

Supplementary Information

Copper-Catalyzed Cross-Coupling and Sequential Allene-Mediated Cyclization For 1,2,3-Triazolo[1,5-*a*]quinolines

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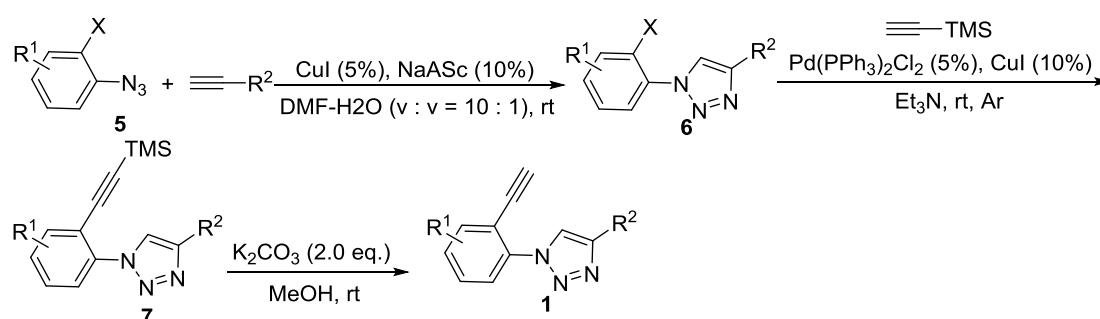
Table of Contents

1. General Information.....	S2
2. General Procedure for the synthesis of 1-(2-ethynylaryl)-1,4- Disubstituted-1,2,3-triazoles 1	S2
3. General Procedure for the synthesis of <i>N</i> -tosylhydrazones 2	S2
4. General Procedure for the synthesis of 1,2,3-Triazolo[1,5- <i>a</i>]quinolines 3 and 4	S3
5. Spectral Data of the Compounds	S4
6. X-ray Data of 3a	S16
7. ¹ H and ¹³ C NMR Spectra of the Compounds.....	S17

1. General Information

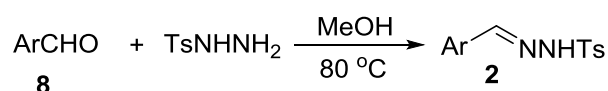
^1H and ^{13}C NMR spectra were recorded with a Bruker ACF600 spectrometer (600 MHz) in CDCl_3 with TMS as an internal standard. All reactions were monitored by TLC with Huanghai GF 254 silica gel coated plates. Column chromatography was carried out using 200–300 mesh silica gel at medium pressure. Infrared spectra were taken on a Bruker Vertex Series FTIR (KBr) and are reported in reciprocal centimeters (cm^{-1}). Melting points were obtained using a Büchi melting point apparatus and are uncorrected. HRMS spectra were recorded on Waters Micromass Premier Q-TOF spectrometer.

2. General Procedure for the synthesis of 1-(2-ethynylaryl)-1,4-disubstituted-1,2,3-triazoles **1**



To a 100 mL round-bottomed flask was added aryl azide **5** (5.0 mmol), alkyne, CuI (0.25 mmol), NaASc (0.5) and $\text{DMF-H}_2\text{O}$ ($v:v = 10:1$) (40 mL). The system was then stirred at room temperature for overnight. After consumption of the aryl azide and alkyne monitored by TLC analysis, the mixture was added with H_2O (40 mL) and extracted with EtOAc (3×20 mL), and the combined organic layer was washed with brine (3×10 mL), dried over Na_2SO_4 and concentrated under reduced pressure to afford a crude product. Purification by column chromatography on silica gel afforded the desired substrates **6**. Next, to a 100 mL round-bottomed flask was **6**, trimethylsilylacetylene (1.5 eq.), $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (5%), CuI (10%), Et_3N (15 mL). The system was then stirred at room temperature for overnight in an argon atmosphere. Intermediate **7** was obtained with the same post-treatment steps. Finally, To a 100 mL round-bottomed flask was added **7**, K_2CO_3 (2.0 eq.), MeOH (15 mL). The system was then stirred at room temperature for overnight. Desired product **1** was obtained with the same post-treatment steps.

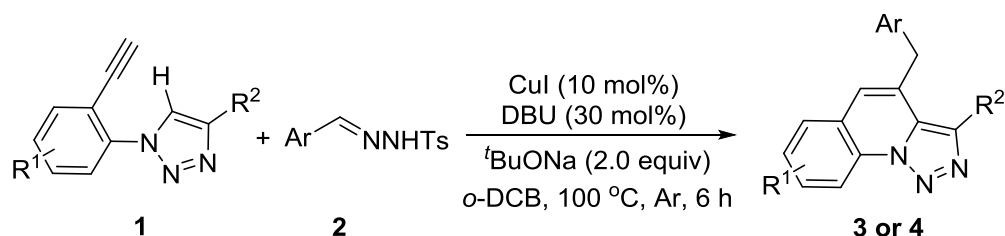
3. General Procedure for the synthesis of *N*-tosylhydrazones **2**



To a 50 mL pressure tube was added aromatic **8** (5.0 mmol), and TsNHNH_2 (5.5 mmol), MeOH (15 mL). The system was then stirred at 80°C for overnight. The

mixture was concentrated under reduced pressure to precipitate crystals, filtered and washed with a small amount of MeOH (2-3 mL) to obtain compound **2**.

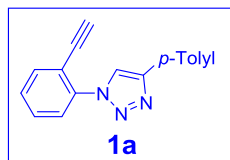
4. General Procedure for the synthesis of 1,2,3-Triazolo[1,5-*a*]quinolines **3** and **4**



To a 50 mL pressure tube was added 1,4-disubstitued 1,2,3-triazoles **1** (0.3 mmol), CuI (5.3 mg, 0.03 mmol, 10%), 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) (13.7 mg, 0.09 mmol, 30%), ^tBuONa (57.6 mg, 0.60 mmol, 2.0 equiv), and 1,2-dichlorobenzene (*o*-DCB) (3.0 mL) under Ar atmosphere. The system was then stirred at 100 °C for 6 hours. After consumption of the 1,4-disubstitued 1,2,3-triazoles and *N*-tosylhydrazones monitored by TLC analysis, the mixture was added with H₂O (15 mL) and extracted with EtOAc (3 × 15 mL), and the combined organic layer was washed with brine (3 × 5 mL), dried over Na₂SO₄ and concentrated under reduced pressure to afford a crude product. Purification by column chromatography on silica gel afforded the desired products **3** or **4**.

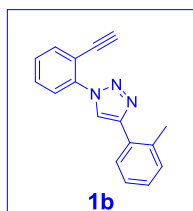
5. Spectral Data of the Compounds

1-(2-Ethynylphenyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (1a)



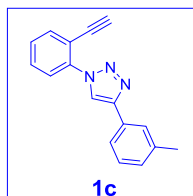
Yield: 932.79 mg (72%); yellow solid; ^1H NMR (600 MHz, CDCl_3) δ 8.45 (s, 1H), 7.80 (d, $J = 8.1$ Hz, 2H), 7.78 (d, $J = 8.1$ Hz, 1H), 7.69 (dd, $J = 7.8, 1.3$ Hz, 1H), 7.54 (t, $J = 7.9, 1.4$ Hz, 1H), 7.45 (t, $J = 7.6, 1.1$ Hz, 1H), 7.27 (d, $J = 7.9$ Hz, 2H), 3.29 (s, 1H), 2.40 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 147.64, 138.50, 138.32, 134.54, 130.31, 129.70, 129.07, 127.65, 125.90, 125.29, 120.68, 116.26, 83.93, 79.27, 77.37, 77.16, 76.95, 21.45; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{14}\text{N}_3$ [(M + H) $^+$]: 260.1182, found 260.1180.

1-(2-Ethynylphenyl)-4-(*o*-tolyl)-1*H*-1,2,3-triazole (1b)



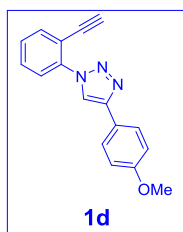
Yield: 1063.2 mg (82%); white solid; ^1H NMR (600 MHz, CDCl_3) δ 8.32 (s, 1H), 7.79 (d, $J = 6.9$ Hz, 1H), 7.71 (d, $J = 8.1$ Hz, 1H), 7.56 (dd, $J = 7.8, 1.1$ Hz, 1H), 7.42 (dd, $J = 11.1, 4.5$ Hz, 1H), 7.32 (td, $J = 7.7, 1.1$ Hz, 1H), 7.18 (t, $J = 3.7$ Hz, 2H), 3.20 (s, 1H), 2.41 (s, 3H); ^{13}C NMR (151 MHz, CDCl_3) δ 146.45, 138.17, 135.48, 134.42, 130.92, 130.24, 129.63, 128.90, 128.29, 126.18, 125.00, 123.14, 115.89, 83.88, 79.28, 21.39; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{14}\text{N}_3$ [(M + H) $^+$]: 260.1182, found 260.1184.

1-(2-Ethynylphenyl)-4-(*m*-tolyl)-1*H*-1,2,3-triazole (1c)



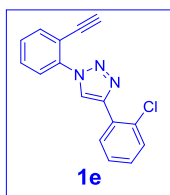
Yield: 1011.3 mg (78%); white solid; ^1H NMR (600 MHz, CDCl_3) δ 8.36 (s, 1H), 7.68 – 7.62 (m, 2H), 7.57 (t, $J = 7.6$ Hz, 2H), 7.41 (dd, $J = 11.3, 4.3$ Hz, 1H), 7.32 (dd, $J = 11.1, 4.2$ Hz, 1H), 7.23 (t, $J = 7.6$ Hz, 1H), 7.06 (d, $J = 7.6$ Hz, 1H), 3.19 (s, 1H), 2.31 (s, 3H); ^{13}C NMR (151 MHz, CDCl_3) δ 146.48, 137.57, 137.26, 133.39, 129.17 (d, $J = 6.1$ Hz), 128.04 (d, $J = 14.3$ Hz), 127.79, 125.49, 124.11, 121.95, 119.91, 115.15, 82.92, 78.08, 20.46; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{14}\text{N}_3$ [(M + H) $^+$]: 260.1182, found 260.1182.

1-(2-Ethynylphenyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (1d)



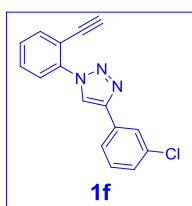
Yield: 1087.5 mg (79%); white solid; ^1H NMR (600 MHz, CDCl_3) δ 8.33 (s, 1H), 7.78 – 7.73 (m, 2H), 7.69 (dd, $J = 8.1, 0.8$ Hz, 1H), 7.61 (dd, $J = 7.8, 1.3$ Hz, 1H), 7.46 (td, $J = 7.9, 1.4$ Hz, 1H), 7.37 (td, $J = 7.7, 1.2$ Hz, 1H), 6.94 – 6.88 (m, 2H), 3.77 (s, 3H), 3.22 (s, 1H); ^{13}C NMR (151 MHz, CDCl_3) δ 159.79, 147.40, 138.47, 134.53, 130.29, 129.04, 127.28, 125.24, 123.12, 120.20, 116.22, 114.38, 83.92, 79.26, 55.44; HRMS (ESI) calcd for $\text{C}_{17}\text{H}_{14}\text{N}_3\text{O}$ [(M + H) $^+$]: 276.1131, found 276.1138.

4-(2-Chlorophenyl)-1-(2-ethynylphenyl)-1*H*-1,2,3-triazole (1e)



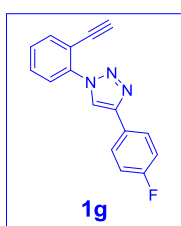
Yield: 979.0 mg (79%); white solid; ^1H NMR (600 MHz, CDCl_3) δ 8.85 (s, 1H), 8.22 (dd, $J = 7.8, 1.5$ Hz, 1H), 7.70 (d, $J = 8.0$ Hz, 1H), 7.58 (d, $J = 7.7$ Hz, 1H), 7.44 (dd, $J = 11.4, 4.1$ Hz, 1H), 7.38 – 7.31 (m, 2H), 7.31 – 7.27 (m, 1H), 7.21 – 7.16 (m, 1H), 3.23 (s, 1H); ^{13}C NMR (151 MHz, CDCl_3) δ 143.61, 138.15, 134.43, 131.32, 130.27 (d, $J = 11.1$ Hz), 129.90, 129.21, 129.04 (d, $J = 4.1$ Hz), 127.25, 125.08, 124.53, 116.15, 84.20, 79.03; HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{11}\text{ClN}_3$ [(M + H) $^+$]: 280.0636, found 280.0632.

4-(3-Chlorophenyl)-1-(2-ethynylphenyl)-1H-1,2,3-triazole (1f)



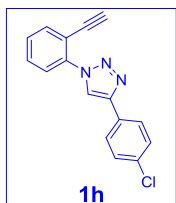
Yield: 951.2mg (68%); white solid; ^1H NMR (600 MHz, CDCl_3) δ 8.50 (s, 1H), 7.90 (t, $J = 1.7$ Hz, 1H), 7.79 (dd, $J = 7.7, 1.0$ Hz, 1H), 7.75 (dd, $J = 8.1, 0.6$ Hz, 1H), 7.69 (dd, $J = 7.8, 1.1$ Hz, 1H), 7.54 (td, $J = 7.8, 1.3$ Hz, 1H), 7.45 (td, $J = 7.7, 1.1$ Hz, 1H), 7.37 (t, $J = 7.8$ Hz, 1H), 7.34 – 7.30 (m, 1H), 3.32 (s, 1H); ^{13}C NMR (151 MHz, CDCl_3) δ 146.14, 138.09, 134.83, 134.50, 132.14, 130.28 (t, $J = 7.9$ Hz), 129.21, 128.33 (d, $J = 9.4$ Hz), 125.87, 125.13, 123.96, 121.39 (d, $J = 9.0$ Hz), 116.18, 84.09, 79.04; HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{11}\text{ClN}_3$ [(M + H) $^+$]: 280.0636, found 280.0635.

1-(2-Ethynylphenyl)-4-(4-fluorophenyl)-1H-1,2,3-triazole (1g)



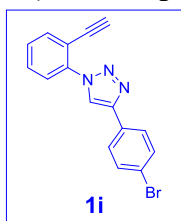
Yield: 961.0 mg (73%); red solid; ^1H NMR (600 MHz, CDCl_3) δ 8.48 – 8.43 (m, 1H), 7.86 (ddd, $J = 11.2, 7.2, 4.0$ Hz, 2H), 7.69 (dd, $J = 11.7, 8.3$ Hz, 1H), 7.63 (t, $J = 9.4$ Hz, 1H), 7.51 – 7.44 (m, 1H), 7.43 – 7.37 (m, 1H), 7.12 – 7.05 (m, 2H), 3.32 (s, 1H); ^{13}C NMR (151 MHz, CDCl_3) δ 162.58 (d, $J = 247.4$ Hz), 146.41, 138.04, 134.36, 130.09, 129.01, 127.50 (d, $J = 8.1$ Hz), 126.50 (d, $J = 3.3$ Hz), 124.98, 120.71, 115.77 (d, $J = 21.7$ Hz), 116.08, 83.98, 78.97; HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{11}\text{FN}_3$ [(M + H) $^+$]: 264.0932, found 264.0930.

4-(4-Chlorophenyl)-1-(2-ethynylphenyl)-1H-1,2,3-triazole (1h)



Yield: 993.0mg (80%); white solid; ^1H NMR (600 MHz, CDCl_3) δ 8.49 (s, 1H), 7.84 (dd, $J = 8.7, 2.0$ Hz, 2H), 7.76 (d, $J = 8.0$ Hz, 1H), 7.70 (dd, $J = 7.7, 1.0$ Hz, 1H), 7.54 (dd, $J = 7.8, 1.0$ Hz, 1H), 7.47 (dd, $J = 7.7, 0.8$ Hz, 1H), 7.42 (d, $J = 8.4$ Hz, 2H), 3.31 (s, 1H).; ^{13}C NMR (151 MHz, CDCl_3) δ 146.49, 138.25, 134.58, 134.14, 130.34, 129.38 – 129.14 (m), 128.96, 127.19, 125.24, 121.07, 116.25, 84.05, 79.15; HRMS (ESI) calcd for $\text{C}_{16}\text{H}_{11}\text{ClN}_3$ [(M + H) $^+$]: 280.0636, found 280.0634.

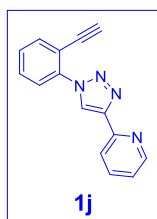
4-(4-Bromophenyl)-1-(2-ethynylphenyl)-1H-1,2,3-triazole (1i)



Yield: 1118.4mg (80%); white solid; ^1H NMR (600 MHz, CDCl_3) δ 8.49 (s, 1H), 7.77 (d, $J = 8.5$ Hz, 2H), 7.74 (d, $J = 8.1$ Hz, 1H), 7.68 (d, $J = 7.7$ Hz, 1H), 7.57 – 7.51 (m, 3H), 7.47 – 7.42 (m, 1H), 3.31 (s, 1H).; ^{13}C NMR (151 MHz, CDCl_3) δ 146.41, 138.13, 134.51, 132.07,

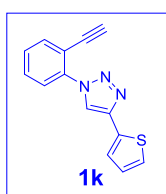
130.27, 129.34, 129.19, 127.40, 125.14, 122.22, 121.07, 116.17, 84.06, 79.08; HRMS (ESI) calcd for C₁₆H₁₁BrN₃ [(M + H)⁺]: 324.0131, found 324.0133.

2-(1-(2-Ethynylphenyl)-1H-1,2,3-triazol-4-yl)pyridine (1j)



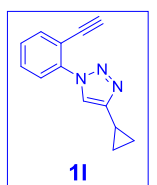
Yield: 923.5 mg (75%); white solid; ¹H NMR (600 MHz, CDCl₃) δ 8.93 – 8.79 (m, 1H), 8.61 (d, *J* = 4.8 Hz, 1H), 8.25 (dd, *J* = 11.1, 4.1 Hz, 1H), 7.82 – 7.74 (m, 2H), 7.69 (dd, *J* = 11.8, 4.6 Hz, 1H), 7.53 (dd, *J* = 15.9, 8.2 Hz, 1H), 7.48 – 7.41 (m, 1H), 7.23 (dd, *J* = 8.0, 4.3 Hz, 1H), 3.38 (s, 1H); ¹³C NMR (151 MHz, CDCl₃) δ 149.96 (d, *J* = 2.0 Hz), 149.46, 147.98, 138.12, 136.84, 134.35, 130.04, 129.09, 125.09, 123.27, 122.92, 120.32, 116.35 (d, *J* = 1.9 Hz), 84.25, 78.76; HRMS (ESI) calcd for C₁₅H₁₁N₄ [(M + H)⁺]: 247.0978, found 247.0983.

1-(2-Ethynylphenyl)-4-(thiophen-2-yl)-1H-1,2,3-triazole (1k)



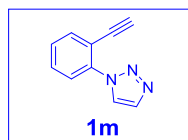
¹H NMR (600 MHz, CDCl₃) δ 8.39 (s, 1H), 7.79 (d, *J* = 8.1 Hz, 2H), 7.61 (d, *J* = 8.2 Hz, 1H), 7.46 (d, *J* = 0.9 Hz, 1H), 7.30 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.24 (d, *J* = 7.9 Hz, 2H), 3.24 (s, 1H), 2.38 (s, 3H), 2.38 (s, 3H); ¹³C NMR (151 MHz, CDCl₃) δ 142.64, 138.16, 134.51, 132.64, 130.29, 129.24, 127.79, 125.38, 125.29, 124.55, 120.43, 116.32, 84.10, 79.03; HRMS (ESI) calcd for C₁₄H₁₀N₃S [(M + H)⁺]: 252.0590, found 252.0582.

4-Cyclopropyl-1-(2-ethynylphenyl)-1H-1,2,3-triazole (1l)



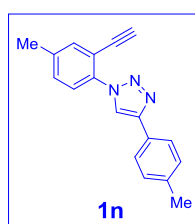
Yield: 680.1 mg (80%); red liquid; ¹H NMR (600 MHz, CDCl₃) δ 7.98 (dd, *J* = 2.9, 2.2 Hz, 1H), 7.70 – 7.59 (m, 2H), 7.51 – 7.44 (m, 1H), 7.42 – 7.35 (m, 1H), 3.32 (d, *J* = 1.4 Hz, 1H), 2.03 (ddd, *J* = 8.1, 6.4, 3.3 Hz, 1H), 1.02 – 0.96 (m, 2H), 0.93 (d, *J* = 1.6 Hz, 2H); ¹³C NMR (151 MHz, CDCl₃) δ 149.63, 138.28, 134.24, 129.96, 128.59, 124.91, 121.07, 115.85, 83.66, 79.06, 7.76, 6.58; HRMS (ESI) calcd for C₁₃H₁₂N₃ [(M + H)⁺]: 210.1026, found 210.1020.

1-(2-Ethynylphenyl)-1H-1,2,3-triazole (1m)



Yield: 507.6 mg (60%); white solid; ¹H NMR (600 MHz, CDCl₃) δ 8.31 (s, 1H), 7.83 (d, *J* = 3.3 Hz, 1H), 7.74 – 7.69 (m, 1H), 7.67 (d, *J* = 7.7 Hz, 1H), 7.52 (dt, *J* = 7.2, 6.4 Hz, 1H), 7.46 – 7.42 (m, 1H), 3.30 (s, 1H); ¹³C NMR (151 MHz, CDCl₃) δ 138.15, 134.47, 134.29, 134.08, 133.36, 130.08, 129.09, 128.96, 125.17, 124.99, 116.21, 83.78, 78.89; HRMS (ESI) calcd for C₁₀H₈N₃ [(M + H)⁺]: 170.0713, found 170.0709.

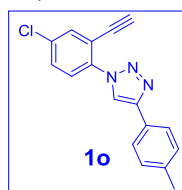
1-(2-Ethynyl-4-methylphenyl)-4-(*p*-tolyl)-1H-1,2,3-triazole (1n)



¹H NMR (600 MHz, CDCl₃) δ 8.39 (s, 1H), 7.79 (d, *J* = 8.1 Hz, 2H), 7.61 (d, *J* = 8.2 Hz, 1H), 7.46 (d, *J* = 0.9 Hz, 1H), 7.30 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.24 (d, *J* = 7.9 Hz, 2H), 3.24 (s, 1H), 2.38 (s, 3H), 2.38 (s, 3H); ¹³C NMR (151 MHz, CDCl₃) δ 147.40, 139.25, 138.12,

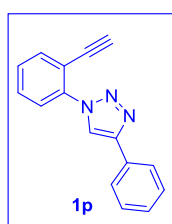
136.07, 134.68, 130.98, 129.59, 127.64, 125.77, 124.97, 120.64, 115.88, 83.37, 79.32, 21.37, 20.94; HRMS (ESI) calcd for C₁₈H₁₆N₃ [(M + H)⁺]: 274.1339, found 274.1341.

1-(4-Chloro-2-ethynylphenyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (1o)



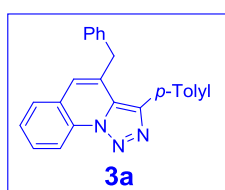
Yield: 851.9 mg (58%); white solid; ¹H NMR (600 MHz, CDCl₃) δ 8.34 (s, 1H), 7.68 (d, *J* = 8.1 Hz, 2H), 7.61 (dd, *J* = 8.6, 3.2 Hz, 1H), 7.55 (d, *J* = 2.3 Hz, 1H), 7.39 (dd, *J* = 8.6, 2.3 Hz, 1H), 7.16 (d, *J* = 7.9 Hz, 2H), 3.26 (s, 1H), 2.29 (s, 3H); ¹³C NMR (151 MHz, CDCl₃) δ 147.75, 138.40, 136.89, 134.75, 134.02, 130.50, 129.67, 127.35, 126.32, 125.84, 120.43, 117.46, 85.16, 78.04, 21.41; HRMS (ESI) calcd for C₁₇H₁₃ClN₃ [(M + H)⁺]: 294.0793, found 294.0787.

1-(2-Ethynylphenyl)-4-phenyl-1*H*-1,2,3-triazole (1p)



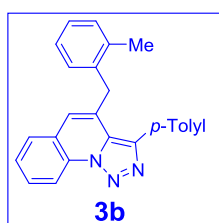
Yield: 981.1 mg (80%); white solid; ¹H NMR (600 MHz, CDCl₃) δ 8.38 (s, 1H), 7.81 (dd, *J* = 8.2, 1.1 Hz, 2H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.57 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.41 (td, *J* = 7.9, 1.4 Hz, 1H), 7.37 – 7.30 (m, 3H), 7.27 – 7.22 (m, 1H), 3.19 (s, 1H); ¹³C NMR (151 MHz, CDCl₃) δ 147.38, 138.24, 134.41, 130.33, 130.18, 128.97 (d, *J* = 18.7 Hz), 128.32, 125.84, 125.11, 120.96, 116.15, 83.95, 79.08; HRMS (ESI) calcd for C₁₆H₁₂N₃ [(M + H)⁺]: 246.1026, found 246.1031.

4-Benzyl-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3a)



Yield: 62.9 mg (60%); Light yellow solid; Mp. 188.8-189.7 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.72 (d, *J* = 8.6 Hz, 1H), 7.62 (t, *J* = 7.1 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 7.8 Hz, 2H), 7.12 – 7.08 (m, 3H), 6.97 (s, 1H), 6.80 (dd, *J* = 7.1, 2.3 Hz, 2H), 3.94 (s, 2H), 2.35 (s, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 141.67, 138.42, 137.86, 131.17, 130.57, 129.53, 129.43, 129.24, 129.20, 129.09, 128.93, 128.55, 128.02, 127.16, 126.65, 125.75, 124.24, 116.31, 77.37, 77.16, 76.95, 38.17, 21.50; IR (KBr): 2919, 1544, 1457, 1255, 1214, 1163, 1030, 995, 824, 750, 703, 558, 513 cm⁻¹; HRMS (ESI) calcd for C₂₄H₂₀N₃ [(M + H)⁺]: 350.1652, found 350.1650.

