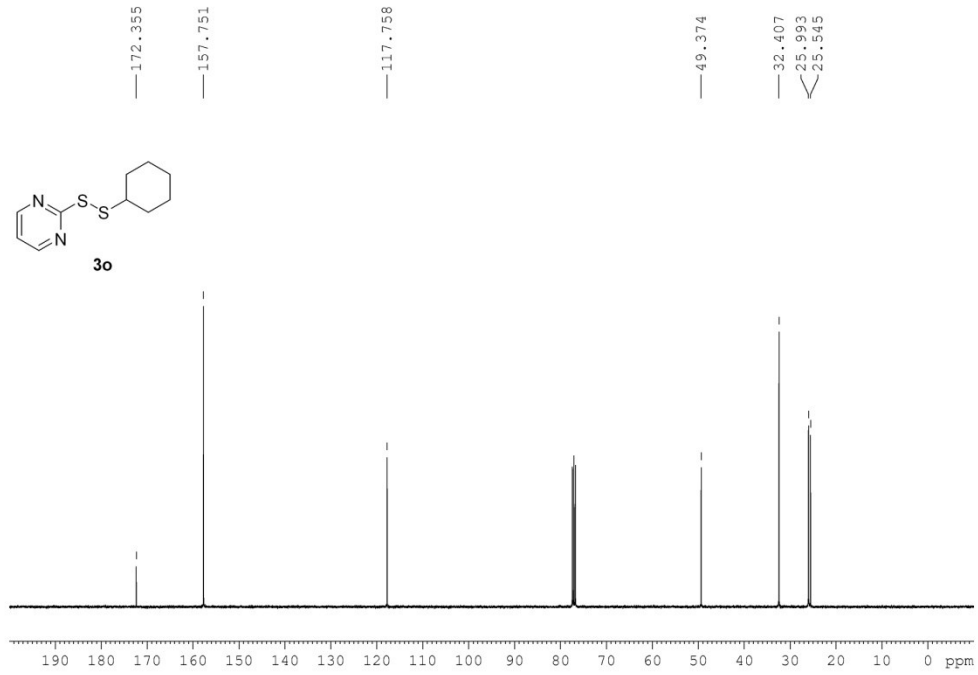
2.188
1.092
5.276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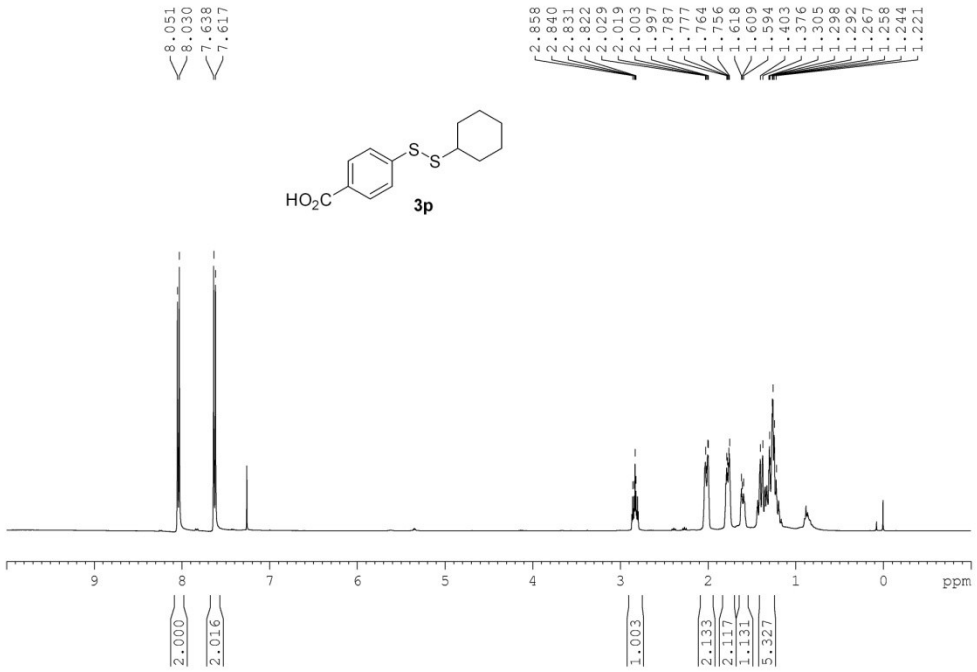
157.751
117.758
49.374
32.407
25.993
25.545
3o
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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2.840
2.831
2.822
2.029
2.019
2.003
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1.787
1.777
1.764
1.756
1.618
1.609
1.594
1.403
1.376
1.305
1.298
1.292
1.267
1.258
1.244
1.221
HO2C
S
S
3p
9
8
7
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5
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2
1
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1.003
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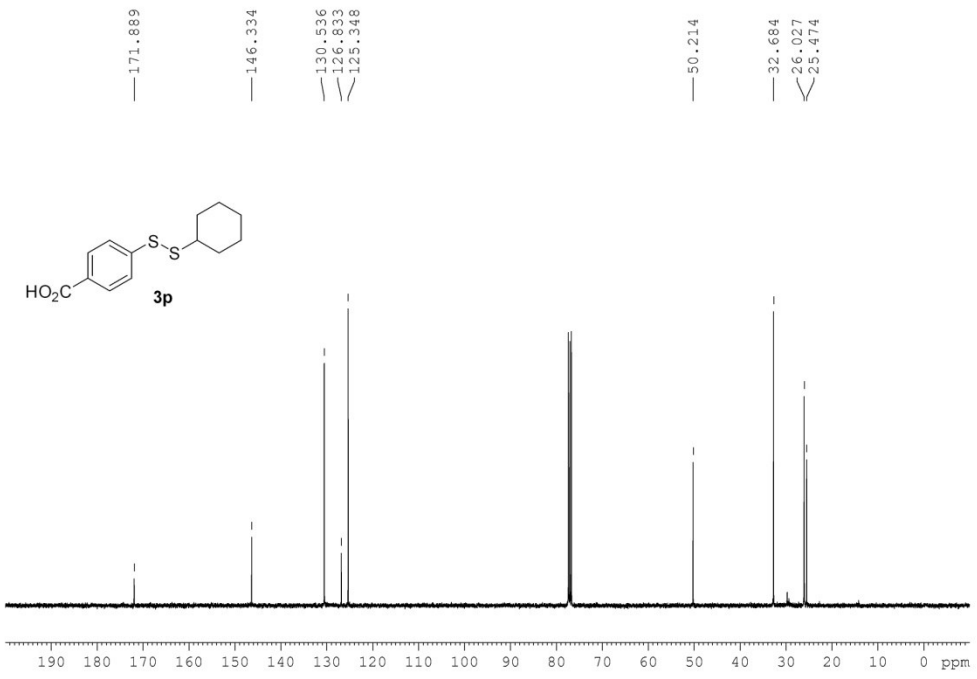
5.327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125.348
