Supporting Information

Palladium-Catalyzed Dehydrogenative Direct Arylations of 1,2,3-Triazoles

Lutz Ackermann,* Rajkumar Jeyachandran, Harish K. Potukuchi, Petr Novák, and Lea Büttner

Institut für Organische und Biomolekulare Chemie

Georg-August-Universitaet, Tammannstrasse 2, D-37077 (Germany)

Fax: +49/ 551-39-6777

http://www.org.chemie.uni-goettingen.de/ackermann/

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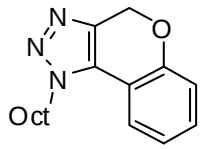
General remarks:

Ruthenium-catalyzed catalytic reactions were carried out under a N_2 atmosphere using pre-dried glassware. Chemicals were obtained from commercial sources, and were used without further purification. Toluene was dried over sodium. Yields refer to isolated compounds, estimated to be >95% pure as determined by ^{1}H-NMR and GC. Flash chromatography: Macherey-Nagel silica gel 60 (70-230 mesh). NMR: Spectra were recorded on Varian-NMR 300 and Varian-NMR 500 in the solvent indicated; chemical shifts (δ) are given in ppm.

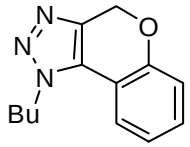
Representative Procedure A: Palladium-Catalyzed Dehydrogenative Direct Arylations of 1,2,3-Triazoles 1 (Table 1, entry 9):

$Pd(OAc)_2$ (11.2 mg, 0.05 mmol, 5.0 mol %), $Cu(OAc)_2{\cdot}H_2O$ (200 mg, 1.00 mmol), PivOH (500 mg, 4.90 mmol) and triazole **1a** (287 mg, 1.00 mmol) in dry toluene (3 mL) were stirred in a sealed tube at 140 °C for 20 h. H_2O (50 mL) was added at ambient temperature, and the resulting mixture was extracted with EtOAc (3 x 50 mL). The combined organic layers were washed with sat. aq. NH_4Cl (50 mL), H_2O (50 mL) and brine (50 mL), dried over Na_2SO_4, filtered and concentrated *in vacuo*. The remaining residue was purified by column chromatography on silica gel (*n*-hexane/EtOAc = 10/1 → 5/1) to yield **2a** (274 mg, 96%) as a yellow oil.



2a

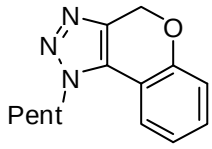
1-*n*-Octyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2a): ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.41 (dd, J = 8.0, 1.6 Hz, 1 H), 7.30–7.23 (m, 1 H), 7.08–7.01 (m, 2 H), 5.44 (s, 2 H), 4.58 (t, J = 7.4 Hz, 2 H), 2.02–1.88 (m, 2 H), 1.47–1.13 (m, 10 H), 0.85 (t, J = 6.9 Hz, 3 H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 153.6 (C_q), 139.4 (C_q), 130.4 (CH), 126.9 (C_q), 122.1 (CH), 122.0 (CH), 118.1 (CH), 114.2 (C_q), 64.5 (CH_2), 49.9 (CH_2), 31.7 (CH_2), 29.7 (CH_2), 29.0 (CH_2), 28.9 (CH_2), 26.5 (CH_2), 22.6 (CH_2), 14.1 (CH_3). IR (film): 2954, 2926, 2855, 1519, 1464, 1446, 1335, 1200, 1123, 1022, 839 cm^{-1}. MS (EI) *m/z* (relative intensity) 285 (100) [M^+], 269 (6), 228 (10), 214 (30), 158 (50), 145 (34), 103 (12), 77 (8), 55 (10), 43 (18), 41 (26). HR-MS (ESI) *m/z* calcd for $C_{17}H_{23}N_3O+H^+$ 286.1914, found 286.1915.



2b

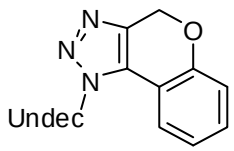
1-*n*-Butyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2b): The representative procedure A was followed, using 1-*n*-butyl-4-(phenoxymethyl)-1*H*-1,2,3-triazole (230 mg, 0.99 mmol). After 20 h, purification by column chromatography (*n*-hexane/EtOAc = 10/1 → 5/1) yielded **2b** (213 mg, 93%) as a yellow oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.42 (dd, J = 8.0, 1.8 Hz, 1 H), 7.30–7.23 (m, 1 H), 7.08–7.01 (m, 2 H), 5.44 (s, 2 H), 4.59 (t, J = 7.4 Hz, 2 H), 1.99–1.87 (m, 2 H), 1.52–1.36 (m, 2 H), 0.98 (t, J = 7.4 Hz, 3 H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 153.6 (C_q), 139.4 (C_q), 130.4 (CH), 126.9 (C_q), 122.1 (CH), 122.0 (CH), 118.1 (CH), 114.2 (C_q), 64.4 (CH_2), 49.6 (CH_2), 31.6 (CH_2), 19.7 (CH_2), 13.5 (CH_3). IR (film): 2961, 2872, 1619, 1559, 1520, 1460, 1336, 1201, 1124, 1022 cm^{-1}. MS (EI) *m/z* (relative intensity) 229

(74) [M^+], 186 (12), 172 (24), 158 (100), 145 (40), 144 (34), 130 (16), 118 (28), 103 (32), 89 (24), 77 (26), 63 (12), 51 (8), 41 (28). HR-MS (ESI) *m/z* calcd for $C_{13}H_{15}N_3O+H^+$ 230.1288, found 230.1287.



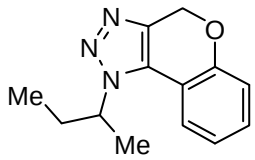
2c

1-*n*-Pentyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2c): The representative procedure A was followed, using 1-*n*-pentyl-4-(phenoxymethyl)-1*H*-1,2,3-triazole (245 mg, 1.00 mmol). After 20 h, purification by column chromatography (*n*-hexane/EtOAc = 10/1 → 5/1) yielded **2c** (213 mg, 88%) as a yellow oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.42 (dd, J = 8.0, 1.6 Hz, 1 H), 7.31–7.23 (m, 1 H), 7.10–7.01 (m, 2 H), 5.45 (s, 2 H), 4.60 (t, J = 7.1 Hz, 2 H), 2.02–1.90 (m, 2 H), 1.47–1.30 (m, 4 H), 0.91 (t, J = 6.9 Hz, 3 H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 153.6 (C_q), 139.4 (C_q), 130.4 (CH), 126.9 (C_q), 122.1 (CH), 122.0 (CH), 118.1 (CH), 114.2 (C_q), 64.5 (CH_2), 49.9 (CH_2), 29.4 (CH_2), 28.6 (CH_2), 22.1 (CH_2), 13.8 (CH_3). IR (film): 3064, 2961, 2872, 2726, 1708, 1617, 1560, 1371, 1299, 840 cm^{-1}. MS (EI) *m/z* (relative intensity) 243 (60) [M^+], 214 (18), 186 (29), 172 (52), 158 (100), 145 (76), 131 (20), 118 (38), 103 (26), 89 (21), 77 (23), 43 (46). HR-MS (ESI) *m/z* calcd for $C_{14}H_{17}N_3O+Na^+$ 266.1264, found 266.1267.



2d

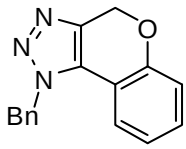
1-*n*-Undecyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2d): The representative procedure A was followed, using 4-(phenoxymethyl)-1-*n*-undecyl-1*H*-1,2,3-triazole (329 mg, 1.00 mmol). After 20 h, purification by column chromatography (*n*-hexane/EtOAc = 10/1 → 5/1) yielded **2d** (266 mg, 81%) as a brown solid. m.p.: 40 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.42 (dd, J = 8.0, 1.6 Hz, 1 H), 7.31–7.23 (m, 1 H), 7.09–7.01 (m, 2 H), 5.45 (s, 2 H), 4.60 (t, J = 7.6 Hz, 2 H), 2.02–1.88 (m, 2 H), 1.48–1.02 (m, 16 H), 0.87 (t, J = 6.7 Hz, 3 H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 153.7 (C_q), 139.4 (C_q), 130.4 (CH), 126.9 (C_q), 122.1 (CH), 122.0 (CH), 118.1 (CH), 114.3 (C_q), 64.5 (CH_2), 49.9 (CH_2), 31.9 (CH_2), 29.7 (CH_2), 29.5 (CH_2), 29.5 (CH_2), 29.4 (CH_2), 29.3 (CH_2), 29.0 (CH_2), 26.5 (CH_2), 22.6 (CH_2), 14.1 (CH_3). IR (KBr): 3051, 1618, 1559, 1520, 1464, 1447, 1404, 1376, 1264, 1201, 1124, 1039, 992, 842 cm^{-1}. MS (EI) *m/z* (relative intensity) 327 (100) [M^{+}], 311 (6), 228 (8), 220 (14), 214 (28), 186 (44), 158 (30), 145 (24), 103 (4), 43 (6). HR-MS (ESI) *m/z* calcd for $C_{20}H_{29}N_3O$+H^{+} 328.2383, found 328.2383.



2e

1-*sec*-Butyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2e): The representative procedure A was followed, using 1-*sec*-butyl-4-(phenoxymethyl)-1*H*-1,2,3-triazole

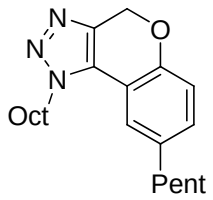
(231 mg, 1.00 mmol). After 20 h, purification by column chromatography (*n*-hexane/EtOAc = 10/1 → 5/1) yielded **2e** (130 mg, 57%) as a yellow oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.48 (dd, J = 1.5, 8.2 Hz, 1 H), 7.27 (t, J = 7.8 Hz, 1 H), 7.09–7.01 (m, 2 H), 5.42 (d, J = 2.3 Hz, 2 H), 4.79–4.70 (m, 1 H), 2.32–2.17 (m, 1 H), 2.09–1.92 (m, 1 H), 1.71 (d, J = 6.7 Hz, 3 H), 0.93 (t, J = 7.4 Hz, 3 H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 153.7 (C_q), 139.1 (C_q), 130.2 (CH), 127.0 (C_q), 122.1 (CH), 122.0 (CH), 118.2 (CH), 114.6 (C_q), 64.3 (CH_2), 58.2 (CH), 29.5 (CH_2), 20.5 (CH_3), 10.5 (CH_3). IR (film): 2974, 2871, 1766, 1712, 1614, 1508, 1382, 1205, 1023, 759 cm^{-1}. MS (EI) *m/z* (relative intensity) 229 (52) [M^+], 186 (10), 172 (100), 145 (58), 118 (32), 116 (16), 102 (20), 89 (22), 77 (16), 63 (12), 57 (26), 41 (48). HR-MS (ESI) *m/z* calcd for $C_{13}H_{15}N_3O+H^+$ 230.1288, found 230.1292.



2f

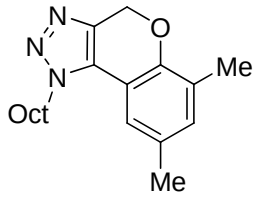
1-Benzyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2f): The representative procedure A was followed, using 1-benzyl-4-(phenoxymethyl)-1*H*-1,2,3-triazole (265 mg, 1.00 mmol). After 20 h, purification by column chromatography (*n*-hexane/EtOAc = 10/1 → 5/1) yielded **2f** (158 mg, 60%) as a white solid. m.p.: 143-144 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.41–7.14 (m, 7 H), 7.04–6.97 (m, 1 H), 6.96–6.84 (m, 1 H), 5.82 (s, 2 H), 5.48 (s, 2 H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 153.6 (C_q), 139.7 (C_q), 134.6 (C_q), 130.5 (CH), 129.1 (CH), 128.3 (CH), 127.7 (C_q), 126.4 (CH), 122.5 (CH), 122.0 (CH), 117.9 (CH), 113.8 (C_q), 64.4 (CH_2), 53.0 (CH_2). IR (KBr): 2725, 2361, 1699, 1653, 1617, 1558, 1337, 1197, 1110, 1024, 848,

768 cm^{-1}. MS (EI) *m/z* (relative intensity) 263 (14) [M^+], 234 (8), 91 (100), 65 (16), 57 (8), 43 (6), 41 (6). HR-MS (ESI) *m/z* calcd for $C_{16}H_{13}N_3O+Na^+$ 286.0951, found 286.0953.



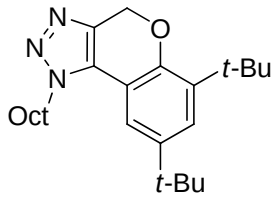
2g

1-*n*-Octyl-8-pentyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2g): The representative procedure A was followed, using 1-*n*-octyl-4-((4-pentylphenoxy)methyl)-1*H*-1,2,3-triazole (366 mg, 1.02 mmol). After 20 h, purification by chromatography (*n*-hexane/EtOAc = 10/1 → 5/1 → 3/1) yielded **2g** (307 mg, 85%) as a yellow oil. ^{1}H-NMR (300 Hz, $CDCl_3$) δ = 7.21 (d, J = 1.7 Hz, 1H), 7.08 (dd, J = 8.3, 1.7 Hz, 1H), 6.96 (d, J = 8.3 Hz, 1H), 5.40 (s, 2H), 4.59 (t, J = 7.3 Hz, 2H), 2.59 (t, J = 7.3 Hz, 2H), 2.05 – 1.86 (m, 2H), 1.68 – 1.52 (m, 2H), 1.51 – 1.15 (m, 14H), 0.94 – 0.83 (m, 6H). ^{13}C-NMR (75 MHz, $CDCl_3$) δ = 151.6 (C_q), 139.6 (C_q), 136.6 (C_q), 130.0 (CH), 127.2 (C_q), 121.8 (CH), 117.8 (CH), 114.0 (C_q), 64.4 (CH_2), 49.9 (CH_2), 35.2 (CH_2), 31.7 (CH_2), 31.3 (CH_2), 31.2 (CH_2), 29.7 (CH_2), 29.1 (CH_2), 29.0 (CH_2), 26.5 (CH_2), 22.6 (CH_2), 22.5 (CH_2), 14.0 (CH_3), 14.0 (CH_3). IR (film): 2925, 2859, 2360, 1519, 1460, 1330, 1200, 1132, 1003, 829 cm^{-1}. MS (EI) *m/z* (relative intensity) 355 (17) [M^+], 284 (22), 270 (22), 228 (33), 186 (22), 172 (23), 158 (100), 131 (25), 115 (36), 55 (36), 41 (93). HR-MS (ESI): *m/z* calcd for $C_{22}H_{33}N_3O+H^+$ 356.2696, found 356.2694.



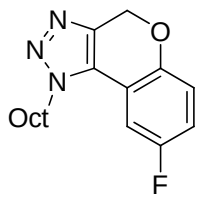
2h

6,8-Dimethyl-1-*n*-octyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2h): The representative procedure A was followed, using 4-{(2,4-dimethylphenoxy)methyl}-1-*n*-octyl-1*H*-1,2,3-triazole (315 mg, 1.00 mmol). After 20 h, purification by chromatography (*n*-hexane/EtOAc = 10/1 → 5/1) yielded **2h** (291 mg, 93%) as a yellow solid. m.p.: 55-57 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ = 7.05 (s, 1H), 6.96 (s, 1H), 5.40 (s, 2H), 4.57 (t, J = 7.4 Hz, 2H), 2.30 (s, 3H), 2.21 (s, 3H), 1.99 – 1.90 (m, 2H), 1.43 – 1.19 (m, 10H), 0.86 (m, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 149.5 (C_q), 139.6 (C_q), 132.6 (CH), 130.7 (C_q), 127.4 (C_q), 127.3 (C_q), 120.0 (CH), 113.5 (C_q), 64.2 (CH_2), 49.7 (CH_2), 31.6 (CH_2), 29.6 (CH_2), 29.0 (CH_2), 28.9 (CH_2), 26.4 (CH_2), 22.5 (CH_2), 20.8 (CH_3), 16.3 (CH_3), 14.0 (CH_3). IR (film): 2926, 2361, 2338, 1762, 1652, 1558, 1457, 1329, 1265, 1190, 1126, 1008, 860, 737 cm^{-1}. MS (EI) *m/z* (relative intensity) 313 (37) [M^{+}], 242 (26), 228 (19), 214 (19), 200 (33), 186 (58), 173 (100), 115 (19), 91 (15), 55 (21), 41 (45). HR-MS (ESI): *m/z* calcd for $C_{19}H_{27}N_3O$+Na^{+} 336.2046, found 336.2039.



2i

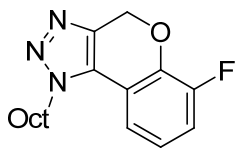
6,8-Di-*tert*-butyl-1-*n*-octyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2i): The representative procedure A was followed, using 4-((2,4-di-tert-butylphenoxy)methyl)-1-octyl-1*H*-1,2,3-triazole (400 mg, 1.00 mmol). After 20 h, purification by chromatography (*n*-hexane/EtOAc = 10/1 → 5/1 → 3/1) yielded **2i** (214 mg, 54%) as a yellow oil. ^{1}H-NMR (300 Hz, $CDCl_3$) δ = 7.34 (dd, J = 5.7, 2.3 Hz, 2H), 5.37 (s, 2H), 4.60 (t, J = 7.6 Hz, 2H), 2.03 – 1.88 (m, 2H), 1.50 – 1.18 (m, 10H), 1.41 (s, 9 H), 1.35 (s, 9H), 0.91 – 0.80 (m, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$) δ = 149.7 (C_q), 144.1 (C_q), 139.8 (C_q), 139.2 (C_q), 128.0 (C_q), 125.0 (CH), 117.0 (CH), 114.7 (C_q), 63.4 (2 C_q), 63.4 (C_q), 63.4 (C_q), 50.0 (CH_2), 35.2 (CH_2), 34.5 (CH_2), 31.6 (CH_2), 31.4 (CH_3), 29.9 (CH_2), 29.8 (CH_3), 29.1 (CH_2), 26.7 (CH_2), 22.5 (CH_2), 14.0 (CH_3). IR (film): 2957, 2861, 1770, 1702, 1466, 1364, 1198, 1098, 1004, 868 cm^{-1}. MS (EI) *m/z* (relative intensity) 397 (34) [M^{+}], 354 (17), 326 (33), 298 (12), 270 (31), 242 (92), 214 (13), 57 (100), 41 (66). HRMS (ESI): *m/z* calcd for $C_{25}H_{39}N_3O$+Na^{+} 420.2985, found 420.2975.



2j

8-Fluoro-1-*n*-octyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2j): The representative procedure A was followed, using 4-{(4-fluorophenoxy)methyl}-1-octyl-1*H*-1,2,3-triazole (307 mg, 1.00 mmol). After 20 h, purification by chromatography (*n*-hexane/EtOAc = 10/1 → 5/1 → 3/1) yielded **2j** (212 mg, 70%) as a yellow solid. m.p. = 41 °C. ^{1}H-NMR (300 Hz, $CDCl_3$) δ = 7.08 (ddd, J = 8.6, 2.6,

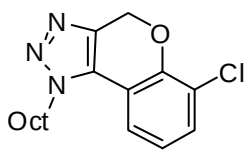
0.7 Hz, 1H), 7.04 – 6.92 (m, 2H), 5.41 (s, 2H), 4.56 (t, J = 7.5 Hz, 2H), 2.01-1.88 (m, 2H), 1.46 – 1.18 (m, 10H), 0.84 (t, J = 6.9 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$) δ = 157.6 (C_q, $^1J_{C\text{-}F}$ = 241 Hz), 149.5 (C_q), 140.0 (C_q), 126.5 (C_q), 119.2 (CH, $^2J_{C\text{-}F}$ = 8.3 Hz), 116.6 (CH, $^3J_{C\text{-}F}$ = 24.0 Hz), 114.9 (C_q, $^3J_{C\text{-}F}$ = 9.5 Hz), 108.7 (CH, $^2J_{C\text{-}F}$ = 24.8 Hz), 64.4 (CH_2), 49.8 (CH_2), 31.6 (CH_2), 29.7 (CH_2), 29.0 (CH_2), 28.9 (CH_2), 26.4 (CH_2), 22.5 (CH_2), 14.0 (CH_3). ^{19}F-NMR (282 MHz, $CDCl_3$) δ = 120.28 – 120.36 (m). IR (KBr): 2926, 2857, 2360, 1635, 1521, 1461, 1292, 1177, 994, 845, 727 cm^{-1}. MS (EI) *m/z* (relative intensity) 303 (26) [M$^+$], 232 (26), 204 (50), 176 (91), 149 (28), 121 (28), 101 (31), 57 (41), 41 (100). HRMS (ESI): *m/z* calcd for $C_{17}H_{22}FN_3O$+H$^+$ 304.1820, found 304.1818.



2k

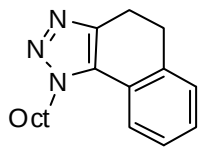
6-Fluoro-1-*n*-octyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2k): The representative procedure A was followed, using 4-{(2-fluorophenoxy)methyl}-1-octyl-1*H*-1,2,3-triazole (305 mg, 1.00 mmol). After 20 h, purification by chromatography (*n*-hexane/EtOAc = 10/1 → 5/1) yielded **2k** (258 mg, 85%) as a yellow solid. m.p. = 52-53 °C. ^{1}H-NMR (300 MHz, $CDCl_3$) δ = 7.29 – 6.95 (m, 3H), 5.52 (s, 2H), 4.58 (t, J = 7.4 Hz, 2H), 1.93 (quint, J = 7.3 Hz, 2H), 1.43 – 1.19 (m, 10H), 0.85 (m, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ = 152.3 (C_q, $^1J_{C\text{-}F}$ = 241 Hz), 141.4 (C_q, $^2J_{C\text{-}F}$ = 11 Hz), 139.5 (C_q), 126.2 (C_q, $^4J_{C\text{-}F}$ = 4 Hz), 122.0 (CH, $^3J_{C\text{-}F}$ = 8 Hz), 117.4 (CH, $^2J_{C\text{-}F}$ = 22 Hz), 117.2 (CH, $^4J_{C\text{-}F}$ = 3 Hz), 116.4 (C_q, $^3J_{C\text{-}F}$ = 2 Hz), 65.0 (CH_2), 49.9 (CH_2), 31.6 (CH_2), 29.6 (CH_2), 29.0 (CH_2), 28.9 (CH_2), 26.4 (CH_2), 22.5

(CH_2), 14.0 (CH_3). ^{19}F-NMR (282 MHz, $CDCl_3$) δ = 131.9 (m). IR (KBr): 3053, 2928, 2857, 2361, 1594, 1522, 1439, 1334, 1263, 1202, 1130, 1001, 896, 736 cm^{-1}. MS (EI) *m/z* (relative intensity) 303 (24) [M$^+$], 246 (11), 232 (27), 204 (59), 190 (45), 176 (91), 163 (67), 149 (27), 136 (27), 121 (19), 101 (21), 69 (21), 55 (51), 41 (100). HRMS (ESI): *m/z* calcd for $C_{17}H_{22}FN_3O+H^+$ 326.1639, found 326.1631.



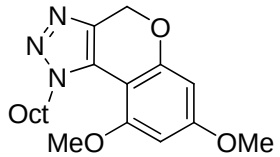
2l

6-Chloro-1-*n*-octyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2l): The representative procedure A was followed, using 1-*n*-octyl-4-{(2-chlorophenoxy)methyl)}-1*H*-1,2,3-triazole (322 mg, 1.00 mmol). After 20 h, purification by column chromatography (*n*-hexane/EtOAc = 10/1 → 5/1) yielded **2l** (182 mg, 57%) as a yellow oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.36–7.30 (m, 2 H), 6.99 (t, J = 8.0 Hz, 1 H), 5.56 (s, 2 H), 4.59 (t, J = 7.4 Hz, 2 H), 1.99–1.89 (m, 2 H), 1.47–1.15 (m, 10 H), 0.86 (t, J = 7.1 Hz, 3 H). ^{13}C-NMR (75 MHz, $CDCl_3$): 149.4 (C_q), 131.0 (CH), 130.4 (C_q), 123.5 (C_q), 122.3 (CH), 120.3 (CH), 118.1 (C_q), 115.7 (C_q), 65.2 (CH_2), 50.0 (CH_2), 31.6 (CH_2), 29.6 (CH_2), 29.0 (CH_2), 28.9 (CH_2), 26.4 (CH_2), 22.6 (CH_2), 14.0 (CH_3). IR (KBr): 2655, 2557, 1615, 1584, 1406, 1365, 1331, 1314, 756 cm^{-1}. MS (EI) *m/z* (relative intensity) 319 (26) [M$^+$], 248 (10), 234 (14), 220 (10), 207 (10), 197 (18), 192 (28), 179 (20), 57 (20), 55 (24), 41 (100). HR-MS (ESI) *m/z* calcd for $C_{17}H_{22}ClN_3O+H^+$ 320.1524, found 320.1525.



2m

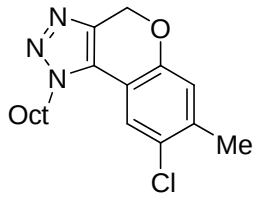
1-*n*-Octyl-4,5-dihydro-1*H*-naphtho[1,2-*d*]-1,2,3-triazole (2m): The representative procedure A was followed, using 1-*n*-octyl-4-phenethyl-1*H*-1,2,3-triazole (285 mg, 1.00 mmol). After 20 h, purification by column chromatography (*n*-hexane/EtOAc = 10/1 → 5/1) yielded **2m** (257 mg, 91%) as a brown oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.46 (d, J = 7.7 Hz, 1 H), 7.36–7.19 (m, 3 H), 4.59 (t, J = 7.5 Hz, 2 H), 3.09–2.89 (m, 4 H), 2.01–1.86 (m, 2 H), 1.48–1.10 (m, 10 H), 0.84 (t, J = 6.7 Hz, 3 H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 145.4 (C_q), 137.2 (C_q), 130.7 (C_q), 129.3 (CH), 128.3 (CH), 127.1 (CH), 125.4 (C_q), 121.9 (CH), 50.0 (CH_2), 31.7 (CH_2), 30.3 (CH_2), 29.7 (CH_2), 29.0 (CH_2), 29.0 (CH_2), 26.5 (CH_2), 22.6 (CH_2), 20.7 (CH_2), 14.0 (CH_3). IR (KBr): 3056, 2364, 1712, 1509, 1374, 1306, 1196, 1085, 1013, 723 cm^{-1}. MS (EI) *m/z* (relative intensity) 283 (42) [M^{+}], 226 (16), 184 (76), 171 (32), 156 (16), 143 (100), 128 (14), 115 (22), 43 (8). HR-MS (ESI) *m/z* calcd for $C_{18}H_{25}N_3$+Na^{+} 306.1941, found 306.1938.



2n

7,9-Dimethoxy-1-*n*-octyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2n): The representative procedure A was followed, using 4-{(3,5-dimethoxyphenoxy)methyl}-1-*n*-octyl-1*H*-1,2,3-triazole (325 mg, 0.94 mmol). After 20 h, purification by

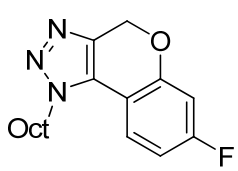
chromatography (*n*-hexane/EtOAc = 10/1 → 5/1 → 3/1) yielded **2n** (217 mg, 67%) as a yellow solid. m.p. = 93 °C. ^{1}H-NMR (300 Hz, $CDCl_3$) δ = 6.30 (d, J = 2.4 Hz, 1H), 6.20 (d, J = 2.4 Hz, 1H), 5.24 (s, 2H), 4.64 (t, J = 7.5 Hz, 2H), 3.89 (s, 3H), 3.81 (s, 3H), 1.81-1.68 (m, 2H), 1.30 – 1.15 (m, 10H), 0.85 (t, J = 6.8 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$) δ = 161.9 (C_q), 156.5 (C_q), 155.7 (C_q), 139.0 (C_q), 126.9 (C_q), 99.0 (C_q), 95.6 (CH), 93.3 (CH), 64.5 (CH_2), 55.5 (CH_3), 55.3 (CH_3), 51.8 (CH_2), 31.7 (CH_2), 30.1 (CH_2), 29.1 (CH_2), 29.1 (CH_2), 26.6 (CH_2), 22.6 (CH_2), 14.0 (CH_3). IR (KBr): 3070, 2916, 2855, 2360, 1615, 1464, 1423, 1308, 1210, 1154, 1109, 928, 837 cm^{-1}. MS (EI) *m/z* (relative intensity) 345 (24) [M$^+$], 233 (27), 218 (37), 204 (100), 190 (22), 176 (14), 146 (17), 69 (28), 55 (28), 41 (66). HRMS (ESI): *m/z* calcd for $C_{19}H_{27}N_3O_3Na$ 368.1945, found 368.1947.



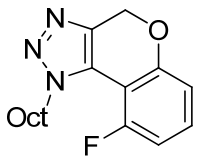
2o

8-Chloro-7-methyl-1-*n*-octyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2o): The representative procedure was followed, using 4-{(4-chloro-3-methylphenoxy)methyl}-1-*n*-octyl-1*H*-1,2,3-triazole (351 mg, 1.05 mmol). After 20 h, purification by chromatography (*n*-hexane/EtOAc = 10/1 → 5/1 → 3/1) yielded **2o** (282 mg, 80%) as a colourless oil. ^{1}H-NMR (300 Hz, $CDCl_3$) δ = 7.34 (s, 1H), 6.89 (s, 1H), 5.41 (s, 2H), 4.55 (t, J = 7.5 Hz, 2H), 2.34 (s, 3H), 2.03 – 1.85 (m, 2H), 1.49-1.13 (m, 10H), 0.84 (t, J = 6.9 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$) δ = 151.9 (C_q), 139.2 (C_q), 138.4 (C_q), 127.2 (C_q), 126.2 (C_q), 122.0 (CH), 120.2 (CH), 113.0

(C_q), 64.5 (CH_2), 49.7 (CH_2), 31.6 (CH_2), 29.5 (CH_2), 29.0 (CH_2), 28.9 (CH_2) 26.3 (CH_2), 22.5 (CH_2), 20.2 (CH_3), 14.0 (CH_3). IR (KBr): 2956, 2859, 1622, 1518, 1547, 1389, 1231, 1158, 1027, 932, 874, 693 cm^{-1}. MS (EI) *m/z* (relative intensity) 333 (11) [M^+], 234 (17), 220 (25), 206 (46), 192 (46), 115 (44), 101 (13), 77 (16), 55 (39), 41 (100). HRMS (ESI): *m/z* calcd for $C_{18}H_{23}ClN_3O+Na^+$ 356.1500, found 356.1492.



2p



2q

7-Fluoro-1-*n*-octyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2p) and **9-Fluoro-1-*n*-octyl-1,4-dihydrochromeno[4,3-*d*]-1,2,3-triazole (2q):** The representative procedure A was followed, using 4-{(3-fluorophenoxy)methyl}-1-*n*-octyl-1*H*-1,2,3-triazole (305 mg, 1.00 mmol). After 20 h, purification by chromatography (*n*-hexane/EtOAc = 10/1 → 5/1 → 3/1) yielded **2p** and **2q** as a colourless oil (252 mg, 83%). Additional purification by HPLC (Nucleodur 100-10 column, CH_2Cl_2, 8.0 mL/min, t_R = 25.2 min) yielded **2p** as an off-white solid and **2q** as a colourless oil.

