Electronic Supplementary Material (ESI) for ChemComm.


Supporting Information for

# Convenient Preparation of 4-Diazoisochroman-3-imines and 3-Substituted 3,5-Dihydroisochromeno[3,4-*d*][1,2,3]triazoles

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## Content

# General Information

$^{1}H$ NMR spectra were obtained on 600 or 400 MHz in $CDCl_3$. The chemical shifts were quoted in parts per million (ppm) referenced to 0.0 ppm for tetramethylsilaneas (TMS) an internal standard. $^{13}C$ NMR spectra were recorded on 150 or 100 MHz in $CDCl_3$. The chemical shifts were reported in ppm referenced to the internal solvent signals (77.00 ppm for $CDCl_3$,). The following abbreviations were used to describe peak patterns where appropriate: b= broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants *J* were reported in hertz unit (Hz). Infrared spectra were obtained on an FTIR spectrometer. High-resolution mass spectra (HRMS) data were obtained by using EI ionization on time-of-flight (TOF) mass spectrometer or ESI ionization on LCMS-IT-TOF mass spectrometer. EPR measurements were carried out at temperatures of ambient with microwave power of 20 mW, modulation amplitude of 1.00G, microwave frequency of 9.866 GHz. Melting points were measured with a micromelting point apparatus. Flash column chromatography was performed employing 300-400 mesh silica gel. Thin layer chromatography (TLC) was performed on silica gel HSGF254.

Methyl cyanide, dichloromethane (DCE) and dichloromethane (DCM) was dried by distillation over $CaH_2$.

(2-Ethynylphenyl)methanols were synthesized according to literature procedure.[1,2]

# General Procedure for the Synthesis of 3

To an oven-dried Schlenk tube equipped with a magnetic stirring bar was added **1** (0.2 mmol), **2** (0.44 mmol), CuBr (0.02 mmol), $NEt_3$ (0.4 mmol) and dry MeCN (2 mL) under $N_2$ atmosphere. The mixture was stirred at room temperature for 2 hours. After removal of the solvent in vacuum, the residue was dissolved in DCM (10 mL) and then washed with aqueous $NaHCO_3$ solution. The organic layer was dried over anhydrous $Na_2SO_4$ and concentrated in vacuum. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate/dichloromethane = 5:1:2, v/v) to give pure product **3**.

# General Procedure for the Synthesis of 5

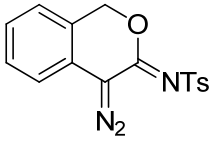
To an oven-dried Sealed tube equipped with a magnetic stirring bar was added **3** (0.1 mmol), **4** (0.22 mmol) and dry MeCN (1 mL). The mixture was stirred at 50 $^{o}$C for 3~12 hours (monitoring by TLC). The solvent was removed in vacuum and the residue was purified by column chromatography on silica gel (generally petroleum ether/ethyl acetate = 5:1, v/v) to give pure product **5**.

# References


1. H. Wu, Y. P. He and L. Z. Gong, *Org. Lett.* 2013, **15**, 460.
2. Alejandro Varela-Fernández, Carlos Saá, *Org. Lett.,* 2009*,* **11** , 5350–5353

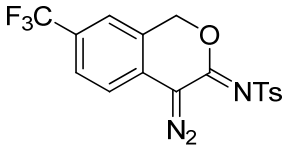
# Characterization Data for Products

*N*-(4-Diazoisochroman-3-ylidene)-4-methylbenzenesulfonamide (**3a**):



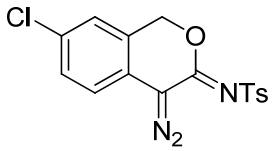

Yellow solid (53.5 mg), Isolated yield = 82%; m.p. 173.1 – 173.4 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.89 (d, *J* = 8.0 Hz, 2H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.21 - 7.14 (m, 2H), 6.94 (d, *J* = 8.0 Hz, 1H), 5.30 (s, 2H), 2.42 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 163.5, 143.0, 139.1, 129.5, 129.1, 127.2, 126.3, 124.8, 124.5, 120.7, 118.8, 71.2, 21.5; IR (film): 2925, 2103, 1747, 1552, 1404, 1318, 1161, 814, 754 cm$^{-1}$; HRMS (ESI) calcd for $C_{16}H_{13}N_3O_3SNa$ (M+Na$^{+}$): 350.0570; found: 350.0549.

*N*-(4-Diazo-7-trifluoromethylisochroman-3-ylidene)-4-methylbenzenesulfonamide (**3b**)



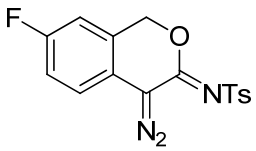

Yellow solid (49.0 mg), Isolated yield = 62%; m.p. 186.1 - 187.8 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.4 Hz, 2H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.42 (s, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.06 (d,*J* = 8.4 Hz, 2H), 5.35 (s, 2H),2.42 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 162.0, 143.3, 138.8, 129.2, 127.3, 126.6(*J* = 3.8 Hz), 124.8, 121.9 (*J* = 3.7 Hz), 119.0, 70.6, 21.5; IR (film):2125, 1580, 1393, 1274, 1112, 814, 686cm$^{-1}$; HRMS (MALDI) calcd for $C_{17}H_{13}F_3N_3O_3S$ (M+H$^{+}$): 396.0624; found: 396.0620.

*N*-(4-Diazo-7-chloroisochroman-3-ylidene)-4-methylbenzenesulfonamide (**3c**)




Yellow solid (32.5 mg), Isolated yield = 45%; m.p. 169.4 - 170.3 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.0 Hz, 2H), 7.36 (dd, $J_1$ = 8.4 Hz, $J_2$ = 2.0 Hz, 1H), 7.29 (d,*J* = 8.0 Hz, 2H), 7.17 (d, *J* = 1.6 Hz, 1H), 6.88 (d,*J* = 8.4 Hz, 1H), 5.27 (s, 2H),2.42 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 162.7, 143.1, 138.9, 132.0, 129.7, 129.2, 127.2, 126.0, 125.2, 120.1, 119.4, 70.4, 21.5; IR (film):2110, 1557, 1380, 1270, 1144, 1085, 802, 709 cm$^{-1}$; HRMS (ESI) calcd for $C_{16}H_{13}ClN_3O_3SNa$ (M+Na$^{+}$): 384.0180; found: 384.0162.

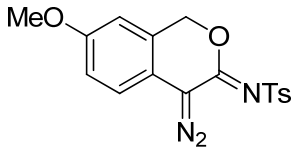
*N*-(4-Diazo-7-fluoroisochroman-3-ylidene)-4-methylbenzenesulfonamide (**3d**)




Yellow solid (43.8mg), Isolated yield = 64%; m.p.169.7 – 170.5 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ

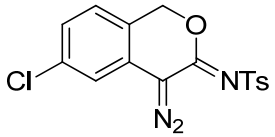
7.88 (d, $J$ = 8.4 Hz, 2H), 7.30 (d, $J$ = 8.4 Hz, 2H), 7.11 (td, $J_1$ = 8.4 Hz, $J_2$ = 2.4 Hz, 1H), 6.95 – 6.91 (m, 2H), 5.28 (s, 2H),2.43 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ163.1, 160.9 ($J$ = 246.7 Hz),143.0, 138.9, 129.1, 127.2, 126.4 ($J$ = 7.5 Hz),120.6 ($J$ = 8.2 Hz), 116.8 ($J$ = 22.7 Hz),116.5 ($J$ = 3.0 Hz),112.6 ($J$ = 23.7 Hz), 70.5 ($J$ = 2.1 Hz), 21.5; IR (film): 1686, 1583, 1492, 1399, 1310, 1212, 860, 725 cm$^{-1}$; HRMS (ESI) calcd for $C_{16}H_{13}FN_3O_3SNa$ (M+Na$^+$): 368.0476; found: 368.0453.

*N*-(4-Diazo-7-methoxyisochroman-3-ylidene)-4-methylbenzenesulfonamide (**3e**)



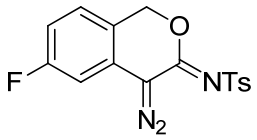

Yellow solid (45.7 mg), Isolated yield = 64%; m.p. 173.4 - 174.5 $^o$C; $^1$H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, $J$ = 8.4 Hz, 2H), 7.28 (d, $J$ = 8.4 Hz, 2H), 6.94 – 6.91 (dd,$J_1$ = 8.4 Hz, $J_2$ = 2.4 Hz, 1H), 6.84 (d, $J$ = 8.4 Hz, 1H), 6.71(d, $J$ = 2.4 Hz, 1H),5.26 (s, 2H), 3.80 (s, 3H), 2.41 (s, 3H); $^{13}$C NMR (400MHz, $CDCl_3$): δ 164.0, 158.4, 142.9, 139.2, 129.1, 127.2, 126.0, 120.3, 115.3, 111.7, 110.8, 71.1, 55.6, 21.5; IR (film): 3056, 2841, 2100, 1557, 1495, 1403, 1319, 1263, 1150, 810, 740cm$^{-1}$; HRMS (ESI) calcd for $C_{17}H_{16}N_3O_4SNa$ (M+Na$^+$):380.0676 ; found: 380.0669.

*N*-(4-Diazo-6-chloroisochroman-3-ylidene)-4-methylbenzenesulfonamide (**3f**)



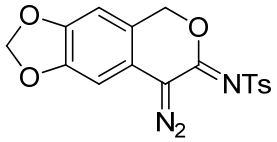

Yellow solid (36.8 mg), Isolated yield = 51%; m.p. 140.1 - 140.6 $^o$C; $^1$H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, $J$ = 8.0 Hz, 2H), 7.29 (d, $J$ = 8.0 Hz, 2H), 7.16 (dd,$J_1$ = 8.2 Hz, $J_2$ = 1.6 Hz, 1H), 7.10 – 7.08 (d, $J$ = 8.4 Hz, 1H), 6.92(d, $J$ = 1.6 Hz, 1H),5.27 (s, 2H),2.42 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 162.6, 143.1, 138.9, 135.6, 129.2, 127.2, 126.3, 126.2, 123.0, 122.7, 118.8, 70.7, 21.5; IR (film):2926, 2108, 1557, 1392, 1316, 1153, 1085, 856, 746 cm$^{-1}$; HRMS (ESI) calcd for $C_{16}H_{13}ClN_3O_3SNa$ (M+Na$^+$): 384.0180; found: 384.0157.

*N*-(4-Diazo-6-fluoroisochroman-3-ylidene)-4-methylbenzenesulfonamide (**3g**)



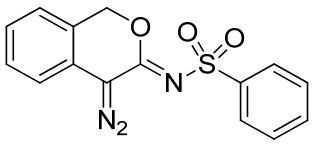

Yellow solid (18.7 mg), Isolated yield = 27%; m.p. 169.3 - 170.0 $^o$C; $^1$H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, $J$ = 8.4 Hz, 2H), 7.29 (d, $J$ = 8.0 Hz, 2H), 7.13 (dd, $J_1$ = 8.4 Hz, $J_2$ = 4.8 Hz, 1H),6.89 (td, $J_1$ = 8.4 Hz, $J_2$ = 2.4 Hz, 1H),6.66 (dd, $J_1$ = 8.4 Hz, $J_2$ = 2.4 Hz, 1H),5.28 (s, 2H), 2.42 (s, 3H); $^{13}$C NMR (100MHz, $CDCl_3$): δ 163.2 ($J$ = 247.8 Hz), 162.6, 143.21 138.9, 129.2, 127.2, 126.8 ($J$ = 9.0 Hz), 123.4 ($J$ = 9.2 Hz), 120.2 ($J$ = 3.1 Hz), 113.4 ($J$ = 22.2 Hz), 106.2 ($J$ = 25.5 Hz), 70.7, 21.5; IR (film): 3066,2924, 2109, 1707, 1557, 1397, 1319, 1151, 1085, 907, 814, 750 cm$^{-1}$; HRMS (ESI) calcd for $C_{16}H_{14}FN_3O_3S$ (M+H$^+$): 346.0656; found: 346.0640.

*N*-( 4-Diazo-6,7-(Methylenedioxyisochroman-3-ylidene)-4-methylbenzenesulfonamide (**3h**)



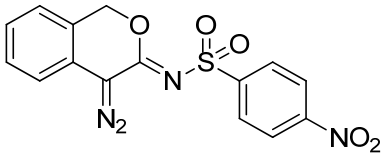
Orange solid (38.1 mg), Isolated yield = 51%; m.p. 169.1 – 170.0 $^{o}$C; $^{1}$H NMR (600 MHz, $CDCl_3$): δ 7.87 (d, *J* = 7.8 Hz, 2H), 7.27 (d, *J* = 7.8 Hz, 2H), 6.63 (s, 1H), 6.39 (s, 1H), 5.99 (s, 2H), 5.17 (s, 2H), 2.41 (s, 3H); $^{13}$C NMR (150 MHz, $CDCl_3$): δ 163.8, 148.9, 146.6, 142.9, 139.1, 129.1, 127.2, 117.9, 113.5, 105.9, 101.8, 99.8, 71.1, 21.5; IR (film): 3041, 2916, 2099, 1560, 1391, 1307, 1237, 1164, 1085, 1036, 977, 842, 762, 684 cm$^{-1}$; HRMS (ESI) calcd for $C_{17}H_{13}N_3O_5SN$ (M+Na$^{+}$): 394.0468; found: 394.0479.

*N*-(4-Diazoisochroman-3-ylidene)-benzenesulfonamide (**3i**)



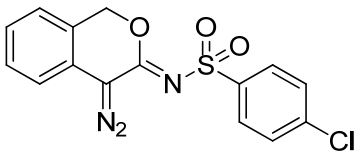
Yellow solid (35.4 mg), Isolated yield = 53%; m.p. 171.7 - 172.5 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.02 – 7.99 (m, 2H), 7.57 – 7.47 (m, 3H),7.38 (td, $J_1$ = 7.6 Hz, $J_2$ = 1.6 Hz, 1H), 7.19 (td, $J_1$ = 7.6 Hz, $J_2$ = 0.8 Hz, 2H), 6.93 (dd, $J_1$ = 7.6 Hz, $J_2$ = 0.8 Hz, 1H), 6.93 (d, *J* = 7.6 Hz, 1H), 5.28 (s, 2H); $^{13}$C NMR (100MHz, $CDCl_3$): δ 163.8, 142.0, 132.2, 129.5, 128.5, 127.1,126.3, 124.8, 124.3, 120.5, 118.8, 71.2; IR (film): 2106, 1548, 1319, 1288, 1149, 1084, 823, 752 cm$^{-1}$; HRMS (MALDI) calcd for $C_{15}H_{11}N_3O_3SNa$ (M+Na$^{+}$): 336.0413; found: 336.0414.

*N*-(4-Diazoisochroman-3-ylidene)-4-nitrobenzenesulfonamide (**3j**)



Yellow solid (35.6 mg), Isolated yield = 57%; m.p. 169.7 - 170.4 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.34 (d, *J* = 9.2 Hz, 2H), 8.18 (d, *J* = 8.8 Hz, 2H), 7.42 (t, J = 7.6 Hz, 1H),7.24 (td, $J_1$ = 7.2 Hz, $J_2$ = 0.8 Hz, 2H), 6.97 (d, *J* = 8.0 Hz, 1H), 5.28 (s, 2H); $^{13}$C NMR (100MHz, $CDCl_3$): δ 165.0, 149.8, 147.7, 129.8, 128.5, 126.7, 124.9, 124.1, 123.9, 120.1, 118.9, 71.7;IR (film):2924, 2107, 1750, 1531, 1407, 1350, 1313, 1152, 1085, 966, 812, 756 cm$^{-1}$; HRMS (ESI) calcd for $C_{15}H_{10}N_4O_5SNa$ (M+Na$^{+}$): 381.0264; found: 381.0258.

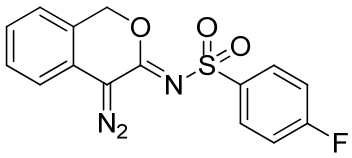
4-Chloro-*N*-(4-diazoisochroman-3-ylidene)benzenesulfonamide (**3k**)



Yellow solid (52.1mg), Isolated yield = 75%; m.p. 165.0 - 165.8 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.94 (d, *J* = 8.8 Hz, 2H), 7.46 (d, *J* = 8.8 Hz, 2H), 7.39 (td, $J_1$ = 7.6 Hz, $J_2$ = 0.8 Hz, 1H), 7.21 (td, $J_1$ = 7.6 Hz, $J_2$ = 1.2 Hz, 1H), 7.16 (dd, $J_1$ = 7.6 Hz, $J_2$ = 0.8 Hz, 1H), 6.95 (d, *J* = 7.6 Hz, 1H), 5.28 (s, 2H);

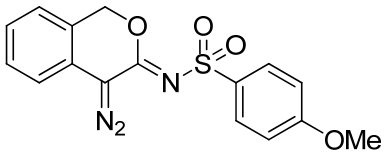
$^{13}$C NMR (100MHz, $CDCl_3$): δ 164.1, 140.6, 138.7, 129.6, 128.8, 128.7, 126.4, 124.9, 124.3, 120.4, 118.9, 71.4; IR (film): 2923, 2104, 1557, 1407, 1316, 1149, 1087, 811, 755 cm$^{-1}$; HRMS (ESI) calcd for $C_{15}H_{11}ClN_3O_3SNa$ (M+Na$^+$): 370.0024; found: 369.9999.

*N*-(4-Diazoisochroman-3-ylidene)-4-fluorobenzenesulfonamide (**3l**)



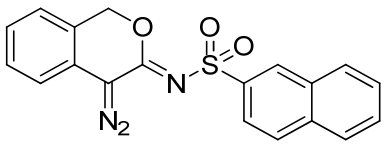
Yellow solid (48.7 mg), Isolated yield = 74%; m.p. 168.2 – 168.8 $^o$C; $^1$H NMR (400 MHz, $CDCl_3$): δ 8.01 (dd, $J_1$ = 8.4 Hz, $J_2$ = 5.2 Hz, 2H), 7.39 (t, $J$ = 7.4 Hz, 1H), 7.22– 7.14 (m, 4H), 6.94 (d, $J$ = 8.0 Hz, 1H), 5.31 (s, 2H); $^{13}$C NMR (100MHz, $CDCl_3$): δ 164.8 ($J$ = 252.2 Hz), 164.0, 138.1 ($J$ = 3.1 Hz), 129.9 ($J$ = 9.2 Hz), 129.5, 126.3, 124.8, 124.2, 120.3, 118.8, 115.6 ($J$ = 22.3 Hz), 71.3; IR (film): 2923, 2108, 1557, 1404, 1316, 1148, 1085, 968, 839, 757 cm$^{-1}$; HRMS (MALDI) calcd for $C_{15}H_{10}FN_3O_3SNa$ (M+Na$^+$): 354.0319; found: 354.0323.

*N*-(4-Diazoisochroman-3-ylidene)-4-methoxybenzenesulfonamide (**3m**)



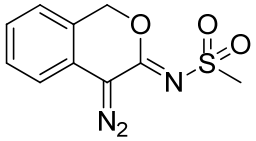
Yellow solid (37.2 mg), Isolated yield = 53%; m.p. 163.1 - 163.5 $^o$C; $^1$H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, $J$ = 8.8 Hz, 2H), 7.37 (td, $J_1$= 8.0 Hz, $J_2$= 0.8 Hz, 1H), 7.21 – 7.14 (m, 2H), 6.96 (d, $J$ = 9.2 Hz, 2H), 6.94 (d, $J$ = 8.4 Hz, 1H), 5.28 (s, 2H), 3.86 (s, 3H); $^{13}$C NMR (100MHz, $CDCl_3$): δ 163.3, 162.5, 133.8, 129.5, 129.3, 126.2, 124.8, 124.4, 120.6, 118.8, 113.6, 71.1, 55.5; IR (film): 3263, 2104, 1747, 1597, 1499, 1335, 1263, 1158, 1025, 834, 740 cm$^{-1}$; HRMS (ESI) calcd for $C_{16}H_{14}N_3O_4S$ (M+H$^+$): 344.0700; found: 344.0681.

*N*-(4-Diazoisochroman-3-ylidene)naphthalene-2-sulfonamide (**3n**)



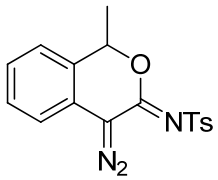
Yellow solid (33.9 mg), Isolated yield = 46%; m.p.182.3 - 182.9$^o$C; $^1$H NMR (400 MHz, $CDCl_3$): δ 8.56 (s, 1H), 8.00 – 7.87 (m, 4H), 7.61 – 7.55 (m, 2H),7.34 (t, $J$ = 7.6 Hz, 1H), 7.16 (t, $J$ = 7.6 Hz, 1H), 7.10 (d, $J$ = 7.2 Hz, 1H), 6.89 (d, $J$ = 7.6 Hz, 1H), 5.26 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 163.8, 138.9, 134.6, 132.0, 129.5,129.2, 128.6, 128.4, 128.0, 127.7, 127.1, 126.2, 124.7, 124.3, 122.9, 120.4,118.8, 71.2; IR (film): 2103, 1557, 1417, 1287, 1123, 1069, 806, 745 cm$^{-1}$; HRMS (MALDI) calcd for $C_{19}H_{12}N_3O_3SNa$ (M+Na$^+$): 386.0570; found: 386.0571.

N-(4-Diazoisochroman-3-ylidene)methanesulfonamide (**3o**)



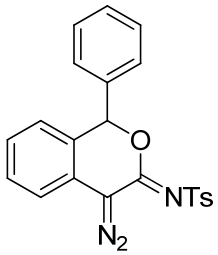
Orange solid (9.8 mg), Isolated yield = 8 %; m.p. 166.2 - 166.9 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.42 (td, $J_1$ = 7.6 Hz, $J_2$ = 0.8 Hz, 1H), 7.26 – 7.19 (m, 2H), 6.99 (d, $J$ = 8.0 Hz, 1H), 5.42 (s, 2H), 3.10 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 163.6, 129.6, 126.4, 124.9, 124.5, 120.6, 118.9, 71.4, 42.6; IR (film): 2928, 2104, 1747, 1568, 1403, 1317, 1138, 965, 825, 757 cm$^{-1}$; HRMS (ESI) calcd for $C_{10}H_{10}N_3O_3SNa$ (M+Na$^+$): 274.0257; found: 274.0239.

*N*-( 4-Diazo-1-Methylisochroman-3-ylidene)-4-methylbenzenesulfonamide (**3p**)



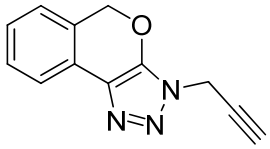

Orange solid (48.0 mg), Isolated yield = 70%; m.p. 191.2 - 191.9 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.90 (d, $J$ = 8.0 Hz, 2H), 7.37 (td, $J_1$ = 7.6 Hz, $J_2$ = 0.8 Hz, 1H), 7.29 (d, $J$ = 8.0 Hz, 2H), 7.19 (td, $J_1$ = 7.6 Hz, $J_2$ = 1.2 Hz, 1H), 7.11 (d, $J$ = 7.6 Hz, 1H), 5.48 (q, $J$ = 6.4 Hz, 1H), 2.42 (s, 3H), 1.49 (d, $J$ = 6.4 Hz, 3H); $^{13}$C NMR (100MHz, $CDCl_3$): δ 163.2, 142.9, 139.3, 129.29, 129.26, 129.0, 127.5, 126.3, 124.4, 119.6, 119.0, 79.3, 21.5, 21.2; IR (film): 2101, 1557, 1395, 1316, 1152, 1086, 915, 818, 786, 756 cm$^{-1}$; HRMS (ESI) calcd for $C_{17}H_{15}N_3O_3SNa$ (M+Na$^+$): 364.0726; found: 364.0730.

*N*-( 4-Diazo-1-phenylisochroman-3-ylidene)-4-methylbenzenesulfonamide (**3q**)




Orange solid (44.8 mg), Isolated yield = 56 %; m.p. 176.8 – 177.5 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, $J$ = 8.4 Hz, 2H), 7.42 – 7.31 (m, 4H), 7.17 – 7.07 (m, 5H), 6.98 (d, $J$ = 7.6 Hz, 1H), 6.89 (d, $J$ = 7.6 Hz, 1H), 6.31 (s, 1H), 2.36 (s, 3H); $^{13}$C NMR (100MHz, $CDCl_3$): δ 162.7, 142.7, 138.9, 136.4, 129.6, 129.3, 128.9, 128.7, 127.8, 127.5, 126.5, 126.1, 120.7, 118.9, 83.9, 21.5; IR (film): 3067, 2916, 2107, 1545, 1388, 1314, 1149, 1086, 969, 804, 759 cm$^{-1}$; HRMS (ESI) calcd for $C_{22}H_{17}N_3O_3SNa$ (M+Na$^+$): 426.0883; found: 426.0882.

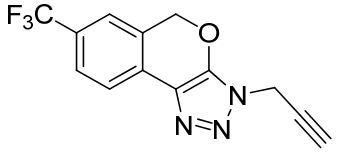
3-(Prop-2-yn-1-yl)-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5a**)




Colorless solid (18.9 mg), Isolated yield = 90%; m.p. 145.3 – 146.0 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, $J$ = 7.6 Hz, 2H), 7.38 (t, $J$ = 7.6 Hz, 1H), 7.23 (td, $J_1$ = 7.6 Hz, $J_2$ = 1.2 Hz, 1H), 7.12 (d, $J$ = 7.6 Hz, 1H), 5.51 (s, 2H), 5.00 (d, $J$ = 2.4 Hz, 2H), 2.45 (t, $J$ = 2.6 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 147.9, 129.2, 127.2, 127.1, 126.7, 126.0, 124.4, 120.3, 75.1, 74.3, 73.6, 35.9; IR (film): 3234, 2962, 2932, 2127, 1625, 1597, 1548, 1454, 1405, 1351, 1298, 1210, 1088, 966, 771, 730, 693

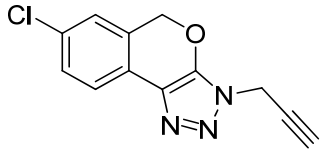
$cm^{-1}$; HRMS (EI) calcd for $C_{12}H_9N_3O$ ($M^+$): 211.0746; found: 211.0744;

7-Trifluoromethyl-3-(2-propyn-1-yl)- 3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5b**)



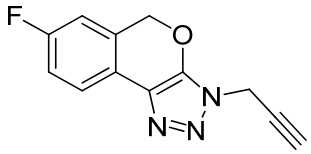
Colorless solid (26.2 mg), Isolated yield = 94%; m.p. 136.9 – 137.8 $^oC$; $^1H$ NMR (400 MHz, $CDCl_3$): δ 7.89 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.38 (s, 1H), 5.57 (s, 2H), 5.02 (d, *J* = 2.8 Hz, 1H), 2.48 (t, *J* = 2.6 Hz, 1H); $^{13}C$ NMR (100 MHz, $CDCl_3$): δ 148.6, 130.1, 129.1(*J* = 32.6 Hz), 126.4 (*J* = 3.8 Hz), 126.3, 126.1, 123.8 (*J* = 270.3 Hz), 121.6 (*J* = 3.8 Hz), 120.4, 74.8, 74.6, 73.2, 36.0; IR (film): 3085, 1608, 1571, 1551, 1417, 1331, 1292, 1161, 1117, 1072, 952, 881, 842, 706 $cm^{-1}$; HRMS (EI) calcd for $C_{13}H_8F_3N_3O$ ($M^+$): 279.0619; found: 279.0615.

7-Chloro-3-(2-propyn-1-yl)-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5c**)



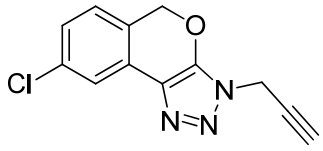
Colorless solid(21.0 mg), Isolated yield = 86%; m.p. 175.5 – 176.0 $^oC$;$^1H$ NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.0 Hz, 1H), 7.34 (dd, $J_1$ = 8.0 Hz, $J_2$ = 2.0 Hz, 1H), 7.11 (d, *J* = 1.6 Hz, 1H), 5.47 (s, 2H), 5.00 (d, *J* = 2.8 Hz, 1H), 2.46 (t, *J* = 2.4 Hz, 1H); $^{13}C$ NMR (100 MHz, $CDCl_3$): δ 147.8, 132.7, 129.3, 127.6, 126.4, 125.3, 124.8, 121.6, 74.9, 74.5, 72.9, 36.0; IR (film): 3284, 2922, 1625, 1590, 1547, 1402, 1292, 1209, 956, 869, 824, 730 $cm^{-1}$; HRMS (EI) calcd for $C_{12}H_8ClN_3O$ ($M^+$): 245.0356; found: 245.0355.

7-Fluoro-3-(2-propyn-1-yl)- 3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5d**)



Colorless solid (19.8 mg), Isolated yield = 86%; m.p. 130.8 – 131.7 $^oC$;$^1H$ NMR (400 MHz, $CDCl_3$): δ7.77 – 7.73 (m, 1H), 7.07 (t, *J* = 8.6 Hz,1H), 6.85 (d, *J* = 8.8 Hz, 1H), 5.48 (s, 2H), 5.00 (s, 2H), 2.47 (s, 1H); $^{13}C$ NMR (100 MHz, $CDCl_3$): δ 161.8 (*J* = 245.5 Hz), 147.4, 128.1 (*J* = 7.4 Hz), 126.5, 123.0 (*J* = 3.1 Hz), 122.0 (*J* = 8.2 Hz), 115.9 (*J* = 21.6 Hz), 112.1 (*J* = 23.6 Hz), 75.0, 74.4, 73.0 (*J* = 2.1 Hz),36.0; IR (film): 3296, 1629, 1586, 1549, 1497, 1421, 1295, 1265, 1253, 1207, 1158, 1087, 1013, 967, 927, 873, 824, 754, 697 $cm^{-1}$; HRMS (EI) calcd for $C_{12}H_8FN_3O$ ($M^+$): 229.0651; found:229.0647.

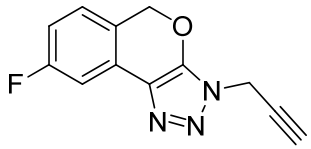
8-Chloro-3-(2-propyn-1-yl)- 3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5e**)



Colorless solid (20.2 mg), Isolated yield = 82%; m.p. 163.6 – 164.4 $^oC$; $^1H$ NMR (400 MHz,

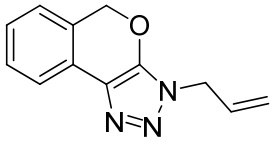
$CDCl_3$): δ 7.77 (d, $J$ = 2.0 Hz, 1H), 7.19 (dd, $J_1$ = 8.0 Hz, $J_2$ = 2.0 Hz, 1H), 7.05 (d, $J$ = 8.0 Hz, 1H), 5.48 (s, 2H), 5.00 (d, $J$ = 2.8 Hz, 1H), 2.46 (t, $J$ = 1.2 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 148.2, 135.3, 128.3, 127.0, 126.2, 125.8, 124.1, 120.4, 74.9, 74.5, 73.2, 36.0; IR (film): 3267, 2923, 1618, 1593, 1432, 1295, 1210, 1087, 942, 814, 706, 669 cm$^{-1}$； HRMS (EI) calcd for $C_{12}H_8ClN_3O$ ($M^+$): 245.0356; found: 245.0357.

8-Fluoro-3-(prop-2-yn-1-yl)- 3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5f**)



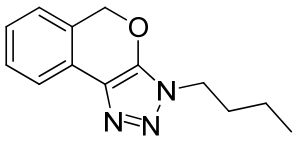

Colorless solid(18.9 mg),Isolated yield = 83%; m.p. 175.5 – 176.0 $^{o}$C;$^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.48 (dd, $J_1$ = 8.8 Hz, $J_2$ = 2.8 Hz, 1H),7.11 – 7.08 (m, 1H), 6.91 (td, $J_1$ = 8.4 Hz,$J_2$ = 2.4 Hz, 1H), 5.48 (s, 2H), 5.00 (d,$J$ = 2.8 Hz, 2H), 2.47 (t, $J$ = 2.6 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 163.3 ($J$ = 245.9 Hz), 148.2, 128.9 ($J$ = 9.6 Hz), 126.6 ($J$ = 2.5 Hz), 126.3 ($J$ = 8.8 Hz), 121.5 ($J$ = 3.2 Hz), 113.7 ($J$ = 22.3 Hz), 107.7 ($J$ = 24.3 Hz), 74.9, 74.4, 73.3, 36.0; IR (film): 3284, 2922, 1604, 1547, 1495, 1446, 1265, 1208, 948, 867, 808, 739 cm$^{-1}$; HRMS (EI) calcd for $C_{12}H_8FN_3O$ ($M^+$): 229.0651; found:229.0652.

3-Allyl-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5g**)



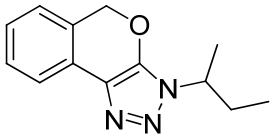

Colorless solid(20.1mg), Isolated yield = 94%; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, $J$ = 7.6 Hz, 1H), 7.37 (t, $J$ = 7.6 Hz, 1H), 7.22 (t, $J$ = 7.6 Hz, 1H), 7.10 (d, $J$ = 7.6 Hz, 1H), 6.05 – 5.95 (m, 1H), 5.45 (s, 2H), 5.31 – 5.22 (m, 2H), 4.81 (dd, $J_1$ = 5.6 Hz, $J_2$ = 1.2 Hz, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 148.0, 130.7, 129.1, 127.0, 126.9, 126.1, 124.4, 120.2, 119.0, 73.4, 48.6; IR (film): 3055, 2923, 2856, 1623, 1594, 1546, 1454, 1298, 1265, 1212, 962, 734 cm$^{-1}$; HRMS (EI) calcd for $C_{12}H_{11}N_3O$ ($M^+$): 213.0902; found: 213.0905;

3-Butyl-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole(**5h**)



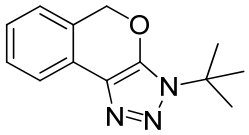

Light yellowoil(19.1 mg),Isolated yield = 83%;$^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, $J$ = 7.6 Hz, 1H), 7.36 (t, $J$ = 7.6 Hz, 1H), 7.21 (t, $J$ = 7.6 Hz, 1H), 7.11 (d, $J$ = 7.2 Hz, 1H), 5.45 (s, 2H), 4.19 (t, $J$ = 7.0 Hz, 2H), 1.90 – 1.83 (m, 2H), 1.42– 1.33 (m, 2H), 0.95 (t, $J$ = 7.4 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 148.0, 129.1, 127.1, 126.90, 126.86, 126.1, 124.4, 120.2, 73.3, 46.2, 31.2, 19.6, 13.4; IR (film): 2959, 2872, 1623, 1593, 1545, 1454, 1300, 1258, 1211, 1042, 963, 765, 731 cm$^{-1}$; HRMS (EI) calcd for $C_{13}H_{15}N_3O$: 229.1215 ($M^+$); found: 229.1213.

3-(*sec*-Butyl)-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5i**)



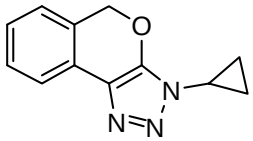
Light yellow oil (18.5 mg),Isolated yield = 81%; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.21 (t, *J* = 7.4 Hz, 1H), 7.11 (d, *J* = 7.6 Hz, 1H), 5.43 (s, 2H), 4.47 – 4.38 (m, 1H), 2.07 – 1.98 (m, 1H),1.91 – 1.80 (m, 1H),1.58 (d, *J* = 6.8 Hz, 3H), 0.88 (t, *J* = 7.4 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 147.7, 129.1, 127.2, 126.8, 126.2, 124.4, 120.2, 73.1, 56.4, 29.6, 28.7, 19.6, 10.6; IR (film): 2969, 2934, 2877, 1622, 1592, 1538, 1454, 1299, 1238, 1220, 964, 765, 731 $cm^{-1}$; HRMS (EI) calcd for $C_{13}H_{15}N_3O$: 229.1215 ($M^+$); found: 229.1211.

3-*tert*-Butyl-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5j**)



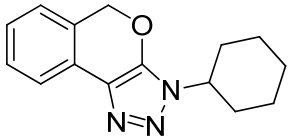
Light yellow oil (16.6 mg, 0.2 mmol), Isolated yield = 36%; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.8 Hz, 1H), 7.20 (t, *J* = 7.8 Hz, 1H), 7.10 (d, *J* = 7.6 Hz, 1H), 5.41(s, 2H), 1.68 (s, 9H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 148.0, 129.1, 128.1, 127.3, 126.8, 126.0, 124.3, 120.2, 72.9, 59.6, 28.5; IR (film): 2984, 2929, 1621, 1590, 1529, 1452, 1387, 1234, 963, 766, 732 $cm^{-1}$; HRMS (EI) calcd for $C_{13}H_{15}N_3O$: 229.1215 ($M^+$); found: 229.1213.

3-Cyclopropyl-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5k**)



Colorless solid (19.0 mg), Isolated yield = 89%; m.p. 113.0 – 113.7 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$):7.77 (d, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.21 (td, $J_1$ = 7.6 Hz, $J_1$ = 1.2 Hz, 1H), 7.10 (d, *J* = 7.6 Hz, 1H), 5.46 (s, 2H),3.52 – 3.46 (m, 1H), 1.31 – 1.28 (m, 2H), 1.16 – 1.10 (m, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 149.1, 129.1, 126.93, 126.89, 126.1, 124.4, 120.1, 73.2, 27.5, 5.85; IR (film): 3054, 3016, 2928, 2874, 1622, 1597, 1542, 1448, 1298, 1260, 1224,1038, 940, 763, 727 $cm^{-1}$; HRMS (EI) calcd for $C_{12}H_{11}N_3O$: 213.0902 ($M^+$); found: 213.0899.

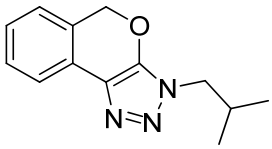
3-Cyclohexyl-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5l**)



Colorless solid (20.6 mg), Isolated yield = 81%; m.p. 86.9 – 87.7 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$):7.79 (d, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.4 Hz, 1H), 7.21 (td, $J_1$ = 7.6 Hz, $J_1$ = 0.8 Hz, 1H), 7.11 (d, *J* = 7.6 Hz, 1H), 5.43 (s, 2H), 4.33 – 4.25 (m, 1H), 2.10 – 1.91 (m, 6H), 1.76 (m, 1H), 1.47 – 1.26 (m, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 147.4, 129.1, 127.25, 127.21, 126.8, 126.2, 124.4, 120.2, 73.1, 57.8, 31.7, 25.3, 25.0; IR (film): 3053, 2935, 2857, 1622, 1592, 1538, 1453, 1258, 1235, 1217, 1060,

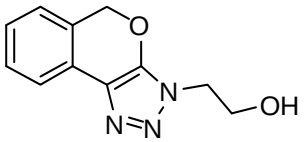
962, 765, 732 $cm^{-1}$; HRMS (EI) calcd for $C_{15}H_{17}N_3O$ ($M^+$): 255.1372; found: 255.1372.

3-Isobutyl-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5m**)



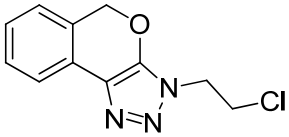
Light yellowoil(20.8 mg), Isolated yield = 91%; $^1$H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 7.2 Hz, 1H), 7.29 (t, *J* = 7.4 Hz, 1H), 7.13 (td, $J_1$ = 7.6 Hz, $J_2$ = 0.8 Hz, 1H), 7.03 (d, *J* = 7.6 Hz, 1H), 5.36 (s, 2H), 3.92 (d, *J* = 7.2 Hz, 2H), 2.23 – 2.13 (m, 1H), 0.89 (s, 3H), 0.88 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 148.2, 129.1, 127.1, 126.9, 126.7, 126.1, 124.4, 120.2, 73.3, 53.5, 29.6, 28.8, 19.8; IR (film): 2963, 2873, 1766, 1622, 1593, 1545, 1454, 1403, 1297, 1238, 1216, 1042, 963, 765, 731 $cm^{-1}$; HRMS (EI) calcd for $C_{13}H_{15}N_3O$ ($M^+$): 229.1215; found: 229.1211.

