Supporting Information

***Org. Commun.* X:X (202X) XX-XX**

Synthesis and biological evaluation of [1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a] indoles: One-pot reaction under microwave irradiation

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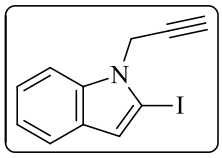
Table of Contents	Page

S1 : **Experimental Section and Spectral Data**

*Synthesis of 2-iodo-1-(prop-2-yn-1-yl)-1H-indole (**2**)*

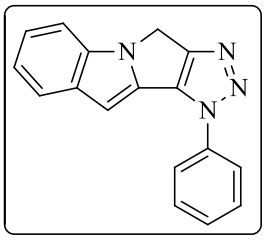


For 6 hours, a combination of 2-iodo-1*H*-indole (**1**) (5g, 0.02 mol), K_2CO_3 (0.06 mol), and propargyl bromide (0.026 mol) in DMF (60 mL) was agitated at 60 °C. After the reaction was completed, the mixture was diluted with water (50 mL) and extracted with ethyl acetate (2 50 mL). The mixed organic layer was washed with brine (2x50 mL), dried with anhydrous Na_2SO_4, and then concentrated under vacuum to yield compound **(2)** (72%). ^{1}H NMR (400MHz, DMSO-d_6; in ppm): 7.70 (d, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.35 - 7.30 (m, 1H), 7.20 (s, 1H), 7.10 - 7.05 (m, 1H), 3.75 (d, *J* = 4.0 Hz, 2H , NC*H*$_2$), 2.21 (t, *J* = 4.0 Hz, 1H, alkyne-H); ESI-MS(*m/z*): 200 $[M+H]^+$.

*2.3.3. Synthesis of 1-(aryl)-1,4-dihydro[1,2,3]triazolo-[4',5':3,4]pyrrolo-[1,2-a]indole (**4a-4p**):*

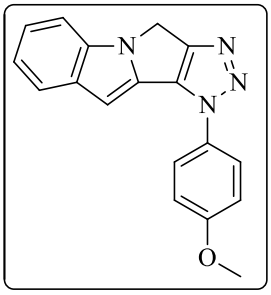
CuI (10 mol%) was added to a solution of 2-iodo-1-(prop-2-yn-1-yl)-1H-indole (2) (1.0 mmol), aryl azide (1.2 mmol), and ^{t}BuOK (3.0 mmol) in a microwave reactor vessel (10 mL). The mixture was heated at 100 °C for 30-40 minutes. TLC was used to track the course of the reaction. The reaction mixture was carefully emptied into ice-cold water (10 mL) and the product was extracted with ethyl acetate (2x15 mL) after the container was allowed to cool at room temperature. The organic layers were washed in brine and dried over anhydrous Na_2SO_4. Following filtration, the solvent was evaporated under vacuum, and the crude product produced was refined using column chromatography (hexane/ethyl acetate gradient) to yield the pure needed product.

*1-phenyl-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole(**4a**)*



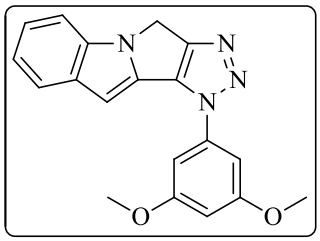
Color: White crystalline solid (74% yield); M.P: 122-124 °C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 7.71 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.60 - 7.56 (m, 2H, Ar-H), 7.52 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.43 - 7.39 (m, 3H, Ar-H), 7.33 - 7.28 (m, 1H, Ar-H), 7.21 (s, 1H, Ar-H), 7.10 - 7.05 (m, 1H, Ar-H), 5.23 (s, 2H, C*H*$_2$); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 161.24, 139.54, 136.50, 135.33, 129.67(2C), 128.40, 127.34, 124.80, 124.23(2C), 123.49, 122.32, 121.35, 110.76, 107.79, 42.23; ESI-MS(*m/z*): 273 [M+H]. Anal.Cal for $C_{17}H_{12}N_4$; C, 74.98; H, 4.44; N, 20.58; found C, 74.94; H, 4.46; N, 20.60.

*1-(4-methoxyphenyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4b**)*



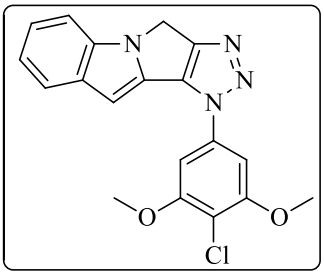
Color: White crystalline solid (71% yield); M.P: 130-132 ^{o}C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 7.78 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.70 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.54 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.35 - 7.31 (m, 1H, Ar-H), 7.19 (s, 1H, Ar-H), 7.10 - 7.06 (m, 1H, Ar-H), 6.99 (d, *J* = 8.0 Hz, 2H, Ar-H), 5.25 (s, 2H, C*H*$_2$), 3.84 (s, 3H, -OCH$_3$); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 161.66, 159.79, 139.60, 135.09, 131.39, 127.85, 126.37(2C), 124.33, 123.42, 122.52, 121.21, 114.88(2C), 110.45, 108.39, 56.21, 42.36; ESI-MS(m/z): 303 [M+H]. Anal.Cal for $C_{18}H_{14}N_4O$; C, 71.51; H, 4.67; N, 18.53; found C, 71.54; H, 4.65; N, 18.51.

*1-(3,5-dimethoxyphenyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4c**)*



Color: Pale yellow solid (68% yield), M.P: 156-158 ^{o}C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 7.72 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.60 (s, 2H, Ar-H), 7.52 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.30 - 7.26 (m, 1H, Ar-H), 7.22 (s, 1H, Ar-H), 7.11 - 7.06 (m, 1H, Ar-H), 7.02 (s, 1H, Ar-H), 5.23 (s, 2H, C*H*$_2$), 3.83 (s, 6H, 2-OCH$_3$); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 161.45, 159.24(2C), 139.67, 138.37, 135.35, 127.51, 124.26, 123.35, 122.70, 121.51, 110.72, 107.21, 104.92(2C), 102.96, 56.18(2C), 42.28; ESI-MS(*m/z*): 333 [M+H]. Anal.Cal for $C_{19}H_{16}N_4O_2$; C, 68.66; H, 4.85; N, 16.86; found C, 68.69; H, 4.83; N, 16.84.

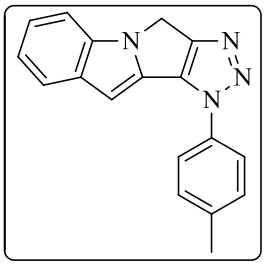
*1-(4-chloro-3,5-dimethoxyphenyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4d**)*



Color: Yellow crystalline solid (78 % yield), M.P: 164-166 ^{o}C, ^{1}H-NMR (400 MHz, DMSO-

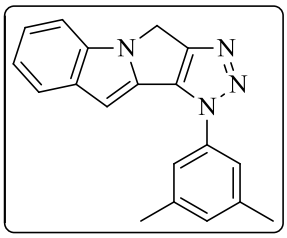
d_6; δ in ppm): 7.73 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.51 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.36 - 7.32 (m, 1H, Ar-H), 7.21 (s, 1H, Ar-H), 7.15 (s, 2H, Ar-H), 7.09 - 7.05 (m, 1H, Ar-H), 5.24 (s, 2H, CH_2), 3.85 (s, 6H, 2-OCH_3); ^{13}C-NMR (100 MHz, DMSO-d_6) 161.53, 156.57(2C), 139.30, 138.09, 135.25, 127.30, 124.19, 123.29, 122.56, 121.08, 118.42, 110.54, 107.72, 104.70(2C), 56.66(2C), 42.27; ESI-MS(*m/z*): 367 [M+H]. Anal.Cal for $C_{19}H_{15}ClN_4O_2$; C, 62.21; H, 4.12; N, 15.27; found C, 62.23; H, 4.14; N, 15.23.

