Electronic Supplementary Information

Four-component, three-step cascade reaction: An effective synthesis of indazole fused triazolo[5,1-*c*]quinoxalines

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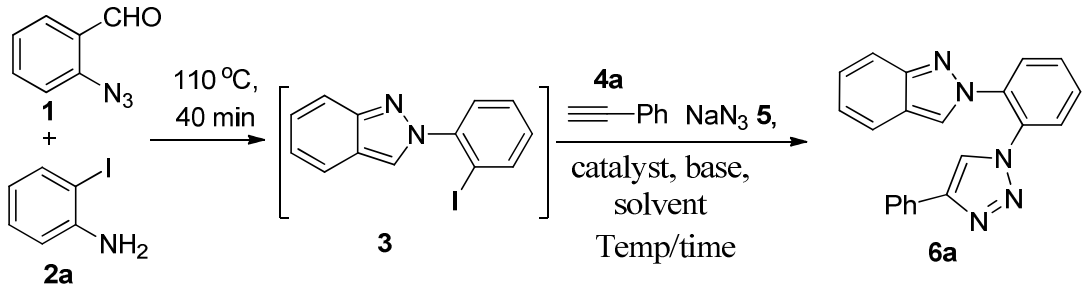
1. Optimization Data:

Initially, CuI and K_2CO_3 in DMF at 120 °C. The reaction was completedwithin 2 h affording the desired 2-(2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)phenyl)-2*H*-indazole**6a** in 88% yield (entry 1, Table 1). The use of other Cu catalysts, e.g. $Cu(OAc)_2$, $Cu(OAc)_2$. H_2O and CuClwas found to be less effective (entries 2-4, Table 1). The use of other bases e.g. Cs_2CO_3,Na_2CO_3 and DBUwas found to be less effective (entries5-7, Table 1). Further, the solvents, such as DMSO, CH_3CN, toluene and ethanol (entries 8-11, Table 1) were also studied but found to be less effective then DMF. By lowering the reaction temperature to 90 °C led to poor substrate conversion (entry 12, Table 1). By lowering or increased the reaction time led to poor yield (entry 13 and 14, Table 1).Overall, the combination ofCuI and K_2CO_3 in DMF at 120 °C under air for 2 h (entry 1, Table 1) is the optimised condition for the synthesis of **6a**.

2. Table S1: Optimization of reaction conditionsfor the formation of intermediate **6a**[a]

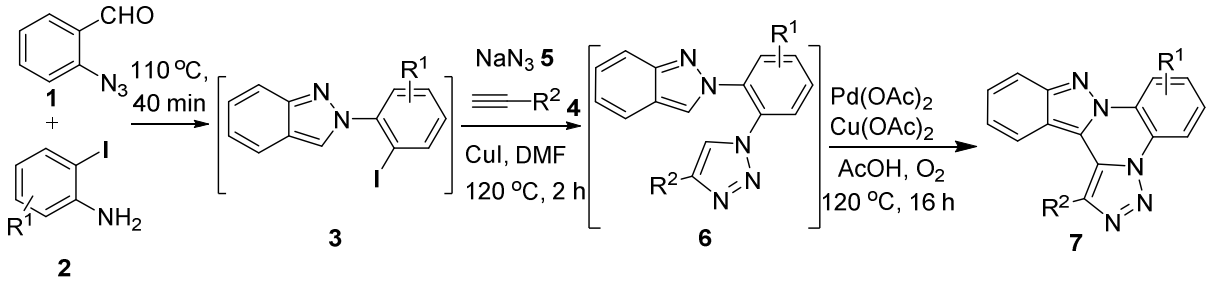


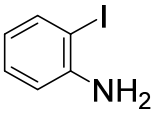
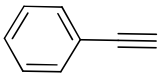
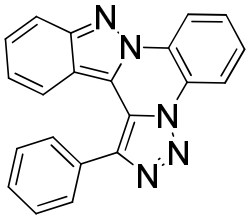
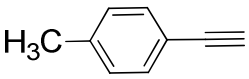
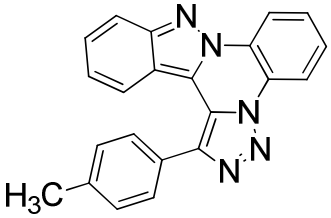
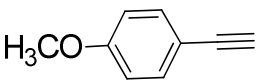
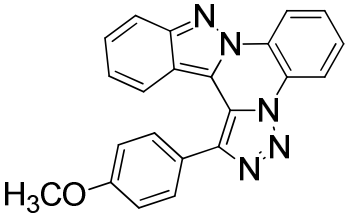
Entry	Catalyst	Base	Solvent	Temp (°C)/ Time (h)	% Yield[b]
1	CuI	K_2CO_3	DMF	2/120	88
2	$Cu(OAc)_2$	K_2CO_3	DMF	2/120	55
3	$Cu(OAc)_2$. H_2O	K_2CO_3	DMF	2/120	42
4	CuCl	K_2CO_3	DMF	2/120	52
5	CuI	Cs_2CO_3	DMF	2/120	55
6	CuI	Na_2CO_3	DMF	2/120	60
7	CuI	DBU	DMF	2/120	45
8	CuI	K_2CO_3	DMSO,	2/120	70
9	CuI	K_2CO_3	CH_3CN,	2/85	52
10	CuI	K_2CO_3	toluene	2/111	60
11	CuI	K_2CO_3	ethanol	2/120	50
12	CuI	K_2CO_3	DMF	2/90	65
13	CuI	K_2CO_3	DMF	1/120	54

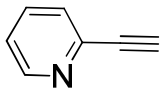
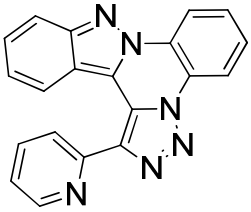
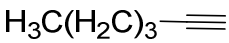
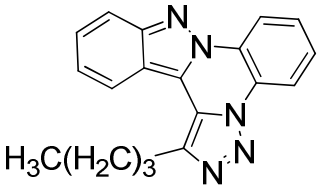
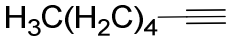
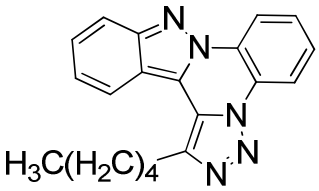
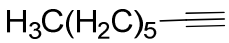
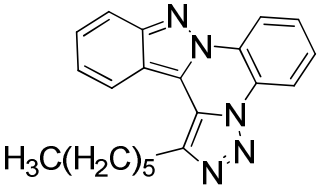
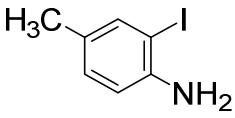
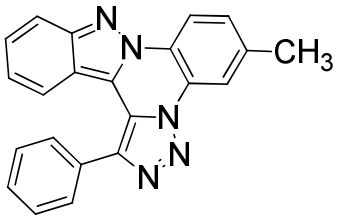
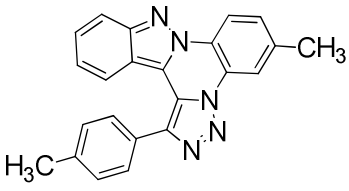
14	CuI	K_2CO_3	DMF	3/120	78

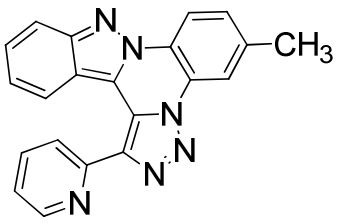
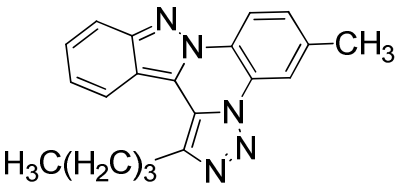
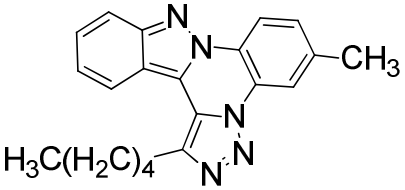
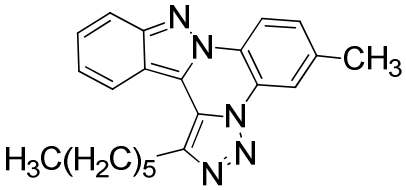
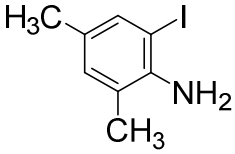
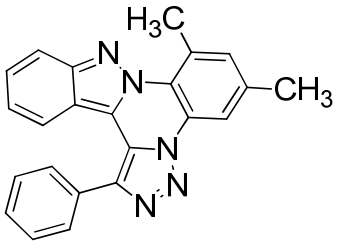
[a]Reaction conditions: **1a** (0.67 mmol) and **2a** (0.67 mmol) was heated at 110 °C, 40 min, and then **4a** (0.67 mmol), **5** (0.67 mmol), catalyst (10 mol%), base (0.81 mmol), solvent (3 mL), air. [b]Isolated yields.

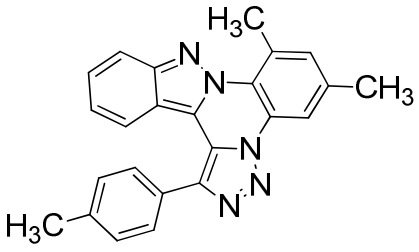
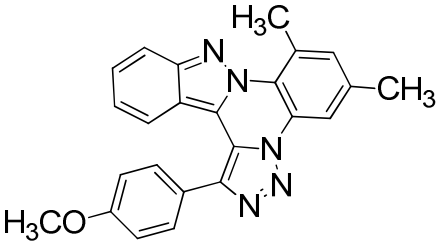
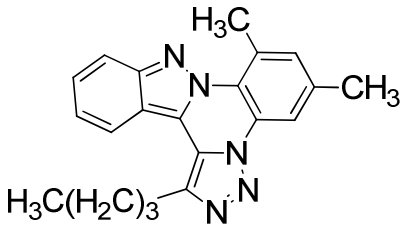
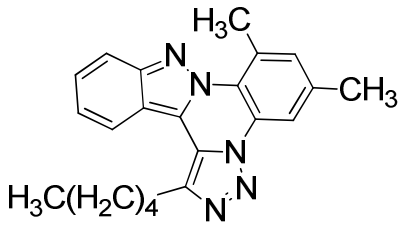
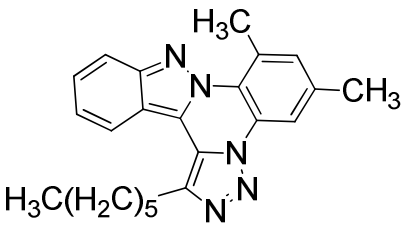
3. Table S2: One-pot sequential cascade synthesis of indazole fused triazolo[5,1-*c*]quinoxalines (7):

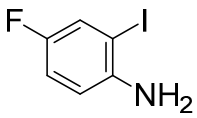
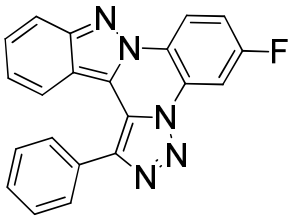
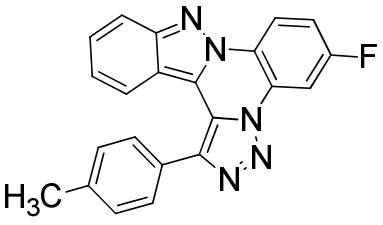
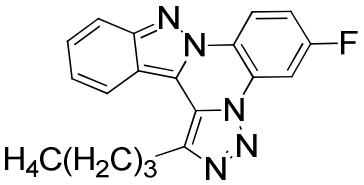
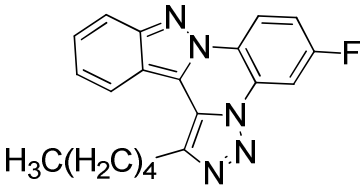


Entry	*o*-Iodoaniline (2)	Acetylene (4)	Indazole fused triazolo[5,1 c]quinoxalines (7)	Yield[b] (%)
1	 **2a**	 **4a**	 **7a**	71
2	**2a**	 **4b**	 **7b**	68
3	**2a**	 **4c**	 **7c**	68

4	**2a**	 **4d**	 **7d**	65
5	**2a**	 **4e**	 **7e**	62
6	**2a**	 **4f**	 **7f**	68
7	**2a**	 **4g**	 **7g**	67
8	 **2b**	**4a**	 **7h**	70
9	**2b**	**4b**	 **7i**	66

10	**2b**	**4d**	 **7j**	65
11	**2b**	**4e**	 **7k**	65
12	**2b**	**4f**	 **7l**	68
13	**2b**	**4g**	 **7m**	68
14	 **2c**	**4a**	 **7n**	65
15				60

	2c	**4b**	 **7o**	
16	**2c**	**4c**	 **7p**	65
17	**2c**	**4e**	 **7q**	65
18	**2c**	**4f**	 **7r**	62
19	**2c**	**4g**	 **7s**	60

20	 **2d**	**4a**	 **7t**	61
21	**2d**	**4b**	 **7u**	62
22	**2d**	**4e**	 **7v**	62
23	**2d**	**4f**	 **7w**	65

[a]Reaction conditions: **1a** (0.67 mmol) and **2a** (0.67 mmol) was heated at 110 °C, 40 min, and then **4a** (0.67 mmol), **5** (0.67 mmol), CuI (10 mol%), K_2CO_3 (0.81 mmol), DMF (3 mL), air, 2 h followed by Pd catalyst (10 mol %), $Cu(OAc)_2$ (1.01 mmol), AcOH (2.03 mmol), O_2additive at 120 ^oC for 16 h. [b]Isolated yields.

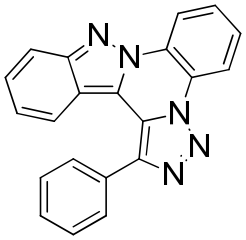
Chemistry

General methods: Unless stated otherwise, solvents and chemicals were obtained from commercial sources and were used without further purification. Reactions were monitored by thin layer chromatography (TLC) on silica gel plates (60 F254), visualizing with ultraviolet light or iodine spray. Flash chromatography was performed on silica gel (100-200 mesh) using hexane and ethyl acetate. ^{1}Hand ^{13}C NMR spectra were determined in $CDCl_3$, DMSO-d_6 and TFA solutions by using 400 or 100 MHz spectrometers, respectively. Proton chemical shifts (δ) are relative to tetramethylsilane (TMS, δ = 0.00) as internal standard and expressed in ppm. Spin multiplicities are given as s (singlet), d (doublet), t (triplet) and m (multiplet) as well as b (broad). Coupling constants (*J*) are given in hertz. Melting points were determined using a melting point apparatus and are uncorrected. MS spectra were obtained on a mass spectrometer. HRMS data were recorded by electrospray ionization with a Q-TOF mass analyzer. 2-Azidobenzaldehyde[1] were prepared according to the known procedure.

General Procedure for theOne-pot sequential cascade synthesis of indazole fused triazolo[5,1-*c*]quinoxalines (7):

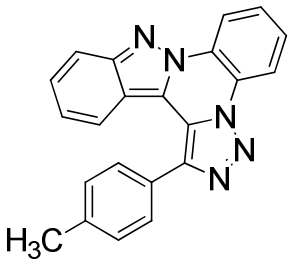
2-Azidobenzaldehyde (**1a)** (0.67 mmol), 2-Iodoaniline (**2a)** (0.67 mmol) were taken in a oven dried Schlenck tube and it was closed with nitrogen balloon and stirred for 40 minat 110 ^{o}C. The completion of first step was monitored by TLC. Upon cooling to room temperature, Alkyne **(4)** (0.67 mmol), NaN_3 **(5)** (0.67 mmol), CuI (10 mol%), K_2CO_3 (0.81 mmol) and DMF (3 ml) solvent were added in same pot and the resulting reaction mixture was heated at 120 ^{o}C for 2 h under open air. After completion of the reaction was monitored by TLC, to the same pot $Pd(OAc)_2$ (10 mol%), $Cu(OAc)_2$ (1.01 mmol), AcOH (2.03 mmol) was added. Subsequently, the vessel was placed under vacuum and backfilled with O_2. The resulting reaction mixture was stirred at 120 ^{o}C for16h. Then, it was quenched with saturated NH_4Cl (10 mL) and extracted with EtOAc (10 mL × 3). The combined EtOAc layer was collected, dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified using column chromatography over silica gel with EtOAc / hexane to give desired product of (**7)**

1-Phenylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7a):



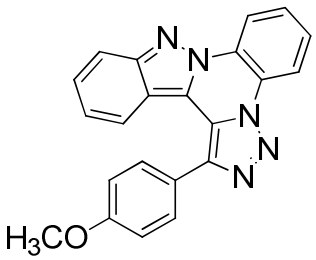
Yellow solid; Yield:71%; mp: 198-201 °C; R_f= 0.4 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.81 (d, *J* = 7.6 Hz, 2H), 7.89 (d, *J* = 8.8 Hz, 1H), 7.80-7.75 (m, 4H), 7.62 (d, *J* = 6.4 Hz, 3H), 7.42 (t, *J* = 7.6 Hz, 1H), 6.99 (t, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$ -TFA-*d*): δ 159.7, 149.2, 131.0, 130.8, 130.6 (2C), 129.6, 129.4, 129.2 (2C), 127.7, 126.0, 124.4, 123.6, 121.5, 121.4, 118.3, 117.6, 117.4, 117.1, 113.5; HR-MS (ESI+) m/z calculated for $[C_{21}H_{14}N_5]^+ = [M + H]^+$ 336.1250, found 336.1249.

1-(*p*-Tolyl)indazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7b):



Yellow solid; Yield: 68%; mp: 221-223 °C; R_f= 0.5 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.82-8.79 (m, 2H), 7.88 (d, *J* = 8.8 Hz, 1H), 7.79-7.72 (m, 2H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.42 (t, *J* = 7.8 Hz, 3H), 7.03-6.95 (m, 2H), 2.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.5, 141.8, 139.5, 130.4 (2C), 129.3 (2C), 128.9, 128.4, 128.0, 127.7, 125.8, 125.7, 124.3, 123.0, 122.7, 121.9, 118.3, 117.5, 117.3, 117.0, 21.6; HR-MS (ESI+) m/z calculated for $[C_{22}H_{16}N_5]^+ = [M + H]^+$ 350.1400, found 350.1406.

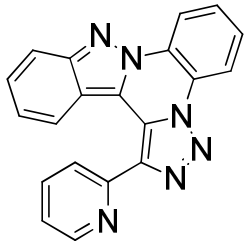
1-(4-Methoxyphenyl)indazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7c):



White color solid; Yield: 68%; mp: 235-240 °C; R_f= 0.4 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.80-8.79 (m, 2H),7.88 (d, *J* = 8.4 Hz, 1H),7.75 (t, *J* = 5.6 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.42 (t, *J* = 7.4 Hz, 1H), 7.13 (d, *J* = 8.4 Hz, 2H), 7.04-6.97 (m,2H), 3.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.7, 149.6, 141.6 (2C), 131.9 (2C), 128.9,

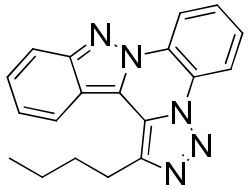
128.4, 128.1, 125.8, 124.3, 123.1, 123.0, 122.7, 121.9, 118.3, 117.6, 117.3, 117.1, 114.1 (2C), 55.5; HR-MS (ESI+) m/z calculated for $[C_{22}H_{16}N_5O]^+$ = $[M + H]^+$ 366.1363, found 366.1355.

1-(Pyridin-2-yl)indazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7d):



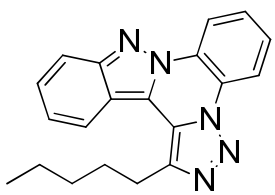
Yellow solid; Yield: 65%; mp: 158-160 °C; R_f= 0.5 (50% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.95-8.90 (m, 3H), 8.18 (d, J = 7.6 Hz, 1H), 7.99 (t, J = 7.0 Hz, 1H), 7.92 (d, J = 8.8 Hz, 1H), 7.81-7.73 (m, 2H), 7.51-7.45 (m, 3H), 7.12 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.7, 149.7, 149.4, 141.3, 137.0, 129.1, 128.4, 128.0, 125.8, 124.8, 124.0, 123.8, 123.2, 122.9, 122.7, 121.4, 118.3, 118.1, 117.6, 117.1; HR-MS (ESI+) m/z calculated for $[C_{20}H_{13}N_6]^+$ = $[M + H]^+$ 337.1198, found 337.1202.

1-Butylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline(7e):



Pale yellow solid; Yield:62%; mp: 166-168 °C; R_f= 0.6 (10% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76 (dd, J_1 = 9.2 Hz, J_2 = 9.2 Hz, 2H), 8.18 (d, J = 8.8 Hz, 1H), 7.94 (d, J = 8.8 Hz, 1H), 7.76-7.68 (m, 2H), 7.53 (t, J = 7.8 Hz, 1H), 7.34 (t, J = 7.6 Hz, 1H), 3.47 (t,J = 7.8 Hz,2H), 2.00-1.96 (m, 2H), 1.62-1.52 (m, 2H), 1.02 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.3, 141.7, 128.6, 128.2, 128.0, 125.4, 124.2, 123.4, 122.8, 122.1, 120.0, 118.2, 117.9, 117.0, 116.8, 32.1, 26.9, 22.4, 13.9; HR-MS (ESI+) m/z calculated for $[C_{19}H_{18}N_5]^+$ = $[M + H]^+$ 316.1555, found 316.1562.

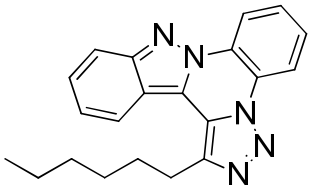
1-Pentylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7f):



White solid: Yield: 68%; mp: 158-160 °C; R_f= 0.4 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.74 (dd, J_1 = 8.0 Hz, J_2 = 8.8 Hz, 2H), 8.15 (d, J = 8.4 Hz, 1H), 7.92 (d, J =

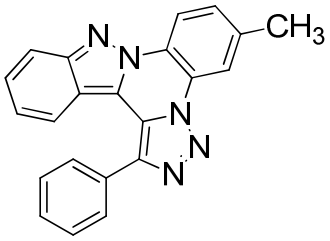
8.8 Hz, 1H), 7.74-7.68 (m, 2H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 3.45 (t, *J* = 7.8 Hz, 2H), 2.01-1.94 (m, 2H), 1.57-1.52 (m, 2H), 1.48-1.38 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.5,141.9, 128.7, 128.3, 128.1, 125.6, 124.3, 123.5, 122.9, 122.2 , 120.1, 118.2, 118.0, 117.1, 116.9, 31.5, 29.8, 27.2, 22.5, 14.0; HR-MS (ESI+) m/z calculated for $[C_{20}H_{20}N_5]^+ = [M + H]^+$ 330.1716, found 330.1719.

1-Hexylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7g):



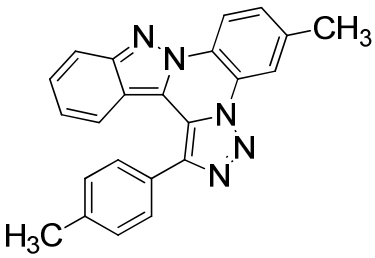
Pale yellow solid; Yield: 67%; mp: 132-135 °C; R_f= 0.4 (10% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71 (dd, J_1 = 9.6 Hz, J_2 = 9.6 Hz, 2H), 8.12 (d, *J* = 8.8 Hz, 1H), 7.89 (d, *J* = 8.8 Hz, 1H), 7.73-7.66 (m, 2H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 1H), 3.42 (t, *J* = 7.8 Hz, 2H), 1.99-1.92 (m, 2H), 1.60-1.53 (m, 2H), 1.42-1.30 (m, 4H), 0.90 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.4, 141.8, 128.6, 128.2, 128.0, 125.5, 124.2, 123.4, 122.8, 122.1, 120.0, 118.2, 117.9, 117.0, 116.8, 31.6, 30.0, 29.0, 27.2, 22.6, 14.1; HR-MS (ESI+) m/z calculated for $[C_{21}H_{22}N_5]^+ = [M + H]^+$ 344.1882, found 344.1875.

6-Methyl-1-phenylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7h):



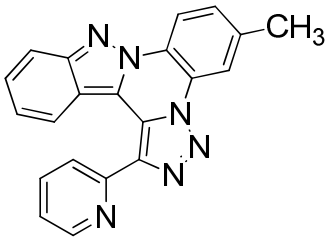
Light yellow solid; Yield: 70%; mp: 213-215 °C; R_f= 0.5 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67 (d, *J* = 8.8 Hz, 1H), 8.61 (s, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 6.0 Hz, 2H), 7.59 (t, *J* = 12.0 Hz, 4H),7.41 (t, *J* = 7.6 Hz, 1H), 6.98 (t, *J* = 7.4 Hz, 1H), 6.86 (d, *J* = 8.8 Hz, 1H), 2.65 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6): δ 153.8, 146.0, 144.0, 135.4, 135.3 (2C), 134.8, 134.3, 133.3 (2C), 132.5, 128.5, 128.2, 127.6, 127.5, 126.3, 125.7, 122.6, 122.1, 121.7, 121.3, 26.3; HR-MS (ESI+) m/z calculated for $[C_{22}H_{16}N_5]^+ = [M + H]^+$ 350.1402, found 350.1406.

6-Methyl-1-(*p*-tolyl)indazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7i):



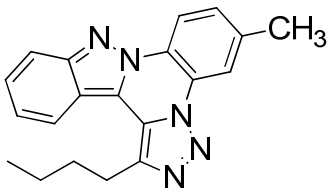
White solid; Yield: 66%; mp: 215-217 °C; R_f= 0.6 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.68 (d, *J* = 8.4 Hz, 1H), 8.61 (s, 1H), 7.88 (d, *J* = 8.8 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.41 (t, *J* = 7.4 Hz, 3H), 7.03-6.95 (m, 2H), 2.65 (s, 3H), 2.54 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.3, 141.6, 139.4, 139.2, 130.4 (2C), 129.9, 129.2 (2C), 127.8, 127.7, 123.9, 123.5, 122.7 (2C),121.9, 121.4, 117.9, 117.4, 117.1, 116.7, 21.6 (2C); HR-MS (ESI+) m/z calculated for $[C_{23}H_{18}N_5]^+$ = $[M + H]^+$ 364.1561, found 364.1562.

6-Methyl-1-(pyridin-2-yl)indazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7j):



Yellow solid; Yield: 65%; mp: 197-200 °C; R_f= 0.6 (50% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.85 (d, *J* = 4.4 Hz, 1H), 8.69 (d, *J* = 8.4 Hz, 1H),8.61 (s, 1H), 8.17 (d, *J* = 8.0 Hz, 1H), 7.98 (t, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.51-7.43 (m, 3H), 7.10 (t, *J* = 7.6 Hz, 1H), 2.65 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.7, 149.5, 149.4, 141.1, 139.2, 137.0, 130.2, 127.7, 124.8, 123.7 (2C), 123.2, 122.7 (2C), 121.4, 118.0 (2C), 117.4, 116.8 (2C), 21.6; HR-MS (ESI+) m/z calculated for $[C_{21}H_{15}N_6]^+$ = $[M + H]^+$ 351.1357, found 351.1358.

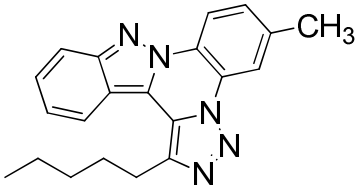
1-Butyl-6-methylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7k):



Whitesolid; Yield:65%; mp: 177-179 °C; R_f= 0.5 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.63 (d, *J* = 8.4 Hz, 1H), 8.52 (s, 1H),8.16 (d, *J* = 8.8 Hz, 1H), 7.92 (d, *J* = 8.8 Hz, 1H),7.51 (t, *J* = 9.6 Hz, 2H), 7.32 (t, *J* = 7.8 Hz, 1H),3.45 (t, *J* = 7.8 Hz, 2H), 2.62 (s, 3H), 2.0-1.92 (m, 2H), 1.62-1.57 (m, 2H),1.02 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz,

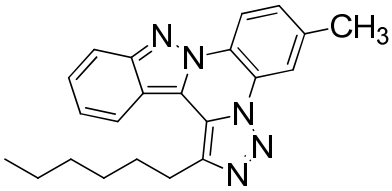
$CDCl_3$): δ 149.2, 141.6, 139.0, 129.7, 127.8, 124.0, 123.3, 123.2, 122.9, 121.7, 120.0, 117.9, 117.8, 116.9, 116.6, 32.1, 26.9, 22.4, 21.5, 13.9; HR-MS (ESI+) m/z calculated for $[C_{20}H_{20}N_5]^+ = [M + H]^+$ 330.1714, found 330.1719.

