Supporting Information

For

Divergent Synthesis of Polycyclic (aza)Fluorenes via Conditions-Controlled Tandem Reaction of ortho-Hydroxyphenyl-Substituted Indene-Dienes

Yin-Fu Zhang,[#a] Shuqi Zhang,[#b] Yan Zhao,[a] Jiying Xu,[b] Xiao-Qing Wang,[a] Qiu-Xia Han,[a] Chuan-Bao Zhang,*[a,c] Lili Zhao,*[b] Ji-Ya Fu*[a]

[†] College of Chemistry and Molecular Sciences, Henan University, Kaifeng 475004, China; Email: fujiya@126.com.

[‡] State Key Laboratory of Material-Oriented Chemical Engineering, School of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211816, China; Email: ias_llzhao@njtech.edu.cn.

[※] School of Pharmacy, Zhengzhou Railway Vocational & Technical College, Zhengzhou 450052; Email: China. zhangchuanbao@zzrvtc.edu.cn.

[#] These two authors contribute equally to this work.

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1. General experimental information

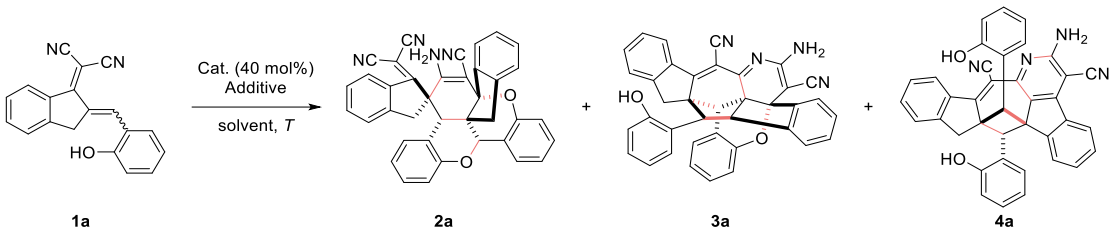
All reagents including starting materials and solvent commercially available were used directly. Compounds **1** were synthesized according to the literatures.[1] Column chromatography was performed using silica gel (HG-/T2354). NMR spectra were recorded with tetramethylsilane as the internal standard. ^{1}H NMR and ^{13}C NMR spectra of DMSO-d_6 solutions were recorded either at 500 and 125 MHz (Bruker Avance) at ambient temperature respectively, and resonances (δ) are given in parts per million (ppm) with tetramethylsilan as reference. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet) and coupling constants in hertz (Hz). High resolution mass spectra (HRMS) were recorded on Q-TOF-Premier mass spectrometer by using ESI method. The X-ray crystal-structure determinations of **2a, 3a**, **4a**, **5**, **8** and **11** were obtained on a Bruker APEX DUO system. All melting points are uncorrected. Reactions were monitored by TLC and visualized with ultraviolet light.

References:

1. (a) X.-H. Chen, Z. Zhao, Y. Liu, P. Lu, and Y.-G. Wang. *Chem. Lett.* **2008**, *37*, 570. (b) N. Almonasya, M. Nepraša, L. Burgerta, A. Lyčkab. *Dyes Pigm*. **2002**, *53*, 21. (c) Y.-H. Deng, L. Qin, R. Li, Y.-B. Wang, J.-Y. Zhu, J.-Y. Fu, C.-B. Zhang and L. Zhao, *Org. Lett*., **2022**, *24*, 8277. (d) Y.-H. Deng, W.-L. Xu, L. Wang, C.-Y. Tang, J.-Y. Fu and C.-B. Zhang, *Org. Biomol. Chem*. **2023**, *21*, 6681. (e) Alex E. Crolais, Neil D. Dolinski, Nicholas R. Boynton, Julia M. Radhakrishnan, Scott A. Snyder, and Stuart J. Rowan.*J. Am. Chem. Soc*. **2023**, *145*, 14427. (f) W.-L. Xu, Y.-H. Zhang, J.-R. Yuan, D. Jing, C.-Y. tang, C.-B. Zhang, Q.-X. Han, J.-Y. Fu, *Org. Lett*., **2024**, *26*, 7999.

2. Optimization of the reaction conditions

Table S1 | Optimization of the reaction conditions of tandem cyclization/rearrangement reaction of ortho-hydroxyphenyl-substituted indene-dienes[a]



1a 2a 3a 4a

Entry	Cat.	Additive	Solvent	Temp (°C)	Time (h)	Yield (%)		
						2a	**3a**	**4a**
1	DBN	-	DCM	25	96	23	-	-
2	DMAP	-	DCM	25	120	trace	-	-
3	DIPEA	-	DCM	25	120	15	-	-
4	K_2CO_3	-	DCM	25	120	nr.	-	-
5	Cs_2CO_3	-	DCM	25	120	nr.	-	-
6	Na_2CO_3	-	DCM	25	120	nr.	-	-
7	DABCO	-	DCM	25	120	nr.	-	-
8	DBU	-	DCM	25	96	32	-	-
9	TMG	-	DCM	25	96	41	-	-
10	Et_3N	-	DCM	25	168	trace	-	-
11	TMG	-	MeCN	25	120	33	-	-
12	TMG	-	PhCl	25	120	nr.	-	-
13	TMG	-	toluene	25	120	nr.	-	-
14	TMG	-	THF	25	120	trace	-	-
15	TMG	-	$CHCl_3$	25	120	32	-	-
16	TMG	-	Et_2O	25	120	trace	-	-
17	TMG	-	DCE	25	72	38	-	-
18	TMG	-	PhCN	25	48	35	-	-
19	TMG	-	DMF	25	2	-	71	-
20[b]	TMG	-	DCM	25	96	26	-	-
21[c]	TMG	-	DCM	25	96	38	-	-
22	TMG	-	DCM	10	144	31	-	-
23	TMG	-	DCM	30	72	41	-	-
24	TMG	-	DCM	40	48	34	-	-
25[d]	TMG	-	DCM	30	72	35	-	-
26[e]	TMG	-	DCM	30	72	24	-	-

27	TMG	3Å MS (50 mg)	DCM	30	72	40	-	-
28	TMG	4Å MS (50 mg)	DCM	30	72	39	-	-
29	TMG	5Å MS (50 mg)	DCM	30	72	34	-	-
30	TMG	$MgSO_4$ （2.0 eq.）	DCM	30	72	43	-	-
31	TMG	$MgSO_4$ （3.0 eq.）	DCM	30	72	50	-	-
32	TMG	$MgSO_4$ （4.0 eq.）	DCM	30	72	60	-	-
33	TMG	$MgSO_4$ （5.0 eq.）	DCM	30	72	54	-	-
34	TMG	Na_2SO_4 （4.0 eq.）	DCM	30	72	40	-	-
35	TMG	-	DMF	40	2	-	44[f]	5[f]
36	TMG	-	DMF	60	48	-	12[f]	66[f]
37	TMG	-	DMF	80	4	-	-	71
38	TMG	-	DMF	100	0.5	-	-	81
39	TMG	-	DMF	110	0.5	-	-	71
40	TMG	-	DMF	120	0.5	-	-	61
41[g]	TMG	-	DMF	100	0.5	-	-	72
42[h]	TMG	-	DMF	100	0.5	-	-	79
43	TMG	$MgSO_4$ （4.0 eq.）	DMF	100	0.5	-	-	76

[a] Reaction conditions: **1a** (0.2 mmol), TMG (40 mol%), solvent (1.5 mL), 25 °C, 96 h. [b] 1.0 mL DCM was used. [c] 2.0 mL DCM was used. [d] 30 mol% TMG was used. [e] 50 mol% TMG was used. [f] determined by ^{1}H NMR of isolated mixture of *o*-HPIDs **3a** and **4a**. [g] 1.0 mL DMF was used. [h] 2.0 mL DMF was used.

To improve the efficiency of the reaction, a variety of other organic or inorganic bases were evaluated, and it was discovered that TMG was the best base for facilitating the Tandem reaction (Table S1, entries 1-10). After screening other reaction solvents, we noted that dichloromethane was suitable for the production of **2a**. Very interestingly, when using DMF as a solvent, an unexpected tandem reaction of o-HPIDs **1a** occurred generating **3a** with indenyl[b]bicyclo [3.2.1] octane and azafluorene skeletons in 71%

yield (Table S1, entry 19). In contrast, the predicted tandem reaction product **2a** was not detected. This outcome furnished us crucial clues as to the solvent-controlled divergent reaction pathways to generate various complex indene-based polycyclic compounds. Then, the influence of the temperature on the reaction was investigated. Although the improvements in yield of **2a** was not achieved upon raising reaction temperature to 30 °C, the reaction time could be foreshortened from 96 h to 72 h (Table S1, entry 23).

To further improve the yield of product **2a**, the additives were estimated (Table S1 in ESI, entries 27-34). When 4.0 equiv. of anhydrous magnesium sulfate was used, the yield of **2a** could be increased to 60% (Table S1, entry 32). Additionally, since indenyl[b]bicyclo [3.2.1] octane and azafluorene skeletons are valuable motifs in many drug molecules and natural products, we also made some effort to meliorate the yields of product **3a** in DMF. When raising the temperature to 40 °C, the target product **3a** was obtained in 44% yield. Concurrently, an uncommon rearrangement reaction of **3a** occurred, resulting in the more stable product 4a with bicyclo [4.1.1] octane and azafluorene skeletons (Table S1, entry 35). Inspired by these results, we further evaluated the influence of reaction temperature in DMF solvent on the reaction (Table S1, entries 36-40). As anticipated, raising reaction temperature is advantageous for rearrangement reaction of **3a** into product **4a**. Notably, upon elevating the temperature to 80 °C, only rearrangement product **4a** was obtained, and product **3a** was not observed (71% yield, Table S1, entry 37). When we further heated the reaction to 100 °C, the reaction time was shortened to 0.5 hours, and the yield of rearrangement product **4a** could be increased to 81% (Table S1, entry 38). Nevertheless, a lower yield was obtained by adjusting the reaction temperature to 120 °C (Table S1, entry 40). Meanwhile, we found that introducing anhydrous magnesium sulfate into the reaction solution led to a lessened yield of product **4a** (Table S1, entry 43). Thus, the conditions employed in entries 23, 19 and 38 were chosen as the optimal reaction conditions for the synthesis of products **2**, **3** and rearrangement products **4**, respectively.

3. Photophysical property investigations

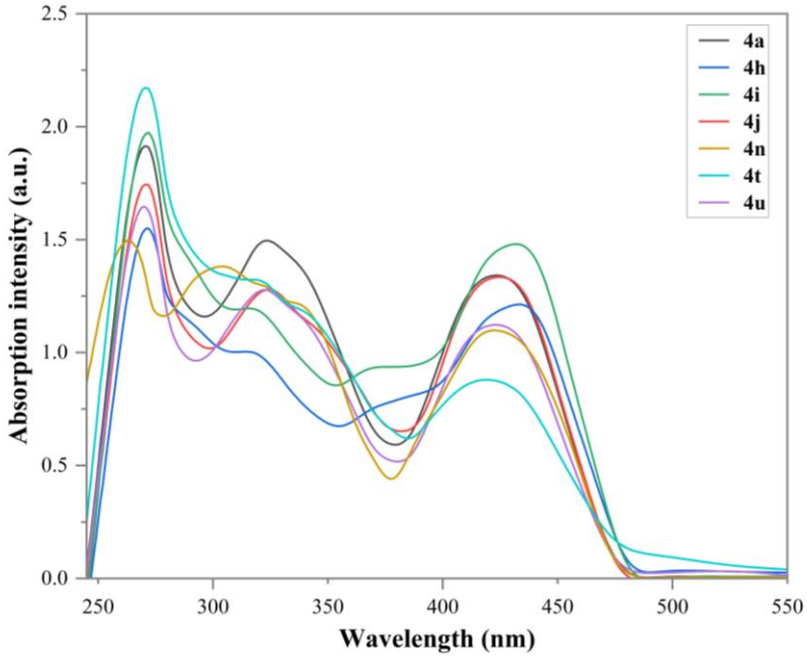


Fig. S1 UV-bis absorption spectra in ethyl acetate at 298 K ([C] = 1×10^{-4} M)

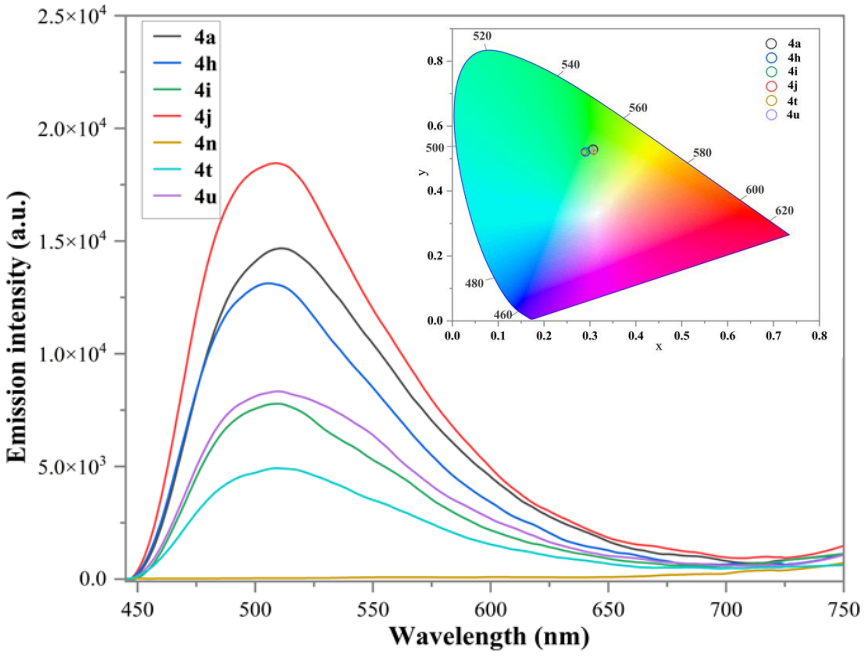


Fig. S2 Steady-state PL spectra in ethyl acetate at 298 K ([C] = 1×10^{-4} M) (the excitation wavelength (λex) was set at 323 nm)

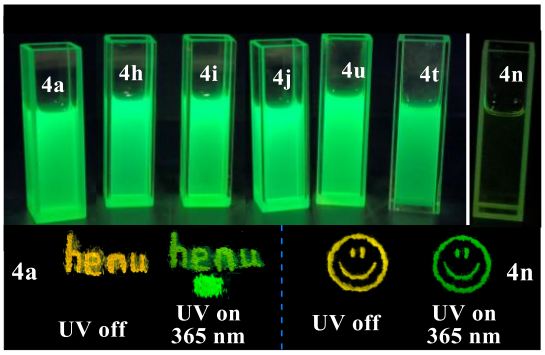


Fig. S3 Fluorescence images under 365 nm light irradiation in ethyl acetate at 298 K ([C] = 1×10^{-4} M) and Solid fluorescence images of **4a** and **4n**.

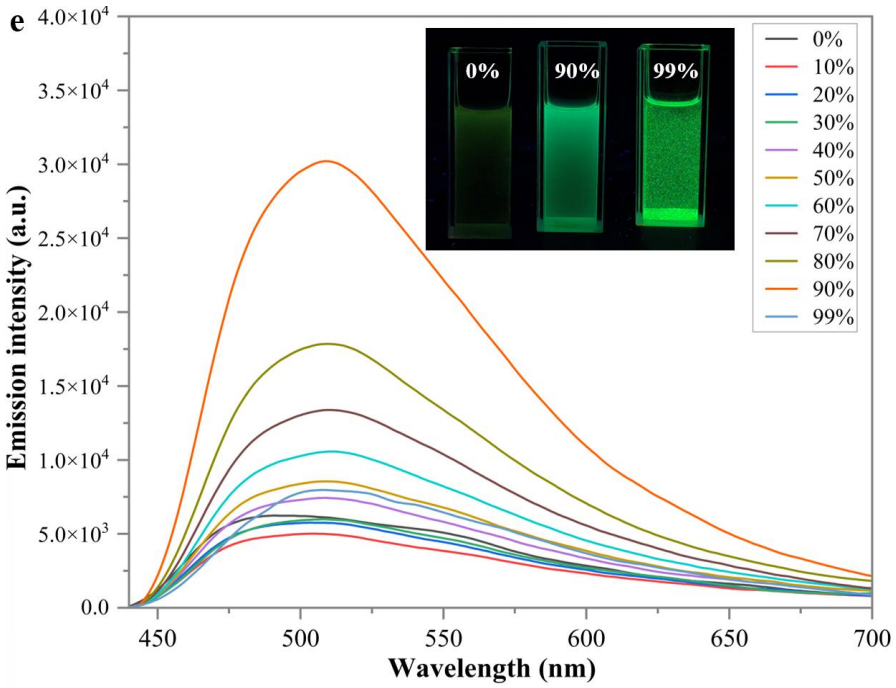


Fig. S4 PL spectra of **4n** in ethyl acetate with different petroleum ether ratios ([C] = 1×10^{-4} M).

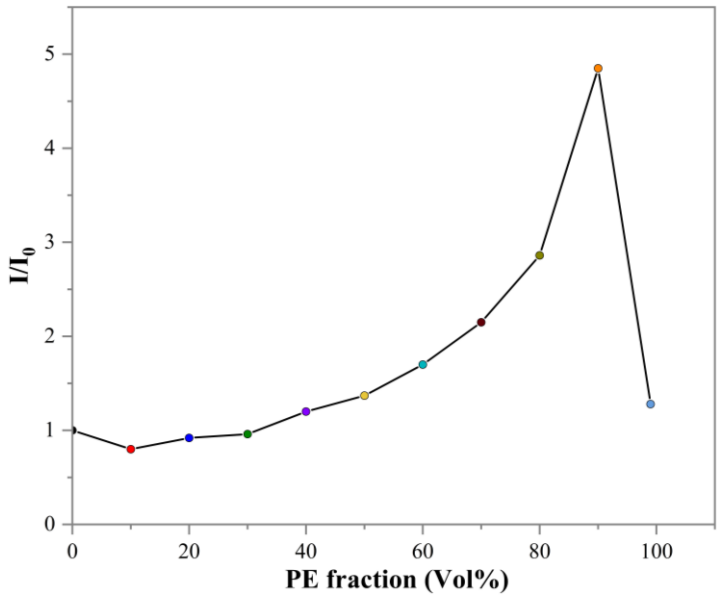


Fig. S5 Dependence of I/I_0 ratios of **4n** in ethyl acetate with different petroleum ether

4. Control experiments

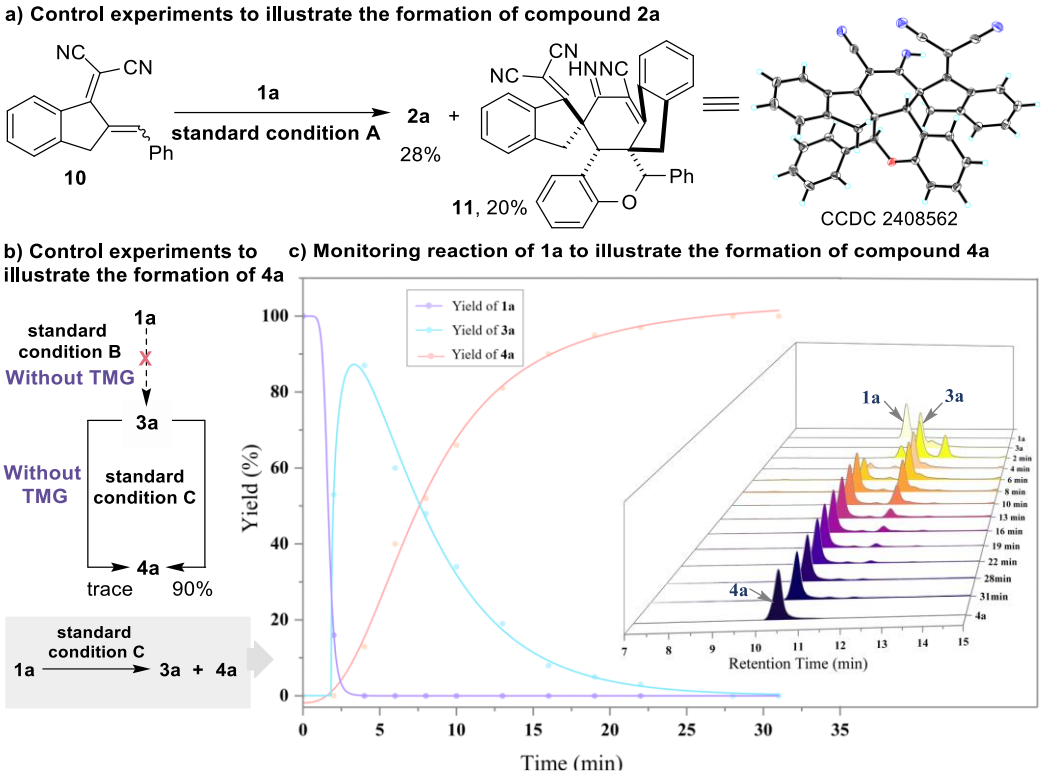
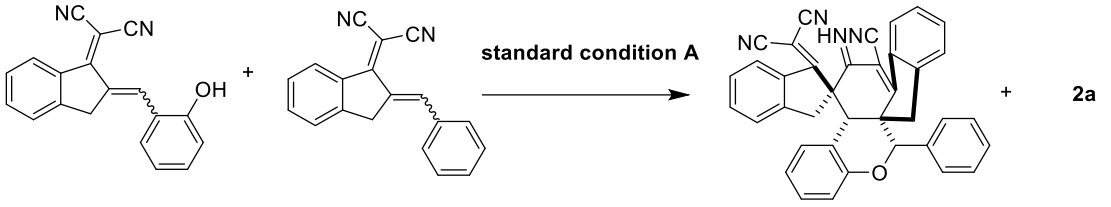


Fig. S6 Mechanistic studies.

Experimental procedure for the tandem cyclization reaction of ortho-hydroxyphenyl-substituted indene-diene with phenyl-substituted indene-diene



1a **10** **11**, 20% 28%

To a solution of ortho-hydroxyphenyl-substituted indene-diene **1a** (0.20 mmol, 1.0 equiv), phenyl-substituted indene-diene **10** (0.20 mmol, 1.0 equiv) and anhydrous sodium sulfate (0.80 mmol, 4.0 equiv) in dichloromethane (3.0 mL), tetramethylguanidine (0.08 mmol, 0.40 equiv) was added at 30 ºC. Then, the resulting mixture was stirred at 30 ºC in oil bath for 96 hours. Upon completion (monitored by TLC), the reaction solution was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : DCM = 1 : 1 to 1 : 10) to afford pure products **2a** as a yellow solid (32.2 mg, 28% yield) and pure products **11** as a white solid (21.8 mg, 20% yield).

2-(7-cyano-6-imino-13-phenyl-6,12-dihydro-4bH,13H-spiro[fluoreno[9a,1-c]chromene-5,2'-inden]-1'(3'H)-ylidene)malononitrile (11): white solid, 21.8 mg, 20% yield, R_f = 0.40 (petroleum ether/dichloromenthane = 1:4). m.p. 254-255 °C.

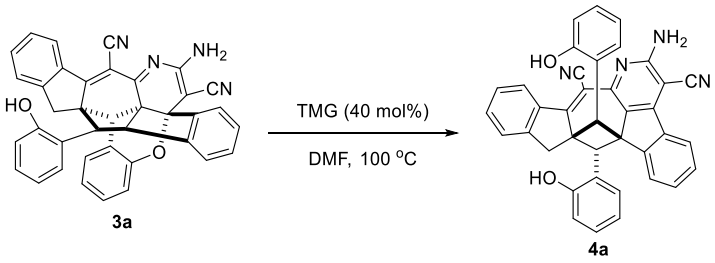
^{1}H NMR (500 MHz, $CDCl_3$) δ 10.65 (s, 1H), 8.52 (d, *J* = 8.1 Hz, 1H), 8.04 (d, *J* = 7.9 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.38 (t, *J* = 7.7 Hz, 1H), 7.19 – 7.07 (m, 5H), 7.05 – 7.00 (m, 5H), 6.86 (d, *J* = 7.5 Hz, 1H), 6.53 – 6.45 (m, 2H), 5.48 (s, 1H), 3.89 (s, 1H), 3.72 – 3.59 (m, 2H), 3.27 (d, *J* = 17.0 Hz, 1H), 2.64 (d, *J* = 17.1 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 173.1, 166.1, 153.9, 151.7, 148.2, 136.3, 136.2, 136.1, 135.2, 133.7, 130.2, 129.3, 128.8, 128.5, 127.9, 127.8, 126.5, 125.8, 125.2, 125.0, 124.8, 120.8, 116.9, 116.7, 114.1, 113.5, 80.1, 61.3, 50.9, 49.8, 46.4, 39.3.

IR (KBr) υ: 3421, 3069, 2923, 2222, 1594, 1553, 1483, 1459, 1362, 1315, 1235, 1162, 1016, 898, 749, 702 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{25}N_4O^+$ $[M + H]^+$ 553.2023; Found 553.2020.

Control experiments to illustrate the formation of compound 4a.



To a solution of **3a** (0.1 mmol, 1.0 equiv) in N, N-dimethylformamide (0.75 mL), tetramethylguanidine (0.04 mmol, 0.40 equiv) was added. Then, the resulting reaction mixture was stirred at 100 °C in oil bath for 0.5 hours. Upon completion (monitored by TLC), the reaction solution was cooled to room temperature. Water was added (10 mL) and the mixture was extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with brine (15 mL), dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 2 : 1) to afford pure products **4a**, 51.2 mg, 90% yield.

5. Mechanism study

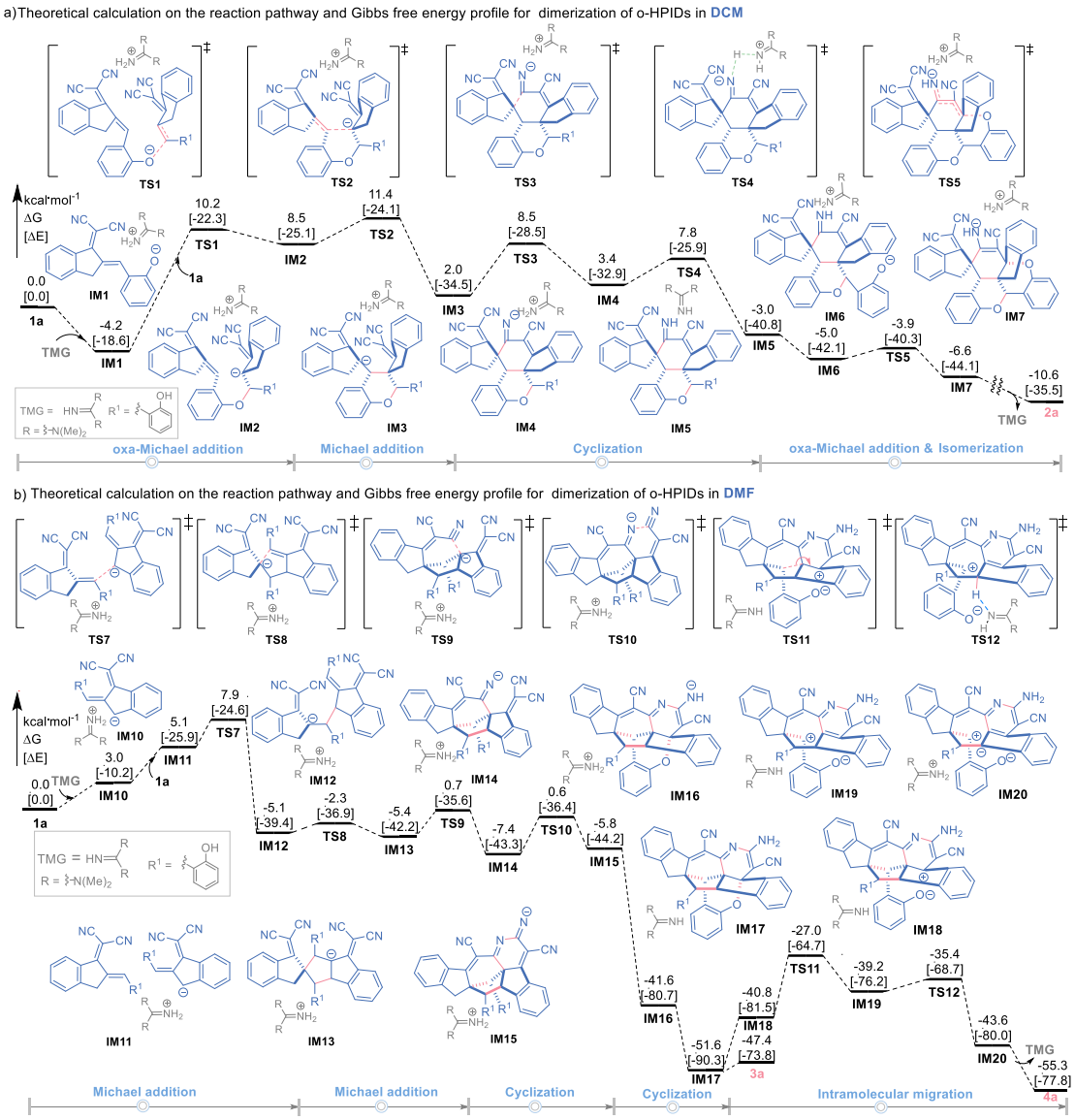


Fig. S7 DFT calculations on the reaction pathway and Gibbs free energy profile for the tandem reaction.

Density functional theory (DFT) calculations were performed to gain mechanistic insight into the dimerization of *o*-HPIDs. As illustrated in Figure S7a, the overall reaction pathway in DCM can be divided into four main stages.

Firstly, dehydrogenation of the hydroxyl group in *o*-HPIDs **1a** occurs in the presence of the base TMG, yielding a more stable intermediate **IM1**. In the following, the involvement of another substrate **1a** facilitates an intermolecular oxa-Michael addition via transition state **TS1**, with a free energy barrier of 14.4 kcal/mol^{-1}, generating the carbanion intermediate **IM2**. Secondly, **IM2** undergoes an intramolecular Michael addition via **TS2**, with a small barrier of 2.9 kcal/mol, leading to the formation of stable intermediate, **IM3**. In the third stage, **IM3** undergoes an intramolecular ring-closing reaction through **TS3** with a barrier of 6.5 kcal/mol, producing the intermediate **IM4**. Subsequent protonation of **IM4** via **TS4** yields a slightly more stable intermediate **IM5**. Finally, with the assistance of TMG, **IM6** undergoes a second intramolecular oxa-Michael addition via a very low free energy barrier of 1.1 kcal/mol (**IM6→TS5**), followed by isomerization process to form **IM7**. Protonation of **IM7** ultimately provides the final product **2a** (See Figure S8 for details), with exergonic by 10.6 kcal/mol. Among all these steps, the first intermolecular oxa-Michael addition, with a free energy barrier of 14.4 kcal/mol, is identified as the rate-determining step (RDS) for the formation of **2a**. These findings are in good agreement with the experimentally observed mild reaction conditions (see Table S1).

Alternatively, we investigated the reaction mechanism of the tandem transformation in DMF. As depicted in S7b, the process is initiated by dehydrogenation at the methylene position of *o*-HPIDs **1a**, generating the carbanion intermediate **IM10** (See Figure S9 for details). The subsequent addition of a second equivalent of substrate **1a** yields the slightly less stable intermediate **IM11**, which then undergoes a Michael addition via **TS7** to produce the thermodynamically more stable carbanion intermediate **IM12**. Next, an intramolecular Michael addition occurs readily through a five-membered ring

transition state (**TS8**), forming intermediate **IM13**. This is followed by an intramolecular ring-closing step via **TS9**, with a relatively low free energy barrier, leading to the iminium intermediate **IM14** featuring a seven-membered ring structure. Subsequently, a nucleophilic attack of the iminium group on the cyano group takes place via **TS10**, leading to the intermediate **IM16**. A subsequent proton transfer step yields the final product **3a**, with an overall exergonicity of -47.4 kcal/mol, providing a strong thermodynamic driving force for the reaction. The highest free energy barrier encountered in this pathway is 8.0 kcal/mol (**IM14 → TS10**), making it the rate-determining step (RDS) for the formation of **3a**. This low barrier aligns well with the mild experimental conditions observed (25 °C). On the other hand, intermediate **IM17** may undergo a structural transformation into **IM18**, which then proceeds through a C–C bond cleavage via **TS11** to generate the slightly less stable intermediate **IM19**. However, the following deprotonation step occurs readily, with a small barrier of 3.8 kcal/mol, yielding the more stable intermediate **IM20**. This intermediate then provides the final product **4a** in a highly exergonic step (−55.3 kcal/mol) and concurrently regenerates TMG for the next catalytic cycle. Remarkably, the rate-determining step (RDS) for the formation of product **4a** exhibits a much higher free energy barrier of 24.6 kcal/mol (**IM17→TS11**) compared to that of product **3a** (8.0 kcal/mol, **IM14 → TS10**), which aligns well with the experimentally observed higher reaction temperature (100 °C) for producing product **4a**.

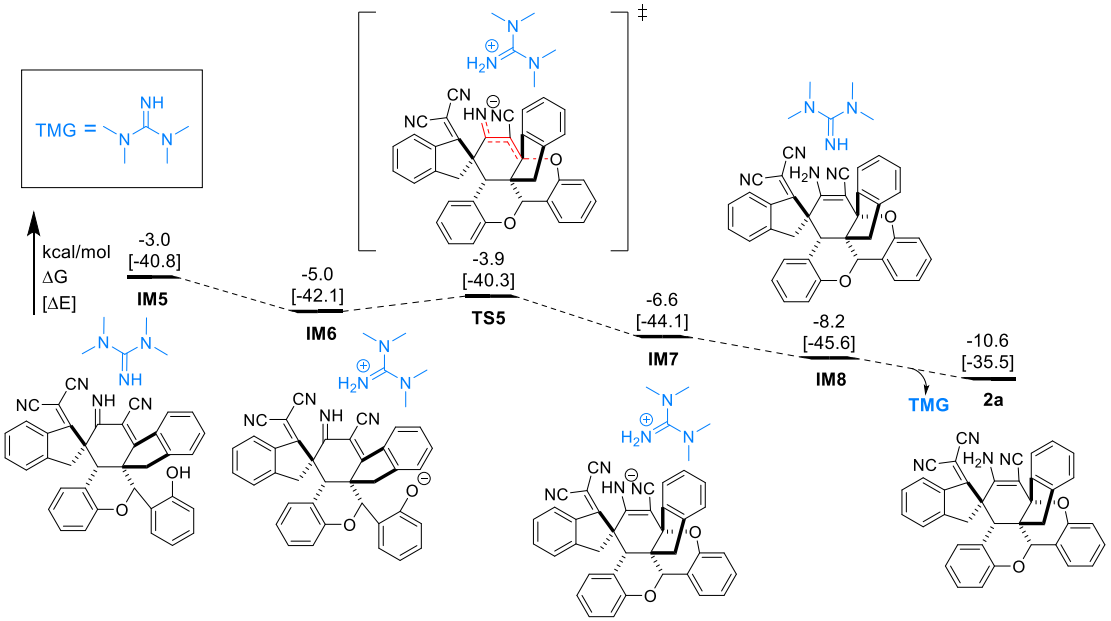


Fig. S8 Free energy and electronic energy profile for the stage III at BP86+D3BJ/def2-TZVPP (IEFPCM,Solvent = Dichloromethane)//BP86+D3BJ/def2-SVP(IEFPCM, Solvent= Dichloromethane) level.

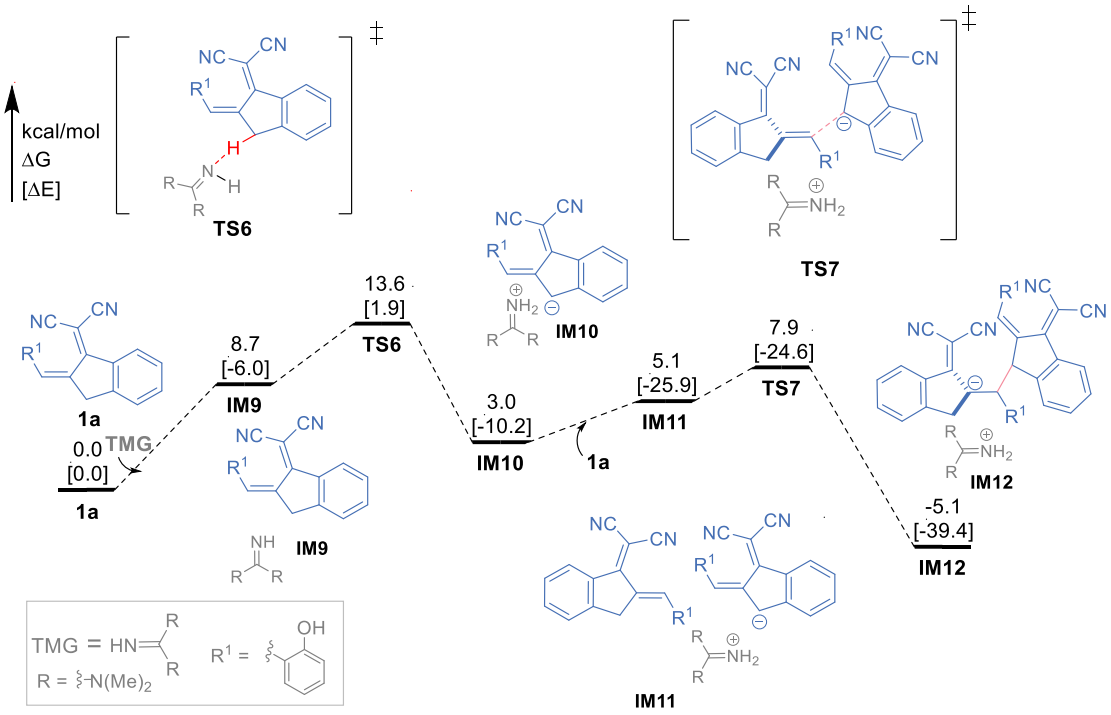
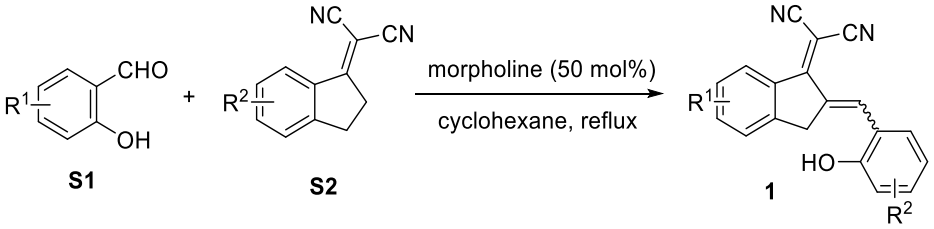


Fig. S9 Free energy and electronic energy profile for the stage I at the BP86+D3BJ/def2-TZVPP(SMD, Solvent = N,N-dimethylformamide) //BP86+D3BJ/def2-SVP(IEFPCM,Solvent= N,N-dimethylformamide) level.

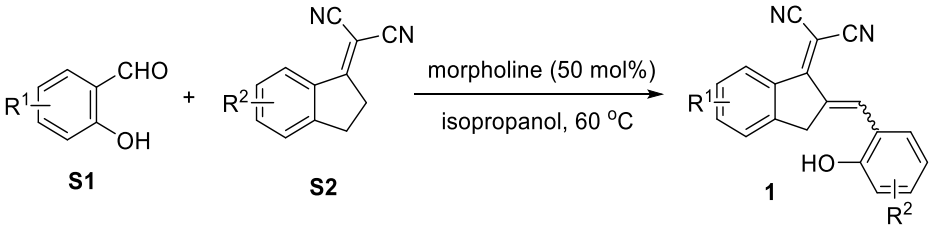
6. Procedure for the synthesis of compounds 1 and characteristic data

General synthetic procedure 1:



To a solution of substituted 2-hydroxybenzaldehyde **S1** (1.2 equiv) in cyclohexane (0.2 M), substituted 2-(2,3-dihydro-1H-inden-1-ylidene)malononitrile **S2** (1.0 equiv) was added to a sealed reaction tube equipped with a stir bar. Then, the reaction temperature was elevated to 80 ^{o}C in oil bath, after which morpholine (0.5 equiv) was added. The resulting mixture was stirred at 80 ^{o}C in oil bath for 0.5 - 6 hours. Upon completion (monitored by TLC), the reaction mixture was cooled to room temperature, and then filtered in vacuo. The residue was subsequently washed with petroleum ether for three times, and allowed to dry at room temperature to afford desired products **1**.

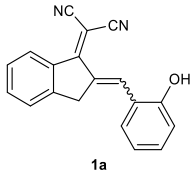
General synthetic procedure 2:



To a solution of substituted 2-hydroxybenzaldehyde **S1** (1.2 equiv) in isopropanol (0.2 M), substituted 2-(2,3-dihydro-1H-inden-1-ylidene)malononitrile **S2** (1.0 equiv) and morpholine (0.5 equiv) were added at 25 ^{o}C. Then, the resulting mixture was stirred at 60 ^{o}C in oil bath for 10 min to 1 hour. Upon completion (monitored by TLC), the reaction mixture was cooled to room temperature, and then filtered in vacuo. The

residue was subsequently washed with petroleum ether for three times, and allowed to dry at room temperature to afford desired products **1**.

2-(2-(2-hydroxybenzylidene)-2,3-dihydro-1H-inden-1-ylidene)malononitrile (1a)



1a

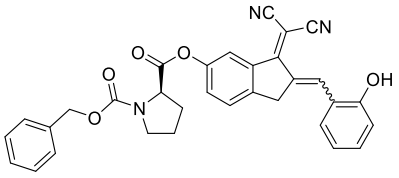
The compound **1a** was prepared according to general procedure **1**. R_f = 0.31 (dichloromethane/ethyl acetate = 40:1). Orange solid, 1226.0 mg, 78% yield, reaction time = 4.5 h, m.p. 171-172 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 10.37 (s, 1H), 8.61 (s, 1H), 8.40 (d, *J* = 8.0 Hz, 1H), 7.72 – 7.67 (m, 2H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.55 (t, *J* = 7.8 Hz, 1H), 7.32 (t, *J* = 7.7 Hz, 1H), 6.98 – 6.92 (m, 2H), 4.08 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 167.5, 157.4, 148.5, 135.8, 135.7, 134.6, 132.3, 131.8, 130.1, 128.0, 126.0, 124.8, 122.0, 119.5, 115.9, 115.6, 115.3, 66.9, 36.8.

HRMS (ESI) m/z: Calcd for $C_{19}H_{13}N_2O^+$ $[M + H]^+$ 285.1022; Found 285.1023.

1-benzyl 2-(3-(dicyanomethylene)-2-(2-hydroxybenzylidene)-2,3-dihydro-1H-inden-5-yl) (R)-pyrrolidine-1,2-dicarboxylate (1aa)



1aa

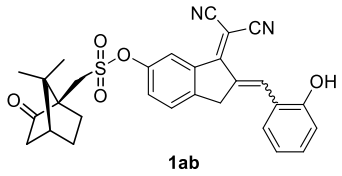
The compound **1aa** was prepared according to general procedure **2**. Upon completion (monitored by TLC), the reaction solution was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 3 : 1) to afford pure products **1aa**. R_f = 0.25 (petroleum ether/ethyl acetate = 3:1). Orange oil, 347.9 mg, 44% yield, reaction time = 1 h.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 18.0 Hz, 1H), 8.17 (d, *J* = 5.1 Hz, 1H), 7.50 (dd, *J* = 17.4, 7.9 Hz, 1H), 7.44 – 7.28 (m, 8H), 6.97 (q, *J* = 7.2 Hz, 1H), 6.93 – 6.76 (m, 2H), 5.43 – 5.22 (m, 1H), 5.21 – 5.07 (m, 1H), 4.71 – 4.54 (m, 1H), 3.93 (s, 1H), 3.84 (d, *J* = 14.9 Hz, 1H), 3.79 – 3.51 (m, 2H), 2.47 – 2.35 (m, 1H), 2.32 – 2.21 (m, 1H), 2.15 – 1.94 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6, 171.4, 166.7, 166.5, 156.5, 156.4, 155.5, 154.6, 150.3, 150.0, 145.3, 145.2, 137.8, 137.7, 136.5, 135.9, 135.8, 133.2, 132.9, 132.4, 132.3, 130.0, 128.7, 128.5, 128.4, 128.3, 128.0, 128.0, 126.2, 126.0, 122.6, 122.5, 120.8, 120.6, 118.4, 118.2, 116.5, 115.2, 115.2, 114.8, 114.8, 69.3, 69.1, 67.7, 67.6, 59.6, 59.0, 47.3, 46.9, 36.9, 36.8, 31.2, 30.3, 24.6, 23.8.

HRMS (ESI) m/z: Calcd for $C_{32}H_{26}N_3O_5^+$ $[M + H]^+$ 532.1867; Found 532.1864.

3-(dicyanomethylene)-2-(2-hydroxybenzylidene)-2,3-dihydro-1H-inden-5-yl ((1R, 4S)-7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methanesulfonate (1ab)



1ab

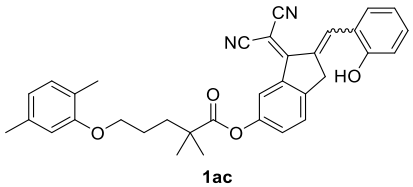
The compound **1ab** was prepared according to general procedure **2**. R_f = 0.20 (petroleum ether/ethyl acetate = 3:1). Orange solid, 555.0 mg, 72% yield, reaction time = 10 min, m.p. 132-133 °C.

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 10.47 (s, 1H), 8.64 (s, 1H), 8.27 (d, *J* = 2.1 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.72 – 7.67 (m, 2H), 7.37 – 7.30 (m, 1H), 7.01 – 6.91 (m, 2H), 4.11 (s, 2H), 3.75 (d, *J* = 15.2 Hz, 1H), 3.64 (d, *J* = 15.3 Hz, 1H), 2.43 – 2.32 (m, 1H), 2.32 – 2.26 (m, 1H), 2.09 (t, *J* = 4.5 Hz, 1H), 1.97 (d, *J* = 18.5 Hz, 2H), 1.70 – 1.56 (m, 1H), 1.49 – 1.39 (m, 1H), 1.05 (s, 3H), 0.84 (s, 3H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 213.4, 166.3, 157.7, 148.0, 147.2, 137.2, 135.7, 132.7, 132.3, 130.2, 128.5, 127.6, 121.9, 119.7, 118.4, 116.0, 115.4, 115.0, 68.3, 57.6, 48.2, 47.8, 42.2, 42.0, 36.6, 26.3, 25.0, 19.2, 19.2.

HRMS (ESI) m/z: Calcd for $C_{29}H_{27}N_2O_5S^+$ $[M + H]^+$ 515.1635; Found 515.1629.

3-(dicyanomethylene)-2-(2-hydroxybenzylidene)-2,3-dihydro-1H-inden-5-yl 5-(2, 5-dimethylphenoxy)-2,2-dimethylpentanoate (1ac)



1ac

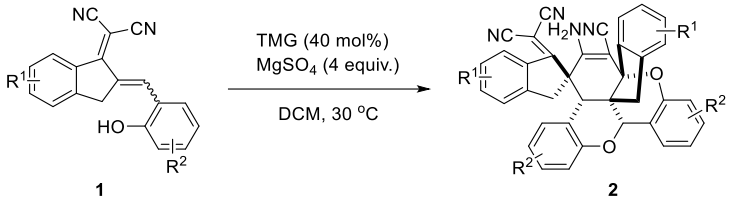
The compound **1ac** was prepared according to general procedure **2**. R_f = 0.15 (petroleum ether/ dichloromethane = 1:2). Red solid, 300.0 mg, 80% yield, reaction time = 0.5 h, m.p. 158-159 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.77 (s, 1H), 8.22 (d, *J* = 1.0 Hz, 1H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.46 (d, *J* = 8.3 Hz, 1H), 7.33 – 7.27 (m, 1H), 7.23 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.02 – 6.96 (m, 2H), 6.87 (d, *J* = 8.2 Hz, 1H), 6.69 – 6.62 (m, 2H), 6.48 (s, 1H), 4.00 (t, *J* = 5.4 Hz, 2H), 3.95 (s, 2H), 2.31 (s, 3H), 2.17 (s, 3H), 1.96 – 1.84 (m, 4H), 1.41 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 176.9, 167.0, 157.0, 156.4, 150.7, 145.1, 137.9, 136.7, 135.8, 132.5, 132.4, 130.4, 129.9, 128.4, 126.2, 123.7, 122.5, 121.0, 120.9, 118.9, 116.4, 115.3, 114.8, 112.1, 68.8, 67.8, 42.7, 37.3, 36.9, 25.4, 25.2, 21.5, 16.0.

HRMS (ESI) m/z: Calcd for $C_{34}H_{33}N_2O_4^+$ $[M + H]^+$ 533.2435; Found 533.2439.

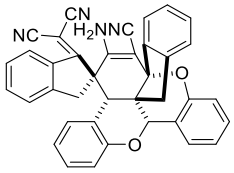
7. Procedure for the synthesis of compounds 2 and characteristic data



General synthetic procedure 3:

To a solution of ortho-hydroxyphenyl-substituted indene-dienes **1** (0.2 mmol, 1.0 equiv) and anhydrous sodium sulfate (0.80 mmol, 4.0 equiv) in dichloromethane (1.5 mL), tetramethylguanidine (0.08 mmol, 0.40 equiv) was added at 30 °C. Then, the resulting mixture was stirred at 30 °C in oil bath for 12 - 144 hours. Upon completion (monitored by TLC), the reaction solution was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 2 : 1) to afford pure products **2**.

2-(18'-amino-19'-cyano-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2a)



The compound **2a** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.32 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 34.3 mg, 60% yield, reaction time = 48 h, m.p. 270-271 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.23 (d, *J* = 7.8 Hz, 1H), 7.92 (d, *J* = 7.8 Hz, 1H), 7.60 (d, *J* = 7.4 Hz, 1H), 7.50 – 7.36 (m, 2H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.20 (t, *J* = 7.4 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 1H), 7.07 – 7.02 (m, 2H), 7.03 – 6.99 (m, 2H), 6.97 (d, *J*

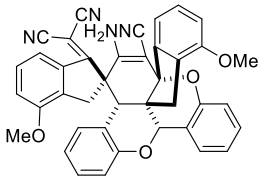
= 7.5 Hz, 1H), 6.71 (d, *J* = 8.0 Hz, 1H), 6.58 (d, *J* = 7.7 Hz, 1H), 6.52 (s, 2H), 6.33 – 6.24 (m, 1H), 5.76 (s, 1H), 3.51 (d, *J* = 18.1 Hz, 1H), 3.38 (s, 1H), 3.26 (s, 1H), 2.60 (d, *J* = 17.1 Hz, 1H), 2.12 (d, *J* = 17.1 Hz, 1H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 178.9, 156.5, 152.9, 152.4, 150.6, 143.2, 138.8, 137.0, 135.4, 131.6, 129.4, 129.3, 128.3, 127.9, 127.4, 125.2, 125.0, 124.8, 124.8, 124.1, 121.7, 119.3, 119.2, 117.1, 116.7, 115.9, 114.1, 111.6, 87.3, 79.2, 77.6, 68.7, 57.3, 47.0, 47.0, 43.2, 40.4.

IR (KBr) υ: 3455, 3231, 3037, 2923, 2202, 1729, 1639, 1598, 1555, 1482, 1365, 1310, 1238, 1122, 1046, 948, 899, 756 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{25}N_4O_2^+$ $[M + H]^+$ 569.1972; Found 569.1970.

2-(18'-amino-19'-cyano-4,14'-dimethoxy-5a'H,15'H,16'H-spiro[indene-2,17'-[10a, 16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2b)



2b

The compound **2b** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.24 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 30.6 mg, 49% yield, reaction time = 48 h, m.p. 270-271 °C.

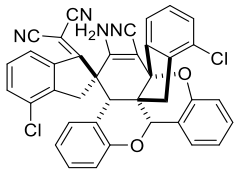
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.81 (d, *J* = 8.1 Hz, 1H), 7.59 (d, *J* = 7.5 Hz, 1H), 7.51 (d, *J* = 7.9 Hz, 1H), 7.37 (t, *J* = 8.1 Hz, 1H), 7.28 (t, *J* = 8.0 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 1H), 7.09 – 6.94 (m, 4H), 6.78 (d, *J* = 8.2 Hz, 1H), 6.68 (d, *J* = 7.9 Hz, 1H), 6.61 (d, *J* = 7.7 Hz, 1H), 6.47 (s, 2H), 6.29 (t, *J* = 7.1 Hz, 1H), 5.71 (s, 1H), 3.63 (s, 3H), 3.56 (s, 3H), 3.36 (d, *J* = 18.3 Hz, 1H), 3.23 (s, 1H), 3.18 (d, *J* = 18.0 Hz, 1H), 2.34 (d, *J* = 17.1 Hz, 1H), 2.00 (d, *J* = 17.0 Hz, 1H).

^{13}C NMR (150 MHz, DMSO-d_6) δ 178.9, 156.5, 155.1, 154.9, 153.0, 152.3, 144.8, 138.5, 138.4, 131.4, 129.9, 129.4, 129.4, 128.4, 126.2, 125.7, 124.1, 121.8, 119.3, 119.3, 117.1, 116.9, 116.5, 116.2, 115.8, 114.1, 111.6, 110.5, 87.9, 79.4, 78.2, 68.8, 57.5, 55.8, 54.9, 47.1, 47.1, 40.1, 37.8.

IR (KBr) υ: 3448, 2927, 2846, 2201, 1727, 1643, 1597, 1555, 1483, 1365, 1266, 1079, 962, 760 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{29}N_4O_4^+$ $[M + H]^+$ 629.2183; Found 629.2181.

2-(18'-amino-4,14'-dichloro-19'-cyano-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2c)



2c

The compound **2c** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-4:1 as eluent. R_f = 0.50 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 28.9 mg, 45% yield, reaction time = 48 h, m.p. 282-283 °C.

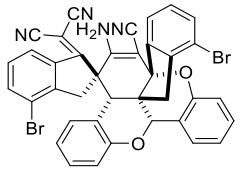
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, *J* = 8.0 Hz, 1H), 7.97 (d, *J* = 7.7 Hz, 1H), 7.66 (d, *J* = 7.4 Hz, 1H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.31 (t, *J* = 7.9 Hz, 1H), 7.27 – 7.23 (m, 1H), 7.20 – 7.13 (m, 1H), 7.15 – 7.04 (m, 3H), 6.82 (d, *J* = 8.0 Hz, 1H), 6.46 – 6.37 (m, 2H), 5.67 (s, 1H), 4.46 (s, 2H), 3.66 (d, *J* = 18.3 Hz, 1H), 3.46 (s, 1H), 3.37 (d, *J* = 18.4 Hz, 1H), 2.80 (d, *J* = 17.7 Hz, 1H), 2.32 (d, *J* = 17.7 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 178.2, 153.6, 153.1, 152.4, 147.9, 144.3, 137.7, 137.6, 135.7, 131.8, 130.6, 130.5, 130.4, 129.9, 129.9, 129.8, 128.8, 124.4, 124.1, 123.9, 122.3, 120.3, 117.6, 117.4, 117.4, 116.1, 112.6, 110.3, 86.7, 85.4, 80.0, 69.2, 56.9, 47.8, 47.7, 42.5, 40.3.

IR (KBr) υ: 3435, 3236, 3072, 2926, 2504, 2207, 1727, 1644, 1599, 1562, 1486, 1457, 1370, 1241, 1145, 955, 778 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Cl_2N_4O_2^+$ $[M + H]^+$ 637.1193; Found 637.1193.

2-(18'-amino-4,14'-dibromo-19'-cyano-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2d)



2d

The compound **2d** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-4:1 as eluent. R_f = 0.46 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 40.2 mg, 55% yield, reaction time = 24 h, m.p. 277-279 °C.

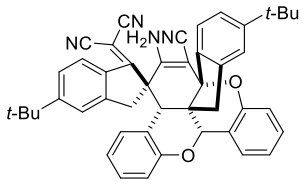
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.44 (d, *J* = 8.1 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.67 (d, *J* = 7.5 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.42 (d, *J* = 7.9 Hz, 1H), 7.30 (t, *J* = 8.0 Hz, 1H), 7.26 – 7.20 (m, 1H), 7.16 (t, *J* = 7.7 Hz, 1H), 7.13 – 7.04 (m, 3H), 6.82 (d, *J* = 8.0 Hz, 1H), 6.45 – 6.35 (m, 2H), 5.68 (s, 1H), 4.49 (s, 2H), 3.62 (d, *J* = 18.3 Hz, 1H), 3.44 (s, 1H), 3.34 (d, *J* = 18.3 Hz, 1H), 2.78 (d, *J* = 17.6 Hz, 1H), 2.28 (d, *J* = 17.6 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 178.4, 153.6, 153.1, 152.5, 149.9, 144.1, 139.7, 138.8, 137.4, 133.0, 130.6, 130.4, 130.0, 129.9, 128.8, 124.7, 124.4, 124.3, 122.3, 120.5, 120.3, 119.7, 117.6, 117.4, 117.4, 116.1, 112.6, 110.3, 86.9, 85.4, 80.0, 69.2, 56.7, 47.8, 47.4, 44.7, 42.2.

IR (KBr) υ: 3435, 3202, 2926, 2848, 2207, 1722, 1641, 1597, 1566, 1486, 1455, 1332, 1289, 1241, 1134, 954, 761 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Br_2N_4O_2^+$ $[M + H]^+$ 725.0182; Found 725.0183.

2-(18'-amino-5,13'-di-tert-butyl-19'-cyano-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2e)



2e

The compound **2e** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-4:1 as eluent. R_f = 0.66 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 29.6 mg, 43% yield, reaction time = 96 h, m.p. 288-290 °C.

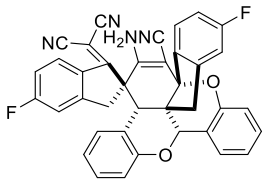
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.7 Hz, 1H), 7.95 (d, *J* = 8.3 Hz, 1H), 7.62 (d, *J* = 7.4 Hz, 1H), 7.45 – 7.38 (m, 1H), 7.34 (d, *J* = 7.9 Hz, 1H), 7.17 – 7.09 (m, 1H), 7.08 – 6.98 (m, 4H), 6.94 – 6.80 (m, 2H), 6.43 – 6.33 (m, 2H), 5.65 (s, 1H), 4.40 (s, 2H), 3.62 (d, *J* = 17.7 Hz, 1H), 3.49 (s, 1H), 3.36 (d, *J* = 17.6 Hz, 1H), 2.86 (d, *J* = 16.9 Hz, 1H), 2.23 (d, *J* = 16.9 Hz, 1H), 1.23 (s, 18H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 178.3, 161.7, 153.6, 153.3, 153.0, 153.0, 151.0, 139.5, 138.7, 133.9, 130.5, 129.6, 128.4, 126.8, 125.5, 125.4, 124.9, 124.8, 124.1, 121.8, 121.7, 121.4, 120.0, 117.9, 117.7, 117.3, 116.9, 113.6, 110.8, 86.4, 85.4, 76.6, 69.5, 57.6, 48.3, 47.5, 43.3, 40.8, 35.8, 34.9, 31.4, 30.9.

IR (KBr) υ: 3434, 3238, 2962, 2213, 1641, 1608, 1553, 1486, 1366, 1241, 1042, 946, 827, 753 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{46}H_{41}N_4O_2^+$ $[M + H]^+$ 681.3224; Found 681.3222.

2-(18'-amino-19'-cyano-5,13'-difluoro-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2f)



2f

The compound **2f** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.41 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 25.4 mg, 42% yield, reaction time = 48 h, m.p. 270-271 °C.

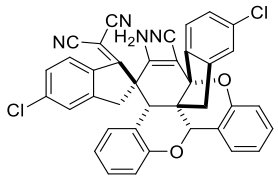
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (dd, *J* = 9.1, 4.8 Hz, 1H), 8.02 (dd, *J* = 8.7, 5.0 Hz, 1H), 7.62 (d, *J* = 7.5 Hz, 1H), 7.21 – 7.09 (m, 3H), 7.09 – 6.99 (m, 3H), 6.82 (d, *J* = 8.0 Hz, 1H), 6.77 (d, *J* = 7.5 Hz, 1H), 6.57 (d, *J* = 8.4 Hz, 1H), 6.47 (t, *J* = 7.4 Hz, 1H), 6.43 (d, *J* = 7.3 Hz, 1H), 5.59 (s, 1H), 4.43 (s, 2H), 3.64 (d, *J* = 18.1 Hz, 1H), 3.53 (s, 1H), 3.40 (d, *J* = 18.0 Hz, 1H), 2.84 (d, *J* = 17.4 Hz, 1H), 2.23 (d, *J* = 17.4 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 177.2, 167.6 (d, *J* = 263.9 Hz), 164.0 (d, *J* = 248.2 Hz), 153.8 (d, *J* = 10.4 Hz), 153.6, 153.2, 152.5, 141.5 (d, *J* = 9.1 Hz), 138.3 (d, *J* = 2.7 Hz), 132.6 (d, *J* = 2.3 Hz), 130.3, 130.2, 128.8, 128.3 (d, *J* = 10.5 Hz), 127.3 (d, *J* = 9.7 Hz), 124.8, 124.2, 122.2, 120.4, 117.7, 117.6, 117.5, 117.3, 116.6, 115.7, 115.5, 113.1, 112.4 (d, *J* = 22.5 Hz), 111.6 (d, *J* = 22.5 Hz), 110.6, 85.7, 85.2, 69.4, 57.6, 48.6, 47.4, 43.0, 40.7.

IR (KBr) υ: 3482, 3240, 2928, 2202, 1730, 1645, 1606, 1558, 1486, 1449, 1371, 1245, 1110, 1044, 952, 855, 759 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}F_2N_4O_2^+$ $[M + H]^+$ 605.1784; Found 605.1780.

2-(18'-amino-5,13'-dichloro-19'-cyano-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2g)



2g

The compound **2g** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.51 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 25.5 mg, 40% yield, reaction time = 48 h, m.p. 274-276 °C.

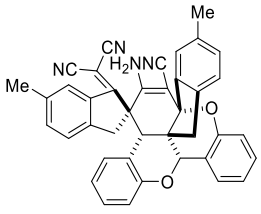
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41 (d, *J* = 8.7 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.62 (d, *J* = 7.5 Hz, 1H), 7.37 (d, *J* = 8.7 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 1H), 7.20 – 7.10 (m, 2H), 7.10 – 7.03 (m, 3H), 6.87 (s, 1H), 6.81 (d, *J* = 8.0 Hz, 1H), 6.48 (t, *J* = 7.3 Hz, 1H), 6.42 (d, *J* = 6.7 Hz, 1H), 5.58 (s, 1H), 4.46 (s, 2H), 3.62 (d, *J* = 17.9 Hz, 1H), 3.52 (s, 1H), 3.39 (d, *J* = 18.0 Hz, 1H), 2.82 (d, *J* = 17.4 Hz, 1H), 2.23 (d, *J* = 17.3 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 177.3, 153.5, 153.3, 152.6, 151.8, 143.4, 141.0, 141.0, 135.8, 134.6, 130.4, 130.2, 129.9, 128.8, 128.5, 126.8, 126.7, 125.6, 125.0, 124.6, 124.3, 122.3, 120.5, 117.7, 117.6, 117.3, 116.5, 112.9, 110.5, 85.7, 85.0, 78.5, 69.3, 57.3, 48.3, 47.5, 42.8, 40.5.

IR (KBr) υ: 3434, 3245, 3075, 2882, 2818, 2212, 1908, 1640, 1601, 1560, 1482, 1329, 1240, 1075, 949, 824, 757, 670 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Cl_2N_4O_2^+$ $[M + H]^+$ 637.1193; Found 637.1192.

2-(18'-amino-19'-cyano-5,12'-dimethyl-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-3(1H)-ylidene)malononitrile (2h)



2h

The compound **2h** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.39 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 25.4 mg, 43% yield, reaction time = 48 h, m.p. 318-319 °C.

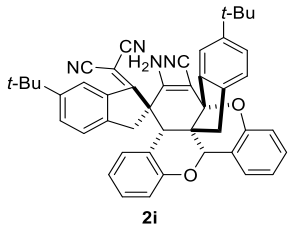
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.83 (s, 1H), 7.62 (d, *J* = 7.5 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.13 (t, *J* = 7.7 Hz, 1H), 7.10 – 7.00 (m, 4H), 6.98 (d, *J* = 7.9 Hz, 1H), 6.83 (d, *J* = 8.1 Hz, 1H), 6.78 (d, *J* = 7.7 Hz, 1H), 6.48 – 6.42 (m, 2H), 5.62 (s, 1H), 4.36 (s, 2H), 3.60 (d, *J* = 17.8 Hz, 1H), 3.56 (s, 1H), 3.33 (d, *J* = 17.7 Hz, 1H), 2.82 (d, *J* = 16.8 Hz, 1H), 2.40 (s, 6H), 2.21 (d, *J* = 16.9 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 178.8, 153.7, 153.5, 152.8, 148.1, 142.6, 139.3, 138.1, 137.7, 136.4, 136.0, 130.8, 130.2, 129.9, 128.6, 126.0, 125.5, 125.1, 124.6, 124.5, 124.2, 121.8, 120.3, 118.0, 117.6, 117.3, 117.0, 113.3, 111.0, 86.3, 85.1, 77.7, 69.4, 57.3, 48.3, 47.4, 43.1, 40.3, 21.7, 21.6.

IR (KBr) υ: 3433, 3239, 3037, 2927, 2216, 1727, 1641, 1603, 1552, 1487, 1453, 1369, 1299, 1242, 1110, 1047, 954, 911, 808, 757 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{29}N_4O_2^+$ $[M + H]^+$ 597.2285; Found 597.2283.

2-(18'-amino-5,12'-di-tert-butyl-19'-cyano-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-3(1H)-ylidene)malononitrile (2i)



2i

The compound **2i** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.66 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 31.9 mg, 47% yield, reaction time = 96 h, m.p. 285-287 °C.

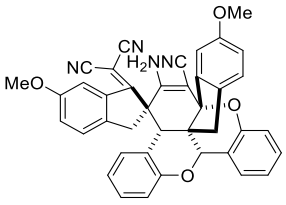
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.7 Hz, 1H), 7.95 (d, *J* = 8.3 Hz, 1H), 7.62 (d, *J* = 7.4 Hz, 1H), 7.41 (d, *J* = 8.6 Hz, 1H), 7.34 (d, *J* = 8.2 Hz, 1H), 7.13 (t, *J* = 7.5 Hz, 1H), 7.07 – 6.99 (m, 4H), 6.86 (s, 1H), 6.83 (d, *J* = 8.0 Hz, 1H), 6.42 – 6.34 (m, 2H), 5.65 (s, 1H), 4.41 (s, 2H), 3.61 (d, *J* = 17.7 Hz, 1H), 3.49 (s, 1H), 3.36 (d, *J* = 17.6 Hz, 1H), 2.85 (d, *J* = 16.9 Hz, 1H), 2.23 (d, *J* = 17.0 Hz, 1H), 1.23 (s, 18H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 178.3, 161.7, 153.6, 153.3, 153.0, 152.9, 150.9, 139.5, 138.7, 133.9, 130.5, 129.6, 128.4, 126.8, 125.5, 125.4, 124.9, 124.8, 124.1, 121.8, 121.7, 121.3, 119.9, 117.9, 117.7, 117.3, 116.9, 113.6, 110.8, 86.4, 85.4, 76.6, 69.5, 57.6, 48.3, 47.5, 43.3, 40.8, 35.8, 34.9, 31.5, 30.9.

IR (KBr) υ: 3435, 3243, 3044, 2963, 2350, 2213, 1642, 1609, 1552, 1487, 1367, 1241, 1043, 949, 824, 752 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{46}H_{41}N_4O_2^+$ $[M + H]^+$ 681.3224; Found 681.3222.

2-(18'-amino-19'-cyano-5,12'-dimethoxy-5a'H,15'H,16'H-spiro[indene-2,17'-[10a, 16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-3(1H)-ylidene)malononitrile (2j)



2j

The compound **2j** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.24 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 33.9 mg, 54% yield, reaction time = 48 h, m.p. 206-207 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 – 7.92 (m, 1H), 7.62 (d, *J* = 7.5 Hz, 1H), 7.57 (s, 1H), 7.14 (t, *J* = 7.7 Hz, 1H), 7.11 – 7.04 (m, 2H), 7.05 – 7.00 (m, 2H), 6.98 (d, *J* = 8.6 Hz, 1H), 6.88 – 6.83 (m, 1H), 6.82 – 6.77 (m, 2H), 6.51 – 6.42 (m, 2H), 5.60 (s, 1H),

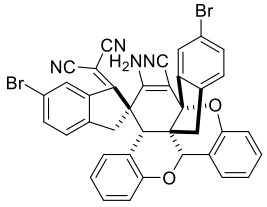
4.39 (s, 2H), 3.87 (s, 3H), 3.85 (s, 3H), 3.60 – 3.53 (m, 2H), 3.31 (d, *J* = 17.6 Hz, 1H), 2.79 (d, *J* = 16.6 Hz, 1H), 2.19 (d, *J* = 16.7 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 178.9, 160.3, 159.8, 153.7, 153.6, 152.8, 143.8, 143.7, 137.3, 130.9, 130.1, 129.9, 128.6, 126.3, 126.1, 125.5, 124.7, 124.2, 121.9, 120.3, 117.9, 117.6, 117.3, 117.1, 113.4, 110.9, 109.4, 106.7, 86.3, 84.9, 77.8, 69.4, 57.6, 55.9, 55.7, 48.7, 47.6, 42.8, 40.0.

IR (KBr) υ: 3431, 3245, 2951, 2833, 2210, 1724, 1643, 1600, 1552, 1491, 1294, 1240, 1159, 1104, 1032, 952, 817, 757 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{29}N_4O_4^+$ $[M + H]^+$ 629.2183; Found 629.2182.

2-(18'-amino-5,12'-dibromo-19'-cyano-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-3(1H)-ylidene)malononitrile (2k)



2k

The compound **2k** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.43 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 40.7 mg, 56% yield, reaction time = 48 h, m.p. 308-310 °C.

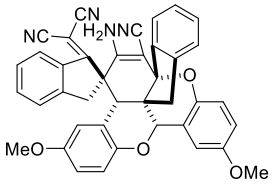
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.44 (d, *J* = 8.1 Hz, 1H), 8.01 (d, *J* = 7.7 Hz, 1H), 7.67 (d, *J* = 7.5 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.42 (d, *J* = 7.9 Hz, 1H), 7.30 (t, *J* = 8.0 Hz, 1H), 7.23 (t, *J* = 8.0 Hz, 1H), 7.16 (t, *J* = 7.7 Hz, 1H), 7.14 – 7.05 (m, 3H), 6.82 (d, *J* = 8.0 Hz, 1H), 6.50 – 6.35 (m, 2H), 5.68 (s, 1H), 4.49 (s, 2H), 3.62 (d, *J* = 18.4 Hz, 1H), 3.44 (s, 1H), 3.34 (d, *J* = 18.3 Hz, 1H), 2.78 (d, *J* = 17.6 Hz, 1H), 2.28 (d, *J* = 17.6 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 178.4, 153.6, 153.1, 152.5, 149.9, 144.1, 139.7, 138.8, 137.4, 133.0, 130.6, 130.4, 130.0, 129.9, 128.8, 124.7, 124.4, 124.3, 122.3, 120.5, 120.3, 119.7, 117.6, 117.4, 117.4, 116.1, 112.6, 110.3, 86.9, 85.4, 80.0, 69.2, 56.7, 47.8, 47.4, 44.7, 42.2.

IR (KBr) υ: 3442, 3242, 3072, 2928, 2600, 2351, 2210, 1722, 1640, 1600, 1565, 1485, 1456, 1289, 1240, 1133, 1050, 953, 763 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Br_2N_4O_2^+$ $[M + H]^+$ 725.0182; Found 725.0181.

2-(18'-amino-19'-cyano-2',7'-dimethoxy-5a'H,15'H,16'H-spiro[indene-2,17'-[10a, 16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2l)



2l

The compound **2l** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.23 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 35.0 mg, 56% yield, reaction time = 48 h, m.p. 271-272 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (d, *J* = 8.2 Hz, 1H), 8.07 (d, *J* = 7.8 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.26 – 7.23 (m, 1H), 7.18 – 7.13 (m, 2H), 6.94 (d, *J* = 9.0 Hz, 1H), 6.90 (d, *J* = 7.5 Hz, 1H), 6.72 (d, *J* = 8.7 Hz, 1H), 6.68 – 6.61 (m, 2H), 5.96 (d, *J* = 3.0 Hz, 1H), 5.54 (s, 1H), 4.39 (s, 2H), 3.79 (s, 3H), 3.70 (d, *J* = 18.0 Hz, 1H), 3.54 (s, 1H), 3.47 – 3.34 (m, 4H), 2.83 (d, *J* = 17.1 Hz, 1H), 2.26 (d, *J* = 17.1 Hz, 1H).

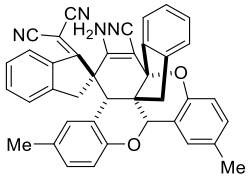
^{13}C NMR (125 MHz, $CDCl_3$) δ 179.1, 155.1, 153.4, 152.9, 151.0, 147.5, 146.2, 142.5, 139.2, 136.7, 136.2, 129.8, 129.1, 128.0, 126.8, 125.6, 125.5, 124.7, 118.5, 117.9, 117.3,

117.1, 113.8, 113.2, 113.1, 110.7, 110.2, 86.5, 85.5, 78.2, 69.6, 57.0, 55.9, 55.6, 48.3, 47.9, 43.3, 41.1.

IR (KBr) υ: 3410, 3244, 2942, 2836, 2196, 1644, 1604, 1559, 1492, 1432, 1364, 1310, 1222, 1163, 1039, 950, 892, 817, 732 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{29}N_4O_4^+$ $[M + H]^+$ 629.2183; Found 629.2183.

2-(18'-amino-19'-cyano-2',7'-dimethyl-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2m)



2m

The compound **2m** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.40 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 30.3 mg, 51% yield, reaction time = 48 h, m.p. 279-280 °C.

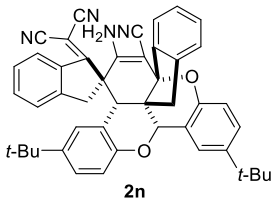
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (d, *J* = 8.2 Hz, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.43 – 7.36 (m, 2H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 7.4 Hz, 1H), 7.09 (d, *J* = 7.7 Hz, 1H), 6.94 – 6.87 (m, 3H), 6.84 (d, *J* = 8.1 Hz, 1H), 6.69 (d, *J* = 8.2 Hz, 1H), 6.17 (s, 1H), 5.58 (s, 1H), 4.41 (s, 2H), 3.66 (d, *J* = 17.8 Hz, 1H), 3.44 (s, 1H), 3.39 (d, *J* = 17.8 Hz, 1H), 2.85 (d, *J* = 17.0 Hz, 1H), 2.33 (s, 3H), 2.26 (d, *J* = 17.1 Hz, 1H), 1.84 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 179.1, 153.3, 151.4, 150.7, 150.6, 142.6, 139.2, 136.5, 136.4, 131.3, 131.0, 130.6, 129.8, 129.4, 129.0, 128.9, 127.9, 125.6, 125.4, 125.4, 124.8, 124.7, 124.6, 118.0, 117.3, 116.6, 116.5, 113.2, 110.6, 86.2, 85.5, 78.1, 69.3, 57.3, 48.2, 47.6, 43.3, 40.9, 21.1, 20.1.

IR (KBr) υ: 3451, 3229, 2923, 2855, 2196, 1643, 1601, 1559, 1492, 1376, 1304, 1236, 1144, 1046, 949, 901, 822, 739 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{29}N_4O_2^+$ $[M + H]^+$ 597.2285; Found 597.2287.

2-(18'-amino-2',7'-di-tert-butyl-19'-cyano-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2n)



2n

The compound **2n** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-4:1 as eluent. R_f = 0.64 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 34.5 mg, 51% yield, reaction time = 24 h, m.p. 266-268 °C.

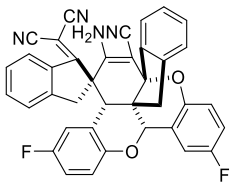
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (d, *J* = 8.2 Hz, 1H), 8.06 (d, *J* = 7.8 Hz, 1H), 7.61 (d, *J* = 1.3 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.29 – 7.23 (m, 1H), 7.16 – 7.06 (m, 3H), 7.00 (d, *J* = 8.7 Hz, 1H), 6.95 (d, *J* = 7.5 Hz, 1H), 6.74 (d, *J* = 8.4 Hz, 1H), 6.42 (d, *J* = 2.4 Hz, 1H), 5.62 (s, 1H), 4.37 (s, 2H), 3.70 (d, *J* = 18.0 Hz, 1H), 3.57 (s, 1H), 3.37 (d, *J* = 18.0 Hz, 1H), 2.89 (d, *J* = 17.1 Hz, 1H), 2.31 (d, *J* = 17.0 Hz, 1H), 1.32 (s, 9H), 0.94 (s, 9H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 179.4, 153.4, 151.3, 151.0, 150.4, 144.8, 143.1, 142.8, 139.3, 136.4, 136.1, 129.7, 128.9, 128.0, 127.3, 126.3, 125.9, 125.6, 125.5, 125.3, 124.9, 123.8, 120.9, 117.9, 116.9, 116.7, 116.2, 113.1, 110.9, 86.1, 85.4, 78.2, 69.5, 57.0, 48.2, 47.9, 43.4, 40.8, 34.6, 33.8, 31.7, 31.3.

IR (KBr) υ: 3458, 3234, 3040, 2960, 2926, 2861, 2206, 1722, 1640, 1603, 1559, 1495, 1365, 1305, 1243, 1139, 1044, 959, 903, 826, 759 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{46}H_{41}N_4O_2^+$ $[M + H]^+$ 681.3224; Found 681.3227.

2-(18'-amino-19'-cyano-2',7'-difluoro-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2o)



2o

The compound **2o** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.40 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 24.5 mg, 41% yield, reaction time = 48 h, m.p. 284-285 °C.

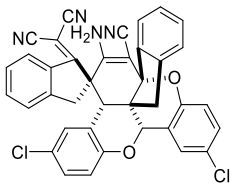
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (d, *J* = 8.2 Hz, 1H), 8.07 (d, *J* = 7.9 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.45 (t, *J* = 7.7 Hz, 1H), 7.38 – 7.25 (m, 3H), 7.14 (d, *J* = 7.7 Hz, 1H), 7.02 – 6.96 (m, 1H), 6.92 (d, *J* = 7.5 Hz, 1H), 6.85 – 6.73 (m, 3H), 6.16 (dd, *J* = 8.5, 3.0 Hz, 1H), 5.57 (s, 1H), 4.43 (s, 2H), 3.63 (d, *J* = 17.9 Hz, 1H), 3.52 (s, 1H), 3.45 (d, *J* = 17.9 Hz, 1H), 2.82 (d, *J* = 17.1 Hz, 1H), 2.25 (d, *J* = 17.2 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 178.2, 158.4 (d, *J* = 240.3 Hz), 156.2 (d, *J* = 241.5 Hz), 153.2, 150.2, 149.5 (d, *J* = 2.2 Hz), 148.4 (d, *J* = 1.9 Hz), 142.0, 138.7, 136.9, 136.0, 130.1, 129.5, 128.2, 126.7 (d, *J* = 8.1 Hz), 125.9, 125.6, 125.5, 124.8, 119.0 (d, *J* = 8.0 Hz), 118.2 (d, *J* = 7.9 Hz), 117.9 (d, *J* = 7.0 Hz), 117.7, 117.2 (d, *J* = 23.0 Hz), 116.3 (d, *J* = 23.6 Hz), 115.2 (d, *J* = 23.3 Hz), 112.9, 111.3 (d, *J* = 25.7 Hz), 110.6, 86.8, 85.2, 78.4, 69.6, 56.8, 47.9, 47.5, 43.2, 41.0.

IR (KBr) υ: 3454, 3234, 3075, 2927, 2200, 1720, 1643, 1601, 1558, 1489, 1437, 1360, 1309, 1241, 1154, 1044, 947, 819, 764 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}F_2N_4O_2^+$ $[M + H]^+$ 605.1784; Found 605.1785.

2-(18'-amino-2',7'-dichloro-19'-cyano-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2p)



2p

The compound **2p** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.51 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 34.2 mg, 54% yield, reaction time = 96 h, m.p. 290-291 °C.

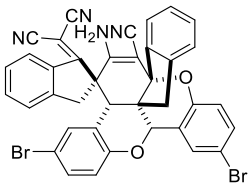
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 (d, *J* = 8.2 Hz, 1H), 8.03 (d, *J* = 7.8 Hz, 1H), 7.56 (d, *J* = 2.5 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 7.5 Hz, 1H), 7.15 – 7.07 (m, 2H), 7.03 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.98 (d, *J* = 8.8 Hz, 1H), 6.93 (d, *J* = 7.5 Hz, 1H), 6.75 (d, *J* = 8.6 Hz, 1H), 6.37 (d, *J* = 2.4 Hz, 1H), 5.59 (s, 1H), 4.51 (s, 2H), 3.57 (d, *J* = 17.9 Hz, 1H), 3.48 – 3.41 (m, 2H), 2.84 (d, *J* = 17.1 Hz, 1H), 2.25 (d, *J* = 17.1 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 178.0, 153.3, 151.9, 151.2, 149.9, 141.9, 138.5, 136.8, 136.2, 130.2, 130.1, 130.1, 129.5, 128.7, 128.2, 127.3, 126.1, 125.7, 125.7, 125.4, 125.3, 124.9, 124.3, 119.1, 118.4, 118.3, 117.6, 112.9, 110.5, 86.9, 84.9, 78.4, 69.5, 57.0, 47.7, 47.3, 43.2, 40.8.

IR (KBr) υ: 3440, 3244, 2927, 2207, 1725, 1643, 1604, 1558, 1477, 1424, 1371, 1242, 1174, 1095, 1043, 823, 761 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Cl_2N_4O_2^+$ $[M + H]^+$ 637.1193; Found 637.1192.

2-(18'-amino-2',7'-dibromo-19'-cyano-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2q)



2q

The compound **2q** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.45 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 29.0 mg, 40% yield, reaction time = 96 h, m.p. 316-318 °C.

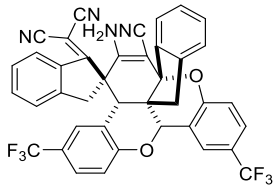
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (d, *J* = 8.1 Hz, 1H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.70 (s, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.29 (d, *J* = 7.5 Hz, 1H), 7.25 – 7.21 (m, 1H), 7.16 (dd, *J* = 8.8, 2.3 Hz, 1H), 7.11 (d, *J* = 7.7 Hz, 1H), 6.95 – 6.90 (m, 2H), 6.71 (d, *J* = 8.6 Hz, 1H), 6.50 (d, *J* = 2.3 Hz, 1H), 5.59 (s, 1H), 4.49 (s, 2H), 3.56 (d, *J* = 17.8 Hz, 1H), 3.49 – 3.34 (m, 2H), 2.85 (d, *J* = 17.1 Hz, 1H), 2.25 (d, *J* = 17.1 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 177.9, 153.1, 152.4, 151.8, 149.8, 141.9, 138.5, 136.8, 136.2, 133.2, 132.9, 131.7, 130.2, 129.6, 128.3, 127.2, 126.4, 125.7, 125.7, 125.3, 125.0, 119.6, 118.8, 118.8, 117.5, 114.6, 112.9, 112.5, 110.5, 86.9, 85.0, 78.4, 69.4, 57.1, 47.7, 47.3, 43.2, 40.8.

IR (KBr) υ: 3446, 3228, 3075, 2881, 2204, 1729, 1642, 1604, 1559, 1476, 1418, 1366, 1241, 1180, 1132, 951, 820, 753 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Br_2N_4O_2^+$ $[M + H]^+$ 725.0182; Found 725.0181.

2-(18'-amino-19'-cyano-2',7'-bis(trifluoromethyl)-5a'H,15'H,16'H-spiro[indene-2, 17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2r)



2r

To a solution of ortho-hydroxyphenyl-substituted indene-diene **1** (0.1 mmol, 1.0 equiv) and anhydrous sodium sulfate (0.40 mmol, 4.0 equiv) in dichloromethane (0.75 mL), tetramethylguanidine (0.04 mmol, 0.40 equiv) was added at 30 °C. Then, the resulting mixture was stirred at 30 °C in oil bath for 144 hours. Upon completion (monitored by TLC), the reaction solution was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 3 : 1) to afford pure product **2r**. R_f = 0.45 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 11.0 mg, 31% yield, reaction time = 144 h, m.p. 215-216 °C.

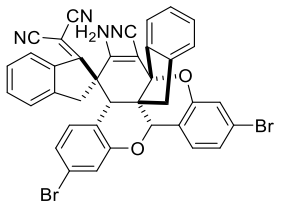
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.0 Hz, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 7.88 (s, 1H), 7.52 – 7.41 (m, 3H), 7.40 – 7.28 (m, 3H), 7.19 (d, *J* = 8.7 Hz, 1H), 7.03 (d, *J* = 7.5 Hz, 1H), 6.95 (t, *J* = 8.8 Hz, 2H), 6.62 (s, 1H), 5.73 (s, 1H), 4.57 (s, 2H), 3.52 – 3.42 (m, 3H), 2.89 (d, *J* = 17.1 Hz, 1H), 2.28 (d, *J* = 17.1 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 177.5, 155.6, 155.3, 153.1, 149.2, 141.6, 138.0, 136.7, 135.9, 130.3, 129.5, 128.3, 127.6 (q, *J* = 5.3 Hz), 127.1 (q, *J* = 3.5 Hz), 126.2 (q, *J* = 3.8 Hz), 125.8, 125.7, 125.0, 124.1 (q, *J* = 32.9 Hz), 123.3 (q, *J* = 270.0 Hz), 122.71 (q, *J* = 33.4 Hz), 121.8 (q, *J* = 3.9 Hz), 121.0 (q, *J* = 269.7 Hz), 123.6, 117.8, 117.6, 117.3, 117.2, 112.6, 110.3, 87.0, 84.4, 78.4, 69.4, 56.9, 47.4, 47.3, 43.0, 40.4.

IR (KBr) υ: 3452, 3234, 3072, 2926, 2207, 1720, 1630, 1560, 1500, 1440, 1332, 1247, 1167, 1124, 1074, 903, 832, 748 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{23}F_6N_4O_2^+$ $[M + H]^+$ 705.1720; Found 705.1724.

2-(18'-amino-3',8'-dibromo-19'-cyano-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2s)



2s

To a solution of ortho-hydroxyphenyl-substituted indene-diene **1** (0.2 mmol, 1.0 equiv) and anhydrous sodium sulfate (0.80 mmol, 4.0 equiv) in dichloromethane (1.5 mL), tetramethylguanidine (0.16 mmol, 0.80 equiv) was added at 30 °C. Then, the resulting mixture was stirred at 30 °C in oil bath for 96 hours. Upon completion (monitored by TLC), the reaction solution was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 3 : 1) to afford pure product **2s**. R_f = 0.42 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 36.9 mg, 51% yield, m.p. 238-240 °C.

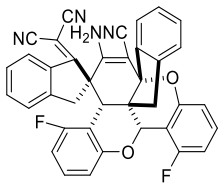
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (d, *J* = 8.2 Hz, 1H), 8.03 (d, *J* = 7.8 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.48 – 7.41 (m, 2H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 2.0 Hz, 1H), 7.20 – 7.13 (m, 2H), 7.04 – 7.00 (m, 1H), 6.94 (d, *J* = 7.4 Hz, 1H), 6.57 (dd, *J* = 8.2, 2.0 Hz, 1H), 6.29 (d, *J* = 8.3 Hz, 1H), 5.56 (s, 1H), 4.43 (s, 2H), 3.57 (d, *J* = 17.8 Hz, 1H), 3.51 (s, 1H), 3.44 (d, *J* = 17.9 Hz, 1H), 2.85 (d, *J* = 17.1 Hz, 1H), 2.24 (d, *J* = 17.1 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 178.2, 154.1, 153.4, 153.3, 150.1, 142.0, 138.5, 137.0, 135.9, 131.2, 130.3, 129.4, 128.3, 125.8, 125.7, 125.6, 125.5, 125.1, 125.0, 123.6, 123.2, 123.1, 122.0, 120.9, 120.4, 117.4, 116.2, 113.0, 110.6, 87.0, 84.7, 78.4, 69.6, 56.7, 47.8, 47.0, 43.3, 40.6.

IR (KBr) υ: 3448, 3228, 2984, 2936, 2871, 2201, 1725, 1641, 1599, 1561, 1478, 1409, 1368, 1231, 1047, 952, 866, 759 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Br_2N_4O_2^+$ $[M + H]^+$ 725.0182; Found 725.0182.

2-(18'-amino-19'-cyano-1',6'-difluoro-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2t)



2t

The compound **2t** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.41 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 41.6 mg, 69% yield, reaction time = 48 h, m.p. 228-230 °C.

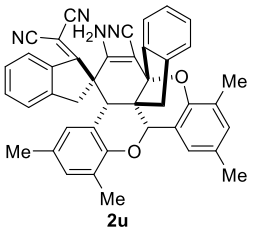
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.46 (d, *J* = 8.1 Hz, 1H), 8.02 (d, *J* = 7.7 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.38 (q, *J* = 7.7 Hz, 2H), 7.31 (t, *J* = 7.1 Hz, 1H), 7.13 – 7.05 (m, 2H), 7.04 – 6.93 (m, 2H), 6.84 (d, *J* = 8.4 Hz, 1H), 6.72 (dd, *J* = 10.9, 8.3 Hz, 1H), 6.64 (d, *J* = 8.2 Hz, 1H), 6.16 (t, *J* = 8.9 Hz, 1H), 5.94 (s, 1H), 4.51 (s, 2H), 3.75 – 3.63 (m, 2H), 3.46 (d, *J* = 17.6 Hz, 1H), 3.07 (d, *J* = 17.0 Hz, 1H), 2.33 (d, *J* = 17.0 Hz, 1H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 179.9, 160.7 (d, *J* = 249.6 Hz), 160.6 (d, *J* = 237.2 Hz), 156.6, 154.7 (d, *J* = 6.3 Hz), 154.4 (d, *J* = 6.7 Hz), 150.0, 142.4, 138.3, 136.0, 135.7, 130.8 (d, *J* = 10.8 Hz), 129.6, 128.0, 127.5, 125.3, 125.1, 125.0, 124.5, 118.7, 113.9, 113.2 (d, *J* = 3.2 Hz), 112.8 (d, *J* = 2.3 Hz), 111.6, 111.0 (d, *J* = 13.1 Hz), 110.1 (d, *J* = 22.4 Hz), 107.0 (d, *J* = 20.9 Hz), 106.8 (d, *J* = 22.5 Hz), 106.7 (d, *J* = 21.1 Hz), 87.0, 79.2, 78.3, 75.6, 75.5 69.5, 57.9, 45.9, 43.2, 41.7.

IR (KBr) υ: 3452, 3247, 2929, 2215, 1722, 1624, 1468, 1357, 1234, 1038, 779, 676 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}F_2N_4O_2^+$ $[M + H]^+$ 605.1784; Found 605.1786.

2-(18'-amino-19'-cyano-2',4',7',9'-tetramethyl-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2u)



2u

The compound **2u** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.44 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 25.4 mg, 41% yield, reaction time = 24 h, m.p. >320 °C.

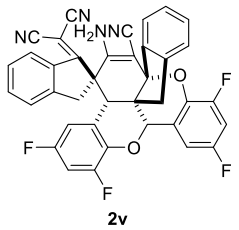
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (d, *J* = 8.2 Hz, 1H), 8.13 (d, *J* = 7.8 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H), 7.26 – 7.19 (m, 2H), 7.11 (d, *J* = 7.7 Hz, 1H), 6.86 (d, *J* = 7.5 Hz, 1H), 6.77 (s, 1H), 6.71 (s, 1H), 6.05 (s, 1H), 5.52 (s, 1H), 4.41 (s, 2H), 3.63 (d, *J* = 17.8 Hz, 1H), 3.50 (s, 1H), 3.37 (d, *J* = 17.7 Hz, 1H), 2.78 (d, *J* = 17.1 Hz, 1H), 2.34 (s, 3H), 2.29 (s, 3H), 2.22 (d, *J* = 17.0 Hz, 1H), 2.01 (s, 3H), 1.82 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 179.5, 153.5, 150.9, 149.5, 148.3, 143.0, 139.5, 136.6, 136.4, 131.8, 131.0, 130.3, 129.7, 128.9, 128.6, 128.4, 127.9, 127.0, 125.9, 125.8, 125.5, 125.4, 125.2, 124.6, 121.9, 118.0, 115.8, 113.2, 110.7, 86.4, 85.7, 78.1, 69.9, 57.2, 48.1, 47.9, 43.3, 41.3, 21.2, 20.1, 16.4, 15.4.

IR (KBr) υ: 3432, 3263, 3020, 2919, 2350, 2231, 2196, 1734, 1655, 1601, 1556, 1476, 1382, 1308, 1226, 1158, 943, 856, 759, 671 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{42}H_{33}N_4O_2^+$ $[M + H]^+$ 625.2598; Found 625.2599.

2-(18'-amino-19'-cyano-2',4',7',9'-tetrafluoro-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene)malononitrile (2v)



2v

The compound **2v** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.22 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 16.4 mg, 26% yield, reaction time = 144 h, m.p. 245-246 °C.

