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Dual C–H activation: Rh(III)-catalyzed cascade π–extended annulation of 2-arylindole with benzoquinone

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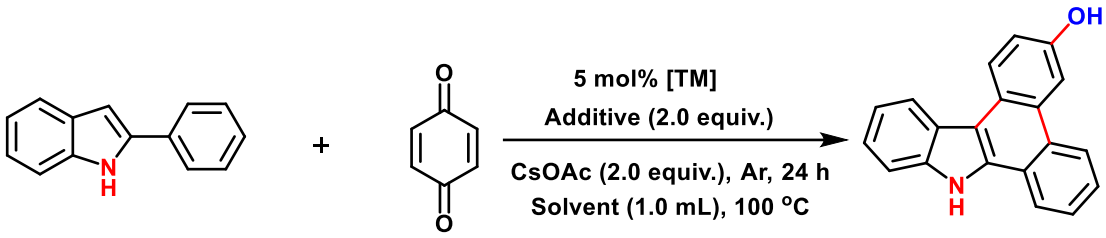
General Methods and Materials:

Unless specified, all reactions were carried out under air using commercial available solvents as received. Dichloro(η^5-pentamethylcyclopentadienyl)rhodium(III) dimer was synthesized according to a previous literature.[1] 2-phenyl indole was purchased from Alfa Aesar and used directly. All 2-aryl indole starting materials are synthesized according to literatures.[2] All other reagents were purchased and used without further purification unless specified otherwise. Solvents for chromatography were technical grade and distilled prior to use. Column chromatography was performed using silica gel Merck 60 (particle size 0.063–0.2 mm). Analytical thin-layer chromatography (TLC) was performed on Merck silica gel aluminium plates with GF-254 indicator. Visualization of the developed chromatogram was performed by UV absorbance (254 nm). ^{1}H NMR and ^{13}C NMR data were recorded on Varian VNMR 600, Varian VNMR 400 or Mercury 300 spectrometer. Chemical shifts (δ) in ppm are reported as quoted relative to the residual signals of dimethyl sulfoxide (^{1}H 2.49 ppm or ^{13}C 39.60 ppm). Multiplicities are described as: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet); and coupling constants (*J*) are reported in Hertz (Hz). ^{13}C NMR spectra were recorded with total proton decoupling. High-resolution mass spectra (HRMS) was collected in ESI mode by using a MicrOTOF mass spectrometer.

Conditions Screening: [a]



1a, 1.0 equiv. + **2a**, 1.0 equiv. → **3a**

Entry	Solvent	Catalyst	Additive	Results
1	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2·H_2O$	55%
2	DMF	$[RhCp^*Cl_2]_2$	–	<5%
3	DMF	–	$Cu(OAc)_2·H_2O$	–
4[b]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2.H_2O$	40%
5	Dioxane	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2·H_2O$	48%
6	*t*-AmOH	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2·H_2O$	–
7	MeCN	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2.H_2O$	52%
8	DCE	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2·H_2O$	43%
9	*o*-xylene	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2·H_2O$	54%
10	DMAc	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2·H_2O$	<5%
11	DMSO	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2·H_2O$	trace
12	DME	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2·H_2O$	40%
13	NMP	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2·H_2O$	7%
14	DMF	$[RuCl_2(p\text{-cymene})]_2$	$Cu(OAc)_2·H_2O$	–
15	DMF	$Pd(OAc)_2$	$Cu(OAc)_2·H_2O$	–
16	DMF	$PdCl_2$	$Cu(OAc)_2·H_2O$	–
17	DMF	$PdCl_2(MeCN)_2$	$Cu(OAc)_2·H_2O$	<5%
18	DMF	$[RhCp^*(OAc)_2]$	$Cu(OAc)_2·H_2O$	47%
19	DMF	$RhCl(PPh_3)_3$	$Cu(OAc)_2·H_2O$	<5%
20	DMF	$[Rh(coe)Cl]_2$	$Cu(OAc)_2·H_2O$	<5%
21	DMF	$Cp^*CoI_2(CO)$	$Cu(OAc)_2·H_2O$	–
22	DMF	$[RhCp^*Cl_2]_2$	AgOAc	–

23	DMF	$[RhCp^*Cl_2]_2$	Ag_2O	–
24	DMF	$[RhCp^*Cl_2]_2$	$Cu(acac)_2$	trace
25	DMF	$[RhCp^*Cl_2]_2$	$CuCl_2$	17%
26	DMF	$[RhCp^*Cl_2]_2$	Copper 2-ethylhexoate	28%
27	DMF	$[RhCp^*Cl_2]_2$	CuOAc	12%
28	DMF	$[RhCp^*Cl_2]_2$	$Fe(OAc)_2$	<5%
29[c]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	50%
30[d]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	59%
31[e]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	54%
32	DMF	$[RhCp^*Cl_2]_2$	O_2	–
33[f, g]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$ (10 mol%)	33%
34[e, h]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	59%
35[e, g, h]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	0%
36[e, i]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	45%
37[e, h, j]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	47%
38[e, h, k]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	59%
39[e, h]	DMF	$[RhCp^*Cl_2]_2$	$PhI(OAc)_2$	–
40[e, h, l]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	65%
41[e, h, l]	DMF/DCE (4:1)	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	69%
42[e, h, l]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	60% (48 h)
43[d, e, h, l]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	62%
44[e, h, l, m]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	62%
45[e, h, l]	DMF/DCE (1:1)	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	67%
46[h, l, n]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	47%
47[e, h, l, o]	DMF/DCE (4:1)	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	52%
48[e, h, l]	DMF/DCE (2:1)	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	74%
49[e, h, l, p]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	42%
50[e, l, q]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	67%
51[e, h, l]	DMF/*o*-xylene (2:1)	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2 \cdot H_2O$	62%

52[e, q, r]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2·H_2O$	70%
53[e, l, q]	DMF	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2·H_2O$	57%
54[e, l, q]	DMF/DCE (2:1)	$[RhCp^*Cl_2]_2$	$Cu(OAc)_2·H_2O$	74%
55[e, q, r, s]	**DMF/DCE (2:1)**	**$[RhCp^*Cl_2]_2$**	**$Cu(OAc)_2·H_2O$**	**84% (36 h)**

[a.] 0.2 mmol scale, isolated yield;

[b.] without CsOAc;

[c.] 0.5 equiv. CsOAc;

[d.] 0.3 equiv. AgOAc;

[e.] NaOAc instead of CsOAc;

[f.] Na_2CO_3 instead of CsOAc;

[g.] under air;

[h.] 2.0 equiv. BQ;

[i.] 3.0 equiv. $Cu(OAc)_2·H_2O$;

[j.] 80 °C;

[k.] 120 °C;

[l.] 1.0 equiv. $Cu(OAc)_2·H_2O$;

[m.] 0.2 equiv. $AgSbF_6$;

[n.] 1.0 equiv. NaOAc;

[o.] 90 °C;

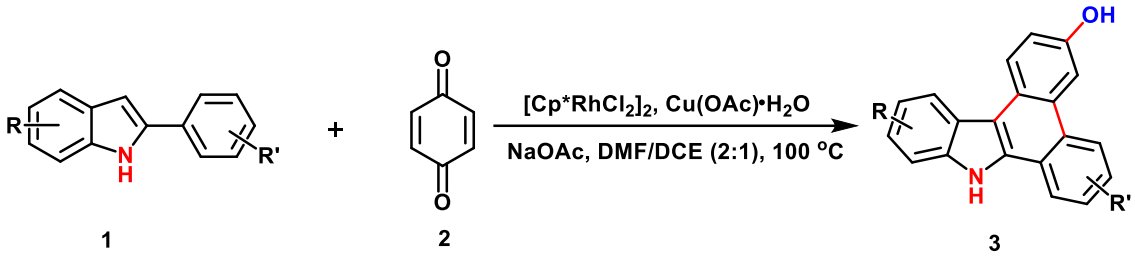
[p.] 0.5 equiv. NaOAc;

[q.] 1.5 equiv. **1a** and 1 equiv. **2a**;

[r.] 2.1 equiv. $Cu(OAc)_2·H_2O$;

[s.] 0.3 mmol scale.

General Procedure for Dual C–H Activation



1 2 3

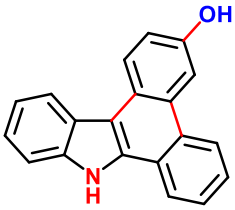
Condition A:

$[Cp^*RhCl_2]_2$ (0.015 mmol, 9.3 mg, 5 mol %), NaOAc (0.6 mmol, 49.2 mg, 2.0 equiv.), $Cu(OAc)_2 \cdot H_2O$ (0.63 mmol, 125.8 mg, 2.1 equiv.) and 2-aryl indole substrate **1** (0.45 mmol, 1.5 equiv.) were weighed into a Schlenk tube. The reaction vessel was capped and subjected to three vacuum-purge/argon-flush cycles. A solution of benzoquione (0.3 mmol, 1.0 equiv.) in DMF/DCE (2:1, 1.5 mL) was then added through the side-arm by syringe. The reaction was stirred under argon at 100 °C. Upon complete of the reaction, it was cooled to room temperature. 30 mL water was added and then extracted with EtOAc (3 times), dried over $MgSO_4$ and the obtained solvent was removed by rotary evaporation and the residue was purified by silica gel flash chromatography using *n*-Hexane/EtOAc (10:1 to 6:1) to afford product **3**.

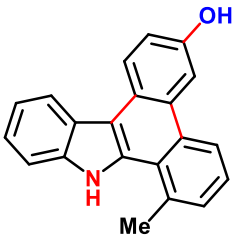
Condition B:

$[Cp^*RhCl_2]_2$ (0.015 mmol, 9.3 mg, 5 mol%), NaOAc (0.6 mmol, 49.2 mg, 2.0 equiv.), $Cu(OAc)_2 \cdot H_2O$ (0.63 mmol, 125.8 mg, 2.1 equiv.) and 2-aryl indole substrate **1** (0.30 mmol, 1.0 equiv.) were weighed into a Schlenk tube. The reaction vessel was capped and subjected to three vacuum-purge/argon-flush cycles. A solution of benzoquione (0.6 mmol, 2.0 equiv.) in DMF/DCE (2:1, 1.5 mL) was then added through the side-arm by syringe. The reaction was stirred under argon at 60 °C. Upon complete of the reaction, it was cooled to room temperature. 30 mL water was added and then extracted with EtOAc (3 times), dried over $MgSO_4$ and the obtained solvent was removed by rotary evaporation and the residue was purified by silica gel flash chromatography using *n*-Hexane/EtOAc (10:1 to 6:1) to afford product **3**.

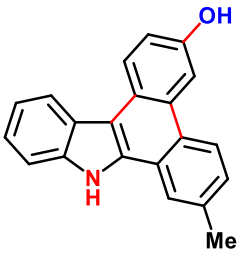
Characterization of Products:



9H-dibenzo[*a,c*]carbazol-3-ol (**3a**).[3] **Condition A**, 36 h, yield: 84%, gray solid. ^{1}H NMR (d_6-DMSO, 600 MHz): δ 12.20 (s, 1H), 9.65 (s, 1H), 8.70 (d, *J* = 8.2 Hz, 1H), 8.65 (d, *J* = 8.6 Hz, 1H), 8.54 (d, *J* = 7.9 Hz, 1H), 8.50 (d, *J* = 7.9 Hz, 1H), 8.16 (s, 1H), 7.74 (t, *J* = 7.2 Hz, 1H), 7.68 – 7.66 (m, 2H), 7.39 (t, *J* = 7.3 Hz, 1H), 7.33 (d, *J* = 7.1 Hz, 1H), 7.27 (d, *J* = 7.4 Hz, 1H); ^{13}C NMR (d_6-DMSO, 150 MHz): δ 154.0, 138.6, 132.5, 128.8, 128.0, 127.0, 126.2, 124.8, 123.9, 123.5, 123.5, 123.1, 122.8, 122.3, 121.4, 119.8, 117.6, 111.8, 111.7, 108.2.

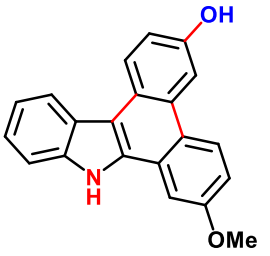


8-methyl-9H-dibenzo[*a,c*]carbazol-3-ol (**3b**).[3] **Condition B**, 48 h, yield: 57%, gray solid. ^{1}H NMR (d_6-DMSO, 600 MHz): δ 11.10 (s, 1H), 9.62 (s, 1H), 8.73 (d, *J* = 8.8 Hz, 1H), 8.61 (d, *J* = 8.1 Hz, 1H), 8.56 (d, *J* = 8.0 Hz, 1H), 8.50 (d, *J* = 7.9 Hz, 1H), 8.16 (s, 1H), 7.92 (t, *J* = 8.1 Hz, 1H), 7.56 – 7.51 (m, 2H), 7.40 (d, *J* = 7.4 Hz, 1H), 7.34 (d, *J* = 8.6 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 3.17 (s, 3H); ^{13}C NMR (d_6-DMSO, 150 MHz): δ 154.1, 138.8, 133.0, 132.2, 129.9, 129.7, 128.4, 125.5, 124.6, 123.3, 122.9, 122.7, 122.4, 122.0, 121.1, 120.0, 117.7, 113.0, 112.9, 108.3, 24.2.



7-methyl-9H-dibenzo[*a,c*]carbazol-3-ol (**3c**).[3] **Condition B**, 45.5 h, yield: 53%, gray solid. ^{1}H NMR (d_6-DMSO, 600 MHz): δ 12.10 (s, 1H), 9.57 (s, 1H), 8.62 (d, *J* = 8.7 Hz, 1H), 8.57 (d, *J* = 8.5 Hz, 1H), 8.47 (d, *J* = 8.0 Hz, 1H), 8.34 (s, 1H), 8.10 (d, *J* = 2.3 Hz, 1H), 7.66 (d, *J* = 8.0 Hz,

1H), 7.50 (d, *J* = 8.4 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 1H), 7.29 – 7.25 (m, 2H), 2.59 (s, 3H); ^{13}C NMR (*d*$_6$-DMSO, 150 MHz): δ 153.9, 138.5, 136.3, 132.4, 128.1, 127.7, 126.7, 124.7, 123.8, 123.5, 123.4, 123.1, 122.4, 121.9, 121.2, 119.7, 117.1, 111.7, 108.0, 21.4.