6-Methyl-1-pentylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7l):



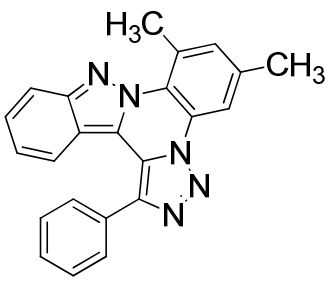
White solid; Yield: 68%; mp: 126-128 °C; R_f= 0.4 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60 (d, *J* = 8.0 Hz, 1H), 8.50 (s, 1H), 8.13 (d, *J* = 8.8 Hz, 1H), 7.89 (d, *J* = 8.8 Hz, 1H), 7.51 (t, *J* = 4.6 Hz, 2H), 7.30 (t, *J* = 7.8 Hz, 1H), 3.43 (t, *J* = 7.8 Hz, 2H), 2.61 (s, 3H), 1.99-1.94 (m, 2H), 1.59-1.53 (m, 2H), 1.45-1.39 (m, 2H), 0.93 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.2, 141.6, 139.0, 129.7, 127.8, 124.0, 123.3, 123.2, 122.9, 121.7, 120.0, 117.9, 117.8, 116.9, 116.6, 31.5, 29.7, 27.2, 22.5, 21.5, 14.1; HR-MS (ESI+) m/z calculated for $[C_{21}H_{22}N_5]^+ = [M + H]^+$ 344.1880, found 344.1875.

1-Hexyl-6-methylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7m):



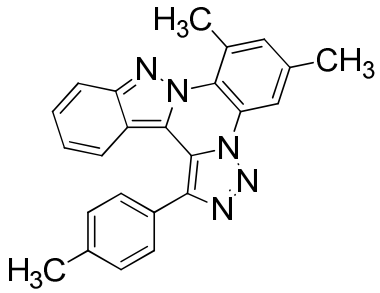
White solid; Yield: 68%; mp: 125-127 °C; R_f= 0.4 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60 (d, *J* = 8.0 Hz, 1H), 8.50 (s, 1H), 8.13 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.2 Hz, 2H), 7.30 (t, *J* = 9.2 Hz, 1H), 3.43 (t, *J* = 7.6 Hz, 2H), 2.61 (s, 3H), 1.99-1.92 (m, 2H), 1.59-1.53 (m, 2H), 1.42-1.32 (m, 4H), 0.89 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.2, 141.6, 139.0, 129.7, 127.7, 124.0, 123.3, 123.2, 122.9, 121.7, 120.0, 117.9, 117.7, 116.9, 116.6, 31.6, 30.0, 29.0, 27.2, 22.6, 21.5,14.1; HR-MS (ESI+) m/z calculated for $[C_{22}H_{24}N_5]^+ = [M + H]^+$ 358.2030, found 358.2032.

6,8-Dimethyl-1-phenylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7n):



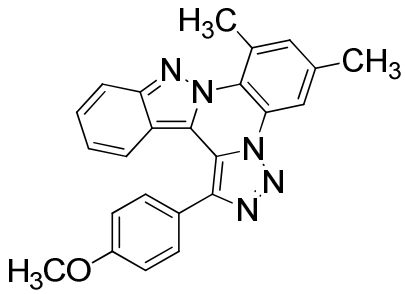
Off white solid; Yield: 65%; mp: 205-210 °C; R_f= 0.6 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.54 (s, 1H), 7.83 (d, *J* = 8.8 Hz, 1H),7.75-7.73 (m, 2H), 7.60-7.57 (m,3H), 7.34 (d, *J* = 10.0 Hz, 2H),6.95 (t, *J* = 7.6 Hz, 1H), 6.84 (d, *J* = 8.8 Hz, 1H), 3.23 (s, 3H), 2.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.5, 140.9, 138.2, 133.6, 131.2, 131.0, 130.6 (2C), 129.4, 128.5 (2C), 127.2, 125.1, 122.8, 122.6, 122.5, 121.7, 121.4, 117.7, 116.0, 114.9, 24.6, 21.2; HR-MS (ESI+) m/z calculated for $[C_{23}H_{18}N_5]^+ = [M + H]^+$ 364.1554, found 364.1562.

6,8-Dimethyl-1-(*p*-tolyl)indazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7o):



Yellow solid; Yield: 60%; mp: 203-205 °C; R_f= 0.6 (10% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.47 (s, 1H), 7.82 (d, *J* = 8.8 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.41 (d, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.30 (s, 1H), 6.97 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 8.4 Hz, 1H), 3.17 (s, 3H), 2.56 (s, 3H), 2.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.6, 141.1, 139.3, 138.2,133.7, 131.3, 130.4 (2C), 129.2 (2C), 128.1, 127.2, 125.2, 122.7 (2C), 122.4, 122.0, 121.7, 117.7, 116.1, 114.9, 24.6, 21.6, 21.2; HR-MS (ESI+) m/z calculated for $[C_{24}H_{20}N_5]^+ = [M + H]^+$ 378.1730, found 378.1719.

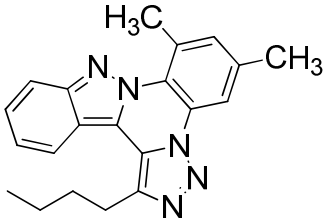
1-(4-Methoxyphenyl)-6,8-dimethylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7p):



Pale yellow solid; Yield: 65%; mp: 215-217 °C; R_f= 0.4 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.42 (s, 1H), 7.79 (d, *J* = 6.8 Hz, 1H), 7.66 (d, *J* = 6.4 Hz, 2H), 7.34 (t, *J* = 5.8 Hz, 1H), 7.26 (s, 1H), 7.12 (d, *J* = 6.4 Hz, 2H), 6.97-6.90 (m, 2H), 3.97 (s, 3H), 3.13 (s, 3H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.5, 148.6, 140.8, 138.2, 133.6, 131.8 (2C), 131.2, 127.2, 125.2, 123.3, 122.8,122.6, 122.3, 122.0, 121.5, 117.7, 116.0, 114.9, 114.0

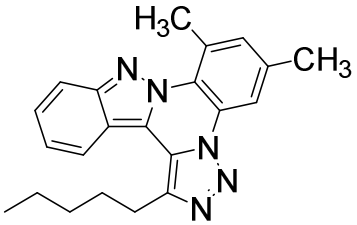
(2C), 55.5, 24.6, 21.2; HR-MS (ESI+) m/z calculated for $[C_{24}H_{20}N_5O]^+$ = $[M + H]^+$ 394.1677, found 394.1668.

1-Butyl-6,8-dimethylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7q):



Off white solid; Yield:65%; mp: 136-138 °C; R_f= 0.6 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.46 (s, 1H), 8.16 (d, J = 8.8 Hz, 1H),7.90 (d, J = 8.8 Hz, 1H), 7.47 (t, J = 7.6 Hz, 1H), 7.32-7.28 (m, 2H), 3.44 (t, J = 7.8 Hz, 2H), 3.20 (s, 3H), 2.55 (s, 3H), 1.99-1.91 (m, 2H), 1.62-1.54 (m, 2H), 1.02 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6): δ 149.2, 141.8, 138.9, 134.4, 132.1, 128.2, 126.2, 124.3, 123.6, 123.4, 123.3, 120.8, 119.2, 116.9, 115.8, 34.3, 29.3, 27.0, 24.7, 23.5, 16.3; HR-MS (ESI+) m/z calculated for $[C_{21}H_{22}N_5]^+$ = $[M + H]^+$ 344.1870, found 344.1875.

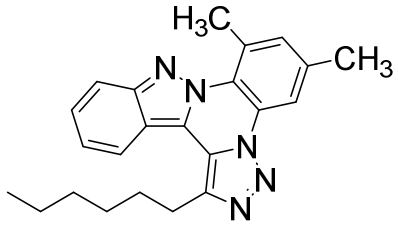
6,8-Dimethyl-1-pentylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7r):



Chemical Formula: $C_{22}H_{23}N_5$
Exact Mass: 357.1953

Whitesolid; Yield: 62%; mp: 138-141 °C; R_f= 0.5 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.49 (s, 1H), 8.18 (d, J = 8.4 Hz, 1H), 7.92 (d, J = 8.8 Hz, 1H), 7.49 (t, J = 7.4 Hz, 1H), 7.34-7.30 (m, 3H), 3.45 (t, J = 7.8 Hz, 2H), 3.23 (s, 3H), 2.56 (s, 3H), 2.01-1.93 (m, 2H), 1.57-1.52 (m, 2H), 1.46-1.40 (m, 2H), 0.93 (t, J =7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$ + DMSO-d_6): δ 149.1, 141.7, 138.9, 134.4, 132.1, 128.2, 126.1, 124.3, 123.6, 123.4, 123.3, 120.8, 119.1, 116.9, 115.8, 33.6, 31.9, 29.5, 26.9, 24.7, 23.5, 16.4; HR-MS (ESI+) m/z calculated for $[C_{22}H_{24}N_5]^+$ = $[M + H]^+$ 358.2036, found 358.2032.

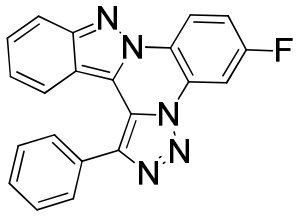
1-Hexyl-6,8-dimethylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7s):



Chemical Formula: $C_{23}H_{25}N_5$
Exact Mass: 371.2110

Yellow solid; Yield: 60%; mp: 148-150 °C; R_f= 0.6 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.44 (s, 1H), 8.13 (d, *J* = 8.4 Hz, 1H), 7.88 (d, *J* = 8.8 Hz, 1H),7.46 (t, *J* = 7.8 Hz, 1H),7.30-7.26 (m, 2H), 3.42 (t, *J* = 7.8 Hz, 2H), 3.18 (s, 3H), 2.53 (s, 3H), 1.99-1.91 (m, 2H), 1.59-1.52 (m, 2H), 1.40-1.33 (m, 4H), 0.89 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.3,140.9, 137.9, 133.3, 131.0, 127.1, 125.1, 123.1, 122.4, 122.2, 119.7, 119.6, 118.0, 115.7, 114.7, 31.6, 30.0, 29.0, 27.4, 24.7, 22.6, 21.1, 14.1; HR-MS (ESI+) m/z calculated for $[C_{23}H_{26}N_5]^+ = [M + H]^+$ 372.2184, found 372.2188.

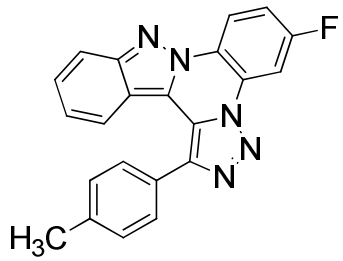
6-Fluoro-1-phenylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7t):



Chemical Formula: $C_{21}H_{12}FN_5$
Exact Mass: 353.1077

White solid; Yield: 61%; mp: 231-233 °C; R_f= 0.5 (10% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71 (d, *J* = 4.0 Hz, 1H), 8.42 (d, *J* = 6.0 Hz, 1H), 7.80-7.62 (m, 6H), 7.45-7.37 (m, 2H), 6.93 (d, *J* = 6.0 Hz, 1H), 6.77(d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$-TFA-*d*): δ 163.0 (d, *J* = 249.8 Hz), 149.4, 141.6, 130.6 (2C), 129.9 (2C), 128.7 (2C), 128.2, 124.9 (d, *J* = 11.5 Hz), 123.4, 123.3, 122.4, 121.6, 121.1, 120.6 (d, *J* = 9.3 Hz), 117.5, 117.3 (d, *J* = 7.6 Hz), 117.0, 104.4 (d, *J* = 28.3 Hz); HR-MS (ESI+) m/z calculated for $[C_{21}H_{13}FN_5]^+ = [M + H]^+$ 354.1150, found 354.1155.

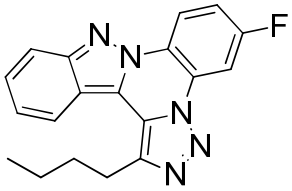
6-Fluoro-1-(*p*-tolyl)indazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7u):



Chemical Formula: $C_{22}H_{14}FN_5$
Exact Mass: 367.1233

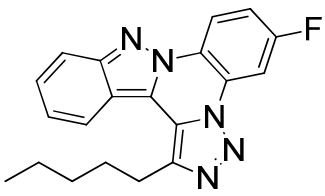
Light yellow solid; Yield: 62%; mp: 234-236 °C; R_f= 0.6 (10% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.80-8.77 (m, 1H), 8.47 (dd, J_1 = 2.4 Hz, J_2 = 2.4 Hz, 1H), 7.86 (d, J = 8.8 Hz, 1H), 7.63 (d, J = 8.0 Hz, 2H), 7.50-7.45 (m, 1H), 7.42 (t, J = 8.0Hz, 3H), 7.01 (t, J = 7.4 Hz, 1H), 6.95 (d, J = 8.8 Hz, 1H), 2.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.9 (d, J = 249.2 Hz), 149.5, 141.9, 139.7, 130.4 (2C), 129.3 (2C), 128.1, 127.5, 125.2 (d, J = 11.4 Hz), 123.2, 123.0, 122.4, 121.9, 121.4, 120.5 (d, J = 9.3 Hz), 117.5, 117.3, 116.9 (d, J = 23.8 Hz), 104.4 (d, J = 28.3 Hz), 21.6; HR-MS (ESI+) m/z calculated for $[C_{22}H_{15}FN_5]^+$ = $[M + H]^+$ 368.1306, found 368.1311.

1-Butyl-6-fluoroindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7v):



White solid; Yield: 62%; mp: 187-189 °C; R_f= 0.4 (10% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.77-8.73 (m, 1H), 8.39 (dd, J_1 = 2.8 Hz, J_2 = 2.8 Hz, 1H), 8.13 (d, J = 8.4 Hz, 1H), 7.90 (d, J = 8.8 Hz, 1H), 7.52 (t, J = 7.6 Hz, 1H), 7.46-7.41 (m, 1H), 7.33 (t, J = 7.6 Hz, 1H), 3.44 (t, J = 7.8 Hz, 2H), 1.99-1.91 (m, 2H), 1.63-1.54 (m, 2H), 1.02 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.9 (d, J = 251.2 Hz), 149.3, 141.9, 128.1, 125.1 (d, J = 11.4 Hz), 123.6, 123.1, 122.0, 121.7, 120.4 (d, J = 9.1 Hz), 120.0, 117.9, 117.0, 116.6 (d, J = 23.9 Hz), 104.1 (d, J = 28.3 Hz), 32.0, 26.9, 22.4, 13.9; HR-MS (ESI+) m/z calculated for $[C_{19}H_{17}FN_5]^+$ = $[M + H]^+$ 334.1468, found 334.1468.

6-Fluoro-1-pentylindazolo[2,3-*a*][1,2,3]triazolo[5,1-*c*]quinoxaline (7w):

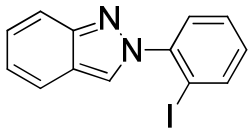


Yellow solid; Yield: 65%; mp: 157-159 °C; R_f= 0.3 (10% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.74-8.70 (m, 1H), 8.37 (dd, J_1 = 2.8 Hz, J_2 = 2.8 Hz, 1H), 8.10 (d, J = 8.4 Hz, 1H), 7.87 (d, J = 8.8 Hz, 1H),7.50 (t, J = 7.8 Hz, 1H), 7.45-7.40 (m, 1H), 7.32 (t, J = 7.6 Hz, 1H), 3.41 (t, J = 7.8 Hz, 2H), 1.99-1.92 (m, 2H), 1.58-1.51 (m, 2H), 1.47-1.38 (m, 2H), 0.93 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.9 (d, J = 249.2 Hz), 149.3, 141.9, 128.1, 125.1 (d, J = 11.6 Hz), 123.7, 123.1, 122.0, 121.7, 120.4 (d, J = 9.2 Hz), 120.0, 117.9, 117.0, 116.6 (d, J = 23.8 Hz), 104.1 (d, J = 28.2 Hz), 31.4, 29.7, 27.1, 22.5, 14.0; HR-MS (ESI+) m/z calculated for $[C_{20}H_{19}FN_5]^+ = [M + H]^+$ 348.1623, found 348.1624.

Procedure for the synthesis of synthesis of compound 3a[1]:

2-Azidobenzaldehyde (**1)** (0.67 mmol) and 2-iodoaniline (**2**) (0.67 mmol) were taken in a 10mL oven dried Schlenck tube and it was closed with nitrogen balloon and stirred for 40 min at 110 ^{o}C. After completion of the reaction was monitored by TLC. The reaction mixture was cooled to room temperature and was purified by column chromatography on silica gel with EtOAc / Hexane to give desired product of **3a**.

2-(2-Iodophenyl)-*2H*-indazole (3a):

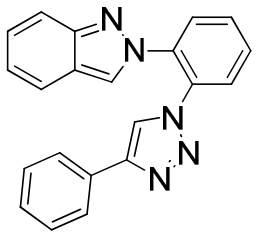


Yellowsolid;Yield:70%;mp: 99-101 °C;R_f= 0.5 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.62 (s, 1H), 8.06 (d, J = 7.6 Hz, 1H),7.79 (d, J = 8.8 Hz, 1H), 7.69 (d, J = 8.4 Hz, 1H),7.61-7.56 (m, 2H), 7.35-7.29 (m, 2H), 7.11 (t, J = 7.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ149.4, 143.8, 140.0, 130.8, 129.0, 128.3, 126.8, 124.9, 122.4, 122.0, 120.5, 118.0, 94.2;HR-MS (ESI+) m/z calculated for $[C_{13}H_{10}IN_2]^+ = [M + H]^+$ 320.9885, found 320.9889.

Procedure for the synthesis of synthesis of compound 6a:

To a round bottom flask containing 2-(2-iodophenyl)-2*H*-indazole (**3a**) (0.67 mmol), phenyl acetylene (**4a**) (0.67 mmol) and sodium azide **(5)** (0.67 mmol) in DMF (3 mL). Then after CuI (10 mol%), K_2CO_3 (0.81 mmol) were added reaction mixture. The reaction mixture was stirred at 120 ^{o}C for 2h under open air. After completion of the reaction was monitored by TLC. The reaction mixture was cooled to room temperature and diluted with water extracted extracted with EtOAc (20 mL × 3). The combined EtOAc layer wascollected, dried over anhydrous Na_2SO_4, filtered and concentrated.The residue was purified using column chromatographyover silica gel with EtOAc / hexane to give desired product of (**6)**

2-(2-(4-Phenyl-*1H*-1,2,3-triazol-1-yl)phenyl)-*2H*-indazole (6):



Brown colour solid; Yield: 60%; mp: 126-128 °C; R_f= 0.3 (20% EtOAc/ *n*-hexane); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88-7.85 (m, 2H), 7.78 (s, 1H), 7.75 (d, J = 8.8 Hz, 1H), 7.72-7.70 (m,2H), 7.55-7.53 (m, 3H), 7.35-7.27 (m,5H), 7.07 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.8, 148.2, 134.9, 132.1, 130.5, 130.2, 129.7, 128.8 (2C), 128.4, 128.1,127.4, 126.9, 125.8 (2C), 125.0, 122.8, 122.6, 120.7, 120.6, 117.7; HR-MS (ESI+) m/z calculated for $[C_{21}H_{16}N_5]^+ = [M + H]^+$ 338.1412, found 338.1406.

Single crystal X-ray data for compound (7q):

X-ray intensity data measurements of all sulphonamides were carried out on a Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer equipped with Incoatech multilayer mirrors optics. The intensity measurements were carried out with Mo micro-focus sealed tube diffraction source (Mo-Kα = 0.72 Å) at 100(2) K temperature. The X-ray generator was operated at 50 kV and 1.4 mA. A preliminary set of cell constants and an orientation matrix were calculated from two sets of 20 frames. Data were collected with ω scan width of 0.5° at different settings of φ and 2θ with a frame time of 40 seconds keeping the sample–to-detector distance fixed at 4.00 cm. The X-ray data collection was monitored by APEX3 program (Bruker, 2016).All the data were corrected for Lorentzian, polarization and absorption effects using SAINT and SADABS programs (Bruker, 2016). SHELX-97 was used for structure solution and full matrix least-squares refinement on F^2. Molecular diagrams were generated using ORTEP-33 and Mercury programs. Geometrical calculations were performed using SHELXTLand PLATON. All the hydrogen atoms were placed in geometrically idealized position and constrained to ride on their parent atoms. An ORTEP III view of both compounds were drawn with 50% probability displacement ellipsoids and H–atoms are shown as small spheres of arbitrary radii.

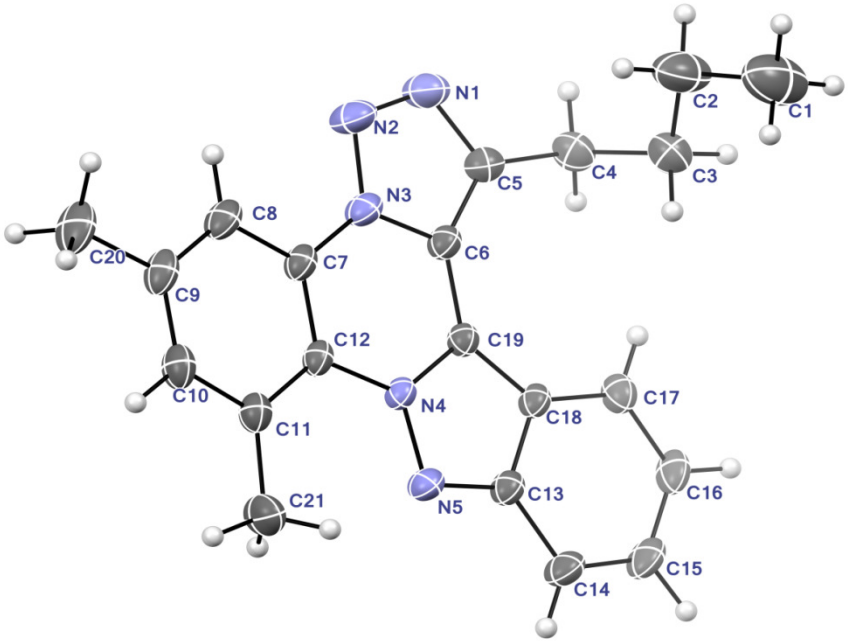


Fig. S-1 X-ray crystal structure of**7q** (ORTEP diagram). Thermal ellipsoidsare drawn at the 50% probability level.

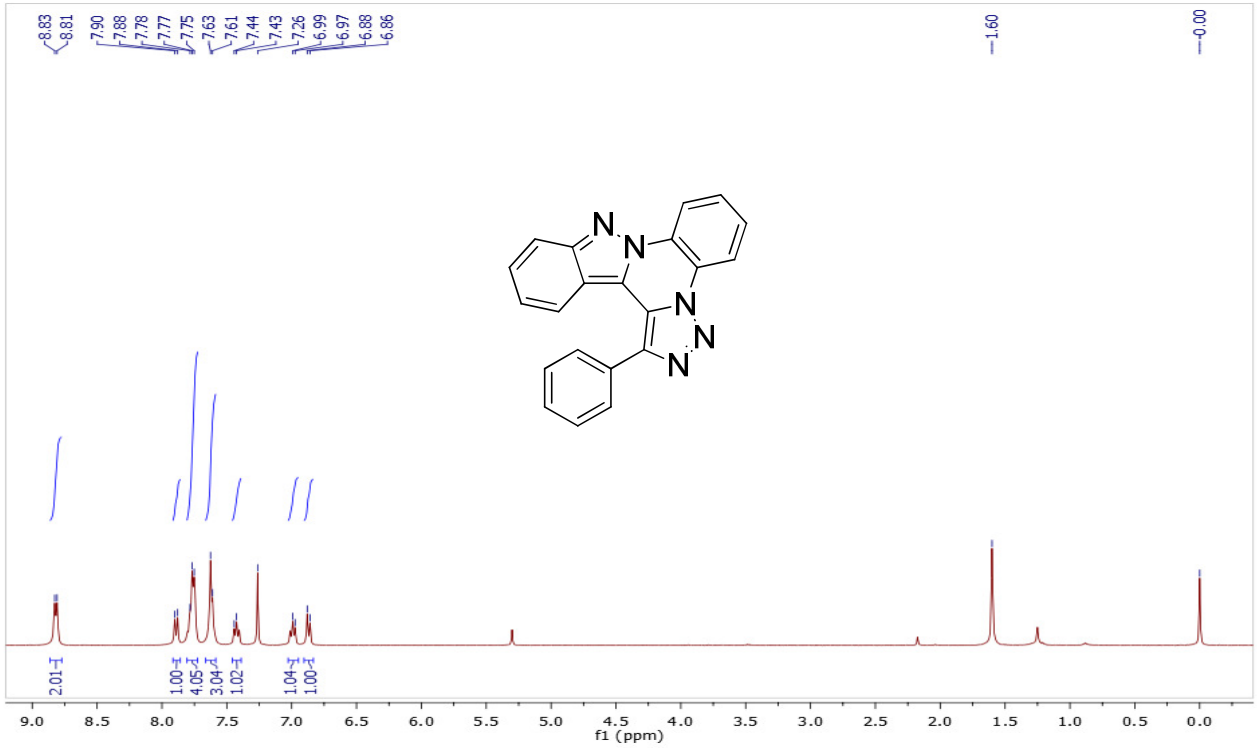
Crystallographic data for **7q** ($C_{21}H_{21}N_5$): M = 343.43, Crystal dimensions 0.490 x 0.270 x 0.130mm3, Monoclinic, space groupC 2/c, a = 12.2671(5)Å, b = 18.1570(8)Å, c = 15.9123(7)Å, α = 90° β = 96.146(2)°□ = 90°, V = 3523.8(3)Å3, Z = 8, ρcalcd = 1.295 Mg/m3, μ (Cu-Kα) = 0.080mm-1, F(000) = 1456, $2\theta_{max}$ = 28.725°,T = 100(2) K, 54074 reflections collected, 4570 unique reflections (R(int) = 0.0669), 4570 observed (I > 2σ (I)) reflections, multi-scan absorption correction, *T*min = 0.962, *T*max = 0.990,238refined parameters, No. of restraints 0, S = 1.069, R1 = = 0.0633, wR2 = 0.1532 (all data R1 = 0.0842, wR2 = 0.1666), maximum and minimum residual electron densities; Δρmax = 0.282, Δρmin= -0.216 ($eÅ^{-3}$). Crystallographic data for compound intermediate deposited with the Cambridge Crystallographic Data Centre as supplementary publication no CCDC 1863988

