Supporting Information

belonging to the paper

A Metalloradical Approach to 2*H*-Chromenes

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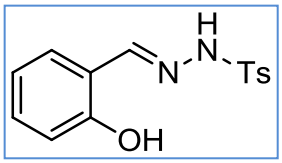
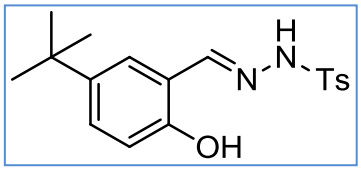
NMR Data

Salicyl tosylhydrazone (1a) [1]



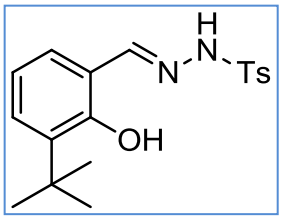
^{1}H NMR (500 MHz, DMSO-d6): δ 2.35 (s, 3H), 6.85 (m, 3H), 7.23 (dt, *J* = 6.5 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.48 (dd, *J* = 6.0 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 2H), 8.20 (s, 1H), 10.24 (s, 1H), 11.50 (s, 1H). **^{13}C NMR (125 MHz, DMSO-d6):** δ 21.47, 116.66, 119.50, 119.89, 127.65, 127.93, 130.23, 131.91, 136.30, 144.09, 146.58, 156.97.

5-*tert-butyl* salicyl tosylhydrazone (1b)



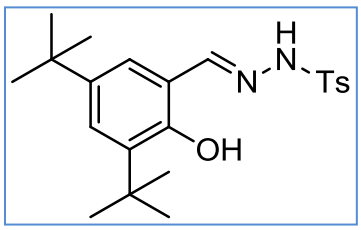
^{1}H NMR (500 MHz, DMSO-d6): δ 1.22 (s, , 9H), 2.36 (s, 3H), 6.80 (d, *J* = 8.6 , 1H), 7.28 (dd, *J* = 6.2 Hz, 1H), 7.42 (d, *J* = 8.2 Hz, 3H), 7.76 (d, *J* = 8.2 Hz, 2H), 8.16 (s, 1H), 10.08 (s, 1H), 11.47 (s, 1H). **^{13}C NMR (125 MHz, DMSO-d6):** δ 21.47, 31.62, 34.17, 116.34, 118.46, 124.61, 127.68, 129.14, 130.18, 136.19, 141.94, 144.13, 147.59, 154.89. MS (EI): m/z=346 (M^+); HR-MS (EI): m/z = 346.1481, calcd. for $C_{18}H_{22}N_2O_3S$ (M^+): 346.1351. (C, H, N)-analysis: C = 62.39; H = 6.37; N = 8.08; calcd. for $C_{18}H_{22}N_2O_3S$: C = 62.40; H = 6.40; N = 8.09.

3-*tert-butyl* salicyl tosylhydrazone (1c)



^{1}H NMR (500 MHz, DMSO-d6): δ 1.35 (s, 9H), 2.35 (s, 3H), 6.83 (t, *J* = Hz, 1H), 7.20 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.25 (dd, *J* = 7.5, 1 Hz, 1H), 7.43 (d, *J* = 8.1,1H), 7.77 (d, *J* = 8.3 Hz, 1H), 8.14 (s, 1H), 11.17 (s, 1H), 11.76 (s, 1H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 21.47, 29.64, 34.92, 117.90, 119.49, 127.59, 129.18, 129.98, 130.38, 135.75, 136.74, 144.50, 151.96, 156.72. MS (EI): m/z = 346 (M^+); HR-MS (EI): m/z = 346.1377, calcd. for $C_{18}H_{22}N_2O_3S$ (M^+): 346.1351. (C, H, N)-analysis: C = 62.43; H = 6.36; N = 8.06; calcd. for $C_{18}H_{22}N_2O_3S$: C = 62.40; H = 6.40; N = 8.09.

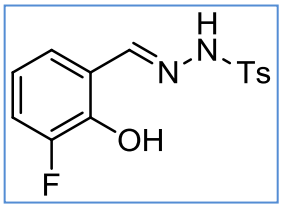
3,5-*di-tert-butyl* salicyl tosylhydrazone (1d)



^{1}H NMR (500 MHz, DMSO-d6): δ 1.22 (s, 9H), 1.36 (s, 9H), 2.35 (s, 3H), 7.17 (s, 1H), 7.26 (s, 1H), 7.43(d, J = 7.9 Hz,1H), 7.76 (d, *J* = 8.1 Hz), 8.14 (s, 1H), 11.01 (s, 1H), 11.72 (s, 1H). **^{13}C NMR (125 MHz, DMSO-d6):** δ 21.46, 29.70, 31.68, 34.33, 35.08, 117.22, 126.13, 126.40, 127.58, 130.34, 135.76, 135.99, 141.18, 144.44, 152.45, 154.50. MS (EI): m/z=402 (M^+); HR-MS (EI): m/z = 402.2122,

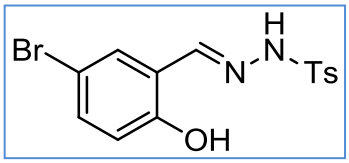
calcd. for $C_{22}H_{30}N_2O_3S$ (M^+): 402.1977. (C, H, N)-analysis: C = 65.64; H = 7.52; N = 6.94; calcd. for $C_{22}H_{30}N_2O_3S$: C = 65.64; H = 7.51; N=6.96.

3-*fluoro* salicyl tosylhydrazone (1e)



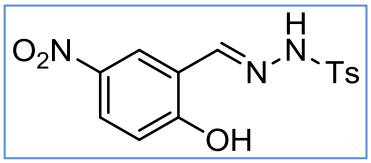
^{1}H NMR (500 MHz, DMSO-d6): δ 2.34 (s, 3H), 6.83 (q, *J* = 7.3, 6.7 Hz, 1H), 7.21 (t, *J* = 9.5 Hz, 1H), 7.32 (d, *J* = 7.8 Hz, 1H), 7.42 (d, *J* = 7.5 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 2H), 8.23 (s, 1H), 10.46 (s, 1H), 11.69 (s, 1H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 21.44, 117.81 (d, *J* = 18 Hz), 119.91 (d, *J* = 7.0), 122.41 (*J* = 3.4 Hz), 123.29 (d, *J* = 3.1 Hz), 127.63, 130.28, 136.22, 144.20, 144.65 (d, *J* = 14.6 Hz), 145.59 (d, *J* = 4.0 Hz), 150.71, 152.62. MS (EI): m/z=308 (M^+); HR-MS (EI): m/z = 308.0646, calcd. for $C_{14}H_{13}FN_2O_3S$ (M^+): 308.0631. (C, H, N)-analysis: C = 54.55; H = 4.18; N = 9.09; calcd. for $C_{14}H_{13}FN_2O_3S$: C = 54.54; H = 4.25; N = 9.09.

5-*bromo* salicyl tosylhydrazone (1f) [1]



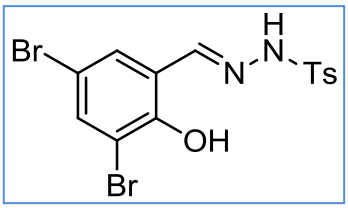
^{1}H NMR (500 MHz, DMSO-d6): δ 2.32 (s, 3H), 6.85 (d, *J* = 8.5 Hz, 1H), 7.35 (d, *J* = 8.6 Hz, 1H), 7.39 (d, *J* = 6.9, 2H), 7.61 (s, 1H), 7.78 (d, *J* = 7.1, 2H), 8.17 (s, 1H), 10.49 (s, 1H), 11.65 (s, 1H). **^{13}C NMR (125 MHz, DMSO-d6):** δ 21.45, 111.12, 118.96, 122.00, 127.61, 129.09, 130.23, 134.09, 136.36, 144.10, 156.07.

5-*bromo* salicyl tosylhydrazone (1g) [1]



^{1}H NMR (500 MHz, DMSO-d6): δ 2.23 (s, 3H), 6.96 (m, 1H), 7.33 (m, 2H), 7.76 (s, 2H, br), 8.01 (m, 1H), 8.22 (s, 1H), 8.32 (d, *J* = 11.4 Hz), 11.80 (s, 2H, br). **^{13}C NMR (500 MHz, DMSO-d6):** δ 21.28, 117.14 (d, *J* = 7.3 Hz), 120.48 (d, *J* = 15.7 Hz), 122.65 (d, *J* = 16.1 Hz), 126.87 (d, *J* = 13.7 Hz), 127.53, 130.14 (d, *J* = 7.5 Hz), 136.13 (d, *J* = 5.1 Hz), 140.27 (d, *J* = 5.9 Hz), 142.89, 143.14, 144.12 (d, *J* = 7.0 Hz), 162.24.

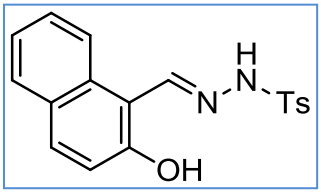
3,5-*di-tert-butyl* salicyl tosylhydrazone (1h)



^{1}H NMR (500 MHz, **DMSO-d6**): δ 2.32 (s, 3H), 7.41 (d, *J* = 7.8 Hz, 2H), 7.62 (s, 1H. br), 7.69 (s, 1H, br), 7.77 (*J* = 7.9 Hz, 2H), 8.13 (s, 1H), 11.16 (s, 1H), 12.11 (s, 1H). **^{13}C NMR (125 MHz, DMSO-d6**): δ 21.48, 111.37, 112.00, 121.76, 127.55, 130.44, 131.59, 135.84, 136.11, 144.52, 146.93, 153.16. MS (EI): m/z = 447 (M^+); HR-MS (EI): m/z = 447.8925, calcd. for $C_{14}H_{12}Br_2N_2O_3S$ (M^+):

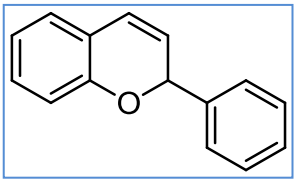
447.8915. (C, H, N)-analysis: C = 37.56; H = 2.67; N = 6.24; calcd. for $C_{14}H_{12}Br_2N_2O_3S$: C = 37.52; H = 2.70; N = 6.25.

2-*hydroxy* napthyl tosylhydrazone (1i) [1]



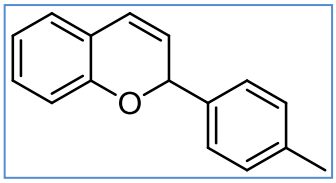
^{1}H NMR (400 MHz, $CDCl_3$): δ 2.30 (s, 3H), 7.19 (d, *J* = 8.9 Hz, 1H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.49 (t, *J* = 7.7 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.84 (d, *J* = 9.0 Hz, 2H), 8.39 (d, *J* = 8.6 Hz, 1H), 8.90 (s, 1H), 11.27 (s, 1H), 11.65 (s, 1H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 21.43, 109.70, 118.75, 122.85, 123.95, 127.84, 128.18, 128.39, 129.16, 130.26, 131.62, 133.22, 136.17, 144.24, 147.32, 157.57.

2-phenyl-*2H*-chromene (3a) [2]



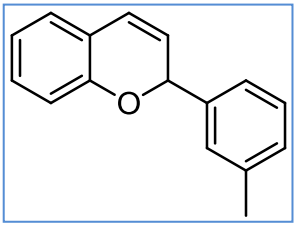
^{1}H NMR (400 MHz, $CDCl_3$): δ 5.83 (dd, *J* = 9.8, 3.4 Hz, 1H), 5.94 (dd, *J* = 3.2, 2.0 Hz, 1H), 6.56 (dd, *J* = 9.8, 1.7 Hz, 1H), 6.81 (d, *J* = 8.1 Hz, 1H), 6.89 (td, *J* = 7.4, 1.1 Hz, 1H), 7.04 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.14 (td, *J* = 7.8, 1.7 Hz, 1H), 7.43 – 7.32 (m, 3H), 7.48 (dd, *J* = 8.1, 1.3 Hz, 2H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 77.18, 116.00, 121.19, 121.32, 124.02, 124.88, 126.60, 127.03, 128.38, 128.68, 129.48, 140.84, 153.17.

2-(*p*-tolyl)-*2H*-chromene (3b) [2]



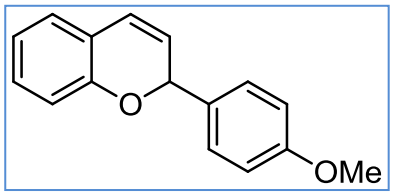
^{1}H NMR (500 MHz, $CDCl_3$): δ 2.39 (s, 3H), 5.83 (dd, *J* = 9.8, 3.4 Hz, 1H), 5.93 (dd, *J* = 3.2, 2.0 Hz, 1H), 6.57 (dd, *J* = 9.8, 1.4 Hz, 1H), 6.82 (d, *J* = 8.1 Hz, 1H), 6.90 (td, *J* = 7.4, 1.1 Hz, 1H), 7.05 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.15 (td, *J* = 7.8, 1.7 Hz, 1H), 7.22 (d, *J* = 7.8 Hz, 2H), 7.39 (d, *J* = 8.1 Hz, 2H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 21.23, 77.27, 116.05, 121.12, 121.39, 123.96, 124.99, 126.57, 127.13, 129.36, 129.44, 137.87, 138.25, 153.21.

2-*(m-tolyl)-2H*-chromene (3c)



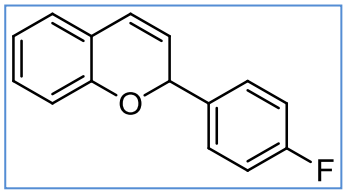
^{1}H NMR (300 MHz, $CDCl_3$): δ 2.28 (s, 3H), 5.71 (dd, *J* = 9.8, 3.3 Hz, 1H), 5.83 – 5.80 (m, 1H), 6.45 (dd, *J* = 9.9, 1.8 Hz, 1H), 6.72 (d, *J* = 8.1 Hz, 1H), 6.79 (td, *J* = 7.4, 0.9 Hz, 1H), 6.94 (dd, *J* = 7.4, 1.5 Hz, 1H), 7.03 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.09 – 7.04 (m, 1H), 7.18 (m, 3H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 21.47, 77.32, 115.97, 121.14, 121.31, 123.94, 124.15, 125.00, 126.59, 127.77, 128.59, 129.16, 129.44, 138.39, 140.79, 153.23. MS (EI): m/z=222 (M^+); HR-MS (EI): m/z= 222.1009.

2-(4-methoxyphenyl)-*2H*-chromene (3d) [2]



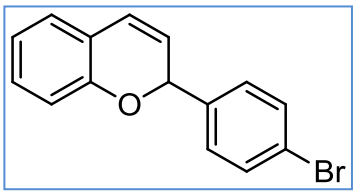
^{1}H NMR (300 MHz, $CDCl_3$): δ 3.83 (s, 3H), 5.81 (dd, *J* = 9.8, 3.4 Hz, 1H), 5.90 (dd, *J* = 3.3, 1.9 Hz, 1H), 6.60 – 6.50 (m, 1H), 6.78 (d, *J* = 8.1 Hz, 1H), 6.89 (td, *J* = 7.4, 1.1 Hz, 1H), 6.94 – 6.91 (m, 2H), 7.04 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.12 (td, *J* = 7.9, 1.6 Hz, 1H), 7.43 – 7.37 (m, 2H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 55.33, 77.25, 114.01, 116.07, 121.10, 121.38, 124.04, 124.93, 126.53, 128.69, 129.43, 132.86, 153.08, 159.73.

2-(4-fluorophenyl)-2H-chromene **(3e)** [2a]



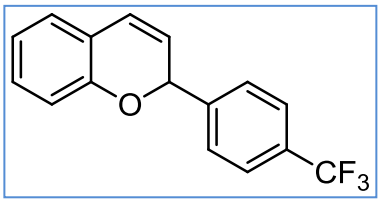
^{1}H NMR (500 MHz, $CDCl_3$): δ 5.81 (dd, *J* = 9.8, 3.4 Hz, 1H), 5.93 (s, 1H, br), 6.58 (d, *J* = 9.8 Hz, 1H), 6.80 (d, *J* = 8.0 Hz, 1H), 6.90 (t, *J* = 7.4 Hz, 1H), 7.10 – 7.02 (m, 3H), 7.18 – 7.11 (m, 1H), 7.46 (dd, *J* = 8.5, 5.4 Hz, 2H) . **^{13}C NMR (125 MHz, $CDCl_3$):** δ 76.40, 115.44, 115.62, 116.05, 121.24, 121.32, 124.30, 124.52, 126.62, 126.65, 128.90, 128.94, 128.97, 129.02, 129.55, 129.57, 129.59, 129.60, 136.56, 136.58, 152.90, 161.75, 163.71.

2-(4-bromophenyl)-*2H*-chromene (3f) [2]



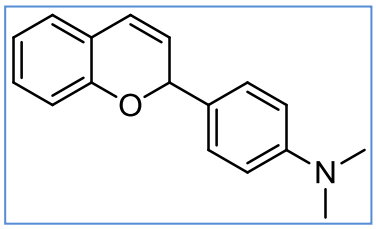
^{1}H NMR (500 MHz, $CDCl_3$): δ 5.75 (dd, *J* =10.0, 3.2 Hz, 1H), 5.85–5.86 (m, 1H), 6.53 (dd, *J* = 10.0, 2.0 Hz, 1H), 6.77 (d, *J* = 8.4 Hz, 1H), 6.86 (t, J = 7.2 Hz, 1H), 7.00 (dd, *J* = 7.2, 2.0 Hz, 1H), 7.10 (t, *J* = 8.0 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 2H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ 76.2, 116.0, 121.1, 121.3, 122.3, 124.1, 124.4, 126.6, 128.7, 129.6, 131.7, 139.7, 152.8.

2-(4-(trifluoromethyl)phenyl)-*2H*-chromene (3g) [2a]



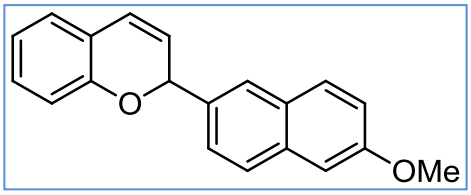
^{1}H NMR (500 MHz, $CDCl_3$): δ 5.71 (dd, *J* = 9.8, 3.5 Hz, 1H), 5.88 (s, 1H, br), 6.48 (dd, *J* = 9.8, 1.6 Hz, 1H), 6.73 (d, *J* = 8.1 Hz, 1H), 6.81 (td, *J* = 7.4, 1.0 Hz, 1H), 6.94 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.05 (td, *J* = 7.9, 1.6 Hz, 1H), 7.48 (d, *J* = 8.2 Hz, 2H), 7.54 (d, *J* = 8.3 Hz, 2H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 76.24, 116.04, 121.15, 121.56, 123.93, 124.58, 125.61, 125.64, 125.67, 125.70, 126.80, 127.15, 129.76, 144.75, 152.86.

4-(*2H*-chromen-2-yl)-N,N-dimethylaniline (3h) [3]



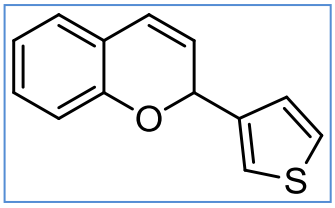
^{1}H NMR (500 MHz, $CDCl_3$): δ 2.87 (s, 3H), 5.71 (dd, *J* = 9.8, 3.5 Hz, 1H), 5.75 (dd, *J* = 3.4, 1.7 Hz, 1H), 6.46 (dd, *J* = 9.7, 1.3 Hz, 1H), 6.65 (m, 3H), 6.76 (td, *J* = 7.4, 1.1 Hz, 1H), 6.93 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.00 (td, *J* = 7.8, 1.7 Hz, 1H), 7.28 – 7.21 (m, 2H). **^{13}C NMR (125 MHz, $CDCl_3$):** 40.57, 77.18, 112.40, 116.12, 120.86, 121.51, 123.82, 125.21, 126.42, 128.55, 129.27, 153.25. MS (EI): m/z=251 (M^+); HR-MS (EI): m/z = 251.1345, calcd. for $C_{17}H_{17}NO$ (M^+): 251.1310.

2-(6-methoxynaphthalen-2-yl)-*2H*-chromene (3i)



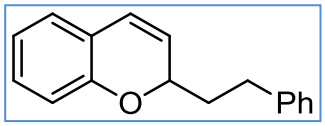
^{1}H NMR (500 MHz, $CDCl_3$): δ 3.95 (s, 3H), 5.89 (dd, *J* = 9.8, 3.4 Hz, 1H), 6.08 (dd, *J* = 3.2, 2.0 Hz, 1H), 6.62 (dd, *J* = 9.9, 1.7 Hz, 1H), 6.82 (d, *J* = 8.1 Hz, 1H), 6.90 (td, *J* = 7.4, 1.1 Hz, 1H), 7.06 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.13 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.20 – 7.15 (m, 2H), 7.59 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.76 (t, *J* = 9.0 Hz, 2H), 7.85 – 7.81 (m, 1H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 55.33, 77.35, 105.68, 116.04, 119.05, 121.17, 121.38, 124.18, 124.84, 125.61, 126.07, 126.62, 127.44, 128.64, 129.49, 129.68, 134.55, 135.79, 157.97. MS (EI): 288; HR-MS (EI): m/z=288.1181, calcd. for $C_{20}H_{16}O_2$ (M^+): 288.1150. (C, H, N)-analysis: C=83.35; H=5.55; calcd. for $C_{20}H_{16}O_2$: C=83.31; H=5.59.

2-(thiophen-3-yl)-*2H*-chromene (3j) [4]



^{1}H NMR (500 MHz, $CDCl_3$): δ 5.90 (dd, *J* = 9.8, 3.7 Hz, 1H), 6.00 (dd, *J* = 3.5, 1.5 Hz, 1H), 6.57 (d, *J* = 9.8 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 1H), 6.90 (td, *J* = 7.4, 1.0 Hz, 1H), 7.04 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.14 (td, *J* = 7.9, 1.6 Hz, 1H), 7.22 – 7.17 (m, 1H), 7.36 – 7.31 (m, 2H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 72.47, 116.18, 121.29, 121.55, 123.19, 124.19, 124.35, 126.38, 126.52, 126.61, 129.45, 141.73, 152.99.

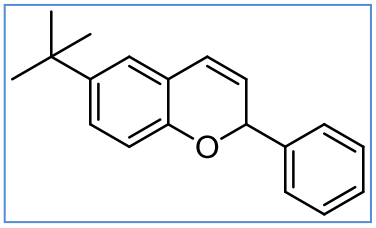
2-(3-phenylpropyl)-*2H*-chromene (3k) [5]



^{1}H NMR (500 MHz, $CDCl_3$): δ 1.97 (dddd, *J* = 14.1, 9.7, 6.9, 4.5 Hz, 1H), 2.31 – 2.07 (m, 1H), 3.00 – 2.70 (m, 2H) 4.89 (dt, *J* = 4.9, 3.1 Hz, 1H), 5.71 (dd, *J* = 9.8, 3.4 Hz, 1H), 6.44 (dd, *J* = 9.8, 1.2 Hz, 1H), 6.84 (d, *J* = 8.0 Hz, 1H), 6.88 (td, *J* = 7.4, 1.1 Hz, 1H), 6.99 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.14 (td, *J* = 7.8, 1.7 Hz, 1H), 7.27 – 7.19 (m, 3H),

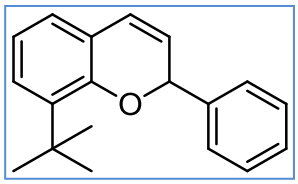
7.20 (d, *J* = 7.4 Hz, 2H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 31.16, 36.93, 74.16, 77.24, 116.04, 121.05, 122.01, 124.21, 125.66, 125.90, 126.49, 128.41, 128.55, 129.17, 153.34.

6-(tert-butyl)-2-phenyl-*2H*-chromene (3m) [6]



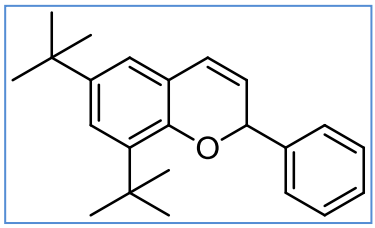
^{1}H NMR (500 MHz, $CDCl_3$): δ 1.33 (s, 9H), 5.82 (dd, *J* = 9.8, 4.4 Hz, 1H), 5.97 – 5.90 (m, 1H), 6.56 (d, *J* = 9.8 Hz, 1H), 6.77 (d, *J* = 8.4 Hz, 1H), 7.09 – 6.99 (m, 1H), 7.18 (dt, *J* = 8.4, 1.8 Hz, 1H), 7.38 – 7.34 (m, 1H), 7.44 – 7.38 (m, 2H), 7.53 – 7.47 (m, 2H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 31.49, 34.10, 77.20, 115.34, 120.62, 123.58, 124.48, 124.76, 126.36, 127.04, 128.29, 128.65, 141.10, 143.92, 150.93. MS (EI): 264.

8-(tert-butyl)-2-phenyl-*2H*-chromene (3n)



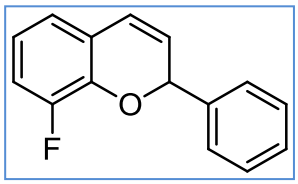
^{1}H NMR (500 MHz, $CDCl_3$): δ 1.33 (s, 9H), 5.82 (dd, *J* = 9.7, 3.1 Hz, 1H), 5.96 – 5.90 (m, 1H), 6.58 (dd, *J* = 9.7, 2.0 Hz, 1H), 6.89 (t, *J* = 7.6 Hz, 1H), 6.97 (dd, *J* = 7.3, 1.5 Hz, 1H), 7.20 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.44 – 7.36 (m, 3H), 7.54 – 7.48 (m, 2H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 29.73, 34.47, 76.99, 120.76, 122.30, 124.96, 125.01, 125.03, 126.96, 127.08, 128.23, 128.60, 137.56, 140.45, 151.65. MS (EI): 264; HR-MS (EI): m/z = 264.1564, calcd. For $C_{19}H_{20}O$ (M^+): 264.1514.

6,8-di-tert-butyl-2-phenyl-*2H*-chromene (3o) [7]



^{1}H NMR (500 MHz, $CDCl_3$): δ 1.25-1.25 (d, br, 18H), 5.67 (dd, *J* = 9.7, 2.8 Hz, 1H), 5.78 (s, 1H, br), 6.45 (dd, *J* = 9.7, 2.0 Hz, 1H), 6.90 – 6.81 (m, 1H), 7.12 (d, *J* = 2.2 Hz, 1H), 7.31 (t, *J* = 7.5 Hz, 2H), 7.40 (t, *J* = 8.0 Hz, 3H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 29.45, 29.81, 31.46, 31.57, 76.92, 121.55, 121.74, 124.04, 124.98, 125.50, 126.99, 128.05, 128.54, 136.63, 140.87, 143.03, 149.36, 156.86, 165.29.

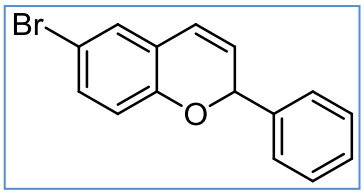
8-fluoro-2-phenyl-*2H*-chromene (3p)



^{1}H NMR (500 MHz, $CDCl_3$): δ 5.93 (dd, *J* = 9.9, 3.6 Hz, 1H), 6.01 (dd, *J* = 3.4, 1.8 Hz, 1H), 6.60 (dt, *J* = 9.9, 1.8 Hz, 1H), 6.82 (dd, *J* = 6.7, 3.6 Hz, 2H), 7.00 – 6.89 (m, 1H), 7.43 – 7.35 (m, 3H), 7.51 – 7.47 (m, 2H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 116.43, 116.58, 120.72, 120.77, 121.73, 121.75, 123.44, 123.47, 123.57, 123.59, 125.60,

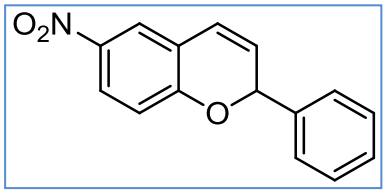
127.03, 128.58, 128.72, 140.08, 149.94, 151.89. MS (EI): 226; HR-MS (EI): m/z = 226.0946; calcd. for $C_{15}H_{11}OF$ (M^+): 226.0794.

6-bromo-2-phenyl-2H-chromene (3q) [2b]



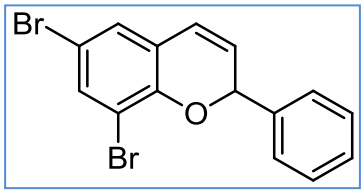
^{1}H NMR (500 MHz, $CDCl_3$): δ 5.75 (dd, *J* =10.0, 3.2 Hz, 1 H), 5.85–5.86 (m, 1 H), 6.53 (dd, *J* =10.0, 2.0 Hz, 1 H), 6.77 (d, *J* = 8.4 Hz, 1 H), 6.86 (t, *J* = 7.2 Hz, 1 H), 7.00 (dd, *J* = 7.2, 2.0 Hz, 1 H), 7.10 (t, *J* = 8.0 Hz, 1 H), 7.31 (d, *J* = 8.4 Hz, 2 H), 7.48 (d, *J* = 8.4 Hz, 2H); **^{13}C NMR (125 MHz, $CDCl_3$):** δ 76.2, 116.0, 121.1, 121.3, 122.3, 124.1, 124.4, 126.6, 128.7, 129.6, 131.7, 139.7, 152.8.

6-nitro-2-phenyl-*2H*-chromene (3r) [8]



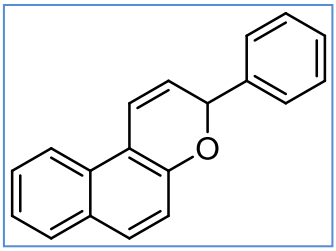
^{1}H NMR (500 MHz, $CDCl_3$): δ 5.94 (dd, *J* = 10, 3 Hz, 1H), 6.07 (dd, *J* = 3, 2 Hz, 1H), 6.59 (dd, *J* = 10, 2 Hz, 1H), 6.81 (d, *J* = 9 Hz, 1H), 7.35−7.46 (m, 5H), 7.93 (d, *J* = 3 Hz, 1H), 8.01 (dd, *J* = 9, 3 Hz, 1H). **^{13}C NMR (125 MHz, $CDCl_3$)**: δ 78.5, 116.3, 120.9, 122.3, 122.4, 125.6, 127.2, 129.0, 129.1, 139.5, 141.8, 158.6.

6,8-dibromo-2-phenyl-*2H*-chromene (3s)

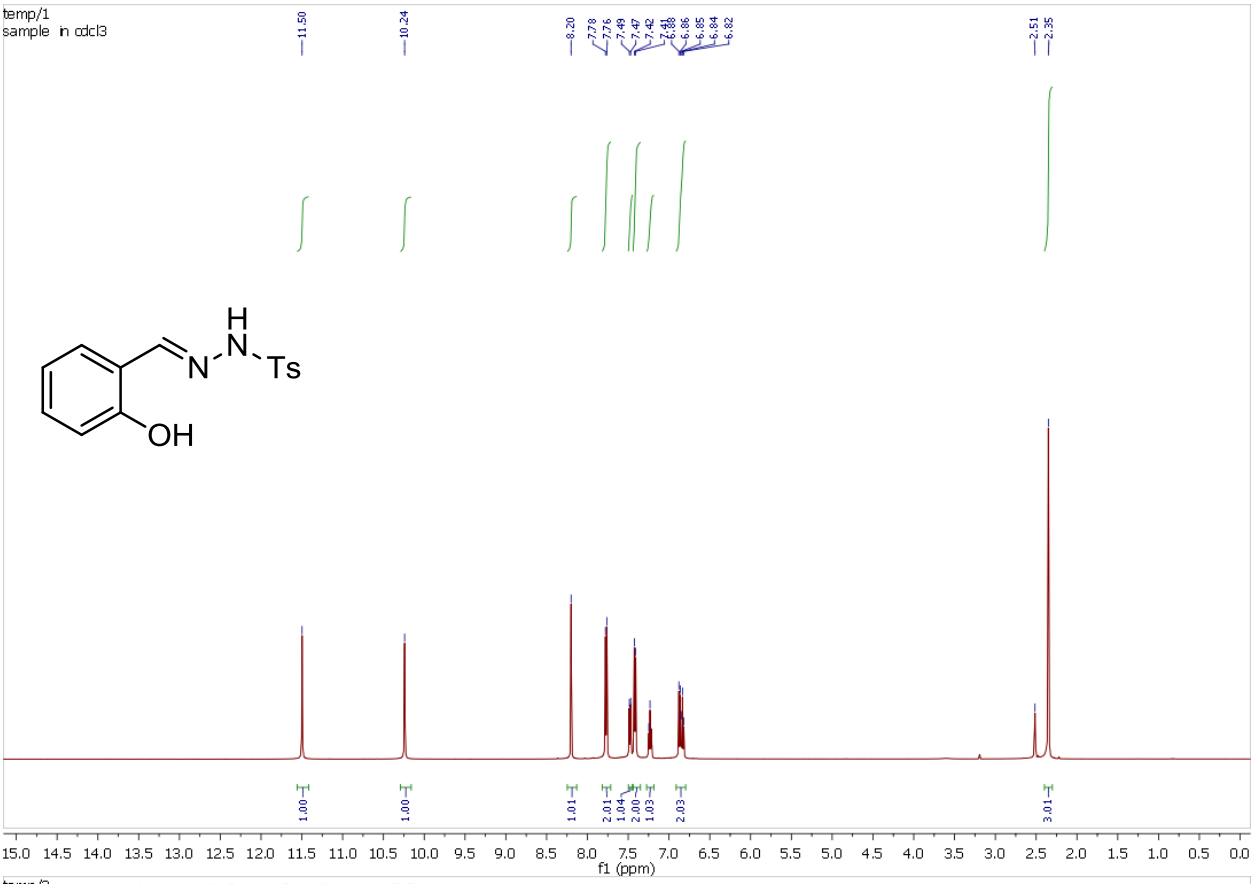


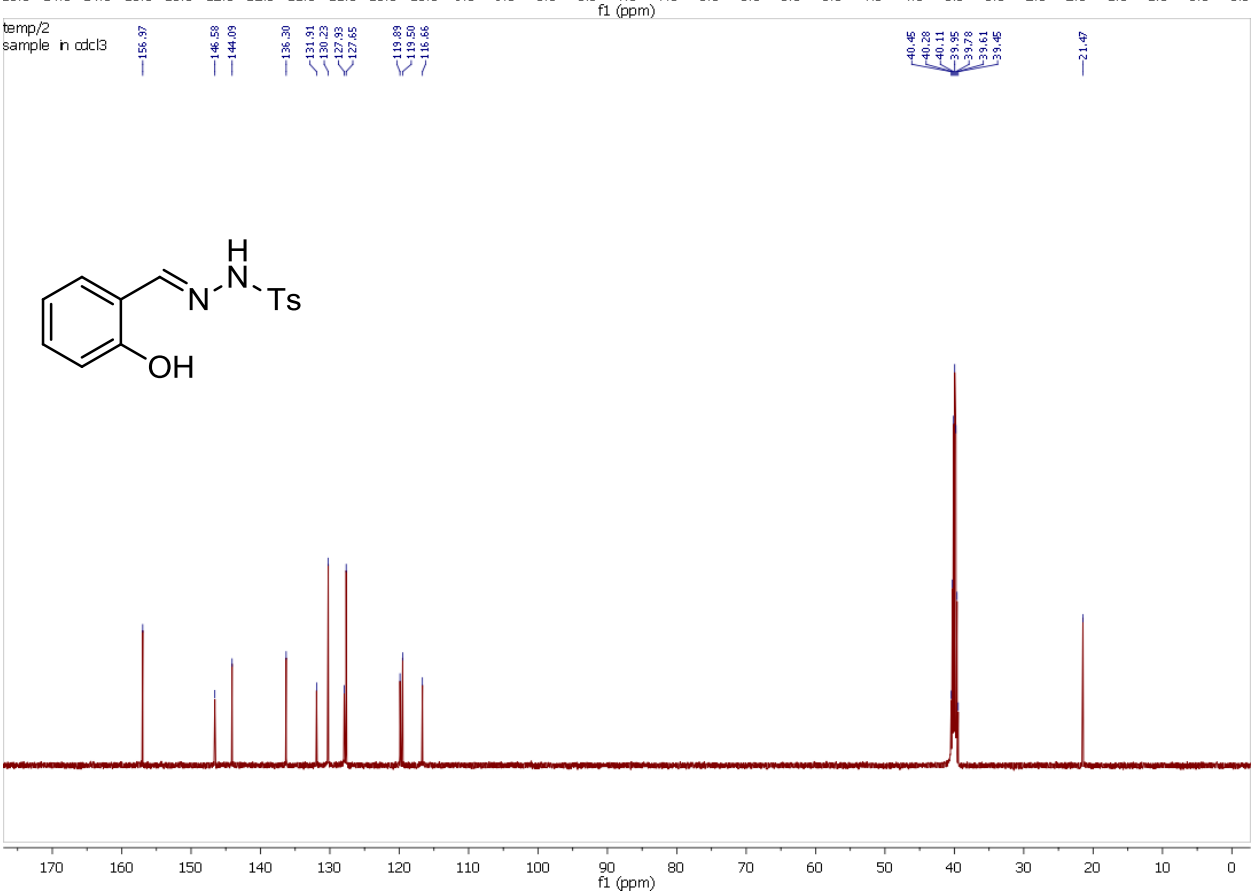
^{1}H NMR (500 MHz, $CDCl_3$): δ 6.00 (dd, *J* = 9.9, 3.8 Hz, 1H), 6.08 (dd, *J* = 3.7, 1.4 Hz, 1H), 6.49 (dd, *J* = 9.9, 1.6 Hz, 1H), 7.10 (d, *J* = 2.3 Hz, 1H), 7.42 – 7.36 (m, 3H), 7.49 – 7.44 (m, 3H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 77.44, 110.93, 113.08, 122.62, 124.09, 126.60, 126.64, 127.38, 128.25, 128.61, 128.74, 134.65, 139.71, 149.09. MS (EI): 366; HR-MS (EI): m/z=365.9116, calcd. For $C_{15}H_{10}Br_2O$ (M^+): 365.9078. (C, H, N)-analysis: C=48.98; H=2.73; calcd. for $C_{15}H_{10}Br_2O$: C=49.22; H=2.75.