*1-(p-tolyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4e**)*



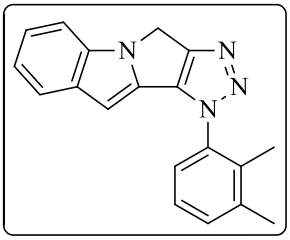
Color: White solid (70 % yield); M.P: 127-129 °C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 7.72 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.66 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.51 (d, *J* = 8.0 Hz, 1H, Ar-H), 7. 42 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.35 - 7.30 (m, 1H, Ar-H), 7.22 (s, 1H, Ar-H), 7.10 - 7.06 (m, 1H, Ar-H), 5.25 (s, 2H, CH_2), 2.31 (s, 3H, -CH_3); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 161.61, 139.38, 138.49, 136.87, 135.18, 130.05 (2C), 127.63, 125.77(2C), 124.08, 123.03, 122.08, 121.09, 110.61, 107.48, 42.37, 21.36; ESI-MS(*m/z*): 287 [M+H]. Anal.Cal for $C_{18}H_{14}N_4$; C, 75.50; H, 4.93; N, 19.57; found C, 75.55; H, 4.90; N, 19.55.

*1-(3,5-dimethylphenyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4f**)*



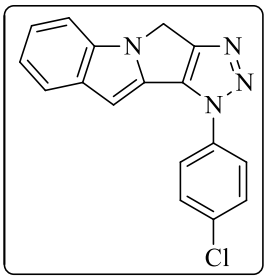
Color: Pale red solid (69 % yield); M.P: 130-132 °C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 7.71 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.52 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.45 (s, 1H, Ar-H), 7.35 - 7.30 (m, 1H, Ar-H), 7.22 (s, 1H, Ar-H), 7. 15 (s, 1H, Ar-H), 7.08 - 7.04 (m, 1H, Ar-H), 5.23 (s, 2H, CH_2), 2.37 (s, 6H, 2-CH3); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 161.47, 140.24(2C), 139.11, 137.01, 135.14, 128.47, 127.24, 125.37(2C), 124.24, 123.02, 122.07, 121.05, 110.32, 107.65, 42.47, 21.65(2C); ESI-MS(δ): 301 [M+H]. Anal.Cal for $C_{19}H_{16}N_4$; C, 75.98; H, 5.37; N, 18.65; found C, 75.94; H, 5.39; N, 18.67.

*1-(2,3-dimethylphenyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4g**)*



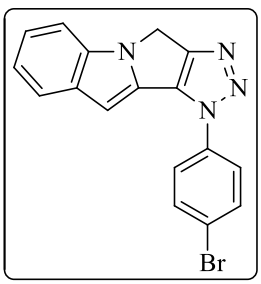
Color: Pale red solid (66 % yield); M.P: 124-126 ^{o}C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 7.73 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.51 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.44 - 7.40 (m, 2H, Ar-H), 7.35 - 7.27 (m, 3H, Ar-H), 7.22 (s, 1H, Ar-H), 7.09 - 7.05 (m, 1H, Ar-H), 5.23 (s, 2H, CH_2), 2.19 (s, 3H, -CH_3), 1.93 (s, 3H, -CH_3); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 161.57, 139.38, 138.46, 137.50, 135.43, 131.24, 128.61, 127.46, 125.82, 125.33, 124.80, 123.69, 121.62, 120.56, 110.20, 107.39, 42.41, 19.63, 15.78; ESI-MS(*m/z*): 301 [M+H]. Anal.Cal for $C_{19}H_{16}N_4$; C, 75.98; H, 5.37; N, 18.65; found C, 75.95; H, 5.39; N, 18.66.

*1-(4-chlorophenyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4h**)*



Color: Pale Yellow solid (76 % yield); M.P: 135-137 ^{o}C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 7.80 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.71 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.53 (d, *J* = 8.0 Hz, 1H, Ar-H), 7. 41 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.34 - 7.30 (m, 1H, Ar-H), 7.19 (s, 1H, Ar-H), 7.09 - 7.05 (m, 1H, Ar-H), 5.24 (s, 2H, CH_2); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 161.57, 139.38, 136.41, 135.29, 134.27, 128.62(2C), 127.32, 125.29(2C), 124.41, 123.64, 122.08, 121.36, 110.91, 107.55, 42.47; ESI-MS(*m/z*): 307 [M+H]. Anal.Cal for $C_{17}H_{11}ClN_4$; C, 66.56; H, 3.61; N, 18.26; found C, 66.53; H, 3.63; N, 18.28.

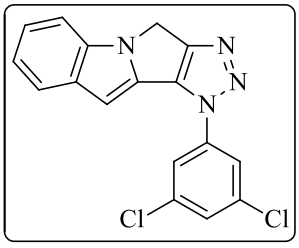
*1-(4-bromophenyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4i**)*



Color: White solid (67 % yield); M.P: 143-145 ^{o}C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 7.73 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.66 - 7.60 (m, 4H, Ar-H), 7.51 (d, *J* = 8.0 Hz, 1H, Ar-

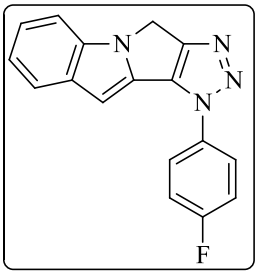
H), 7.34 - 7.29 (m, 1H, Ar-H), 7.21 (s, 1H, Ar-H), 7.10-7.04 (m, 1H, Ar-H), 5.24 (s, 2H, CH_2); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 161.30, 139.51, 135.53, 133.88, 131.23(2C), 127.36, 124.80, 124.11(2C), 123.07, 122.42, 121.22, 120.74, 110.64, 107.56, 42.33; ESI-MS(*m/z*): 351 [M+H] & 353[M+3H]. Anal.Cal for $C_{17}H_{11}BrN_4$; C, 58.14; H, 3.16; N, 15.95; found C, 58.17; H, 3.14; N, 15.93.