3-(2-Hydroxylethyl)-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5n**)



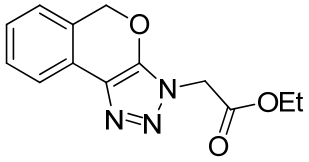
Colorless solid (17.0 mg), Isolated yield = 78%; m.p. 154.2 – 154.9 $^o$C; $^1$H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, *J* = 7.6 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.15 (t, *J* = 7.4 Hz, 1H), 6.95 (d, *J* = 7.6 Hz, 1H), 5.31 (s, 2H), 4.28 (t, *J* = 4.2 Hz, 2H), 4.13 (t, *J* = 4.4 Hz, 2H), 1.82 (s, 1H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 148.4, 129.0, 127.1, 126.5, 126.4, 126.3, 124.3, 120.2, 73.3, 60.5, 49.0, 29.7; IR (film):3252, 2955, 2910, 2863, 1623, 1596, 1569, 1549, 1455, 1426, 1412, 1379, 1301, 1265, 1236, 1211, 1195,1112, 1076, 1023, 955, 862, 768, 734 $cm^{-1}$; HRMS (ESI) calcd for $C_{11}H_{11}N_3O_2Na$ ($M+Na^+$): 240.0743; found: 240.0720.

3-(2-Chloroethyl)-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5o**)



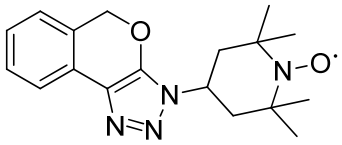
Colorless solid (18.4 mg),Isolated yield = 78%; m.p. 87.3 – 88.0 $^o$C;$^1$H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, *J* = 7.6 Hz, 1H), 7.38 (tt, $J_1$ = 7.6 Hz, $J_2$ = 0.6 Hz, 1H), 7.23 (td, $J_1$ = 7.4 Hz, $J_2$ = 1.2 Hz, 1H), 7.13 (d, *J* = 7.2 Hz, 1H), 5.49 (s, 2H), 4.52 (t, *J* = 6.2 Hz, 2H), 3.94 (t, *J* = 6.4 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 148.5, 129.2, 127.2, 126.9, 126.8, 126.1, 124.5, 120.3, 73.6, 47.6, 41.3; IR (film): 3062, 3011, 2966, 2852, 1623, 1595, 1571, 1547, 1492, 1453, 1438, 1409, 1301, 1278, 1220, 1193, 1155, 1086, 1013, 968, 908, 767, 732 $cm^{-1}$; HRMS (EI) calcd for $C_{11}H_{10}ClN_3O$ ($M^+$): 235.0512; found: 235.0515.

Ethyl 2-(isochromeno[3,4-d][1,2,3]triazol-3(5H)-yl)acetate (**5p**)

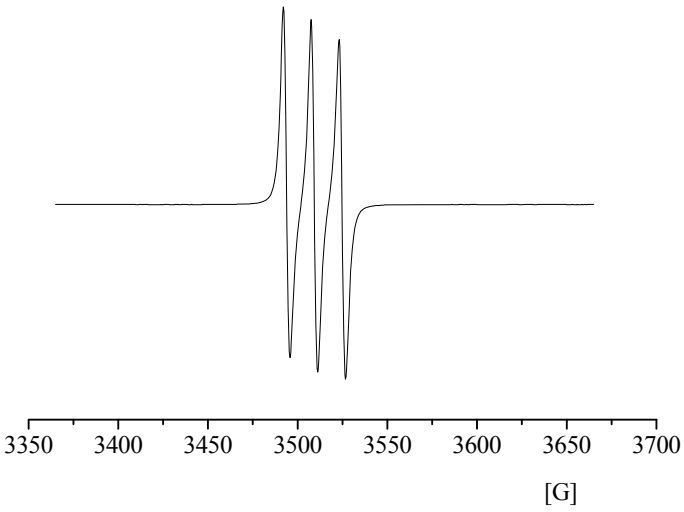


Colorless solid (18.4 mg), Isolated yield = 71%; m.p. 93.8 – 94.5 $^{o}$C;$^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, *J* = 7.6 Hz, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H),7.11 (d, *J* = 7.6 Hz, 1H), 5.48 (s, 2H), 4.99 (s, 2H), 4.27 (q, *J* = 7.2, 2H), 1.30 (t, *J* = 6.8, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 165.8, 148.7, 129.2, 127.1, 126.9, 126.8, 126.0, 124.4, 120.3, 73.6, 62.3, 47.2, 14.0; IR (film): 2985, 2860, 1748, 1625, 1596, 1549, 1455, 1375, 1412, 1375, 1300, 1221, 1085, 1011, 962,766, 731 cm$^{-1}$; HRMS (EI) calcd for $C_{13}H_{13}N_3O_3$ ($M^+$):259.0957; found: 259.0956.

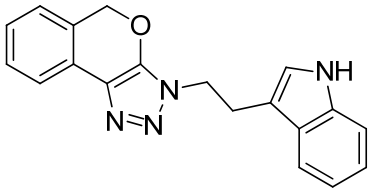
3-(2,2,6,6-Tetramethyl-1-N-oxylpiperidin-4-yl)-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5q**)



Colorless solid (28.1 mg), Isolated yield = 86%; m.p. 149.6 – 150.4 $^{o}$C; IR (film): 2972, 2926, 1622, 1593, 1538, 1455, 1379, 1366, 1323, 1300, 1242, 1188, 1063, 961, 765, 734 cm$^{-1}$; HRMS (EI) calcd for $C_{18}H_{23}N_4O_2$ ($M^+$): 327.1821; found: 327.1825. EPR (1× $10^{-4}$ M in DCM): 3 lines, A = 15.6 G, $\Delta H_0$ = 3.5 G, $g_0$ = 2.00571.



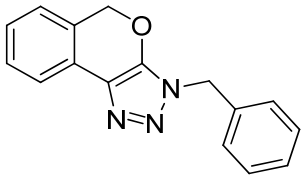

3-(2-(1*H*-Indol-3-yl)ethyl)-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5r**)



Colorless solid (25.7 mg), Isolated yield = 81%; m.p. 136.9 – 137.8 $^{o}$C; $^{1}$H NMR (400 MHz,

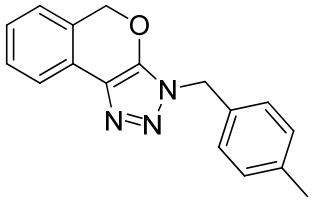
$CDCl_3$): δ 8.15 (s, 1H), 7.77 (d, *J* = 7.6 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.36 – 7.32 (m, 2H),7.20 – 7.16 (m, 2H), 7.12 (tt, $J_1$ = 7.4 Hz, $J_2$ = 0.8 Hz, 1H), 7.03 (d, *J* = 7.6 Hz, 1H), 6.95 (d, *J* = 1.2 Hz, 1H), 5.11 (s, 2H), 4.48 (t, *J* = 7.4 Hz, 2H), 3.36 (t, *J* = 7.0 Hz, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 148.3, 136.2, 129.1, 127.04, 127.00, 126.9, 126.2, 124.4, 122.4, 122.1, 120.2, 119.5, 118.4, 111.3, 111.2, 73.1, 46.9, 25.6; IR (film): 3358, 3313, 3262, 3052, 2919, 1624, 1594, 1550, 1459, 1305, 1161, 1098, 1015, 988, 969, 768, 743 $cm^{-1}$; HRMS (EI) calcd for $C_{19}H_{16}N_4O$ ($M^+$): 316.1324; found: 316.1324.

3-Benzyl-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5s**)



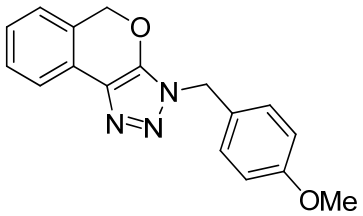
Colorless solid (23.7 mg),Isolated yield = 90%; m.p. 106.2 – 106.9 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 7.2 Hz, 2H), 7.37 – 7.30 (m, 6H), 7.20 (td, $J_1$ = 7.6 Hz, $J_2$ = 0.8 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 5.42 (s, 2H), 5.37 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 148.0, 134.5, 129.1, 128.8, 128.3, 127.8, 127.2, 127.0, 126.9, 126.1, 124.4, 120.2, 73.4, 50.1; IR (film): 3032, 2923, 2858, 1622, 1594, 1545, 1454, 1300, 1210, 963, 731, 701 $cm^{-1}$; HRMS (EI) calcd for $C_{16}H_{13}N_3O$ ($M^+$): 263.1059; found: 263.1056.

3-(4-Methylbenzyl)-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5t**)



Colorless solid (24.4 mg), Isolated yield = 88%; m.p. 109.9– 110.4$^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.8 Hz, 1H), 7.23 – 7.17 (m, 3H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 7.6 Hz, 1H), 5.41 (s, 2H), 5.32 (s, 2H), 2.31 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 147.9, 138.1, 131.5, 129.5, 129.1, 127.8, 127.1, 127.0, 126.9, 126.1, 124.4, 120.1, 73.3, 49.9, 21.1; IR (film): 3025, 2922, 2858, 1623, 1594, 1547, 1454, 1299, 1210, 959, 764, 731 $cm^{-1}$; HRMS (EI) calcd for $C_{17}H_{15}N_3O_2$ ($M^+$): 277.1215; found: 277.1215.

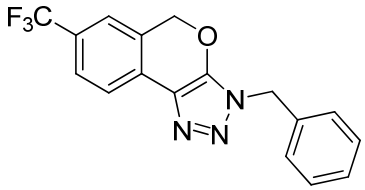
3-(4-Methoxybenzyl)-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5u**)



Yellow oil (24.4 mg), Isolated yield = 83%; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.77 (d, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 8.8 Hz, 2H), 7.19 (td, $J_1$ = 7.6 Hz, $J_2$ = 1.2 Hz, 1H), 7.07 (d, *J* = 7.6 Hz, 1H), 6.86 (d, *J* = 8.8 Hz, 2H), 5.42 (s, 2H), 5.30 (s, 2H),3.77 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 159.6, 147.8, 129.4, 129.1, 127.2, 127.0, 126.9, 126.6, 126.1, 124.4, 120.1, 114.1, 73.4, 55.2,

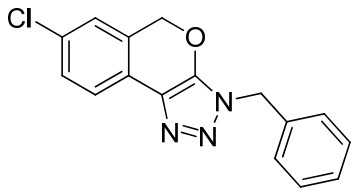
49.7; IR (film): 2934, 2836, 1622, 1539, 1515, 1454, 1265, 1030, 961, 736 $cm^{-1}$; HRMS (EI) calcd for $C_{17}H_{15}N_3O_2$: 293.1164 ($M^+$); found: 293.1167.

3-Benzyl-7-(trifluoromethyl)-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5v**)



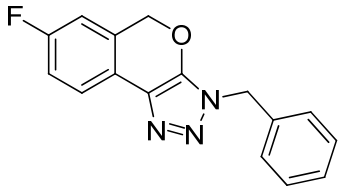
Colorless solid (28.7 mg), Isolated yield = 87%; m.p. 133.3 – 134.0 $^oC$; $^1H$ NMR (400 MHz, $CDCl_3$): δ 7.86 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.37 – 7.32 (m, 6H), 5.47 (s, 2H), 5.38 (s, 2H); $^{13}C$ NMR (100 MHz, $CDCl_3$): δ 148.7, 134.2, 130.4, 128.92, 128.89 (*J* = 32.6 Hz), 128.5, 127.9, 126.37, 126.32(*J* = 4.0 Hz), 126.2, 123.84(*J* = 270.4 Hz), 121.58(*J* = 3.7 Hz), 120.3,73.0, 50.3; IR (film): 3036, 2920, 2846, 1602, 1567, 1410, 1328, 1298, 1213, 1166, 1117, 1072, 969, 848, 734 $cm^{-1}$; HRMS (EI) calcd for $C_{17}H_{12}F_3N_3O$: 331.0932 ($M^+$); found:331.0928.

3-Benzyl-7-chloro-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5w**)



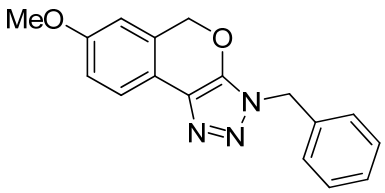
Colorless solid (25.7 mg), Isolated yield =87%; m.p. 118.4 – 119.0 $^oC$; $^1H$ NMR (400 MHz, $CDCl_3$): δ 7.69 (d, *J* = 8.0 Hz, 1H), 7.36 – 7.30 (m, 6H), 7.07 (s,1H), 5.37 (s, 2H), 5.36 (s, 2H); $^{13}C$ NMR (100 MHz, $CDCl_3$): δ 147.8, 134.3, 132.4, 129.2, 128.9, 128.4, 127.8, 127.7, 126.4, 125.5, 124.7, 121.4, 72.7, 50.2; IR (film): 3029, 2968, 2938, 1624, 1586, 1548, 1494, 1455, 1405, 1265, 1208, 1084, 960, 821, 717$cm^{-1}$; HRMS (EI) calcd for $C_{16}H_{12}ClN_3O$: 297.0669 ($M^+$); found: 297.0665.

3-Benzyl-7-fluoro-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5x**)



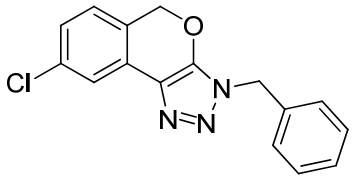
Colorless solid (22.7 mg), Isolated yield = 81%; m.p. 103.9– 104.7$^oC$; $^1H$ NMR (400 MHz, $CDCl_3$): δ 7.74 (dd, $J_1$ = 8.4 Hz, $J_2$ = 5.2 Hz, 1H), 7.36 – 7.30 (m, 5H), 7.05 (td, $J_1$ = 8.6 Hz, $J_2$ = 2.4 Hz, 1H), 6.81 (dd, $J_1$ = 8.8 Hz, $J_2$ = 2.0 Hz, 1H), 5.39 (s, 2H), 5.36 (s, 2H); $^{13}C$ NMR (100 MHz, $CDCl_3$): δ 161.7 (*J* = 245.2 Hz), 147.5, 134.4, 128.9, 128.4, 128.2 (*J* = 7.3 Hz), 127.8, 126.6, 123.2 (*J* = 3.2 Hz), 121.9 (*J* = 8.1 Hz), 115.8 (*J* = 21.6 Hz),112.0 (*J* = 23.5 Hz), 72.8 (*J* = 2.1 Hz), 50.2; IR (film): 3033, 2933, 1633, 1586, 1549, 1495, 1455, 1426, 1274, 1244, 1206, 1158, 1088, 971, 927, 819, 731 $cm^{-1}$.HRMS (EI) calcd for $C_{16}H_{12}FN_3O$ ($M^+$): 281.0964; found: 281.0965.

3-Benzyl -7-methoxy-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5y**)



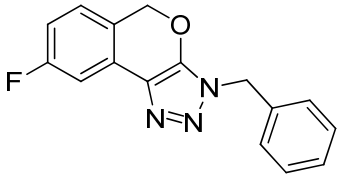
Colorless oil (23.9 mg), Isolated yield = 82%; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, $J$ = 8.4 Hz, 1H), 7.36 – 7.28 (m, 5H), 6.88 (dd, $J_1$ = 8.4 Hz, $J_2$ = 2.4 Hz, 1H), 6.64 (d, $J$ = 2.4 Hz, 1H), 5.37 (s, 2H), 5.36 (s, 2H),3.79 (s, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 158.8, 147.0, 134.6, 128.8, 128.3, 127.9, 127.8, 127.2, 121.5, 119.8, 113.6, 111.0, 73.2, 55.4, 50.1; IR (film): 3032, 2932, 2836, 1622, 1598, 1549, 1497, 1455, 1249, 1168, 1039, 972, 730, 702 cm$^{-1}$; HRMS (EI) calcd for $C_{17}H_{15}N_3O_2$ ($M^+$): 293.1164; found: 293.1165.

3-Benzyl-8-chloro-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5z**)



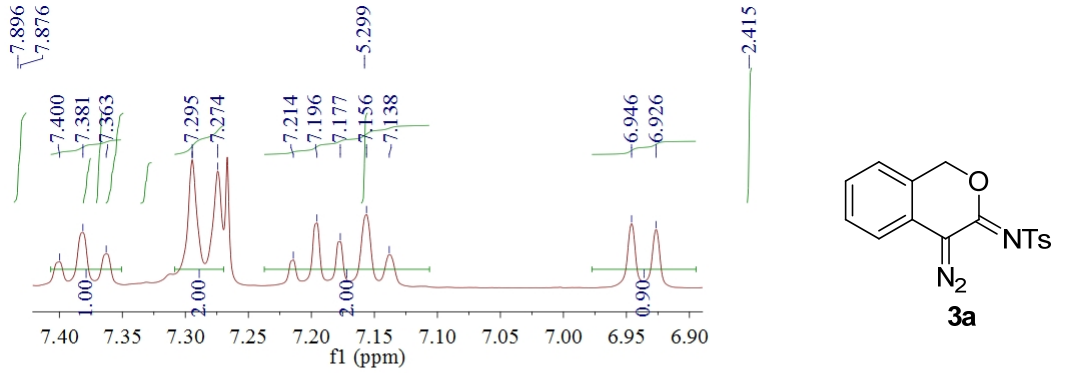
Colorless solid (24.4 mg), Isolated yield = 82%; m.p. 103.2 – 104.1 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.74 (s, 1H), 7.36 – 7.29 (m, 5H), 7.14 (d, $J$ = 8.0 Hz,1H), 6.99 (d, $J$ = 8.0 Hz,1H), 5.38 (s, 2H), 5.36 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ 148.2, 135.2, 134.3, 128.9, 128.6, 128.4, 127.8, 126.8, 126.2, 125.8, 124.2, 120.3, 72.9, 50.2; IR (film): 3064, 3036, 2923, 2855, 1620, 1591, 1546, 1424, 1273, 1211, 1080, 966, 823, 703 cm$^{-1}$; HRMS (EI) calcd for $C_{16}H_{12}ClN_3O$ ($M^+$): 297.0669; found: 297.0668.

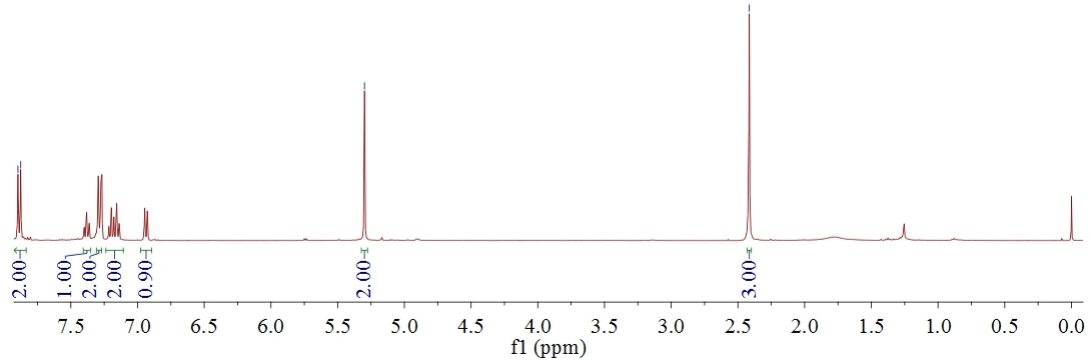
3-Benzyl-8-fluoro-3,5-dihydroisochromeno[3,4-d][1,2,3]triazole (**5A**)

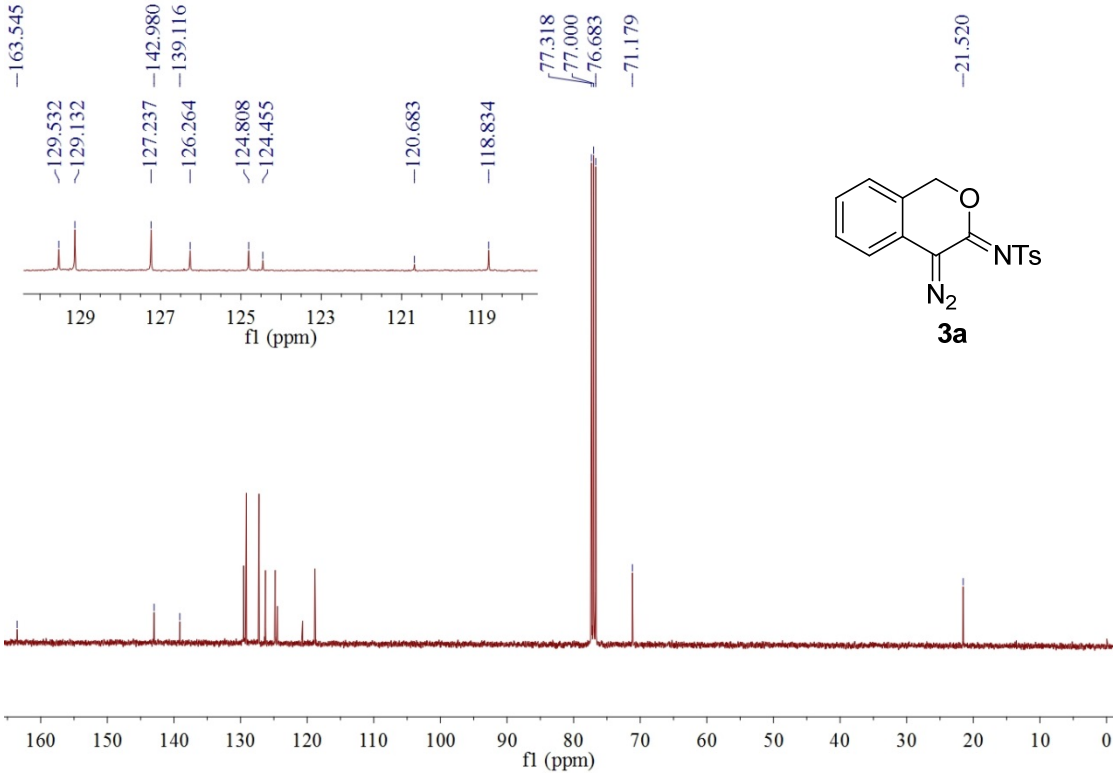


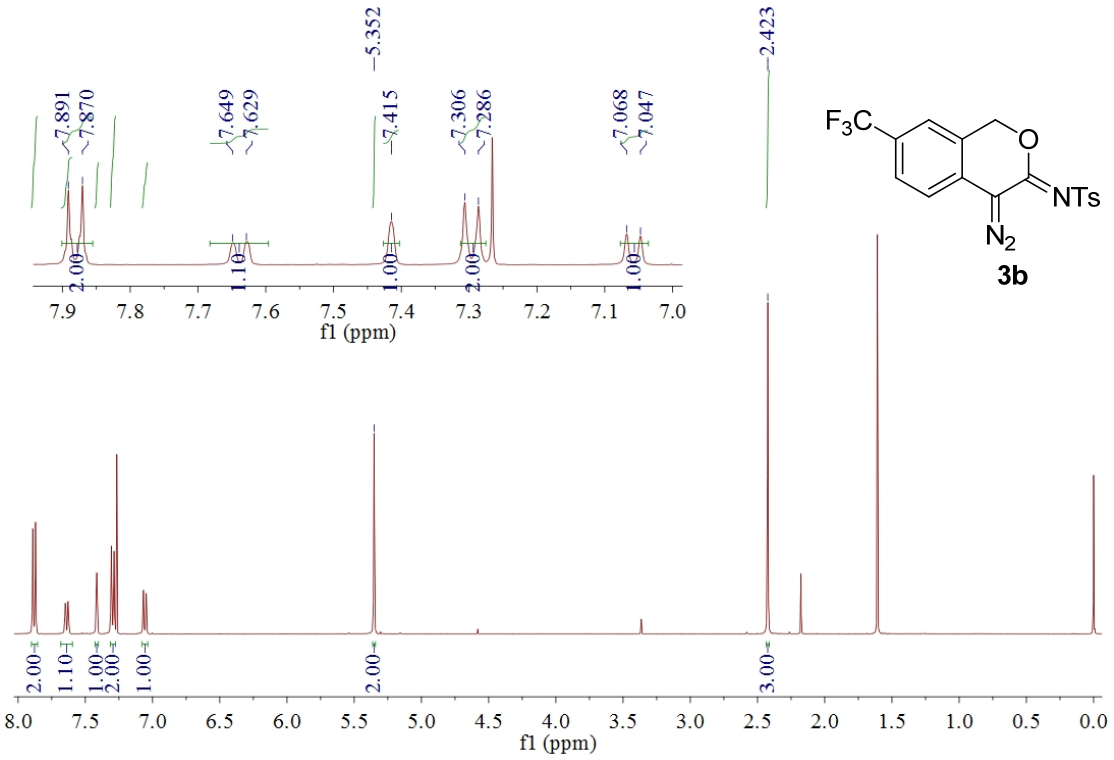
Colorless solid (19.5 mg), Isolated yield = 69%; m.p. 120.5 – 121.0 $^{o}$C; $^{1}$H NMR (400 MHz, $CDCl_3$): δ 7.74 (dd, $J_1$ = 8.8 Hz, $J_2$ = 2.4 Hz, 1H), 7.36 – 7.30 (m, 5H),7.06 (dd, $J_1$ = 8.4 Hz, $J_2$ = 5.2 Hz, 1H), 6.88 (td, $J_1$ = 8.4 Hz, $J_2$ = 2.8 Hz, 1H), 5.39 (s, 2H), 5.37 (s, 2H); $^{13}$C NMR (100 MHz, $CDCl_3$): δ163.3 ($J$ = 245.7 Hz), 148.3, 134.4, 129.2 ($J$ = 9.6 Hz), 128.9, 128.4, 127.9, 126.7 ($J$ = 2.7 Hz), 126.2 ($J$ = 8.8 Hz), 121.6 ($J$ = 3.3 Hz), 113.6 ($J$ =22.2 Hz), 107.6 ($J$ = 24.1 Hz),73.1, 50.2; IR (film):3065, 3034, 2924, 2861, 1622, 1549, 1495, 1455, 1266, 1209, 1089, 965, 883, 809, 736 cm$^{-1}$.HRMS (EI) calcd for $C_{16}H_{12}FN_3O$ ($M^+$): 281.0964; found: 281.0962.

# Copies of NMR Spectra

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7.649
7.629
5.352
7.415
7.306
7.286
7.068
7.047
2.423
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1.00
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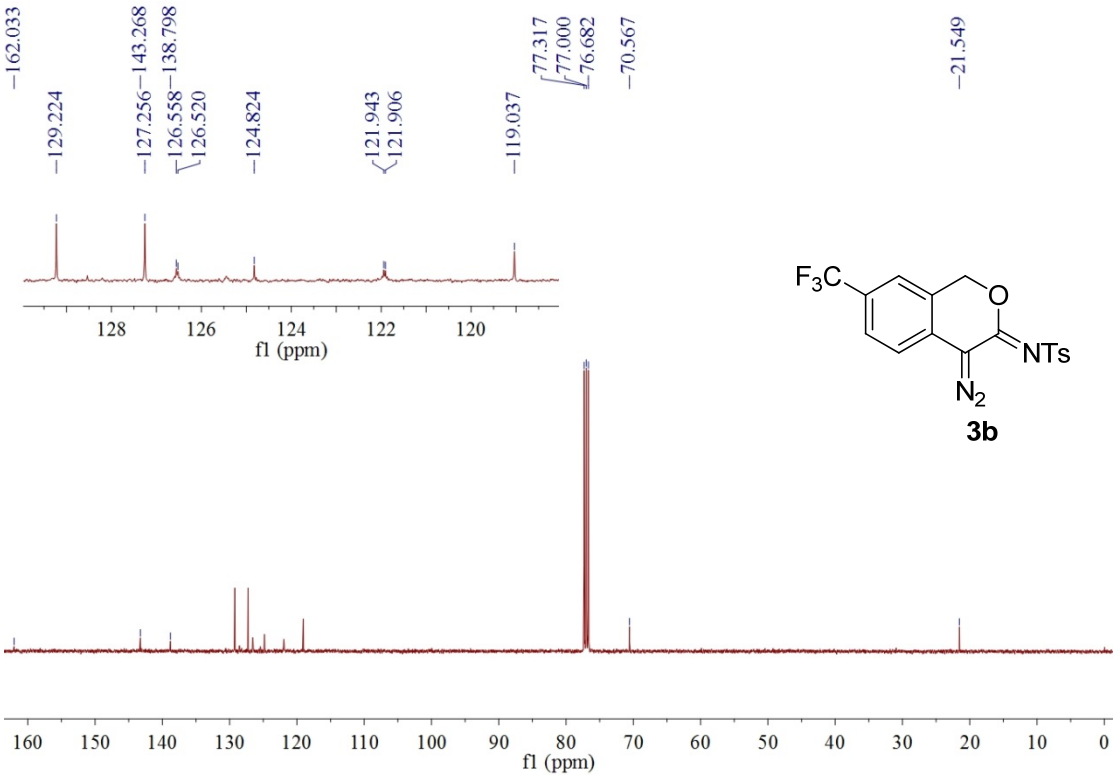
1.00
3.00
f1 (ppm)
F3C
O
NTs
N2
3b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138.798
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124.824
121.943
121.906
119.037
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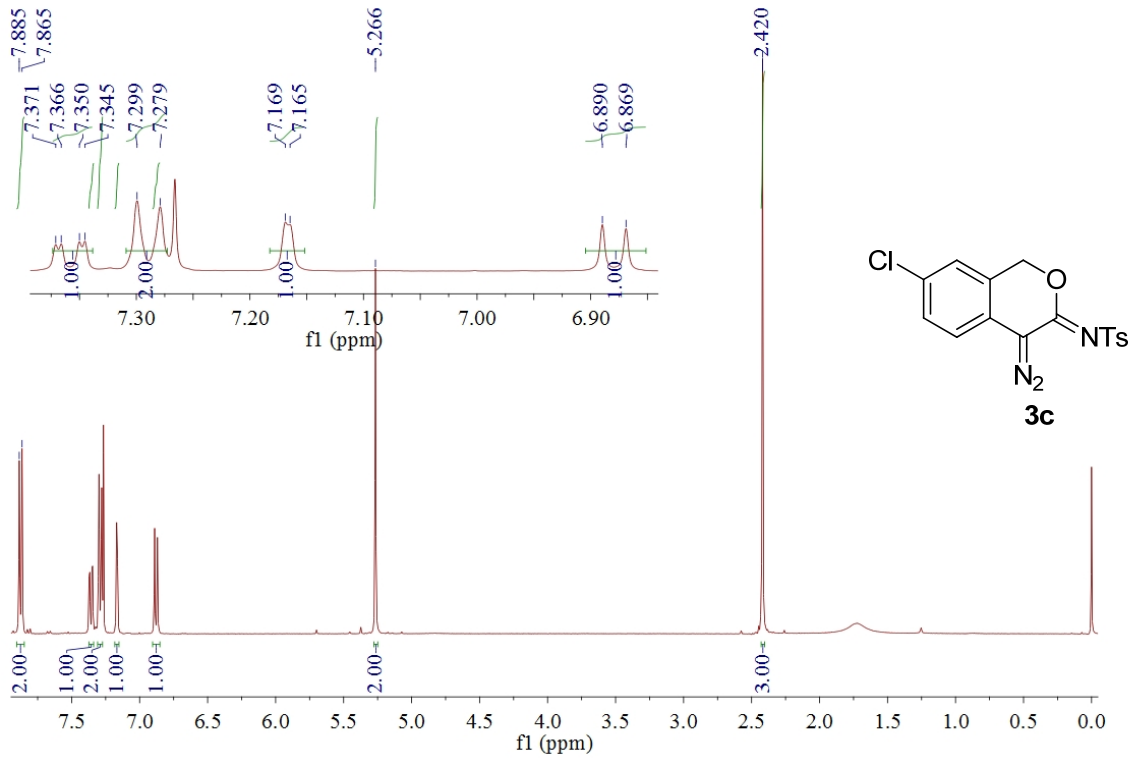
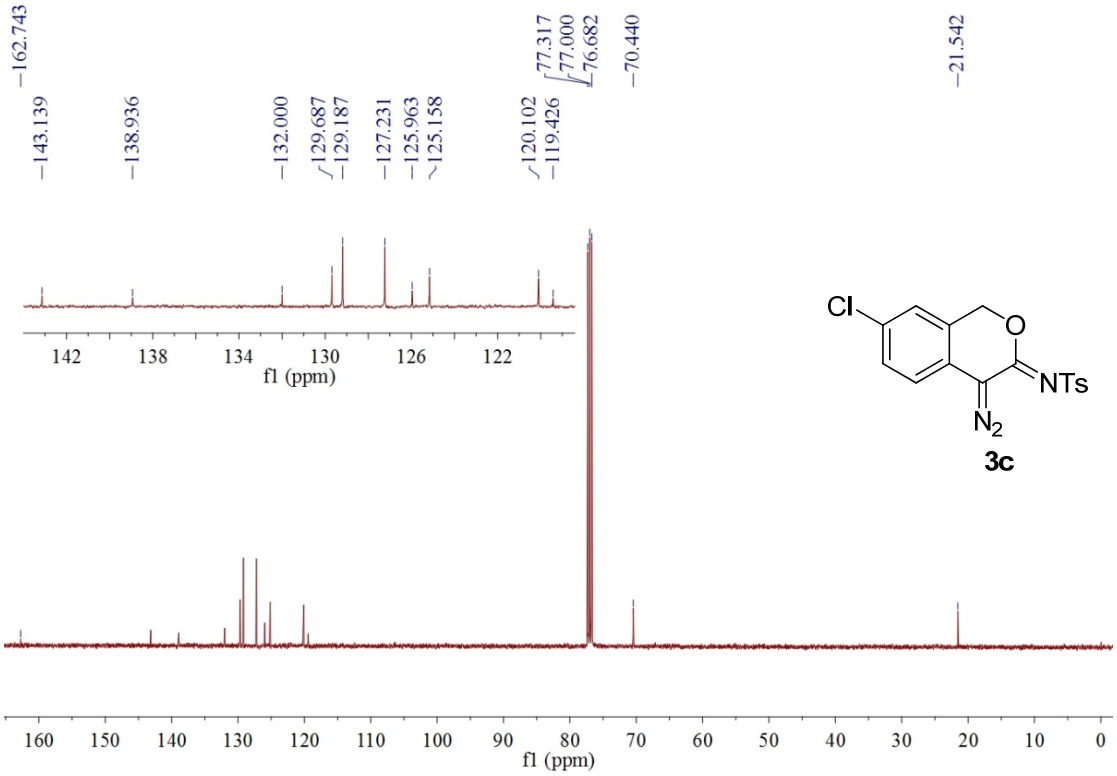
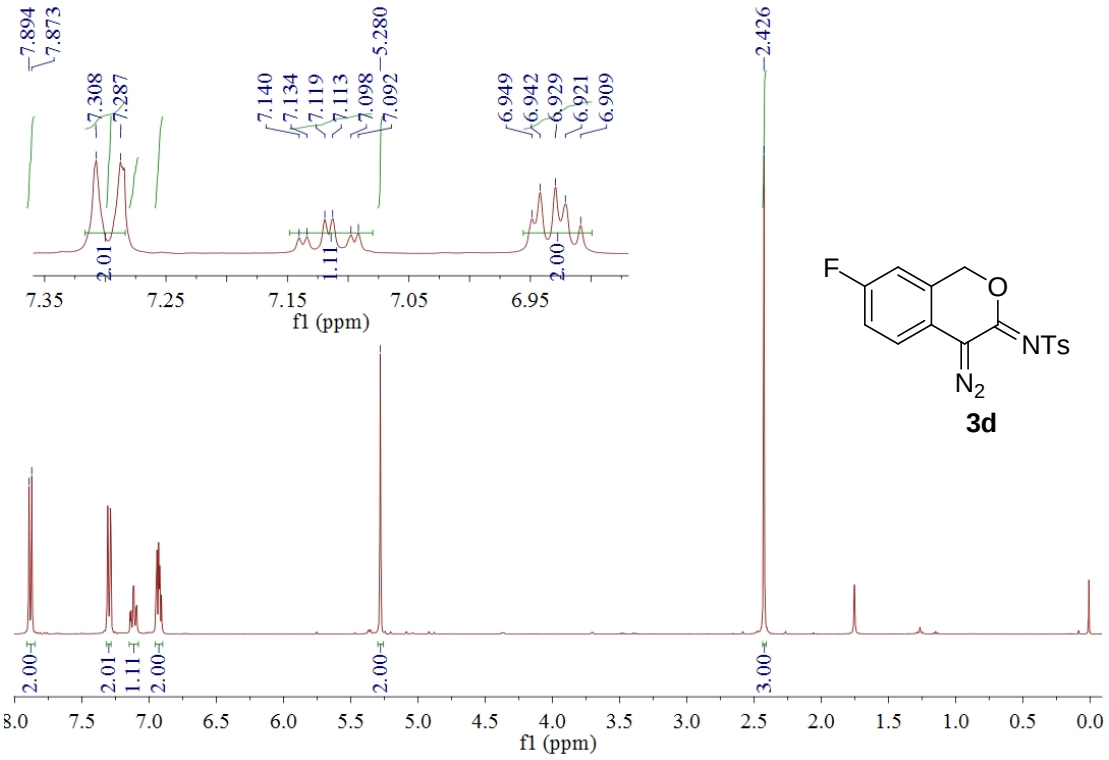
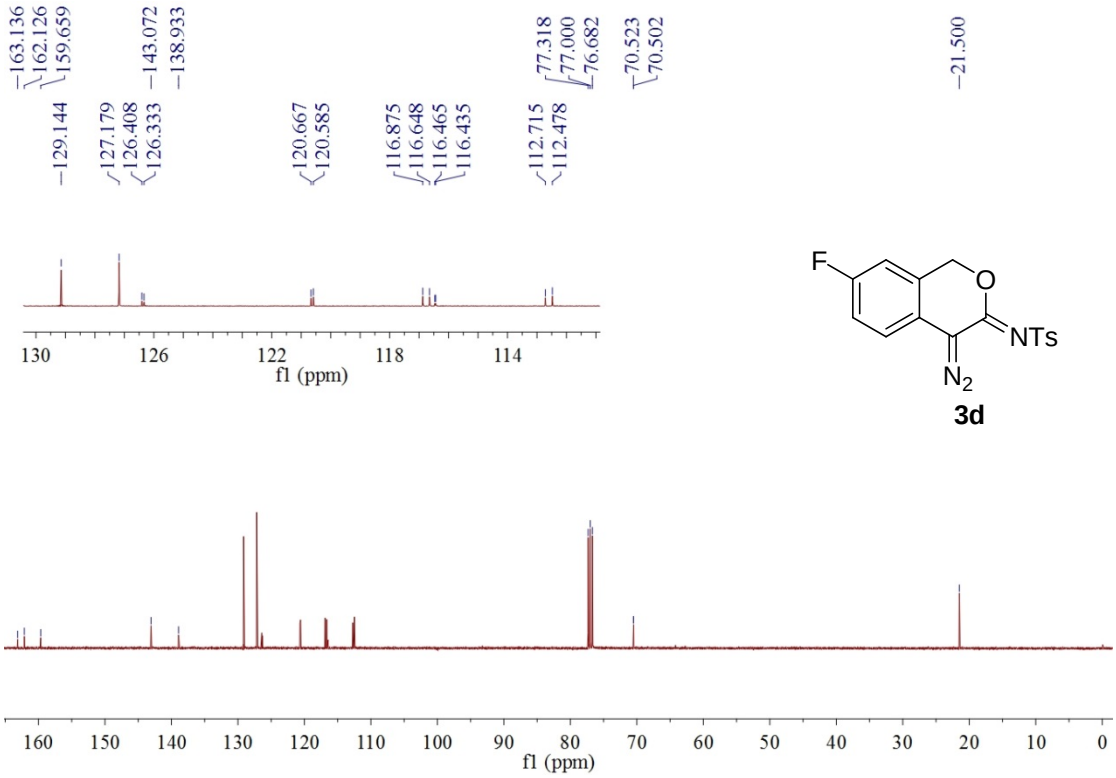
76.682
70.567
21.549
f1 (ppm)
F3C
O
NTs
N2
3b