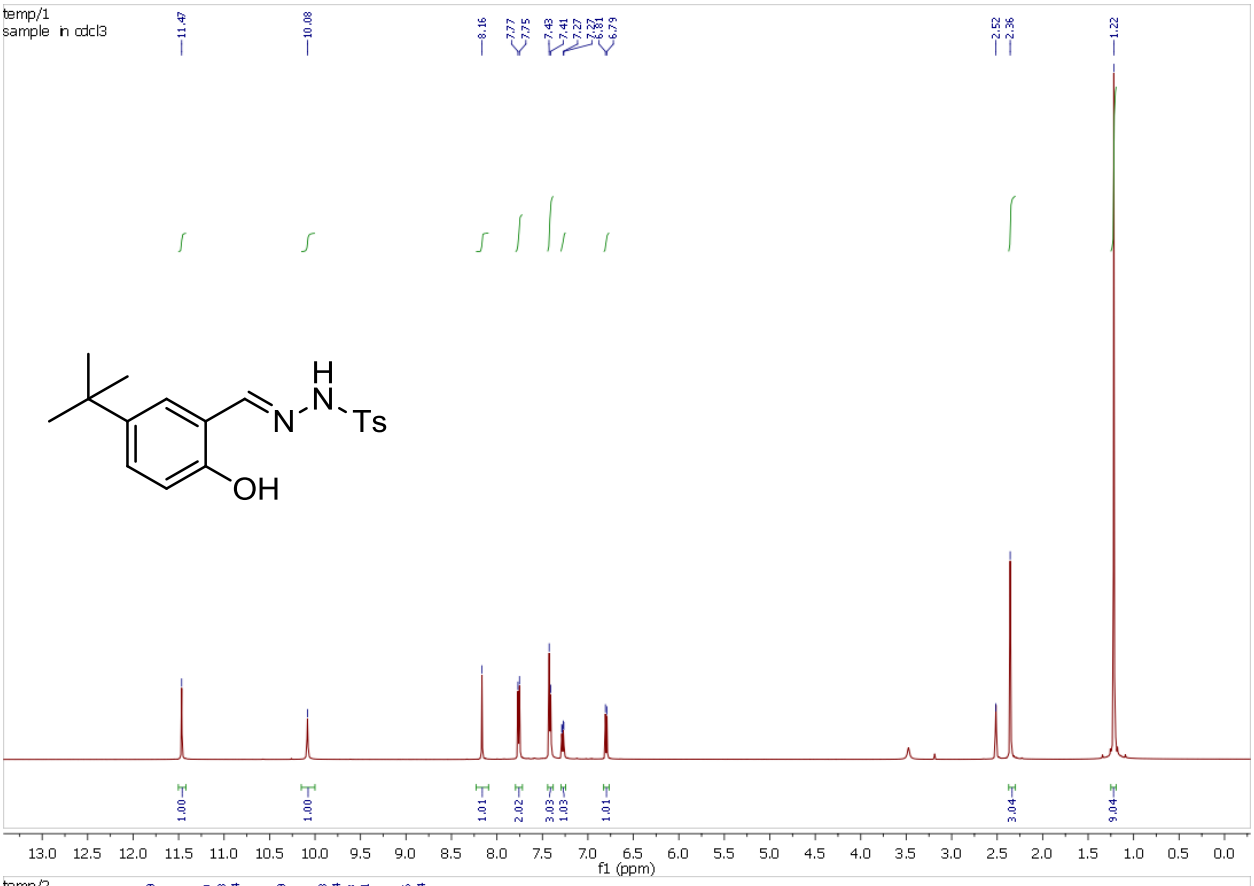
3-phenyl-3H-benzo[f]chromene (3t) [9]

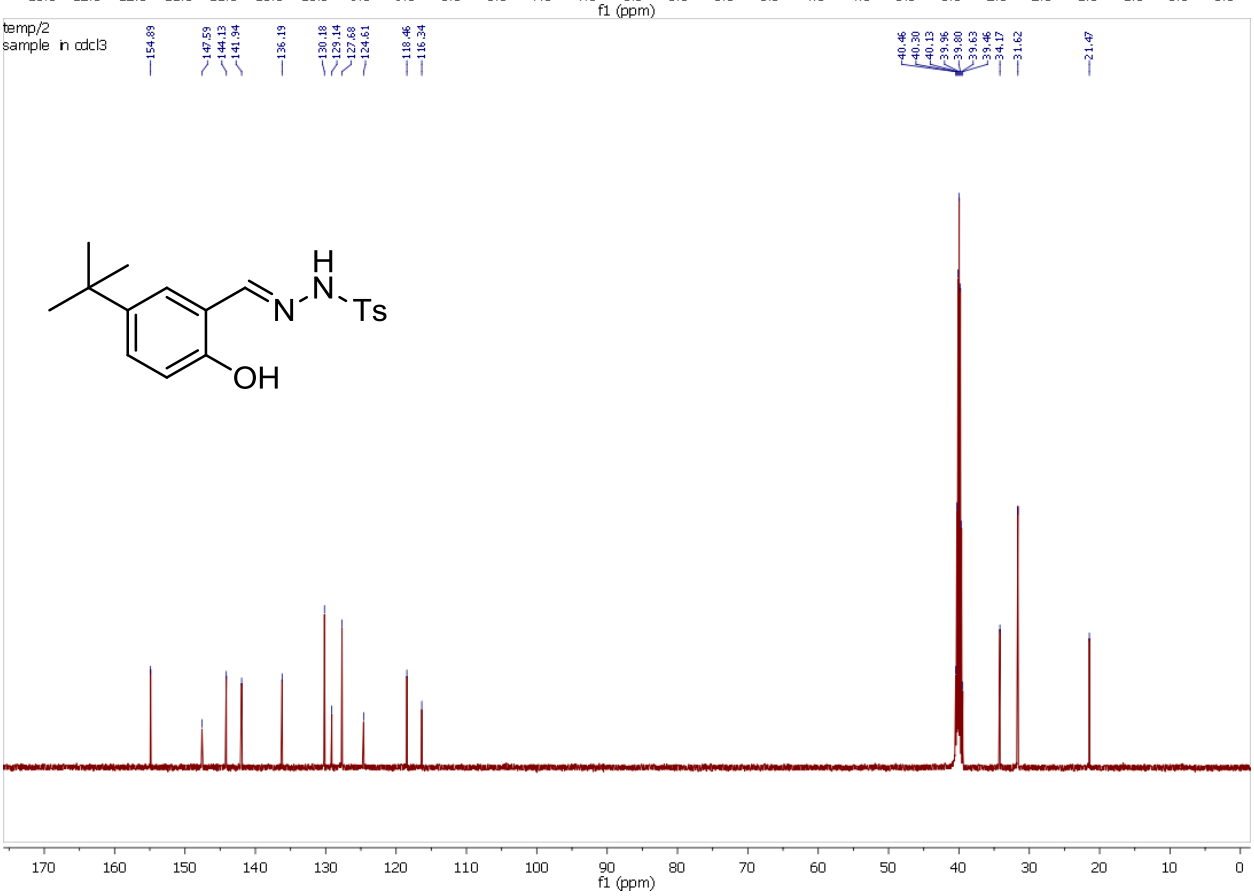


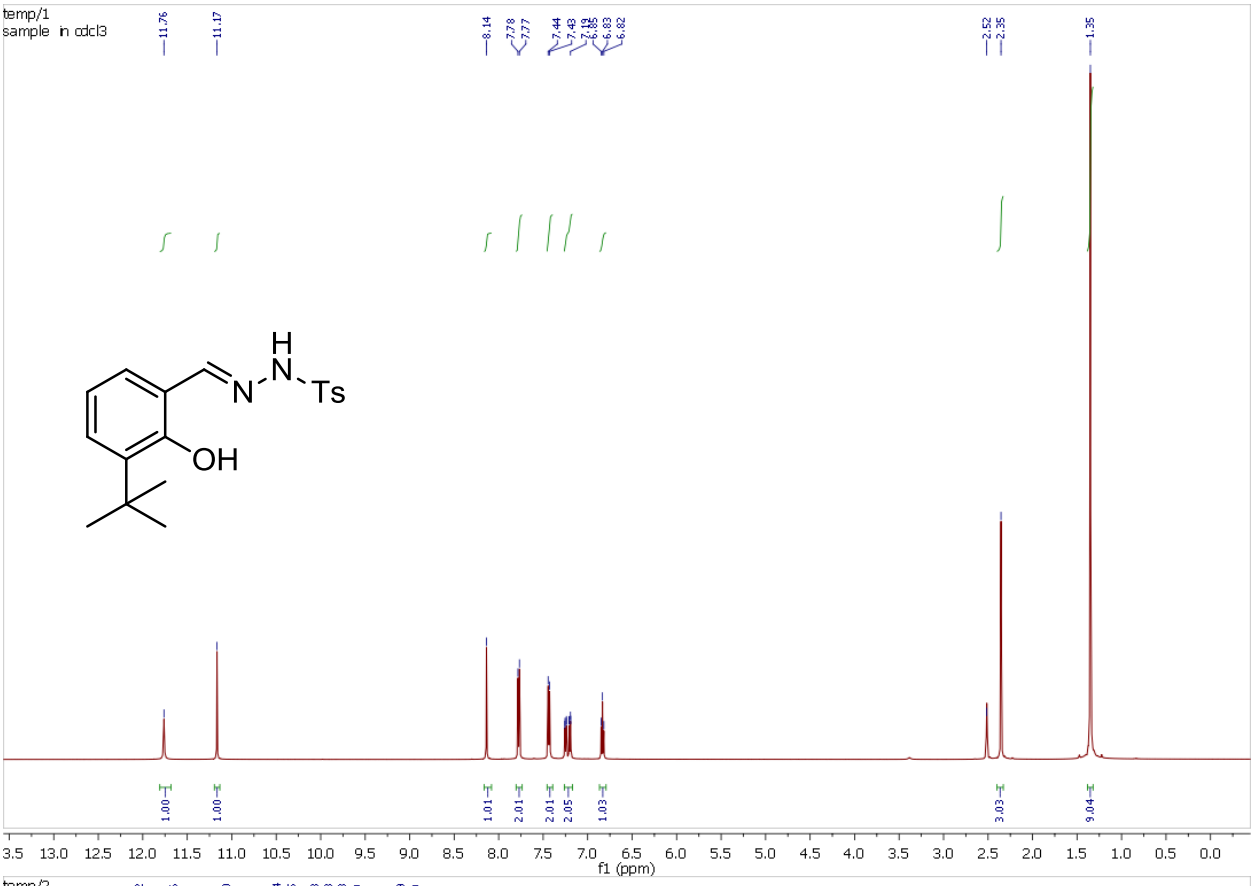
^{1}H NMR (500 MHz, $CDCl_3$): δ 5.95 (dd, *J* = 9.8, 3.7 Hz, 1H), 5.99 (m, 1H), 7.08 (d, *J* = 8.9 Hz, 1H), 7.39 – 7.32 (m, 5H), 7.51 (d, *J* = 7.0 Hz, 3H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.98 (d, *J* = 8.5 Hz, 1H). **^{13}C NMR (125 MHz, $CDCl_3$):** δ 76.93, 114.15, 118.01, 120.28, 121.27, 123.47, 123.61, 126.69, 127.12, 128.43, 128.57, 128.65, 129.38, 129.72, 129.88, 140.60, 151.31.

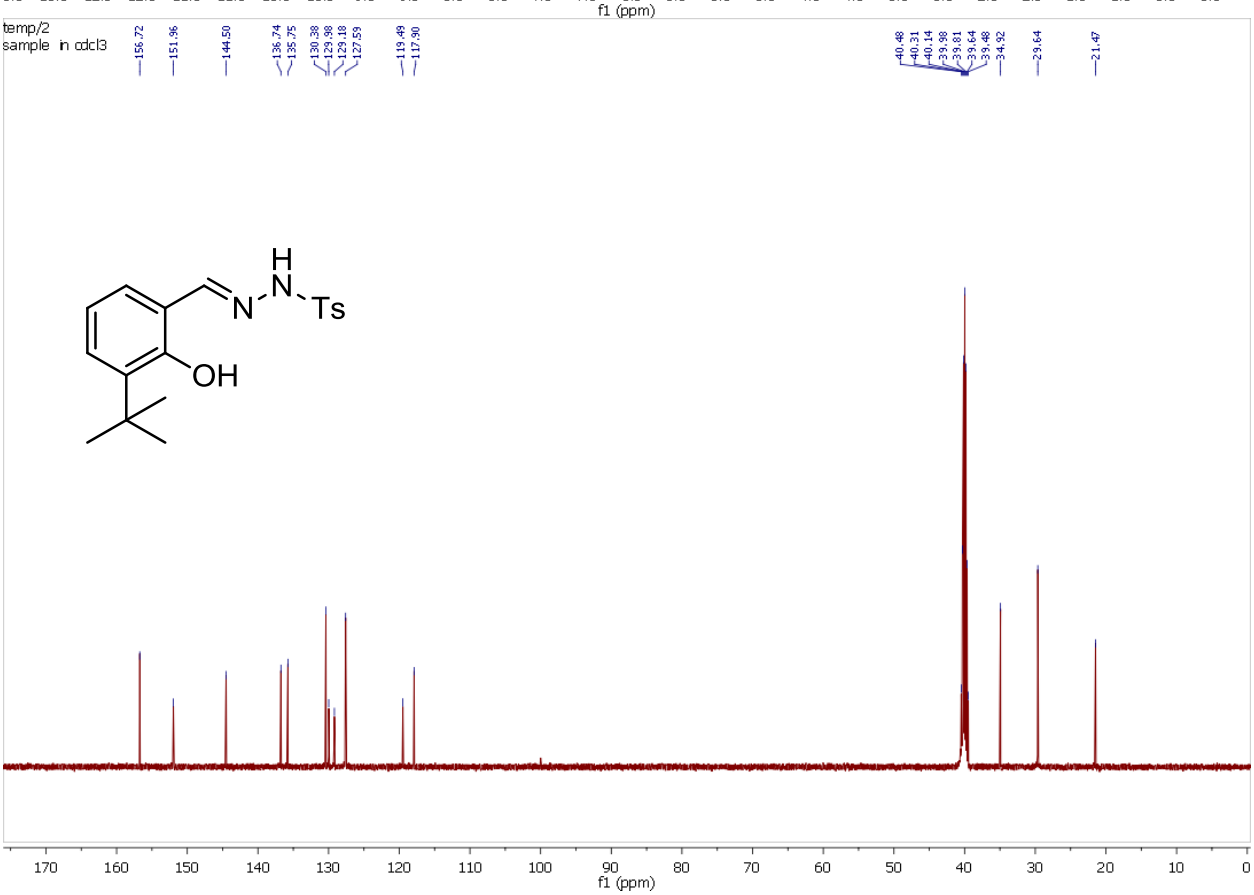

temp/1
sample in cdcl3
11.50
10.24
8.20
7.78
7.76
7.49
7.47
7.42
7.41
6.88
6.86
6.85
6.84
6.82
2.51
2.35
H
N
N
Ts
OH
1.00
1.00
1.01
2.01
1.04
2.00
1.03
2.03
3.01
15.0 14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

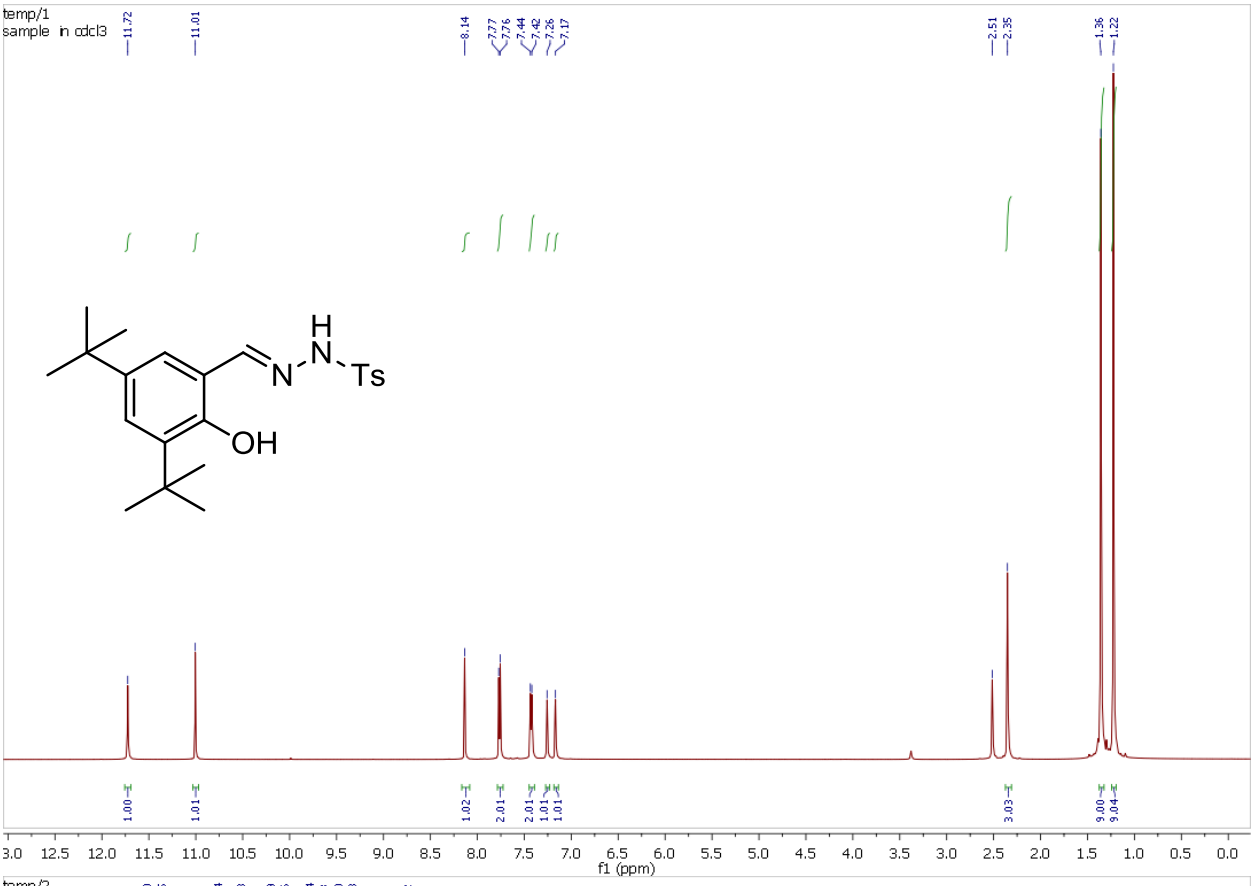

temp/2
sample in cdcl3
156.97
146.58
144.09
136.30
131.91
130.23
127.93
127.65
119.89
119.50
116.66
40.45
40.28
40.11
39.95
39.78
39.61
39.45
21.47
H
N
N
Ts
OH
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

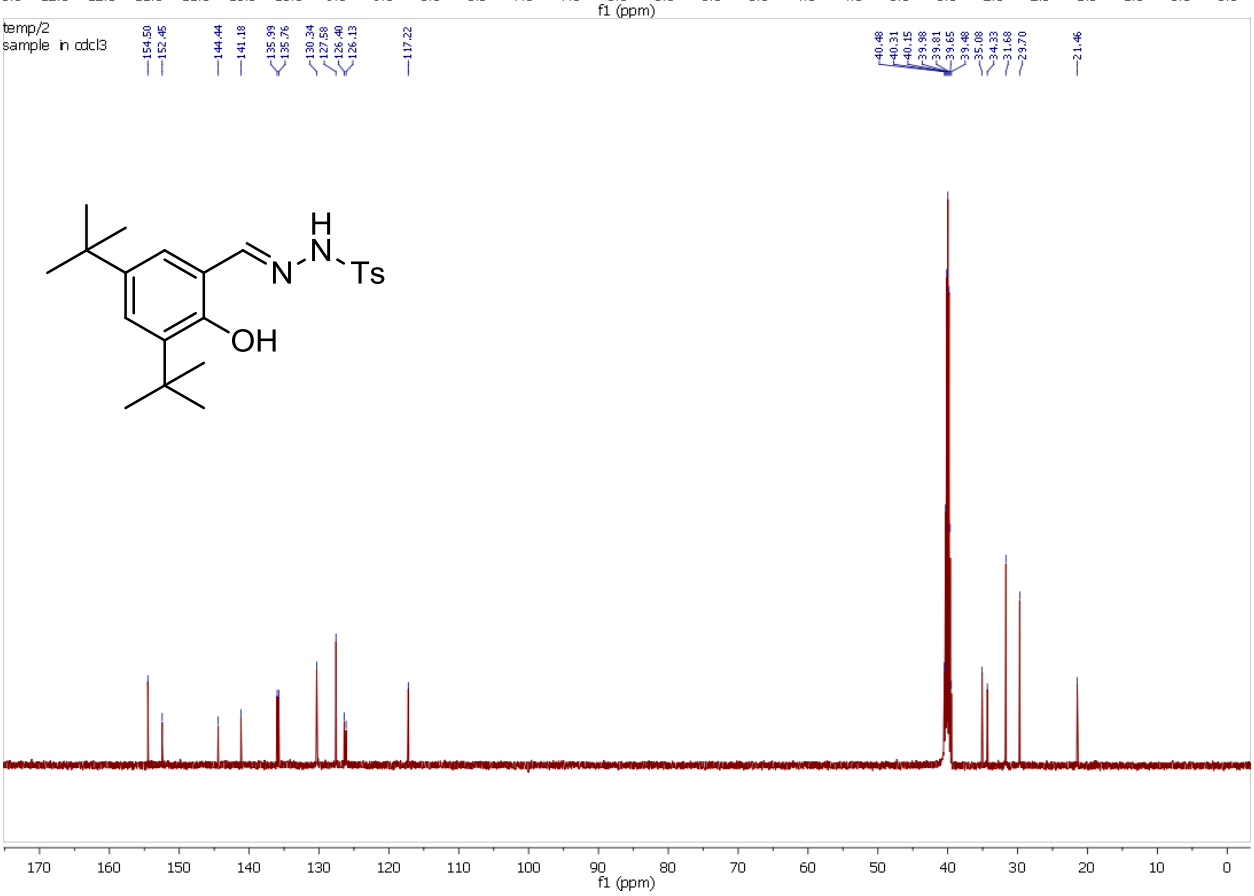

temp/1
sample in cdcl3
11.47
10.08
8.16
7.77
7.75
7.43
7.41
7.27
7.27
6.81
6.79
2.52
2.36
1.22
1.00
1.00
1.01
2.02
3.03
1.03
1.01
3.04
9.04
H
N
N
Ts
OH
f1 (ppm)

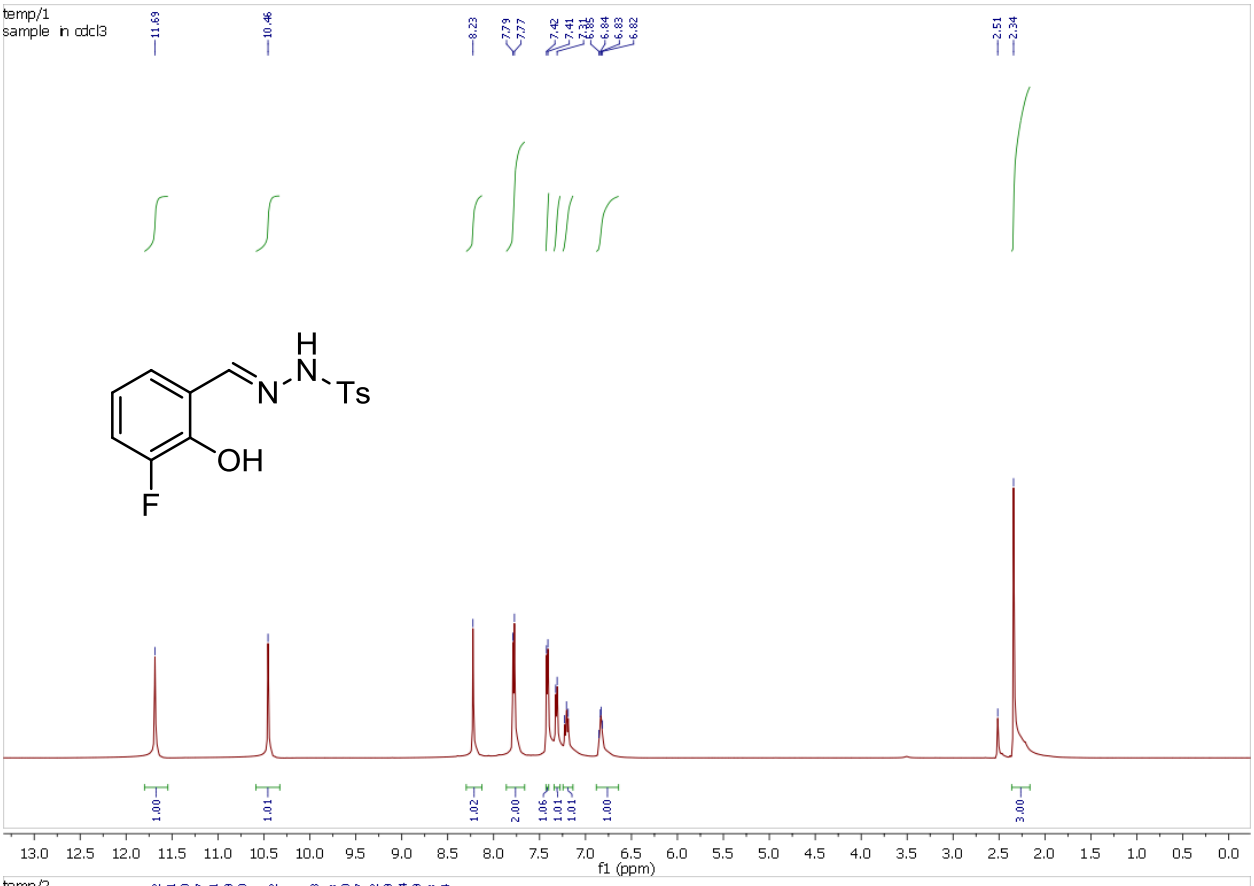

temp/2
sample in cdcl3
154.89
147.59
144.13
141.34
136.19
130.18
129.14
127.68
124.61
118.46
116.34
40.46
40.30
40.13
39.96
39.80
39.63
39.46
34.17
31.62
21.47
H
N
N
Ts
OH
f1 (ppm)

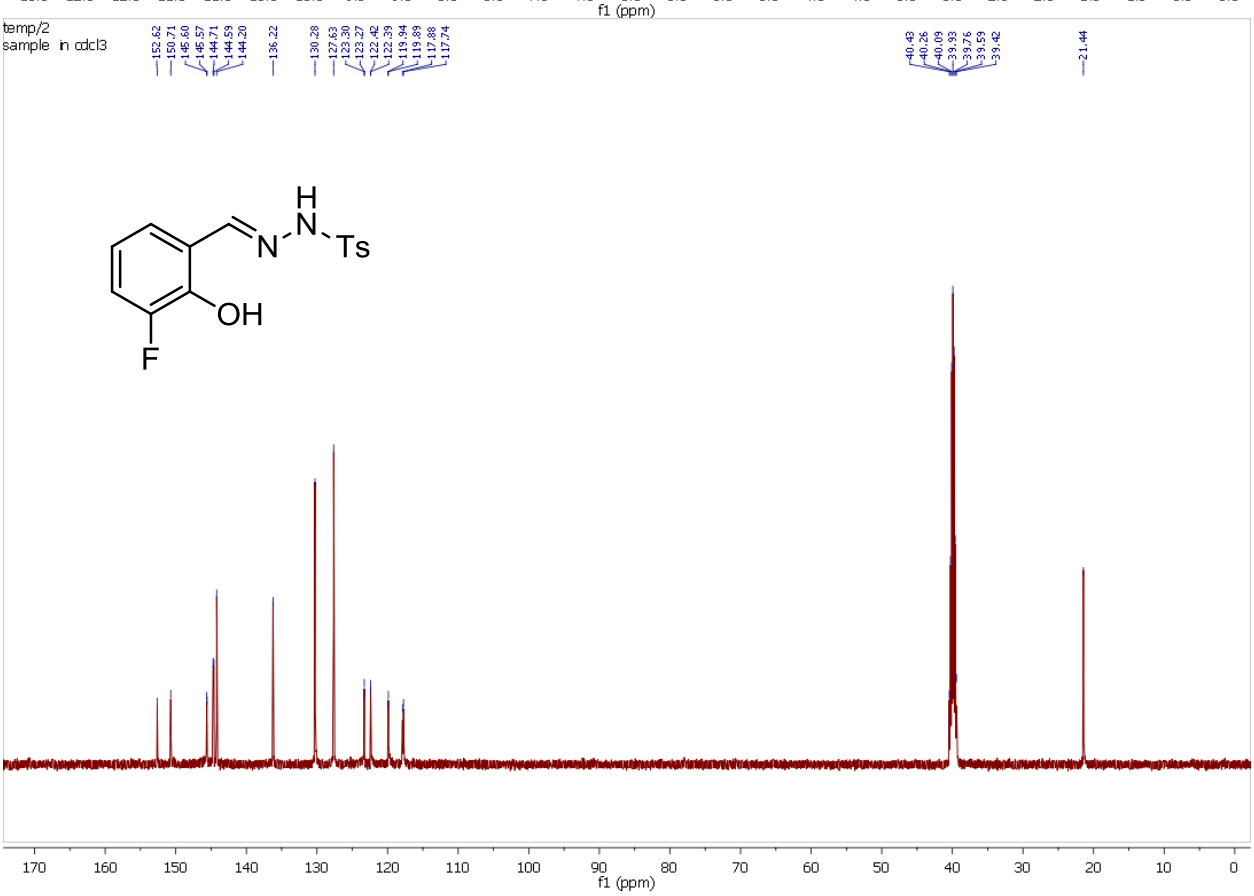

temp/1
sample in cdcl3
11.76
11.17
8.14
7.78
7.77
7.44
7.43
6.83
6.82
2.52
2.35
1.35
H
N
N
Ts
OH
1.00
1.00
1.01
2.01
2.01
2.05
1.03
3.03
9.04
f1 (ppm)

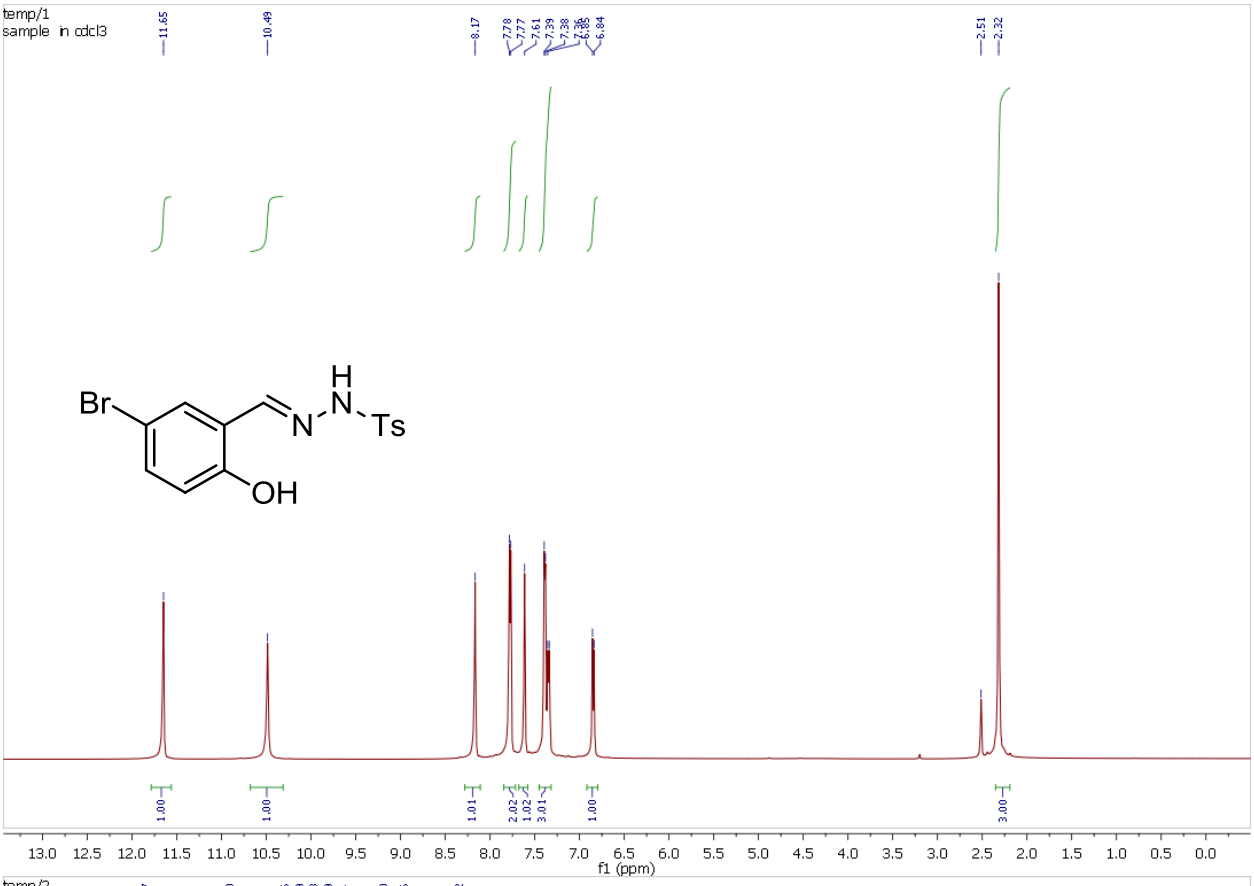

temp/2
sample in cdcl3
156.72
151.96
144.50
136.74
135.75
130.38
129.98
129.18
127.59
119.49
117.90
40.48
40.31
40.14
39.98
39.81
39.64
39.48
34.92
29.64
21.47
H
N
N
Ts
OH
f1 (ppm)

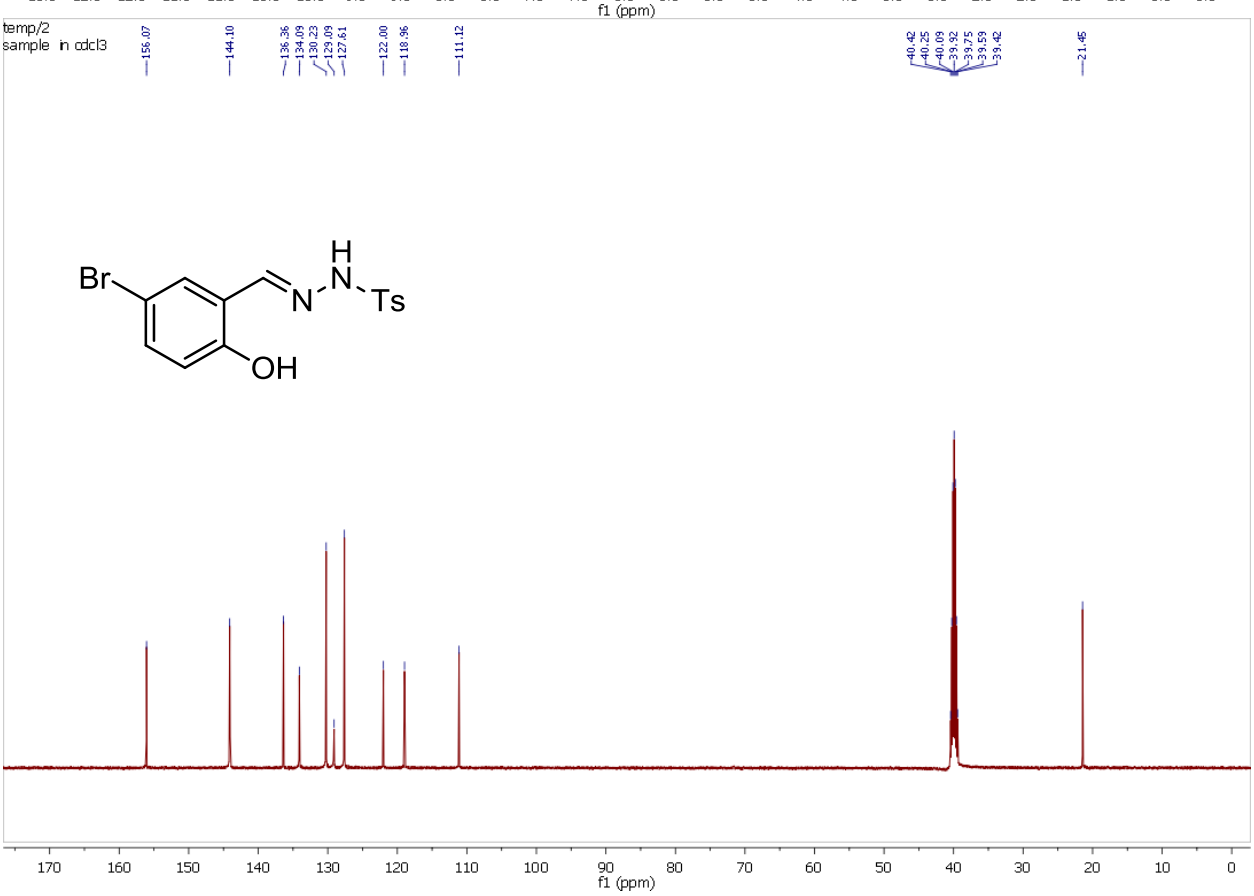

temp/1
sample in cdcl3
11.72
11.01
8.14
7.77
7.76
7.44
7.42
7.26
7.17
2.51
2.35
1.36
1.22
1.00
1.01
1.02
2.01
2.01
1.01
1.01
3.03
9.00
9.04
H
N
N
Ts
OH
f1 (ppm)