*1-(3,5-dichlorophenyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4j**)*



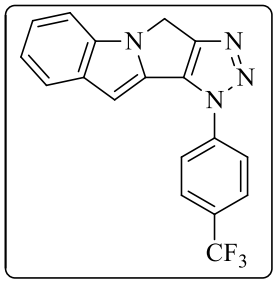
Color: Pale Yellow solid (77 % yield); M.P: 151-153 °C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 7.82 (s, 2H, Ar-H), 7.72 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.55 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.42 (s, 1H, Ar-H), 7.33 - 7.27 (m, 1H, Ar-H), 7.23 (s, 1H, Ar-H), 7.11-7.06 (m, 1H, Ar-H), 5.26 (s, 2H, CH_2); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 161.73, 139.38, 135.44, 134.48, 131.43(2C), 127.42, 124.81, 124.12(2C), 123.33, 122.52, 121.31, 120.22, 110.98, 107.12, 42.22; ESI-MS(*m/z*): 341 [M+H]. Anal.Cal for $C_{17}H_{10}Cl_2N_4$; C, 59.84; H, 2.95; N, 16.42; found C, 59.81; H, 2.94; N, 16.45.

*1-(4-fluorophenyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4k**)*



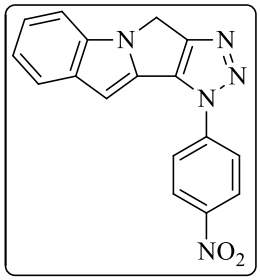
Color: Pale red solid (73 % yield); M.P: 127-129 °C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 8.10 (d, *J* = 8.0 Hz, 2H), 7.90 (d, *J* = 8.0 Hz, 2H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.37 - 7.33 (m, 1H), 7.21 (s, 1H), 7.11 - 7.06 (m, 1H), 5.27 (s, 2H, CH_2); ESI-MS(*m/z*): 291 [M+H]. Anal.Cal for $C_{17}H_{11}FN_4$; C, 70.34; H, 3.82; N, 19.30; found C, 70.37; H, 3.80; N, 19.32.

*1-(4-(trifluoromethyl)phenyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4l**)*



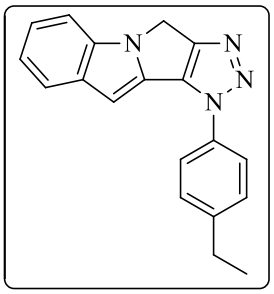
Color: Pale red solid (67 % yield), ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 8.16 (d, *J* = 8.0 Hz, 2H, Ar-H), 8.05 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.75 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.52 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.38 - 7.33 (m, 1H, Ar-H), 7.22 (s, 1H, Ar-H), 7.11 - 7.05 (m, 1H, Ar-H), 5.26 (s, 2H, C*H*$_2$); ESI-MS(*m/z*): 341 [M+H]. Anal.Cal for $C_{18}H_{11}F_3N_4$; C, 63.53; H, 3.26; N, 16.46; found C, 63.56; H, 3.28; N, 16.42.

*1-(4-nitrophenyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4m**)*



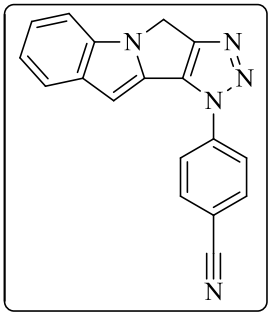
Color: Yellow solid (80 % yield); M.P: 150-152 ^{o}C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 8.41 (d, *J* = 8.0 Hz, 2H), 8.21 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.36 - 7.31 (m, 1H), 7.21 (s, 1H), 7.10 - 7.06 (m, 1H), 5.27 (s, 2H, C*H*$_2$); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 161.77, 147.65, 140.19, 139.14, 135.03, 127.55, 126.17(2C), 124.07, 123.45(2C), 122.95, 122.08, 121.08, 110.72, 107.12, 42.37; ESI-MS(*m/z*): 318 [M+H]. Anal.Cal for $C_{17}H_{11}N_5O_2$; C, 64.35; H, 3.49; N, 22.07; found C, 64.38; H, 3.47; N, 22.05.

*1-(4-ethylphenyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4n**)*



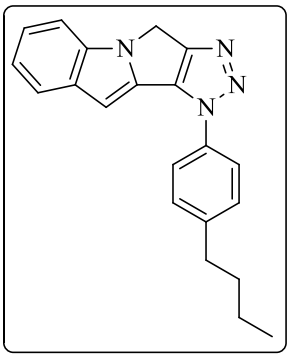
Color: White red solid (72 % yield); M.P: 134-136 ^{o}C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 7.70 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.60 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.50 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.38 - 7.34 (m, 1H, Ar-H), 7.28 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.18 (s, 1H, Ar-H), 7.09-7.05 (m, 1H, Ar-H), 5.23 (s, 2H, C*H*$_2$), 2.28 (q, *J* = 4.0 Hz, 2H. -CH_2), 1.68 (t, *J* = 4.0 Hz, 2H. –CH_3); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 161.73, 141.27, 139.41, 138.10, 135.21, 129.61(2C), 127.83, 127.23(2C), 124.81, 123.66, 122.53, 121.24, 110.53, 107.28, 42.33, 23.20, 13.78; ESI-MS(*m/z*): 301 [M+H]. Anal.Cal for $C_{19}H_{16}N_4$; C, 75.98; H, 5.37; N, 18.65; found C, 75.94; H, 5.39; N, 18.67.

*4-([1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indol-1(4H)-yl)benzonitrile (**4o**)*



Color: White solid (72 % yield); M.P: 141-143 ^{o}C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 7.80 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.72 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.50 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.41 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.36 - 7.31 (m, 1H, Ar-H), 7.21 (s, 1H, Ar-H), 7.11 - 7.06 (m, 1H, Ar-H), 5.24 (s, 2H, C*H*$_2$); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 161.48, 139.42, 138.12, 135.38, 127.63, 127.11(2C), 126.10(2C), 124.19, 123.32, 122.42, 121.43, 119.53, 117.54, 110.41, 107.25, 42.22; ESI-MS(*m/z*): 298 [M+H]. Anal.Cal for $C_{18}H_{11}N_5$; C, 72.72; H, 3.73; N, 23.56; found C, 72.76; H, 3.71; N, 23.54.

*1-(4-butylphenyl)-1,4-dihydro-[1,2,3]triazolo[4',5':3,4]pyrrolo[1,2-a]indole (**4p**)*



Color: Pale Yellow solid (66 % yield), M.P: 146-148 ^{o}C, ^{1}H-NMR (400 MHz, DMSO-d_6; δ in ppm): 7.72 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.64 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.50 (d, *J* = 8.0 Hz, 1H, Ar-H), 7.35 - 7.30 (m, 1H, Ar-H), 7.24 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.18 (s, 1H, Ar-H), 7.10 - 7.05 (m, 1H, Ar-H), 5.25 (s, 2H, C*H*$_2$), 2.68 (t, *J* = 4.0 Hz, 2H, -CH_2), 1.68 - 1.58 (m, 2H, -CH_2), 1.38 - 1.29 (m, 2H, -CH_2), 0.94 (t, *J* = 4.0 Hz, 3H, -CH_3); ^{13}C-NMR (100 MHz, DMSO-d_6) δ 161.37, 139.33, 138.14(2C), 135.78, 130.01, 129.14(2C), 128.07, 127.03, 124.22, 123.02, 122.38, 121.44, 110.58, 107.53, 42.47, 34.21, 32.89, 21.65, 13.70; ESI-MS(*m/z*): 329 [M+H]. Anal.Cal for $C_{21}H_{20}N_4$; C, 76.80; H, 6.14; N, 17.06; found C, 76.84; H, 6.16; N, 17.00.