7.885
7.865
7.371
7.366
7.350
7.345
7.299
7.279
7.169
7.165
6.890
6.869
5.266
2.420
1.00
2.00
1.00
1.00
7.30
7.20
7.10
7.00
6.90
f1 (ppm)
Cl
O
NTs
N2
3c
2.00
1.00
2.00
1.00
1.00
2.00
3.00
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)

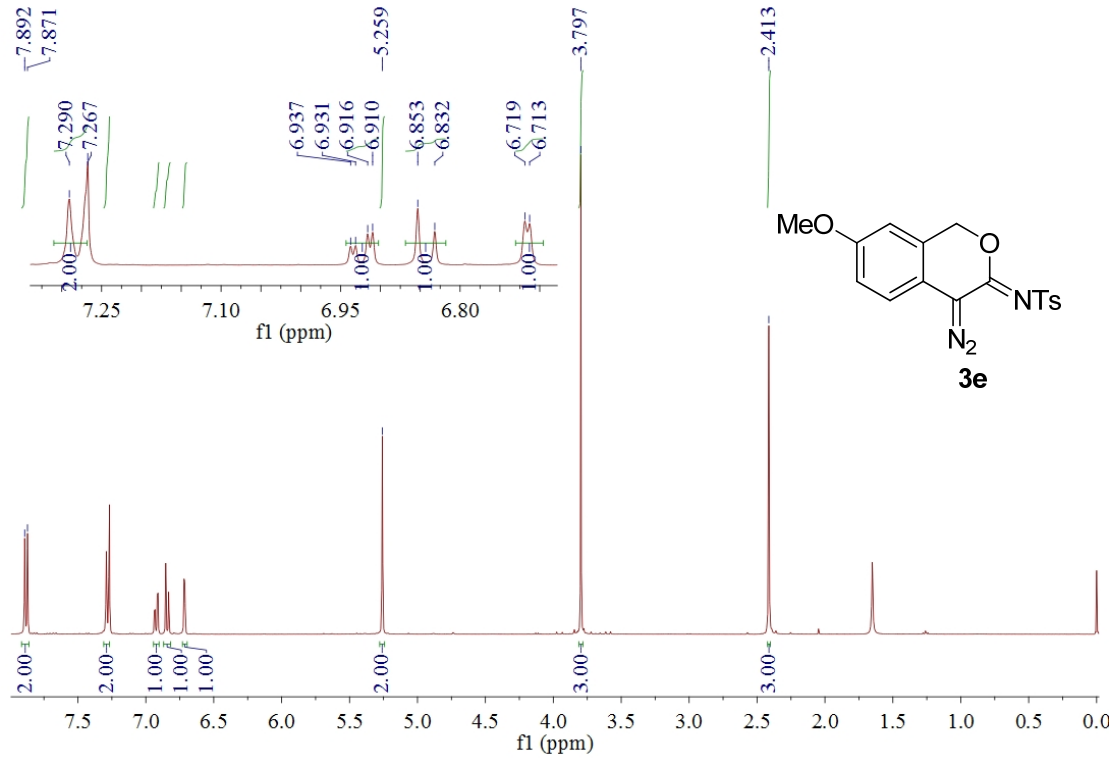

162.743
143.139
138.936
132.000
129.687
129.187
127.231
125.963
125.158
120.102
119.426
77.317
77.000
76.682
70.440
21.542
142
138
134
130
126
122
f1 (ppm)
Cl
O
NTs
N2
3c
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

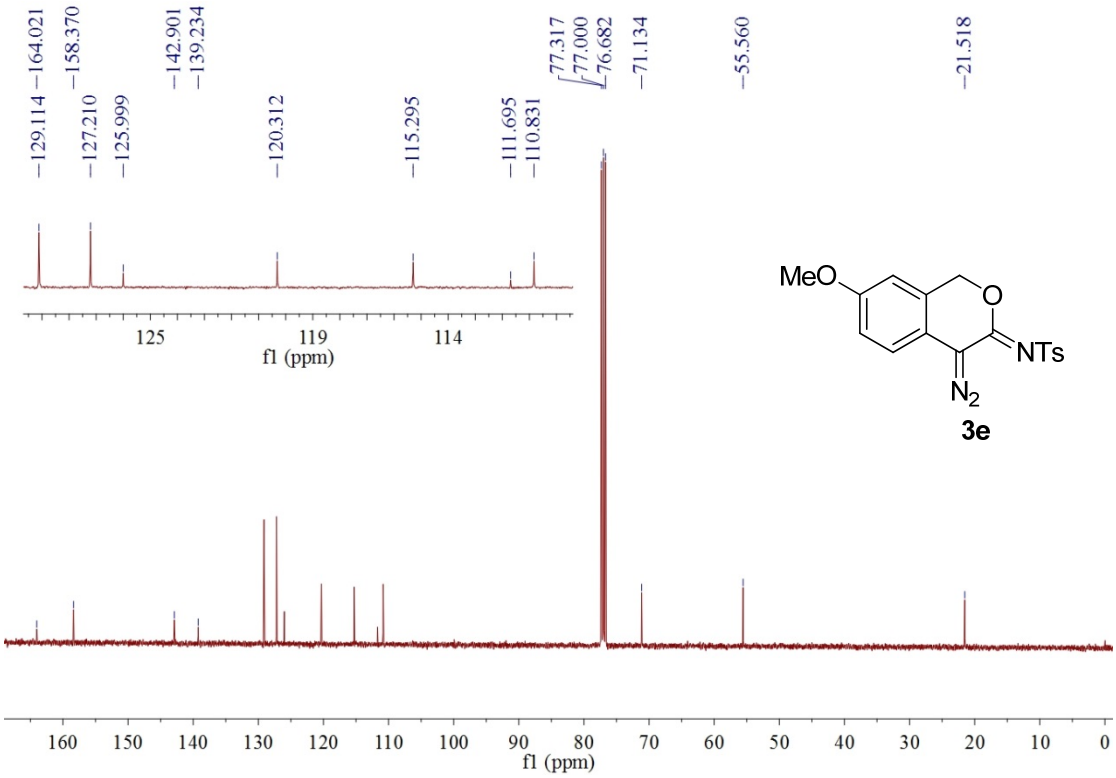

7.894
7.873
7.308
7.287
7.140
7.134
7.119
7.113
7.098
7.092
5.280
6.949
6.942
6.929
6.921
6.909
2.426
2.01
1.11
2.00
7.35
7.25
7.15
7.05
6.95
f1 (ppm)
F
O
NTs
N2
2.00
2.01
1.11
2.00
2.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

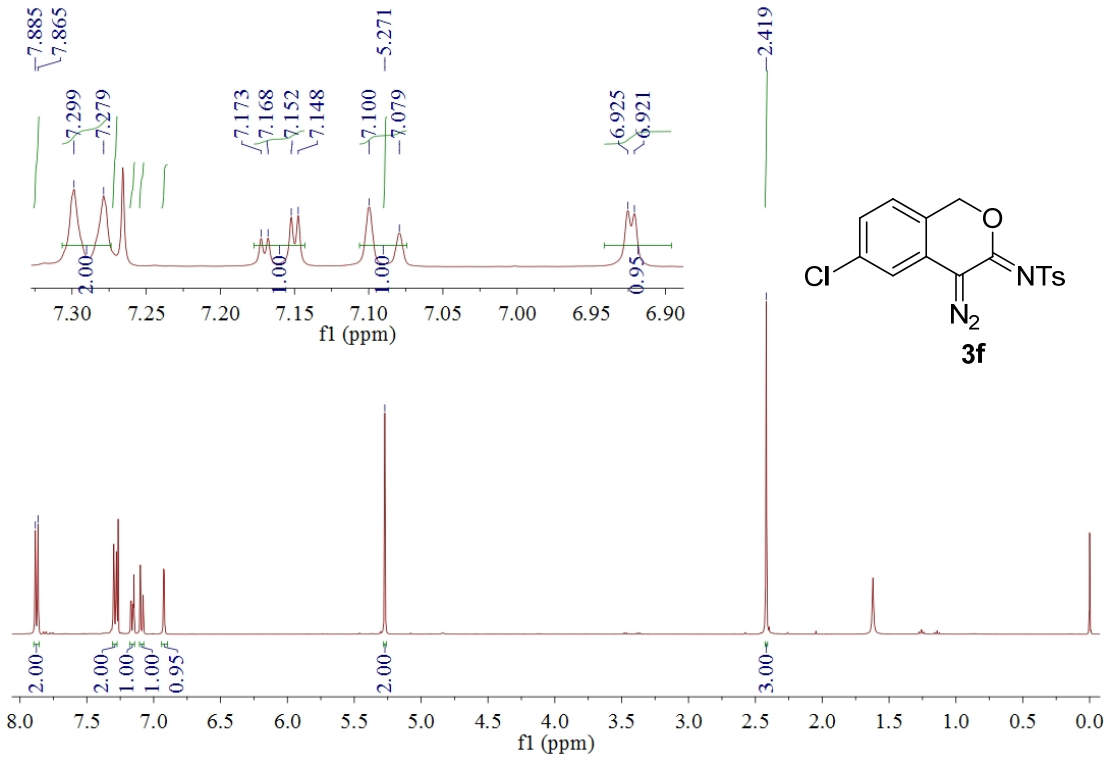
**3d**

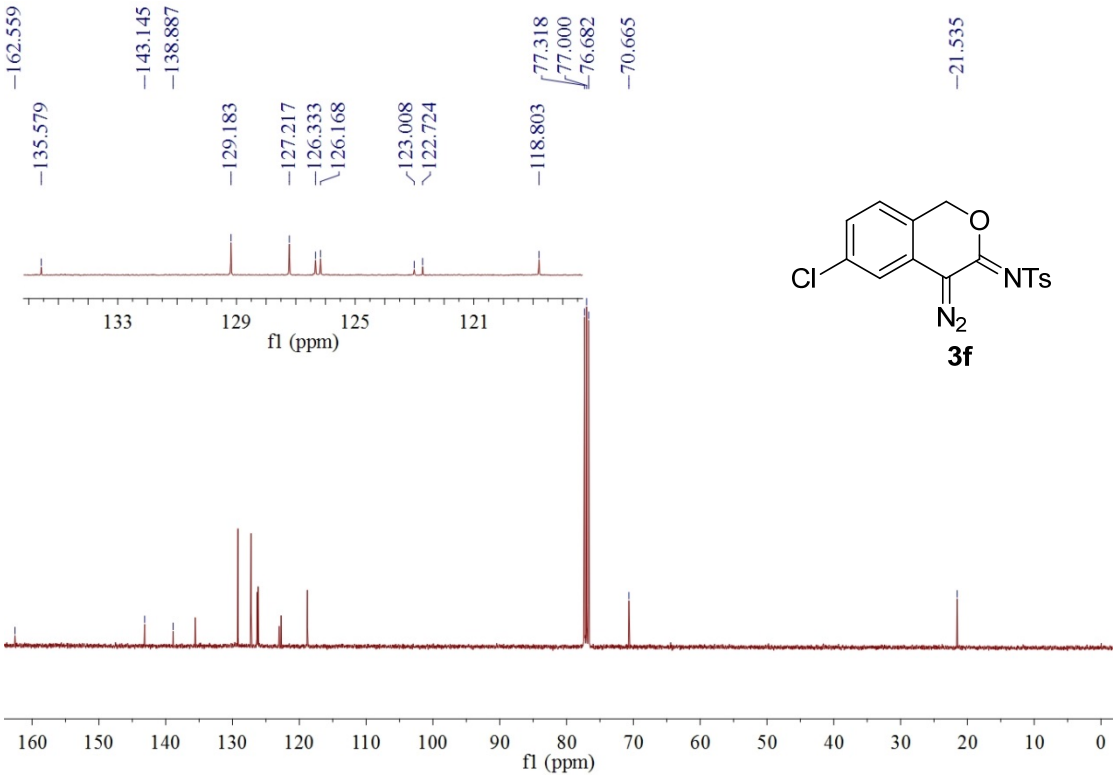

163.136
162.126
159.659
143.072
138.933
129.144
127.179
126.408
126.333
120.667
120.585
116.875
116.648
116.465
116.435
112.715
112.478
77.318
77.000
76.682
70.523
70.502
21.500
130
126
122
118
114
f1 (ppm)
F
O
NTs
N2
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

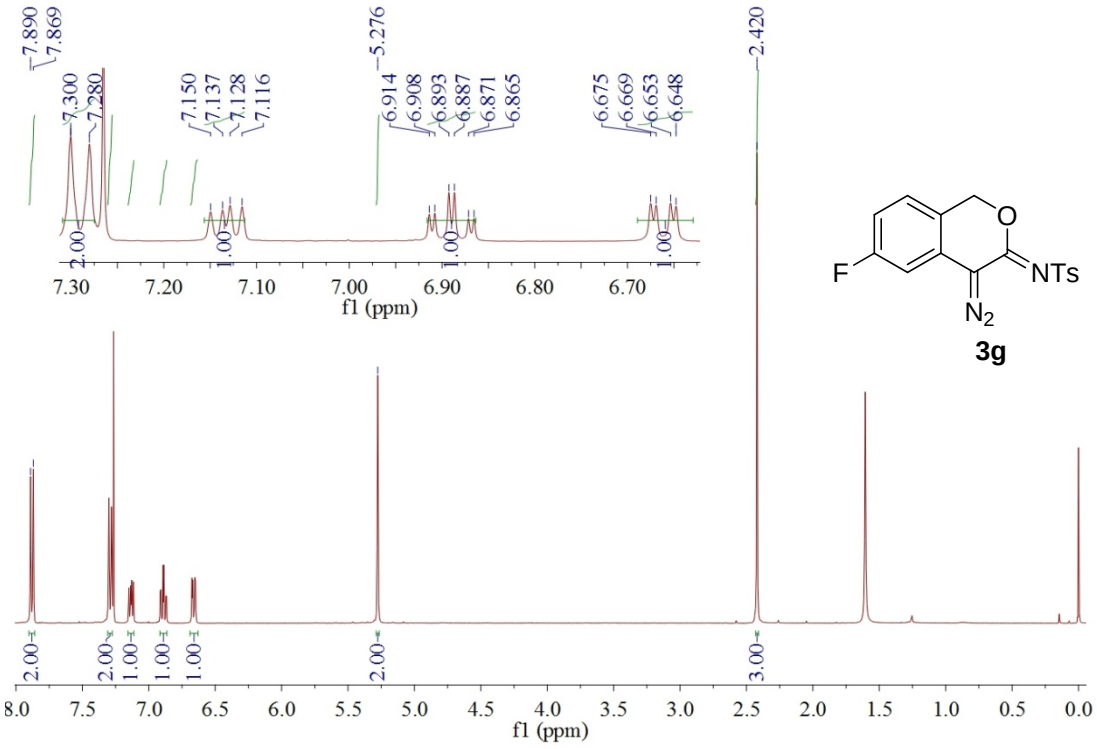
**3d**


7.892
7.871
7.290
7.267
6.937
6.931
6.916
6.910
6.853
6.832
6.719
6.713
5.259
3.797
2.413
2.00
1.00
1.00
1.00
7.25
7.10
6.95
6.80
f1 (ppm)
MeO
O
NTs
N2
3e
2.00
2.00
1.00
1.00
1.00
2.00
3.00
3.00
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)

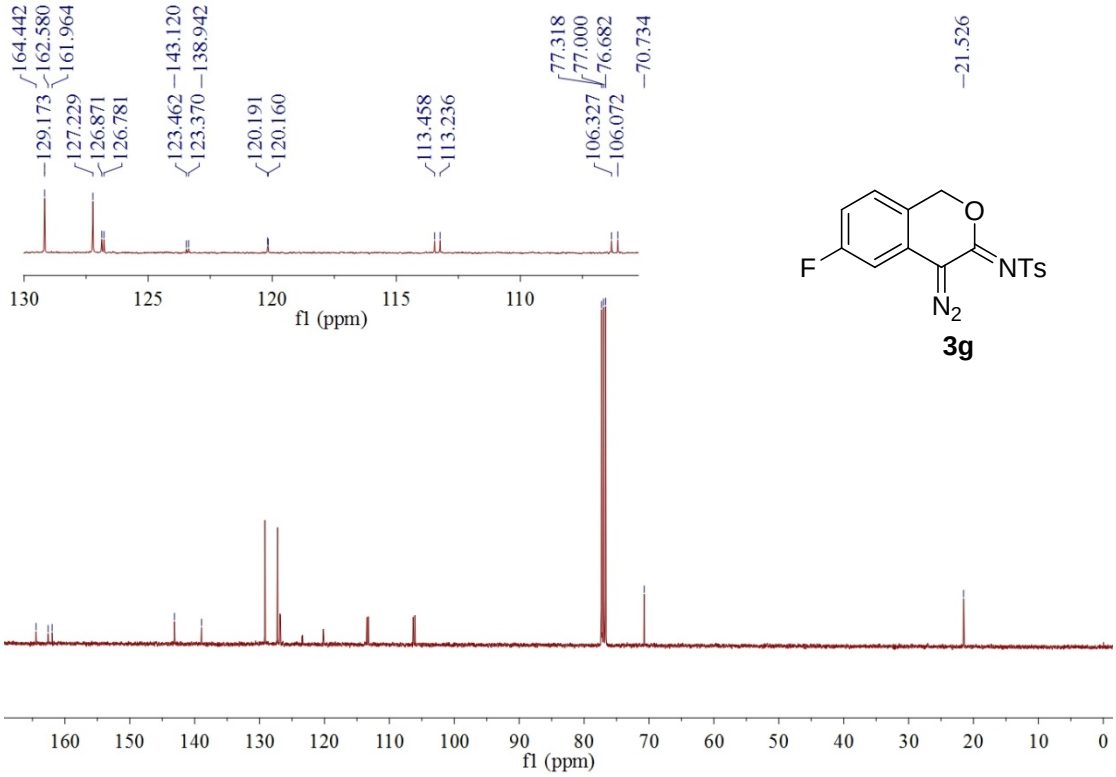

164.021
158.370
142.901
139.234
129.114
127.210
125.999
120.312
115.295
111.695
110.831
77.317
77.000
76.682
71.134
55.560
21.518
125
119
114
f1 (ppm)
MeO
O
NTs
N2
3e
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

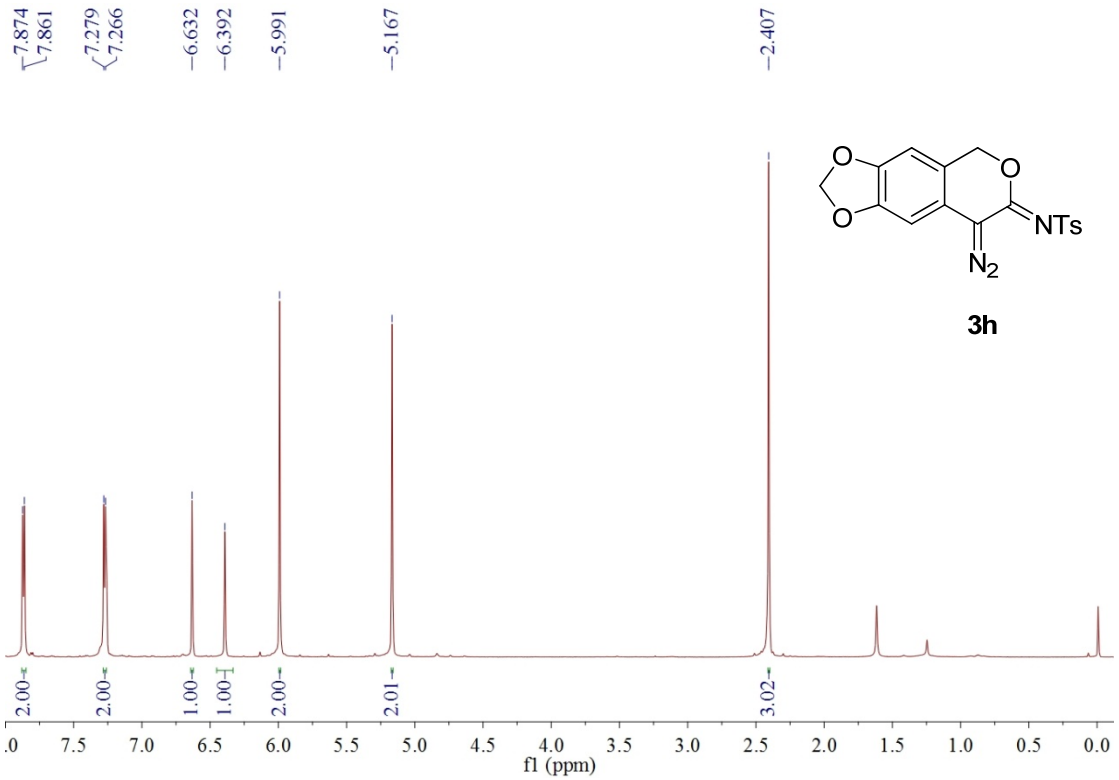

7.885
7.865
7.299
7.279
7.173
7.168
7.152
7.148
7.100
7.079
6.925
6.921
5.271
2.419
2.00
1.00
1.00
0.95
7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90
f1 (ppm)
2.00
2.00
1.00
1.00
0.95
2.00
3.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
Cl
O
NTs
N2
3f


162.559
143.145
138.887
135.579
129.183
127.217
126.333
126.168
123.008
122.724
118.803
77.318
77.000
76.682
70.665
21.535
133 129 125 121
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
Cl
O
NTs
N2
3f

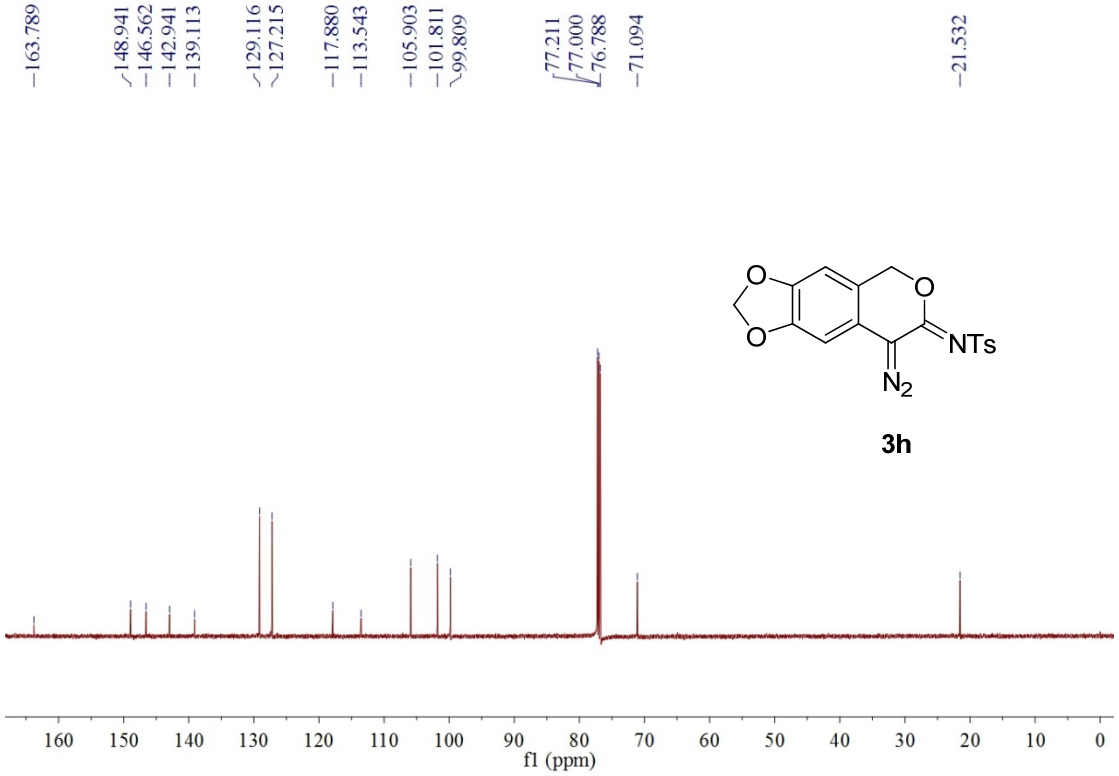

7.890
7.869
7.300
7.280
7.150
7.137
7.128
7.116
5.276
6.914
6.908
6.893
6.887
6.871
6.865
6.675
6.669
6.653
6.648
2.420
2.00
1.00
1.00
1.00
7.30
7.20
7.10
7.00
6.90
6.80
6.70
f1 (ppm)
2.00
2.00
1.00
1.00
1.00
2.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
O
F
NTs
N2
3g

RAN6-129-3

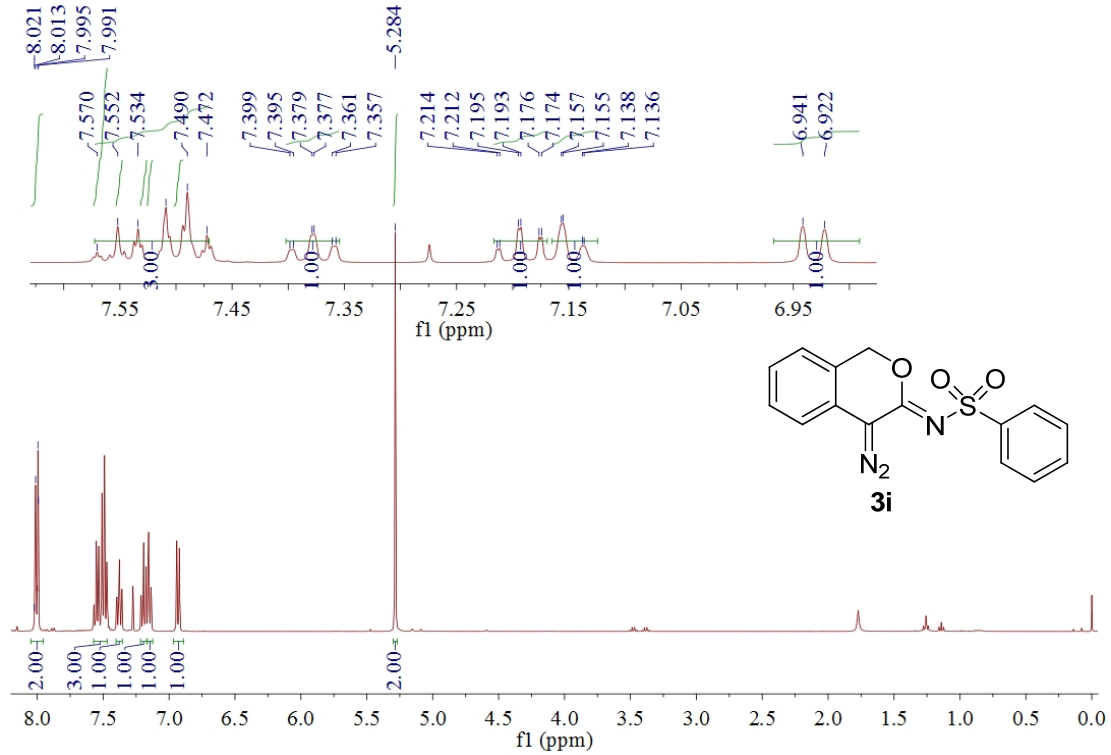

164.442
162.580
161.964
129.173
127.229
126.871
126.781
123.462
143.120
123.370
138.942
120.191
120.160
113.458
113.236
77.318
77.000
76.682
106.327
106.072
70.734
21.526
130
125
120
115
110
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
F
NTs
N2
3g

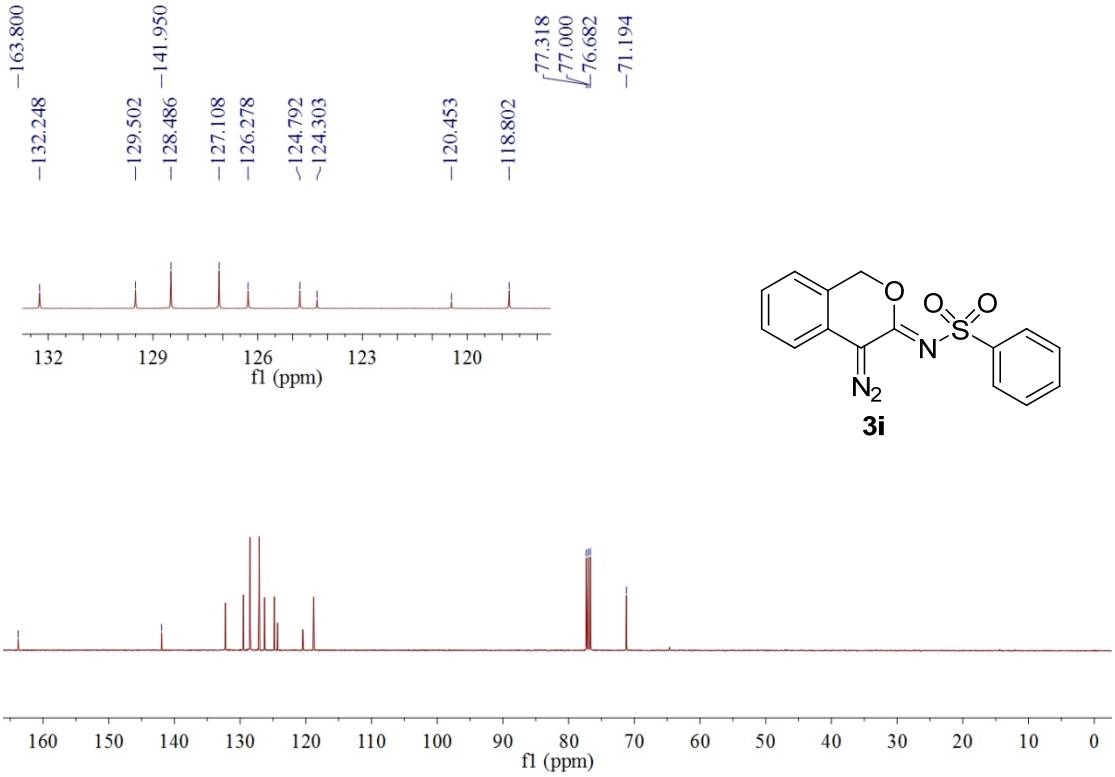

7.874
7.861
7.279
7.266
6.632
6.392
5.991
5.167
2.407
O
O
O
NTs
N2
2.00
2.00
1.00
1.00
2.00
2.01
3.02
fl (ppm)

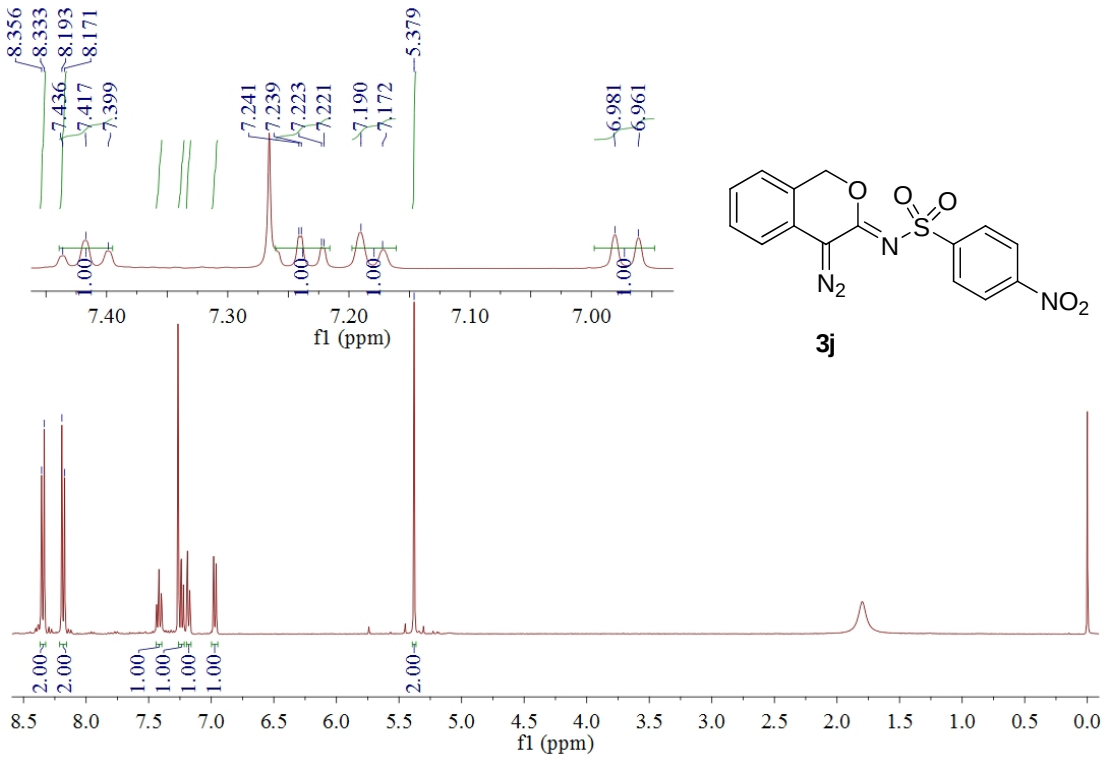
**3h**


163.789
148.941
146.562
142.941
139.113
129.116
127.215
117.880
113.543
105.903
101.811
99.809
77.211
77.000
76.788
71.094
21.532
O
O
O
NTs
N2
fl (ppm)

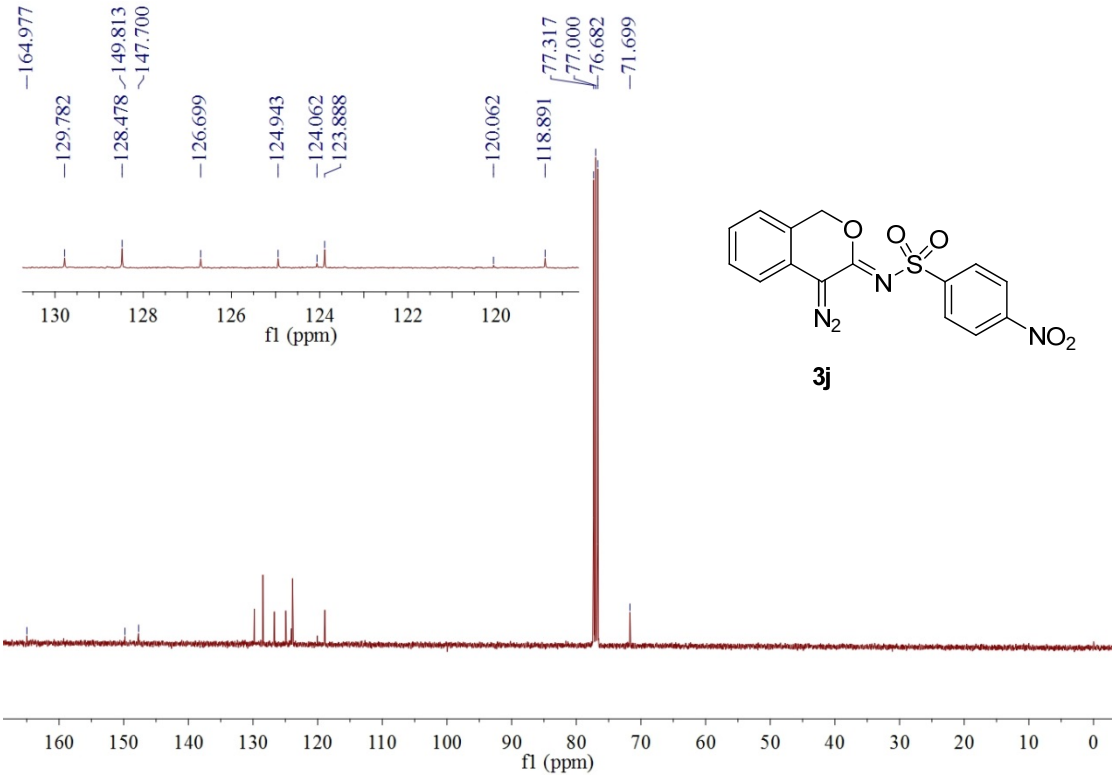
**3h**


8.021
8.013
7.995
7.991
5.284
7.570
7.552
7.534
7.490
7.472
7.399
7.395
7.379
7.377
7.361
7.357
7.214
7.212
7.195
7.193
7.176
7.174
7.157
7.155
7.138
7.136
6.941
6.922
3.00
1.00
1.00
1.00
1.00
7.55
7.45
7.35
7.25
7.15
7.05
6.95
f1 (ppm)
O
O
O
S
N
N2
3i
2.00
3.00
1.00
1.00
1.00
1.00
2.00
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)

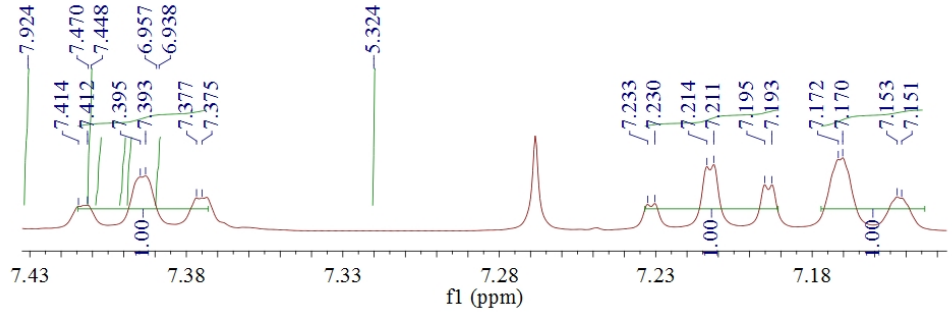

163.800
141.950
132.248
129.502
128.486
127.108
126.278
124.792
124.303
120.453
118.802
77.318
77.000
76.682
71.194
132
129
126
123
120
f1 (ppm)
O
O
O
S
N
N2
3i
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

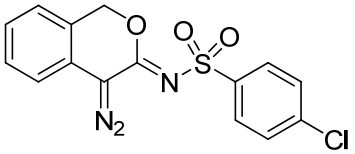

8.356
8.333
8.193
8.171
7.436
7.417
7.399
7.241
7.239
7.223
7.221
7.190
7.172
5.379
6.981
6.961
1.00
7.40
7.30
7.20
7.10
7.00
f1 (ppm)
2.00
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
O
O
O
N
S
N2
NO2

**3j**

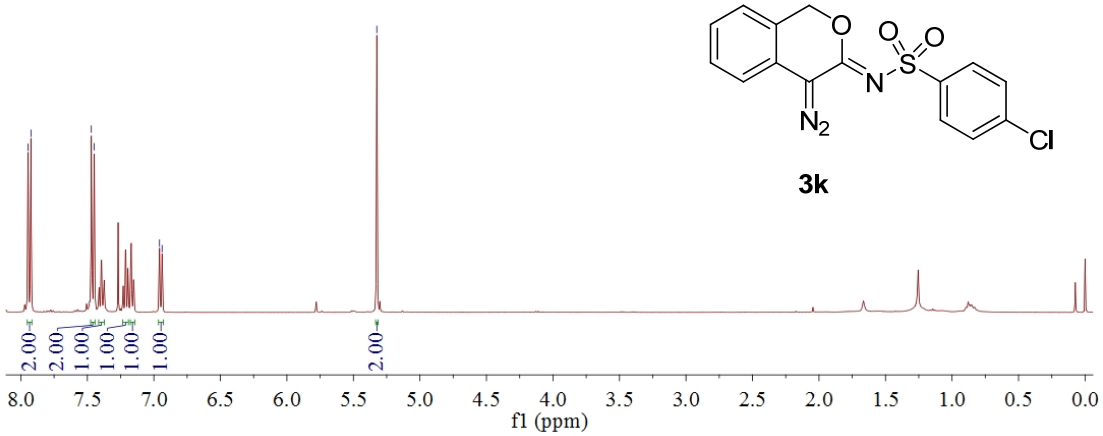

164.977
129.782
128.478
149.813
147.700
126.699
124.943
124.062
123.888
120.062
118.891
77.317
77.000
76.682
71.699
130
128
126
124
122
120
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
O
O
O
N
S
N2
NO2