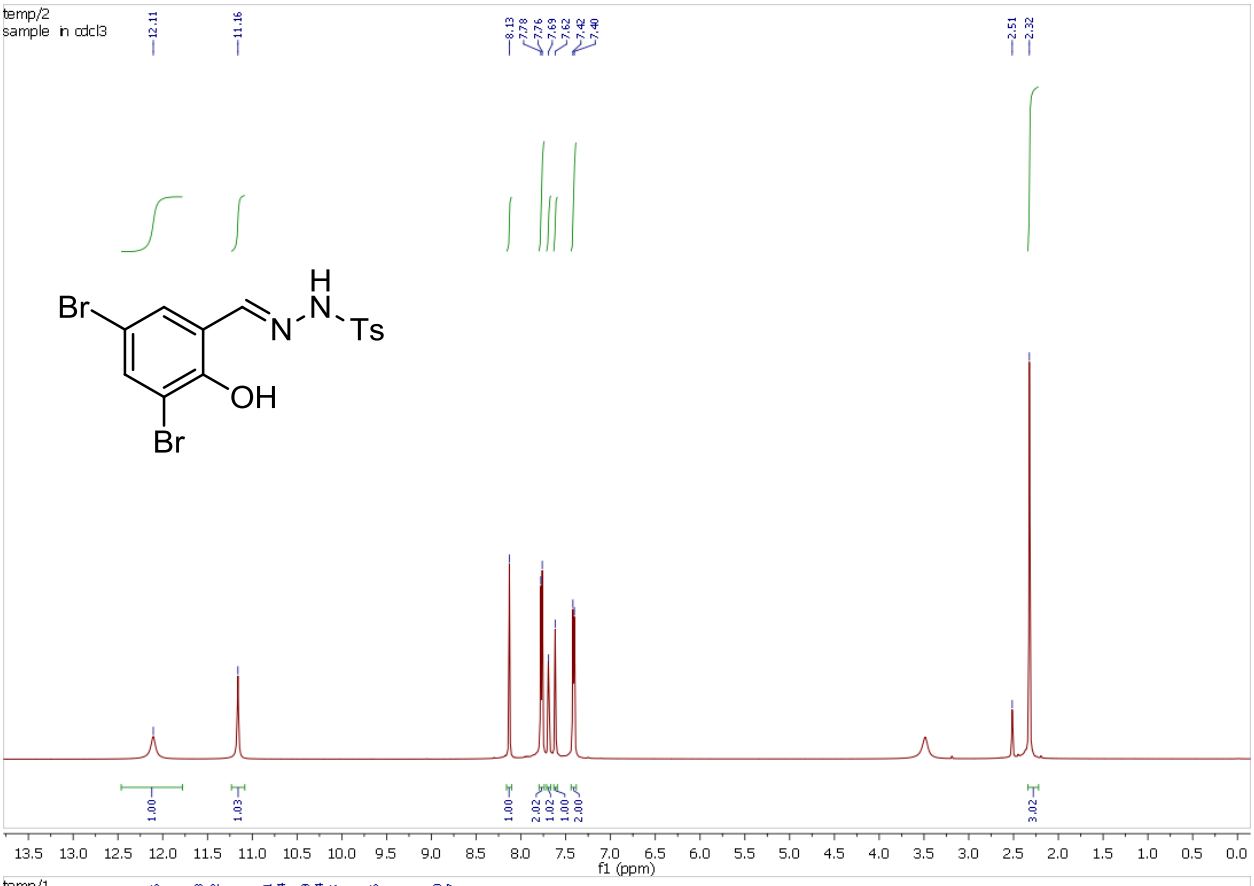

temp/2
sample in cdcl3
154.50
152.46
144.44
141.18
135.39
135.76
130.34
127.58
126.40
126.13
117.22
40.48
40.31
40.15
39.98
39.81
39.65
39.48
35.08
34.33
31.68
29.70
21.46
H
N
N
Ts
OH
f1 (ppm)

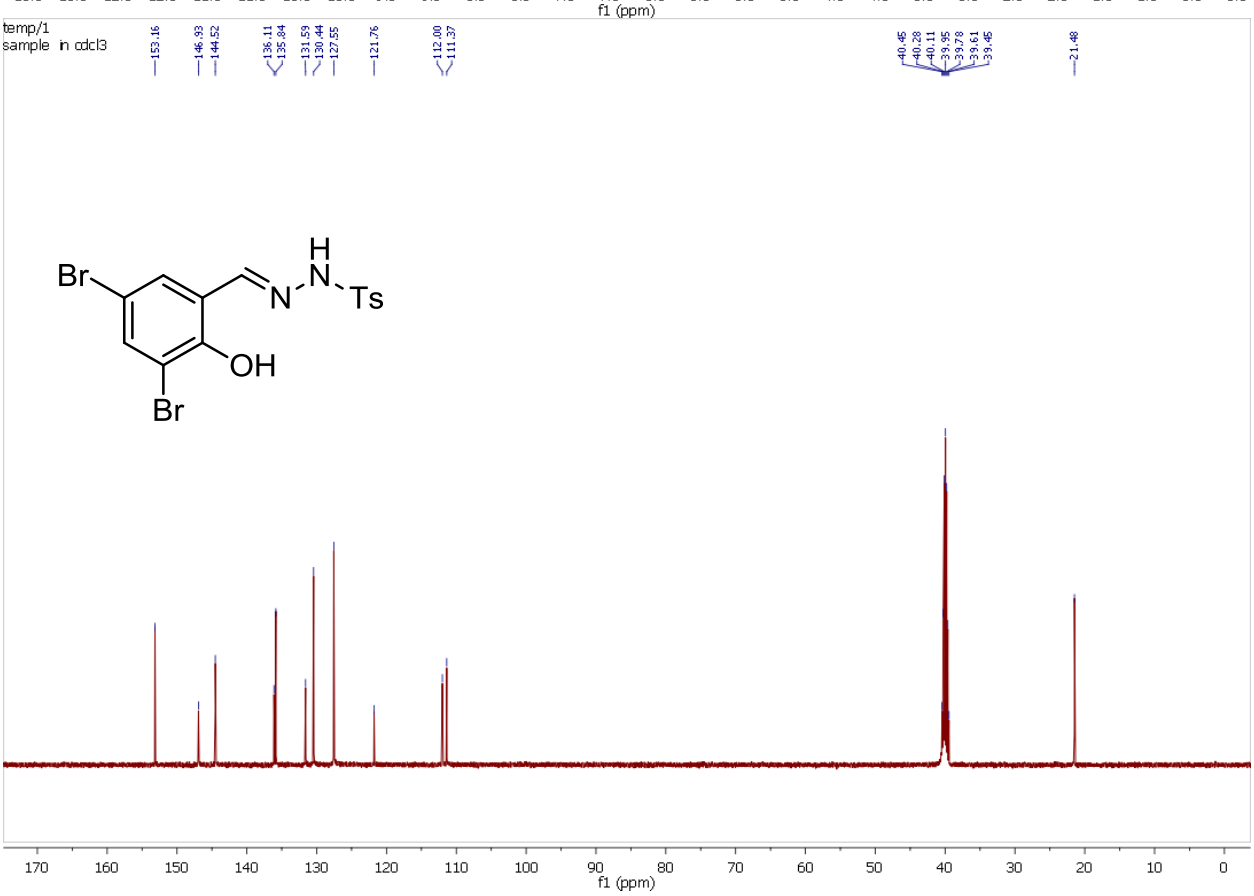

temp/1
sample in cdcl3
11.69
10.46
8.23
7.79
7.77
7.42
7.41
7.39
6.84
6.83
6.82
2.51
2.34
H
N
N
Ts
OH
F
1.00
1.01
1.02
2.00
1.06
1.01
1.01
1.00
3.00
f1 (ppm)

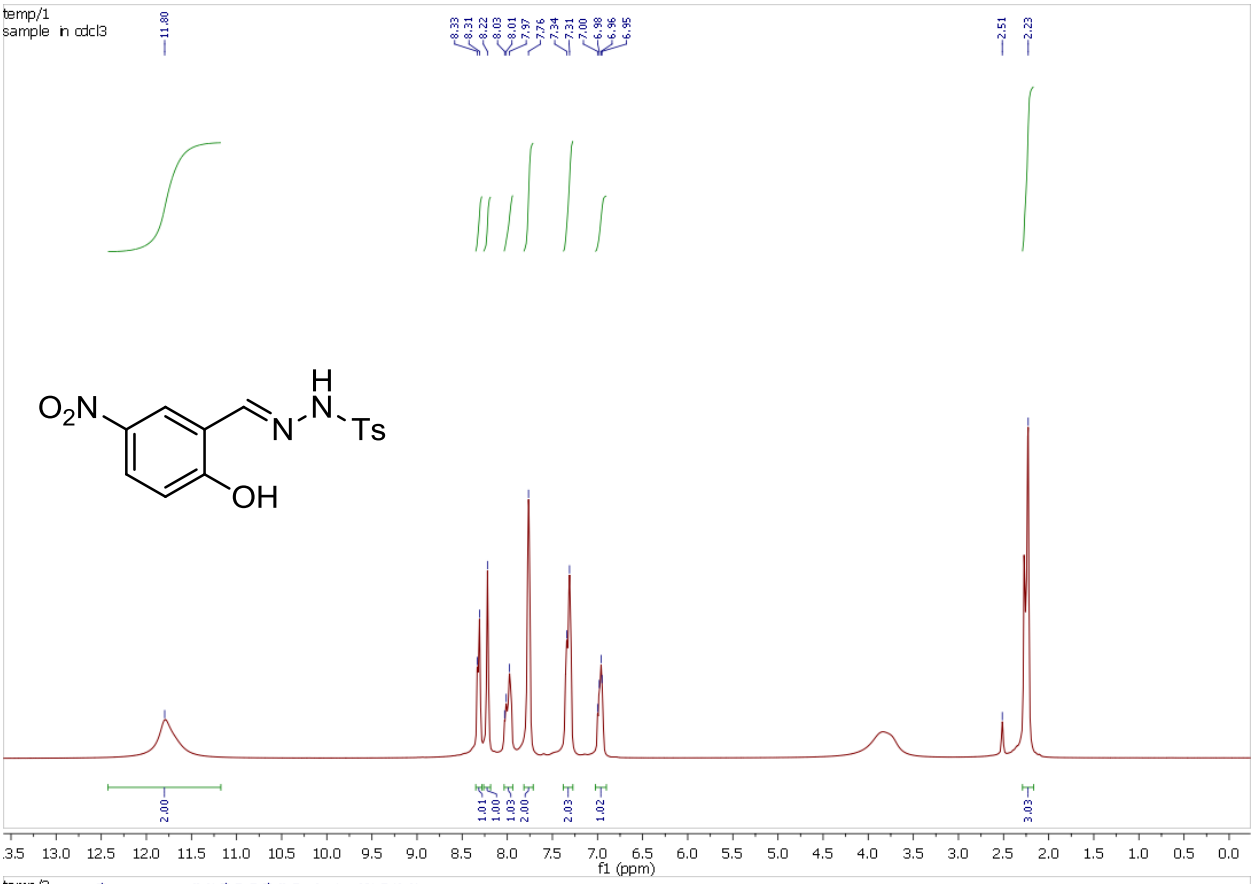

temp/2
sample in cdcl3
152.82
150.71
146.60
146.57
144.71
144.59
144.20
136.22
130.28
127.63
123.30
123.27
122.42
122.39
119.94
119.89
117.88
117.74
40.43
40.26
40.09
39.93
39.76
39.59
39.42
21.44
H
N
N
Ts
OH
F
f1 (ppm)

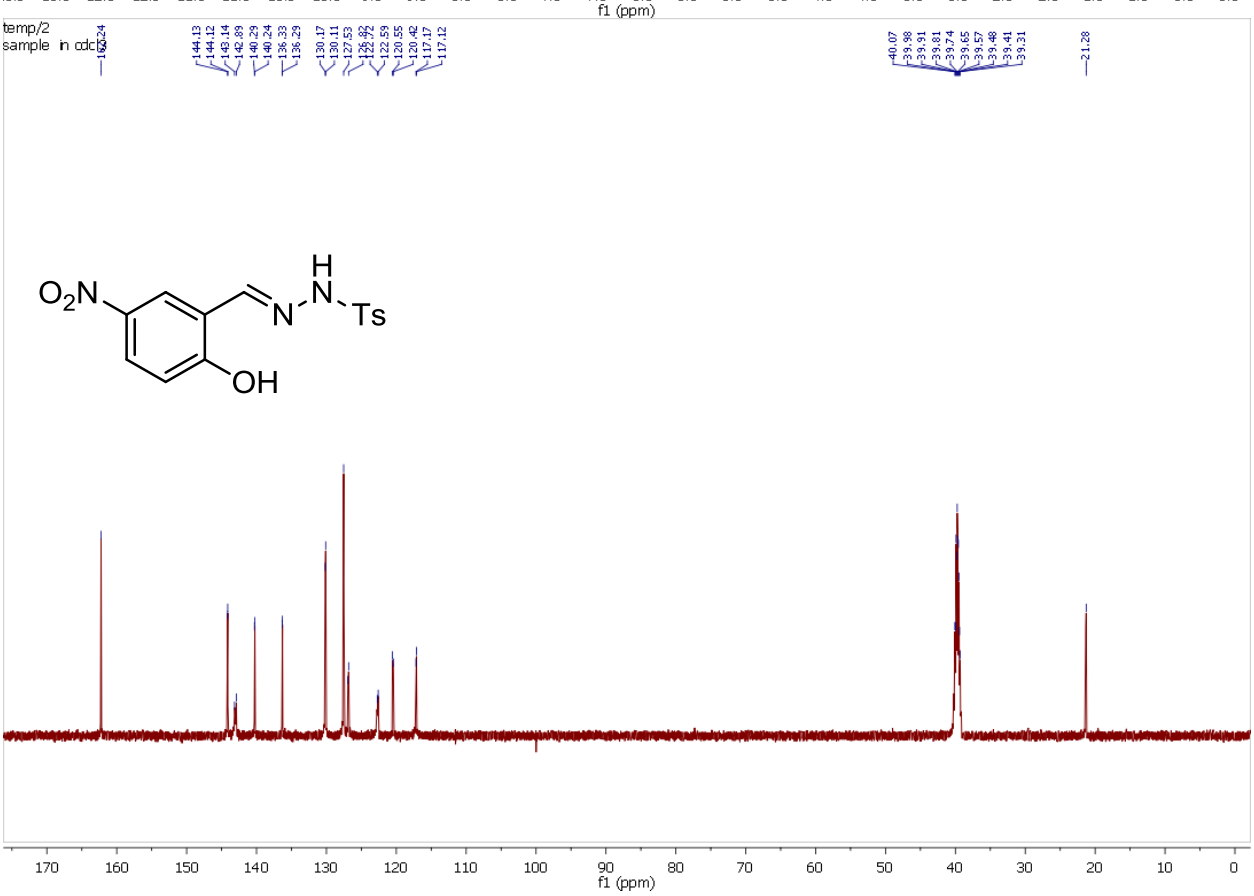

temp/1
sample in cdcl3
11.65
10.49
8.17
7.78
7.77
7.61
7.39
7.38
7.36
6.85
6.84
2.51
2.32
Br
H
N
N
Ts
OH
1.00
1.00
1.01
2.02
1.02
3.01
1.00
3.00
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

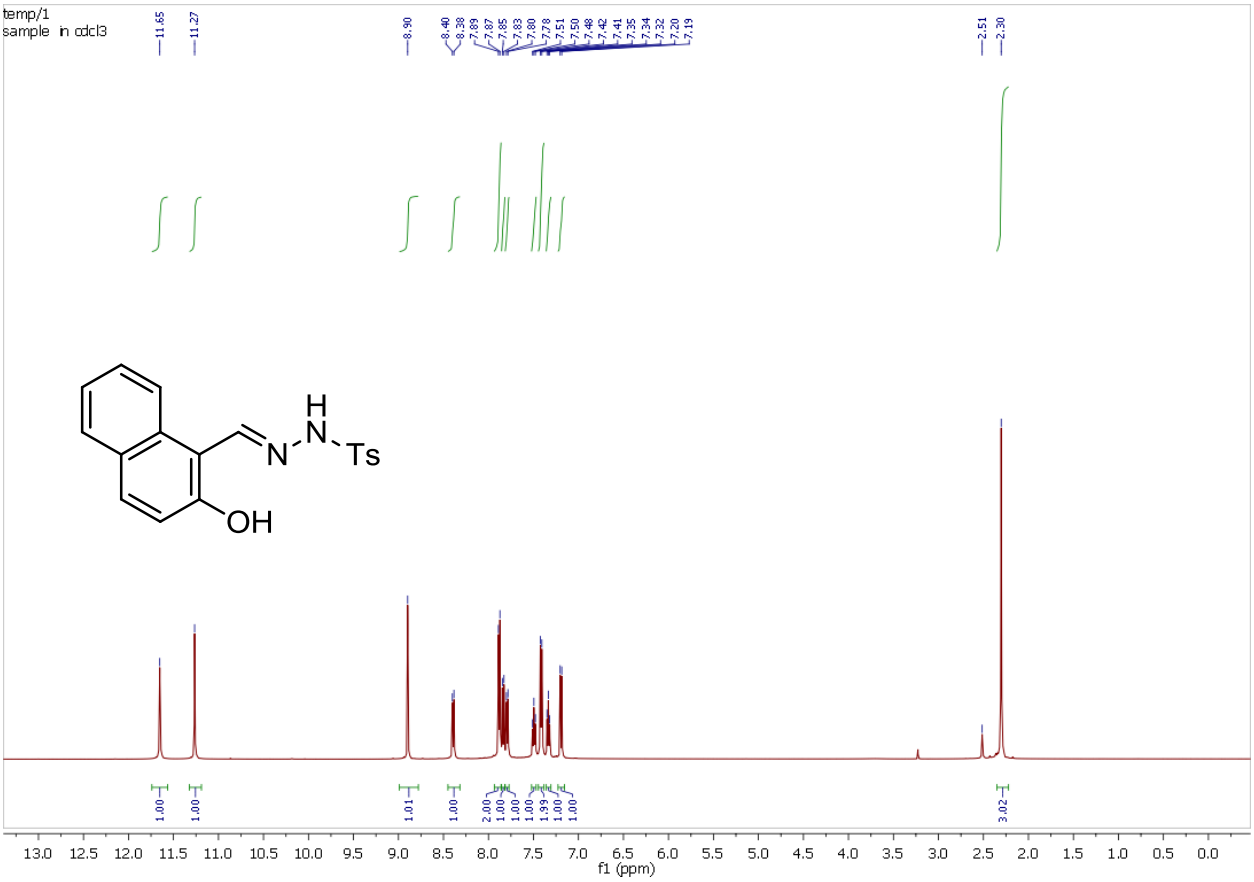

temp/2
sample in cdcl3
156.07
144.10
136.36
134.09
130.23
129.09
127.61
122.00
118.96
111.12
40.42
40.25
40.09
39.92
39.75
39.59
39.42
21.45
Br
H
N
N
Ts
OH
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

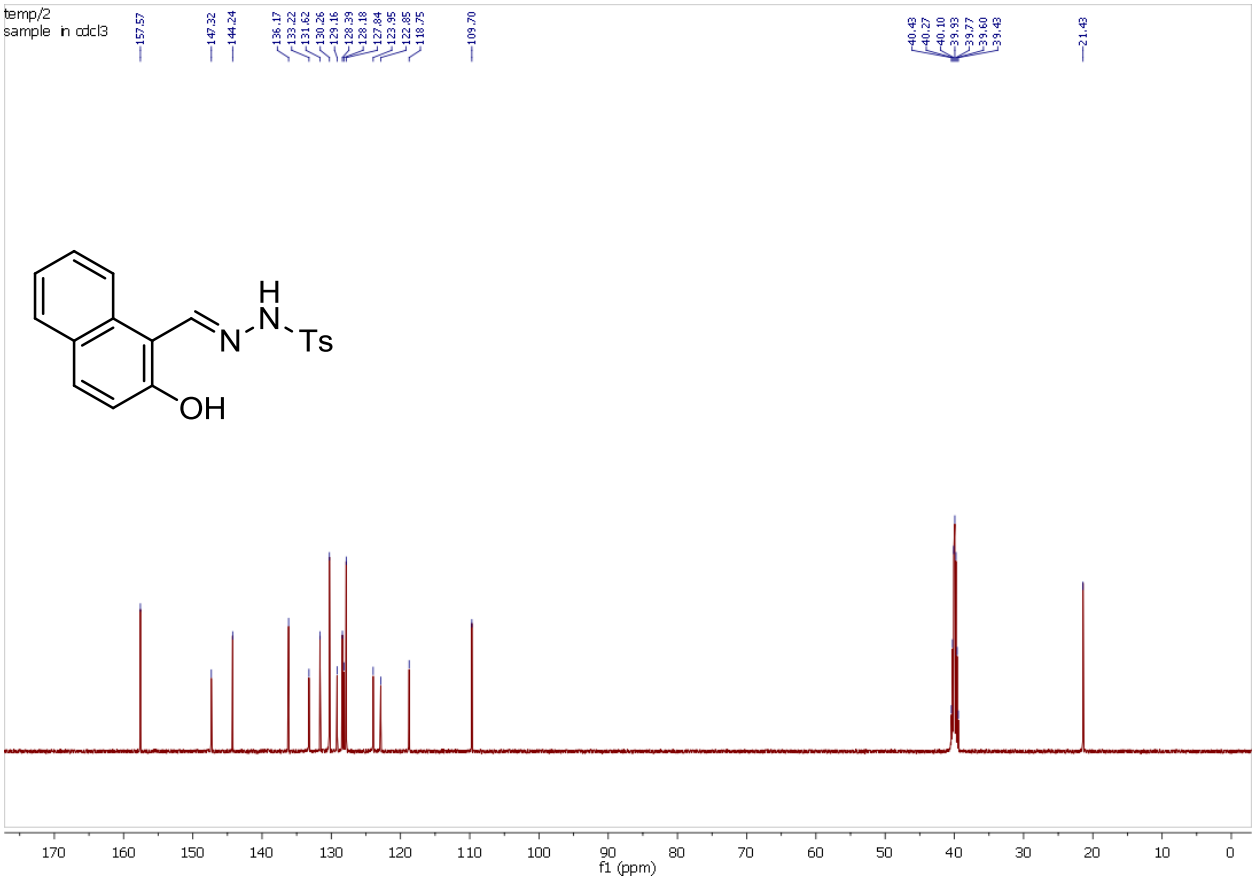

temp/2
sample in cdcl3
12.11
11.16
8.13
7.78
7.76
7.65
7.62
7.42
7.40
2.51
2.32
Br
H
N
N
Ts
OH
Br
1.00
1.03
1.00
2.02
1.02
1.00
2.00
3.02
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

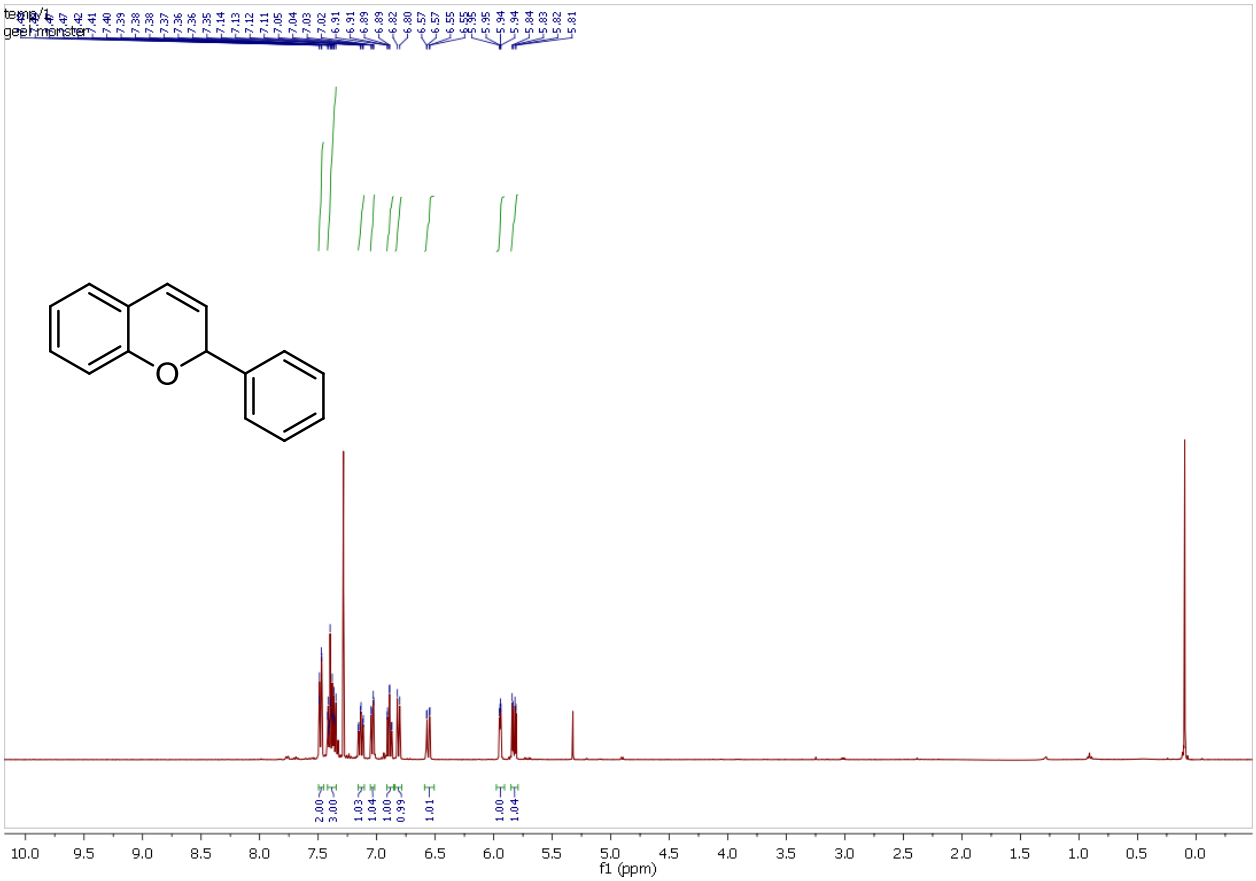

temp/1
sample in cdcl3
153.16
146.33
144.52
136.11
135.84
131.59
130.44
127.55
121.76
112.00
111.37
40.45
40.28
40.11
39.95
39.78
39.61
39.45
21.48
Br
H
N
N
Ts
OH
Br
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

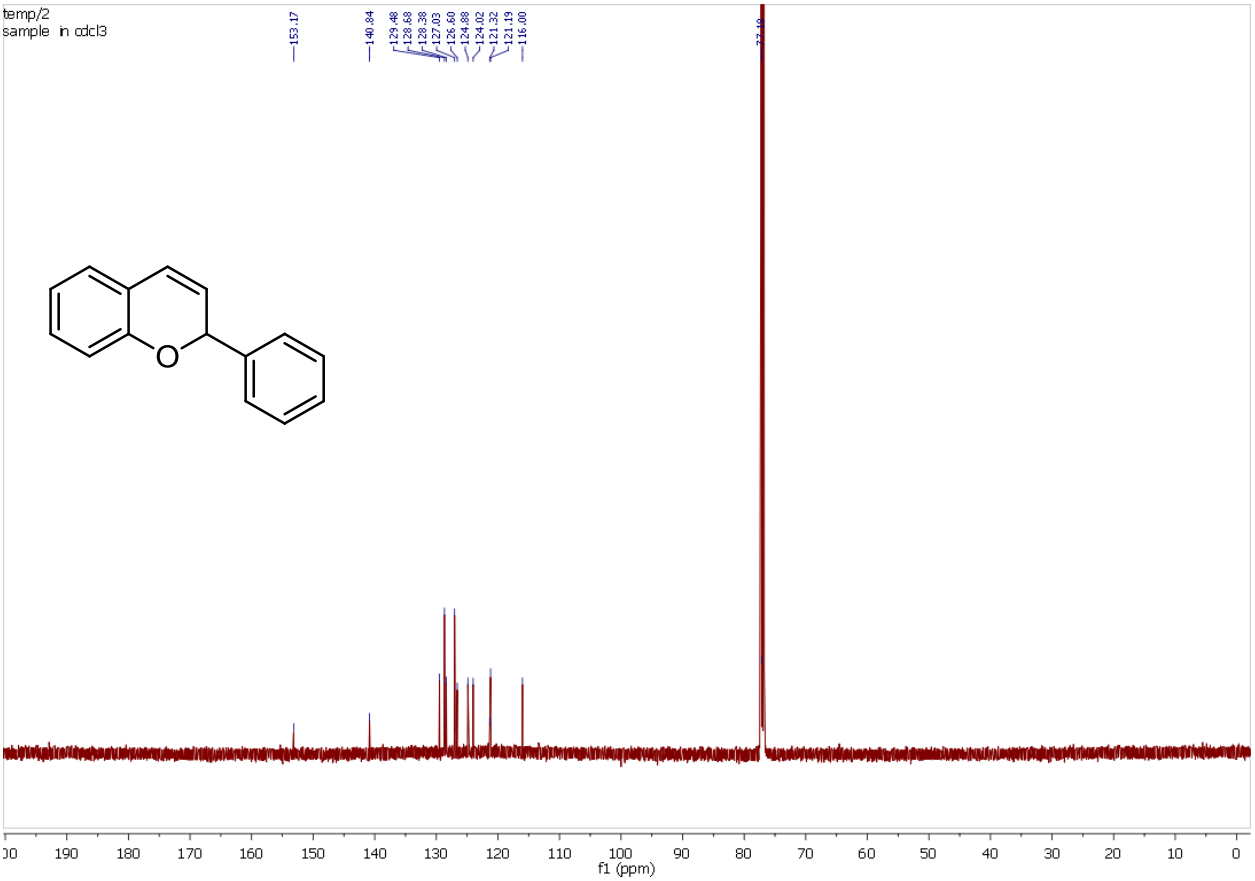

temp/1
sample in cdcl3
11.80
8.33
8.31
8.22
8.03
8.01
7.97
7.76
7.34
7.31
7.00
6.98
6.96
6.95
2.51
2.23
O2N
H
N
N
Ts
OH
2.00
1.01
1.00
1.03
2.00
2.03
1.02
3.03
f1 (ppm)

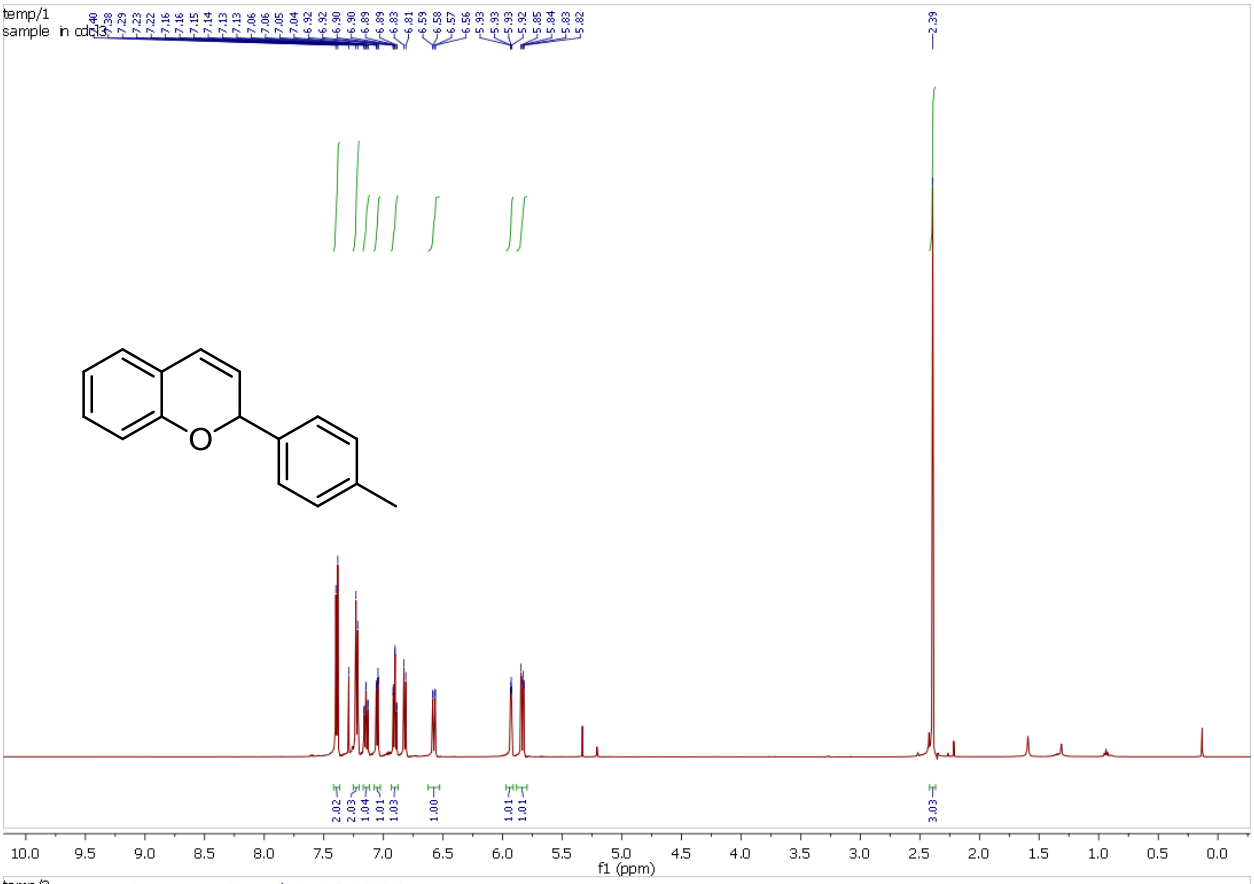

temp/2
sample in cdcl3
162.24
144.13
144.12
143.14
142.89
140.29
140.24
136.33
136.29
130.17
130.11
127.53
125.92
123.59
120.55
120.42
117.17
117.12
40.07
39.98
39.91
39.81
39.74
39.65
39.57
39.48
39.41
39.31
21.28
O2N
H
N
N
Ts
OH
f1 (ppm)