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26.027
25.474
HO2C
S
S
3p
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180
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160
150
140
130
120
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100
90
80
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60
50
40
30
20
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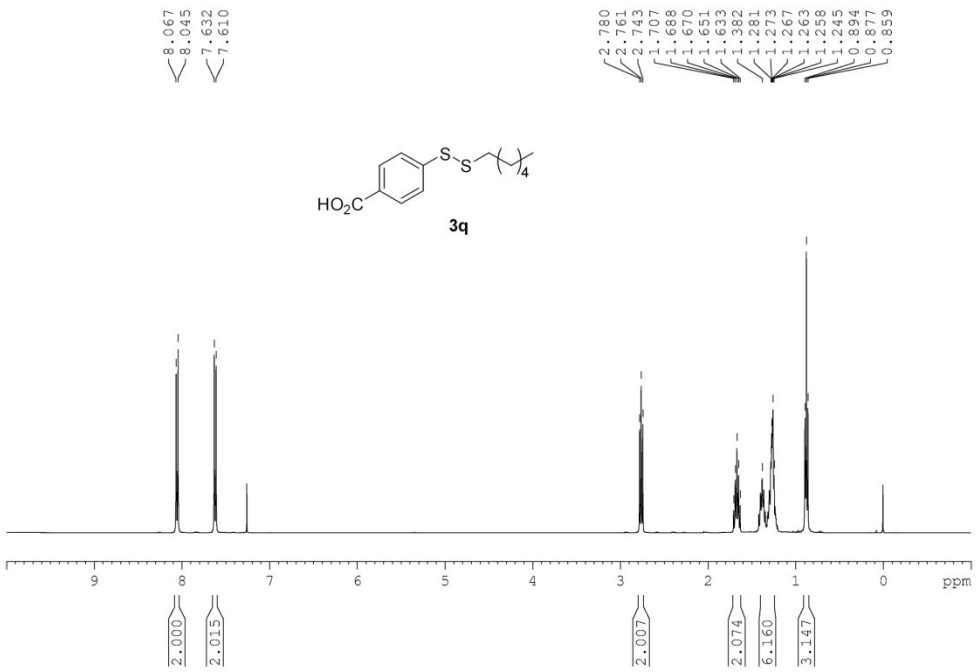
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1.707
1.688
1.670
1.651
1.633
1.382
1.281
1.273
1.267
1.263
1.258
1.245
0.894
0.877
0.859
HO2C
S
S
4
3q
9
8
7
6
5
4
3
2
1
0
ppm
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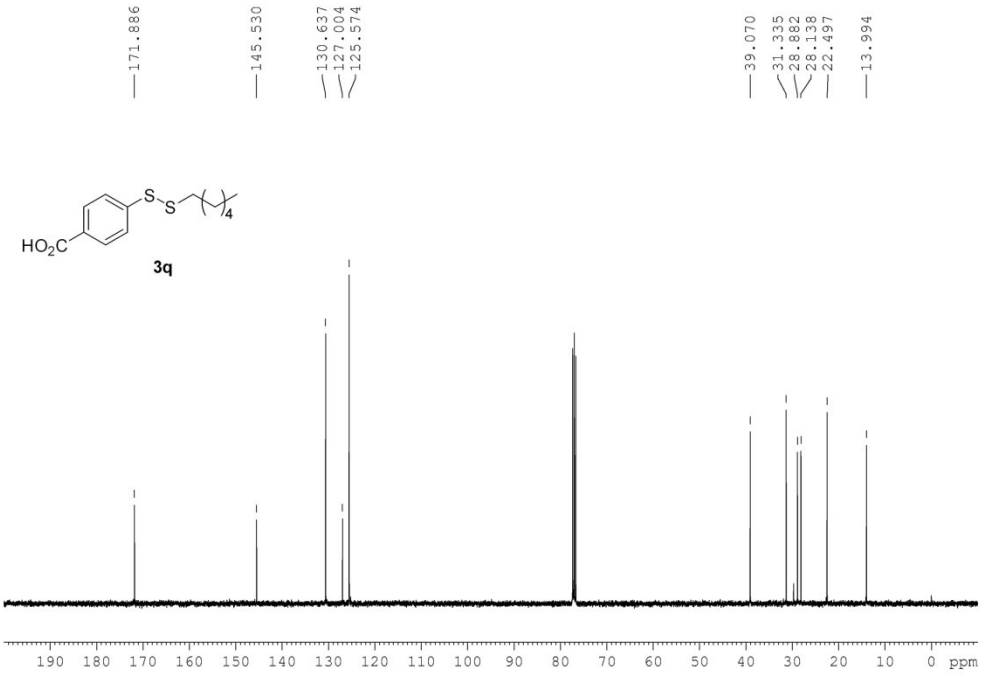
2.015
2.007
2.074
6.160
3.147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39.070
31.335
28.882
28.138