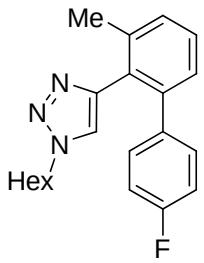
2p: m.p. = 59 °C. ^{1}H-NMR (300 MHz, $CDCl_3$) δ = 7.36 (dd, J = 9.5, 6.0 Hz, 1 H), 6.80 – 6.71 (m, 2H), 5.44 (s, 2H), 4.54 (t, J = 7.5 Hz, 2H), 2.00 – 1.82 (m, 2H), 1.46-1.14 (m, 10H), 0.86 (t, J = 6.9 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$) δ = 163.6 (C_q, $^1J_{C\text{-}F}$ = 250 Hz), 155.3 (C_q, $^3J_{C\text{-}F}$ = 12 Hz), 138.5 (C_q), 126.5 (C_q), 123.0 (CH, $^3J_{C\text{-}F}$ = 10 Hz), 110.7 (C_q), 109.2 (CH, $^2J_{C\text{-}F}$ = 25 Hz), 106.0 (CH, $^2J_{C\text{-}F}$ = 25 Hz), 64.9 (CH_2), 49.9 (CH_2), 31.6 (CH_2), 29.6 (CH_2), 29.0 (CH_2), 28.9 (CH_2), 26.4 (CH_2), 22.6 (CH_2), 14.0 (CH_3). ^{19}F-NMR (283 MHz, $CDCl_3$) δ = -108.57 (m) IR (KBr): 3074,

2929, 2856, 2357, 1627, 1584, 1521, 1465, 1325, 1270, 1116, 1016, 830 cm^{-1}. MS (EI) *m/z* (relative intensity) 303 (35) [M^+], 232 (41), 204 (100), 191 (52), 176 (96), 163 (60), 149 (27), 136 (29), 101 (20), 69 (18), 55 (38), 41 (81). HRMS (ESI): *m/z* calcd for $C_{17}H_{22}FN_3O+H^+$ 304.1820, found 304.1819.

2q: ^{1}H-NMR (300 MHz, $CDCl_3$) δ = 7.27 – 7.17 (ddd, J = 8.9, 7.3, 1.9 Hz, 1H), 6.92–6.76 (m, 2H), 5.34 (s, 2H), 4.70–4.57 (m, 2H), 1.87–1.77 (m, 2H), 1.33–1.20 (m, 10H), 0.84 (t, J = 6.9 Hz, 3H). ^{13}C-NMR (125 MHz, $CDCL_3$) δ = 157.0 (C_q, $^1J_{C-F}$ = 249 Hz), 154.9 (C_q, $^3J_{C-F}$ = 7 Hz), 140.3 (C_q), 130.5 (CH, $^3J_{C-F}$ = 11 Hz), 124.7 (C_q), 114.1 (CH, $^4J_{C-F}$ = 3 Hz), 109.6 (CH, $^2J_{C-F}$ = 23 Hz), 104.7 (C_q, $^2J_{C-F}$ = 19 Hz), 64.5 (CH_2), 51.4 (CH_2), 31.7 (CH_2), 30.4 (CH_2), 29.1 (CH_2), 29.0 (CH_2), 26.5 (CH_2), 22.7 (CH_2), 14.1 (CH_3).^{19}F-NMR (282 MHz, $CDCl_3$) δ = -108.6 (m). IR (film): 2926, 2856, 2361, 2335, 1629, 1588, 1555, 1510, 1336, 1304, 1093, 1044, 951, 787 cm^{-1}. MS (EI) *m/z* (relative intensity) 303 (47) [M^+], 246 (23), 232 (30), 204 (91), 191 (72), 176 (100), 163 (64), 149 (26), 136 (32), 101 (22), 55 (41), 41 (81). HRMS (ESI): *m/z* calcd for $C_{17}H_{22}FN_3O+H^+$ 304.1820, found 304.1820.

Representative procedure B: Ruthenium-catalyzed direct arylation of 4-aryltriazoles 3 (Table 2, entry 3).

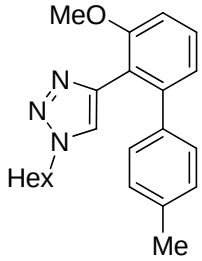
A suspension of $[RuCl_2(p\text{-cymene})]_2$ (15.4 mg, 0.025 mmol, 2.5 mol %), 2,4,6-trimethylbenzoic acid (49.2 mg, 0.30 mmol, 30 mol %), K_2CO_3 (276 mg, 2.0 mmol), 1-*n*-hexyl-4-*o*-tolyl-1*H*-1,2,3-triazole (243 mg, 1.00 mmol) and 1-chloro-4-fluorobenzene (196 mg, 1.50 mmol) in PhMe (4 mL) was stirred under N_2 for 20 h at 120 °C. EtOAc (50 mL) and H_2O (50 mL) were added to the cold reaction mixture. The separated aqueous phase was extracted with EtOAc (2 × 50 mL). The combined organic layers were washed with H_2O (50 mL) and brine (50 mL), dried over Na_2SO_4 and concentrated in vacuum. The remaining residue was purified by column chromatography on silica gel (*n*-hexane/EtOAc = 5/1) to yield **5c** (300 mg, 89%) as a colourless oil.



5c

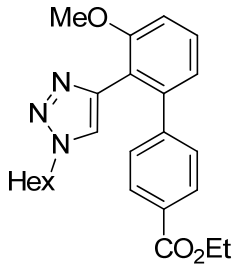
4-(4'-Fluoro-3-methylbiphenyl-2-yl)-1-*n*-hexyl-1*H*-1,2,3-triazole (5c): ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.35 – 7.21 (m, 2H), 7.21 – 7.12 (m, 1H), 7.08 – 6.95 (m, 2H), 6.92 – 6.73 (m, 3H), 4.20 (t, J = 6.9 Hz, 2H), 2.25 (s, 3H), 1.77 – 1.57 (m, 2H), 1.32 – 1.14 (m, 4H), 1.08 (m, 2H), 0.84 (t, J = 6.8 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 161.5 (C_q, $^1J_{C\text{-}F}$ = 246 Hz), 145.4 (C_q), 141.6 (C_q), 138.6 (C_q), 137.6 (C_q, $^4J_{C\text{-}F}$ = 3 Hz), 131.0 (CH, $^3J_{C\text{-}F}$ = 8 Hz), 129.4 (CH), 129.1 (CH), 128.3 (CH), 127.1 (CH), 122.6 (CH), 114.4 ($^2J_{C\text{-}F}$ = 21 Hz, CH), 49.9 (CH_2), 30.9 (CH_2), 30.1 (CH_2),

25.7 (CH_2), 22.2 (CH_2), 20.8 (CH_3), 13.8 (CH_3). IR (NaCl): 2930, 1641, 1550, 1223 cm^{-1}. MS (EI): *m/z* (relative intensity) 337 (100) [M^+], 309 (44), 238 (89). HRMS (ESI): *m/z* calcd. for $C_{21}H_{24}FN_3+H^+$ 338.2022, found 338.2025.



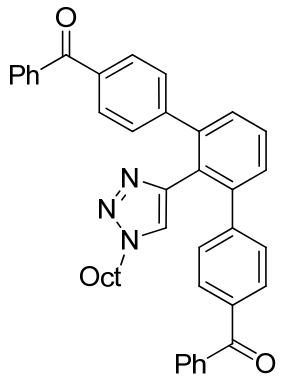
5a

1-*n*-Hexyl-4-(3-methoxy-4'-methylbiphenyl-2-yl)-1*H*-1,2,3-triazole (5a): The representative procedure B was followed, using 1-*n*-hexyl-4-(2-methoxyphenyl)-1*H*-1,2,3-triazole (259 mg, 1.00 mmol) and 1-chloro-4-methylbenzene (190 mg, 1.50 mmol) at 120 °C. After 20 h, purification by chromatography (*n*-hexane/EtOAc = 5/1) yielded **5a** (259 mg, 74 %) as a colourless oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.45 – 7.32 (m, 1H), 7.07 – 6.90 (m, 7H), 4.22 (t, J = 7.0 Hz, 2H), 3.80 (s, 3H), 2.27 (s, 3H), 1.69 (m, 2H), 1.31 – 1.07 (m, 6H), 0.86 (t, J = 6.9 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 158.0 (C_q), 144.0 (C_q), 142.7 (C_q), 138.2 (C_q), 136.1 (C_q), 129.4 (CH), 129.3 (CH), 128.4 (CH), 123.3 (CH), 122.4 (CH), 118.8 (C_q), 109.8 (CH), 56.0 (CH_3), 50.0 (CH_2), 31.1 (CH_2), 30.1 (CH_2), 25.9 (CH_2), 22.4 (CH_2), 21.0 (CH_3), 14.0 (CH_3). IR (NaCl): 2923, 2855, 1699, 1642, 1459, 1366 cm^{-1}. MS (EI): *m/z* (relative intensity) 349 (100) [M^+], 321 (45), 250 (86). HRMS (ESI): *m/z* calcd. for $C_{22}H_{27}N_3O+H^+$ 350.2222, found 350.2225.



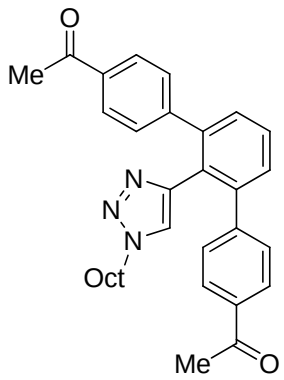
5b

2'-(1-*n*-hexyl-1*H*-1,2,3-triazol-4-yl)-3'-methoxybiphenyl-4-carboxylicacid ethyl ester (5b): The representative procedure B was followed, using 1-*n*-hexyl-4-(2-methoxyphenyl)-1*H*-1,2,3-triazole (259 mg, 1.00 mmol) and 4-chlorobenzoicacid ethyl ester (277 mg, 1.50 mmol) at 120 °C. After 20 h, purification by chromatography (*n*-hexane/EtOAc = 5/1) yielded **5b** (273 mg, 67 %) as a colourless oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.92 – 7.80 (m, 2H), 7.40 (t, J = 8.0 Hz, 1H), 7.23 – 7.13 (m, 2H), 7.09 (s, 1H), 6.99 (d, J = 8.0 Hz, 2H), 4.32 (q, J = 6.9 Hz, 2H), 4.22 (t, J = 7.0 Hz, 2H), 3.80 (s, 3H), 1.81 – 1.64 (m, 2H), 1.34 (t, J = 7.1 Hz, 3H), 1.29 – 1.02 (m, 6H), 0.84 (t, J = 6.9 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.7 (C_q), 158.2 (C_q), 146.3 (C_q), 143.2 (C_q), 142.3 (C_q), 129.9 (CH), 129.7 (CH), 129.2 (CH), 128.9 (C_q), 123.7 (CH), 122.5 (CH), 119.0 (C_q), 110.7 (CH), 61.1 (CH_2), 56.2 (CH_3), 50.3 (CH_2), 31.3 (CH_2), 30.3 (CH_2), 26.1 (CH_2), 22.6 (CH_2), 14.5 (CH_3), 14.2 (CH_3). IR (NaCl): 2926, 1711, 1641, 1363, 1270 cm^{-1}. MS (EI): *m/z* (relative intensity) 407 (95) [M^+], 379 (100), 308 (61). HRMS (ESI): *m/z* calcd. for $C_{24}H_{29}N_3O_3$+H^+ 408.2282, found 408.2281.



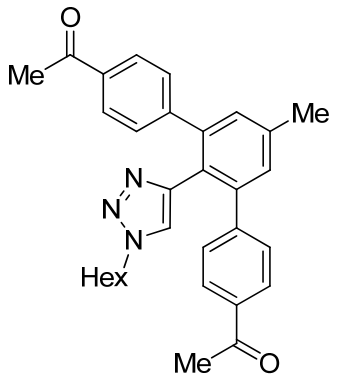
5d

4-{2',6'-Di-(4"-phenylcarbonylphenyl)-phenyl}-1-*n*-octyl-1*H*-1,2,3-triazole (5d): The representative procedure B was followed, using 1-*n*-octyl-4-phenyl-1*H*-1,2,3-triazole (259 mg, 1.00 mmol) and (4-chlorophenyl)(phenyl)methanone (650 mg, 3.00 mmol) at 120 °C. After 20 h, purification by chromatography (*n*-hexane/EtOAc = 5/1) yielded **5d** (482 mg, 78 %) as a white solid. m.p.: 136 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.75 (dd, J = 8.0, 1.0 Hz, 4H), 7.72 – 7.63 (m, 4H), 7.63 – 7.52 (m, 3H), 7.52 – 7.40 (m, 6H), 7.29 (d, J = 8.1 Hz, 4H), 6.83 (s, 1H), 4.11 (t, J = 7.0 Hz, 2H), 1.60 (m, 2H), 1.21 – 1.06 (m, 8H), 1.01 (m, 2H), 0.79 (t, J = 6.8 Hz, 3H). ^{13}C-NMR (125 MHz, $CDCl_3$): δ = 196.2 (C_q), 145.6 (C_q), 144.4 (C_q), 142.5 (C_q), 137.6 (C_q), 135.7 (C_q), 132.3 (CH), 129.9 (CH), 129.6 (CH), 129.5 (CH, 2x), 128.8 (C_q), 128.2 (CH), 128.1 (CH), 123.3 (CH), 49.9 (CH_2), 31.6 (CH_2), 30.2 (CH_2), 28.9 (CH_2), 28.7 (CH_2), 26.0 (CH_2), 22.5 (CH_2), 14.0 (CH_3). IR (NaCl): 2926, 1649, 1277, 927 cm^{-1}. MS (EI): *m/z* (relative intensity) 617 (5) [M^+], 589 (7), 105 (100). HRMS (ESI): *m/z* calcd. for $C_{42}H_{39}N_3O_2$+H^+ 618.3115, found 618.3112.



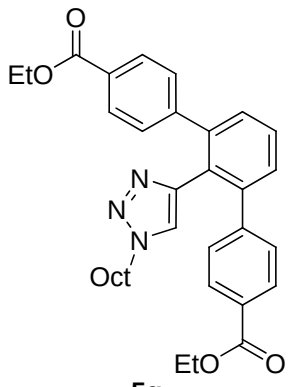
5e

4-{2',6'-Di-(4"-methylcarbonylphenyl)-phenyl}-1-*n*-octyl-1*H*-1,2,3-triazole (5e): The representative procedure B was followed, using 1-*n*-octyl-4-phenyl-1*H*-1,2,3-triazole (259 mg, 1.00 mmol) and 1-(4-chlorophenyl)ethanone (464 mg, 3.00 mmol) at 120°C. After 20 h, purification by chromatography (*n*-hexane/EtOAc 5:1) yielded **5e** (350 mg, 71 %) as a white solid. m.p.: 169 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.87 – 7.73 (m, 4H), 7.54 (dd, *J* = 8.5, 6.7 Hz, 1H), 7.43 (dd, *J* = 7.6, 0.8 Hz, 2H), 7.31 – 7.19 (m, 4H), 6.77 (s, 1H), 4.08 (t, *J* = 7.0 Hz, 2H), 2.56 (s, 6H), 1.64 – 1.48 (m, 2H), 1.30 – 1.10 (m, 8H), 0.96 (m, 2H), 0.85 (t, *J* = 6.9 Hz, 3H). ^{13}C-NMR (125 MHz, $CDCl_3$): δ = 197.6 (C_q), 146.1 (C_q), 144.4 (C_q), 142.4 (C_q), 135.4 (C_q), 129.8 (CH), 129.6 (CH), 128.8 (CH), 128.0 (C_q), 127.8 (CH), 123.2 (CH), 49.9 (CH_2), 31.7 (CH_2), 30.1 (CH_2), 29.0 (CH_2), 28.7 (CH_2), 26.5 (CH_3), 25.9 (CH_2), 22.5 (CH_2), 14.0 (CH_3). IR (NaCl): 2924, 2090, 1642, 1364, 1254 cm^{-1}. MS (EI): *m/z* (relative intensity) = 493 (100) [M^+], 279 (44), 239 (76). HRMS (ESI): *m/z* calcd. for $C_{32}H_{35}N_3O_2$+H^+ 494.2794, found 494.2802.



5f

4-{2',6'-Di-(4"-methylcarbonylphenyl)-*p*-tolyl}-1-*n*-hexyl-1*H*-1,2,3-triazole (5f): The representative procedure B was followed, using 1-*n*-hexyl-4-*p*-tolyl-1*H*-1,2,3-triazole (229 mg, 1.00 mmol) and 1-(4-chlorophenyl)ethanone (464 mg, 3.00 mmol) at 120 °C. After 20 h, purification by chromatography (*n*-hexane/EtOAc = 5/1) yielded **5f** (317 mg, 66 %) as a white solid. m.p.: 164 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.76 (d, J = 8.3 Hz, 4H), 7.32 – 7.14 (m, 6H), 6.78 (s, 1H), 4.06 (t, J = 6.8 Hz, 2H), 2.50 (s, 6H), 2.43 (s, 3H), 1.63 – 1.46 (m, 2H), 1.21 – 1.07 (m, 4H), 0.93 (m, 2H), 0.79 (t, J = 6.7 Hz, 3H). ^{13}C-NMR (125 MHz, $CDCl_3$): δ = 197.2 (C_q), 146.0 (C_q), 144.1 (C_q), 142.0 (C_q), 138.4 (C_q), 135.0 (C_q), 130.0 (CH), 129.5 (CH), 127.5 (CH), 124.9 (C_q), 123.1 (CH), 49.7 (CH_2), 30.8 (CH_2), 29.9 (CH_2), 26.4 (CH_3), 25.4 (CH_2), 22.2 (CH_2), 21.1 (CH_3), 13.8 (CH_3). IR (NaCl): 2926, 1678, 1361, 1264, 837 cm^{-1}. MS (EI): *m/z* (relative intensity) = 479 (64) [M^+], 478 (74), 451 (100), 409 (6), 380 (16), 297 (26), 255 (12), 43 (38). HRMS (ESI): *m/z* calcd. for $C_{31}H_{33}N_3O_2$+H^+ 480.2646, found 480.2645.

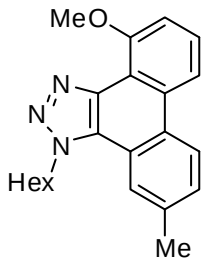


5g

4-{2',6'-Di-(4"-ethoxycarbonylphenyl)-phenyl}-1-*n*-octyl-1*H*-1,2,3-triazole (5g): The representative procedure B was followed, using 1-*n*-octyl-4-phenyl-1*H*-1,2,3-triazole (257 mg, 1.00 mmol) and 4-chlorobenzoicacid ethyl ester (552 mg, 3.00 mmol) at 120 °C. After 20 h, purification by chromatography (*n*-hexane/EtOAc = 5/1) yielded **5g** (354 mg, 64 %) as a white solid. m.p: 134-136 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.87 (m, 4H), 7.53 (dd, J = 8.6, 6.7 Hz, 1H), 7.48 – 7.38 (m, 2H), 7.28 – 7.17 (m, 4H), 6.75 (s, 1H), 4.32 (q, J = 7.1 Hz, 4H), 4.07 (t, J = 6.9 Hz, 2H), 1.63 – 1.45 (m, 2H), 1.35 (t, J = 7.1 Hz, 6H), 1.28 – 1.09 (m, 8H), 0.95 (m, 2H), 0.85 (t, J = 6.9 Hz, 3H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 166.4 (C_q), 145.9 (C_q), 144.4 (C_q), 142.5 (C_q), 129.5 (CH), 129.0 (CH), 129.0 (CH), 128.8 (C_q), 128.7 (CH), 128.1 (C_q), 123.2 (CH), 60.9 (CH_2), 49.9 (CH_2), 31.7 (CH_2), 30.1 (CH_2), 28.9 (CH_2), 28.6 (CH_2), 25.9 (CH_2), 22.5 (CH_2), 14.3 (CH_3), 14.0 (CH_3). IR (NaCl): 2925, 2855, 1706, 1642, 1270, 1108 cm^{-1}. MS (EI): *m/z* (relative intensity) = 553 (13) [M^+], 525 (19), 43 (100). HRMS (ESI): *m/z* calcd. for $C_{34}H_{39}N_3O_4$+H^+ 554.3013, found 554.3010.

Representative Procedure C: Palladium-Catalyzed Cyclodehydrogenative Direct Arylations of 1,2,3-Triazoles 5 (Table 2, entry 1):

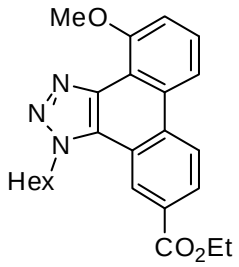
$Pd(OAc)_2$ (5.6 mg, 0.025 mmol, 5.0 mol %), $Cu(OAc)_2$ (100 mg, 0.50 mmol), PivOH (250 mg, 2.45 mmol) and triazole (**5a**) (175 mg, 0.50 mmol) in dry toluene (1.5 mL) were stirred under air at 140 °C for 20 h. H_2O (50 mL) was added at ambient temperature, and the resulting mixture was extracted with EtOAc (3 x 50 mL). The combined organic layers were washed with sat. aq. NH_4Cl (50 mL), H_2O (50 mL) and brine (50 mL), dried over Na_2SO_4, filtered and concentrated *in vacuo*. The remaining residue was purified by column chromatography on silica gel (*n*-hexane/EtOAc = 10/1 → 5/1 → 1/1) to yield **6a** (124 mg, 71%) as a yellow solid.



6a

1-*n*-Hexyl-4-methoxy-10-methyl-1*H*-phenanthro[9,10-*d*]-1,2,3-triazole (6a): m.p.: 113-114 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): $\delta = 8.64$ (d, $J = 8.6$ Hz, 1 H), 8.24 (d, $J = 8.2$ Hz, 1 H), 8.04 (s, 1 H), 7.67–7.48 (m, 2 H), 7.22 (d, $J = 8.0$ Hz, 1 H), 5.14–5.00 (m, 2 H), 4.22 (s, 3 H), 2.62 (s, 3 H), 2.16–1.98 (m, 2 H), 1.56–1.19 (m, 6 H), 0.88 (t, $J = 7.1$ Hz, 3 H). ^{13}C-NMR (75 MHz, $CDCl_3$): $\delta = 156.8$ (C_q), 141.1 (C_q), 137.5 (C_q), 137.5 (C_q), 130.9 (C_q), 128.8 (CH), 128.6 (C_q), 127.8 (C_q), 126.9 (CH), 124.9 (CH), 122.2 (CH), 120.8 (C_q), 115.3 (CH), 108.7 (CH), 56.2 (CH_3), 50.9 (CH_2), 31.2 (CH_2), 29.4 (CH_2), 26.1 (CH_2), 22.4 (CH_2), 21.8 (CH_3), 13.9 (CH_3). IR (KBr):

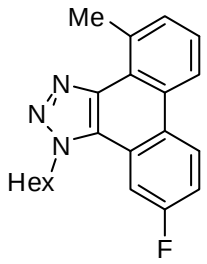
3050, 2859, 1625, 1584, 1533, 1438, 1393, 1224, 1020, 799 cm^{-1}. MS (EI) *m/z* (relative intensity) 347 (100) [M^+], 318 (20), 263 (12), 248 (54), 234 (56), 220 (54), 204 (10), 190 (24), 176 (12), 55 (12), 43 (32). HR-MS (ESI) *m/z* calcd for $C_{22}H_{25}N_3$+Na^+ 370.1890, found 370.1891.



6b

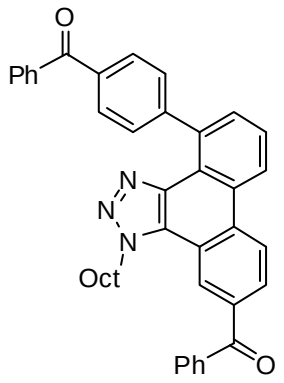
1-*n*-Hexyl-4-methoxy-1*H*-phenanthro[9,10-*d*]-1,2,3-triazole-10-carboxylicacid ethyl ester (6b): The representative procedure C was followed, using **5b** (204 mg, 0.50 mmol). After 20 h, purification by column chromatography (*n*-hexane/EtOAc = 10/1 → 5/1 → 1/1) yielded **6b** (138 mg, 68%) as a green solid. m.p.: 125 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.73 (s, 1 H), 8.51 (d, J = 8.9 Hz, 1 H), 8.11 (dd, J = 8.7, 1.5 Hz, 1 H), 8.03 (d, J = 8.4 Hz, 1 H), 7.47 (t, J = 8.2 Hz, 1 H), 7.14 (d, J = 8.1 Hz, 1 H), 4.96 (t, J = 7.5 Hz, 2 H), 4.43 (q, J = 7.1 Hz, 2 H), 4.13 (s, 3 H), 2.08–1.93 (m, 2 H), 1.53–1.10 (m, 6 H), 1.48 (t, J = 7.1 Hz, 3 H), 0.83 (t, J = 7.0 Hz, 3 H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 165.5 (C_q), 156.4 (C_q), 140.7 (C_q), 133.4 (C_q), 129.7 (C_q), 128.6 (C_q), 127.4 (C_q), 126.9 (CH), 124.7 (CH), 123.8 (CH), 119.8 (C_q), 116.1 (C_q), 115.7 (CH), 109.7 (CH), 61.3 (CH_2), 56.1 (CH_3), 50.9 (CH_2), 31.2 (CH_2), 29.2 (CH_2), 26.2 (CH_2), 22.4 (CH_2), 14.3 (CH_3), 13.9 (CH_3). IR (KBr): 3053, 2933, 2866, 1662, 1616, 1581, 1464, 1311, 1210, 1157, 1110, 1021, 896 cm^{-1}. MS (EI) *m/z* (relative intensity) 406 (42) [M^+], 379 (26), 362 (11), 308 (36), 281 (12), 239 (36),

207 (100), 191 (14), 165 (42), 96 (19), 43 (66). HR-MS (ESI) *m/z* calcd for $C_{24}H_{27}N_3O_3$+H^+ 406.2125, found 406.2125.



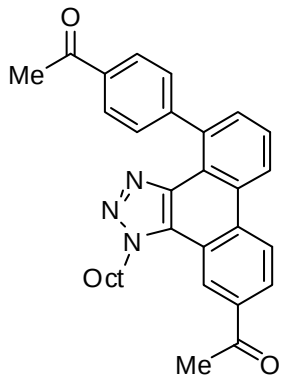
6c

10-Fluoro-1-*n*-hexyl-4-methyl-1*H*-phenanthro[9,10-*d*]-1,2,3-triazole (6c): The representative procedure C was followed, using **5c** (169 mg, 0.50 mmol). After 20 h, purification by column chromatography (*n*-hexane/EtOAc = 20/1) yielded **6c** (110 mg, 66%) as a white solid. m.p.: 91 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.69 (dd, J = 9.1, 5.6 Hz, 1 H), 8.43–8.36 (m, 1 H), 7.81 (dd, J = 9.9, 2.6 Hz, 1 H), 7.58–7.50 (m, 2 H), 7.45–7.37 (m, 1 H), 4.96 (t, J = 7.4 Hz, 2 H), 3.22 (s, 3 H), 2.15–2.00 (m, 2 H), 1.56–1.22 (m, 6 H), 0.89 (t, J = 7.0 Hz, 3 H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 161.4 (C_q, $^1J_{C\text{-}F}$ = 247 Hz), 143.4 (C_q), 136.0 (C_q), 136.0 (C_q), 130.2 (CH), 129.0 (C_q), 127.5 (C_q, $^3J_{C\text{-}F}$ = 12 Hz), 127.0 (CH, $^3J_{C\text{-}F}$ = 9 Hz), 126.3 (CH), 123.5 (C_q), 121.2 (C_q, $^4J_{C\text{-}F}$ = 9 Hz), 120.7 (CH), 115.5 (CH, $^2J_{C\text{-}F}$ = 23 Hz), 107.6 (CH, $^2J_{C\text{-}F}$ = 24 Hz), 50.6 (CH_2), 31.1 (CH_2), 29.3 (CH_2), 26.1 (CH_2), 24.1 (CH_2), 22.4 (CH_3), 13.9 (CH_3). ^{19}F-NMR (282 MHz, $CDCl_3$): δ = -112.8 – -113.0 (m). IR (KBr): 3052, 2959, 2858, 1624, 1529, 1465, 1364, 1264, 1194, 1159, 1030, 892, 791 cm^{-1}. MS (EI) *m/z* (relative intensity) 335 (40) [M^+], 251 (18), 223 (24), 207 (16), 183 (8) 57 (32), 43 (100), 41 (64). HR-MS (ESI) *m/z* calcd for $C_{21}H_{22}FN_3$+H^+ 336.1871, found 336.1871.



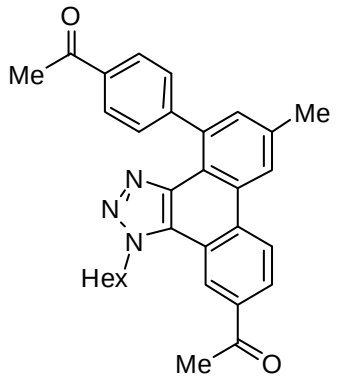
6d

10-Phenylcarbonyl-4-(4'-phenylcarbonylphenyl)-1-*n*-octyl-1*H*-phenanthro [9,10-*d*]-1,2,3-triazole (6d): The representative procedure C was followed, using **5d** (309 mg, 0.50 mmol). After 20 h, purification by column chromatography (*n*-hexane/EtOAc = 5/1 → 2/1) yielded **6d** (210 mg, 68%) as a yellow oil. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.91 (d, J = 8.9 Hz, 1 H), 8.76 (d, J = 8.6 Hz, 1 H), 8.69 (s, 1 H), 8.20 (d, J = 8.7 Hz, 1 H), 8.02–7.86 (m, 6 H), 7.81–7.44 (m, 10 H), 4.82 (t, J = 7.7 Hz, 2 H), 2.01–1.86 (m, 2 H), 1.33–1.09 (m, 10 H), 0.83 (t, J = 6.8 Hz, 3 H). ^{13}C-NMR (125 MHz, $CDCl_3$): δ = 196.4 (C_q), 195.5 (C_q), 147.0 (C_q), 142.0 (C_q), 138.7 (C_q), 137.9 (C_q), 137.3 (C_q), 136.1 (C_q), 136.0 (C_q), 133.8 (C_q), 132.7 (CH), 132.0 (CH), 131.8 (CH), 130.0 (CH), 129.9 (CH), 129.9 (CH), 129.5 (CH), 129.0 (C_q), 128.5 (CH), 128.2 (CH), 128.2 (C_q), 128.1 (CH), 126.4 (CH), 125.0 (CH), 123.9 (CH), 123.8 (C_q), 120.1 (C_q), 51.0 (CH_2), 31.7 (CH_2), 29.5 (CH_2), 29.0 (2 x CH_2), 26.5 (CH_2), 22.7 (CH_2), 14.1 (CH_3). IR (film): 3055, 2929, 2860, 2306, 1657, 1597, 1450, 1151, 1108, 934 cm^{-1}. MS (EI): *m/z* (relative intensity) = 614 (100) [M^+-H^+], 105 (56), 77 (12), 43 (4). HR-MS (ESI) *m/z* calcd for $C_{42}H_{37}N_3O_2$+H^+ 616.2959, found 616.2957.