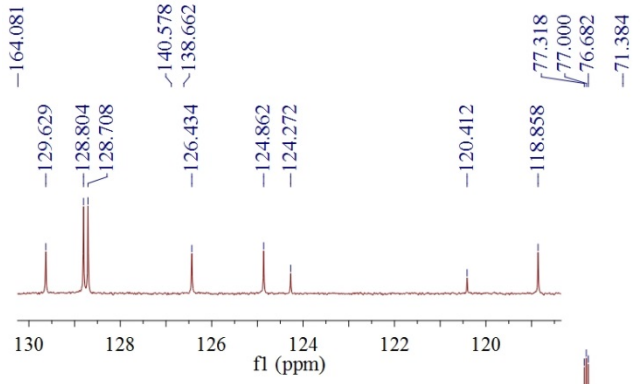
**3j**

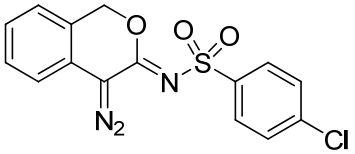

7.924
7.470
7.448
6.957
6.938
5.324
7.414
7.412
7.395
7.393
7.377
7.375
7.233
7.230
7.214
7.211
7.195
7.193
7.172
7.170
7.153
7.151
1.00
1.00
1.00
7.43
7.38
7.33
7.28
7.23
7.18
f1 (ppm)


O
O
O
S
N
N2
Cl

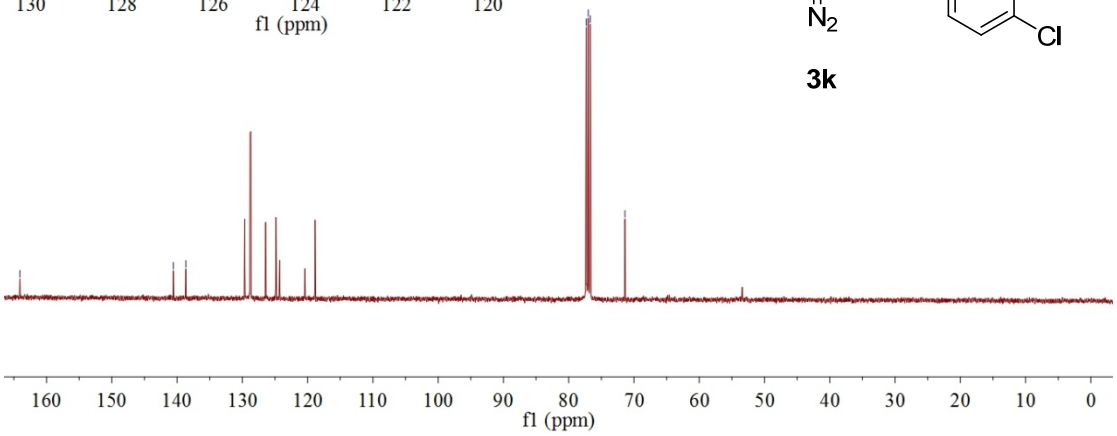
**3k**

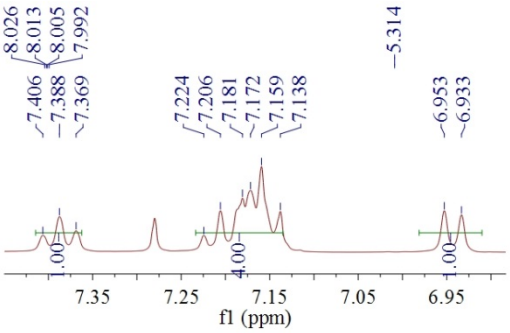

2.00
2.00
1.00
1.00
1.00
1.00
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

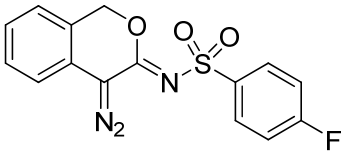

164.081
140.578
138.662
129.629
128.804
128.708
126.434
124.862
124.272
120.412
118.858
77.318
77.000
76.682
71.384
130
128
126
124
122
120
f1 (ppm)


O
O
O
S
N
N2
Cl

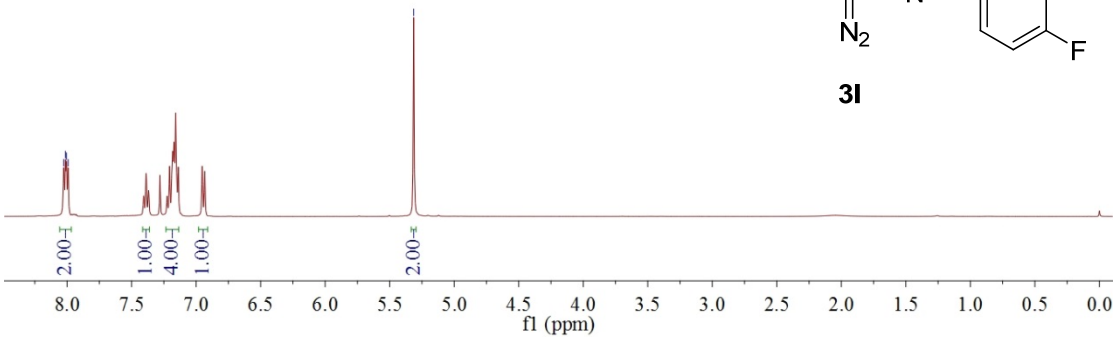
**3k**

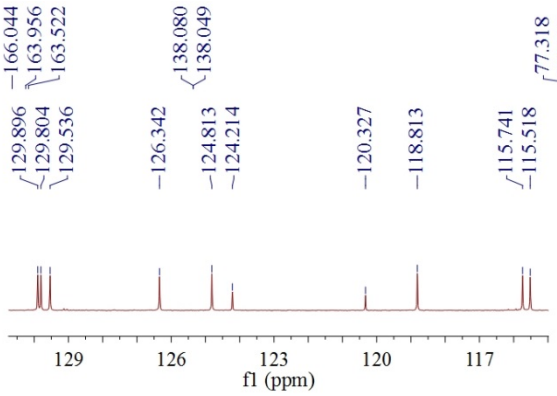

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

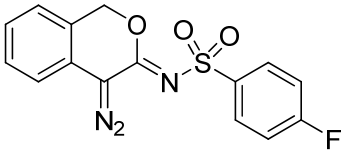

8.026
8.013
8.005
7.992
7.406
7.388
7.369
7.224
7.206
7.181
7.172
7.159
7.138
5.314
6.953
6.933
1.00
4.00
1.00
7.35
7.25
7.15
7.05
6.95
f1 (ppm)


O
O
O
S
N
N2
F

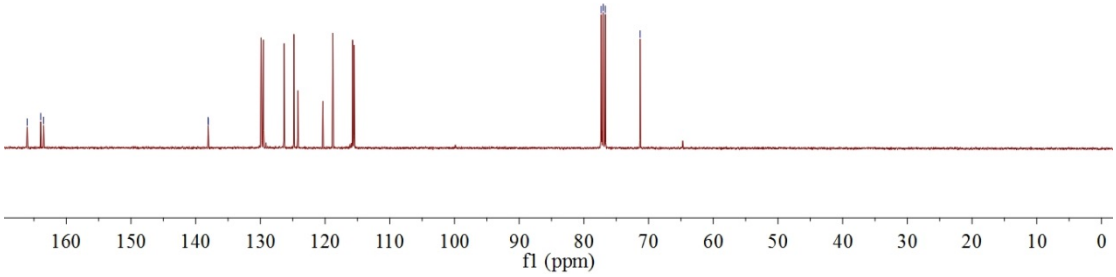
**3l**

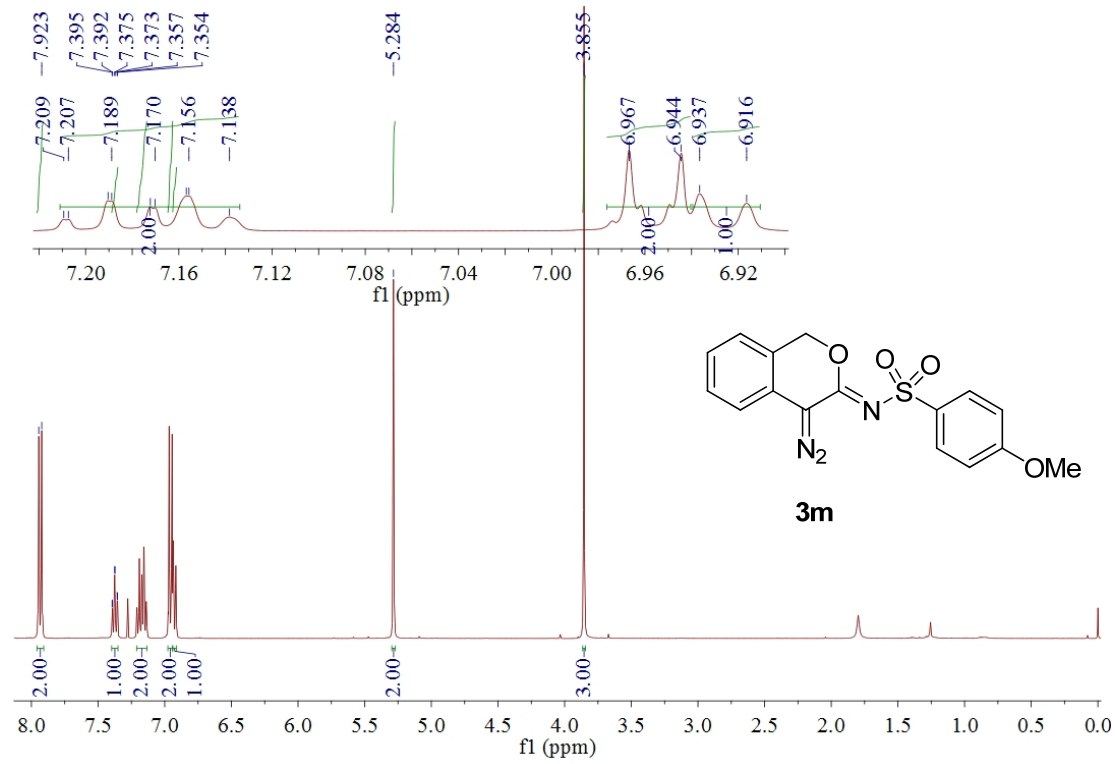

2.00
1.00
4.00
1.00
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


166.044
163.956
163.522
138.080
138.049
77.318
77.000
76.682
71.301
129.896
129.804
129.536
126.342
124.813
124.214
120.327
118.813
115.741
115.518
129
126
123
120
117
f1 (ppm)

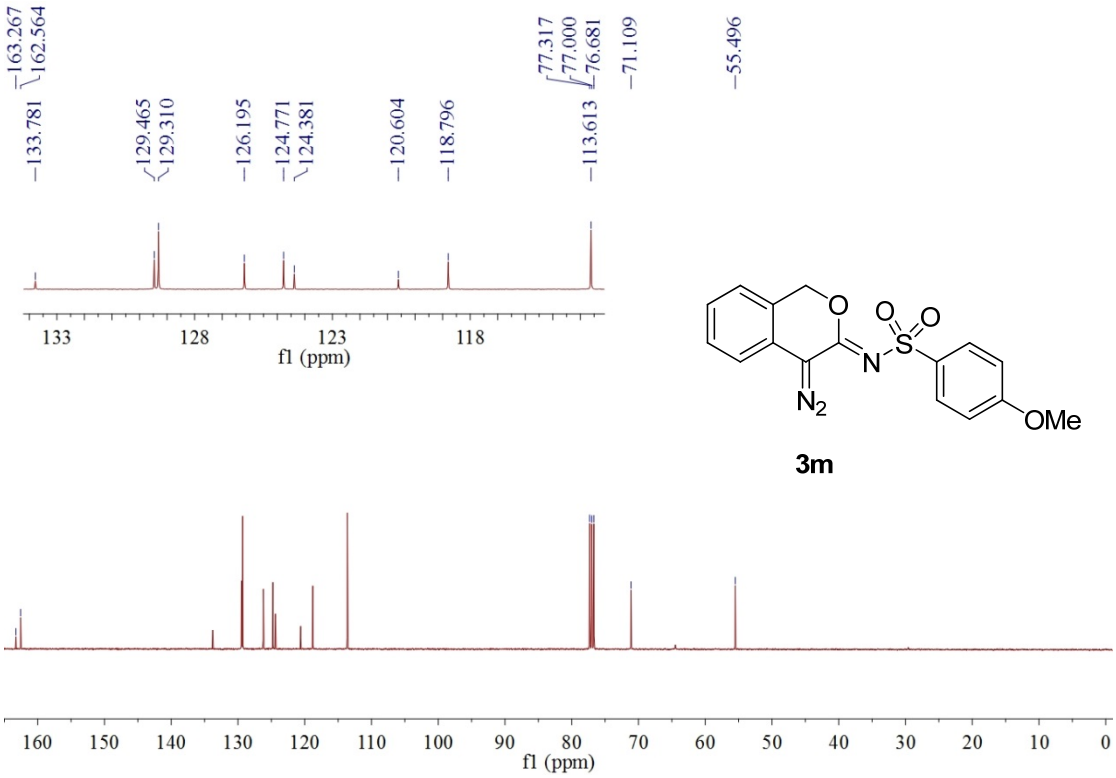

O
O
O
S
N
N2
F

**3l**

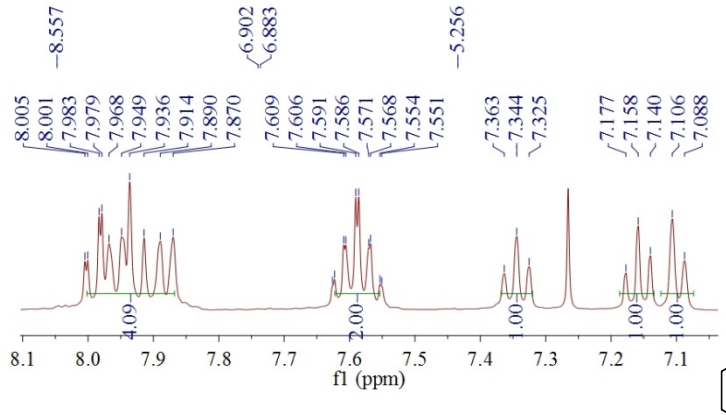

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

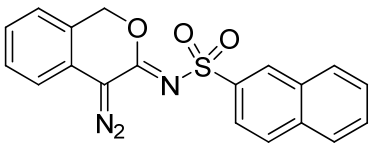

7.923
7.395
7.392
7.375
7.373
7.357
7.354
5.284
3.855
7.209
7.207
7.189
7.170
7.156
7.138
6.967
6.944
6.937
6.916
2.00
2.00
1.00
7.20
7.16
7.12
7.08
7.04
7.00
6.96
6.92
f1 (ppm)
O
O
O
S
N
N2
OMe
2.00
1.00
2.00
2.00
1.00
2.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

**3m**

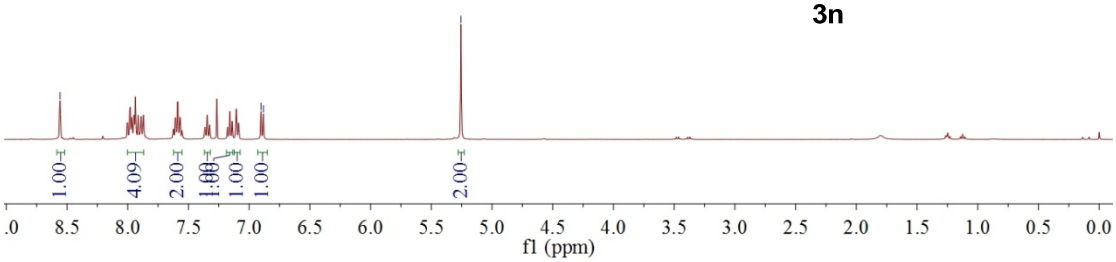

163.267
162.564
133.781
129.465
129.310
126.195
124.771
124.381
120.604
118.796
77.317
77.000
76.681
113.613
71.109
55.496
133
128
123
118
f1 (ppm)
O
O
O
S
N
N2
OMe
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

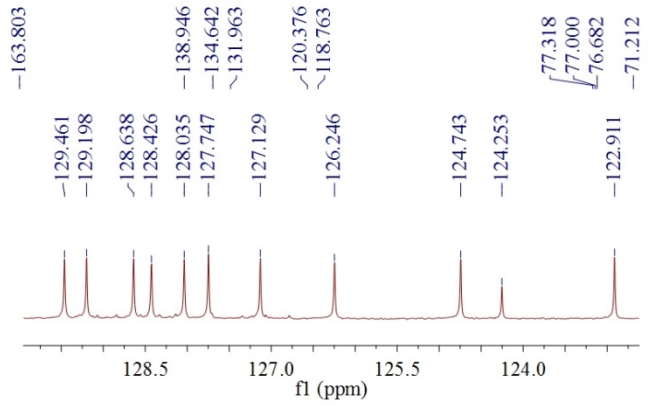
**3m**

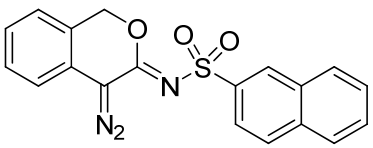

8.557
6.902
6.883
5.256
8.005
8.001
7.983
7.979
7.968
7.949
7.936
7.914
7.890
7.870
7.609
7.606
7.591
7.586
7.571
7.568
7.554
7.551
7.363
7.344
7.325
7.177
7.158
7.140
7.106
7.088
4.09
2.00
1.00
1.00
1.00
f1 (ppm)



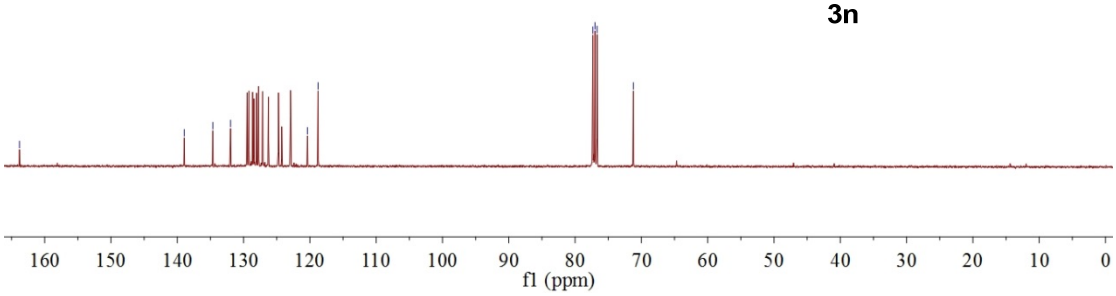
**3n**

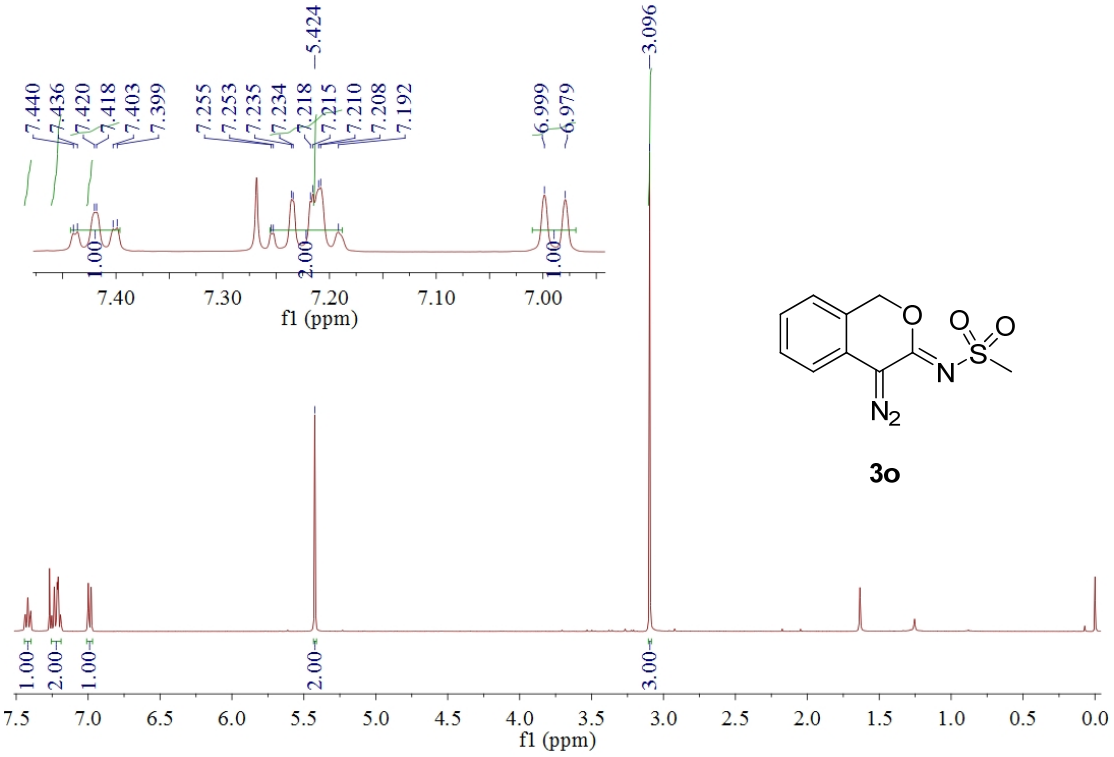

1.00
4.09
2.00
1.00
1.00
2.00
f1 (ppm)


163.803
138.946
134.642
131.963
120.376
118.763
77.318
77.000
76.682
71.212
129.461
129.198
128.638
128.426
128.035
127.747
127.129
126.246
124.743
124.253
122.911
f1 (ppm)

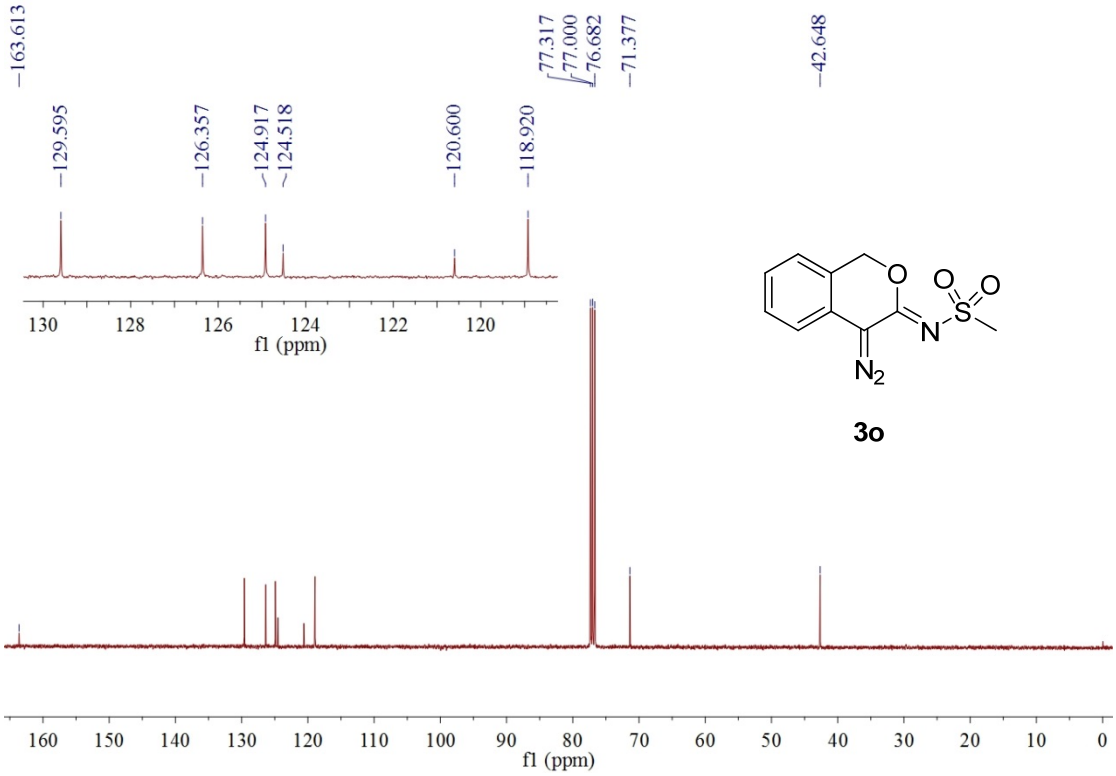


**3n**

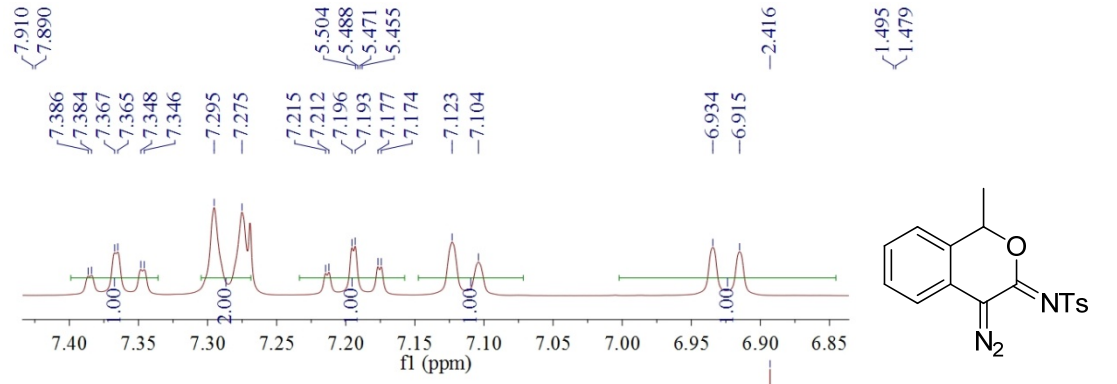

f1 (ppm)


7.440
7.436
7.420
7.418
7.403
7.399
7.255
7.253
7.235
7.234
7.218
7.215
7.210
7.208
7.192
6.999
6.979
5.424
3.096
1.00
2.00
1.00
7.40
7.30
7.20
7.10
7.00
f1 (ppm)
O
O
O
S
N
N2
1.00
2.00
1.00
2.00
3.00
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)

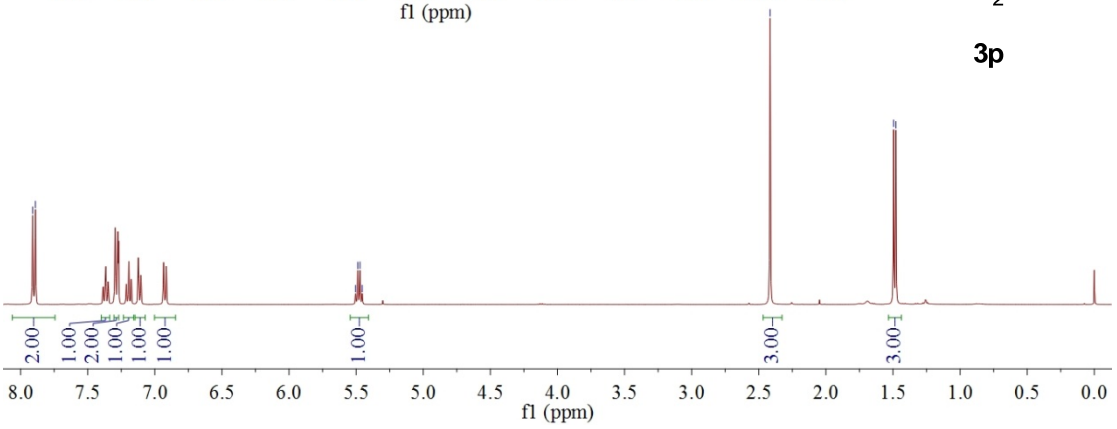
**3o**

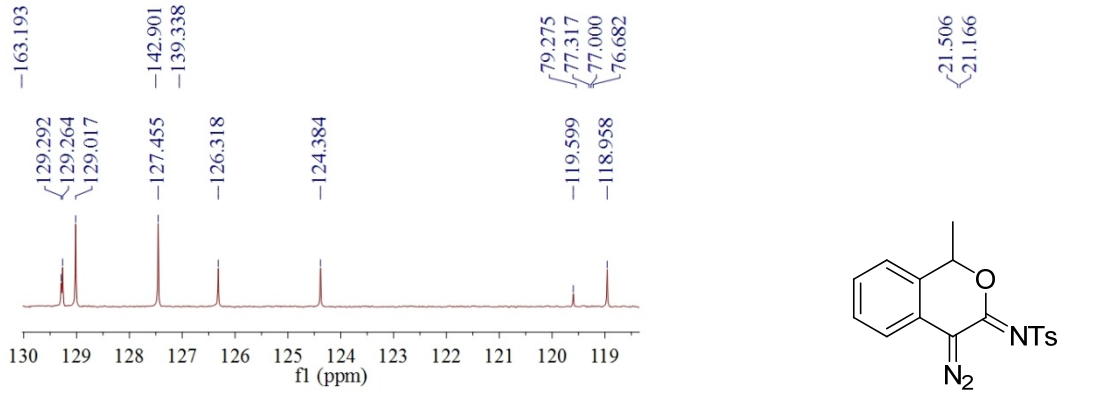

163.613
129.595
126.357
124.917
124.518
120.600
118.920
77.317
77.000
76.682
71.377
42.648
130
128
126
124
122
120
f1 (ppm)
O
O
O
S
N
N2
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

**3o**

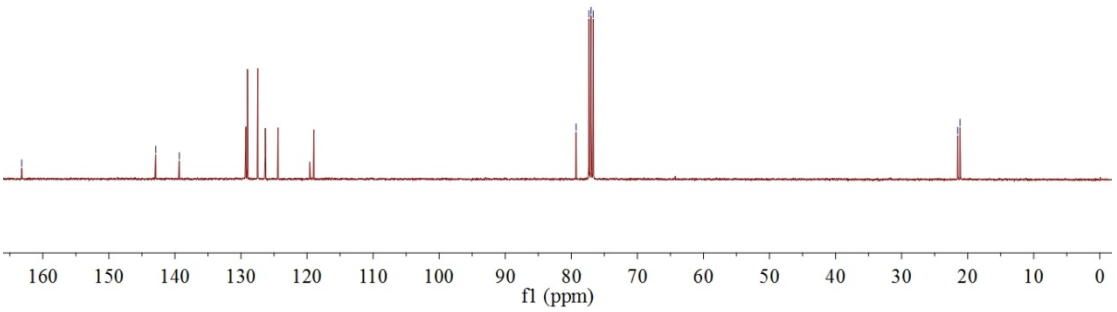

7.910
7.890
5.504
5.488
5.471
5.455
2.416
1.495
1.479
7.386
7.384
7.367
7.365
7.348
7.346
7.295
7.275
7.215
7.212
7.196
7.193
7.177
7.174
7.123
7.104
6.934
6.915
1.00
2.00
1.00
1.00
7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85
f1 (ppm)
O
NTs
N2

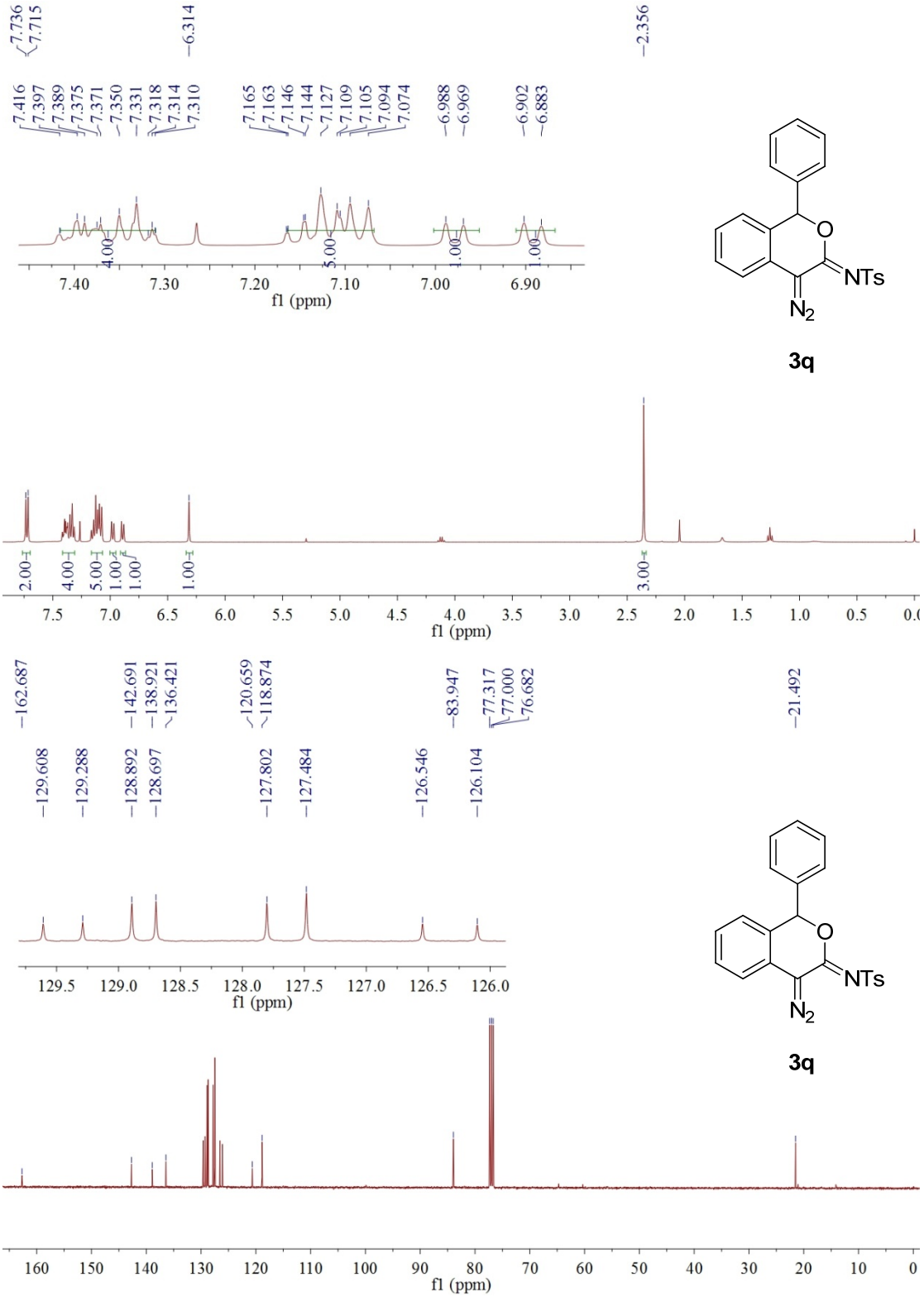
**3p**

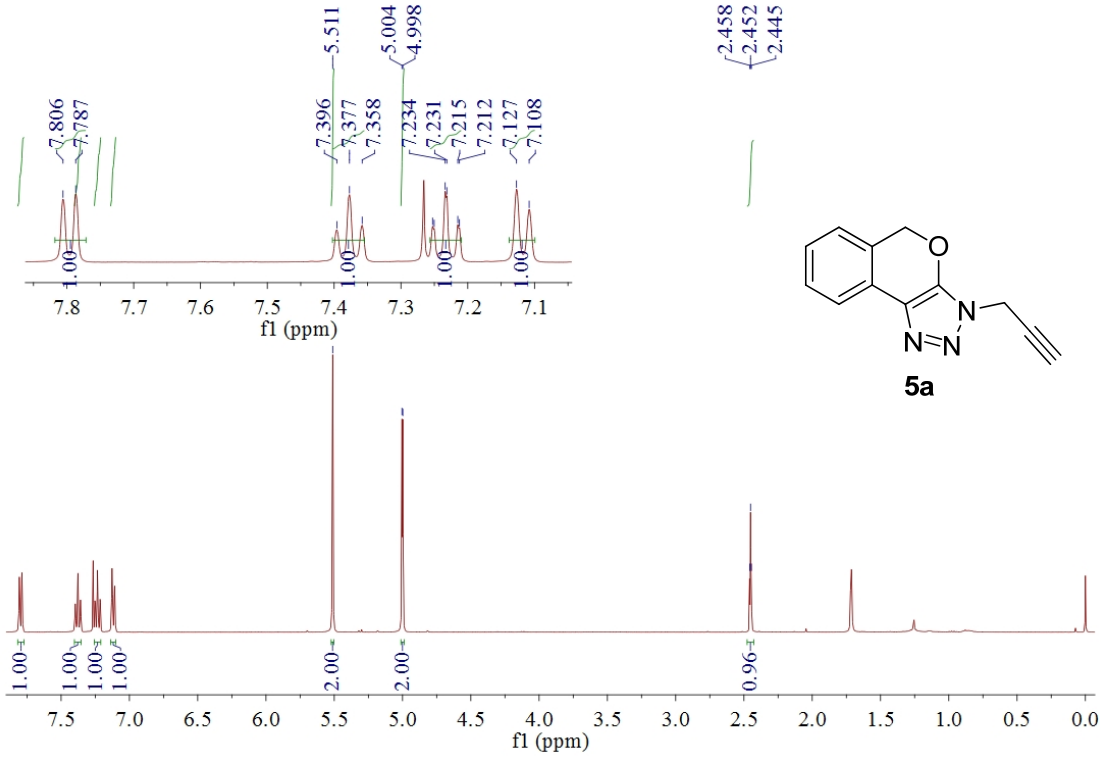

2.00
1.00
2.00
1.00
1.00
1.00
1.00
3.00
3.00
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

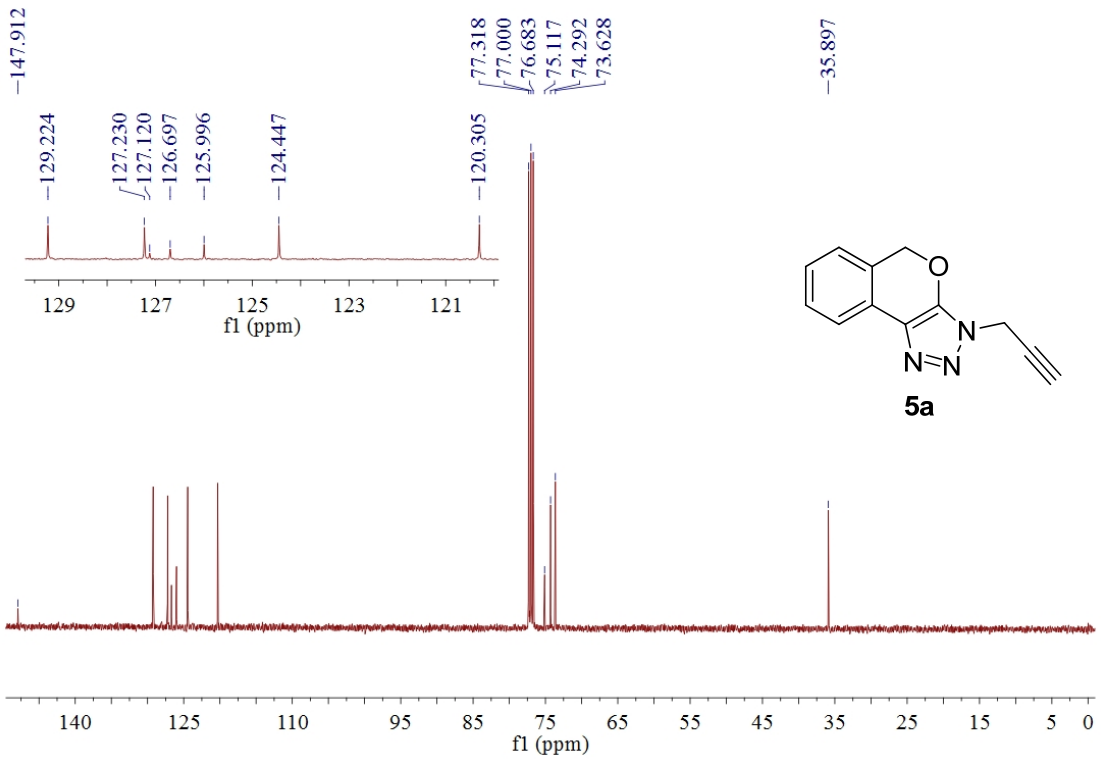

163.193
142.901
139.338
79.275
77.317
77.000
76.682
21.506
21.166
129.292
129.264
129.017
127.455
126.318
124.384
119.599
118.958
130 129 128 127 126 125 124 123 122 121 120 119
f1 (ppm)
O
NTs
N2