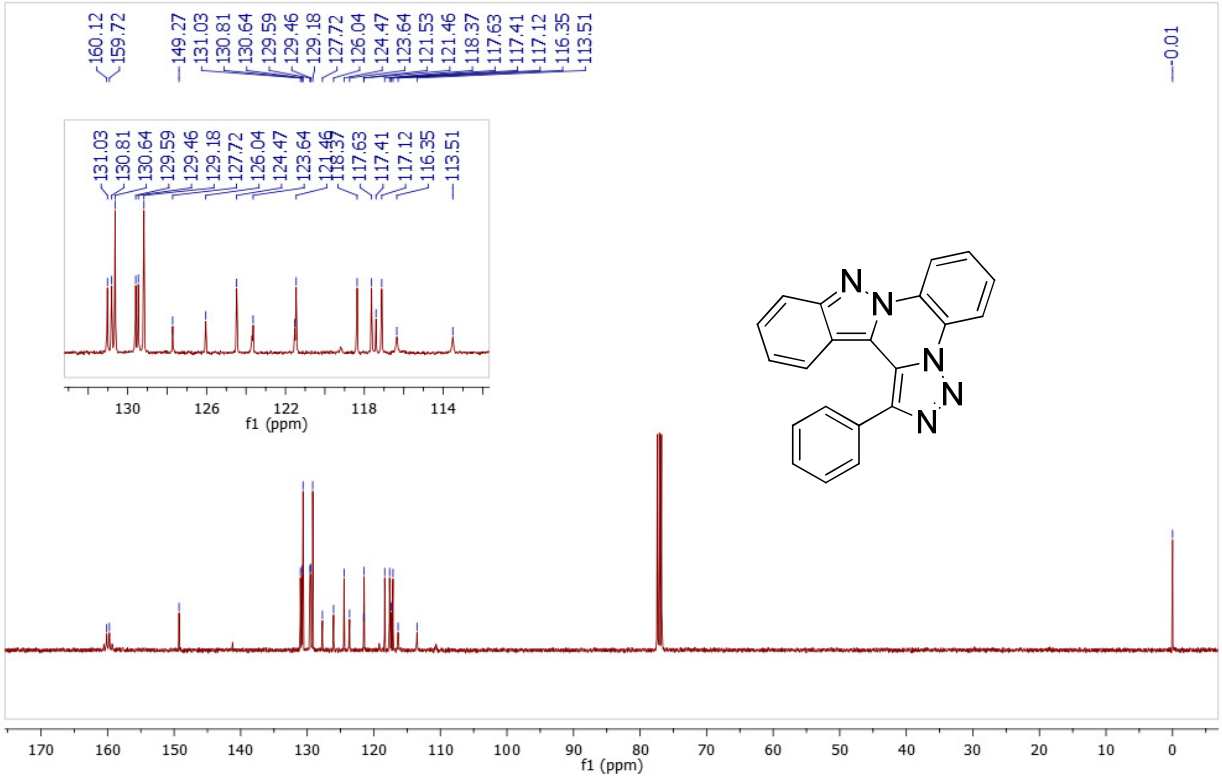
References:

1. S. Vidyacharan, A. Murugan and D. S. Sharada*, J. Org. Chem.*, 2016, 81, 2837

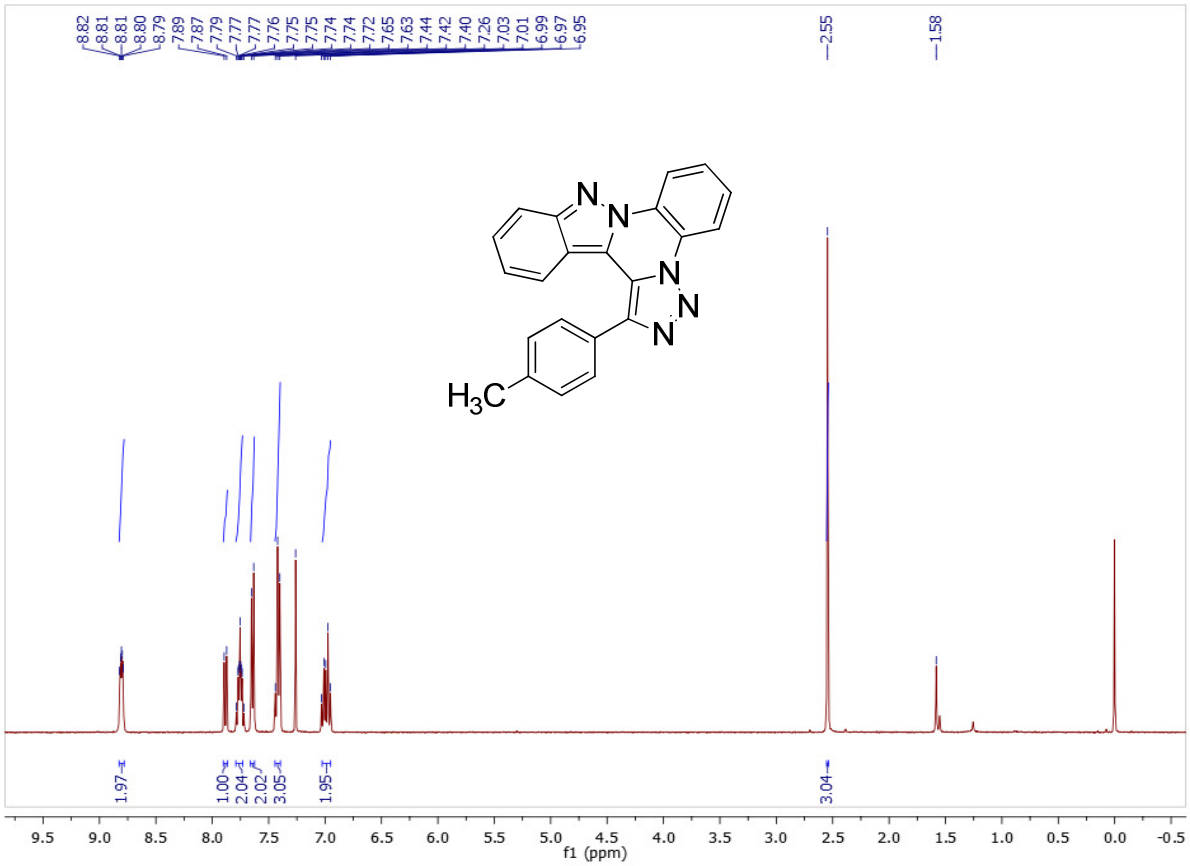
Copies of ^{1}H and ^{13}C NMR spectra of product

Compound- **7a**





Compound- **7b**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8.81
8.80
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7.89
7.87
7.79
7.77
7.77
7.76
7.75
7.75
7.74
7.74
7.72
7.65
7.63
7.44
7.42
7.40
7.26
7.03
7.01
6.99
6.97
6.95
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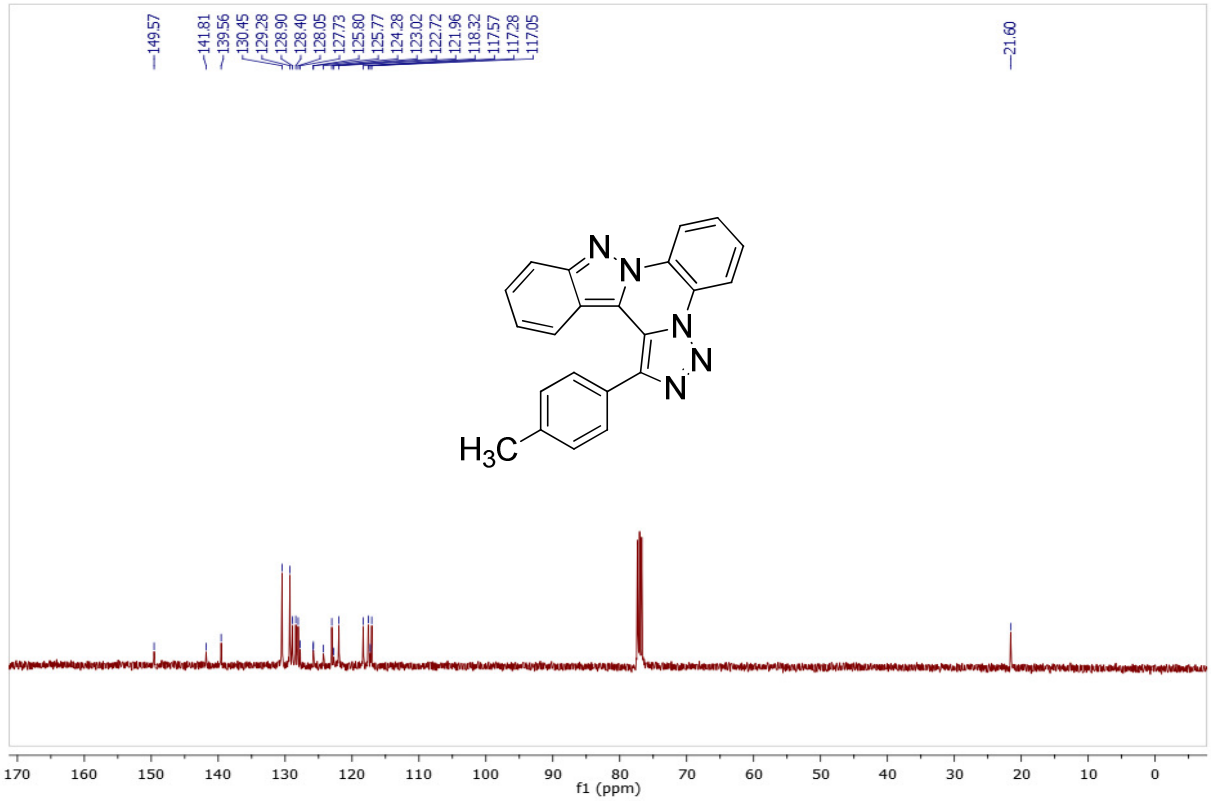
1.58
1.97
1.00
2.04
2.02
3.05
1.95
3.04
f1 (ppm)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139.56
130.45
129.28
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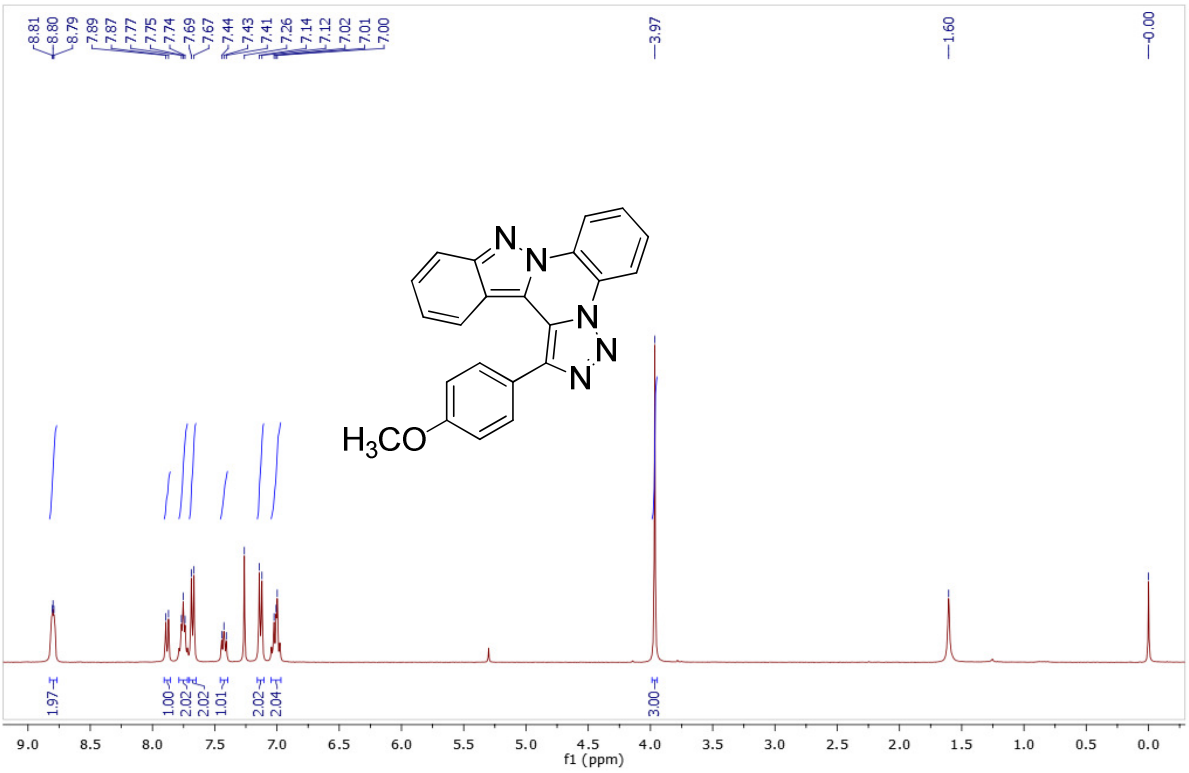
128.05
127.73
125.80
125.77
124.28
123.02
122.72
121.96
118.32
117.57
117.28
117.05
21.60
f1 (ppm)

Compound-**7c**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8.80
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7.77
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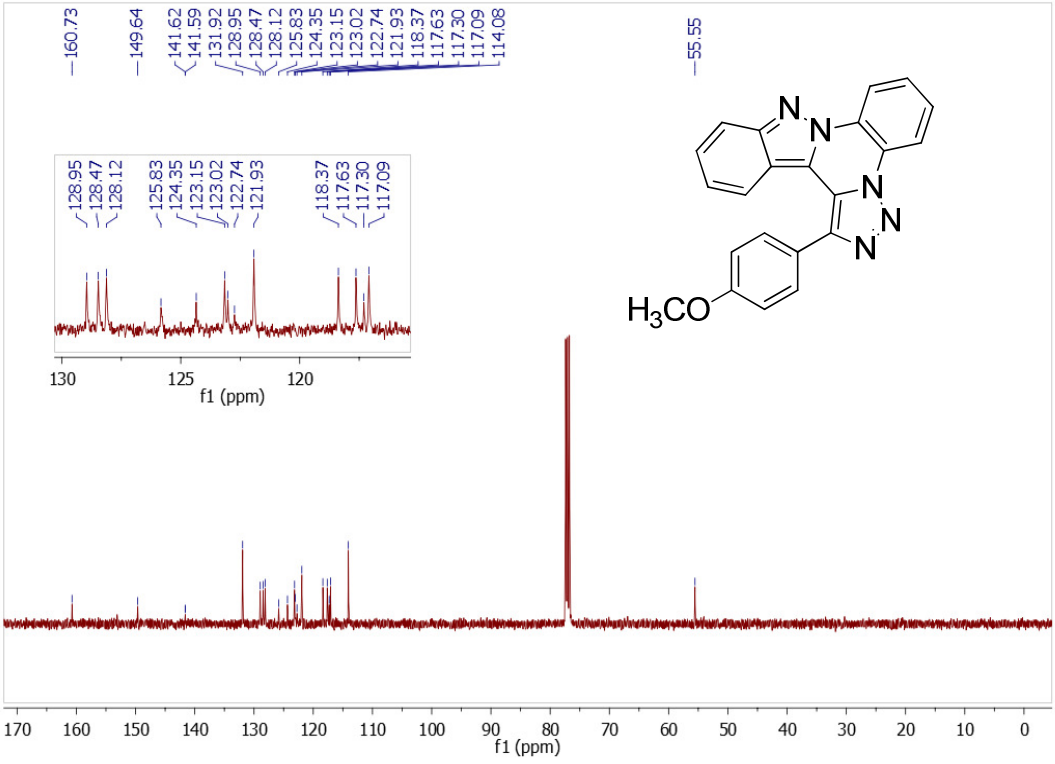
7.74
7.69
7.67
7.44
7.43
7.41
7.26
7.14
7.12
7.02
7.01
7.00
3.97
1.60
0.00
1.97
1.00
2.02
2.02
1.01
2.02
2.04
3.00
N
N
N
N
N
H3CO
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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141.59
131.92
128.95
128.47
128.12
125.83
124.35
123.15
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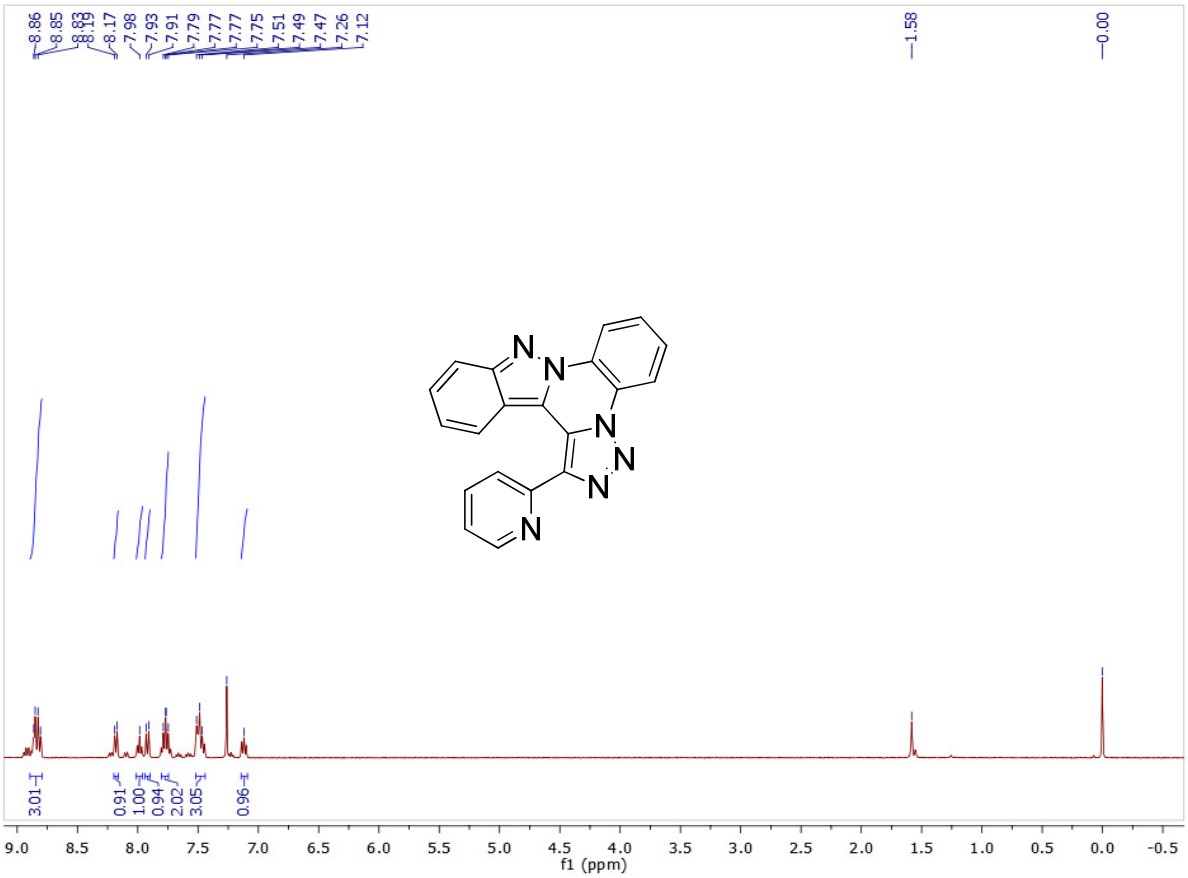
122.74
121.93
118.37
117.63
117.30
117.09
114.08
55.55
128.95
128.47
128.12
125.83
124.35
123.15
123.02
122.74
121.93
118.37
117.63
117.30
117.09
130
125
120
f1 (ppm)
N
N
N
N
N
H3CO
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Compound- **7d**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7.77
7.77
7.75
7.51
7.49
7.47
7.26
7.12
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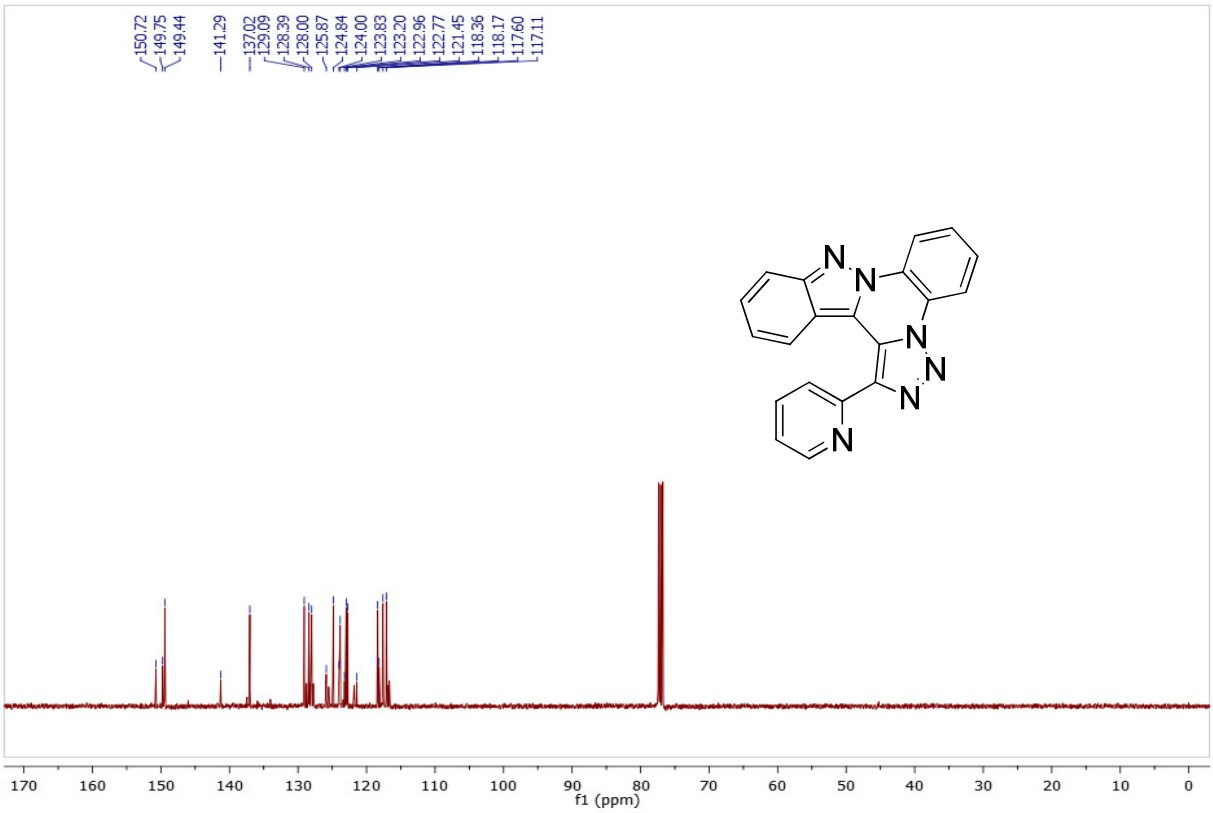
1.00
0.94
2.02
3.05
0.96
f1 (ppm)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141.29
137.02
129.09
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128.00
125.87
124.84
124.00
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123.20
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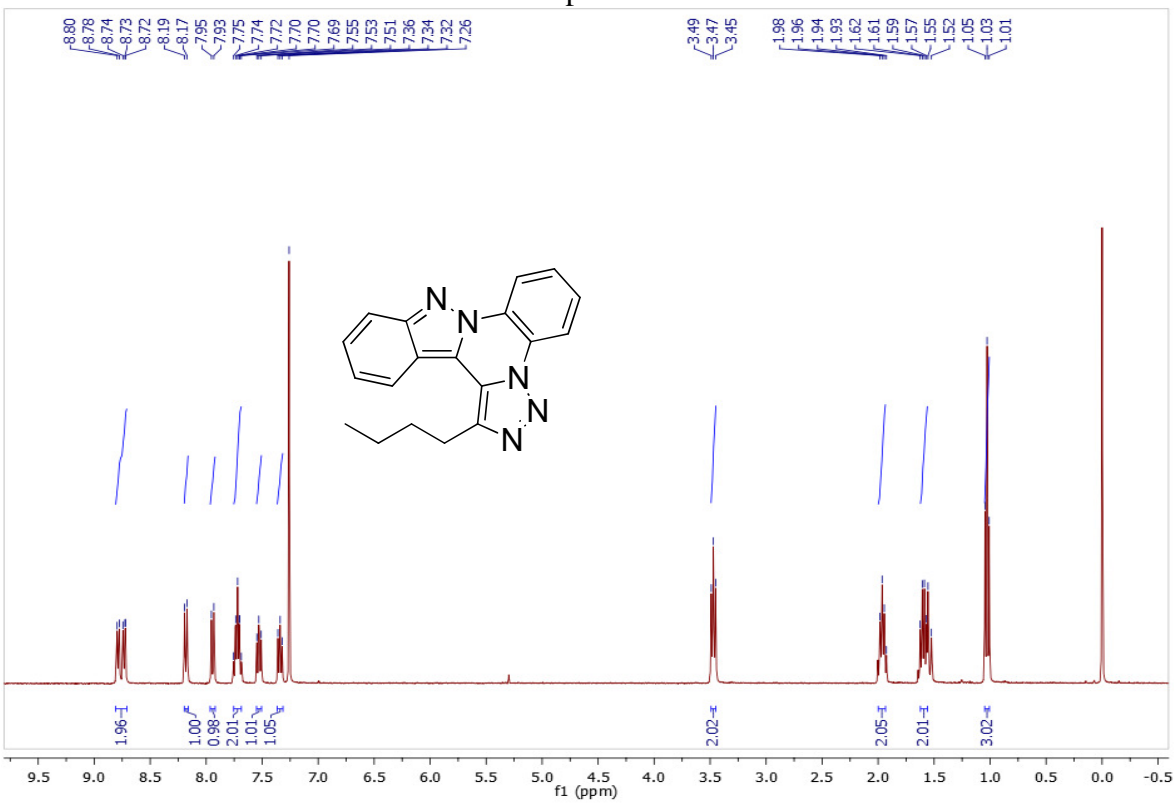
122.77
121.45
118.36
118.17
117.60
117.11
f1 (ppm)