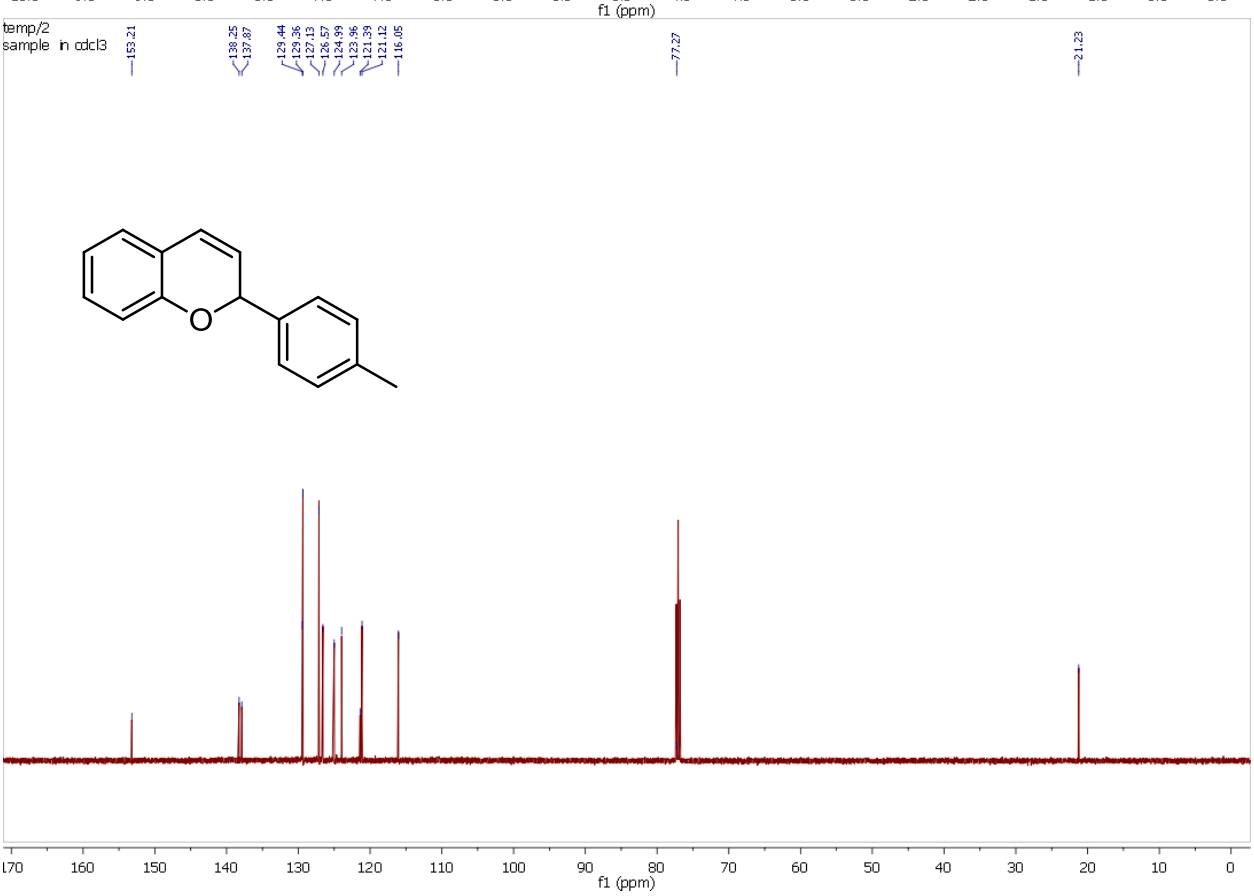

temp/1
sample in cdcl3
11.65
11.27
8.90
8.40
8.38
7.89
7.87
7.85
7.83
7.80
7.78
7.51
7.50
7.48
7.42
7.41
7.35
7.34
7.32
7.20
7.19
2.51
2.30
H
N
N
Ts
OH
1.00
1.00
1.01
1.00
2.00
1.00
1.00
1.99
1.00
1.00
3.02
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

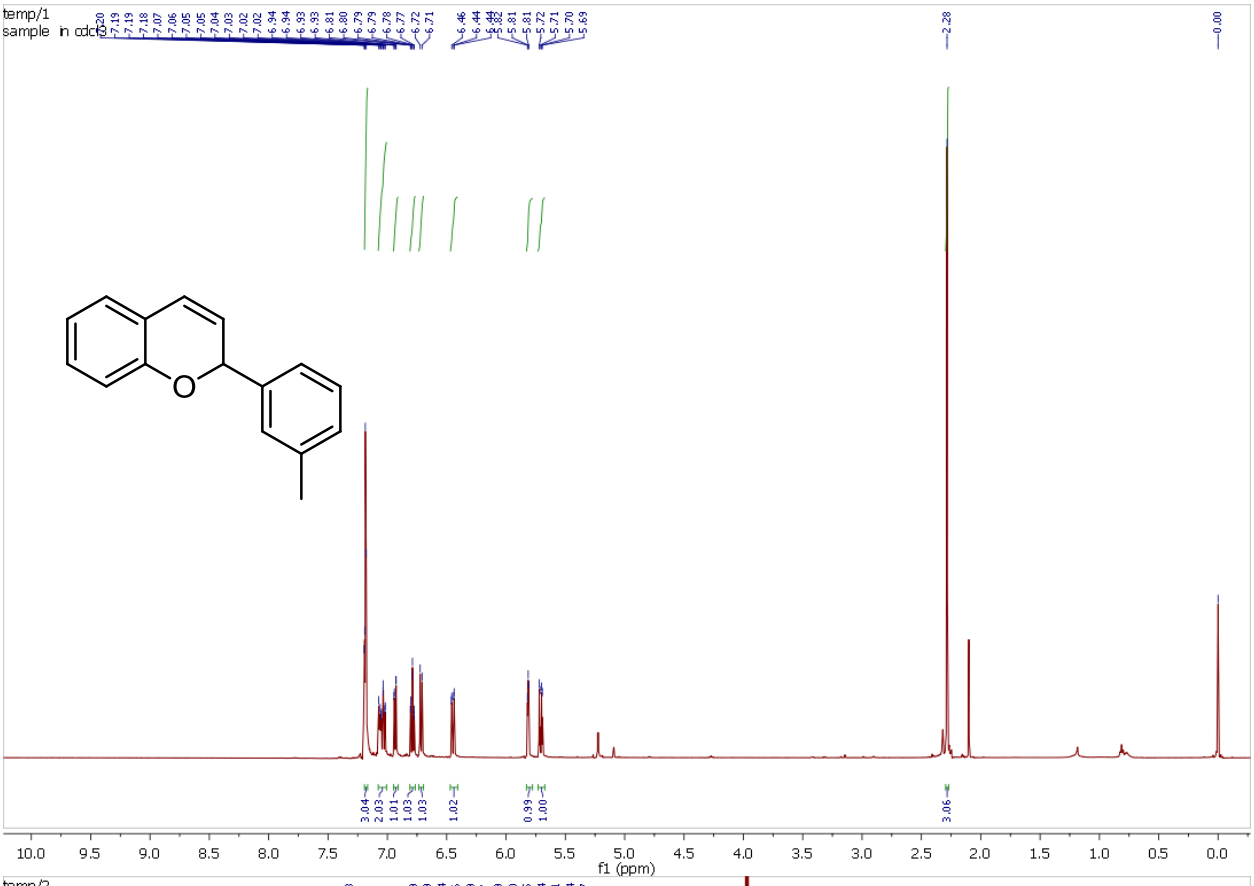

temp/2
sample in cdcl3
157.57
147.32
144.24
136.17
133.22
131.62
130.26
129.16
128.39
128.18
127.84
123.95
122.85
118.75
109.70
40.43
40.27
40.10
39.93
39.77
39.60
39.43
21.43
H
N
N
Ts
OH
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

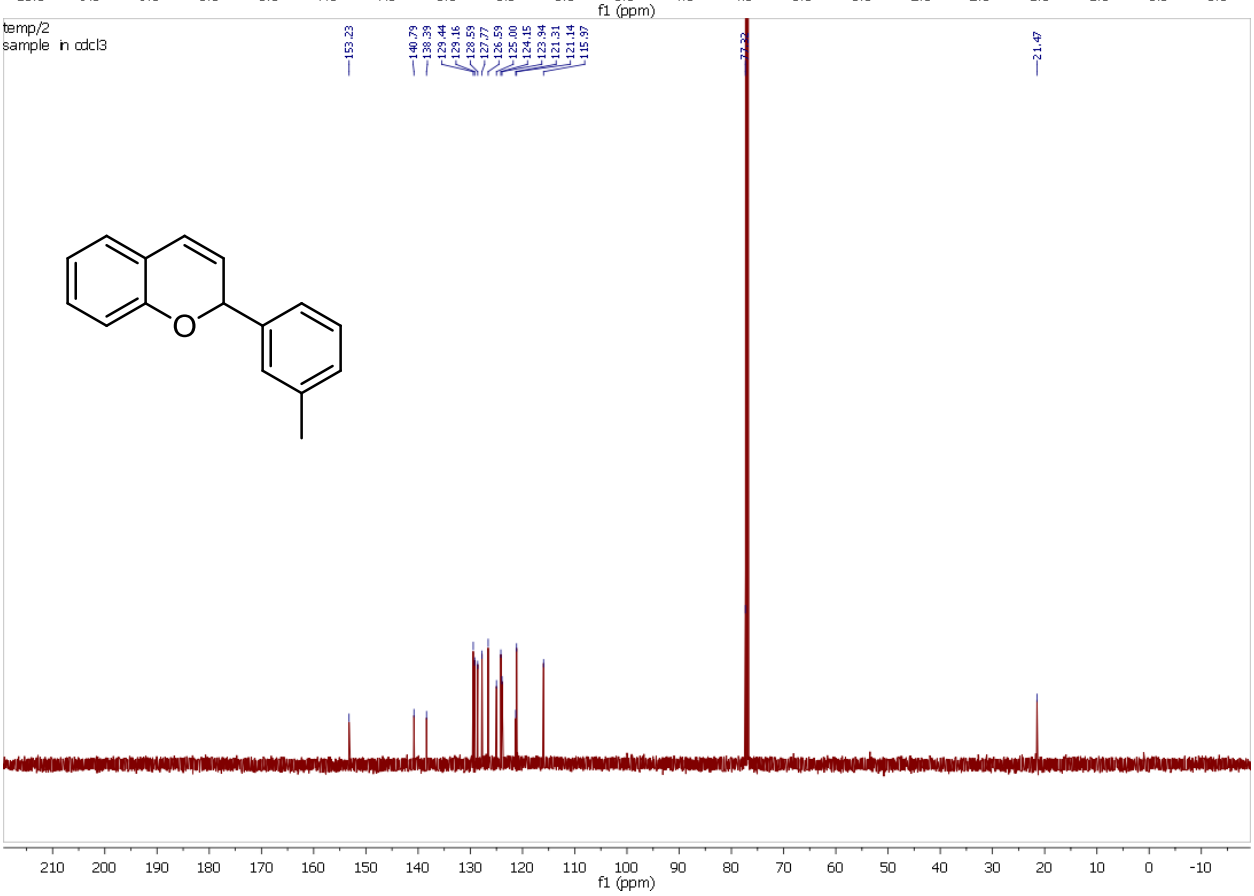

temp/1
geeh monster
7.47
7.42
7.41
7.40
7.39
7.38
7.38
7.37
7.36
7.36
7.35
7.14
7.13
7.12
7.11
7.05
7.04
7.03
7.02
6.91
6.89
6.89
6.82
6.80
6.57
6.57
6.55
6.55
5.95
5.94
5.94
5.84
5.83
5.82
5.81
O
2.00
3.00
1.03
1.04
1.00
0.93
1.01
1.00
1.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

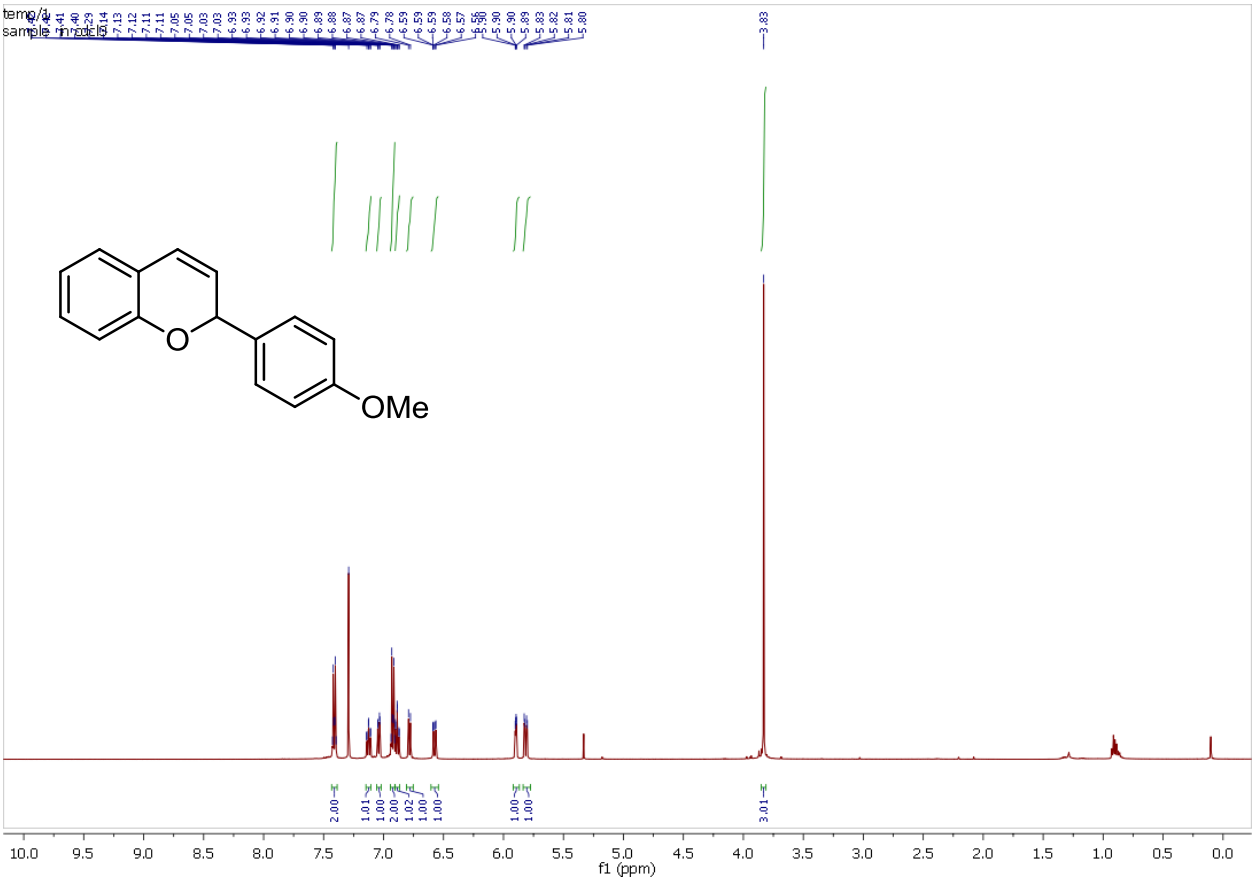

temp/2
sample in cdcl3
153.17
140.84
129.48
128.68
128.38
127.03
126.60
124.88
124.02
121.32
121.19
116.00
77.49
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

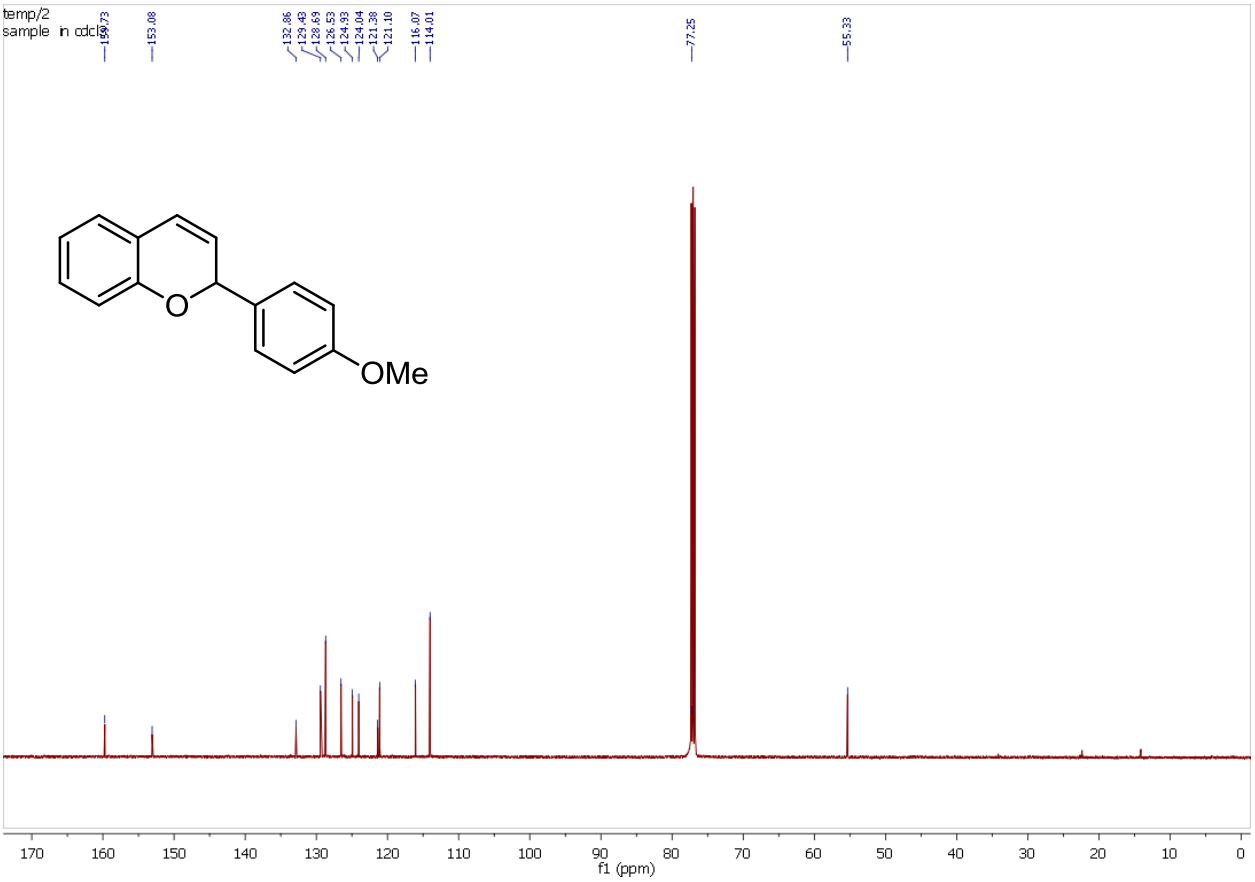

temp/1
sample in cdcl3
7.40
7.38
7.29
7.23
7.22
7.16
7.16
7.15
7.14
7.13
7.13
7.06
7.06
7.05
7.04
6.92
6.90
6.90
6.89
6.89
6.83
6.81
6.59
6.58
6.57
6.56
5.93
5.93
5.93
5.92
5.85
5.84
5.83
5.82
2.39
O
2.02
2.03
1.04
1.01
1.03
1.00
1.01
1.01
3.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

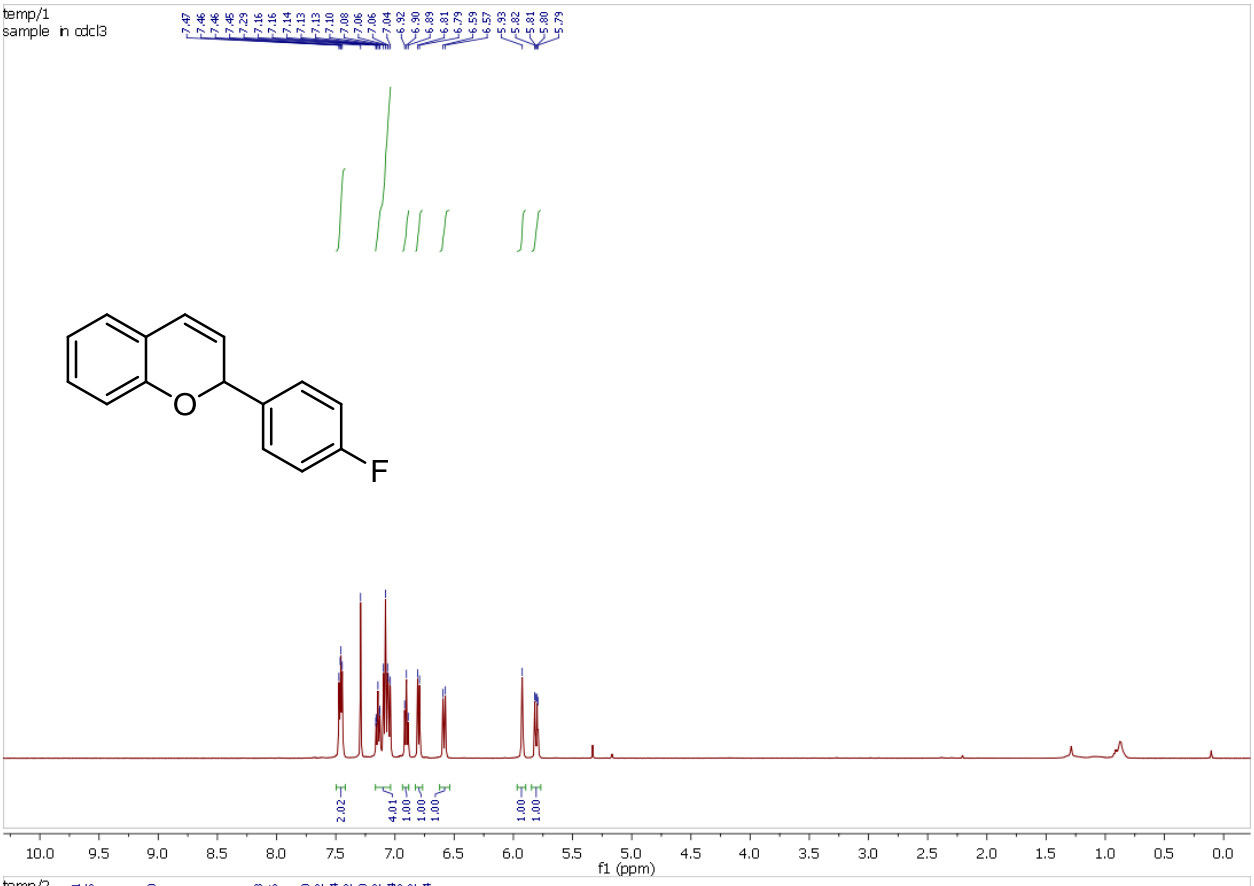

temp/2
sample in cdcl3
153.21
138.25
137.87
129.44
129.36
127.13
126.57
124.99
123.96
121.39
121.12
116.05
77.27
21.23
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

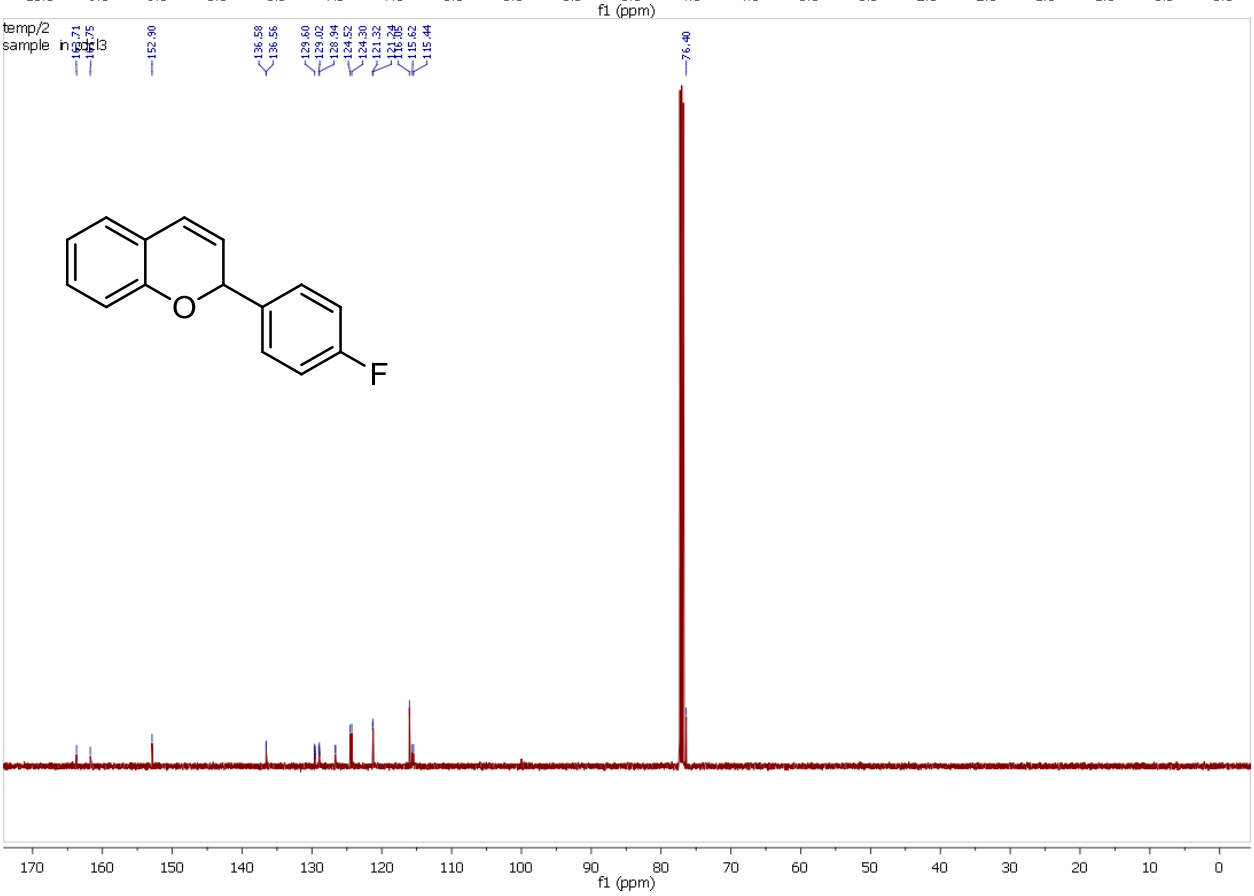

temp/1
sample in cdcl3
7.20
7.19
7.19
7.18
7.07
7.06
7.05
7.05
7.04
7.03
7.02
7.02
6.94
6.94
6.93
6.93
6.81
6.80
6.79
6.79
6.78
6.77
6.72
6.71
6.46
6.44
6.44
5.82
5.81
5.81
5.72
5.71
5.70
5.69
2.28
0.00
3.04
2.03
1.01
1.03
1.03
1.02
0.99
1.00
3.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

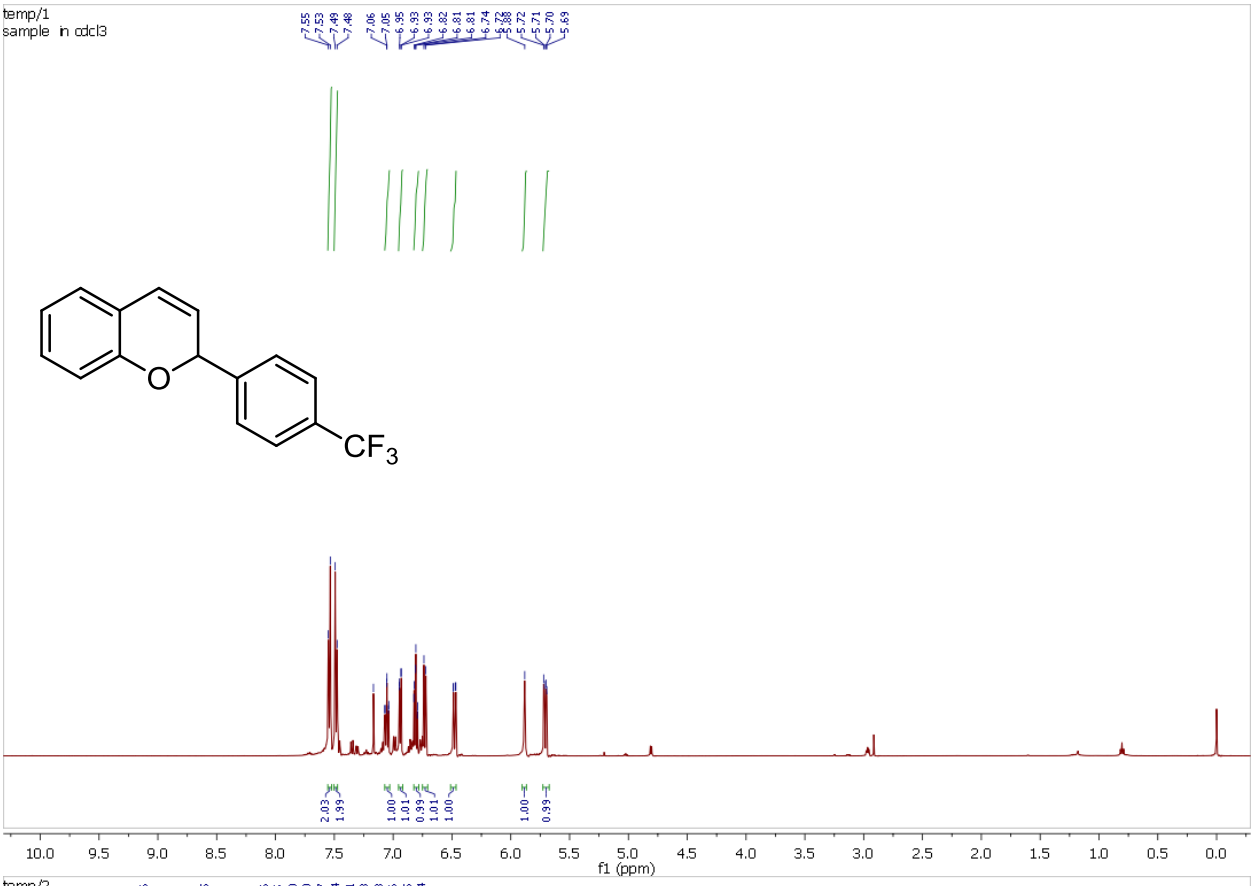

temp/2
sample in cdcl3
153.23
140.79
138.39
129.44
129.16
128.59
127.77
126.59
125.00
124.15
123.94
121.31
121.14
115.97
77.32
21.47
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

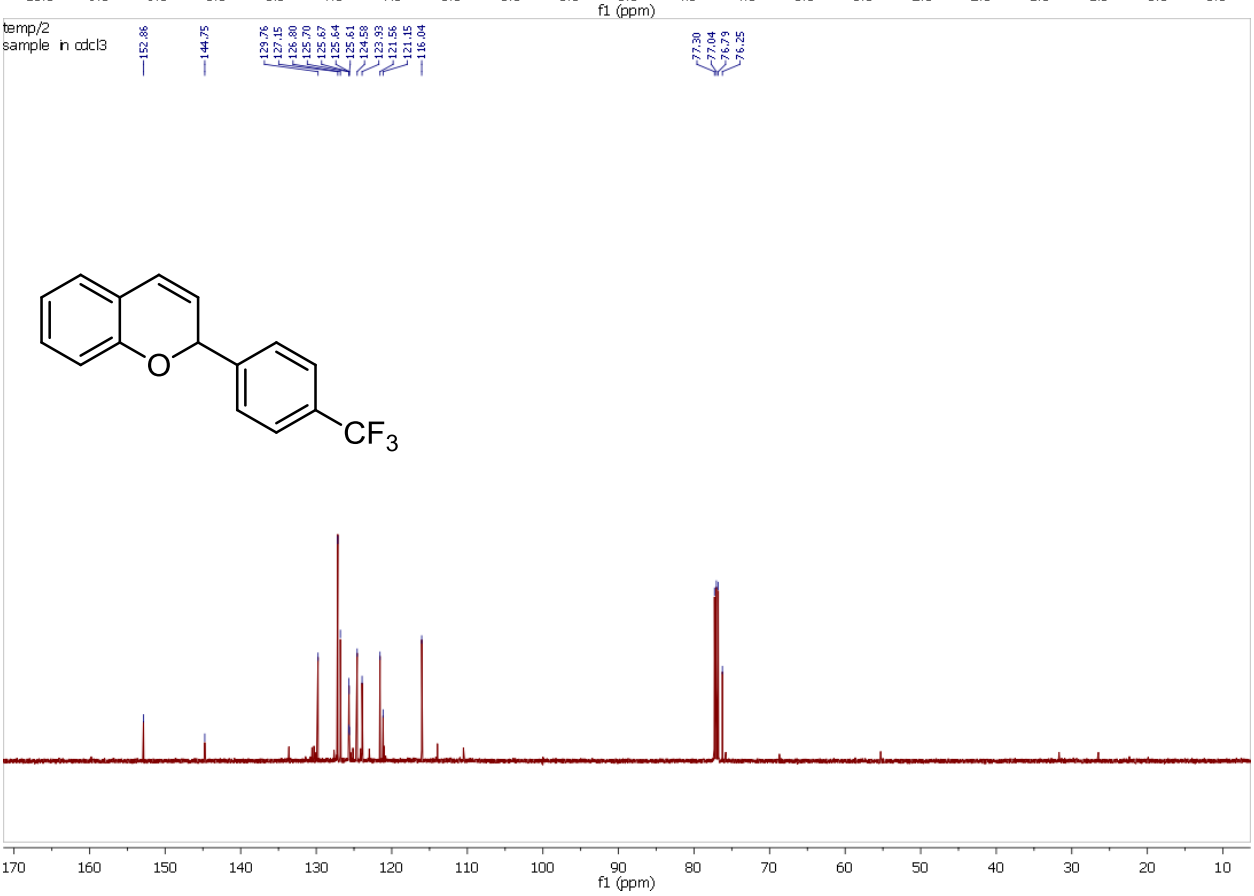

temp/1
sample in cdcl3
3.83
O
OMe
f1 (ppm)

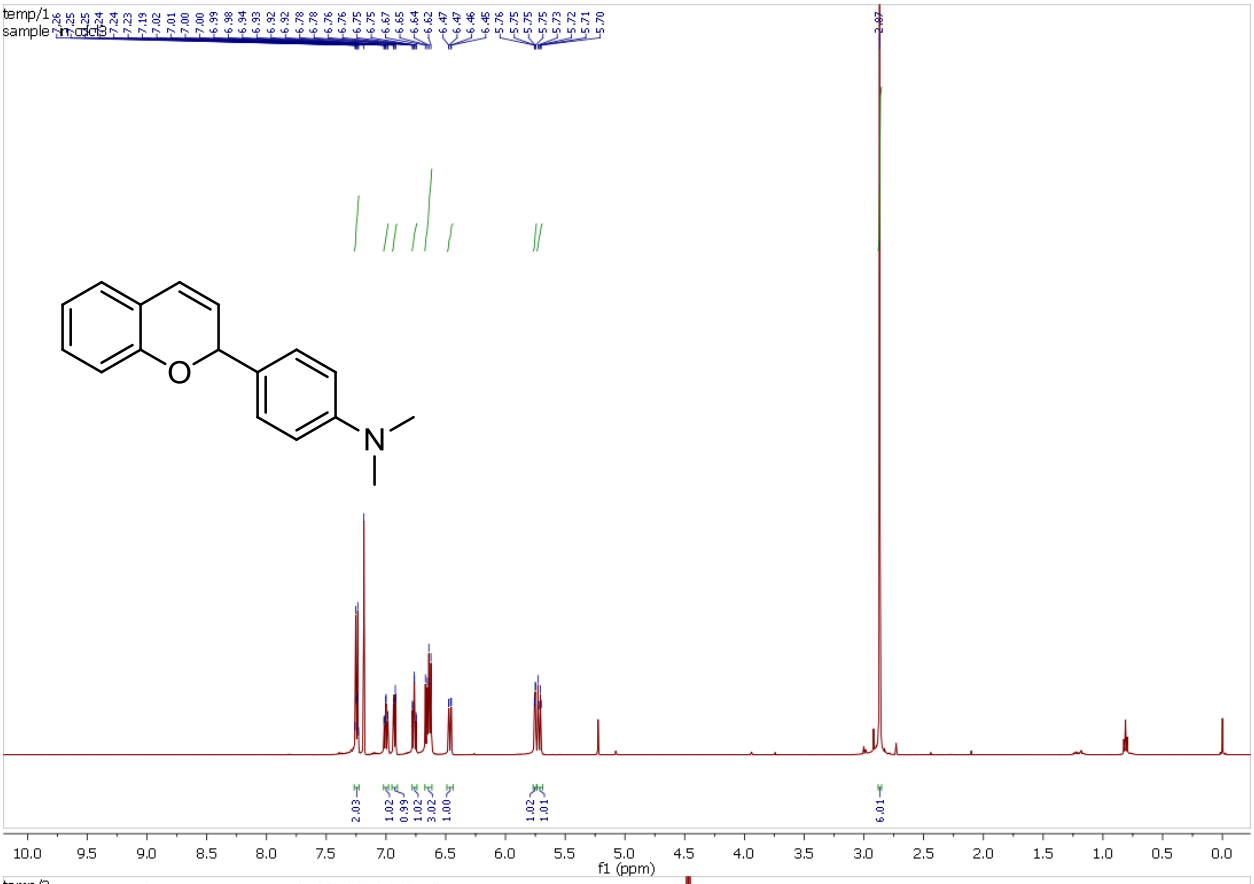

temp/2
sample in cdcl3
159.73
153.08
132.86
129.48
128.69
126.53
124.93
124.04
121.38
121.10
116.07
114.01
77.25
55.33
O
OMe
f1 (ppm)