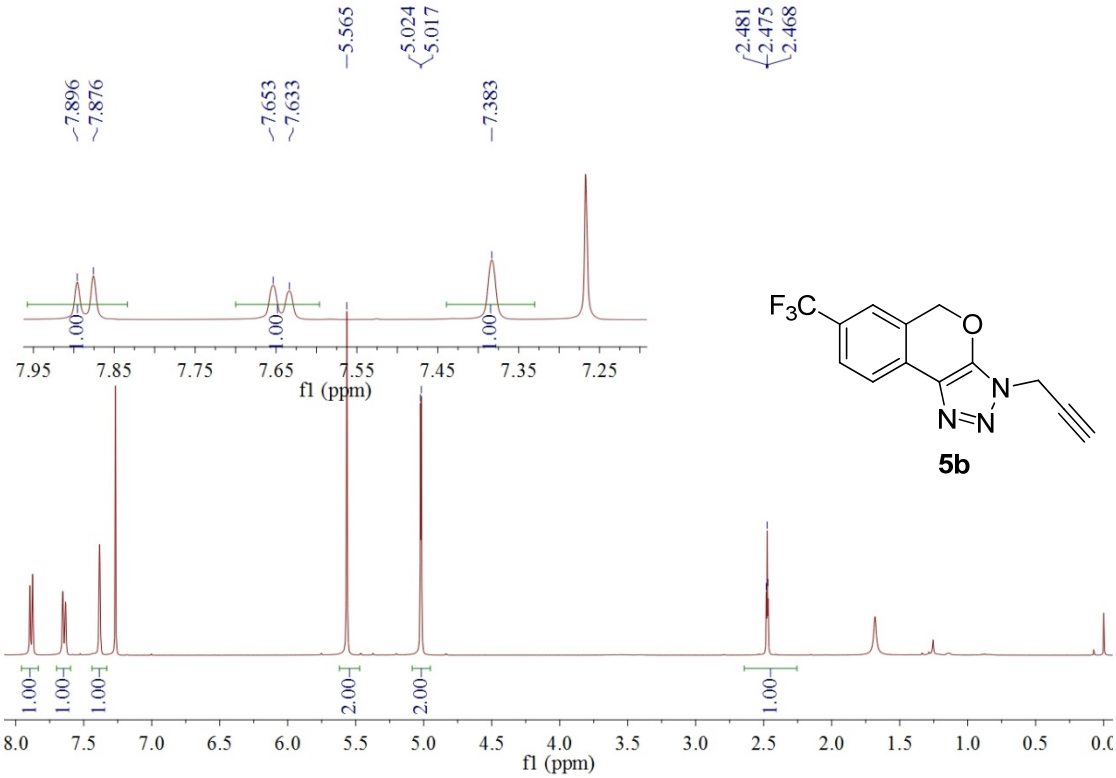
**3p**

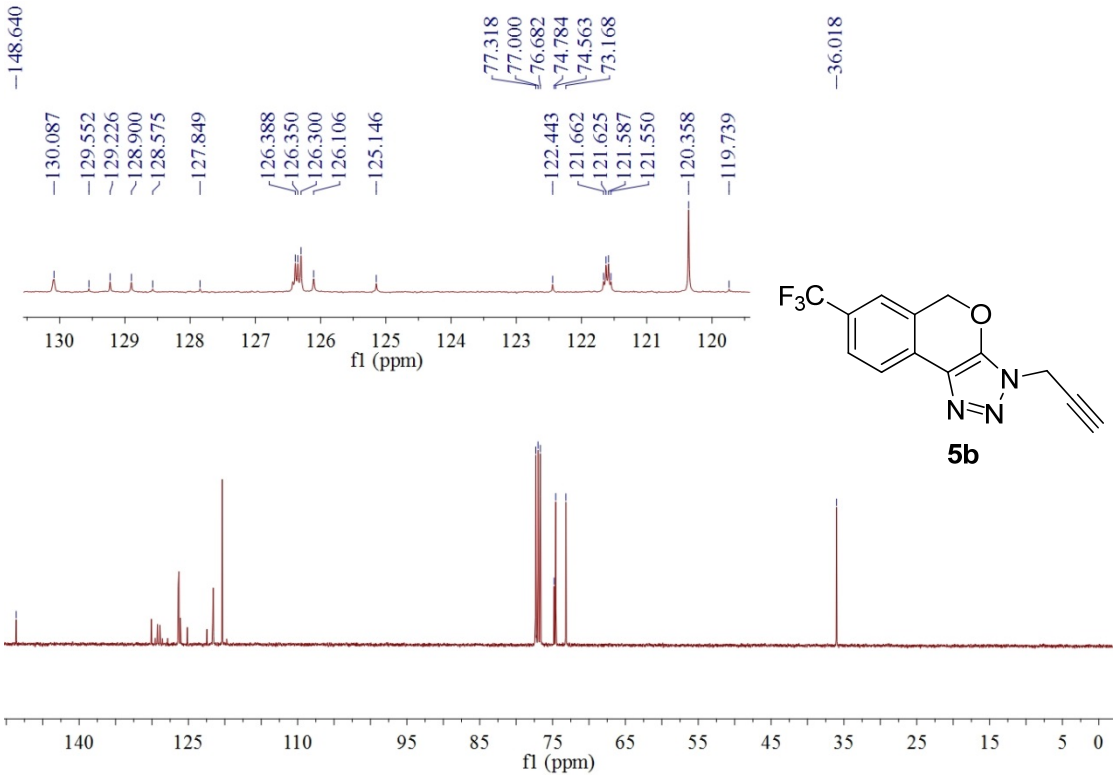

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

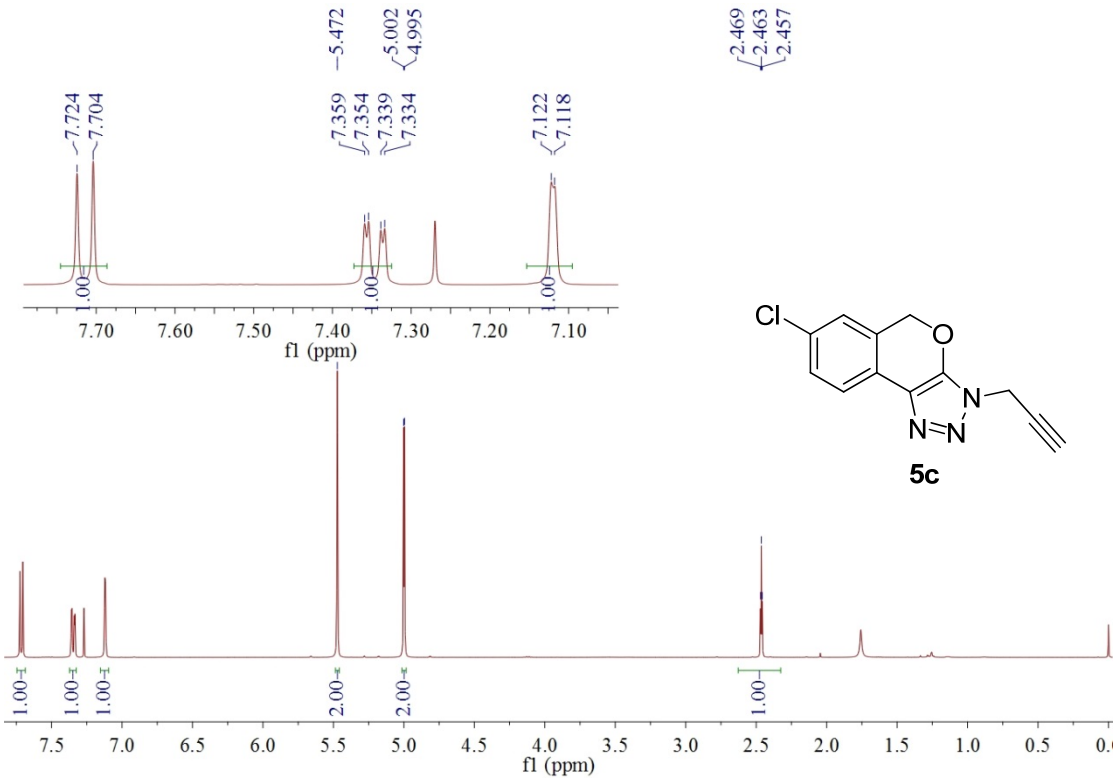

7.736
7.715
6.314
2.356
7.416
7.397
7.389
7.375
7.371
7.350
7.331
7.318
7.314
7.310
7.165
7.163
7.146
7.144
7.127
7.109
7.105
7.094
7.074
6.988
6.969
6.902
6.883
4.00
5.00
1.00
1.00
7.40
7.30
7.20
7.10
7.00
6.90
f1 (ppm)
O
NTs
N2
3q
2.00
4.00
5.00
1.00
1.00
1.00
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)
162.687
142.691
138.921
136.421
120.659
118.874
83.947
77.317
77.000
76.682
21.492
129.608
129.288
128.892
128.697
127.802
127.484
126.546
126.104
129.5
129.0
128.5
128.0
127.5
127.0
126.5
126.0
f1 (ppm)
O
NTs
N2
3q
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

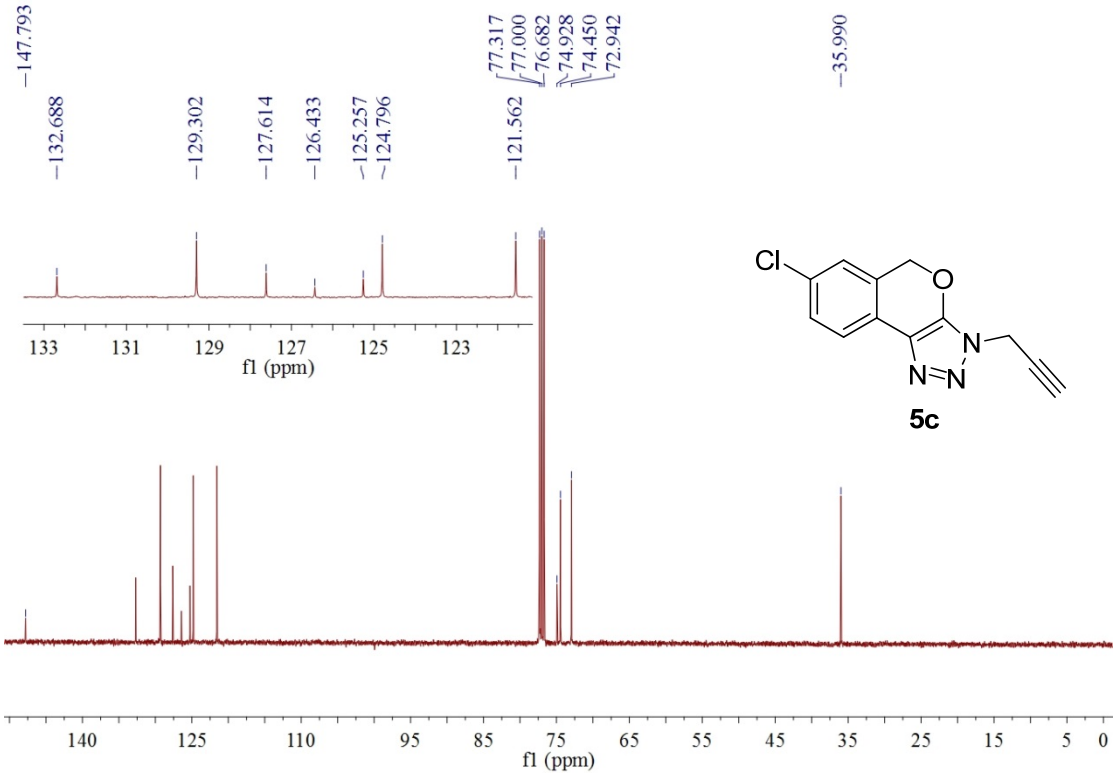

7.806
7.787
5.511
5.004
4.998
7.396
7.377
7.358
7.234
7.231
7.215
7.212
7.127
7.108
2.458
2.452
2.445
1.00
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
O
N
N=N
5a
1.00 1.00 1.00 1.00 2.00 2.00 0.96
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

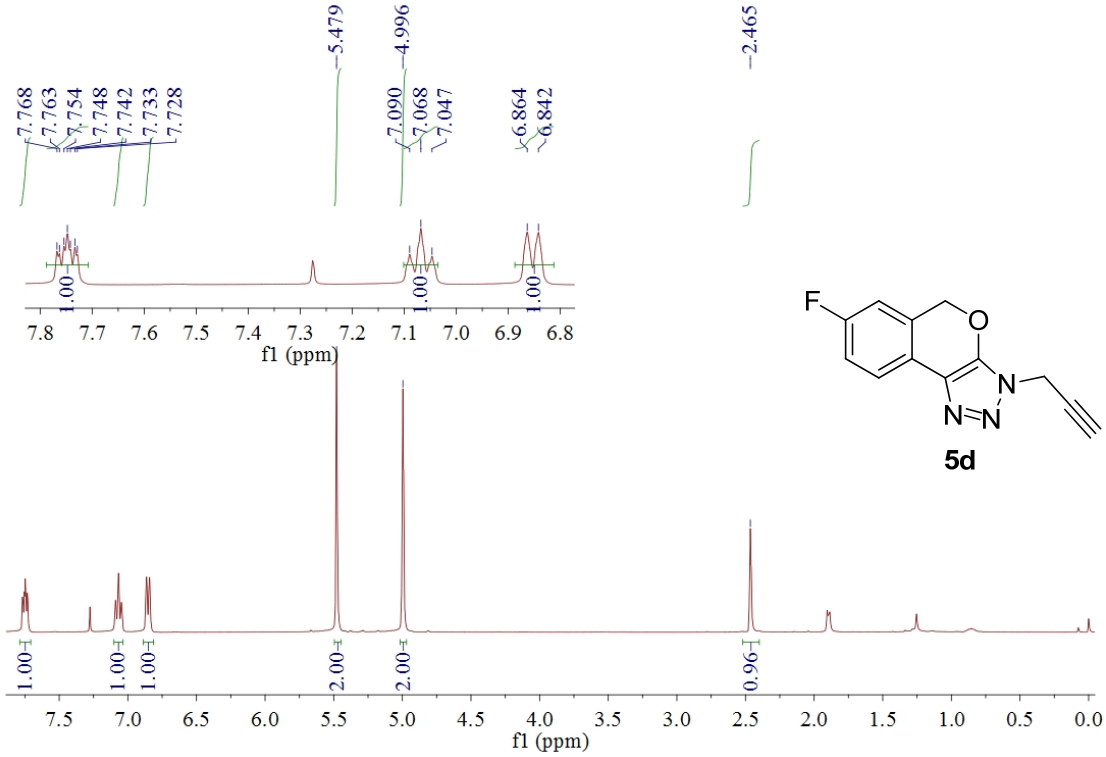

147.912
129.224
127.230
127.120
126.697
125.996
124.447
120.305
77.318
77.000
76.683
75.117
74.292
73.628
35.897
129 127 125 123 121
f1 (ppm)
O
N
N=N
5a
140 125 110 95 85 75 65 55 45 35 25 15 5 0
f1 (ppm)


7.896
7.876
7.653
7.633
5.565
5.024
5.017
7.383
2.481
2.475
2.468
1.00
1.00
1.00
7.95
7.85
7.75
7.65
7.55
7.45
7.35
7.25
f1 (ppm)
F3C
O
N
N=N
5b
1.00
1.00
1.00
2.00
2.00
1.00
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)

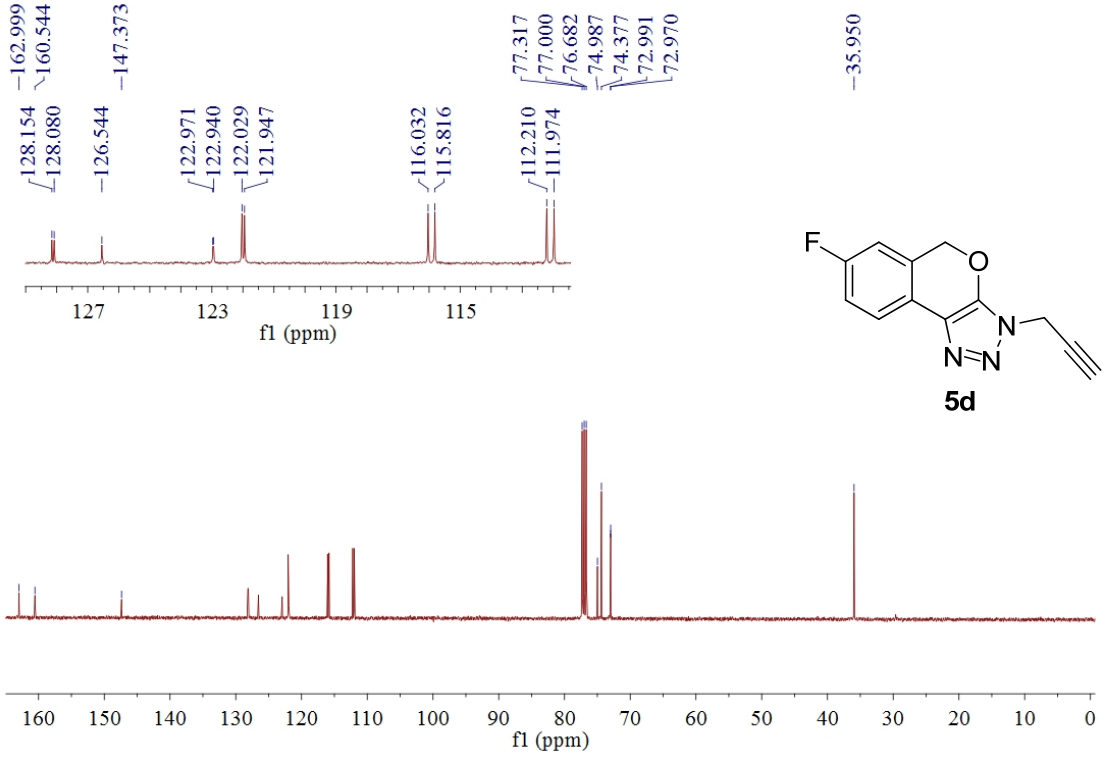

148.640
77.318
77.000
76.682
74.784
74.563
73.168
36.018
130.087
129.552
129.226
128.900
128.575
127.849
126.388
126.350
126.300
126.106
125.146
122.443
121.662
121.625
121.587
121.550
120.358
119.739
130
129
128
127
126
125
124
123
122
121
120
f1 (ppm)
F3C
O
N
N=N
5b
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)


7.724
7.704
5.472
7.359
7.354
7.339
7.334
5.002
4.995
7.122
7.118
2.469
2.463
2.457
Cl
O
N
N=N
5c
fl (ppm)

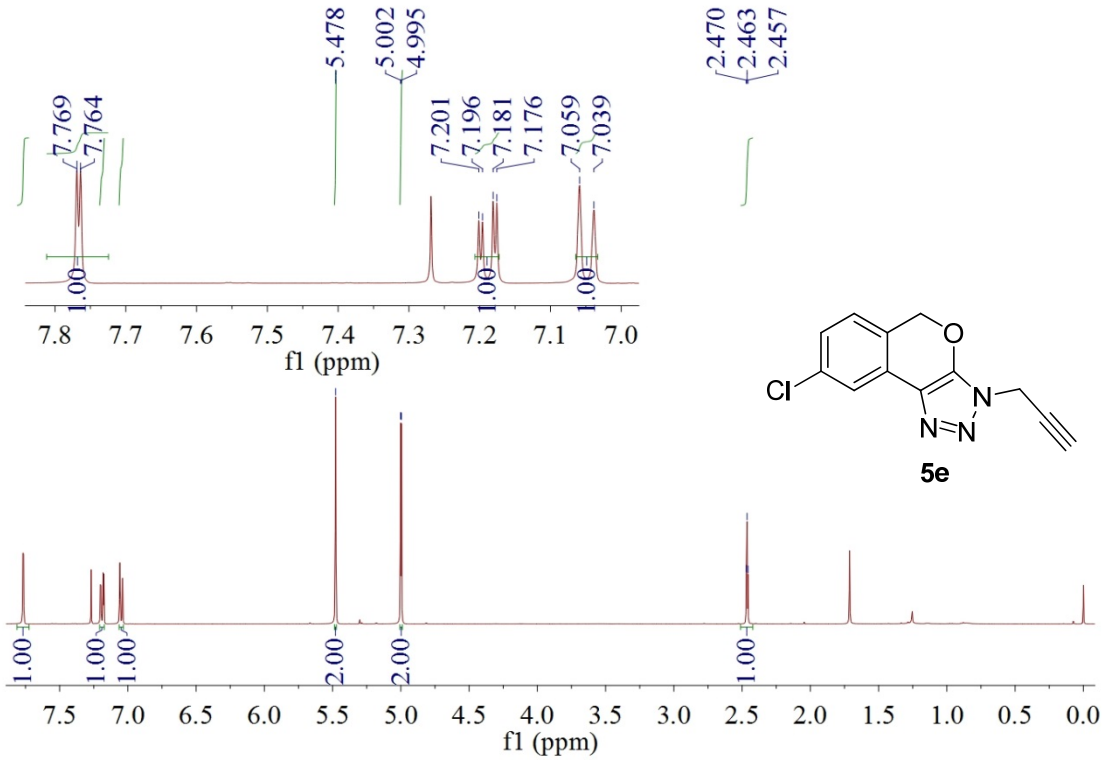

147.793
132.688
129.302
127.614
126.433
125.257
124.796
121.562
77.317
77.000
76.682
74.928
74.450
72.942
35.990
Cl
O
N
N=N
5c
fl (ppm)

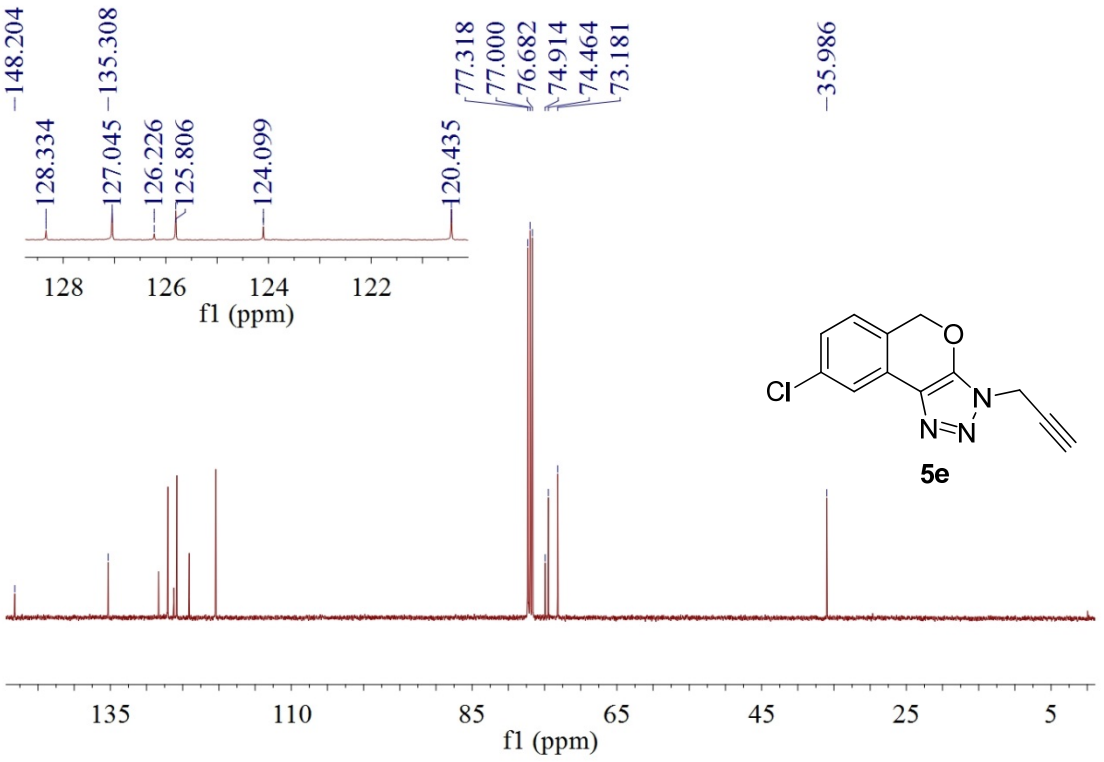

7.768
7.763
7.754
7.748
7.742
7.733
7.728
5.479
4.996
7.090
7.068
7.047
6.864
6.842
2.465
1.00
1.00
1.00
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)
F
O
N
N=N
1.00
1.00
1.00
2.00
2.00
0.96
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

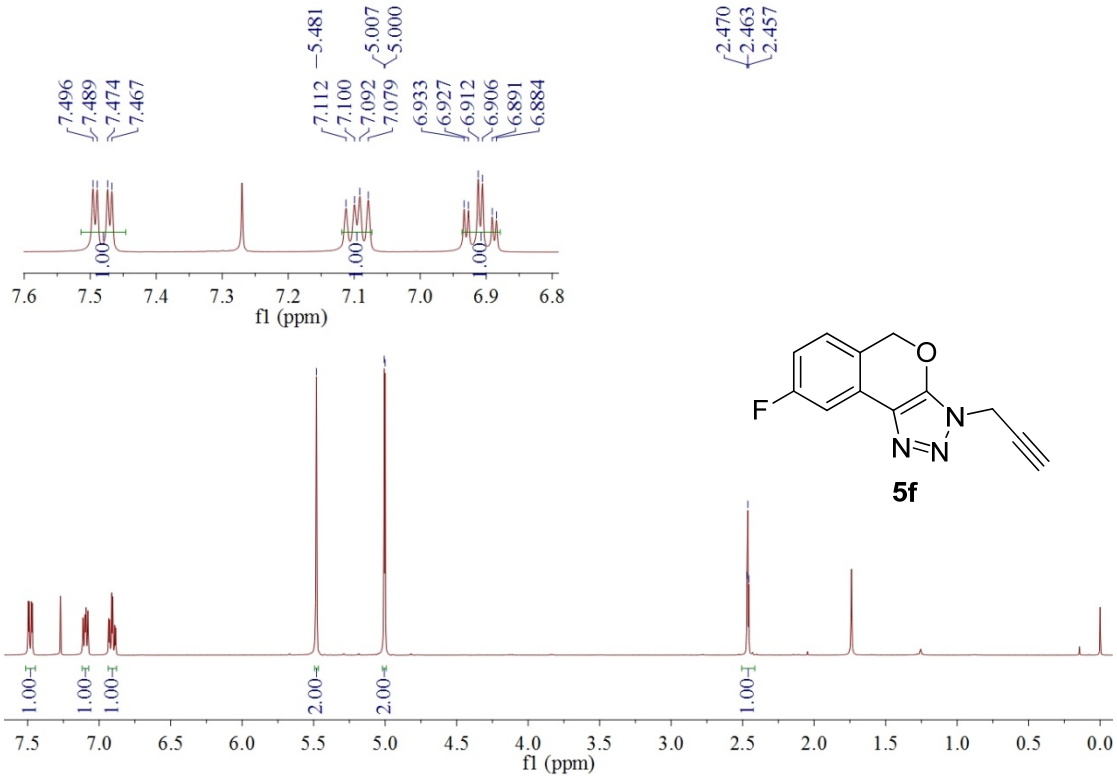
**5d**

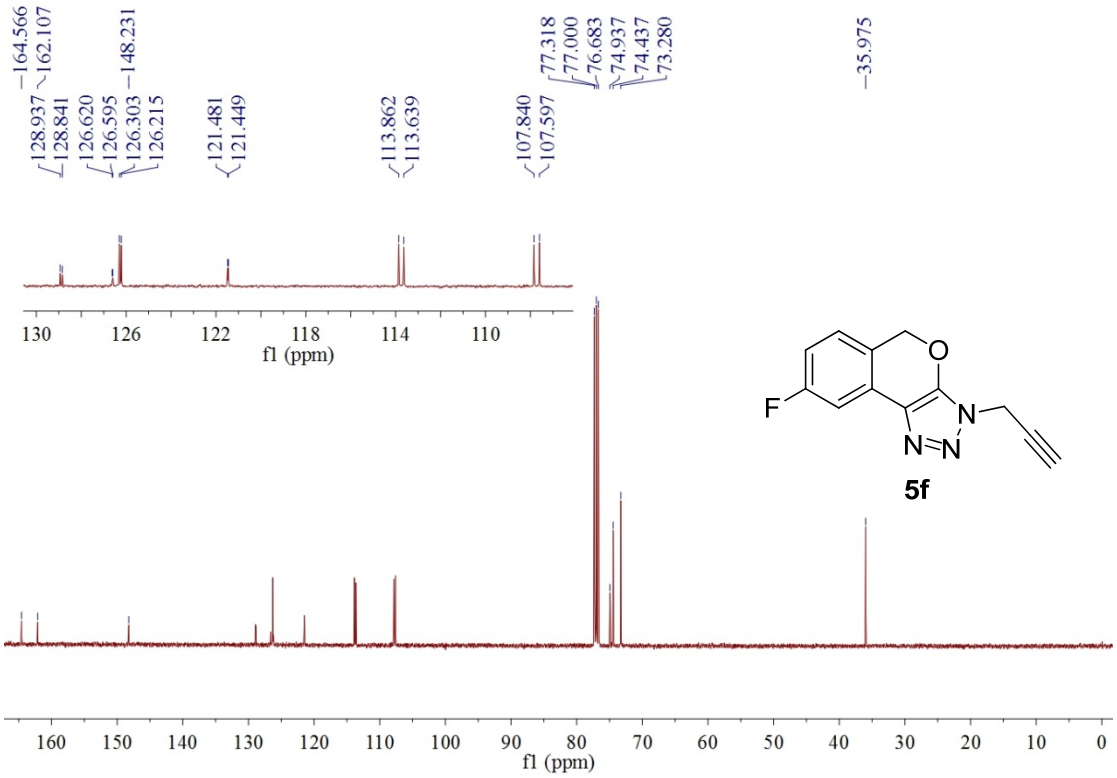

162.999
160.544
147.373
128.154
128.080
126.544
122.971
122.940
122.029
121.947
116.032
115.816
112.210
111.974
77.317
77.000
76.682
74.987
74.377
72.991
72.970
35.950
127 123 119 115
f1 (ppm)
F
O
N
N=N
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

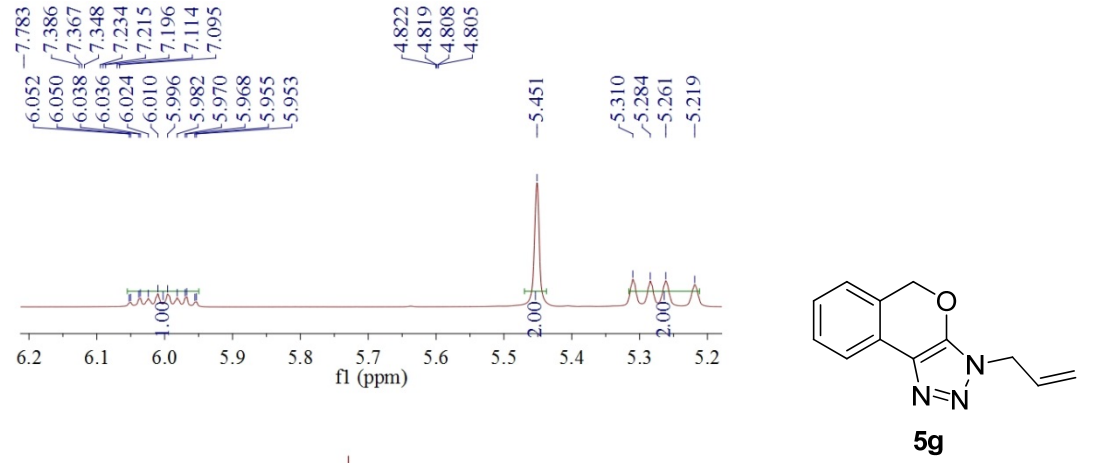
**5d**


5.478
5.002
4.995
2.470
2.463
2.457
7.769
7.764
7.201
7.196
7.181
7.176
7.059
7.039
1.00
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
Cl
O
N
N=N
5e
1.00 1.00 1.00 2.00 2.00 1.00
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)


148.204
135.308
128.334
127.045
126.226
125.806
124.099
120.435
77.318
77.000
76.682
74.914
74.464
73.181
35.986
128 126 124 122
f1 (ppm)
Cl
O
N
N=N
5e
135 110 85 65 45 25 5
f1 (ppm)

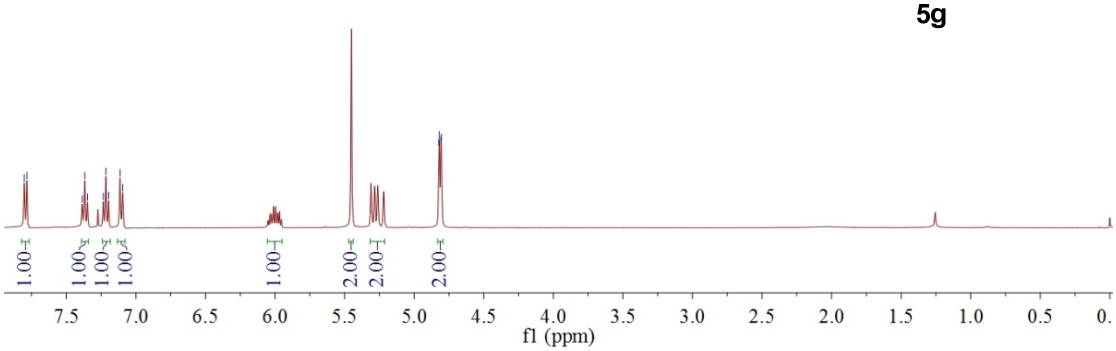

7.496
7.489
7.474
7.467
7.112
7.100
5.481
7.092
7.079
5.007
5.000
6.933
6.927
6.912
6.906
6.891
6.884
2.470
2.463
2.457
1.00
2.00
fl (ppm)
F
O
N
N=N
5f

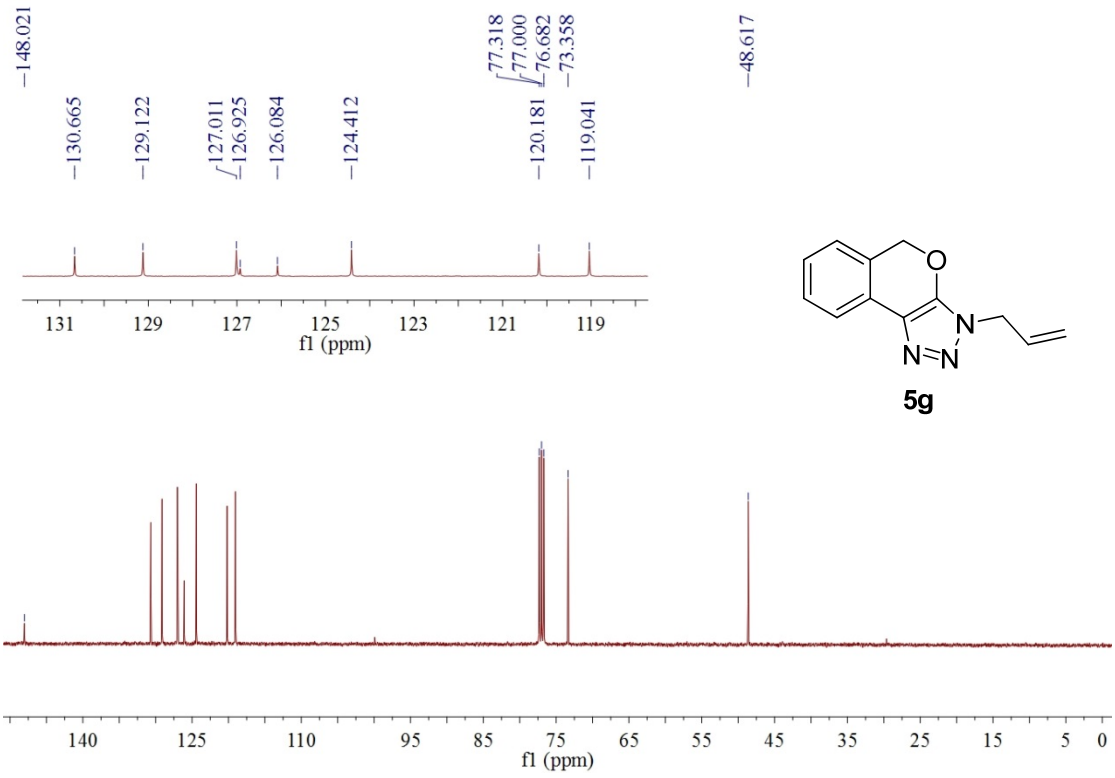

164.566
162.107
128.937
128.841
126.620
126.595
126.303
148.231
126.215
121.481
121.449
113.862
113.639
107.840
107.597
77.318
77.000
76.683
74.937
74.437
73.280
35.975
fl (ppm)
F
O
N
N=N
5f


7.783
7.386
7.367
7.348
7.234
7.215
7.196
7.114
7.095
6.052
6.050
6.038
6.036
6.024
6.010
5.996
5.982
5.970
5.968
5.955
5.953
4.822
4.819
4.808
4.805
5.451
5.310
5.284
5.261
5.219
1.00
2.00
2.00
6.2
6.1
6.0
5.9
5.8
5.7
5.6
5.5
5.4
5.3
5.2
f1 (ppm)


