Electronic Supporting Information

Brønsted Acid Mediated Mono- and Di-substitution of Quinoxalines with Indoles: A Pathway to Indolocarbazole-Quinoxaline Scaffolds

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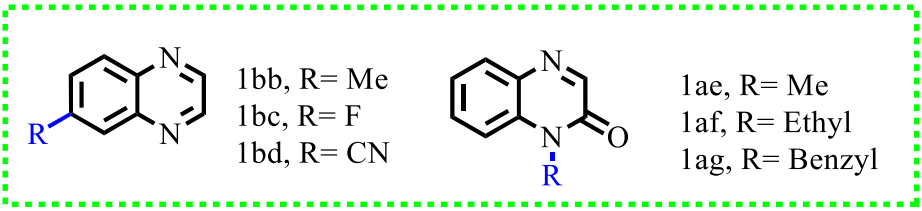
1. General Information:

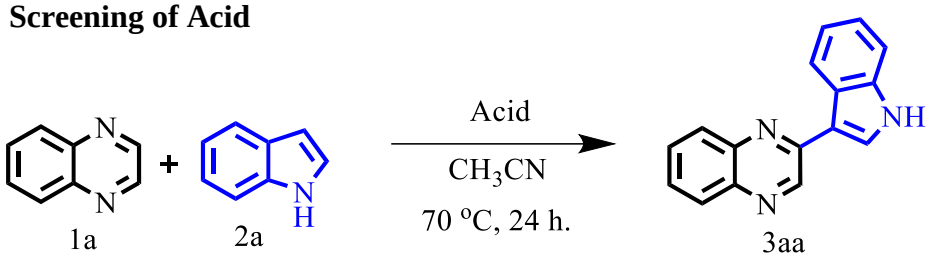
All reactions were performed in an oven-dried glassware using a clean seal reaction tube, ^{1}H, and ^{13}C were recorded on a JEOL, RESONANCE ECZ600R (500 MHz, 600MHz) and BRUKER AVANCE III HD (200MHz), and Chemical shifts (δ) are reported in ppm, coupling constants (J) were given in Hz. using the residual solvent peak in $CDCl_3$ (H: δ = 7.26 and C: δ = 77.16 ppm), DMSO-d6 (H: δ =2.50, and 3.33 ppm and C: δ 49.25 ppm) and Tetramethyl silane (TMS) (for ^{1}H, δ = 0), as the internal standard. IR spectra were recorded on a Perkin Elmer, G-FTIR. HRMS ESI (*m/z*) were recorded on a LC Waters, MS Micromass. X-ray diffraction data were recorded on a Bruker Kappa Apex-II CCD diffractometer at 296 K. Melting points of solid compounds were measured by a Thermo Scientific MEL TEMP instrument. the reaction was carried inside a wooden box. Progress of the reactions was monitored by thin-layer chromatography (TLC). All products were purified through column chromatography using silica gel 100−200 mesh size using hexane/ethyl acetate as an eluent, unless otherwise indicated.

All chemical reagents, substrates, and catalysts were purchased from commercial suppliers (like TCI, Sigma Aldrich, Spectrochem, BLD Pharma etc.), and were used without further purification. The starting substrates **1bb, 1bc, 1bd, 1ae**, **1af**, and **1ag** were prepared according to the literature procedure[1,2].



2. Optimization of reaction conditions for mono-substitution of quinoxaline and indole:

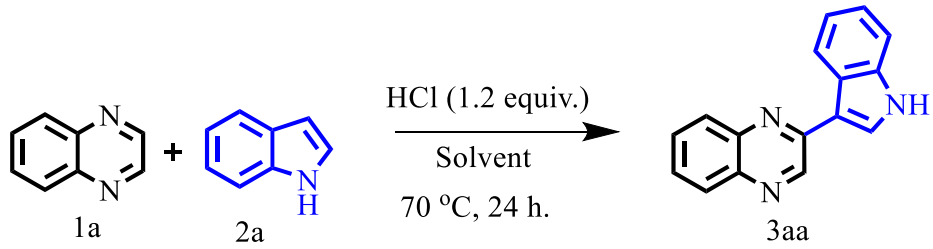
Table S1: Screening of Acid



Entry	Variations of Acid (equiv.)	Yield (%) [a]
1	H_2SO_4 (1.2)	42
2	$Et_2O(BF_3)$ (1.2)	trace
3	$FeCl_3$ (1.2)	trace
4	p-TSA (1.2)	47
5	HBr (1.2)	53
6	**HCl (1.2)**	**65**
7	CH_3COOH (1.2)	nr
8	HCl (0.3)	36
9	HCl (0.5)	40
10	HCl (1.0)	39
11	HCl (1.5)	47
12	HCl (2.0)	48

[a] Reaction Condition: 0.3 mmol of **1a** (1.0 equiv), 0.3 mmol of **2a** (1.0 equiv), Acid in Acetonitrile (1mL) at 70 °C for 24 h, isolated yield.

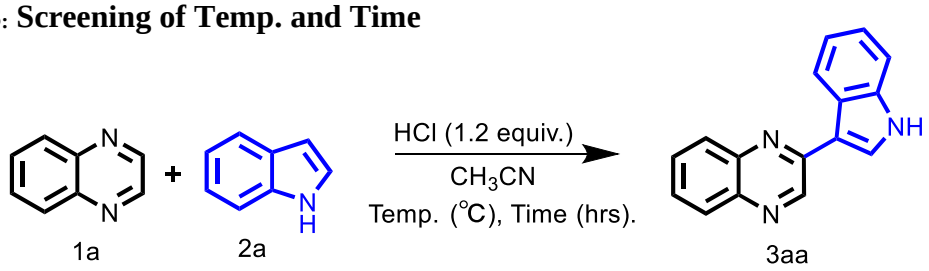
Table S2: Screening of Solvent



Entry	Variations of Solvent (1mL)	Yield (%) [a]
1	DMF	24
2	DCE	nr
3	**CH_3CN**	**65**
4	Toluene	nr
5	1,4 Dioxane	10
6	Ethyl Acetate	nr
7	Methanol	15
8	Acetone	nr

[a] Reaction Condition: 0.3 mmol of **1a** (1.0 equiv.), 0.3 mmol of **2a** (1.0 equiv.), Hydrochloric acid (1.2 equiv.) in Solvent at 70 °C for 24 h, isolated yield.

Table S3: Screening of Temp. and Time

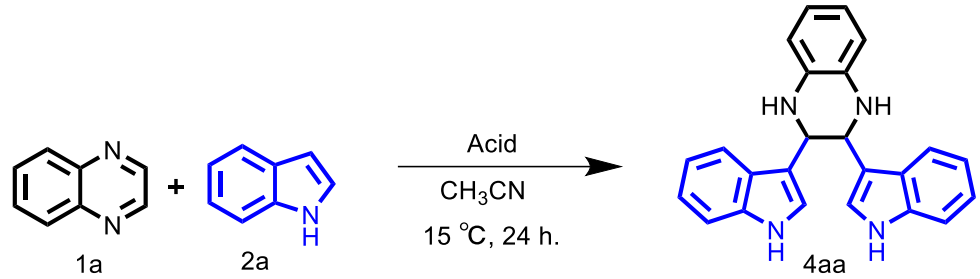


Entry	Temp. (°C)	Time (h)	Yield (%) [a]
1	00	24	trace
2	rt	24	49
3	50	24	50
4	**70**	**24**	**65**
5	100	24	59
6	120	24	57
7	70	12	45
8	70	35	50
9	80	24	64

[a] Reaction Condition: 0.3 mmol of **1a** (1.0 equiv.), 0.3 mmol of **2a** (1.0 equiv.), and Hydrochloric acid (1.2 equiv.) in the acetonitrile (1mL) temp. and time, isolated yield.

2a. Optimization of reaction conditions for di-substitution of quinoxaline and indole:

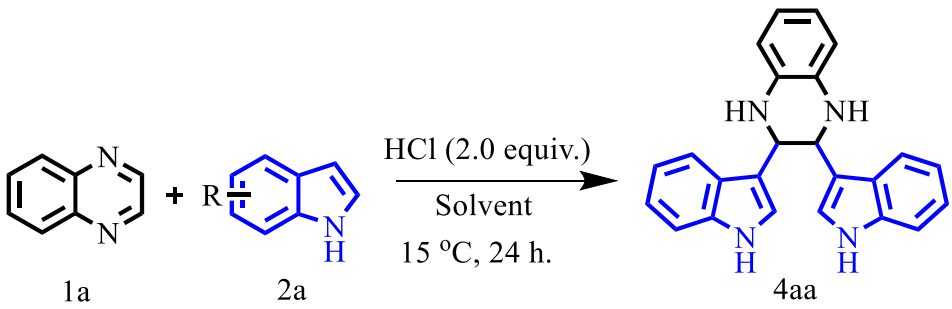
Table S4: Screening of Acid



Entry	Acid (equiv.)	Yield [a]
1	HBr (2.0)	30
2	H_2SO_4 (2.0)	53
3	CH_3COOH (2.0)	nr
4	$Et_2O(BF_3)$ (2.0)	nr
5	$FeCl_3$ (2.0)	nr
6	**HCl (2.0)**	**66**
7	HCl (1.2)	42
8	HCl (1.5)	48
9	HCl (3.0)	46

[a] Reactions condition: 0.3 mmol of **1a** (1.0 equiv.), 0.6 mmol of **2a** (2.0 equiv.), and Acid in the acetonitrile (2mL) at 15 ℃ for 24 h, isolated yield.

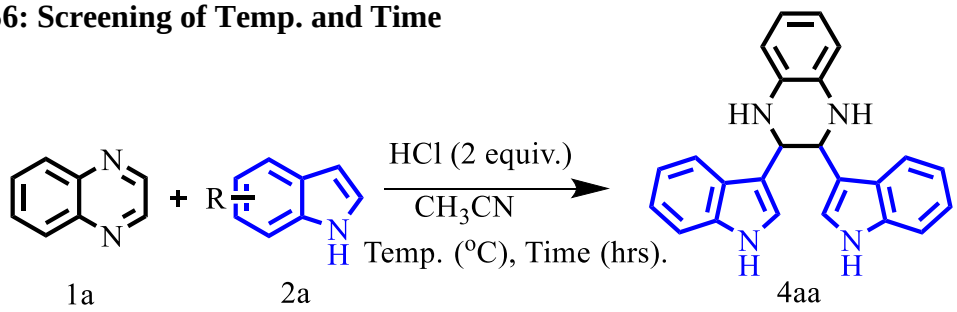
Table S5: Screening of Solvent



Entry	Solvent (2mL)	Yield [a]
1	THF	35
2	**CH_3CN**	**66**
3	THF: CH_3CN (1:1)	25
4	H_2O	nr
5	Acetone	nr
6	Toluene	nr
7	DCE	nr

[a] Reactions condition: 0.3 mmol of **1a** (1.0 equiv.), 0.6 mmol of **2a** (2.0 equiv.), and Hydrochloric Acid (2.0 equiv.) in the solvent at 15 ℃ for 24 h, isolated yield.

Table S6: Screening of Temp. and Time

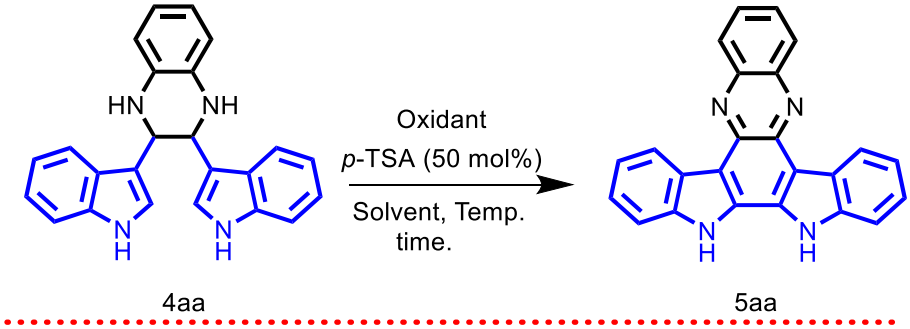


Entry	Temp (℃)	Time (h)	Yield [a]
1	-20	24	11
2	00	24	47
3	10	24	48
4	**15**	**24**	**66**
5	**18**	**24**	**66**
6	20	24	41
7	rt	24	31
8	50	24	nr
9	00	12	14

10	18	48	70
11	15	36	67

[a] Reactions condition: 0.3 mmol of **1a** (1.0 equiv.), 0.6 mmol of **2a** (2.0 equiv.) and Hydrochloric Acid (2.0 equiv.) in Acetonitrile (2mL) at Temp. ℃ for Time h, Isolated yield

Table S7: Optimization of reaction conditions for Indolocarbazole-quinoxalines:



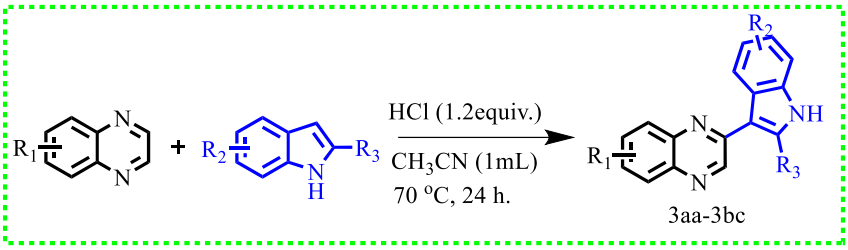
Entry	Oxidant (2.0 equiv.)	Solvent (1mL)	Temp. (℃)	Time (h.)	Yield [a] (%)
1	DDQ	Benzene	80	6	70
2[b]	DDQ	Benzene	80	12	53
3	DDQ (1.0 equiv.)	Benzene	80	12	40
4	DDQ	Benzene	80	4	47
5	DDQ	Benzene	80	8	71
6	**DDQ**	**Benzene**	**80**	**12**	**86**
7	DDQ	Benzene	80	16	71
8	DDQ	Benzene	rt	12	trace
9	DDQ	Benzene	110	12	72
10	DDQ	Toluene	80	12	65
11	DDQ	DCE	80	12	40
12	DDQ	CH_3CN	80	12	nr
13	DDQ	1.4-Dioxane	80	12	nr
14	DDQ	Toluene	110	12	60

16	DDQ	Xylene	80	12	38
17	DDQ	Benzene: H_2O (4:1)	80	12	62
18	DDQ	Ethanol	80	12	trace
19	DDQ	Trifluorobenzene	100	12	25
20	I_2	Benzene	80	12	trace
21	PIDA	Benzene	80	12	trace
22	TBPB	Benzene	80	12	nr
23	DDQ	o-DCB	80	12	37
24	DDQ	Chlorobenzene	80	12	34

[a] Reaction condition: 0.1 mmol of **4aa**, 0.2 mmol of oxidative, and p-TSA (50 mol%) in 1 mL solvent. Isolated yield. [b] Reaction were performed without additive (*p*-TSA).

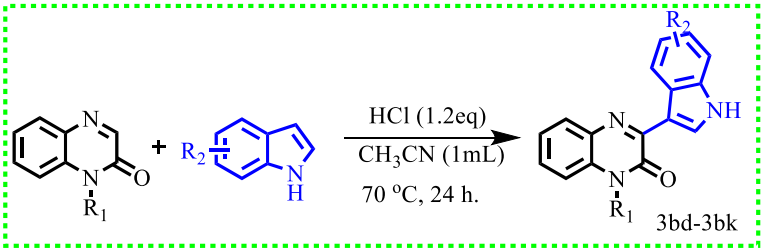
3. Experimental procedure:

3a. General reaction procedure for the synthesis of 3aa-3bc



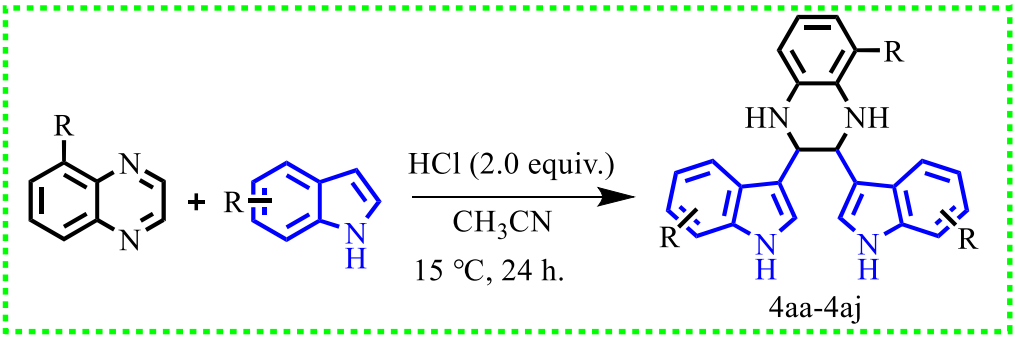
The reaction was performed 0.3 mmol quinoxaline (1.0 equiv.), and 0.3 mmol indole (1.0 equiv.), added into the clean oven dried reaction tube with cap, acetonitrile was used as a solvent, then 25.1 µl of HCl (35%) (1.2 equiv.) was added dropwise at room temperature and the reaction mixture stirred in an oil bath at 70 ℃ up to 24 h. After cooling and quenching the reaction with water (10mL), the reaction mixture was extracted with ethyl acetate (10-15 mL three times) and the combined organic layer were dried over anhydrous Na_2SO_4. The organic solvent was removed under reduced pressure, the crude product leftover was purified by column chromatography using silica gel having 100-200 mesh size.

3b. General reaction procedure for the synthesis of 3bd-3bk



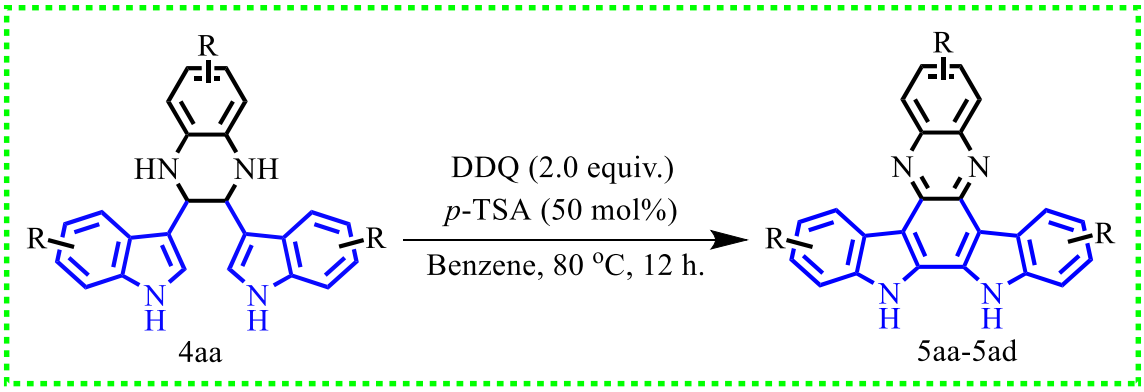
The reaction was performed 0.3 mmol quinoxalinone (1.0 equiv.), and 0.3 mmol indole (1.0 equiv.), added into the clean oven dried reaction tube with cap, acetonitrile was used as a solvent, then 25.1 µl of HCl (35%) (1.2 equiv.) was added dropwise at room temperature and the reaction mixture stirred in an oil bath at 70 ℃ up to 24 h. After cooling and quenching the reaction with water (10mL), the reaction mixture was extracted with ethyl acetate (10-15 mL three times) and the combined organic layer were dried over anhydrous Na_2SO_4. The organic solvent was removed under reduced pressure, the crude product leftover was purified by column chromatography using silica gel having 100-200 mesh size.

3c. General reaction procedure for the synthesis of 4aa- 4aj



The reaction was performed with 0.3 mmol of quinoxaline (1.0 equiv.) and 0.6 mmol of indole (2.0 equiv.) was added in a clean reaction tube, with 2.0 mL of acetonitrile, the reaction mixture was cooled to 15 -18 ℃, then 42 µl of HCl (35%) (2.0 equiv. w.r.t. quinoxaline) was added dropwise into the reaction mixture, and the reaction mixture was stirred at same temperature for 24 h. After quenching with water (10mL), the reaction mixture was extracted with ethyl acetate (15 mL three times), and the combined organic layer was dried over anhydrous Na_2SO_4. After the removal of solvent under reduced pressure, the crude product leftover was purified by column chromatography using silica gel with 100-200 mesh size.

3d. General reaction procedure for the synthesis of 5aa-5ad



The reaction was performed with 0.1 mmol of **4aa** and 0.2 mmol DDQ (2.0 equiv.) and the catalytic amount 8.61 mg of *p*-TSA (50 mol %) were added in to a sealed tube containing 1.0 mL of benzene, then the reaction mixture was stirred at 80 ℃ for 12 h on carousel reactor. After cooling the reaction was quenched with water (10 mL), and reaction mixture was extracted with ethyl acetate (15 mL three times) and the combined organic layer was dried over anhydrous Na_2SO_4. After recovery of solvent under reduced pressure, the crude product leftover was purified by column chromatography using silica gel having 100-200 mesh size.

3e. Large-Scale-Reaction

Synthesis of 2-(1H-indol-3-yl) quinoxaline (3aa)

The reaction was performed at 1.30 g of **1a** (10 mmol) and 1.18 g of **2a** (10 mmol) added into the clean 100 mL round bottom flask, acetonitrile was used as a solvent (10 mL), then 840 µl of HCl (35%) was added dropwise at room temperature and the reaction mixture was stirred in an oil bath at 70 ℃ up to 24 h. After cooling the reaction, it was quenched with water (40 mL), the reaction mixture was extracted with ethyl acetate (70 mL three times) and the combined organic layer was dried over anhydrous Na_2SO_4. Removal of the solvent under reduced pressure, the crude product leftover was purified by column chromatography (hexane: ethyl acetate= 7.5:2.5) using silica gel (100-200 mesh size) and the desired product was obtained (1.15 g) in 47% yield.

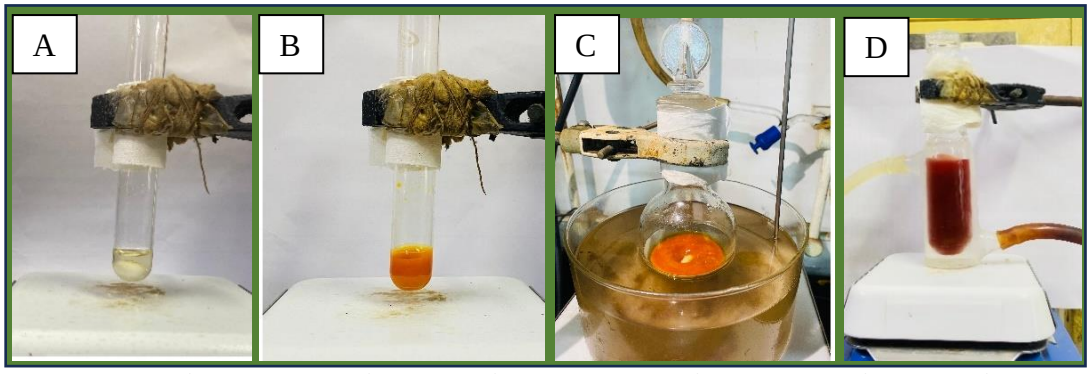


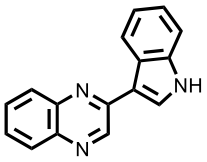
Fig S1: (A) Photograph of reaction mixture before addition of HCl **(B)** Photograph of reaction mixture after addition of HCl **(C)** Photograph of reaction setup at gram scale for 3aa **(D)** Photograph of reaction setup at gram scale for 4aa.

Synthesis of 2-(1H-indol-3-yl) quinoxaline (4aa)

The reaction was performed at 1.30 g (10 mmol) of **1a** and 2.34 g (20 mmol) of **2a** was added in to a 25 mL reaction tube containing 15 ml of acetonitrile, the reaction mixture was cooled to 15 -18 ℃ and then 1.40 mL of HCl (35%) (2.0 equiv., w.r.t. quinoxaline) was added dropwise into the reaction mixture. The reaction mixture was stirred at same temperature for 48 h in reaction tube, and the reaction was quenched with water (40 mL), and it was extracted with ethyl acetate (70 mL three times) and the combined organic layer was dried over anhydrous Na_2SO_4. After the recovery of the solvent under reduced pressure, the crude product leftover was purified by column chromatography (hexane: ethyl acetate= 7.0:3.0) using silica gel (having 100-200 mesh size). The desired product was obtained 49% yield (1.78 gm) (w.r.t. quinoxaline).

4. Spectroscopic data:

Synthesis of 2-(1H-indol-3-yl) quinoxaline (3aa)



Prepared according to the general procedure (3a) mentioned above in 65% yield (47.8mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 184-186 ℃.

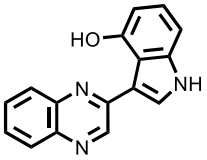
^{1}H NMR (600 MHz, $CDCl_3$) δ 11.07 (s, 1H), 9.35 (s, 1H), 8.78 (d, *J* = 8.4 Hz, 1H), 8.56 (s, 1H), 8.19 (dd, *J* = 24.3, 8.4 Hz, 2H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.93 – 7.90 (m, 1H), 7.87 (t, *J* = 7.5 Hz, 1H), 7.65 (t, *J* = 8.0 Hz, 1H), 7.17 (t, *J* = 7.7 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 195.8, 159.8, 149.6, 145.0, 143.1, 140.8, 140.4, 135.8, 135.2, 132.3, 131.2, 130.4, 129.5, 122.9, 122.0, 121.2.

IR (cm^{-1}): νmax; 3173, 3015,1617, 1550, 1121, 737.

HRMS (ESI): calcd for $C_{16}H_{11}N_3$ $[M+H]^-$: 246.1031; found: 246.1032.

Synthesis of 3-(quinoxalin-2-yl)-1H-indol-4-ol (3ab)



Prepared according to the general procedure (3a) mentioned above in 78% yield (61.1mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 270-272 ℃.

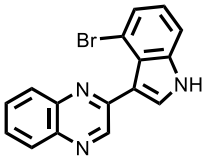
^{1}H NMR (600 MHz, DMSO-d_6) δ 13.48 (s, 1H), 12.00 (s, 1H), 9.61 (s, 1H), 8.62 (d, *J* = 3.0 Hz, 1H), 8.00 (d, *J* = 8.1 Hz, 1H), 7.79 (dd, *J* = 5.0, 1.8 Hz, 2H), 7.67 (ddd, *J* = 8.1, 5.7, 2.6 Hz, 1H), 7.04 (t, *J* = 7.8 Hz, 1H), 6.86 (d, *J* = 8.0 Hz, 1H), 6.45 (d, *J* = 7.8 Hz, 1H).

^{13}C NMR (151 MHz, DMSO-d_6) δ 152.81, 149.3, 145.9, 140.1, 139.9, 139.1, 131.6, 130.2, 129.4, 128.7, 126.3, 125.8, 115.0, 114.1, 106.7, 103.4.

IR (cm^{-1}): νmax; 3305, 3131, 3059, 1632, 1588, 1257, 1155, 1124, 897.

HRMS (ESI): calcd for $C_{16}H_{11}N_3O$: 262.0980 $[M+H]^+$; found: 262.0980

Synthesis of 2-(4-bromo-1H-indol-3-yl) quinoxaline (3ac)



Prepared according to the general procedure (3a) mentioned above in 42% yield (40.8 mg), eluent (30% EtOAc/hexane) to afford a yellowish brown solid, mp= 216-218 ℃.

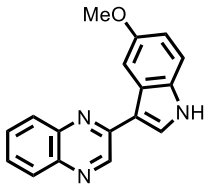
^{1}H NMR (600 MHz, DMSO-d_6) δ 12.10 (s, 1H), 9.18 (s, 1H), 8.12 – 8.09 (m, 2H), 7.98 (d, *J* = 2.8 Hz, 1H), 7.87 – 7.81 (m, 2H), 7.60 (d, *J* = 8.1 Hz, 1H), 7.37 (d, *J* = 7.5 Hz, 1H), 7.16 (t, *J* = 7.8 Hz, 1H).

^{13}C NMR (151 MHz, DMSO-d_6) δ 150.3, 148.5, 141.9, 140.5, 138.3, 130.6, 130.3, 129.6, 129.3, 129.3, 125.1, 124.6, 123.6, 114.8, 113.3, 112.5.

IR (cm^{-1}): νmax**;** 3139, 3029, 1617, 1530, 1238, 1104, 725, 608.

HRMS (ESI): calcd for $C_{16}H_{10}BrN_3$ [M+Na] $^+$:345.9956; found:345.9951.

Synthesis of 2-(5-methoxy-1H-indol-3-yl) quinoxaline (3ad)



Prepared according to the general procedure (3a) mentioned above in 83% yield (68.5mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 192-194 ℃.

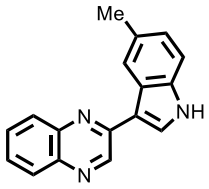
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.70 (s, 1H), 8.35 (d, *J* = 2.6 Hz, 1H), 8.12 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.05 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.95 (d, *J* = 2.9 Hz, 1H), 7.76 – 7.72 (m, 1H), 7.67 – 7.63 (m, 1H), 7.34 (d, *J* = 8.9 Hz, 1H), 6.99 (dd, *J* = 8.8, 2.5 Hz, 1H), 3.98 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 155.6, 150.4, 143.6, 142.5, 140.1, 131.8, 129.8, 128.9, 128.0, 128.0, 126.2, 126.0, 114.6, 113.7, 112.0, 104.1, 55.7.

IR (cm^{-1}): νmax**;** 3052, 1610, 1550, 1455, 1337, 1225, 1122, 737.

HRMS (ESI): calcd for $C_{17}H_{13}N_3O$ [M+Na] $^+$:276.1137; found: 276.1118.

Synthesis of 2-(5-methyl-1H-indol-3-yl) quinoxaline (3ae)



Prepared according to the general procedure (3a) mentioned above in 82% yield (63.7mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp=118-120 ℃.

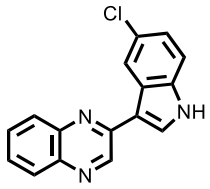
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.23 (s, 1H), 8.56 (s, 1H), 8.53 (s, 1H), 8.16 (dd, *J* = 8.3, 1.4 Hz, 1H), 8.04 (dd, *J* = 8.4, 1.4 Hz, 1H), 7.96 (d, *J* = 2.7 Hz, 1H), 7.73 (t, *J* = 6.8 Hz, 1H), 7.67 – 7.63 (m, 1H), 7.35 (d, *J* = 8.2 Hz, 1H), 7.15 (dd, *J* = 8.5, 1.7 Hz, 1H), 2.55 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 150.6, 144.0, 142.8, 140.3, 135.3, 131.3, 130.0, 129.1, 129.0, 128.1, 128.1, 125.9, 125.2, 121.9, 114.6, 111.2, 21.8.

IR (cm^{-1}): νmax**;** 3122, 3023, 1612, 1548, 1439, 1234, 1138, 750.

HRMS (ESI): calcd for $C_{17}H_{13}N_3$ [M+H] $^-$:258.1031; found: 258.1043.

Synthesis of 2-(5-chloro-1H-indol-3-yl) quinoxaline (3af)



Prepared according to the general procedure (3a) mentioned above in 59% yield (49.5 mg), eluent (30% EtOAc/hexane) to afford a yellow solid, mp= 218-220 ℃.

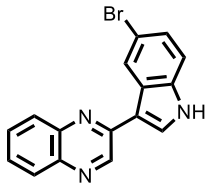
^{1}H NMR (600 MHz, DMSO-d_6) δ 12.10 (s, 1H), 9.50 (s, 1H), 8.81 (d, *J* = 2.2 Hz, 1H), 8.70 (d, *J* = 2.9 Hz, 1H), 8.11 (d, *J* = 8.2 Hz, 1H), 8.02 (d, *J* = 8.1 Hz, 1H), 7.81 (t, *J* = 7.7 Hz, 1H), 7.71 (t, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 8.6 Hz, 1H), 7.28 (d, *J* = 8.5 Hz, 1H).

^{13}C NMR (151 MHz, DMSO-d_6) δ 150.2, 144.2, 141.5, 139.3, 135.4, 130.2, 129.9, 128.6, 128.3, 127.8, 126.4, 125.3, 122.5, 121.2, 113.4, 112.3.

IR (cm^{-1}): νmax**;** 3157, 3044, 1621, 1549, 1230, 1132, 741, 704.

The chemical compounds have been described.[3]

Synthesis of 2-(5-bromo-1H-indol-3-yl) quinoxaline (3ag)



Prepared according to the general procedure (3a) mentioned above in 68% yield (72.0 mg), eluent (30% EtOAc/hexane) to afford a yellow solid, mp= 240-242 ℃.

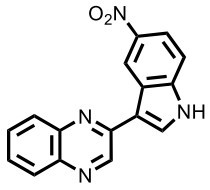
^{1}H NMR (600 MHz, DMSO-d_6) δ 12.13 (s, 1H), 9.52 (s, 1H), 8.98 (d, *J* = 2.2 Hz, 1H), 8.70 (d, *J* = 2.2 Hz, 1H), 8.11 (dd, *J* = 8.4, 1.3 Hz, 1H), 8.04 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.83 – 7.80 (m, 1H), 7.73 – 7.70 (m, 1H), 7.53 (d, *J* = 8.6 Hz, 1H), 7.41 (dd, *J* = 8.6, 2.2 Hz, 1H).

^{13}C NMR (151 MHz, DMSO-d_6) δ 150.87, 144.93, 142.22, 140.08, 136.41, 130.77, 130.63, 129.29, 129.01, 128.52, 127.79, 125.78, 124.93, 114.60, 114.16, 112.99.

IR (cm^{-1}): νmax**;** 3143, 3031, 1619, 1548, 1229, 1123, 744;

HRMS (ESI): calcd for $C_{16}H_{10}BrN_3$ [M+H] $^+$:324.0136; found: 324.0129.

Synthesis of 2-(5-nitro-1H-indol-3-yl) quinoxaline (3ah)



Prepared according to the general procedure (3a) mentioned above in 38% yield (33.1 mg), eluent (30% EtOAc/hexane) to afford a yellow solid, mp= 262-264 ℃.

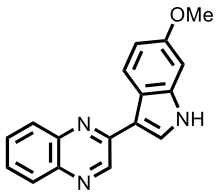
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 12.47 (s, 1H), 9.63 (d, *J* = 2.4 Hz, 1H), 9.47 (s, 1H), 8.79 (d, *J* = 2.6 Hz, 1H), 8.08 (dd, *J* = 8.9, 2.4 Hz, 1H), 8.03 (d, *J* = 8.2 Hz, 1H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.78 (s, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.64 (d, *J* = 8.9 Hz, 1H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 150.2, 144.8, 142.6, 142.0, 140.7, 140.3, 132.7, 130.9, 129.3, 129.1, 129.0, 125.3, 119.6, 118.5, 115.2, 113.2.

IR (cm^{-1}): νmax**;** 3160, 3060, 1618, 1579, 1548, 1240, 1140, 743.

HRMS (ESI): calcd for $C_{16}H_{10}N_3O_2$ [M+Na] $^+$; 313.0701; found: 313.0711

Synthesis of 2-(6-methoxy-1H-indol-3-yl) quinoxaline (3ai)



Prepared according to the general procedure (3a) mentioned above in 69% yield (66.9mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 190-192 ℃.

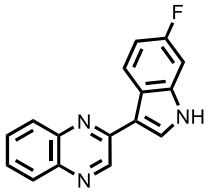
^{1}H NMR (600 MHz, CDCl$_3$) δ 9.19 (s, 1H), 8.68 (d, *J* = 8.9 Hz, 1H), 8.61 (s, 1H), 8.13 (d, *J* = 8.5 Hz, 1H), 8.04 (d, *J* = 8.1 Hz, 1H), 7.87 (d, *J* = 2.7 Hz, 1H), 7.76 – 7.71 (m, 1H), 7.67 – 7.63 (m, 1H), 7.00 (dd, *J* = 8.8, 2.3 Hz, 1H), 6.91 (d, *J* = 2.3 Hz, 1H), 3.88 (s, 3H).

^{13}C NMR (151 MHz, CDCl$_3$) δ 157.3, 150.2, 143.7, 142.6, 140.1, 137.7, 129.8, 128.9, 128.8, 128.0, 124.4, 123.2, 119.8, 115.0, 111.4, 94.7, 55.5.

IR (cm^{-1}): νmax**;**3181, 3068, 1628, 1550, 1453, 1250, 1151, 1125, 757.

HRMS (ESI): calcd for $C_{17}H_{13}N_3O$ [M+H] $^+$:276.1137; found: 276.1122.

Synthesis of 2-(6-fluoro-1H-indol-3-yl) quinoxaline (3aj)



Prepared according to the general procedure (3a) mentioned above in 71% yield (56.1mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 216-218 ℃.

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 11.96 (s, 1H), 9.50 (s, 1H), 8.80 (dd, *J* = 8.8, 5.7 Hz, 1H), 8.63 (d, *J* = 3.0 Hz, 1H), 8.09 (d, *J* = 8.1 Hz, 1H), 8.02 (d, *J* = 8.1 Hz, 1H), 7.80 (t, *J* = 7.6 Hz, 1H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.32 (dd, *J* = 9.8, 2.5 Hz, 1H), 7.13 – 7.08 (m, 1H).

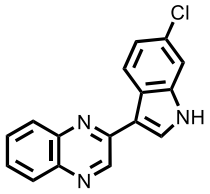
^{13}C NMR (151 MHz, DMSO-d$_6$) δ 160.7, 159.1, 151.0, 144.9, 142.2, 140.0, 137.7, 130.6, 130.1, 129.2, 128.9, 128.4, 124.0, 124.0, 122.8, 113.5, 109.8, 109.6, 98.7, 98.5.

^{19}F NMR (471 MHz, DMSO-d$_6$): -119.89.

IR (cm^{-1}): νmax**;** 3153, 3038, 1614, 1551, 1230, 1172, 11023, 755.

HRMS: (ESI) calcd for $C_{16}H_{10}FN_3$ [M+H] $^+$:264.0937; found: 264.0936.

Synthesis of 2-(6-chloro-1H-indol-3-yl) quinoxaline (3ak)



Prepared according to the general procedure (3a) mentioned above in 54% yield (45.3 mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 236-238 ℃.

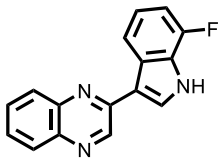
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 12.02 (s, 1H), 9.50 (s, 1H), 8.79 (d, *J* = 8.5 Hz, 1H), 8.66 (d, *J* = 2.8 Hz, 1H), 8.09 (d, *J* = 8.0 Hz, 1H), 8.02 (d, *J* = 8.2 Hz, 1H), 7.81 (dd, *J* = 8.3, 6.7 Hz, 1H), 7.72 (d, *J* = 7.6 Hz, 1H), 7.58 (d, *J* = 2.0 Hz, 1H), 7.27 (dd, *J* = 8.4, 2.0 Hz, 1H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 150.8, 144.9, 142.2, 140.0, 138.1, 130.6, 130.4, 129.2, 129.0, 128.5, 127.8, 124.8, 124.1, 121.7, 113.5, 112.2.

IR (cm^{-1}): νmax**;** 3151, 3043, 1609, 1549, 1265, 1125, 753, 710.

HRMS (ESI): calcd for $C_{16}H_{10}ClN_3$ [M+Na] $^+$:302.0461; found: 302.0458.

Synthesis of 2-(7-fluoro-1H-indol-3-yl) quinoxaline (3al)



Prepared according to the general procedure (3a) mentioned above in 54% yield (42.6mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 236-238 ℃.

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 12.40 (s, 1H), 9.54 (s, 1H), 8.70 (d, *J* = 3.0 Hz, 1H), 8.62 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 8.2 Hz, 1H), 8.02 (d, *J* = 8.2 Hz, 1H), 7.81 (t, *J* = 7.6 Hz, 1H), 7.72 (d, *J* = 7.7 Hz, 1H), 7.22 (td, *J* = 7.9, 4.8 Hz, 1H), 7.11 (dd, *J* = 11.4, 7.7 Hz, 1H).

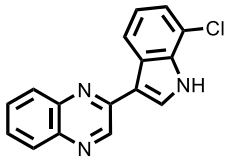
^{13}C NMR (151 MHz, DMSO-d$_6$) δ 161.3, 161.1, 159.5, 154.8, 153.0, 151.0, 140.5, 140.4, 139.7, 139.5, 139.1, 138.9, 138.6, 132.0, 132.0, 129.6, 125.6, 118.3, 118.2.

^{19}F NMR (471 MHz, DMSO-d$_6$): -132.97.

IR (cm^{-1}): νmax**;** 3058, 3021, 1639, 1547, 1227, 1181, 1130, 757.

HRMS: (ESI) calcd for $C_{16}H_{10}FN_3$ $[M+H]^+$:264.0937; found: 264.0939.

Synthesis of 2-(7-chloro-1H-indol-3-yl) quinoxaline (3am)



Prepared according to the general procedure (3a) mentioned above in 40% yield (33.5 mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 270-272 ℃.

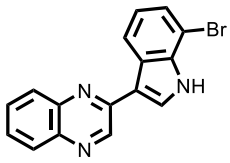
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 12.26 (s, 1H), 9.56 (s, 1H), 8.79 (d, *J* = 7.9 Hz, 1H), 8.71 (d, *J* = 2.9 Hz, 1H), 8.11 (d, *J* = 8.2 Hz, 1H), 8.03 (d, *J* = 8.5 Hz, 1H), 7.81 (t, *J* = 7.5 Hz, 1H), 7.72 (t, *J* = 7.7 Hz, 1H), 7.35 (d, *J* = 7.5 Hz, 1H), 7.26 (t, *J* = 7.8 Hz, 1H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 150.8, 145.1, 142.2, 140.1, 134.5, 130.6, 130.5, 129.3, 129.0, 128.6, 128.0, 122.7, 122.4, 121.9, 116.8, 114.5.

IR (cm^{-1}): νmax**;** 3166, 3061, 1621, 1563, 1260, 1118, 748, 702.

HRMS (ESI): calcd for $C_{16}H_{10}ClN_3$ $[M+H]^+$:280.0642; found: 280.0635.

Synthesis of 2-(7-bromo-1H-indol-3-yl) quinoxaline (3an)



Prepared according to the general procedure (3a) mentioned above in 50% yield (48.6mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 260-262 ℃.

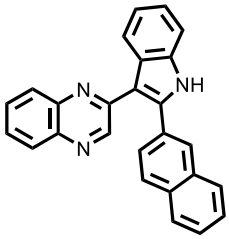
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 12.12 (s, 1H), 9.57 (s, 1H), 8.84 (d, *J* = 7.9 Hz, 1H), 8.70 (d, *J* = 2.9 Hz, 1H), 8.11 (d, *J* = 7.6 Hz, 1H), 8.03 (d, *J* = 8.5 Hz, 1H), 7.86 – 7.78 (m, 1H), 7.76 – 7.68 (m, 1H), 7.49 (d, *J* = 7.5 Hz, 1H), 7.21 (t, *J* = 7.8 Hz, 1H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 150.8, 145.1, 142.2, 140.1, 136.0, 130.6, 130.5, 129.3, 129.0, 128.6, 127.8, 125.8, 122.8, 122.3, 114.5, 105.1.

IR (cm^{-1}): νmax**;** 3204, 3041, 1608, 1524, 1238, 1147, 745, 650.

HRMS (ESI): calcd for $C_{16}H_{10}BrN_3$ $[M+H]^+$:324.0136; found:324.0133.

Synthesis of 2-(2-(naphthalen-2-yl)-1H-indol-3-yl) quinoxaline (3ao)



Prepared according to the general procedure (3a) mentioned above in 60% yield (66.8mg), eluent (20% EtOAc/hexane) to afford a yellow solid, mp= 168-170 ℃.

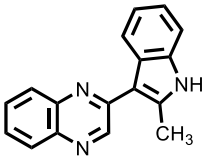
^{1}H NMR (500 MHz, DMSO-d$_6$) δ 12.18 (s, 1H), 8.54 (s, 1H), 8.37 (d, *J* = 7.9 Hz, 1H), 8.27 (d, *J* = 1.8 Hz, 1H), 8.14 (dd, *J* = 8.5, 1.4 Hz, 1H), 8.05 – 7.95 (m, 4H), 7.84 (ddd, *J* = 8.4, 7.0, 1.5 Hz, 1H), 7.75 (ddd, *J* = 8.3, 7.0, 1.4 Hz, 1H), 7.67 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.63 – 7.55 (m, 3H), 7.33 – 7.29 (m, 1H), 7.26 – 7.22 (m, 1H).

^{13}C NMR (126 MHz, DMSO-d$_6$) δ 151.5, 146.4, 142.6, 139.7, 139.7, 137.1, 133.4, 133.2, 130.6, 130.1, 129.1, 129.1, 129.0, 128.7, 128.7, 128.2, 128.0, 127.4, 127.3, 127.3, 123.4, 121.4, 121.2, 112.2, 110.7.

IR (cm^{-1}): νmax**;** 3146, 3017, 1616, 1544, 1132, 739.

HRMS (ESI): calcd for $C_{26}H_{17}N_3$ [M+Na] $^+$: 394.1320; found: 394.1340.

Synthesis of 2-(2-methyl-1H-indol-3-yl) quinoxaline (3ap)



Prepared according to the general procedure (3a) mentioned above in 67% yield (52.1mg), eluent (20-25% EtOAc/hexane) to afford a yellow solid, mp= 142-144 ℃.

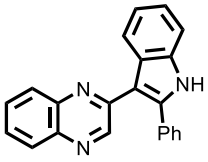
^{1}H NMR (600 MHz, CDCl$_3$) δ 9.23 (s, 1H), 8.90 (s, 1H), 8.14 – 8.09 (m, 3H), 7.73 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.67 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.29 (d, *J* = 7.4 Hz, 1H), 7.24 – 7.18 (m, 2H), 2.67 (s, 3H).

^{13}C NMR (151 MHz, CDCl$_3$) δ 151.0, 145.5, 142.7, 139.9, 137.0, 135.3, 129.8, 128.8, 128.7, 128.3, 126.9, 122.2, 121.0, 119.3, 110.8, 110.6, 13.5.

IR (cm^{-1}): νmax**;** 3154, 3051, 1620, 1578, 1431, 1274, 1126, 731.

HRMS (ESI): calcd for $C_{17}H_{13}N_3$ [M+Na] $^+$:282.1007; found: 282.1012.

Synthesis of 2-(2-phenyl-1H-indol-3-yl) quinoxaline (3aq)



Prepared according to the general procedure (3a) mentioned above in 49% yield (47.2mg), eluent (20-25% EtOAc/hexane) to afford a yellow solid, mp= 218-220 ℃.

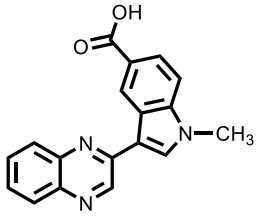
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 12.04 (s, 1H), 8.51 (s, 1H), 8.33 (d, *J* = 8.0 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.84 (t, *J* = 7.5 Hz, 1H), 7.75 (t, *J* = 7.6 Hz, 1H), 7.63 – 7.61 (m, 2H), 7.54 – 7.51 (m, 4H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.21 (t, *J* = 7.5 Hz, 1H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 151.6, 146.5, 142.6, 139.8, 139.7, 137.0, 132.7, 130.6, 129.7, 129.6, 129.5, 129.2, 129.1, 128.0, 123.4, 121.4, 121.2, 112.2, 110.4.

IR (cm^{-1}): νmax**;** 3232, 3050, 1649, 1546, 1237, 1103, 749.

HRMS (ESI): calcd for $C_{22}H_{15}N_3$[M+H] $^+$:322.1344; found: 322.1349.

Synthesis of 1-methyl-3-(quinoxalin-2-yl)-1H-indole-5-carboxylic acid (3ar)



Prepared according to the general procedure (3a) mentioned above in 36% yield (32.7mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 246-248 ℃.

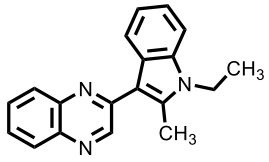
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 12.26 (s, 1H), 9.54 (s, 1H), 9.51 (d, *J* = 1.7 Hz, 1H), 8.75 (d, *J* = 2.8 Hz, 1H), 8.08 (dd, *J* = 8.4, 1.4 Hz, 1H), 8.05 (dd, *J* = 8.4, 1.4 Hz, 1H), 7.90 (dd, *J* = 8.3, 1.9 Hz, 1H), 7.85 (td, *J* = 7.4, 1.6 Hz, 1H), 7.76 – 7.73 (m, 1H), 7.62 (d, *J* = 8.6 Hz, 1H), 3.94 (s, 3H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 167.7, 150.8, 145.0, 142.2, 140.2, 140.1, 131.1, 130.7, 129.3, 128.9, 128.7, 125.6, 125.4, 124.1, 122.9, 114.4, 112.6, 52.4.

IR (cm^{-1}): νmax**;**3278, 3057, 1690, 1624, 1551, 1458, 1231, 1163, 1124, 743.

HRMS (ESI): calcd for $C_{18}H_{13}N_3O_2$ [M+Na] $^+$:326.0905; found: 326.0906.

Synthesis of 2-(1-ethyl-2-methyl-1H-indol-3-yl) quinoxaline (3as)



Prepared according to the general procedure (3a) mentioned above in 67% yield (57.7 mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 138-140 ℃.

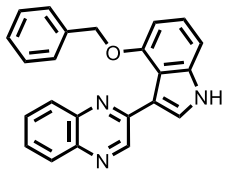
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.24 (s, 1H), 8.11 (dd, *J* = 11.5, 8.5 Hz, 2H), 8.04 (d, *J* = 7.9 Hz, 1H), 7.74 (t, *J* = 7.7 Hz, 1H), 7.69 (t, *J* = 7.7 Hz, 1H), 7.39 (d, *J* = 8.1 Hz, 1H), 7.28 – 7.22 (m, 2H), 4.26 (q, *J* = 7.2 Hz, 2H), 2.79 (s, 3H), 1.43 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 151.3, 146.3, 142.9, 140.2, 137.8, 136.0, 129.9, 129.2, 129.0, 128.4, 126.7, 122.0, 121.1, 119.2, 110.9, 109.4, 38.1, 15.1, 11.6.

IR (cm^{-1}): νmax**;** 3043, 1613, 1538, 1418, 1232, 1153, 736.

HRMS (ESI): calcd for $C_{19}H_{17}N_3$ $[M+Na]^+$:310.1320; found:310.1321

Synthesis of 2-(4-(benzyloxy)-1H-indol-3-yl) quinoxaline (3at)



Prepared according to the general procedure (3a) mentioned above in 76% yield (80.0mg), eluent (20% EtOAc/hexane) to afford a yellow solid, mp=154-156 ℃.

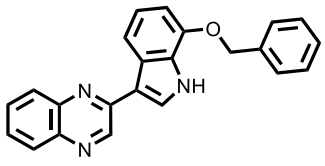
^{1}H NMR (200 MHz, $CDCl_3$) δ 10.02 (s, 1H), 9.37 (s, 1H), 8.11 – 8.00 (m, 2H), 7.70 – 7.55 (m, 3H), 7.13 (d, *J* = 2.9 Hz, 6H), 6.94 (d, *J* = 8.2 Hz, 1H), 6.64 (d, *J* = 7.7 Hz, 1H), 5.14 (s, 2H).

^{13}C NMR (50 MHz, $CDCl_3$) δ 153.1, 150.8, 148.3, 141.9, 140.4, 138.7, 136.7, 129.8, 128.9, 128.6, 128.5, 128.3, 127.7, 127.5, 127.2, 126.4, 123.6, 115.7, 115.1, 105.6, 102.7, 70.4.

IR (cm^{-1}): νmax**;** 3096, 3048, 1634, 1542, 1470, 1232, 1141, 730.

HRMS (ESI): calcd for $C_{23}H_{17}N_3O$ [M+ Na] +:374.1269; found:374.1277

Synthesis of 2-(7-(benzyloxy)-1H-indol-3-yl) quinoxaline (3au)



Prepared according to the general procedure (3a) mentioned above in 68% yield (71.6 mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 184-186 ℃.

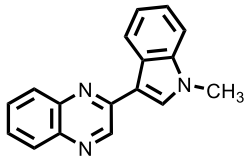
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.23 (s, 1H), 8.95 (s, 1H), 8.33 (d, *J* = 8.1 Hz, 1H), 8.14 – 8.11 (m, 1H), 8.04 (dd, *J* = 8.6, 1.5 Hz, 1H), 7.94 (d, *J* = 2.8 Hz, 1H), 7.72 (td, *J* = 7.4, 1.4 Hz, 1H), 7.65 – 7.61 (m, 1H), 7.50 – 7.47 (m, 2H), 7.42 – 7.35 (m, 3H), 7.26 – 7.24 (m, 1H), 6.85 (d, *J* = 7.6 Hz, 1H), 5.23 (s, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 150.4, 145.4, 143.9, 142.8, 140.4, 136.8, 129.9, 129.1, 129.0, 128.7, 128.7, 128.3, 128.2, 128.0, 127.8, 127.1, 125.2, 122.3, 115.6, 115.1, 104.6, 70.5.

IR (cm^{-1}): νmax**;** 3141, 3057, 1624, 1549, 1448, 1237, 1190, 1135, 721.

HRMS (ESI): calcd for $C_{23}H_{17}N_3O$ [M+H] $^+$:352.1450; found:352.1456.

Synthesis of 2-(1-methyl-1H-indol-3-yl) quinoxaline (3av)



Prepared according to the general procedure (3a) mentioned above in 62% yield (48.2mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 74-76 ℃.

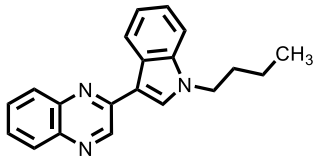
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.80 – 8.76 (m, 1H), 8.11 (dd, *J* = 8.3, 1.4 Hz, 1H), 8.05 – 8.01 (m, 1H), 7.79 (s, 1H), 7.72 (ddd, *J* = 8.5, 6.9, 1.5 Hz, 1H), 7.65 – 7.61 (m, 1H), 7.36 (d, *J* = 3.4 Hz, 3H), 3.84 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 150.4, 143.8, 142.8, 140.2, 137.9, 130.2, 129.9, 129.0, 127.9, 126.4, 123.1, 122.6, 121.6, 113.4, 109.7, 33.4.

IR (cm^{-1}): νmax**;** 3052, 1610, 1550, 1455, 1337, 1225, 1122, 737.

HRMS (ESI) calcd for $C_{17}H_{13}N_3$ [M+H] $^+$:322.1344; found: 322.1349.

Synthesis of 2-(1-butyl-1H-indol-3-yl) quinoxaline (3aw)



Prepared according to the general procedure (3a) mentioned above in 50% yield (45.2mg), eluent (15-20% EtOAc/hexane) to afford a yellow solid, mp= 88-90 ℃.

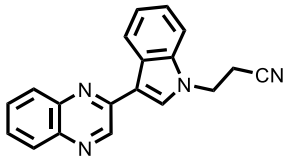
^{1}H NMR (600 MHz, DMSO-d_6) δ 9.45 (s, 1H), 8.83 (d, *J* = 7.5 Hz, 1H), 8.67 (s, 1H), 8.08 (dd, *J* = 8.7, 1.5 Hz, 1H), 8.01 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.81 – 7.78 (m, 1H), 7.71 – 7.67 (m, 1H), 7.62 (d, *J* = 7.7 Hz, 1H), 7.32 – 7.27 (m, 2H), 4.30 (t, *J* = 7.1 Hz, 2H), 1.88 – 1.84 (m, 2H), 1.36 – 1.31 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (151 MHz, DMSO-d_6) δ 151.0, 144.9, 142.4, 139.9, 137.5, 132.3, 130.5, 129.2, 128.9, 128.3, 126.5, 123.2, 123.1, 121.6, 112.5, 111.0, 46.3, 32.2, 20.0, 14.0.

IR (cm^{-1}): νmax**;** 3057, 1613, 1546, 1455, 1217, 1199, 733

HRMS (ESI): calcd for $C_{20}H_{19}N_3$ [M+H] $^+$:302.1657; found: 302.1663.

Synthesis of 3-(3-(quinoxalin-2-yl)-1H-indol-1-yl) propanenitrile (3ax)



Prepared according to the general procedure (3a) mentioned above in 43% yield (38.4mg), eluent (20% EtOAc/hexane) to afford a yellow solid, mp= 104-106 ℃.

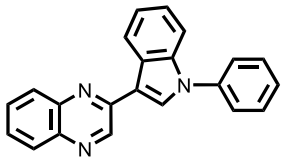
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 9.42 (s, 1H), 8.82 (d, *J* = 7.7 Hz, 1H), 8.71 (s, 1H), 8.11 (d, *J* = 8.2 Hz, 1H), 8.03 (d, *J* = 8.3 Hz, 1H), 7.82 (t, *J* = 7.6 Hz, 1H), 7.77 – 7.70 (m, 2H), 7.34 (dt, *J* = 18.6, 7.1 Hz, 2H), 4.65 (t, *J* = 6.6 Hz, 2H), 3.21 (t, *J* = 6.7 Hz, 2H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 150.7, 144.7, 142.3, 140.0, 137.3, 132.1, 130.7, 129.3, 129.0, 128.6, 126.5, 123.5, 123.1, 122.0, 119.2, 113.3, 111.1, 42.3, 19.0.

IR (cm^{-1}): νmax; 3054, 2247, 1614, 1506, 1458, 1395, 1250, 1096, 695.

HRMS (ESI): calcd for $C_{19}H_{14}N_4$ [M+Na] $^+$:321.1116; found: 321.1111.

Synthesis of 2-(1-phenyl-1H-indol-3-yl) quinoxaline (3ay)



Prepared according to the general procedure (3a) mentioned above in 39% yield (37.6mg), eluent (20% EtOAc/hexane) to afford a yellow solid, mp= 88-90 ℃.

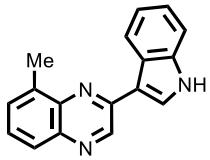
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 9.60 (s, 1H), 8.96 (d, *J* = 3.5 Hz, 2H), 8.15 (dd, *J* = 8.4, 1.5 Hz, 1H), 8.06 – 8.03 (m, 1H), 7.85 – 7.82 (m, 1H), 7.78 – 7.72 (m, 3H), 7.70 – 7.66 (m, 2H), 7.63 (dd, *J* = 6.5, 2.3 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.40 – 7.36 (m, 2H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 150.6, 145.2, 142.2, 140.2, 138.8, 137.0, 132.1, 130.7, 130.5, 129.3, 129.1, 128.8, 128.0, 127.2, 125.0, 124.4, 123.5, 122.6, 114.8, 111.4.