Compound- **7e**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7.93
7.75
7.74
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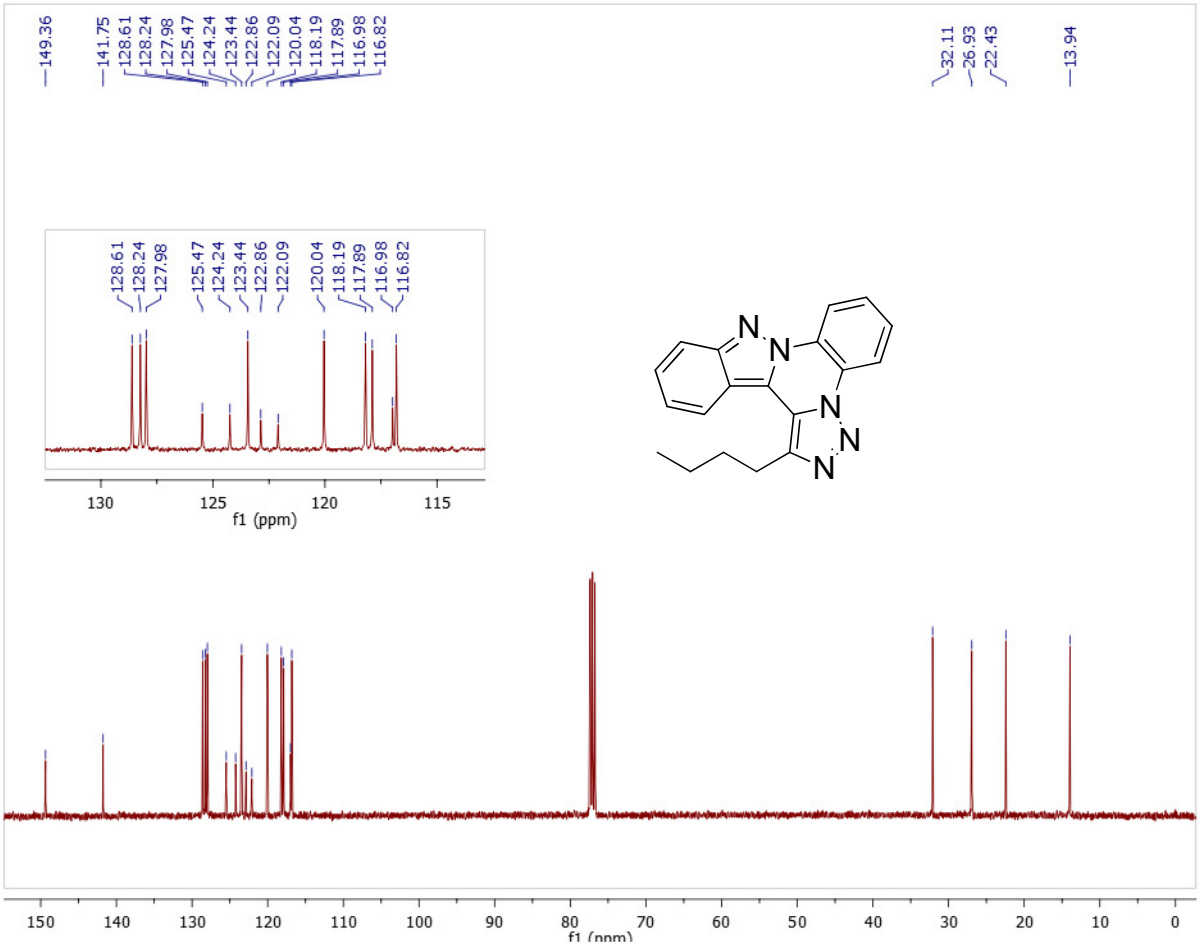
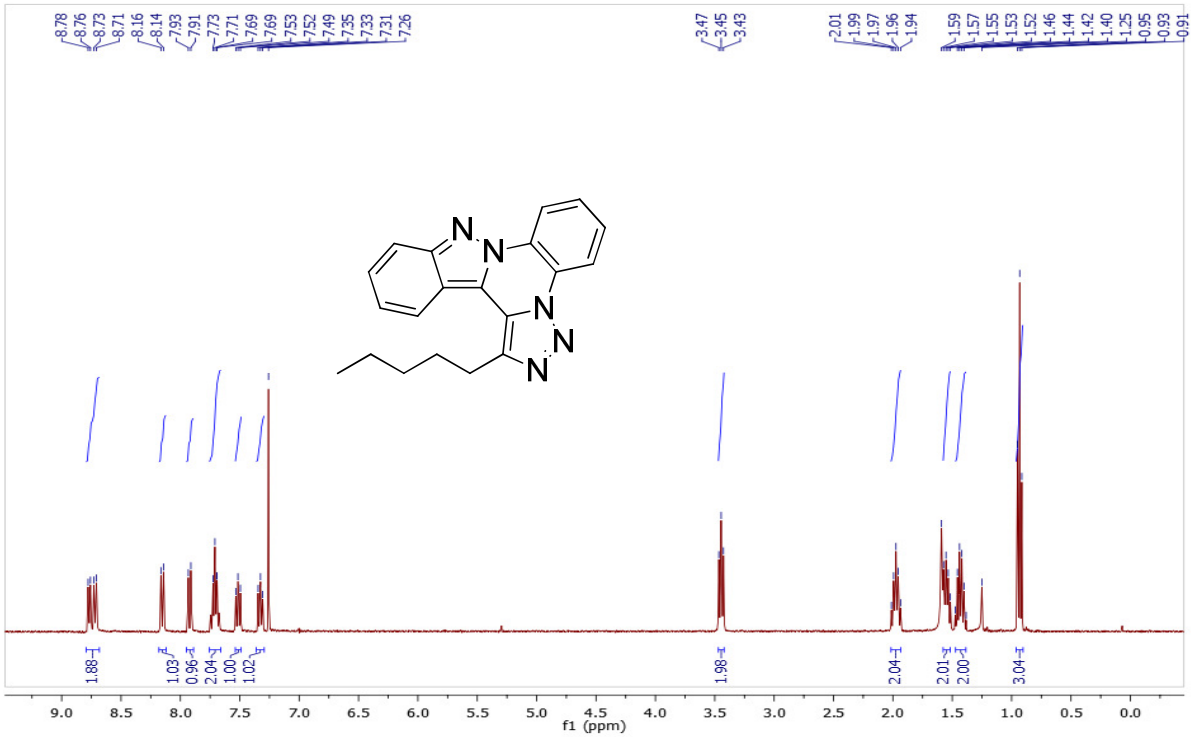
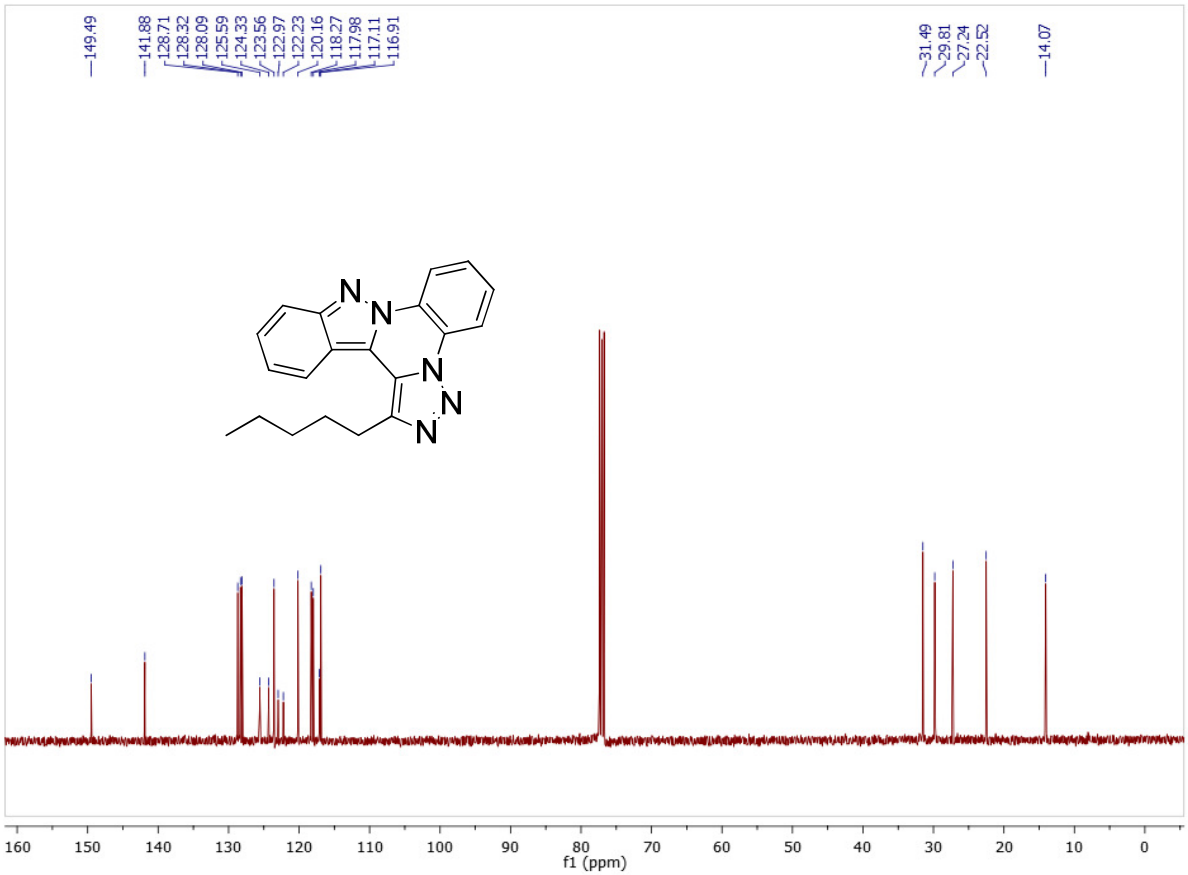
7.70
7.69
7.55
7.53
7.51
7.36
7.34
7.32
7.26
3.49
3.47
3.45
1.98
1.96
1.94
1.93
1.62
1.61
1.59
1.57
1.55
1.52
1.05
1.03
1.01
1.96
1.00
0.98
2.01
1.01
1.05
2.02
2.05
2.01
3.02
f1 (ppm)

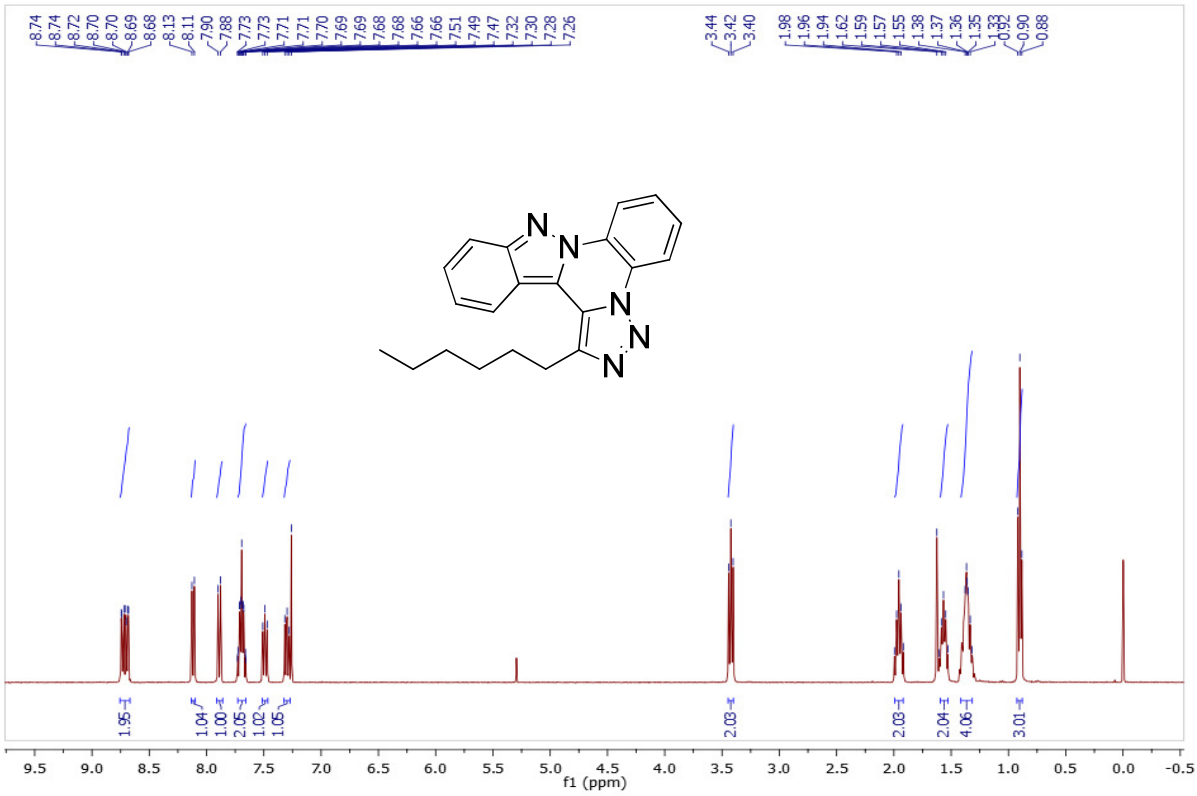

149.36
141.75
128.61
128.24
127.98
125.47
124.24
123.44
122.86
122.09
120.04
118.19
117.89
116.98
116.82
32.11
26.93
22.43
13.94
f1 (ppm)
f1 (ppm)

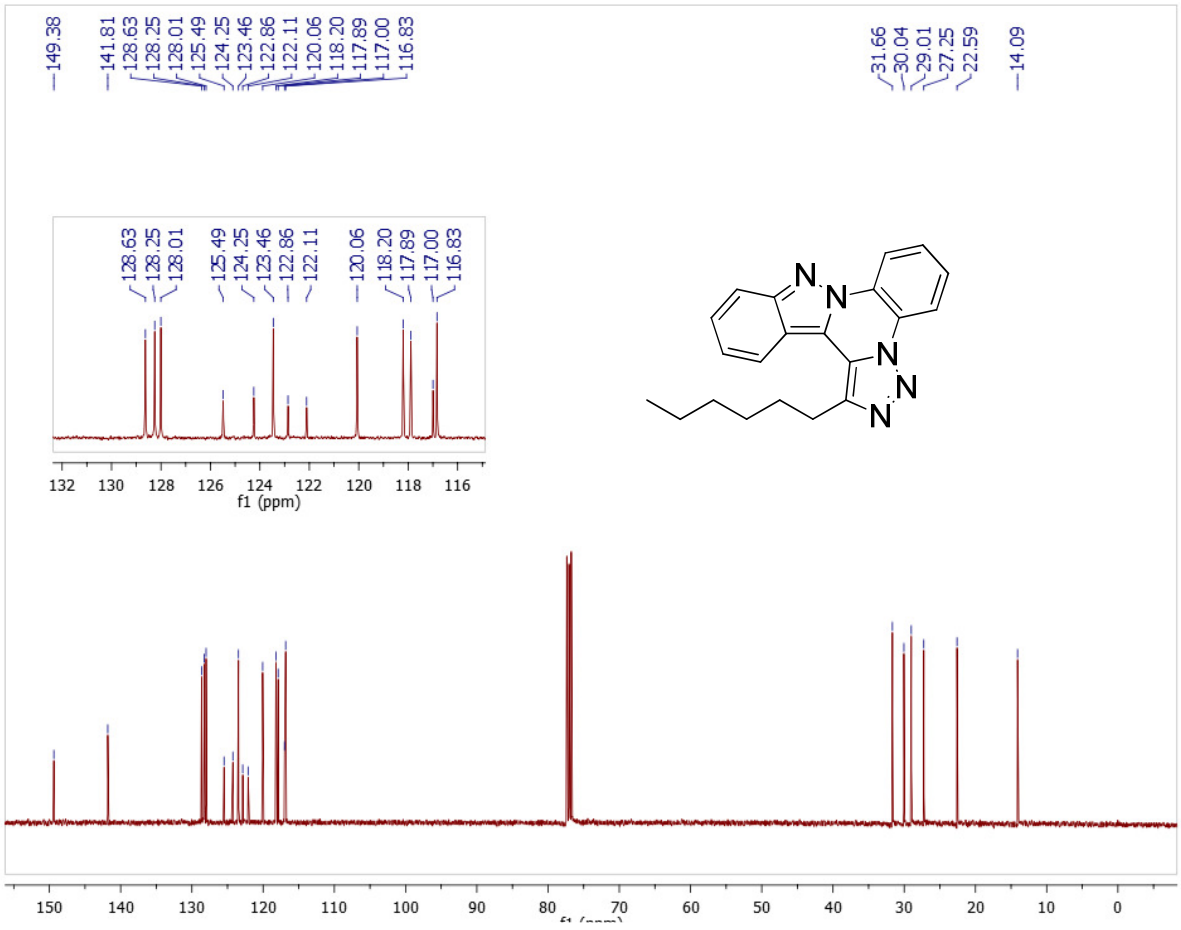
Compound- **7f**


8.78
8.76
8.73
8.71
8.16
8.14
7.93
7.91
7.73
7.71
7.69
7.69
7.53
7.52
7.49
7.35
7.33
7.31
7.26
3.47
3.45
3.43
2.01
1.99
1.97
1.96
1.94
1.59
1.57
1.55
1.53
1.52
1.46
1.44
1.42
1.40
1.25
0.95
0.93
0.91
1.88
1.03
0.96
2.04
1.00
1.02
1.98
2.04
2.01
2.00
3.04
f1 (ppm)

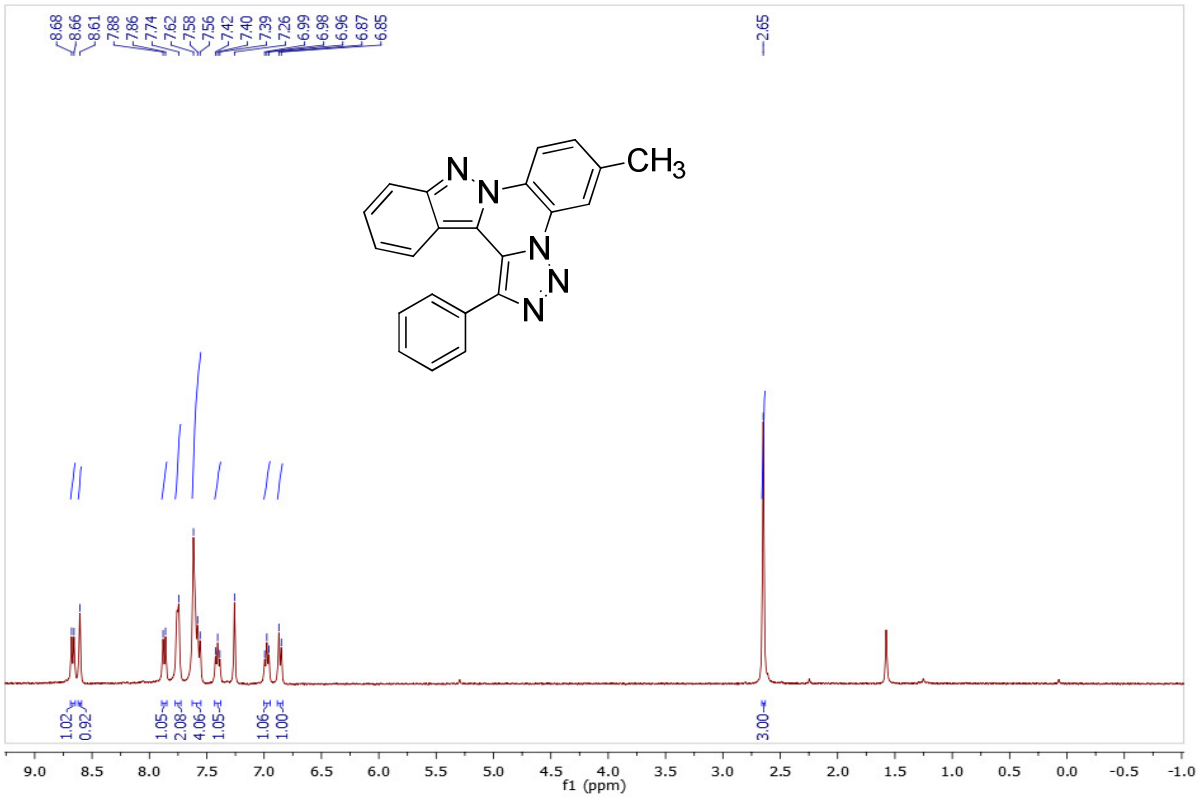

149.49
141.88
128.71
128.32
128.09
125.59
124.33
123.56
122.97
122.23
120.16
118.27
117.98
117.11
116.91
31.49
29.81
27.24
22.52
14.07
f1 (ppm)

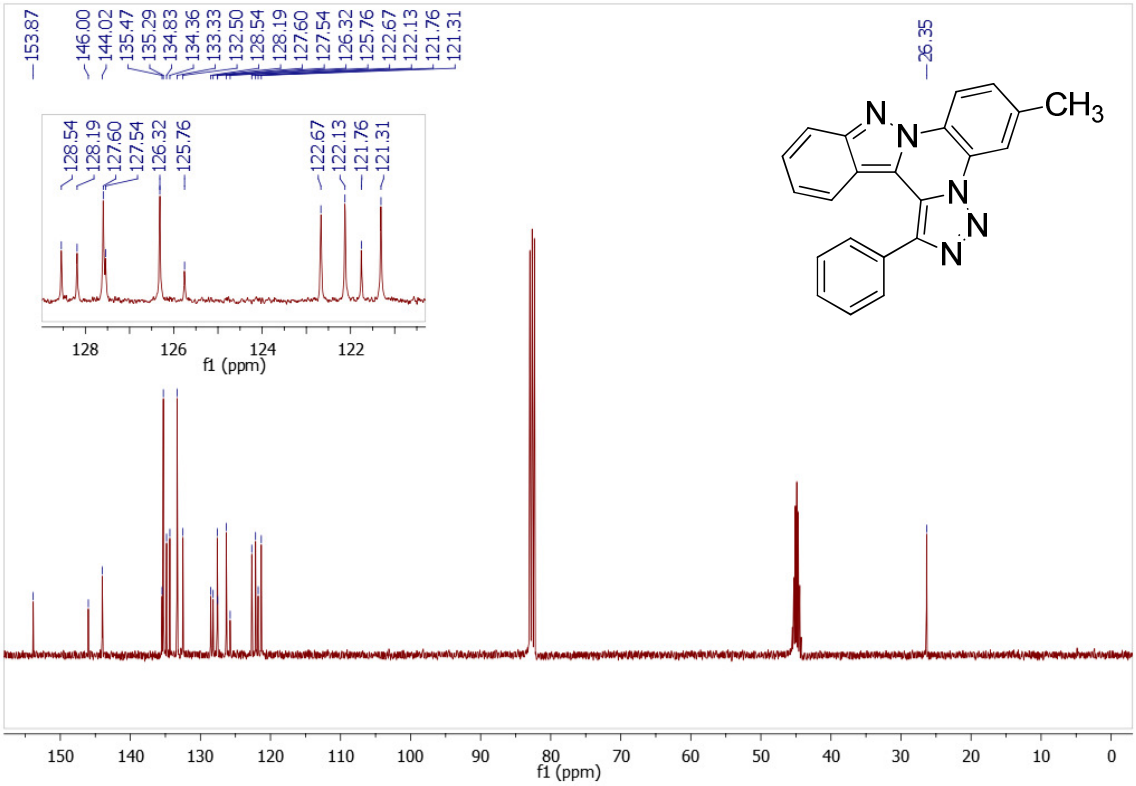
Compound- **7g**


8.74
8.74
8.72
8.70
8.70
8.69
8.68
8.13
8.11
7.90
7.88
7.73
7.73
7.71
7.71
7.70
7.69
7.69
7.68
7.68
7.66
7.66
7.51
7.49
7.47
7.32
7.30
7.28
7.26
3.44
3.42
3.40
1.98
1.96
1.94
1.62
1.59
1.57
1.55
1.38
1.37
1.36
1.35
0.92
0.90
0.88
N
N
N
N
N
1.95
1.04
1.00
2.05
1.02
1.05
2.03
2.03
2.04
4.06
3.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

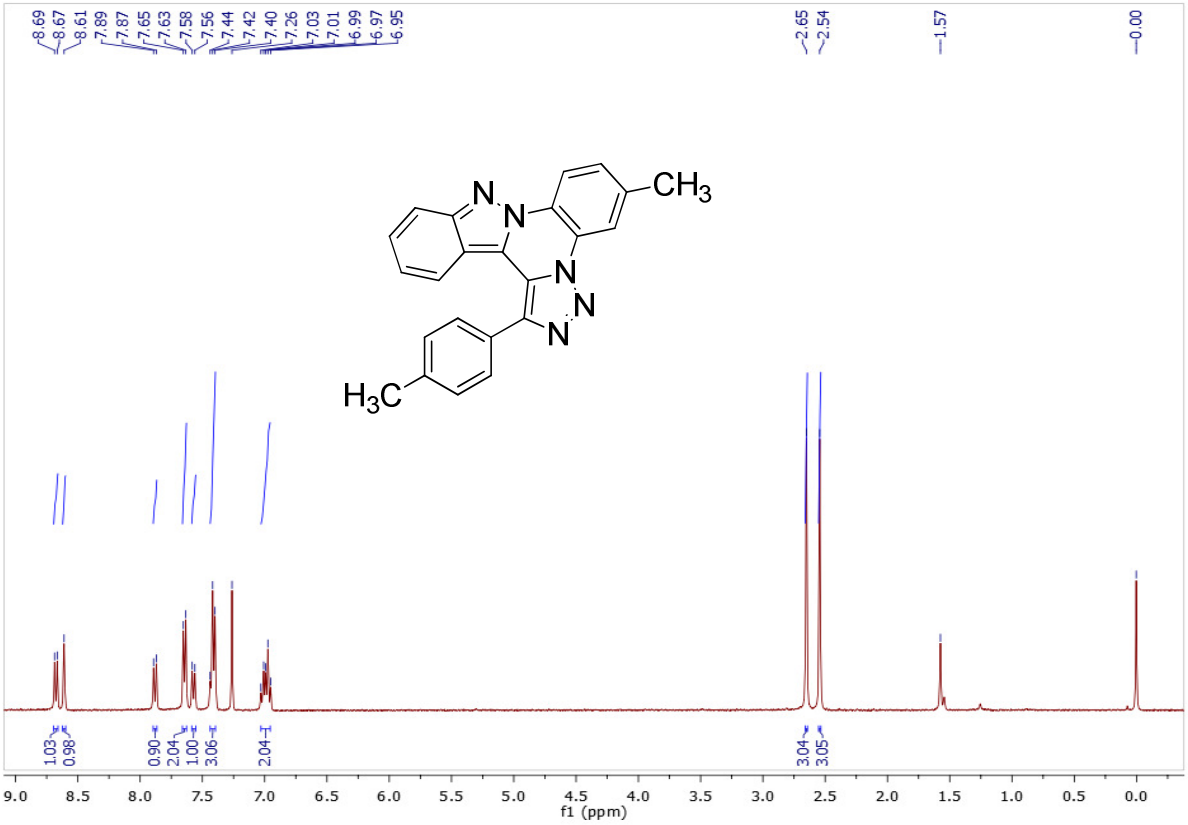

149.38
141.81
128.63
128.25
128.01
125.49
124.25
123.46
122.86
122.11
120.06
118.20
117.89
117.00
116.83
31.66
30.04
29.01
27.25
22.59
14.09
N
N
N
N
N
132
130
128
126
124
122
120
118
116
f1 (ppm)
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

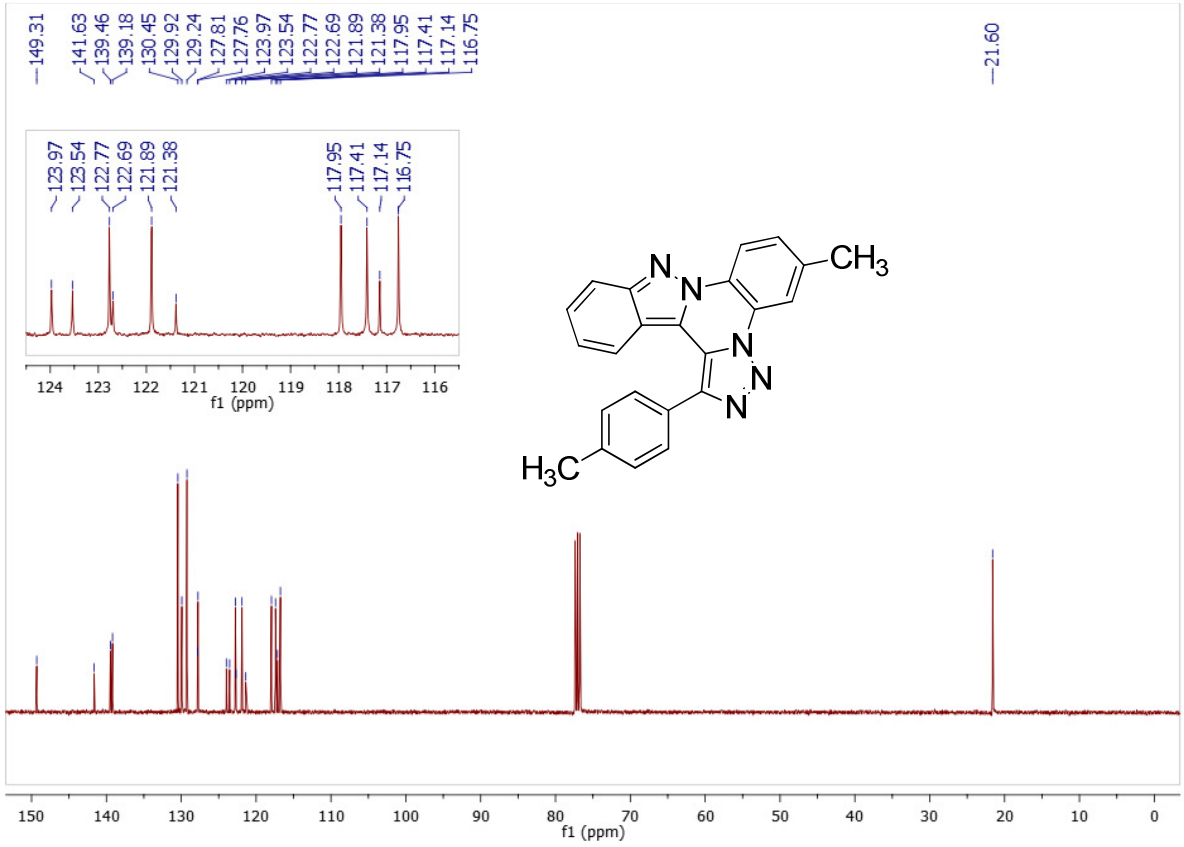
Compound- **7h**


8.68
8.66
8.61
7.88
7.86
7.74
7.62
7.58
7.56
7.42
7.40
7.39
7.26
6.99
6.98
6.96
6.87
6.85
2.65
CH3
N
N
N
N
N
1.02
0.92
1.05
2.08
4.06
1.05
1.06
1.00
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