22.497
13.994
HO2C
S
S
4
3q
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180
170
160
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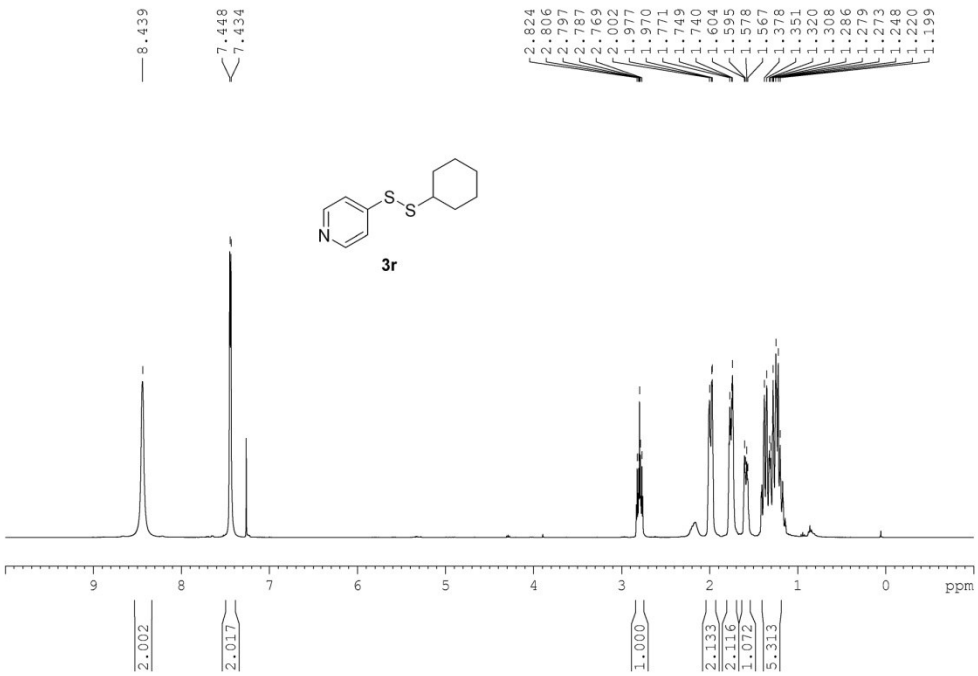
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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2.806
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2.769
2.002
1.977
1.970
1.771
1.749
1.740
1.604
1.595
1.578
1.567
1.378
1.351
1.320
1.308
1.286
1.279
1.273
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1.199
3r
ppm
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1.000
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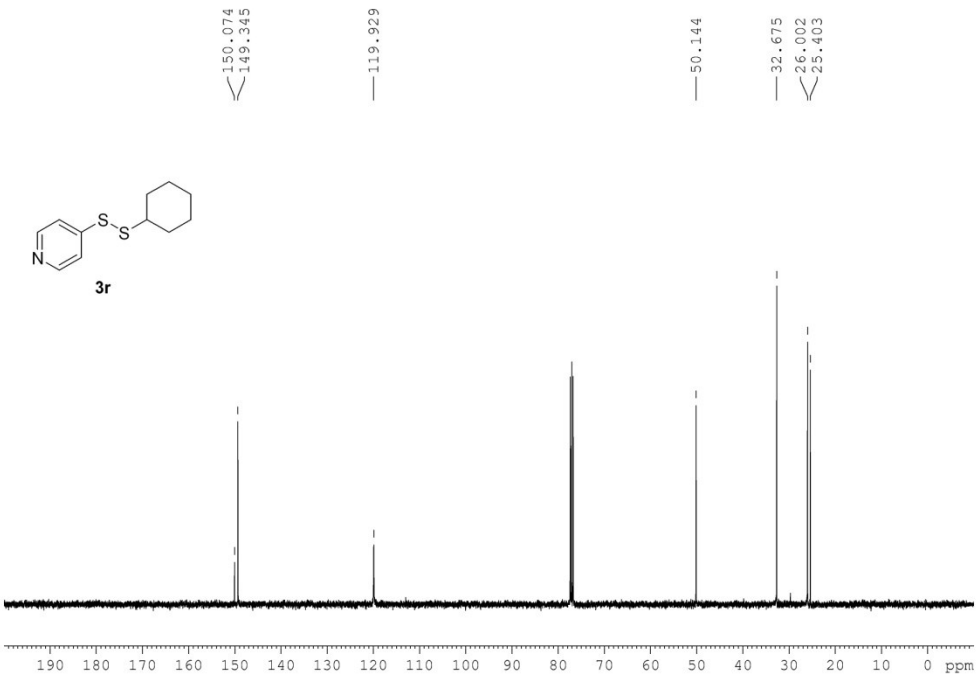
2.116
1.072
5.313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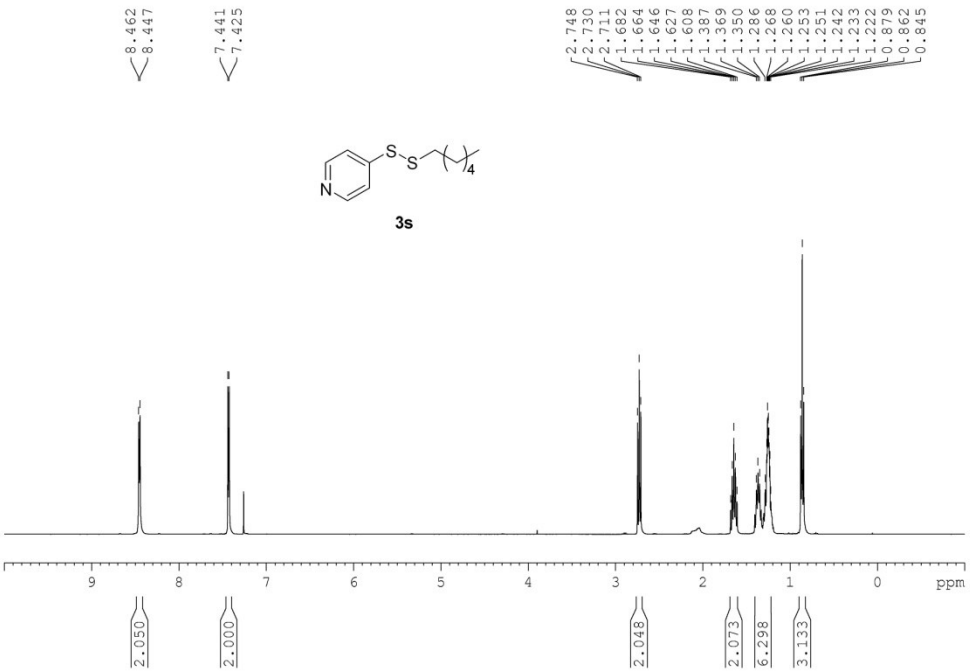
25.403
3r