IR (cm^{-1}): νmax; 3044, 1595, 1539, 1215, 1141, 739.

HRMS (ESI): calcd for $C_{22}H_{15}N_3$ [M+Na] $^+$:344.1164; found: 344.1176

Synthesis of 2-(1H-indol-3-yl)-8-methylquinoxaline (3az)



Prepared according to the general procedure (3a) mentioned above in 44% yield (34.2mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp=152-154 ℃.

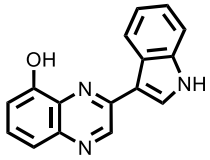
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 11.90 (s, 1H), 9.50 (s, 1H), 8.80 (dd, *J* = 6.0, 3.3 Hz, 1H), 8.63 (d, *J* = 2.9 Hz, 1H), 7.84 (d, *J* = 8.2 Hz, 1H), 7.66 (d, *J* = 7.0 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.54 (dd, *J* = 6.0, 3.1 Hz, 1H), 7.27 (dd, *J* = 6.0, 3.0 Hz, 2H), 2.86 (s, 3H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 150.2, 144.5, 141.2, 139.9, 137.7, 136.6, 130.3, 129.3, 127.8, 127.1, 126.0, 123.2, 122.7, 121.5, 113.8, 112.5, 17.8.

IR (cm^{-1}): νmax**;** 3130, 3053, 1617, 1547, 1446, 1239, 1139, 736

HRMS (ESI): calcd for calcd for $C_{17}H_{13}N_3$ [M+H] $^+$:260.1188; found:260.1202

Synthesis of 3-(1H-indol-3-yl) quinoxalin-5-ol (3ba)



Prepared according to the general procedure (3a) mentioned above in 42% yield (33.0mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp=270-272 ℃.

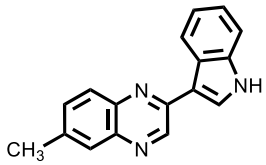
^{1}H NMR (200 MHz, DMSO-d$_6$) δ 11.91 (s, 1H), 10.17 (s, 1H), 9.39 (s, 1H), 8.82 – 8.75 (m, 1H), 8.63 (d, *J* = 2.9 Hz, 1H), 7.65 – 7.49 (m, 3H), 7.30 – 7.22 (m, 2H), 7.03 (dd, *J* = 7.5, 1.6 Hz, 1H).

^{13}C NMR (50 MHz, DMSO-d$_6$) δ 154.1, 151.4, 143.3, 142.2, 137.6, 131.0, 130.7, 129.3, 126.0, 123.1, 122.7, 121.3, 118.8, 113.3, 112.4, 111.2.

IR (cm^{-1}): νmax**;** 3340, 3137, 3022, 1627, 1555, 1207, 1167, 1104, 697.

HRMS (ESI): calcd for $C_{16}H_{11}N_3$ [M+Na] $^+$:284.0800; found: 284.0812.

Synthesis of 2-(1H-indol-3-yl)-6-methylquinoxaline (3bb)



Prepared according to the general procedure (3a) mentioned above in 71% yield (55.2mg), eluent (25% EtOAc/hexane) to afford a brownish yellow solid mp=154-156 ℃.

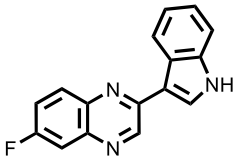
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 11.10 (s, 1H), 8.64 (s, 1H), 8.07 – 8.01 (m, 1H), 7.79 (d, *J* = 2.9 Hz, 1H), 7.18 – 7.03 (m, 2H), 6.76 (dd, *J* = 5.4, 3.1 Hz, 1H), 6.69 (dd, *J* = 8.4, 2.1 Hz, 1H), 6.49 – 6.45 (m, 2H), 1.74 (s, 3H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 151.3, 144.0, 142.4, 140.4, 138.3, 137.6, 132.4, 130.2, 129.1, 128.7, 127.9, 126.1, 123.1, 121.3, 113.5, 112.5, 21.7.

IR (cm^{-1}): νmax**;** 3187, 3074, 1598, 1548, 1482, 1233, 1109, 742.

The chemical compounds have been described.[3]

Synthesis of 6-fluoro-2-(1H-indol-3-yl) quinoxaline (3bc)



Prepared according to the general procedure (3a) mentioned above in 71% yield (56.1mg), eluent (25% EtOAc/hexane) to afford a yellow solid, mp= 164-166 ℃.

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 11.96 – 11.89 (m, 1H), 9.44 (s, 1H), 8.77 – 8.75 (m, 1H), 8.60 (d, *J* = 2.9 Hz, 1H), 8.00 (dd, *J* = 9.1, 5.9 Hz, 1H), 7.78 (dd, *J* = 9.7, 2.6 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.24 – 7.19 (m, 2H).

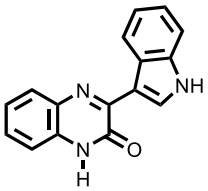
^{13}C NMR (151 MHz, DMSO-d$_6$) δ 163.6, 162.0, 152.1, 144.5, 143.4, 143.3, 137.7, 137.1, 131.6, 131.5, 130.1, 126.0, 123.3, 122.9, 121.5, 117.8, 117.6, 113.2, 112.6, 112.4.

^{19}F NMR (471 MHz DMSO-d$_6$): -109.62.

IR (cm^{-1}): 3167 3047, 1615, 1543, 1243, 1168, 1143, 737.

HRMS (ESI): calcd for $C_{16}H_{10}N_3F$ [M+H] $^{+}$:264.0937; found: 264.0947.

Synthesis of 3-(1H-indol-3-yl) quinoxalin-2(1H)-one (3bd)



Prepared according to the general procedure (3b) mentioned above in 57% yield (44.6mg), eluent (20-25% EtOAc/hexane) to afford an orange solid, mp=300-302 ℃.

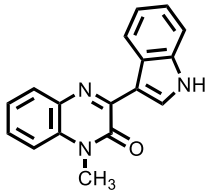
^{1}H NMR (200 MHz, DMSO-d$_6$) δ 12.42 (s, 1H), 11.80 (s, 1H), 8.96 (d, *J* = 2.9 Hz, 1H), 8.90 (dd, *J* = 6.4, 3.0 Hz, 1H), 7.88 (d, *J* = 7.7 Hz, 1H), 7.56 – 7.40 (m, 2H), 7.37 – 7.22 (m, 4H).

^{13}C NMR (50 MHz, DMSO-d$_6$) δ 154.8, 152.4, 136.7, 133.5, 133.1, 130.6, 128.4, 128.0, 126.6, 123.7, 123.4, 123.0, 121.4, 115.4, 112.3, 111.7.

IR (cm^{-1}): νmax**;** 3130, 3053, 1617, 1547, 1446, 1239, 1139, 736

The chemical compounds have been described.[4]

Synthesis of 3-(1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3be)



Prepared according to the general procedure (3b) mentioned above in 75% yield (61.9mg), eluent (20% EtOAc/hexane) to afford an orange solid, mp= 250-252 ℃.

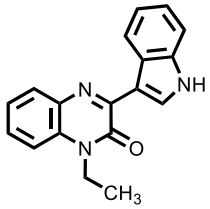
^{1}H NMR (200 MHz, DMSO-d$_6$) δ 10.97 (s, 1H), 8.09 (dd, *J* = 9.6, 3.2 Hz, 2H), 7.08 (d, *J* = 7.6 Hz, 1H), 6.70 (dd, *J* = 6.5, 3.0 Hz, 3H), 6.56 (dd, *J* = 7.7, 4.3 Hz, 1H), 6.43 (dd, *J* = 6.1, 3.2 Hz, 2H), 2.89 (s, 3H).

^{13}C NMR (50 MHz, DMSO-d$_6$) δ 154.1, 151.0, 136.7, 133.6, 133.4, 131.9, 128.8, 128.7, 126.7, 123.8, 123.4, 123.0, 121.4, 114.8, 112.3, 111.8, 29.5.

IR (cm^{-1}): *ν*max**;** 3254, 3032, 1736, 1625, 1532, 1429, 1175, 741.

HRMS (ESI) calcd for $C_{17}H_{13}N_3O$ [M+Na] $^+$:298.0956; found: 298.0969.

Synthesis of 1-ethyl-3-(1H-indol-3-yl) quinoxalin-2(1H)-one (3bf)



Prepared according to the general procedure (3b) mentioned above in 73% yield (63.3mg), eluent (20% EtOAc/hexane) to afford a brownish solid, mp=188-190 ℃.

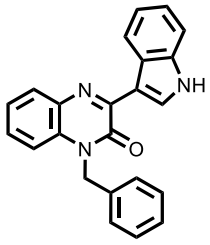
^{1}H NMR (200 MHz, DMSO-d$_6$) δ 11.82 (s, 1H), 8.94 (dd, *J* = 11.8, 3.1 Hz, 2H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 6.3 Hz, 3H), 7.42 – 7.33 (m, 1H), 7.26 (dd, *J* = 6.1, 3.2 Hz, 2H), 4.37 (q, *J* = 6.9 Hz, 2H), 1.30 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (50 MHz, DMSO-d$_6$) δ 153.6, 151.1, 136.7, 133.7, 133.6, 130.7, 129.1, 128.8, 126.8, 123.8, 123.4, 123.0, 121.4, 114.5, 112.3, 111.8, 37.34, 12.8.

IR (cm^{-1}): *ν*max**;** 3242, 3028, 1633, 1575, 1453, 1431, 1216, 1113, 737.

The chemical compounds have been described.[5]

Synthesis of 1-benzyl-3-(1H-indol-3-yl) quinoxalin-2(1H)-one (3bg)



Prepared according to the general procedure (3b) mentioned above in 80% yield (84.3mg), eluent (20% EtOAc/hexane) to afford a brownish solid, mp=194-196 ℃.

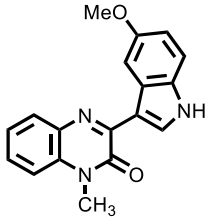
^{1}H NMR (200 MHz, $CDCl_3$) δ 9.08 – 9.01 (m, 1H), 8.96 (d, *J* = 2.9 Hz, 1H), 8.70 (s, 1H), 8.05 – 7.97 (m, 1H), 7.40 – 7.30 (m, 5H), 7.30 – 7.21 (m, 6H), 5.59 (s, 2H).

^{13}C NMR (50 MHz, $CDCl_3$) δ 154.6, 151.0, 136.1, 135.5, 134.0, 132.4, 131.0, 129.5, 128.9, 128.4, 127.5, 126.6, 123.7, 123.4, 123.2, 121.8, 114.2, 112.9, 111.2, 46.0.

IR (cm^{-1}): νmax**;** 3108, 3047, 1682, 1627, 1533, 1237, 1129, 743

The chemical compounds have been described.[4]

Synthesis of 3-(5-methoxy-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3bh)



Prepared according to the general procedure (3b) mentioned above in 60% yield (55.0mg), eluent (20% EtOAc/hexane) to afford an orange solid, mp= 264-266 ℃.

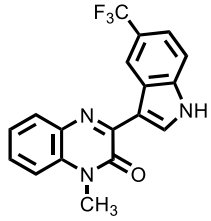
^{1}H NMR (200 MHz, DMSO-d_6) δ 11.67 (s, 1H), 8.89 (d, *J* = 3.0 Hz, 1H), 8.48 (d, *J* = 2.6 Hz, 1H), 7.90 (d, *J* = 7.7 Hz, 1H), 7.53 (d, *J* = 3.9 Hz, 2H), 7.42 (d, *J* = 8.7 Hz, 2H), 6.90 (dd, *J* = 8.8, 2.6 Hz, 1H), 3.89 (s, 3H), 3.73 (s, 3H).

^{13}C NMR (50 MHz, DMSO-d_6) δ 155.3, 154.1, 151.1, 133.9, 133.4, 131.8, 131.6, 128.7, 128.6, 127.4, 123.9, 114.8, 112.9, 112.5, 111.6, 105.5, 55.7, 29.5.

IR (cm^{-1}): νmax**;** 3149, 2935, 1641, 1527, 1411, 1196, 1137, 741.

The chemical compounds have been described.[5]

Synthesis of 1-methyl-3-(5-(trifluoromethyl)-1H-indol-3-yl) quinoxalin-2(1H)-one (3bi)



Prepared according to the general procedure (3b) mentioned above in 79% yield (81.3mg), eluent (20% EtOAc/hexane) to afford a brownish solid, mp=288-290 ℃.

^{1}H NMR (200 MHz, DMSO-d_6) δ 12.15 (s, 1H), 9.23 (s, 1H), 9.03 (s, 1H), 7.83 (d, *J* = 7.8 Hz, 1H), 7.72 (d, *J* = 8.5 Hz, 1H), 7.54 (d, *J* = 5.5 Hz, 3H), 7.44 – 7.35 (m, 1H), 3.71 (s, 3H).

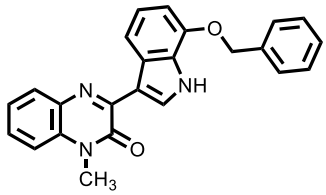
^{13}C NMR (50 MHz, DMSO-d_6) δ 153.9, 150.6, 138.3, 135.3, 133.0, 132.0, 129.1, 128.8, 126.1, 123.9, 123.6, 122.2, 120.7, 119.4, 114.9, 113.1, 112.3, 29.5.

^{19}F NMR (471 MHz, DMSO-d$_6$) δ -58.67.

IR (cm^{-1}): νmax**;** 3204, 3066, 1712, 1602, 1560, 1454, 1196, 1087, 741.

HRMS (ESI): calcd for $C_{18}H_{12}F_3N_3O_2$ [M+Na] $^+$:366.0830; found: 366.0854.

Synthesis of 3-(7-(benzyloxy)-1H-indol-3-yl)-1-methylquinoxalin-2(1H)-one (3bj)



Prepared according to the general procedure (3b) mentioned above in 51% yield (58.3mg), eluent (20% EtOAc/hexane) to afford an orange solid, mp= 228-230 ℃.

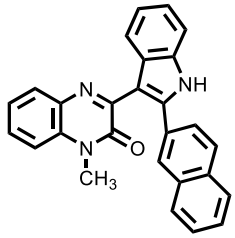
^{1}H NMR (200 MHz, DMSO-d$_6$) δ 11.84 (s, 1H), 8.76 (d, *J* = 3.0 Hz, 1H), 8.41 (d, *J* = 8.0 Hz, 1H), 7.80 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.55 – 7.47 (m, 2H), 7.43 – 7.24 (m, 6H), 7.06 (t, *J* = 7.9 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 1H), 5.20 (s, 2H), 3.61 (s, 3H).

^{13}C NMR (50 MHz, DMSO-d$_6$) δ 154.1, 151.0, 145.6, 137.6, 133.4, 133.0, 131.9, 128.8, 128.8, 128.7, 128.5, 128.3, 128.1, 126.9, 123.8, 122.0, 116.4, 114.8, 112.4, 105.1, 69.8, 29.5.

IR (cm^{-1}): νmax**;** 3199, 3043, 1625, 1603, 1247, 1179, 1096, 727.

HRMS (ESI): calcd for $C_{24}H_{19}N_3O_2$ [M+Na] $^+$:404.1375; found: 404.1383.

Synthesis of 1-methyl-3-(2-(naphthalen-2-yl)-1H-indol-3-yl) quinoxalin-2(1H)-one (3bk)



Prepared according to the general procedure (3b) mentioned above in 53% yield (63.8mg), eluent (20% EtOAc/hexane) to afford an orange solid, mp=168-170 ℃.

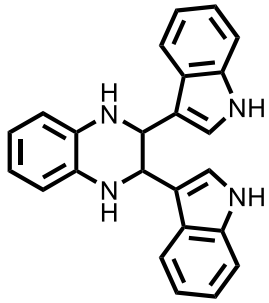
^{1}H NMR (200 MHz, DMSO-d$_6$) δ 11.92 (s, 1H), 8.09 (s, 1H), 7.85 – 7.63 (m, 5H), 7.54 – 7.40 (m, 6H), 7.33 – 7.24 (m, 1H), 7.17 – 6.98 (m, 2H), 3.47 (s, 3H).

^{13}C NMR (50 MHz, DMSO-d$_6$) δ 154.2, 153.8, 139.7, 136.6, 133.5, 133.3, 133.2, 132.8, 131.3, 130.2, 129.4, 129.1, 128.5, 128.0, 128.0, 127.0, 126.8, 126.7, 123.8, 122.7, 120.9, 120.5, 120.2 115.0, 111.9, 110.0, 29.7.

IR (cm^{-1}): νmax**;** 3245, 3022, 1738, 1644, 1577, 1446, 1145, 740.

The chemical compounds have been described.[4]

Synthesis of 5,6,10c,11,16,16a-hexahydrodiindolo[3,2-a:2',3'-c] phenazine (4aa)



Prepared according to the general procedure (3c) mentioned above in 66% yield (72.0mg), eluent (25-30% EtOAc/hexane) to afford off white solid, mp= 193-195 ℃.

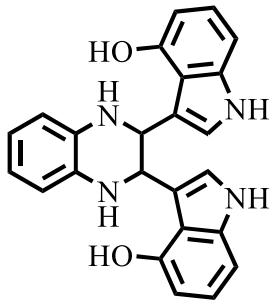
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 10.72 (s, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 8.2 Hz, 2H), 7.04 (d, *J* = 2.3 Hz, 2H), 6.97 (t, *J* = 7.5 Hz, 2H), 6.83 (t, *J* = 7.4 Hz, 2H), 6.56 (dd, *J* = 5.8, 3.4 Hz, 2H), 6.40 (dd, *J* = 5.7, 3.4 Hz, 2H), 5.60 (s, 2H), 4.82 (s, 2H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 135.7, 134.0, 126.0, 122.9, 120.3, 118.7, 117.8, 116.3, 115.3, 112.5, 110.9, 52.9.

IR (cm^{-1}): νmax**;** 3394, 3165, 3018, 1503, 1366, 1230, 1094, 736.

HRMS (ESI): calcd for $C_{24}H_{18}N_4$ $[M+Na]^+$: 387.1586; found: 387.1584.

Synthesis of 3,3'-(1,2,3,4-tetrahydroquinoxaline-2,3-diyl) bis(1H-indol-4-ol) (4ab)



Prepared according to the general procedure (3c) mentioned above in 34% yield (40.4mg), eluent (25-30% EtOAc/hexane) to afford a bluish grey solid, mp= 220-222 ℃.

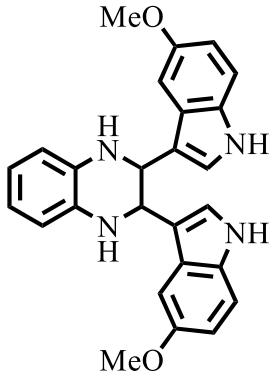
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 10.60 (s, 2H), 10.50 (s, 2H), 6.88 (t, *J* = 7.8 Hz, 2H), 6.81 (dd, *J* = 5.8, 3.4 Hz, 2H), 6.76 (d, *J* = 8.1 Hz, 2H), 6.74 – 6.69 (m, 4H), 6.37 – 6.32 (m, 4H), 4.65 (s, 2H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 150.1, 137.9, 132.8, 121.7, 121.7, 119.5, 116.0, 115.1, 103.3, 102.3, 53.7.

IR (cm^{-1}): νmax**;** 3264, 3120, 3076, 2920, 1578, 1243, 1159, 1085, 746.

HRMS (ESI): calcd for $C_{24}H_{20}N_4O_2$ $[M+Na]^+$: 419.1484; found: 419.1479.

Synthesis of 2,3-bis(4-methoxy-1H-indol-3-yl)-1,2,3,4-tetrahydroquinoxaline (4ac)



Prepared according to the general procedure (3c) mentioned above in 60% yield (76.4mg), eluent (25-30% EtOAc/hexane) to afford an off white solid, mp= 126-128 ℃.

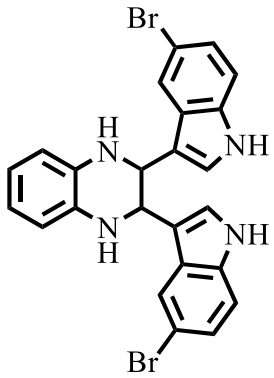
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 10.58 (s, 2H), 7.11 (d, *J* = 8.6 Hz, 2H), 7.02 (d, *J* = 2.7 Hz, 2H), 6.76 (d, *J* = 2.6 Hz, 2H), 6.62 – 6.53 (m, 4H), 6.40 (s, 2H), 5.57 (s, 2H), 4.71 (s, 2H), 3.50 (s, 6H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 152.9, 134.7, 131.5, 127.2, 124.1, 116.9, 115.7, 113.1, 112.1, 111.2, 101.0, 55.2, 54.0.

IR (cm^{-1}): νmax**;** 3358, 3179, 3066, 1503, 1485, 1384, 1277, 1195, 1120, 720.

HRMS (ESI): calcd for $C_{26}H_{24}N_4O_2$ $[M+Na]^+$:447.1797; found 447.1798.

Synthesis of 2,3-bis(4-bromo-1H-indol-3-yl)-1,2,3,4-tetrahydroquinoxaline (4ad)



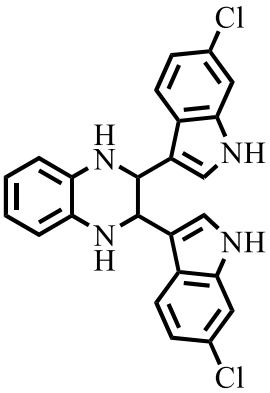
Prepared according to the general procedure (3c) mentioned above in 50% yield (78.3mg), eluent (25-30% EtOAc/hexane) to afford a brownish yellow solid, mp= 202-204 ℃.

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 10.98 (d, *J* = 2.5 Hz, 2H), 7.37 (s, 2H), 7.22 (d, *J* = 8.6 Hz, 2H), 7.07 (dt, *J* = 5.5, 2.5 Hz, 4H), 6.58 (s, 2H), 6.43 (s, 2H), 5.73 (s, 2H), 4.66 (s, 2H).
^{13}C NMR (151 MHz, DMSO-d$_6$) δ 135.3, 134.7, 128.7, 125.5, 123.6, 121.8, 117.4, 115.6, 113.8, 113.5, 111.4, 54.1.

IR (cm^{-1}): νmax**;** 3244, 3181, 3020, 1608, 1503, 1366, 1229, 1100, 739, 624.

HRMS (ESI): calcd for $C_{24}H_{18}Br_2N_4$ [M+K]$^+$: 558.9535; found 558.9531

Synthesis of 2,3-bis(6-chloro-1H-indol-3-yl)-1,2,3,4-tetrahydroquinoxaline (4ae)



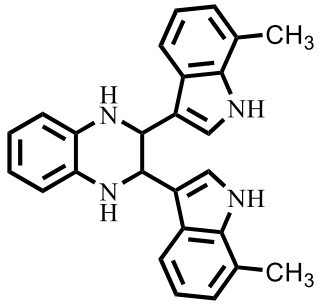
Prepared according to the general procedure (3c) mentioned above in 57% yield (74.1 mg), eluent (25-30% EtOAc/hexane) to afford a brownish yellow solid, mp= 202-204 ℃.

^{1}H NMR (500 MHz, DMSO-d$_6$) δ 10.90 (s, 2H), 7.35 – 7.25 (m, 4H), 7.07 (d, *J* = 2.5 Hz, 2H), 6.82 (dd, *J* = 8.4, 2.0 Hz, 2H), 6.56 (dd, *J* = 5.7, 3.3 Hz, 2H), 6.41 (dd, *J* = 5.8, 3.4 Hz, 2H), 5.70 (s, 2H), 4.72 (s, 2H).
^{13}C NMR (126 MHz, DMSO-d$_6$) δ 135.79, 133.63, 124.69, 124.54, 123.84, 119.71, 117.88, 116.21, 115.03, 112.37, 110.26, 52.86.

IR (cm^{-1}): νmax**;** 3345, 3120, 3010, 1548, 1265, 1148, 752, 698

HRMS (ESI): calcd for $C_{24}H_{18}Cl_2N_4$ [M+Na]$^+$:433.0987; found 433.0969.

Synthesis of 2,3-bis(7-methyl-1H-indol-3-yl)-1,2,3,4-tetrahydroquinoxaline (4af)



Prepared according to the general procedure (3c) mentioned above in 69% yield (81.2mg), eluent (25-30% EtOAc/hexane) to afford a brownish yellow solid, mp=196-198 ℃.

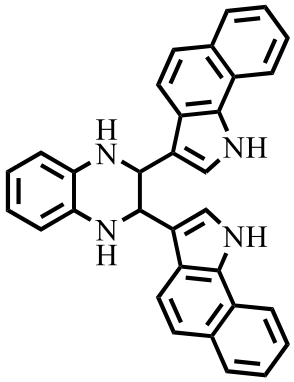
^{1}H NMR (500 MHz, DMSO-d$_6$) δ 10.63 (s, 2H), 7.27 – 7.23 (m, 2H), 6.97 (d, J = 2.6 Hz, 2H), 6.71 (d, J = 6.0 Hz, 4H), 6.48 (dd, J = 5.7, 3.4 Hz, 2H), 6.33 (dd, J = 5.7, 3.4 Hz, 2H), 5.47 (s, 2H), 4.78 (s, 2H), 2.30 (s, 6H).

^{13}C NMR (126 MHz, DMSO-d$_6$) δ 136.0, 134.7, 126.5, 123.5, 121.6, 120.7, 118.9, 117.2, 117.0, 116.5, 113.2, 53.4, 17.2.

IR (cm^{-1}): νmax**;** 3287, 3104, 3026, 1525, 1430, 1241, 1150, 710

HRMS (ESI): calcd for $C_{26}H_{24}N_4$ $[M+Na]^+$: 415.1899; found 415.1912.

Synthesis of 2,3-bis(1H-benzo[f]indol-3-yl)-1,2,3,4-tetrahydroquinoxaline (4ag)



Prepared according to the general procedure (3c) mentioned above in 43% yield (59.9mg), eluent (25-30% EtOAc/hexane) to afford a brownish yellow solid, mp=230-232 ℃.

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 10.81 (s, 2H), 7.36 (d, *J* = 8.1 Hz, 2H), 6.95 (d, *J* = 8.1 Hz, 2H), 6.67 (d, *J* = 8.7 Hz, 2H), 6.58 (t, *J* = 7.6 Hz, 2H), 6.47 (t, *J* = 7.5 Hz, 2H), 6.38 (d, *J* = 8.6

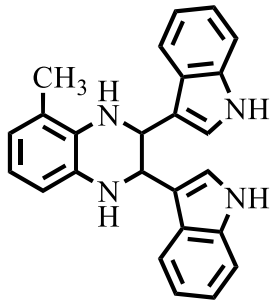
Hz, 2H), 6.26 (d, *J* = 2.5 Hz, 2H), 5.79 – 5.75 (m, 2H), 5.59 (dd, *J* = 5.8, 3.5 Hz, 2H), 4.90 (s, 2H), 4.05 (s, 2H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 134.9, 130.9, 130.0, 128.6, 125.4, 123.7, 122.8, 122.5, 122.0, 120.9, 120.3, 119.3, 117.9, 117.2, 113.5, 54.5.

IR (cm^{-1}): νmax**;** 3325, 3148, 3034, 1592, 1217, 1116, 739.

HRMS (ESI): calcd for $C_{32}H_{24}N_4$ $[M+Na]^+$: 487.1899 found 487.1924.

Synthesis of 2,3-di(1H-indol-3-yl)-5-methyl-1,2,3,4-tetrahydroquinoxaline (4ah)



Prepared according to the general procedure (3c) mentioned above in 30% yield (34.0mg), eluent (25-30% EtOAc/hexane) to afford an off white solid, mp= 188-190 ℃.

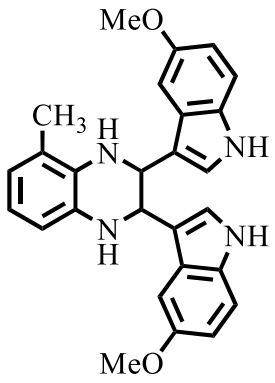
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 10.72 (d, *J* = 8.3 Hz, 2H), 7.42 (dd, *J* = 17.8, 8.0 Hz, 2H), 7.23 (d, *J* = 8.1 Hz, 2H), 7.03 (dd, *J* = 8.7, 2.5 Hz, 2H), 6.96 (td, *J* = 7.5, 3.7 Hz, 2H), 6.83 (dt, *J* = 11.2, 7.3 Hz, 2H), 6.46 (d, *J* = 7.4 Hz, 1H), 6.35 (dt, *J* = 15.2, 7.4 Hz, 2H), 5.60 (s, 1H), 4.91 (d, *J* = 6.4 Hz, 1H), 4.77 (d, *J* = 7.1 Hz, 1H), 4.53 (s, 1H), 2.02 (s, 3H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 135.6, 133.7, 131.0, 129.2, 128.3, 127.4, 125.9, 125.9, 122.8, 122.7, 120.2, 119.9, 118.6, 118.4, 118.1, 117.7, 116.2, 115.6, 115.3, 110.9, 110.9, 110.8, 53.3, 52.3, 16.7.

IR (cm^{-1}): νmax**;** 3396, 3175, 3052, 1605, 1426, 1259, 1168, 735.

HRMS (ESI): calcd for $C_{25}H_{22}N_4$ $[M+Na]^+$: 417.1482; found 417.1475.

Synthesis of 2,3-bis(5-methoxy-1H-indol-3-yl)-5-methyl-1,2,3,4-tetrahydroquinoxaline (4ai)



Prepared according to the general procedure (3c) mentioned above in 43% yield (56.5mg), eluent (25-30% EtOAc/hexane) to afford a white solid, mp= 130-132 ℃.

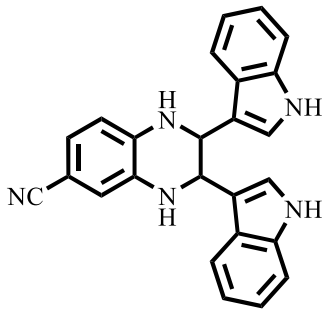
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (s, 2H), 7.14 – 7.09 (m, 2H), 6.88 (d, *J* = 4.6 Hz, 3H), 6.82 (s, 1H), 6.75 (td, *J* = 9.3, 2.5 Hz, 2H), 6.61 (d, *J* = 6.7 Hz, 2H), 6.55 (dd, *J* = 6.9, 2.4 Hz, 1H), 4.92 (d, *J* = 7.9 Hz, 1H), 4.85 (d, *J* = 7.9 Hz, 1H), 3.57 (s, 3H), 3.54 (s, 2H), 2.16 (d, *J* = 11.6 Hz, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 153.9, 131.9, 131.3, 127.0, 123.4, 123.3, 120.2, 117.8, 116.4, 112.6, 112.0, 111.9, 111.8, 101.1, 101.0, 55.7, 55.4, 54.6, 30.9, 17.2.

IR (cm^{-1}): νmax = 3378, 3141, 3041, 1611, 1420, 1344, 1254, 1199, 1162, 730.

HRMS (ESI): calcd for $C_{27}H_{24}N_4O_2$ $[M+Na]^+$: 461.1953; found 461.1978.

Synthesis of 2,3-di(1H-indol-3-yl)-1,2,3,4-tetrahydroquinoxaline-6-carbonitrile (4aj)



Prepared according to the general procedure (3c) mentioned above in 80% yield (93.4 mg), eluent (25% EtOAc/hexane) to afford a off white solid, mp= 130-132 ℃.

^{1}H NMR (500 MHz, DMSO-d_6) δ 10.82 (s, 2H), 7.43 (dd, *J* = 14.5, 8.0 Hz, 2H), 7.26 (dd, *J* = 8.2, 2.9 Hz, 2H), 7.08 (dd, *J* = 5.1, 2.5 Hz, 2H), 6.99 (qd, *J* = 6.9, 1.2 Hz, 2H), 6.92 – 6.78

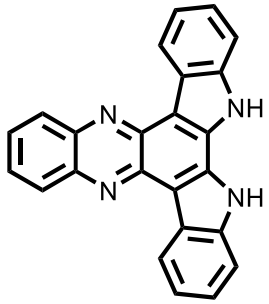
(m, 5H), 6.63 (d, *J* = 7.9 Hz, 1H), 6.19 (s, 1H), 4.94 (d, *J* = 7.4 Hz, 1H), 4.78 (d, *J* = 7.5 Hz, 1H).

^{13}C NMR (126 MHz, DMSO-d$_6$) δ 139.5, 136.6, 136.5, 134.5, 126.7, 126.5, 124.1, 124.0, 122.7, 121.9, 121.3, 121.3, 119.4, 118.9, 118.9, 115.0, 114.8, 114.7, 112.1, 111.9, 111.8, 96.3, 53.7, 52.2.

IR (cm^{-1}): *ν*max **=** 3302, 3142, 3062, 2235, 1507, 1230, 1120, 733

HRMS (ESI): calcd for $C_{25}H_{19}N_5$ $[M+Na]^+$: 412.1538; found 412.1545

Synthesis of 5,6-dihydrodiindolo[3,2-a:2',3'-c] phenazine (5aa)



Prepared according to the general procedure (3d) mentioned above in 86% yield (30.8mg), eluent (25-30% EtOAc/hexane) to afford a reddish brown solid, mp= 380-382 ℃.

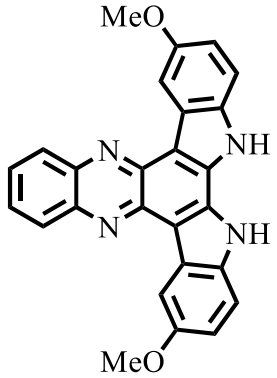
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 12.01 (s, 2H), 9.10 (d, *J* = 7.1 Hz, 2H), 8.41 (dd, *J* = 6.3, 3.4 Hz, 2H), 7.92 – 7.88 (m, 4H), 7.50 – 7.44 (m, 4H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 139.9, 139.4, 137.8, 129.7, 128.5, 128.0, 124.6, 124.0, 122.1, 121.0, 112.3, 111.8.

IR (cm^{-1}): *ν*max**;** 3159, 3041, 1623, 1584, 1123, 711.

HRMS (ESI): calcd for $C_{24}H_{14}N_4$ $[M+Na]^+$: 381.1116; found 381.1109.

Synthesis of 2,9-dimethoxy-5,6-dihydrodiindolo[3,2-a:2',3'-c] phenazine (5ab)



Prepared according to the general procedure (3d) mentioned above in 67% yield (28.0mg), eluent (25-30% EtOAc/hexane) to afford a reddish brown solid, mp= 300-302 ℃.

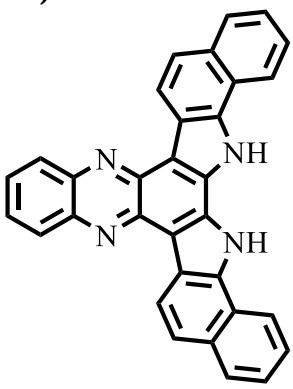
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 11.82 (s, 2H), 8.59 (d, *J* = 2.5 Hz, 2H), 8.38 (dd, *J* = 6.3, 3.4 Hz, 2H), 7.87 (dd, *J* = 6.8, 3.4 Hz, 2H), 7.77 (d, *J* = 8.7 Hz, 2H), 7.11 (dd, *J* = 8.7, 2.7 Hz, 2H), 3.99 (s, 6H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 155.3, 140.7, 139.7, 133.2, 130.7, 129.1, 128.3, 125.8, 113.9, 113.6, 111.9, 104.7, 55.8.

IR (cm^{-1}): νmax**;** 3114, 3039, 1613, 1555, 1204, 1140, 717.

HRMS (ESI): calcd for $C_{24}H_{18}N_4O_2$ $[M+H]^+$: 419.1508; found 419.1519.

Synthesis of 1,20-dihydrobenzo [5,6] indolo[3,2-a] benzo [5,6] indolo[2,3-c] phenazine (5ac)



Prepared according to the general procedure (3d) mentioned above in 58% yield (26.6mg), eluent (25-30% EtOAc/hexane) to afford a reddish brown solid, mp= 308-310 ℃.

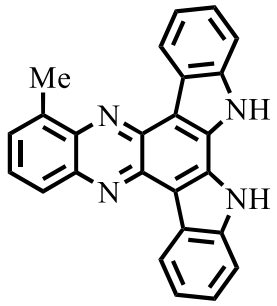
^{1}H NMR (600 MHz, DMSO-d$_6$) δ 12.63 (s, 2H), 9.17 (d, *J* = 8.6 Hz, 2H), 8.44 – 8.41 (m, 4H), 8.14 (d, *J* = 8.0 Hz, 2H), 7.93 – 7.90 (m, 4H), 7.77 (t, *J* = 7.4 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 2H).

^{13}C NMR (151 MHz, DMSO-d$_6$) δ 141.0, 140.2, 133.5, 131.5, 129.4, 129.2, 128.9, 126.8, 125.5, 122.5, 122.1, 121.6, 121.1, 113.5.

IR (cm^{-1}): νmax**;** 3155, 3054, 1619, 1562, 1140, 705.

HRMS (ESI): calcd for $C_{32}H_{18}N_4$ [M+Na] $^+$: 481.1429; found 481.1440.

Synthesis of 12-methyl-5,6-dihydrodiindolo[3,2-a:2',3'-c] Phenazine (5ad)



Prepared according to the general procedure (3d) mentioned above in 75% yield (27.9mg), eluent (25-30% EtOAc/hexane) to afford a reddish brown solid. mp= 304-306 ℃.

^{1}H NMR (600 MHz, DMSO-d$_6$) δ 11.98 (d, *J* = 6.6 Hz, 2H), 9.10 – 9.02 (m, 2H), 8.23 (d, *J* = 8.4 Hz, 1H), 7.90 – 7.87 (m, 2H), 7.80 – 7.75 (m, 2H), 7.49 – 7.42 (m, 4H), 3.07 (s, 3H).

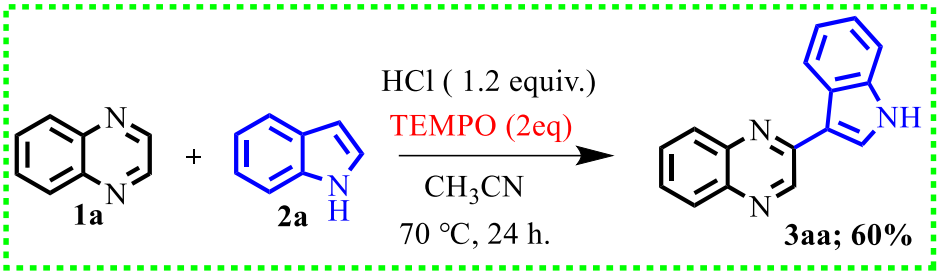
^{13}C NMR (151 MHz, DMSO-d$_6$) δ 140.2, 139.3, 138.6, 136.8, 130.3, 128.5, 127.3, 125.4, 124.7, 122.9, 122.8, 121.9, 121.8, 113.1, 113.0, 18.0.

IR (cm^{-1}): νmax**;** 3126, 3070, 1649, 1530, 1402, 1103, 698

HRMS (ESI): calcd for $C_{25}H_{16}N_4$ [M+Na] $^+$: 395.1273; found.395.1255

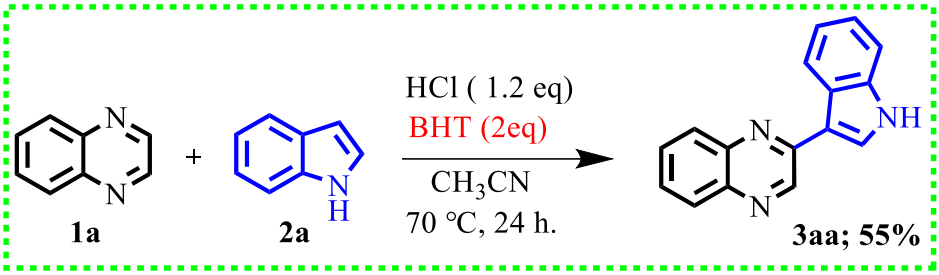
5. Mechanistic studies:

5a. The Radical scavenging experiment in the presence of (2,2,6,6 Tetramethylpiperidin-1-yl) oxyl (TEMPO)



The reaction was performed with 39.0 mg of **1a** (0.3mmol), 35.1 mg of **2a** (0.3mmol), and 93.7 mg of TEMPO (0.6mmol) added into the oven dried clean reaction tube, in acetonitrile (1mL), after that 26 µl of HCl was added dropwise into the reaction mixture at room temperature, and the reaction mixture stirred in an oil bath at 70 ℃ up to 24 hrs, our desired product observed in 60% yield.

5b. The radical scavenging experiment in the presence of 3,5-Di-tert-4-butylhydroxytoluene (BHT)



The reaction was performed with 39.0 mg of **1a** (0.3mmol), 35.1 mg of **2a** (0.3mmol), and 132.2 mg of BHT (0.6mmol) added in to the oven dried clean reaction tube, in acetonitrile,(1mL) after that 26 µl of HCl was added dropwise into the reaction mixture at room temperature, and the reaction mixture stirred in an oil bath at 70 ℃ up to 24 hrs, our desired product observed less than 55%.

5c. Intermediate detected by HRMS

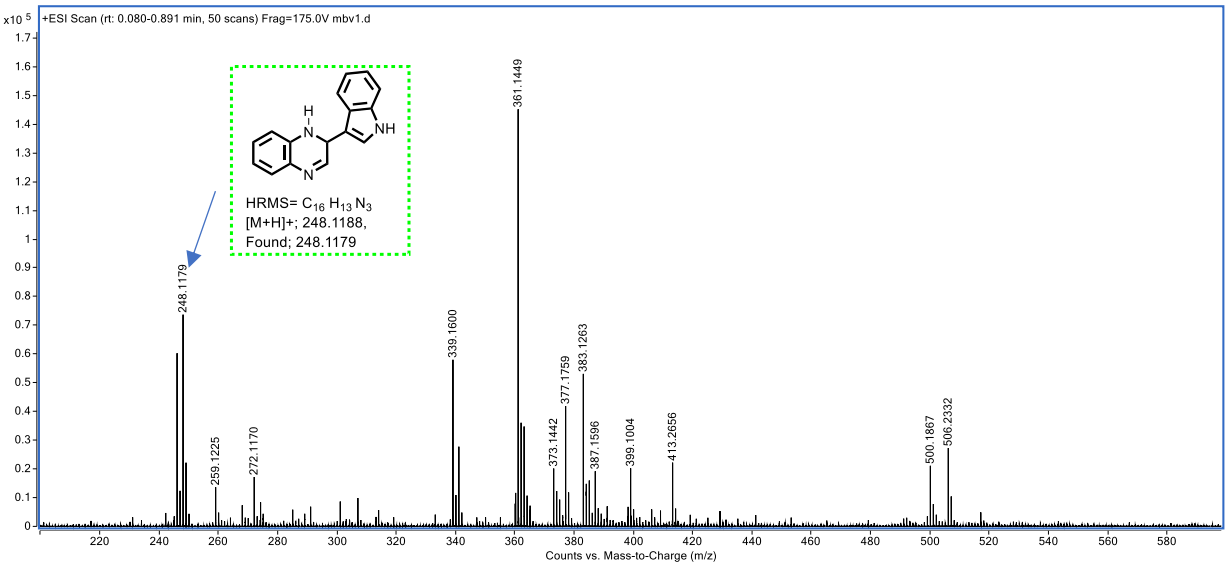
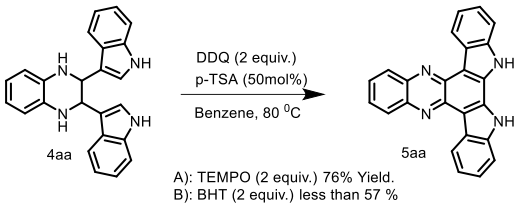
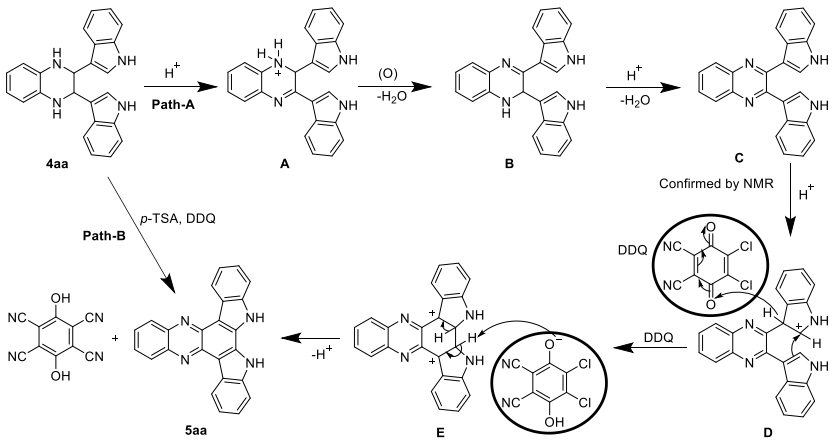


Fig.S2: Spectra of HRMS

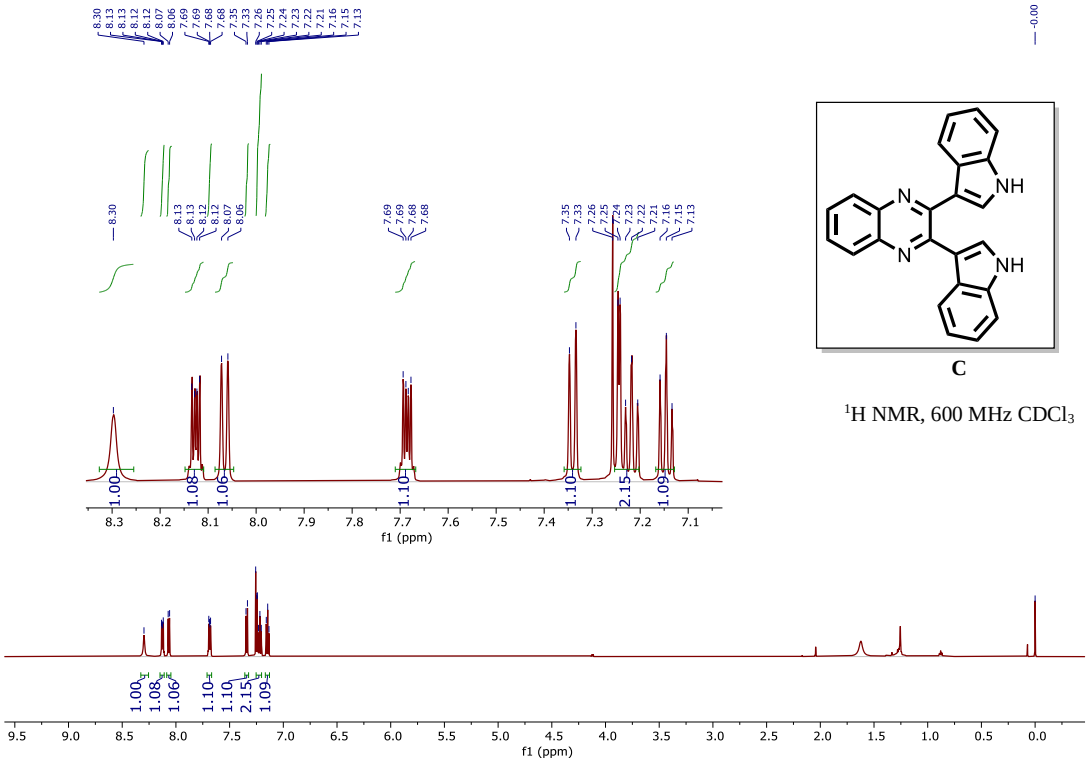
5d. Mechanism of oxidative cyclisation of 4aa



Based on control experiments and literature reports,[6] we proposed a two plausible reaction mechanisms Path-A and B (Scheme S1). Initially, **4aa** in presence of p-TSA, generates intermediate **A,** and its oxidation generates another intermediate **B.** Intermediate **B,** under similar conditions may provide stable intermediate **C,** which was isolated and confirmed by NMR. In presence of acid, intermediate **C** will generate carbocationic intermediate **D** and its reaction with DDQ will generate another intermediate **E.** Finally aromatisation of **E** give the desired product **5aa**.[6] Through Path-B, **4aa** may directly transformed to **5aa** by DDQ through oxidative cyclisation as per the reported literature.[6]



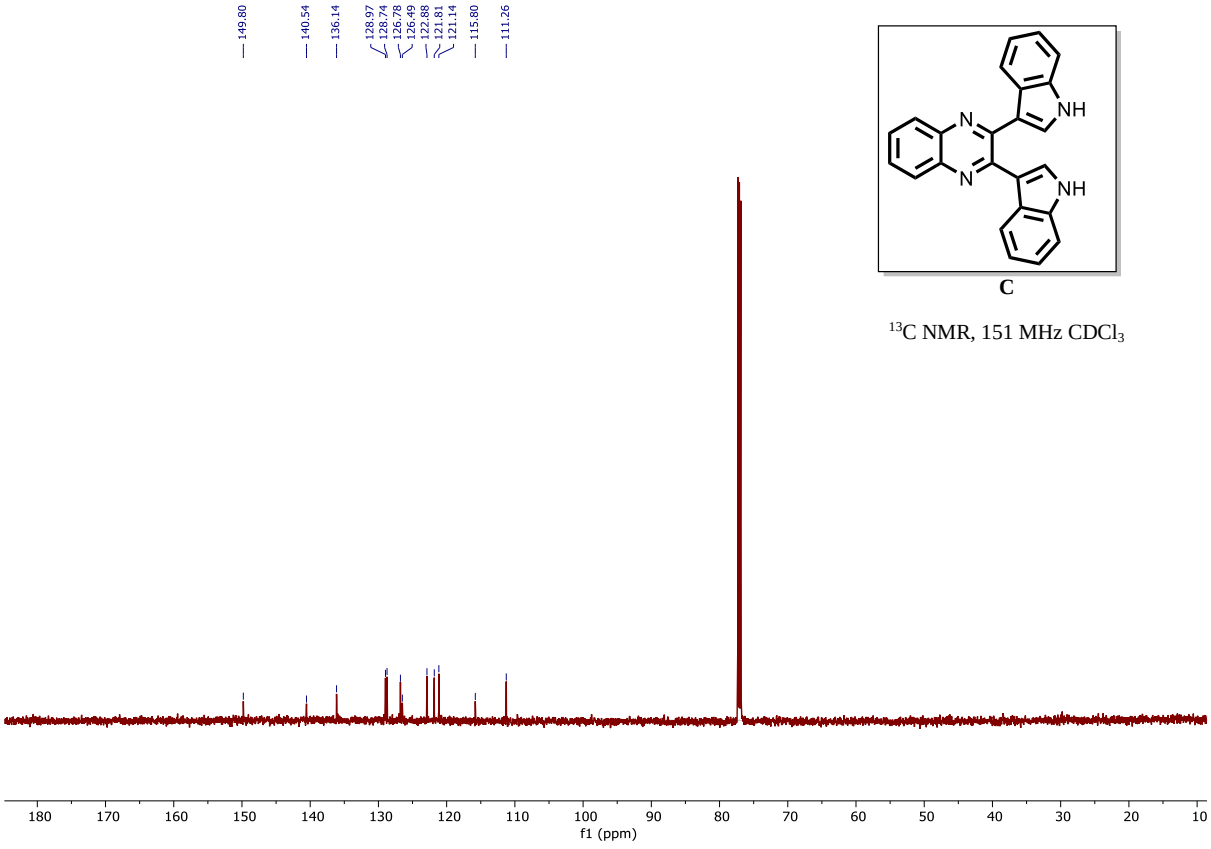
Scheme S1: Plausible mechanism



C

^{1}H NMR, 600 MHz $CDCl_3$

^{1}H NMR of Intermediate C



C

^{13}C NMR, 151 MHz $CDCl_3$

^{13}C NMR of Intermediate C

6. X-ray Structure and Data

6a. Procedure for the crystal growth

15–20 mg of the pure substance was taken and diluted in 1-2 mL of solvent (hexane and ethyl acetate) in a glass vial (5 mL), it was kept for slow evaporation at room temperature. After 2-3 days small crystals were begun to form. X-ray diffraction data were collected on a Bruker Kappa Apex-II CCD diffractometer at 296 K.

Table S8: Crystal Data and Refinement Parameters (Experimental: X-ray part).