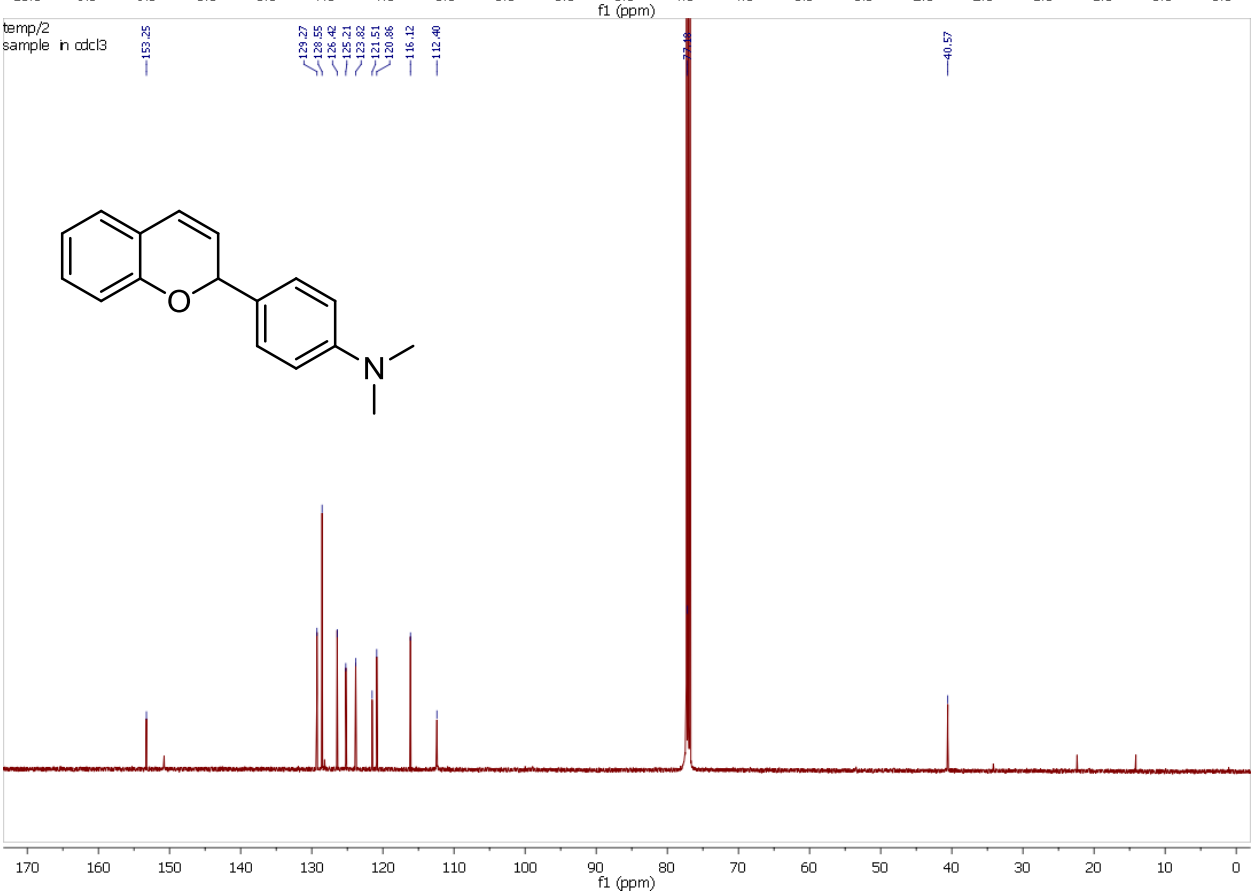

temp/1
sample in cdcl3
7.47
7.46
7.46
7.45
7.29
7.16
7.16
7.14
7.13
7.10
7.08
7.06
7.06
7.04
6.92
6.90
6.89
6.81
6.79
6.59
6.57
5.93
5.82
5.81
5.80
5.79
O
F
2.02
4.01
1.00
1.00
1.00
1.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

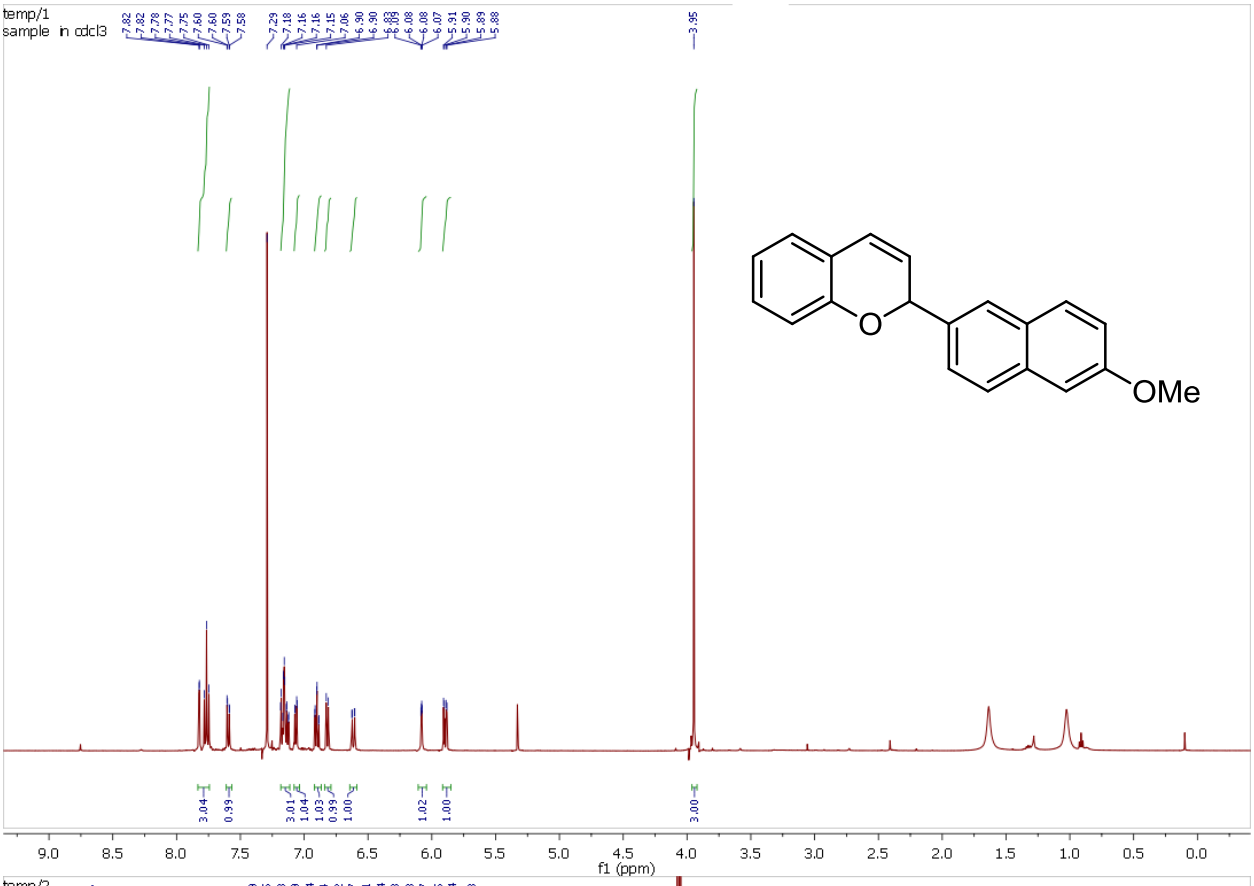

temp/2
sample in cdcl3
163.71
161.75
152.90
136.58
136.56
129.60
129.02
128.94
124.52
124.30
121.32
121.24
121.20
115.82
115.44
76.40
O
F
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

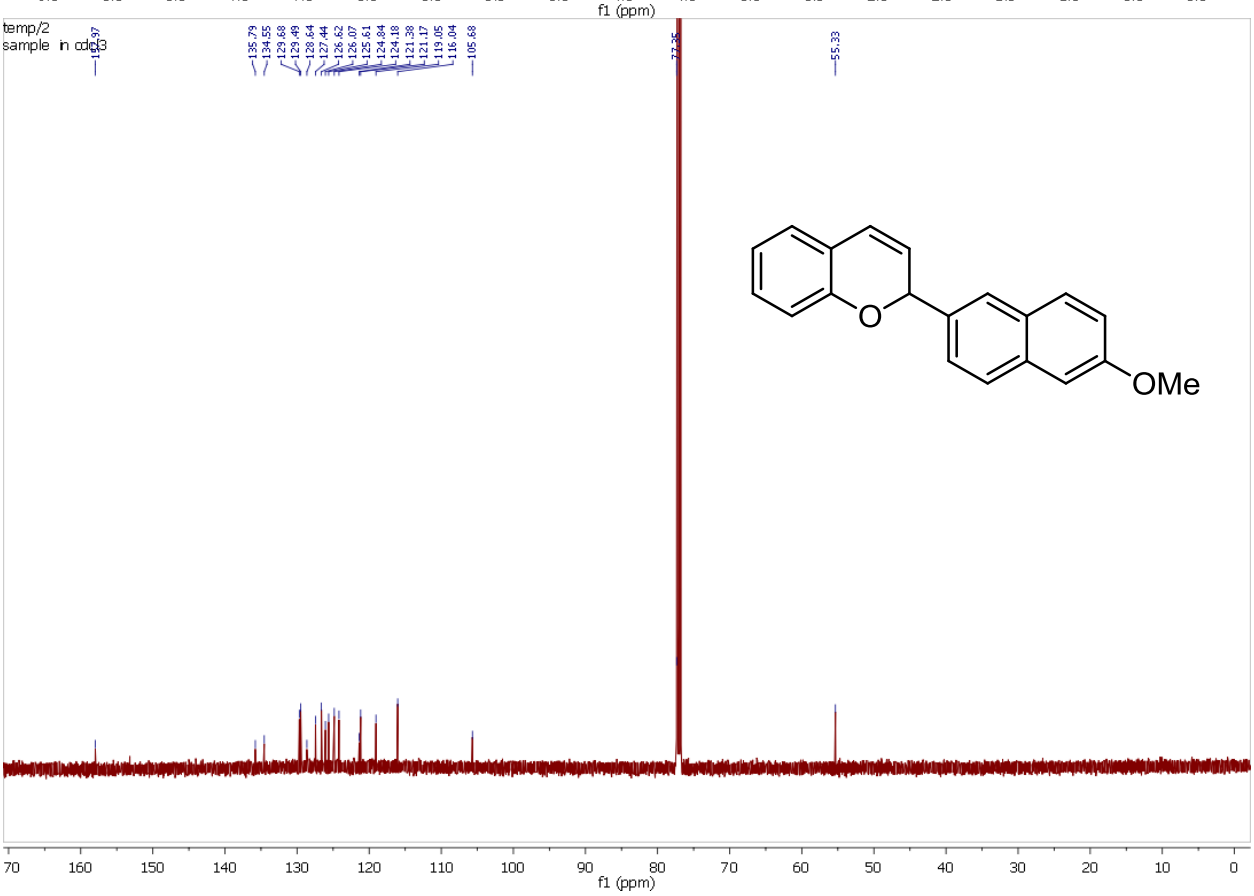

temp/1
sample in cdcl3
7.55
7.53
7.49
7.48
7.06
7.05
6.55
6.53
6.53
6.52
6.51
6.51
6.74
6.73
5.72
5.71
5.70
5.69
O
CF3
2.03
1.99
1.00
1.01
0.99
1.01
1.00
1.00
0.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

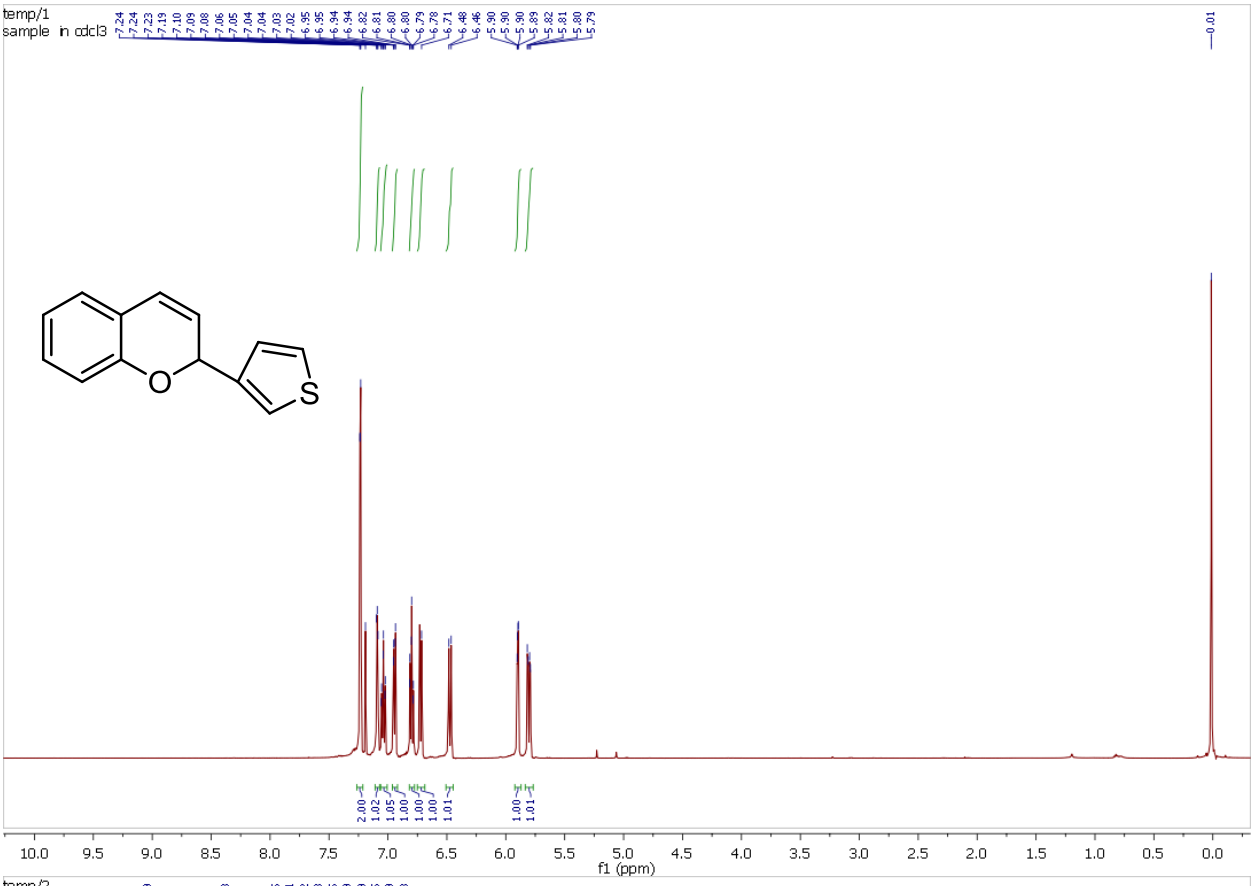

temp/2
sample in cdcl3
152.86
144.75
129.76
127.15
126.80
125.70
125.67
125.64
125.61
124.58
123.93
121.56
121.15
116.04
77.30
77.04
76.79
76.25
O
CF3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

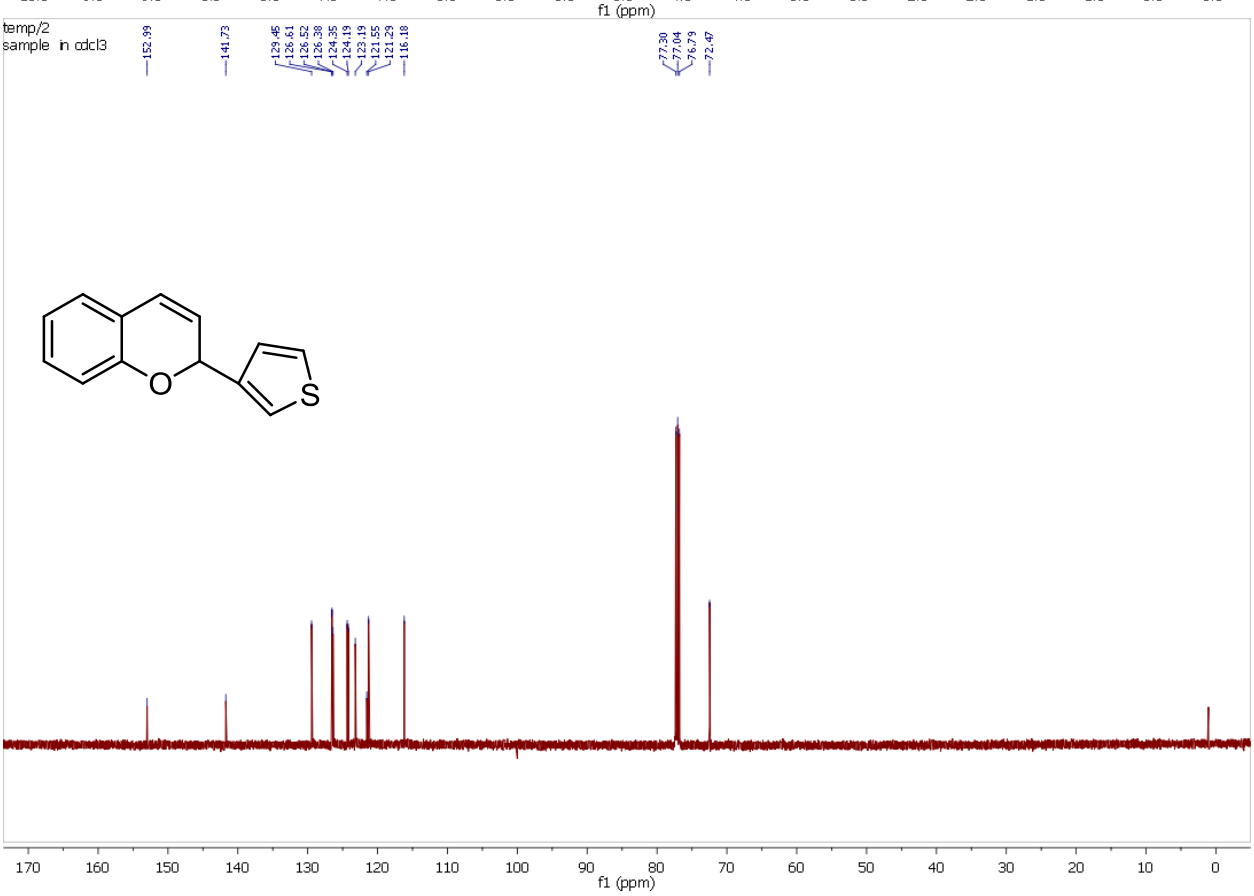

temp/1
sample in cdcl3
7.26
7.25
7.25
7.24
7.24
7.23
7.19
7.02
7.01
7.00
7.00
6.99
6.98
6.94
6.93
6.92
6.78
6.78
6.76
6.76
6.75
6.75
6.67
6.65
6.64
6.62
6.47
6.47
6.46
6.45
5.76
5.75
5.75
5.75
5.73
5.72
5.71
5.70
2.87
O
N
2.03
1.02
0.99
1.02
3.02
1.00
1.02
1.01
6.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

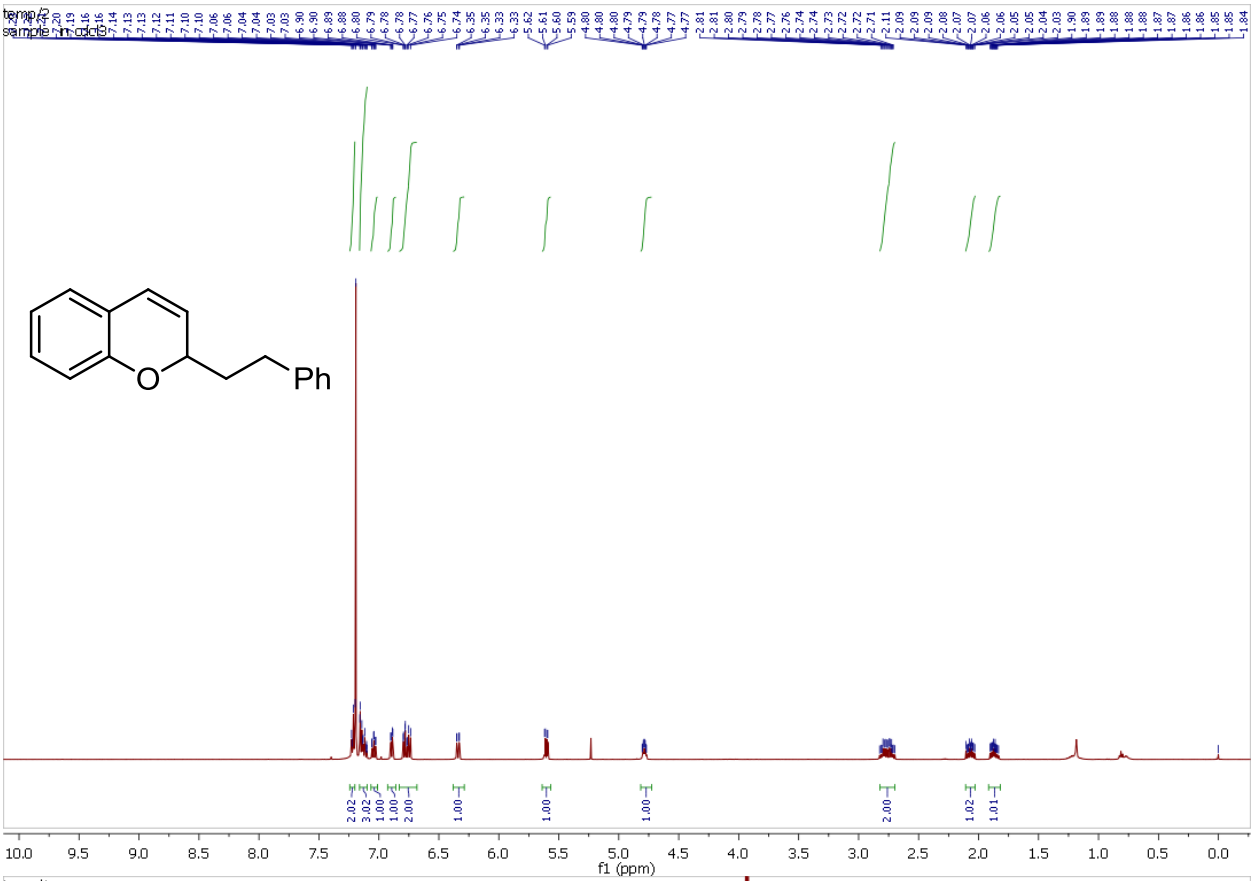

temp/2
sample in cdcl3
153.25
129.27
128.55
126.42
125.21
123.82
121.51
120.86
116.12
112.40
77.48
40.57
O
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

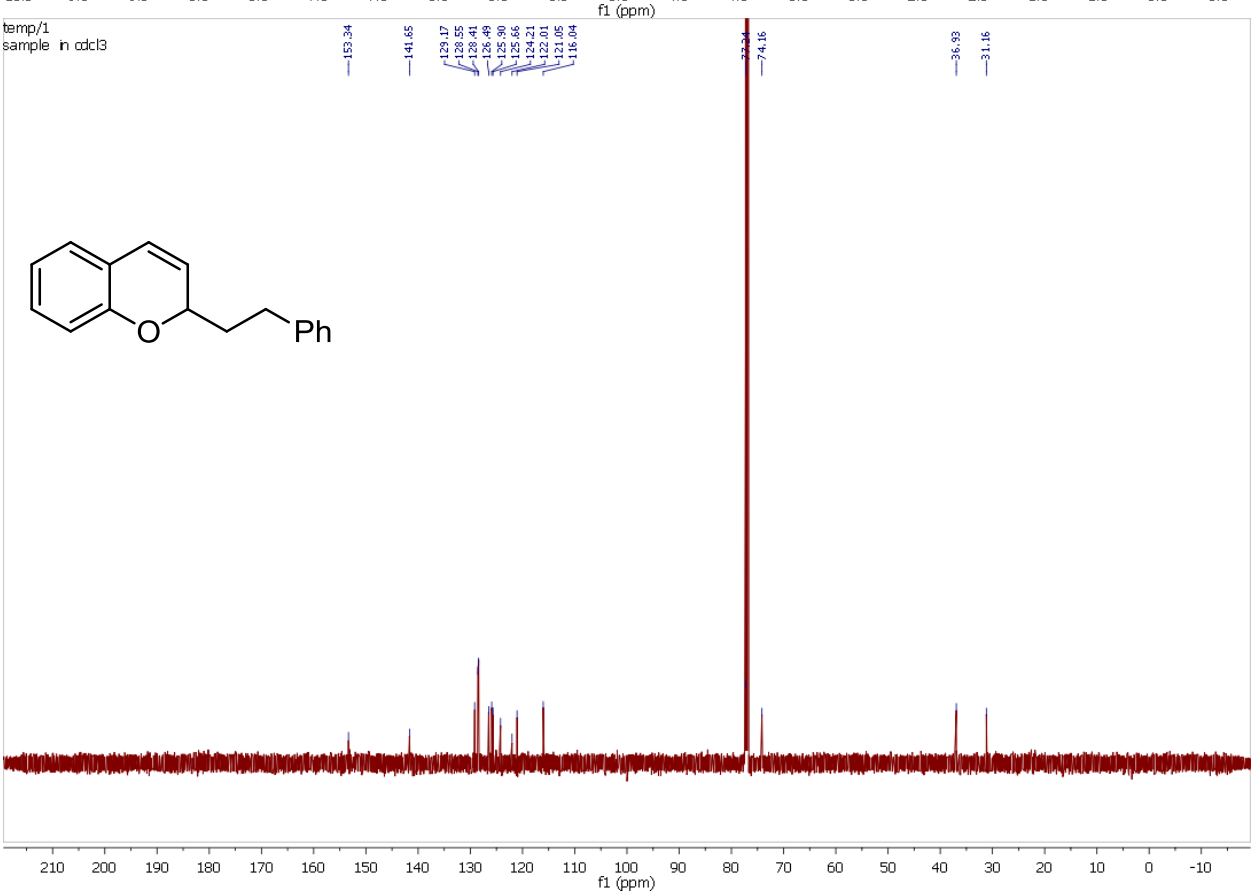

temp/1
sample in cdcl3
7.82
7.82
7.78
7.77
7.75
7.60
7.60
7.59
7.58
7.29
7.18
7.16
7.16
7.15
7.06
6.90
6.90
6.88
6.88
6.08
6.07
5.91
5.90
5.89
5.88
3.95
3.04
0.99
3.01
1.04
1.03
0.99
1.00
1.02
1.00
3.00
O
OMe
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

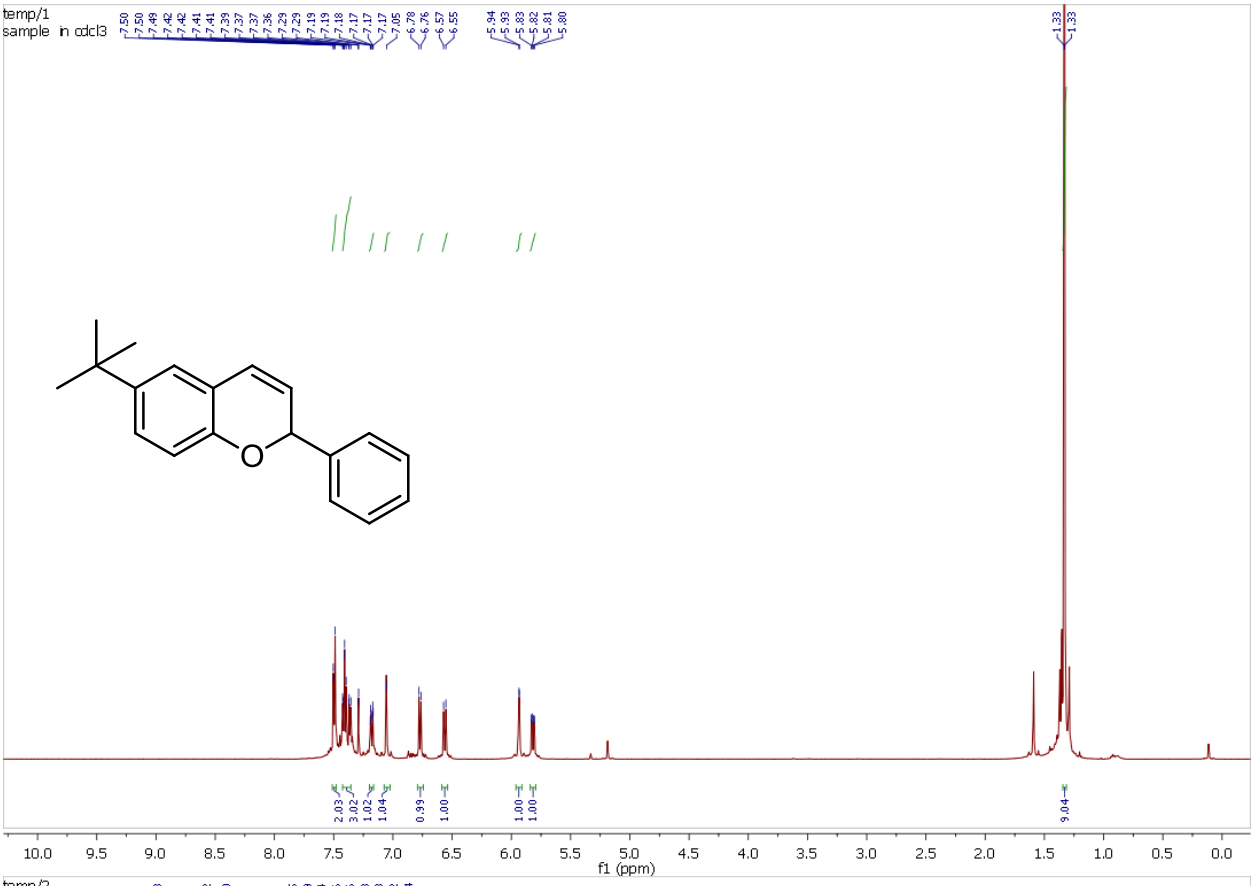

temp/2
sample in cdcl3
162.97
135.79
134.55
129.68
129.49
128.64
127.44
126.62
126.07
125.61
124.84
124.18
121.38
121.17
119.05
116.04
105.68
77.36
55.33
O
OMe
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

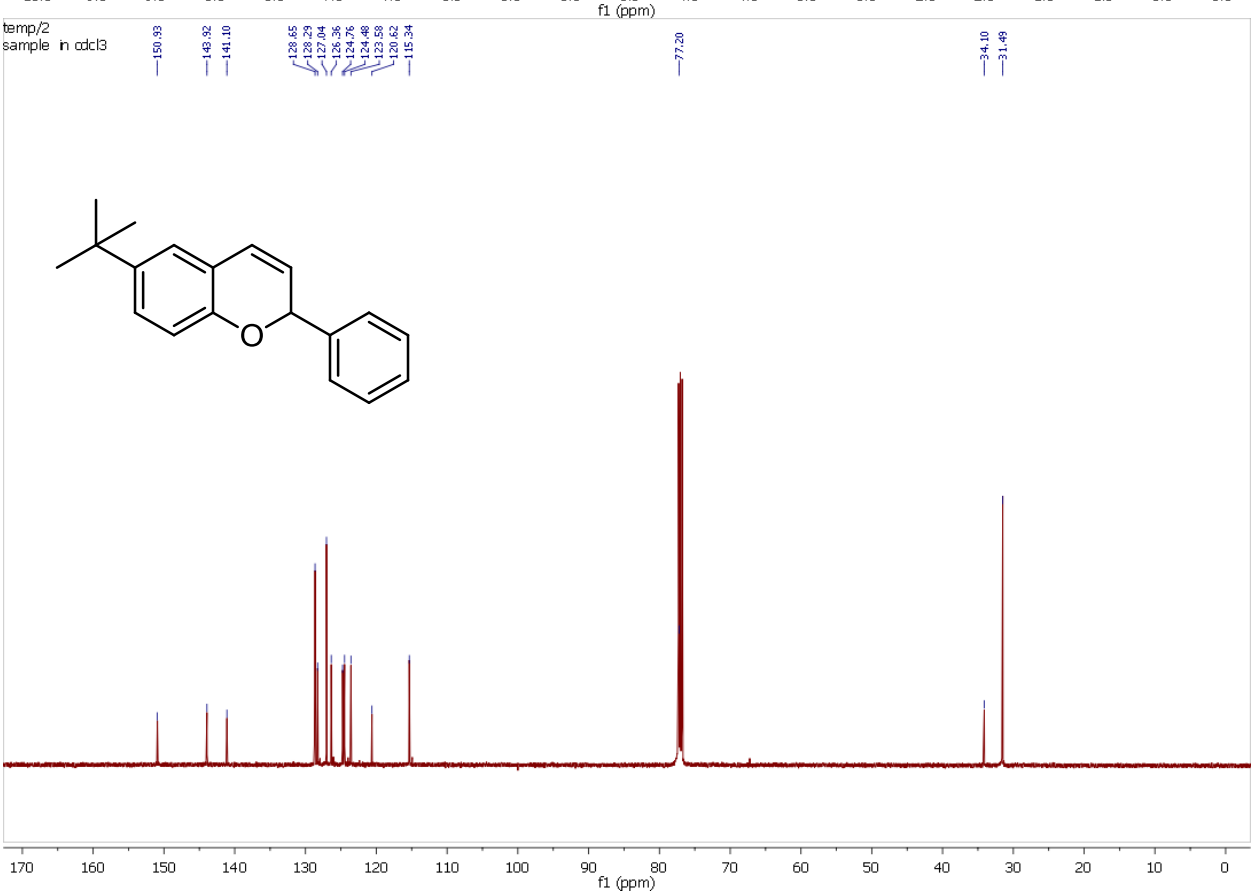

temp/1
sample in cdcl3
7.24
7.24
7.23
7.19
7.10
7.09
7.08
7.06
7.05
7.04
7.04
7.03
7.02
6.95
6.95
6.94
6.94
6.82
6.81
6.80
6.80
6.79
6.78
6.71
6.48
6.46
5.90
5.90
5.89
5.82
5.81
5.80
5.79
0.01
O
S
2.00
1.02
1.05
1.00
1.00
1.01
1.00
1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

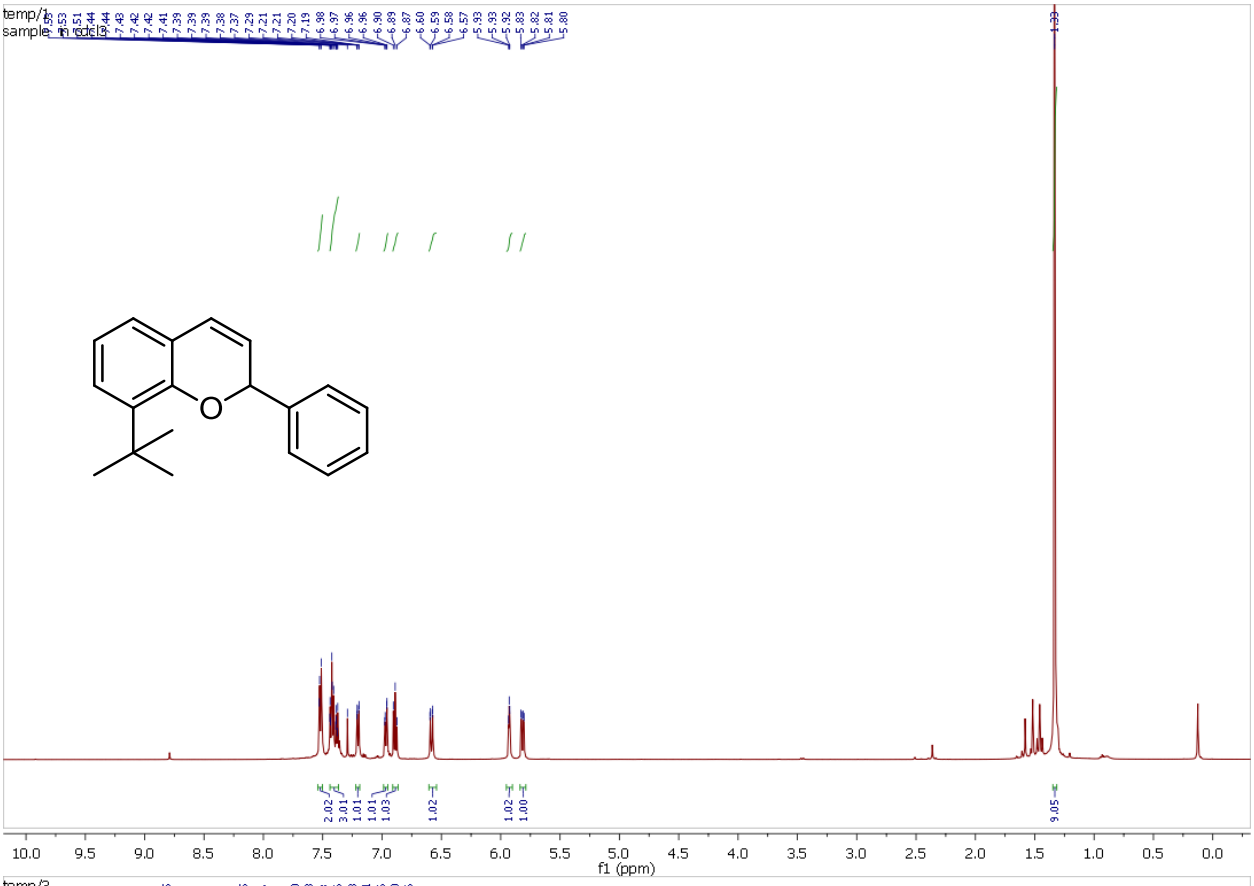

temp/2
sample in cdcl3
152.99
141.73
129.45
126.61
126.52
126.38
124.35
124.19
123.19
121.55
121.29
116.18
77.30
77.04
76.79
72.47
O
S
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