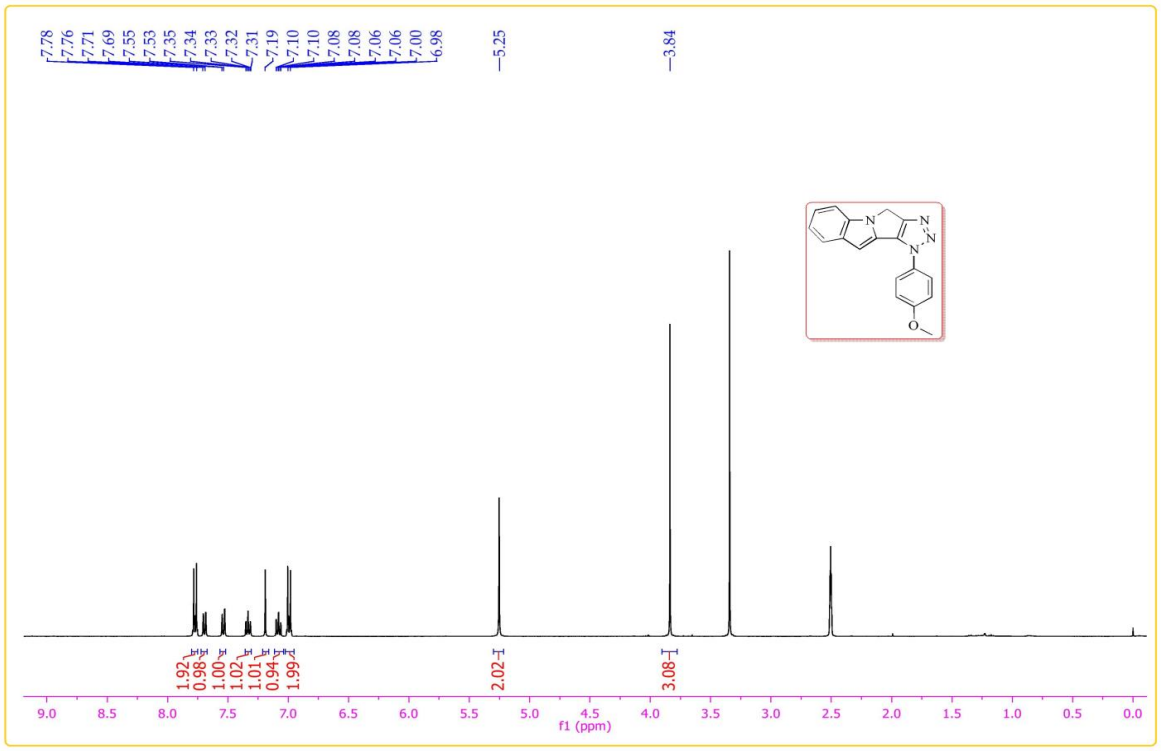


Figure S1: ^{1}H-NMR Spectrum of **4b**

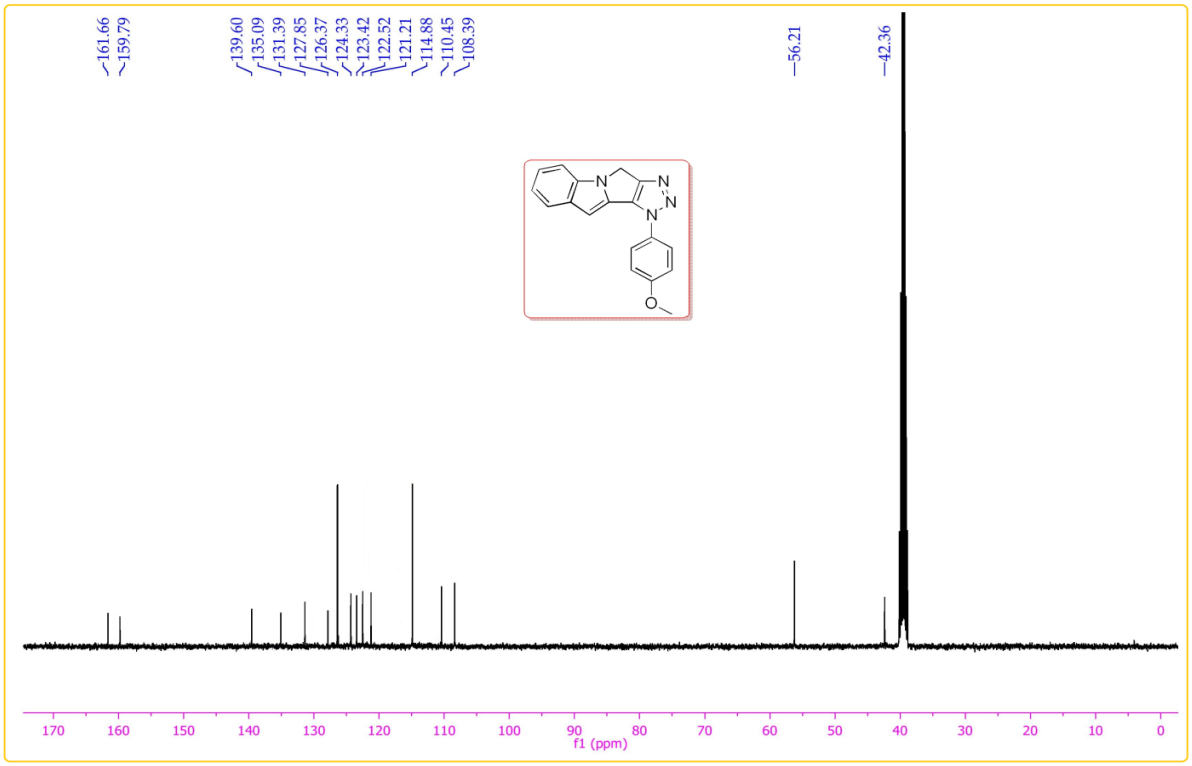


Figure S2: ^{13}C-NMR Spectrum of **4b**

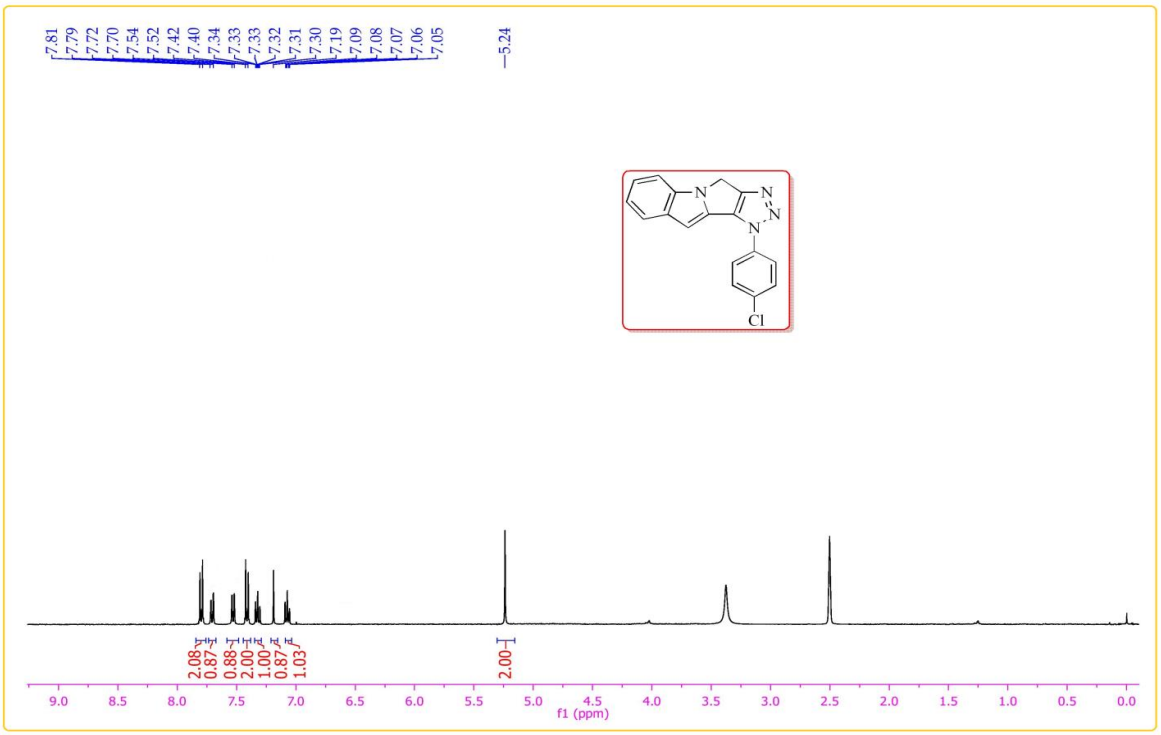