ppm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2.711
1.682
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1.646
1.627
1.608
1.387
1.369
1.350
1.286
1.268
1.260
1.253
1.251
1.242
1.233
1.222
0.879
0.862
0.845
3s
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8
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5
4
3
2
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0
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2.000
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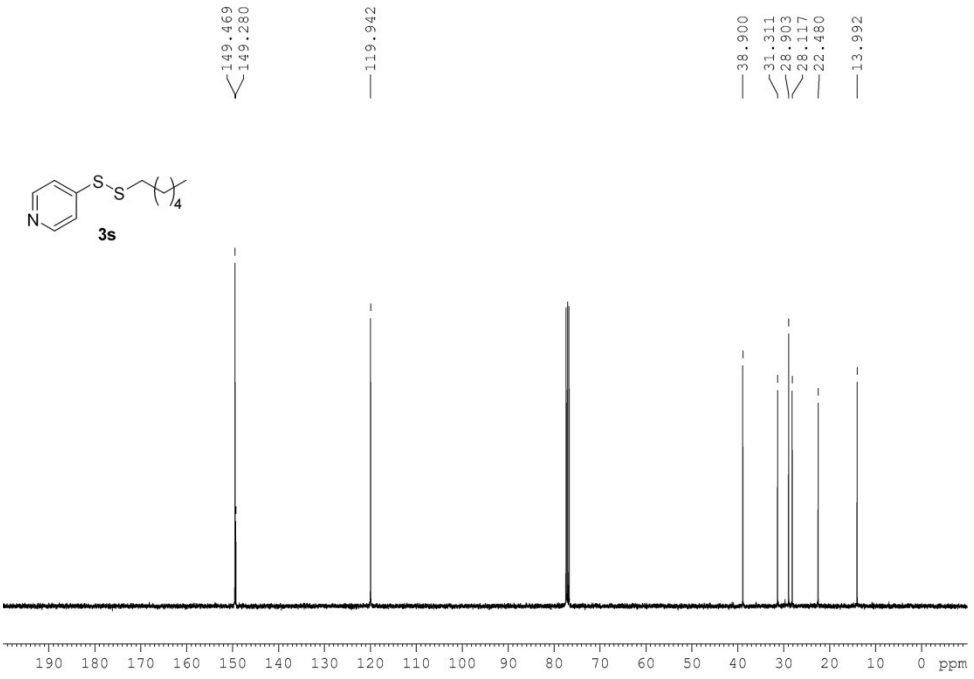
2.073
6.298
3.133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119.942
38.900
31.311
28.903
28.117
22.480
13.992
3s
190
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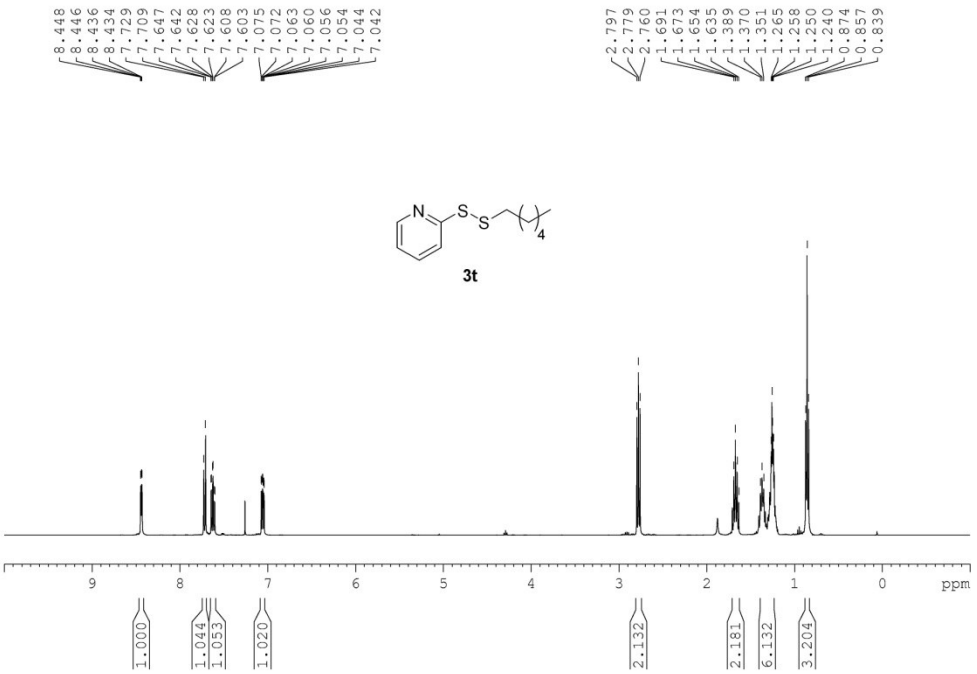
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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8.434