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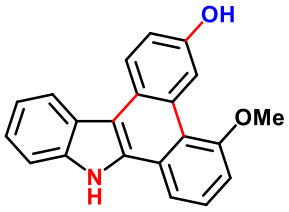
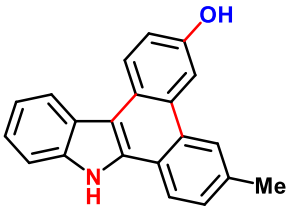
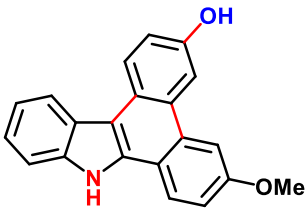


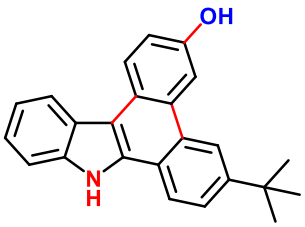
7-methoxy-9H-dibenzo[*a,c*]carbazol-3-ol (**3d**) and 5-methoxy-9H-dibenzo[*a,c*]carbazol-3-ol (**3d'**). **Condition B**, 45.5 h, yield: 68%, isolated as an inseparable mixture, ratio = 5:3, gray solid. ^{1}H NMR (*d*$_6$-DMSO, 400 MHz): δ 12.10 (s, 1H), 12.10 (s, 0.7H), 9.55 (s, 1H), 9.41 (s, 0.7H), 9.22 (d, *J* = 2.5 Hz, 0.7H), 8.65 (d, *J* = 8.8 Hz, 0.7H), 8.61 (d, *J* = 7.8 Hz, 1.7H), 8.58 (s, 0.6H), 8.49 (d, *J* = 8.0 Hz, 1.7H), 8.16 (d, *J* = 8.0 Hz, 0.7H), 8.06 – 8.04 (m, 2H), 7.70 – 7.65 (m, 2.3H), 7.41 – 7.37 (m, 1.7H), 7.29 – 7.24 (m, 4.8H), 6.57 (s, 0.7H), 4.12 (s, 1.8H), 4.01 (s, 3H); ^{13}C NMR (*d*$_6$-DMSO, 150 MHz): δ 159.0, 158.4, 154.0, 153.3, 149.8, 138.8, 138.5, 132.7, 132.4, 128.2, 127.9, 127.4, 125.6, 125.2, 124.7, 124.3, 123.9, 123.6, 123.5, 123.2, 123.1, 122.8, 121.7, 121.5, 121.4, 119.7, 118.7, 116.5, 116.3, 115.8, 115.7, 114.8, 114.4, 112.3, 112.1, 111.7, 108.7, 107.7, 103.6, 56.0, 55.6. HRMS (ESI) calcd. for $C_{21}H_{14}NO_2$ $[M–H]^-$: 312.1030, found: 312.1026.



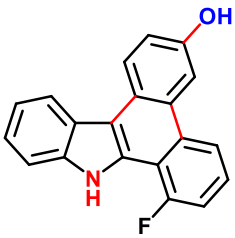
6-methyl-9H-dibenzo[*a,c*]carbazol-3-ol (**3e**).[3] **Condition B**, 48 h, yield: 47%, gray solid. ^{1}H NMR (*d*$_6$-DMSO, 600 MHz): δ 12.10 (s, 1H), 9.56 (s, 1H), 8.62 (d, *J* = 8.8 Hz, 1H), 8.57 (d, *J* = 8.5 Hz, 1H), 8.50 (s, 1H), 8.47 (d, *J* = 8.0 Hz, 1H), 8.43 (d, *J* = 8.2 Hz, 1H), 8.16 (d, *J* = 2.2 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.37 (t, *J* = 7.4 Hz, 1H), 7.31 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.26 (t, *J* = 7.6 Hz, 1H), 2.61 (s, 3H); ^{13}C NMR (*d*$_6$-DMSO, 150 MHz): δ 153.8, 138.4, 135.4, 132.7, 128.9, 128.4, 127.8, 124.7, 123.6, 123.6, 123.2, 123.0, 122.3, 121.1, 120.9, 119.7, 117.5, 111.7, 111.1, 108.2, 21.8.



6-methoxy-9H-dibenzo[*a,c*]carbazol-3-ol (**3f**).[3] **Condition B**, 45.5 h, yield: 59%, gray solid. ^{1}H NMR (*d*$_6$-DMSO, 600 MHz): δ 12.10 (s, 1H), 9.55 (s, 1H), 8.61 (d, *J* = 8.7 Hz, 1H), 8.46 (d, *J* = 8.8 Hz, 1H), 8.44 (d, *J* = 8.0 Hz, 1H), 8.13 (d, *J* = 2.2 Hz, 1H), 8.08 (d, *J* = 2.1 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.41 (dd, *J* = 8.8, 2.3 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.31 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.25 (t, *J* = 7.7 Hz, 1H), 4.02 (s, 3H); ^{13}C NMR (*d*$_6$-DMSO, 150 MHz): δ 157.9, 153.7, 138.3, 132.9, 130.4, 127.5, 124.7, 123.9, 123.6, 123.2, 122.9, 120.9, 119.6, 117.7, 117.3, 116.6, 111.5, 110.1, 108.5, 105.8, 55.5.

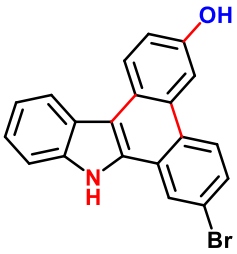


6-(tert-butyl)-9H-dibenzo[*a,c*]carbazol-3-ol (**3g**)**. Condition B**, 48 h, yield: 59%, gray solid. ^{1}H NMR (*d*$_6$-DMSO, 600 MHz): δ 12.10 (s, 1H), 9.57 (s, 1H), 8.63 (d, *J* = 8.8 Hz, 2H), 8.48 (t, *J* = 8.5 Hz, 1H), 8.21 (d, *J* = 1.9 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.37 (t, *J* = 7.4 Hz, 1H), 7.31 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.27 (t, *J* = 7.5 Hz, 1H), 1.49 (s, 9H); ^{13}C NMR (*d*$_6$-DMSO, 150 MHz): δ 153.8, 148.3, 138.5, 132.6, 128.4, 128.1, 125.1, 124.8, 123.6, 123.2, 123.0, 122.2, 121.2, 120.9, 119.6, 119.2, 117.4, 111.7, 111.2, 108.0, 35.1, 31.4. HRMS (ESI) calcd. for $C_{24}H_{20}NO$ $[M–H]^-$: 338.1550, found: 338.1557.

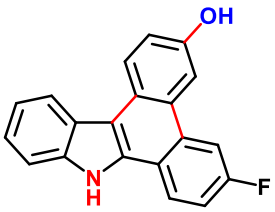


8-fluoro-9H-dibenzo[*a,c*]carbazol-3-ol (**3h**). **Condition A**, 48 h, yield: 68%, white solid. ^{1}H NMR (*d*$_6$-DMSO, 400 MHz): δ 11.73 (d, *J* = 2.9 Hz, 1H), 9.74 (s, 1H), 8.73 (d, *J* = 8.9 Hz, 1H), 8.55 (t, *J* = 8.9 Hz, 2H), 8.16 (d, *J* = 2.4 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.67 (td, *J* = 8.0, 6.1 Hz, 1H), 7.59 (dd, *J* = 11.8, 8.0 Hz, 1H), 7.43 – 7.37 (s, 2H), 7.30 (td, *J* = 8.1, 1.0 Hz, 1H); ^{19}F NMR

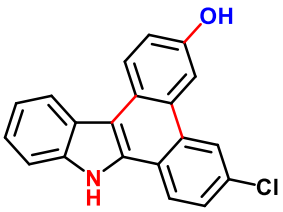
(d_6-DMSO, 564 MHz): δ -116.3 (m, 1F); ^{13}C NMR (d_6-DMSO, 150 MHz): δ 158.3 (d, J_{1F} = 246.0 Hz), 154.3, 138.9 (d, J_{4F} = 2.2 Hz), 131.2 (d, J_{3F} = 4.7 Hz), 127.8, 127.1, 126.2 (d, J_{3F} = 8.8 Hz), 125.0, 123.7, 123.0, 122.2, 121.2, 120.0, 120.0, 120.0, 118.5, 112.8, 112.5 (d, J_{2F} = 14.2 Hz), 112.3 (d, J_{2F} = 20.2 Hz), 108.6. HRMS (ESI) calcd. for $C_{20}H_{11}FNO$ $[M–H]^-$: 300.0830, found: 300.0824.



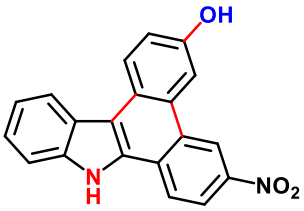
7-bromo-9H-dibenzo[*a,c*]carbazol-3-ol (**3i**).[3] **Condition A**, 48 h, yield: 64%, white solid. ^{1}H NMR (d_6-DMSO, 400 MHz): δ 12.26 (s, 1H), 9.69 (s, 1H), 8.80 (d, *J* = 2.0 Hz, 2H), 8.65 (t, *J* = 7.4 Hz, 2H), 8.50 (d, *J* = 8.0 Hz, 1H), 8.12 (d, *J* = 2.2 Hz, 1H), 7.78 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.35 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.28 (t, *J* = 7.7 Hz, 1H); ^{13}C NMR (d_6-DMSO, 100 MHz): δ 154.2, 138.7, 131.2, 128.6, 127.5, 126.3, 125.0, 124.6, 124.5, 124.0, 123.2, 122.7, 121.5, 120.4, 119.9, 118.1, 112.8, 111.9, 108.2.



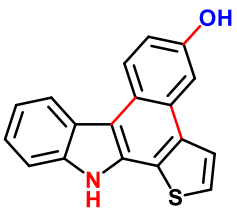
6-fluoro-9H-dibenzo[a,c]carbazol-3-ol (**3j**).[3] **Condition A**, 48 h, yield: 56%, white solid. ^{1}H NMR (d_6-DMSO, 600 MHz): δ 12.21 (s, 1H), 9.65 (s, 1H), 8.65 (d, *J* = 8.8 Hz, 1H), 8.58 (dd, *J* = 8.9, 5.9 Hz, 1H), 8.49 (d, *J* = 8.0 Hz, 1H), 8.45 (dd, *J* = 11.8, 2.3 Hz, 1H), 8.09 (d, *J* = 2.3 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.65 (td, *J* = 8.5, 2.4 Hz, 1H), 7.38 (td, *J* = 7.9, 0.7 Hz, 1H), 7.35 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.27 (td, *J* = 7.9, 0.8 Hz, 1H); ^{19}F NMR (d_6-DMSO, 564 MHz): δ -114.1 (m, 1F); ^{13}C NMR (d_6-DMSO, 150 MHz): δ 160.8 (d, J_{1F} = 241.5 Hz), 154.0, 138.5, 132.2, 130.7 (d, J_{3F} = 8.0 Hz), 127.4 (d, J_{4F} = 3.3 Hz), 124.8, 124.8 (d, J_{3F} = 9.0 Hz), 123.5, 123.4, 123.2, 121.3, 120.0, 119.8, 118.4, 115.6 (d, J_{2F} = 23.6 Hz), 111.8, 111.3, 109.3 (d, J_{2F} = 22.3 Hz), 108.7.



6-chloro-9H-dibenzo[*a,c*]carbazol-3-ol (**3k**).[3] **Condition A**, 48 h, yield: 60%, gray solid. ^{1}H NMR (*d*$_6$-DMSO, 600 MHz): δ 12.26 (s, 1H), 9.67 (s, 1H), 8.70 (s, 1H), 8.67 (d, *J* = 8.7 Hz, 1H), 8.56 (d, *J* = 8.5 Hz, 1H), 8.50 (d, *J* = 8.0 Hz, 1H), 8.14 (s, 1H), 7.80 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.68 (d, *J* = 8.1 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.37 – 7.36 (m, 1H), 7.28 (t, *J* = 7.9 Hz, 1H); ^{13}C NMR (*d*$_6$-DMSO, 150 MHz): δ 154.2, 138.6, 131.9, 130.9, 130.1, 127.1, 127.0, 124.9, 124.3, 123.8, 123.4, 123.3, 123.2, 121.6, 121.4, 119.9, 118.4, 112.2, 111.8, 108.4.

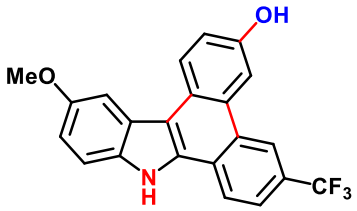


6-nitro-9H-dibenzo[*a,c*]carbazol-3-ol (**3l**). **Condition A**, 48 h, yield: 62%, yellow solid. ^{1}H NMR (*d*$_6$-DMSO, 600 MHz): δ 12.42 (s, 1H), 9.83 (s, 1H), 9.42 (d, *J* = 1.9 Hz, 1H), 8.69 (d, *J* = 8.8 Hz, 1H), 8.65 (d, *J* = 8.9 Hz, 1H), 8.53 (d, *J* = 8.1 Hz, 1H), 8.48 (dd, *J* = 8.9, 2.1 Hz, 1H), 8.17 (d, *J* = 2.2 Hz, 1H), 7.69 (d, *J* = 8.2 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.38 (dd, *J* = 8.6, 2.2 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (*d*$_6$-DMSO, 150 MHz): δ 154.7, 144.6, 139.4, 131.1, 127.8, 127.7, 126.7, 125.3, 125.0, 123.6, 123.0, 122.8, 122.0, 120.7, 120.2, 119.8, 118.9, 115.2, 112.1, 108.2. HRMS (ESI) calcd. for $C_{20}H_{11}N_2O_3$ $[M–H]^-$: 327.0775, found: 327.0769.

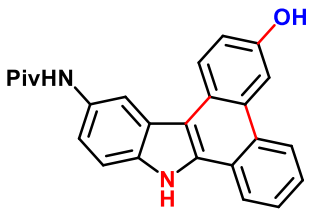


12H-benzo[c]thieno[2,*3-a*]carbazol-5-ol (**3m**).[3] **Condition A**, 52 h, yield: 53%, gray solid. ^{1}H NMR (*d*$_6$-DMSO, 600 MHz): δ 12.10 (s, 1H), 9.69 (s, 1H), 8.68 (d, *J* = 8.8 Hz, 1H), 8.50 (d, *J* = 8.0 Hz, 1H), 7.98 (d, *J* = 5.2 Hz, 1H), 7.91 (d, *J* = 5.3 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 2.3 Hz, 1H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.25 (dd, *J* = 8.8, 2.4 Hz, 1H); ^{13}C NMR (*d*$_6$-DMSO, 150 MHz): δ 153.6, 138.0, 134.9, 131.5, 126.6, 126.4, 125.8, 125.4, 123.4,

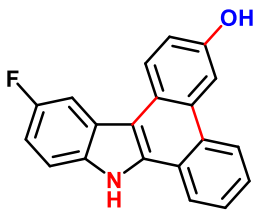
123.3, 122.2, 121.3, 121.1, 119.6, 117.6, 111.7, 111.6, 107.4.



