Supporting Information

Divergent Synthesis of Pyrrolidone Fused Pyrimido[1,2-*b*]indazole through Selective Trapping of Enone Intermediate by 1*H*-indazol-3-amine

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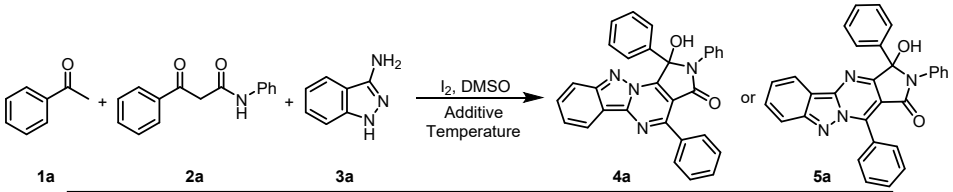
1. General

All the materials and solvents were commercially available and used without further purification. TLC analysis was performed using pre-coated glass plates. Column chromatography was performed using silica gel (200–300 mesh). ^{1}H spectra were recorded in $CDCl_3$ and DMSO-d_6 on 400 MHz NMR spectrometers and resonances (δ) are given in parts per million relative to tetramethylsilane. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz) and integration. ^{13}C spectra were recorded in $CDCl_3$ and DMSO-d_6 on 100 MHz NMR spectrometers and resonances (δ) are given in ppm. ^{19}F spectra were recorded in $CDCl_3$ and DMSO-d_6 on 376 MHz NMR using TMS as internal standard. HRMS were obtained on an Agilent LC1290-TOF 6224 equipped with an electrospray source. The X-ray crystal-structure determinations of **4b** and **5i** were obtained on a Bruker SMART APEX CCD system. Melting points were determined using XT-4 apparatus and not corrected.

2. Screening of reaction conditions

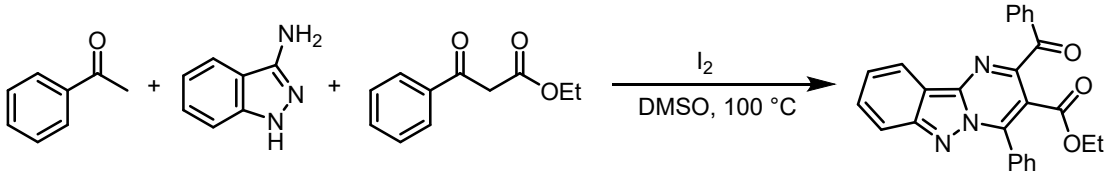


Entry	Additives (eq.)	Temp (°C)	Yield (%)[b]	
			4a	5a
1	**-**	**100**	**74**	**13**
2	$ZnCl_2$ (1.0)	100	65	15
3	$Cu(OTf)_2$ (1.0)	100	46	33
4	AcOH (1.0)	100	67	20
5	TsOH (1.0)	100	60	17
6	Na_2CO_3 (1.0)	100	45	trace
7	DBU (1.0)	100	63	16
8	TBHP (70 %) (1.0)	100	54	10
9	DTBP (1.0)	100	64	15
10	$Na_2S_2O_8$ (1.0)	100	trace	58
11	$PhI(OAc)_2$ (1.0)	100	70	15
12	MnO_2 (1.0)	110	nd	nd
13	$Na_2S_2O_8$ (0.5)	100	10	50
14	$Na_2S_2O_8$ (1.5)	100	trace	63
15	**$Na_2S_2O_8$ (2.0)**	**100**	**trace**	**67**
16	$Na_2S_2O_8$ (2.5)	100	trace	62
17	-	80	55	10
18	-	120	66	14
19	-	140	61	11
20	$Na_2S_2O_8$ (2.0)	80	trace	43
21	$Na_2S_2O_8$ (2.0)	120	11	62
22	$Na_2S_2O_8$ (2.0)	140	13	56

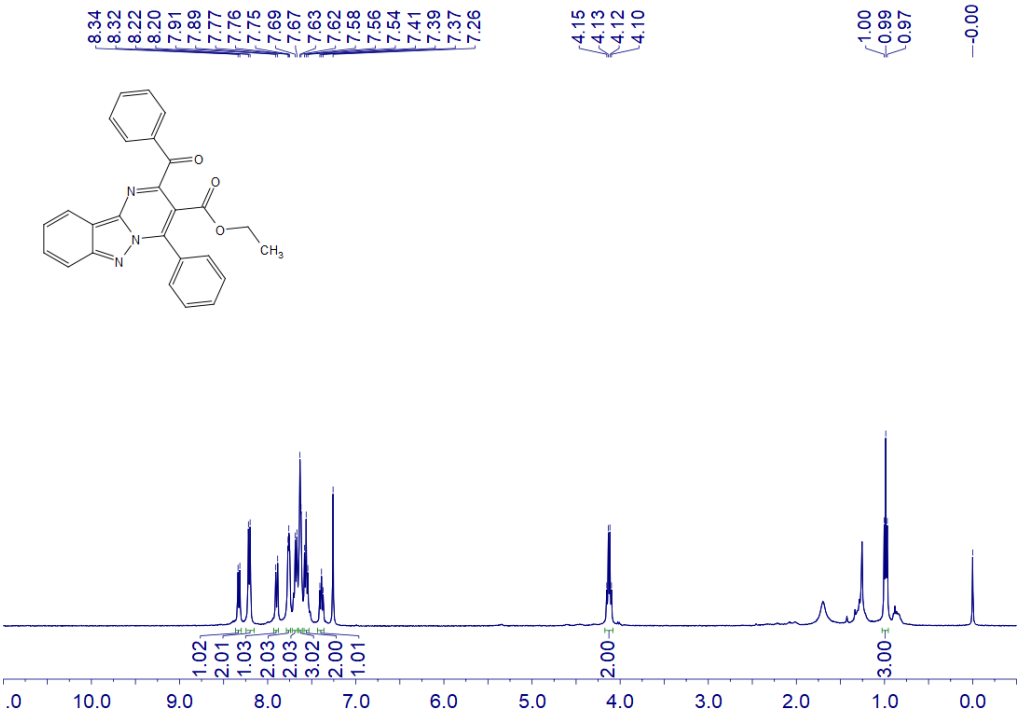
[a]Reaction conditions: **1a** (1.0 mmol), **2a** (1.0 mmol), **3a** (1.0 mmol), I_2 (1.0 mmol), additive (x equiv.), 4 h, DMSO (4.0 mL), indicated temperature, unless otherwise noted. [b]Isolated yields.

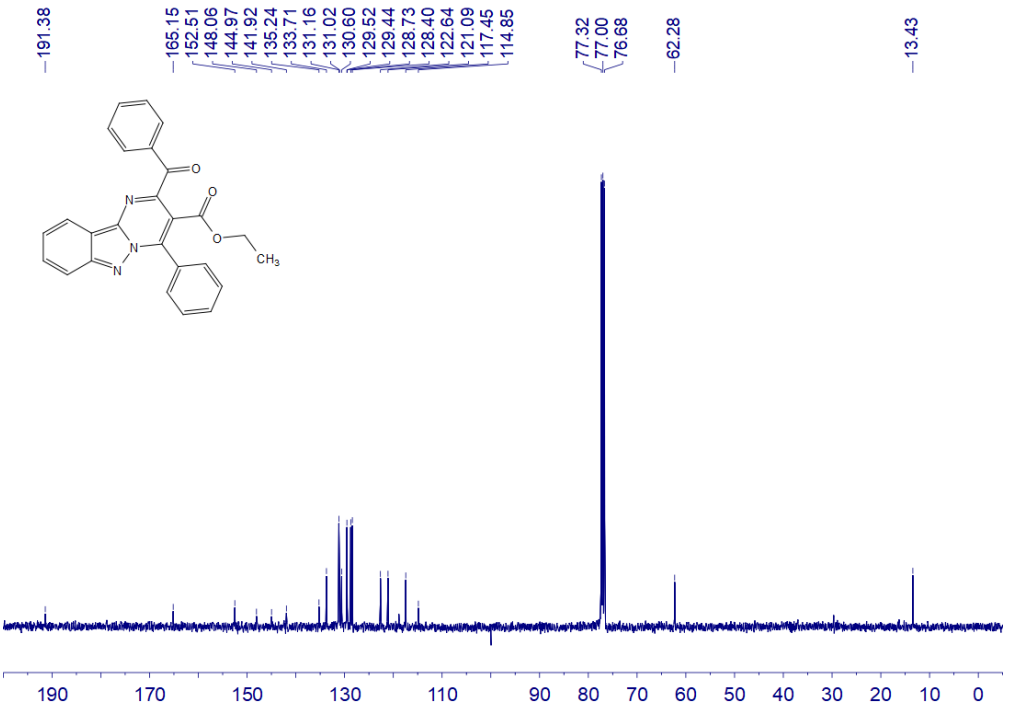
3. Synthesis steps and methods of operation

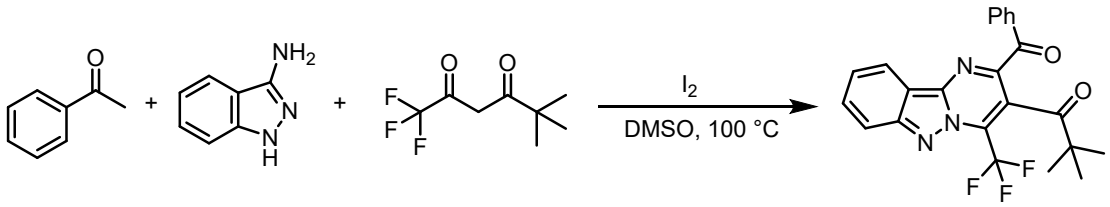
Some attempts (presumed structure)



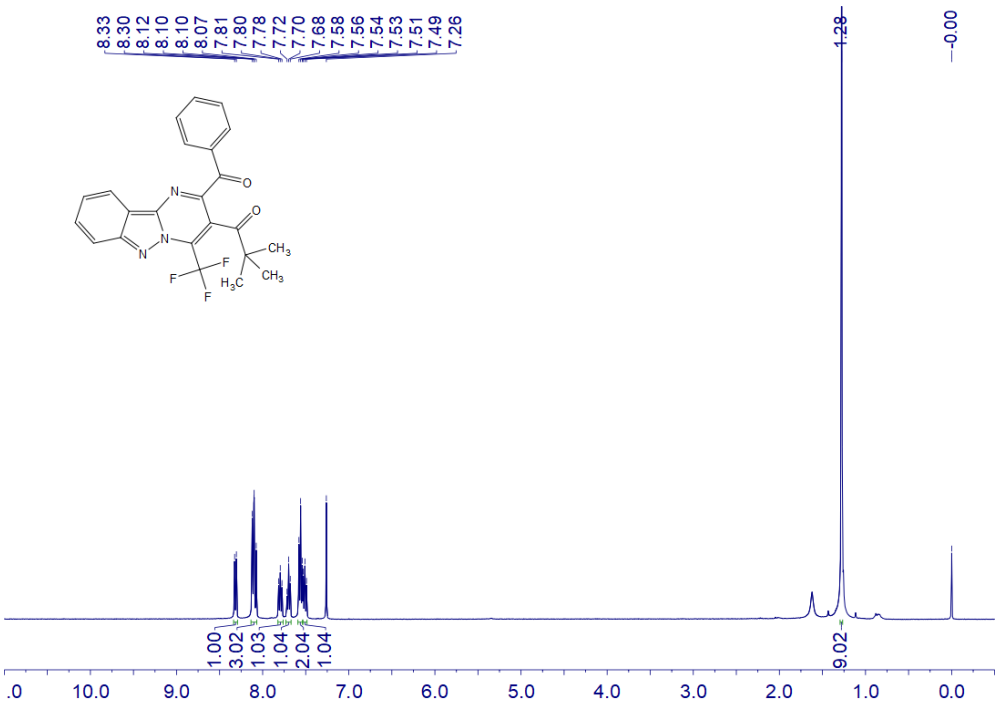
HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{26}H_{20}N_3O_3^+$: 422.1499; found: 422.1491.

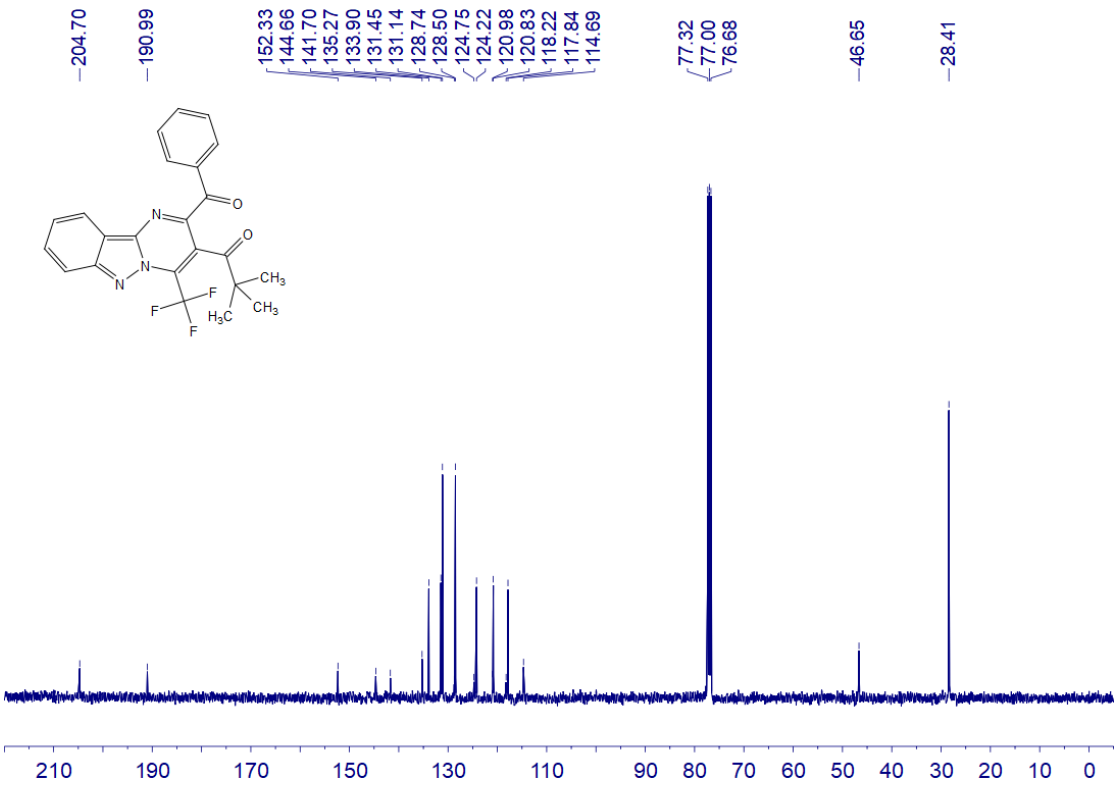


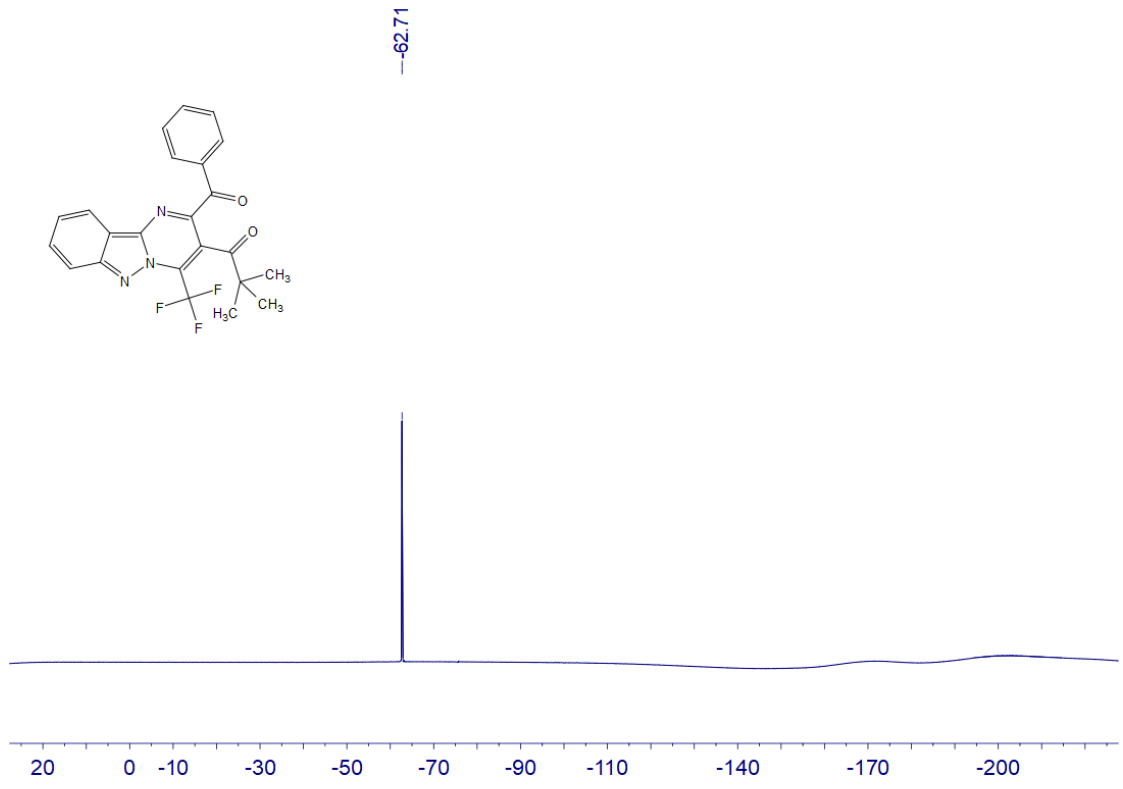




HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{23}H_{19}F_3N_3O_2^+$: 426.1424; found: 426.1418.






-62.71
O
N
O
N
N
F
F
F
H3C
CH3
CH3
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0
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-50
-70
-90
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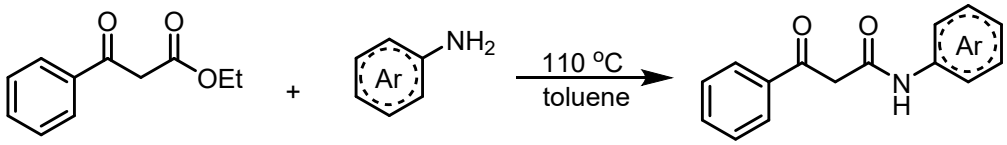
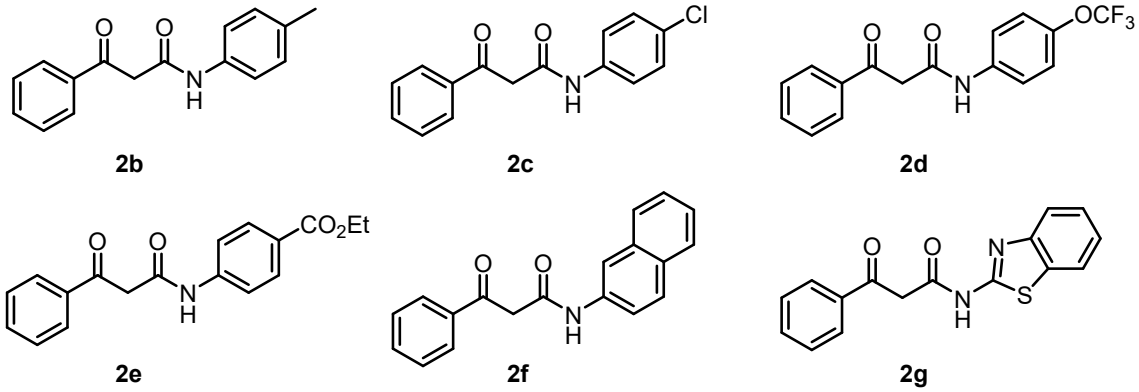
-170
-200

Synthetic methods of benzoylacetanilides



2a-2g

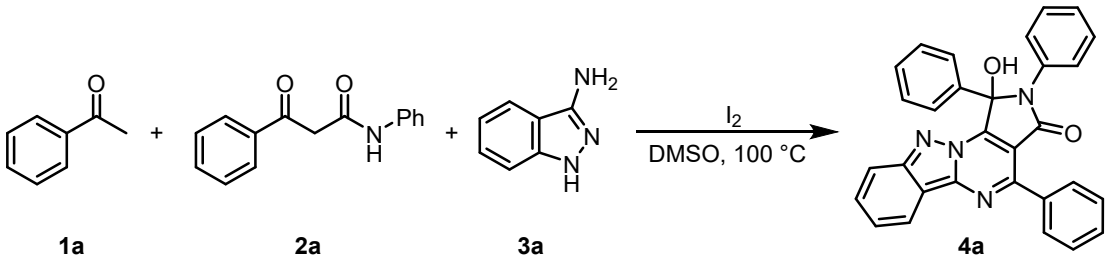
Ethyl benzoylacetate (1 mmol) and aryl amine (1.1 mmol) were heated in toluene solvent (2 ml, 18.8 mmol) and reacted under reflux conditions for 12 hours. After the completion of the reaction, the solvent was removed under reduced pressure to obtain a crude residue. The crude product was purified by column chromatography on silica gel (200−300 mesh) to afford the product **2b**-**2g** in 90% yields.[1]



2b **2c** **2d**

2e **2f** **2g**

General procedure for the synthesis of 4 and 5 (4a or 5a as example)

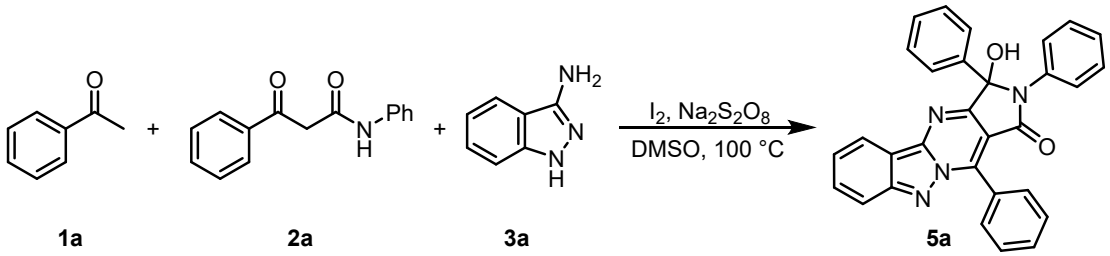


1a **2a** **3a** **4a**

1.0 mmol scale: The reactions did not require the protection of inert gases. In a 35 mL sealed tube were added acetophenone (**1a**) (120 mg, 1.0 mmol), iodine (254 mg, 1.0 mmol) and dimethyl sulfoxide (4 mL) and the resulting mixture was stirred at 100 ℃ (heating block), the reaction tube was removed after about 1 hour. Then additional **2a** (240 mg, 1.0 mmol), **3a** (133 mg, 1.0 mmol) were added at room temperature, followed by reaction at 100 ℃ for 4 hours until substrate conversion was almost complete by TLC analysis. The reaction mixture was quenched with saturated $Na_2S_2O_3$ solution (50 mL) and NaCl solution (150 mL), then the mixture was extracted with EtOAc (150 mL x 2), the organic layers were separated and combined,

dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 8:1) to afford the product **4a** (346 mg, 74% yield).

5.0 mmol scale: The reactions did not require the protection of inert gases. In a 100 mL round flask were added acetophenone (**1a**) (600 mg, 5.0 mmol), iodine (1270 mg, 5.0 mmol) and dimethyl sulfoxide (30 mL) and the resulting mixture was stirred in oil bath heating at 100 ℃, the round flask was removed after about 1.5 hours. Then additional **2a** (1200 mg, 5.0 mmol), **3a** (665 mg, 5.0 mmol) were added at room temperature, followed by reaction at 100 ℃ for 6 hours until substrate conversion was almost complete by TLC analysis. The reaction mixture was quenched with saturated $Na_2S_2O_3$ solution (150 mL) and NaCl solution (300 mL), then the mixture was extracted with EtOAc (300 mL x 2), the organic layers were separated and combined, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 7:1) to afford the product **4a** (1470 mg, 63% yield).



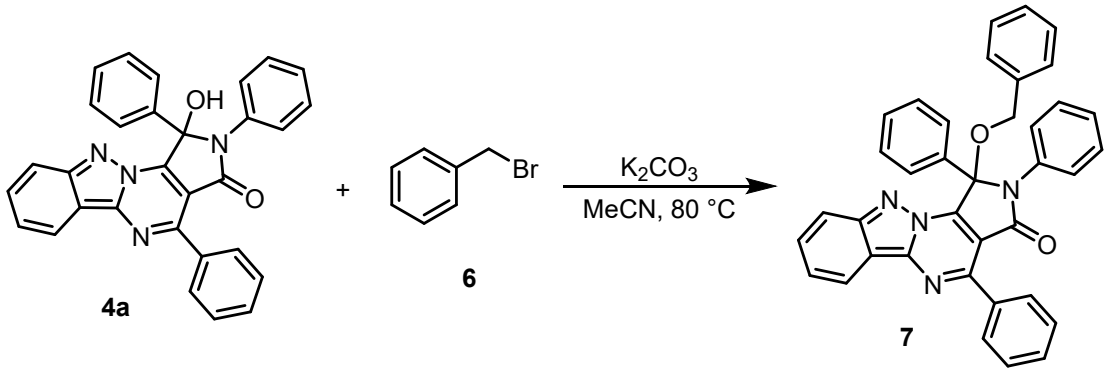
1a **2a** **3a** **5a**

1.0 mmol scale: The reactions did not require the protection of inert gases. In a 35 mL sealed tube were added acetophenone (**1a**) (120 mg, 1.0 mmol), iodine (254 mg, 1.0 mmol) and dimethyl sulfoxide (4 mL) and the resulting mixture was stirred at 100 ℃ (heating block), the reaction tube was removed after about 1 hour. Then additional **2a** (240 mg, 1 .0 mmol), **3a** (133 mg, 1.0 mmol), $Na_2S_2O_8$ (476 mg, 2.0 mmol) were added at room temperature, followed by reaction at 100 ℃ for 4 hours until substrate conversion was almost complete by TLC analysis. The reaction mixture was quenched with saturated $Na_2S_2O_3$ solution (50 mL) and NaCl solution (150 mL), then the mixture was extracted with EtOAc (150 mL x 2), the organic layers were separated and combined, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1) to afford the product **5a** (313 mg, 67% yield).

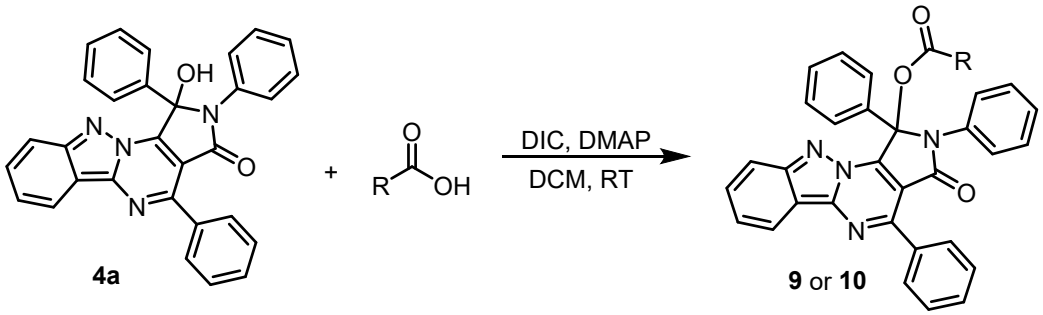
5.0 mmol scale: The reactions did not require the protection of inert gases. In a 100 mL round flask were added acetophenone (**1a**) (600 mg, 5.0 mmol), iodine (1270 mg, 5.0 mmol) and dimethyl sulfoxide (30 mL) and the resulting mixture was stirred in oil bath heating at 100 ℃, the round flask was removed after about 1.5 hours. Then additional **2a** (1200 mg, 5.0 mmol), **3a** (665 mg, 5.0 mmol), $Na_2S_2O_8$ (2380 mg, 10.0 mmol) were added at room temperature, followed by reaction at 100 ℃ for 6 hours

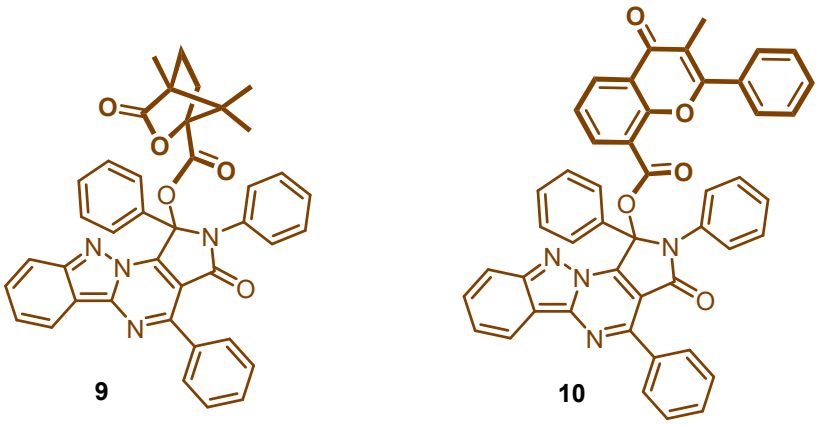
until substrate conversion was almost complete by TLC analysis. The reaction mixture was quenched with saturated $Na_2S_2O_3$ solution (150 mL) and NaCl solution (300 mL), then the mixture was extracted with EtOAc (300 mL x 2), the organic layers were separated and combined, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1) to afford the product **5a** (1380 mg, 59% yield).

Coupling of products and transformation of drug molecules

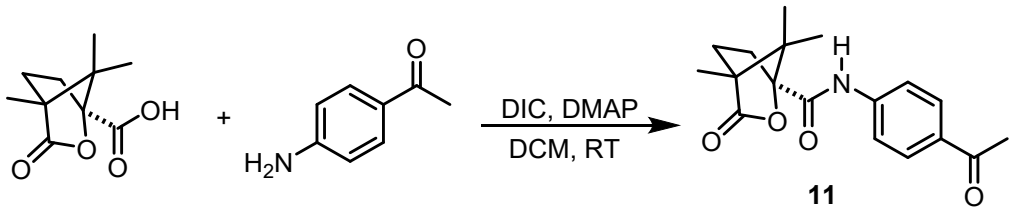


4a (140.0 mg, 0.3 mmol), benzyl bromide **6** (77 mg, 0.45 mmol) and K_2CO_3 (83.0 mg, 0.6 mmol) were dissolved in MeCN (4 mL) and heated at 80℃ for 7 hours. After substrate conversion was almost complete by TLC analysis, EtOAc and NaCl solution were added to the reaction mixture and extracted twice. The combined organic layers were dried with anhydrous Na_2SO_4 and then concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 20:1) to afford the product **7** (155 mg, 93% yield).[2]





4a (0.3 mmol, 141 mg), (1*S*)-(-)-Camphanic acid (0.3 mmol, 59 mg), [or flavoxate acid (0.3 mmol, 84 mg)] and 4-dimethylaminopyridine (DMAP, 0.1 mmol, 12.2 mg) were added to a 35 mL sealed tube, then 3 mL of dichloromethane was added and mixed well to form a solution, and add the condensation reagent *N, N*-diisopropylcarbodiimide (DIC, 0.45 mmol, 57 mg) while stirring the solution. Keep the mixture stirred at room temperature for 4 hours using a magnetic stirrer to complete the reaction. After the reaction, the crude product was obtained by extracting with ethyl acetate and NaCl aqueous solution and concentrating under reduced pressure. Finally, the pure target product was obtained by column chromatography separation.[3]



(1*S*)-(-)-Camphanic acid (10 mmol, 1980 mg), 1-(4-aminophenyl)ethan-1-one (10 mmol, 1350 mg) and 4-dimethylaminopyridine (DMAP, 3 mmol, 366 mg) were added to a 100 mL round-bottomed flask, then 50 mL of dichloromethane was added and mixed well to form a solution, and add the condensation reagent *N, N*-diisopropylcarbodiimide (DIC, 15 mmol, 1890 mg) while stirring the solution. Keep the mixture stirred at room temperature for 6 hours using a magnetic stirrer to complete the reaction. At the end of the reaction, the organic phase was extracted and

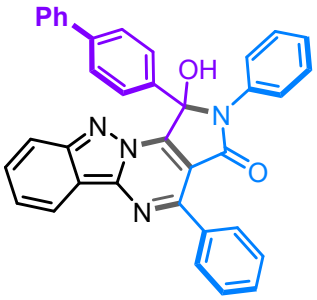
partitioned with ethyl acetate and NaCl aqueous solution, and the crude product mixture was obtained after rotary evaporation under reduced pressure. The crude product was purified by column chromatography on silica gel (200−300 mesh) to afford the product (more than 90% yield).[3]

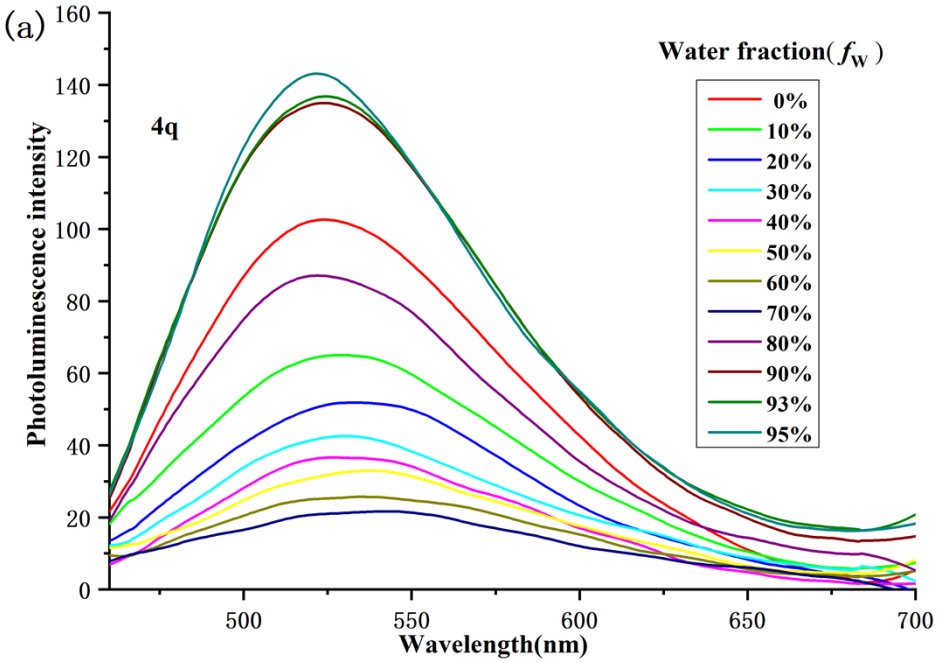
1. S. Pal, R. Nandi, A. S. Manna, S. Aich and D. K. Maiti, *J. Org. Chem.* **2024**, *89*, 2703-2717.
2. Cao, L.; Hu, F.; Sun, H.; Zhang, X.; Li, S. S. *Org. Chem. Front.* **2022**, *9*, 1668-1674.
3. (a) Seeberger, Peter H. ; Pereira, Claney L.; Khan, Naeem; Xiao, Guozhi; Diago-Navarro, Elizabeth. *Angew. Chem. Int. Ed.*, **2017**, *56*, 13973-13978. (b) Rochon, Kristina; Proteau-Gagne, Arnaud; Bourassa, Philippe; Nadon, Jean-Francois; Cote, Jerome. *ACS Chemical Neuroscience*, **2013**, *4*, 1204-1216.

4. Testing of AIE properties of molecules

The 2.3 mg of product **4q** was added to a 10 mL volumetric flask and THF was added to the scale to completely form a homogeneous solution to obtain a mother liquor with a concentration of 0.5 mmol/L. Prepare thirteen 10 mL centrifuge tubes, accurately add water (H_2O) and acetonitrile (MeCN) to form a mixed solvent system with equal total volume and increasing water fractions (f_w), then add 0.1 mL of the mother liquor and mix well to form AIE solutions (5.0 mL) of equal concentration and different water fractions of 0.01 mmol/L. Use a fluorometer to excite the solution to be tested under the UV light of 360 nm, the data, after processing and intensity normalization, to obtain the fluorescence emission curves as shown in the figure below.

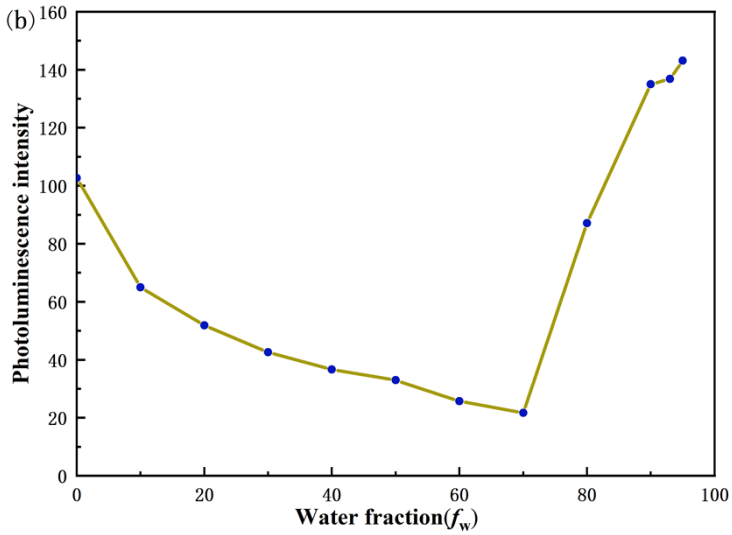
f_w (%)	0	10	20	30	40	50	60	70	80	90	93	95
mother liquor (mL)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
MeCN (mL)	4.9	4.4	3.9	3.4	2.9	2.4	1.9	1.4	0.9	0.4	0.25	0.15
H_2O (mL)	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	4.65	4.75





Fluorescence emission curve of AIE

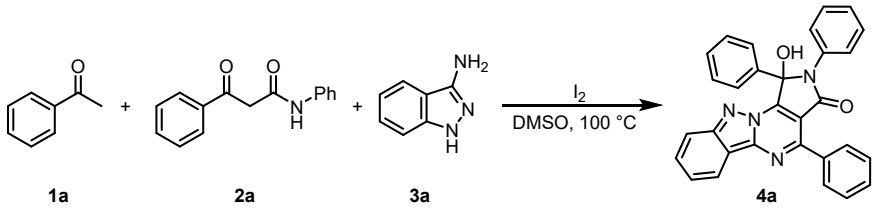
In the fluorescence data and graphs of AIE, the maximum fluorescence intensity at each water fraction was obtained, which was plotted against the number of water fractions to obtain a graph of the trend of AIE intensity.



Water fraction and maximum luminous intensity

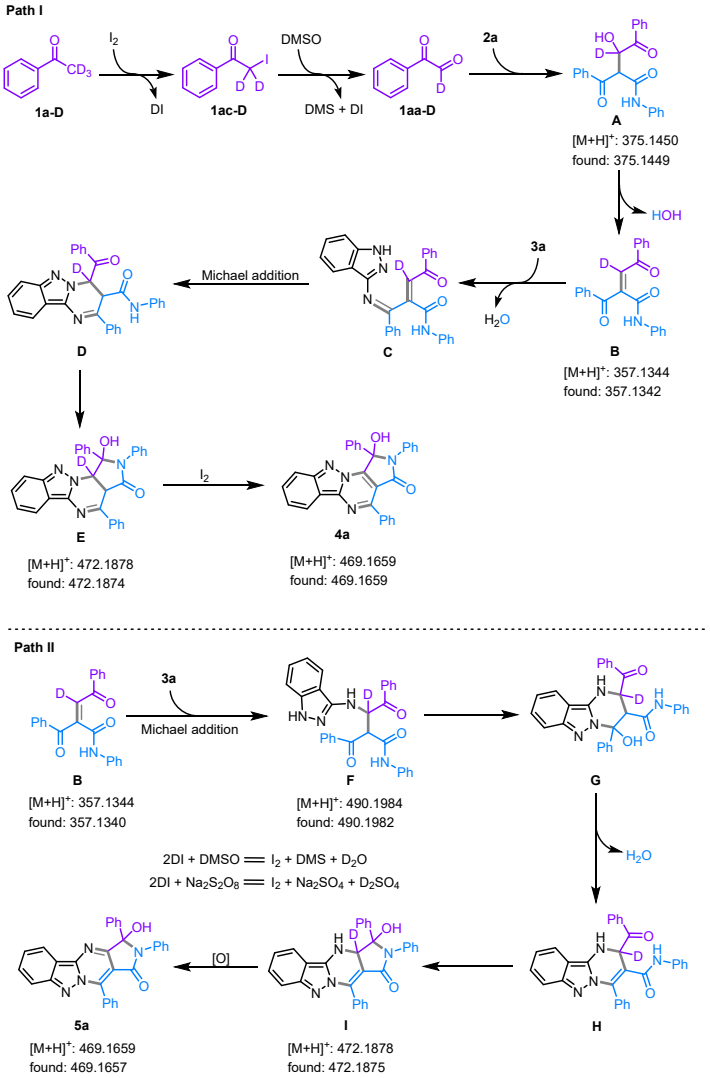
5. Mechanistic studies

The mechanism of HRMS (4a as an example)



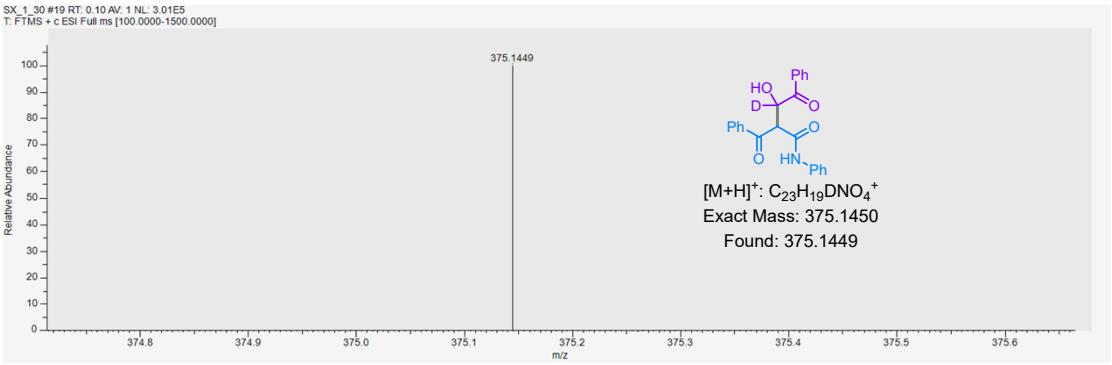
1a 2a 3a 4a

The reactions did not require the protection of inert gases. In a 35 mL sealed tube were added acetophenone (**1a**) (120.0 mg, 1.0 mmol), iodine (254.0 mg, 1.0 mmol) and dimethyl sulfoxide (4 mL) and the resulting mixture was stirred at 100 ℃ (heating block), the reaction tube was removed after about 1 hour. Then additional **2a** (239 mg, 1.0 mmol), **3a** (133 mg, 1.0 mmol) were added at room temperature, followed by reaction at 100 ℃ for 0.5 hours, then wait for the reaction to cool to room temperature. Take 0.5 mL of reaction solution and dilute it with 4 mL of CH_2Cl_2. Then 1.5 mL of the extraction solution was added into the test bottle, the samples were immediately monitored by Agilent LC1290-TOF 6224 high resolution mass spectrometers.

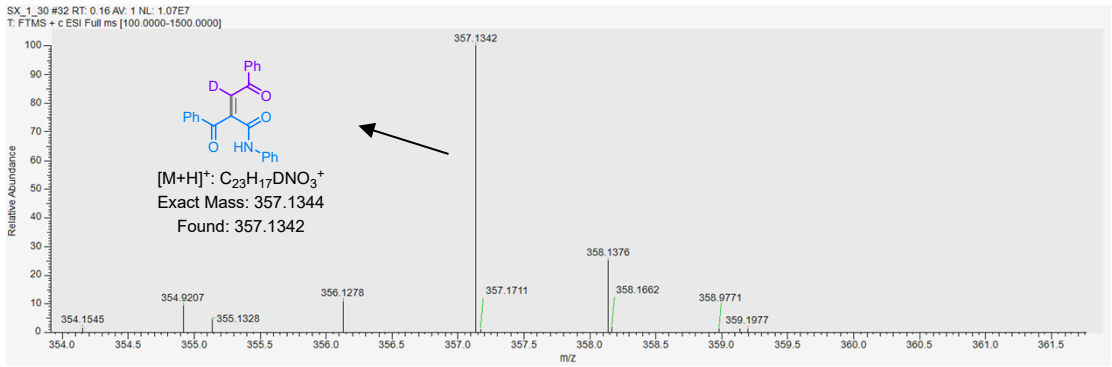


Spectrum of HRMS:

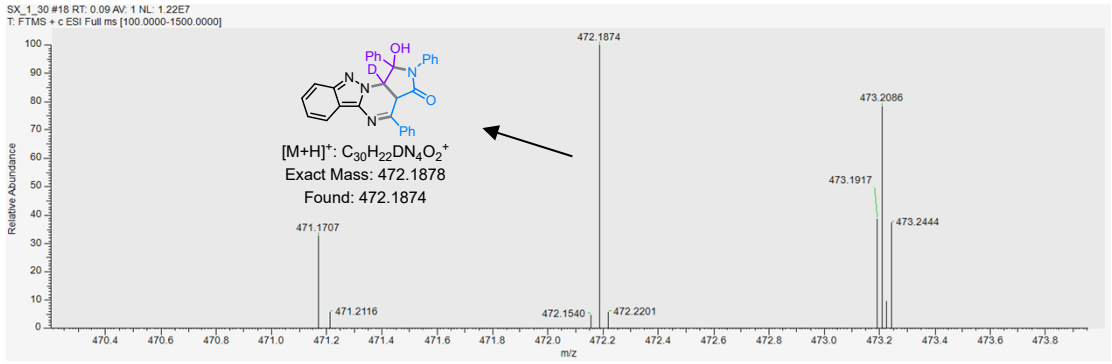
A



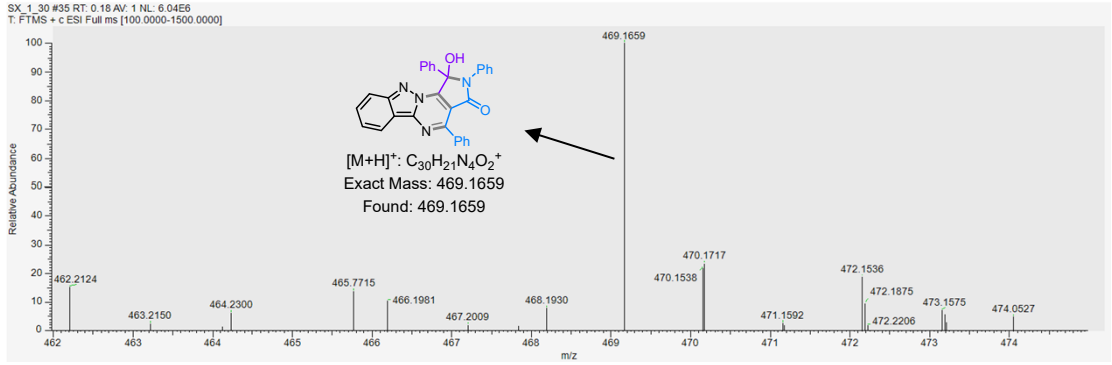
B



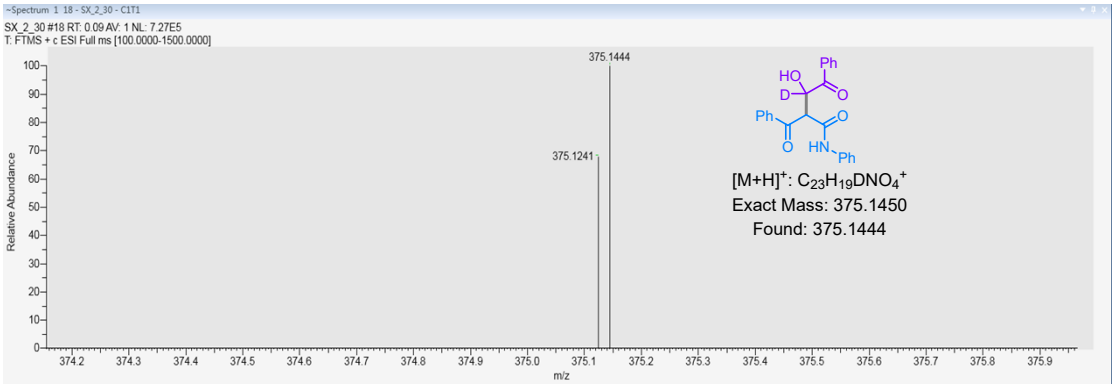
E



4a



A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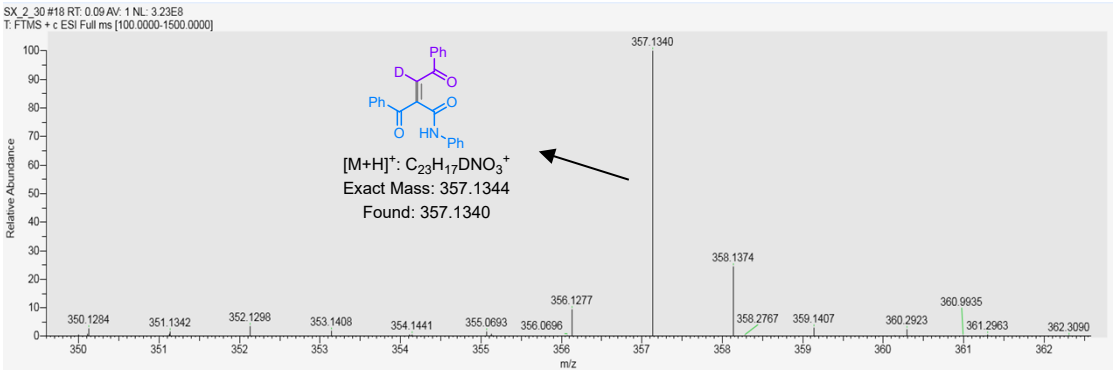
T: FTMS + c ESI Full ms [100.0000-1500.0000]
375.1444
375.1241
Relative Abundance
m/z
[M+H]+: C23H19DNO4+
Exact Mass: 375.1450
Found: 375.1444

B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351.1342
352.1298
353.1408
354.1441
355.0693
356.0696
358.2767
359.1407
360.2923
361.2963
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Relative Abundance
m/z
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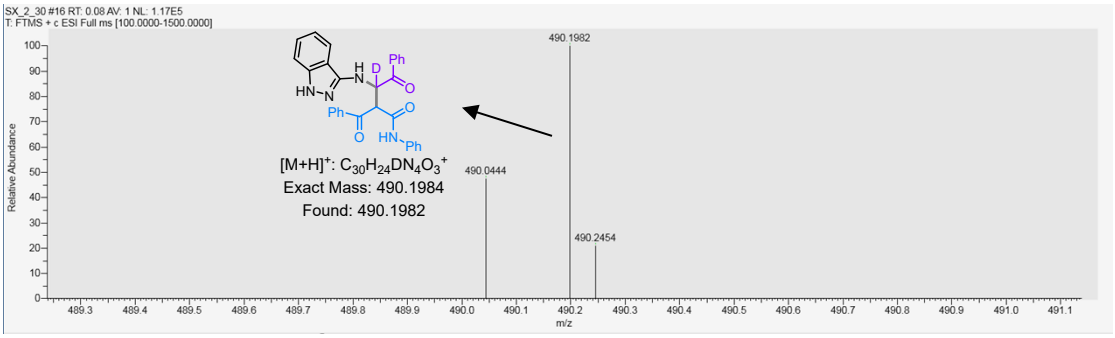
Exact Mass: 357.1344
Found: 357.1340

F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T: FTMS + c ESI Full ms [100.0000-1500.0000]
490.1982
490.0444
490.2454
Relative Abundance
m/z
[M+H]+: C30H24DN4O3+
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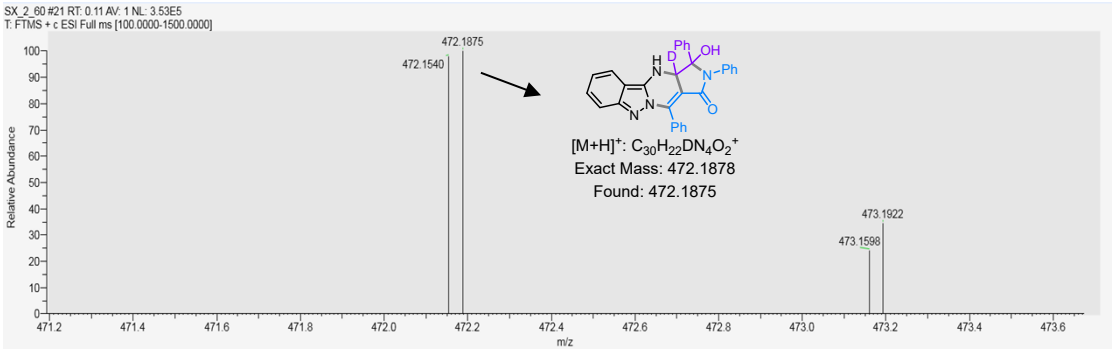
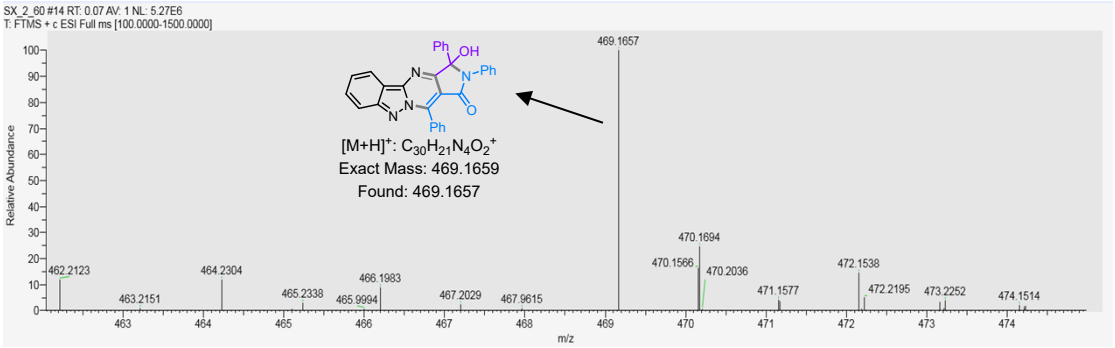
Found: 490.1982

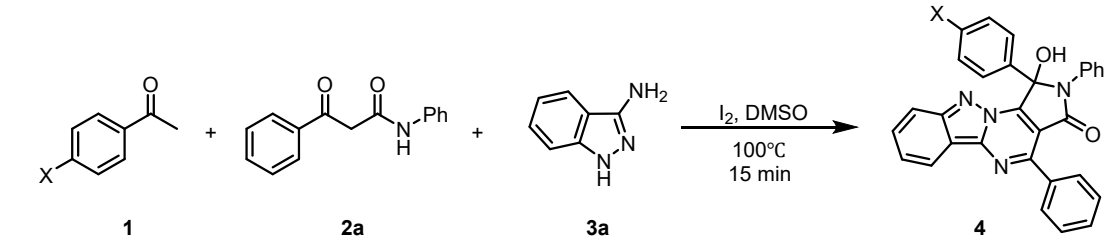
I


SX_2_60 #21 RT: 0.11 AV: 1 NL: 3.53E5
T: FTMS + c ESI Full ms [100.0000-1500.0000]
472.1875
472.1540
473.1922
473.1598
Relative Abundance
m/z
[M+H]+: C30H22DN4O2+
Exact Mass: 472.1878
Found: 472.1875

5a



Hammett-Analysis



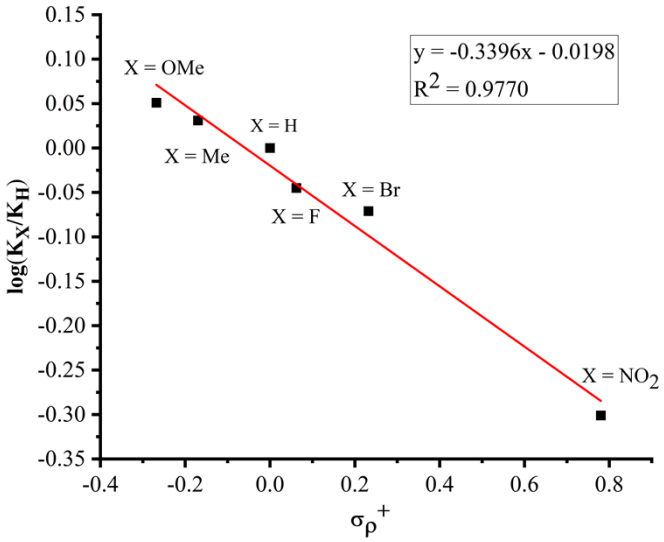
1 **2a** **3a** **4**

X = OMe, Me, H, F, Br, NO_2

The reactions did not require the protection of inert gases. In a 35 mL sealed tube were added acetophenone (**1**) (1.0 mmol), iodine (254 mg, 1.0 mmol) and dimethyl sulfoxide (4 mL) and the resulting mixture was stirred at 100 ℃ (heating block), the reaction tube was removed after about 1 hour. Then additional **2a** (240 mg, 1.0 mmol), **3a** (133 mg, 1.0 mmol) were added at room temperature, followed by reaction at 100 ℃ for 15 min. The reaction mixture was quenched with saturated $Na_2S_2O_3$ solution (50 mL) and NaCl solution (150 mL), then the mixture was extracted with EtOAc (150 mL x 2), the organic layers were separated and combined, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was obtained. According to the literature[4], we understand that the Hammett equation ($(\log (K_X/K_H) = \rho\sigma_x$, K_H is the reference reaction rate of the unsubstituted reactant, and K_X that of a substituted reactant)

Substituent X	σ_x^+	K_{X1}/K_{H1}	K_{X2}/K_{H2}	K_X/K_H	$\log (K_X/K_H)$
OMe	-0.268	1.198	1.052	1.125	0.051
Me	-0.170	0.993	1.157	1.075	0.031
H	0.000	1.000	1.000	1.000	0.000
F	0.062	0.867	0.933	0.900	-0.045
Br	0.232	0.824	0.876	0.850	-0.071
NO_2	0.780	0.472	0.528	0.500	-0.301

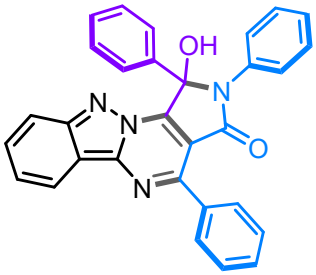
The values of log (K_X /K_H) were plotted versus the σ_x^+ value and a linear fit was created to obtain the Hammett-slope ρ = - 0.3396. The results indicate that the electron donating group benefits the reaction.



[4] (a) S. Chen, Y. Zhang, S. Liu and X. Shen, *Sci. China Chem.*, 2023, **66**, 3141-3147;

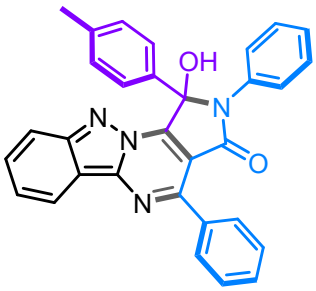
(b) D. Tian, G. Chen, X. Wang and H. J. Zhang, *J. Am. Chem. Soc.*, 2024, **146**, 18011-18018.

6. Characterization data for compounds



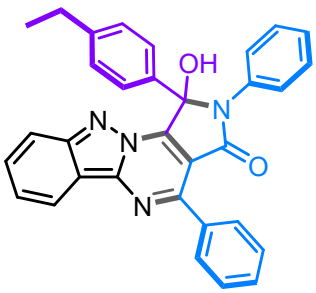
(*S*)-1-hydroxy-1,2,4-triphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4a):

Yield 74%; 346 mg; yellow solid; column chromatography, silica gel (PE:EA, 8:1); mp 185–187 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.24 (d, J = 8.4 Hz, 1H), 8.04 (dd, J = 8.4, 2.8 Hz, 3H), 7.82 (d, J = 8.8 Hz, 1H), 7.74-7.64 (m, 4H), 7.64-7.59 (m, 2H), 7.42 (d, J = 7.6 Hz, 2H), 7.36-7.26 (m, 6H), 7.18 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.0, 153.0, 152.4, 150.8, 144.5, 135.6, 135.1, 131.0, 130.7, 130.1, 128.9, 128.5, 128.3, 127.8, 127.24, 127.17, 126.9, 122.0, 121.0, 116.9, 113.0, 111.9, 89.4. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{30}H_{21}N_4O_2^+$: 469.1659; found: 469.1656.



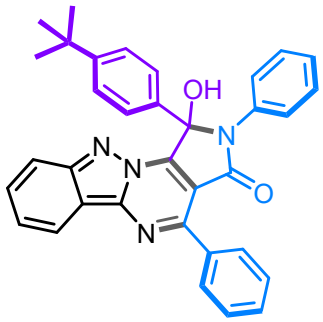
(*S*)-1-hydroxy-2,4-diphenyl-1-(*p*-tolyl)-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4b):

Yield 75%; 361 mg; orange solid; column chromatography, silica gel (PE:EA, 8:1); mp 210–212 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (d, J = 8.4 Hz, 1H), 8.28-8.15 (m, 3H), 7.85 (d, J = 8.8 Hz, 1H), 7.73-7.66 (m, 1H), 7.64-7.56 (m, 5H), 7.46-7.31 (m, 5H), 7.22 (t, J = 7.2 Hz, 1H), 7.12 (d, J = 8.0 Hz, 2H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.9, 152.9, 152.5, 150.8, 144.4, 138.2, 135.5, 135.1, 132.0, 131.0, 130.6, 130.1, 128.8, 128.5, 127.8, 127.1, 126.8, 122.0, 121.0, 116.9, 112.9, 111.8, 89.4, 20.7. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{23}N_4O_2^+$: 483.1816; found: 483.1815.



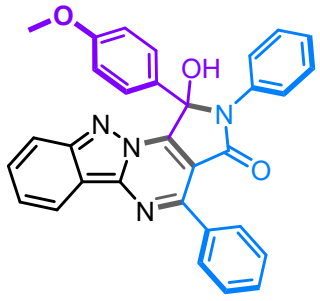
(*S*)-1-(4-ethylphenyl)-1-hydroxy-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4c):

Yield 71%; 352 mg; yellow solid; column chromatography, silica gel (PE:EA, 8:1); mp 220–222 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (d, J = 8.4 Hz, 1H), 8.24 (dd, J = 8.0, 4.0 Hz, 3H), 7.86 (d, J = 8.8 Hz, 1H), 7.69 (d, J = 7.6 Hz, 1H), 7.66-7.59 (m, 5H), 7.46 (d, J = 7.6 Hz, 2H), 7.39-7.31 (m, 3H), 7.22 (t, J = 7.6 Hz, 1H), 7.16 (d, J = 8.4 Hz, 2H), 2.58-2.51 (m, 2H), 1.09 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.0, 152.9, 152.5, 150.8, 144.4, 144.2, 135.5, 135.2, 132.2, 131.0, 130.6, 130.1, 128.5, 127.8, 127.6, 127.2, 127.1, 126.8, 122.0, 121.0, 116.9, 112.9, 111.7, 89.5, 27.7, 15.0. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{32}H_{25}N_4O_2^+$: 497.1972; found: 497.1974.



(*S*)-1-(4-(tert-butyl)phenyl)-1-hydroxy-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4d):

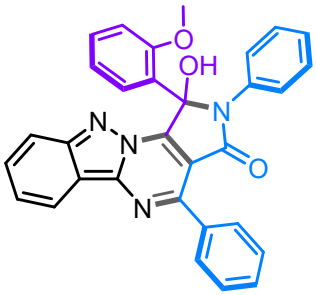
Yield 75%; 393 mg; yellow solid; column chromatography, silica gel (PE:EA, 8:1); mp 228–230 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.35 (d, J = 8.4 Hz, 1H), 8.24-8.20 (m, 3H), 7.86 (d, J = 8.8 Hz, 1H), 7.67 (q, J = 2.4 Hz, 3H), 7.63-7.59 (m, 3H), 7.46 (d, J = 7.6 Hz, 2H), 7.38-7.31 (m, 5H), 7.22 (t, J = 7.6 Hz, 1H), 1.19 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.9, 152.9, 152.5, 151.1, 150.8, 144.4, 135.5, 135.1, 132.0, 131.0, 130.6, 130.1, 128.5, 127.8, 127.1, 126.8, 125.0, 121.9, 121.0, 116.9, 112.9, 111.6, 89.5, 34.3, 31.0. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{34}H_{29}N_4O_2^+$: 525.2285; found: 525.2281.



(*S*)-1-hydroxy-1-(4-methoxyphenyl)-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4e):

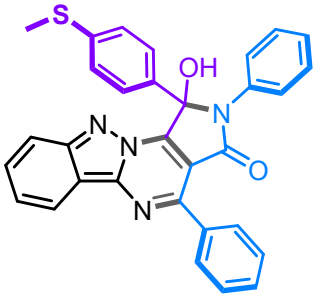
Yield 75%; 498 mg; yellow solid; column chromatography, silica gel (PE:EA, 7:1); mp 219–221 ℃. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.36 (d, J = 8.4 Hz, 1H), 8.21 (dd, J = 6.8, 2.8 Hz, 2H), 8.18 (s, 1H), 7.84 (d, J = 8.8 Hz, 1H), 7.71-7.67 (m, 1H), 7.64-7.59 (m, 5H), 7.44-7.37 (m, 3H), 7.33 (t, J = 8.0 Hz, 2H), 7.22 (t, J = 7.2 Hz, 1H), 6.85 (d, J = 8.8 Hz, 2H), 3.68 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.9, 159.4, 152.9, 152.5, 150.8, 144.4, 135.6,

135.2, 131.0, 130.6, 130.1, 128.7, 128.5, 127.8, 127.1, 126.8, 126.7, 122.0, 121.0, 116.9, 113.5, 112.9, 111.7, 89.3, 55.0. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{23}N_4O_3^+$: 499.1765; found: 499.1763.



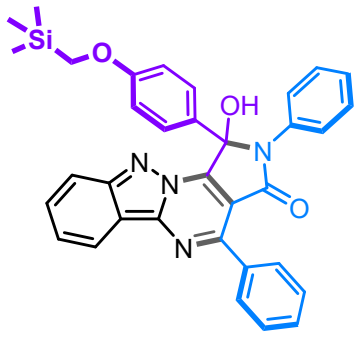
(*S*)-1-hydroxy-1-(2-methoxyphenyl)-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4f):

Yield 69%; 343 mg; orange solid; column chromatography, silica gel (PE:EA, 8:1); mp 259–261 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.40 (d, J = 8.4 Hz, 1H), 8.23 (s, 1H), 8.21 (dd, J = 7.6, 2.0 Hz, 2H), 8.03 (dd, J = 8.0, 1.6 Hz, 1H), 7.82 (d, J = 8.8 Hz, 1H), 7.68 (d, J = 7.6 Hz, 1H), 7.66-7.61 (m, 3H), 7.40-7.29 (m, 5H), 7.28-7.17 (m, 2H), 7.03 (t, J = 7.6 Hz, 1H), 6.79 (d, J = 8.4 Hz, 1H), 3.34 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.4, 155.6, 153.4, 152.9, 150.7, 144.2, 135.7, 135.1, 130.9, 130.6, 130.3, 130.1, 128.4, 128.0, 127.1, 127.0, 122.7, 121.7, 121.0, 120.5, 116.8, 112.7, 112.5, 111.3, 87.0, 55.5. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{23}N_4O_3^+$: 499.1765; found: 499.1762.