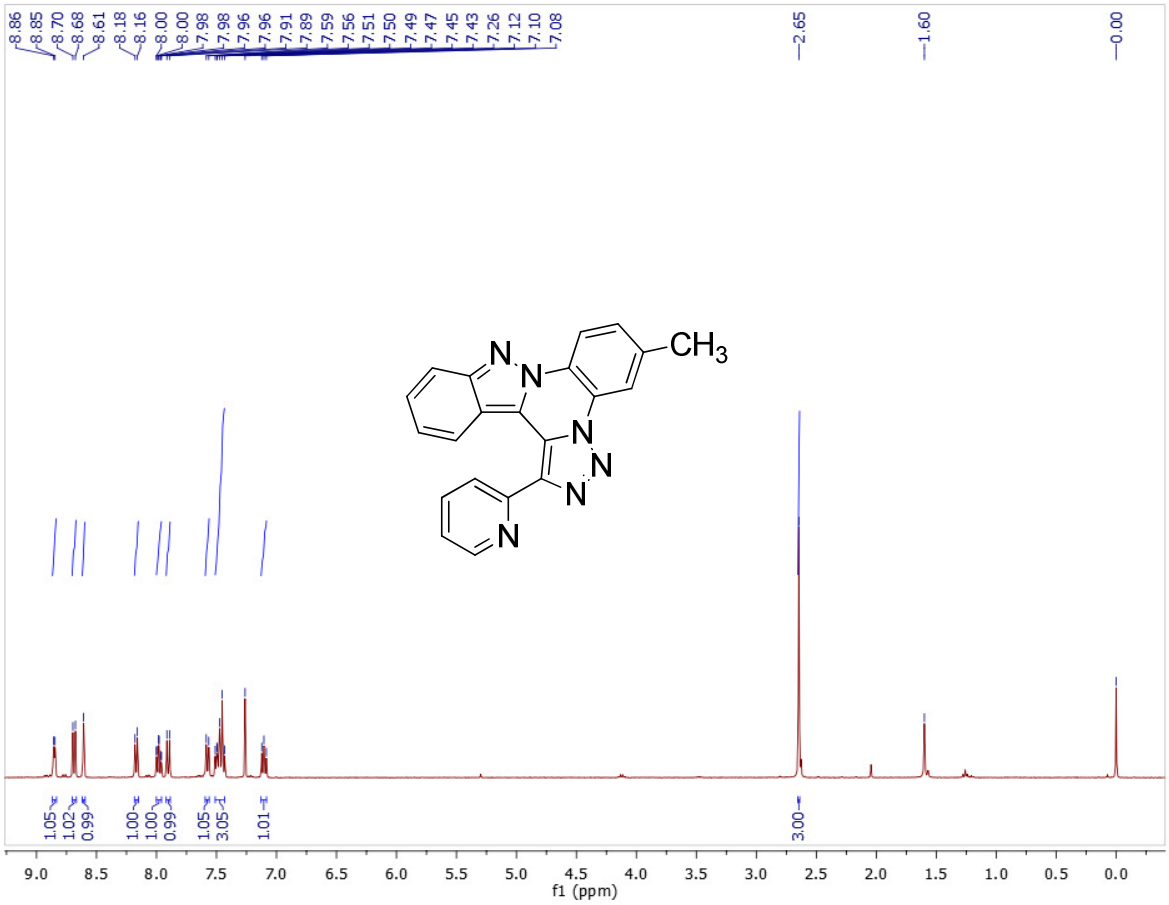

153.87
146.00
144.02
135.47
135.29
134.83
134.36
133.33
132.50
128.54
128.19
127.60
127.54
126.32
125.76
122.67
122.13
121.76
121.31
26.35
CH3
N
N
N
N
N
128 126 124 122
f1 (ppm)
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

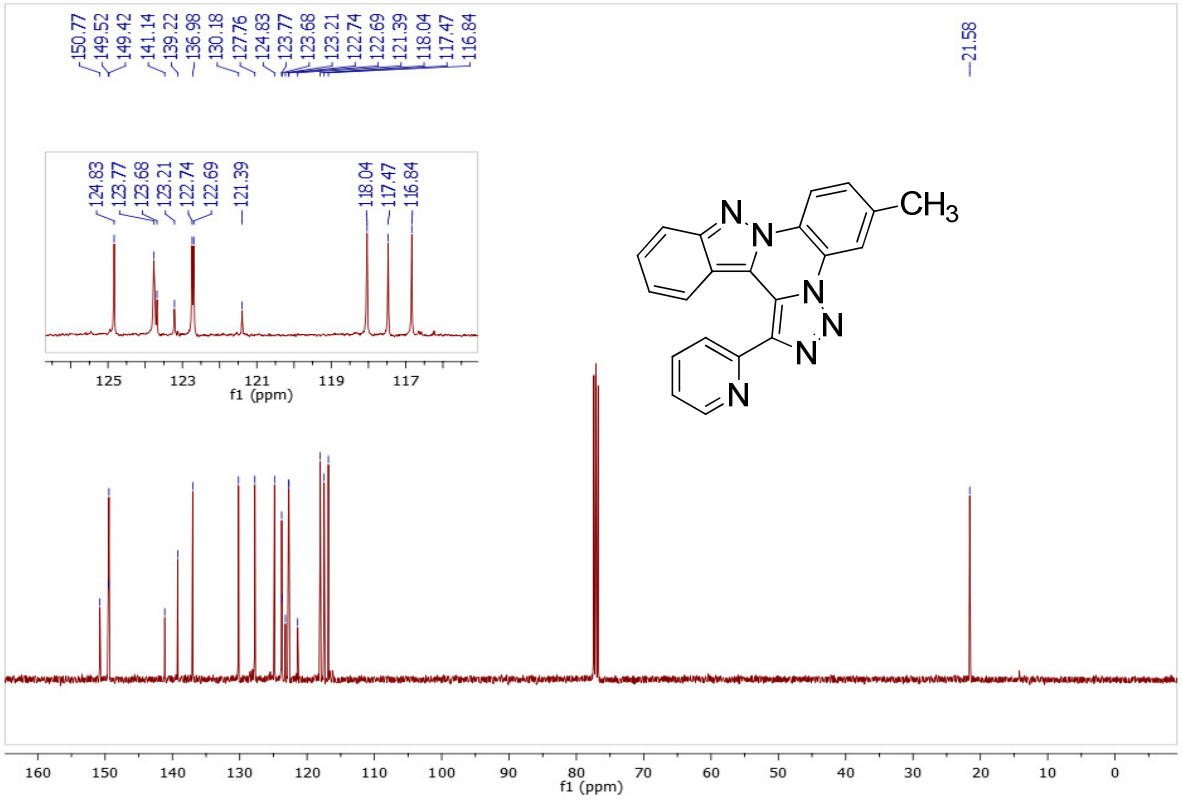
Compound- **7i**


8.69
8.67
8.61
7.89
7.87
7.65
7.63
7.58
7.56
7.44
7.42
7.40
7.26
7.03
7.01
6.99
6.97
6.95
2.65
2.54
1.57
0.00
CH3
H3C
1.03
0.98
0.90
2.04
1.00
3.06
2.04
3.04
3.05
f1 (ppm)

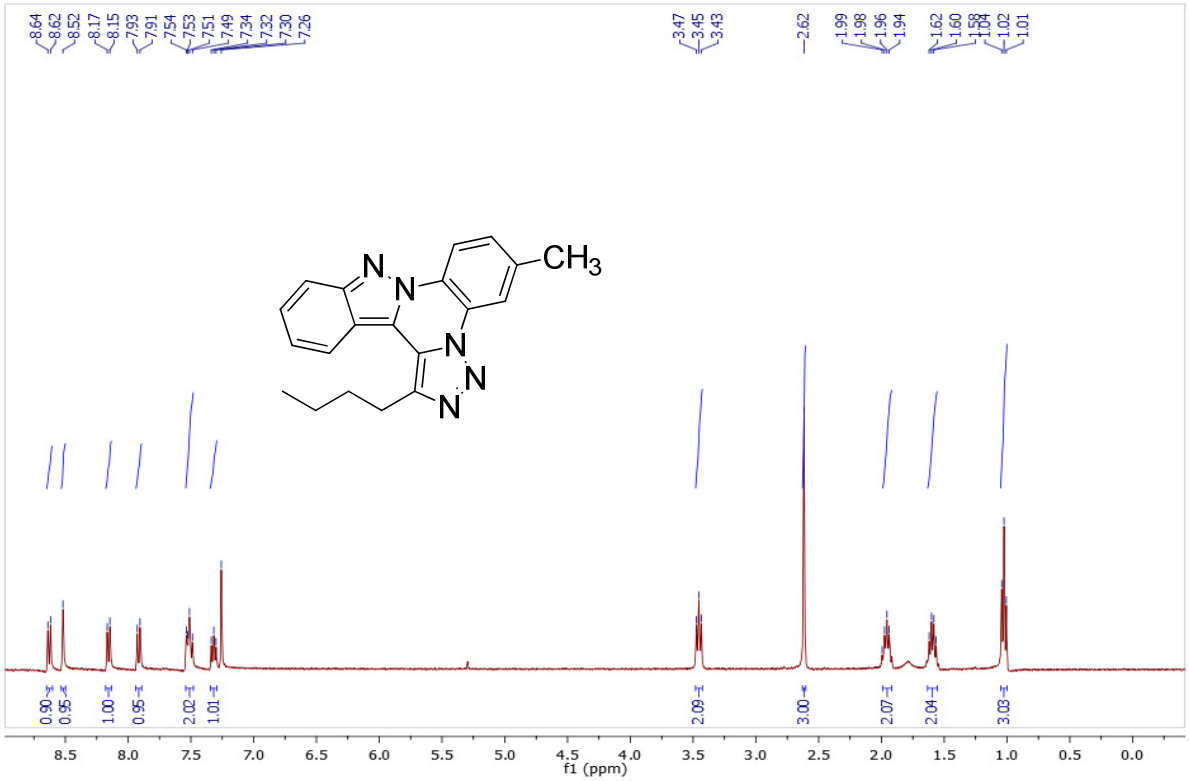

149.31
141.63
139.46
139.18
130.45
129.92
129.24
127.81
127.76
123.97
123.54
122.77
122.69
121.89
121.38
117.95
117.41
117.14
116.75
21.60
CH3
H3C
f1 (ppm)

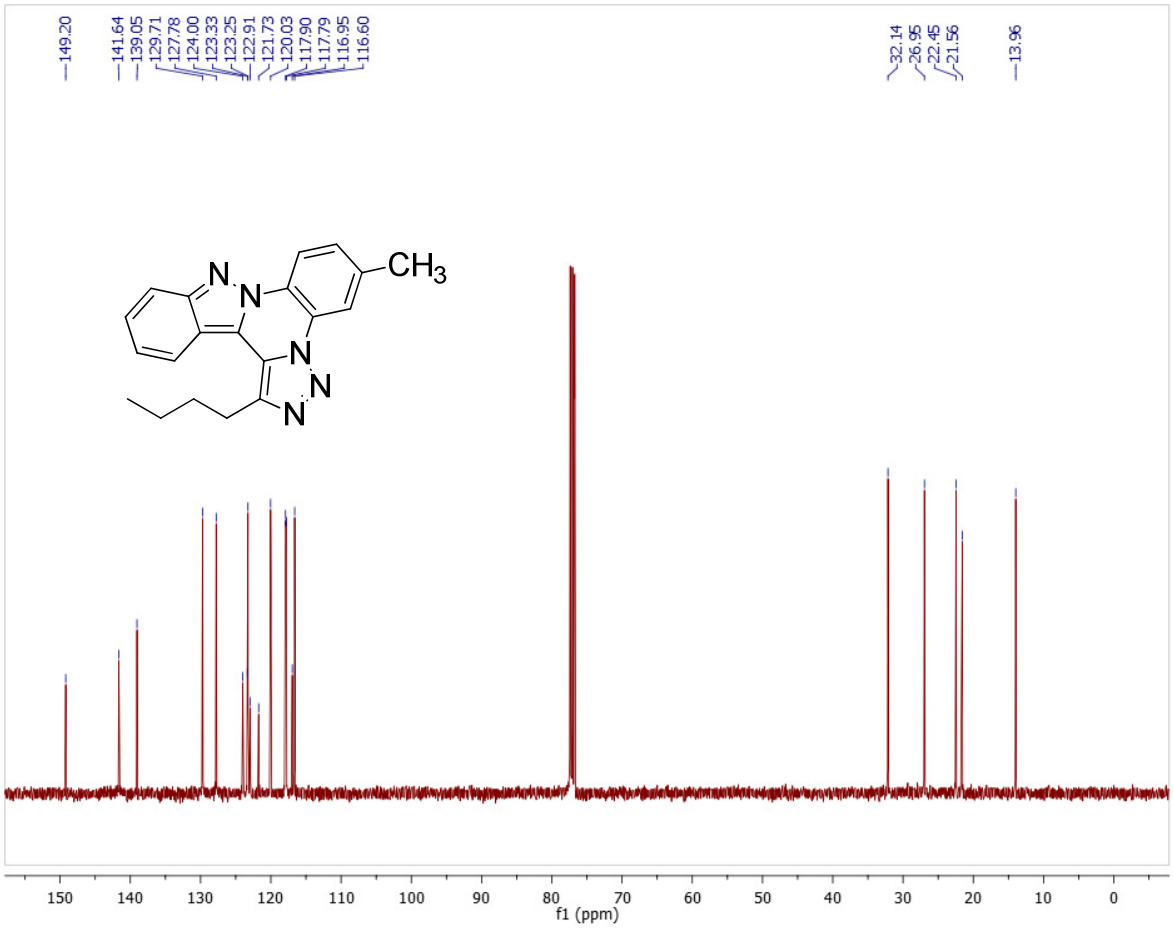
Compound- **7j**


8.86
8.85
8.70
8.68
8.61
8.18
8.16
8.00
8.00
7.98
7.98
7.96
7.96
7.91
7.89
7.59
7.56
7.51
7.50
7.49
7.47
7.45
7.43
7.26
7.12
7.10
7.08
2.65
1.60
0.00
CH3
1.05
1.02
0.99
1.00
1.00
0.99
1.05
3.05
1.01
3.00
f1 (ppm)

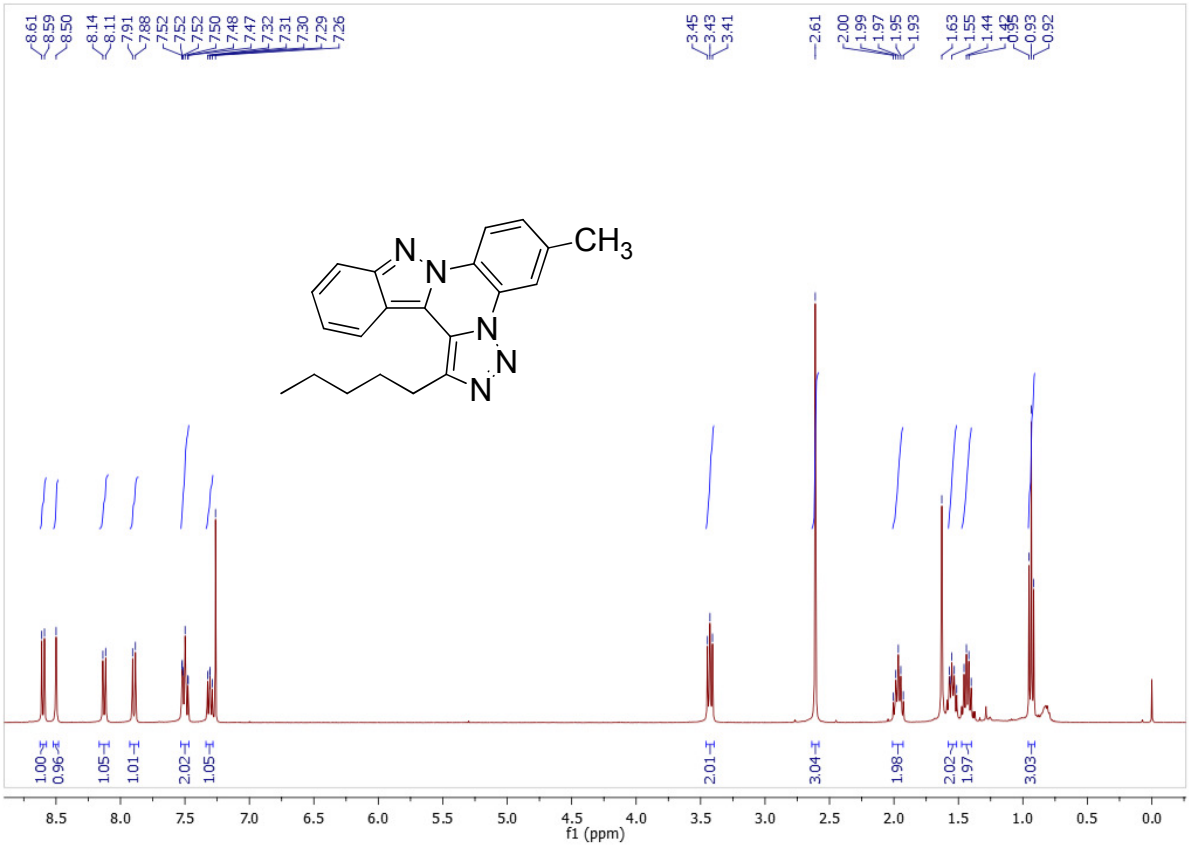

150.77
149.52
149.42
141.14
139.22
136.98
130.18
127.76
124.83
123.77
123.68
123.21
122.74
122.69
121.39
118.04
117.47
116.84
21.58
CH3
f1 (ppm)
f1 (ppm)

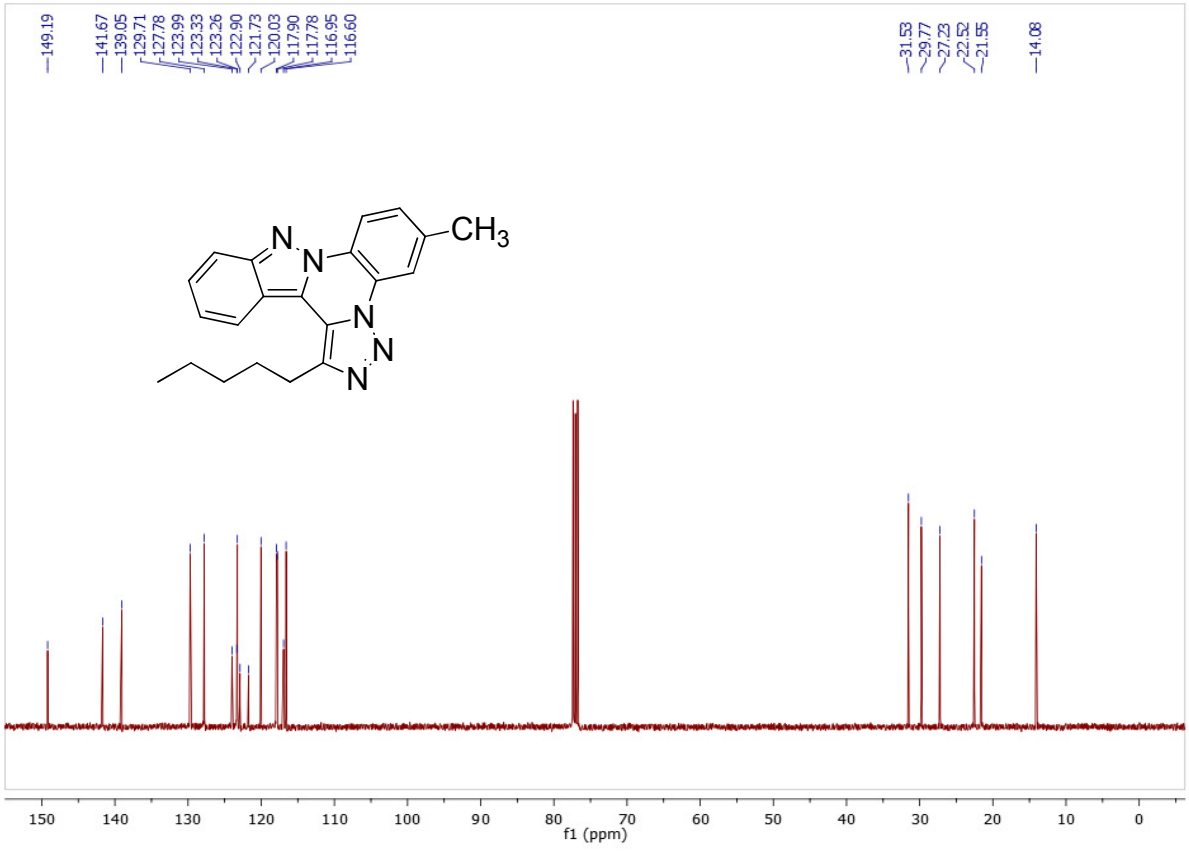
Compound- **7k**


8.64
8.62
8.52
8.17
8.15
7.93
7.91
7.54
7.53
7.51
7.49
7.34
7.32
7.30
7.26
3.47
3.45
3.43
2.62
1.99
1.98
1.96
1.94
1.62
1.60
1.58
1.04
1.02
1.01
CH3
0.90
0.95
1.00
0.95
2.02
1.01
2.09
3.00
2.07
2.04
3.03
f1 (ppm)

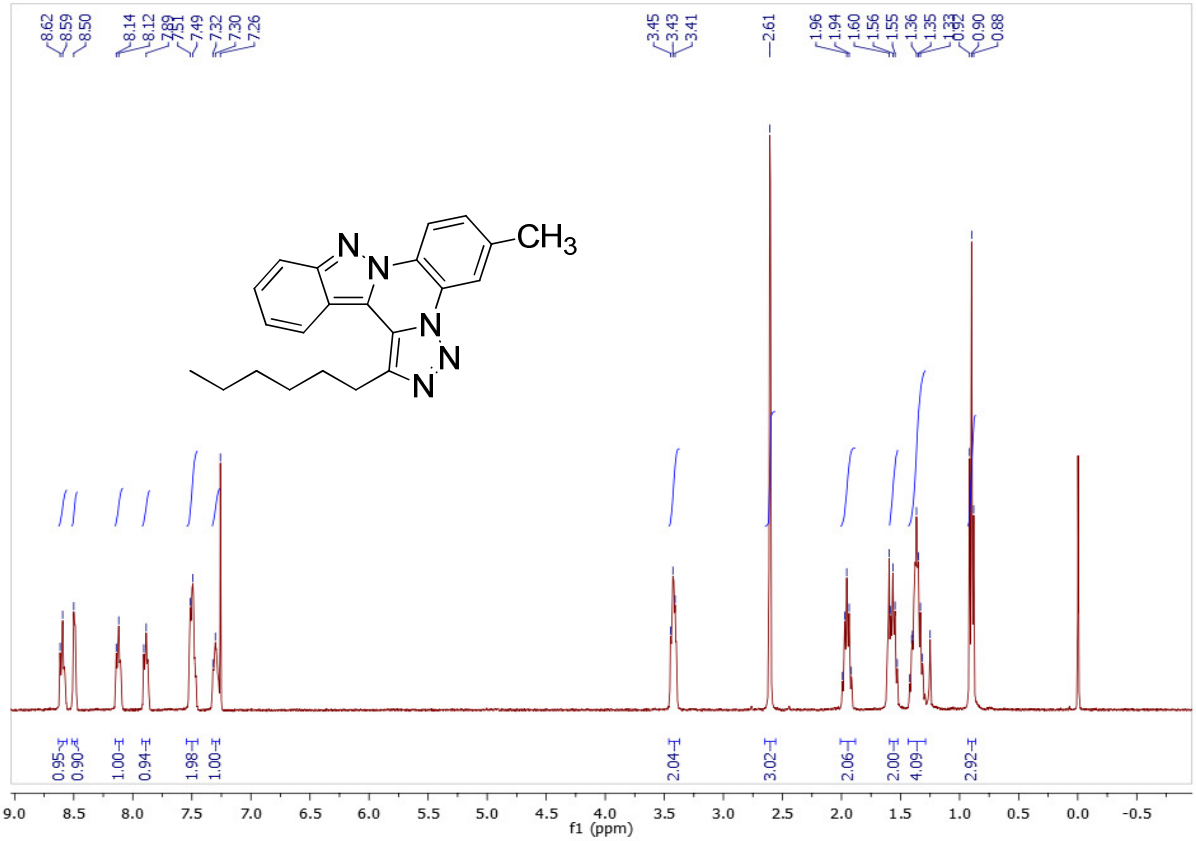

149.20
141.64
139.05
129.71
127.78
124.00
123.33
123.25
122.91
121.73
120.03
117.90
117.79
116.95
116.60
32.14
26.95
22.45
21.56
13.96
CH3
f1 (ppm)

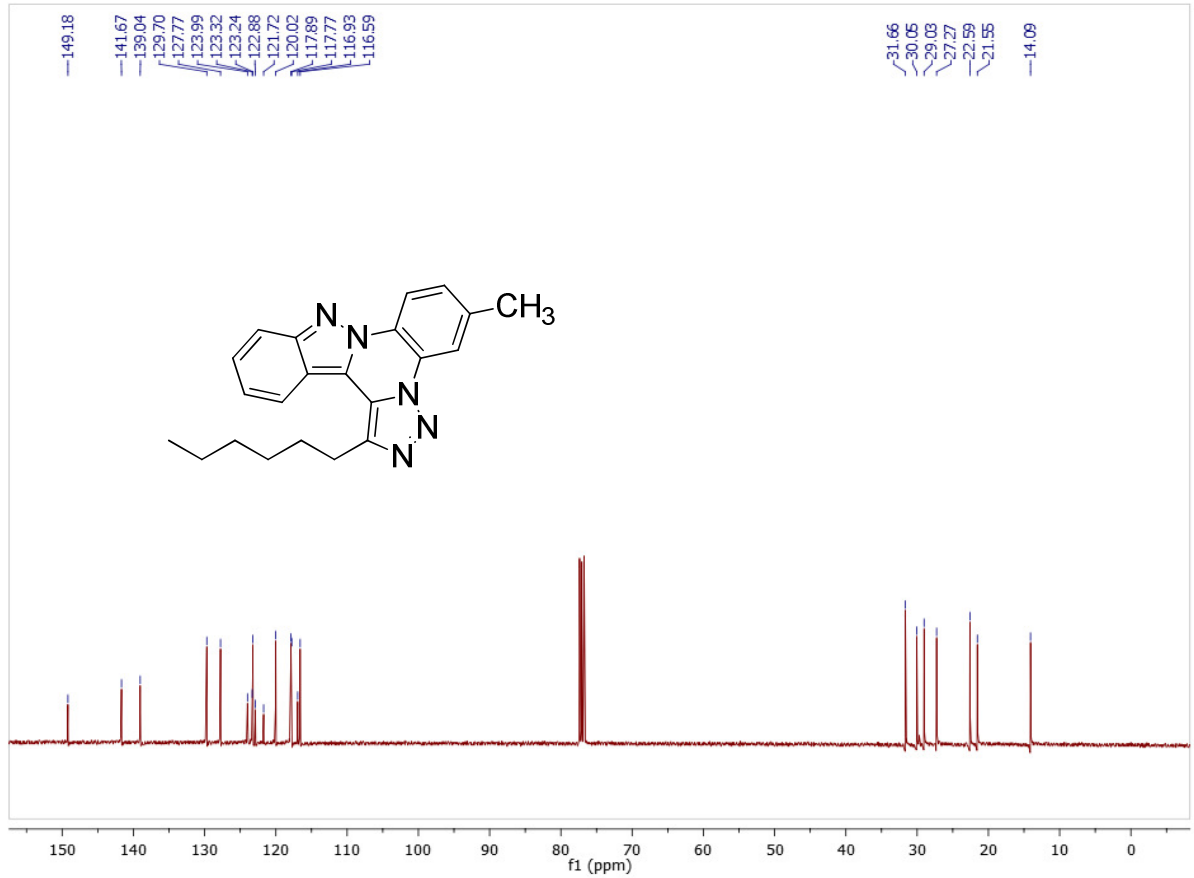
Compound- **7l**


8.61
8.59
8.50
8.14
8.11
7.91
7.88
7.52
7.52
7.52
7.50
7.48
7.47
7.32
7.31
7.30
7.29
7.26
3.45
3.43
3.41
2.61
2.00
1.99
1.97
1.95
1.93
1.63
1.55
1.44
0.95
0.93
0.92
CH3
N
N
N
N
N
1.00
0.96
1.05
1.01
2.02
1.05
2.01
3.04
1.98
2.02
1.97
3.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