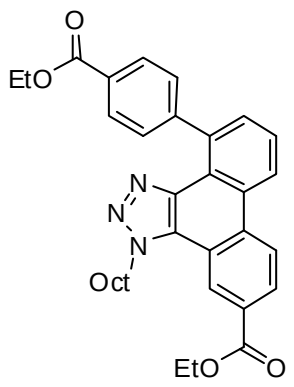
6e

10-Phenylcarbonyl-4-(4'-methylcarbonylphenyl)-1-*n*-octyl-1*H*-phenanthro [9,10-*d*]-1,2,3-triazole (6e): The representative procedure A was followed, using **5e** (247 mg, 0.50 mmol). After 20 h, purification by column chromatography (*n*-hexane/EtOAc = 5/1 → 2/1) yielded **6e** (178 mg, 72%) as a yellow solid. m.p.: 90-91 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.94–8.87 (m, 2 H), 8.76 (d, J = 8.1 Hz, 1 H), 8.29 (dd, J = 8.8, 1.6 Hz, 1 H), 8.10 (d, J = 8.1 Hz, 2 H), 7.80–7.71 (m, 1 H); 7.65–7.58 (m, 3 H), 5.00 (t, J = 7.4 Hz, 2 H), 2.80 (s, 3 H), 2.70 (s, 3 H), 2.15–2.01 (m, 2 H), 1.55–1.18 (m, 10 H), 0.90–0.80 (m, 3 H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 198.0 (C_q), 196.8 (C_q), 147.6 (C_q), 142.0 (C_q), 138.7 (C_q), 136.0 (C_q), 135.5 (C_q), 134.3 (C_q), 131.8 (CH), 129.9 (CH), 129.1 (C_q), 128.4 (C_q), 128.1 (CH), 126.8 (CH); 126.4 (CH); 125.3 (CH); 124.0 (CH), 123.9 (C_q), 122.8 (CH), 120.5 (C_q), 51.1 (CH_2), 31.6 (CH_2), 29.3 (CH_2), 29.0 (CH_2), 29.0 (CH_2), 26.7 (CH_3), 26.7 (CH_3), 26.6 (CH_2), 22.5 (CH_2), 14.0 (CH_3). IR (KBr): 3448, 2928, 2861, 2358, 2253, 1708, 1610, 1363, 1228, 1098, 909, 734 cm^{-1}. MS (EI) *m/z* (relative intensity) 491 (52) [M$^+$], 490 (100), 351 (2), 280 (8), 57 (2), 43 (38), 41 (14). HR-MS (ESI) *m/z* calcd for $C_{32}H_{33}N_3O_2$+Na$^+$ 514.2465, found 514.2473.



6f

8-Methyl-10-phenylcarbonyl-4-(4'-methylcarbonylphenyl)-1-*n*-hexyl-1*H*-phenanthro[9,10-*d*]-1,2,3-triazole (6f): The representative procedure A was followed, using **5f** (240 mg, 0.50 mmol). After 20 h, purification by column chromatography (*n*-Hexan/EtOAc = 5/1 → 2/1) yielded **6f** (155 mg, 65%) as a white solid. m.p.: 99-100 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.78 (d, J = 8.4 Hz, 2 H), 8.45 (s, 1 H), 8.17 (d, J = 8.9 Hz, 1 H), 8.07 (d, J = 8.2 Hz, 2 H), 7.59 (d, J = 8.2 Hz, 2 H), 7.43 (s, 1 H), 4.89 (t, J = 7.5 Hz, 2 H), 2.74 (s, 3 H), 2.67 (s, 3 H), 2.63 (s, 3 H), 2.11–1.96 (m, 2 H), 1.55–1.20 (m, 6 H), 0.85 (t, J = 7.0 Hz, 3 H). ^{13}C-NMR (75 MHz, $CDCl_3$): δ = 197.7 (C_q), 196.5 (C_q), 147.4 (C_q), 141.8 (C_q), 138.3 (C_q), 136.0 (C_q), 135.7 (C_q), 135.0 (C_q), 133.8 (C_q), 133.0 (CH), 129.7 (CH), 129.0 (C_q), 127.9 (CH), 127.7 (C_q), 126.3 (CH), 125.0 (CH), 123.8 (CH), 122.5 (CH), 121.4 (C_q), 120.3 (C_q), 50.9 (CH_2), 31.2 (CH_2), 29.2 (CH_2), 26.7 (CH_3), 26.7 (CH_3), 26.3 (CH_2), 22.4 (CH_2), 21.8 (CH_3), 13.9 (CH_3). IR (KBr): 3054, 2958, 2931, 2859, 1605, 1582, 1457, 1422, 1357, 1236, 1182, 1033, 1017, 959, 833 cm^{-1}. MS (EI): *m/z* (relative intensity) = 477 (56) [M^+], 476 (100), 350 (4), 336 (8), 294 (12), 278 (6), 43 (10). HR-MS (ESI) *m/z* calcd for $C_{31}H_{31}N_3O_2$+H^+ 478.2489, found 478.2489.

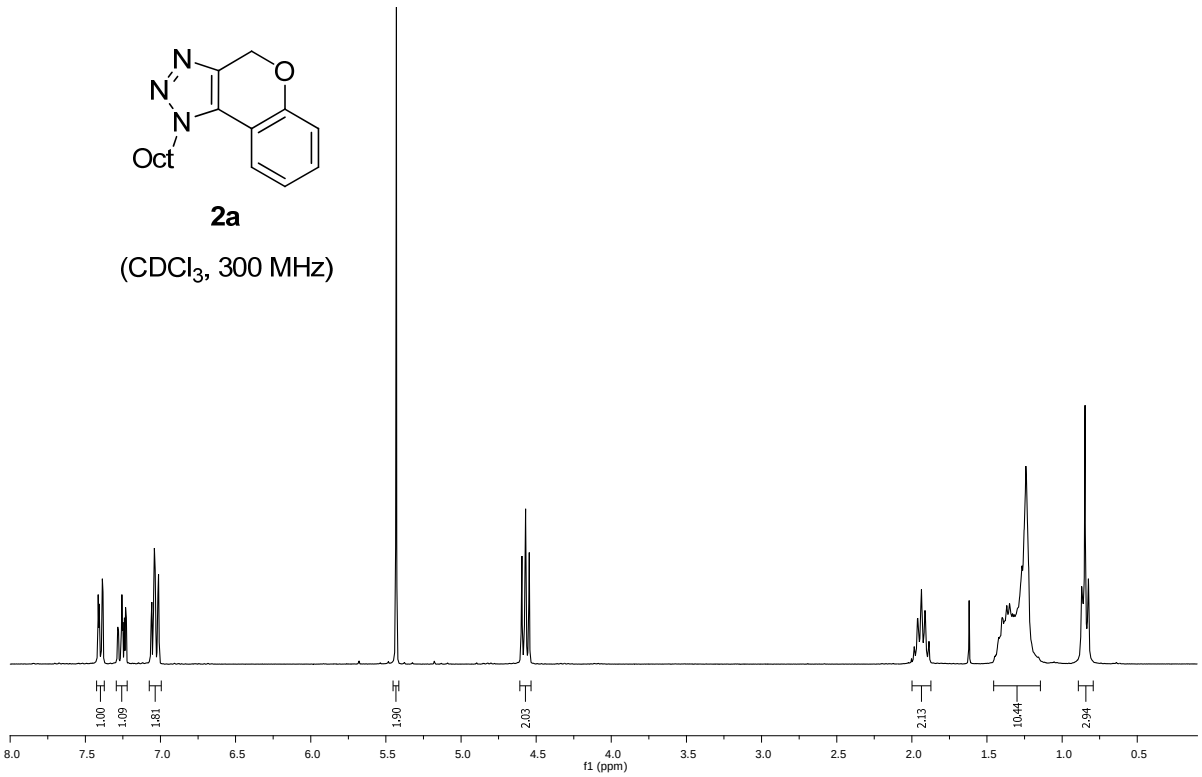


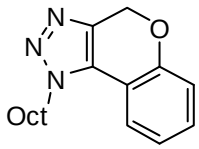
6g

10-Ethoxycarbonyl-4-(4'-ethoxycarbonylphenyl)-1-*n*-octyl-1*H*-phenanthro [9,10-*d*]-1,2,3-triazole (6g): The representative procedure A was followed, using **5g** (277 mg, 0.50 mmol). After 20 h, purification by column chromatography (*n*-hexane/EtOAc = 5/1 → 2/1) yielded **6g** (266 mg, 96%) as a white solid. m.p.: 80-82 °C. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 8.95 (s, 1 H), 8.85 (d, J = 8.9 Hz, 1 H), 8.73 (d, J = 7.9 Hz, 1 H), 8.35 (dd, J = 8.7, 1.6 Hz, 1 H), 8.17 (d, J = 8.2 Hz, 2 H), 7.76–7.67 (m, 1 H), 7.64–7.53 (m, 3 H), 5.02–4.90 (m, 2 H), 4.56–4.36 (m, 4 H), 2.14–1.99 (m, 2 H), 1.58–1.10 (m, 16 H), 0.89–0.79 (m, 3 H). ^{13}C-NMR (125 MHz, $CDCl_3$): δ = 166.6 (C_q), 165.7 (C_q), 147.2 (C_q), 141.8 (C_q), 138.7 (C_q), 134.0 (C_q), 131.5 (CH), 129.5 (CH), 129.3 (C_q), 129.2 (CH), 129.1 (C_q), 129.0 (C_q), 128.1 (C_q), 127.5 (CH), 126.2 (CH), 124.9 (CH), 124.2 (CH), 123.8 (C_q), 123.7 (CH), 120.1 (C_q), 61.5 (CH_2), 60.8 (CH_2), 51.0 (CH_2), 31.7 (CH_2), 29.4 (CH_2), 29.1 (CH_2), 29.1 (CH_2), 26.7 (CH_2), 22.6 (CH_2), 14.5 (CH_3), 14.5 (CH_3), 14.1 (CH_3). IR (KBr): 3053, 2724, 2361, 1720, 1373, 1264, 1110, 1026, 740 cm^{-1}. MS (EI): *m/z* (relative intensity) = 551 (48) [M^{+}], 550 (100), 506 (4), 351 (8), 278 (4). HR-MS (ESI) *m/z* calcd for $C_{34}H_{37}N_3O_4$+H^{+} 552.2857, found 552.2858.

2a

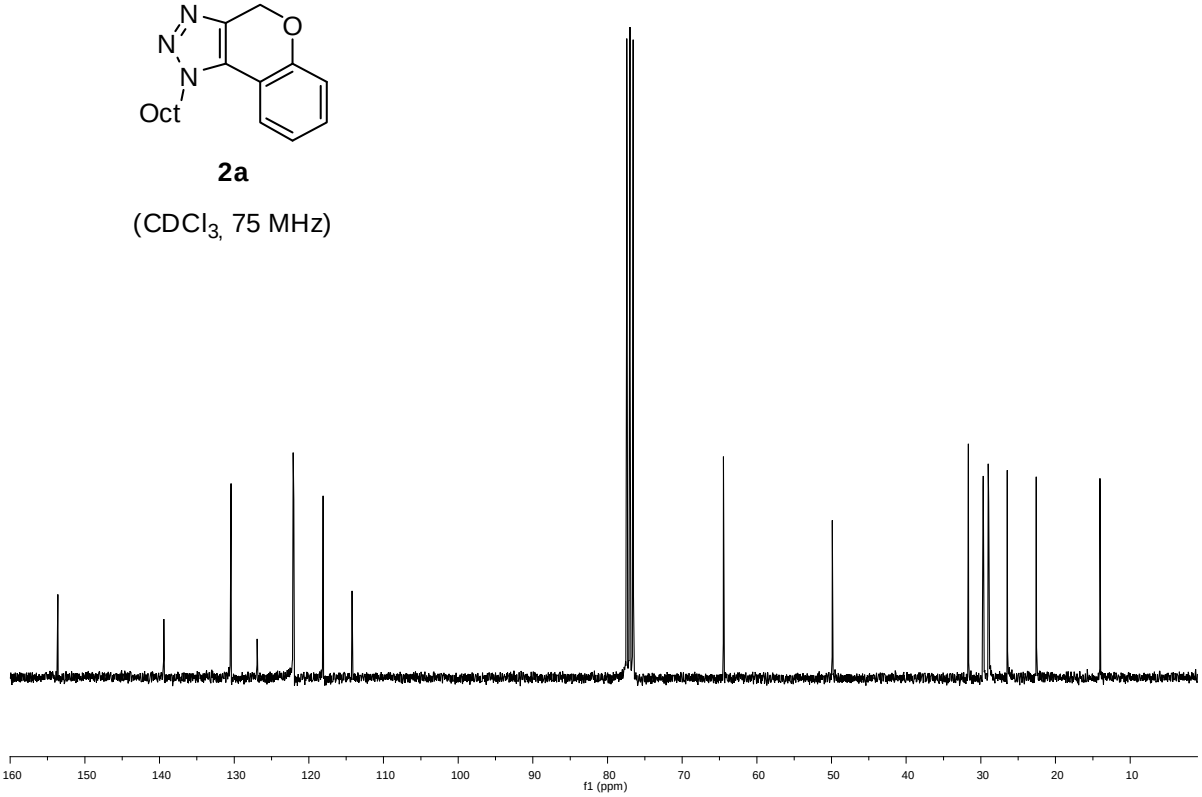
($CDCl_3$, 300 MHz)

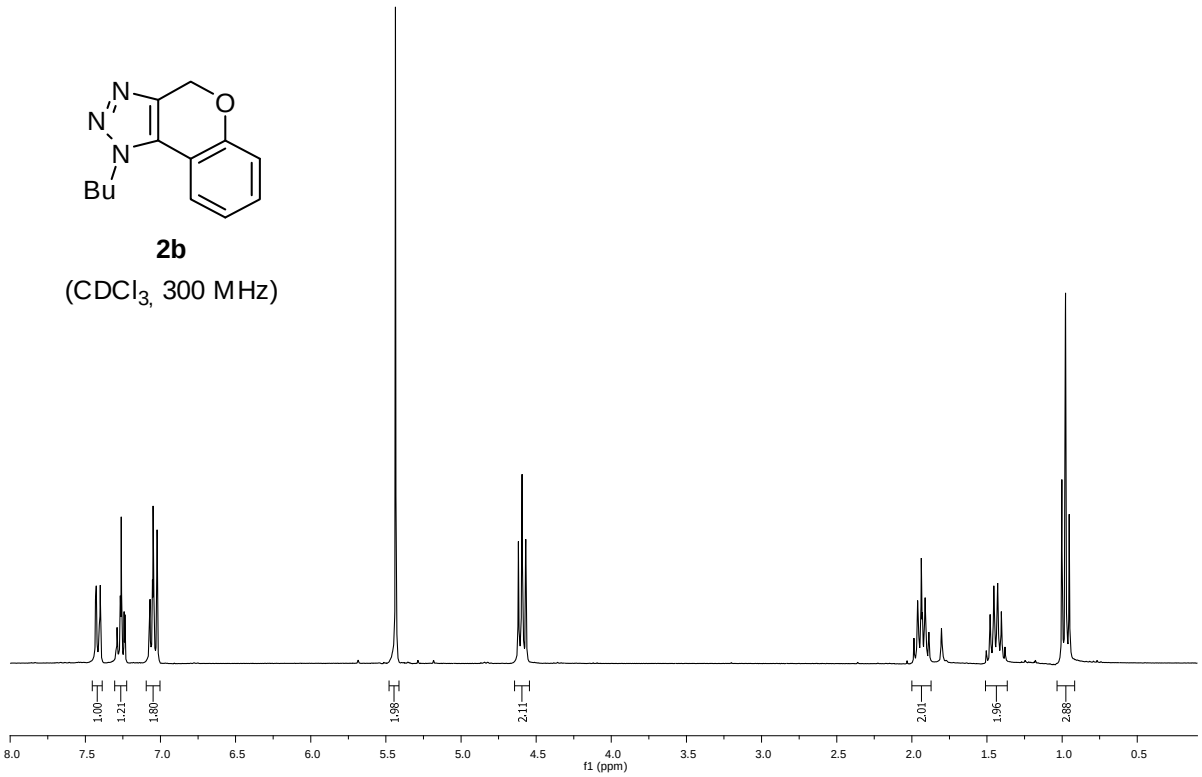


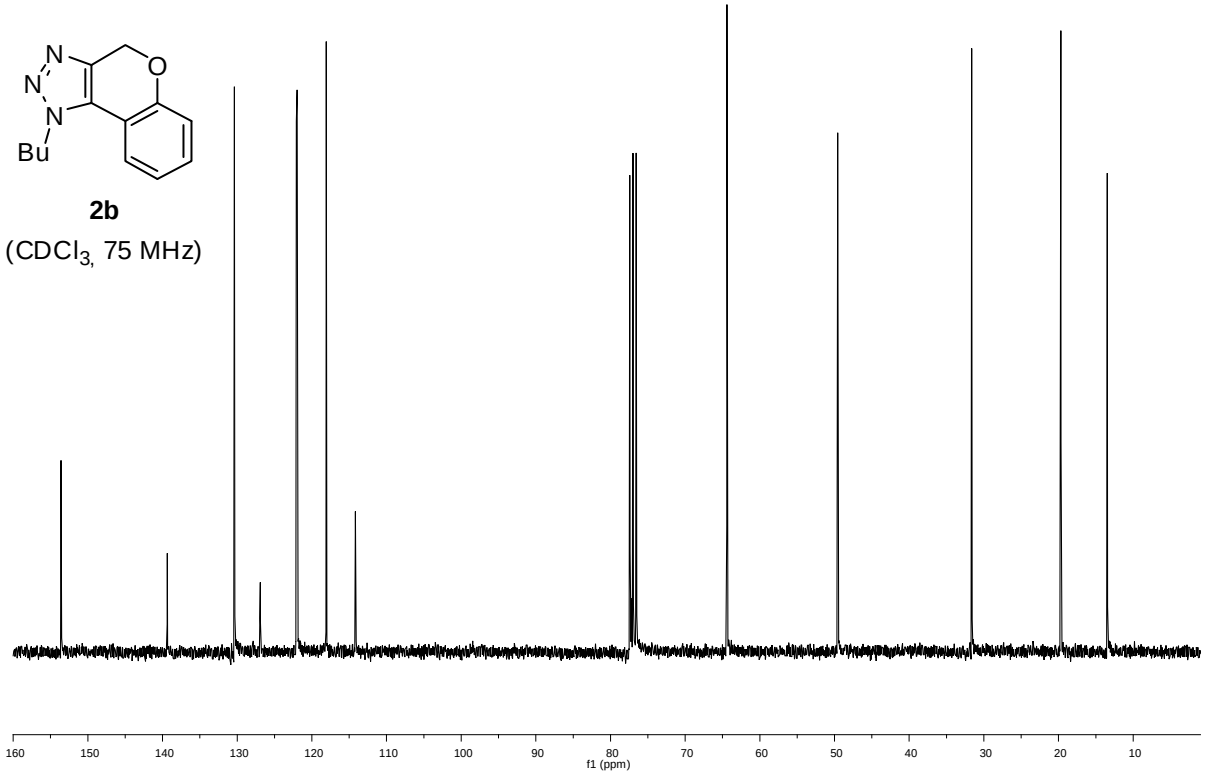


2a

($CDCl_{3,}$ 75 MHz)

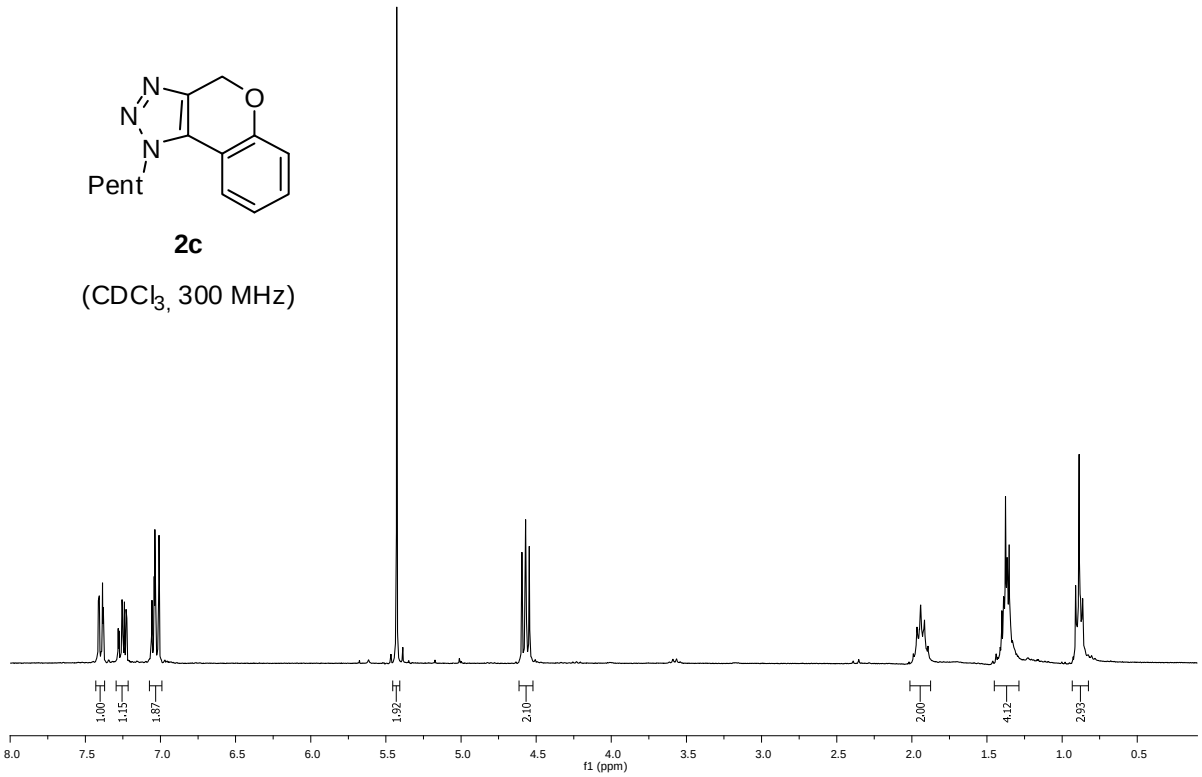



N
N
N
O
Bu
2b
(CDCl3, 300 MHz)
1.00
1.21
1.80
1.98
2.11
2.01
1.96
2.88
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


N
N
N
O
Bu
2b
(CDCl3, 75 MHz)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

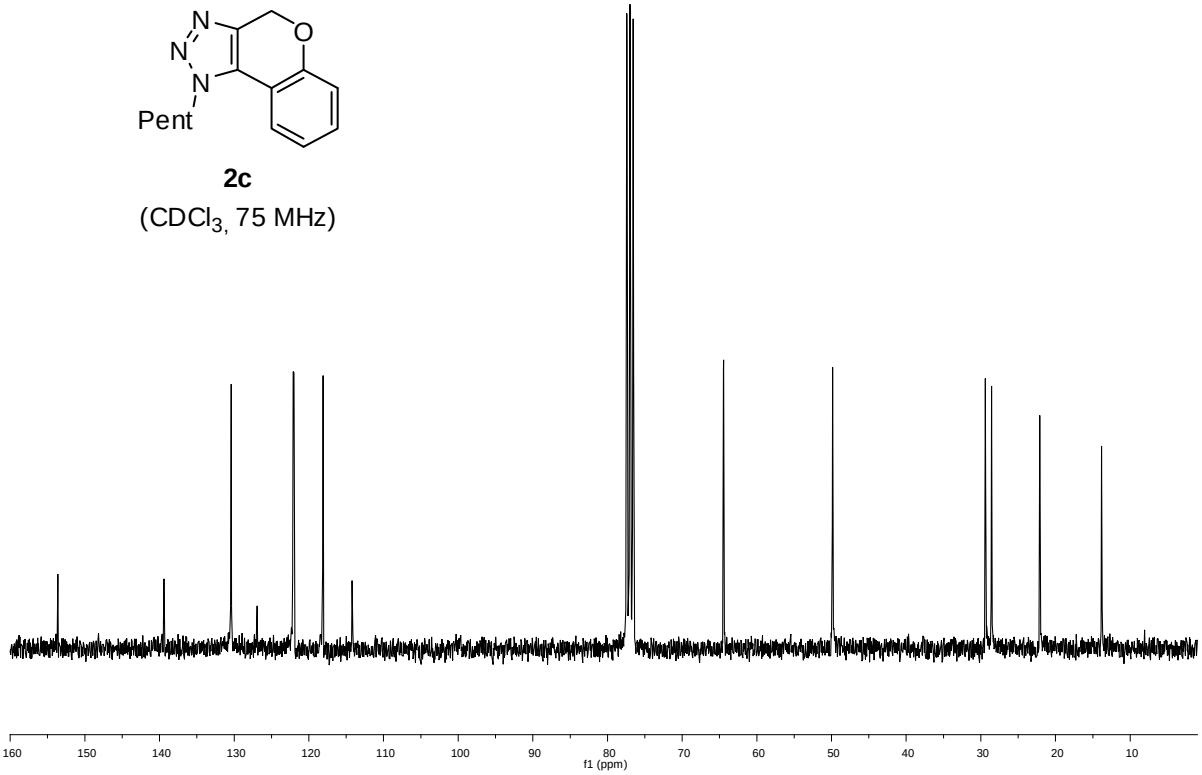
2c

($CDCl_3$, 300 MHz)



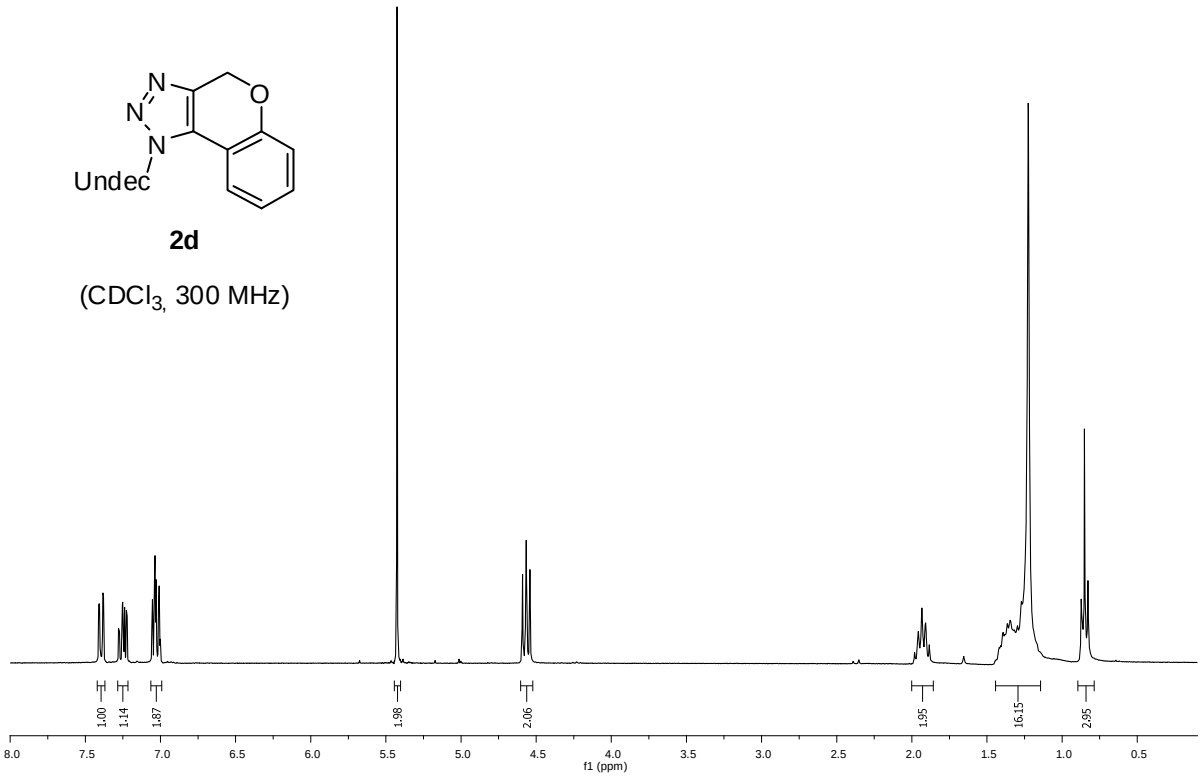
2c

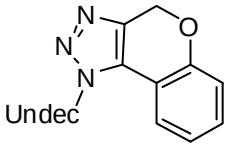
($CDCl_3$, 75 MHz)



2d

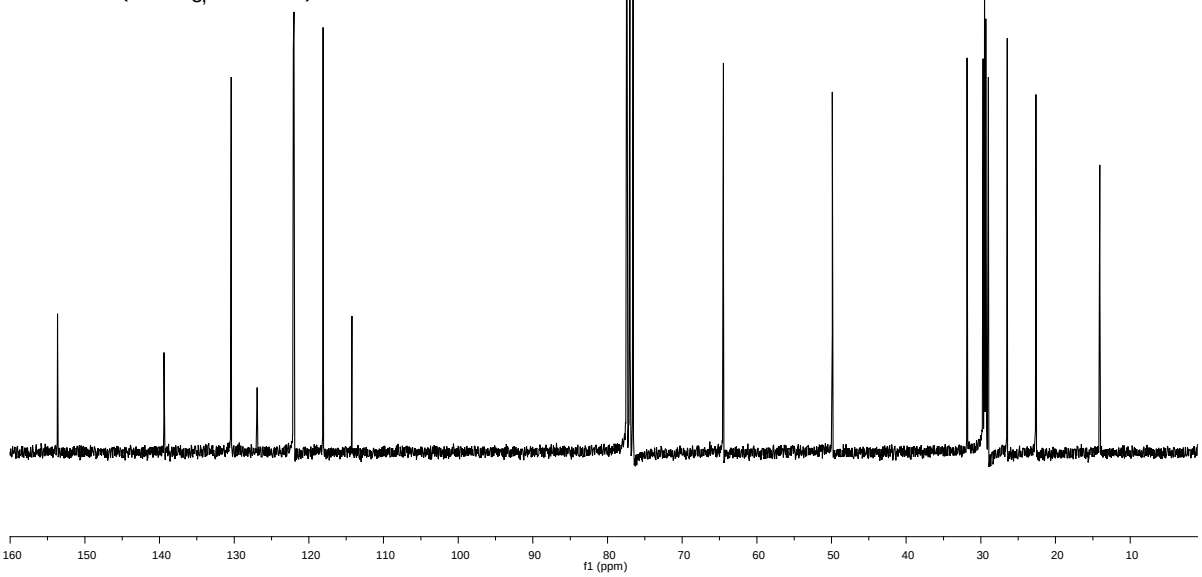
($CDCl_3$, 300 MHz)