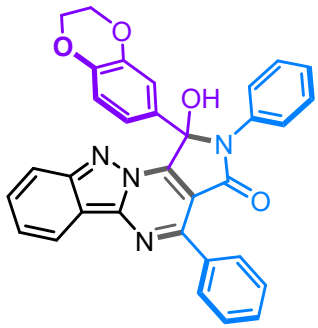
(*S*)-1-hydroxy-1-(4-(methylthio)phenyl)-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4g):

Yield 71%; 365 mg; yellow solid; column chromatography, silica gel (PE:EA, 5:1); mp 243–245 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.38 (d, J = 8.4 Hz, 1H), 8.28 (s, 1H), 8.24 (dd, J = 6.4, 3.2 Hz, 2H), 7.86 (d, J = 8.8 Hz, 1H), 7.72-7.65 (m, 3H), 7.64-7.59 (m, 3H), 7.46 (d, J = 7.6 Hz, 2H), 7.40-7.33 (m, 3H), 7.24 (t, J = 7.6 Hz, 1H), 7.17 (d, J = 8.8 Hz, 2H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.0, 152.9, 152.3, 150.8, 144.4, 139.2, 135.5, 135.1, 131.2, 131.0, 130.6, 130.1, 128.6, 127.8, 127.1, 126.9, 124.9, 122.0, 121.0, 116.9, 112.9, 111.8, 89.2, 13.9. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{23}N_4O_2S^+$: 515.1536; found: 515.1533.



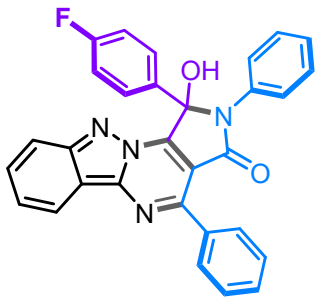
(*S*)-1-hydroxy-2,4-diphenyl-1-(4-((trimethylsilyl)methoxy)phenyl)-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4h):

Yield 67%; 382 mg; orange solid; column chromatography, silica gel (PE:EA, 7:1); mp 205–208 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (d, J = 8.4 Hz, 1H), 8.23 (dd, J = 6.4, 2.8 Hz, 2H), 8.16 (s, 1H), 7.84 (d, J = 8.8 Hz, 1H), 7.71-7.66 (m, 1H), 7.64-7.57 (m, 5H), 7.44 (d, J = 8.0 Hz, 2H), 7.40-7.31 (m, 3H), 7.23 (d, J = 7.2 Hz, 1H), 6.89 (d, J = 8.8 Hz, 2H), 3.54 (q, J = 12.8 Hz, 2H), 0.06 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.9, 161.2, 152.9, 152.5, 150.8, 144.4, 135.5, 135.2, 130.9, 130.6, 130.1, 128.8, 128.5, 127.8, 127.1, 126.7, 126.3, 121.9, 121.0, 118.2, 116.8, 113.7, 112.9, 111.7, 89.3, 60.6, -3.15. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{34}H_{31}N_4O_3Si^+$: 571.2160; found: 571.2160.



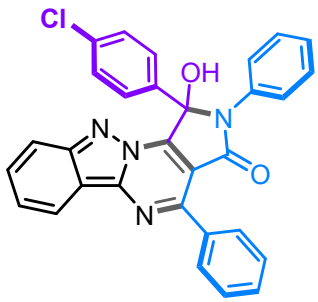
(*S*)-1-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-1-hydroxy-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4i):

Yield 71%; 373 mg; yellow solid; column chromatography, silica gel (PE:EA, 6:1); mp 185–187 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (d, J = 8.4 Hz, 1H), 8.22 (d, J = 3.6 Hz, 2H), 8.16 (s, 1H), 7.88 (d, J = 8.8 Hz, 1H), 7.72-7.67 (m, 1H), 7.62-7.57 (m, 3H), 7.44 (d, J = 8.0 Hz, 2H), 7.40-7.33 (m, 3H), 7.25 (d, J = 7.6 Hz, 2H), 7.16 (d, J = 8.4 Hz, 1H), 6.77 (d, J = 8.4 Hz, 1H), 4.17 (d, J = 3.6 Hz, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.9, 152.9, 152.3, 150.8, 144.4, 143.7, 142.9, 135.5, 135.1, 131.0, 130.7, 130.1, 128.6, 127.8, 127.0, 126.8, 122.0, 121.0, 120.2, 116.9, 116.8, 116.3, 112.9, 111.7, 89.1, 64.0, 63.9. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{32}H_{23}N_4O_4^+$: 527.1714; found: 527.1713.



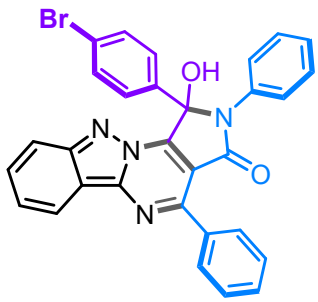
(*S*)-1-(4-fluorophenyl)-1-hydroxy-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4j):

Yield 73%; 354 mg; yellow solid; column chromatography, silica gel (PE:EA, 7:1); mp 188–190 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.38 (d, J = 8.4 Hz, 1H), 8.33 (s, 1H), 8.28-8.21 (m, 2H), 7.85 (d, J = 8.8 Hz, 1H), 7.78 (dd, J = 8.4, 5.6 Hz, 2H), 7.72-7.66 (m, 1H), 7.61 (d, J = 3.6 Hz, 3H), 7.42 (d, J = 8.0 Hz, 2H), 7.39-7.30 (m, 3H), 7.24 (t, J = 7.2 Hz, 1H), 7.14 (t, J = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.9, 162.2 (d, J = 244.0 Hz, $^{1}J_{CF}$), 152.9, 152.0, 150.8, 144.4, 135.5, 134.9, 131.28, 131.2 (d, J = 3.0 Hz, $^{4}J_{CF}$), 130.7, 130.6, 130.1, 129.6 (d, J = 7.0 Hz, $^{3}J_{CF}$), 128.6, 127.8, 127.3, 127.0, 122.0, 121.0, 116.8, 115.1 (d, J = 23.0 Hz, $^{2}J_{CF}$), 113.0, 111.9, 88.9. ^{19}F NMR (376 MHz, DMSO-d_6) δ -113.03. HRMS (ESI): m/z [M+H]$^{+}$ calcd for $C_{30}H_{20}FN_4O_2^{+}$: 487.1565; found: 487.1566.



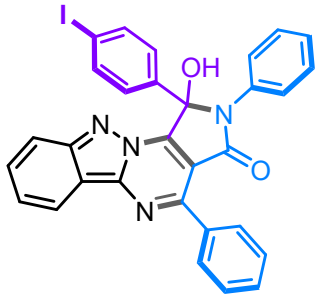
(*S*)-1-(4-chlorophenyl)-1-hydroxy-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4k):

Yield 75%; 376 mg; yellow solid; column chromatography, silica gel (PE:EA, 6:1); mp 200–202 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (d, J = 8.4 Hz, 1H), 8.34 (s, 1H), 8.26-8.19 (m, 2H), 7.84 (d, J = 8.8 Hz, 1H), 7.76-7.66 (m, 3H), 7.64-7.58 (m, 3H), 7.42-7.33 (m, 7H), 7.24 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.9, 152.9, 151.8, 150.8, 144.4, 135.4, 134.8, 134.2, 133.6, 131.0, 130.6, 130.1, 129.2, 128.6, 128.2, 127.8, 127.2, 127.0, 122.0, 121.0, 116.8, 112.9, 111.9, 88.8. HRMS (ESI): m/z [M+H]$^{+}$ calcd for $C_{30}H_{20}ClN_4O_2^{+}$: 503.1269; found: 503.1270.



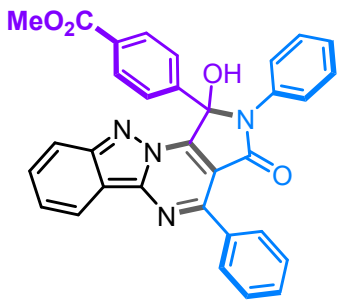
(*S*)-1-(4-bromophenyl)-1-hydroxy-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4l):

Yield 72%; 393 mg; yellow solid; column chromatography, silica gel (PE:EA, 6:1); mp 210–212 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (d, J = 10.8 Hz, 2H), 8.24 (dd, J = 6.4, 2.8 Hz, 2H), 7.85 (d, J = 8.8 Hz, 1H), 7.74-7.65 (m, 3H), 7.65-7.57 (m, 3H), 7.51 (d, J = 8.4 Hz, 2H), 7.45-7.32 (m, 5H), 7.25 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.9, 152.9, 151.8, 150.8, 144.4, 135.4, 134.8, 134.6, 131.2, 131.1, 130.6, 130.1, 129.6, 128.7, 127.8, 127.3, 127.0, 122.4, 122.0, 121.0, 116.8, 113.0, 112.0, 88.8. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{30}H_{20}BrN_4O_2^+$: 547.0764; found: 547.0766.



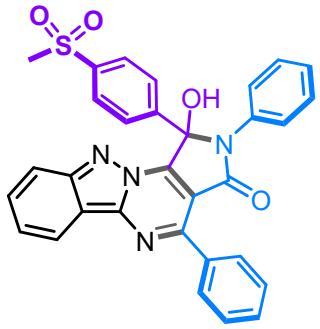
(*S*)-1-hydroxy-1-(4-iodophenyl)-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4m):

Yield 70%; 415 mg; yellow solid; column chromatography, silica gel (PE:EA, 8:1); mp 206–208 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (d, J = 8.4 Hz, 1H), 8.33 (s, 1H), 8.22 (dd, J = 6.4, 2.8 Hz, 2H), 7.85 (d, J = 8.8 Hz, 1H), 7.71-7.66 (m, 3H), 7.63-7.59 (m, 3H), 7.52 (d, J = 8.4 Hz, 2H), 7.40 (t, J = 7.6 Hz, 3H), 7.37-7.33 (m, 2H), 7.24 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.9, 152.9, 151.8, 150.8, 144.4, 137.0, 135.4, 135.0, 134.8, 131.1, 130.6, 130.1, 129.5, 128.7, 127.8, 127.2, 127.0, 122.0, 121.0, 116.8, 112.9, 111.9, 95.9, 89.0. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{30}H_{20}IN_4O_2^+$: 595.0625; found: 595.0626.



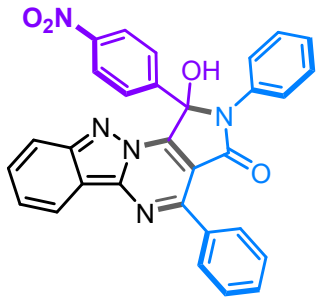
methyl(*S*)-4-(1-hydroxy-3-oxo-2,4-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-1-yl)benzoate (4n):

Yield 62%; 326 mg; yellow solid; column chromatography, silica gel (PE:EA, 5:1); mp 196–198 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.48 (s, 1H), 8.39 (d, J = 8.4 Hz, 1H), 8.32-8.26 (m, 2H), 7.92 (s, 4H), 7.84 (d, J = 8.8 Hz, 1H), 7.68 (d, J = 7.2 Hz, 1H), 7.65-7.60 (m, 3H), 7.43 (d, J = 8.0 Hz, 2H), 7.40-7.32 (m, 3H), 7.24 (t, J = 7.2 Hz, 1H), 3.78 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.8, 163.1, 153.0, 151.8, 150.8, 144.4, 140.4, 135.5, 134.8, 131.1, 130.7, 130.2, 130.1, 129.1, 128.7, 127.9, 127.7, 127.4, 127.2, 122.1, 121.0, 116.8, 113.0, 112.1, 88.9, 52.2. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{32}H_{23}N_4O_4^+$: 527.1714; found: 527.1711.



(*S*)-1-hydroxy-1-(4-(methylsulfonyl)phenyl)-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4o):

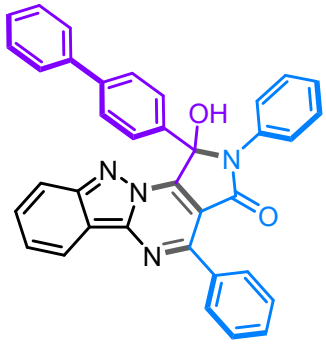
Yield 80%; 437 mg; yellow solid; column chromatography, silica gel (PE:EA, 3:1); mp 229–231 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.55 (s, 1H), 8.38 (d, J = 8.4 Hz, 1H), 8.29-8.24 (m, 2H), 8.05 (d, J = 8.4 Hz, 2H), 7.90 (d, J = 8.4 Hz, 2H), 7.85 (d, J = 8.8 Hz, 1H), 7.71-7.67 (m, 1H), 7.63 (d, J = 3.6 Hz, 3H), 7.44 (d, J = 7.6 Hz, 2H), 7.41-7.34 (m, 3H), 7.25 (t, J = 7.2 Hz, 1H), 3.20 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.0, 153.0, 151.6, 150.9, 144.4, 141.2, 140.8, 135.4, 134.7, 131.2, 130.7, 130.2, 128.8, 128.5, 127.9, 127.4, 127.2, 126.9, 122.1, 121.0, 116.9, 113.0, 112.1, 88.8, 43.2. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{31}H_{23}N_4O_4S^+$: 547.1435; found: 547.1436.



(*S*)-1-hydroxy-1-(4-nitrophenyl)-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4p):

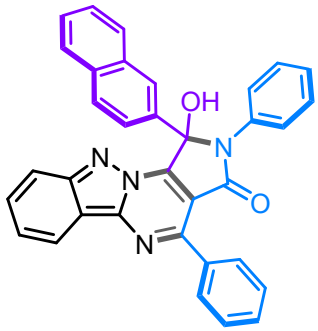
Yield 55%; 282 mg; yellow solid; column chromatography, silica gel (PE:EA, 4:1); mp 212–214 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.62 (s, 1H), 8.39 (d, J = 8.4 Hz, 1H), 8.30-8.24 (m, 2H), 8.17 (d, J = 8.8 Hz, 2H), 8.05 (d, J = 8.8 Hz, 2H), 7.83 (d, J = 8.8 Hz, 1H), 7.71-7.66 (m, 1H), 7.65-7.60 (m, 3H), 7.45-7.34 (m, 5H), 7.25 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz,

DMSO-d_6) δ 163.1, 153.0, 151.4, 150.9, 147.8, 144.5, 142.5, 135.4, 134.6, 131.2, 130.6, 130.2, 128.9, 128.8, 127.9, 127.4, 127.3, 123.4, 122.1, 121.0, 116.8, 113.0, 112.2, 88.5. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{30}H_{20}N_5O_4^+$: 514.1510; found: 514.1511.



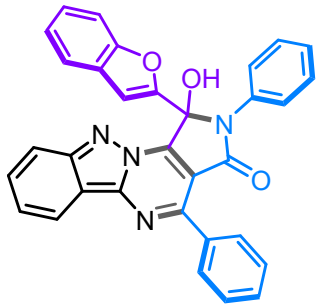
(*S*)-1-([1,1'-biphenyl]-4-yl)-1-hydroxy-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4q):

Yield 70%; 380 mg; yellow solid; column chromatography, silica gel (PE:EA, 7:1); mp 187–189 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.38 (d, J = 8.4 Hz, 1H), 8.33 (s, 1H), 8.29-8.24 (m, 2H), 7.84 (dd, J = 8.0, 6.4 Hz, 3H), 7.71-7.65 (m, 2H), 7.64-7.60 (m, 6H), 7.49 (d, J = 7.6 Hz, 2H), 7.43-7.37 (m, 3H), 7.36-7.29 (m, 3H), 7.23 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.0, 152.9, 152.3, 150.8, 144.4, 140.3, 139.1, 135.5, 135.1, 134.2, 131.0, 130.7, 130.1, 128.9, 128.6, 127.9, 127.8, 127.7, 127.2, 126.9, 126.6, 126.4, 122.0, 121.0, 116.9, 113.0, 111.9, 89.3. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{36}H_{25}N_4O_2^+$: 545.1972; found: 545.1969.



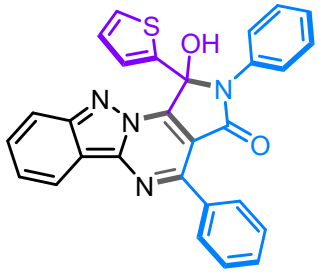
(*S*)-1-hydroxy-1-(naphthalen-2-yl)-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4r):

Yield 74%; 383 mg; orange solid; column chromatography, silica gel (PE:EA, 7:1); mp 220–222 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.51 (s, 1H), 8.49 (s, 1H), 8.40 (d, J = 8.4 Hz, 1H), 8.35 (d, J = 6.8 Hz, 2H), 8.01 (d, J = 5.2 Hz, 1H), 7.89-7.84 (m, 2H), 7.80 (t, J = 9.2 Hz, 2H), 7.65 (t, J = 10.0 Hz, 4H), 7.51 (d, J = 2.0 Hz, 2H), 7.50 (s, 2H), 7.37-7.30 (m, 3H), 7.19 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.2, 152.9, 152.4, 150.9, 144.5, 135.6, 135.1, 133.0, 132.6, 131.0, 130.7, 130.2, 128.6, 128.4, 128.0, 127.9, 127.5, 127.4, 127.2, 127.0, 126.8, 126.3, 124.2, 122.0, 121.0, 116.8, 113.0, 112.1, 89.5. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{34}H_{23}N_4O_2^+$: 519.1816; found: 519.1814.



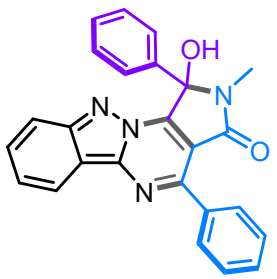
(*R*)-1-(benzofuran-2-yl)-1-hydroxy-2,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4s):

Yield 58%; 294 mg; orange solid; column chromatography, silica gel (PE:EA, 6:1); mp 200–202 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.64 (s, 1H), 8.38 (d, J = 8.4 Hz, 1H), 8.19 (dd, J = 6.4, 2.4 Hz, 2H), 7.87 (d, J = 8.8 Hz, 1H), 7.70 (d, J = 6.8 Hz, 1H), 7.66 (d, J = 5.2 Hz, 1H), 7.63-7.60 (m, 3H), 7.43 (d, J = 5.2 Hz, 1H), 7.40-7.34 (m, 4H), 7.30 (d, J = 8.0 Hz, 3H), 7.25-7.21 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.8, 154.2, 153.2, 150.5, 150.2, 150.0, 144.5, 135.2, 134.3, 131.3, 130.5, 130.3, 128.9, 128.0, 127.8, 127.3, 125.2, 123.3, 122.3, 121.8, 121.1, 116.9, 113.0, 112.0, 111.5, 108.9, 86.1. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{32}H_{21}N_4O_3^+$: 509.1608; found: 509.1608.



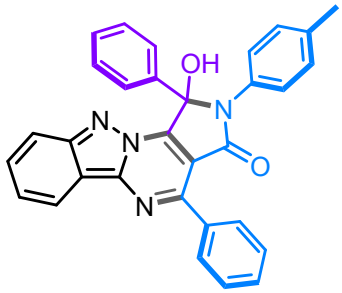
(*R*)-1-hydroxy-2,4-diphenyl-1-(thiophen-2-yl)-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4t):

Yield 65%; 308 mg; orange solid; column chromatography, silica gel (PE:EA, 6:1); mp 233–235 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.47 (s, 1H), 8.38 (d, J = 8.4 Hz, 1H), 8.20 (dd, J = 6.4, 2.8 Hz, 2H), 7.90 (d, J = 8.8 Hz, 1H), 7.74-7.69 (m, 1H), 7.62-7.58 (m, 3H), 7.50 (d, J = 5.2 Hz, 1H), 7.45 (d, J = 8.0 Hz, 2H), 7.39 (d, J = 7.6 Hz, 3H), 7.29 (d, J = 7.2 Hz, 1H), 7.25 (d, J = 2.8 Hz, 1H), 6.92 (dd, J = 4.8, 4.0 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.4, 153.0, 151.6, 150.7, 144.5, 139.2, 135.4, 134.8, 131.1, 130.6, 130.2, 128.6, 127.8, 127.7, 127.2, 127.0, 126.9, 122.1, 121.0, 119.8, 116.9, 112.9, 111.3, 87.9. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{28}H_{19}N_4O_2S^+$: 475.1223; found: 475.1224.



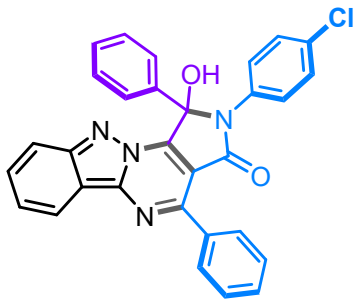
1-hydroxy-2-methyl-1,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4u):

Yield 70%; 284 mg; yellow solid; column chromatography, silica gel (PE:EA, 7:1); mp 279–281 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.34 (d, J = 7.2 Hz, 1H), 8.25-8.20 (m, 2H), 7.83 (d, J = 8.8 Hz, 1H), 7.71 (d, J = 5.6 Hz, 3H), 7.68–7.58 (m, 4H), 7.44 (t, J = 7.2 Hz, 2H), 7.41–7.32 (m, 2H), 2.78 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.0, 152.8, 152.7, 150.5, 144.1, 135.5, 134.7, 130.9, 130.5, 130.0, 129.0, 128.5, 127.8, 127.0, 121.8, 120.9, 116.7, 112.8, 112.3, 87.6, 23.5. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{25}H_{19}N_4O_2^+$: 407.1503; found: 407.1503.



(*S*)-1-hydroxy-1,4-diphenyl-2-(*p*-tolyl)-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4v):

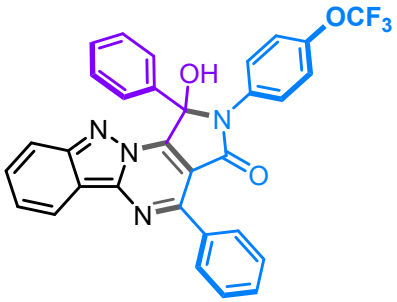
Yield 74%; 356 mg; yellow solid; column chromatography, silica gel (PE:EA, 8:1); mp 207–209 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (d, J = 8.4 Hz, 1H), 8.24 (d, J = 4.0 Hz, 2H), 8.20 (s, 1H), 7.84 (d, J = 8.8 Hz, 1H), 7.74-7.66 (m, 3H), 7.61 (d, J = 4.0 Hz, 3H), 7.38-7.23 (m, 6H), 7.12 (d, J = 8.0 Hz, 2H), 2.24 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.9, 152.9, 152.4, 150.8, 144.4, 136.3, 135.5, 135.1, 132.3, 131.0, 130.6, 130.1, 129.1, 128.8, 128.2, 127.8, 127.3, 127.1, 121.9, 121.0, 116.8, 112.9, 112.0, 89.2, 20.6. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{31}H_{23}N_4O_2^+$: 483.1816; found: 483.1816.



(*S*)-2-(4-chlorophenyl)-1-hydroxy-1,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4w):

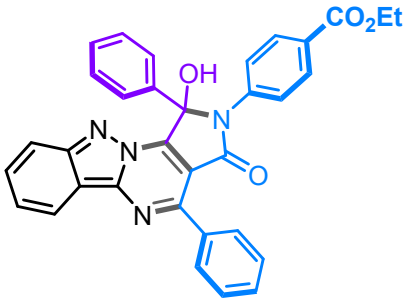
Yield 68%; 341 mg; orange solid; column chromatography, silica gel (PE:EA, 8:1); mp 235–237 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.40 (s, 1H), 8.37 (d, J = 8.4 Hz, 1H), 8.26 (dd, J = 7.2, 2.0 Hz, 2H), 7.85 (d, J = 8.8 Hz, 1H), 7.76 (d, J = 7.2 Hz, 2H), 7.70-7.65 (m, 1H), 7.64-7.60 (m, 3H), 7.52 (d, J = 8.8 Hz, 2H), 7.41 (d, J = 8.8 Hz, 2H), 7.39-7.32 (m, 3H), 7.30 (d, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.0, 153.0, 152.3, 150.8, 144.5, 135.5, 134.8, 134.1, 131.11, 131.07, 130.6, 130.2, 129.0, 128.7, 128.3, 127.9, 127.2, 122.0, 121.0,

116.9, 113.0, 111.7, 89.4. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{30}H_{20}ClN_4O_2^+$: 503.1269; found: 503.1268.



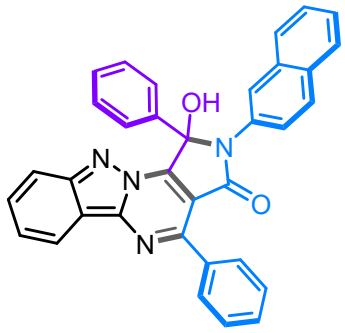
(*S*)-1-hydroxy-1,4-diphenyl-2-(4-(trifluoromethoxy)phenyl)-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4x):

Yield 69%; 380 mg; orange solid; column chromatography, silica gel (PE:EA, 7:1); mp 218–220 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.41 (s, 1H), 8.38 (d, J = 8.4 Hz, 1H), 8.31-8.23 (m, 2H), 7.85 (d, J = 8.8 Hz, 1H), 7.79 (d, J = 7.6 Hz, 2H), 7.70-7.65 (m, 1H), 7.65-7.57 (m, 5H), 7.41-7.33 (m, 5H), 7.32-7.28 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.1, 153.0, 152.3, 150.8, 146.5, 144.5, 135.5, 134.8, 134.2, 131.0, 130.6, 130.1, 129.0, 128.5, 128.3, 127.8, 127.2, 122.0, 121.2, 120.9, 120.0 (q, J = 255.0 Hz, $^1J_{CF}$), 116.8, 113.0, 111.6, 89.5. ^{19}F NMR (376 MHz, DMSO-d_6) δ -56.91. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{20}F_3N_4O_3^+$: 553.1482; found: 553.1483.



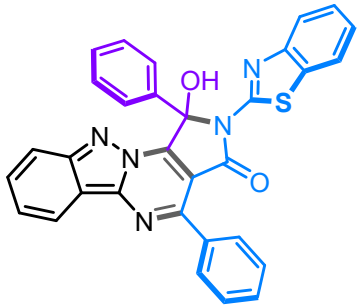
ethyl(*S*)-4-(1-hydroxy-3-oxo-1,4-diphenyl-1,3-dihydro-2*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-2-yl)benzoate (4y):

Yield 60%; 324 mg; orange solid; column chromatography, silica gel (PE:EA, 6:1); mp 233–235 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.48 (s, 1H), 8.36 (d, J = 8.4 Hz, 1H), 8.23 (dd, J = 6.4, 2.8 Hz, 2H), 7.90 (d, J = 8.8 Hz, 2H), 7.85 (d, J = 8.8 Hz, 1H), 7.77 (t, J = 7.6 Hz, 4H), 7.71-7.67 (m, 1H), 7.65-7.61 (m, 3H), 7.40-7.36 (m, 1H), 7.35-7.26 (m, 3H), 4.28 (q, J = 7.2 Hz, 2H), 1.28 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.1, 163.0, 152.9, 152.1, 150.8, 144.4, 139.9, 135.4, 134.6, 131.1, 130.5, 130.1, 129.4, 128.9, 128.2, 127.8, 127.2, 127.1, 125.0, 122.0, 120.9, 116.8, 112.9, 111.4, 89.7, 60.7, 14.1. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{33}H_{25}N_4O_4^+$: 541.1870; found: 541.1868.



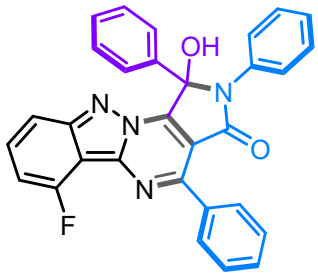
(*S*)-1-hydroxy-2-(naphthalen-2-yl)-1,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4z):

Yield 71%; 367 mg; yellow solid; column chromatography, silica gel (PE:EA, 8:1); mp 217–219 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.43 (s, 1H), 8.39 (d, J = 8.4 Hz, 1H), 8.28 (dd, J = 7.6, 2.0 Hz, 2H), 8.02 (d, J = 1.2 Hz, 1H), 7.85 (t, J = 8.4 Hz, 4H), 7.78 (d, J = 7.6 Hz, 2H), 7.71-7.66 (m, 1H), 7.66-7.61 (m, 3H), 7.59 (d, J = 2.0 Hz, 1H), 7.49 (dd, J = 6.4, 3.2 Hz, 2H), 7.41-7.36 (m, 1H), 7.30 (t, J = 7.6 Hz, 2H), 7.24 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.2, 152.9, 152.4, 150.8, 144.5, 135.6, 135.0, 132.8, 132.7, 131.4, 131.0, 130.6, 130.1, 128.9, 128.2, 128.0, 127.85, 127.77, 127.5, 127.2, 126.4, 126.2, 125.4, 125.0, 122.0, 121.0, 116.9, 113.0, 111.9, 89.6. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{34}H_{23}N_4O_2^+$: 519.1816; found: 519.1819.



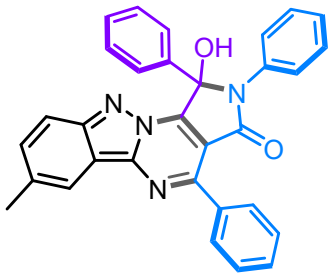
(*S*)-2-(benzo[d]thiazol-2-yl)-1-hydroxy-1,4-diphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4aa):

Yield 50%; 262 mg; orange solid; column chromatography, silica gel (PE:EA, 7:1); mp 264–266 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.52 (s, 1H), 8.35 (d, J = 8.4 Hz, 1H), 8.24 (dd, J = 7.2, 2.0 Hz, 2H), 8.01-7.96 (m, 3H), 7.89 (d, J = 8.8 Hz, 1H), 7.70-7.65 (m, 5H), 7.41-7.37 (m, 4H), 7.31 (s, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.8, 153.24, 153.15, 152.7, 150.9, 148.5, 144.7, 135.2, 134.6, 131.4, 131.2, 130.5, 130.4, 128.9, 128.0, 127.9, 127.4, 126.2, 124.2, 122.4, 121.5, 121.4, 121.0, 117.0, 113.0, 109.8, 91.0. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{31}H_{20}N_5O_2S^+$: 526.1332; found: 526.1334.



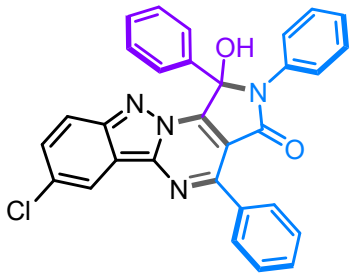
(*S*)-6-fluoro-1-hydroxy-1,2,4-triphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4ab):

Yield 66%; 320 mg; yellow solid; column chromatography, silica gel (PE:EA, 6:1); mp 208–210 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.29 (s, 1H), 8.23 (dd, J = 6.4, 2.8 Hz, 2H), 7.71 (d, J = 6.8 Hz, 2H), 7.67-7.60 (m, 5H), 7.39 (d, J = 7.6 Hz, 2H), 7.36-7.28 (m, 5H), 7.23 (t, J = 7.2 Hz, 1H), 7.15-7.08 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.7, 156.3 (d, J = 255.0 Hz, $^{1}J_{CF}$), 154.4 (d, J = 4.0 Hz, $^{4}J_{CF}$), 152.4, 152.0, 142.8 (d, J = 6.0 Hz, $^{3}J_{CF}$), 135.3, 134.9 (d, J = 5.0 Hz, $^{3}J_{CF}$), 131.6 (d, J = 7.0 Hz, $^{3}J_{CF}$), 130.7, 130.3, 129.0, 128.6, 128.3, 127.9, 127.3, 127.2, 127.0, 113.1, 112.3, 105.6 (d, J = 17.0 Hz, $^{2}J_{CF}$), 103.3 (d, J = 18.0 Hz, $^{2}J_{CF}$), 89.4. ^{19}F NMR (376 MHz, DMSO-d_6) δ -115.78. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{30}H_{20}FN_4O_2^+$: 487.1565; found: 487.1567.



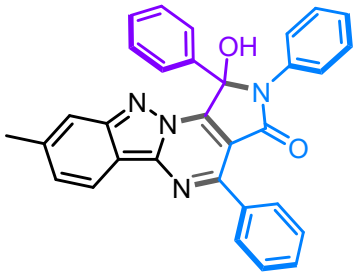
(*S*)-1-hydroxy-7-methyl-1,2,4-triphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4ac):

Yield 74%; 356 mg; yellow solid; column chromatography, silica gel (PE:EA, 8:1); mp 251–253 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.30 (s, 1H), 8.29-8.27 (m, 2H), 8.15 (s, 1H), 7.77 (d, J = 8.4 Hz, 3H), 7.65-7.60 (m, 3H), 7.51 (dd, J = 9.2, 1.2 Hz, 1H), 7.46 (d, J = 7.6 Hz, 2H), 7.37-7.29 (m, 5H), 7.23 (t, J = 7.6 Hz, 1H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.1, 152.4, 151.9, 150.2, 143.8, 135.7, 135.1, 133.6, 131.3, 130.6, 130.0, 128.9, 128.5, 128.2, 127.8, 127.20, 127.16, 126.8, 119.1, 116.7, 113.1, 111.5, 89.4, 21.3. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{23}N_4O_2^+$: 483.1816; found: 483.1820.



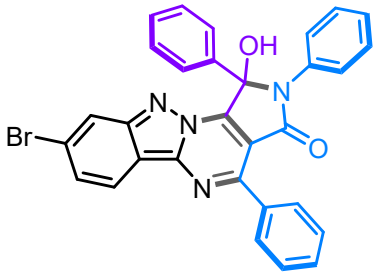
(*S*)-7-chloro-1-hydroxy-1,2,4-triphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4ad):

Yield 68%; 341 mg; yellow solid; column chromatography, silica gel (PE:EA, 8:1); mp 227–229 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.38 (s, 1H), 8.32-8.26 (m, 3H), 7.86 (d, J = 9.2 Hz, 1H), 7.75 (d, J = 7.2 Hz, 2H), 7.64-7.59 (m, 4H), 7.43 (d, J = 7.6 Hz, 2H), 7.36-7.29 (m, 5H), 7.23 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.8, 152.8, 151.5, 151.1, 143.9, 135.3, 135.0, 134.9, 131.6, 130.7, 130.3, 129.0, 128.6, 128.3, 127.8, 127.3, 127.2, 127.0, 126.2, 119.8, 118.9, 113.5, 112.5, 89.3. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{30}H_{20}ClN_4O_2^+$: 503.1269; found: 503.1271.



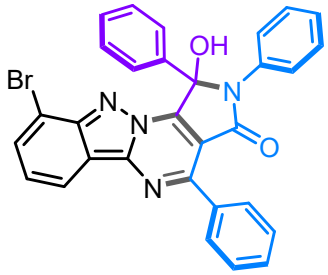
(*S*)-1-hydroxy-8-methyl-1,2,4-triphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4ae):

Yield 76%; 366 mg; yellow solid; column chromatography, silica gel (PE:EA, 8:1); mp 244–246 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.28 (s, 1H), 8.25 (d, J = 8.4 Hz, 3H), 7.73 (d, J = 7.2 Hz, 2H), 7.62 (d, J = 3.6 Hz, 4H), 7.43 (d, J = 8.0 Hz, 2H), 7.37-7.28 (m, 5H), 7.26-7.19 (m, 2H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.1, 153.6, 152.3, 150.7, 144.3, 141.3, 135.6, 135.1, 130.6, 130.1, 128.8, 128.5, 128.2, 127.8, 127.2, 126.8, 124.6, 120.5, 115.4, 111.4, 111.1, 89.3, 22.1. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{31}H_{23}N_4O_2^+$: 483.1816; found: 483.1814.



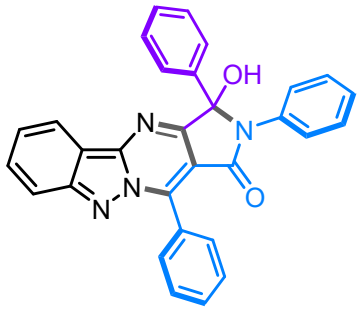
(*S*)-8-bromo-1-hydroxy-1,2,4-triphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4af):

Yield 71%; 387 mg; yellow solid; column chromatography, silica gel (PE:EA, 8:1); mp 227–229 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.31 (s, 1H), 8.30-8.22 (m, 3H), 8.07 (s, 1H), 7.74 (d, J = 7.2 Hz, 2H), 7.65-7.59 (m, 3H), 7.46-7.38 (m, 3H), 7.37-7.28 (m, 5H), 7.23 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.8, 153.3, 152.7, 151.9, 144.6, 135.3, 134.94, 134.86, 130.7, 130.3, 128.9, 128.5, 128.2, 127.8, 127.24, 127.18, 127.0, 125.1, 124.5, 122.8, 119.0, 112.4, 111.7, 89.3. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{30}H_{20}BrN_4O_2^+$: 547.0764; found: 547.0768.



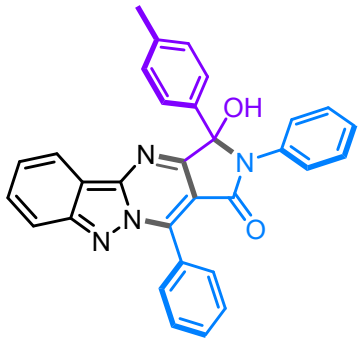
(*S*)-9-bromo-1-hydroxy-1,2,4-triphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (4ag):

Yield 66%; 360 mg; yellow solid; column chromatography, silica gel (PE:EA, 8:1); mp 183–185 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (s, 1H), 8.34 (d, J = 6.4 Hz, 1H), 8.31 (s, 1H), 8.29 (s, 1H), 7.93-7.87 (m, 3H), 7.65-7.62 (m, 3H), 7.56 (d, J = 7.6 Hz, 2H), 7.38-7.30 (m, 5H), 7.25-7.19 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.9, 153.0, 151.9, 150.8, 145.0, 135.24, 135.20, 134.5, 133.5, 130.7, 130.4, 129.0, 128.6, 128.1, 127.8, 127.7, 126.8, 126.7, 122.6, 120.6, 114.2, 112.3, 109.7, 89.5. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{30}H_{20}BrN_4O_2^+$: 547.0764; found: 547.0763.



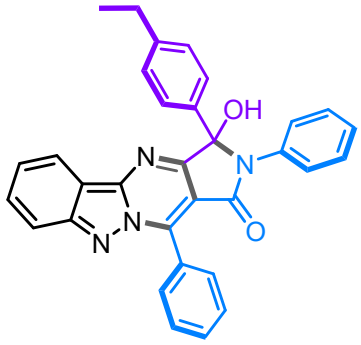
(*S*)-3-hydroxy-2,3,11-triphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5a):

Yield 67%; 313 mg; orange solid; column chromatography, silica gel (PE:EA, 6:1); mp 191–193 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.24 (d, J = 8.4 Hz, 1H), 8.04 (dd, J = 8.4, 2.8 Hz, 3H), 7.82 (d, J = 8.8 Hz, 1H), 7.72-7.64 (m, 4H), 7.61 (d, J = 7.2 Hz, 2H), 7.42 (d, J = 7.6 Hz, 2H), 7.36-7.27 (m, 6H), 7.18 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.4, 162.3, 151.8, 145.2, 144.5, 138.2, 135.6, 131.2, 131.1, 130.7, 128.4, 128.2, 127.7, 127.0, 126.8, 126.7, 121.7, 120.9, 116.6, 112.5, 111.3, 90.8. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{30}H_{21}N_4O_2^+$: 469.1659; found: 469.1661.



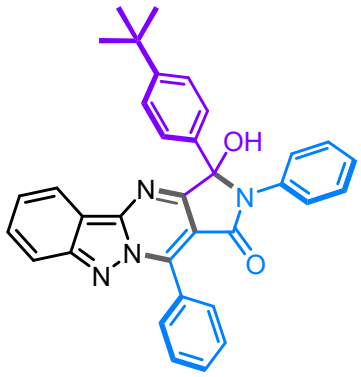
(*S*)-3-hydroxy-2,11-diphenyl-3-(*p*-tolyl)-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5b):

Yield 69%; 332 mg; orange solid; column chromatography, silica gel (PE:EA, 6:1); mp 238–240 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.24 (d, J = 8.4 Hz, 1H), 8.09-8.03 (m, 2H), 8.00 (s, 1H), 7.83 (d, J = 8.8 Hz, 1H), 7.71-7.63 (m, 4H), 7.50 (d, J = 8.0 Hz, 2H), 7.46 (d, J = 8.0 Hz, 2H), 7.35-7.27 (m, 3H), 7.18 (t, J = 7.6 Hz, 1H), 7.14 (d, J = 8.0 Hz, 2H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.6, 162.3, 151.8, 145.2, 144.4, 137.7, 135.7, 135.2, 131.3, 131.1, 130.7, 128.9, 128.4, 127.7, 127.0, 126.8, 126.6, 121.7, 120.9, 116.6, 112.5, 111.2, 90.8, 20.7. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{31}H_{23}N_4O_2^+$: 483.1816; found: 483.1816.



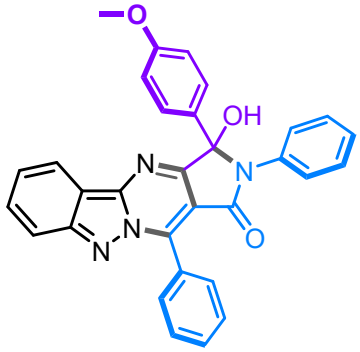
(*S*)-3-(4-ethylphenyl)-3-hydroxy-2,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5c):

Yield 68%; 337 mg; orange solid; column chromatography, silica gel (PE:EA, 6:1); mp 227–230 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 (d, J = 8.4 Hz, 1H), 8.06 (dd, J = 7.2, 2.4 Hz, 2H), 8.03 (s, 1H), 7.83 (d, J = 8.8 Hz, 1H), 7.70-7.63 (m, 4H), 7.55 (d, J = 8.4 Hz, 2H), 7.49 (d, J = 7.6 Hz, 2H), 7.34-7.28 (m, 3H), 7.19 (t, J = 7.2 Hz, 3H), 2.55 (q, J = 7.6 Hz, 2H), 1.13 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.6, 162.3, 151.8, 145.2, 144.5, 143.8, 135.8, 135.4, 131.3, 131.1, 130.7, 128.4, 127.72, 127.67, 127.0, 126.8, 126.6, 121.7, 120.9, 116.6, 112.5, 111.2, 90.9, 27.8, 15.2. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{32}H_{25}N_4O_2^+$: 497.1972; found: 497.1972.



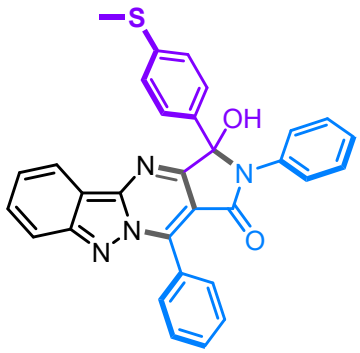
(*S*)-3-(4-(tert-butyl)phenyl)-3-hydroxy-2,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5d):

Yield 71%; 372 mg; orange solid; column chromatography, silica gel (PE:EA, 6:1); mp 245–247 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 (d, J = 8.4 Hz, 1H), 8.01 (d, J = 6.8 Hz, 2H), 7.99 (s, 1H), 7.81 (d, J = 8.8 Hz, 1H), 7.70-7.63 (m, 4H), 7.54 (d, J = 8.4 Hz, 2H), 7.49 (d, J = 8.0 Hz, 2H), 7.35 (d, J = 8.4 Hz, 2H), 7.29 (d, J = 7.6 Hz, 3H), 7.19 (t, J = 7.2 Hz, 1H), 1.22 (s, 9H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.5, 162.3, 151.7, 150.6, 145.1, 144.5, 135.8, 135.1, 131.2, 131.1, 130.7, 128.4, 127.7, 126.8, 126.7, 126.55, 126.47, 125.1, 121.7, 120.9, 116.6, 112.5, 111.0, 90.9, 34.3, 31.0. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{34}H_{29}N_4O_2^+$: 525.2285; found: 525.2288.



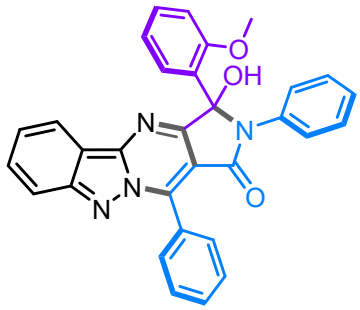
(*S*)-3-hydroxy-3-(4-methoxyphenyl)-2,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5e):

Yield 71%; 353 mg; orange solid; column chromatography, silica gel (PE:EA, 5:1); mp 206–208 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.26 (d, J = 8.4 Hz, 1H), 8.10-8.03 (m, 2H), 8.00 (s, 1H), 7.83 (d, J = 8.8 Hz, 1H), 7.72-7.63 (m, 4H), 7.56 (d, J = 8.8 Hz, 2H), 7.48 (d, J = 8.0 Hz, 2H), 7.32 (t, J = 8.0 Hz, 3H), 7.20 (t, J = 7.2 Hz, 1H), 6.90 (d, J = 8.8 Hz, 2H), 3.71 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.7, 162.3, 159.1, 151.8, 145.2, 144.4, 135.8, 131.3, 131.1, 130.7, 130.0, 128.4, 127.7, 126.8, 126.6, 121.7, 120.8, 116.6, 113.6, 112.5, 111.3, 90.8, 55.0. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{23}N_4O_3^+$: 499.1765; found: 499.1765.



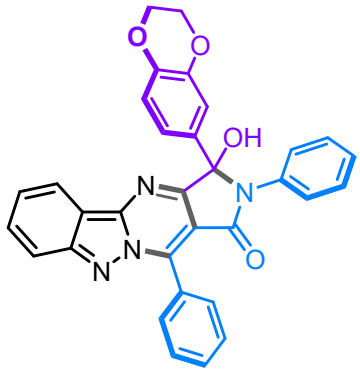
(*S*)-3-hydroxy-3-(4-(methylthio)phenyl)-2,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5f):

Yield 67%; 344 mg; orange solid; column chromatography, silica gel (PE:EA, 5:1); mp 241–243 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.27 (d, J = 8.4 Hz, 1H), 8.09 (s, 2H), 8.07 (d, J = 3.6 Hz, 1H), 7.84 (d, J = 8.8 Hz, 1H), 7.71-7.64 (m, 4H), 7.59 (d, J = 8.4 Hz, 2H), 7.51 (d, J = 8.0 Hz, 2H), 7.33 (t, J = 7.6 Hz, 3H), 7.21 (t, J = 7.6 Hz, 3H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.4, 162.3, 151.8, 145.2, 144.5, 138.7, 135.7, 134.5, 131.3, 131.1, 130.7, 128.4, 127.7, 127.6, 126.8, 126.7, 126.5, 125.2, 121.7, 120.8, 116.6, 112.5, 111.2, 90.7, 14.2. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{23}N_4O_2S^+$: 515.1536; found: 515.1536.



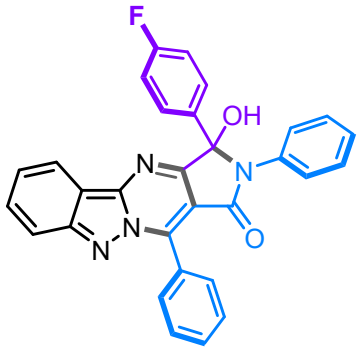
(*S*)-3-hydroxy-3-(2-methoxyphenyl)-2,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5g):

Yield 60%; 298 mg; orange solid; column chromatography, silica gel (PE:EA, 5:1); mp 203–205 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.27 (d, J = 8.4 Hz, 1H), 8.04 (s, 1H), 8.03-7.99 (m, 2H), 7.93 (dd, J = 8.0, 1.6 Hz, 1H), 7.85 (d, J = 8.8 Hz, 1H), 7.73-7.69 (m, 3H), 7.68-7.63 (m, 1H), 7.40-7.36 (m, 2H), 7.33-7.26 (m, 4H), 7.17 (t, J = 7.2 Hz, 1H), 7.02-6.97 (m, 1H), 6.86 (d, J = 8.0 Hz, 1H), 3.47 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.4, 162.5, 155.5, 151.5, 144.7, 143.7, 135.6, 131.0, 130.9, 130.5, 129.1, 128.3, 127.9, 126.9, 126.8, 126.5, 125.3, 121.6, 120.8, 120.1, 116.6, 112.6, 112.5, 111.5, 88.8, 55.6. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{23}N_4O_3^+$: 499.1765; found: 499.1764.



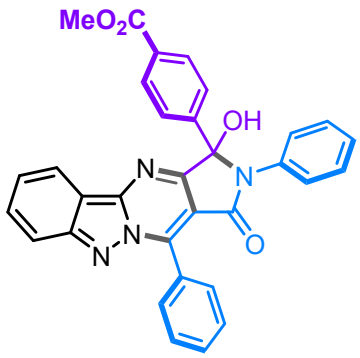
(*S*)-3-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-3-hydroxy-2,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5h):

Yield 73%; 384 mg; yellow solid; column chromatography, silica gel (PE:EA, 5:1); mp 189–191 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.27 (d, J = 8.0 Hz, 1H), 8.03 (d, J = 5.2 Hz, 2H), 7.96 (s, 1H), 7.82 (d, J = 8.4 Hz, 1H), 7.67 (s, 4H), 7.46 (d, J = 7.2 Hz, 2H), 7.32 (t, J = 7.2 Hz, 3H), 7.22 (d, J = 6.8 Hz, 1H), 7.11 (s, 1H), 7.04 (d, J = 8.0 Hz, 1H), 6.79 (d, J = 8.4 Hz, 1H), 4.19 (s, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.4, 162.3, 151.7, 145.2, 144.4, 143.4, 142.9, 135.7, 131.3, 131.1, 130.7, 128.4, 127.7, 126.8, 126.6, 126.5, 121.7, 120.9, 120.0, 116.8, 116.7, 116.0, 112.5, 111.2, 90.5, 64.01, 63.95. HRMS (ESI): m/z [M+H]$^{+}$ calcd for $C_{32}H_{23}N_4O_4^{+}$: 527.1714; found: 527.1714.



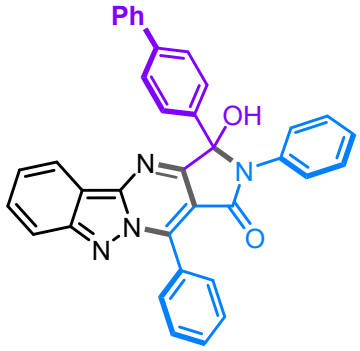
(*S*)-3-(4-fluorophenyl)-3-hydroxy-2,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5i):

Yield 64%; 311 mg; orange solid; column chromatography, silica gel (PE:EA, 5:1); mp 196–198 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 (d, J = 8.4 Hz, 1H), 8.12 (s, 1H), 8.05 (dd, J = 7.2, 2.0 Hz, 2H), 7.83 (d, J = 8.8 Hz, 1H), 7.73-7.61 (m, 6H), 7.41 (d, J = 7.6 Hz, 2H), 7.36-7.28 (m, 3H), 7.25-7.11 (m, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.3, 162.2, 162.0 (d, J = 244.0 Hz, $^{1}J_{CF}$), 151.8, 145.2, 144.5, 135.4, 134.4 (d, J = 2.0 Hz, $^{4}J_{CF}$), 131.2, 131.1, 130.7, 129.3 (d, J = 9.0 Hz, $^{3}J_{CF}$), 128.4, 127.7, 126.8, 121.7, 120.8, 116.6, 115.0 (d, J = 22.0 Hz, $^{2}J_{CF}$), 112.5, 111.3, 90.4. ^{19}F NMR (376 MHz, DMSO-d6) δ -113.67. HRMS (ESI): m/z [M+H]$^{+}$ calcd for $C_{30}H_{20}FN_4O_2^{+}$: 487.1565; found: 487.1565.



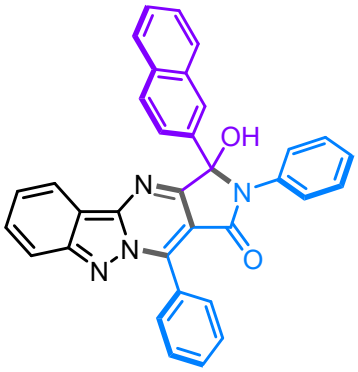
methyl(*S*)-4-(3-hydroxy-1-oxo-2,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-3-yl)benzoate (5j):

Yield 51%; 268 mg; orange solid; column chromatography, silica gel (PE:EA, 4:1); mp 182–184 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.24 (s, 1H), 8.22 (s, 1H), 8.04 (d, J = 6.0 Hz, 2H), 7.90 (d, J = 8.4 Hz, 2H), 7.83 (d, J = 8.8 Hz, 1H), 7.76 (d, J = 8.4 Hz, 2H), 7.70-7.64 (m, 4H), 7.39 (d, J = 8.0 Hz, 2H), 7.30 (d, J = 8.0 Hz, 3H), 7.19 (t, J = 7.6 Hz, 1H), 3.81 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.8, 162.4, 161.9, 151.8, 145.2, 144.6, 143.4, 135.3, 131.3, 131.2, 130.8, 129.7, 129.1, 128.5, 127.7, 127.6, 126.9, 126.8, 126.7, 121.8, 120.8, 116.7, 112.5, 111.2, 90.4, 52.2. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{32}H_{23}N_4O_4^+$: 527.1714; found: 527.1712.



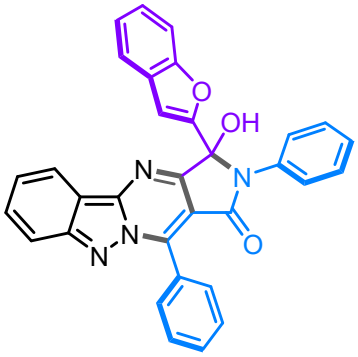
(*S*)-3-([1,1'-biphenyl]-4-yl)-3-hydroxy-2,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5k):

Yield 66%; 359 mg; orange solid; column chromatography, silica gel (PE:EA, 5:1); mp 192–194 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 (d, J = 8.4 Hz, 1H), 8.14 (s, 1H), 8.08 (d, J = 4.4 Hz, 2H), 7.84 (d, J = 8.8 Hz, 1H), 7.74 (d, J = 8.0 Hz, 2H), 7.69 (d, J = 4.8 Hz, 3H), 7.67-7.62 (m, 5H), 7.53 (d, J = 7.6 Hz, 2H), 7.42 (t, J = 7.6 Hz, 2H), 7.36-7.29 (m, 4H), 7.20 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.4, 151.8, 145.2, 144.5, 140.1, 139.3, 137.3, 135.7, 131.3, 131.1, 130.7, 130.6, 129.2, 128.9, 128.5, 127.7, 127.3, 127.2, 126.8, 126.7, 126.6, 126.5, 121.7, 120.9, 116.7, 112.5, 111.2, 90.8. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{36}H_{25}N_4O_2^+$: 545.1972; found: 545.1972.



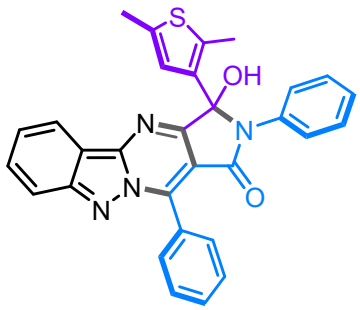
(*S*)-3-hydroxy-3-(naphthalen-2-yl)-2,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5l):

Yield 66%; 342 mg; orange solid; column chromatography, silica gel (PE:EA, 5:1); mp 215–217 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.35 (s, 1H), 8.21 (s, 2H), 8.09 (s, 2H), 7.99 (s, 1H), 7.84 (d, J = 8.8 Hz, 3H), 7.70 (s, 3H), 7.66-7.58 (m, 2H), 7.51 (s, 2H), 7.47 (d, J = 7.6 Hz, 2H), 7.31-7.21 (m, 3H), 7.15 (d, J = 6.8 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.5, 162.4, 151.8, 145.2, 144.5, 135.6, 135.5, 132.7, 132.5, 131.3, 131.1, 130.7, 128.4, 128.3, 127.9, 127.7, 127.5, 126.8, 126.7, 126.6, 126.4, 124.5, 121.7, 120.8, 116.6, 112.5, 111.4, 90.9. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{34}H_{23}N_4O_2^+$: 519.1816; found: 519.1816.



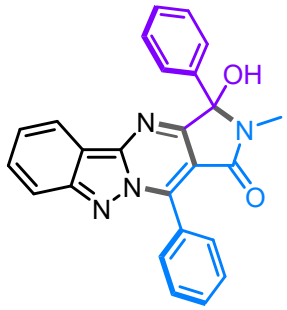
(*R*)-3-(benzofuran-2-yl)-3-hydroxy-2,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5m):

Yield 58%; 294 mg; orange solid; column chromatography, silica gel (PE:EA, 4:1); mp 223–225 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.40 (s, 1H), 8.27 (d, J = 8.4 Hz, 1H), 8.04-8.00 (m, 2H), 7.84 (d, J = 8.8 Hz, 1H), 7.70-7.64 (m, 5H), 7.48 (d, J = 7.6 Hz, 1H), 7.37-7.31 (m, 5H), 7.28-7.23 (m, 4H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.2, 159.6, 154.4, 152.9, 151.8, 145.1, 144.8, 135.0, 131.3, 131.2, 130.8, 128.8, 127.8, 127.5, 127.4, 127.1, 126.6, 125.1, 123.3, 122.0, 121.7, 120.9, 116.8, 112.7, 111.5, 110.9, 107.9, 87.8. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{32}H_{21}N_4O_3^+$: 509.1608; found: 509.1608.



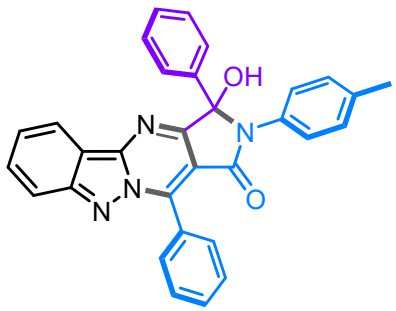
(*S*)-3-(2,5-dimethylthiophen-3-yl)-3-hydroxy-2,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5n):

Yield 60%; 301 mg; yellow solid; column chromatography, silica gel (PE:EA, 5:1); mp 197–199 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.33 (d, J = 8.4 Hz, 1H), 8.02-7.96 (m, 2H), 7.84 (d, J = 8.8 Hz, 1H), 7.78 (s, 1H), 7.70-7.64 (m, 4H), 7.45 (d, J = 8.0 Hz, 2H), 7.39-7.33 (m, 3H), 7.26 (t, J = 7.2 Hz, 1H), 6.76 (s, 1H), 2.27 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 161.8, 161.7, 151.8, 145.3, 144.4, 135.7, 134.0, 133.3, 131.2, 131.1, 130.7, 128.5, 127.7, 126.9, 126.8, 126.2, 121.7, 121.0, 116.7, 112.6, 111.2, 90.3, 14.7, 13.8. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{30}H_{23}N_4O_2S^+$: 503.1536; found: 503.1537.



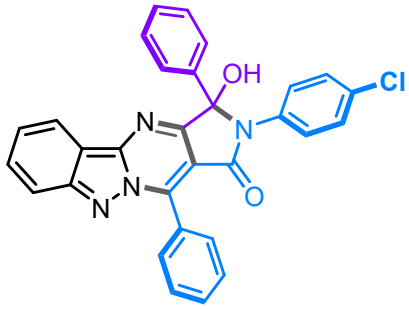
3-hydroxy-2-methyl-3,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5o):

Yield 73%; 296 mg; orange solid; column chromatography, silica gel (PE:EA, 5:1); mp 263–265 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.22 (d, J = 8.4 Hz, 1H), 7.98 (dd, J = 7.6, 1.6 Hz, 2H), 7.79 (d, J = 8.8 Hz, 1H), 7.69-7.64 (m, 3H), 7.63-7.57 (m, 3H), 7.47-7.42 (m, 3H), 7.40 (d, J = 7.2 Hz, 1H), 7.32-7.26 (m, 1H), 2.75 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.7, 162.3, 151.5, 144.7, 143.8, 137.7, 131.2, 131.0, 130.4, 128.6, 128.5, 127.7, 126.9, 126.7, 121.6, 120.7, 116.6, 112.5, 111.7, 88.8, 24.0. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{25}H_{19}N_4O_2^+$: 407.1503; found: 407.1505



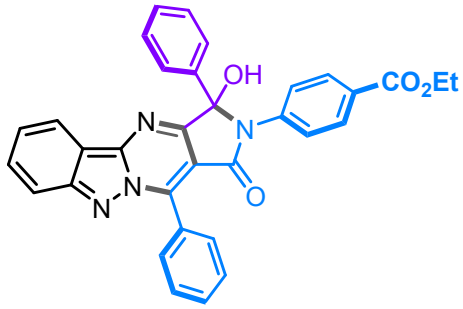
(*S*)-3-hydroxy-3,11-diphenyl-2-(*p*-tolyl)-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5p):

Yield 63%; 303 mg; orange solid; column chromatography, silica gel (PE:EA, 6:1); mp 256–258 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.24 (d, J = 8.4 Hz, 1H), 8.08-8.02 (m, 2H), 8.00 (s, 1H), 7.82 (d, J = 8.8 Hz, 1H), 7.74-7.63 (m, 4H), 7.63-7.58 (m, 2H), 7.37-7.27 (m, 6H), 7.09 (d, J = 8.4 Hz, 2H), 2.23 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.5, 162.3, 151.7, 145.2, 144.4, 138.2, 136.0, 132.9, 131.2, 131.0, 130.6, 128.9, 128.3, 128.2, 127.7, 127.0, 126.8, 126.6, 121.7, 120.8, 116.6, 112.5, 111.4, 90.7, 20.6. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{23}N_4O_2^+$: 483.1816; found: 483.1816.



(*S*)-2-(4-chlorophenyl)-3-hydroxy-3,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5q):

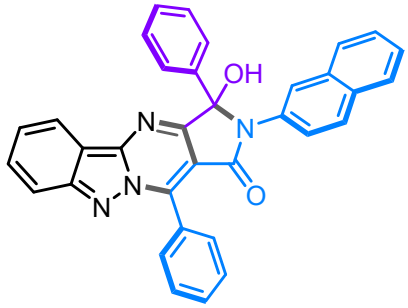
Yield 60%; 301 mg; orange solid; column chromatography, silica gel (PE:EA, 5:1); mp 193–195 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.24 (d, J = 8.4 Hz, 1H), 8.14 (s, 1H), 8.06-8.01 (m, 2H), 7.82 (d, J = 8.8 Hz, 1H), 7.70-7.63 (m, 4H), 7.61 (d, J = 7.2 Hz, 2H), 7.50 (d, J = 8.8 Hz, 2H), 7.38-7.33 (m, 4H), 7.30 (d, J = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.3, 162.1, 151.8, 145.2, 144.6, 137.8, 134.7, 131.3, 131.2, 130.79, 130.77, 128.6, 128.5, 128.3, 127.8, 127.7, 127.0, 126.7, 121.8, 120.9, 116.7, 112.5, 111.0, 90.8. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{30}H_{20}ClN_4O_2^+$: 503.1269; found: 503.1269.



ethyl(*S*)-4-(3-hydroxy-1-oxo-3,11-diphenyl-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-2(3*H*)-yl)benzoate (5r):

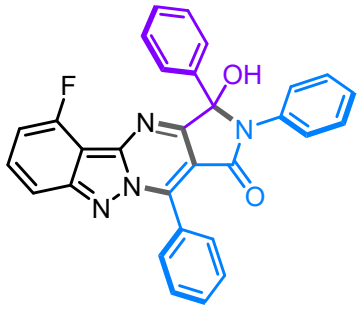
Yield 58%; 313 mg; orange solid; column chromatography, silica gel (PE:EA, 5:1); mp 184–186 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 (s, 1H), 8.23 (s, 1H), 8.06-8.03 (m, 2H), 7.89-7.80 (m, 4H), 7.77 (d, J = 8.8 Hz, 2H), 7.69 (d, J = 6.8 Hz, 3H), 7.64 (d, J = 7.2 Hz, 2H), 7.34 (t, J = 7.2 Hz, 3H), 7.29 (d, J = 8.8 Hz, 1H), 4.26 (d, J = 7.2 Hz, 2H), 1.28 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 165.1, 162.4, 161.8, 151.8, 145.3, 144.8, 140.4, 137.8, 131.2, 130.8, 129.5, 129.3, 128.5, 128.3, 127.7, 126.9, 126.7, 124.7, 121.8, 120.8,

116.6, 112.5, 110.8, 91.2, 60.6, 14.1. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{33}H_{25}N_4O_4^+$: 541.1870; found: 541.1870.



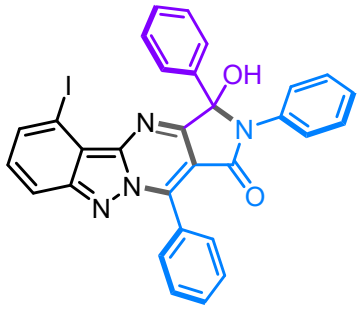
(*S*)-3-hydroxy-2-(naphthalen-2-yl)-3,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5s):

Yield 55%; 284 mg; orange solid; column chromatography, silica gel (PE:EA, 5:1); mp 227–229 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.26 (d, J = 8.4 Hz, 1H), 8.24 (s, 1H), 8.08 (d, J = 7.6 Hz, 3H), 7.83 (t, J = 8.0 Hz, 4H), 7.71-7.62 (m, 7H), 7.47 (dd, J = 6.0, 3.2 Hz, 2H), 7.32 (t, J = 7.6 Hz, 3H), 7.24 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.6, 162.4, 151.8, 145.3, 144.6, 138.1, 133.5, 132.7, 131.3, 131.1, 130.7, 128.4, 128.3, 127.82, 127.77, 127.4, 127.1, 126.9, 126.4, 126.2, 124.9, 124.2, 121.8, 120.9, 116.7, 112.6, 111.3, 91.1. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{34}H_{23}N_4O_2^+$: 519.1816; found: 519.1816.



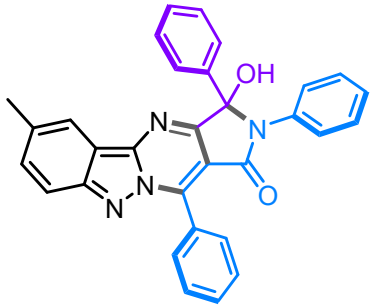
(*S*)-5-fluoro-3-hydroxy-2,3,11-triphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5t):

Yield 62%; 301 mg; orange solid; column chromatography, silica gel (PE:EA, 5:1); mp 208–210 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.10 (s, 1H), 8.05 (d, J = 6.8 Hz, 2H), 7.71-7.66 (m, 3H), 7.65-7.58 (m, 4H), 7.43 (d, J = 7.6 Hz, 2H), 7.37-7.28 (m, 5H), 7.20 (t, J = 7.2 Hz, 1H), 7.09-7.03 (m, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.5, 162.1, 156.0 (d, J = 255.0 Hz, $^1J_{CF}$), 153.2 (d, J = 4.0 Hz, $^4J_{CF}$), 144.7, 143.6 (d, J = 6.0 Hz, $^3J_{CF}$), 138.0, 135.5, 131.3, 128.5, 128.4, 128.3, 127.7, 127.0, 126.8, 126.7, 126.6, 113.0, 111.6, 105.1 (d, J = 17.0 Hz, $^2J_{CF}$), 103.1 (d, J = 18.0 Hz, $^2J_{CF}$), 90.9. ^{19}F NMR (376 MHz, DMSO-d6) δ -115.53. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{30}H_{20}FN_4O_2^+$: 487.1565; found: 487.1568.