Figure S3: ^{1}H-NMR Spectrum of **4h**

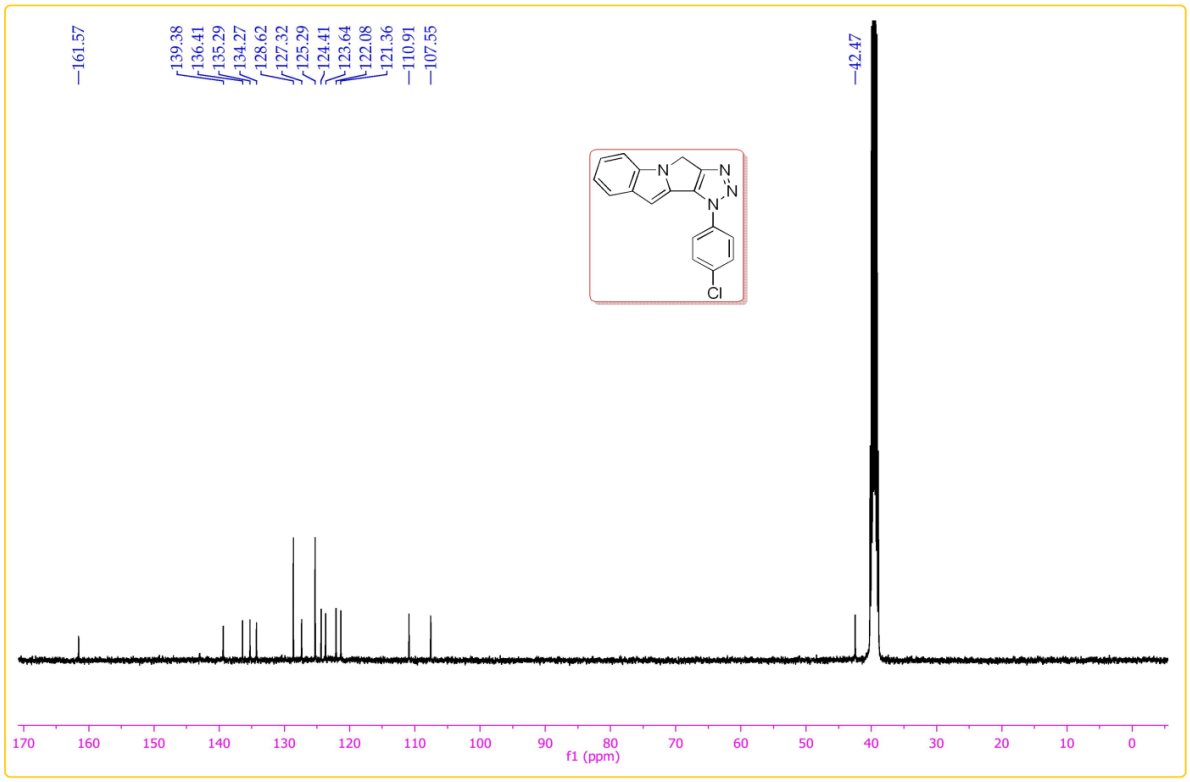


Figure S4: ^{13}C-NMR Spectrum of **4h**

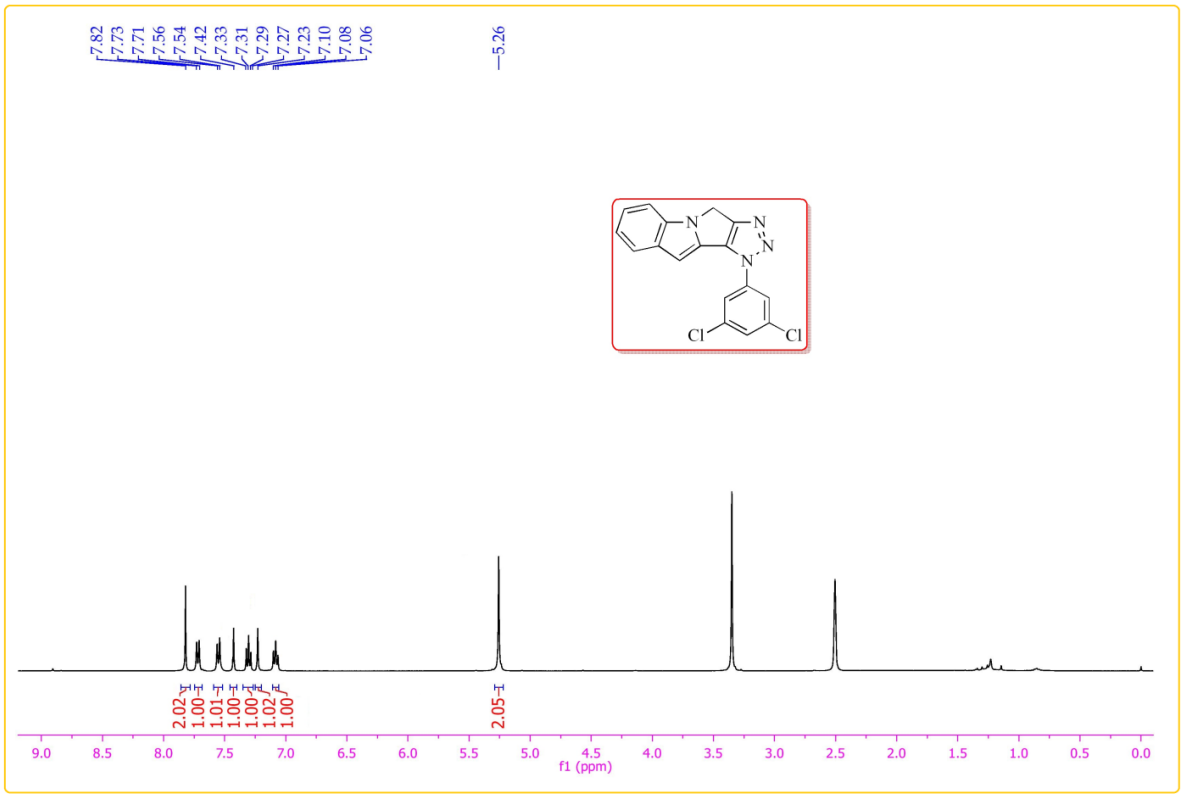