O
N
N=N

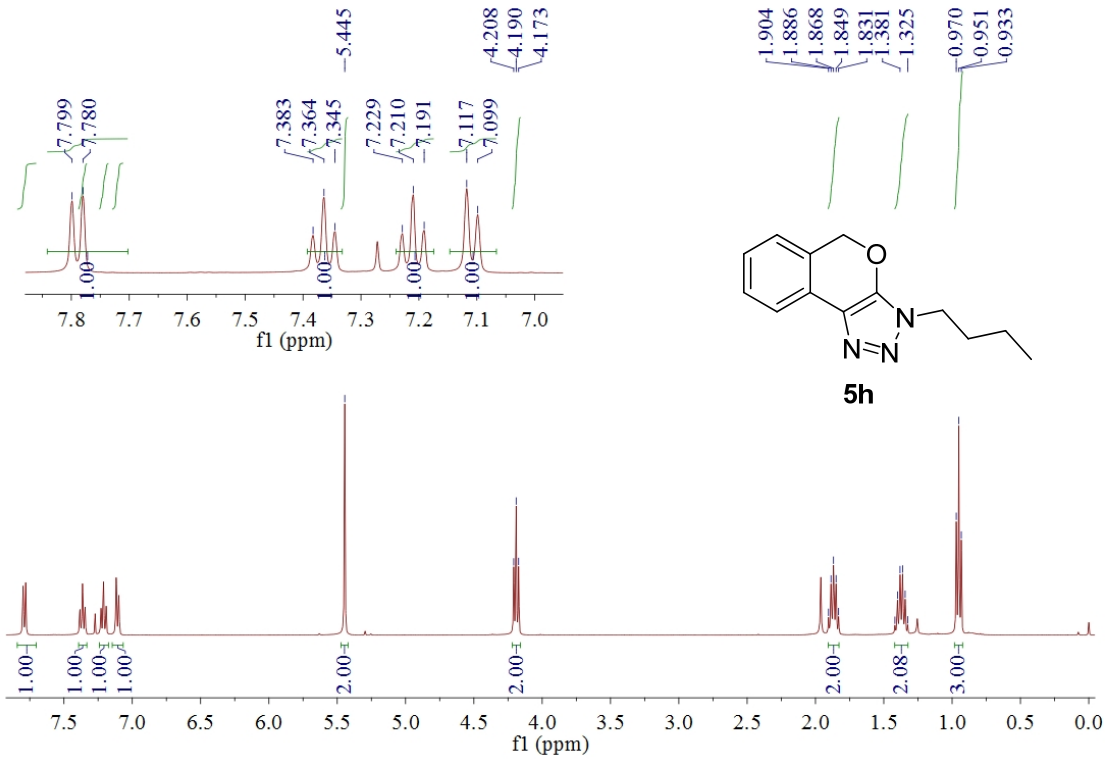
**5g**

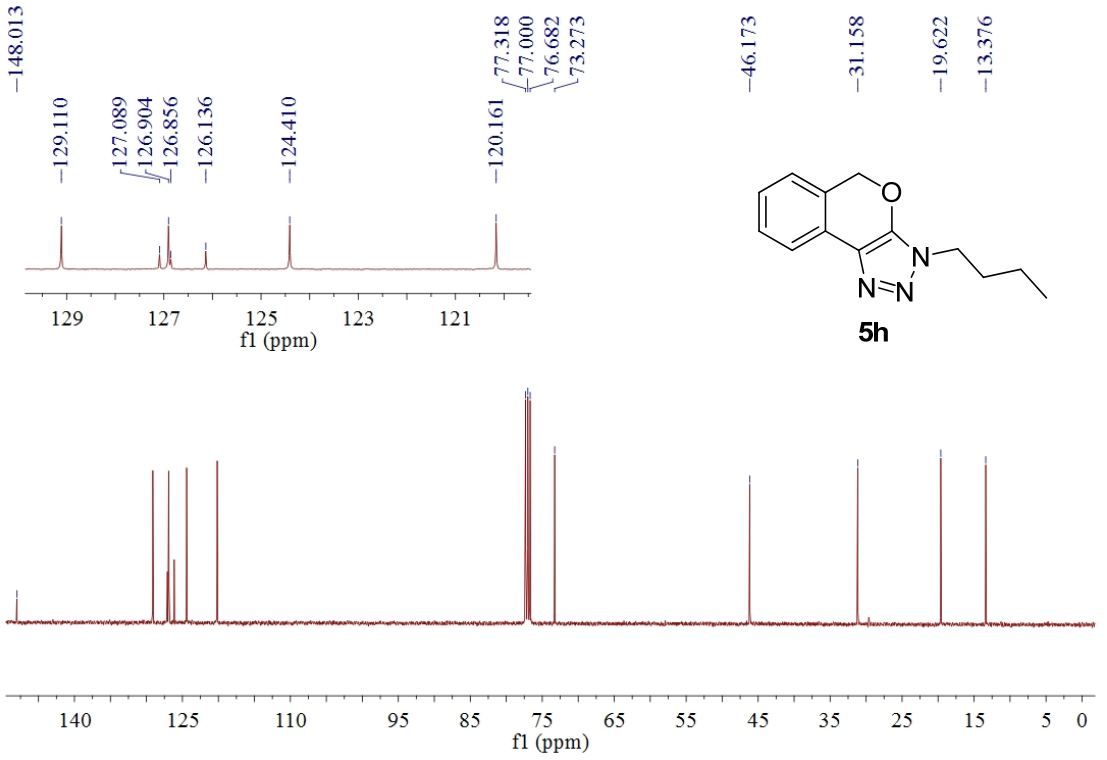

1.00
1.00
1.00
1.00
1.00
2.00
2.00
2.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

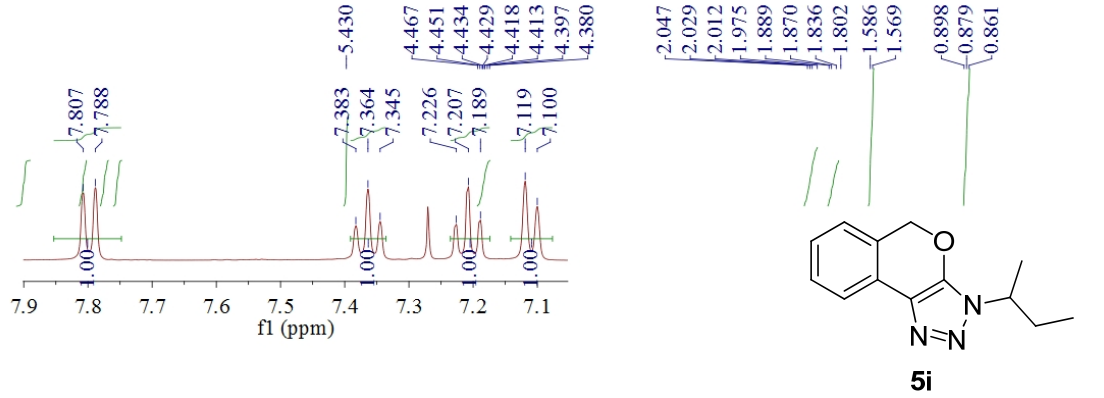

148.021
130.665
129.122
127.011
126.925
126.084
124.412
77.318
77.000
76.682
120.181
73.358
119.041
48.617
131
129
127
125
123
121
119
f1 (ppm)
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)


O
N
N=N

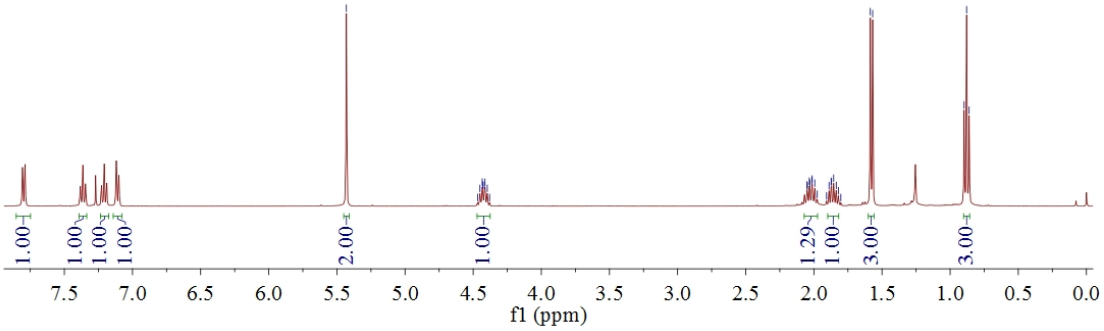
**5g**

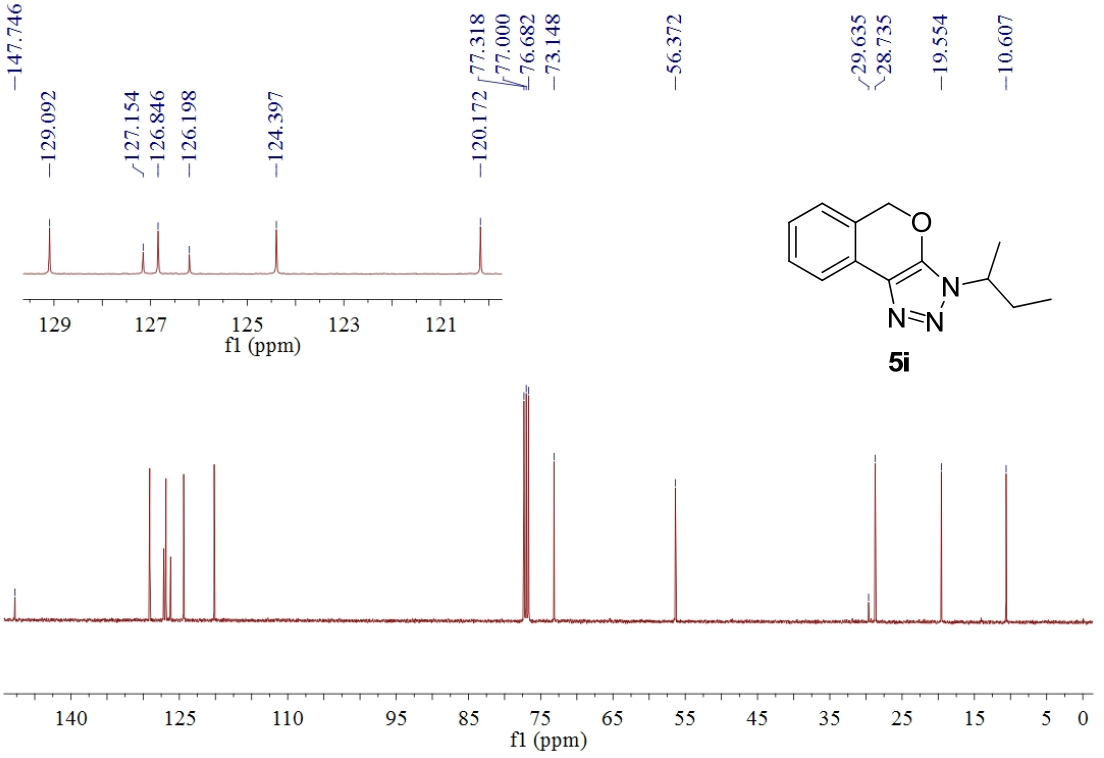

7.799
7.780
7.383
7.364
7.345
7.229
7.210
7.191
7.117
7.099
5.445
4.208
4.190
4.173
1.904
1.886
1.868
1.849
1.831
1.381
1.325
0.970
0.951
0.933
1.00
2.00
2.08
3.00
f1 (ppm)
5h


148.013
129.110
127.089
126.904
126.856
126.136
124.410
120.161
77.318
77.000
76.682
73.273
46.173
31.158
19.622
13.376
f1 (ppm)
5h


5.430
4.467
4.451
4.434
4.429
4.418
4.413
4.397
4.380
2.047
2.029
2.012
1.975
1.889
1.870
1.836
1.802
1.586
1.569
0.898
0.879
0.861
7.807
7.788
7.383
7.364
7.345
7.226
7.207
7.189
7.119
7.100
1.00
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
O
N
N=N

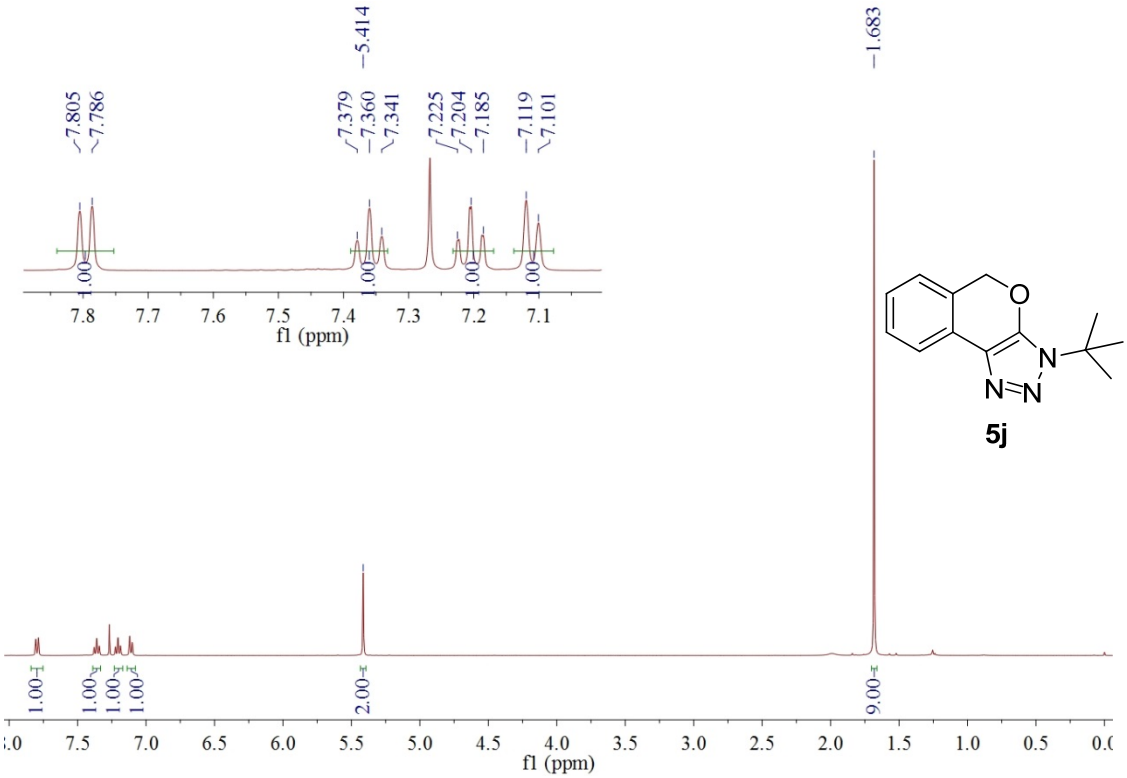
**5i**


1.00
1.00
1.00
1.00
2.00
1.00
1.29
1.00
3.00
3.00
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)


147.746
129.092
127.154
126.846
126.198
124.397
120.172
77.318
77.000
76.682
73.148
56.372
29.635
28.735
19.554
10.607
129 127 125 123 121
f1 (ppm)
O
N
N=N

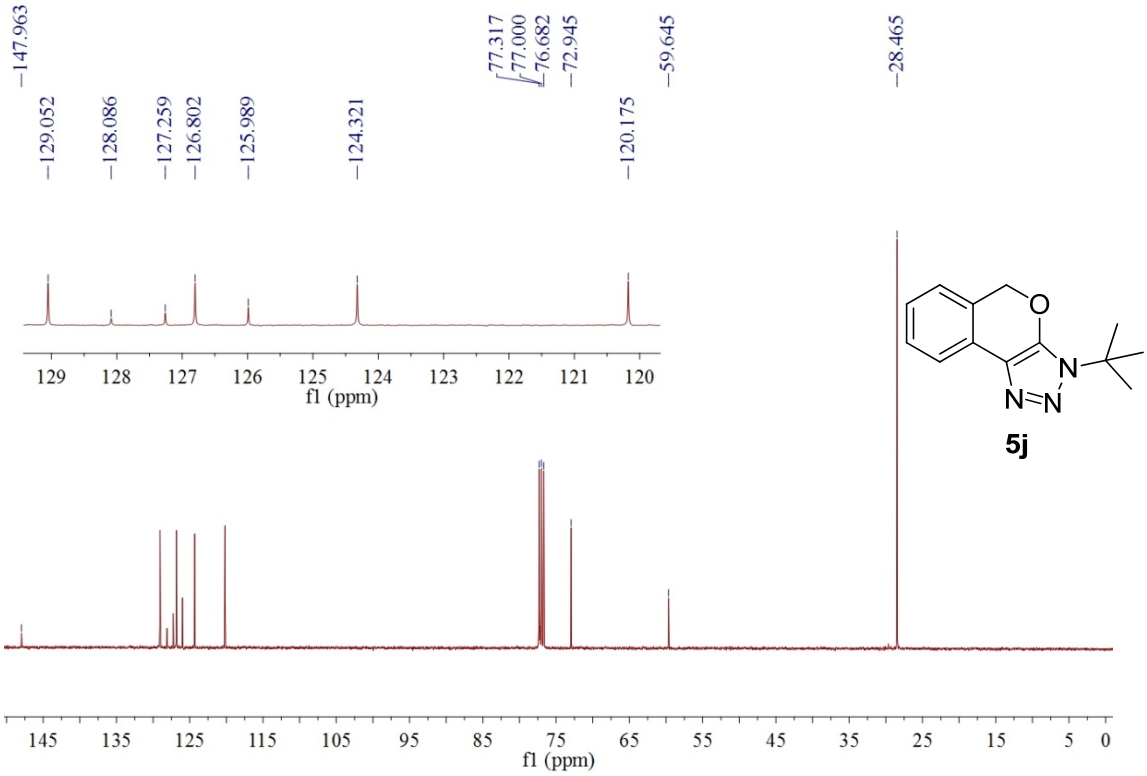
**5i**


140 125 110 95 85 75 65 55 45 35 25 15 5 0
f1 (ppm)


7.805
7.786
5.414
7.379
7.360
7.341
7.225
7.204
7.185
7.119
7.101
1.683
1.00
2.00
9.00
fl (ppm)

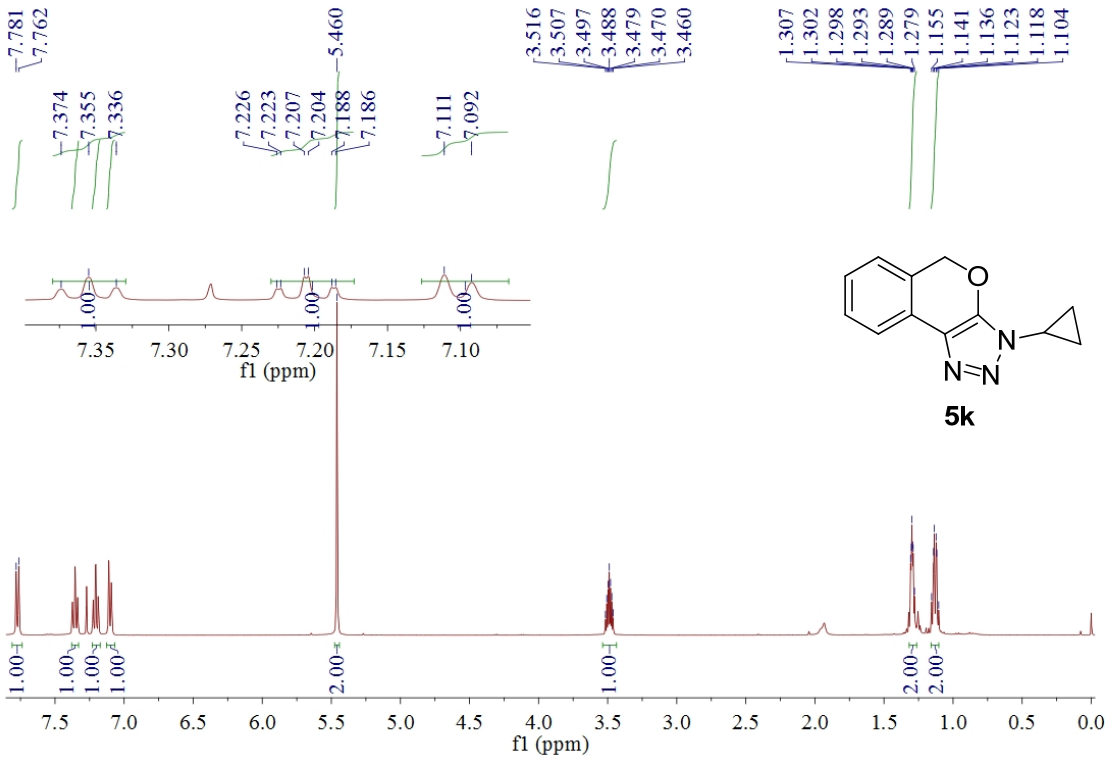


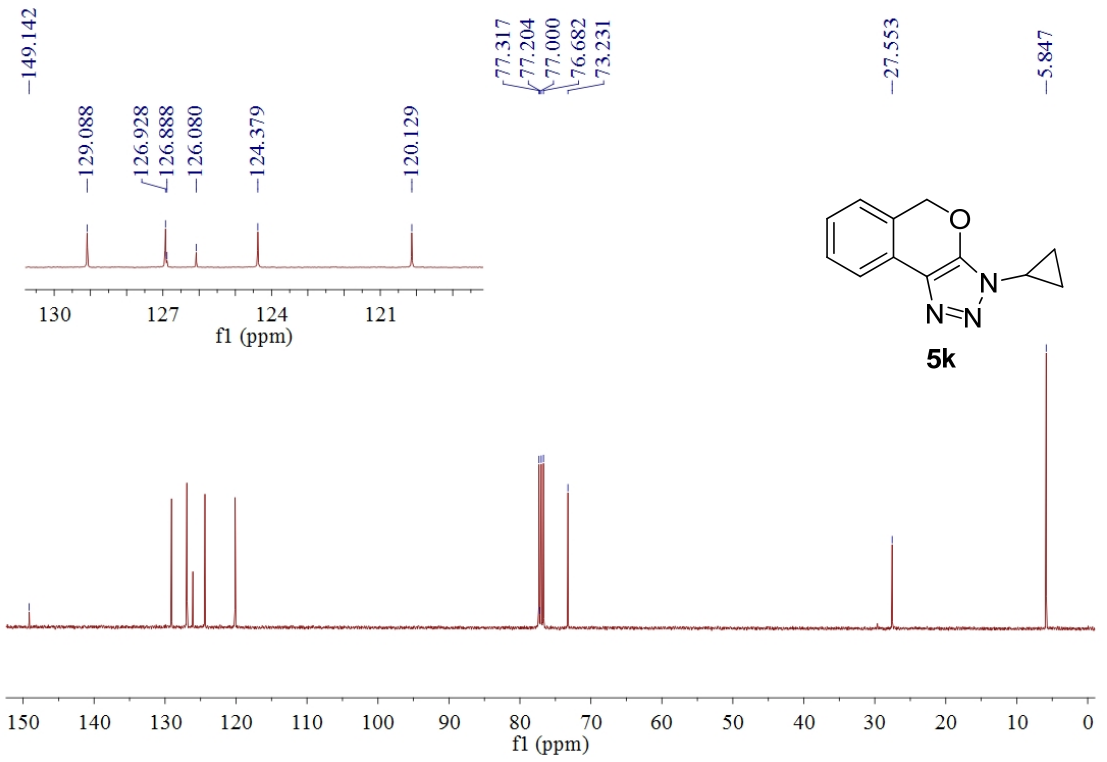
**5j**

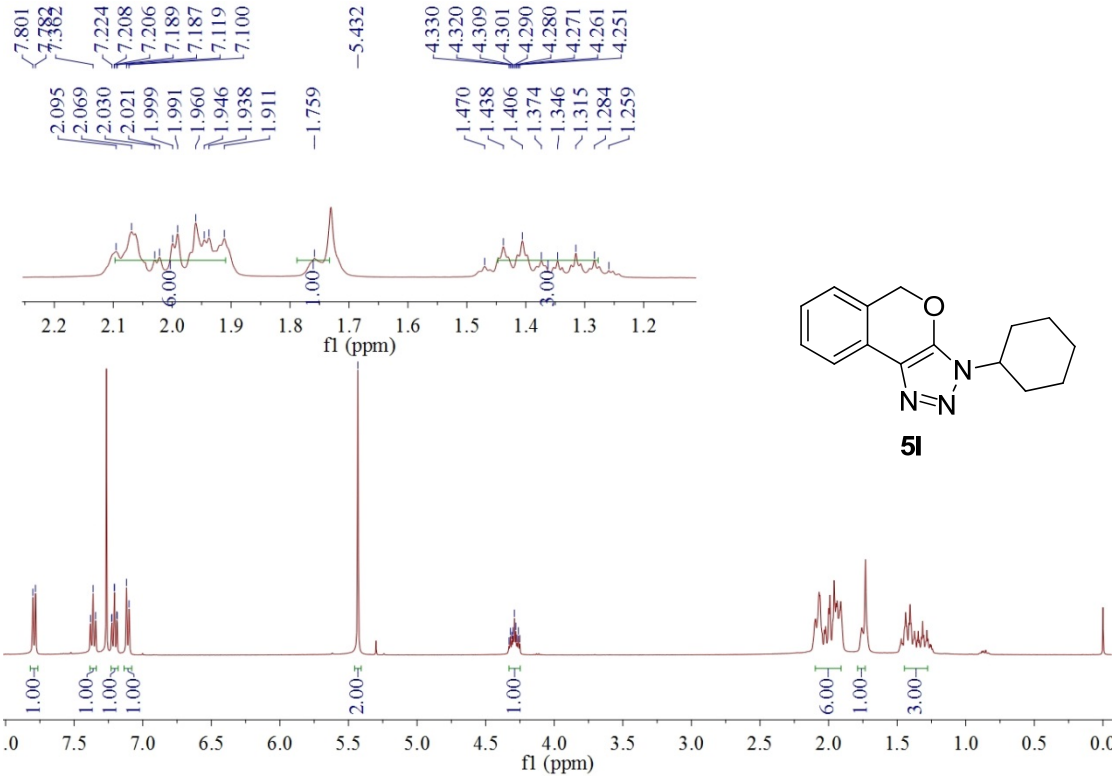

147.963
129.052
128.086
127.259
126.802
125.989
124.321
77.317
77.000
76.682
72.945
120.175
59.645
28.465
fl (ppm)



**5j**

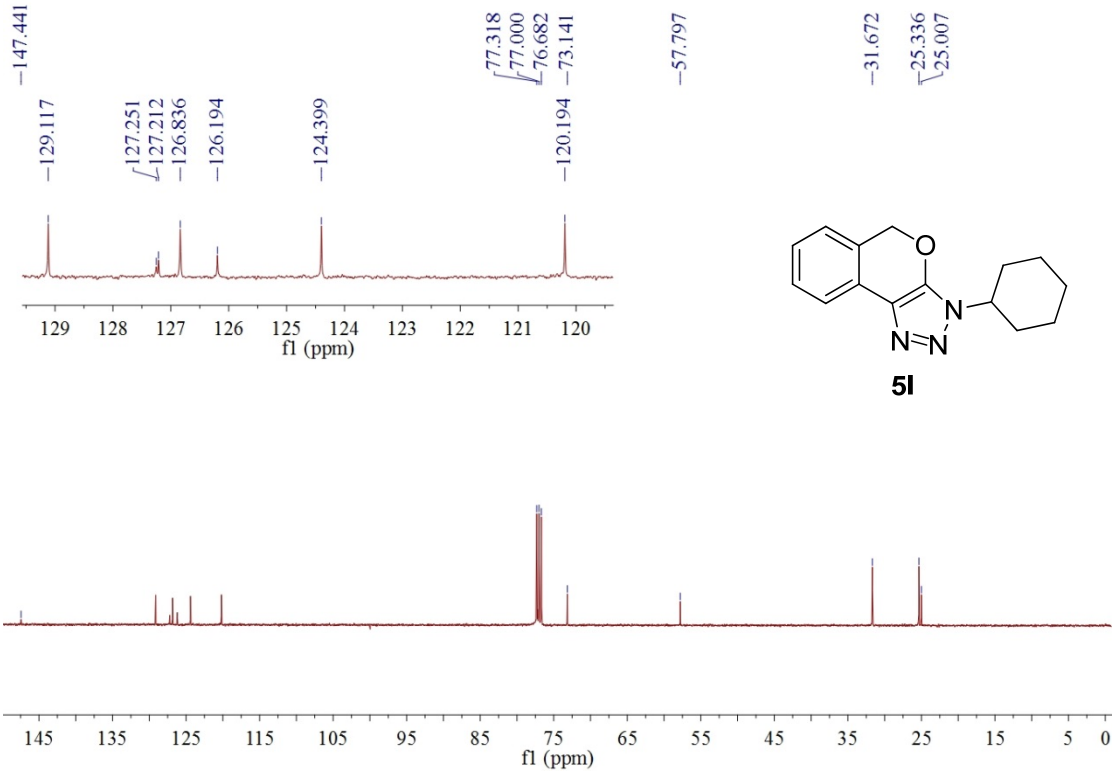

7.781
7.762
7.374
7.355
7.336
7.226
7.223
7.207
7.204
7.188
7.186
5.460
7.111
7.092
3.516
3.507
3.497
3.488
3.479
3.470
3.460
1.307
1.302
1.298
1.293
1.289
1.279
1.155
1.141
1.136
1.123
1.118
1.104
1.00
1.00
1.00
7.35
7.30
7.25
7.20
7.15
7.10
f1 (ppm)
O
N
N=N
5k
1.00
1.00
1.00
1.00
2.00
1.00
2.00
2.00
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)


149.142
129.088
126.928
126.888
126.080
124.379
120.129
77.317
77.204
77.000
76.682
73.231
27.553
5.847
130
127
124
121
f1 (ppm)
O
N
N=N
5k
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.801
7.782
7.382
7.224
7.208
7.206
7.189
7.187
7.119
7.100
5.432
4.330
4.320
4.309
4.301
4.290
4.280
4.271
4.261
4.251
2.095
2.069
2.030
2.021
1.999
1.991
1.960
1.946
1.938
1.911
1.759
1.470
1.438
1.406
1.374
1.346
1.315
1.284
1.259
6.00
1.00
3.00
fl (ppm)
1.00
1.00
1.00
1.00
2.00
1.00
6.00
1.00
3.00
fl (ppm)



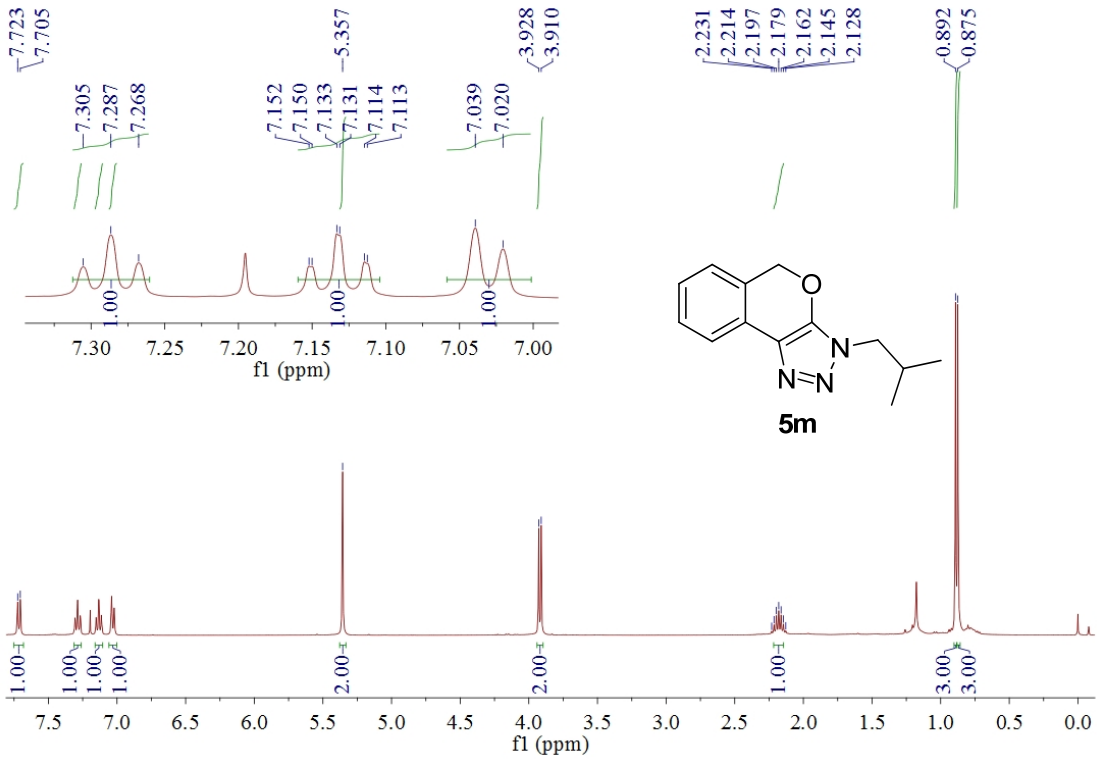
**5l**

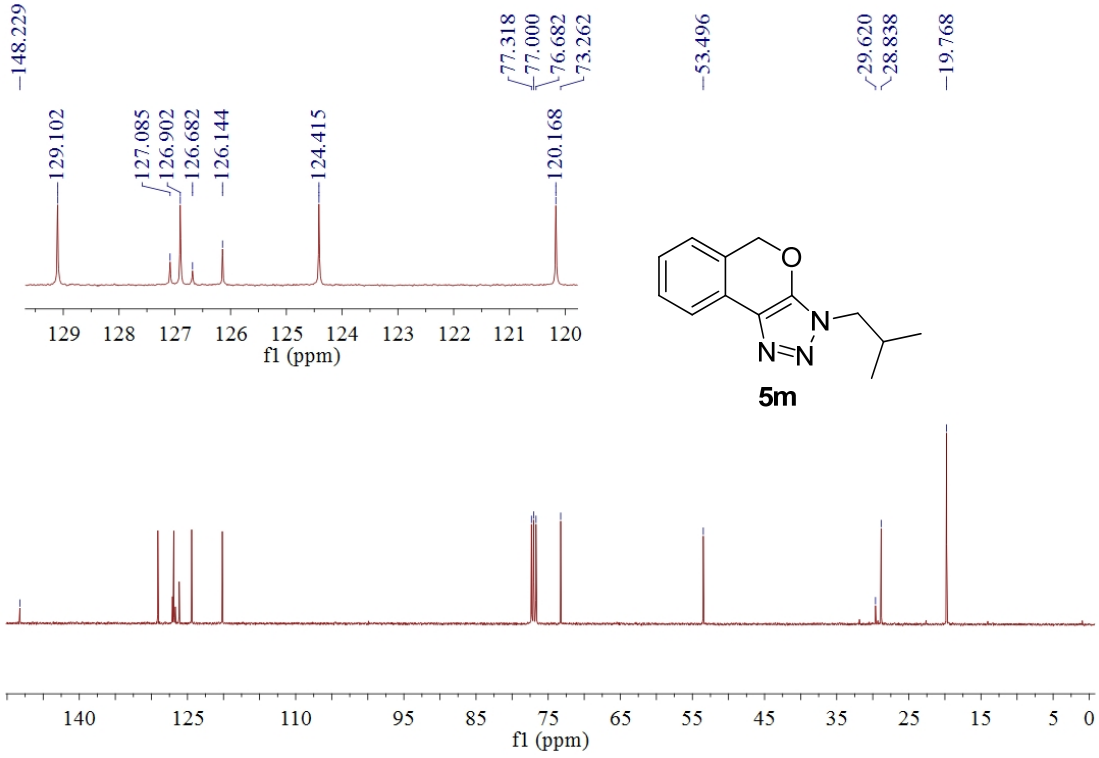

147.441
129.117
127.251
127.212
126.836
126.194
124.399
77.318
77.000
76.682
73.141
120.194
57.797
31.672
25.336
25.007
fl (ppm)
fl (ppm)

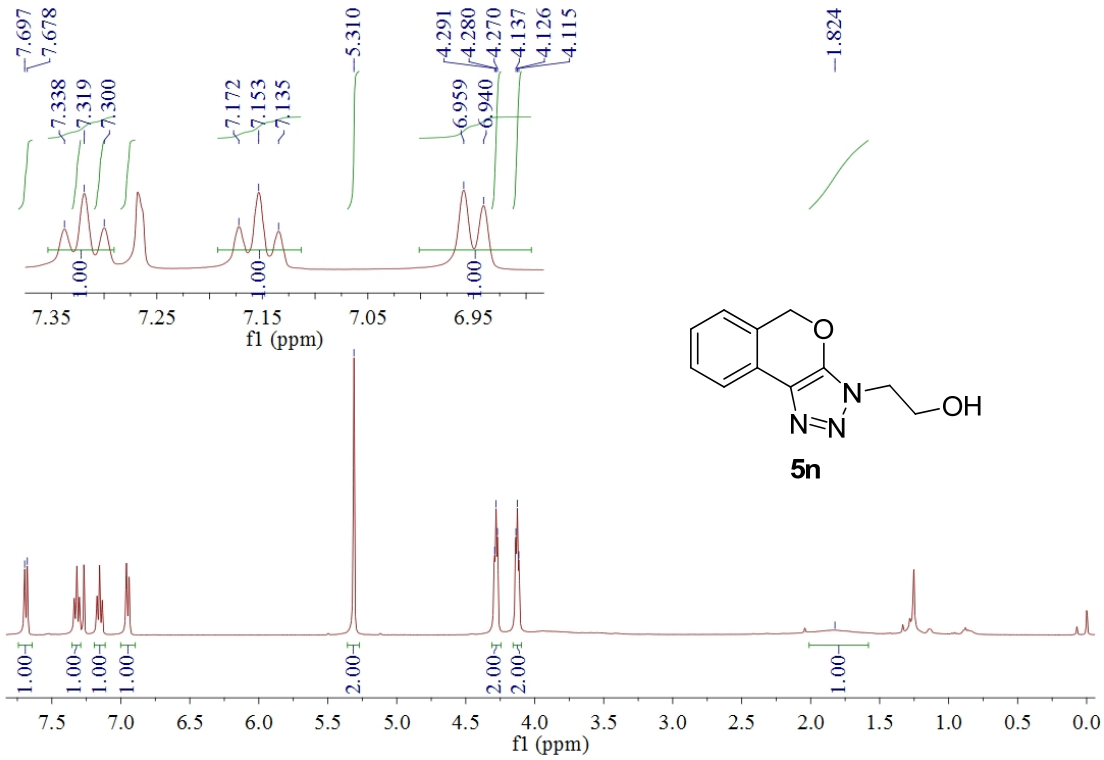


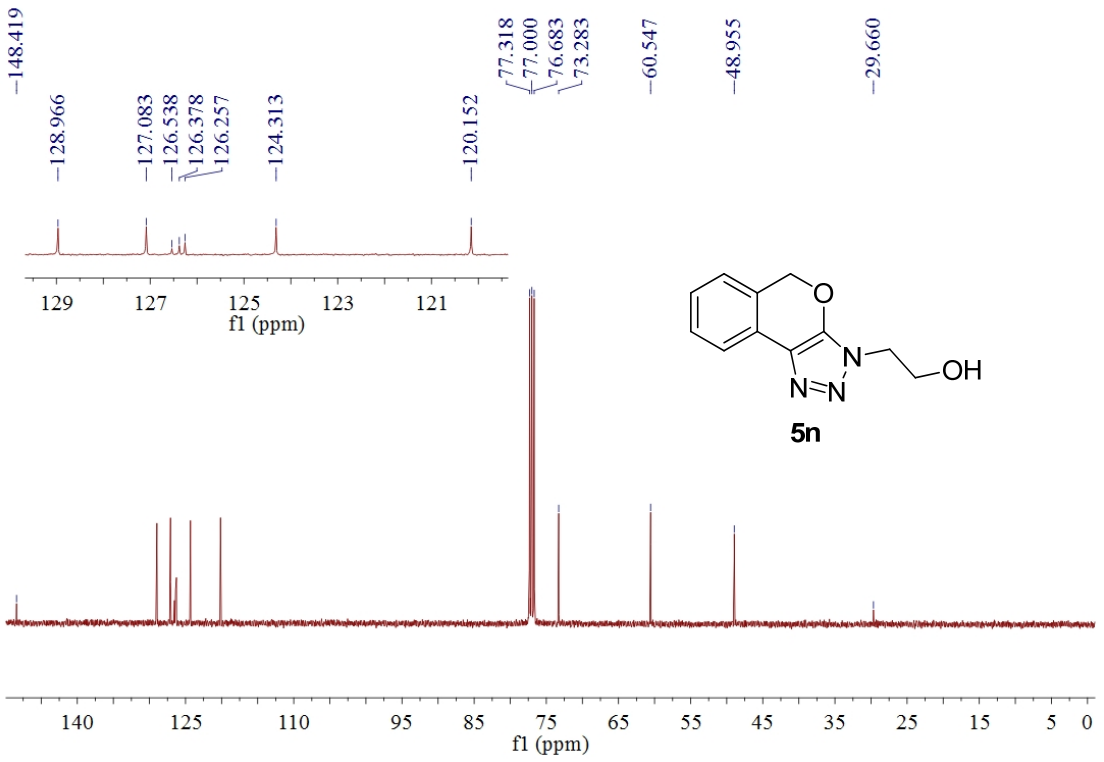
**5l**

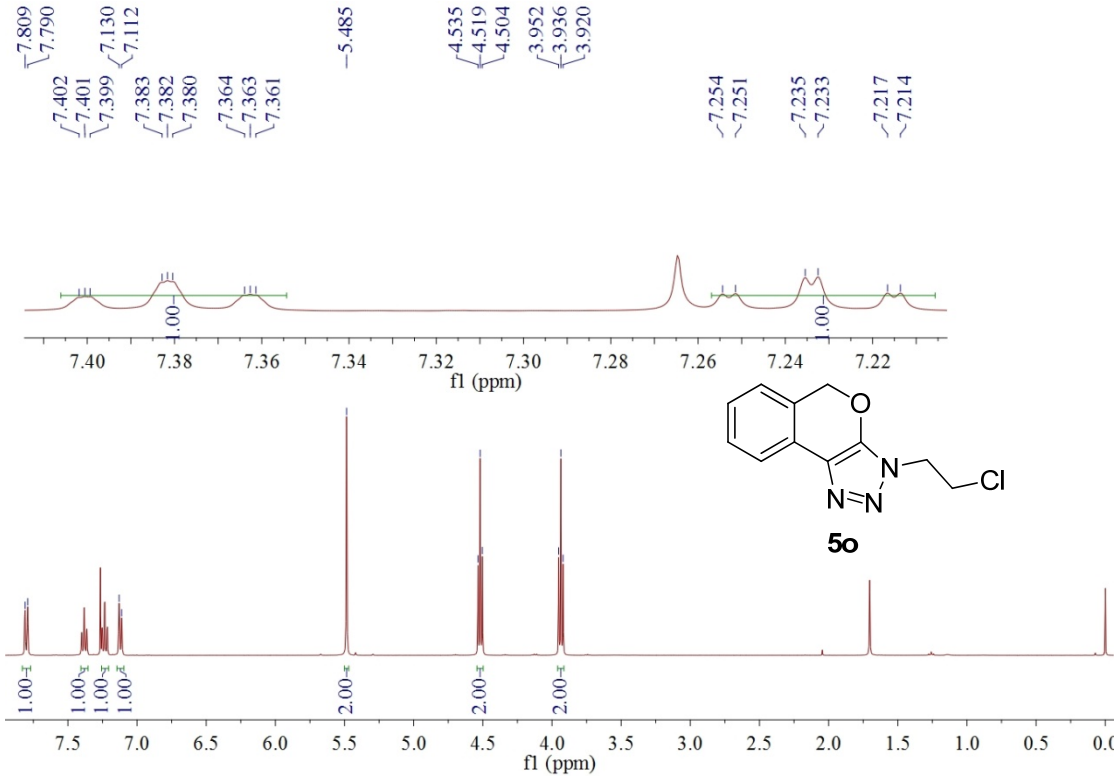

fl (ppm)