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7.642
7.628
7.623
7.608
7.603
7.075
7.072
7.063
7.060
7.056
7.054
7.044
7.042
2.797
2.779
2.760
1.691
1.673
1.654
1.635
1.389
1.370
1.351
1.265
1.258
1.250
1.240
0.874
0.857
0.839
3t
9
8
7
6
5
4
3
2
1
0
ppm
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1.044
1.053
1.020
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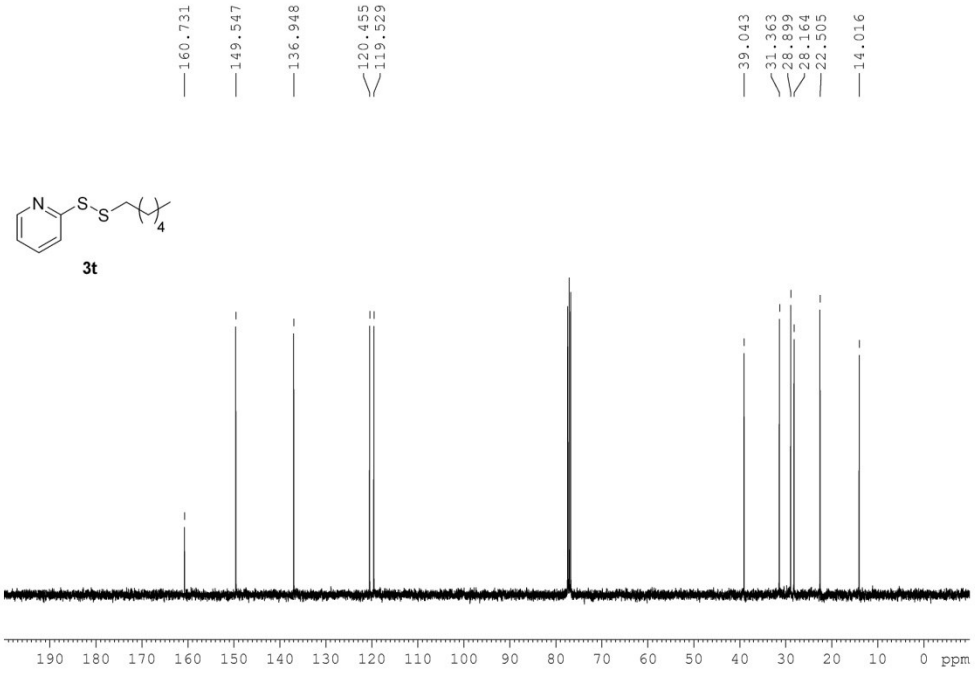
2.181
6.132
3.204


160.731
149.547
136.948
120.455
119.529
39.043
31.363
28.899
28.164
22.505
14.016
3t
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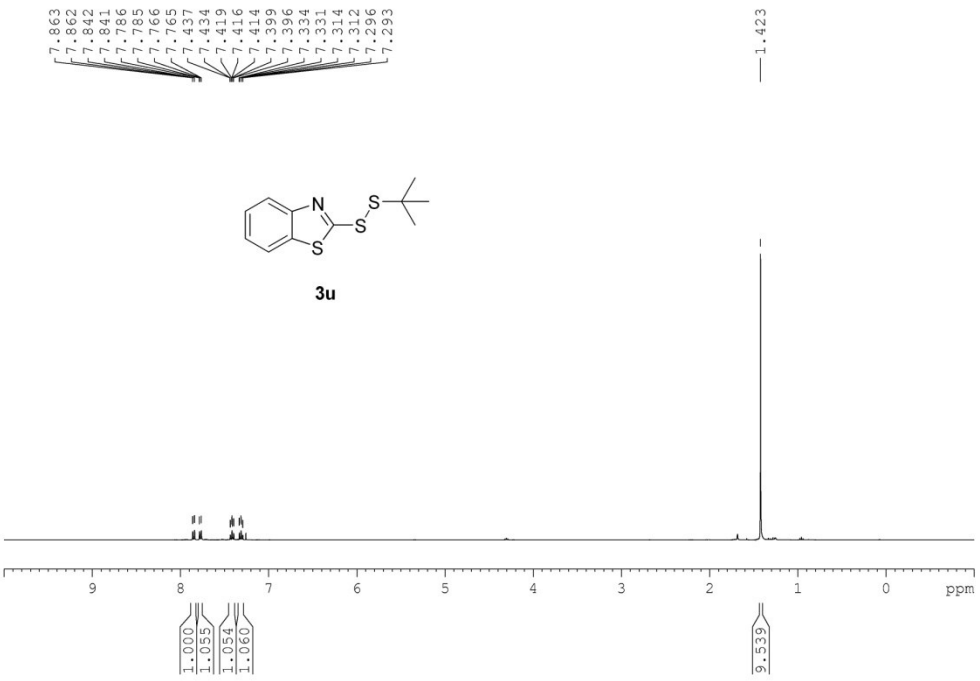
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.785
7.766
7.765
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7.434
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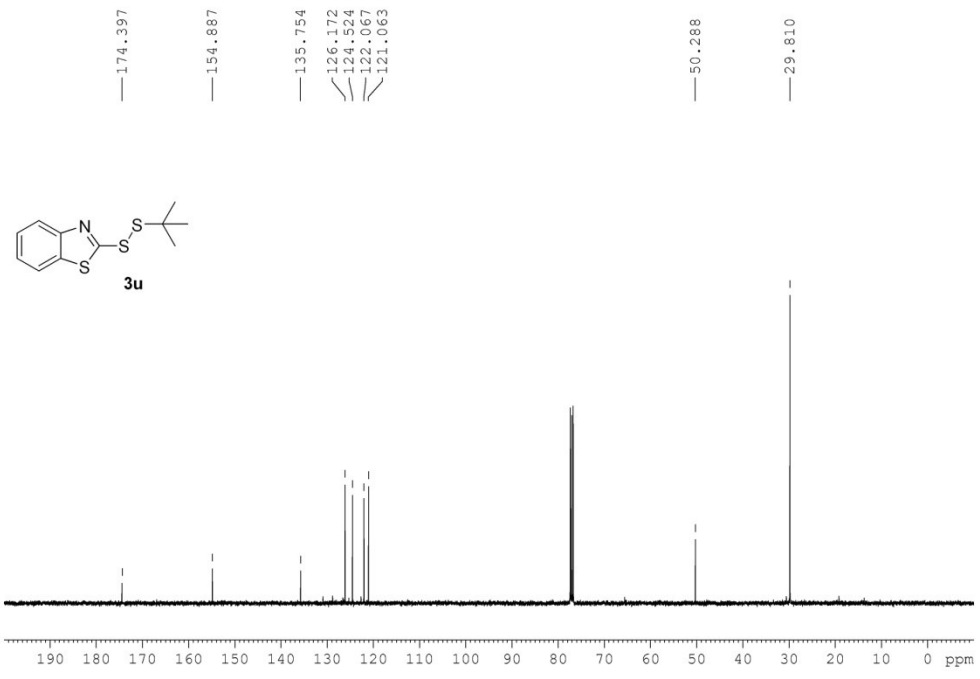