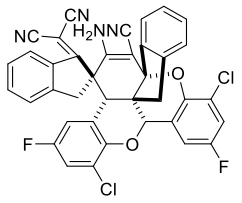
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (d, *J* = 8.2 Hz, 1H), 8.11 (d, *J* = 7.9 Hz, 1H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 7.3 Hz, 1H), 7.22 (d, *J* = 7.7 Hz, 1H), 7.16 (d, *J* = 7.7 Hz, 1H), 6.93 (d, *J* = 7.5 Hz, 1H), 6.77 – 6.66 (m, 2H), 6.04 (d, *J* = 8.5 Hz, 1H), 5.58 (s, 1H), 4.53 (s, 2H), 3.66 – 3.55 (m, 2H), 3.50 (d, *J* = 17.9 Hz, 1H), 2.83 (d, *J* = 17.1 Hz, 1H), 2.26 (d, *J* = 17.2 Hz, 1H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 177.3, 157.2, 156.6 (dd, *J* = 241.4, 11.0 Hz), 154.2 (dd, *J* = 239.1, 11.1 Hz), 150.8 (dd, *J* = 248.5, 12.6 Hz), 150.3, 149.8 (dd, *J* = 247.2, 13.4 Hz), 142.7, 138.9, 138.1 (dd, *J* = 11.1, 2.7 Hz), 137.4, 136.6 (dd, *J* = 12.4, 2.6 Hz), 135.8, 130.2, 129.7 (dd, *J* = 9.3, 2.8 Hz), 128.5, 128.1, 125.5, 125.24, 125.21, 125.0, 120.6 (dd, *J* = 9.3, 2.7 Hz), 119.3, 114.5, 114.1 (dd, *J* = 25.0, 1.6 Hz), 111.9, 106.7 (dd, *J* = 25.3, 2.2 Hz), 105.2 (dd, *J* = 28.0, 20.9 Hz), 104.4 (dd, *J* = 26.5, 22.7 Hz), 89.6, 79.1, 78.9, 69.7, 57.4, 47.3, 46.7, 43.4, 40.9.

IR (KBr) υ: 3471, 3246, 3080, 2209, 1642, 1603, 1558, 1492, 1364, 1306, 1234, 1124, 1058, 991, 948, 842, 758, 719 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{21}F_4N_4O_2^+$ $[M + H]^+$ 641.1595; Found 641.1591.

2-(18'-amino-4',9'-dichloro-19'-cyano-2',7'-difluoro-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-1(3H)-ylidene) malononitrile (2w)



2w

The compound **2w** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.36 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 24.7 mg, 37% yield, reaction time = 144 h, m.p. 263-265 °C.

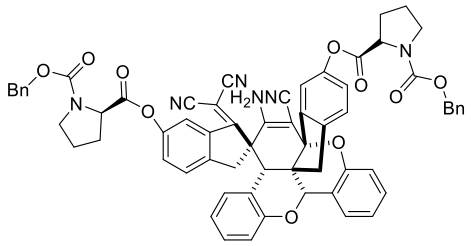
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.23 (d, *J* = 7.9 Hz, 1H), 8.02 (d, *J* = 7.8 Hz, 1H), 7.50 (t, *J* = 7.3 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.36 – 7.29 (m, 2H), 7.29 – 7.20 (m, 3H), 7.13 (d, *J* = 7.6 Hz, 1H), 6.98 (d, *J* = 7.5 Hz, 1H), 6.71 (s, 2H), 6.67 (dd, *J* = 9.3, 3.0 Hz, 1H), 5.89 (s, 1H), 3.42 (s, 2H), 3.38 (s, 1H), 2.56 (d, *J* = 17.4 Hz, 1H), 2.13 (d, *J* = 17.4 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 176.9, 157.7, 156.5 (d, *J* = 237.2 Hz), 154.1 (d, *J* = 236.0 Hz), 149.9, 144.9 (d, *J* = 2.4 Hz), 144.3 (d, *J* = 2.6 Hz), 142.3, 138.4, 137.0, 135.5, 129.7, 129.2 (d, *J* = 9.0 Hz), 128.1, 127.6, 124.9, 124.8, 124.8, 124.6, 122.0 (d, *J* = 10.9 Hz), 120.2 (d, *J* = 11.5 Hz), 119.7 (d, *J* = 8.7 Hz), 118.7, 117.4 (d, *J* = 24.1 Hz), 117.1 (d, *J* = 24.1 Hz), 115.7 (d, *J* = 26.2 Hz), 114.0, 111.4, 109.6 (d, *J* = 25.2 Hz), 89.5, 78.8, 78.7, 70.1, 56.8, 46.6, 46.6, 42.9, 40.7.

IR (KBr) υ: 3427, 3247, 2939, 2883, 2820, 2378, 2214, 2000, 1721, 1624, 1535, 1462, 1320, 1160, 940, 758, 672 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{21}Cl_2F_2N_4O_2^+$ $[M + H]^+$ 673.1004; Found 673.1004.

2-(18'-amino-12'-((((benzyloxy)carbonyl)-L-prolyl)oxy)-19'-cyano-1-(dicyanomethylene)-1,3-dihydro-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-6-yl) 1-benzyl (R)-pyrrolidine-1,2-dicarboxylate (2x)



2x

The compound **2x** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-2:1 as eluent. R_f = 0.23 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 64.7 mg, 61% yield, reaction time = 19 h, m.p. 204-205 °C.

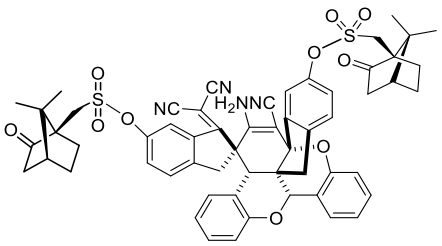
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 – 7.73 (m, 2H), 7.69 – 7.59 (m, 2H), 7.48 – 7.27 (m, 8H), 7.25 – 7.19 (m, 1H), 7.16 – 6.92 (m, 7H), 6.91 – 6.72 (m, 3H), 6.50 – 6.41 (m, 2H), 5.59 – 5.53 (m, 1H), 5.23 – 5.09 (m, 3H), 4.91 – 4.40 (m, 4H), 3.65 (m, 2H), 3.58 – 3.40 (m, 4H), 3.34 – 3.08 (m, 1H), 2.88 – 2.76 (m, 1H), 2.43 – 2.28 (m, 2H), 2.27 – 2.18 (m, 2H), 2.11 – 1.94 (m, 5H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 179.3, 179.2, 171.5, 171.4, 171.4, 171.3, 157.2, 155.4, 155.4, 155.2, 155.2, 154.7, 154.7, 153.5, 152.6, 150.3, 150.2, 150.1, 144.3, 142.9, 142.9, 137.4, 137.4, 136.8, 136.8, 136.5, 136.5, 130.3, 129.9, 129.9, 128.7, 128.7, 128.6, 128.3, 128.2, 128.2, 128.0, 126.1, 125.6, 124.4, 124.4, 123.2, 123.1, 122.0, 120.4, 118.2, 118.1, 117.5, 117.5, 117.5, 117.1, 117.1, 116.9, 116.9, 113.3, 113.3, 111.3, 110.1, 110.1, 110.1, 86.1, 82.7, 69.1, 67.6, 67.6, 67.5, 59.6, 59.5, 59.1, 59.0, 57.6, 57.5, 48.5, 48.4, 47.3, 47.2, 47.2, 46.8, 46.8, 42.8, 40.2, 31.1, 30.2, 24.6, 24.5, 23.8.

IR (KBr) υ: 3446, 3245, 3036, 2957, 2209, 1764, 1694, 1640, 1553, 1489, 1356, 1308, 1235, 1161, 912, 754 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{64}H_{51}N_6O_{10}^+$ $[M + H]^+$ 1063.3661; Found 1063.3663.

18'-amino-19'-cyano-1-(dicyanomethylene)-12'-(((((1R,4R)-7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methyl)sulfonyl)oxy)-1,3-dihydro-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromen]-6-yl ((1R,4S)-7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methanesulfonate (2y)



2y

The compound **2y** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-2:1 as eluent. R_f = 0.33 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 41.6 mg, 40% yield, reaction time = 20 h, m.p. 220-221 °C.

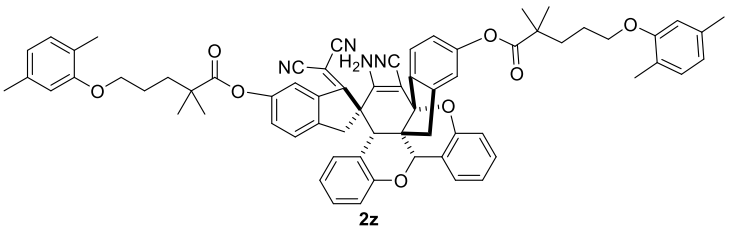
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (dd, *J* = 19.8, 2.1 Hz, 1H), 7.84 (dd, *J* = 16.2, 2.3 Hz, 1H), 7.62 (d, *J* = 7.5 Hz, 1H), 7.39 (d, *J* = 7.2 Hz, 1H), 7.29 – 7.21 (m, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 7.11 – 6.99 (m, 4H), 6.94 (dd, *J* = 8.3, 3.2 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 1H), 6.49 – 6.29 (m, 2H), 5.63 (d, *J* = 9.6 Hz, 1H), 4.83 (s, 2H), 3.86 – 3.73 (m, 1H), 3.69 – 3.57 (m, 2H), 3.54 – 3.44 (m, 1H), 3.41 (d, *J* = 11.4 Hz, 1H), 3.22 (td, *J* = 14.5, 5.4 Hz, 2H), 2.82 (d, *J* = 17.2 Hz, 1H), 2.55 – 2.34 (m, 4H), 2.24 (d, *J* = 17.3 Hz, 1H), 2.16 (t, *J* = 4.5 Hz, 1H), 2.14 – 2.05 (m, 3H), 2.01 – 1.90 (m, 2H), 1.85 – 1.73 (m, 3H), 1.52 – 1.38 (m, 2H), 1.19 (s, 1H), 1.14 (s, 4H), 0.94 – 0.82 (m, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 214.2, 214.1, 214.1, 214.0, 178.0, 177.9, 154.0, 154.0, 153.4, 153.4, 152.5, 152.5, 149.4, 149.3, 149.1, 149.0, 149.0, 148.9, 144.5, 144.4, 138.0, 137.6, 137.5, 130.5, 130.5, 130.4, 130.2, 128.7, 126.6, 126.6, 126.4, 126.4, 124.3, 124.3, 124.2, 124.1, 124.1, 122.1, 122.1, 120.4, 120.3, 118.8, 118.7, 117.7, 117.6, 117.5, 117.4, 117.1, 117.0, 116.5, 116.4, 112.7, 112.6, 110.5, 110.4, 85.7, 85.7, 83.6, 79.8, 79.7, 69.0, 69.0, 58.3, 58.3, 58.2, 58.2, 58.0, 57.9, 48.5, 48.4, 48.4, 48.4, 48.4, 48.3, 48.3, 48.0, 47.7, 47.7, 47.4, 43.1, 43.0, 42.9, 42.8, 42.8, 42.7, 42.6, 42.6, 40.2, 40.1, 27.1, 27.0, 27.0, 25.5, 25.3, 25.3, 25.2, 20.1, 20.0, 19.9, 19.9, 19.8, 19.8, 19.8.

IR (KBr) υ: 3459, 3237, 2962, 2203, 1746, 1641, 1600, 1484, 1373, 1242, 1172, 1054, 964, 837, 729 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{58}H_{53}N_4O_{10}S_2^+$ $[M + H]^+$ 1029.3198; Found 1029.3194.

18'-amino-19'-cyano-1-(dicyanomethylene)-1,3-dihydro-5a'H,15'H,16'H-spiro[indene-2,17'-[10a,16]prop[1]enochromeno[3,2-c]indeno[1,2-b]chromene]-6,13'-diyl bis(5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate) (2z)



2z

The compound **2z** was prepared according to general procedure **3** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.55 (petroleum ether/ethyl acetate = 3:1). Yellow solid, 26.7 mg, 50% yield, reaction time = 36 h, m.p. 120-121 °C.

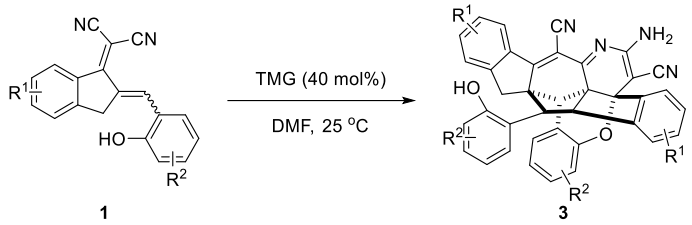
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 – 8.13 (m, 1H), 7.68 (d, *J* = 2.1 Hz, 1H), 7.63 (d, *J* = 7.5 Hz, 1H), 7.15 (t, *J* = 7.7 Hz, 1H), 7.12 – 7.08 (m, 2H), 7.07 – 7.02 (m, 3H), 7.00 (d, *J* = 6.8 Hz, 2H), 6.94 (dd, *J* = 8.1, 2.2 Hz, 1H), 6.92 – 6.81 (m, 2H), 6.69 – 6.64 (m, 3H), 6.63 (s, 1H), 6.51 (t, *J* = 7.4 Hz, 1H), 6.42 (d, *J* = 7.6 Hz, 1H), 5.61 (s, 1H), 4.46 (s, 2H), 4.02 – 3.95 (m, 4H), 3.62 (d, *J* = 17.9 Hz, 1H), 3.55 (s, 1H), 3.37 (d, *J* = 17.8 Hz, 1H), 2.84 (d, *J* = 17.1 Hz, 1H), 2.33 – 2.29 (m, 6H), 2.25 (d, *J* = 17.1 Hz, 1H), 2.20 (s, 3H), 2.16 (s, 3H), 1.95 – 1.79 (m, 8H), 1.47 – 1.35 (m, 12H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 177.9, 176.4, 176.4, 157.1, 156.9, 153.6, 153.6, 153.5, 152.6, 151.3, 150.9, 147.7, 143.9, 137.2, 136.7, 136.6, 136.3, 130.5, 130.5, 130.4, 130.2, 130.1, 128.7, 126.0, 125.5, 124.4, 124.2, 123.8, 123.6, 123.6, 122.0, 120.9, 120.7, 120.5, 118.7, 118.2, 117.7, 117.6, 117.1, 116.8, 112.6, 112.1, 112.1, 110.5, 86.0, 84.4, 79.2, 69.2, 68.0, 67.7, 57.6, 48.5, 47.5, 42.8, 42.7, 42.6, 40.2, 37.3, 37.2, 25.3, 25.3, 25.3, 25.1, 25.1, 21.5, 16.0, 15.9.

IR (KBr) υ: 3450, 3366, 2925, 2874, 2202, 1750, 1644, 1603, 1485, 1245, 1122, 1051, 955, 754 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{68}H_{65}N_4O_8^+$ $[M + H]^+$ 1065.4797; Found 1065.4800.

8. Procedure for the synthesis of compounds 3 and characteristic data

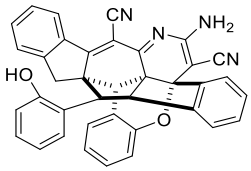


1 3

General synthetic procedure 4:

To a solution of ortho-hydroxyphenyl-substituted indene-dienes **1** (0.4 mmol, 1.0 equiv) in N, N-dimethylformamide (3.0 mL), tetramethylguanidine (0.16 mmol, 0.40 equiv) was added at 25 °C. Then, the resulting mixture was stirred at 25 °C for 1 - 6 hours. Upon completion (monitored by TLC), water was added (15 mL) and the mixture was extracted with ethyl acetate (20 mL × 3). The combined organic layer was washed with brine (15 mL), dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 2 : 1) to afford pure products **3**.

19-amino-21-(2-hydroxyphenyl)-5H,5bH,15H-16,10a-(azenoetheno)-5a,15-methanofluoreno[2,1-c]indeno[1,2-b]chromene-17,20-dicarbonitrile (3a)



3a

The compound **3a** was prepared according to general procedure **4** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-2:1 as eluent. R_f = 0.19 (petroleum ether/ethyl acetate = 2:1). Orange solid, 80.2 mg, 71% yield, >20:1 dr, reaction time = 1 h, m.p. 249-250 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 9.58 (s, 1H), 8.16 (d, J = 7.9 Hz, 1H), 7.49 (d, J = 7.8 Hz, 1H), 7.47 – 7.37 (m, 2H), 7.31 (t, J = 7.2 Hz, 2H), 7.21 – 7.11 (m, 3H), 7.09 –

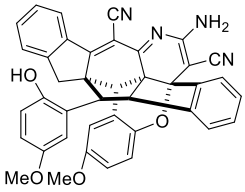
7.01 (m, 2H), 6.98 (t, *J* = 7.4 Hz, 1H), 6.92 (t, *J* = 7.6 Hz, 1H), 6.87 (d, *J* = 7.9 Hz, 1H), 6.79 (t, *J* = 7.7 Hz, 1H), 6.66 – 6.61 (m, 1H), 6.50 – 6.42 (m, 2H), 4.68 (s, 1H), 4.08 – 3.82 (m, 2H), 3.71 (d, *J* = 16.2 Hz, 1H), 3.57 (s, 1H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 177.7, 173.9, 157.1, 156.0, 155.4, 155.3, 152.6, 151.5, 143.2, 142.6, 134.8, 133.9, 128.7, 127.9, 127.8, 127.6, 127.5, 125.1, 124.9, 124.7, 124.6, 124.0, 123.0, 122.7, 120.0, 120.0, 118.8, 115.2, 115.1, 102.3, 84.2, 66.4, 63.8, 63.4, 62.6, 60.6, 60.0, 38.0.

IR (KBr) υ: 3477, 3315, 3215, 3033, 2594, 2228, 2185, 1635, 1589, 1548, 1457, 1402, 1363, 1327, 1238, 1156, 951, 750 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{25}N_4O_2^+$ $[M + H]^+$ 569.1972; Found 569.1978.

19-amino-21-(2-hydroxy-5-methoxyphenyl)-7-methoxy-5H,5bH,15H-16,10a-(azenoetheno)-5a,15-methanofluoreno[2,1-c]indeno[1,2-b]chromene-17,20-dicarbonitrile (3b)



3b

The compound **3b** was prepared according to general procedure **4** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-2:1 as eluent. R_f = 0.16 (petroleum ether/ethyl acetate = 2:1). Orange solid, 60.1 mg, 48% yield, 20:1 dr, reaction time = 5 h, m.p. 284-285 °C.

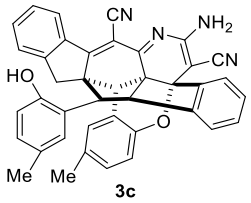
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.10 (s, 1H), 8.18 (d, *J* = 7.9 Hz, 1H), 7.46 – 7.38 (m, 2H), 7.35 (t, *J* = 7.2 Hz, 2H), 7.20 – 7.13 (m, 3H), 7.05 – 6.99 (m, 2H), 6.81 (d, *J* = 8.7 Hz, 1H), 6.64 (dd, *J* = 8.6, 2.7 Hz, 1H), 6.61 – 6.46 (m, 3H), 6.36 (dd, *J* = 8.7, 2.9 Hz, 1H), 4.65 (s, 1H), 4.03 – 3.84 (m, 2H), 3.72 (d, *J* = 16.1 Hz, 1H), 3.66 (s, 3H), 3.53 (s, 3H), 3.48 (s, 1H).

^{13}C NMR (150 MHz, DMSO-d_6) δ 177.2, 173.7, 157.0, 154.3, 151.6, 151.5, 149.1, 146.0, 143.3, 142.8, 134.8, 133.9, 128.7, 128.3, 127.4, 127.4, 125.3, 124.4, 124.0, 122.9, 122.5, 120.4, 120.1, 115.9, 115.2, 114.3, 112.3, 111.9, 111.2, 102.3, 84.1, 66.3, 63.6, 60.2, 56.1, 55.1, 55.0, 52.1, 50.0, 37.6.

IR (KBr) υ: 3411, 3222, 2940, 2835, 2187, 1729, 1632, 1550, 1487, 1430, 1398, 1363, 1269, 1206, 1037, 940, 815, 762 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{29}N_4O_4^+$ $[M + H]^+$ 629.2183; Found 629.2188.

19-amino-21-(2-hydroxy-5-methylphenyl)-7-methyl-5H,5bH,15H-16,10a-(azenoetheno)-5a,15-methanofluoreno[2,1-c]indeno[1,2-b]chromene-17,20-dicarbonitrile (3c)



3c

The compound **3c** was prepared according to general procedure **4** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.27 (petroleum ether/ethyl acetate = 2:1). Orange solid, 66.1 mg, 55% yield, 16:1 dr, reaction time = 5 h, m.p. 294-295 °C.

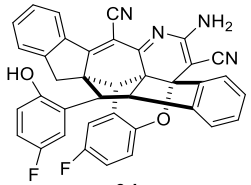
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.28 (s, 1H), 8.18 (d, *J* = 7.8 Hz, 1H), 7.49 – 7.37 (m, 2H), 7.37 – 7.30 (m, 2H), 7.28 (s, 1H), 7.20 – 7.12 (m, 3H), 7.00 (t, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 8.2 Hz, 1H), 6.80 (s, 1H), 6.76 (d, *J* = 8.1 Hz, 1H), 6.55 (d, *J* = 8.0 Hz, 1H), 6.51 (d, *J* = 7.6 Hz, 2H), 4.62 (s, 1H), 3.91 – 3.82 (m, 2H), 3.72 (d, *J* = 16.2 Hz, 1H), 3.44 (s, 1H), 2.19 (s, 3H), 1.94 (s, 3H).

^{13}C NMR (150 MHz, DMSO-d_6) δ 177.7, 173.9, 156.9, 153.0, 151.5, 150.2, 143.3, 142.8, 135.1, 133.9, 131.4, 128.7, 128.4, 128.3, 128.1, 127.4, 127.3, 127.2, 126.9, 125.4, 125.1, 124.2, 123.9, 122.8, 121.4, 120.1, 119.6, 115.2, 114.8, 102.2, 83.9, 66.5, 63.5, 60.3, 56.6, 51.7, 49.6, 38.0, 21.0, 20.1.

IR (KBr) υ: 3560, 3489, 2908, 2371, 2193, 1625, 1546, 1359, 1328, 1257, 1110, 1045, 945 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{29}N_4O_2^+$ $[M + H]^+$ 597.2285; Found 597.2293.

19-amino-7-fluoro-21-(5-fluoro-2-hydroxyphenyl)-5H,5bH,15H-16,10a-(azenoetheno)-5a,15-methanofluoreno[2,1-c]indeno[1,2-b]chromene-17,20-dicarbonitrile (3d)



3d

The compound **3d** was prepared according to general procedure **4** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-2:1 as eluent. R_f = 0.22 (petroleum ether/ethyl acetate = 2:1). Orange solid, 48.4 mg, 40% yield, >20:1 dr, reaction time = 4 h, m.p. 280-282 °C.

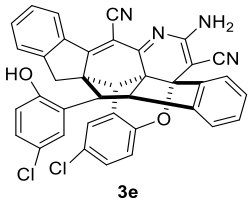
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.64 (s, 1H), 8.17 (s, 1H), 7.39 (d, *J* = 28.8 Hz, 4H), 7.31 – 7.16 (m, 4H), 7.07 – 6.87 (m, 4H), 6.56 (d, *J* = 35.2 Hz, 3H), 4.56 (s, 1H), 4.04 (s, 1H), 3.91 (d, *J* = 16.5 Hz, 1H), 3.72 (d, *J* = 16.2 Hz, 1H), 3.55 (s, 1H).

^{13}C NMR (150 MHz, DMSO-d_6) δ 176.3, 173.3, 157.2 (d, *J* = 236.8 Hz), 157.1, 155.1 (d, *J* = 232.5 Hz), 151.6 (d, *J* = 9.7 Hz), 151.2, 148.9, 143.2, 142.3, 134.7, 134.0, 129.1 (d, *J* = 7.3 Hz), 128.9, 127.6, 127.6, 125.3, 124.3, 124.0, 122.8, 121.4 (d, *J* = 7.9 Hz), 120.0, 115.8 (d, *J* = 7.6 Hz), 115.1, 114.4 (d, *J* = 22.8 Hz), 114.2 (d, *J* = 23.0 Hz), 111.8 (d, *J* = 25.3 Hz), 102.8, 84.6, 66.1, 63.1, 60.1, 55.8, 52.0, 49.8, 37.5.

IR (KBr) υ: 3472, 3217, 3060, 2188, 1708, 1628, 1590, 1545, 1482, 1436, 1364, 1329, 1267, 1183, 1102, 1044, 934, 819, 764 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}F_2N_4O_2^+$ $[M + H]^+$ 605.1784; Found 605.1787.

19-amino-7-chloro-21-(5-chloro-2-hydroxyphenyl)-5H,5bH,15H-16,10a-(azenoet heno)-5a,15-methanofluoreno[2,1-c]indeno[1,2-b]chromene-17,20-dicarbonitrile (3e)



3e

The compound **3e** was prepared according to general procedure **4** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-2:1 as eluent. R_f = 0.24 (petroleum ether/ethyl acetate = 2:1). Orange solid, 61.8 mg, 48% yield, >20:1 dr, reaction time = 6 h, m.p. 285-287 °C.

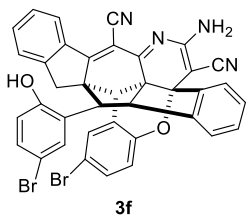
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.65 (s, 1H), 8.17 (s, 1H), 7.39 (d, *J* = 29.0 Hz, 4H), 7.33 – 7.15 (m, 4H), 7.10 – 6.86 (m, 4H), 6.56 (d, *J* = 35.1 Hz, 3H), 4.56 (s, 1H), 4.04 (s, 1H), 3.91 (d, *J* = 16.4 Hz, 1H), 3.72 (d, *J* = 16.3 Hz, 1H), 3.55 (s, 1H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 176.2, 173.1, 157.1, 151.6, 151.0, 143.2, 142.2, 134.7, 134.1, 129.6, 129.0, 127.8, 127.6, 127.6, 126.4, 125.3, 124.8, 124.7, 124.2, 123.9, 122.9, 122.6, 121.8, 121.8, 119.9, 116.5, 115.0, 102.7, 84.7, 66.1, 63.0, 60.1, 54.4, 51.7, 49.5, 37.6.

IR (KBr) υ: 3499, 3321, 3066, 2705, 2189, 1624, 1546, 1477, 1422, 1362, 1270, 1172, 1112, 1039, 919, 821, 751 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Cl_2N_4O_2^+$ $[M + H]^+$ 637.1193; Found 637.1192.

19-amino-7-bromo-21-(5-bromo-2-hydroxyphenyl)-5H,5bH,15H-16,10a-(azenoet heno)-5a,15-methanofluoreno[2,1-c]indeno[1,2-b]chromene-17,20-dicarbonitrile (3f)



3f

The compound **3f** was prepared according to general procedure **4** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-2:1 as eluent. R_f = 0.24 (petroleum ether/ethyl acetate = 2:1). Orange solid, 113.6 mg, 78% yield, >20:1 dr, reaction time = 4 h, m.p. 272-273 °C.

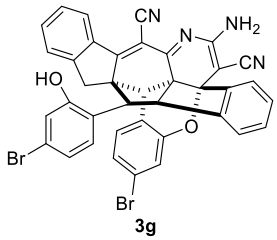
^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 10.00 (s, 1H), 8.18 (s, 1H), 7.54 (s, 1H), 7.41 (d, *J* = 17.9 Hz, 4H), 7.32 – 7.13 (m, 5H), 7.07 – 7.02 (m, 1H), 6.94 – 6.86 (m, 2H), 6.55 (s, 2H), 4.53 (s, 1H), 4.08 (s, 1H), 3.77 (q, *J* = 16.5, 15.9 Hz, 2H), 3.57 (s, 1H).

^{13}C NMR (150 MHz, DMSO-*d*$_6$) δ 176.2, 173.1, 157.1, 154.6, 152.0, 151.0, 143.2, 142.2, 134.7, 134.1, 130.8, 130.5, 130.1, 129.1, 127.7, 127.6, 125.3, 124.4, 124.3, 123.9, 123.0, 122.2, 119.9, 116.9, 115.0, 114.4, 110.4, 102.7, 84.7, 66.2, 63.0, 60.1, 55.6, 51.6, 49.4, 37.6.

IR (KBr) υ: 3465, 3320, 3222, 2945, 2503, 2311, 2189, 1713, 1637, 1550, 1475, 1411, 1364, 1327, 1272, 1172, 1113, 1040, 819, 753 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Br_2N_4O_2^+$ $[M + H]^+$ 725.0182; Found 725.0187.

19-amino-8-bromo-21-(4-bromo-2-hydroxyphenyl)-5H,5bH,15H-16,10a-(azenoetheno)-5a,15-methanofluoreno[2,1-c]indeno[1,2-b]chromene-17,20-dicarbonitrile (3g)



3g

The compound **3g** was prepared according to general procedure **4** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.25 (petroleum ether/ethyl acetate = 2:1). Orange solid, 90.0 mg, 62% yield, 10:1 dr, reaction time = 4 h, m.p. 290-291 °C.

^{1}H NMR (400 MHz, DMSO-*d*$_6$, a mixture of two isomers) δ 10.26 (s, 1H, isomer B), 10.13 (s, 1H, isomer A), 8.17 (d, *J* = 7.8 Hz, 1H, isomer A), 8.08 (d, *J* = 8.0 Hz, 1H,

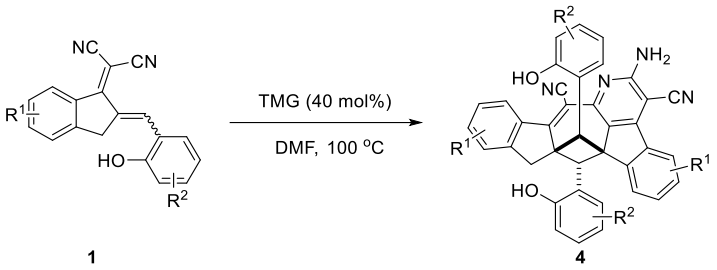
isomer B), 7.76 (d, *J* = 7.7 Hz, 1H, isomer B), 7.57 (t, *J* = 7.4 Hz, 1H, isomer B), 7.52 – 7.32 (m, 5H, isomer A), 7.29 (s, 2H, isomer A), 7.26 – 7.18 (m, 1H for isomer A and 3H for isomer B, overlapped), 7.18 – 7.09 (m, 2H for isomer A and 4H for isomer B, overlapped), 7.09 – 6.94 (m, 2H for isomer A and 4H for isomer B, overlapped), 6.83 – 6.73 (m, 1H for isomer A and 1H for isomer B, overlapped), 6.67 – 6.57 (m, 1H, isomer A), 6.51 (d, *J* = 7.6 Hz, 1H, isomer A), 6.28 (d, *J* = 8.1 Hz, 1H, isomer B), 4.65 (d, *J* = 5.7 Hz, 1H, isomer B), 4.52 (s, 1H, isomer A), 4.03 – 3.82 (m, 2H, isomer A), 3.82 – 3.66 (m, 1H for isomer A and 2H for isomer B, overlapped), 3.62 – 3.44 (m, 1H for isomer A and 2H for isomer B, overlapped).

^{13}C NMR (150 MHz, DMSO-d_6, a mixture of two isomers) δ 176.70 (isomer A), 173.38 (isomer A), 172.73 (isomer B), 170.62 (isomer B), 157.15 (isomer A), 156.95 (isomer B), 156.55 (isomer A), 156.28 (isomer B), 153.69 (isomer A), 151.24 (isomer A), 151.17 (isomer A), 144.32, 143.05 (isomer A), 142.22 (isomer B), 142.09 (isomer A), 135.34 (isomer B), 134.86 (isomer A), 134.67 (isomer B), 134.12 (isomer A), 130.48 (isomer B), 129.86 (isomer B), 129.40 (isomer B), 129.10 (isomer A), 128.16 (isomer B), 128.06 (isomer B), 127.74 (isomer A), 127.69 (isomer A), 126.95 (isomer A), 126.71 (isomer A), 126.07 (isomer B), 125.98 (isomer A), 125.30 (isomer B), 125.18 (isomer A), 125.30 (isomer B), 125.01 (isomer B), 124.82 (isomer B), 124.76 (isomer B), 124.63 (isomer A), 123.94 (isomer A), 122.81 (isomer A), 122.72 (isomer A), 122.32 (isomer B), 121.70 (isomer B), 121.65 (isomer B), 121.55 (isomer A), 121.19 (isomer B), 120.31 (isomer B), 120.06 (isomer A), 119.95 (isomer B), 119.81 (isomer A), 119.59 (isomer B), 117.67 (isomer B), 117.55 (isomer A), 115.04 (isomer A), 114.23 (isomer B), 102.61 (isomer A), 101.59 (isomer B), 87.59 (isomer B), 85.00 (isomer A), 66.01 (isomer A), 63.34 (isomer B), 62.87 (isomer A), 62.36 (isomer B), 60.10 (isomer A), 59.61 (isomer B), 56.34 (isomer A), 54.95 (isomer B), 54.55 (isomer B), 51.55 (isomer A), 50.07 (isomer B), 49.58 (isomer A), 37.89 (isomer A), 36.93 (isomer B).

IR (KBr) υ: 3648, 2957, 2926, 2361, 2342, 1698, 1653, 1540, 1507, 1457, 1418, 1363, 1086, 797 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Br_2N_4O_2^+$ $[M + H]^+$ 725.0182; Found 725.0192.

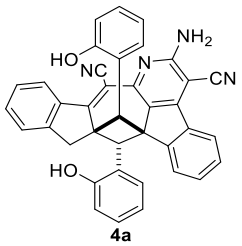
9. Procedure for the synthesis of compounds 4 and characteristic data



General synthetic procedure 5:

To a solution of ortho-hydroxyphenyl-substituted indene-dienes **1** (0.2 mmol, 1.0 equiv) in N, N-dimethylformamide (1.5 mL), tetramethylguanidine (0.08 mmol, 0.40 equiv) was added. Then, the resulting reaction mixture was stirred at 100 °C in oil bath for 0.5 - 6 hours. Upon completion (monitored by TLC), the reaction solution was cooled to room temperature. Water was added (10 mL) and the mixture was extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with brine (15 mL), dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 2 : 1) to afford pure products **4**.

2-amino-8,15-bis(2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4a)



The compound **4a** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f

= 0.14 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 46.2 mg, 81% yield, reaction time = 0.5 h, m.p. 278-279 °C.

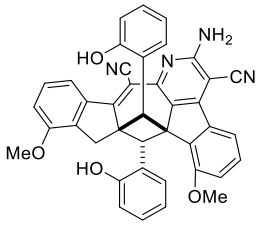
^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 9.03 (s, 2H), 8.59 (d, *J* = 8.2 Hz, 1H), 8.29 (d, *J* = 7.6 Hz, 1H), 8.18 (d, *J* = 7.5 Hz, 1H), 7.73 – 7.65 (m, 1H), 7.64 – 7.58 (m, 1H), 7.58 – 7.50 (m, 2H), 7.44 – 7.33 (m, 1H), 6.79 (s, 2H), 6.73 (t, *J* = 7.7 Hz, 2H), 6.47 (d, *J* = 8.0 Hz, 2H), 6.24 (t, *J* = 7.6 Hz, 2H), 5.87 (d, *J* = 7.7 Hz, 2H), 4.55 (s, 2H), 4.10 (s, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 168.8, 159.0, 155.7, 152.3, 151.3, 150.63, 150.3, 139.0, 136.5, 132.5, 130.8, 128.8, 128.2, 127.4, 127.2, 126.7, 125.1, 124.9, 124.5, 122.9, 122.1, 117.8, 117.4, 116.9, 114.8, 104.6, 79.9, 60.8, 56.4, 45.9, 43.0.

IR (KBr) υ: 3489, 2878, 2814, 2216, 1633, 1595, 1543, 1451, 1389, 1291, 1154, 1091, 756, 613 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{25}N_4O_2^+$ $[M + H]^+$ 569.1972; Found 569.1974.

2-amino-8,15-bis(2-hydroxyphenyl)-7,10-dimethoxy-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4b)



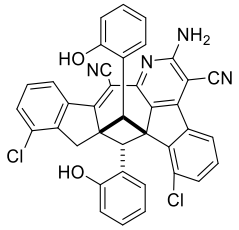
4b

The compound **4b** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.19 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 49.0 mg, 78% yield, reaction time = 2 h, m.p. 292-293 °C.

^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.98 (s, 2H), 8.18 (d, *J* = 8.1 Hz, 1H), 7.92 (d, *J* = 7.7 Hz, 1H), 7.59 (t, *J* = 8.0 Hz, 1H), 7.36 (t, *J* = 8.1 Hz, 1H), 7.27 (d, *J* = 8.2 Hz, 1H), 7.15 (d, *J* = 8.1 Hz, 1H), 6.76 – 6.70 (m, 4H), 6.47 (d, *J* = 8.0 Hz, 2H), 6.24 (t, *J* = 7.5 Hz, 2H), 5.91 (d, *J* = 7.7 Hz, 2H), 5.00 (s, 2H), 4.01 (s, 3H), 3.95 (s, 2H), 3.90 (s, 3H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.9, 158.9, 158.1, 155.7, 155.1, 151.1, 150.5, 140.4, 140.0, 137.9, 135.4, 130.0, 129.1, 128.3, 127.2, 127.2, 123.2, 117.76, 117.1, 116.9, 116.7, 114.8, 114.6, 113.6, 113.5, 104.9, 80.0, 61.2, 56.7, 55.8, 55.4, 43.7, 40.3.
IR (KBr) υ: 3451, 2978, 2884, 2211, 1711, 1627, 1581, 1541, 1456, 1385, 1263, 1172, 1069, 752 cm^{-1}.
HRMS (ESI) m/z: Calcd for $C_{40}H_{29}N_4O_4^+$ $[M + H]^+$ 629.2183; Found 629.2184.

2-amino-7,10-dichloro-8,15-bis(2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4c)



4c

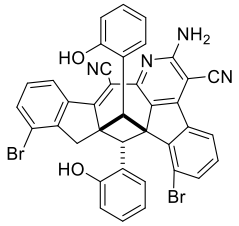
To a solution of ortho-hydroxyphenyl-substituted indene-diene **1** (0.2 mmol, 1.0 equiv) in N, N-dimethylformamide (1.5 mL), tetramethylguanidine (0.12 mmol, 0.60 equiv) was added. Then, the resulting reaction mixture was stirred at 100 °C for 1 hours. Upon completion (monitored by TLC), the reaction solution was cooled to room temperature. Water was added (10 mL) and the mixture was extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with brine (15 mL), dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 2 : 1) to afford pure products **4c**. R_f = 0.23 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 32.6 mg, 51% yield, reaction time = 1 h, m.p. 309-310 °C.
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.11 (s, 2H), 8.54 (d, *J* = 8.1 Hz, 1H), 8.34 (dd, *J* = 6.0, 2.6 Hz, 1H), 7.73 – 7.64 (m, 3H), 7.48 (t, *J* = 8.0 Hz, 1H), 6.94 (s, 2H), 6.77 (t, *J* = 7.6 Hz, 2H), 6.49 (d, *J* = 8.0 Hz, 2H), 6.29 (t, *J* = 7.5 Hz, 2H), 5.88 (d, *J* = 7.7 Hz, 2H), 5.20 (s, 2H), 4.09 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 167.2, 159.0, 155.6, 150.3, 149.9, 149.3, 143.7, 140.9, 139.3, 132.3, 131.9, 131.6, 130.3, 129.8, 129.0, 128.6, 127.6, 127.1, 123.5, 122.5, 121.5, 118.0, 116.6, 116.5, 114.9, 106.1, 80.0, 59.7, 57.7, 46.3.

IR (KBr) υ: 3441, 2985, 2875, 2393, 2215, 1626, 1595, 1548, 1456, 1284, 1139, 940, 756 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Cl_2N_4O_2^+$ $[M + H]^+$ 637.1193; Found 637.1191.

2-amino-7,10-dibromo-8,15-bis(2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4d)



4d

To a solution of ortho-hydroxyphenyl-substituted indene-diene **1** (0.2 mmol, 1.0 equiv) in N, N-dimethylformamide (1.5 mL), tetramethylguanidine (0.12 mmol, 0.60 equiv) was added. Then, the resulting reaction mixture was stirred at 100 ^{o}C for 1 hours. Upon completion (monitored by TLC), the reaction solution was cooled to room temperature. Water was added (10 mL) and the mixture was extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with brine (15 mL), dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 2 : 1) to afford pure products **4d**. R_f = 0.22 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 43.6 mg, 60% yield, reaction time = 1 h, m.p. 290-291 °C.

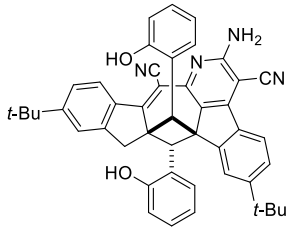
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.09 (s, 2H), 8.57 (d, *J* = 8.1 Hz, 1H), 8.39 (d, *J* = 7.7 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 7.8 Hz, 1H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.40 (t, *J* = 8.0 Hz, 1H), 6.87 (s, 2H), 6.76 (t, *J* = 7.7 Hz, 2H), 6.49 (d, *J* = 8.0 Hz, 2H), 6.28 (t, *J* = 7.6 Hz, 2H), 5.86 (d, *J* = 7.7 Hz, 2H), 5.31 (s, 2H), 4.06 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 167.4, 158.9, 155.6, 151.2, 150.2, 149.6, 144.7, 140.6, 139.5, 135.6, 134.8, 130.4, 129.1, 128.7, 127.5, 127.1, 123.9, 122.4, 122.0, 120.2, 119.3, 117.9, 116.5, 116.5, 114.9, 106.1, 79.8, 59.2, 58.2, 48.6.

IR (KBr) υ: 3479, 3064, 2925, 2212, 1703, 1614, 1545, 1455, 1274, 1226, 1103, 1045, 931, 883, 815, 754 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Br_2N_4O_2^+$ $[M + H]^+$ 725.0182; Found 725.0180.

2-amino-6,11-di-tert-butyl-8,15-bis(2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4e)



4e

The compound **4e** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.30 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 61.0 mg, 90% yield, reaction time = 1 h, m.p. 306-308 °C.

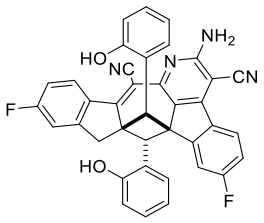
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.01 (s, 2H), 8.50 (d, *J* = 8.6 Hz, 1H), 8.22 (s, 1H), 8.17 (d, *J* = 8.1 Hz, 1H), 7.65 (d, *J* = 8.1 Hz, 1H), 7.49 (s, 1H), 7.42 (d, *J* = 8.6 Hz, 1H), 6.76 – 6.69 (m, 4H), 6.49 (d, *J* = 8.0 Hz, 2H), 6.23 (t, *J* = 7.5 Hz, 2H), 5.89 (d, *J* = 7.8 Hz, 2H), 4.61 (s, 2H), 4.08 (s, 2H), 1.39 (s, 9H), 1.35 (s, 9H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.8, 158.9, 155.8, 155.6, 154.2, 152.5, 151.3, 150.7, 150.2, 136.6, 133.9, 128.7, 127.3, 125.4, 124.6, 124.4, 123.1, 121.6, 121.4, 117.9, 117.6, 116.9, 114.8, 103.8, 79.5, 61.4, 56.6, 46.0, 42.7, 35.3, 35.0, 31.3, 31.0.

IR (KBr) υ: 3483, 2961, 2866, 2213, 1607, 1537, 1450, 1391, 1293, 1256, 1196, 1139, 923, 832, 753, 618 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{46}H_{41}N_4O_2^+$ $[M + H]^+$ 681.3224; Found 681.3219.

2-amino-6,11-difluoro-8,15-bis(2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2, 3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4f)



4f

The compound **4f** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-2:1 as eluent. R_f = 0.16 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 48.4 mg, 80% yield, reaction time = 2 h, m.p. 287-288 °C.

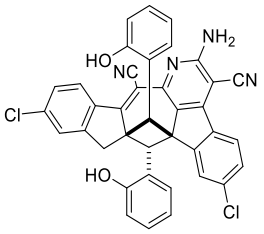
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.02 (s, 2H), 8.60 (dd, *J* = 9.0, 5.2 Hz, 1H), 8.28 (dd, *J* = 8.6, 5.0 Hz, 1H), 8.16 (dd, *J* = 9.1, 2.5 Hz, 1H), 7.47 (td, *J* = 8.9, 2.5 Hz, 1H), 7.42 (dd, *J* = 8.7, 2.6 Hz, 1H), 7.25 (td, *J* = 9.0, 2.7 Hz, 1H), 6.80 (s, 2H), 6.75 (t, *J* = 7.7 Hz, 2H), 6.47 (d, *J* = 8.0 Hz, 2H), 6.26 (t, *J* = 7.5 Hz, 2H), 5.88 (d, *J* = 7.7 Hz, 2H), 4.56 (s, 2H), 4.05 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 167.3, 164.7 (d, *J* = 250.6 Hz), 164.1 (d, *J* = 245.6 Hz), 158.9, 155.6, 155.6 (d, *J* = 9.5 Hz), 153.7 (d, *J* = 9.6 Hz), 150.3, 150.2, 135.5 (d, *J* = 2.3 Hz), 132.8 (d, *J* = 1.6 Hz), 128.5, 127.5, 127.1, 127.0 (d, *J* = 10.2 Hz), 123.9 (d, *J* = 9.1 Hz), 122.7, 117.8, 117.2, 116.7, 115.5 (d, *J* = 24.7 Hz), 114.8, 114.4 (d, *J* = 22.7 Hz), 112.2 (d, *J* = 22.9 Hz), 111.8 (d, *J* = 22.2 Hz), 104.2 (d, *J* = 2.2 Hz), 79.7, 60.7, 56.4 (d, *J* = 2.5 Hz), 45.7, 43.1.

IR (KBr) υ: 3454, 2922, 2850, 2210, 1625, 1594, 1454, 1394, 1258, 1176, 1095, 952, 823, 757 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}F_2N_4O_2^+$ $[M + H]^+$ 605.1784; Found 605.1784.

2-amino-6,11-dichloro-8,15-bis(2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2, 3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4g)



4g

The compound **4g** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.24 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 43.5 mg, 68% yield, reaction time = 3 h, m.p. 300-301 °C.

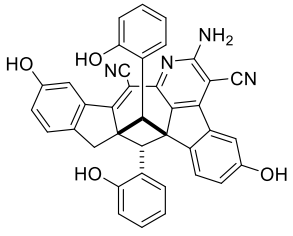
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.03 (s, 2H), 8.55 (d, *J* = 8.7 Hz, 1H), 8.40 (s, 1H), 8.25 (d, *J* = 8.3 Hz, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.67 (s, 1H), 7.47 (d, *J* = 8.7 Hz, 1H), 6.86 (s, 2H), 6.75 (t, *J* = 7.7 Hz, 2H), 6.47 (d, *J* = 8.0 Hz, 2H), 6.26 (t, *J* = 7.5 Hz, 2H), 5.84 (d, *J* = 7.7 Hz, 2H), 4.59 (s, 2H), 4.05 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 167.4, 159.0, 155.6, 154.5, 152.7, 150.3, 150.3, 138.0, 137.2, 135.7, 135.3, 128.6, 128.4, 127.5, 127.1, 127.1, 126.2, 125.1, 123.5, 122.7, 117.9, 117.0, 116.6, 114.8, 105.1, 80.0, 60.4, 56.4, 45.5, 42.9.

IR (KBr) υ: 3471, 2889, 2213, 1707, 1618, 1594, 1543, 1452, 1387, 1209, 1198, 1079, 898, 829, 756 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Cl_2N_4O_2^+$ $[M + H]^+$ 637.1193; Found 637.1192.

2-amino-5,12-dihydroxy-8,15-bis(2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo [2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4h)



4h

The compound **4h** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-2:1 as eluent. R_f

= 0.11 (petroleum ether/ethyl acetate = 1:2). Yellow solid, 46.6 mg, 78% yield, reaction time = 2 h, m.p. >320 °C.

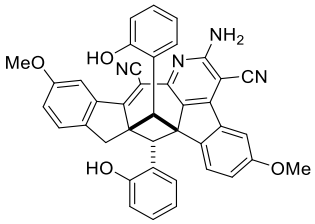
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.91 (s, 1H), 9.56 (s, 1H), 8.99 (s, 2H), 8.02 (d, *J* = 1.9 Hz, 1H), 7.90 (d, *J* = 8.3 Hz, 1H), 7.73 (d, *J* = 2.2 Hz, 1H), 7.28 (d, *J* = 8.2 Hz, 1H), 7.05 (dd, *J* = 8.3, 2.3 Hz, 1H), 6.97 (dd, *J* = 8.2, 2.3 Hz, 1H), 6.73 (t, *J* = 7.6 Hz, 2H), 6.66 (s, 2H), 6.48 (d, *J* = 8.0 Hz, 2H), 6.25 (t, *J* = 7.5 Hz, 2H), 5.92 (d, *J* = 7.8 Hz, 2H), 4.44 (s, 2H), 3.94 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 169.1, 158.9, 157.6, 156.0, 155.8, 151.2, 150.6, 143.1, 141.1, 140.1, 137.6, 129.6, 127.3, 127.3, 125.4, 125.1, 123.1, 120.9, 118.4, 117.8, 117.3, 116.8, 114.8, 110.8, 108.6, 104.3, 79.7, 61.6, 55.9, 45.2, 43.2.

IR (KBr) υ: 3462, 2880, 2582, 2208, 1617, 1539, 1451, 1295, 1206, 1095, 925, 823, 756 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{25}N_4O_4^+$ $[M + H]^+$ 601.1870; Found 601.1868.

2-amino-8,15-bis(2-hydroxyphenyl)-5,12-dimethoxy-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4i)



4i

The compound **4i** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-2:1 as eluent. R_f = 0.19 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 24.6 mg, 39% yield, reaction time = 2 h, m.p. 299-301 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 9.01 (s, 2H), 8.17 (d, *J* = 2.4 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 7.80 (d, *J* = 2.3 Hz, 1H), 7.42 (d, *J* = 8.4 Hz, 1H), 7.25 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.16 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.79 (s, 2H), 6.73 (t, *J* = 7.6 Hz, 2H), 6.48 (d,

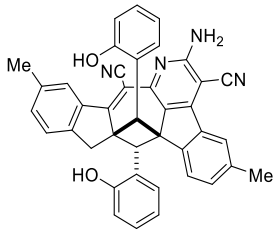
J = 8.0 Hz, 2H), 6.25 (t, *J* = 7.5 Hz, 2H), 5.89 (d, *J* = 7.8 Hz, 2H), 4.50 (s, 2H), 3.99 (s, 2H), 3.88 (s, 3H), 3.78 (s, 3H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 169.3, 159.8, 159.3, 158.5, 156.2, 151.4, 151.0, 145.2, 143.1, 140.5, 138.0, 130.0, 127.8, 127.6, 126.0, 125.8, 123.4, 120.0, 118.3, 117.8, 117.2, 115.2, 109.4, 107.4, 105.1, 80.2, 62.0, 56.3, 55.9, 55.7, 45.6, 43.5.

IR (KBr) υ: 3489, 2885, 2831, 2212, 1609, 1581, 1540, 1490, 1448, 1340, 1291, 1240, 1024, 818, 753, 621 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{29}N_4O_4^+$ $[M + H]^+$ 629.2183; Found 629.2182.

2-amino-8,15-bis(2-hydroxyphenyl)-5,12-dimethyl-8H,9H-7b,8a-methanobenzo[2, 3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4j)



4j

The compound **4j** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-2:1 as eluent. R_f = 0.11 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 47.0 mg, 79% yield, reaction time = 1 h, m.p. 293-294 °C.

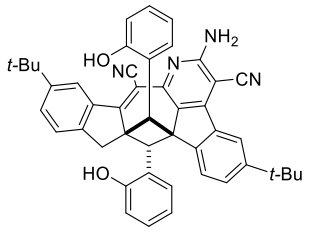
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.01 (s, 2H), 8.41 (s, 1H), 8.08 (s, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 7.7 Hz, 1H), 7.36 (d, *J* = 7.8 Hz, 1H), 6.77 (s, 2H), 6.72 (t, *J* = 7.6 Hz, 2H), 6.47 (d, *J* = 8.0 Hz, 2H), 6.24 (t, *J* = 7.5 Hz, 2H), 5.87 (d, *J* = 7.8 Hz, 2H), 4.50 (s, 2H), 4.02 (s, 2H), 2.49 (s, 3H), 2.35 (s, 3H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.7, 159.0, 155.7, 151.1, 150.6, 149.7, 147.7, 139.2, 137.5, 136.7, 135.6, 133.6, 131.7, 129.1, 127.3, 127.2, 125.0, 124.8, 124.2, 122.9, 122.4, 117.8, 117.4, 116.9, 114.8, 104.4, 79.8, 61.1, 56.1, 45.6, 43.0, 21.4, 21.4.

IR (KBr) υ: 3487, 2876, 2826, 2218, 1708, 1614, 1586, 1541, 1487, 1448, 1367, 1289, 1141, 1100, 1042, 818, 754, 635 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{29}N_4O_2^+$ $[M + H]^+$ 597.2285; Found 597.2281.

2-amino-5,12-di-tert-butyl-8,15-bis(2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4k)



4k

The compound **4k** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.30 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 70.3 mg, 99% yield, reaction time = 1 h, m.p. 301-303 °C.

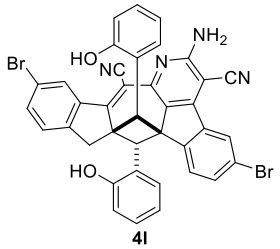
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.01 (s, 2H), 8.50 (d, J = 8.6 Hz, 1H), 8.23 (s, 1H), 8.17 (d, J = 8.2 Hz, 1H), 7.68 – 7.62 (m, 1H), 7.49 (s, 1H), 7.42 (d, J = 8.6 Hz, 1H), 6.76 – 6.69 (m, 4H), 6.49 (d, J = 8.0 Hz, 2H), 6.24 (t, J = 7.5 Hz, 2H), 5.89 (d, J = 7.7 Hz, 2H), 4.62 (s, 2H), 4.09 (s, 2H), 1.39 (s, 9H), 1.35 (s, 9H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.8, 158.9, 155.8, 155.6, 154.1, 152.5, 151.2, 150.7, 150.2, 136.6, 133.9, 128.7, 127.3, 127.3, 125.4, 124.6, 124.4, 123.1, 121.6, 121.4, 121.4, 117.9, 117.6, 116.9, 114.8, 103.8, 79.5, 61.4, 56.6, 46.0, 42.7, 35.3, 35.0, 31.3, 31.0.

IR (KBr) υ: 3485, 2961, 2897, 2313, 2212, 1723, 1609, 1537, 1451, 1391, 1255, 1201, 1044, 1000, 883, 833, 753 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{46}H_{41}N_4O_2^+$ $[M + H]^+$ 681.3224; Found 681.3223.

2-amino-5,12-dibromo-8,15-bis(2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4l)



4l

The compound **4l** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.22 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 35.4 mg, 49% yield, reaction time = 6 h, m.p. >320 °C.

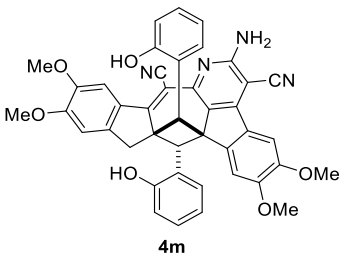
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.00 (s, 2H), 8.74 (d, *J* = 1.8 Hz, 1H), 8.39 (d, *J* = 1.8 Hz, 1H), 8.20 (d, *J* = 8.2 Hz, 1H), 7.88 (dd, *J* = 8.2, 1.9 Hz, 1H), 7.75 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.53 (d, *J* = 8.1 Hz, 1H), 6.90 (s, 2H), 6.77 (td, *J* = 7.7, 1.6 Hz, 2H), 6.49 (d, *J* = 8.0 Hz, 2H), 6.29 (t, *J* = 7.5 Hz, 2H), 5.86 (d, *J* = 7.8 Hz, 2H), 4.57 (s, 2H), 4.03 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 167.1, 158.9, 155.5, 151.4, 150.2, 149.8, 149.6, 141.3, 138.6, 134.8, 133.2, 129.1, 127.5, 127.1, 127.0, 127.0, 126.6, 124.6, 122.5, 121.0, 119.7, 117.9, 116.7, 116.4, 114.9, 105.7, 80.2, 60.6, 56.2, 45.5, 42.8.

IR (KBr) υ: 3481, 2977, 2885, 2215, 1701, 1614, 1544, 1455, 1361, 1277, 1147, 1083, 1044, 1005, 882, 819, 752, 604 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Br_2N_4O_2^+$ $[M + Na]^+$ 747.0002; Found 747.0006.

2-amino-8,15-bis(2-hydroxyphenyl)-5,6,11,12-tetramethoxy-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4m)



4m

The compound **4m** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-2:1 as eluent. R_f = 0.22 (petroleum ether/ethyl acetate = 1:2). Yellow solid, 55.2 mg, 80% yield, reaction time = 1 h, m.p. >320 °C.

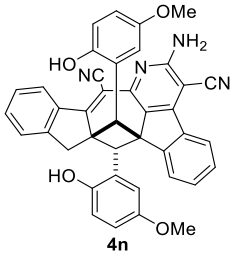
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.98 (s, 2H), 8.20 (s, 1H), 7.82 (d, *J* = 30.4 Hz, 2H), 7.13 (s, 1H), 6.74 (t, *J* = 7.7 Hz, 2H), 6.60 (s, 2H), 6.49 (d, *J* = 8.0 Hz, 2H), 6.26 (t, *J* = 7.6 Hz, 2H), 5.94 (d, *J* = 7.7 Hz, 2H), 4.54 (s, 2H), 4.03 (s, 2H), 3.95 (s, 3H), 3.90 (s, 3H), 3.89 (s, 3H), 3.76 (s, 3H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.8, 158.8, 155.8, 153.3, 151.9, 151.5, 150.2, 149.0, 147.7, 147.6, 144.5, 131.1, 128.4, 128.2, 127.3, 123.4, 118.4, 117.8, 117.4, 114.7, 107.6, 107.1, 107.1, 104.3, 101.7, 78.5, 61.5, 56.3, 56.1, 55.9, 55.6, 55.4, 45.8, 43.5.

IR (KBr) υ: 3425, 2933, 2852, 2210, 1706, 1612, 1583, 1501, 1454, 1325, 1273, 1218, 1112, 1018, 859, 805, 757 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{42}H_{33}N_4O_6^+$ $[M + H]^+$ 689.2395; Found 689.2397.

2-amino-8,15-bis(2-hydroxy-5-methoxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4n)



4n

The compound **4n** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.19 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 38.3 mg, 61% yield, reaction time = 1 h, m.p. 264-266 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.62 (d, *J* = 8.2 Hz, 1H), 8.59 (s, 2H), 8.29 (d, *J* = 7.7 Hz, 1H), 8.20 (d, *J* = 7.5 Hz, 1H), 7.69 (t, *J* = 7.4 Hz, 1H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.57 – 7.51 (m, 2H), 7.41 – 7.35 (m, 1H), 6.85 (s, 2H), 6.38 (d, *J* = 8.7 Hz, 2H), 6.32

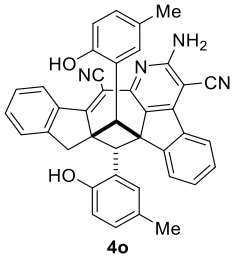
(dd, *J* = 8.7, 2.9 Hz, 2H), 5.45 (d, *J* = 2.9 Hz, 2H), 4.54 (s, 2H), 4.10 (s, 2H), 3.12 (s, 6H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.9, 159.0, 152.2, 151.4, 150.7, 150.7, 150.3, 149.5, 139.3, 136.4, 132.5, 130.9, 128.6, 128.3, 126.7, 125.1, 124.8, 124.6, 123.4, 121.9, 117.3, 116.7, 115.3, 112.8, 112.6, 104.7, 79.7, 60.8, 56.4, 54.3, 46.0, 43.1.

IR (KBr) υ: 3463, 2937, 2835, 2212, 1704, 1625, 1519, 1467, 1429, 1377, 1277, 1211, 1037, 819, 759 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{29}N_4O_4^+$ $[M + H]^+$ 629.2183; Found 629.2182.

2-amino-8,15-bis(2-hydroxy-5-methylphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4o)



4o

The compound **4o** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.12 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 44.3 mg, 74% yield, reaction time = 1 h, m.p. 300-302 °C.

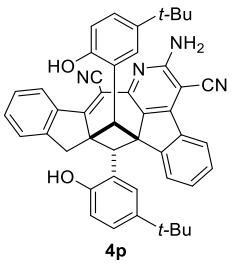
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.76 (s, 2H), 8.60 (d, *J* = 8.2 Hz, 1H), 8.31 (d, *J* = 7.6 Hz, 1H), 8.17 (d, *J* = 7.4 Hz, 1H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.56 – 7.49 (m, 2H), 7.38 (t, *J* = 7.4 Hz, 1H), 6.79 (s, 2H), 6.52 (d, *J* = 8.1 Hz, 2H), 6.34 (d, *J* = 8.1 Hz, 2H), 5.65 (s, 2H), 4.49 (s, 2H), 4.09 (s, 2H), 1.66 (s, 6H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.9, 158.9, 153.4 152.2, 151.5, 150.7, 150.5, 139.4, 136.5, 132.3, 130.8, 128.9, 128.2, 128.2, 127.6, 126.7, 125.5, 125.0, 124.7, 124.5, 122.6, 121.9, 117.4, 116.8, 114.6, 104.6, 79.5, 60.8, 56.4, 46.1, 43.0, 20.1.

IR (KBr) υ: 3492, 3062, 2931, 2215, 1610, 1537, 1467, 1430, 1284, 1203, 1116, 1031, 812, 758, 602 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{29}N_4O_2^+$ $[M + H]^+$ 597.2285; Found 597.2283.

2-amino-8,15-bis(5-(tert-butyl)-2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4p)



4p

The compound **4p** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.32 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 26.3 mg, 39% yield, reaction time = 1 h, m.p. 307-309 °C.

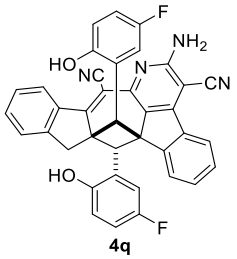
^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.76 (s, 2H), 8.62 (d, *J* = 8.2 Hz, 1H), 8.32 (d, *J* = 7.7 Hz, 1H), 8.18 (d, *J* = 7.5 Hz, 1H), 7.69 (t, *J* = 7.4 Hz, 1H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.52 (d, *J* = 4.3 Hz, 2H), 7.37 (dt, *J* = 8.4, 4.3 Hz, 1H), 6.73 (s, 2H), 6.70 (dd, *J* = 8.3, 2.4 Hz, 2H), 6.36 (d, *J* = 8.4 Hz, 2H), 5.95 – 5.91 (m, 2H), 4.52 (s, 2H), 4.11 (s, 2H), 0.74 (s, 18H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 169.0, 158.9, 153.1, 152.2, 151.4, 150.8, 150.7, 139.6, 139.5, 136.6, 132.2, 130.8, 129.1, 128.0, 126.5, 124.9, 124.4, 123.6, 122.1, 122.0, 117.4, 116.7, 114.1, 104.6, 80.0, 60.7, 56.5, 46.3, 43.4, 33.1, 30.8.

IR (KBr) υ: 3406, 2956, 2874, 2210, 1701, 1607, 1542, 1469, 1436, 1374, 1276, 1131, 1041, 821, 758, 619 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{46}H_{41}N_4O_2^+$ $[M + H]^+$ 681.3224; Found 681.3222.

2-amino-8,15-bis(5-fluoro-2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4q)



4q

The compound **4q** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.16 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 43.9 mg, 73% yield, reaction time = 2 h, m.p. 296-298 °C.

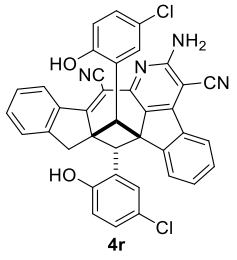
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.10 (s, 2H), 8.60 (d, *J* = 8.2 Hz, 1H), 8.31 (d, *J* = 7.6 Hz, 1H), 8.23 (d, *J* = 7.5 Hz, 1H), 7.71 (t, *J* = 7.4 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.60 – 7.51 (m, 2H), 7.40 (t, *J* = 7.6 Hz, 1H), 6.92 (s, 2H), 6.60 (td, *J* = 8.4, 3.1 Hz, 2H), 6.45 (dd, *J* = 8.9, 5.0 Hz, 2H), 5.55 (dd, *J* = 10.5, 3.1 Hz, 2H), 4.58 (s, 2H), 4.09 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.4, 159.2, 155.0, 153.1, 152.11, 152.06 (d, *J* = 1.3 Hz), 151.4, 150.5, 149.7, 138.8, 136.2, 132.7, 131.1, 128.6, 127.7, 125.8 (d, *J* = 274.2 Hz), 125.1, 124.8, 124.2 (d, *J* = 6.9 Hz), 122.2, 117.1, 116.6, 115.5 (d, *J* = 8.3 Hz), 113.7 (d, *J* = 22.4 Hz), 113.4 (d, *J* = 24.1 Hz), 104.6, 79.9, 60.7, 56.2, 45.8, 42.5.

IR (KBr) υ: 3494, 2881, 2817, 2217, 1629, 1541, 1505, 1434, 1388, 1266, 1176, 877, 817, 760 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}F_2N_4O_2^+$ $[M + H]^+$ 605.1784; Found 605.1785.

2-amino-8,15-bis(5-chloro-2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4r)



4r

The compound **4r** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.24 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 42.1 mg, 66% yield, reaction time = 2 h, m.p. 312-313 °C.

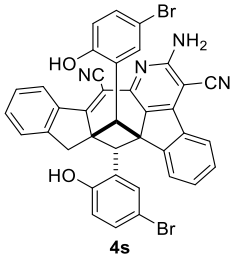
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.38 (s, 2H), 8.61 (d, *J* = 8.2 Hz, 1H), 8.32 (d, *J* = 7.6 Hz, 1H), 8.23 (d, *J* = 7.5 Hz, 1H), 7.71 (t, *J* = 7.4 Hz, 1H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.60 – 7.52 (m, 2H), 7.41 (t, *J* = 7.3 Hz, 1H), 6.92 (s, 2H), 6.79 (dd, *J* = 8.6, 2.6 Hz, 2H), 6.47 (d, *J* = 8.6 Hz, 2H), 5.78 (d, *J* = 2.6 Hz, 2H), 4.56 (s, 2H), 4.08 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.3, 159.1, 154.7, 152.1, 151.5, 150.4, 149.7, 138.9, 136.3, 132.7, 131.1, 128.6, 127.6, 127.1, 126.9, 125.1, 124.9, 124.8, 124.7, 122.1, 121.0, 117.1, 116.6, 116.3, 104.6, 79.7, 60.4, 56.1, 45.9, 42.5.

IR (KBr) υ: 3498, 2879, 2693, 2214, 1615, 1583, 1538, 1496, 1438, 1405, 1280, 1167, 1111, 1044, 878, 814, 755, 655 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Cl_2N_4O_2^+$ $[M + H]^+$ 637.1193; Found 637.1193.

2-amino-8,15-bis(5-bromo-2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4s)



4s

The compound **4s** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.23 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 37.2 mg, 51% yield, reaction time = 2 h, m.p. 312-313 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 9.39 (s, 2H), 8.61 (d, *J* = 8.2 Hz, 1H), 8.32 (d, *J* = 7.6 Hz, 1H), 8.22 (d, *J* = 7.5 Hz, 1H), 7.71 (t, *J* = 7.4 Hz, 1H), 7.67 (t, *J* = 7.5 Hz, 1H),

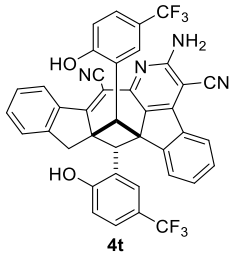
7.60 – 7.51 (m, 2H), 7.40 (t, *J* = 7.5 Hz, 1H), 6.93 – 6.86 (m, 4H), 6.42 (d, *J* = 8.6 Hz, 2H), 5.93 – 5.89 (m, 2H), 4.55 (s, 2H), 4.08 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.3, 159.1, 155.1, 152.1, 151.6, 150.5, 149.8, 139.0, 136.3, 132.7, 131.1, 130.2, 130.0, 128.7, 127.6, 126.9, 125.5, 125.1, 124.8, 124.8, 122.1, 117.1, 116.9, 116.6, 108.6, 104.6, 79.7, 60.4, 56.1, 46.0, 42.5.

IR (KBr) υ: 3483, 2882, 2822, 2214, 1612, 1537, 1484, 1437, 1400, 1278, 1166, 1108, 997, 876, 814, 757, 635 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Br_2N_4O_2^+$ $[M + H]^+$ 725.0182; Found 725.0185.

2-amino-8,15-bis(2-hydroxy-5-(trifluoromethyl)phenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4t)



4t

The compound **4t** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-2:1 as eluent. R_f = 0.11 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 50.2 mg, 71% yield, reaction time = 1 h, m.p. 290-292 °C.

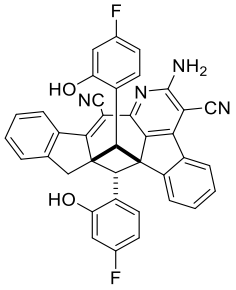
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.98 (s, 2H), 8.61 (d, *J* = 8.2 Hz, 1H), 8.34 (d, *J* = 7.6 Hz, 1H), 8.27 (d, *J* = 7.5 Hz, 1H), 7.73 (t, *J* = 7.4 Hz, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.62 – 7.56 (m, 2H), 7.46 – 7.38 (m, 1H), 7.10 (dd, *J* = 8.6, 1.3 Hz, 2H), 6.84 (s, 2H), 6.62 (d, *J* = 8.4 Hz, 2H), 6.13 (s, 2H), 4.63 (s, 2H), 4.14 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.1, 159.1, 158.9, 152.0, 151.7, 150.4, 149.8, 139.0, 136.3, 132.7, 131.2, 128.7, 127.5, 126.9, 125.0, 124.9 (d, *J* = 3.8 Hz), 124.8 (d, *J* = 5.2 Hz), 124.2 (q, *J* = 269.2 Hz), 123.7, 122.2, 118.2 (q, *J* = 31.7 Hz), 116.9, 116.4, 115.2, 104.7, 79.9, 60.0, 56.0, 46.1, 42.6.

IR (KBr) υ: 3452, 2923, 2854, 2216, 1703, 1622, 1529, 1468, 1440, 1328, 1290, 1164, 1118, 1080, 825, 757, 617 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{23}F_6N_4O_2^+$ $[M + H]^+$ 705.1720; Found 705.1722.

2-amino-8,15-bis(4-fluoro-2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4u)



4u

The compound **4u** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.16 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 52.8 mg, 87% yield, reaction time = 2 h, m.p. 307-308 °C.

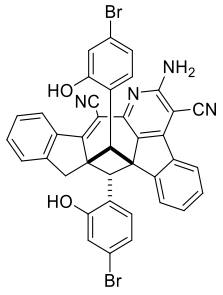
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.56 (s, 2H), 8.60 (d, *J* = 8.2 Hz, 1H), 8.29 (d, *J* = 7.6 Hz, 1H), 8.18 (d, *J* = 7.5 Hz, 1H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.59 – 7.51 (m, 2H), 7.39 (t, *J* = 7.3 Hz, 1H), 6.85 (s, 2H), 6.24 (dd, *J* = 10.7, 2.7 Hz, 2H), 6.13 (td, *J* = 8.5, 2.6 Hz, 2H), 5.85 (t, *J* = 7.7 Hz, 2H), 4.50 (s, 2H), 4.06 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.4, 161.9, 159.9, 159.0, 157.2 (d, *J* = 10.6 Hz), 152.1, 151.2, 150.5, 149.9, 138.8, 136.3, 132.6, 130.8, 128.3, 128.15, 128.14 (d, *J* = 10.3 Hz), 125.8 (d, *J* = 244.0 Hz), 125.0, 124.5, 122.2, 119.3 (d, *J* = 2.9 Hz), 117.2, 116.7, 104.6, 104.4 (d, *J* = 21.1 Hz), 101.8 (d, *J* = 23.4 Hz), 80.0, 60.5, 56.2, 45.8, 42.3.

IR (KBr) υ: 3453, 2945, 2890, 2215, 1708, 1607, 1540, 1469, 1432, 1388, 1284, 1221, 1153, 1100, 979, 846, 761, 612 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}F_2N_4O_2^+$ $[M + H]^+$ 605.1784; Found 605.1783.

2-amino-8,15-bis(4-bromo-2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4v)



4v

The compound **4v** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.24 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 72.8 mg, 99% yield, reaction time = 1 h, m.p. >320 °C.

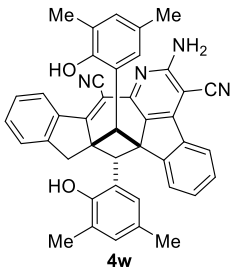
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.57 (s, 2H), 8.60 (d, *J* = 8.1 Hz, 1H), 8.30 (d, *J* = 7.5 Hz, 1H), 8.19 (d, *J* = 7.4 Hz, 1H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.59 – 7.50 (m, 2H), 7.39 (t, *J* = 7.5 Hz, 1H), 6.86 (s, 2H), 6.63 (d, *J* = 2.1 Hz, 2H), 6.47 (dd, *J* = 8.4, 2.0 Hz, 2H), 5.78 (d, *J* = 8.4 Hz, 2H), 4.50 (s, 2H), 4.05 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.3, 159.1, 156.9, 152.1, 151.3, 150.4, 149.8, 138.7, 136.3, 132.7, 130.9, 128.8, 128.4, 128.0, 126.9, 125.1, 124.9, 124.6, 122.5, 122.3, 120.7, 119.6, 117.4, 117.2, 116.7, 104.6, 80.2, 60.4, 56.1, 45.8, 42.5.

IR (KBr) υ: 3451, 2883, 2827, 2218, 1633, 1588, 1541, 1442, 1404, 1261, 1037, 889, 860, 794, 757 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{23}Br_2N_4O_2^+$ $[M + H]^+$ 725.0182; Found 725.0192.

2-amino-8,15-bis(2-hydroxy-3,5-dimethylphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4w)



4w

The compound **4w** was prepared according to general procedure **5** and purified by silica gel column chromatography using petroleum ether/ ethyl acetate = 5:1-3:1 as eluent. R_f = 0.35 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 46.1 mg, 74% yield, reaction time = 1 h, m.p. 308-310 °C.

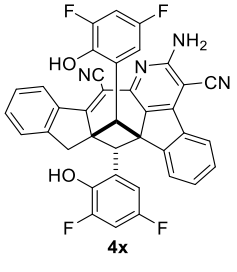
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.58 (d, *J* = 8.2 Hz, 1H), 8.27 (d, *J* = 7.6 Hz, 1H), 8.12 (d, *J* = 7.5 Hz, 1H), 7.65 (t, *J* = 7.4 Hz, 1H), 7.62 – 7.57 (m, 3H), 7.56 – 7.47 (m, 2H), 7.36 (t, *J* = 7.6 Hz, 1H), 6.79 (s, 2H), 6.45 (s, 2H), 5.60 (s, 2H), 4.58 (s, 2H), 4.09 (s, 2H), 1.84 (s, 6H), 1.65 (s, 6H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 168.8, 159.0, 151.6, 151.3, 151.2, 150.7, 150.1, 139.1, 136.6, 132.4, 130.7, 129.5, 129.0, 128.1, 126.7, 126.2, 125.8, 125.2, 124.8, 124.3, 123.9, 123.8, 122.0, 117.4, 116.8, 104.8, 79.6, 61.7, 57.0, 45.6, 42.8, 20.2, 16.8.

IR (KBr) υ: 3562, 2962, 2889, 2210, 1625, 1533, 1473, 1387, 1194, 1157, 1095, 1044, 811, 756 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{42}H_{33}N_4O_2^+$ $[M + H]^+$ 625.2598; Found 625.2594.

2-amino-8,15-bis(3,5-difluoro-2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3] indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4x)



4x

To a solution of ortho-hydroxyphenyl-substituted indene-diene **1** (0.1 mmol, 1.0 equiv) in N, N-dimethylformamide (0.75 mL), tetramethylguanidine (0.04 mmol, 0.40 equiv)

was added. Then, the resulting reaction mixture was stirred at 100 °C for 1 hours. Upon completion (monitored by TLC), the reaction solution was cooled to room temperature. Water was added (10 mL) and the mixture was extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with brine (15 mL), dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 3 : 1) to afford pure product **4x**. R_f = 0.24 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 22.4 mg, 70% yield, m.p. 190-192 °C.

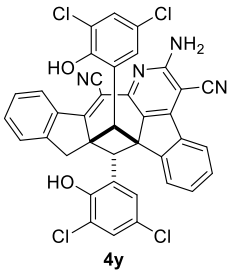
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.27 (s, 2H), 8.59 (d, *J* = 8.2 Hz, 1H), 8.30 (d, *J* = 7.6 Hz, 1H), 8.24 (d, *J* = 7.5 Hz, 1H), 7.71 (t, *J* = 7.4 Hz, 1H), 7.65 (t, *J* = 7.6 Hz, 1H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 1H), 6.96 (s, 2H), 6.88 – 6.80 (m, 2H), 5.45 (d, *J* = 10.0 Hz, 2H), 4.70 (s, 2H), 4.10 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 167.7, 159.3, 152.9 (dd, *J* = 235.8, 11.9 Hz), 152.6, 151.5, 150.5 (dd, *J* = 241.2, 13.6 Hz), 150.2, 149.1, 139.8 (dd, *J* = 15.2, 3.1 Hz), 138.4, 136.2, 132.9, 131.2, 128.7, 127.1, 127.1, 127.0 (dd, *J* = 8.4, 3.6 Hz), 125.4, 124.9, 124.7, 122.4, 116.9, 116.5, 108.7 (dd, *J* = 23.2, 2.5 Hz), 104.7, 102.6 (dd, *J* = 26.3, 23.0 Hz), 80.2, 60.9, 56.3, 45.5, 42.2.

IR (KBr) υ: 3498, 2960, 2866, 2218, 1720, 1630, 1541, 1493, 1448, 1361, 1226, 1121, 1082, 989, 853, 762, 604 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{21}F_4N_4O_2^+$ $[M + H]^+$ 641.1595; Found 641.1601.

2-amino-8,15-bis(3,5-dichloro-2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2, 3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4y)



4y

To a solution of ortho-hydroxyphenyl-substituted indene-diene **1** (0.1 mmol, 1.0 equiv) in N, N-dimethylformamide (0.75 mL), tetramethylguanidine (0.04 mmol, 0.40 equiv) was added. Then, the resulting reaction mixture was stirred at 100 °C for 1 hours. Upon completion (monitored by TLC), the reaction solution was cooled to room temperature. Water was added (10 mL) and the mixture was extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with brine (15 mL), dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 3 : 1) to afford pure products **4y**. R_f = 0.30 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 25.1 mg, 71% yield, m.p. >320 °C.

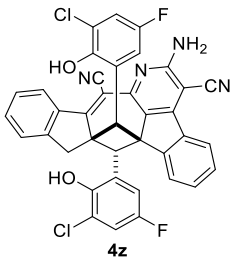
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.27 (s, 2H), 8.59 (d, *J* = 8.2 Hz, 1H), 8.31 (d, *J* = 7.6 Hz, 1H), 8.22 (d, *J* = 7.5 Hz, 1H), 7.71 (t, *J* = 7.4 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.58 (t, *J* = 7.3 Hz, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.11 (d, *J* = 2.2 Hz, 2H), 6.98 (s, 2H), 5.82 (d, *J* = 2.5 Hz, 2H), 4.69 (s, 2H), 4.09 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 167.6, 159.3, 151.7, 151.3, 150.4, 150.2, 149.0, 138.4, 136.2, 133.0, 131.2, 128.8, 127.8, 127.2, 127.1, 126.9, 126.1, 125.5, 124.9, 124.7, 122.4, 122.0, 121.4, 116.8, 116.5, 104.7, 80.1, 61.0, 56.4, 45.4, 42.3.

IR (KBr) υ: 3496, 3076, 2974, 2881, 2216, 1624, 1580, 1536, 1465, 1443, 1314, 1234, 1159, 1047, 858, 752 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{21}Cl_4N_4O_2^+$ $[M + H]^+$ 705.0413; Found 705.0412.

2-amino-8,15-bis(3-chloro-5-fluoro-2-hydroxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4z)



4z

To a solution of ortho-hydroxyphenyl-substituted indene-diene **1** (0.1 mmol, 1.0 equiv) in N, N-dimethylformamide (0.75 mL), tetramethylguanidine (0.04 mmol, 0.40 equiv) was added. Then, the resulting reaction mixture was stirred at 100 °C for 1 hours. Upon completion (monitored by TLC), the reaction solution was cooled to room temperature. Water was added (10 mL) and the mixture was extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with brine (15 mL), dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 3 : 1) to afford pure product **4z**. R_f = 0.28 (petroleum ether/ethyl acetate = 2:1). Yellow solid, 29.4 mg, 87% yield, m.p. 217-218 °C.

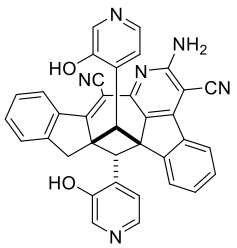
^{1}H NMR (500 MHz, DMSO-d_6) δ 8.94 (s, 2H), 8.58 (d, *J* = 8.2 Hz, 1H), 8.30 (d, *J* = 7.6 Hz, 1H), 8.22 (d, *J* = 7.5 Hz, 1H), 7.70 (t, *J* = 7.4 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.58 (t, *J* = 7.3 Hz, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.01 – 6.96 (m, 4H), 5.61 (dd, *J* = 10.0, 3.1 Hz, 2H), 4.72 (s, 2H), 4.09 (s, 2H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 167.6, 159.3, 154.6, 152.7, 151.6, 151.3, 150.2, 148.9, 148.0 (d, *J* = 2.5 Hz), 138.2, 136.2, 133.0, 131.2, 128.7, 127.4 (d, *J* = 7.5 Hz), 127.1, 126.9, 125.5, 124.7, 123.6 (d, *J* = 272.7 Hz), 121.0 (d, *J* = 11.8 Hz), 116.8, 116.5, 114.8 (d, *J* = 25.6 Hz), 112.6 (d, *J* = 23.9 Hz), 104.7, 80.3, 61.2, 56.5, 45.2, 42.4.

IR (KBr) υ: 3458, 3217, 3075, 2926, 2850, 2213, 1717, 1624, 1591, 1458, 1309, 1230, 1161, 1041, 863, 756 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{21}Cl_2F_2N_4O_2^+$ $[M + H]^+$ 673.1004; Found 673.1001.

2-amino-8,15-bis(3-hydroxypyridin-4-yl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (4a')



4a'

The compound **4a'** was prepared according to general procedure **5** and purified by silica gel column chromatography using dichloromethane/ ethyl acetate = 3:1-1:1 to dichloromethane/ methyl alcohol = 20:1 as eluent. R_f = 0.33 (dichloromethane/methyl alcohol = 20:1). Yellow solid, 46.2 mg, 81% yield, reaction time = 0.5 h, m.p. 312-313 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 9.55 (s, 2H), 8.59 (d, *J* = 8.2 Hz, 1H), 8.34 (d, *J* = 7.6 Hz, 1H), 8.27 (d, *J* = 7.4 Hz, 1H), 7.79 (s, 2H), 7.75 – 7.64 (m, 2H), 7.60 – 7.55 (m, 2H), 7.50 (d, *J* = 5.0 Hz, 2H), 7.45 – 7.37 (m, 1H), 6.91 (s, 2H), 5.76 (d, *J* = 5.1 Hz, 2H), 4.65 (s, 2H), 4.12 (s, 2H).

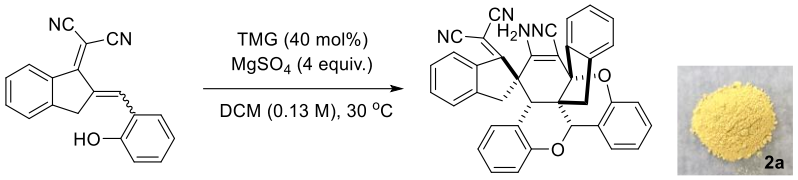
^{13}C NMR (125 MHz, DMSO-d_6) δ 168.3, 159.6, 152.5, 152.4, 152.0, 150.5, 149.8, 139.9, 139.1, 137.7, 136.8, 133.2, 131.5, 131.0, 129.1, 127.7, 127.4, 125.5, 125.3, 125.3, 122.9, 122.0, 117.4, 117.1, 105.0, 80.7, 60.4, 55.9, 46.2, 42.6.

IR (KBr) υ: 3458, 3360, 3073, 2379, 2210, 1717, 1605, 1546, 1428, 1308, 1267, 1076, 807 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{36}H_{22}N_6O_2Na^+$ $[M + Na]^+$ 593.1696; Found 593.1698.

10. Experimental procedure for gram scale synthesis of compounds 2a, 4a and 4v

Experimental procedure for gram scale synthesis of compound 2a

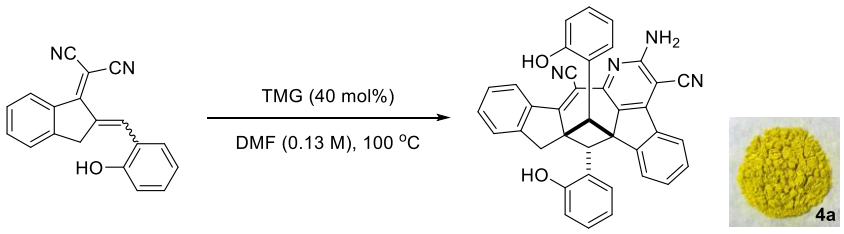


1a, 3 mmol

2a, 0.460 g, 54%

To a solution of ortho-hydroxyphenyl-substituted indene-diene **1a** (3.0 mmol, 1.0 equiv) and anhydrous sodium sulfate (12 mmol, 4.0 equiv) in dichloromethane (22.5 mL), tetramethylguanidine (1.2 mmol, 0.40 equiv) was added at 30 °C. Then, the resulting mixture was stirred at 30 °C in oil bath for 96 hours. Upon completion (monitored by TLC), the reaction solution was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent DCM to DCM : EtOAc = 20 : 1) to afford pure product **2a** as a yellow solid (0.460 g, 54% yield).

Experimental procedure for gram scale synthesis of compound 4a



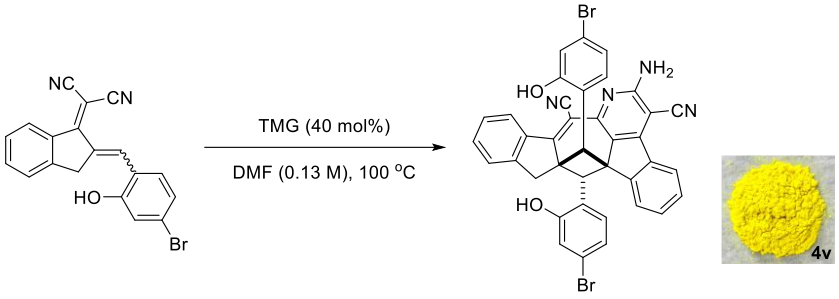
1a, 3 mmol

4a, 0.634 g, 74%

To a solution of ortho-hydroxyphenyl-substituted indene-diene **1a** (3.0 mmol, 1.0 equiv) in N, N-dimethylformamide (22.5 mL), tetramethylguanidine (1.2 mmol, 0.40 equiv) was added. Then, the reaction temperature was elevated to 100 °C and the reaction mixture was stirred at 100 °C for 1 hour. Upon completion (monitored by TLC), the

reaction solution was cooled to room temperature. Water was added (30 mL) and the mixture was extracted with ethyl acetate (30 mL × 3). The combined organic layer was washed with brine (60 mL), dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 2 : 1) to afford pure product **4a** as a yellow solid (0.634 g, 74% yield).

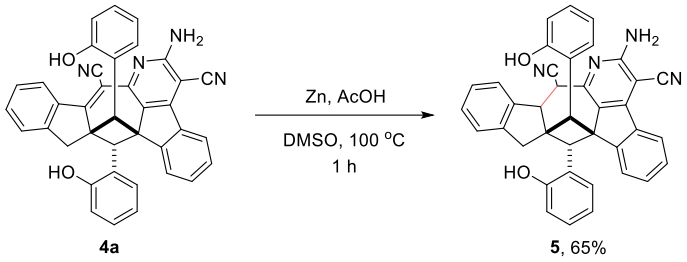
Experimental procedure for gram scale synthesis of compound 4v



To a solution of 4-bromo-2-hydroxyphenyl-substituted indene-diene **1v** (3.0 mmol, 1.0 equiv) in N, N-dimethylformamide (22.5 mL), tetramethylguanidine (1.2 mmol, 0.40 equiv) was added. Then, the reaction temperature was elevated to 100 °C and the reaction mixture was stirred at 100 °C for 0.5 hour. Upon completion (monitored by TLC), the reaction solution was cooled to room temperature. Water was added (30 mL) and the mixture was extracted with ethyl acetate (30 mL × 3). The combined organic layer was washed with brine (60 mL), dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 2 : 1) to afford pure product **4v** as a yellow solid (0.987 g, 91% yield).

11. Synthetic Derivatization of products

Synthetic procedure and characterization data of compound 5:



4a **5**, 65%

To the solution of **4a** (0.05 mmol, 1.0 equiv) and zinc (0.25 mmol, 5.0 equiv) in dimethyl sulfoxide (1.5 mL), acetic acid (1.0 mL) was added. Then, the reaction mixture was stirred at 100 °C in oil bath for 1 hour. Upon completion (monitored by TLC), the reaction solution was cooled to room temperature, and then filtered in vacuo. The residue was washed with ethyl acetate. The mixture was extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with brine (15 mL), dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 2 : 1) to afford pure products **5** as a yellow solid (18.5 mg, 65% yield).

2-amino-8,15-bis(2-hydroxyphenyl)-13b,14-dihydro-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (5): Yellow solid, 18.5 mg, 65% yield, R_f = 0.20 (petroleum ether/ethyl acetate = 2:1). m.p. 235-236 °C.

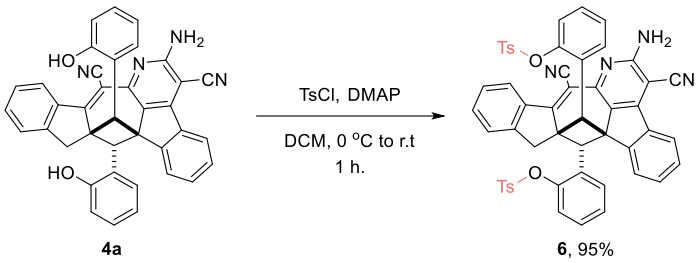
^{1}H NMR (500 MHz, DMSO-d_6) δ 9.70 (s, 1H), 8.70 (s, 1H), 8.29 (d, *J* = 7.7 Hz, 1H), 8.06 (d, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 7.7 Hz, 1H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.35 (d, *J* = 7.3 Hz, 1H), 7.30 (t, *J* = 7.3 Hz, 1H), 7.24 (t, *J* = 7.4 Hz, 1H), 7.03 (s, 2H), 6.87 (t, *J* = 7.5 Hz, 1H), 6.76 – 6.68 (m, 2H), 6.42 – 6.33 (m, 2H), 6.13 (t, *J* = 7.5 Hz, 1H), 5.95 (t, *J* = 8.2 Hz, 2H), 4.70 (s, 1H), 4.48 (s, 1H), 4.28 (d, *J* = 16.9 Hz, 1H), 4.02 (d, *J* = 11.7 Hz, 1H), 3.91 (d, *J* = 11.6 Hz, 1H), 3.71 (d, *J* = 17.1 Hz, 1H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 158.9, 155.7, 155.4, 153.1, 151.2, 150.8, 143.3, 143.2, 135.7, 131.1, 128.2, 128.1, 127.8, 127.8, 127.6, 126.8, 126.4, 124.2, 124.2, 123.8, 122.9, 122.6, 122.2, 120.6, 118.7, 117.8, 117.7, 116.4, 115.5, 114.9, 81.8, 58.7, 57.2, 55.5, 51.2, 47.0, 45.6, 41.7.

IR (KBr) υ: 3451, 3241, 3032, 2939, 2883, 2378, 2217, 1707, 1629, 1596, 1569, 1451, 1371, 1272, 1154, 1098, 1043, 846, 754 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{38}H_{27}N_4O_2^+$ $[M + H]^+$ 571.2129; Found 571.2125.

Synthetic procedure and characterization data of compound 6:



4a **6**, 95%

To the solution of **4a** (0.2 mmol, 1.0 equiv) and tosyl chloride (0.50 mmol, 2.5 equiv) in dry dichloromethane (2.0 mL), 4-dimethylaminopyridine (0.60 mmol, 3.0 equiv) was added dropwise at 0 °C. And then the reaction mixture was warmed to room temperature and stirred at room temperature for 1 hour. Upon completion (monitored by TLC), the reaction solution was diluted with water (15 mL) and extracted with dichloromethane (15 mL × 3). Then, the combined organic layer was dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo to afford the crude product. The crude product was purified by column chromatography on silica gel (eluent PE : DCM = 1 : 1 to DCM) to afford pure product **6** as a yellow solid (166.1 mg, 95% yield).