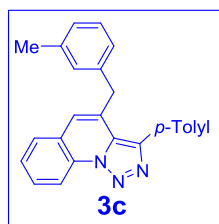
4-(2-Methylbenzyl)-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3b)



Yield: 83.9 mg (77%); Light yellow solid; Mp. 182.8-183.6 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.81 (d, *J* = 8.4 Hz, 1H), 7.69 (t, *J* = 8.4, 7.3, 1.3 Hz, 1H), 7.65 – 7.61 (m, 1H), 7.55 – 7.49 (m, 1H), 7.44 – 7.36 (m, 2H), 7.21 (d, *J* = 7.8 Hz, 2H), 7.18 (dd, *J* = 4.6, 2.8 Hz, 1H), 7.16 – 7.11 (m, 2H), 6.99 (d, *J* = 7.5 Hz, 1H), 6.83 (s, 1H), 3.90 (s, 2H), 2.40 (s, 3H), 2.00 (s, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 141.66, 138.43, 136.85, 136.16, 131.09, 130.43, 130.42, 129.85, 129.38, 129.33, 129.16, 128.94, 128.89, 128.02, 127.15, 127.11, 126.26, 124.81, 124.29, 116.26, 77.37, 77.16, 76.95, 36.02, 21.44, 19.34; IR (KBr): 2955, 2911, 1558, 1462, 1430, 1388, 1329, 1242, 1209, 1155, 1112, 1022, 993, 950, 897, 851, 818, 747, 624,

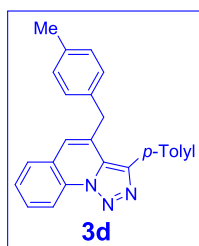
561, 509 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{22}\text{N}_3$ $[(\text{M} + \text{H})^+]$: 364.1808, found 364.1810.

4-(3-Methylbenzyl)-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3c)



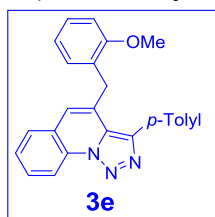
Yield: 82.9 mg (76%); Light yellow solid; Mp. 149.6-150.7 $^{\circ}\text{C}$; ^1H NMR (600 MHz, CDCl_3) δ 8.82 (d, $J = 8.3$ Hz, 1H), 7.72 (dd, $J = 15.8, 7.5$ Hz, 2H), 7.59 – 7.54 (m, 1H), 7.37 (d, $J = 8.0$ Hz, 2H), 7.24 (d, $J = 7.8$ Hz, 2H), 7.10 (s, 1H), 7.07 (t, $J = 7.6$ Hz, 1H), 6.98 (d, $J = 7.6$ Hz, 1H), 6.68 (d, $J = 7.6$ Hz, 1H), 6.60 (s, 1H), 3.99 (s, 2H), 2.44 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 141.69, 138.38, 138.15, 137.77, 131.22, 130.64, 129.90, 129.66, 129.42, 129.29, 129.26, 128.92, 128.38, 128.05, 127.35, 127.17, 125.97, 125.75, 124.30, 116.36, 77.37, 77.16, 76.95, 38.20, 21.52, 21.47; IR (KBr): 2910, 2860, 1463, 1243, 1160, 1110, 1029, 990, 948, 902, 858, 817, 756, 693, 560, 509 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{22}\text{N}_3$ $[(\text{M} + \text{H})^+]$: 364.1808, found 364.1806.

4-(4-Methylbenzyl)-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3d)



Yield: 85.1 mg (78%); Light yellow solid; Mp. 162.5-163.4 $^{\circ}\text{C}$; ^1H NMR (600 MHz, CDCl_3) δ 8.81 (d, $J = 8.6$ Hz, 1H), 7.73 – 7.67 (m, 2H), 7.57 – 7.52 (m, 1H), 7.41 (d, $J = 8.0$ Hz, 2H), 7.24 (d, $J = 7.8$ Hz, 2H), 7.05 (s, 1H), 7.02 (d, $J = 7.8$ Hz, 2H), 6.80 (d, $J = 7.9$ Hz, 2H), 3.98 (s, 2H), 2.43 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 141.66, 138.42, 136.25, 134.75, 132.19, 131.14, 130.62, 129.95, 129.36, 129.27, 129.06, 128.94, 128.02, 127.51, 127.13, 125.55, 124.31, 116.32, 77.37, 77.16, 76.95, 37.73, 21.51, 21.17.; IR (KBr): 2919, 1454, 1298, 1220, 1167, 1106, 1038, 948, 913, 825, 755, 560 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{22}\text{N}_3$ $[(\text{M} + \text{H})^+]$: 364.1808, found 364.1807.

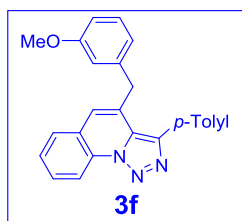
4-(2-Methoxybenzyl)-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3e)



Yield: 75.1 mg (66%); Light yellow solid; Mp. 191.6-192.5 $^{\circ}\text{C}$; ^1H NMR (600 MHz, CDCl_3) δ 8.81 (d, $J = 8.3$ Hz, 1H), 7.71 – 7.62 (m, 2H), 7.54 – 7.49 (m, 1H), 7.41 (d, $J = 8.0$ Hz, 2H), 7.24 – 7.17 (m, 3H), 6.95 (s, 1H), 6.88 (dd, $J = 7.4, 1.5$ Hz, 1H), 6.83 (t, $J = 7.4$ Hz, 1H), 6.80 (d, $J = 8.2$ Hz, 1H), 3.97 (s, 2H), 3.66 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 157.36, 141.68, 138.04, 131.10, 130.46, 130.42, 129.45, 129.36, 129.27, 129.13, 128.78, 128.20, 127.95, 127.01, 126.38, 124.88, 124.42, 120.49, 116.26, 110.24, 77.37, 77.16, 76.95, 55.21, 32.61, 21.49; IR (KBr): 2909, 1603, 1551, 1461, 1323, 1284, 1247, 1157, 1110, 1027, 990, 941, 824, 753, 645, 557 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{22}\text{N}_3\text{O}$ $[(\text{M} + \text{H})^+]$: 380.1757, found 380.1754.

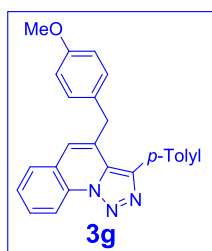
4-(3-Methoxybenzyl)-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3f)

Yield: 69.4 mg (61%); Light yellow solid; Mp. 163.8-165.4 $^{\circ}\text{C}$; ^1H NMR (600 MHz, CDCl_3) δ 8.82 (d, $J = 8.2$ Hz, 1H), 7.76 – 7.68 (m, 2H), 7.60 – 7.53 (m, 1H), 7.38 (d,



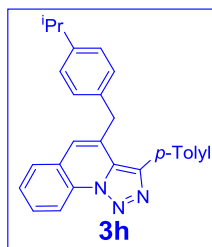
$J = 7.9$ Hz, 2H), 7.23 (d, $J = 7.8$ Hz, 2H), 7.14 – 7.08 (m, 2H), 6.73 (dd, $J = 8.2, 2.3$ Hz, 1H), 6.48 (d, $J = 7.6$ Hz, 1H), 6.41 (s, 1H), 4.01 (s, 2H), 3.71 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 159.77, 141.67, 139.49, 138.42, 131.23, 130.59, 129.52, 129.48, 129.30, 129.25, 129.21, 128.95, 128.07, 127.19, 125.85, 124.27, 121.39, 116.37, 114.80, 112.00, 77.37, 77.16, 76.95, 55.23, 38.23, 21.51; IR (KBr): 2922, 1729, 1593, 1462, 1256, 1159, 1038, 950, 909, 865, 822, 759, 697, 551 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{22}\text{N}_3\text{O}$ $[(\text{M} + \text{H})^+]$: 380.1757, found 380.1759.

4-(4-Methoxybenzyl)-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3g)



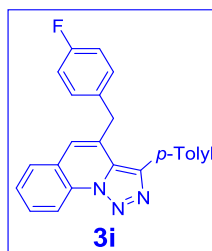
Yield: 76.3 mg (67%); Light yellow solid; Mp. 166.2-163.2 °C; ^1H NMR (600 MHz, CDCl_3) δ 8.81 (d, $J = 8.6$ Hz, 1H), 7.74 – 7.67 (m, 2H), 7.55 (t, $J = 7.6$ Hz, 1H), 7.43 – 7.38 (m, 2H), 7.25 (d, $J = 7.7$ Hz, 2H), 7.05 (s, 1H), 6.83 – 6.78 (m, 2H), 6.76 – 6.72 (m, 2H), 3.96 (s, 2H), 3.78 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 158.37, 141.67, 138.43, 131.17, 130.62, 130.16, 130.10, 129.82, 129.39, 129.29, 129.27, 128.95, 128.92, 128.03, 127.16, 125.50, 124.31, 116.35, 113.96, 77.37, 77.16, 76.95, 55.40, 37.37, 21.53; IR (KBr): 2969, 2915, 2843, 1507, 1457, 1302, 1244, 1178, 1093, 1039, 954, 887, 817, 758, 600, 556 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{22}\text{N}_3\text{O}$ $[(\text{M} + \text{H})^+]$: 380.1757, found 380.1755.

4-(4-Isopropylbenzyl)-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3h)



Yield: 79.9 mg (68%); Light yellow solid; Mp. 167.4-168.2 °C; ^1H NMR (600 MHz, CDCl_3) δ 8.80 (d, $J = 8.2$ Hz, 1H), 7.74 – 7.65 (m, 2H), 7.57 – 7.50 (m, 1H), 7.38 (d, $J = 8.0$ Hz, 2H), 7.22 (d, $J = 7.8$ Hz, 2H), 7.10 – 7.00 (m, 3H), 6.80 (d, $J = 8.1$ Hz, 2H), 3.99 (s, 2H), 2.85 (m, 1H), 2.42 (s, 3H), 1.22 (d, $J = 6.9$ Hz, 6H); ^{13}C NMR (150 MHz, CDCl_3) δ 147.26, 141.67, 138.34, 135.13, 131.14, 130.57, 129.83, 129.33, 129.29, 129.24, 129.02, 128.89, 128.02, 127.10, 126.57, 125.58, 124.29, 116.29, 77.37, 77.16, 76.95, 37.81, 33.80, 24.15, 21.49; IR (KBr): 2965, 1908, 1507, 1460, 1296, 1102, 1042, 1003, 944, 898, 863, 815, 756, 560 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{27}\text{H}_{26}\text{N}_3$ $[(\text{M} + \text{H})^+]$: 392.2121, found 392.2123.

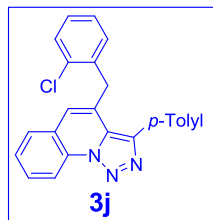
4-(4-Fluorobenzyl)-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3i)



Yield: 57.3 mg (52%); Light yellow solid; Mp. 197.4-198.2 °C; ^1H NMR (600 MHz, CDCl_3) δ 8.81 (d, $J = 8.1$ Hz, 1H), 7.76 – 7.68 (m, 2H), 7.57 (t, $J = 7.0$ Hz, 1H), 7.35 (d, $J = 8.0$ Hz, 2H), 7.23 (d, $J = 7.7$ Hz, 2H), 7.08 (s, 1H), 6.90 – 6.81 (m, 2H), 6.81 – 6.74 (m, 2H), 4.00 (s, 2H), 2.44 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 161.63 (d, $J = 244.9$ Hz), 141.62, 138.47, 133.46 (d, $J = 3.2$ Hz), 131.21, 130.53, 130.37 (d, $J = 7.9$ Hz), 129.56, 129.17 (d, $J = 11.6$ Hz), 129.05, 128.92, 128.02, 127.23, 125.82, 124.13, 116.32, 115.34, 115.20,

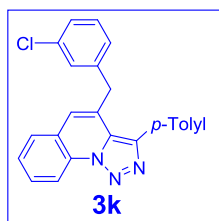
37.44, 21.49; IR (KBr): 2922, 1608, 1548, 1507, 1463, 1298, 1228, 1158, 1096, 1043, 1001, 955, 923, 888, 859, 820, 759, 597, 511 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{19}\text{FN}_3$ $[(\text{M} + \text{H})^+]$: 368.01558, found 368.1555.

4-(2-Chlorobenzyl)-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3j)



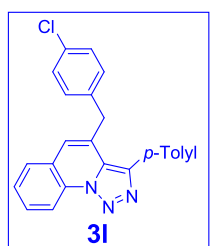
Yield: 54.1 mg (47%); Light yellow solid; Mp. 164.2-165.9 $^{\circ}\text{C}$; ^1H NMR (600 MHz, CDCl_3) δ 8.82 (d, $J = 8.3$ Hz, 1H), 7.74 – 7.69 (m, 1H), 7.66 (d, $J = 7.9$ Hz, 1H), 7.56 – 7.51 (m, 1H), 7.39 (d, $J = 8.0$ Hz, 2H), 7.33 (dd, $J = 7.9, 1.2$ Hz, 1H), 7.20 (dd, $J = 11.8, 4.8$ Hz, 3H), 7.16 (t, $J = 6.8$ Hz, 1H), 7.00 (dd, $J = 7.5, 1.5$ Hz, 1H), 6.88 (s, 1H), 4.06 (s, 2H), 2.41 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 141.75, 138.45, 135.82, 134.65, 131.22, 131.05, 130.34, 129.69, 129.51, 129.18, 128.98, 128.96, 128.45, 128.09, 127.94, 127.17, 127.03, 125.15, 124.22, 116.32, 36.09, 21.48; IR (KBr): 2913, 1919, 1468, 1298, 1240, 1165, 1097, 1043, 993, 945, 828, 756, 686, 567, 521 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{19}\text{ClN}_3$ $[(\text{M} + \text{H})^+]$: 384.1262, found 384.1265.

4-(3-chlorobenzyl)-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3k)



Yield: 62.2 mg (54%); Light yellow solid; Mp. 204.6-206.0 $^{\circ}\text{C}$; ^1H NMR (600 MHz, CDCl_3) δ 8.83 (d, $J = 8.3$ Hz, 1H), 7.77 (d, $J = 7.8$ Hz, 1H), 7.76 – 7.70 (m, 1H), 7.63 – 7.56 (m, 1H), 7.28 (t, $J = 8.3$ Hz, 2H), 7.23 (d, $J = 7.8$ Hz, 2H), 7.17 (s, 1H), 7.11 (d, $J = 8.4$ Hz, 1H), 7.05 (t, $J = 7.7$ Hz, 1H), 6.66 (d, $J = 8.6$ Hz, 2H), 4.02 (s, 2H), 2.45 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 141.70, 139.89, 138.67, 134.25, 131.38, 130.52, 129.72, 129.59, 128.99, 128.95, 128.94, 128.34, 128.11, 127.31, 126.73, 126.72, 126.27, 124.10, 116.41, 77.37, 77.16, 76.95, 38.01, 21.55; IR (KBr): 2916, 1463, 1295, 946, 758 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{19}\text{ClN}_3$ $[(\text{M} + \text{H})^+]$: 384.1262, found 384.1260.

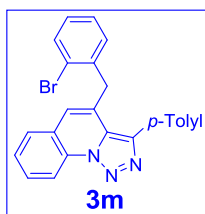
4-(4-Chlorobenzyl)-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3l)



Yield: 53.0 mg (46%); Light yellow solid; Mp. 185.5-187.2 $^{\circ}\text{C}$; ^1H NMR (600 MHz, CDCl_3) δ 8.81 (d, $J = 8.3$ Hz, 1H), 7.73 (t, $J = 8.1$ Hz, 2H), 7.58 (dd, $J = 11.0, 4.0$ Hz, 1H), 7.34 (d, $J = 7.9$ Hz, 2H), 7.23 (d, $J = 7.8$ Hz, 2H), 7.12 (d, $J = 8.4$ Hz, 2H), 7.09 (s, 1H), 6.75 (d, $J = 8.3$ Hz, 2H), 4.00 (s, 2H), 2.44 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 141.64, 138.55, 136.35, 132.44, 131.27, 130.56, 130.27, 129.65, 129.10, 129.03, 128.96, 128.85, 128.59, 128.55, 128.05, 127.28, 125.96, 124.12, 116.37, 77.37, 77.16, 76.95, 37.59, 21.52; IR (KBr): 2918, 2852, 1083, 1538, 1459, 1297, 1252, 1213, 1165, 1096, 1003, 957, 912, 869, 800, 751, 727, 665 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{19}\text{ClN}_3$ $[(\text{M} + \text{H})^+]$: 384.1262, found 384.1264.

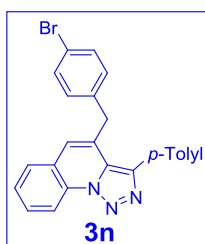
4-(2-Bromobenzyl)-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3m)

Yield: 57.8 mg (45%); Light yellow solid; Mp. 179.6-180.7 $^{\circ}\text{C}$; ^1H NMR (600 MHz,



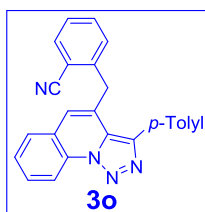
CDCl₃) δ 8.83 (d, *J* = 8.4 Hz, 1H), 7.74 – 7.69 (m, 1H), 7.67 (d, *J* = 7.9 Hz, 1H), 7.58 – 7.48 (m, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.22 (t, *J* = 5.8 Hz, 3H), 7.13 (t, *J* = 6.9 Hz, 1H), 7.02 (dd, *J* = 7.6, 1.4 Hz, 1H), 6.87 (s, 1H), 4.06 (s, 2H), 2.41 (s, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 141.78, 138.48, 137.57, 133.04, 131.23, 131.13, 130.36, 129.54, 129.20, 129.02, 128.93, 128.66, 128.12, 128.00, 127.68, 127.19, 125.33, 125.19, 124.24, 116.35, 77.37, 77.16, 76.95, 38.73, 21.50; IR (KBr): 2975, 1919, 1924, 1735, 1462, 1326, 1280, 1211, 1089, 1049, 942, 882, 825, 755, 657, 567 cm⁻¹; HRMS (ESI) calcd for C₂₄H₁₉BrN₃ [(M + H)⁺]: 428.0757, found 428.0754.

4-(4-Bromobenzyl)-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinoline (3n)



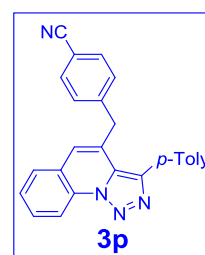
Yield: 51.4 mg (40%); Light yellow solid; Mp. 194.0-195.7 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.82 (d, *J* = 8.2 Hz, 1H), 7.73 (t, *J* = 8.3 Hz, 2H), 7.58 (t, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 7.9 Hz, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 7.8 Hz, 2H), 7.09 (s, 1H), 6.69 (d, *J* = 8.3 Hz, 2H), 3.99 (s, 2H), 2.44 (s, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 141.62, 138.54, 136.86, 131.53, 131.25, 130.64, 130.53, 129.64, 129.06, 129.00, 128.94, 128.73, 128.04, 127.27, 125.95, 124.09, 120.49, 116.36, 37.64, 21.50; IR (KBr): 2918, 1923, 1803, 1473, 1298, 1256, 1212, 1165, 1043, 1002, 956, 912, 931, 797, 750 cm⁻¹; HRMS (ESI) calcd for C₂₄H₁₉BrN₃ [(M + H)⁺]: 428.0757, found 428.0759.

2-((3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinolin-4-yl)methyl)benzonitrile (3o)



Yield: 33.7 mg (30%); Light yellow solid; Mp. 189.2-190.8 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.84 (d, *J* = 8.3 Hz, 1H), 7.82 (d, *J* = 7.7 Hz, 1H), 7.80 – 7.73 (m, 1H), 7.67 – 7.58 (m, 1H), 7.38 (d, *J* = 7.7 Hz, 1H), 7.27 (s, 1H), 7.22 (q, *J* = 8.1 Hz, 4H), 7.17 (t, *J* = 7.8 Hz, 1H), 6.93 (d, *J* = 7.9 Hz, 1H), 6.76 (s, 1H), 4.11 (s, 2H), 2.49 (s, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 141.61, 139.38, 139.01, 132.66, 132.31, 131.53, 130.51, 130.16, 130.01, 129.07, 129.05, 128.85, 128.69, 128.14, 127.47, 127.39, 126.75, 123.92, 118.77, 116.47, 112.35, 77.37, 77.16, 76.95, 38.08, 21.55; IR (KBr): 2923, 2856, 2222, 1911, 1841, 1810, 1611, 1552, 1448, 1392, 1262, 1164, 1034, 996, 712, 859, 753, 694, 561 cm⁻¹; HRMS (ESI) calcd for C₂₅H₁₉N₄ [(M + H)⁺]: 375.1604, found 375.1606.

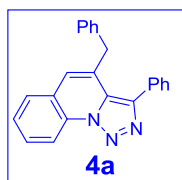
4-((3-(*p*-tolyl)-[1,2,3]triazolo[1,5-*a*]quinolin-4-yl)methyl)benzonitrile (3p)



Yield: 33.8 mg (30%); Light yellow solid; Mp. 190.4-191.6 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.83 (d, *J* = 8.3 Hz, 1H), 7.82 – 7.72 (m, 2H), 7.66 – 7.54 (m, 1H), 7.39 (d, *J* = 8.3 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.22 – 7.17 (m, 3H), 6.83 (d, *J* = 8.2 Hz, 2H), 4.12 (s, 2H), 2.44 (s, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 143.55, 141.55, 138.62, 132.12, 132.08, 131.38, 130.46, 130.43, 129.93, 129.76, 129.37, 129.33, 128.92, 128.81, 128.71, 128.06, 127.39, 127.31, 126.61, 123.88, 118.88, 116.38, 110.34, 38.33, 21.47; IR (KBr): 2917, 2858, 2221,

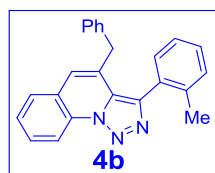
1609, 1554, 1504, 1464, 1417, 1383, 1326, 1246, 1204, 1160, 1112, 1070, 1023, 993, 941, 886, 812, 757, 729, 597, 551, 507 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{25}\text{H}_{19}\text{N}_4$ [(M + H)⁺]: 375.1604, found 375.1602.

4-Benzyl-3-phenyl-[1,2,3]triazolo[1,5-a]quinoline (4a)



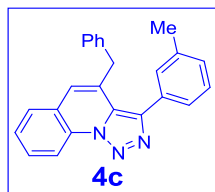
Yield: 56.3 mg (56%); Light yellow solid, Mp. 187.5-189.0 °C; ¹H NMR (600 MHz, CDCl_3) δ 8.83 (d, J = 8.1 Hz, 1H), 7.72 (dd, J = 12.4, 4.4 Hz, 2H), 7.57 (t, J = 7.1 Hz, 1H), 7.51 – 7.46 (m, 2H), 7.46 – 7.39 (m, 3H), 7.17 (dd, J = 6.6, 3.7 Hz, 3H), 7.12 (s, 1H), 6.83 (dd, J = 6.5, 3.0 Hz, 2H), 4.03 (s, 2H); ¹³C NMR (150 MHz, CDCl_3) δ 141.65, 137.77, 132.19, 131.18, 130.73, 129.52, 129.30, 129.27, 128.95, 128.60, 128.56, 128.23, 128.06, 127.24, 126.63, 126.05, 124.23, 116.36, 77.37, 77.16, 76.95, 38.25; IR (KBr): 2924, 2856, 1951, 1890, 1821, 1605, 1549, 1551, 1393, 1215, 1161, 1072, 990, 920, 854, 751, 700, 565, 510 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{18}\text{N}_3$ [(M + H)⁺]: 336.1495, found 336.1493.

4-benzyl-3-(*o*-tolyl)-[1,2,3]triazolo[1,5-a]quinoline (4b)



Yield: 80.7 mg (77%); Light yellow solid; Mp. 155.7-157.0 °C; ¹H NMR (600 MHz, CDCl_3) δ 8.83 (d, J = 8.3 Hz, 1H), 7.76 (d, J = 8.0 Hz, 1H), 7.73 (t, J = 7.5 Hz, 1H), 7.58 (t, J = 7.6 Hz, 1H), 7.35 (t, J = 7.3 Hz, 1H), 7.25 (t, J = 5.8 Hz, 1H), 7.24 – 7.20 (m, 2H), 7.16 (s, 1H), 7.15 – 7.09 (m, 3H), 6.69 (d, J = 6.9 Hz, 2H), 3.87 (s, 2H), 1.91 (s, 3H); ¹³C NMR (150 MHz, CDCl_3) δ 140.49, 139.01, 137.70, 131.58, 131.37, 131.30, 130.19, 129.51, 129.49, 129.14, 129.11, 128.69, 128.40, 128.10, 127.22, 126.58, 125.93, 125.38, 124.29, 116.28, 77.37, 77.16, 76.95, 37.92, 20.05; IR (KBr): 2920, 2858, 1919, 1815, 1609, 1542, 1455, 1390, 1326, 1213, 1163, 1117, 1031, 991, 946, 908, 954, 748, 627, 572 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{20}\text{N}_3$ [(M + H)⁺]: 350.1652, found 350.1649.

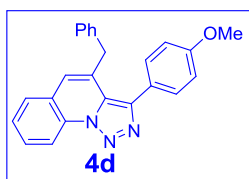
4-Benzyl-3-(*m*-tolyl)-[1,2,3]triazolo[1,5-a]quinoline (4c)



Yield: 76.5 mg (73%); Light yellow solid; Mp. 181.5-182.9 °C; ¹H NMR (600 MHz, CDCl_3) δ 8.82 (d, J = 8.2 Hz, 1H), 7.75 – 7.68 (m, 2H), 7.56 (dd, J = 11.0, 4.2 Hz, 1H), 7.33 – 7.26 (m, 2H), 7.24 (d, J = 8.8 Hz, 2H), 7.20 – 7.15 (m, 3H), 7.12 (s, 1H), 6.83 (dd, J = 6.5, 2.8 Hz, 2H), 4.04 (s, 2H), 2.35 (s, 3H); ¹³C NMR (150 MHz, CDCl_3) δ 141.77, 137.90, 137.87, 131.99, 131.39, 131.18, 129.47, 129.33, 129.24, 129.22, 128.89, 128.50, 128.03, 127.77, 127.19, 126.54, 126.03, 124.22, 116.33, 77.37, 77.16, 76.95, 38.17, 21.50; IR (KBr): 2921, 2856, 1604, 1558, 1492, 1422, 1323, 1240, 1206, 1155, 1107, 1028, 989, 948, 871, 792, 745, 690, 627, 585, 542 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{20}\text{N}_3$ [(M + H)⁺]: 350.1652, found 350.1653.