12-methoxy-6-(trifluoromethyl)-9H-dibenzo[*a,c*]carbazol-3-ol (**3n**). **Condition A**, 48 h, yield: 61%, white solid. ^{1}H NMR (*d*$_6$-DMSO, 600 MHz): δ 12.26 (s, 1H), 9.71 (s, 1H), 8.68 (t, *J* = 9.1 Hz, 1H), 8.22 (s, 1H), 8.04 (d, *J* = 8.3 Hz, 1H), 7.95 (s, 1H), 7.61 (d, *J* = 8.7 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.11 (d, *J* = 8.6 Hz, 1H), 3.95 (s, 3H); ^{19}F NMR (*d*$_6$-DMSO, 564 MHz): δ -60.0 (s, 3F); ^{13}C NMR (*d*$_6$-DMSO, 150 MHz): δ 154.2 (d, J_{2F} = 33.0 Hz), 134.0, 132.0, 128.0, 127.3, 125.8, 125.8 (q, J_{1F} = 31.5 Hz), 125.5, 125.1, 124.0, 123.5, 123.2, 123.2, 122.7, 121.0, 118.5, 114.4, 113.6, 112.7, 108.3, 103.9, 55.9. HRMS (ESI) calcd. for $C_{22}H_{13}F_3NO_2$ $[M–H]^-$: 380.0904, found: 380.0895.

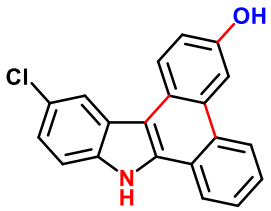


N-(3-hydroxy-9H-dibenzo[*a,c*]carbazol-12-yl)pivalamide (**3o**). **Condition A**, 45.5 h, yield: 64%, white solid. ^{1}H NMR (*d*$_6$-DMSO, 600 MHz): δ 12.10 (s, 1H), 9.64 (s, 1H), 9.26 (s, 1H), 8.76 (s, 1H), 8.68 (d, *J* = 8.3 Hz, 1H), 8.50 (t, *J* = 8.3 Hz, 1H), 8.15 (d, *J* = 2.2 Hz, 1H), 7.91 (d, *J* = 5.3 Hz, 1H), 7.73 (t, *J* = 7.4 Hz, 1H), 7.70 (dd, *J* = 8.7, 1.6 Hz, 1H), 7.66 (t, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.6 Hz, 1H), 7.34 (dd, *J* = 8.6, 2.3 Hz, 1H), 1.30 (s, 9H); ^{13}C NMR (*d*$_6$-DMSO, 150 MHz): δ 176.3, 153.9, 135.2, 133.1, 132.2, 128.7, 127.9, 127.0, 126.1, 124.2, 123.9, 123.1, 123.0, 122.8, 122.3, 118.2, 117.5, 112.9, 111.6, 111.2, 108.3, 78.4, 27.6. HRMS (ESI) calcd. for $C_{25}H_{21}N_2O_2$ $[M–H]^-$: 381.1608, found: 381.1601.

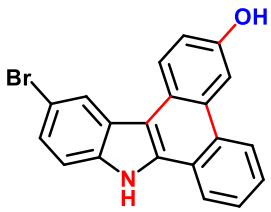


12-fluoro-9H-dibenzo[*a,c*]carbazol-3-ol (**3p**).[3] **Condition A**, 62 h, yield: 76%, white solid. ^{1}H

NMR (d_6-DMSO, 600 MHz): δ 12.28 (s, 1H), 9.65 (s, 1H), 8.70 (d, J = 8.3 Hz, 1H), 8.59 (d, J = 8.8 Hz, 1H), 8.52 (dd, J = 8.0, 0.7 Hz, 1H), 8.28 (dd, J = 10.5, 2.2 Hz, 1H), 8.15 (d, J = 2.3 Hz, 1H), 7.74 (td, J = 7.7, 0.7 Hz, 1H), 7.70 – 7.65 (m, 2H), 7.33 (dd, J = 8.6, 2.3 Hz, 1H), 7.24 (td, J = 9.1, 2.4 Hz, 1H); ^{19}F NMR (d_6-DMSO, 564 MHz): δ -123.6 (m, 1F); ^{13}C NMR (d_6-DMSO, 150 MHz): δ 157.3 (d, J_{1F} = 230.3 Hz), 154.1, 135.1, 134.1, 129.1, 127.9, 127.0, 126.5, 124.8, 123.9, 123.4 (d, J_{3F} = 9.9 Hz), 123.0, 122.4, 117.7, 115.7, 112.6 (d, J_{3F} = 9.6 Hz), 111.8 (d, J_{4F} = 4.4 Hz), 111.4 (d, J_{2F} = 25.5 Hz), 108.3, 106.5 (d, J_{2F} = 24.2 Hz).



12-chloro-9H-dibenzo[*a,c*]carbazol-3-ol (**3q**).[3] **Condition A**, 62 h, yield: 60%, white solid. ^{1}H NMR (d_6-DMSO, 600 MHz): δ 12.39 (s, 1H), 9.66 (s, 1H), 8.70 (d, J = 8.3 Hz, 1H), 8.60 (d, J = 8.8 Hz, 1H), 8.52 – 8.51 (m, 2H), 8.14 (d, J = 2.3 Hz, 1H), 7.75 (t, J = 7.7 Hz, 1H), 7.70 (td, J = 8.1, 1.0 Hz, 1H), 7.68 (d, J = 8.6 Hz, 1H), 7.40 (dd, J = 8.5, 1.9 Hz, 1H), 7.33 (dd, J = 8.6, 2.4 Hz, 1H); ^{13}C NMR (d_6-DMSO, 150 MHz): δ 154.3, 137.0, 133.7, 129.1, 128.1, 127.1, 126.6, 124.9, 124.4, 124.2, 124.0, 123.4, 122.8, 122.4, 122.2, 120.4, 117.8, 113.2, 111.2, 108.3.

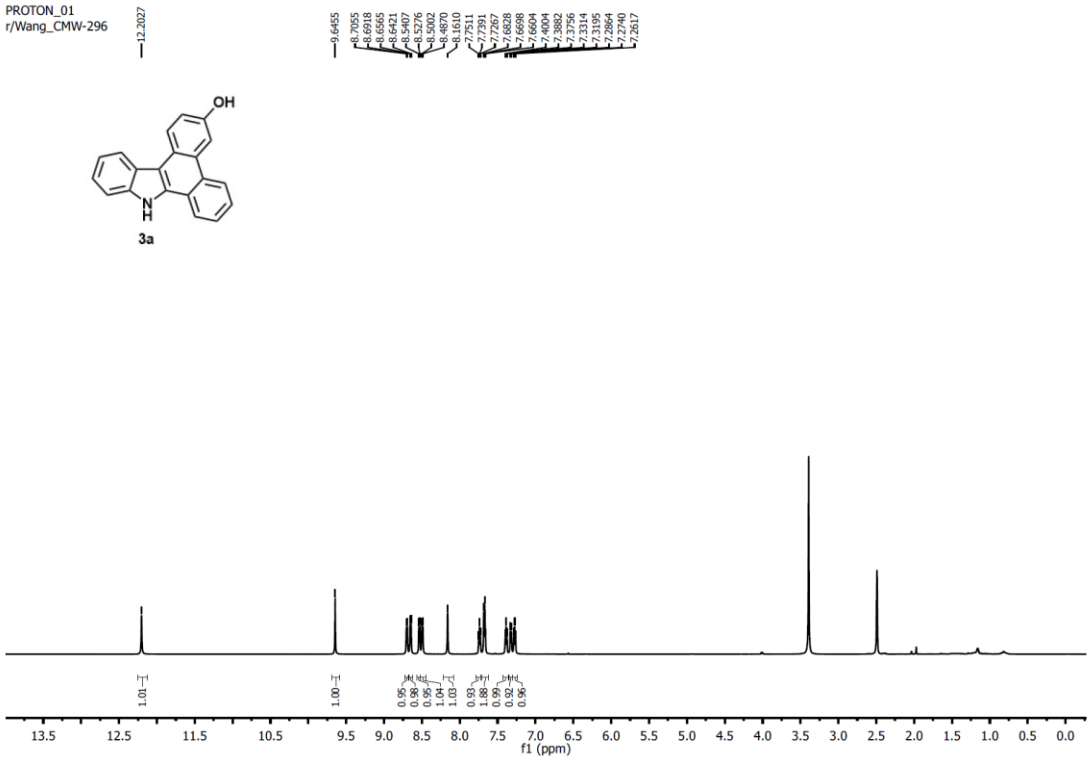


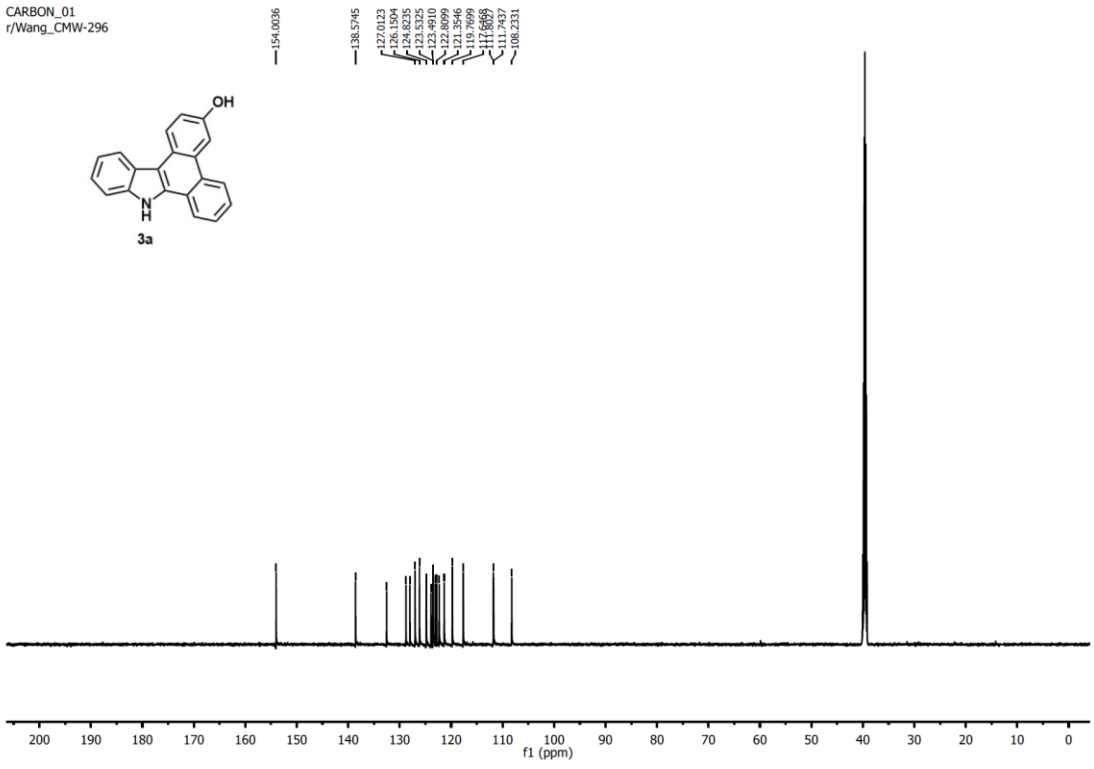
12-bromo-9H-dibenzo[*a,c*]carbazol-3-ol (**3r**).[3] **Condition A**, 62 h, yield: 58%, gray solid. ^{1}H NMR (d_6-DMSO, 600 MHz): δ 12.40 (s, 1H), 9.66 (s, 1H), 8.70 (d, J = 8.3 Hz, 1H), 8.64 (d, J = 1.4 Hz, 1H), 8.59 (d, J = 8.8 Hz, 1H), 8.51 (d, J = 7.1 Hz, 1H), 8.14 (d, J = 2.3 Hz, 1H), 7.75 (t, J = 7.7 Hz, 1H), 7.69 (t, J = 8.0 Hz, 1H), 7.63 (d, J = 8.5 Hz, 1H), 7.51 (dd, J = 8.5, 1.7 Hz, 1H), 7.33 (dd, J = 8.6, 2.2 Hz, 1H); ^{13}C NMR (d_6-DMSO, 150 MHz): δ 154.3, 137.2, 133.5, 129.1, 128.1, 127.1, 126.7, 126.0, 125.1, 124.9, 124.0, 123.3, 122.8, 122.4, 122.2, 117.8, 113.6, 112.1, 111.1, 108.3.

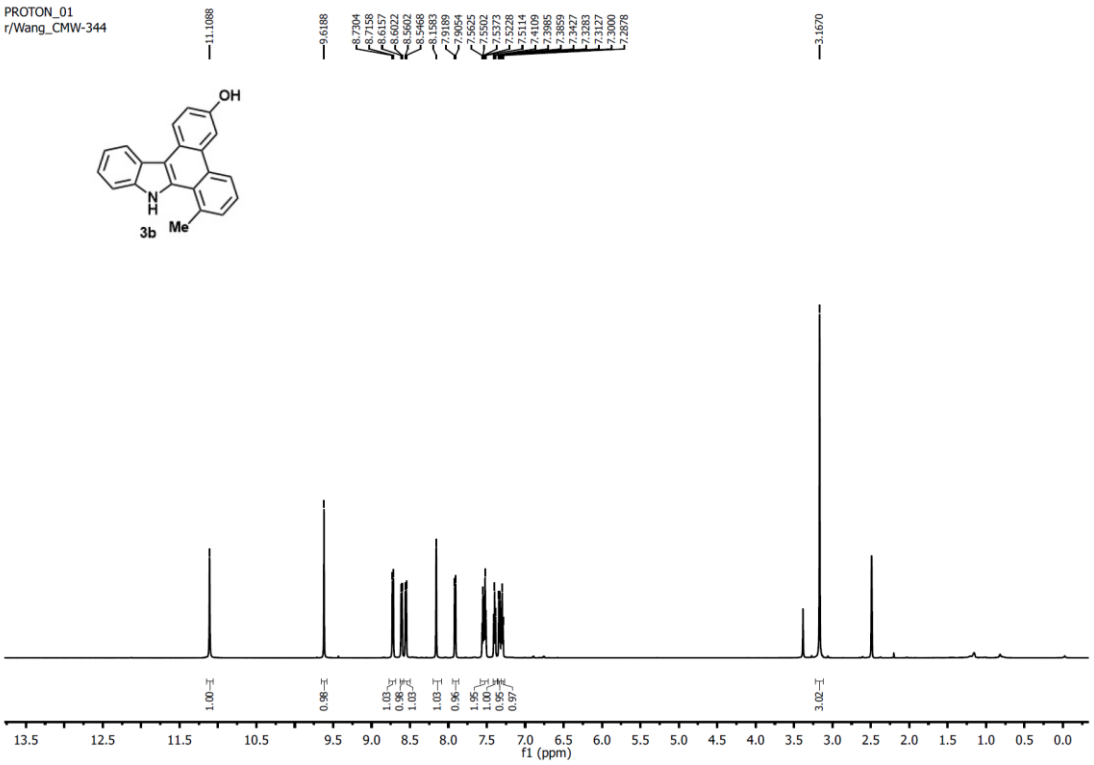
References

1. C. White, A. Yates and P. M. Maitlis, *Inorg. Syn.*, 1992, **29**, 228.
2. X. Yu, E.-J. Park, T. P. Kondratyuk, J. M. Pezzuto and D. Sun, *Org. Biomol. Chem.*, 2012, **10**, 8835.
3. S. Guo, Y. Liu, L. Zhao, X. Zhang and X. Fan, *Org. Lett.*, 2019, **21**, 6437.