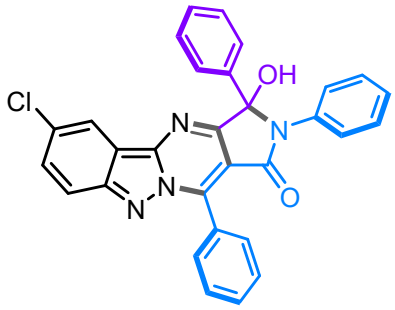
(*S*)-3-hydroxy-5-iodo-2,3,11-triphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5u):

Yield 58%; 344 mg; orange solid; column chromatography, silica gel (PE:EA, 6:1); mp 240–242 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.06 (s, 1H), 7.99 (dd, J = 7.6, 2.0 Hz, 2H), 7.83 (t, J = 8.0 Hz, 2H), 7.69-7.63 (m, 5H), 7.51 (d, J = 7.6 Hz, 2H), 7.38-7.35 (m, 1H), 7.34-7.28 (m, 5H), 7.20 (t, J = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.3, 161.7, 152.1, 145.4, 144.6, 138.0, 135.8, 132.3, 131.5, 131.2, 131.1, 128.44, 128.39, 128.2, 127.7, 127.0, 126.7, 126.5, 126.3, 116.5, 113.8, 111.7, 91.2, 86.0. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{30}H_{20}IN_4O_2^+$: 595.0625; found: 595.0625.



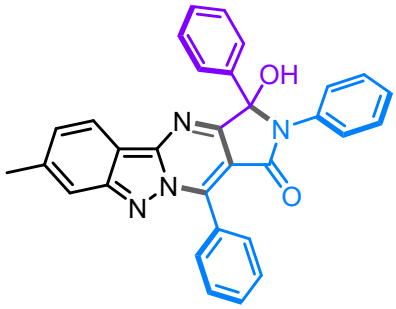
(*S*)-3-hydroxy-6-methyl-2,3,11-triphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5v):

Yield 70%; 337 mg; orange solid; column chromatography, silica gel (PE:EA, 5:1); mp 238–240 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.06 (d, J = 1.6 Hz, 1H), 8.05-8.01 (m, 3H), 7.74 (d, J = 8.8 Hz, 1H), 7.70-7.62 (m, 5H), 7.51-7.44 (m, 3H), 7.37-7.27 (m, 5H), 7.19 (t, J = 7.6 Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.4, 162.0, 150.7, 144.5, 144.3, 138.3, 135.7, 133.3, 131.2, 131.1, 131.0, 128.4, 128.2, 127.7, 127.0, 126.9, 126.6, 118.9, 116.4, 112.7, 110.9, 90.8, 21.2. HRMS (ESI): m/z [M+H]$^+$ calcd for $C_{31}H_{23}N_4O_2^+$: 483.1816; found: 483.1816.



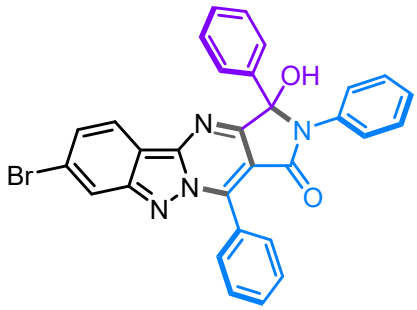
(*S*)-6-chloro-3-hydroxy-2,3,11-triphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5w):

Yield 60%; 301 mg; orange solid; column chromatography, silica gel (PE:EA, 5:1); mp 267–269 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.29 (d, J = 1.6 Hz, 1H), 8.06 (s, 1H), 8.02 (dd, J = 7.6, 1.6 Hz, 2H), 7.87 (d, J = 9.2 Hz, 1H), 7.70-7.66 (m, 3H), 7.63 (d, J = 2.0 Hz, 1H), 7.61 (d, J = 1.6 Hz, 1H), 7.59 (s, 1H), 7.41 (d, J = 1.2 Hz, 1H), 7.39 (s, 1H), 7.35-7.27 (m, 5H), 7.19 (t, J = 7.2 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.1, 162.1, 149.9, 144.9, 144.6, 138.0, 135.5, 131.4, 131.2, 128.44, 128.40, 128.2, 127.7, 127.0, 126.8, 126.7, 126.5, 126.0, 124.5, 119.6, 118.8, 113.0, 111.8, 90.8. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{30}H_{20}ClN_4O_2^+$: 503.1269; found: 503.1266.



(*S*)-3-hydroxy-7-methyl-2,3,11-triphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5x):

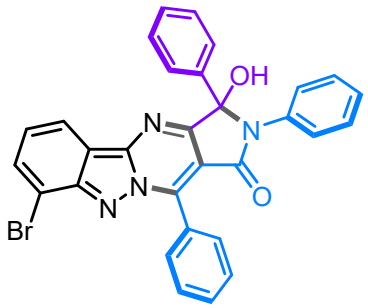
Yield 60%; 289 mg; orange solid; column chromatography, silica gel (PE:EA, 6:1); mp 196–198 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.12 (d, J = 8.4 Hz, 1H), 8.04-7.99 (m, 3H), 7.67 (q, J = 5.6 Hz, 3H), 7.60 (d, J = 8.0 Hz, 3H), 7.41 (d, J = 8.0 Hz, 2H), 7.35-7.26 (m, 5H), 7.20-7.14 (m, 2H), 2.50 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 162.4, 152.5, 145.1, 144.4, 140.9, 138.2, 135.7, 131.2, 131.1, 128.4, 128.2, 127.7, 127.0, 126.8, 126.6, 124.5, 120.4, 115.1, 110.8, 110.7, 90.7, 22.2. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{23}N_4O_2^+$: 483.1816; found: 483.1816.



(*S*)-7-bromo-3-hydroxy-2,3,11-triphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5y):

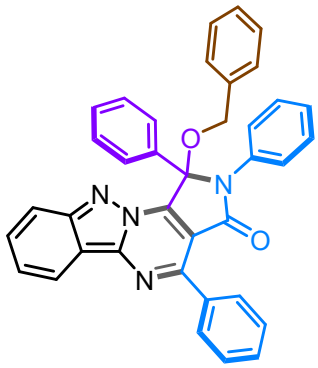
Yield 57%; 311 mg; yellow solid; column chromatography, silica gel (PE:EA, 6:1); mp 186–188 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.21 (d, J = 8.8 Hz, 1H), 8.13 (d, J = 0.8 Hz, 1H), 8.08 (s, 1H), 8.06-8.01 (m, 2H), 7.71-7.65 (m, 3H), 7.63-7.60 (m, 2H), 7.42 (d, J = 7.6 Hz, 2H), 7.39 (dd, J = 8.8, 1.6 Hz, 1H), 7.35 (d, J = 6.8 Hz, 1H), 7.33-7.26 (m, 4H), 7.19 (t, J = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.5, 162.1, 152.2, 145.4, 145.0, 137.9,

135.5, 131.2, 128.5, 128.4, 128.3, 127.8, 127.0, 126.8, 126.7, 126.6, 124.9, 124.2, 122.9, 118.8, 111.8, 111.3, 90.8. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{30}H_{20}BrN_4O_2^+$: 547.0764; found: 547.0764.



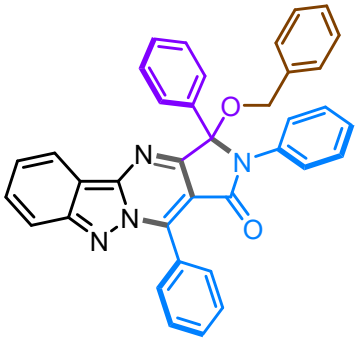
(*S*)-8-bromo-3-hydroxy-2,3,11-triphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (5z):

Yield 63%; 344 mg; orange solid; column chromatography, silica gel (PE:EA, 6:1); mp 190–192 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.27 (d, J = 8.4 Hz, 1H), 8.11 (s, 3H), 7.93 (d, J = 7.2 Hz, 1H), 7.70 (d, J = 6.4 Hz, 3H), 7.64 (d, J = 7.2 Hz, 2H), 7.44 (d, J = 7.6 Hz, 2H), 7.37-7.28 (m, 5H), 7.23-7.18 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 163.6, 162.1, 149.7, 146.0, 145.2, 137.9, 135.5, 133.3, 131.5, 131.4, 128.5, 128.4, 128.3, 127.7, 127.0, 126.8, 126.7, 126.3, 122.4, 120.6, 113.8, 112.0, 109.5, 90.7. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{30}H_{20}BrN_4O_2^+$: 547.0764; found: 547.0764.



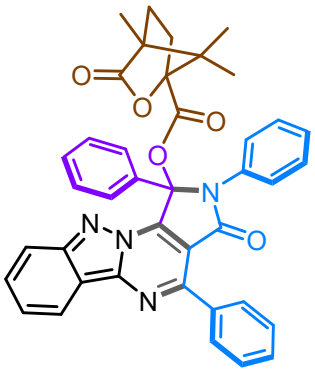
(*S*)-1-(benzyloxy)-1,2,4-triphenyl-1,2-dihydro-3*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-3-one (7):

Yield 93%; 155 mg; yellow solid; column chromatography, silica gel (PE:EA, 20:1); mp 211–213 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, J = 8.4 Hz, 1H), 8.45 (d, J = 7.6 Hz, 2H), 8.01 (d, J = 8.8 Hz, 1H), 7.88 (d, J = 7.6 Hz, 2H), 7.77-7.67 (m, 6H), 7.44-7.36 (m, 8H), 7.31-7.29 (m, 1H), 7.27-7.23 (m, 3H), 4.97 (d, J = 10.8 Hz, 1H), 4.39 (d, J = 10.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0, 154.0, 150.5, 149.3, 144.8, 135.3, 134.9, 133.7, 130.7, 130.5, 130.3, 129.3, 128.7, 128.3, 128.04, 127.99, 127.9, 127.1, 126.5, 124.9, 122.0, 121.1, 117.3, 113.7, 112.1, 93.8, 66.8. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{37}H_{27}N_4O_2^+$: 559.2129; found: 559.2127.



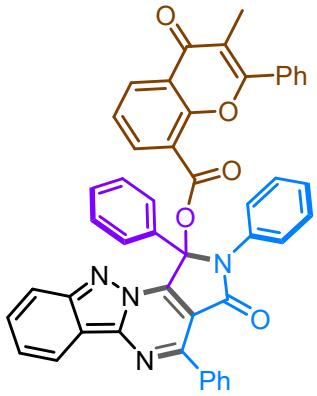
(*S*)-3-(benzyloxy)-2,3,11-triphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-1-one (8):

Yield 82%; 137 mg; orange solid; column chromatography, silica gel (PE:EA, 15:1); mp 190–192 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.4 Hz, 1H), 8.11 (dd, *J* = 6.4, 2.8 Hz, 2H), 7.83 (d, *J* = 8.8 Hz, 1H), 7.70-7.67 (m, 3H), 7.63 (t, *J* = 8.0 Hz, 3H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.36-7.32 (m, 4H), 7.30 (d, *J* = 9.2 Hz, 4H), 7.26 (d, *J* = 4.4 Hz, 1H), 7.23 (d, *J* = 7.6 Hz, 4H), 7.14 (t, *J* = 7.2 Hz, 1H), 4.73 (d, *J* = 10.8 Hz, 1H), 4.46 (d, *J* = 10.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.5, 158.3, 152.9, 146.2, 145.1, 137.2, 136.5, 135.6, 132.0, 131.3, 130.9, 128.9, 128.7, 128.6, 128.3, 128.1, 127.9, 127.8, 126.8, 126.4, 126.1, 124.7, 121.9, 121.5, 117.0, 113.5, 111.0, 95.2, 65.8. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{37}H_{27}N_4O_2^+$: 559.2129; found: 559.2129.



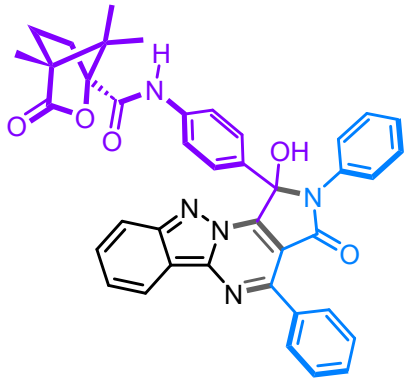
(*S*)-3-oxo-1,2,4-triphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-1-yl (1*R*,4*S*)-4,7,7-trimethyl-3-oxo-2-oxabicyclo[2.2.1]heptane-1-carboxylate (9):

Yield 90%; 175 mg; yellow solid; column chromatography, silica gel (PE:EA, 10:1); mp 226–228 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.4 Hz, 1H), 8.29 (d, *J* = 6.4 Hz, 2H), 7.86-7.80 (m, 2H), 7.77-7.72 (m, 1H), 7.61-7.55 (m, 4H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.32-7.27 (m, 3H), 7.25-7.18 (m, 4H), 2.58-2.39 (m, 1H), 1.94-1.83 (m, 2H), 1.68-1.61 (m, 1H), 1.06 (d, *J* = 4.0 Hz, 3H), 0.93 (s, 3H), 0.74 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.7, 165.2, 164.3, 154.0, 151.4, 150.3, 144.8, 135.2, 133.8, 132.3, 131.0, 130.5, 130.4, 130.3, 130.2, 129.1, 129.0, 128.1, 127.6, 126.8, 126.1, 121.9, 121.5, 116.8, 113.7, 110.9, 90.7, 55.0, 54.6, 31.3, 28.6, 16.3, 16.2, 9.6. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{40}H_{33}N_4O_5^+$: 649.2445; found: 649.2448.



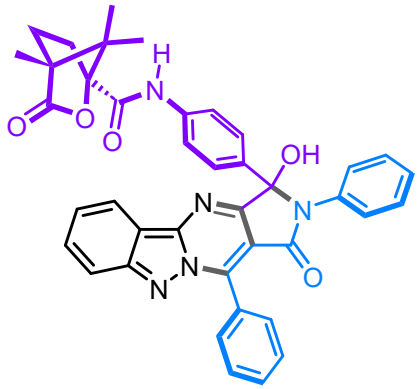
(*S*)-3-oxo-1,2,4-triphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-1-yl 3-methyl-4-oxo-2-phenyl-4*H*-chromene-8-carboxylate (10):

Yield 88%; 192 mg; orange solid; column chromatography, silica gel (PE:EA, 10:1); mp 238–240 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (dd, *J* = 12.4, 8.0 Hz, 4H), 8.24-8.19 (m, 1H), 7.90 (d, *J* = 7.6 Hz, 2H), 7.81 (d, *J* = 8.8 Hz, 1H), 7.70-7.63 (m, 3H), 7.60-7.51 (m, 3H), 7.40-7.35 (m, 3H), 7.33-7.28 (m, 8H), 7.22 (t, *J* = 7.6 Hz, 2H), 2.24 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.4, 164.5, 161.8, 160.8, 154.0, 153.9, 151.2, 150.8, 144.7, 136.2, 135.2, 133.5, 132.0, 131.9, 131.4, 130.7, 130.5, 130.21, 130.16, 129.7, 129.0, 128.9, 128.4, 127.9, 127.8, 127.5, 126.8, 123.9, 123.0, 121.6, 121.2, 118.7, 117.6, 116.7, 113.5, 111.2, 91.4, 11.6. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{47}H_{31}N_4O_5^+$: 731.2289; found: 731.2293.



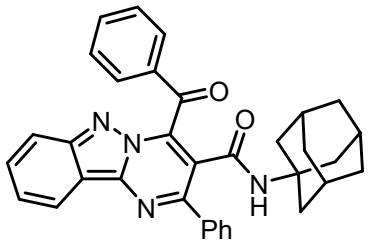
(4*S*)-*N*-(4-((*S*)-1-hydroxy-3-oxo-2,4-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':5,6]pyrimido[1,2-*b*]indazol-1-yl)phenyl)-4,7,7-trimethyl-3-oxo-2-oxabicyclo[2.2.1]heptane-1-carboxamide (12):

Yield 69%; 457 mg; yellow solid; column chromatography, silica gel (PE:EA, 5:1); mp 265–267 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.84 (s, 1H), 8.37 (d, *J* = 8.4 Hz, 1H), 8.32 (s, 1H), 8.25-8.23 (m, 2H), 7.86 (d, *J* = 8.8 Hz, 1H), 7.74-7.67 (m, 6H), 7.62-7.60 (m, 2H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.39-7.33 (m, 3H), 7.24 (d, *J* = 7.2 Hz, 1H), 2.01-1.95 (m, 1H), 1.93-1.85 (m, 1H), 1.59-1.53 (m, 1H), 1.27-1.19 (m, 1H), 1.01 (s, 3H), 1.00 (s, 3H), 0.88-0.85 (m, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 177.8, 165.4, 162.9, 152.9, 152.3, 150.8, 144.4, 138.3, 135.5, 135.1, 131.0, 130.6, 130.1, 128.5, 127.8, 127.6, 127.1, 126.8, 122.0, 121.0, 120.4, 120.3, 116.9, 112.9, 111.8, 91.7, 89.2, 54.6, 53.6, 30.1, 28.4, 16.5, 16.3, 9.5. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{40}H_{34}N_5O_5^+$: 664.2554; found: 664.2553.



(4*S*)-*N*-(4-((*S*)-3-hydroxy-1-oxo-2,11-diphenyl-2,3-dihydro-1*H*-pyrrolo[3',4':4,5]pyrimido[1,2-*b*]indazol-3-yl)phenyl)-4,7,7-trimethyl-3-oxo-2-oxabicyclo[2.2.1]heptane-1-carboxamide (13):

Yield 60%; 397 mg; yellow solid; column chromatography, silica gel (PE:EA, 4:1); mp 211–213 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.84 (s, 1H), 8.24 (d, J = 8.4 Hz, 1H), 8.04 (dd, J = 7.6, 2.0 Hz, 2H), 8.01 (s, 1H), 7.82 (d, J = 8.8 Hz, 1H), 7.71-7.64 (m, 6H), 7.56 (d, J = 8.8 Hz, 2H), 7.46 (dd, J = 8.4, 1.2 Hz, 2H), 7.34-7.27 (m, 3H), 7.19 (t, J = 7.6 Hz, 1H), 2.01-1.95 (m, 1H), 1.92-1.84 (m, 1H), 1.60-1.54 (m, 1H), 1.23 (s, 1H), 1.02 (s, 3H), 1.01 (s, 3H), 0.87 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 177.9, 165.4, 162.4, 162.3, 151.7, 145.2, 144.4, 139.1, 137.8, 135.7, 133.7, 131.2, 131.1, 130.7, 128.4, 127.7, 127.3, 126.8, 126.5, 121.7, 120.8, 120.5, 116.6, 112.5, 111.2, 91.8, 90.7, 54.6, 53.6, 30.0, 28.4, 16.5, 16.3, 9.5. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{40}H_{34}N_5O_5^+$: 664.2554; found: 664.2551.



***N*-((3R,5R)-adamantan-1-yl)-4-benzoyl-2-phenylpyrimido[1,2-*b*]indazole-3-carboxamide (14):**

Yield 68%; 357 mg; yellow solid; column chromatography, silica gel (PE:EA, 8:1); mp 292–294 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.36 (d, J = 8.4 Hz, 1H), 7.96 (d, J = 6.0 Hz, 5H), 7.77 (t, J = 8.0 Hz, 2H), 7.68-7.63 (m, 1H), 7.60-7.54 (m, 5H), 7.37 (t, J = 7.6 Hz, 1H), 1.86 (s, 3H), 1.61-1.50 (m, 9H), 1.43 (d, J = 11.6 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 187.5, 162.3, 152.5, 151.6, 142.4, 139.6, 137.5, 135.3, 134.3, 130.4, 129.9, 129.7, 129.2, 129.0, 128.2, 121.5, 120.9, 120.7, 116.3, 112.5, 51.9, 35.8, 28.5. HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{34}H_{31}N_4O_2^+$: 527.2442; found: 527.2434.

7. Crystallographic data and molecular structure of 4b and 5i

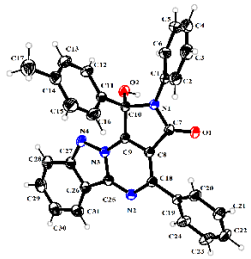


Figure 1. Molecular structure of **4b** with 30% probability ellipsoids

Crystal Data for Compound **4b**: CCDC 2367465 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic.

Sample preparation: In a 10 mL glass bottle, 15 mg of pure **4b** or **5i** was completely dissolved in the mixed solvent of 3 mL EtOAc, 1 mL EtOH, 1 mL $CHCl_3$; and then 2 mL of n-hexane was added slowly. After a week of solvent evaporation, some colorless transparent crystals were obtained. The crystals were mounted on a glass fiber for diffraction experiments. Intensity data were collected on a Bruker SMART APEX CCD diffractometer with Mo Kα radiation (0.71073 Å) at room temperature.

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Bond precision:   C-C = 0.0028 A          Wavelength=0.71073

Cell:             a=18.947(3)     b=16.244(3)          c=15.993(3)
                  alpha=90        beta=104.238(2)      gamma=90
Temperature:      296 K

                 Calculated                  Reported
Volume           4771.1(15)                  4771.1(13)
Space group      C 2/c                       C 1 2/c 1
Hall group       -C 2yc                      -C 2yc
Moiety formula   C31 H22 N4 O2               C31 H22 N4 O2
Sum formula      C31 H22 N4 O2               C31 H22 N4 O2
Mr               482.53                      482.52
Dx,g cm-3        1.344                       1.344
Z                8                           8
Mu (mm-1)        0.086                       0.086
F000             2016.0                      2016.0
F000'            2016.79
h,k,lmax         23,20,20                    23,20,20
Nref             4933                        4920
Tmin,Tmax        0.980,0.991                 0.681,0.745
Tmin'            0.975

Correction method= # Reported T Limits: Tmin=0.681 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.997            Theta(max)= 26.475

R(reflections)= 0.0444( 3773)                wR2(reflections)=
                                             0.1456( 4920)
S = 1.026                  Npar= 337
```

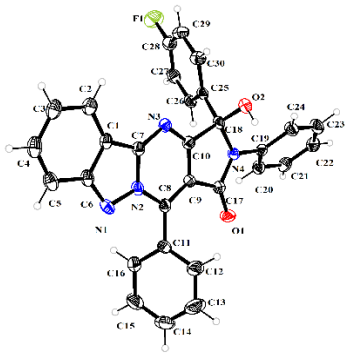


Figure 2. Molecular structure of **5i** with 30% probability ellipsoids

Crystal Data for Compound **5i**: CCDC 2367548 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic.

```
Bond precision:   C-C = 0.0056 A          Wavelength=0.71073

Cell:             a=12.761(2)     b=11.663(2)          c=19.570(3)
                  alpha=90        beta=107.371(3)      gamma=90
Temperature:      296 K

                  Calculated                  Reported
Volume            2779.8(8)                   2779.6(8)
Space group       P 21/n                      P 1 21/n 1
Hall group        -P 2yn                      -P 2yn
Moiety formula    C30 H20 F N4 O2, C2 H6 O S  C30 H20 F N4 O2, C2 H6 O S
Sum formula       C32 H26 F N4 O3 S           C32 H26 F N4 O3 S
Mr                565.63                      565.63
Dx,g cm-3         1.352                       1.352
Z                 4                           4
Mu (mm-1)         0.165                       0.165
F000              1180.0                      1180.0
F000'             1181.01
h,k,lmax          15,13,23                    15,13,23
Nref              4912                        4899
Tmin,Tmax         0.961,0.984                 0.671,0.745
Tmin'             0.949

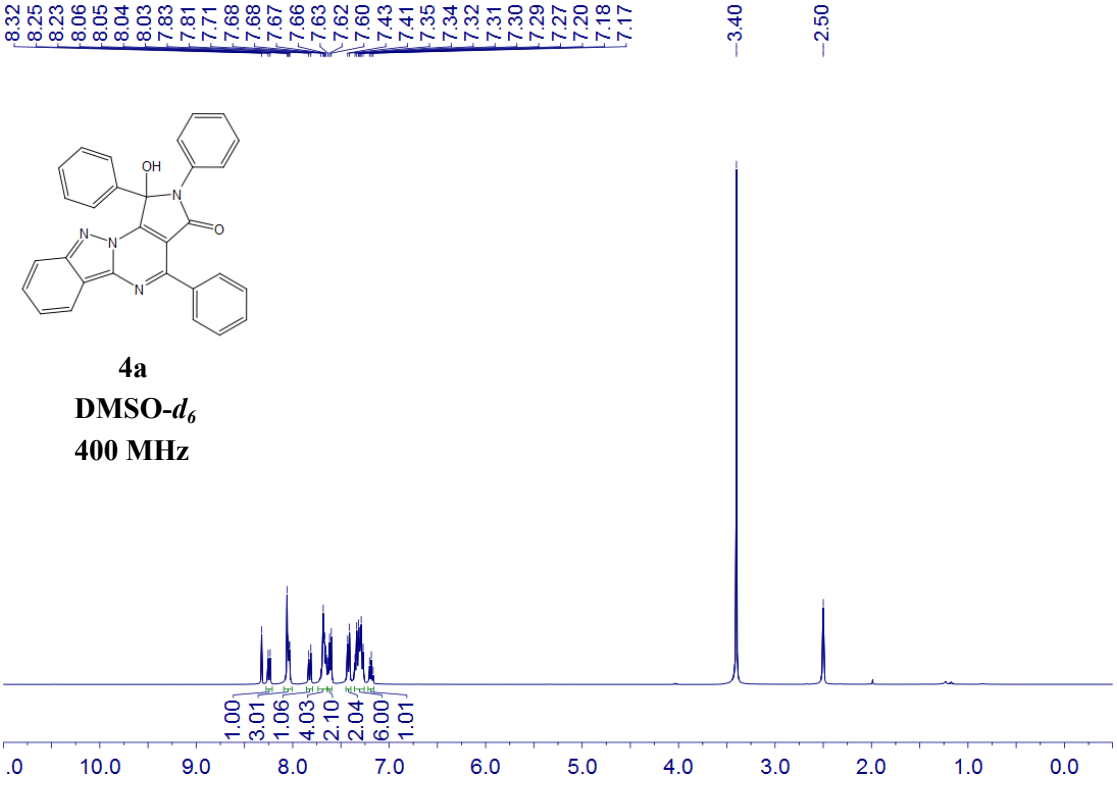
Correction method= # Reported T Limits: Tmin=0.671 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.997          Theta(max)= 24.999