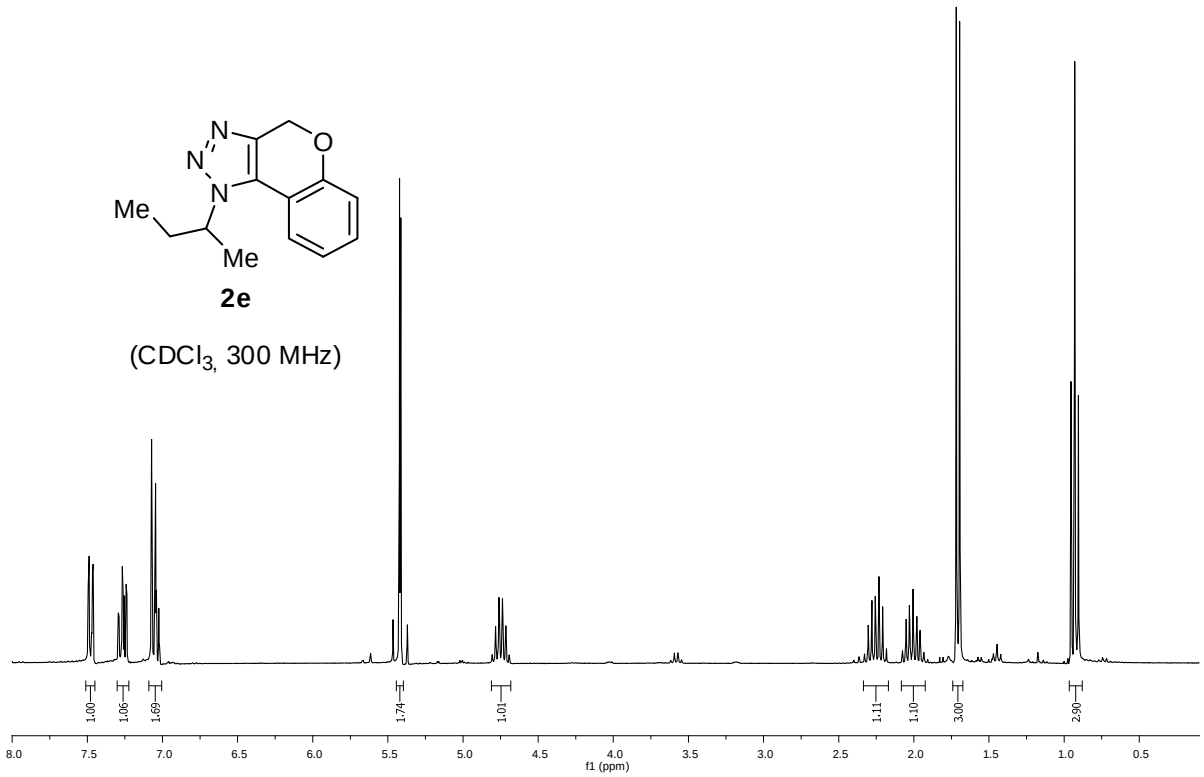


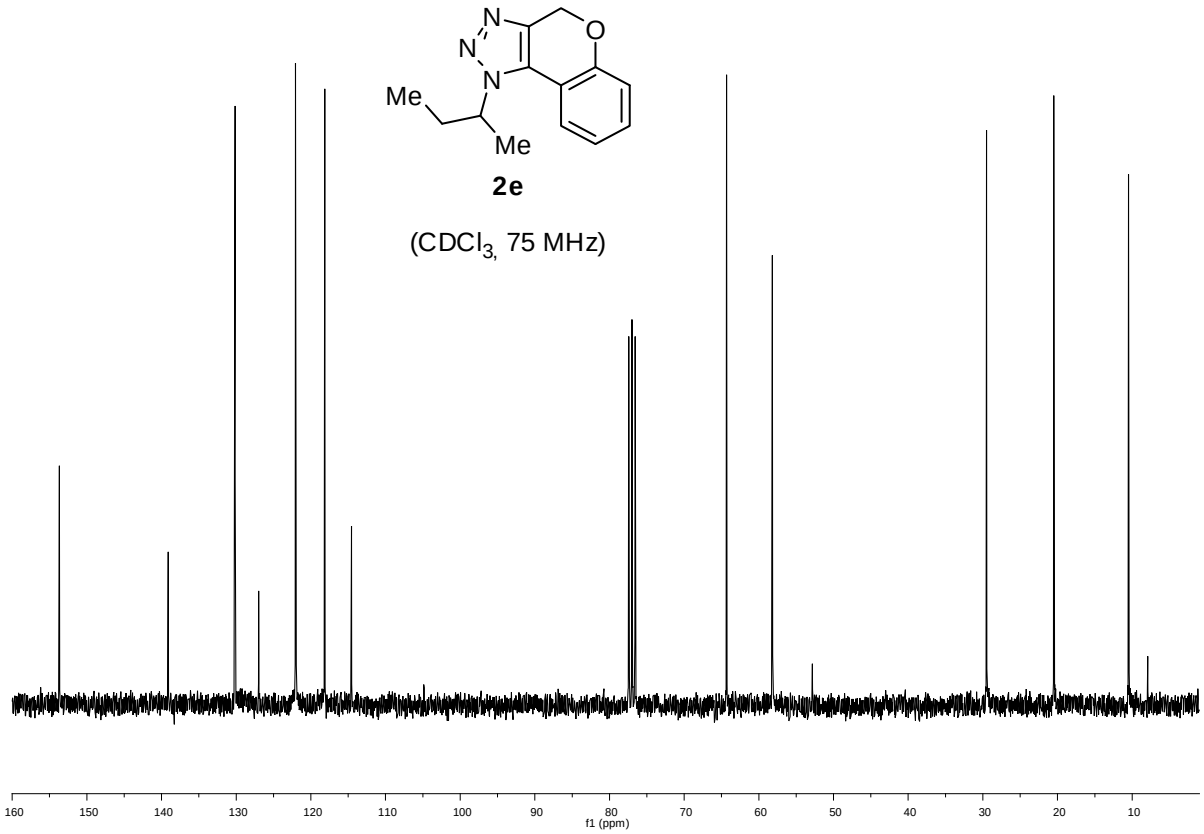


2d

($CDCl_3$, 75 MHz)

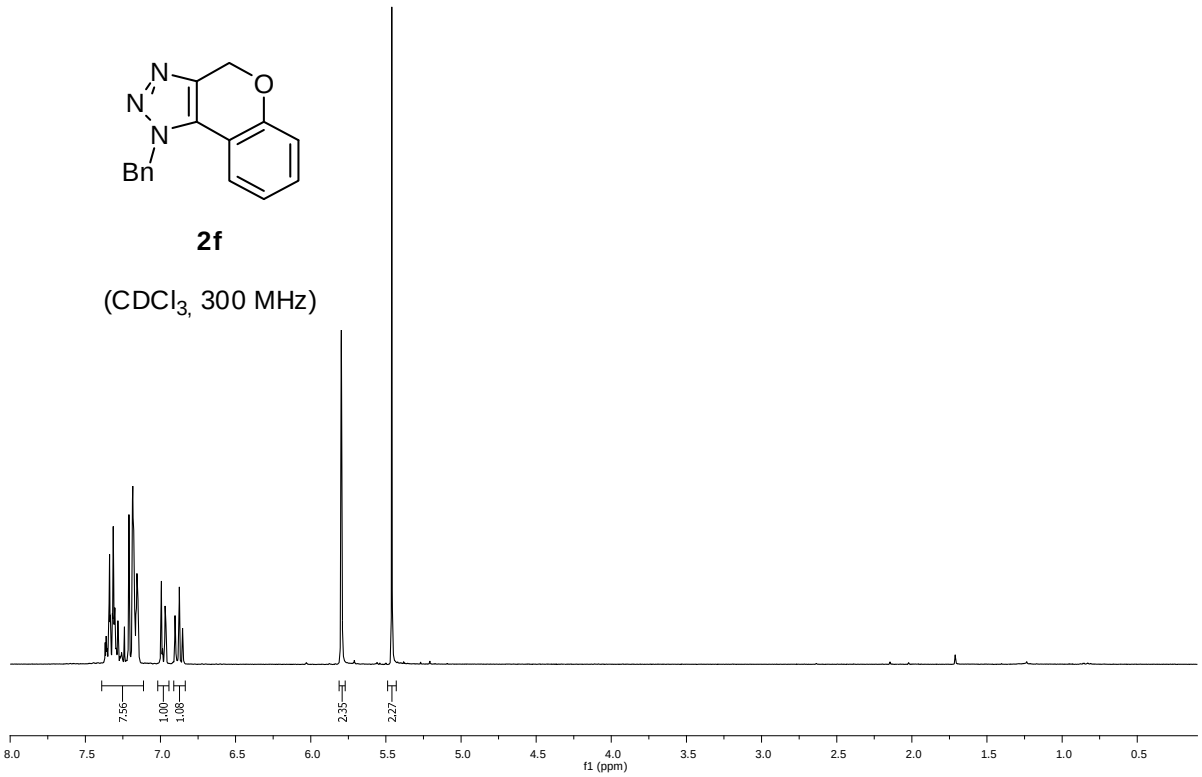


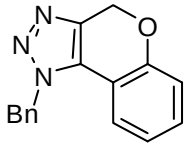

N
N
N
O
Me
Me
2e
(CDCl3, 300 MHz)
1.00
1.06
1.69
1.74
1.01
1.11
1.10
3.00
2.90
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


N
N
N
O
Me
Me
2e
(CDCl3, 75 MHz)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

2f

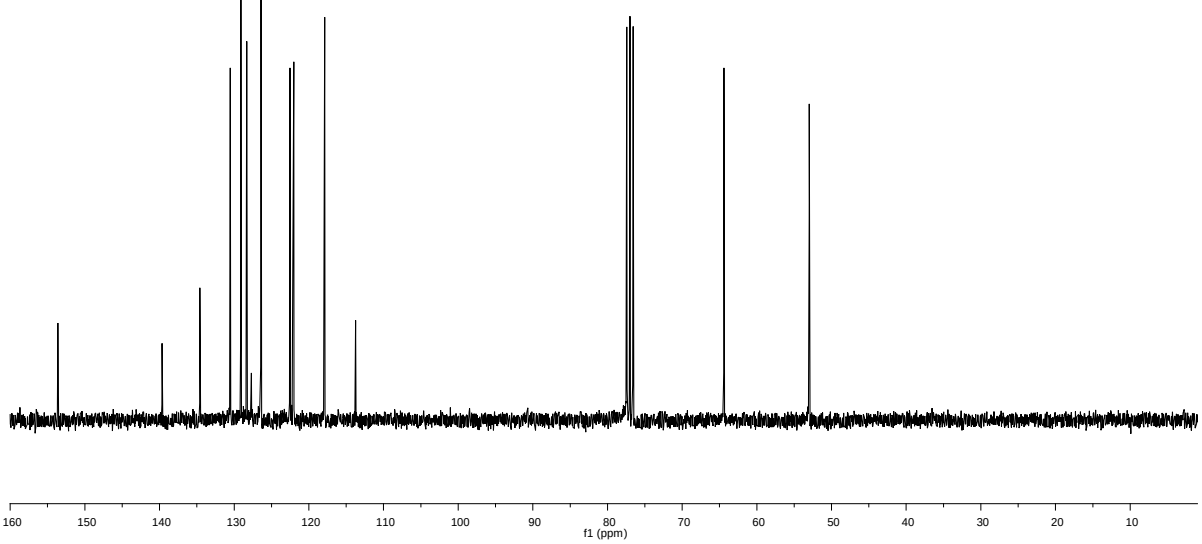
($CDCl_3$, 300 MHz)

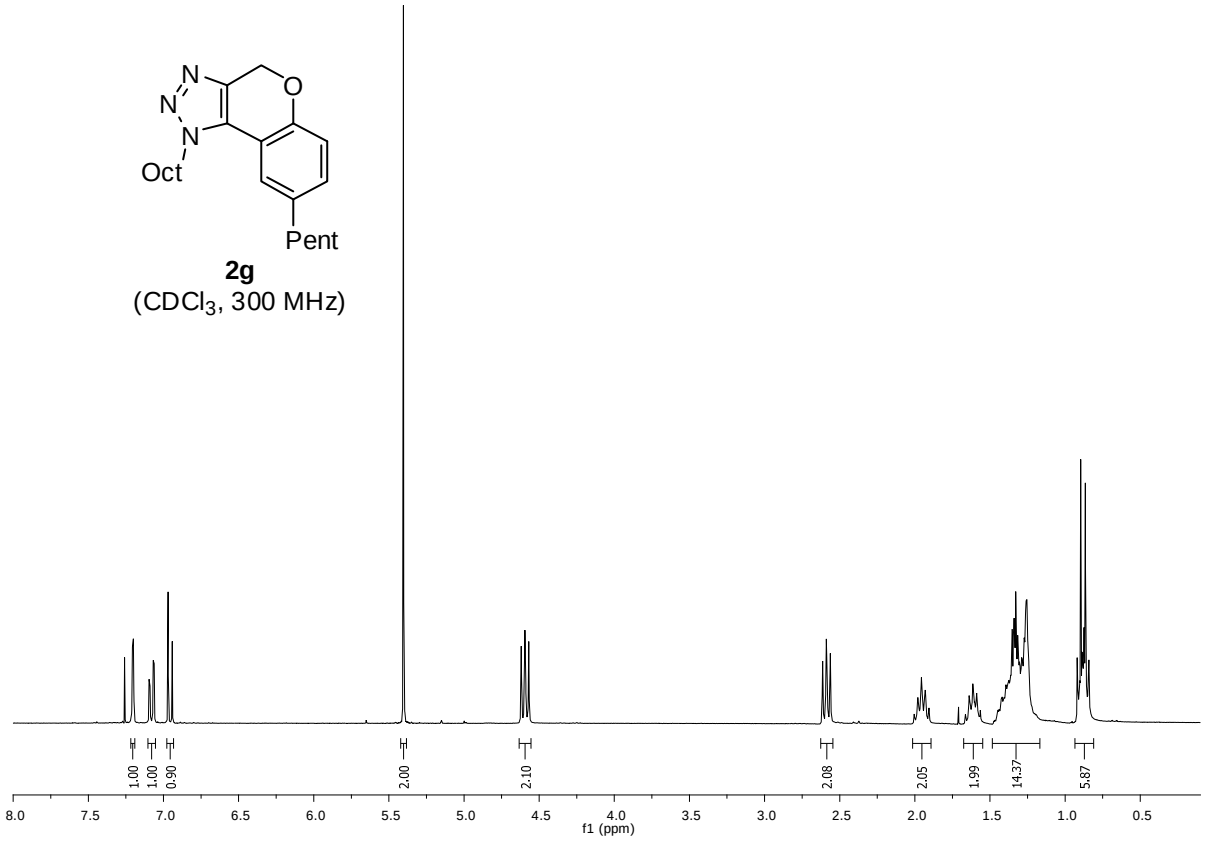


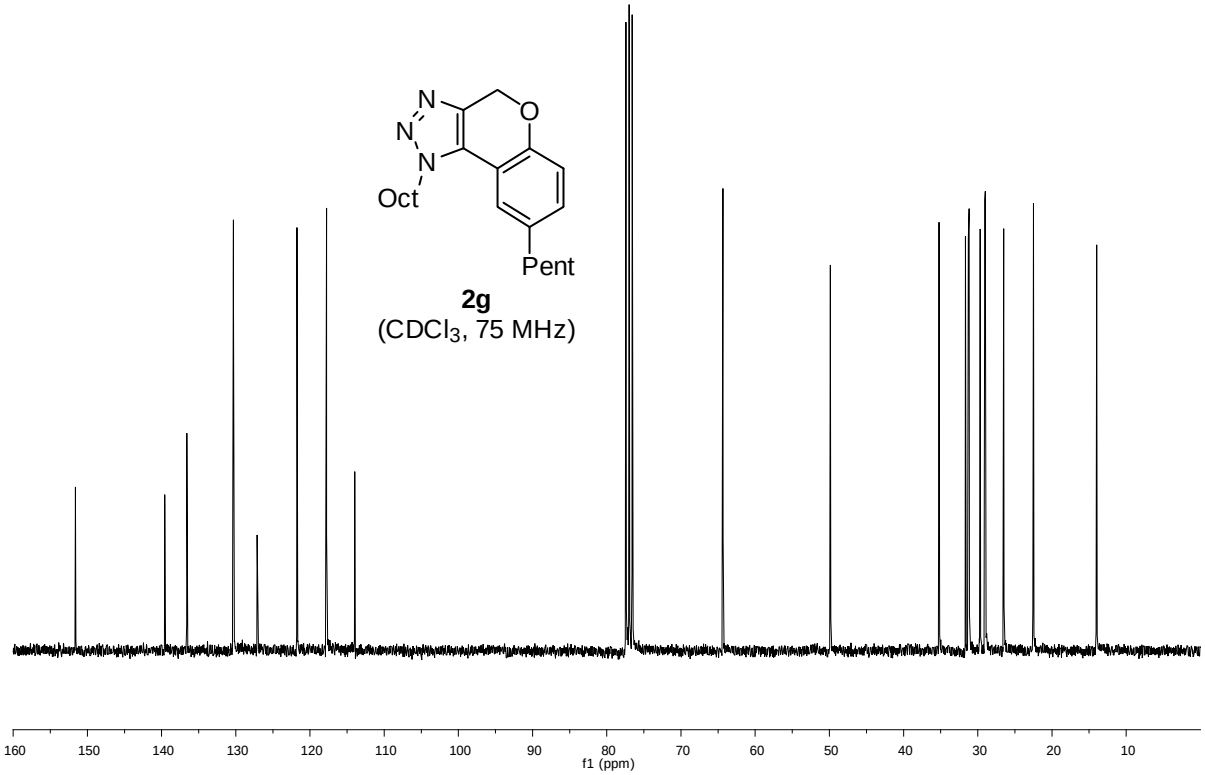


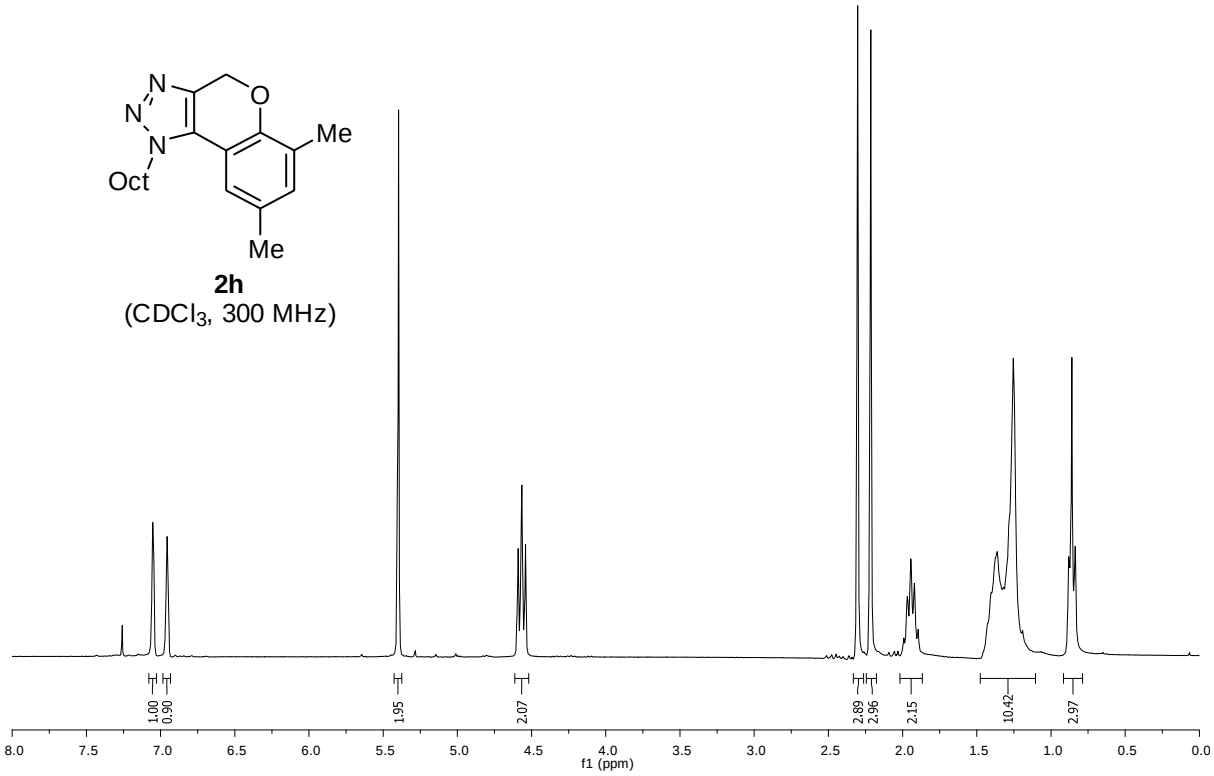
2f

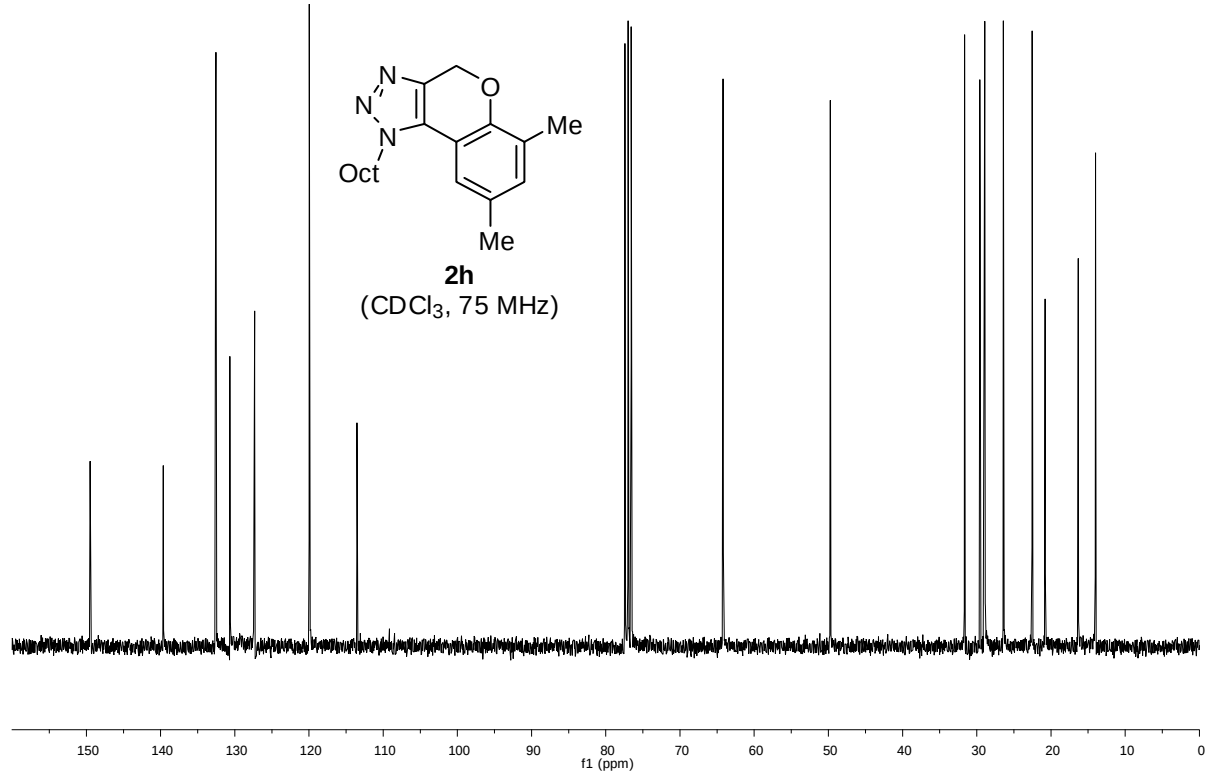
($CDCl_3$, 75 MHz)



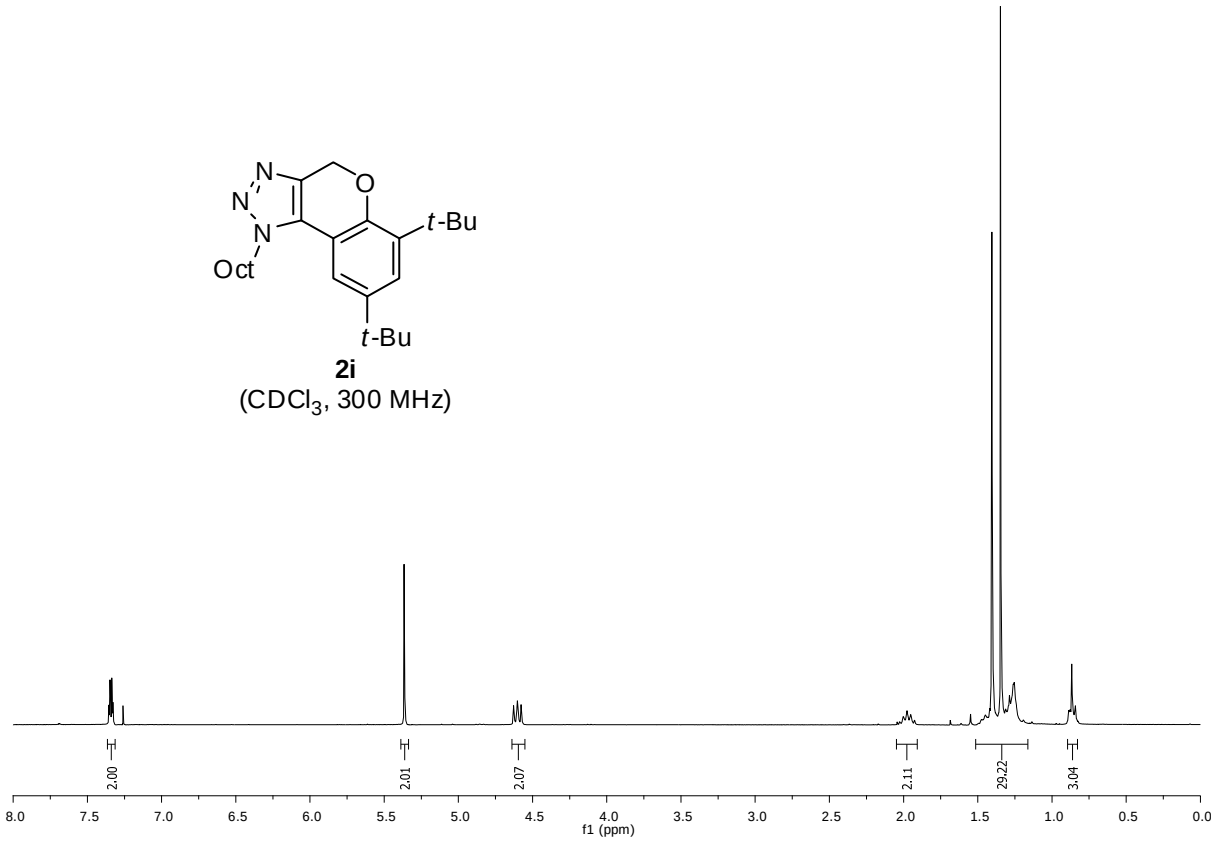

N
N
N
O
Oct
Pent
2g
(CDCl3, 300 MHz)
1.00
1.00
0.90
2.00
2.10
2.08
2.05
1.99
14.37
5.87
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


N
N
N
O
Oct
Pent
2g
(CDCl3, 75 MHz)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

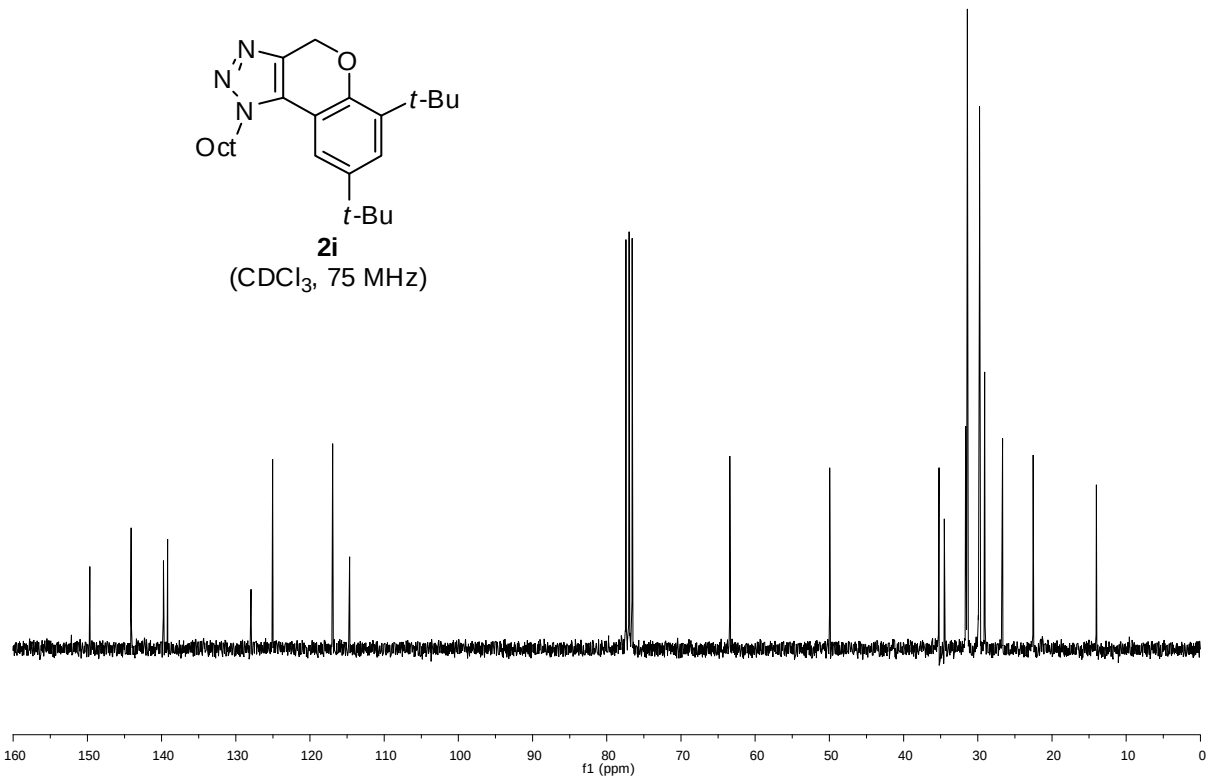

N
N
N
O
Me
Oct
Me
2h
(CDCl3, 300 MHz)
1.00
0.90
1.95
2.07
2.89
2.96
2.15
10.42
2.97
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


N
N
N
O
Me
Oct
Me
2h
(CDCl3, 75 MHz)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

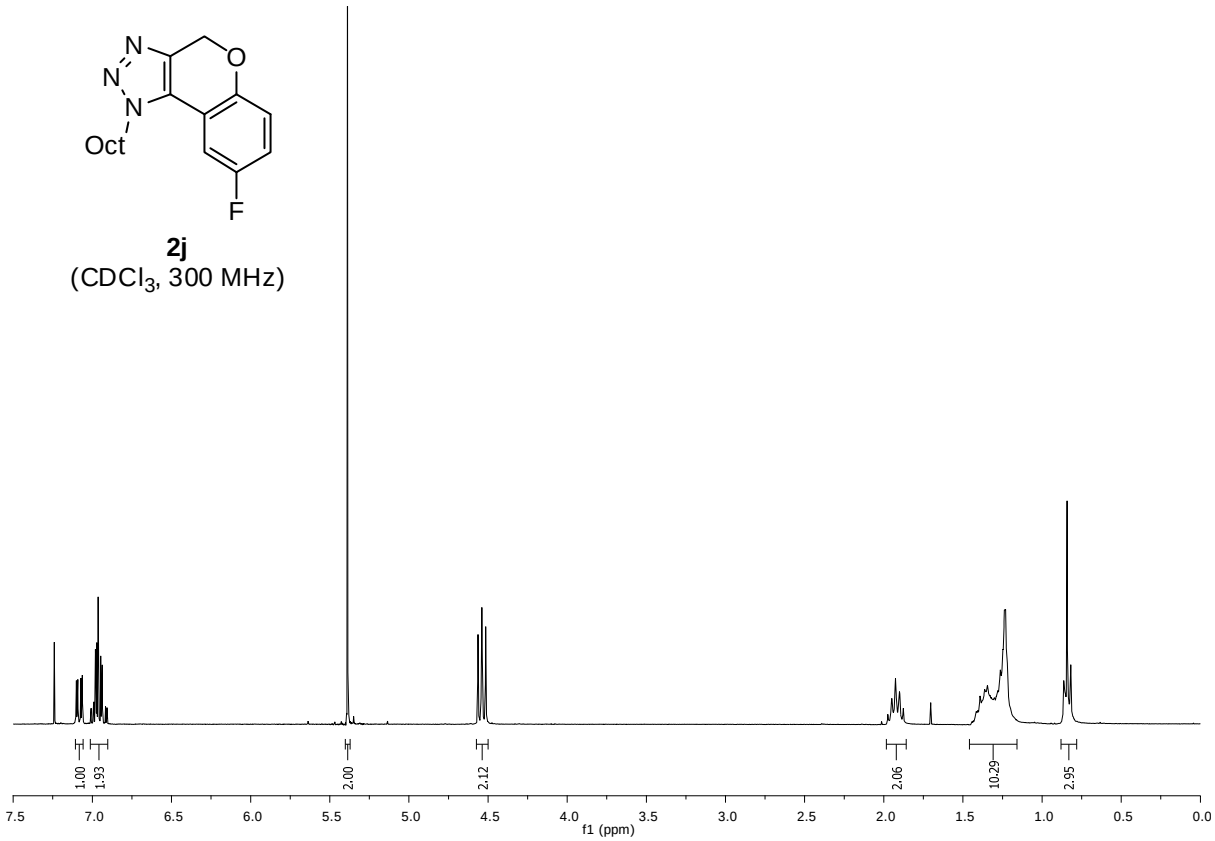
2i
($CDCl_3$, 300 MHz)