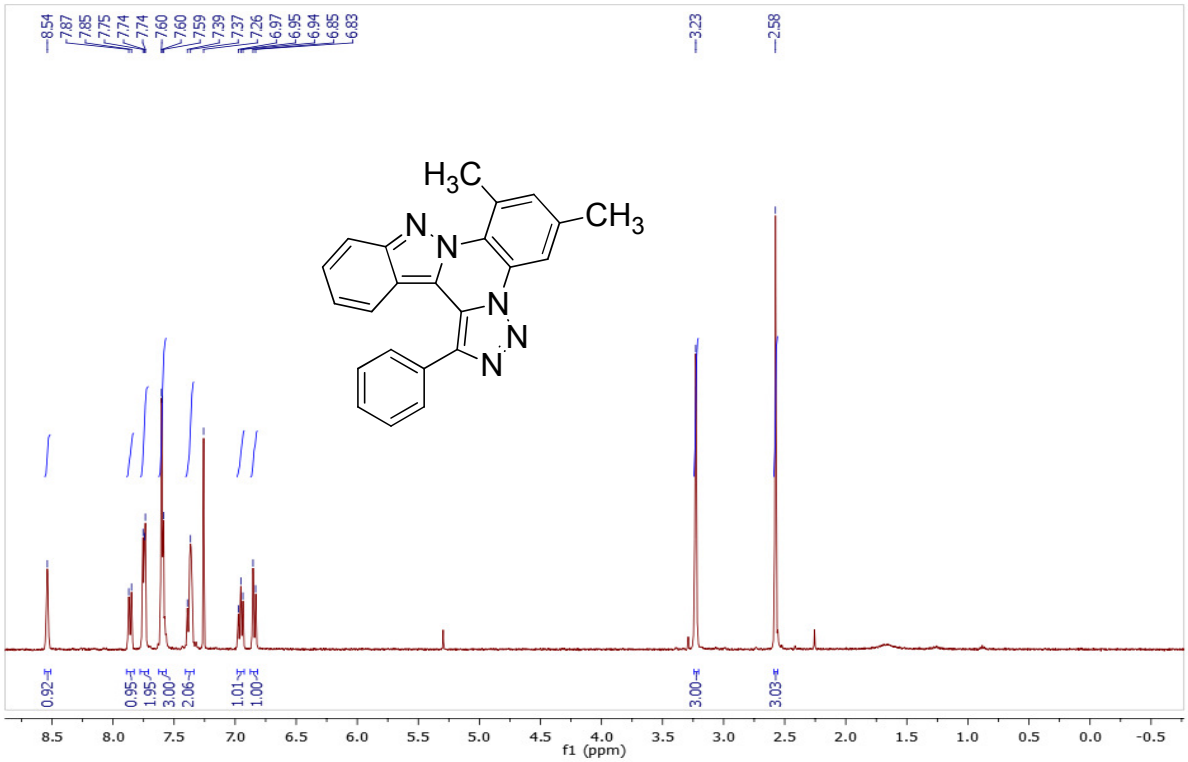

149.19
141.67
139.05
129.71
127.78
123.99
123.33
123.26
122.90
121.73
120.03
117.90
117.78
116.95
116.60
31.53
29.77
27.23
22.52
21.55
14.08
CH3
N
N
N
N
N
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Compound- **7m**

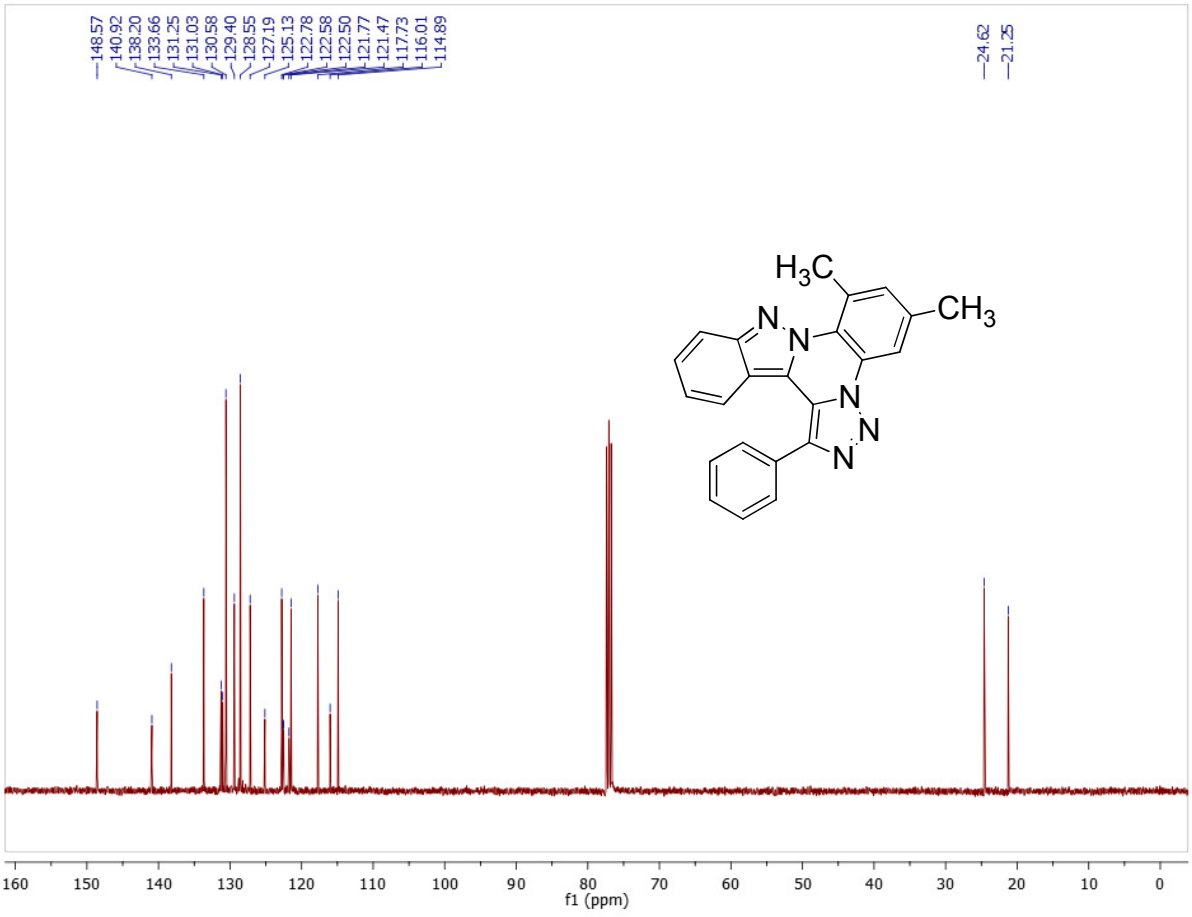

8.62
8.59
8.50
8.14
8.12
7.89
7.51
7.49
7.32
7.30
7.26
3.45
3.43
3.41
2.61
1.96
1.94
1.60
1.56
1.55
1.36
1.35
0.92
0.90
0.88
CH3
N
N
N
N
N
0.95
0.90
1.00
0.94
1.98
1.00
2.04
3.02
2.06
2.00
4.09
2.92
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


149.18
141.67
139.04
129.70
127.77
123.99
123.32
123.24
122.88
121.72
120.02
117.89
117.77
116.93
116.59
31.66
30.05
29.03
27.27
22.59
21.55
14.09
CH3
N
N
N
N
N
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

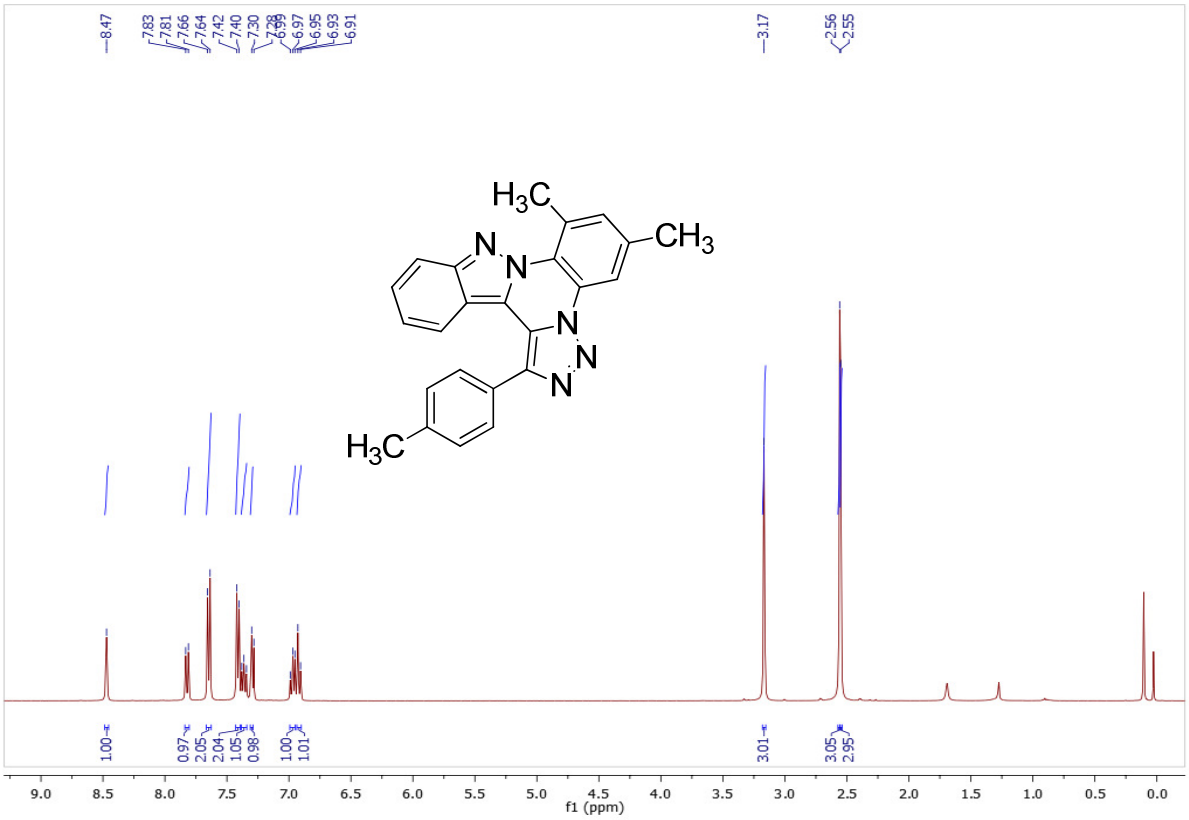
Compound-**7n**

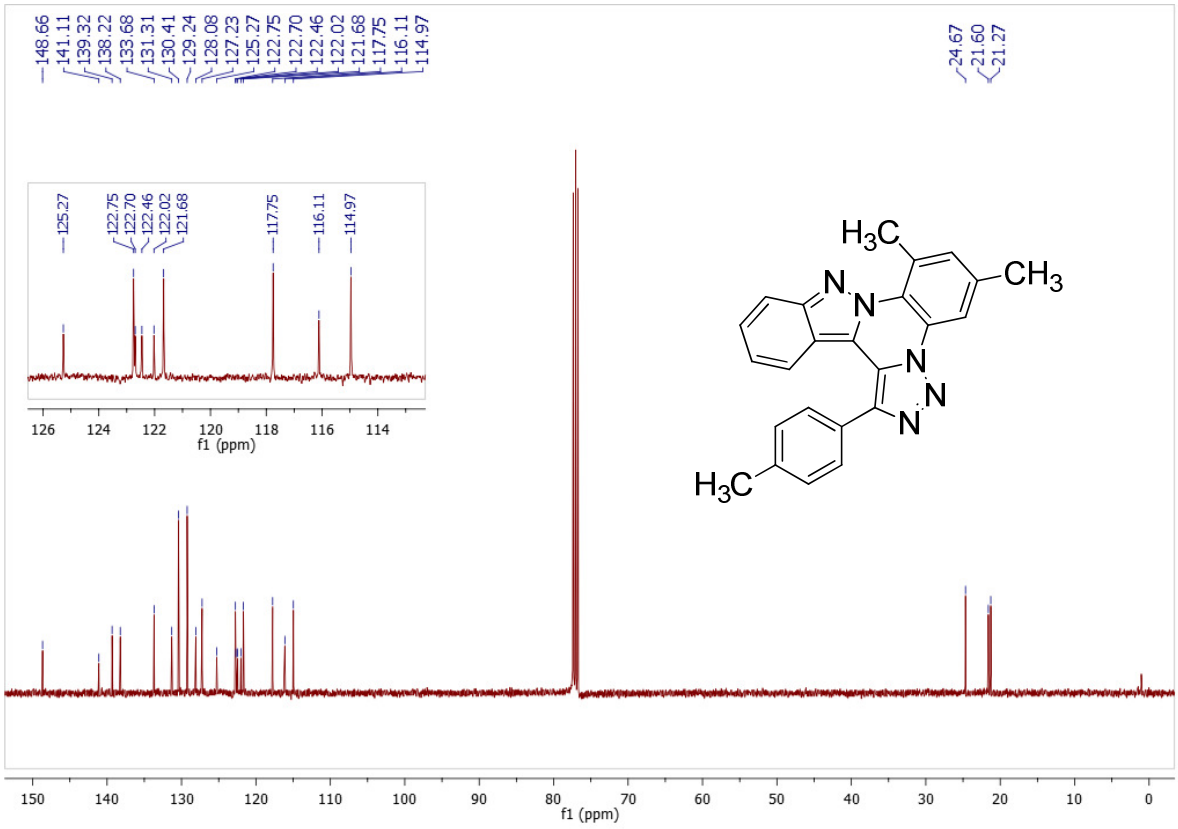

8.54
7.87
7.85
7.75
7.74
7.74
7.60
7.60
7.59
7.39
7.37
7.26
6.97
6.95
6.94
6.85
6.83
3.23
2.58
H3C
CH3
N
N
N
N
N
0.92
0.95
1.95
3.00
2.06
1.01
1.00
3.00
3.03
f1 (ppm)

•

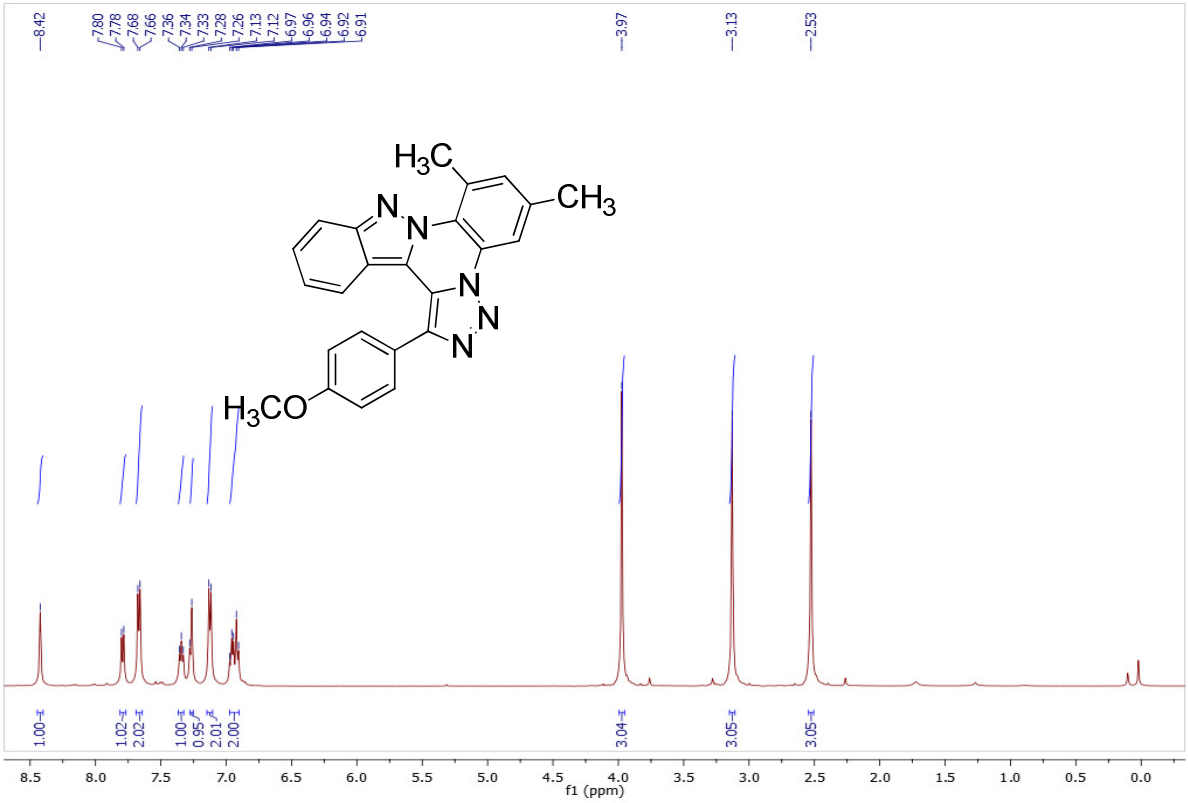

148.57
140.92
138.20
133.66
131.25
131.03
130.58
129.40
128.55
127.19
125.13
122.78
122.58
122.50
121.77
121.47
117.73
116.01
114.89
24.62
21.25
H3C
CH3
N
N
N
N
N
f1 (ppm)

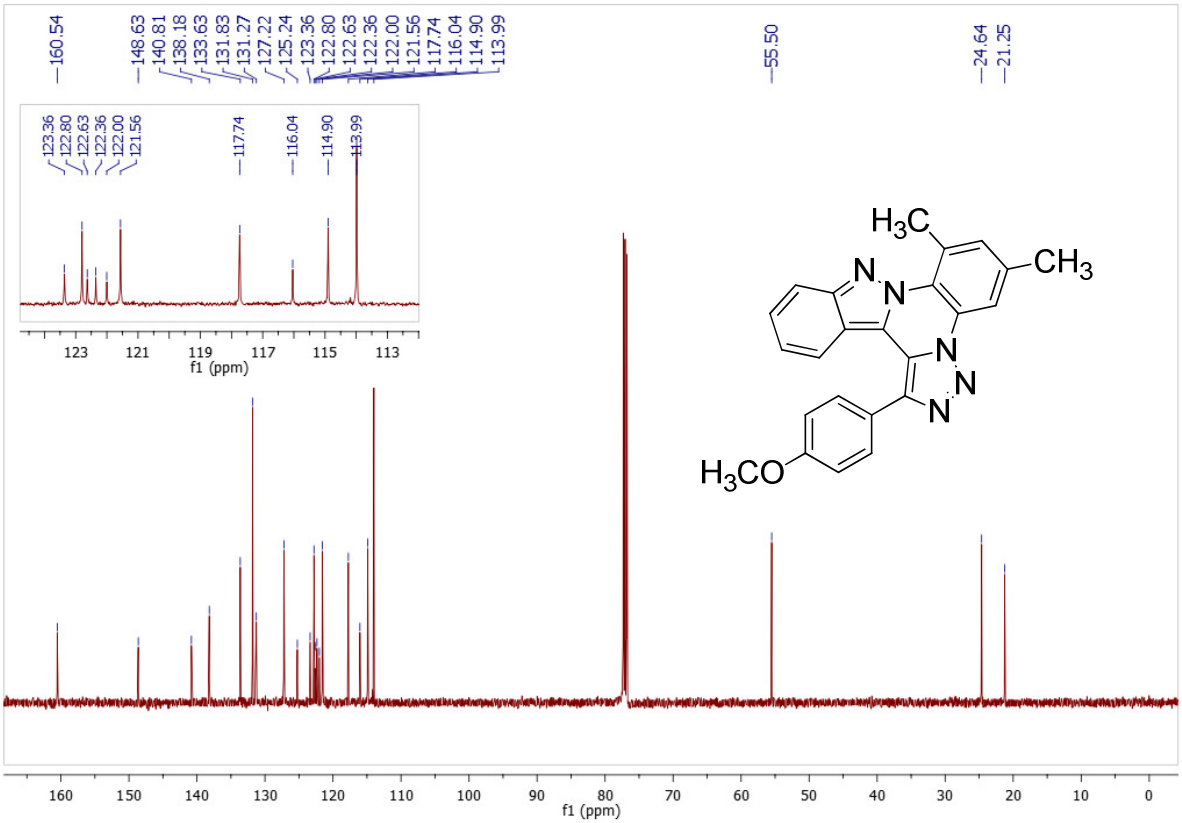
Compound- **7o**


8.47
7.83
7.81
7.66
7.64
7.42
7.40
7.30
6.97
6.95
6.93
6.91
3.17
2.56
2.55
H3C
CH3
N
N
N
N
N
H3C
1.00
0.97
2.05
2.04
1.05
0.98
1.00
1.01
3.01
3.05
2.95
f1 (ppm)

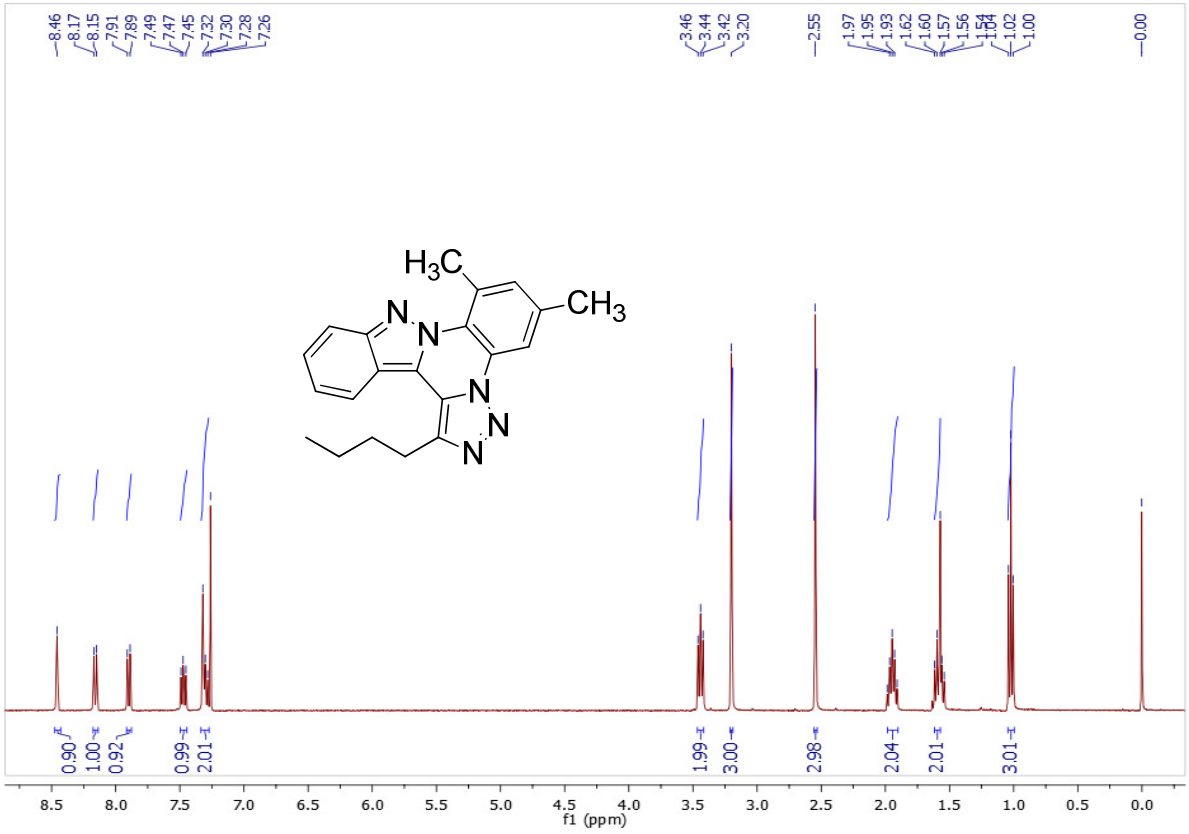

148.66
141.11
139.32
138.22
133.68
131.31
130.41
129.24
128.08
127.23
125.27
122.75
122.70
122.46
122.02
121.68
117.75
116.11
114.97
24.67
21.60
21.27
f1 (ppm)
H3C
CH3
N
N
N
N
N
H3C

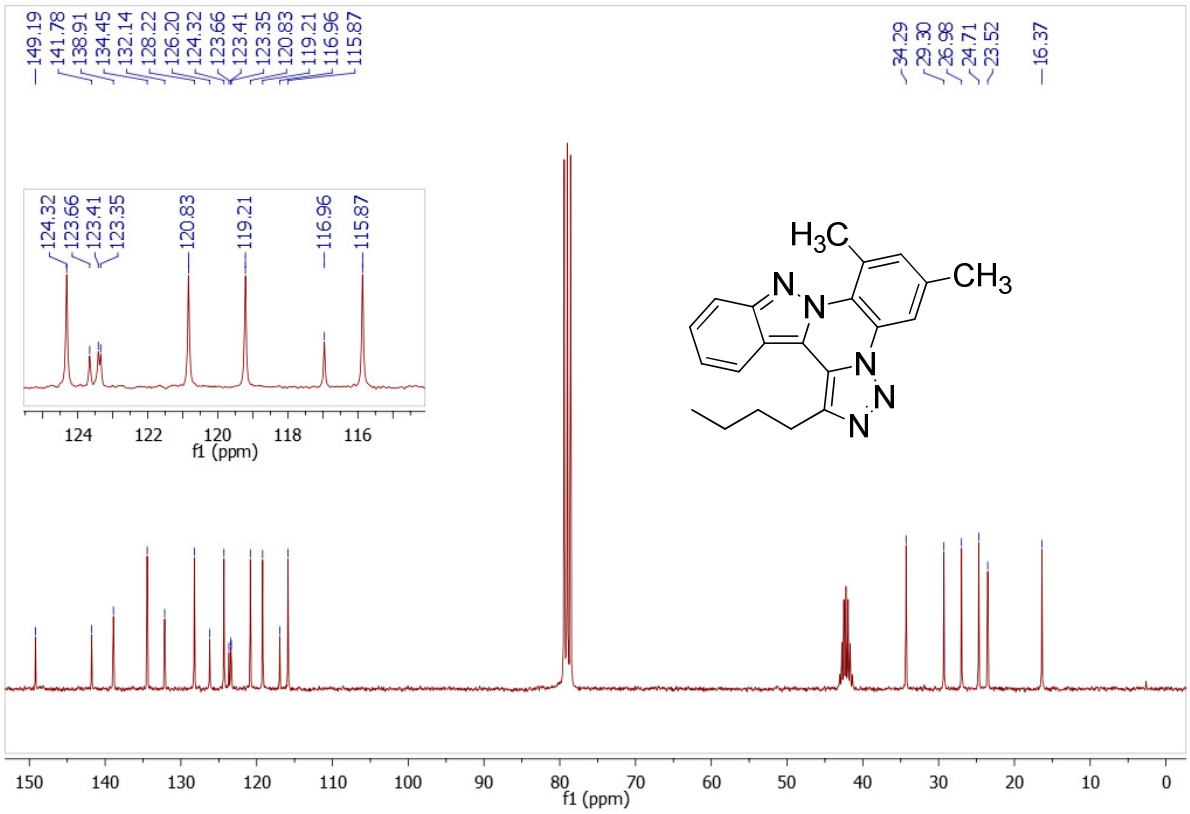
Compound- **7p**


8.42
7.80
7.78
7.68
7.66
7.36
7.34
7.33
7.28
7.26
7.13
7.12
6.97
6.96
6.94
6.92
6.91
3.97
3.13
2.53
H3C
CH3
N
N
N
N
H3CO
1.00
1.02
2.02
1.00
0.95
2.01
2.00
3.04
3.05
3.05
f1 (ppm)