Identification code	**4aa**	**3au**
Empirical formula	$C_{24}H_{20}N_4$	$C_{23}H_{17}N_3O$
Formula weight	364.44	351.39
Temperature/K	298	298
Crystal system	triclinic	orthorhombic
Space group	P-1	$P2_12_12_1$
a/Å	9.2942(8)	9.6588(4)
b/Å	10.9020(8)	13.5399(5)
c/Å	11.0378(9)	14.1363(5)
α/°	62.717(3)	90
β/°	71.571(4)	90
γ/°	89.138(3)	90
Volume/Å^3	931.76(13)	1848.73(12)
Z	2	4
ρ_{calc}g/cm^3	1.299	1.262
μ/mm^{-1}	0.079	0.079
F(000)	384.0	736.0

Crystal size/mm^3	0.13 × 0.12 × 0.08	0.29 × 0.2 × 0.06
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.254 to 50	4.166 to 66.486
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -13 ≤ l ≤ 13	-14 ≤ h ≤ 14, -20 ≤ k ≤ 20, -21 ≤ l ≤ 21
Reflections collected	45073	165909
Independent reflections	3266 [R_{int} = 0.0938, R_{sigma} = 0.0364]	7107 [R_{int} = 0.1160, R_{sigma} = 0.0409]
Data/restraints/parameters	3266/0/253	7107/0/244
Goodness-of-fit on F^2	1.086	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0512, wR_2 = 0.1322	R_1 = 0.0447, wR_2 = 0.1004
Final R indexes [all data]	R_1 = 0.0831, wR_2 = 0.1620	R_1 = 0.0919, wR_2 = 0.1301
Largest diff. peak/hole / e $Å^{-3}$	0.28/-0.27	0.16/-0.23
CCDC	**2408003**	**2410123**

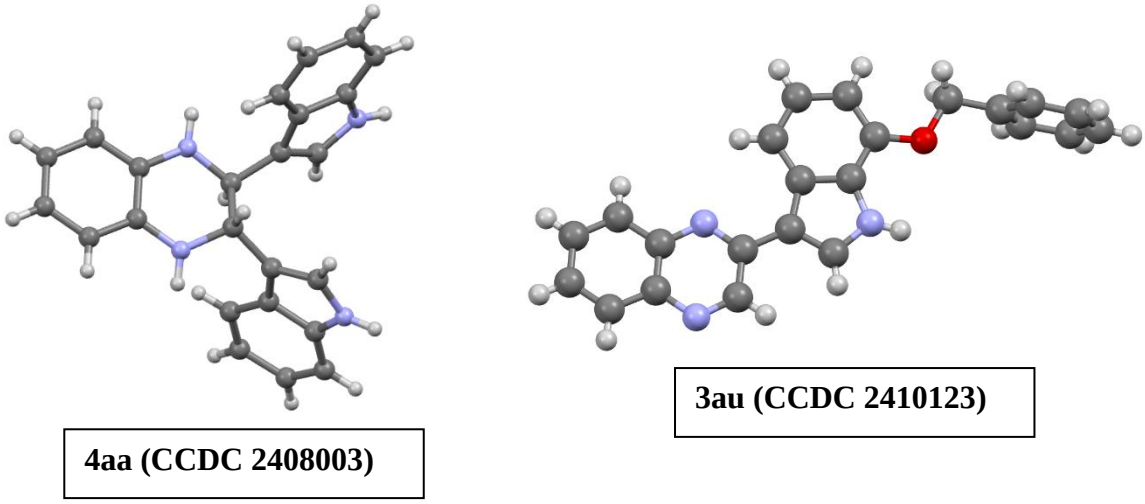
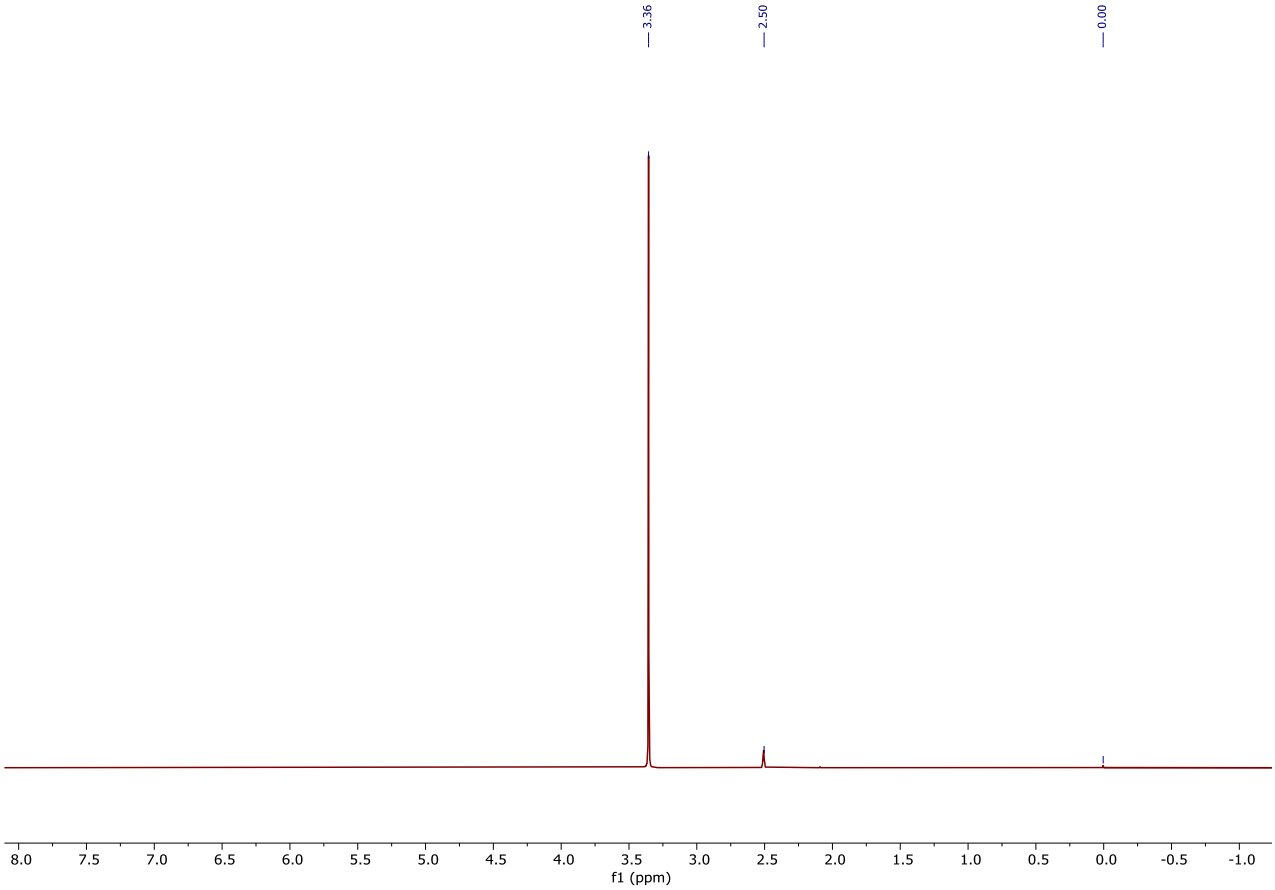


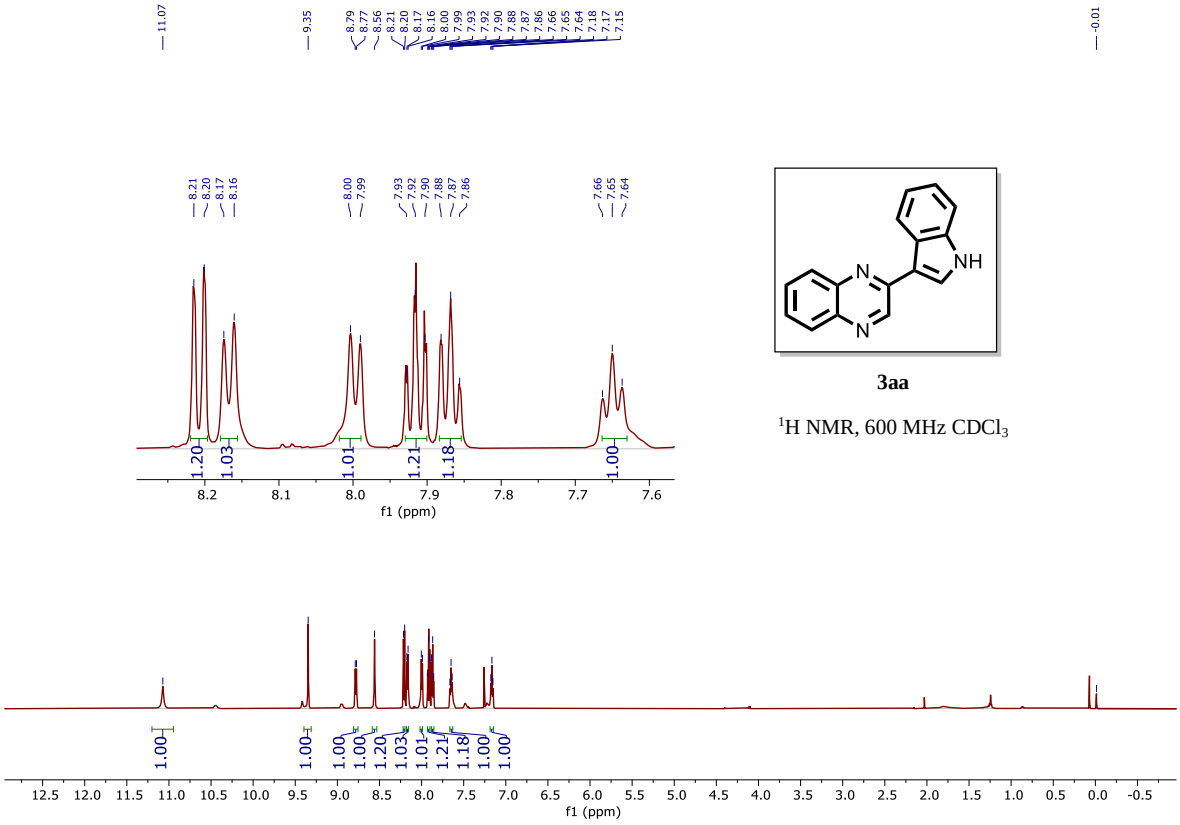
Fig. S3. (a) Thermal ellipsoid plot for the crystal structure **4aa (CCDC 2408003).** (b) Thermal ellipsoid plot for the crystal structure **3au (CCDC 2410123).**

Copies of ^{1}H, ^{13}C & ^{19}F NMR



^{1}H NMR OF DMSO-d_6 (blank for reference)

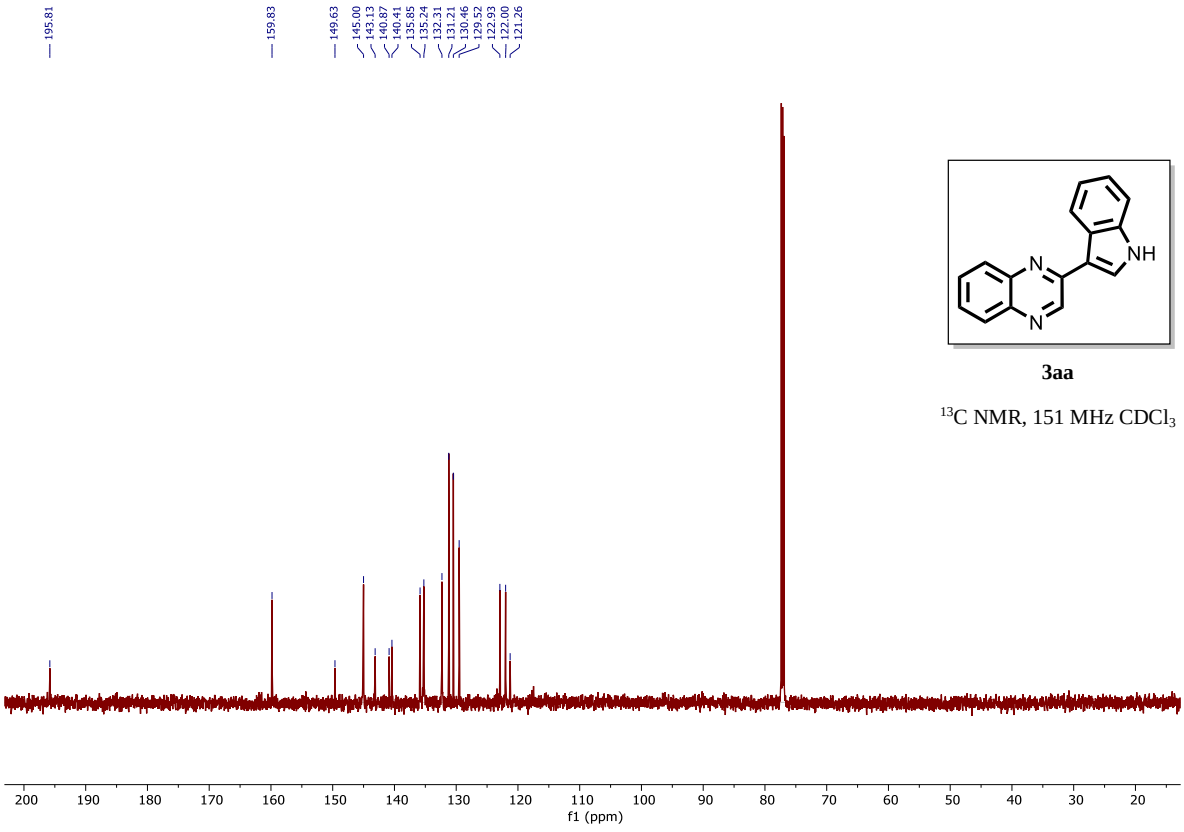
The spectrum shows a characteristic water peak at 3.36 ppm and 2.50 ppm are attributed to residual water in the solvent (DMSO-d_6). Hence these peaks appears in the spectra wherever DMSO is used as solvent for recording NMR and these peaks may be ignored during integration.



3aa

^{1}H NMR, 600 MHz $CDCl_3$

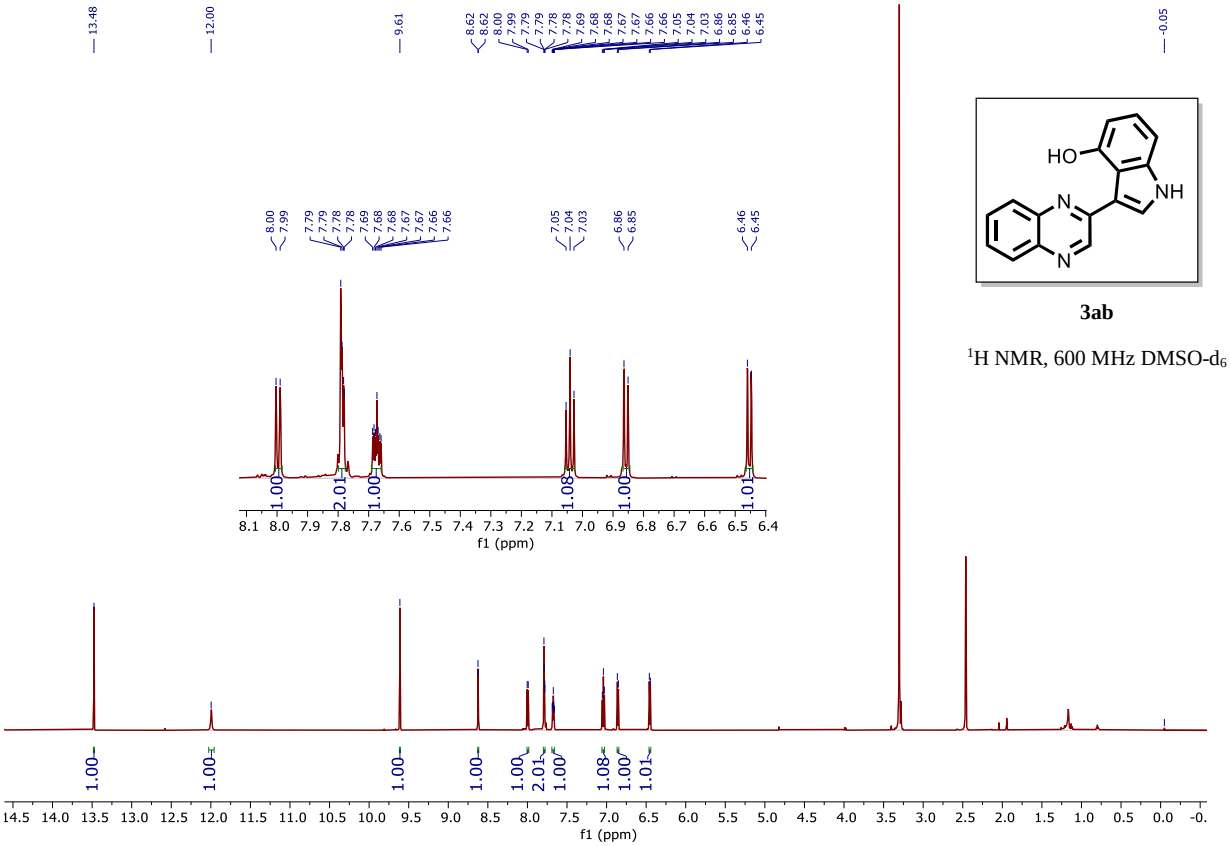
^{1}H NMR of 3aa



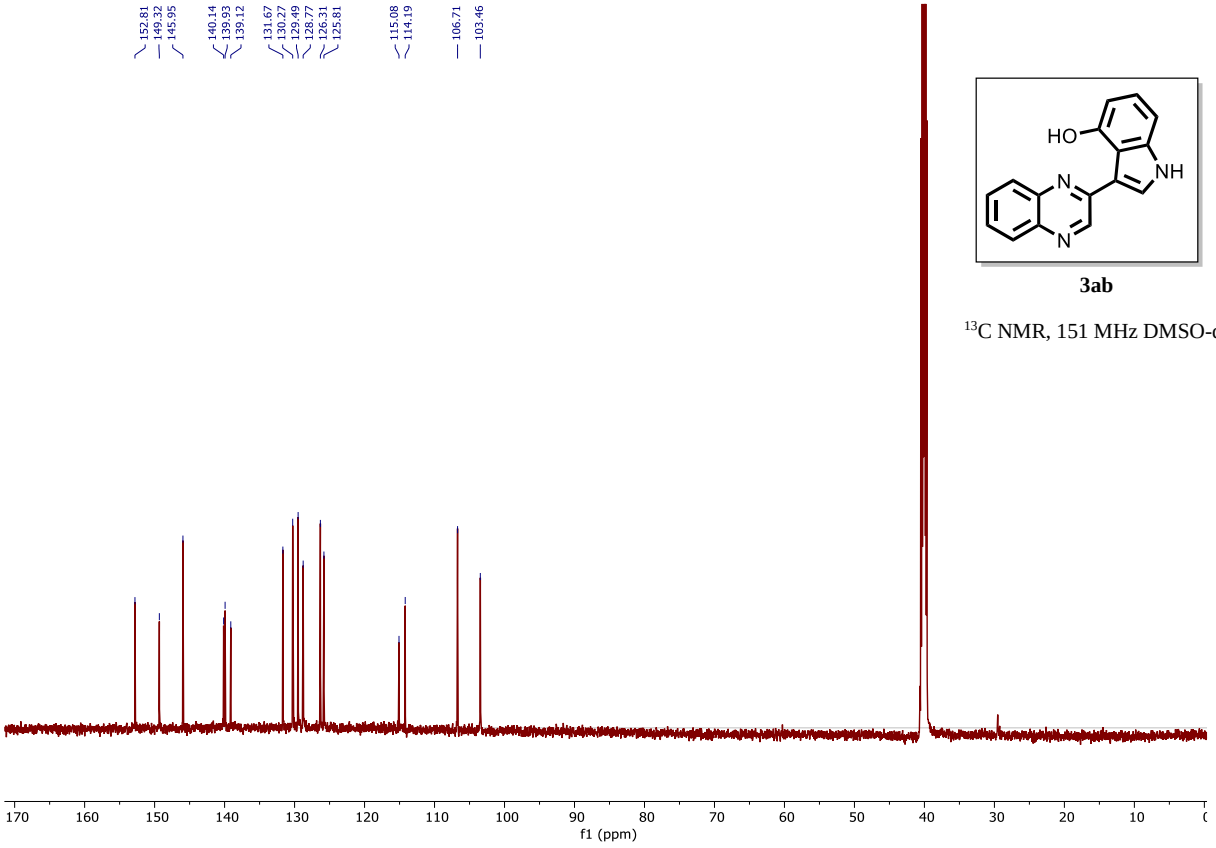
3aa

^{13}C NMR, 151 MHz $CDCl_3$

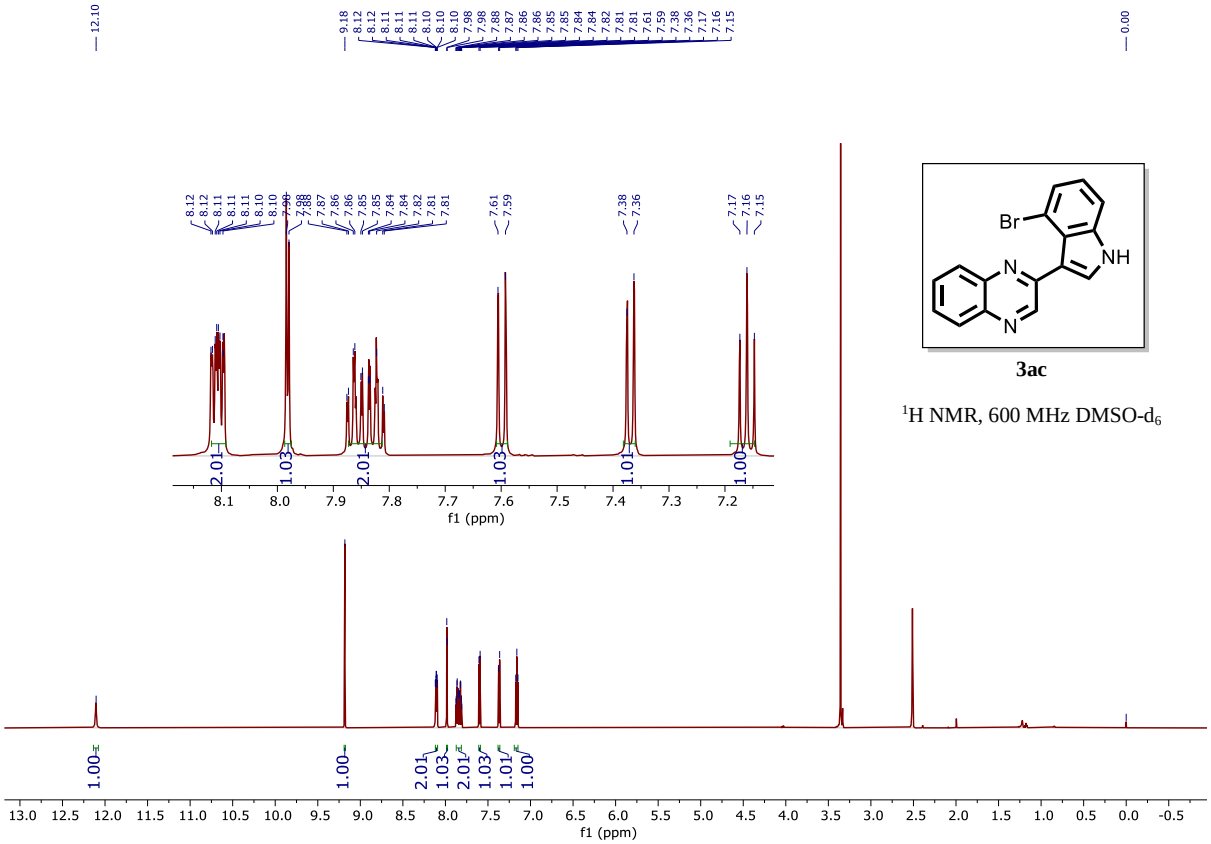
^{13}C NMR of 3aa



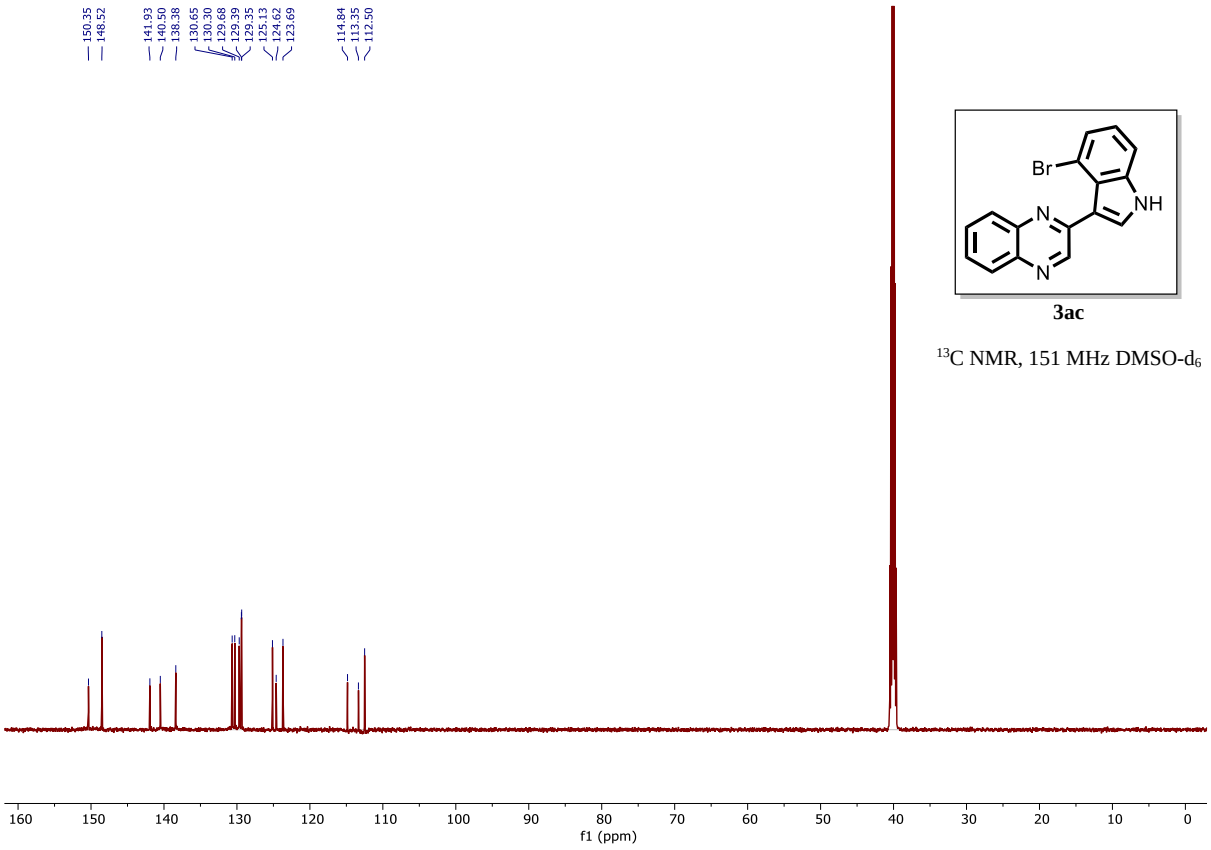
^{1}H NMR of 3ab



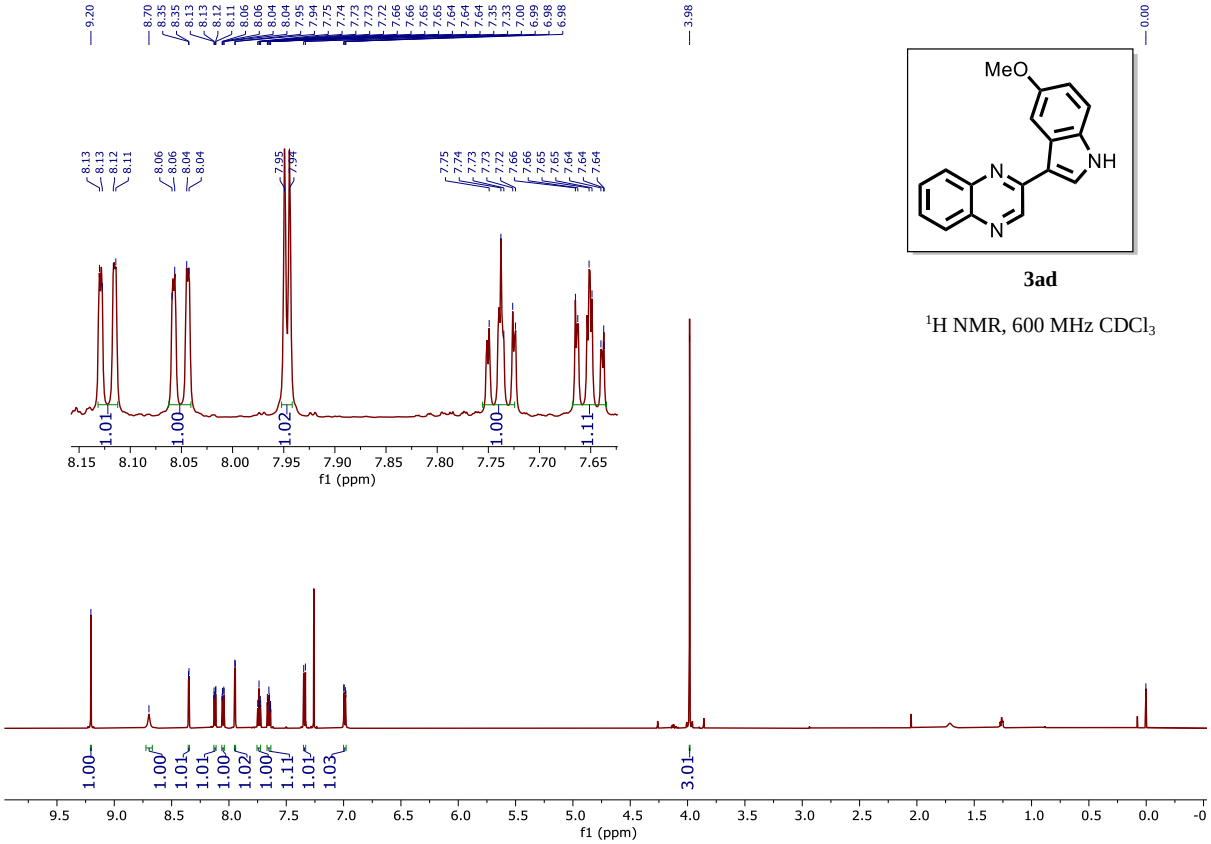
^{13}C NMR of 3ab



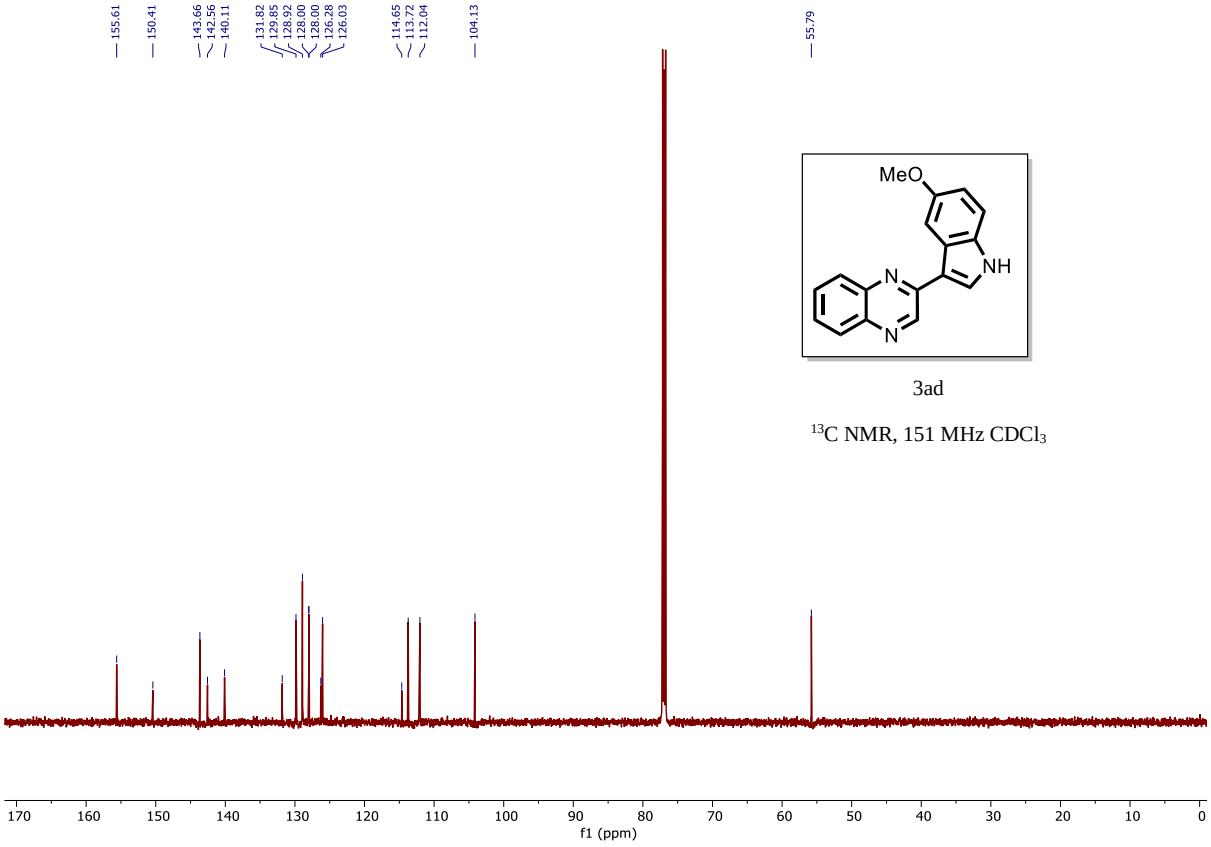
^{1}H NMR of 3ac



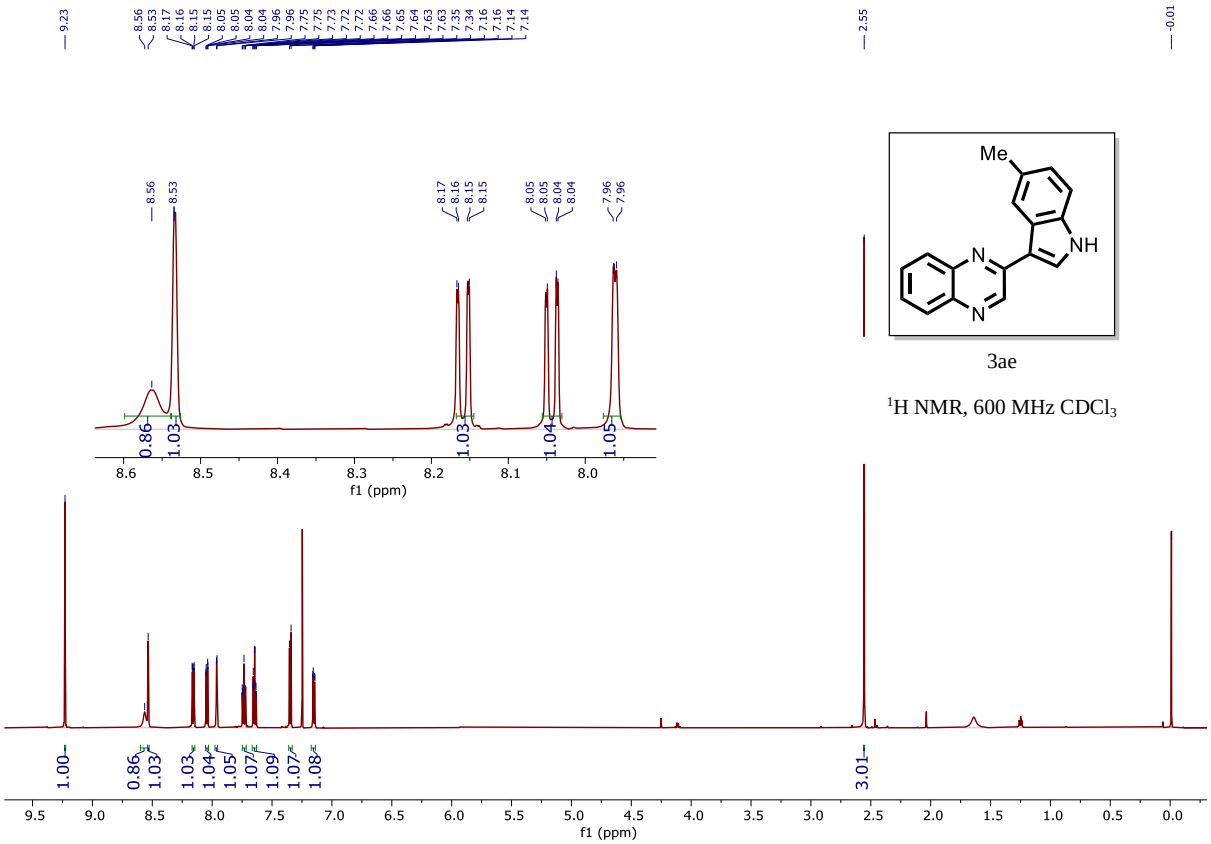
^{13}C NMR of 3ac



^{1}H NMR of 3ad



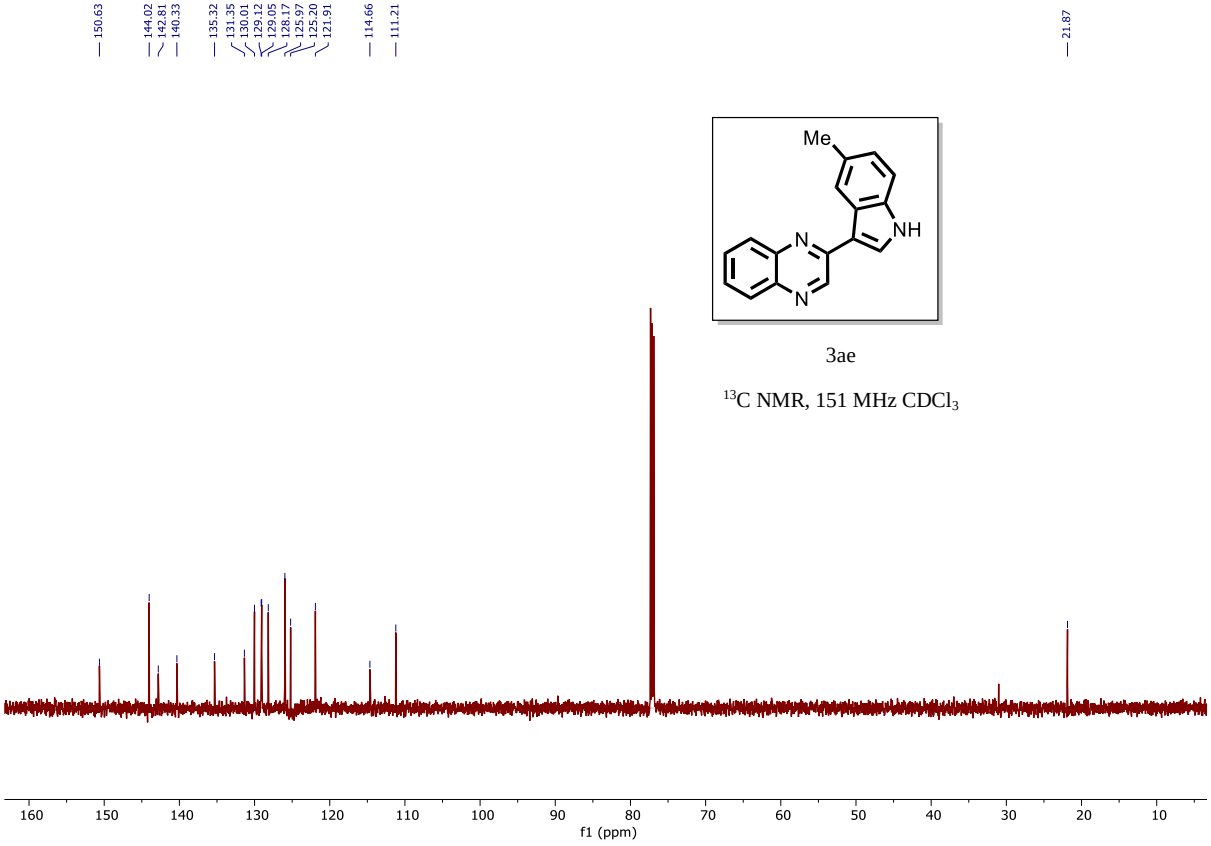
^{13}C NMR of 3ad



3ae

^{1}H NMR, 600 MHz $CDCl_3$

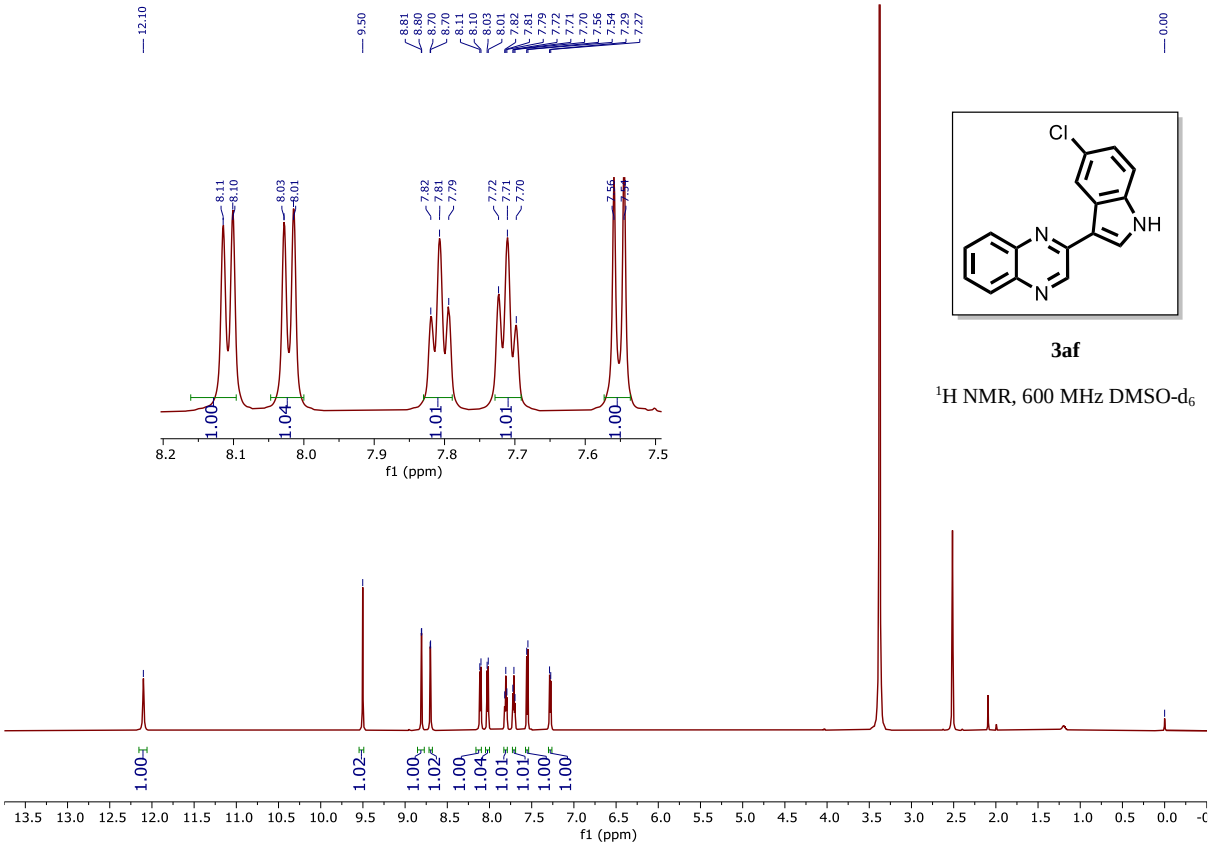
^{1}H NMR of 3ae



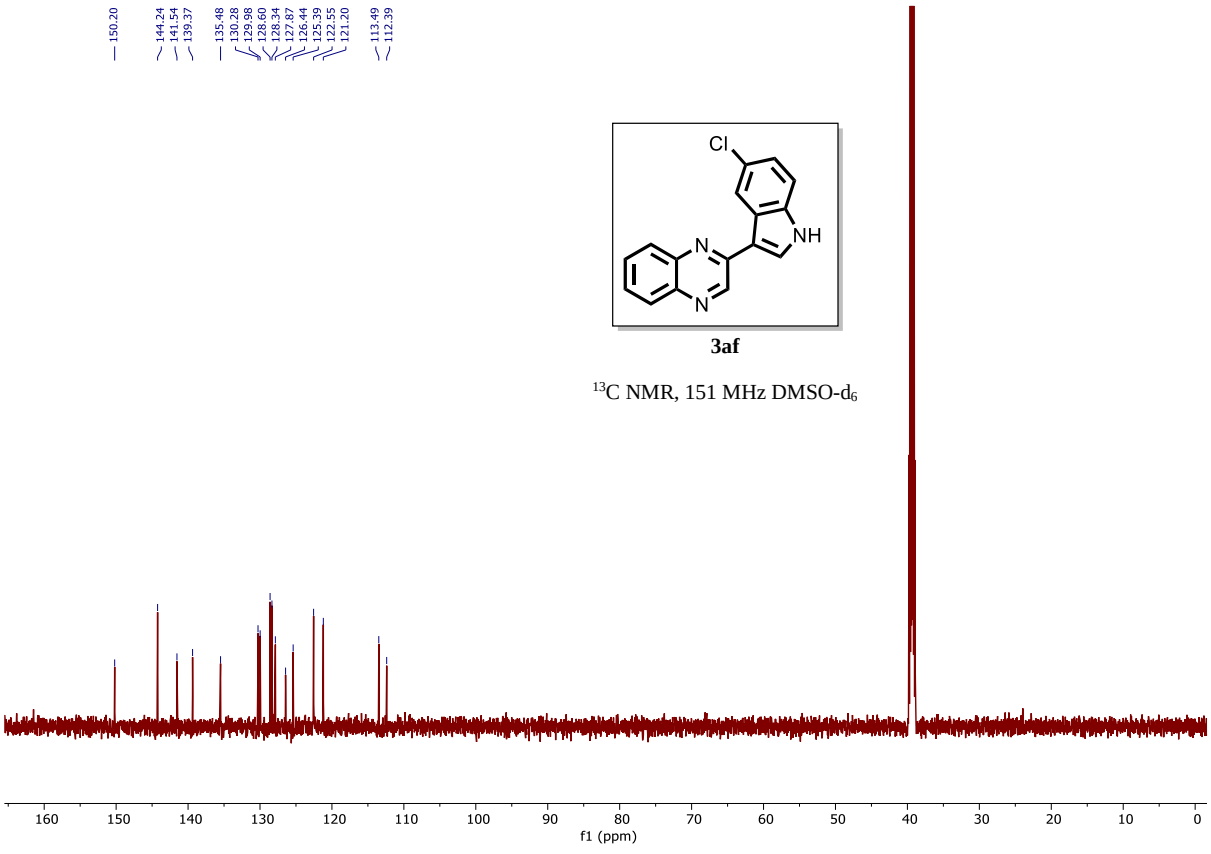
3ae

^{13}C NMR, 151 MHz $CDCl_3$

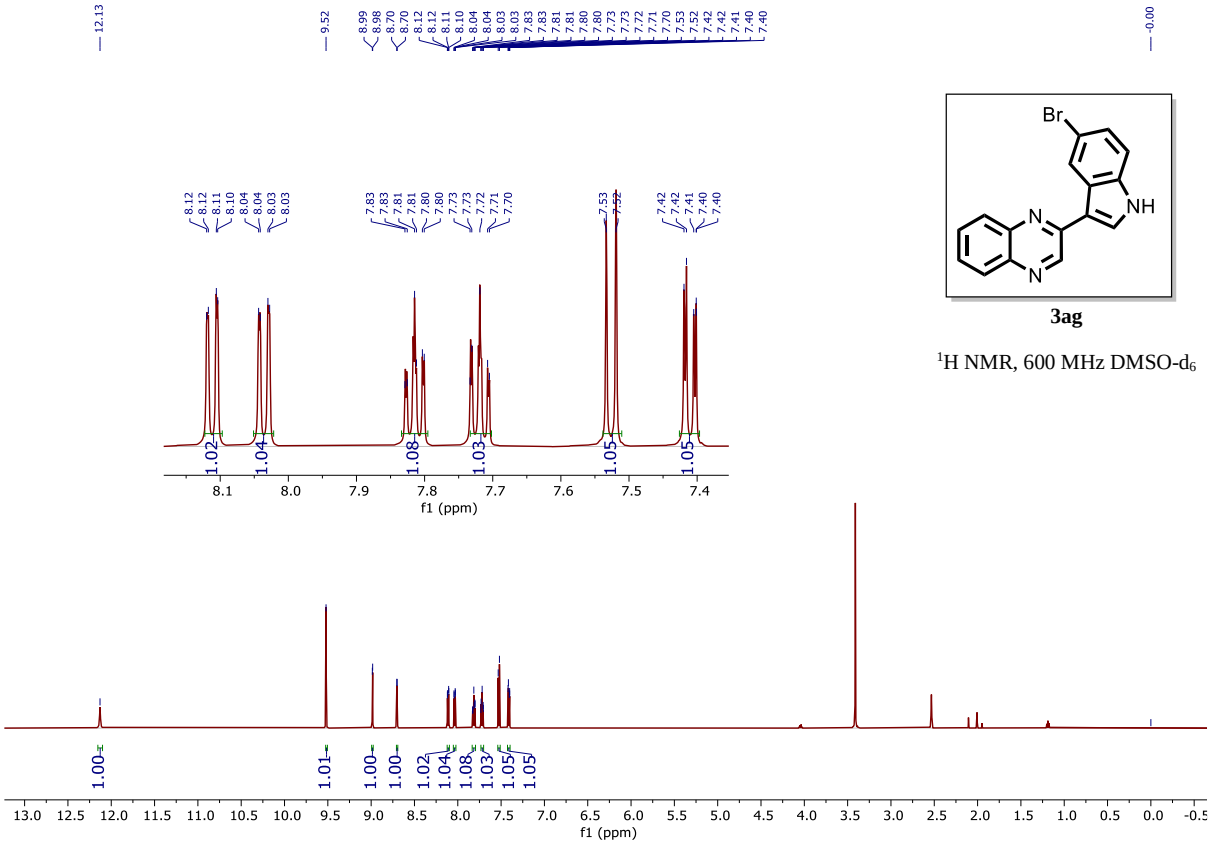
^{13}C NMR of 3ae



^{1}H NMR of 3af



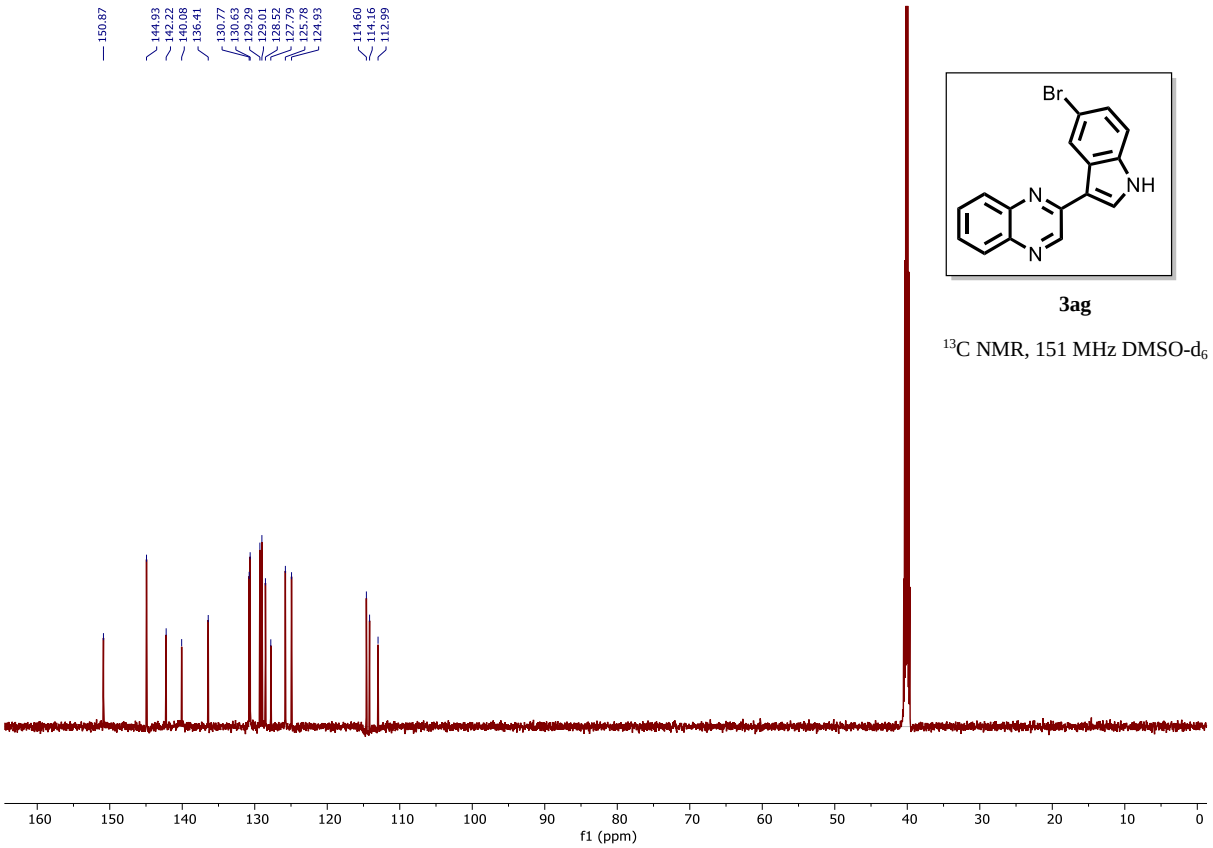
^{13}C NMR of 3af



3ag

^{1}H NMR, 600 MHz DMSO-d_6

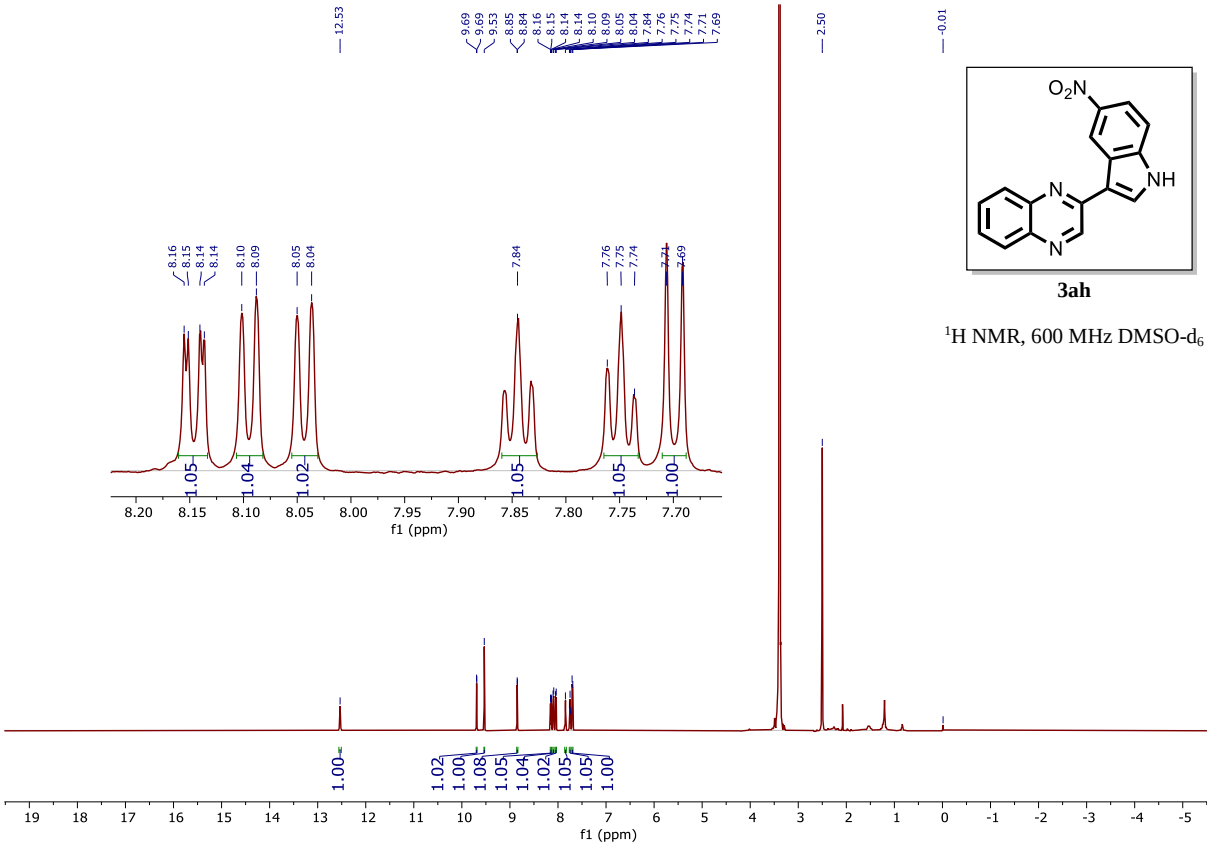
^{1}H NMR of 3ag



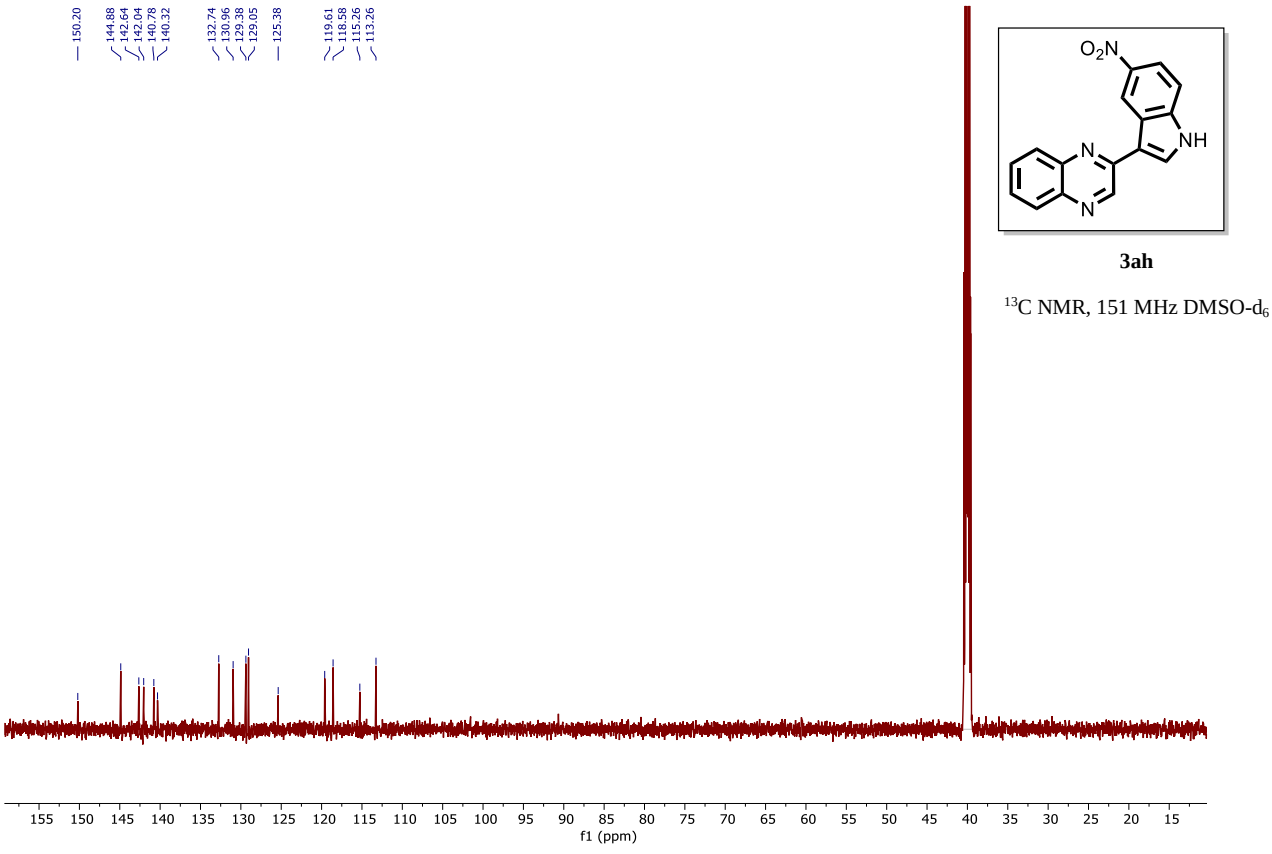
3ag

^{13}C NMR, 151 MHz DMSO-d_6

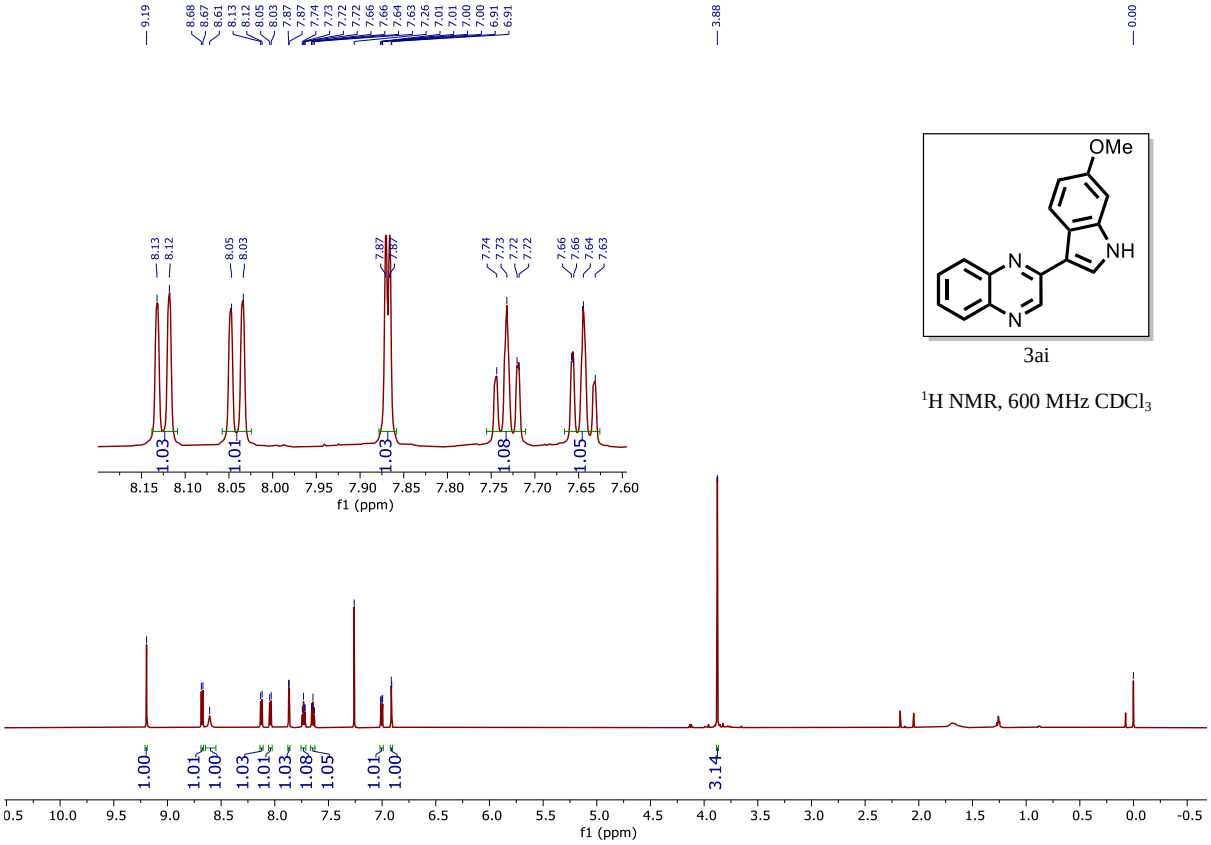
^{13}C NMR of 3ag



^{1}H NMR of 3ah

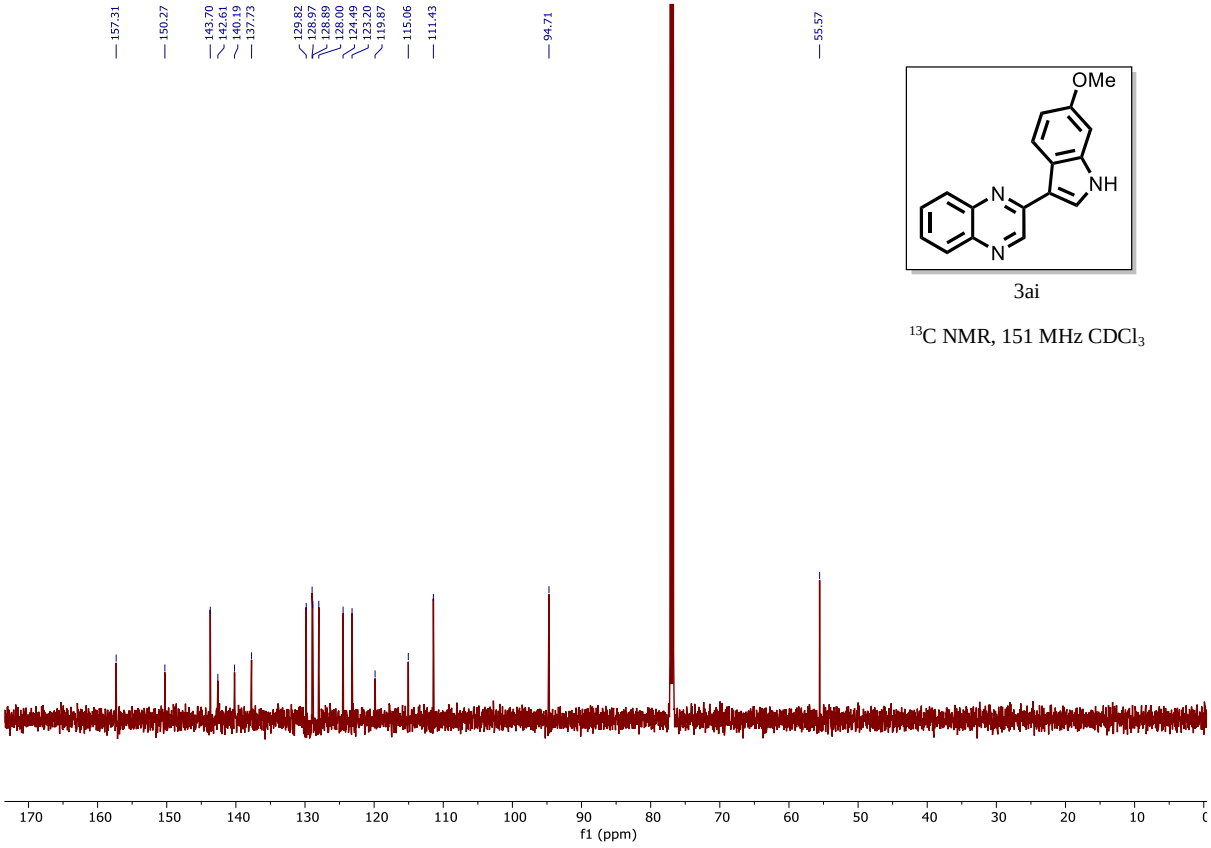


^{13}C NMR of 3ah



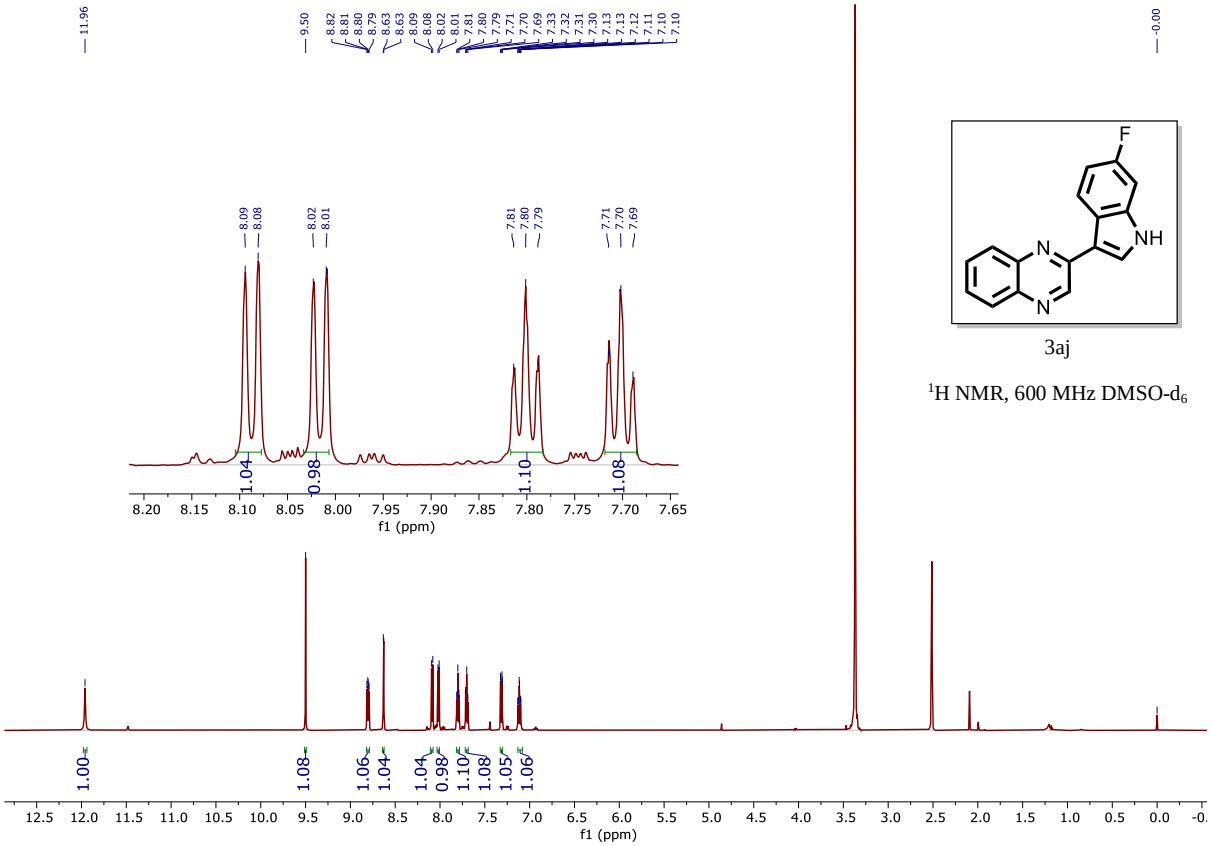
^{1}H NMR, 600 MHz $CDCl_3$

^{1}H NMR of 3ai

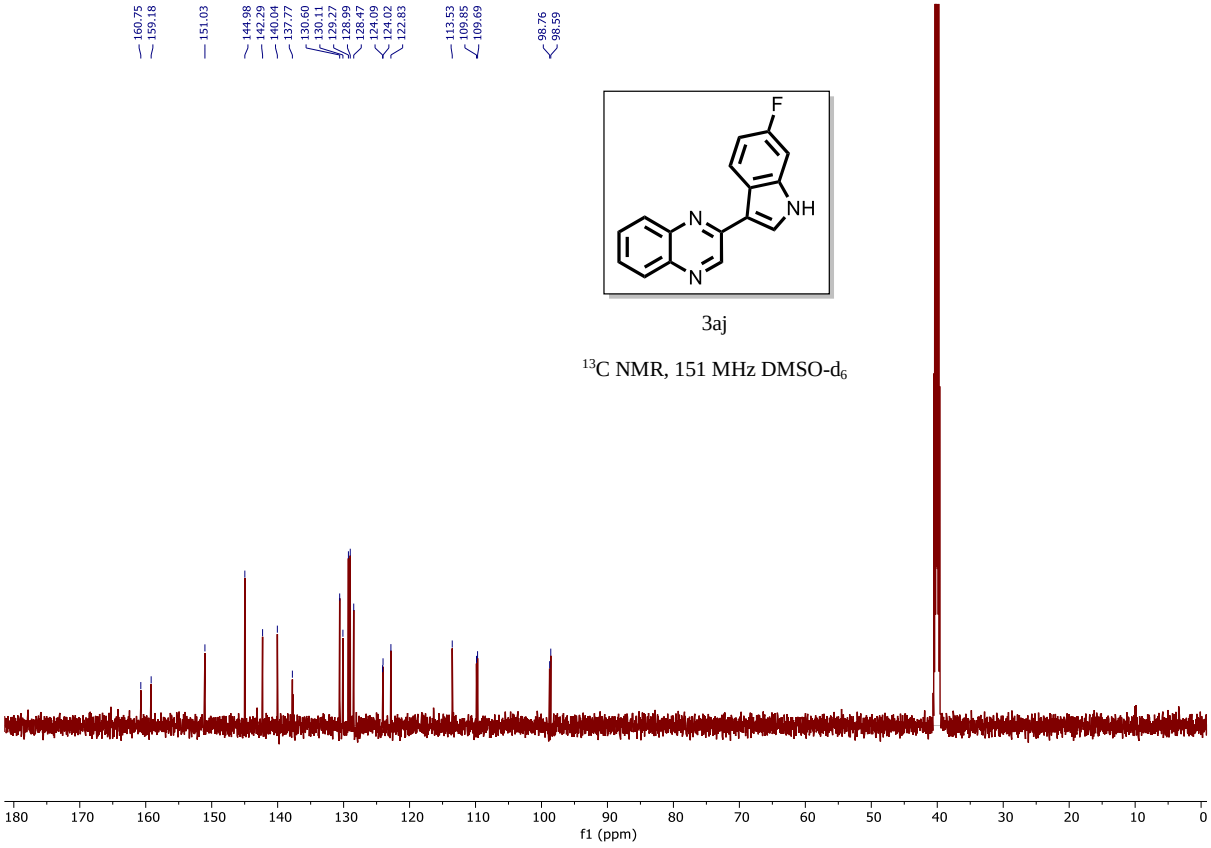


^{13}C NMR, 151 MHz $CDCl_3$

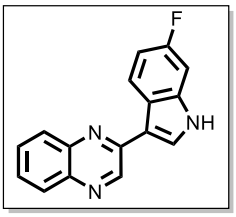
^{13}C NMR of 3ai



^{1}H NMR of 3aj



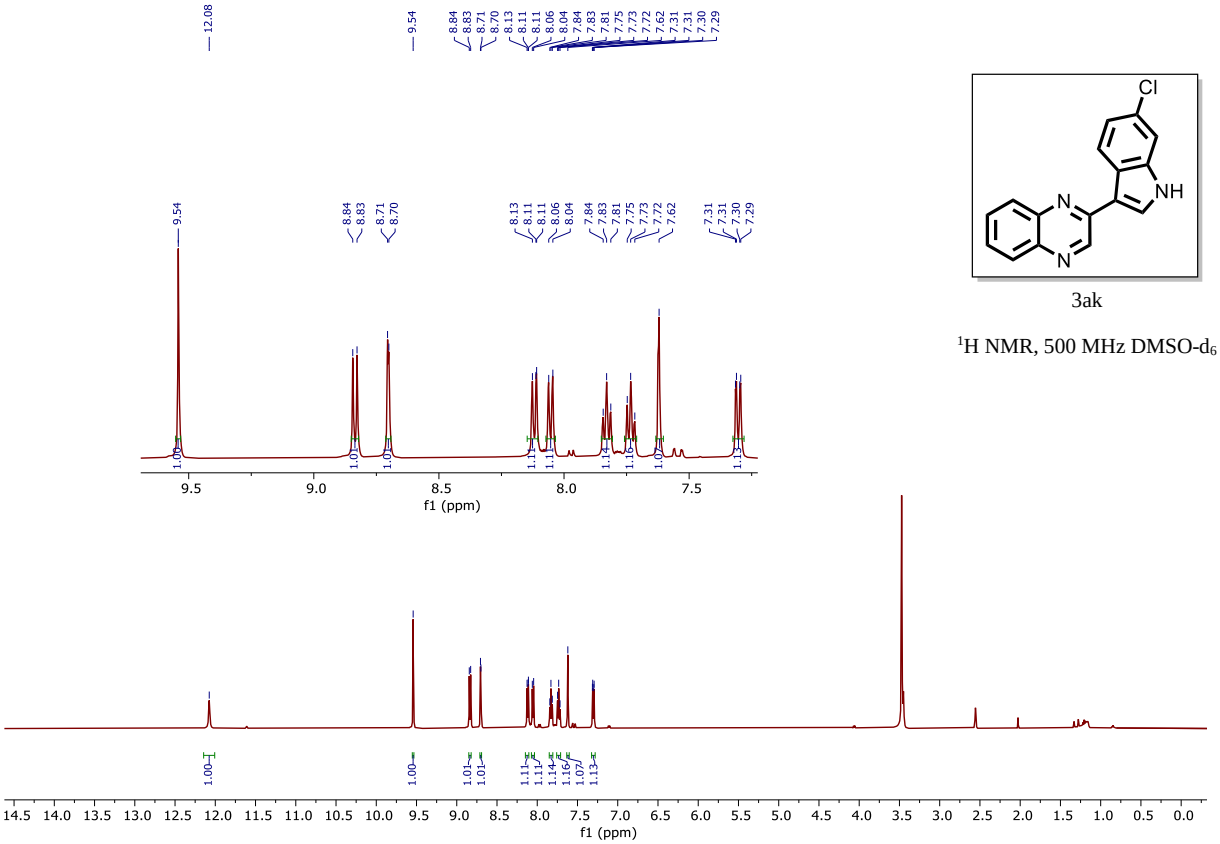
^{13}C NMR of 3aj



3aj

^{19}F NMR, 471 MHz DMSO-d_6

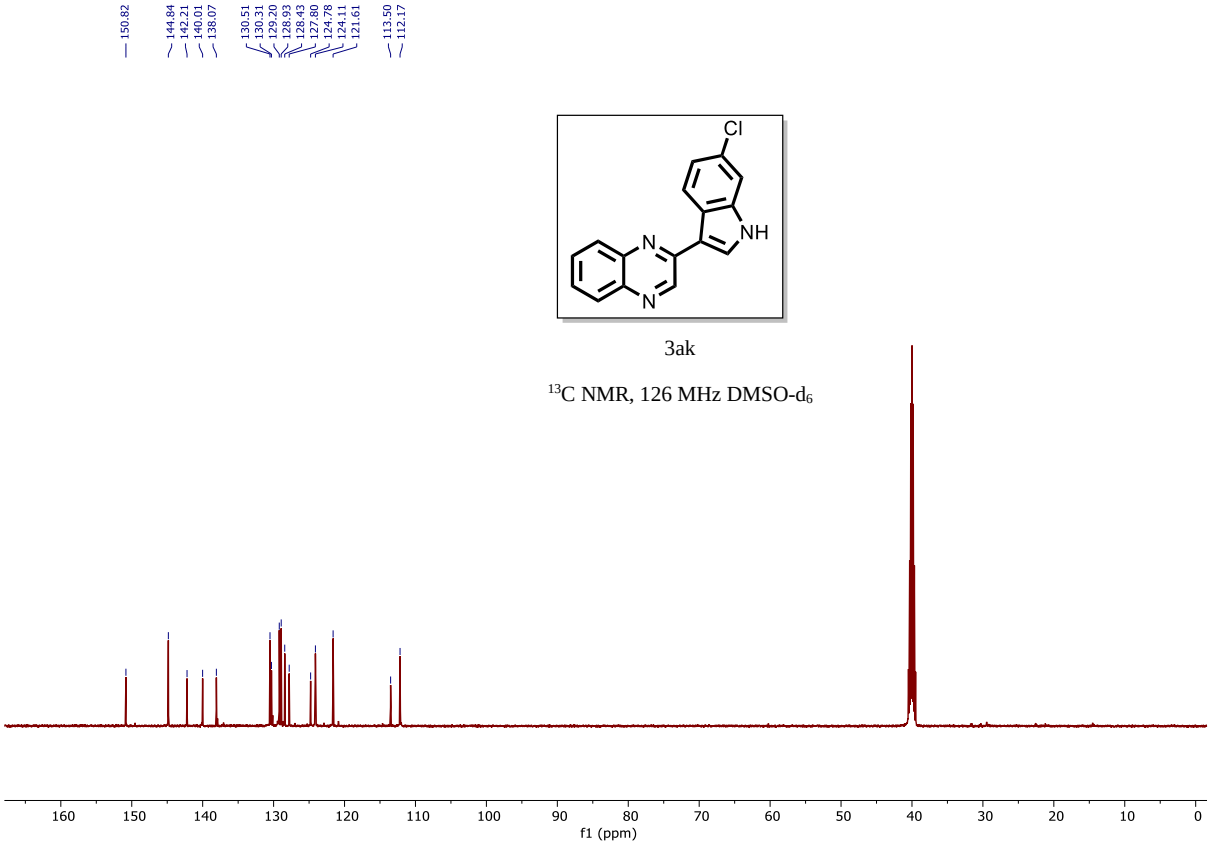
^{19}F NMR of 3aj



3ak

^{1}H NMR, 500 MHz DMSO-d_6

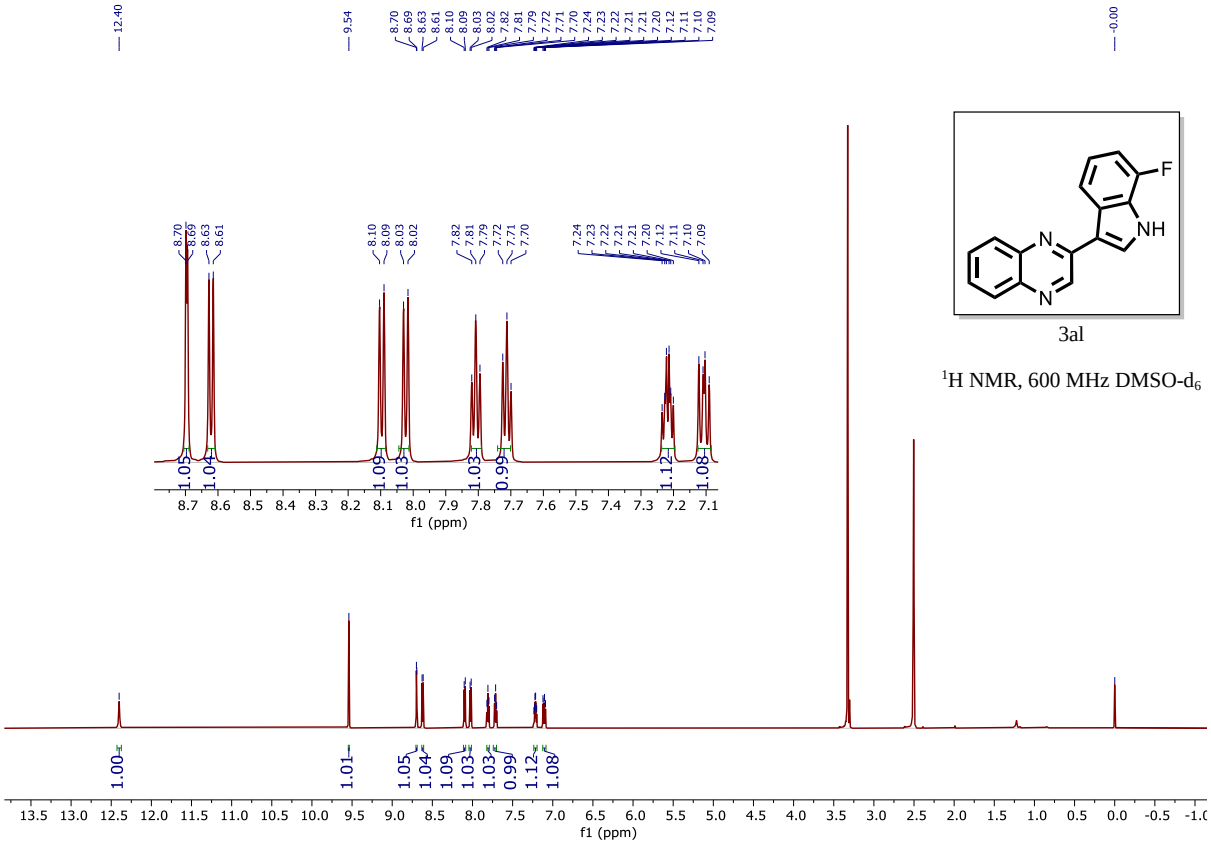
^{1}H NMR of 3ak



3ak

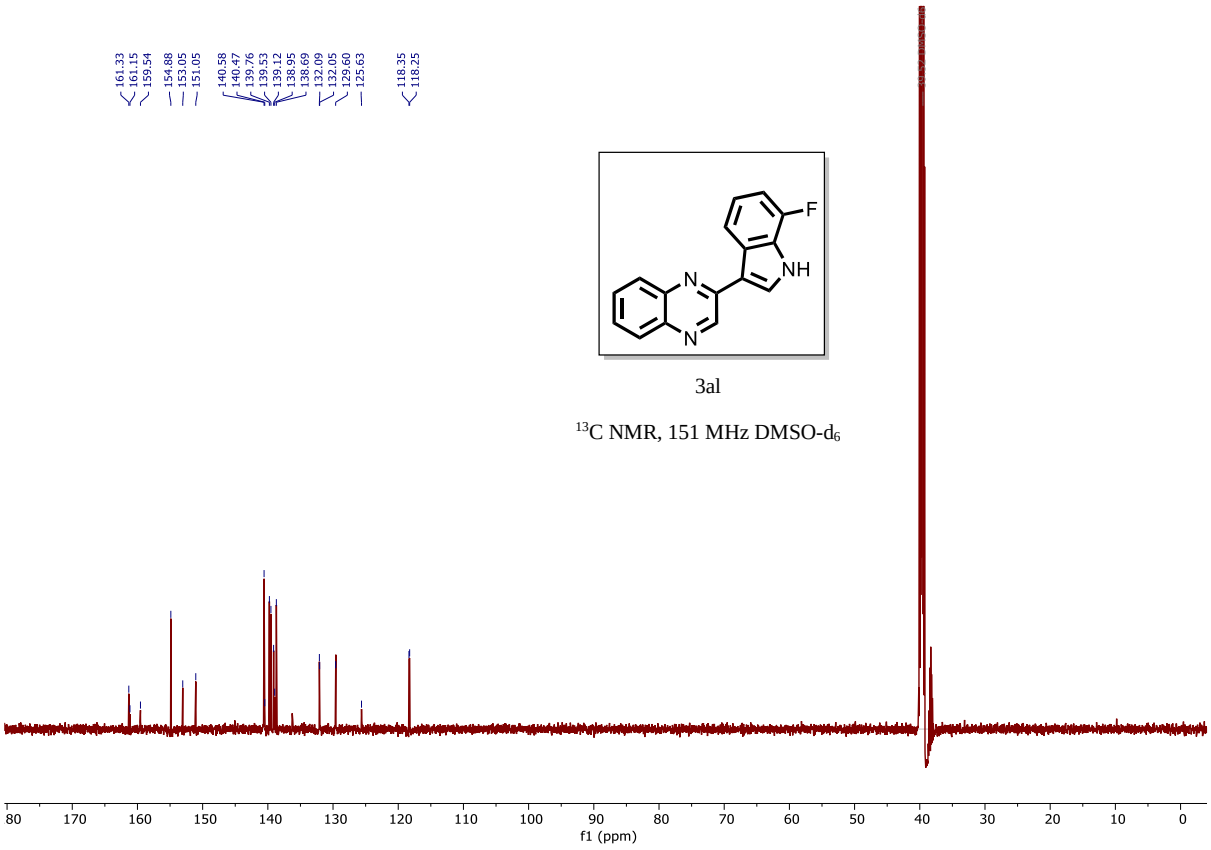
^{13}C NMR, 126 MHz DMSO-d_6

^{13}C NMR of 3ak



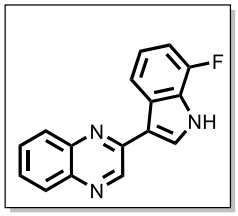
^{1}H NMR, 600 MHz DMSO-d_6

^{1}H NMR of 3al



^{13}C NMR, 151 MHz DMSO-d_6

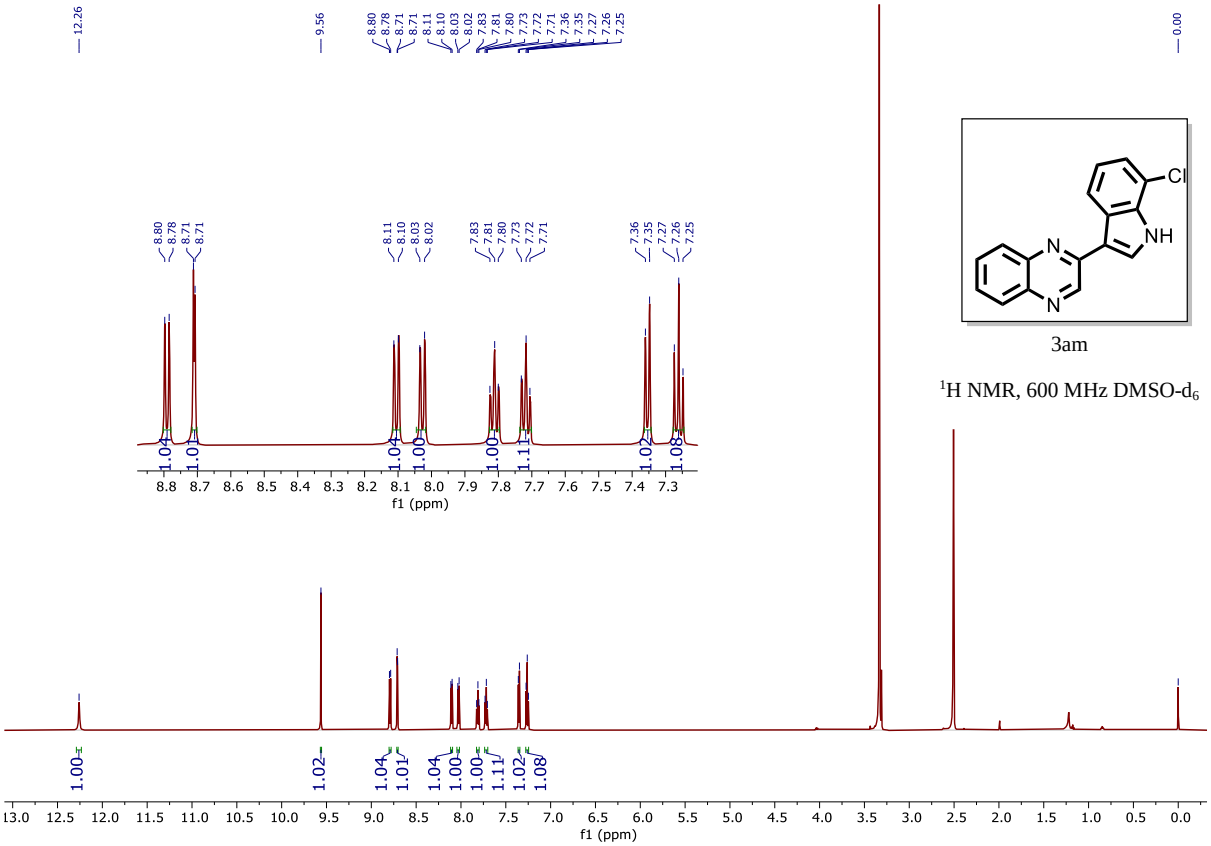
^{13}C NMR of 3al



3al

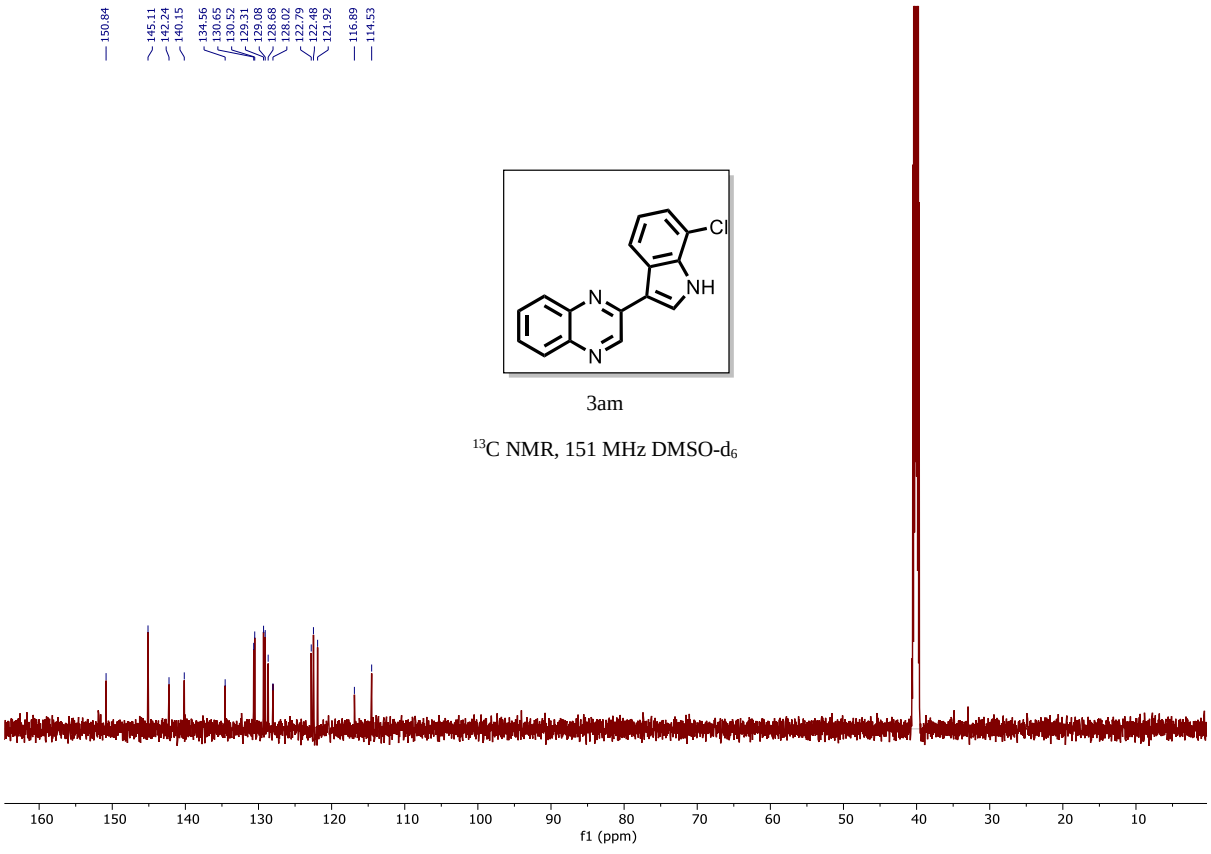
^{19}F NMR, 471MHz, DMSO-d_6

^{19}F NMR of 3al



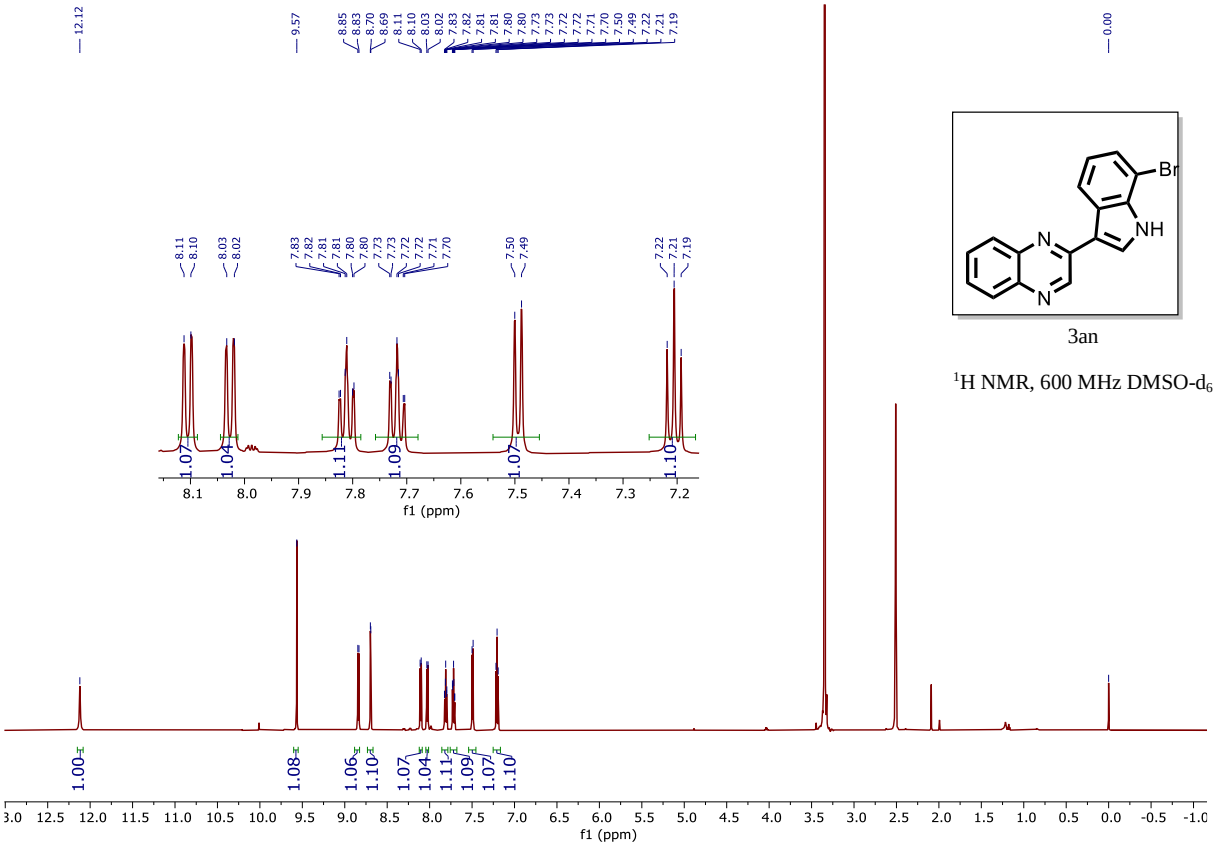
^{1}H NMR, 600 MHz DMSO-d_6

^{1}H NMR of 3am



^{13}C NMR, 151 MHz DMSO-d_6

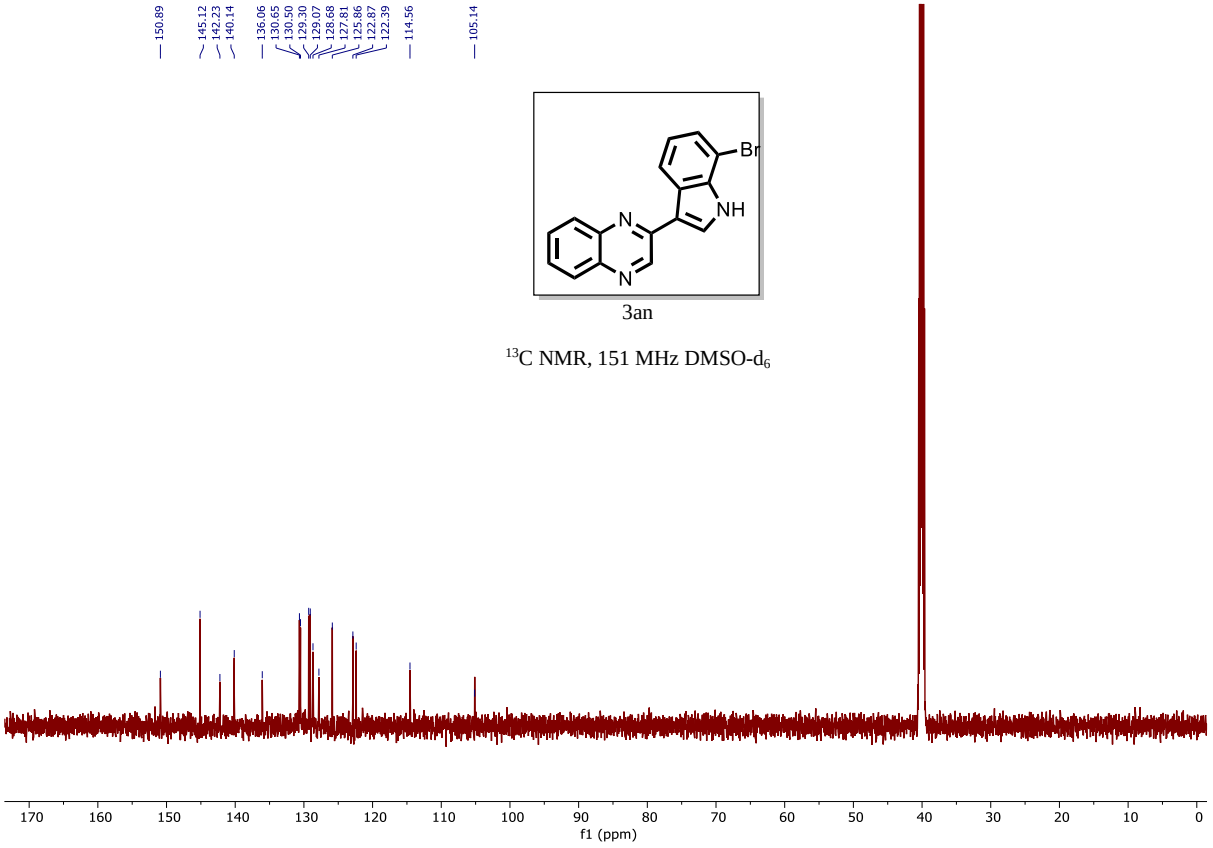
^{13}C NMR of 3am



3an

^{1}H NMR, 600 MHz DMSO-d_6

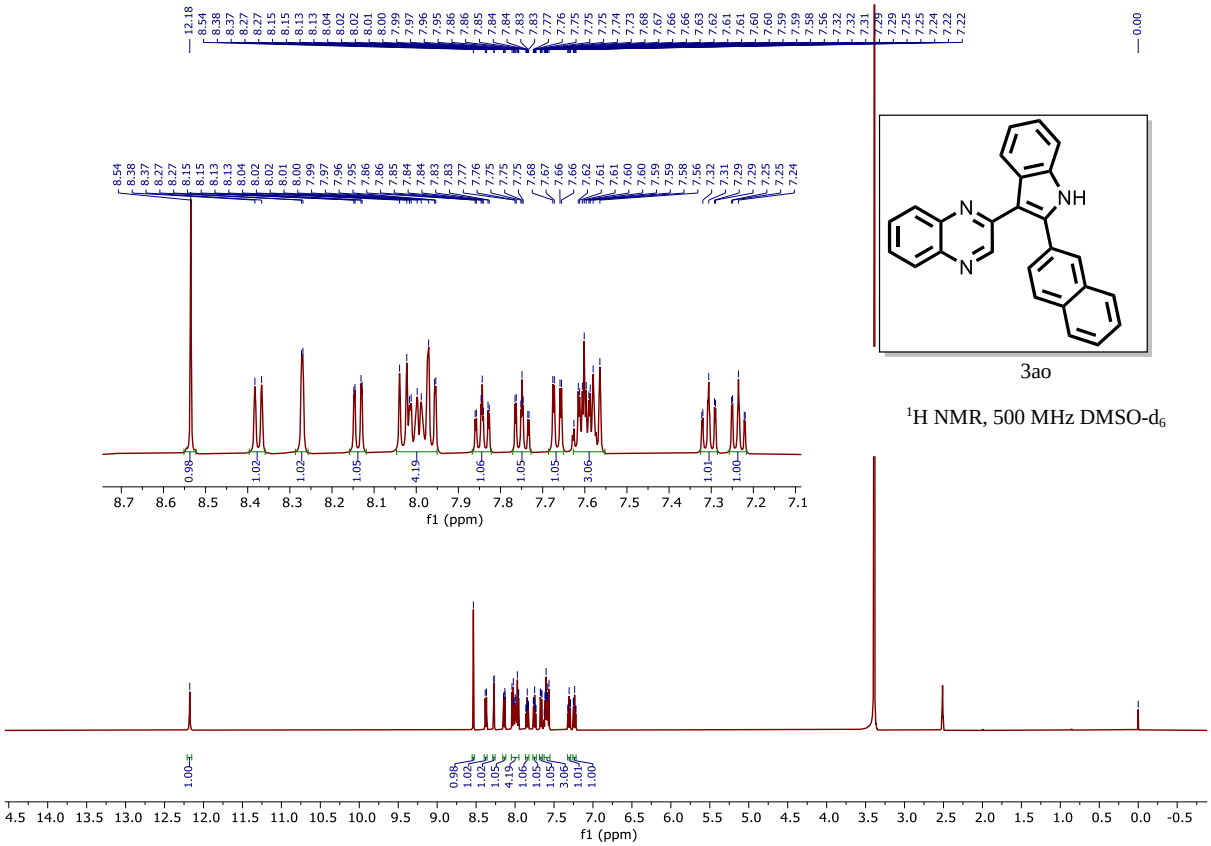
^{1}H NMR of 3an



3an

^{13}C NMR, 151 MHz DMSO-d_6

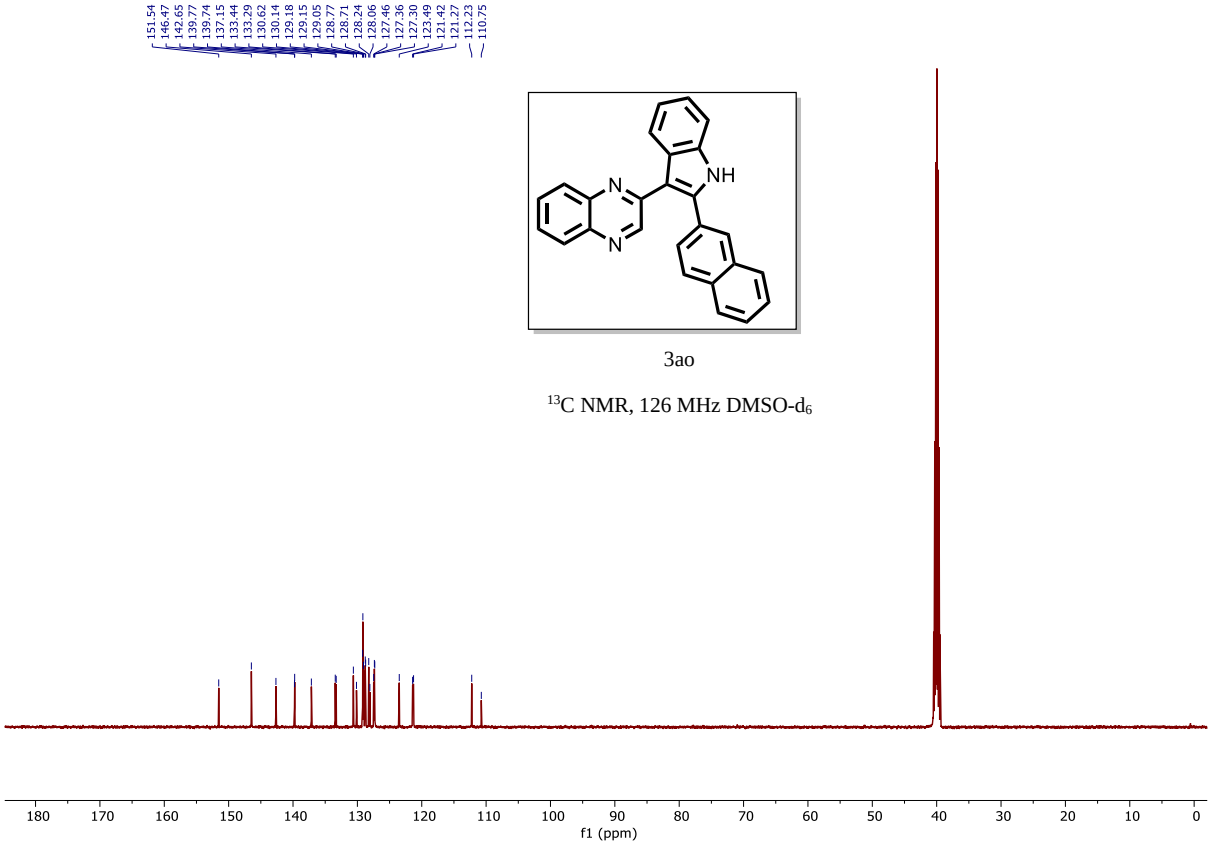
^{13}C NMR of 3an



3ao

^{1}H NMR, 500 MHz DMSO-d_6

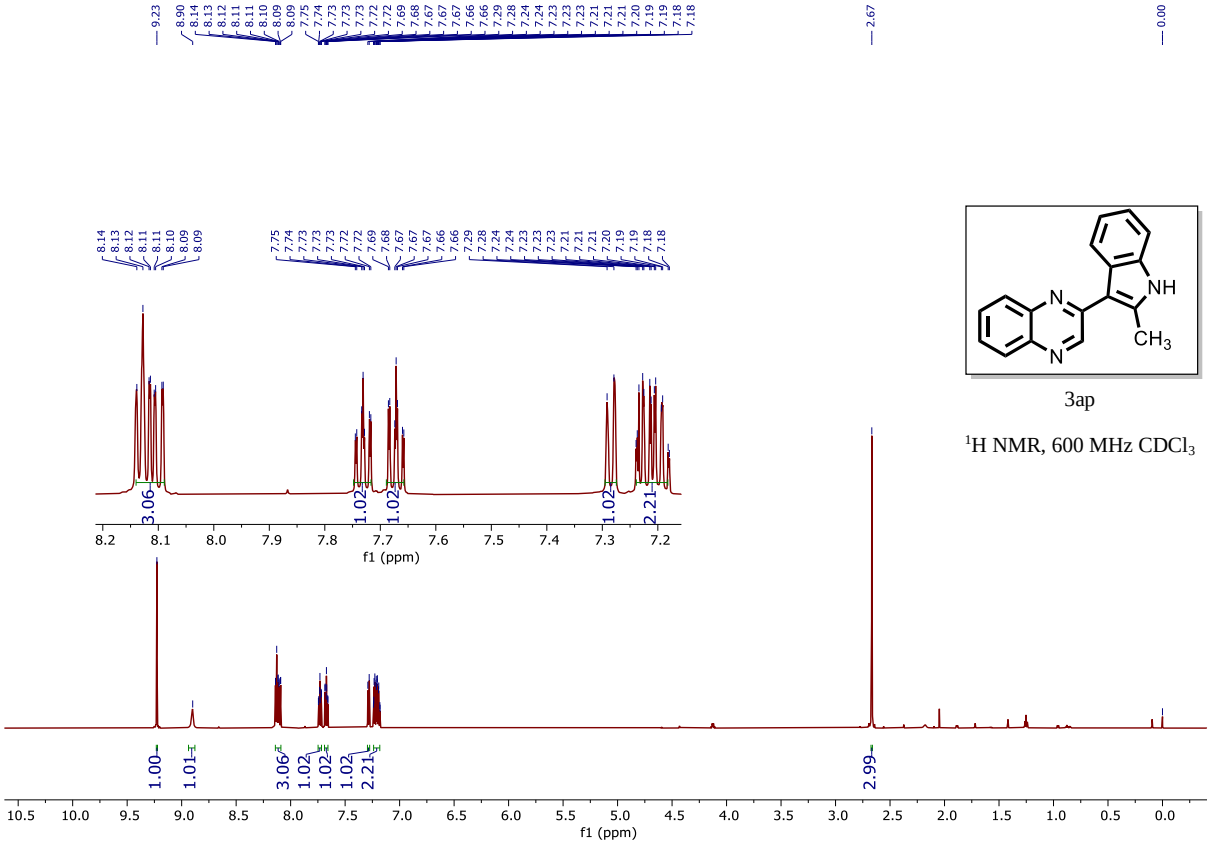
^{1}H NMR of 3ao



3ao

^{13}C NMR, 126 MHz DMSO-d_6

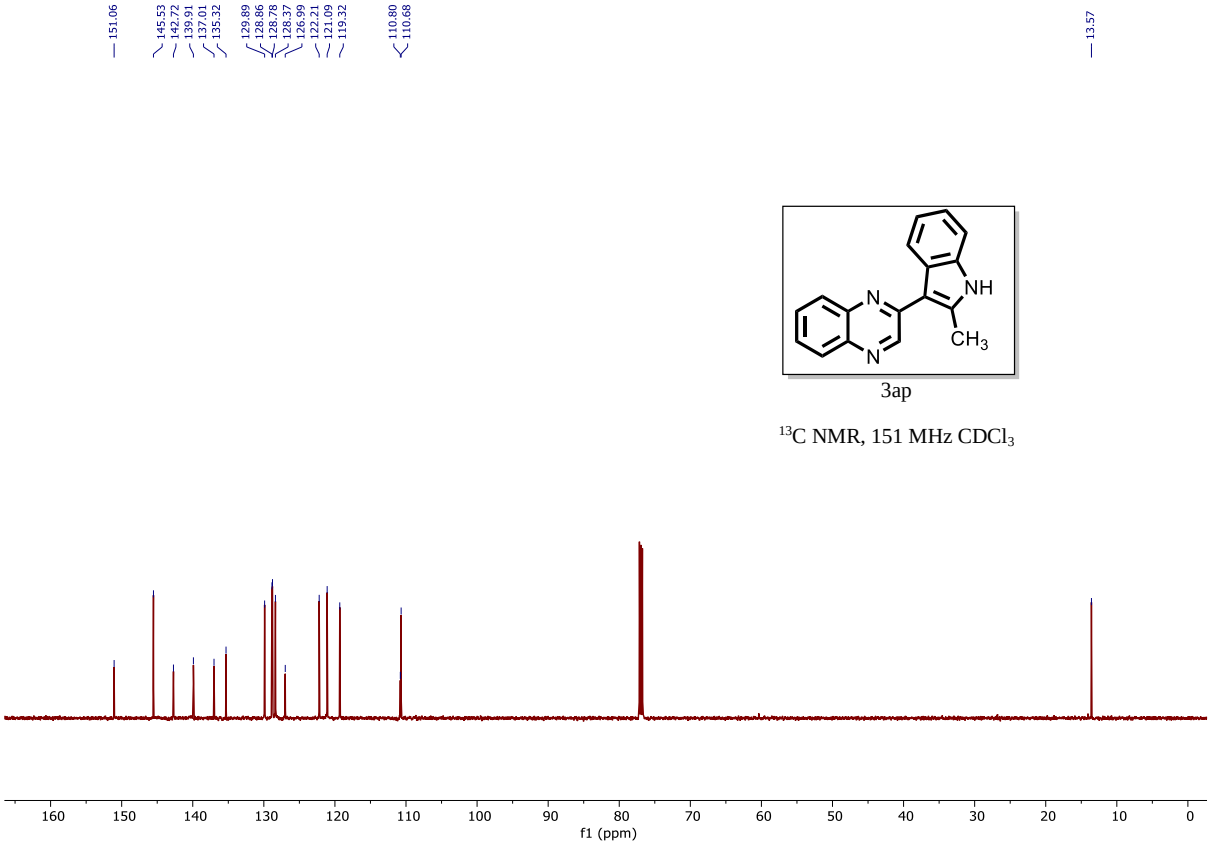
^{13}C NMR of 3ao



3ap

^{1}H NMR, 600 MHz $CDCl_3$

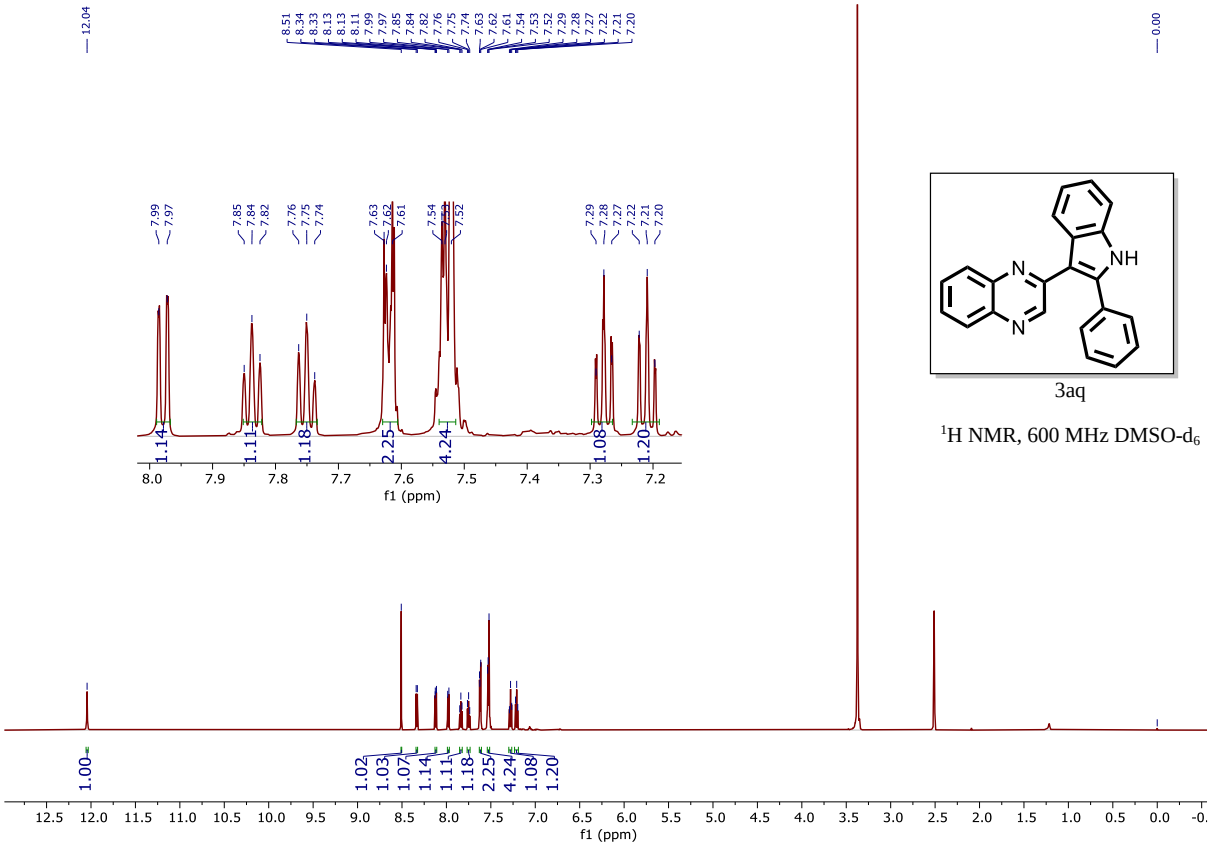
^{1}H NMR of 3ap



3ap

^{13}C NMR, 151 MHz $CDCl_3$

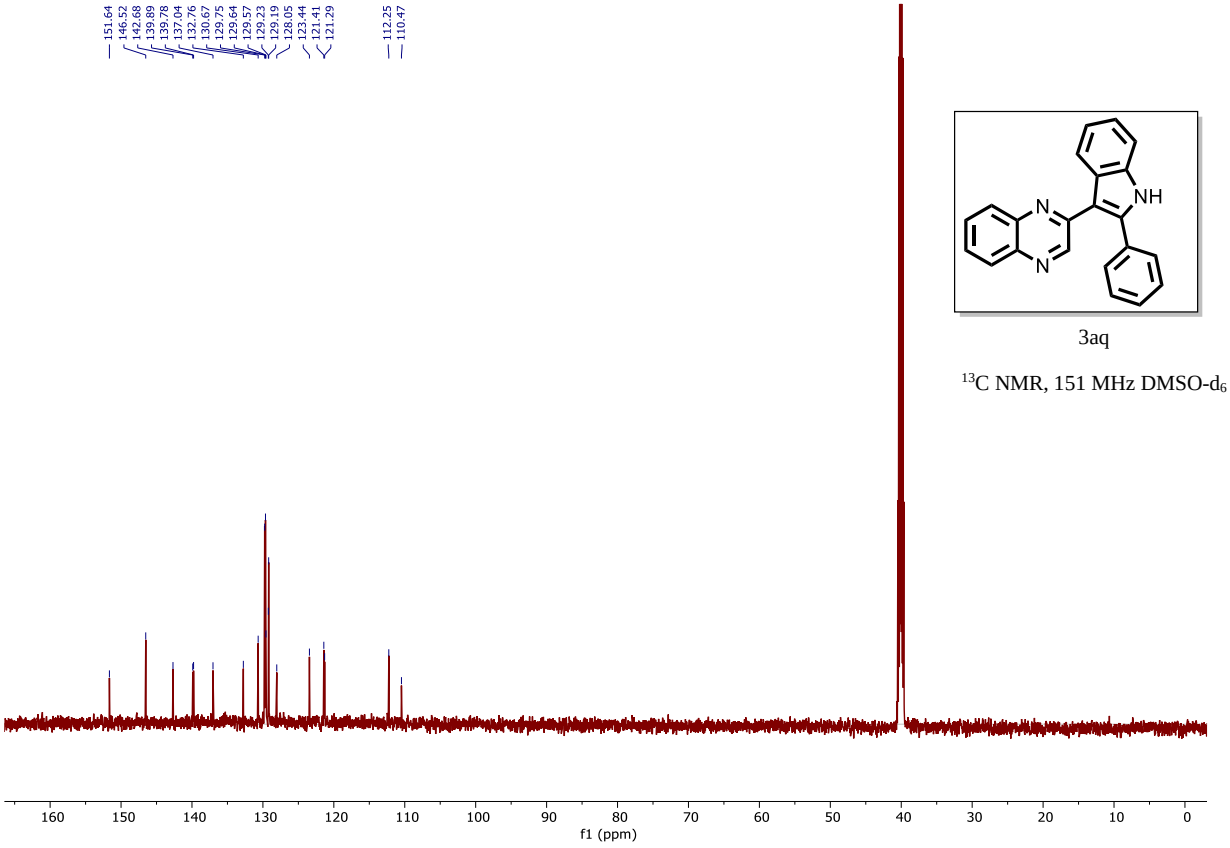
^{13}C NMR of 3ap



3aq

^{1}H NMR, 600 MHz DMSO-d_6

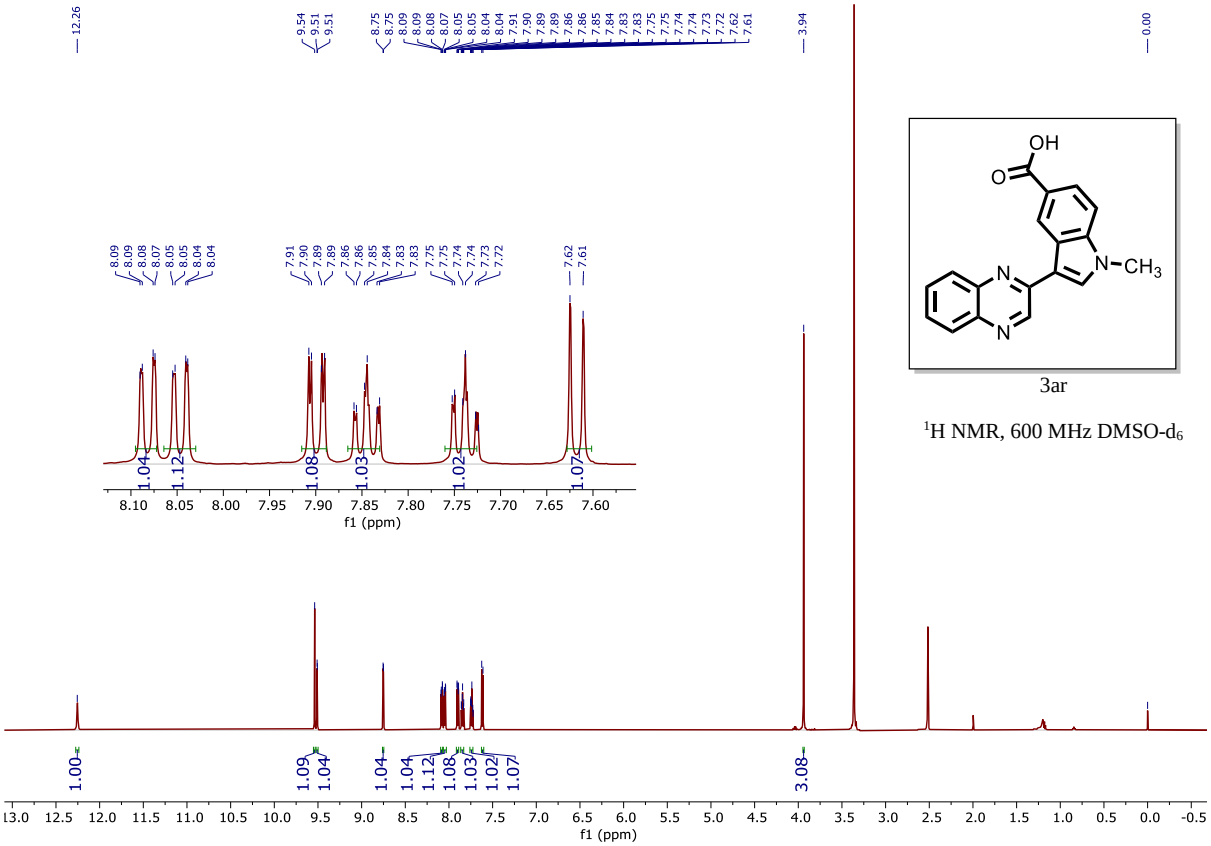
^{1}H NMR of 3aq



3aq

^{13}C NMR, 151 MHz DMSO-d_6

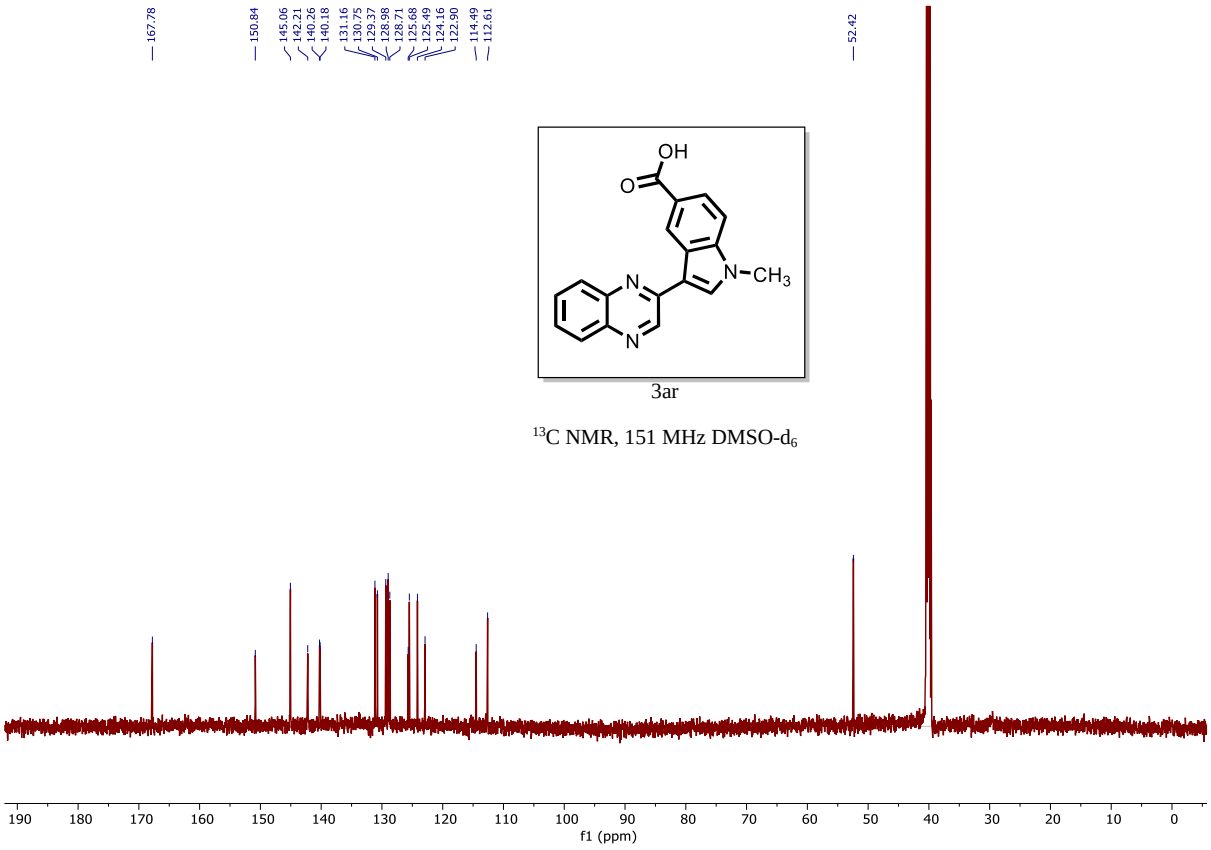
^{13}C NMR of 3aq



3ar

^{1}H NMR, 600 MHz DMSO-d_6

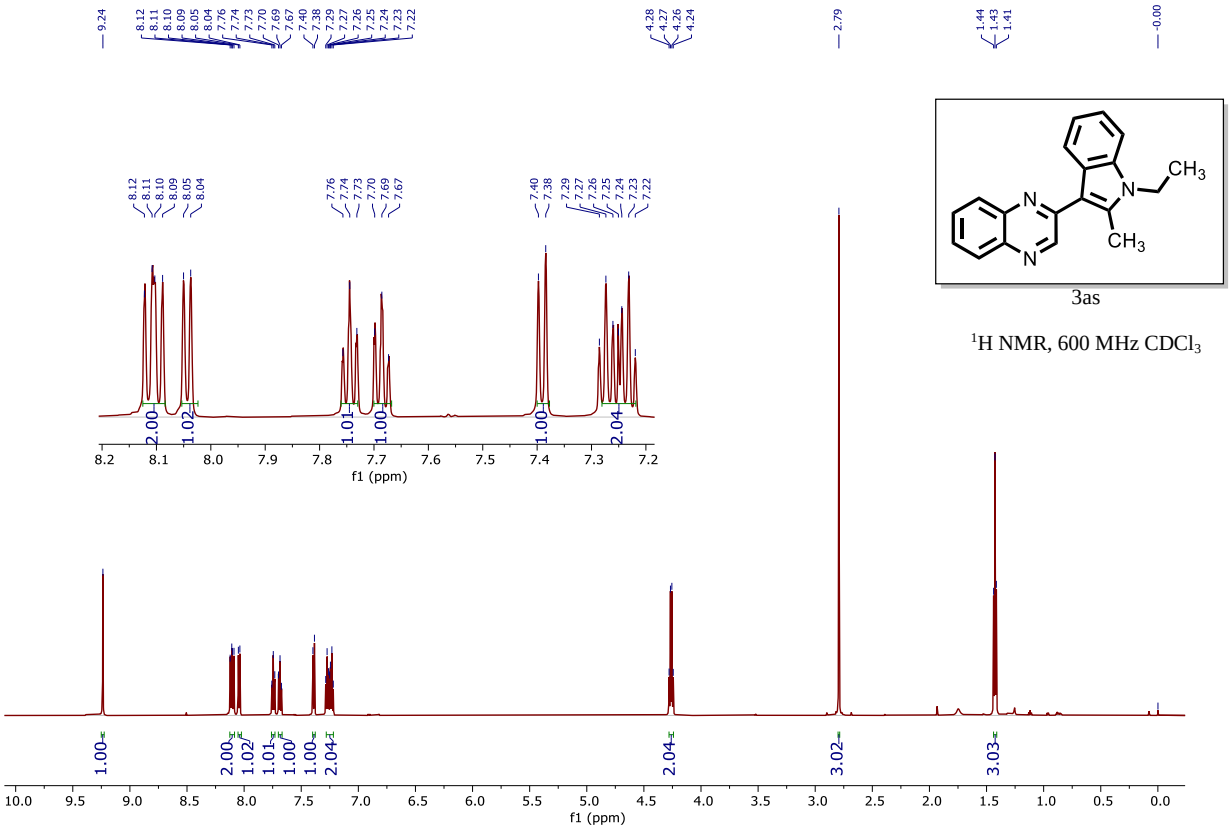
^{1}H NMR of 3ar



3ar

^{13}C NMR, 151 MHz DMSO-d_6

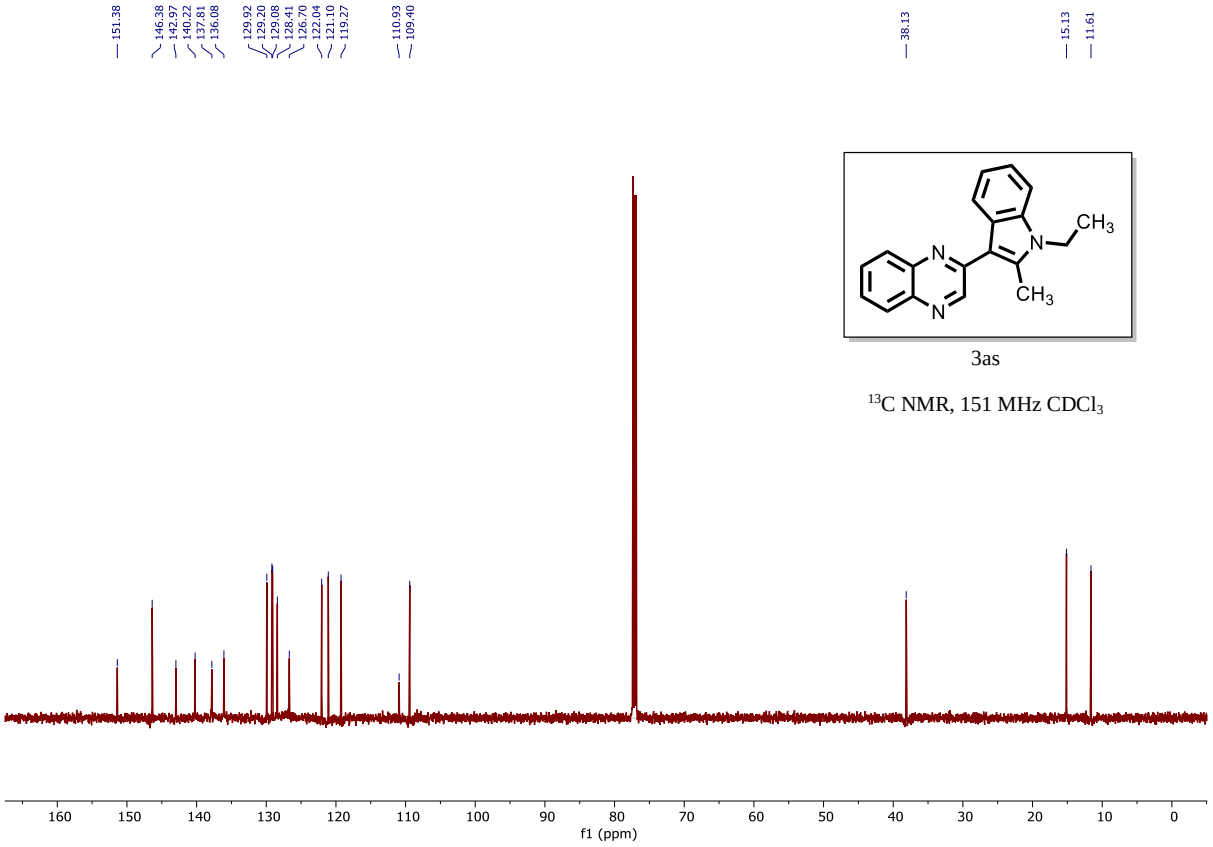
^{13}C NMR of 3ar



3as

^{1}H NMR, 600 MHz $CDCl_3$

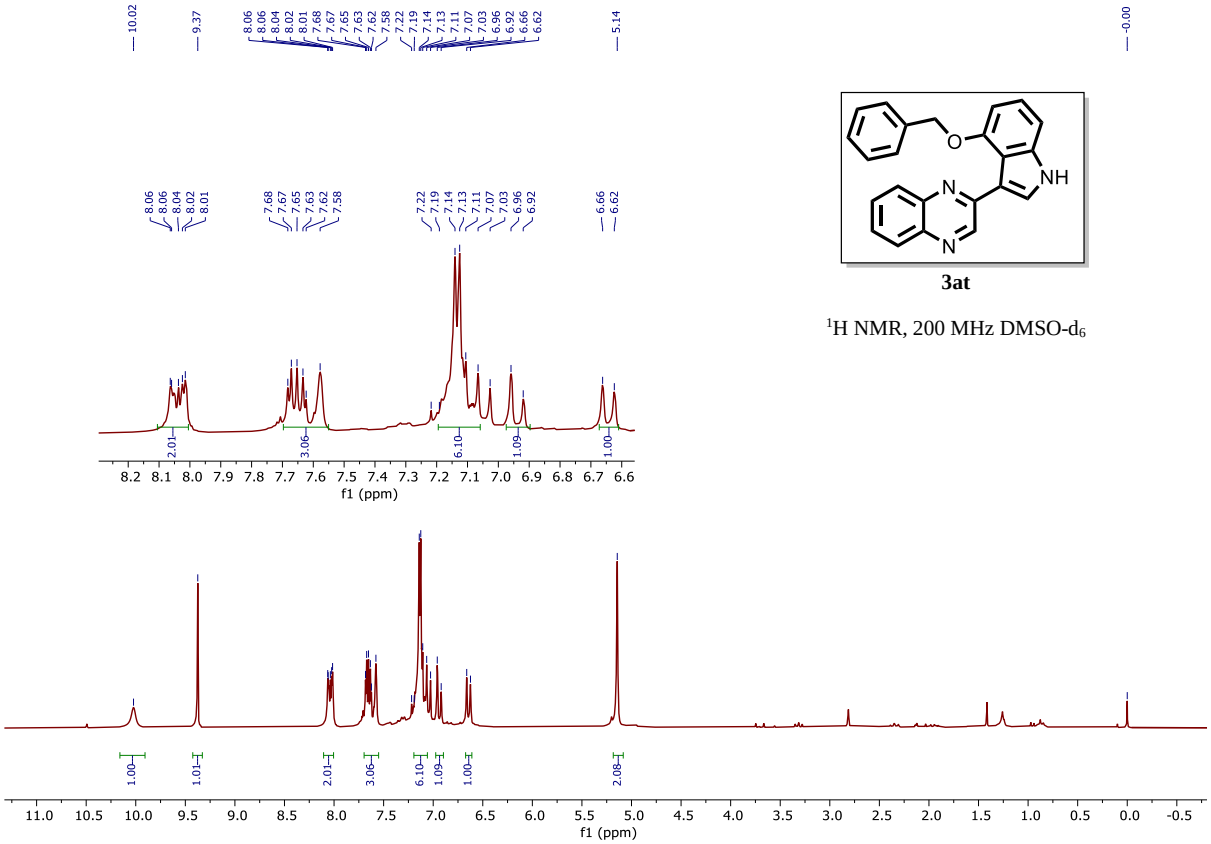
^{1}H NMR of 3as



3as

^{13}C NMR, 151 MHz $CDCl_3$

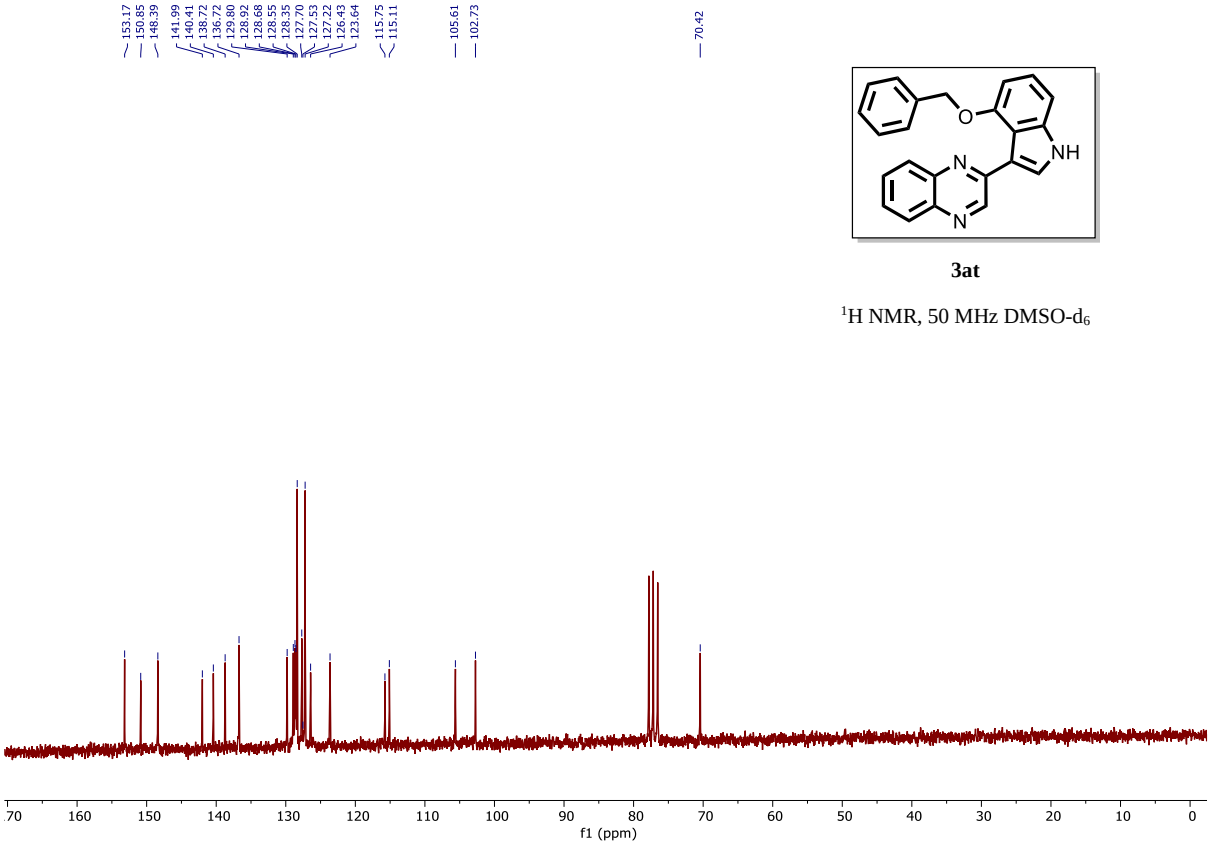
^{13}C NMR of 3as



3at

^{1}H NMR, 200 MHz DMSO-d_6

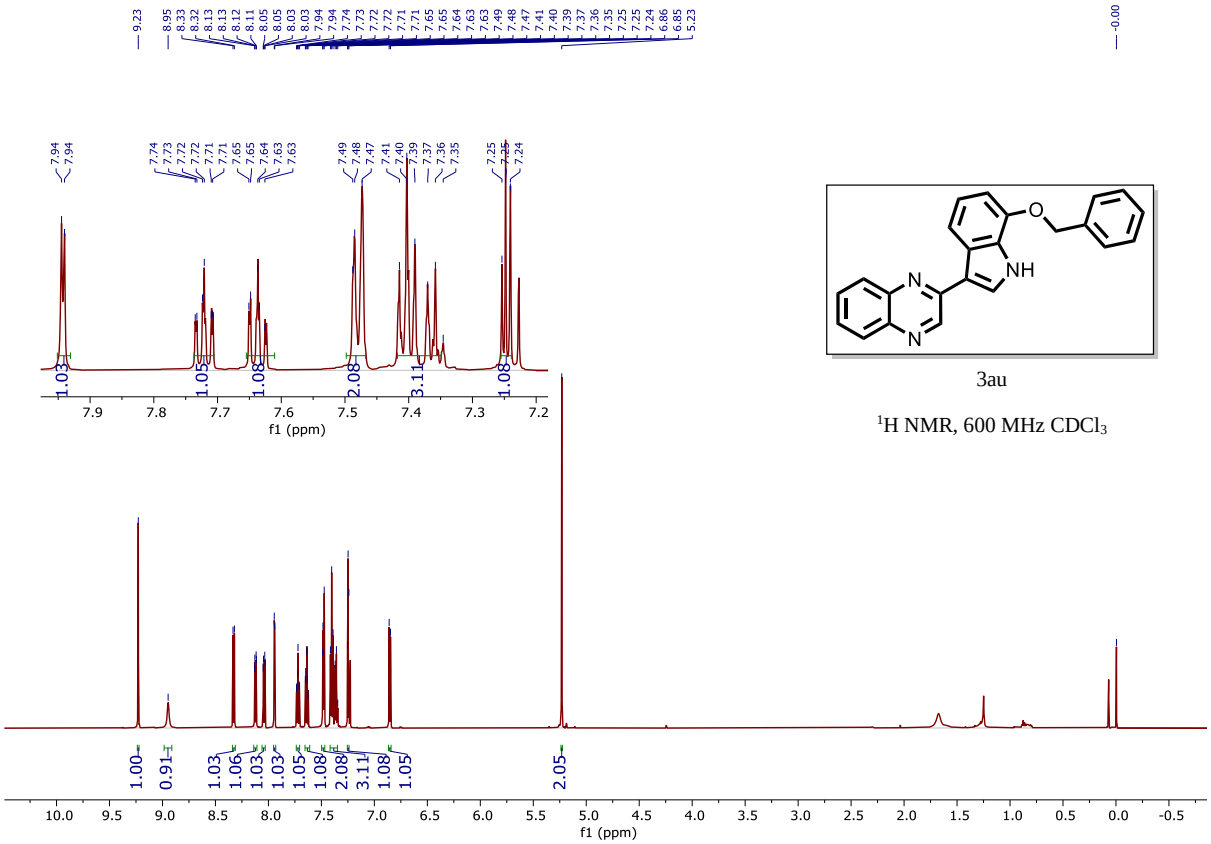
^{1}H NMR of 3at



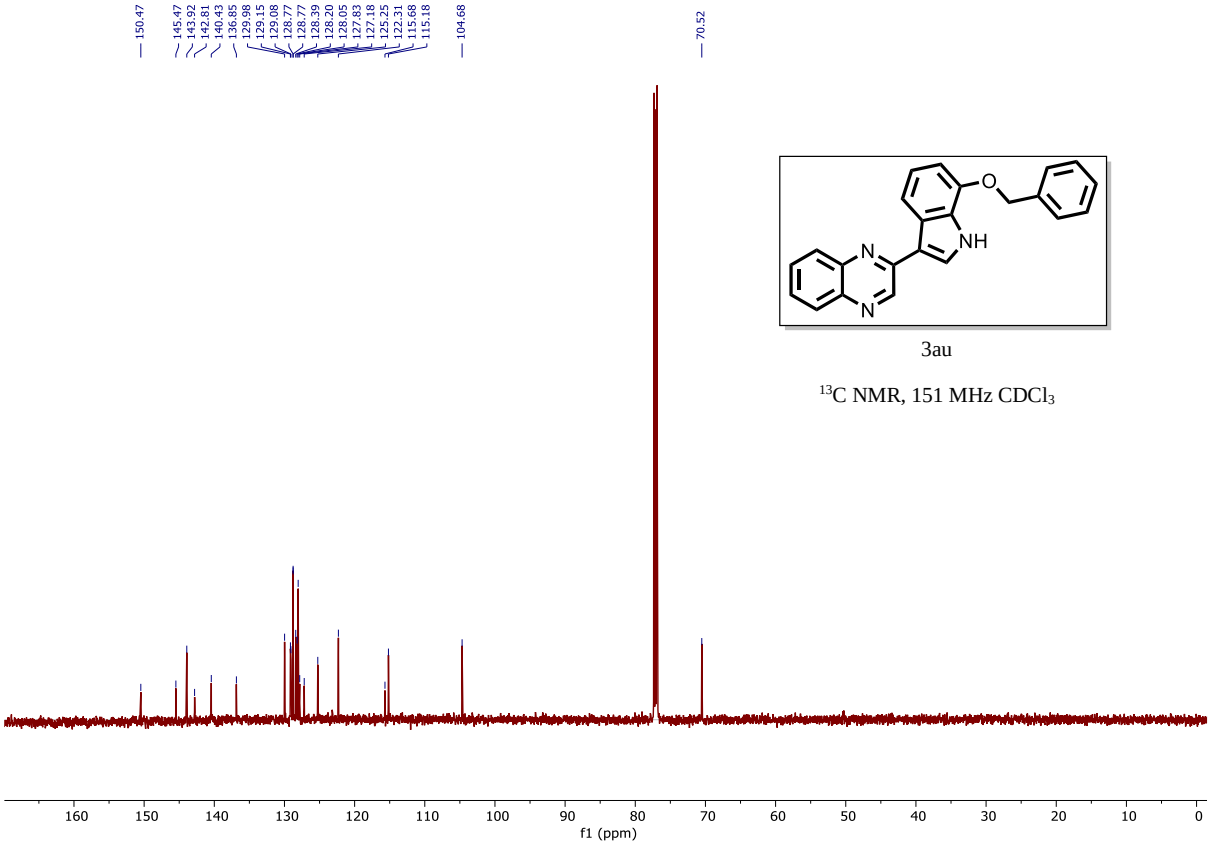
3at

^{1}H NMR, 50 MHz DMSO-d_6

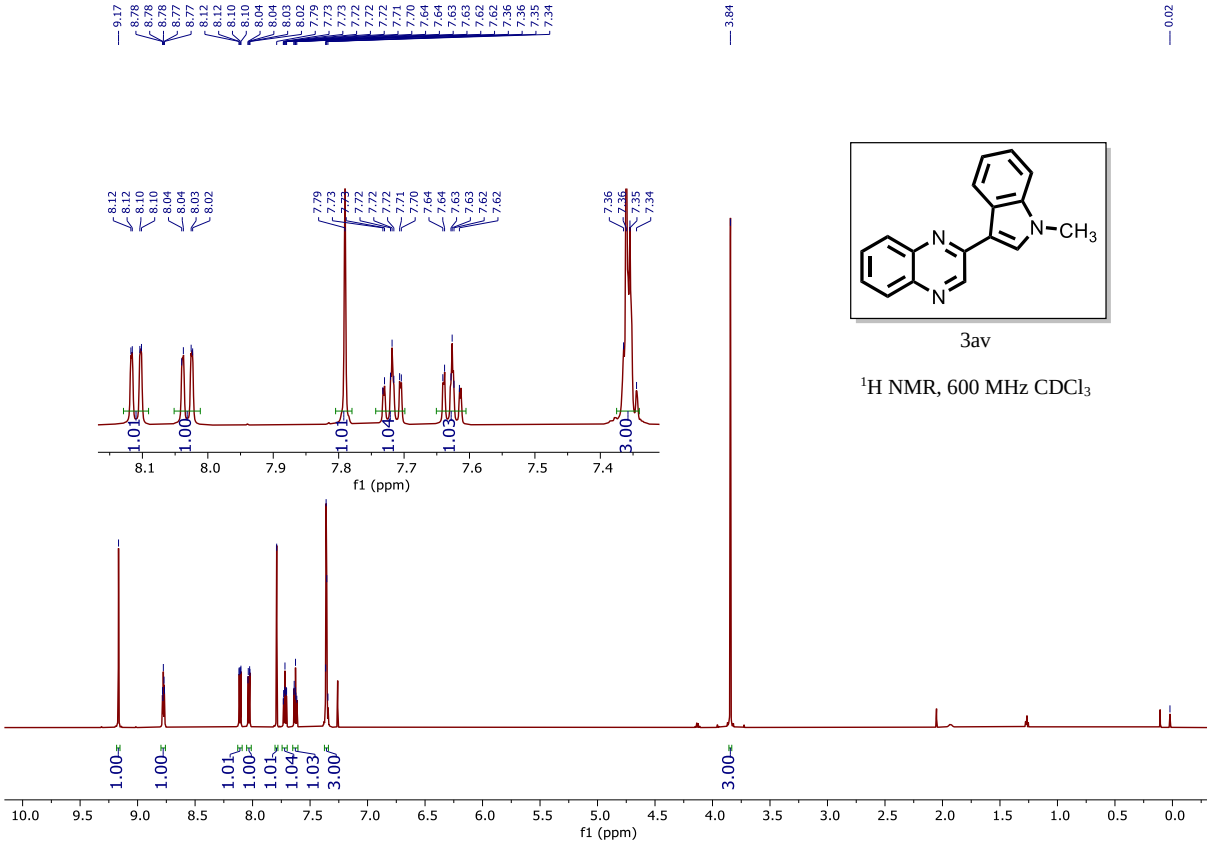
^{13}C NMR of 3at



^{1}H NMR of 3au



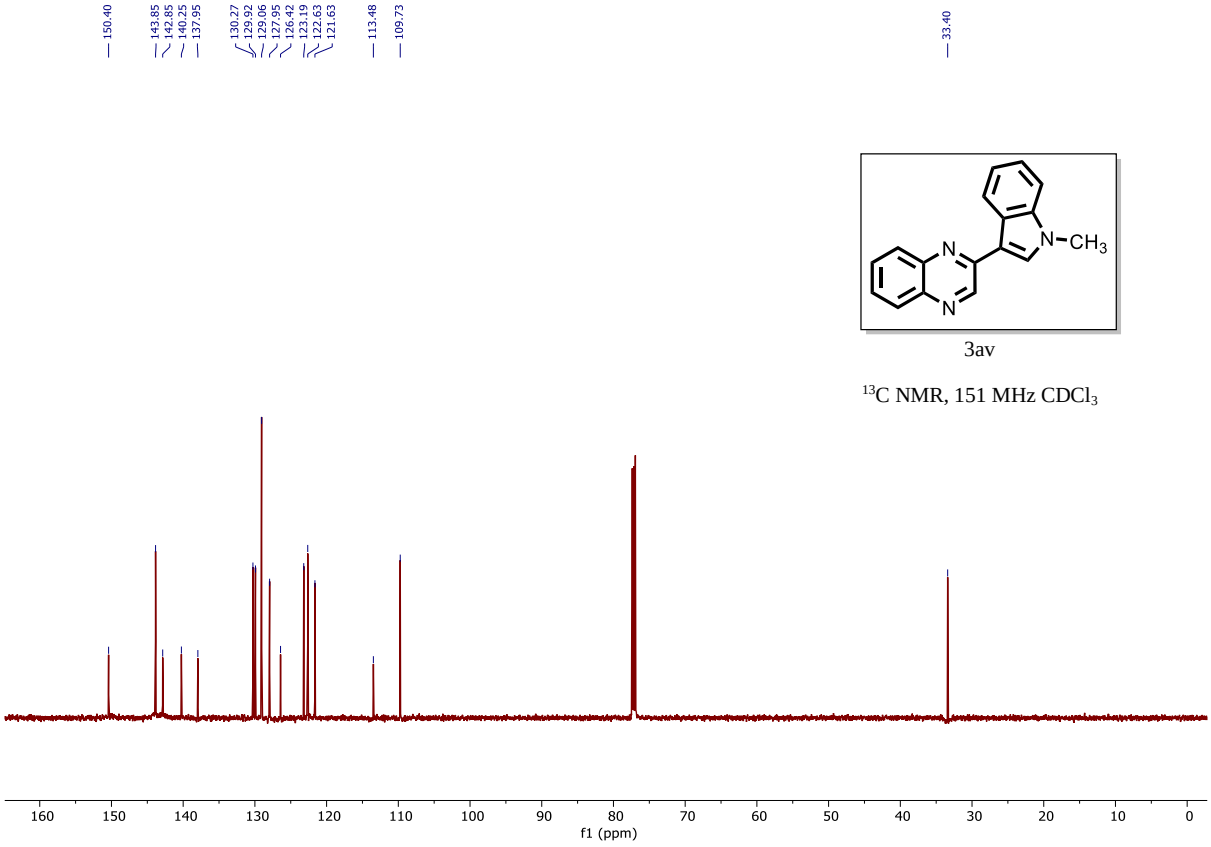
^{13}C NMR of 3au



3av

^{1}H NMR, 600 MHz $CDCl_3$

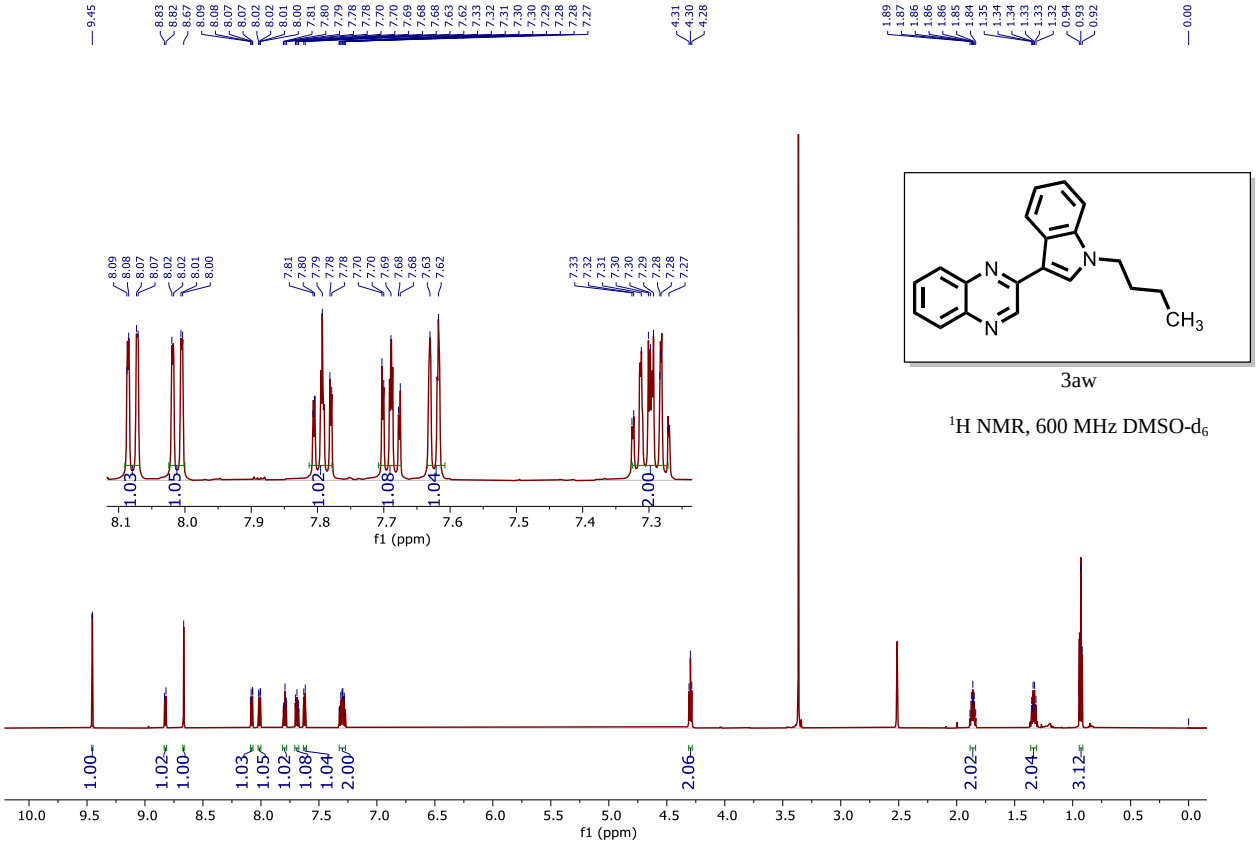
^{1}H NMR of 3av



3av

^{13}C NMR, 151 MHz $CDCl_3$

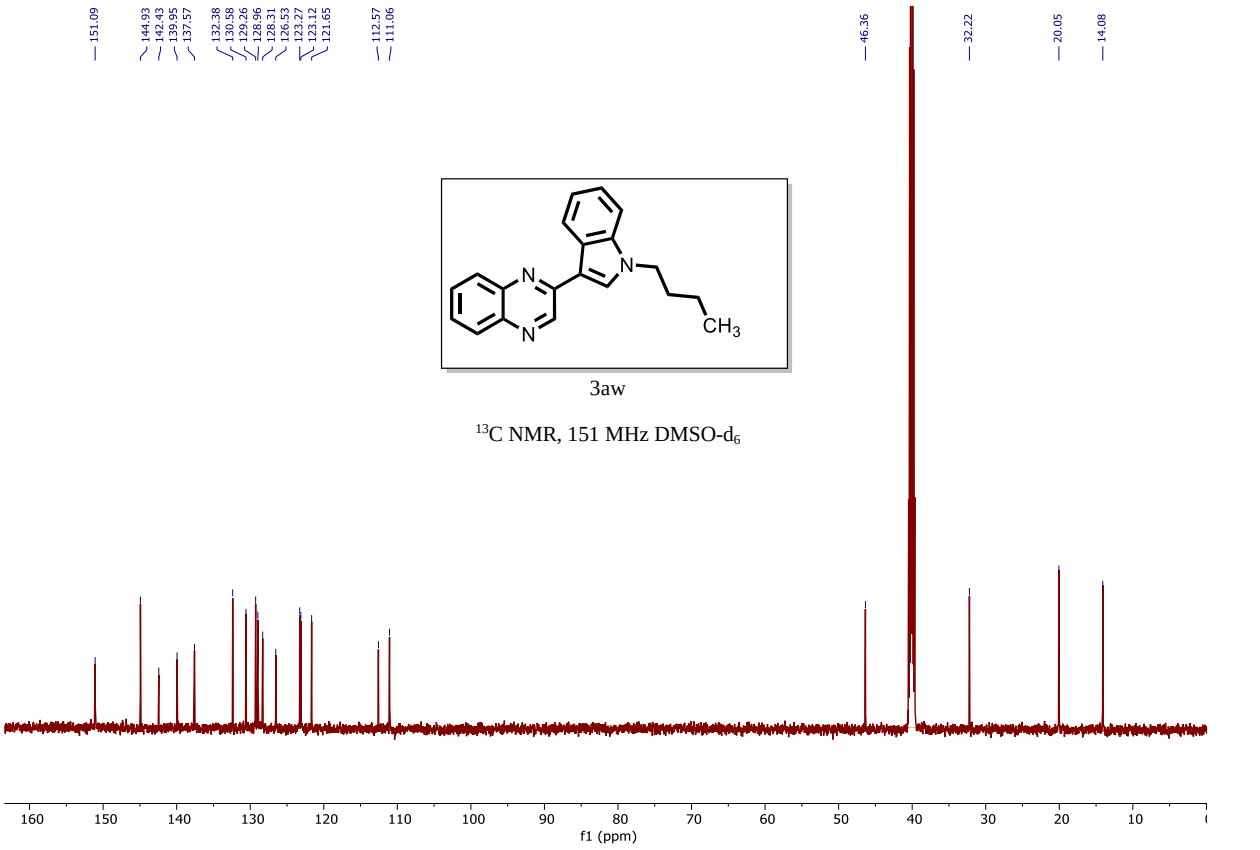
^{13}C NMR of 3av



3aw

^{1}H NMR, 600 MHz DMSO-d_6