7.416
7.414
7.399
7.396
7.334
7.331
7.314
7.312
7.296
7.293
1.423
N
S
S
S
3u
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.055
1.054
1.060
9.539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154.887
135.754
126.172
124.524
122.067
121.063
50.288
29.810
N
S
S
S
3u
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
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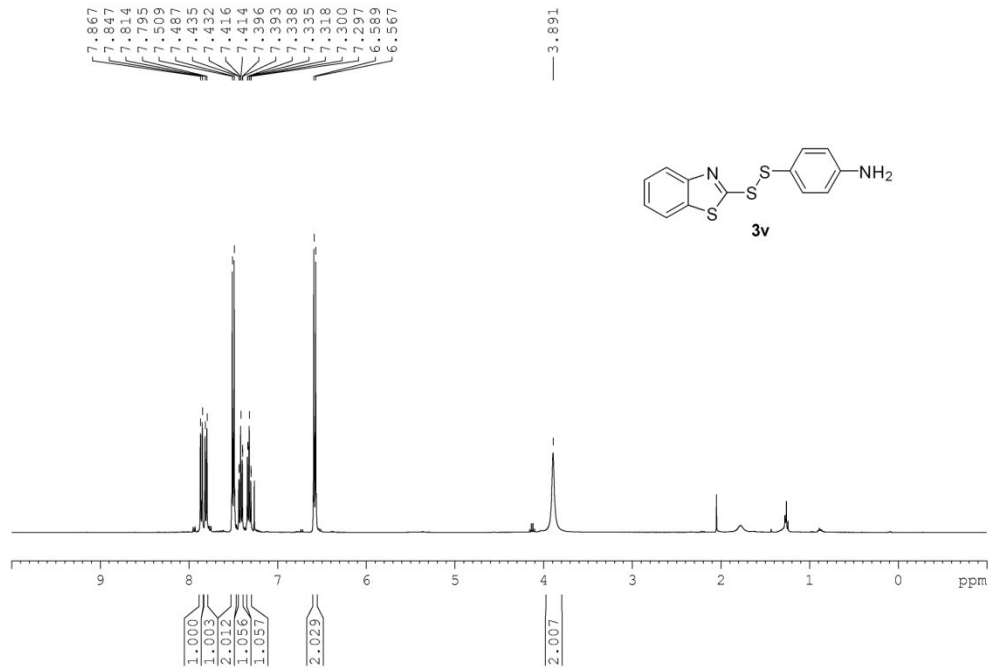
30
20
10
0
ppm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7.795
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7.435
7.432
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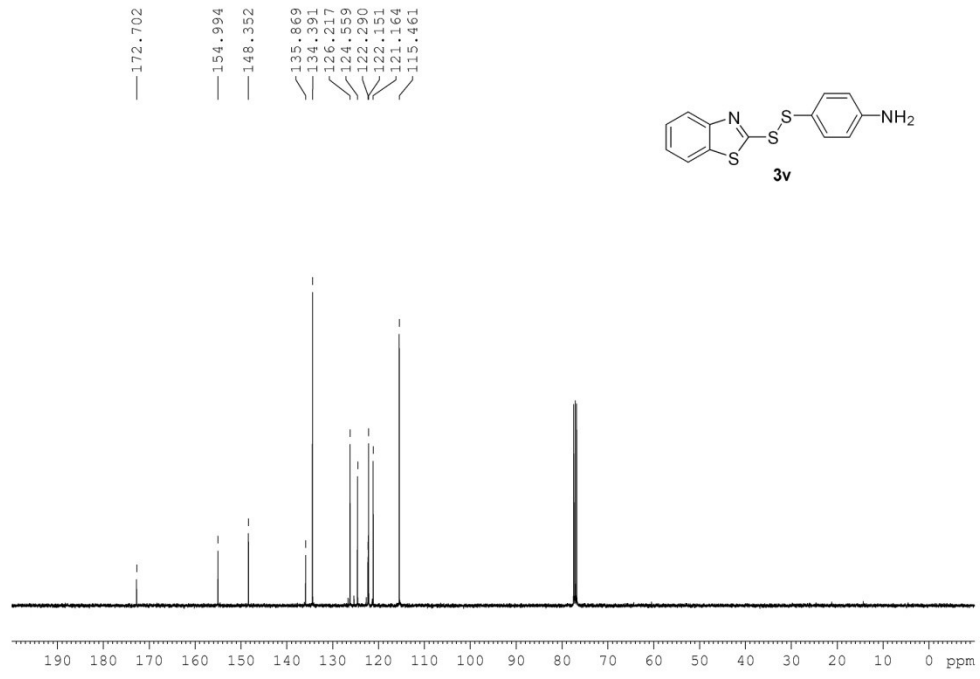
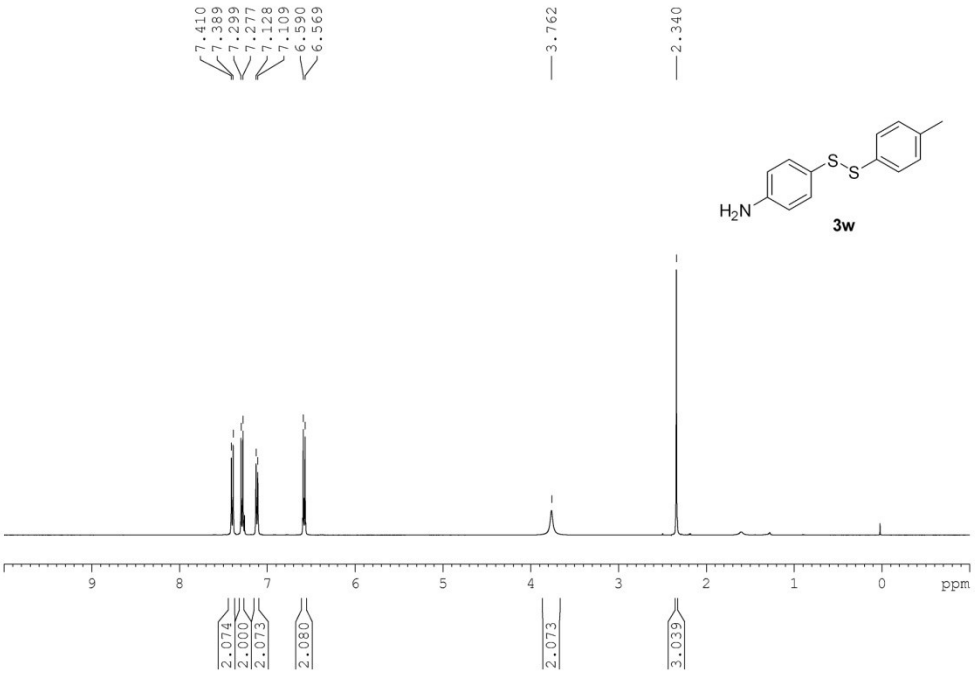
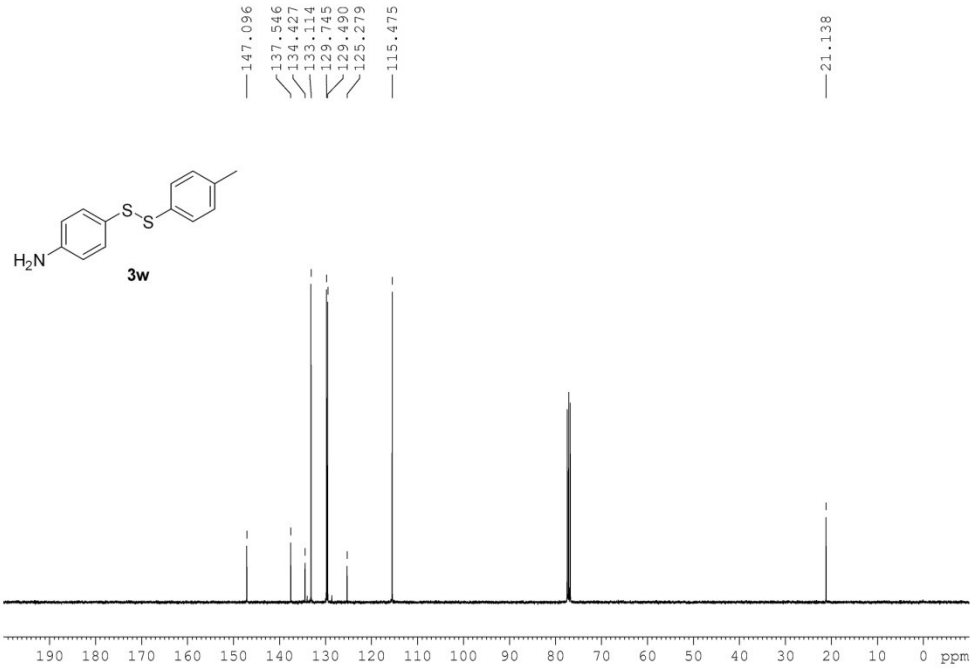
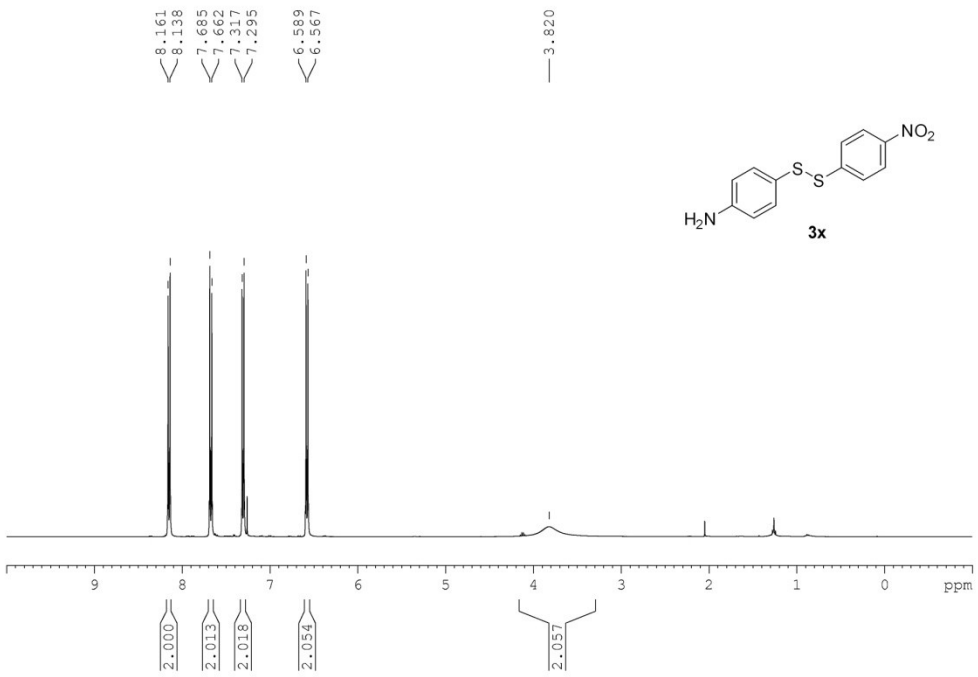