Figure S5: ^{1}H-NMR Spectrum of **4j.**

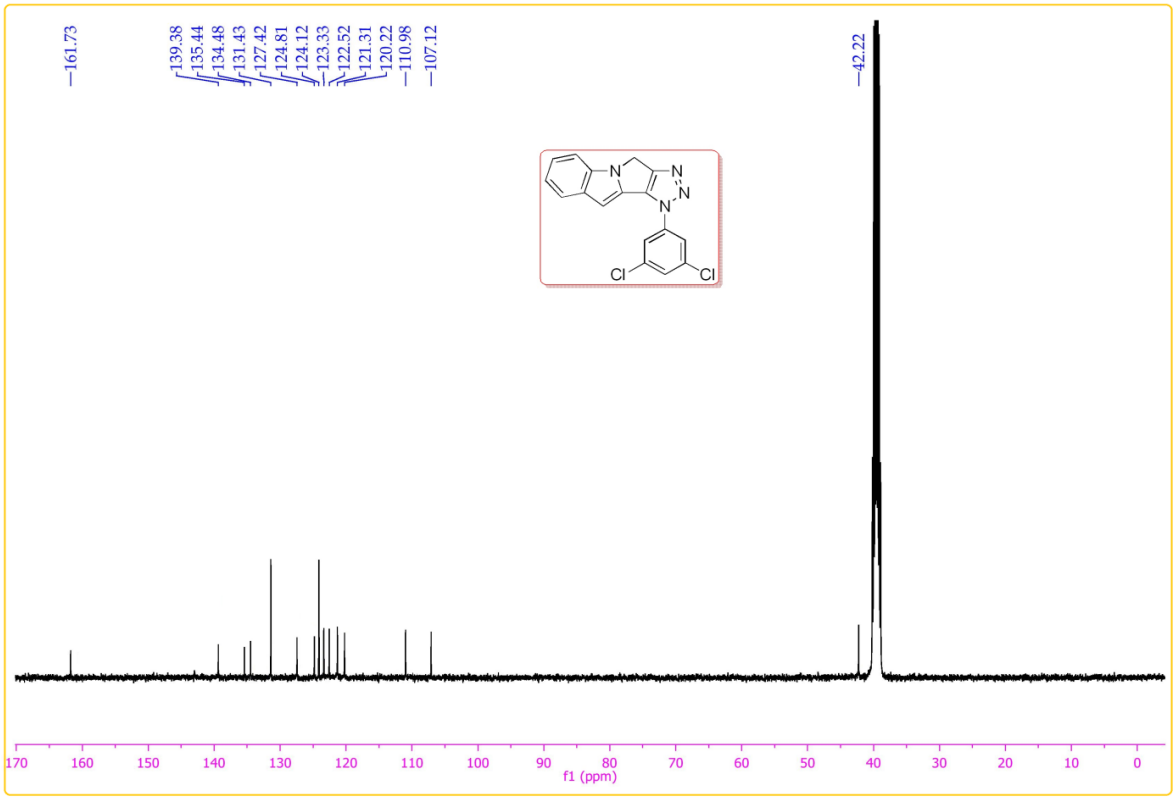


Figure S6: ^{13}C-NMR Spectrum of **4j**

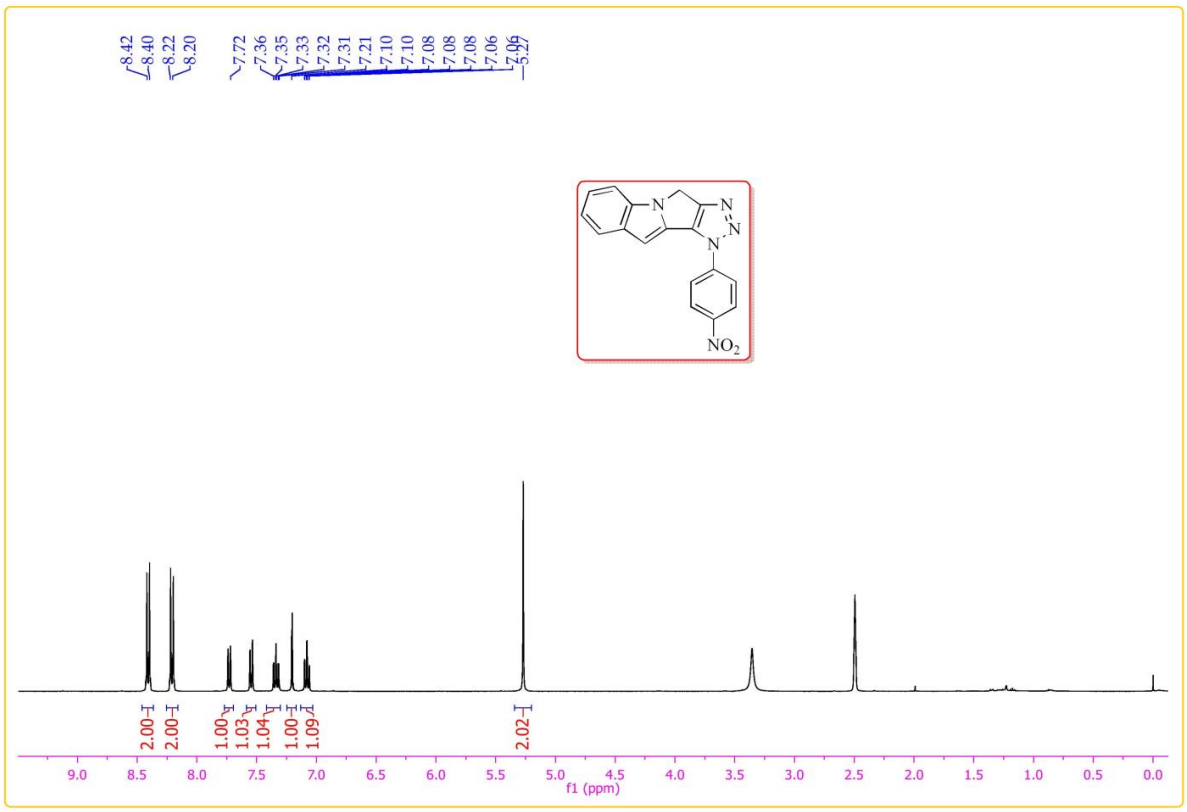


Figure S7: ^{1}H-NMR Spectrum of **4m**