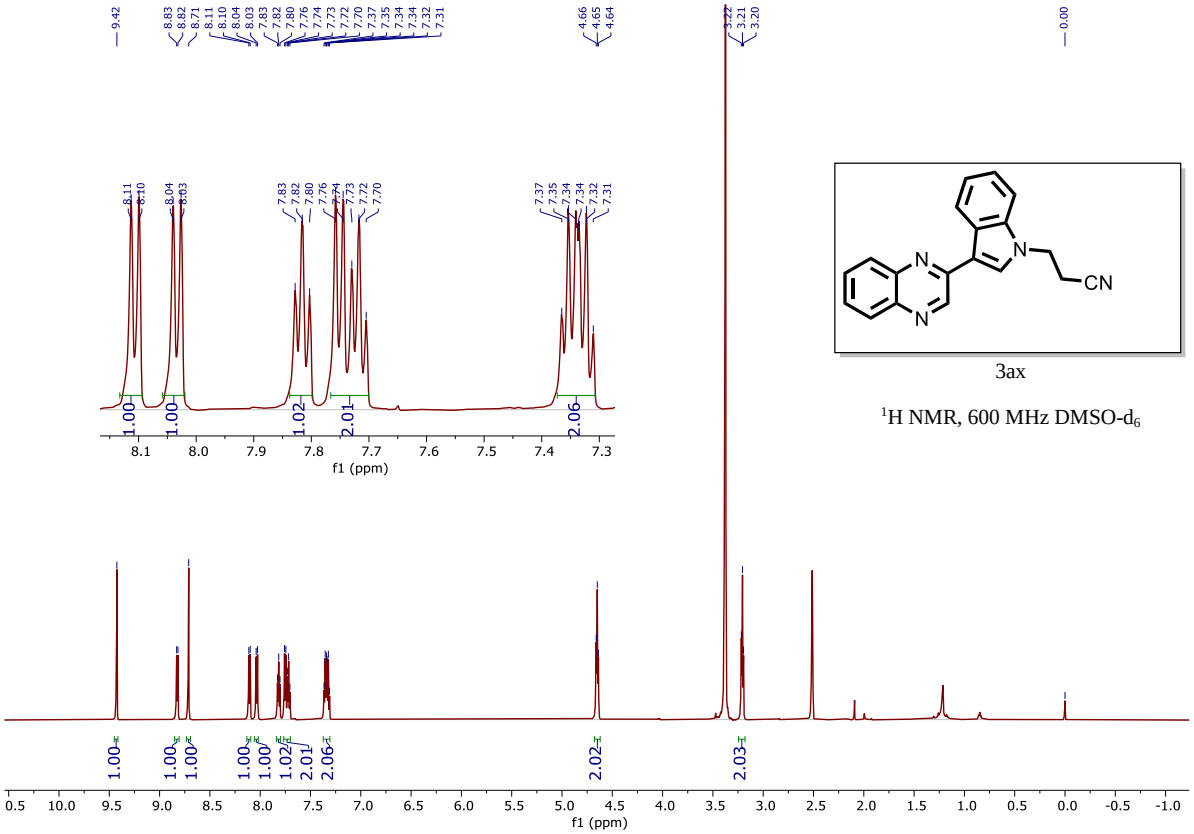
^{1}H NMR of 3aw



3aw

^{13}C NMR, 151 MHz DMSO-d_6

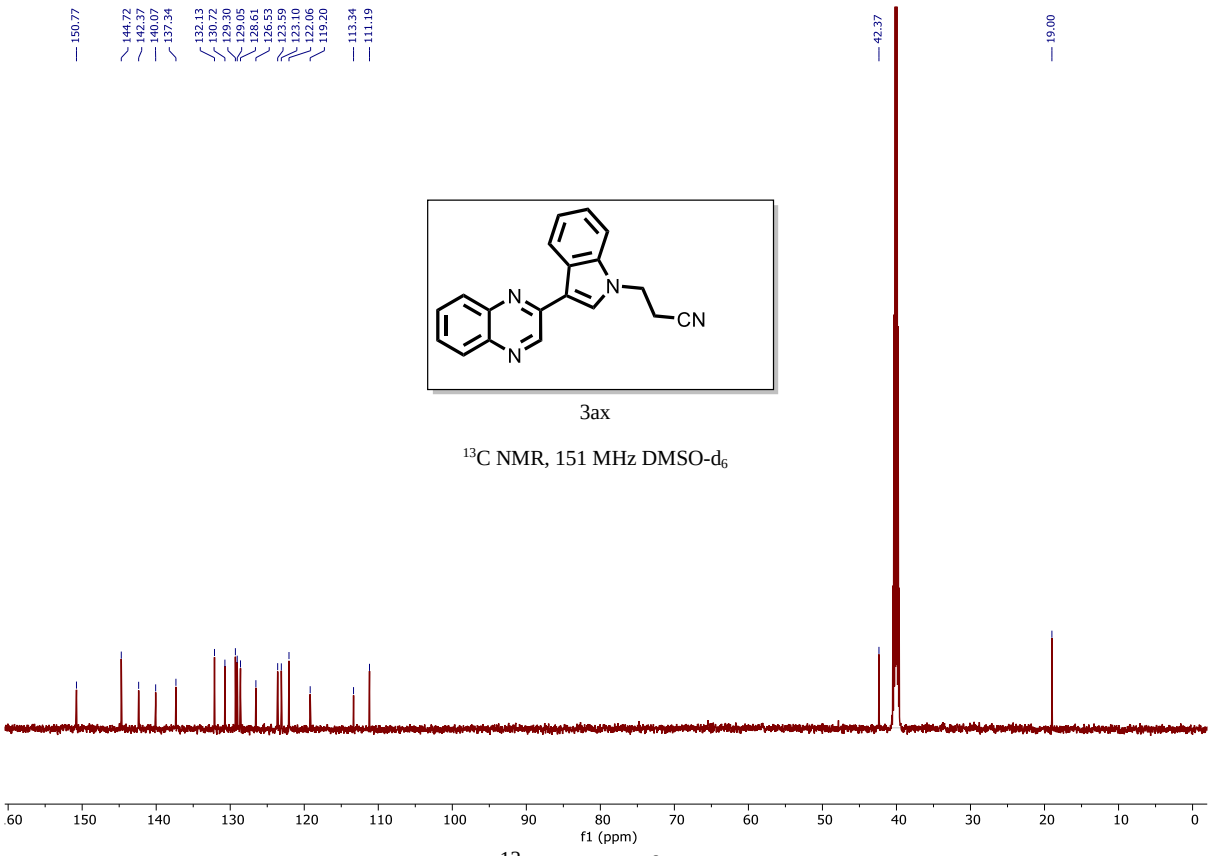
^{13}C NMR of 3aw



3ax

^{1}H NMR, 600 MHz DMSO-d_6

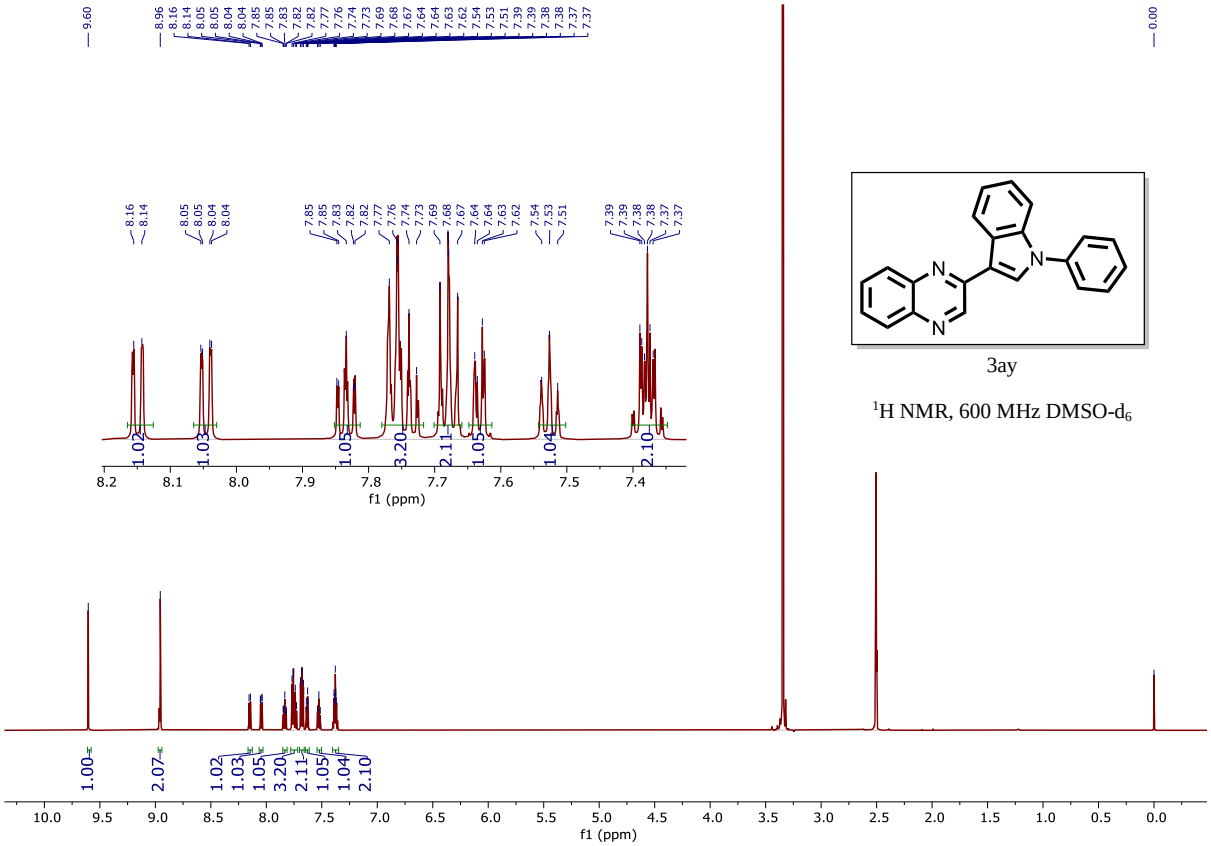
^{1}H NMR of 3ax



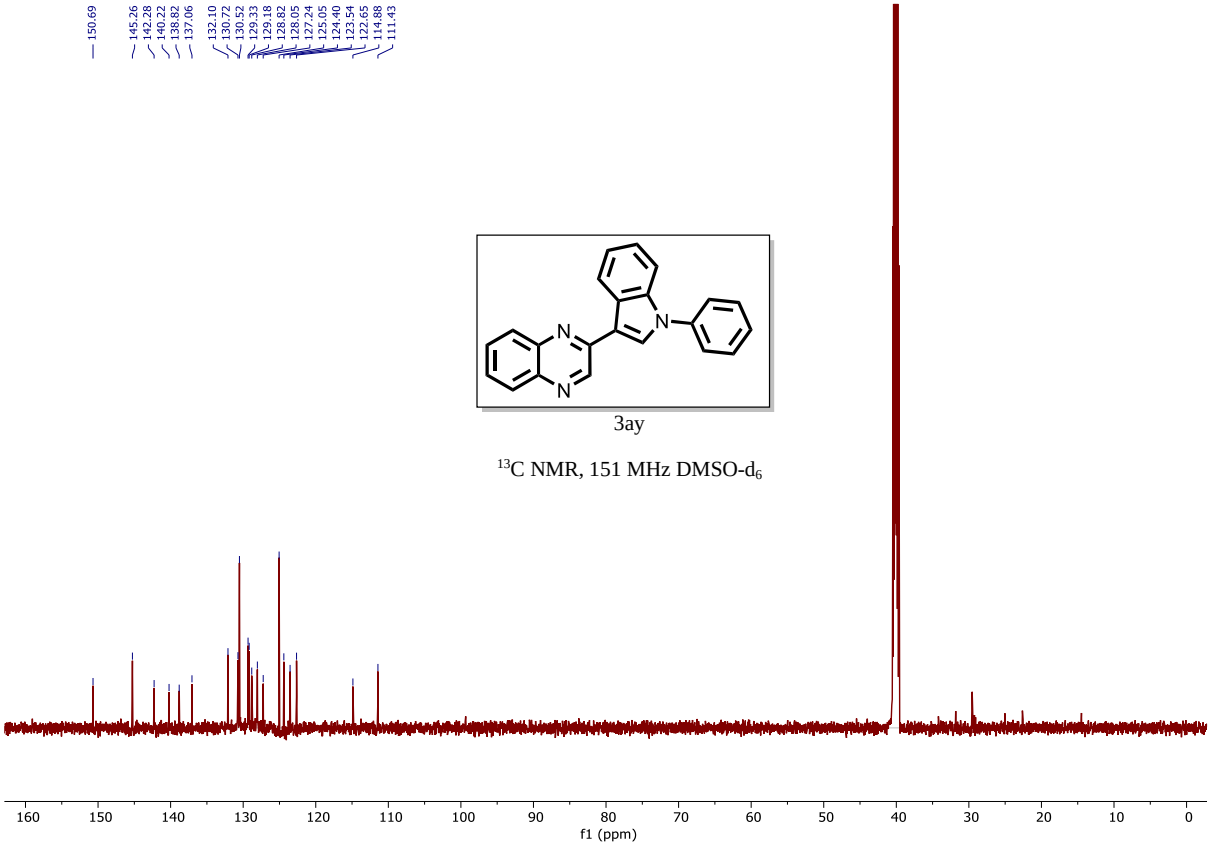
3ax

^{13}C NMR, 151 MHz DMSO-d_6

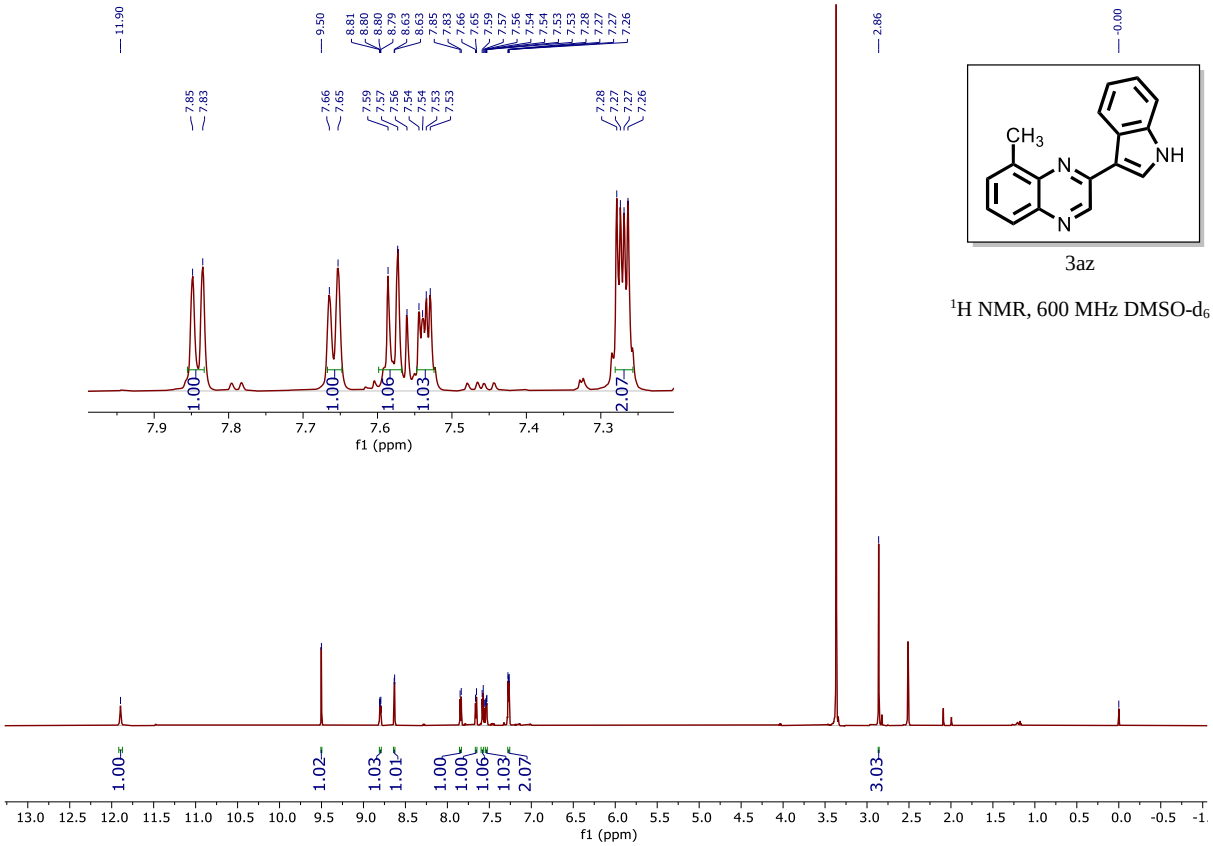
^{13}C NMR of 3ax



^{1}H NMR of 3ay



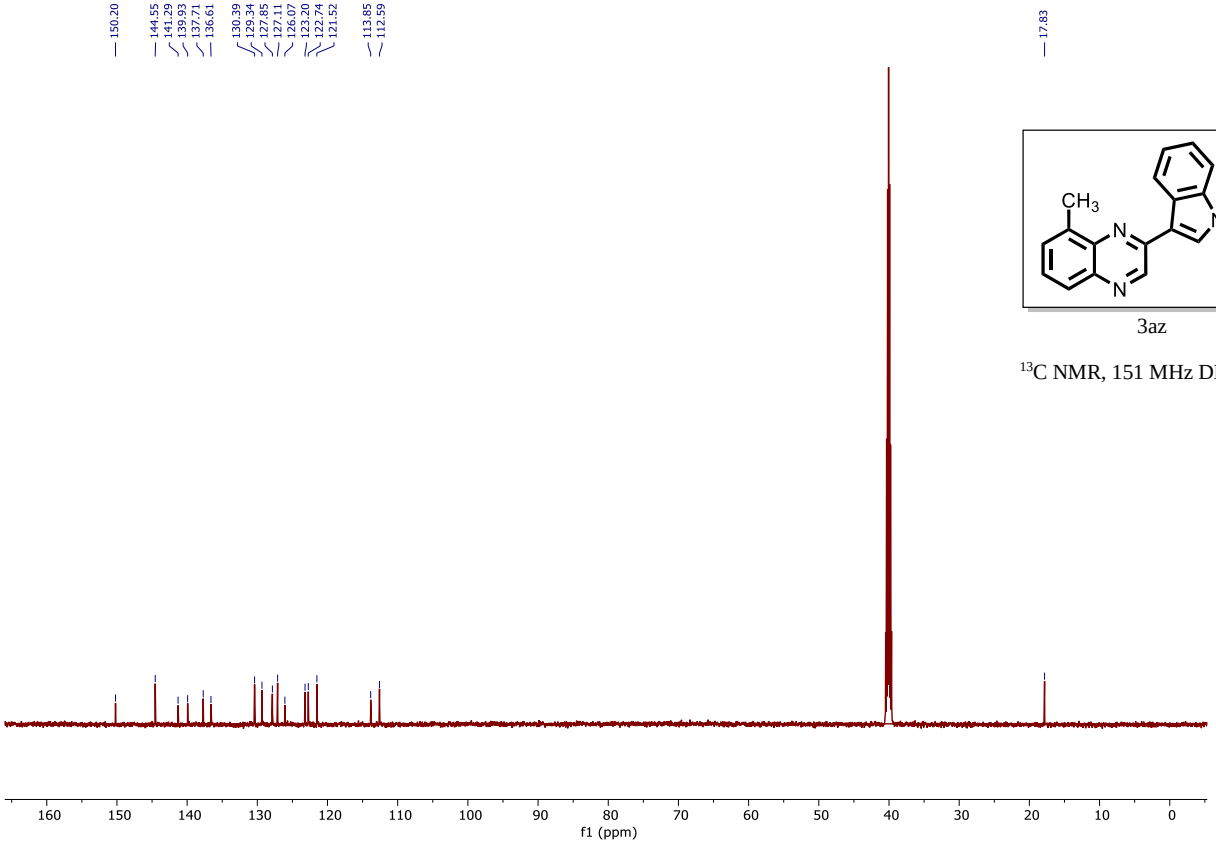
^{13}C NMR of 3ay



3az

^{1}H NMR, 600 MHz DMSO-d_6

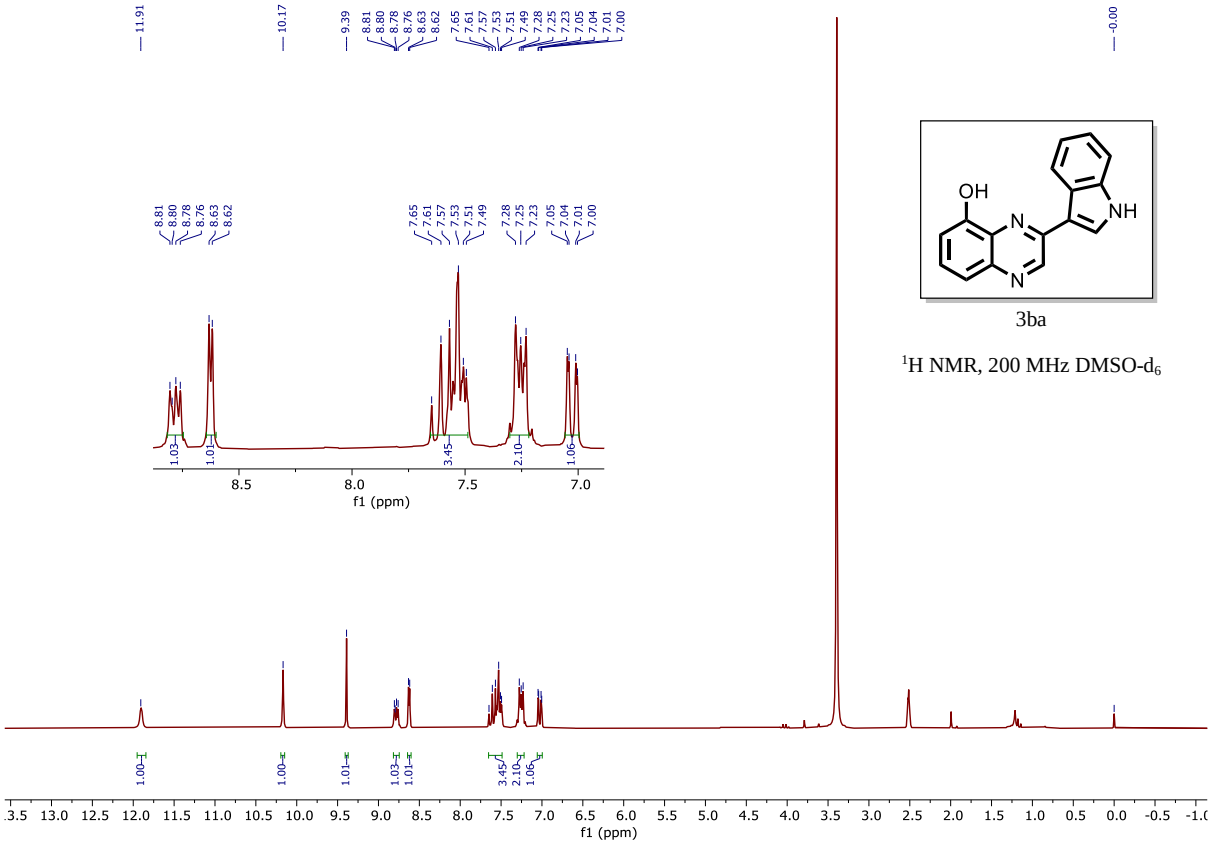
^{1}H NMR of 3az



3az

^{13}C NMR, 151 MHz DMSO-d_6

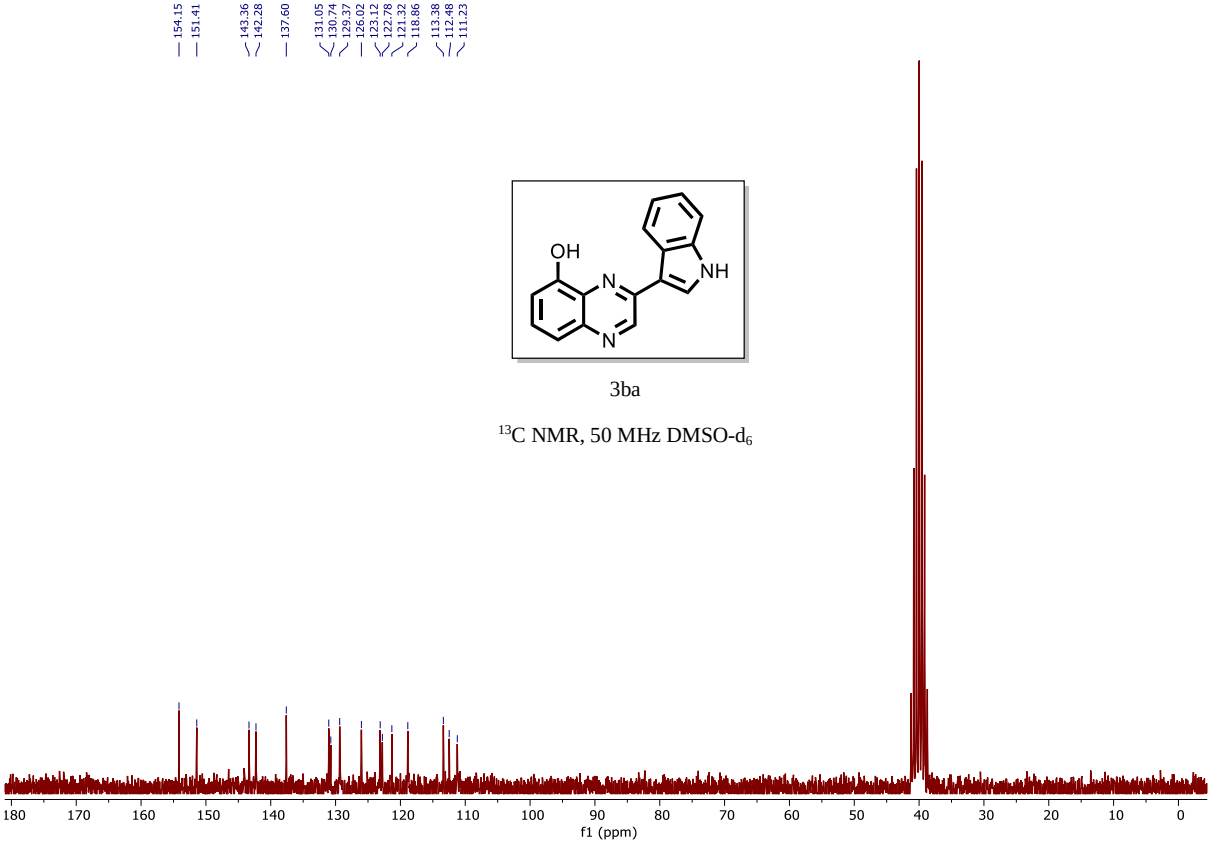
^{13}C NMR of 3az



3ba

^{1}H NMR, 200 MHz DMSO-d_6

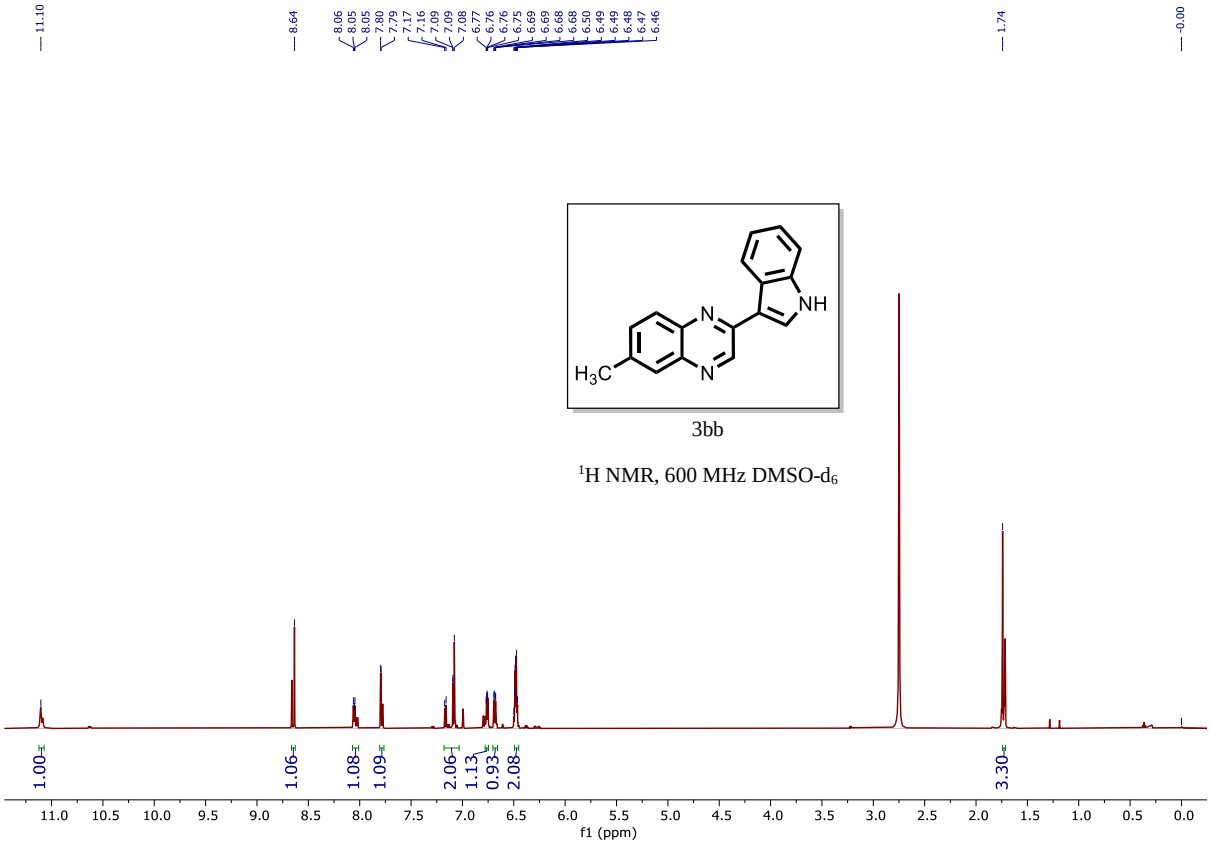
^{1}H NMR of 3ba



3ba

^{13}C NMR, 50 MHz DMSO-d_6

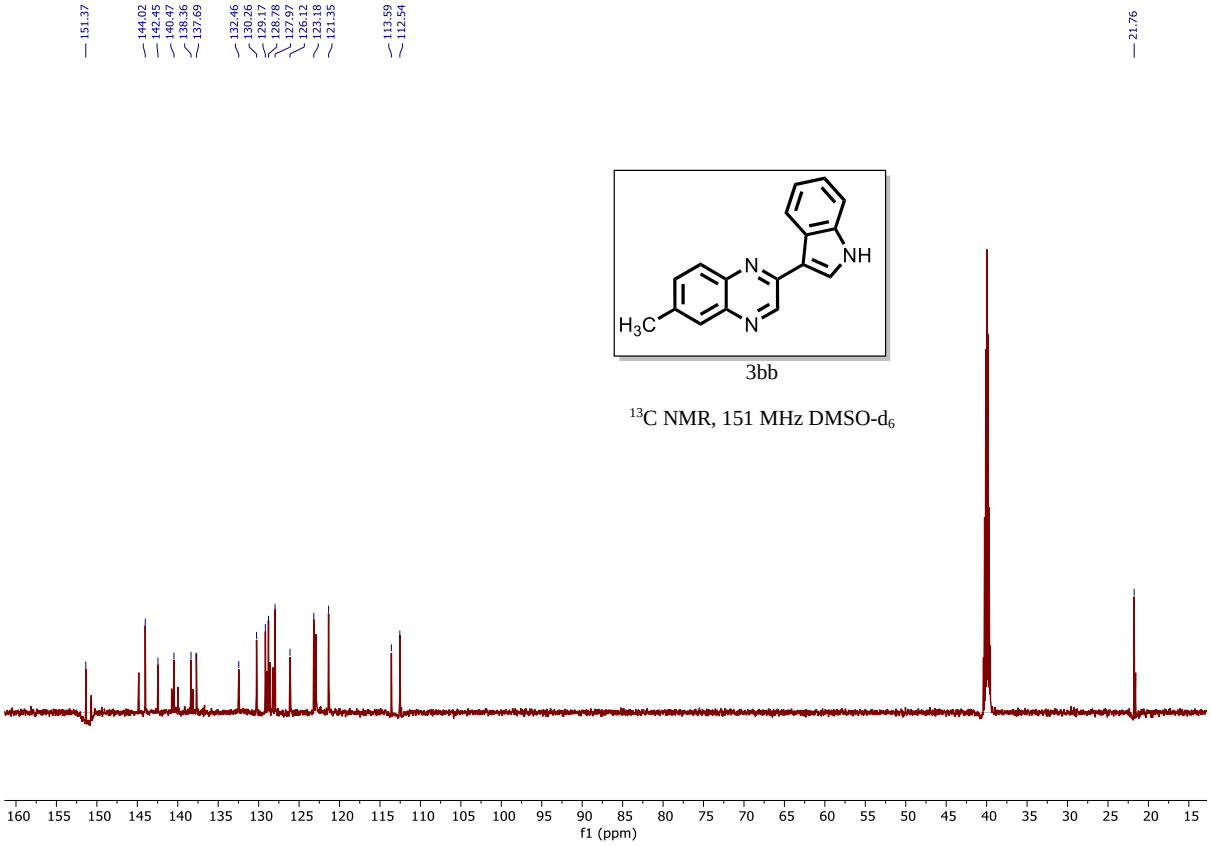
^{13}C NMR of 3ba



3bb

^{1}H NMR, 600 MHz DMSO-d_6

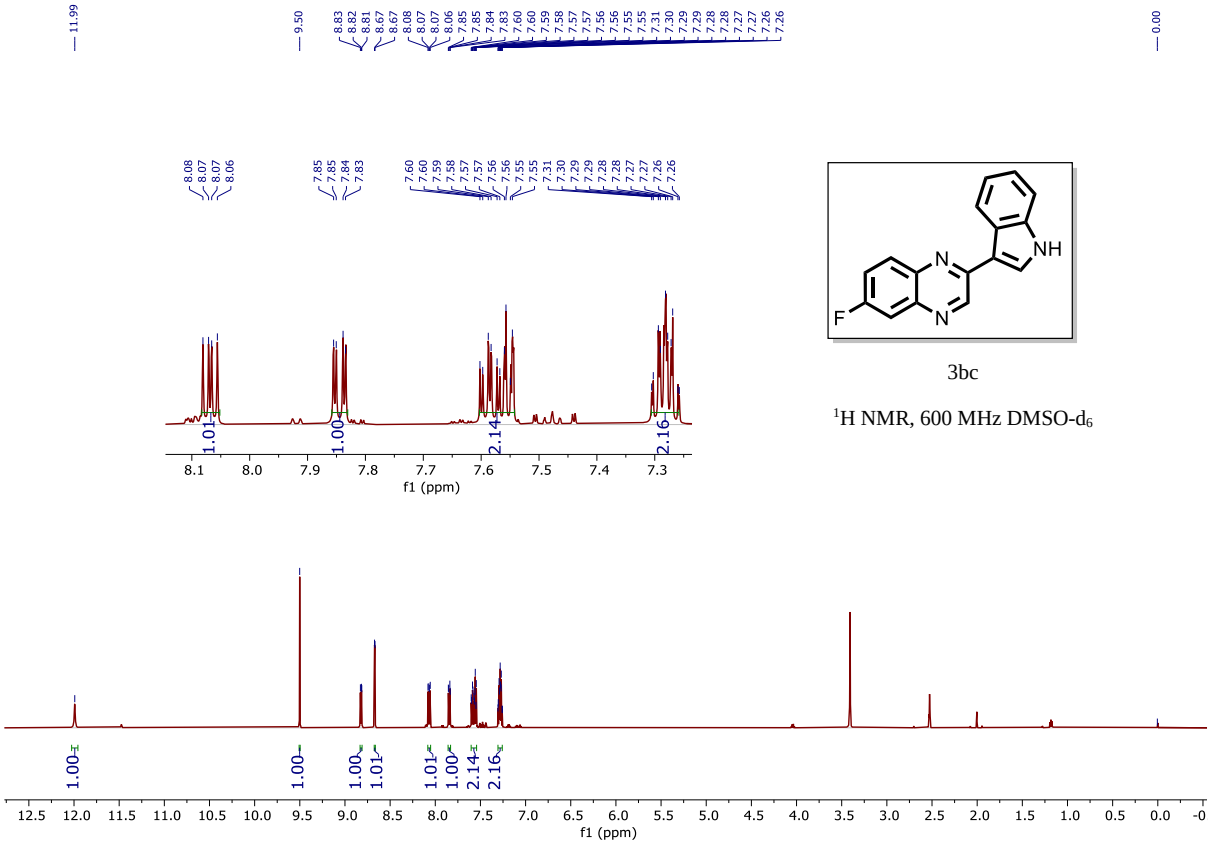
^{1}H NMR of 3bb



3bb

^{13}C NMR, 151 MHz DMSO-d_6

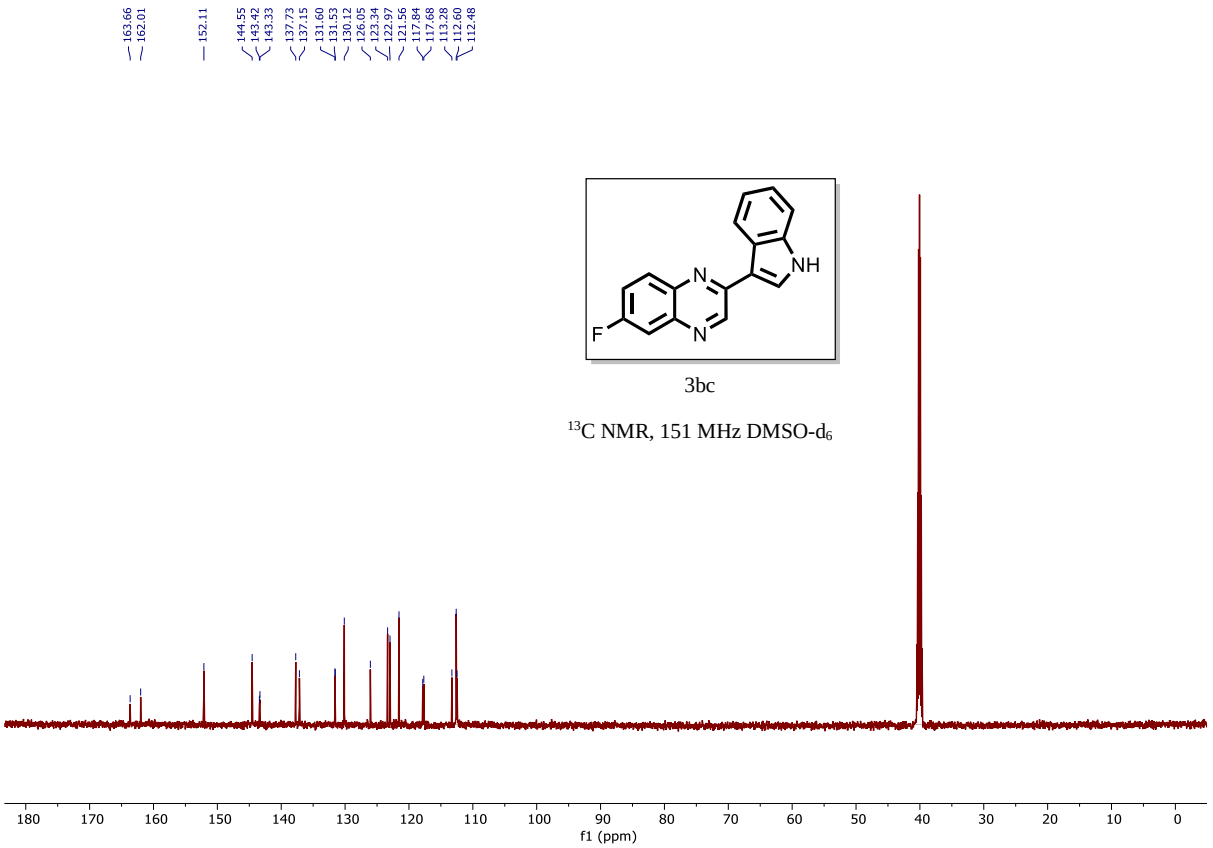
^{13}C NMR of 3bb



3bc

^{1}H NMR, 600 MHz DMSO-d_6

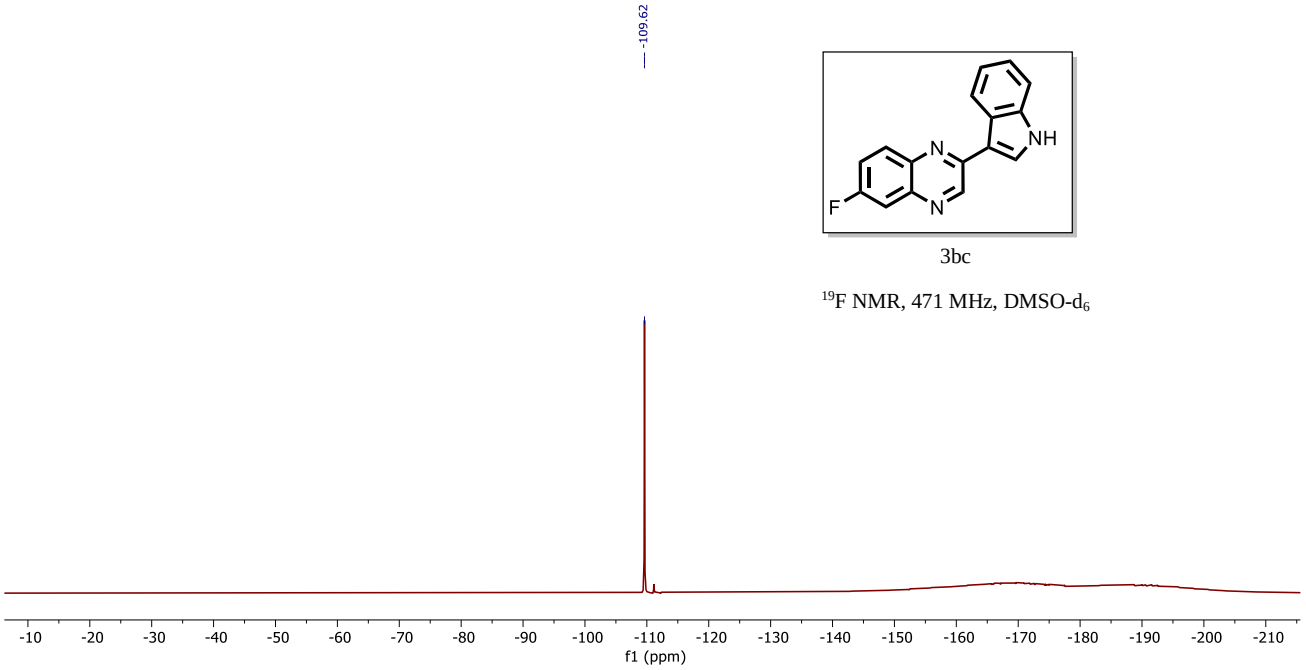
^{1}H NMR of 3bc



3bc

^{13}C NMR, 151 MHz DMSO-d_6

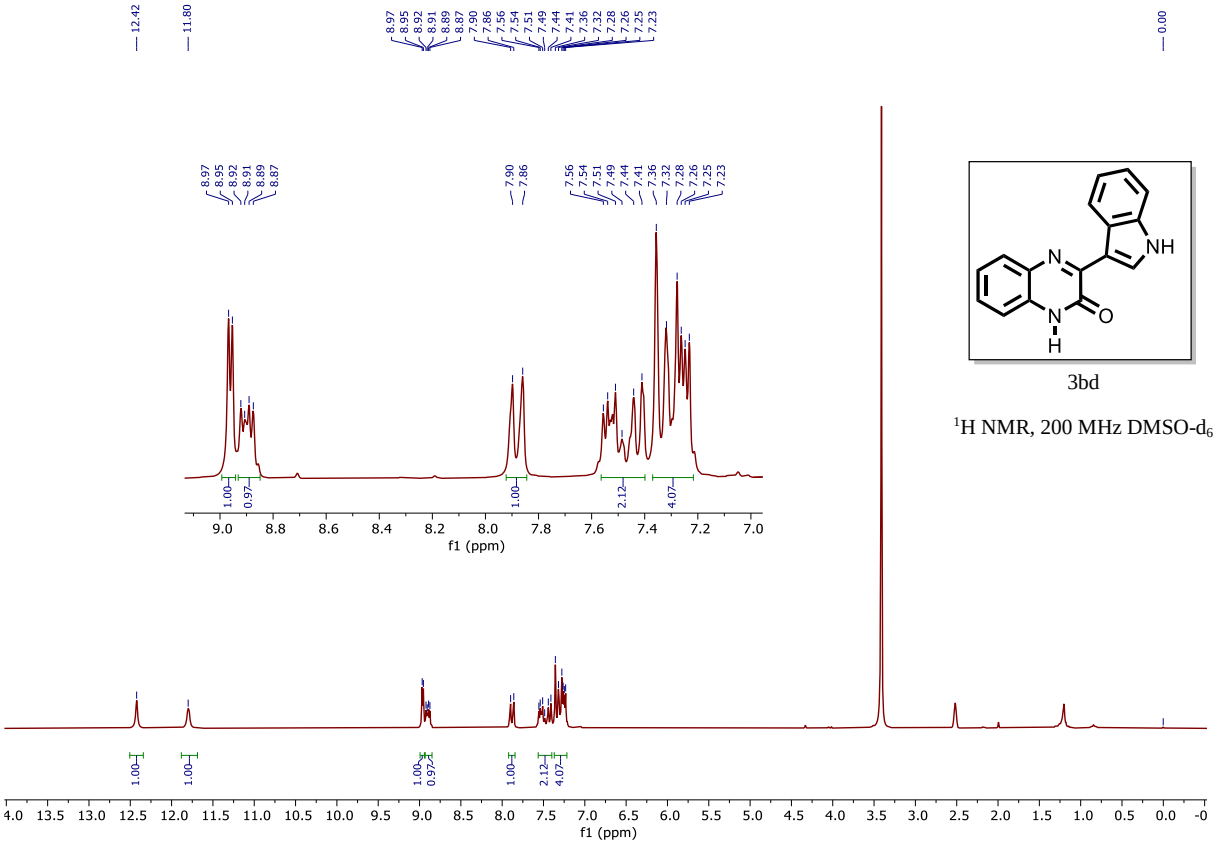
^{13}C NMR of 3bc



3bc

^{19}F NMR, 471 MHz, DMSO-d_6

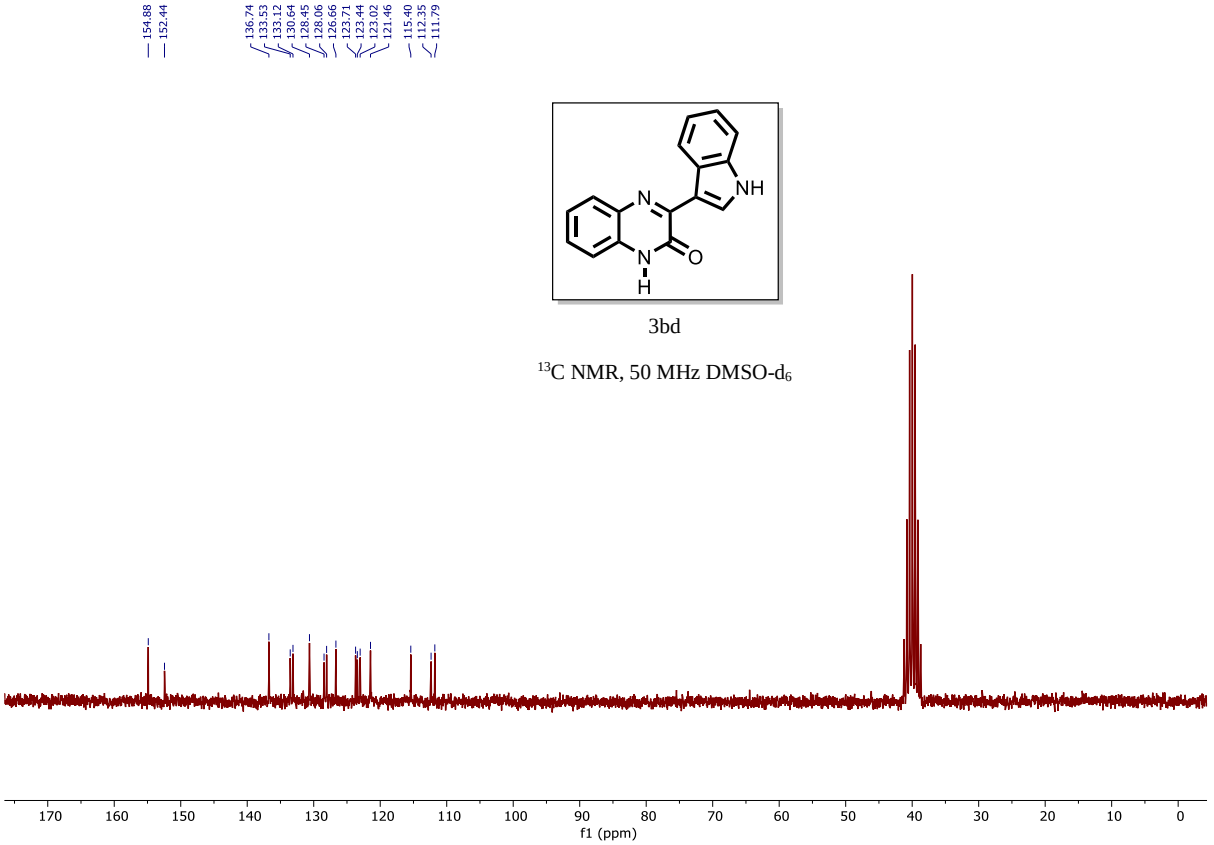
^{19}F NMR of 3bc



3bd

^{1}H NMR, 200 MHz DMSO-d_6

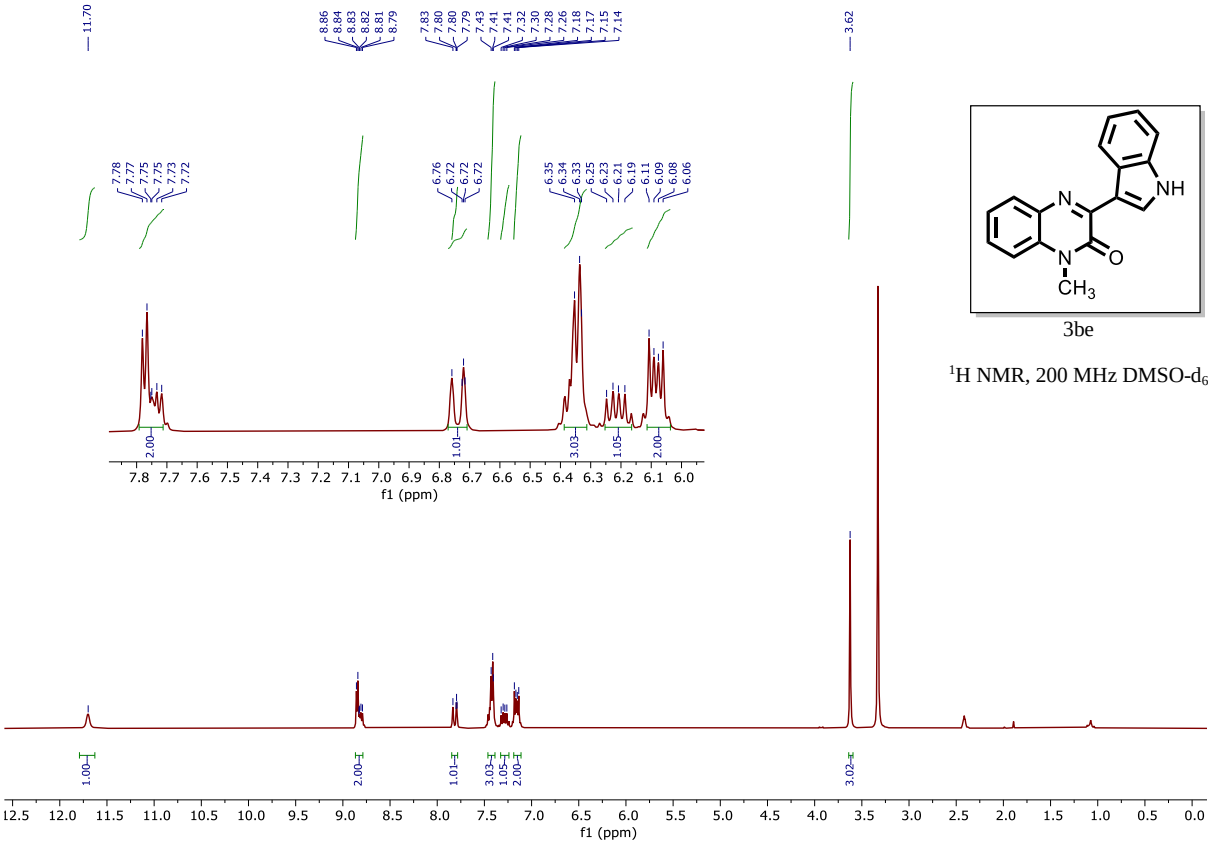
^{1}H NMR of 3bd



3bd

^{13}C NMR, 50 MHz DMSO-d_6

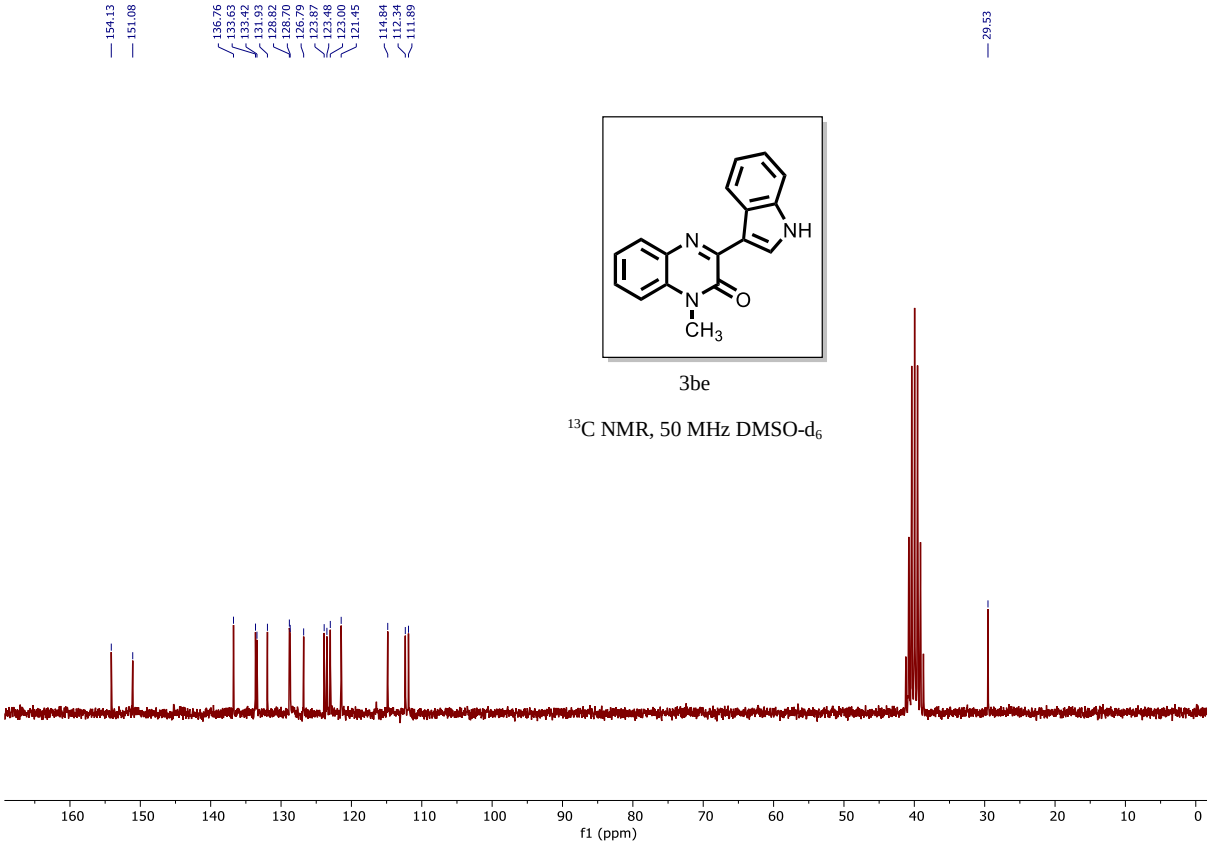
^{13}C NMR of 3bd



3be

^{1}H NMR, 200 MHz DMSO-d_6

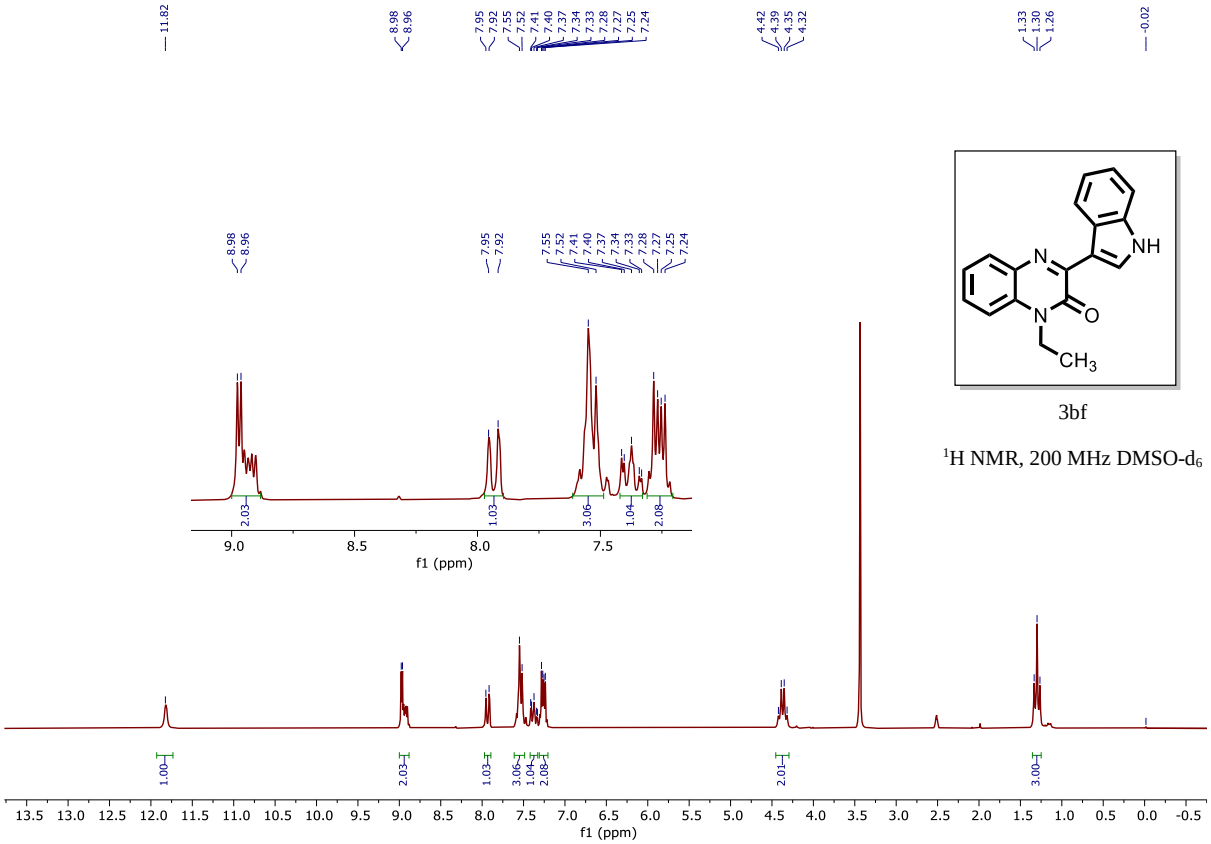
^{1}H NMR of 3be



3be

^{13}C NMR, 50 MHz DMSO-d_6

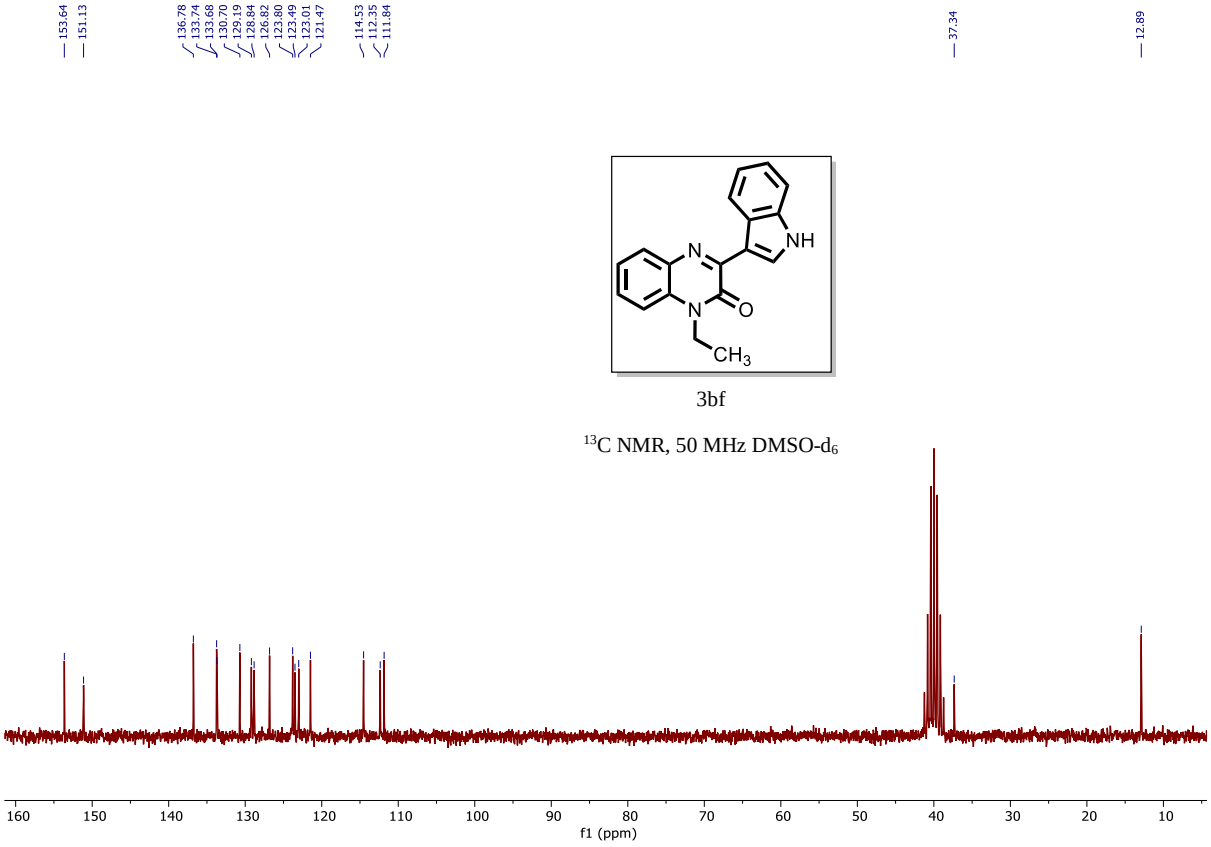
^{13}C NMR of 3be



3bf

^{1}H NMR, 200 MHz DMSO-d_6

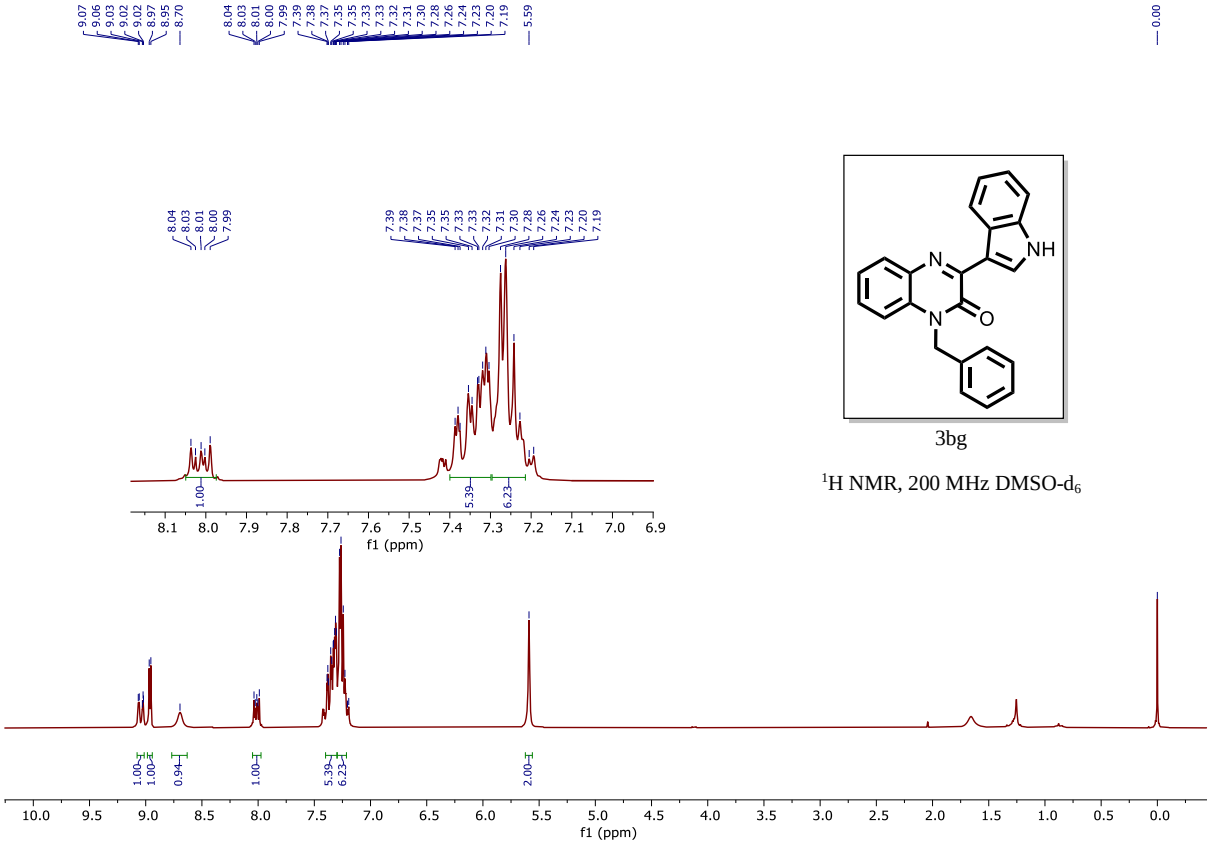
^{1}H NMR of 3bf



3bf

^{13}C NMR, 50 MHz DMSO-d_6

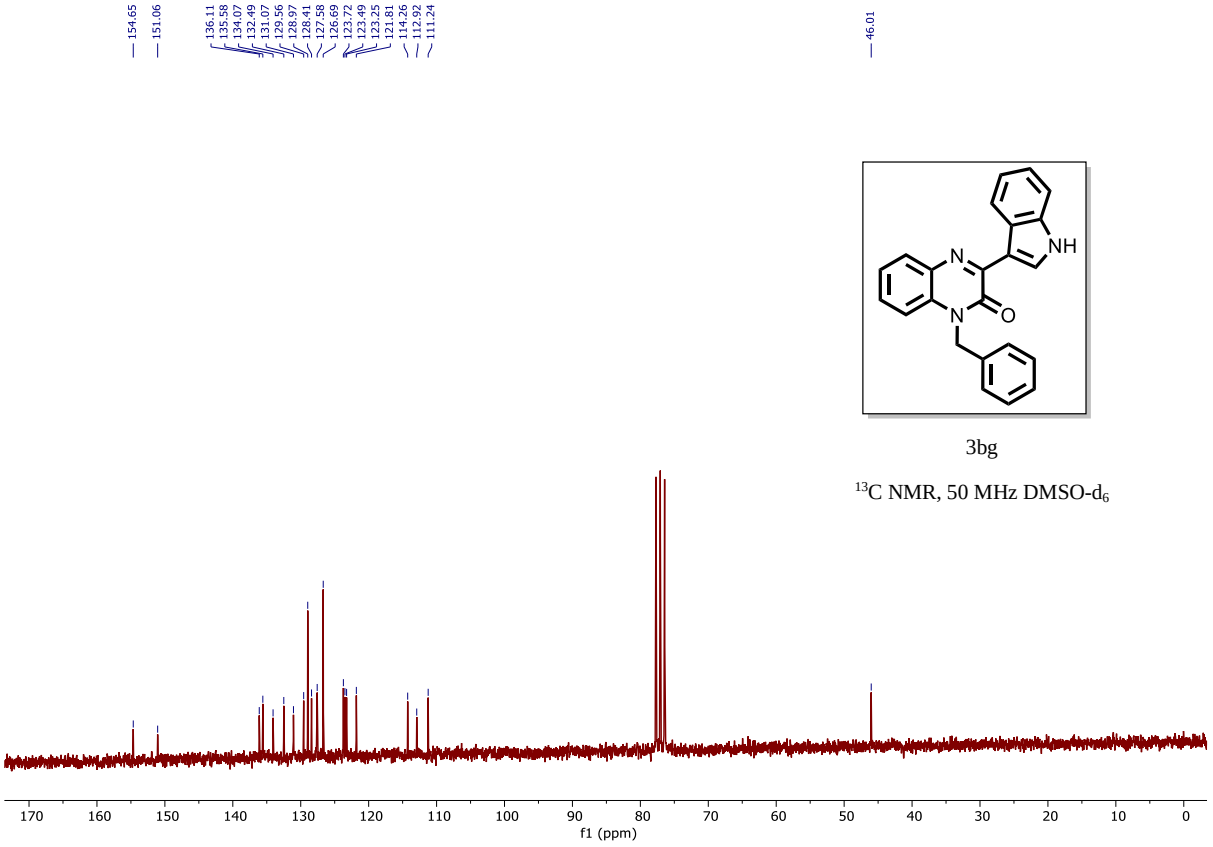
^{13}C NMR of 3bf



3bg

^{1}H NMR, 200 MHz DMSO-d_6