(2-amino-3,14-dicyano-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno [8,1-bc]pyridine-8,15-diyl)bis(2,1-phenylene) bis(4-methylbenzenesulfonate) (6):

Yellow solid, 166.1 mg, 95% yield, R_f = 0.36 (dichloromethane). m.p. 279-280 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.45 (d, *J* = 8.2 Hz, 1H), 8.20 (d, *J* = 7.7 Hz, 1H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.66 – 7.58 (m, 3H), 7.56 (s, 8H), 7.45 – 7.38 (m, 2H), 7.03 (t,

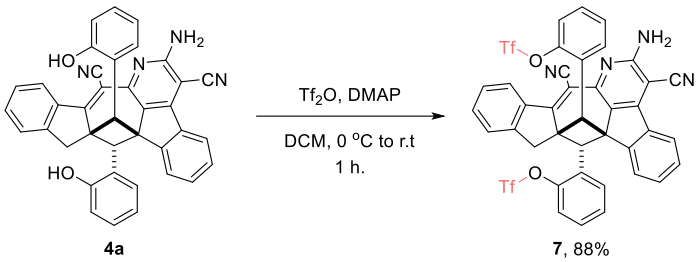
J = 7.7 Hz, 2H), 6.92 (s, 2H), 6.87 (t, *J* = 7.6 Hz, 2H), 6.81 (d, *J* = 8.1 Hz, 2H), 6.22 (d, *J* = 7.7 Hz, 2H), 3.93 (s, 2H), 3.62 (s, 2H), 2.52 (s, 6H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 165.4, 159.2, 150.6, 150.2, 149.8, 147.2, 146.4, 146.3, 137.0, 135.8, 133.4, 131.7, 131.5, 130.4, 129.1, 128.6, 128.1, 128.1, 127.9, 127.6, 126.6, 126.5, 125.8, 124.9, 124.4, 122.3, 121.7, 116.4, 116.3, 105.7, 80.6, 60.4, 56.8, 44.3, 42.1, 21.3.

IR (KBr) υ: 3487, 3070, 2952, 2581, 2314, 2212, 1746, 1610, 1543, 1443, 1375, 1297, 1167, 1089, 853, 769, 730, 664 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{52}H_{37}N_4O_6S_2^+$ $[M + H]^+$ 877.2149; Found 877.2151.

Synthetic procedure and characterization data of compound 7:



To the solution of **4a** (0.05 mmol, 1.0 equiv) and 4-dimethylaminopyridine (0.15 mmol, 3.0 equiv) in dichloromethane (1.5 mL), triflic anhydride (0.11 mmol, 2.2 equiv) was added dropwise at 0 °C. And then the reaction mixture was warmed to room temperature and stirred at room temperature for 1 hour. Upon completion (monitored by TLC), the reaction solution was diluted with water (10 mL) and extracted with dichloromethane (10 mL × 3). Then, the combined organic layer was dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo to afford the crude product. The crude product was purified by column chromatography on silica gel (eluent PE : DCM = 1 : 4 to DCM : EtOAc = 20 : 1) to afford pure products **7** as a yellow solid (36.4 mg, 88% yield).

2-amino-3,14-dicyano-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno [8,1-bc]pyridine-8,15-diyl)bis(2,1-phenylene) bis(trifluoromethanesulfonate) (7):

Yellow solid, 36.4 mg, 88% yield, R_f = 0.25 (petroleum ether/ dichloromethane = 1:4). m.p. 287-288 °C.

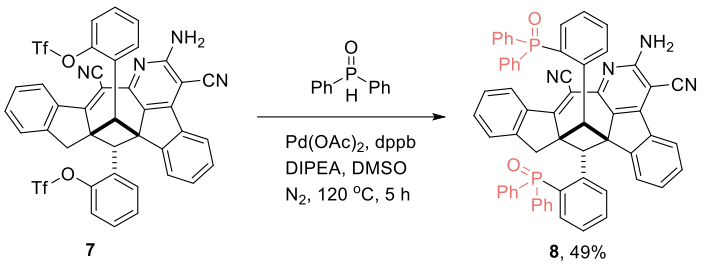
^{1}H NMR (500 MHz, DMSO-*d*$_6$) δ 8.50 (d, *J* = 8.2 Hz, 1H), 8.28 (dd, *J* = 7.7, 3.7 Hz, 2H), 7.72 (t, *J* = 7.5 Hz, 1H), 7.69 – 7.59 (m, 2H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.20 (t, *J* = 7.8 Hz, 2H), 7.10 – 7.02 (m, 4H), 7.00 (s, 2H), 6.46 (d, *J* = 7.9 Hz, 2H), 4.98 (s, 2H), 4.06 (s, 2H).

^{13}C NMR (125 MHz, DMSO-*d*$_6$) δ 165.2, 159.3, 150.9, 149.8, 149.7, 147.4, 146.5, 137.0, 136.0, 133.5, 131.6, 129.5, 129.3, 129.1, 127.9, 127.7, 126.5, 125.8, 125.3, 124.9, 122.3, 120.6, 117.9 (q, *J* = 319.5 Hz), 116.3, 116.2, 106.0, 80.7, 60.8, 57.3, 43.8, 41.6.

IR (KBr) υ: 3442, 3249, 2505, 2311, 2212, 1629, 1539, 1475, 1422, 1215, 1139, 1082, 869, 760, 603 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{23}F_6N_4O_6S^+$ $[M + H]^+$ 833.0958; Found 833.0960.

Synthetic procedure and characterization data of compound 8:



Under nitrogen atmosphere, DMSO (1.5 mL) was added to the mixture of **7** (0.1 mmol, 1.0 equiv), $Ph_2P(O)H$ (0.8 mmol, 8.0 equiv), $Pd(OAc)_2$ (0.06 mmol, 0.6 equiv) and dppb (0.06 mmol, 0.6 equiv). Then, DIPEA (1.0 mmol, 10.0 equiv) was added to the reaction mixture, which was stirred at 120 °C in oil bath for 5 h. Upon completion (monitored by TLC), the reaction solution was diluted with water (15 mL) and extracted with ethyl acetate (10 mL × 3). Then, the combined organic layer was dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo to afford the crude product. The crude product was purified by column chromatography on silica

gel (eluent DCM : EtOAc = 3 : 1 to 1 : 1) to afford pure products **8** as a yellow solid (45.6 mg, 49% yield).

2-amino-8,15-bis(2-(diphenylphosphoryl)phenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno[2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (8): Yellow solid, 45.6 mg, 49% yield, R_f = 0.50 (dichloromethane/ethyl acetate = 2:1). m.p. 224-226 °C.

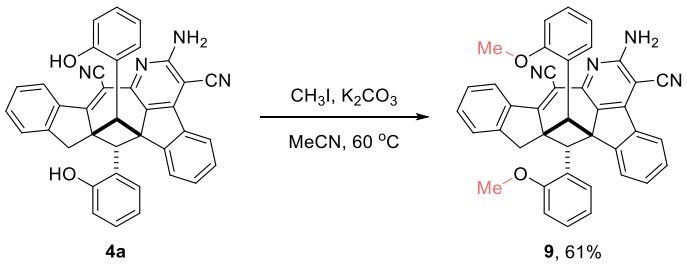
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.25 – 9.17 (m, 1H), 8.59 (d, *J* = 8.1 Hz, 1H), 8.06 – 7.85 (m, 2H), 7.53 – 7.48 (m, 3H), 7.48 – 7.41 (m, 5H), 7.41 – 7.32 (m, 2H), 7.29 – 7.21 (m, 3H), 7.21 – 7.13 (m, 4H), 7.13 – 7.06 (m, 5H), 7.07 – 7.02 (m, 1H), 7.00 – 6.93 (m, 5H), 6.86 (t, *J* = 7.6 Hz, 1H), 6.82 – 6.67 (m, 3H), 5.44 (s, 2H), 4.92 (s, 1H), 4.04 (d, *J* = 18.7 Hz, 1H), 3.08 (d, *J* = 18.5 Hz, 1H), 2.19 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 158.5, 150.4, 150.1, 150.0, 144.8, 142.6, 142.5, 141.6, 141.5, 137.1, 137.1, 134.8, 134.7, 134.7, 134.6, 134.3, 134.2, 133.9, 133.6, 133.2, 133.2, 133.2, 133.0, 132.8, 132.4, 132.4, 132.3, 132.2, 132.2, 132.2, 132.1, 132.1, 132.0, 131.9, 131.8, 131.6, 131.6, 131.5, 131.4, 131.3, 130.9, 130.8, 130.5, 130.5, 130.3, 130.2, 129.0, 128.9, 128.8, 128.7, 128.5, 128.5, 128.4, 128.4, 127.9, 127.2, 127.1, 127.1, 126.5, 126.5, 126.4, 125.9, 124.9, 122.9, 117.7, 116.8, 106.5, 82.3, 77.4, 63.6, 59.2, 53.2, 53.1, 39.8, 38.3, 38.2.

IR (KBr) υ: 3471, 3296, 3056, 2209, 1587, 1536, 1436, 1385, 1300, 1177, 1112, 993, 911, 840, 721 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{62}H_{43}N_4O_2P_2^+$ $[M + H]^+$ 937.2856; Found 937.2851.

Synthetic procedure and characterization data of compound 9:



To the solution of **4a** (0.04 mmol, 1.0 equiv) and potassium carbonate (0.16 mmol, 4.0 equiv) in acetonitrile (1.0 mL), iodomethane (0.16 mmol, 4.0 equiv) was added at room temperature. Then, the reaction mixture was stirred at 60 ºC for 6 hours. Upon completion (monitored by TLC), the reaction solution was diluted with water (10 mL) and extracted with ethyl acetate (10 mL × 3). Then, the combined organic layer was dried over anhydrous sodium sulfate, and filtered. The filtrate was concentrated in vacuo to afford the crude product. The crude product was purified by column chromatography on silica gel (eluent PE : EtOAc = 5 : 1 to 4 : 1) to afford pure product **9** as a yellow solid (14.6 mg, 61% yield).

2-amino-8,15-bis(2-methoxyphenyl)-8H,9H-7b,8a-methanobenzo[2,3]indeno [2',1':5,6]azuleno[8,1-bc]pyridine-3,14-dicarbonitrile (9): Yellow solid, 14.6 mg, 61% yield, R_f = 0.42 (petroleum ether/ethyl acetate = 3:1). m.p. 290-291 °C.

^{1}H NMR (500 MHz, DMSO-d_6) δ 8.60 (d, *J* = 8.2 Hz, 1H), 8.35 (d, *J* = 7.7 Hz, 1H), 8.23 (d, *J* = 7.6 Hz, 1H), 7.74 (t, *J* = 7.5 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.7 Hz, 1H), 6.92 (t, *J* = 7.8 Hz, 2H), 6.75 (s, 2H), 6.60 (d, *J* = 8.2 Hz, 2H), 6.42 (t, *J* = 7.5 Hz, 2H), 5.95 (d, *J* = 7.7 Hz, 2H), 4.54 (s, 2H), 4.00 (s, 2H), 2.83 (s, 6H).

^{13}C NMR (125 MHz, DMSO-d_6) δ 167.9, 158.9, 156.8, 151.4, 151.1, 150.6, 150.1, 138.9, 136.1, 132.4, 130.9, 128.3, 128.1, 127.8, 127.0, 125.3, 124.8, 124.5, 124.3, 122.2, 119.3, 116.9, 116.6, 110.1, 1047, 79.9, 59.7, 56.5, 53.6, 46.0, 43.3.

IR (KBr) υ: 3433, 2962, 2916, 2850, 2212, 1733, 1538, 1459, 1261, 1096, 1026, 869, 856, 702 cm^{-1}.

HRMS (ESI) m/z: Calcd for $C_{40}H_{29}N_4O_2^+$ $[M + H]^+$ 597.2285; Found 597.2284.

12. X-ray crystallographic data for compounds 2a, 3a, 4a, 5, 8 and 11

X-ray crystallographic data for compound 2a

Crystal data for compound **2a**: $C_{42}H_{32}N_4O_4$, M = 656.71, a = 12.5542(6) Å, b = 14.0614(7) Å, c = 18.8278(10) Å, α = 90°, β = 96.095(2)°, γ = 90°, V = 3304.9(3) Å^3, T = 150.(2) K, space group $P121/n1$, Z = 4, μ(Cu Kα) = 0.690 mm^{-1}, 21704 reflections measured, 6027 independent reflections (R_{int} = 0.0706). The final R_1 values were 0.0523 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1402 ($I > 2\sigma(I)$). The final R_1 values were 0.0766 (all data). The final $wR(F^2)$ values were 0.1482 (all data). The goodness of fit on F^2 was 1.082.

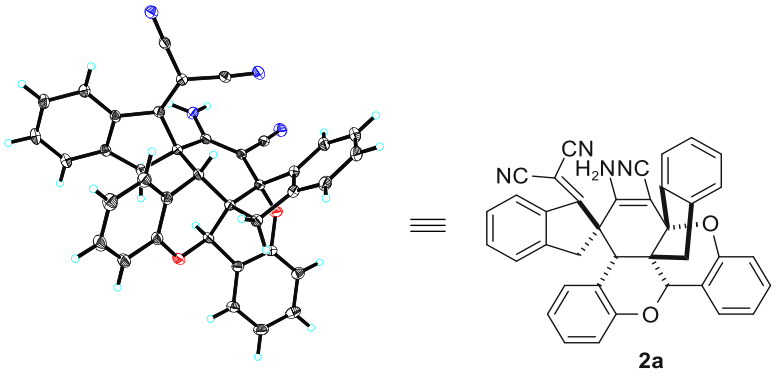


Fig. S10 View of a molecule of compound **2a** with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

Table S2 Crystal data and structure refinement for compound **2a**.

Identification code	global	
Empirical formula	C42 H32 N4 O4	
Formula weight	656.71	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 12.5542(6) Å	α= 90°.
	b = 14.0614(7) Å	β= 96.095(2)°.

	c = 18.8278(10) Å γ = 90°.
Volume	3304.9(3) Å^3
Z	4
Density (calculated)	1.320 Mg/m^3
Absorption coefficient	0.690 mm^{-1}
F(000)	1376
Crystal size	0.350 x 0.200 x 0.160 mm^3
Theta range for data collection	3.93 to 68.39°.
Index ranges	-15<=h<=15, -16<=k<=16, -22<=l<=22
Reflections collected	21704
Independent reflections	6027 [R(int) = 0.0706]
Completeness to theta = 68.39°	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.90 and 0.67
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6027 / 0 / 453
Goodness-of-fit on F^2	1.082
Final R indices [I>2sigma(I)]	R1 = 0.0523, wR2 = 0.1402
R indices (all data)	R1 = 0.0766, wR2 = 0.1482
Largest diff. peak and hole	0.550 and -0.357 e.Å^{-3}

X-ray crystallographic data for compound 3a

Crystal data for **compound 3a**: $C_{38}H_{24}N_4O_2 \bullet C_4H_8O_2$, M = 656.71, a = 10.2680(5) Å, b = 11.7261(6) Å, c = 14.8370(7) Å, α = 104.156(2)°, β = 106.691(2)°, γ = 100.305(2)°, V = 1598.40(14) Å^3, T = 150.(2) K, space group P-1, Z = 2, μ(Cu Kα) = 0.714 mm^{-1}, 25053 reflections measured, 5832 independent reflections (R_{int} = 0.0561). The final R_1 values were 0.0451 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1172 ($I > 2\sigma(I)$). The final R_1 values were 0.0524 (all data). The final $wR(F^2)$ values were 0.1225 (all data). The goodness of fit on F^2 was 1.027.

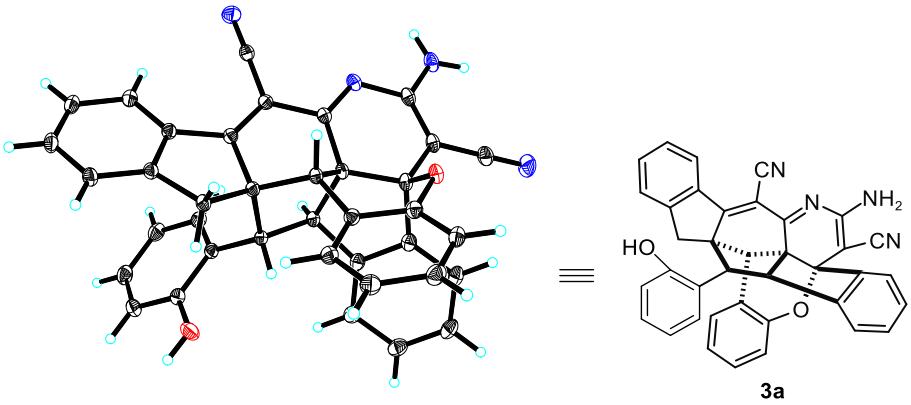


Fig. S11 View of a molecule of compound **3a** with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

Table S3 Crystal data and structure refinement for compound **3a**.

Identification code	global	
Empirical formula	C42 H32 N4 O4	
Formula weight	656.71	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.2680(5) Å	α=104.156(2)°.
	b = 11.7261(6) Å	β=106.691(2)°.
	c = 14.8370(7) Å	γ=100.305(2)°.
Volume	1598.40(14) $Å^3$	
Z	2	
Density (calculated)	1.364 Mg/m^3	
Absorption coefficient	0.714 mm^{-1}	
F(000)	688	
Crystal size	0.250 x 0.130 x 0.100 mm^3	
Theta range for data collection	4.04 to 68.30°.	
Index ranges	-12<=h<=12, -14<=k<=13, -17<=l<=17	
Reflections collected	25053	
Independent reflections	5832 [R(int) = 0.0561]	

Completeness to theta = 68.30°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.93 and 0.74
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5832 / 0 / 454
Goodness-of-fit on F^2	1.027
Final R indices [I>2sigma(I)]	R1 = 0.0451, wR2 = 0.1172
R indices (all data)	R1 = 0.0524, wR2 = 0.1225
Largest diff. peak and hole	0.499 and -0.350 e.Å^{-3}

X-ray crystallographic data for compound 4a

Crystal data for **compound 4a**: $C_{38}H_{24}N_4O_2 \bullet C_4H_8O_2$, M = 656.71, a = 14.0567(8) Å, b = 12.8429(7) Å, c = 19.1088(9) Å, α = 90°, β = 111.022(3)°, γ = 90°, V = 3220.1(3) Å^3, T = 150.(2) K, space group $P121/c1$, Z = 4, μ(Cu Kα) = 0.709 mm^{-1}, 68374 reflections measured, 5936 independent reflections (R_{int} = 0.6224). The final R_1 values were 0.1828 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.4364 ($I > 2\sigma(I)$). The final R_1 values were 0.2950 (all data). The final $wR(F^2)$ values were 0.5537 (all data). The goodness of fit on F^2 was 1.058.

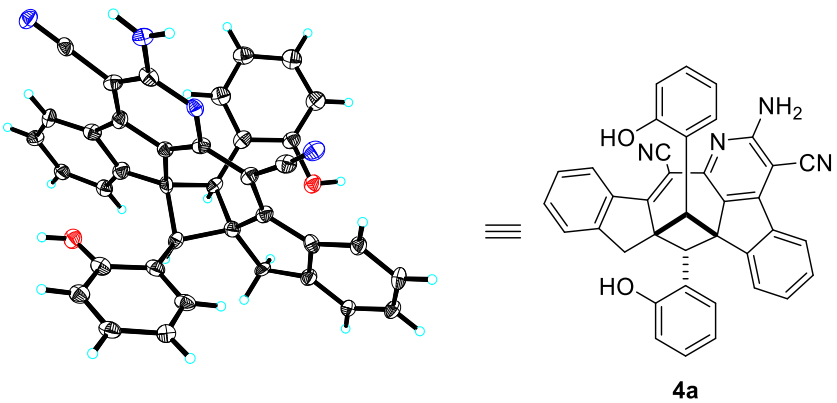


Fig. S12 View of a molecule of **compound 4a** with the atom-labelling scheme. Displacement ellipsoids are drawn at the 10% probability level.

Table S4 Crystal data and structure refinement for **compound 4a**.

Identification code	global	
Empirical formula	C42 H32 N4 O4	
Formula weight	656.71	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 14.0567(8) Å	α= 90°.
	b = 12.8429(7) Å	β=111.022(3)°.
	c = 19.1088(9) Å	γ = 90°.
Volume	3220.1(3) $Å^3$	
Z	4	
Density (calculated)	1.355 Mg/m^3	
Absorption coefficient	0.709 mm^{-1}	
F(000)	1376	
Crystal size	0.270 x 0.050 x 0.020 mm^3	
Theta range for data collection	3.37 to 69.04°.	
Index ranges	-16<=h<=16, -15<=k<=15, -23<=l<=23	
Reflections collected	68374	
Independent reflections	5936 [R(int) = 0.6224]	
Completeness to theta = 69.04°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.99 and 0.37	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5936 / 0 / 456	
Goodness-of-fit on F^2	1.058	
Final R indices [I>2sigma(I)]	R1 = 0.1828, wR2 = 0.4364	
R indices (all data)	R1 = 0.2950, wR2 = 0.5537	
Extinction coefficient	0.011(2)	
Largest diff. peak and hole	0.325 and -0.297 $e.Å^{-3}$	

X-ray crystallographic data for compound 5

Crystal data for **compound 5**: $C_{38}H_{26}N_4O_2 \bullet C_2H_6O$, $M = 616.69$, $a = 12.1304(4)$ Å, $b = 10.3755(4)$ Å, $c = 25.2295(9)$ Å, $\alpha = 90°$, $\beta = 102.9180(10)°$, $\gamma = 90°$, $V = 3094.99(19)$ Å^3, $T = 150.(2)$ K, space group $P12/c1$, $Z = 4$, μ(Cu Kα) = 0.675 mm^{-1}, 27808 reflections measured, 5666 independent reflections ($R_{int} = 0.1189$). The final R_1 values were 0.0824 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1902 ($I > 2\sigma(I)$). The final R_1 values were 0.1041 (all data). The final $wR(F^2)$ values were 0.2110 (all data). The goodness of fit on F^2 was 1.077.

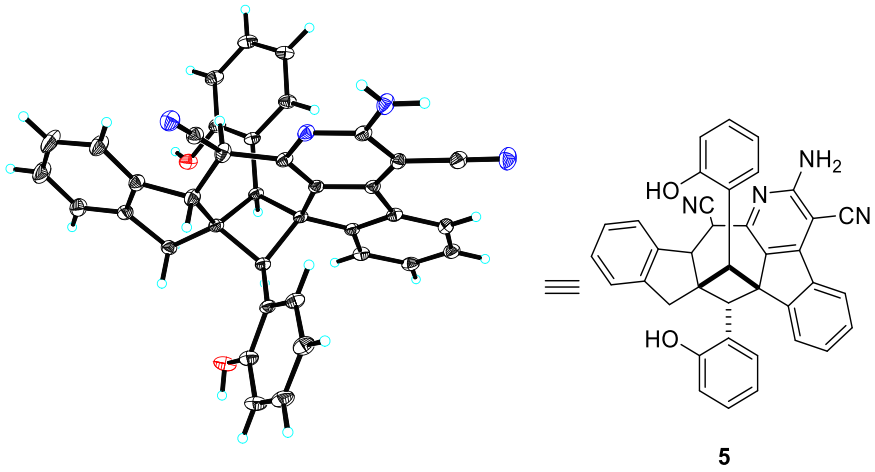


Fig. S13 View of a molecule of **compound 5** with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

Table S5 Crystal data and structure refinement for **compound 5**.

Identification code	global	
Empirical formula	C40 H32 N4 O3	
Formula weight	616.69	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 1 2/c 1	
Unit cell dimensions	a = 12.1304(4) Å	α= 90°.
	b = 10.3755(4) Å	β= 102.9180(10)°.
	c = 25.2295(9) Å	γ = 90°.

Volume	3094.99(19) $Å^3$
Z	4
Density (calculated)	1.323 Mg/m^3
Absorption coefficient	0.675 mm^{-1}
F(000)	1296
Crystal size	0.500 x 0.240 x 0.170 mm^3
Theta range for data collection	3.60 to 68.28°.
Index ranges	-14<=h<=14, -12<=k<=12, -27<=l<=30
Reflections collected	27808
Independent reflections	5666 [R(int) = 0.1189]
Completeness to theta = 68.28°	99.4 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.89 and 0.61
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5666 / 0 / 429
Goodness-of-fit on F^2	1.077
Final R indices [I>2sigma(I)]	R1 = 0.0824, wR2 = 0.1902
R indices (all data)	R1 = 0.1041, wR2 = 0.2110
Extinction coefficient	0.0055(7)
Largest diff. peak and hole	0.762 and -0.582 $e.Å^{-3}$

X-ray crystallographic data for compound 8

Crystal data for **compound 8**: $C_{62}H_{42}N_4O_2P_2$, M = 936.93, a = 14.0167(6) Å, b = 23.1649(10) Å, c = 32.3543(15) Å, α = 90°, β = 90°, γ = 90°, V = 10505.3(8) $Å^3$, T = 150.(2) K, space group *Pbca*, Z = 8, μ(Cu Kα) = 1.116 mm^{-1}, 60910 reflections measured, 9584 independent reflections (R_{int} = 0.0850). The final R_1 values were 0.0591 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1606 ($I > 2\sigma(I)$). The final R_1 values were 0.0625 (all data). The final $wR(F^2)$ values were 0.1634 (all data). The goodness of fit on F^2 was 1.057.

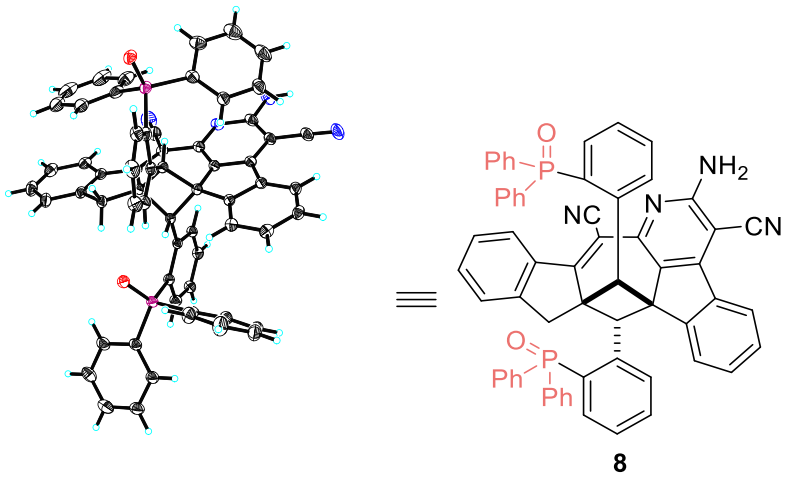


Fig. S14 View of a molecule of compound **8** with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

Table S6 Crystal data and structure refinement for compound **8**.

Identification code	global	
Empirical formula	C62 H42 N4 O2 P2	
Formula weight	936.93	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 14.0167(6) Å	α= 90°.
	b = 23.1649(10) Å	β= 90°.
	c = 32.3543(15) Å	γ = 90°.
Volume	10505.3(8) $Å^3$	
Z	8	
Density (calculated)	1.185 Mg/m^3	
Absorption coefficient	1.116 mm^{-1}	
F(000)	3904	
Crystal size	0.440 x 0.260 x 0.110 mm^3	
Theta range for data collection	2.73 to 68.26°.	

Index ranges	-16<=h<=16, -27<=k<=27, -38<=l<=38
Reflections collected	60910
Independent reflections	9584 [R(int) = 0.0850]
Completeness to theta = 68.26°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.89 and 0.53
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9584 / 0 / 631
Goodness-of-fit on F^2	1.057
Final R indices [I>2sigma(I)]	R1 = 0.0591, wR2 = 0.1606
R indices (all data)	R1 = 0.0625, wR2 = 0.1634
Largest diff. peak and hole	0.592 and -0.459 e.Å^{-3}

X-ray crystallographic data for compound 11

Crystal data for **compound 11**: $C_{38}H_{24}N_4O{\bullet}CH_2Cl_2$, M = 637.54, a = 11.1010(3) Å, b = 10.5875(3) Å, c = 26.8424(7) Å, α = 90°, β = 96.4050(10)°, γ = 90°, V = 3135.14(15) Å^3, T = 150.(2) K, space group $P121/n1$, Z = 4, μ(Cu Kα) = 2.169 mm^{-1}, 26650 reflections measured, 5763 independent reflections (R_{int} = 0.0806). The final R_1 values were 0.0580 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.1644 ($I > 2\sigma(I)$). The final R_1 values were 0.0692 (all data). The final $wR(F^2)$ values were 0.1722 (all data). The goodness of fit on F^2 was 1.066.

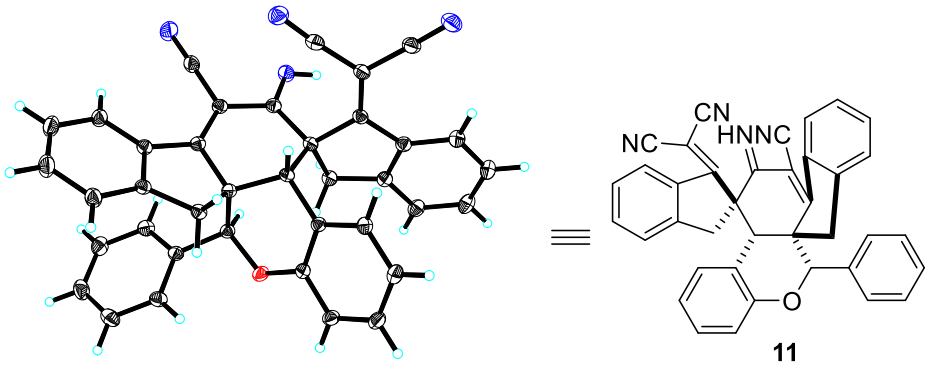


Fig. S15 View of a molecule of compound **11** with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.

Table S7 Crystal data and structure refinement for compound **11**.

Identification code	global	
Empirical formula	C39 H26 Cl2 N4 O	
Formula weight	637.54	
Temperature	150(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 11.1010(3) Å	α= 90°.
	b = 10.5875(3) Å	β= 96.4050(10)°.
	c = 26.8424(7) Å	γ = 90°.
Volume	3135.14(15) $Å^3$	
Z	4	
Density (calculated)	1.351 Mg/m^3	
Absorption coefficient	2.169 mm^{-1}	
F(000)	1320	
Crystal size	0.350 x 0.300 x 0.090 mm^3	
Theta range for data collection	3.31 to 68.63°.	
Index ranges	-12<=h<=13, -12<=k<=12, -32<=l<=31	
Reflections collected	26650	
Independent reflections	5763 [R(int) = 0.0806]	
Completeness to theta = 68.63°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.83 and 0.44	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5763 / 0 / 416	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0580, wR2 = 0.1644	
R indices (all data)	R1 = 0.0692, wR2 = 0.1722	
Largest diff. peak and hole	0.441 and -0.533 $e.Å^{-3}$	

13. Computational Details

Geometry optimizations were carried out with the BP86[1, 2] functional and the def2-SVP[3] basis set and IEFPCM[4] solvent model and dispersion corrections by Grimme with Becke-Johnson damping (D3BJ)[5, 6], which is termed as BP86+D3BJ/def2-SVP(IEFPCM,Solvent=Dichloromethane)//BP86+D3BJ/def2-SVP(IEFPCM,Solvent=n,n-dimethylformamide). Vibrational frequency calculations were performed at the same level of theory to confirm the stationary points as transition states (only one imaginary frequency) or minima (no imaginary frequencies) and used to obtain the zero-point energy (ZPE)-corrected enthalpies and free energies at 298.15 K and 1 atm. Intrinsic reaction coordinate (IRC)[7] analysis was conducted to evaluate the correct connections between the transition states and corresponding minima if necessary. The energetics was further improved by using the larger basis set def2-TZVPP[8, 9] single point calculations and SMD[5, 6] solvent model, denoted as BP86+D3BJ/def2-TZVPP(SMD, Solvent = Dichloromethane) //BP86+D3BJ/ def2-SVP (IEFPCM, Solvent = Dichloromethane)/BP86+D3BJ/def2-TZVPP(SMD, Solvent = N,N-dimethylformamide) // BP86+D3BJ/def2-SVP (IEFPCM,Solvent= N,N-dimethylformamide). Gibbs free energies (in kcal/mol) are used in the following discussion, and the electronic energies without ZPE corrections are also given in the related schemes for reference. All calculations were performed by using the Gaussian 16 program.

References

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Table S8 Coordinates and free energies and electronic energies (in hatree) of the calculated structures at the BP86-D3(BJ) /def2-TZVPP (SMD, Solvent = Dichloromethane) //BP86-D3(BJ)/def2-SVP (IEFPCM, Solvent = Dichloromethane) level.

1a				C	-3.631918	0.548727	-0.312708
N	-0.390341	3.703881	0.490125	C	-4.937876	0.019681	-0.314253
H	-4.227309	2.301502	-0.817485	H	-5.782823	0.671653	-0.589431
N	3.784835	3.152935	-0.003198	C	-5.155730	-1.320845	0.028691
O	-3.383829	1.839468	-0.640532	H	-6.181466	-1.720926	0.024242
C	0.057051	-0.212640	0.109707	C	0.424470	2.868819	0.325236
C	-1.197060	0.348975	0.019202	C	1.486752	1.931626	0.135075
H	-1.243939	1.437596	-0.119549	C	2.761433	2.572373	0.056526
C	-2.505436	-0.275931	0.032945	C	1.320064	0.536340	0.061267

C	0.377230	-1.696593	0.173318
H	0.067293	-2.141909	1.145565
H	-0.150062	-2.272442	-0.618066
C	1.871070	-1.753834	0.019454
C	2.416434	-0.441847	-0.043776
C	3.814285	-0.269541	-0.184215
H	4.265525	0.728577	-0.240338
C	4.633801	-1.404277	-0.258712
H	5.721347	-1.278552	-0.372184
C	4.083204	-2.701924	-0.191354
H	4.745870	-3.579285	-0.251286
C	2.695933	-2.882889	-0.050167
H	2.264794	-3.894496	0.003066
C	-4.070770	-2.149259	0.381567
H	-4.242675	-3.198708	0.663093
C	-2.773149	-1.630813	0.380001
H	-1.946110	-2.283348	0.681317

IM1

H	-0.479306	-2.843747	0.500526
N	-2.459808	3.777319	1.777471
O	-1.725880	-1.848867	0.312421
N	1.431690	5.209416	0.760933
C	3.630519	1.790013	-1.498303
H	4.604540	2.302995	-1.491832
C	2.517773	2.417167	-0.913911
H	2.632958	3.407960	-0.456974
C	1.273094	1.748413	-0.916954
C	-0.032051	2.101941	-0.318582
C	-0.946997	1.007252	-0.574264
C	-2.309210	0.987105	-0.281508
H	-2.766836	1.955060	-0.018880
C	3.514189	0.517337	-2.094482
H	4.397876	0.043191	-2.549538
C	2.274592	-0.149173	-2.111352
H	2.178616	-1.139615	-2.580699
C	1.164674	0.461661	-1.515631
C	-0.218637	-0.080432	-1.330947
H	-0.252747	-1.031872	-0.758297
H	-0.724362	-0.308086	-2.296532
C	-2.875650	-1.511009	-0.142975
C	-3.910478	-2.490550	-0.382474
H	-3.629804	-3.549970	-0.266851
C	-5.215614	-2.124646	-0.686344
H	-5.979343	-2.906175	-0.836321
C	-5.588129	-0.753316	-0.779885
H	-6.630634	-0.473707	-0.995212

C	-4.615641	0.223232	-0.602657
H	-4.885831	1.289552	-0.687408
C	-3.240585	-0.100745	-0.365164
C	-0.281507	3.273662	0.439820
C	-1.493669	3.519916	1.151074
C	0.673997	4.319041	0.601540
C	1.540777	-2.438904	0.893445
N	0.506887	-3.232518	0.565409
N	2.782198	-2.676239	0.383356
N	1.345167	-1.403983	1.748442
C	4.003960	-2.422719	1.146546
H	4.622410	-3.344533	1.153824
H	4.604788	-1.601649	0.701678
H	3.755570	-2.168296	2.191525
C	2.955934	-3.417309	-0.862682
H	3.184495	-4.491133	-0.680940
H	2.044283	-3.340363	-1.482857
H	3.800688	-2.976078	-1.429062
C	2.116174	-0.162550	1.673493
H	2.776185	-0.033470	2.556852
H	2.721698	-0.138164	0.751442
H	1.409487	0.690741	1.639581
C	0.191755	-1.379630	2.651548
H	-0.110202	-2.414306	2.897505
H	0.486127	-0.857411	3.583148
H	-0.671792	-0.867499	2.179483
H	0.699594	-4.144990	0.151091

TS1

N	1.224512	1.119696	-1.044861
H	-1.137958	4.590571	-2.298328
H	2.954736	1.511851	-0.856591
N	1.139744	-2.790111	-2.480151
O	-1.365315	3.735476	-1.883525
N	-0.480708	-4.347765	0.712066
O	-2.014073	1.713056	1.086720
N	3.728466	-3.657215	0.291332
C	4.680702	0.410284	2.218101
H	5.768841	0.244792	2.227523
C	3.830066	-0.614340	1.778336
H	4.258399	-1.571690	1.461026
C	2.431890	-0.402925	1.791703
C	1.304029	-1.301373	1.473998
C	0.066174	-0.577324	1.767689
C	-1.214226	-1.093705	1.720110
H	-1.316664	-2.167404	1.503363
C	-2.656934	0.069630	-0.910990

C	-2.300520	1.443573	-0.658401	C	-2.550514	-2.207675	-1.467205
H	-1.275125	1.692974	-0.959699	C	-2.172702	-3.515254	-1.840286
C	-3.228499	2.566182	-0.952580	H	-1.133436	-3.760305	-2.087777
C	-2.694251	3.731891	-1.577192	C	-3.152679	-4.521717	-1.880362
C	-3.521870	4.835152	-1.867045	H	-2.861373	-5.544622	-2.165563
H	-3.085911	5.718135	-2.363462	C	-4.493454	-4.244566	-1.548521
C	-4.881923	4.810071	-1.522711	H	-5.243726	-5.050403	-1.580571
H	-5.516569	5.680032	-1.753188	C	-4.877723	-2.942594	-1.174297
C	4.156613	1.641997	2.662740	H	-5.924201	-2.718877	-0.912669
H	4.838891	2.428847	3.020819	C	-5.423391	3.680417	-0.884361
C	2.768556	1.863928	2.674638	H	-6.485950	3.657110	-0.598795
H	2.356848	2.820477	3.032178	C	-4.600676	2.577229	-0.609203
C	1.912774	0.840109	2.248781	H	-5.029567	1.714908	-0.086133
C	0.417710	0.821376	2.225637	C	-2.760508	0.950369	1.878633
H	-0.020081	1.573169	1.534206	C	-3.945485	1.487137	2.455393
H	-0.027593	1.052220	3.219221	H	-4.129244	2.563482	2.319710
C	0.453333	0.246706	-1.249351	C	-4.865407	0.669515	3.118814
C	-0.350844	-0.878041	-1.539650	H	-5.781381	1.107450	3.546713
C	0.427391	-1.945565	-2.058140	C	-4.643686	-0.725089	3.197385
C	-1.766391	-0.960309	-1.307117	H	-5.387068	-1.379268	3.678155
C	-4.062620	-0.483640	-0.796623	C	-3.464756	-1.267577	2.680452
H	-4.493851	-0.355449	0.222522	H	-3.273148	-2.349526	2.765576
H	-4.767107	0.022638	-1.495032	C	-2.463167	-0.449541	2.081258
C	-3.906925	-1.935109	-1.141565	C	1.445412	-2.620034	0.993624

C	0.365023	-3.535193	0.827531
C	2.703110	-3.177756	0.621606
C	5.037020	1.120175	-1.005378
N	3.935301	1.878472	-0.902578
N	6.259881	1.668786	-0.749484
N	4.949268	-0.183626	-1.363010
C	7.443936	1.303709	-1.530514
H	7.882356	2.223757	-1.970819
H	8.217761	0.811909	-0.905069
H	7.163747	0.630393	-2.358906
C	6.385492	2.876313	0.062148
H	6.416714	3.798080	-0.561435
H	5.542638	2.942019	0.773298
H	7.327759	2.822197	0.643541
C	5.914970	-1.187048	-0.907091
H	6.588085	-1.515302	-1.726561
H	6.522466	-0.781505	-0.078801
H	5.357728	-2.073909	-0.542013
C	3.761223	-0.706773	-2.035443
H	3.039914	-1.138810	-1.312817
H	3.259975	0.094029	-2.607652
H	4.066501	-1.509473	-2.733403
H	4.028787	2.893884	-0.948634

IM2

N	-1.336732	-1.204858	-1.039547
H	1.332954	-2.302963	-3.732619
H	-3.069273	-1.510795	-0.880353
N	-1.068604	2.689179	-2.469416
O	1.488271	-2.070465	-2.796266
N	0.799353	4.146818	0.660651
O	2.288626	-1.925860	1.272689
N	-3.476043	3.691646	0.434094
C	-4.559357	-0.395311	2.199202
H	-5.641241	-0.192349	2.200188
C	-3.671016	0.601460	1.769594
H	-4.064203	1.573086	1.451495
C	-2.280593	0.343997	1.791064
C	-1.120237	1.201554	1.471837
C	0.084972	0.436331	1.779259
C	1.385785	0.906300	1.776544
H	1.547708	1.963377	1.521300
C	2.523667	-0.145655	-0.498442
C	2.137673	-1.546506	-0.147882
H	1.064834	-1.700081	-0.367507
C	2.946147	-2.534598	-0.980202
C	2.579549	-2.744400	-2.334691

C	3.336544	-3.610162	-3.149176	H	3.140527	5.122127	-2.702393
H	3.032943	-3.764958	-4.197913	C	4.662394	3.859681	-1.796160
C	4.467657	-4.261036	-2.629013	H	5.462841	4.604979	-1.927092
H	5.052504	-4.932139	-3.277369	C	4.949257	2.620298	-1.189475
C	-4.083577	-1.647894	2.638407	H	5.969421	2.387094	-0.844840
H	-4.795096	-2.413719	2.984992	C	4.846900	-4.052232	-1.292264
C	-2.703842	-1.915635	2.660643	H	5.732778	-4.557060	-0.877827
H	-2.326838	-2.887121	3.016353	C	4.083043	-3.193195	-0.481865
C	-1.811682	-0.917472	2.250260	H	4.367782	-3.026589	0.566056
C	-0.314625	-0.946896	2.256191	C	2.906482	-1.116303	2.180572
H	0.090540	-1.747478	1.603014	C	3.956985	-1.683377	2.932809
H	0.097647	-1.162416	3.267451	H	4.182962	-2.750405	2.785946
C	-0.523851	-0.360258	-1.202919	C	4.709024	-0.900402	3.818912
C	0.324577	0.738563	-1.467065	H	5.526768	-1.360390	4.395185
C	-0.399775	1.818777	-2.028093	C	4.442389	0.478338	3.934536
C	1.727972	0.810980	-1.150992	H	5.053172	1.110988	4.596375
C	3.966243	0.304261	-0.450331	C	3.383097	1.038871	3.211746
H	4.397622	0.295271	0.575550	H	3.150258	2.110617	3.315929
H	4.615019	-0.374792	-1.050951	C	2.548102	0.250805	2.374212
C	3.918202	1.687500	-1.036593	C	-1.216095	2.539775	1.021919
C	2.593358	1.975543	-1.468039	C	-0.094910	3.393587	0.814835
C	2.313408	3.218414	-2.072140	C	-2.457738	3.161601	0.707270
H	1.300860	3.473712	-2.406690	C	-5.127235	-0.985902	-0.979787
C	3.356180	4.148762	-2.234353	N	-4.073396	-1.813788	-0.933238

N	-6.373798	-1.464301	-0.697375
N	-4.969012	0.319427	-1.306472
C	-7.556478	-1.010220	-1.432126
H	-8.063813	-1.891725	-1.877456
H	-8.278982	-0.486981	-0.771742
H	-7.260899	-0.336180	-2.254609
C	-6.547652	-2.681338	0.090894
H	-6.649263	-3.585216	-0.551423
H	-5.691182	-2.812368	0.776342
H	-7.469499	-2.586943	0.699204
C	-5.855752	1.369081	-0.797856
H	-6.528361	1.761546	-1.589145
H	-6.466222	0.981723	0.036968
H	-5.233016	2.209373	-0.427381
C	-3.772190	0.789157	-2.001781
H	-3.020822	1.189022	-1.291806
H	-3.316786	-0.033030	-2.581561
H	-4.054216	1.605042	-2.694831
H	-4.235000	-2.819587	-0.995855

TS2

N	-1.290692	-1.000529	-1.414054
H	1.582213	-0.942624	-4.230265
H	-3.072982	-1.259215	-1.264036
N	-1.083457	3.119523	-1.984349
O	1.674768	-1.045852	-3.262933
N	0.909755	3.697884	1.712967
O	2.314366	-2.304761	0.622271
N	-3.383643	3.438121	1.360474
C	-4.581448	-0.935791	2.002935
H	-5.653625	-0.706156	2.101967
C	-3.663290	0.114087	1.844592
H	-4.023848	1.148533	1.832620
C	-2.284472	-0.181816	1.743778
C	-1.093673	0.694802	1.652633
C	0.073354	-0.155348	1.709552
C	1.414640	0.239910	1.819079
H	1.618927	1.316277	1.914915
C	2.452230	0.042138	-0.308777
C	2.189859	-1.424762	-0.540990
H	1.147859	-1.556336	-0.887787
C	3.126889	-1.958636	-1.619933
C	2.828454	-1.715733	-2.984390
C	3.710977	-2.153689	-3.992671
H	3.460151	-1.958905	-5.048624
C	4.896271	-2.825197	-3.652050
H	5.578415	-3.158541	-4.449703

C	-4.147572	-2.276006	2.051000	H	5.764501	2.728793	0.193397
H	-4.880835	-3.085436	2.192243	C	5.205373	-3.067483	-2.302540
C	-2.778829	-2.581786	1.950403	H	6.131908	-3.593946	-2.027637
H	-2.431689	-3.625404	2.006666	C	4.318704	-2.633993	-1.301393
C	-1.857690	-1.536357	1.812707	H	4.549099	-2.823077	-0.243126
C	-0.362555	-1.606667	1.784475	C	2.820590	-1.874012	1.813064
H	0.008290	-2.202155	0.923411	C	3.741840	-2.720319	2.464544
H	0.047202	-2.111279	2.688321	H	3.984490	-3.686538	1.996860
C	-0.502955	-0.122999	-1.321782	C	4.340764	-2.321245	3.667699
C	0.309356	1.037628	-1.286622	H	5.058166	-2.990820	4.167282
C	-0.422677	2.191305	-1.672807	C	4.049061	-1.056419	4.214726
C	1.671809	1.097506	-0.861975	H	4.537135	-0.725319	5.144000
C	3.865309	0.536345	-0.053019	C	3.121895	-0.222586	3.574201
H	4.225457	0.330640	0.978143	H	2.870344	0.760330	4.003468
H	4.587968	0.026612	-0.729645	C	2.453371	-0.631690	2.394758
C	3.785485	2.006662	-0.350014	C	-1.154557	2.117523	1.608598
C	2.493261	2.327398	-0.850096	C	-0.010328	2.960275	1.651431
C	2.201440	3.657470	-1.221606	C	-2.377213	2.830612	1.480096
H	1.212335	3.940177	-1.600749	C	-5.118798	-0.686656	-1.221192
C	3.201000	4.636429	-1.093412	N	-4.078453	-1.516042	-1.395930
H	2.977479	5.675154	-1.382666	N	-6.376036	-1.201813	-1.096362
C	4.473812	4.312114	-0.585353	N	-4.933822	0.653922	-1.175094
H	5.240268	5.096752	-0.484893	C	-7.540889	-0.537878	-1.685797
C	4.770730	2.988949	-0.204371	H	-8.058598	-1.251692	-2.360349

H	-8.262218	-0.201067	-0.912338
H	-7.222351	0.329962	-2.288751
C	-6.579905	-2.586272	-0.677863
H	-6.691385	-3.273876	-1.546503
H	-5.733279	-2.919557	-0.050962
H	-7.505761	-2.646031	-0.071260
C	-5.812583	1.542874	-0.409691
H	-6.466354	2.147443	-1.072537
H	-6.441461	0.954533	0.281548
H	-5.182406	2.238718	0.181384
C	-3.698047	1.258499	-1.667454
H	-2.947659	1.357209	-0.857309
H	-3.269749	0.649810	-2.483795
H	-3.917197	2.271637	-2.052800
H	-4.253394	-2.462267	-1.735592

IM3

N	1.281312	-0.532249	-1.617062
H	-1.311382	-2.210244	-3.307301
H	3.098094	-0.546831	-1.649045
N	0.380287	-3.896607	0.331646
O	-1.553328	-1.398413	-2.820226
N	-1.047689	-0.666052	3.536767
O	-3.151996	2.010874	-1.363124
N	3.252204	-0.603980	3.760903
C	4.842790	1.943900	0.247015
H	5.895297	1.848124	0.557566
C	3.835607	1.363903	1.038376
H	4.105424	0.834437	1.959581
C	2.485762	1.503760	0.648969
C	1.219255	1.054603	1.278905
C	0.159861	1.527335	0.491433
C	-1.294606	1.529093	0.880912
H	-1.333988	1.390182	1.978100
C	-2.246415	0.420460	0.305001
C	-2.526796	0.730261	-1.211543
H	-1.544709	0.742407	-1.732871
C	-3.436500	-0.294634	-1.864144
C	-2.897733	-1.381593	-2.598765
C	-3.744718	-2.396951	-3.089224
H	-3.303756	-3.242471	-3.642499
C	-5.130612	-2.322456	-2.887561
H	-5.778606	-3.124321	-3.274333
C	4.524098	2.649835	-0.929989
H	5.325467	3.109563	-1.529950
C	3.180781	2.792628	-1.327564
H	2.923405	3.356655	-2.238370

C	2.173572	2.233180	-0.532831	H	-5.262134	0.656832	-1.209962
C	0.682677	2.325841	-0.682962	C	-2.783345	3.041087	-0.537793
H	0.346864	1.931933	-1.669216	C	-3.341961	4.303469	-0.834438
H	0.341328	3.385293	-0.647719	H	-4.006115	4.390095	-1.707686
C	0.425317	-0.758930	-0.834499	C	-3.045593	5.406477	-0.024325
C	-0.515870	-1.473230	-0.019605	H	-3.481504	6.388973	-0.264096
C	-0.066640	-2.816643	0.191417	C	-2.196454	5.258313	1.091531
C	-1.743222	-1.013130	0.437831	H	-1.962684	6.121903	1.732577
C	-3.571177	0.438079	1.127293	C	-1.653541	3.998313	1.379778
H	-3.396230	0.958246	2.093383	H	-0.982787	3.866206	2.244561
H	-4.390650	0.987222	0.627162	C	-1.931827	2.873939	0.575694
C	-3.892213	-1.000316	1.387043	C	1.152907	0.234835	2.477597
C	-2.792367	-1.830497	1.040973	C	-0.060952	-0.242894	3.035796
C	-2.875247	-3.229316	1.242649	C	2.303083	-0.206945	3.170855
H	-2.043154	-3.895127	0.983243	C	5.027170	-1.120627	-0.988985
C	-4.052332	-3.769526	1.774823	N	4.104424	-0.708031	-1.871587
H	-4.127916	-4.856600	1.929642	N	6.350283	-0.944357	-1.269633
C	-5.143475	-2.937568	2.107958	N	4.657850	-1.719860	0.167622
H	-6.062417	-3.383500	2.519581	C	7.353748	-1.949409	-0.913077
C	-5.067478	-1.547414	1.916160	H	7.909159	-2.242909	-1.828577
H	-5.917230	-0.897625	2.176056	H	8.082597	-1.562422	-0.170724
C	-5.684469	-1.220153	-2.214326	H	6.865093	-2.851881	-0.506907
H	-6.772953	-1.138243	-2.076326	C	6.786369	0.077396	-2.217710
C	-4.835015	-0.219406	-1.717401	H	6.919754	-0.334157	-3.243666

H	6.054583	0.904859	-2.241886
H	7.760753	0.485907	-1.882337
C	5.470878	-1.636285	1.384476
H	5.985935	-2.595384	1.602702
H	6.223664	-0.834853	1.280811
H	4.805971	-1.392794	2.239669
C	3.324315	-2.296634	0.328403
H	2.626271	-1.578629	0.809292
H	2.917069	-2.597116	-0.653263
H	3.394563	-3.194928	0.971369
H	4.383014	-0.533452	-2.837221

TS3

N	1.285128	-0.664813	-1.430752
H	-1.537107	-2.280713	-3.160280
H	2.941849	-0.773757	-1.625358
N	0.201888	-3.878402	0.121748
O	-1.746630	-1.436394	-2.715772
N	-0.941111	-0.506787	3.563769
O	-3.175275	2.063851	-1.304886
N	3.313083	-0.187996	3.925770
C	4.948614	1.885066	0.130988
H	5.998330	1.844671	0.460750
C	3.940617	1.407096	0.979095
H	4.205348	1.006517	1.964560
C	2.591674	1.471902	0.554015
C	1.341534	1.050107	1.196347
C	0.260138	1.248947	0.241655
C	-1.166323	1.503152	0.768093
H	-1.116642	1.447407	1.871288
C	-2.242629	0.478063	0.345115
C	-2.598225	0.757959	-1.163033
H	-1.643063	0.720399	-1.731403
C	-3.567386	-0.246432	-1.746476
C	-3.082614	-1.375399	-2.455125
C	-3.974099	-2.385716	-2.870751
H	-3.578125	-3.265714	-3.404058
C	-5.348267	-2.266112	-2.613851
H	-6.031453	-3.065839	-2.939958
C	4.634221	2.423312	-1.136736
H	5.439811	2.810141	-1.780533
C	3.300871	2.490532	-1.571063
H	3.051311	2.922662	-2.552768
C	2.285165	2.025247	-0.723102
C	0.800439	2.121382	-0.893151
H	0.455737	1.801721	-1.896552
H	0.480948	3.176703	-0.754433

C	0.415809	-0.495045	-0.594735	C	-2.608963	5.492965	-0.180140
C	-0.561228	-1.388736	0.056792	H	-2.976798	6.501423	-0.426073
C	-0.165809	-2.759959	0.100883	C	-1.656785	5.314275	0.844419
C	-1.800661	-0.969963	0.478809	H	-1.275556	6.179251	1.408085
C	-3.507517	0.570954	1.247580	C	-1.204445	4.021639	1.144092
H	-3.227552	1.017531	2.226381	H	-0.461442	3.865113	1.943573
H	-4.302130	1.213899	0.822658	C	-1.671225	2.894215	0.436434
C	-3.933611	-0.858208	1.445988	C	1.241821	0.393789	2.460809
C	-2.907938	-1.748253	1.026679	C	0.024972	-0.082979	3.031908
C	-3.085696	-3.144883	1.142150	C	2.379789	0.093649	3.257324
H	-2.304547	-3.844142	0.814982	C	4.900504	-1.322698	-0.948617
C	-4.290533	-3.631057	1.669690	N	3.970686	-0.960602	-1.839632
H	-4.446952	-4.717324	1.756311	N	6.226793	-1.209175	-1.261737
C	-5.306525	-2.743327	2.083805	N	4.547563	-1.809690	0.267892
H	-6.247296	-3.145381	2.491579	C	7.200312	-2.223418	-0.852319
C	-5.131725	-1.351524	1.976069	H	7.708914	-2.622563	-1.755432
H	-5.927287	-0.661246	2.297050	H	7.972349	-1.806919	-0.171973
C	-5.847135	-1.126404	-1.959927	H	6.690314	-3.063949	-0.350710
H	-6.926078	-1.015794	-1.774859	C	6.671287	-0.298302	-2.311604
C	-4.953851	-0.129230	-1.537805	H	6.761804	-0.807417	-3.298161
H	-5.333376	0.770454	-1.032825	H	5.967583	0.549125	-2.396900
C	-2.626720	3.092155	-0.586097	H	7.668327	0.104550	-2.041546
C	-3.096175	4.388615	-0.889851	C	5.393214	-1.641813	1.450859
H	-3.844545	4.500526	-1.688955	H	5.879826	-2.593847	1.751533

H	6.170894	-0.882513	1.255217
H	4.763687	-1.293238	2.295203
C	3.221487	-2.373529	0.507418
H	2.559132	-1.645837	1.022046
H	2.747754	-2.662319	-0.446353
H	3.319271	-3.273048	1.147433
H	4.245501	-0.880152	-2.819465

IM4

N	-3.264693	0.455674	-2.508992
H	-1.306337	3.499583	-3.273548
H	4.782647	-1.278276	-1.330941
N	-3.434919	3.784793	0.007701
O	-0.954175	2.629879	-2.999440
N	-0.033450	-0.941084	3.295037
O	1.256846	-0.773309	-2.371352
N	-3.483557	1.823781	3.338656
C	-6.642718	-1.011907	0.893258
H	-7.560165	-0.685965	1.408759
C	-5.386872	-0.653441	1.418904
H	-5.316032	-0.050336	2.335997
C	-4.226669	-1.068022	0.737887
C	-2.795728	-0.855517	1.034431
C	-2.047142	-1.418532	0.004766
C	-0.558865	-1.289234	-0.083060
H	-0.189937	-1.456076	0.947859
C	0.058226	0.160371	-0.414183
C	0.370820	0.280669	-1.952759
H	-0.581346	0.185390	-2.516025
C	1.081165	1.575252	-2.329776
C	0.383068	2.725818	-2.781149
C	1.080506	3.929544	-3.025448
H	0.511203	4.815183	-3.352460
C	2.472551	3.992888	-2.881627
H	2.997080	4.940506	-3.079471
C	-6.740876	-1.781116	-0.283582
H	-7.733157	-2.049290	-0.679803
C	-5.578327	-2.207851	-0.959691
H	-5.657074	-2.811323	-1.878400
C	-4.327075	-1.844401	-0.451197
C	-2.941379	-2.155372	-0.963233
H	-2.802897	-1.815502	-2.012482
H	-2.747708	-3.253051	-0.968117
C	-2.678248	0.921670	-1.599060
C	-2.047947	1.647405	-0.539799
C	-2.793833	2.818211	-0.193245
C	-0.820276	1.328952	0.035085

C	1.369831	0.318125	0.413861	C	-0.045349	-3.721178	-0.564132
H	1.557733	-0.578096	1.034731	H	-0.725778	-3.968688	0.266605
H	2.253424	0.447548	-0.236263	C	0.118793	-2.360372	-0.907955
C	1.158331	1.516388	1.288932	C	-2.265358	-0.174223	2.211698
C	-0.122759	2.088744	1.067597	C	-1.051115	-0.575648	2.807640
C	-0.530596	3.216072	1.821555	C	-2.943091	0.900391	2.831095
H	-1.523493	3.661289	1.687000	C	4.274861	-1.373882	0.671998
C	0.351889	3.752164	2.769130	N	4.074865	-1.558395	-0.650755
H	0.040647	4.624707	3.363752	N	3.626471	-2.151438	1.566998
C	1.629677	3.188396	2.971692	N	5.120570	-0.395053	1.086526
H	2.310350	3.629677	3.716260	C	3.236705	-1.664717	2.896169
C	2.035813	2.063414	2.231858	H	2.133794	-1.736877	3.013170
H	3.031463	1.621587	2.389794	H	3.731585	-2.253904	3.694814
C	3.189323	2.840447	-2.515912	H	3.507377	-0.601748	3.008144
H	4.287111	2.862262	-2.442952	C	3.075180	-3.451457	1.180244
C	2.488017	1.653717	-2.255911	H	2.005216	-3.374791	0.893881
H	3.040065	0.734513	-2.013957	H	3.646248	-3.875503	0.334116
C	1.004680	-2.049596	-1.961919	H	3.157944	-4.141100	2.042422
C	1.731109	-3.068336	-2.623166	C	5.985100	-0.568984	2.257988
H	2.409880	-2.779986	-3.440424	H	5.741020	0.158362	3.059481
C	1.553382	-4.409079	-2.255362	H	5.891596	-1.595296	2.653488
H	2.115590	-5.196178	-2.780938	H	7.039203	-0.410867	1.948987
C	0.650340	-4.742218	-1.227055	C	5.419579	0.758770	0.237330
H	0.500785	-5.792201	-0.934393	H	6.319711	0.592914	-0.394679

H	4.553738	0.995738	-0.406907
H	5.609859	1.634864	0.887338
H	3.261957	-2.073517	-1.008060

TS4

N	2.041484	-0.046279	-1.109300
H	3.361314	-1.045437	-0.928077
H	2.300063	0.942460	-1.248491
N	1.830679	-3.473098	-0.526047
O	-1.768825	-2.492353	-1.505422
N	1.826994	-0.436096	2.595487
O	-3.672259	1.044495	-0.926769
N	3.229902	3.644679	2.618204
C	0.607349	5.871121	-0.625241
H	0.888489	6.889813	-0.318416
C	1.074403	4.775189	0.107291
H	1.708272	4.934250	0.989184
C	0.681018	3.473554	-0.292382
C	0.893615	2.184705	0.339170
C	0.008764	1.126188	-0.350630
C	-1.211092	0.865730	0.615186
H	-0.768344	0.691901	1.617260
C	-2.032104	-0.401301	0.284402
C	-2.896234	-0.159209	-0.997566
H	-2.179991	-0.086730	-1.846938
C	-3.802320	-1.320236	-1.277317
C	-3.092906	-2.531850	-1.526444
C	-3.836720	-3.717680	-1.764956
H	-3.287747	-4.655908	-1.940490
C	-5.239768	-3.673573	-1.778894
H	-5.808727	-4.597373	-1.974591
C	-0.236886	5.685796	-1.744152
H	-0.604898	6.564635	-2.296025
C	-0.615027	4.397149	-2.158549
H	-1.274073	4.257592	-3.028653
C	-0.147078	3.293223	-1.435817
C	-0.412915	1.838195	-1.681162
H	0.217097	1.464195	-2.516665
H	-1.461538	1.657113	-1.972311
C	0.822425	-0.153741	-0.615785
C	0.253455	-1.424457	-0.266874
C	1.100942	-2.552189	-0.402143
C	-1.128281	-1.633836	0.080349
C	-2.960842	-0.746774	1.491585
H	-2.703507	-0.119927	2.372811
H	-4.027760	-0.546946	1.265040
C	-2.696599	-2.201730	1.775516

C	-1.603603	-2.683097	1.019352	C	1.741218	0.603208	2.051311
C	-1.174066	-4.018332	1.161622	C	2.516234	2.875894	2.085447
H	-0.343562	-4.407048	0.557531	C	5.439237	-1.474714	-0.570071
C	-1.840883	-4.852546	2.071848	N	4.153022	-1.764284	-0.751173
H	-1.516659	-5.898579	2.188544	N	6.399062	-2.429800	-0.746381
C	-2.931505	-4.370464	2.826942	N	5.820988	-0.212730	-0.217344
H	-3.449176	-5.041813	3.530157	C	7.596140	-2.485923	0.093042
C	-3.364996	-3.041879	2.680819	H	7.640828	-3.473231	0.600049
H	-4.218476	-2.663712	3.265547	H	8.524444	-2.357100	-0.502523
C	-5.929115	-2.468685	-1.530243	H	7.552219	-1.703321	0.870707
H	-7.030061	-2.449135	-1.534551	C	6.119782	-3.621012	-1.543817
C	-5.203050	-1.289395	-1.272915	H	5.757002	-4.467565	-0.918768
H	-5.719294	-0.336896	-1.077284	H	5.359242	-3.390783	-2.312692
C	-3.284872	2.088644	-0.134687	H	7.051505	-3.941238	-2.051998
C	-4.114345	3.230500	-0.162479	C	7.056129	0.391704	-0.712843
H	-4.993882	3.223577	-0.823532	H	7.776696	0.597015	0.107208
C	-3.807410	4.336458	0.639590	H	7.532256	-0.271866	-1.456227
H	-4.454542	5.226814	0.605107	H	6.814587	1.354820	-1.210927
C	-2.689327	4.305085	1.496743	C	4.905876	0.680732	0.484455
H	-2.455092	5.164816	2.141988	H	5.460665	1.227886	1.274122
C	-1.874749	3.165165	1.518719	H	4.453457	1.431728	-0.199753
H	-0.999812	3.127621	2.186363	H	4.099079	0.092360	0.955698
C	-2.137040	2.054894	0.689708	H	3.814453	-2.731718	-0.668029
C	1.680347	1.903462	1.450709				

IM5

N	0.920626	-2.328846	-1.200854
H	-3.891089	-1.802387	-2.869037
H	1.876579	-1.898019	-1.347922
N	-1.711286	-4.557171	-0.753845
O	-3.419136	-1.082014	-2.406870
N	0.399293	-2.922501	2.432713
O	-1.981303	2.396467	-0.774037
N	4.086554	-0.868938	3.406313
C	4.218735	2.836227	0.478813
H	5.090792	3.311093	0.953017
C	3.766334	1.596657	0.949524
H	4.273152	1.111036	1.793016
C	2.626779	1.017646	0.344198
C	1.832676	-0.137568	0.725680
C	0.524202	-0.129181	-0.079683
C	-0.559835	0.524352	0.891952
H	-0.419584	0.041602	1.880302
C	-2.014367	0.233193	0.475822
C	-2.350353	1.005036	-0.855724
H	-1.754836	0.529382	-1.664015
C	-3.813868	0.954557	-1.245256
C	-4.315117	-0.143665	-1.988526
C	-5.693634	-0.244923	-2.260756
H	-6.068605	-1.116226	-2.822094
C	-6.574999	0.753810	-1.819701
H	-7.650722	0.659017	-2.034915
C	3.559440	3.489716	-0.584691
H	3.920528	4.472643	-0.924647
C	2.454629	2.895386	-1.222992
H	1.950252	3.401322	-2.059781
C	2.000033	1.655784	-0.763165
C	0.868445	0.816535	-1.277583
H	1.223756	0.196579	-2.126379
H	0.021246	1.419708	-1.644634
C	0.121657	-1.549107	-0.561511
C	-1.240015	-2.043048	-0.251940
C	-1.472222	-3.427993	-0.529230
C	-2.237474	-1.250809	0.264529
C	-3.047836	0.604948	1.579076
H	-2.566004	0.539556	2.579022
H	-3.444685	1.633566	1.481685
C	-4.104189	-0.463141	1.433877
C	-3.592395	-1.571211	0.700984
C	-4.396881	-2.706252	0.461838
H	-4.009100	-3.561713	-0.107625
C	-5.716164	-2.705307	0.937467

H	-6.364729	-3.573670	0.744549	N	5.774761	-0.396819	-1.536064
C	-6.225734	-1.599152	1.651137	N	4.979400	-2.223017	-0.287273
H	-7.267942	-1.615645	2.006472	C	7.107028	-0.939777	-1.798099
C	-5.420742	-0.473652	1.908756	H	7.341726	-0.880404	-2.886197
H	-5.823757	0.387974	2.462728	H	7.892921	-0.379754	-1.246432
C	-6.084674	1.869931	-1.120011	H	7.154539	-2.002280	-1.502138
H	-6.768549	2.665705	-0.788651	C	5.493155	0.851737	-2.223627
C	-4.710959	1.962482	-0.845958	H	5.463396	0.735012	-3.334959
H	-4.310601	2.835504	-0.310234	H	4.528006	1.266215	-1.883121
C	-1.085750	2.857805	0.154129	H	6.285502	1.590868	-1.984862
C	-0.883736	4.253078	0.184483	C	5.951870	-2.040260	0.783044
H	-1.442154	4.882255	-0.524534	H	6.819876	-2.731106	0.687577
C	0.019727	4.803389	1.102966	H	6.323708	-0.999599	0.775488
H	0.182210	5.892450	1.115008	H	5.475044	-2.220907	1.768560
C	0.705611	3.975367	2.013904	C	4.085563	-3.364324	-0.169048
H	1.405476	4.408372	2.743855	H	3.254067	-3.189058	0.550572
C	0.491850	2.591233	1.978598	H	3.631672	-3.585032	-1.152481
H	1.024788	1.930182	2.679882	H	4.661125	-4.247954	0.176001
C	-0.381554	2.010297	1.037427	H	3.522640	-0.540345	-2.577379
C	2.055364	-1.015101	1.781799				
C	1.136384	-2.062160	2.115416				
C	3.179979	-0.921945	2.657817	**IM6**			
C	4.710593	-1.248441	-1.229438	N	2.076393	-0.164402	-0.980389
N	3.513157	-1.161916	-1.757593	H	3.384598	-1.253454	-0.823312

H	2.381613	0.800493	-1.184749	C	-0.021090	5.629674	-1.882156
N	1.743473	-3.546232	-0.203697	H	-0.364354	6.492645	-2.473555
O	-1.865943	-2.494123	-1.706992	C	-0.429830	4.334269	-2.243112
N	1.840590	-0.361549	2.709527	H	-1.088369	4.173715	-3.109881
O	-3.546909	1.128268	-0.946015	C	0.007119	3.251661	-1.470707
N	3.385262	3.684621	2.576705	C	-0.291399	1.793812	-1.655132
C	0.822059	5.842622	-0.767183	H	0.340520	1.368204	-2.463994
H	1.126615	6.866511	-0.503107	H	-1.339157	1.619733	-1.952388
C	1.257996	4.768550	0.014999	C	0.863010	-0.182700	-0.482786
H	1.890860	4.949459	0.893451	C	0.242630	-1.425910	-0.075052
C	0.834070	3.461167	-0.331064	C	1.053998	-2.592390	-0.139539
C	1.009888	2.197269	0.357794	C	-1.104889	-1.527908	0.311034
C	0.094769	1.137068	-0.285199	C	-2.973382	-0.601323	1.561309
C	-1.150787	0.973546	0.677467	H	-2.602822	-0.145359	2.505988
H	-0.729624	0.845670	1.695917	H	-3.987840	-0.195848	1.378990
C	-1.985602	-0.292898	0.397924	C	-2.939225	-2.104295	1.656915
C	-2.823671	-0.116983	-0.931257	C	-1.787626	-2.619572	1.002692
H	-2.081688	-0.131168	-1.760560	C	-1.516529	-4.005623	1.027849
C	-3.788461	-1.236667	-1.178339	H	-0.644084	-4.416544	0.502993
C	-3.153517	-2.466770	-1.585481	C	-2.406967	-4.854695	1.697727
C	-4.008581	-3.603519	-1.775828	H	-2.216626	-5.939183	1.712626
H	-3.538351	-4.556899	-2.066838	C	-3.557983	-4.340046	2.337145
C	-5.392009	-3.500834	-1.591728	H	-4.251468	-5.028194	2.845678
H	-6.026314	-4.390461	-1.745908	C	-3.828337	-2.961847	2.322140

H	-4.725623	-2.560034	2.818016
C	-5.990124	-2.279429	-1.204678
H	-7.080207	-2.212797	-1.063357
C	-5.176620	-1.149716	-0.998471
H	-5.619336	-0.185999	-0.699400
C	-3.164320	2.199352	-0.193110
C	-3.968718	3.355214	-0.300079
H	-4.830560	3.332272	-0.983670
C	-3.658458	4.494210	0.452753
H	-4.285616	5.394258	0.355875
C	-2.562550	4.486422	1.339308
H	-2.326327	5.374529	1.944122
C	-1.773345	3.333199	1.441699
H	-0.915061	3.312486	2.131839
C	-2.041350	2.187150	0.665243
C	1.786853	1.940091	1.482610
C	1.800023	0.664408	2.135332
C	2.650658	2.913556	2.076950
C	5.449308	-1.704941	-0.522137
N	4.155389	-1.985279	-0.680003
N	6.396832	-2.659793	-0.744067
N	5.841212	-0.453129	-0.149775
C	7.623560	-2.731837	0.050444
H	7.692215	-3.734411	0.523022
H	8.528904	-2.576987	-0.573358
H	7.601382	-1.974598	0.853624
C	6.098174	-3.827466	-1.569712
H	5.763083	-4.695114	-0.958912
H	5.311070	-3.578556	-2.305158
H	7.014591	-4.124316	-2.118214
C	7.064687	0.161941	-0.661986
H	7.811433	0.334794	0.141777
H	7.513158	-0.477594	-1.442663
H	6.812959	1.142790	-1.118178
C	4.955272	0.418263	0.615736
H	5.541134	0.933912	1.404175
H	4.484429	1.195719	-0.024761
H	4.161806	-0.181501	1.095476
H	3.809604	-2.947460	-0.587650

TS5

N	2.041484	-0.046279	-1.109300
H	3.361314	-1.045437	-0.928077
H	2.300063	0.942460	-1.248491
N	1.830679	-3.473098	-0.526047
O	-1.768825	-2.492353	-1.505422
N	1.826994	-0.436096	2.595487

O	-3.672259	1.044495	-0.926769	C	-0.147078	3.293223	-1.435817
N	3.229902	3.644679	2.618204	C	-0.412915	1.838195	-1.681162
C	0.607349	5.871121	-0.625241	H	0.217097	1.464195	-2.516665
H	0.888489	6.889813	-0.318416	H	-1.461538	1.657113	-1.972311
C	1.074403	4.775189	0.107291	C	0.822425	-0.153741	-0.615785
H	1.708272	4.934250	0.989184	C	0.253455	-1.424457	-0.266874
C	0.681018	3.473554	-0.292382	C	1.100942	-2.552189	-0.402143
C	0.893615	2.184705	0.339170	C	-1.128281	-1.633836	0.080349
C	0.008764	1.126188	-0.350630	C	-2.960842	-0.746774	1.491585
C	-1.211092	0.865730	0.615186	H	-2.703507	-0.119927	2.372811
H	-0.768344	0.691901	1.617260	H	-4.027760	-0.546946	1.265040
C	-2.032104	-0.401301	0.284402	C	-2.696599	-2.201730	1.775516
C	-2.896234	-0.159209	-0.997566	C	-1.603603	-2.683097	1.019352
H	-2.179991	-0.086730	-1.846938	C	-1.174066	-4.018332	1.161622
C	-3.802320	-1.320236	-1.277317	H	-0.343562	-4.407048	0.557531
C	-3.092906	-2.531850	-1.526444	C	-1.840883	-4.852546	2.071848
C	-3.836720	-3.717680	-1.764956	H	-1.516659	-5.898579	2.188544
H	-3.287747	-4.655908	-1.940490	C	-2.931505	-4.370464	2.826942
C	-5.239768	-3.673573	-1.778894	H	-3.449176	-5.041813	3.530157
H	-5.808727	-4.597373	-1.974591	C	-3.364996	-3.041879	2.680819
C	-0.236886	5.685796	-1.744152	H	-4.218476	-2.663712	3.265547
H	-0.604898	6.564635	-2.296025	C	-5.929115	-2.468685	-1.530243
C	-0.615027	4.397149	-2.158549	H	-7.030061	-2.449135	-1.534551
H	-1.274073	4.257592	-3.028653	C	-5.203050	-1.289395	-1.272915

H	-5.719294	-0.336896	-1.077284
C	-3.284872	2.088644	-0.134687
C	-4.114345	3.230500	-0.162479
H	-4.993882	3.223577	-0.823532
C	-3.807410	4.336458	0.639590
H	-4.454542	5.226814	0.605107
C	-2.689327	4.305085	1.496743
H	-2.455092	5.164816	2.141988
C	-1.874749	3.165165	1.518719
H	-0.999812	3.127621	2.186363
C	-2.137040	2.054894	0.689708
C	1.680347	1.903462	1.450709
C	1.741218	0.603208	2.051311
C	2.516234	2.875894	2.085447
C	5.439237	-1.474714	-0.570071
N	4.153022	-1.764284	-0.751173
N	6.399062	-2.429800	-0.746381
N	5.820988	-0.212730	-0.217344
C	7.596140	-2.485923	0.093042
H	7.640828	-3.473231	0.600049
H	8.524444	-2.357100	-0.502523
H	7.552219	-1.703321	0.870707
C	6.119782	-3.621012	-1.543817
H	5.757002	-4.467565	-0.918768
H	5.359242	-3.390783	-2.312692
H	7.051505	-3.941238	-2.051998
C	7.056129	0.391704	-0.712843
H	7.776696	0.597015	0.107208
H	7.532256	-0.271866	-1.456227
H	6.814587	1.354820	-1.210927
C	4.905876	0.680732	0.484455
H	5.460665	1.227886	1.274122
H	4.453457	1.431728	-0.199753
H	4.099079	0.092360	0.955698
H	3.814453	-2.731718	-0.668029

IM7

N	1.916292	0.403098	-1.210533
H	3.267908	-0.366239	-1.034270
H	1.957164	1.428031	-1.299691
N	2.179837	-3.111828	-1.363670
O	-1.177949	-3.161081	-0.584913
N	1.888904	-0.066906	2.457098
O	-3.824737	0.052981	-1.133316
N	2.271429	4.218384	2.523260
C	-0.862255	5.813234	-0.646820
H	-0.831185	6.865056	-0.324667

C	-0.154243	4.847701	0.076787	C	0.741561	-0.004163	-0.736502
H	0.419184	5.138636	0.966576	C	0.422246	-1.375386	-0.567710
C	-0.227339	3.496033	-0.342103	C	1.366859	-2.332266	-0.993829
C	0.284876	2.284248	0.270410	C	-0.798309	-1.907446	0.135810
C	-0.328772	1.058693	-0.425884	C	-2.806732	-1.370361	1.465098
C	-1.475737	0.532201	0.525787	H	-3.306832	-0.520984	1.972921
H	-1.045721	0.512742	1.548883	H	-3.607999	-2.076439	1.159180
C	-1.978626	-0.899742	0.228130	C	-1.777654	-2.058780	2.330356
C	-2.763311	-0.913686	-1.091844	C	-0.619285	-2.349164	1.583041
H	-2.043546	-0.676044	-1.909266	C	0.483263	-2.985112	2.168121
C	-3.312422	-2.289250	-1.344924	H	1.389443	-3.187652	1.578262
C	-2.439869	-3.363594	-1.048980	C	0.410099	-3.342909	3.526887
C	-2.860563	-4.691966	-1.264461	H	1.266948	-3.839525	4.008645
H	-2.165053	-5.509641	-1.022973	C	-0.744737	-3.053365	4.281299
C	-4.145173	-4.941702	-1.772761	H	-0.782628	-3.327563	5.347527
H	-4.466136	-5.981877	-1.941130	C	-1.846115	-2.404823	3.688663
C	-1.631011	5.450713	-1.776571	H	-2.743074	-2.170267	4.283966
H	-2.190825	6.226235	-2.322117	C	-5.023206	-3.877562	-2.052437
C	-1.692361	4.114859	-2.209776	H	-6.033879	-4.077322	-2.439955
H	-2.293150	3.836413	-3.088745	C	-4.601651	-2.553948	-1.832403
C	-0.984132	3.141825	-1.494751	H	-5.270161	-1.705172	-2.037953
C	-0.888015	1.669789	-1.760967	C	-3.753641	1.179107	-0.355609
H	-0.158820	1.474811	-2.576635	C	-4.842868	2.070051	-0.451540
H	-1.852010	1.243142	-2.086827	H	-5.661913	1.825641	-1.144415

C	-4.863759	3.234655	0.327022
H	-5.714594	3.928339	0.240233
C	-3.813560	3.509147	1.224744
H	-3.833900	4.414709	1.849150
C	-2.736734	2.616190	1.313385
H	-1.909725	2.818075	2.012155
C	-2.672075	1.457030	0.514372
C	1.147282	2.176490	1.355000
C	1.528763	0.918315	1.924692
C	1.749142	3.308830	1.990138
C	5.417880	-0.608716	-0.768114
N	4.161403	-1.018162	-0.888051
N	6.466351	-1.422935	-1.100860
N	5.688055	0.650074	-0.306734
C	7.719075	-1.414921	-0.345953
H	7.905768	-2.428625	0.069032
H	8.584356	-1.135121	-0.983713
H	7.648591	-0.706651	0.498282
C	6.255520	-2.571494	-1.976456
H	6.030209	-3.500089	-1.404510
H	5.418979	-2.369775	-2.671045
H	7.174422	-2.746917	-2.571380
C	6.794701	1.446276	-0.832393
H	7.537046	1.695608	-0.044258
H	7.302899	0.900910	-1.647365
H	6.398124	2.397812	-1.247714
C	4.708174	1.365097	0.503211
H	5.239769	1.976919	1.260266
H	4.073620	2.044579	-0.108057
H	4.053211	0.641670	1.020411
H	3.947381	-2.021459	-0.977526

IM8

N	1.886046	0.429527	-1.240490
H	2.810014	-0.144508	-1.209108
H	2.019218	1.442229	-1.283780
N	2.127343	-3.143268	-1.374818
O	-1.209448	-3.086111	-0.732073
N	1.833058	-0.133224	2.458385
O	-3.835787	0.134723	-1.136327
N	2.313357	4.157820	2.579788
C	-0.768687	5.833753	-0.598403
H	-0.719486	6.881899	-0.267084
C	-0.075231	4.850625	0.114964
H	0.504850	5.123892	1.005897
C	-0.171731	3.504344	-0.316578
C	0.317775	2.280484	0.289292

C	-0.318520	1.071029	-0.422344	C	-2.831447	-1.339319	1.438762
C	-1.471725	0.550213	0.521406	H	-3.275988	-0.481251	1.982468
H	-1.040525	0.509257	1.543186	H	-3.676046	-1.988430	1.124939
C	-1.998632	-0.868565	0.204191	C	-1.833064	-2.111043	2.266689
C	-2.798700	-0.855409	-1.109706	C	-0.684191	-2.412634	1.510330
H	-2.084234	-0.635381	-1.937222	C	0.386160	-3.127408	2.066020
C	-3.381444	-2.219420	-1.350092	H	1.285494	-3.347064	1.472018
C	-2.503140	-3.300496	-1.106613	C	0.289460	-3.548629	3.404431
C	-2.939514	-4.625435	-1.294937	H	1.120559	-4.107014	3.862675
H	-2.236758	-5.447806	-1.094616	C	-0.856563	-3.247803	4.167980
C	-4.254170	-4.864600	-1.728668	H	-0.913226	-3.575147	5.218145
H	-4.592987	-5.901810	-1.878355	C	-1.925110	-2.524059	3.605079
C	-1.545862	5.493927	-1.729417	H	-2.815819	-2.283245	4.206877
H	-2.094189	6.283369	-2.266428	C	-5.138724	-3.793750	-1.955963
C	-1.630080	4.163593	-2.175496	H	-6.171361	-3.987190	-2.284173
H	-2.237041	3.903345	-3.055605	C	-4.698780	-2.471674	-1.760650
C	-0.935605	3.173404	-1.471358	H	-5.373023	-1.618780	-1.926293
C	-0.867149	1.702547	-1.753662	C	-3.739507	1.250376	-0.345823
H	-0.151860	1.500544	-2.579371	C	-4.810827	2.163828	-0.428969
H	-1.841244	1.294869	-2.073326	H	-5.636500	1.943390	-1.121870
C	0.715102	-0.010788	-0.732124	C	-4.805431	3.320056	0.361773
C	0.417673	-1.361391	-0.561703	H	-5.642086	4.031804	0.284918
C	1.354212	-2.335594	-0.995408	C	-3.747651	3.563697	1.259597
C	-0.838281	-1.899787	0.085272	H	-3.748367	4.462366	1.894031

C	-2.689174	2.648519	1.336072
H	-1.857468	2.825692	2.035804
C	-2.650509	1.497465	0.523426
C	1.167094	2.146330	1.380886
C	1.512040	0.874107	1.943315
C	1.782558	3.262001	2.032798
C	5.478506	-0.629625	-0.790789
N	4.230518	-0.947075	-1.025914
N	6.566349	-1.434812	-1.113485
N	5.792227	0.585324	-0.197357
C	7.694500	-1.584800	-0.197331
H	7.692401	-2.600726	0.260730
H	8.666392	-1.445173	-0.718890
H	7.617463	-0.843336	0.617770
C	6.368359	-2.538437	-2.039555
H	5.987425	-3.461853	-1.540091
H	5.647881	-2.245797	-2.827706
H	7.335143	-2.789591	-2.522302
C	6.909333	1.395940	-0.669238
H	7.556159	1.730313	0.171080
H	7.522801	0.816043	-1.381804
H	6.535967	2.305094	-1.195729
C	4.750792	1.308114	0.510955
H	5.206458	1.918121	1.318807
H	4.180268	2.001699	-0.152655
H	4.039596	0.588299	0.954088
H	4.095029	-1.949186	-1.223059

2a

N	-0.909088	2.045458	-2.682137
H	-0.395836	2.707779	-3.267831
H	-1.926730	2.110153	-2.694860
N	2.399797	3.004610	-3.135123
O	3.080832	0.175659	-1.175995
N	-0.307876	3.837350	0.575437
O	0.420564	-2.809760	-0.002856
N	-4.613737	3.591823	1.010492
C	-5.741347	-0.789557	-0.341785
H	-6.774950	-0.759984	0.034344
C	-4.895926	0.303009	-0.123055
H	-5.260732	1.177779	0.430332
C	-3.562009	0.234157	-0.596446
C	-2.443351	1.138957	-0.405701
C	-1.147475	0.440713	-0.867184
C	-0.407654	-0.046969	0.441282
H	-0.435152	0.807571	1.148531
C	1.080924	-0.429324	0.262454

C	1.201618	-1.735962	-0.542137	C	2.401597	1.548707	0.685676
H	0.845588	-1.530515	-1.579018	C	2.938832	2.843122	0.632044
C	2.648730	-2.134870	-0.618440	H	2.993092	3.394247	-0.318096
C	3.544816	-1.083654	-0.919161	C	3.400497	3.428793	1.824043
C	4.926673	-1.330198	-1.009358	H	3.820304	4.446483	1.805140
H	5.601402	-0.492850	-1.241099	C	3.318005	2.727861	3.044128
C	5.408831	-2.633261	-0.799013	H	3.675407	3.203333	3.971087
H	6.490479	-2.827083	-0.871914	C	2.775057	1.430011	3.091317
C	-5.278552	-1.937413	-1.024768	H	2.705411	0.887279	4.047268
H	-5.958448	-2.790796	-1.171917	C	4.524498	-3.681063	-0.482054
C	-3.963202	-2.004875	-1.515853	H	4.909434	-4.697160	-0.306537
H	-3.606140	-2.900433	-2.046085	C	3.143752	-3.426702	-0.388110
C	-3.111843	-0.914309	-1.306865	H	2.434192	-4.228214	-0.136114
C	-1.685220	-0.752046	-1.737923	C	-0.685259	-2.538004	0.760943
H	-1.634530	-0.478090	-2.813180	C	-1.385770	-3.656594	1.257543
H	-1.106290	-1.683823	-1.620967	H	-1.024454	-4.661866	0.994433
C	-0.266812	1.356540	-1.702558	C	-2.513599	-3.470809	2.067195
C	1.104163	1.428523	-1.522701	H	-3.059174	-4.349729	2.444322
C	1.838882	2.281751	-2.390665	C	-2.937880	-2.172185	2.410675
C	1.885920	0.691792	-0.461581	H	-3.812904	-2.023125	3.060364
C	1.708567	-0.520903	1.689979	C	-2.233765	-1.067488	1.913697
H	0.947290	-0.777509	2.454127	H	-2.552392	-0.046915	2.177380
H	2.482552	-1.315824	1.734198	C	-1.119957	-1.225930	1.064350
C	2.319251	0.842192	1.900800	C	-2.449429	2.401989	0.173829

C	-1.254345	3.168991	0.375060	C	-3.645930	3.042909	0.629715

Table S9 Coordinates and free energies and electronic energies (in hatree) of the calculated structures at the BP86+D3BJ/def2-TZVPP(SMD, Solvent = N,N-dimethylformamide) //BP86+D3BJ/def2-SVP(IEFPCM,Solvent=N,N-dimethylformamide) level

TMG

C	-0.006240	0.569863	-0.006985
N	-0.068062	1.872206	0.001262
N	1.165995	-0.199838	0.067984
N	-1.181942	-0.184423	-0.074516
C	1.355291	-1.343618	-0.821444
H	2.010511	-1.076177	-1.685033
H	1.827221	-2.196405	-0.286775
H	0.379817	-1.671245	-1.223049
C	2.393745	0.467702	0.462458
H	2.881256	1.026538	-0.375586
H	2.191871	1.180936	1.285901
H	3.121152	-0.287131	0.826153
C	-1.369068	-1.338502	0.799697
H	-1.874120	-2.170628	0.262989
H	-0.391934	-1.695628	1.170601
H	-1.996570	-1.073365	1.684786
C	-2.409765	0.510967	-0.420284
H	-3.143603	-0.218783	-0.822696
H	-2.876524	1.021685	0.457171
H	-2.198267	1.282722	-1.182915
H	0.873483	2.263392	-0.155312

1a

N	1.523746	3.717377	-0.484118
N	-1.954241	1.535499	-1.859221
C	1.462123	-2.168854	-0.454391
H	1.560074	-2.524369	-1.506283
C	2.682641	-1.387005	-0.044781
C	3.983203	-1.848322	0.194600
H	4.223723	-2.918457	0.099656
C	4.975228	-0.921647	0.563163
H	6.000396	-1.270786	0.762216
C	4.670947	0.451891	0.685819
H	5.459052	1.159654	0.984845
C	-0.974577	-1.510915	-0.186988
C	0.339303	-1.141567	-0.331224
C	0.954549	0.189097	-0.269993
C	2.372391	-0.000557	0.068890
C	3.375734	0.925999	0.435390
H	3.153114	1.995848	0.540668
C	0.352425	1.396962	-0.658739
C	1.012036	2.659100	-0.561031
C	-0.927545	1.452464	-1.288943
C	-2.092629	-0.734253	0.332135

C	-3.407914	-1.000019	-0.152023	C	2.774153	0.393915	-0.373469
C	-1.939116	0.227214	1.362794	C	3.944330	0.598395	0.412976
C	-4.515573	-0.303847	0.374913	H	3.965058	1.380590	1.185248
C	-3.037027	0.916068	1.885782	C	1.191059	2.331513	0.189075
H	-0.932369	0.404904	1.769745	C	1.965488	2.887772	1.240941
C	-4.328563	0.650781	1.383464	C	0.151728	3.171188	-0.282269
H	-5.523667	-0.514648	-0.017501	C	-1.856353	0.810354	-0.880199
H	-2.895602	1.647603	2.695303	C	-3.144601	0.755989	-1.512996
H	-5.200892	1.187355	1.787752	C	-1.836017	1.157123	0.499657
O	-3.523953	-1.921160	-1.142200	C	-4.322248	1.014340	-0.785139
H	-4.469368	-2.050094	-1.359306	C	-3.003999	1.397526	1.225928
H	-1.208601	-2.565208	-0.421364	H	-0.867558	1.197599	1.011884
H	1.293410	-3.068186	0.172230	C	-4.256631	1.329050	0.579928
IM9				H	-5.295533	0.956778	-1.299326
N	2.587130	3.351218	2.134005	H	-2.943128	1.643506	2.296689
N	-0.709647	3.886633	-0.661915	H	-5.184819	1.523859	1.138716
C	1.506873	-0.664109	-2.043645	O	-3.178330	0.411211	-2.828125
H	1.172802	-1.346786	-2.836262	H	-4.109687	0.343871	-3.119814
C	2.764349	-0.652276	-1.407657	H	-1.009355	-0.228754	-2.527836
C	3.925464	-1.473340	-1.571203	C	-0.401315	-2.072059	0.957779
H	3.926988	-2.277535	-2.324734	N	0.896948	-2.091910	0.591566
C	5.041070	-1.248154	-0.774210	N	-0.761157	-1.543450	2.154649
H	5.935722	-1.879490	-0.903079	N	-1.317841	-2.620158	0.122205
C	5.059145	-0.212911	0.217294	C	-2.720152	-2.204444	0.077019
H	5.960850	-0.066862	0.832011	H	-2.983401	-1.967373	-0.973077
C	-0.713725	0.352310	-1.636344	H	-3.393904	-3.010921	0.434077
C	0.663167	0.330727	-1.405048	H	-2.874796	-1.293451	0.678449
C	1.512068	1.070939	-0.417497	C	-0.899423	-3.536013	-0.940113

H	0.051907	-4.025743	-0.664953
H	-1.680732	-4.310521	-1.070772
H	-0.766274	-3.001987	-1.905424
C	0.100330	-0.569262	2.826048
H	-0.537416	0.171233	3.347588
H	0.759858	-1.051464	3.580288
H	0.722275	-0.030151	2.086176
C	-1.875249	-2.062397	2.949700
H	-2.240130	-3.013315	2.524822
H	-1.514528	-2.261779	3.979646
H	-2.712174	-1.334969	3.004278
H	1.152696	-1.867817	-0.396788
H	1.606833	-1.851596	1.284293

IM10

N	3.533669	3.447276	1.428127
N	-0.057262	3.987443	-0.948177
C	1.439182	-0.945764	-1.899983
H	1.651351	-0.756586	-2.977252
C	2.709967	-1.085044	-1.108317
C	3.648899	-2.124654	-1.129962
H	3.513565	-2.985058	-1.803279
C	4.760794	-2.055333	-0.271286
H	5.501594	-2.870078	-0.271677
C	4.935635	-0.955864	0.597811
H	5.807127	-0.925722	1.269436
C	-0.595820	0.436851	-1.325436
C	0.762572	0.252245	-1.242987
C	1.760509	0.954328	-0.431955
C	2.886740	0.030084	-0.236944
C	4.009451	0.096217	0.620050
H	4.154127	0.940670	1.306612
C	1.721997	2.307678	-0.056811
C	2.726460	2.917481	0.753046
C	0.724624	3.208460	-0.538024
C	-1.488872	1.190997	-0.460479
C	-2.731022	1.651212	-0.987195
C	-1.250835	1.358994	0.926803
C	-3.683396	2.262899	-0.147102
C	-2.196669	1.956846	1.763169
H	-0.313341	0.975554	1.349663
C	-3.416895	2.412667	1.220347
H	-4.637688	2.611387	-0.574033
H	-1.995264	2.056859	2.840009
H	-4.170966	2.883462	1.869864
O	-2.947167	1.455389	-2.314145
H	-3.854023	1.743473	-2.542261
H	-1.109691	-0.155211	-2.103761
C	-1.224414	-2.547532	0.368380
N	-0.258831	-3.092736	-0.326985
N	-1.064932	-1.899803	1.597715
N	-2.530310	-2.597629	-0.114740
C	-3.453519	-1.475640	0.014197
H	-3.590919	-0.966648	-0.967546
H	-4.453777	-1.815954	0.361485
H	-3.063193	-0.729352	0.726623
C	-2.801972	-3.469945	-1.244853

H	-2.177280	-4.378671	-1.173371	C	-0.435032	2.370714	-1.927381
H	-3.875925	-3.751561	-1.239668	C	-0.957781	2.760066	-3.190851
H	-2.578212	-2.980168	-2.223408	H	-1.908118	2.331739	-3.544606
C	0.282500	-1.585704	2.037534	C	-0.244009	3.674564	-3.968032
H	0.243425	-0.775269	2.793803	H	-0.640380	3.975987	-4.951053
H	0.804475	-2.455914	2.506697	C	0.990665	4.228147	-3.520793
H	0.893917	-1.232826	1.185546	H	1.528788	4.943062	-4.161653
C	-2.034085	-2.062858	2.677857	C	0.536527	-3.043114	-0.066061
H	-2.923683	-2.604651	2.310765	C	-0.728572	-2.758290	0.477665
H	-1.593753	-2.656886	3.511761	C	1.183136	-4.117810	0.604240
H	-2.356477	-1.079963	3.087645	C	5.316258	-1.296314	-1.568499
H	0.800583	-1.855361	-1.816128	H	6.364430	-0.995515	-1.722008
H	0.594036	-3.162235	0.246887	C	4.282513	-0.592047	-2.214670
IM11				H	4.510409	0.264541	-2.868361
N	-1.727235	-2.495021	1.063280	C	2.957485	-0.992780	-2.007532
N	1.672226	-5.026123	1.179663	C	1.694560	-0.387556	-2.536259
N	3.734159	4.748359	0.329229	H	1.666108	-0.353908	-3.646871
N	1.553449	2.411147	3.349764	H	1.579986	0.667475	-2.199537
C	5.015653	-2.383500	-0.720589	C	0.035255	0.290440	1.003416
H	5.832690	-2.923721	-0.217604	C	0.075914	1.323395	0.072566
C	3.689124	-2.779666	-0.495628	C	1.113198	2.368434	-0.170173
H	3.480023	-3.613664	0.185294	C	0.841075	2.922531	-1.480151
C	2.643519	-2.082214	-1.145153	C	1.530222	3.862687	-2.282149
C	1.180926	-2.208177	-1.042302	H	2.490097	4.286115	-1.954169
C	0.588242	-1.265911	-1.960535	C	1.957826	2.912281	0.828640
C	-0.716714	-1.035832	-2.389691	C	2.921809	3.922164	0.550586
C	-0.918748	1.454722	-0.955518	C	1.771148	2.610917	2.206954
H	-1.851140	0.889655	-1.014279	C	1.049503	-0.333366	1.817665

C	0.644441	-1.159565	2.916860
C	2.442103	-0.258901	1.535112
C	1.596750	-1.825807	3.706471
C	3.382959	-0.928850	2.316590
H	2.773719	0.313865	0.657821
C	2.963391	-1.708603	3.415524
H	1.237687	-2.441329	4.544642
H	4.449763	-0.865114	2.056626
H	3.702929	-2.240736	4.033477
O	-0.685532	-1.276447	3.263489
H	-1.190541	-1.693128	2.486688
H	-0.946243	-0.203622	1.044330
C	-1.906006	-1.869574	-2.276579
C	-3.203539	-1.281585	-2.389590
C	-1.841532	-3.285367	-2.179558
C	-4.364846	-2.075809	-2.330689
C	-2.992812	-4.078130	-2.143111
H	-0.851329	-3.761680	-2.161405
C	-4.261600	-3.468804	-2.202033
H	-5.352735	-1.590976	-2.392878
H	-2.904237	-5.172797	-2.074220
H	-5.176857	-4.079215	-2.160228
O	-3.271480	0.073921	-2.537586
H	-4.205263	0.342394	-2.653161
H	-0.837274	-0.156870	-3.041980
C	-2.669996	1.487152	2.416064
N	-1.758270	1.340276	3.398090
N	-3.505436	0.445543	2.149181
N	-2.774189	2.647077	1.724869
C	-4.038079	3.102205	1.145238
H	-4.209501	4.153566	1.454294
H	-4.015045	3.064231	0.036019
H	-4.875886	2.489090	1.519308
C	-1.673568	3.605086	1.642606
H	-0.728585	3.133844	1.958722
H	-1.555863	3.931044	0.589413
H	-1.872316	4.495373	2.276579
C	-3.875070	-0.528596	3.177483
H	-3.567423	-0.166639	4.173976
H	-4.977519	-0.657115	3.167237
H	-3.411276	-1.516654	2.980448
C	-3.977875	0.126291	0.801161
H	-3.536409	0.811829	0.060660
H	-3.654601	-0.905814	0.550046
H	-5.084441	0.182332	0.734172
H	-1.207869	2.138465	3.719895
H	-1.353110	0.391528	3.540731

IM12

N	-0.981384	-2.851716	1.091150
N	2.437795	-5.231222	-0.405327
N	1.376513	5.928760	0.740554
N	0.303939	2.594374	3.343481
C	5.401746	-1.490370	-0.095118
H	6.197324	-1.962230	0.502806
C	4.125358	-2.080134	-0.137856
H	3.919422	-2.999435	0.428580

C	3.118243	-1.457336	-0.898792	C	0.236650	4.378859	-2.159175
C	1.679012	-1.783648	-1.039876	H	0.783293	5.174510	-1.636663
C	1.070064	-0.780618	-1.791112	C	0.678135	3.427169	0.909674
C	-0.355657	-0.455247	-2.186413	C	1.048652	4.797660	0.798793
C	-0.830637	0.862881	-1.412154	C	0.523276	2.958892	2.243132
H	-1.895803	0.727421	-1.142264	C	1.326930	0.088927	1.702808
C	-0.704007	2.110747	-2.252537	C	1.217543	-0.820093	2.804915
C	-1.175640	2.334260	-3.550815	C	2.567800	0.754939	1.504100
H	-1.734570	1.550948	-4.085866	C	2.313100	-1.004776	3.672800
C	-0.929595	3.580551	-4.158278	C	3.649132	0.556045	2.360338
H	-1.291787	3.770186	-5.180615	H	2.676117	1.415164	0.632495
C	-0.223723	4.588622	-3.469083	C	3.517684	-0.323864	3.456306
H	-0.031533	5.553803	-3.962107	H	2.190252	-1.698780	4.517588
C	1.137082	-2.979367	-0.374441	H	4.603426	1.067373	2.167696
C	-0.035829	-2.949938	0.368270	H	4.366584	-0.489284	4.137852
C	1.853391	-4.202223	-0.380017	O	0.047766	-1.458041	3.118150
C	5.671796	-0.296904	-0.794259	H	-0.355977	-1.990270	2.330861
H	6.676120	0.152124	-0.741978	H	-0.420933	-0.648688	0.673885
C	4.660300	0.334804	-1.547713	C	-1.333315	-1.632200	-2.269001
H	4.862888	1.280799	-2.074902	C	-2.747845	-1.535461	-2.168794
C	3.390894	-0.250422	-1.591905	C	-0.819114	-2.895383	-2.642980
C	2.114938	0.230919	-2.224159	C	-3.565244	-2.677561	-2.306546
H	2.171496	0.281671	-3.336087	C	-1.624399	-4.031289	-2.807348
H	1.866182	1.267263	-1.901889	H	0.261631	-2.977703	-2.817371
C	0.243503	0.223217	0.754523	C	-3.011160	-3.926712	-2.613103
C	-0.044229	1.223459	-0.156809	H	-4.655697	-2.564106	-2.186997
C	0.319086	2.622860	-0.201107	H	-1.165904	-4.992623	-3.084148
C	-0.004425	3.129462	-1.547091	H	-3.665981	-4.805540	-2.718229

O	-3.341459	-0.310847	-1.955822	N	-4.989725	-4.764689	-0.616646
H	-4.310865	-0.412069	-2.037327	N	-0.863555	-3.997423	-2.038506
H	-0.268279	-0.106144	-3.242107	C	3.419512	-0.145996	3.221728
C	-3.009663	0.276746	2.428570	H	4.508109	-0.158346	3.384462
N	-1.934259	0.538668	3.192031	C	2.883878	0.621327	2.179768
N	-3.492057	-0.992399	2.381458	H	3.551769	1.191400	1.522005
N	-3.626479	1.259740	1.723234	C	1.483811	0.610619	1.976074
C	-5.073048	1.257716	1.497674	C	0.677095	1.142508	0.886376
H	-5.490317	2.223531	1.851019	C	-0.708281	0.545911	0.974194
H	-5.320510	1.142893	0.422133	C	-1.985762	1.432090	0.620238
H	-5.547751	0.443555	2.072076	C	-2.688794	0.692205	-0.538587
C	-2.932794	2.495656	1.371752	H	-2.349680	1.144484	-1.503103
H	-1.845697	2.317196	1.331438	C	-4.188813	0.519821	-0.595109
H	-3.263432	2.822484	0.366035	C	-5.220313	1.462199	-0.553577
H	-3.147670	3.311580	2.095638	H	-5.000288	2.532167	-0.412466
C	-3.275164	-1.937900	3.475985	C	-6.556550	1.020643	-0.683661
H	-2.991734	-1.394699	4.395247	H	-7.381108	1.749050	-0.630674
H	-4.220654	-2.487246	3.663400	C	-6.836651	-0.343360	-0.884685
H	-2.485907	-2.673900	3.218700	H	-7.881749	-0.673824	-0.997184
C	-4.055783	-1.559845	1.155659	C	1.124968	1.917640	-0.189214
H	-3.932996	-0.847075	0.322834	C	0.405849	2.032994	-1.418450
H	-3.480574	-2.473389	0.902431	C	2.404989	2.536672	-0.213362
H	-5.129048	-1.816532	1.275179	C	2.579187	-0.915287	4.059294
H	-1.615630	1.496390	3.375231	H	3.025099	-1.523869	4.861304
H	-1.222675	-0.210114	3.327831	C	1.185919	-0.916201	3.875968
IM13				H	0.533768	-1.519733	4.524833
N	-0.094278	2.077175	-2.483975	C	0.641446	-0.149117	2.838277
N	3.457018	3.065856	-0.268756	C	-0.787903	0.042871	2.439695

H	-1.221965	0.855771	3.057133	C	-2.126330	5.005050	-0.852650
H	-1.421667	-0.853618	2.562607	H	-2.870992	3.066721	-1.444941
C	-0.750611	-0.731147	-0.072254	C	-1.385086	5.729328	0.095597
C	-2.182470	-0.724920	-0.487191	H	-0.280893	5.623881	1.975009
C	-3.190211	-1.638129	-0.736776	H	-2.553412	5.509809	-1.732283
C	-4.468964	-0.869043	-0.775665	H	-1.217968	6.810444	-0.029313
C	-5.799267	-1.297548	-0.942936	O	-0.597994	3.025188	2.484568
H	-6.032526	-2.360426	-1.100315	H	-0.051607	3.629064	3.026368
C	-3.061254	-3.066304	-1.007073	H	-2.638107	1.319969	1.513522
C	-4.112598	-3.985665	-0.796516	C	4.724049	0.039138	-1.586284
C	-1.858851	-3.579680	-1.548282	N	5.342273	0.940130	-0.804625
C	-0.139828	-1.967971	0.531019	N	4.809306	-1.298260	-1.283165
C	1.246370	-2.206892	0.358323	N	4.019165	0.466372	-2.658369
C	-0.870680	-2.863950	1.335665	C	2.884105	-0.259025	-3.238357
C	1.873784	-3.301891	0.980875	H	2.027211	0.441160	-3.317807
C	-0.254299	-3.956961	1.964361	H	3.127209	-0.635626	-4.253162
H	-1.950652	-2.696657	1.457283	H	2.573534	-1.093209	-2.589612
C	1.124248	-4.171375	1.787546	C	4.300903	1.767645	-3.273738
H	2.952750	-3.465771	0.834862	H	5.321678	2.099505	-3.012358
H	-0.848643	-4.641561	2.588250	H	4.232883	1.653522	-4.373561
H	1.623665	-5.022577	2.276110	H	3.572115	2.539259	-2.951468
O	1.935217	-1.325287	-0.426646	C	5.359572	-1.702624	0.020852
H	2.885612	-1.567536	-0.480171	H	5.099761	-2.763897	0.193959
H	-0.115859	-0.420339	-0.928697	H	6.468821	-1.622046	0.050356
C	-1.780707	2.926208	0.423123	H	4.918173	-1.098556	0.836254
C	-1.070635	3.688546	1.388558	C	4.997358	-2.293950	-2.356909
C	-2.311310	3.623237	-0.680507	H	4.895987	-1.819567	-3.346476
C	-0.857041	5.070064	1.215740	H	6.019399	-2.719030	-2.281646

H	4.259281	-3.114604	-2.265216
H	4.941078	1.888800	-0.691077
H	6.076997	0.654384	-0.156818

IM14

N	1.284149	3.738936	-2.504683
O	-2.279658	-1.385251	1.086705
H	-3.015764	-1.746676	1.618677
N	6.355175	-0.484735	-0.695106
O	2.107356	-0.756871	1.371852
N	4.431171	3.427421	0.233650
N	-2.764596	5.032714	-2.431662
C	3.011241	-2.659567	-3.314498
H	3.691774	-3.405336	-3.754256
C	3.548598	-1.588790	-2.571703
H	4.635490	-1.499967	-2.435467
C	2.670015	-0.652308	-1.995410
C	2.924009	0.526214	-1.111726
C	1.680262	1.049279	-0.770126
C	1.154986	1.885560	0.374254
H	1.276055	2.974878	0.190278
C	-0.401579	1.551286	0.382194
C	-1.036405	1.386144	1.789610
H	-0.868575	0.381892	2.218768
H	-0.588446	2.122560	2.489816
C	-2.484181	1.703156	1.564907
C	-3.592210	1.372698	2.353103
H	-3.464210	0.807285	3.288608
C	-4.871848	1.756150	1.914334
H	-5.756361	1.492010	2.514719
C	2.776028	1.240712	4.376087
H	3.146436	1.079927	5.400593
C	2.663987	0.151517	3.500048
H	2.952041	-0.865049	3.807989
C	2.189841	0.343570	2.187542
C	1.806943	1.633580	1.733490
C	0.569651	0.368316	-1.521170
H	0.173672	1.034493	-2.325388
C	-0.515852	0.173679	-0.452169
H	-0.172297	-0.603029	0.256791
C	-1.888114	-0.210299	-0.951794
C	-2.757219	-0.971156	-0.128931
C	-4.064524	-1.280293	-0.549543
H	-4.722601	-1.861733	0.115974
C	-4.524245	-0.842250	-1.801024
H	-5.550396	-1.084801	-2.117566
C	-3.673924	-0.103287	-2.640420
H	-4.021385	0.238990	-3.626645
C	-2.371866	0.199767	-2.210852
H	-1.716448	0.785863	-2.871939
C	-5.039433	2.466716	0.705417
H	-6.051220	2.740923	0.370529
C	-3.934325	2.812052	-0.083178
H	-4.085420	3.341239	-1.032319
C	-2.644011	2.425553	0.349686
C	-1.332650	2.564210	-0.285756
C	-1.028032	3.417972	-1.340521

C	0.262263	3.559958	-1.950136
C	4.338968	2.310216	-0.147331
C	4.215421	0.989865	-0.646702
C	5.379107	0.186955	-0.675893
C	1.261059	-0.790628	-2.192526
C	0.735027	-1.837516	-2.958172
H	-0.351104	-1.912857	-3.125130
C	1.622799	-2.789841	-3.506481
H	1.227065	-3.634982	-4.090507
C	-2.001652	4.296596	-1.922408
C	1.962686	2.712443	2.627220
H	1.692252	3.721489	2.276445
C	2.434537	2.532930	3.936732
H	2.534904	3.397088	4.610846
C	-0.243600	-3.764616	0.766403
N	0.783692	-3.041190	0.282287
H	0.775747	-2.721486	-0.694652
N	-0.991159	-4.514282	-0.083905
N	-0.503111	-3.778027	2.096088
C	-1.029323	-4.966195	2.771163
H	-0.372279	-5.203070	3.633272
H	-2.059013	-4.802109	3.151712
H	-1.025096	-5.830181	2.084130
C	-0.074502	-2.689802	2.972830
H	0.103696	-1.771468	2.388748
H	-0.875981	-2.484837	3.710040
H	0.852256	-2.955432	3.525699
C	-0.474305	-4.930688	-1.386059
H	-0.839675	-5.954093	-1.604487
H	-0.820301	-4.256677	-2.198495
H	0.630515	-4.946625	-1.372300
C	-2.429085	-4.700249	0.114500
H	-2.766130	-4.132416	0.996574
H	-2.967532	-4.307891	-0.773770
H	-2.690083	-5.770617	0.244183
H	2.109671	-0.392481	0.438493
H	1.422640	-2.541350	0.914959

IM15

N	1.223158	-1.226141	-2.583363
O	-3.507122	1.508111	2.476991
H	-3.996166	1.972658	3.184582
N	-0.261653	-6.091540	-1.715459
O	2.086161	-0.660954	2.313965
N	2.490545	-3.153708	-0.134091
N	1.026717	2.198591	-4.016948
C	-4.522116	-4.001255	-1.256375
H	-5.109311	-4.927897	-1.350944
C	-3.119839	-4.072325	-1.248187
H	-2.619909	-5.046766	-1.331288
C	-2.374842	-2.876190	-1.115892
C	-0.937822	-2.649678	-0.983818
C	-0.673948	-1.208050	-0.820614
C	0.040775	-0.659423	0.468485
H	1.126610	-0.557608	0.281694
C	-0.573568	0.765924	0.499324
C	-0.284518	1.681429	1.710660

H	-1.078731	1.630024	2.480149	H	0.410544	6.277465	-1.050483
H	0.670503	1.376619	2.191233	C	0.253617	4.113353	-1.094783
C	-0.136052	3.051490	1.093547	H	0.389276	4.043430	-2.183213
C	-0.130833	4.304387	1.719901	C	0.043843	2.953657	-0.316314
H	-0.279123	4.385920	2.808102	C	-0.058921	1.551648	-0.706367
C	0.065018	5.459332	0.938186	C	0.249992	0.913669	-1.892258
H	0.064130	6.449928	1.419513	C	0.351868	-0.602153	-1.950861
C	-0.193364	-2.887488	4.195211	C	1.417052	-3.297044	-0.604401
H	-0.221537	-3.446136	5.143794	C	0.093845	-3.599545	-1.039651
C	0.946676	-2.135073	3.869493	C	-0.114307	-4.963662	-1.407993
H	1.809310	-2.100433	4.555353	C	-3.057656	-1.627928	-0.999140
C	0.997331	-1.416064	2.659263	C	-4.454443	-1.565555	-1.017860
C	-0.095715	-1.444960	1.749808	H	-4.968741	-0.596000	-0.928978
C	-2.065310	-0.505811	-0.901861	C	-5.188260	-2.763122	-1.139134
H	-2.120724	0.076946	-1.845974	H	-6.289000	-2.733143	-1.139470
C	-2.112295	0.466597	0.290124	C	0.692898	1.617071	-3.047425
H	-2.432066	-0.081828	1.197843	C	-1.224469	-2.210616	2.103585
C	-2.977415	1.696337	0.159311	H	-2.075803	-2.266067	1.411251
C	-3.631414	2.211767	1.309669	C	-1.285456	-2.925584	3.312383
C	-4.371017	3.409844	1.240312	H	-2.181707	-3.515667	3.556260
H	-4.867672	3.791272	2.147805	C	4.546342	0.060162	-0.491421
C	-4.469163	4.108892	0.027062	N	3.571137	-0.691948	-1.012500
H	-5.045953	5.046085	-0.013736	H	2.984041	-0.439713	-1.827828
C	-3.837897	3.609327	-1.125081	N	4.634151	1.389589	-0.760456
H	-3.911886	4.148753	-2.081357	N	5.470785	-0.515572	0.326324
C	-3.105954	2.413284	-1.046710	C	6.012270	0.192862	1.487174
H	-2.604444	2.032195	-1.949207	H	5.826054	-0.413225	2.398656
C	0.261226	5.362677	-0.456340	H	7.105846	0.360793	1.396759

H	5.503495	1.165070	1.610433	C	-0.994291	2.247220	-1.230362
C	5.717284	-1.956117	0.280943	C	-0.123300	1.062327	-0.900031
H	5.536076	-2.338130	-0.740482	C	-0.161374	0.530885	0.608938
H	6.775779	-2.143955	0.548465	H	-0.926595	-0.265860	0.673943
H	5.063720	-2.510877	0.988073	C	1.221721	-0.152832	0.658146
C	3.462393	2.151085	-1.179183	C	1.698633	-0.752449	2.004250
H	3.528103	3.175028	-0.761035	H	2.357432	-0.070132	2.571924
H	3.383384	2.229397	-2.285056	H	0.818927	-0.983388	2.645031
H	2.546522	1.676165	-0.786432	C	2.401532	-2.026251	1.599545
C	5.924844	2.067325	-0.888938	C	3.282488	-2.820278	2.342335
H	6.746762	1.331127	-0.848172	H	3.555775	-2.540762	3.371676
H	5.964776	2.579811	-1.872912	C	3.827464	-3.974345	1.746270
H	6.073653	2.826993	-0.093120	H	4.531227	-4.601317	2.315879
H	3.318616	-1.608412	-0.585535	C	-1.438592	3.684630	3.306353
H	2.775330	-0.758838	3.000050	H	-1.792878	4.506651	3.947410
IM16				C	-2.368120	2.925967	2.575945
N	-1.550164	-0.316666	-2.410891	H	-3.447131	3.139342	2.645640
O	4.497110	0.603071	1.630757	C	-1.922728	1.880086	1.748903
H	5.316597	0.404827	2.125285	C	-0.538974	1.583302	1.620180
N	-3.702986	4.019258	-2.693810	C	1.336266	1.645526	-0.997816
O	-2.806395	1.109592	1.029314	H	1.715175	1.537397	-2.035049
N	-3.820978	0.278138	-2.103426	C	2.226803	0.899273	0.022274
N	0.221859	-3.404182	-3.009545	H	2.518016	1.596286	0.830319
C	0.239958	5.745955	-0.251569	C	3.500477	0.273284	-0.510529
H	-0.088546	6.778947	-0.057426	C	4.601696	0.091150	0.366600
C	-0.705852	4.775244	-0.624081	C	5.753187	-0.601779	-0.057719
H	-1.770279	5.036146	-0.717689	H	6.589225	-0.739761	0.647561
C	-0.266986	3.454326	-0.844787	C	5.828037	-1.115395	-1.361715

H	6.730092	-1.661513	-1.678962
C	4.758324	-0.925275	-2.252537
H	4.808898	-1.317103	-3.279565
C	3.614313	-0.234540	-1.819208
H	2.773723	-0.107333	-2.517635
C	3.487550	-4.335155	0.424091
H	3.931210	-5.236999	-0.025151
C	2.602383	-3.549192	-0.327905
H	2.354908	-3.823162	-1.362971
C	2.063049	-2.383548	0.261797
C	1.192280	-1.358049	-0.287521
C	0.411516	-1.340512	-1.432108
C	-0.454563	-0.175991	-1.709509
C	-2.623350	0.658162	-2.213800
C	-2.155194	2.067511	-1.943743
C	-3.000139	3.142019	-2.337731
C	1.108778	3.119515	-0.706636
C	2.046228	4.092918	-0.347476
H	3.111628	3.834399	-0.238751
C	1.603543	5.411444	-0.115046
H	2.328368	6.186839	0.178322
C	0.304490	-2.472580	-2.294977
C	0.365471	2.343592	2.385023
H	1.440867	2.133067	2.316244
C	-0.069043	3.384827	3.223058
H	0.665809	3.966280	3.799743
C	-3.565830	-2.668424	0.313874
N	-2.770706	-1.675244	-0.123703
H	-2.405854	-1.682619	-1.095537
N	-3.196344	-3.956553	0.099743
N	-4.709298	-2.375479	0.983604
C	-5.203780	-3.196689	2.088217
H	-5.368969	-2.545008	2.971673
H	-6.163996	-3.694357	1.838083
H	-4.454624	-3.961944	2.357623
C	-5.404371	-1.106693	0.751185
H	-5.075274	-0.661342	-0.210465
H	-6.495385	-1.299877	0.702204
H	-5.216471	-0.390070	1.580089
C	-1.798818	-4.300445	-0.163721
H	-1.564555	-5.261069	0.337743
H	-1.598019	-4.410901	-1.250310
H	-1.137177	-3.512101	0.239619
C	-4.174698	-5.024339	-0.106164
H	-5.189491	-4.598574	-0.195062
H	-3.935269	-5.550791	-1.053296
H	-4.157693	-5.766002	0.719651
H	-2.956230	-0.719823	0.211698
H	-3.665971	1.569003	0.954372

IM17

N	-1.955993	-0.653780	-0.476376
O	4.848876	1.497416	1.169614
H	5.682887	1.959366	1.385876
N	-1.633547	-5.421903	0.418282
O	0.793027	-3.155861	-1.595551
N	-3.493789	-2.305405	-0.130107

H	-3.655200	-3.307943	0.044566	H	0.469048	-0.139155	1.696784
H	-4.438823	-1.040942	-0.274778	C	2.311405	0.453990	0.630209
N	-2.697579	2.698492	-0.815888	H	3.277756	-0.083192	0.563762
C	2.524328	-4.487252	2.217482	C	2.497958	1.639935	1.545370
H	2.850104	-5.506605	2.478117	C	3.802630	2.160989	1.750816
C	1.650650	-4.290945	1.132542	C	3.997740	3.325374	2.521178
H	1.296340	-5.143012	0.534311	H	5.019660	3.713785	2.663591
C	1.249240	-2.982472	0.816495	C	2.899215	3.982928	3.095889
C	0.323763	-2.537798	-0.312359	H	3.063858	4.894412	3.691396
C	0.523297	-0.998604	-0.352570	C	1.601081	3.475445	2.913554
C	1.552576	-0.537168	-1.444786	H	0.734347	3.982544	3.363388
H	1.011314	-0.393473	-2.407290	C	1.416608	2.313927	2.146277
C	1.960202	0.835184	-0.867613	H	0.396877	1.926963	1.997044
C	3.064442	1.696103	-1.540790	C	1.210861	5.544984	-1.031175
H	4.059909	1.552008	-1.079829	H	0.697002	6.507794	-0.888426
H	3.147527	1.441571	-2.619789	C	0.498752	4.348244	-0.877950
C	2.569747	3.111583	-1.385227	H	-0.566657	4.365418	-0.608979
C	3.273021	4.313323	-1.535702	C	1.187545	3.125474	-1.048127
H	4.344972	4.308635	-1.786196	C	0.738692	1.754886	-0.882594
C	2.586520	5.528238	-1.353535	C	-0.539162	1.241651	-0.750280
H	3.129150	6.480543	-1.460074	C	-0.744169	-0.201393	-0.540007
C	4.335834	-3.725102	-2.403801	C	-2.201513	-2.025954	-0.235569
H	5.004667	-4.553301	-2.686230	C	-1.103063	-2.938174	-0.105743
C	2.968496	-3.971613	-2.197552	C	-1.382913	-4.287442	0.178168
H	2.541250	-4.981182	-2.293281	C	1.730224	-1.886238	1.555122
C	2.120031	-2.911145	-1.837122	C	2.605482	-2.079042	2.635946
C	2.613260	-1.589982	-1.689582	H	2.988381	-1.217517	3.205888
C	1.216057	-0.578397	1.003765	C	2.997207	-3.389986	2.966555

H	3.685188	-3.559257	3.809803
C	-1.714858	2.052103	-0.795321
C	3.991918	-1.371558	-1.868960
H	4.413982	-0.366880	-1.742401
C	4.850851	-2.429562	-2.220421
H	5.925754	-2.235137	-2.356442
C	-6.096254	0.359470	-0.045589
N	-4.875070	-0.030813	-0.399617
H	-4.190535	0.680706	-0.679030
N	-6.609057	1.546743	-0.492184
N	-6.873113	-0.431746	0.750753
C	-8.324783	-0.499319	0.593099
H	-8.624070	-1.555389	0.421637
H	-8.858005	-0.130512	1.495100
H	-8.639667	0.096134	-0.282019
C	-6.276607	-1.460784	1.596447
H	-5.206869	-1.242886	1.763830
H	-6.804369	-1.482854	2.572109
H	-6.355885	-2.468341	1.131724
C	-6.041559	2.185212	-1.678298
H	-6.822194	2.812609	-2.152393
H	-5.163894	2.823730	-1.434272
H	-5.723530	1.411486	-2.402792
C	-7.433885	2.399213	0.364260
H	-7.553123	1.937252	1.360145
H	-6.932614	3.381751	0.499329
H	-8.437887	2.577375	-0.075729

3a

N	-1.200572	3.233887	-0.011968
O	2.299844	-3.133017	0.773671
H	2.927258	-3.875200	0.881140
N	-5.818118	1.926591	0.698105
O	-3.159130	0.186600	-1.434910
N	-3.133303	4.317952	0.560481
H	-4.126403	4.398591	0.778642
H	-2.543275	5.149676	0.586393
N	1.999697	4.638279	-0.409068
C	-3.993823	-2.143831	2.187579
H	-4.922163	-2.682705	2.433093
C	-4.010523	-1.139657	1.203251
H	-4.938543	-0.894800	0.666192
C	-2.813246	-0.468482	0.906827
C	-2.596624	0.621348	-0.140760
C	-1.048194	0.744852	-0.217811
C	-0.439169	-0.052581	-1.423947
H	-0.440533	0.603387	-2.323354
C	1.005559	-0.239191	-0.916906
C	2.037482	-1.076339	-1.719791
H	2.105903	-2.123358	-1.368930
H	1.765086	-1.093252	-2.797428
C	3.333341	-0.332254	-1.531564
C	4.641712	-0.767704	-1.774166
H	4.835153	-1.787749	-2.139687
C	5.706111	0.120576	-1.534017
H	6.741061	-0.211019	-1.711598
C	-3.064375	-3.294974	-2.619469

H	-3.757806	-4.081022	-2.956807
C	-3.563675	-2.033585	-2.255098
H	-4.639860	-1.806376	-2.279526
C	-2.671052	-1.038740	-1.827437
C	-1.275265	-1.269311	-1.763665
C	-0.452515	0.009280	1.050803
H	-0.142561	0.751289	1.814922
C	0.757557	-0.814036	0.542092
H	0.417317	-1.855124	0.377289
C	1.991689	-0.855635	1.410002
C	2.767092	-2.043990	1.457578
C	3.976944	-2.082528	2.180104
H	4.564276	-3.015097	2.200277
C	4.427360	-0.942098	2.862269
H	5.376530	-0.983156	3.418872
C	3.667310	0.240192	2.836195
H	4.011393	1.138052	3.370966
C	2.462703	0.268914	2.115746
H	1.877595	1.200949	2.089599
C	5.468479	1.432083	-1.063548
H	6.318721	2.105829	-0.878224
C	4.163967	1.877701	-0.818375
H	3.985002	2.891946	-0.436427
C	3.090701	0.984295	-1.046165
C	1.667713	1.133467	-0.811591
C	0.921222	2.268625	-0.525453
C	-0.512665	2.154097	-0.259137
C	-2.561370	3.129970	0.252829
C	-3.269953	1.919712	0.211845
C	-4.657075	1.912743	0.476238
C	-1.616414	-0.803027	1.562988
C	-1.596091	-1.809772	2.541892
H	-0.655622	-2.079138	3.047815
C	-2.795768	-2.475345	2.853682
H	-2.797691	-3.267717	3.618453
C	1.504601	3.573382	-0.464106
C	-0.800435	-2.550149	-2.102390
H	0.271526	-2.776093	-2.047490
C	-1.686501	-3.558226	-2.524958
H	-1.292867	-4.552252	-2.786522

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N	-0.861676	-4.151041	-0.419245
O	-1.922806	2.747738	1.183126
H	-2.430791	3.567327	1.345572
N	3.761240	-5.314292	0.478615
O	2.366955	-2.319441	-1.500644
N	0.270753	-6.075184	0.085978
H	1.086909	-6.642698	0.314324
H	-0.644748	-6.518131	0.007832
N	-4.302533	-3.797122	-1.094016
C	4.071633	-1.039237	2.351655
H	5.131623	-1.045179	2.649895
C	3.652673	-1.808161	1.251128
H	4.372984	-2.409762	0.677599
C	2.294844	-1.784289	0.895361
C	1.621624	-2.538811	-0.248798

C	0.209758	-1.896133	-0.318513	C	-4.052938	-0.507060	2.709185
C	0.123391	-0.760046	-1.386197	H	-4.603537	-1.376859	3.097575
H	-0.160836	-1.221132	-2.359685	C	-2.818857	-0.690778	2.065901
C	-1.090676	0.022736	-0.848971	H	-2.440325	-1.717301	1.956430
C	-1.517460	1.350242	-1.525238	C	-5.768821	0.771182	-1.248974
H	-1.095314	2.241768	-1.027176	H	-6.848790	0.581293	-1.155120
H	-1.185034	1.358683	-2.586022	C	-4.863275	-0.287857	-1.105408
C	-3.022115	1.313879	-1.465868	H	-5.222503	-1.304034	-0.892972
C	-3.935485	2.363519	-1.613520	C	-3.480135	-0.010489	-1.206464
H	-3.585240	3.389924	-1.800881	C	-2.325501	-0.863625	-0.996897
C	-5.309997	2.084406	-1.498269	C	-2.224415	-2.241232	-0.866169
H	-6.040942	2.901975	-1.598269	C	-0.932165	-2.854960	-0.550184
C	3.996437	0.811854	-2.523256	C	0.360973	-4.738966	-0.114450
H	4.978452	1.164799	-2.874617	C	1.566466	-4.025549	-0.022921
C	3.811351	-0.545356	-2.212260	C	2.766903	-4.716882	0.250725
H	4.627810	-1.278054	-2.296521	C	1.376997	-0.984107	1.596547
C	2.550254	-0.984594	-1.782648	C	1.795465	-0.204708	2.685544
C	1.458656	-0.091065	-1.638136	H	1.084833	0.446985	3.213959
C	-0.021044	-1.138470	1.046470	C	3.148622	-0.248007	3.065426
H	-0.590826	-1.788745	1.739206	H	3.494639	0.357351	3.917652
C	-0.805135	0.159251	0.717940	C	-3.357644	-3.104634	-0.995345
H	-0.123027	1.028263	0.832316	C	1.680791	1.270884	-1.910684
C	-2.069957	0.382305	1.536907	H	0.871624	1.999092	-1.782782
C	-2.615816	1.682727	1.695829	C	2.936250	1.718047	-2.359989
C	-3.851351	1.880992	2.343671	H	3.085503	2.783789	-2.578817
H	-4.245415	2.905897	2.441743	C	1.819851	3.735703	0.554520
C	-4.574061	0.789650	2.845154	N	1.147964	2.959081	1.358060
H	-5.541992	0.958161	3.341895	H	0.135444	3.134626	1.280178

N	1.306094	4.866043	-0.115968	C	-3.022544	-3.336486	2.187631
N	3.171350	3.495385	0.327395	H	-3.808592	-4.055296	2.465093
C	4.133522	4.582624	0.212714	C	-3.267792	-2.396884	1.173354
H	4.787947	4.626551	1.115226	H	-4.237443	-2.372776	0.655993
H	4.792763	4.452786	-0.674651	C	-2.237596	-1.501851	0.823800
H	3.605803	5.549492	0.127799	C	-2.169832	-0.451937	-0.192303
C	3.722635	2.233844	0.788250	C	-0.848506	0.058147	-0.222576
H	2.984721	1.425522	0.645082	C	0.557559	-1.593996	-1.585871
H	4.636227	1.999671	0.204261	H	0.121149	-1.068312	-2.451181
H	3.990983	2.259626	1.870939	C	1.704997	-0.931244	-0.861956
C	0.006137	5.363171	0.299232	C	3.075475	-1.618326	-1.189068
H	-0.102426	6.418795	-0.024625	H	3.379795	-2.334185	-0.402594
H	-0.843659	4.787621	-0.144973	H	3.000142	-2.183085	-2.143172
H	-0.082617	5.325303	1.402373	C	4.040350	-0.475111	-1.336707
C	1.566527	5.050400	-1.540977	C	5.439857	-0.521570	-1.379488
H	2.561647	4.657689	-1.810202	H	5.969669	-1.482610	-1.291181
H	0.804756	4.528587	-2.171141	C	6.156159	0.680387	-1.523099
H	1.538343	6.129465	-1.801128	H	7.256901	0.660306	-1.549393
IM19				C	-1.437976	-5.247180	-0.826523
N	-1.463471	1.597884	-1.977135	H	-1.972225	-6.183834	-0.596813
O	3.705177	-2.120143	1.831263	C	-1.958971	-4.374870	-1.751524
H	4.544925	-2.427779	2.226164	H	-2.902737	-4.584776	-2.278450
N	-5.609631	-0.739204	-1.131663	C	-1.289458	-3.116888	-2.082458
O	-1.771207	-2.307258	-2.901954	C	-0.008945	-2.828008	-1.332617
N	-3.651045	1.846938	-2.666951	C	-0.047482	-0.477952	0.946852
H	-4.629277	1.563408	-2.705770	H	-0.026673	0.357511	1.681233
H	-3.318952	2.568073	-3.307087	C	1.419767	-0.927379	0.703931
N	1.228998	3.903673	-2.165468	H	1.517115	-1.973501	1.040886

C	2.447270	-0.120674	1.474624
C	3.610384	-0.760611	1.975155
C	4.624429	-0.013202	2.607189
H	5.524395	-0.530532	2.978662
C	4.483449	1.374639	2.762836
H	5.285239	1.948734	3.253295
C	3.317878	2.016721	2.310088
H	3.188710	3.101102	2.448746
C	2.311801	1.268402	1.676314
H	1.390296	1.780526	1.344085
C	5.478032	1.914390	-1.626151
H	6.054748	2.846336	-1.729284
C	4.077996	1.968450	-1.585420
H	3.563168	2.936250	-1.648208
C	3.351191	0.764225	-1.436866
C	1.916999	0.532310	-1.289168
C	0.877130	1.432958	-1.417436
C	-0.531908	1.046267	-1.177675
C	-2.747017	1.189054	-1.898995
C	-3.149868	0.091331	-1.050121
C	-4.487891	-0.379088	-1.082605
C	-0.978768	-1.545257	1.492773
C	-0.751245	-2.470557	2.515501
H	0.218380	-2.507539	3.036184
C	-1.778109	-3.373513	2.851853
H	-1.607486	-4.120654	3.642430
C	1.085354	2.780641	-1.843357
C	0.485852	-3.806583	-0.387005
H	1.445104	-3.630250	0.119686
C	-0.194883	-4.975117	-0.146476
H	0.204565	-5.713991	0.564033
C	-1.846491	3.018283	1.168733
N	-0.542496	2.977823	1.072235
H	-0.199726	3.794788	0.547546
N	-2.686327	3.874992	0.443936
N	-2.510237	2.138633	2.016592
C	-3.871405	1.686219	1.788817
H	-3.912904	0.577055	1.859042
H	-4.591323	2.095722	2.534817
H	-4.201155	1.984689	0.777755
C	-1.838791	1.573098	3.172389
H	-0.822676	2.000603	3.242678
H	-2.404346	1.803724	4.104094
H	-1.757743	0.465462	3.098808
C	-2.138219	4.555593	-0.719293
H	-2.976878	4.923909	-1.344491
H	-1.506081	5.437758	-0.448786
H	-1.540422	3.852065	-1.328420
C	-3.712755	4.644868	1.147941
H	-3.910307	4.211075	2.143612
H	-3.378031	5.697945	1.299844
H	-4.664472	4.665919	0.574693

IM20

N	-0.312496	-1.371027	-3.316922
O	2.300402	1.621794	2.957823
H	2.715163	2.217366	3.612989

N	-5.019453	-2.101558	-2.510699	C	0.000312	-4.074379	1.341701
O	-0.229968	-4.517769	0.196603	C	0.894922	-2.878812	1.579623
N	-2.124871	-1.966025	-4.639251	C	-0.222589	-0.187653	0.315106
H	-3.015334	-2.466039	-4.679986	H	-1.092568	1.591590	-0.473111
H	-1.423328	-2.278502	-5.314045	C	1.126080	0.144630	0.878803
N	2.706346	-0.538990	-4.603896	H	1.069181	-0.018512	1.971710
C	-4.013743	-0.675975	2.163901	C	1.618538	1.561615	0.673871
H	-5.016882	-0.807266	2.598177	C	2.206745	2.268641	1.754819
C	-3.799825	-0.956049	0.807682	C	2.655336	3.593934	1.585815
H	-4.629167	-1.312045	0.177660	H	3.100981	4.127577	2.441311
C	-2.503218	-0.796856	0.268071	C	2.533045	4.225911	0.337777
C	-1.944218	-1.042295	-1.040000	H	2.889584	5.260821	0.217976
C	-0.530839	-0.697358	-0.991674	C	1.955375	3.540830	-0.745343
C	1.378013	-2.260676	0.446192	H	1.851316	4.030447	-1.725193
H	1.129563	-2.784197	-0.492798	C	1.504126	2.223266	-0.564776
C	2.144748	-0.964953	0.343303	H	1.044300	1.688590	-1.407785
C	3.482085	-0.931935	1.153494	C	5.978267	0.989029	-1.757108
H	3.370397	-0.404853	2.121760	H	6.581769	1.479533	-2.536754
H	3.819774	-1.966557	1.378074	C	4.706652	0.495576	-2.080161
C	4.457318	-0.242772	0.244932	H	4.322633	0.607547	-3.102083
C	5.724472	0.262067	0.562596	C	3.928634	-0.128157	-1.072199
H	6.114991	0.178436	1.588986	C	2.557923	-0.631115	-1.094277
C	6.488996	0.877246	-0.445821	C	1.708461	-0.742605	-2.198399
H	7.487842	1.277055	-0.210916	C	0.253882	-0.948443	-2.159002
C	-0.339371	-4.182327	3.797806	C	-1.627295	-1.621408	-3.399329
H	-0.805332	-4.661391	4.674952	C	-2.501065	-1.503974	-2.257344
C	-0.598457	-4.669749	2.537851	C	-3.877574	-1.834261	-2.381945
H	-1.263184	-5.533453	2.378771	C	-1.418467	-0.297282	1.100750

C	-1.658798	-0.038049	2.474452	H	-5.472510	4.115678	-1.252412
H	-0.842966	0.310425	3.127677	H	-5.920308	3.324688	0.301096
C	-2.942035	-0.240499	2.992107	**4a**			
H	-3.131506	-0.052021	4.061014	O	2.556851	1.899266	-1.866824
C	2.246564	-0.633848	-3.524136	H	3.443785	2.307916	-1.823374
C	1.127178	-2.427684	2.937803	N	0.992631	0.555309	2.629903
H	1.801941	-1.577986	3.114127	O	-3.143121	-2.305950	-1.170072
C	0.537578	-3.056564	4.008954	H	-4.033204	-2.671383	-0.997582
H	0.729614	-2.706476	5.034470	N	2.821991	0.649136	4.029911
C	-2.855599	2.611495	-0.141029	H	3.801423	0.483378	4.257520
N	-1.836321	2.172992	-0.907389	H	2.183422	0.946950	4.767206
H	-1.997236	2.013321	-1.902280	N	5.695147	-0.500430	2.218118
N	-4.120626	2.632570	-0.632002	C	4.551176	-0.338298	1.981854
N	-2.591100	3.059140	1.109213	C	3.168127	-0.125962	1.741381
C	-3.576572	2.983512	2.187590	C	2.312775	0.362924	2.804299
H	-3.084447	2.546491	3.078083	C	0.415177	0.319922	1.426982
H	-3.976772	3.983679	2.454835	N	-2.105937	1.107779	3.683938
H	-4.402979	2.311447	1.898332	C	-1.047936	0.526939	1.368146
C	-1.241073	3.461987	1.502892	C	-1.854857	0.459478	0.236607
H	-0.636454	3.703887	0.610487	C	-3.314442	0.619816	0.179210
H	-1.308373	4.358256	2.151193	C	-4.278362	0.757573	1.209124
H	-0.732772	2.652624	2.067775	H	-3.984346	0.771758	2.264948
C	-4.533595	1.705719	-1.685182	C	-5.633713	0.869000	0.869572
H	-5.559579	1.347418	-1.468142	H	-6.383987	0.970660	1.668729
H	-4.536179	2.191805	-2.685094	C	-6.046136	0.850275	-0.479537
H	-3.861379	0.829800	-1.701062	H	-7.115696	0.940673	-0.725866
C	-5.069977	3.698158	-0.306283	C	2.556443	-0.374538	0.492152
H	-4.559258	4.511284	0.238128	C	3.085735	-0.894779	-0.776477

C	4.373188	-1.325163	-1.143555
H	5.204485	-1.308228	-0.423816
C	4.577947	-1.781068	-2.459044
H	5.578400	-2.123345	-2.765766
C	3.517060	-1.809273	-3.387444
H	3.699726	-2.172702	-4.410721
C	2.225546	-1.378720	-3.020498
H	1.402427	-1.402205	-3.752254
C	2.015608	-0.920163	-1.717591
C	0.748178	-0.408997	-1.082077
C	-0.585160	-1.199558	-1.256655
H	-0.649822	-1.530641	-2.315917
C	-1.366134	0.182668	-1.187179
C	-0.029172	0.850646	-1.638255
H	0.003048	0.786941	-2.747962
C	0.312308	2.244278	-1.177414
C	-0.659857	3.116356	-0.649032
H	-1.703937	2.778913	-0.579410
C	-0.334077	4.407773	-0.199565
H	-1.118208	5.059859	0.213597
C	0.997822	4.848388	-0.272771
H	1.275961	5.850486	0.089348
C	1.983601	4.011855	-0.820201
H	3.029010	4.352984	-0.899524
C	1.643238	2.726291	-1.286313
C	-2.579879	0.418079	-2.106914
H	-2.424023	1.334018	-2.718619
H	-2.731580	-0.421985	-2.812698
C	-3.744141	0.590936	-1.178244
C	-5.099348	0.711346	-1.509637
H	-5.417714	0.688473	-2.563481
C	-1.620431	0.844094	2.645194
C	-0.922709	-2.338277	-0.330095
C	-2.246837	-2.848827	-0.296839
C	-2.598900	-3.882061	0.593662
H	-3.639256	-4.246482	0.611496
C	-1.628471	-4.446033	1.437445
H	-1.914569	-5.252420	2.130690
C	-0.301223	-3.989221	1.382955
H	0.471815	-4.437504	2.025157
C	0.036128	-2.944652	0.504383
H	1.075182	-2.591667	0.467448
C	1.173560	-0.136969	0.336195

TS6

N	2.994453	3.532888	1.801096
N	-0.447156	3.908923	-0.781789
C	1.444733	-0.972421	-1.688829
H	1.222009	-1.410850	-2.677080
C	2.789947	-0.866122	-1.161902
C	3.911364	-1.713644	-1.324867
H	3.859769	-2.571262	-2.014180
C	5.078844	-1.452971	-0.599513
H	5.955399	-2.108602	-0.726764
C	5.154234	-0.360012	0.305368
H	6.080470	-0.186008	0.874218
C	-0.658010	0.344680	-1.411832

C	0.707511	0.216078	-1.197371
C	1.625100	1.004083	-0.346895
C	2.871371	0.258531	-0.256555
C	4.062447	0.495690	0.477593
H	4.133530	1.336451	1.180737
C	1.411918	2.329161	0.120350
C	2.292905	2.976439	1.031911
C	0.375737	3.170031	-0.370813
C	-1.703899	1.000205	-0.655162
C	-2.965542	1.230491	-1.287824
C	-1.615240	1.256423	0.739295
C	-4.073536	1.682918	-0.544212
C	-2.714910	1.692970	1.480322
H	-0.659877	1.068435	1.245422
C	-3.950832	1.908667	0.833797
H	-5.036061	1.846720	-1.055441
H	-2.617081	1.859109	2.563474
H	-4.825433	2.253283	1.406748
O	-3.046286	0.963341	-2.617972
H	-3.969534	1.086659	-2.917779
H	-1.045906	-0.279080	-2.238164
C	-0.755356	-2.374159	0.650487
N	0.468542	-2.636276	0.191039
N	-0.982526	-1.833242	1.896086
N	-1.834426	-2.644015	-0.152381
C	-3.096482	-1.915023	-0.086440
H	-3.336120	-1.508688	-1.091570
H	-3.935979	-2.573230	0.226438
H	-3.017701	-1.065420	0.612493
C	-1.680841	-3.522558	-1.305858
H	-0.794821	-4.166366	-1.163910
H	-2.588713	-4.152109	-1.412265
H	-1.548504	-2.943823	-2.247581
C	0.104369	-1.153286	2.589555
H	-0.322631	-0.382336	3.262037
H	0.715429	-1.847341	3.212082
H	0.769752	-0.649689	1.861328
C	-2.109163	-2.235809	2.736370
H	-2.699029	-3.023025	2.235159
H	-1.728320	-2.653826	3.693290
H	-2.774666	-1.377309	2.971315
H	0.919540	-1.938345	-0.825248
H	1.182537	-2.620201	0.928805

TS7

N	-1.310976	2.766620	-1.149300
N	1.992529	5.276558	0.036455
N	3.138164	-5.127242	-0.380967
N	1.547327	-2.322407	-3.360899
C	5.078336	1.889916	1.031341
H	5.939004	2.386939	0.557051
C	3.784549	2.384674	0.801846
H	3.639365	3.252042	0.144727
C	2.685974	1.738873	1.411619
C	1.236389	1.975377	1.281848
C	0.555824	1.001259	2.068458
C	-0.805325	0.708378	2.324952

C	-1.043904	-1.230679	0.832697	C	1.667615	-2.601280	-2.221636
H	-2.002168	-0.733737	0.680806	C	1.360112	0.368631	-1.716123
C	-0.813163	-2.335501	1.728642	C	1.141246	1.251448	-2.825079
C	-1.533656	-2.781893	2.860256	C	2.705917	0.078609	-1.358106
H	-2.462220	-2.270742	3.151676	C	2.229394	1.755652	-3.559664
C	-1.034660	-3.862146	3.601845	C	3.780256	0.590773	-2.085273
H	-1.586810	-4.208934	4.489809	H	2.895445	-0.539789	-0.469493
C	0.168650	-4.515507	3.236401	C	3.543372	1.422741	-3.199818
H	0.541020	-5.353905	3.844241	H	2.017309	2.416034	-4.413778
C	0.731870	3.030624	0.411709	H	4.809269	0.360574	-1.772628
C	-0.409550	2.899581	-0.381753	H	4.387854	1.828122	-3.778450
C	1.438547	4.245289	0.206617	O	-0.128939	1.568778	-3.244888
C	5.288578	0.754271	1.840745	H	-0.647279	2.020679	-2.482955
H	6.310745	0.375628	1.997966	H	-0.676123	0.511063	-1.048197
C	4.196172	0.094665	2.439103	C	-1.956802	1.614296	2.201318
H	4.353714	-0.804147	3.056198	C	-3.295331	1.118343	2.200769
C	2.906430	0.593682	2.225746	C	-1.799854	3.024342	2.233864
C	1.585222	0.061217	2.686399	C	-4.396406	1.993728	2.138301
H	1.495996	0.041262	3.795670	C	-2.891373	3.899881	2.192751
H	1.427926	-0.990413	2.359164	H	-0.784131	3.430461	2.322459
C	0.221299	-0.119009	-0.977794	C	-4.197792	3.382074	2.124703
C	0.050054	-1.192562	-0.113101	H	-5.414999	1.572874	2.108343
C	0.881661	-2.396240	0.112305	H	-2.722874	4.987003	2.221588
C	0.411301	-3.011383	1.351304	H	-5.067130	4.055936	2.077330
C	0.891141	-4.101352	2.106773	O	-3.476850	-0.236526	2.246186
H	1.823601	-4.613659	1.832932	H	-4.434750	-0.433863	2.272712
C	1.709391	-3.002611	-0.854267	H	-0.966493	-0.117644	3.034087
C	2.480417	-4.171558	-0.587678	C	-2.552581	-0.937131	-2.641446

N	-1.526205	-0.880131	-3.513197	C	2.852154	0.381580	2.191860
N	-3.286659	0.189152	-2.432079	H	3.538484	0.947963	1.549274
N	-2.868657	-2.091578	-2.004614	C	1.452081	0.454249	2.012400
C	-4.235950	-2.405059	-1.586325	C	0.647819	1.104203	0.974795
H	-4.496482	-3.415906	-1.961433	C	-0.714307	0.620029	1.081606
H	-4.334495	-2.408186	-0.480611	C	-1.979969	1.361106	0.589020
H	-4.946405	-1.679988	-2.018945	C	-2.562995	0.626701	-0.657075
C	-1.913695	-3.189000	-1.866902	H	-2.163432	1.109293	-1.579519
H	-0.888433	-2.833018	-2.057731	C	-4.067042	0.496274	-0.733108
H	-1.952913	-3.577859	-0.829310	C	-5.058511	1.482720	-0.719529
H	-2.152607	-4.016104	-2.569066	H	-4.791665	2.547696	-0.641270
C	-3.414301	1.225580	-3.458814	C	-6.413065	1.092944	-0.800369
H	-3.047240	0.847982	-4.429112	H	-7.204022	1.859130	-0.780075
H	-4.486573	1.493319	-3.561460	C	-6.756159	-0.266937	-0.910654
H	-2.853206	2.138785	-3.175075	H	-7.815978	-0.558794	-0.981045
C	-3.868190	0.538203	-1.134768	C	1.157263	1.945129	-0.055144
H	-3.615254	-0.217168	-0.373342	C	0.512790	2.101738	-1.312823
H	-3.442942	1.510552	-0.810540	C	2.422708	2.569744	0.026310
H	-4.972696	0.627778	-1.196640	C	2.496742	-1.213143	4.015390
H	-1.039635	-1.729599	-3.805948	H	2.921101	-1.873791	4.787301
H	-1.002840	0.017656	-3.592785	C	1.102409	-1.139694	3.848554
TS8				H	0.429270	-1.740824	4.478047
N	0.063163	2.174390	-2.402313	C	0.585955	-0.306243	2.849763
N	3.470820	3.117814	0.058038	C	-0.834750	-0.062218	2.439637
N	-5.134130	-4.722553	-0.892306	H	-1.314122	0.659755	3.136274
N	-0.911213	-4.234182	-1.913820	H	-1.463745	-0.974879	2.429247
C	3.361894	-0.456277	3.194252	C	-0.687793	-0.942752	-0.278435
H	4.451009	-0.530132	3.338374	C	-2.091901	-0.811952	-0.605658

C	-3.162258	-1.696476	-0.787309	H	-2.444354	5.491930	-1.717157
C	-4.409843	-0.883948	-0.824249	H	-1.513399	6.805168	0.229400
C	-5.761707	-1.265026	-0.931104	O	-1.015491	2.966056	2.687001
H	-6.046590	-2.322354	-1.018223	H	-0.660477	3.598226	3.343106
C	-3.095122	-3.116379	-1.050888	H	-2.718160	1.189902	1.404570
C	-4.215903	-3.978134	-0.967217	C	4.728054	0.252877	-1.604106
C	-1.894641	-3.723888	-1.498650	N	5.317819	1.101588	-0.745699
C	-0.053538	-2.078305	0.397549	N	4.899566	-1.100331	-1.448388
C	1.358974	-2.237846	0.295762	N	3.962473	0.743225	-2.605925
C	-0.754361	-2.957308	1.258696	C	2.869334	0.000090	-3.241119
C	2.028622	-3.229499	1.033855	H	1.972148	0.652151	-3.258855
C	-0.092230	-3.945422	1.996517	H	3.126275	-0.277628	-4.284269
H	-1.846653	-2.854488	1.334599	H	2.617066	-0.901412	-2.660751
C	1.305485	-4.074880	1.887408	C	4.135977	2.115689	-3.090742
H	3.121938	-3.325514	0.948166	H	5.115921	2.512749	-2.771954
H	-0.661998	-4.612437	2.660619	H	4.096924	2.102376	-4.198327
H	1.840301	-4.840972	2.469809	H	3.332116	2.782029	-2.716610
O	2.017489	-1.384029	-0.536674	C	5.489464	-1.610590	-0.201826
H	2.982464	-1.559392	-0.528904	H	5.275972	-2.694011	-0.133617
H	-0.009486	-0.412913	-0.966963	H	6.594765	-1.485825	-0.178765
C	-1.848950	2.875538	0.454906	H	5.043562	-1.107583	0.677517
C	-1.356598	3.638428	1.548686	C	5.102568	-1.971063	-2.621397
C	-2.240163	3.582314	-0.698295	H	4.991157	-1.394631	-3.554391
C	-1.228170	5.038694	1.457586	H	6.133111	-2.381145	-2.593040
C	-2.131950	4.980111	-0.794409	H	4.381773	-2.812382	-2.620470
H	-2.621507	3.024533	-1.564208	H	4.856423	2.004242	-0.503114
C	-1.614941	5.710245	0.287844	H	6.086899	0.785386	-0.154033
H	-0.829118	5.598153	2.319779				

TS9

N	4.318371	1.081189	-1.520899
O	-2.718273	0.450887	1.113826
H	-3.553957	0.603487	1.597024
N	4.911139	-4.138887	-1.187269
O	0.546099	-2.448196	0.929319
N	5.196649	-0.676614	1.464216
N	3.258444	4.605899	-2.156411
C	0.744226	-3.630943	-3.433545
H	0.790541	-4.598313	-3.956979
C	1.789431	-3.267628	-2.566697
H	2.643217	-3.943503	-2.422934
C	1.717580	-2.030340	-1.886114
C	2.606777	-1.409405	-0.884057
C	2.058325	-0.133228	-0.504140
C	1.887494	0.371621	0.949123
H	2.773472	0.961099	1.257832
C	0.724939	1.379556	0.714102
C	-0.009519	2.001615	1.921527
H	-0.884375	1.405576	2.241331
H	0.678460	2.072693	2.791569
C	-0.361377	3.384727	1.432509
C	-1.310710	4.282766	1.934787
H	-1.942092	4.006751	2.793593
C	-1.452297	5.540429	1.318117
H	-2.202674	6.251931	1.696961
C	1.253015	-2.102148	4.502866
H	1.085826	-2.690402	5.418354
C	0.822427	-2.598679	3.267095
H	0.335620	-3.582069	3.185871
C	1.019970	-1.860765	2.081022
C	1.667105	-0.597546	2.107545
C	0.752151	0.074617	-1.289680
H	0.889521	0.892337	-2.030843
C	-0.254258	0.560262	-0.236158
H	-0.593821	-0.297061	0.375196
C	-1.468580	1.306946	-0.732722
C	-2.682861	1.249865	-0.000606
C	-3.807250	1.996287	-0.403077
H	-4.733391	1.944818	0.192307
C	-3.740072	2.810522	-1.544095
H	-4.622723	3.394763	-1.846779
C	-2.551749	2.873085	-2.291289
H	-2.488701	3.506643	-3.188548
C	-1.437261	2.124742	-1.880340
H	-0.506359	2.192652	-2.463170
C	-0.646110	5.899223	0.216709
H	-0.775724	6.885338	-0.255160
C	0.307959	5.006554	-0.293955
H	0.916949	5.285753	-1.164642
C	0.443443	3.737393	0.310954
C	1.270611	2.586856	-0.048995
C	2.364706	2.508428	-0.891801
C	3.191075	1.282064	-1.109393
C	4.580170	-1.199544	0.605122
C	3.846955	-1.896073	-0.402854

C	4.421691	-3.123886	-0.835831
C	0.583950	-1.182955	-2.088048
C	-0.426362	-1.529026	-2.993465
H	-1.259561	-0.834307	-3.186006
C	-0.352959	-2.773751	-3.653782
H	-1.152814	-3.074230	-4.347884
C	2.857540	3.665692	-1.572010
C	2.133526	-0.152149	3.368793
H	2.682849	0.802391	3.406079
C	1.925403	-0.868062	4.554595
H	2.296249	-0.470107	5.511239
C	-3.281696	-2.399600	0.092321
N	-2.002799	-2.495522	-0.304235
H	-1.694746	-2.068801	-1.184667
N	-4.250662	-2.150271	-0.826603
N	-3.607714	-2.583043	1.396411
C	-4.848879	-3.253325	1.794414
H	-4.595375	-4.129119	2.427421
H	-5.510610	-2.579421	2.376847
H	-5.389450	-3.618344	0.903931
C	-2.601062	-2.425302	2.444292
H	-1.874462	-1.643948	2.159862
H	-3.105745	-2.098476	3.373981
H	-2.069945	-3.378765	2.654522
C	-4.005581	-2.359636	-2.251771
H	-4.953707	-2.665743	-2.735645
H	-3.647780	-1.431138	-2.749048
H	-3.263967	-3.166156	-2.399182
C	-5.443099	-1.366254	-0.500021
H	-5.406886	-1.032239	0.550122
H	-5.470743	-0.466508	-1.150030
H	-6.371835	-1.950693	-0.663106
H	1.096975	-2.145055	0.165690
H	-1.237566	-2.760643	0.334587

TS10

N	-1.561246	0.539944	-2.386080
O	4.196449	-1.229855	1.864806
H	4.851814	-1.685222	2.429385
N	-1.073859	5.754518	-2.051800
O	-2.205049	1.971187	1.503614
N	-3.456509	2.640300	-1.214708
N	-0.830144	-2.931349	-3.421258
C	3.343981	4.835585	-0.841717
H	3.662146	5.887031	-0.768055
C	1.979271	4.537114	-0.979475
H	1.243647	5.351599	-1.004510
C	1.577269	3.182655	-1.054690
C	0.245415	2.576155	-1.129952
C	0.381889	1.110724	-0.874053
C	0.038644	0.621836	0.599340
H	-1.015002	0.290624	0.618304
C	0.915442	-0.646537	0.664456
C	1.003189	-1.400911	2.011099
H	1.913025	-1.141725	2.584506
H	0.125777	-1.149694	2.647407

C	0.959075	-2.858027	1.612623	H	0.065979	-4.397405	-1.358119
C	1.256837	-3.989680	2.382248	C	0.532902	-3.000372	0.260795
H	1.595740	-3.883764	3.424751	C	0.348405	-1.676024	-0.318596
C	1.121586	-5.266111	1.802355	C	-0.169432	-1.272216	-1.531787
H	1.360024	-6.162607	2.395994	C	-0.530926	0.190465	-1.756778
C	0.267640	3.914071	3.443919	C	-2.281363	2.665592	-1.375785
H	0.297025	4.777185	4.126877	C	-0.952404	3.223086	-1.423094
C	-0.959246	3.495487	2.907431	C	-0.986404	4.615202	-1.766980
H	-1.893947	4.016759	3.170996	C	2.558580	2.153619	-0.982594
C	-1.008103	2.397090	2.028082	C	3.918382	2.457845	-0.860526
C	0.172741	1.698359	1.653994	H	4.666919	1.651908	-0.806895
C	1.909783	0.797093	-1.035228	C	4.309530	3.808954	-0.785362
H	2.082107	0.354409	-2.038987	H	5.374298	4.065696	-0.671728
C	2.315884	-0.196083	0.077750	C	-0.560374	-2.184821	-2.549229
H	2.835725	0.354437	0.881914	C	1.386228	2.135989	2.225006
C	3.223340	-1.344309	-0.310820	H	2.323328	1.628583	1.965452
C	4.122107	-1.868364	0.656239	C	1.444872	3.224662	3.110524
C	4.903059	-3.006512	0.371420	H	2.413548	3.536626	3.528950
H	5.585382	-3.399626	1.142946	C	-4.399203	-1.000678	-0.021213
C	4.807547	-3.632961	-0.881000	N	-3.307896	-0.276944	-0.308151
H	5.418513	-4.525115	-1.089432	H	-2.842317	-0.279366	-1.246894
C	3.943020	-3.114994	-1.860019	N	-4.544844	-2.243507	-0.551392
H	3.867096	-3.592273	-2.848637	N	-5.347083	-0.509212	0.820327
C	3.167748	-1.981041	-1.565889	C	-6.089740	-1.371704	1.739766
H	2.483160	-1.589985	-2.332794	H	-5.990842	-0.966410	2.768492
C	0.686008	-5.410019	0.467494	H	-7.169373	-1.416545	1.485314
H	0.589609	-6.416270	0.031175	H	-5.669312	-2.392585	1.727249
C	0.387625	-4.283031	-0.313309	C	-5.514328	0.930584	1.015657

H	-5.050391	1.490657	0.180582
H	-6.597315	1.167694	1.047283
H	-5.061376	1.257998	1.977242
C	-3.383544	-3.014772	-0.988936
H	-3.540157	-4.080842	-0.726923
H	-3.223077	-2.942833	-2.085014
H	-2.476767	-2.651378	-0.472388
C	-5.853559	-2.782268	-0.920710
H	-6.629455	-2.003659	-0.816604
H	-5.823015	-3.101621	-1.983430
H	-6.129543	-3.660677	-0.300325
H	-3.090223	0.552891	0.257166
H	-2.869112	2.684199	1.588085

TS11

N	-4.421295	-0.165020	-0.350684
O	2.154317	2.566797	1.009884
H	2.809008	3.289014	1.083993
N	-4.545031	-4.954033	0.362037
O	-1.896539	-2.745746	-2.198009
N	-6.041701	-1.795091	-0.443142
H	-6.383571	-2.753384	-0.366748
H	-6.692479	-1.053731	-0.706292
N	-4.796494	3.339587	-0.640052
C	0.110474	-4.478789	1.872046
H	0.344862	-5.544876	2.012649
C	-1.086413	-4.106865	1.245316
H	-1.792183	-4.868782	0.885571
C	-1.352424	-2.732492	1.070017
C	-2.475018	-2.049062	0.448413
C	-2.106525	-0.656945	0.276836
C	-0.863994	-0.394238	-1.272561
H	-1.660344	-0.372857	-2.036716
C	-0.396499	0.956053	-0.738956
C	0.732158	1.636130	-1.570071
H	1.739873	1.434047	-1.165048
H	0.714266	1.254542	-2.613654
C	0.377184	3.098503	-1.538918
C	1.179750	4.203802	-1.842577
H	2.222694	4.067473	-2.167066
C	0.634214	5.494421	-1.708699
H	1.257685	6.374339	-1.931593
C	1.553253	-3.846542	-1.931443
H	2.178710	-4.734516	-2.123080
C	0.207846	-3.871964	-2.249526
H	-0.267398	-4.765055	-2.685699
C	-0.648962	-2.724760	-1.999855
C	0.002029	-1.518621	-1.429881
C	-0.976659	-0.353295	1.283762
H	-1.452125	-0.048500	2.241039
C	-0.013841	0.754469	0.799881
H	1.030655	0.391049	0.849328
C	-0.104639	2.052483	1.592271
C	0.988858	2.954396	1.615865
C	0.878132	4.217817	2.228072
H	1.745839	4.897501	2.218431

C	-0.325899	4.607010	2.832194
H	-0.404615	5.601090	3.298689
C	-1.417219	3.723033	2.842579
H	-2.366330	4.009406	3.319626
C	-1.292602	2.465376	2.231181
H	-2.163805	1.794388	2.236097
C	-0.700350	5.678224	-1.284099
H	-1.101607	6.697430	-1.176559
C	-1.513981	4.577675	-0.983819
H	-2.544834	4.727017	-0.635615
C	-0.967785	3.279222	-1.107468
C	-1.531684	1.981460	-0.773338
C	-2.837895	1.628814	-0.470291
C	-3.173437	0.243402	-0.128833
C	-4.751758	-1.474176	-0.208121
C	-3.784996	-2.476264	0.171346
C	-4.182472	-3.835662	0.284803
C	-0.419641	-1.747141	1.515149
C	0.774309	-2.126258	2.137335
H	1.524680	-1.376935	2.436962
C	1.028571	-3.499336	2.311907
H	1.962974	-3.820210	2.797186
C	-3.917474	2.561299	-0.574173
C	1.384630	-1.565430	-1.080216
H	1.869629	-0.695973	-0.616692
C	2.153069	-2.690998	-1.340117
H	3.223378	-2.687665	-1.089181
C	4.534741	-0.531254	0.378014
N	3.749883	-0.156490	1.350999
H	3.302151	0.747541	1.134128
N	4.952714	0.262332	-0.703132
N	5.061777	-1.825603	0.366458
C	6.455827	-2.060202	0.000290
H	7.081710	-2.227685	0.908785
H	6.554182	-2.955391	-0.650823
H	6.860432	-1.183149	-0.534746
C	4.520436	-2.778691	1.319935
H	3.424427	-2.662923	1.371611
H	4.762131	-3.807838	0.983161
H	4.933512	-2.638565	2.347688
C	4.825182	1.703739	-0.600539
H	5.544917	2.184642	-1.294800
H	3.805608	2.077404	-0.862039
H	5.065589	2.031655	0.429925
C	4.905183	-0.251647	-2.069549
H	4.902076	-1.355505	-2.063543
H	3.982243	0.089060	-2.596891
H	5.782780	0.097609	-2.655438

TS12

N	-0.465649	-2.307511	-2.715850
O	2.527250	1.937898	2.614312
H	3.079151	2.538559	3.153152
N	-5.190121	-2.485214	-1.716295
O	-1.194346	-4.094941	1.020913
N	-2.318560	-3.239177	-3.739698

H	-3.273343	-3.594718	-3.683827	H	-0.538133	1.276828	-0.672713
H	-1.658604	-3.756970	-4.321501	C	1.079281	0.342546	0.816467
N	2.667174	-1.927502	-4.146603	H	0.914534	0.517838	1.894399
C	-4.077448	0.423146	2.144031	C	1.970397	1.472441	0.340139
H	-5.075093	0.461809	2.607880	C	2.701317	2.234860	1.287237
C	-3.878624	-0.334772	0.982771	C	3.561435	3.270215	0.869376
H	-4.712353	-0.891866	0.530647	H	4.119492	3.847835	1.624595
C	-2.583549	-0.387567	0.419531	C	3.701089	3.560219	-0.496853
C	-2.043781	-1.110481	-0.717462	H	4.378549	4.368895	-0.812827
C	-0.635915	-0.838697	-0.792832	C	2.971642	2.827310	-1.449207
C	0.804865	-2.166030	1.018684	H	3.064578	3.057178	-2.521365
H	0.674955	-2.965937	0.270788	C	2.115472	1.800221	-1.021834
C	1.806477	-1.078971	0.715008	H	1.531629	1.240204	-1.764064
C	3.062297	-1.118003	1.651283	C	6.114069	-0.569936	-1.318520
H	3.007516	-0.352443	2.449810	H	6.863160	-0.430999	-2.113232
H	3.142679	-2.108517	2.148507	C	4.785795	-0.853756	-1.663643
C	4.226479	-0.900762	0.727267	H	4.498328	-0.929487	-2.720340
C	5.555823	-0.613568	1.063930	C	3.828410	-1.018299	-0.633594
H	5.854612	-0.513344	2.118937	C	2.385516	-1.229338	-0.698229
C	6.499620	-0.448294	0.034263	C	1.594371	-1.469821	-1.812778
H	7.546990	-0.217531	0.284290	C	0.117860	-1.526656	-1.779888
C	-1.980253	-2.509310	4.172983	C	-1.797666	-2.501190	-2.714129
H	-2.731131	-2.559588	4.978795	C	-2.647100	-1.947639	-1.687228
C	-2.089918	-3.345321	3.088069	C	-4.037837	-2.235424	-1.686023
H	-2.909879	-4.075175	3.000785	C	-1.500716	0.361118	1.000102
C	-1.110804	-3.325110	1.999087	C	-1.722376	1.119148	2.164713
C	-0.019189	-2.283770	2.115221	H	-0.898695	1.682286	2.631396
C	-0.293669	0.236098	0.161532	C	-3.001839	1.132066	2.736543

H	-3.178137	1.706605	3.659571
C	2.182062	-1.730913	-3.092439
C	0.042302	-1.453463	3.301629
H	0.871856	-0.740898	3.414916
C	-0.893361	-1.566958	4.298896
H	-0.827716	-0.937195	5.198604
C	-2.052665	2.931567	-1.100808
N	-1.072642	2.164184	-1.563212
H	-1.298858	1.712667	-2.457286
N	-3.335817	2.912550	-1.605118
N	-1.795626	3.775415	-0.049193
C	-2.810580	4.124160	0.937747
H	-2.417702	3.914626	1.954182
H	-3.094415	5.198116	0.889315
H	-3.710618	3.501005	0.790442
C	-0.422346	4.120398	0.296068
H	0.235909	3.944464	-0.573052
H	-0.372888	5.187424	0.598120
H	-0.042950	3.501935	1.139533
C	-3.794742	1.753862	-2.359719
H	-4.890693	1.647609	-2.229809
H	-3.586232	1.841582	-3.451505
H	-3.312442	0.836322	-1.973554
C	-4.111720	4.137931	-1.788319
H	-3.529178	5.011704	-1.446804
H	-4.338439	4.279823	-2.867883
H	-5.073886	4.106939	-1.233349

SCAN1

N	-0.032394	1.049531	3.292763
O	2.666970	-1.094014	-3.189155
H	3.163348	-1.459397	-3.948116
N	-4.602192	1.813600	1.867476
O	-1.141305	3.282165	0.328379
N	-1.990453	1.418964	4.424047
N	2.973186	-0.211894	4.615352
C	-3.519635	0.528783	-2.176501
H	-4.440333	0.768480	-2.730526
C	-3.068838	1.394681	-1.163690
H	-3.621959	2.313338	-0.920877
C	-1.890483	1.069452	-0.472248
C	-1.248246	1.819557	0.688157
C	0.163649	1.188831	0.788193
C	1.261275	2.007827	0.023378
H	1.680511	2.772684	0.715639
C	2.307297	0.898061	-0.212843
C	3.594030	1.168988	-1.038713
H	3.490952	0.874650	-2.100362
H	3.852472	2.249853	-1.007274
C	4.655715	0.366469	-0.330643
C	5.926076	-0.007207	-0.786405
H	6.264605	0.273349	-1.795748
C	6.759772	-0.755554	0.065369
H	7.757695	-1.064285	-0.283352
C	-0.490515	4.466100	-3.093100
H	-0.941300	5.133743	-3.844188

C	-1.099268	4.318678	-1.835859	C	-3.410930	1.805951	1.912972
H	-2.033090	4.842137	-1.580674	C	-1.153618	-0.081501	-0.809743
C	-0.521366	3.465063	-0.880330	C	-1.601527	-0.946122	-1.821403
C	0.678735	2.759554	-1.154949	H	-1.012772	-1.835505	-2.096641
C	0.112984	-0.181461	0.004679	C	-2.796572	-0.637549	-2.498955
H	0.053232	-1.028007	0.719654	H	-3.157711	-1.299382	-3.300970
C	1.415893	-0.254446	-0.832060	C	2.551103	0.118479	3.568437
H	1.183519	0.087470	-1.859786	C	1.253582	2.896936	-2.432073
C	2.098166	-1.597702	-0.928666	H	2.170443	2.350743	-2.686610
C	2.754746	-1.960676	-2.133953	C	0.674147	3.739925	-3.398767
C	3.472769	-3.170550	-2.223729	H	1.141815	3.832256	-4.390987
H	3.977568	-3.429879	-3.168757	C	-4.352837	-1.969915	0.316261
C	3.546056	-4.031266	-1.117681	N	-3.866277	-1.000814	1.109312
H	4.114369	-4.970920	-1.198833	H	-2.865830	-0.779124	1.084474
C	2.893883	-3.693992	0.080930	N	-3.578596	-3.050486	0.033478
H	2.943671	-4.363923	0.952355	N	-5.622896	-1.892857	-0.154333
C	2.178687	-2.488168	0.160272	C	-6.463875	-3.080213	-0.322411
H	1.680504	-2.223014	1.105401	H	-5.963286	-3.967365	0.102556
C	6.332257	-1.120609	1.361200	H	-7.414138	-2.922733	0.228663
H	6.999097	-1.710660	2.008321	H	-6.705258	-3.268074	-1.389166
C	5.063259	-0.750200	1.826576	C	-6.313925	-0.607774	-0.253961
H	4.729418	-1.050212	2.829327	H	-5.583375	0.219014	-0.301053
C	4.217494	-0.009105	0.969862	H	-6.918315	-0.597055	-1.182905
C	2.846141	0.442068	1.144929	H	-6.992790	-0.443086	0.610808
C	2.058599	0.499620	2.280623	C	-2.410256	-3.368510	0.851471
C	0.655930	0.951146	2.199162	H	-2.292824	-4.469091	0.897057
C	-1.401487	1.414204	3.251061	H	-1.478642	-2.938726	0.420984
C	-2.020660	1.682020	1.957677	H	-2.547900	-2.984334	1.878519

C	-3.686899	-3.775831	-1.232621
H	-2.684364	-3.820914	-1.705282
H	-4.050351	-4.813712	-1.083172
H	-4.365458	-3.243375	-1.920562
H	-2.978931	1.700749	4.286592
H	-4.450396	-0.207448	1.425584

SCAN2

N	0.805517	4.137972	-0.439744
O	1.936189	-2.745840	1.194941
H	2.444816	-3.564058	1.362114
N	-3.841257	5.228455	0.428898
O	-2.367898	2.252421	-1.412199
N	-0.352618	6.034336	0.109849
H	-1.177150	6.588669	0.339496
H	0.553994	6.492798	0.021221
N	4.248274	3.844600	-1.147904
C	-4.018776	1.016657	2.439434
H	-5.071808	1.009970	2.761803
C	-3.642686	1.745541	1.296700
H	-4.391339	2.305067	0.715983
C	-2.292680	1.742312	0.911061
C	-1.682080	2.469907	-0.309828
C	-0.226039	1.866299	-0.348702
C	-0.113561	0.725446	-1.402907
H	0.168810	1.176093	-2.382077
C	1.109500	-0.032754	-0.856017
C	1.559533	-1.358633	-1.518813
H	1.145493	-2.251996	-1.017385
H	1.235531	-1.378032	-2.582124
C	3.063337	-1.296870	-1.452808
C	3.994960	-2.332384	-1.585301
H	3.662704	-3.366908	-1.760451
C	5.364299	-2.028480	-1.470713
H	6.109366	-2.834600	-1.558806
C	-3.981923	-0.855432	-2.544057
H	-4.964111	-1.206603	-2.895881
C	-3.808547	0.492082	-2.185223
H	-4.632294	1.219477	-2.232480
C	-2.548048	0.917593	-1.752090
C	-1.442394	0.041464	-1.655124
C	0.037389	1.145446	1.027771
H	0.623451	1.814302	1.688444
C	0.821723	-0.156329	0.710821
H	0.136276	-1.022468	0.830360
C	2.084656	-0.376852	1.532882
C	2.628219	-1.677307	1.702012
C	3.862225	-1.872459	2.353961
H	4.254656	-2.897237	2.459938
C	4.585792	-0.778945	2.849413
H	5.552296	-0.945708	3.349547
C	4.067370	0.517646	2.702551
H	4.618866	1.389389	3.085333
C	2.835099	0.698545	2.055081
H	2.458949	1.724873	1.935868
C	5.799736	-0.704563	-1.237252

H	6.876065	-0.494786	-1.143601
C	4.875649	0.340602	-1.109271
H	5.216903	1.365546	-0.909277
C	3.497792	0.038739	-1.209689
C	2.327944	0.875092	-1.013492
C	2.199847	2.252322	-0.902557
C	0.895740	2.845379	-0.585687
C	-0.427430	4.700146	-0.121922
C	-1.623288	3.972279	-0.051813
C	-2.833903	4.648665	0.210054
C	-1.341787	0.995397	1.622367
C	-1.715230	0.256527	2.755706
H	-0.973779	-0.347233	3.299541
C	-3.059935	0.281819	3.166091
H	-3.370452	-0.292555	4.052877
C	3.317030	3.134932	-1.040688
C	-1.650399	-1.310366	-1.983601
H	-0.829013	-2.031607	-1.899864
C	-2.908320	-1.753463	-2.430267
H	-3.048150	-2.810628	-2.693034
C	-1.828457	-3.694483	0.542448
N	-1.129227	-2.922162	1.325897
H	-0.123334	-3.133390	1.253706
N	-1.352229	-4.858515	-0.098442
N	-3.171153	-3.412983	0.311825
C	-4.169188	-4.469089	0.214667
H	-4.824658	-4.476095	1.117454
H	-4.823727	-4.331603	-0.675024
H	-3.674637	-5.454586	0.146319
C	-3.680525	-2.128964	0.760643
H	-2.922349	-1.342156	0.600790
H	-4.592953	-1.876885	0.182662
H	-3.938220	-2.133287	1.845758
C	-0.066174	-5.379979	0.331015
H	0.019254	-6.441883	0.021430
H	0.800029	-4.830421	-0.114784
H	0.017473	-5.329755	1.434121
C	-1.614056	-5.066945	-1.519930
H	-2.597916	-4.654344	-1.800505
H	-0.837390	-4.579375	-2.159483
H	-1.613586	-6.151830	-1.756119

SCAN3

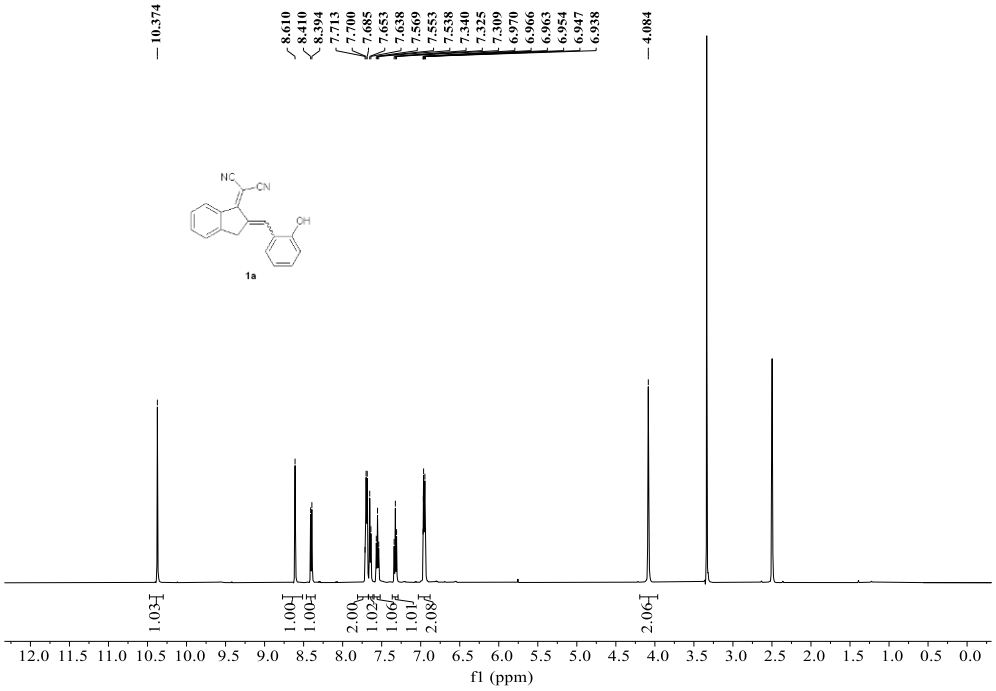
O	-1.596092	2.872262	-1.356873
H	-2.048436	3.674624	-1.029261
N	1.221772	1.079411	2.384100
O	-3.064424	-2.517552	-0.936399
H	-3.953342	-2.895255	-0.785513
N	3.133821	1.395934	3.632487
H	4.137222	1.321578	3.794133
H	2.564337	1.940735	4.279661
N	5.870435	-0.173345	1.925068
C	4.713214	-0.045505	1.736570
C	3.317617	0.134858	1.550904
C	2.544596	0.876558	2.525315
C	0.561559	0.595001	1.305655

N	-1.830748	1.964057	3.436471	C	1.981710	2.137140	-1.580102
C	-0.889857	0.859229	1.266012	H	2.637304	1.285046	-1.812706
C	-1.745138	0.575551	0.205863	C	2.551625	3.389659	-1.308741
C	-3.209773	0.672093	0.193636	H	3.644841	3.513727	-1.329702
C	-4.131088	0.937149	1.235824	C	1.713646	4.477345	-1.001830
H	-3.789476	1.150465	2.255969	H	2.141156	5.465475	-0.770962
C	-5.504943	0.916357	0.956139	C	0.322141	4.308339	-1.002108
H	-6.224951	1.116609	1.764557	H	-0.346013	5.158147	-0.785270
C	-5.973266	0.636934	-0.345223	C	-0.244229	3.048688	-1.294206
H	-7.056273	0.624756	-0.545199	C	-2.554933	0.130347	-2.056543
C	2.616193	-0.375383	0.434757	H	-2.439572	0.989984	-2.750004
C	3.069076	-1.139624	-0.736484	H	-2.697414	-0.784672	-2.662585
C	4.337027	-1.633215	-1.096739	C	-3.692496	0.383558	-1.113941
H	5.211923	-1.476193	-0.449558	C	-5.066107	0.368290	-1.385877
C	4.462288	-2.339824	-2.306431	H	-5.429762	0.142510	-2.400504
H	5.445373	-2.735686	-2.604405	C	-1.398061	1.461319	2.464473
C	3.344869	-2.550490	-3.140593	C	-0.921759	-2.336338	0.073900
H	3.466181	-3.108744	-4.081814	C	-2.234391	-2.878587	0.083820
C	2.075096	-2.053710	-2.783086	C	-2.642554	-3.764419	1.100097
H	1.207159	-2.220210	-3.440975	H	-3.673767	-4.154058	1.092285
C	1.943480	-1.345925	-1.584515	C	-1.739054	-4.152767	2.102437
C	0.703792	-0.693799	-1.001421	H	-2.069117	-4.844833	2.892898
C	-0.534144	-1.348025	-1.006169	C	-0.421505	-3.667559	2.082066
H	-0.701537	-1.841571	-1.990695	H	0.302175	-3.979949	2.850004
C	-1.313316	0.044916	-1.152476	C	-0.029310	-2.768736	1.073936
C	0.036902	0.543202	-1.763150	H	1.002102	-2.392881	1.069383
H	0.005405	0.282050	-2.842807	C	1.229103	-0.153299	0.318343
C	0.585601	1.928716	-1.553049				

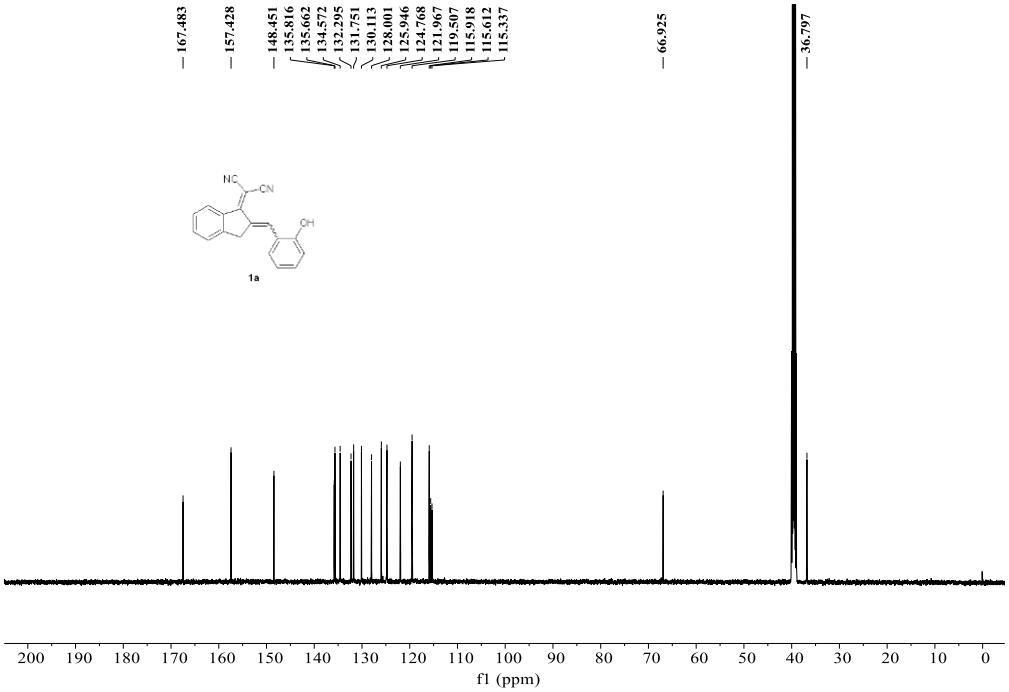
14. NMR Spectra of Products

14.1 NMR spectra for compounds 1

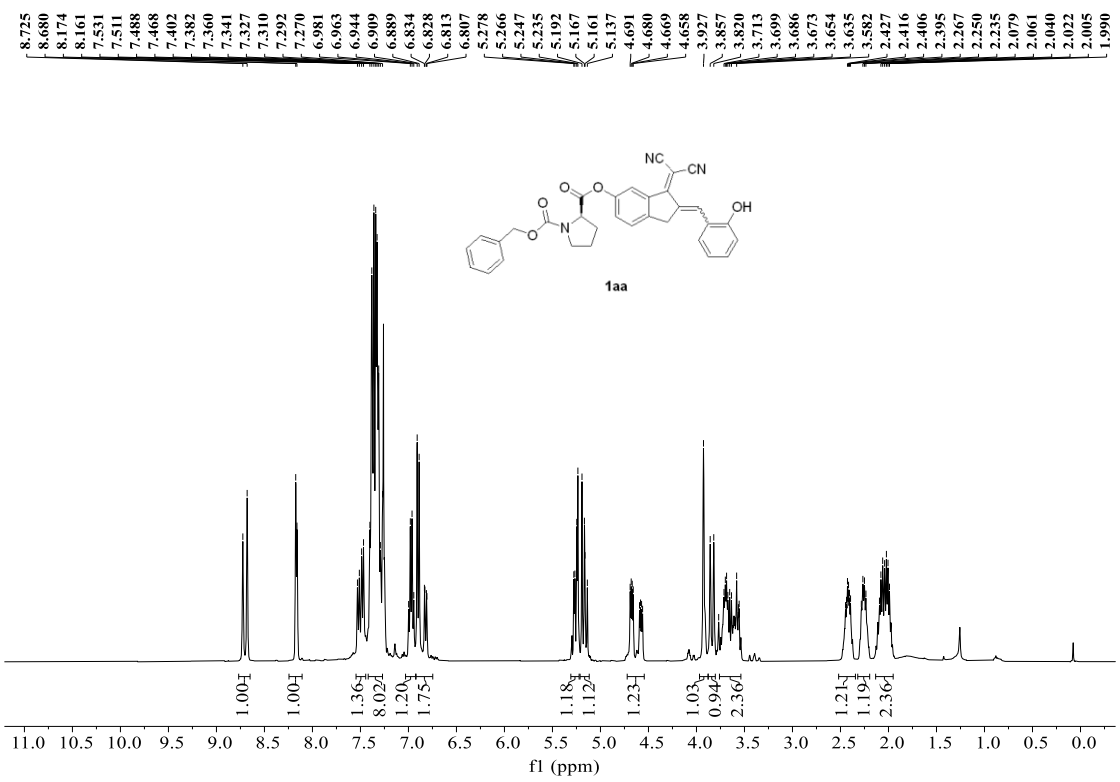
^{1}H NMR spectra of compound **1a** (500 MHz, DMSO-d_6)



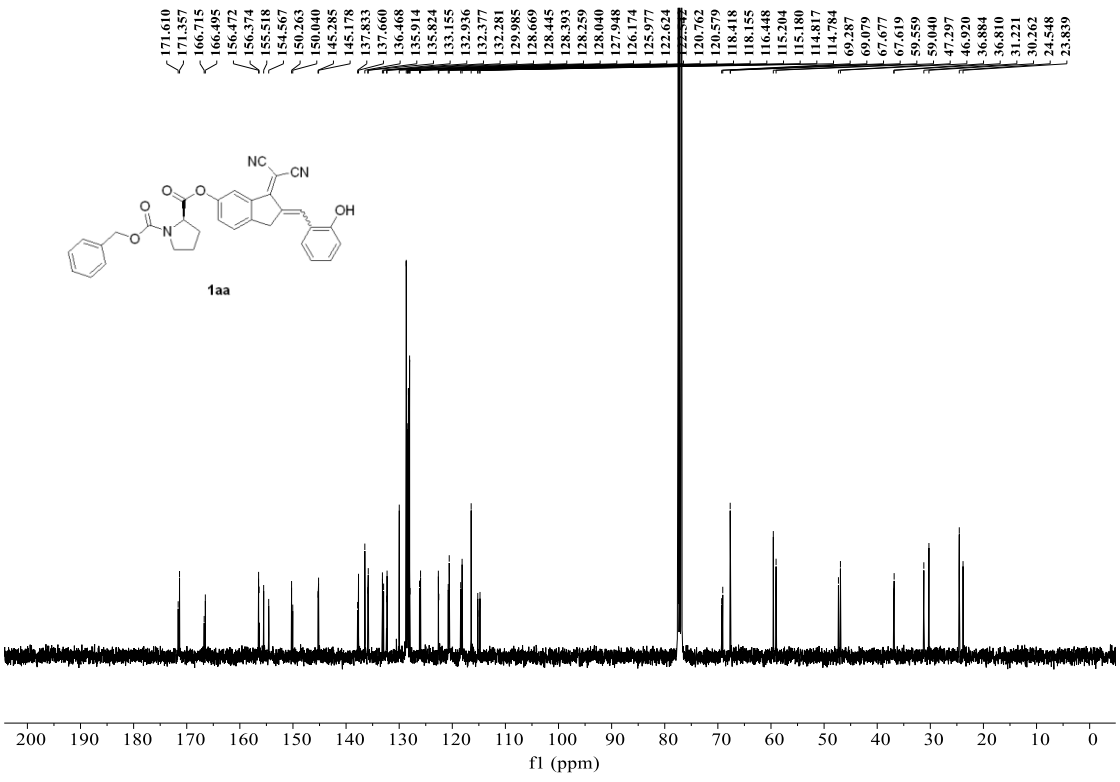
^{13}C NMR spectra of compound **1a** (125 MHz, DMSO-d_6)



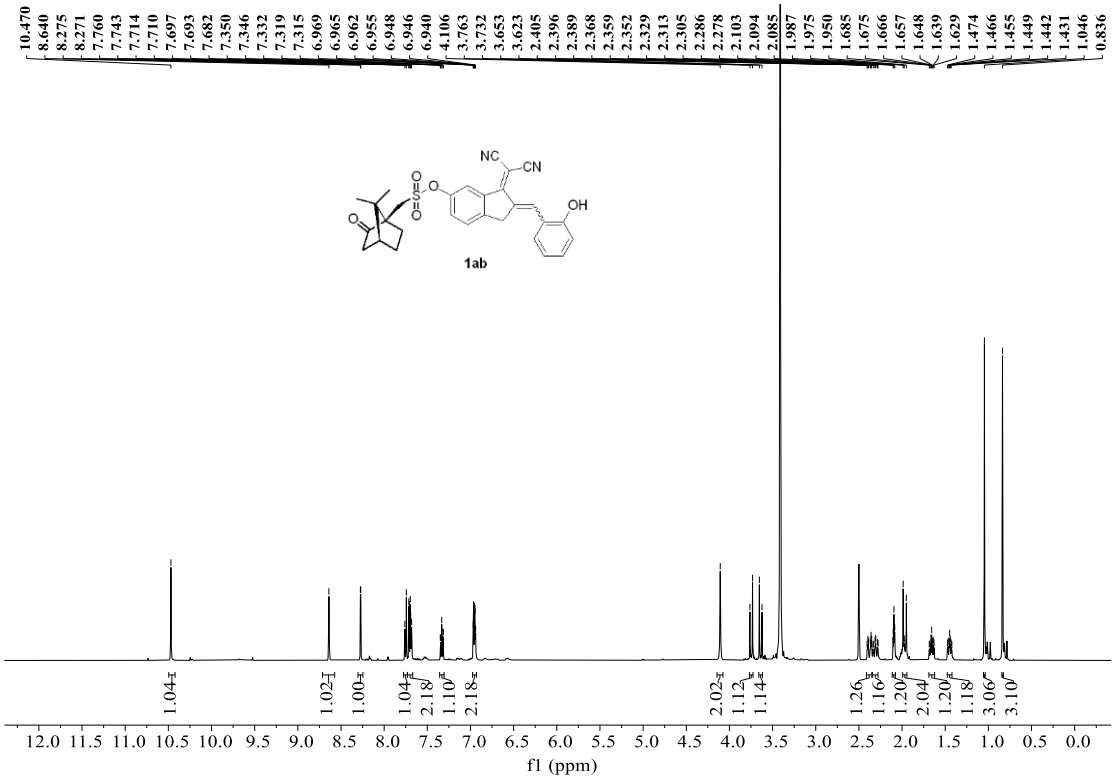
^{1}H NMR spectra of compound **1aa** (400 MHz, $CDCl_3$)



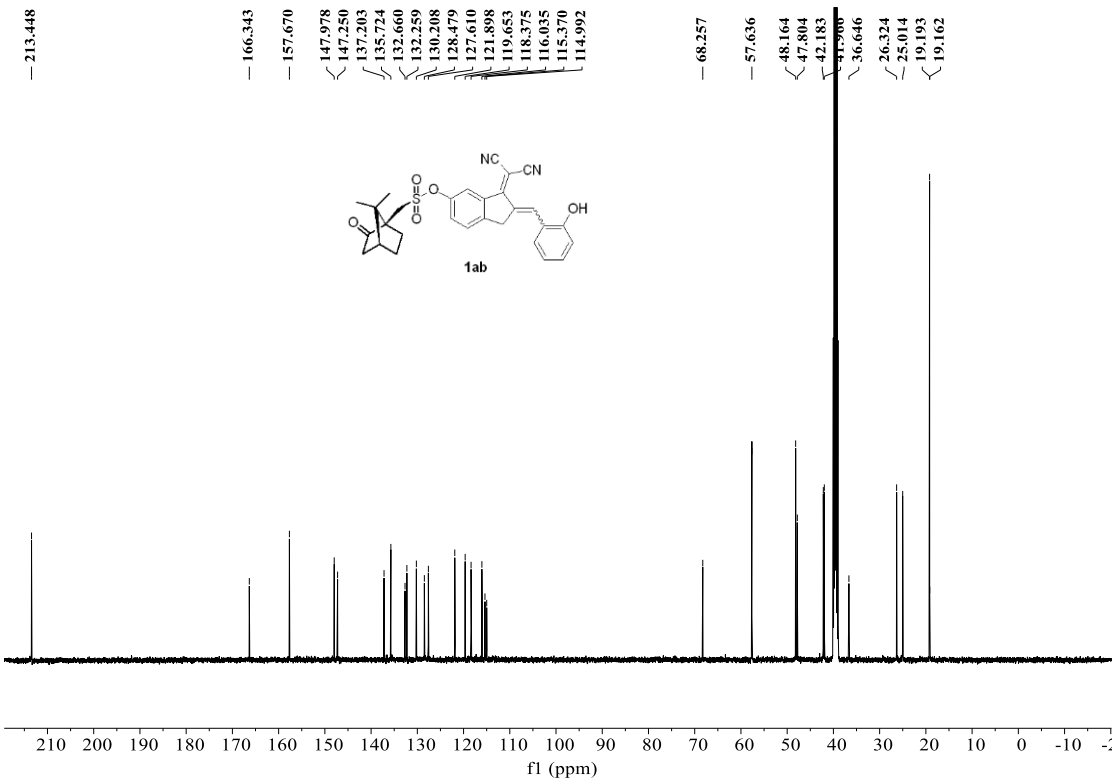
^{13}C NMR spectra of compound **1aa** (100 MHz, $CDCl_3$)



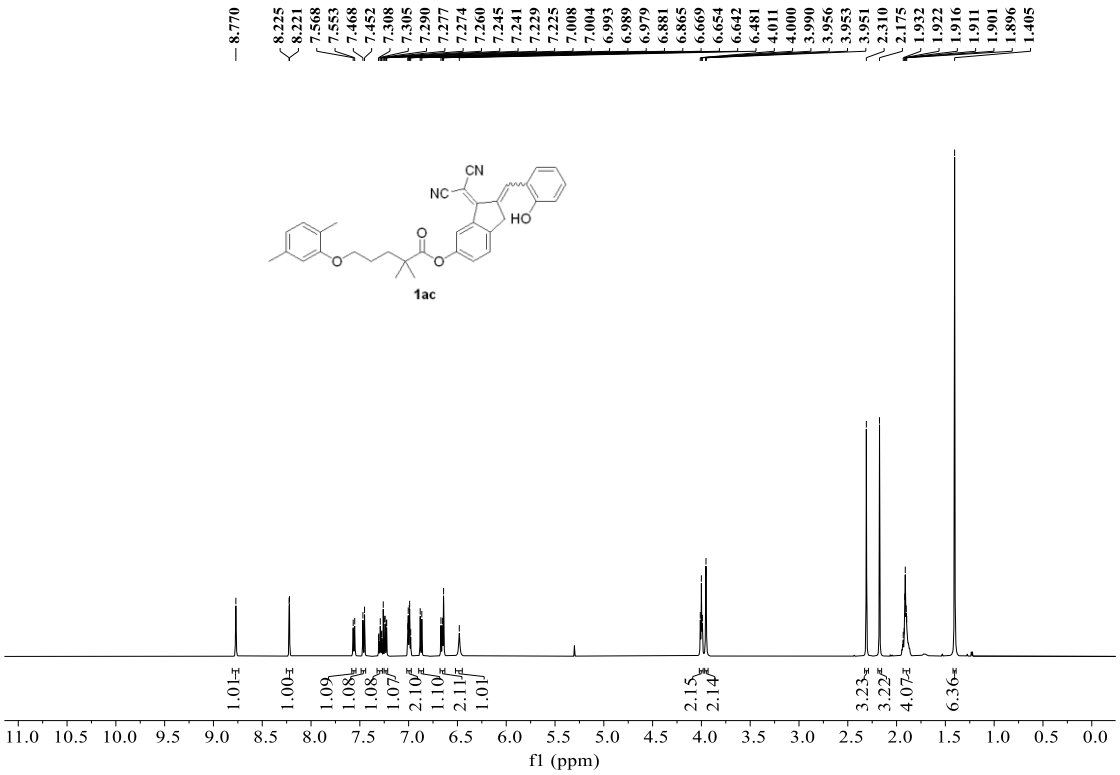
^{1}H NMR spectra of compound **1ab** (500 MHz, DMSO-d_6)



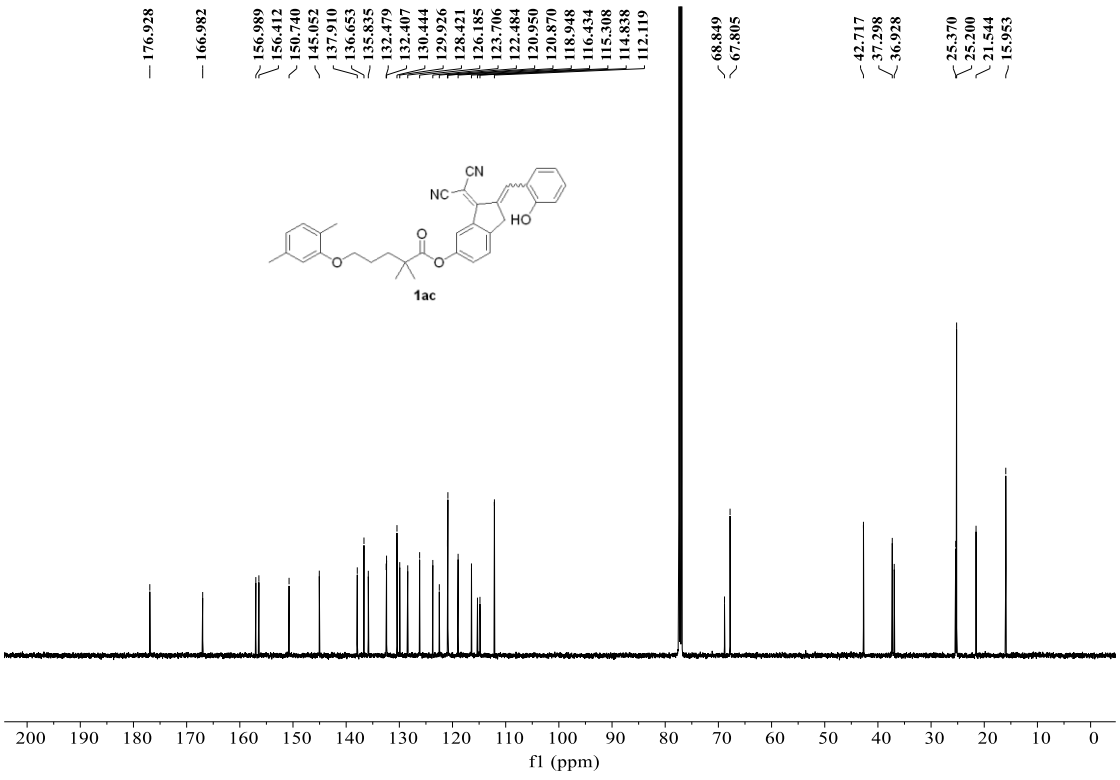
^{13}C NMR spectra of compound **1ab** (125 MHz, DMSO-d_6)



^{1}H NMR spectra of compound **1ac** (500 MHz, $CDCl_3$)

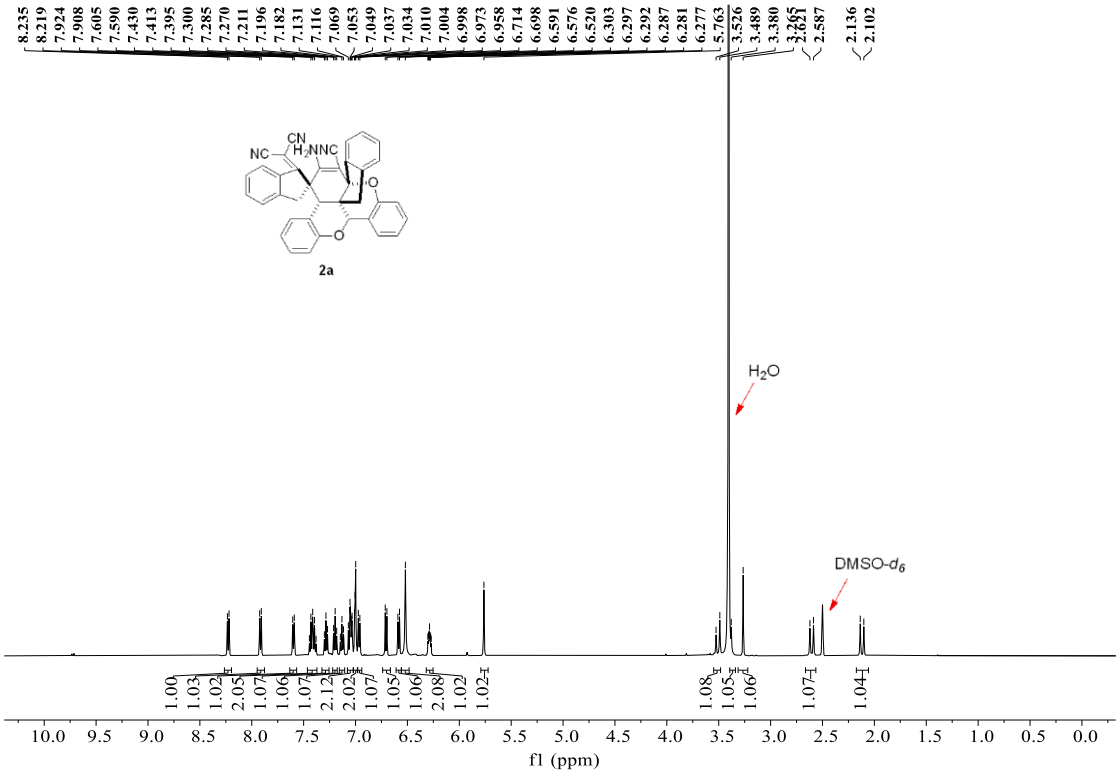


^{13}C NMR spectra of compound **1ac** (125 MHz, $CDCl_3$)

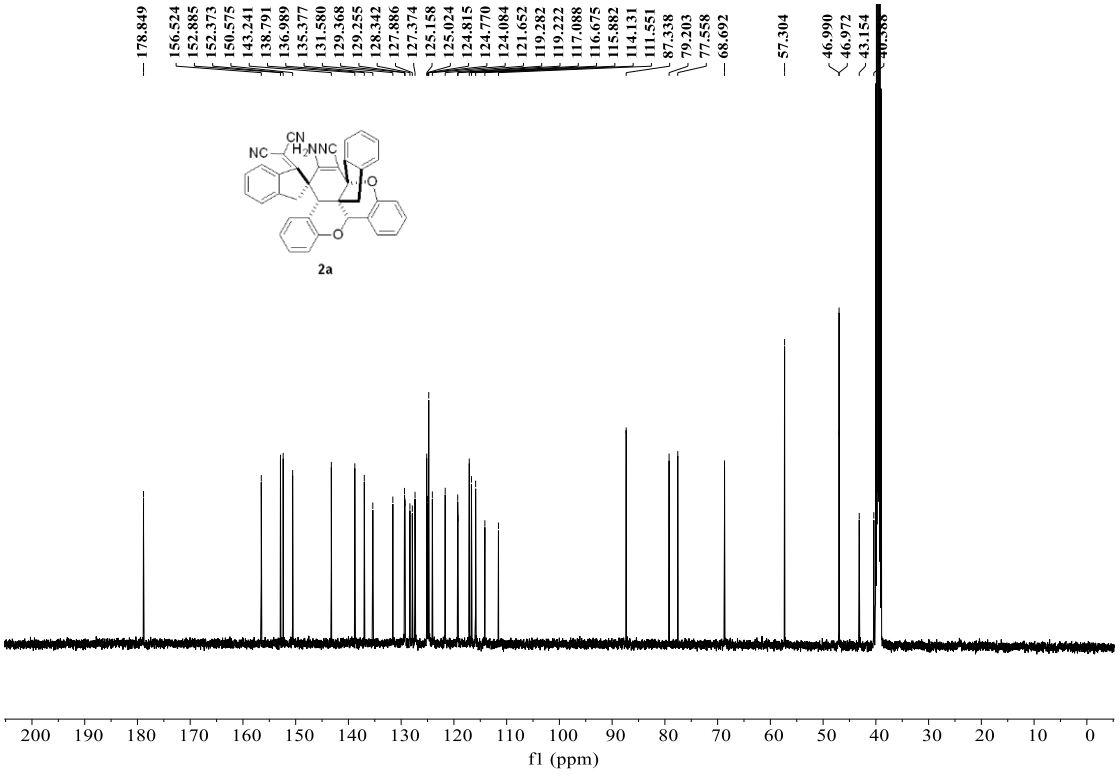


14.2 NMR spectra for compounds 2

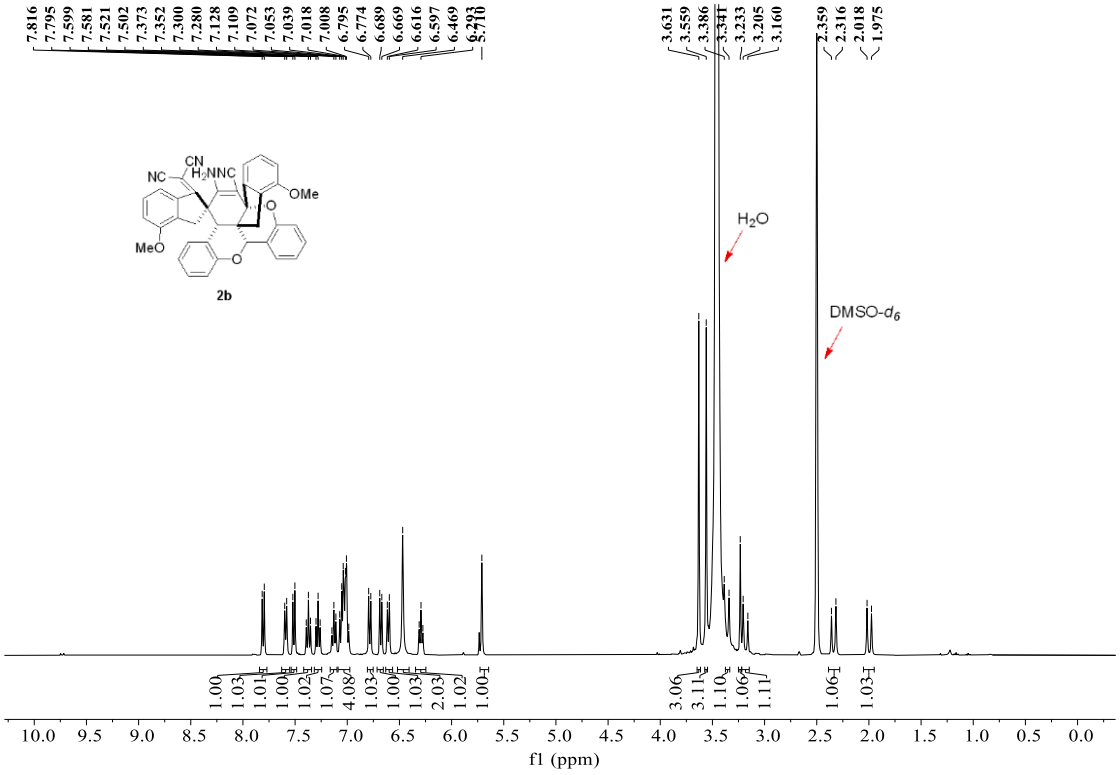
^{1}H NMR spectra of compound **2a** (500 MHz, DMSO-d_6)



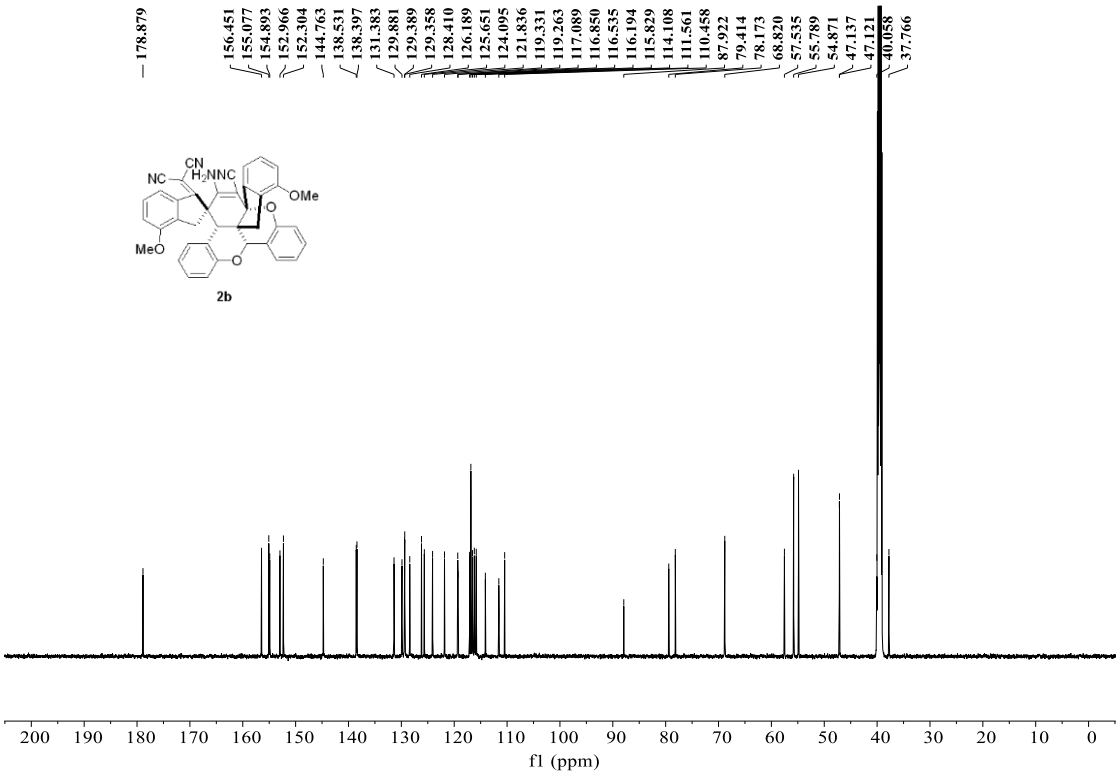
^{13}C NMR spectra of compound **2a** (125 MHz, DMSO-d_6)



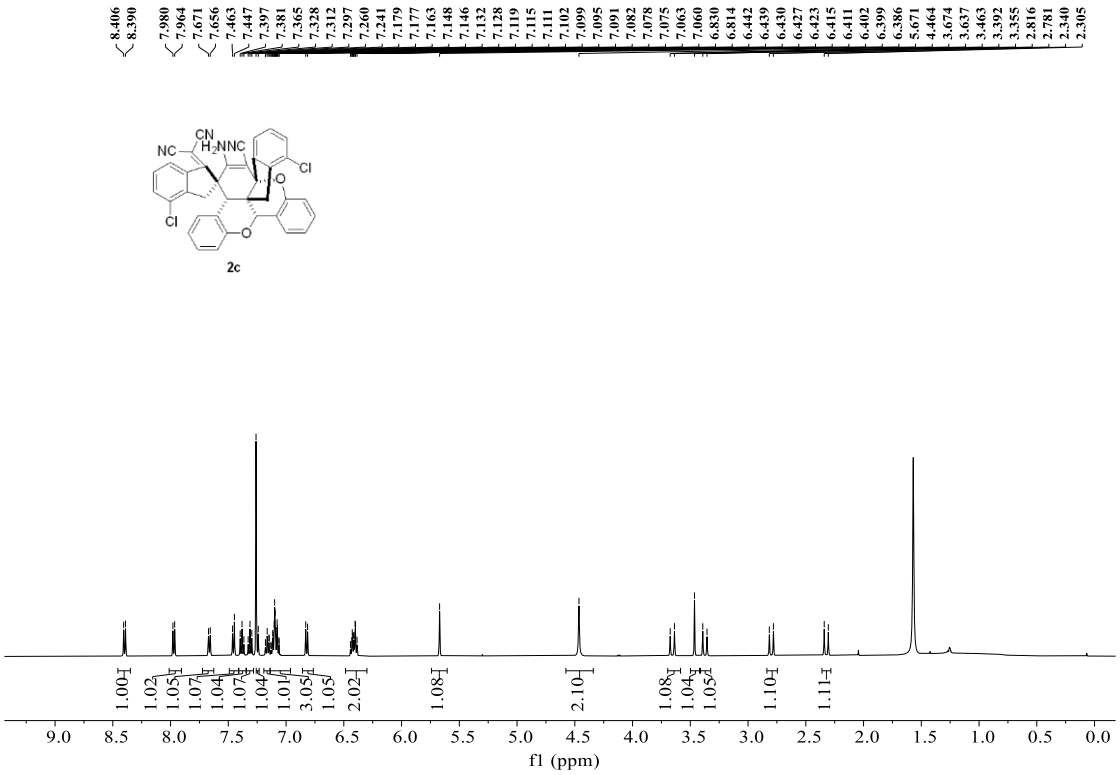
^{1}H NMR spectra for compound **2b** (400 MHz, DMSO-d_6)



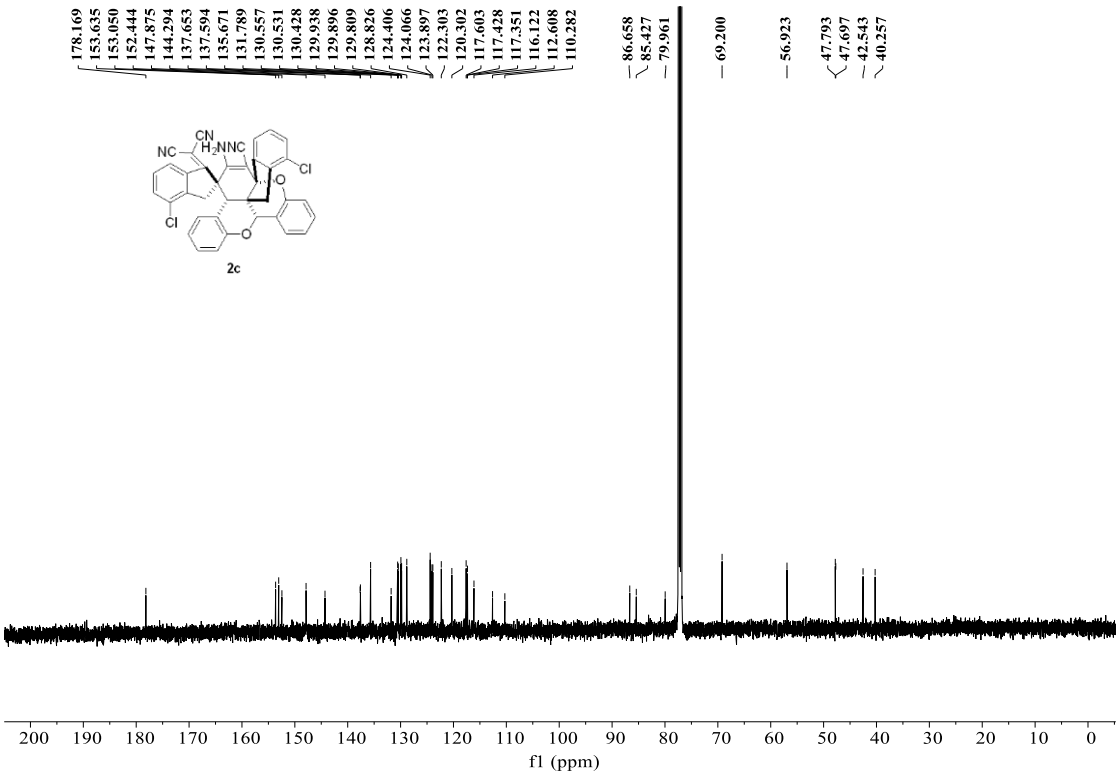
^{13}C NMR spectra for compound **2b** (150 MHz, DMSO-d_6)



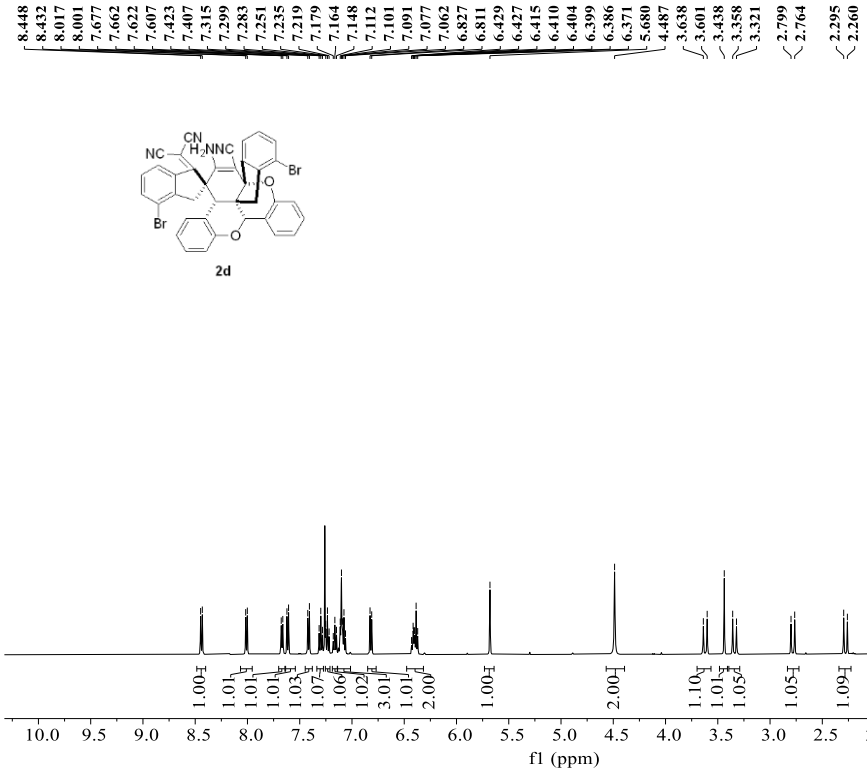
^{1}H NMR spectra for compound **2c** (500 MHz, $CDCl_3$)



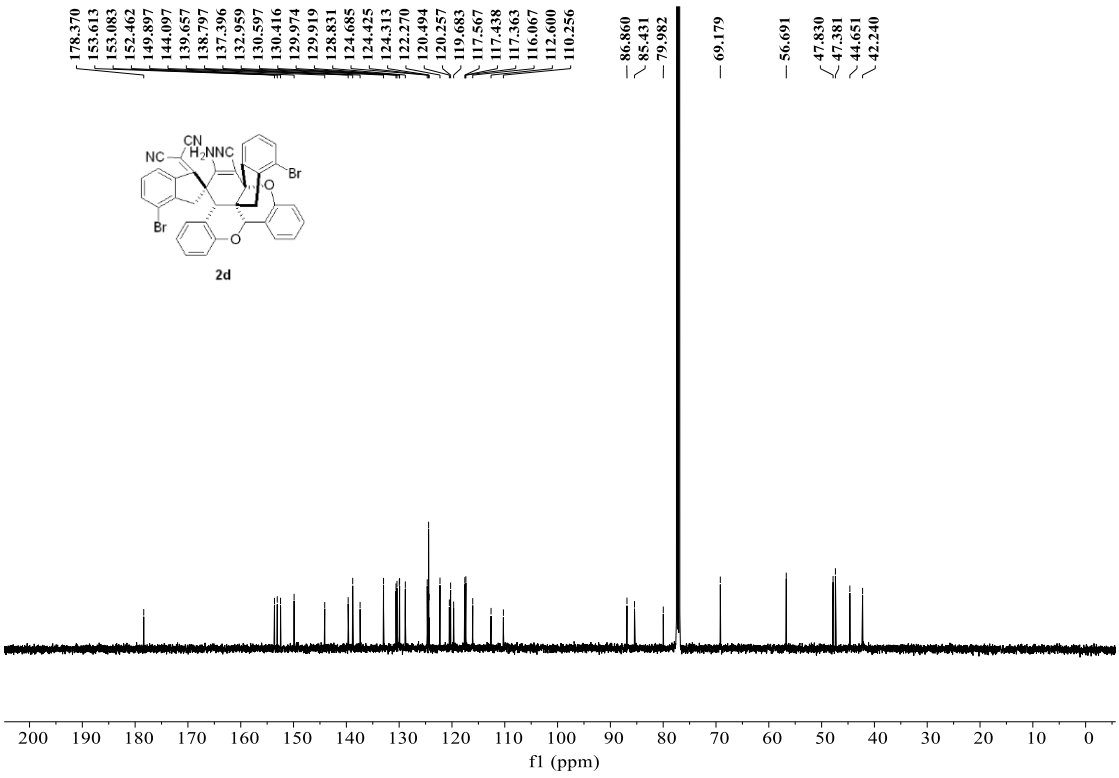
^{13}C NMR spectra for compound **2c** (125 MHz, $CDCl_3$)



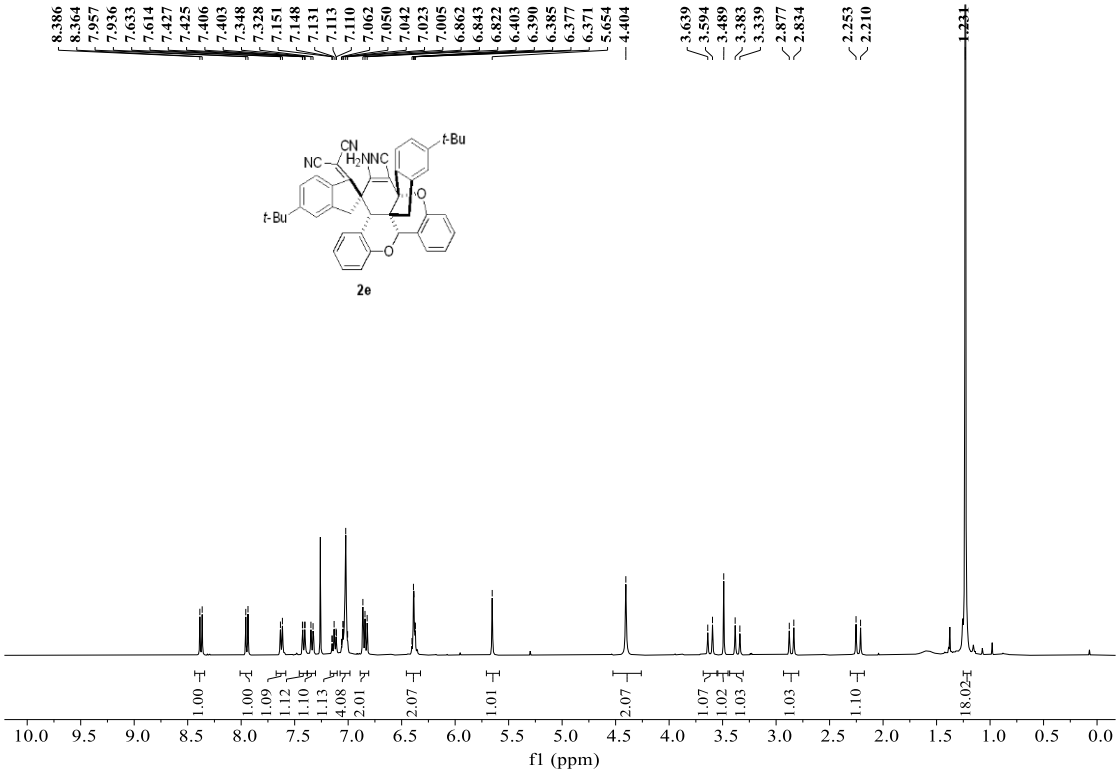
^{1}H NMR spectra for compound **2d** (500 MHz, $CDCl_3$)



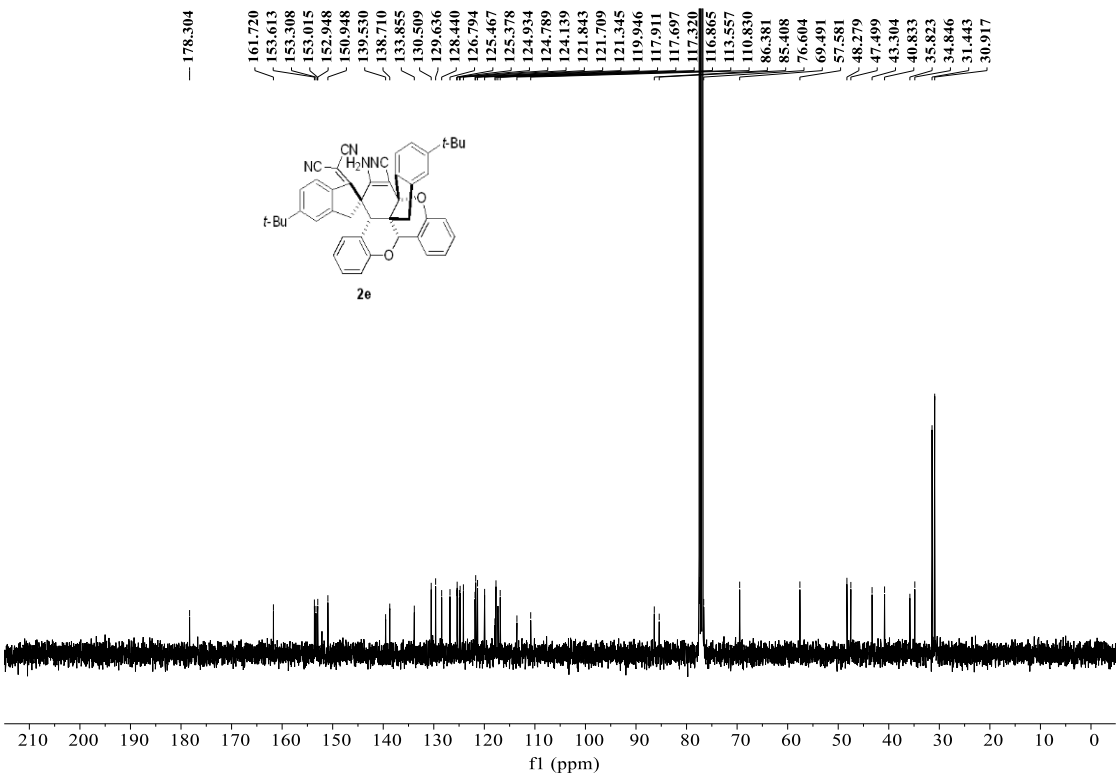
^{13}C NMR spectra for compound **2d** (125 MHz, $CDCl_3$)



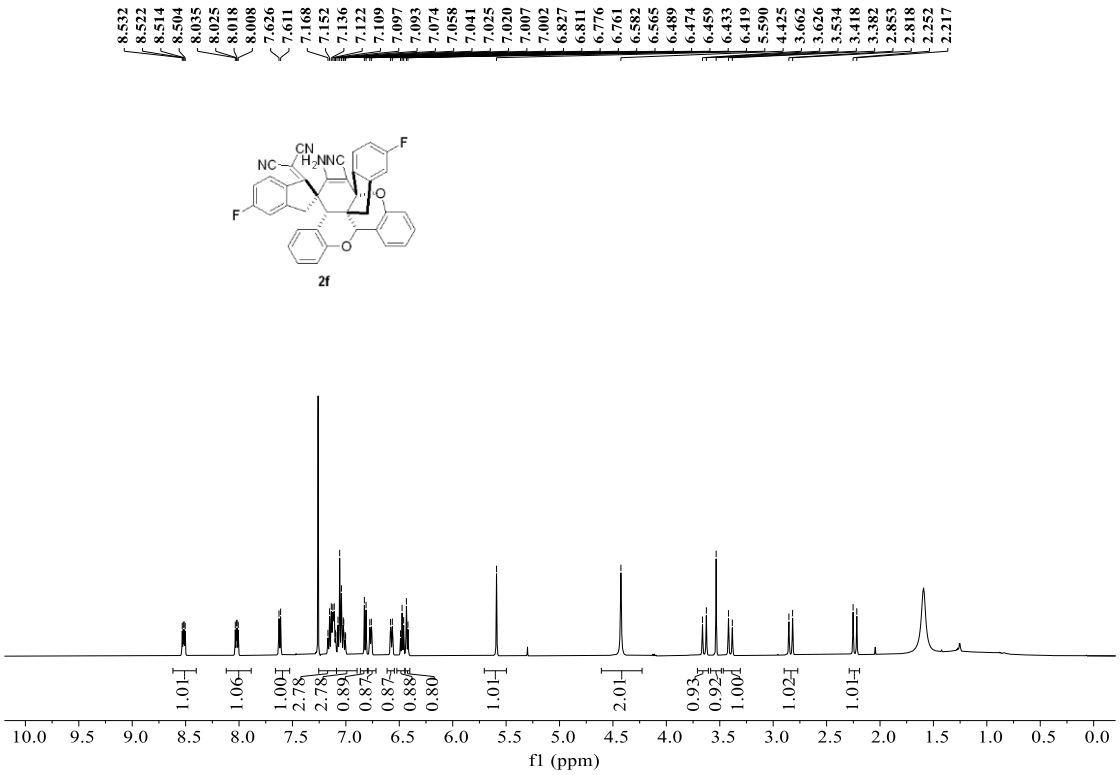
^{1}H NMR spectra for compound **2e** (400 MHz, $CDCl_3$)



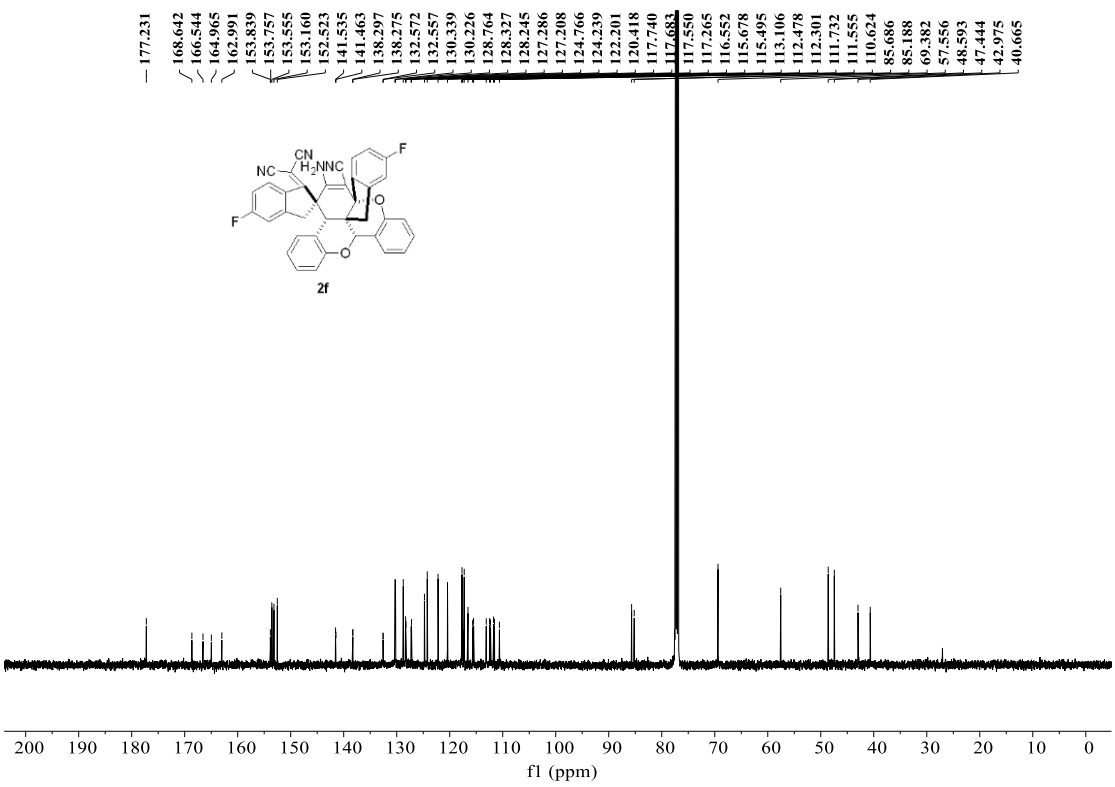
^{13}C NMR spectra for compound **2e** (100 MHz, $CDCl_3$)



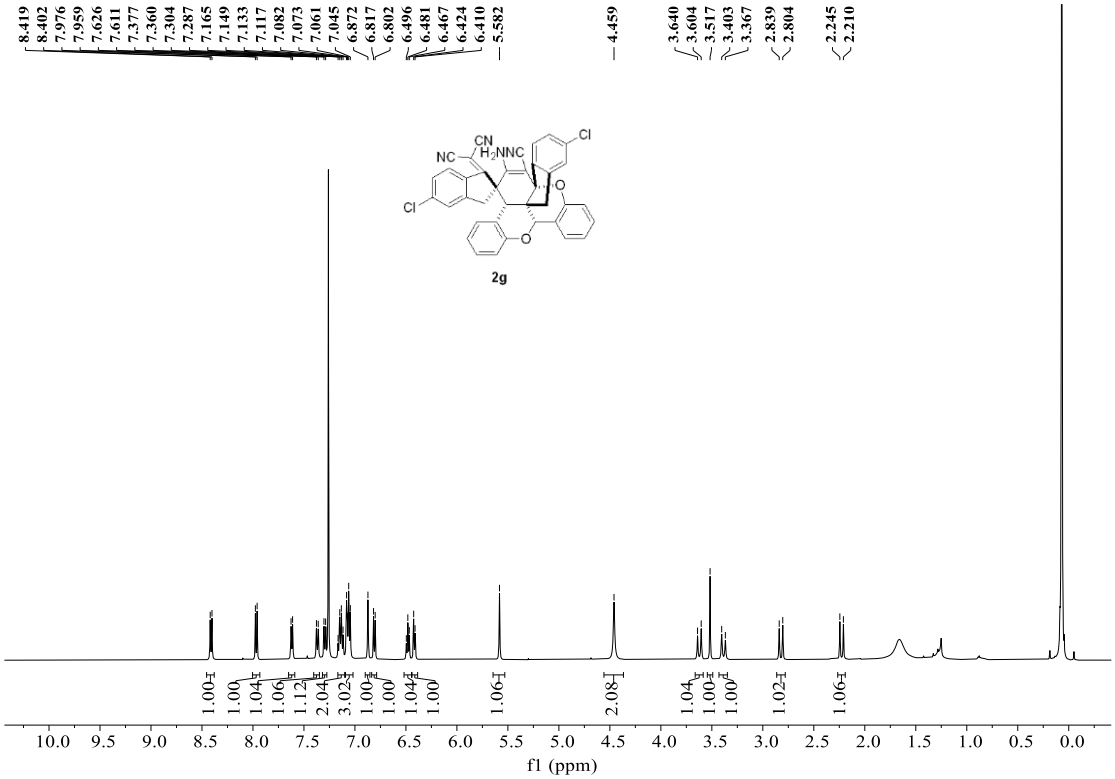
^{1}H NMR spectra for compound **2f** (500 MHz, $CDCl_3$)



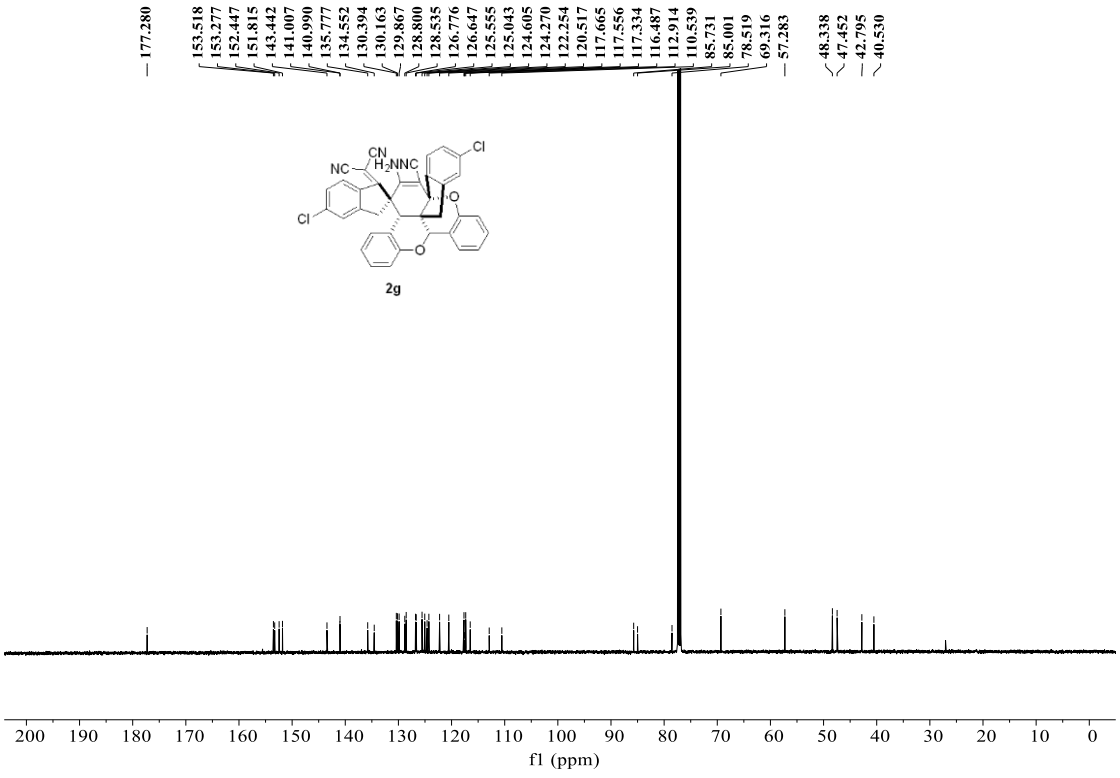
^{13}C NMR spectra for compound **2f** (125 MHz, $CDCl_3$)



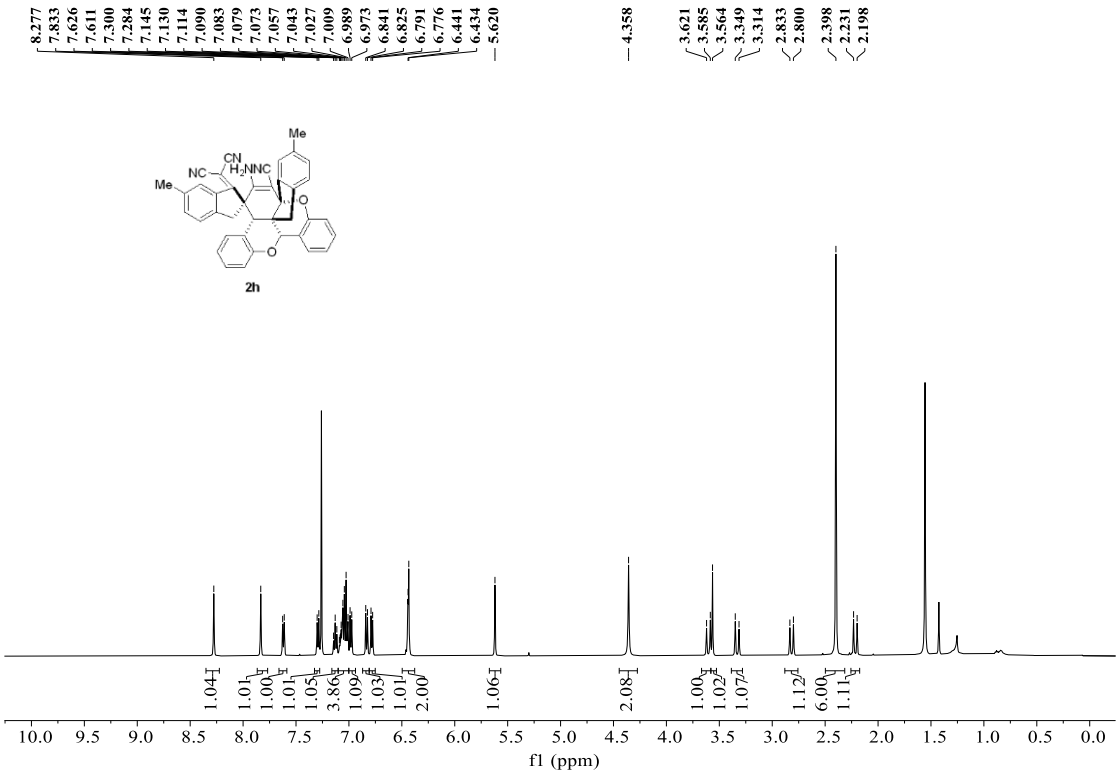
^{1}H NMR spectra for compound **2g** (500 MHz, $CDCl_3$)



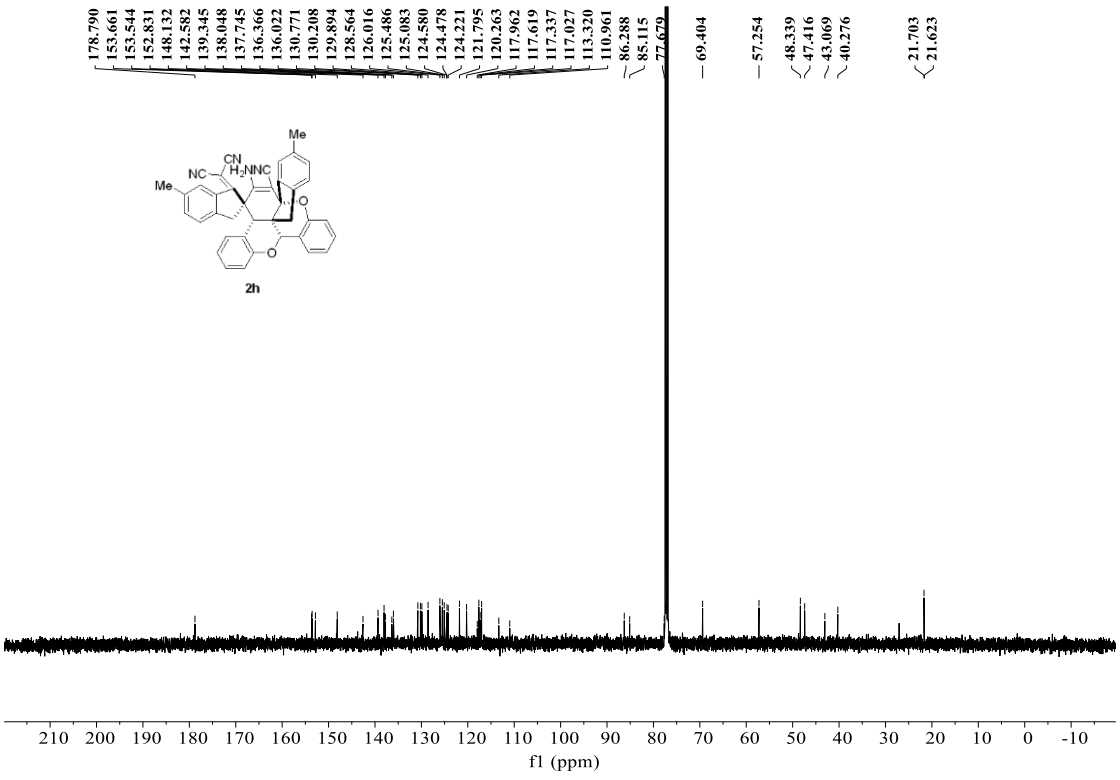
^{13}C NMR spectra for compound **2g** (125 MHz, $CDCl_3$)



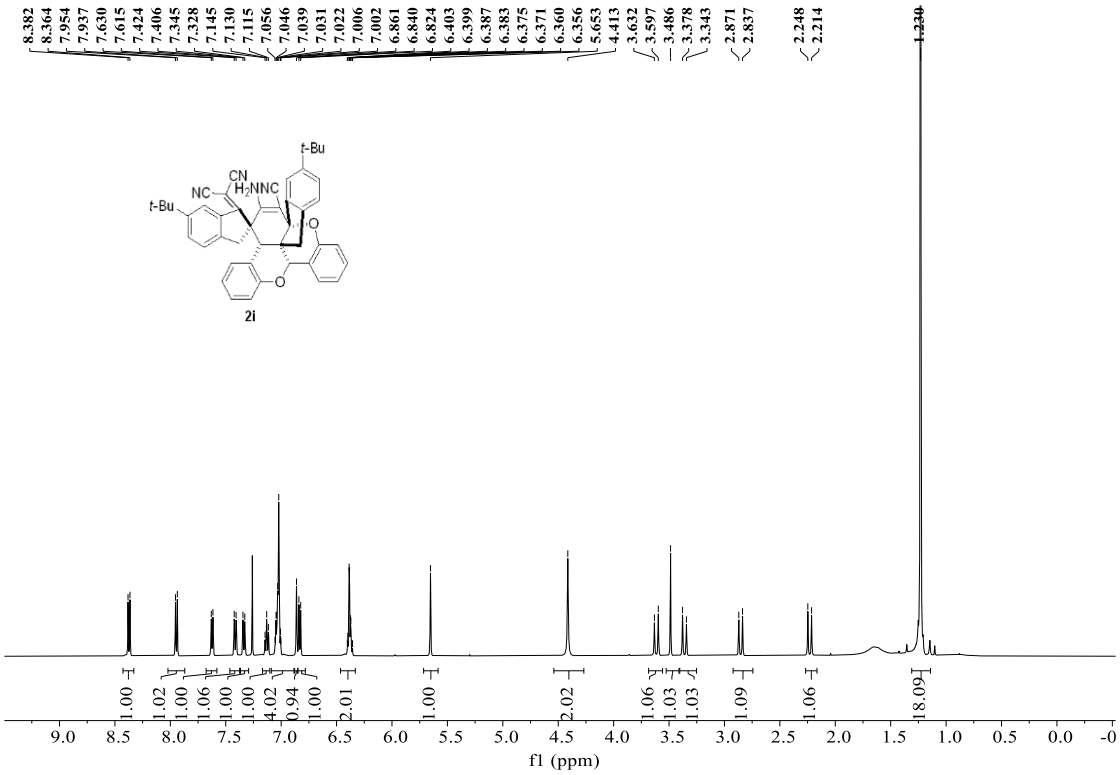
^{1}H NMR spectra for compound **2h** (500 MHz, $CDCl_3$)



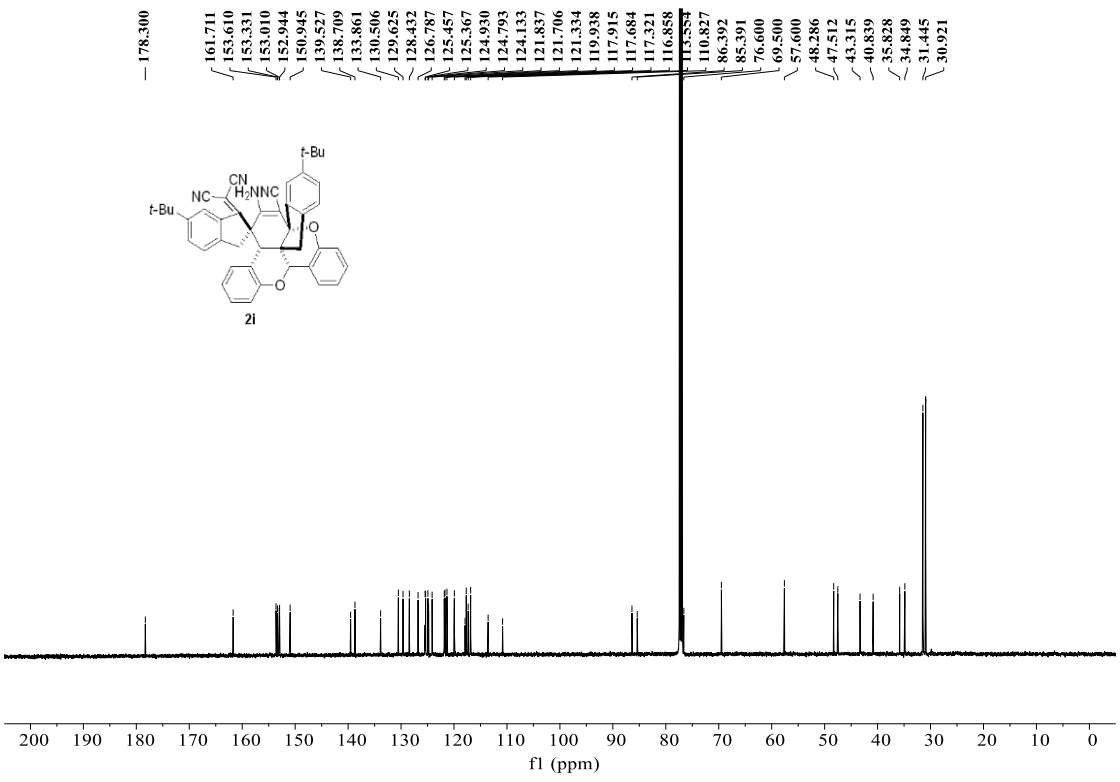
^{13}C NMR spectra for compound **2h** (125 MHz, $CDCl_3$)



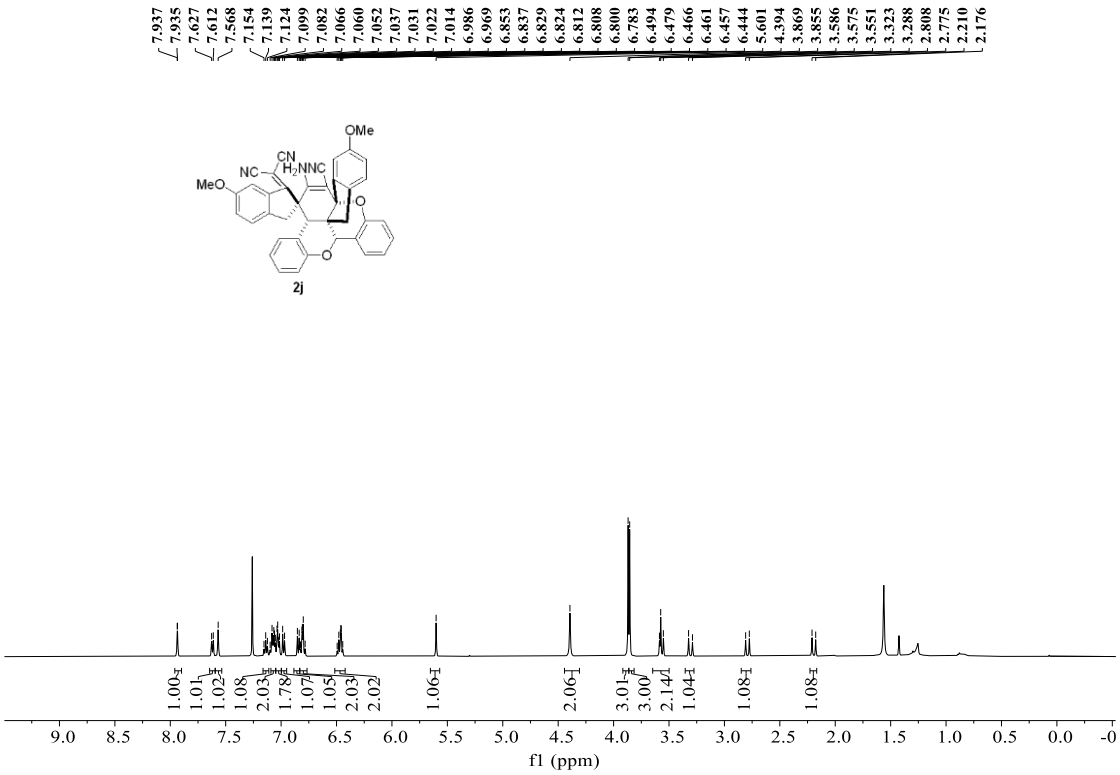
^{1}H NMR spectra for compound **2i** (500 MHz, $CDCl_3$)



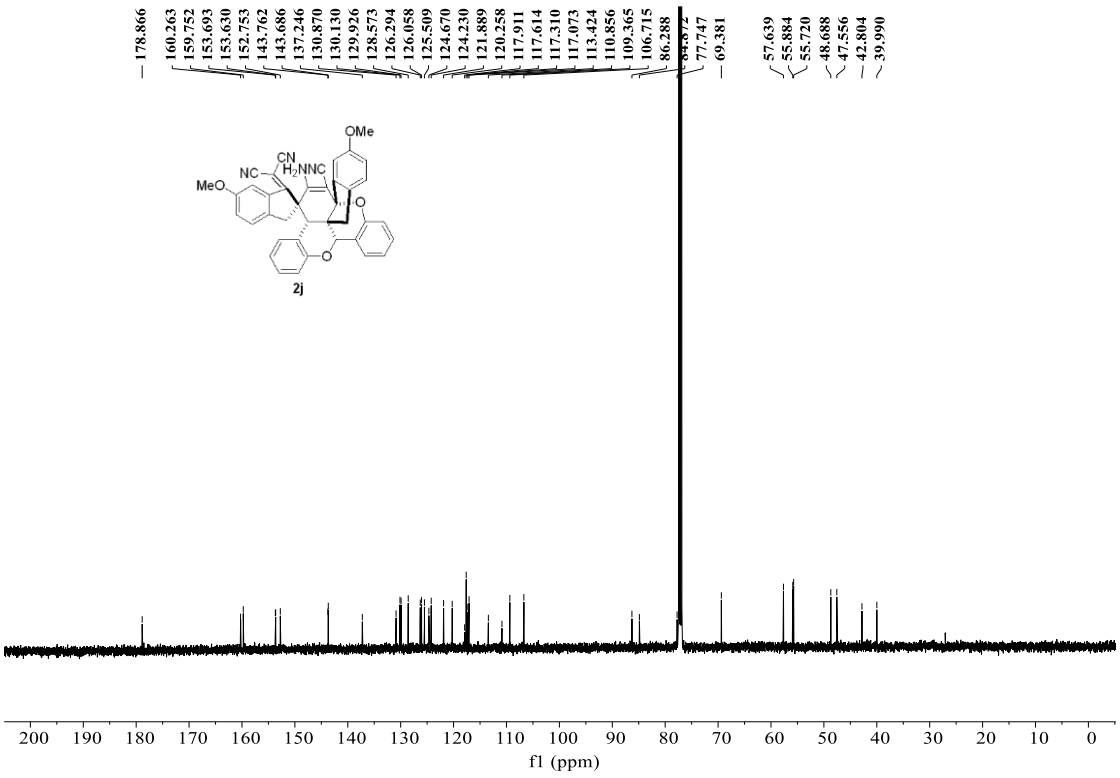
^{13}C NMR spectra for compound **2i** (125 MHz, $CDCl_3$)



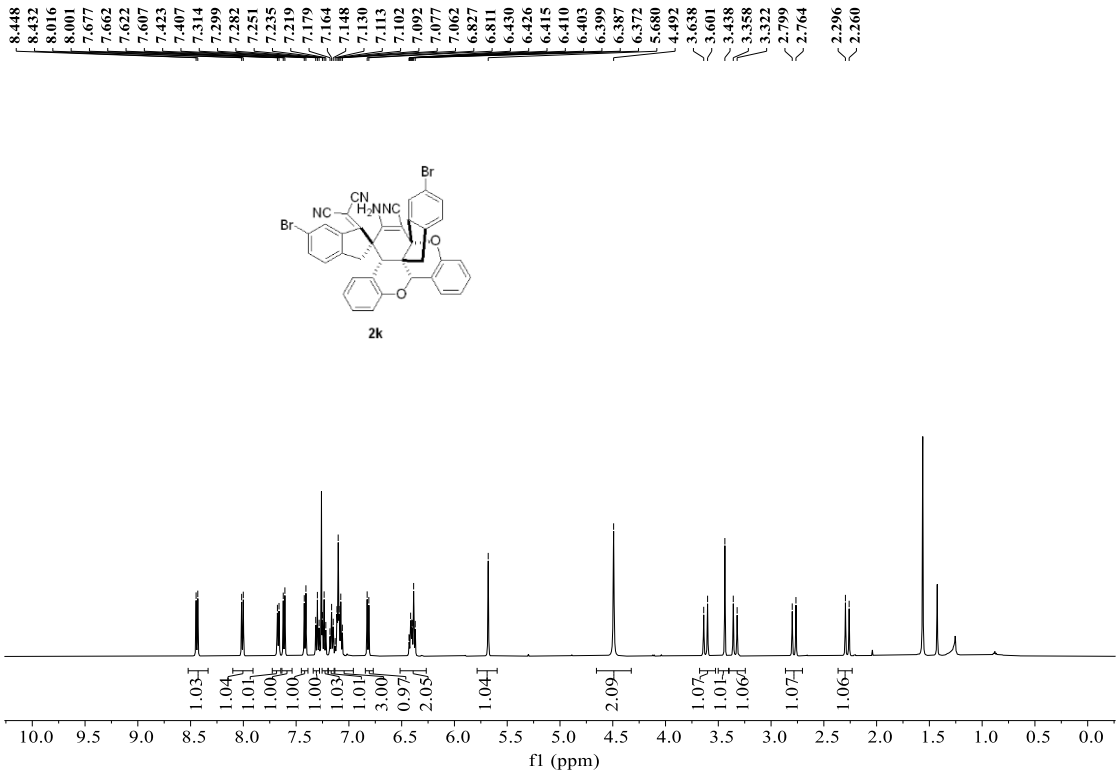
^{1}H NMR spectra for compound **2j** (500 MHz, $CDCl_3$)



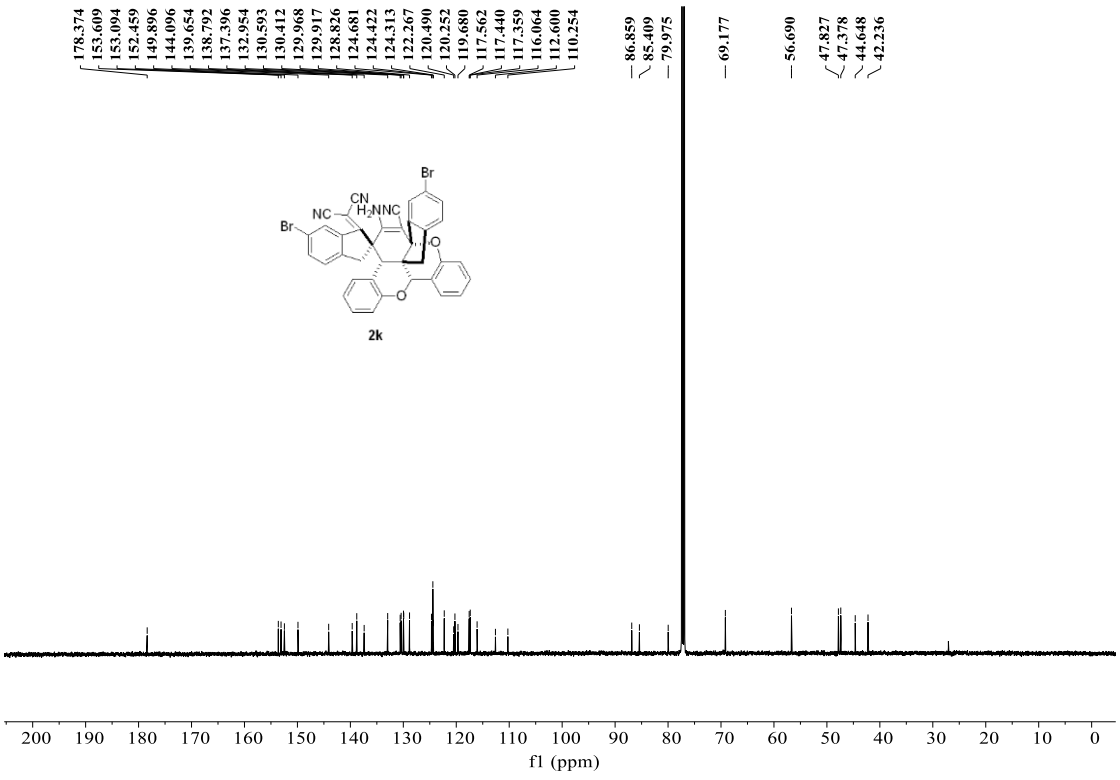
^{13}C NMR spectra for compound **2j** (125 MHz, $CDCl_3$)



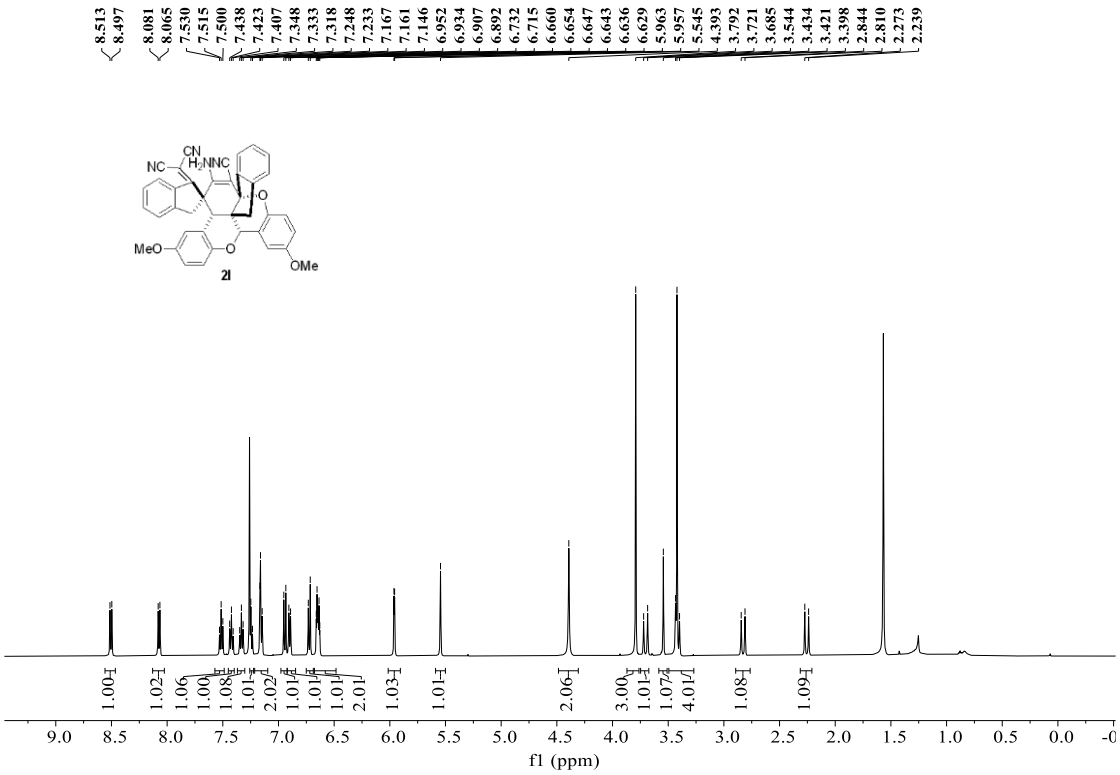
^{1}H NMR spectra for compound **2k** (500 MHz, $CDCl_3$)



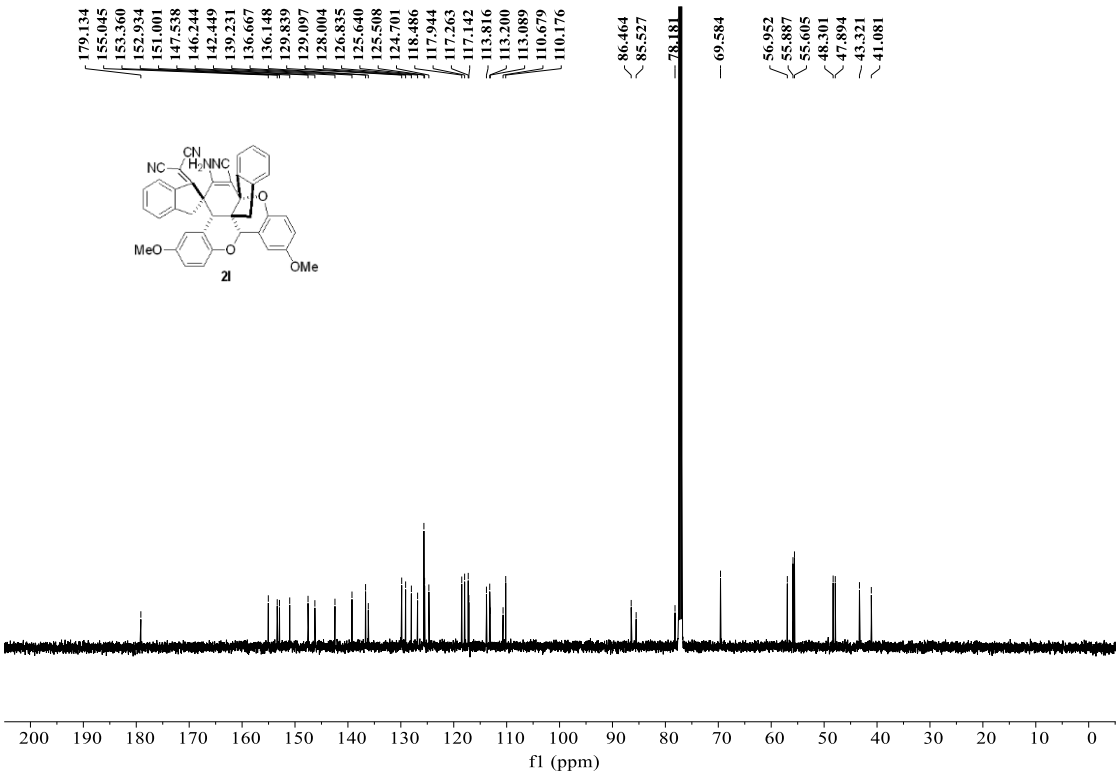
^{13}C NMR spectra for compound **2k** (125 MHz, $CDCl_3$)



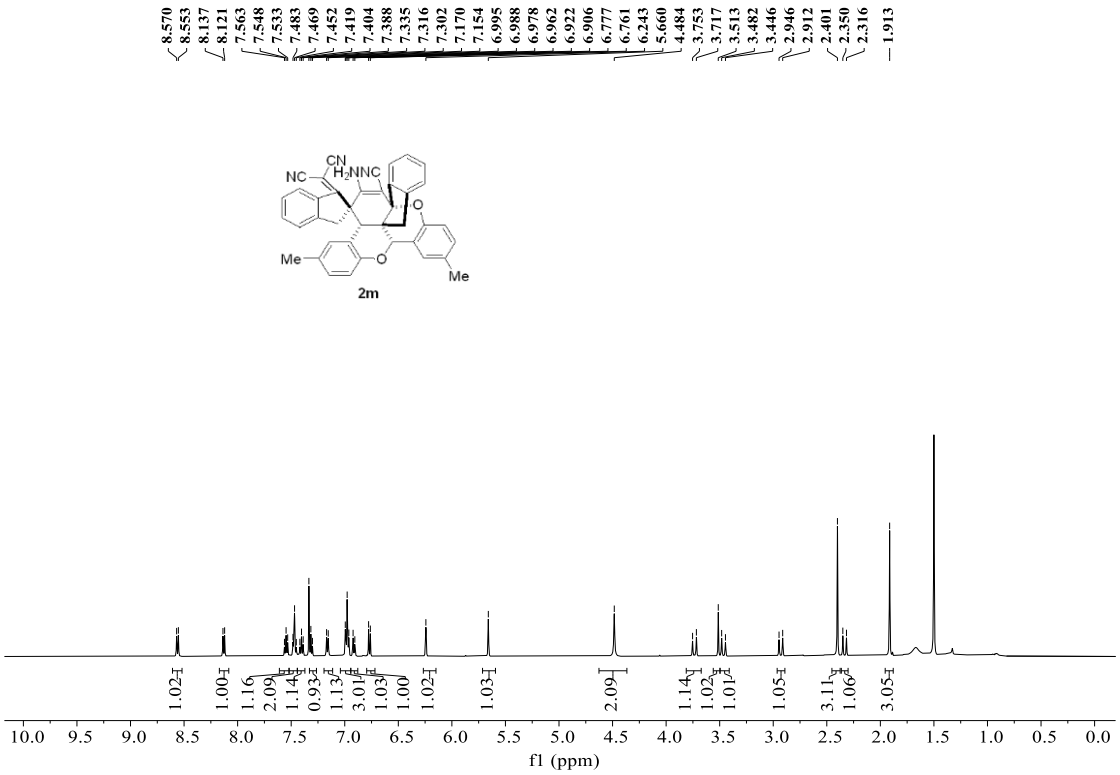
^{1}H NMR spectra for compound **2l** (500 MHz, $CDCl_3$)



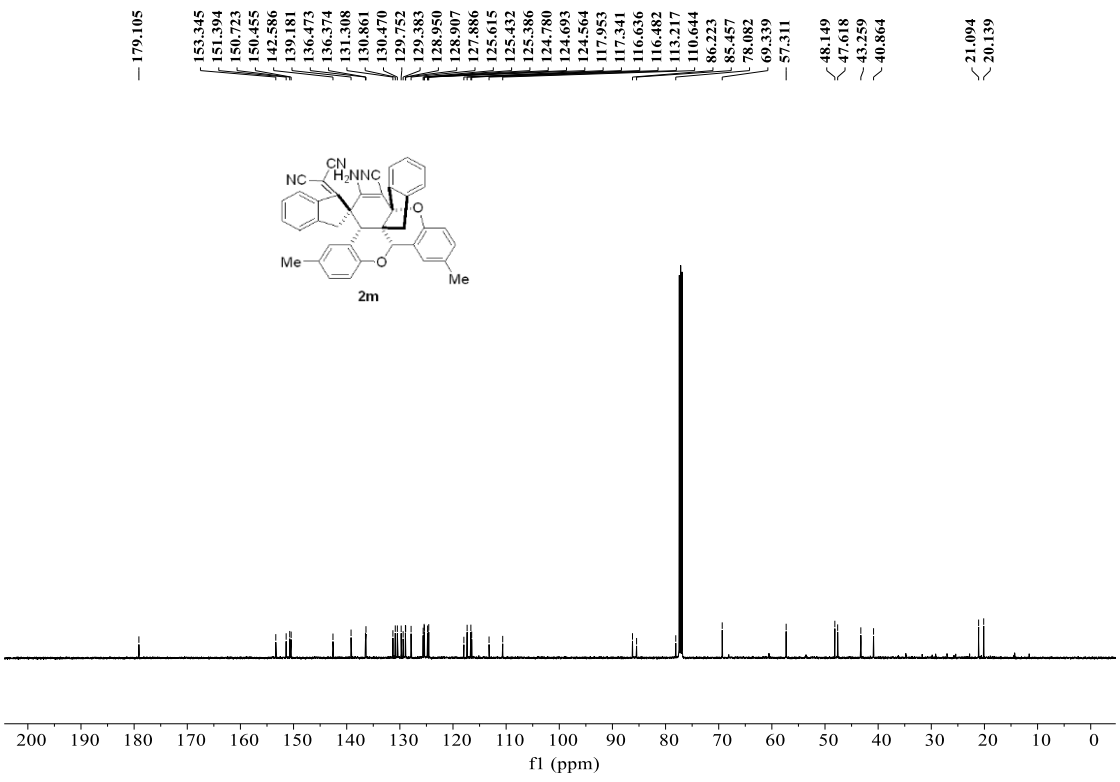
^{13}C NMR spectra for compound **2l** (125 MHz, $CDCl_3$)



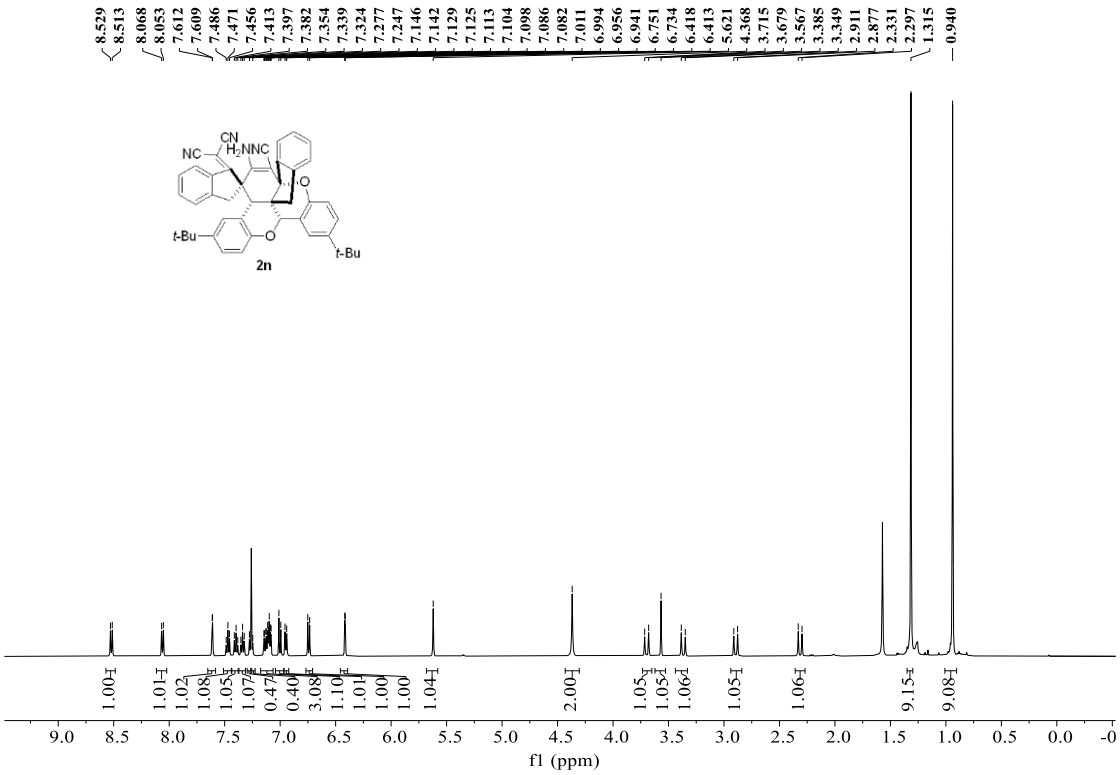
^{1}H NMR spectra for compound **2m** (500 MHz, $CDCl_3$)



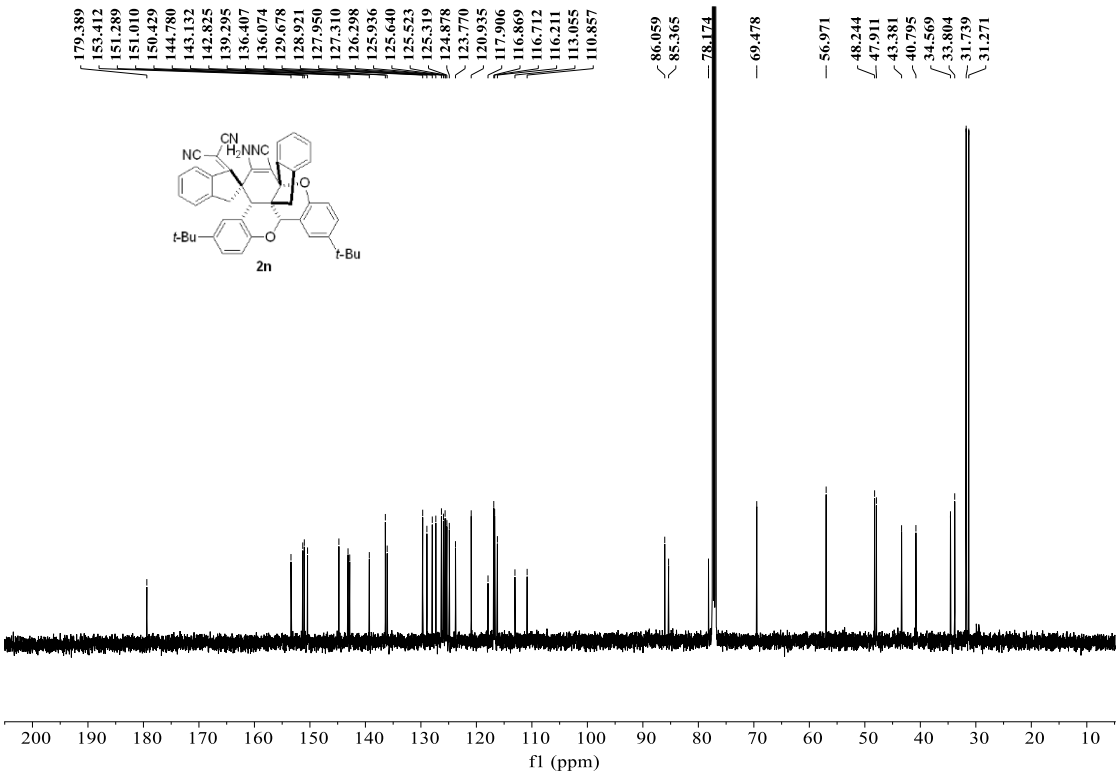
^{13}C NMR spectra for compound **2m** (125 MHz, $CDCl_3$)



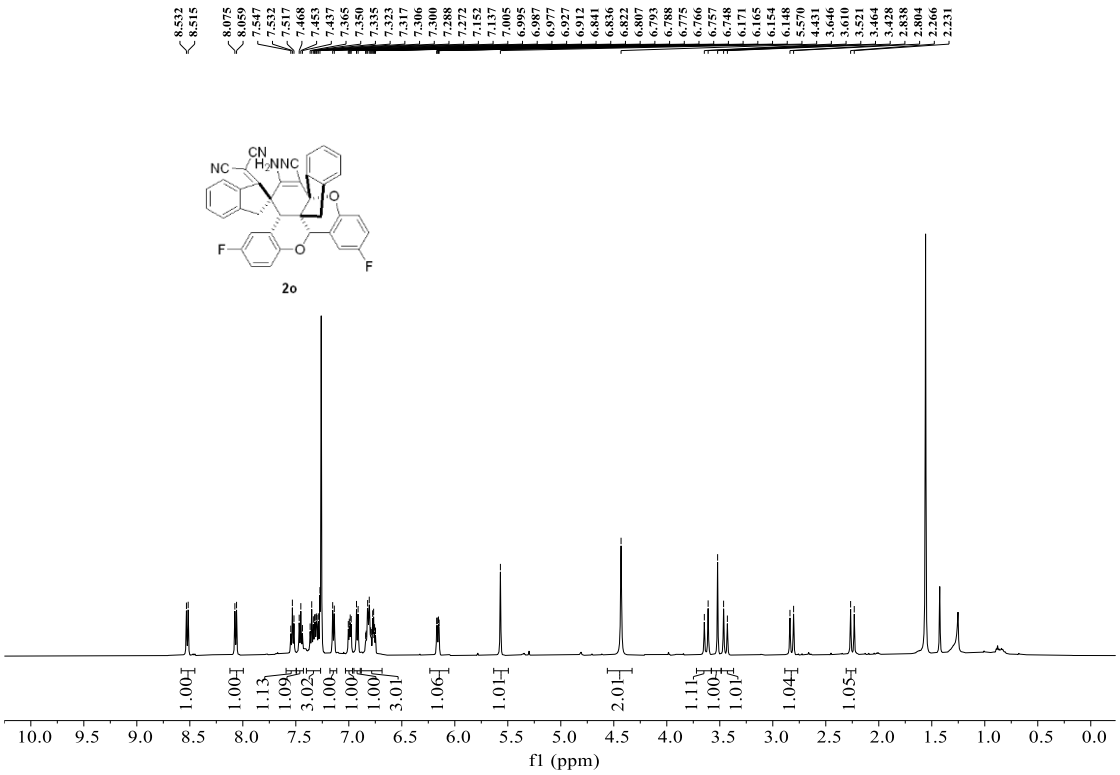
^{1}H NMR spectra for compound **2n** (500 MHz, $CDCl_3$)



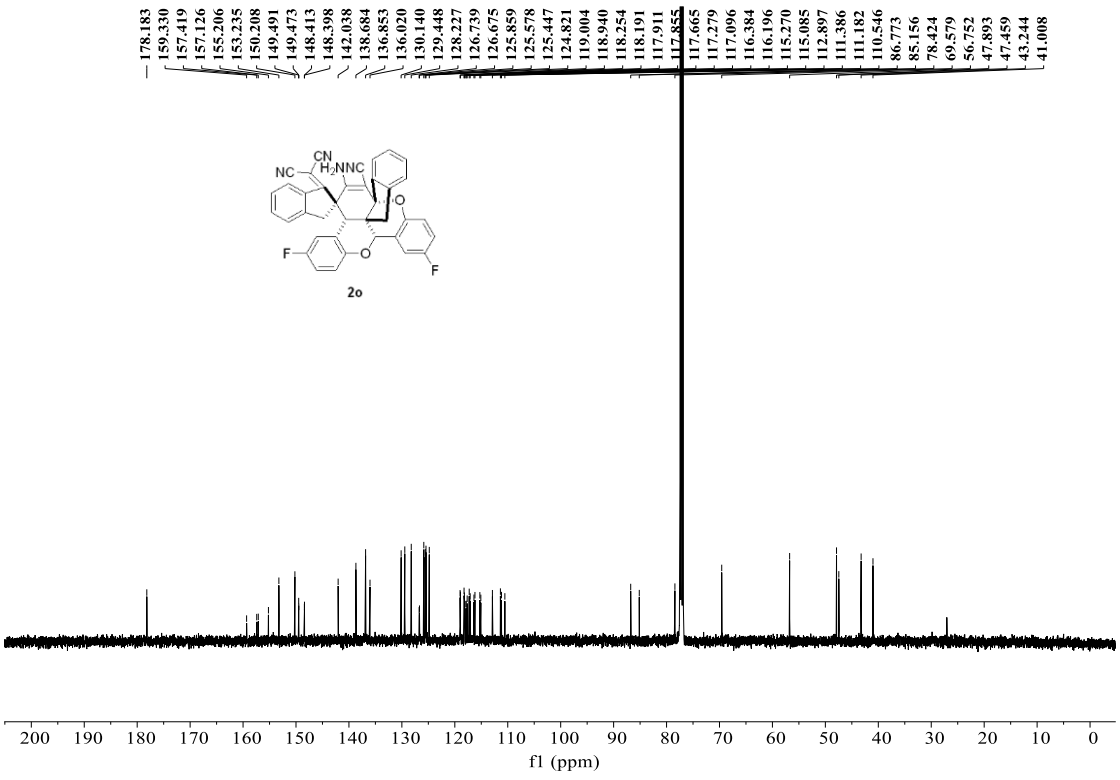
^{13}C NMR spectra for compound **2n** (125 MHz, $CDCl_3$)



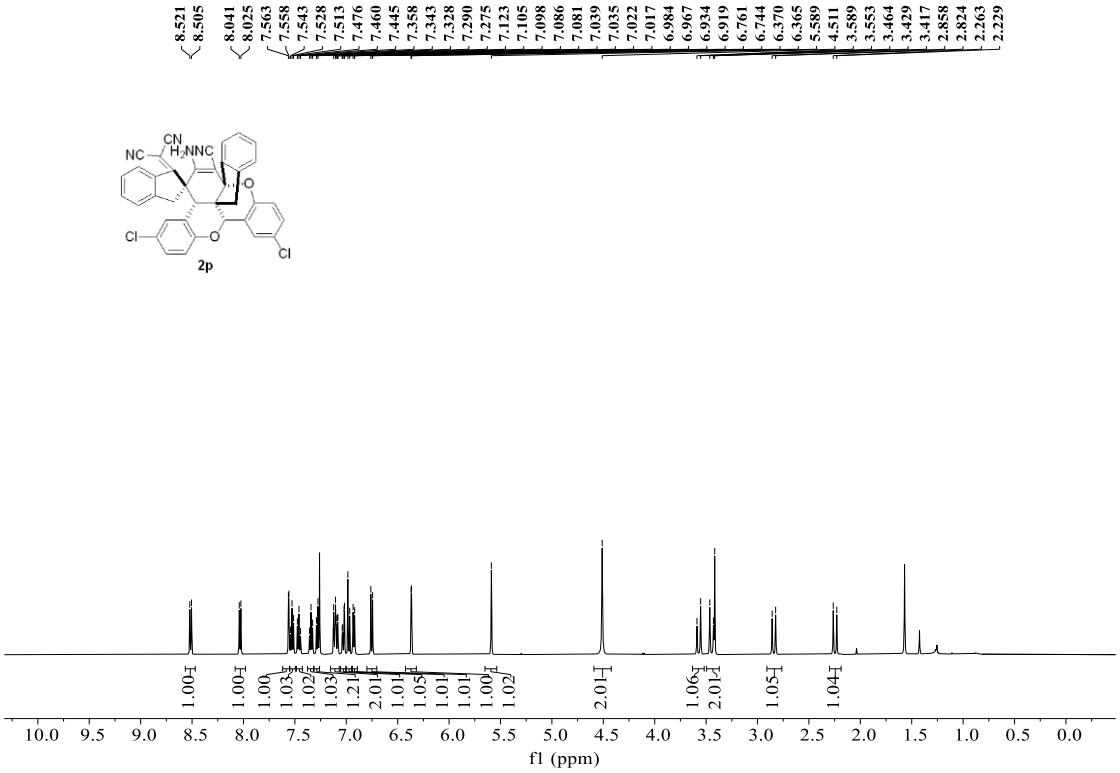
^{1}H NMR spectra for compound **2o** (500 MHz, $CDCl_3$)



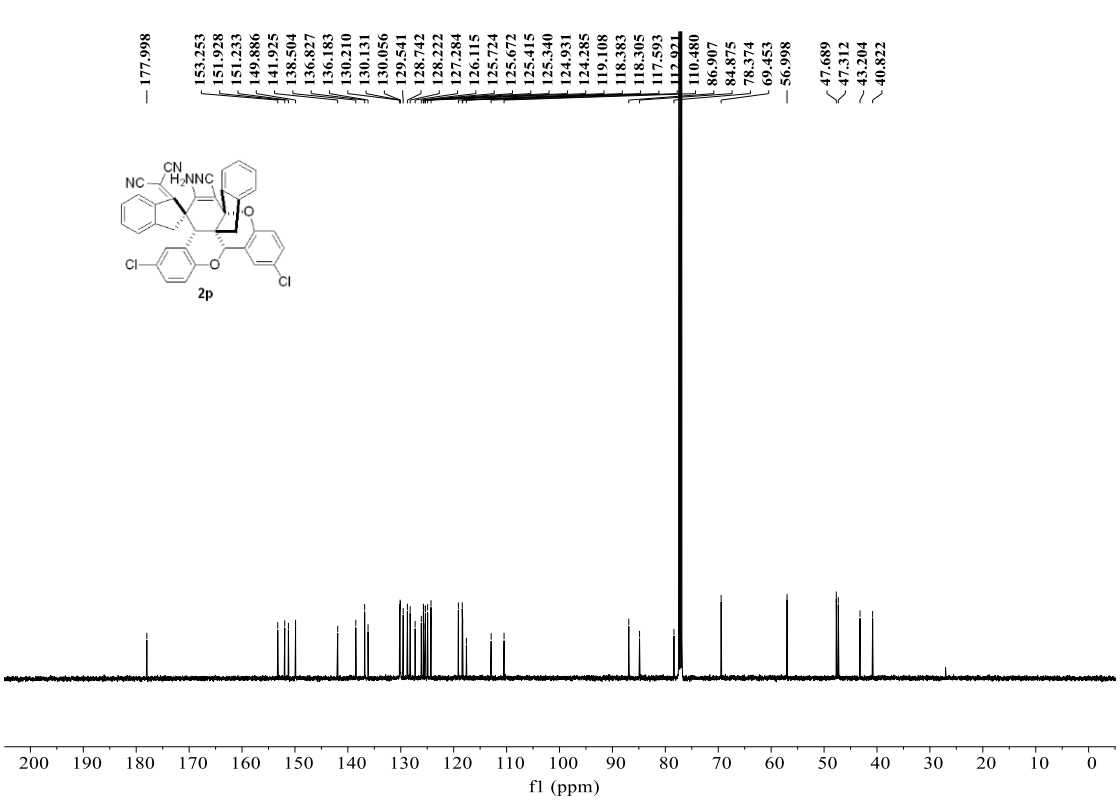
^{13}C NMR spectra for compound **2o** (125 MHz, $CDCl_3$)



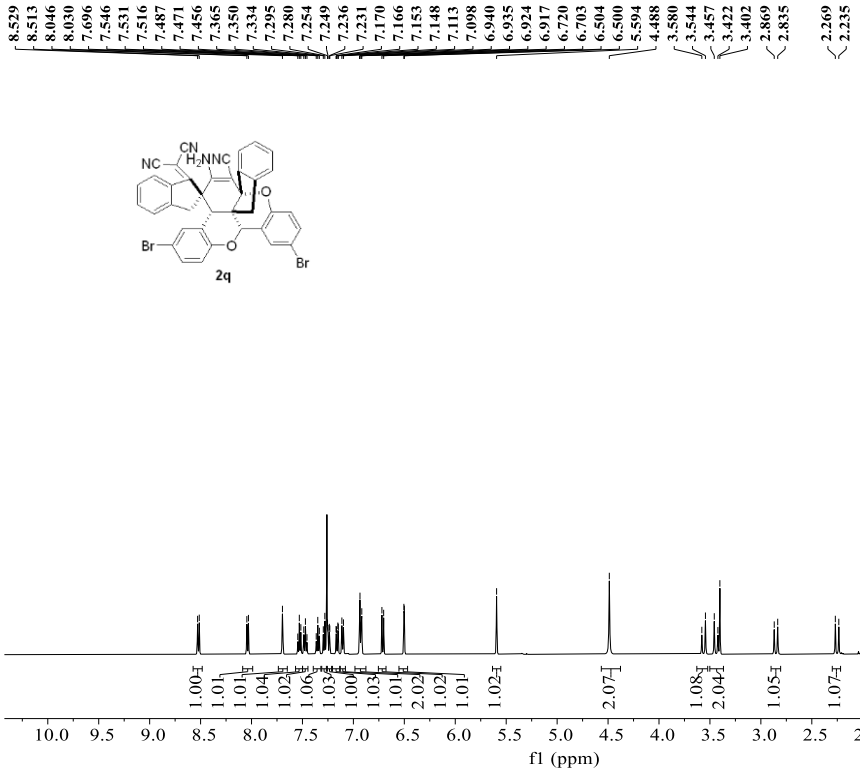
^{1}H NMR spectra for compound **2p** (500 MHz, $CDCl_3$)



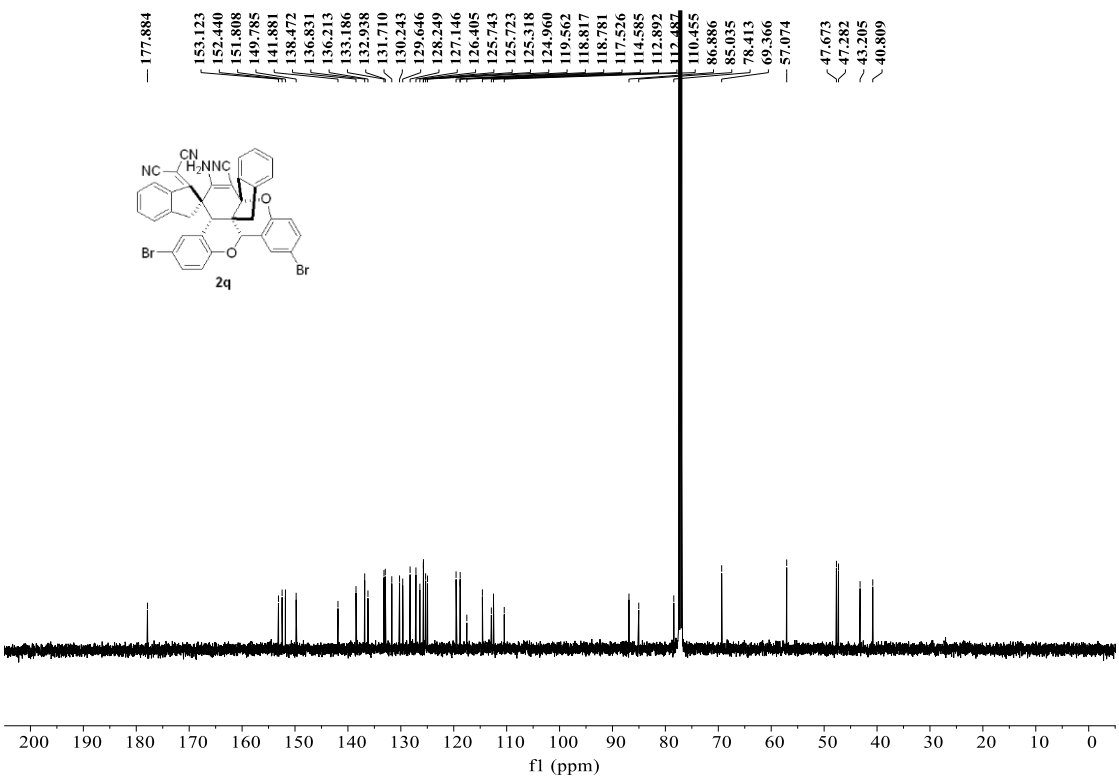
^{13}C NMR spectra for compound **2p** (125 MHz, $CDCl_3$)



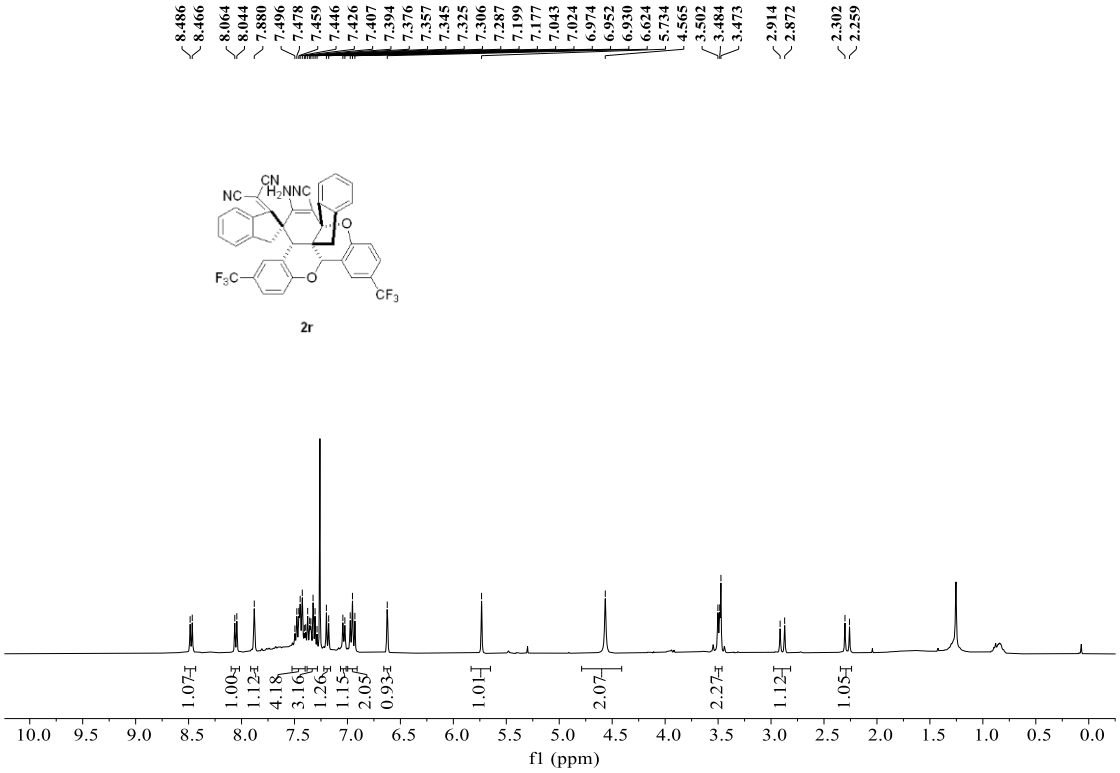
^{1}H NMR spectra for compound **2q** (500 MHz, $CDCl_3$)



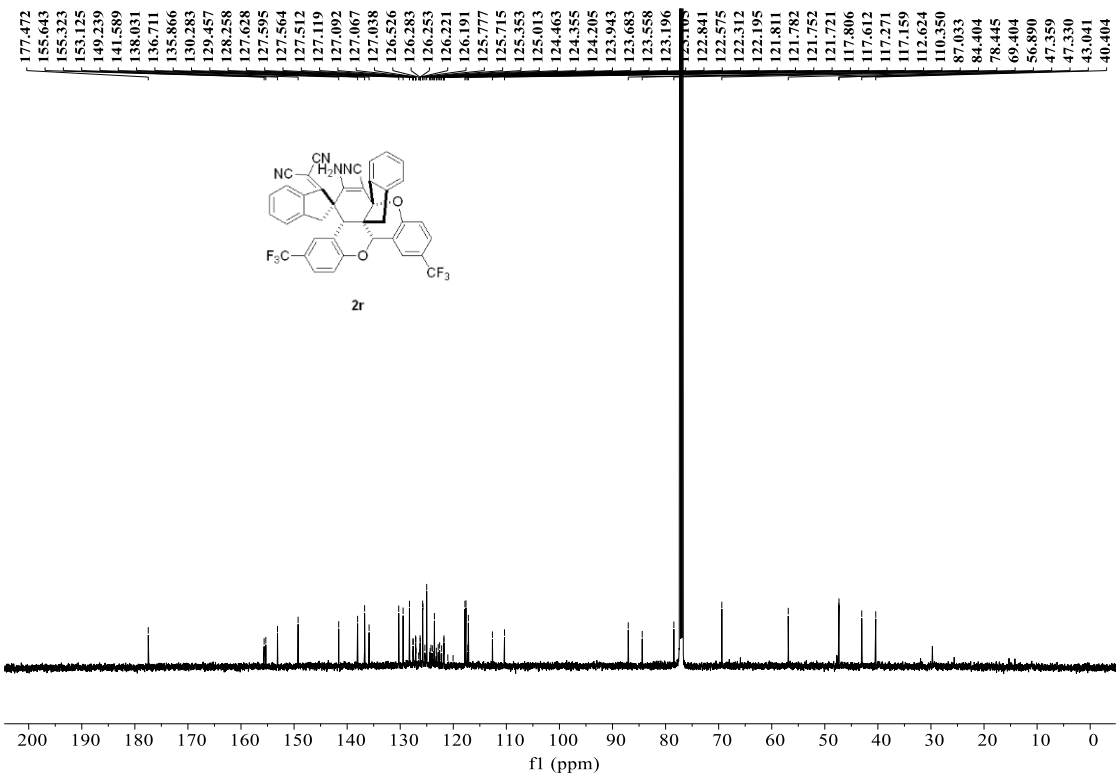
^{13}C NMR spectra for compound **2q** (125 MHz, $CDCl_3$)



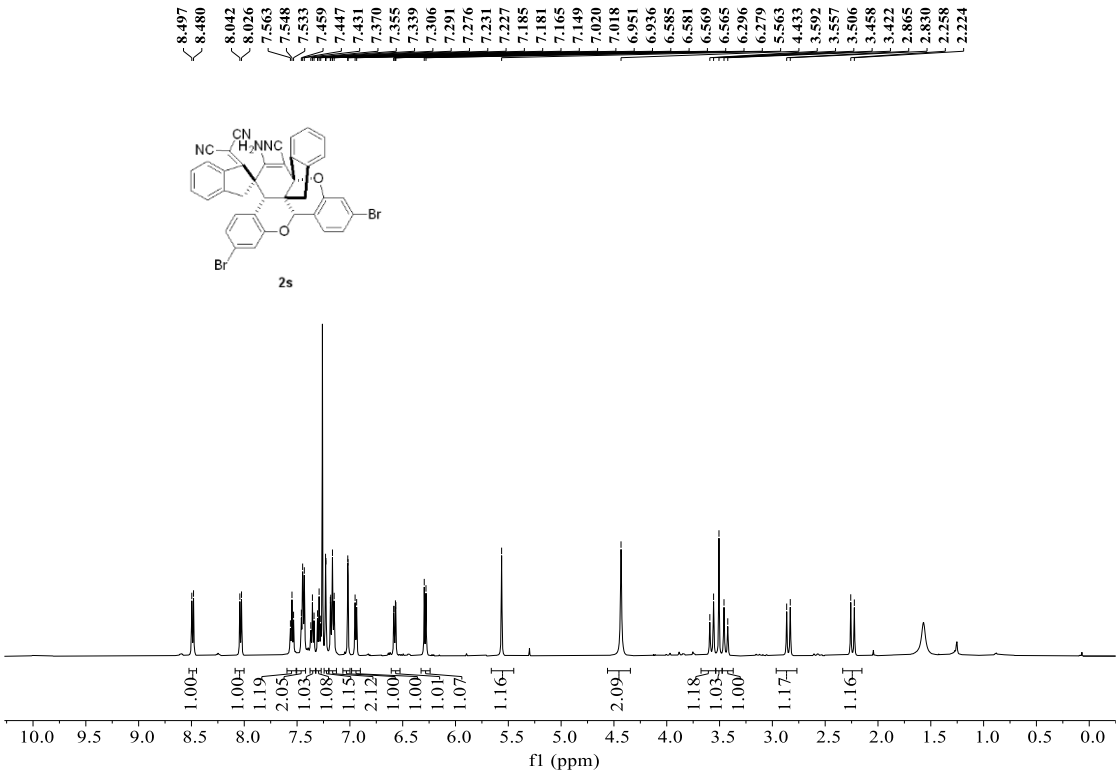
^{1}H NMR spectra for compound **2r** (400 MHz, $CDCl_3$)



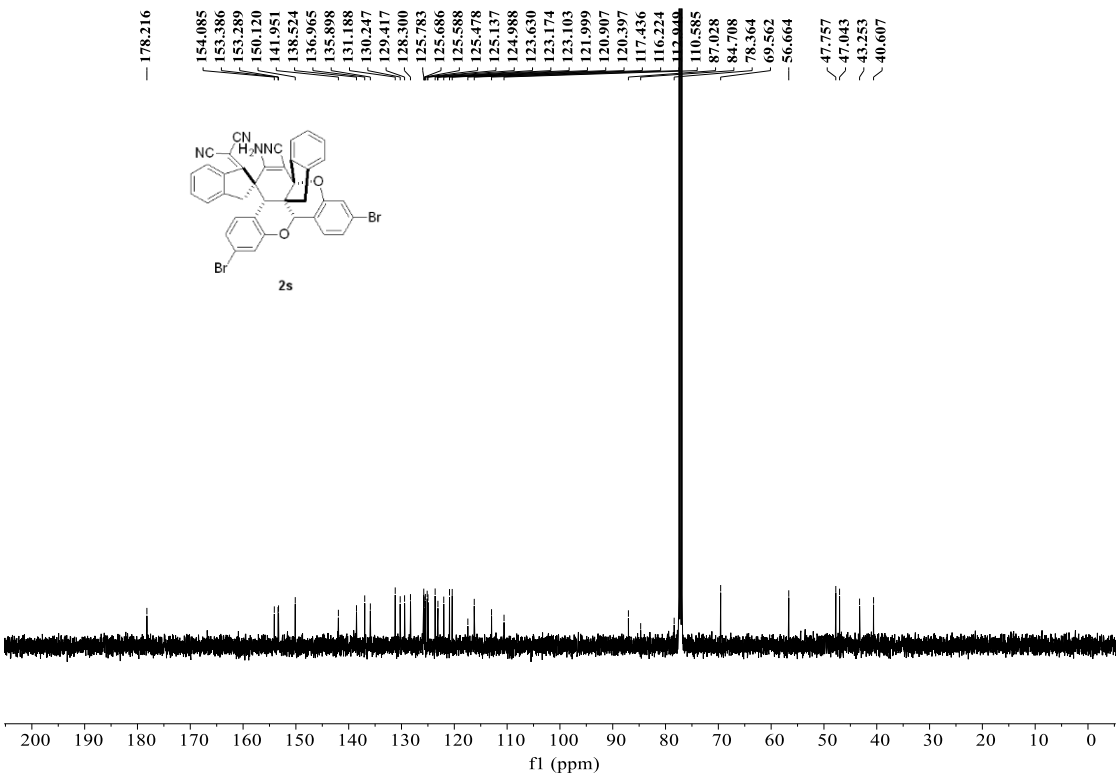
^{13}C NMR spectra for compound **2r** (125 MHz, $CDCl_3$)



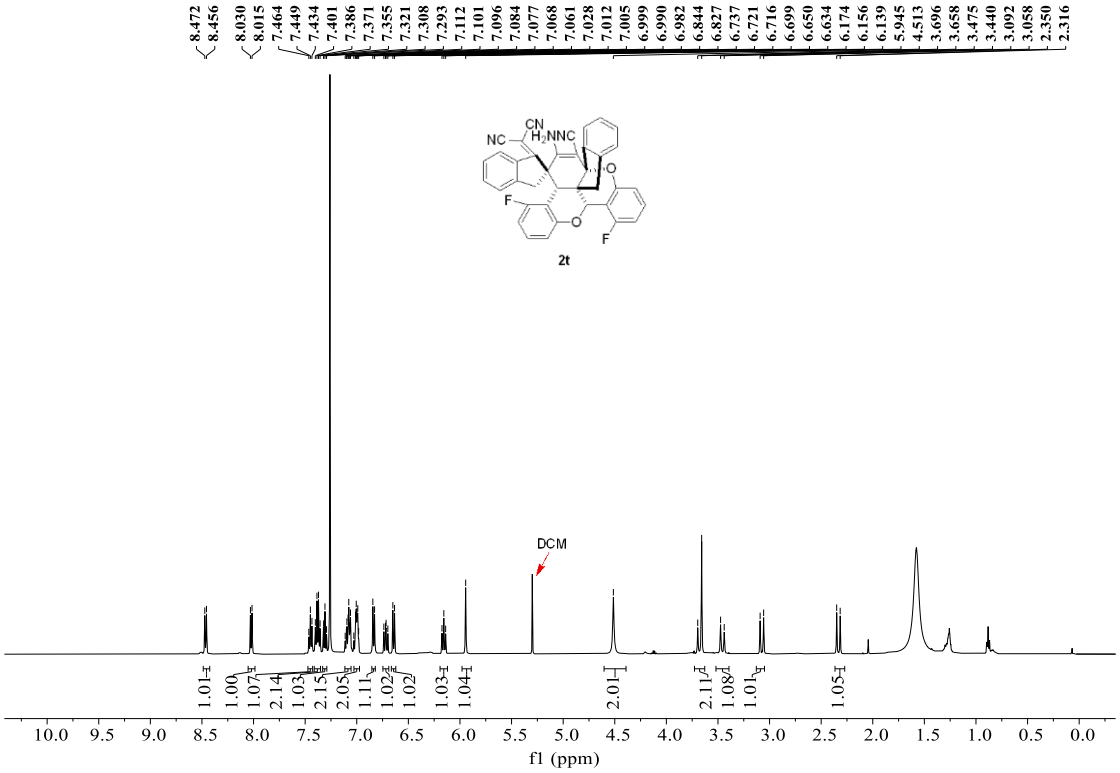
^{1}H NMR spectra for compound **2s** (500 MHz, $CDCl_3$)



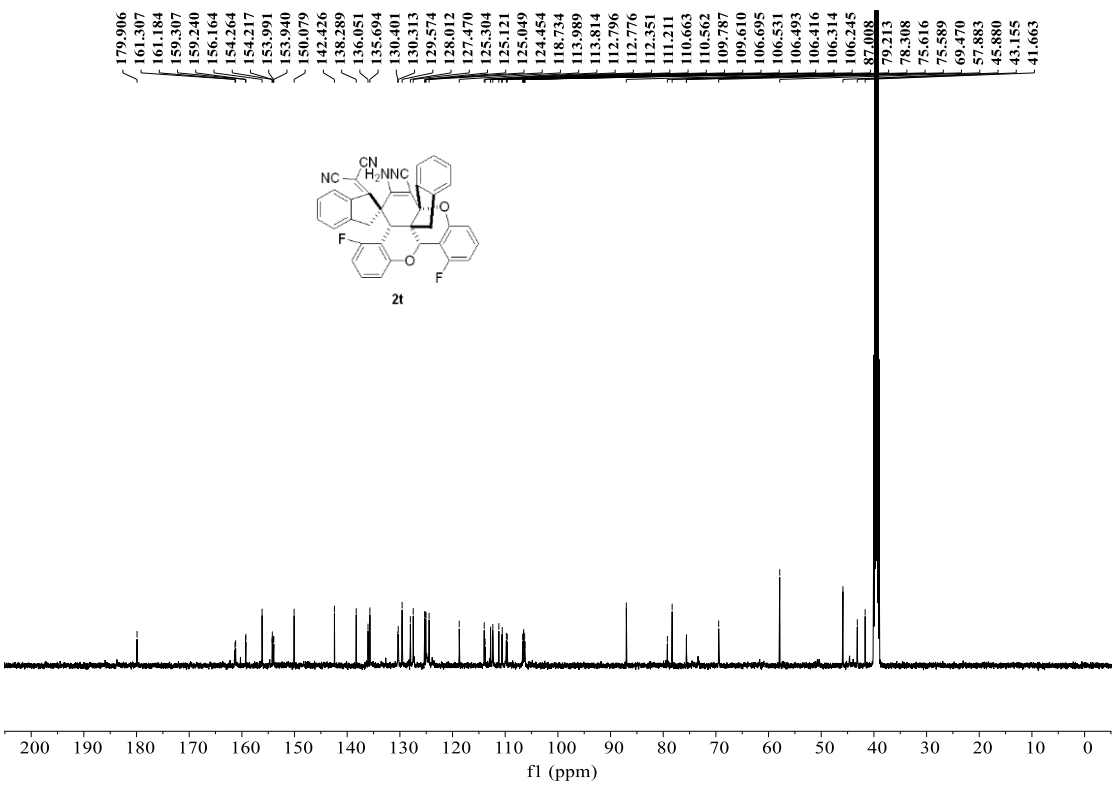
^{13}C NMR spectra for compound **2s** (125 MHz, $CDCl_3$)



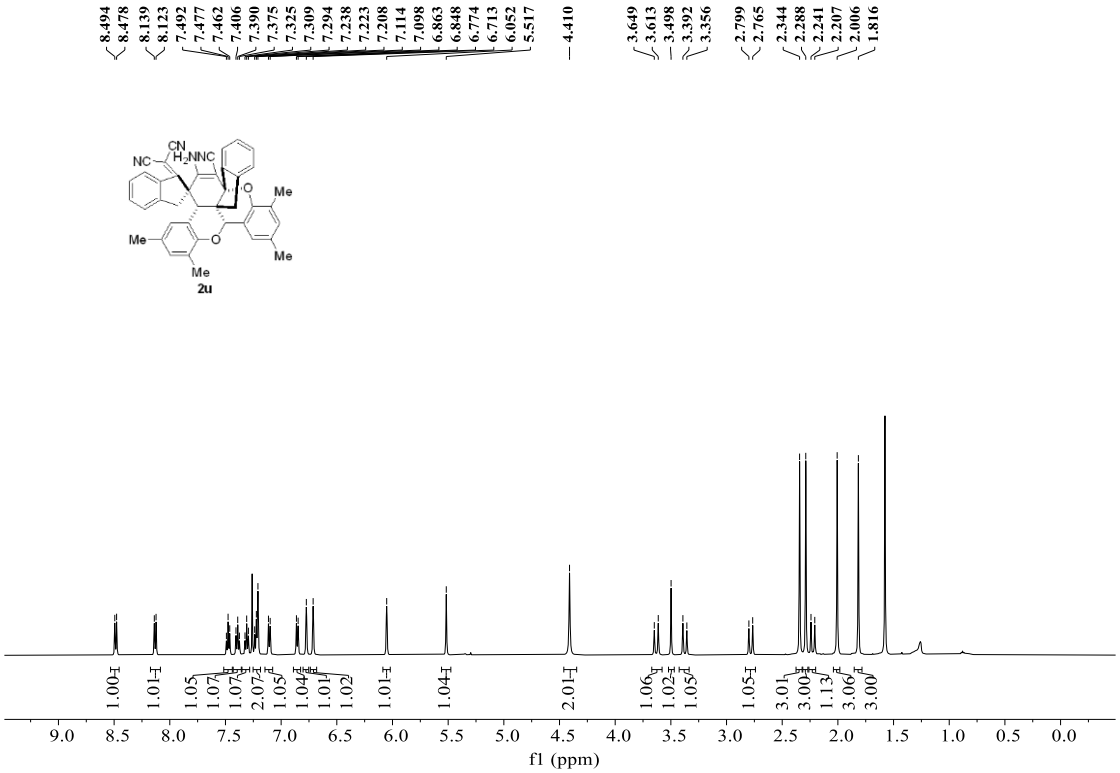
^{1}H NMR spectra for compound **2t** (500 MHz, $CDCl_3$)



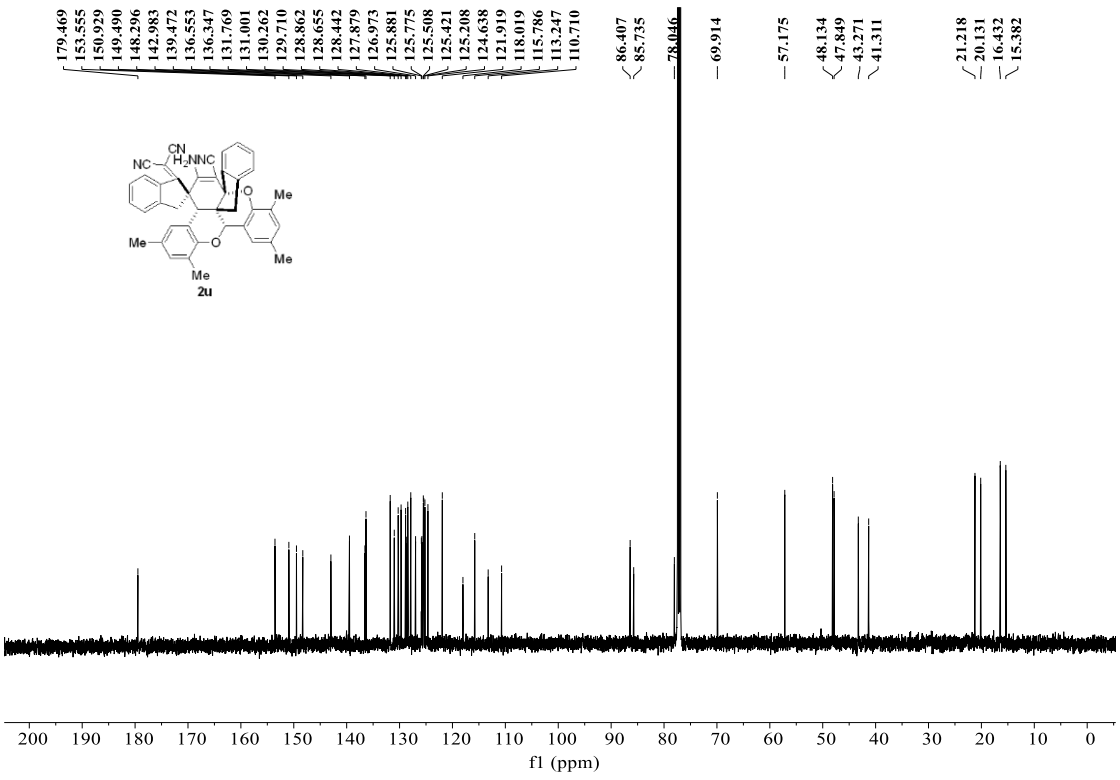
^{13}C NMR spectra for compound **2t** (125 MHz, DMSO-d_6)



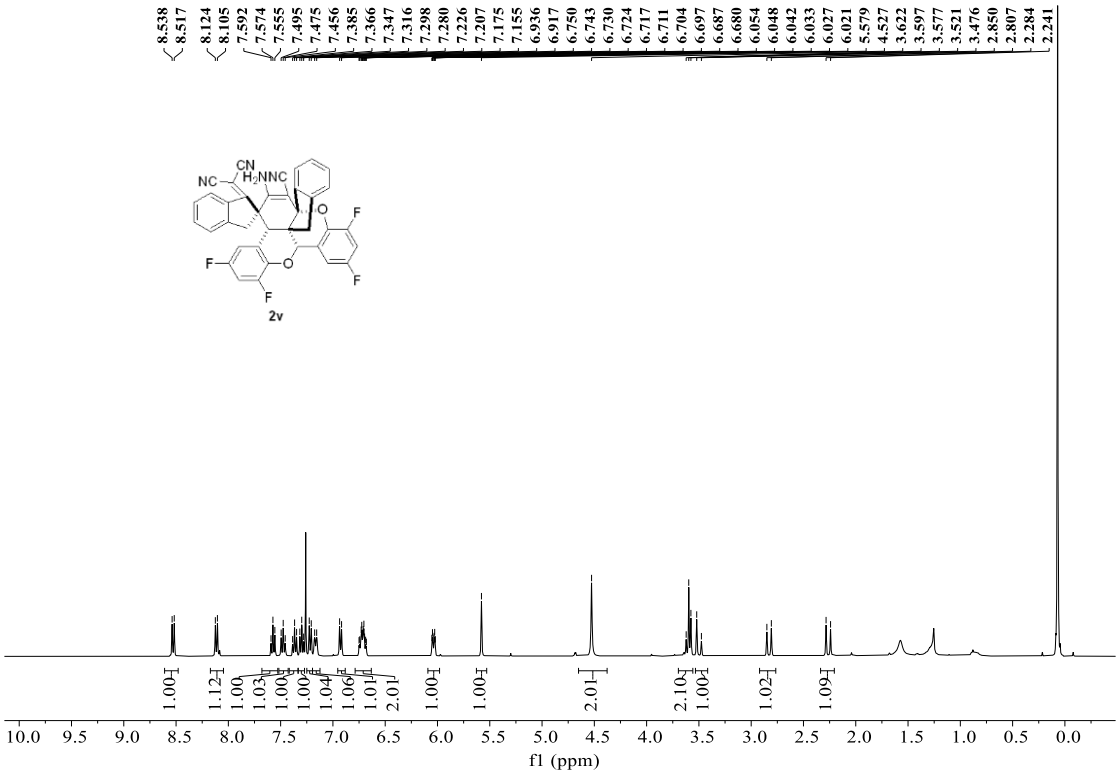
^{1}H NMR spectra for compound **2u** (500 MHz, $CDCl_3$)



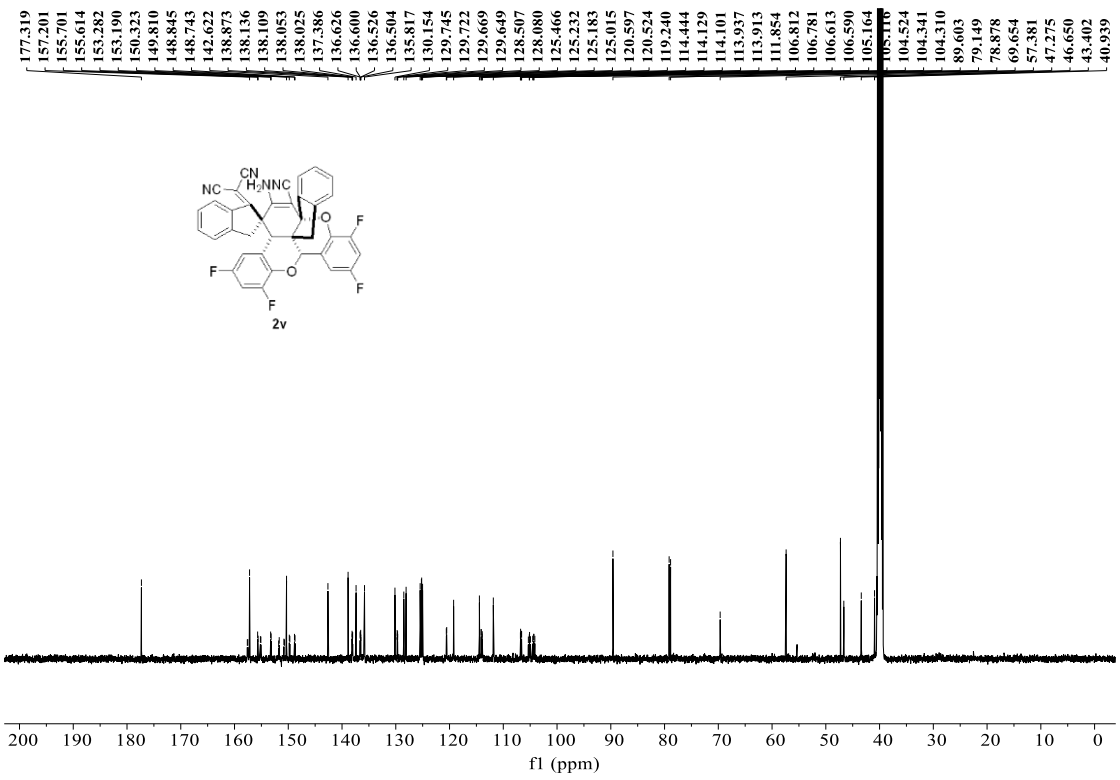
^{13}C NMR spectra for compound **2u** (125 MHz, $CDCl_3$)



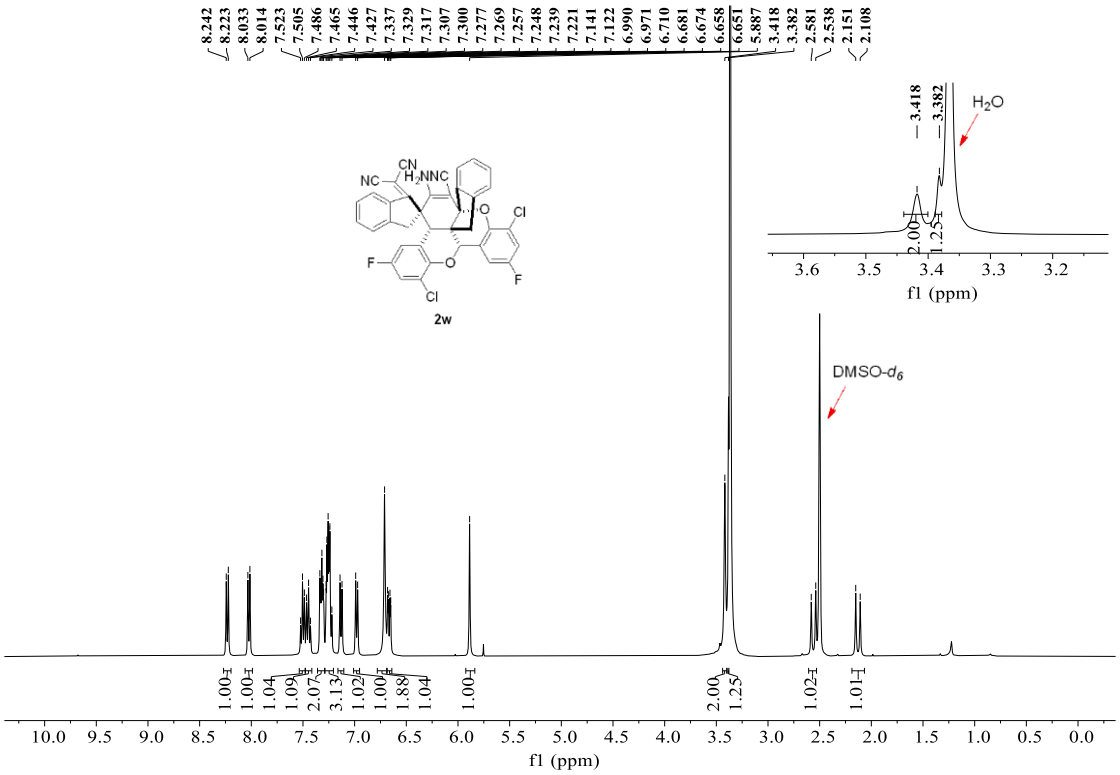
^{1}H NMR spectra for compound **2v** (400 MHz, $CDCl_3$)



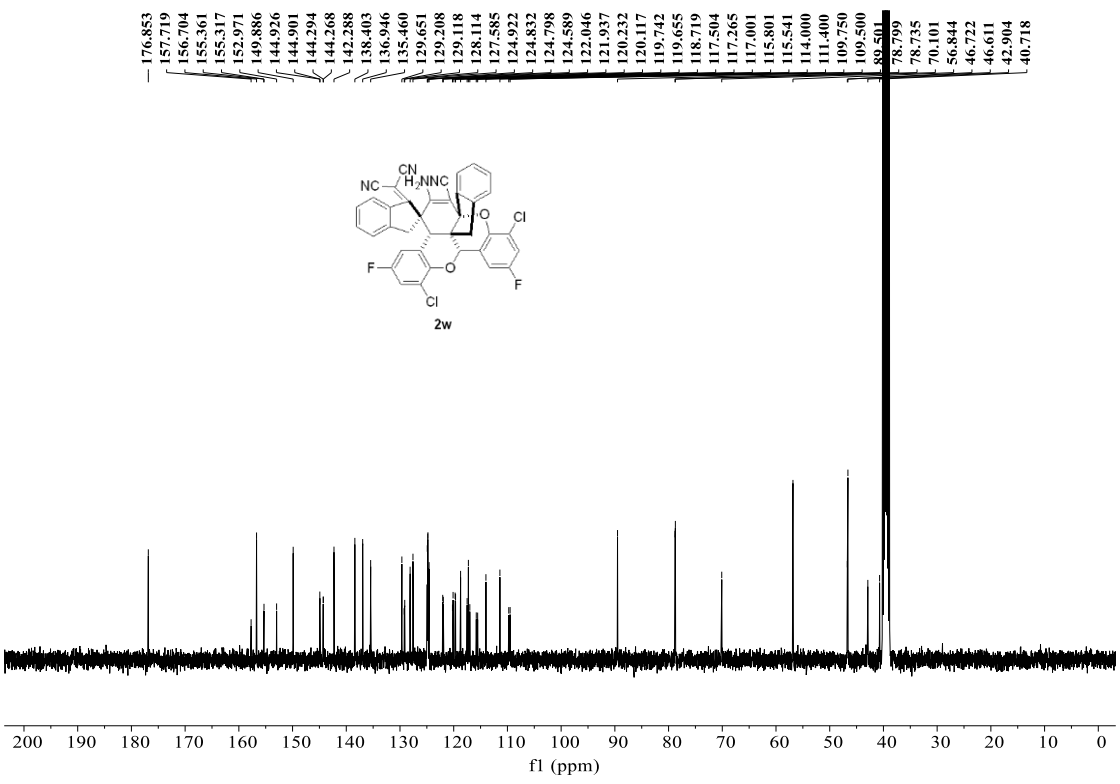
^{13}C NMR spectra for compound **2v** (125 MHz, DMSO-d_6)



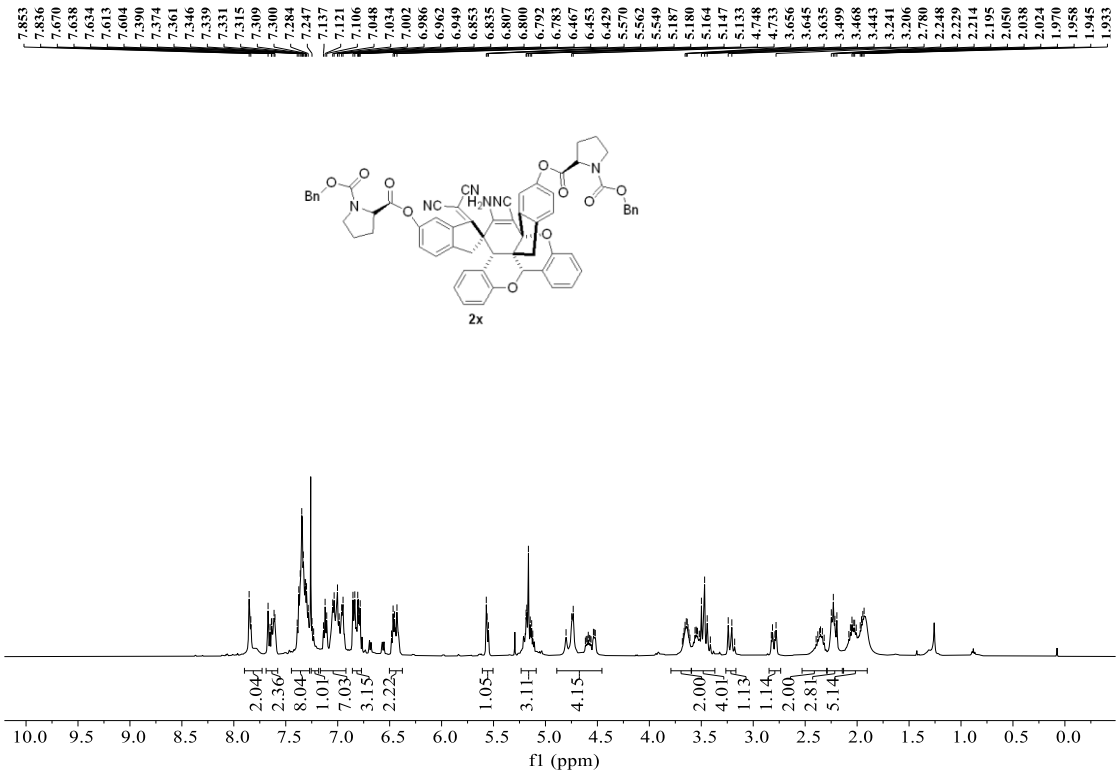
^{1}H NMR spectra for compound **2w** (400 MHz, DMSO-d_6)



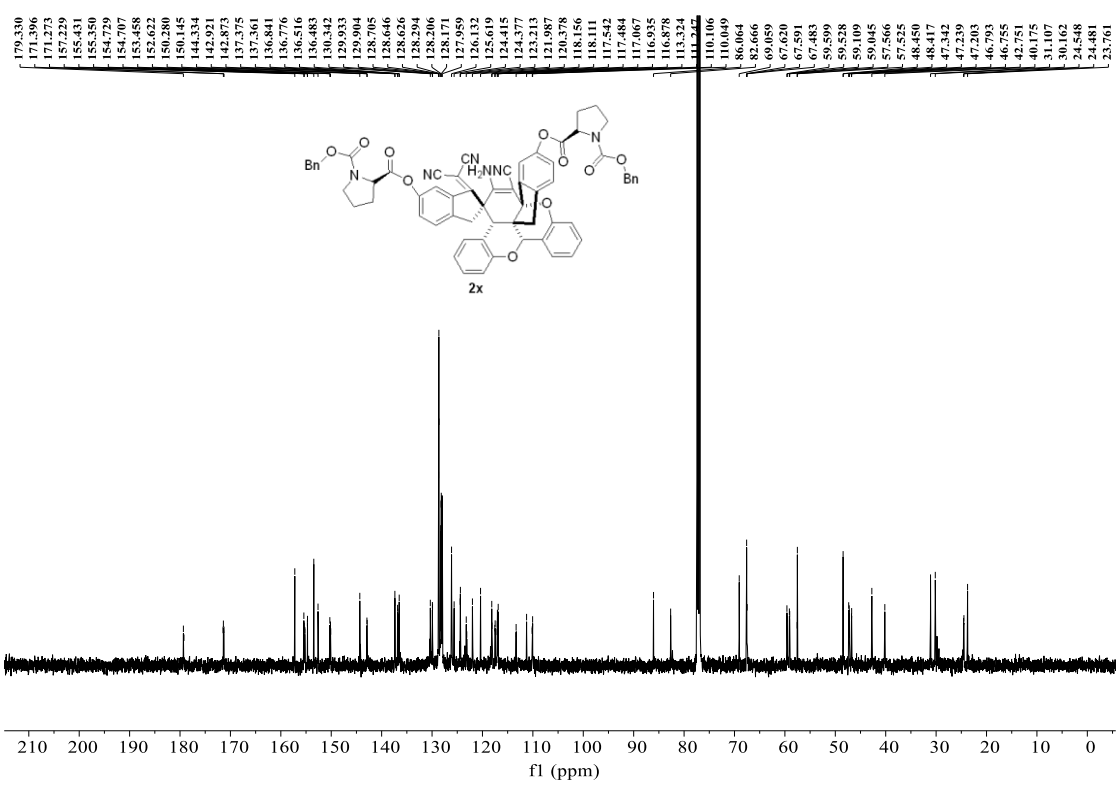
^{13}C NMR spectra for compound **2w** (100 MHz, DMSO-d_6)



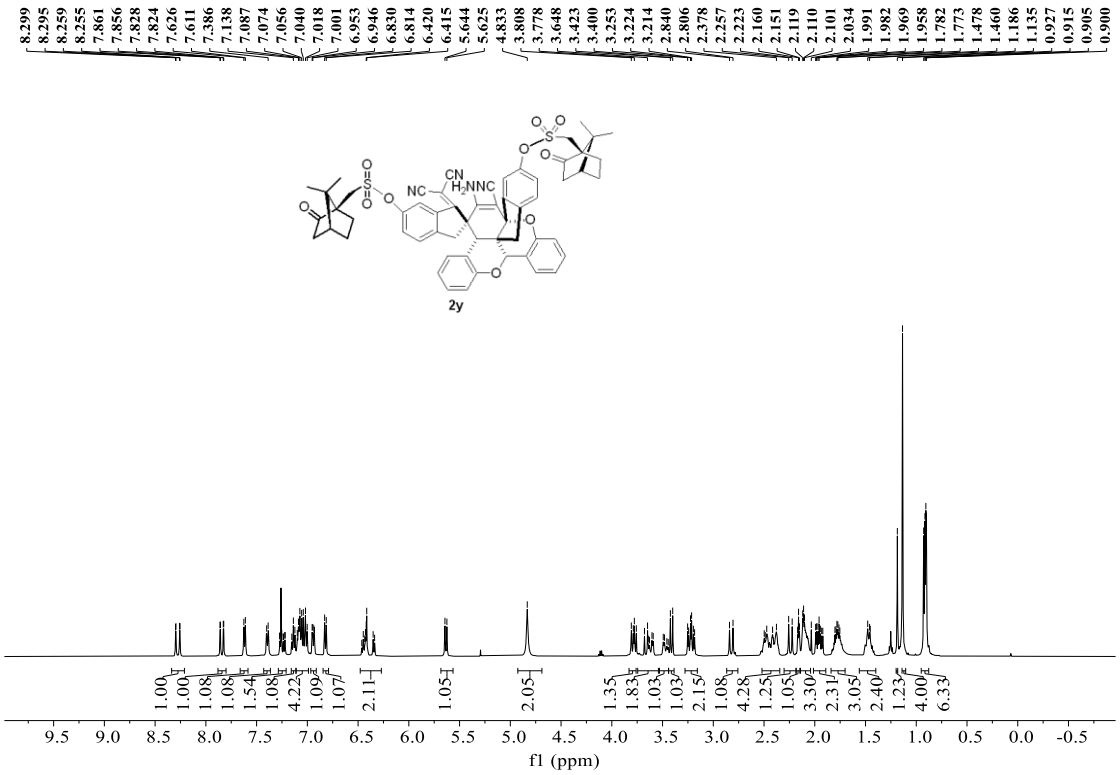
^{1}H NMR spectra for compound **2x** (500 MHz, $CDCl_3$)



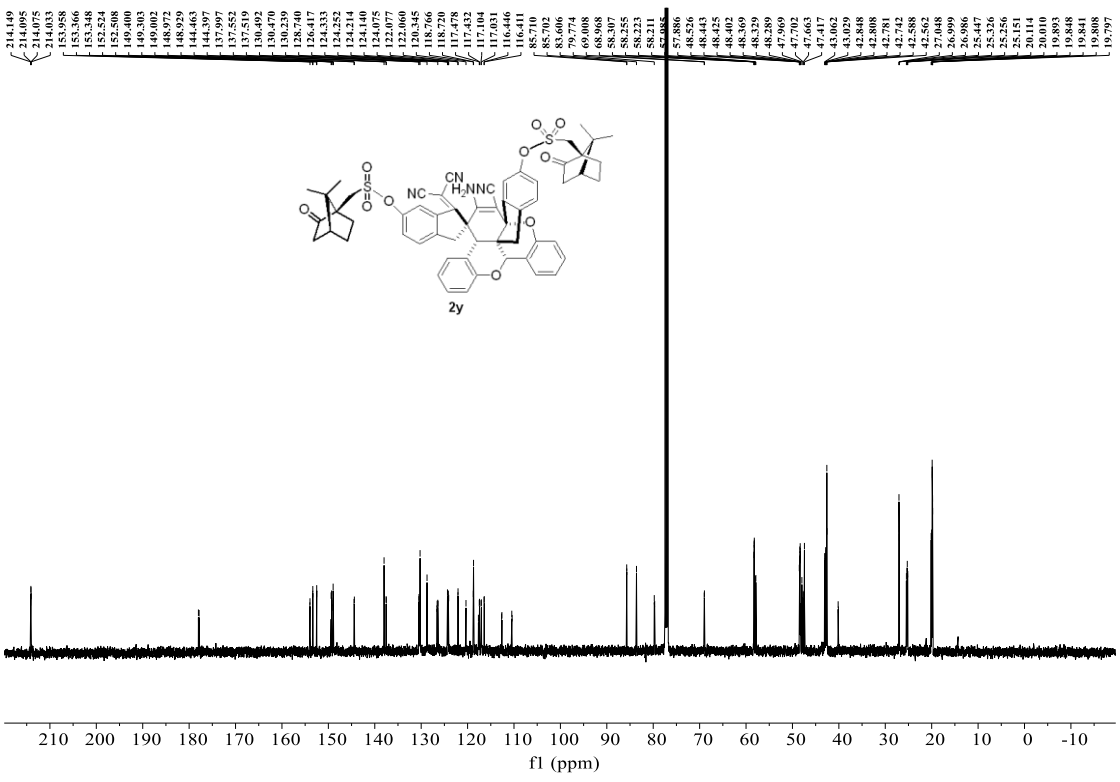
^{13}C NMR spectra for compound **2x** (125 MHz, $CDCl_3$)



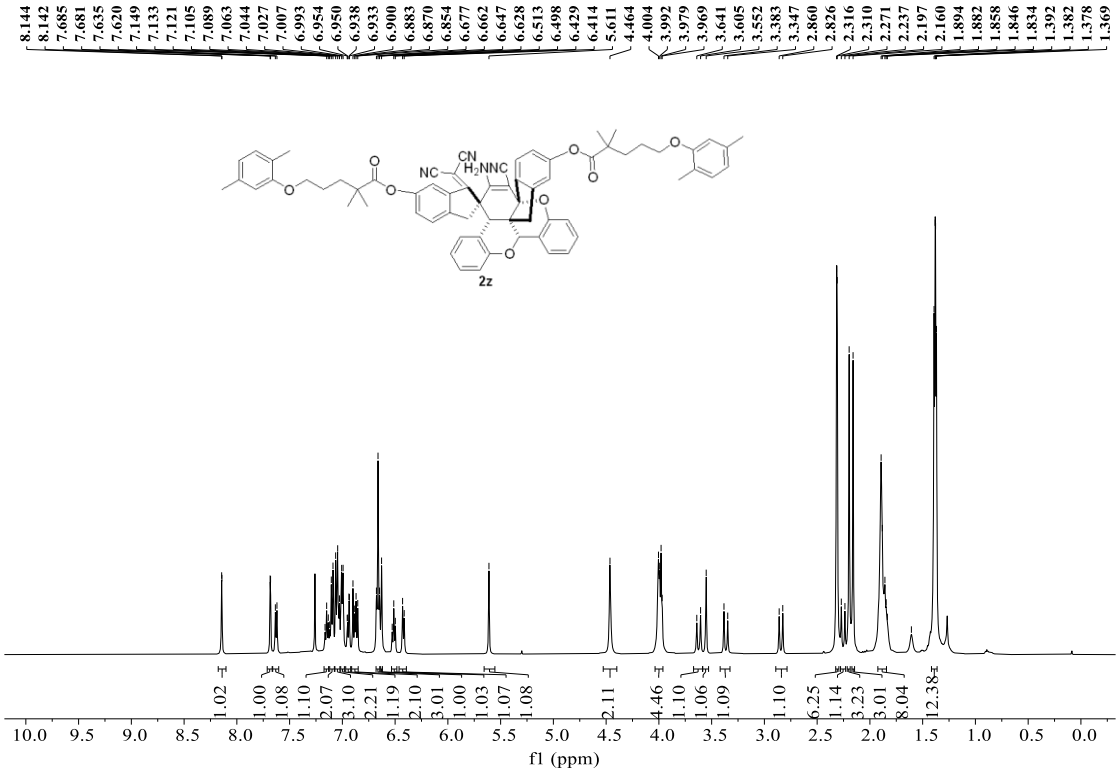
^{1}H NMR spectra for compound **2y** (500 MHz, $CDCl_3$)



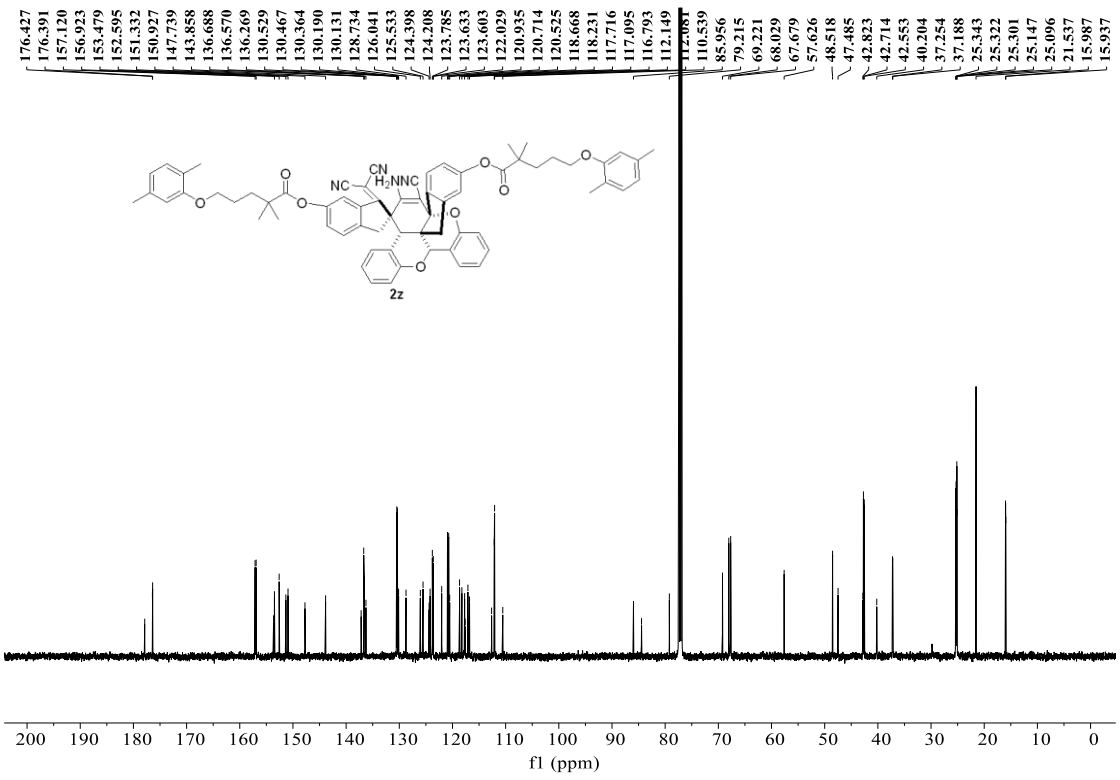
^{13}C NMR spectra for compound **2y** (125 MHz, $CDCl_3$)



^{1}H NMR spectra for compound **2z** (500 MHz, $CDCl_3$)

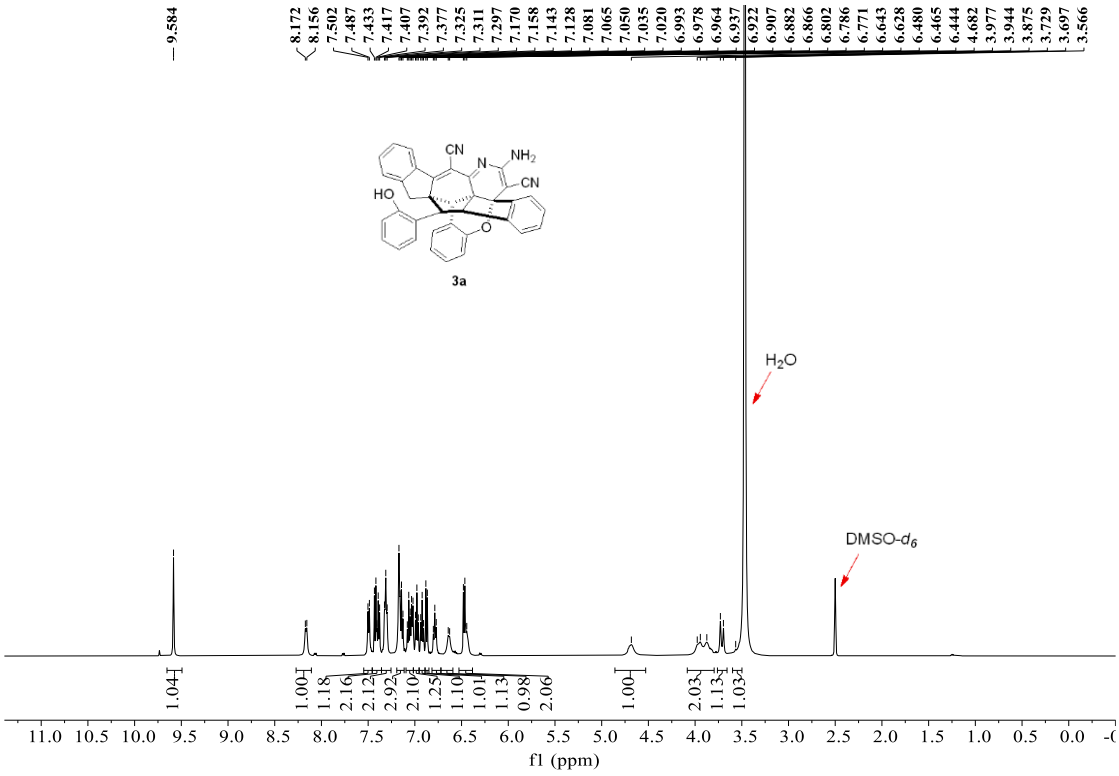


^{13}C NMR spectra for compound **2z** (125 MHz, $CDCl_3$)

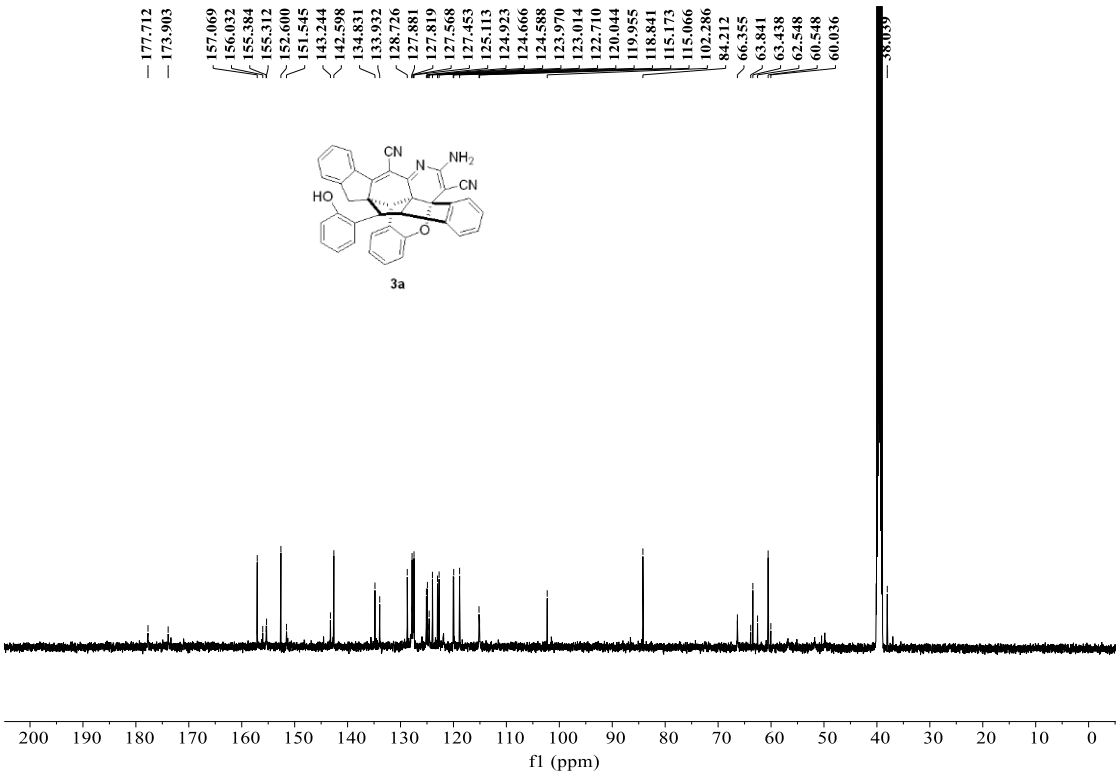


14.3 NMR spectra for compounds 3

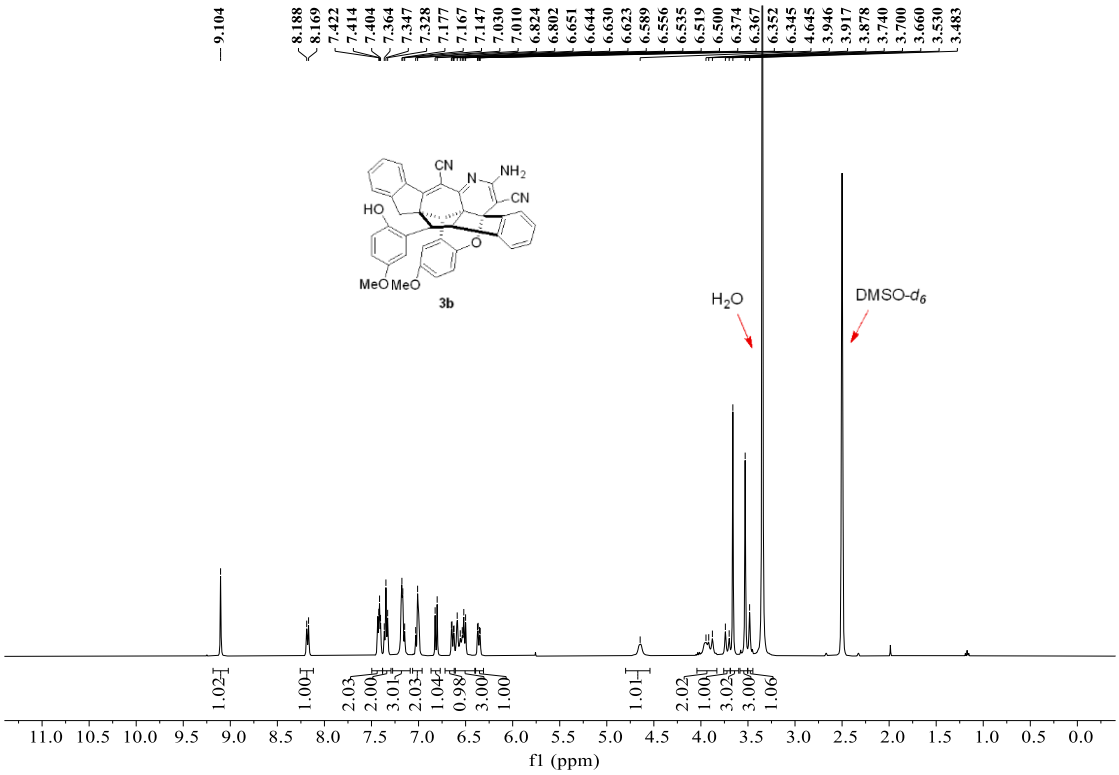
^{1}H NMR spectra for compound **3a** (500 MHz, DMSO-d_6)



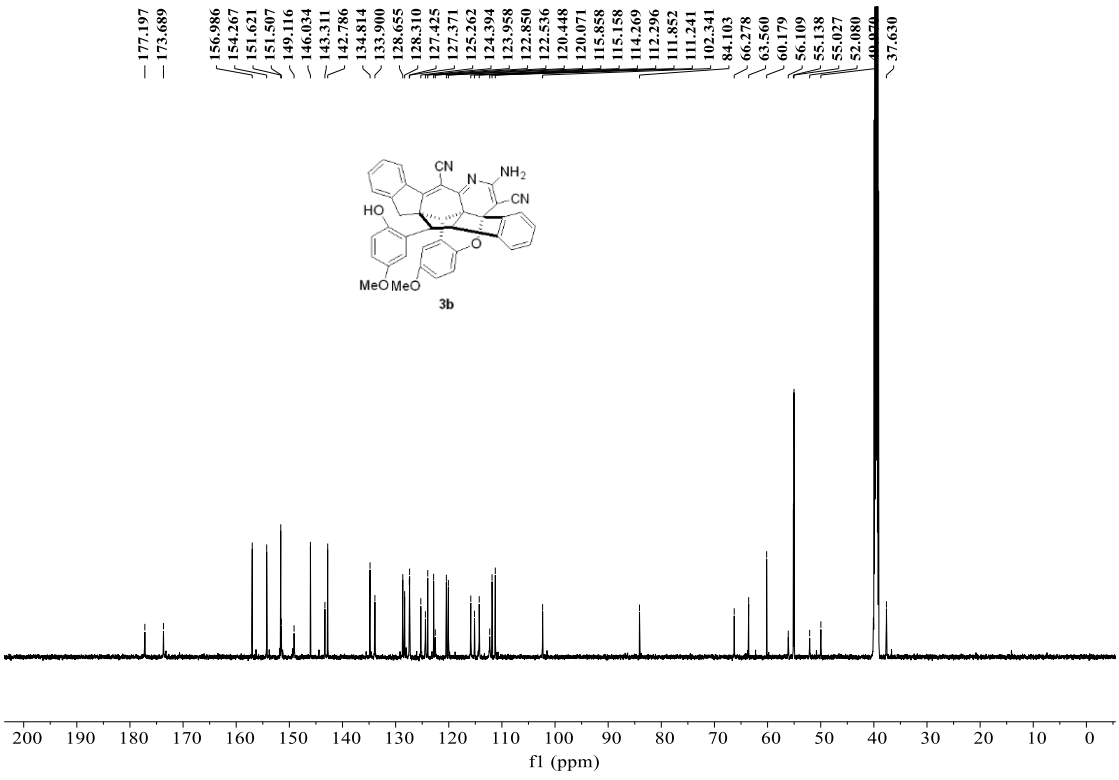
^{13}C NMR spectra for compound **3a** (125 MHz, DMSO-d_6)



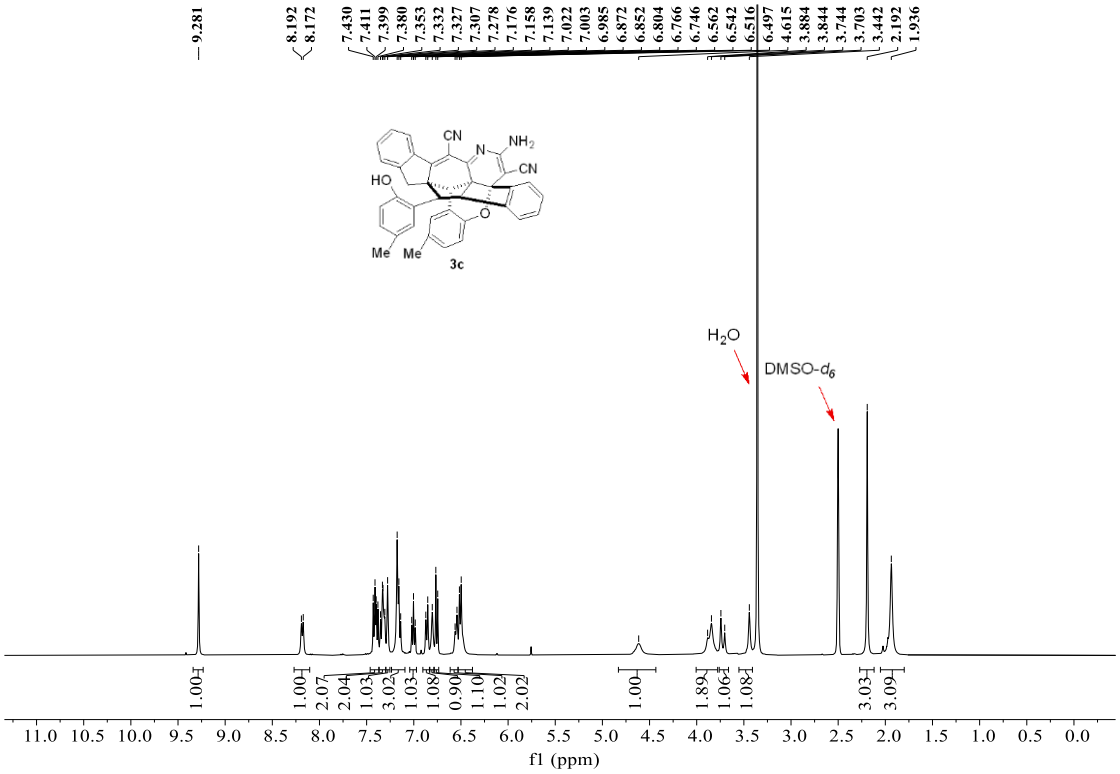
^{1}H NMR spectra for compound **3b** (400 MHz, DMSO-d_6)



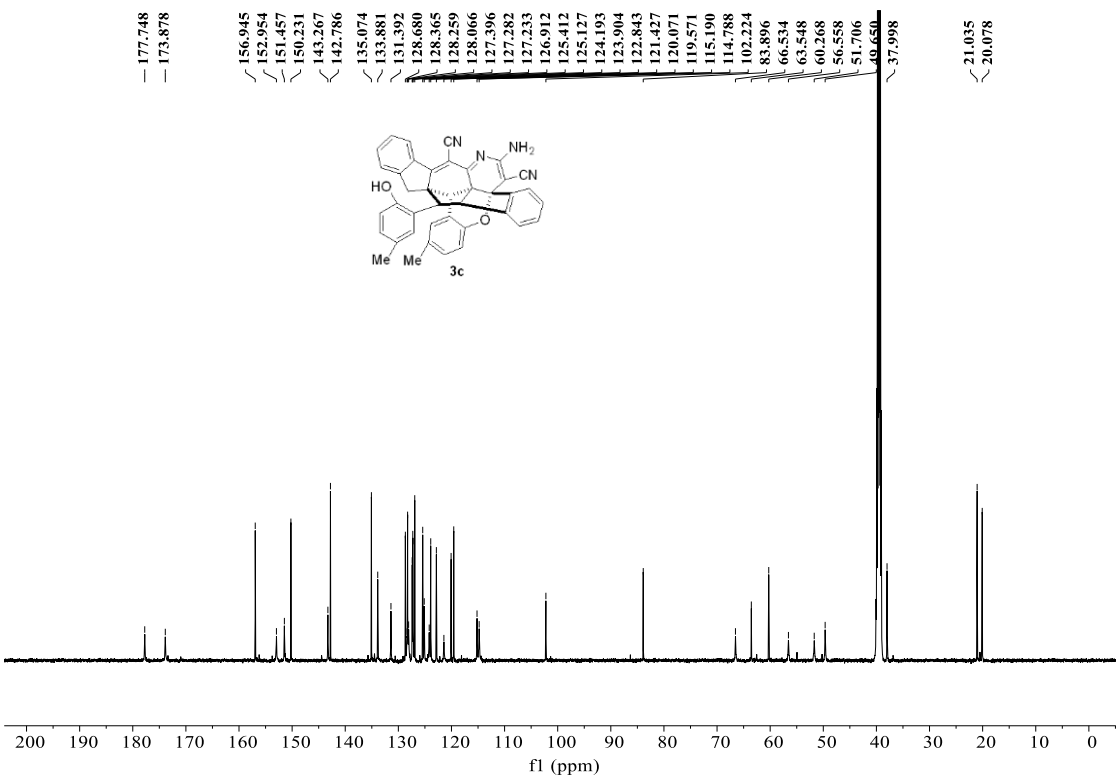
^{13}C NMR spectra for compound **3b** (150 MHz, DMSO-d_6)



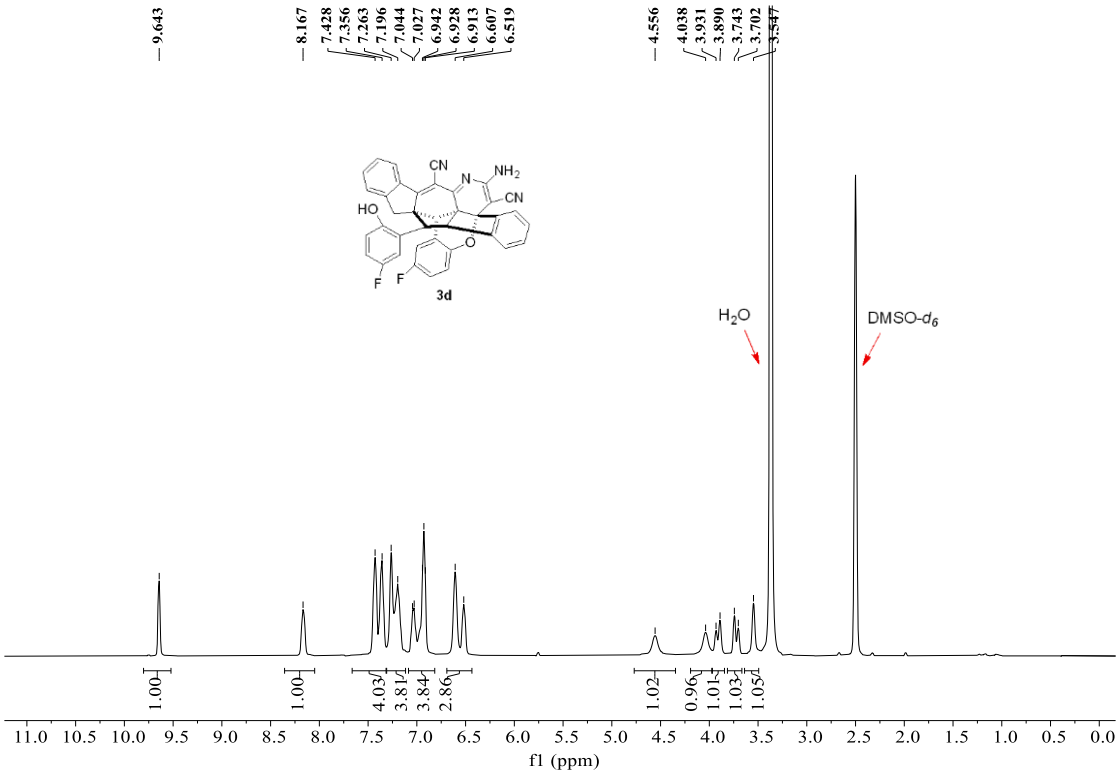
^{1}H NMR spectra for compound **3c** (400 MHz, DMSO-d_6)



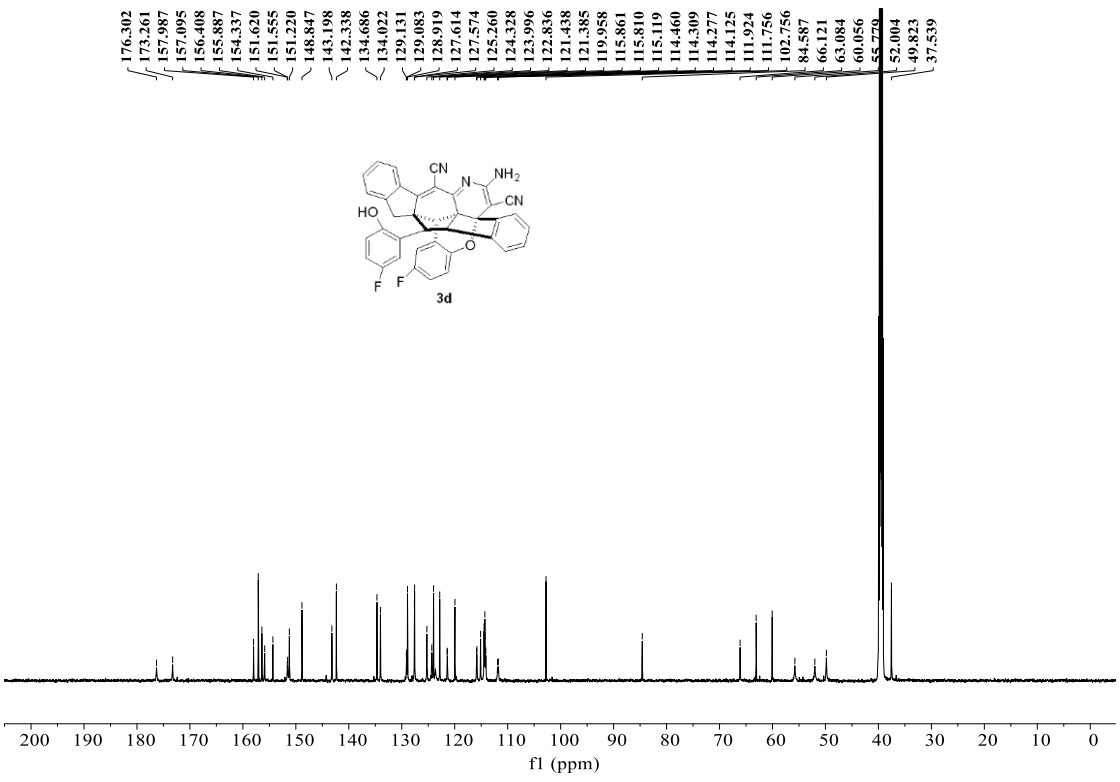
^{13}C NMR spectra for compound **3c** (150 MHz, DMSO-d_6)



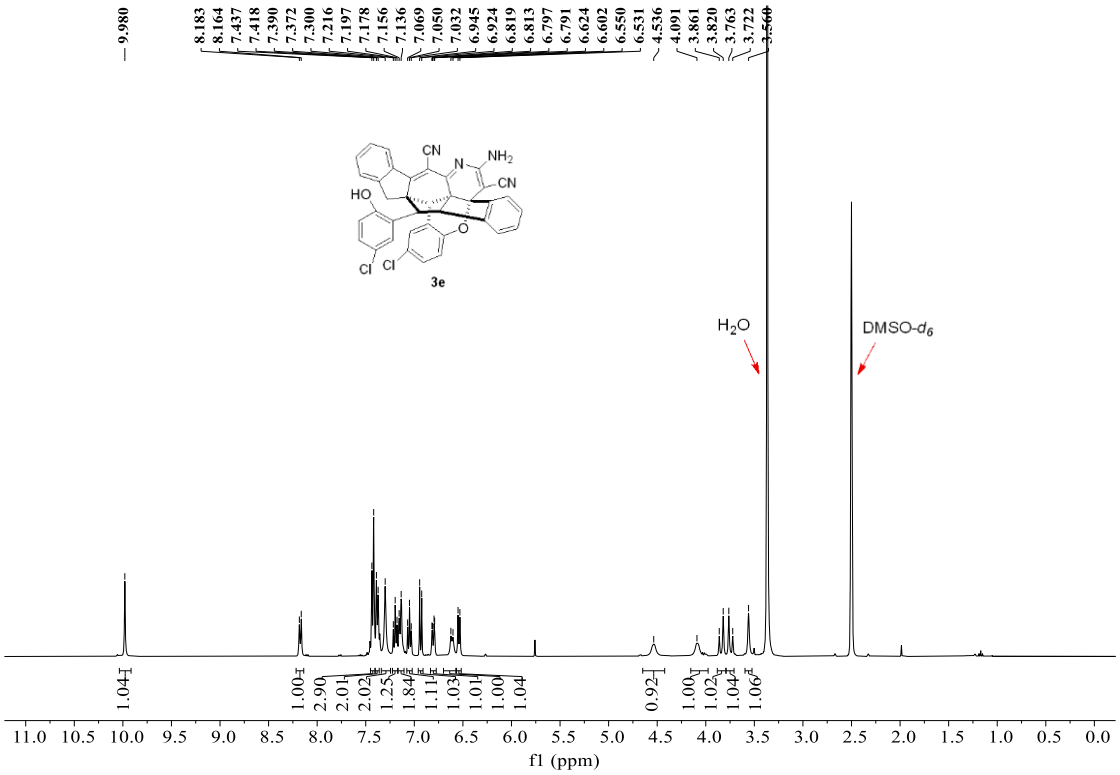
^{1}H NMR spectra for compound **3d** (400 MHz, DMSO-d_6)



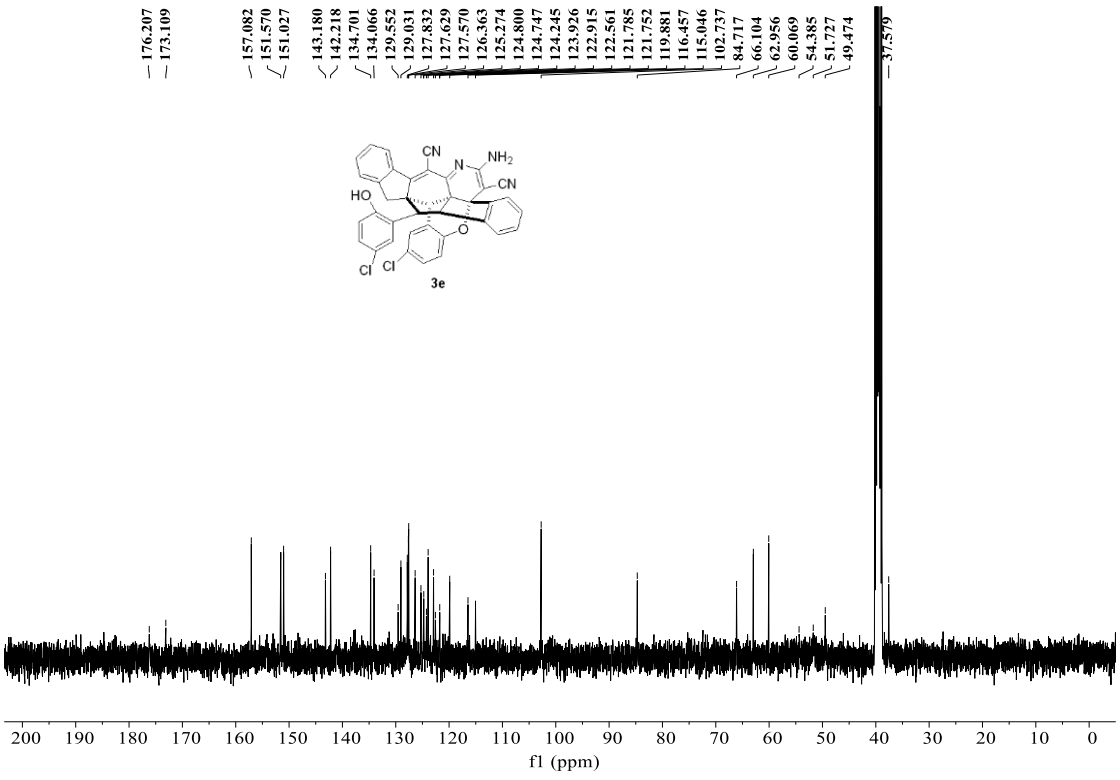
^{13}C NMR spectra for compound **3d** (150 MHz, DMSO-d_6)



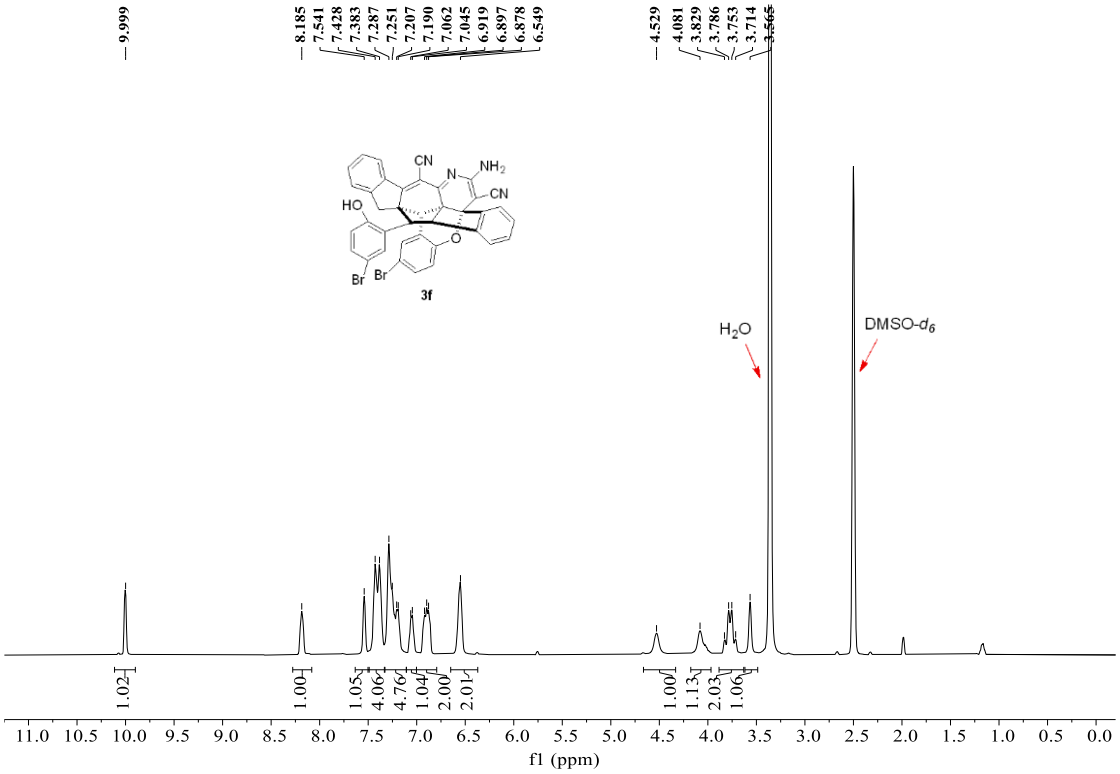
^{1}H NMR spectra for compound **3e** (400 MHz, DMSO-d_6)



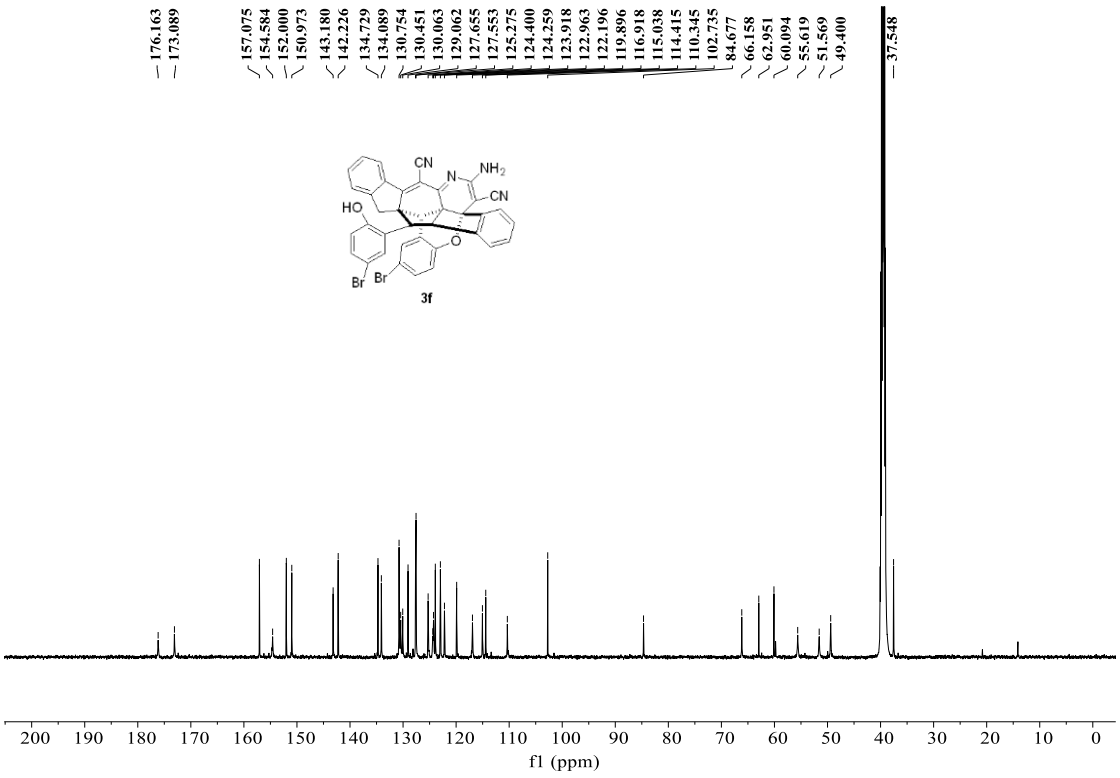
^{13}C NMR spectra for compound **3e** (125 MHz, DMSO-d_6)