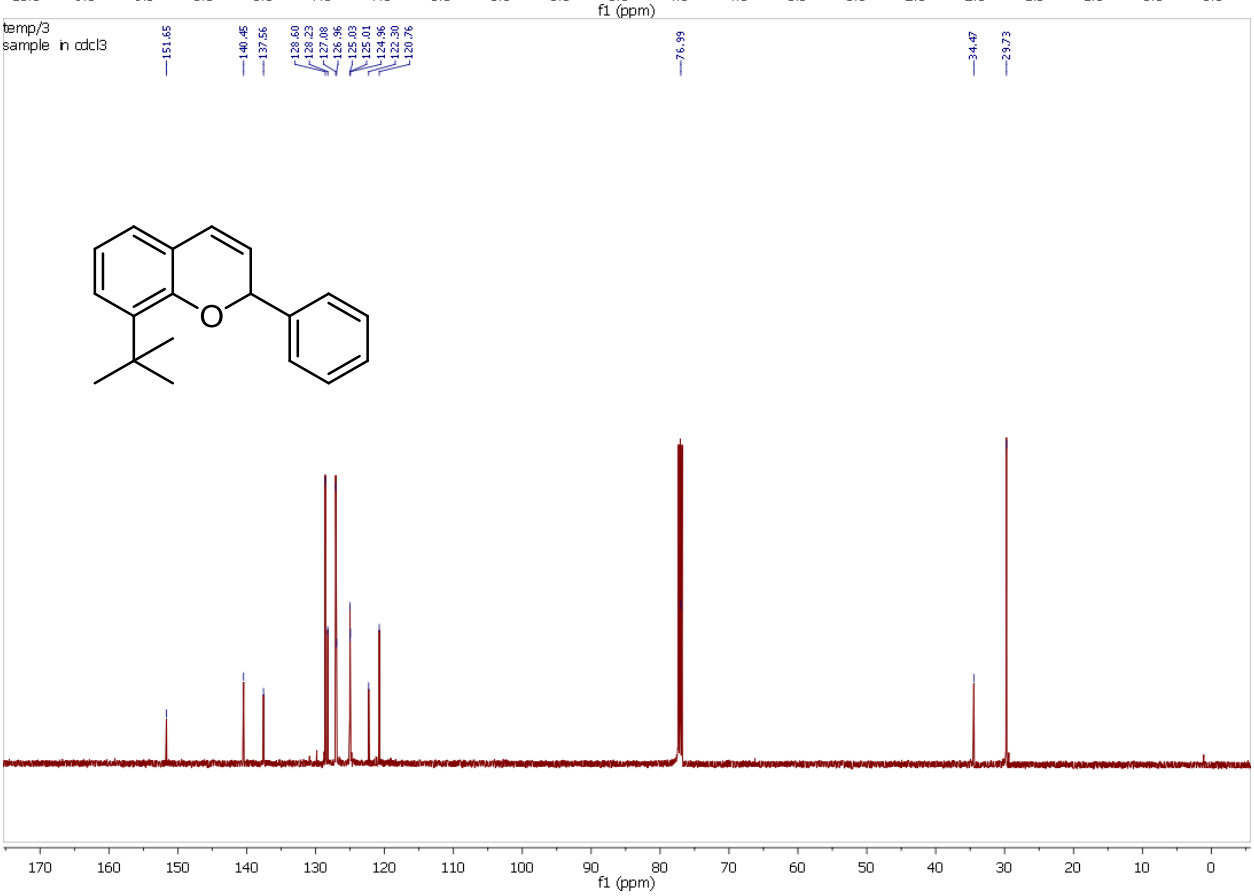

temp/2
sample in cdcl3
O
Ph
f1 (ppm)

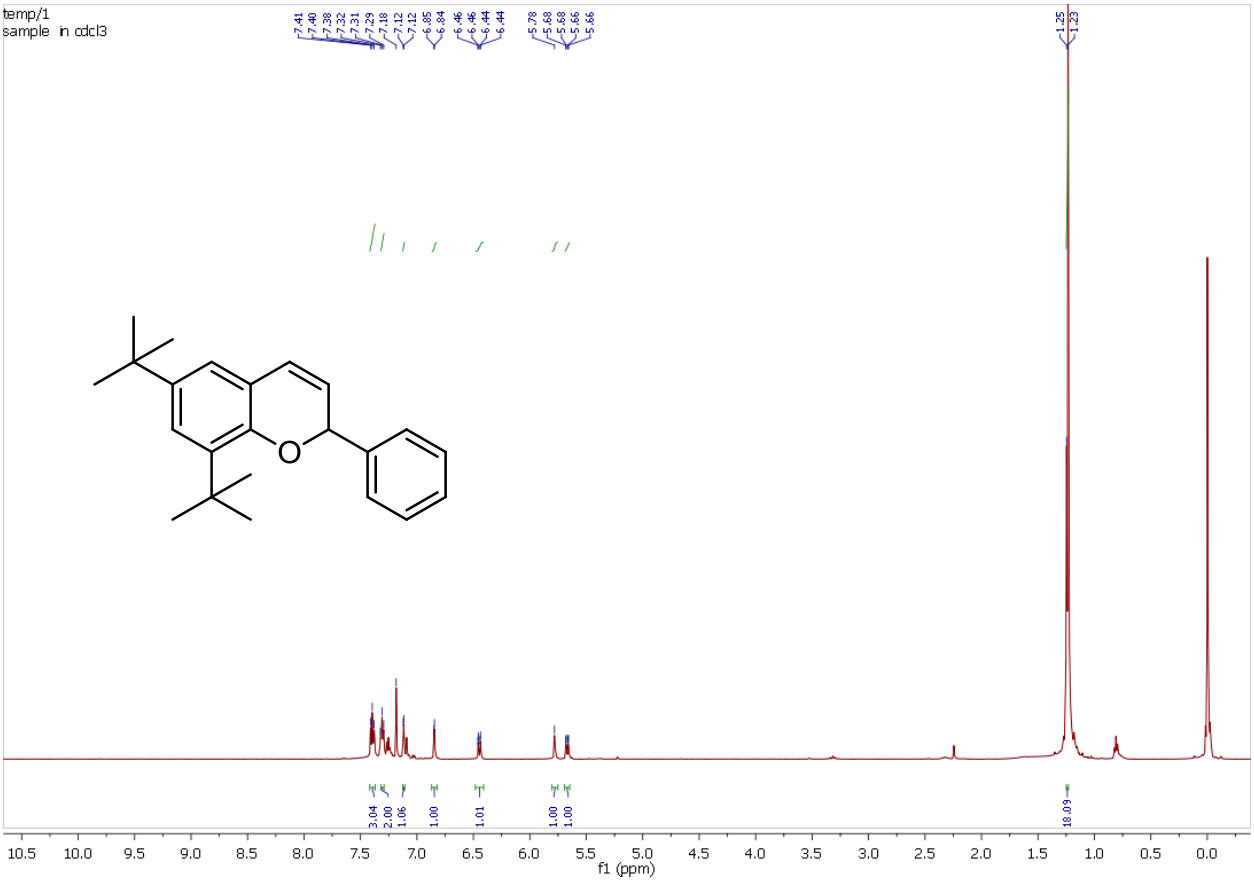

temp/1
sample in cdcl3
153.34
141.65
129.17
128.55
128.41
126.49
125.90
125.66
124.21
122.01
121.05
116.04
77.24
74.16
36.93
31.16
O
Ph
f1 (ppm)

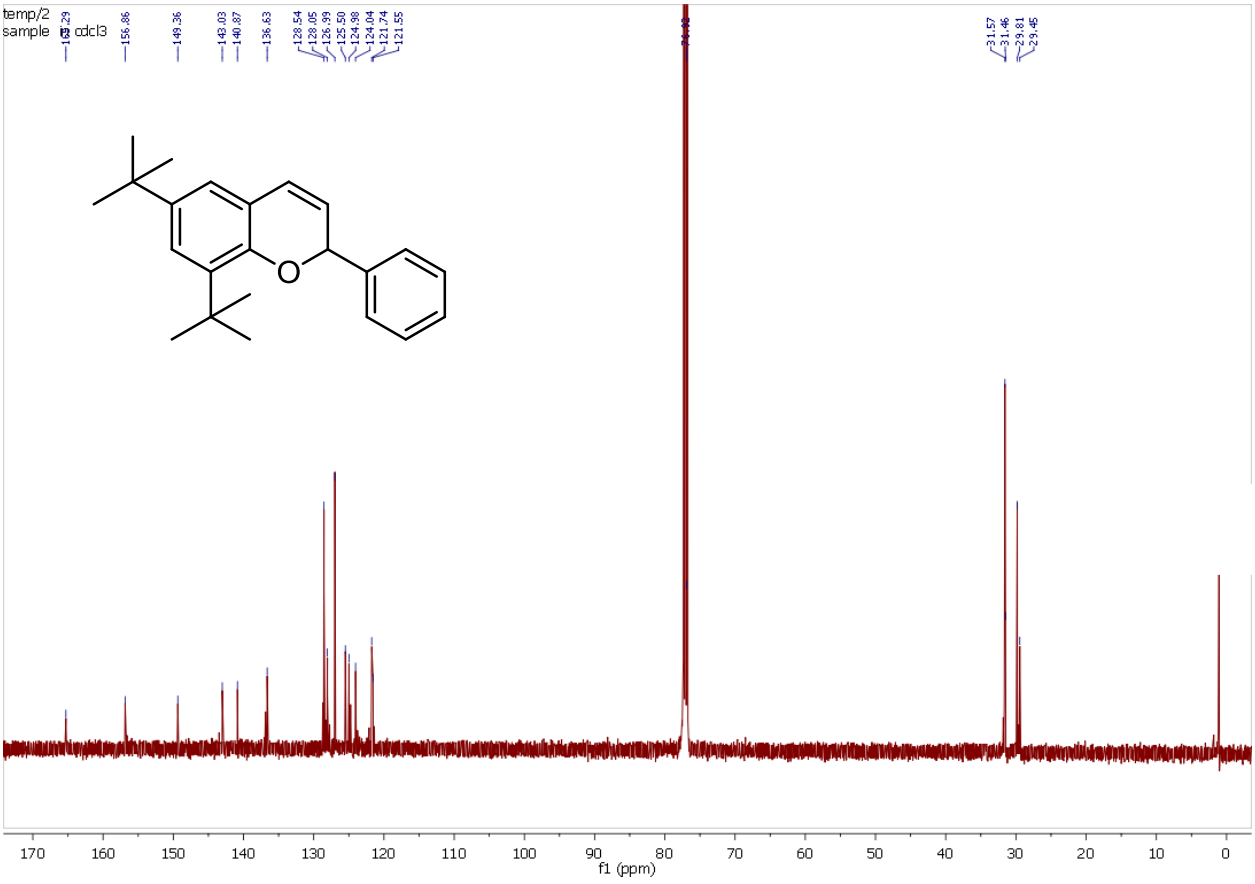

temp/1
sample in cdcl3
7.50
7.50
7.49
7.42
7.42
7.41
7.41
7.39
7.37
7.37
7.36
7.29
7.29
7.19
7.18
7.17
7.17
7.17
7.05
6.78
6.76
6.57
6.55
5.84
5.83
5.82
5.81
5.80
1.33
1.33
2.03
3.02
1.02
1.04
0.99
1.00
1.00
1.00
9.04
f1 (ppm)

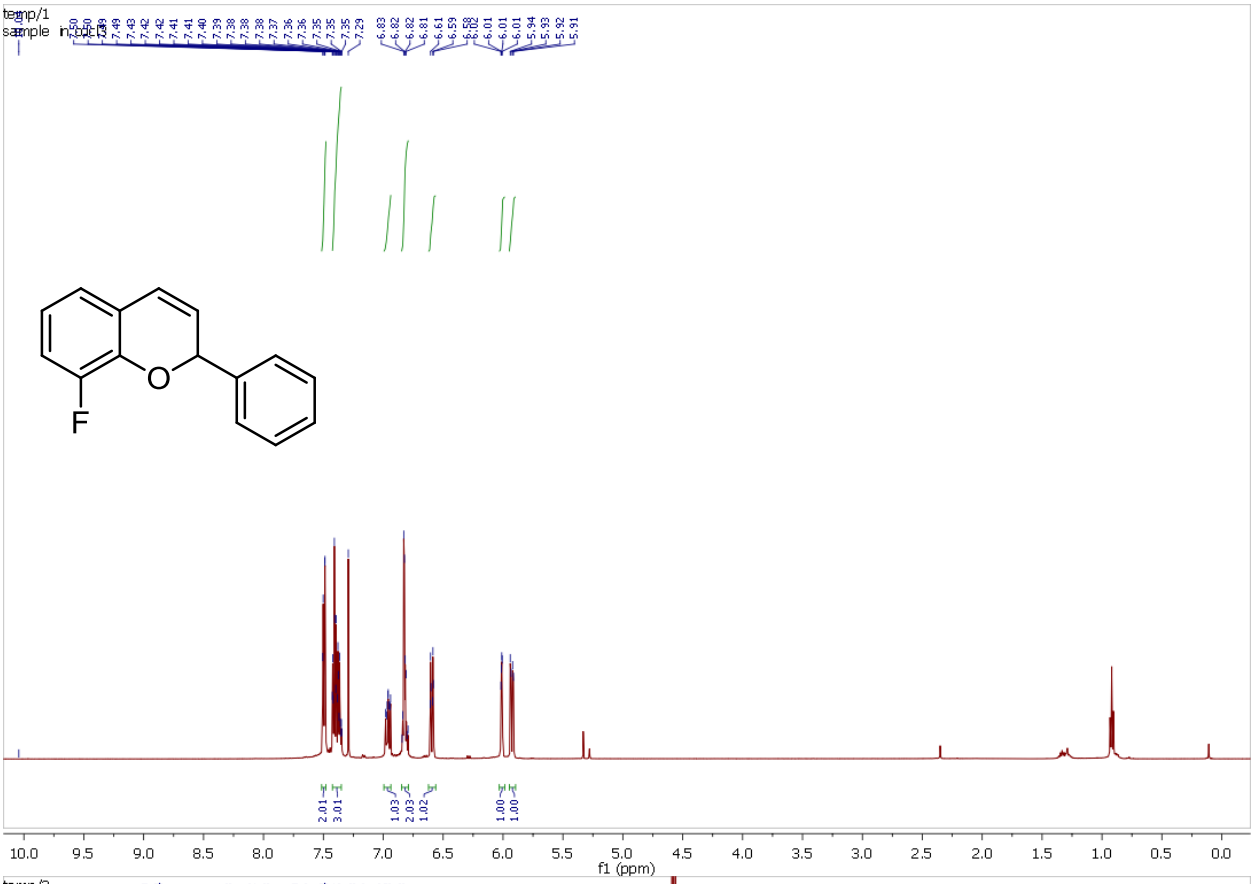

temp/2
sample in cdcl3
150.93
143.92
141.10
128.65
128.29
127.04
126.36
124.76
124.48
123.58
120.62
115.34
77.20
34.10
31.49
f1 (ppm)

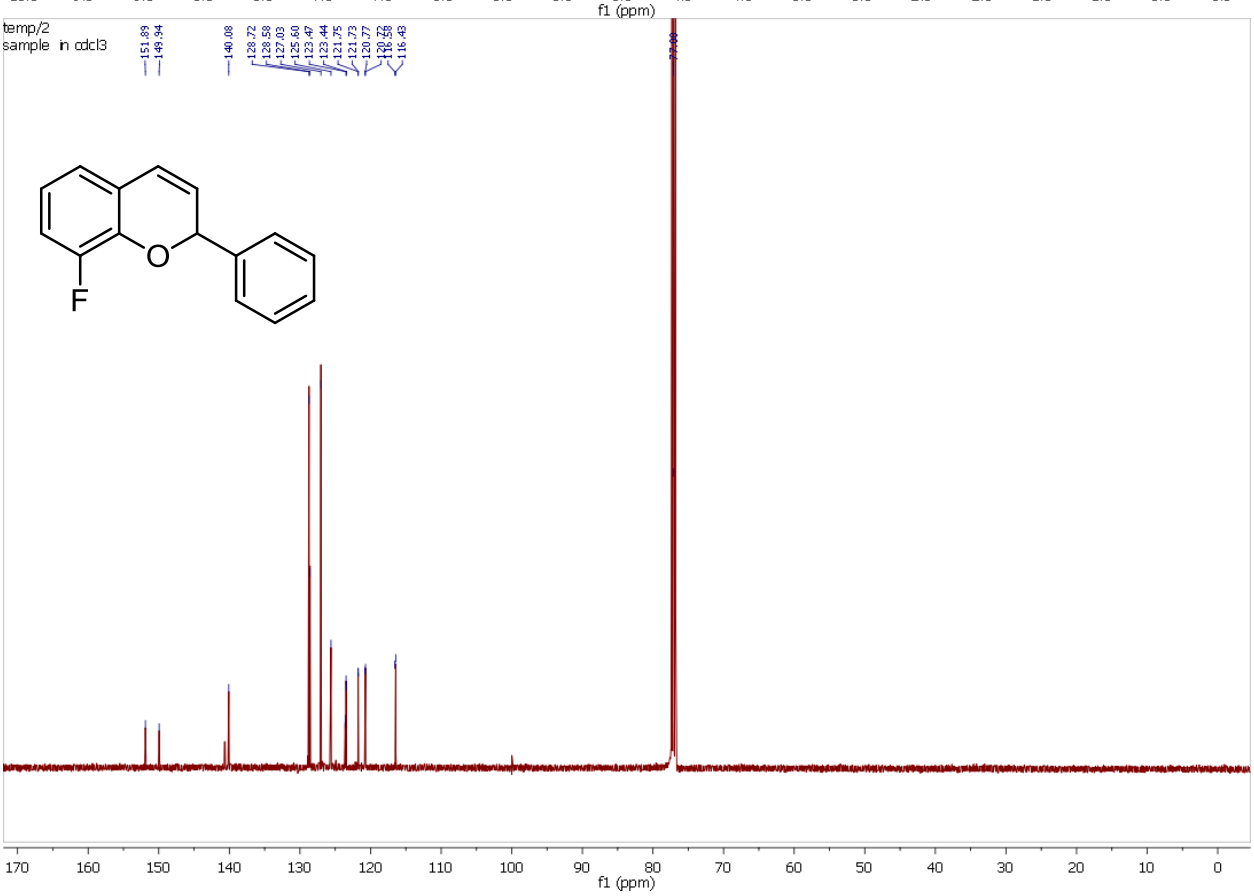

temp/3
sample in cdcl3
7.53
7.51
7.44
7.44
7.43
7.42
7.42
7.41
7.39
7.39
7.39
7.38
7.37
7.29
7.21
7.21
7.20
7.19
6.98
6.97
6.96
6.96
6.90
6.89
6.87
6.60
6.59
6.58
6.57
5.33
5.33
5.32
5.83
5.82
5.81
5.80
1.33
2.02
3.01
1.01
1.01
1.03
1.02
1.02
1.00
9.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

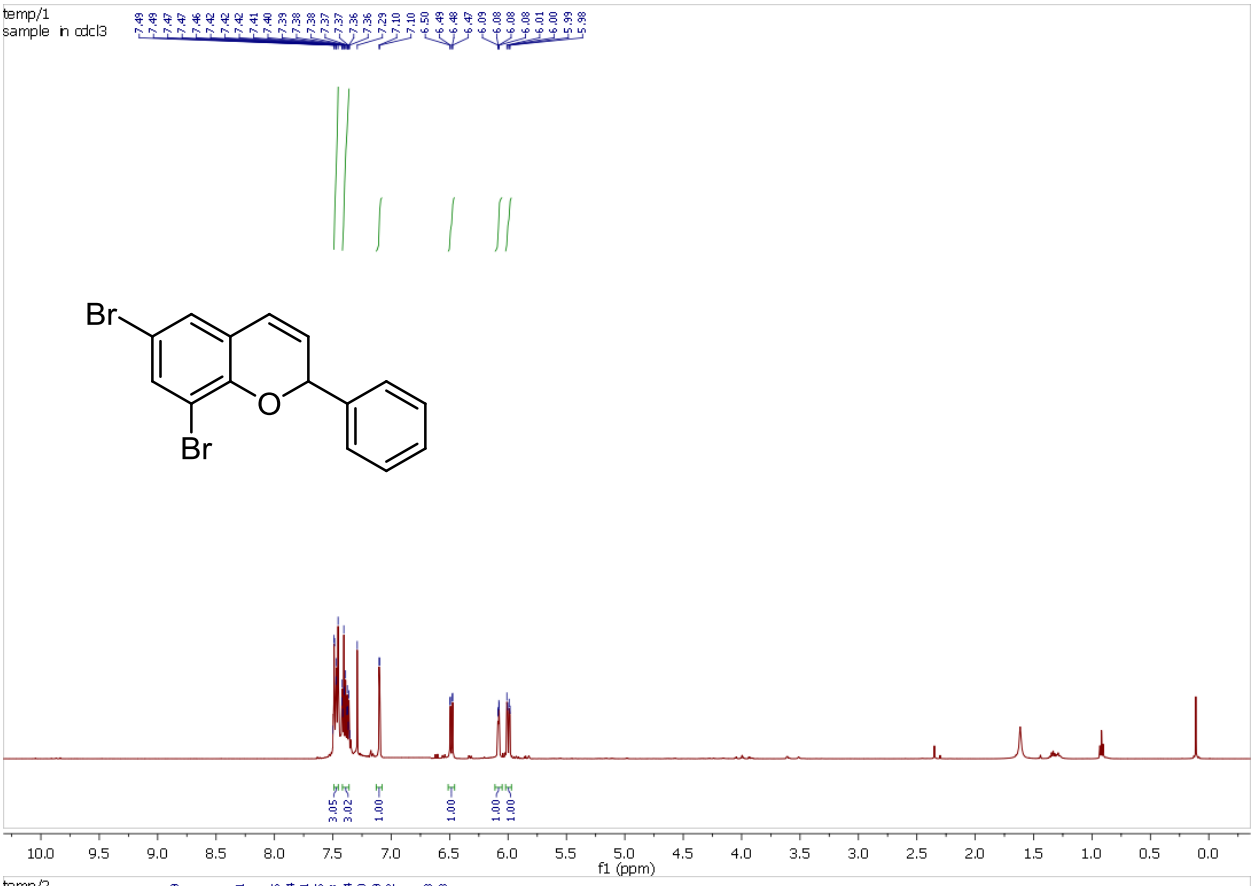

temp/3
sample in cdcl3
151.65
140.45
137.56
128.60
128.23
127.08
126.96
125.03
125.01
124.96
122.30
120.76
76.99
34.47
29.73
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

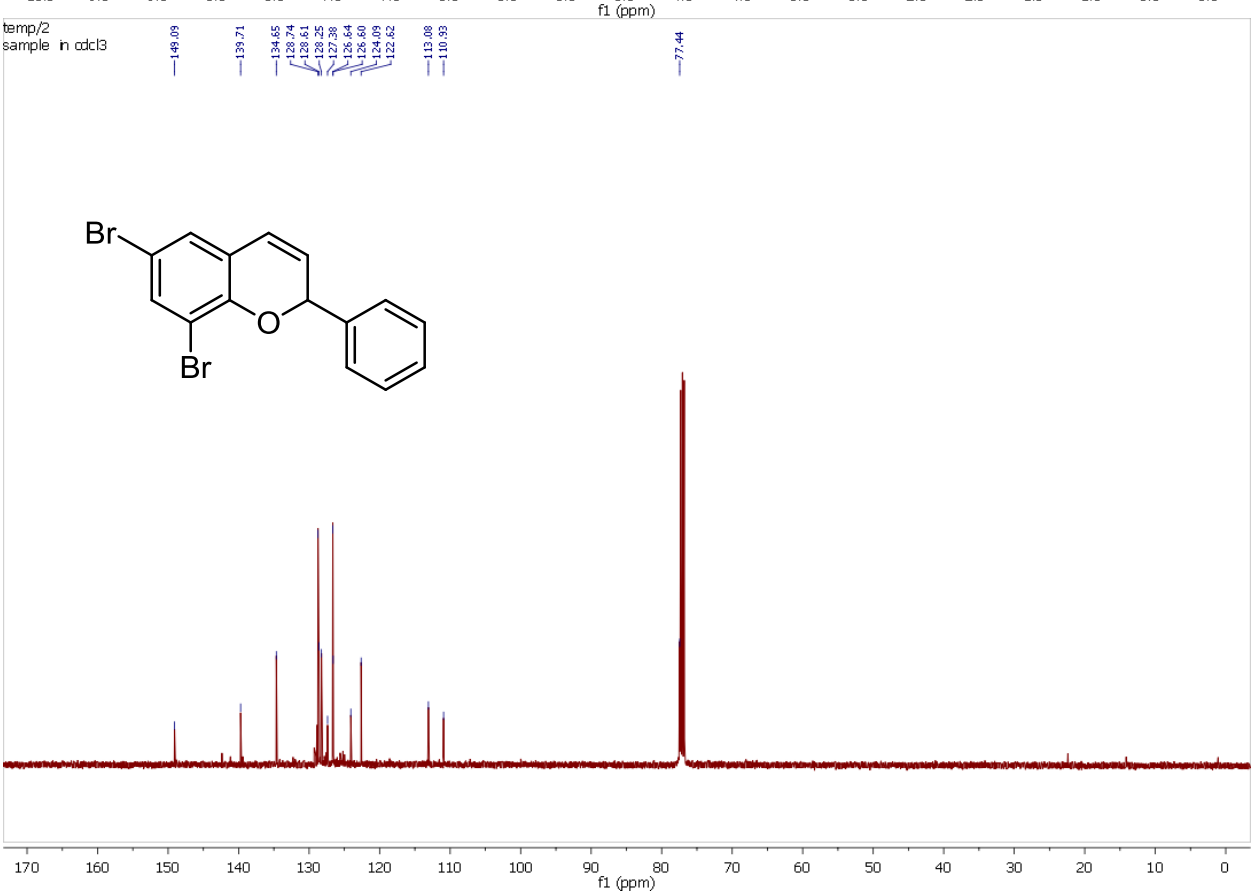

temp/1
sample in cdcl3
7.41
7.40
7.38
7.32
7.31
7.29
7.18
7.12
7.12
6.85
6.84
6.46
6.46
6.44
6.44
5.78
5.68
5.68
5.66
5.66
1.25
1.23
O
3.04
2.00
1.06
1.00
1.01
1.00
1.00
18.09
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

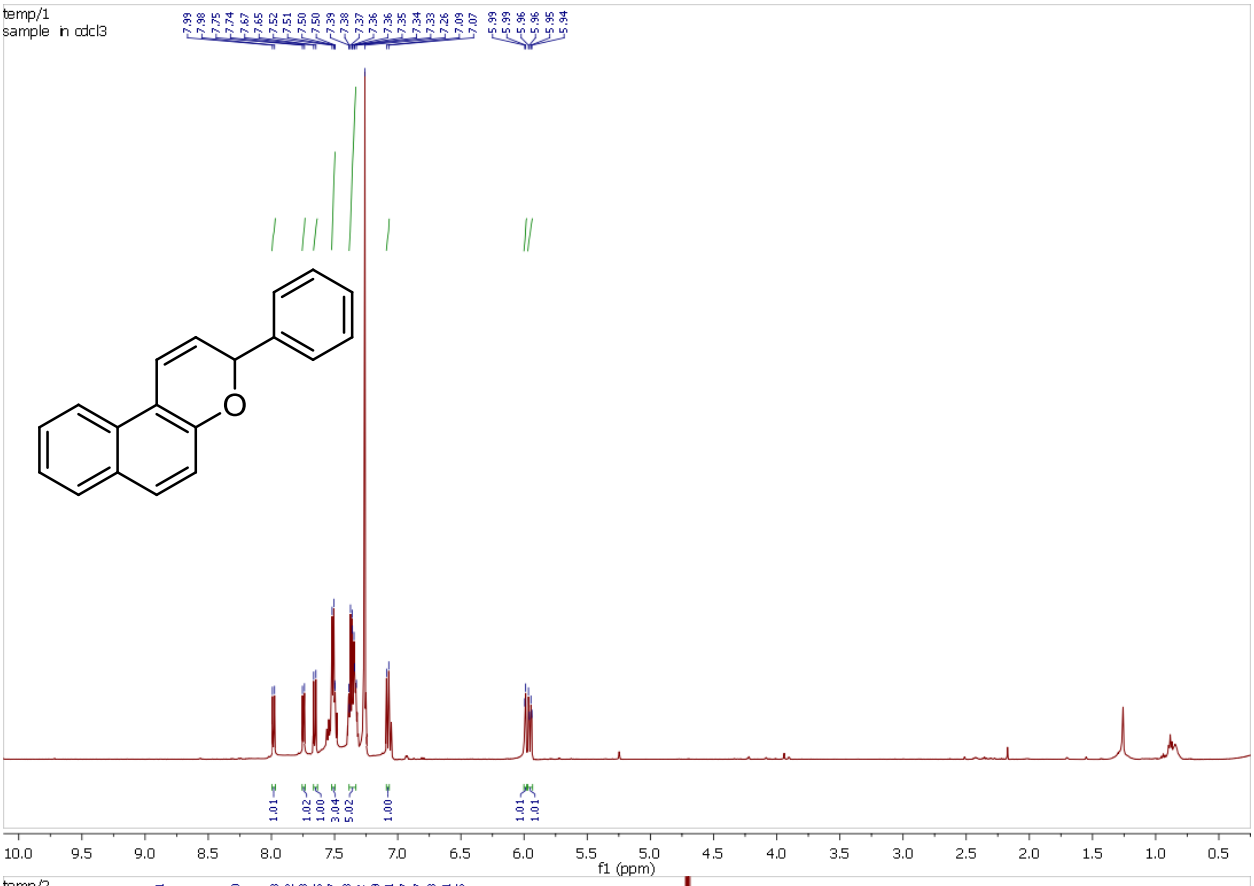

temp/2
sample in cdcl3
156.86
149.36
143.03
140.87
136.63
128.54
128.05
126.99
125.50
124.98
124.04
121.74
121.55
77.48
31.57
31.46
29.81
29.46
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

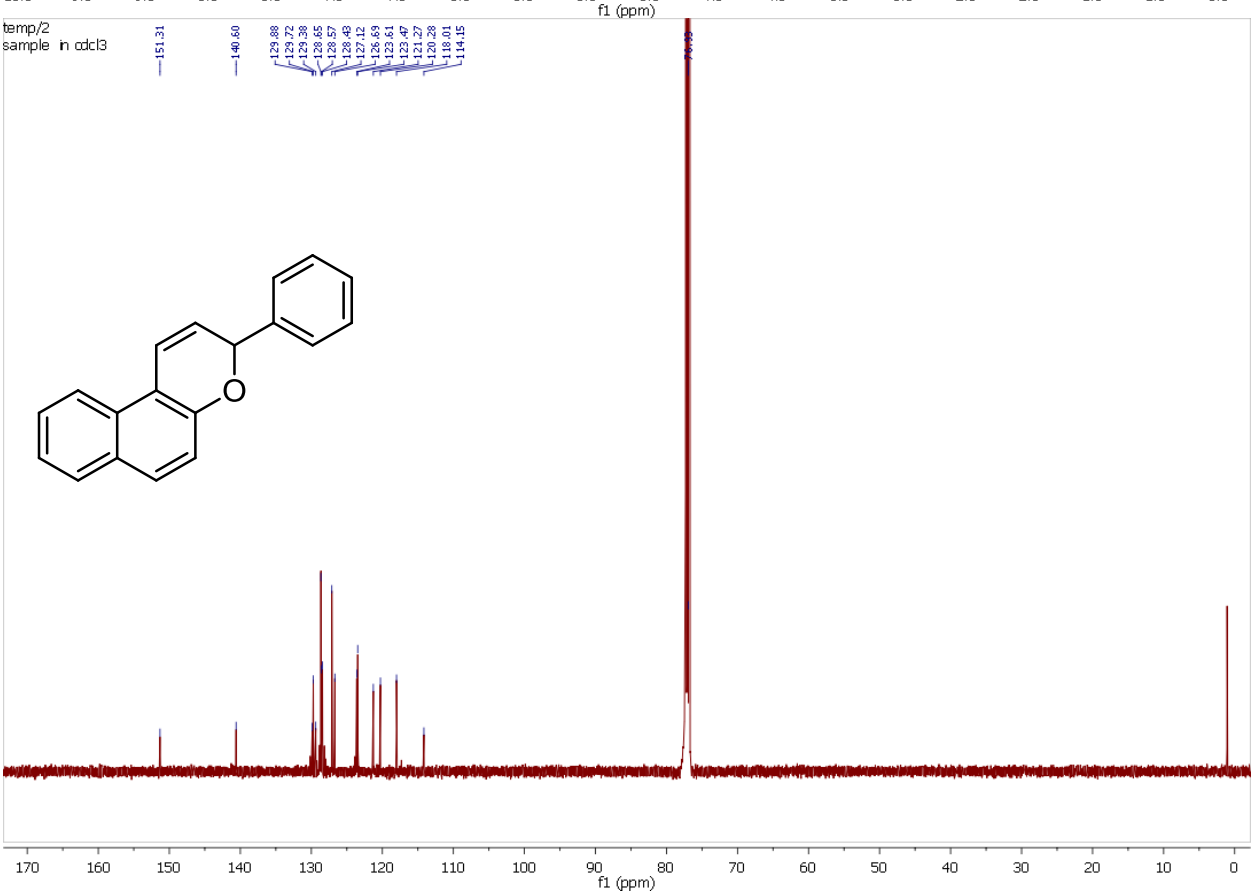

temp/1
sample in cdcl3
7.50
7.50
7.49
7.49
7.43
7.42
7.42
7.41
7.41
7.40
7.39
7.38
7.38
7.37
7.36
7.36
7.35
7.35
7.29
6.83
6.82
6.82
6.81
6.61
6.59
6.58
6.02
6.01
6.01
5.94
5.93
5.92
5.91
O
F
2.01
3.01
1.03
2.03
1.02
1.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


temp/2
sample in cdcl3
151.89
149.94
140.08
128.72
128.58
127.03
125.60
123.47
123.44
121.75
121.73
120.77
120.22
116.58
116.43
77.00
O
F
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


temp/1
sample in cdcl3
7.49
7.49
7.47
7.47
7.46
7.42
7.42
7.42
7.41
7.40
7.39
7.38
7.38
7.37
7.37
7.36
7.36
7.29
7.10
6.50
6.49
6.48
6.47
6.09
6.08
6.08
6.03
6.01
6.00
5.99
5.98
Br
O
Br
3.05
3.02
1.00
1.00
1.00
1.00
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
f1 (ppm)


temp/2
sample in cdcl3
149.09
139.71
134.65
128.74
128.61
128.25
127.38
126.64
126.60
124.09
122.62
113.08
110.93
77.44
Br
O
Br
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


temp/1
sample in cdcl3
7.99
7.98
7.75
7.74
7.67
7.65
7.52
7.51
7.50
7.50
7.39
7.38
7.37
7.36
7.36
7.35
7.34
7.33
7.26
7.09
7.07
5.39
5.39
5.36
5.36
5.35
5.34
1.01
1.02
1.00
3.04
5.02
1.00
1.01
1.01
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
f1 (ppm)


temp/2
sample in cdcl3
151.31
140.60
129.88
129.72
129.38
128.85
128.57
128.43
127.12
126.89
123.61
123.47
121.27
120.28
118.01
114.15
77.33
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Computational Part

Table S1. Energies of the calculated species

		SCF Au	G au	ZPE Au	SCF+ZPE au	Negative Eigen values
Salicyldehyde diazo	**disp3**	-455.24785	-455.16660	0.11494	-455.13291	-
	without disp3	-455.23528	-455.15411	0.11489	-455.12039	-
Co(por) (A)	**disp3**	-2371.97068	-2371.74586	0.26797	-2371.70271	-
	without disp3	-2371.92421	-2371.69951	0.26780	-2371.65641	-
Co(por)_ Salicyldehyde diazo (B) (C-bound)	**disp3**	-2827.24787	-2826.92214	0.38350	-2826.86437	-
	without disp3	-2827.15654	-2826.83007	0.38320	-2826.77334	-
TS1_N_2 elimination	**disp3**	-2827.23547	-2826.90864	0.38200	-2826.85347	-389.2500
	without disp3	-2827.13962	-2826.81466	0.38132	-2826.7583	-395.5900
Co_Carbene (C)	**disp3**	-2717.67378	-2717.35221	0.37478	2717.299	-
	without disp3	-2717.59189	-2717.27157	0.37403	-2717.21786	-
Co_Carbene (bridged)(C')	**disp3**	-2717.67882	-2717.35387	0.37637	-2717.30245	-
	without disp3	-2717.59717	-2717.27228	0.37615	-2717.22102	-
Phenylacetylene	**disp3**	-308.52305	-308.44676	0.10616	-308.41689	-
	without disp3	-308.51484	-308.43855	0.10615	-308.40869	-
TS2_phenylacetylene addition	**disp3**	-3026.20838	-3025.79094	0.48202	-3025.72636	-130.1600
	without disp3	-3026.09766	-3025.68217	0.48080	-3025.61686	-234.8900
N_2	**disp3**	-109.58042	-109.59343	0.00543	-109.57499	-
	without disp3	-109.58042	-109.59343	0.00543	-109.57499	-
Vinly Radical (D)	**disp3**	-3026.25878	-3025.83561	0.48518	-3025.7736	-

	without disp3	-3026.14421	-3025.72288	0.48416	-3025.66005	-
TS3_HAT	**disp3**	-3026.22659	-3025.80777	0.48050	-3025.74609	-1420.4900
	without disp3	-3026.11961	-3025.70156	0.47975	-3025.63986	-1286.3800
***Trans o*-quinone methide (E)**	**disp3**	-654.29807	-654.12213	0.21723	-654.08084	-
	without disp3	-654.27455	-654.09867	0.21710	-654.05745	-
***Cis o*-quinone methide (F)**	**disp3**	-654.29137	-654.11545	0.21737	-654.074	-
	without disp3	-654.26711	-654.09114	0.21733	-654.04978	-
TS4_ring closer	**disp3**	-654.28326	-654.10575	0.21698	-654.06628	-140.2800
	without disp3	-654.25723	-654.07992	0.21684	-654.04039	-159.6700
Chromene (G)	**disp3**	-654.31577	-654.13716	0.21931	-654.09646	-
	without disp3	-654.28987	-654.10867	0.21912	-654.07075	-
TS5_propene formation	**disp3**	-3026.23803	-3025.81743	0.48377	-3025.75426	-383.8300
	without disp3	-3026.12868	-3025.71136	0.48238	-3025.6463	-275.5600
Co(por)-propene (H)	**disp3**	-3026.26598	-3025.84398	0.48582	-3025.78016	-
	without disp3	-3026.15669	-3025.73798	0.48552	-3025.67117	-
Propene (I)	**disp3**	-654.25815	-654.08199	0.21674	-654.04141	-
	without disp3	-654.23213	-654.05632	0.21663	-654.0155	-