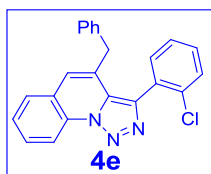
4-Benzyl-3-(4-methoxyphenyl)-[1,2,3]triazolo[1,5-a]quinoline (4d)

Yield: 72.4 mg (66%); Light yellow solid; Mp. 189.4-190.4 °C; ¹H NMR (600 MHz, CDCl_3) δ 8.80 (d, J = 8.6 Hz, 1H), 7.70 (dd, J = 7.8, 6.3 Hz, 2H), 7.59 – 7.49 (m, 1H),



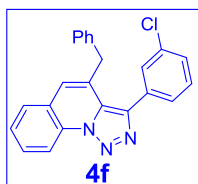
7.42 – 7.36 (m, 2H), 7.22 – 7.14 (m, 3H), 7.07 (s, 1H), 6.96 – 6.92 (m, 2H), 6.87 (dd, $J = 7.2, 2.0$ Hz, 2H), 4.02 (s, 2H), 3.87 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 159.93, 141.35, 137.84, 131.86, 131.14, 129.39, 129.36, 129.20, 128.96, 128.51, 128.00, 127.13, 126.61, 125.77, 124.42, 124.20, 116.24, 113.66, 77.37, 77.16, 76.95, 55.46, 38.12; IR (KBr): 2973, 1915, 1613, 1551, 1464, 1296, 1248, 1171, 1089, 1044, 883, 834, 755, 704, 563 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{24}\text{H}_{20}\text{N}_3\text{O}$ $[(\text{M} + \text{H})^+]$: 366.1601, found 366.1602.

4-Benzyl-3-(2-chlorophenyl)-[1,2,3]triazolo[1,5-a]quinoline (4e)



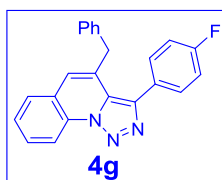
Yield: 61.0 mg (55%); Light yellow solid; Mp. 184.5-186.0 $^{\circ}\text{C}$; ^1H NMR (600 MHz, CDCl_3) δ 8.83 (d, $J = 8.2$ Hz, 1H), 7.78 – 7.71 (m, 2H), 7.62 – 7.55 (m, 1H), 7.49 (dd, $J = 8.1, 0.8$ Hz, 1H), 7.43 – 7.36 (m, 1H), 7.33 – 7.23 (m, 2H), 7.20 – 7.11 (m, 4H), 6.80 (dd, $J = 7.0, 2.4$ Hz, 2H), 3.96 (dd, $J = 62.9, 16.3$ Hz, 2H); ^{13}C NMR (150 MHz, CDCl_3) δ 138.27, 137.63, 135.51, 133.14, 131.41, 131.19, 130.44, 130.22, 129.60, 129.49, 129.10, 128.79, 128.57, 128.15, 127.33, 126.73, 126.66, 126.25, 124.32, 116.38, 77.37, 77.16, 76.95, 37.69; IR (KBr): 2920, 1919, 1830, 1801, 1714, 1610, 1553, 1453, 1323, 1217, 1160, 1117, 1034, 996, 948, 916, 742, 698, 662 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{17}\text{ClN}_3$ $[(\text{M} + \text{H})^+]$: 370.1106, found 370.1104.

4-Benzyl-3-(3-chlorophenyl)-[1,2,3]triazolo[1,5-a]quinoline (4f)



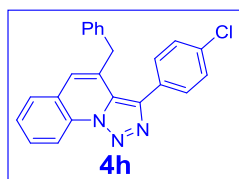
Yield: 54.3 mg (49%); Light yellow solid; Mp. 153.3-154.6 $^{\circ}\text{C}$; ^1H NMR (600 MHz, CDCl_3) δ 8.82 (d, $J = 8.3$ Hz, 1H), 7.82 – 7.70 (m, 2H), 7.66 – 7.55 (m, 1H), 7.44 – 7.37 (m, 2H), 7.36 – 7.29 (m, 2H), 7.20 (s, 1H), 7.19 – 7.15 (m, 3H), 6.80 (dd, $J = 6.3, 2.7$ Hz, 2H), 4.05 (s, 2H); ^{13}C NMR (150 MHz, CDCl_3) δ 140.21, 137.49, 134.11, 133.95, 131.17, 130.69, 129.75, 129.41, 129.40, 128.88, 128.73, 128.70, 128.65, 128.63, 128.15, 127.44, 126.76, 126.72, 124.18, 116.40, 38.44; IR (KBr): 2920, 2859, 1451, 1219, 1158, 1030, 908, 852, 793, 749, 703 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{17}\text{ClN}_3$ $[(\text{M} + \text{H})^+]$: 370.1106, found 370.1108.

4-Benzyl-3-(4-fluorophenyl)-[1,2,3]triazolo[1,5-a]quinoline (4g)



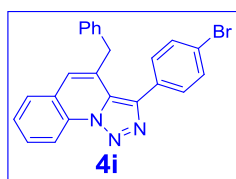
Yield: 45.6 mg (43%); Light yellow solid; Mp. 150.6-151.3 $^{\circ}\text{C}$; ^1H NMR (600 MHz, CDCl_3) δ 8.82 (d, $J = 8.3$ Hz, 1H), 7.77 – 7.72 (m, 2H), 7.61 – 7.55 (m, 1H), 7.43 – 7.36 (m, 2H), 7.16 (m, 4H), 7.12 – 7.06 (m, 2H), 6.82 (dd, $J = 6.5, 2.9$ Hz, 2H), 4.02 (s, 2H); ^{13}C NMR (150 MHz, CDCl_3) δ 163.15 (d, $J = 247.9$ Hz), 140.59, 137.65, 132.43 (d, $J = 8.3$ Hz), 131.22, 129.66, 128.75 (d, $J = 7.8$ Hz), 128.74, 128.60, 128.23 (d, $J = 3.2$ Hz), 128.12, 127.37, 126.71, 126.46, 124.21, 116.38, 115.31, 115.17, 38.31; IR (KBr): 2923, 2857, 1897, 1827, 1606, 1555, 1469, 1300, 1230, 1158, 1089, 996, 944, 836, 753, 705, 619, 557 cm^{-1} ; HRMS (ESI) calcd for $\text{C}_{23}\text{H}_{17}\text{FN}_3$ $[(\text{M} + \text{H})^+]$: 354.1401, found 354.1403.

4-Benzyl-3-(4-chlorophenyl)-[1,2,3]triazolo[1,5-a]quinoline (4h)



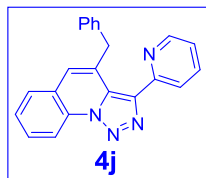
Yield: 58.8 mg (53%); Light yellow solid; Mp. 176.8-178.2 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.82 (d, *J* = 8.3 Hz, 1H), 7.77 – 7.69 (m, 2H), 7.63 – 7.51 (m, 1H), 7.36 (s, 4H), 7.17 (dd, *J* = 7.6, 5.0 Hz, 4H), 6.82 (dd, *J* = 6.5, 2.8 Hz, 2H), 4.02 (s, 2H); ¹³C NMR (150 MHz, CDCl₃) δ 140.39, 137.56, 134.74, 131.91, 131.16, 130.66, 129.69, 129.36, 128.75, 128.71, 128.61, 128.41, 128.11, 127.38, 126.72, 126.58, 124.17, 116.36, 77.37, 77.16, 76.95, 38.34; IR (KBr): 2950, 2900, 1463, 1295, 1246, 1116, 1073, 949, 852, 831, 759, 702, 514 cm⁻¹; HRMS (ESI) calcd for C₂₃H₁₇ClN₃ [(M + H)⁺]: 370.1106, found 370.1105.

4-Benzyl-3-(4-bromophenyl)-[1,2,3]triazolo[1,5-a]quinoline (4i)



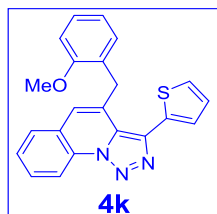
Yield: 58.4 mg (47%); Light yellow solid; Mp. 178.8-179.9 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.81 (d, *J* = 8.2 Hz, 1H), 7.77 – 7.69 (m, 2H), 7.61 – 7.55 (m, 1H), 7.54 – 7.48 (m, 2H), 7.32 – 7.27 (m, 2H), 7.21 – 7.13 (m, 4H), 6.82 (dd, *J* = 6.5, 2.9 Hz, 2H), 4.02 (s, 2H); ¹³C NMR (150 MHz, CDCl₃) δ 140.38, 137.52, 132.18, 131.34, 131.13, 131.11, 129.68, 129.32, 128.74, 128.68, 128.60, 128.10, 127.37, 126.71, 126.59, 124.15, 122.96, 116.33, 77.37, 77.16, 76.95, 38.34; IR (KBr): 2915, 1458, 1250, 1161, 1068, 994, 947, 824, 757, 696, 573, 507 cm⁻¹; HRMS (ESI) calcd for C₂₃H₁₇BrN₃ [(M + H)⁺]: 414.0600, found 414.0602.

4-Benzyl-3-(pyridin-2-yl)-[1,2,3]triazolo[1,5-a]quinoline (4j)



Yield: 66.6 mg (66%); Light yellow solid; Mp. 162.0-163.0 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.82 (d, *J* = 8.3 Hz, 1H), 8.73 (d, *J* = 4.8 Hz, 1H), 7.88 (d, *J* = 7.5 Hz, 1H), 7.78 – 7.68 (m, 3H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.33 – 7.28 (m, 1H), 7.22 (s, 1H), 7.14 (dd, *J* = 9.6, 5.7 Hz, 3H), 6.97 – 6.75 (m, 2H), 4.56 (s, 2H); ¹³C NMR (150 MHz, CDCl₃) δ 151.83, 148.82, 141.27, 138.54, 136.67, 130.92, 130.27, 130.03, 129.53, 128.91, 128.44, 128.02, 127.32, 126.79, 126.38, 125.00, 124.30, 122.77, 116.37, 77.37, 77.16, 76.95, 39.00; IR (KBr): 2975, 1797, 1451, 1300, 1090, 1048, 749 cm⁻¹; HRMS (ESI) calcd for C₂₂H₁₇N₄ [(M + H)⁺]: 337.1448, found 337.1450.

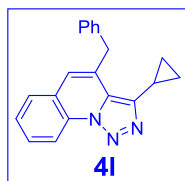
4-(2-Methoxybenzyl)-3-(thiophen-2-yl)-[1,2,3]triazolo[1,5-a]quinoline (4k)



Yield: 72.5 mg (65%); Light yellow solid; Mp. 160.9-162.4 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.80 (d, *J* = 8.3 Hz, 1H), 7.73 – 7.63 (m, 2H), 7.57 – 7.49 (m, 1H), 7.44 – 7.38 (m, 1H), 7.26 – 7.23 (m, 1H), 7.19 (dd, *J* = 3.5, 0.9 Hz, 1H), 7.06 (dd, *J* = 5.1, 3.6 Hz, 1H), 6.99 (s, 1H), 6.93 (dd, *J* = 7.3, 1.3 Hz, 1H), 6.86 (dd, *J* = 14.0, 7.6 Hz, 2H), 4.11 (s, 2H), 3.72 (s, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 157.44, 134.60, 132.58, 131.05, 130.47, 130.14, 129.54, 129.37, 129.15, 128.34, 128.02, 127.36, 127.23, 126.99, 126.26, 125.61, 124.38, 120.63, 116.28, 110.37, 77.37, 77.16, 76.95, 55.32, 32.47; IR (KBr): 2919, 1458, 1301, 1242, 1164, 1111, 1033, 941, 845, 756, 719, 559 cm⁻¹; HRMS (ESI) calcd for C₂₂H₁₈N₃OS [(M + H)⁺]:

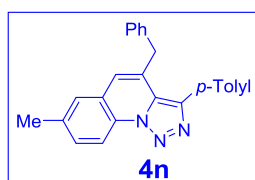
372.1165, found 372.1163.

4-Benzyl-3-cyclopropyl-[1,2,3]triazolo[1,5-a]quinoline (4l)



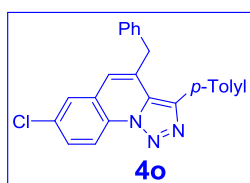
Yield: 53.9 mg (60%); Light yellow solid; Mp. 141.7-142.6 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.72 (d, *J* = 8.3 Hz, 1H), 7.67 (dd, *J* = 15.4, 8.0 Hz, 2H), 7.52 (t, *J* = 7.6 Hz, 1H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.28 (t, *J* = 7.3 Hz, 1H), 7.23 (d, *J* = 7.5 Hz, 2H), 7.01 (s, 1H), 4.50 (s, 2H), 2.19 – 1.91 (m, 1H), 1.15 (dd, *J* = 5.0, 1.7 Hz, 2H), 0.95 (dd, *J* = 8.3, 2.2 Hz, 2H); ¹³C NMR (150 MHz, CDCl₃) δ 142.12, 138.19, 131.34, 130.54, 129.30, 129.21, 128.99, 128.94, 127.97, 127.84, 127.03, 126.95, 124.80, 124.32, 116.22, 77.37, 77.16, 76.95, 38.28, 7.85, 7.75; IR (KBr): 2907, 2848, 1559, 1488, 1451, 1334, 1249, 1202, 1023, 991, 951, 900, 812, 759, 729, 559, 515 cm⁻¹; HRMS (ESI) calcd for C₂₀H₁₈N₃ [(M + H)⁺]: 300.1495, found 300.1495.

4-Benzyl-7-methyl-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-a]quinoline (4n)



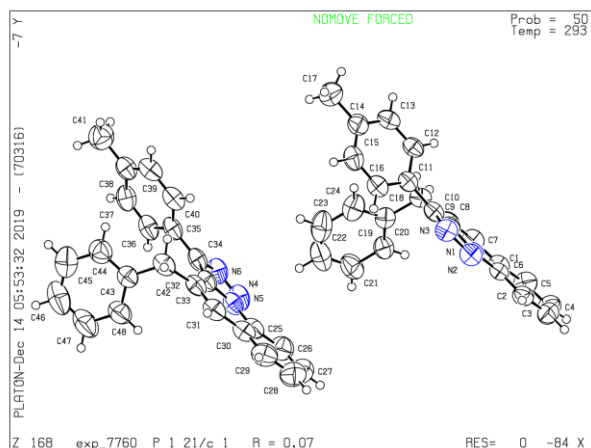
Yield: 58.9 mg (54%); Light yellow solid; Mp. 170.6-171.5 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.69 (d, *J* = 8.5 Hz, 1H), 7.52 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.49 (s, 1H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 7.8 Hz, 2H), 7.20 – 7.15 (m, 3H), 6.99 (s, 1H), 6.88 (dd, *J* = 7.1, 2.3 Hz, 2H), 4.01 (s, 2H), 2.51 (s, 3H), 2.43 (s, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 141.58, 138.35, 137.96, 137.11, 130.82, 130.58, 129.43, 129.31, 129.30, 129.11, 129.09, 128.92, 128.54, 127.66, 126.63, 125.65, 124.30, 116.13, 77.37, 77.16, 76.95, 38.19, 21.51, 21.47; IR (KBr): 2964, 2920, 2855, 1910, 1806, 1731, 1540, 1448, 1261, 1200, 1086, 1042, 998, 958, 897, 818, 736, 699, 561, 520 cm⁻¹; HRMS (ESI) calcd for C₂₅H₂₂N₃ [(M + H)⁺]: 364.1808, found 364.1810.

4-Benzyl-7-chloro-3-(*p*-tolyl)-[1,2,3]triazolo[1,5-a]quinoline (4o)



Yield: 50.6 mg (44%); Light yellow solid; Mp. 143.9-145.0 °C; ¹H NMR (600 MHz, CDCl₃) δ 8.74 (d, *J* = 8.8 Hz, 1H), 7.68 (d, *J* = 2.1 Hz, 1H), 7.64 (dd, *J* = 8.8, 2.2 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 7.8 Hz, 2H), 7.22 – 7.19 (m, 3H), 6.94 (s, 1H), 6.89 (dd, *J* = 6.9, 2.4 Hz, 2H), 4.01 (s, 2H), 2.43 (s, 3H); ¹³C NMR (150 MHz, CDCl₃) δ 142.05, 138.63, 137.40, 132.84, 131.30, 130.54, 129.66, 129.54, 129.14, 129.10, 129.01, 128.88, 128.66, 127.19, 126.84, 125.42, 124.50, 117.84, 77.37, 77.16, 76.95, 38.19, 21.51; IR (KBr): 2968, 2919, 2856, 1913, 1551, 1464, 1422, 1330, 1245, 1195, 1154, 1083, 1045, 990, 895, 821, 761, 737, 700, 551, 506 cm⁻¹; HRMS (ESI) calcd for C₂₄H₁₉ClN₃ [(M + H)⁺]: 384.1262, found 384.1260.

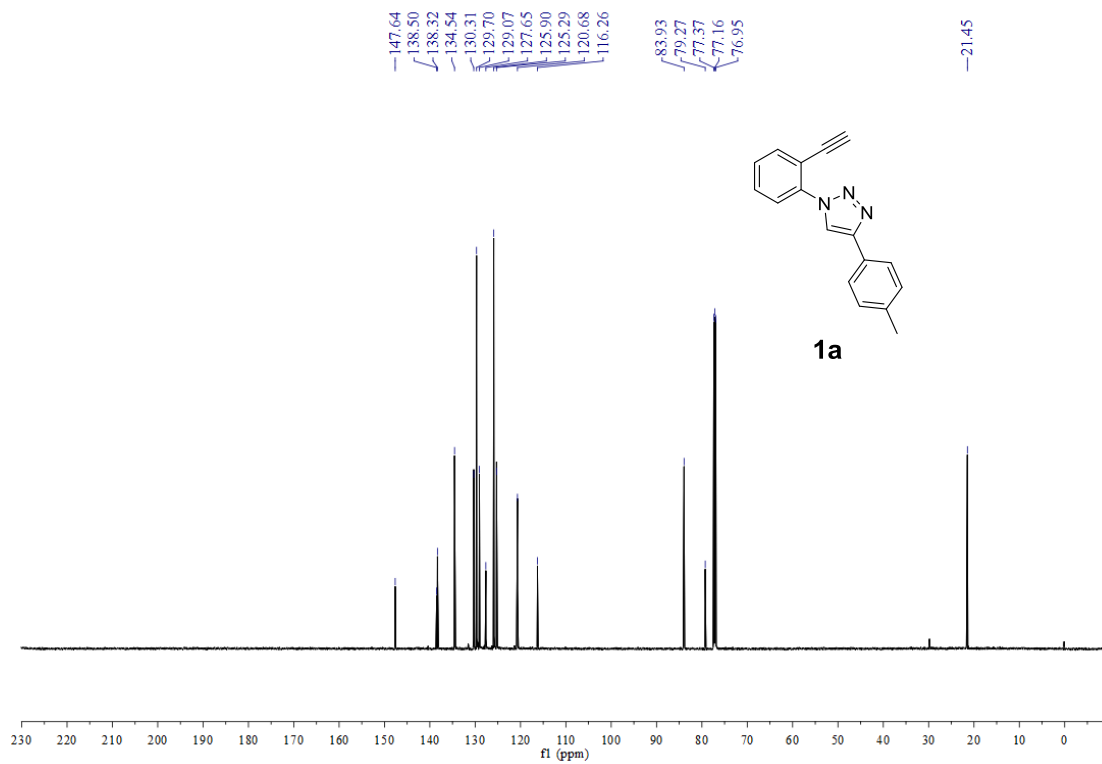
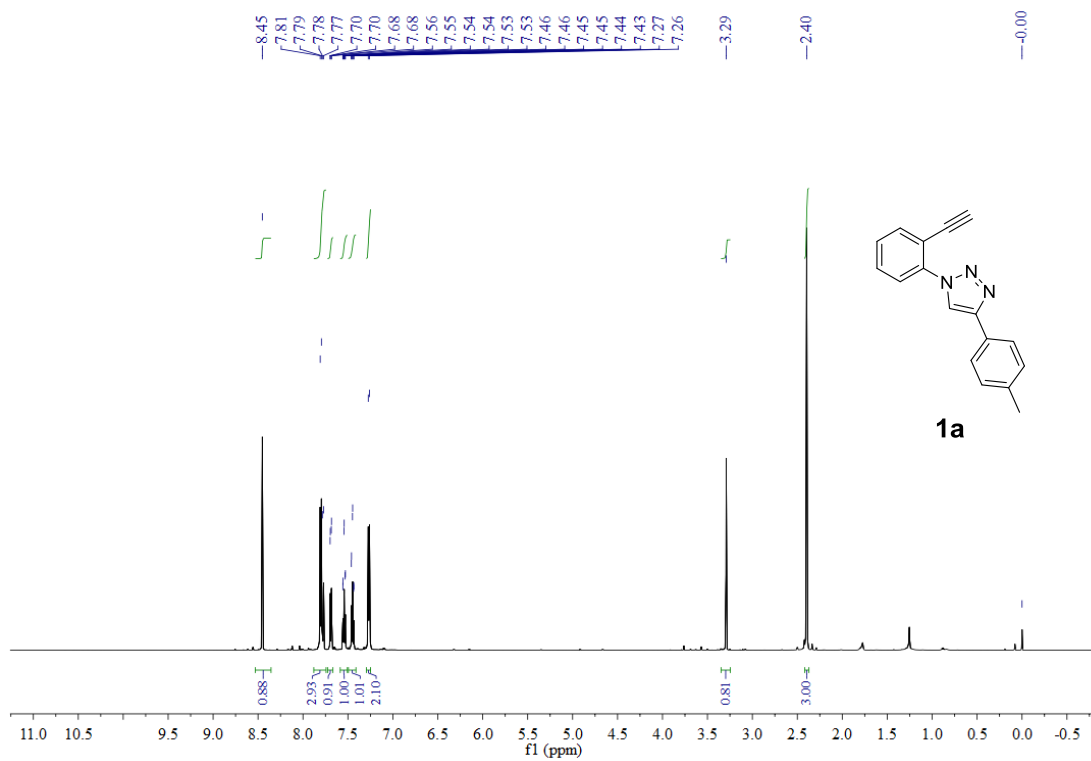
6. X-ray Data of 3a

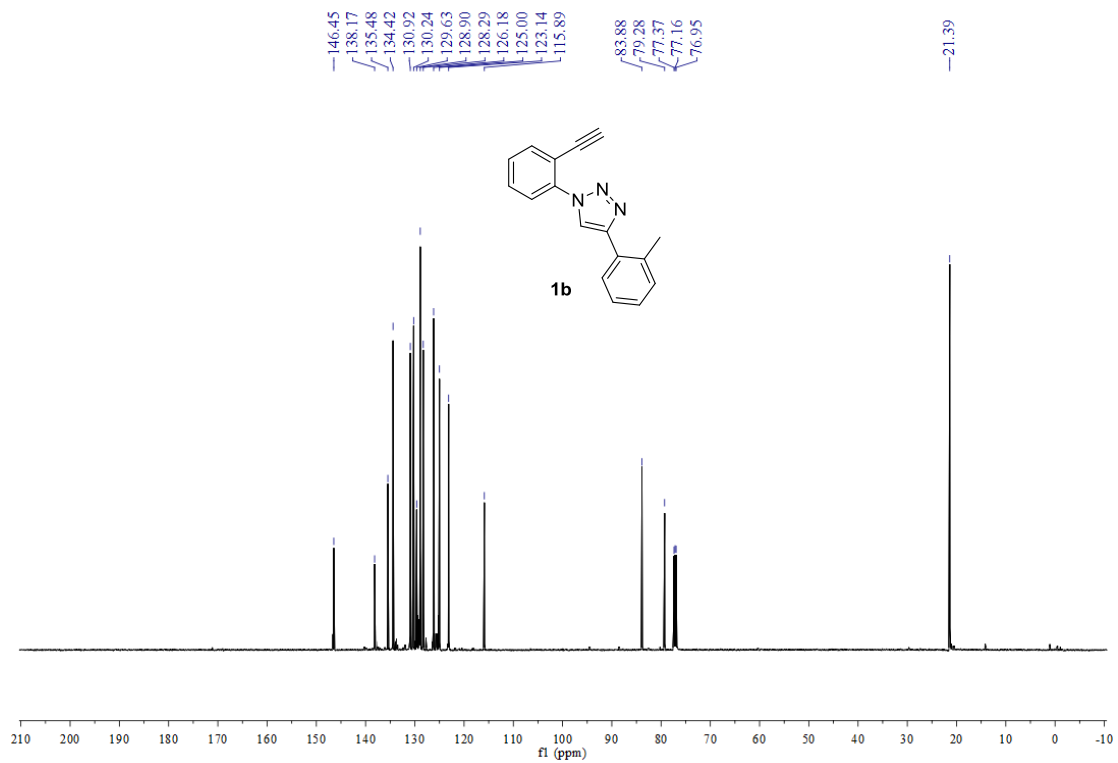
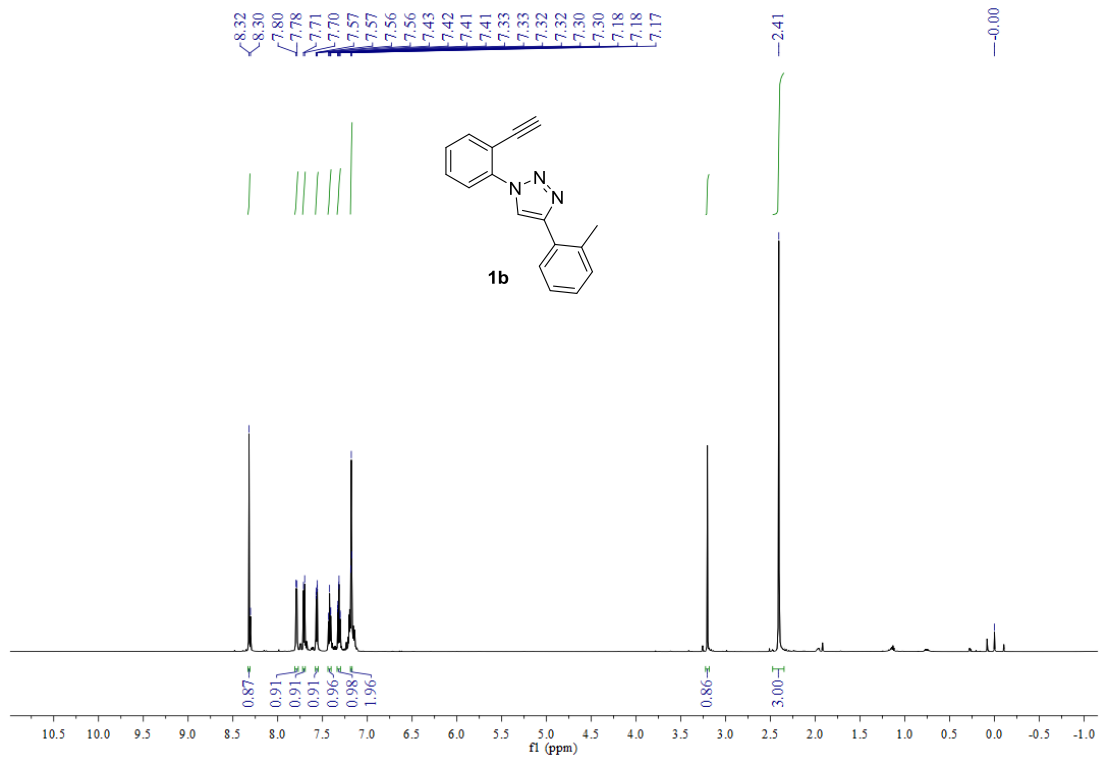


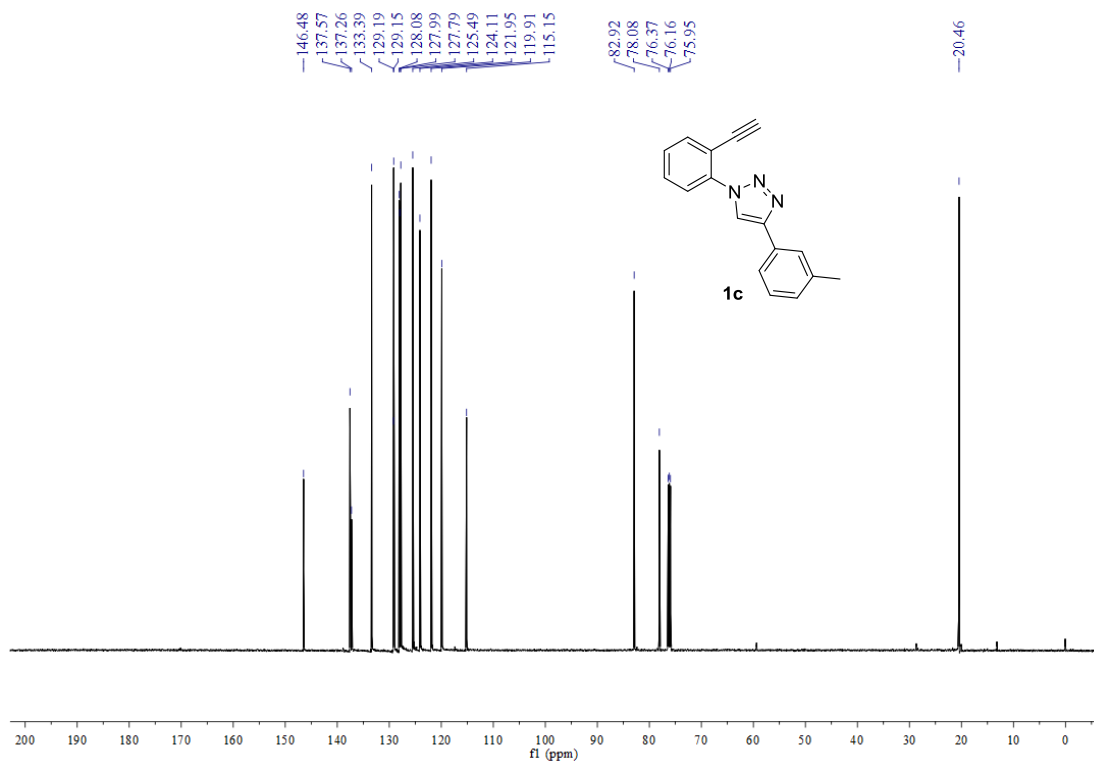
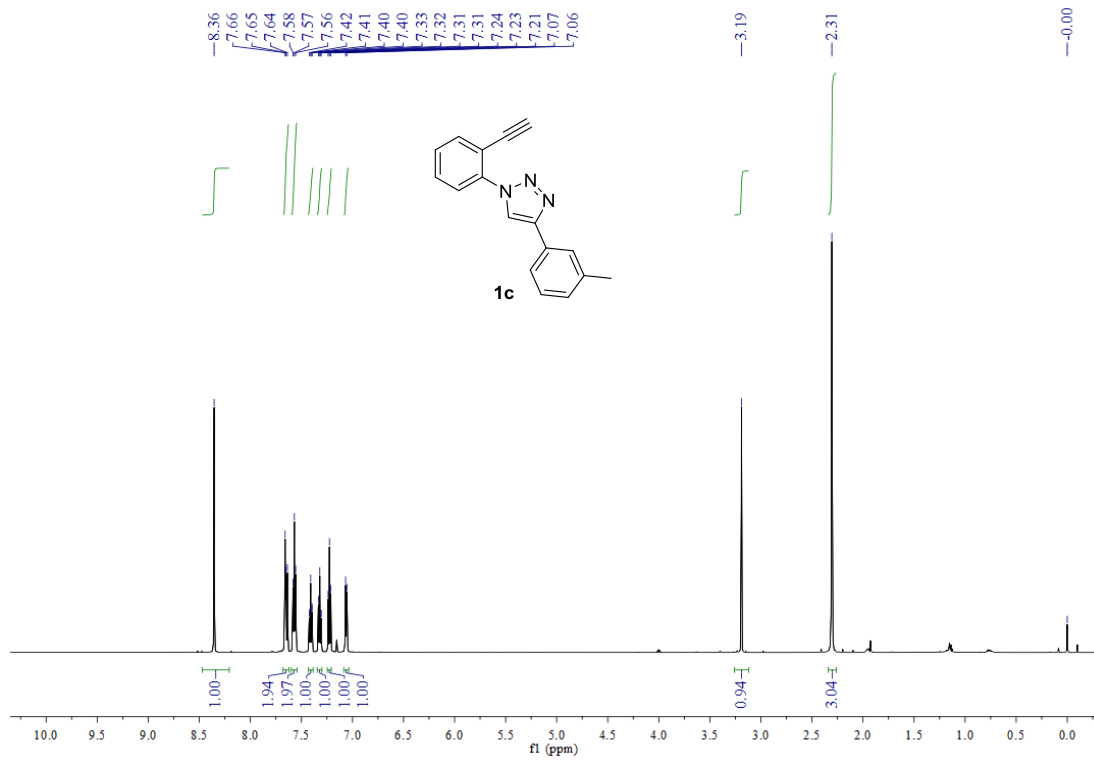
Datablock: exp_7760

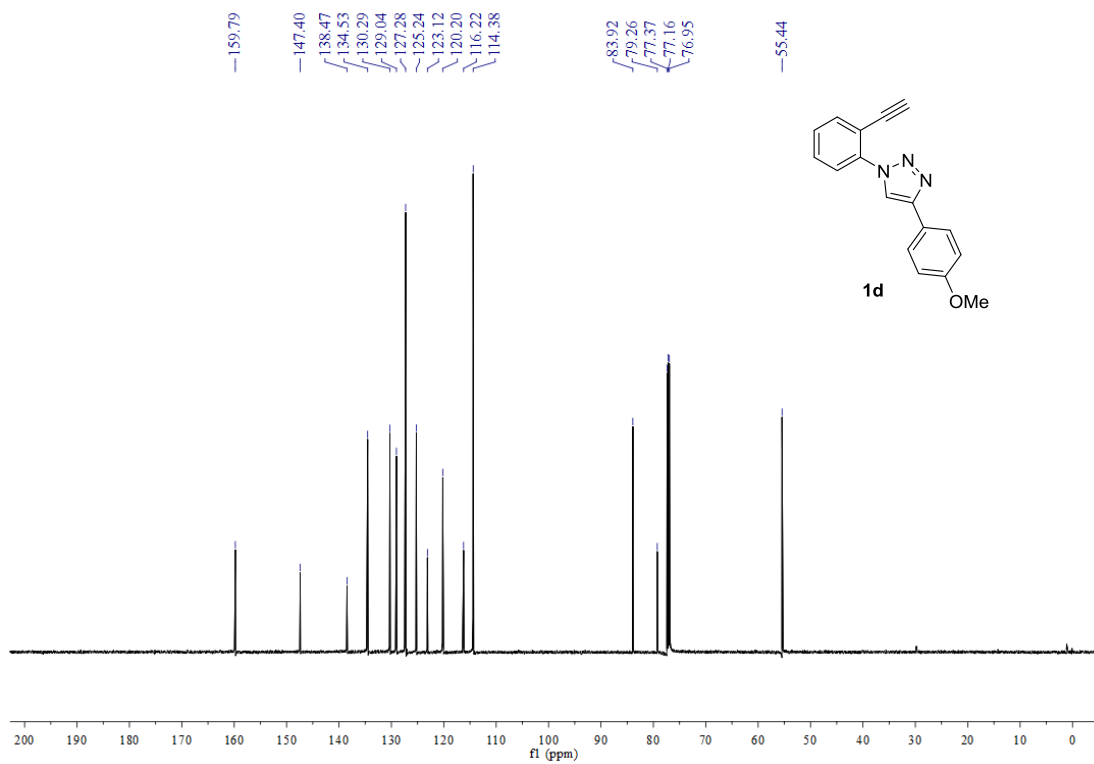
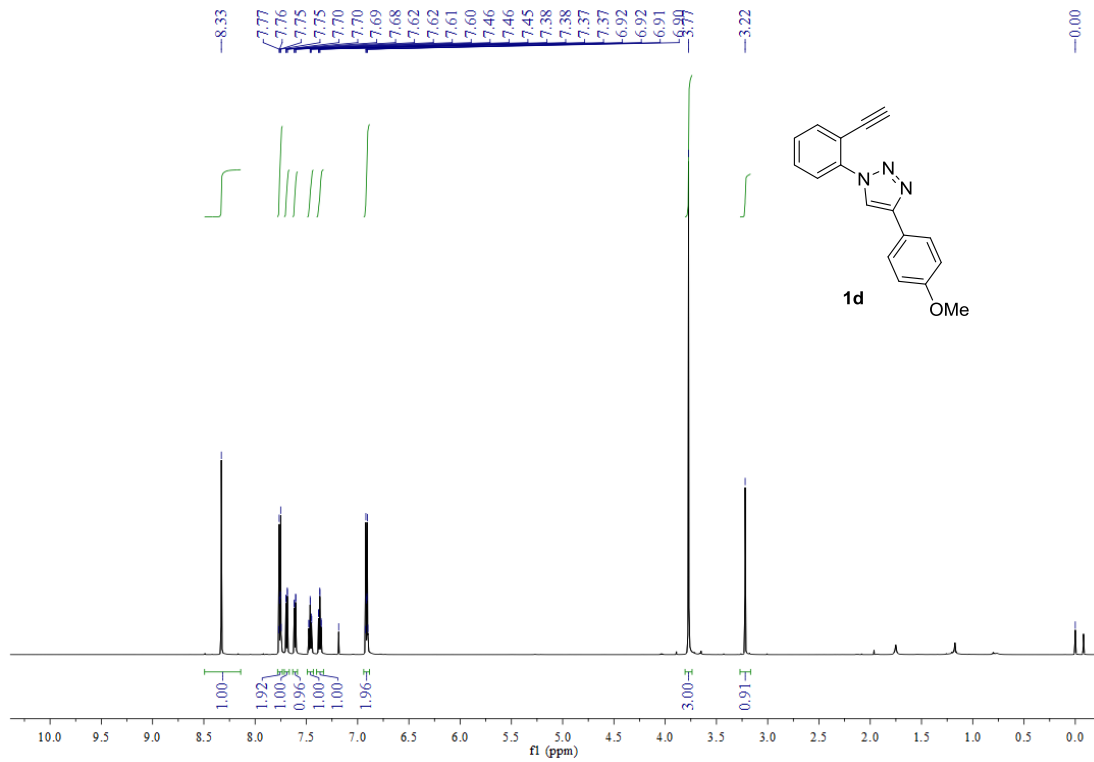
Bond precision:	C-C = 0.0037 Å	Wavelength=0.71073	
Cell:	a=18.4957(13) alpha=90	b=7.8032(5) beta=92.571(7)	c=25.760(2) gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	3714.1(5)	3714.0(5)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C ₂₄ H ₁₉ N ₃	C ₂₄ H ₁₉ N ₃	
Sum formula	C ₂₄ H ₁₉ N ₃	C ₂₄ H ₁₉ N ₃	
Mr	349.42	349.42	
Dx, g cm ⁻³	1.250	1.250	
Z	8	8	
Mu (mm ⁻¹)	0.075	0.075	
F000	1472.0	1472.0	
F000'	1472.49		
h,k,lmax	23,9,32	23,9,32	
Nref	8104	7966	
Tmin,Tmax	0.981,0.992	0.518,1.000	
Tmin'	0.978		
Correction method=	# Reported T Limits: Tmin=0.518 Tmax=1.000		
AbsCorr =	MULTI-SCAN		
Data completeness =	0.983	Theta (max) = 27.000	
R (reflections) =	0.0668(3860)	wR2 (reflections) = 0.1772(7966)	
S =	1.006	Npar = 489	

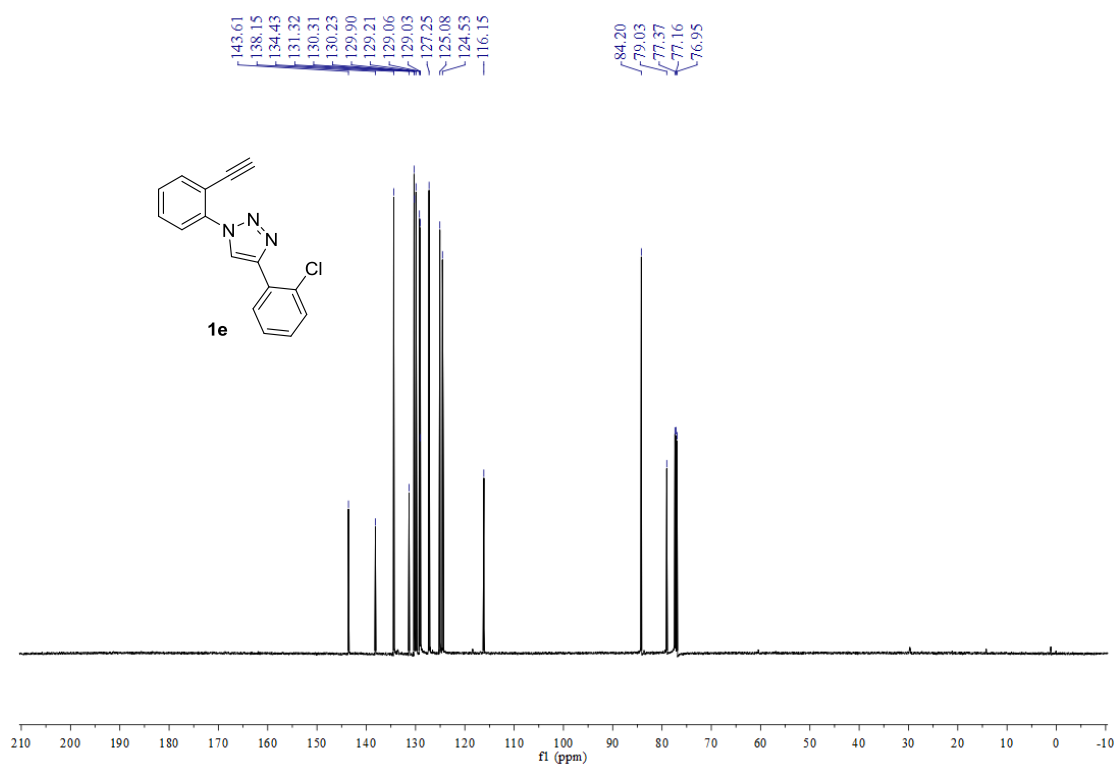
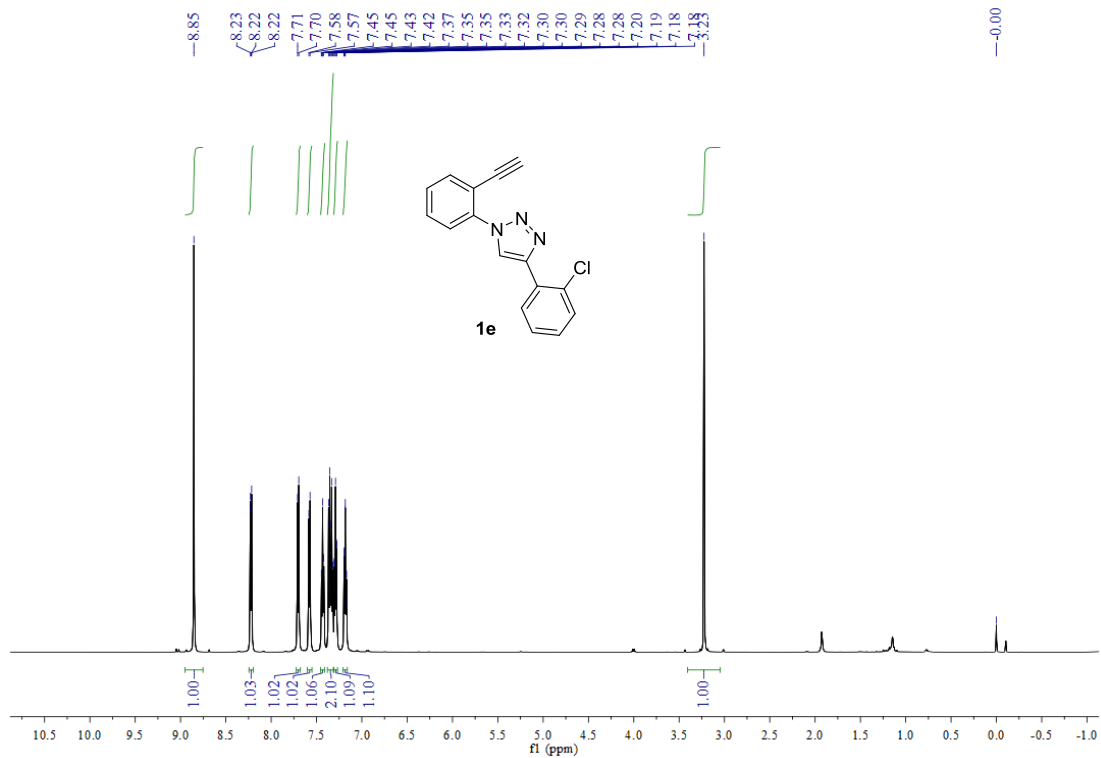
7. ^1H and ^{13}C NMR Spectra of the Compounds

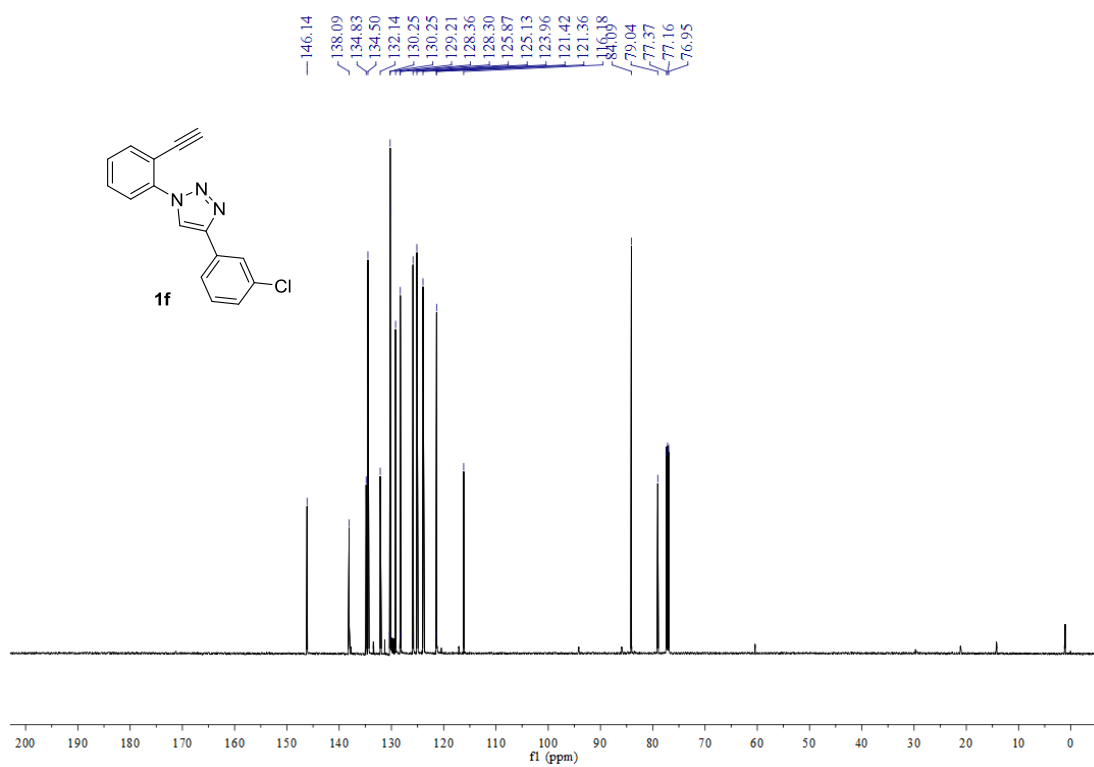
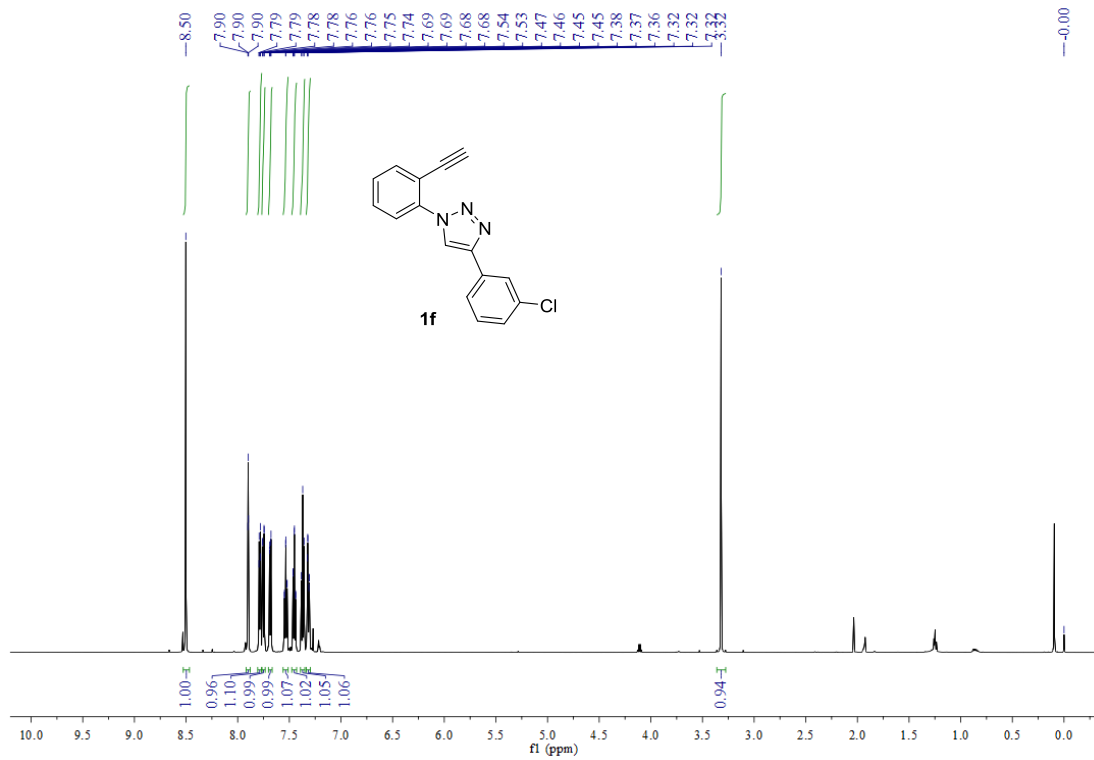


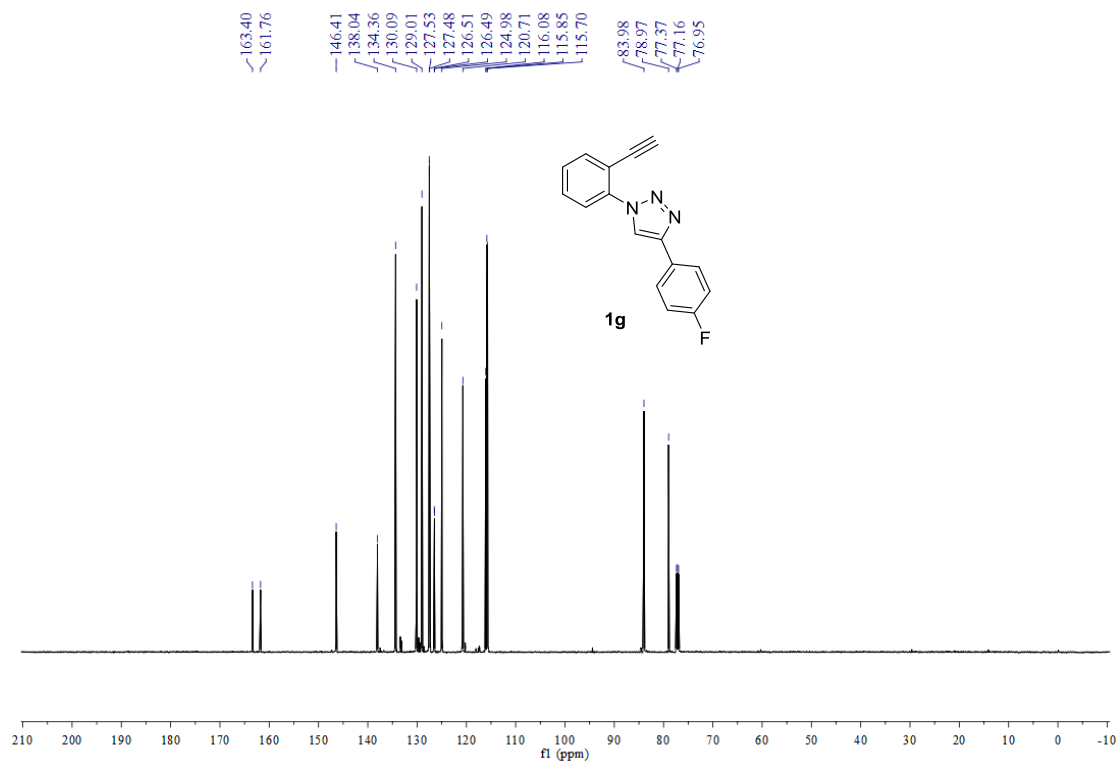
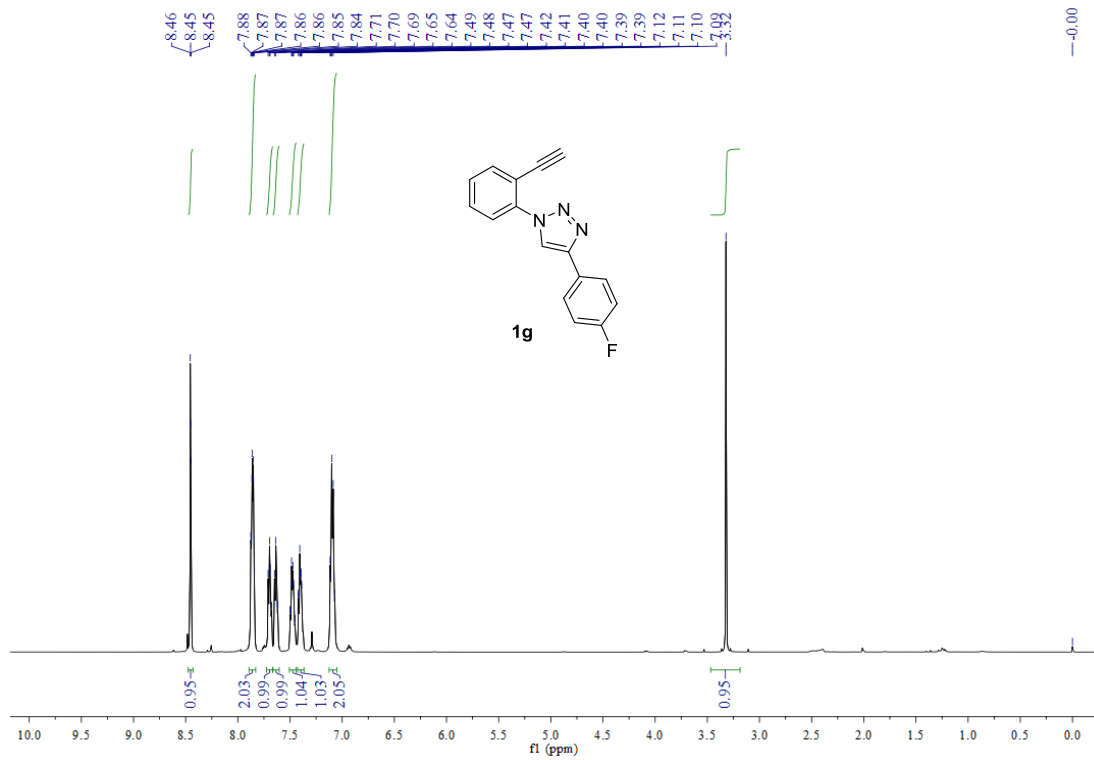


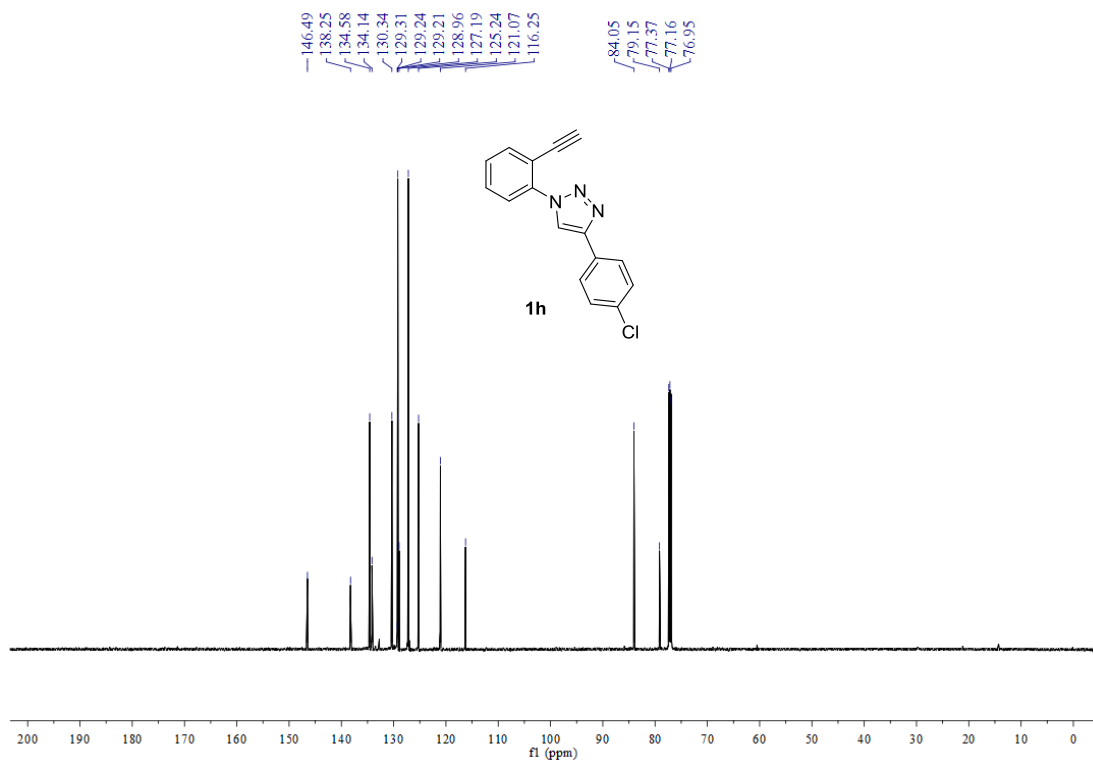
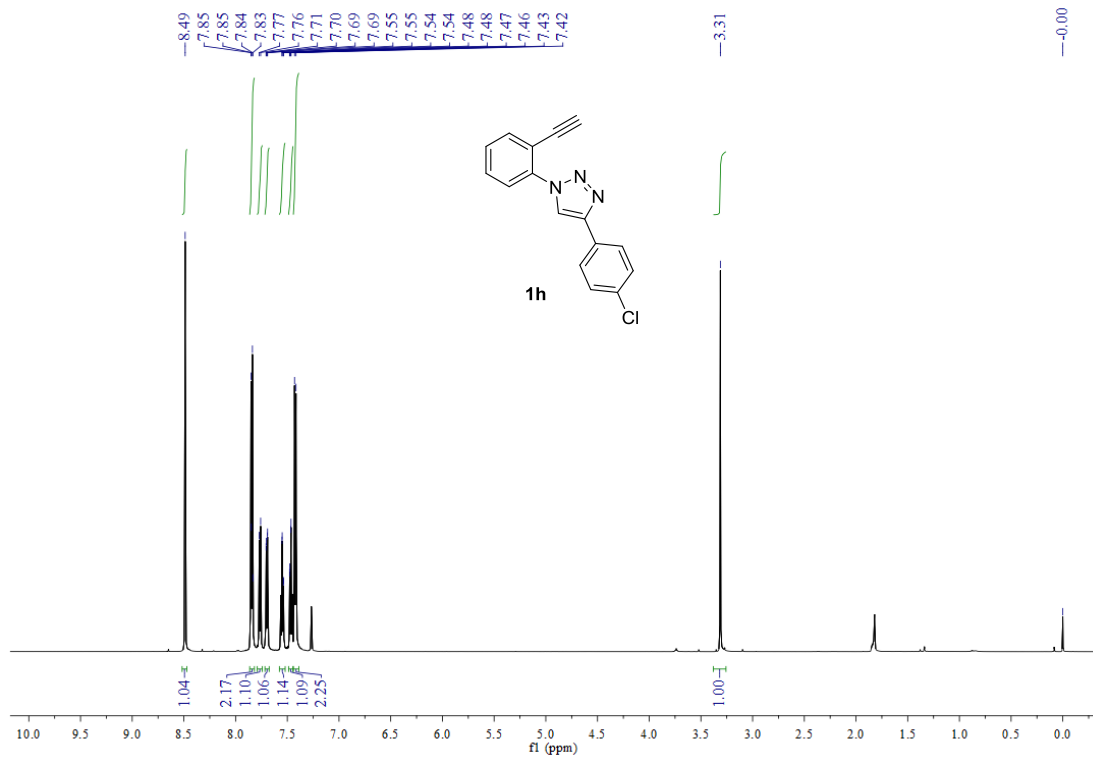


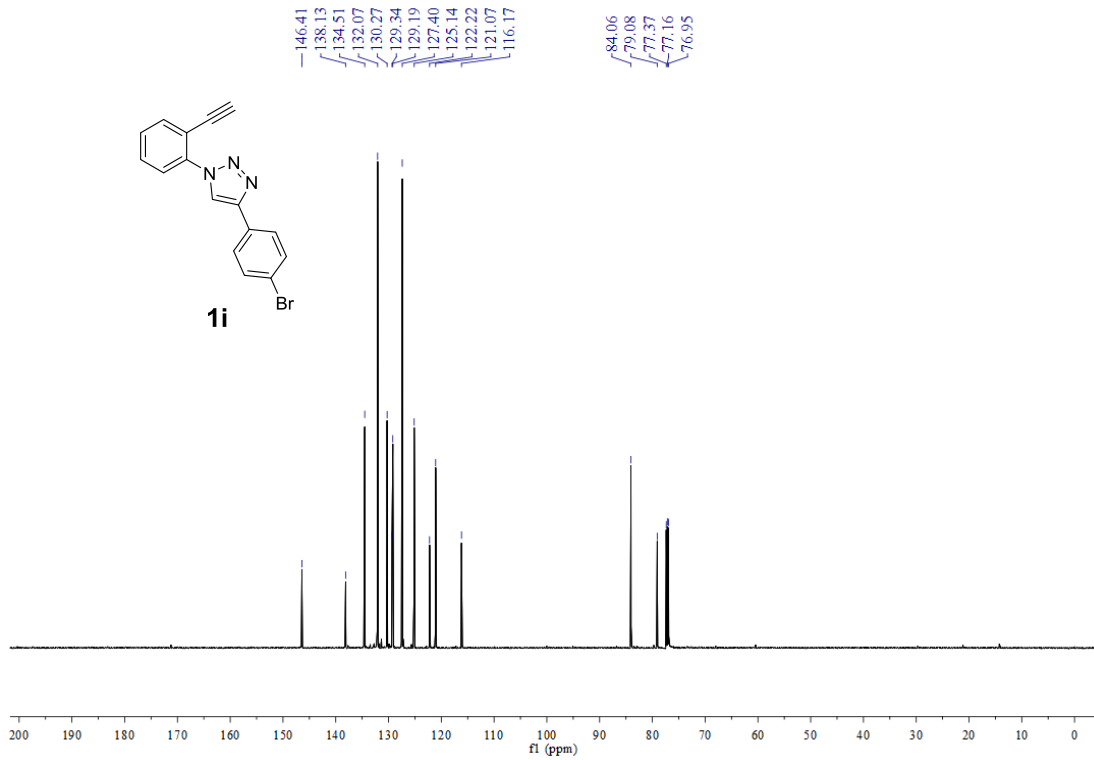
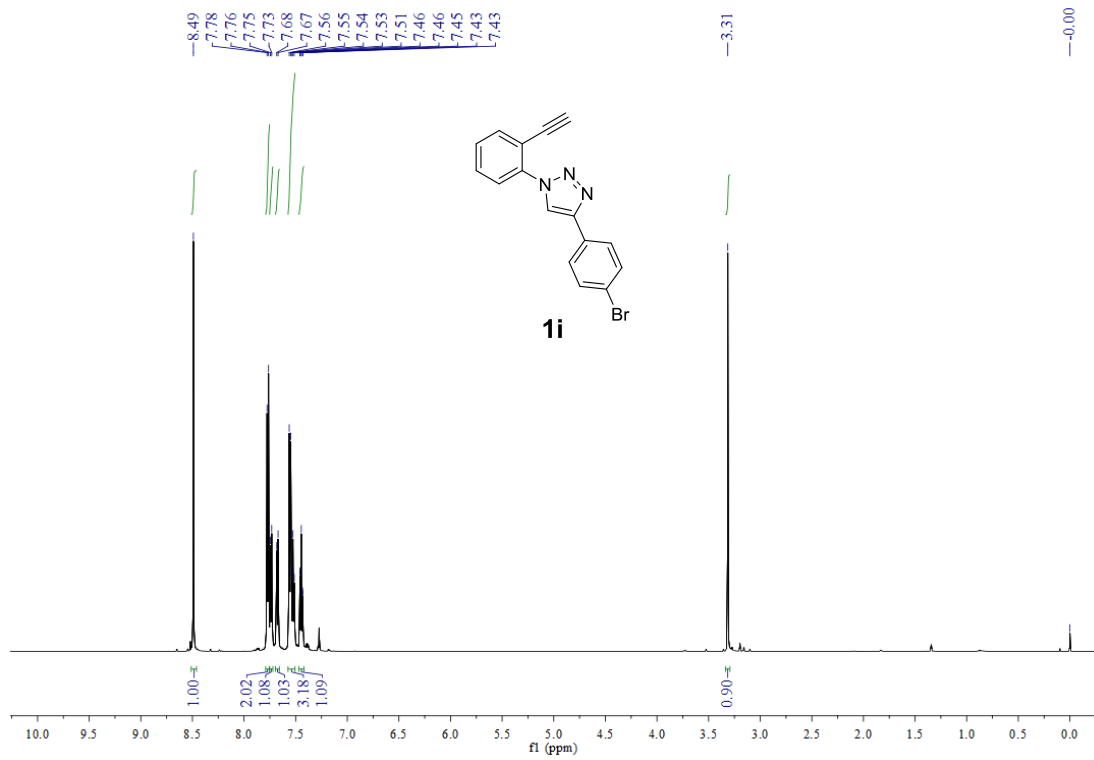


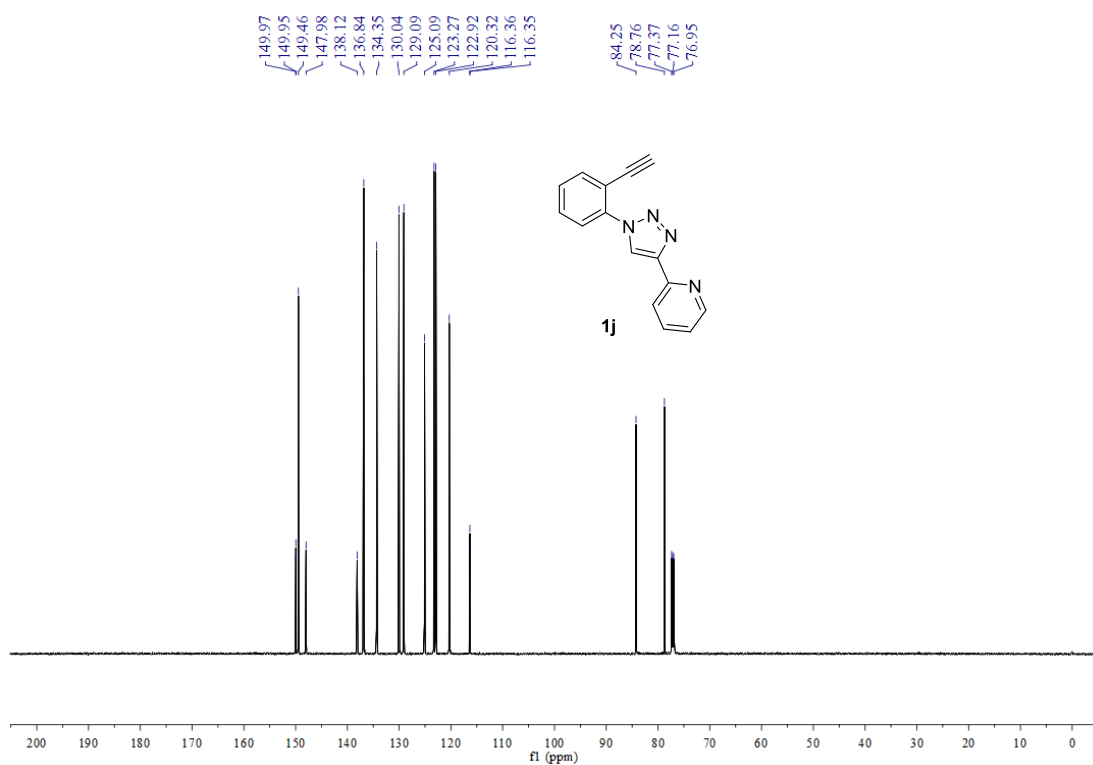
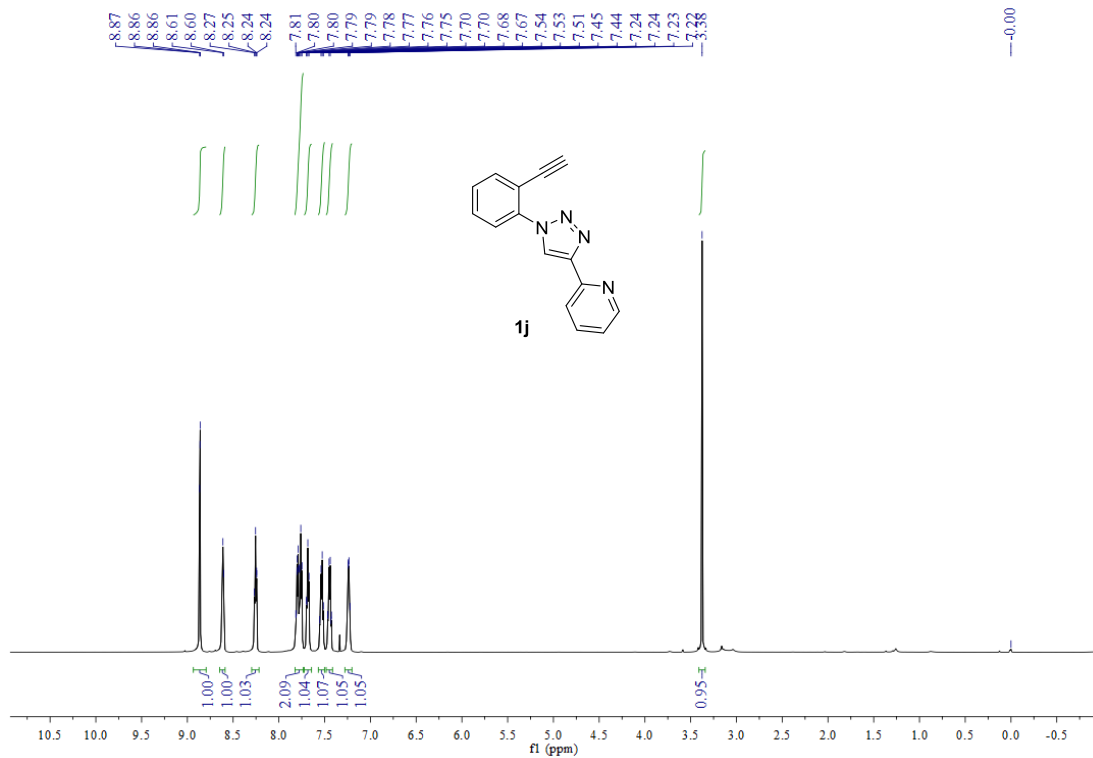


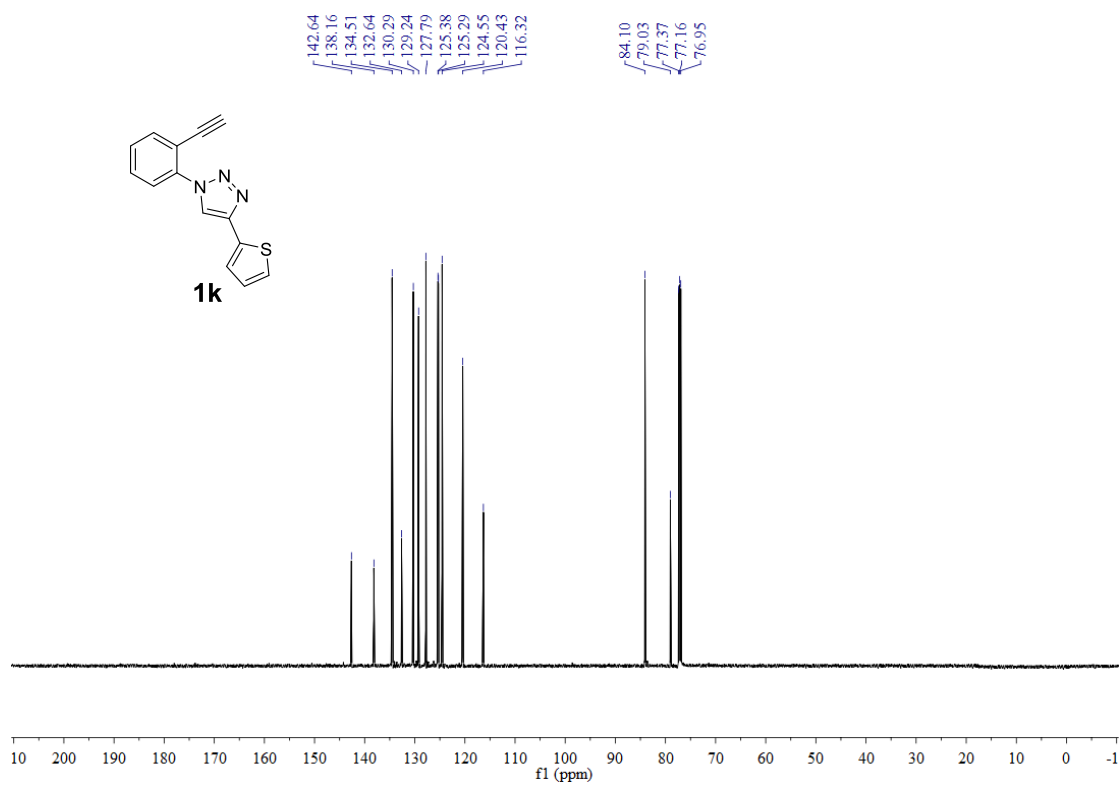
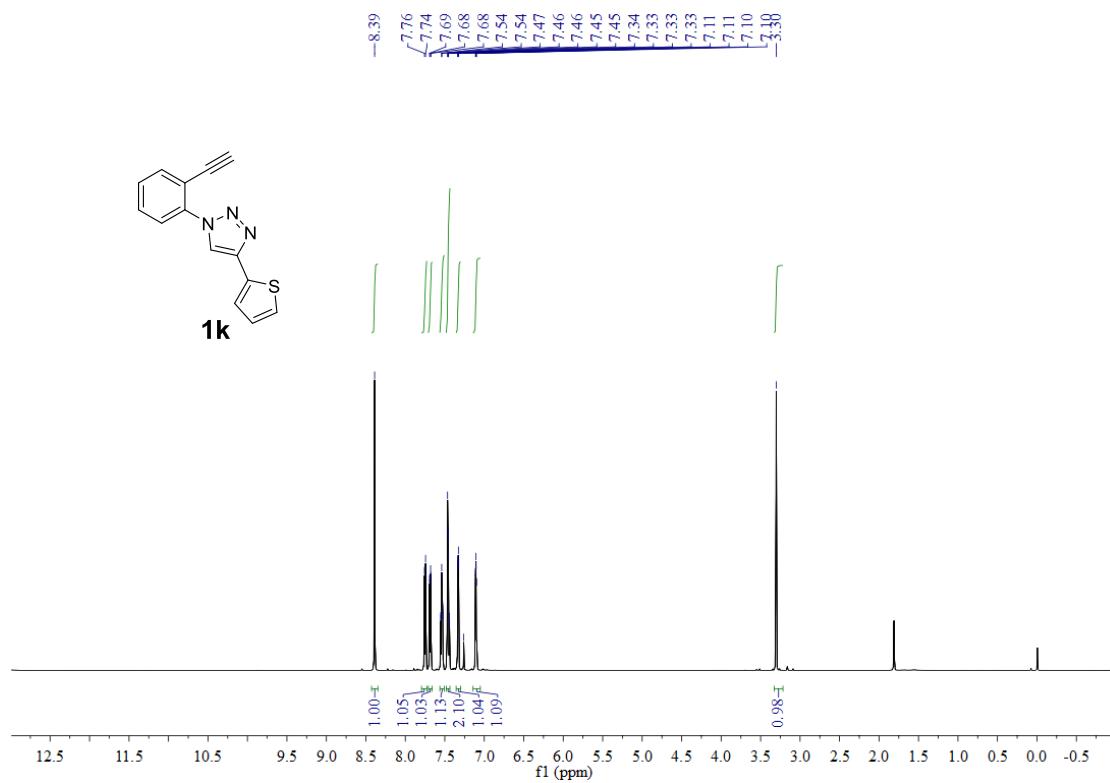


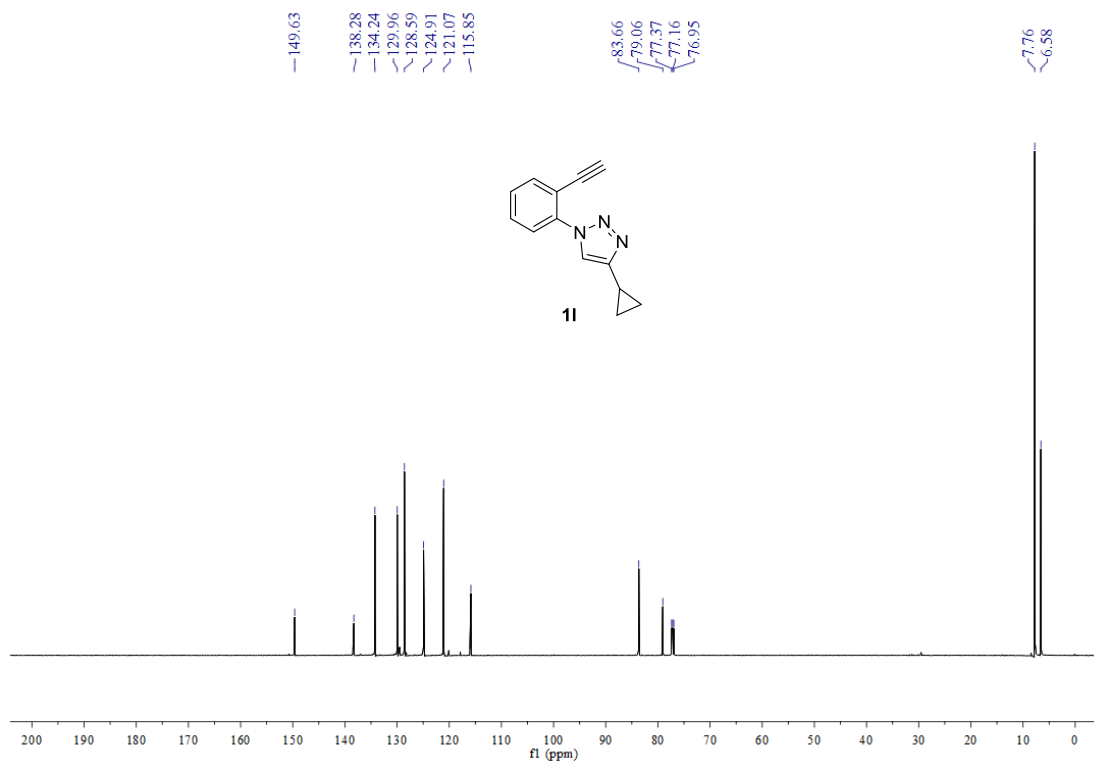
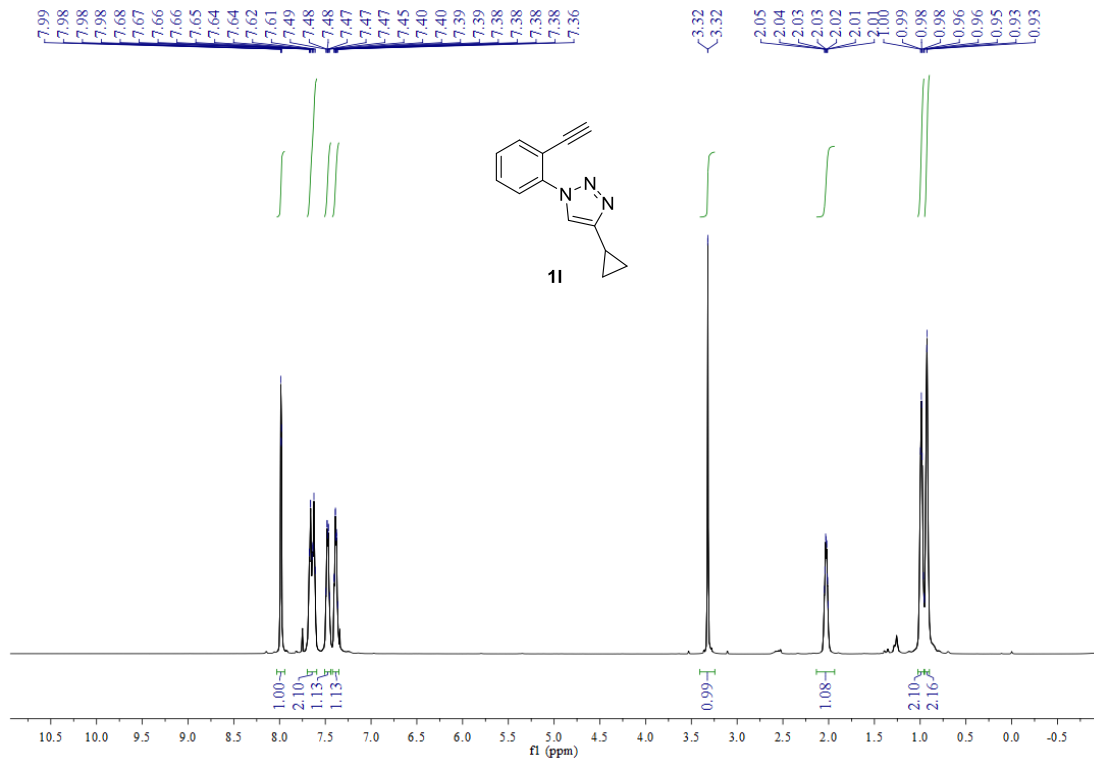


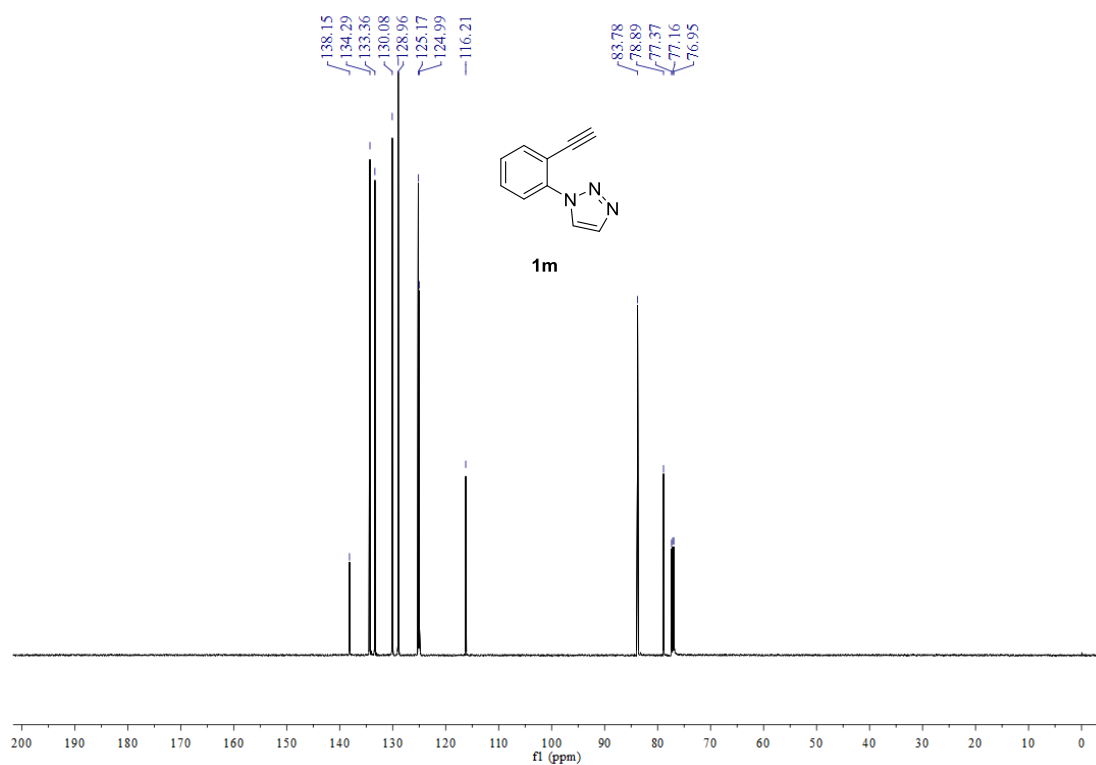
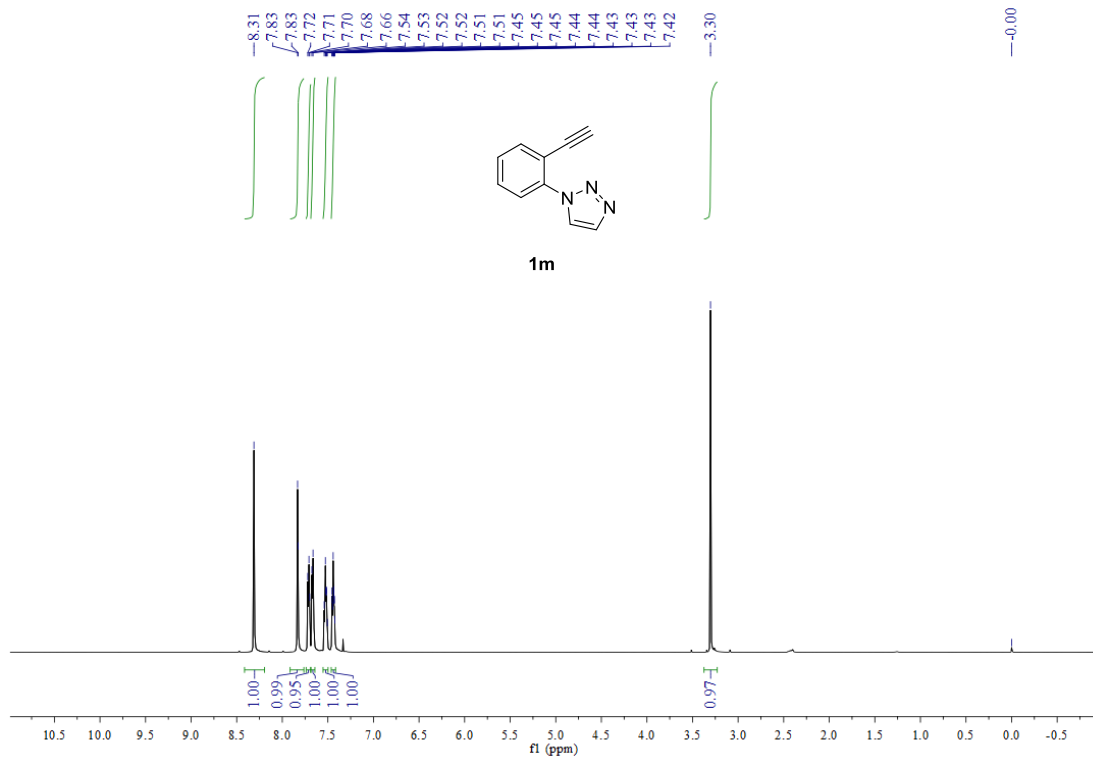


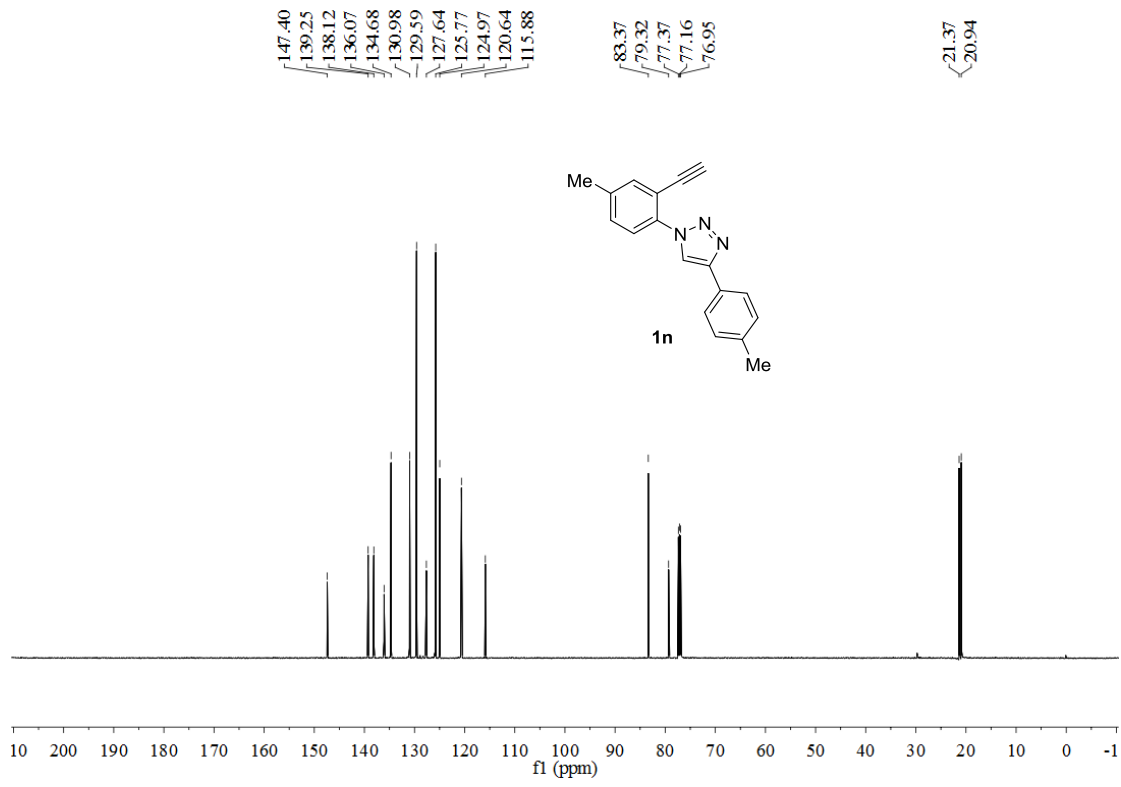
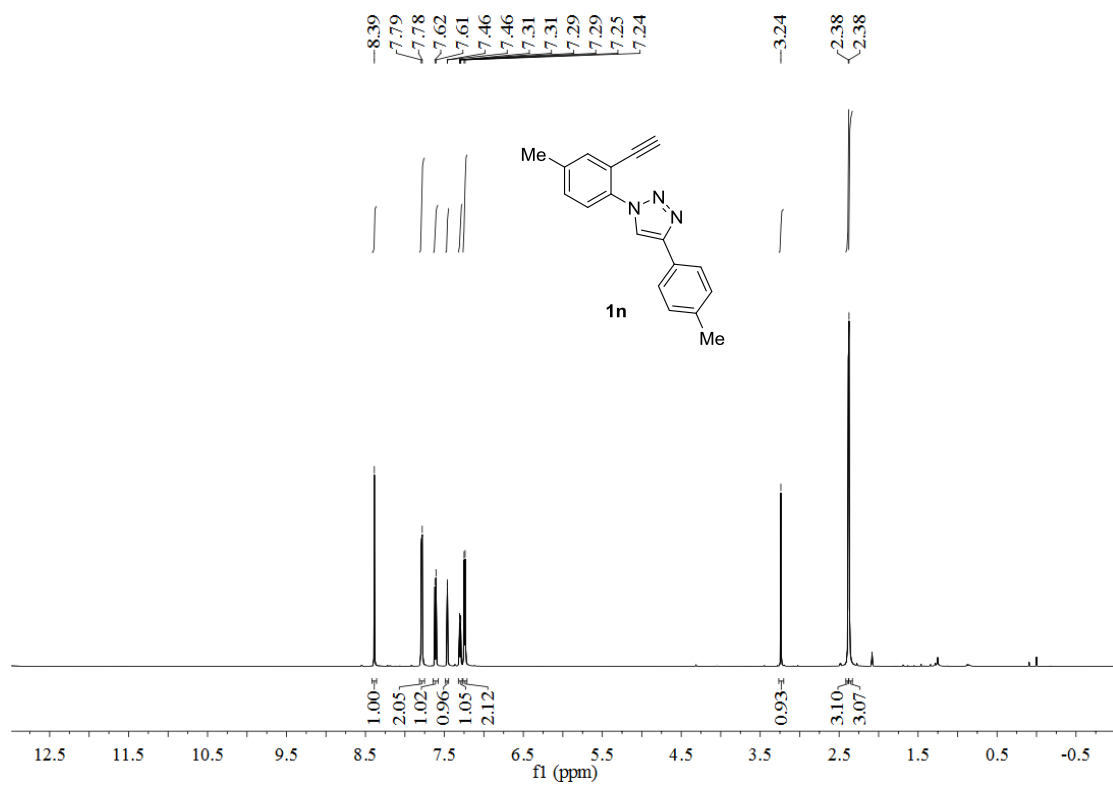


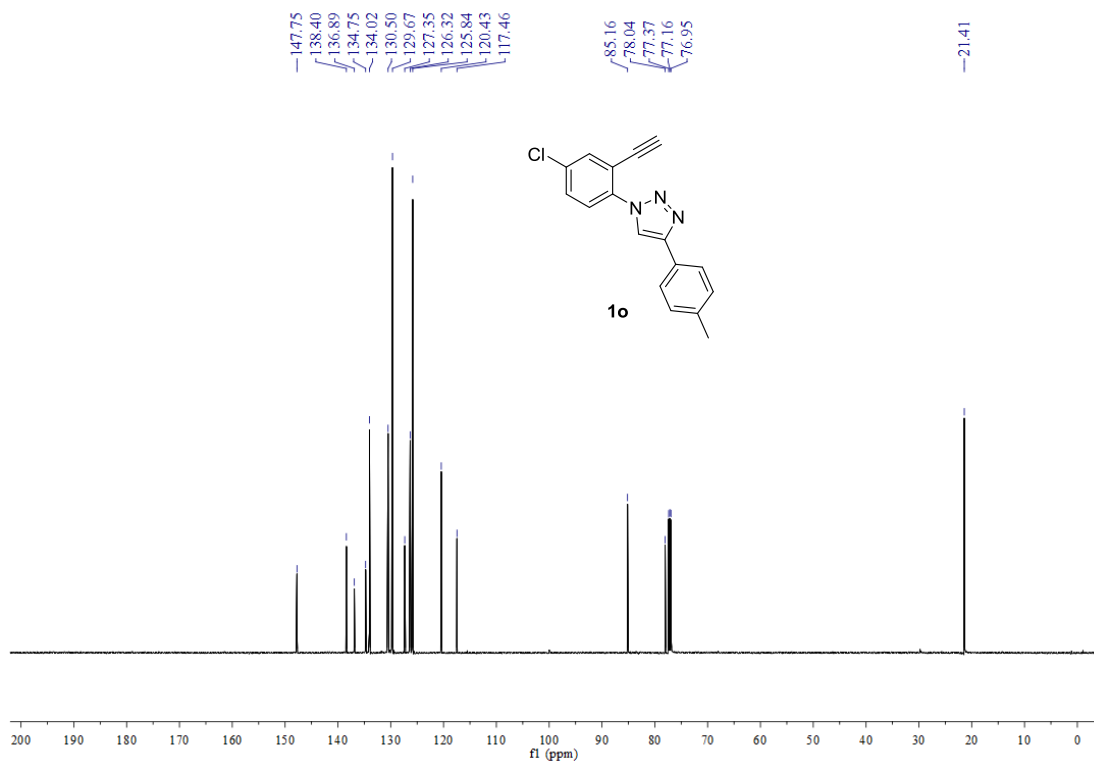
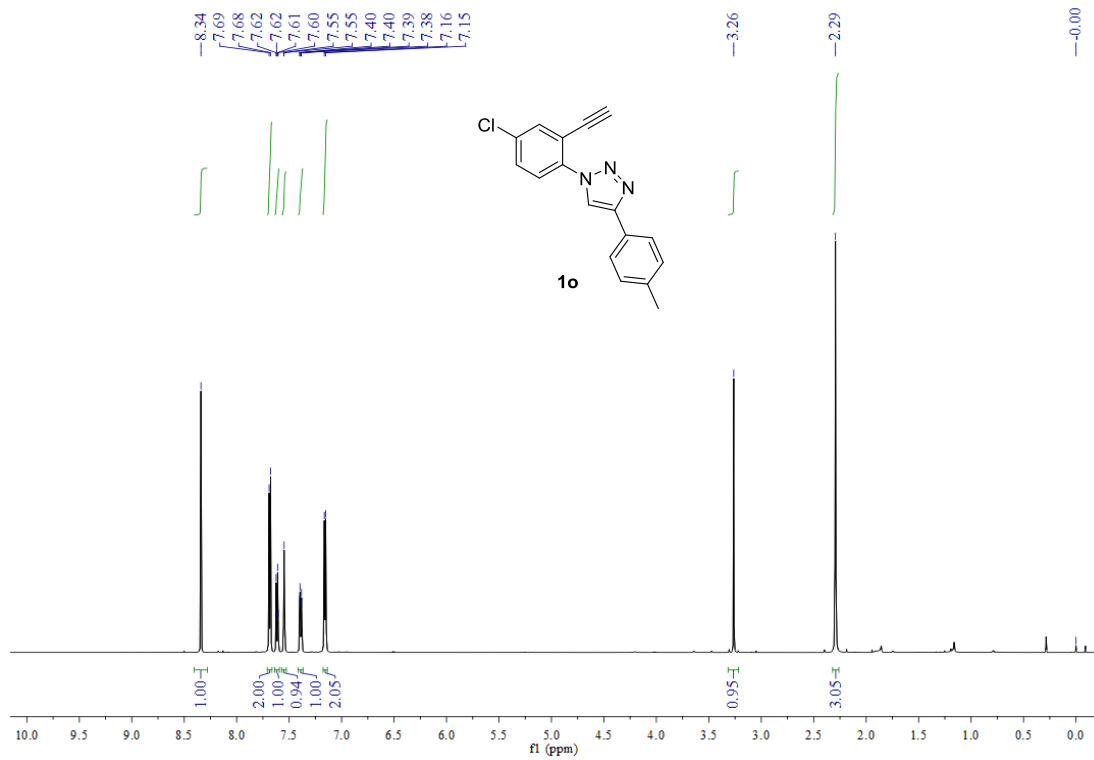


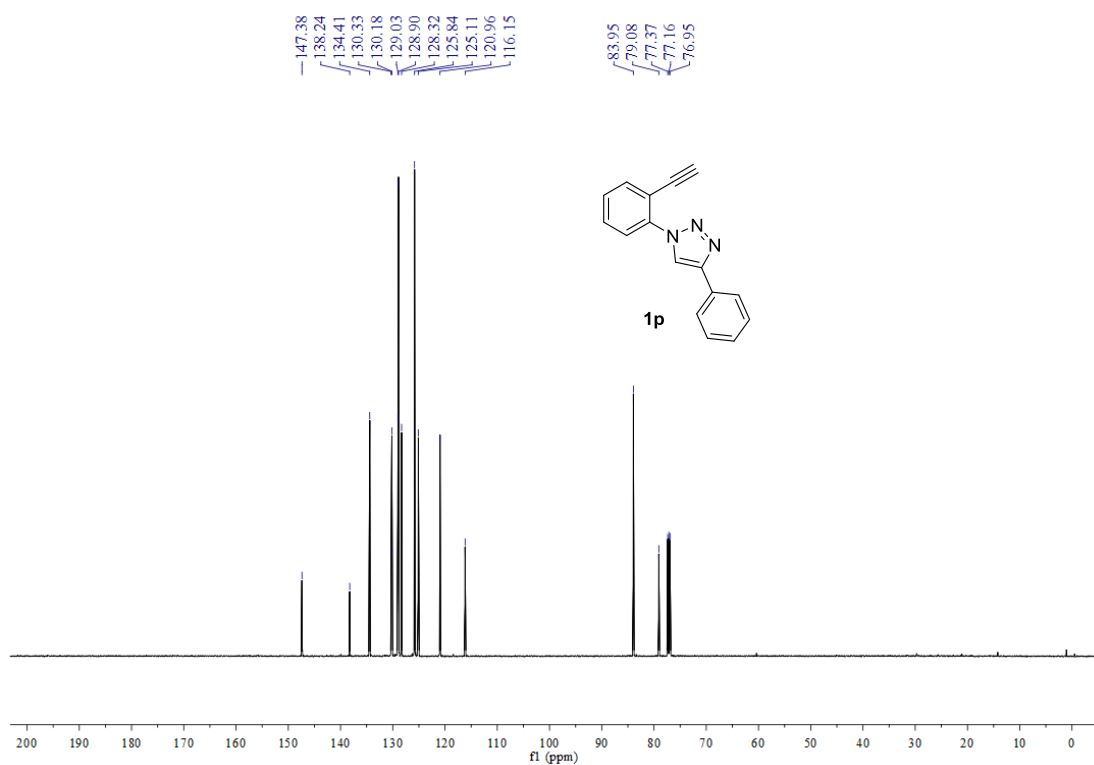
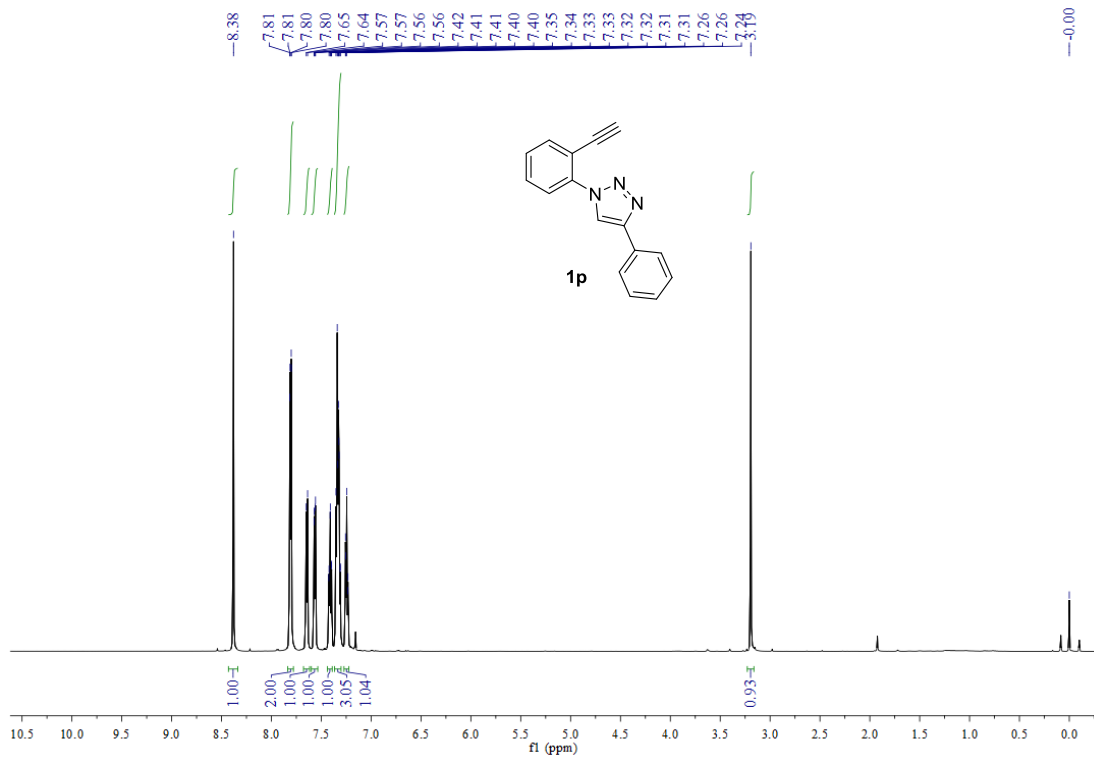


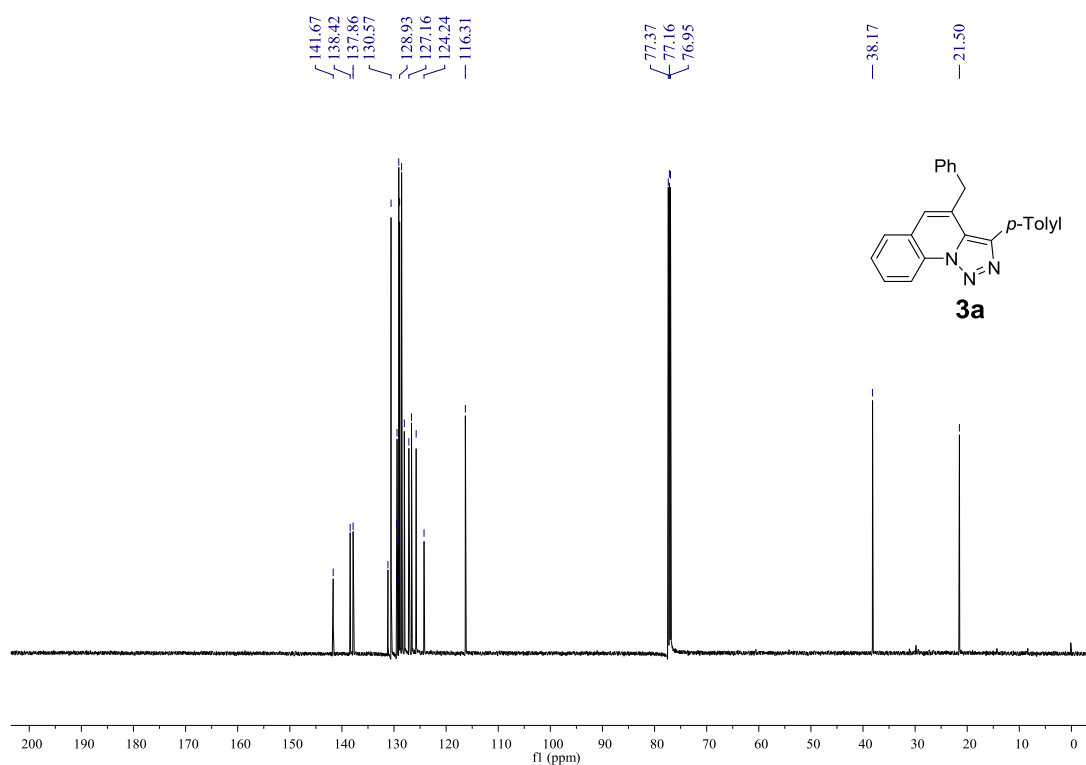
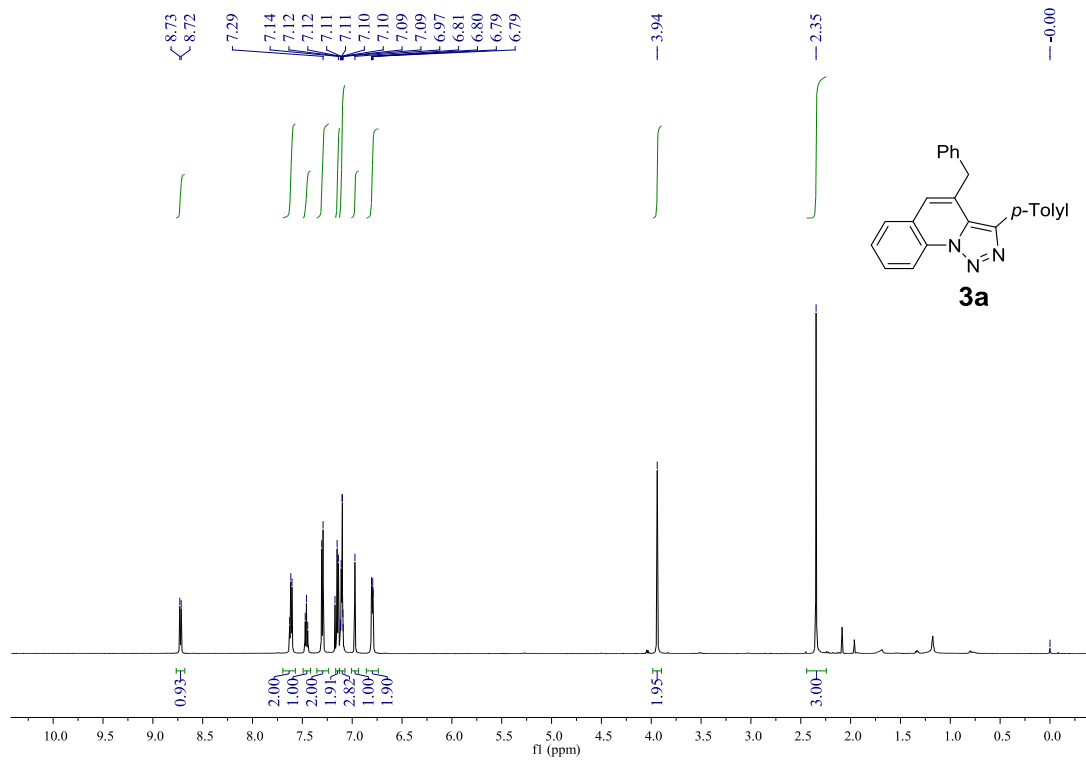


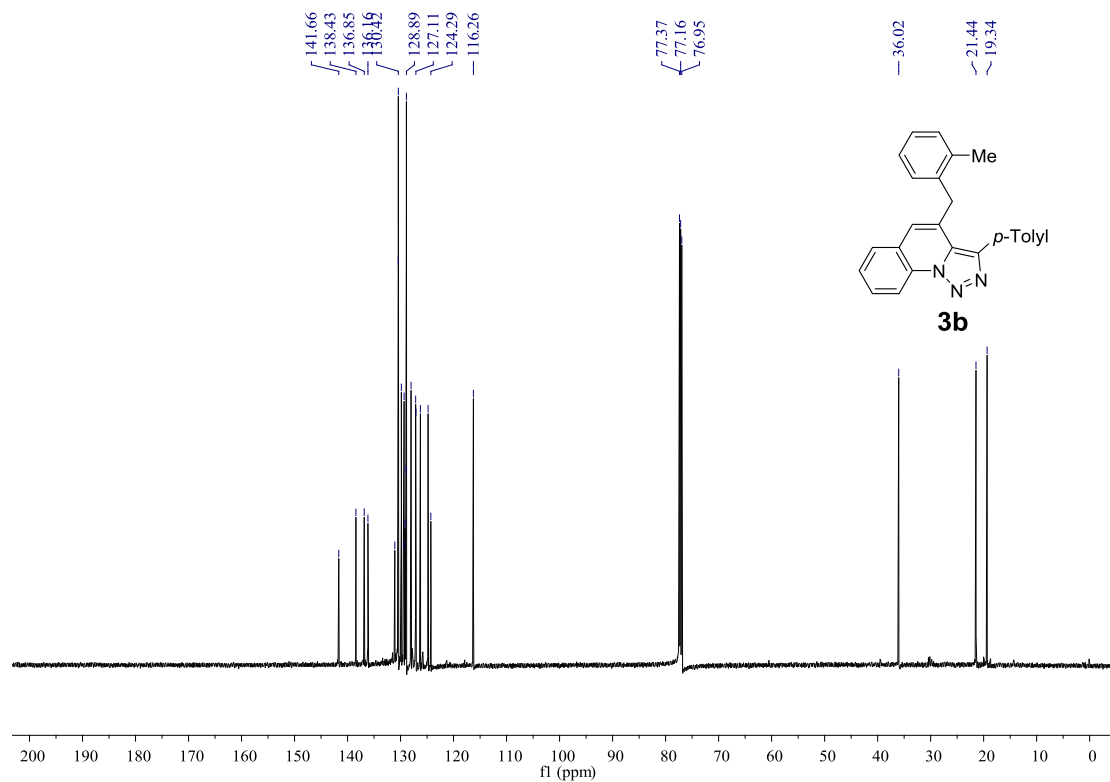
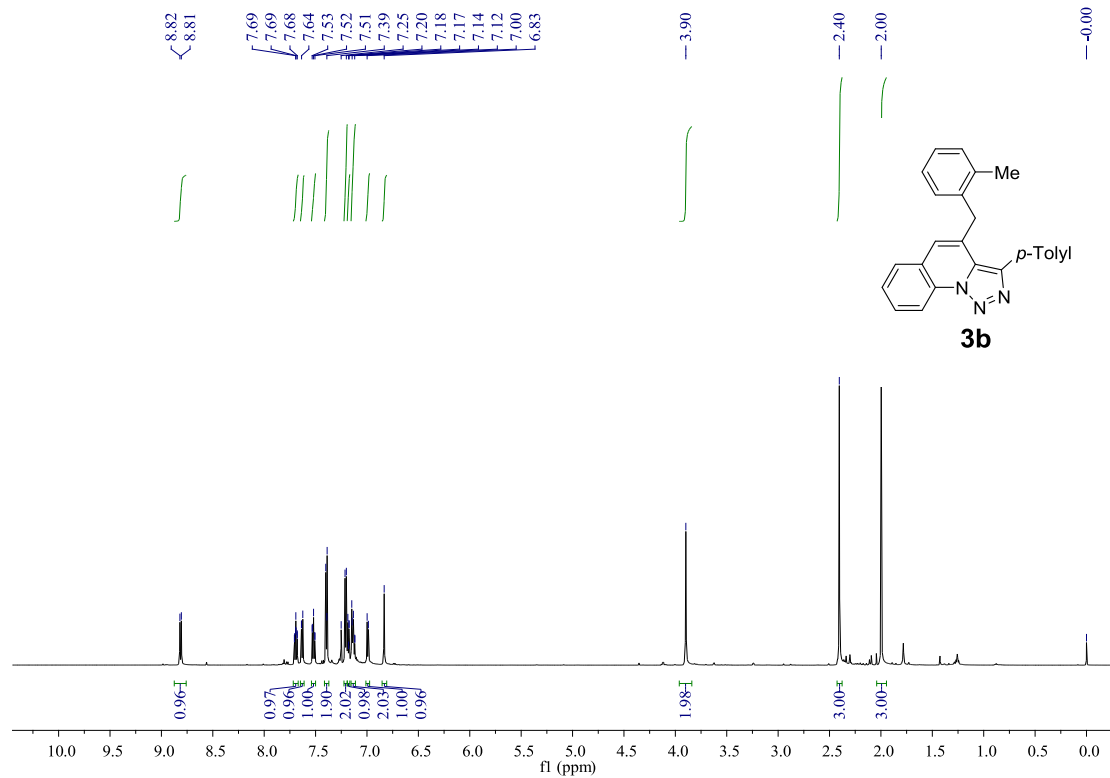


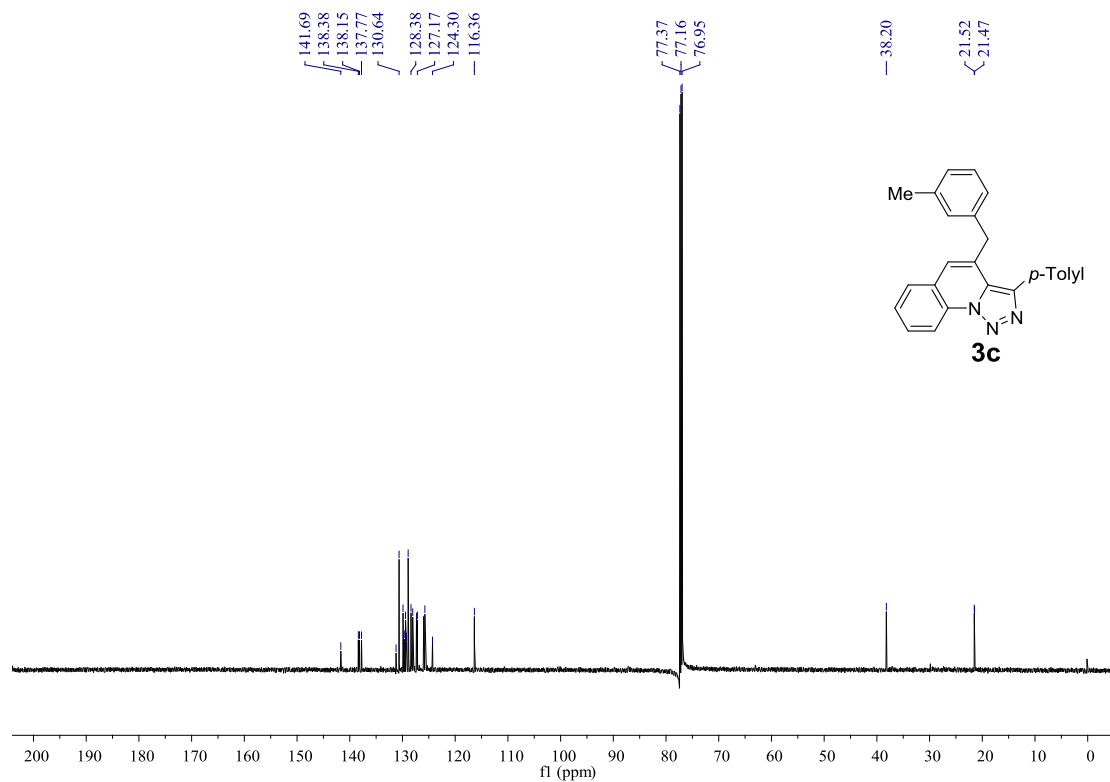
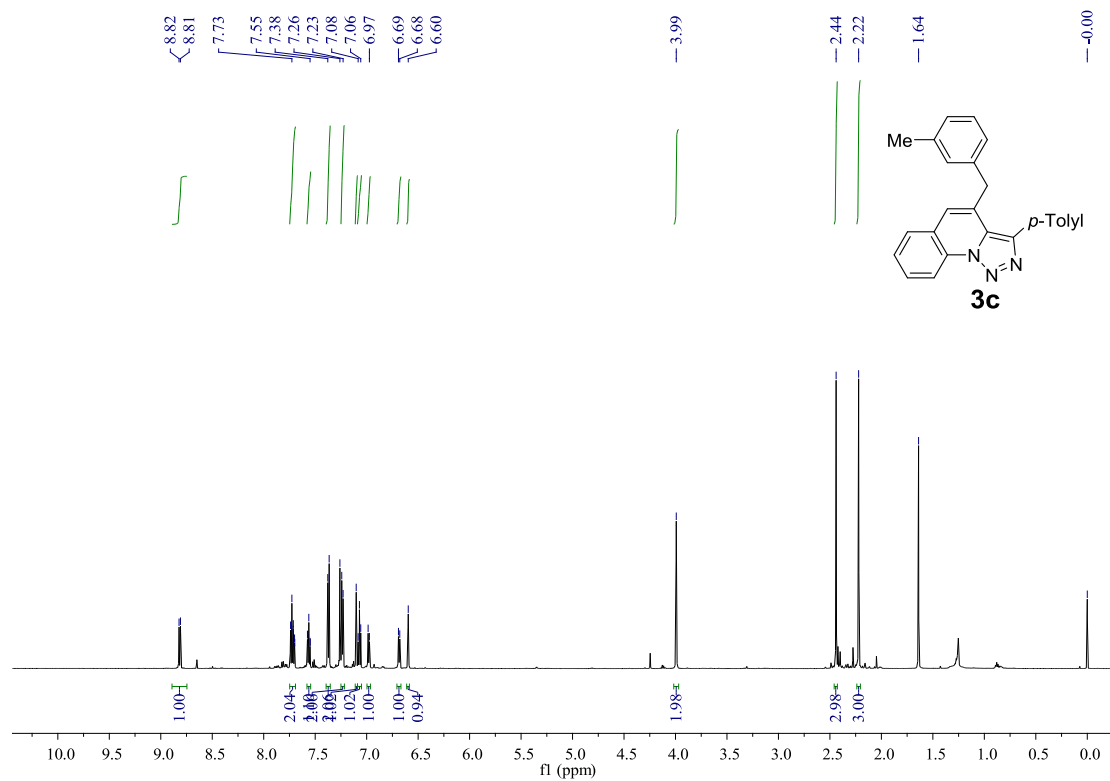


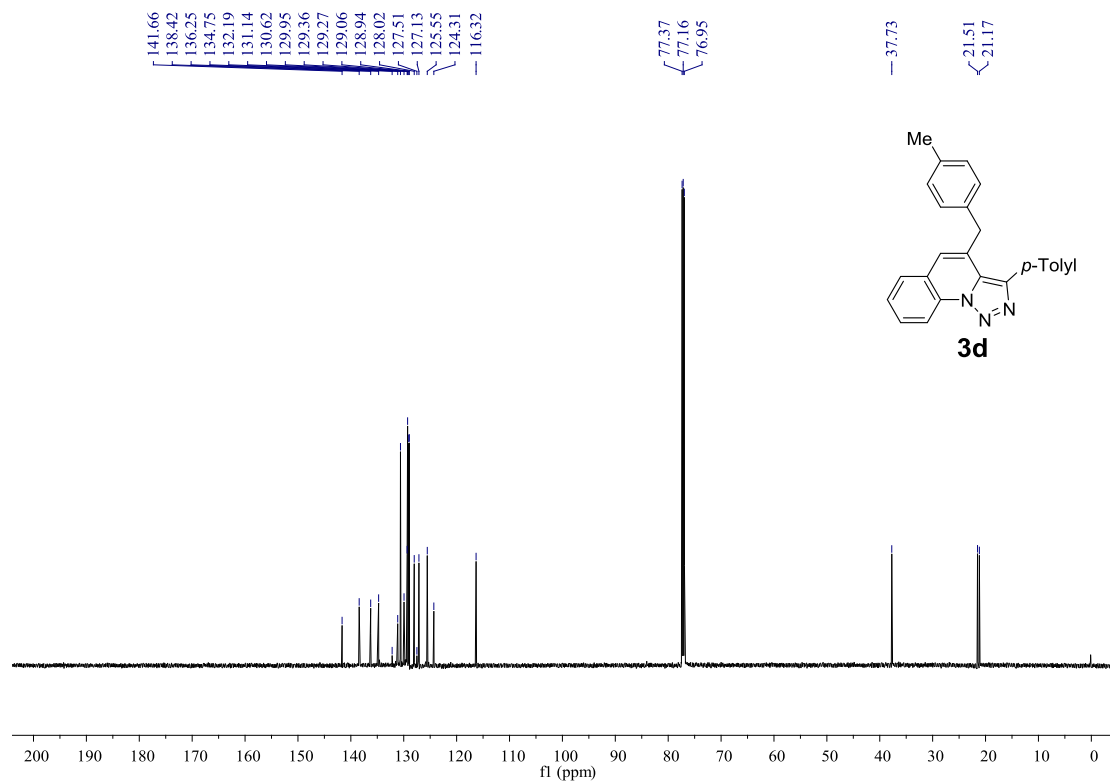
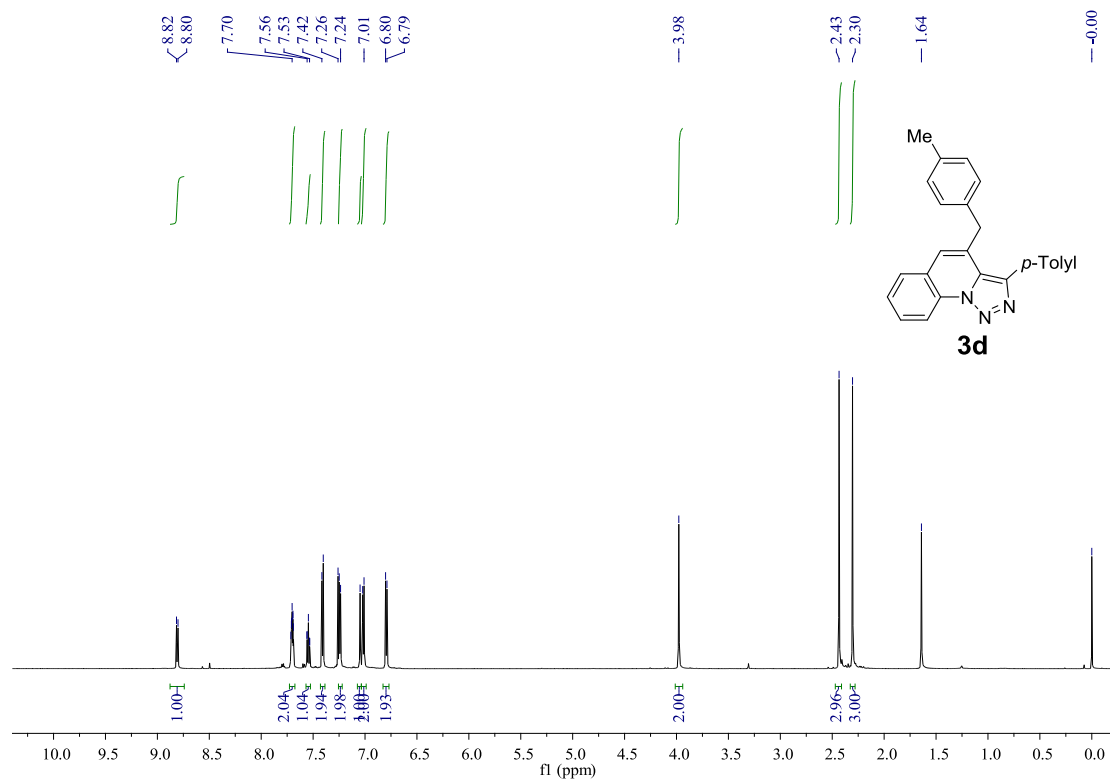


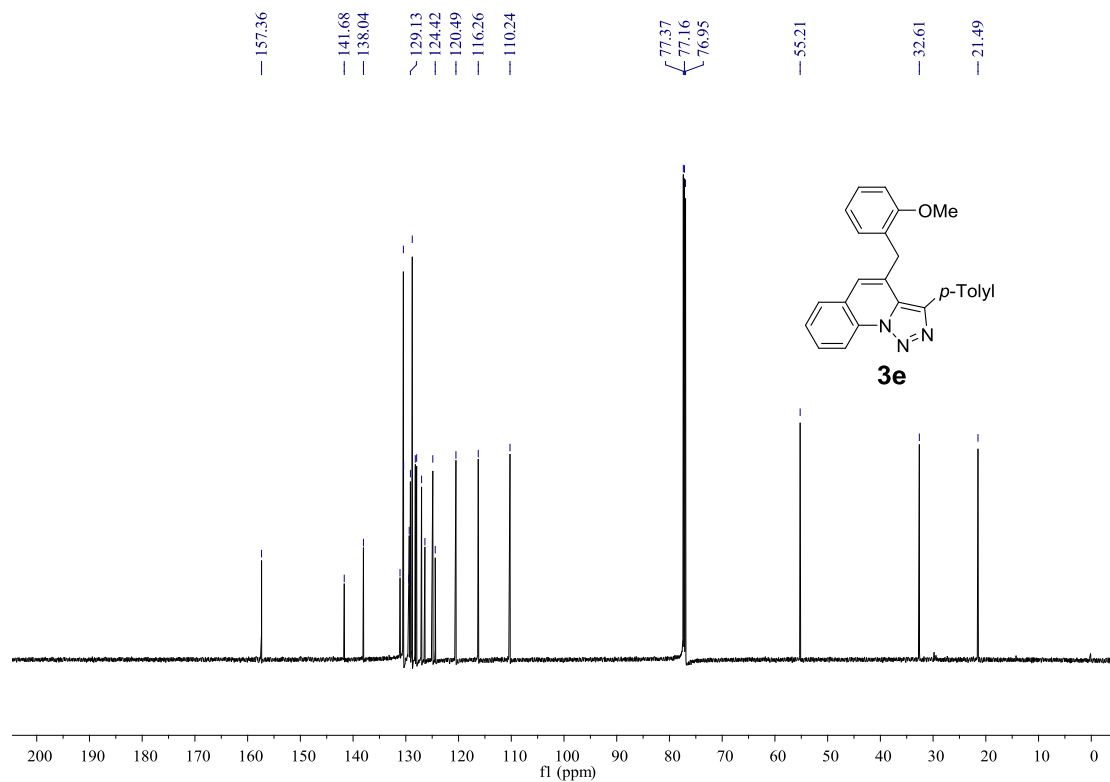
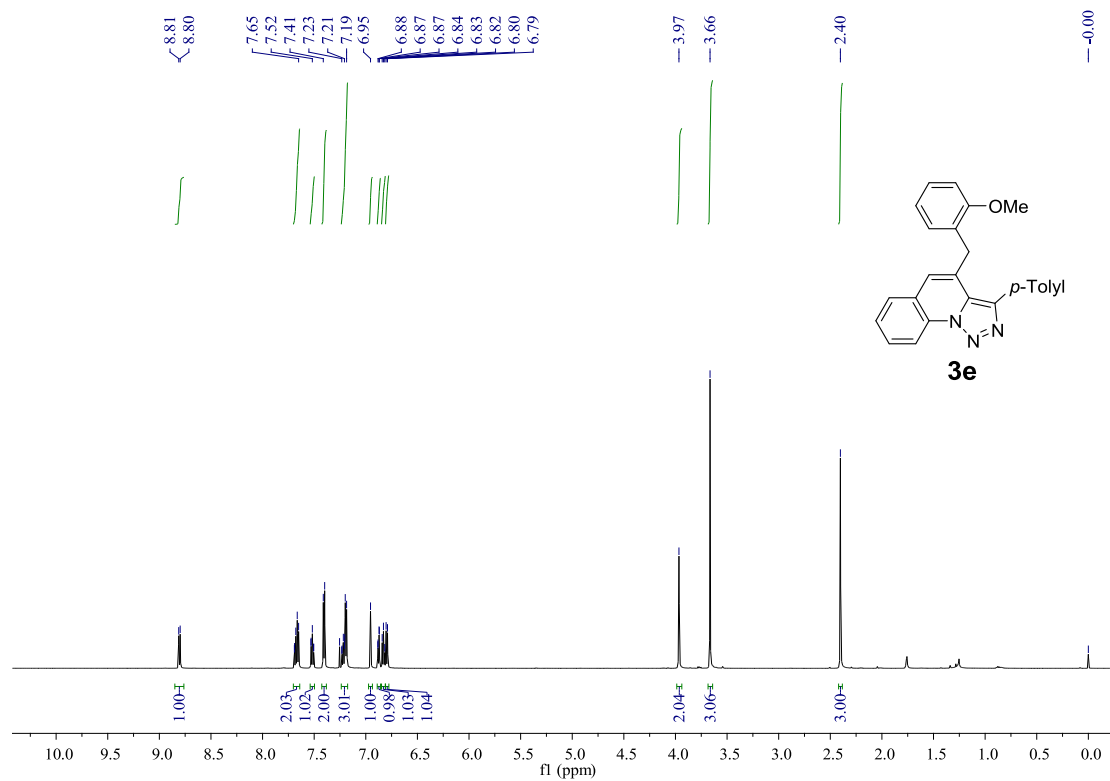


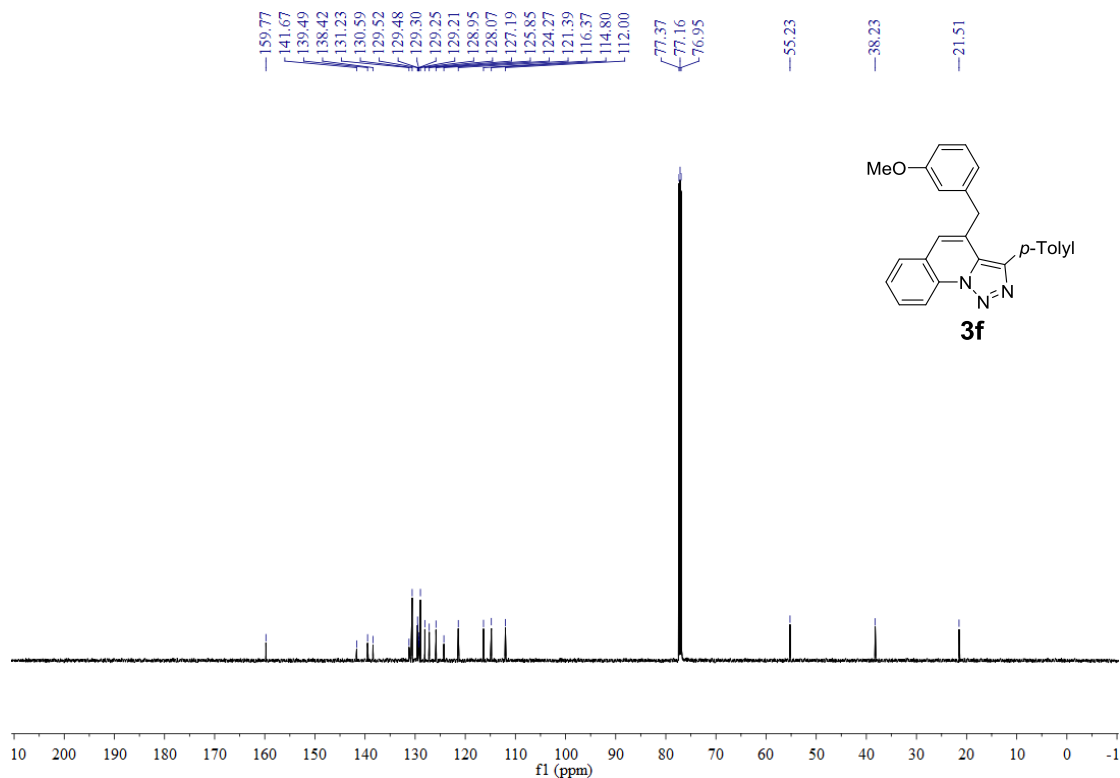
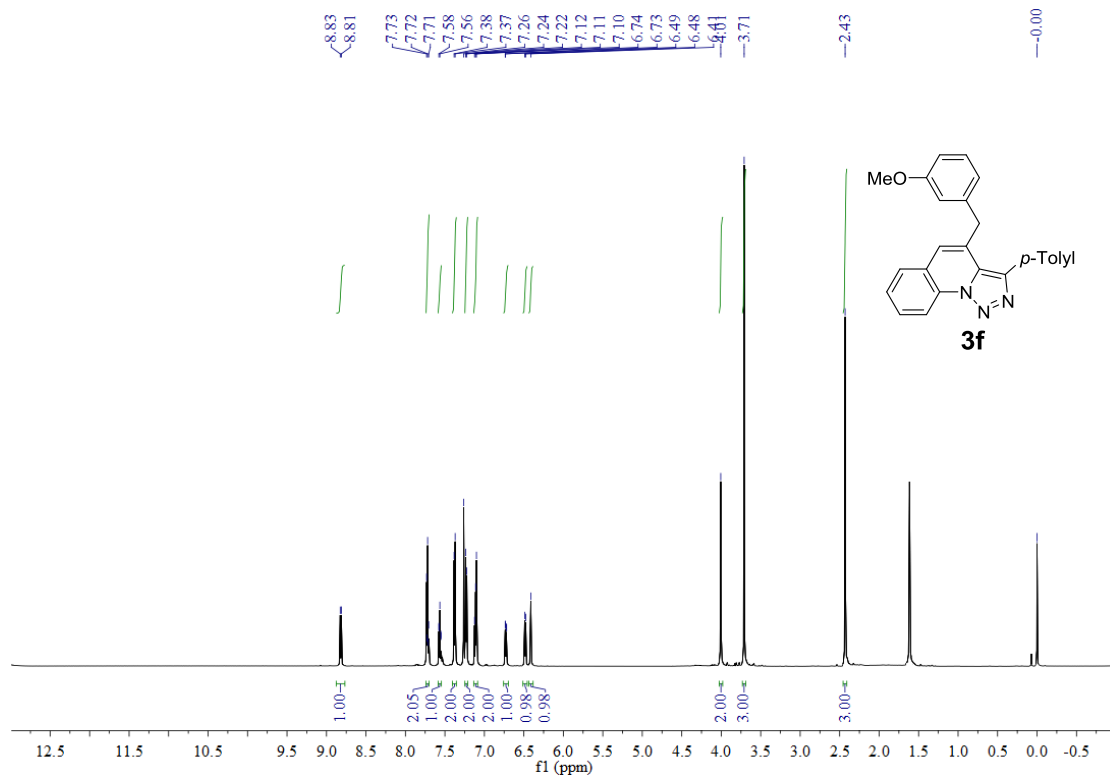


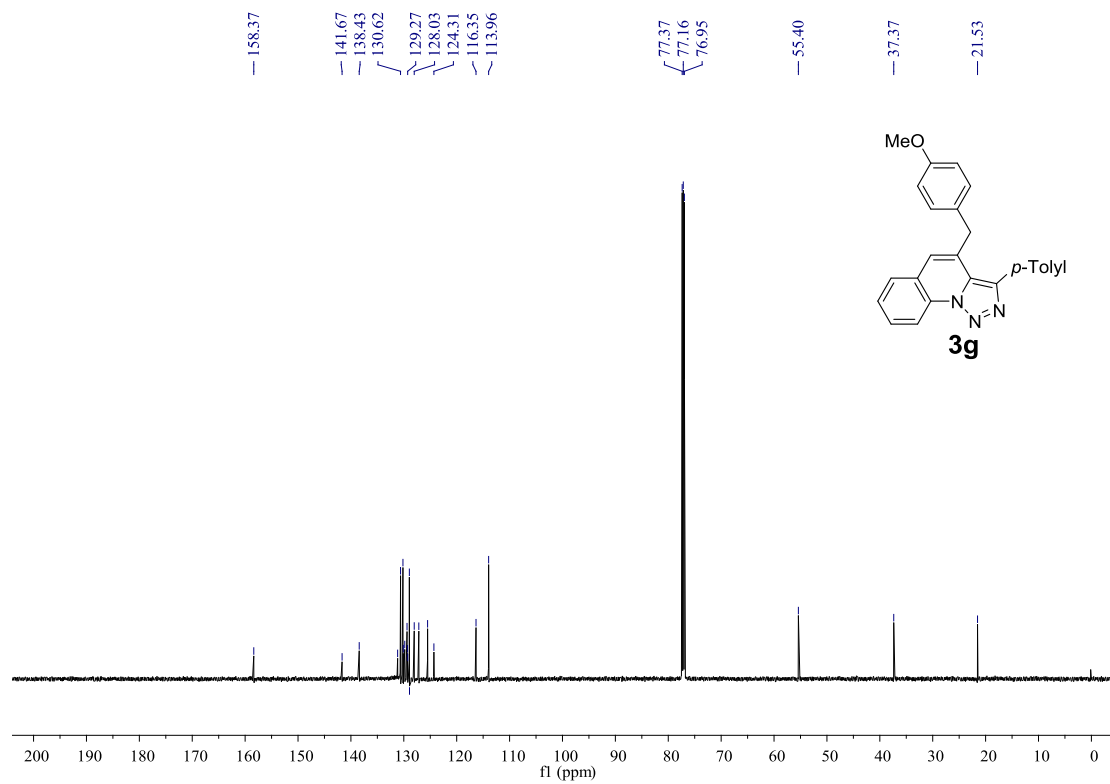
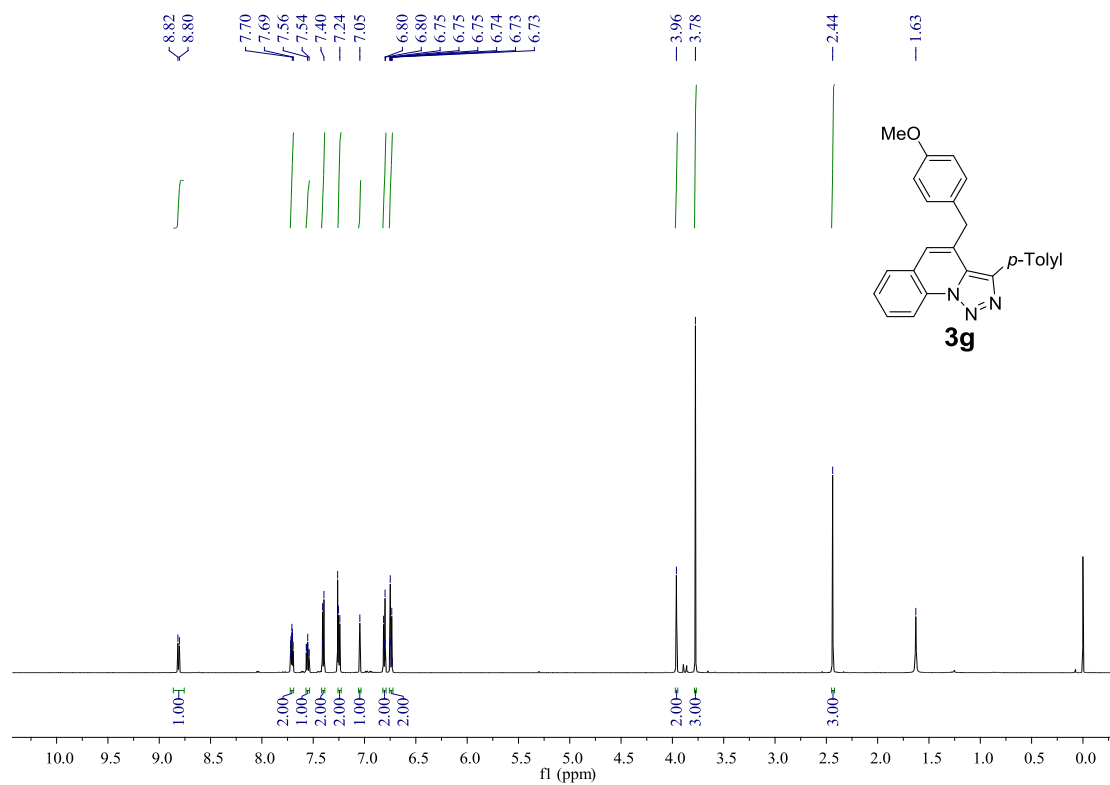


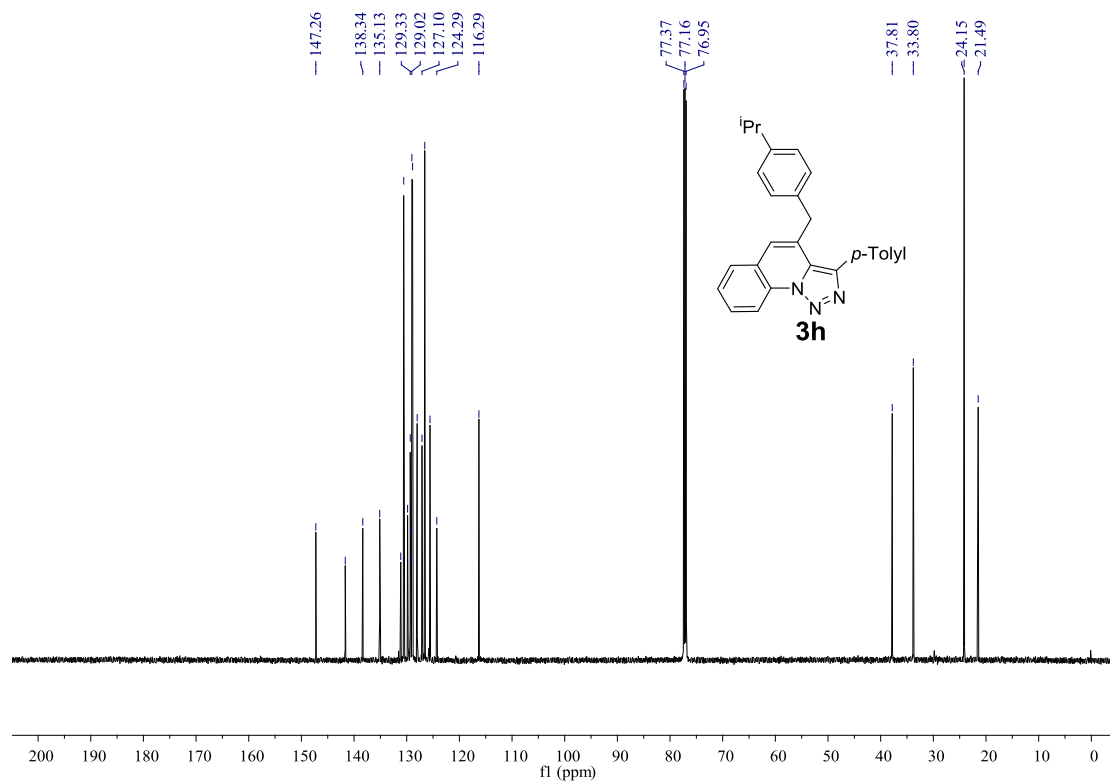
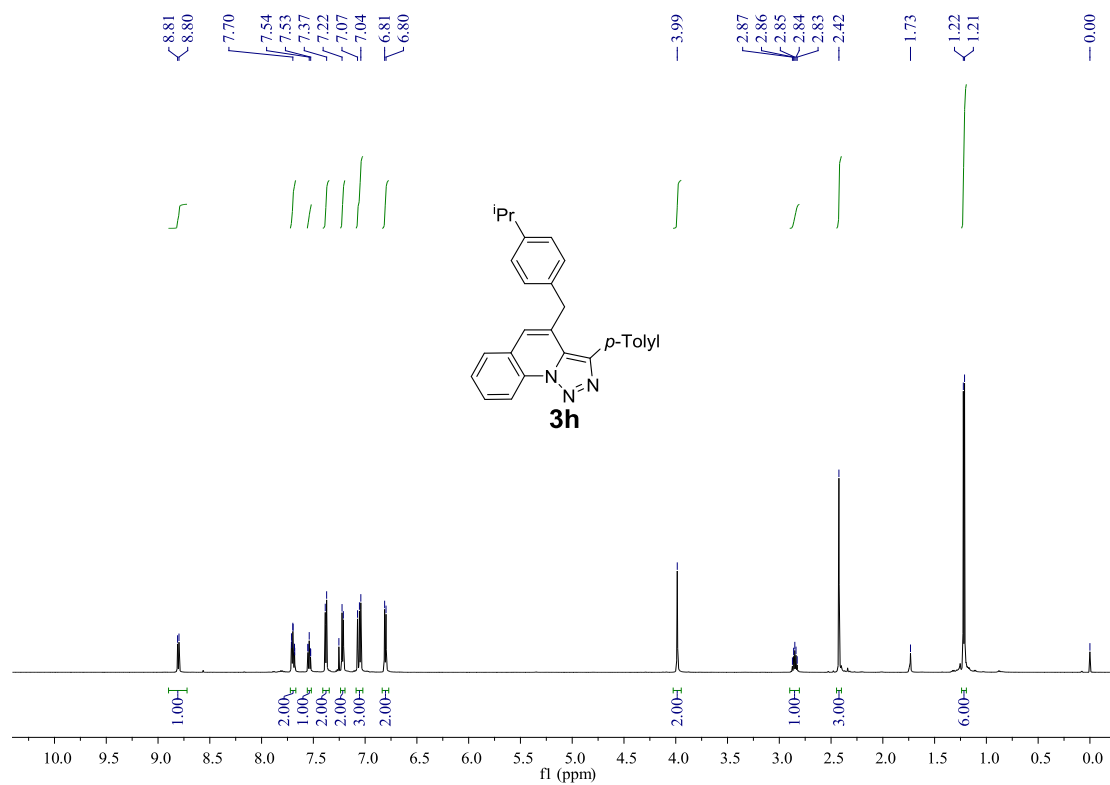


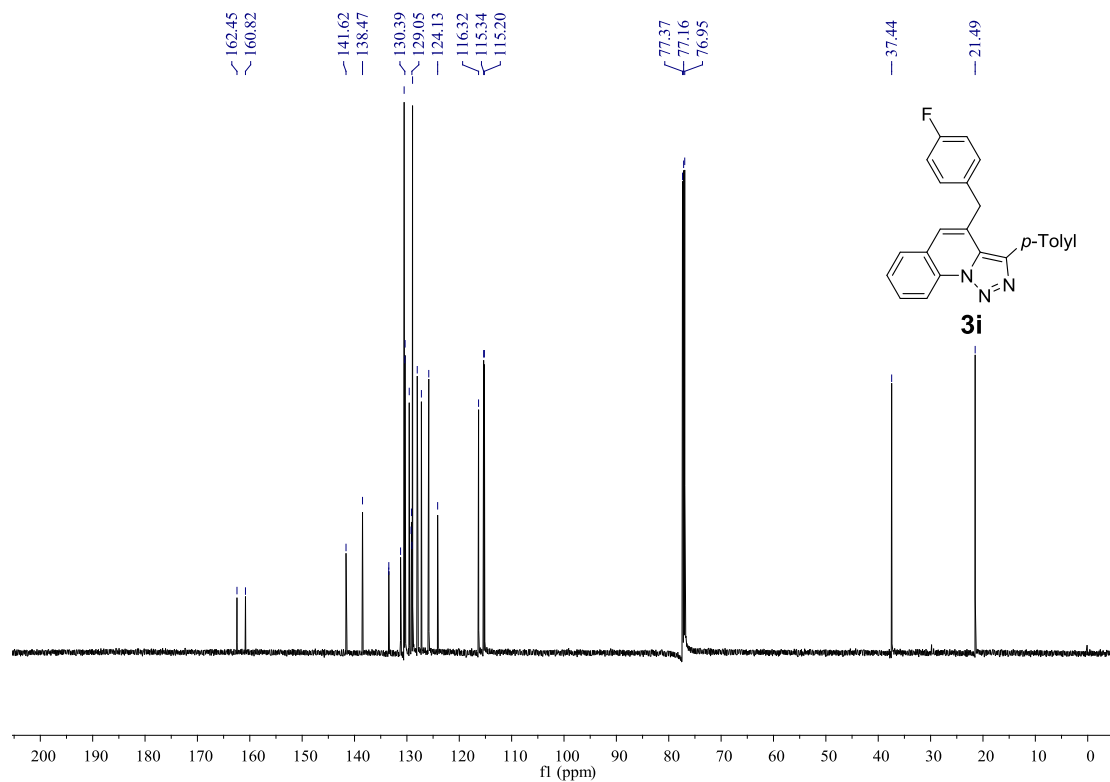
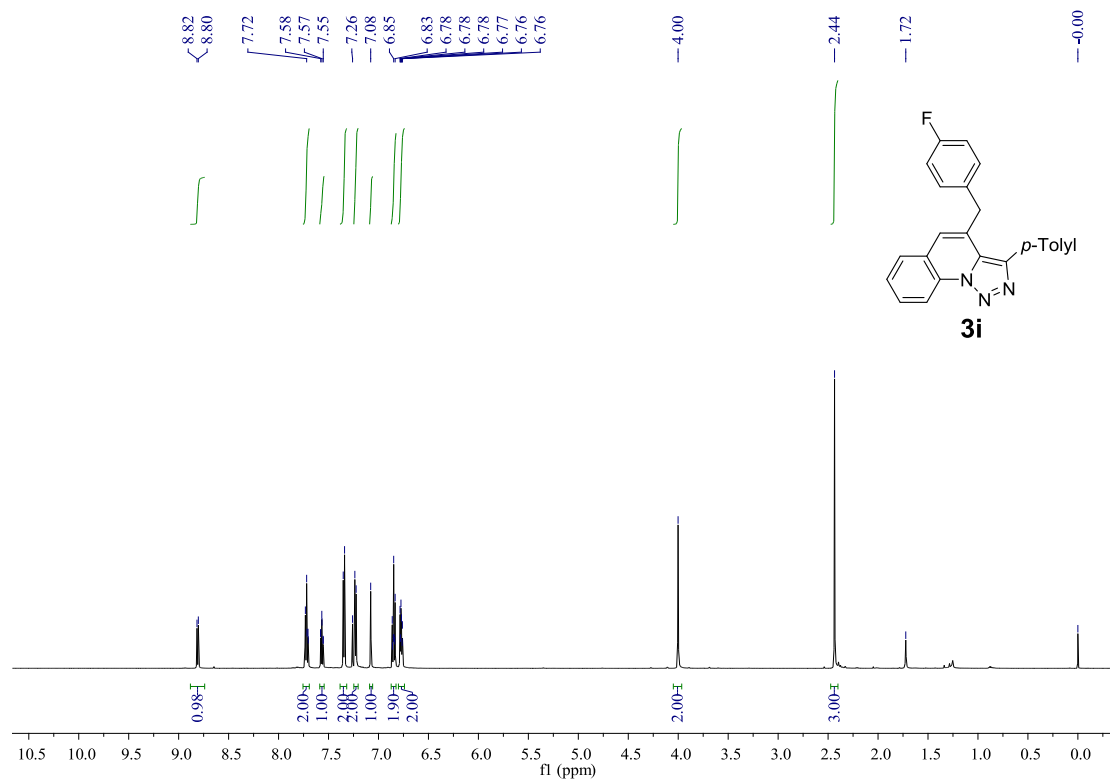




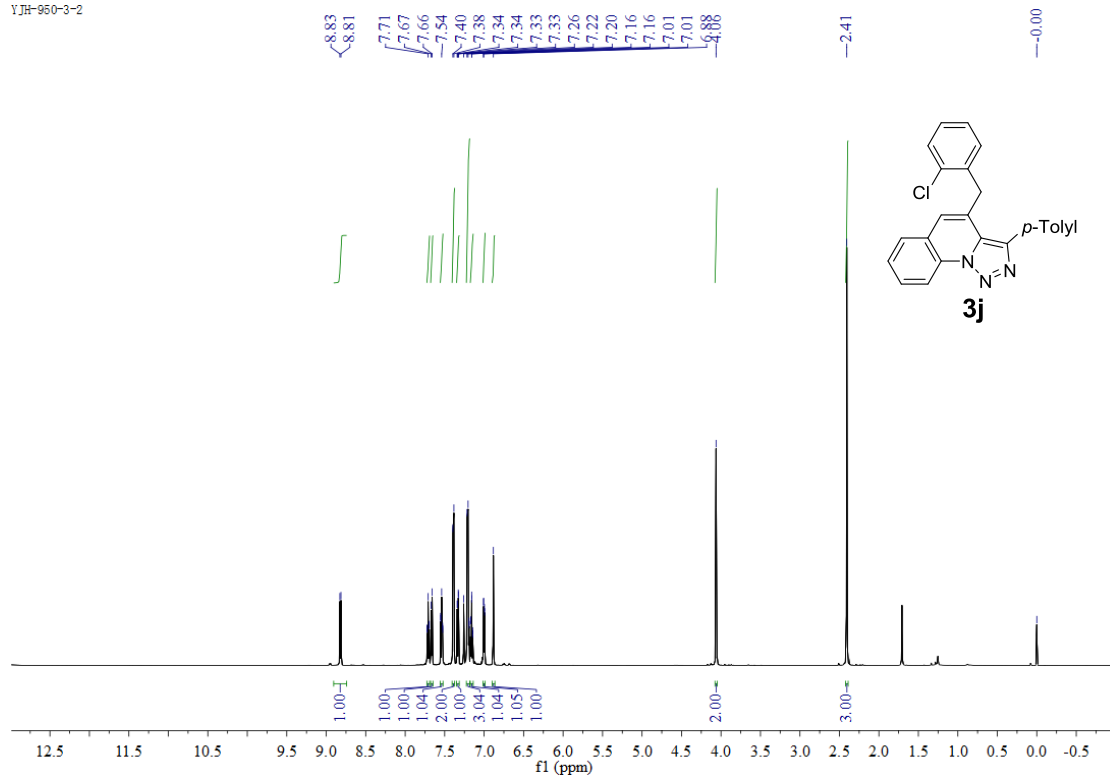








YJH-960-3-2



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