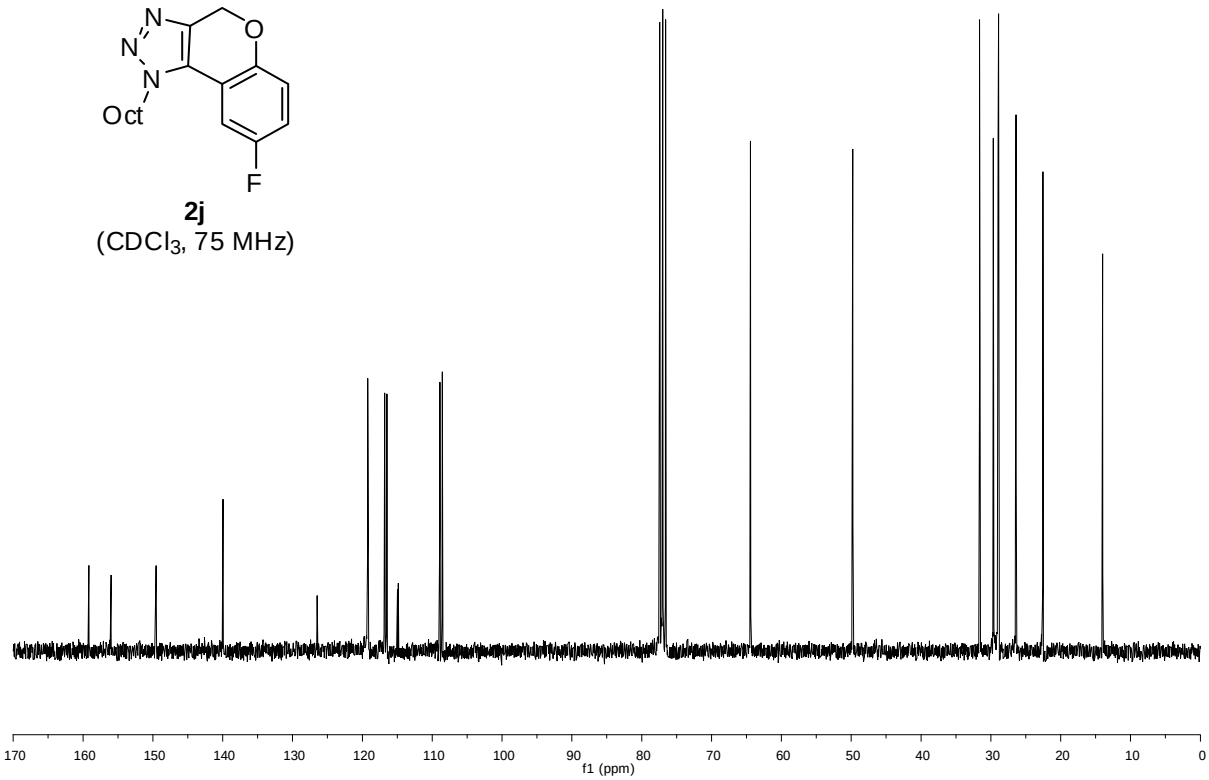
2i
($CDCl_3$, 75 MHz)



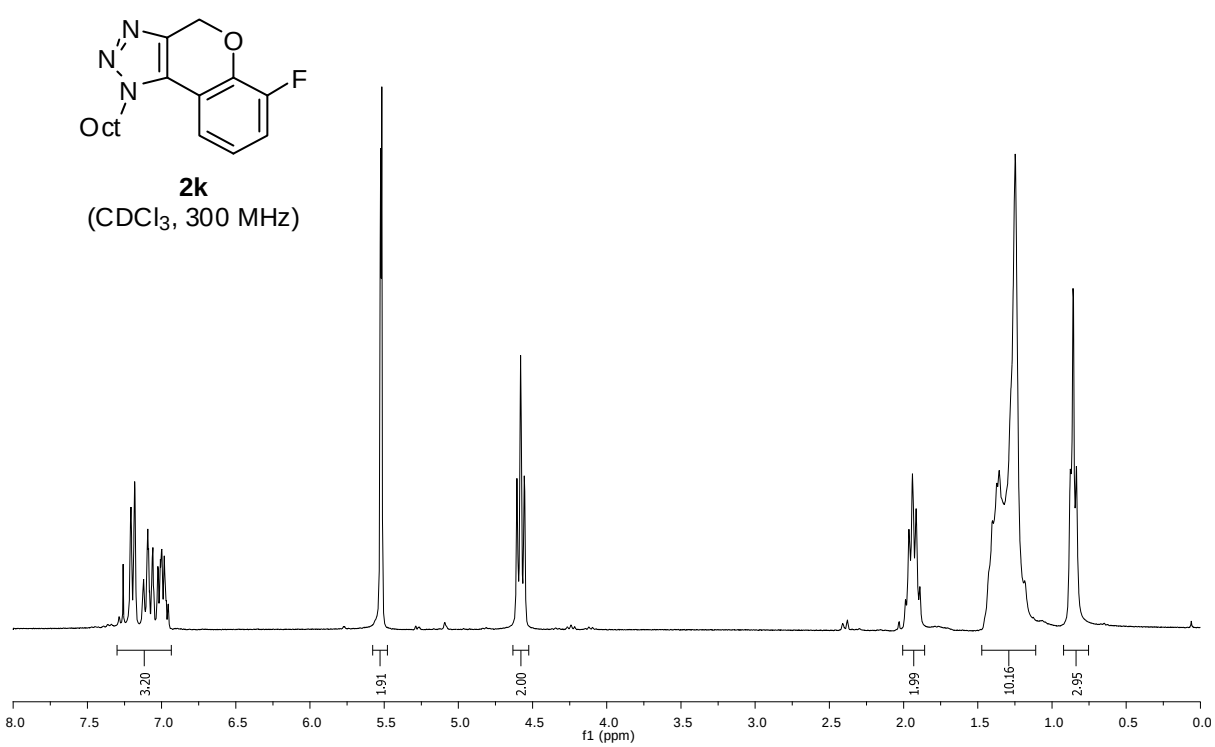
2j
($CDCl_3$, 300 MHz)



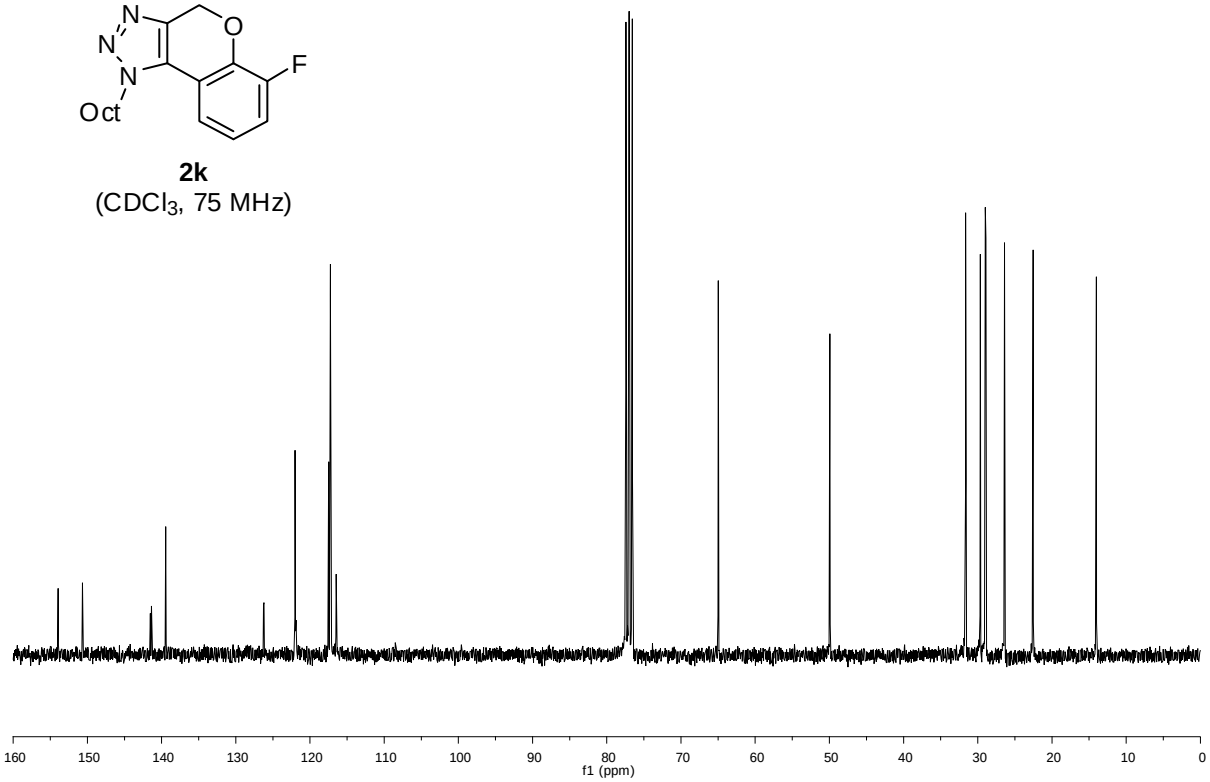
2j
($CDCl_3$, 75 MHz)

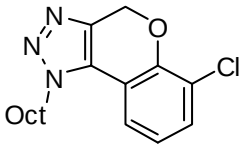


2k
($CDCl_3$, 300 MHz)



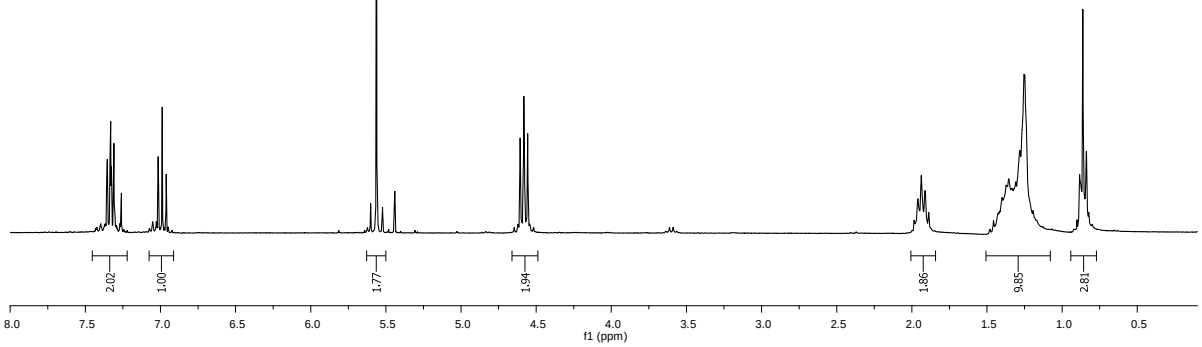
2k
($CDCl_3$, 75 MHz)





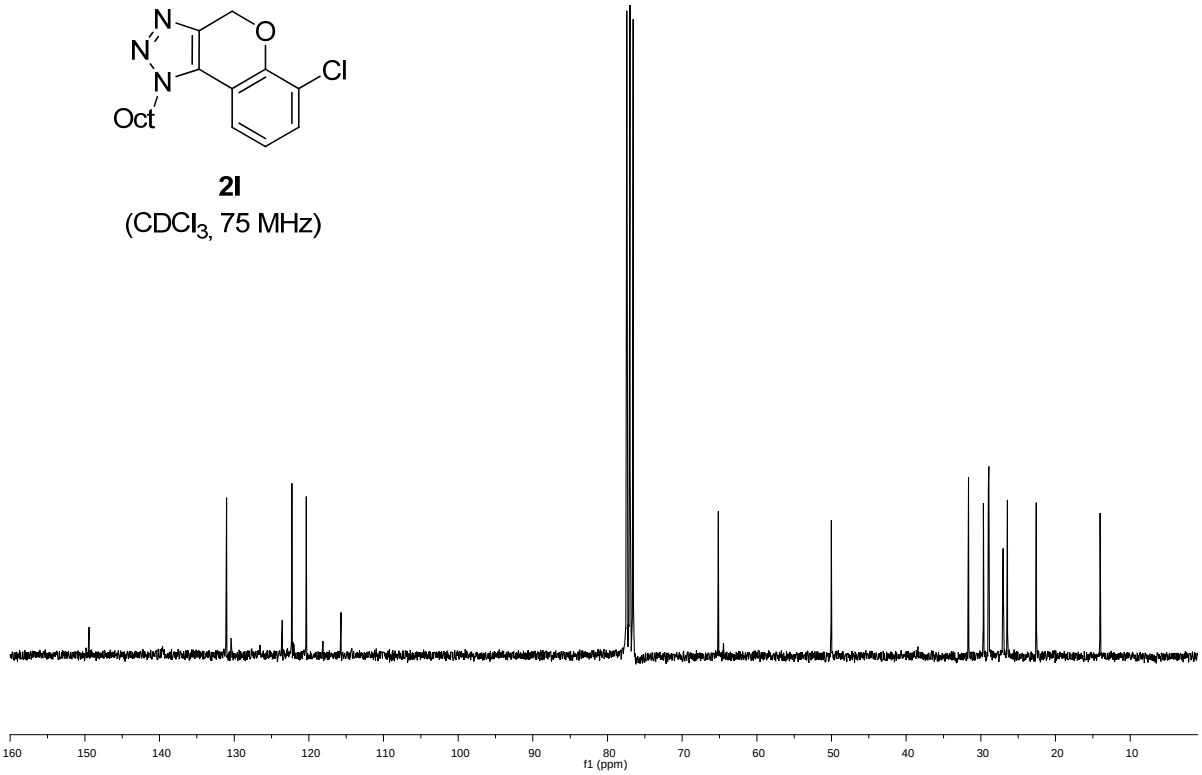
2l

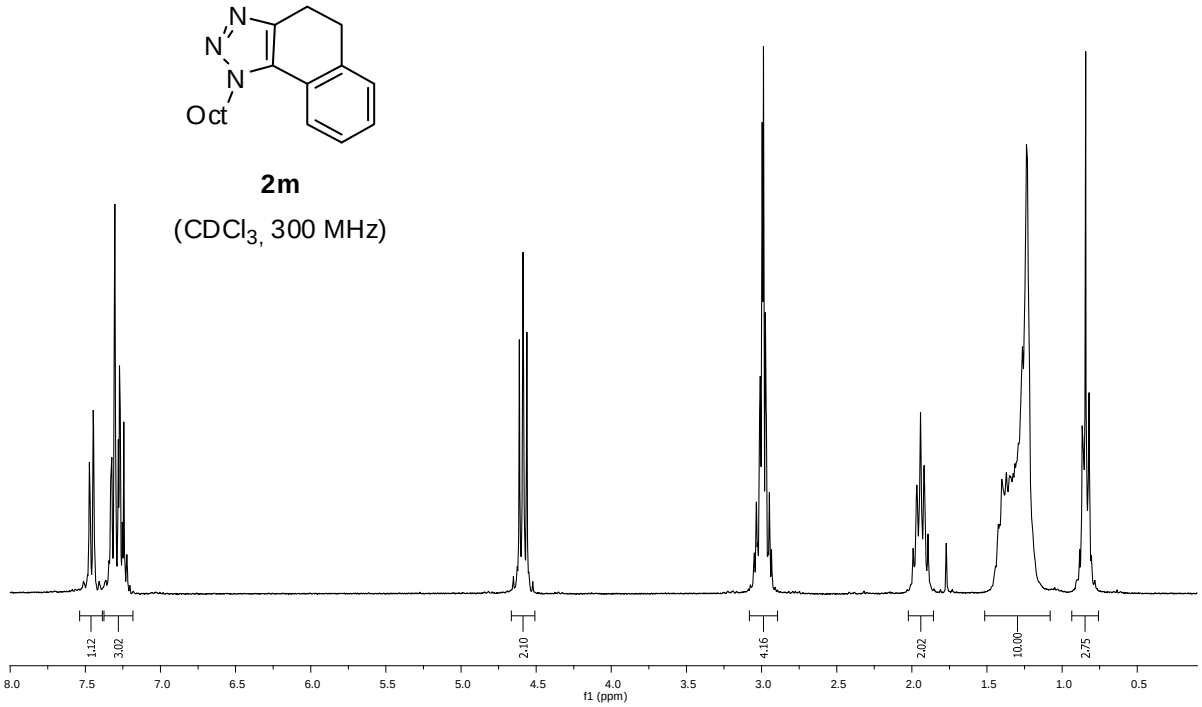
($CDCl_3$, 300 MHz)

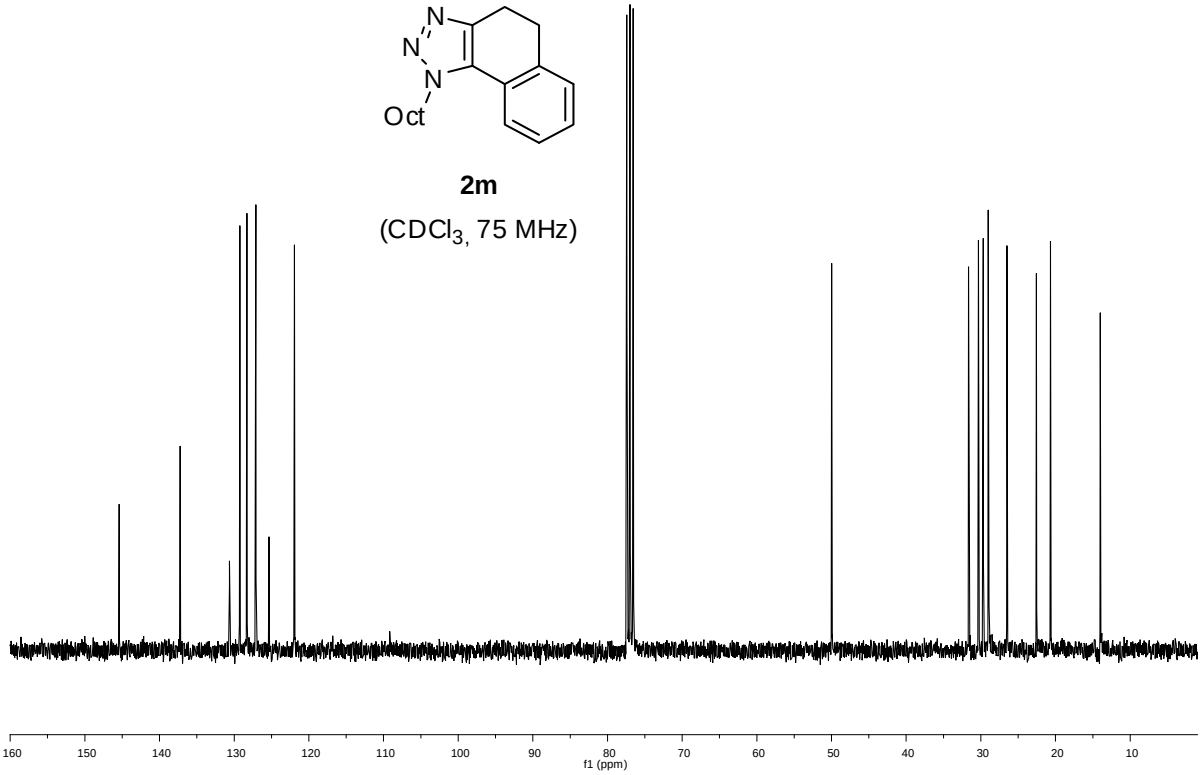


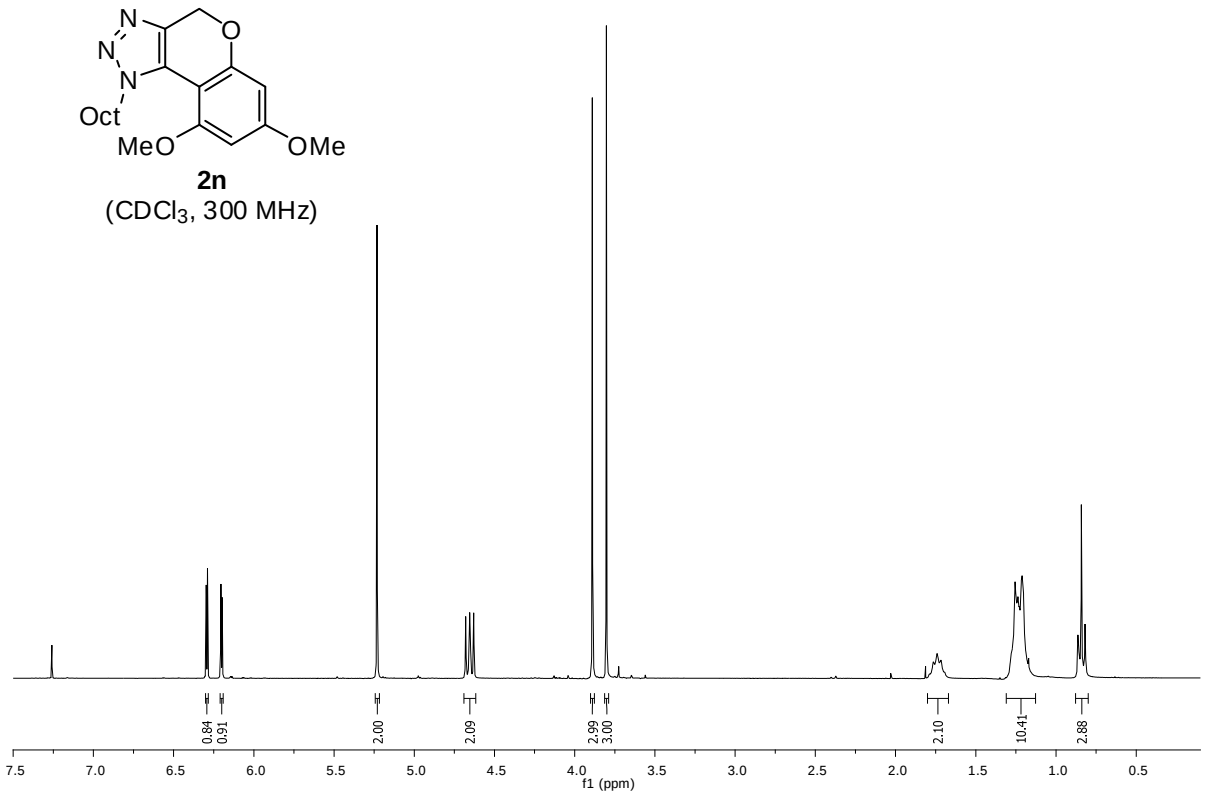
2l

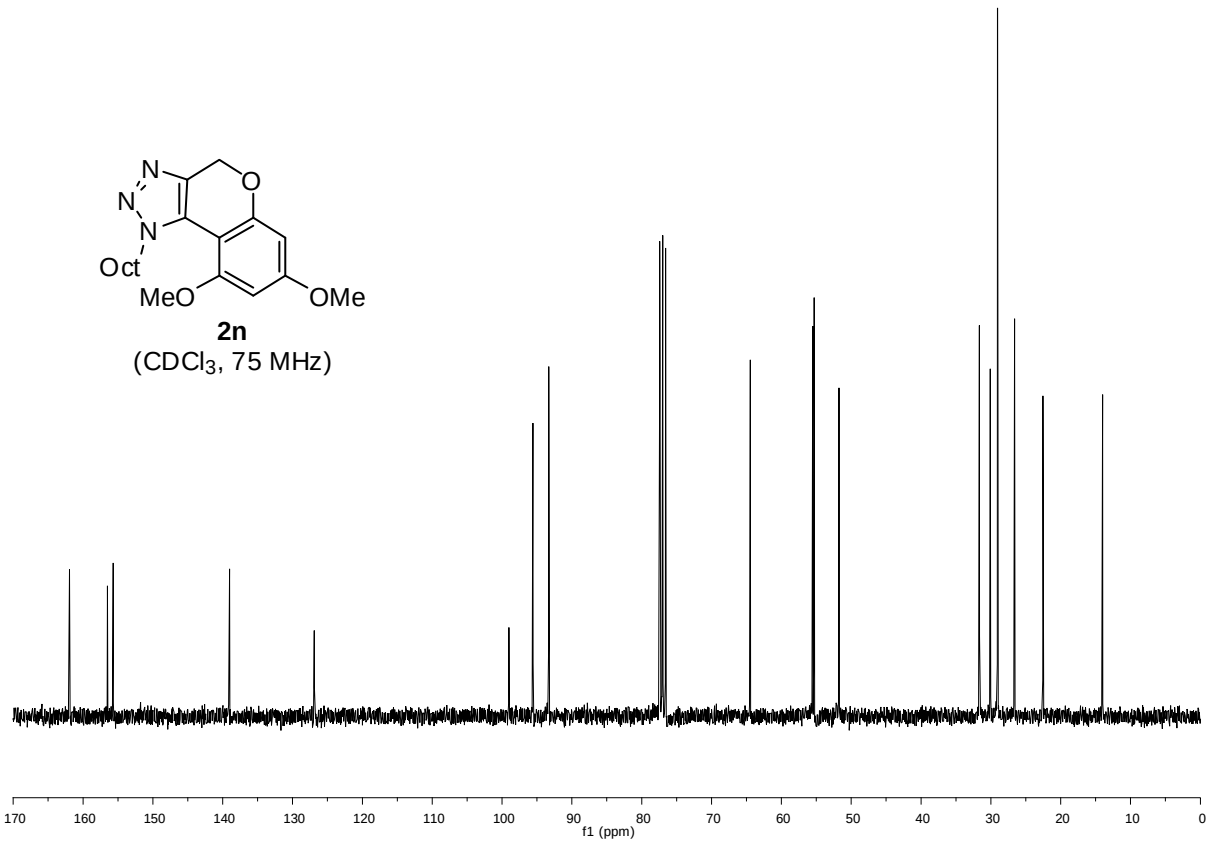
($CDCl_3$, 75 MHz)

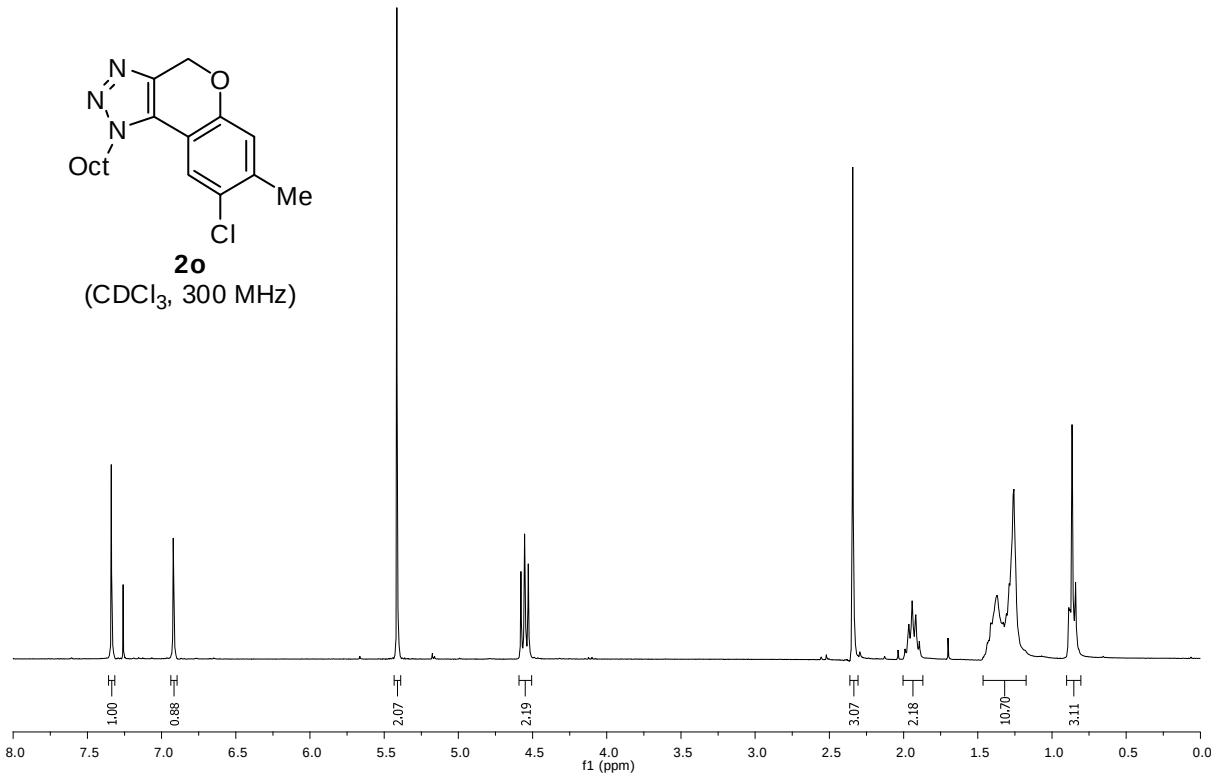



N
N
N
Oct
2m
(CDCl3, 300 MHz)
1.12
3.02
2.10
4.16
2.02
10.00
2.75
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