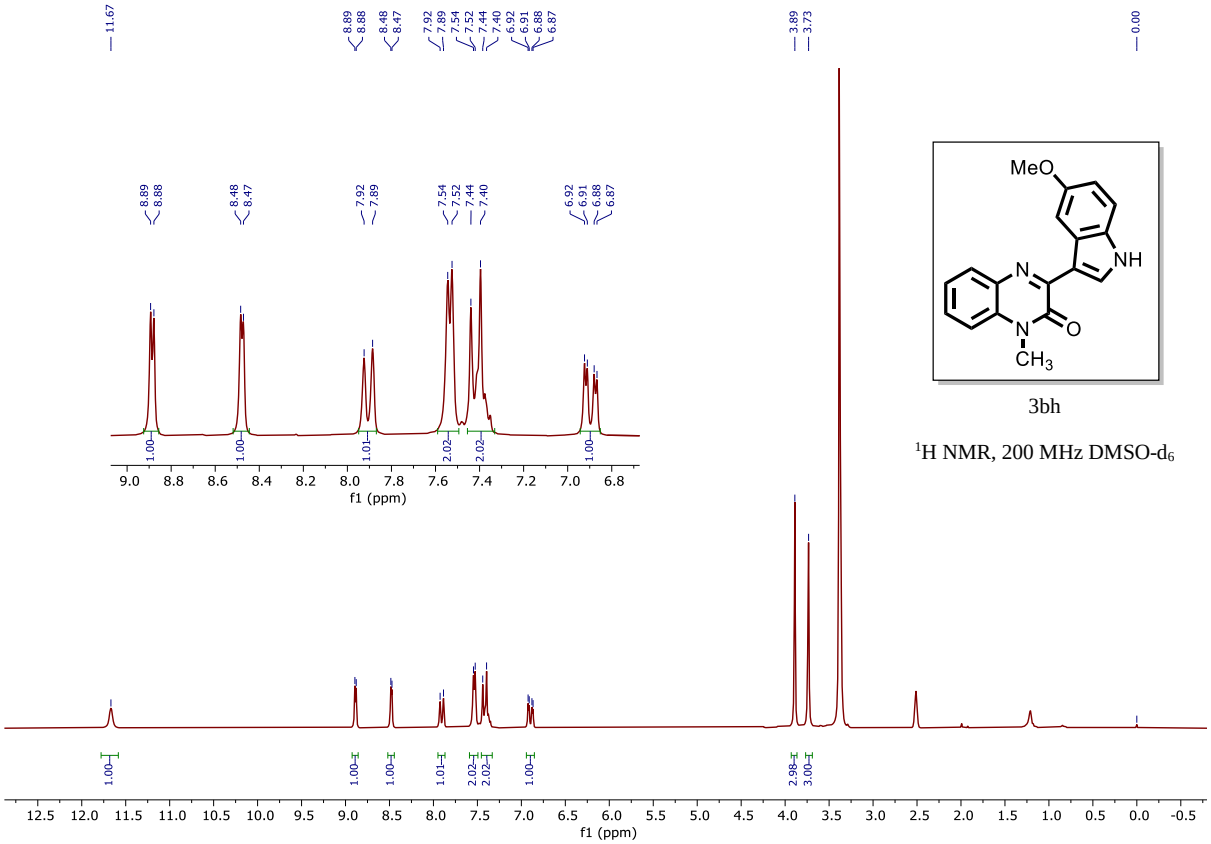
^{1}H NMR of 3bg



3bg

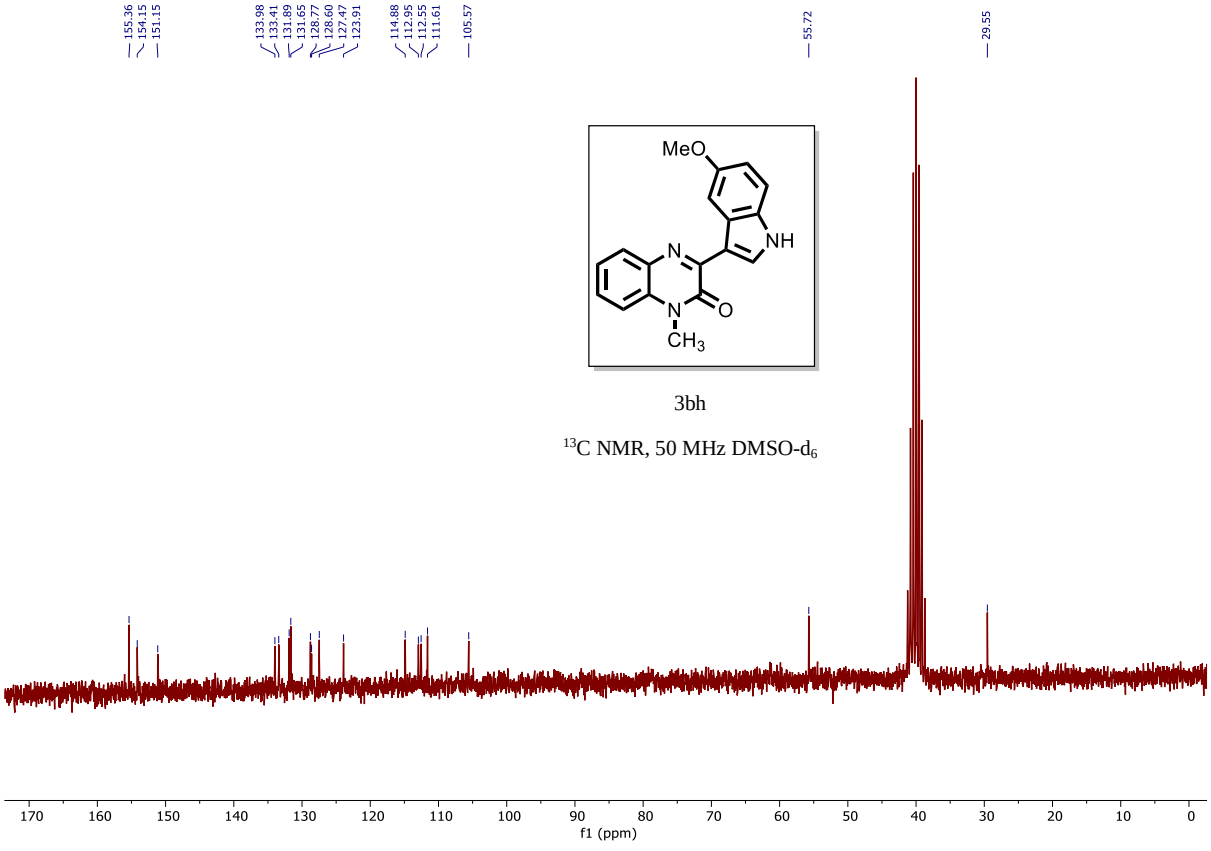
^{13}C NMR, 50 MHz DMSO-d_6

^{13}C NMR of 3bg



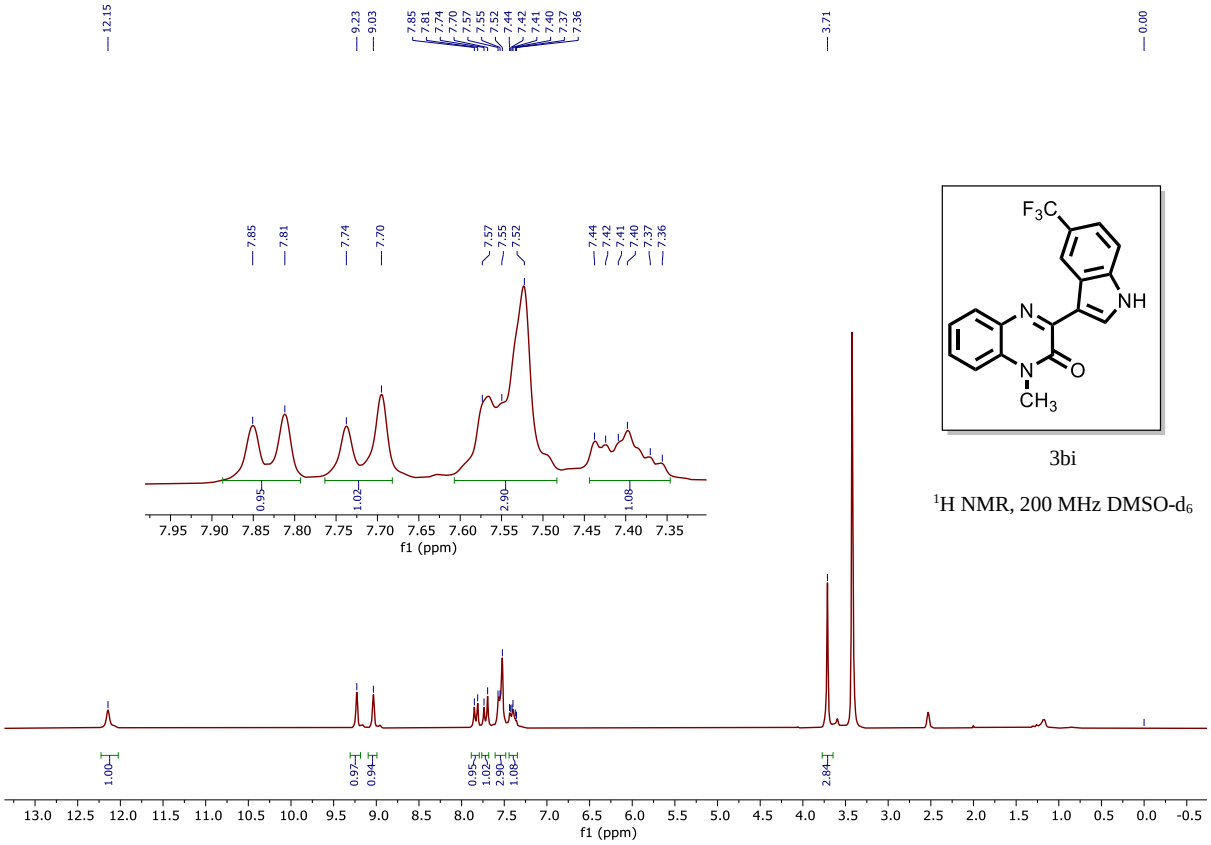
^{1}H NMR, 200 MHz DMSO-d_6

^{1}H NMR of 3bh



^{13}C NMR, 50 MHz DMSO-d_6

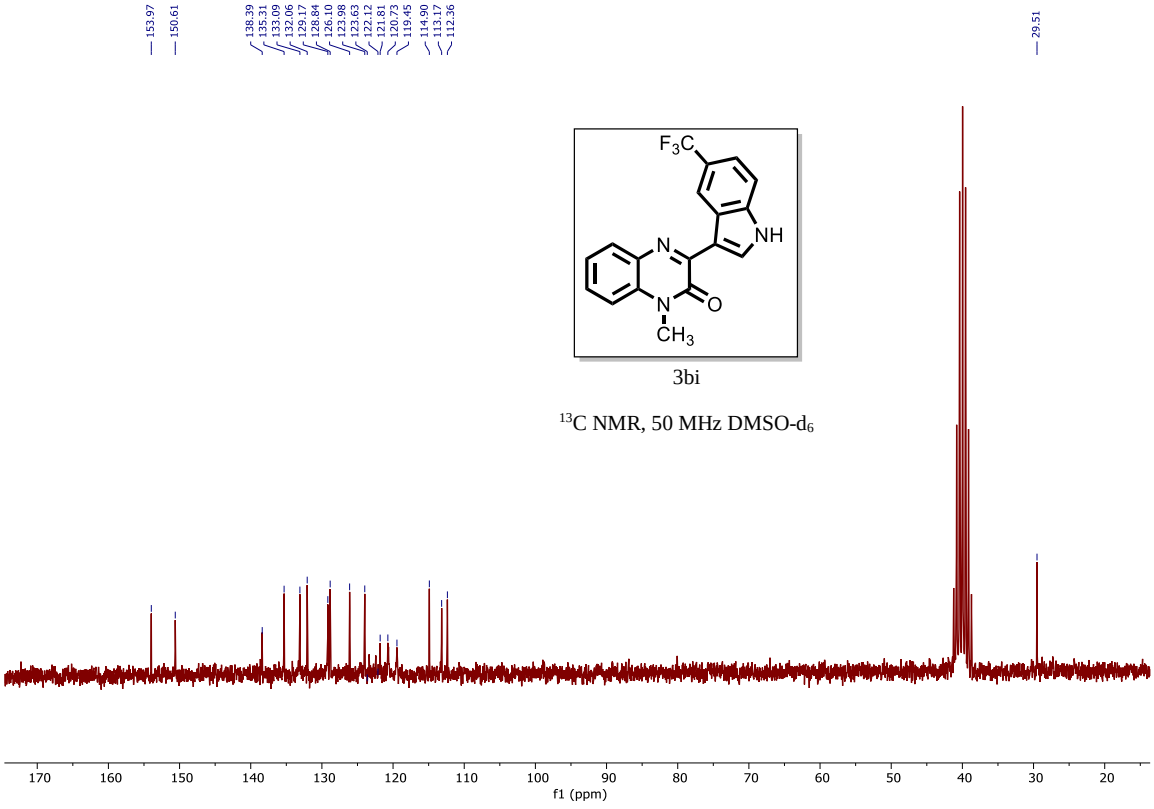
^{13}C NMR of 3bh



3bi

^{1}H NMR, 200 MHz DMSO-d_6

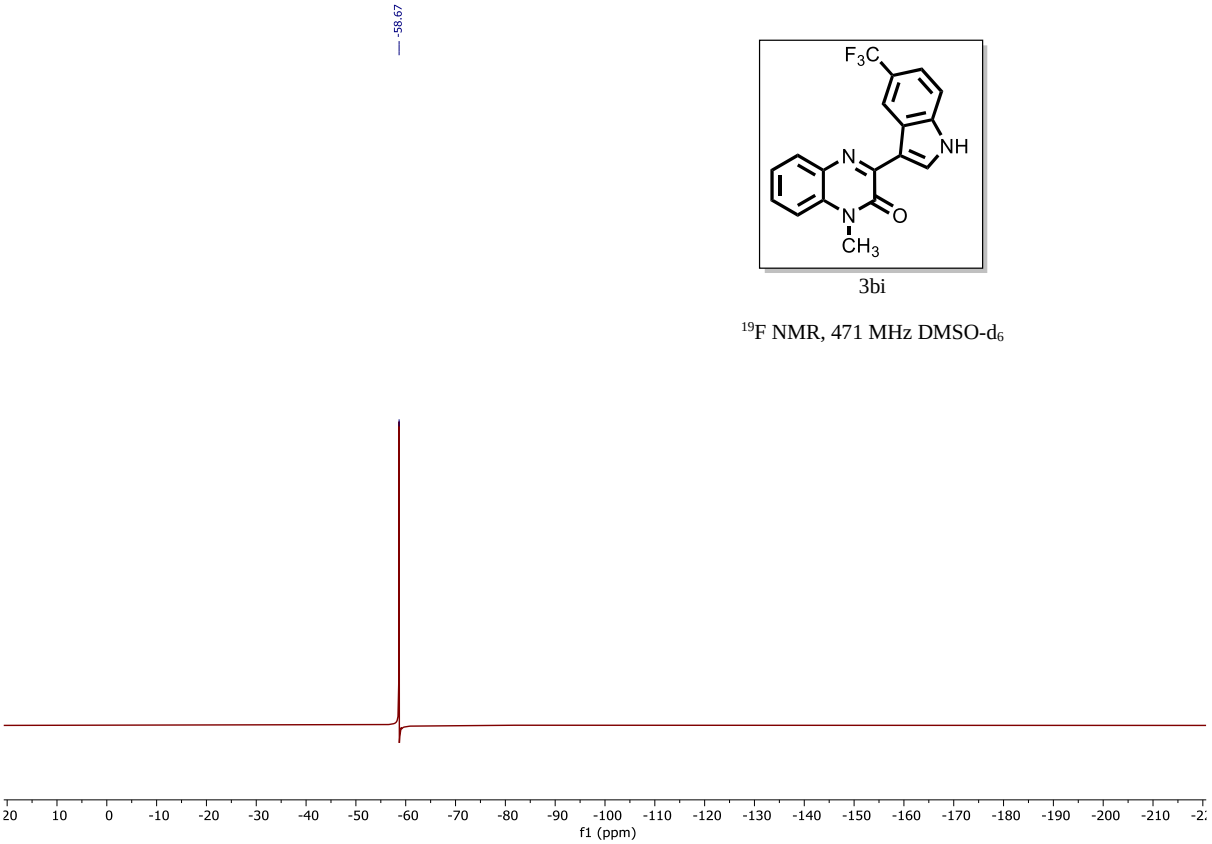
^{1}H NMR of 3bi



3bi

^{13}C NMR, 50 MHz DMSO-d_6

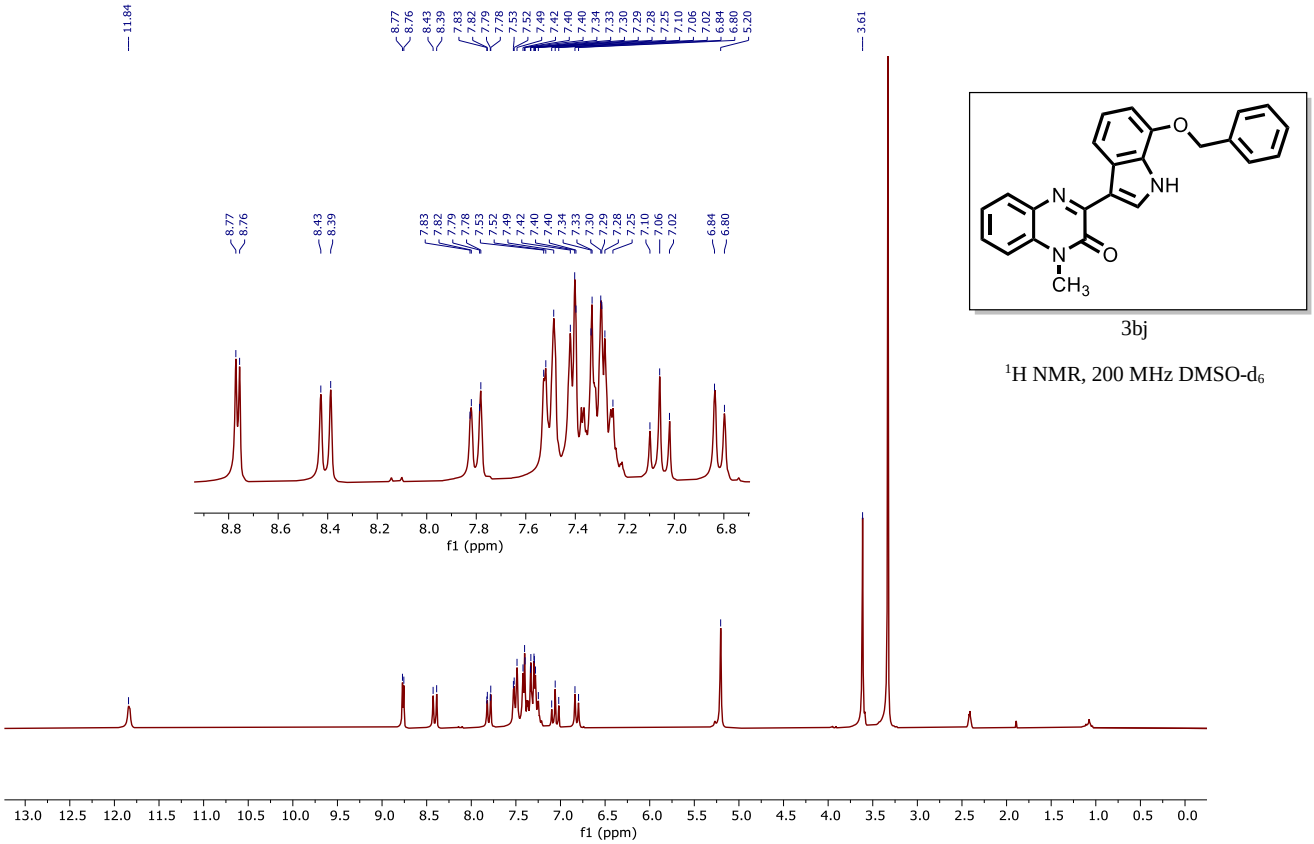
^{13}C NMR of 3bi



3bi

^{19}F NMR, 471 MHz DMSO-d_6

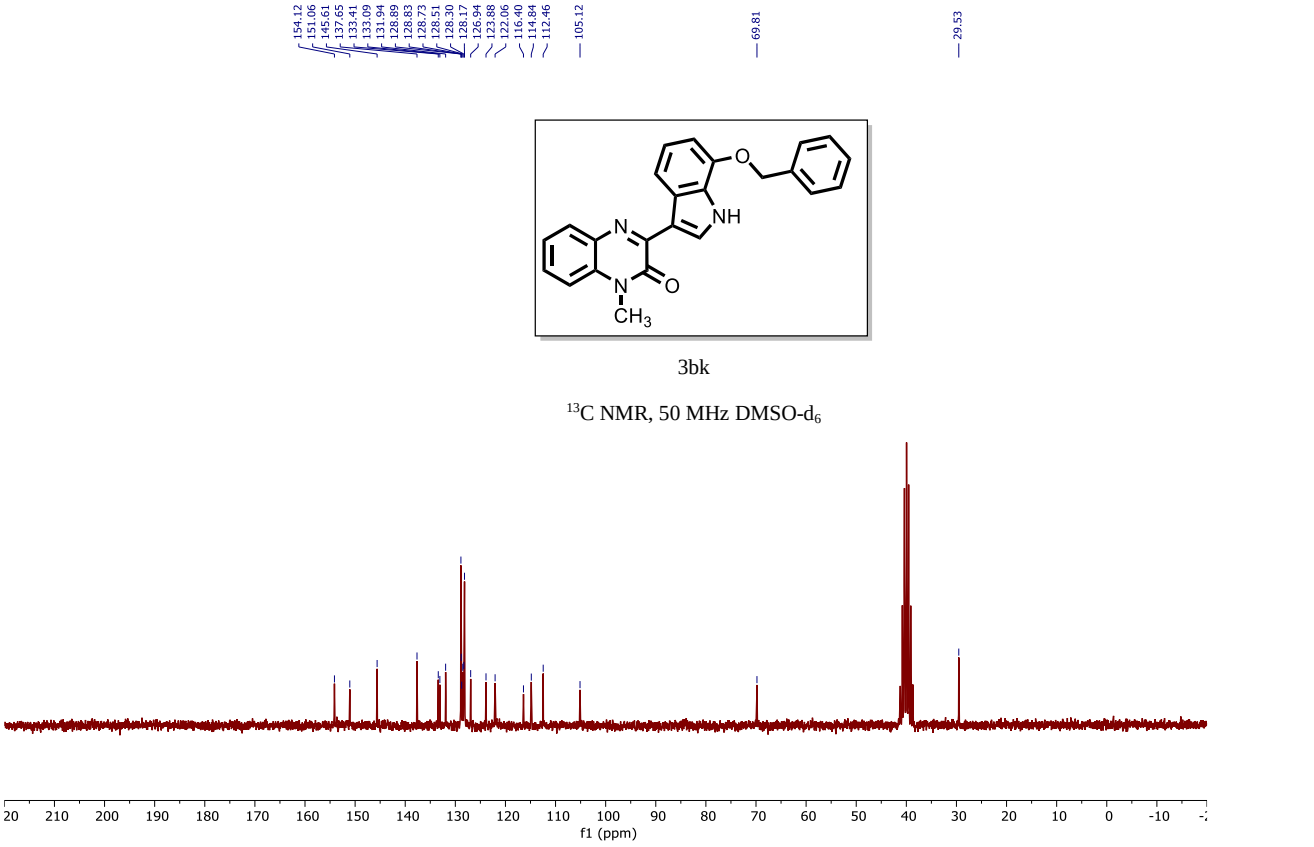
^{19}F NMR of 3bi



3bj

^{1}H NMR, 200 MHz DMSO-d_6

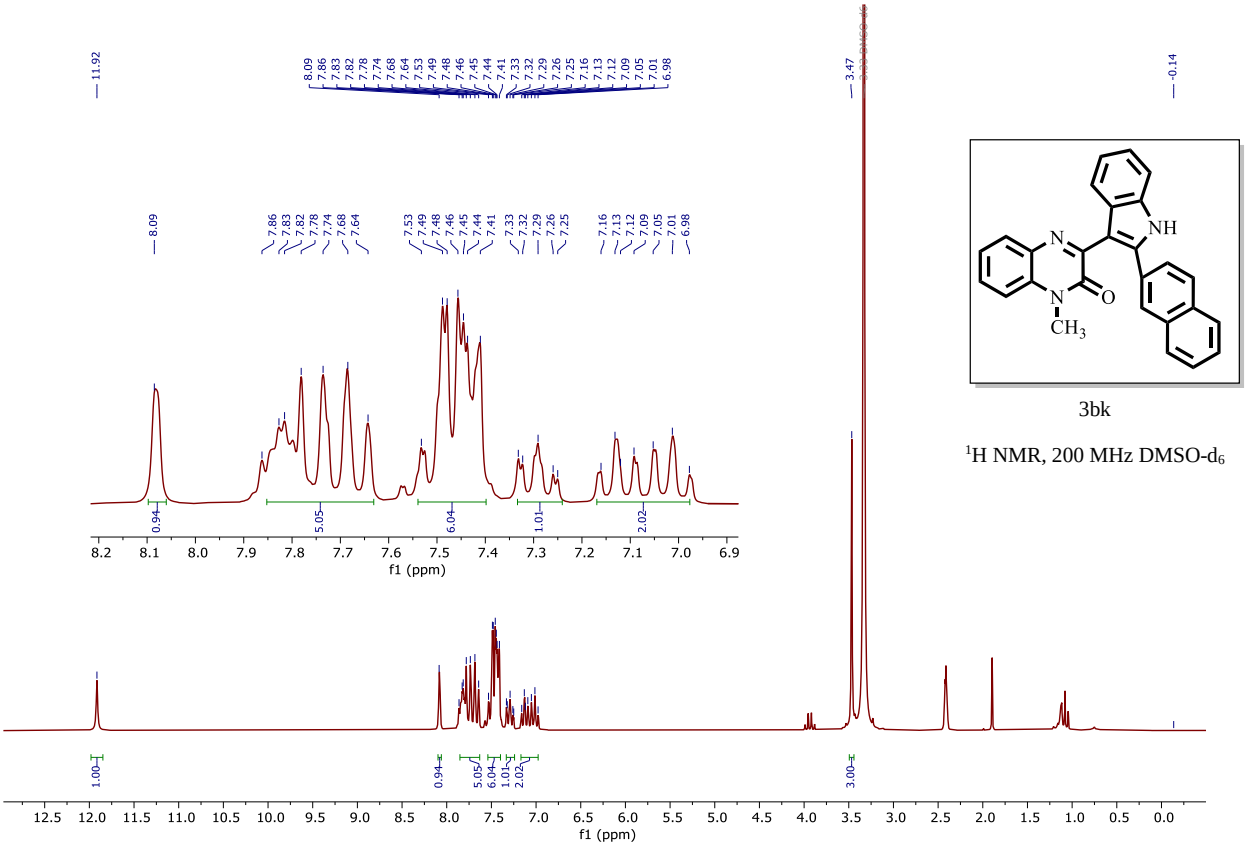
^{1}H NMR of 3bj



3bk

^{13}C NMR, 50 MHz DMSO-d_6

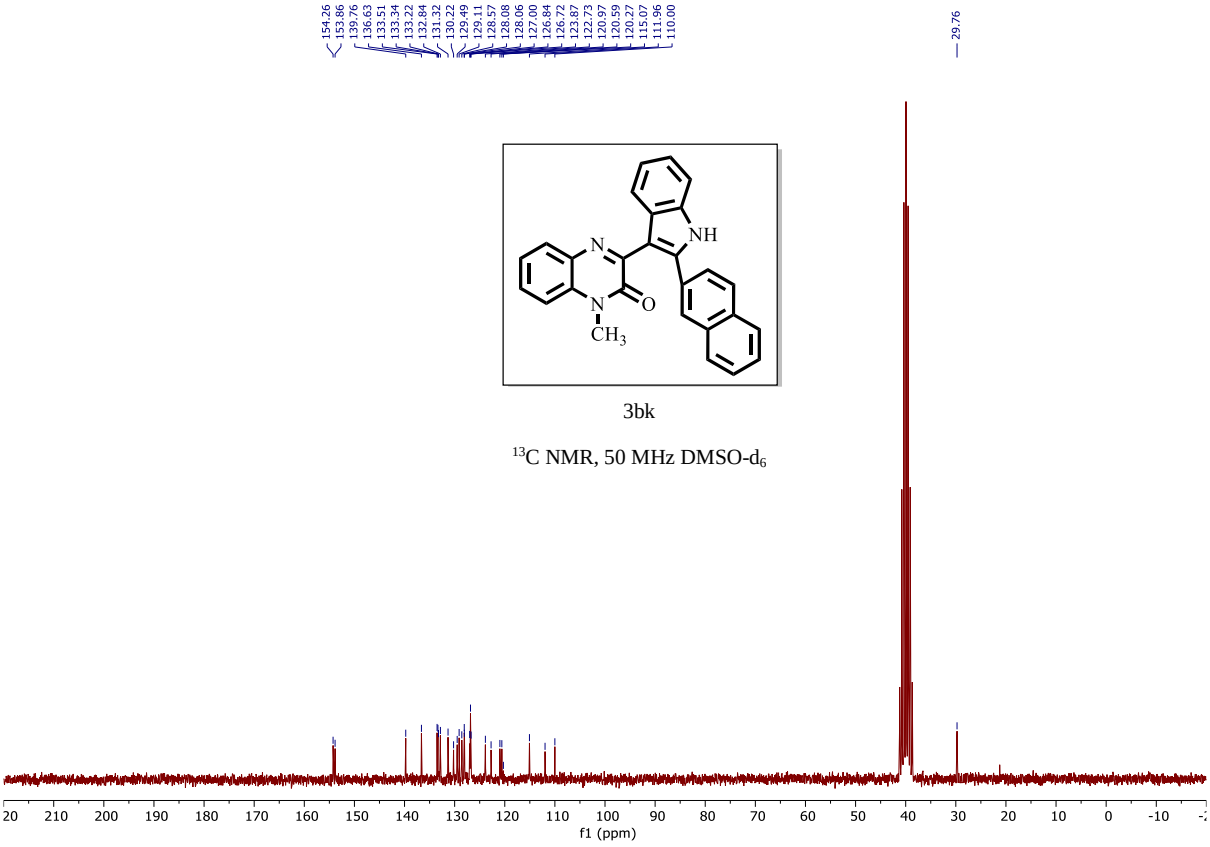
^{13}C NMR of 3bj



3bk

^{1}H NMR, 200 MHz DMSO-d_6

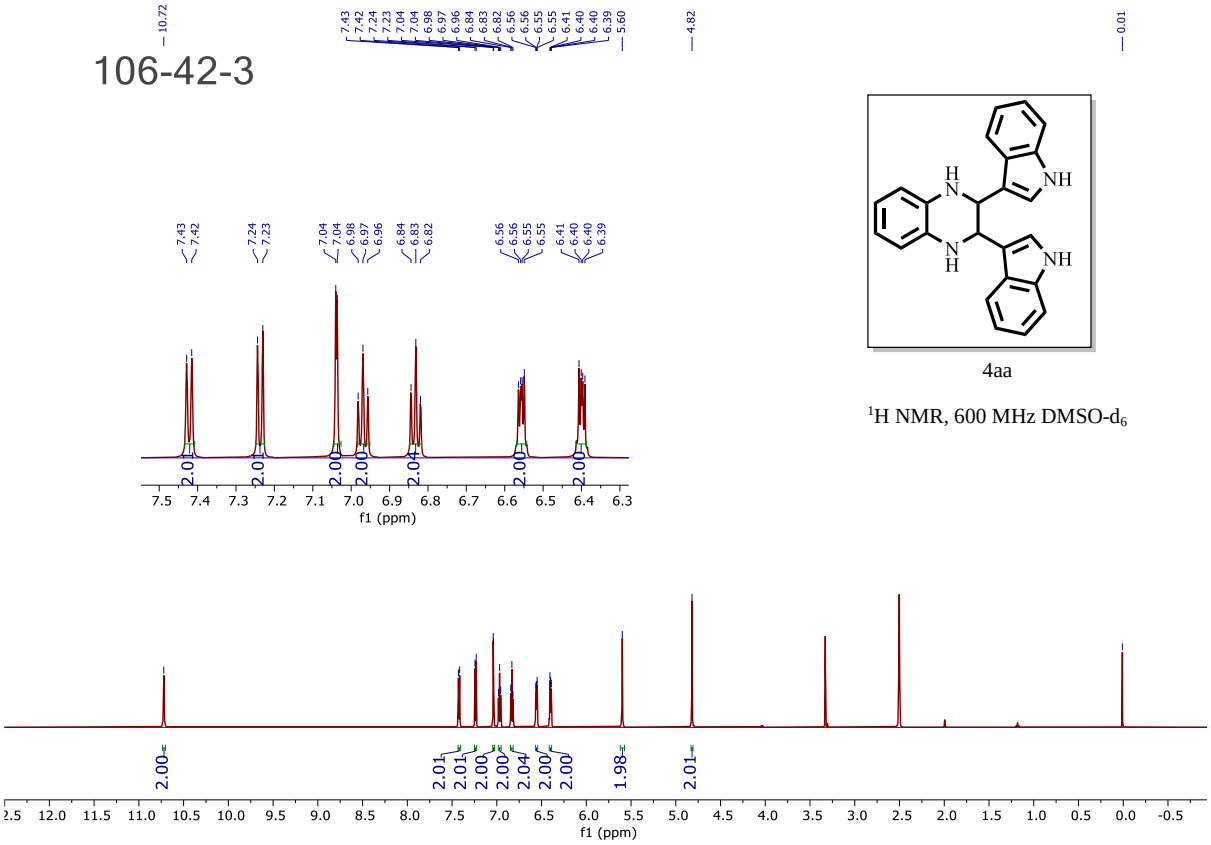
^{1}H NMR of 3bk



3bk

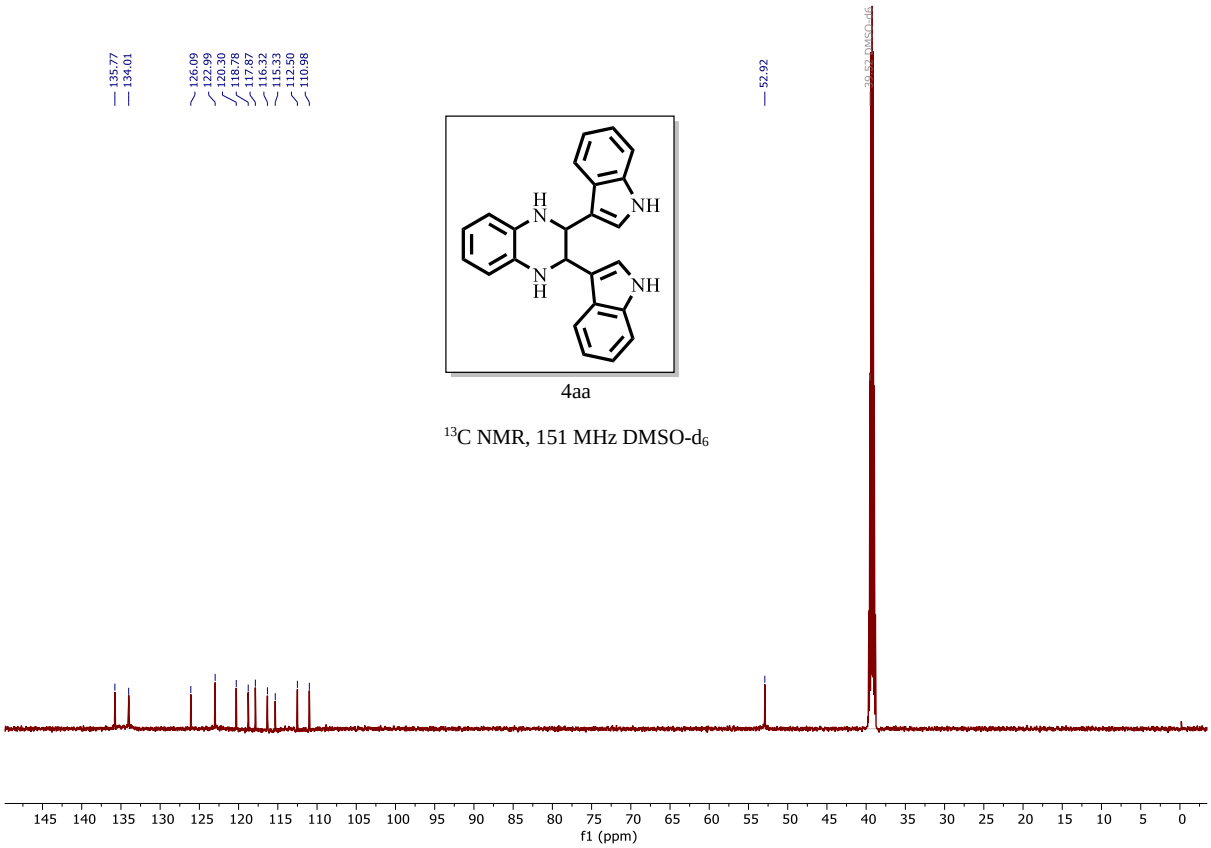
^{13}C NMR, 50 MHz DMSO-d_6

^{13}C NMR of 3bk



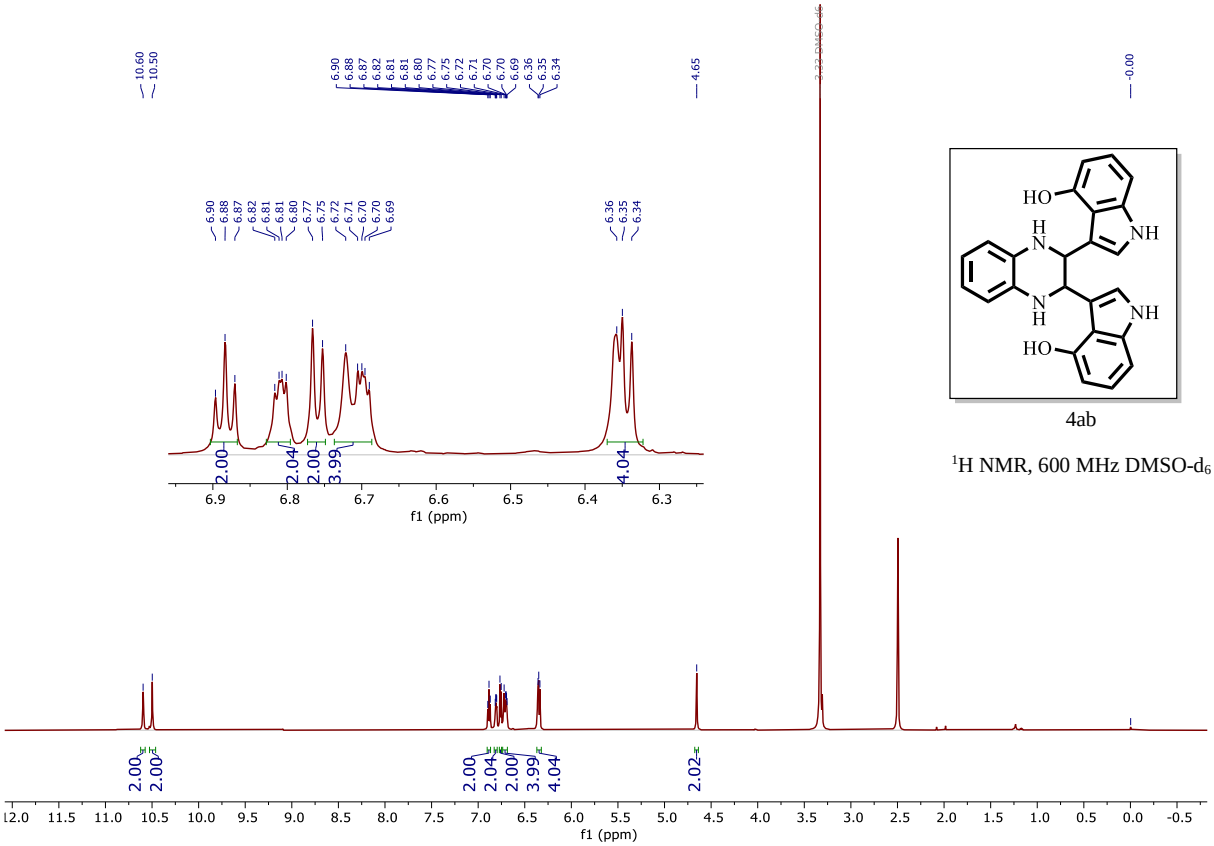
^{1}H NMR, 600 MHz DMSO-d_6

^{1}H NMR of 4aa



^{13}C NMR, 151 MHz DMSO-d_6

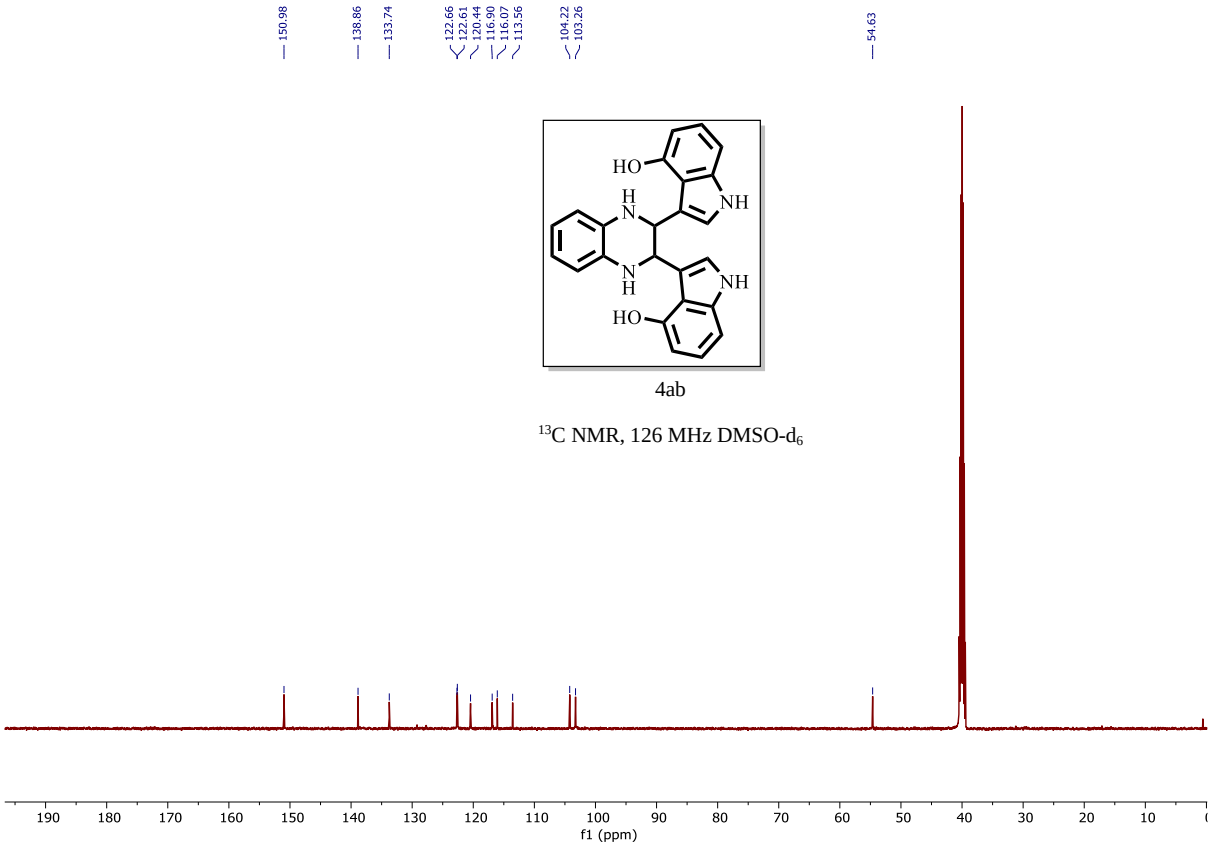
^{13}C NMR of 4aa



4ab

^{1}H NMR, 600 MHz DMSO-d_6

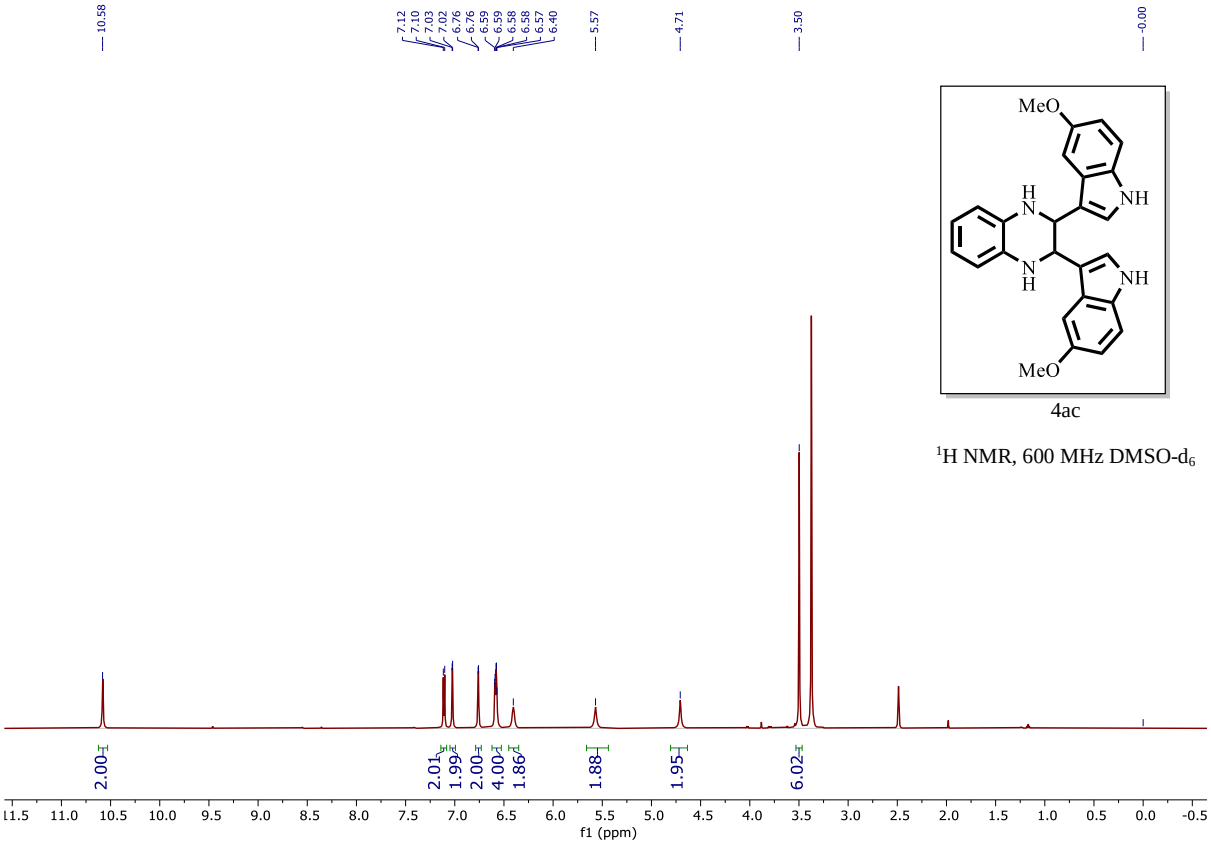
^{1}H NMR of 4ab



4ab

^{13}C NMR, 126 MHz DMSO-d_6

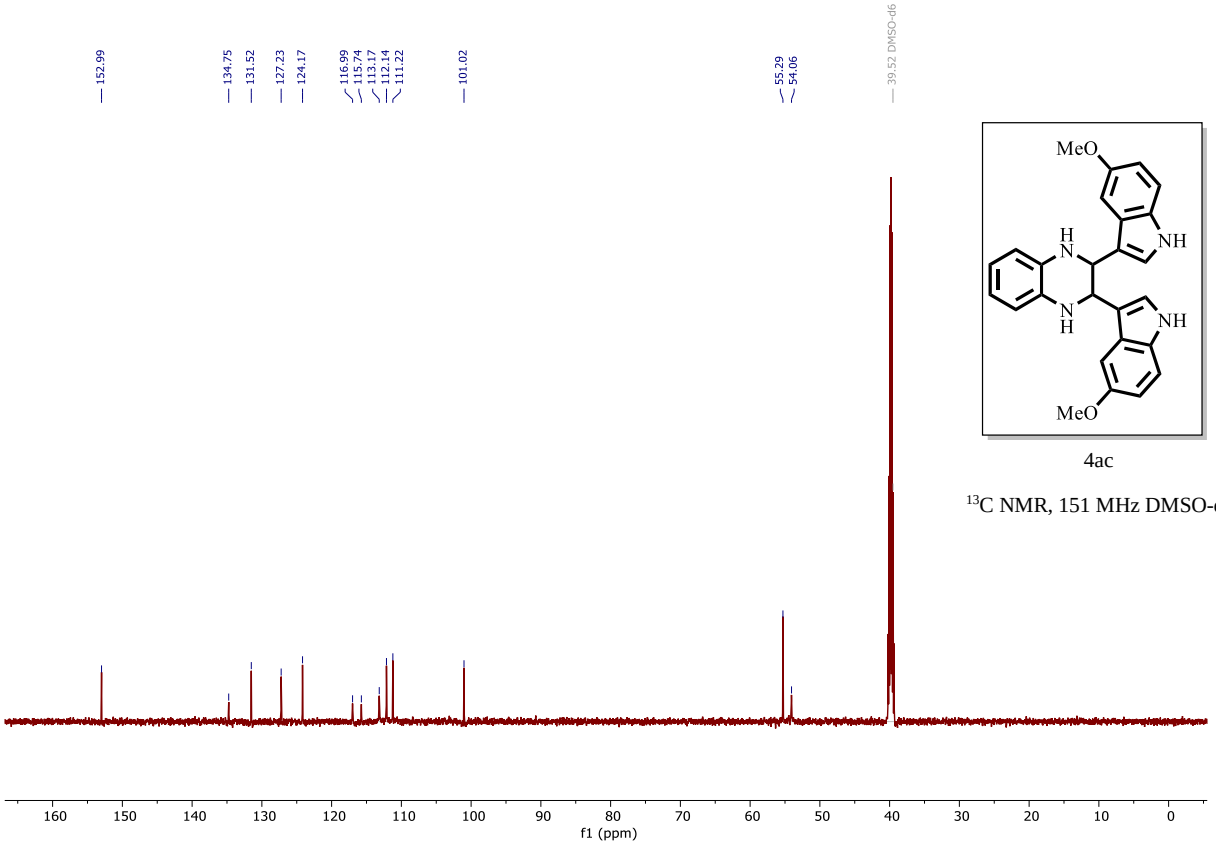
^{13}C NMR of 4ab



4ac

^{1}H NMR, 600 MHz DMSO-d_6

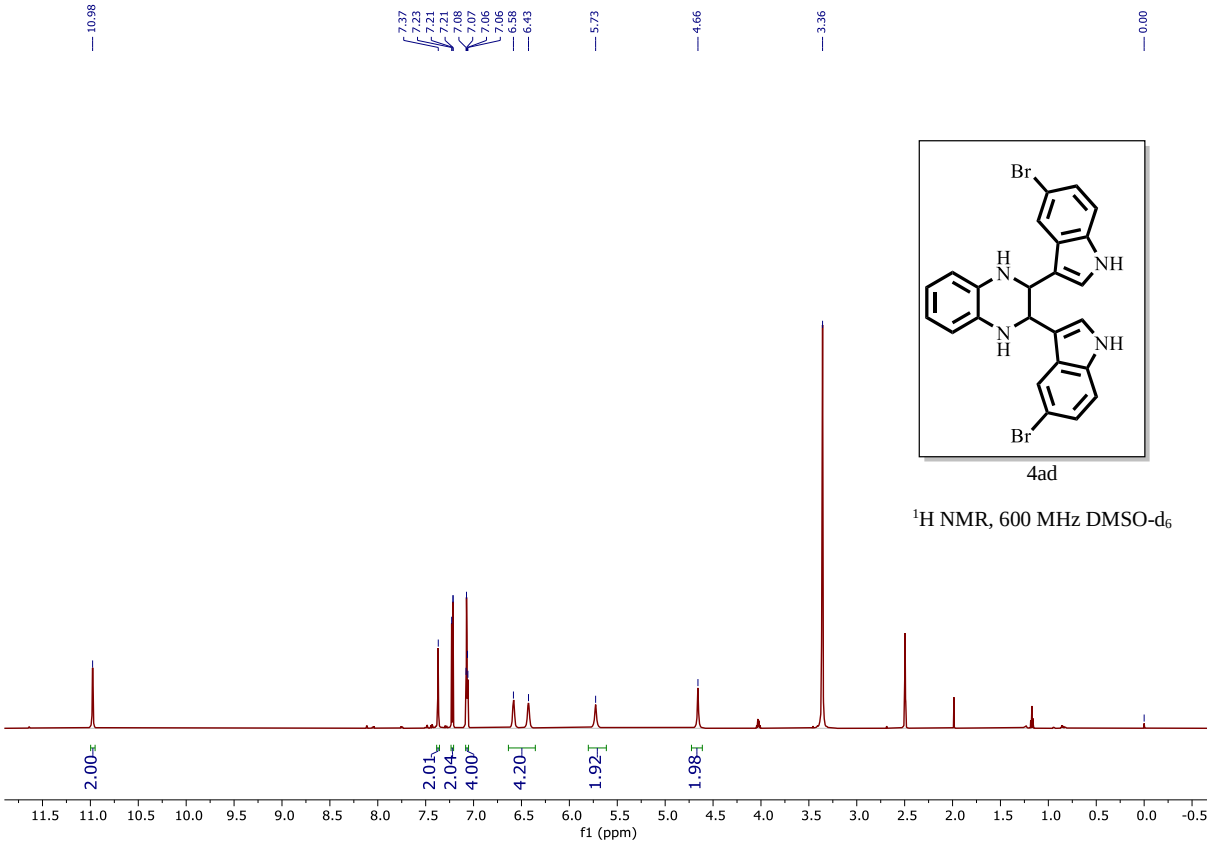
^{1}H NMR of 4ac



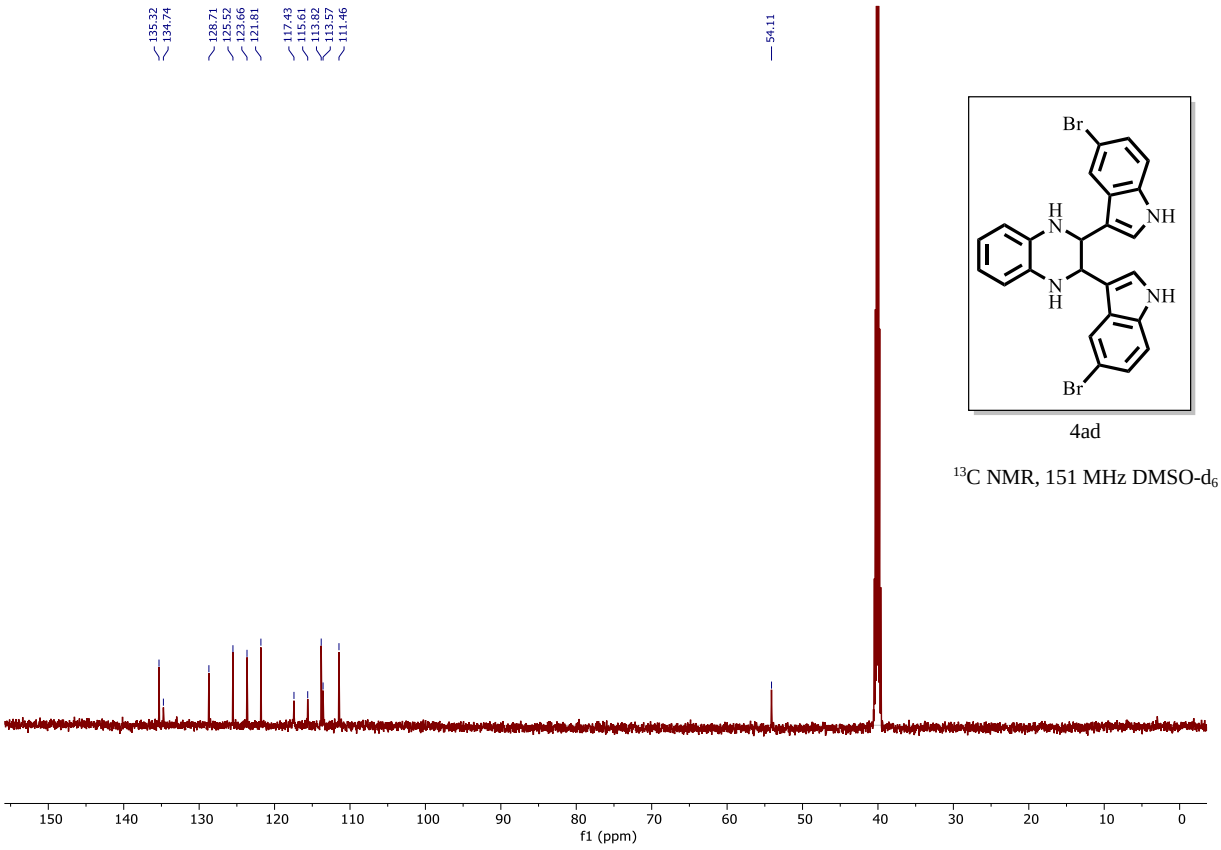
4ac

^{13}C NMR, 151 MHz DMSO-d_6

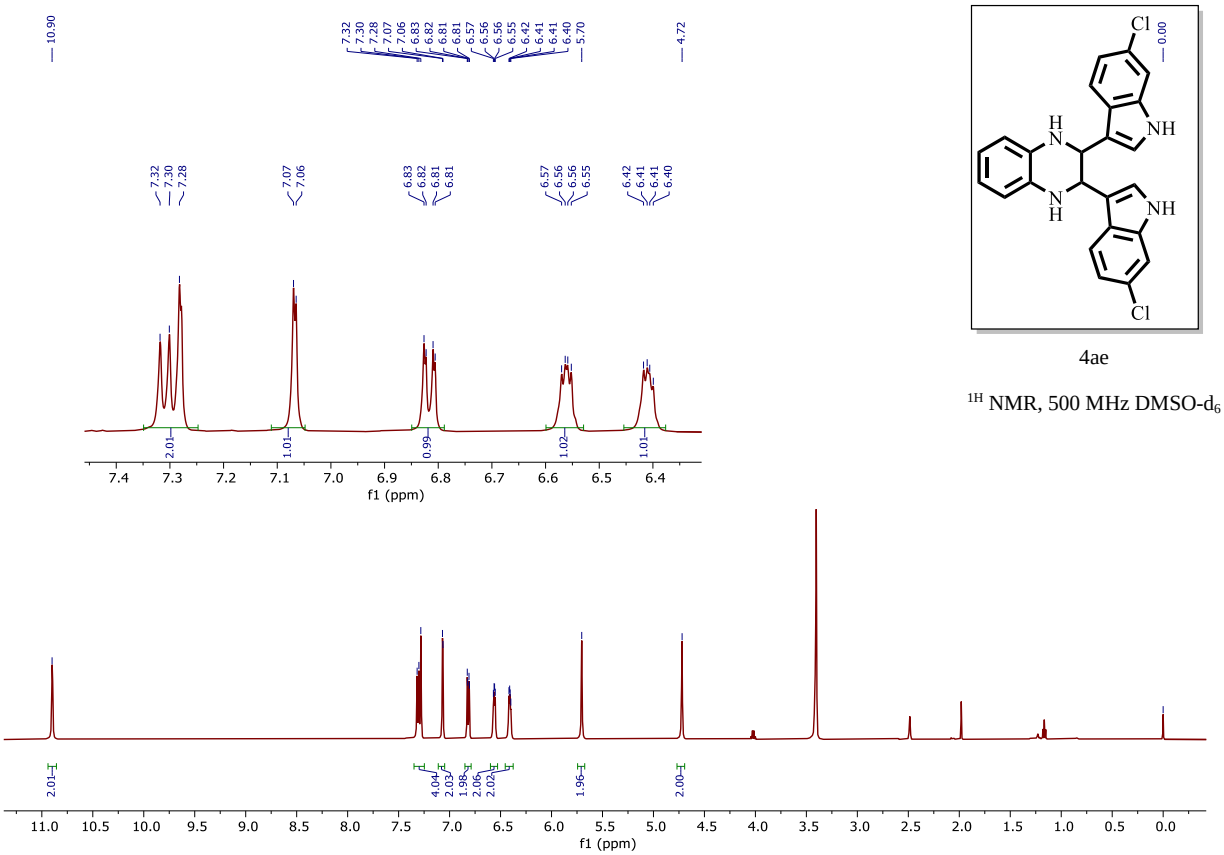
^{13}C NMR of 4ac



^{1}H NMR of 4ad



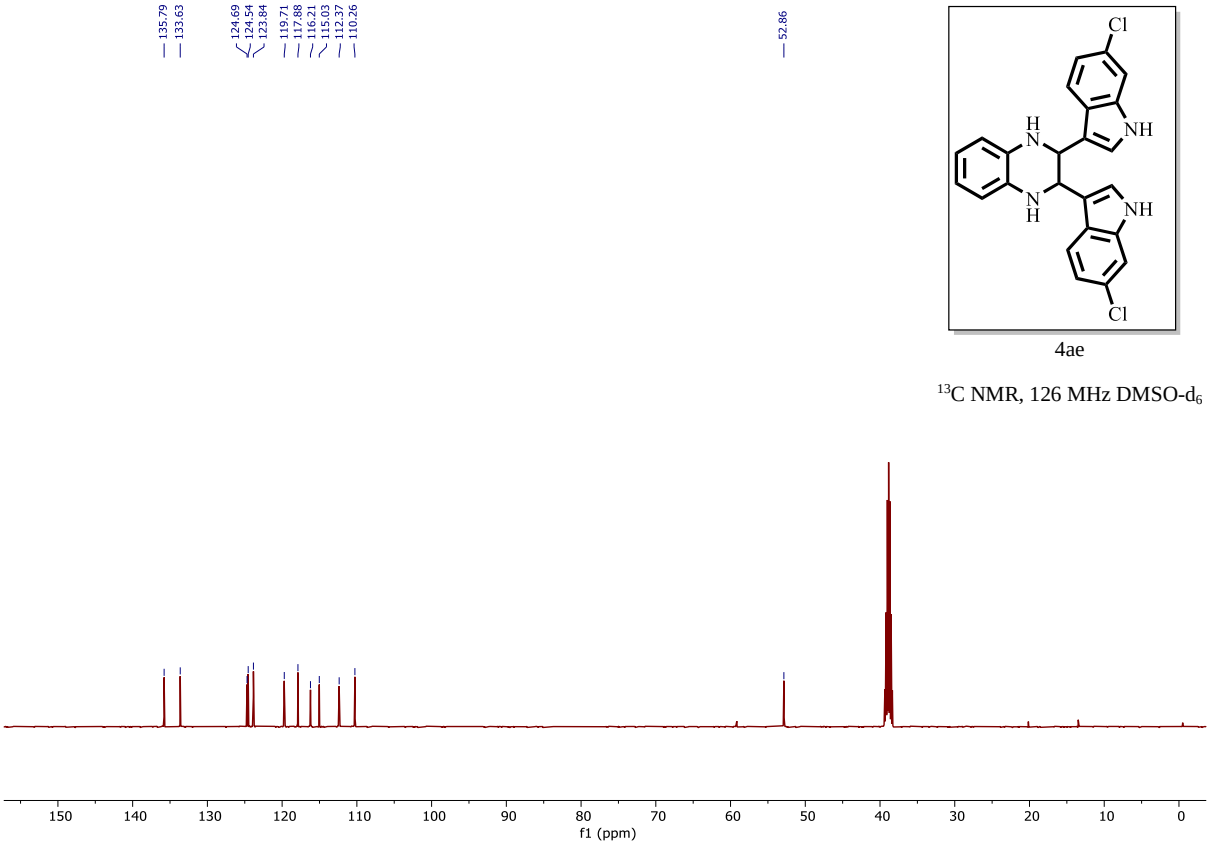
^{13}C NMR of 4ad



4ae

^{1H} NMR, 500 MHz DMSO-d_6

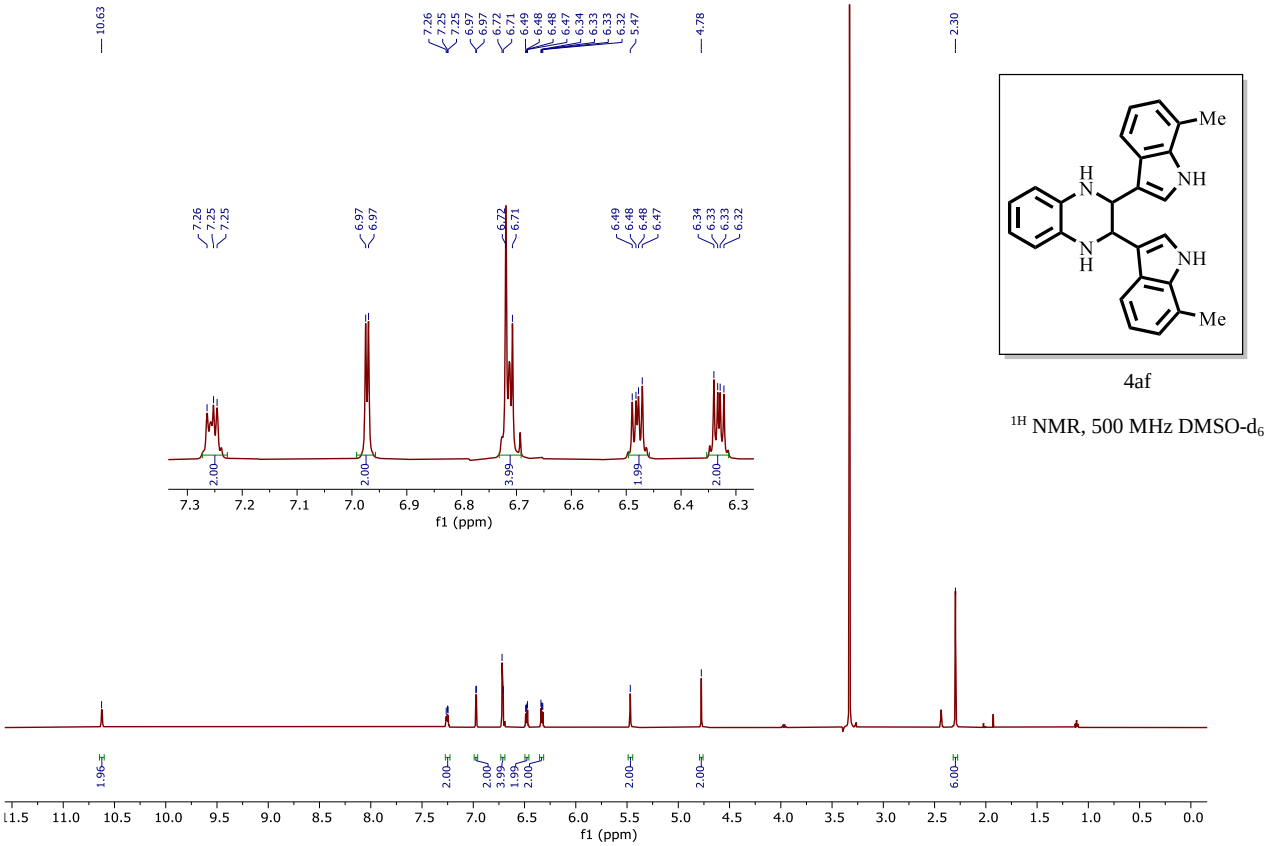
^{1}H NMR of 4ae



4ae

^{13}C NMR, 126 MHz DMSO-d_6

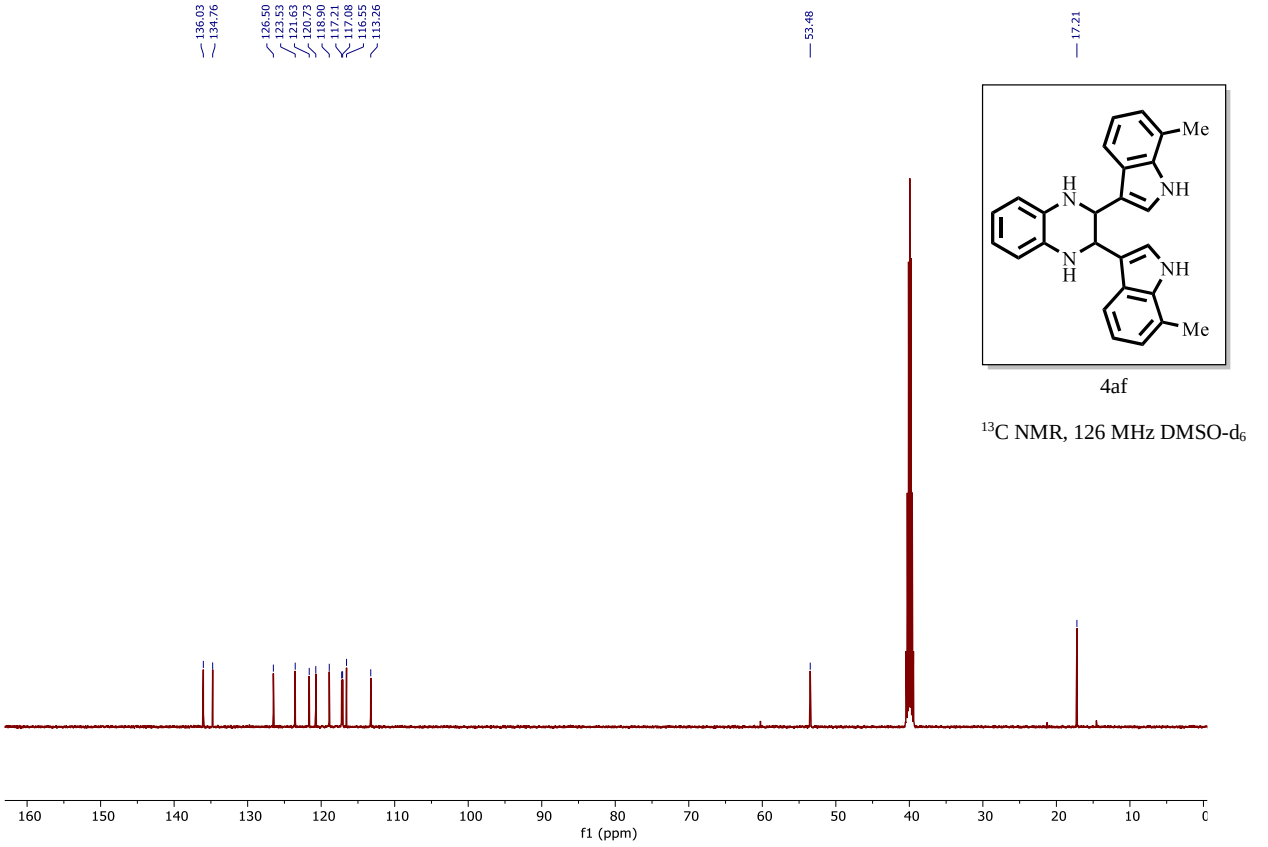
^{13}C NMR of



4af

^{1H} NMR, 500 MHz DMSO-d_6

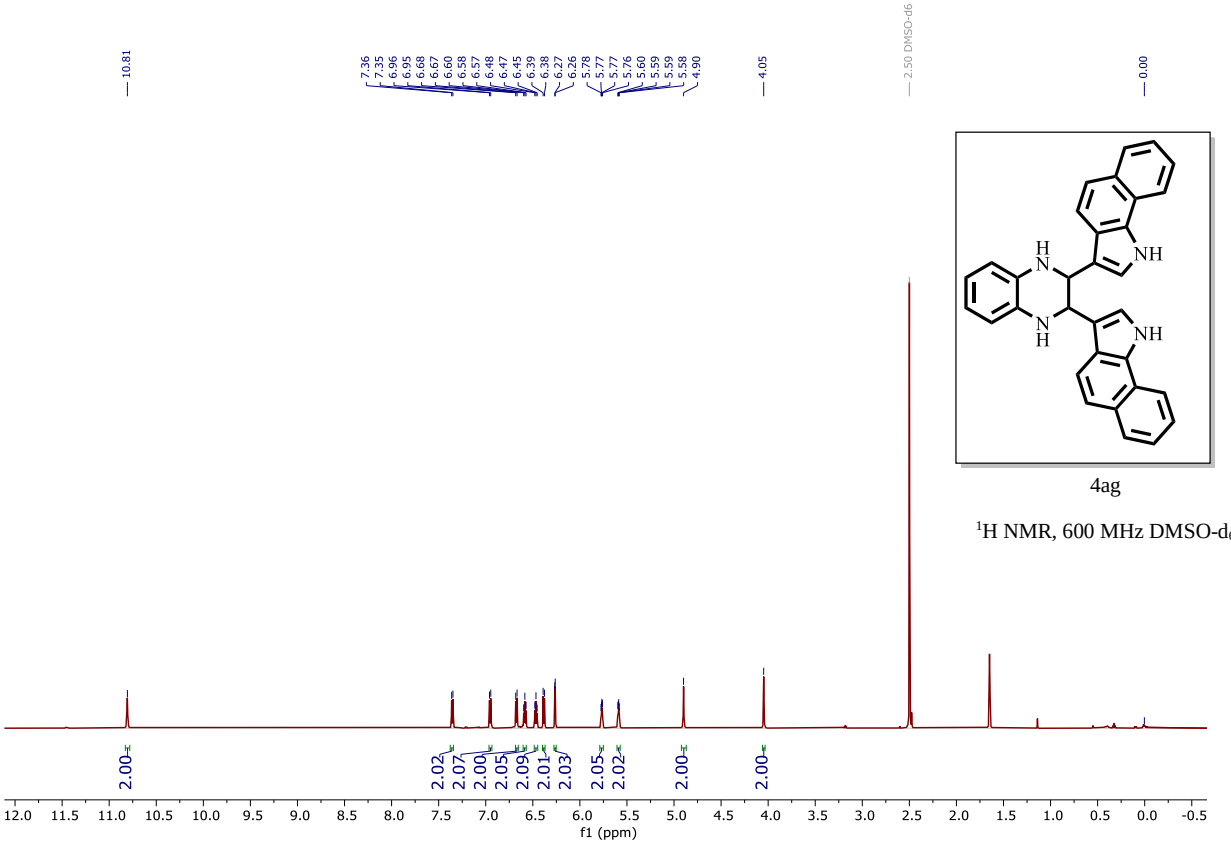
^{1}H NMR of 4af