Cartesian coordinates of the calculated species:

Salicyldehyde diazo

With disp3				Without disp3			
16				16			
Energy = -455.2478496680				Energy = -455.2352774739			
C	0.9444701	-2.9314087	3.5439875	C	0.9406096	-2.9312201	3.5431628
H	2.0146827	-2.7719561	3.6445372	H	2.0115204	-2.7770122	3.6453308
C	0.5346928	-6.4784124	4.7028174	C	0.5357794	-6.4779484	4.7028704
C	-0.8416178	-6.6810459	4.5720021	C	-0.8402653	-6.6836161	4.5730806
C	-1.6496251	-5.6445228	4.0981764	C	-1.6505040	-5.6489305	4.0993971
C	-1.0816917	-4.4175918	3.7592964	C	-1.0854366	-4.4208035	3.7596376
C	0.3020354	-4.1891468	3.8822840	C	0.2979103	-4.1889715	3.8812169
C	1.1050731	-5.2506708	4.3640777	C	1.1028577	-5.2493721	4.3629107
H	1.1781509	-7.2812450	5.0724418	H	1.1811266	-7.2795488	5.0726623
H	-1.2746537	-7.6447156	4.8401073	H	-1.2712750	-7.6480698	4.8420734
H	-2.7246737	-5.7899234	3.9915092	H	-2.7254641	-5.7964204	3.9935783
H	-1.7219508	-3.6142409	3.3901405	H	-1.7279222	-3.6190798	3.3907290
O	2.4552189	-5.0062248	4.4767244	O	2.4526511	-5.0032523	4.4754712
N	0.2567160	-1.9178912	3.0967920	N	0.2603030	-1.9126156	3.0957980
N	-0.3757579	-1.0446403	2.7060955	N	-0.3566463	-1.0285232	2.7040968
H	2.8909307	-5.8063634	4.8170105	H	2.8867554	-5.8046158	4.8159843

Co(por) (A)

With disp3				Without disp3			
37				37			
Energy = -2371.9706760150				Energy = -2371.9242128370			
C	-0.5218465	1.8926277	-7.5020587	C	-0.5210918	1.8893813	-7.5018713
N	0.8606507	1.9747049	-7.5114249	N	0.8605355	1.9742194	-7.5112776
H	-2.0666365	1.6288470	-5.9000788	H	-2.0664368	1.6244997	-5.8997921

C	1.2305937	1.8512061	-6.1826265	C	1.2298029	1.8535072	-6.1827512
C	0.0730343	1.6905570	-5.3413752	C	0.0726177	1.6918400	-5.3410451
H	0.1101668	1.5738897	-4.2617578	H	0.1092233	1.5770737	-4.2611229
C	-1.0155883	1.7181430	-6.1605394	C	-1.0155144	1.7156028	-6.1604389
C	2.5297318	1.8822429	-5.7077965	C	2.5292742	1.8867528	-5.7083758
N	3.6264376	2.2009771	-7.8861025	N	3.6266581	2.2007990	-7.8859571
C	4.9570980	2.3419869	-8.2433536	C	4.9569085	2.3393849	-8.2429824
C	5.8083242	2.2793251	-7.0836645	C	5.8086084	2.2780083	-7.0834843
H	6.8910440	2.3658467	-7.1114647	H	6.8915226	2.3630923	-7.1110353
C	4.9935204	2.0958683	-6.0069913	C	4.9937175	2.0982291	-6.0066588
H	5.2614550	2.0000067	-4.9584292	H	5.2619365	2.0043803	-4.9579081
C	3.6448114	2.0495463	-6.5094975	C	3.6451257	2.0523744	-6.5097402
C	-1.3349062	1.9599358	-8.6194378	C	-1.3335336	1.9553890	-8.6200482
H	-1.1661414	2.3989051	-13.2025601	H	-1.1672177	2.4033691	-13.2021823
C	-0.8993091	2.3191610	-12.1523769	C	-0.8998550	2.3217326	-12.1521909
C	0.4499643	2.3576156	-11.6506844	C	0.4492347	2.3605785	-11.6498480
H	-2.8003517	2.1002437	-11.0426239	H	-2.8004583	2.0976424	-11.0435767
N	0.4666381	2.2308982	-10.2715868	N	0.4664314	2.2311968	-10.2717202
C	-0.8657374	2.1148354	-9.9117557	C	-0.8651964	2.1126517	-9.9126056
C	-1.7164787	2.1701788	-11.0721572	C	-1.7166002	2.1691353	-11.0725661
C	5.4250764	2.5145131	-9.5338466	C	5.4243060	2.5100778	-9.5341461
H	3.9852904	2.8248621	-13.8992891	H	3.9858650	2.8273624	-13.8993342
C	4.0212656	2.7245502	-12.8179982	C	4.0215326	2.7256588	-12.8180808
C	5.1075441	2.7310175	-11.9953092	C	5.1077884	2.7287770	-11.9959020
H	6.1575095	2.8364493	-12.2540687	H	6.1578648	2.8325057	-12.2552361
C	4.6132627	2.5641805	-10.6530500	C	4.6129070	2.5614172	-10.6538382
N	3.2324299	2.4574039	-10.6462352	N	3.2325675	2.4574128	-10.6464283
C	2.8641816	2.5562056	-11.9775546	C	2.8646489	2.5585064	-11.9769586
C	1.5662647	2.5072996	-12.4542092	C	1.5661171	2.5115996	-12.4527387
Co	2.0465432	2.2159811	-9.0788577	Co	2.0465701	2.2158155	-9.0788746

H 6.5007623 2.6125435 -9.6783633	H 6.5002668 2.6062654 -9.6789025
H -2.4119069 1.8810860 -8.4729271	H -2.4105361 1.8745083 -8.4737490
H 2.6841313 1.7735407 -4.6344727	H 2.6835278 1.7802560 -4.6346757
H 1.4131706 2.5968177 -13.5294746	H 1.4128814 2.6029965 -13.5279558

N_2

With disp3	Without disp3
2	2
Energy = -109.5804240180	Energy = -109.5804240180
N 1.9083652 4.4465698 -8.8585874	N 1.9083652 4.4465698 -8.8585874
N 1.6456348 5.4754302 -9.1554126	N 1.6456348 5.4754302 -9.1554126

Co(por)_ Salicyldehyde diazo (B) (C-bound)

With disp3	Without disp3
53	53
Energy = -2827.1565393360	Energy = -2827.1565393360
C 0.3790086 -0.1964625 0.3828159	C 0.3790086 -0.1964625 0.3828159
N 0.1505755 -1.5610185 0.4227677	N 0.1505755 -1.5610185 0.4227677
H -0.8747900 1.5903553 -0.1345152	H -0.8747900 1.5903553 -0.1345152
C -1.1729318 -1.7080476 0.0477075	C -1.1729318 -1.7080476 0.0477075
C -1.7767309 -0.4268198 -0.2204568	C -1.7767309 -0.4268198 -0.2204568
H -2.8073903 -0.2858397 -0.5350853	H -2.8073903 -0.2858397 -0.5350853
C -0.8089592 0.5113048 -0.0235115	C -0.8089592 0.5113048 -0.0235115
C -1.8255006 -2.9195347 -0.1125221	C -1.8255006 -2.9195347 -0.1125221
H -2.8715163 -2.8977102 -0.4183227	H -2.8715163 -2.8977102 -0.4183227
N 0.0970084 -4.3621027 0.4013128	N 0.0970084 -4.3621027 0.4013128
C 0.2716441 -5.7328799 0.3435951	C 0.2716441 -5.7328799 0.3435951
C -0.9425327 -6.3877241 -0.0743339	C -0.9425327 -6.3877241 -0.0743339
H -1.0496171 -7.4615503 -0.2025036	H -1.0496171 -7.4615503 -0.2025036
C -1.8699462 -5.4088701 -0.2665668	C -1.8699462 -5.4088701 -0.2665668

H	-2.9021405	-5.5030749	-0.5931237	H	-2.9021405	-5.5030749	-0.5931237
C	-1.2166329	-4.1566232	0.0227837	C	-1.2166329	-4.1566232	0.0227837
C	1.5740386	0.4250142	0.7061586	C	1.5740386	0.4250142	0.7061586
H	1.6177313	1.5118577	0.6351389	H	1.6177313	1.5118577	0.6351389
H	5.8498862	-0.4715274	2.1819535	H	5.8498862	-0.4715274	2.1819535
C	4.8184919	-0.5675794	1.8530881	C	4.8184919	-0.5675794	1.8530881
C	4.1238870	-1.8209245	1.6985698	C	4.1238870	-1.8209245	1.6985698
H	4.1047979	1.4872080	1.4530819	H	4.1047979	1.4872080	1.4530819
N	2.8281945	-1.6146766	1.2588966	N	2.8281945	-1.6146766	1.2588966
C	2.7138154	-0.2421876	1.1238047	C	2.7138154	-0.2421876	1.1238047
C	3.9455320	0.4126296	1.4856316	C	3.9455320	0.4126296	1.4856316
C	1.4451825	-6.4032485	0.6432883	C	1.4451825	-6.4032485	0.6432883
H	1.4462071	-7.4897591	0.5563945	H	1.4462071	-7.4897591	0.5563945
H	5.7779966	-5.6875289	2.0514726	H	5.7779966	-5.6875289	2.0514726
C	4.7428892	-5.5499216	1.7496777	C	4.7428892	-5.5499216	1.7496777
C	3.8308925	-6.4909479	1.3719824	C	3.8308925	-6.4909479	1.3719824
H	3.9549544	-7.5684562	1.3001187	H	3.9549544	-7.5684562	1.3001187
C	2.6167556	-5.7851922	1.0483726	C	2.6167556	-5.7851922	1.0483726
N	2.7827140	-4.4226787	1.2105043	N	2.7827140	-4.4226787	1.2105043
C	4.0874123	-4.2713266	1.6424178	C	4.0874123	-4.2713266	1.6424178
C	4.7072382	-3.0606775	1.9070612	C	4.7072382	-3.0606775	1.9070612
H	5.7409603	-3.0837452	2.2521276	H	5.7409603	-3.0837452	2.2521276
Co	1.4199897	-2.9957201	0.9653145	Co	1.4199897	-2.9957201	0.9653145
C	0.9661466	-3.0390585	3.1175582	C	0.9661466	-3.0390585	3.1175582
H	2.0141791	-2.9119926	3.4050716	H	2.0141791	-2.9119926	3.4050716
C	0.5140384	-6.4065136	4.8022904	C	0.5140384	-6.4065136	4.8022904
C	-0.8575463	-6.6216413	4.6661109	C	-0.8575463	-6.6216413	4.6661109
C	-1.6541916	-5.6602582	4.0390493	C	-1.6541916	-5.6602582	4.0390493
C	-1.0695485	-4.4973194	3.5403099	C	-1.0695485	-4.4973194	3.5403099
C	0.3080211	-4.2622739	3.6596187	C	0.3080211	-4.2622739	3.6596187

C 1.0965079 -5.2321920 4.3140480	C 1.0965079 -5.2321920 4.3140480
H 1.1427405 -7.1450427 5.3069352	H 1.1427405 -7.1450427 5.3069352
H -1.3008796 -7.5391310 5.0546657	H -1.3008796 -7.5391310 5.0546657
H -2.7264156 -5.8201867 3.9275607	H -2.7264156 -5.8201867 3.9275607
H -1.6890977 -3.7598258 3.0276881	H -1.6890977 -3.7598258 3.0276881
O 2.4315993 -4.9593028 4.4690482	O 2.4315993 -4.9593028 4.4690482
N 0.2845484 -1.9035702 3.3894337	N 0.2845484 -1.9035702 3.3894337
N -0.3349673 -0.9533708 3.4531168	N -0.3349673 -0.9533708 3.4531168
H 2.8857498 -5.7593339 4.7853977	H 2.8857498 -5.7593339 4.7853977

TS1_N_2 elimination

With disp3	Without disp3
53	53
Energy = -2827.2354749600	Energy = -2827.1396189350
C 0.3675738 -0.2134005 0.4144539	C 0.3431970 -0.2204843 0.4551374
N 0.1496594 -1.5809181 0.4493065	N 0.1358980 -1.5893339 0.4604353
H -0.9009721 1.5676625 -0.0748489	H -0.9294739 1.5603837 -0.0280590
C -1.1828509 -1.7313222 0.1016555	C -1.1843402 -1.7434817 0.0737955
C -1.7947386 -0.4531846 -0.1563483	C -1.8030376 -0.4657855 -0.1706641
H -2.8315290 -0.3171458 -0.4515265	H -2.8327893 -0.3320380 -0.4909979
C -0.8288100 0.4884846 0.0279104	C -0.8504572 0.4799952 0.0570688
C -1.8400793 -2.9400410 -0.0350891	C -1.8208942 -2.9569009 -0.1198150
H -2.8938966 -2.9200040 -0.3115968	H -2.8655708 -2.9410167 -0.4301888
N 0.0882283 -4.3731298 0.4746608	N 0.1156860 -4.3841218 0.3805799
C 0.2361122 -5.7487645 0.5217848	C 0.2965808 -5.7546410 0.3255003
C -0.9968201 -6.4098150 0.1782960	C -0.9106577 -6.4164672 -0.0989121
H -1.1252398 -7.4879927 0.1395255	H -1.0099418 -7.4907209 -0.2292882
C -1.9105224 -5.4308914 -0.0708492	C -1.8421738 -5.4429673 -0.2973362
H -2.9525372 -5.5291461 -0.3627206	H -2.8718210 -5.5428837 -0.6302017
C -1.2327247 -4.1736744 0.1190743	C -1.1990076 -4.1880139 -0.0003775

C	1.5573590	0.4152590	0.7317160	C	1.5286993	0.4106271	0.7882958
H	1.5905564	1.5030429	0.6766228	H	1.5546884	1.4995327	0.7499787
H	5.8501144	-0.4662049	2.1561064	H	5.8431497	-0.4626184	2.1517584
C	4.8174240	-0.5655277	1.8330066	C	4.8063685	-0.5642482	1.8423358
C	4.1298345	-1.8222892	1.6755498	C	4.1263482	-1.8227728	1.6664822
H	4.0807298	1.4876140	1.4654209	H	4.0503845	1.4895736	1.5230665
N	2.8319420	-1.6223627	1.2385020	N	2.8206049	-1.6254938	1.2553516
C	2.7035093	-0.2495238	1.1282413	C	2.6819148	-0.2521503	1.1698192
C	3.9331946	0.4112424	1.4859982	C	3.9103896	0.4118757	1.5258574
C	1.3947632	-6.4168634	0.8689200	C	1.4719276	-6.4189217	0.6272429
H	1.3701956	-7.5060398	0.8821773	H	1.4784450	-7.5056711	0.5438797
H	5.7458653	-5.6815830	2.2020249	H	5.8220744	-5.6731861	1.9561771
C	4.7143390	-5.5463236	1.8877531	C	4.7811051	-5.5425799	1.6722927
C	3.7795717	-6.4948718	1.5879132	C	3.8670894	-6.4896441	1.3175877
H	3.8797566	-7.5771583	1.5972290	H	3.9944858	-7.5668506	1.2482914
C	2.5813143	-5.7918642	1.2099922	C	2.6430709	-5.7929462	1.0174689
N	2.7778981	-4.4241622	1.2629794	N	2.8040520	-4.4279103	1.1698268
C	4.0847732	-4.2672515	1.6910252	C	4.1157938	-4.2691132	1.5799501
C	4.7156056	-3.0548947	1.9036446	C	4.7304581	-3.0564007	1.8396744
H	5.7482519	-3.0716555	2.2509997	H	5.7709920	-3.0724321	2.1635271
Co	1.4196907	-2.9975496	1.0037425	Co	1.4188947	-3.0154967	0.9845760
C	1.1026403	-3.0379813	2.9427917	C	1.0970685	-3.1424992	2.9404179
H	2.0637168	-2.8351392	3.4328860	H	2.0821386	-2.9945886	3.3998428
C	0.5643666	-6.4523771	4.4876376	C	0.4358961	-6.3466208	4.8825831
C	-0.8050620	-6.6268796	4.3037903	C	-0.9404851	-6.4910594	4.7244624
C	-1.5755312	-5.6019575	3.7400830	C	-1.6646885	-5.5443448	3.9907032
C	-0.9590105	-4.4222233	3.3430349	C	-0.9970124	-4.4700776	3.4121207
C	0.4255277	-4.2223270	3.4929701	C	0.3930619	-4.2929052	3.5473022
C	1.1785245	-5.2536281	4.1014612	C	1.1007476	-5.2527208	4.3119669
H	1.1682589	-7.2418714	4.9422793	H	1.0046599	-7.0788855	5.4628112

H -1.2735243 -7.5640396 4.6076483	H -1.4481529 -7.3426699 5.1797716
H -2.6477036 -5.7338919 3.5971897	H -2.7430410 -5.6484165 3.8704985
H -1.5422684 -3.6320188 2.8697572	H -1.5559640 -3.7306972 2.8376429
O 2.5169969 -5.0358209 4.2826418	O 2.4478114 -5.0740907 4.4744156
N 0.2133557 -1.6252282 3.6299648	N 0.3211735 -1.7232680 3.6846040
N -0.5392714 -0.8990624 3.1956990	N -0.4118276 -0.9295307 3.3449062
H 2.9684420 -5.8863031 4.4219115	H 2.8034805 -5.8253200 4.9808334

Co_Carbene (C)

With disp3	Without disp3
51	51
Energy = -2717.6737838360	Energy = -2717.5918869220
C 0.1860365 -0.3111737 0.8275010	C 0.1083216 -0.5372069 1.0583661
N 0.1061627 -1.6647286 0.5532266	N 0.1018984 -1.8600767 0.6535682
H -1.2407545 1.4100987 0.6510400	H -1.3934250 1.1275437 0.9987474
C -1.1729316 -1.8539971 0.0627999	C -1.1534104 -2.0571234 0.1054115
C -1.8973135 -0.6087037 0.0296463	C -1.9327244 -0.8469029 0.1618917
H -2.9186170 -0.5006966 -0.3252600	H -2.9464717 -0.7488743 -0.2169370
C -1.0587108 0.3467188 0.5215012	C -1.1568149 0.0908429 0.7750800
C -1.7095485 -3.0736046 -0.3122905	C -1.6264723 -3.2649859 -0.3782466
H -2.7298316 -3.0877933 -0.6944107	H -2.6352467 -3.2920532 -0.7895914
N 0.2264364 -4.4436835 0.3325680	N 0.3646725 -4.5946426 0.1815750
C 0.3923315 -5.8117956 0.4494967	C 0.6201199 -5.9534955 0.1201569
C -0.7887147 -6.5109600 0.0137380	C -0.5183649 -6.6666224 -0.3987045
H -0.8958537 -7.5920336 0.0087653	H -0.5566444 -7.7428070 -0.5430827
C -1.6801734 -5.5626011 -0.3887229	C -1.4674595 -5.7332509 -0.6870213
H -2.6822505 -5.6952935 -0.7870371	H -2.4576887 -5.8780832 -1.1103132
C -1.0565311 -4.2838102 -0.1610657	C -0.9223100 -4.4548674 -0.3081863
C 1.3260387 0.3482302 1.2505952	C 1.2069241 0.1326081 1.5680332
H 1.2611130 1.4221967 1.4240986	H 1.0811646 1.1764628 1.8558547

H	5.8384745	-0.3260058	1.9090888	H	5.7690954	-0.3190279	2.0429082
C	4.7788547	-0.4738245	1.7191349	C	4.7141136	-0.5151957	1.8714898
C	4.1681328	-1.7520932	1.4536837	C	4.1744516	-1.7894038	1.4682168
H	3.8399861	1.5238431	1.8577319	H	3.6582970	1.3841213	2.2805012
N	2.8108280	-1.6087578	1.2251978	N	2.8039844	-1.7128885	1.3057342
C	2.5615358	-0.2585134	1.3927113	C	2.4779126	-0.4114155	1.6374153
C	3.7780877	0.4510614	1.6970647	C	3.6571241	0.3358959	1.9942618
C	1.5445711	-6.4404653	0.8856122	C	1.8349900	-6.5474847	0.4120798
H	1.5367026	-7.5267065	0.9671721	H	1.9084212	-7.6318315	0.3312788
H	5.9739054	-5.5522508	1.8064133	H	6.2472987	-5.4534083	1.1706596
C	4.9146637	-5.4522818	1.5860954	C	5.1695729	-5.4080936	1.0394407
C	3.9721733	-6.4311824	1.4649146	C	4.2911970	-6.4308251	0.8371043
H	4.0931032	-7.5064883	1.5603647	H	4.4938956	-7.4955200	0.7592303
C	2.7287017	-5.7779109	1.1535251	C	2.9859465	-5.8376446	0.7062797
N	2.8998942	-4.4035544	1.1000979	N	3.0573308	-4.4612660	0.8368637
C	4.2412106	-4.1963580	1.3792660	C	4.3963206	-4.1931445	1.0613698
C	4.8456867	-2.9578571	1.5088876	C	4.9278412	-2.9429011	1.3311620
H	5.9145476	-2.9326933	1.7198125	H	6.0037326	-2.8711812	1.4901209
Co	1.4808654	-3.0389954	0.9397884	Co	1.5470747	-3.1935754	0.9033314
C	1.2476242	-3.2538556	2.8066485	C	1.3443474	-3.5759239	2.7527993
H	2.1799989	-3.0036517	3.3383633	H	2.3475484	-3.5414125	3.2012719
C	0.0906659	-6.1909410	4.8652148	C	-0.3760443	-5.4883262	5.4909369
C	-1.2809124	-6.1542993	4.6274134	C	-1.7178301	-5.3191389	5.1504602
C	-1.8298120	-5.1924253	3.7620867	C	-2.0626628	-4.6290809	3.9761871
C	-0.9998102	-4.2631530	3.1558741	C	-1.0715546	-4.0998286	3.1662720
C	0.3986064	-4.2498767	3.3867433	C	0.3138860	-4.2231527	3.4797577
C	0.9310429	-5.2626871	4.2412664	C	0.6284000	-4.9712615	4.6723147
H	0.5363839	-6.9490697	5.5100828	H	-0.0823965	-6.0435893	6.3827349
H	-1.9281985	-6.8874683	5.1110458	H	-2.4946212	-5.7323049	5.7951735
H	-2.9034012	-5.1730807	3.5737207	H	-3.1114877	-4.4992404	3.7062762

H -1.4058865 -3.5010094 2.4905373	H -1.3427808 -3.5401377 2.2736988
O 2.2713989 -5.3860878 4.4568474	O 1.9176313 -5.2121367 5.0503764
H 2.7294868 -4.7767293 3.8404025	H 2.4988960 -4.9051410 4.3246901

Phenylacetylene

With disp3	Without disp3
14	14
Energy = -308.5230504593	Energy = -308.5148399335
C 0.0000000 0.0000002 0.9548009	C 0.0000000 0.0000002 0.9560694
H 0.0000000 0.0000001 2.0247447	H 0.0000000 0.0000001 2.0258633
C 0.0000000 0.0000003 -0.2594158	C 0.0000000 0.0000003 -0.2582813
C 0.0000000 0.0000002 -1.6842608	C 0.0000000 0.0000002 -1.6837684
C 0.0000000 -0.0000003 -4.4952975	C 0.0000000 -0.0000003 -4.4955702
C 0.0000000 1.2149793 -2.4004282	C 0.0000000 1.2146008 -2.4007510
C 0.0000000 -1.2149792 -2.4004279	C 0.0000000 -1.2146007 -2.4007506
C 0.0000000 -1.2096755 -3.7939138	C 0.0000000 -1.2093330 -3.7941562
C 0.0000000 1.2096752 -3.7939142	C 0.0000000 1.2093327 -3.7941566
H 0.0000000 -2.1555577 -1.8492289	H 0.0000000 -2.1555482 -1.8502249
H 0.0000000 -2.1560274 -4.3364346	H 0.0000000 -2.1558137 -4.3365871
H 0.0000000 -0.0000005 -5.5858878	H 0.0000000 -0.0000005 -5.5862018
H 0.0000000 2.1560268 -4.3364353	H 0.0000000 2.1558132 -4.3365878
H 0.0000000 2.1555579 -1.8492295	H 0.0000000 2.1555484 -1.8502255

TS2_(phenylacetylene addition)

With disp3	Without disp3
65	65
Energy = -3026.2083834980	Energy = -3026.0976630000
C -0.2510056 -0.2135064 0.9083535	C -0.2724931 -0.3017679 0.8444696

N	-0.3676876	-1.5792806	0.7141094	N	-0.4040544	-1.6684757	0.6685666
H	-1.6183224	1.5365268	0.6013733	H	-1.6269532	1.4589446	0.5367248
C	-1.6422460	-1.7568986	0.2056565	C	-1.6894386	-1.8378129	0.1844681
C	-2.3329788	-0.4967737	0.1004482	C	-2.3698961	-0.5729295	0.0752299
H	-3.3456176	-0.3796668	-0.2758803	H	-3.3869875	-0.4499153	-0.2874235
C	-1.4682214	0.4621667	0.5386210	C	-1.4889687	0.3821465	0.4871560
C	-2.1835735	-2.9710751	-0.1797132	C	-2.2461110	-3.0502024	-0.1851125
H	-3.1952225	-2.9740088	-0.5845740	H	-3.2665686	-3.0481217	-0.5678476
N	-0.2603029	-4.3630485	0.4593794	N	-0.2970663	-4.4480668	0.3597635
C	-0.0776376	-5.7343173	0.4741752	C	-0.0847618	-5.8120797	0.2691321
C	-1.2262960	-6.4122691	-0.0702224	C	-1.2420924	-6.4804799	-0.2685646
H	-1.3126432	-7.4907187	-0.1689975	H	-1.3086596	-7.5511486	-0.4413384
C	-2.1235048	-5.4482407	-0.4164622	C	-2.1726909	-5.5171360	-0.5114881
H	-3.1091380	-5.5616621	-0.8592995	H	-3.1712838	-5.6234104	-0.9264026
C	-1.5275045	-4.1831568	-0.0681577	C	-1.5847618	-4.2634211	-0.1126399
C	0.8812548	0.4342475	1.3670733	C	0.8783316	0.3413658	1.2651599
H	0.8447005	1.5189175	1.4639487	H	0.8498920	1.4268203	1.3592374
H	5.1927248	-0.3598174	2.7825790	H	5.2632506	-0.4504864	2.4333326
C	4.1757496	-0.4798790	2.4193971	C	4.2244736	-0.5717018	2.1379937
C	3.5565540	-1.7491298	2.1334127	C	3.5977034	-1.8391465	1.8578663
H	3.3330428	1.5583800	2.2421189	H	3.3623244	1.4630919	2.0447106
N	2.2648910	-1.5739821	1.6704383	N	2.2778429	-1.6665906	1.4856754
C	2.0599076	-0.2064874	1.7010729	C	2.0699377	-0.3014254	1.5483088
C	3.2453313	0.4792710	2.1494962	C	3.2741273	0.3846485	1.9434726
C	1.0421020	-6.3885214	0.9537315	C	1.0844144	-6.4647324	0.6154914
H	1.0418516	-7.4778605	0.9401078	H	1.1146404	-7.5489394	0.5095949
H	5.2456027	-5.5831040	2.6648484	H	5.4027739	-5.6521149	2.0041389
C	4.2420026	-5.4644076	2.2660975	C	4.3612008	-5.5382333	1.7160743
C	3.3530476	-6.4271896	1.8904337	C	3.4671801	-6.4991153	1.3490180
H	3.4690396	-7.5069331	1.9162676	H	3.6157651	-7.5727377	1.2718573

C	2.1715190	-5.7479086	1.4287867	C	2.2306854	-5.8247108	1.0512005
N	2.3304062	-4.3750848	1.5148104	N	2.3600137	-4.4581228	1.2288670
C	3.6009050	-4.1944559	2.0411704	C	3.6684857	-4.2774132	1.6455340
C	4.1799454	-2.9704223	2.3246854	C	4.2493804	-3.0575556	1.9473429
H	5.1926960	-2.9678076	2.7265282	H	5.2928810	-3.0553406	2.2617866
Co	0.9436336	-2.9885168	1.2217969	Co	0.9340889	-3.0851223	1.1082022
C	0.5264955	-3.2760864	3.0618082	C	0.6179337	-3.3920876	2.9977759
H	1.4237496	-3.0280871	3.6522275	H	1.6002237	-3.2818147	3.4838023
C	-0.4918909	-6.4009465	4.9229741	C	-0.6397569	-6.2408676	5.1573274
C	-1.8361862	-6.4857083	4.5743194	C	-1.9950840	-6.2317334	4.8452049
C	-2.4113299	-5.5368686	3.7119189	C	-2.4985288	-5.3241617	3.8993518
C	-1.6296904	-4.5071057	3.2141050	C	-1.6359573	-4.4330125	3.2803689
C	-0.2605437	-4.3778715	3.5476792	C	-0.2482905	-4.3975424	3.5695626
C	0.2995498	-5.3644584	4.4115852	C	0.2321537	-5.3422338	4.5294923
H	-0.0259824	-7.1383929	5.5773778	H	-0.2283127	-6.9447179	5.8818475
H	-2.4427202	-7.3005777	4.9729211	H	-2.6652313	-6.9366041	5.3401939
H	-3.4646078	-5.6077146	3.4403038	H	-3.5617863	-5.3153877	3.6583191
H	-2.0576054	-3.7558660	2.5501804	H	-2.0221983	-3.7142642	2.5574393
O	1.6162489	-5.3665884	4.7544974	O	1.5459356	-5.4272949	4.8758418
H	2.0636317	-4.6477631	4.2608940	H	2.0427854	-4.7758384	4.3388991
C	-0.5282649	-1.2360438	4.0840765	C	-0.0991548	-1.4555467	4.1671532
C	0.2560233	-1.1243527	5.0144208	C	0.5854950	-1.2879241	5.1749499
C	1.2969253	-1.1977033	5.9724461	C	1.4433952	-1.2088779	6.2968971
C	3.4111023	-1.4198392	7.8154158	C	3.1406077	-1.0336280	8.5413674
C	1.1246198	-1.9105562	7.1798994	C	1.1409831	-1.9090980	7.4896186
C	2.5483330	-0.5972996	5.7061497	C	2.6169005	-0.4176886	6.2568380
C	3.5908898	-0.7123672	6.6214615	C	3.4505267	-0.3357037	7.3685544
C	2.1752891	-2.0175999	8.0874541	C	1.9839259	-1.8196260	8.5933929
H	0.1643773	-2.3851528	7.3820573	H	0.2399940	-2.5215495	7.5278017
H	2.0316656	-2.5762578	9.0134252	H	1.7376009	-2.3684869	9.5036371

H 4.2306627 -1.5078296 8.5297788	H 3.7967415 -0.9654856 9.4098149
H 4.5535105 -0.2486225 6.4001405	H 4.3513534 0.2785725 7.3216479
H 2.6895485 -0.0637659 4.7663839	H 2.8578061 0.1219022 5.3405528
H -1.2928060 -1.1619529 3.3384868	H -0.8706668 -1.2778598 3.4447886

Vinly Radical (D)

With disp3	Without disp3
65	65
Energy = -3026.2587781870	Energy = -3026.1442121360
C 0.1002396 -0.2426117 1.4304155	C -0.1096365 -0.3612766 1.1421785
N -0.1934600 -1.5717411 1.1812173	N -0.3034776 -1.7272463 1.0215648
H -1.0831460 1.6607656 1.4010860	H -1.4404352 1.4341489 0.9577079
C -1.5428329 -1.5797100 0.8652199	C -1.6489145 -1.8682211 0.7290166
C -2.0938992 -0.2503461 0.9317519	C -2.3030940 -0.5850166 0.6902664
H -3.1304680 -0.0029228 0.7196838	H -3.3576527 -0.4377282 0.4727115
C -1.0688517 0.5824526 1.2688065	C -1.3422368 0.3523285 0.9278671
C -2.2609505 -2.6949223 0.4741553	C -2.2706574 -3.0641824 0.4123864
H -3.3186003 -2.5680745 0.2430281	H -3.3374201 -3.0436621 0.1899689
N -0.3894722 -4.2799084 0.5819230	N -0.2519049 -4.4541835 0.5144840
C -0.2978992 -5.6273625 0.2794423	C -0.0071487 -5.7631813 0.1373593
C -1.5588875 -6.1356148 -0.1979748	C -1.2061954 -6.3873371 -0.3641423
H -1.7296670 -7.1638466 -0.5041456	H -1.2604793 -7.4085876 -0.7310558
C -2.4349141 -5.0934812 -0.1761758	C -2.1988107 -5.4607270 -0.2697103
H -3.4829187 -5.0777361 -0.4622752	H -3.2445230 -5.5524199 -0.5501450
C -1.7047834 -3.9500644 0.3083373	C -1.5969480 -4.2629668 0.2600326
C 1.3348789 0.2421268 1.8211347	C 1.0925558 0.2475088 1.4564917
H 1.4361897 1.3173009 1.9694283	H 1.1153776 1.3360892 1.5063336
H 5.5089058 -1.1638750 3.1668934	H 5.3877204 -0.7247732 2.8126286
C 4.4904672 -1.1338098 2.7900477	C 4.3608259 -0.8026704 2.4661049
C 3.7351092 -2.2921509 2.3865784	C 3.6830100 -2.0446707 2.1948054

H	3.9110199	0.9986449	2.7444695	H	3.6308889	1.2711019	2.2209010
N	2.4729263	-1.9308390	1.9452837	N	2.3925215	-1.8155182	1.7495051
C	2.4374339	-0.5532439	2.0732172	C	2.2576403	-0.4392374	1.7511674
C	3.6924587	-0.0516847	2.5728770	C	3.4821572	0.1957136	2.1677061
C	0.8363124	-6.4041130	0.4239835	C	1.2078290	-6.4148244	0.2488306
H	0.7718952	-7.4558383	0.1475027	H	1.2670276	-7.4469950	-0.0959663
H	5.1710644	-6.2387631	1.9748385	H	5.4567033	-5.8620813	1.9521691
C	4.1604452	-5.9753779	1.6759416	C	4.4287966	-5.6966270	1.6410565
C	3.2089653	-6.7596526	1.0954940	C	3.5832650	-6.5539983	1.0000379
H	3.2683002	-7.8089634	0.8209755	H	3.7647232	-7.5788847	0.6881384
C	2.0419607	-5.9379725	0.9148862	C	2.3420160	-5.8535167	0.8083713
N	2.2758251	-4.6444678	1.3531868	N	2.4224367	-4.5611020	1.3104132
C	3.5792173	-4.6671883	1.8341831	C	3.7166662	-4.4569052	1.8064157
C	4.2455423	-3.5780814	2.3701701	C	4.2876867	-3.2875804	2.2812971
H	5.2590078	-3.7315238	2.7407885	H	5.3116430	-3.3329744	2.6518156
Co	1.0025182	-3.1333800	1.4073947	Co	1.0163538	-3.1602731	1.3184898
C	0.5818497	-3.4976772	3.3972469	C	0.5809367	-3.4192844	3.3545784
H	1.6053124	-3.5669063	3.7919391	H	1.5939697	-3.6664092	3.6980245
C	-0.2497105	-7.1648541	4.0106120	C	-0.7974935	-6.8623986	4.2241810
C	-1.6289046	-7.1708562	3.8421900	C	-2.1611131	-6.6056683	4.3202003
C	-2.3001192	-5.9813540	3.5248611	C	-2.6514808	-5.3216841	4.0502230
C	-1.5784400	-4.8040197	3.3913631	C	-1.7662886	-4.3077292	3.7030827
C	-0.1766341	-4.7596434	3.5395682	C	-0.3746525	-4.5251069	3.6016134
C	0.4800596	-5.9774187	3.8557295	C	0.0917863	-5.8432858	3.8588499
H	0.2994826	-8.0741459	4.2557830	H	-0.3892220	-7.8530185	4.4259975
H	-2.1836084	-8.1033123	3.9555473	H	-2.8436051	-7.4078919	4.6051309
H	-3.3806733	-5.9775935	3.3822737	H	-3.7187766	-5.1117902	4.1248252
H	-2.1043257	-3.8859110	3.1308102	H	-2.1559236	-3.3070741	3.5183855
O	1.8255177	-6.0787501	4.0568042	O	1.4123598	-6.1843388	3.8136191
H	2.2754695	-5.2859147	3.7056447	H	1.9066760	-5.5069090	3.3096889