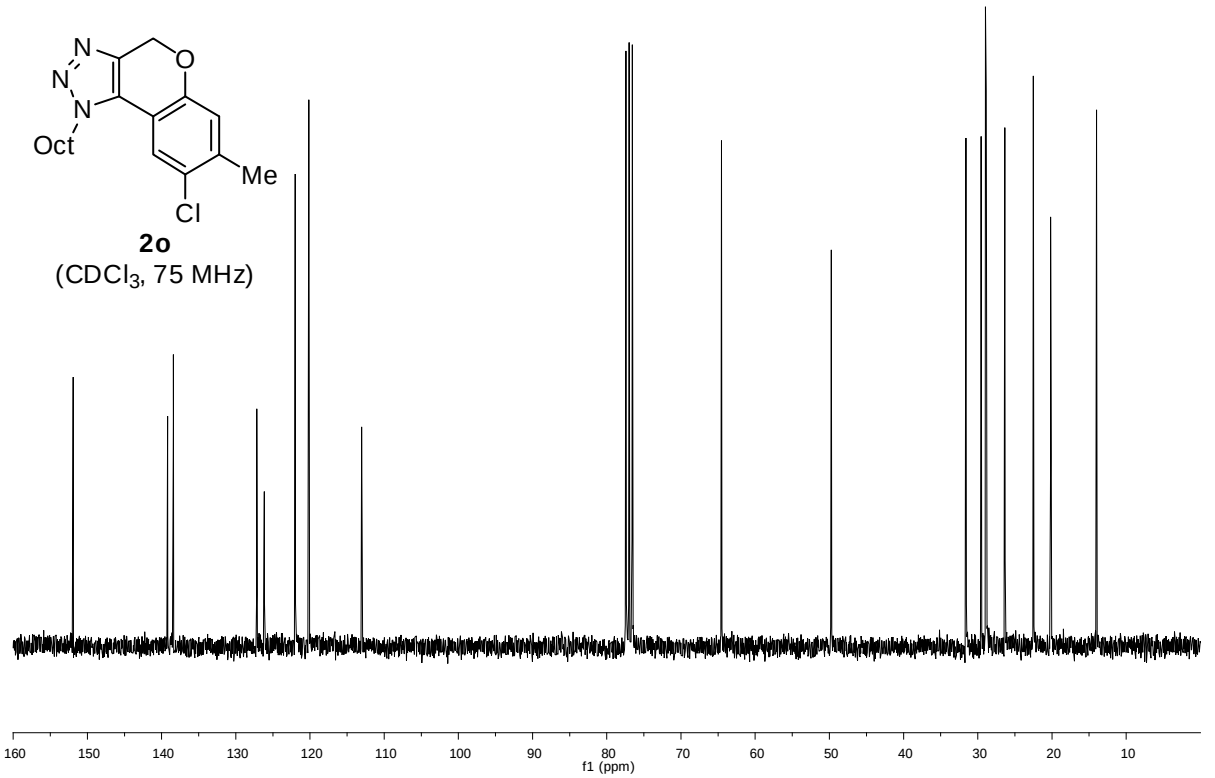

N
N
N
Oct
2m
(CDCl3, 75 MHz)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


N
N
N
O
Oct
MeO
OMe
2n
(CDCl3, 300 MHz)
0.84
0.91
2.00
2.09
2.99
3.00
2.10
10.41
2.88
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)

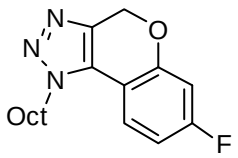

N
N
N
O
Oct
MeO
OMe
2n
(CDCl3, 75 MHz)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



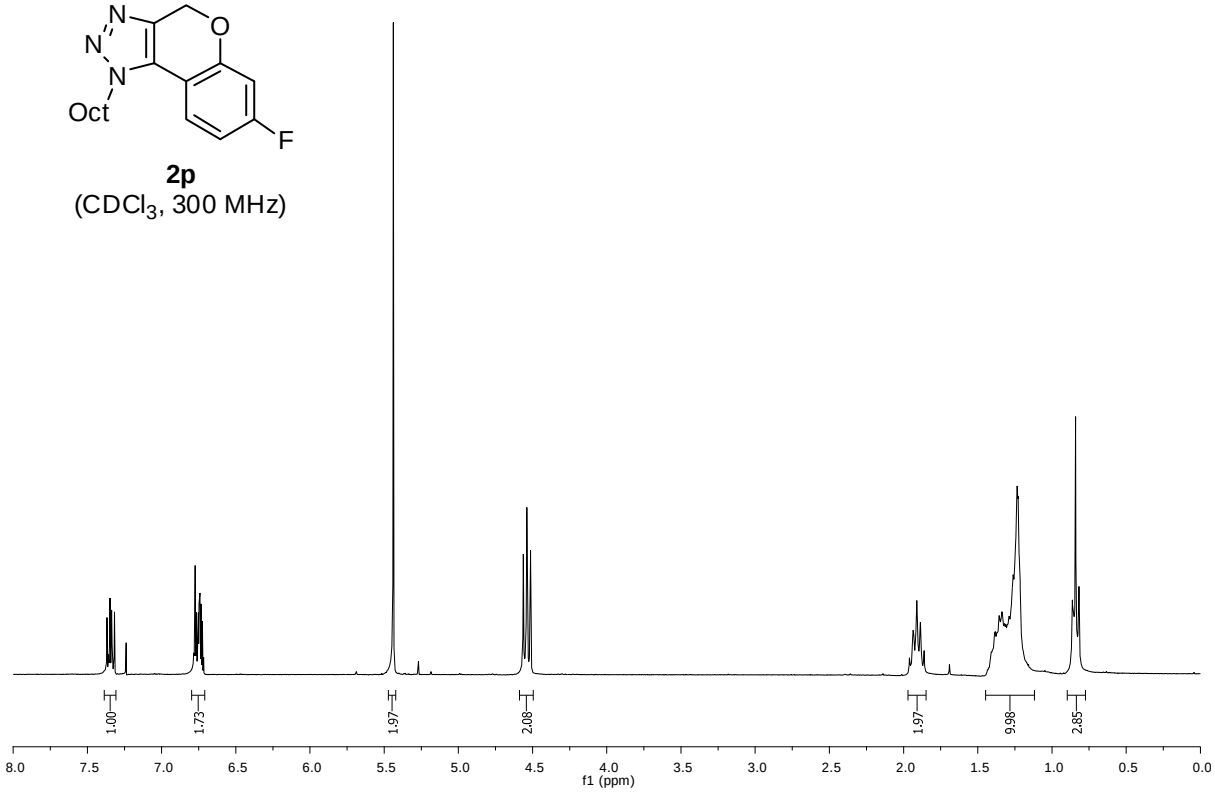
2o
($CDCl_3$, 300 MHz)



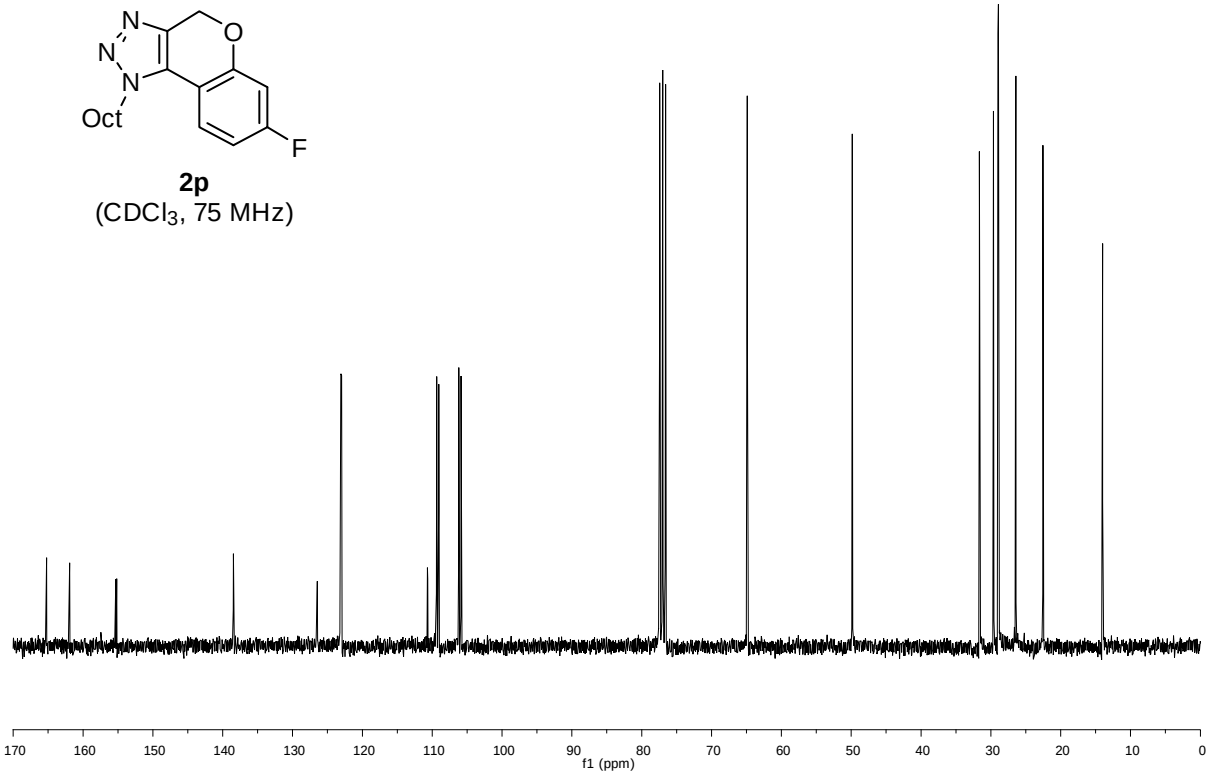
2o
($CDCl_3$, 75 MHz)



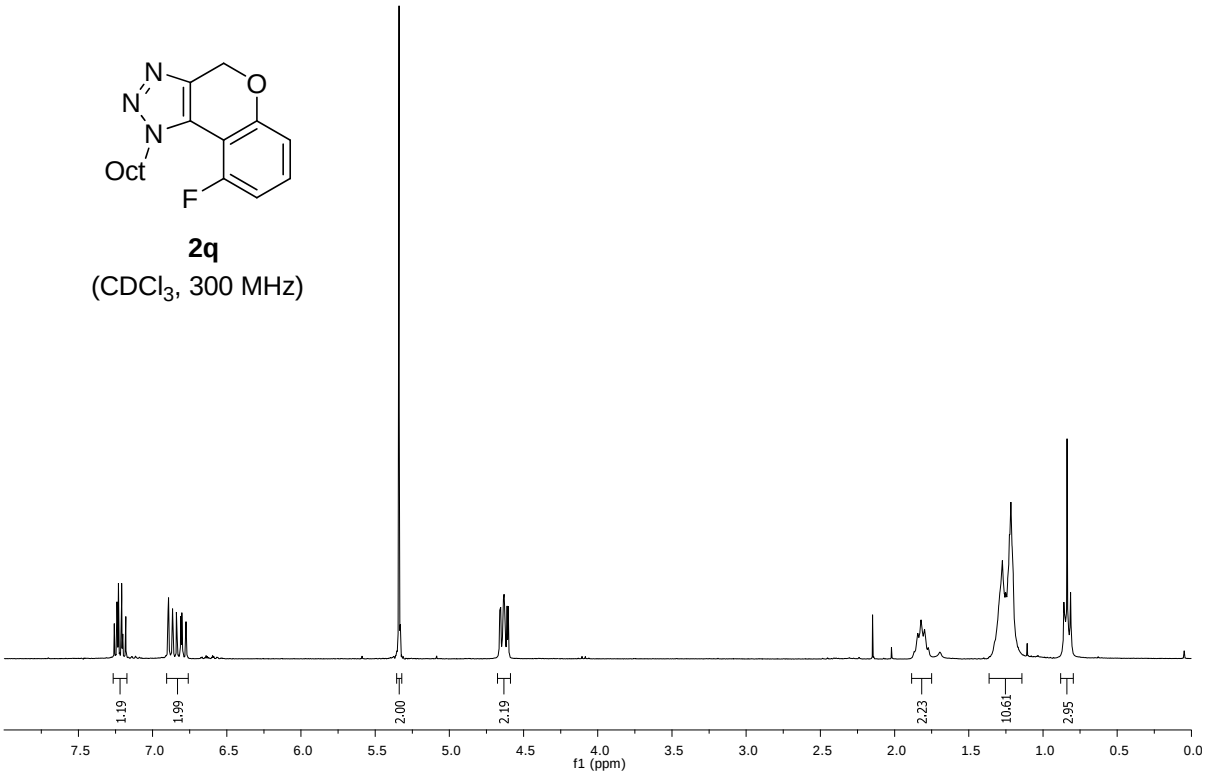
2p
($CDCl_3$, 300 MHz)



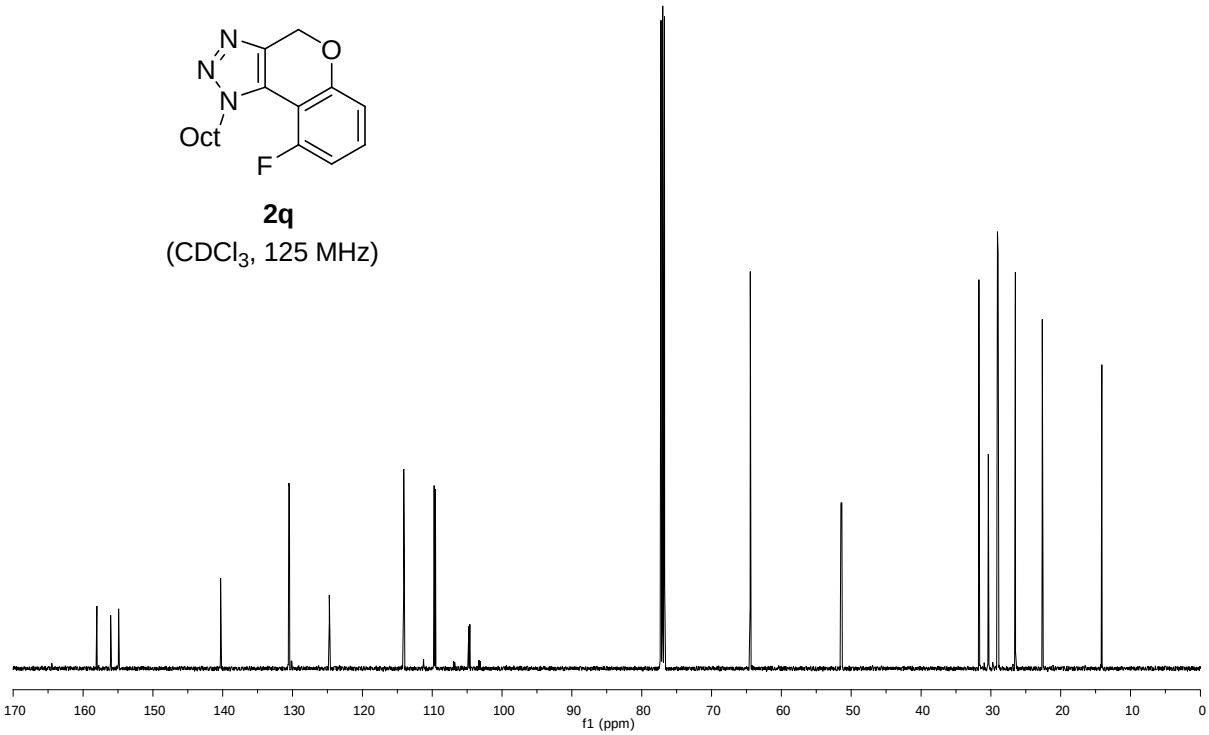
2p
($CDCl_3$, 75 MHz)

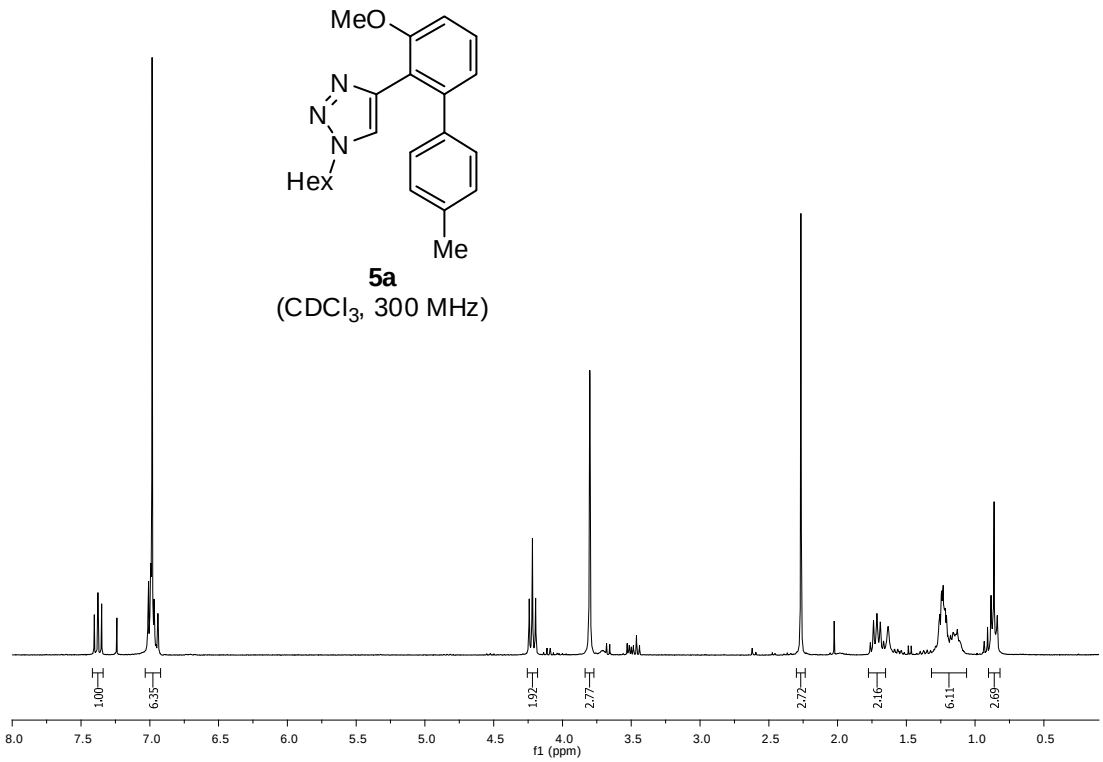


2q
($CDCl_3$, 300 MHz)

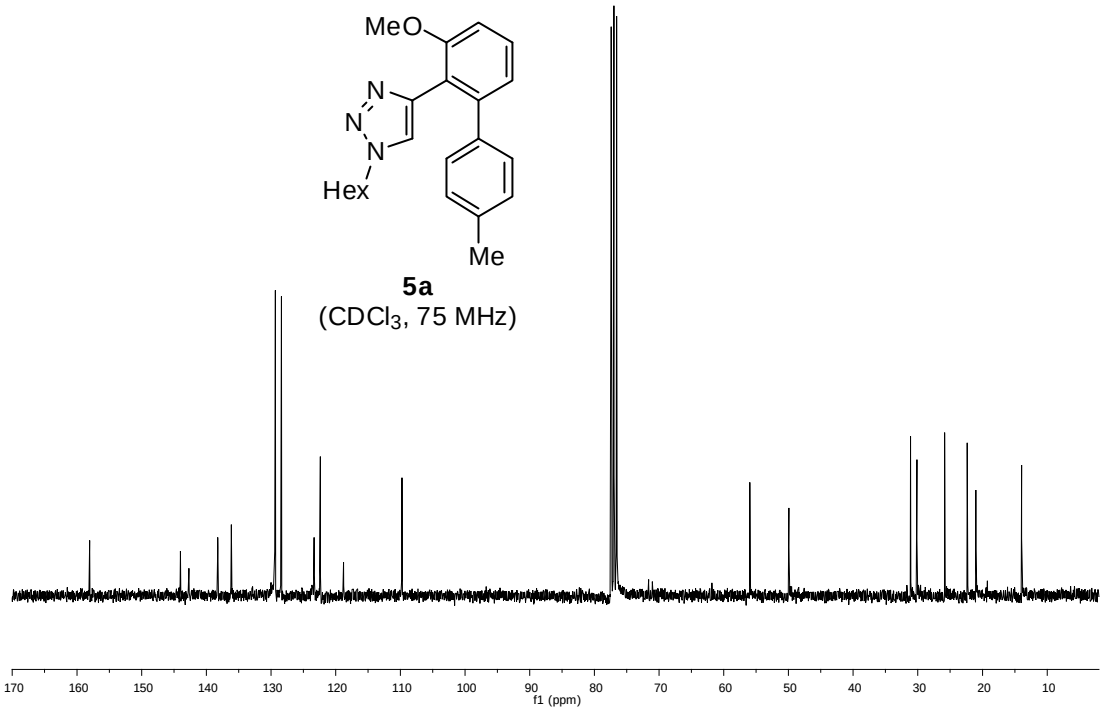


2q
($CDCl_3$, 125 MHz)

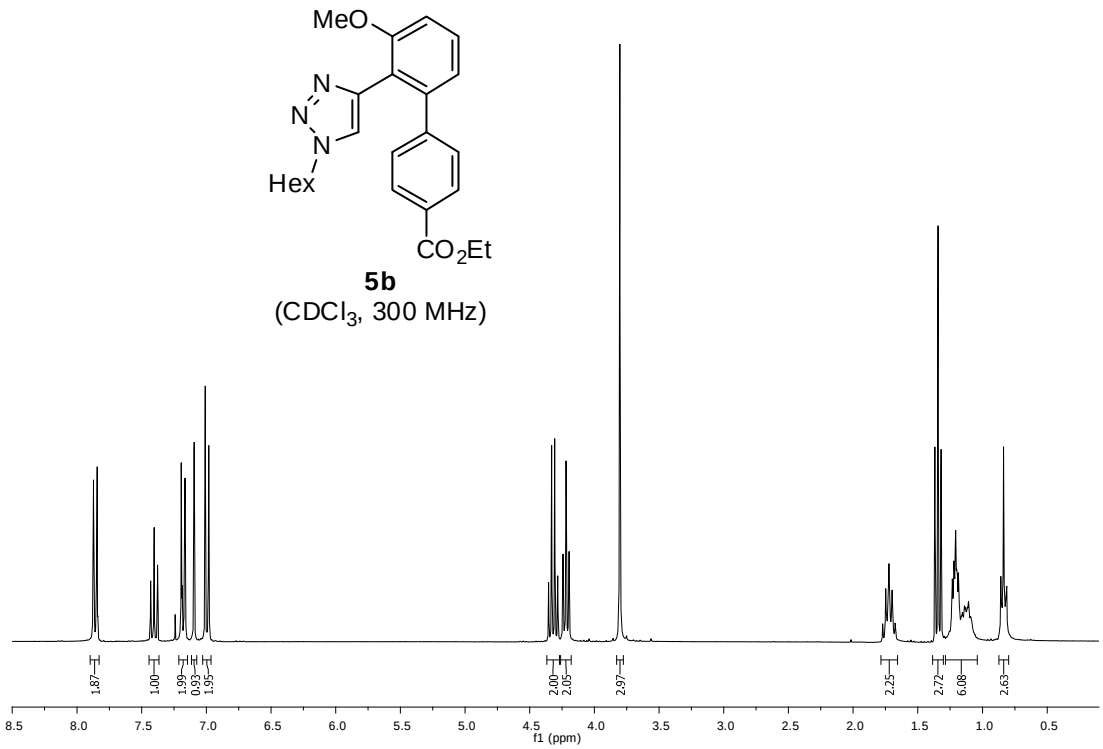


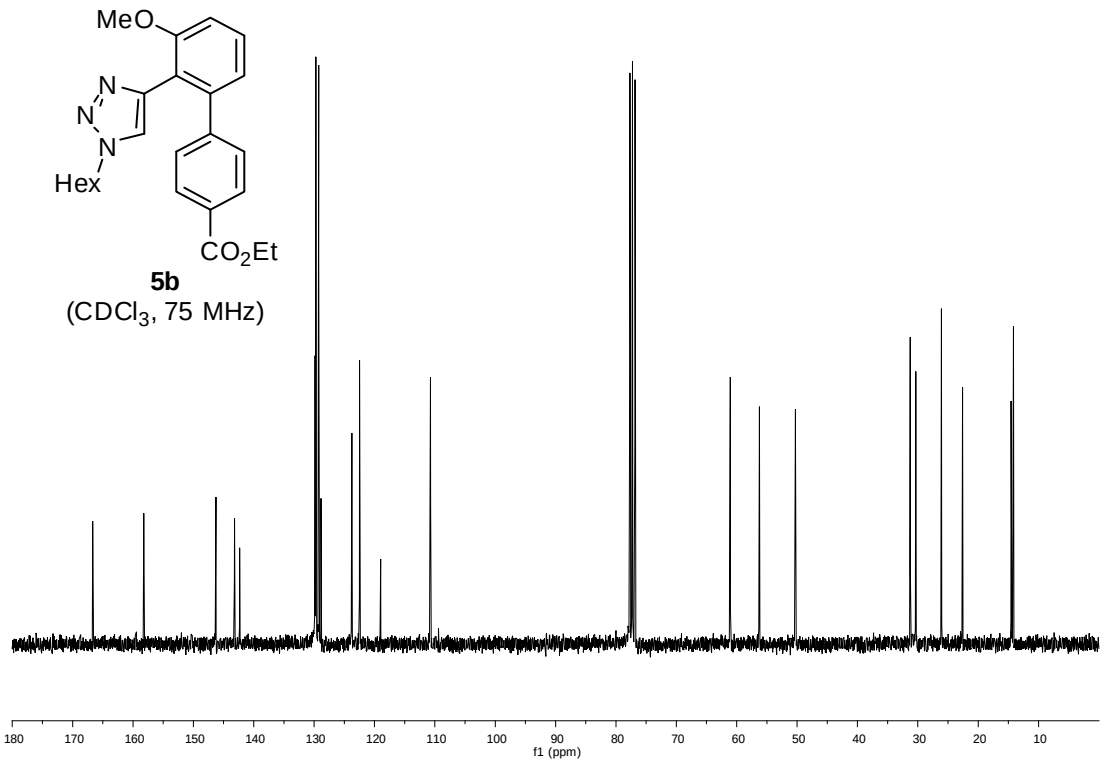


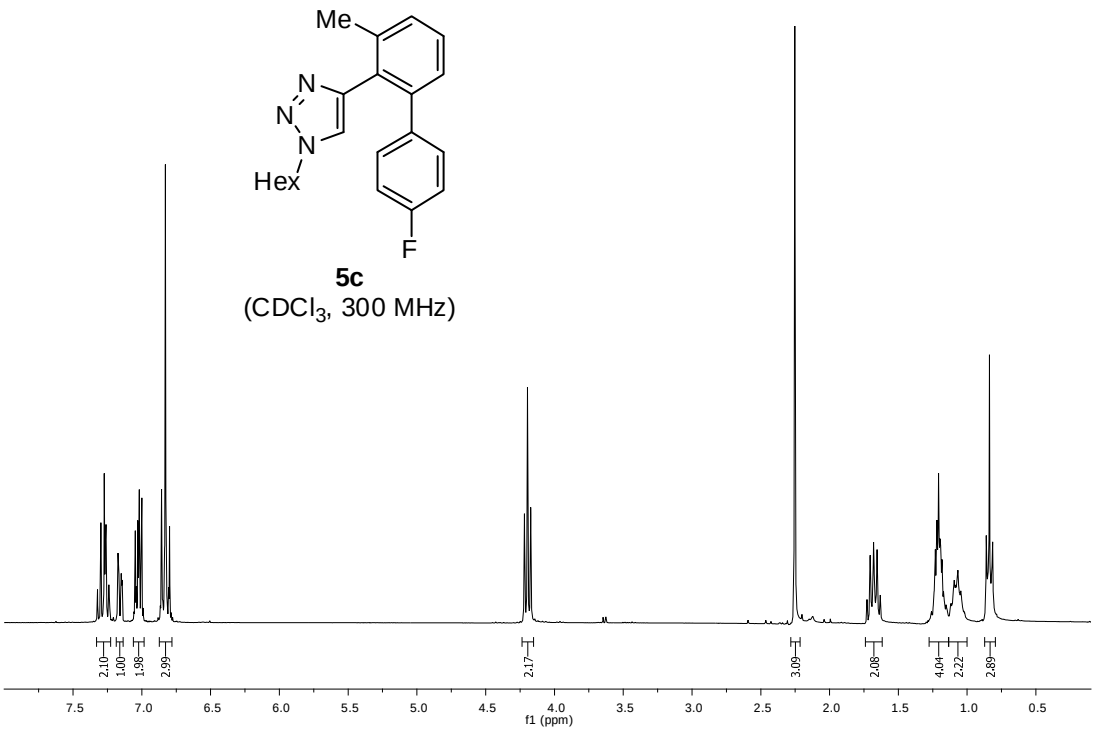
5a
($CDCl_3$, 300 MHz)

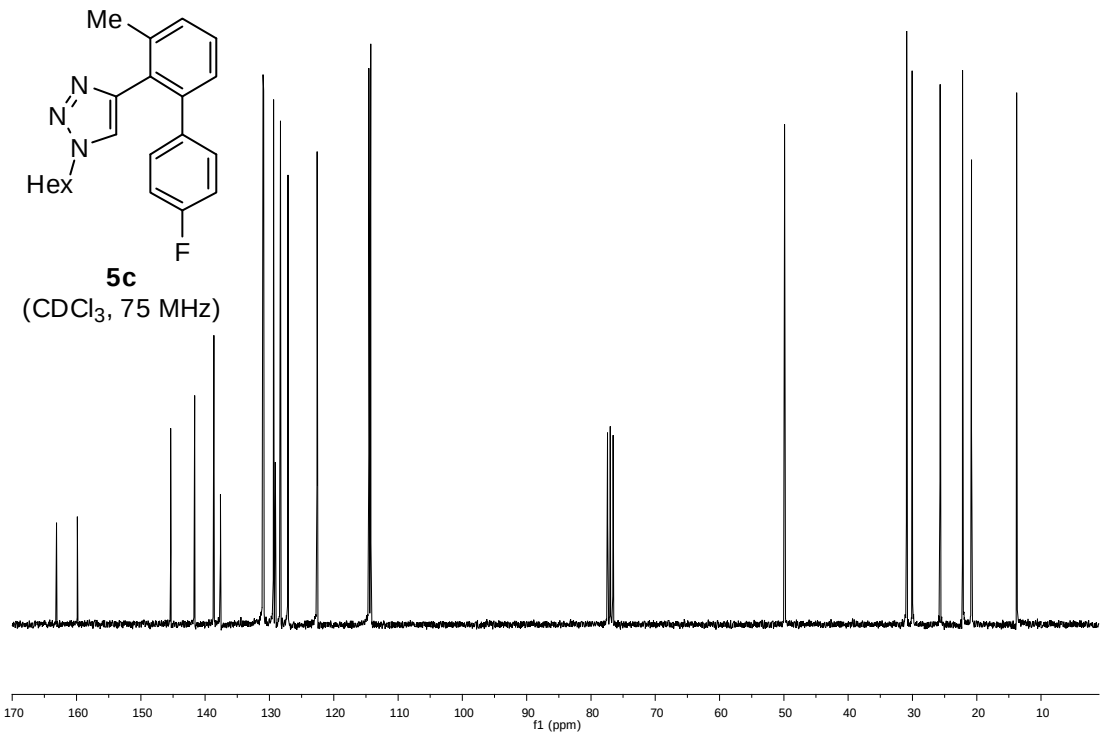


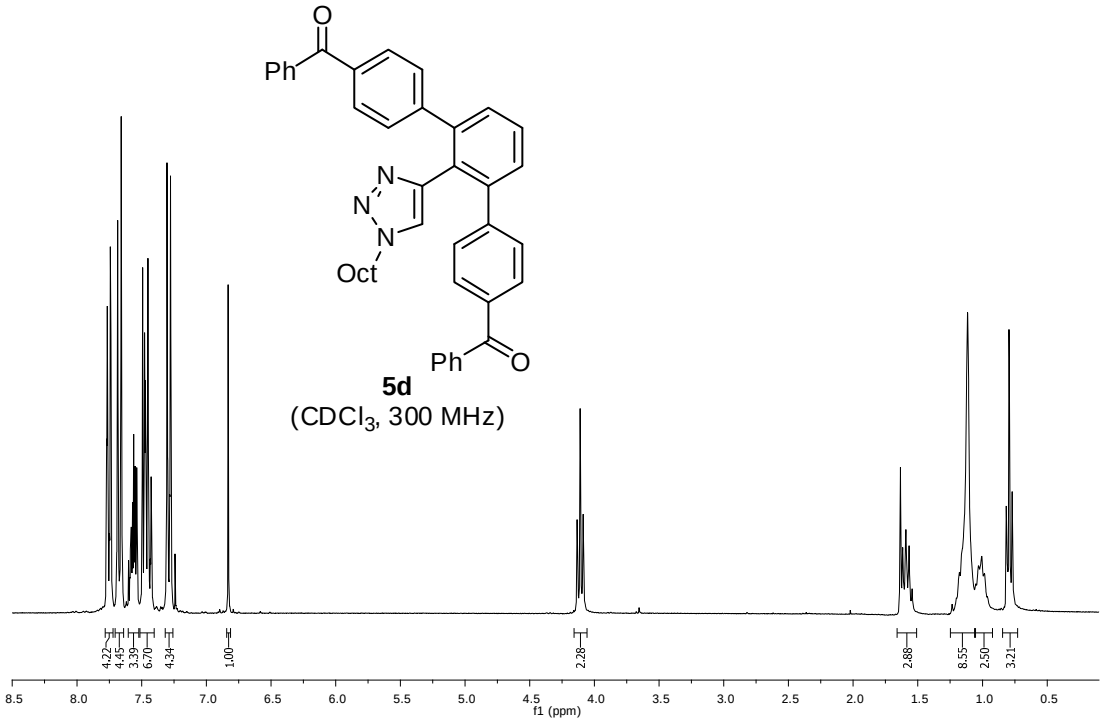
5a
($CDCl_3$, 75 MHz)