NMR Spectra Images of Products



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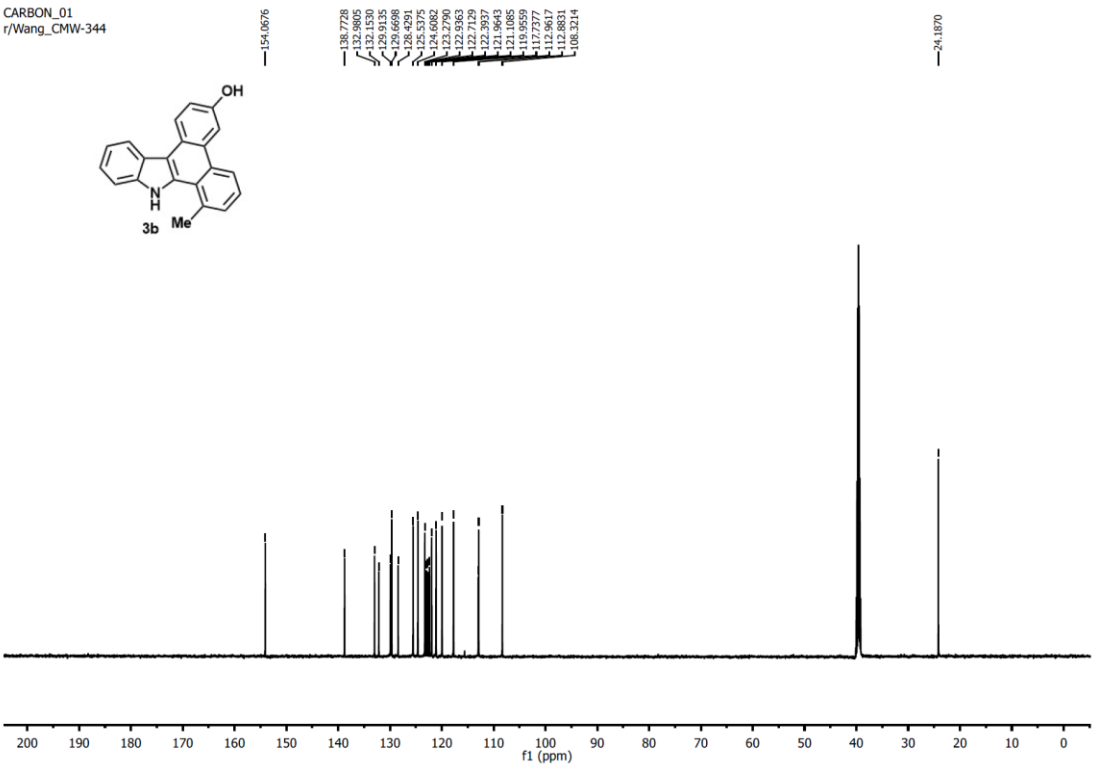
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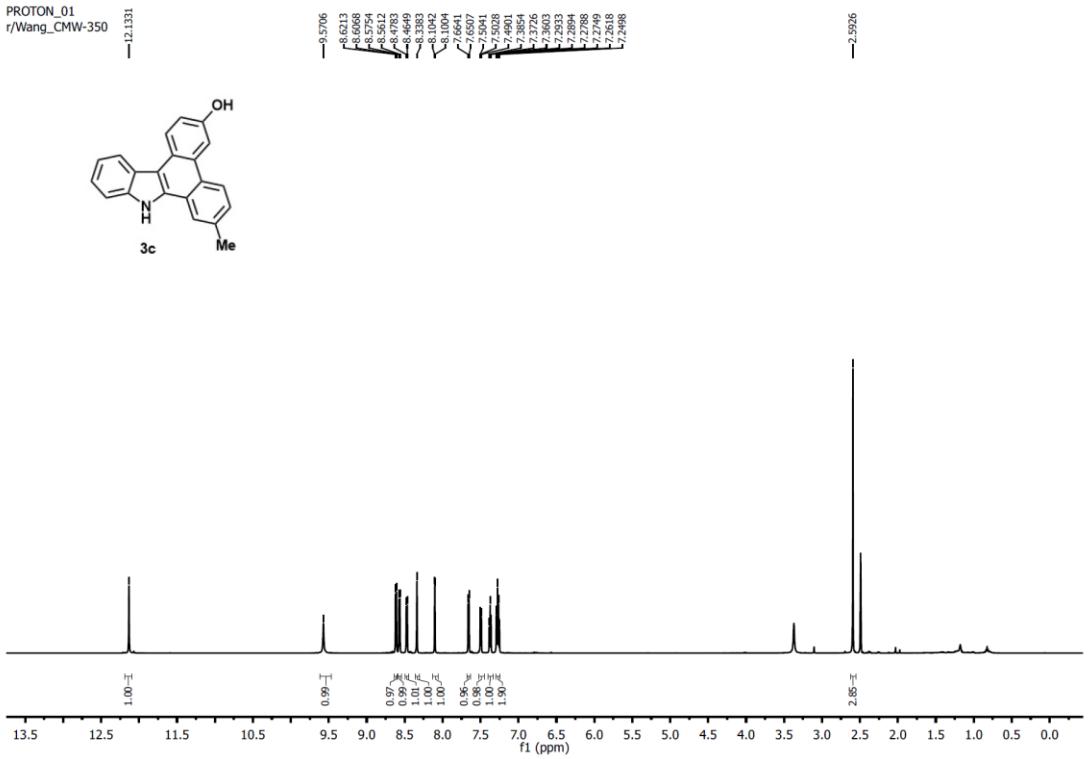
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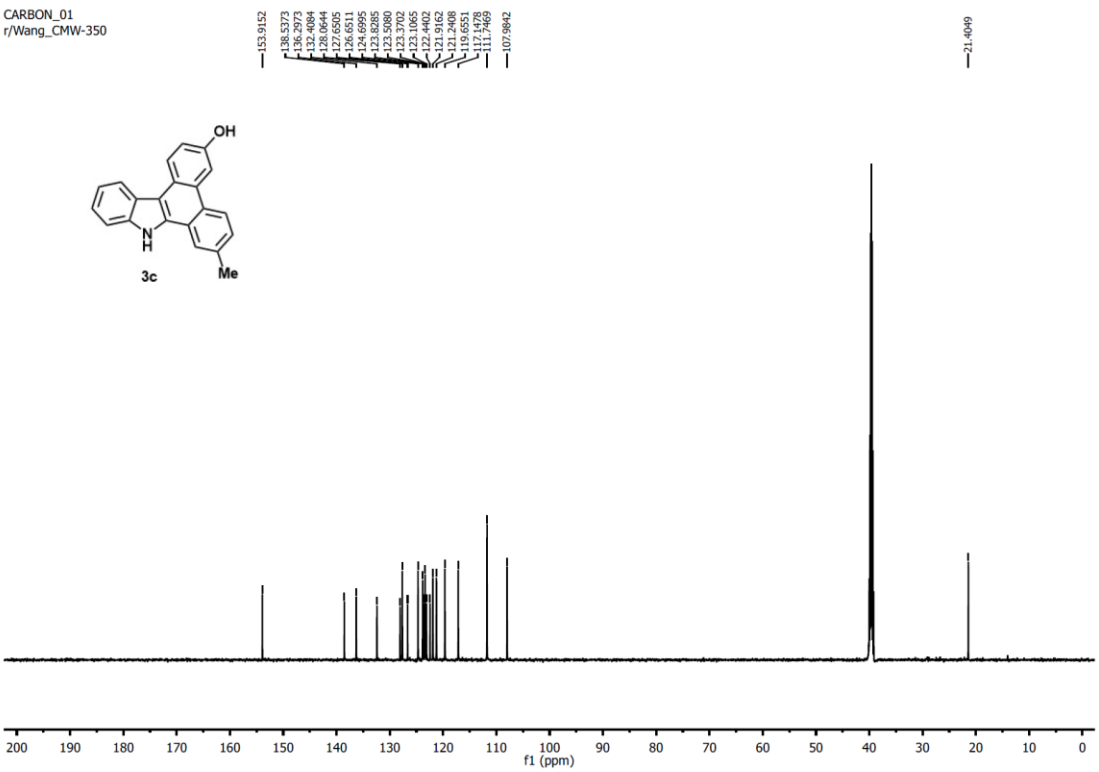
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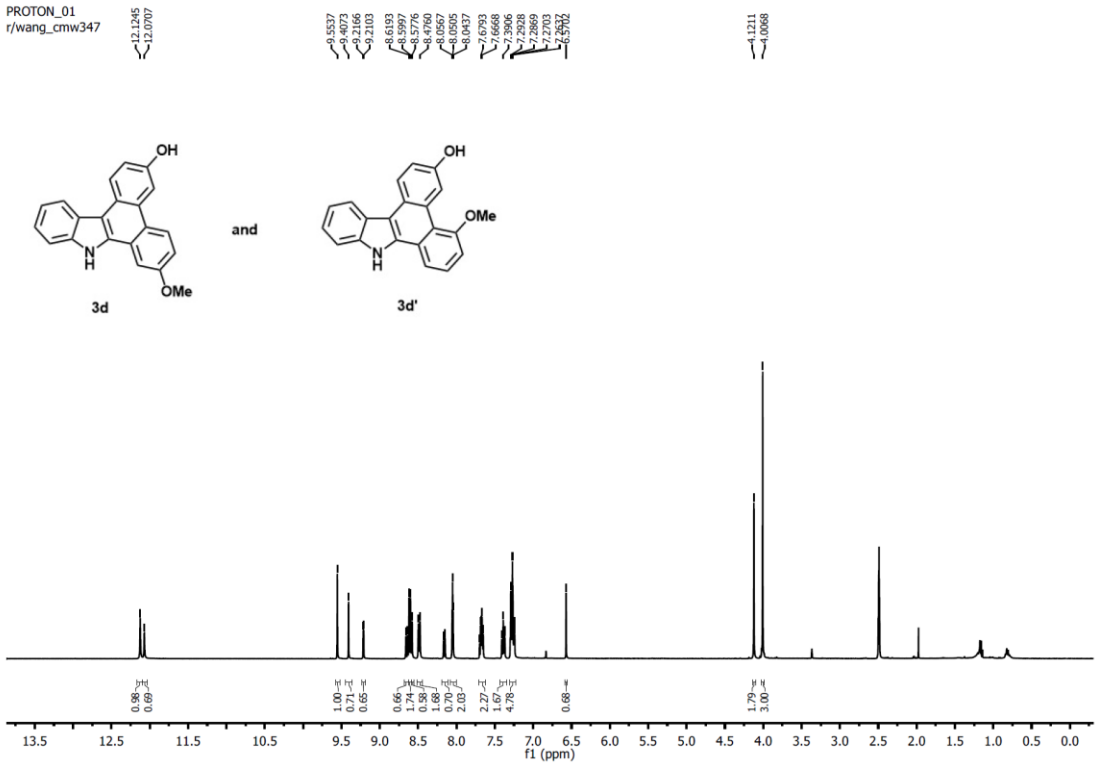
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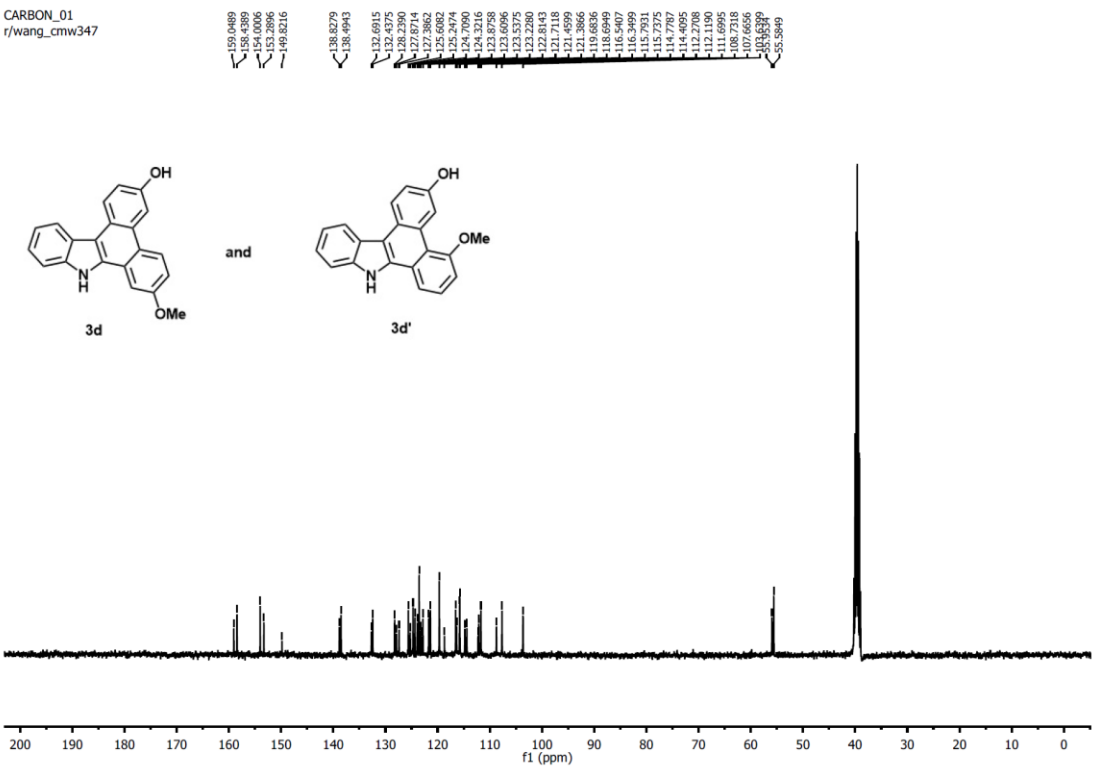
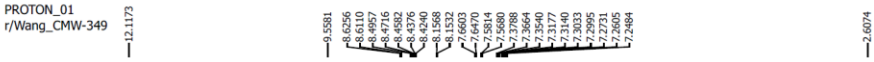
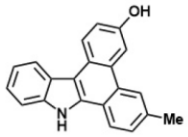
0.58
1.68
0.70
2.03
2.27
1.67
4.78
0.68
1.79
3.00
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