C	-0.0730442	-2.2894276	3.9809673	C	0.1738959	-2.1112669	3.9714940
C	0.5259121	-1.5053572	4.8397958	C	0.8393687	-1.5623899	4.9540544
C	1.2163398	-0.8107123	5.8009350	C	1.4803461	-1.0225247	6.0437332
C	2.6326300	0.5927246	7.8214725	C	2.7677724	0.0813933	8.3198165
C	1.2560376	-1.2912172	7.1548830	C	1.1300525	-1.4384035	7.3739353
C	1.9069816	0.4128031	5.5126808	C	2.5085200	-0.0303151	5.9086821
C	2.5936764	1.0879616	6.5079111	C	3.1257550	0.5026229	7.0288064
C	1.9561348	-0.5997104	8.1292784	C	1.7682563	-0.8934241	8.4755245
H	0.7324075	-2.2168656	7.3942672	H	0.3530650	-2.1930349	7.4969663
H	1.9800102	-0.9893851	9.1482623	H	1.4862272	-1.2265192	9.4758228
H	3.1792226	1.1305220	8.5962552	H	3.2623296	0.5058244	9.1938740
H	3.1111459	2.0176274	6.2641461	H	3.9037315	1.2576890	6.9017806
H	1.8738955	0.7971124	4.4958524	H	2.7961611	0.2888297	4.9072098
H	-1.1165830	-2.0993872	3.7015762	H	-0.7609881	-1.6530594	3.6251235

TS3_(HAT)

With disp3				Without disp3			
65				65			
Energy = -3026.2265934310				Energy = -3026.1196120580			
C	0.3639717	-0.2348510	1.5436692	C	0.3890123	-0.2198938	1.4273963
N	-0.0340925	-1.5075936	1.1653235	N	-0.0262909	-1.5068986	1.1266763
H	-0.6979955	1.7119324	1.8661067	H	-0.6455272	1.7592926	1.6259944
C	-1.4030152	-1.4045369	0.9801426	C	-1.3919648	-1.3938928	0.9267879
C	-1.8627286	-0.0701624	1.2645245	C	-1.8339619	-0.0390272	1.1319186
H	-2.8963693	0.2544659	1.1830444	H	-2.8622624	0.2955654	1.0257768
C	-0.7622117	0.6595497	1.6034284	C	-0.7241361	0.6934623	1.4293595
C	-2.2172834	-2.4161484	0.5059221	C	-2.2151348	-2.4136930	0.4842512
H	-3.2780155	-2.2034271	0.3758235	H	-3.2721329	-2.1927385	0.3370712
N	-0.4491692	-4.1128474	0.2881456	N	-0.4592534	-4.1261750	0.3062208
C	-0.4735582	-5.4196023	-0.1766699	C	-0.4801190	-5.4263888	-0.1741648

C	-1.7854965	-5.7730058	-0.6486835	C	-1.7883083	-5.7747145	-0.6613064
H	-2.0457390	-6.7395544	-1.0710812	H	-2.0448469	-6.7349101	-1.1004975
C	-2.5839468	-4.6866938	-0.4457286	C	-2.5877456	-4.6906060	-0.4531197
H	-3.6405233	-4.5665189	-0.6690321	H	-3.6412484	-4.5661030	-0.6888324
C	-1.7545060	-3.6647748	0.1353451	C	-1.7608803	-3.6744864	0.1422707
C	1.6606412	0.1413574	1.8422075	C	1.6942281	0.1569464	1.6901901
H	1.8423283	1.1824236	2.1093422	H	1.8910088	1.2106240	1.8890193
H	5.8694450	-1.6132060	2.4771636	H	5.9012959	-1.6003020	2.3396147
C	4.8180521	-1.4874597	2.2335705	C	4.8452999	-1.4787298	2.1141705
C	3.9446676	-2.5547263	1.8176437	C	3.9550856	-2.5574772	1.7698581
H	4.3693170	0.6613603	2.5055639	H	4.4220057	0.6856707	2.2756631
N	2.6699775	-2.0789765	1.5613259	N	2.6782262	-2.0856555	1.5212276
C	2.7352914	-0.7275044	1.8534196	C	2.7614961	-0.7213242	1.7364288
C	4.0687516	-0.3497539	2.2452821	C	4.1062308	-0.3352293	2.0791218
C	0.5846024	-6.3067696	-0.1212427	C	0.5854173	-6.3073434	-0.1402945
H	0.4187683	-7.3233611	-0.4766564	H	0.4256943	-7.3167614	-0.5189346
H	4.9716774	-6.6047187	1.2513849	H	4.9838959	-6.6062439	1.1963807
C	3.9720926	-6.2451294	1.0241481	C	3.9799143	-6.2486698	0.9854078
C	2.9207840	-6.9253983	0.4882344	C	2.9302689	-6.9237029	0.4406031
H	2.8677736	-7.9665986	0.1827899	H	2.8831791	-7.9581310	0.1116413
C	1.8306998	-5.9899470	0.3833604	C	1.8333415	-5.9933230	0.3639360
N	2.2078378	-4.7393585	0.8396291	N	2.2045033	-4.7506047	0.8453204
C	3.5276701	-4.8908201	1.2310549	C	3.5284017	-4.9010890	1.2202411
C	4.3405565	-3.8751592	1.7001370	C	4.3456461	-3.8821087	1.6763323
H	5.3672816	-4.1251712	1.9659110	H	5.3771530	-4.1287483	1.9270806
Co	1.0679390	-3.1529667	1.1033884	Co	1.0641594	-3.1623199	1.1146909
C	0.9501746	-3.6432235	3.0344684	C	0.9337662	-3.6205729	3.0750185
H	2.0155456	-3.8035842	3.2381372	H	2.0020331	-3.7752426	3.2649304
C	0.1467781	-6.4433978	5.4429135	C	0.1687391	-6.4166429	5.5125998
C	-0.9769595	-7.0385229	4.8879876	C	-0.9598870	-7.0207092	4.9783831

C -1.5483226 -6.5058364 3.7205732	C -1.5459892 -6.4998922 3.8139137
C -0.9626278 -5.4102234 3.0890234	C -0.9719877 -5.4075127 3.1643168
C 0.2258784 -4.8439523 3.5648955	C 0.2174446 -4.8248724 3.6230791
C 0.7649847 -5.3437226 4.8066850	C 0.7714316 -5.3174630 4.8605692
H 0.5821027 -6.7976336 6.3780085	H 0.6186620 -6.7638111 6.4436757
H -1.4330143 -7.9015325 5.3760218	H -1.4065022 -7.8817190 5.4786686
H -2.4519310 -6.9493083 3.3005414	H -2.4520426 -6.9516892 3.4079270
H -1.4205615 -4.9964854 2.1965733	H -1.4423584 -5.0137507 2.2675631
O 1.8105899 -4.7539555 5.3912595	O 1.8226344 -4.7196587 5.4282174
H 1.6466499 -3.5747640 5.3503115	H 1.6454750 -3.5490892 5.3885288
C 0.4850543 -2.4971234 3.9027392	C 0.4731939 -2.4721747 3.9517992
C 1.1071388 -2.2979445 5.0690940	C 1.0852107 -2.2791286 5.1260701
C 1.1352914 -1.2738139 6.0633042	C 1.0980500 -1.2848156 6.1554510
C 1.1748141 0.7484670 8.0253442	C 1.1199448 0.6698087 8.1915826
C 1.2558336 -1.5984130 7.4370026	C 1.1955867 -1.6550590 7.5204062
C 1.0666906 0.0949274 5.6954739	C 1.0423596 0.0975011 5.8395481
C 1.0765790 1.0882153 6.6692666	C 1.0436802 1.0562162 6.8475184
C 1.2655436 -0.5979714 8.4029353	C 1.1971413 -0.6894738 8.5210580
H 1.3344175 -2.6490172 7.7208080	H 1.2654249 -2.7141670 7.7722622
H 1.3481594 -0.8633157 9.4579996	H 1.2637020 -0.9934766 9.5667292
H 1.1887201 1.5310312 8.7852687	H 1.1278794 1.4252142 8.9785434
H 1.0110674 2.1371953 6.3752837	H 0.9889402 2.1149069 6.5879759
H 1.0004714 0.3445424 4.6353207	H 0.9942874 0.3913351 4.7905447
H -0.4591919 -2.0030423 3.6462212	H -0.4731185 -1.9763884 3.7010178

***Trans o*-quinone methide (E)**

With disp3	Without disp3
28	28
Energy = -654.2980732481	Energy = -654.2745495567
C 0.8990925 -4.2656516 5.0248301	C 0.8849542 -4.2660147 5.0335616

H	1.9315754	-4.5910497	5.1955650	H	1.9148996	-4.5942890	5.2137442
C	-0.1352708	-7.4686792	3.3311406	C	-0.1283919	-7.4732450	3.3381183
C	-1.4394812	-7.1858760	3.0590933	C	-1.4299535	-7.1924292	3.0510298
C	-2.0299082	-5.9249952	3.4256710	C	-2.0257065	-5.9308475	3.4058243
C	-1.2888513	-4.9712674	4.0612846	C	-1.2928852	-4.9743190	4.0468425
C	0.0947279	-5.1911652	4.3838031	C	0.0869479	-5.1923472	4.3856178
C	0.7308720	-6.5056818	4.0102035	C	0.7291811	-6.5060034	4.0221884
H	0.3205834	-8.4208256	3.0576896	H	0.3294373	-8.4268100	3.0720571
H	-2.0625402	-7.9257270	2.5513969	H	-2.0466222	-7.9347866	2.5388977
H	-3.0783697	-5.7402436	3.1893181	H	-3.0716594	-5.7479939	3.1568018
H	-1.7555354	-4.0217442	4.3305042	H	-1.7621762	-4.0237830	4.3078688
O	1.9191119	-6.7614383	4.2622039	O	1.9160206	-6.7559309	4.2869270
H	2.4493101	-2.5327936	6.2465729	H	2.4322686	-2.5401707	6.2604205
C	0.5391740	-2.9692829	5.4768461	C	0.5248768	-2.9678837	5.4811389
C	1.4335660	-2.1471781	6.1053815	C	1.4194417	-2.1490955	6.1143298
C	1.1993862	-0.8111663	6.6183824	C	1.1929867	-0.8103721	6.6244516
C	0.8540963	1.7900091	7.6628853	C	0.8680937	1.7972543	7.6582997
C	2.2623269	-0.1306107	7.2540167	C	2.2632203	-0.1328534	7.2506423
C	-0.0449915	-0.1471248	6.5195322	C	-0.0485895	-0.1405107	6.5305287
C	-0.2122861	1.1331935	7.0345245	C	-0.2057419	1.1432469	7.0403423
C	2.0927952	1.1518593	7.7700385	C	2.1039839	1.1530459	7.7610232
H	3.2311150	-0.6271077	7.3398299	H	3.2292800	-0.6354964	7.3316019
H	2.9280680	1.6561943	8.2575664	H	2.9451867	1.6555163	8.2402268
H	0.7172465	2.7943054	8.0655934	H	0.7393132	2.8043395	8.0568630
H	-1.1805398	1.6282727	6.9485350	H	-1.1719972	1.6431545	6.9578524
H	-0.8881828	-0.6394550	6.0337476	H	-0.8974332	-0.6317988	6.0531147
H	-0.4850904	-2.6237704	5.3178437	H	-0.4969353	-2.6185766	5.3136849

***Cis o*-quinone methide (F)**

With disp3				Without disp3			
28				28			
Energy = -654.2913703095				Energy = -654.2671063182			
C	1.0839024	-4.7385189	4.8014454	C	1.0852748	-4.7473285	4.7994153
H	0.6794602	-3.7479418	5.0418122	H	0.6828074	-3.7560162	5.0401135
C	-0.8516487	-7.5905635	3.1002870	C	-0.8642004	-7.5893576	3.0964095
C	-2.0455172	-6.9479614	2.9524796	C	-2.0551181	-6.9405883	2.9510410
C	-2.2148713	-5.5986512	3.4022025	C	-2.2179914	-5.5912409	3.4028979
C	-1.1701708	-4.9426158	3.9881133	C	-1.1695733	-4.9410499	3.9886066
C	0.1254332	-5.5483732	4.1834548	C	0.1231572	-5.5532732	4.1814254
C	0.3086521	-6.9562270	3.7142013	C	0.2997235	-6.9612602	3.7101426
H	-0.7033714	-8.6173718	2.7641756	H	-0.7227258	-8.6165457	2.7579799
H	-2.8886702	-7.4622370	2.4856335	H	-2.9012552	-7.4502485	2.4843081
H	-3.1769434	-5.1017369	3.2751509	H	-3.1779937	-5.0897386	3.2775622
H	-1.3034299	-3.9130189	4.3305313	H	-1.2951284	-3.9113423	4.3334739
O	1.3786604	-7.5924575	3.8216192	O	1.3678388	-7.6007503	3.8168400
H	2.9137369	-6.8165697	4.6181069	H	2.9224964	-6.8301757	4.6183361
C	2.4447320	-4.8535935	5.2053135	C	2.4467365	-4.8650732	5.2027252
C	3.3087426	-5.9134090	5.0897849	C	3.3125424	-5.9240221	5.0887622
C	4.6881996	-5.9407086	5.5358569	C	4.6924452	-5.9449148	5.5366887
C	7.3824055	-6.1486308	6.3541353	C	7.3870932	-6.1397566	6.3576644
C	5.4224152	-7.1337118	5.3412855	C	5.4323617	-7.1347216	5.3448122
C	5.3472343	-4.8518439	6.1532951	C	5.3461743	-4.8524320	6.1532775
C	6.6736517	-4.9565486	6.5554733	C	6.6728048	-4.9507496	6.5566800
C	6.7509757	-7.2370018	5.7449233	C	6.7610178	-7.2317059	5.7496604
H	4.9261742	-7.9814700	4.8651849	H	4.9395165	-7.9848161	4.8693766
H	7.2972213	-8.1675311	5.5853119	H	7.3115261	-8.1601226	5.5917341
H	8.4231300	-6.2253690	6.6716233	H	8.4279749	-6.2113196	6.6761148
H	7.1647520	-4.1058266	7.0301036	H	7.1596814	-4.0970443	7.0305223

H 4.8143161 -3.9149615 6.3181191	H 4.8088687 -3.9176071 6.3162790
H 2.8218274 -3.9401489 5.6753760	H 2.8249447 -3.9517988 5.6721505

TS4_(ring closer)

With disp3	Without disp3
28	28
Energy = -654.2832618957	Energy = -654.2572319193
C -0.7006249 -3.5614794 4.4831300	C -0.7031993 -3.5595376 4.4874879
H -0.8049242 -3.5711742 3.3926425	H -0.8040859 -3.5634636 3.3967261
C -0.7275409 -6.5195883 6.7554518	C -0.7385127 -6.5199278 6.7553030
C -1.5977653 -7.3367837 6.0735346	C -1.6033754 -7.3393915 6.0676058
C -2.3021001 -6.8733735 4.9298344	C -2.2987197 -6.8792122 4.9184053
C -2.0781754 -5.5934212 4.4806641	C -2.0733412 -5.5985239 4.4700886
C -1.2273015 -4.6796739 5.1715815	C -1.2304830 -4.6840074 5.1680106
C -0.6132836 -5.1136095 6.4480034	C -0.6224190 -5.1162732 6.4438986
H -0.1900221 -6.8661688 7.6382916	H -0.2072354 -6.8668655 7.6419192
H -1.7470804 -8.3635170 6.4149415	H -1.7540582 -8.3656168 6.4101376
H -2.9776325 -7.5404915 4.3945760	H -2.9686585 -7.5480581 4.3782041
H -2.5533933 -5.2466905 3.5597515	H -2.5408367 -5.2521366 3.5450998
O 0.0101676 -4.3573888 7.2550129	O 0.0004633 -4.3558223 7.2513366
C 0.1039330 -2.5760919 5.0488393	C 0.0993788 -2.5798760 5.0616324
C 1.0577966 -1.5141095 7.1377450	C 1.0633898 -1.5248800 7.1497879
C 2.9297051 -0.0057492 8.6005844	C 2.9332512 0.0062939 8.5922002
C 0.7195351 -0.9582091 8.3887581	C 0.7270950 -0.9585054 8.3966859
C 2.3655262 -1.3167869 6.6459885	C 2.3678042 -1.3239078 6.6509691
C 3.2880522 -0.5667338 7.3681248	C 3.2895159 -0.5632233 7.3632878
C 1.6436289 -0.2070154 9.1110249	C 1.6500296 -0.1961815 9.1088141
H -0.2824049 -1.1264361 8.7877764	H -0.2734367 -1.1264565 8.7995567
H 1.3646808 0.2187611 10.0756203	H 1.3721020 0.2378128 10.0701684
H 3.6569394 0.5785543 9.1659677	H 3.6596858 0.5993233 9.1496656

H 4.2966692 -0.4241218 6.9779827	H 4.2956438 -0.4180610 6.9674793
H 2.6615336 -1.7768558 5.7024280	H 2.6609649 -1.7880554 5.7083339
H 0.8057561 -2.0400589 4.4052426	H 0.7952493 -2.0320807 4.4213749
C 0.0647487 -2.2896929 6.4168154	C 0.0674484 -2.3071343 6.4354065
H -0.8914235 -2.4070940 6.9216862	H -0.8886602 -2.4112317 6.9424143

Chromene (G)

With disp3	Without disp3
28	28
Energy = -654.3157709630	Energy = -654.2898713492
C -0.9383137 -3.2463349 4.5406793	C -0.8964101 -3.2833143 4.4873419
H -1.1581099 -3.0187341 3.4952990	H -1.1000241 -3.0826851 3.4330532
C -0.6299271 -6.2556230 6.7482340	C -0.6682399 -6.2309794 6.7852317
C -1.2675686 -7.2393638 5.9877717	C -1.3175771 -7.2244679 6.0479201
C -1.8372273 -6.9237612 4.7494658	C -1.8703852 -6.9353616 4.7957439
C -1.7532362 -5.6172630 4.2673089	C -1.7572266 -5.6457773 4.2760380
C -1.1215446 -4.6101305 5.0124030	C -1.1136819 -4.6284800 4.9974546
C -0.5721798 -4.9457413 6.2701845	C -0.5823321 -4.9361638 6.2700319
H -0.1774892 -6.4838932 7.7134991	H -0.2292611 -6.4416084 7.7608934
H -1.3227898 -8.2592495 6.3709182	H -1.3951522 -8.2315381 6.4603224
H -2.3363033 -7.6939737 4.1614103	H -2.3785542 -7.7134982 4.2259703
H -2.1752574 -5.3616361 3.2927603	H -2.1656180 -5.4119357 3.2900575
O 0.1078845 -4.0242324 7.0225757	O 0.1079444 -4.0034877 7.0000486
C -0.4879059 -2.2969720 5.3769923	C -0.4330430 -2.3174210 5.2983545
C 0.9210243 -1.8045342 7.3936724	C 0.9348517 -1.7841840 7.3521818
C 3.0329140 -0.2216450 8.3425388	C 3.0227833 -0.2243708 8.3958028
C 0.6621630 -0.6805723 8.1844562	C 0.6655900 -0.7511701 8.2565277
C 2.2458925 -2.1338664 7.0809920	C 2.2618794 -2.0332919 6.9752577
C 3.2966538 -1.3496581 7.5584048	C 3.2997095 -1.2610455 7.4980609
C 1.7131568 0.1122353 8.6545059	C 1.7031355 0.0303766 8.7737219

H -0.3693504 -0.4260559 8.4387685	H -0.3655682 -0.5601569 8.5630654
H 1.5002021 0.9848504 9.2734846	H 1.4796478 0.8315842 9.4797183
H 3.8551799 0.3916385 8.7136049	H 3.8354515 0.3792903 8.8023744
H 4.3262771 -1.6175847 7.3165952	H 4.3300649 -1.4674298 7.2039254
H 2.4433652 -3.0163933 6.4718843	H 2.4775750 -2.8448702 6.2786850
H -0.3260788 -1.2669604 5.0589567	H -0.2497131 -1.3021073 4.9454861
C -0.2221610 -2.6205560 6.8292138	C -0.1992584 -2.5984961 6.7641041
H -1.1362704 -2.4099893 7.4244200	H -1.1235874 -2.3634102 7.3336270

TS5_(propene formation)

With disp3	Without disp3
65	65
Energy = -3026.2380331700	Energy = -3026.1286754370
C -0.3831327 -0.4903024 0.4750186	C -0.2011292 -0.3443709 0.5625728
N -0.4066785 -1.8545808 0.7110677	N -0.3231642 -1.7223422 0.6260891
H -1.9705814 1.0652451 0.1658680	H -1.6339708 1.3372433 0.1698294
C -1.7462539 -2.1951639 0.7506087	C -1.6636771 -1.9732962 0.3944112
C -2.5697843 -1.0287079 0.5575918	C -2.3863927 -0.7428232 0.1937391
H -3.6562708 -1.0375083 0.5476355	H -3.4522117 -0.6807192 -0.0090284
C -1.7247218 0.0243169 0.3578379	C -1.4746523 0.2676132 0.2775472
C -2.2334634 -3.4883565 0.8597776	C -2.2301424 -3.2333267 0.2894445
H -3.3130068 -3.6277608 0.9004618	H -3.3035160 -3.2978176 0.1119340
N -0.0505660 -4.6048836 0.7813281	N -0.1366752 -4.4985183 0.4979587
C 0.3188172 -5.9259061 0.5947595	C 0.1694329 -5.8306140 0.2793203
C -0.8465068 -6.7693966 0.5075264	C -1.0156179 -6.5790142 -0.0580215
H -0.8166191 -7.8457308 0.3628987	H -1.0291233 -7.6431928 -0.2772147
C -1.9319219 -5.9620539 0.6766946	C -2.0568739 -5.7020613 -0.0259105
H -2.9841125 -6.2313459 0.6887824	H -3.1091153 -5.8882014 -0.2228032
C -1.4335029 -4.6172145 0.8135332	C -1.5018372 -4.4107022 0.2947441
C 0.7613247 0.2947050 0.4663633	C 0.9626407 0.3636149 0.8164630

H	0.6476327	1.3611223	0.2724317	H	0.9251586	1.4503747	0.7415947
H	5.1702827	0.1271805	1.8100869	H	5.2648823	-0.2158461	2.3715365
C	4.1593263	-0.1416449	1.5156193	C	4.2530165	-0.3884313	2.0141052
C	3.6362959	-1.4854106	1.5201261	C	3.6620188	-1.6905799	1.8300326
H	3.1859364	1.7417219	0.8840993	H	3.4015792	1.6083959	1.5904615
N	2.3234739	-1.4955049	1.0853490	N	2.3680899	-1.5786868	1.3529060
C	2.0217749	-0.1749219	0.8038429	C	2.1527906	-0.2184233	1.2215256
C	3.1676372	0.6668178	1.0418581	C	3.3225910	0.5248401	1.6159168
C	1.6221845	-6.3970232	0.5968164	C	1.4295236	-6.3919727	0.3989836
H	1.7821589	-7.4621624	0.4326729	H	1.5391231	-7.4533777	0.1769742
H	5.8477045	-5.0649095	1.8876785	H	5.6697518	-5.4027543	1.9225336
C	4.7986478	-5.0728426	1.6049471	C	4.6304672	-5.3319641	1.6132864
C	4.0463580	-6.1213437	1.1577010	C	3.8303375	-6.3045409	1.0879939
H	4.3439278	-7.1566696	1.0170674	H	4.0703002	-7.3454589	0.8895412
C	2.7198708	-5.6168774	0.9221911	C	2.5451016	-5.7052121	0.8475258
N	2.6638607	-4.2552003	1.1963058	N	2.5558987	-4.3624539	1.2042785
C	3.9481928	-3.9118314	1.5941175	C	3.8465586	-4.1261842	1.6590619
C	4.3837992	-2.6146315	1.8203259	C	4.3446058	-2.8829965	2.0156626
H	5.4142175	-2.4727752	2.1462835	H	5.3707324	-2.8311659	2.3794394
Co	1.1181523	-3.0434627	1.0178872	Co	1.0898865	-3.0408361	1.0024275
C	0.8468276	-2.7992736	3.4966553	C	0.5042315	-3.0333606	3.6036829
H	1.8634499	-3.1914352	3.4631107	H	1.5632429	-3.2705584	3.5052727
C	-1.0550082	-5.9647486	4.2926554	C	-0.8648151	-6.4249439	4.5644997
C	-2.3317304	-5.4656144	4.5477730	C	-2.1773976	-6.1037962	4.9038887
C	-2.5824747	-4.0930168	4.4359938	C	-2.6325449	-4.7844305	4.7758695
C	-1.5484447	-3.2317867	4.0815975	C	-1.7613639	-3.7979908	4.3298756
C	-0.2432105	-3.7039755	3.8357127	C	-0.4154739	-4.0820513	3.9969262
C	-0.0173396	-5.1009537	3.9336069	C	0.0101743	-5.4365554	4.1019111
H	-0.8388210	-7.0315751	4.3484646	H	-0.4920923	-7.4467426	4.6420879
H	-3.1337491	-6.1517672	4.8231243	H	-2.8488963	-6.8855938	5.2617499

H -3.5816968 -3.6975943 4.6207236	H -3.6616094 -4.5291690 5.0312172
H -1.7377671 -2.1613587 3.9927219	H -2.1058201 -2.7654616 4.2553615
O 1.2069487 -5.6609333 3.6988781	O 1.2783344 -5.8350986 3.7930204
H 1.7162391 -5.0963770 3.0810436	H 1.6955749 -5.1925542 3.1828945
C 0.7069106 -1.3210699 3.6365768	C 0.1707192 -1.5944502 3.7838149
C 1.0918232 -1.4404248 4.8591791	C 0.7311198 -1.5076557 4.9449806
C 1.4802962 -1.6548279 6.1877576	C 1.3736679 -1.4514842 6.1831387
C 2.2454318 -2.1556950 8.8472811	C 2.6730096 -1.3195731 8.6828396
C 0.5449675 -2.1780192 7.1197424	C 0.7132820 -1.8776744 7.3694910
C 2.8065023 -1.3903205 6.6170981	C 2.7037732 -0.9548424 6.2869189
C 3.1732821 -1.6355924 7.9355371	C 3.3314510 -0.8870736 7.5240755
C 0.9360507 -2.4282030 8.4300389	C 1.3659223 -1.8164964 8.5941410
H -0.4691641 -2.3947527 6.7837556	H -0.3056629 -2.2580121 7.2998287
H 0.2128352 -2.8378458 9.1365440	H 0.8492831 -2.1534306 9.4940492
H 2.5419453 -2.3483936 9.8787386	H 3.1750957 -1.2684024 9.6494969
H 4.1939621 -1.4241846 8.2576027	H 4.3487231 -0.4977642 7.5886690
H 3.5264237 -0.9963045 5.8998696	H 3.2155874 -0.6268347 5.3820254
H 0.3210312 -0.5485870 2.9754823	H -0.4339289 -0.9218419 3.1738367

Co(por)_propene (H)

With disp3	Without disp3
65	65
Energy = -3026.2659837180	Energy = -3026.1566891440
C -1.0758995 1.6835175 -8.3451911	C -1.0167877 2.1856381 -8.9308231
N 0.3044724 1.6883380 -8.2516994	N 0.3139909 2.4004697 -8.6158952
H -2.7398154 1.1228905 -6.9486132	H -2.8098359 1.4886150 -7.7800256
C 0.5753009 1.2517936 -6.9675608	C 0.4143757 2.0781466 -7.2729940
C -0.6440516 0.9502744 -6.2615495	C -0.8616000 1.6661348 -6.7475265
H -0.6862667 0.5885345 -5.2380319	H -1.0340745 1.3655803 -5.7176118
C -1.6703810 1.2144183 -7.1180717	C -1.7497197 1.7266345 -7.7789007

C	1.8360408	1.1332728	-6.4109117	C	1.5791024	2.1171839	-6.5276645
N	3.1034614	1.8051185	-8.4081444	N	3.0649742	2.8448695	-8.3462633
C	4.4613635	1.9014515	-8.6564637	C	4.4289370	3.0759323	-8.3936196
C	5.2225913	1.5554109	-7.4819092	C	5.0349448	2.8361593	-7.1092300
H	6.3079541	1.5617053	-7.4293349	H	6.0946732	2.9515277	-6.8981331
C	4.3213424	1.2586757	-6.5038821	C	4.0323561	2.4629894	-6.2656791
H	4.5051612	0.9542683	-5.4772770	H	4.0905852	2.2013711	-5.2126251
C	3.0119695	1.4063772	-7.0856467	C	2.8170960	2.4662833	-7.0381259
C	-1.8041759	2.1086557	-9.4432258	C	-1.5876910	2.3943487	-10.1754269
H	-1.2918052	3.7394129	-13.7236048	H	-0.5982752	3.9501413	-14.3977801
C	-1.1028990	3.3714466	-12.7191893	C	-0.5297710	3.6362501	-13.3598206
C	0.2090876	3.1554077	-12.1635673	C	0.6792457	3.6660076	-12.5777649
H	-3.0861706	3.0428638	-11.7978009	H	-2.5532840	2.9533979	-12.7846317
C	-1.2389496	2.5878228	-10.6129670	C	-0.8979152	2.8776577	-11.2747851
C	-2.0009179	3.0219341	-11.7552366	C	-1.5081870	3.1391192	-12.5534885
C	5.0294429	2.3055191	-9.8524462	C	5.1284626	3.5038546	-9.5082881
H	3.9185062	3.8592306	-14.0486274	H	4.5188430	4.8238835	-13.8800879
C	3.8734940	3.4843115	-13.0298711	C	4.3586601	4.4603353	-12.8687053
C	4.8995697	3.1712065	-12.1887971	C	5.2701915	4.2779179	-11.8726198
H	5.9694102	3.2353497	-12.3678131	H	6.3409118	4.4626392	-11.8876986
C	4.3044847	2.7248647	-10.9547112	C	4.5448303	3.7828186	-10.7314168
N	2.9234408	2.7747540	-11.0298784	N	3.1975883	3.6516651	-11.0224642
C	2.6523187	3.2271041	-12.3098880	C	3.0793503	4.0664003	-12.3378622
C	1.3882760	3.3982753	-12.8472932	C	1.9033233	4.0853791	-13.0671323
Co	1.6176625	2.1236735	-9.6842325	Co	1.7564079	3.0238225	-9.8193309
H	6.1169670	2.3210899	-9.9217195	H	6.2044048	3.6488151	-9.4109214
H	-2.8912868	2.0661212	-9.3826858	H	-2.6515000	2.1864477	-10.2913925
H	1.9087296	0.7859693	-5.3811223	H	1.5214573	1.8362708	-5.4763671
H	1.3152424	3.7566045	-13.8736873	H	1.9480472	4.4343803	-14.0984082
C	1.8476615	-1.3923942	-8.7215555	C	2.1178735	-2.7390124	-8.7141623

C	2.5418404	-2.7210743	-6.3555566	C	3.0040785	-4.3571573	-6.5940187
C	0.8541856	-2.0056435	-7.9312282	C	1.1994646	-3.4826244	-7.9488293
C	3.1951714	-1.4584955	-8.3132062	C	3.4900825	-2.8178654	-8.3983194
C	3.5356271	-2.1199272	-7.1382628	C	3.9256969	-3.6194213	-7.3469009
C	1.2013508	-2.6639626	-6.7552927	C	1.6417078	-4.2860339	-6.8983821
C	1.4691345	-0.6779348	-9.8995454	C	1.6542115	-1.9024694	-9.7937088
C	0.3632811	-0.5098036	-10.8915935	C	0.4141663	-1.4372006	-10.5280989
C	1.7591171	0.1271517	-10.9205555	C	1.8649293	-1.0688478	-10.7785018
C	0.0169546	-1.5992995	-11.8548831	C	-0.3443404	-2.3365427	-11.4583027
C	-0.6691486	-3.5582446	-13.7503421	C	-1.7976492	-4.0251790	-13.1924553
C	-0.4652378	-1.2306022	-13.1290414	C	-1.5056461	-1.8760301	-12.1161968
C	0.1599182	-2.9611545	-11.5636532	C	0.0677909	-3.6538782	-11.7097273
C	-0.1784578	-3.9424007	-12.4982759	C	-0.6410145	-4.4979790	-12.5646034
C	-0.8109479	-2.2078138	-14.0692736	C	-2.2280016	-2.7185271	-12.9700139
O	-0.6034755	0.0805552	-13.5004086	O	-1.9865545	-0.5975495	-11.9640022
H	-0.2671013	0.6586745	-12.7866623	H	-1.3506366	-0.0697622	-11.4445307
N	0.1205579	2.6741796	-10.8667441	N	0.4489160	3.1995321	-11.2946050
H	3.9571649	-0.9619579	-8.9144779	H	4.2056592	-2.2401913	-8.9850701
H	4.5781089	-2.1549431	-6.8203941	H	4.9894384	-3.6717926	-7.1099935
H	2.8130194	-3.2352236	-5.4323201	H	3.3492520	-4.9862305	-5.7721438
H	-0.1871980	-1.9300719	-8.2467192	H	0.1380345	-3.4235302	-8.1934232
H	0.4273938	-3.1272782	-6.1422307	H	0.9206743	-4.8598320	-6.3144274
H	2.5198437	0.4048481	-11.6394434	H	2.5356368	-0.5072724	-11.4180726
H	-0.4711026	0.1515842	-10.6328520	H	-0.2093033	-0.6927923	-10.0064854
H	0.5449200	-3.2489193	-10.5833844	H	0.9689328	-4.0197562	-11.2126254
H	-0.0627633	-4.9979696	-12.2507157	H	-0.2975197	-5.5190552	-12.7341625
H	-0.9389160	-4.3145430	-14.4890998	H	-2.3653885	-4.6725713	-13.8625354
H	-1.1787824	-1.8886491	-15.0449510	H	-3.1188194	-2.3231643	-13.4595116

Propene (I)

With disp3				Without disp3			
28				28			
Energy = -654.2581484799				Energy = -654.2321265232			
C	0.3888392	-0.4791870	0.7724715	C	0.2357843	-0.4351111	0.7794222
C	0.1171597	0.6051501	3.3322020	C	0.1346713	0.6155999	3.3663897
C	0.6622401	-1.2882372	1.8939040	C	0.6577052	-1.2356596	1.8614274
C	-0.0251404	0.8470183	0.9260301	C	-0.2370907	0.8645343	0.9871518
C	-0.1609640	1.3855254	2.2054802	C	-0.2863945	1.3869942	2.2788393
C	0.5237374	-0.7194229	3.1650748	C	0.5981260	-0.6819391	3.1468950
C	1.1183978	-2.6999511	1.6921830	C	1.1540737	-2.6301335	1.6209814
H	0.5438563	-3.2565751	0.9300444	H	0.5917672	-3.1802673	0.8450999
C	1.7528123	-3.5115491	2.7925156	C	1.7707401	-3.4619742	2.7149186
H	1.5712921	-4.0286215	3.7274795	H	1.5684001	-4.0119421	3.6268114
C	2.5794091	-3.0769638	1.8777065	C	2.6151960	-3.0164298	1.8213557
C	3.8830376	-2.8800851	1.3046780	C	3.9416182	-2.8641423	1.2799719
C	6.4177080	-2.4647033	0.1737193	C	6.5238921	-2.5708536	0.2116303
C	4.0381511	-2.0263247	0.1955766	C	4.1569866	-2.0752478	0.1338504
C	5.0178119	-3.5207496	1.8425942	C	5.0439512	-3.5030064	1.8853476
C	6.2730670	-3.3152816	1.2771503	C	6.3215255	-3.3571978	1.3526350
C	5.2991547	-1.8201022	-0.3626755	C	5.4395500	-1.9303662	-0.3941403
H	3.1635659	-1.5147539	-0.2101369	H	3.3091030	-1.5702522	-0.3314384
H	5.4103173	-1.1528302	-1.2181955	H	5.5938527	-1.3137588	-1.2805210
H	7.4033015	-2.3042664	-0.2651239	H	7.5267550	-2.4577534	-0.2023641
H	7.1460712	-3.8174271	1.6964340	H	7.1673156	-3.8568670	1.8272446
H	4.8986098	-4.1808190	2.7028860	H	4.8833533	-4.1142923	2.7745158
H	0.7485927	-1.3377558	4.0373264	H	0.9297428	-1.2927860	3.9901350
H	-0.2259604	1.4406343	0.0337065	H	-0.5540790	1.4514434	0.1243666
H	0.0139428	1.0248513	4.3331448	H	0.0970524	1.0204201	4.3781710
H	-0.4817707	2.4218132	2.3205392	H	-0.6537425	2.4024913	2.4341782

O	0.5382544	-0.9482242	-0.5140056	O	0.2836676	-0.8831151	-0.5217300
H	0.8112480	-1.8832086	-0.4681189	H	0.6132194	-1.8004350	-0.5165547

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