4af

^{13}C NMR, 126 MHz DMSO-d_6

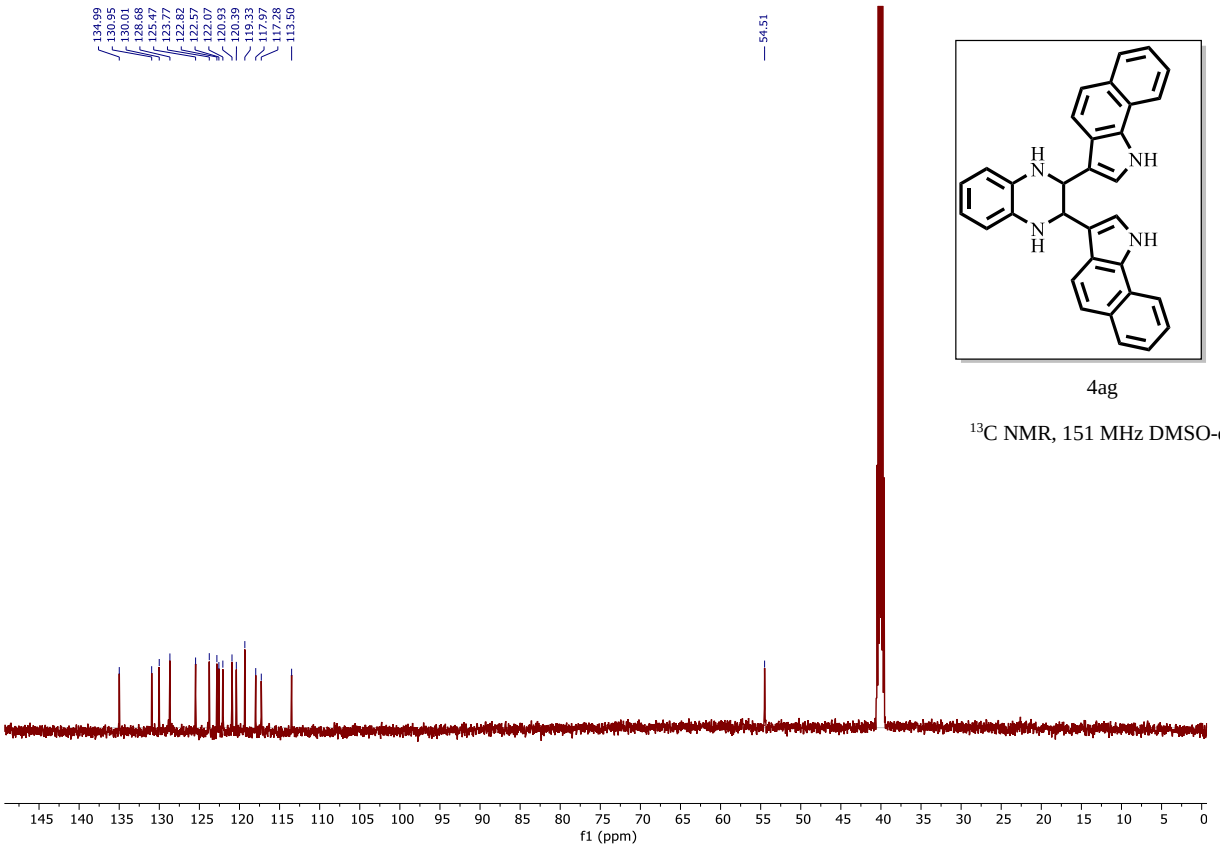
^{13}C NMR of 4af



4ag

^{1}H NMR, 600 MHz DMSO-d_6

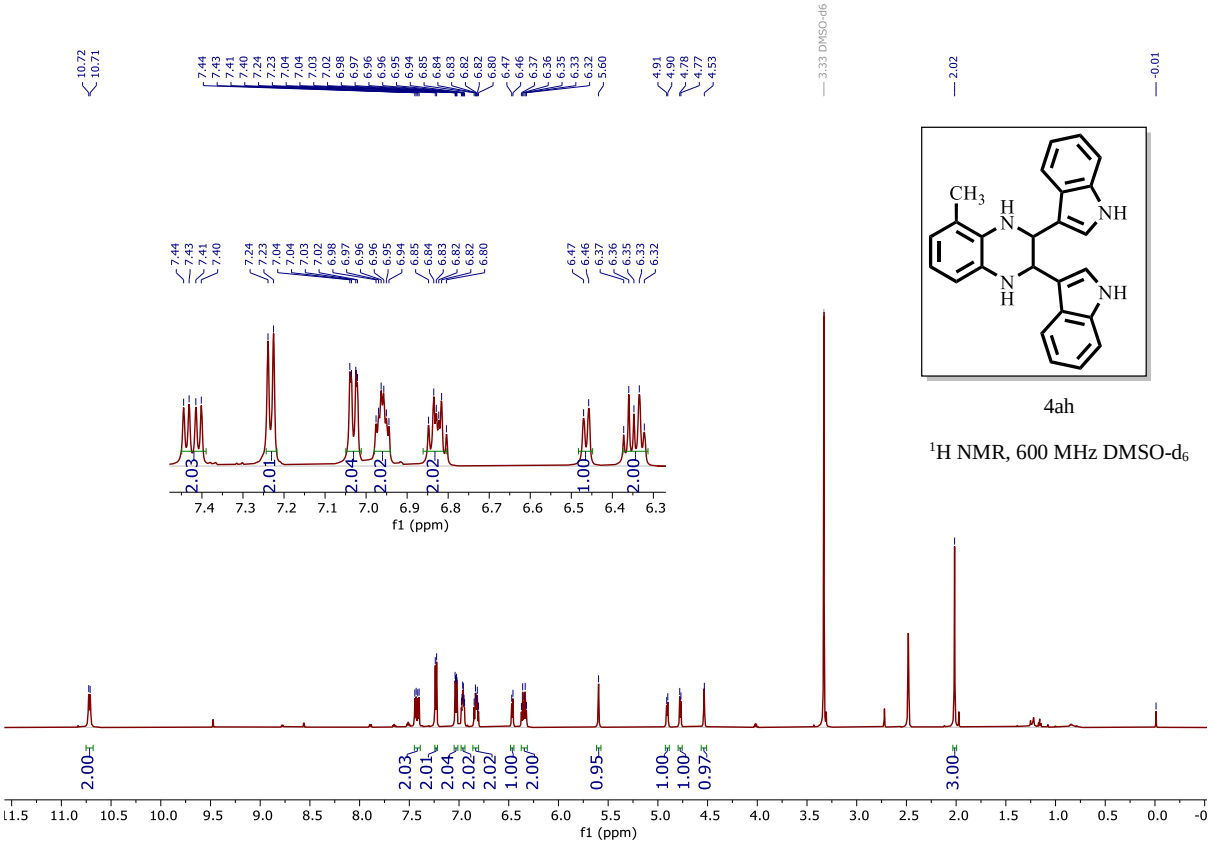
^{1}H NMR of 4ag



4ag

^{13}C NMR, 151 MHz DMSO-d_6

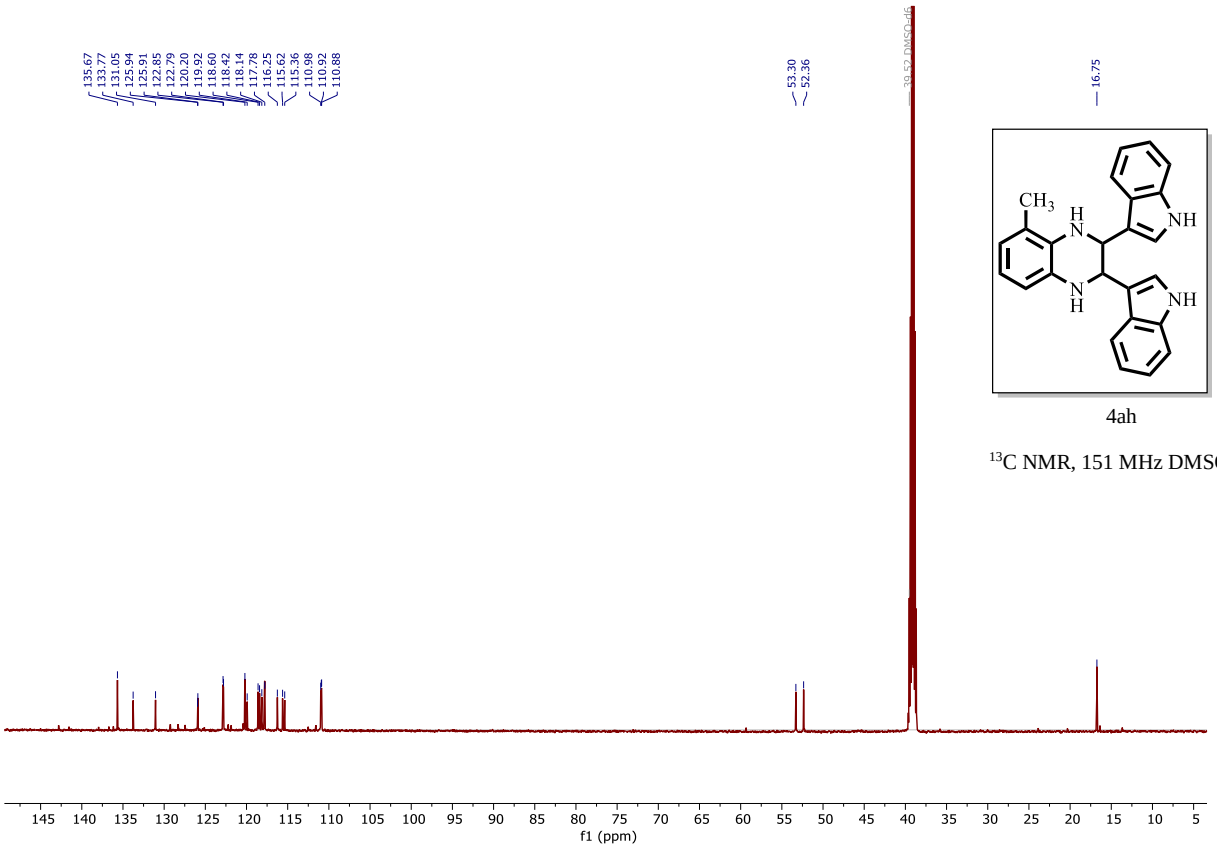
^{13}C NMR of 4ag



4ah

^{1}H NMR, 600 MHz DMSO-d_6

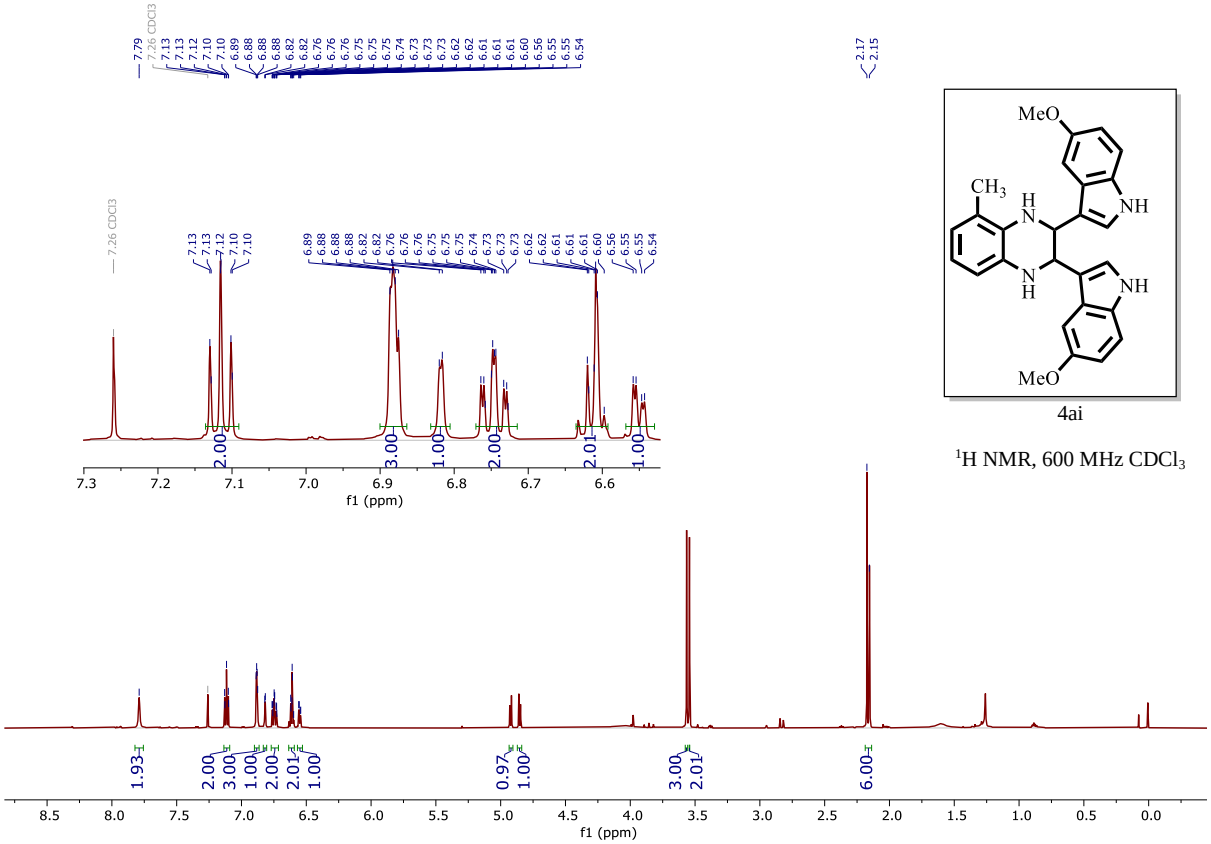
^{1}H NMR of 4ah



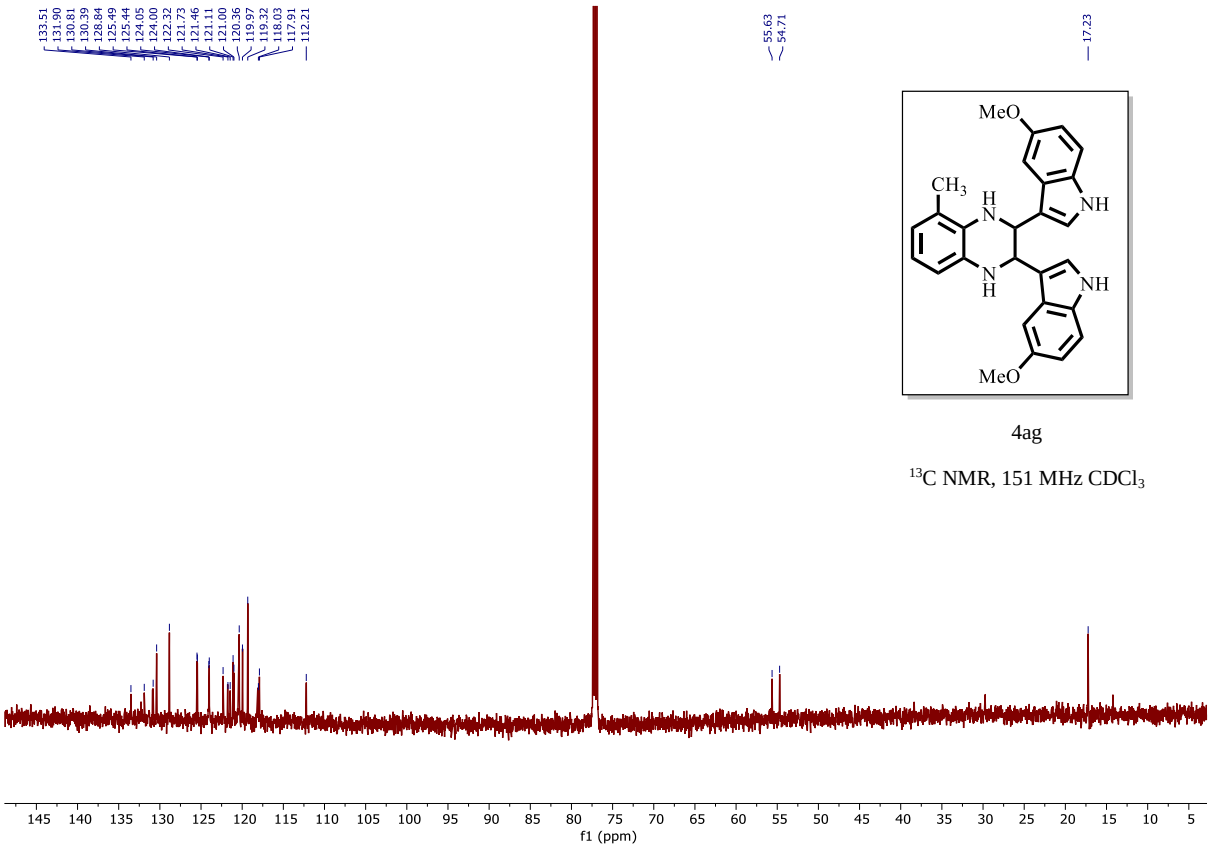
4ah

^{13}C NMR, 151 MHz DMSO-d_6

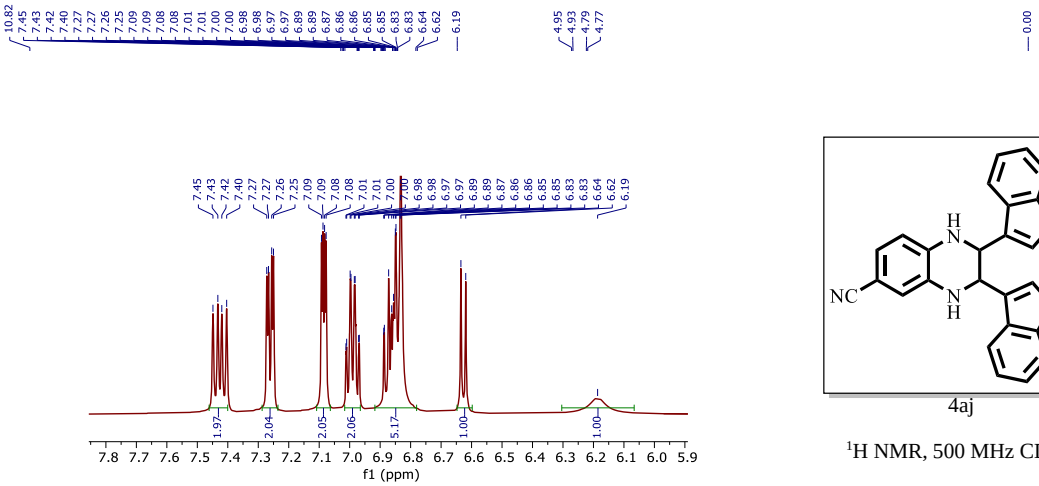
^{13}C NMR of 4ah



^{1}H NMR of 4ai

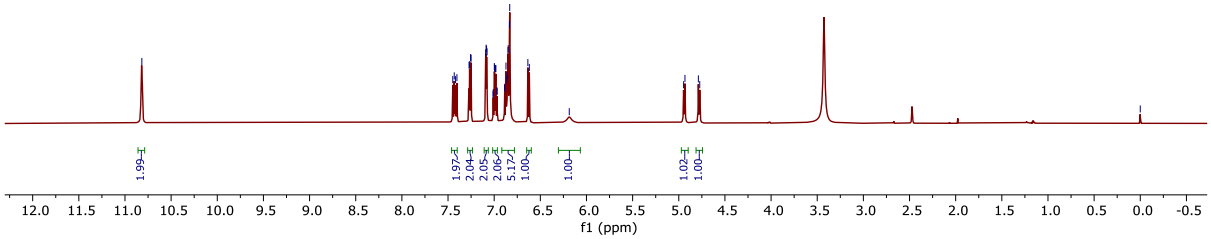


^{13}C NMR of 4ai

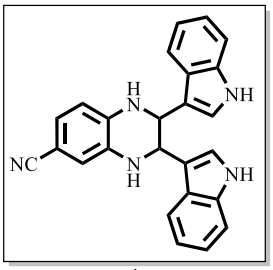


4aj

^{1}H NMR, 500 MHz $CDCl_3$

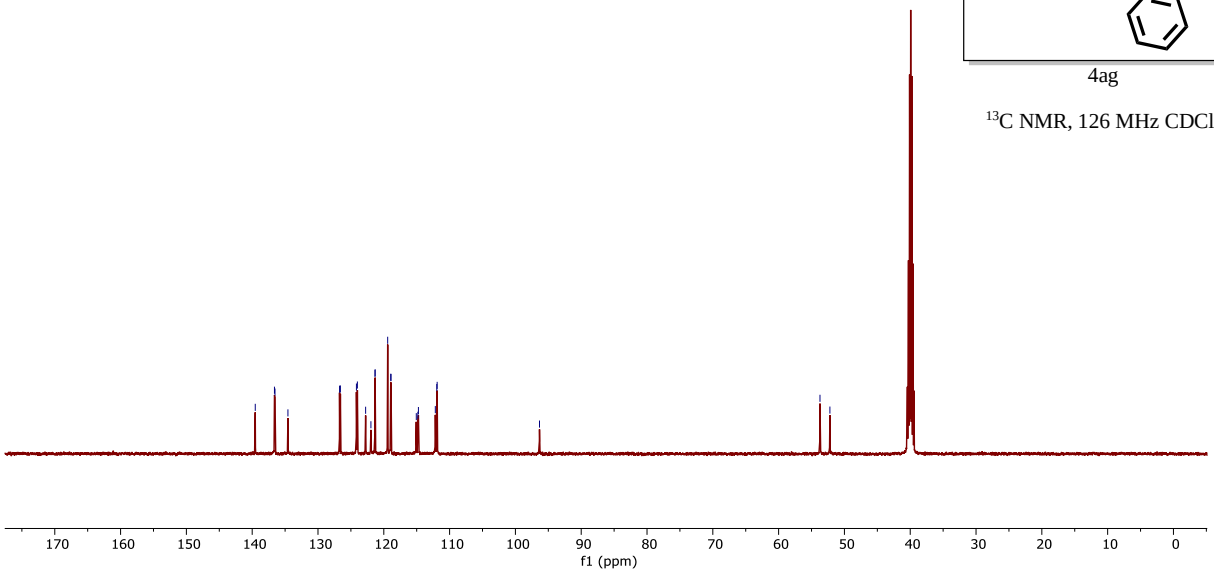


^{1}H NMR of 4aj

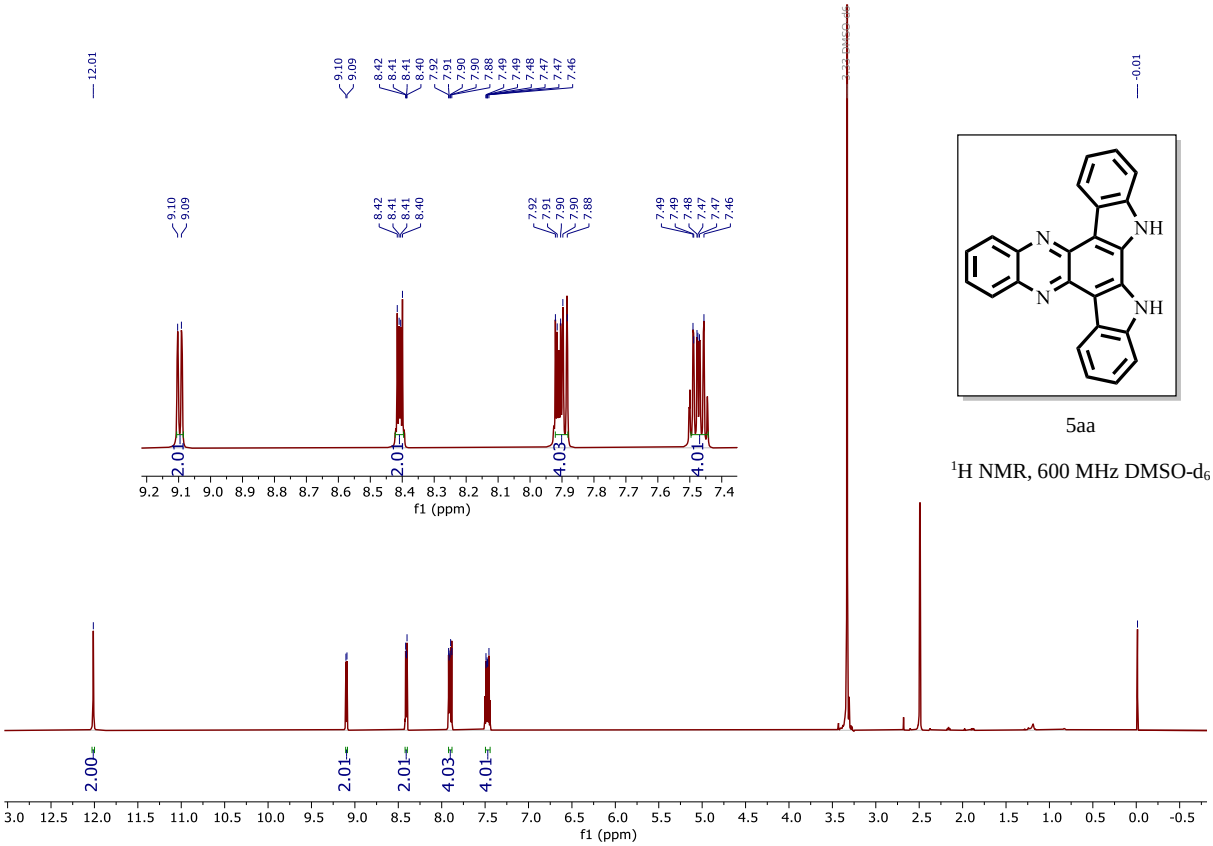


4ag

^{13}C NMR, 126 MHz $CDCl_3$



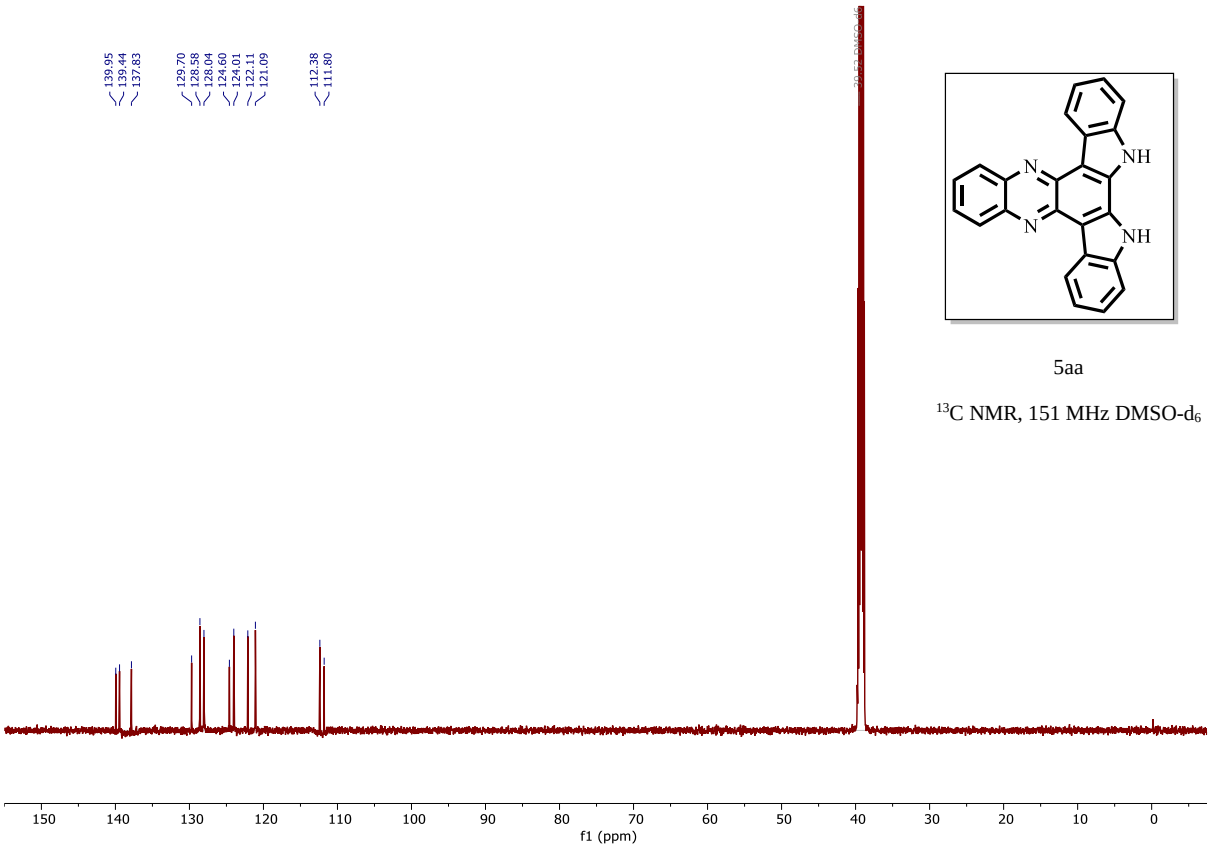
^{13}C NMR of 4aj



5aa

^{1}H NMR, 600 MHz DMSO-d_6

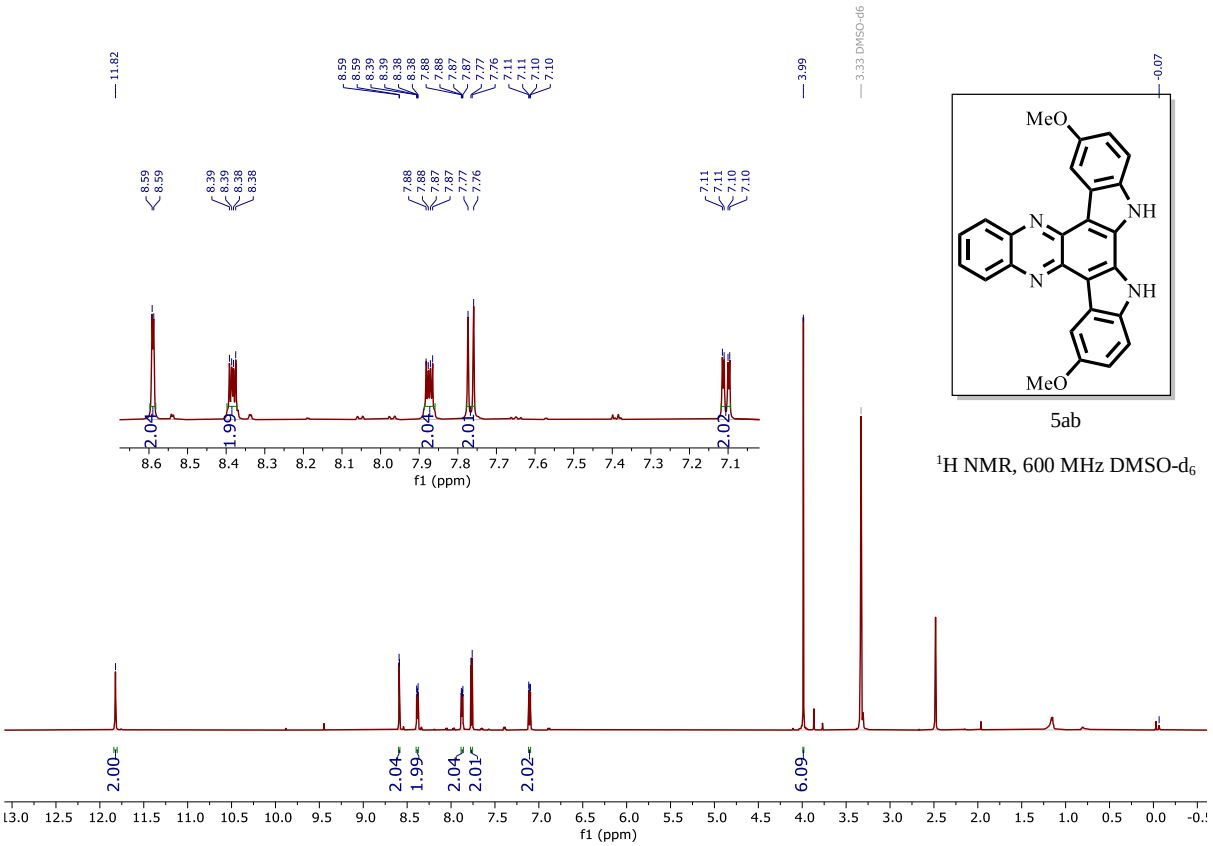
^{1}H NMR of 5aa



5aa

^{13}C NMR, 151 MHz DMSO-d_6

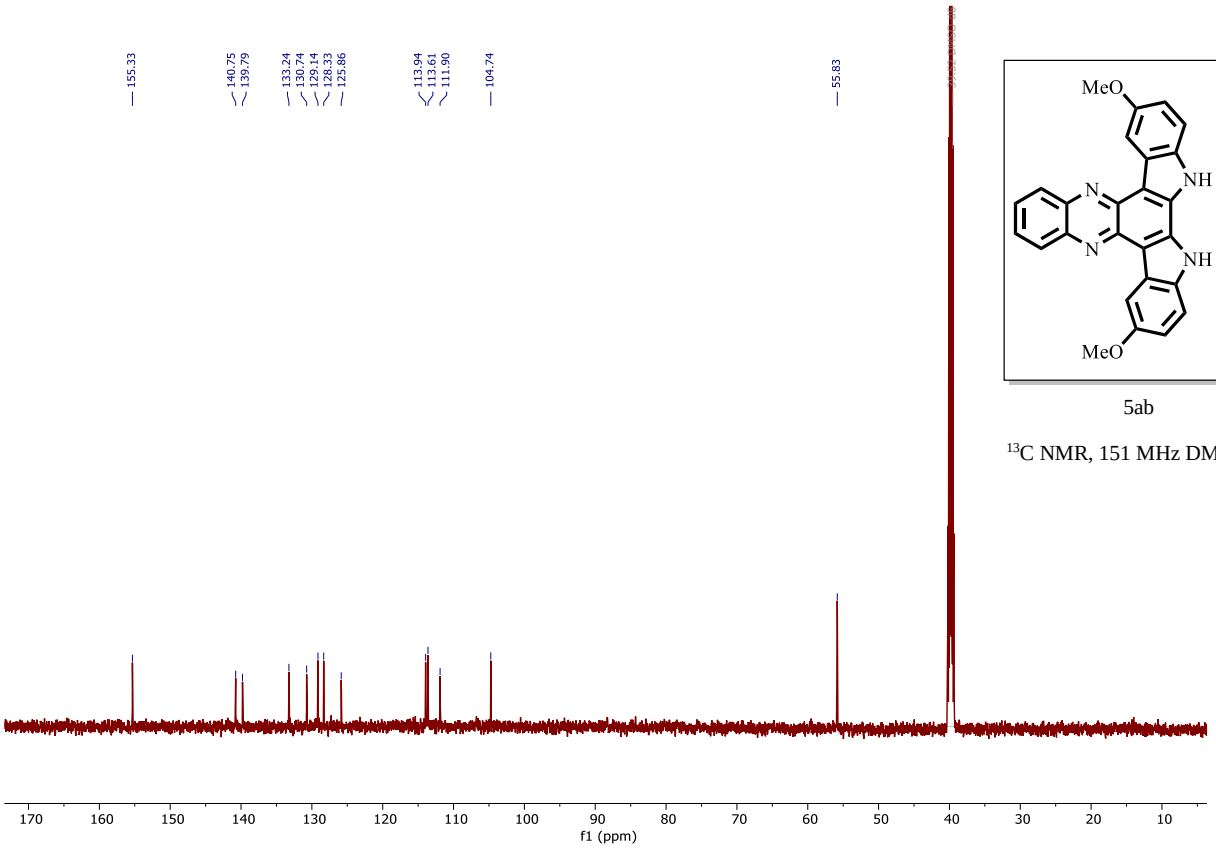
^{13}C NMR of 5aa



5ab

^{1}H NMR, 600 MHz DMSO-d_6

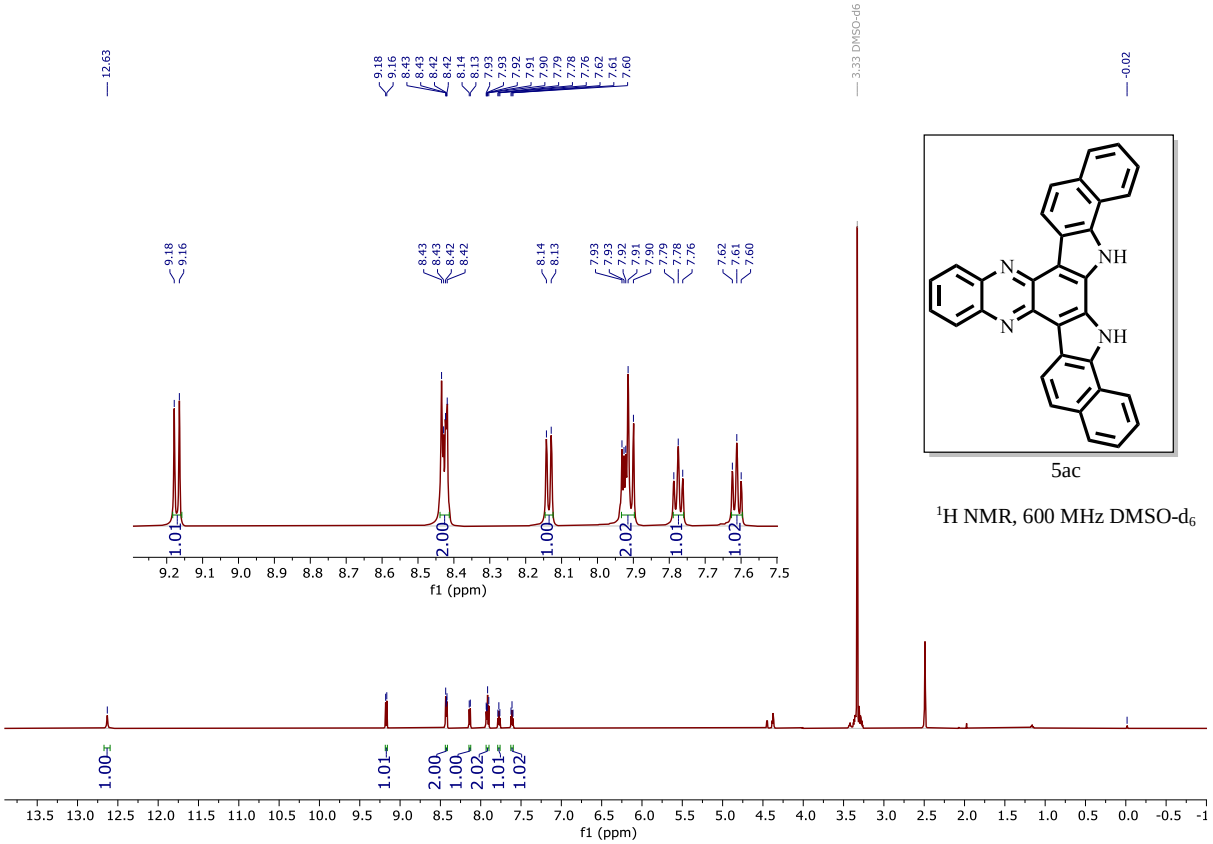
^{1}H NMR of 5ab



5ab

^{13}C NMR, 151 MHz DMSO-d_6

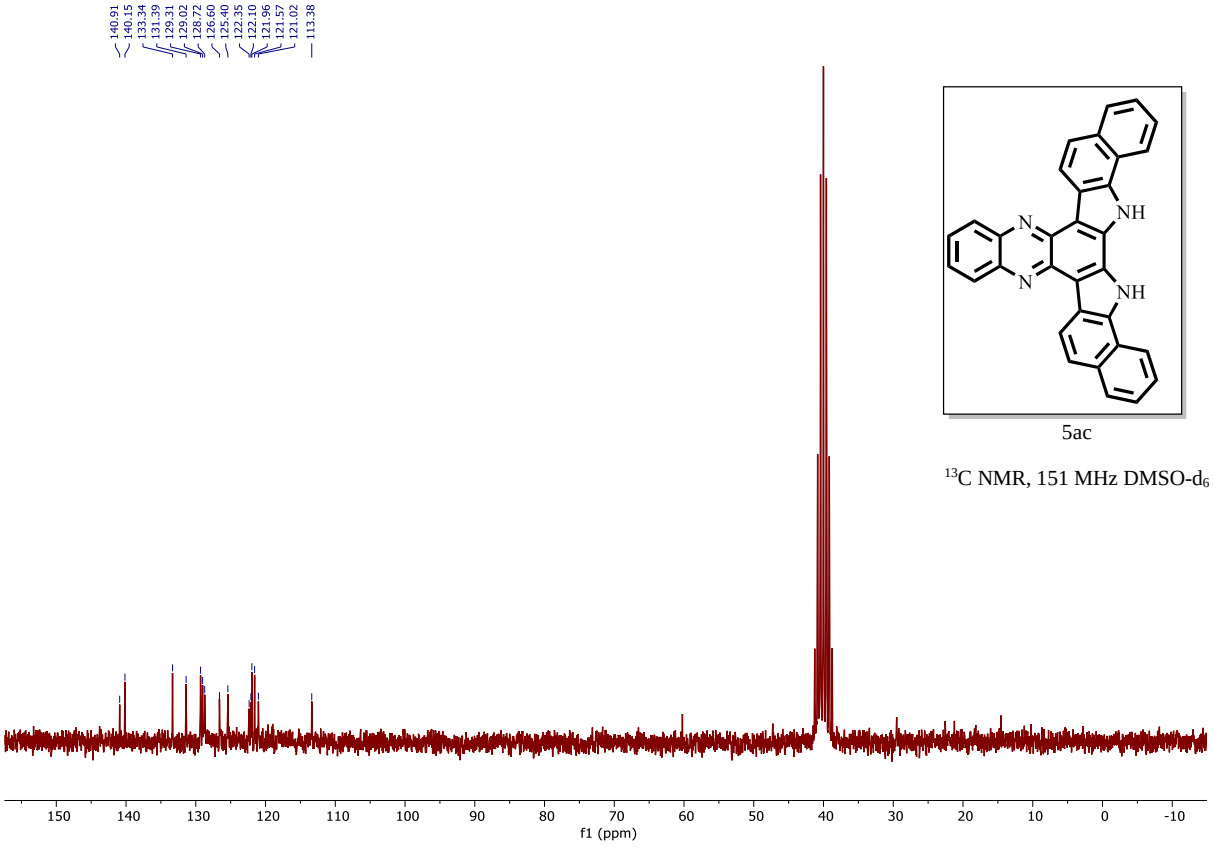
^{13}C NMR of 5ab



5ac

^{1}H NMR, 600 MHz DMSO-d_6

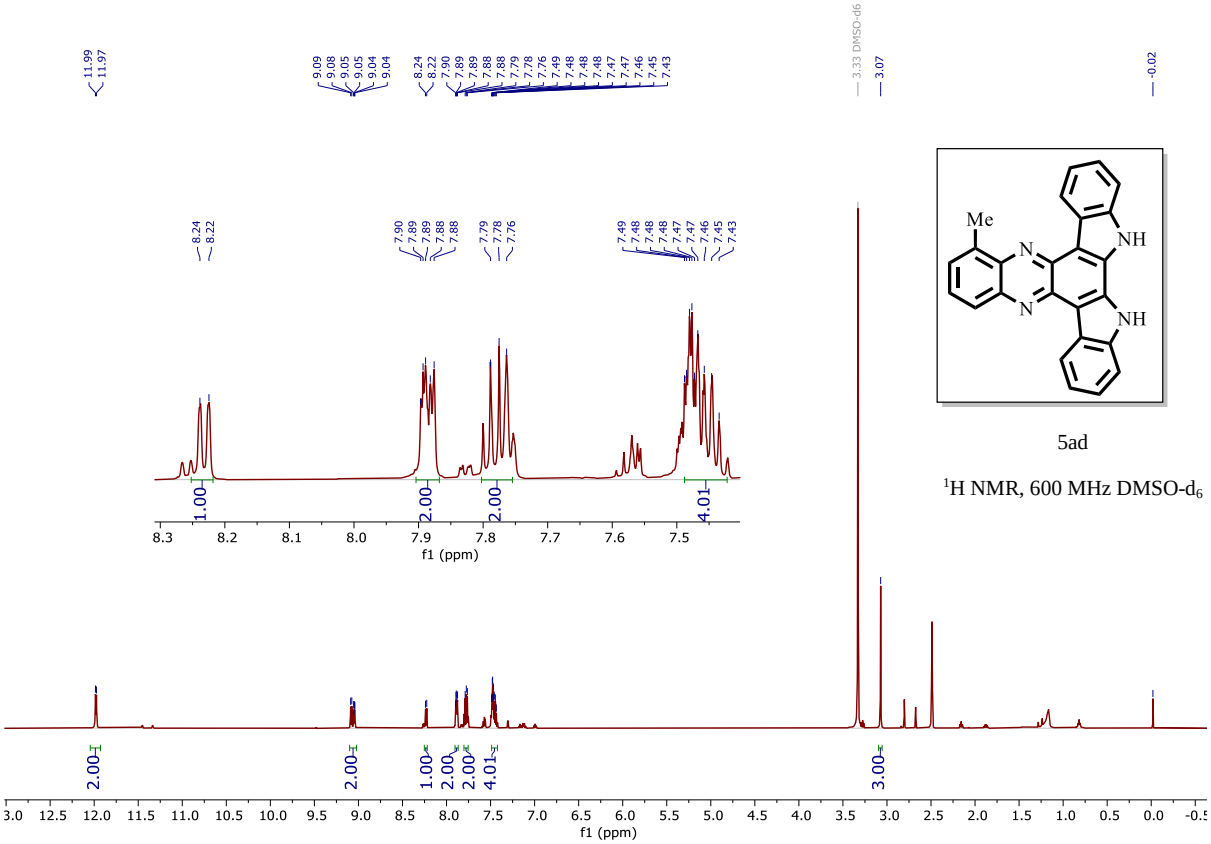
^{1}H NMR of 5ac



5ac

^{13}C NMR, 151 MHz DMSO-d_6

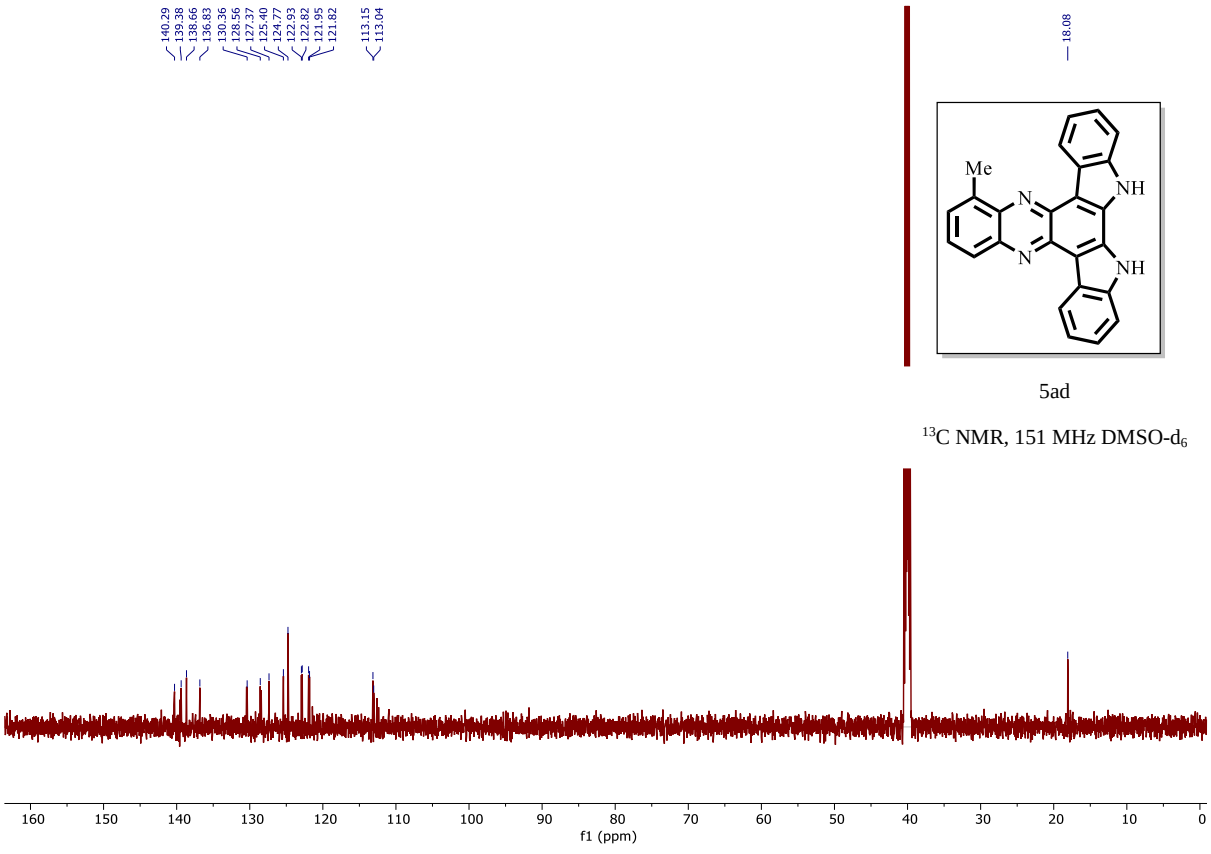
^{13}C NMR of 5ac



5ad

^{1}H NMR, 600 MHz DMSO-d_6

^{1}H NMR of 5ad



5ad

^{13}C NMR, 151 MHz DMSO-d_6

^{13}C NMR of 5ad

8. References

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Note: ***Abbreviations***

1. w. r. t. = with respect to

2. NMR = Nuclear Magnetic Resonance

3. HRMS = High Resolution Mass Spectrometry

4. CCDC = Cambridge Crystallographic Data Centre

5. *p*-TSA = p-Toluenesulfonic acid

6. DDQ = 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone

7. o-DCB = 1,2-Dichlorobenzene