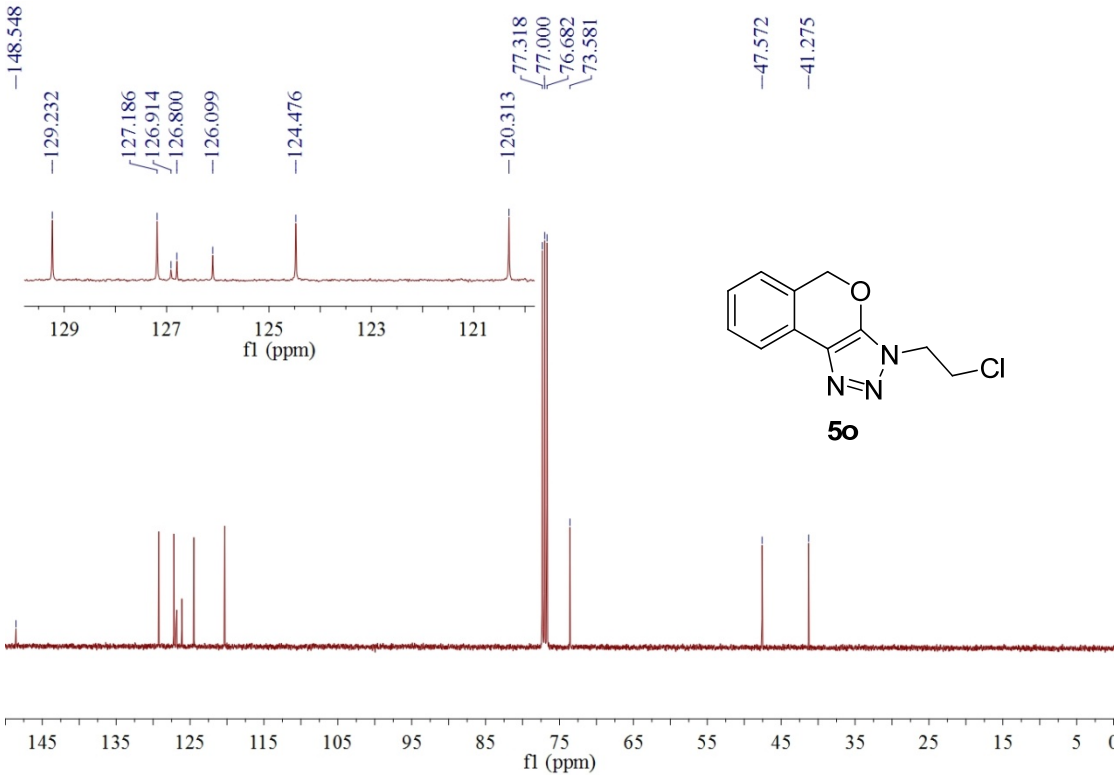

7.723
7.705
7.305
7.287
7.268
7.152
7.150
7.133
5.357
7.131
7.114
7.113
7.039
7.020
3.928
3.910
2.231
2.214
2.197
2.179
2.162
2.145
2.128
0.892
0.875
1.00
7.30 7.25 7.20 7.15 7.10 7.05 7.00
f1 (ppm)
O
N
N=N
5m
1.00 1.00 1.00 1.00 2.00 2.00 1.00 3.00 3.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

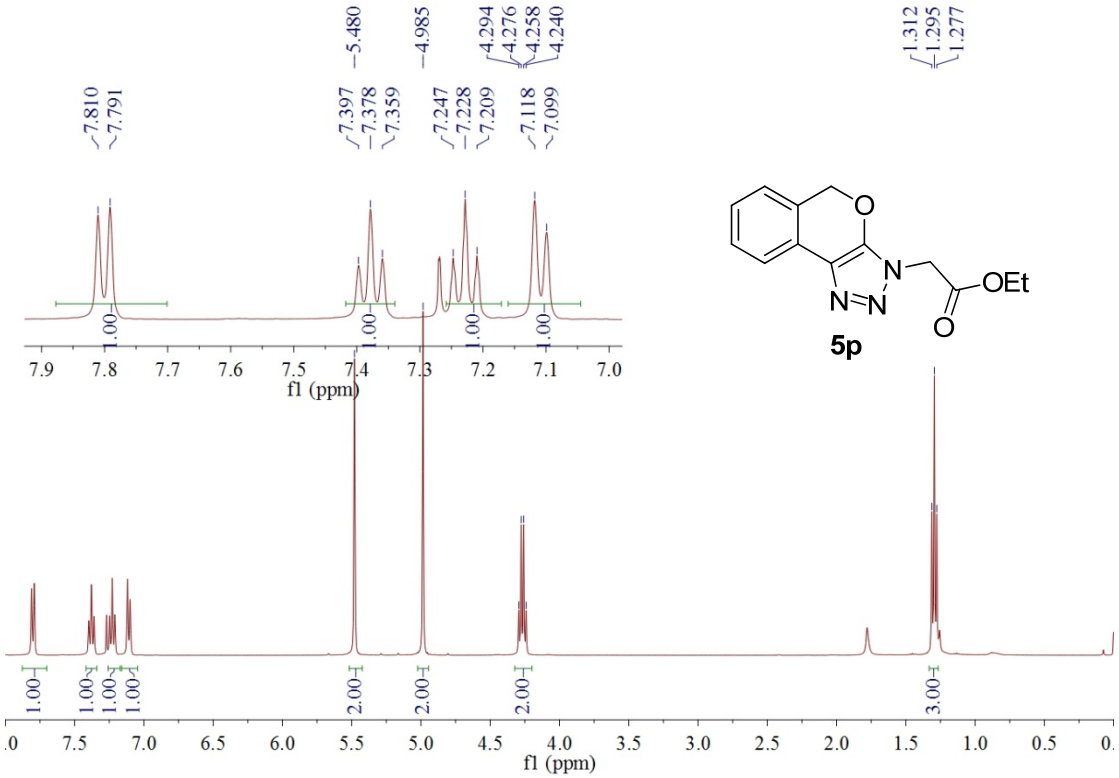

148.229
77.318
77.000
76.682
73.262
53.496
29.620
28.838
19.768
129.102
127.085
126.902
126.682
126.144
124.415
120.168
129 128 127 126 125 124 123 122 121 120
f1 (ppm)
O
N
N=N
5m
140 125 110 95 85 75 65 55 45 35 25 15 5 0
f1 (ppm)

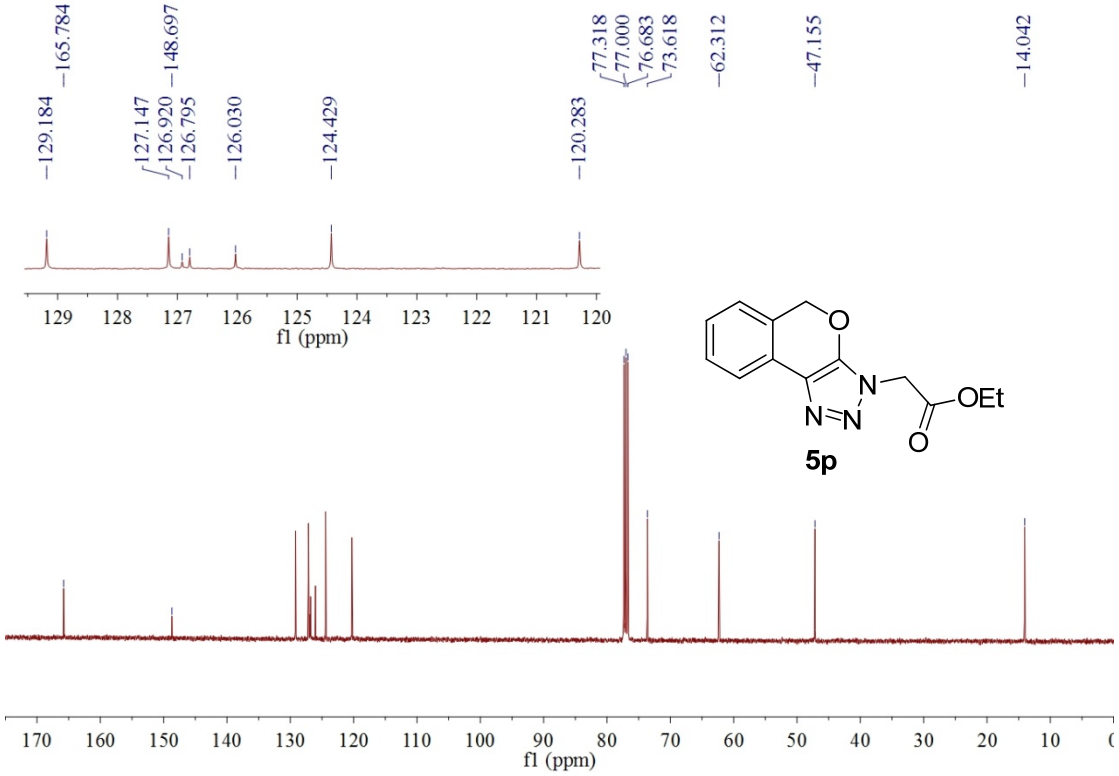

7.697
7.678
7.338
7.319
7.300
7.172
7.153
7.135
5.310
4.291
4.280
4.270
4.137
4.126
4.115
6.959
6.940
1.824
1.00
1.00
1.00
7.35
7.25
7.15
7.05
6.95
f1 (ppm)
O
N
N=N
OH
5n
1.00
1.00
1.00
1.00
2.00
2.00
2.00
1.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

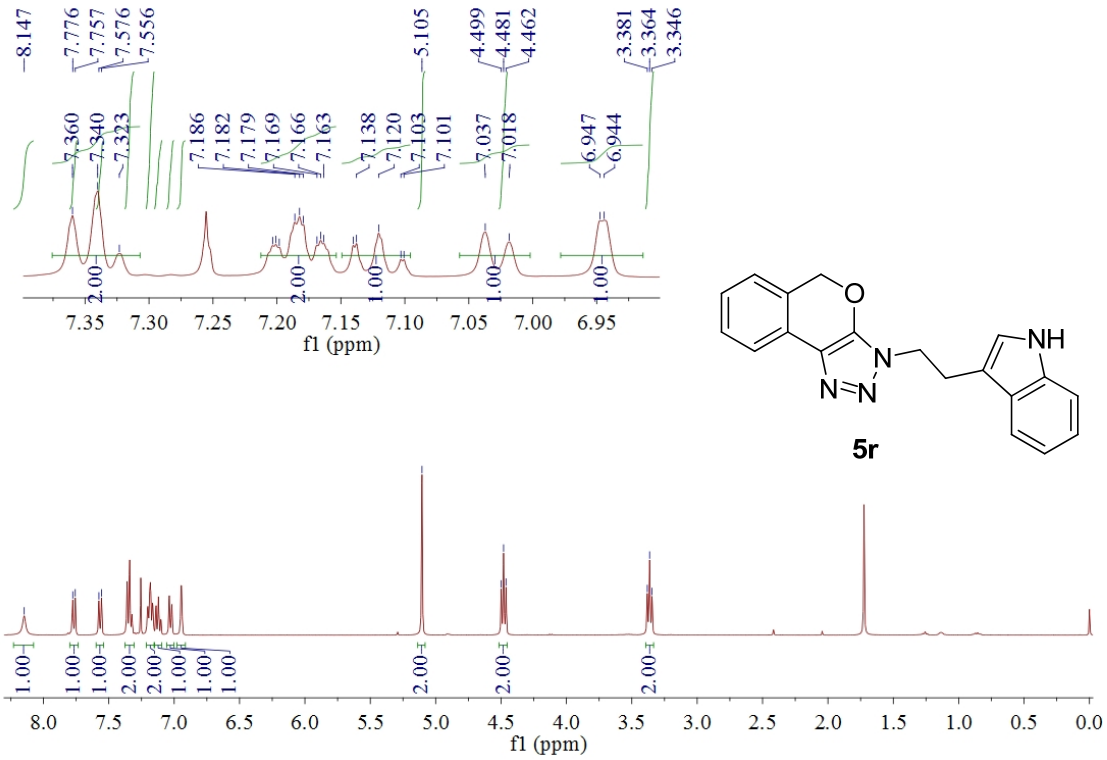

148.419
128.966
127.083
126.538
126.378
126.257
124.313
120.152
77.318
77.000
76.683
73.283
60.547
48.955
29.660
129
127
125
123
121
f1 (ppm)
O
N
N=N
OH
5n
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)

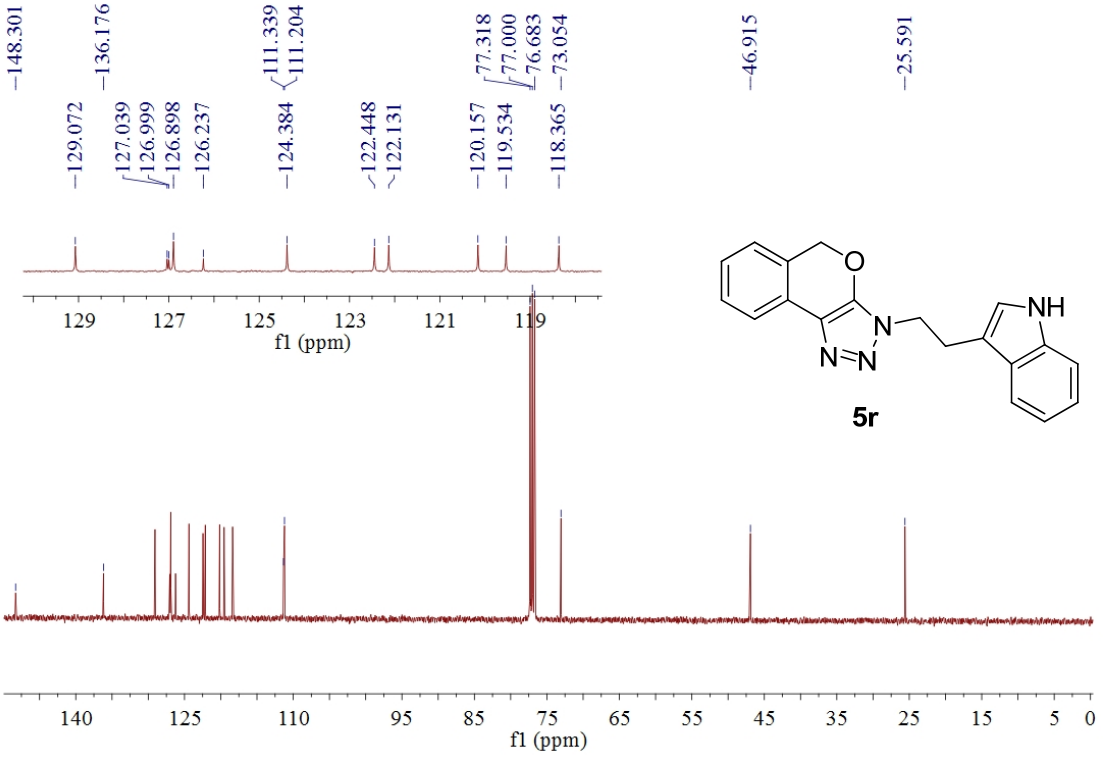

7.809
7.790
7.402
7.401
7.399
7.130
7.112
7.383
7.382
7.380
7.364
7.363
7.361
5.485
4.535
4.519
4.504
3.952
3.936
3.920
7.254
7.251
7.235
7.233
7.217
7.214
1.00
1.00
7.40
7.38
7.36
7.34
7.32
7.30
7.28
7.26
7.24
7.22
f1 (ppm)
O
N
N=N
Cl
5o
1.00
1.00
1.00
1.00
2.00
2.00
2.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

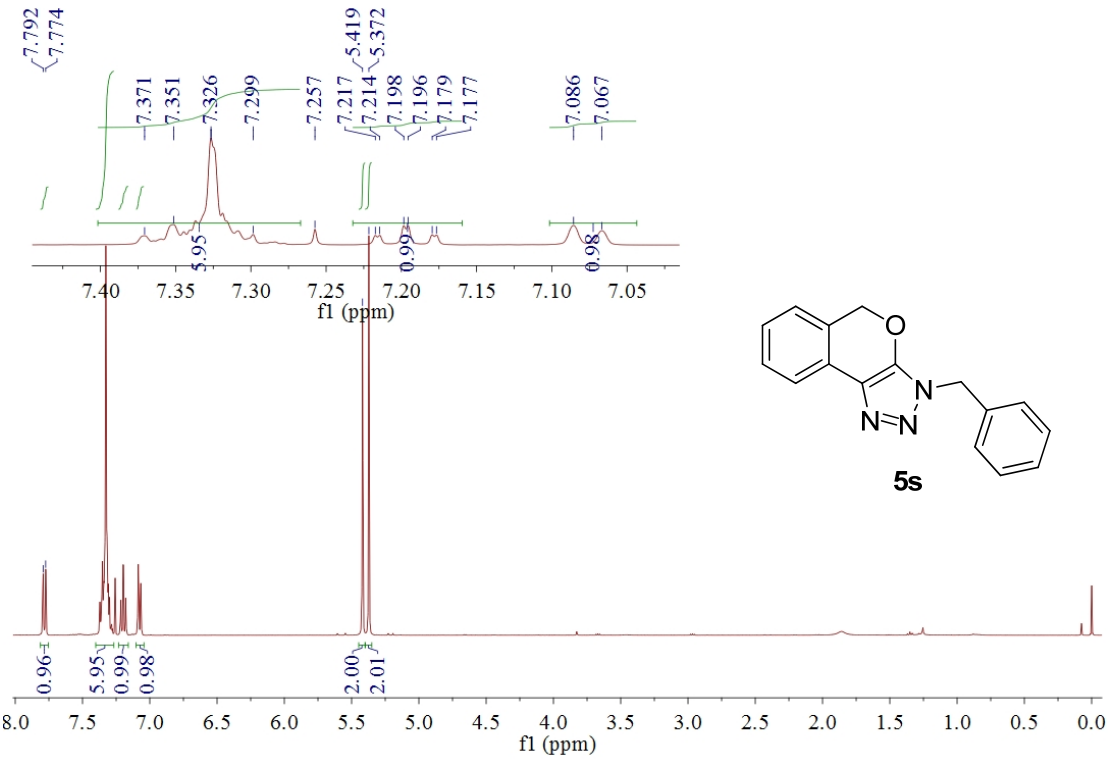

148.548
129.232
127.186
126.914
126.800
126.099
124.476
120.313
77.318
77.000
76.682
73.581
47.572
41.275
129
127
125
123
121
f1 (ppm)
O
N
N=N
Cl
5o
145
135
125
115
105
95
85
75
65
55
45
35
25
15
5
f1 (ppm)

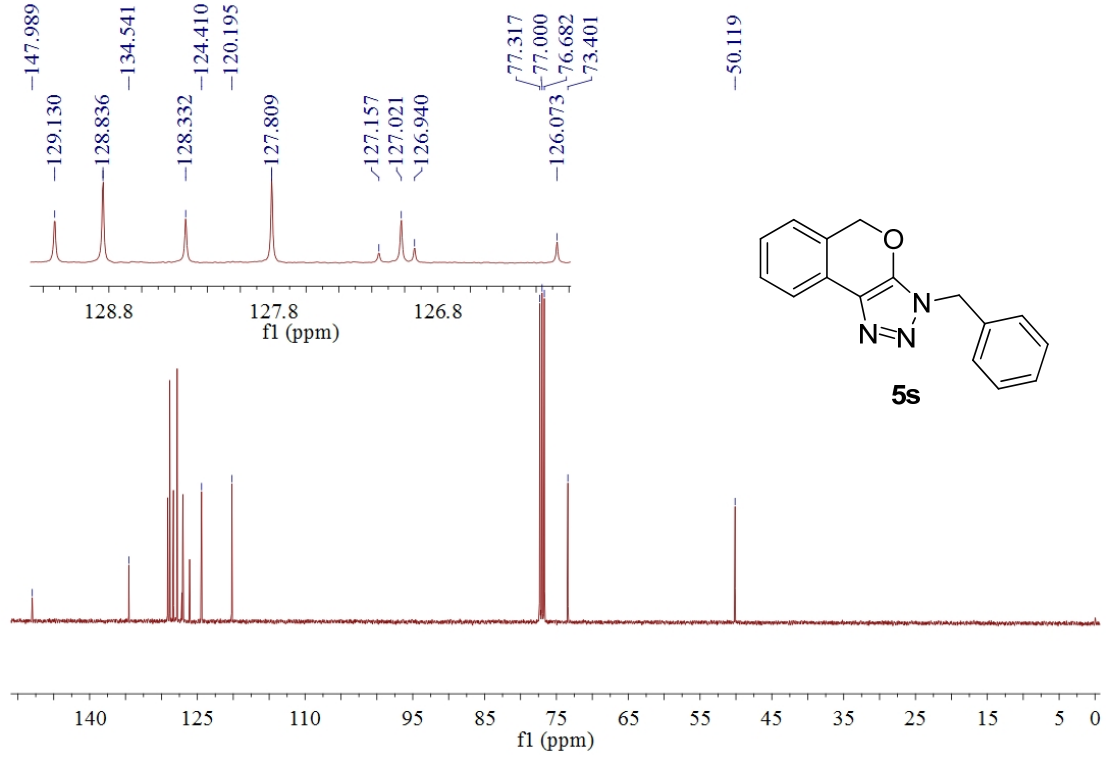

7.810
7.791
5.480
4.985
4.294
4.276
4.258
4.240
7.397
7.378
7.359
7.247
7.228
7.209
7.118
7.099
1.312
1.295
1.277
O
N
N=N
OEt
O
5p
1.00
2.00
3.00
fl (ppm)

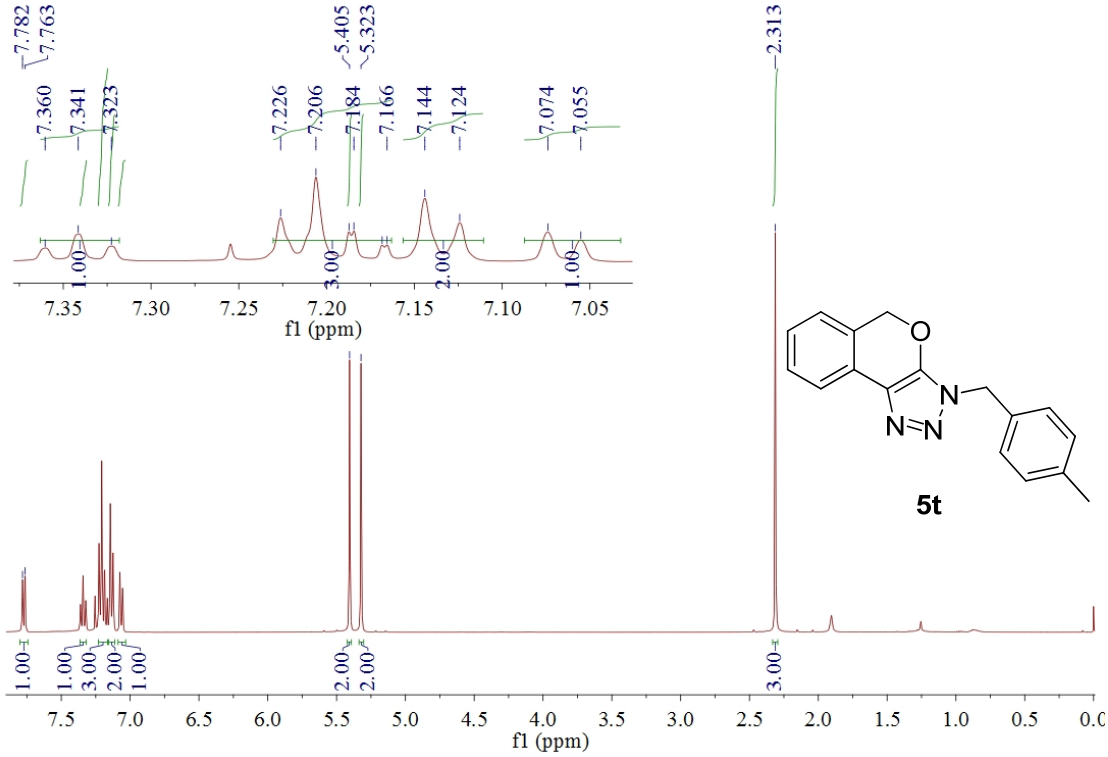

165.784
148.697
129.184
127.147
126.920
126.795
126.030
124.429
120.283
77.318
77.000
76.683
73.618
62.312
47.155
14.042
O
N
N=N
OEt
O
5p
fl (ppm)

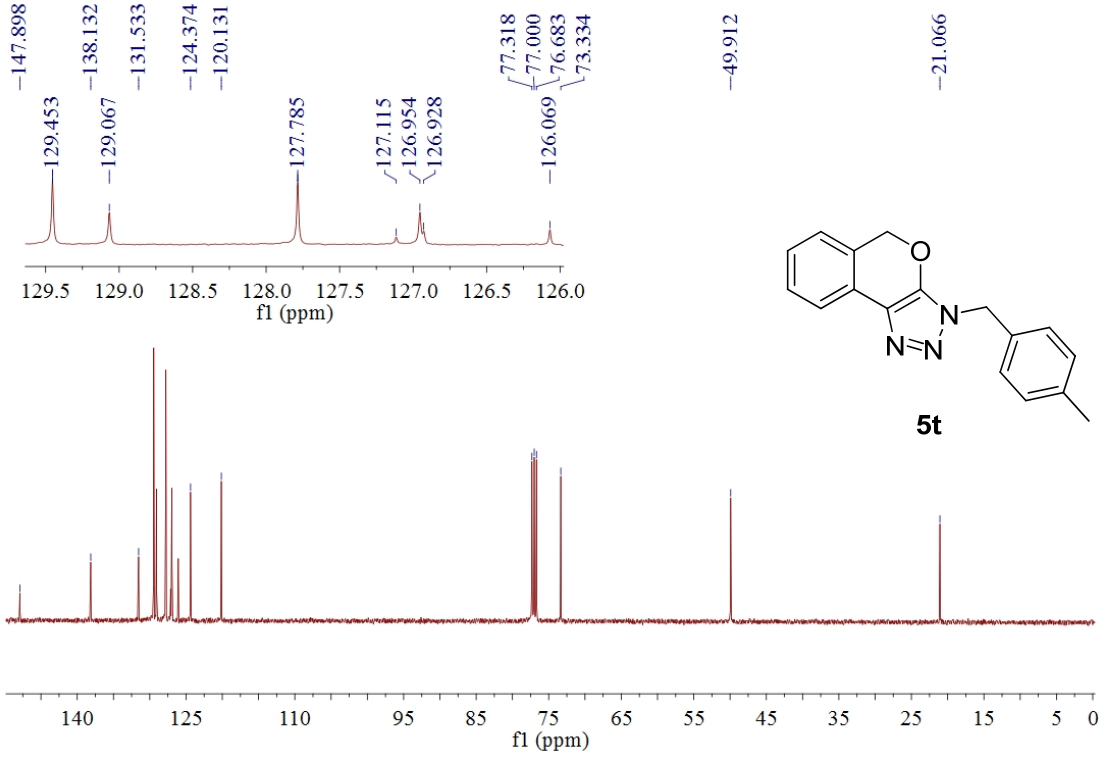

8.147
7.776
7.757
7.576
7.556
7.360
7.340
7.323
7.186
7.182
7.179
7.169
7.166
7.163
7.138
7.120
7.103
7.101
7.037
7.018
6.947
6.944
5.105
4.499
4.481
4.462
3.381
3.364
3.346
2.00
2.00
1.00
1.00
1.00
7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95
f1 (ppm)
O
N
N=N
NH
5r
1.00
1.00
1.00
2.00
2.00
1.00
1.00
2.00
2.00
2.00
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)

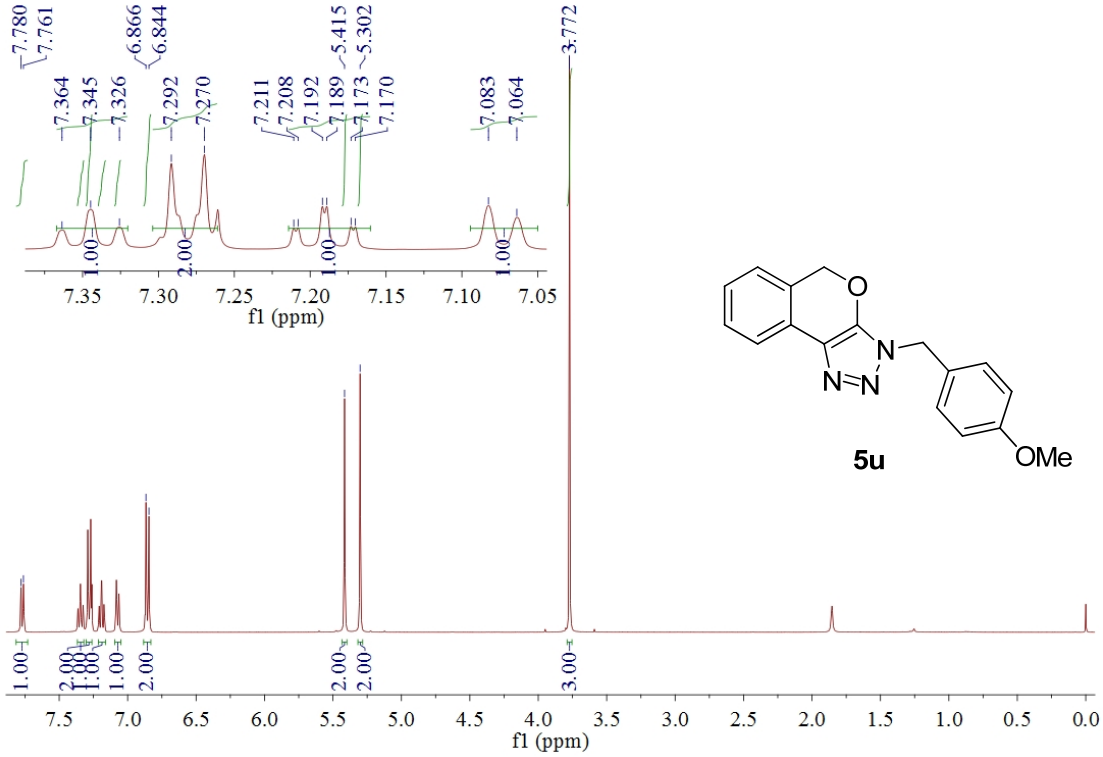

148.301
136.176
129.072
127.039
126.999
126.898
126.237
111.339
111.204
124.384
122.448
122.131
120.157
119.534
118.365
77.318
77.000
76.683
73.054
46.915
25.591
129 127 125 123 121 119
f1 (ppm)
O
N
N=N
NH
5r
140 125 110 95 85 75 65 55 45 35 25 15 5 0
f1 (ppm)

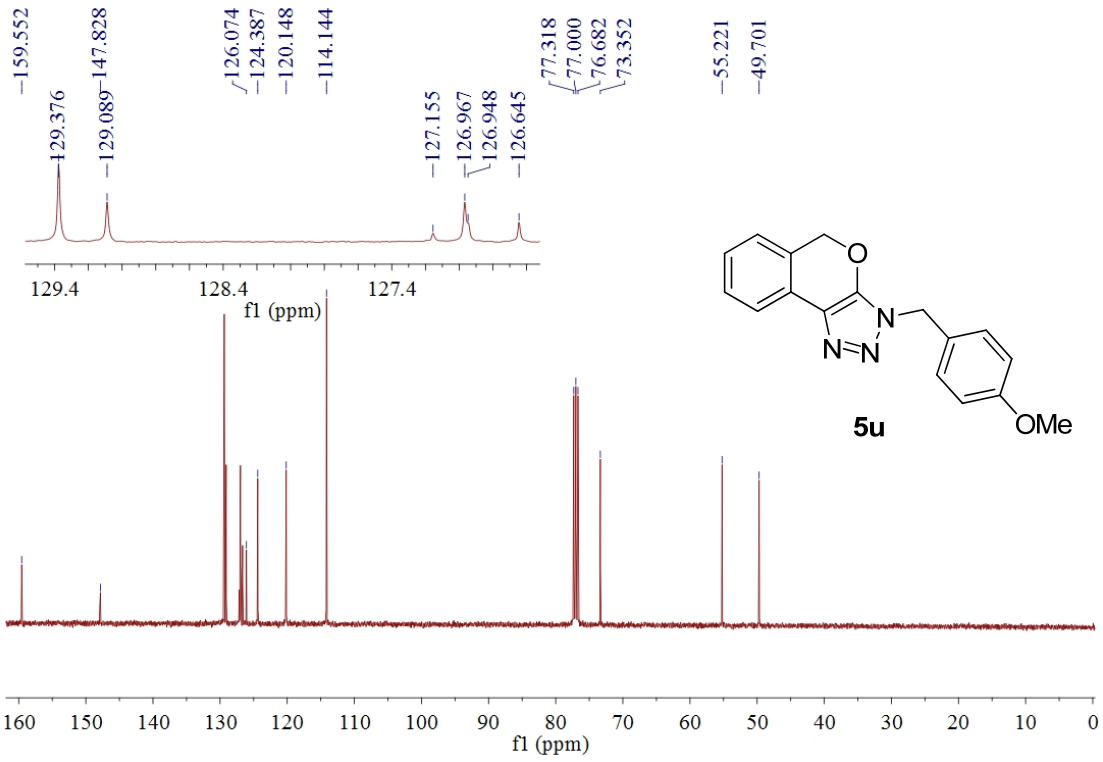

7.792
7.774
7.371
7.351
7.326
7.299
7.257
5.419
5.372
7.217
7.214
7.198
7.196
7.179
7.177
7.086
7.067
5.95
0.99
0.98
f1 (ppm)
0.96
5.95
0.99
0.98
2.00
2.01
f1 (ppm)
O
N
N=N
5s

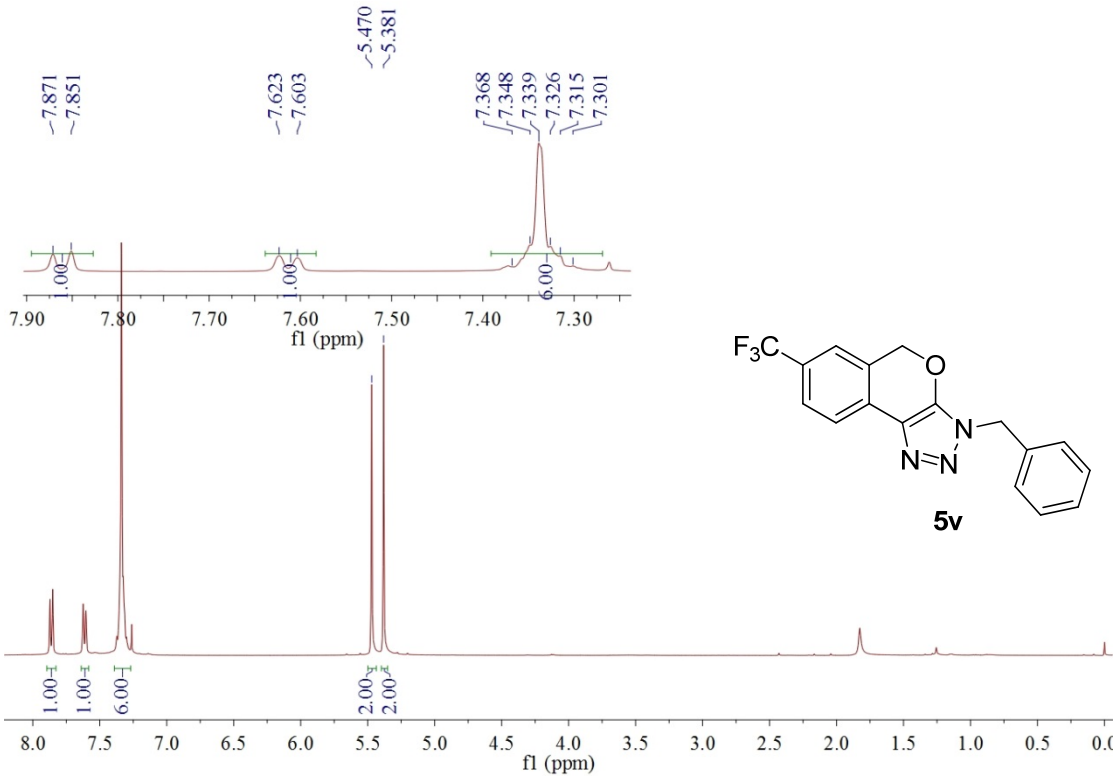

147.989
129.130
128.836
134.541
124.410
128.332
120.195
127.809
127.157
127.021
126.940
77.317
77.000
76.682
73.401
126.073
50.119
f1 (ppm)
f1 (ppm)
O
N
N=N
5s


7.782
7.763
7.360
7.341
7.323
7.226
7.206
7.184
7.166
7.144
7.124
7.074
7.055
5.405
5.323
2.313
1.00
3.00
2.00
1.00
f1 (ppm)
O
N
N=N
5t


147.898
138.132
131.533
124.374
120.131
129.453
129.067
127.785
127.115
126.954
126.928
126.069
77.318
77.000
76.683
73.334
49.912
21.066
f1 (ppm)
O
N
N=N
5t