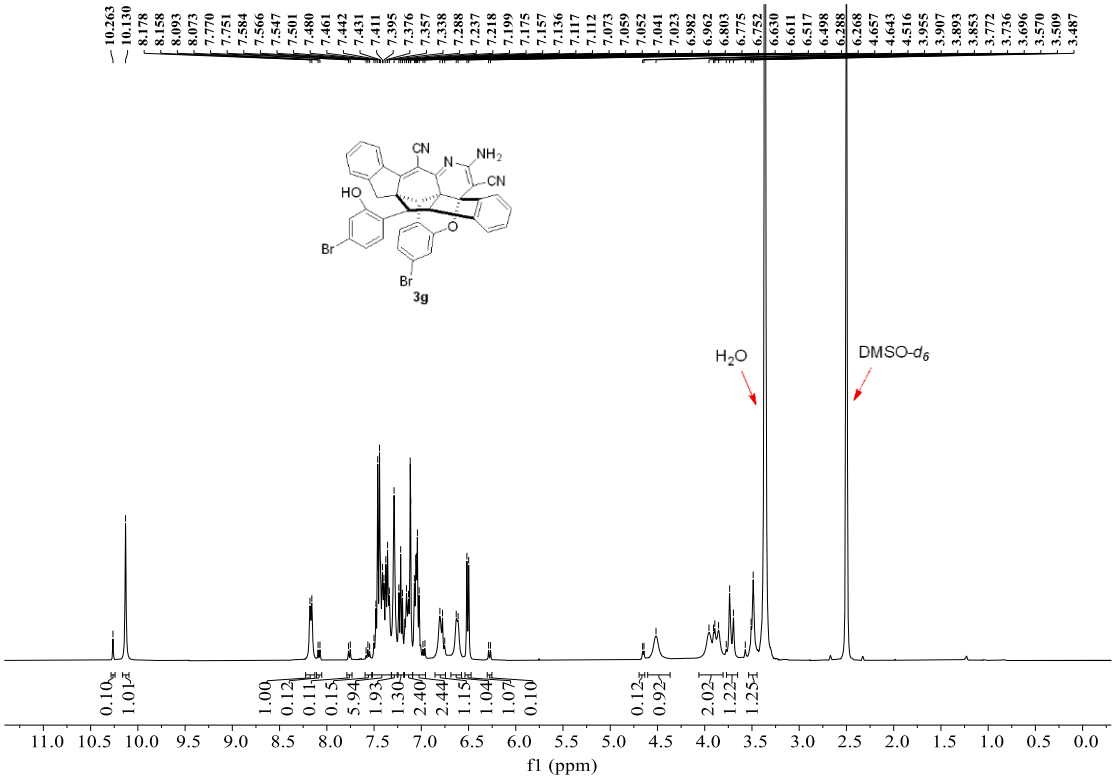
^{1}H NMR spectra for compound **3f** (400 MHz, DMSO-d_6)



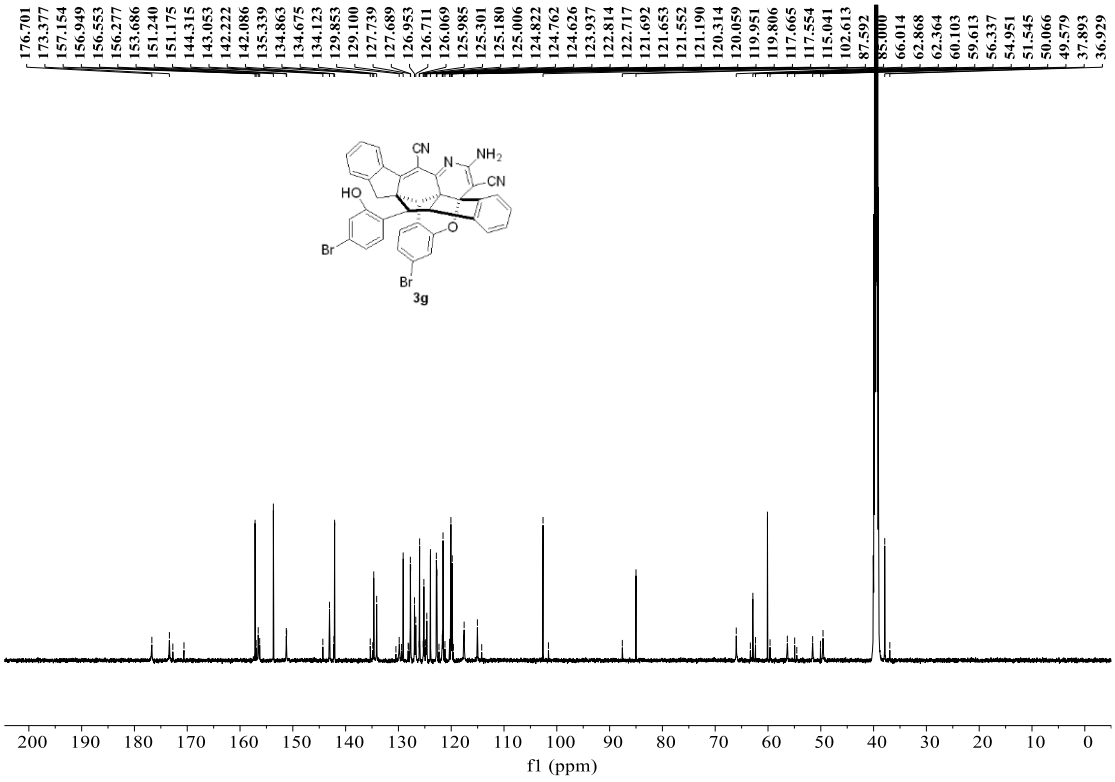
^{13}C NMR spectra for compound **3f** (150 MHz, DMSO-d_6)



^{1}H NMR spectra for compound **3g** (400 MHz, DMSO-d_6, a mixture of two isomers)

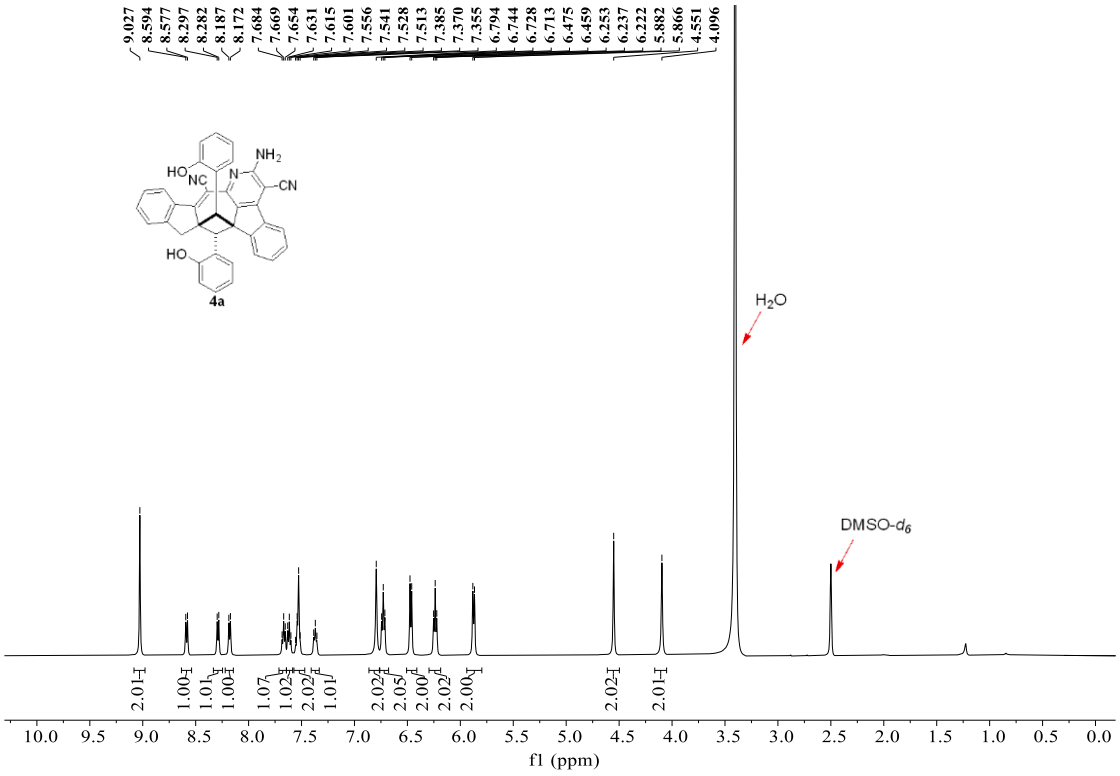


^{13}C NMR spectra for compound **3g** (150 MHz, DMSO-d_6, a mixture of two isomers)

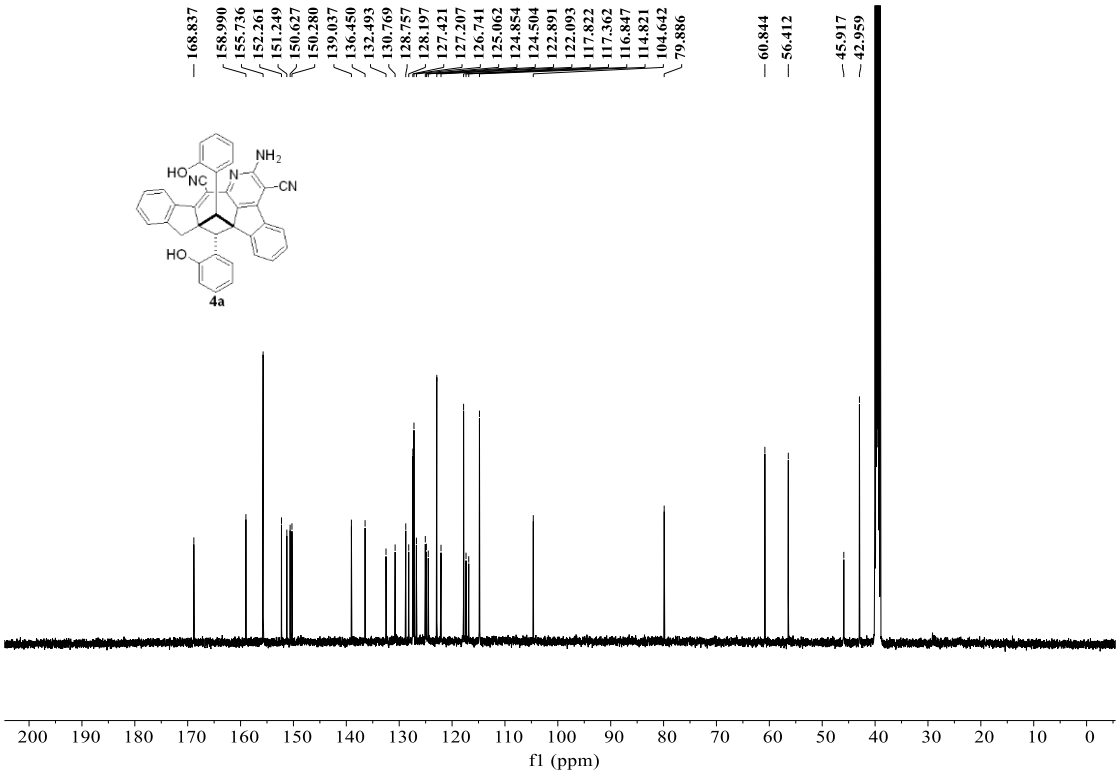


14.4 NMR spectra for compounds 4

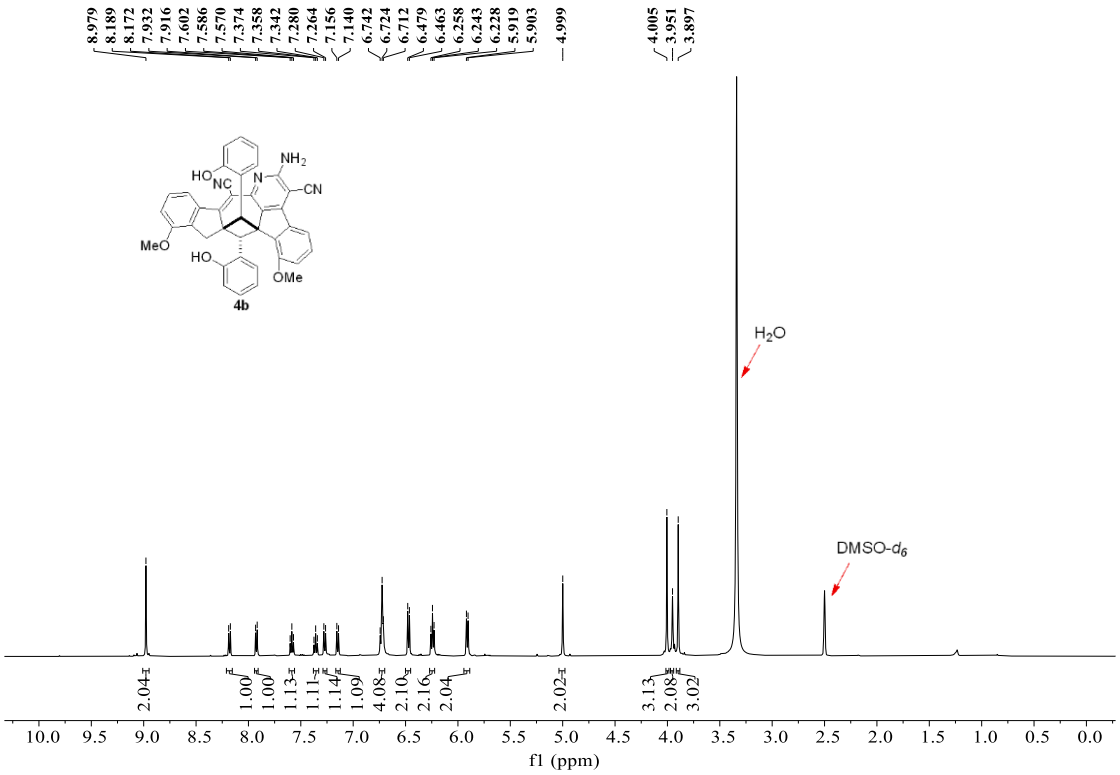
^{1}H NMR spectra for compound **4a** (500 MHz, DMSO-d_6)



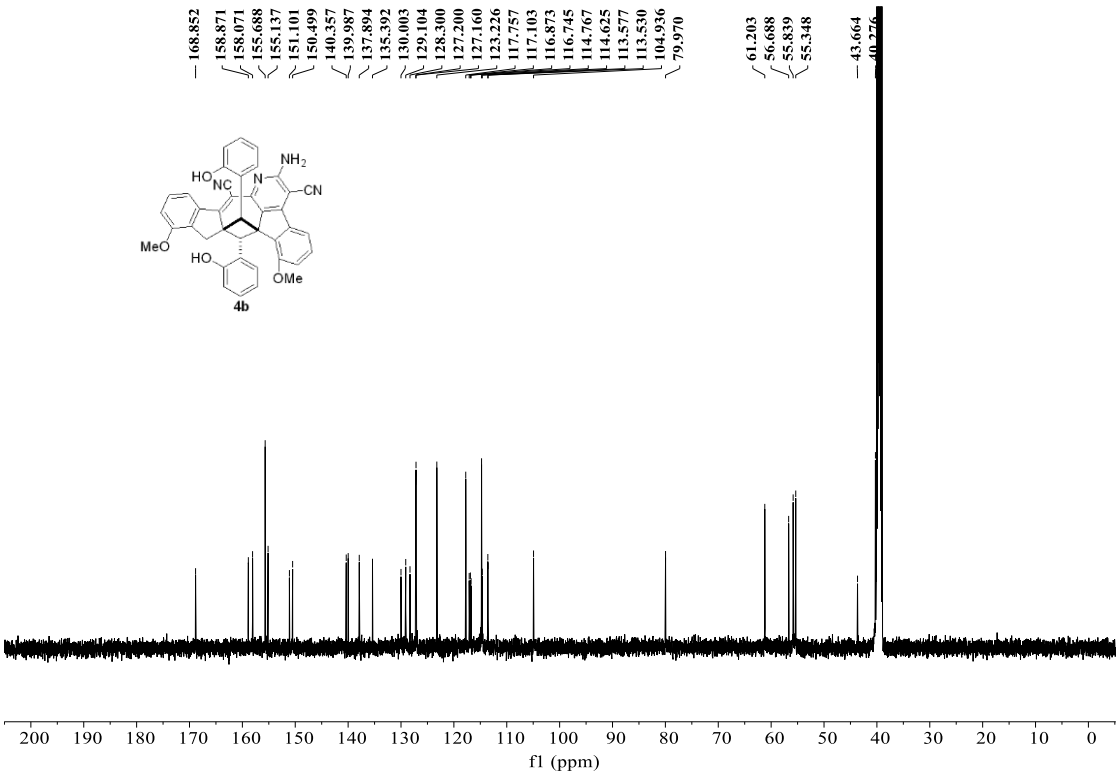
^{13}C NMR spectra for compound **4a** (125 MHz, DMSO-d_6)



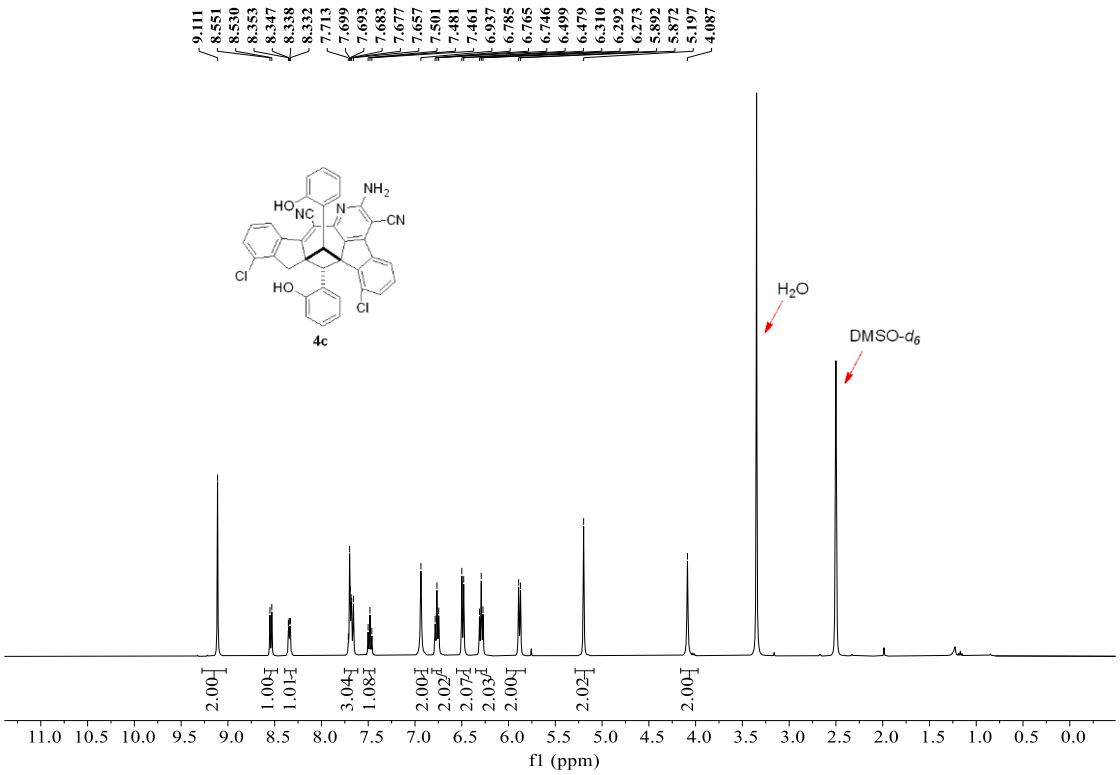
^{1}H NMR spectra for compound **4b** (500 MHz, DMSO-d_6)



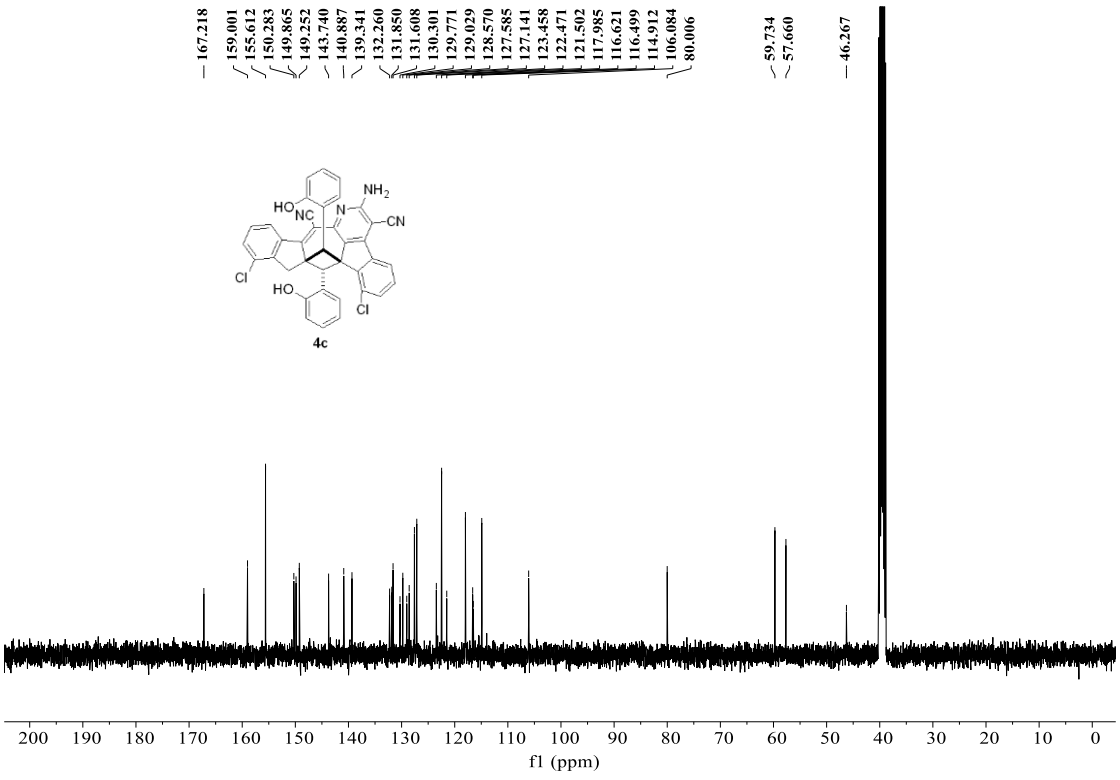
^{13}C NMR spectra for compound **4b** (125 MHz, DMSO-d_6)



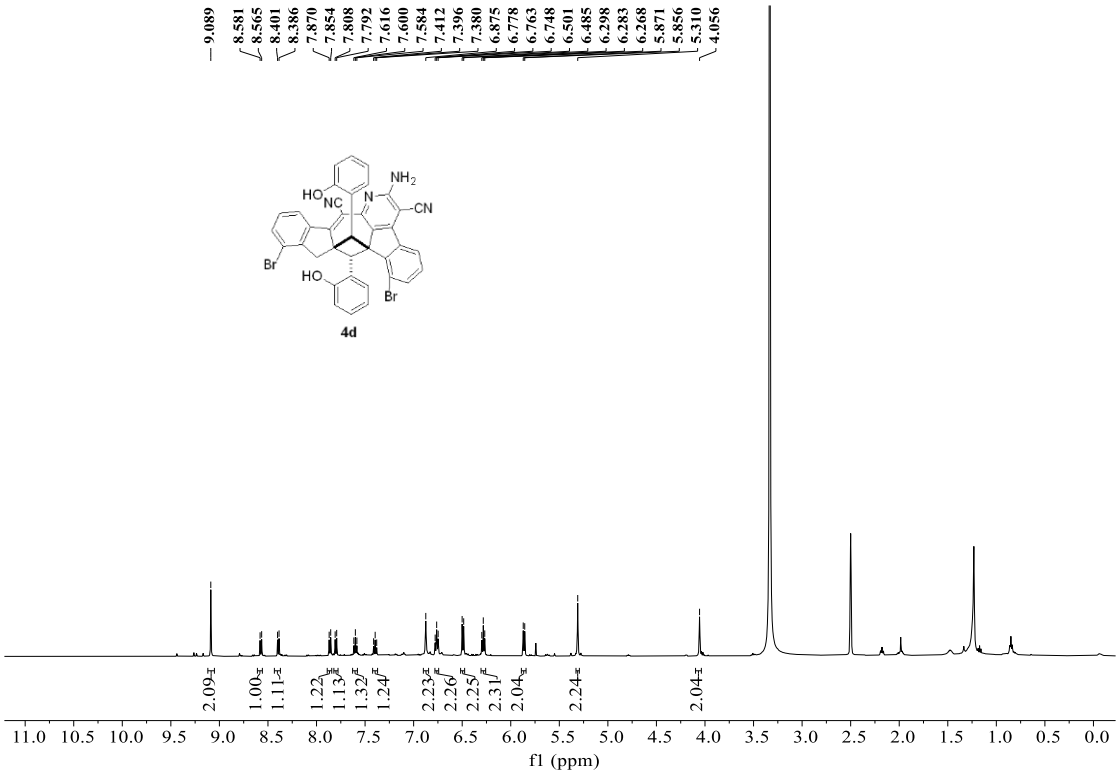
^{1}H NMR spectra for compound **4c** (400 MHz, DMSO-d_6)



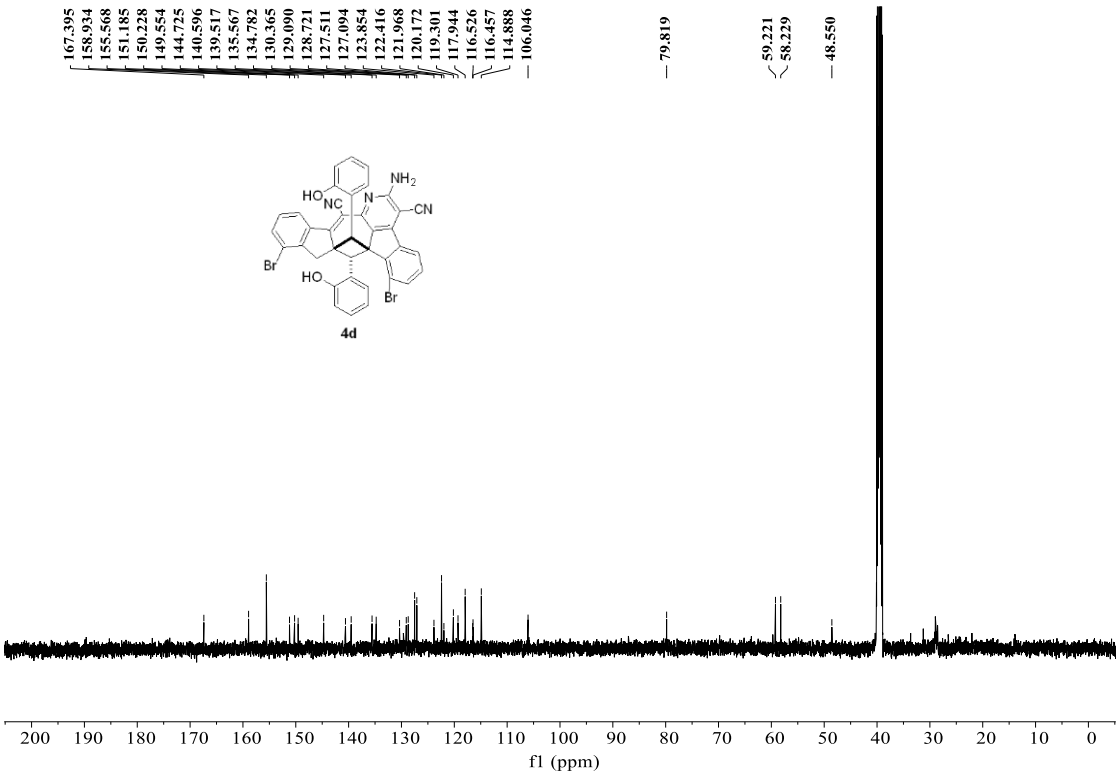
^{13}C NMR spectra for compound **4c** (100 MHz, DMSO-d_6)



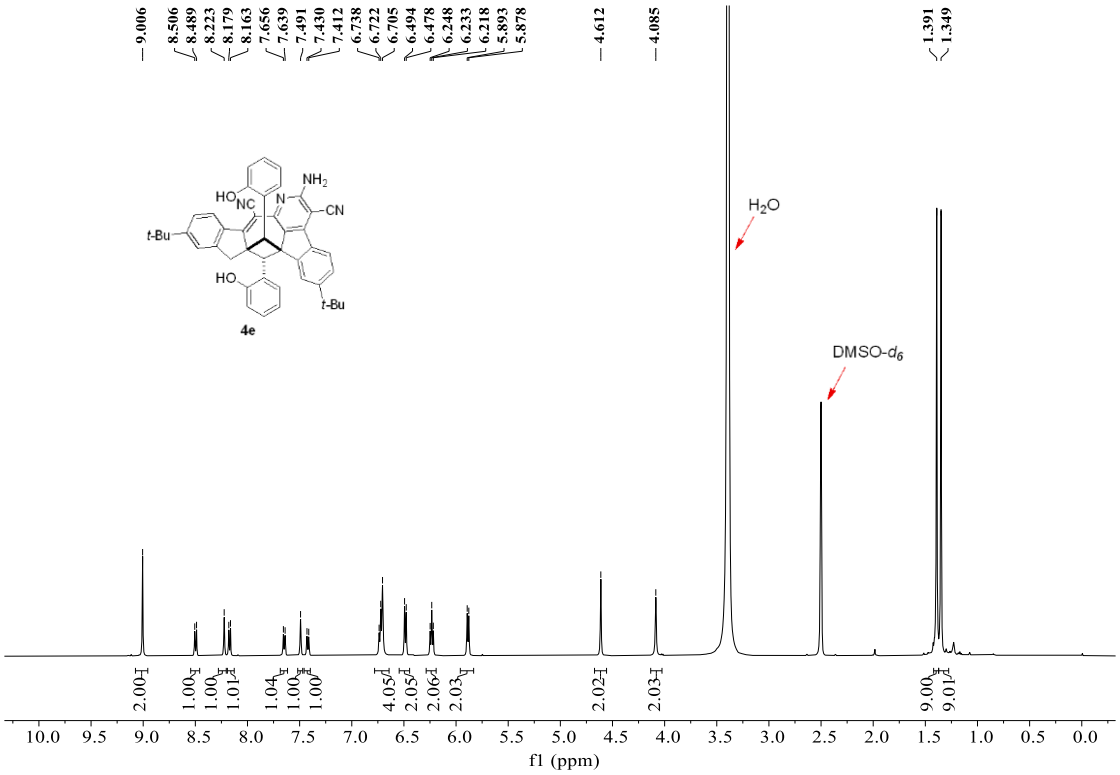
^{1}H NMR spectra for compound **4d** (500 MHz, DMSO-d_6)



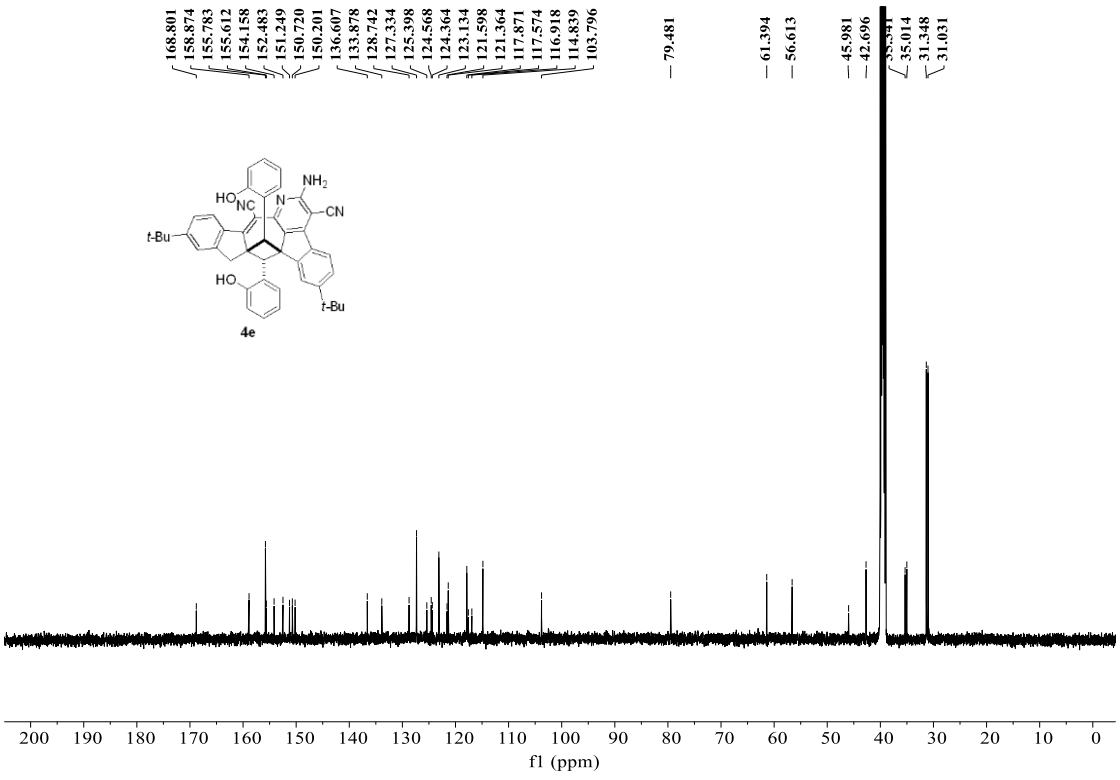
^{13}C NMR spectra for compound **4d** (125 MHz, DMSO-d_6)



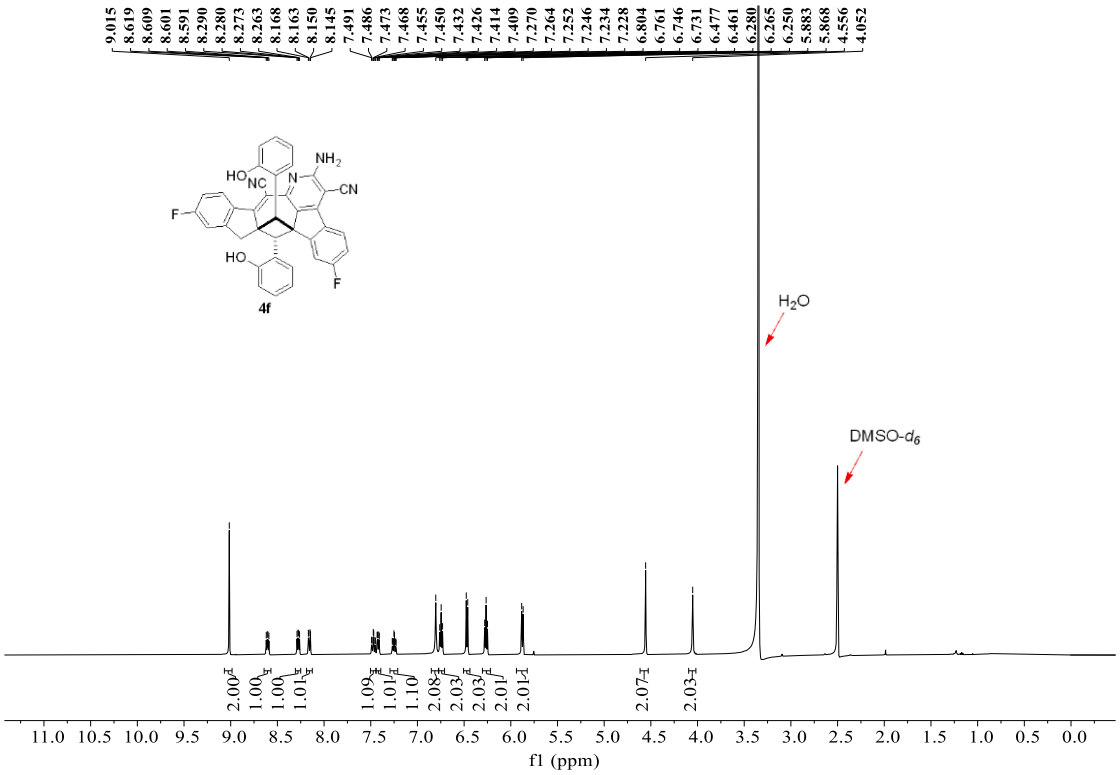
^{1}H NMR spectra for compound **4e** (500 MHz, DMSO-d_6)



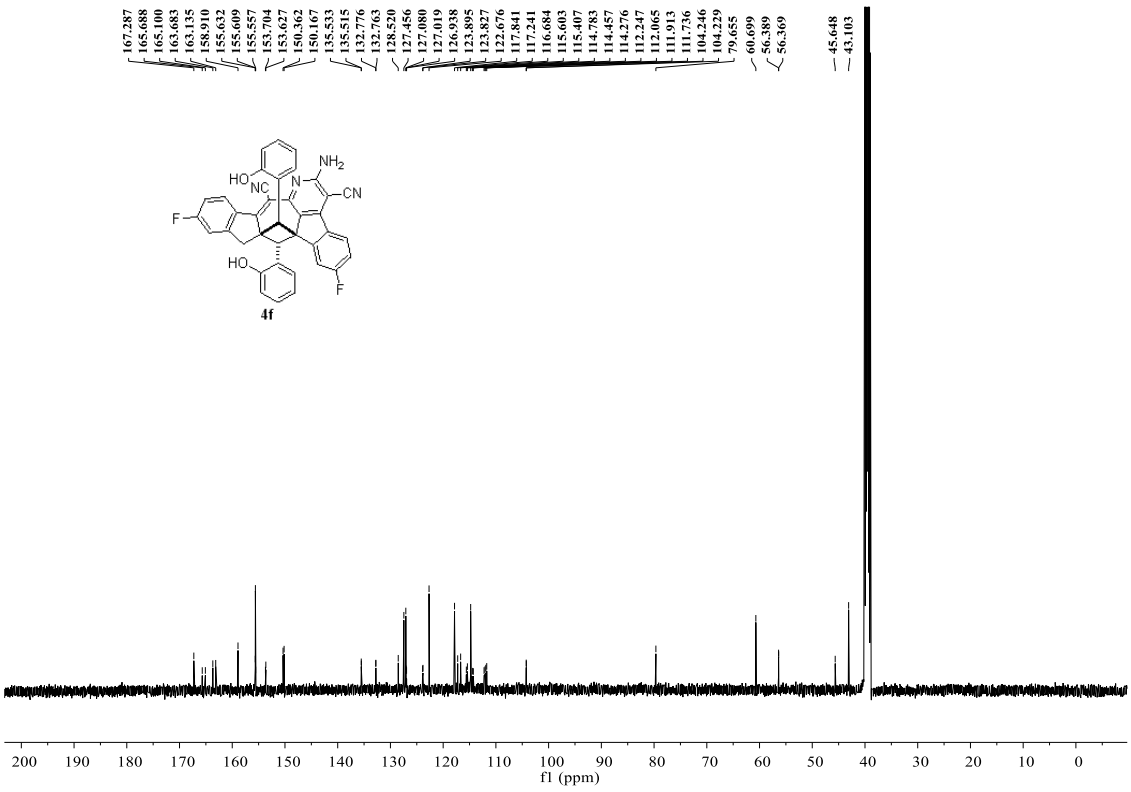
^{13}C NMR spectra for compound **4e** (125 MHz, DMSO-d_6)



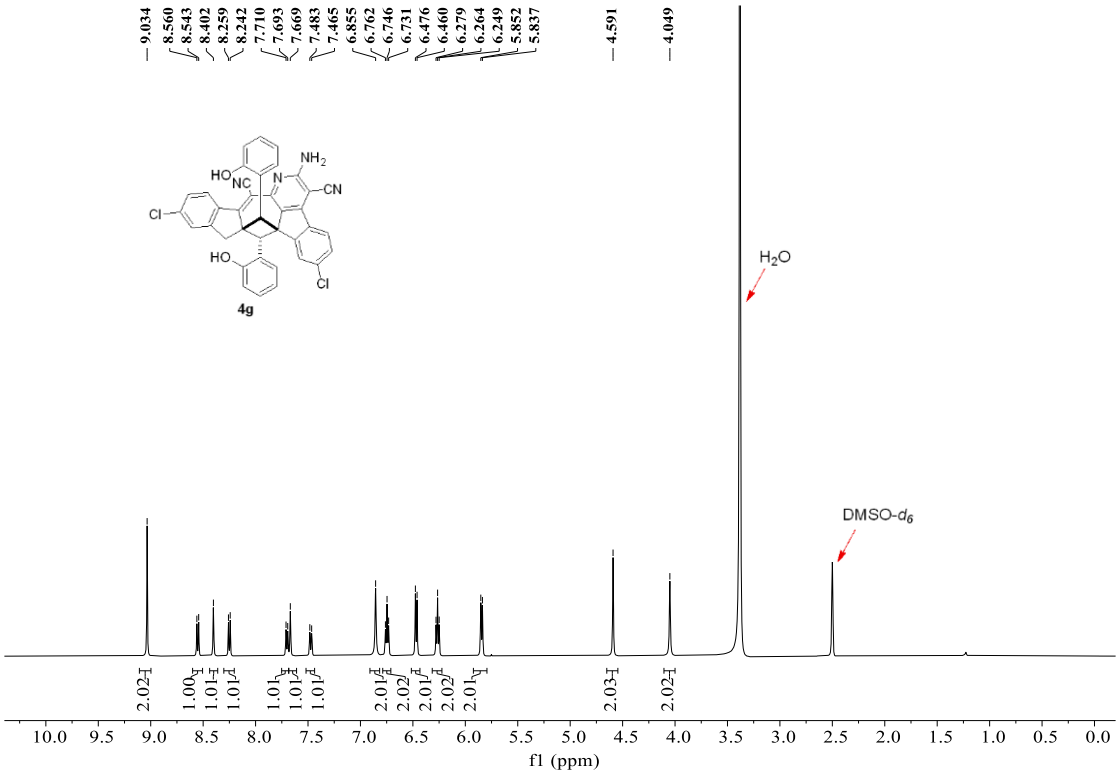
^{1}H NMR spectra for compound **4f** (500 MHz, DMSO-d_6)



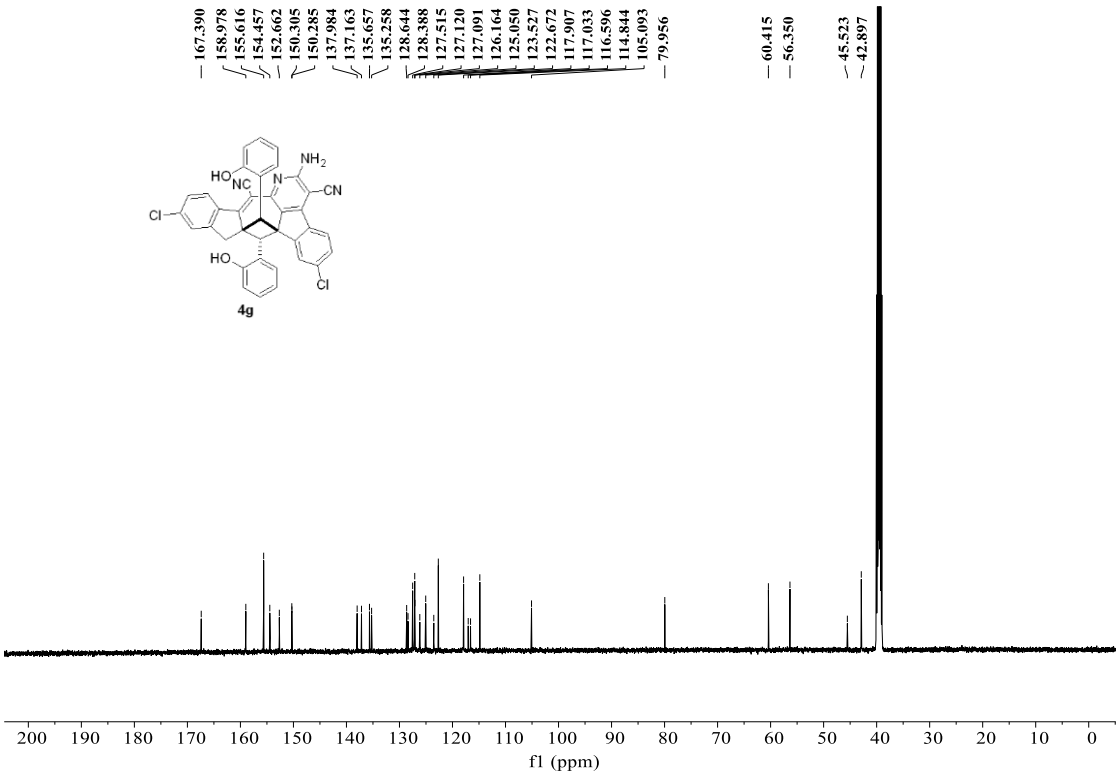
^{13}C NMR spectra for compound **4f** (125 MHz, DMSO-d_6)



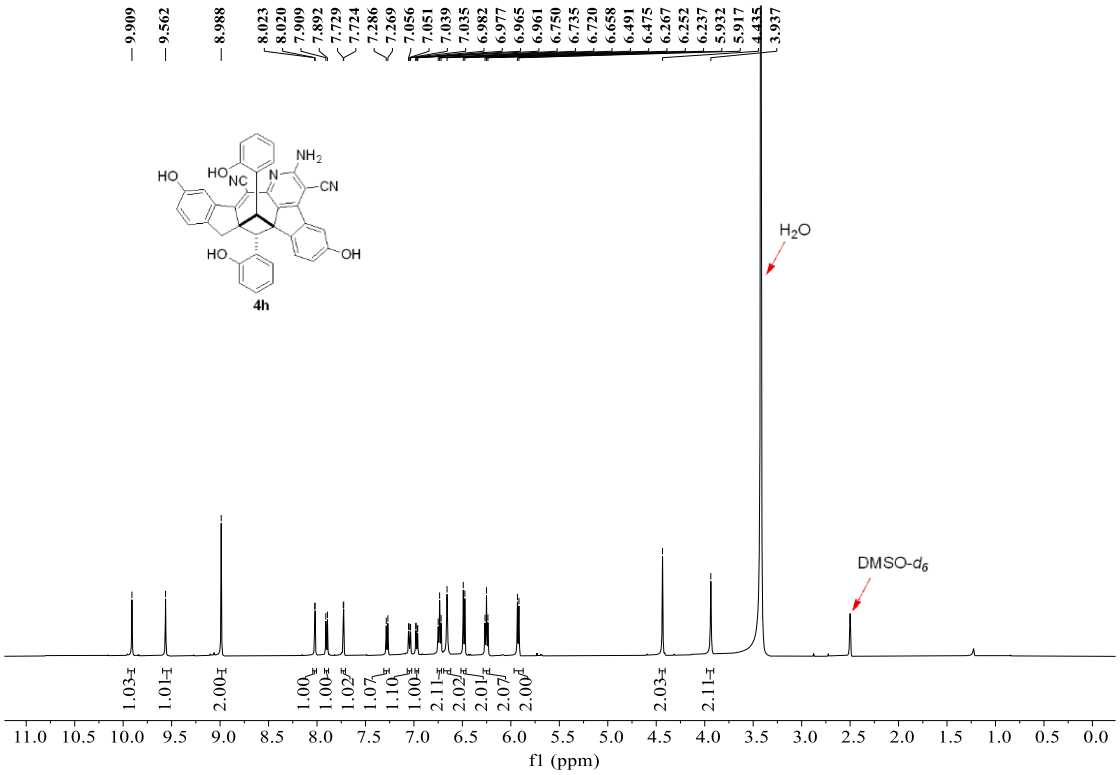
^{1}H NMR spectra for compound **4g** (500 MHz, DMSO-d_6)



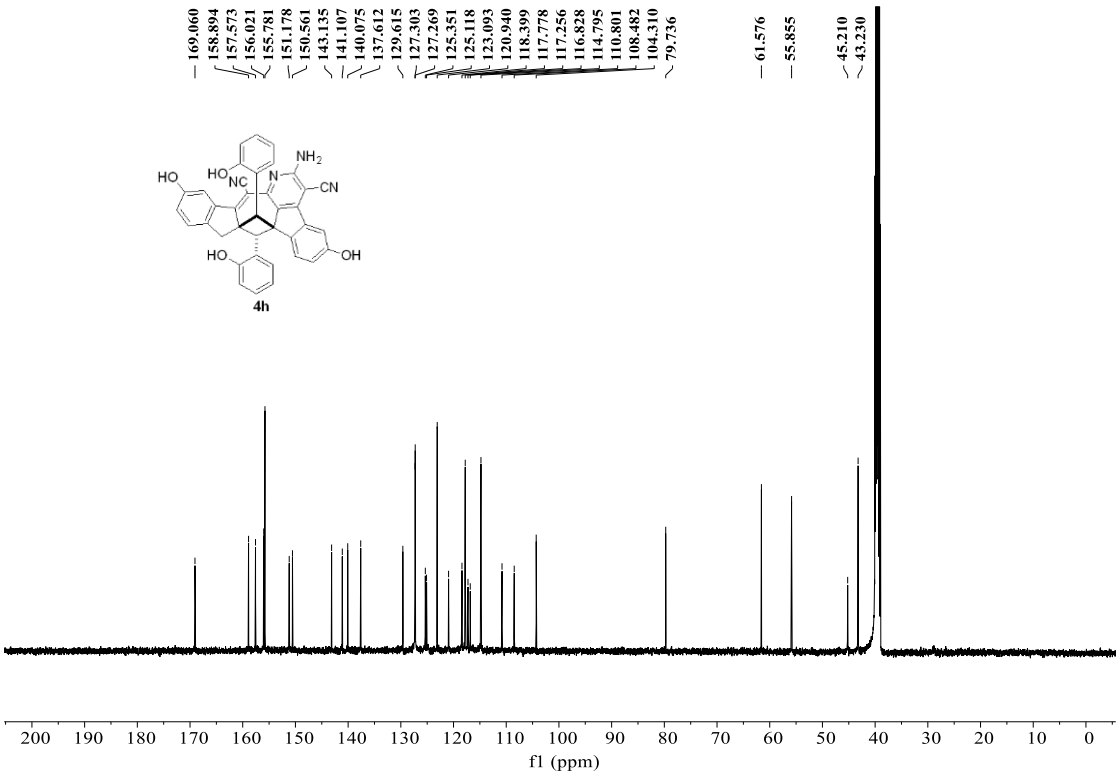
^{13}C NMR spectra for compound **4g** (125 MHz, DMSO-d_6)



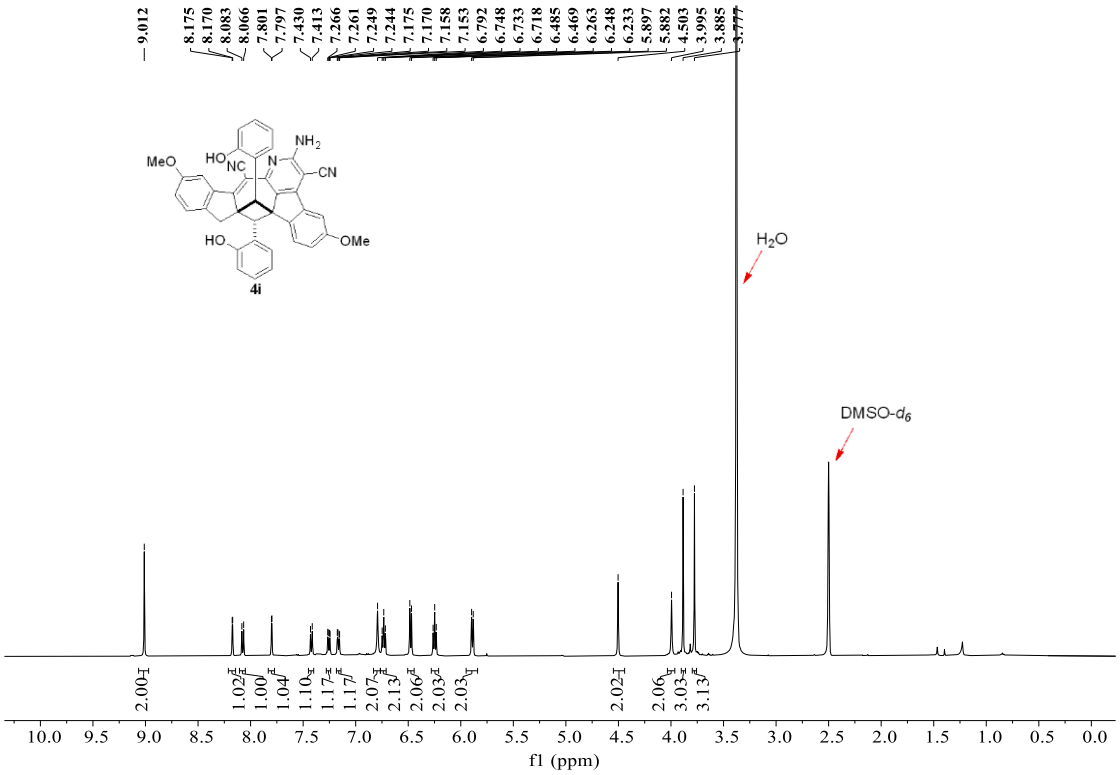
^{1}H NMR spectra for compound **4h** (500 MHz, DMSO-d_6)



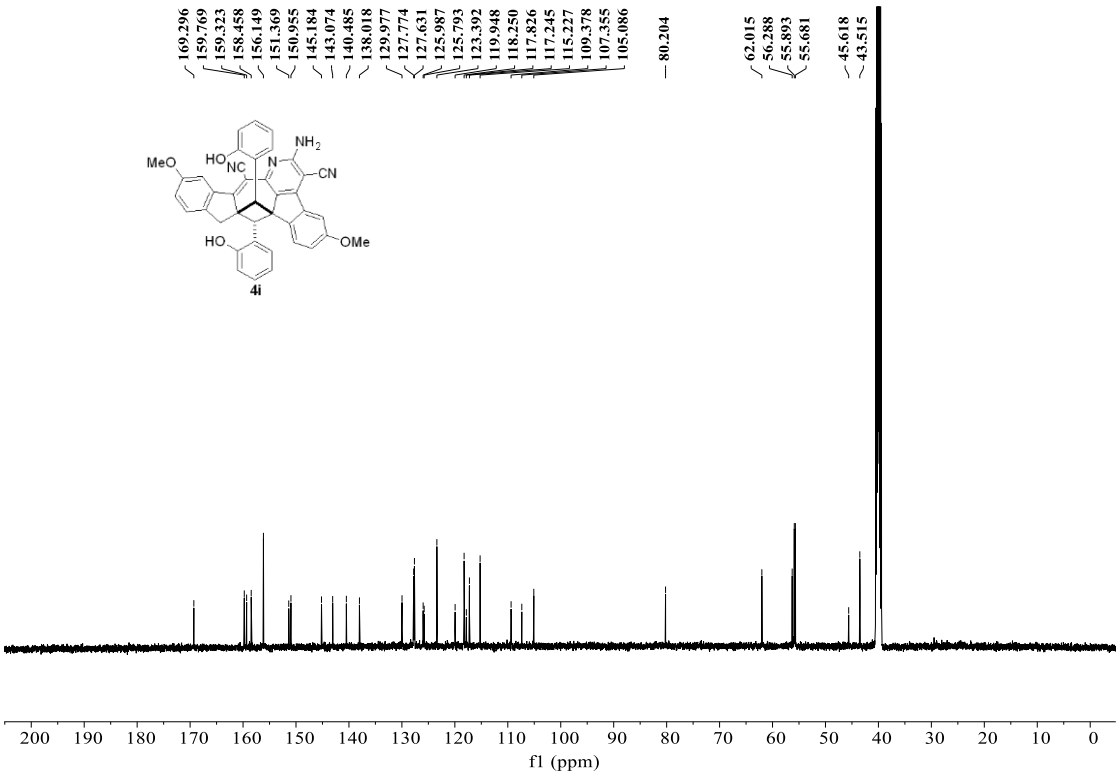
^{13}C NMR spectra for compound **4h** (125 MHz, DMSO-d_6)



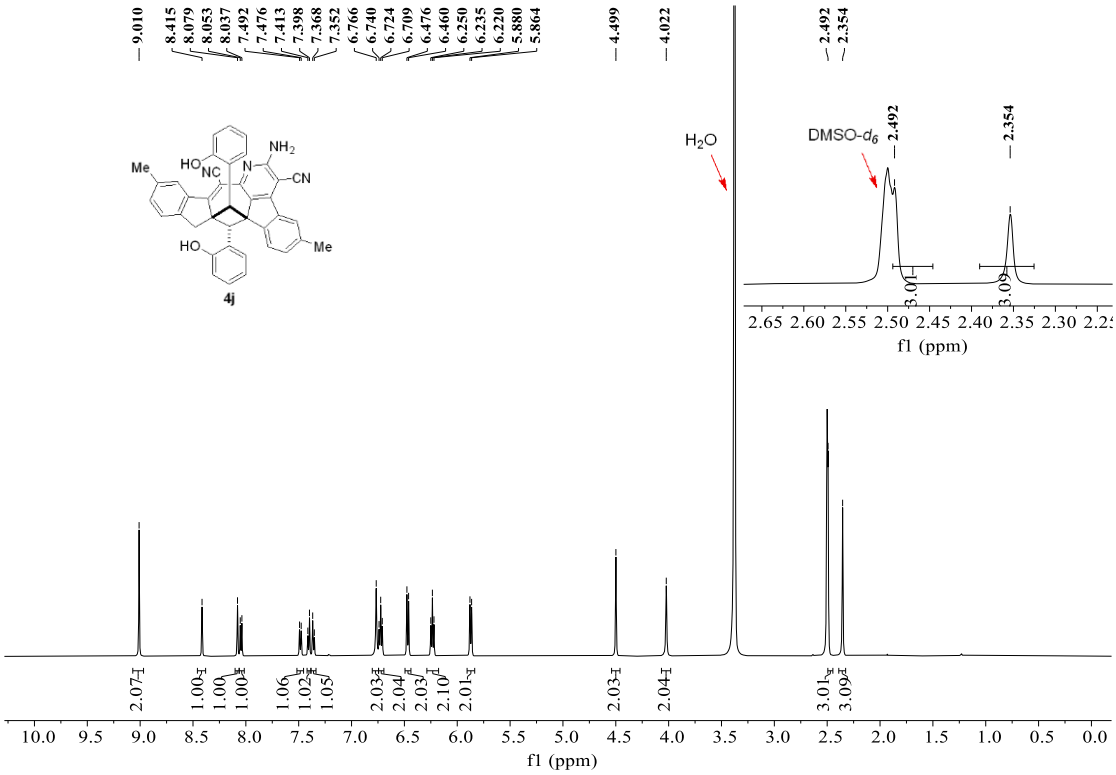
^{1}H NMR spectra for compound **4i** (500 MHz, DMSO-d_6)



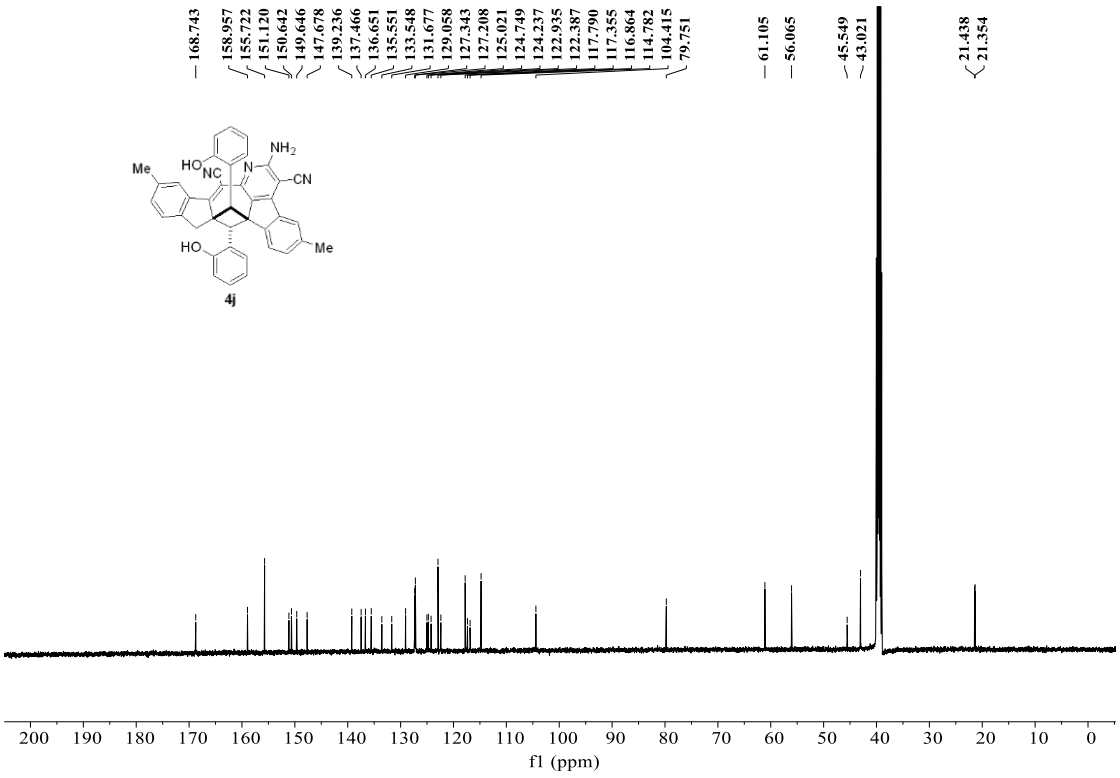
^{13}C NMR spectra for compound **4i** (125 MHz, DMSO-d_6)



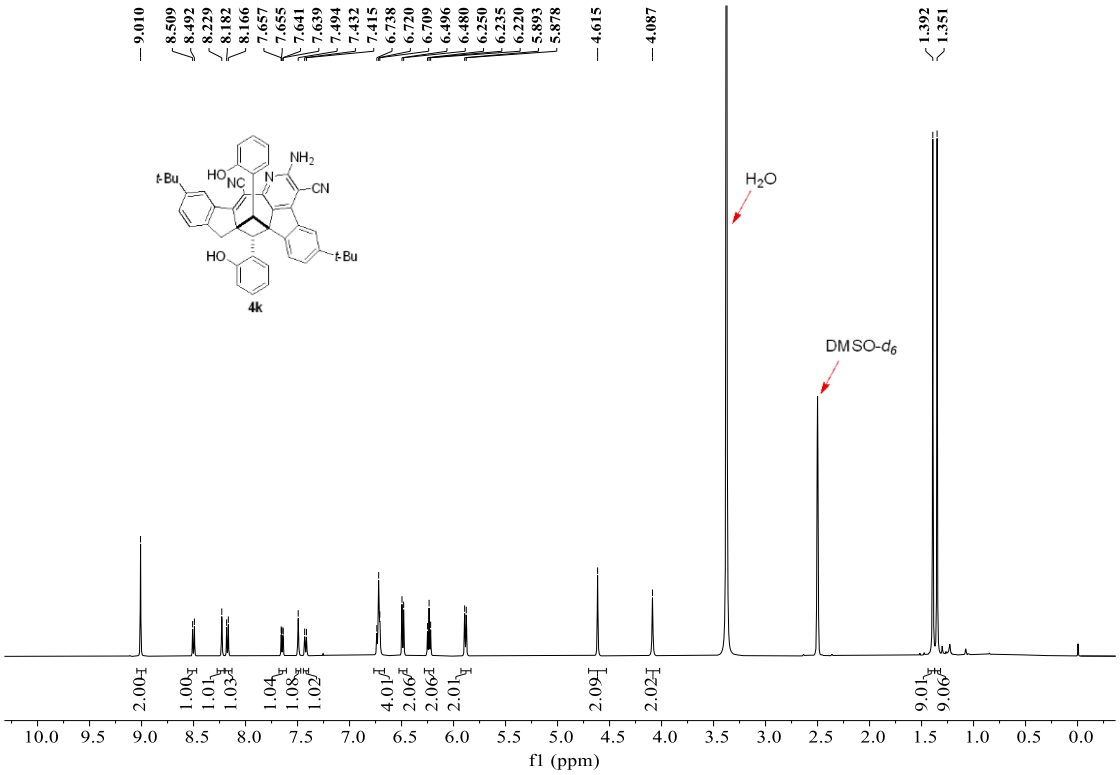
^{1}H NMR spectra for compound **4j** (500 MHz, DMSO-d_6)



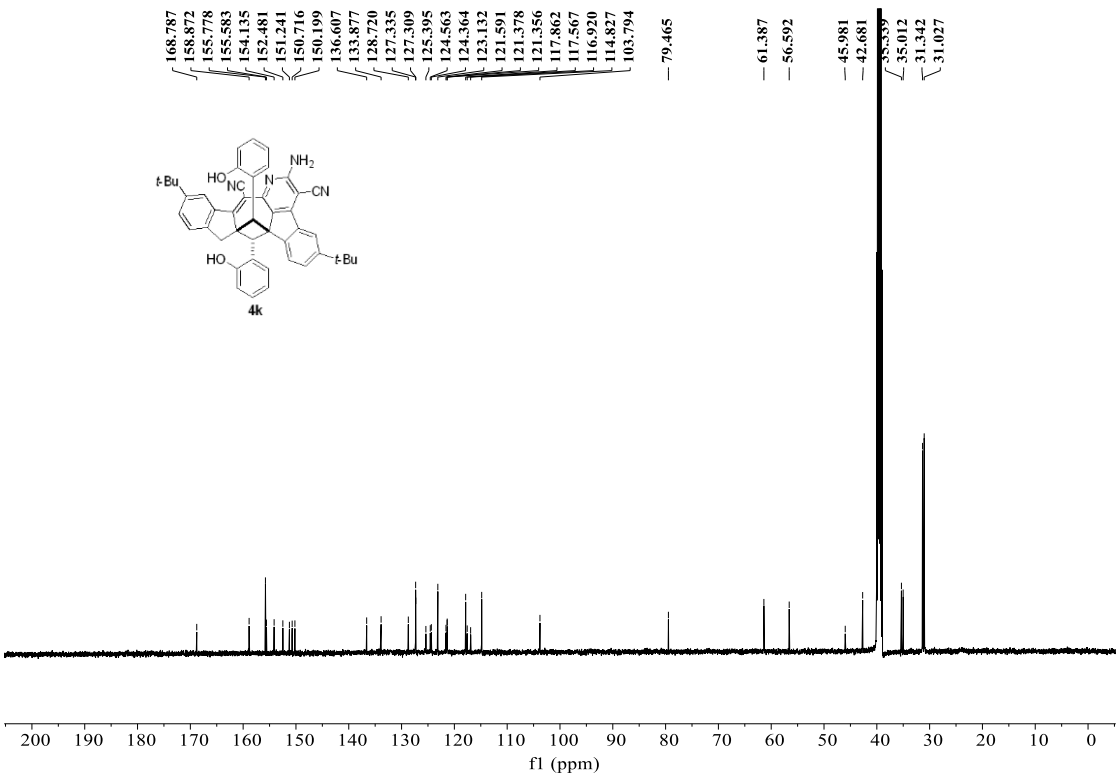
^{13}C NMR spectra for compound **4j** (125 MHz, DMSO-d_6)



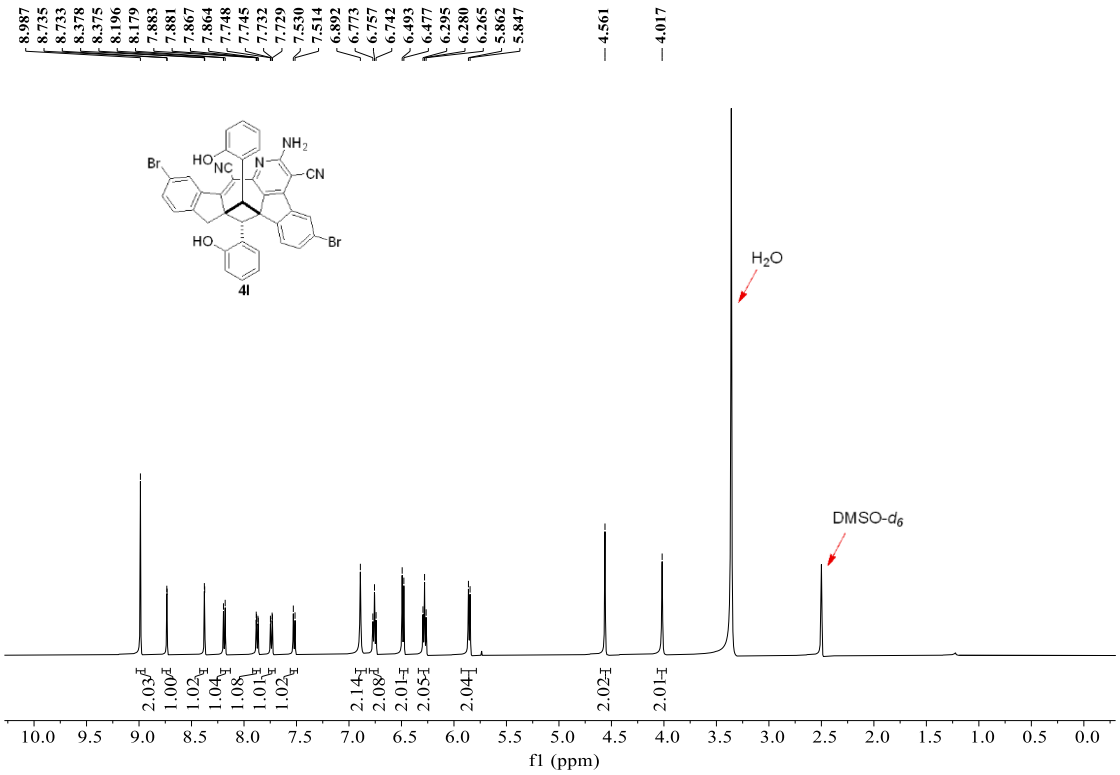
^{1}H NMR spectra for compound **4k** (500 MHz, DMSO-d_6)



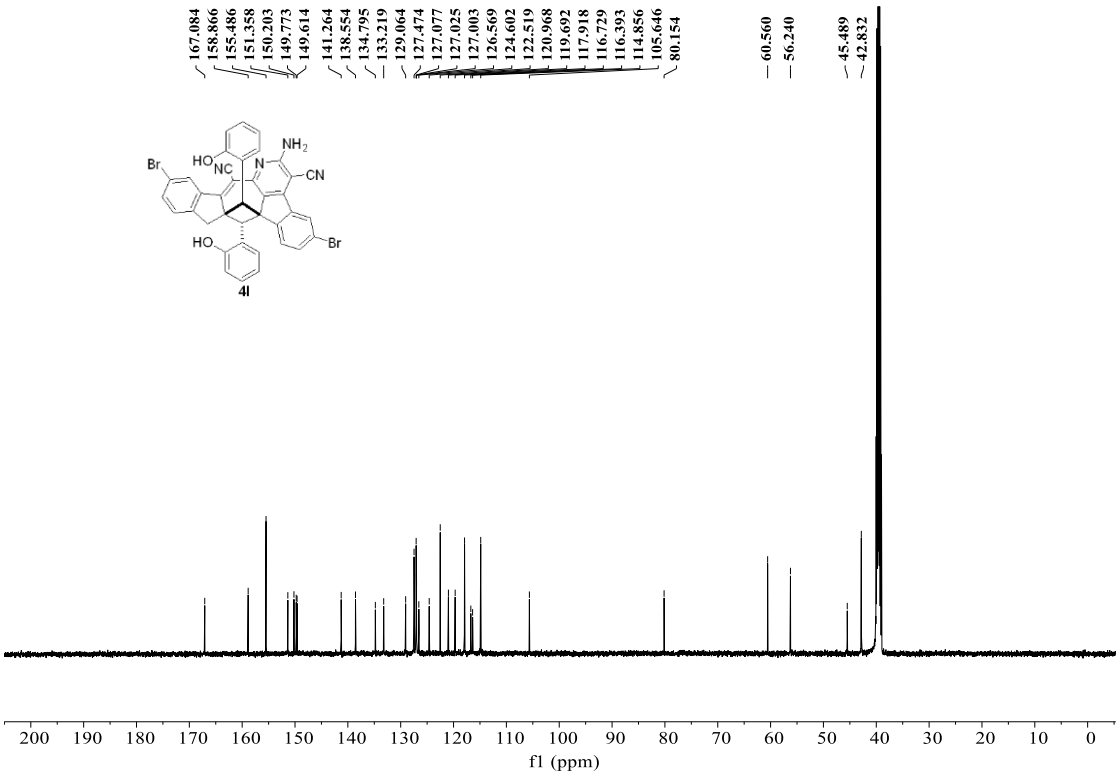
^{13}C NMR spectra for compound **4k** (125 MHz, DMSO-d_6)



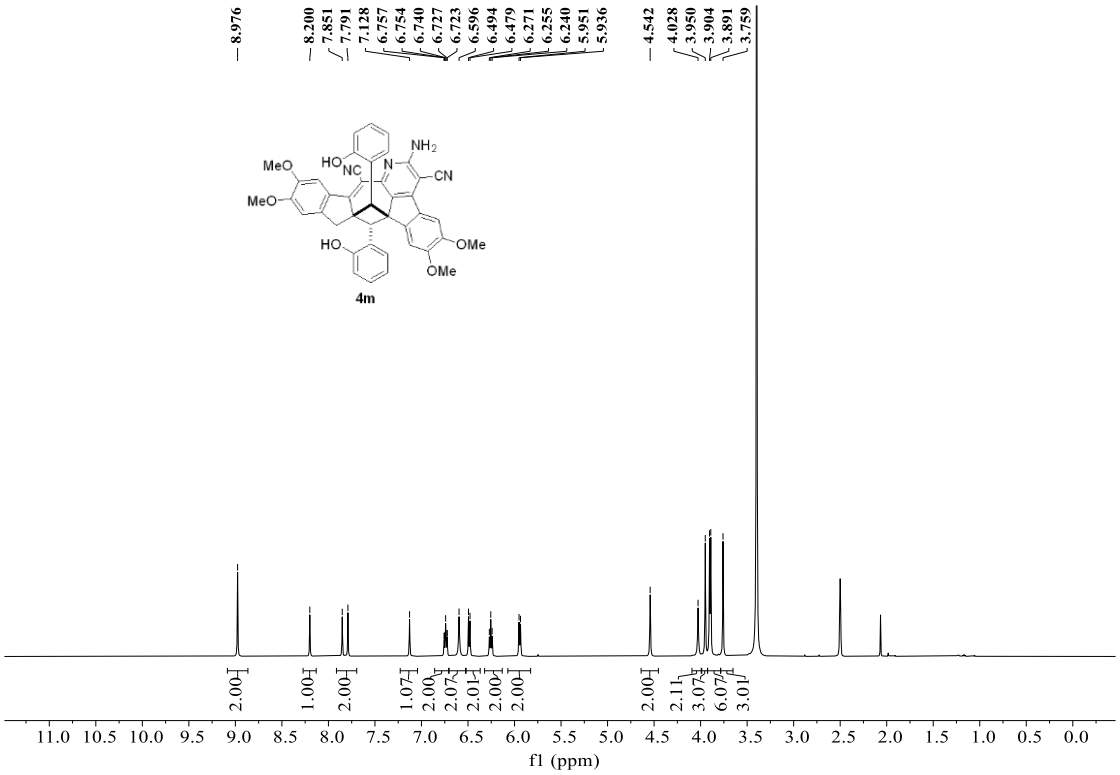
^{1}H NMR spectra for compound **4l** (500 MHz, DMSO-d_6)



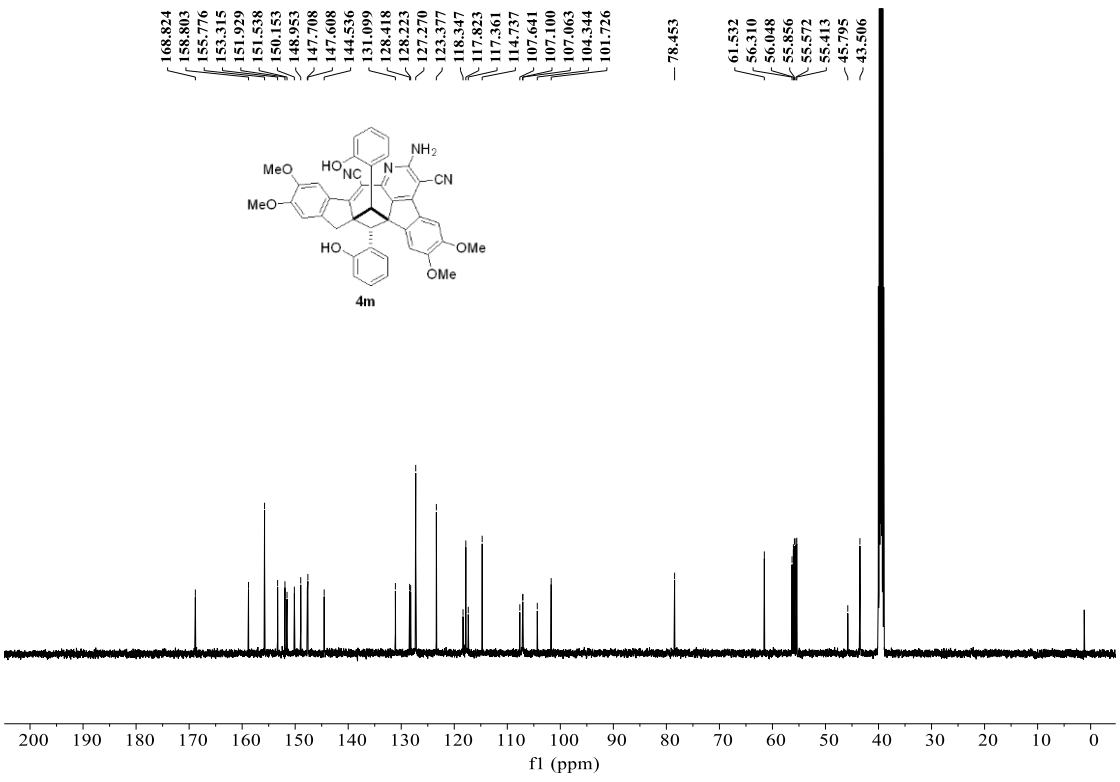
^{13}C NMR spectra for compound **4l** (125 MHz, DMSO-d_6)



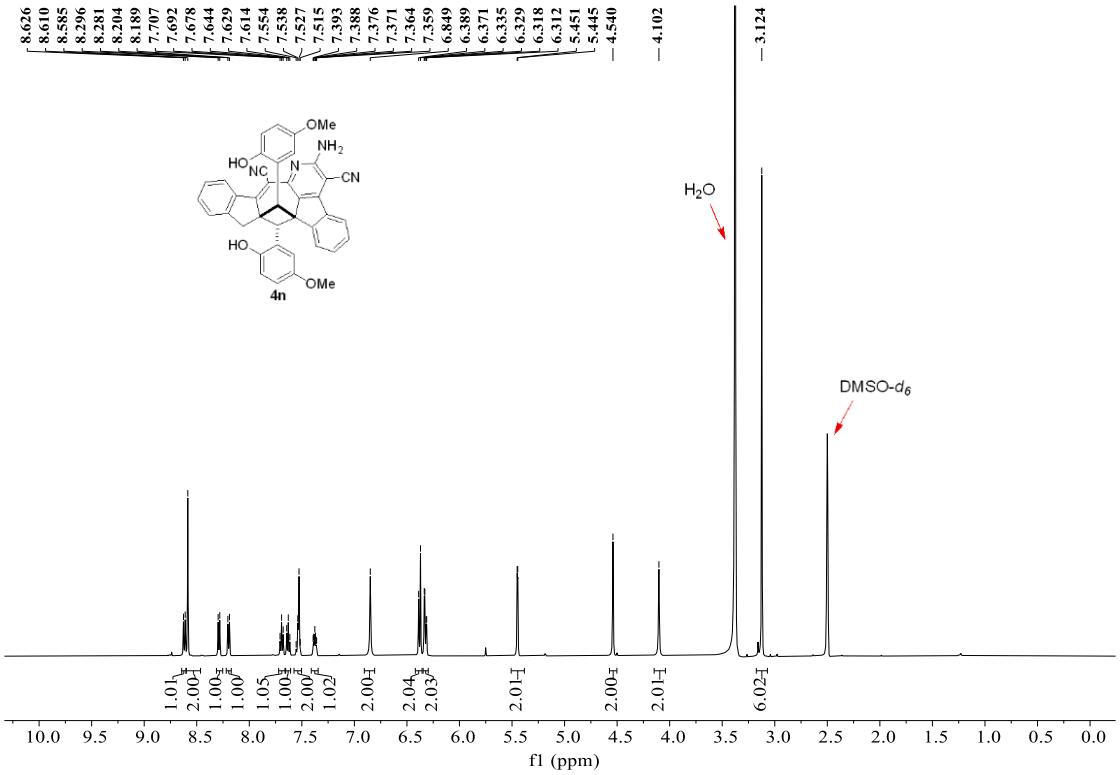
^{1}H NMR spectra for compound **4m** (500 MHz, DMSO-d_6)



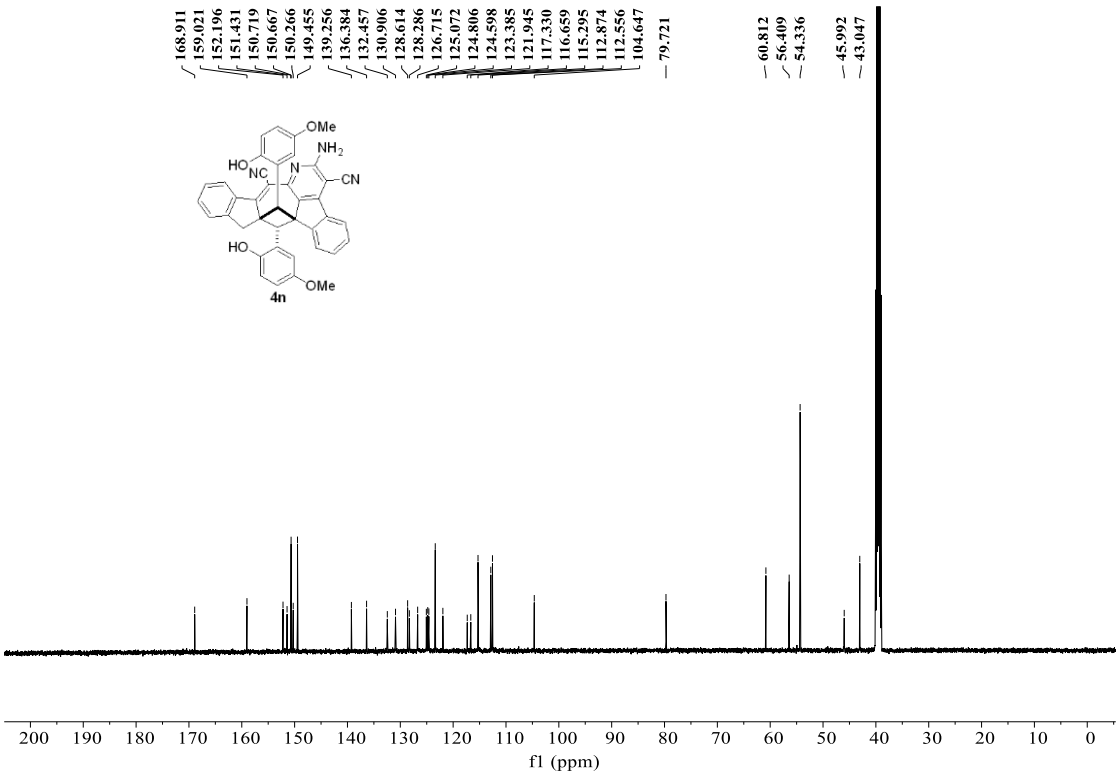
^{13}C NMR spectra for compound **4m** (125 MHz, DMSO-d_6)



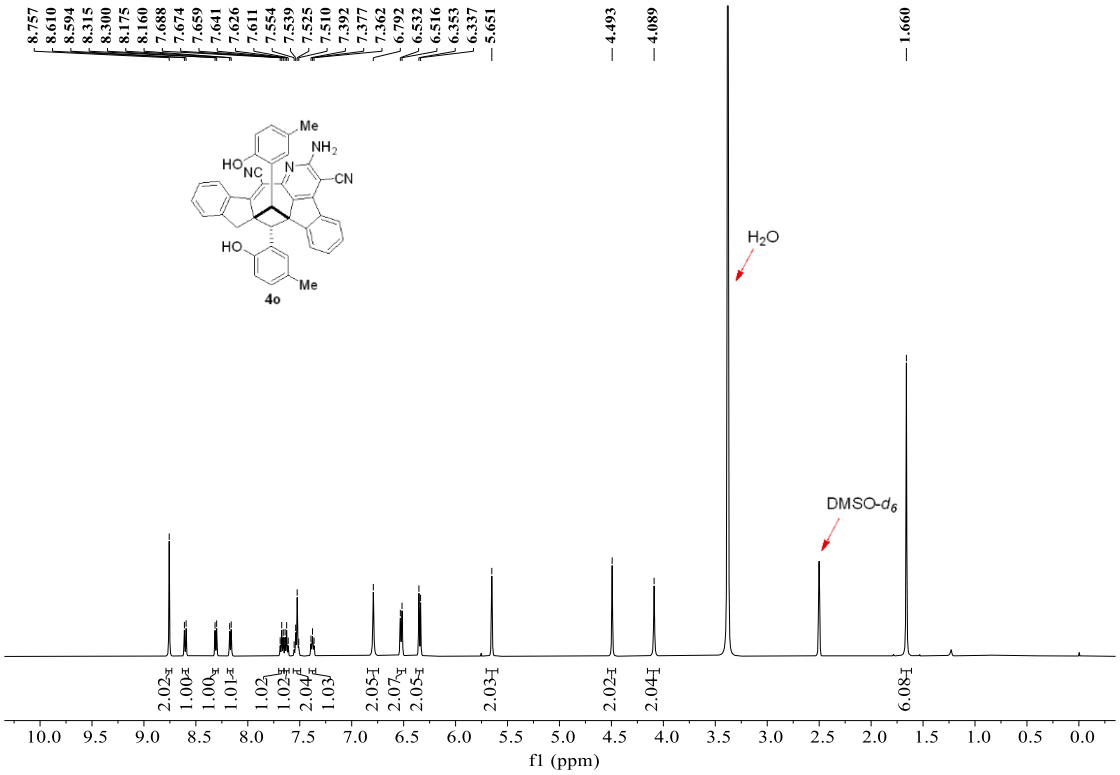
^{1}H NMR spectra for compound **4n** (500 MHz, DMSO-d_6)



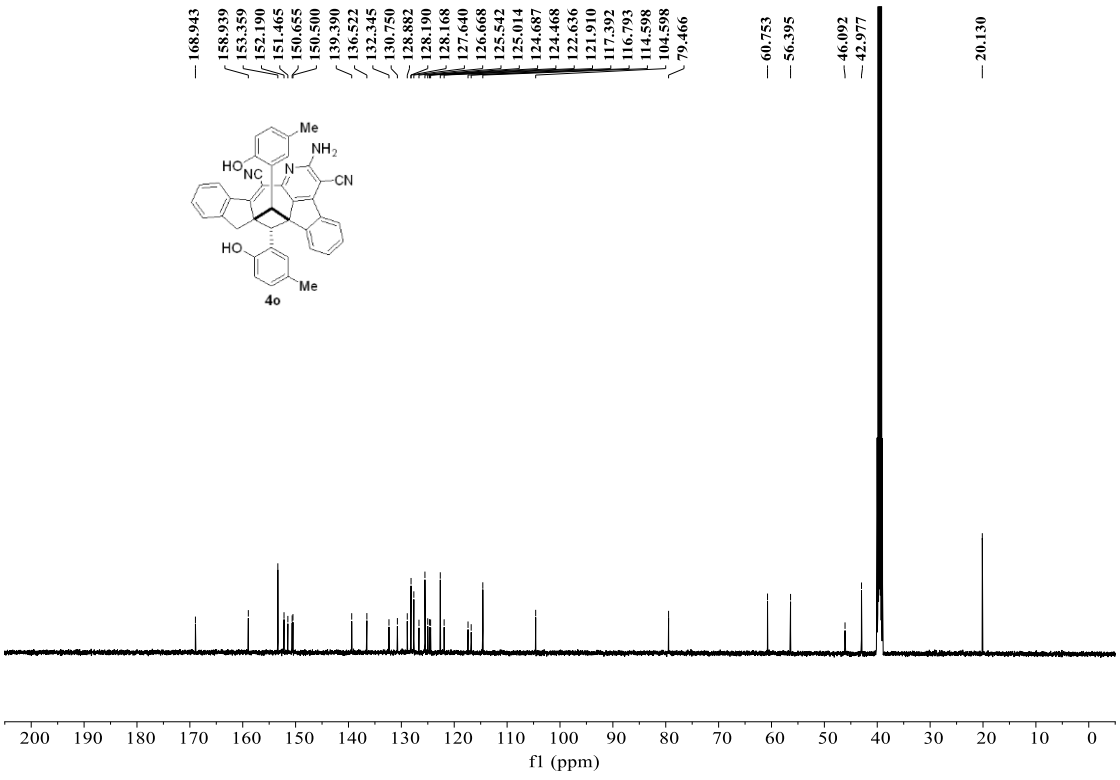
^{13}C NMR spectra for compound **4n** (125 MHz, DMSO-d_6)



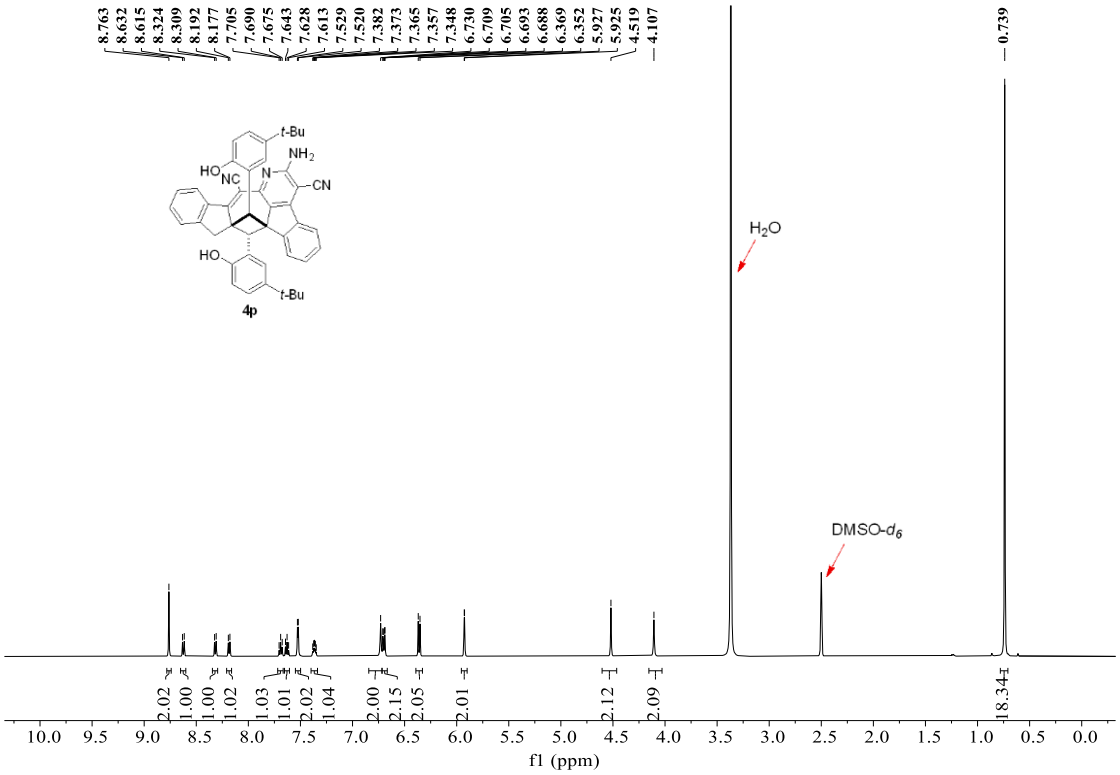
^{1}H NMR spectra for compound **4o** (500 MHz, DMSO-d_6)