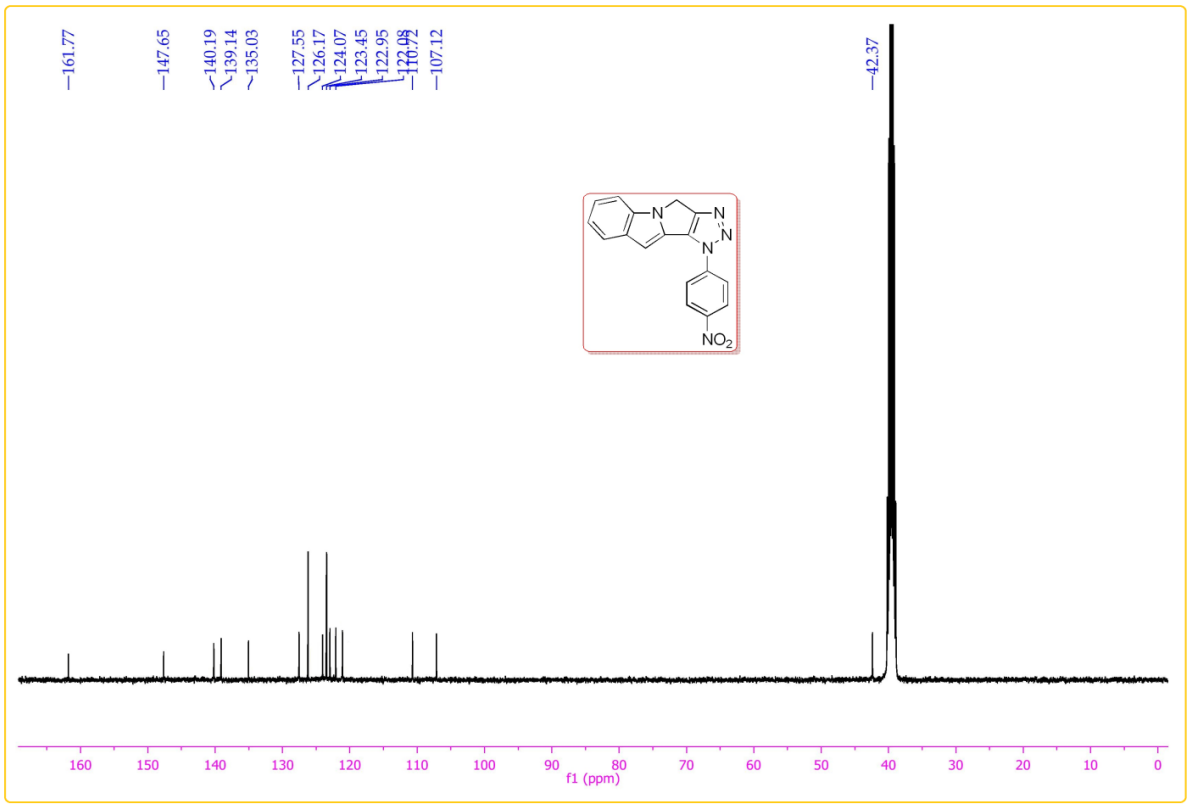


Figure S8: ^{13}C-NMR Spectrum of **4m**

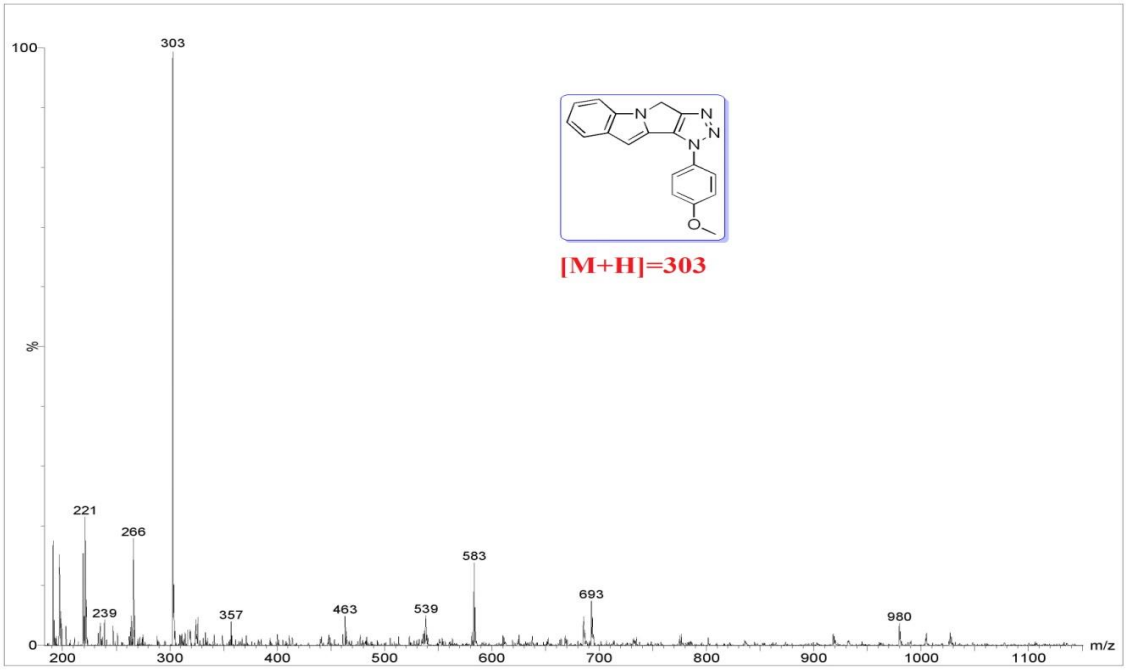


Figure S9: ESI-MS Spectrum of **4b**

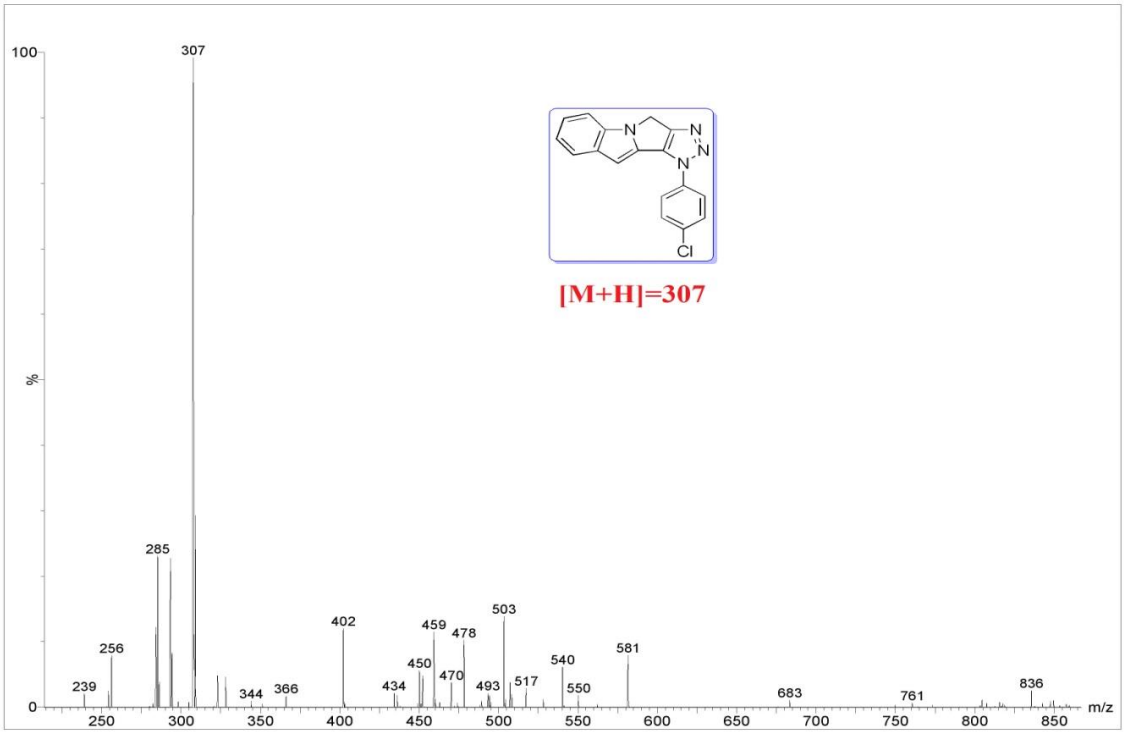