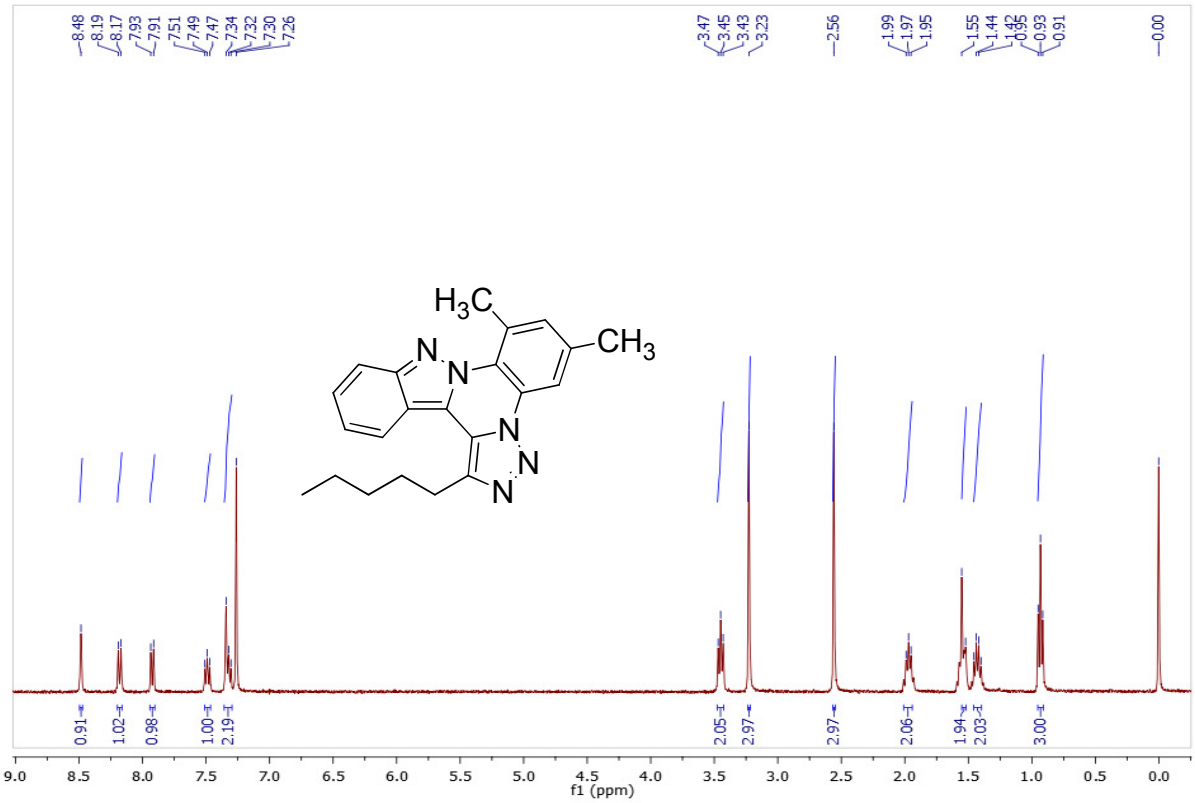

160.54
148.63
140.81
138.18
133.63
131.83
131.27
127.22
125.24
123.36
122.80
122.63
122.36
122.00
121.56
117.74
116.04
114.90
113.99
55.50
24.64
21.25
f1 (ppm)
H3C
CH3
N
N
N
N
H3CO
f1 (ppm)

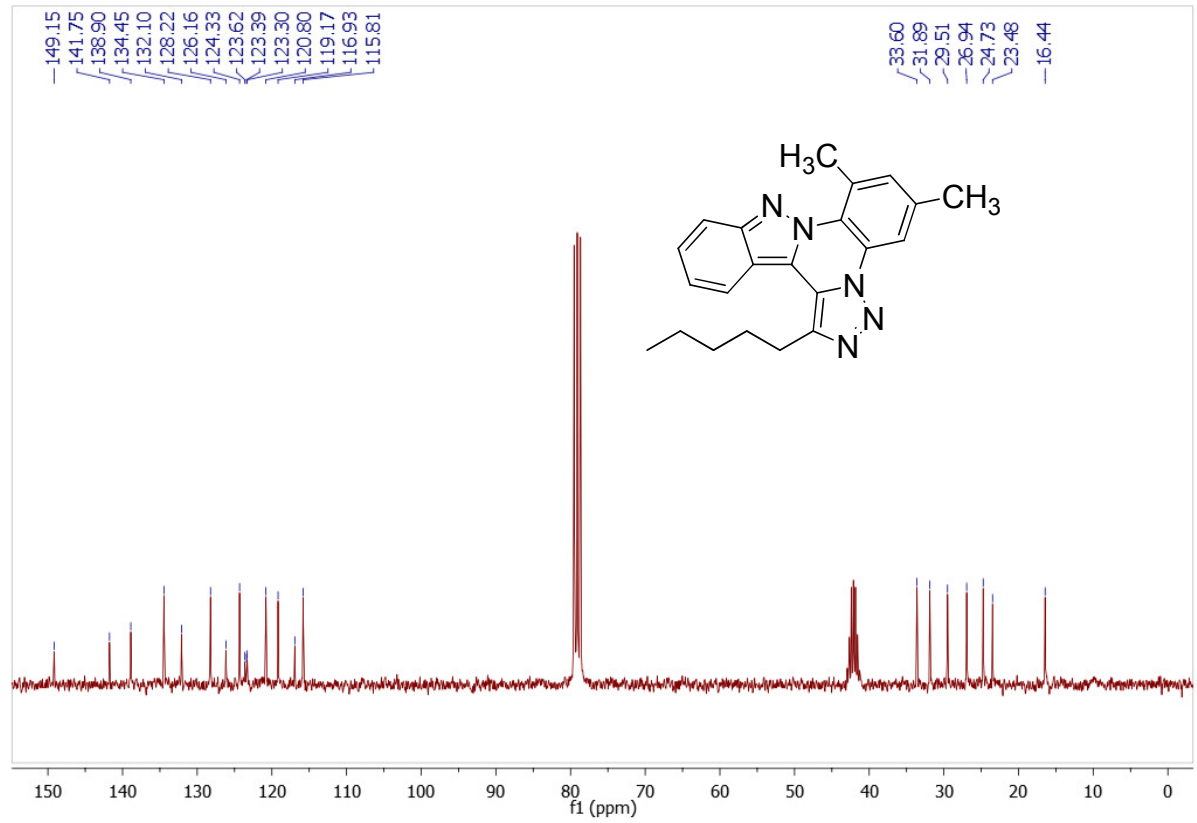
Compound- **7q**


8.46
8.17
8.15
7.91
7.89
7.49
7.47
7.45
7.32
7.30
7.28
7.26
3.46
3.44
3.42
3.20
2.55
1.97
1.95
1.93
1.62
1.60
1.57
1.56
1.54
1.04
1.02
1.00
0.00
0.90
1.00
0.92
0.99
2.01
1.99
3.00
2.98
2.04
2.01
3.01
H3C
CH3
N
N
N
N
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

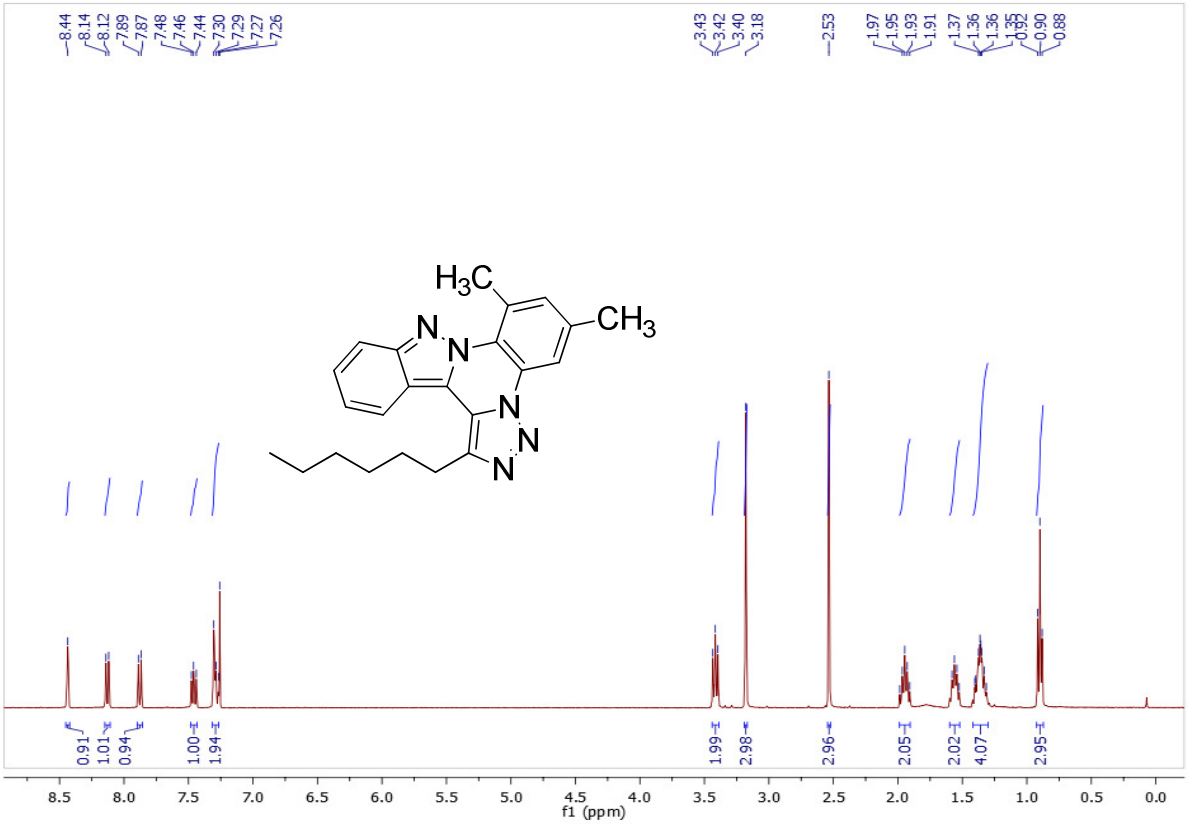

149.19
141.78
138.91
134.45
132.14
128.22
126.20
124.32
123.66
123.41
123.35
120.83
119.21
116.96
115.87
34.29
29.30
26.98
24.71
23.52
16.37
124.32
123.66
123.41
123.35
120.83
119.21
116.96
115.87
124
122
120
118
116
f1 (ppm)
H3C
CH3
N
N
N
N
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

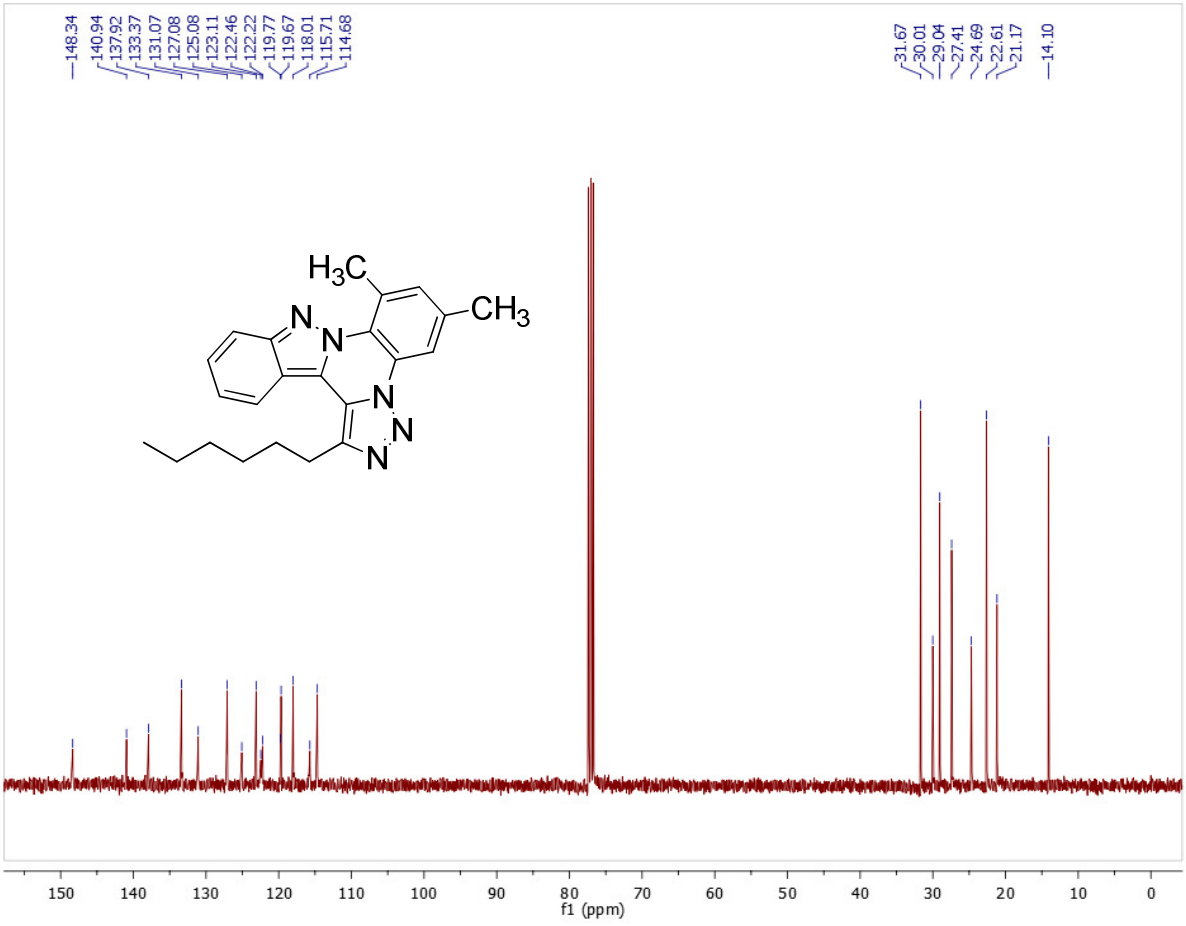
Compound- **7r**


8.48
8.19
8.17
7.93
7.91
7.51
7.49
7.47
7.34
7.32
7.30
7.26
3.47
3.45
3.43
3.23
2.56
1.99
1.97
1.95
1.55
1.44
1.42
0.95
0.93
0.91
0.00
H3C
CH3
N
N
N
N
N
0.91
1.02
0.98
1.00
2.19
2.05
2.97
2.97
2.06
1.94
2.03
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

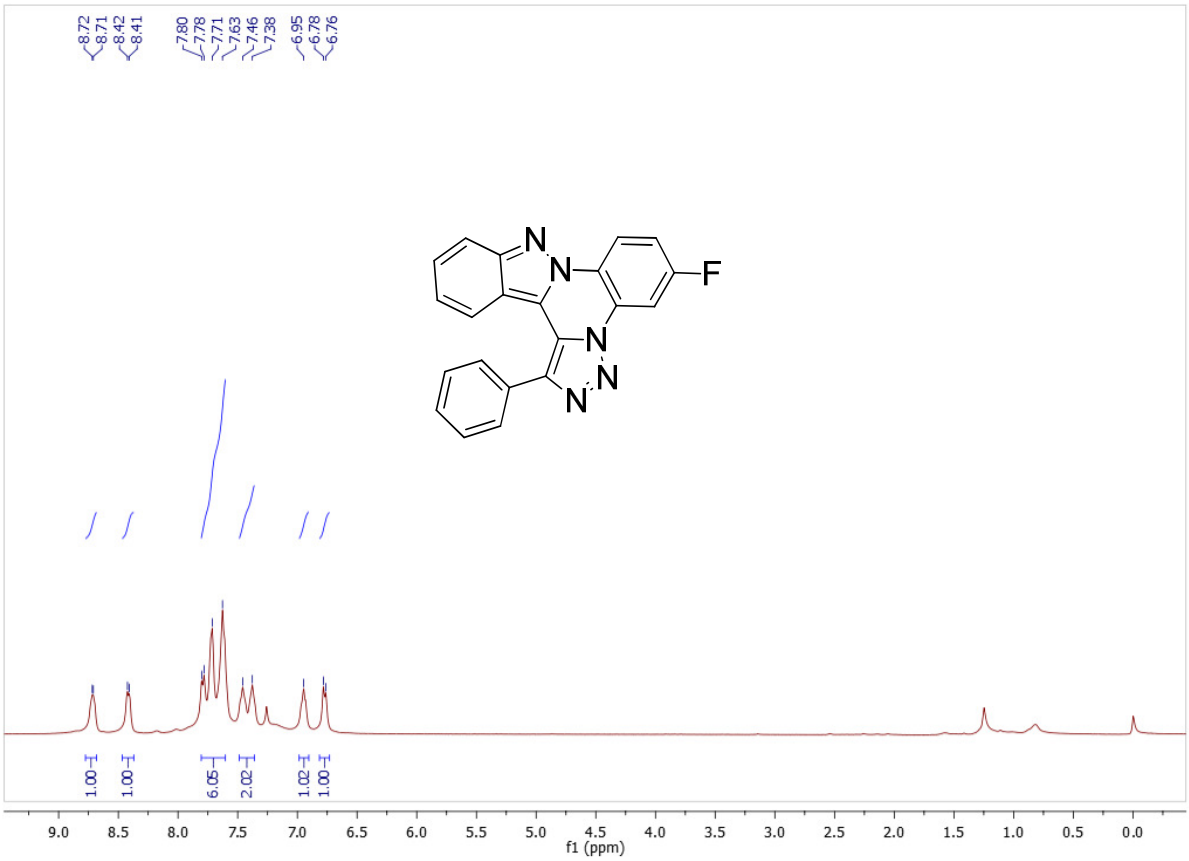

149.15
141.75
138.90
134.45
132.10
128.22
126.16
124.33
123.62
123.39
123.30
120.80
119.17
116.93
115.81
33.60
31.89
29.51
26.94
24.73
23.48
16.44
H3C
CH3
N
N
N
N
N
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

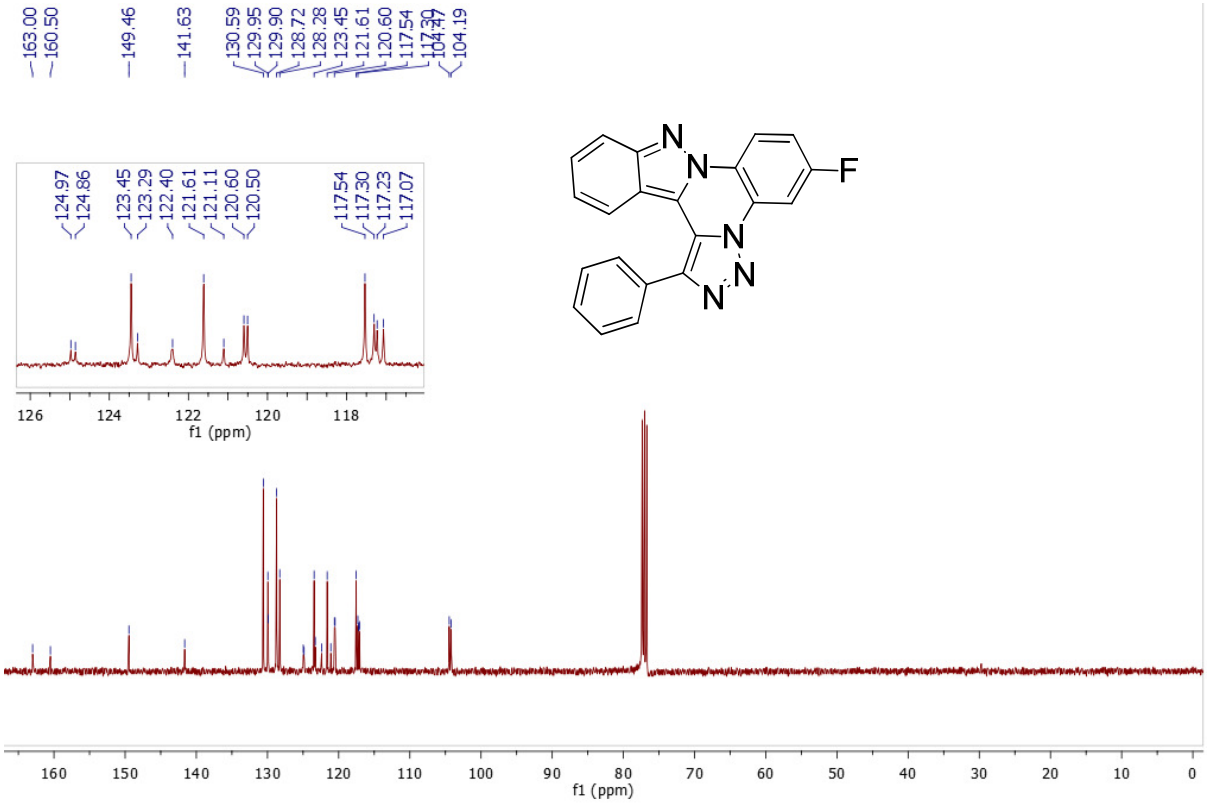
Compound- **7s**


8.44
8.14
8.12
7.89
7.87
7.48
7.46
7.44
7.30
7.29
7.27
7.26
3.43
3.42
3.40
3.18
2.53
1.97
1.95
1.93
1.91
1.37
1.36
1.36
1.35
0.92
0.90
0.88
0.91
1.01
0.94
1.00
1.94
1.99
2.98
2.96
2.05
2.02
4.07
2.95
H3C
CH3
N
N
N
N
N
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

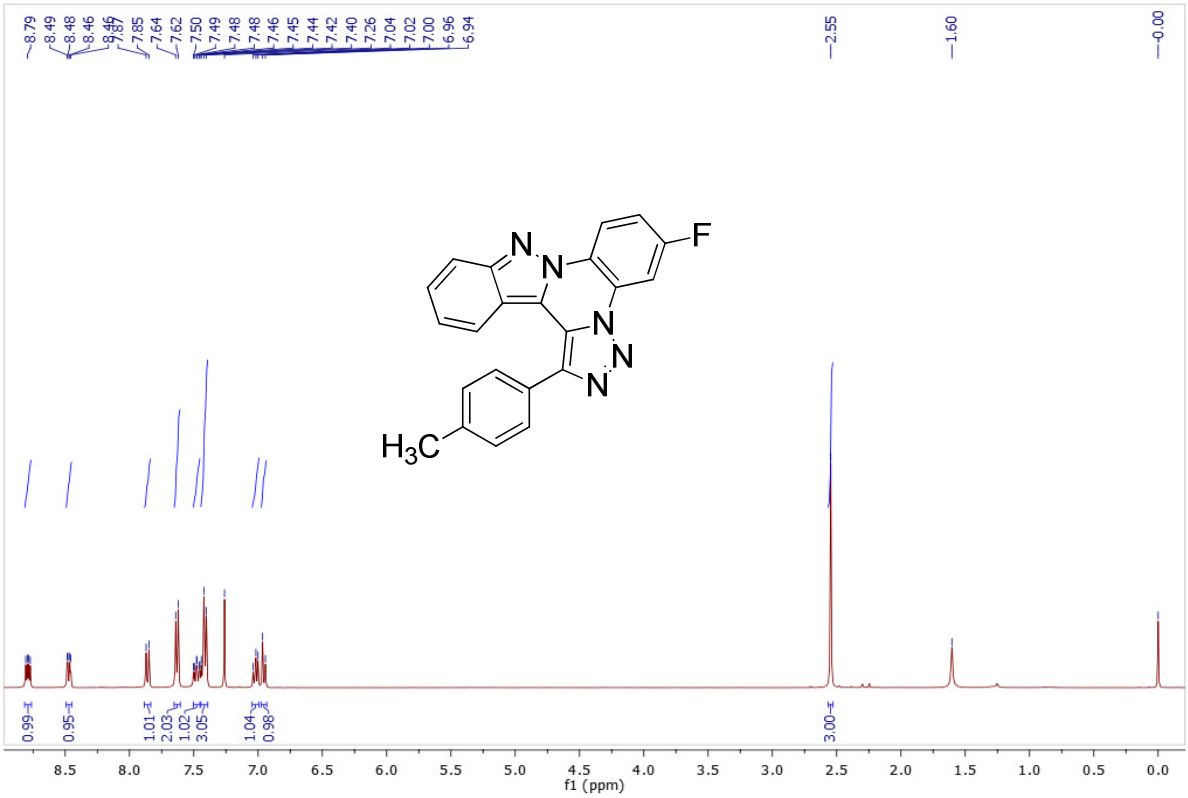

148.34
140.94
137.92
133.37
131.07
127.08
125.08
123.11
122.46
122.22
119.77
119.67
118.01
115.71
114.68
31.67
30.01
29.04
27.41
24.69
22.61
21.17
14.10
H3C
CH3
N
N
N
N
N
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

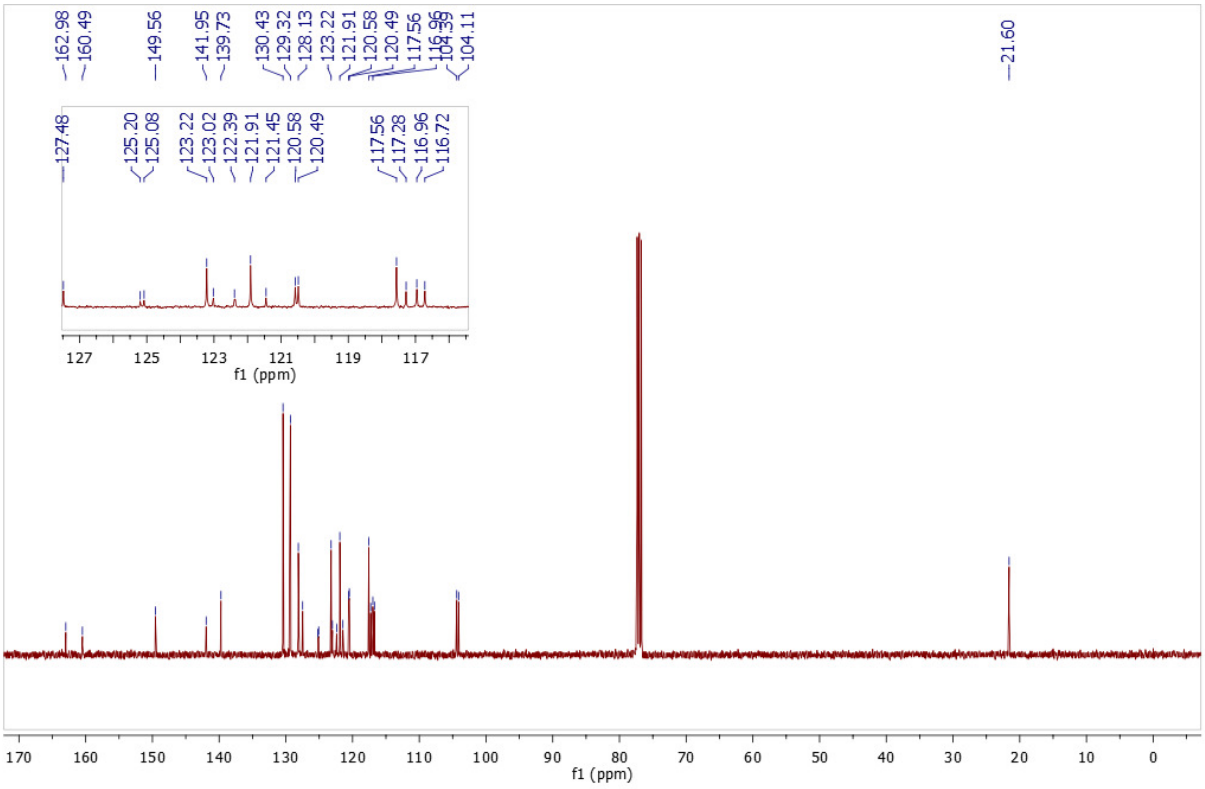
Compound- **7t**


8.72
8.71
8.42
8.41
7.80
7.78
7.71
7.63
7.46
7.38
6.95
6.78
6.76
F
1.00
1.00
6.05
2.02
1.02
1.00
f1 (ppm)