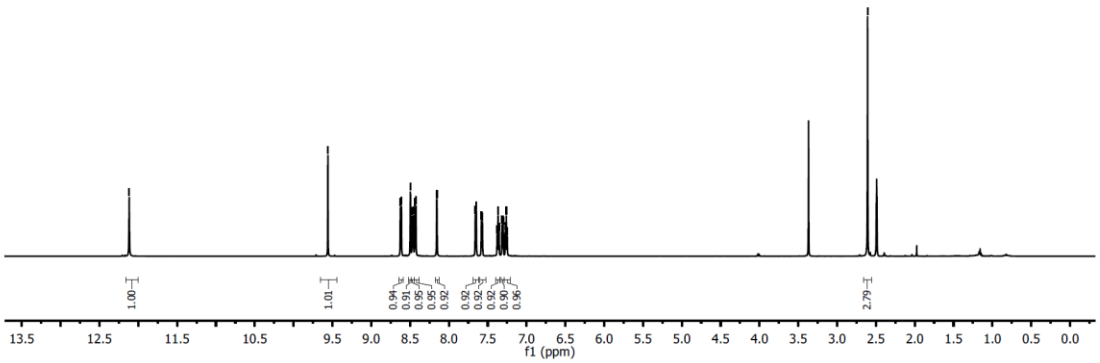

CARBON_01
r/wang_cmw347
159.0489
158.4389
154.3006
153.3896
149.8216
138.8279
138.4943
132.6915
132.4375
128.2390
127.8714
127.3862
125.6002
125.3754
124.7090
124.3216
123.8758
123.6096
123.5375
123.2280
122.8143
121.7118
121.4599
121.3866
119.6836
118.6949
116.5407
116.3499
115.7931
115.7375
114.7787
114.4095
112.2708
112.1190
111.6995
108.7318
107.6566
101.6399
55.9534
55.5849
OH
OMe
N
H
3d
and
OH
OMe
N
H
3d'
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