MeO
N
N
N
Hex
CO2Et
5b
(CDCl3, 300 MHz)
1.87
1.00
1.99
0.93
1.95
2.00
2.05
2.97
2.25
2.72
6.08
2.63
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

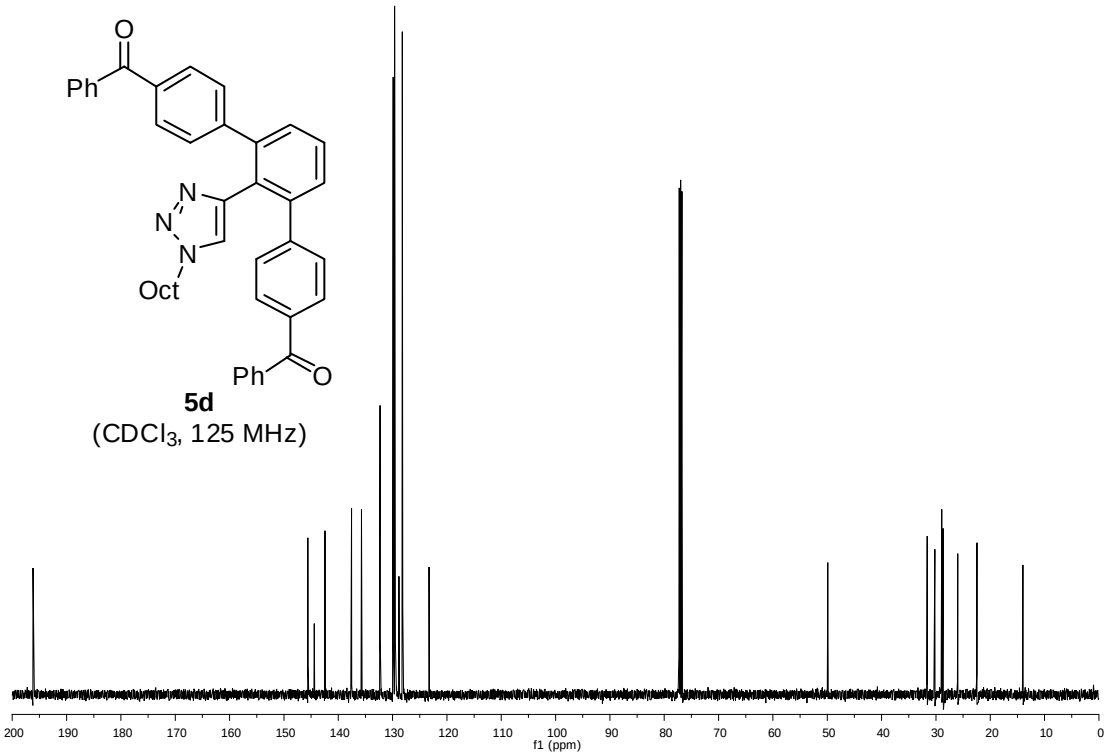

MeO
N
N
N
Hex
CO2Et
5b
(CDCl3, 75 MHz)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


Me
N
N
N
Hex
F
5c
(CDCl3, 300 MHz)
2.10
1.00
1.98
2.99
2.17
3.09
2.08
4.04
2.22
2.89
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)

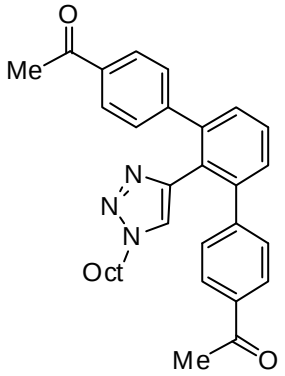

Me
N
N
N
Hex
F
5c
(CDCl3, 75 MHz)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)



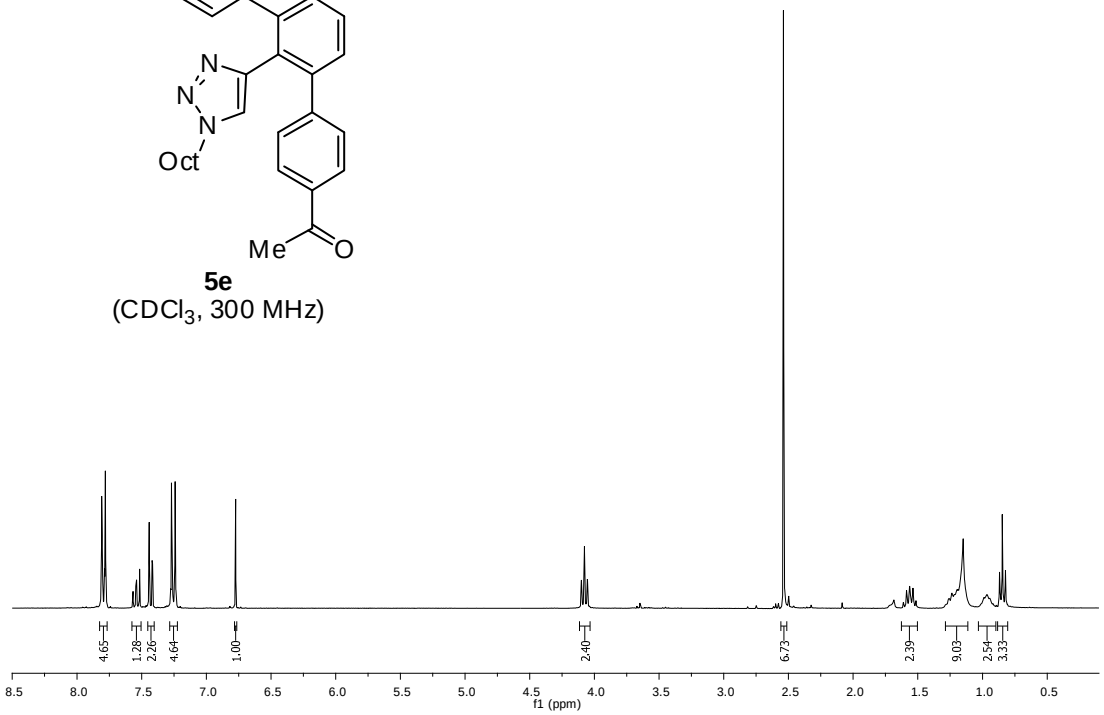
5d
($CDCl_3$, 300 MHz)



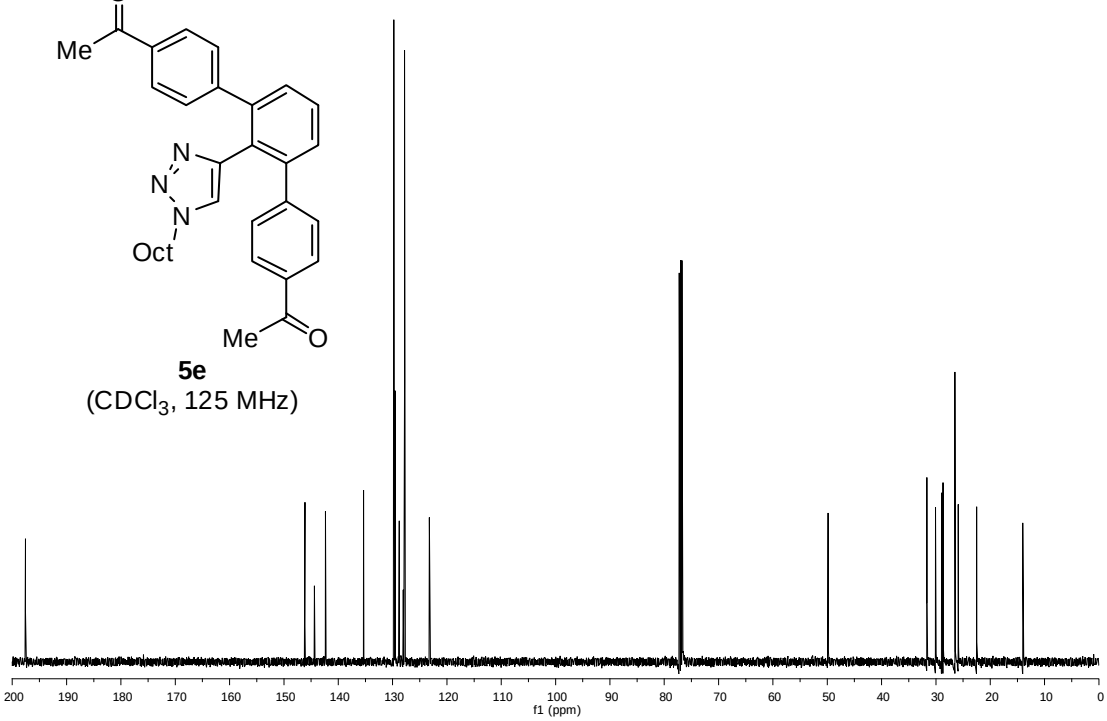
5d
($CDCl_3$, 125 MHz)

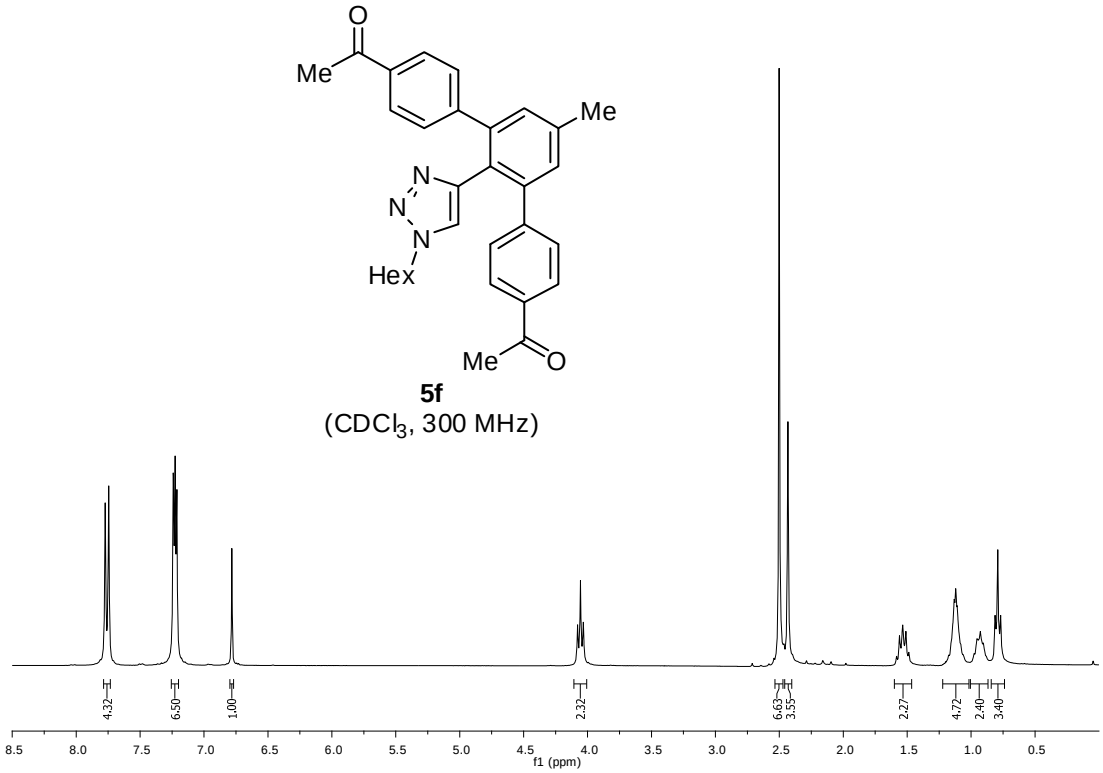


5e
($CDCl_3$, 300 MHz)

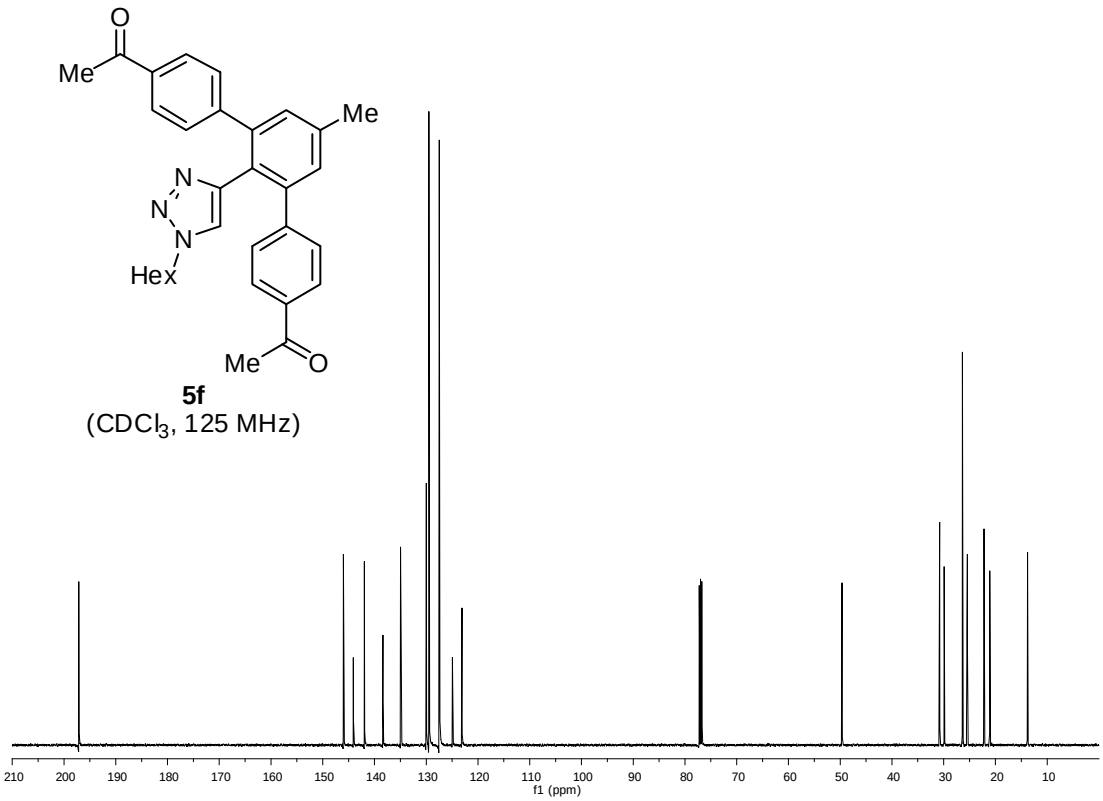


5e
($CDCl_3$, 125 MHz)

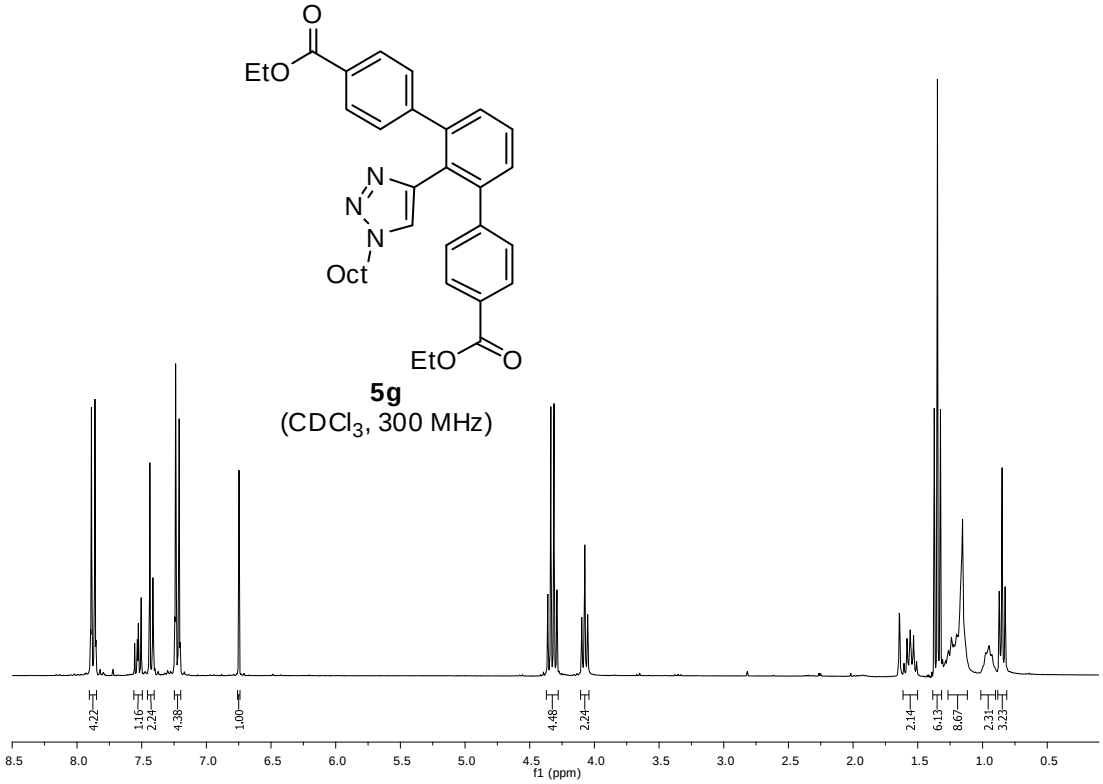


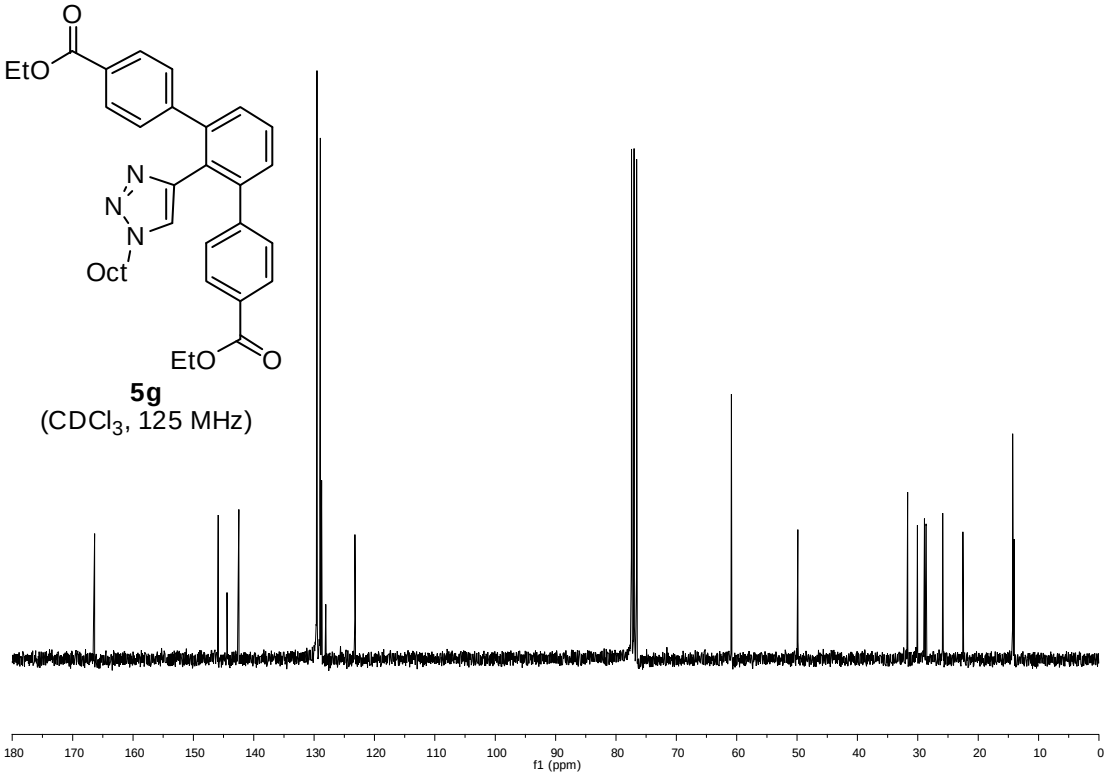


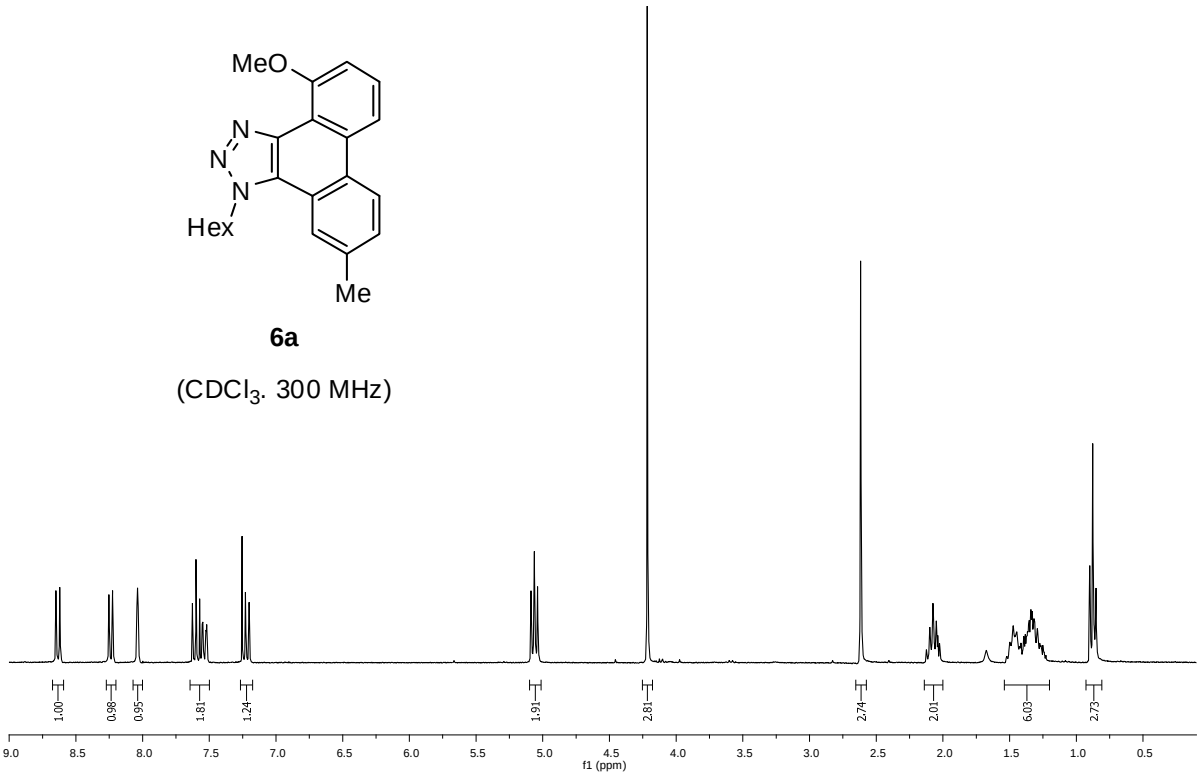
5f
($CDCl_3$, 300 MHz)

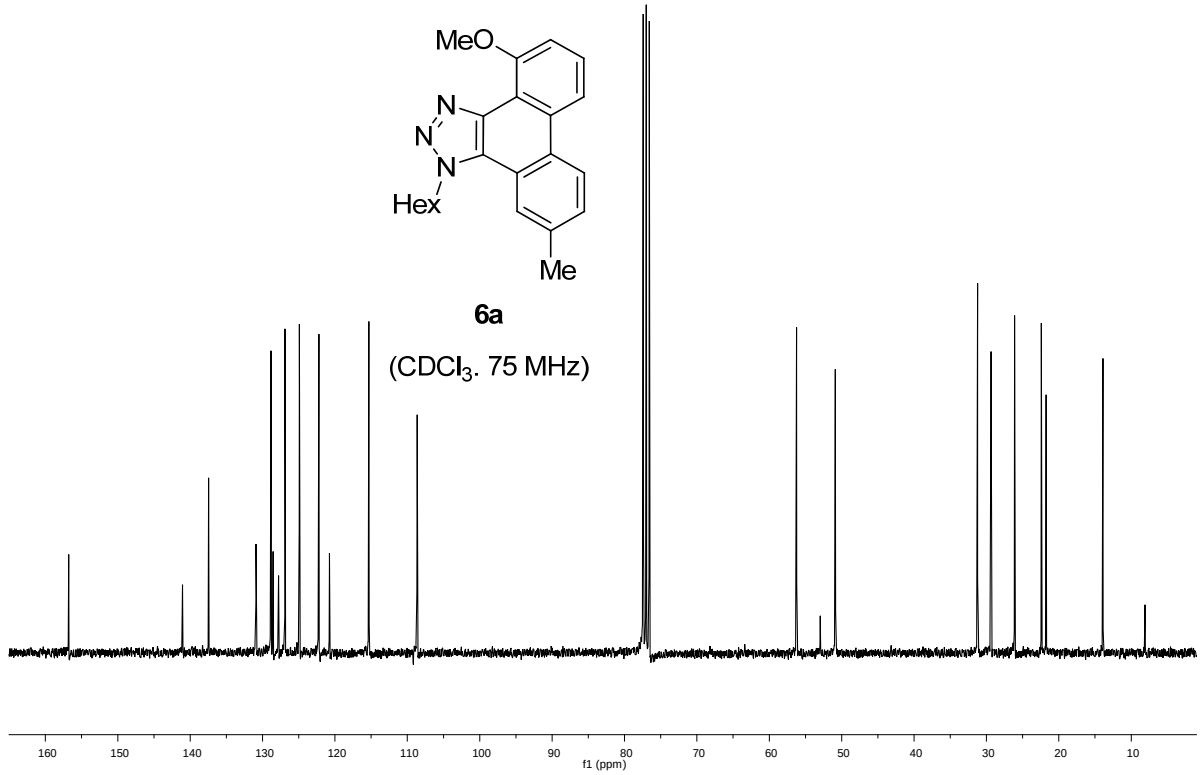


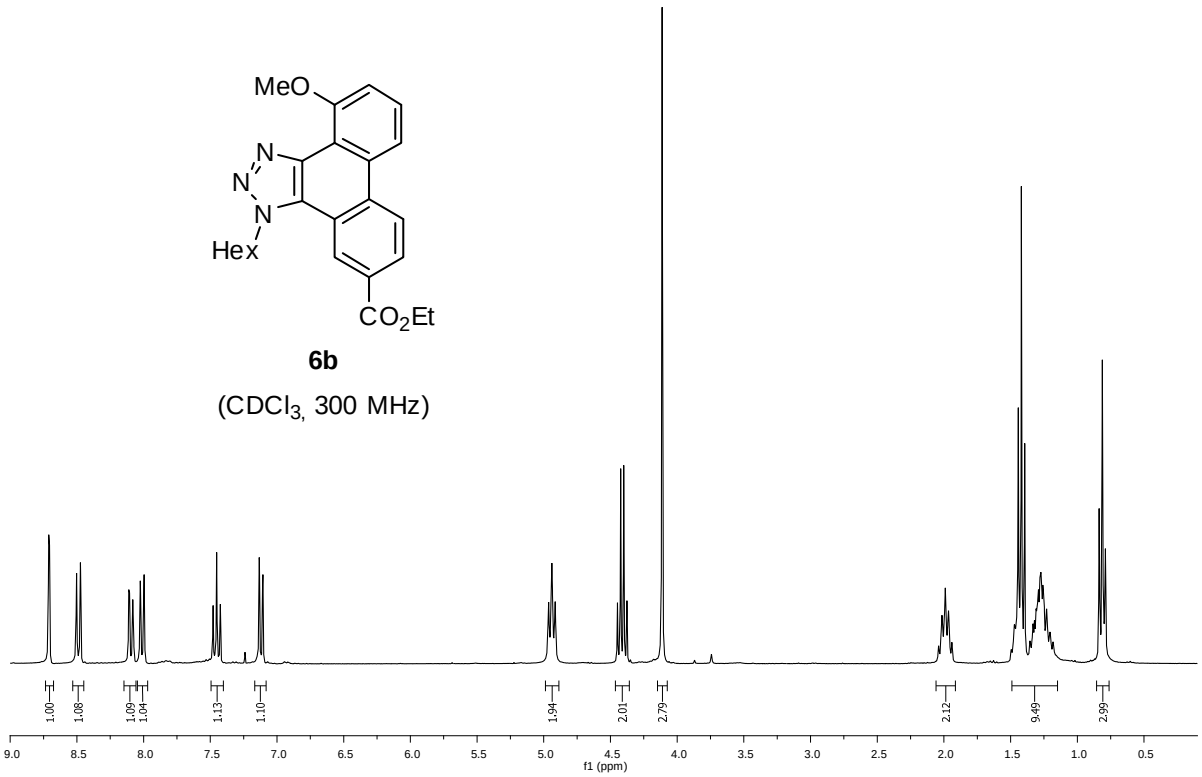
5f
($CDCl_3$, 125 MHz)