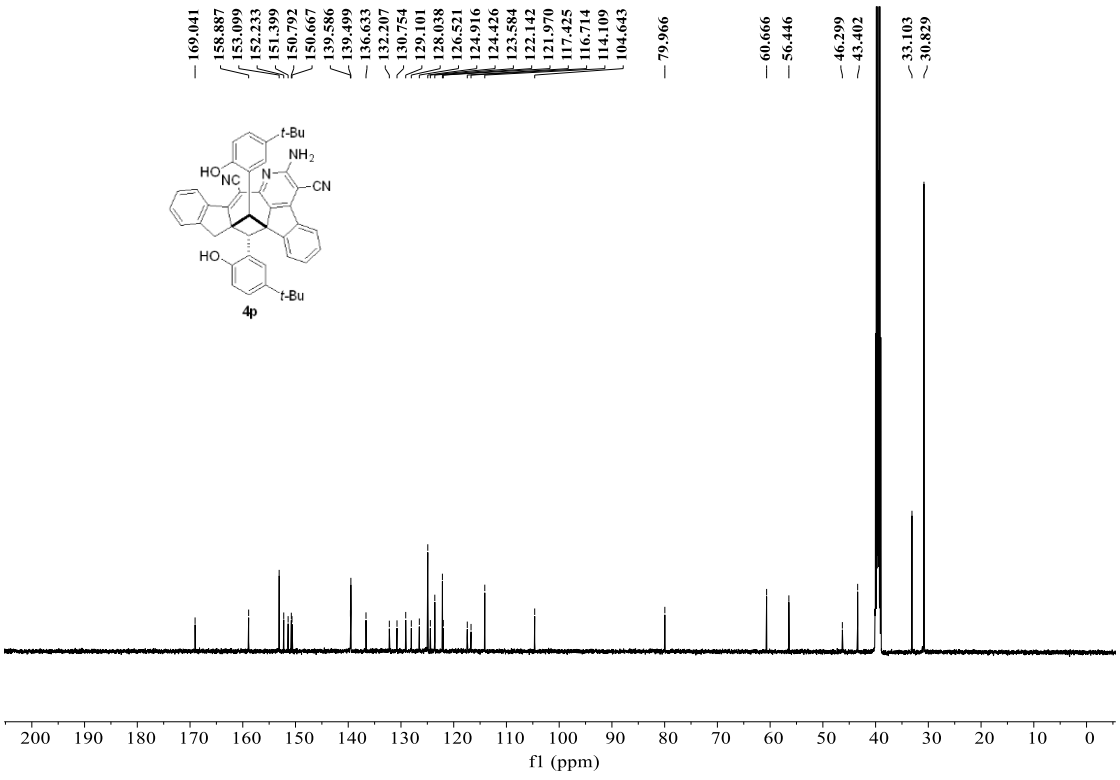
^{13}C NMR spectra for compound **4o** (125 MHz, DMSO-d_6)



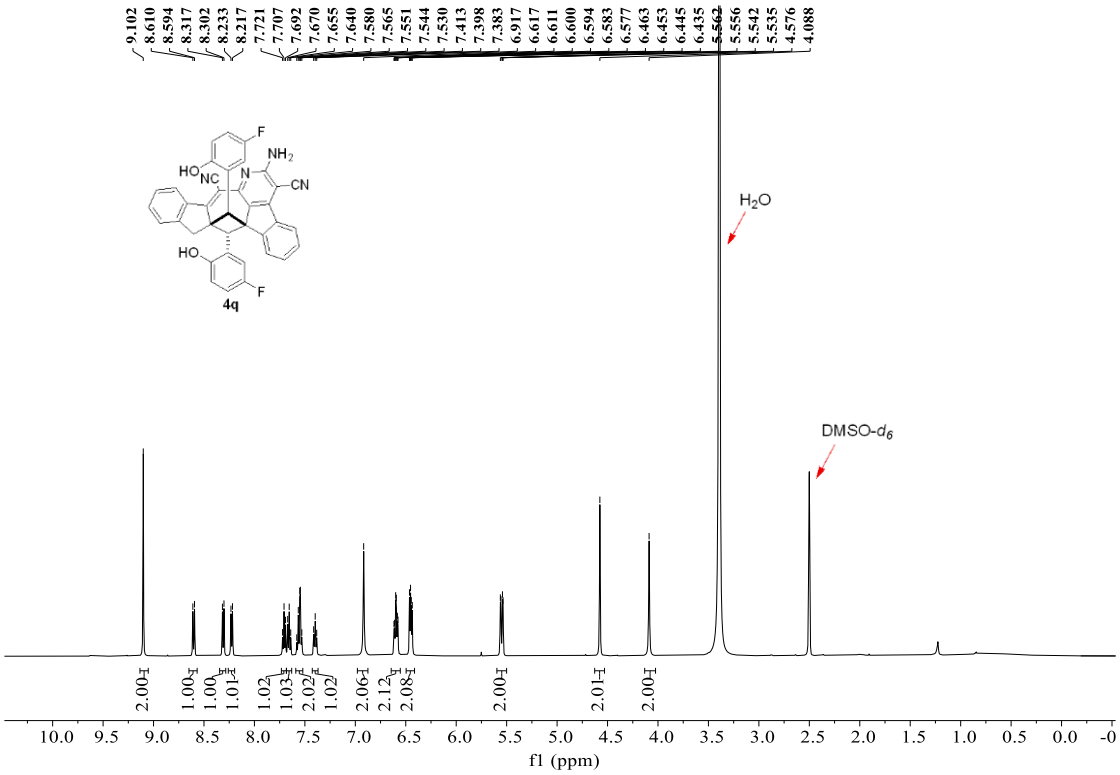
^{1}H NMR spectra for compound **4p** (500 MHz, DMSO-d_6)



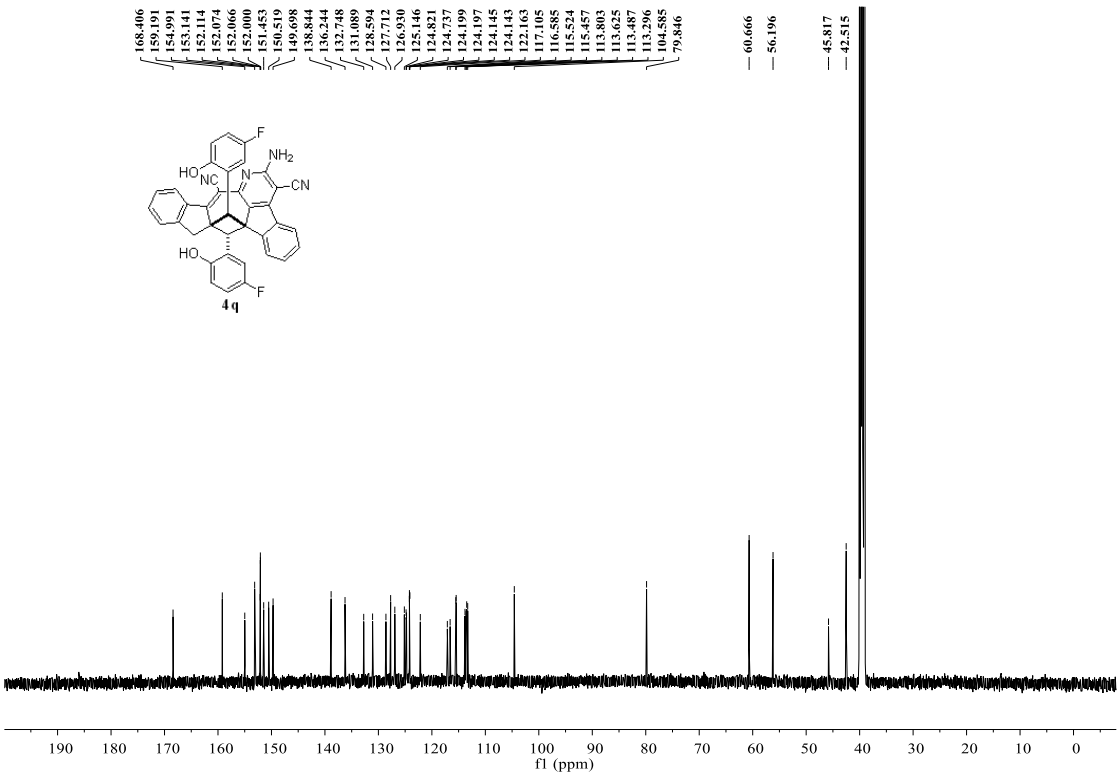
^{13}C NMR spectra for compound **4p** (125 MHz, DMSO-d_6)



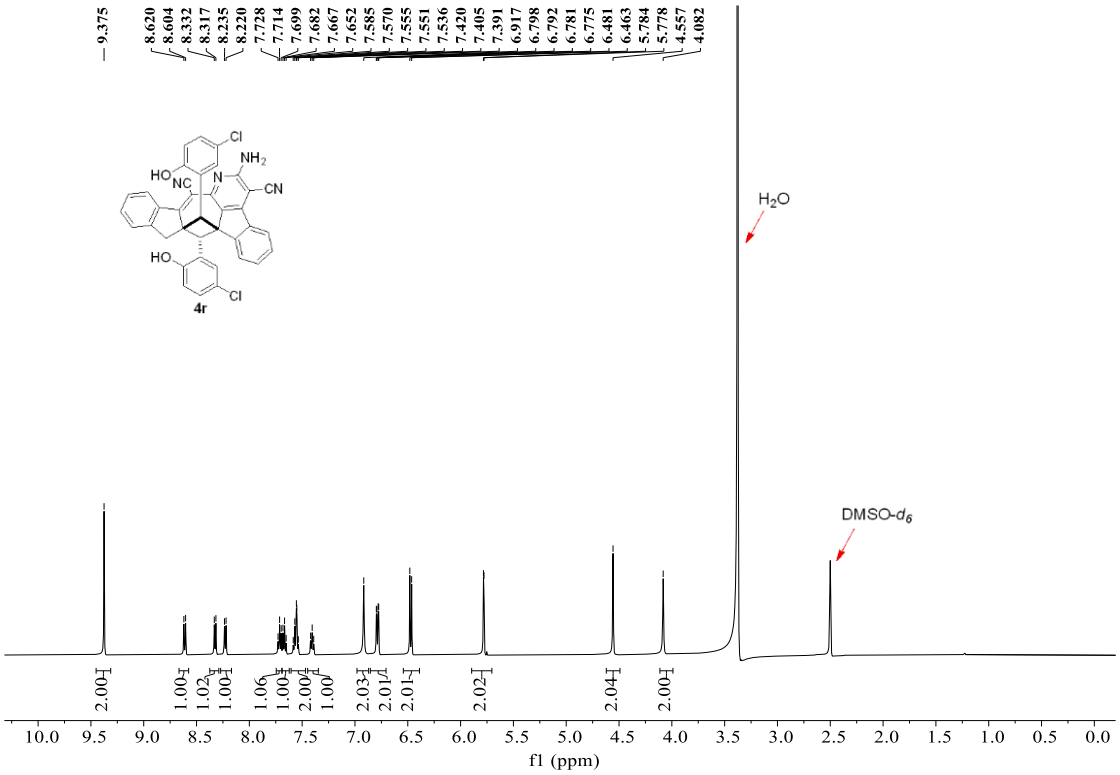
^{1}H NMR spectra for compound **4q** (500 MHz, DMSO-d_6)



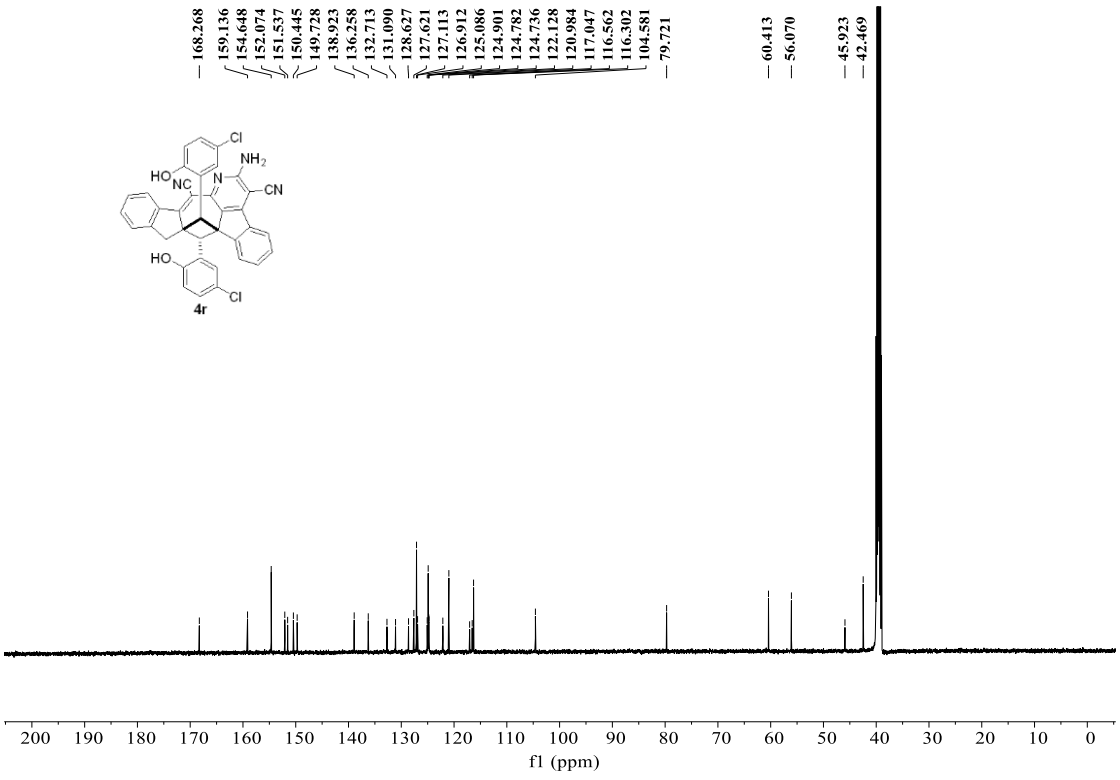
^{13}C NMR spectra for compound **4q** (125 MHz, DMSO-d_6)



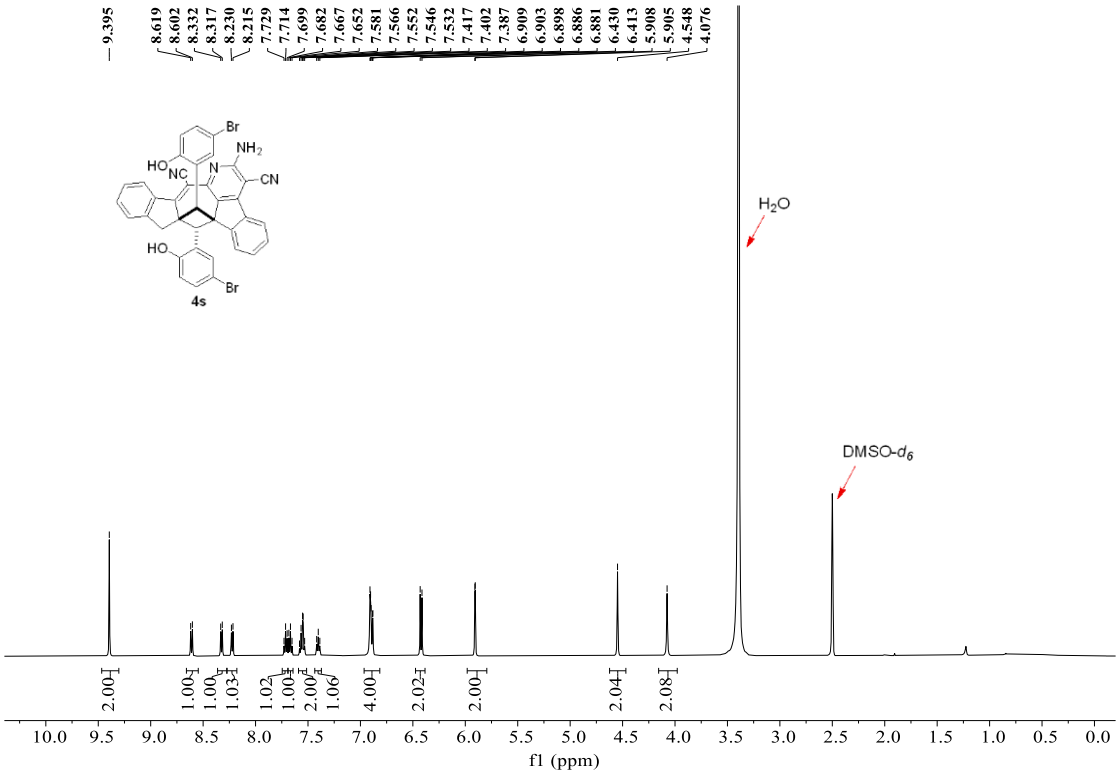
^{1}H NMR spectra for compound **4r** (500 MHz, DMSO-d_6)



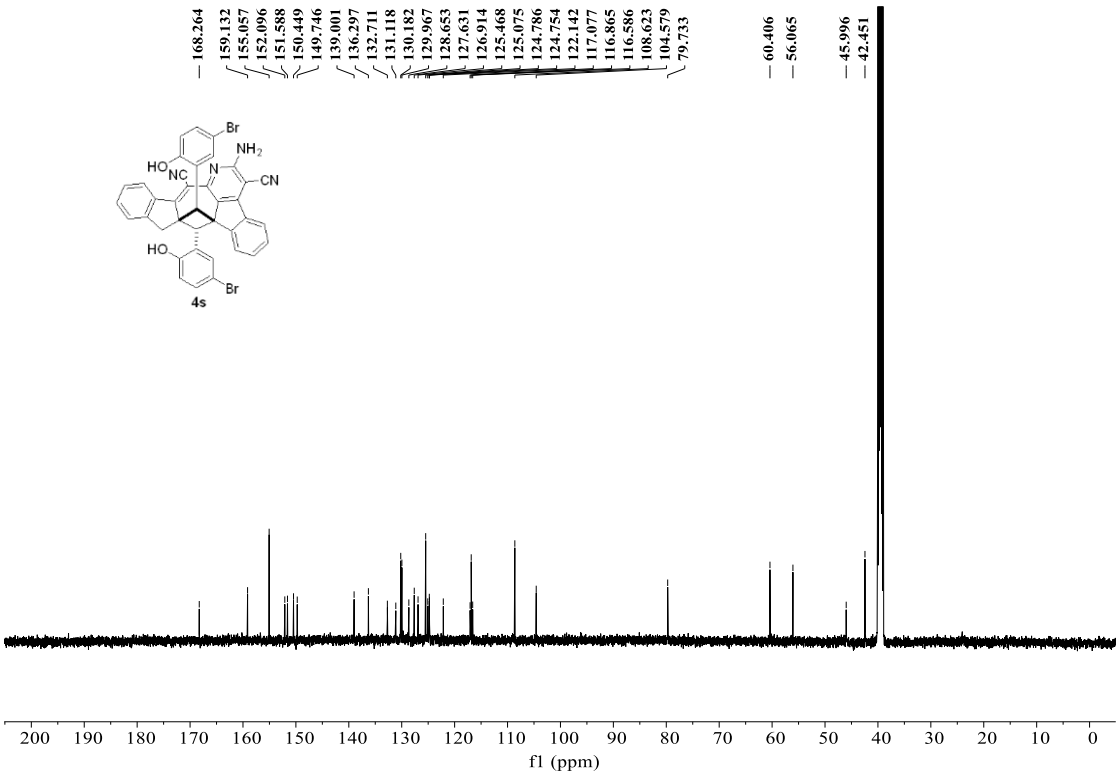
^{13}C NMR spectra for compound **4r** (125 MHz, DMSO-d_6)



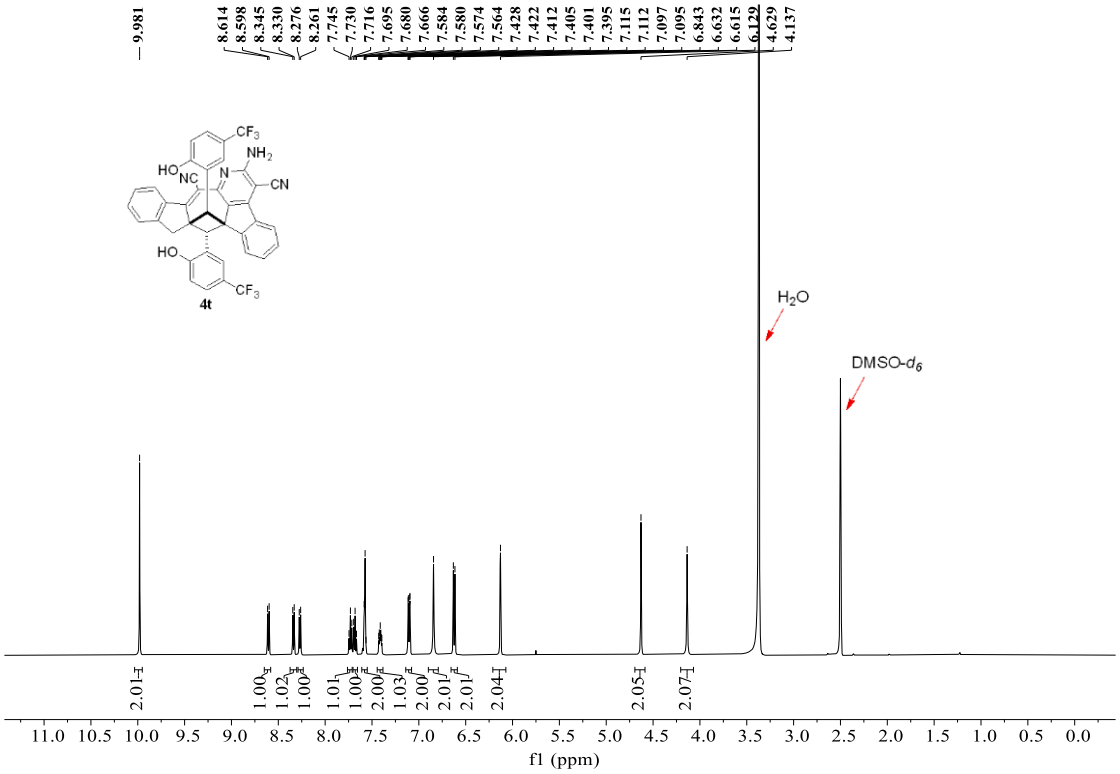
^{1}H NMR spectra for compound **4s** (500 MHz, DMSO-d_6)



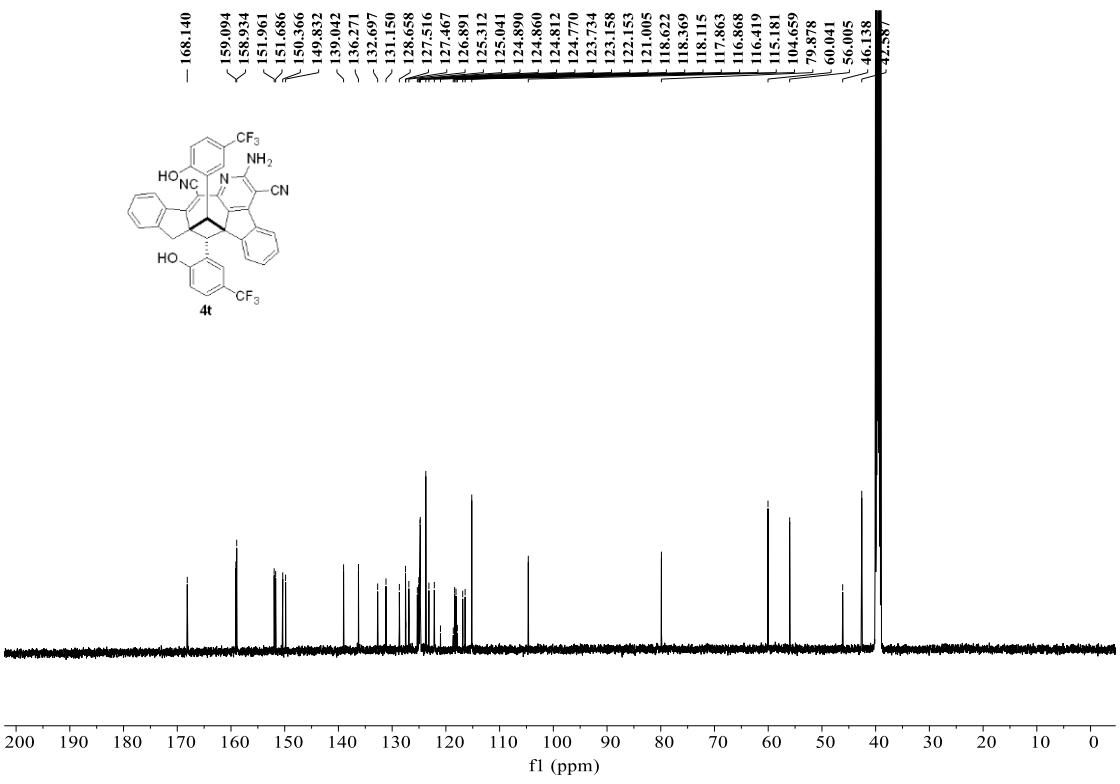
^{13}C NMR spectra for compound **4s** (125 MHz, DMSO-d_6)



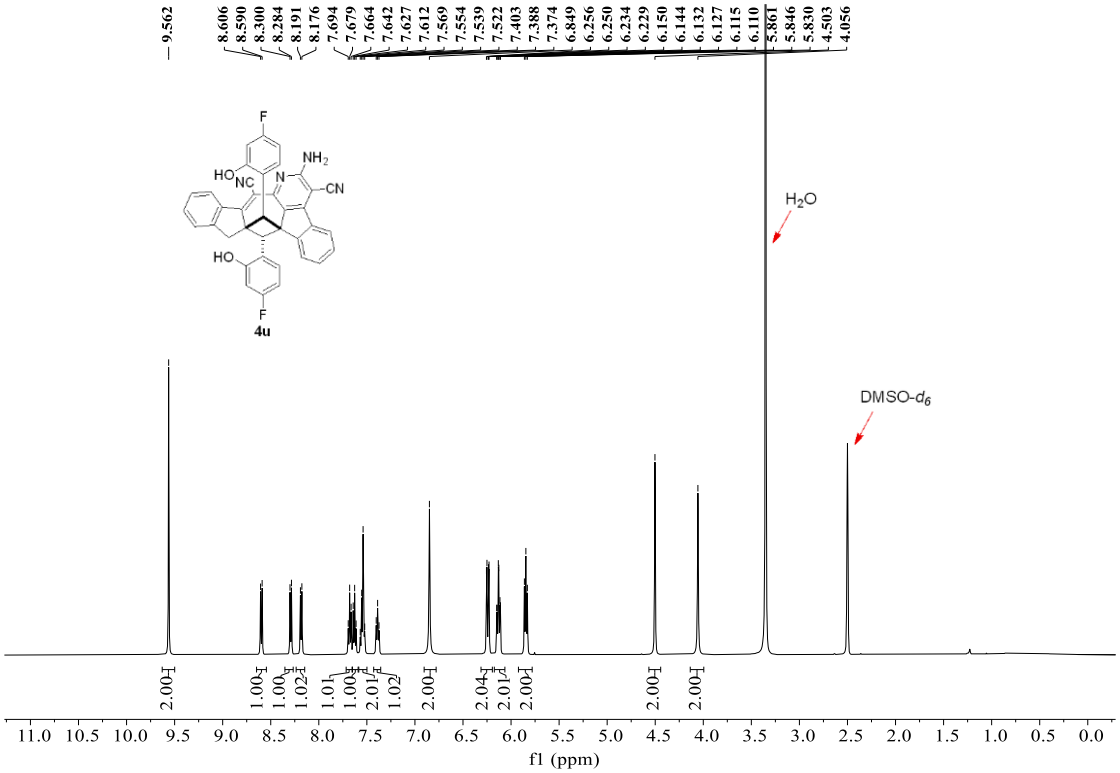
^{1}H NMR spectra for compound **4t** (500 MHz, DMSO-d_6)



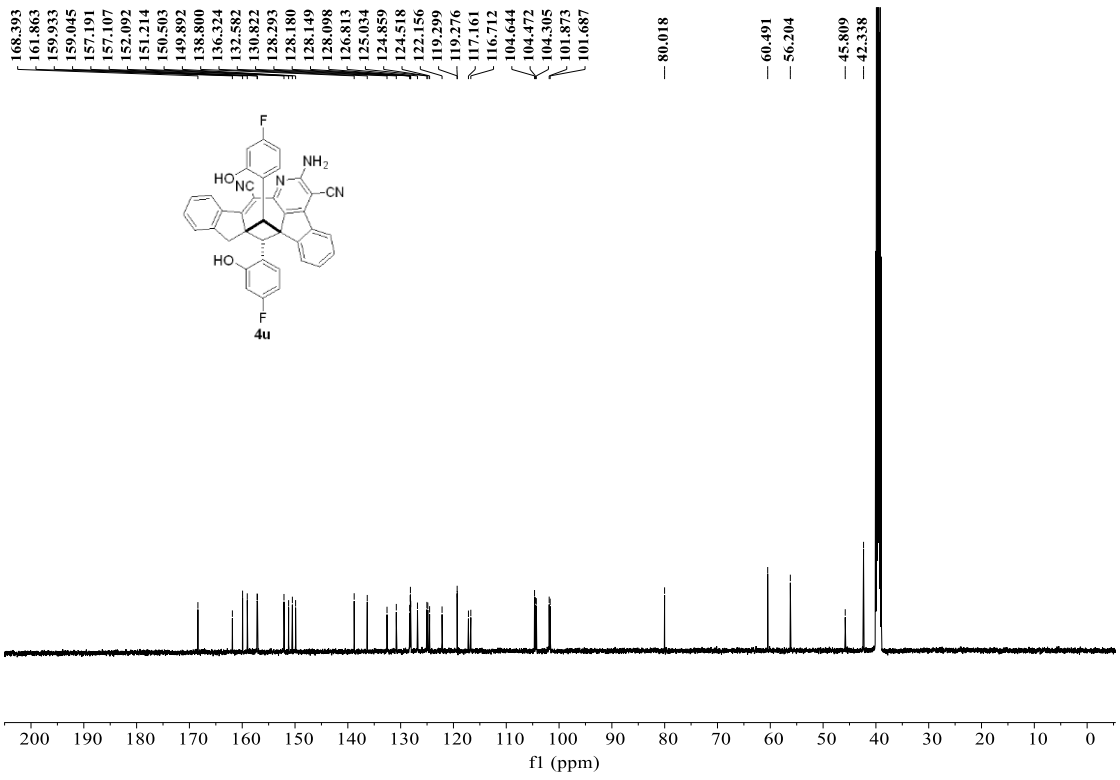
^{13}C NMR spectra for compound **4t** (125 MHz, DMSO-d_6)



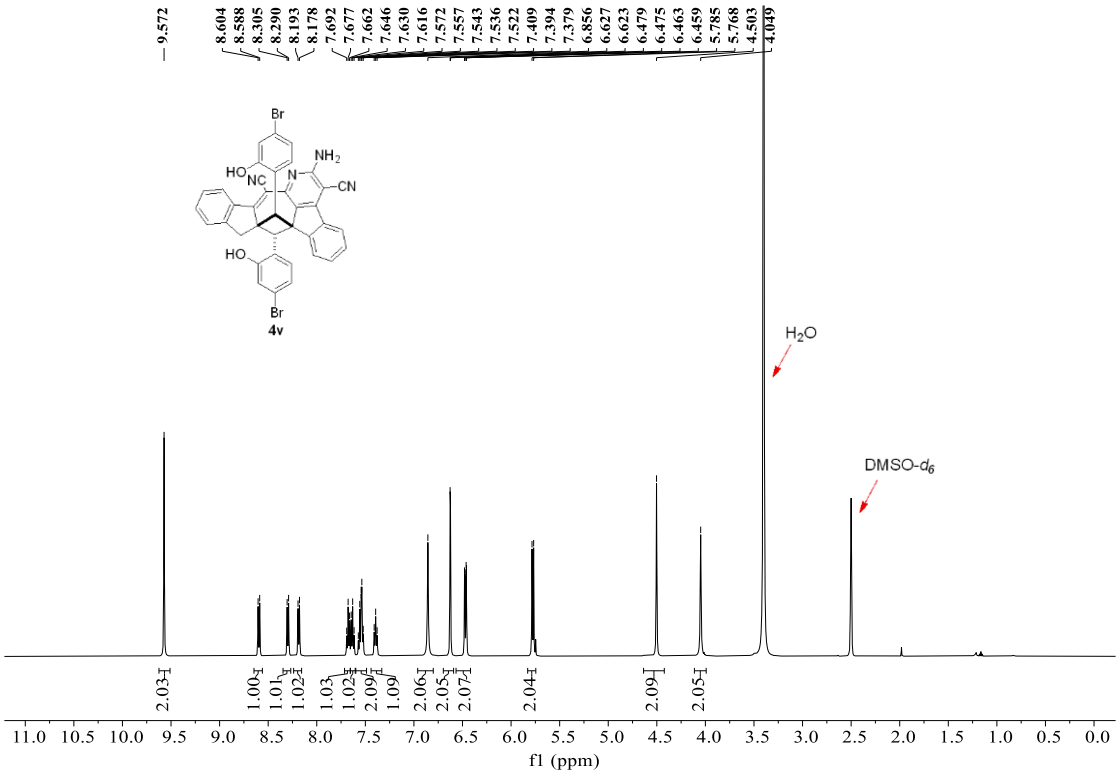
^{1}H NMR spectra for compound **4u** (500 MHz, DMSO-d_6)



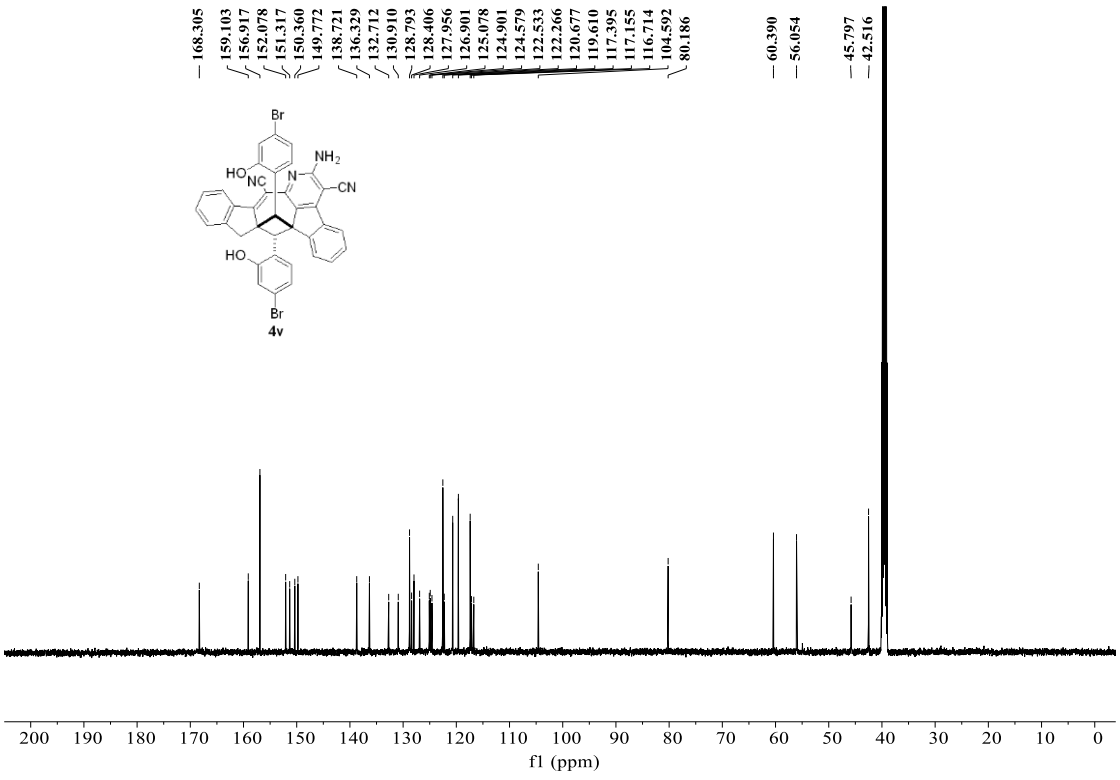
^{13}C NMR spectra for compound **4u** (125 MHz, DMSO-d_6)



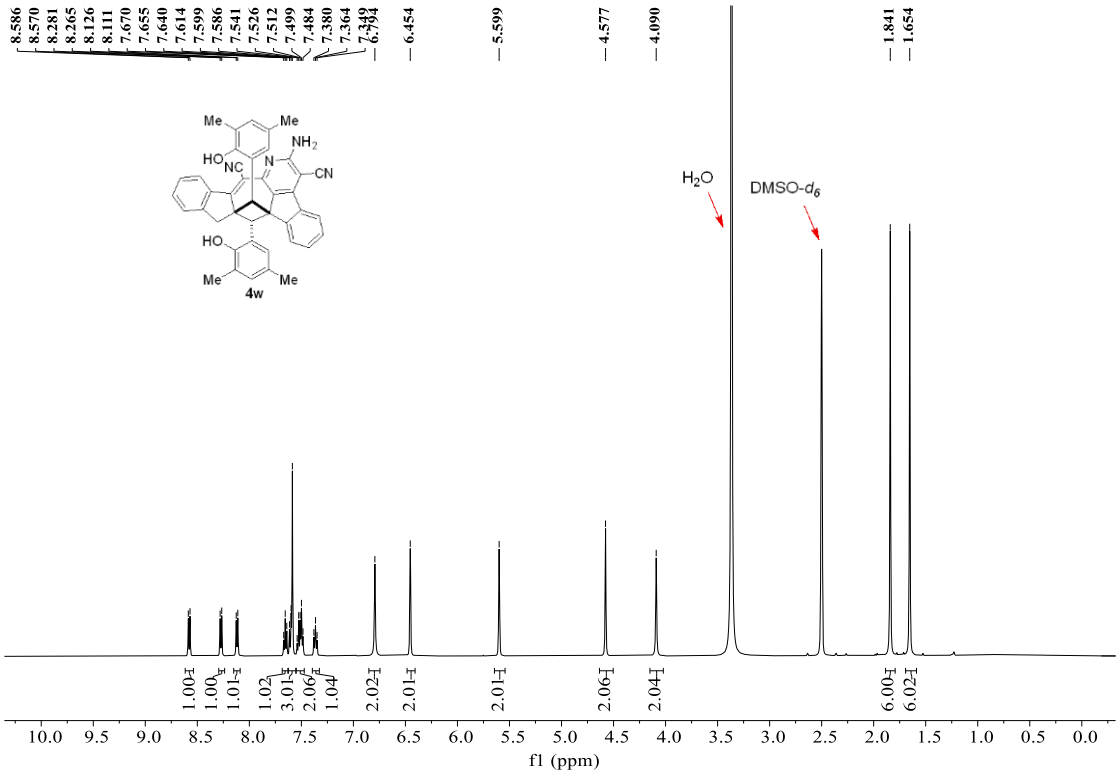
^{1}H NMR spectra for compound **4v** (500 MHz, DMSO-d_6)



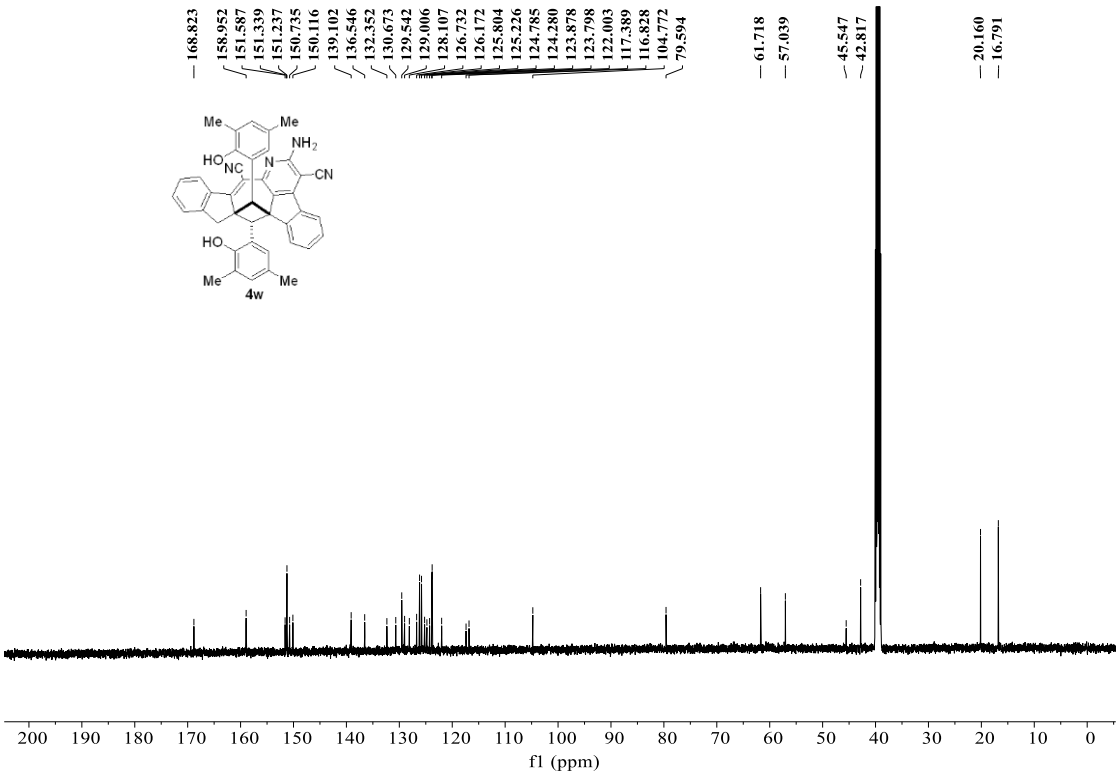
^{13}C NMR spectra for compound **4v** (125 MHz, DMSO-d_6)



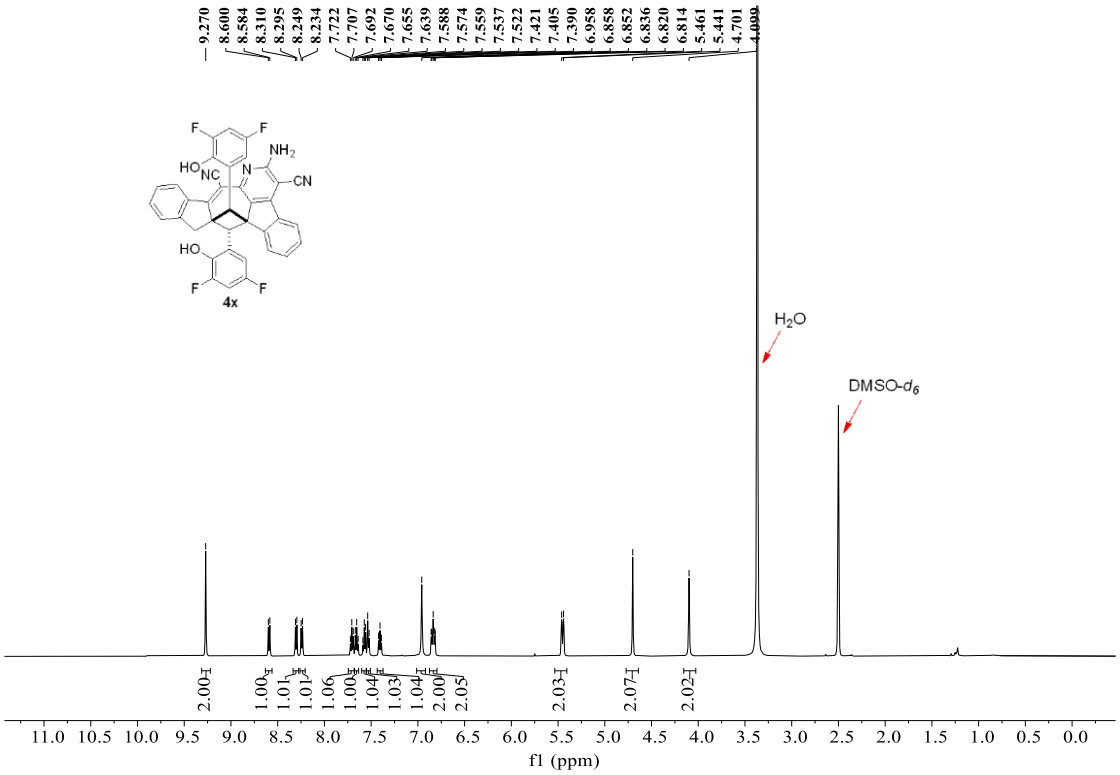
^{1}H NMR spectra for compound **4w** (500 MHz, DMSO-d_6)



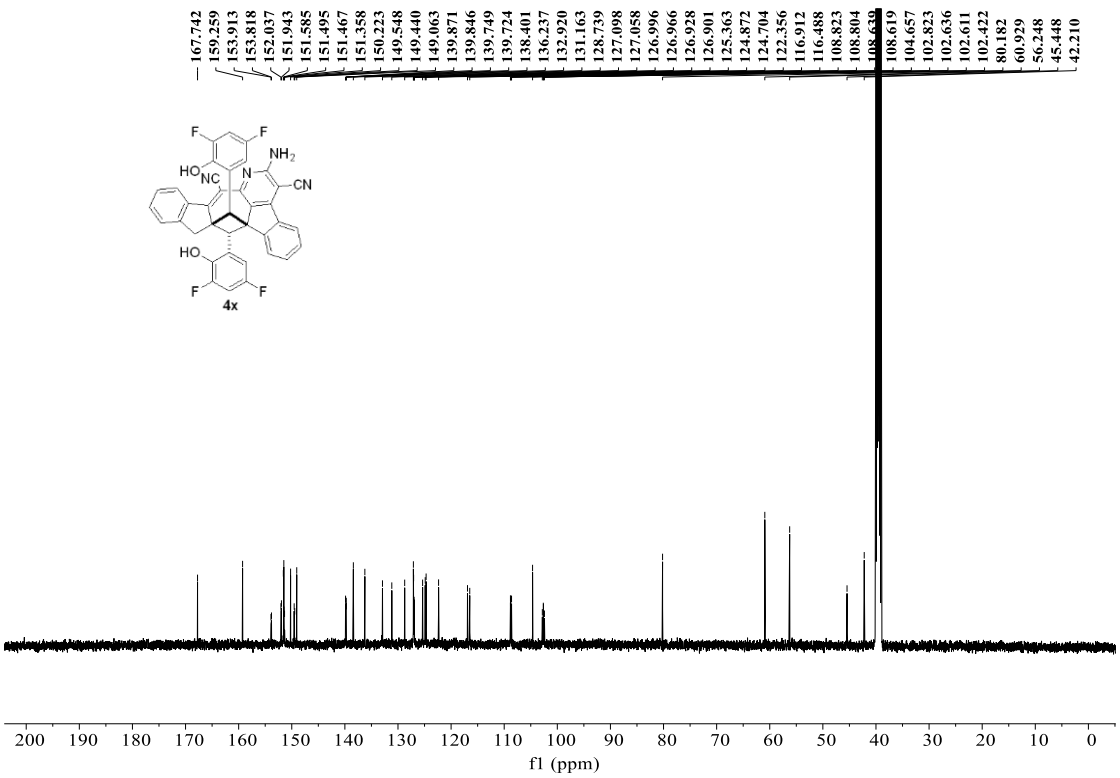
^{13}C NMR spectra for compound **4w** (125 MHz, DMSO-d_6)



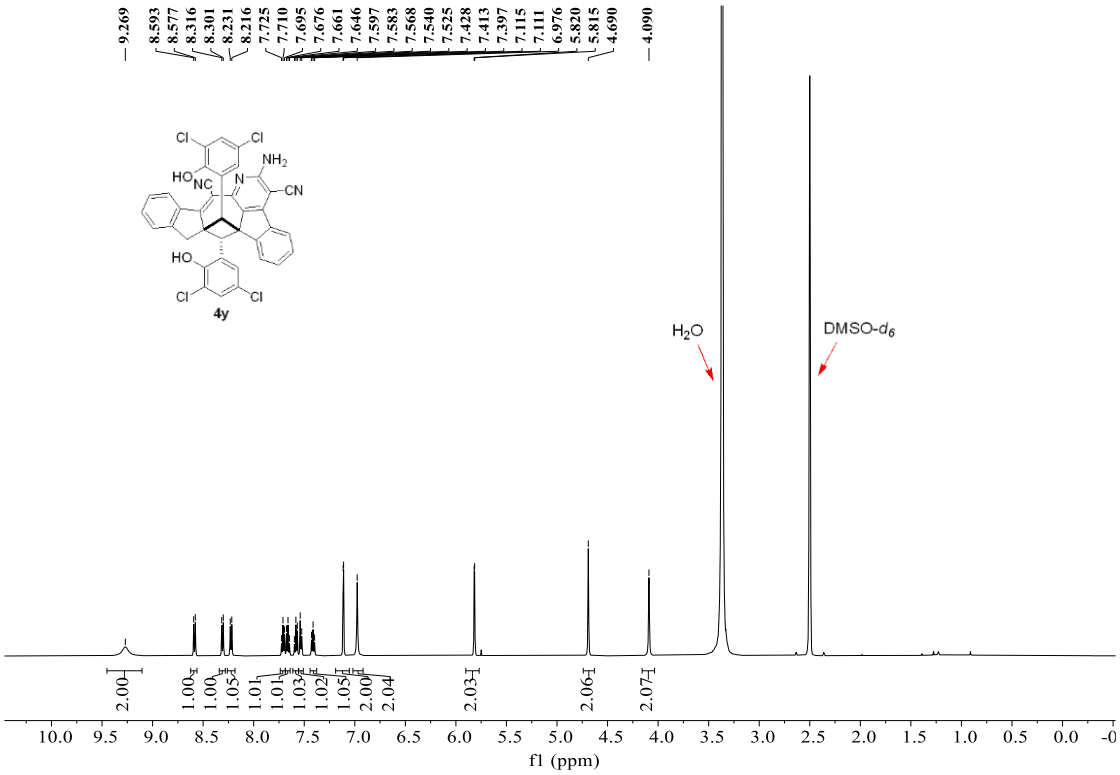
^{1}H NMR spectra for compound **4x** (500 MHz, DMSO-d_6)



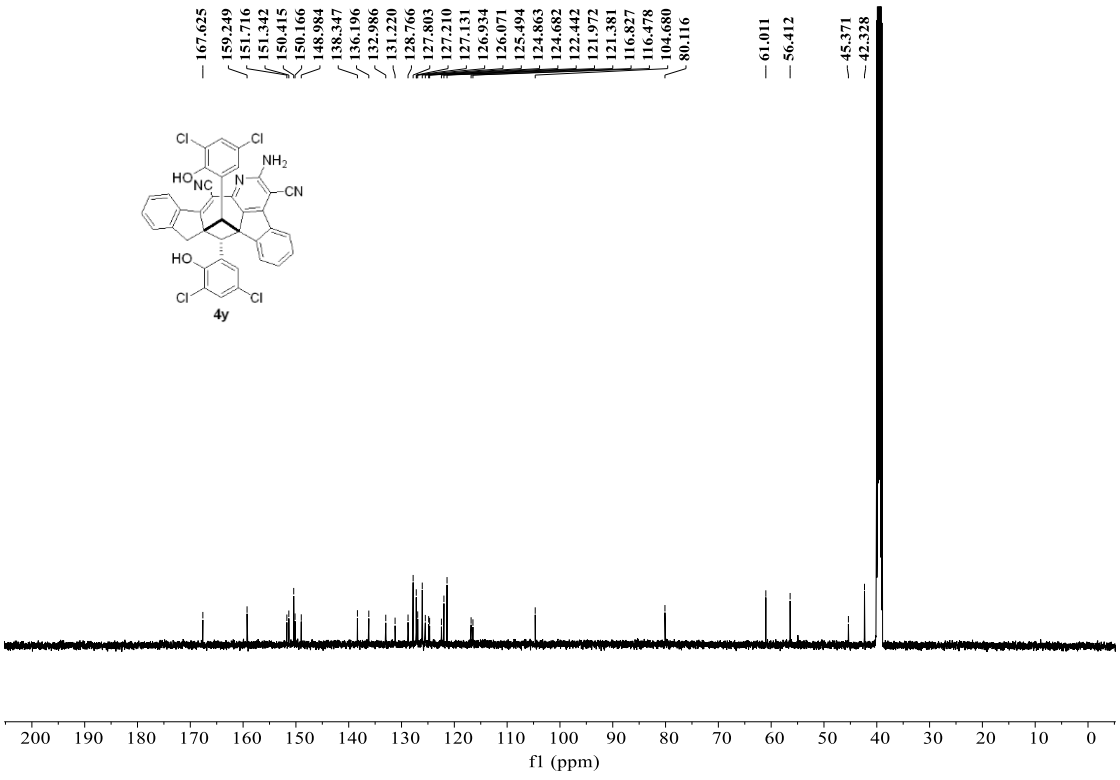
^{13}C NMR spectra for compound **4x** (125 MHz, DMSO-d_6)



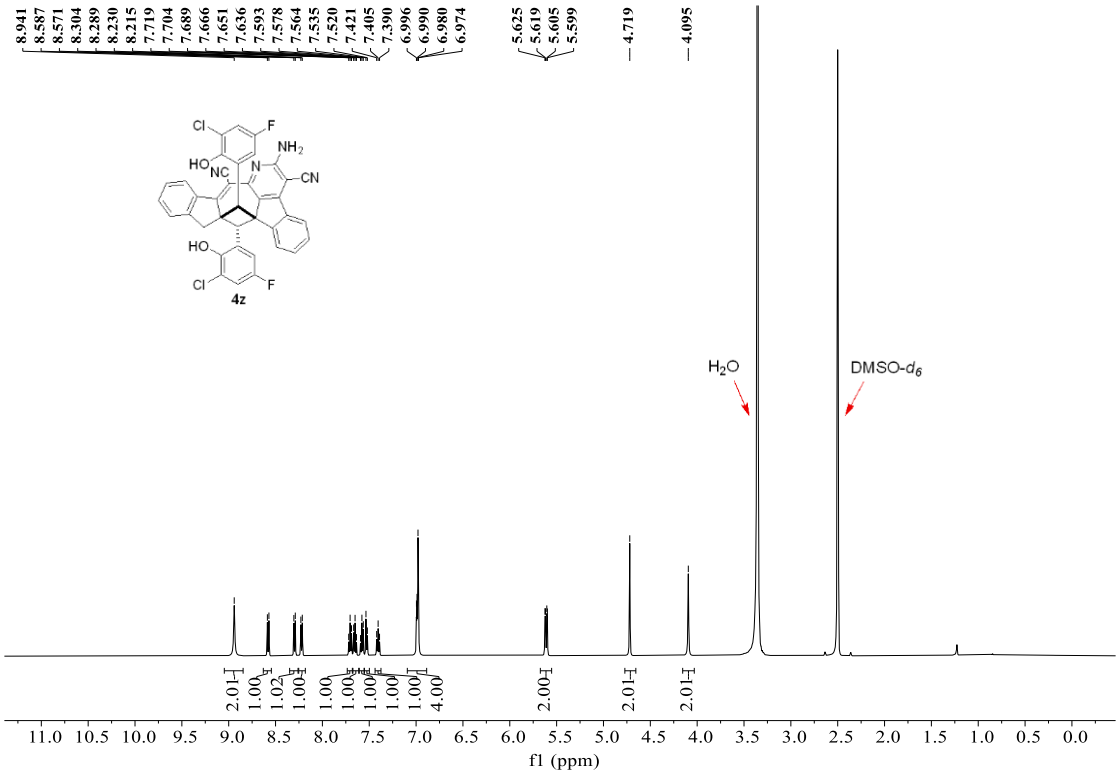
^{1}H NMR spectra for compound **4y** (500 MHz, DMSO-d_6)



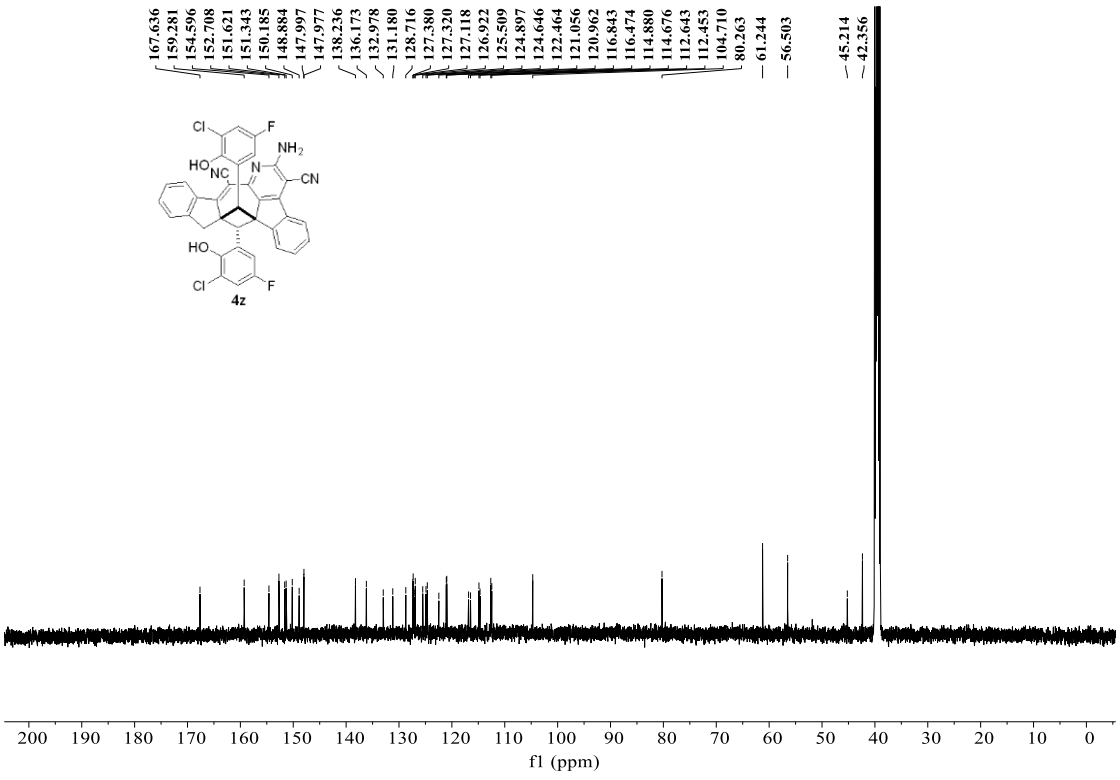
^{13}C NMR spectra for compound **4y** (125 MHz, DMSO-d_6)



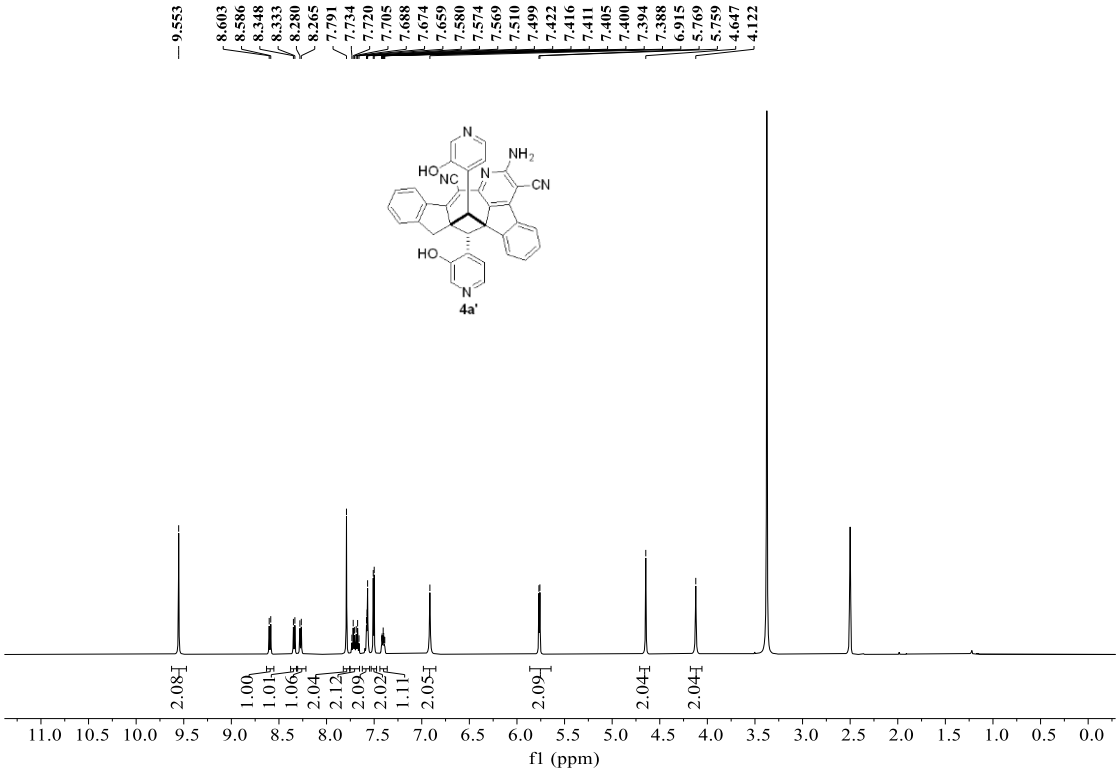
^{1}H NMR spectra for compound 4**z** (500 MHz, DMSO-d_6)



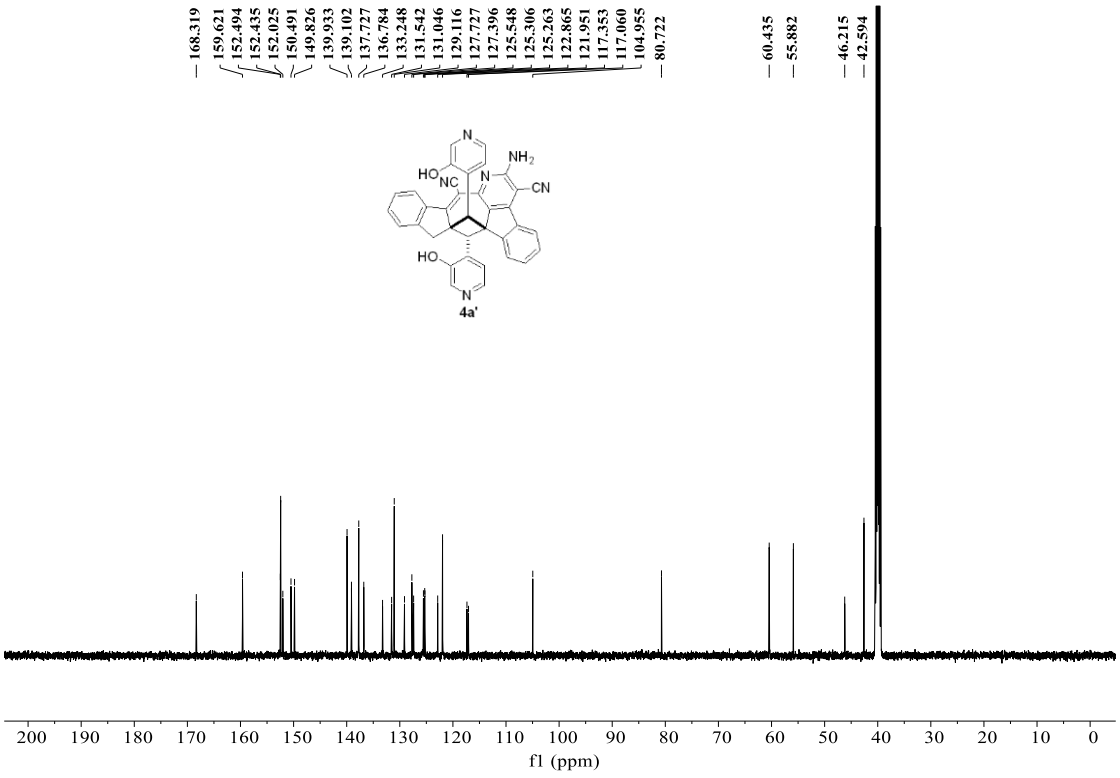
^{13}C NMR spectra for compound **4z** (125 MHz, DMSO-d_6)



^{1}H NMR spectra for compound **4a'** (500 MHz, DMSO-d_6)

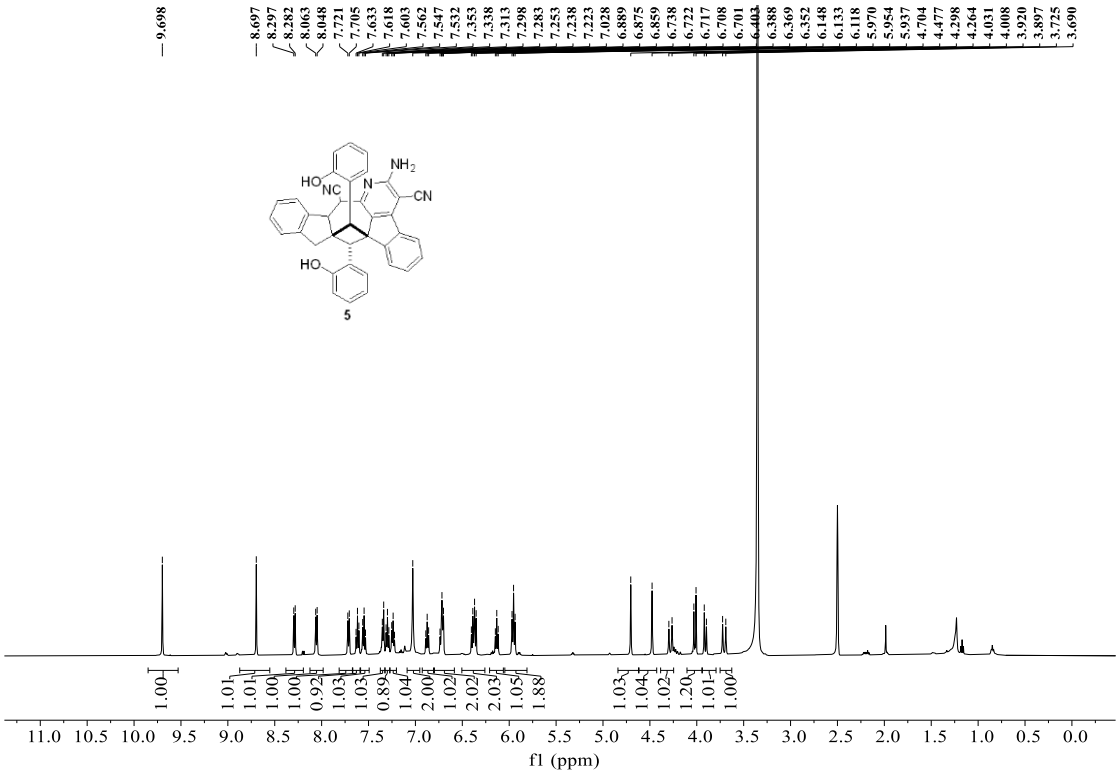


^{13}C NMR spectra for compound **4a'** (125 MHz, DMSO-d_6)

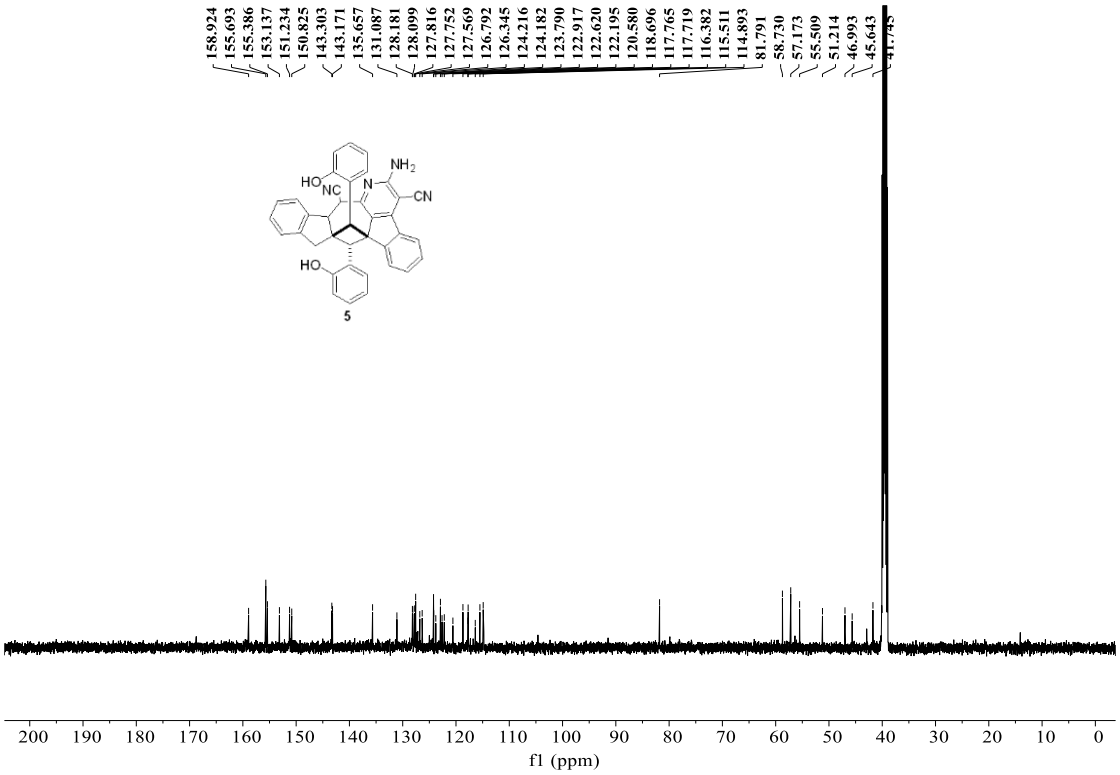


14.5 NMR spectra of all products 5-9, 11

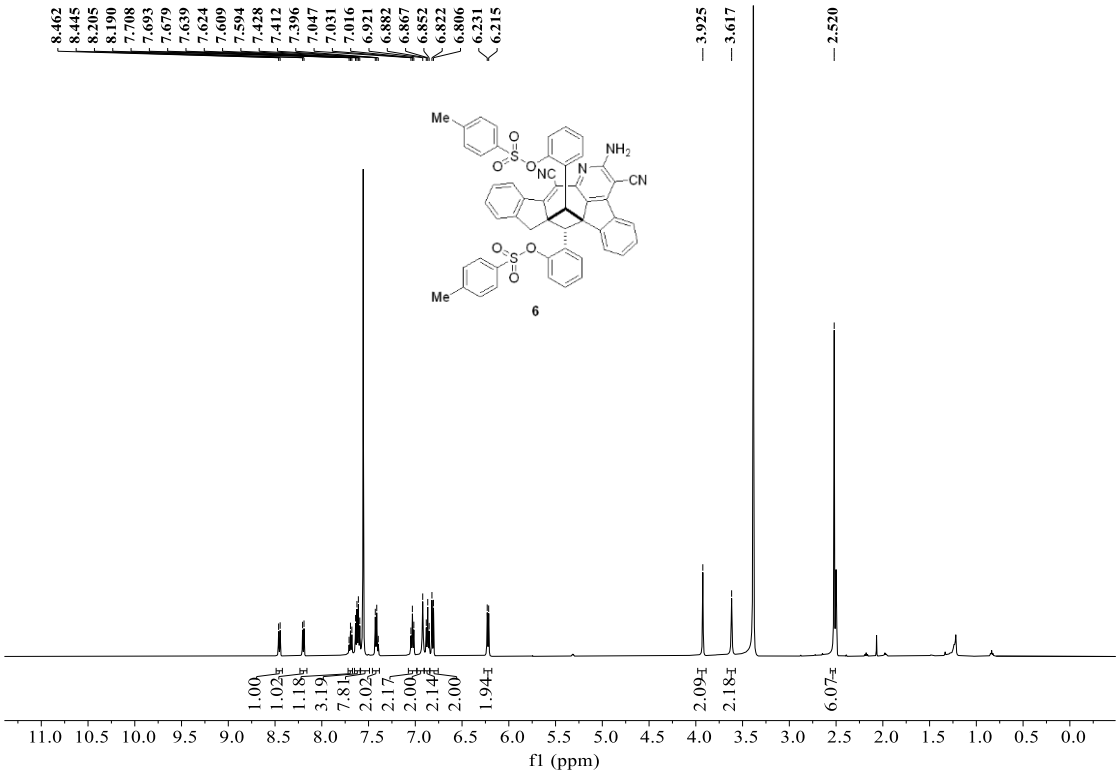
^{1}H NMR spectra for compound **5** (500 MHz, DMSO-d_6)



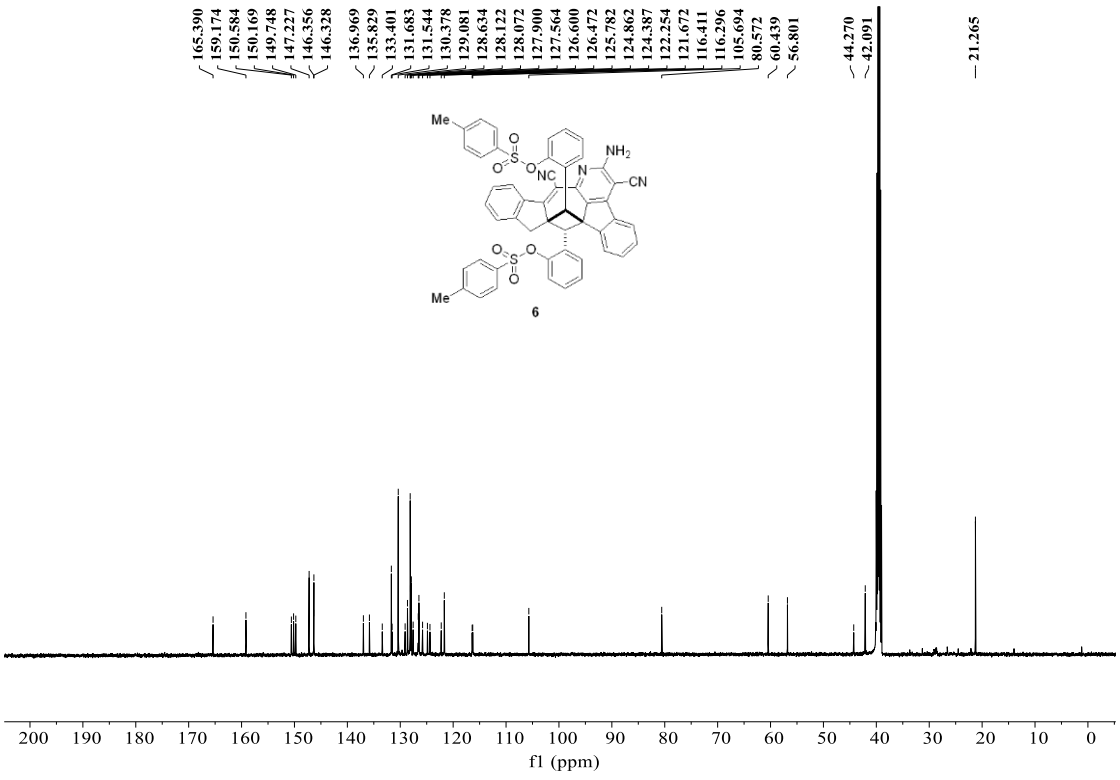
^{13}C NMR spectra for compound **5** (125 MHz, DMSO-d_6)



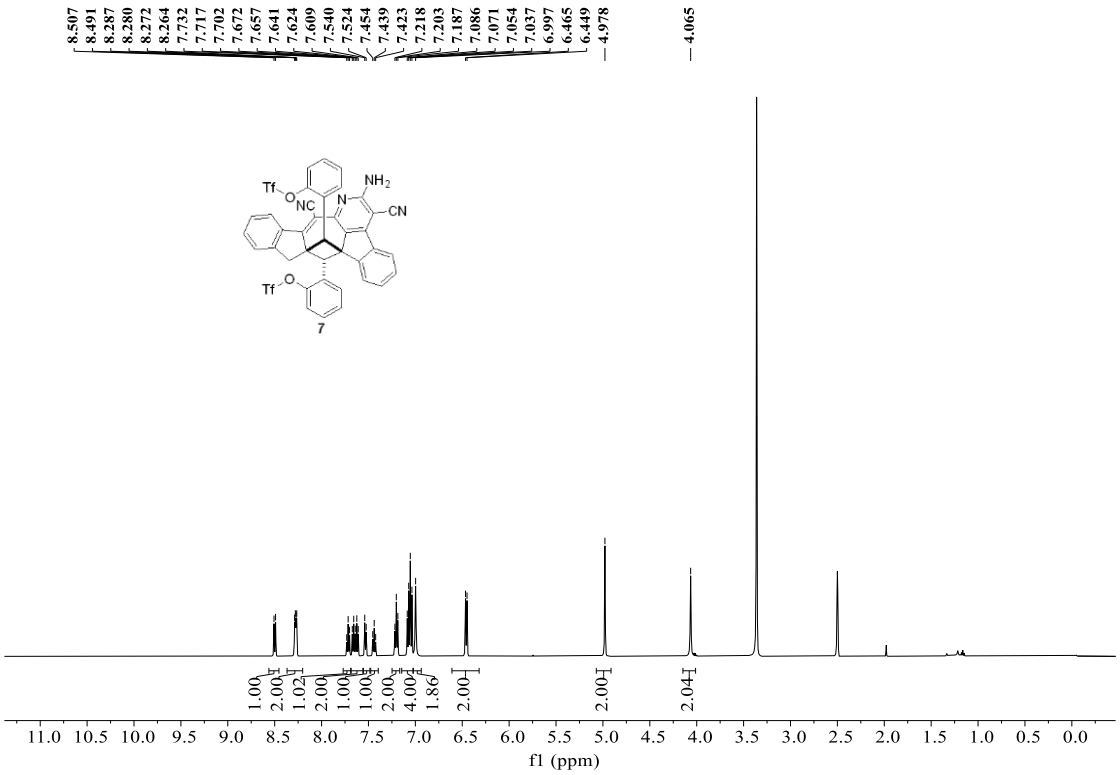
^{1}H NMR spectra for compound **6** (500 MHz, DMSO-d_6)



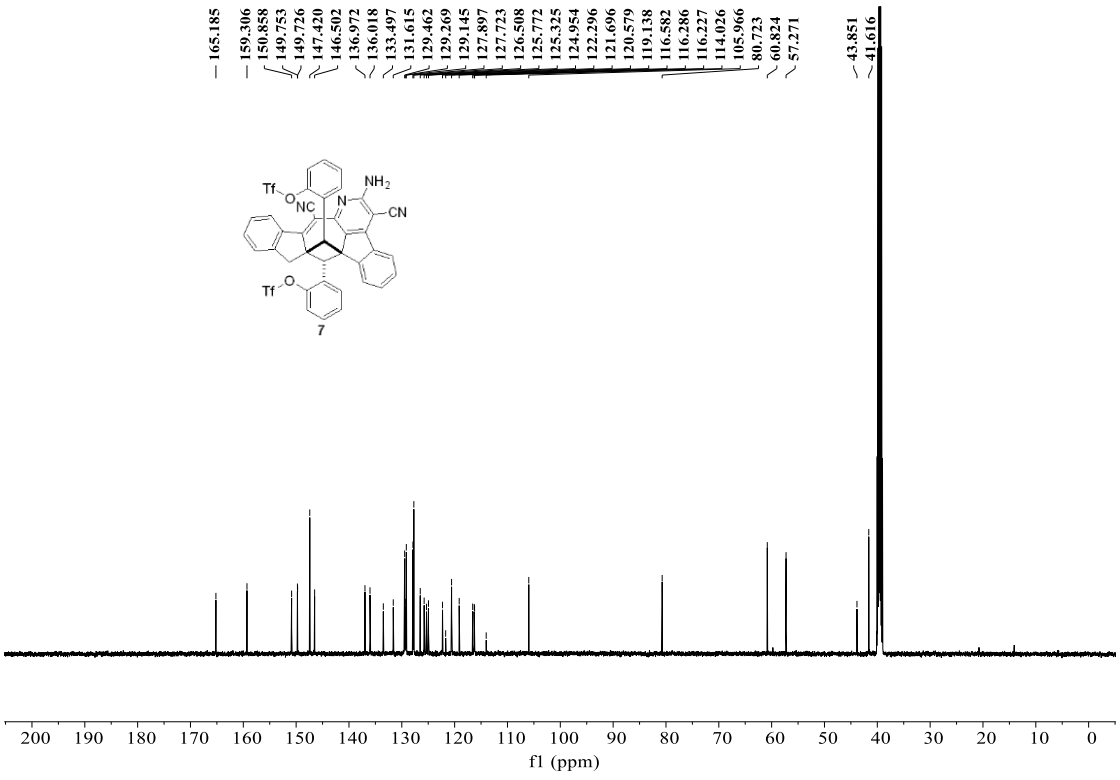
^{13}C NMR spectra for compound **6** (125 MHz, DMSO-d_6)



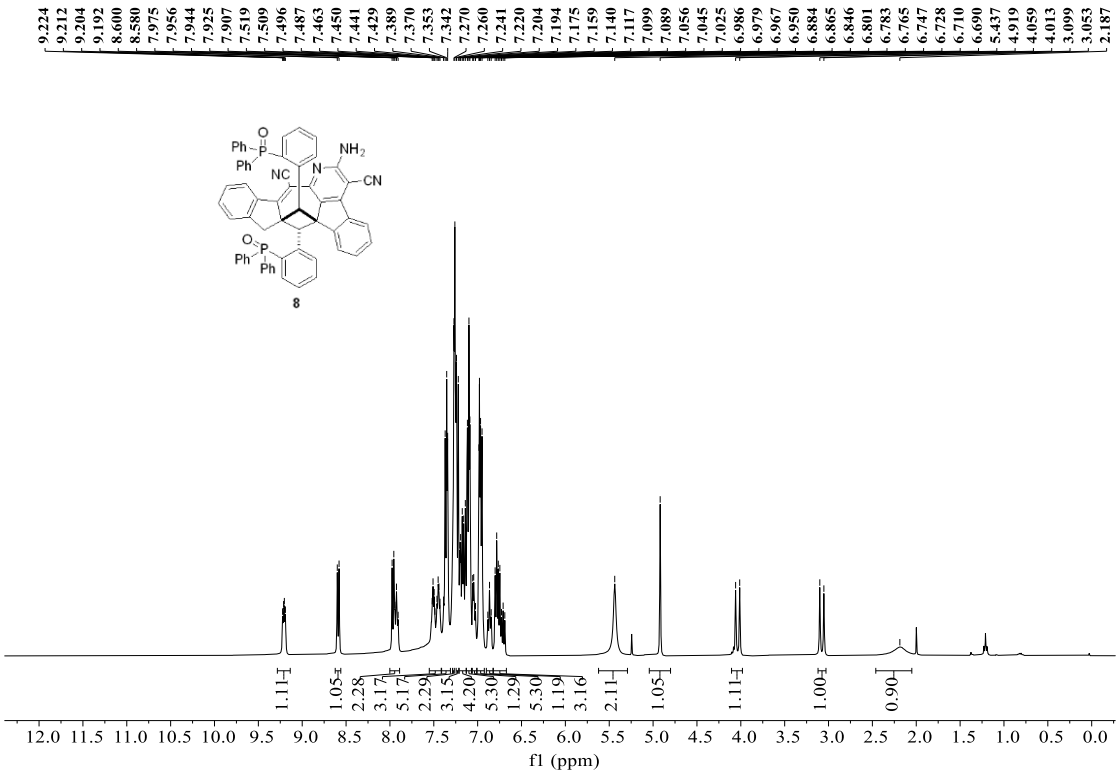
^{1}H NMR spectra for compound **7** (500 MHz, DMSO-d_6)



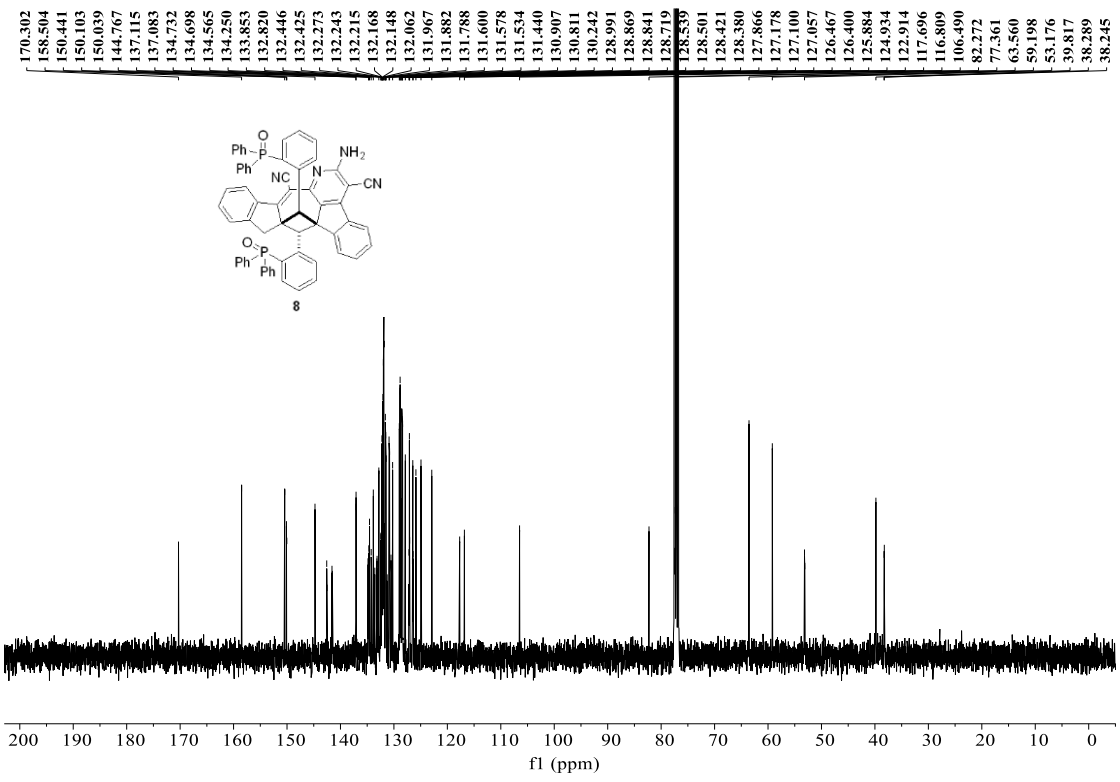
^{13}C NMR spectra for compound **7** (125 MHz, DMSO-d_6)



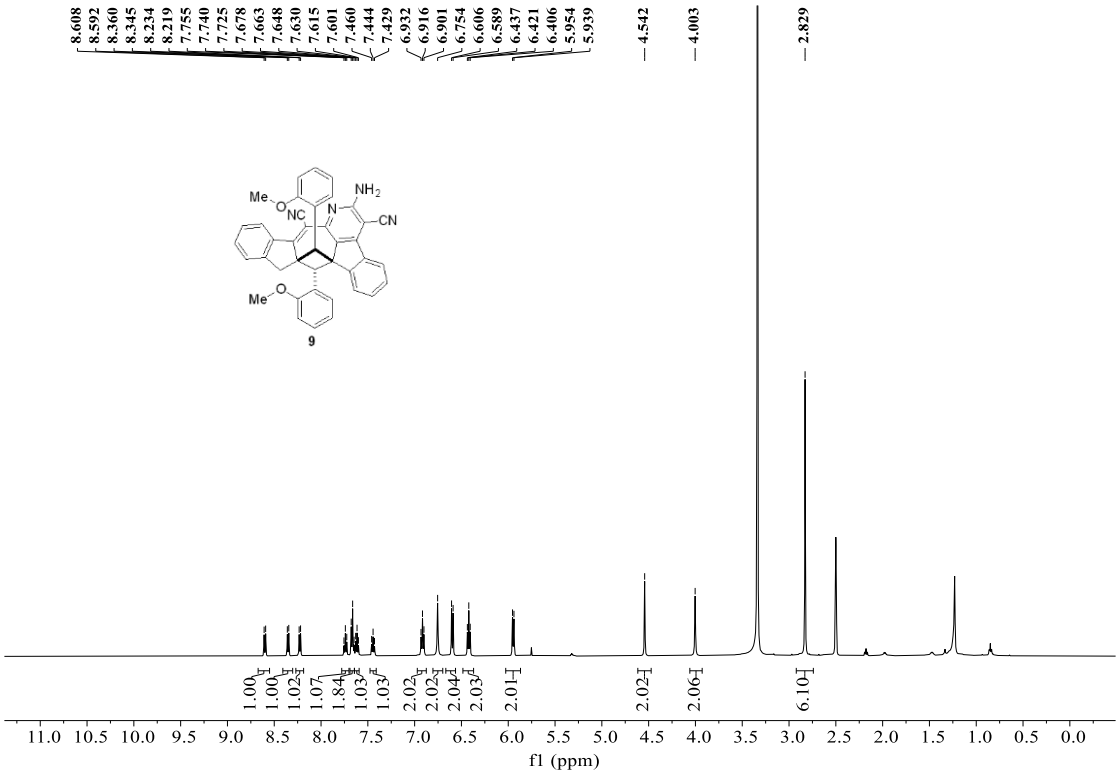
^{1}H NMR spectra for compound **8** (400 MHz, $CDCl_3$)



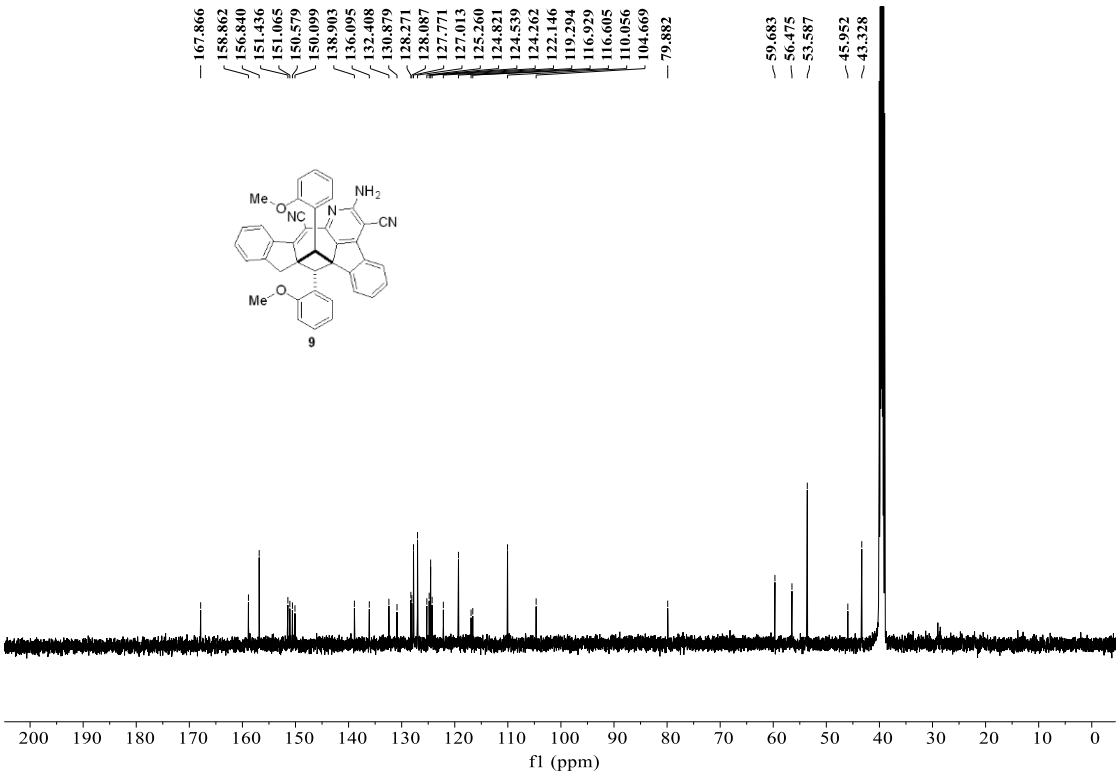
^{13}C NMR spectra for compound **8** (100 MHz, $CDCl_3$)



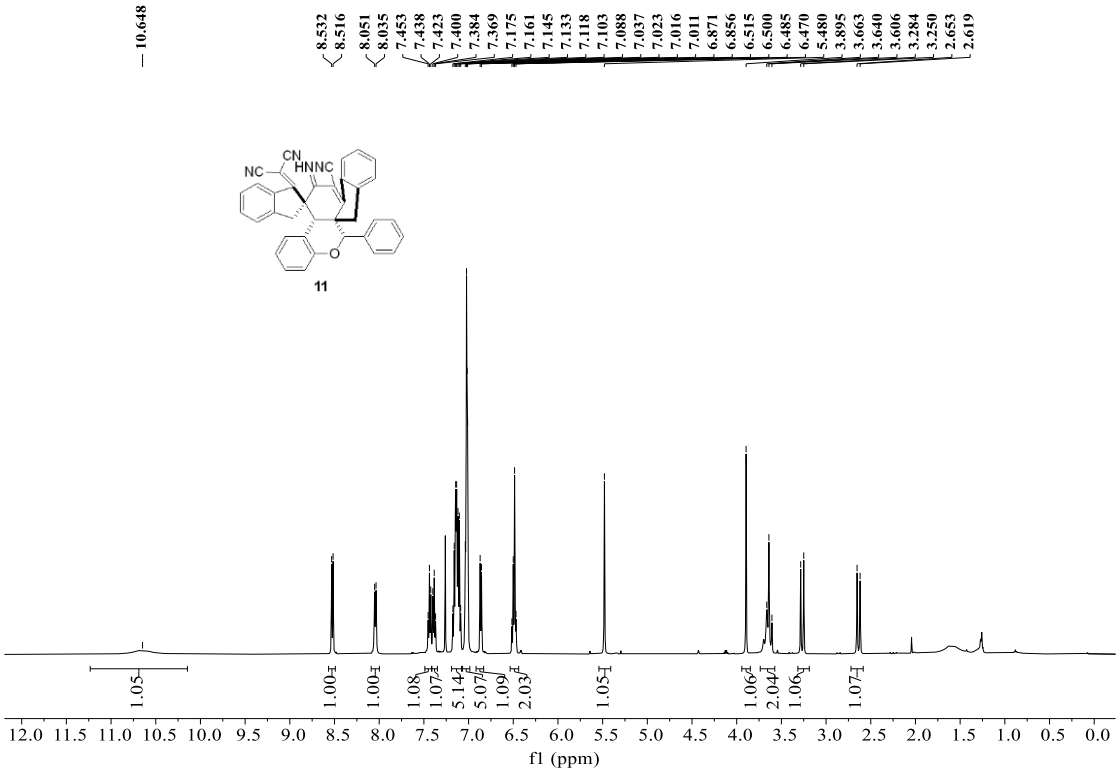
^{1}H NMR spectra for compound **9** (500 MHz, DMSO-d_6)



^{13}C NMR spectra for compound **9** (125 MHz, DMSO-d_6)



^{1}H NMR spectra for compound **11** (500 MHz, $CDCl_3$)



^{13}C NMR spectra for compound **11** (125 MHz, $CDCl_3$)