PROTON_01
r/Wang_CMW-349

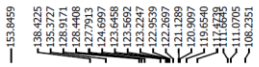


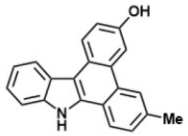


3e

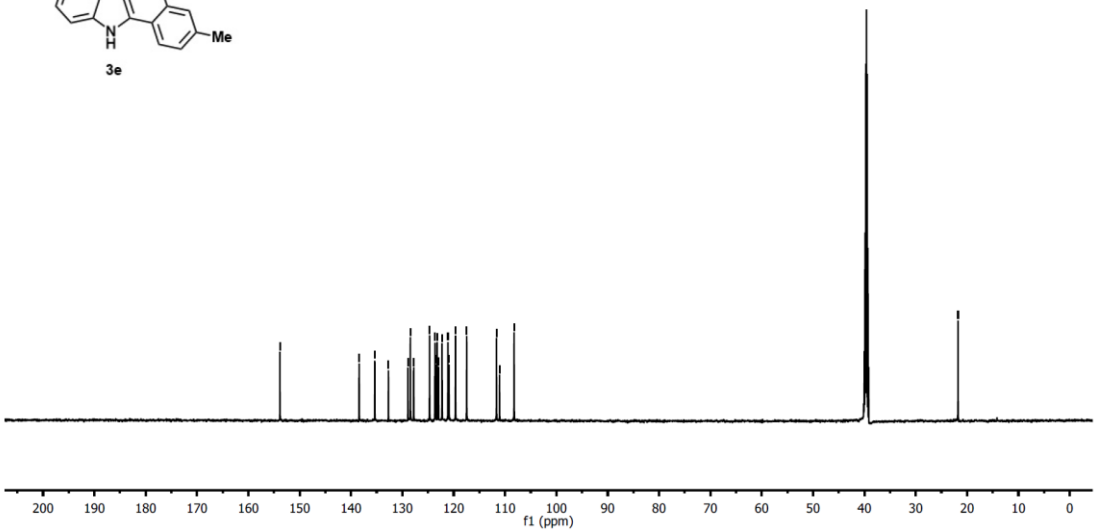


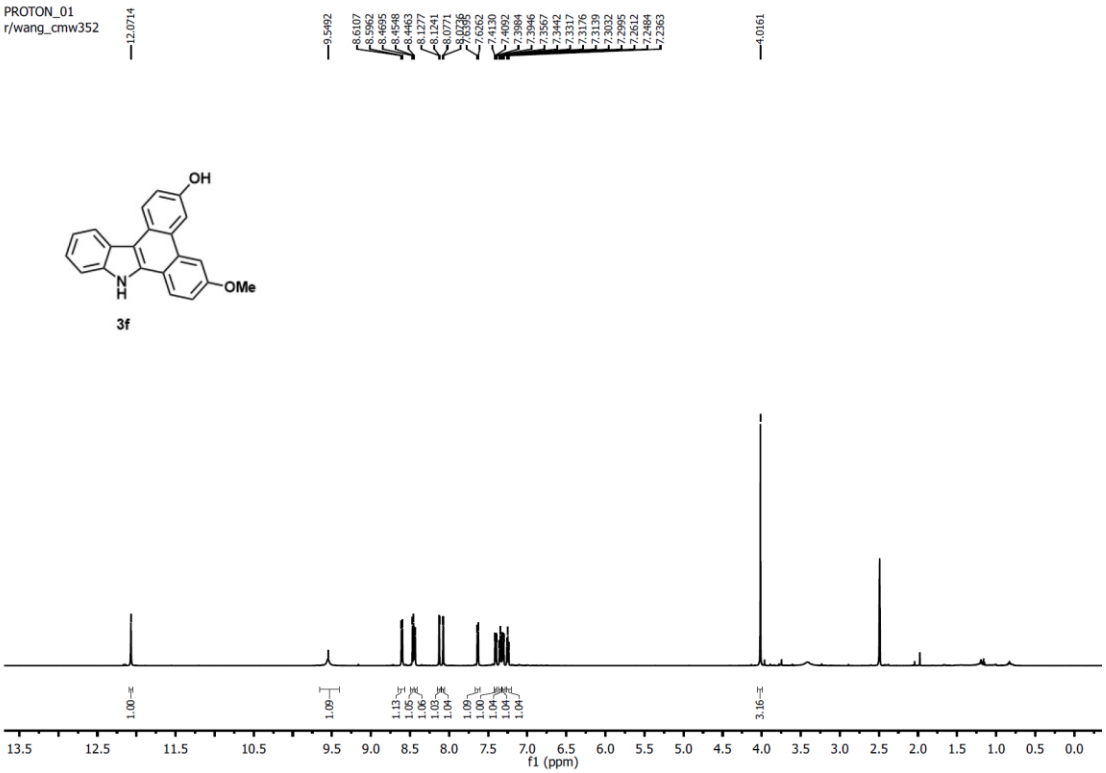
CARBON_01
r/Wang_CMW-349

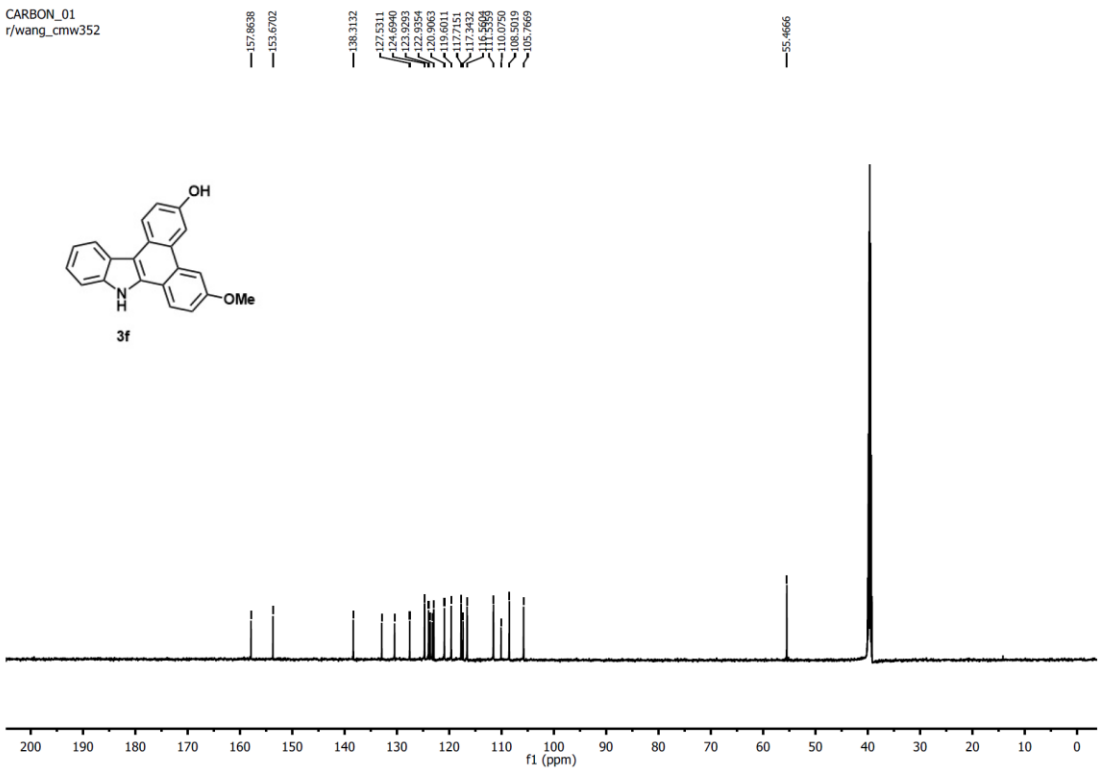


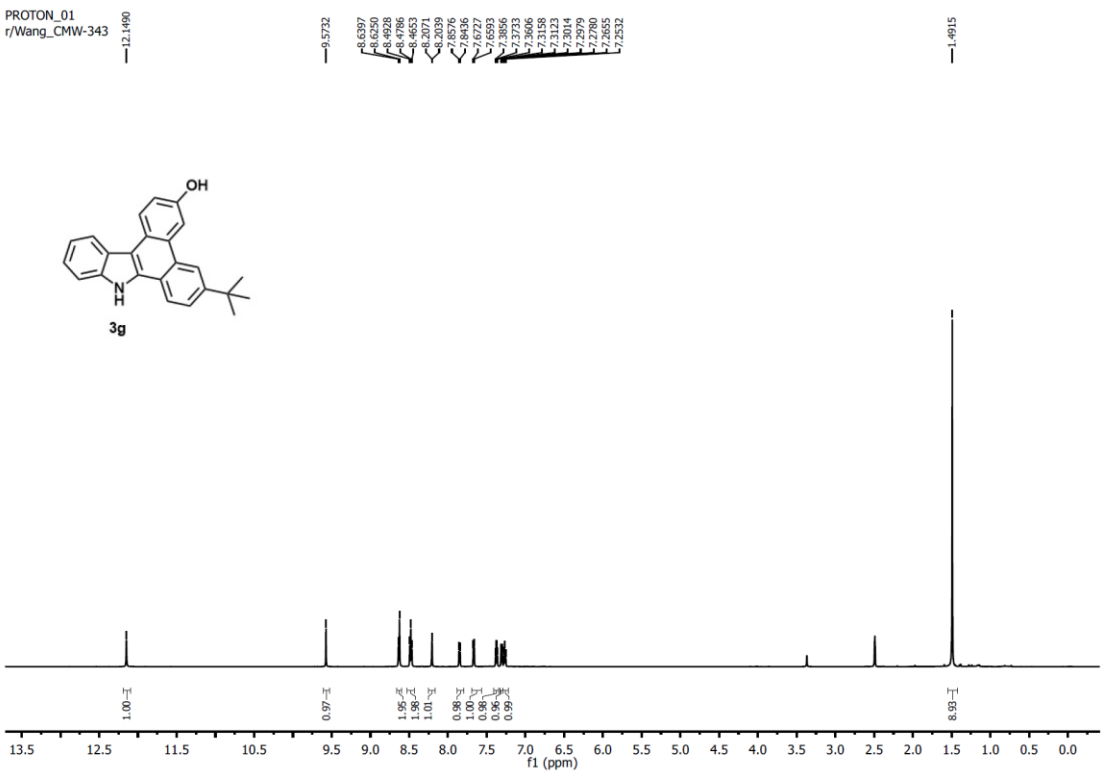


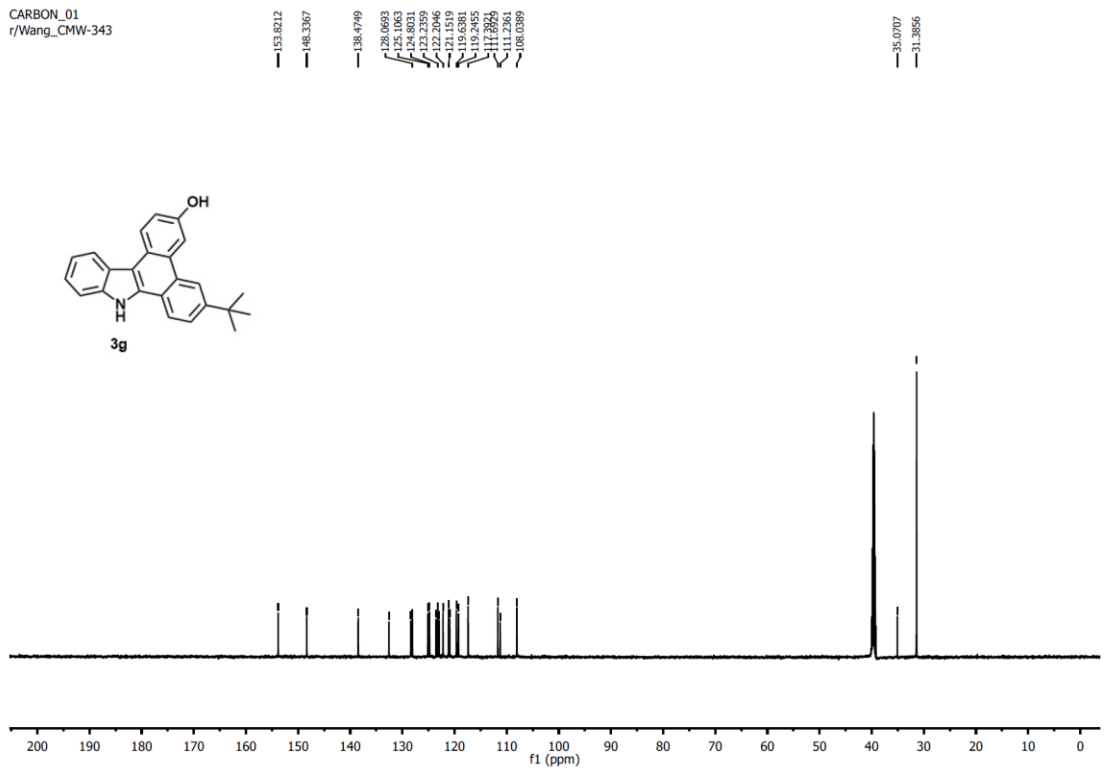
3e



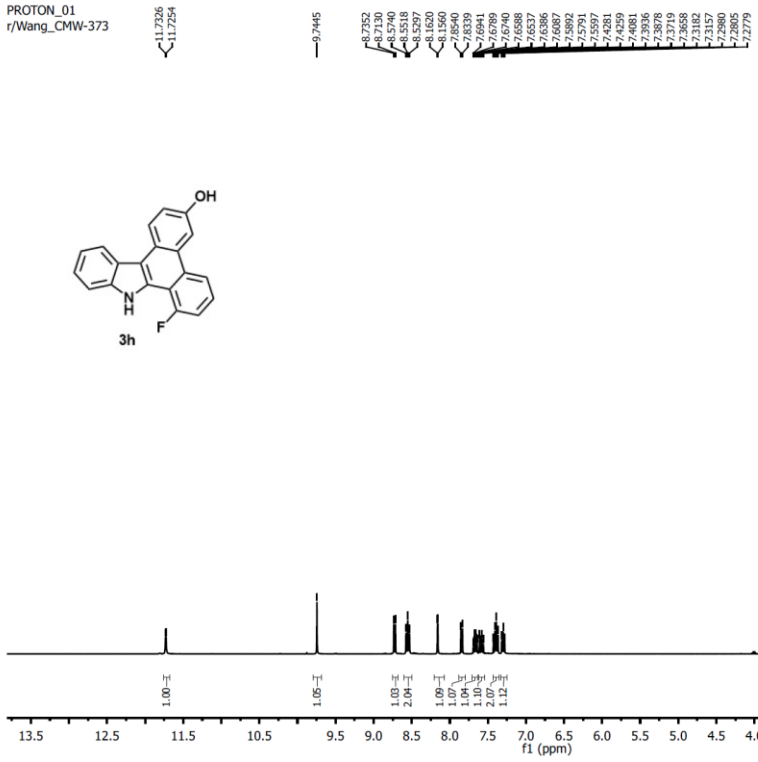

PROTON_01
r/wang_cmw352
12.0714
9.5492
8.6107
8.3962
8.4695
8.4548
8.4463
8.1277
8.1241
8.0771
7.6262
7.4130
7.4092
7.3984
7.3946
7.3567
7.3442
7.3317
7.3176
7.3139
7.3032
7.2895
7.2852
7.2484
7.2363
4.0161
OH
OMe
N
H
3f
1.00
1.09
1.13
1.05
1.06
1.03
1.04
1.00
1.00
1.04
1.04
1.04
3.16
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


CARBON_01
r/wang_cmw352
157.8638
153.6702
138.3132
127.5311
124.6940
123.9293
122.9354
120.9063
119.6011
117.7151
117.3432
110.0750
108.5019
105.7669
55.4666
OH
OMe
N
H
3f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

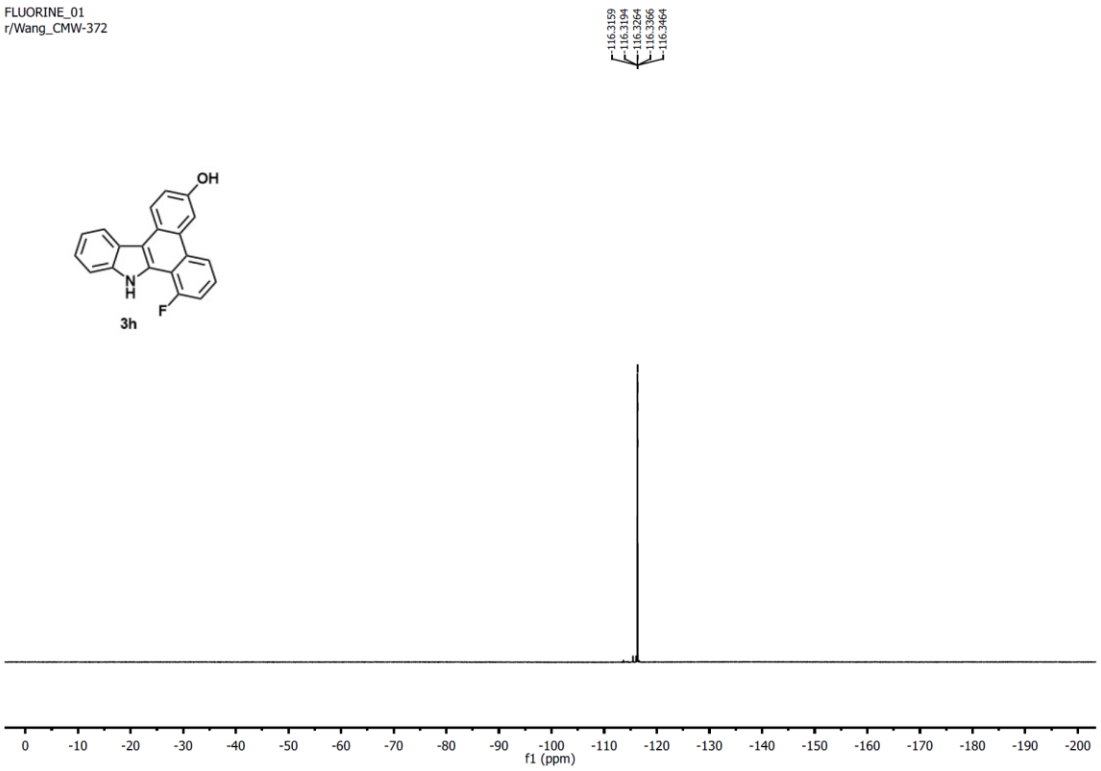

PROTON_01
r/Wang_CMW-343
12.1490
9.5732
8.6397
8.6250
8.4928
8.4786
8.4653
8.2071
8.2039
7.8576
7.8436
7.6727
7.6593
7.3866
7.3733
7.3606
7.3158
7.3123
7.3014
7.2979
7.2780
7.2655
7.2532
1.4915
OH
N
H
3g
1.00
0.97
1.95
1.98
1.01
0.98
1.00
0.98
0.96
0.99
8.93
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


CARBON_01
r/Wang_CMW-343
153.8212
148.3367
138.4749
128.0693
125.1063
124.8031
123.2359
122.2046
121.1519
119.6381
119.2455
111.8925
111.2361
108.0389
35.0707
31.3856
OH
N
H
3g
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

PROTON_01
r/Wang_CMW-373

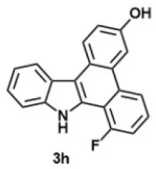


FLUORINE_01
r/Wang_CMW-372

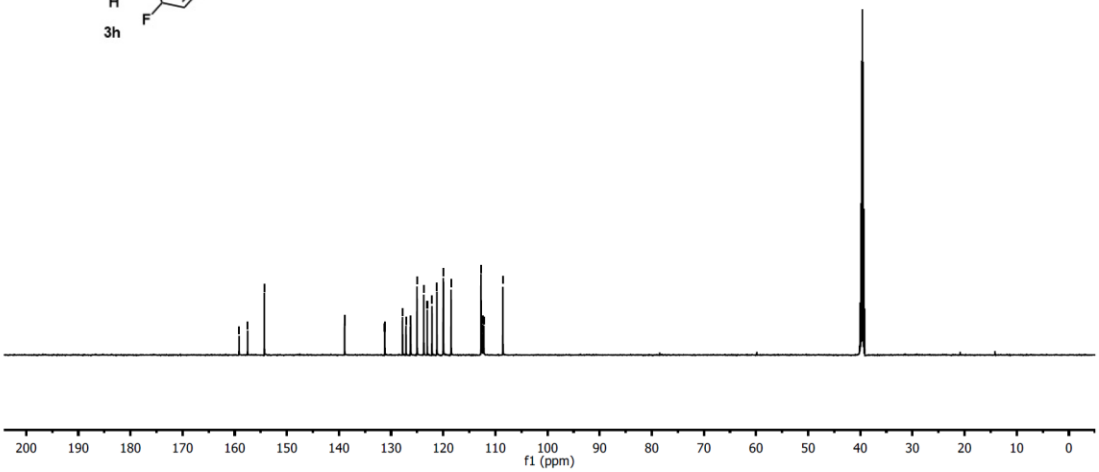


CARBON_01
r/Wang_CMW-372

159.1593
157.5246
154.3156
138.9252
138.9106
125.0291
123.7347
123.0570
122.1657
121.2168
119.9998
119.9783
112.5755
112.4809
112.3434
112.2085
108.5670

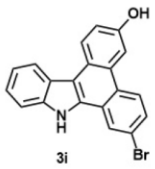


3h

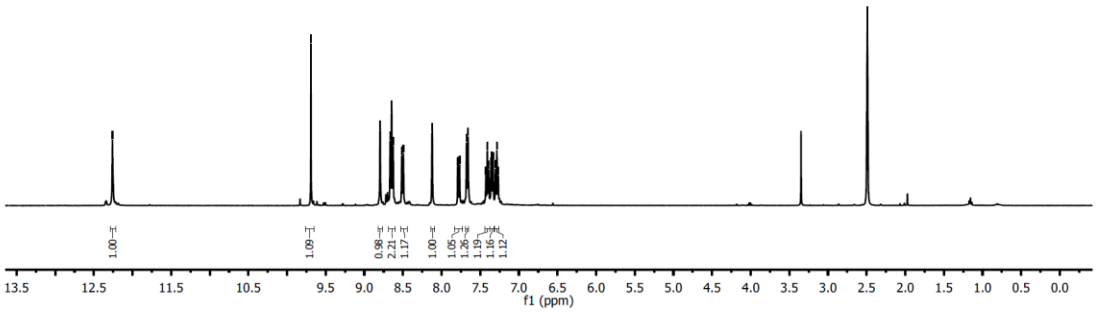


PROTON_01
r/Wang_CMW-374

12.2593
9.6908
8.7986
8.7936
8.6666
8.6482
8.6451
8.6263
8.1253
8.1197
7.7936
7.7876
7.7705
7.7655
7.6774
7.6573
7.4276
7.4085
7.3899
7.3607
7.3551
7.3390
7.3333
7.3042
7.2849
7.2669

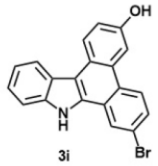


3i



CARBON_01
r/Wang_CMW-374

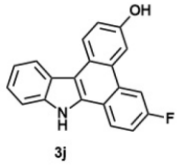
154.2344
138.6722
127.5286
126.3462
124.9525
124.5904
124.5388
123.3864
121.5565
119.9256
118.0000
112.8804
111.8894
108.1963



3i

PROTON_01
r/Wang_CMW-335

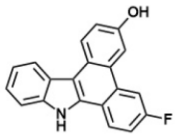
12.2109
9.6518
8.6505
8.6359
8.5819
8.5770
8.5671
8.4896
8.4763
8.4617
8.0880
8.0841
7.6689
7.6618
7.6556
7.6477
7.6438
7.6334
7.6294
7.3971
7.3960
7.3840
7.3720
7.3708
7.3584
7.3544
7.3439
7.3399
7.2871
7.2858
7.2739
7.2621
7.2606



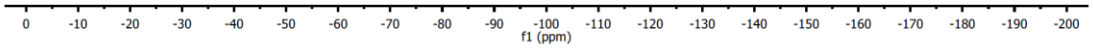
3j

FLUORINE_01
r/Wang_CMW-335

-114.0671
-114.0787
-114.0890
-114.0911
-114.0987
-114.1125

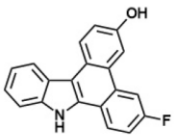


3j



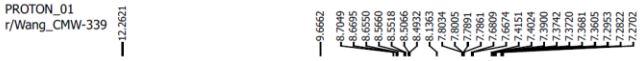
CARBON_01
r/Wang_CMW-335

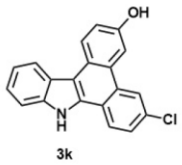
161.5694
159.9634
153.9706
138.4837
132.2023
130.6564
130.6030
127.3964
127.3742
124.8354
124.8038
124.7436
123.5234
123.3859
123.1735
121.2653
119.9700
119.8311
118.3531
115.6757
115.5583
111.7610
111.3123
109.3542
109.2057
108.7008