R(reflections)= 0.0702( 3049)                wR2(reflections)=
                                             0.1845( 4899)
S = 1.040                 Npar= 387
```

8.^{1}H, ^{13}C and ^{19}F NMR spectra of compounds

4a



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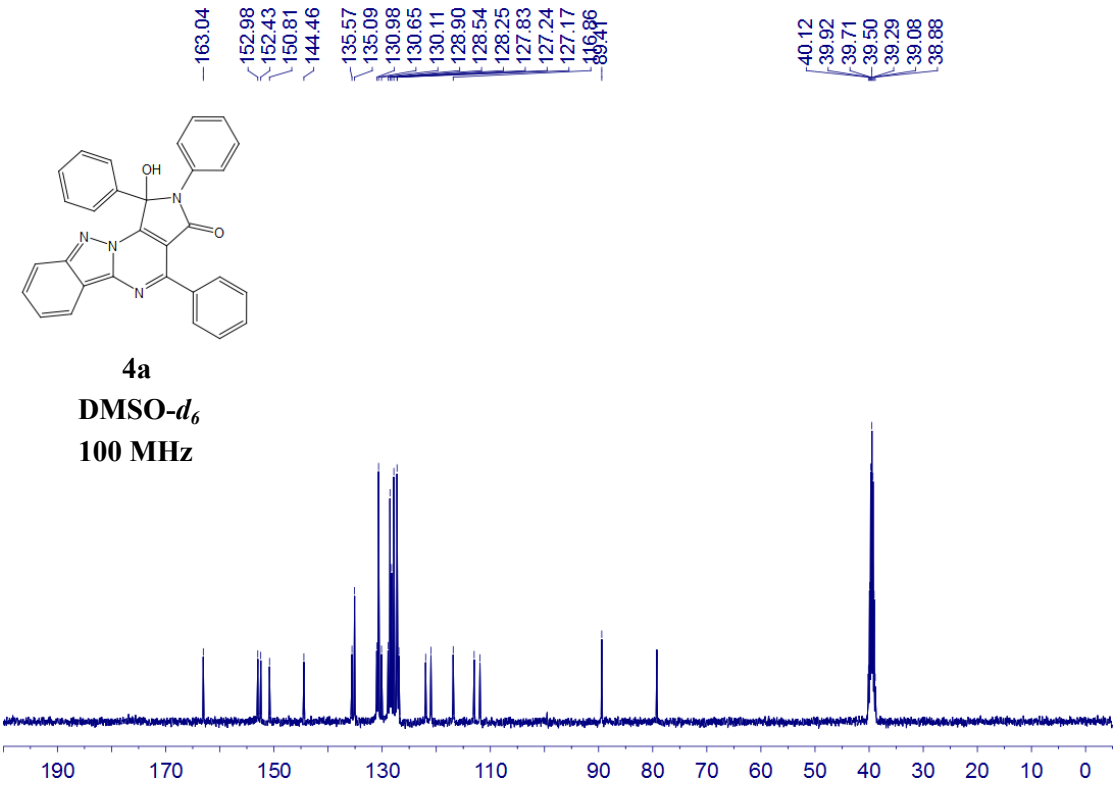

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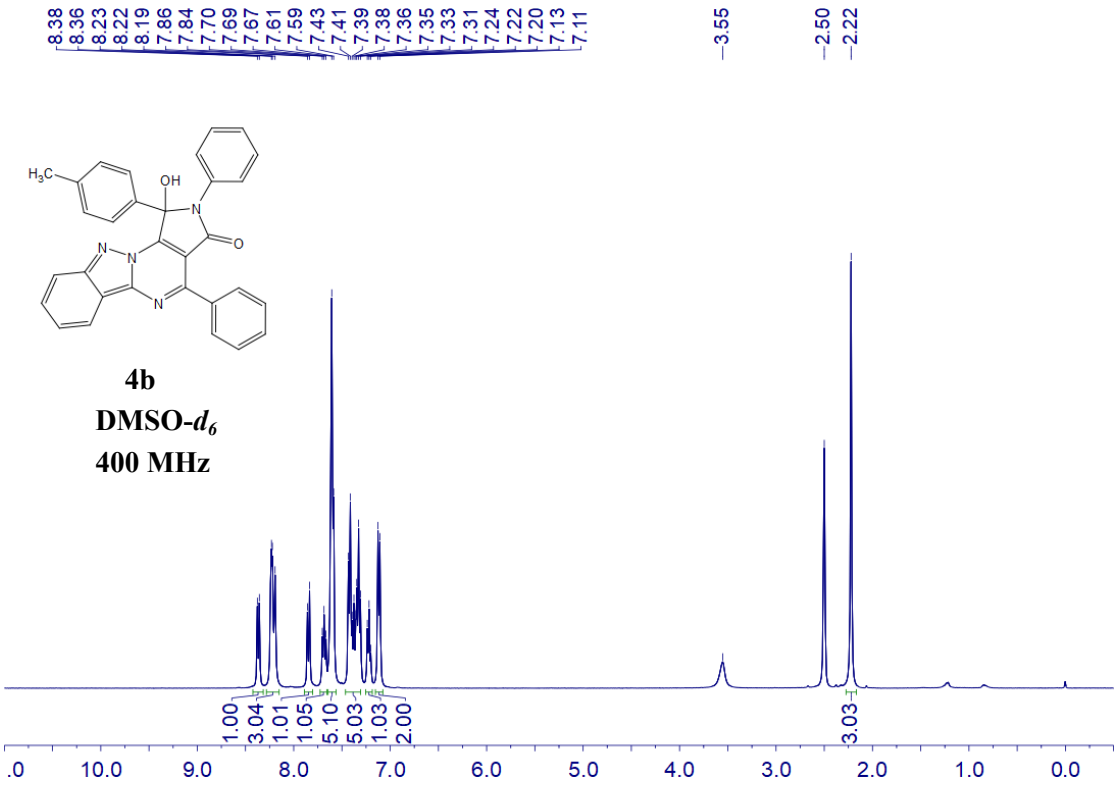
4b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H3C
OH
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O
N
N
N
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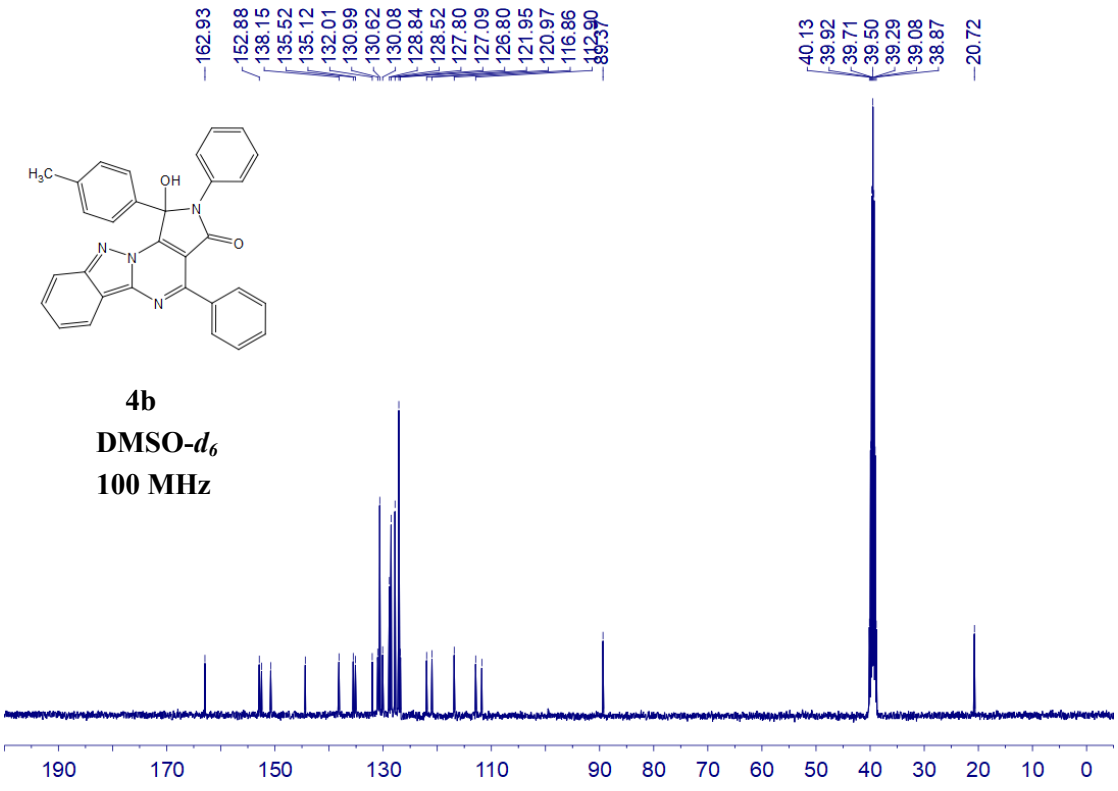
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N
4b
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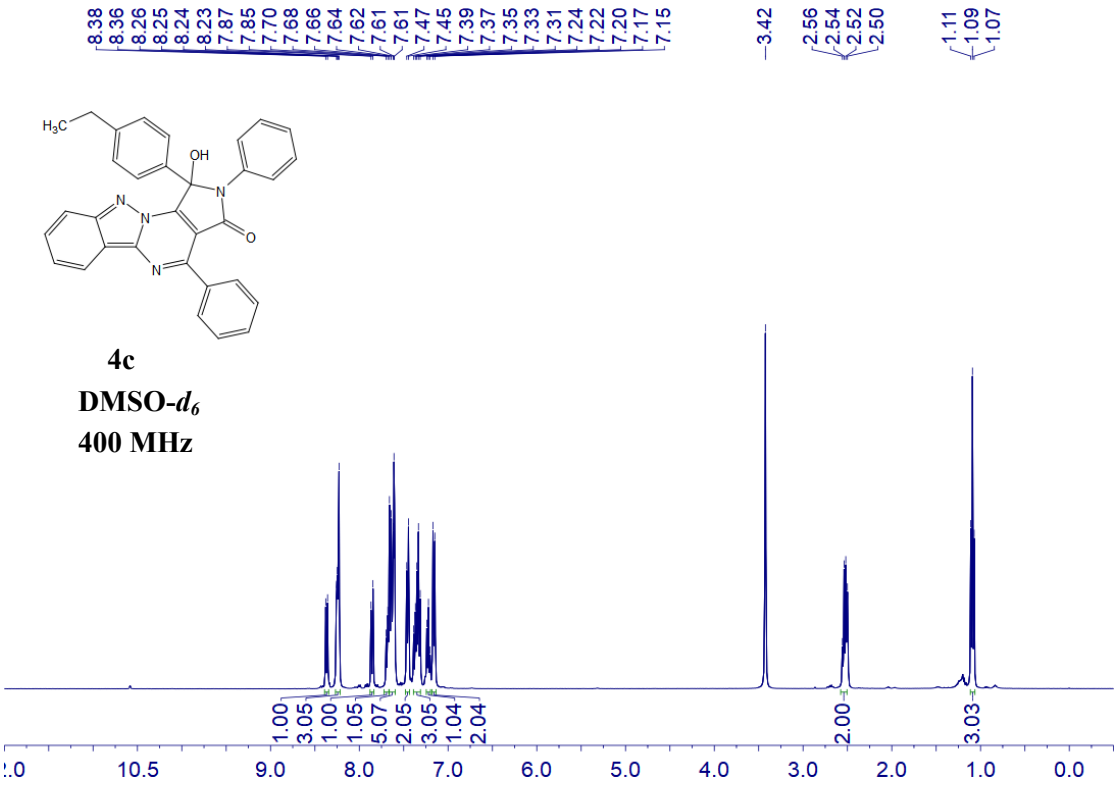
4c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4c
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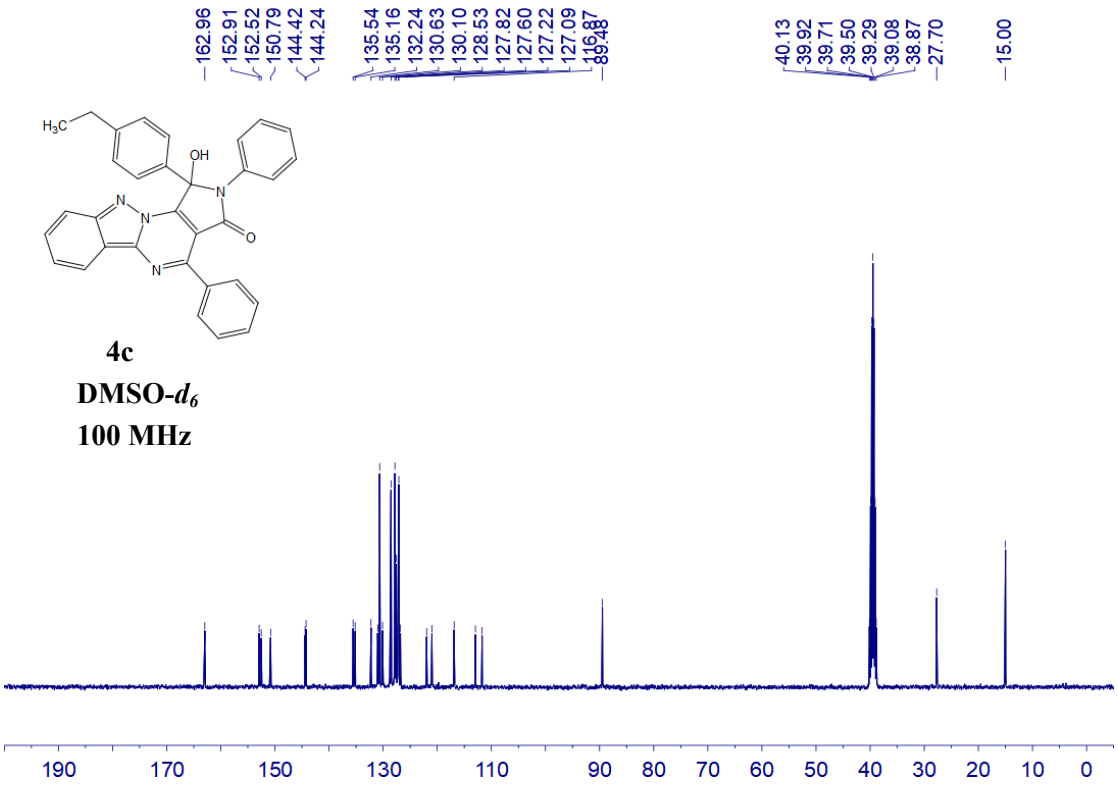
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N
O
N
4c
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10
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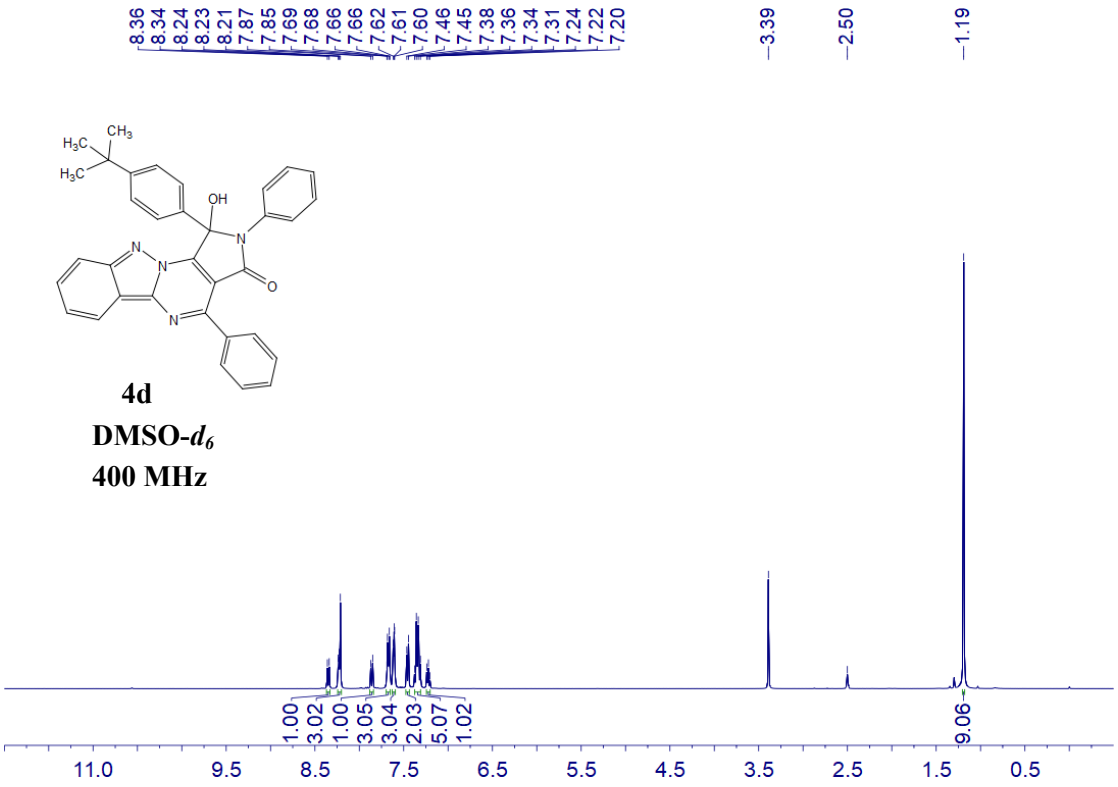
4d



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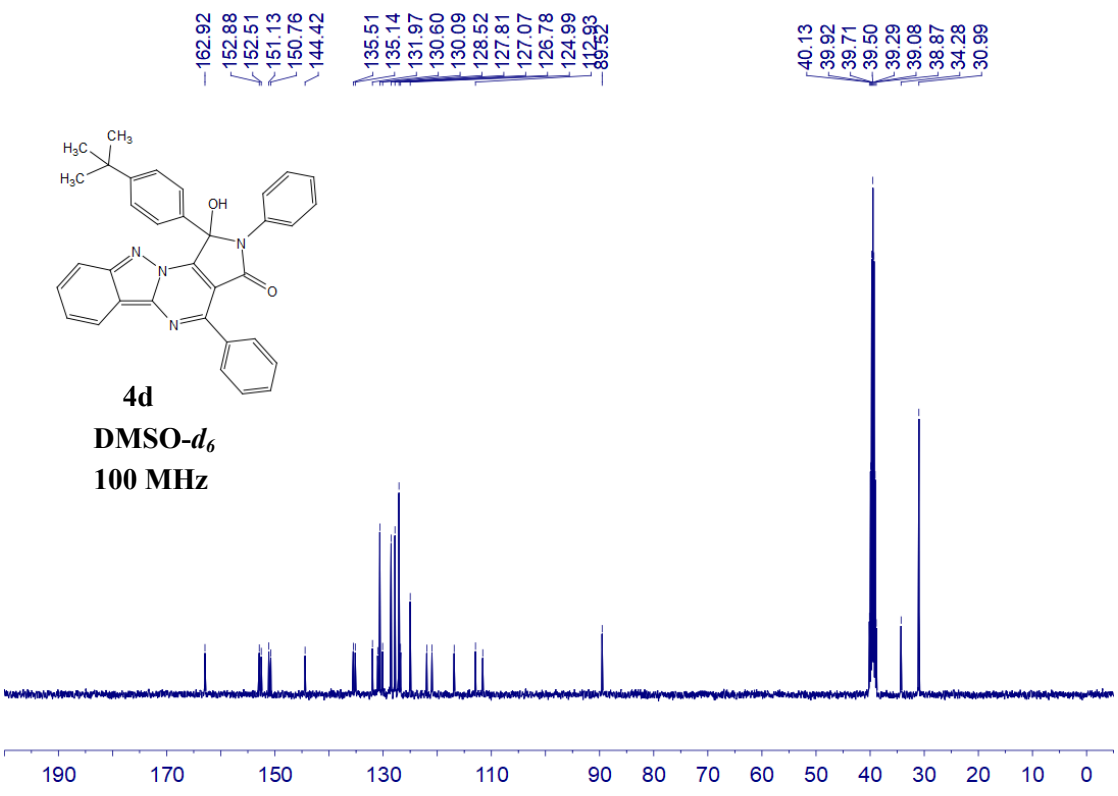

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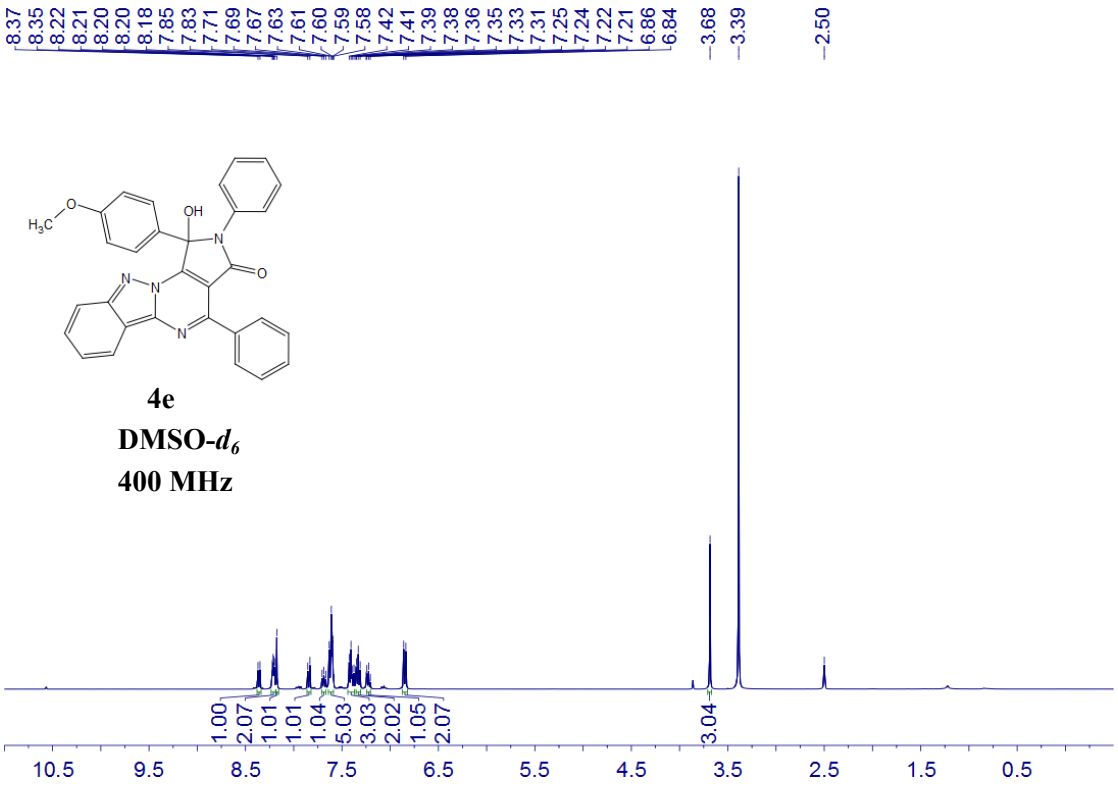

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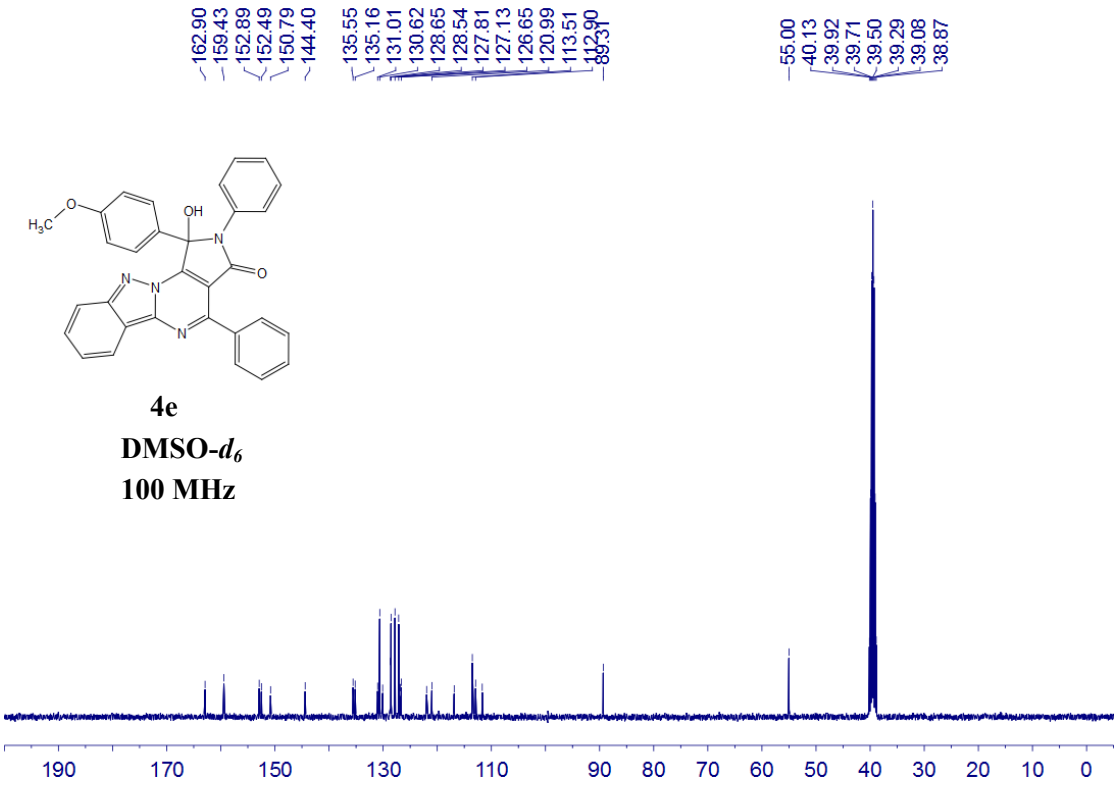

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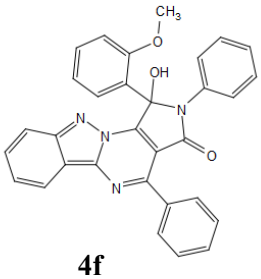

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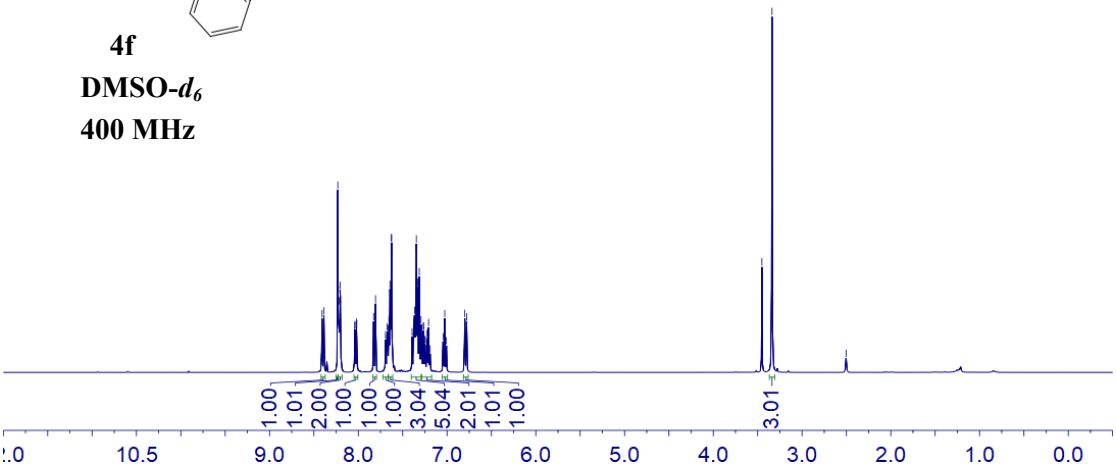

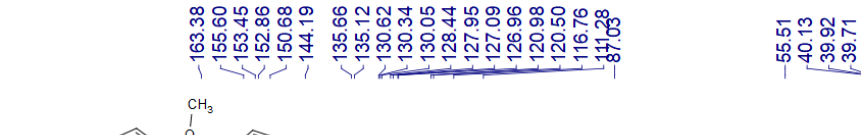

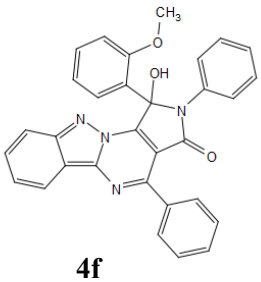

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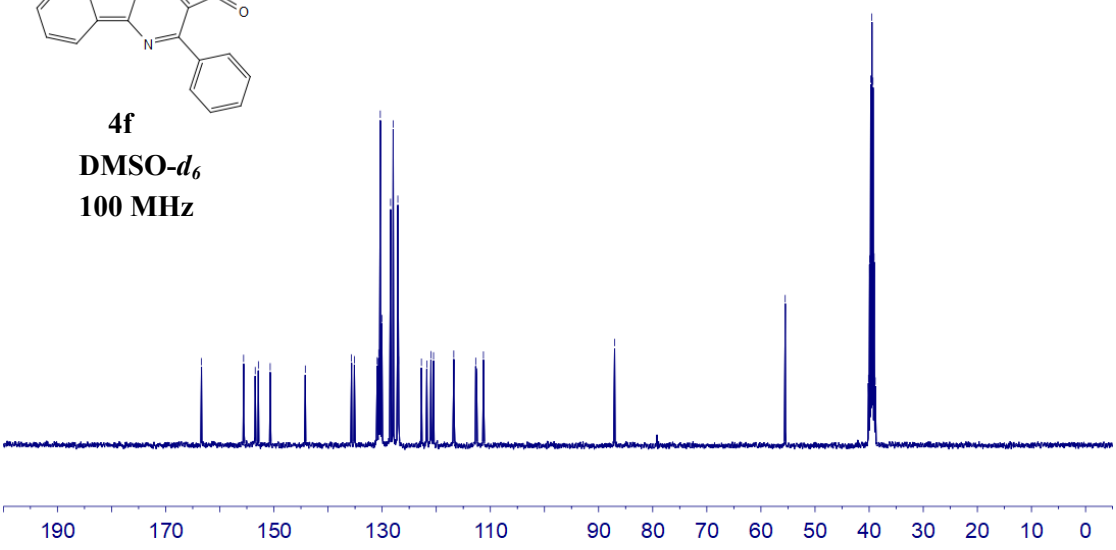

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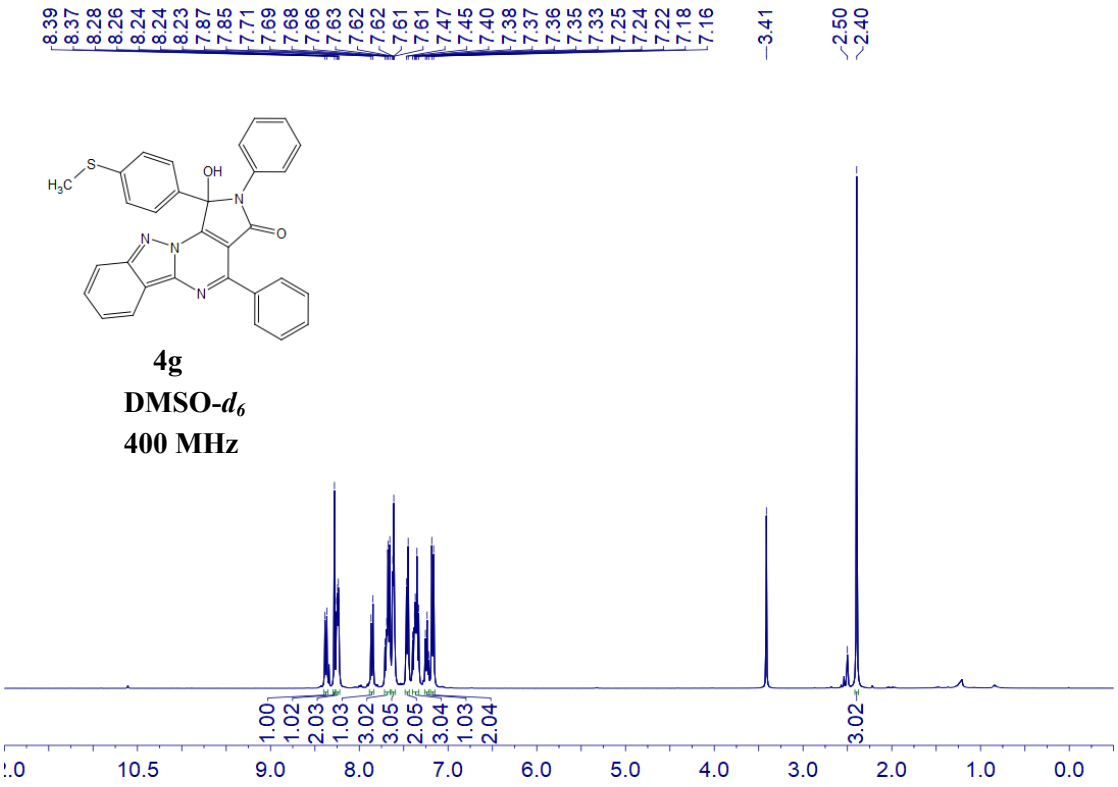

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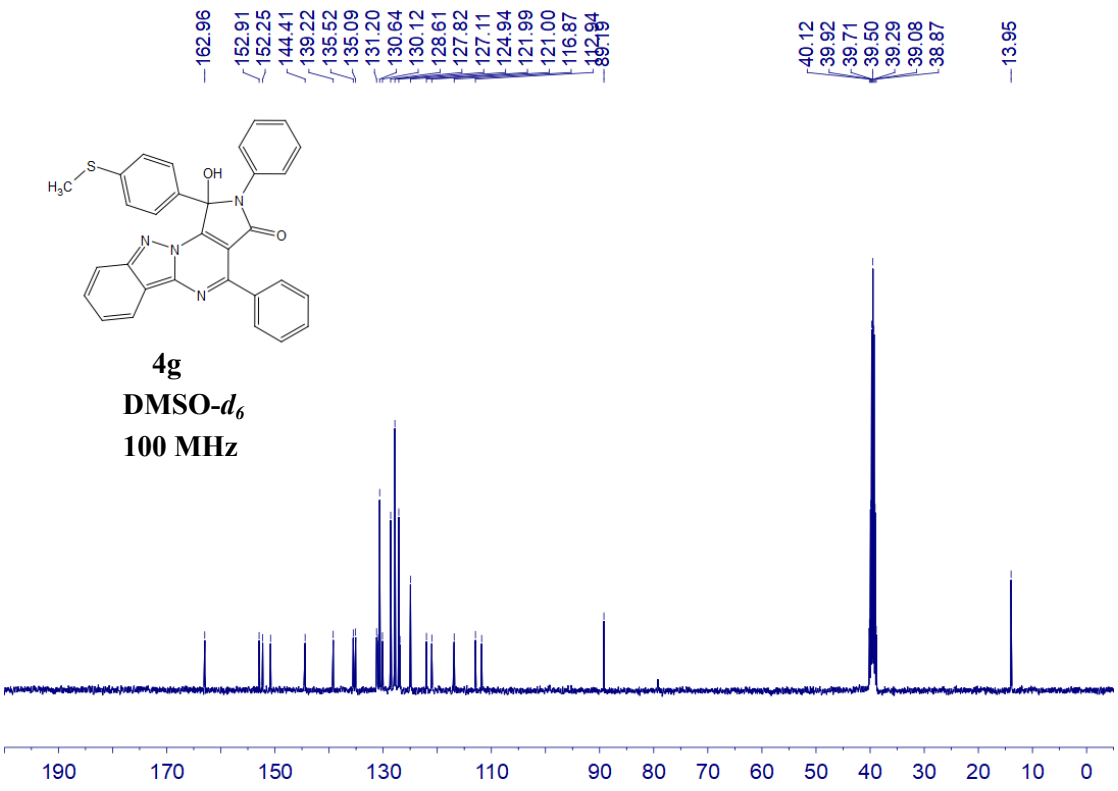

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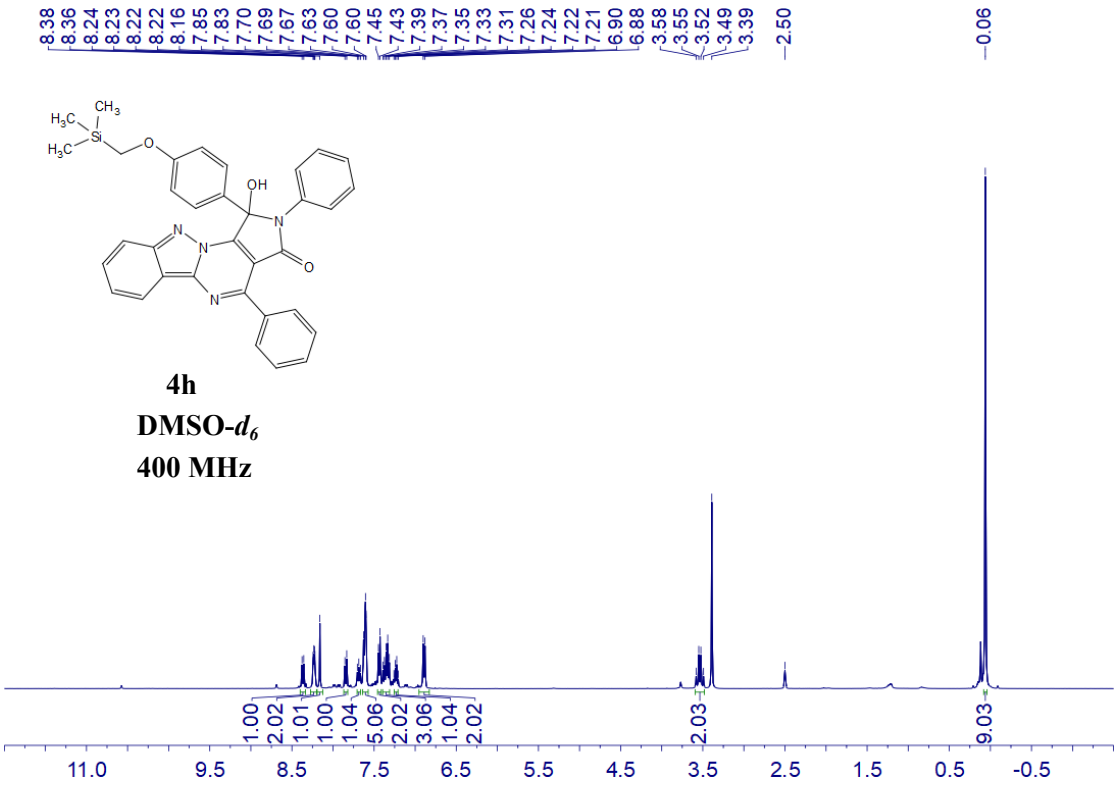

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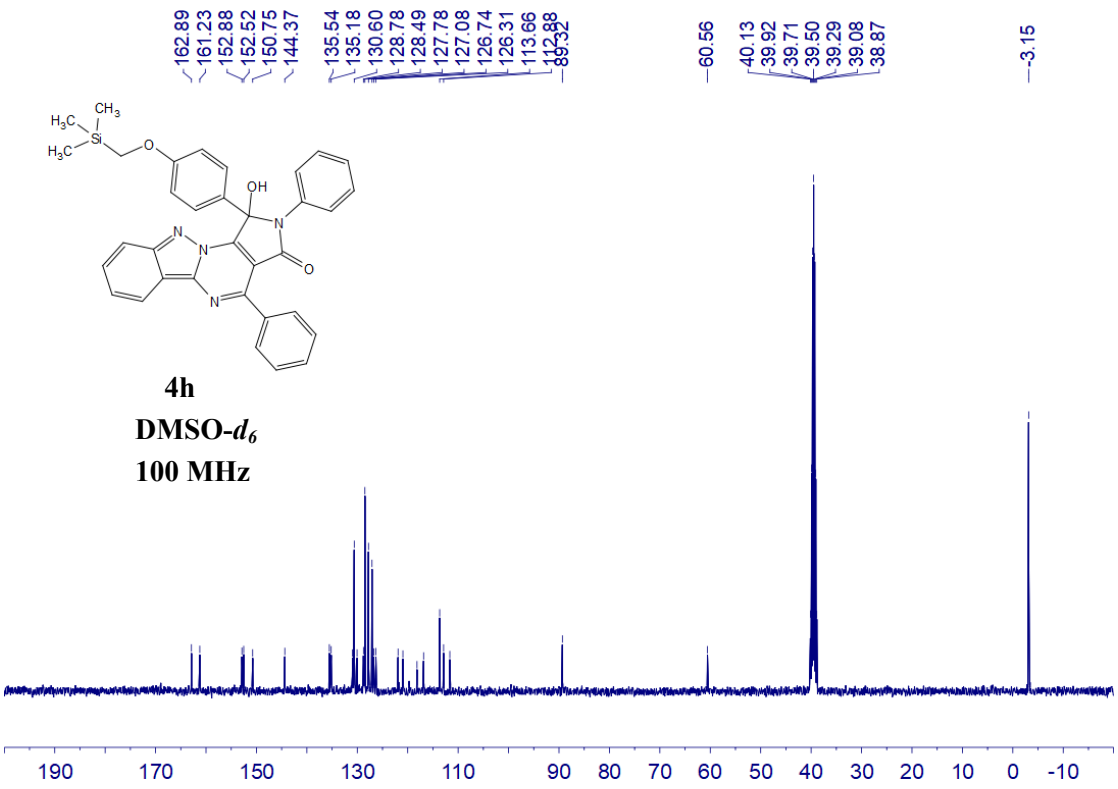

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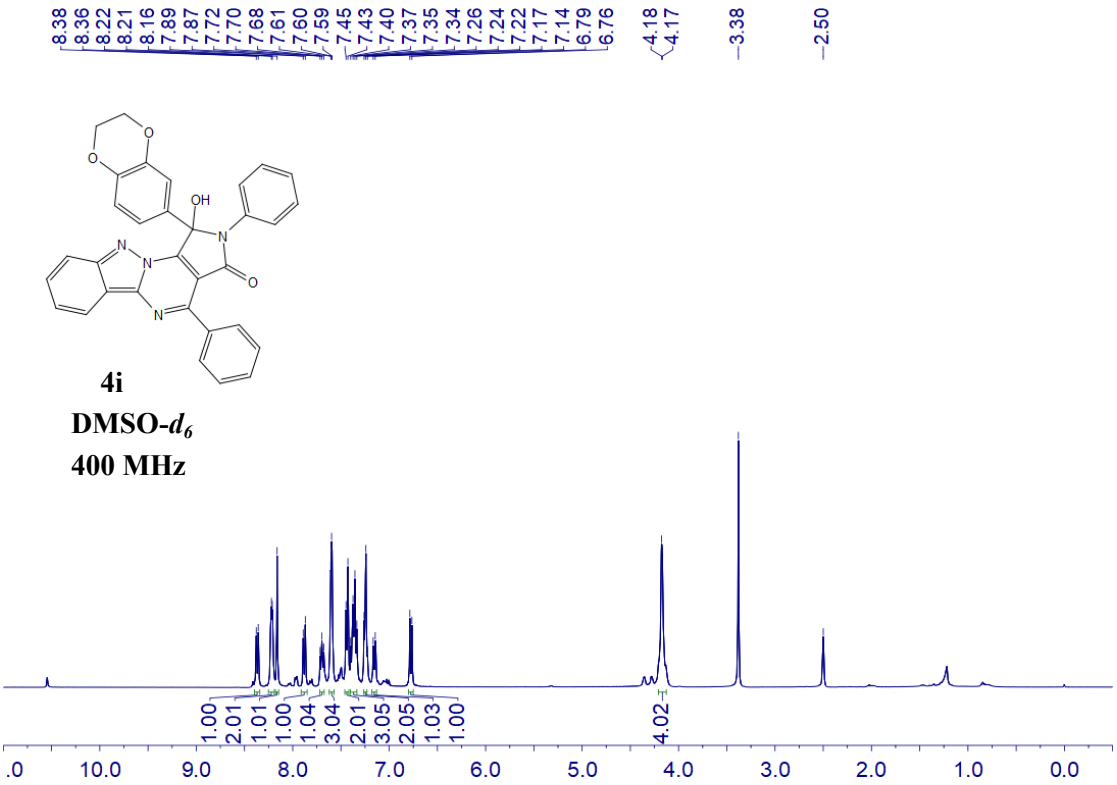
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O
O
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N
N
4i
DMSO-d_6
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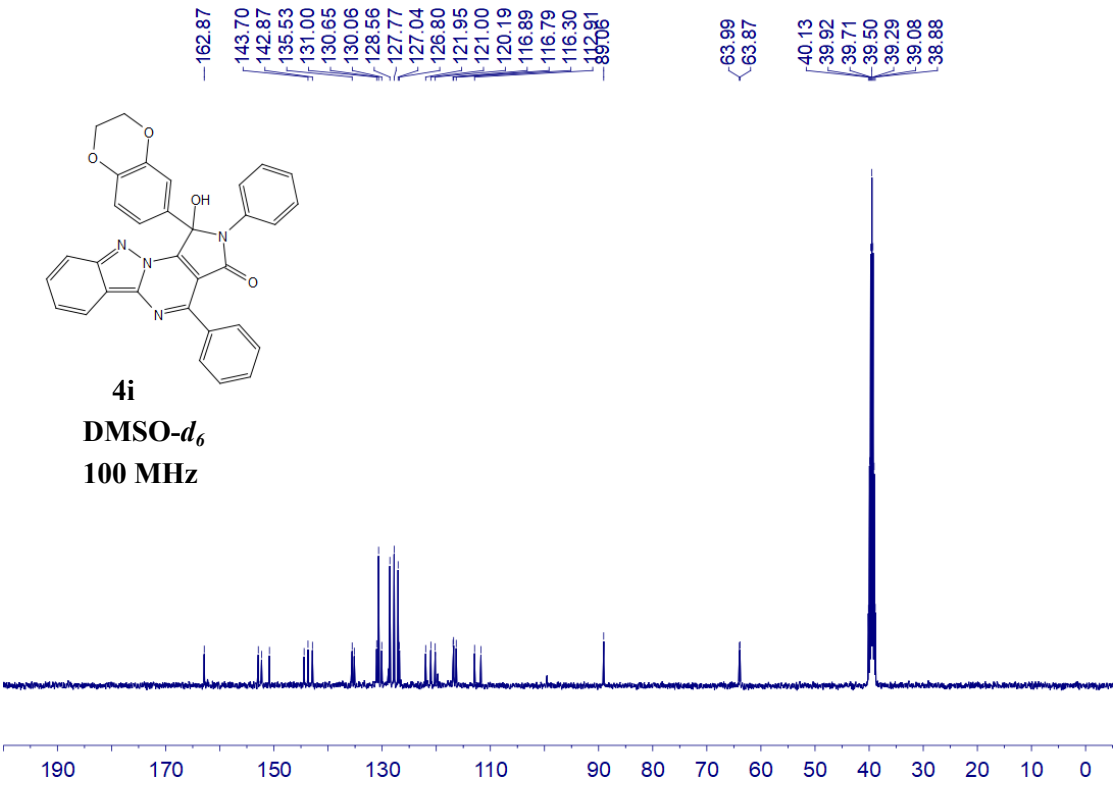
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4i
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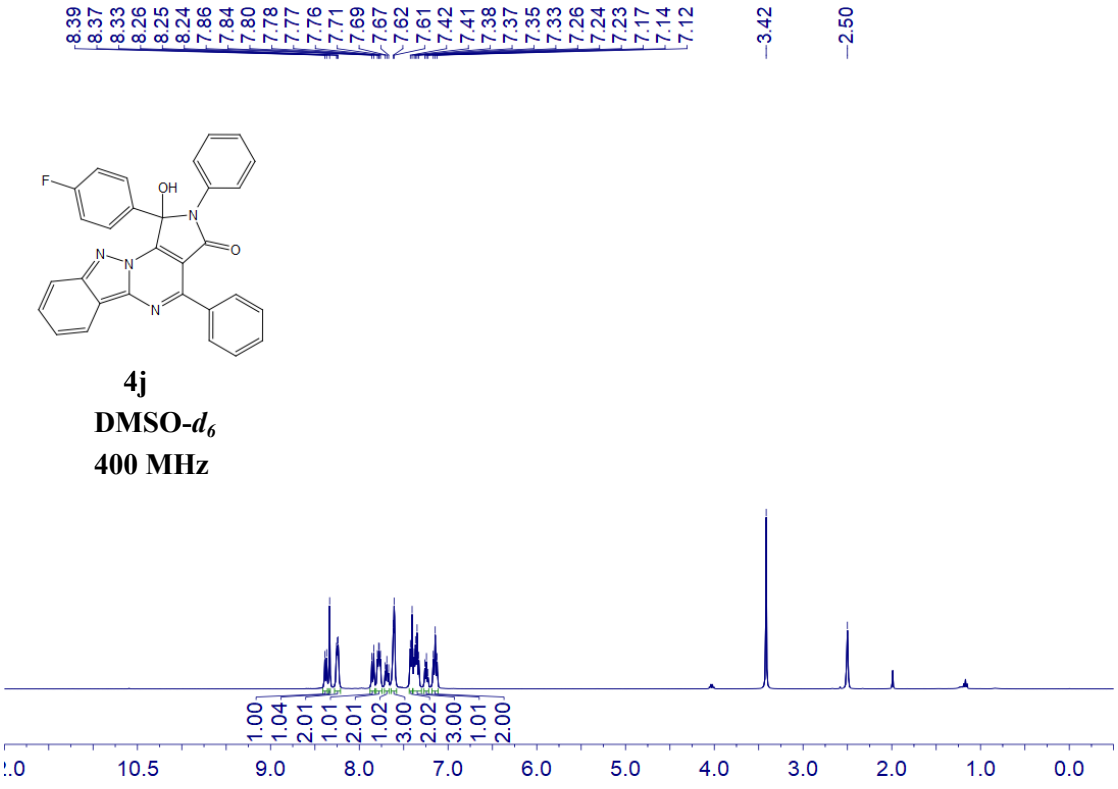
4j



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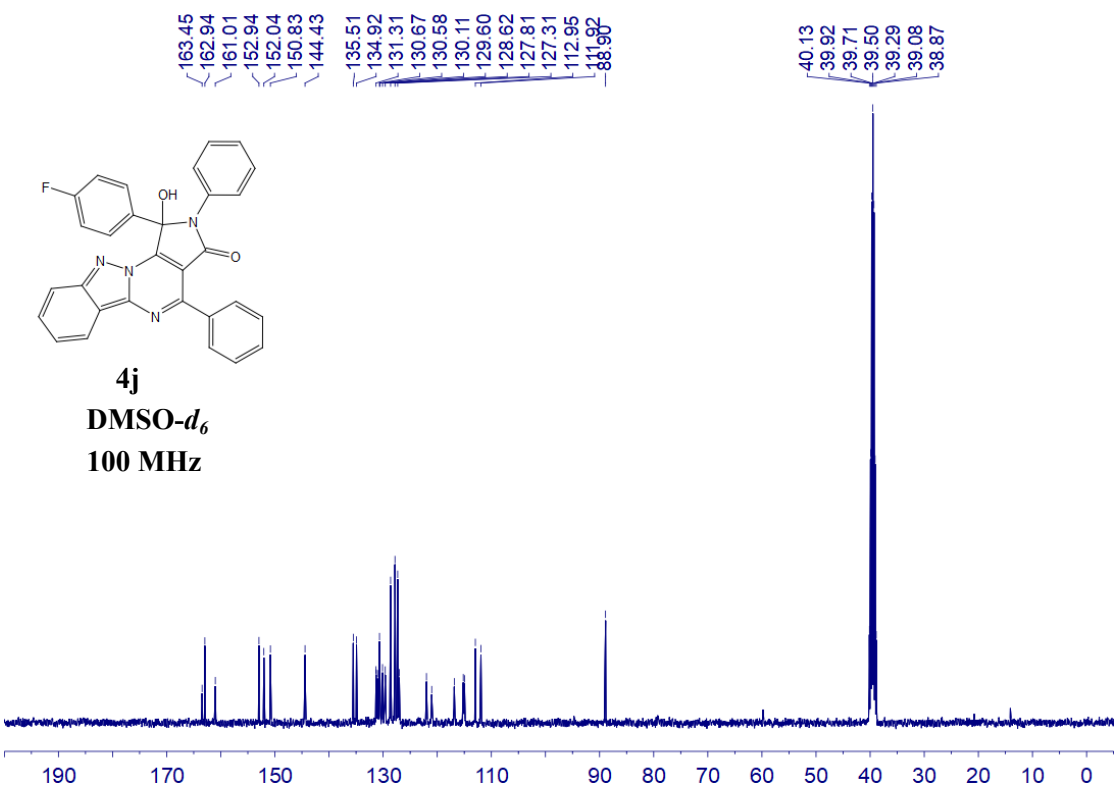

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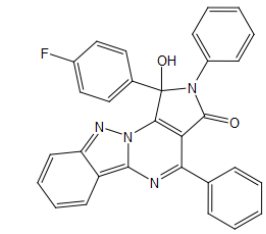

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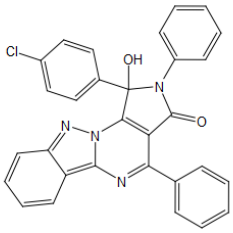
4k



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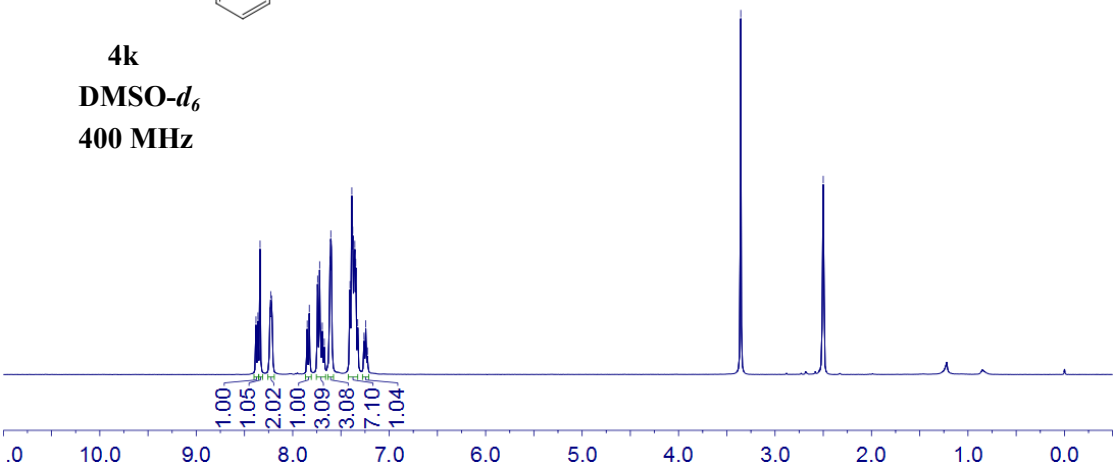

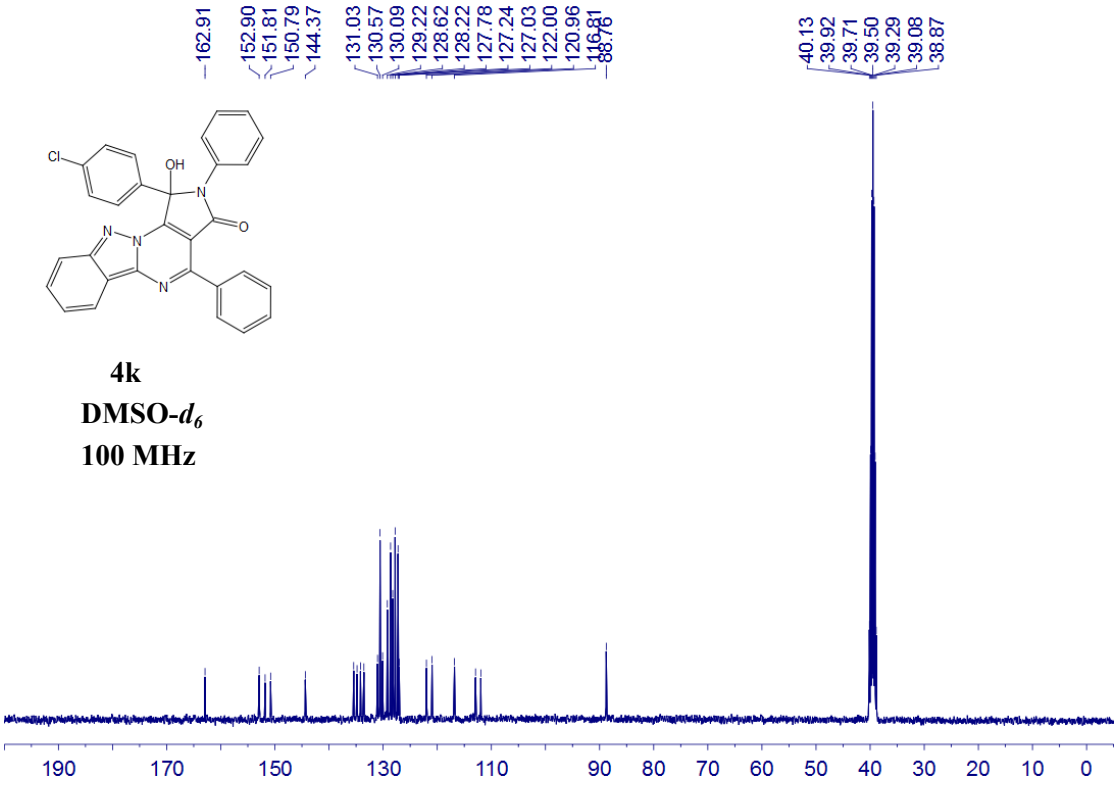

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DMSO-d_6

100 MHz

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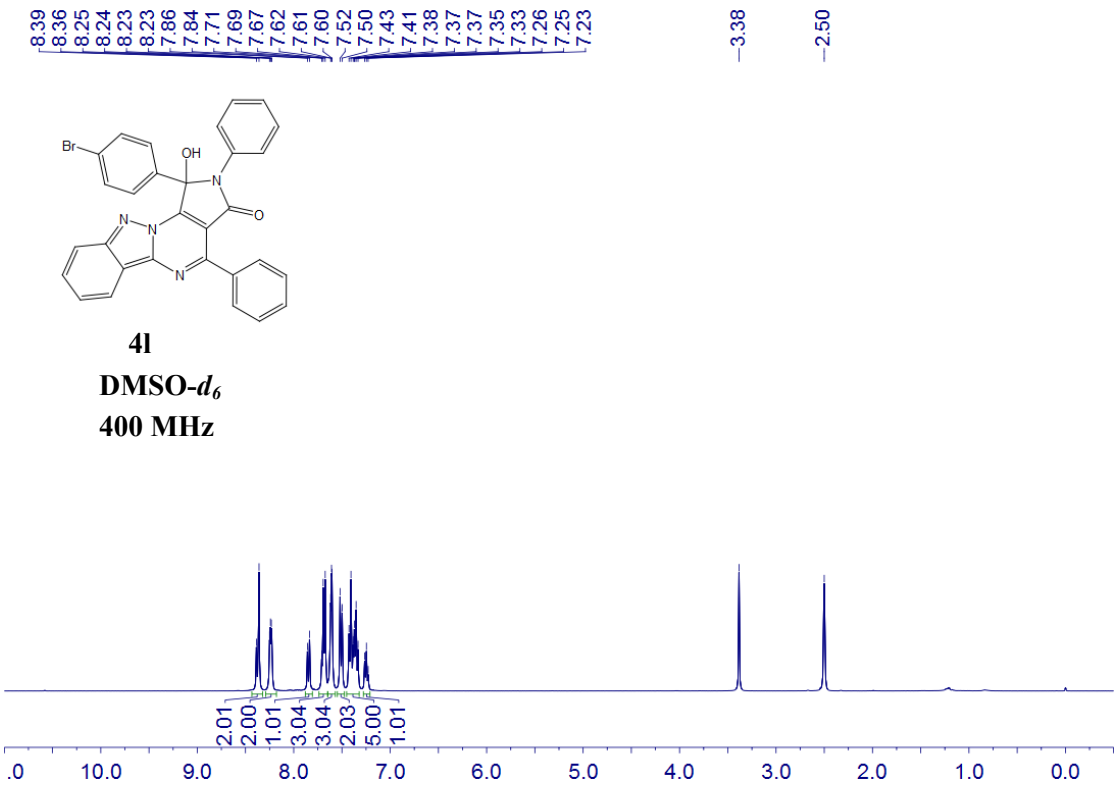