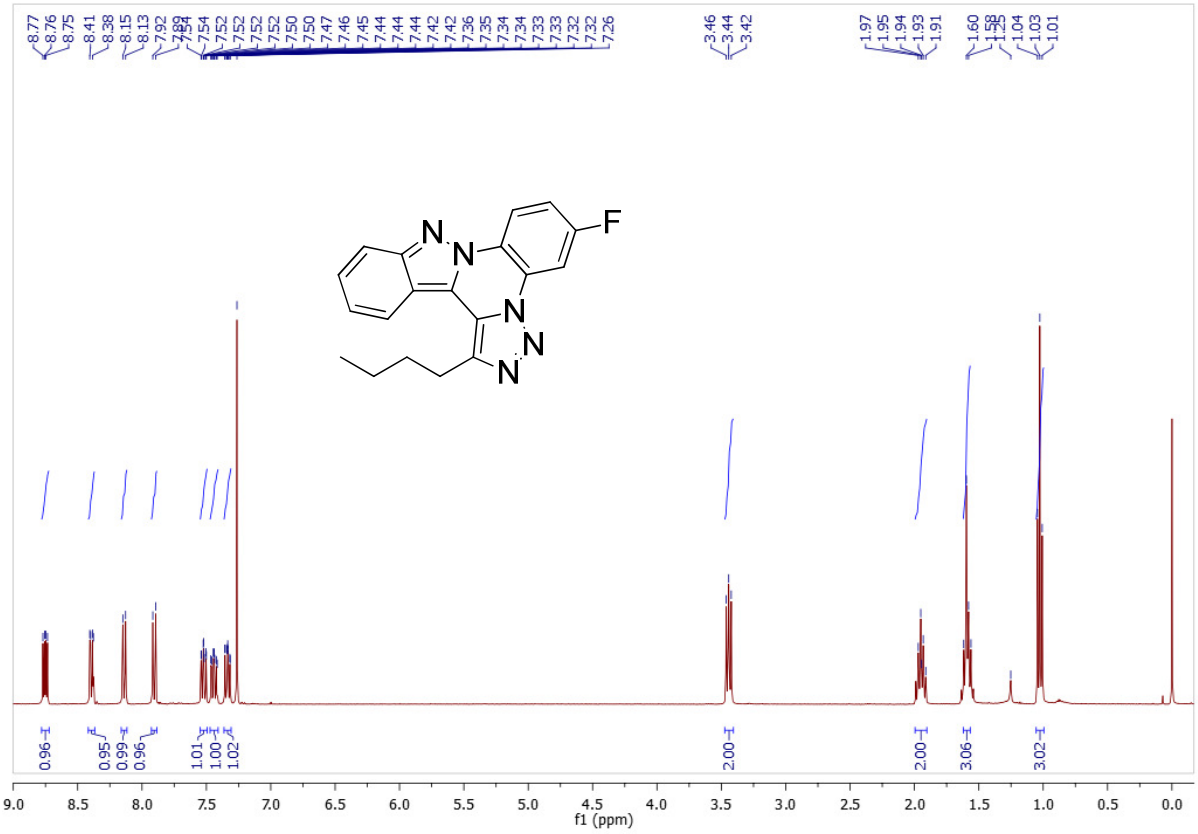

163.00
160.50
149.46
141.63
130.59
129.95
129.90
128.72
128.28
123.45
121.61
120.60
117.54
104.19
124.97
124.86
123.45
123.29
122.40
121.61
121.11
120.60
120.50
117.54
117.30
117.23
117.07
F
f1 (ppm)
f1 (ppm)

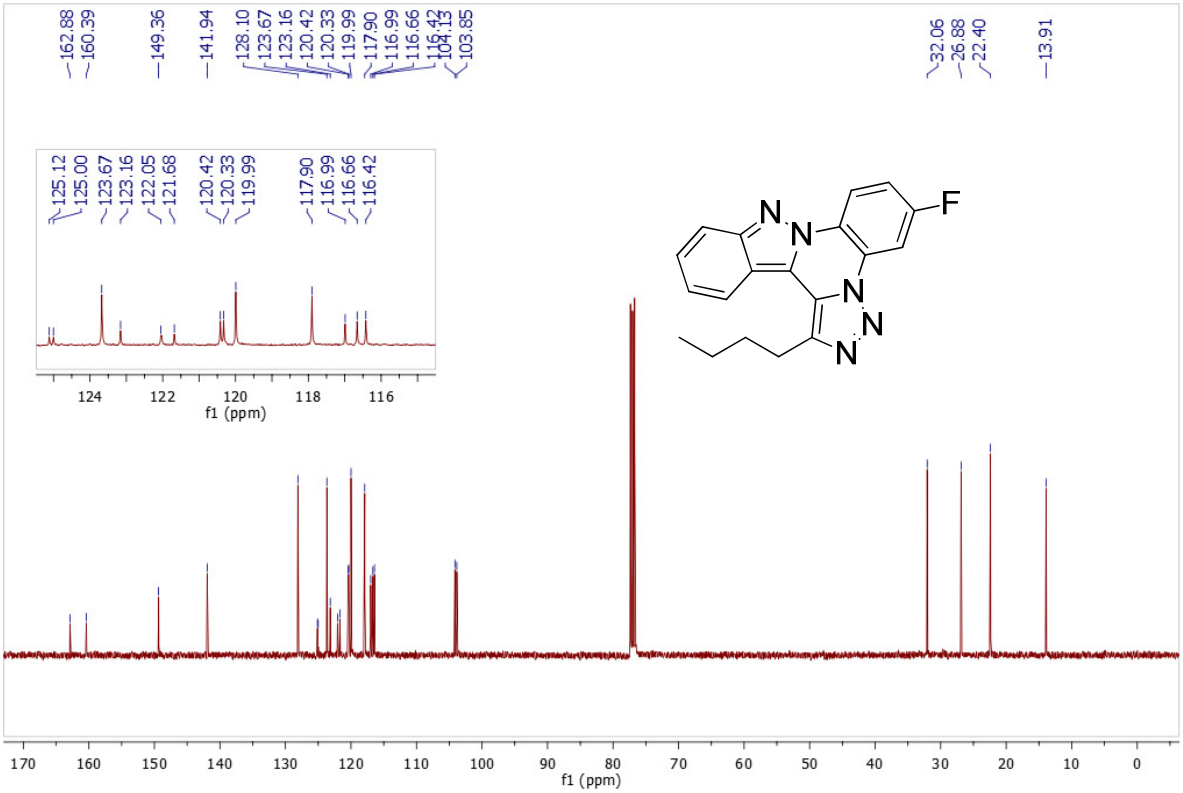
Compound- **7u**


8.79
8.49
8.48
8.46
7.85
7.64
7.62
7.50
7.49
7.48
7.46
7.45
7.44
7.42
7.40
7.26
7.04
7.02
7.00
6.96
6.94
2.55
1.60
0.00
F
N
N
N
N
N
H3C
0.99
0.95
1.01
2.03
1.02
3.05
1.04
0.98
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

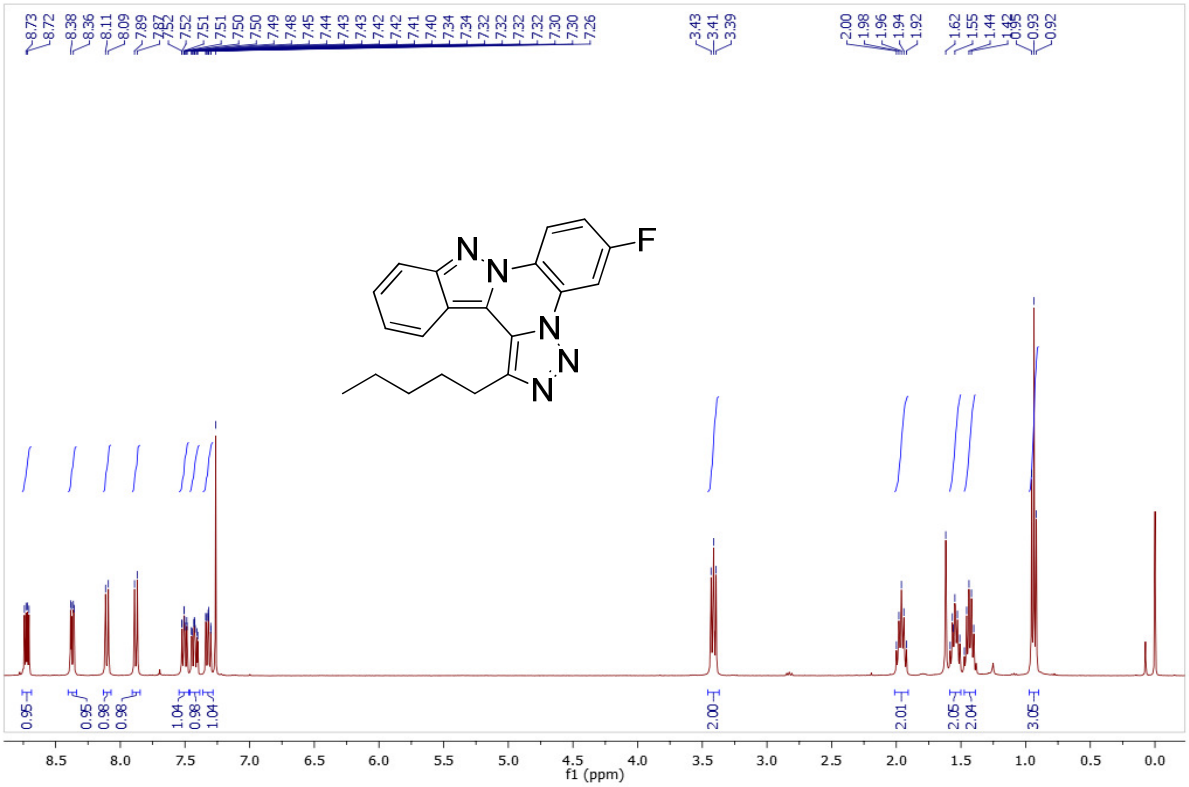

162.98
160.49
149.56
141.95
139.73
130.43
129.32
128.13
123.22
121.91
120.58
120.49
117.56
116.96
104.39
104.11
21.60
127.48
125.20
125.08
123.22
123.02
122.39
121.91
121.45
120.58
120.49
117.56
117.28
116.96
116.72
127
125
123
121
119
117
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

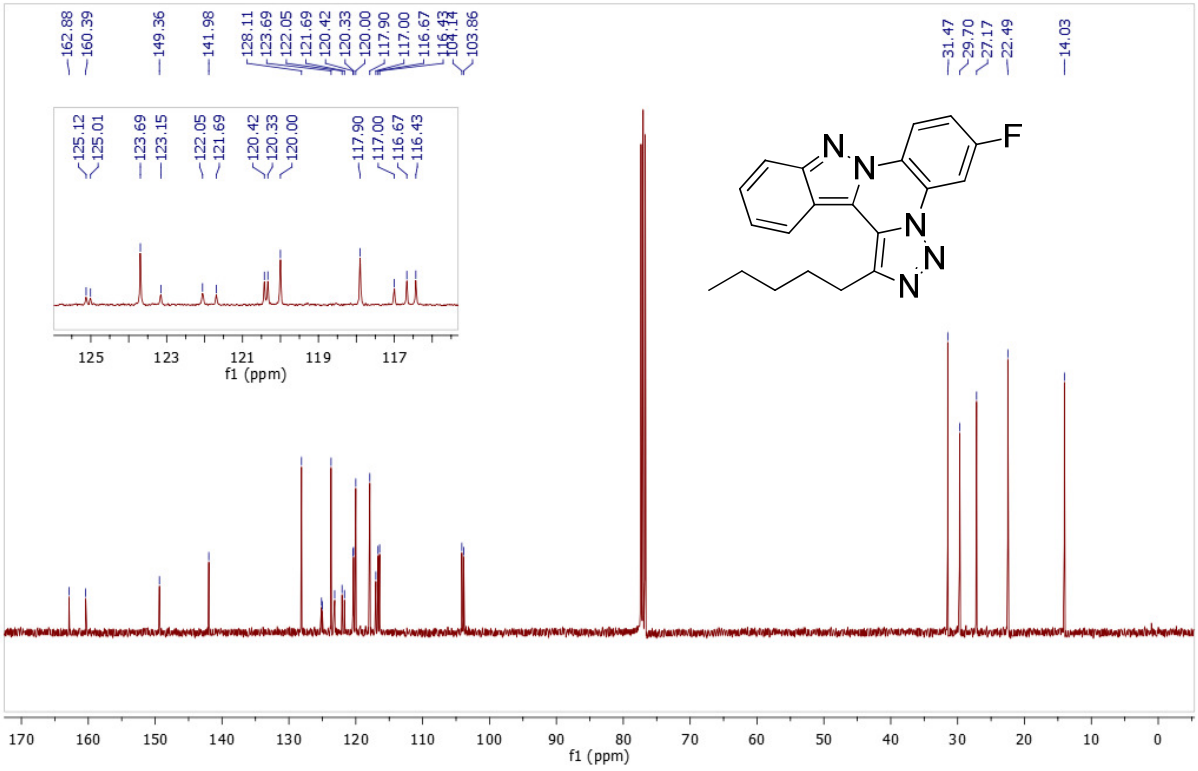
Compound- **7v**


8.77
8.76
8.75
8.41
8.38
8.15
8.13
7.92
7.54
7.52
7.52
7.52
7.50
7.50
7.47
7.46
7.45
7.44
7.44
7.44
7.42
7.42
7.36
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.26
3.46
3.44
3.42
1.97
1.95
1.94
1.93
1.91
1.60
1.58
1.25
1.04
1.03
1.01
F
N
N
N
N
N
0.96
0.95
0.99
0.96
1.01
1.00
1.02
2.00
2.00
3.06
3.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

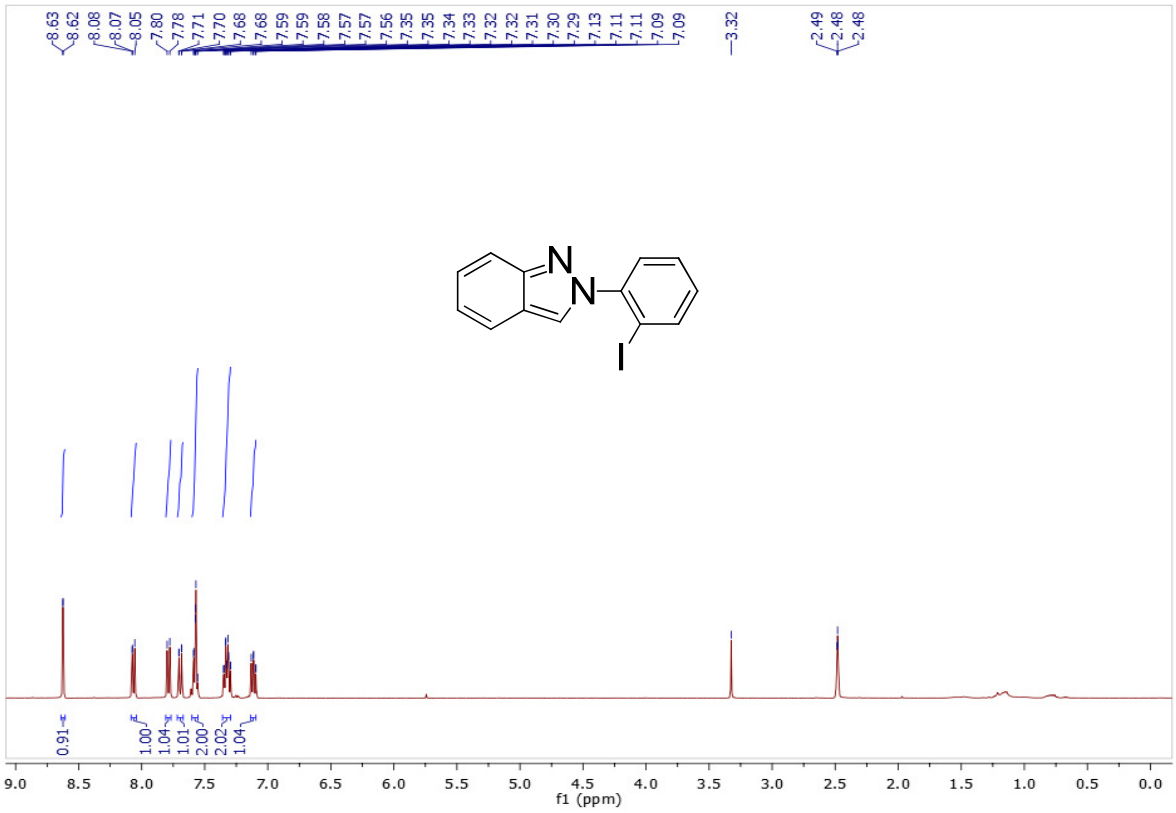

162.88
160.39
149.36
141.94
128.10
123.67
123.16
120.42
120.33
119.99
117.90
116.99
116.66
116.42
104.13
103.85
32.06
26.88
22.40
13.91
125.12
125.00
123.67
123.16
122.05
121.68
120.42
120.33
119.99
117.90
116.99
116.66
116.42
124
122
120
118
116
f1 (ppm)
F
N
N
N
N
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

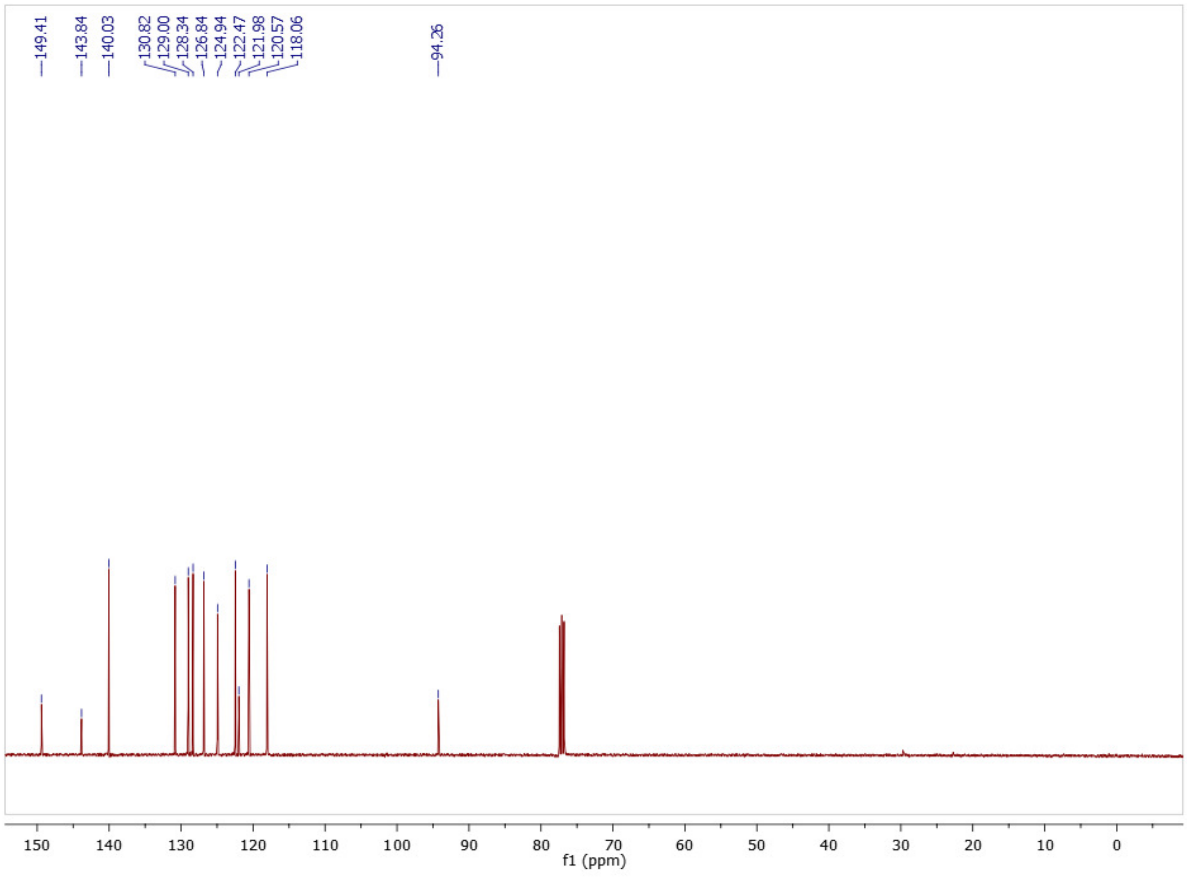
Compound- **7w**


8.73
8.72
8.38
8.36
8.11
8.09
7.89
7.87
7.52
7.51
7.50
7.49
7.48
7.45
7.44
7.43
7.42
7.41
7.40
7.34
7.32
7.30
7.26
3.43
3.41
3.39
2.00
1.98
1.96
1.94
1.92
1.62
1.55
1.44
0.95
0.93
0.92
F
N
0.95
0.95
0.98
0.98
1.04
0.98
1.04
2.00
2.01
2.05
2.04
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

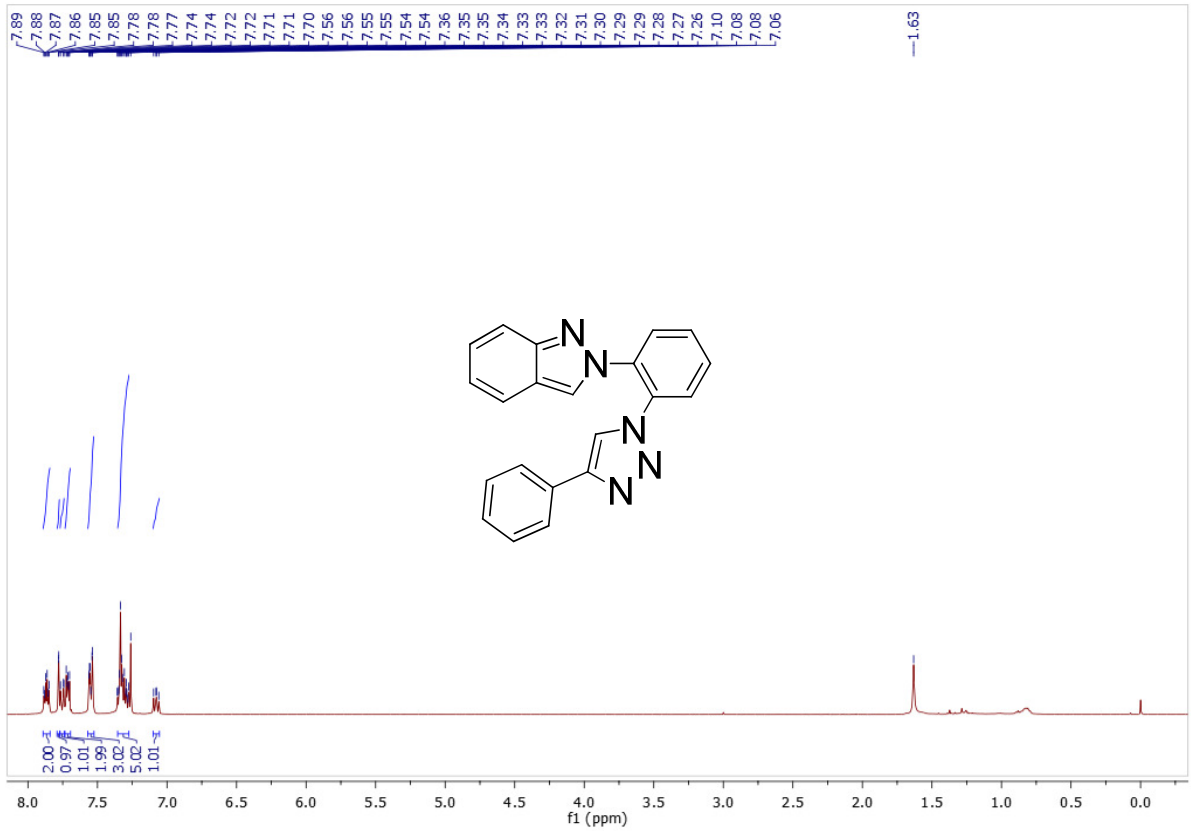

162.88
160.39
149.36
141.98
128.11
123.69
122.05
121.69
120.42
120.33
120.00
117.90
117.00
116.67
103.86
31.47
29.70
27.17
22.49
14.03
125.12
125.01
123.69
123.15
122.05
121.69
120.42
120.33
120.00
117.90
117.00
116.67
116.43
125
123
121
119
117
f1 (ppm)
F
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

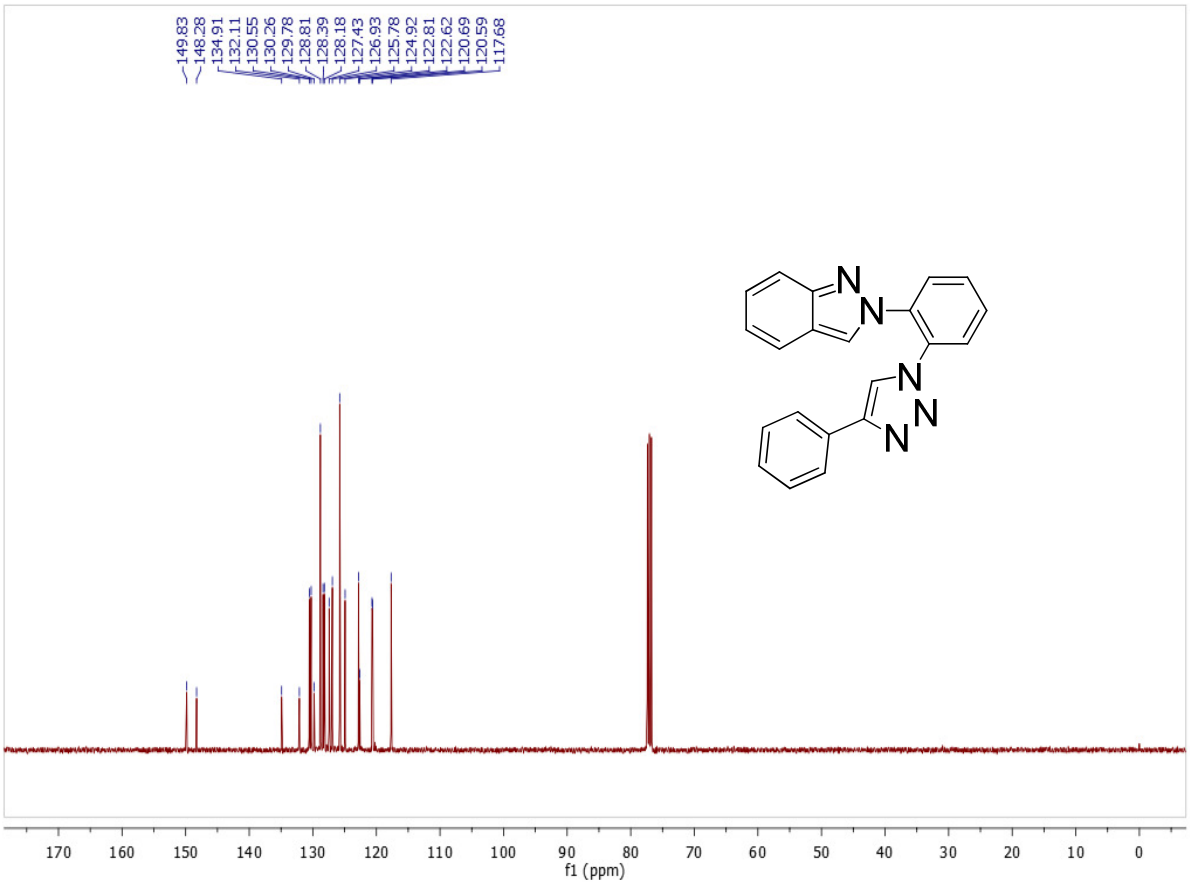
Compound- **3a**


8.63
8.62
8.08
8.07
8.05
7.80
7.78
7.71
7.70
7.68
7.59
7.59
7.58
7.57
7.57
7.56
7.35
7.35
7.34
7.33
7.32
7.32
7.31
7.30
7.29
7.13
7.11
7.11
7.09
7.09
3.32
2.49
2.48
2.48
N
N
I
0.91
1.00
1.04
1.01
2.00
2.02
1.04
f1 (ppm)


149.41
143.84
140.03
130.82
129.00
128.34
126.84
124.94
122.47
121.98
120.57
118.06
94.26
f1 (ppm)

Compound- **6**


7.89
7.88
7.87
7.86
7.85
7.85
7.78
7.78
7.77
7.74
7.74
7.72
7.72
7.71
7.71
7.70
7.56
7.56
7.55
7.55
7.54
7.54
7.36
7.35
7.35
7.34
7.33
7.33
7.32
7.31
7.30
7.29
7.29
7.28
7.27
7.26
7.10
7.08
7.08
7.06
1.63
2.00
0.97
1.01
1.99
3.02
5.02
1.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


149.83
148.28
134.91
132.11
130.55
130.26
129.78
128.81
128.39
128.18
127.43
126.93
125.78
124.92
122.81
122.62
120.69
120.59
117.68
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)