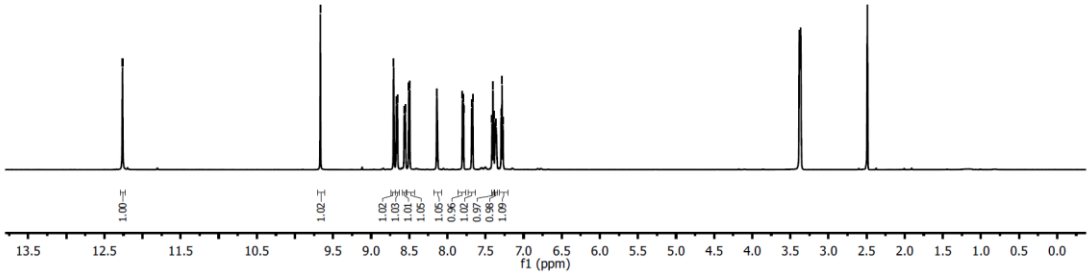
3j

PROTON_01
r/Wang_CMW-339

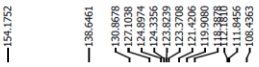


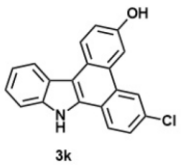


3k

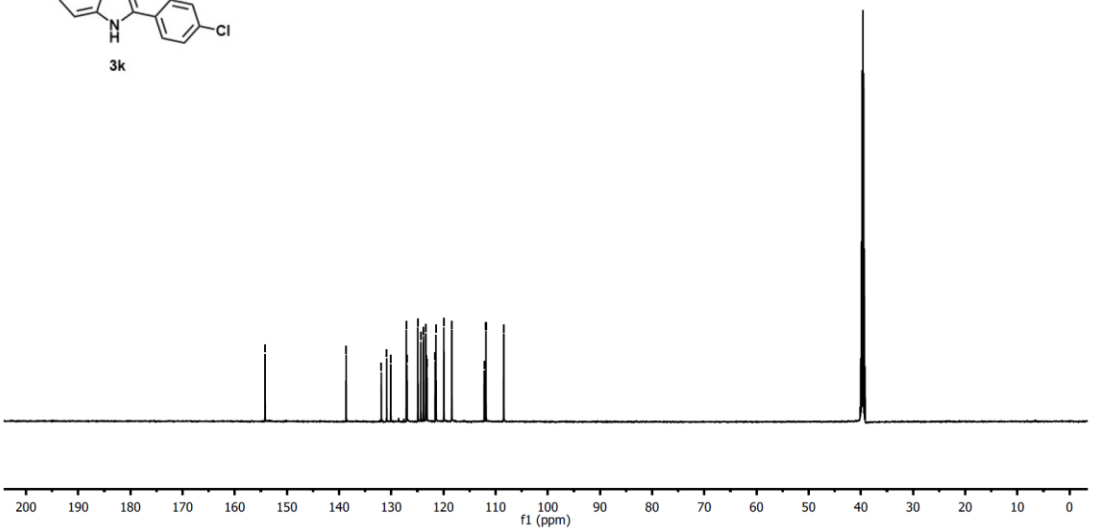


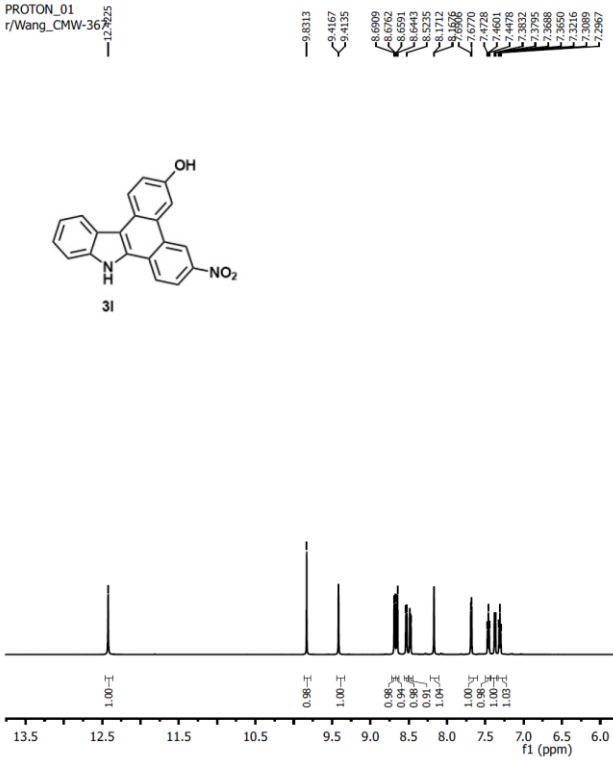
CARBON_01
r/Wang_CMW-339

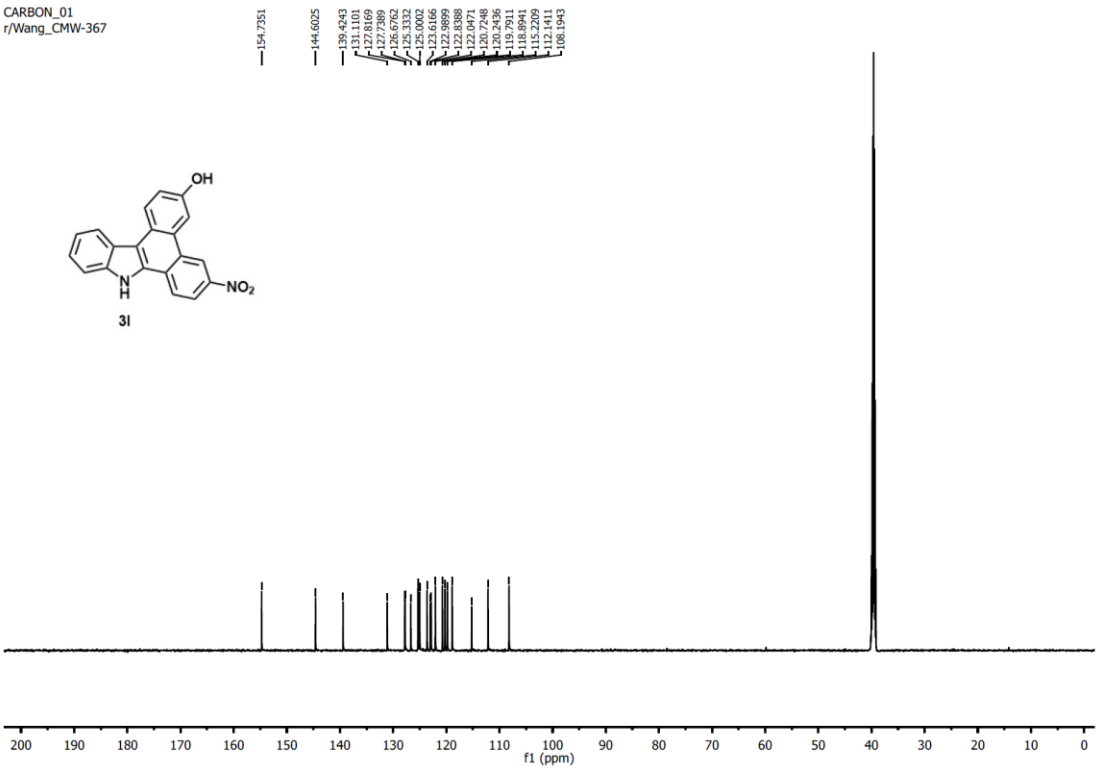


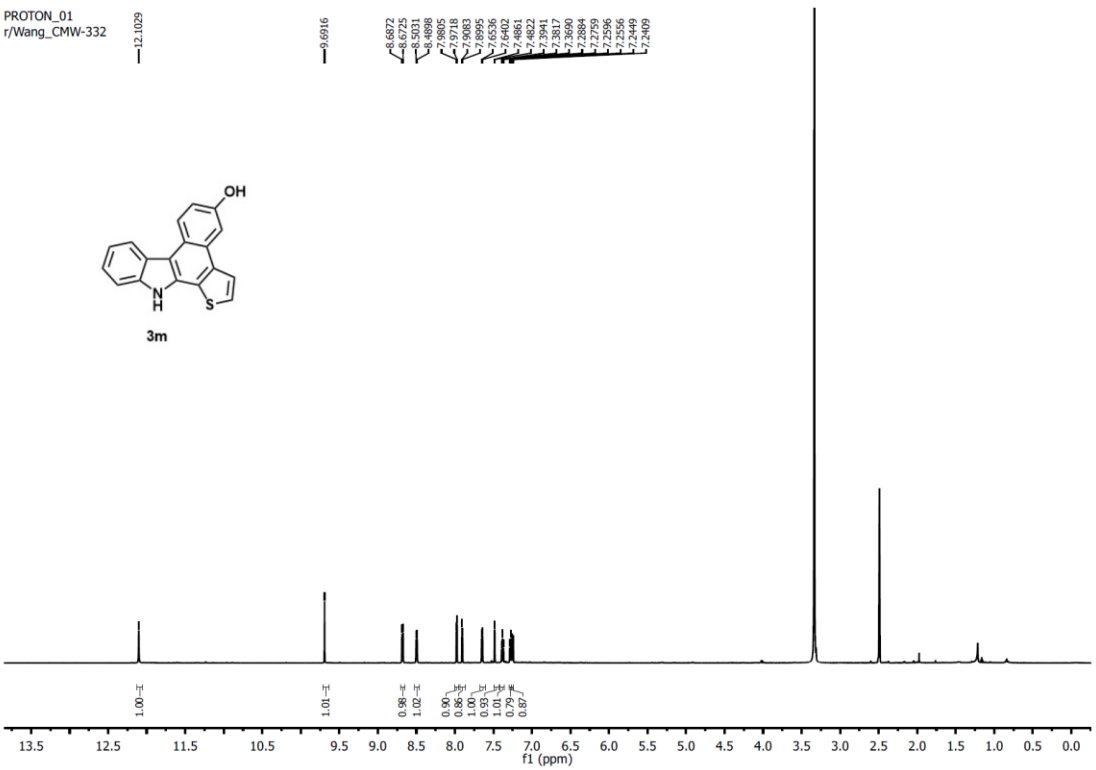


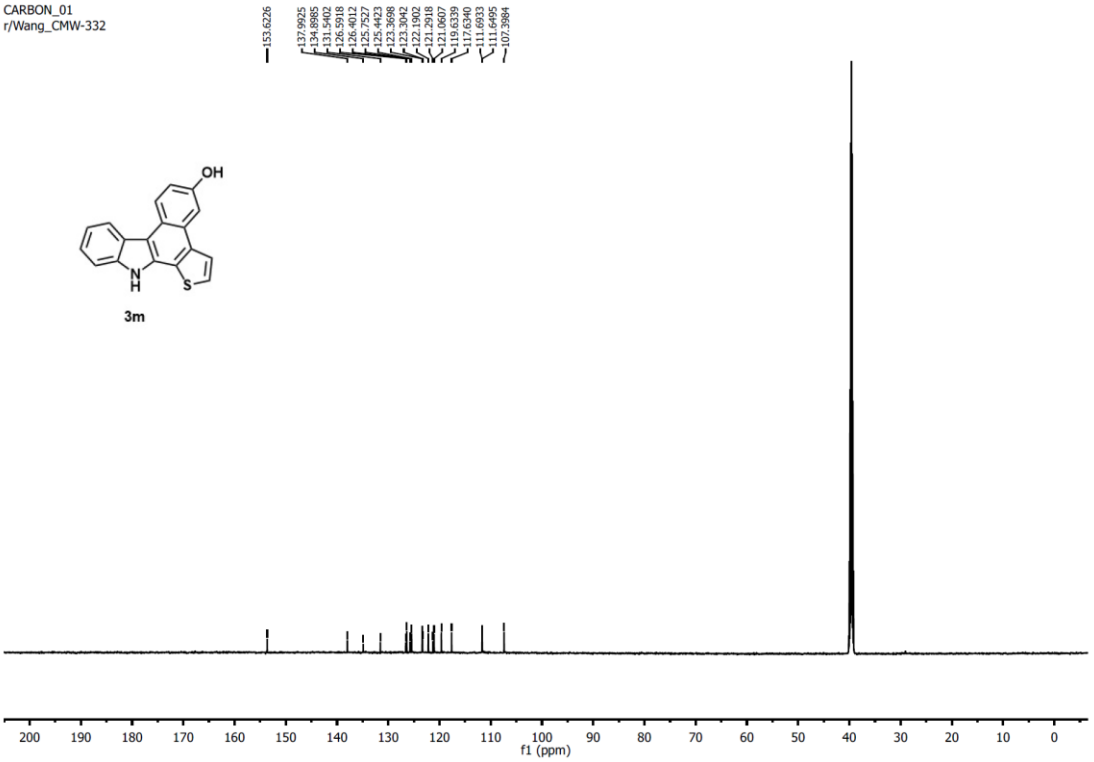
3k

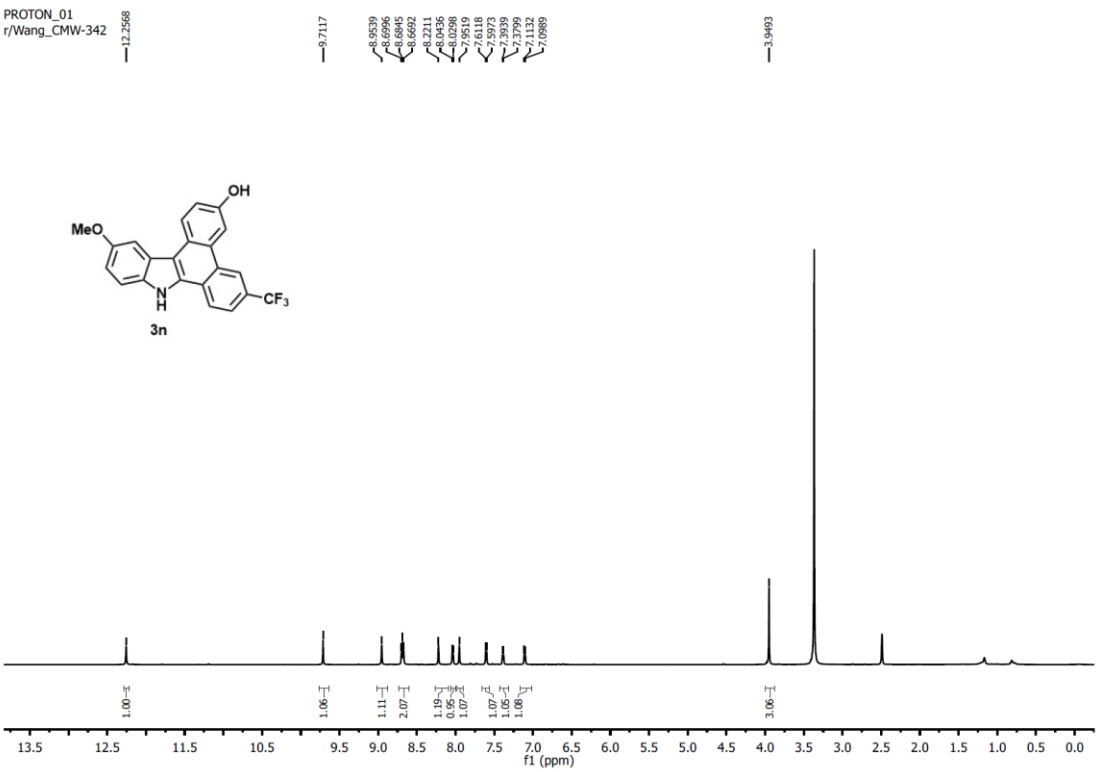


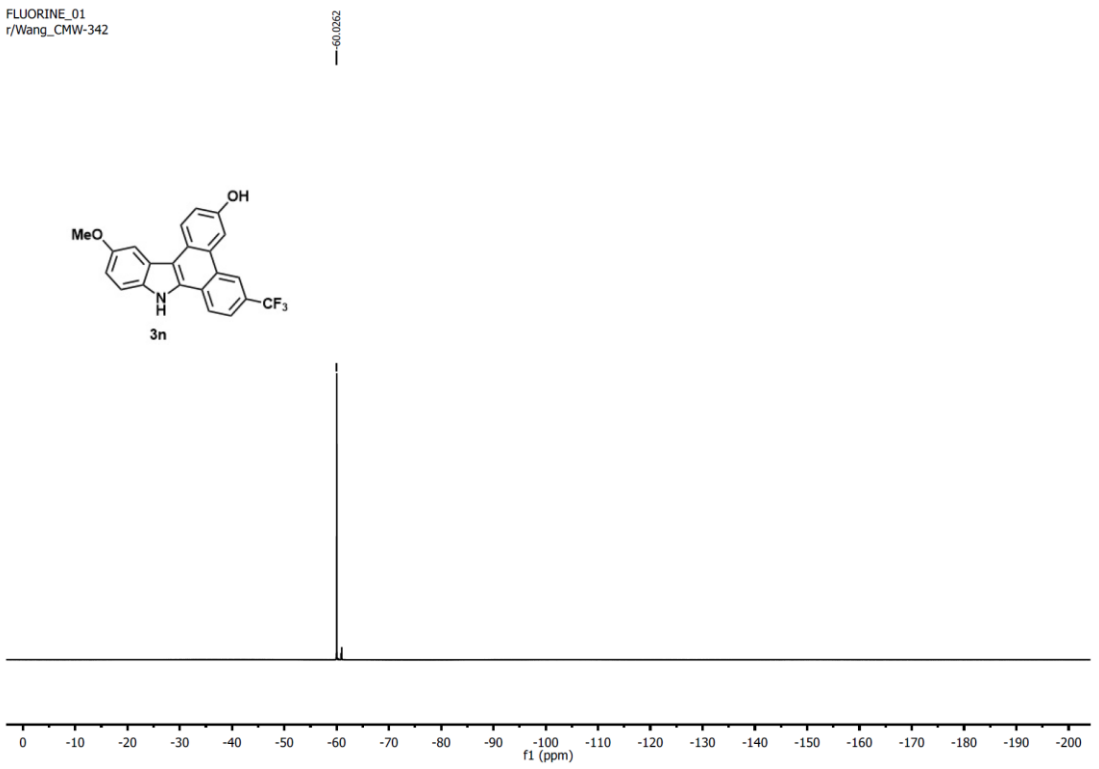

PROTON_01
r/Wang_CMW-367
12.5225
9.8313
9.4167
9.4135
8.6909
8.6762
8.6591
8.6443
8.5335
8.1712
7.6908
7.6770
7.4728
7.4601
7.4478
7.3832
7.3795
7.3688
7.3650
7.3216
7.3089
7.2967
OH
NO2
3l
1.00
0.98
1.00
0.98
0.94
0.98
0.91
1.04
1.00
0.98
1.00
1.03
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