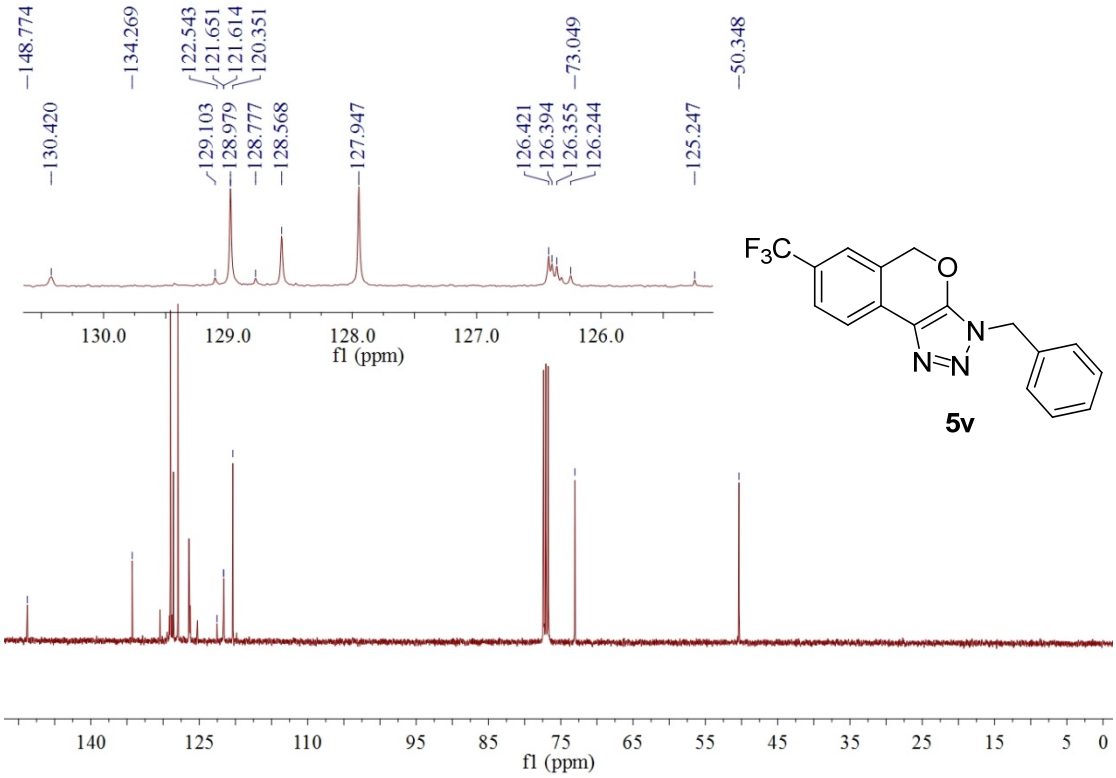

7.780
7.761
6.866
6.844
5.415
5.302
3.772
7.364
7.345
7.326
7.292
7.270
7.211
7.208
7.192
7.189
7.173
7.170
7.083
7.064
1.00
2.00
1.00
1.00
7.35
7.30
7.25
7.20
7.15
7.10
7.05
f1 (ppm)
O
N
N=N
OMe
5u
1.00
2.00
1.00
1.00
2.00
2.00
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


159.552
147.828
129.376
129.089
126.074
124.387
120.148
114.144
127.155
126.967
126.948
126.645
77.318
77.000
76.682
73.352
55.221
49.701
129.4
128.4
127.4
f1 (ppm)
O
N
N=N
OMe
5u
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.871
7.851
7.623
7.603
5.470
5.381
7.368
7.348
7.339
7.326
7.315
7.301
1.00
1.00
6.00
fl (ppm)
1.00
1.00
6.00
2.00
2.00
fl (ppm)

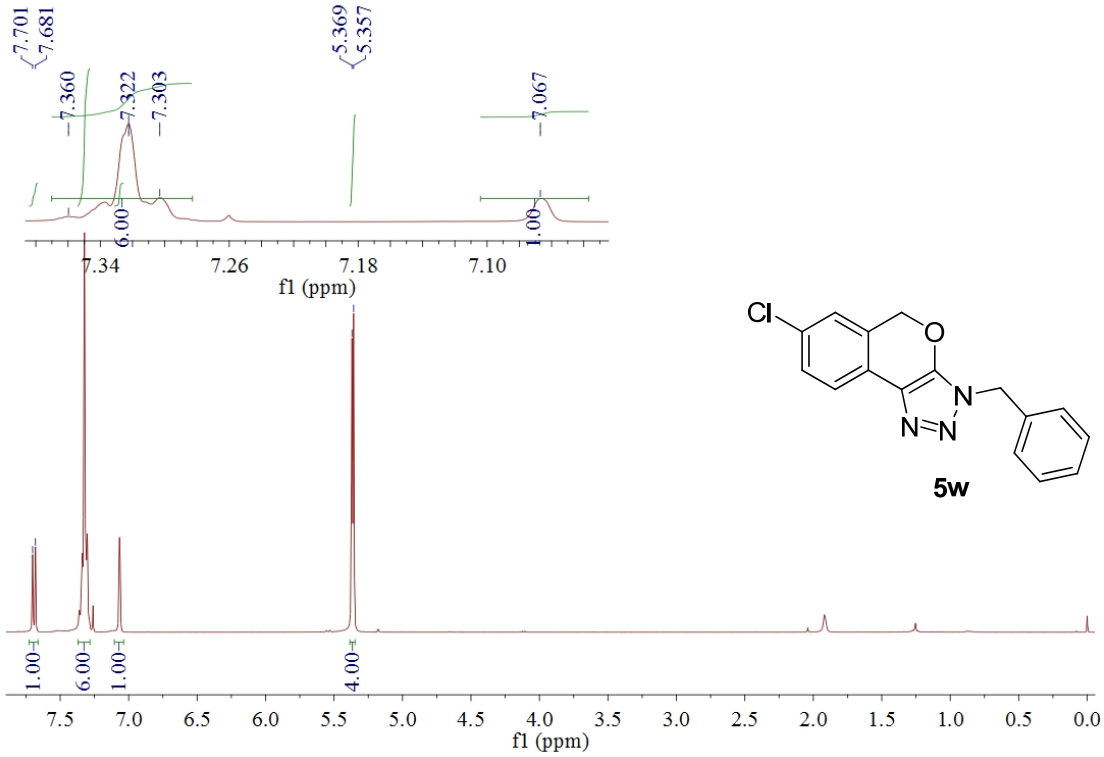

F3C
O
N
N=N

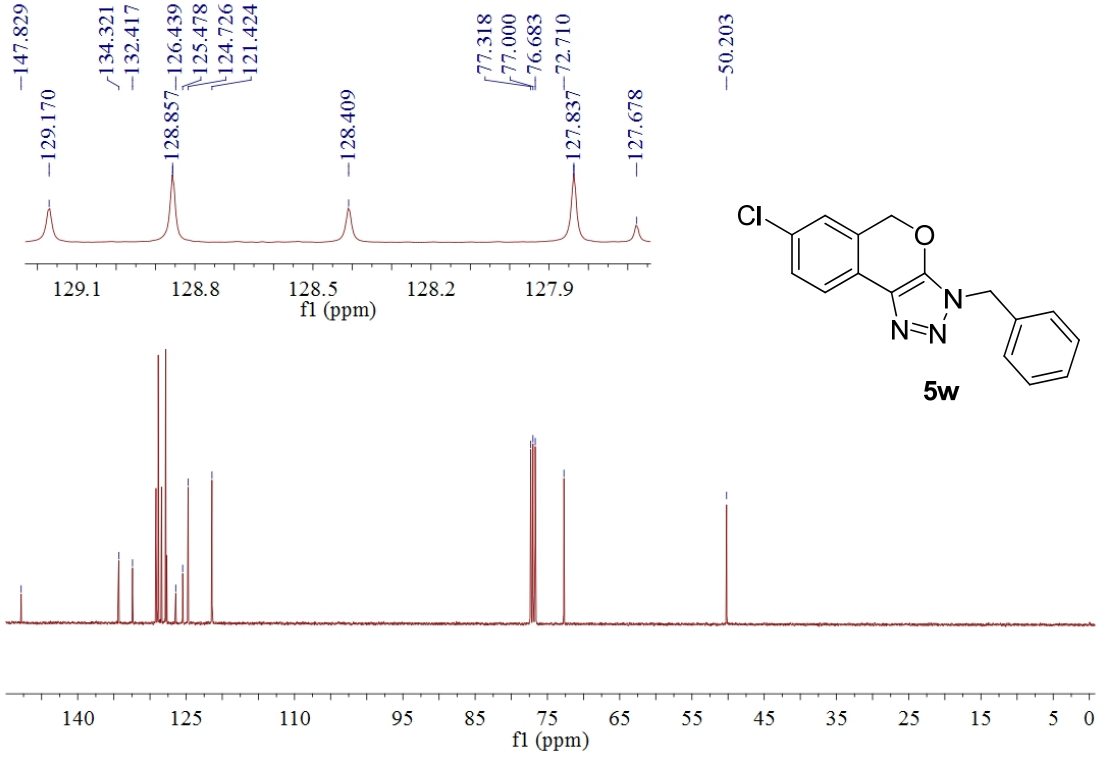
**5v**

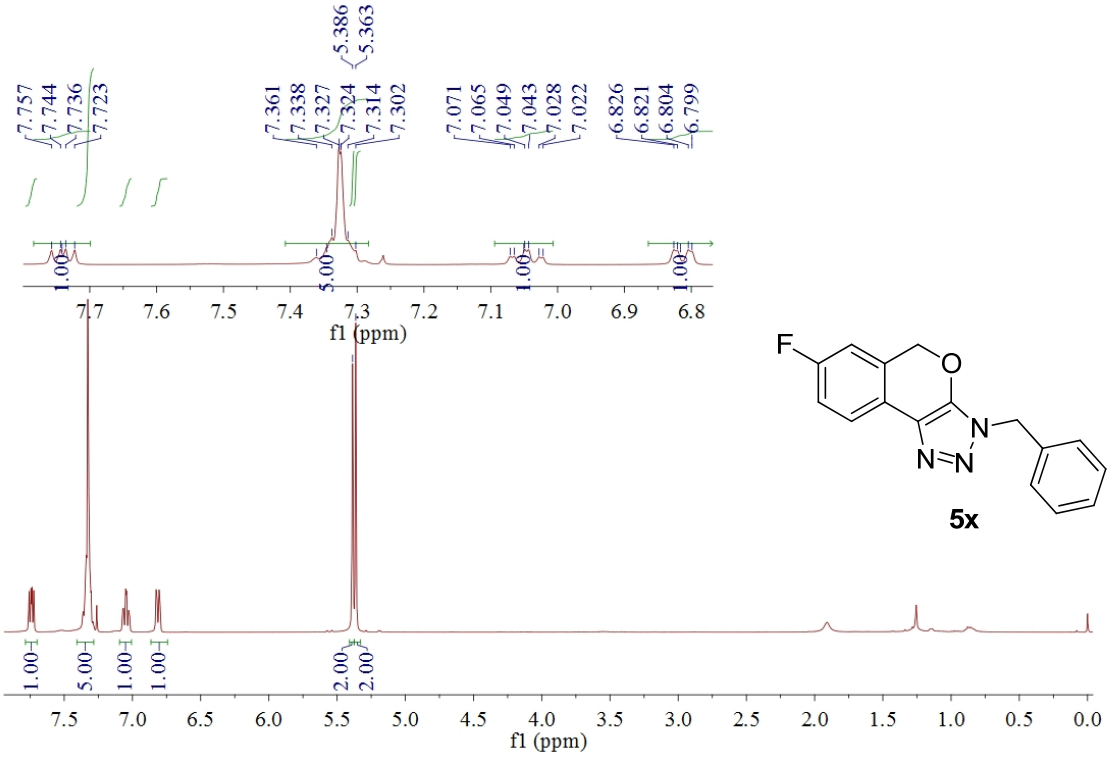

148.774
134.269
122.543
121.651
121.614
120.351
73.049
50.348
130.420
129.103
128.979
128.777
128.568
127.947
126.421
126.394
126.355
126.244
125.247
130.0
129.0
128.0
127.0
126.0
fl (ppm)
140
125
110
95
85
75
65
55
45
35
25
15
5
0
fl (ppm)

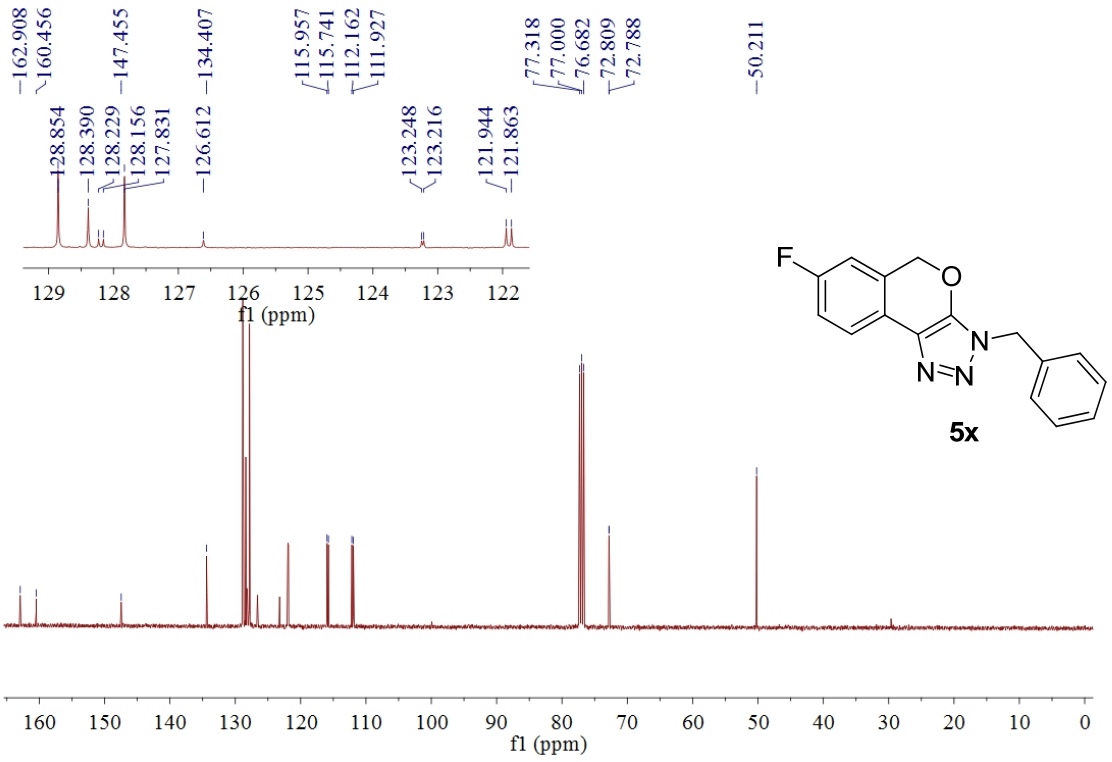

F3C
O
N
N=N

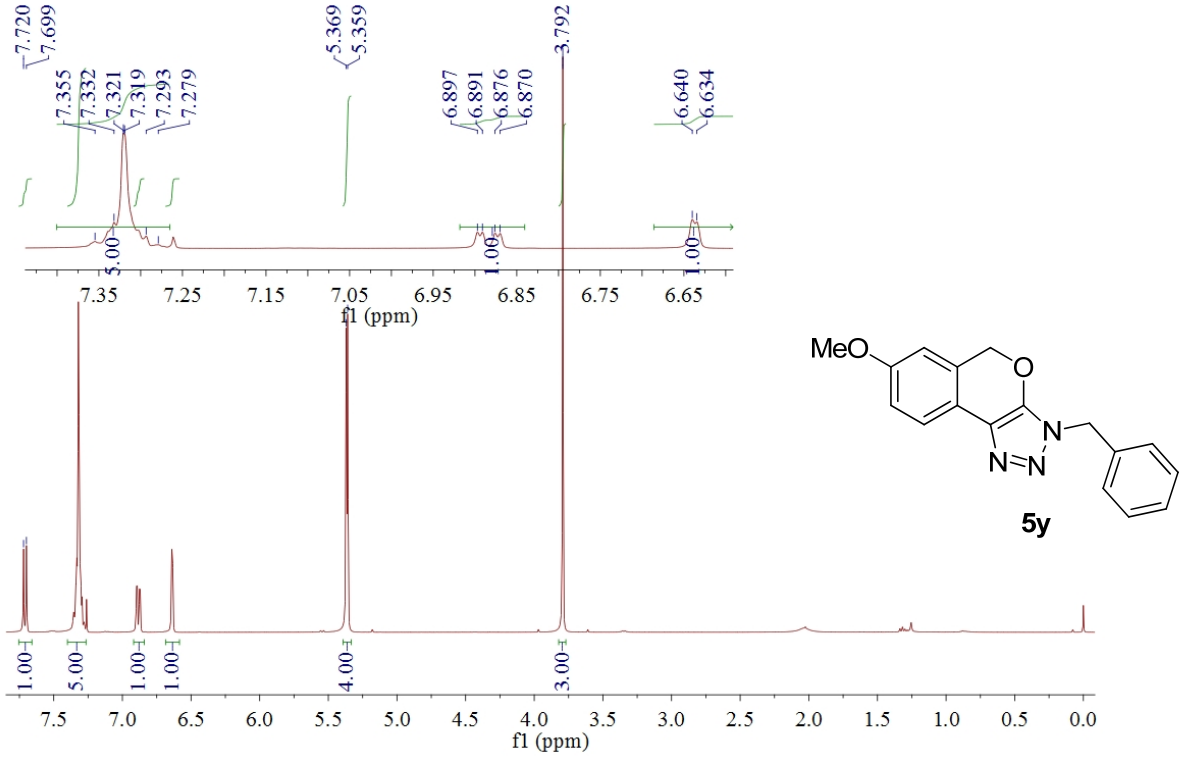
**5v**

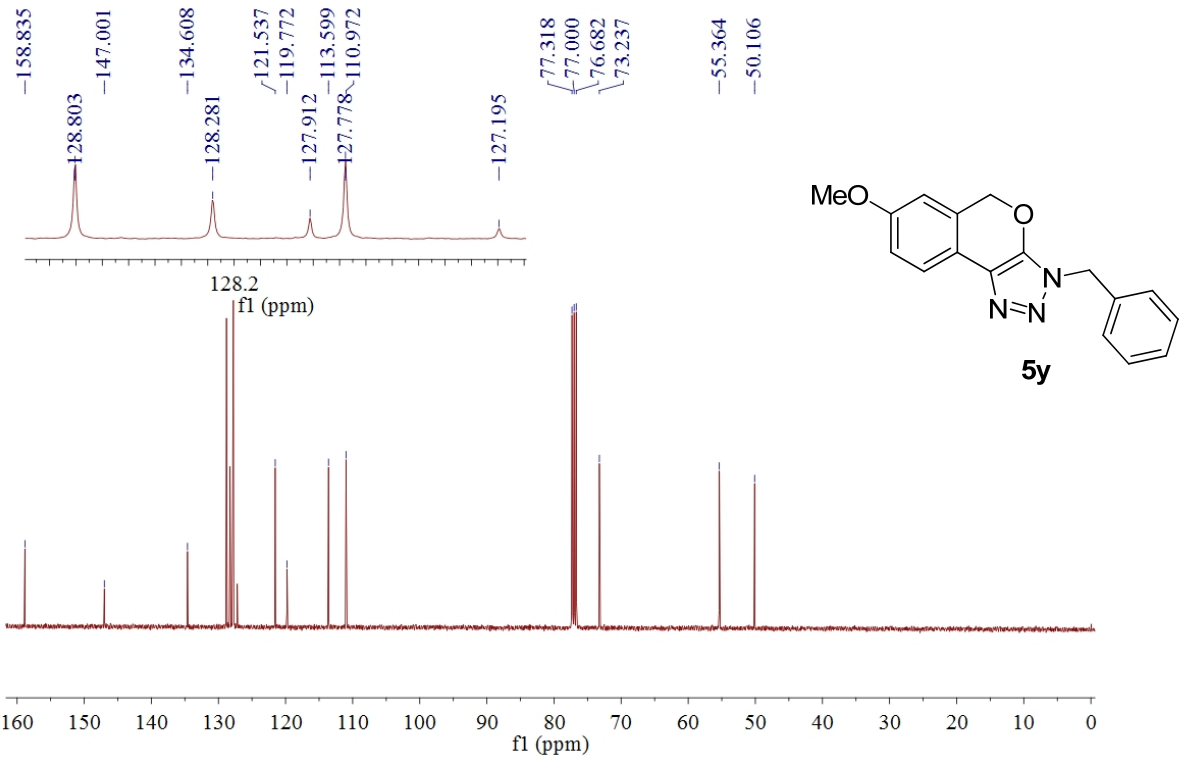

7.701
7.681
7.360
7.322
7.303
5.369
5.357
7.067
6.00
1.00
7.34
7.26
7.18
7.10
f1 (ppm)
Cl
O
N
N=N
5w
1.00
6.00
1.00
4.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

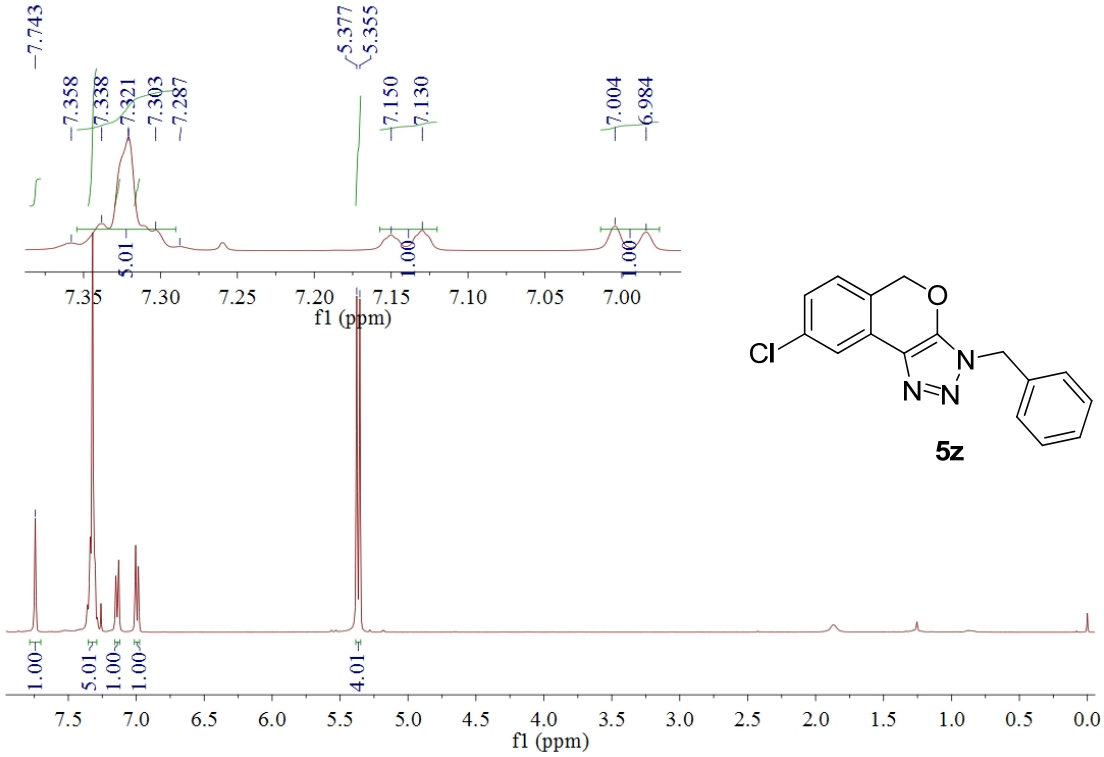

147.829
134.321
132.417
126.439
125.478
124.726
121.424
129.170
128.857
128.409
77.318
77.000
76.683
72.710
127.837
127.678
50.203
129.1
128.8
128.5
128.2
127.9
f1 (ppm)
Cl
O
N
N=N
5w
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)

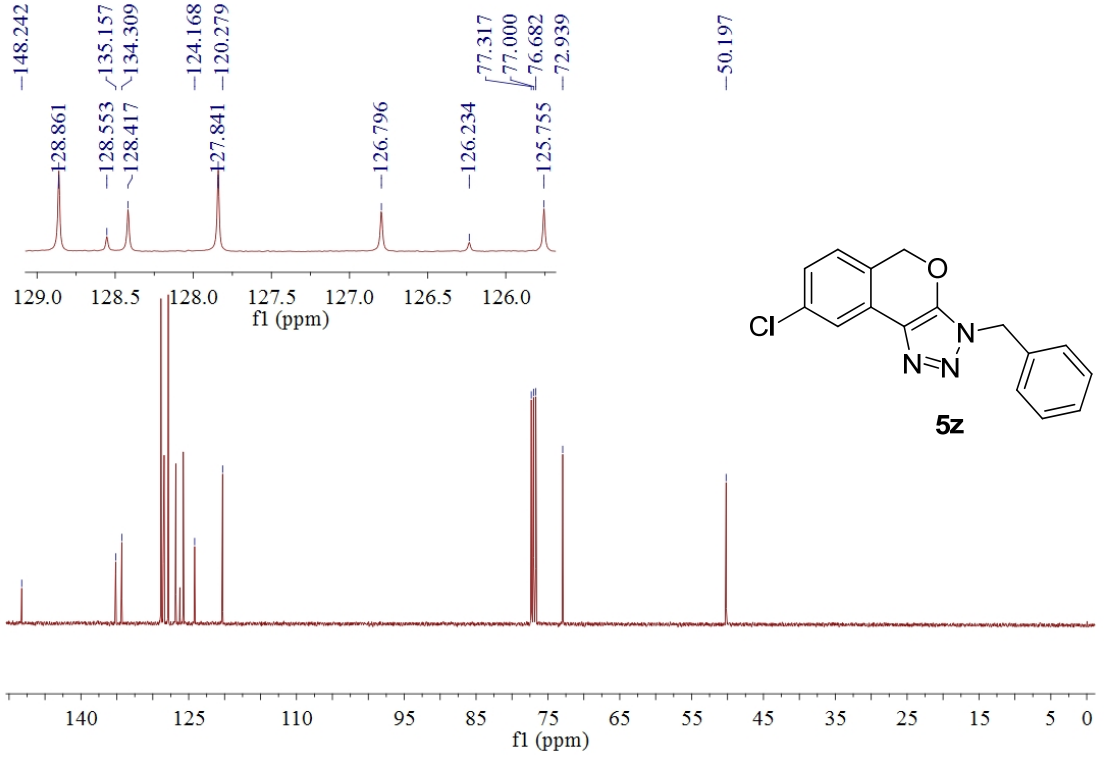

7.757
7.744
7.736
7.723
7.361
7.338
7.327
7.324
7.314
7.302
5.386
5.363
7.071
7.065
7.049
7.043
7.028
7.022
6.826
6.821
6.804
6.799
1.00
5.00
1.00
1.00
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
f1 (ppm)
F
O
N
N=N
5x
1.00
5.00
1.00
1.00
2.00
2.00
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

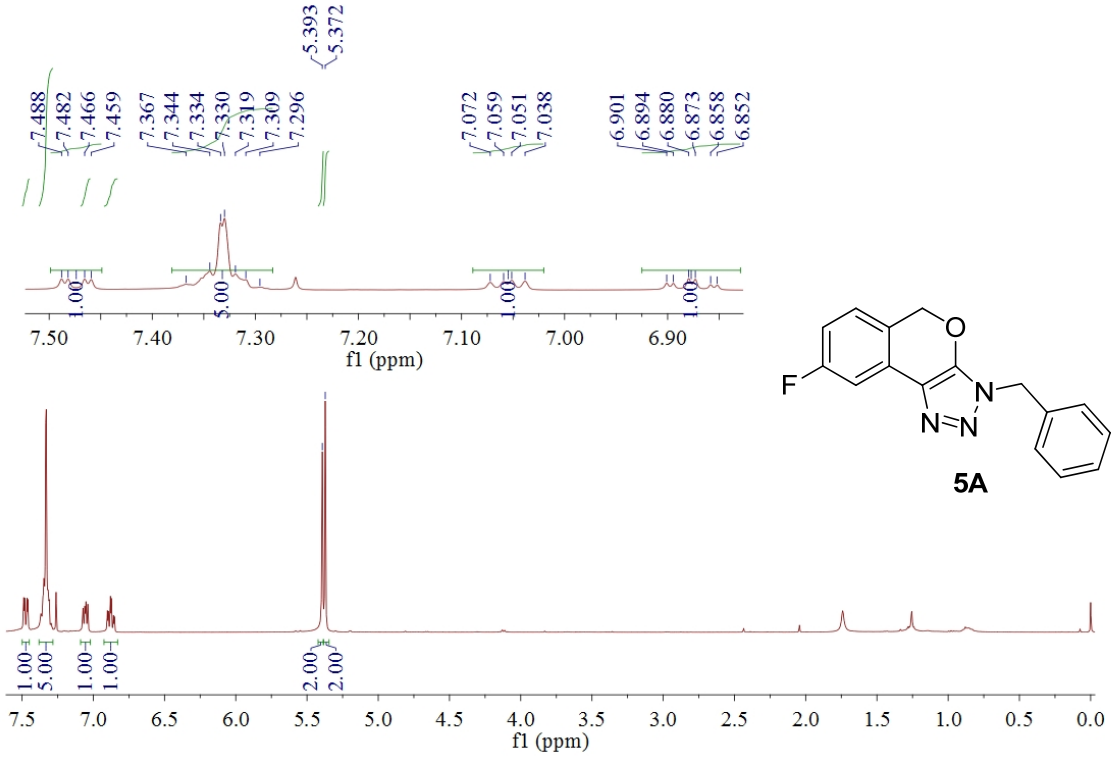

162.908
160.456
147.455
134.407
115.957
115.741
112.162
111.927
77.318
77.000
76.682
72.809
72.788
50.211
128.854
128.390
128.229
128.156
127.831
126.612
123.248
123.216
121.944
121.863
129 128 127 126 125 124 123 122
f1 (ppm)
F
O
N
N=N
5x
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

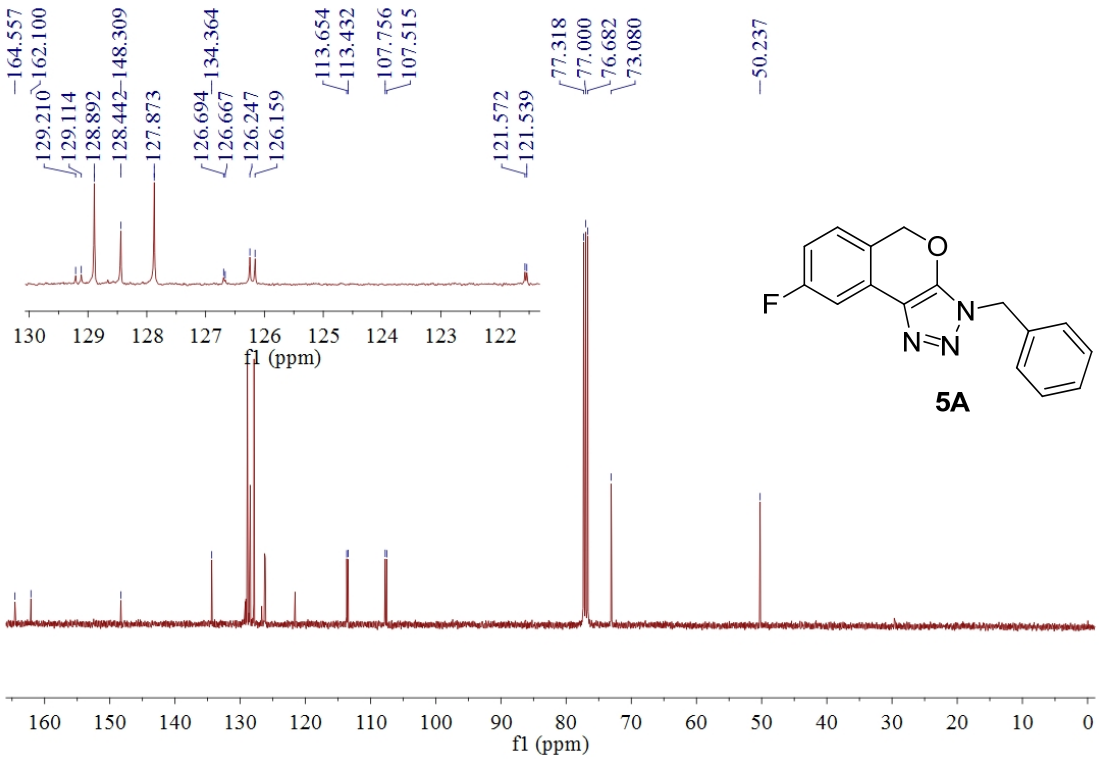

7.720
7.699
7.355
7.332
7.321
7.319
7.293
7.279
5.369
5.359
6.897
6.891
6.876
6.870
3.792
6.640
6.634
5.00
1.00
1.00
7.35
7.25
7.15
7.05
6.95
6.85
6.75
6.65
f1 (ppm)
MeO
O
N
N=N
5y
1.00
5.00
1.00
1.00
4.00
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


158.835
147.001
134.608
121.537
119.772
113.599
110.972
128.803
128.281
127.912
127.778
127.195
77.318
77.000
76.682
73.237
55.364
50.106
128.2
f1 (ppm)
MeO
O
N
N=N
5y
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

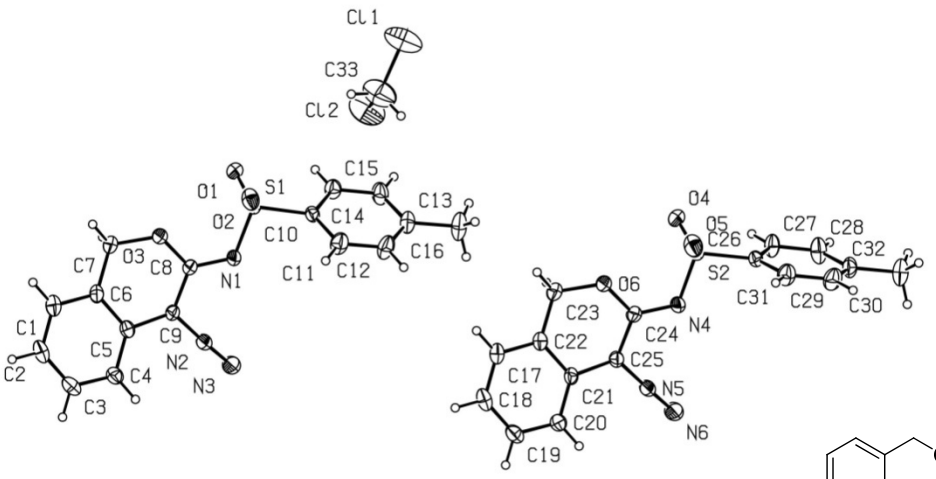

7.743
7.358
7.338
7.321
7.303
7.287
5.377
5.355
7.150
7.130
7.004
6.984
5.01
1.00
1.00
f1 (ppm)
1.00
5.01
1.00
1.00
4.01
f1 (ppm)
Cl
O
N
N=N
5z

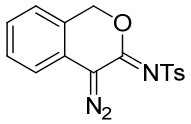

148.242
135.157
134.309
124.168
120.279
128.861
128.553
128.417
127.841
126.796
126.234
125.755
77.317
77.000
76.682
72.939
50.197
f1 (ppm)
f1 (ppm)
Cl
O
N
N=N
5z


5.393
5.372
7.488
7.482
7.466
7.459
7.367
7.344
7.334
7.330
7.319
7.309
7.296
7.072
7.059
7.051
7.038
6.901
6.894
6.880
6.873
6.858
6.852
1.00
5.00
1.00
1.00
7.50
7.40
7.30
7.20
7.10
7.00
6.90
f1 (ppm)
F
O
N
N=N
5A
1.00
5.00
1.00
1.00
2.00
2.00
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)


164.557
162.100
129.210
129.114
128.892
128.442
148.309
127.873
126.694
134.364
126.667
126.247
126.159
113.654
113.432
107.756
107.515
121.572
121.539
77.318
77.000
76.682
73.080
50.237
130
129
128
127
126
125
124
123
122
f1 (ppm)
F
O
N
N=N
5A
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

# The ORTEP diagram and Crystal Parameters of 3a




3a

## checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

## Datablock: 150312_ran6_71

---

```
Bond precision:  C-C = 0.0046 A          Wavelength=0.71073

Cell:          a=8.3200(6)       b=8.9410(5)       c=24.9526(17)
               alpha=83.367(5)   beta=81.578(6)    gamma=67.510(6)
Temperature:   293 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 1692.9(2) | 1692.94(19) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | 2(C16 H13 N3 O3 S), C H2 Cl2 | 2(C16 H13 N3 O3 S), C H2 Cl2 |
| Sum formula | C33 H28 Cl2 N6 O6 S2 | C33 H28 Cl2 N6 O6 S2 |
| Mr | 739.63 | 739.63 |
| Dx,g cm-3 | 1.451 | 1.451 |
| Z | 2 | 2 |
| Mu (mm-1) | 0.370 | 0.370 |
| F000 | 764.0 | 764.0 |
| F000' | 765.39 | |
| h,k,lmax | 10,10,30 | 10,10,30 |
| Nref | 6179 | 6156 |
| Tmin,Tmax | 0.837,0.918 | 0.858,1.000 |
| Tmin' | 0.837 | |

```
Correction method= # Reported T Limits: Tmin=0.858 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996          Theta(max)= 25.350

R(reflections)= 0.0580( 3927)     wR2(reflections)= 0.1815( 6156)

S = 1.027                 Npar= 444
```

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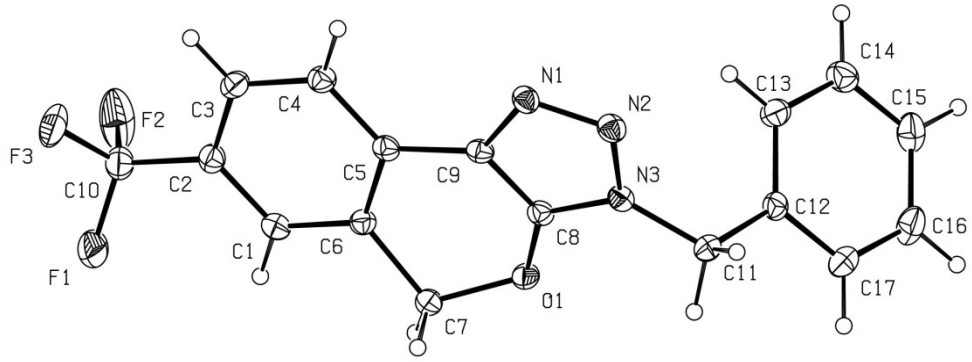
# The ORTEP diagram and Crystal Parameters of 5v




## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 160606_ran3_31_2

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

## Datablock: 160606_ran3_31_2

---

```
Bond precision:  C-C = 0.0040 A          Wavelength=0.71073

Cell:            a=8.6016(6)     b=27.4748(15)     c=6.1928(3)
                 alpha=90        beta=90           gamma=90
Temperature:     170 K

                 Calculated                Reported
Volume           1463.53(15)               1463.51(14)
Space group      P n a 21                  P n a 21
Hall group       P 2c -2n                  P 2c -2n
Moiety formula   C17 H12 F3 N3 O           C17 H12 F3 N3 O
Sum formula      C17 H12 F3 N3 O           C17 H12 F3 N3 O
Mr               331.30                    331.30
Dx,g cm-3        1.504                     1.504
Z                4                         4
Mu (mm-1)        0.123                     0.123
F000             680.0                     680.0
F000'            680.41
h,k,lmax         10,33,7                   10,33,7
Nref             2681[ 1475]               1470
Tmin,Tmax        0.950,0.970               0.953,1.000
Tmin'            0.950

Correction method= # Reported T Limits: Tmin=0.953 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.00/0.55      Theta(max)= 25.350

R(reflections)= 0.0331( 1362)     wR2(reflections)= 0.0812( 1470)

S = 1.036                 Npar= 217
```

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