Figure S10: ESI-MS Spectrum of **4h**

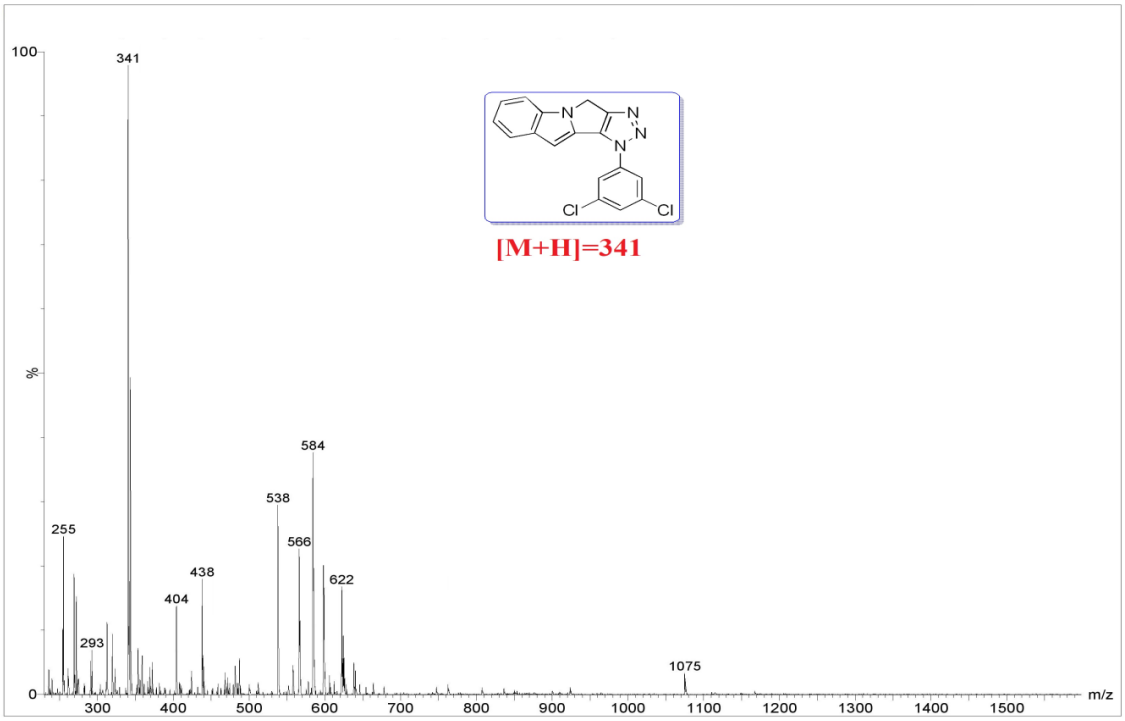


Figure S11: ESI-MS Spectrum of **4j**

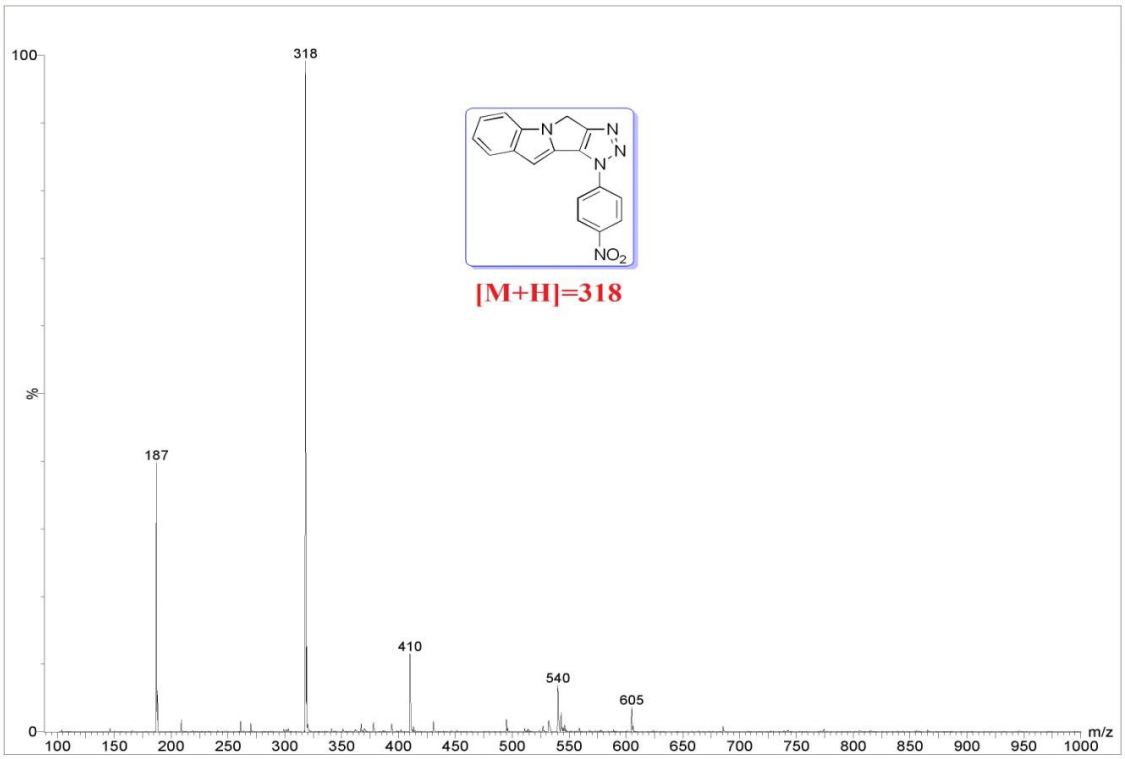


Figure S12: ESI-MS Spectrum of **4m**