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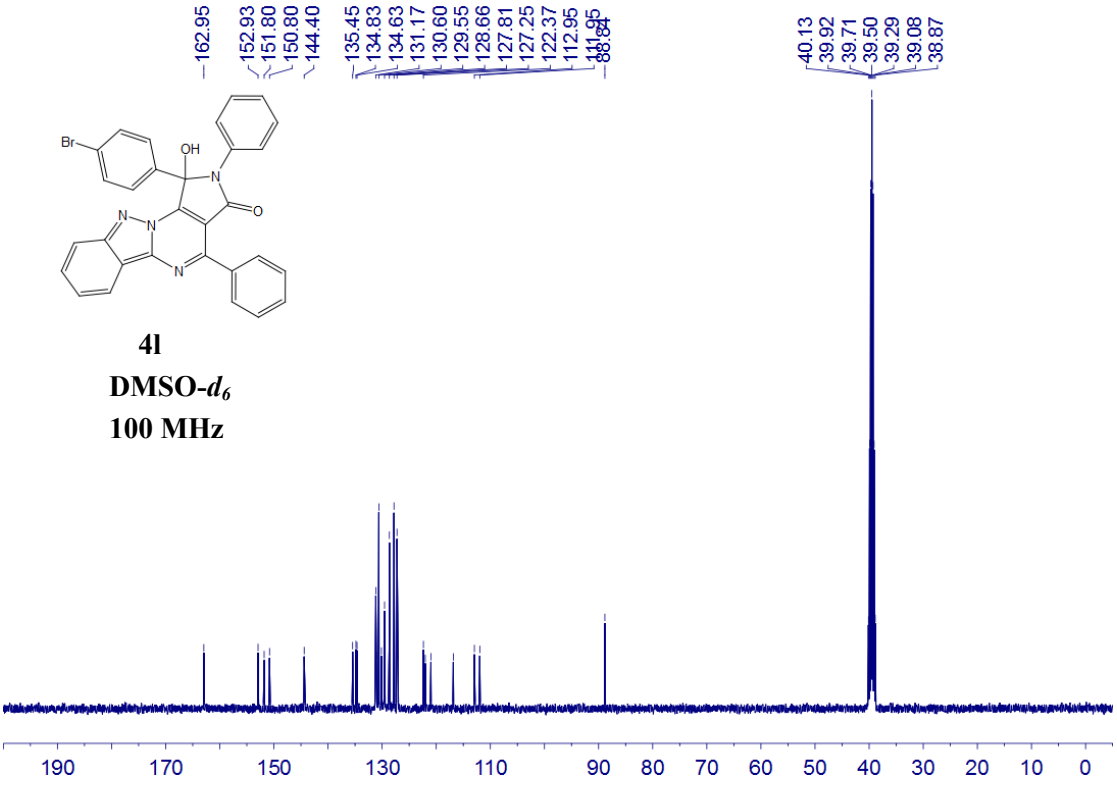

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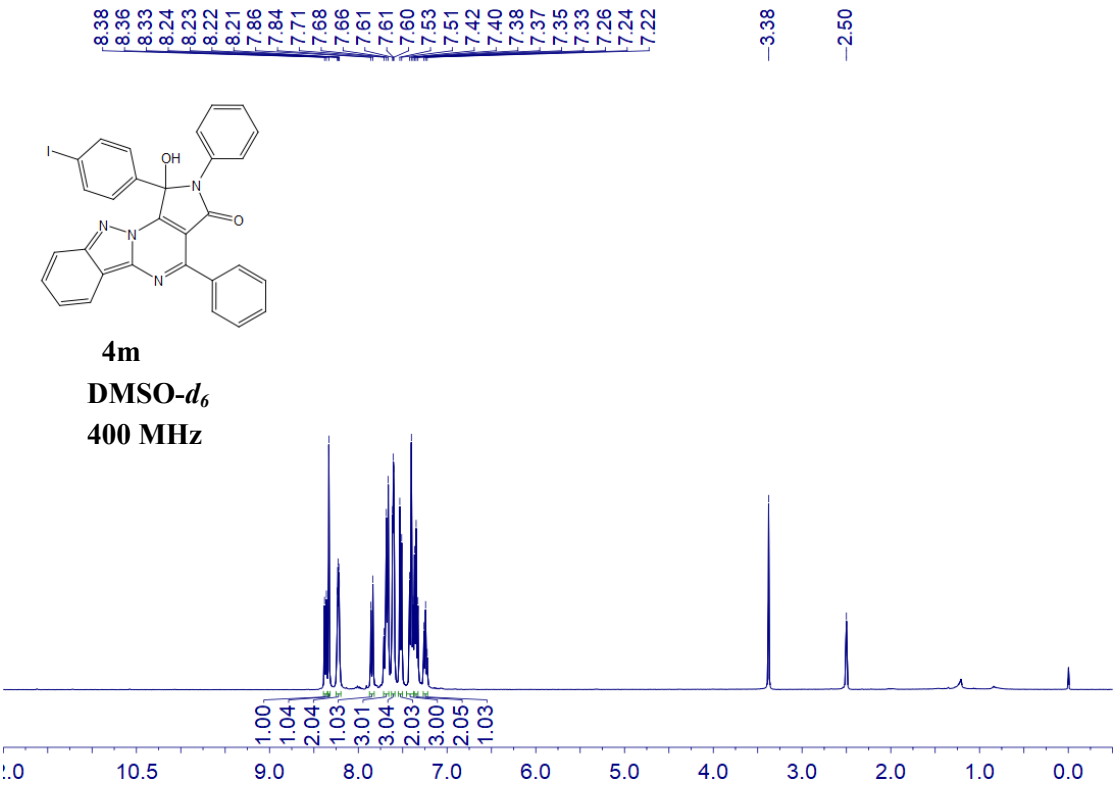

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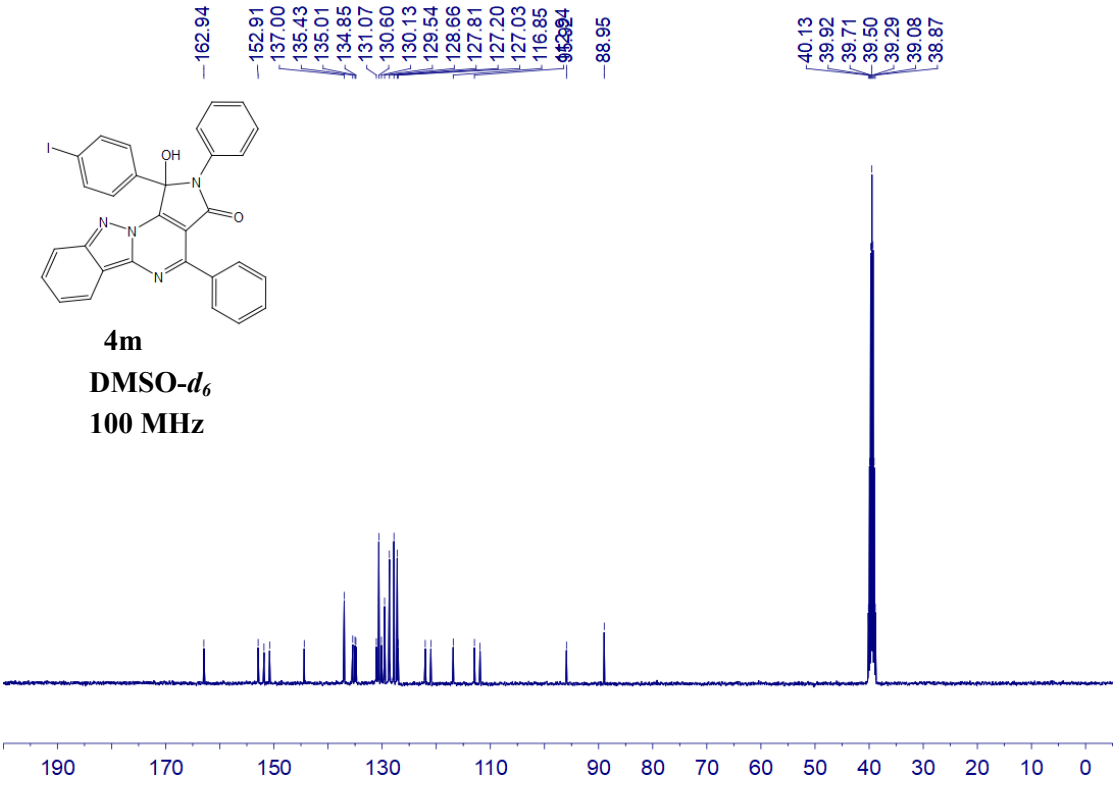

4m

DMSO-d_6

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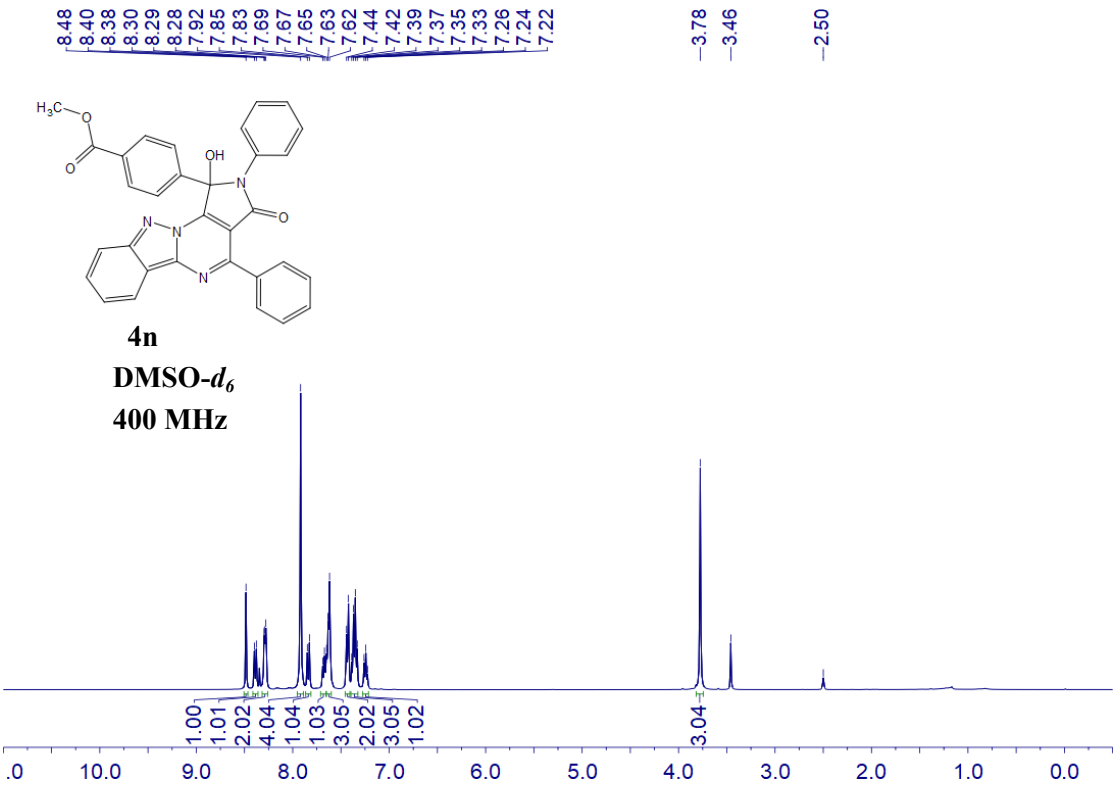

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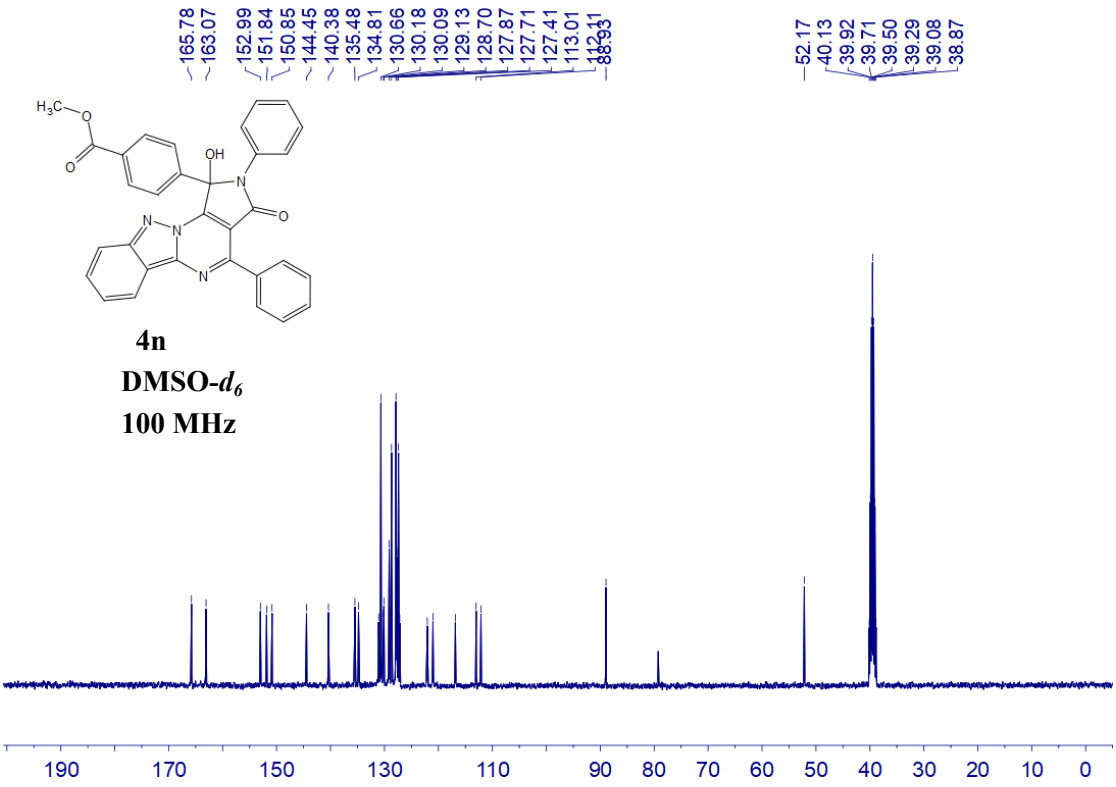

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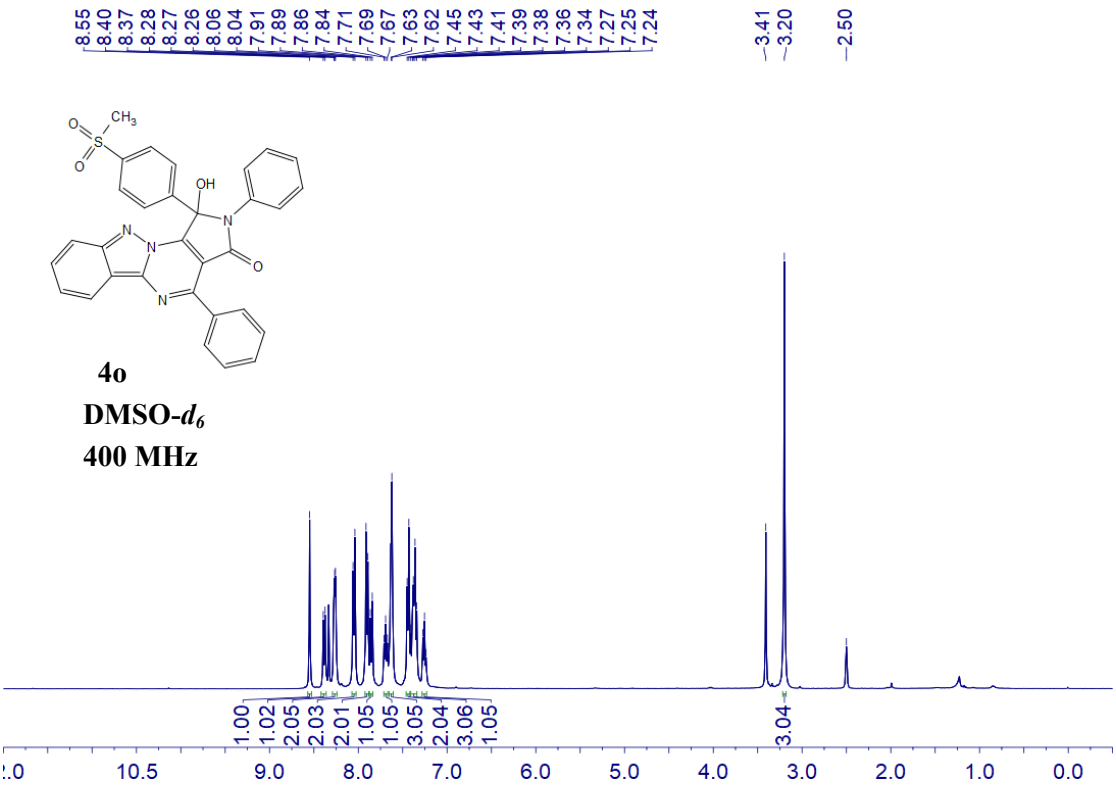
100 MHz

4o



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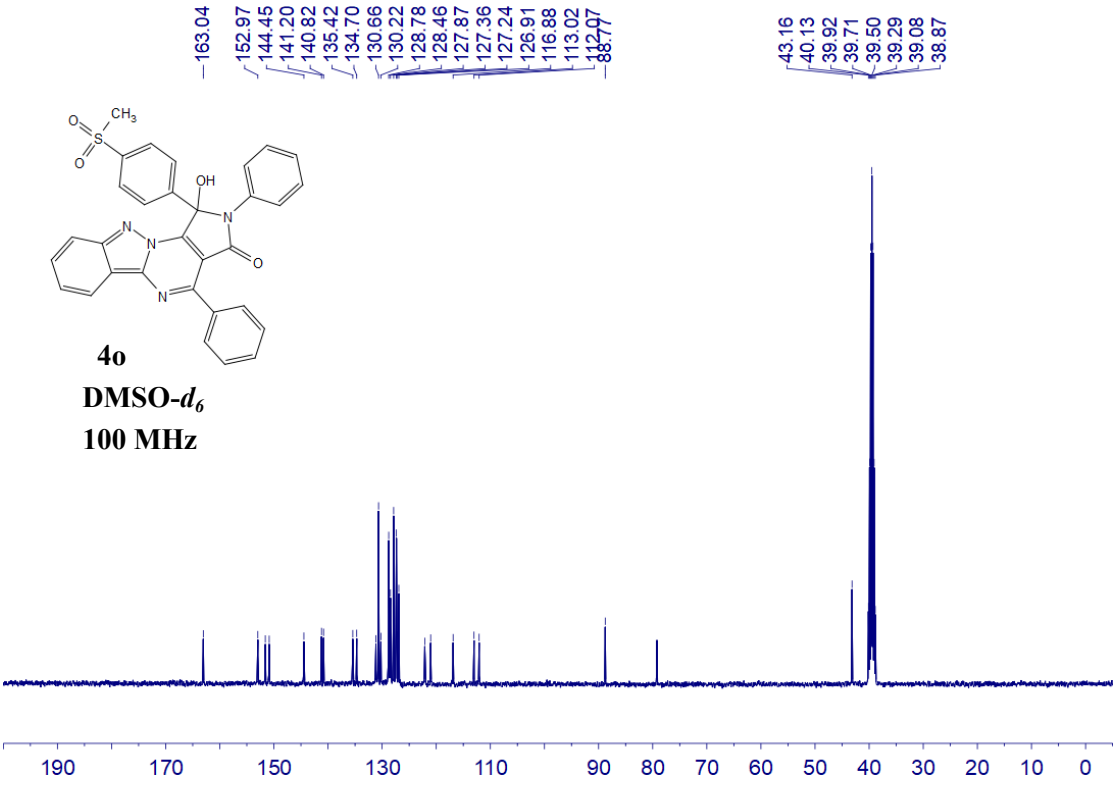
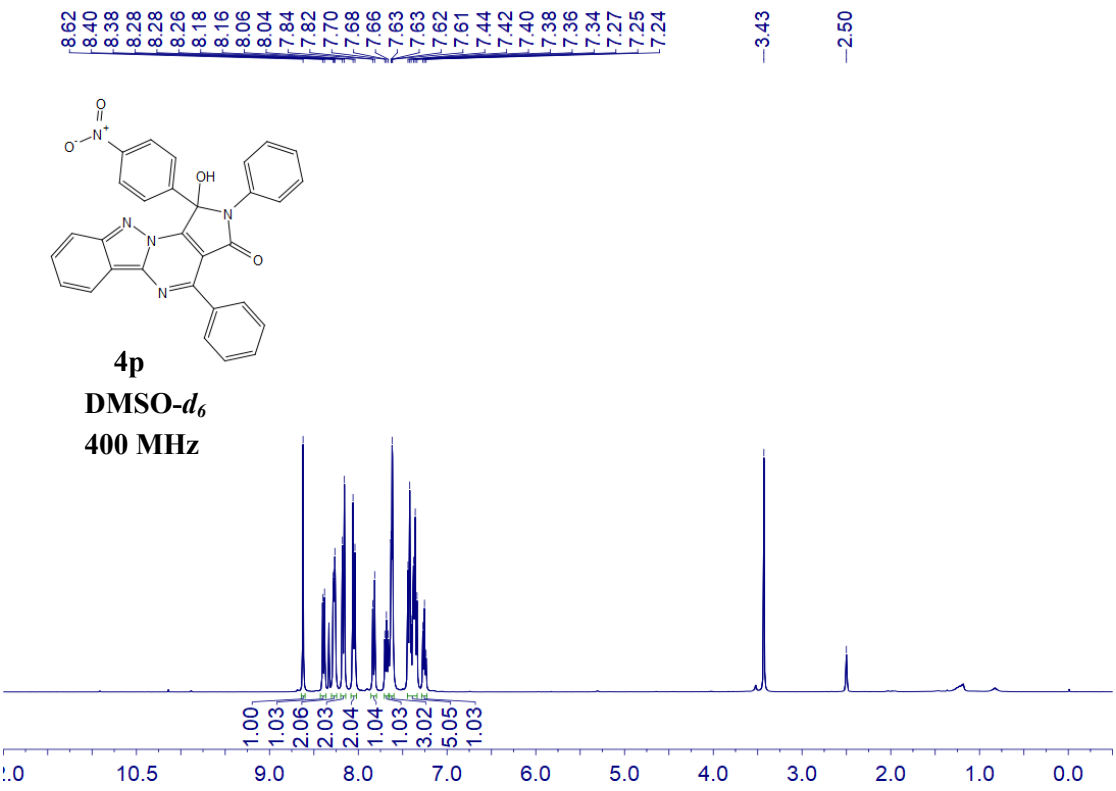


4o

DMSO-d_6

100 MHz

4p



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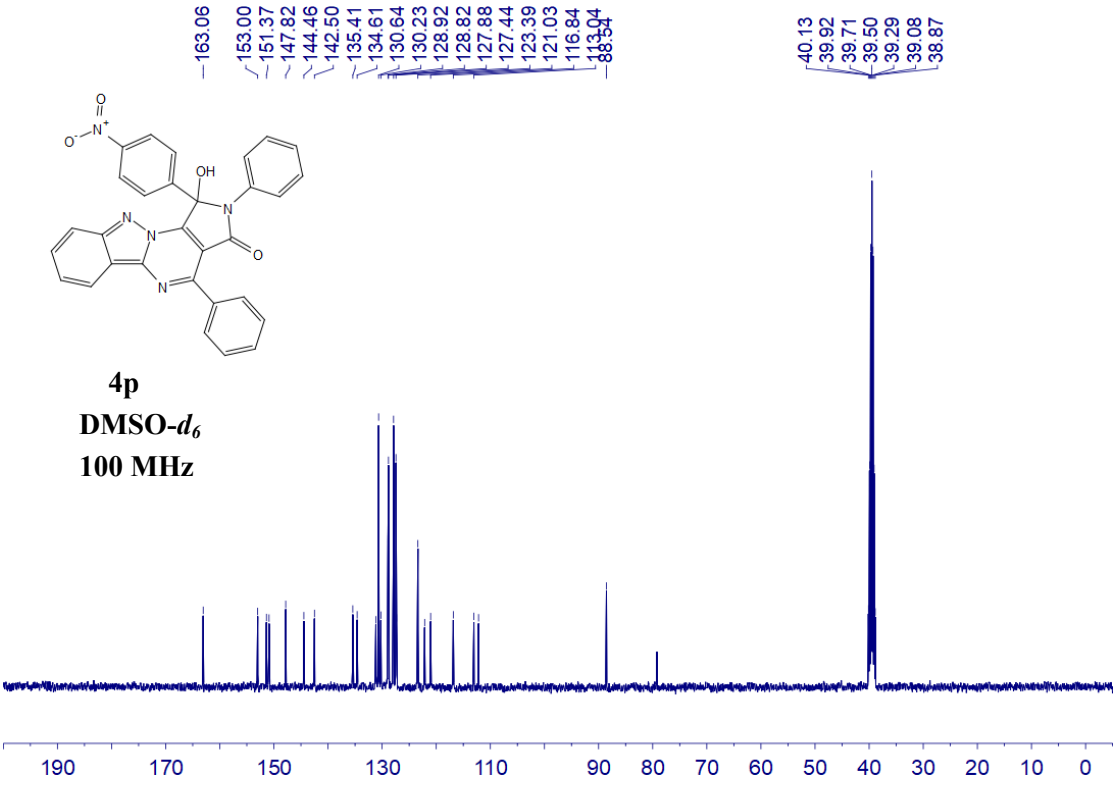

4p

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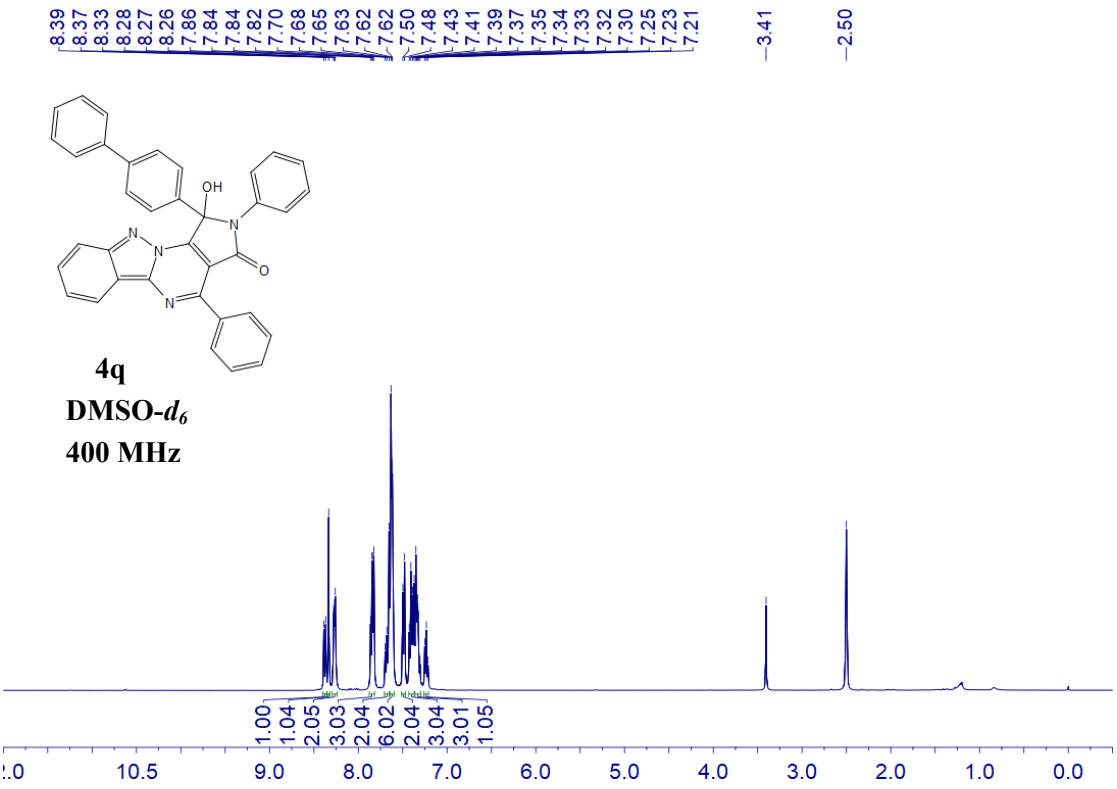
100 MHz

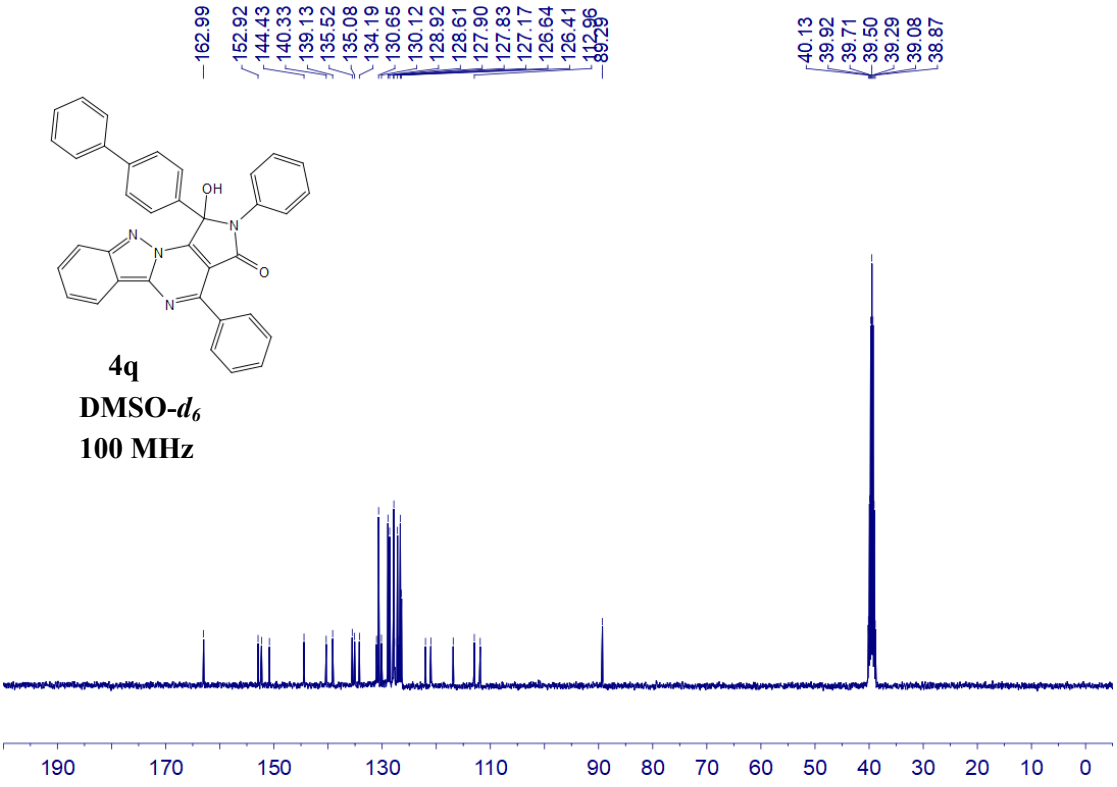
4q



4q

DMSO-d_6

400 MHz

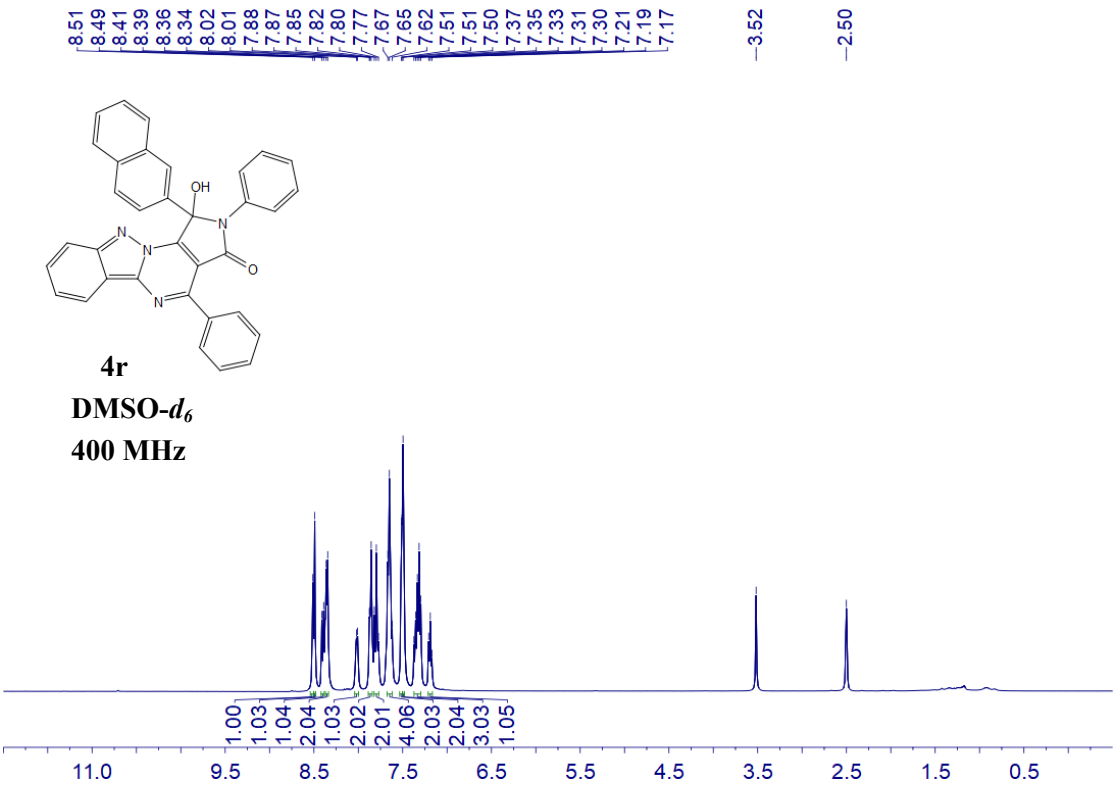


4q

DMSO-d_6

100 MHz

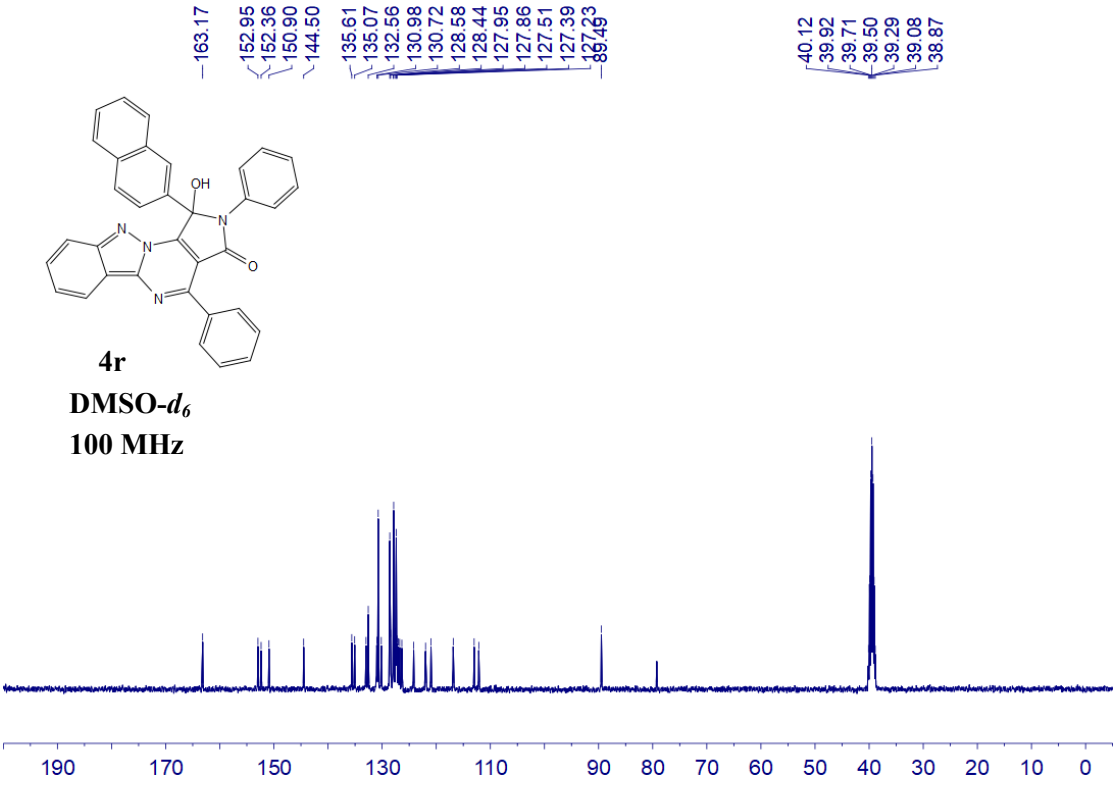
4r



4r

DMSO-d_6

400 MHz

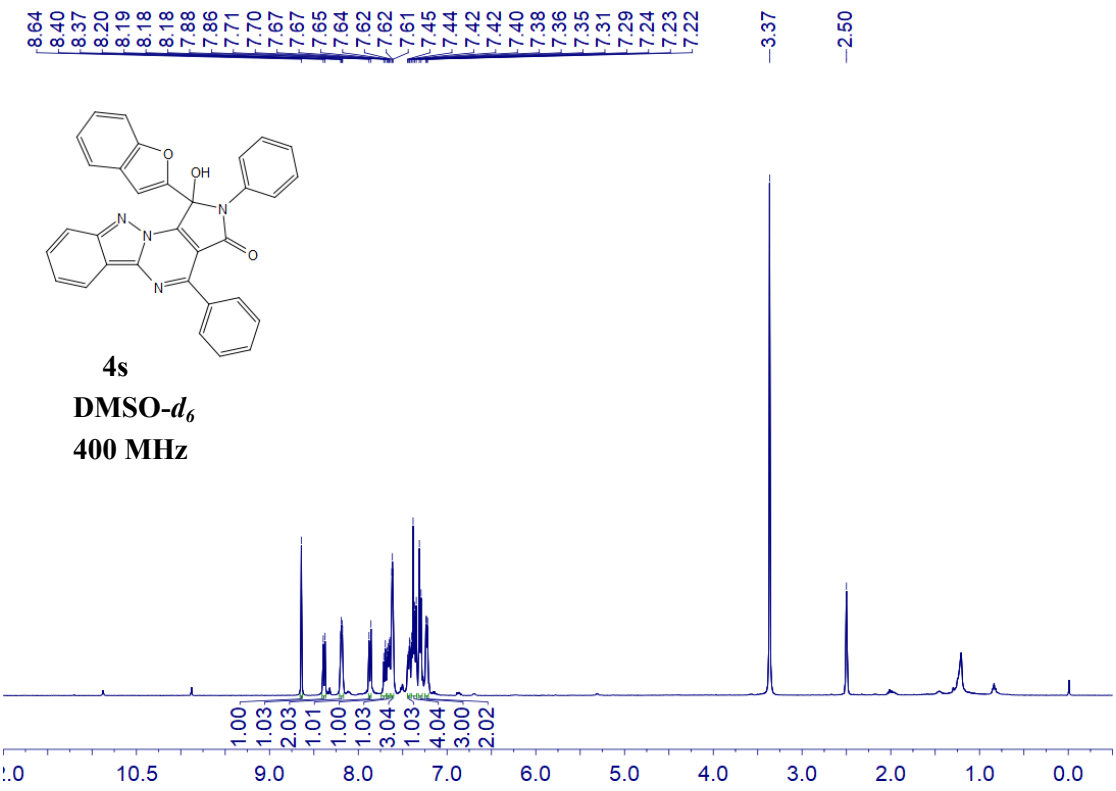


4r

DMSO-d_6

100 MHz

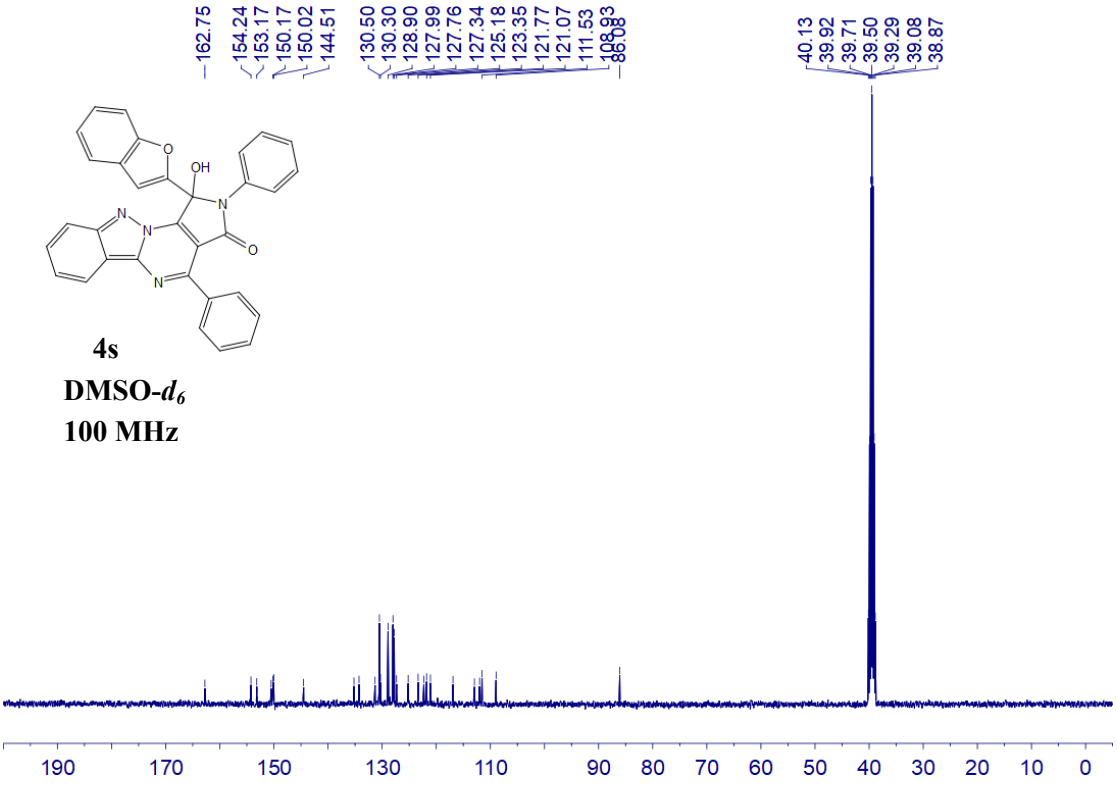
4s



4s

DMSO-d_6

400 MHz

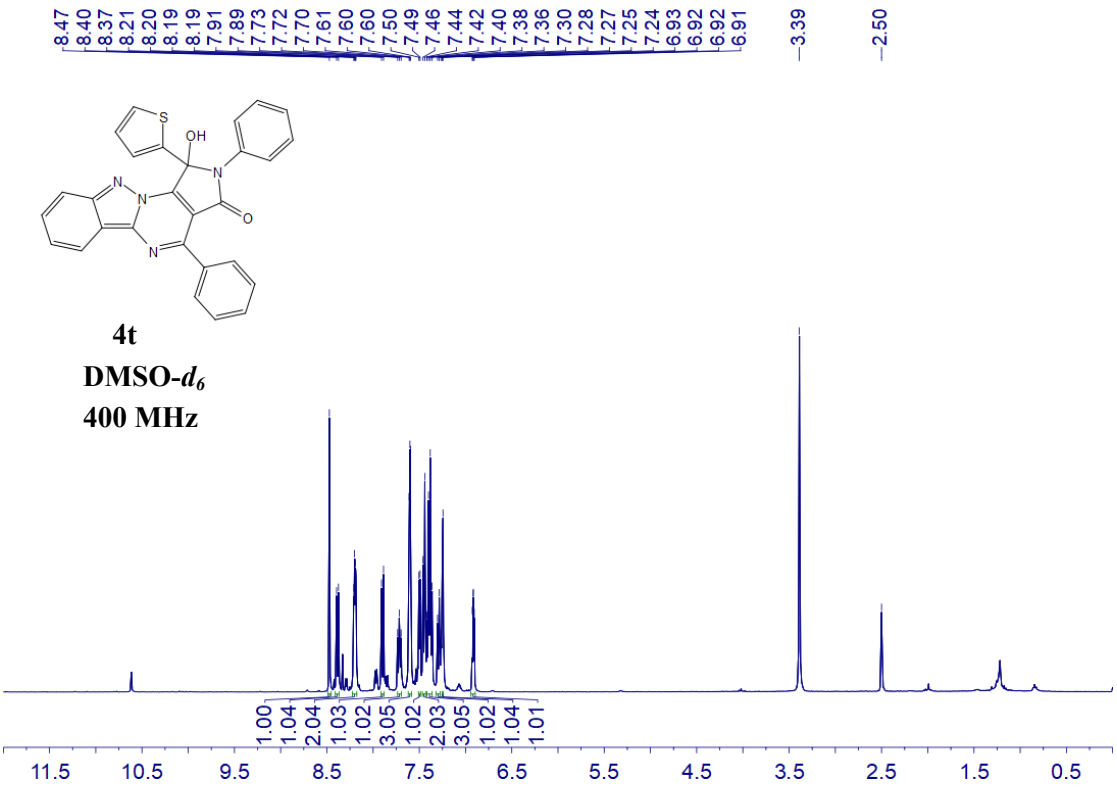


4s

DMSO-d_6

100 MHz

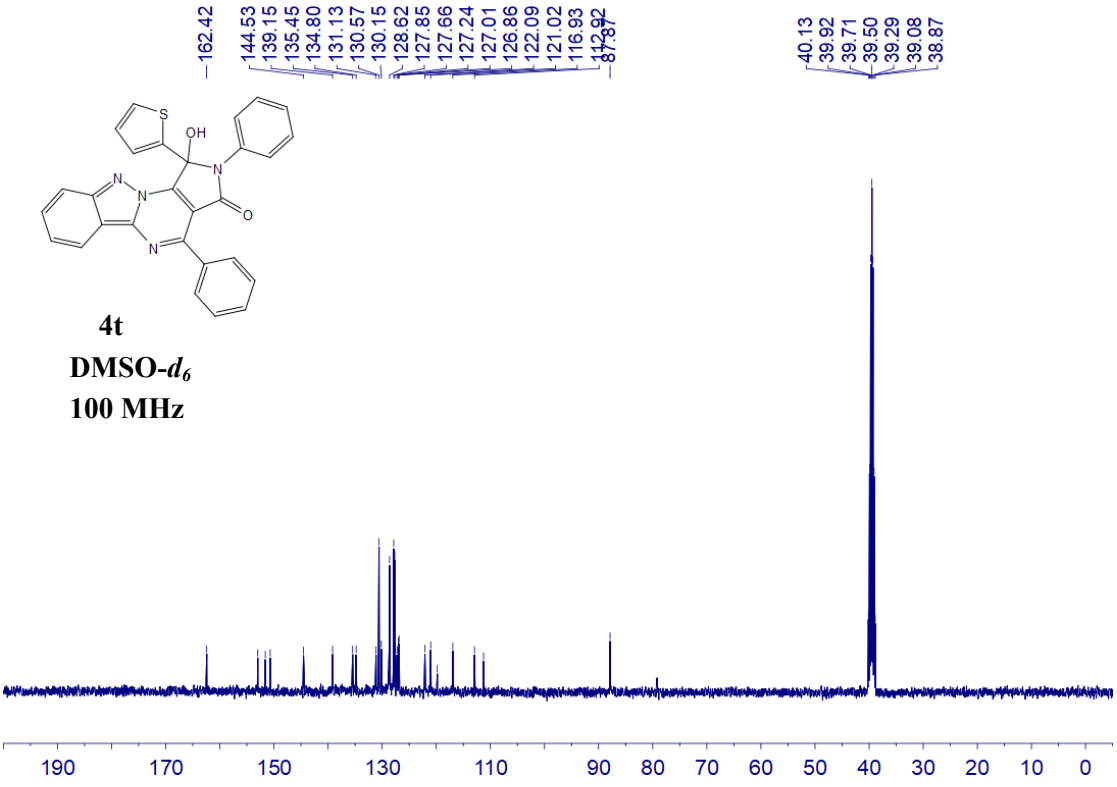
4t



4t

DMSO-d_6

400 MHz

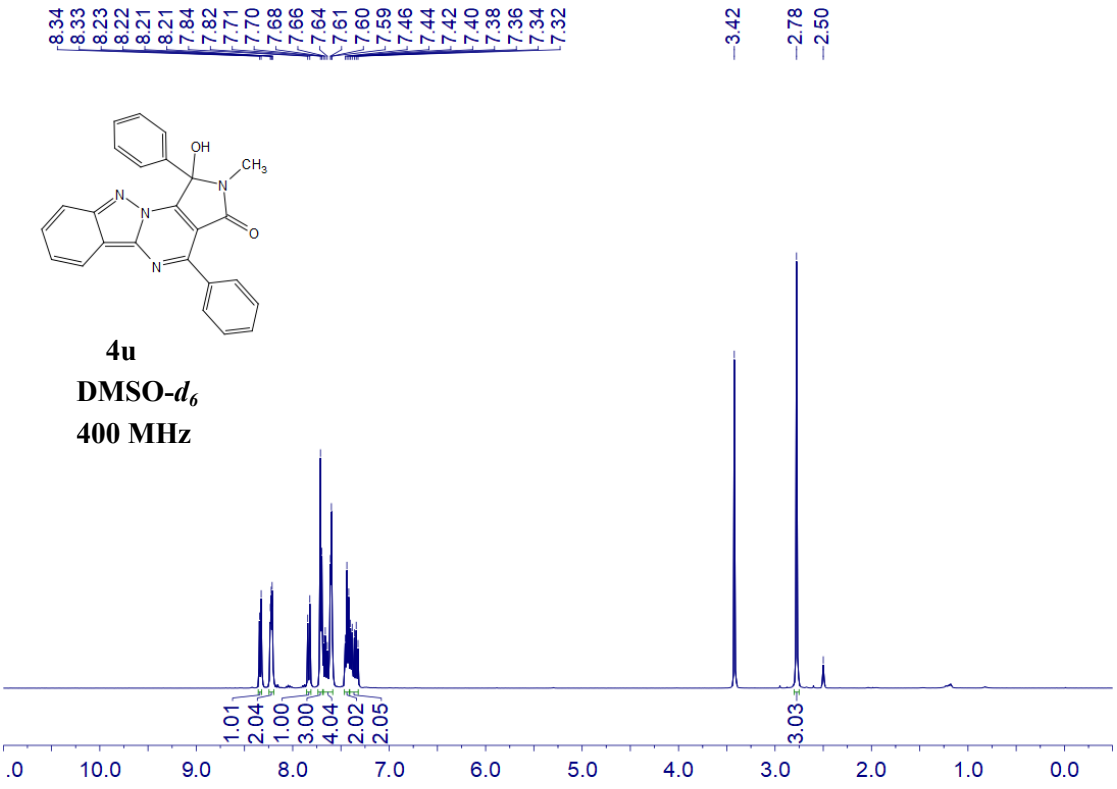


4t

DMSO-d_6

100 MHz

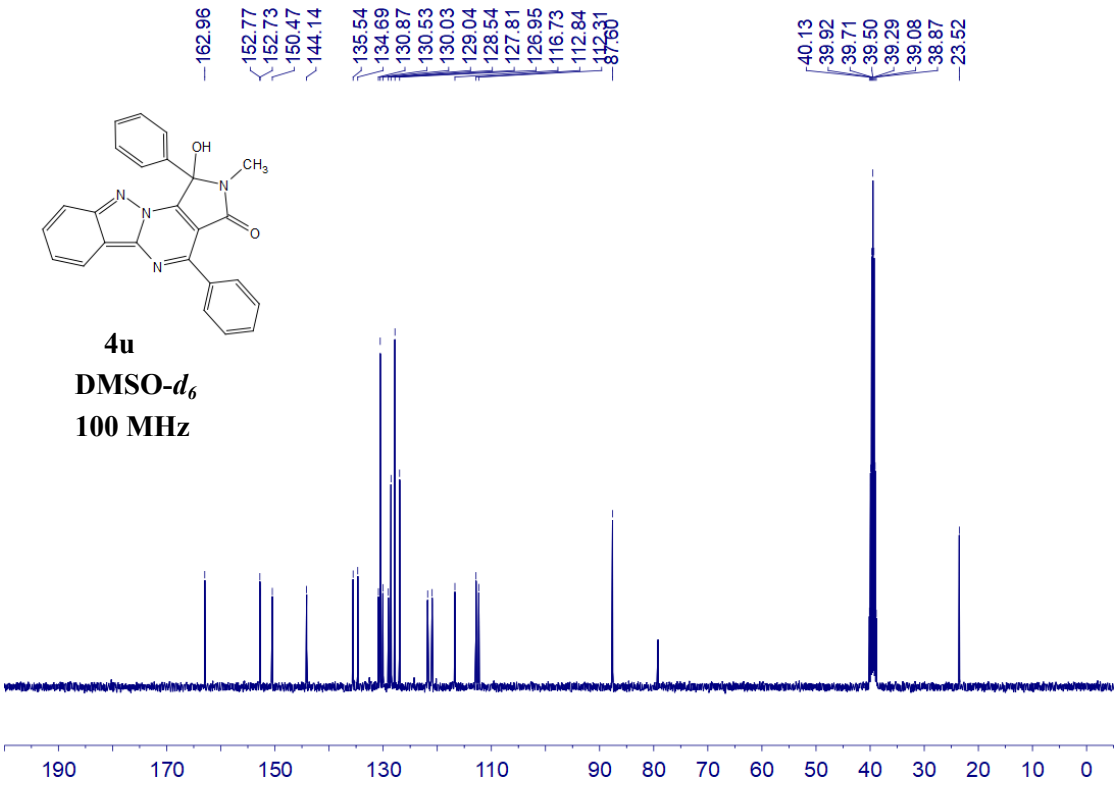
4u



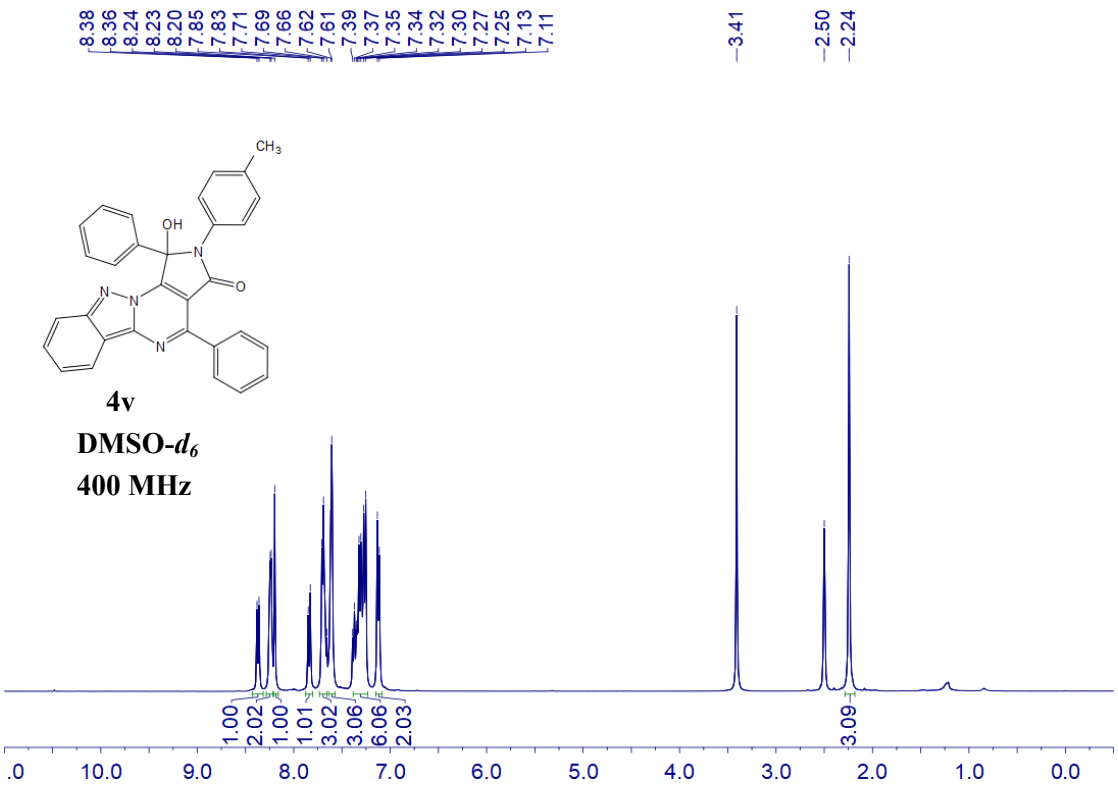
4u

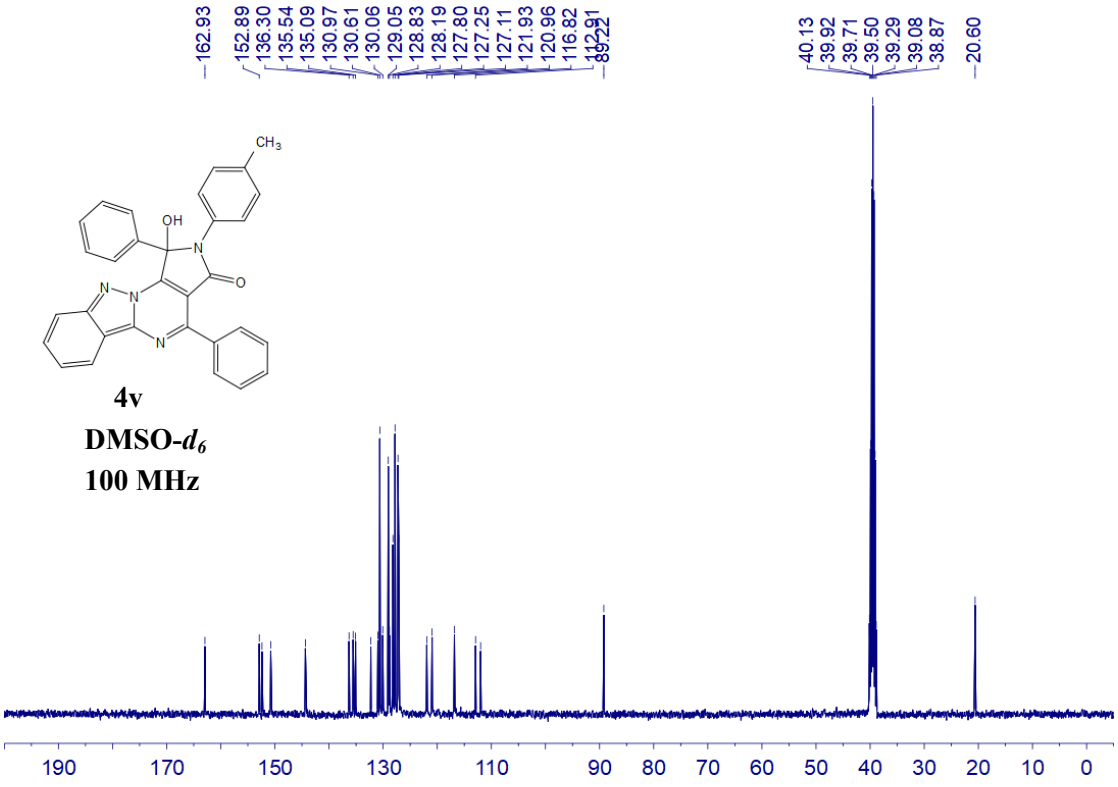
DMSO-d_6

400 MHz


162.96
152.77
152.73
150.47
144.14
135.54
134.69
130.87
130.53
130.03
129.04
128.54
127.81
126.95
116.73
112.84
112.31
87.60
40.13
39.92
39.71
39.50
39.29
39.08
38.87
23.52
OH
CH3
N
N
N
O
4u
DMSO-d6
100 MHz
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

4v


8.38
8.36
8.24
8.23
8.20
7.85
7.83
7.71
7.69
7.66
7.62
7.61
7.39
7.37
7.35
7.34
7.32
7.30
7.27
7.25
7.13
7.11
3.41
2.50
2.24
CH3
OH
N
N
N
O
4v
DMSO-d6
400 MHz
1.00
2.02
1.00
1.01
3.02
3.06
6.06
2.03
3.09
.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

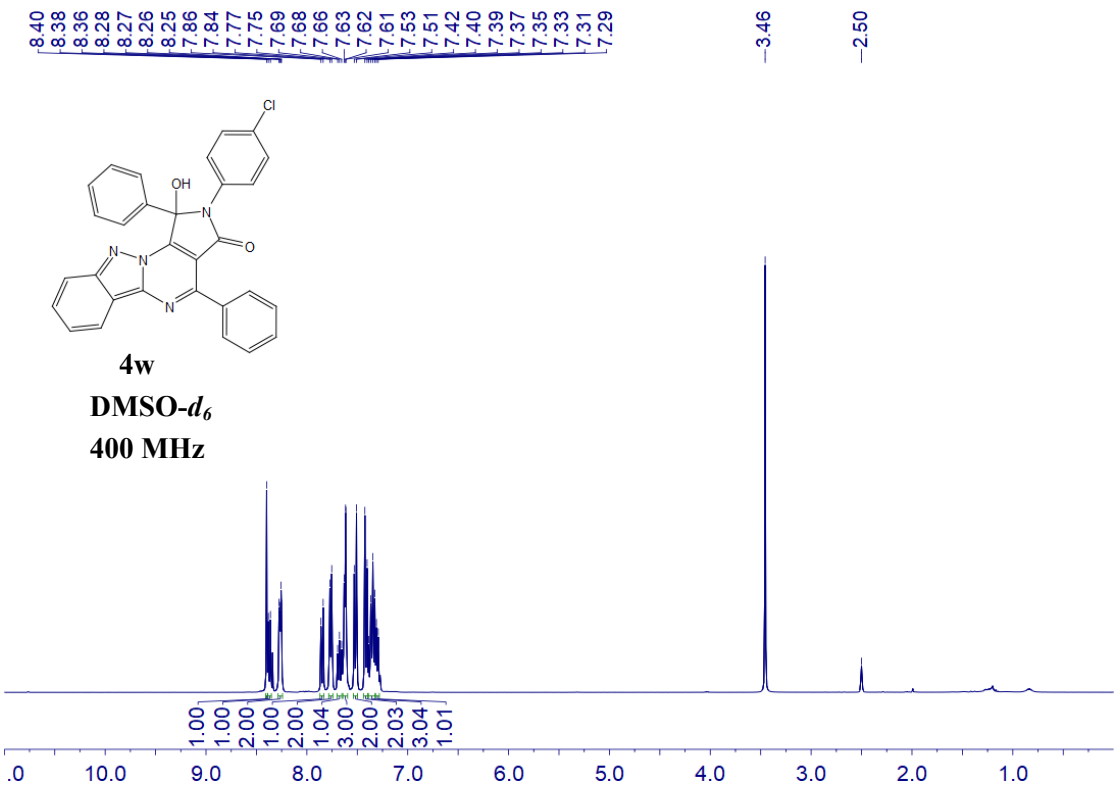


4v

DMSO-*d*$_6$

100 MHz

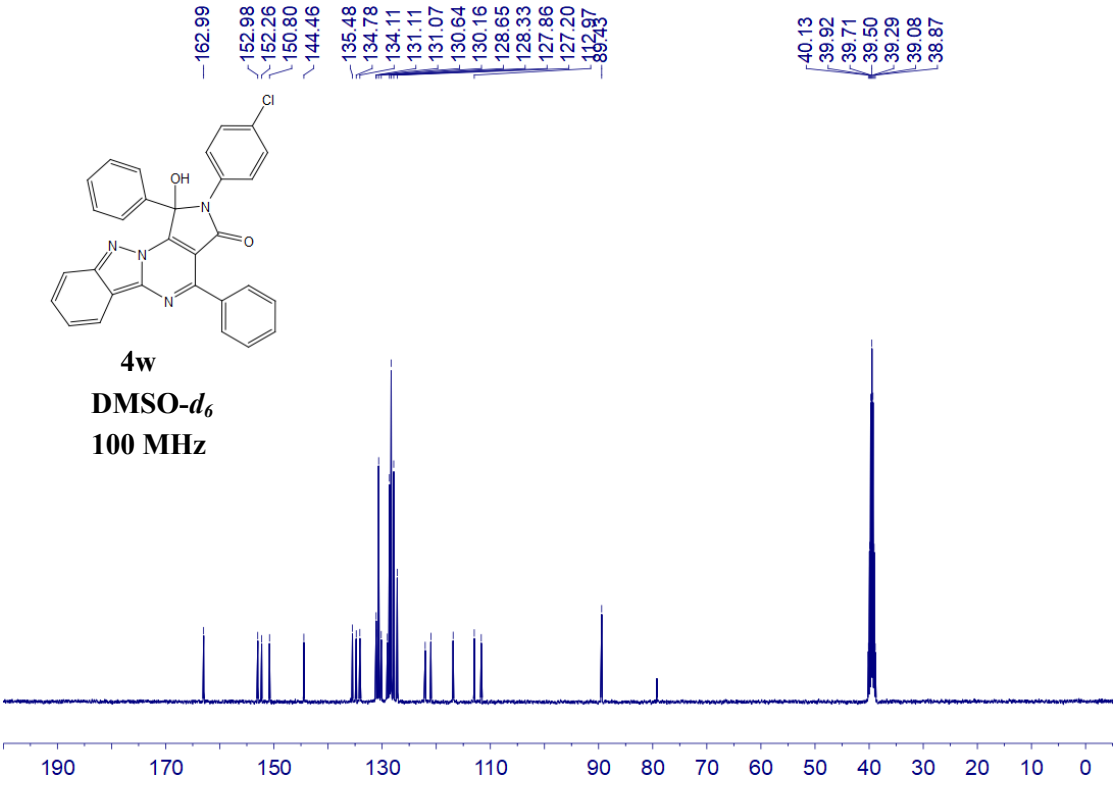
4w



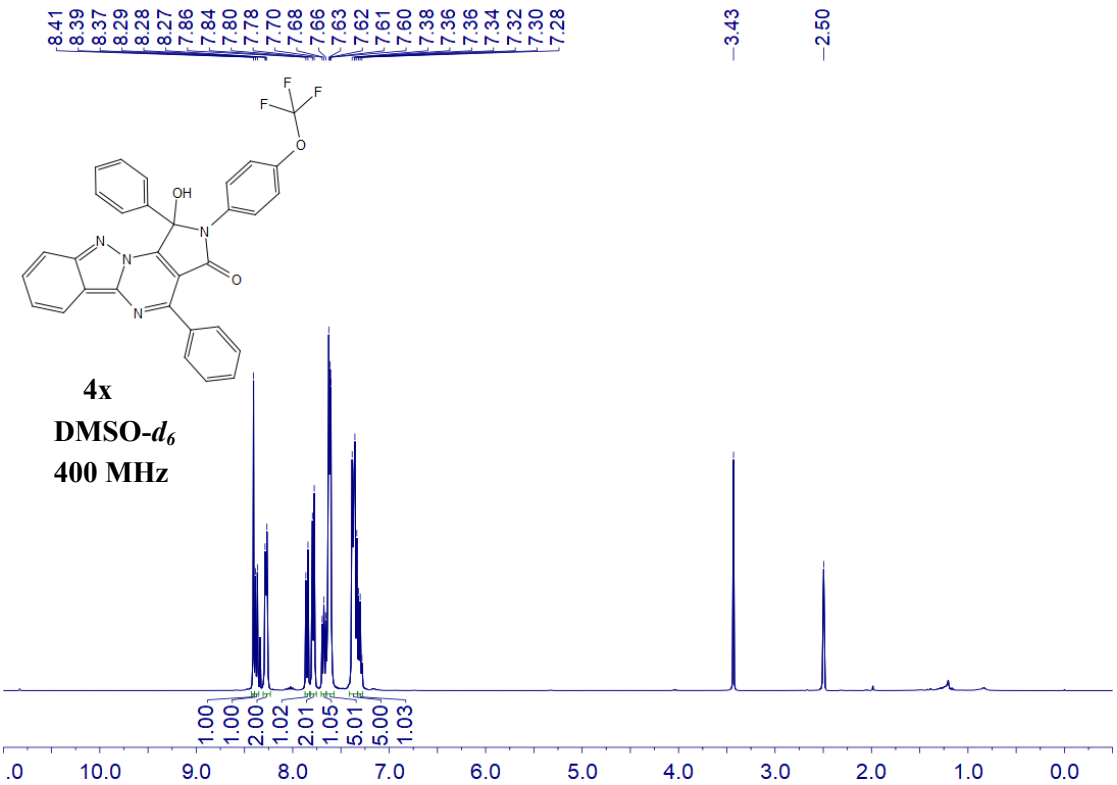
4w

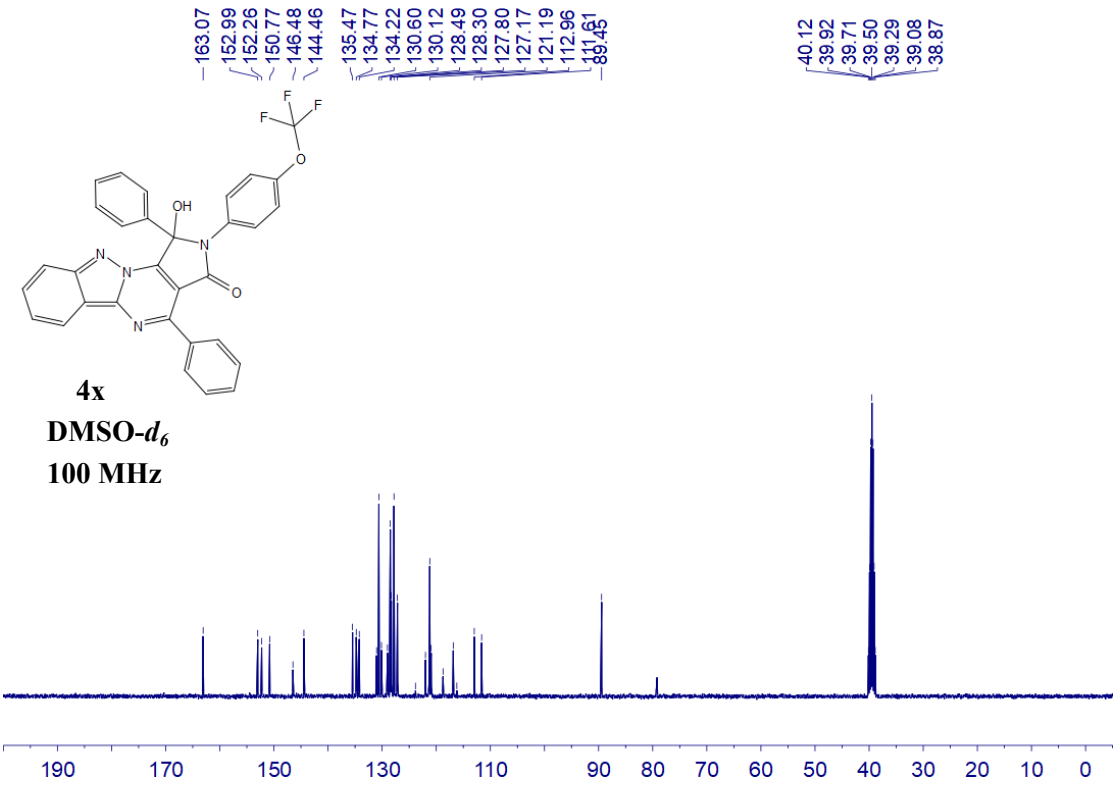
DMSO-*d*$_6$

400 MHz

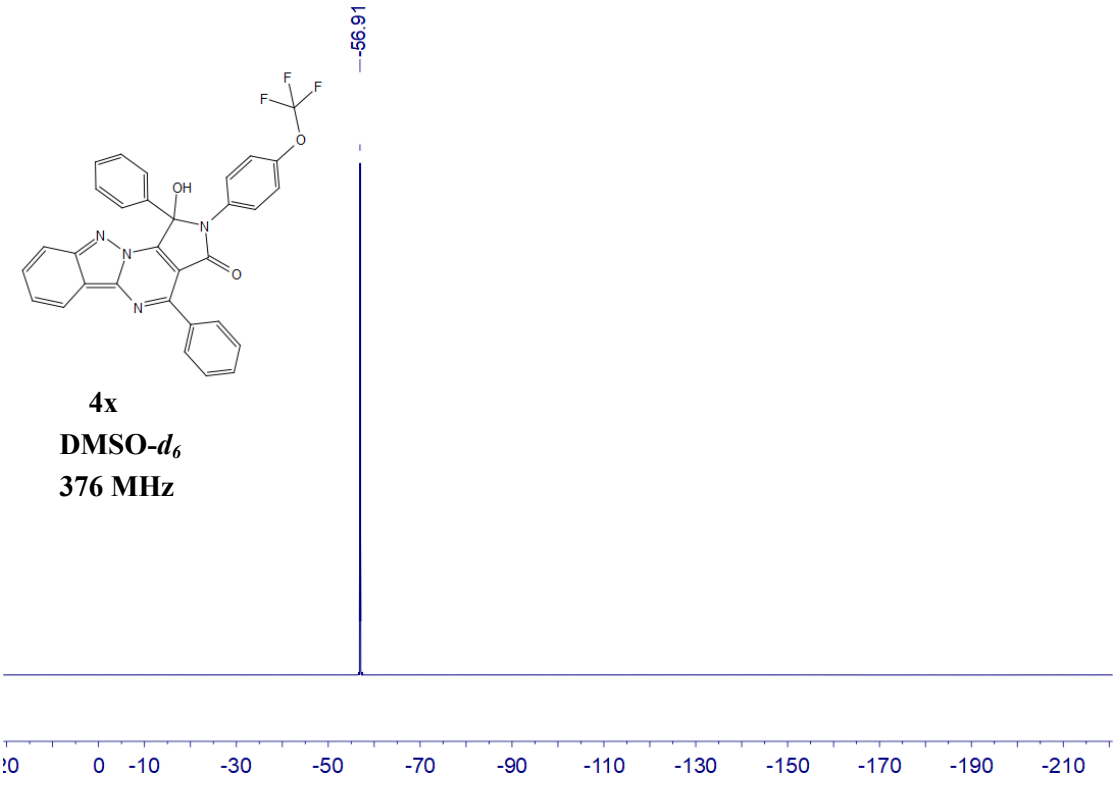

162.99
152.98
152.26
150.80
144.46
135.48
134.78
134.11
131.11
131.07
130.64
130.16
128.65
128.33
127.86
127.20
112.97
89.43
40.13
39.92
39.71
39.50
39.29
39.08
38.87
Cl
OH
N
O
N
N
N
4w
DMSO-d6
100 MHz
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

4x


8.41
8.39
8.37
8.29
8.28
8.27
7.86
7.84
7.80
7.78
7.70
7.68
7.66
7.63
7.62
7.61
7.60
7.38
7.36
7.36
7.34
7.32
7.30
7.28
3.43
2.50
F
F
F
O
OH
N
O
N
N
N
4x
DMSO-d6
400 MHz
1.00
1.00
2.00
1.02
2.01
1.05
5.01
5.00
1.03
.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

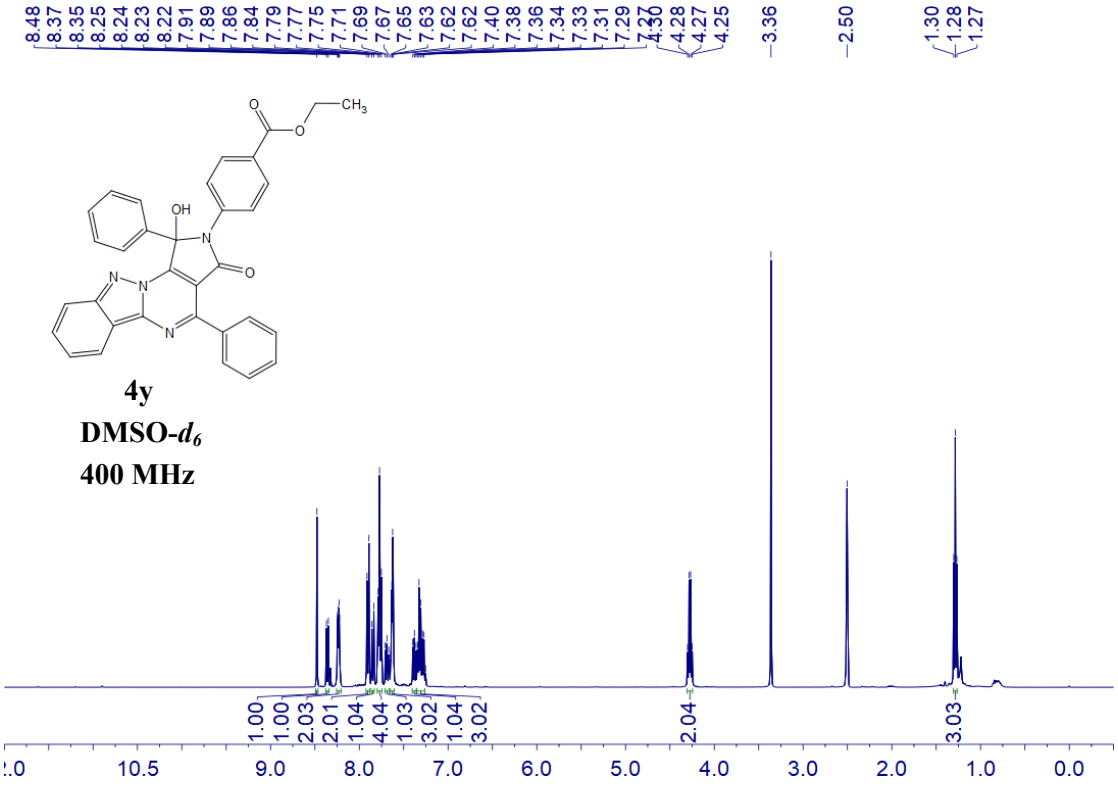


4x
DMSO-d_6
100 MHz

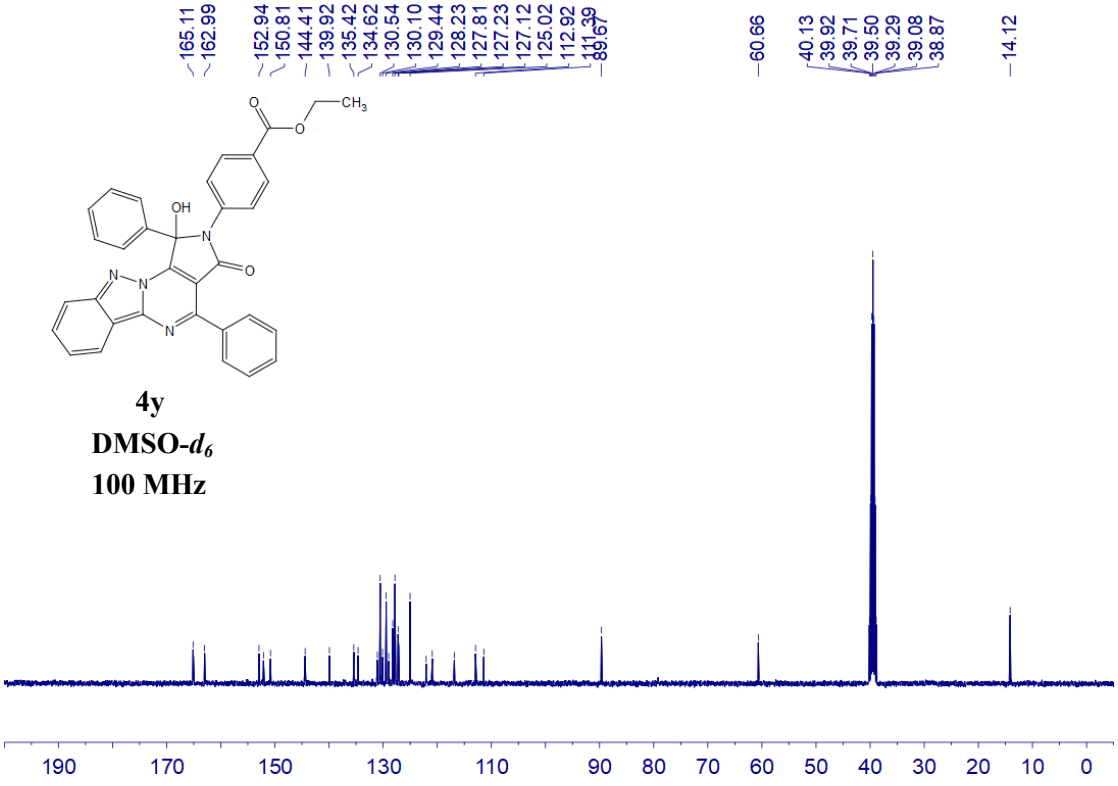


4x
DMSO-d_6
376 MHz

4y

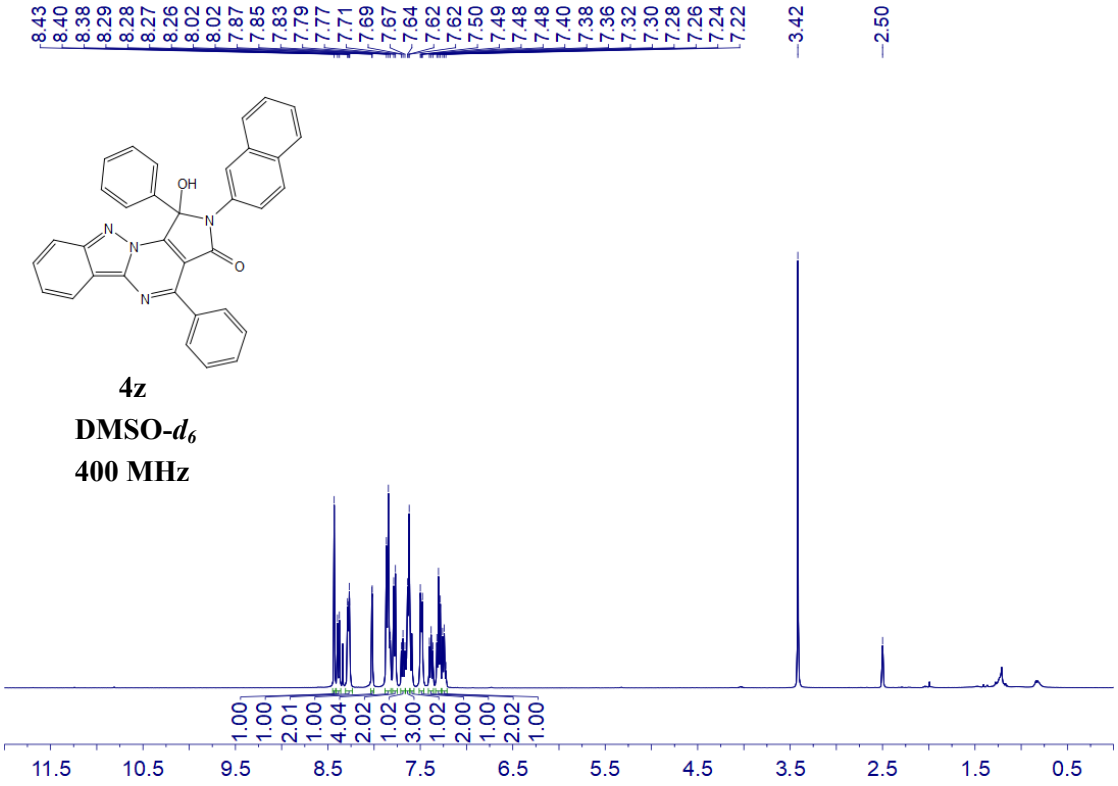


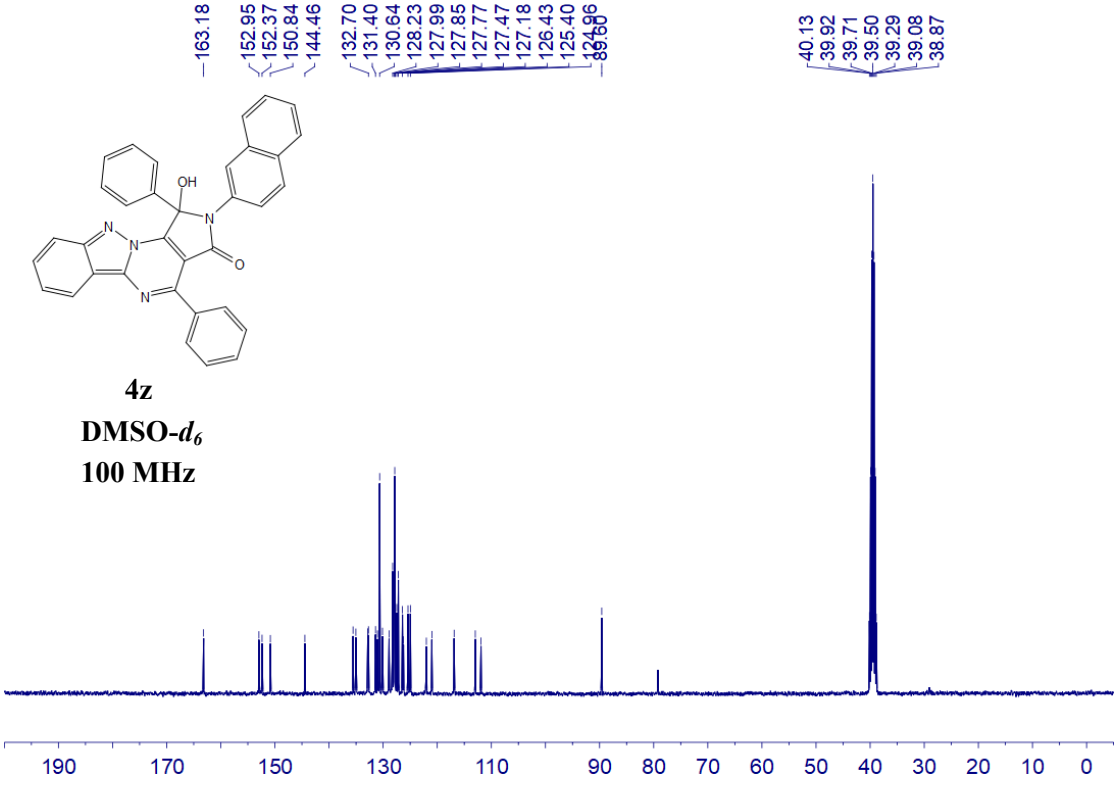
4y
DMSO-*d*$_6$
400 MHz