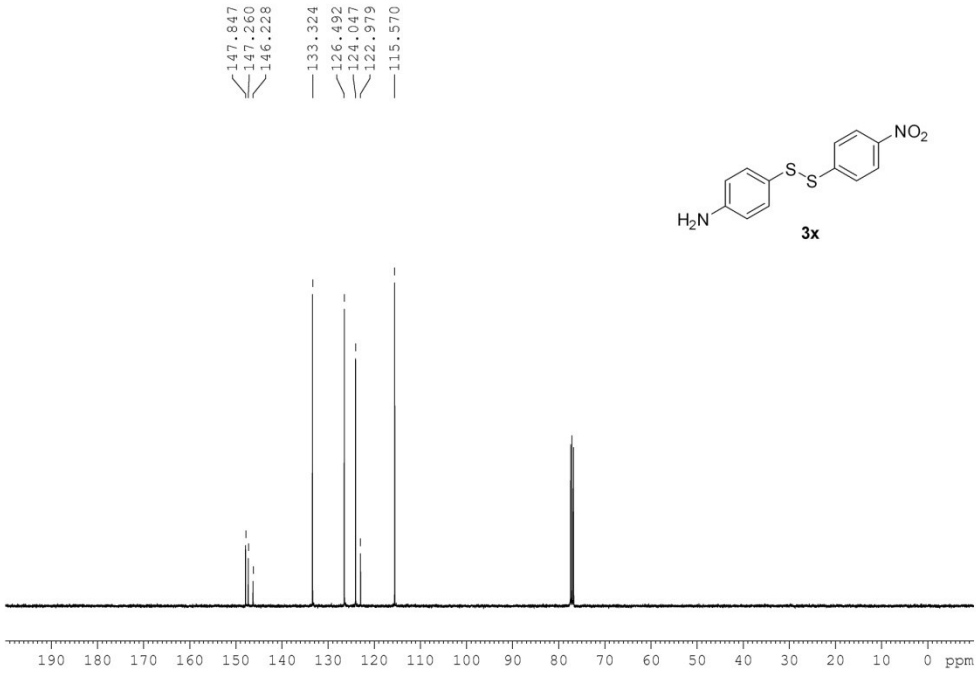
7.414
7.396
7.393
7.338
7.335
7.318
7.300
7.297
6.589
6.567
3.891
NH2
3v
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.003
2.012
1.056
1.057
2.029
2.007

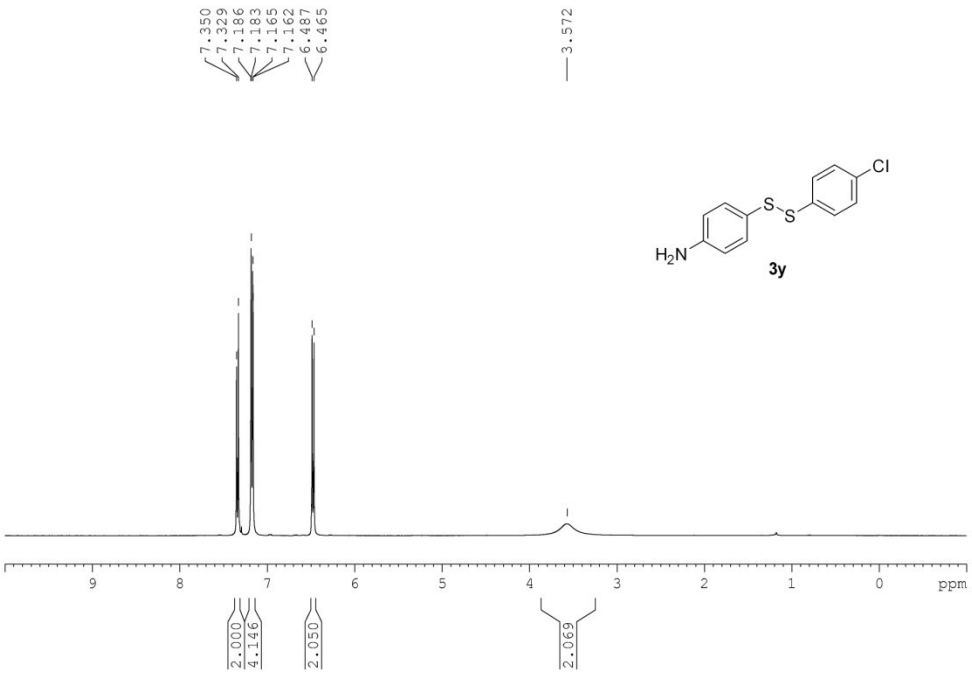

172.702
154.994
148.352
135.869
134.391
126.217
124.559
122.290
122.151
121.164
115.461
NH2
3v
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

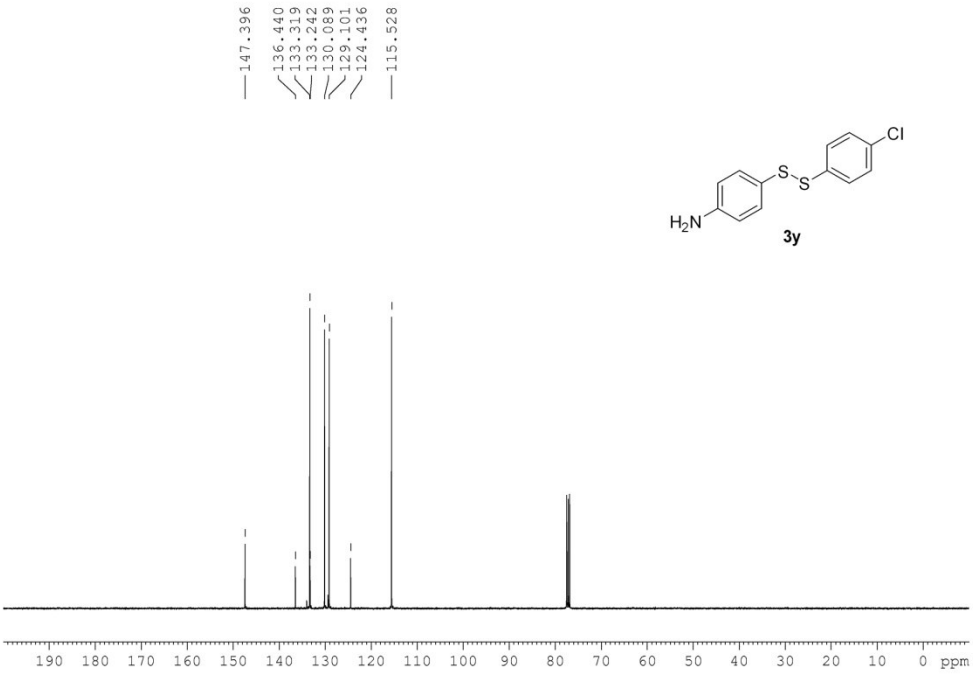

7.410
7.389
7.299
7.277
7.128
7.109
6.590
6.569
3.762
2.340
S
S
H_2N
3w
9
8
7
6
5
4
3
2
1
0
ppm
2.074
2.000
2.073
2.080
2.073
3.039

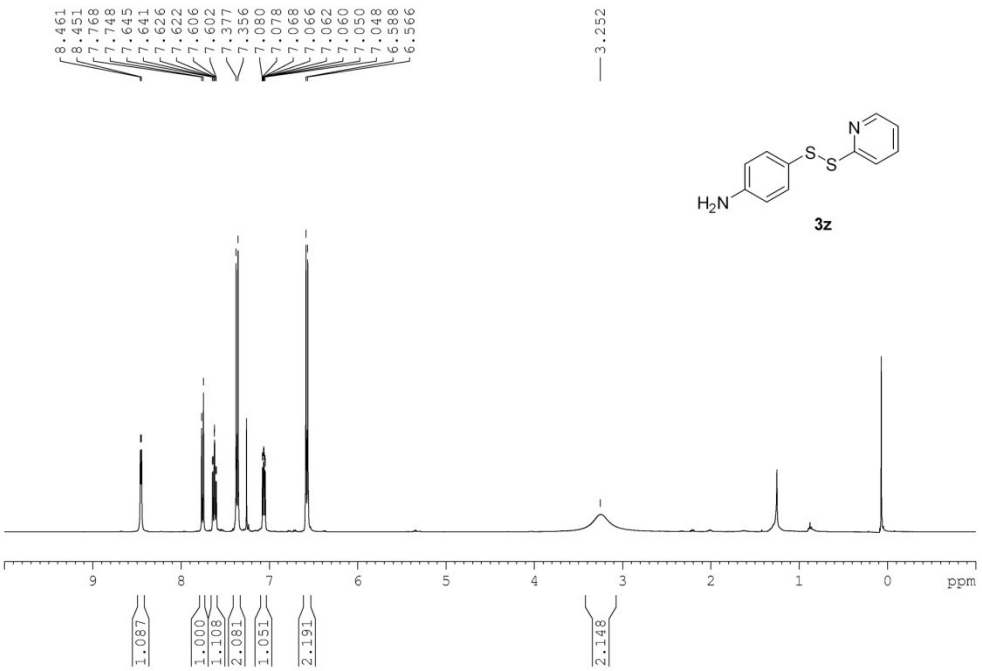

147.096
137.546
134.427
133.114
129.745
129.490
125.279
115.475
21.138
S
S
H_2N
3w
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

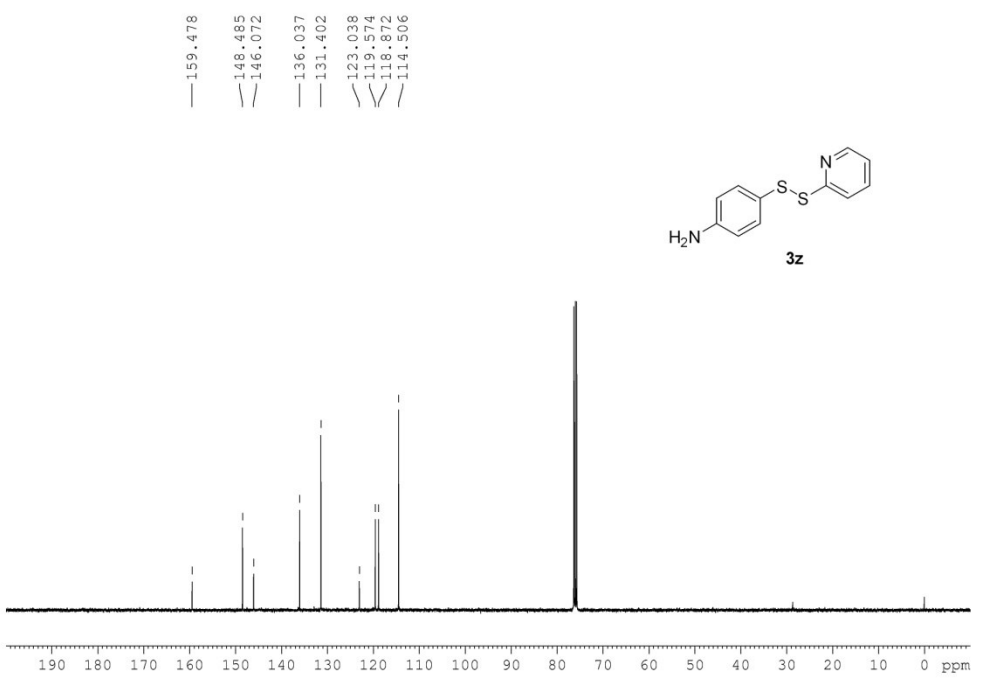

8.161
8.138
7.685
7.662
7.317
7.295
6.589
6.567
3.820
NO2
S
S
H2N
3x
9
8
7
6
5
4
3
2
1
0
ppm
2.000
2.013
2.018
2.054
2.057


147.847
147.260
146.228
133.324
126.492
124.047
122.979
115.570
NO2
S
S
H2N
3x
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.350
7.329
7.186
7.183
7.165
7.162
6.487
6.465
3.572
Cl
S
S
H2N
3y
9
8
7
6
5
4
3
2
1
0
ppm
2.000
4.146
2.050
2.069


147.396
136.440
133.319
133.242
130.089
129.101
124.436
115.528
Cl
S
S
H2N
3y
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


8.461
8.451
7.768
7.748
7.645
7.641
7.626
7.622
7.606
7.602
7.377
7.356
7.080
7.078
7.068
7.066
7.062
7.060
7.050
7.048
6.588
6.566
3.252
N
S
S
H2N
3z
9
8
7
6
5
4
3
2
1
0
ppm
1.087
1.000
1.108
2.081
1.051
2.191
2.148


159.478
148.485
146.072
136.037
131.402
123.038
119.574
118.872
114.506
N
S
S
H2N
3z
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm