

# Selective Synthesis of 2-(1,2, 3-Triazolyl) Quinazolinones through Copper-Catalyzed Multicomponent Reaction

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**Abstract:** We describe here our results from the copper-catalyzed three component reaction of 2-azidobenzaldehyde, anthranilamide and terminal alkynes, using Et<sub>3</sub>N as base, and DMSO as solvent. Depending on the temperature and amount of Et<sub>3</sub>N used in the reactions, 1,2,3-triazolyl-quinazolinones or 1,2,3-triazolyl-dihydroquinazolinone could be obtained. When the reactions were performed at 100 °C using 2 equiv. of Et<sub>3</sub>N, 1,2,3-triazolyl-dihydroquinazolinone was formed in 82% yield, whereas reactions carried out at 120 °C using 1 equiv. of Et<sub>3</sub>N provided 1,2,3-triazolyl-quinazolinones in moderate-to-good yields.

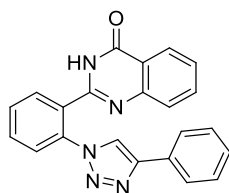
**Keywords:** 1,2,3-triazoles; quinazolinones; copper catalysis; cycloaddition; multicomponent

**General Information:** The reactions were monitored by TLC carried out on Merck silica gel (60 F<sub>254</sub>) by using UV light as visualizing agent and 5% vanillin in 10% H<sub>2</sub>SO<sub>4</sub> and heat as developing agents. Baker silica gel (particle size 0.040–0.063 mm) was used for flash chromatography. Hydrogen nuclear magnetic resonance spectra (<sup>1</sup>H NMR) were obtained at 400 MHz on Bruker DPX 400 spectrometer. Spectra were recorded in DMSO-*d*<sub>6</sub> solutions. Chemical shifts are reported in ppm, referenced to tetramethylsilane (TMS) as the external reference. Coupling constants (*J*) are reported in Hertz. Abbreviations to denote the multiplicity of a particular signal are s (singlet), d (doublet), dd (double doublet), t (triplet), q (quartet), quin (quintet), sex (sextet) and m (multiplet). Carbon-13 nuclear magnetic resonance spectra (<sup>13</sup>C NMR) were obtained at 100 MHz on Bruker DPX 400 spectrometer. Chemical shifts are reported in ppm, referenced to the solvent peak of DMSO-*d*<sub>6</sub>. Selenium -77 nuclear magnetic resonance spectra (<sup>77</sup>Se NMR) were obtained at 77 MHz on Bruker DPX 400 spectrometer. Spectra were recorded in DMSO-*d*<sub>6</sub> solutions. Low-resolution mass spectra were obtained with a Shimadzu GC-MS-QP2010 mass spectrometer. High resolution mass spectra (HRMS) were recorded on a Bruker Micro TOF-QII spectrometer 10416. Single crystal X-ray diffraction data of compound **6a** were collected on a Bruker D8 Quest diffractometer equipped with a Photon 100 detector, Incoatec microfocus Montel optic X-ray tube with Cu-Kα radiation (1.54178 Å). Absorption correction was performed by the multiscan (SADABS) method.<sup>1</sup> Structure solutions and refinements were done through direct methods, with the SHELX program package.<sup>2,3</sup> The graphical representation of the crystal structure was performed using the DIAMOND program (version 4.6.0).<sup>4</sup> The crystallographic information file (CIF) for the compound **6a**

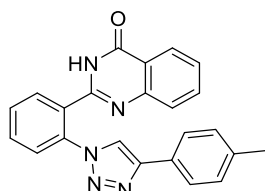
was deposited at the Cambridge Crystallographic Data Centre (CCDC) under identification number 2106971.

**General procedure for the synthesis of tri-azoylquinazolin-4(3H)-ones 6a-n:** In a test tube was added 2-azidobenzaldehyde (**1**, 0.5 mmol), anthranilamide (**2**, 0.5 mmol), CuI (10 mol%). Then, DMSO (1.5 mL) was added, followed by triethylamine (0.5 mmol) and the terminal alkyne **3a-n** (0.5 mmol). The system was heated to 120 °C under a nitrogen atmosphere and magnetic stirring for 16 h. Afterwards, the organic phase was received in water (20 mL), extracted with dichloromethane (3x 10 mL), dried with MgSO<sub>4</sub>, and concentrated on a rotary evaporator followed by a vacuum pump. Finally, a purification by column chromatography of silica gel as a stationary phase, and a mixture of hexanes/ethyl acetate as eluant (50/50) was performed, providing the desired products **6a-n** (20-87%).

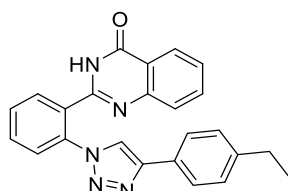
## Spectral data of the products:



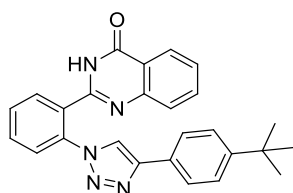
**2-(2-(4-Phenyl-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (6a):** Yield: 0.159 g (87%); white solid, mp 243 – 246 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  12.56 (s, 1H); 9.10 (s, 1H); 8.13 – 8.11 (m, 1H); 7.92 – 7.89 (m, 3H); 7.85 – 7.82 (m, 2H); 7.80 – 7.72 (m, 2H); 7.53 – 7.45 (m, 4H); 7.38 – 7.34 (m, 1H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ )  $\delta$  161.6; 152.1; 148.6; 146.3; 134.9; 134.5; 131.5; 131.2; 130.2; 129.4; 129.4; 129.0 (2C); 128.2; 127.3; 126.8; 125.8; 125.3 (2C); 124.8; 122.8; 121.0. MS (relative intensity)  $m/z$ : 336 ( $\text{M}^+ - 28$ , 100); 360 (36); 334 (27); 102 (10), 90 (20). HRMS calculated for  $\text{C}_{22}\text{H}_{16}\text{N}_5\text{O}$  [ $\text{M} + \text{H}$ ] $^+$ : 366.1349. Found: 366.1349.



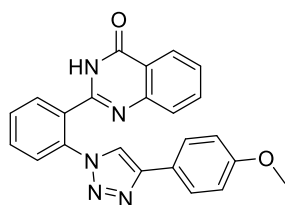
**2-(2-(4-(*p*-Tolyl)-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (6b):** Yield: 0.102 g (54%); yellow solid; mp 226 – 228 °C.  $^1\text{H}$  NMR (400 MHz,  $\text{DMSO}-d_6$ )  $\delta$  12.54 (s, 1H); 9.02 (s, 1H); 8.11 (d,  $J = 7.6$  Hz, 1H); 7.89 (d,  $J = 7.6$  Hz, 1H); 7.82 – 7.70 (m, 6H); 7.52 – 7.48 (m, 2H); 7.26 (d,  $J = 7.9$  Hz, 2H); 2.33 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{DMSO}-d_6$ )  $\delta$  161.6; 152.1; 148.6; 146.4; 137.5; 134.9; 134.4; 131.5; 131.2; 129.5 (2C); 129.31; 129.30; 127.4; 127.3; 126.8; 125.8; 125.2 (2C); 124.8; 122.4; 121.0; 20.8. MS (relative intensity)  $m/z$ : 350 ( $\text{M}^+ - 28$ , 100); 335 (27); 324 (24); 260 (41), 234 (26), 119 (10), 103 (15), 90 (12). HRMS calculated for  $\text{C}_{23}\text{H}_{18}\text{N}_5\text{O}$  [ $\text{M} + \text{H}$ ] $^+$ : 380.1506. Found: 380.1495.



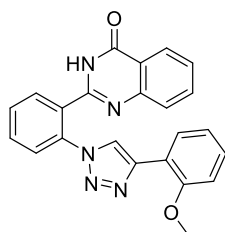
**2-(2-(4-(4-Ethylphenyl)-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (6c):** Yield: 0.132 g (67%); yellow solid; mp 241 – 243 °C.  $^1\text{H}$  NMR (400 MHz;  $\text{DMSO}-d_6$ )  $\delta$  1.57 (s, 1H); 9.03 (s, 1H); 8.12 (d,  $J = 7.5$  Hz, 1H); 7.90 (d,  $J = 7.5$  Hz, 1H); 7.84 – 7.77 (m, 4H); 7.76 – 7.70 (m, 2H); 7.52 – 7.49 (m, 2H); 7.29 (d,  $J = 7.9$  Hz, 2H); 2.62 (q,  $J = 7.6$  Hz, 2H); 1.18 (t,  $J = 7.6$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz;  $\text{DMSO}-d_6$ )  $\delta$  161.6; 152.1; 148.6; 146.5; 143.8; 135.0; 134.5; 131.5; 131.2; 129.4; 128.3 (2C); 127.7; 127.30; 127.31; 126.8; 125.8; 125.3 (2C); 124.8; 122.4; 121.1; 28.0; 15.5. MS (relative intensity)  $m/z$ : 393 ( $\text{M}^+$ , 4); 367 (77); 351 (43); 349 (48); 338 (100); 323 (41); 320 (28); 307 (48); 281 (20); 261 (80); 247 (86); 204 (51). HRMS calculated for  $\text{C}_{24}\text{H}_{20}\text{N}_5\text{O}$  [ $\text{M} + \text{H}$ ] $^+$ : 366.1662. Found: 366.1657.



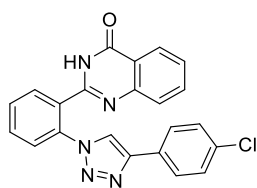
**2-(2-(4-(4-tert-Butylphenyl)-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (6d):** Yield: 0.107 g (51%); yellow solid; mp 206–208 °C.  $^1\text{H}$  NMR (400 MHz;  $\text{DMSO}-d_6$ )  $\delta$  12.56 (s, 1H); 9.03 (s, 1H); 8.12 (d,  $J = 7.5$  Hz, 1H); 7.89 (d,  $J = 7.5$  Hz, 1H); 7.84–7.77 (m, 4H); 7.75–7.70 (m, 2H); 7.52–7.46 (m, 4H); 1.29 (s, 9H).  $^{13}\text{C}$  NMR (100 MHz;  $\text{DMSO}-d_6$ )  $\delta$  161.6; 152.1; 150.7; 148.6; 146.4; 135.0; 134.5; 131.4; 131.1; 129.38; 129.36; 127.5; 127.3; 126.8; 125.8; 125.7 (2C); 125.8; 125.1 (2C); 122.4; 121.0; 34.4; 31.0 (3C). MS (relative intensity)  $m/z$ : 393 ( $\text{M}^+ - 28$ , 83); 392(100); 336 (31); 366 (37); 260 (70); 234 (36); 175 (27); 131(94); 119 (34); 91 (36). HRMS calculated for  $\text{C}_{26}\text{H}_{24}\text{N}_5\text{O}$  [ $\text{M} + \text{H}$ ] $^+$ : 422.1975. Found: 422.1972.



**2-(2-(4-(4-Methoxyphenyl)-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (6e):** Yield: 0.130 g (66%); yellow solid; mp 255–257 °C.  $^1\text{H}$  NMR (400 MHz;  $\text{DMSO}-d_6$ )  $\delta$  12.55 (s, 1H); 8.97 (s, 1H); 8.12 (d,  $J = 7.6$  Hz, 1H); 7.90 (d,  $J = 7.6$  Hz, 1H); 7.83–7.70 (m, 6H); 7.52–7.49 (m, 2H); 7.02 (d,  $J = 8.4$  Hz, 2H); 3.78 (s, 3H).  $^{13}\text{C}$  NMR (100 MHz;  $\text{DMSO}-d_6$ )  $\delta$  161.6; 159.2; 152.1; 148.7; 146.3; 135.0; 134.5; 131.5; 131.2; 129.3; 129.3; 127.3; 126.8; 126.7 (2C); 125.8; 124.7; 122.8; 121.8; 121.1; 114.4 (2C); 55.2. MS (relative intensity)  $m/z$ : 395 ( $\text{M}^+$ , 2); 367 (100); 352 (63); 340 (46); 260 (39); 234 (27); 120 (14); 90 (21). HRMS calculated for  $\text{C}_{23}\text{H}_{18}\text{N}_5\text{O}$  [ $\text{M} + \text{H}$ ] $^+$ : 396.1455. Found: 396.1451.

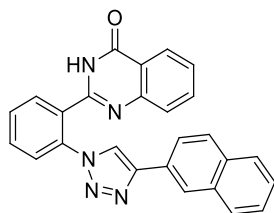


**2-(2-(4-(2-Methoxyphenyl)-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (6f):** Yield: 0.0808 g (42%); yellow oil.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  11.47–11.40 (s, 1H); 8.29 (s, 1H); 8.22–8.19 (m, 1H); 8.17–8.14 (m, 1H); 7.79–7.76 (m, 1H); 7.71–7.63 (m, 3H); 7.58–7.49 (m, 2H); 7.45–7.41 (m, 1H); 7.26–7.22 (m, 1H); 7.01–6.97 (m, 1H); 6.81–6.79 (m, 1H); 3.53–3.52 (m, 3H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  163.1; 155.7; 151.1; 149.0; 143.3; 135.4; 134.8; 131.7; 131.1; 129.7; 129.2; 127.9; 127.7; 127.6; 127.2; 126.5; 125.8; 124.5; 121.0; 120.9; 118.7; 110.7; 54.9. MS (relative intensity)  $m/z$ : 368 ( $\text{M}^+ - 28$ , 23), 338 (26), 262 (28), 248 (98), 234 (29), 219 (83), 205 (13), 147 (26), 131 (17), 120 (100), 92 (67). HRMS calculated for  $\text{C}_{23}\text{H}_{17}\text{N}_5\text{NaO}_2$  [ $\text{M} + \text{Na}$ ] $^+$ : 418.1274. Found: 418.1261.

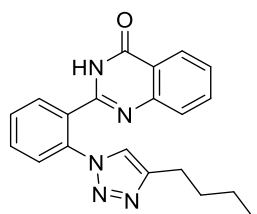


**2-(2-(4-(4-Chlorophenyl)-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (6g):** Yield: 0.119g (60%); yellow solid; mp 188–190 °C.  $^1\text{H}$

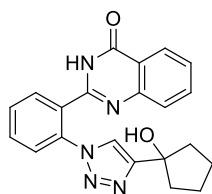
NMR (400 MHz; DMSO- $d_6$ )  $\delta$  12.56 (s, 1H); 9.14 (s, 1H); 8.12–8.10 (m, 1H); 7.92–7.90 (m, 3H); 7.83–7.81 (m, 2H); 7.77–7.72 (m, 2H); 7.54–7.47 (m, 4H).  $^{13}\text{C}$  NMR (100 MHz; DMSO- $d_6$ )  $\delta$  161.6; 151.9; 148.6; 145.2; 134.9; 134.5; 132.6; 131.5; 131.2; 129.5; 129.4; 129.2; 129.1 (2C); 127.3; 126.9 (2C); 126.8; 125.8; 124.9; 123.3; 121.0. MS (relative intensity)  $m/z$ : 371 ( $M^+ - 28$ , 29); 370 (100); 360 (29); 344 (30); 335 (53); 329 (14); 260 (61); 253 (33); 234 (47); 147 (30); 120 (96); 92 (76). HRMS calculated for  $\text{C}_{22}\text{H}_{15}\text{ClN}_5\text{O}$  [ $M + H$ ] $^+$ : 400.0960. Found: 400.0956.



**2-(2-(4-(Naphthalen-2-yl)-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (6h)**: Yield: 0.131 g (63%); yellow solid; mp 247–250 °C.  $^1\text{H}$  NMR (400 MHz; DMSO- $d_6$ )  $\delta$  12.59 (s, 1H); 9.23 (s, 1H); 8.47 (s, 1H); 8.14–8.11 (m, 1H); 8.06–7.00 (m, 2H); 7.97–7.91 (m, 3H); 7.89–7.81 (m, 2H); 7.77–7.73 (m, 2H); 7.56–7.48 (m, 4H).  $^{13}\text{C}$  NMR (100 MHz; DMSO- $d_6$ )  $\delta$  161.6; 152.1; 148.6; 146.4; 135.0; 134.5; 133.1; 132.7; 131.5; 131.2; 129.5; 129.4; 128.6; 128.0; 127.72; 127.70; 127.3; 126.8; 126.7; 126.3; 125.8; 124.8; 123.7; 123.6; 123.3; 121.1. MS (relative intensity)  $m/z$ : 415 ( $M^+$ ; 2); 386 (100); 360 (29); 269 (12); 260 (30); 234 (13); 139 (17). HRMS calculated for  $\text{C}_{26}\text{H}_{18}\text{N}_5\text{O}$  [ $M + H$ ] $^+$ : 416.1506. Found: 416.1506.

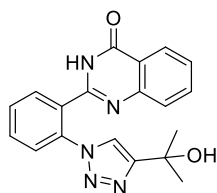


**2-(2-(4-Butyl-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (6i)**: Yield: 0.0983 g (57%); yellow solid; mp 188–190 °C.  $^1\text{H}$  NMR (400 MHz; DMSO- $d_6$ )  $\delta$  12.49 (s, 1H); 8.21 (s, 1H); 8.12 (d,  $J = 7.9$  Hz, 1H); 7.84 (d,  $J = 7.9$  Hz, 1H); 7.79–7.66 (m, 4H); 7.53–7.47 (m, 2H); 2.61 (t,  $J = 7.4$  Hz, 2H); 1.52 (quint,  $J = 7.4$  Hz, 2H); 1.21 (sext,  $J = 7.4$  Hz, 2H); 0.80 (t,  $J = 7.3$  Hz, 3H).  $^{13}\text{C}$  NMR (100 MHz; DMSO- $d_6$ )  $\delta$  161.6; 152.0; 148.5; 146.9; 135.3; 134.3; 131.3; 130.9; 129.5; 129.1; 127.2; 126.7; 125.7; 124.9; 123.3; 121.0; 30.9; 24.4; 21.4; 13.6. MS (relative intensity)  $m/z$ : 316 ( $M^+ - 28$ , 36); 274 (100); 260 (14); 248 (13); 136 (10); 119 (37); 92 (12). HRMS calculated for  $\text{C}_{20}\text{H}_{20}\text{N}_5\text{O}$  [ $M + H$ ] $^+$ : 346.1662. Found: 346.1663.

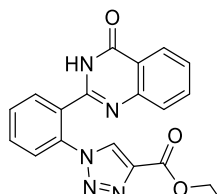


**2-(2-(4-(1-Hydroxycyclopentyl)-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (6j)**: Yield: determined for  $^1\text{H}$  NMR (27%); white solid. Mixture of compounds (reason 2:1). Asterisk denotes the chemical displacement of the compound **6b**.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$  12.51 (s, 1H); 8.34 (s, 1H)\*; 8.23 (s, 1H); 8.16 (s, 1H)\*; 8.13–8.10 (m, 1H); 8.02–8.00 (m, 1H)\*; 7.84 (d,  $J = 7.5$  Hz, 1H); 7.80–7.74 (m, 2H); 7.71–7.67 (m, 1H); 7.65–7.60 (m, 1H); 7.53–7.48 (m, 2H); 7.29–7.24 (m, 1H)\*; 6.89 (s, 1H)\*; 6.74–6.71 (m, 2H)\*; 5.54 (s, 1H)\*; 5.19 (s, 1H)\*; 5.09 (s, 1H); 1.94–1.60 (m, 8H).  $^{13}\text{C}$  NMR (100 MHz, DMSO)  $\delta$  163.5\*; 161.6; 154.9\*; 154.6\*; 152.0; 148.6; 148.0\*; 135.4\*; 135.2; 134.4; 134.4\*; 133.5\*; 131.4; 130.9; 130.2; 130.2\*; 130.0\*; 129.5\*; 129.5; 129.1; 129.1\*; 127.4;

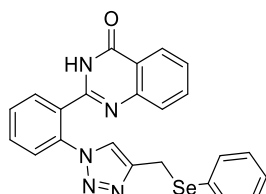
127,3; 126,8; 126,1\*; 125,7; 124,8\*; 123,8\*; 122,5; 121,0; 117,7\*; 114,6\*; 77,4\*; 77,4; 62,3\*; 40,8 (2C); 40,7\*; 23,3 (2C).



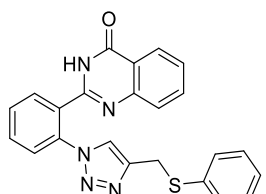
**2-(2-(4-(2-Hydroxypropan-2-yl)-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (6k):** Yield: 0.0908 g (52%); white solid, mp 243 – 246 °C. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.51 (s, 1H); 8.22 (s, 1H); 8.11 (dd, *J* = 7.9, 1.6 Hz, 1H); 7.88 – 7.81 (m, 1H); 7.82 – 7.72 (m, 3H); 7.74 – 7.64 (m, 1H); 7.55 – 7.45 (m, 2H); 5.18 (s, 1H); 1.42 (s, 6H). <sup>13</sup>C NMR (100 MHz, DMSO) δ 161.6; 155.9; 151.9; 148.5; 135.2; 134.4; 131.4; 130.9; 129.5; 129.1; 127.3; 126.8; 125.7; 124.9; 121.8; 121.8; 121.0; 67.0; 30.6. MS (relative intensity) *m/z*: 319 (*M*<sup>+</sup> -28, 9); 304 (27); 372 (11); 262 (100); 248 (38); 234 (11); 129 (10); 119 (77); 92 (28). HRMS calculated for C<sub>19</sub>H<sub>18</sub>N<sub>5</sub>O<sub>2</sub> [*M* + *H*]<sup>+</sup>: 348.1455. Found: 348.1457.



**Ethyl-1-(2-(4-oxo-3,4-dihydroquinazolin-2-yl)phenyl)-1H-1,2,3-triazole-4-carboxylate (6l):** Yield: 0.036 g (20%); orange solid; mp 219 – 222 °C. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.51 (s, 1H); 9.25 (s, 1H); 8.10 (d, *J* = 7.9 Hz, 1H); 7.94 – 7.88 (m, 1H); 7.86 – 7.72 (m, 4H); 7.55 – 7.48 (m, 1H); 7.48 – 7.40 (m, 1H); 4.33 (q, *J* = 7.0 Hz, 2H); 1.30 (t, *J* = 7.0 Hz, 3H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>) δ 161.6; 160.1; 151.5; 148.4; 138.7; 134.5; 134.3; 131.5; 131.1; 130.8; 130.1; 129.6; 127.2; 126.9; 125.7; 125.6; 120.9; 60.8; 14.1. MS (relative intensity) *m/z*: 332 (*M*<sup>+</sup> -28); 260 (100); 248 (42); 230 (13); 119 (14); 102 (22); 90 (17). HRMS calculated for C<sub>19</sub>H<sub>16</sub>N<sub>5</sub>O<sub>3</sub> [*M* + *H*]<sup>+</sup>: 362.1248. Found: 362.1248.

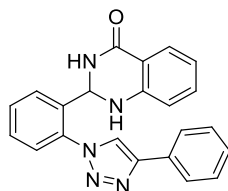


**2-(2-(4-((Phenylselanyl)methyl)-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (6m):** Yield: 0.122 g (53%); yellow solid; mp 183 – 186 °C. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 12.52 (s, 1H); 8.28 (s, 1H); 8.11 (d, *J* = 7.5 Hz, 1H); 7.85 – 7.83 (m, 1H); 7.76 – 7.64 (m, 4H); 7.53 – 7.43 (m, 4H); 7.26 – 7.24 (m, 3H); 4.24 (s, 2H). <sup>13</sup>C NMR (100 MHz; DMSO-*d*<sub>6</sub>) δ 161.6; 151.8; 148.5; 144.6; 134.9; 134.4; 131.7 (2C); 131.4; 1310; 130.3; 129.4; 129.3; 129.2 (2C); 127.4; 126.9; 126.8; 125.7; 125.0; 124.2; 121.0; 19.4. <sup>77</sup>Se RMN (77 MHz; DMSO-*d*<sub>6</sub>) δ 351.35. MS (relative intensity) *m/z*: 459 (*M*<sup>+</sup>; 12); 274 (100); 248 (54); 156 (30); 119 (21); 92 (20). HRMS calculated for C<sub>23</sub>H<sub>18</sub>N<sub>5</sub>OSe [*M* + *H*]<sup>+</sup>: 460.0671. Found: 460.0679.



**2-(2-(4-((Phenylthio)methyl)-1H-1,2,3-triazol-1-yl)phenyl)quinazolin-4(3H)-one (6n):** Yield: 0.113 g (55%); yellow solid; mp 188 – 190 °C. <sup>1</sup>H

NMR (400 MHz; DMSO-*d*<sub>6</sub>)  $\delta$  12.54 (s, 1H), 8.38 (s, 1H); 8.14 – 8.11 (m, 1H); 7.86 – 7.84 (m, 1H); 7.78 – 7.74 (m, 2H); 7.71 – 7.67 (m, 2H); 7.53 – 7.49 (m, 1H); 7.41 (d, *J* = 8.0 Hz, 1H); 7.35 – 7.33 (m, 2H); 7.29 – 7.25 (m, 2H); 7.20 – 7.16 (m, 1H); 4.29 (s, 2H). <sup>13</sup>C NMR (100 MHz; DMSO-*d*<sub>6</sub>)  $\delta$  161.6; 151.8; 148.5; 143.8; 135.7; 134.9; 134.4; 131.4; 131.0; 129.5; 129.4; 129.0 (2C); 128.3 (2C); 127.4; 126.8; 126.0; 125.7; 125.0; 124.6; 121.0; 27.1. MS (relative intensity) *m/z*: 411 (*M*<sup>+</sup>; 3); 274 (100); 156 (17); 129 (11); 119 (35); 102 (14); 92 (22). HRMS calculated for C<sub>23</sub>H<sub>18</sub>N<sub>5</sub>OS [*M* + *H*]<sup>+</sup>: 412.1226. Found: 412.1227.

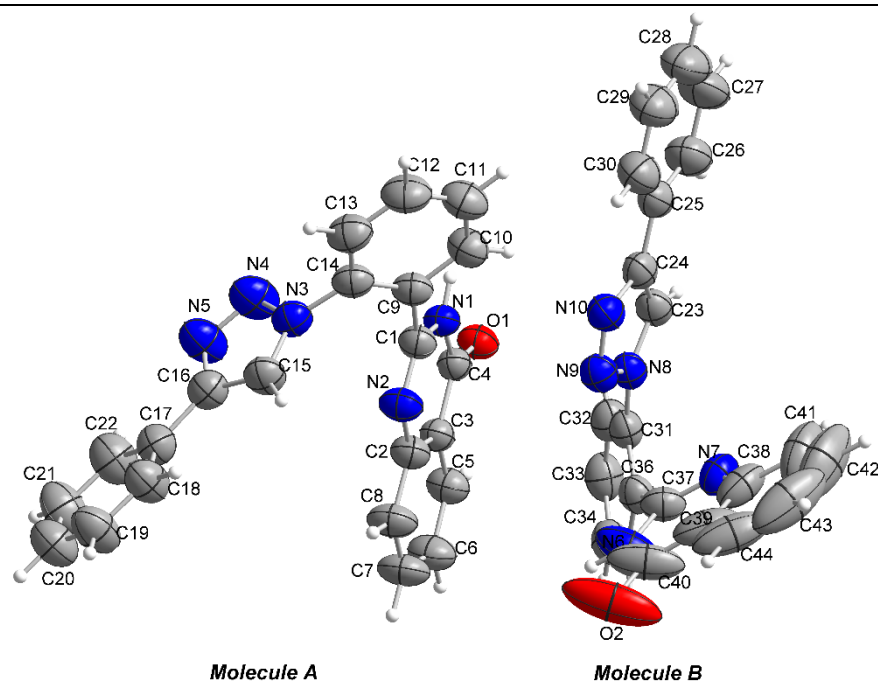


**2-(2-(4-Phenyl-1H-1,2,3-triazol-1-yl)phenyl)-2,3-dihydroquinazolin-4(1H)-one (5a)**: Yield: 0.150 g (82%); white solid; mp 187 – 189 °C. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  8.99 (s, 1H); 8.13 (s, 1H); 8.01 – 7.98 (m, 1H); 7.94 – 7.92 (m, 2H); 7.73 – 7.61 (m, 4H); 7.52 – 7.48 (m, 2H); 7.41 – 7.37 (m, 1H), 7.28 – 7.24 (m, 1H); 6.90 (s, 1H); 6.76 – 6.69 (m, 2H); 5.68 (s, 1H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  163.4; 147.8; 146.7; 135.7; 134.9; 133.5; 130.4; 130.1; 130.0; 129.0 (2C); 128.9; 128.3; 127.4; 126.1; 125.4 (2C); 123.8; 117.7; 114.6; 114.6; 62.3. MS (relative intensity) *m/z*: 339 (*M*<sup>+</sup> -28,17); 336 (100); 260 (35); 234 (32); 219 (49); 192 (13); 147 (18); 120 (57); 102 (15); 92 (50). HRMS calculated for C<sub>22</sub>H<sub>18</sub>N<sub>5</sub>O [*M* + *H*]<sup>+</sup>: 368.1506. Found: 368.1508

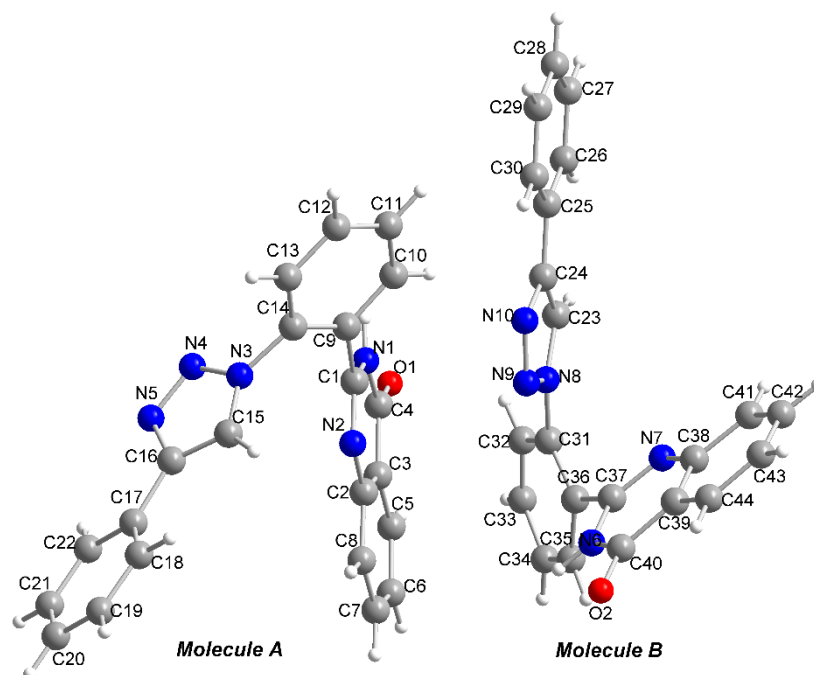
**Table S1.** Crystallographic and structure refinement data for compound **6a**.

Formula	C <sub>22</sub> H <sub>15</sub> N <sub>5</sub> O
CCDC n°	2106971
F.W. (g·mol <sup>-1</sup> )	365.39
Crystal system	Triclinic
Space group	<i>P</i> -1
<i>a</i> (Å)	12.6964(3)
<i>b</i> (Å)	12.7328(3)
<i>c</i> (Å)	12.7938(3)
$\alpha$ (°)	73.6450(10)
$\beta$ (°)	66.9090(10)
$\gamma$ (°)	78.5480(10)
T (K)	296(2)
V (Å <sup>3</sup> )	1816.45(8)
Z	4
<i>r</i> calc. (g·cm <sup>-3</sup> )	1.336
$\mu$ (mm <sup>-1</sup> )	0.695
<i>F</i> (000)	760
Collected reflections	34182
Independent reflections [ <i>R</i> <sub>int</sub> ]	6893 [ <i>R</i> (int) = 0.0407]
<i>R</i> <sub>I</sub> [ <i>I</i> > 2σ( <i>I</i> )]	0.0577
<i>wR</i> <sub>2</sub> [ <i>I</i> > 2σ( <i>I</i> )]	0.1466
<i>R</i> <sub>I</sub> (all data) <sup>[a]</sup>	0.0798
<i>wR</i> <sub>2</sub> (all data) <sup>[b]</sup>	0.1665
GOOF on <i>F</i> <sup>2</sup>	1.041
Largest diff. peak and hole (e.Å <sup>-3</sup> )	0.380 and -0.301

<sup>[a]</sup>*R*<sub>1</sub> =  $\sum ||F_o| - |F_c|| / \sum |F_o|$ ; <sup>[b]</sup>*wR*<sub>2</sub> =  $\{\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)\}^{1/2}$ .



**Figure S1.** Ellipsoid representations (50% probability) of **6a**.

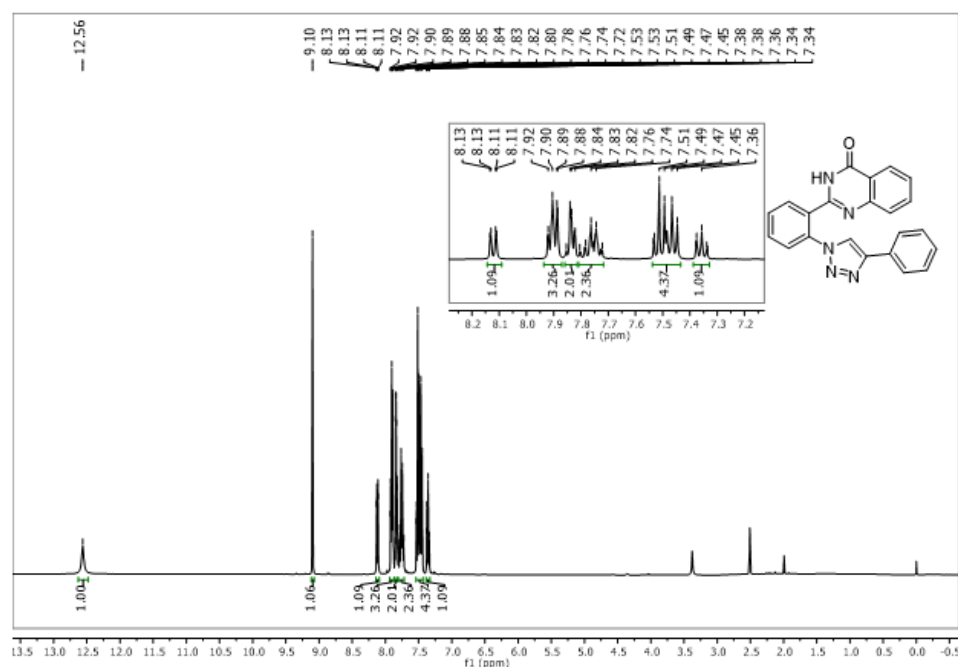


**Figure S2.** Molecular structure of **6a** determined by single-crystal X-ray crystallography.

**Table S2.** Selected bond lengths (Å) and angles (°) of both independent molecules present in the compound **6a**.

A			B		
Bond lengths			Bond lengths		
O1–C4	1.236(2)		O2–C40	1.228(4)	
C1–N2	1.288(2)		N7–C37	1.281(3)	
C1–N1	1.370(2)		N6–C37	1.360(3)	
N1–C4	1.373(2)		N6–C40	1.383(3)	
N3–C14	1.436(3)		N8–C31	1.426(3)	
N3–C15	1.342(3)		N8–C23	1.347(2)	
N3–N4	1.340(3)		N9–N8	1.353(2)	
N4–N5	1.309(3)		N9–N10	1.308(2)	
N2–C2	1.391(3)		N7–C38	1.393(3)	
N5–C16	1.356(3)		N10–C24	1.368(3)	
Angles			Angles		
N2–C1–N1	124.31(18)		N7–C37–N6	123.3(2)	
N2–C1–C9	119.61(17)		N7–C37–C36	119.38(19)	
C1–N1–C4	123.24(16)		C37–N6–C40	124.0(3)	
N4–N3–C15	110.16(18)		C23–N8–N9	110.46(17)	
N4–N3–C14	118.79(17)		N9–N8–C31	119.76(16)	
C15–N3–C14	131.04(18)		C23–N8–C31	129.64(17)	
N5–N4–N3	107.41(17)		N10–N9–N8	107.14(16)	
O1–C4–N1	120.56(16)		O2–C40–N6	120.4(4)	
N1–C4–C3	114.18(16)		N6–C40–C39	114.0(3)	
C1–N2–C2	116.51(17)		C37–N7–C38	116.5(2)	
N5–C16–C15	107.55(19)		N10–C24–C23	107.68(18)	
N5–C16–C17	120.82(19)		N10–C24–C25	121.3(2)	
N4–N5–C16	109.23(19)		N9–N10–C24	109.36(17)	
N3–C15–C16	105.66(19)		N8–C23–C24	105.34(18)	

## Spectra of the compounds

**Figure S3.** <sup>1</sup>H NMR (400 MHz) spectrum for compound **6a** in DMSO-*d*<sub>6</sub>.

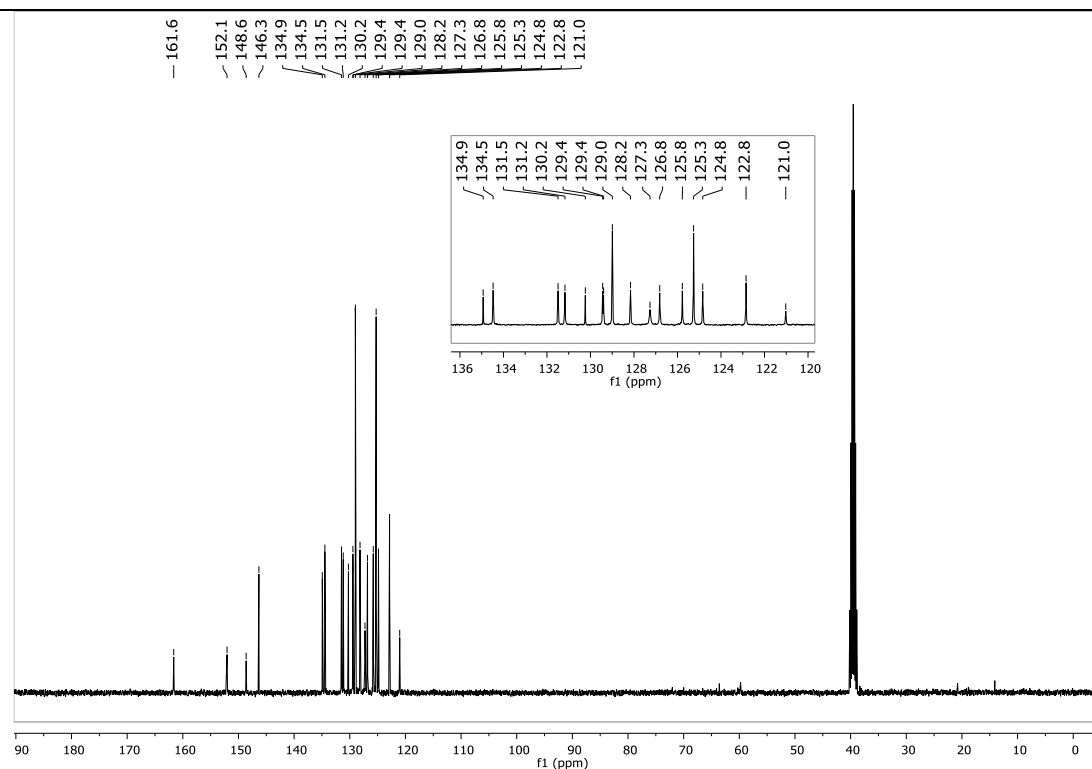


Figure S4. <sup>13</sup>C NMR (100 MHz) spectrum for compound **6a** in DMSO-*d*<sub>6</sub>.

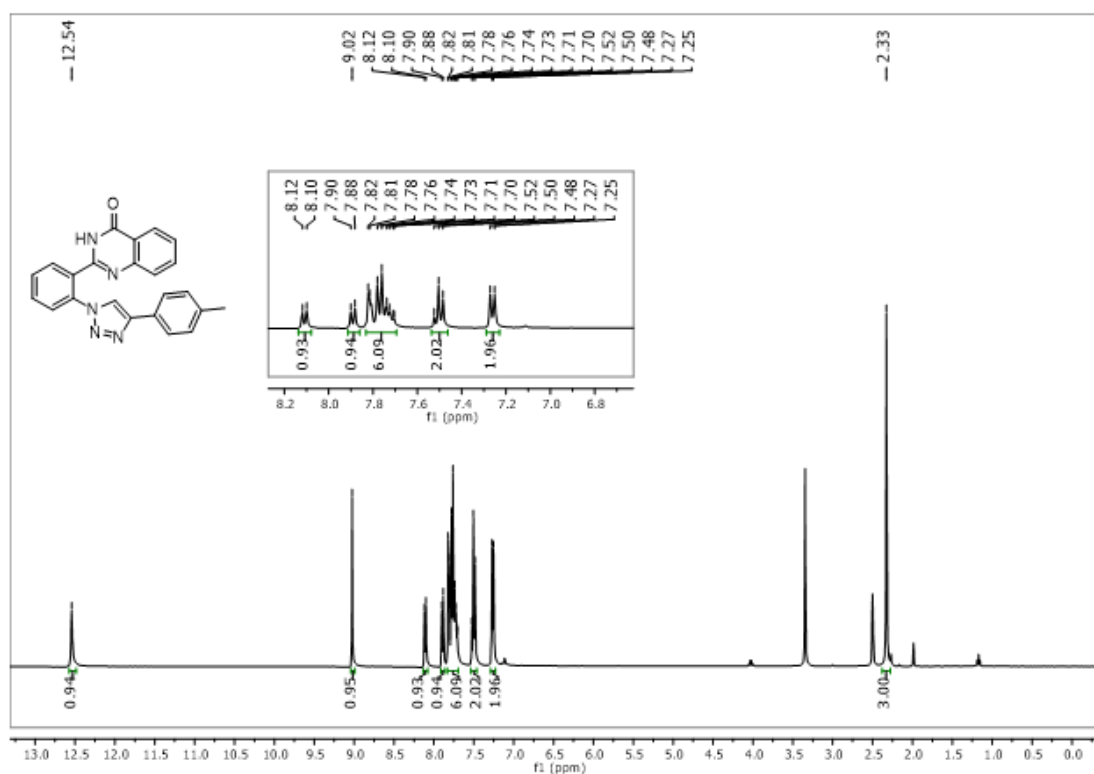


Figure S5. <sup>1</sup>H NMR (400 MHz) spectrum for compound **6b** in DMSO-*d*<sub>6</sub>.

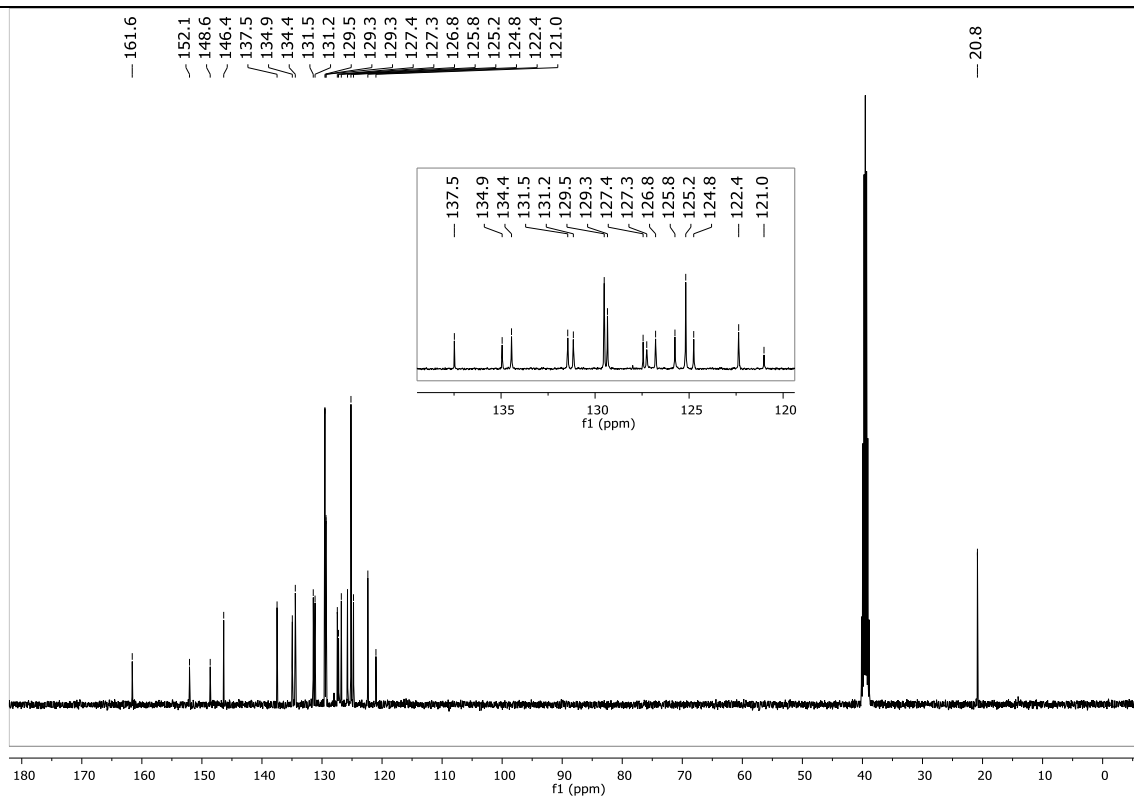


Figure S6. <sup>13</sup>C NMR (100 MHz) spectrum for compound **6b** in DMSO-d<sub>6</sub>.

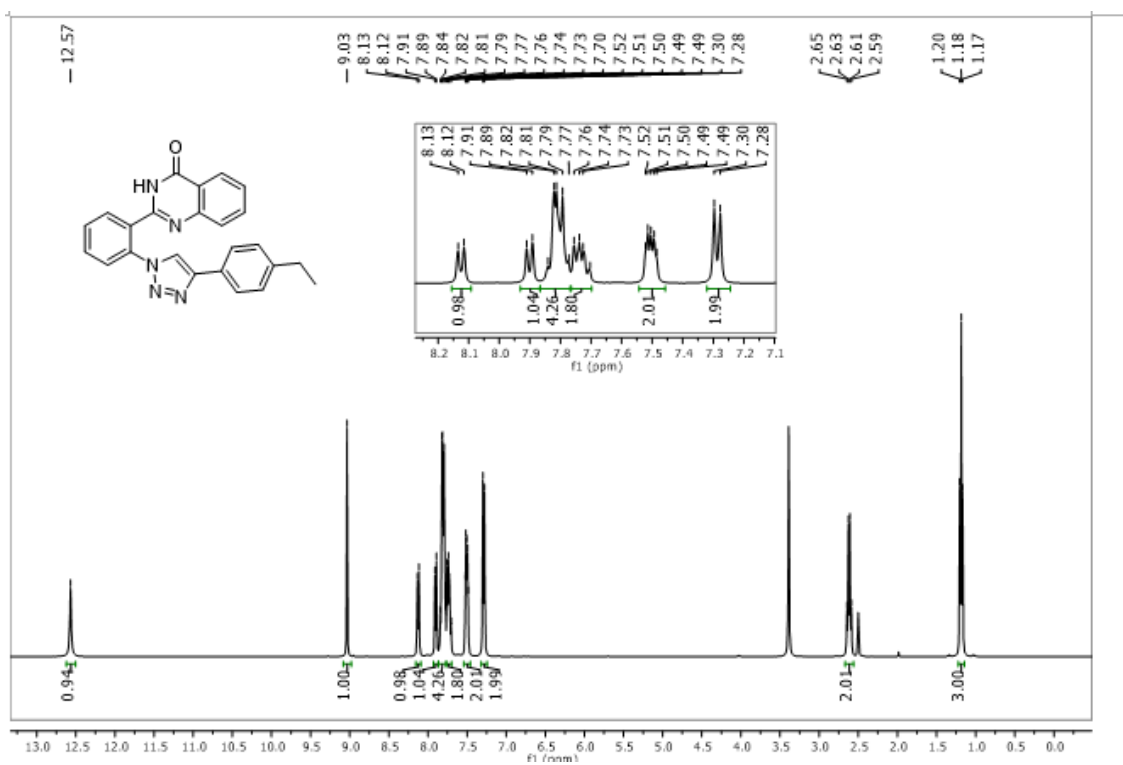


Figure S7. <sup>1</sup>H NMR (400 MHz) spectrum for compound **6c** in DMSO-d<sub>6</sub>.

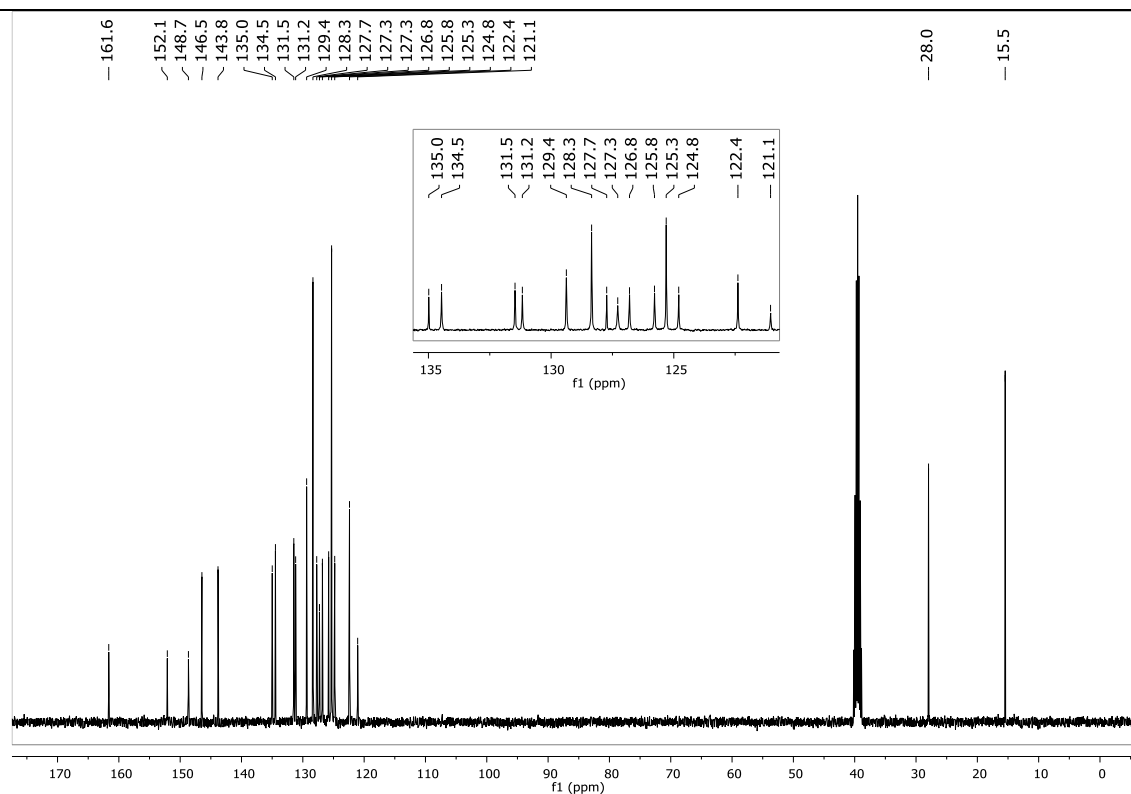


Figure S8. <sup>13</sup>C NMR (100 MHz) spectrum for compound **6c** in DMSO-d<sub>6</sub>.

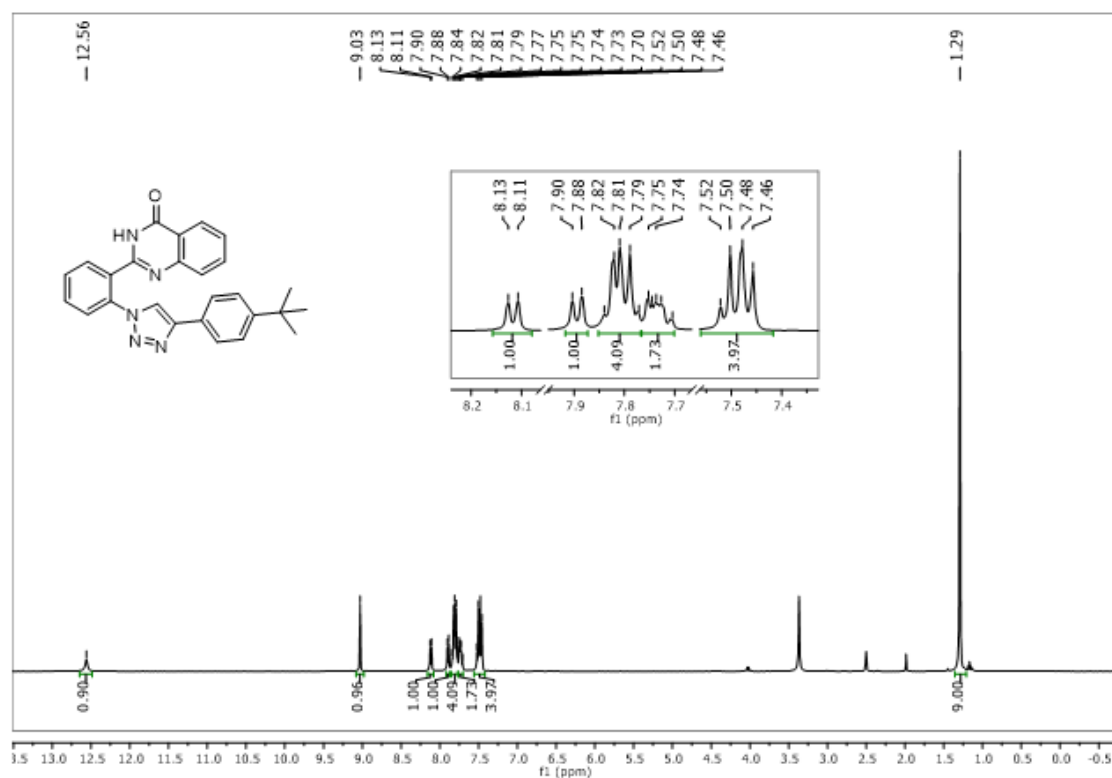


Figure S9. <sup>1</sup>H NMR (400 MHz) spectrum for compound **6d** in DMSO-d<sub>6</sub>.

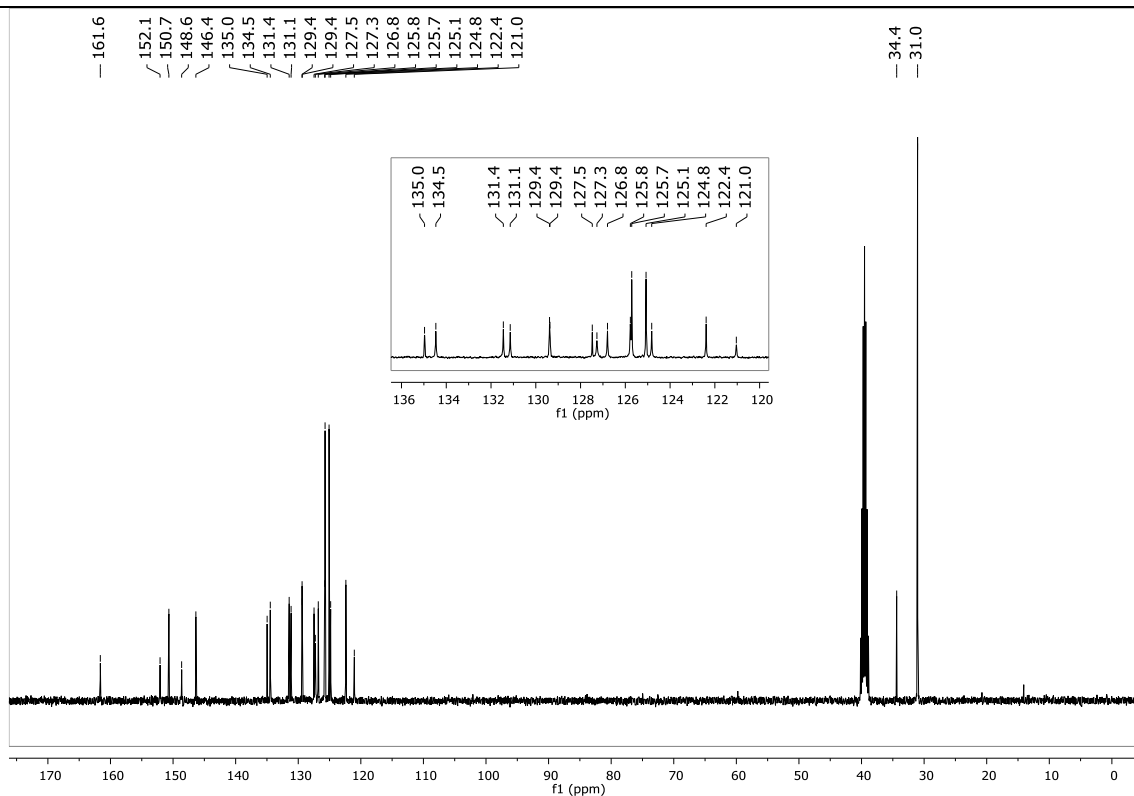


Figure S10. <sup>13</sup>C NMR (100 MHz) spectrum for compound **6d** in DMSO-d<sub>6</sub>.

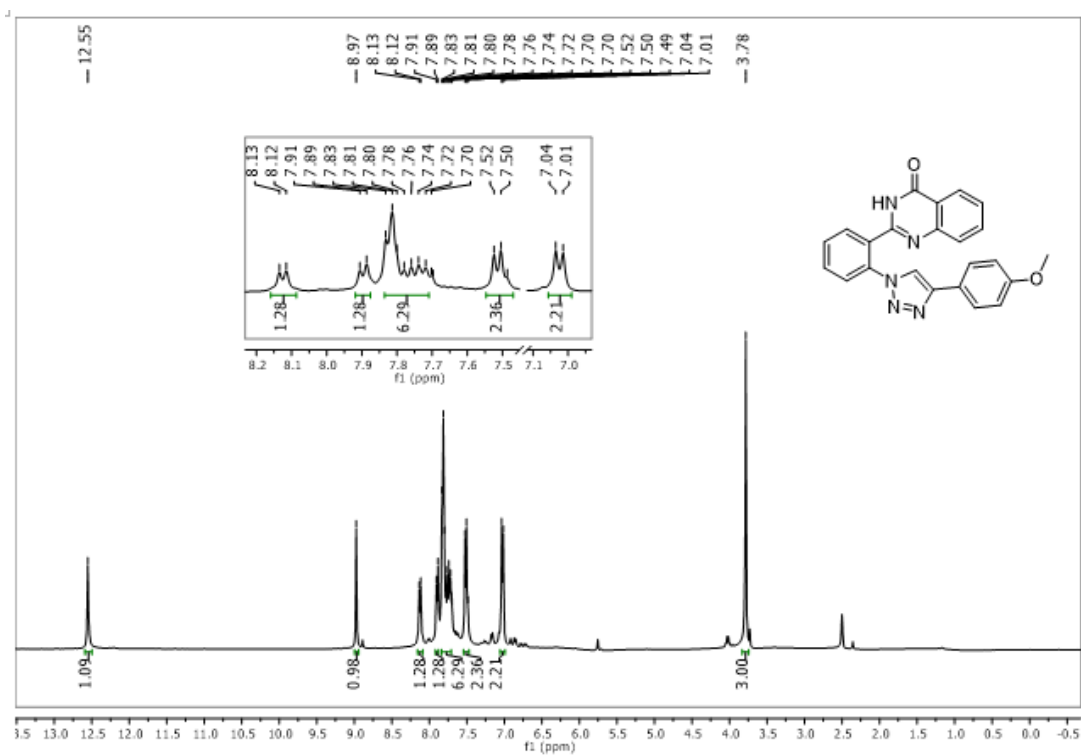


Figure S11. <sup>1</sup>H NMR (400 MHz) spectrum for compound **6e** in DMSO-d<sub>6</sub>.

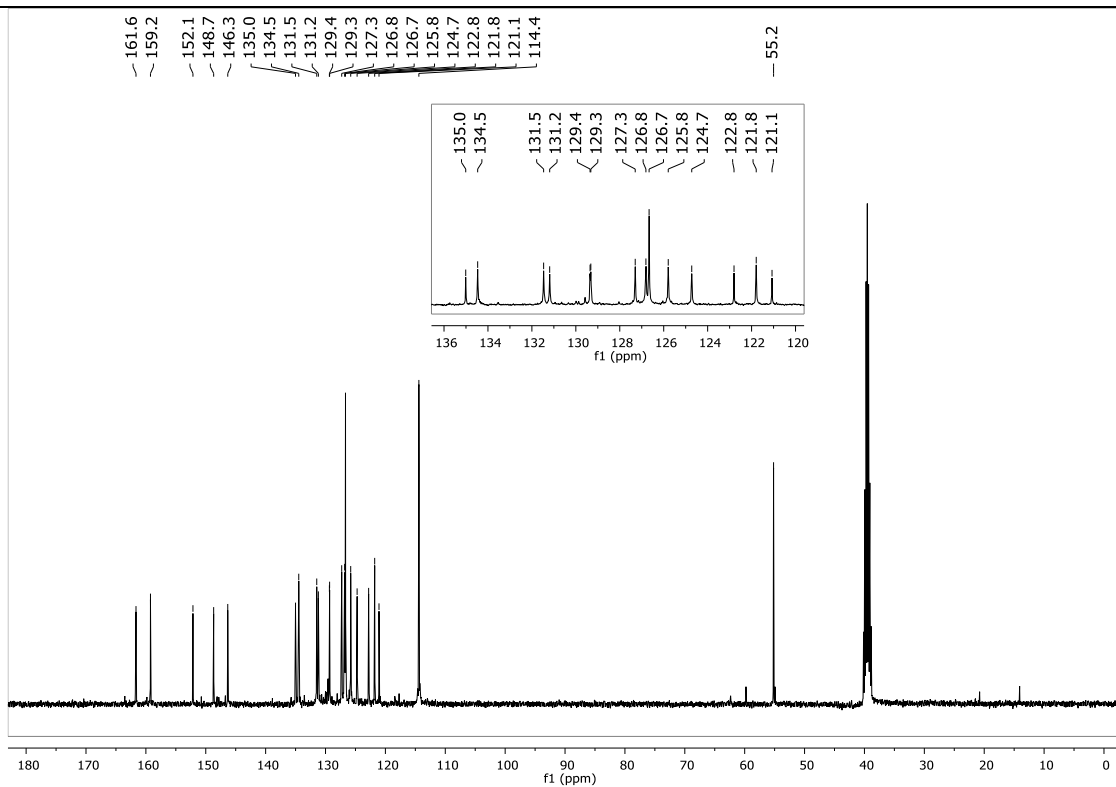


Figure S12. <sup>13</sup>C NMR (100 MHz) spectrum for compound **6e** in DMSO-d<sub>6</sub>.

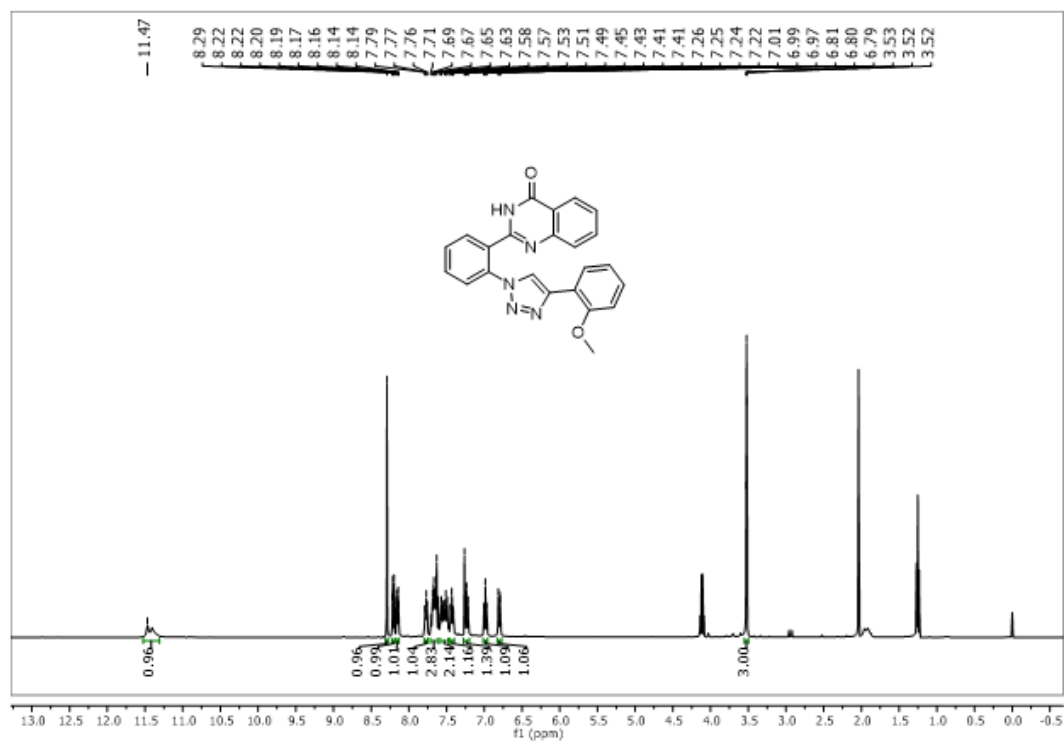


Figure S13. <sup>1</sup>H NMR (400 MHz) spectrum for compound **6f** in DMSO-d<sub>6</sub>.

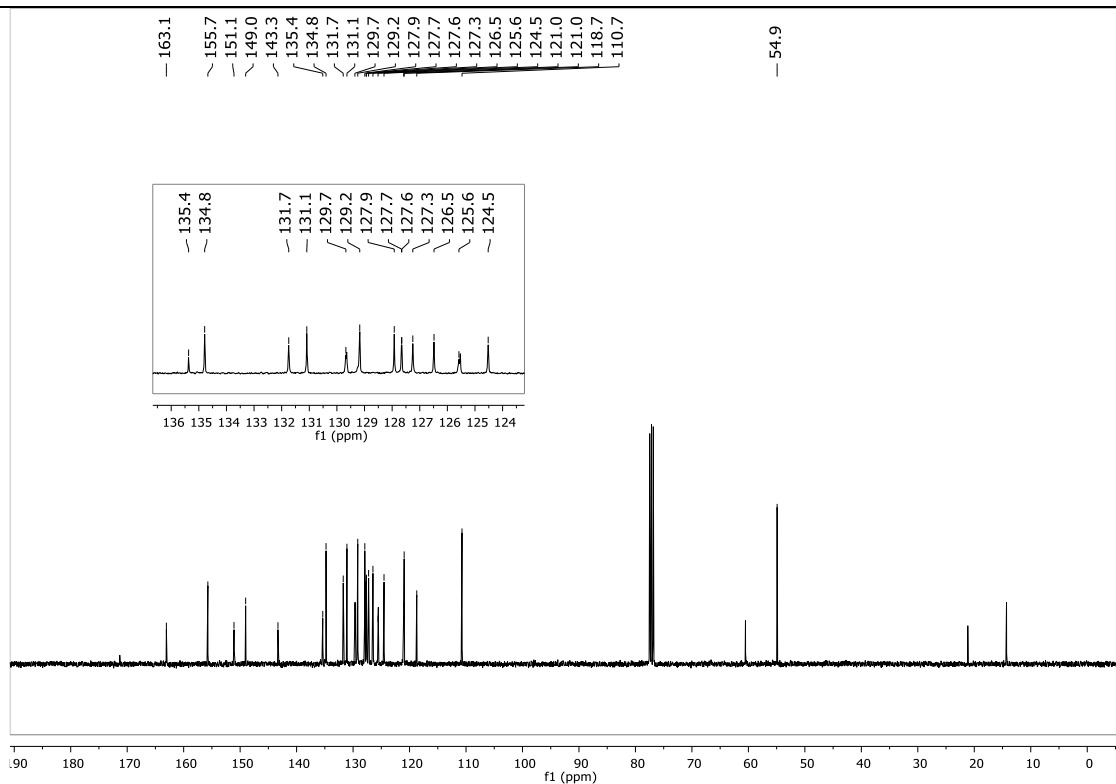


Figure S14:  $^{13}\text{C}$  NMR (100 MHz) spectrum for compound **6f** in  $\text{DMSO-d}_6$ .

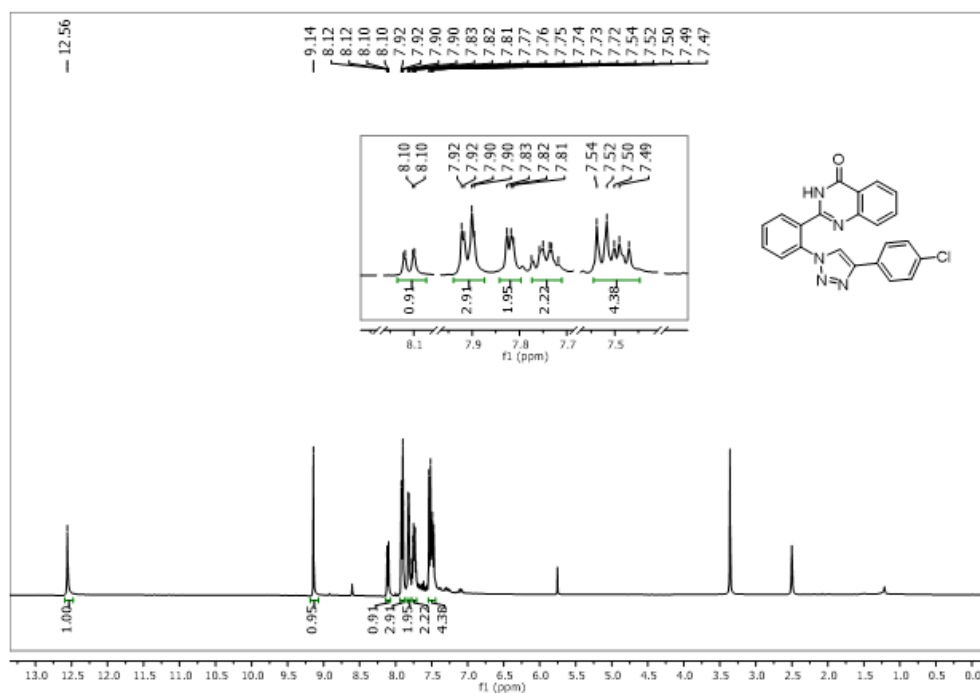


Figure S15:  $^1\text{H}$  NMR (400 MHz) spectrum for compound **6g** in  $\text{DMSO-d}_6$ .

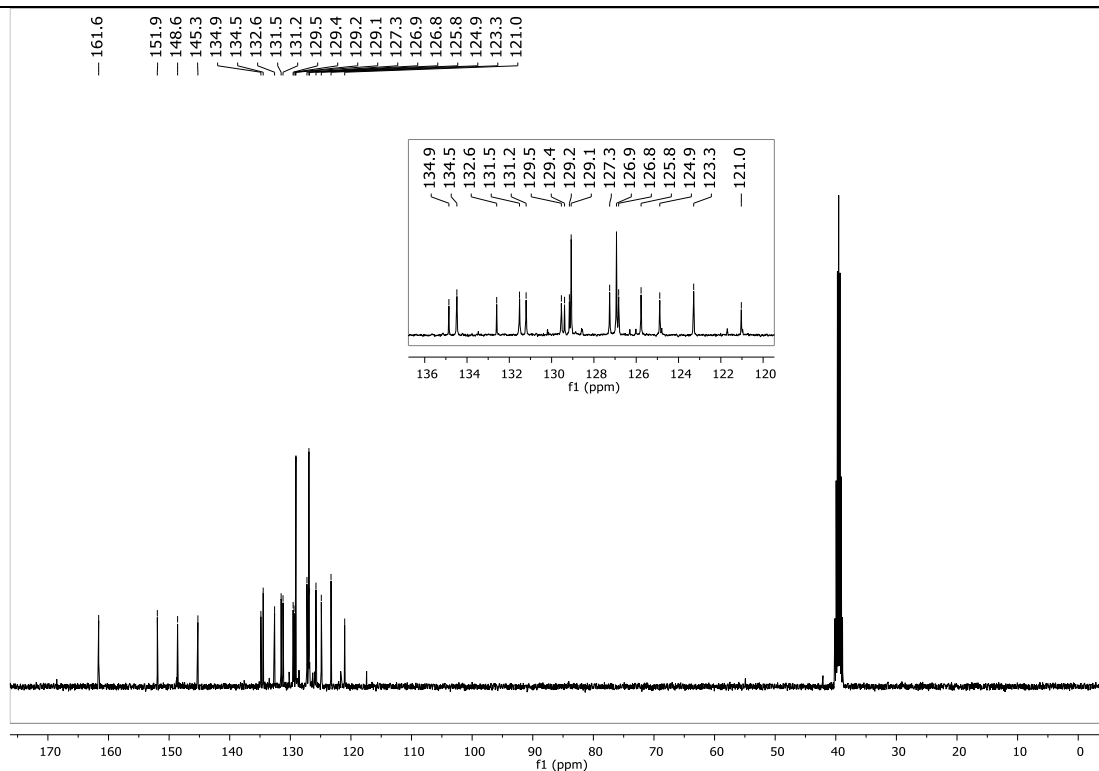


Figure S16. <sup>13</sup>C NMR (100 MHz) spectrum for compound **6g** in DMSO-d<sub>6</sub>.

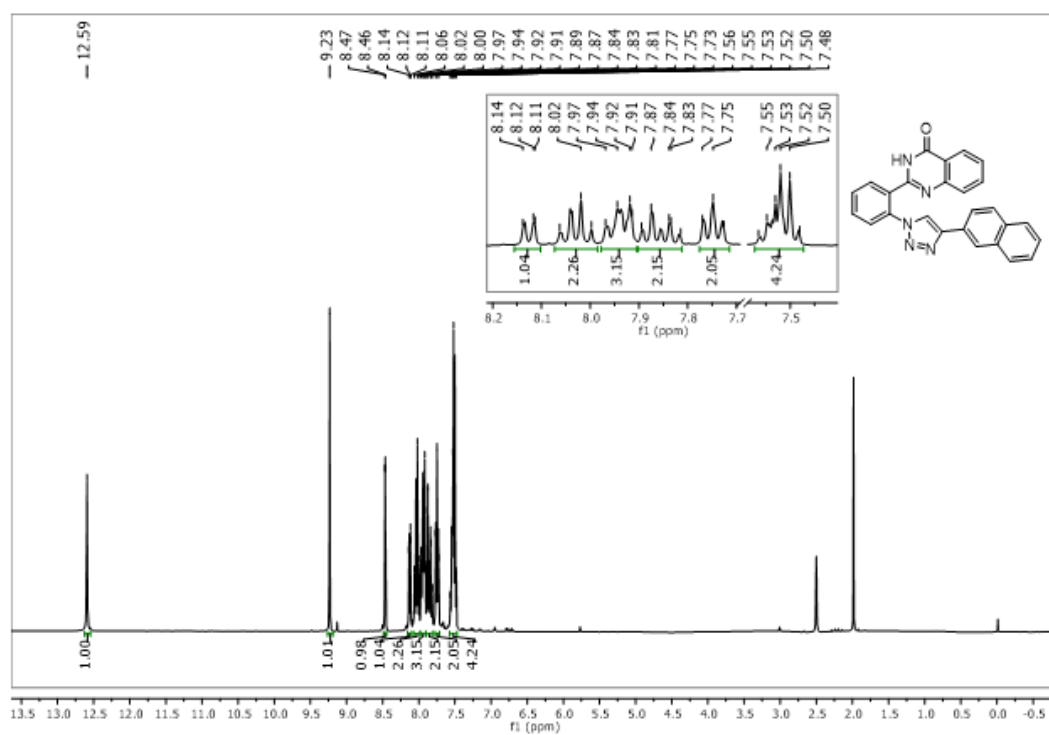


Figure S17. <sup>1</sup>H NMR (400 MHz) spectrum for compound **6h** in DMSO-d<sub>6</sub>.

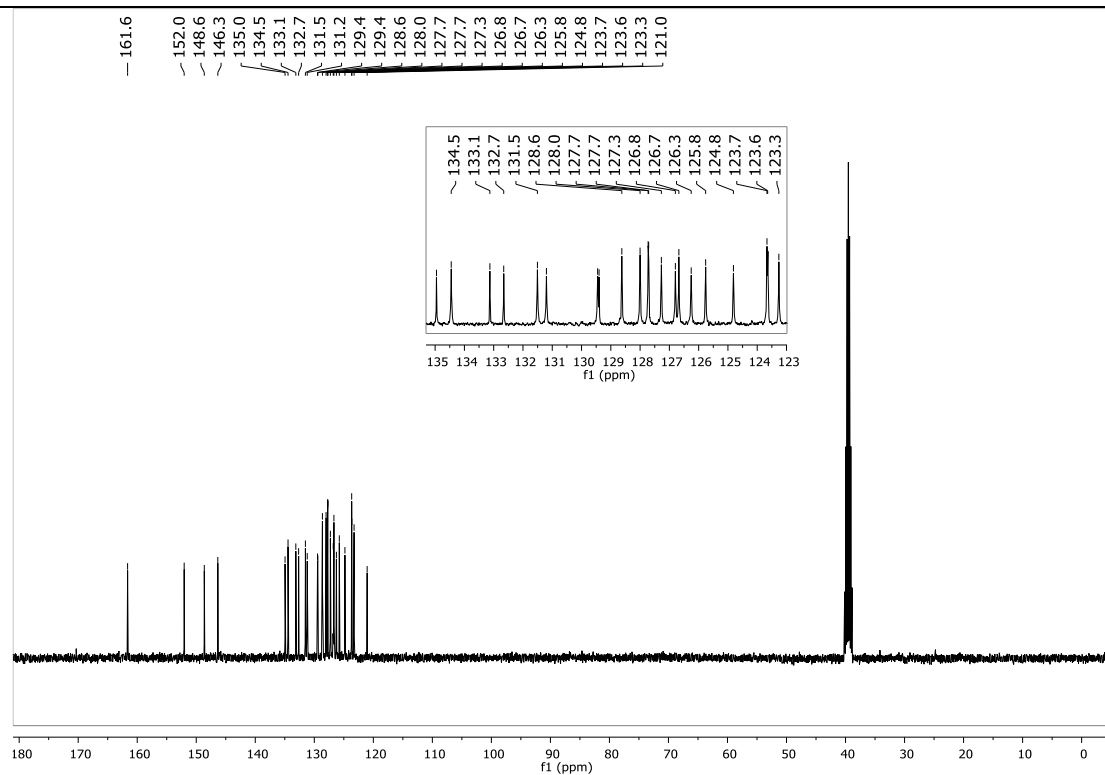


Figure S18. <sup>13</sup>C NMR (100 MHz) spectrum for compound **6h** in DMSO-d<sub>6</sub>.

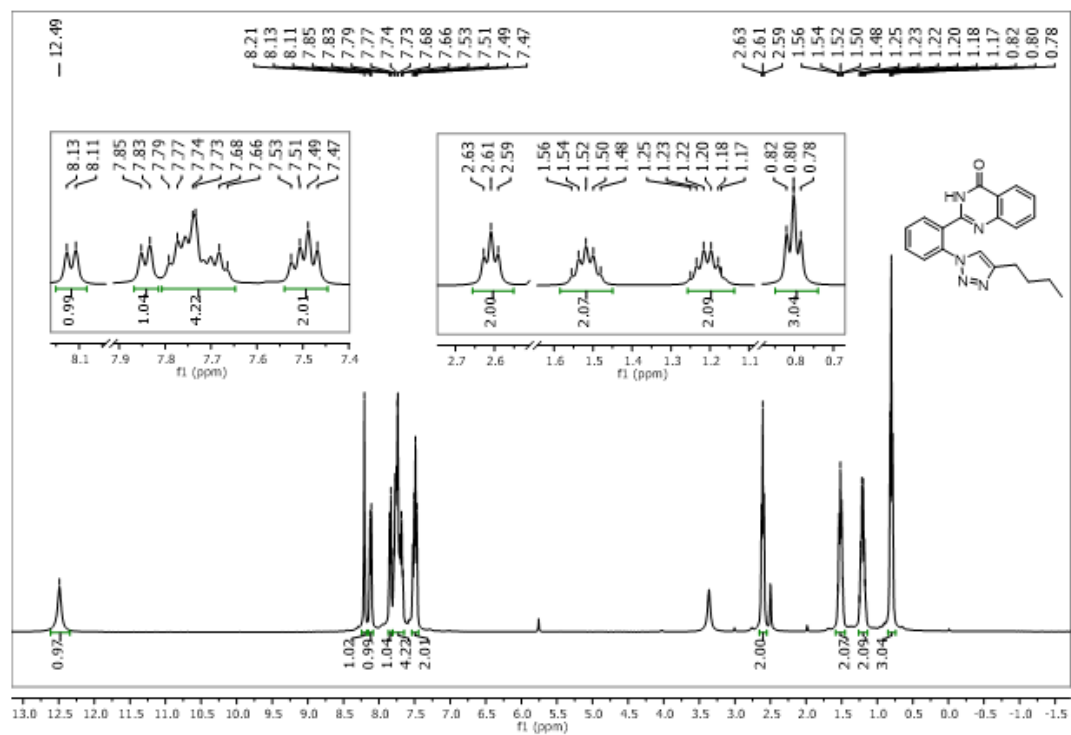


Figure S19. <sup>1</sup>H NMR (400 MHz) spectrum for compound **6i** in DMSO-d<sub>6</sub>.

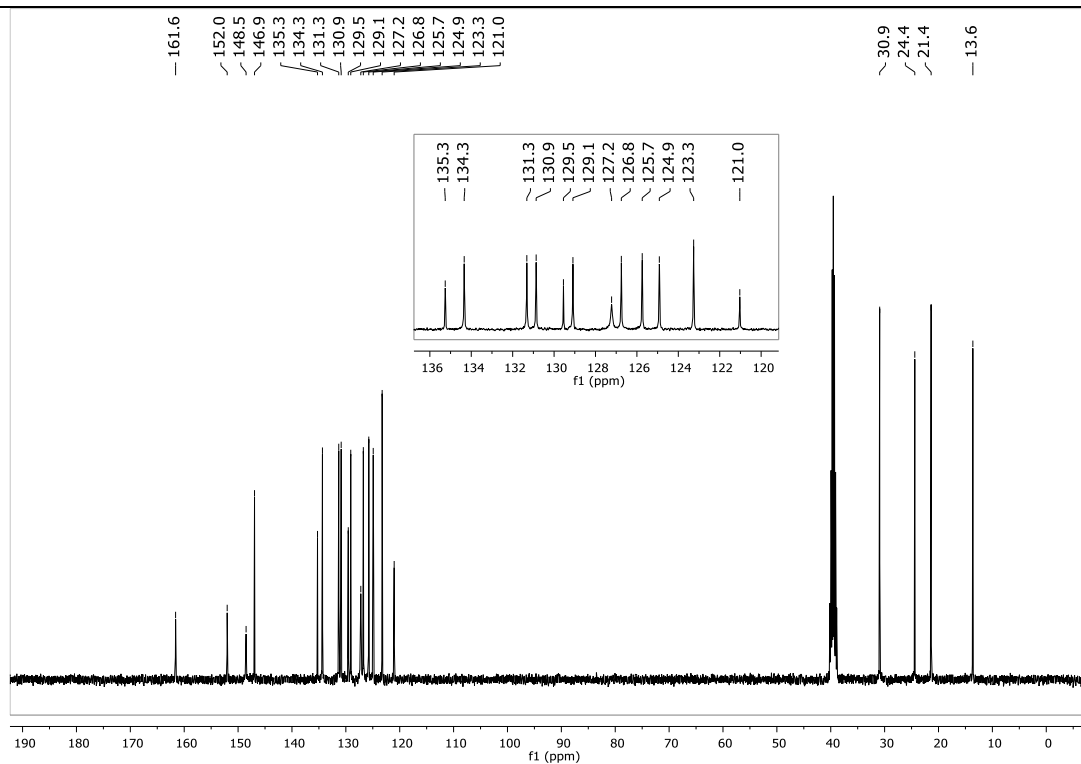


Figure S20. <sup>13</sup>C NMR (100 MHz) spectrum for compound **6i** in DMSO-d<sub>6</sub>.

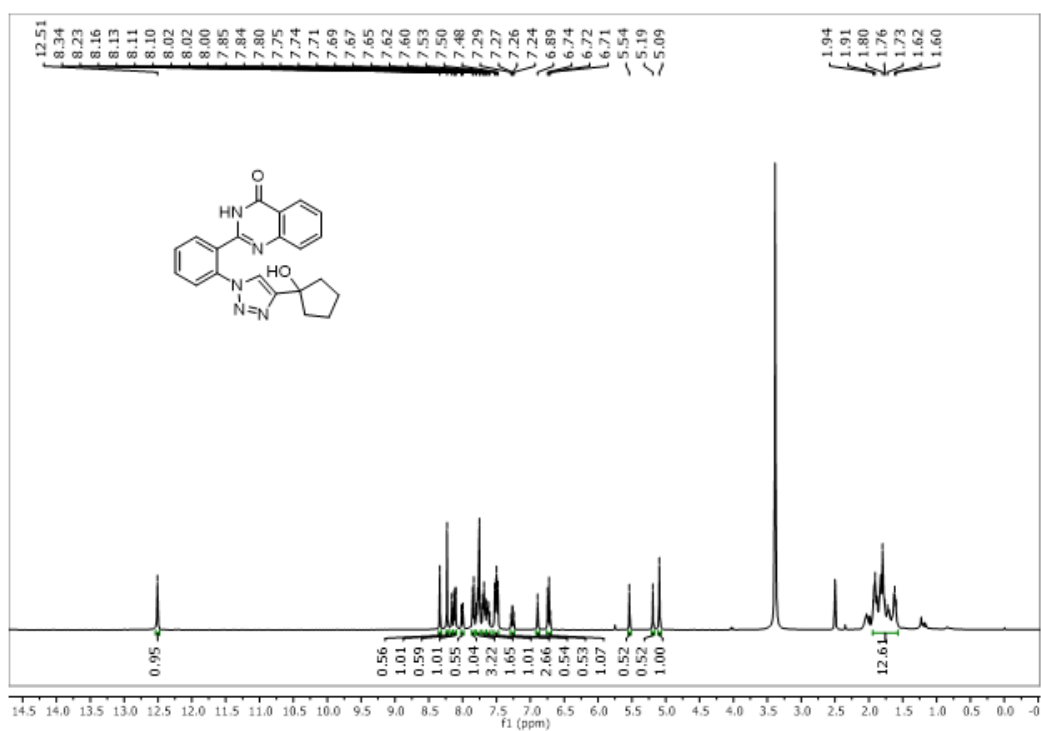


Figure S21. <sup>1</sup>H NMR (400 MHz) spectrum for compound **6j** in DMSO-d<sub>6</sub>.

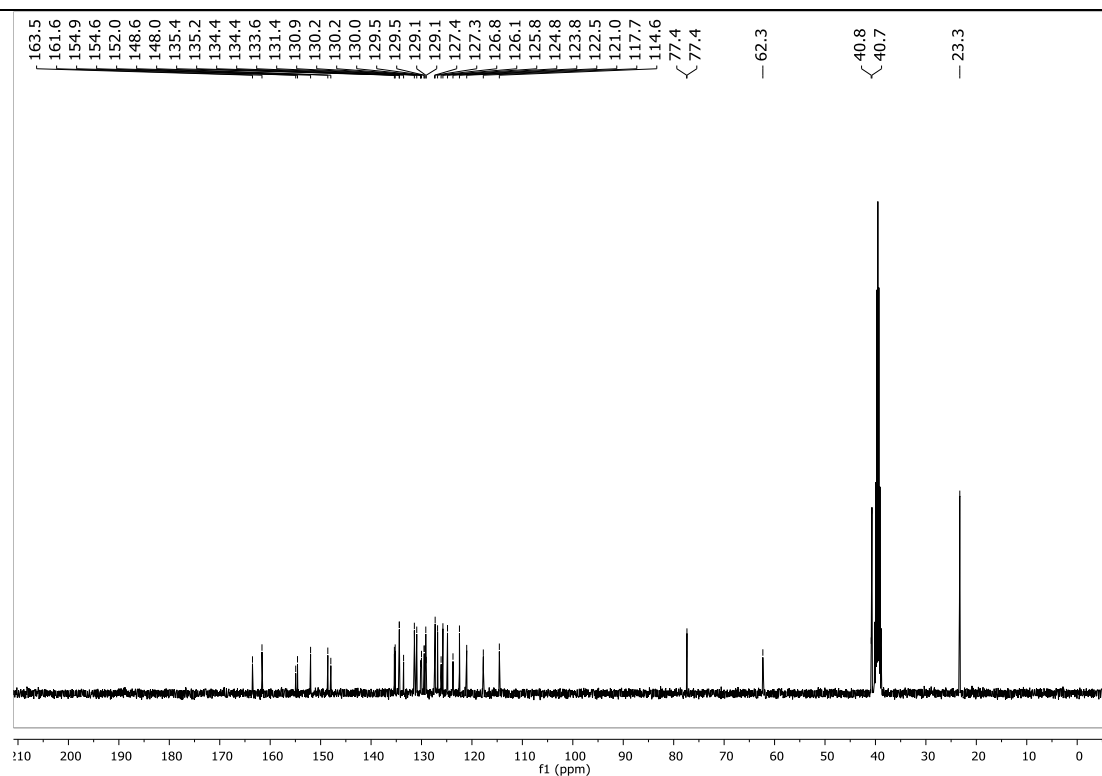


Figure S22. <sup>13</sup>C NMR (100 MHz) spectrum for compound **6j** in DMSO-d<sub>6</sub>.

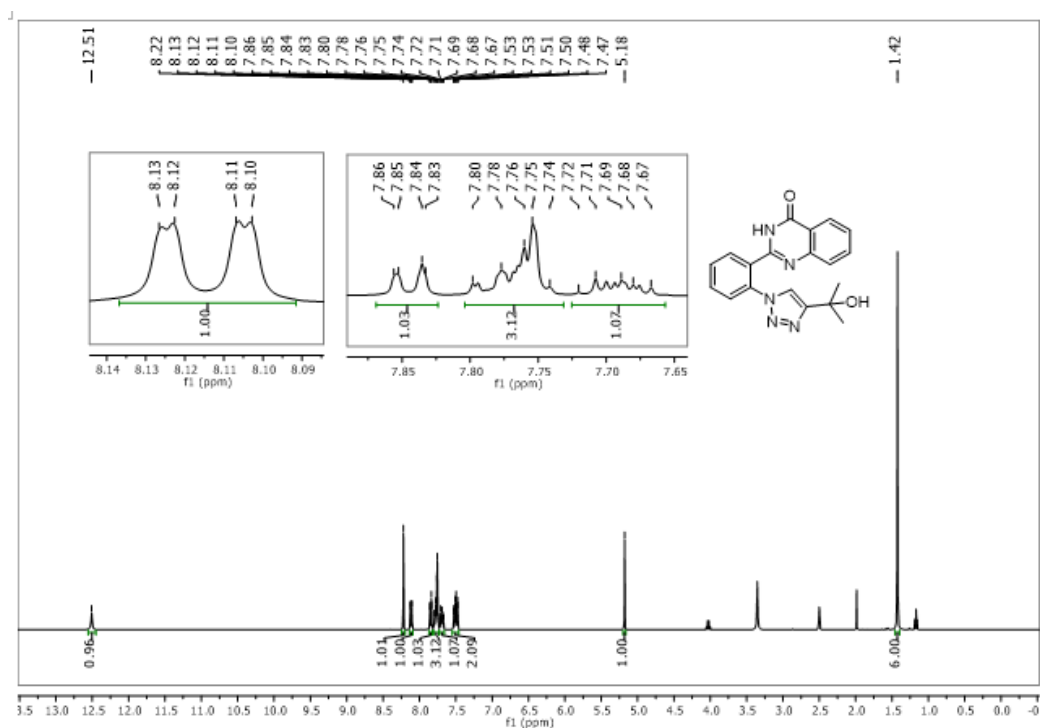


Figure S23. <sup>1</sup>H NMR (400 MHz) spectrum for compound **6k** in DMSO-d<sub>6</sub>.

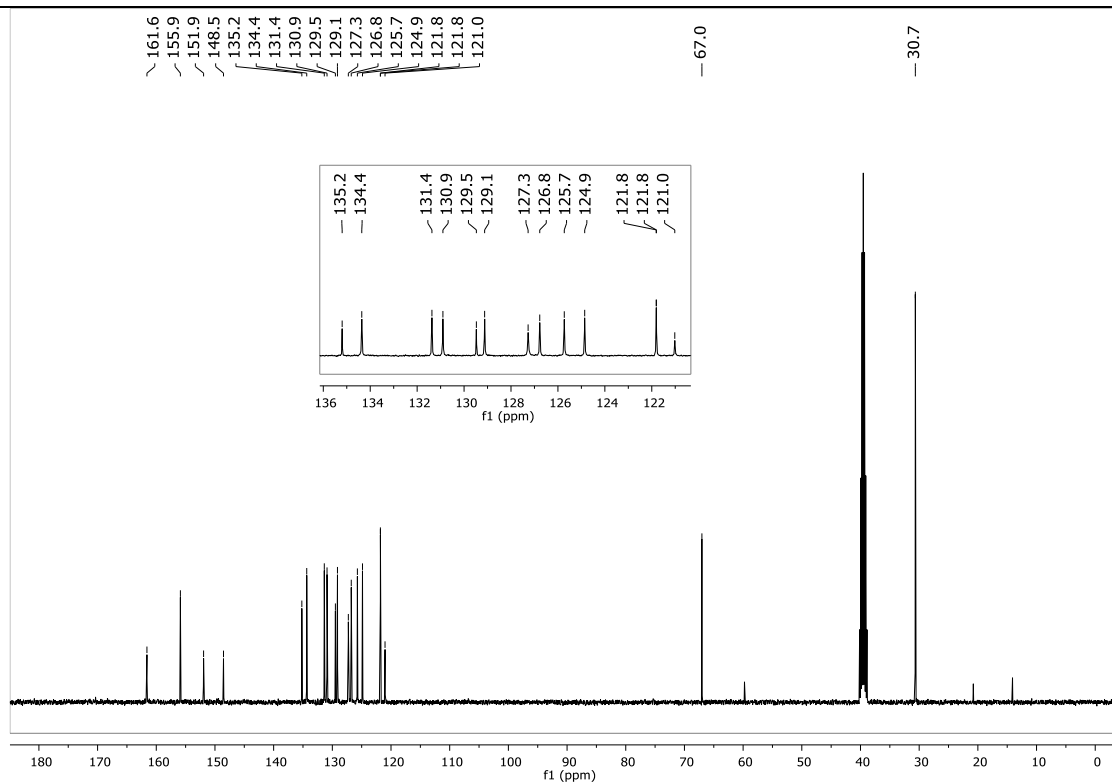


Figure S24. <sup>13</sup>C NMR (100 MHz) spectrum for compound **6i** in DMSO-d<sub>6</sub>.

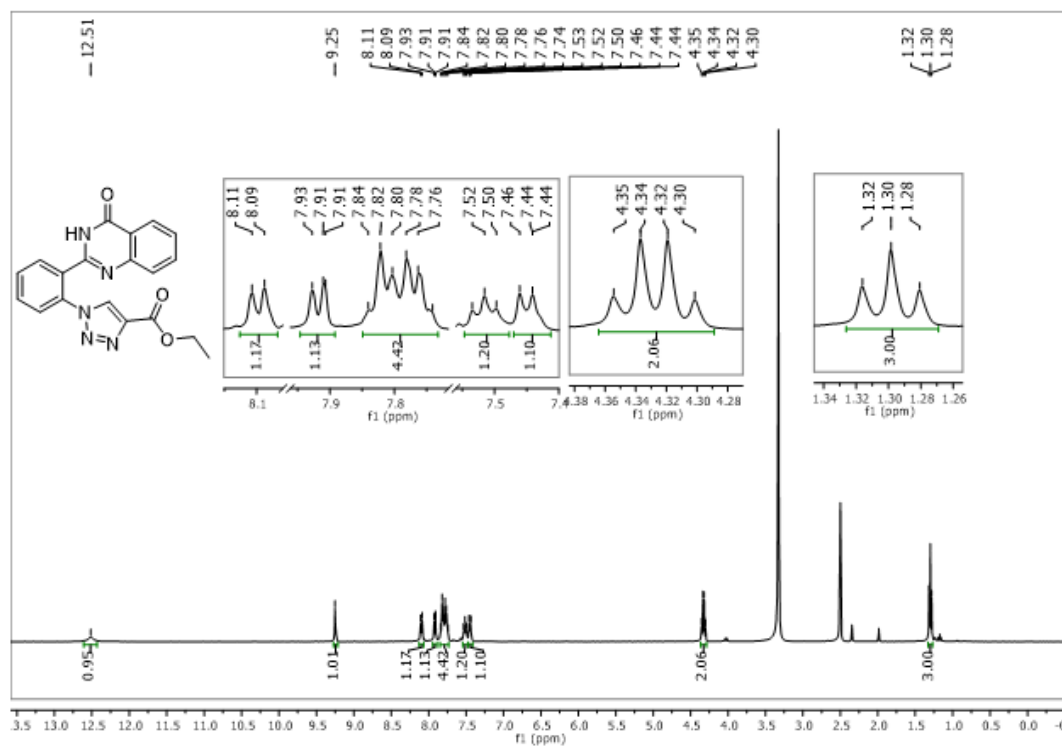


Figure S25. <sup>1</sup>H NMR (400 MHz) spectrum for compound **6l** in DMSO-d<sub>6</sub>.

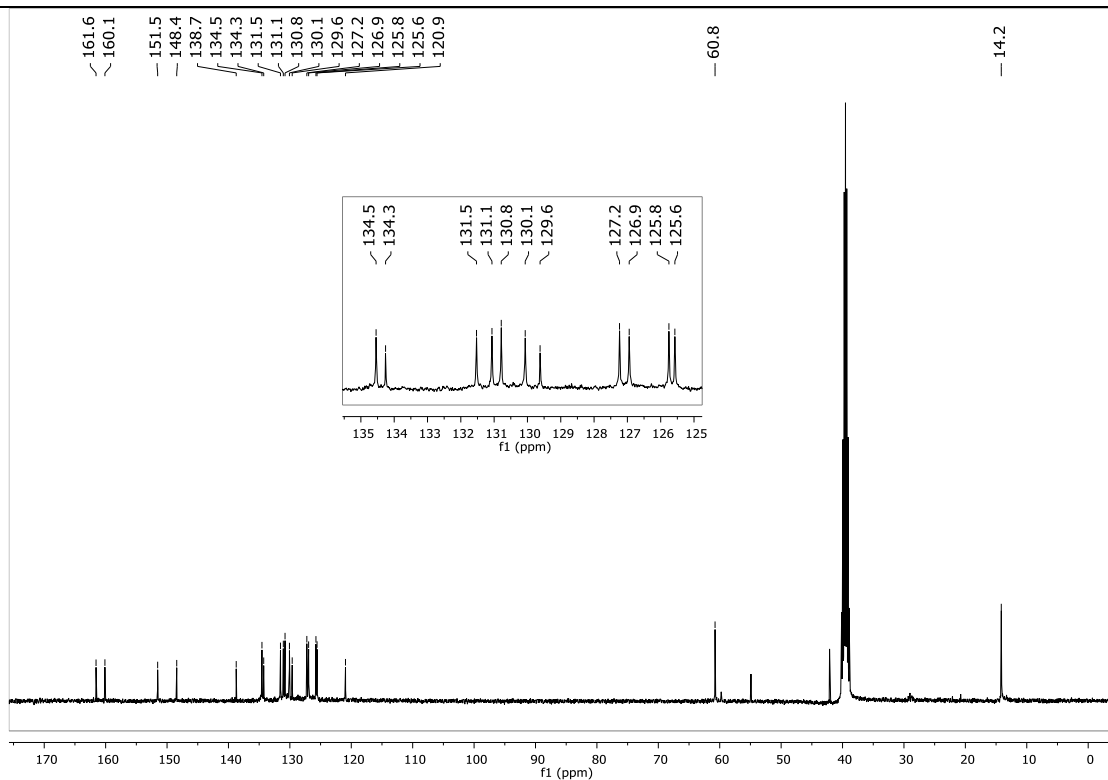


Figure S26. <sup>13</sup>C NMR (100 MHz) spectrum for compound **6l** in DMSO-d<sub>6</sub>.

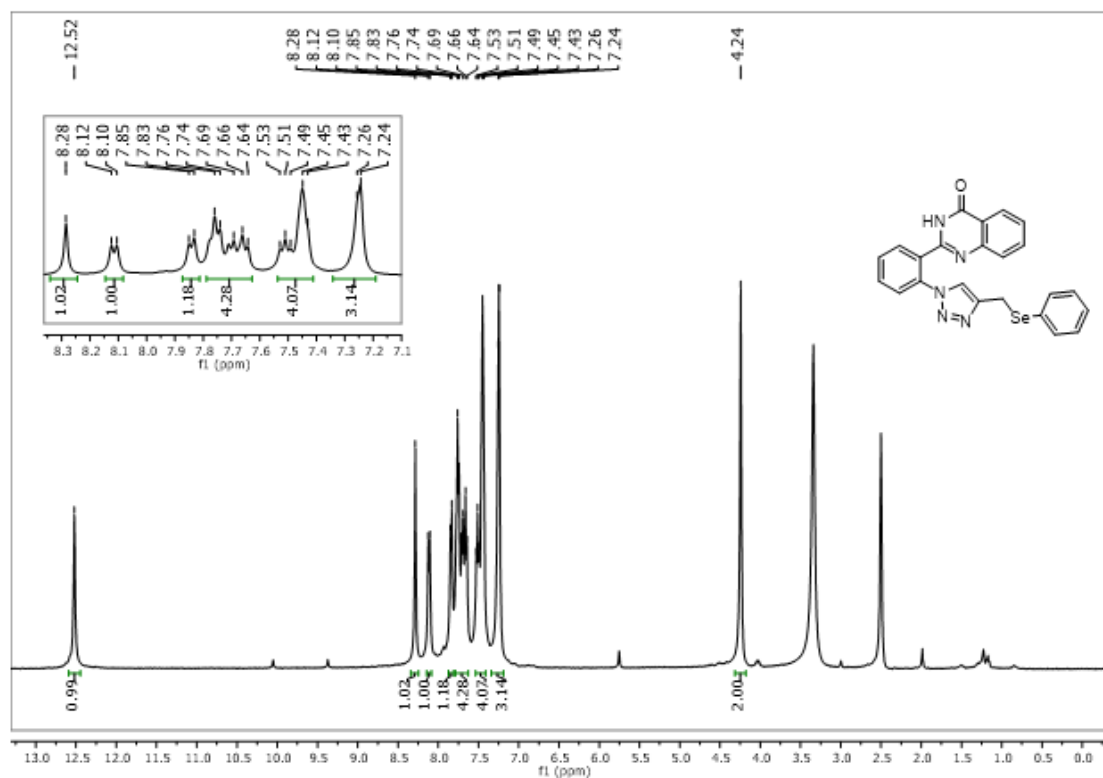


Figure S27. <sup>1</sup>H NMR (400 MHz) spectrum for compound **6m** in DMSO-d<sub>6</sub>.

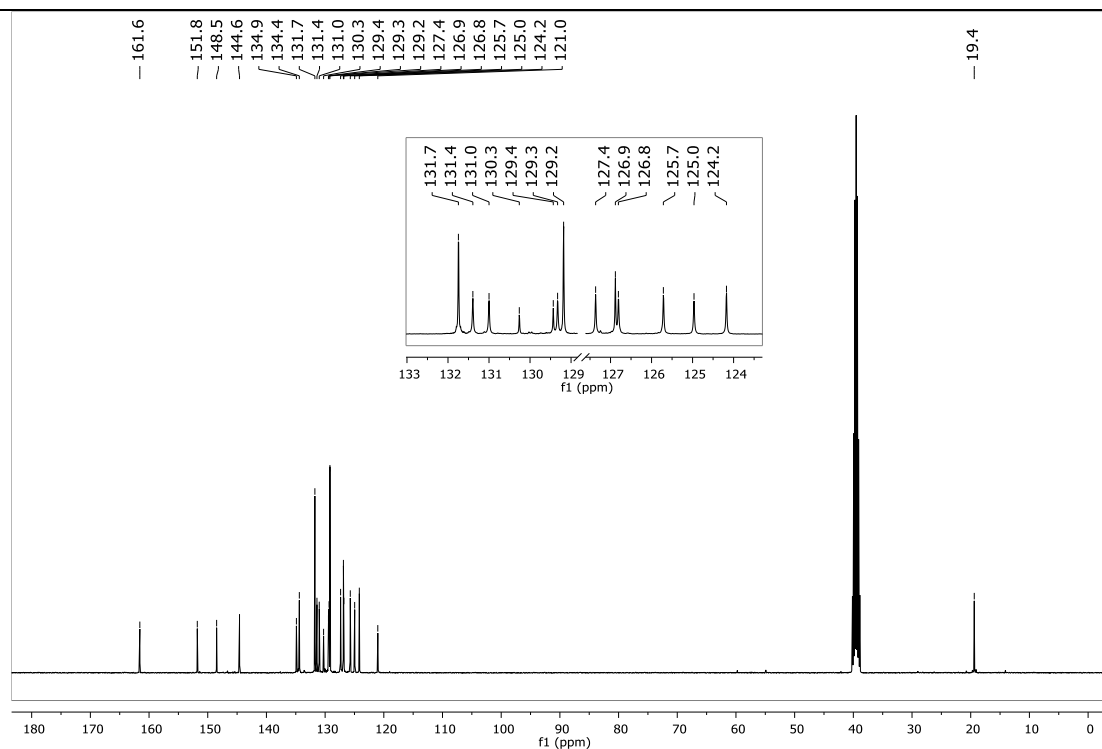


Figure S28. <sup>13</sup>C NMR (100 MHz) spectrum for compound **6m** in DMSO-d<sub>6</sub>.

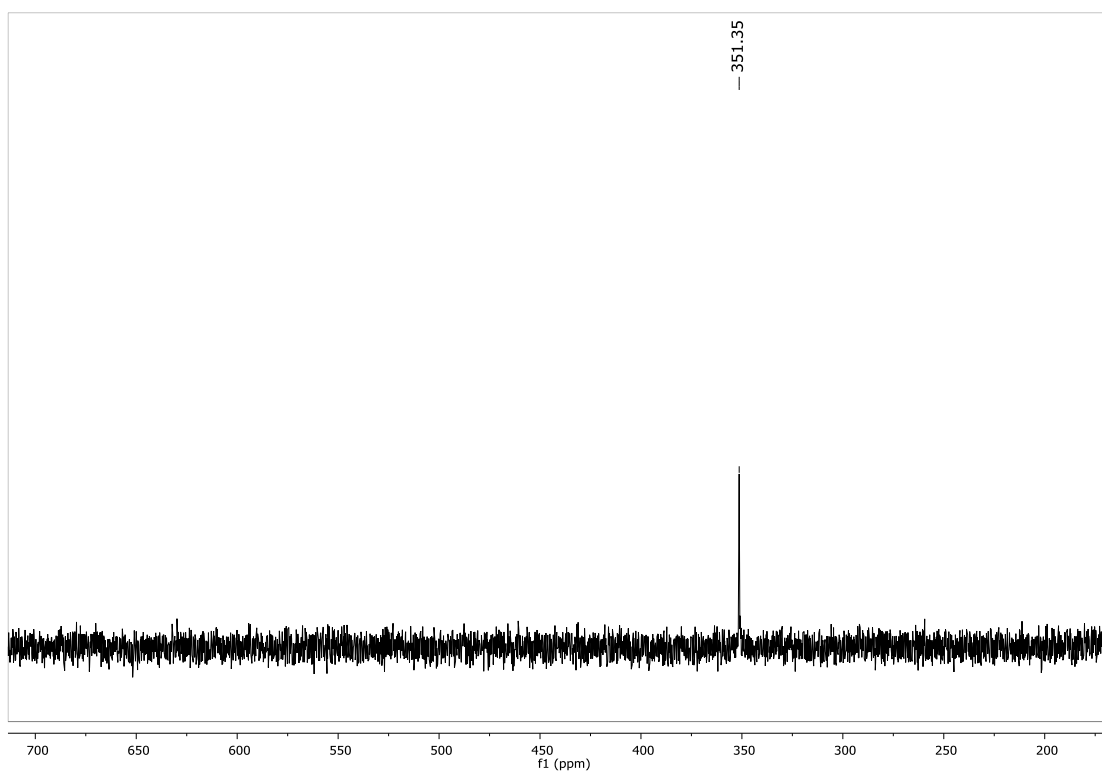


Figure S29. <sup>77</sup>Se NMR (77 MHz) spectrum for compound **6m** in DMSO-d<sub>6</sub>.

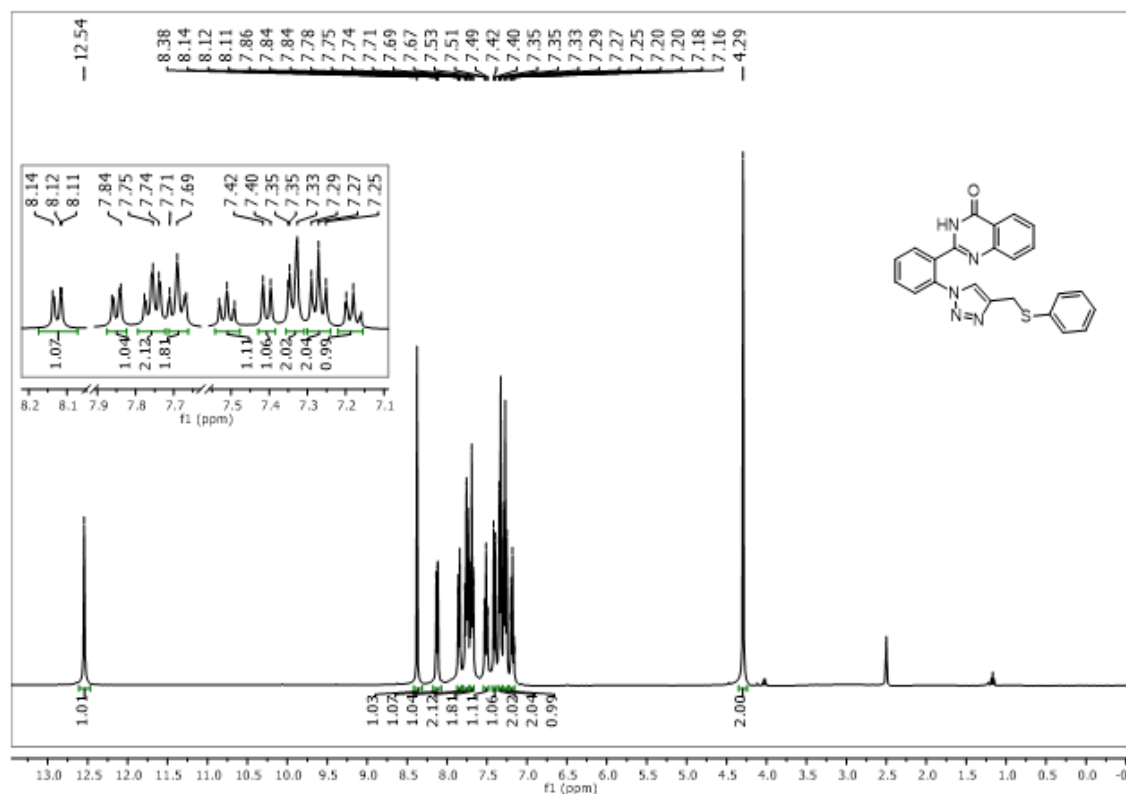


Figure S30. NMR (400 MHz) spectrum for compound **6n** in DMSO-d<sub>6</sub>.

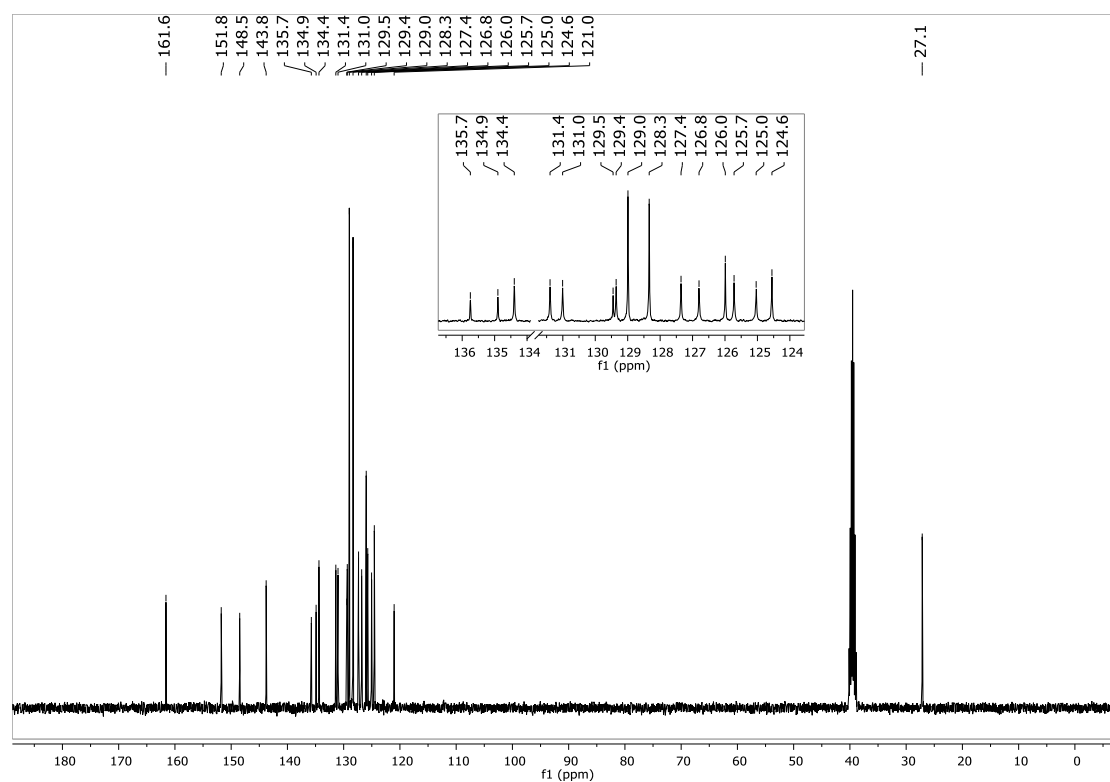
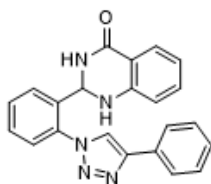
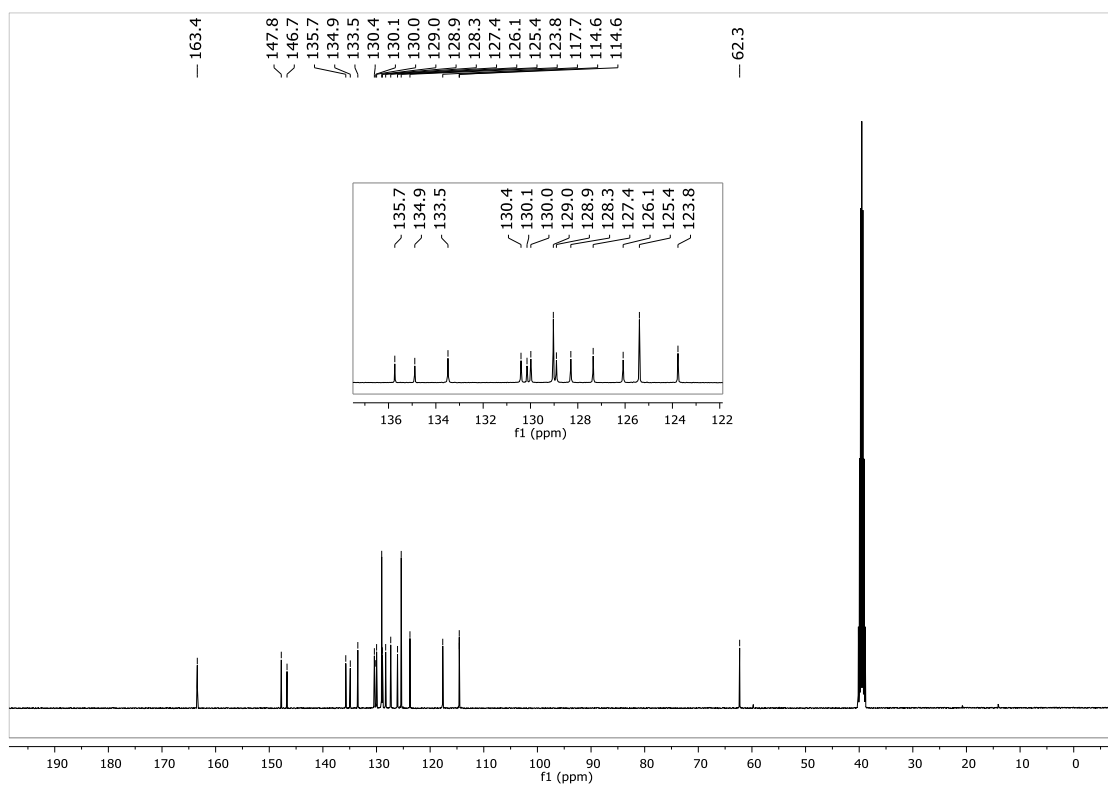


Figure S31. <sup>13</sup>C NMR (100 MHz) spectrum for compound **6n** in DMSO-d<sub>6</sub>.



**Figure S32.**  $^1\text{H}$  NMR (400 MHz) spectrum for compound **5a** in DMSO- $d_6$ .



**Figure S33.**  $^{13}\text{C}$  NMR (100 MHz) spectrum for compound **5a** in DMSO- $d_6$ .

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## References

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2. G. M. Sheldrick, *Acta Crystallogr. Sect. C Struct. Chem.*, **2015**, 71, 3–8.
3. G. M. Sheldrick, *Acta Crystallogr. Sect. A Found. Crystallogr.*, **2008**, 64, 112–122.
4. K. Brandenburg and H. Putz, Diamond - Crystal and Molecular Structure Visualization, Crystal Impact GbR-Bonn, Germany.