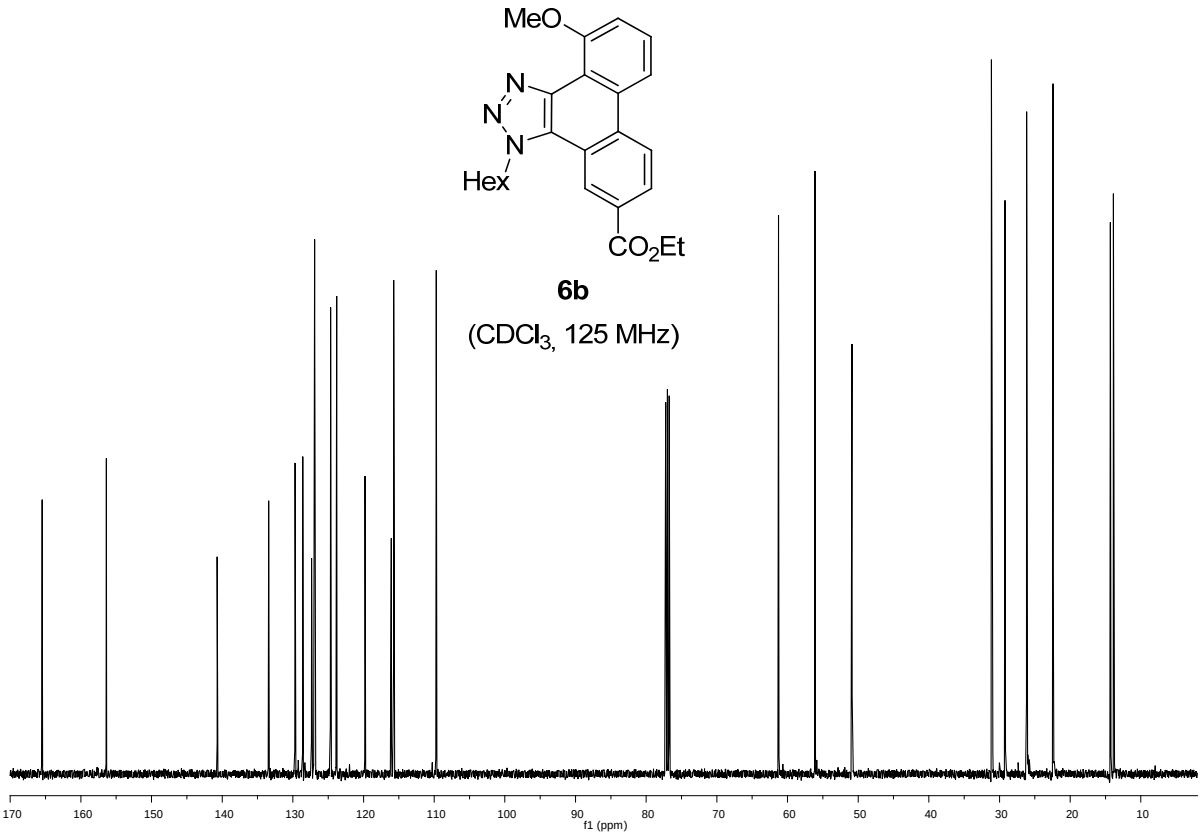

O
EtO
N
N
N
Oct
EtO
O
5g
(CDCl3, 300 MHz)
4.22
1.16
2.24
4.38
1.00
4.48
2.24
2.14
6.13
8.67
2.31
3.23
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


O
EtO
N
N
N
Oct
EtO
O
5g
(CDCl3, 125 MHz)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


MeO
N
N
N
Hex
Me
6a
(CDCl3. 300 MHz)
1.00
0.98
0.95
1.81
1.24
1.91
2.81
2.74
2.01
6.03
2.73
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

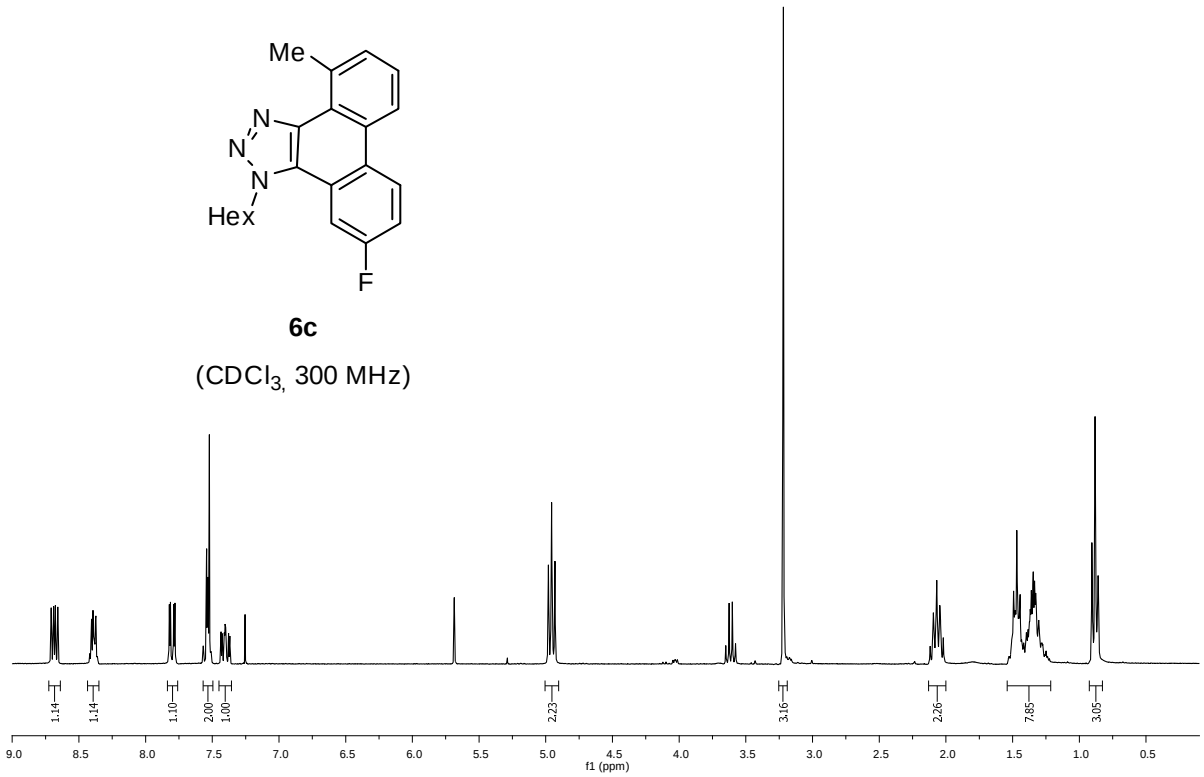

MeO
N
N
N
Hex
Me
6a
(CDCl3. 75 MHz)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


MeO
N
N
N
Hex
CO2Et
6b
(CDCl3, 300 MHz)
1.00
1.08
1.09
1.04
1.13
1.10
1.94
2.01
2.79
2.12
9.49
2.99
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


MeO
N
N
N
Hex
CO2Et
6b
(CDCl3, 125 MHz)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

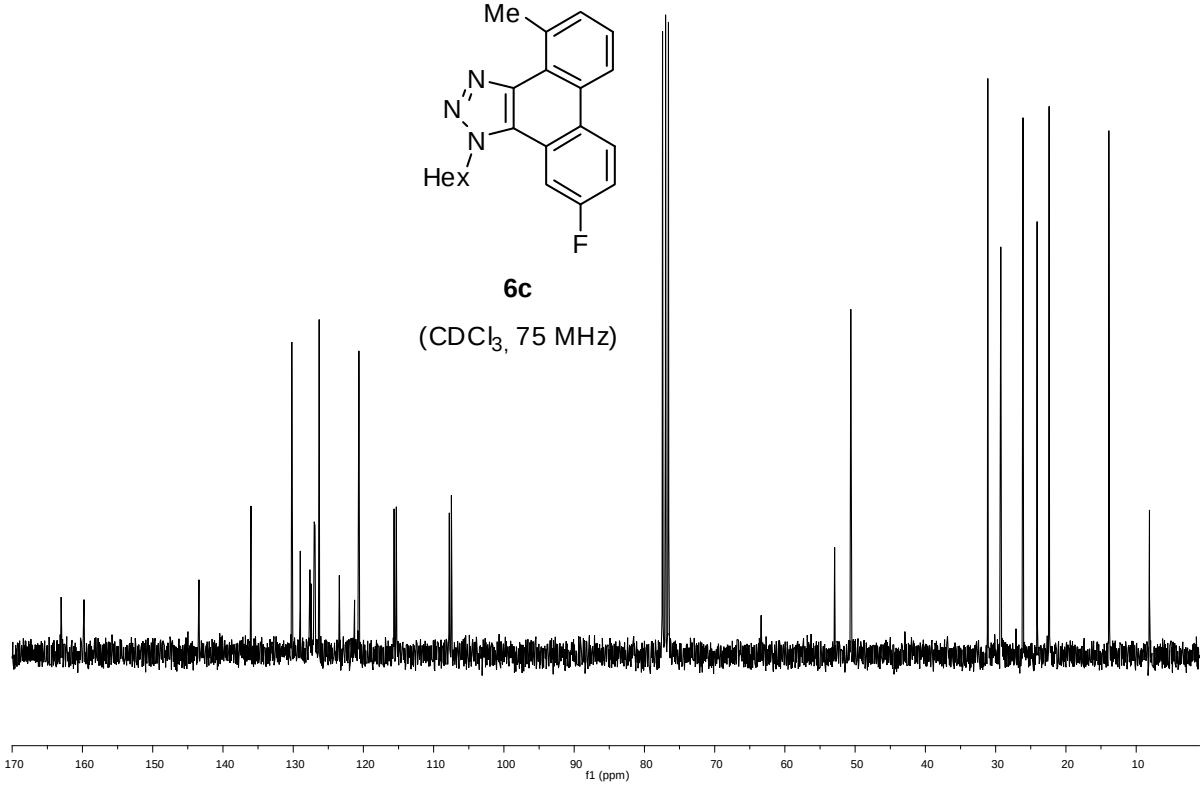
6c

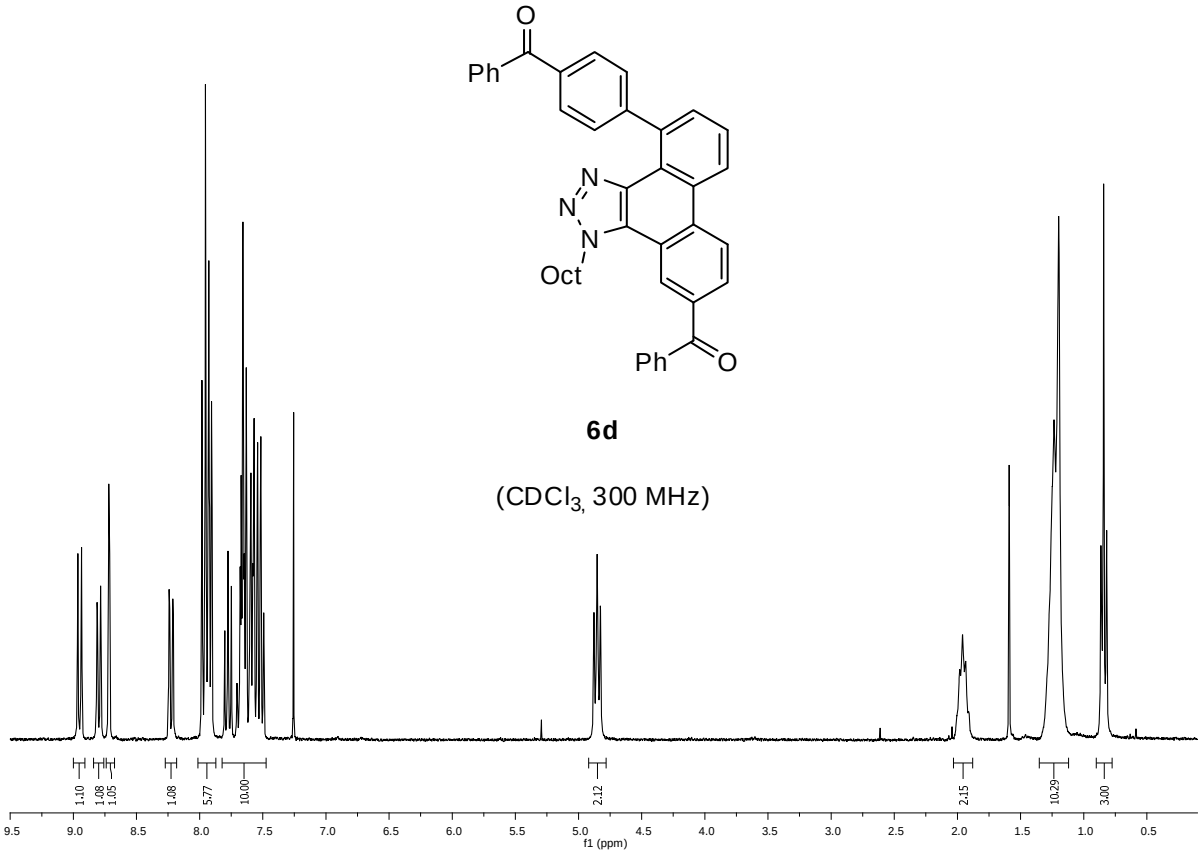
($CDCl_3$, 300 MHz)



6c

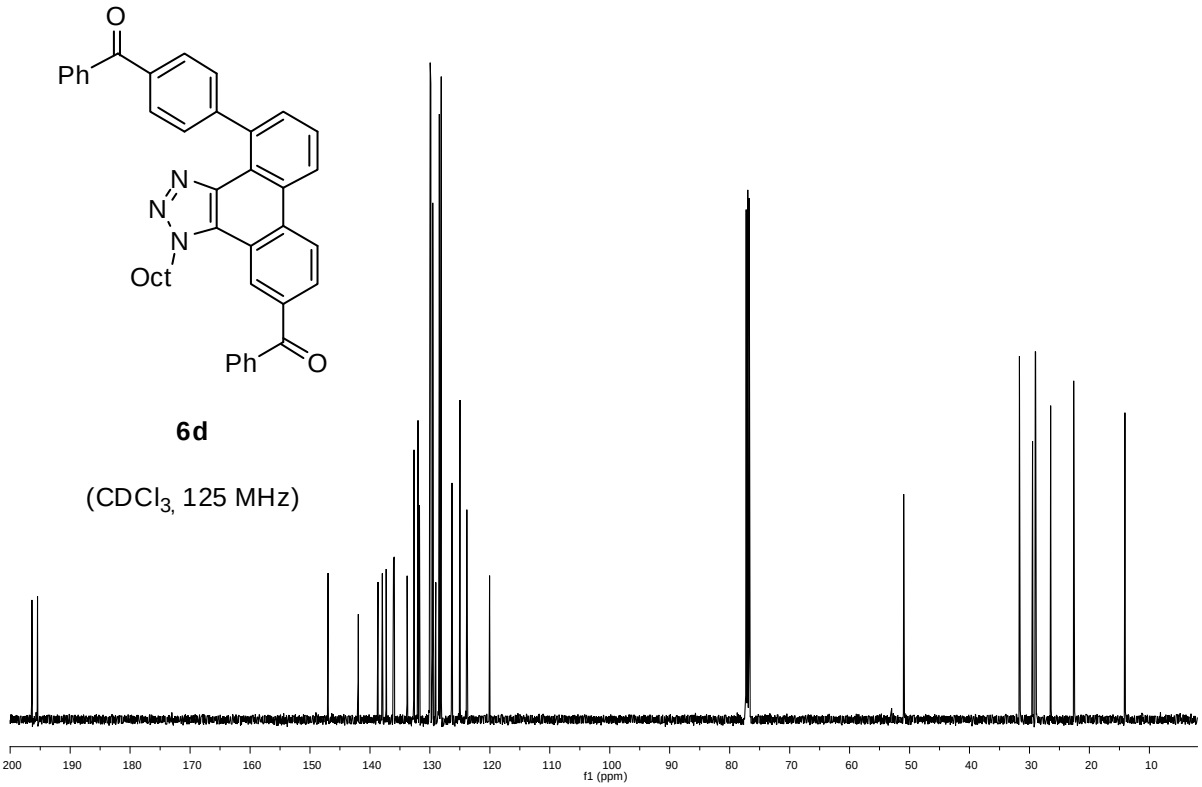
($CDCl_3$, 75 MHz)





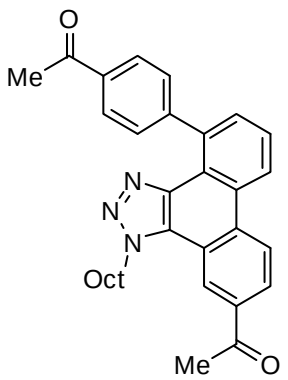
6d

($CDCl_3$, 300 MHz)



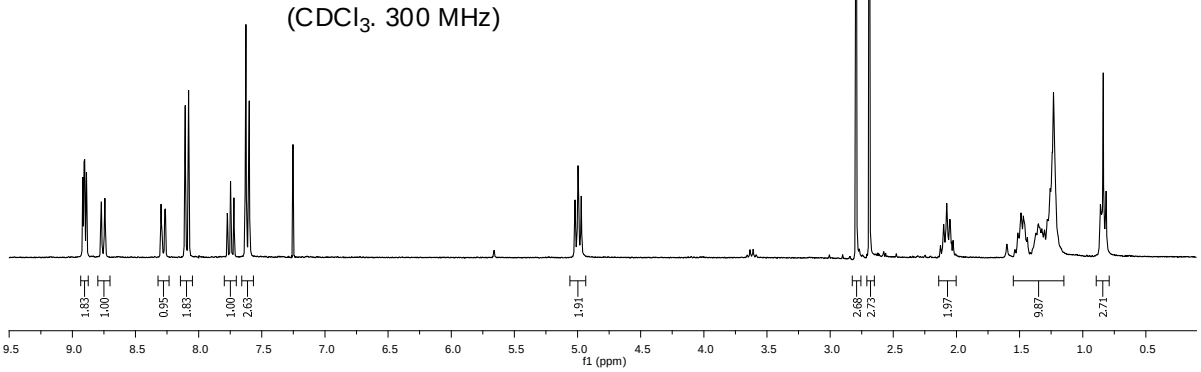
6d

($CDCl_3$, 125 MHz)



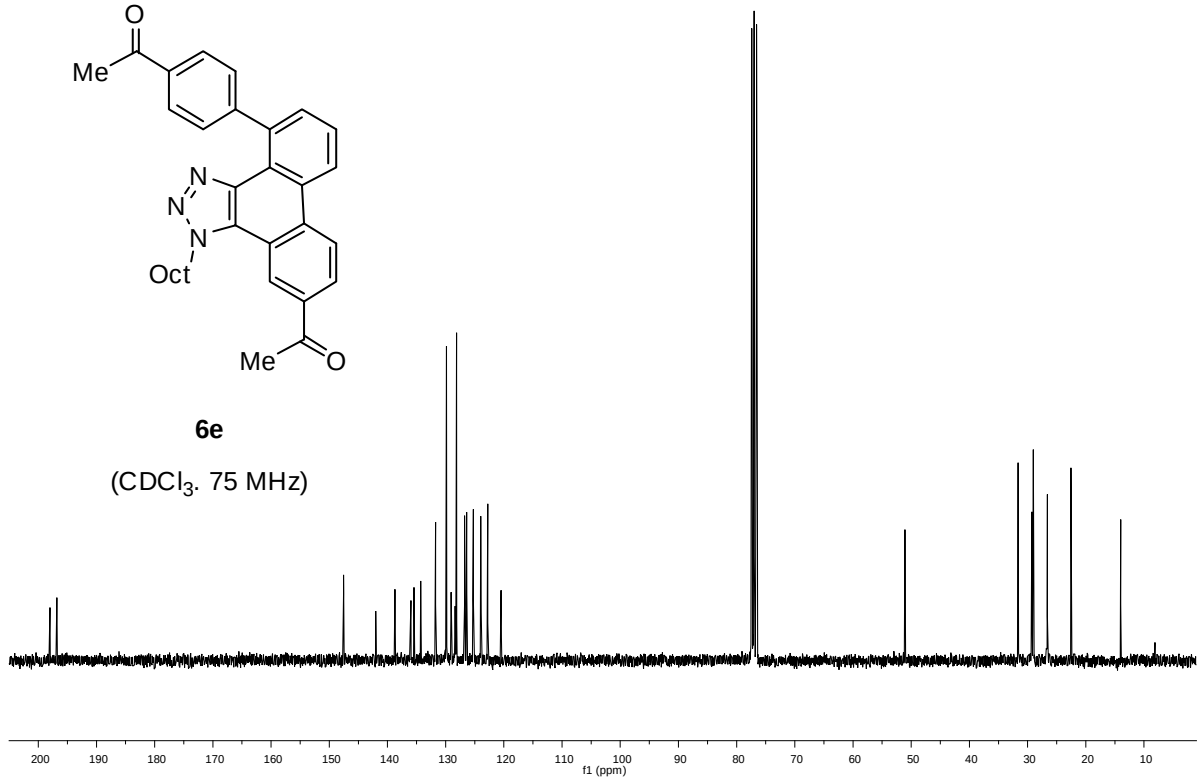
6e

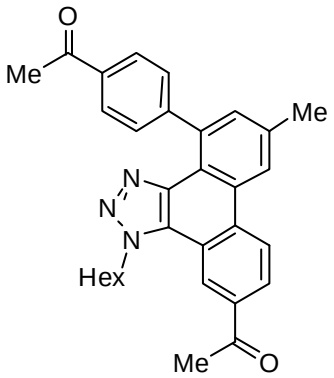
($CDCl_3$. 300 MHz)



6e

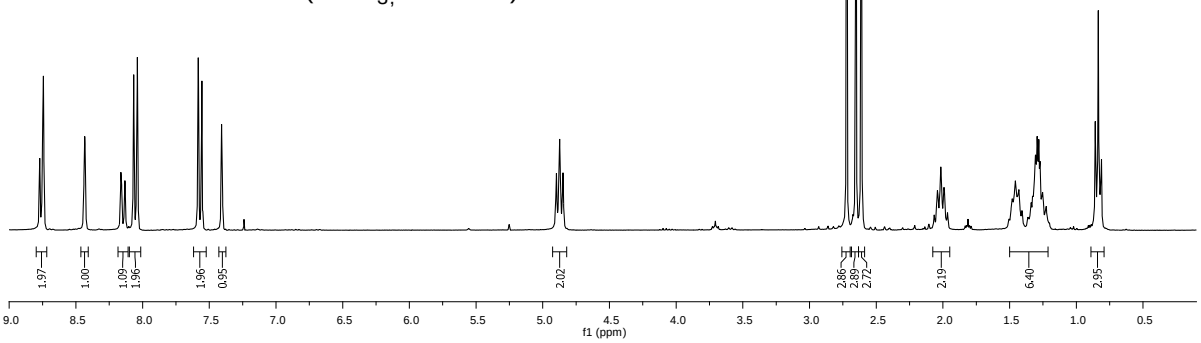
($CDCl_3$. 75 MHz)

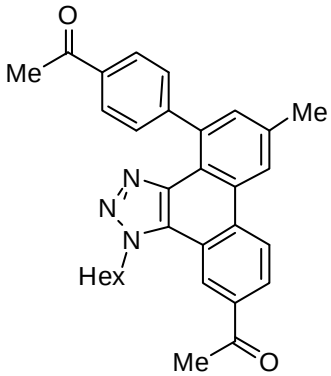




6f

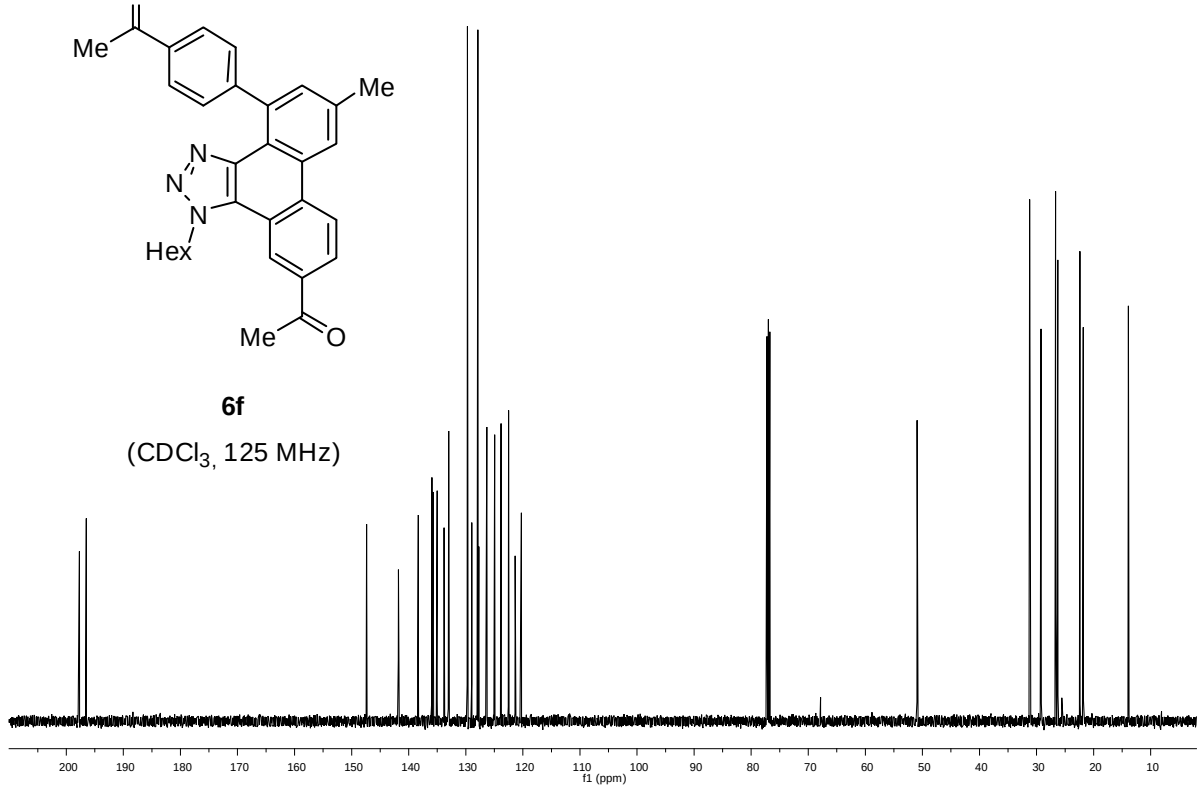
($CDCl_3$, 300 MHz)

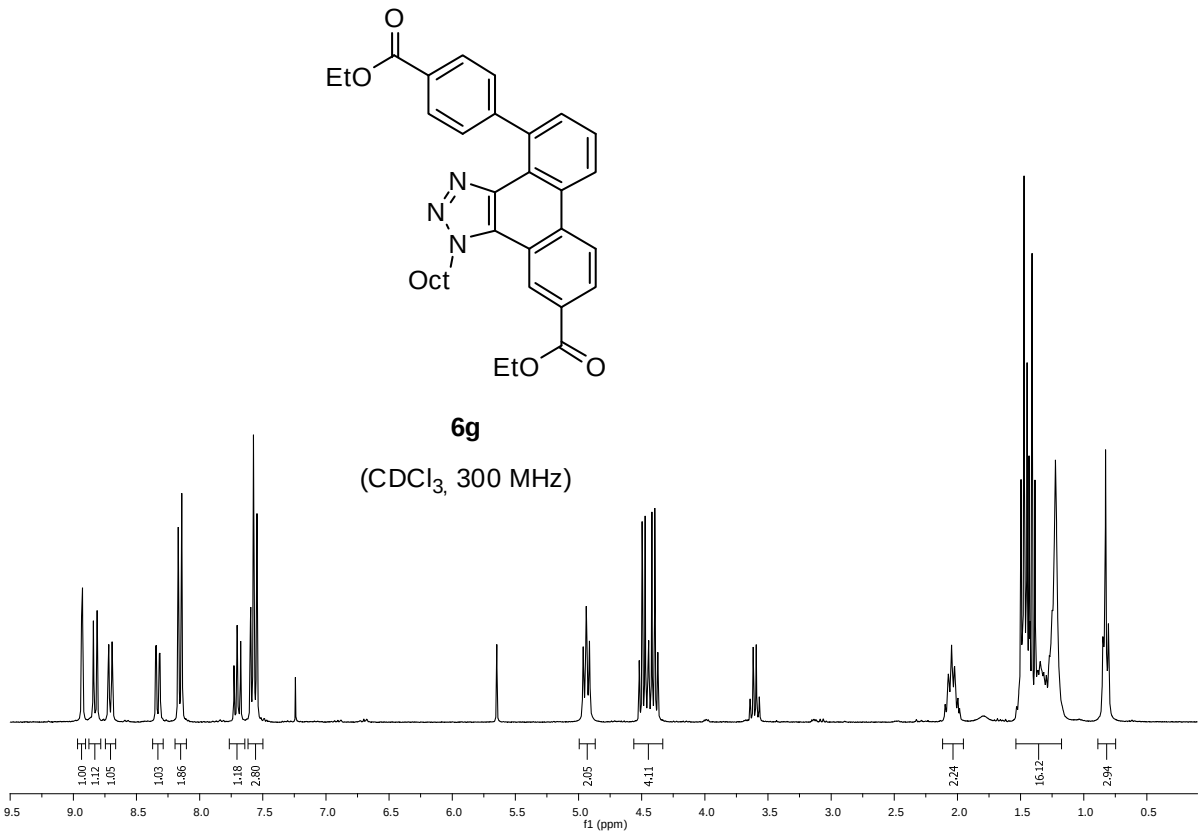


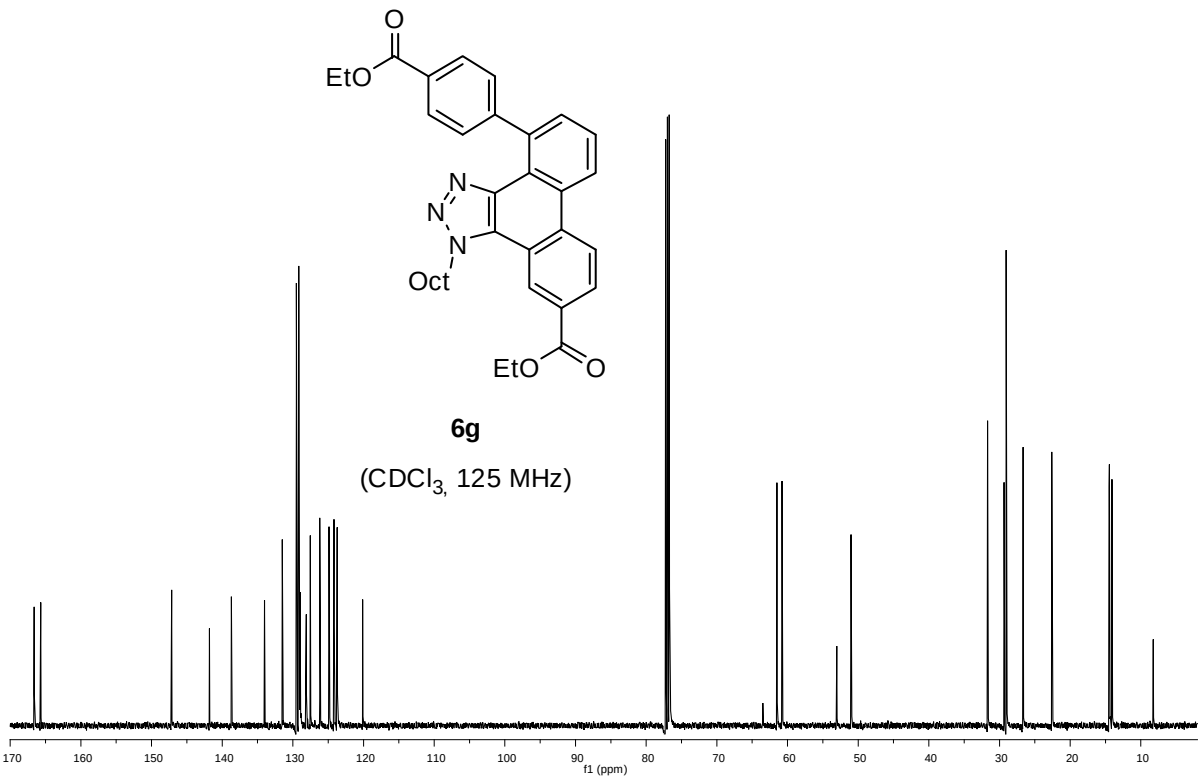


6f

($CDCl_3$, 125 MHz)




O
EtO
N
N
N
Oct
EtO
O
6g
(CDCl3, 300 MHz)
1.00
1.12
1.05
1.03
1.86
1.18
2.80
2.05
4.11
2.24
16.12
2.94
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


O
EtO
N
N
N
Oct
EtO
O
6g
(CDCl3, 125 MHz)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)