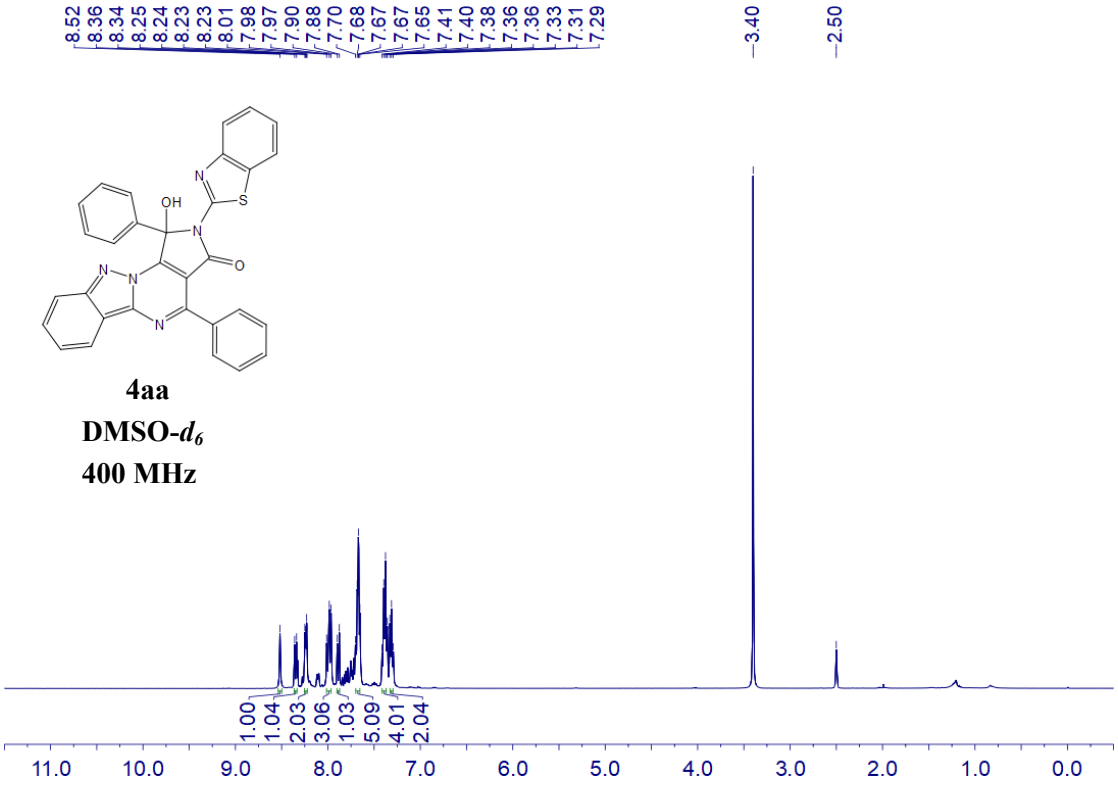
4y
DMSO-*d*$_6$
100 MHz

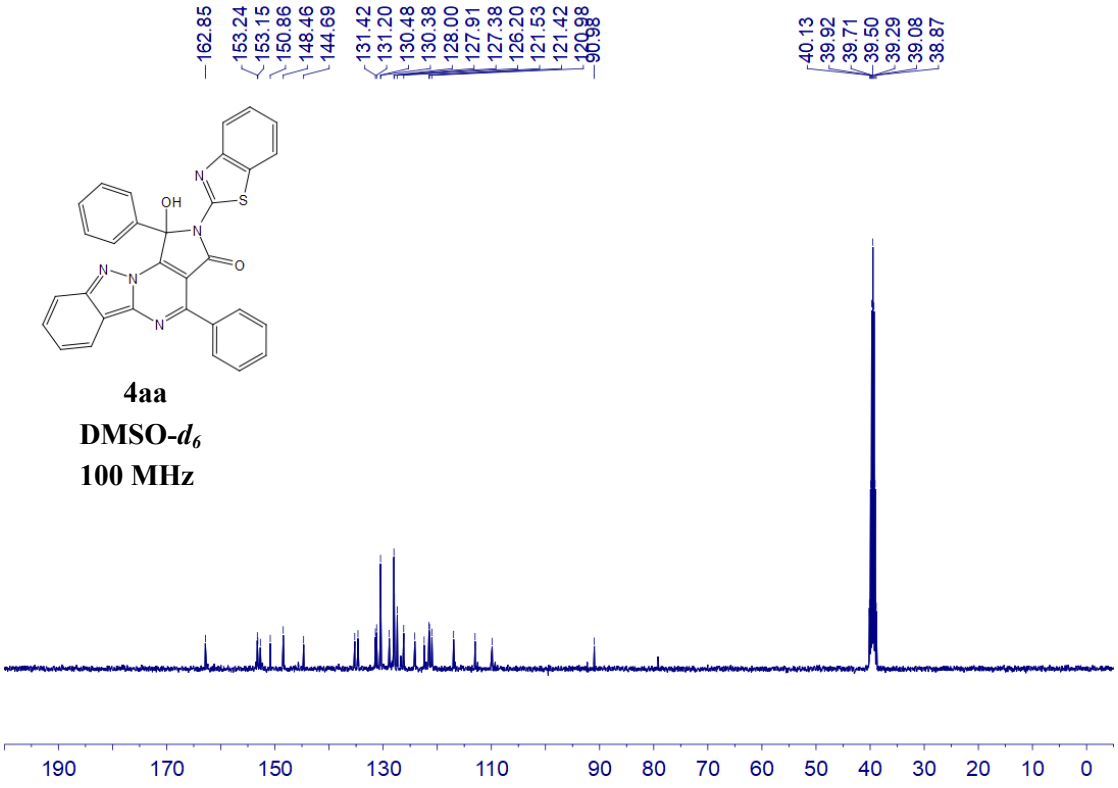
4z


8.43
8.40
8.38
8.29
8.28
8.27
8.26
8.02
8.02
7.87
7.85
7.83
7.79
7.77
7.71
7.69
7.67
7.64
7.62
7.62
7.50
7.49
7.48
7.48
7.40
7.38
7.36
7.32
7.30
7.28
7.26
7.24
7.22
3.42
2.50
OH
N
N
N
O
N
4z
DMSO-d_6
400 MHz
1.00
1.00
2.01
1.00
4.04
2.02
1.02
3.00
1.02
2.00
1.00
2.02
1.00
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

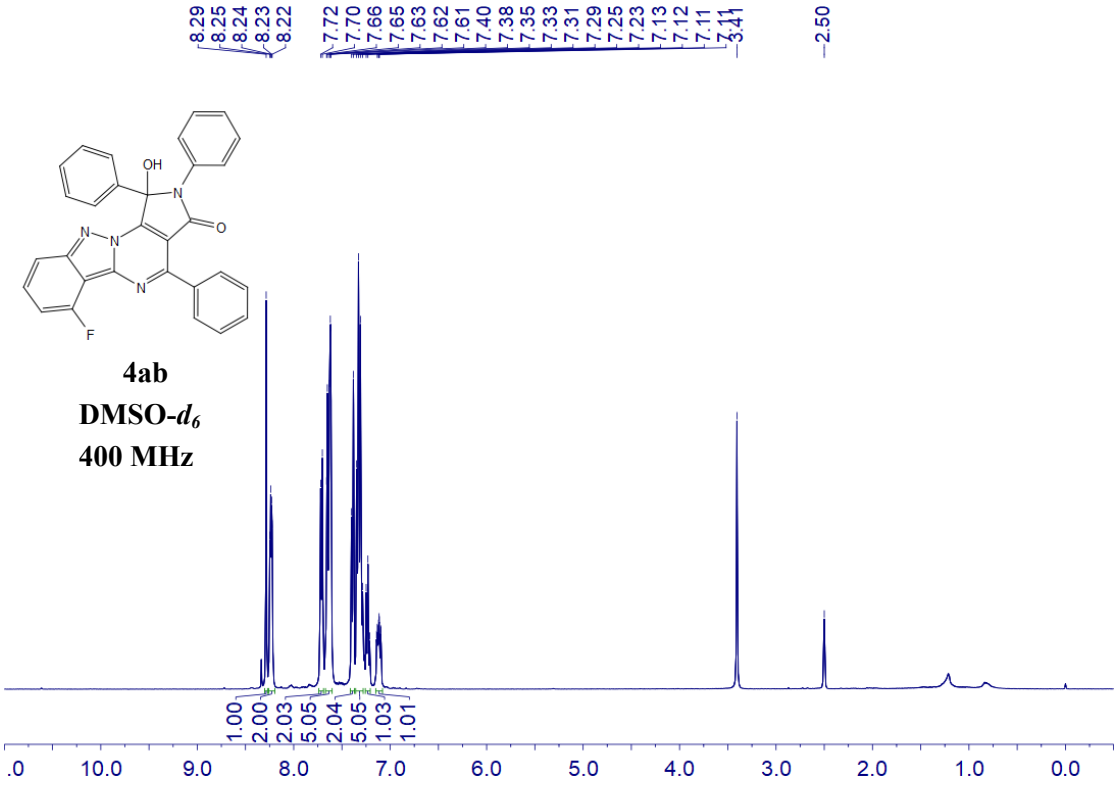

163.18
152.95
152.37
150.84
144.46
132.70
131.40
130.64
128.23
127.99
127.85
127.77
127.47
127.18
126.43
125.40
40.13
39.92
39.71
39.50
39.29
39.08
38.87
OH
N
N
N
O
N
4z
DMSO-d_6
100 MHz
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

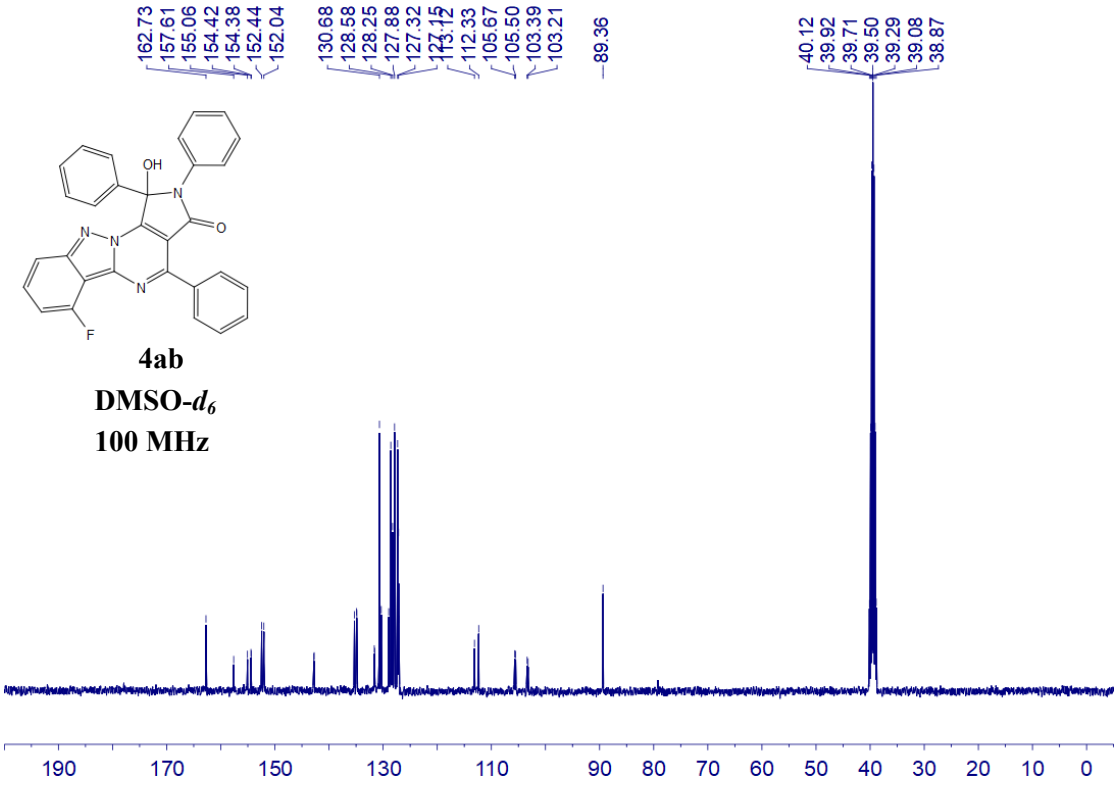
4aa

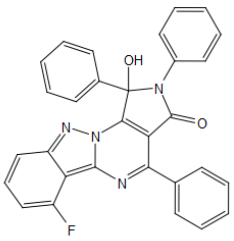

8.52
8.36
8.34
8.25
8.24
8.23
8.23
8.01
7.98
7.97
7.90
7.88
7.70
7.68
7.67
7.67
7.65
7.41
7.40
7.38
7.36
7.36
7.33
7.31
7.29
3.40
2.50
OH
N
S
N
O
N
N
N
4aa
DMSO-d_6
400 MHz
1.00
1.04
2.03
3.06
1.03
5.09
4.01
2.04
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


162.85
153.24
153.15
150.86
148.46
144.69
131.42
131.20
130.48
130.38
128.00
127.91
127.38
126.20
121.53
121.42
120.98
120.88
40.13
39.92
39.71
39.50
39.29
39.08
38.87
OH
N
S
N
O
N
N
N
4aa
DMSO-d_6
100 MHz
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

4ab

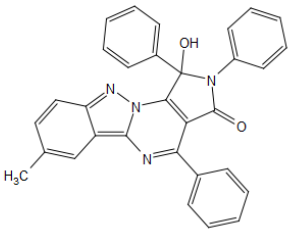

8.29
8.25
8.24
8.23
8.22
7.72
7.70
7.66
7.65
7.63
7.62
7.61
7.40
7.38
7.35
7.33
7.31
7.29
7.25
7.23
7.13
7.12
7.11
3.41
2.50
OH
N
O
N
N
N
F
4ab
DMSO-d6
400 MHz
1.00
2.00
2.03
5.05
2.04
5.05
1.03
1.01
.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


162.73
157.61
155.06
154.42
154.38
152.44
152.04
130.68
128.58
128.25
127.88
127.32
112.33
105.67
105.50
103.39
103.21
89.36
40.12
39.92
39.71
39.50
39.29
39.08
38.87
OH
N
O
N
N
N
F
4ab
DMSO-d6
100 MHz
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

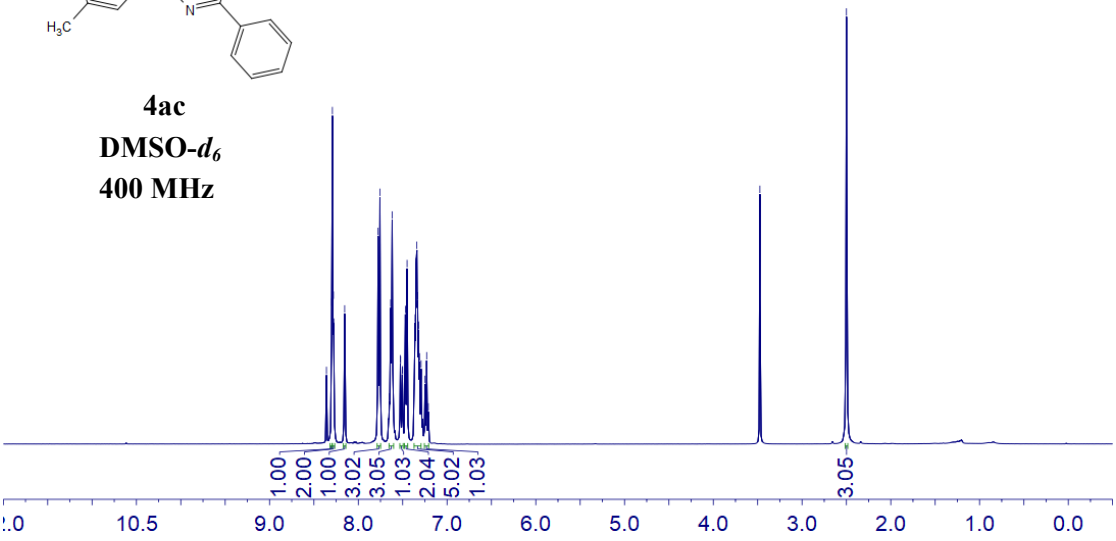


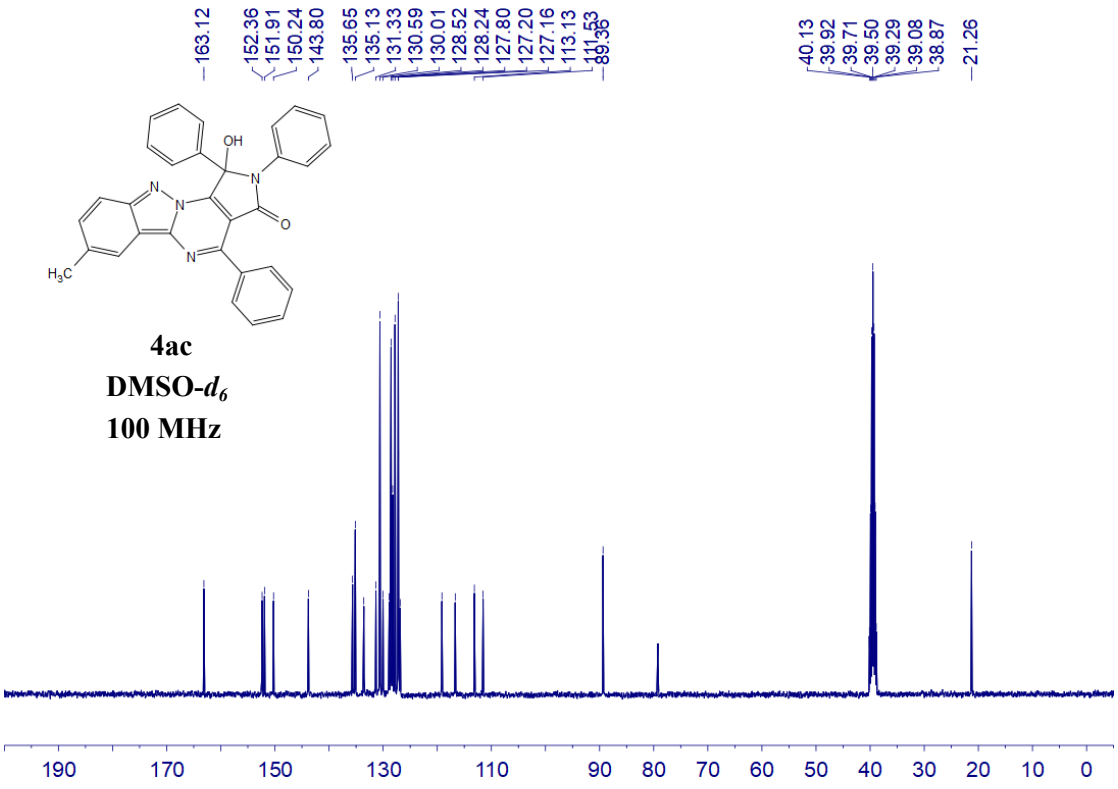
4ab
DMSO-d_6
376 MHz

4ac



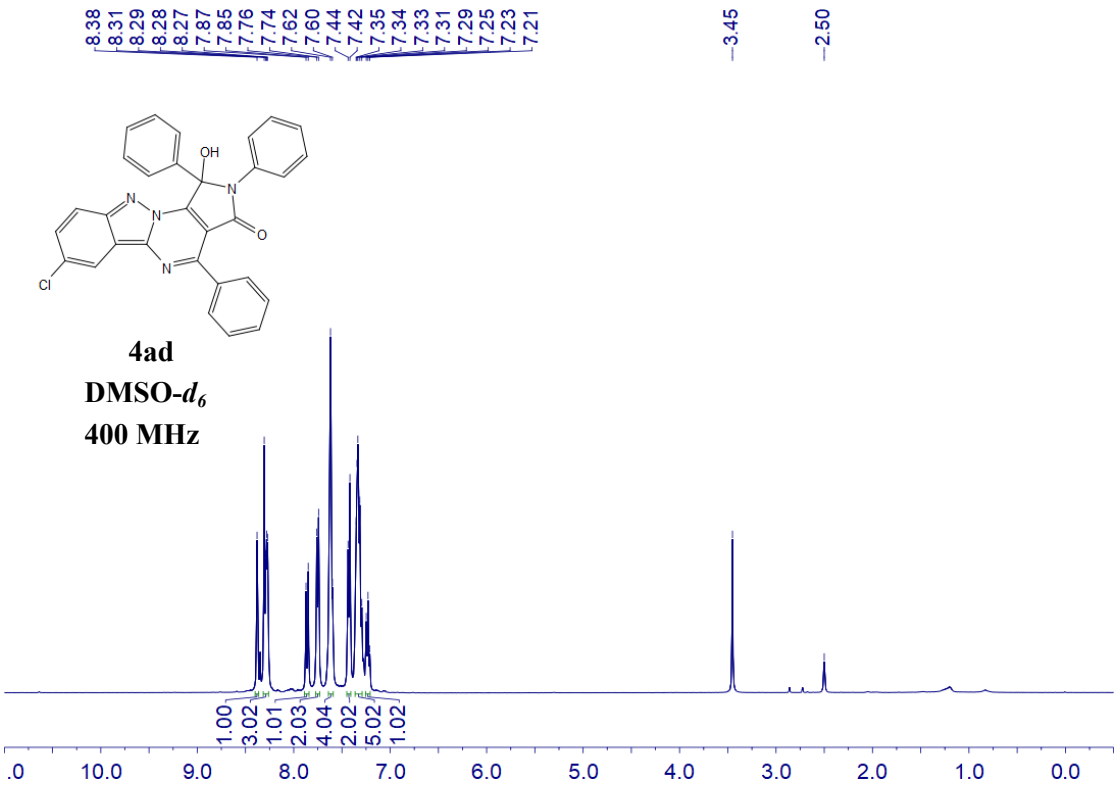
4ac
DMSO-d_6
400 MHz



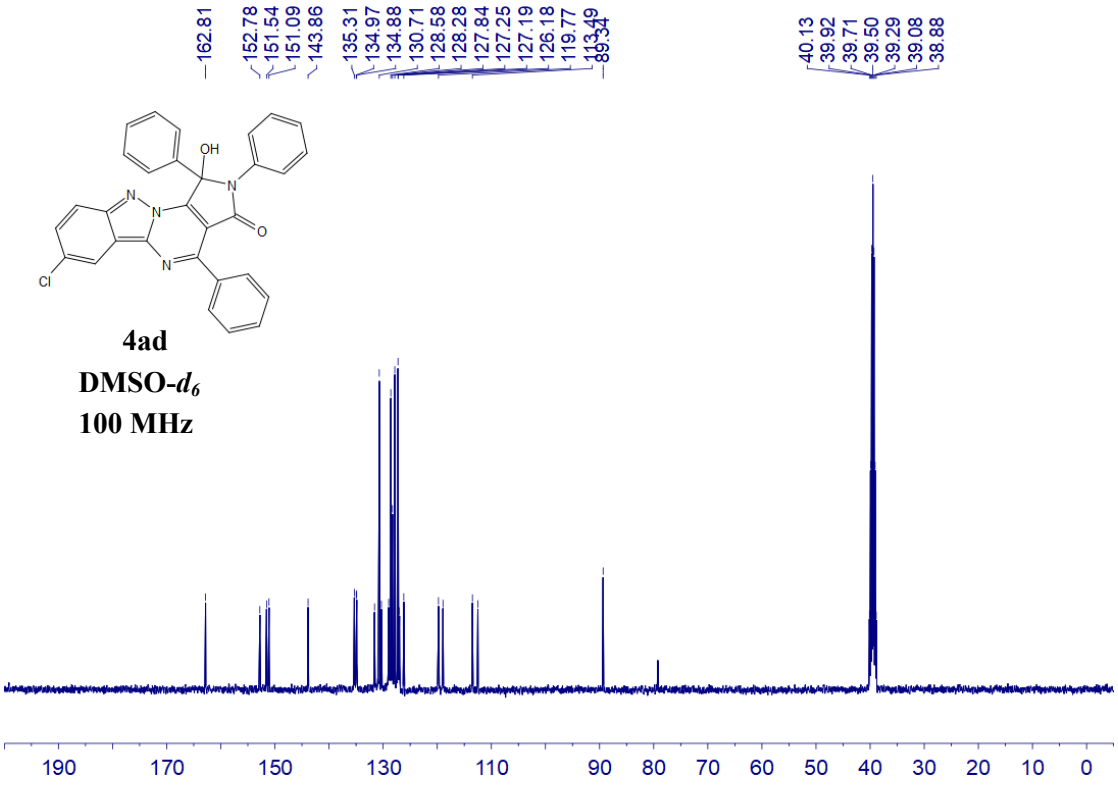


4ac
DMSO-d_6
100 MHz

4ad

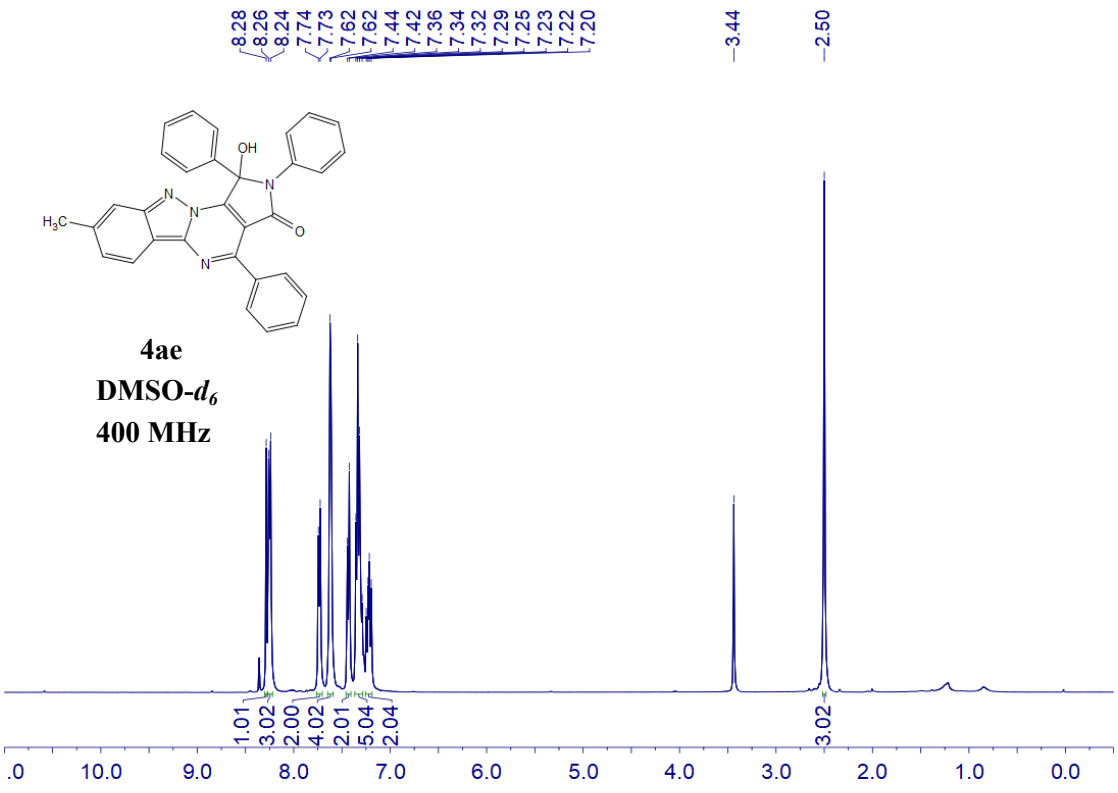


4ad
DMSO-d_6
400 MHz

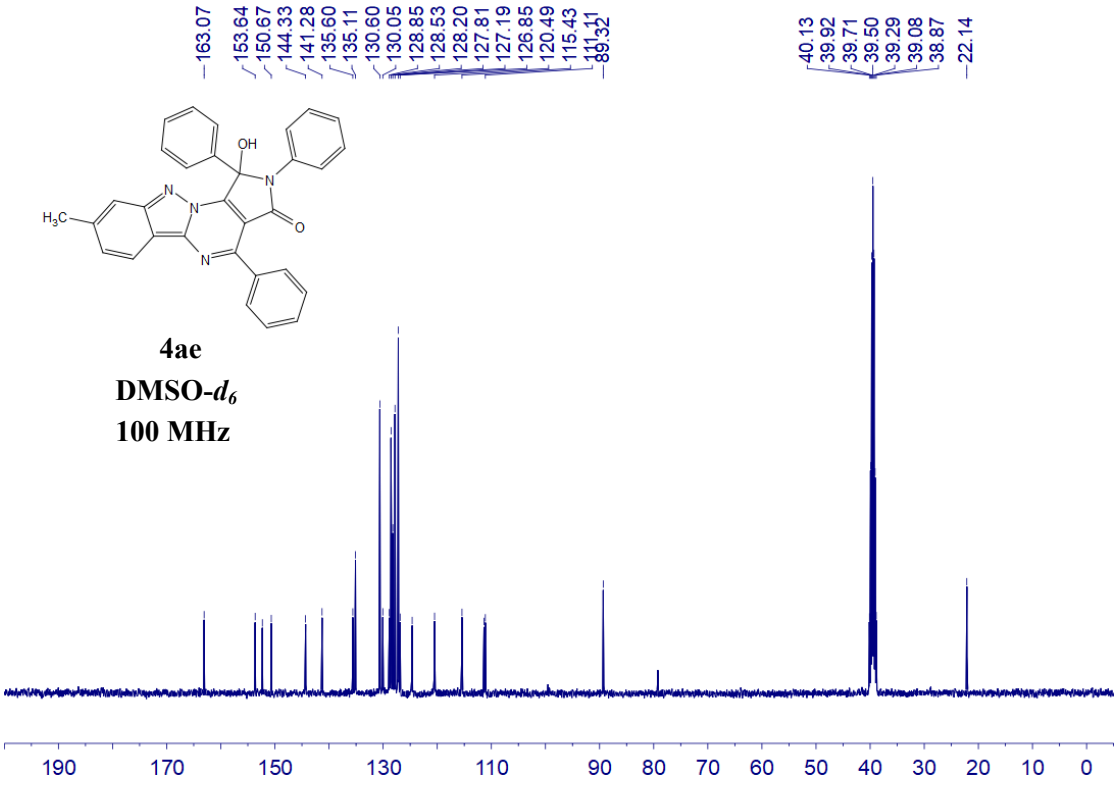


4ad
DMSO-d_6
100 MHz

4ae



4ae
DMSO-d_6
400 MHz

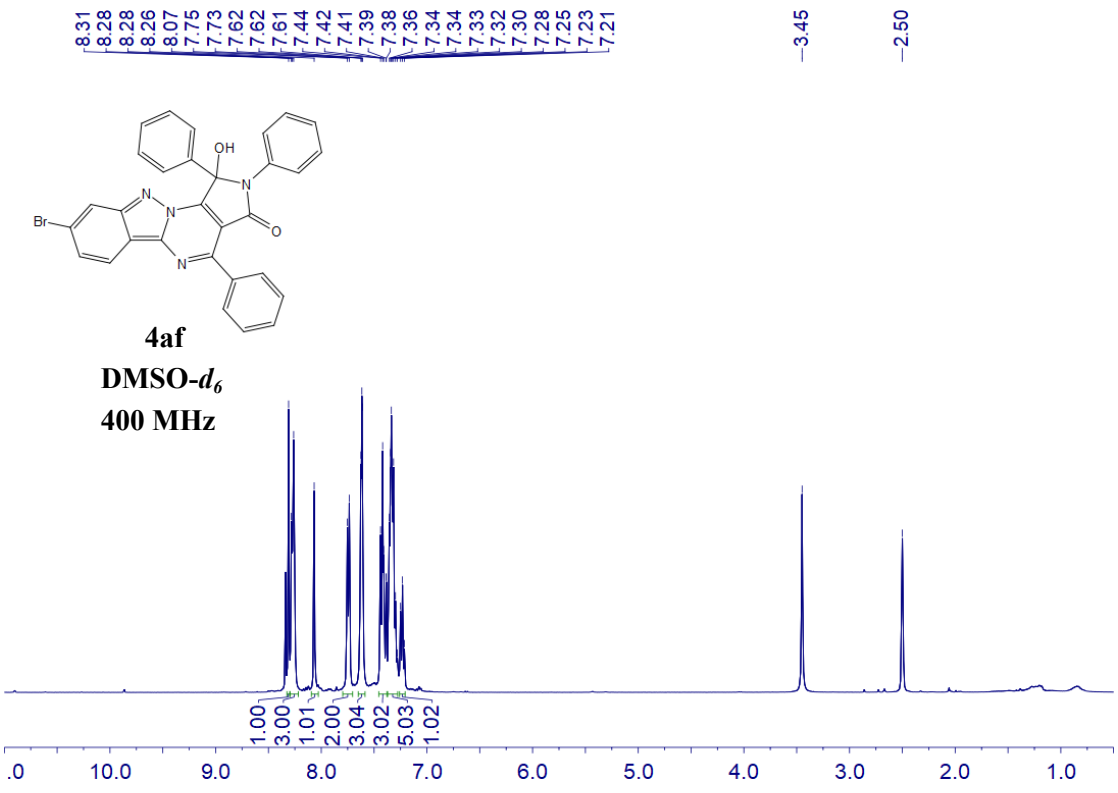


4ae

DMSO-*d*$_6$

100 MHz

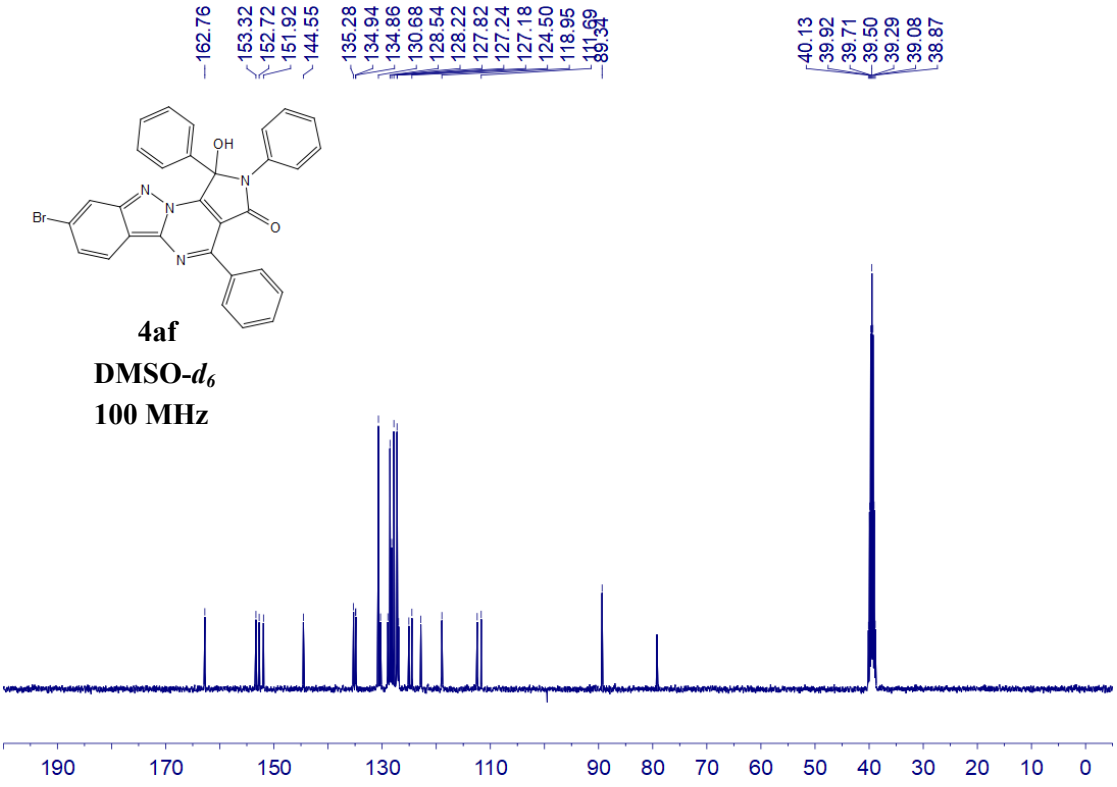
4af



4af

DMSO-*d*$_6$

400 MHz

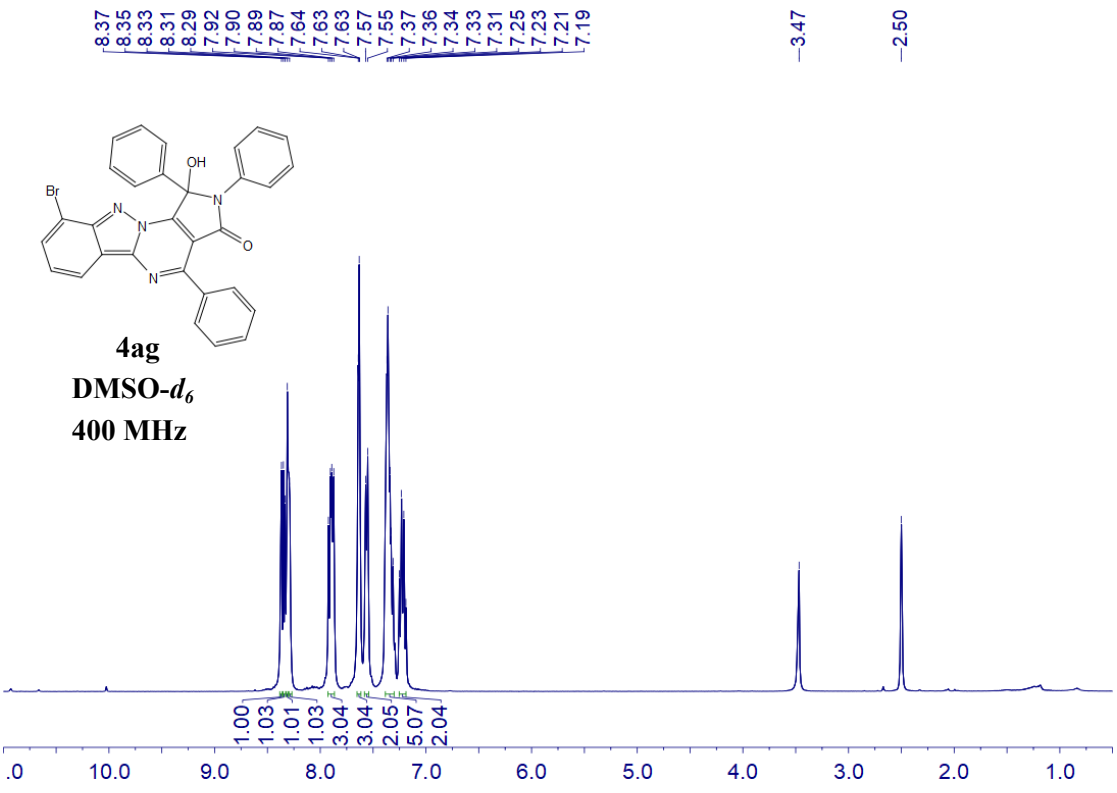


4af

DMSO-*d*$_6$

100 MHz

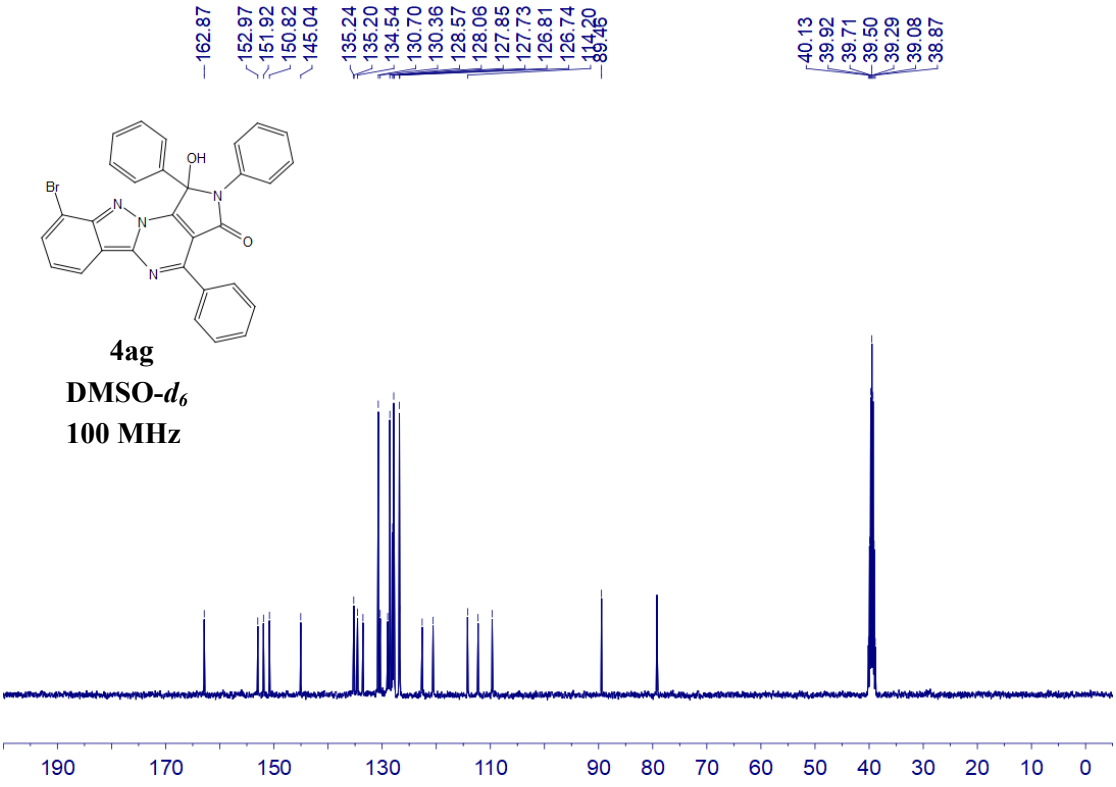
4ag



4ag

DMSO-*d*$_6$

400 MHz

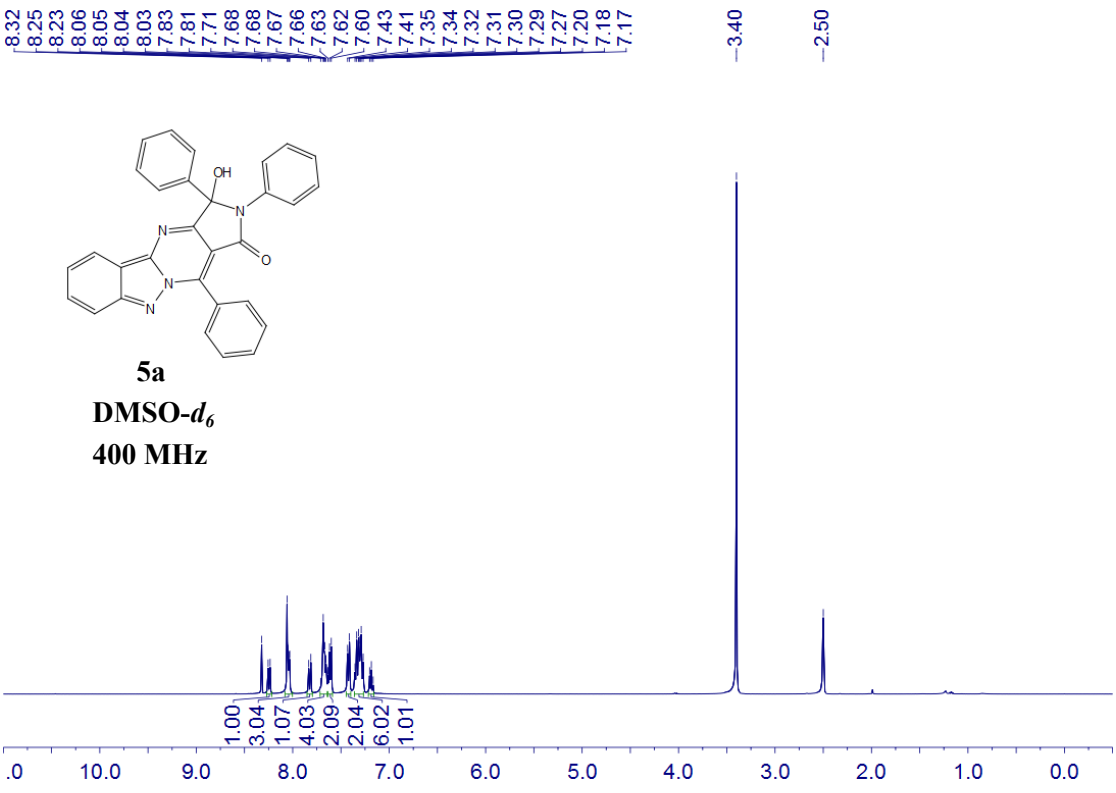


4ag

DMSO-d_6

100 MHz

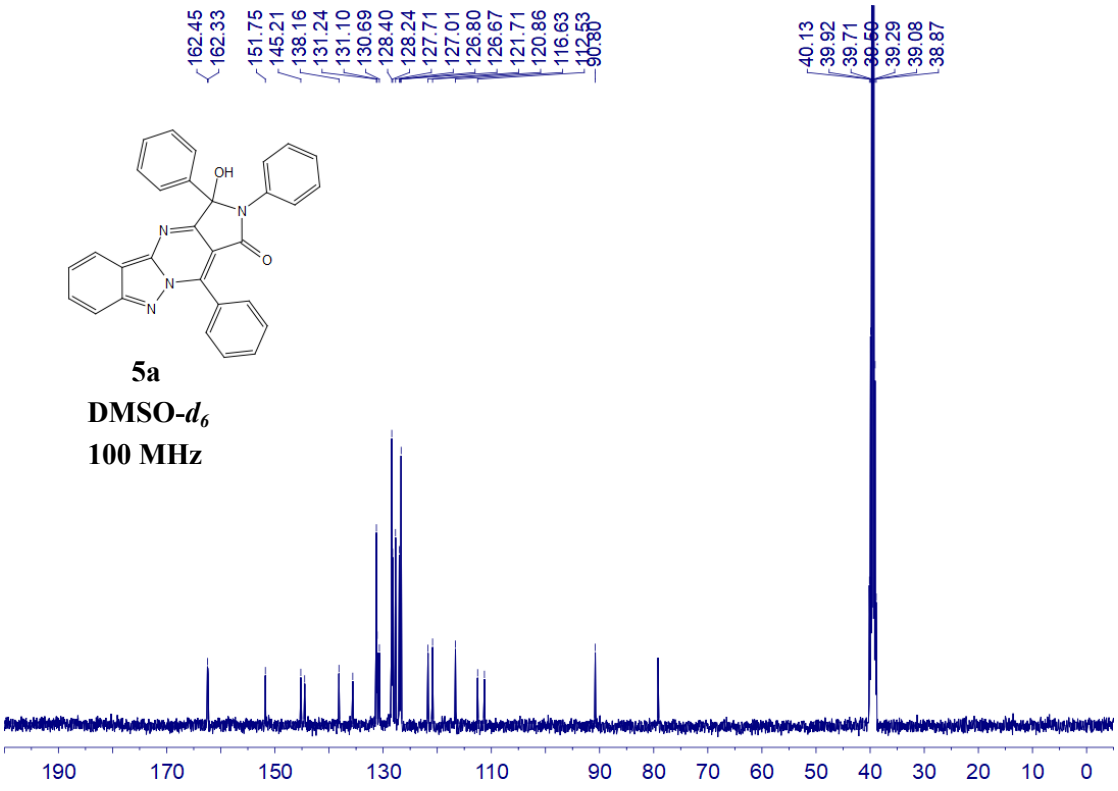
5a



5a

DMSO-d_6

400 MHz

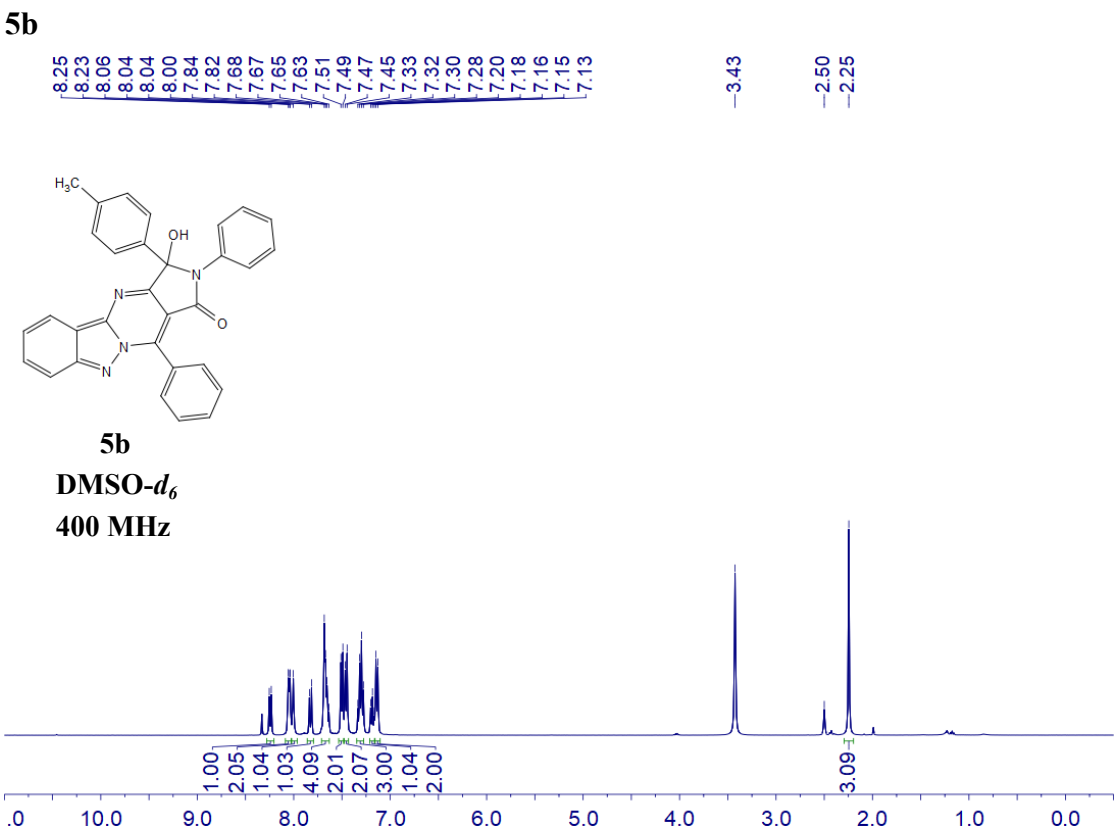


5a

DMSO-*d*$_6$

100 MHz

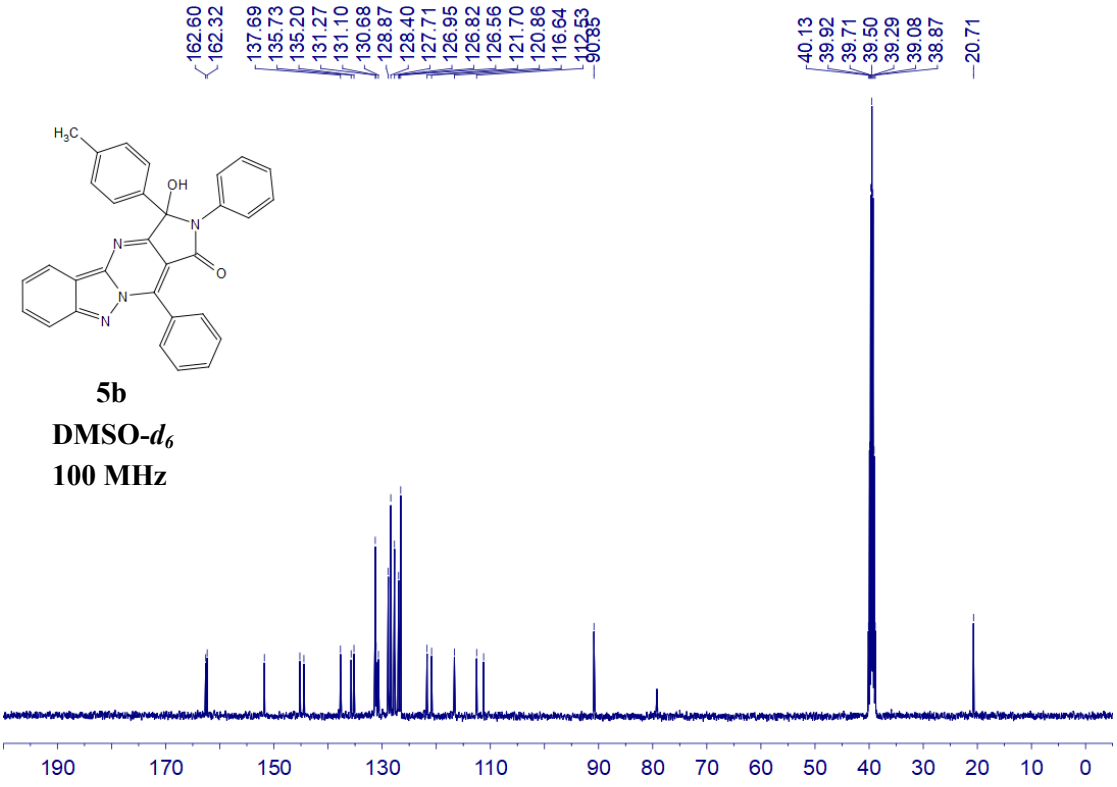
5b



5b

DMSO-*d*$_6$

400 MHz

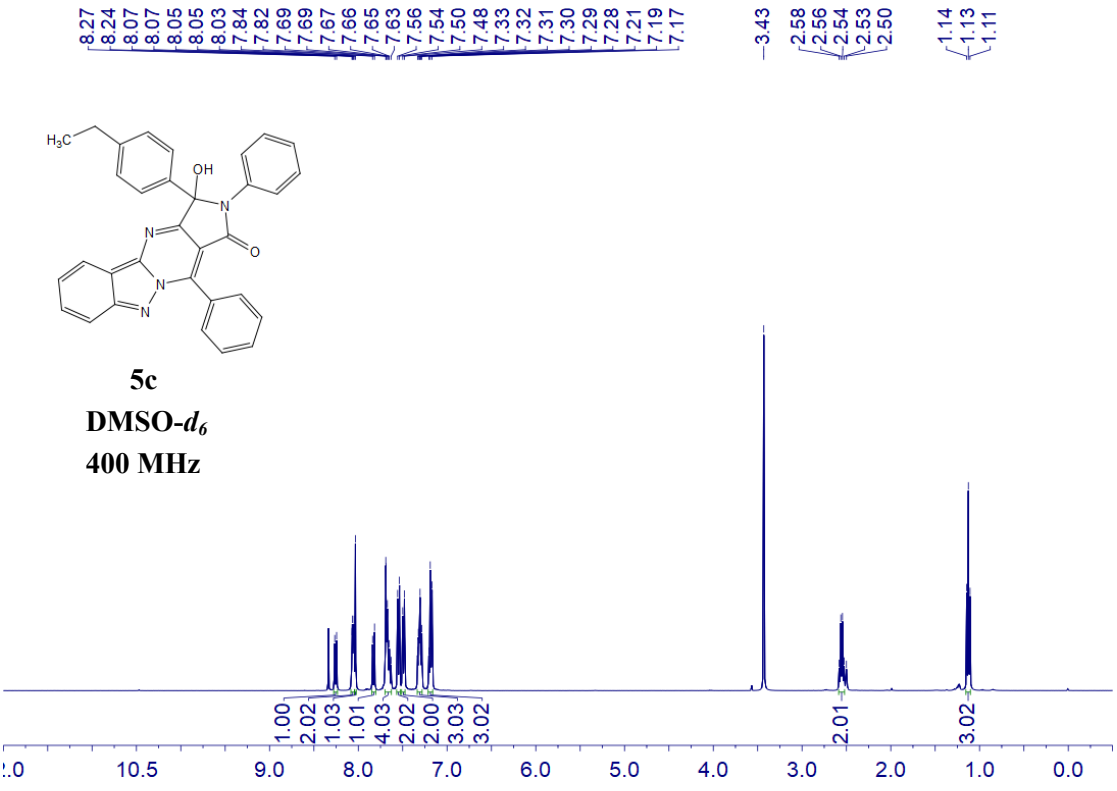


5b

DMSO-d_6

100 MHz

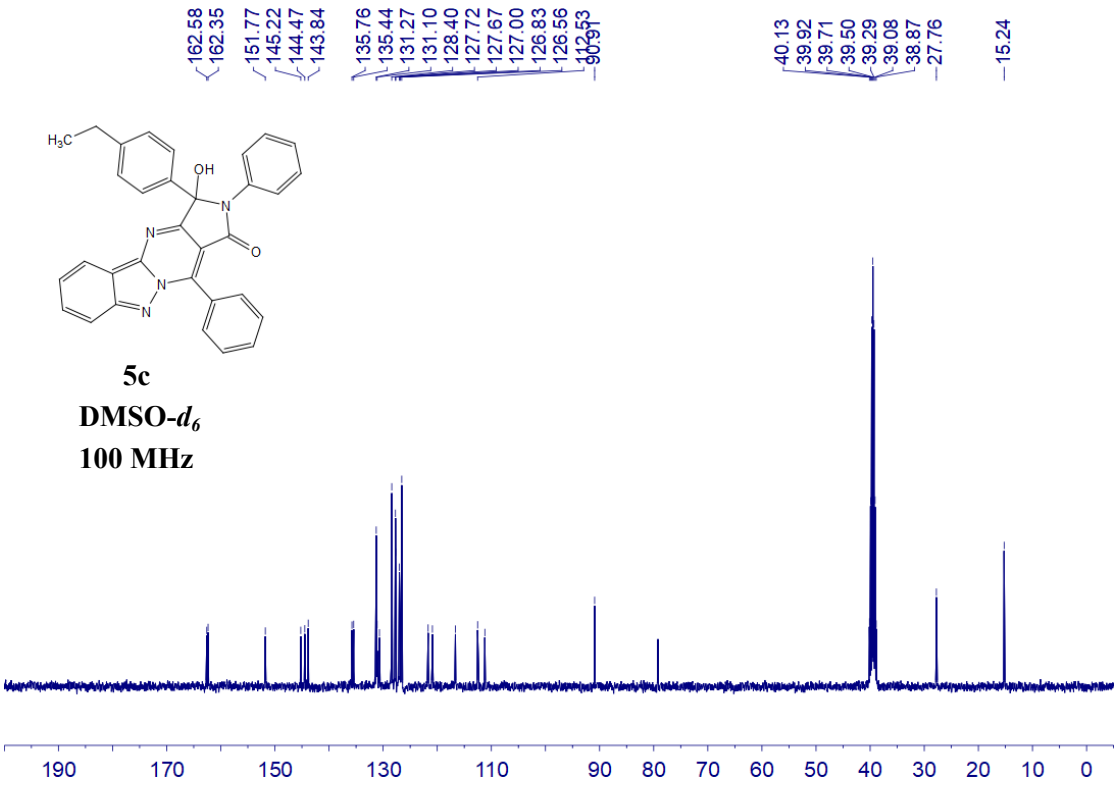
5c



5c

DMSO-d_6

400 MHz

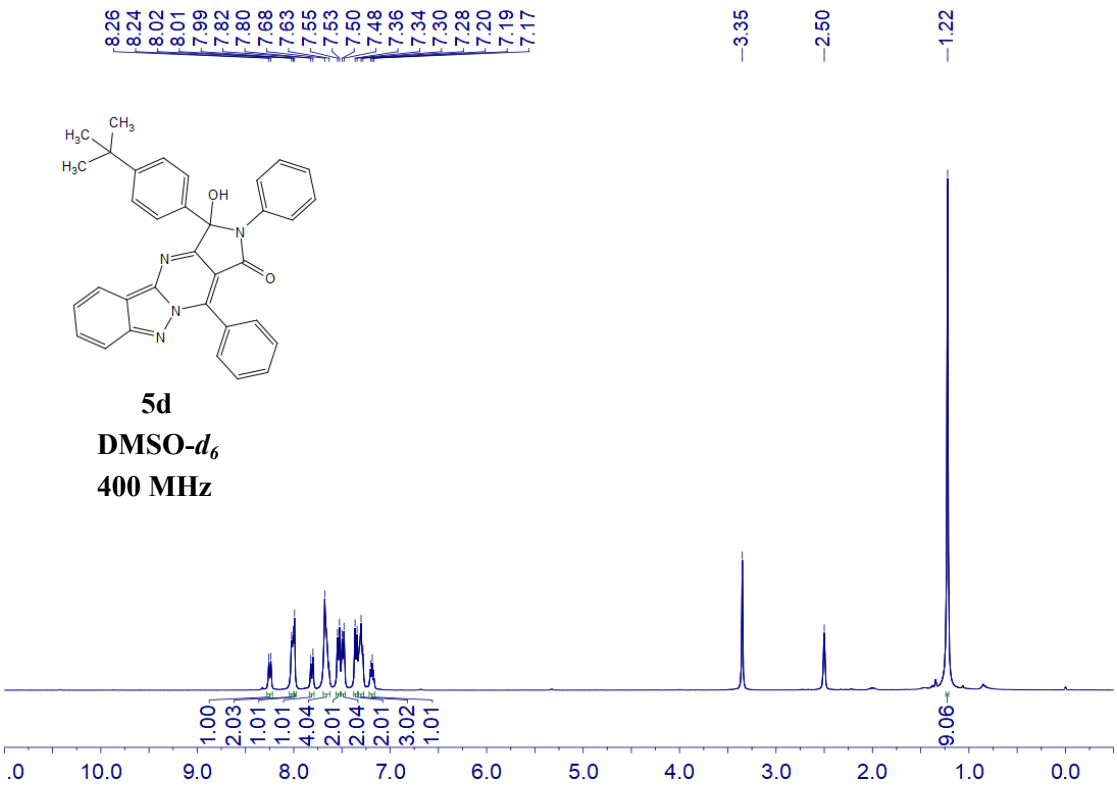


5c

DMSO-d_6

100 MHz

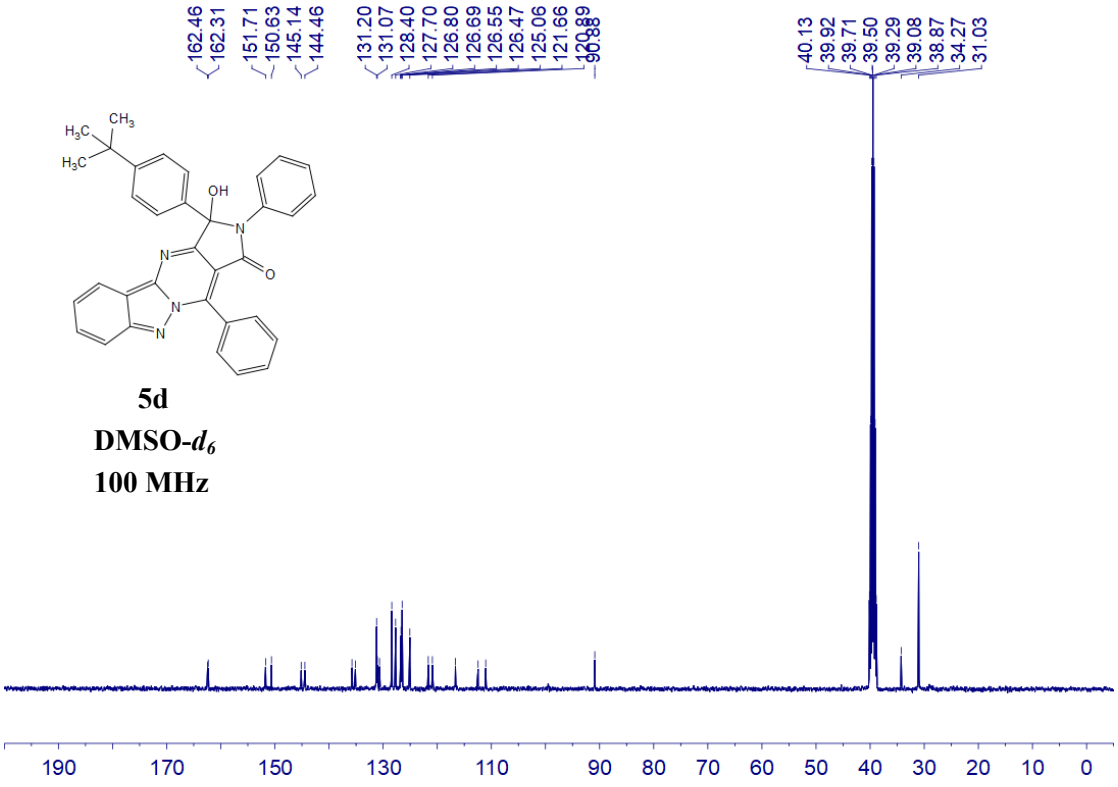
5d



5d

DMSO-d_6

400 MHz

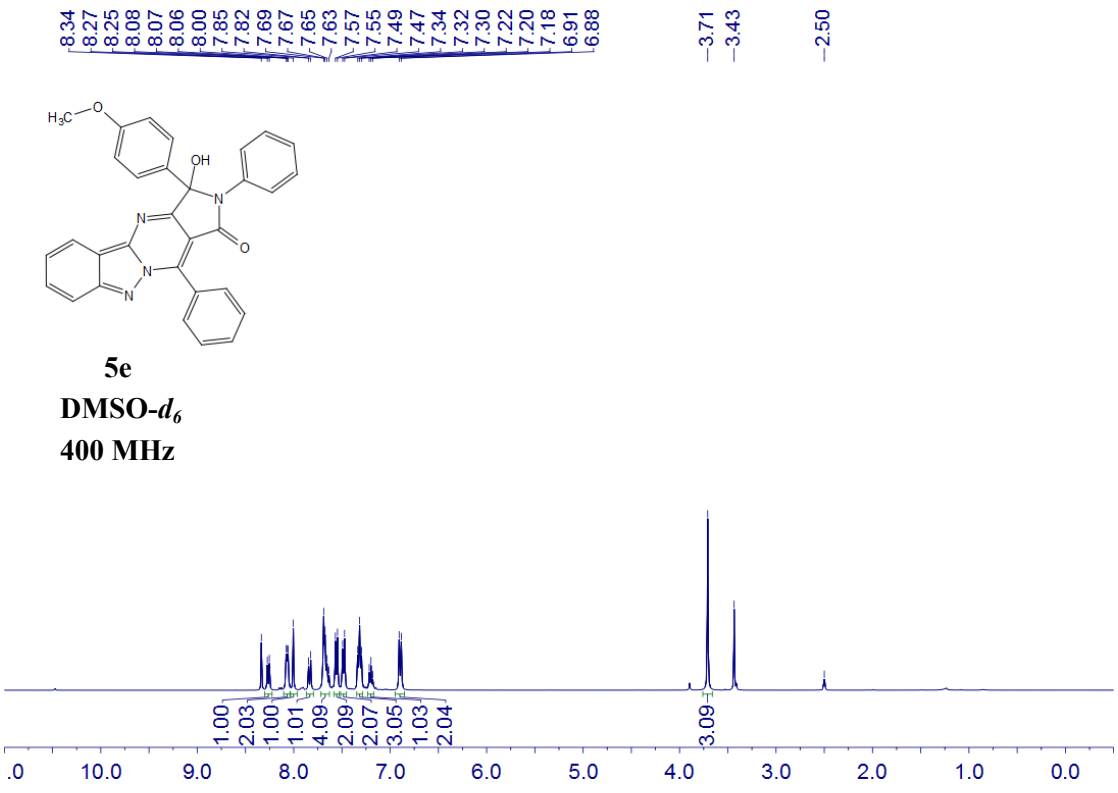


5d

DMSO-d_6

100 MHz

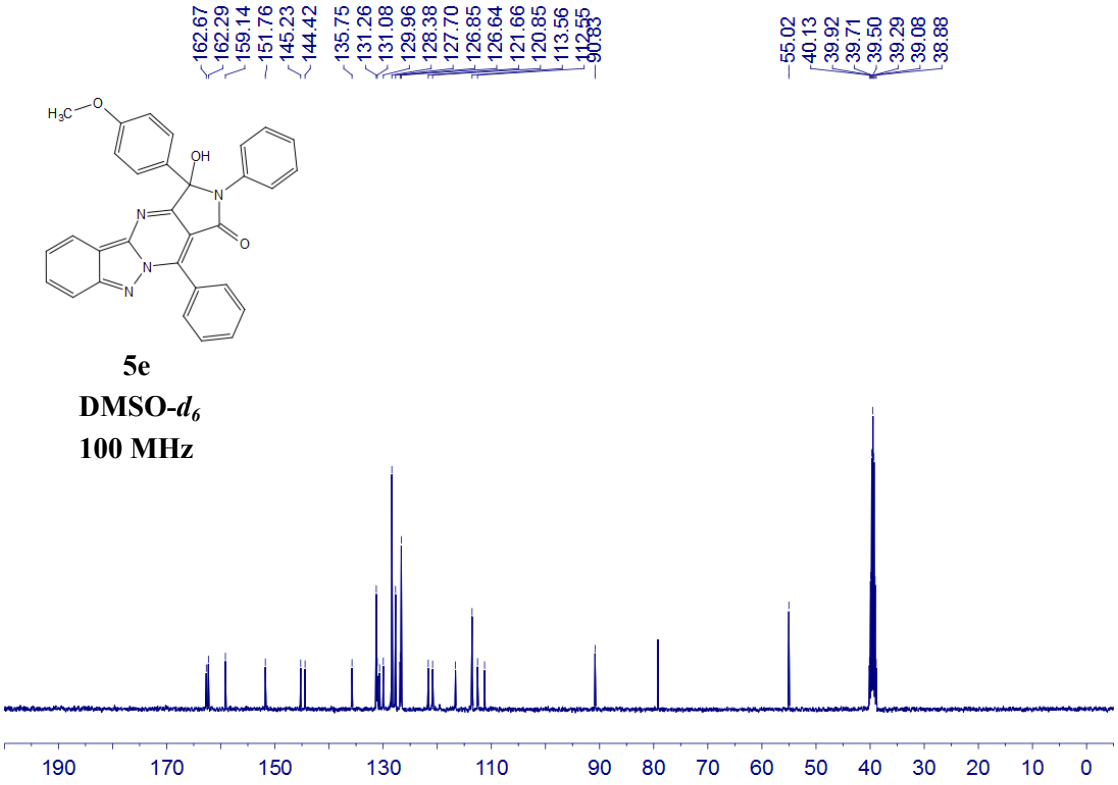
5e



5e

DMSO-d_6

400 MHz

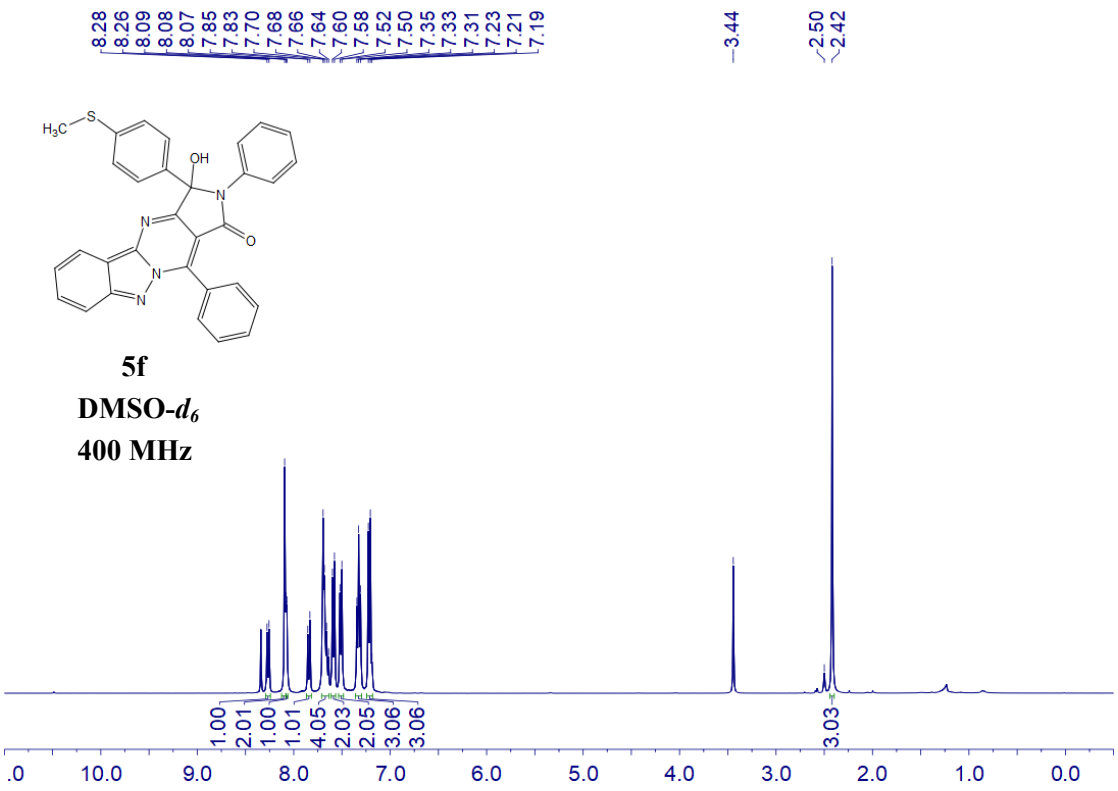


5e

DMSO-d_6

100 MHz

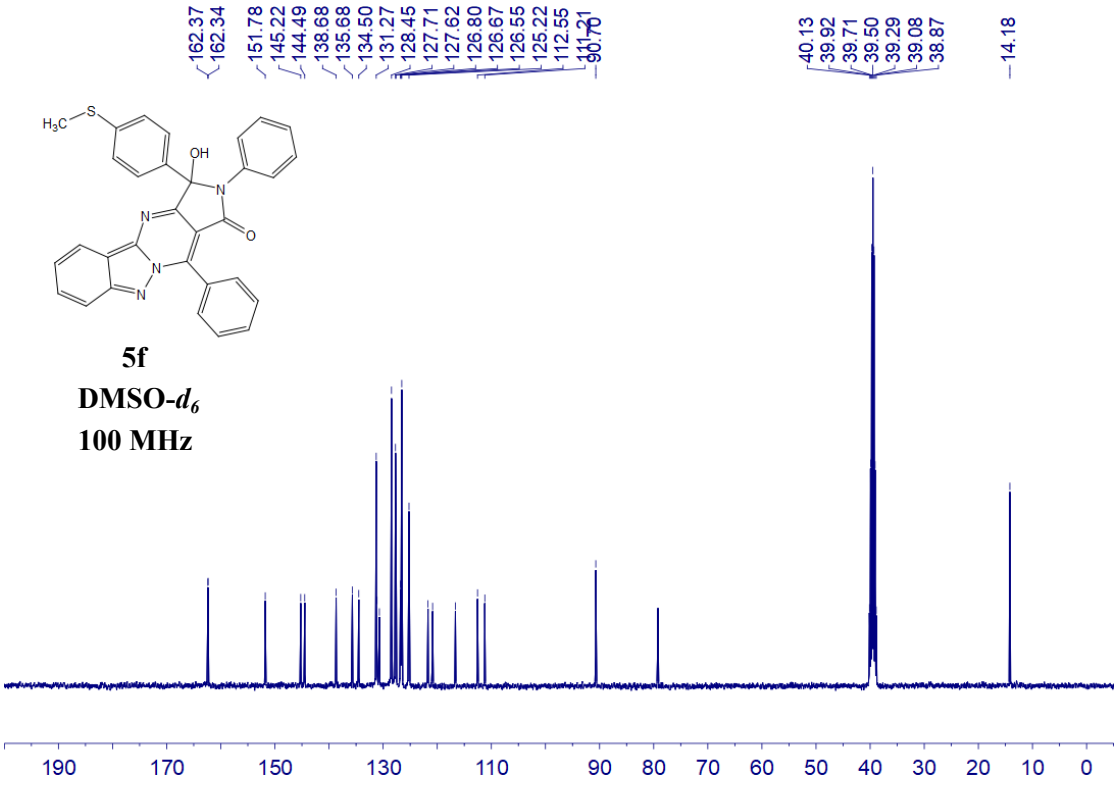
5f



5f

DMSO-d_6

400 MHz

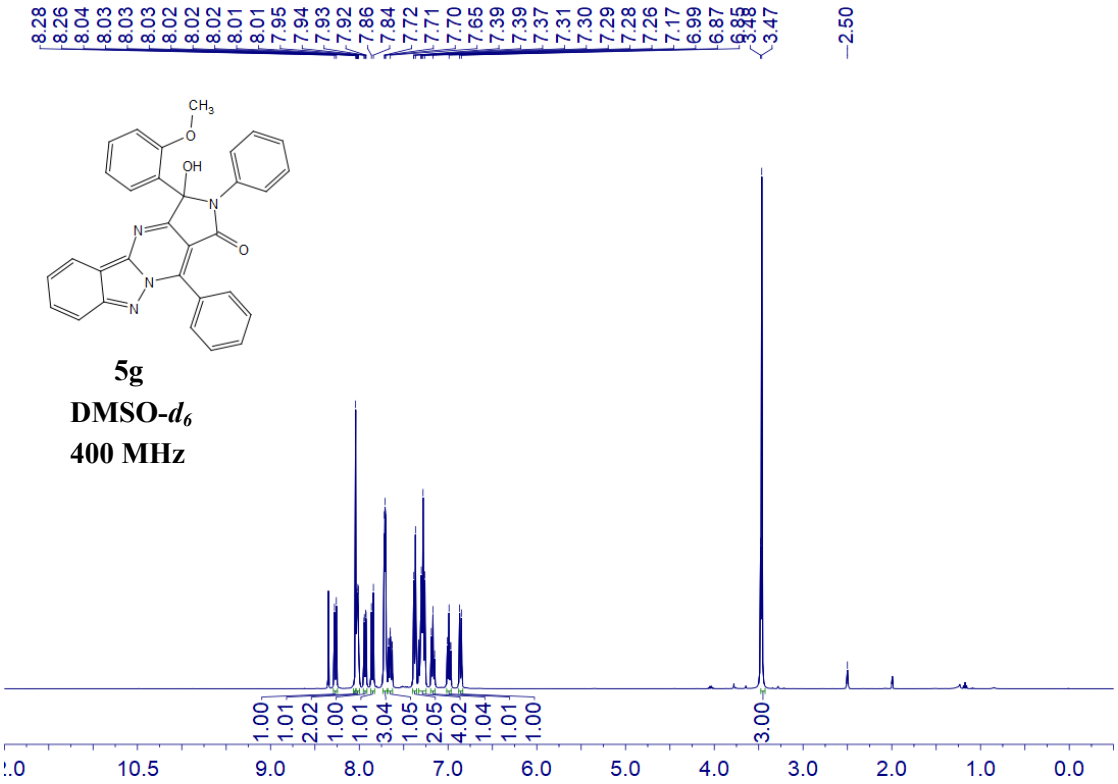


5f

DMSO-d_6

100 MHz

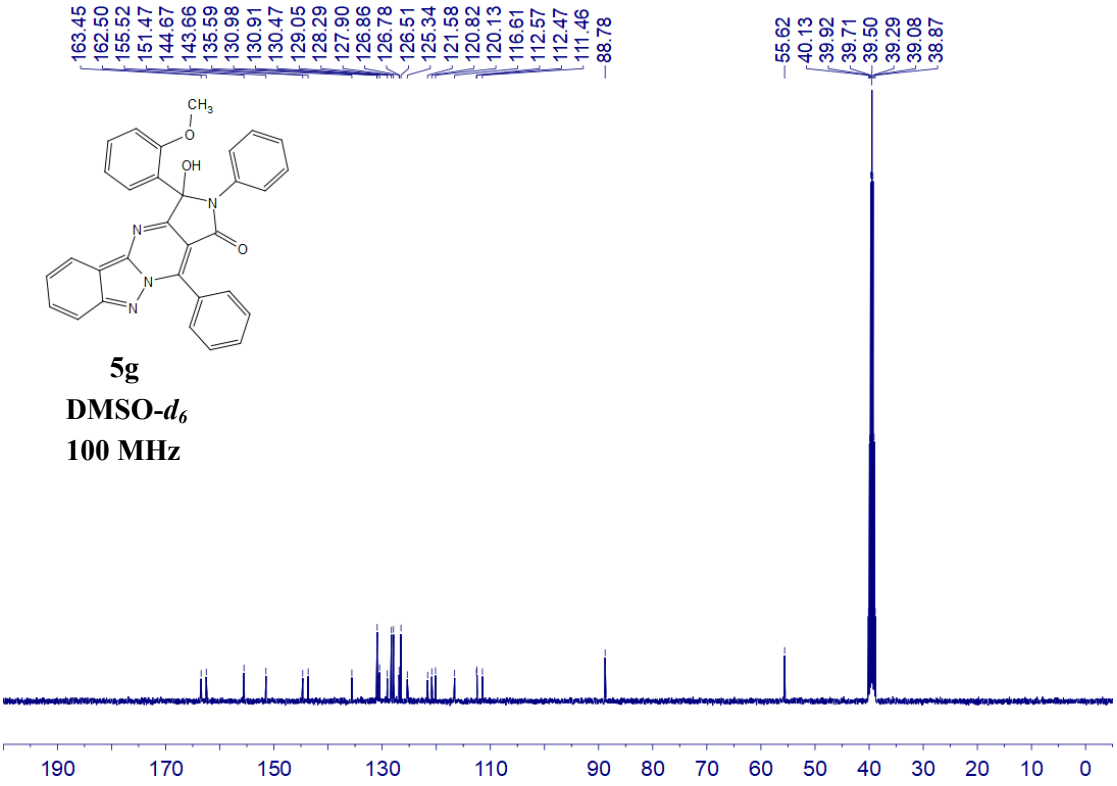
5g



5g

DMSO-d_6

400 MHz

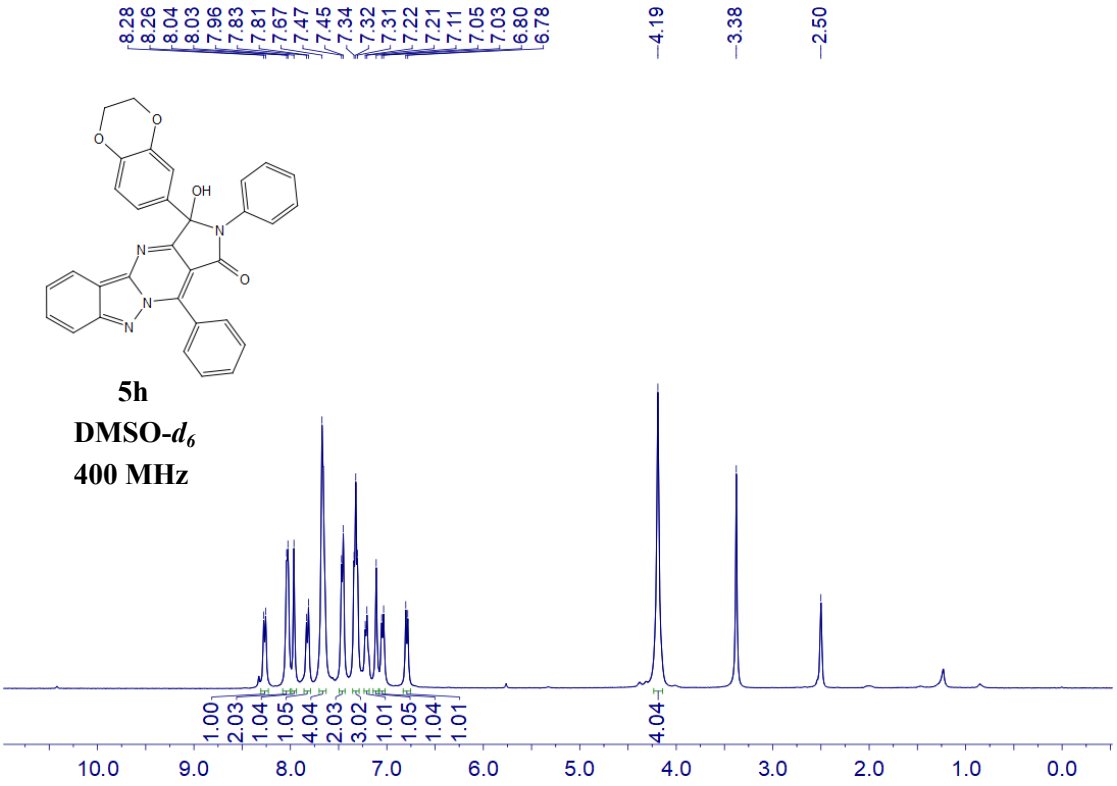


5g

DMSO-d_6

100 MHz

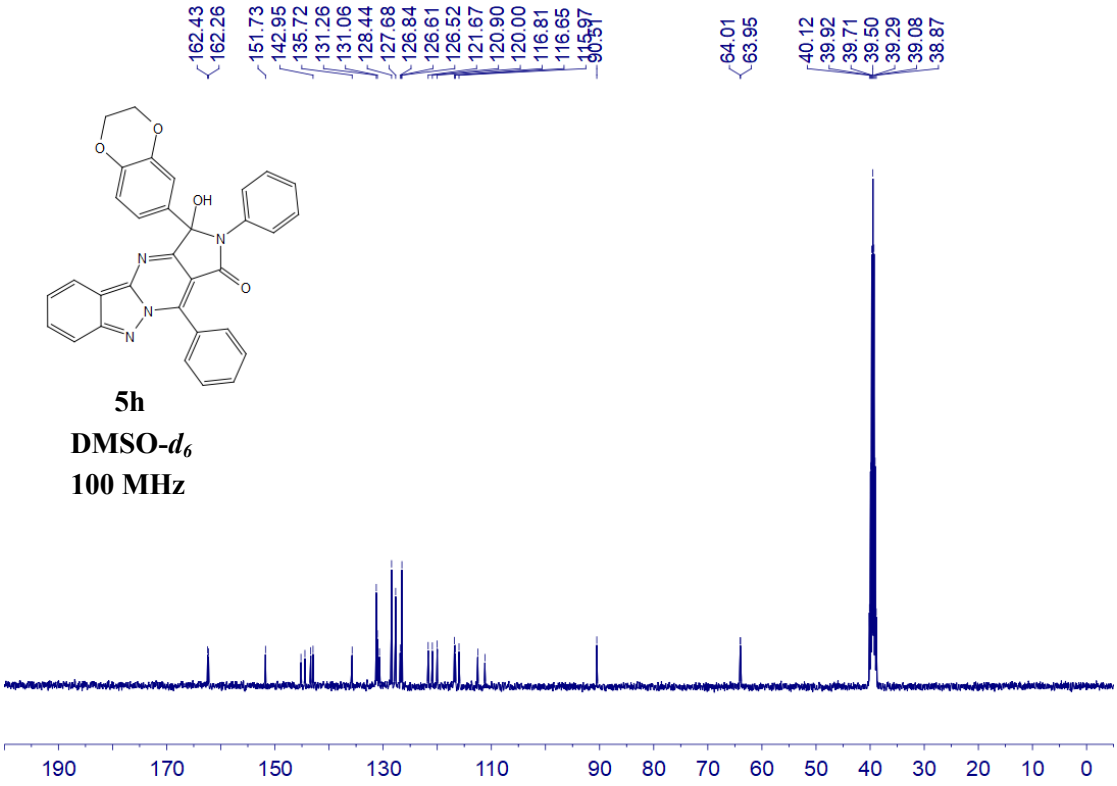
5h



5h

DMSO-d_6

400 MHz

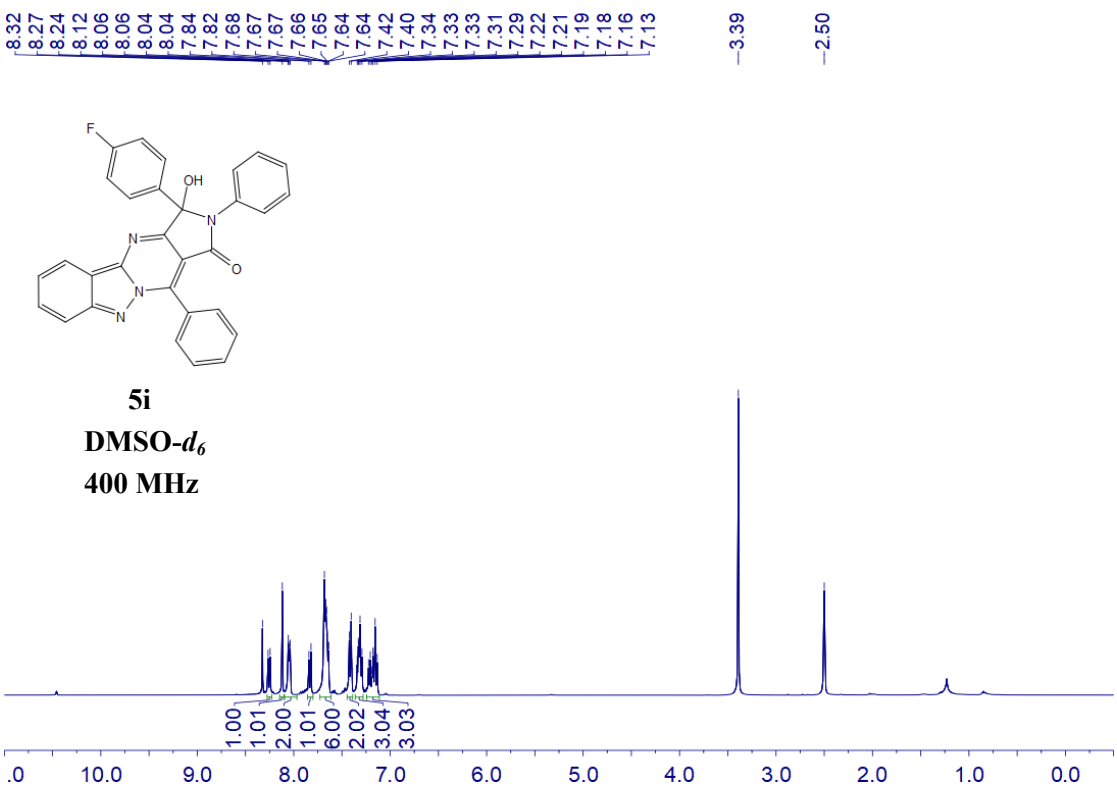


5h

DMSO-d_6

100 MHz

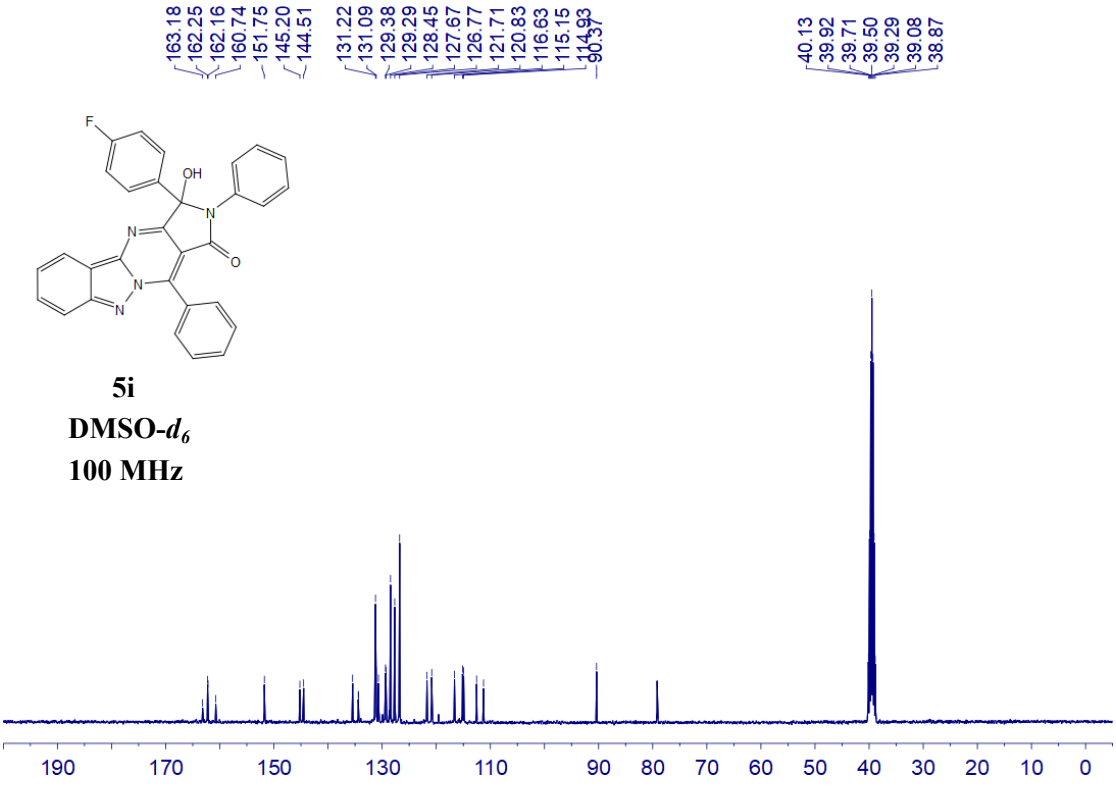
5i



5i

DMSO-d_6

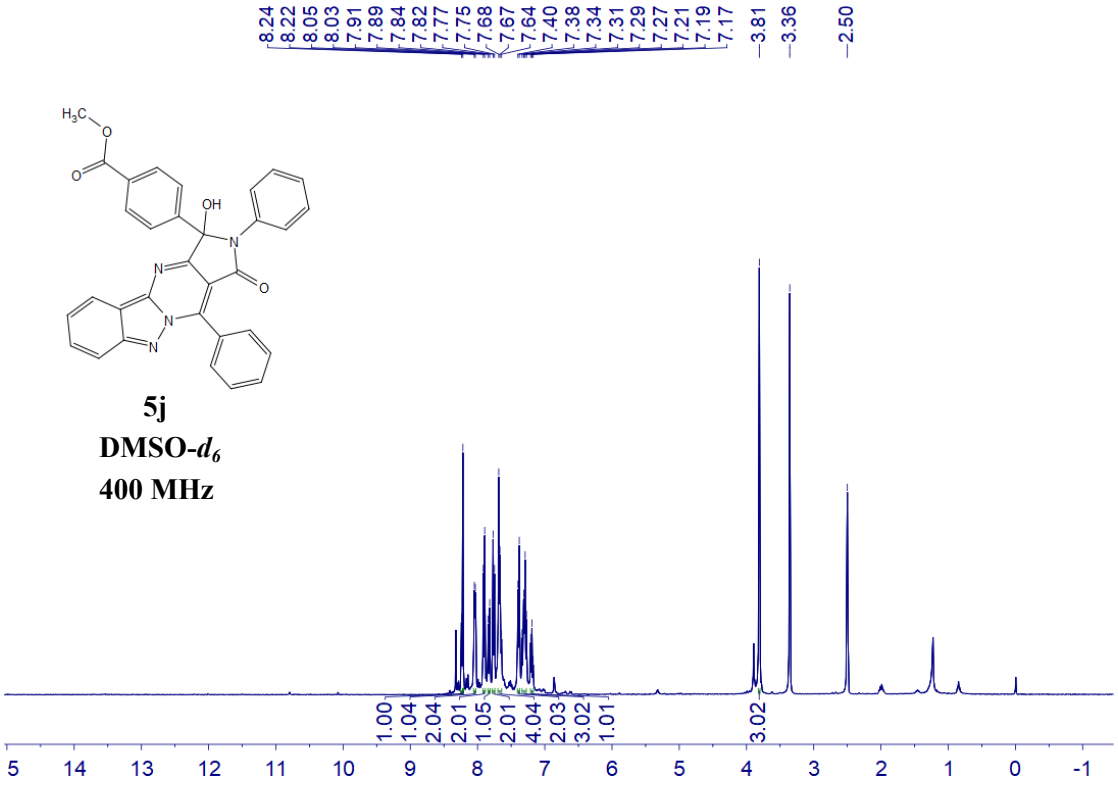
400 MHz



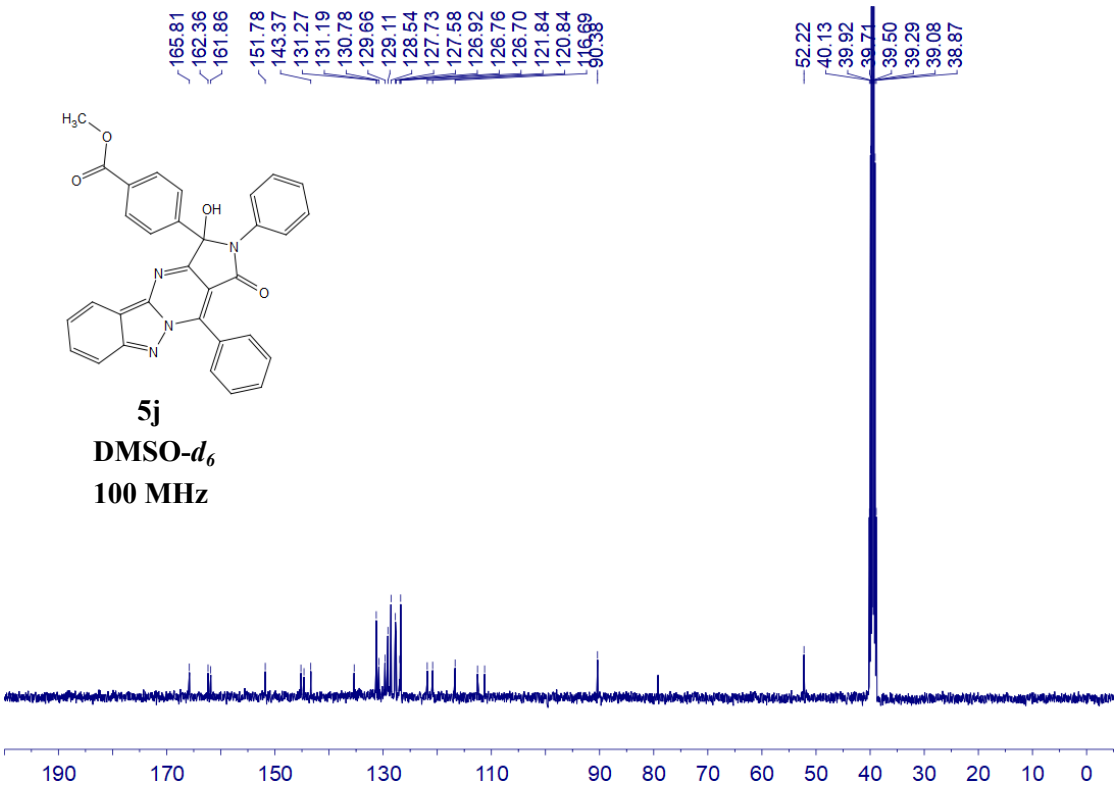
5i
DMSO-d_6
100 MHz

5i
DMSO-d_6
376 MHz

5j

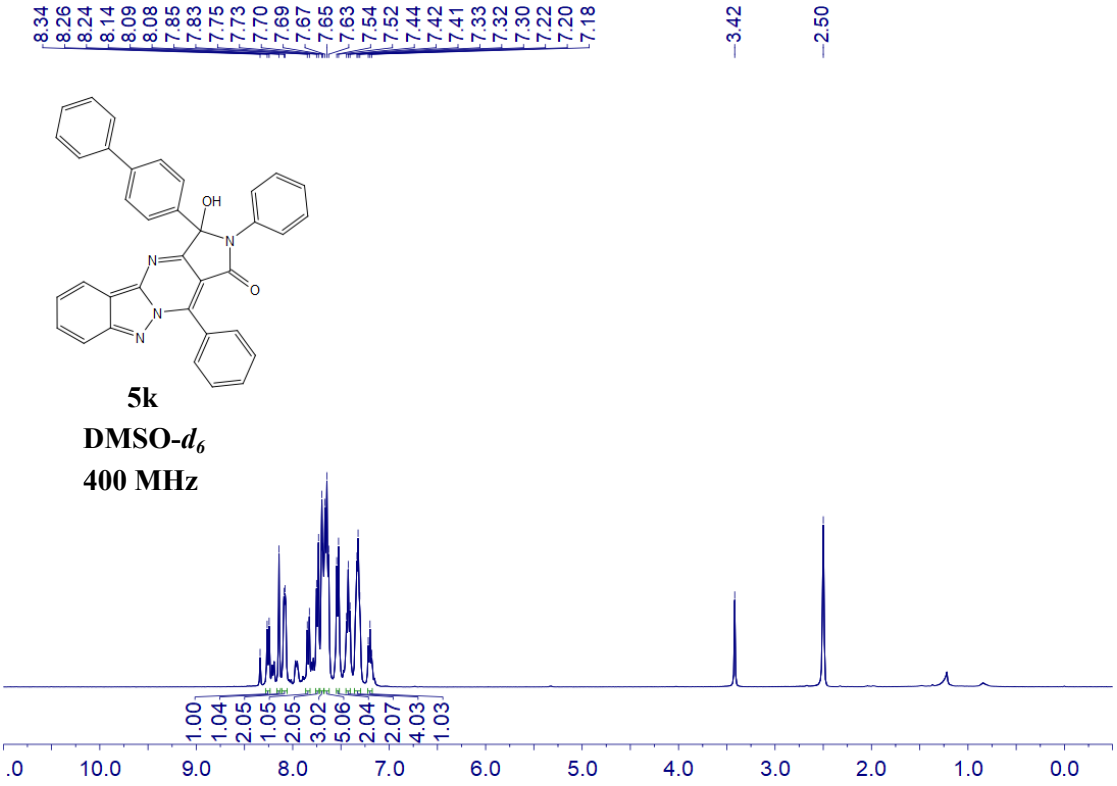


5j
DMSO-d_6
400 MHz



5j
DMSO-d_6
100 MHz

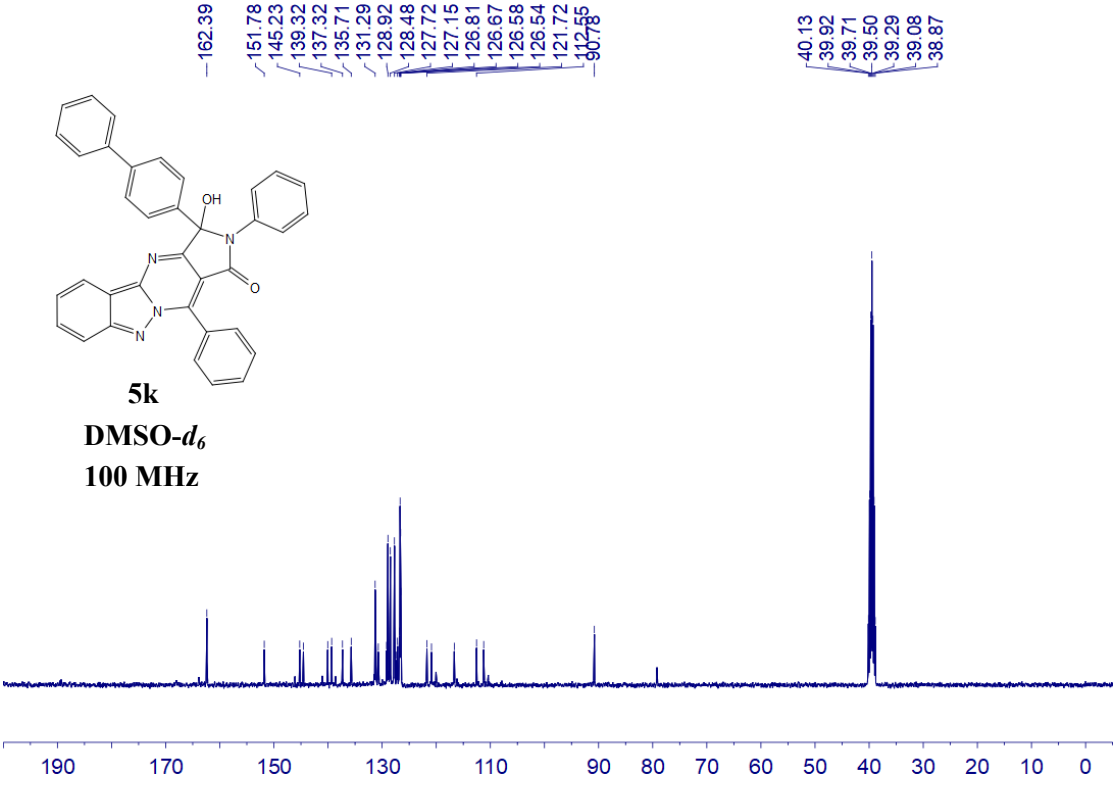
5k



5k

DMSO-d_6

400 MHz

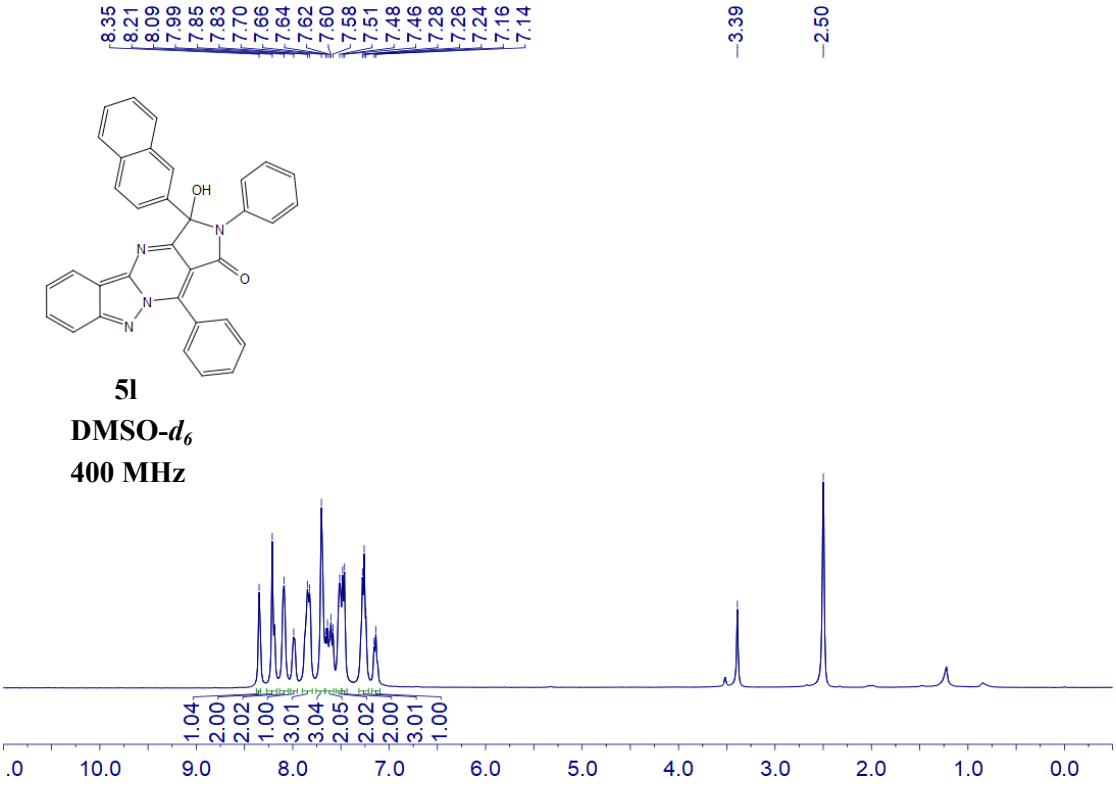


5k

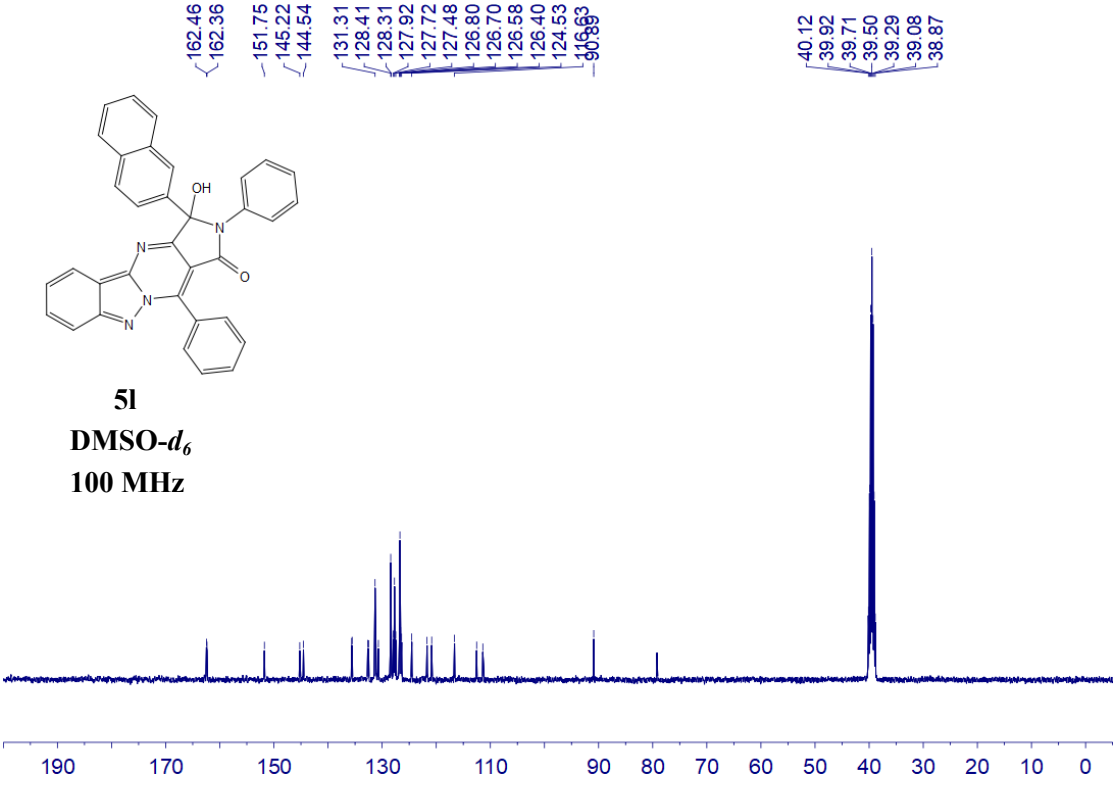
DMSO-d_6

100 MHz

5l

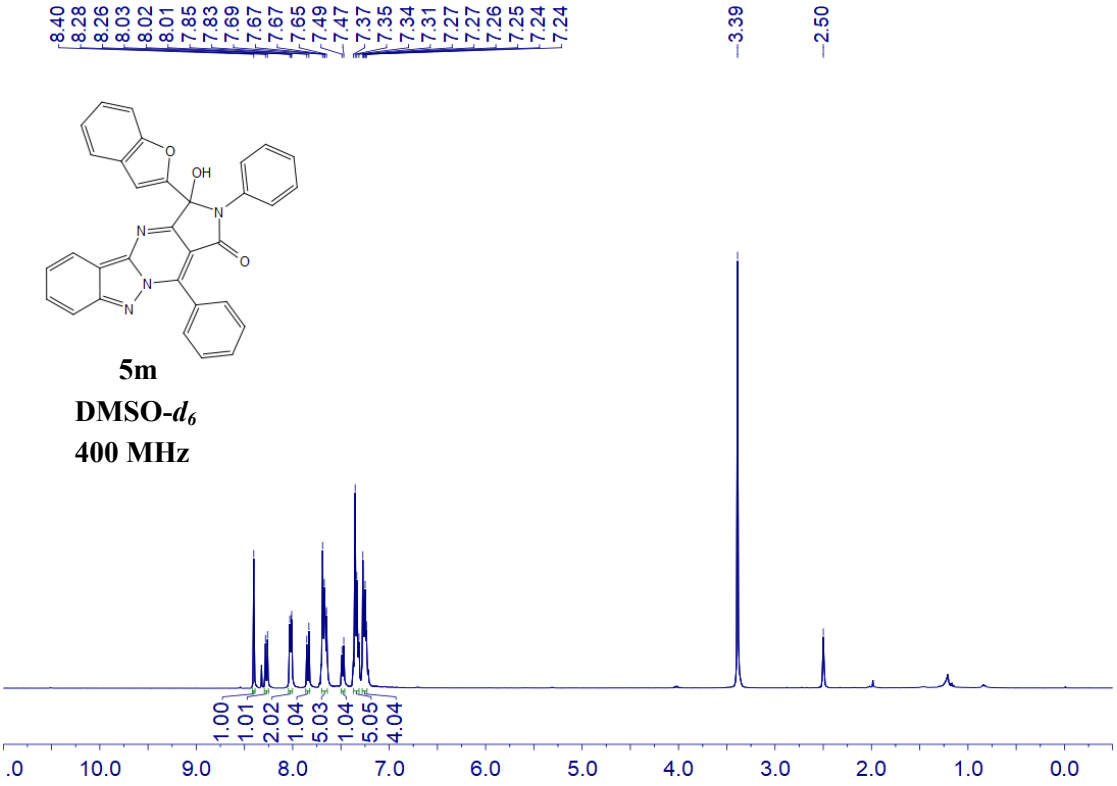


5l
DMSO-d_6
400 MHz

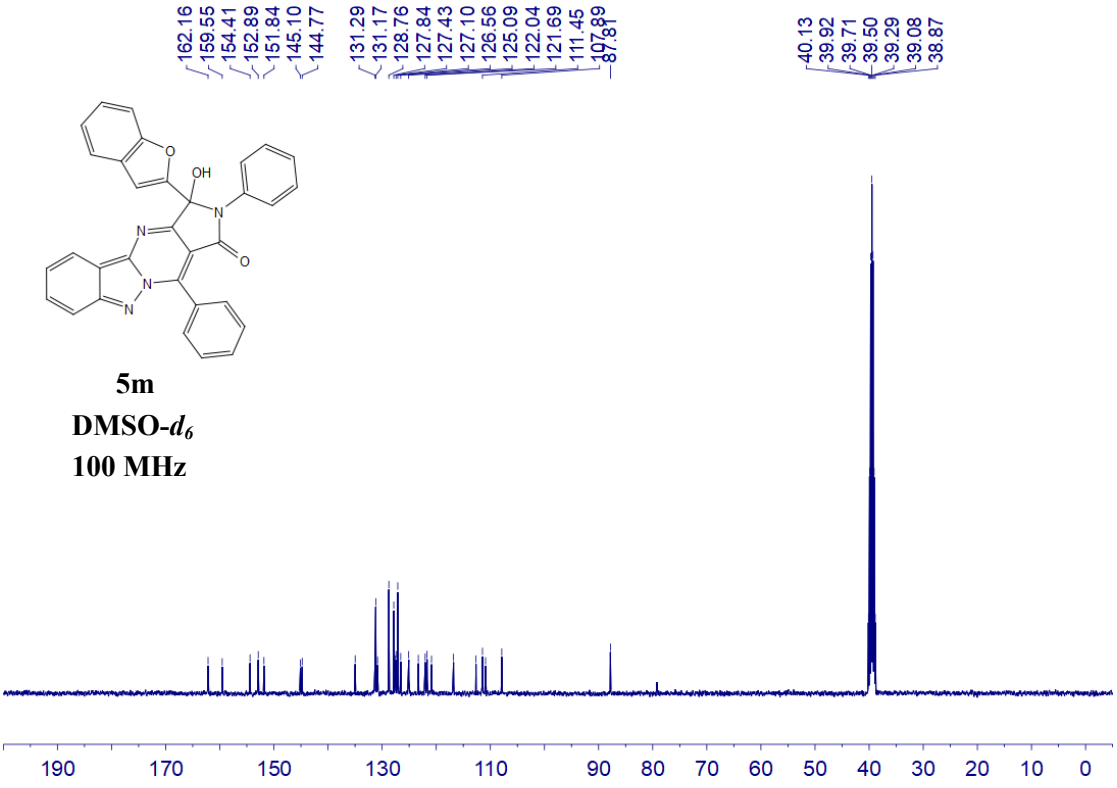


5l
DMSO-d_6
100 MHz

5m

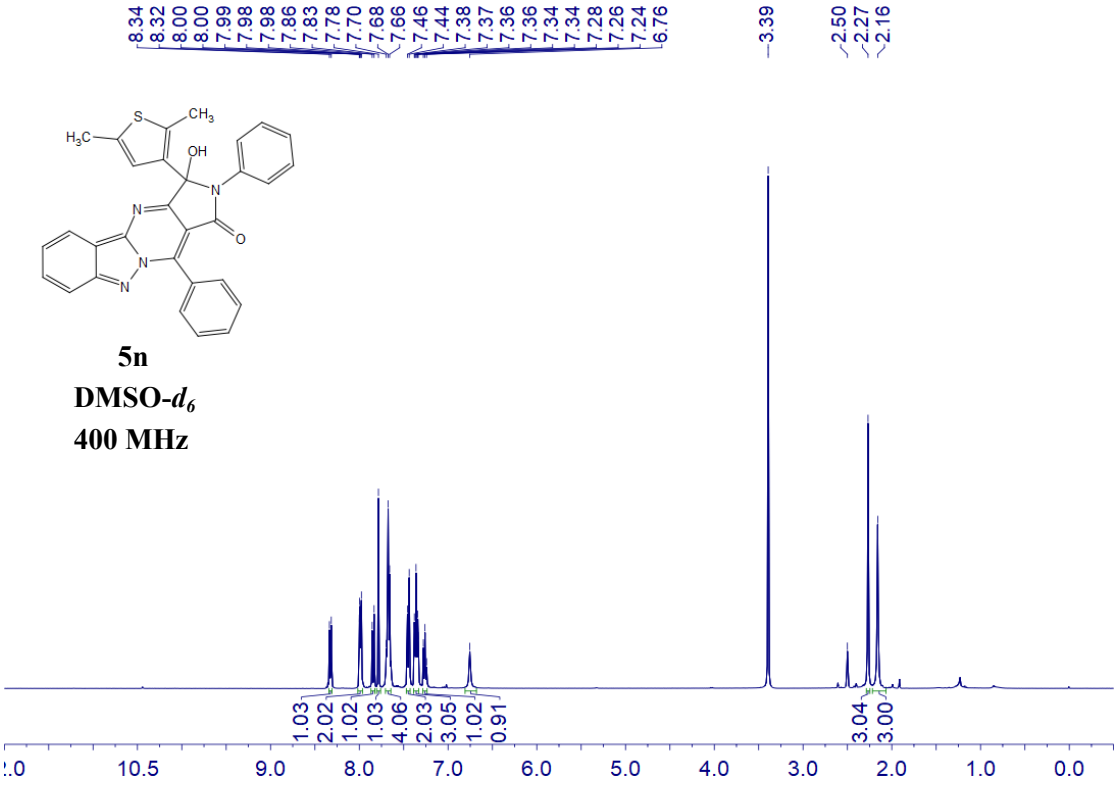


5m
DMSO-d_6
400 MHz

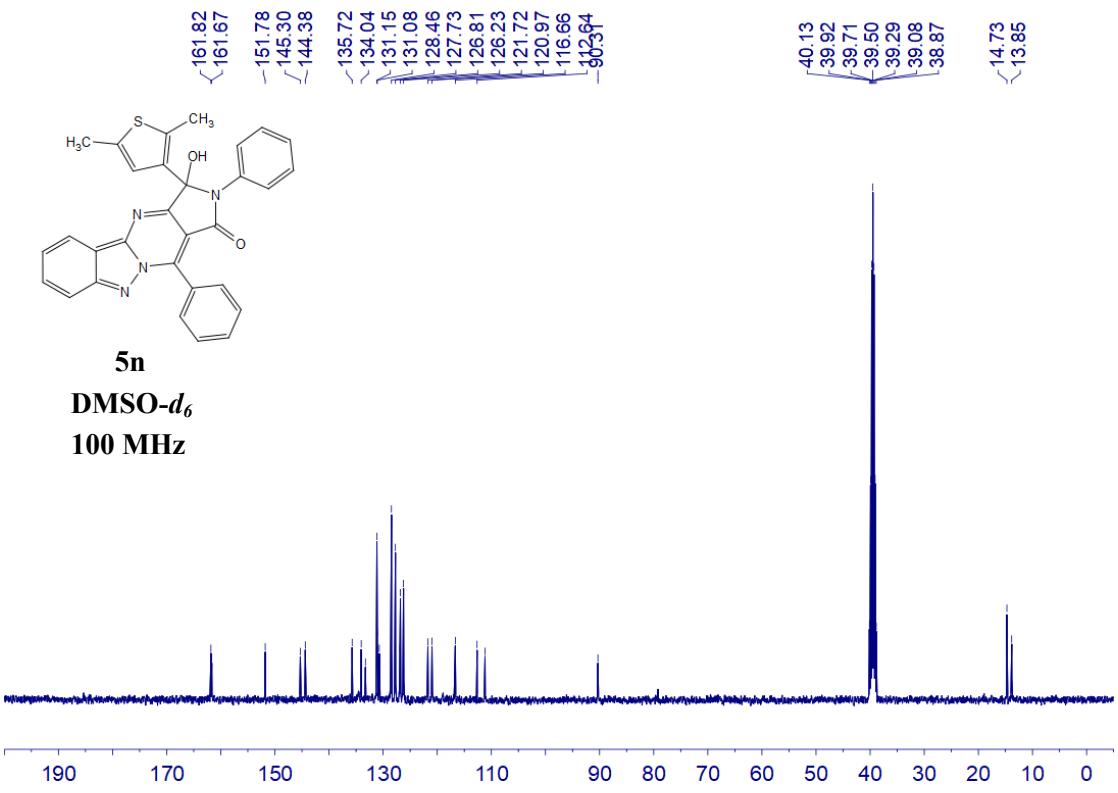


5m
DMSO-d_6
100 MHz

5n

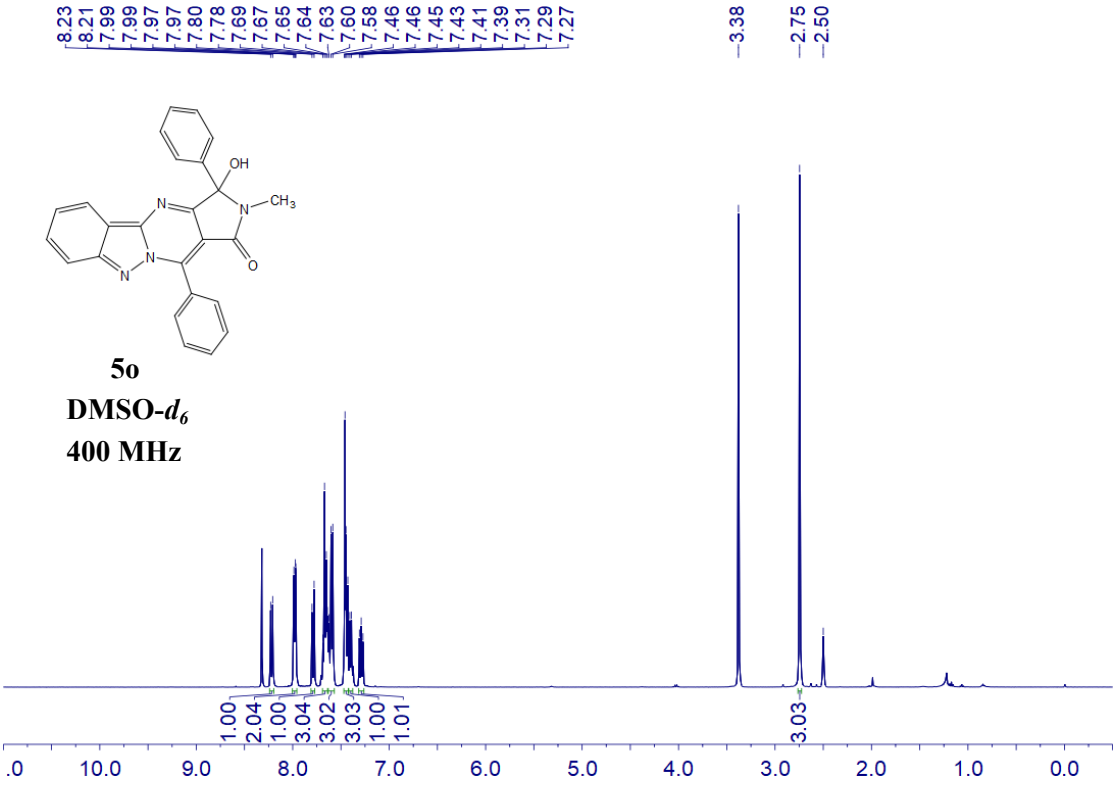


5n
DMSO-d_6
400 MHz

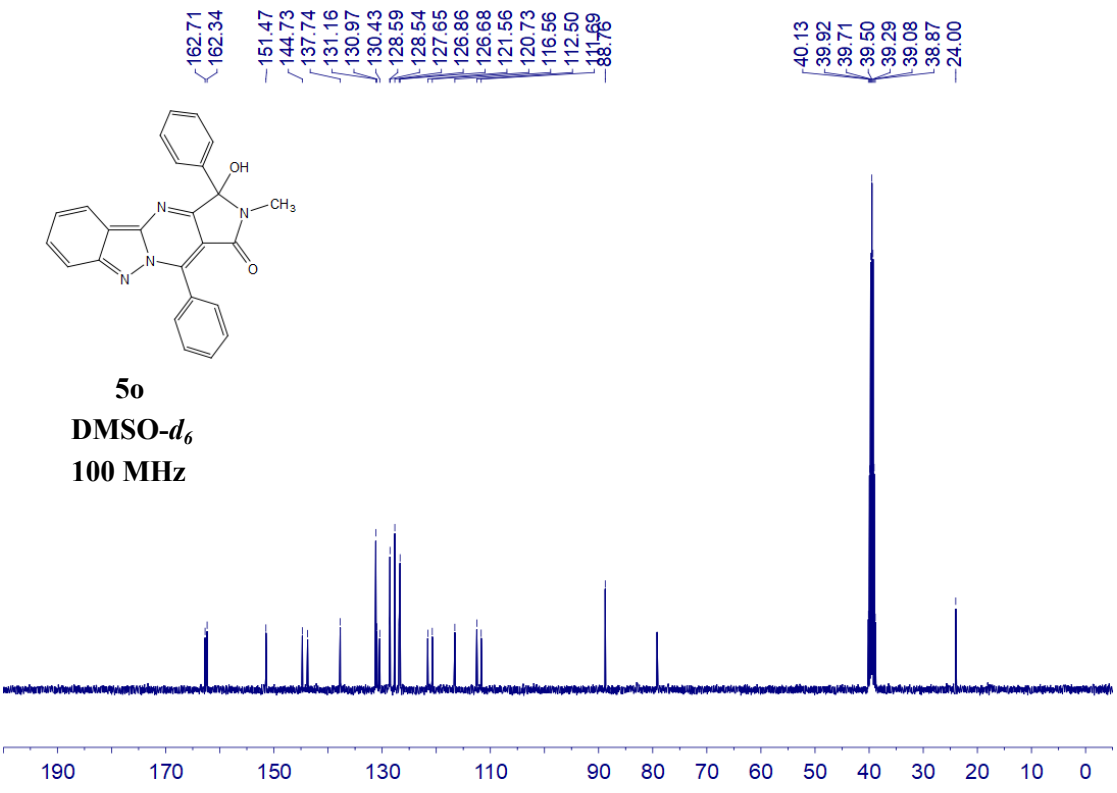


5n
DMSO-d_6
100 MHz

5o

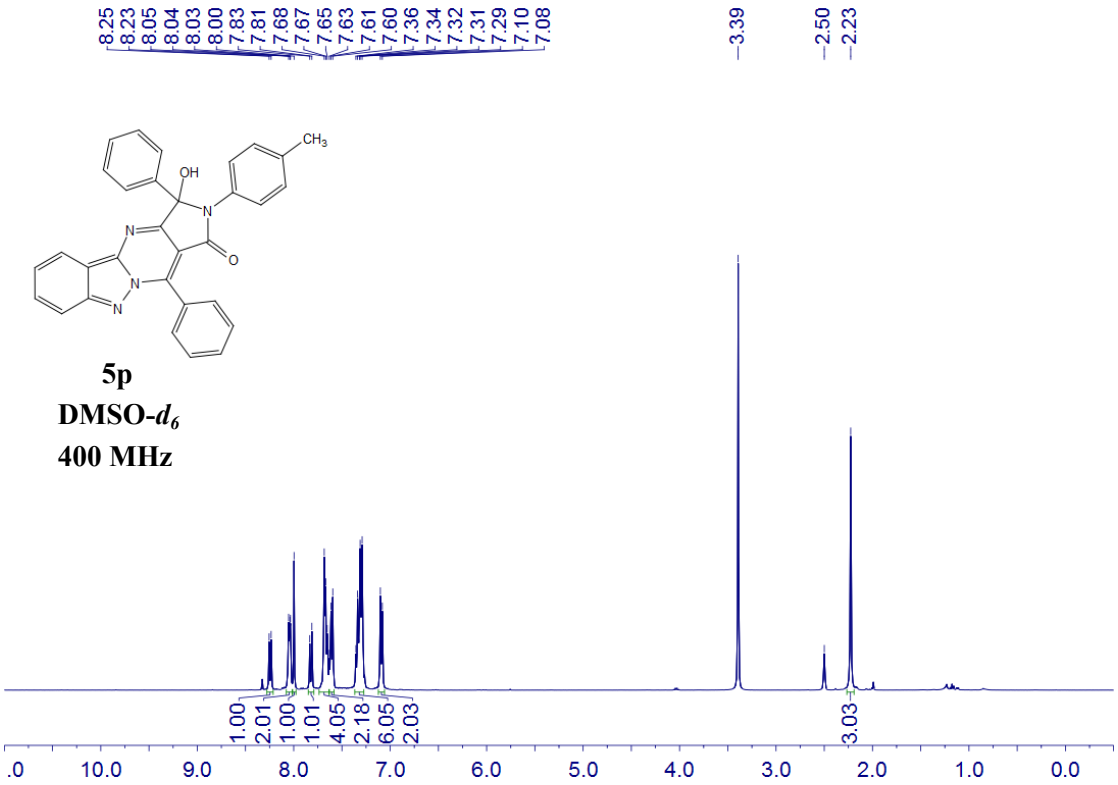


5o
DMSO-d_6
400 MHz

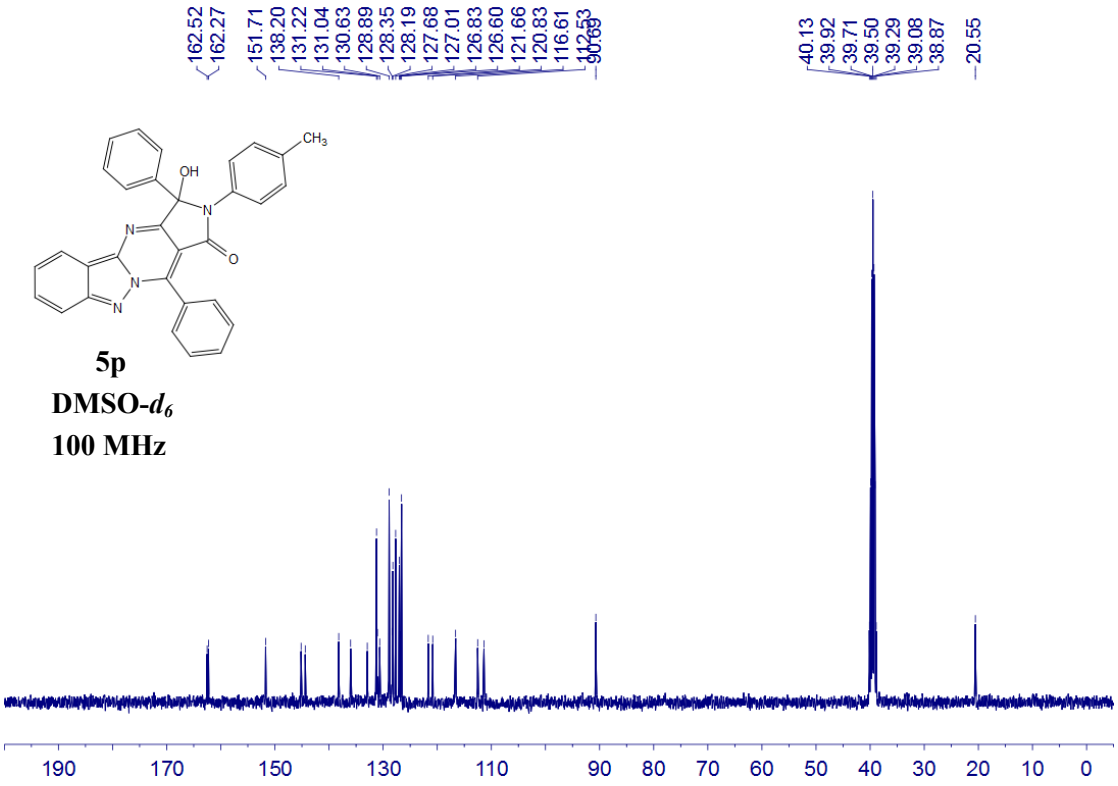


5o
DMSO-d_6
100 MHz

5p

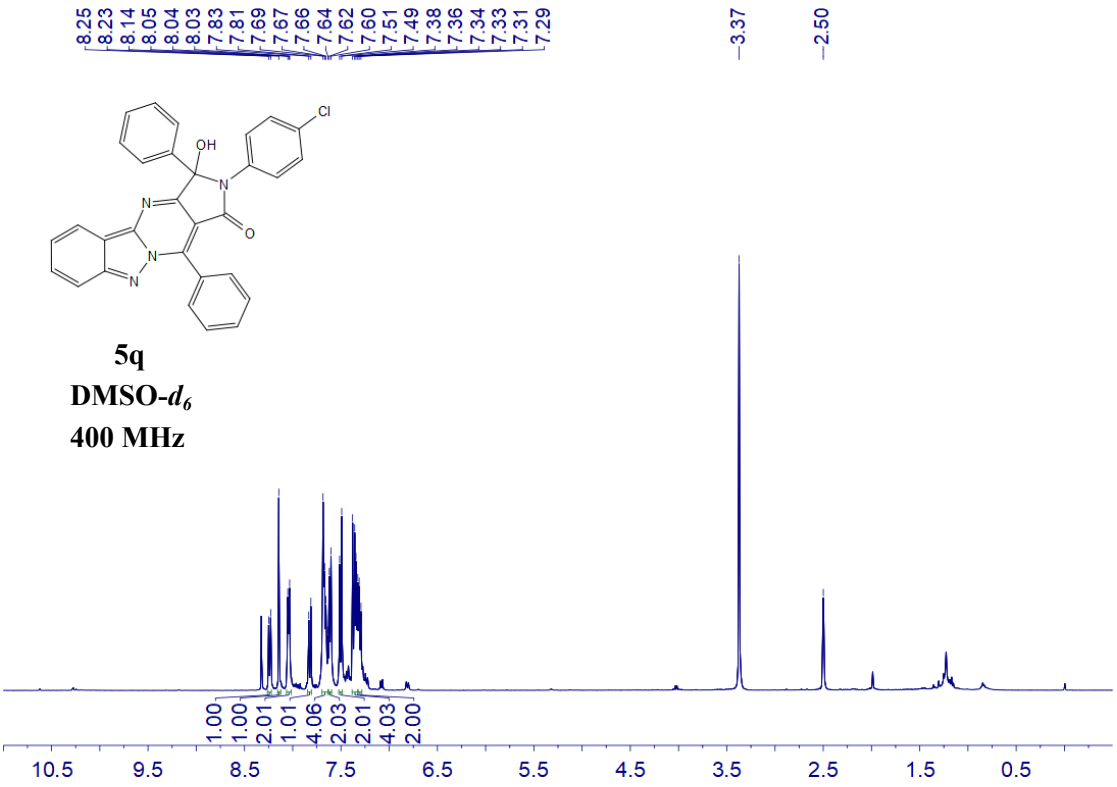


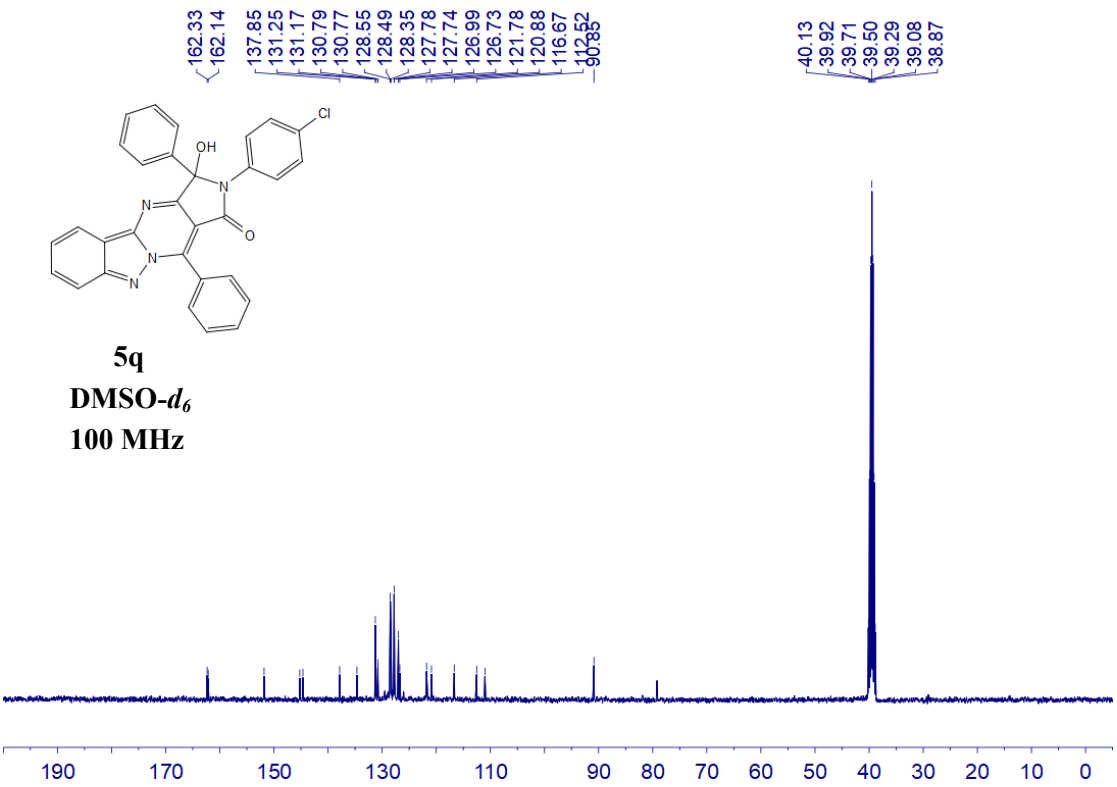
5p
DMSO-*d*$_6$
400 MHz



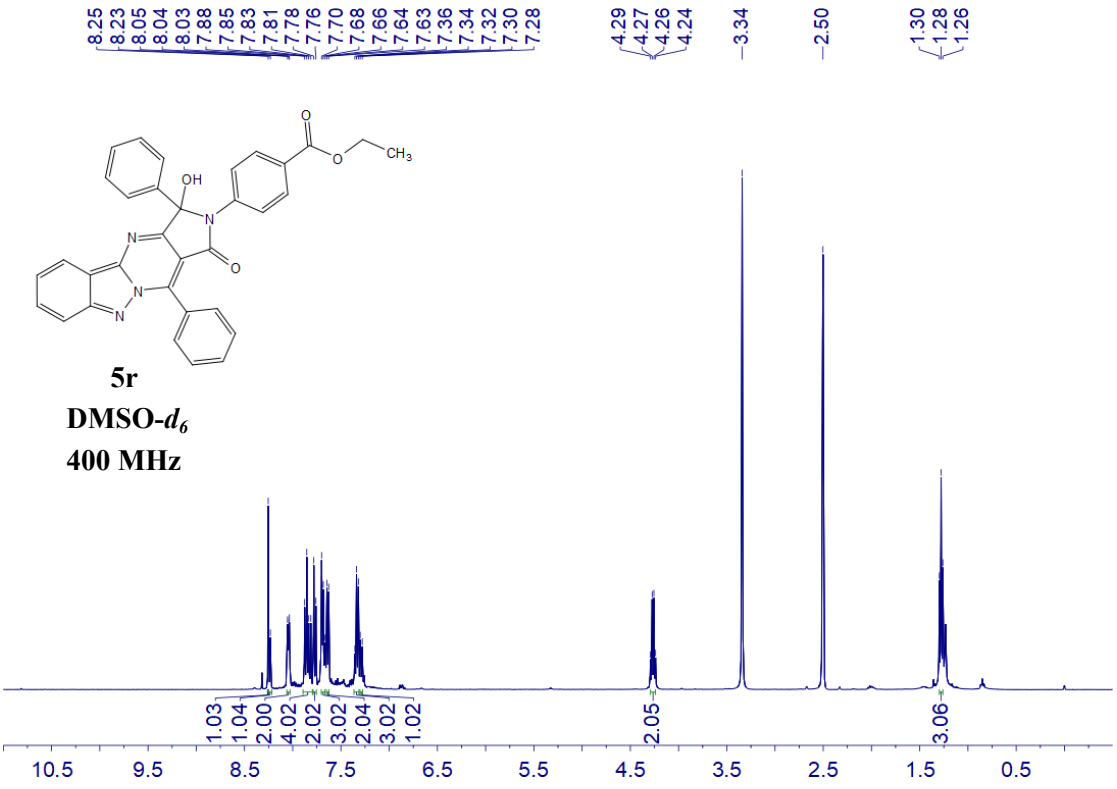
5p
DMSO-*d*$_6$
100 MHz

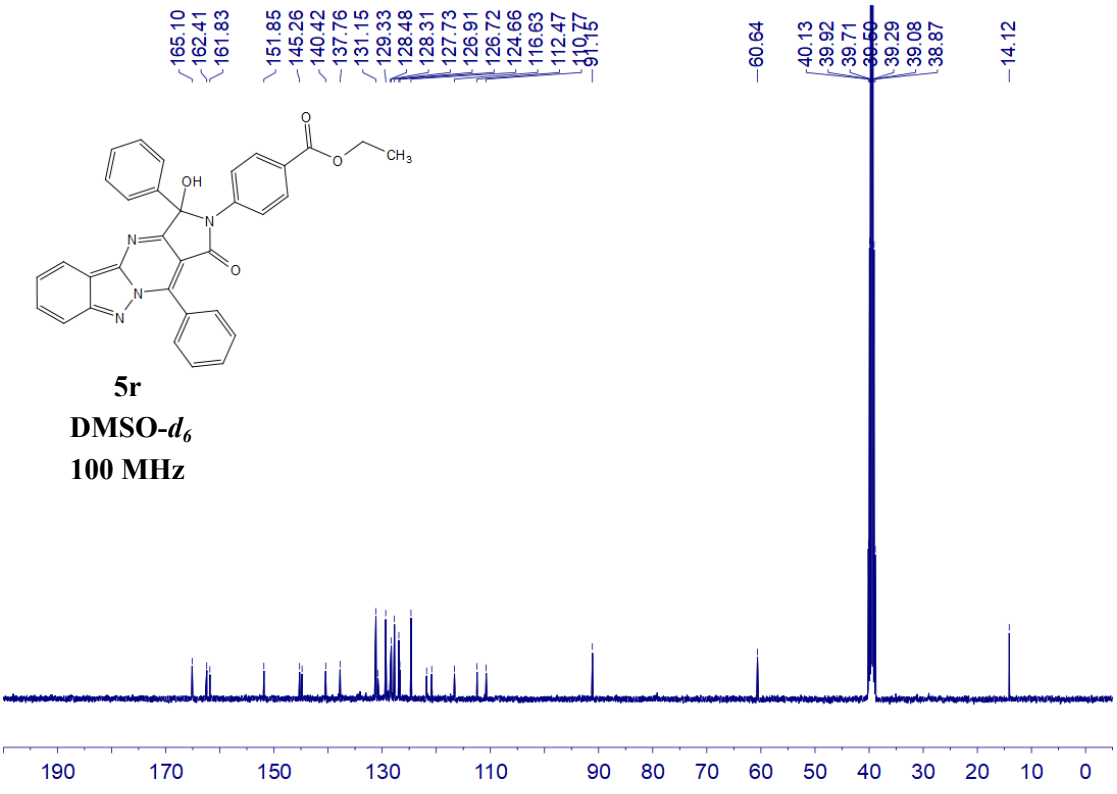
5q


8.25
8.23
8.14
8.05
8.04
8.03
7.83
7.81
7.69
7.67
7.66
7.64
7.62
7.60
7.51
7.49
7.38
7.36
7.34
7.33
7.31
7.29
3.37
2.50
OH
Cl
N
O
N
N
5q
DMSO-d_6
400 MHz
1.00
1.00
2.01
1.01
4.06
2.03
2.01
4.03
2.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

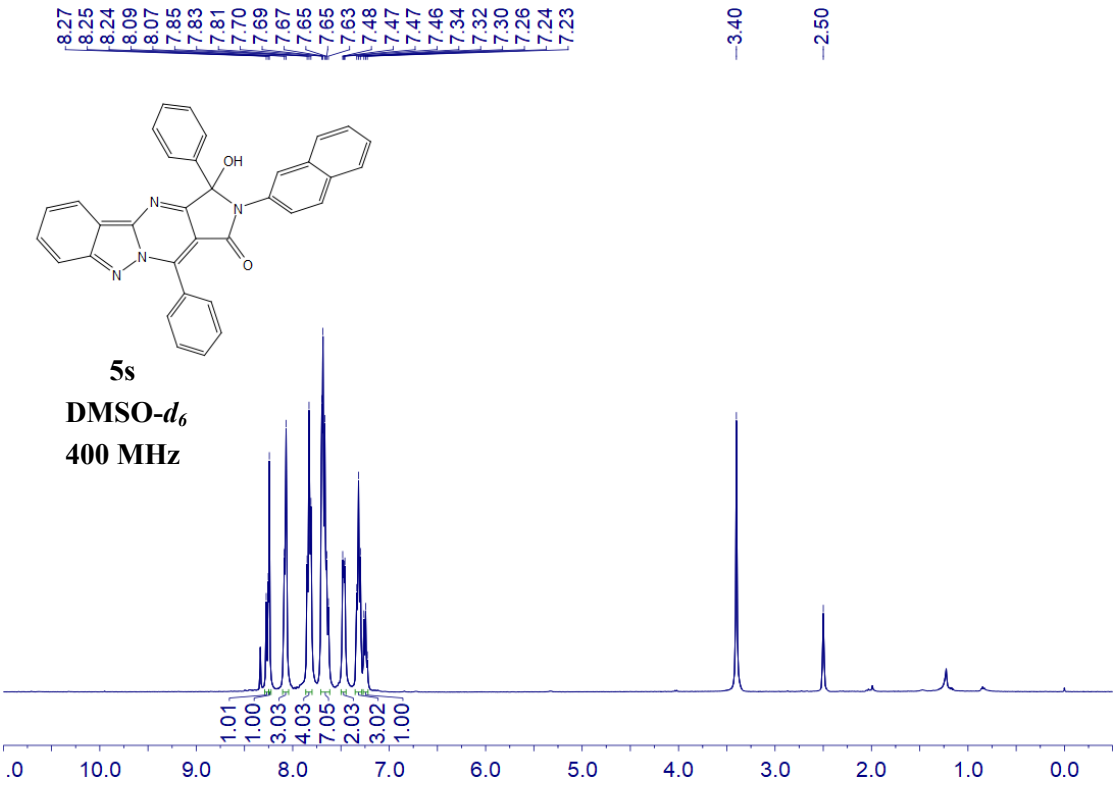

162.33
162.14
137.85
131.25
131.17
130.79
130.77
128.55
128.49
128.35
127.78
127.74
126.99
126.73
121.78
120.88
116.67
112.52
90.85
40.13
39.92
39.71
39.50
39.29
39.08
38.87
OH
Cl
N
O
N
N
5q
DMSO-d_6
100 MHz
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

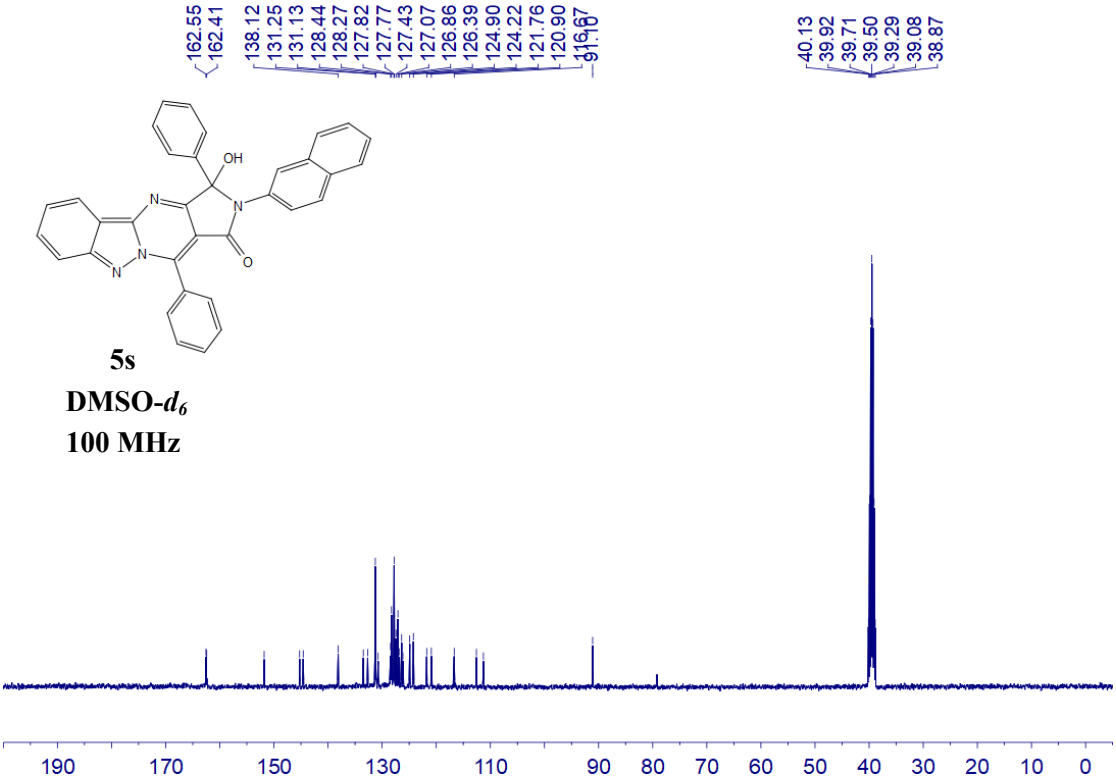
5r


8.25
8.23
8.05
8.04
8.03
7.88
7.85
7.83
7.81
7.78
7.76
7.70
7.68
7.66
7.64
7.63
7.36
7.34
7.32
7.30
7.28
4.29
4.27
4.26
4.24
3.34
2.50
1.30
1.28
1.26
OH
O
CH3
N
O
N
N
5r
DMSO-d6
400 MHz
1.03
1.04
2.00
4.02
2.02
3.02
2.04
3.02
1.02
2.05
3.06
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

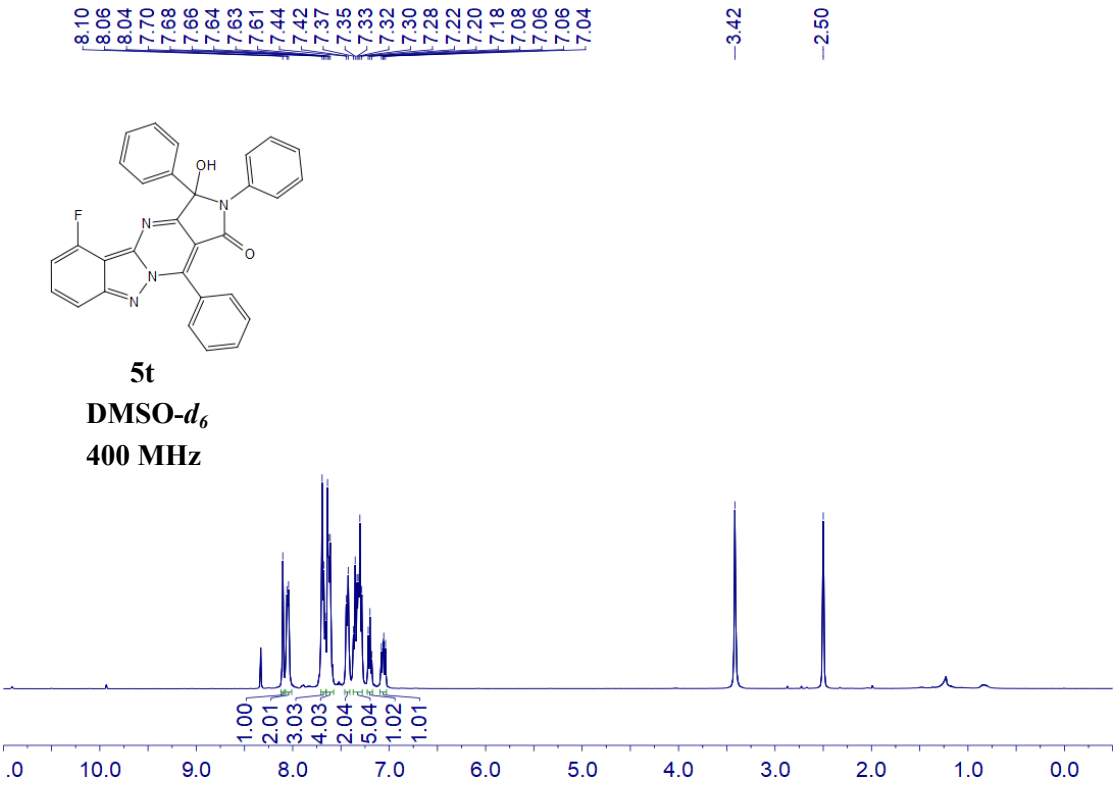

165.10
162.41
161.83
151.85
145.26
140.42
137.76
131.15
129.33
128.48
128.31
127.73
126.91
126.72
124.66
116.63
112.47
110.77
91.15
60.64
40.13
39.92
39.71
39.50
39.29
39.08
38.87
14.12
OH
O
CH3
N
O
N
N
5r
DMSO-d6
100 MHz
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

5s

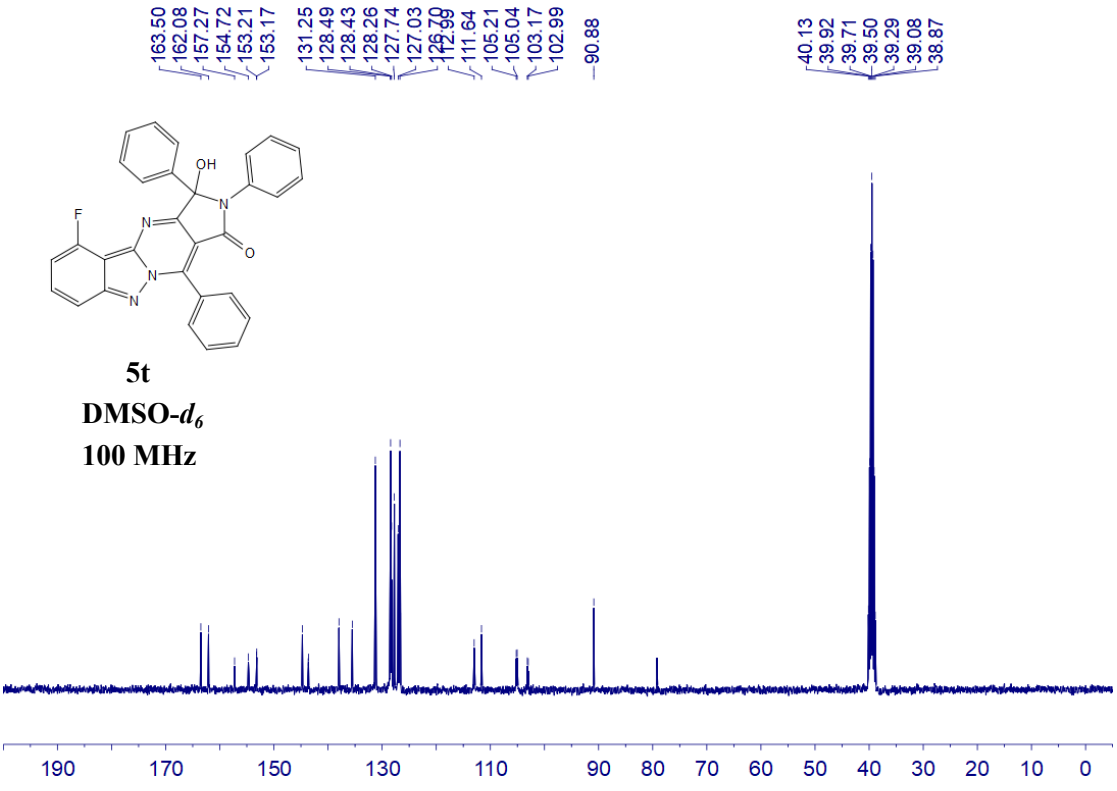

8.27
8.25
8.24
8.09
8.07
7.85
7.83
7.81
7.70
7.69
7.67
7.65
7.65
7.63
7.48
7.47
7.47
7.46
7.34
7.32
7.30
7.26
7.24
7.23
3.40
2.50
OH
N
N
N
O
5s
DMSO-d6
400 MHz
1.01
1.00
3.03
4.03
7.05
2.03
3.02
1.00
.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


162.55
162.41
138.12
131.25
131.13
128.44
128.27
127.82
127.77
127.43
127.07
126.86
126.39
124.90
124.22
121.76
120.90
116.67
91.10
40.13
39.92
39.71
39.50
39.29
39.08
38.87
OH
N
N
N
O
5s
DMSO-d6
100 MHz
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

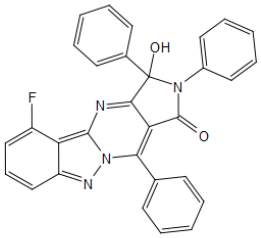
5t



5t
DMSO-d_6
400 MHz



5t
DMSO-d_6
100 MHz

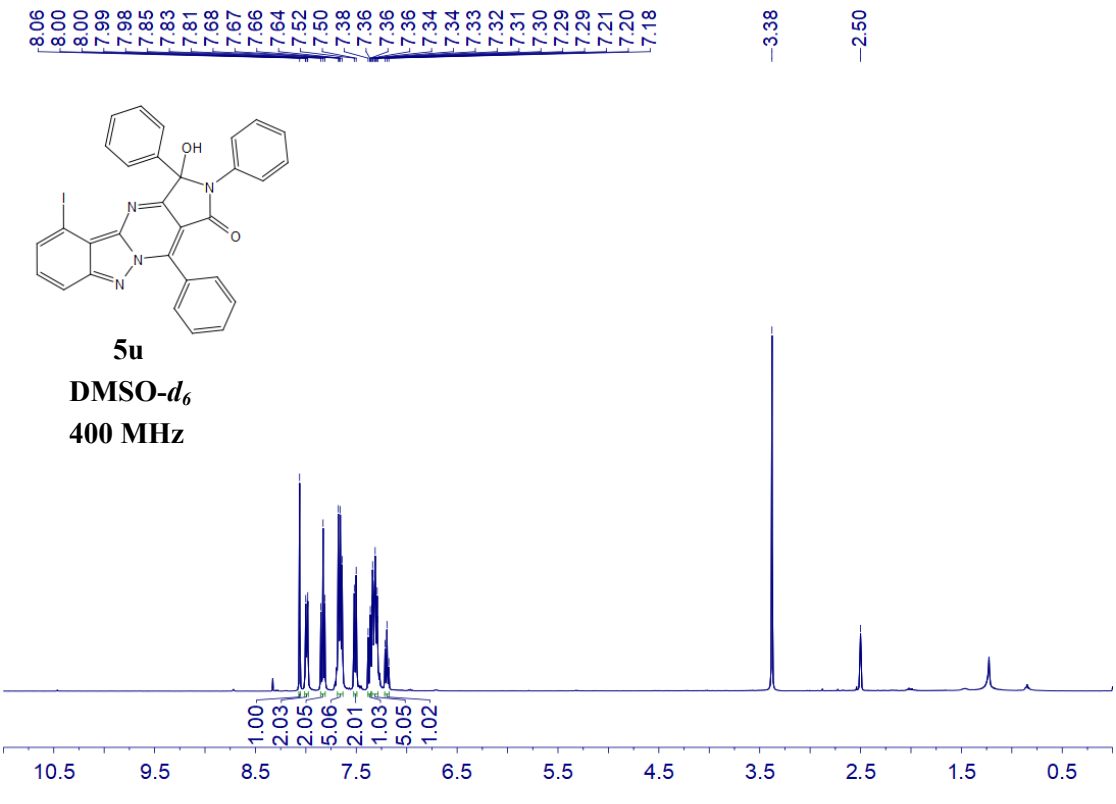


5t

DMSO-d_6

376 MHz

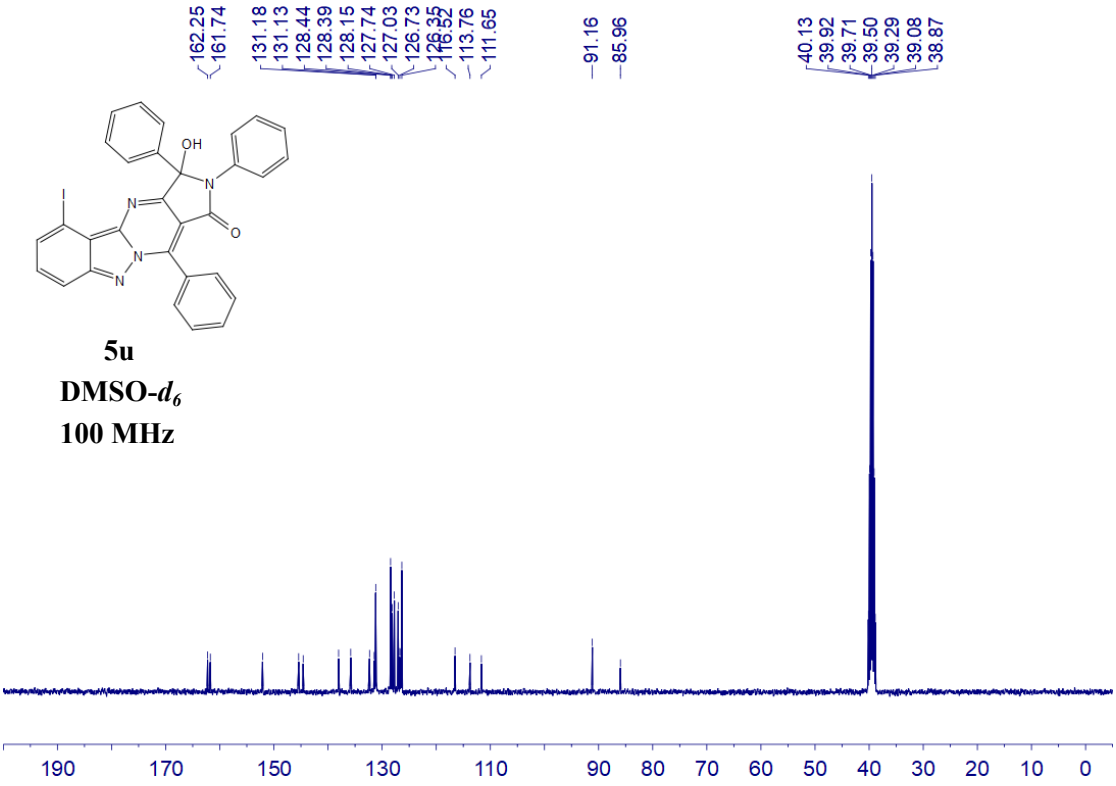
5u



5u

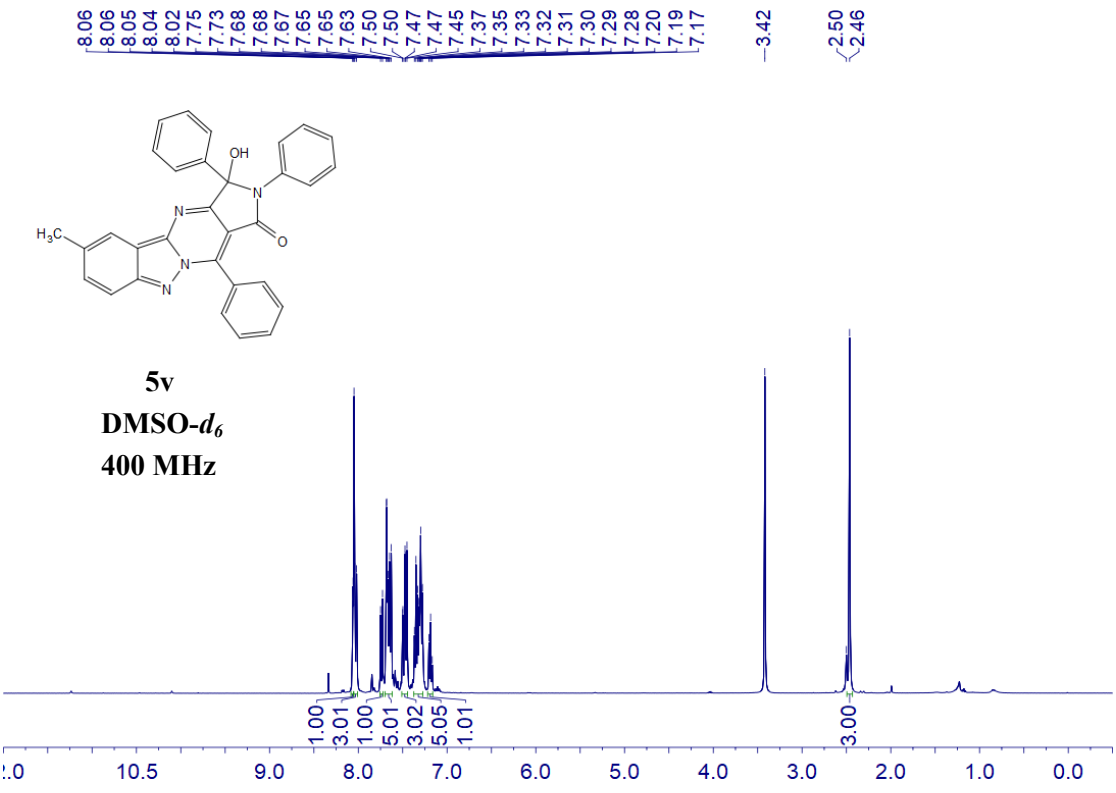
DMSO-d_6

400 MHz

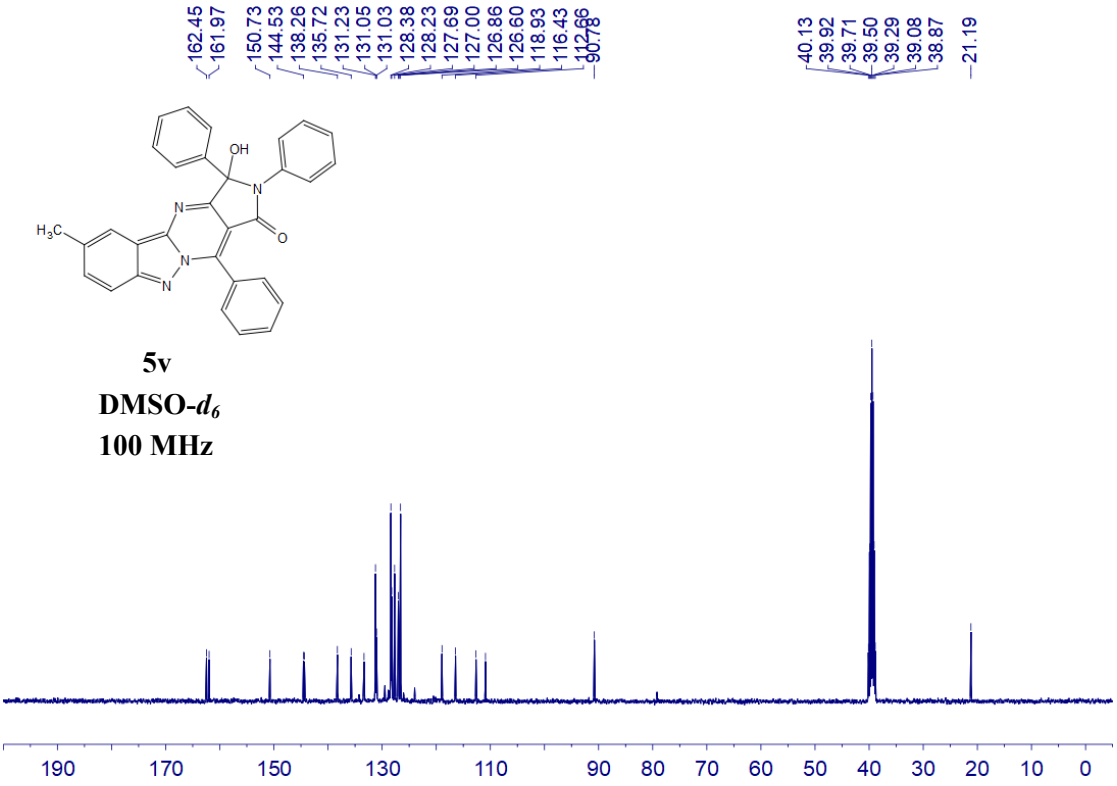


5u
DMSO-*d*$_6$
100 MHz

5v



5v
DMSO-*d*$_6$
400 MHz

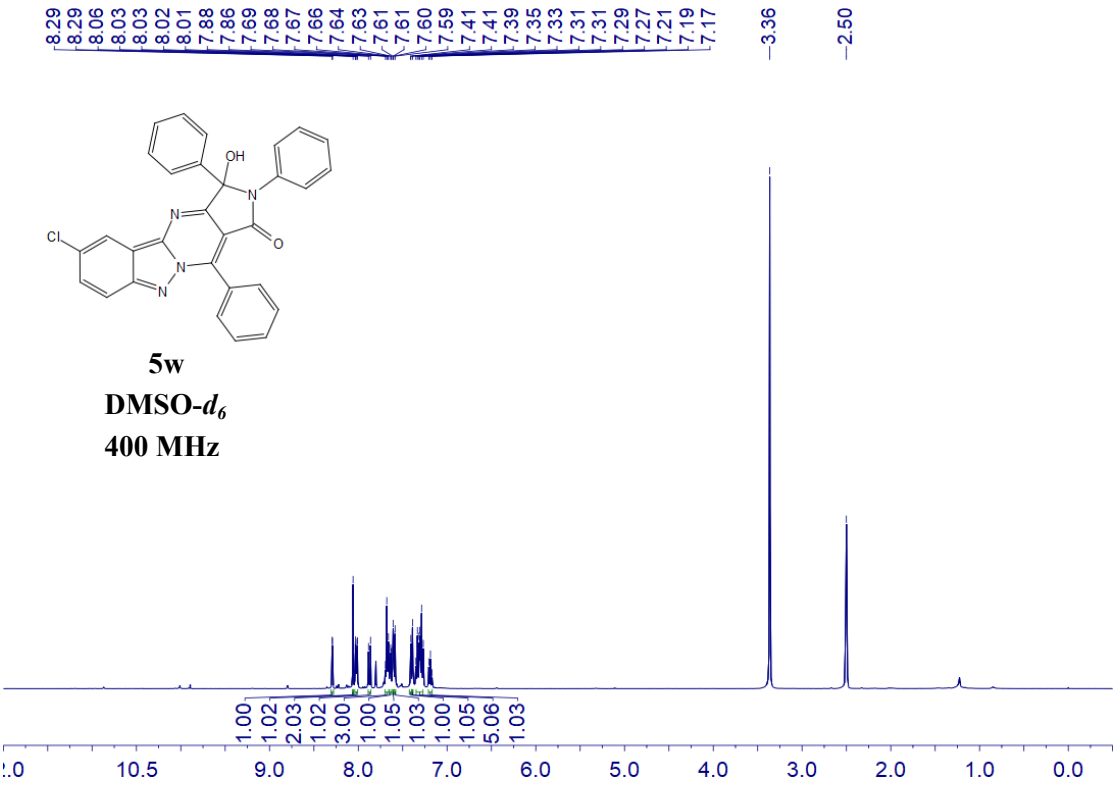


5v

DMSO-d_6

100 MHz

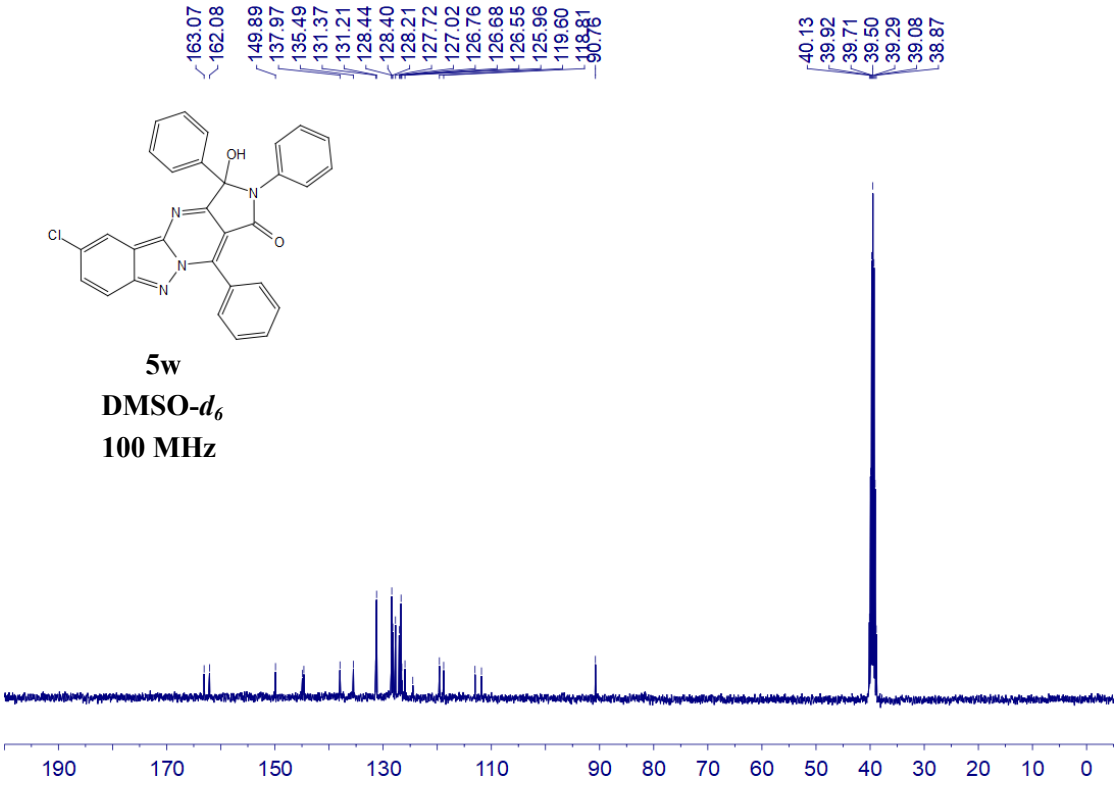
5w



5w

DMSO-d_6

400 MHz

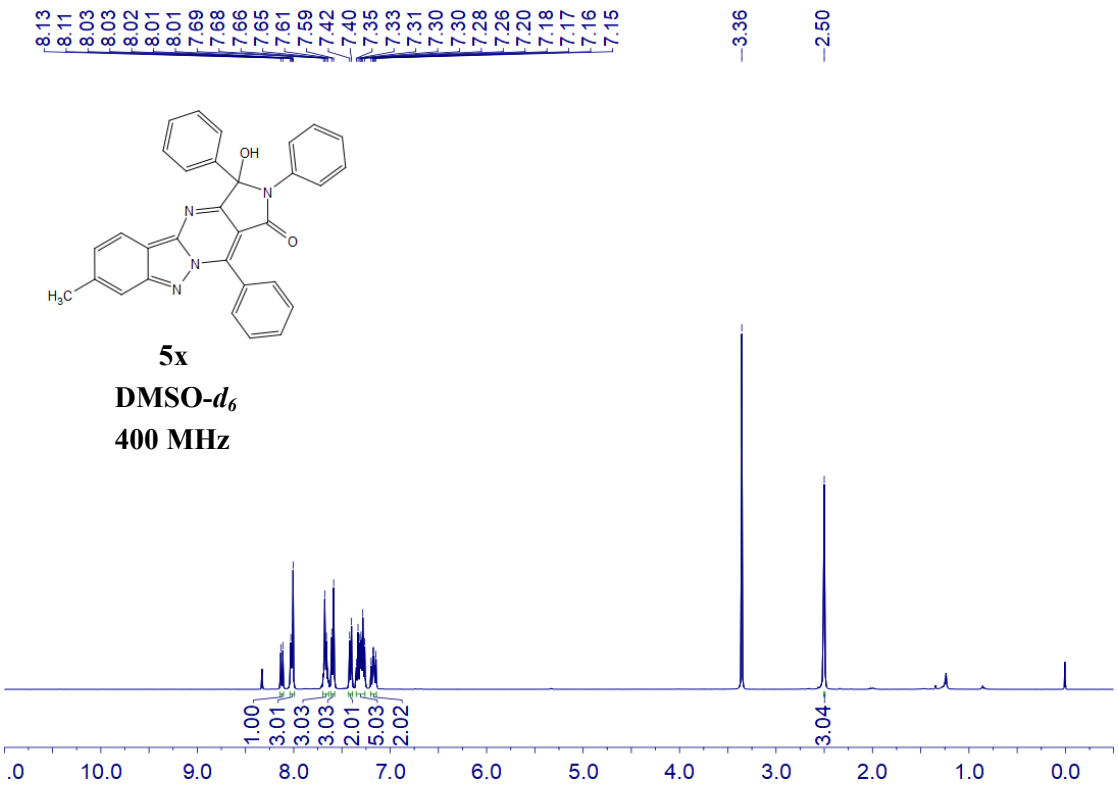


5w

DMSO-d_6

100 MHz

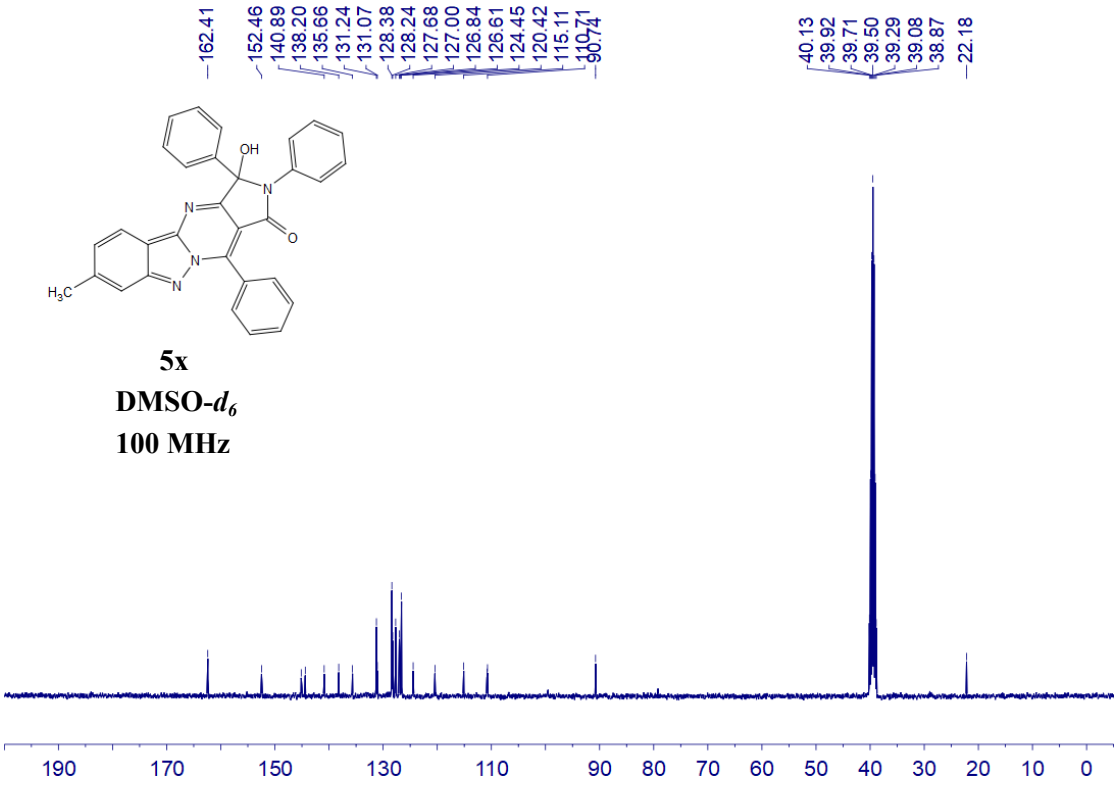
5x



5x

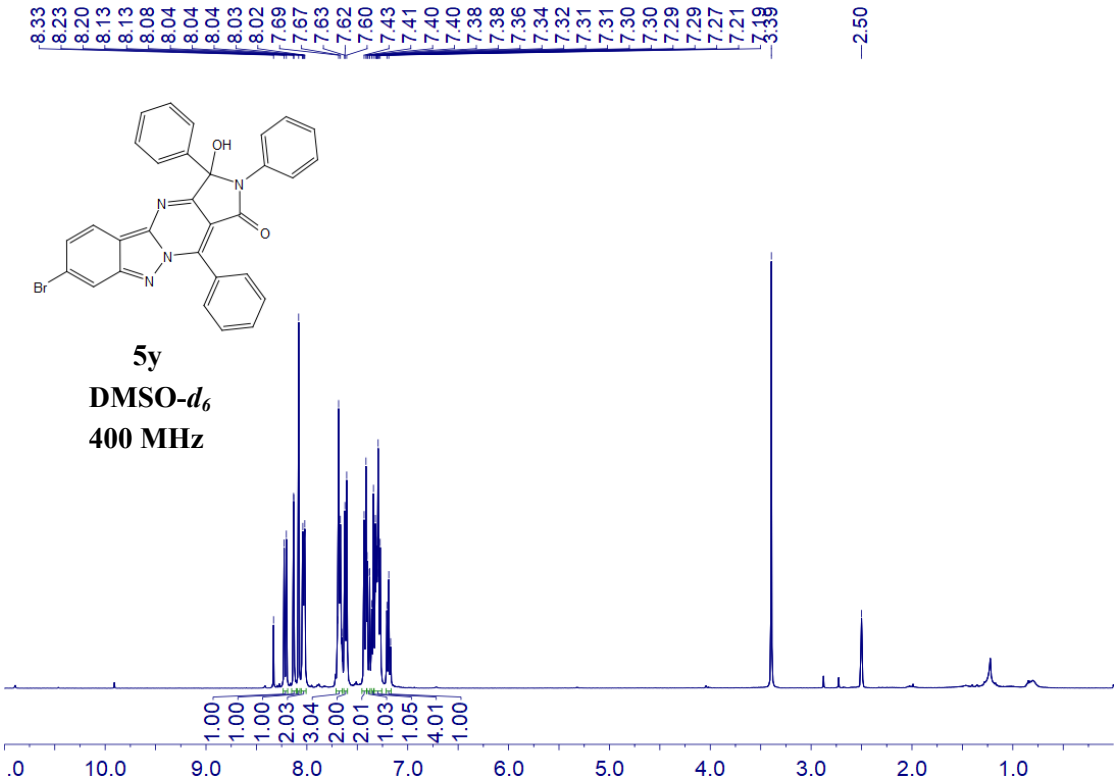
DMSO-d_6

400 MHz

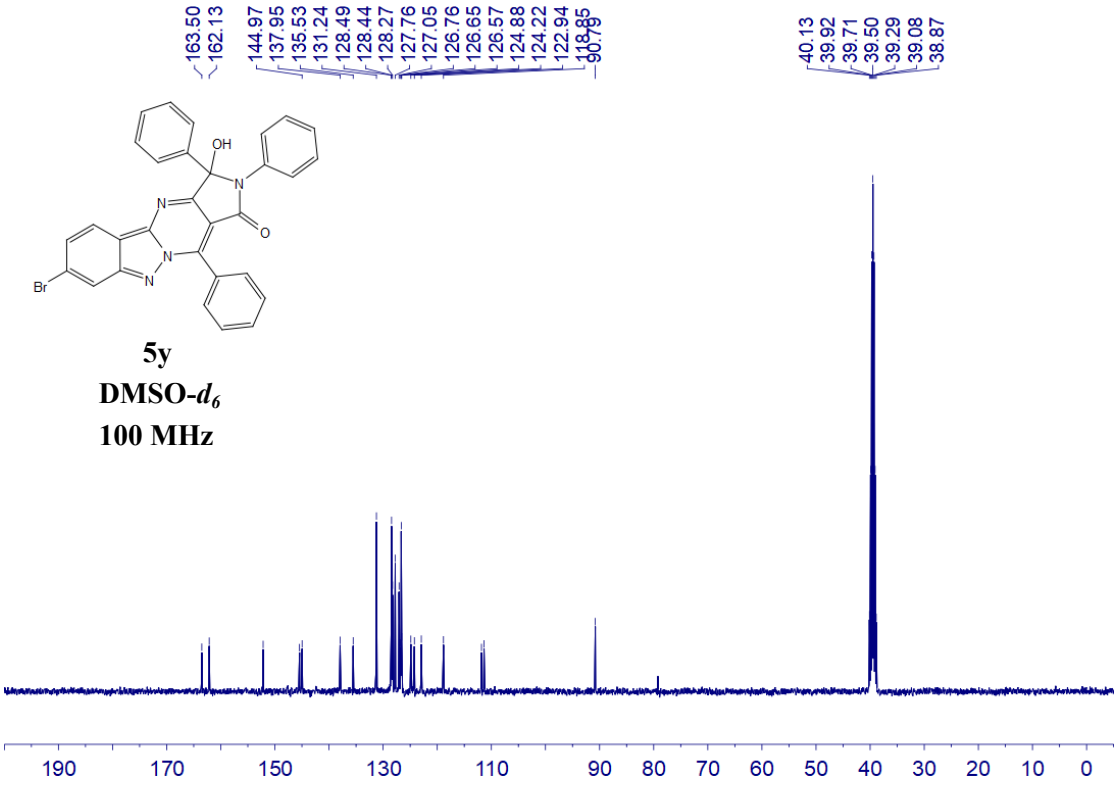


5x
DMSO-*d*$_6$
100 MHz

5y

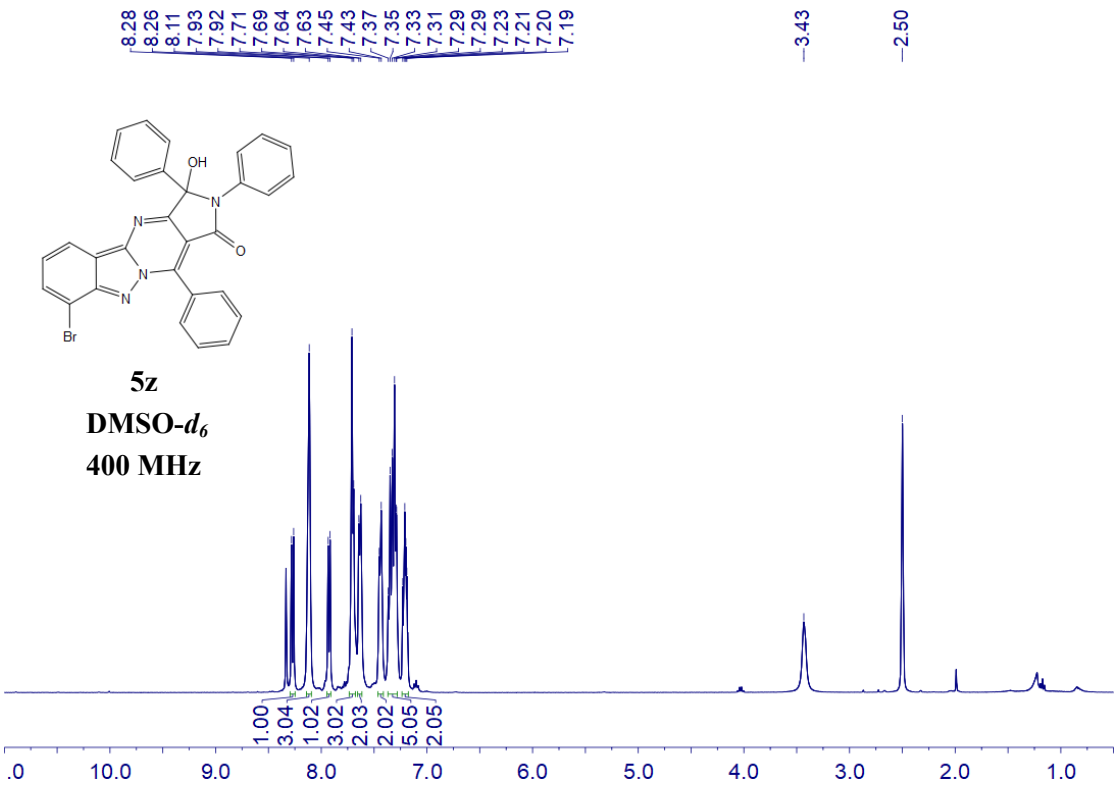


5y
DMSO-*d*$_6$
400 MHz

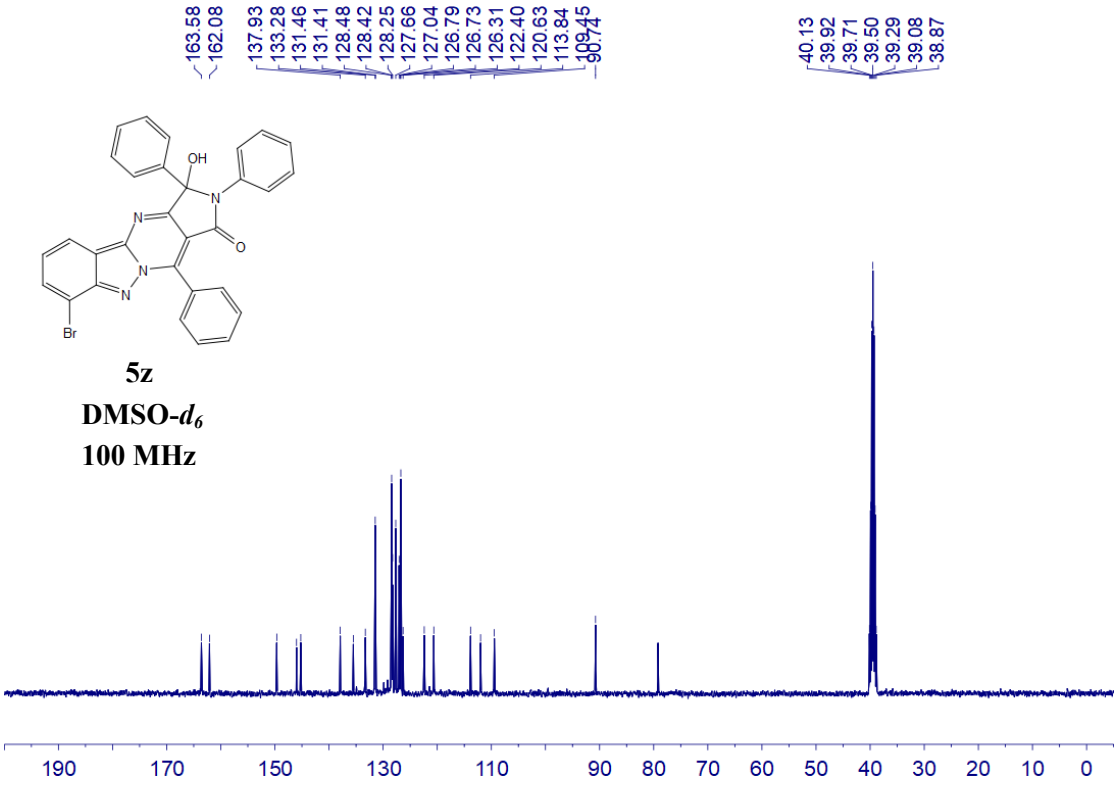


5y
DMSO-d_6
100 MHz

5z



5z
DMSO-d_6
400 MHz

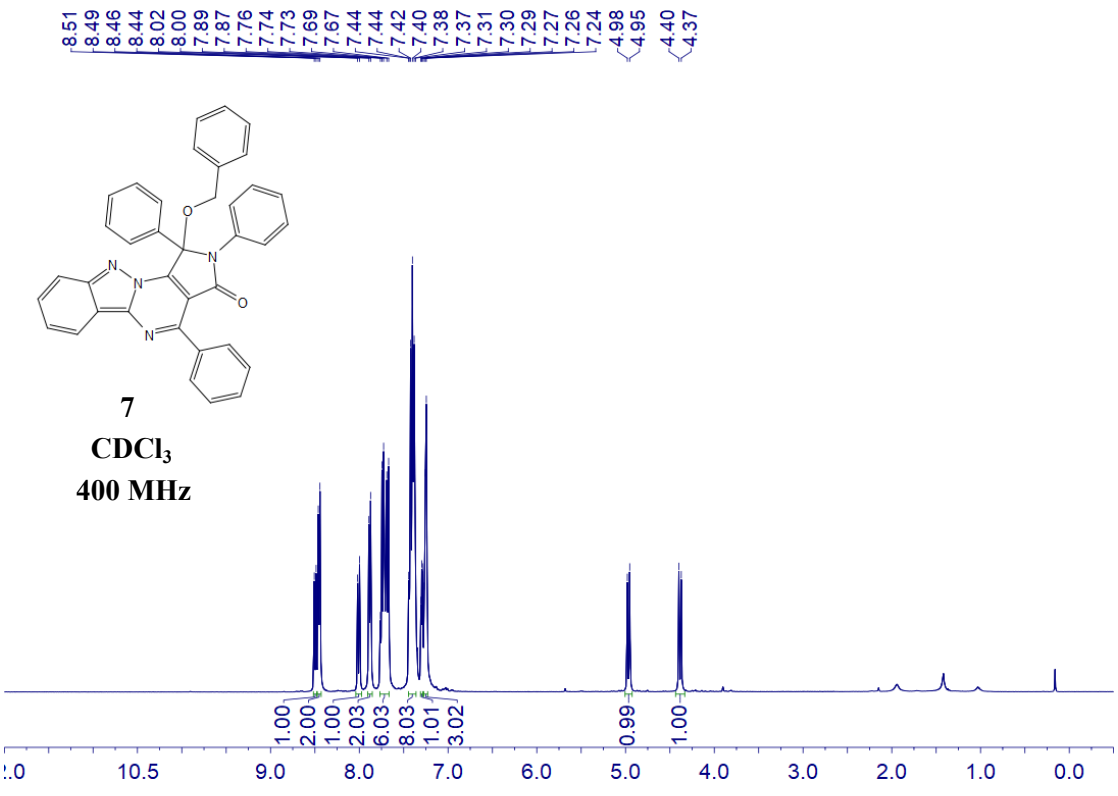


5z

DMSO-d_6

100 MHz

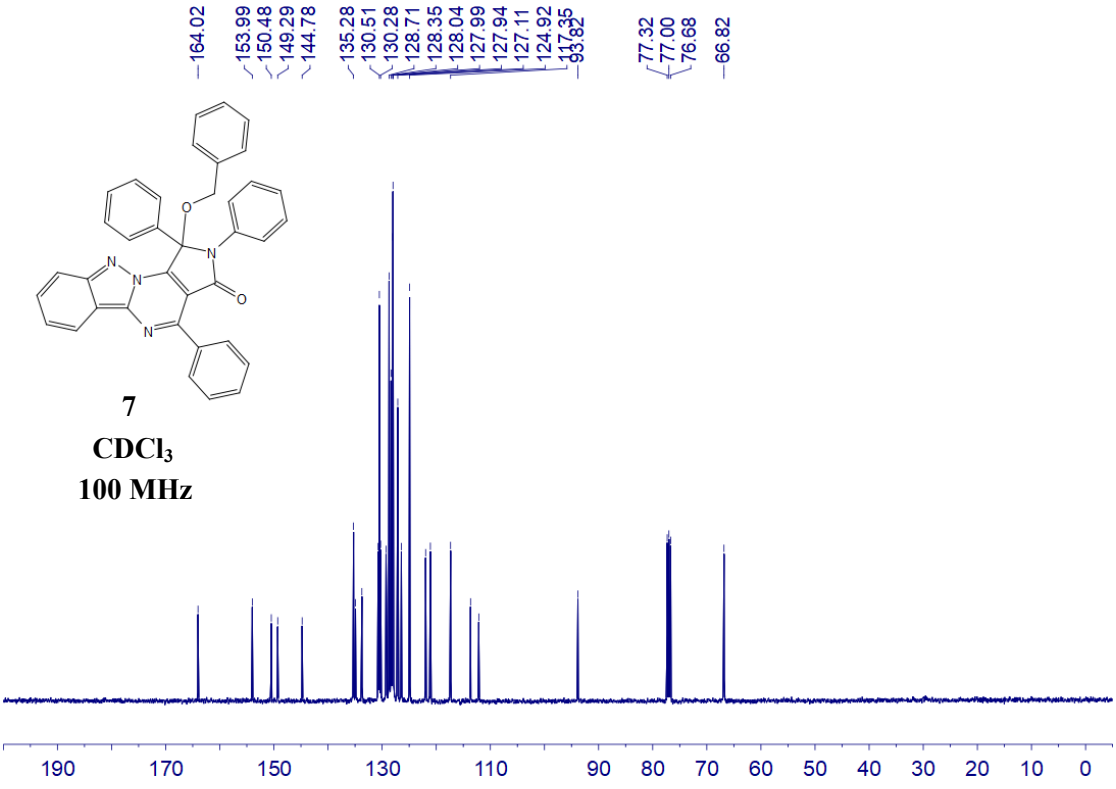
7



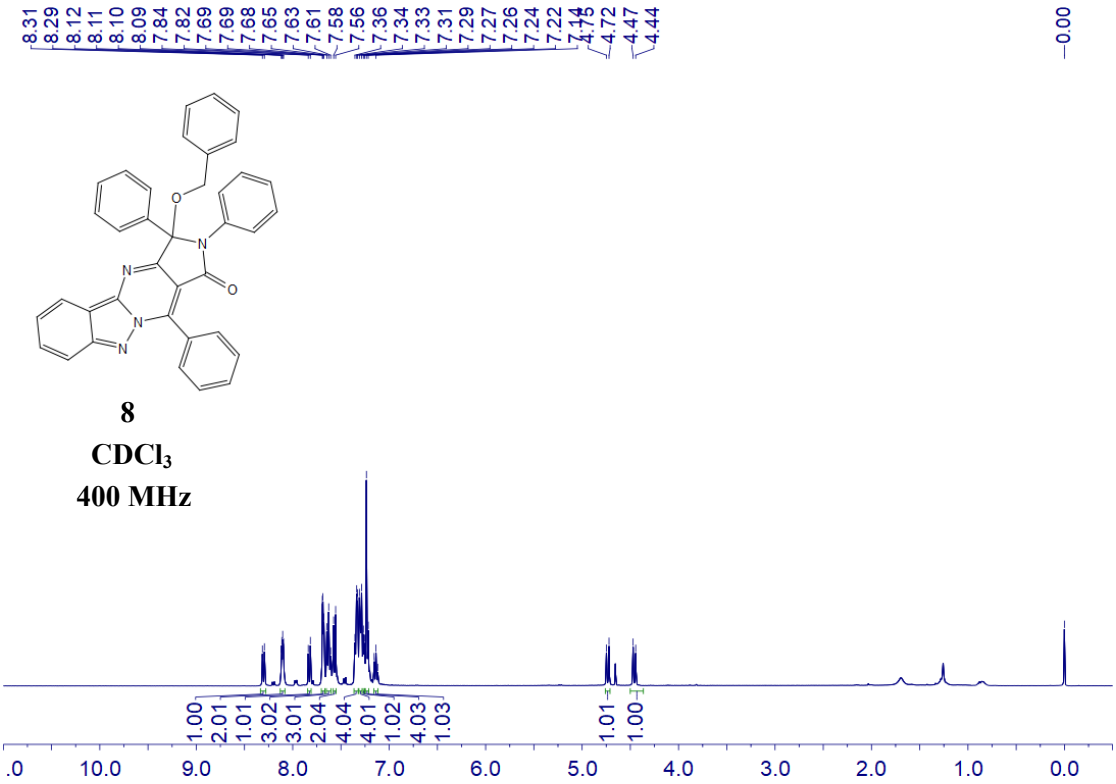
7

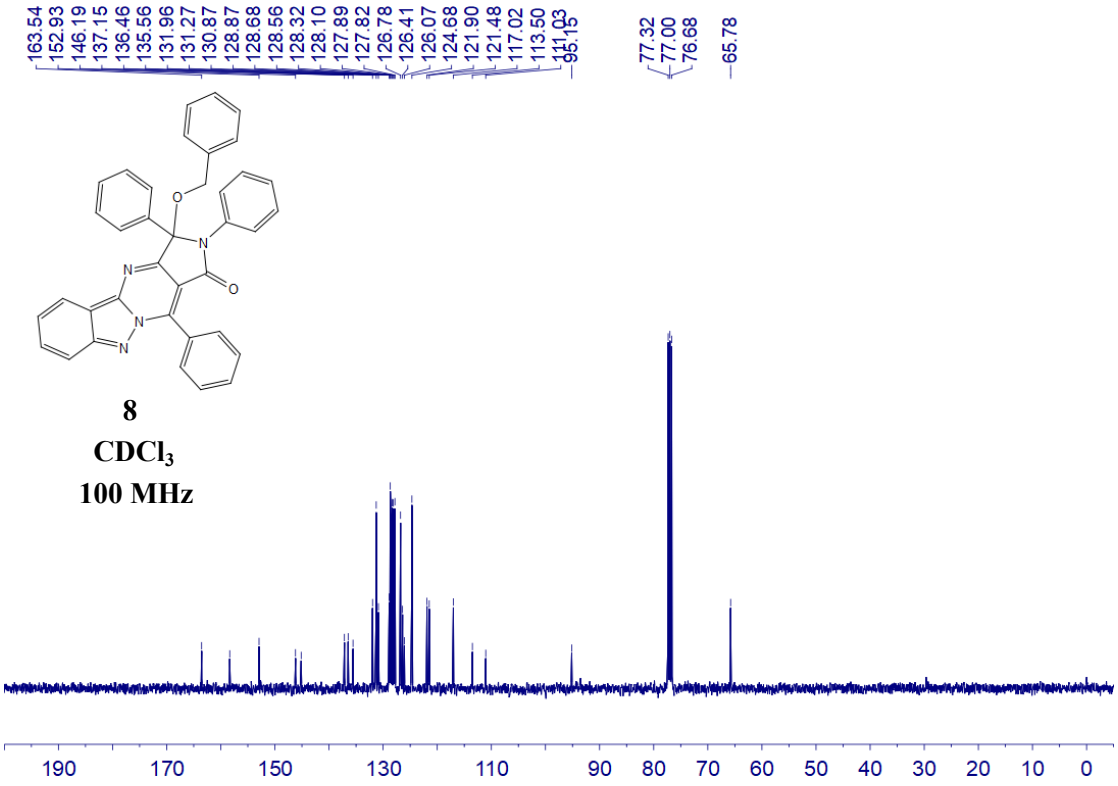
$CDCl_3$

400 MHz


164.02
153.99
150.48
149.29
144.78
135.28
130.51
130.28
128.71
128.35
128.04
127.99
127.94
127.11
124.92
93.82
77.32
77.00
76.68
66.82
O
N
N
N
N
O
7
CDCl3
100 MHz
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

8


8.31
8.29
8.12
8.11
8.10
8.09
7.84
7.82
7.69
7.69
7.68
7.65
7.63
7.61
7.58
7.56
7.36
7.34
7.33
7.31
7.29
7.27
7.26
7.24
7.22
4.72
4.47
4.44
0.00
O
N
N
N
N
O
8
CDCl3
400 MHz
1.00
2.01
1.01
3.02
3.01
2.04
4.04
4.01
1.02
4.03
1.03
1.01
1.00
.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0

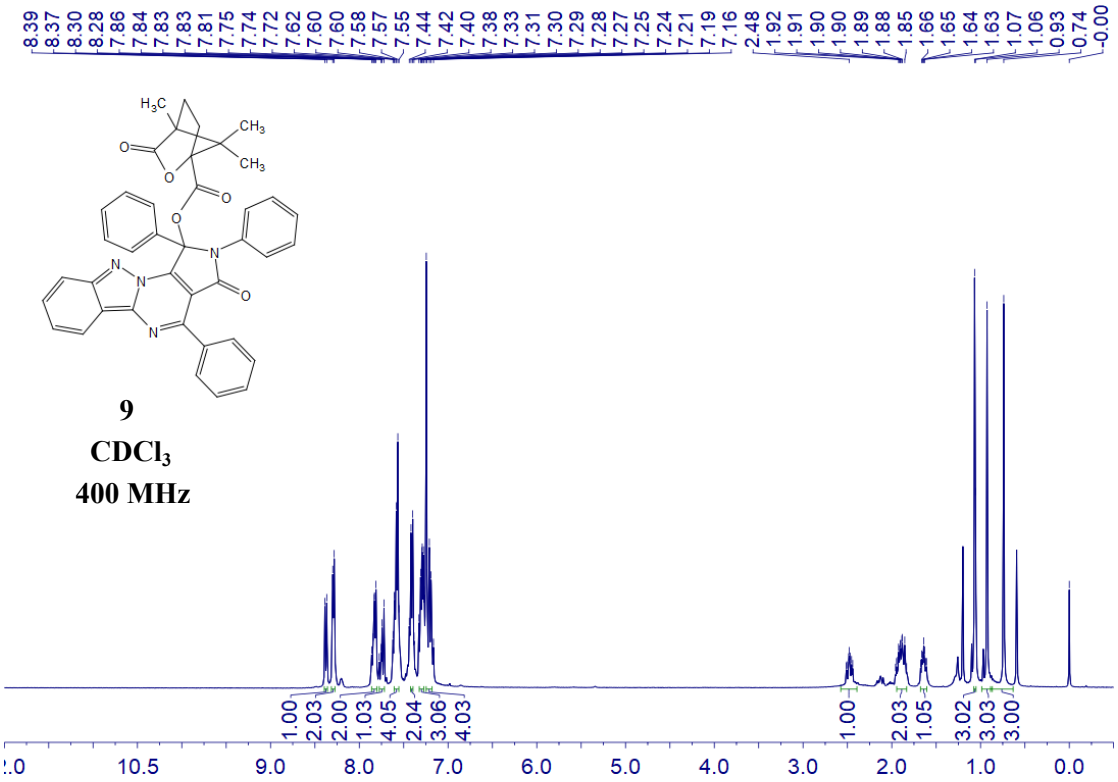


8

$CDCl_3$

100 MHz

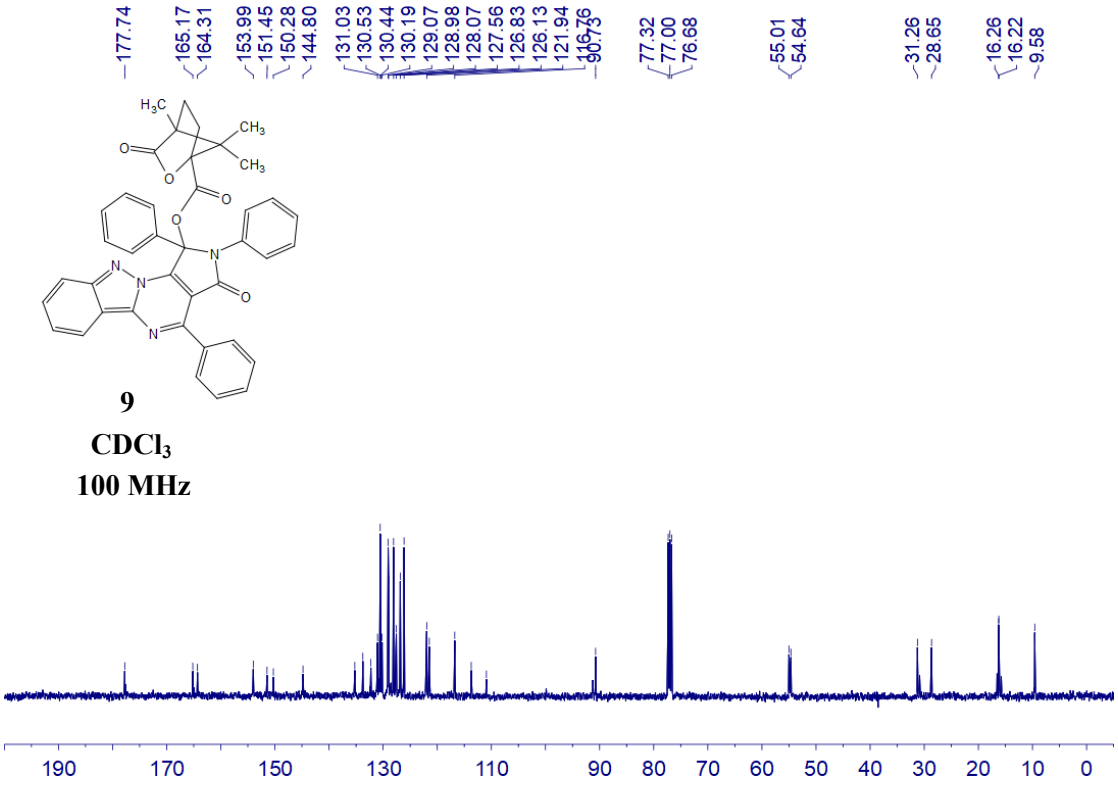
9



9

$CDCl_3$

400 MHz

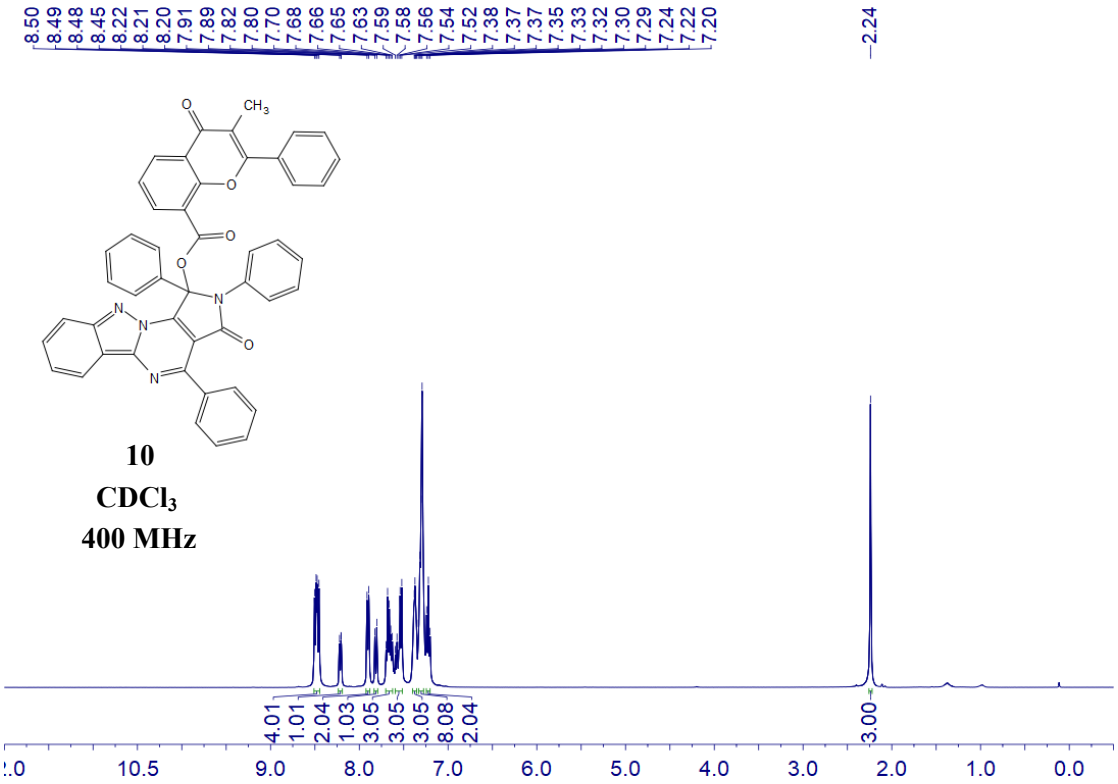


9

$CDCl_3$

100 MHz

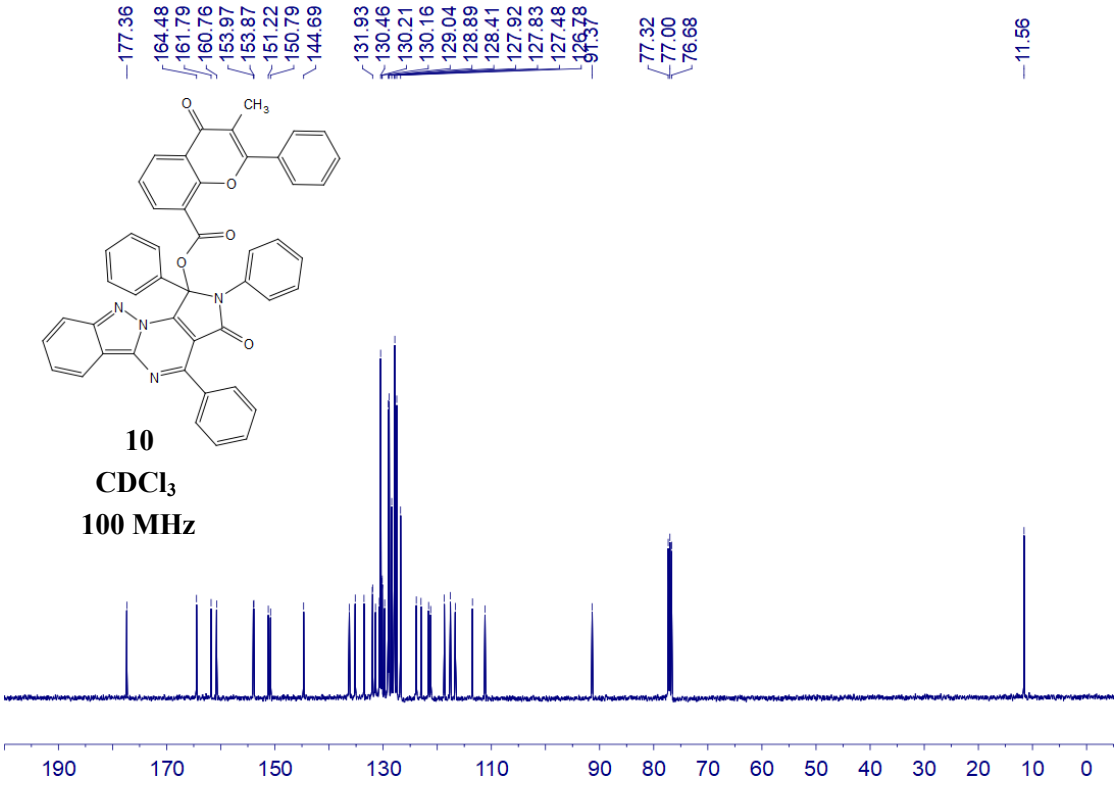
10



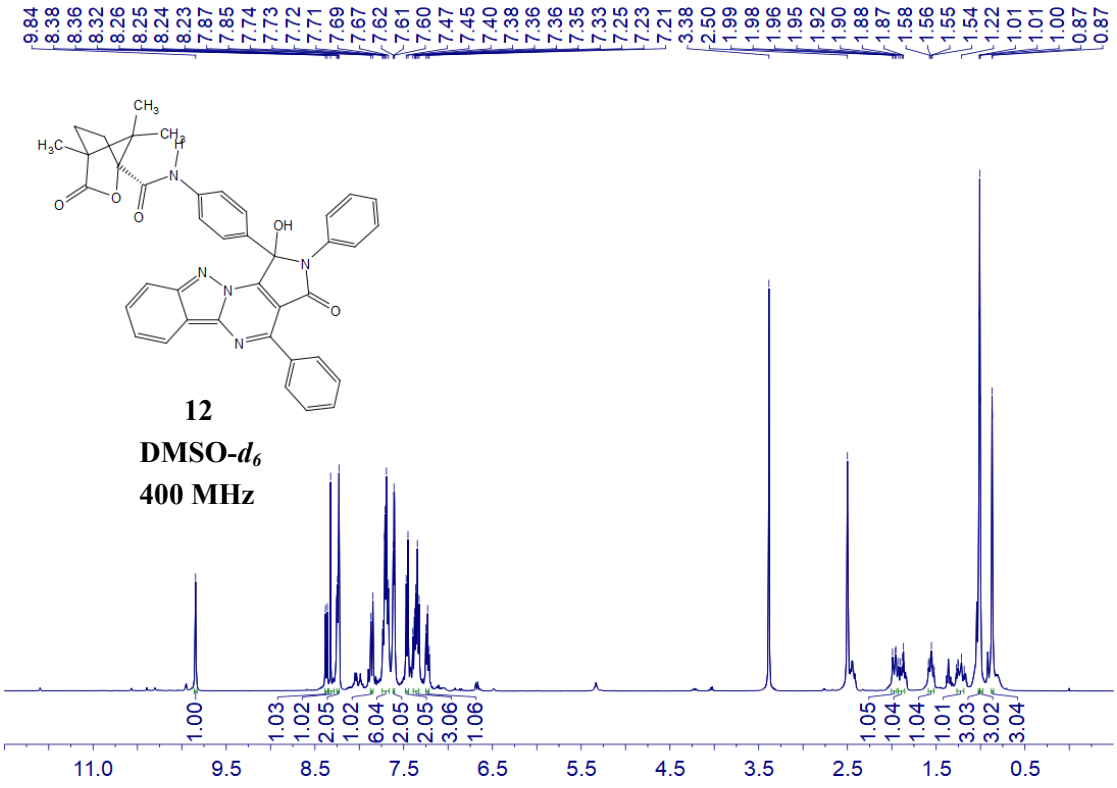
10

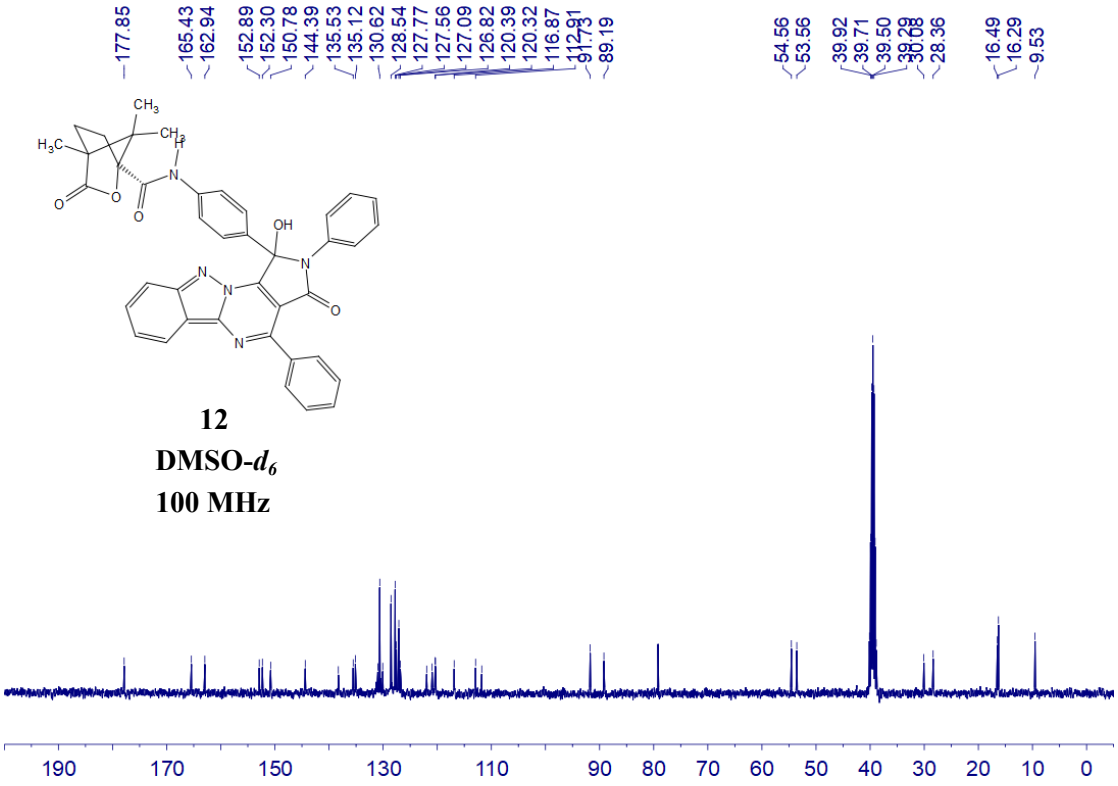
$CDCl_3$

400 MHz


177.36
164.48
161.79
160.76
153.97
153.87
151.22
150.79
144.69
131.93
130.46
130.21
130.16
129.04
128.89
128.41
127.92
127.83
127.48
126.78
91.37
77.32
77.00
76.68
11.56
10
CDCl3
100 MHz
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

12


9.84
8.38
8.36
8.32
8.26
8.25
8.24
8.23
7.87
7.85
7.74
7.73
7.72
7.71
7.69
7.67
7.62
7.61
7.60
7.47
7.45
7.40
7.38
7.36
7.36
7.35
7.33
7.25
7.23
7.21
3.38
2.50
1.99
1.98
1.96
1.95
1.92
1.90
1.88
1.87
1.58
1.56
1.55
1.54
1.22
1.01
1.01
1.00
0.87
0.87
12
DMSO-d6
400 MHz
1.00
1.03
1.02
2.05
1.02
6.04
2.05
2.05
3.06
1.06
1.05
1.04
1.01
3.03
3.02
3.04
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5

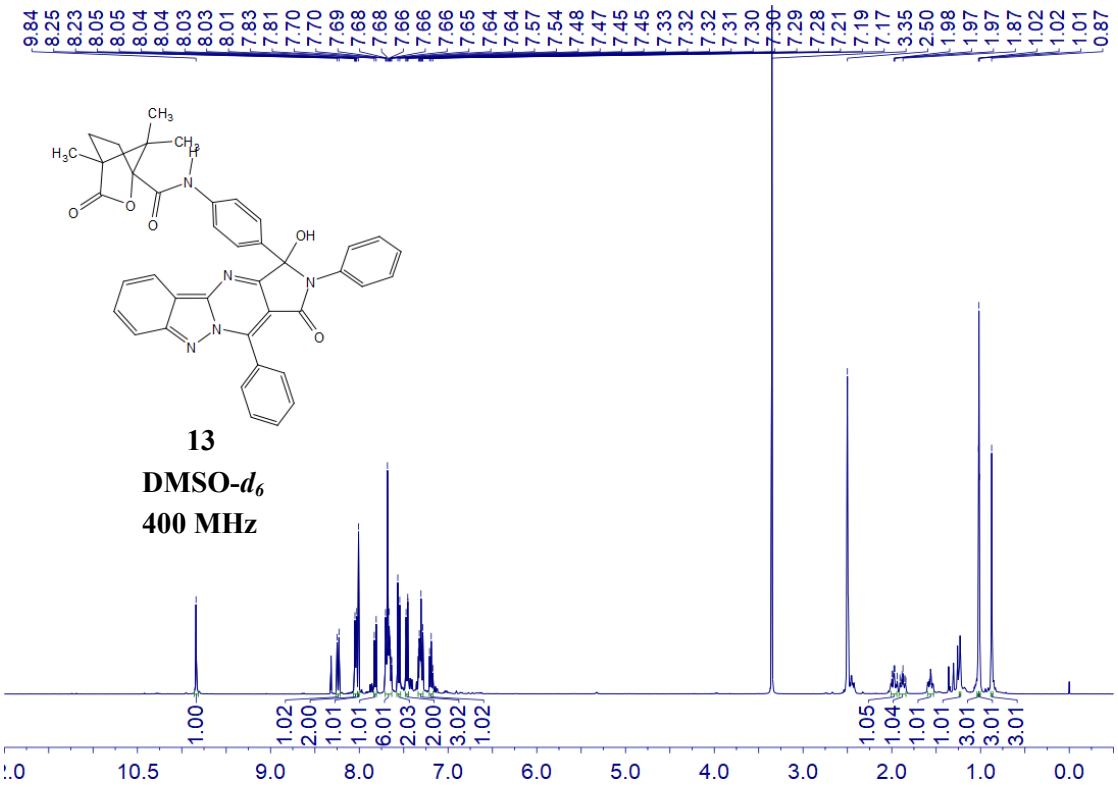


12

DMSO-*d*$_6$

100 MHz

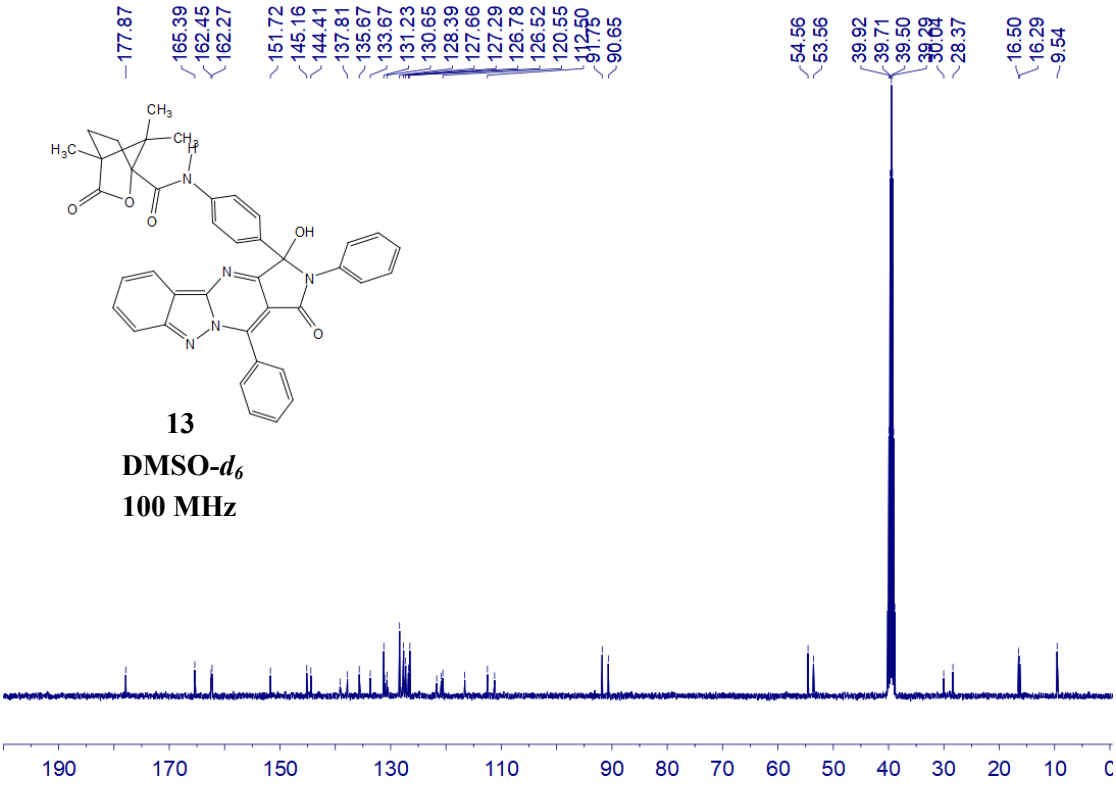
13



13

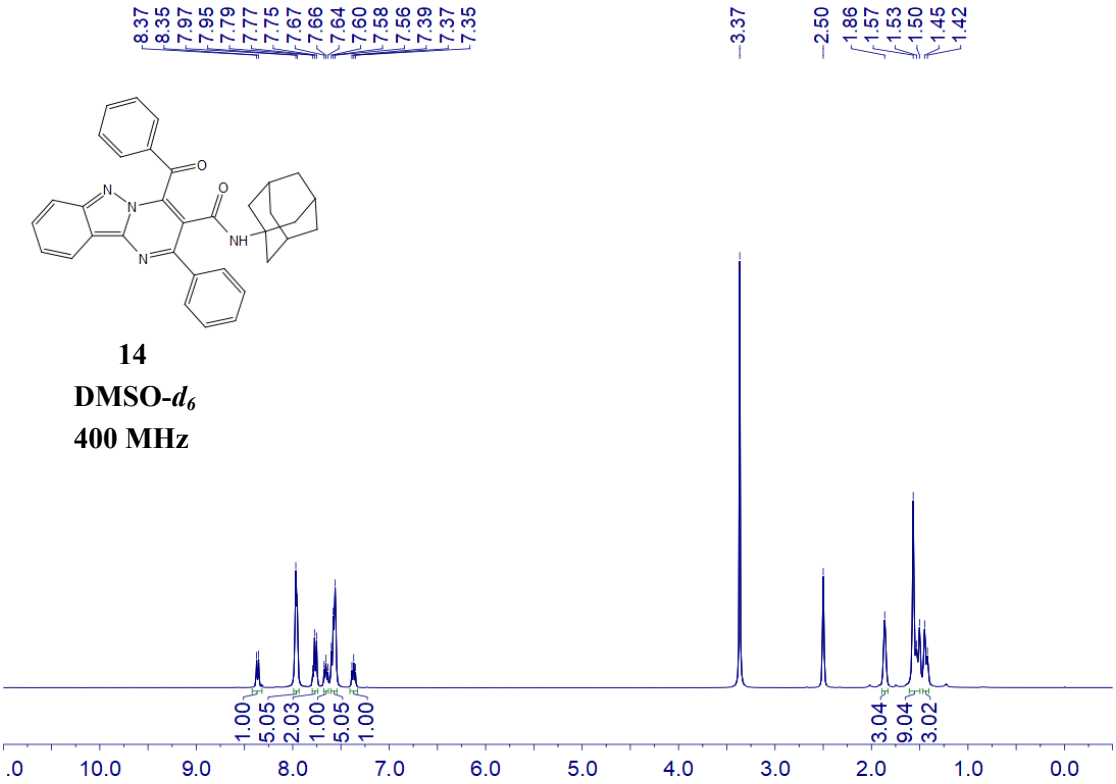
DMSO-*d*$_6$

400 MHz

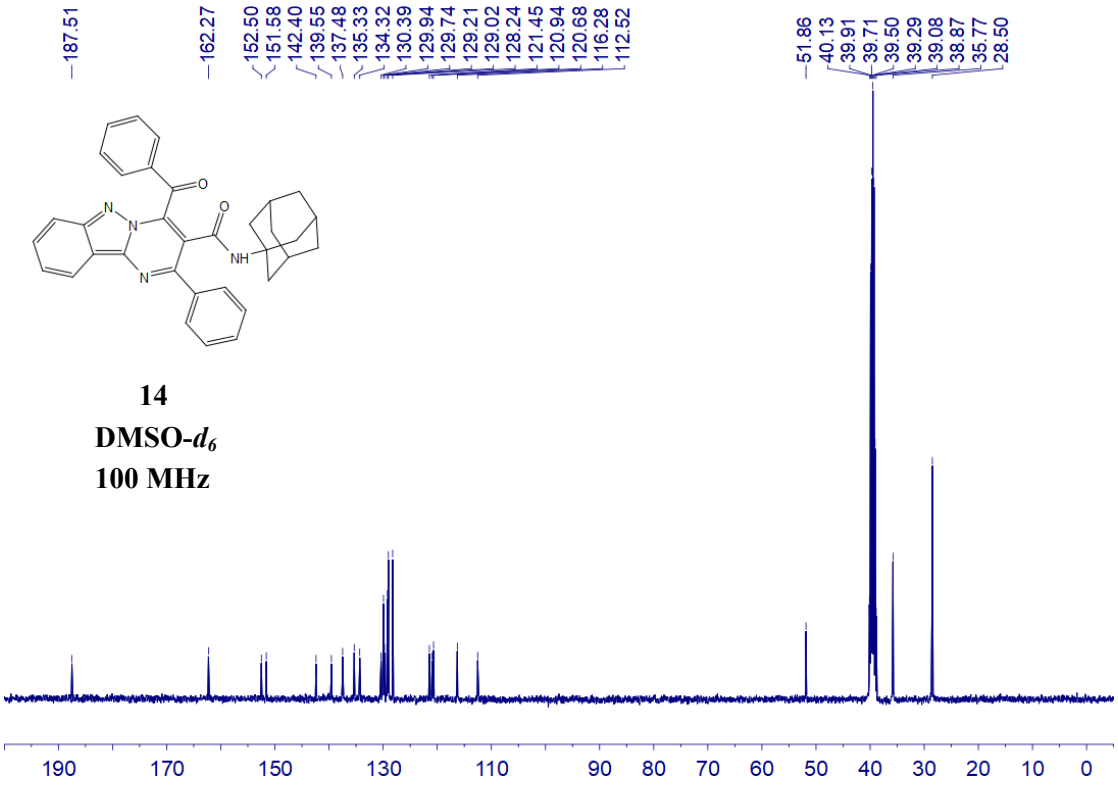


13
DMSO-d_6
100 MHz

14



14
DMSO-d_6
400 MHz



14
DMSO-d_6
100 MHz