CARBON_01
r/Wang_CMW-367
154.7351
144.6025
139.4243
131.1101
127.8169
127.7389
126.6762
125.3332
125.0002
123.6166
122.9899
122.8388
122.6471
120.7248
120.2436
119.7911
118.8941
115.2209
112.1411
108.1943
OH
NO2
3l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

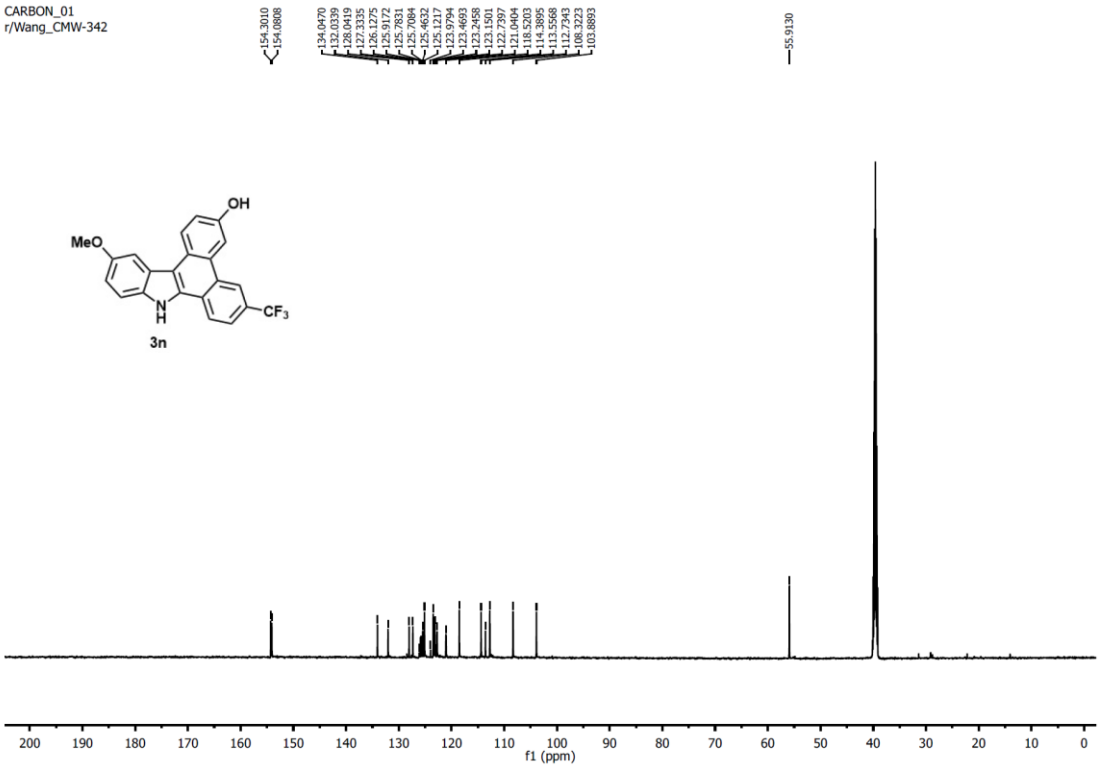

PROTON_01
r/Wang_CMW-332
12.1029
9.6916
8.6872
8.6725
8.5031
8.4898
7.9805
7.9718
7.9003
7.8995
7.6536
7.6402
7.4861
7.4822
7.3941
7.3817
7.3690
7.2884
7.2759
7.2596
7.2555
7.2449
7.2409
OH
N
H
S
3m
1.00
1.01
0.98
1.02
0.90
0.86
1.00
0.93
1.01
0.79
0.87
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


CARBON_01
r/Wang_CMW-332
153.6226
137.9925
134.9895
131.5402
126.5918
126.4012
125.7527
125.4423
123.3698
123.3042
122.1902
121.2918
121.0607
119.6539
117.6240
111.6933
111.6495
107.3984
OH
N
H
S
3m
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

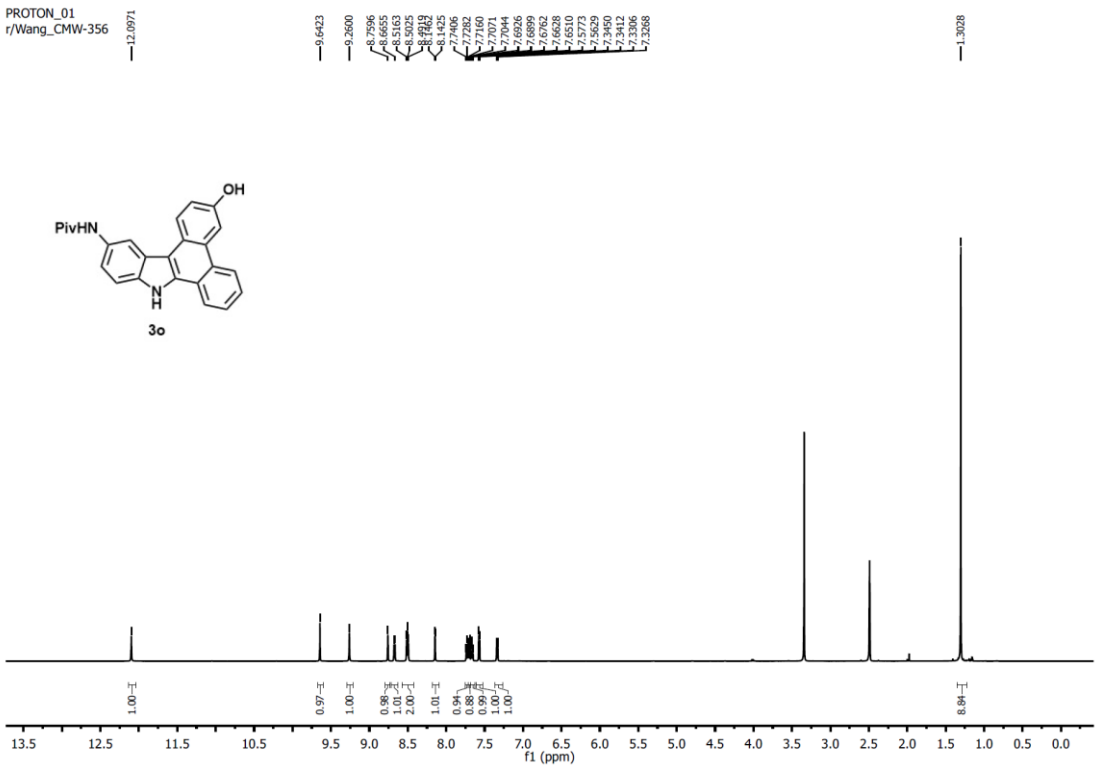

PROTON_01
r/Wang_CMW-342
12.2568
9.7117
8.9539
8.6996
8.6845
8.6692
8.2211
8.0496
8.0288
7.9519
7.6118
7.5973
7.3939
7.3799
7.1132
7.0989
3.9493
OH
MeO
N
H
CF3
3n
1.00
1.06
1.11
2.07
1.19
0.95
1.07
1.07
1.05
1.08
3.06
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

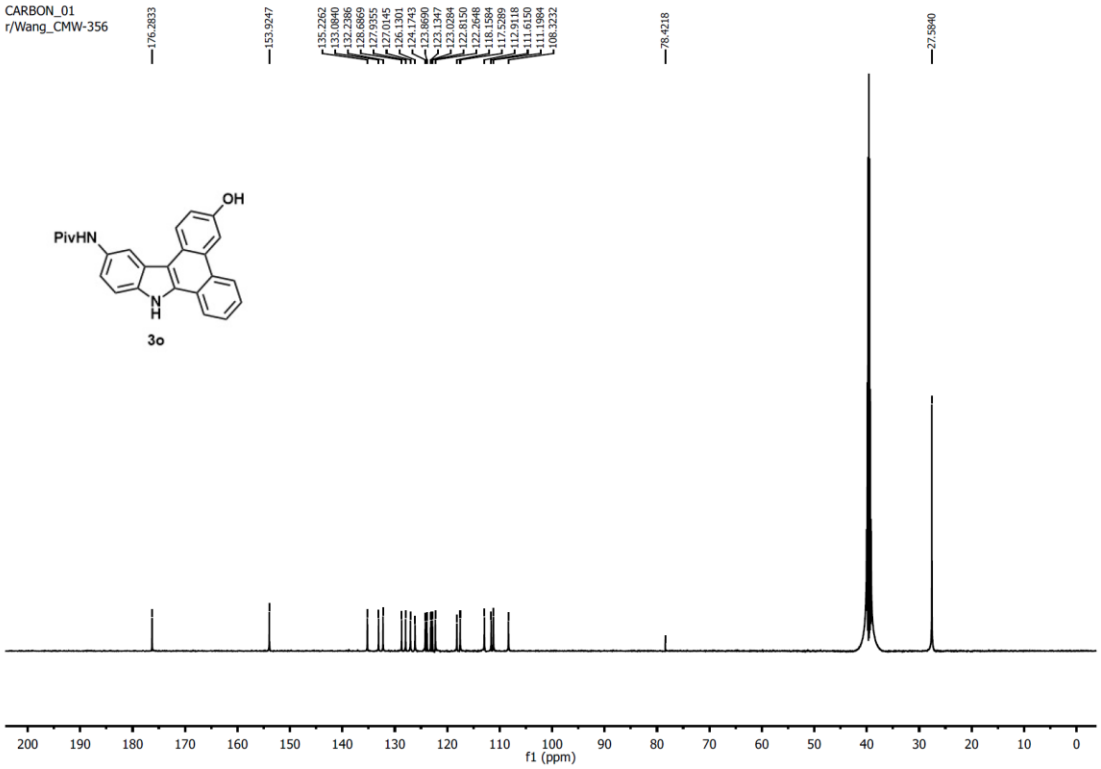

FLUORINE_01
r/Wang_CMW-342
-60.0262
OH
MeO
N
H
CF3
3n
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)

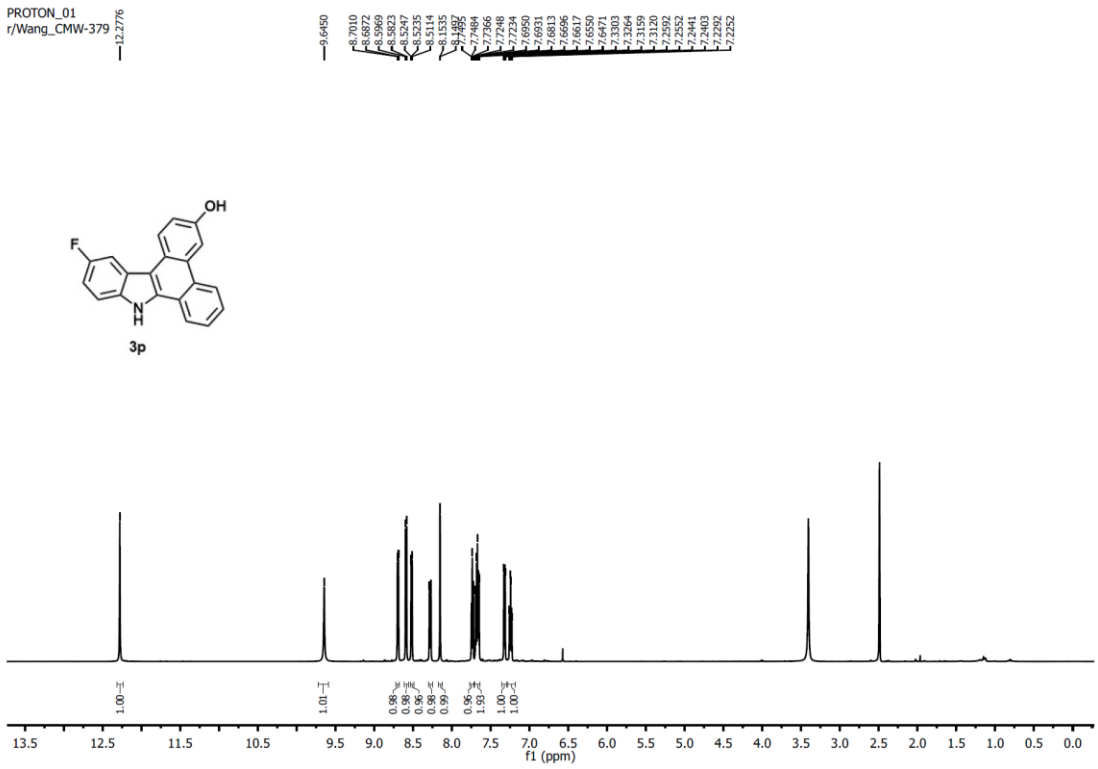
CARBON_01
r/Wang_CMW-342



PROTON_01
r/Wang_CMW-356

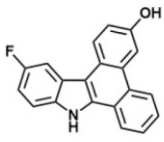



CARBON_01
r/Wang_CMW-356
176.2833
153.9247
135.2262
133.0840
132.2386
128.6869
127.9355
127.0145
126.1301
124.1743
123.9660
123.1347
123.0284
122.8150
122.2648
118.1584
117.5289
112.9118
111.6150
111.1984
108.3232
78.4218
27.5840
OH
PivHN
N
H
3o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

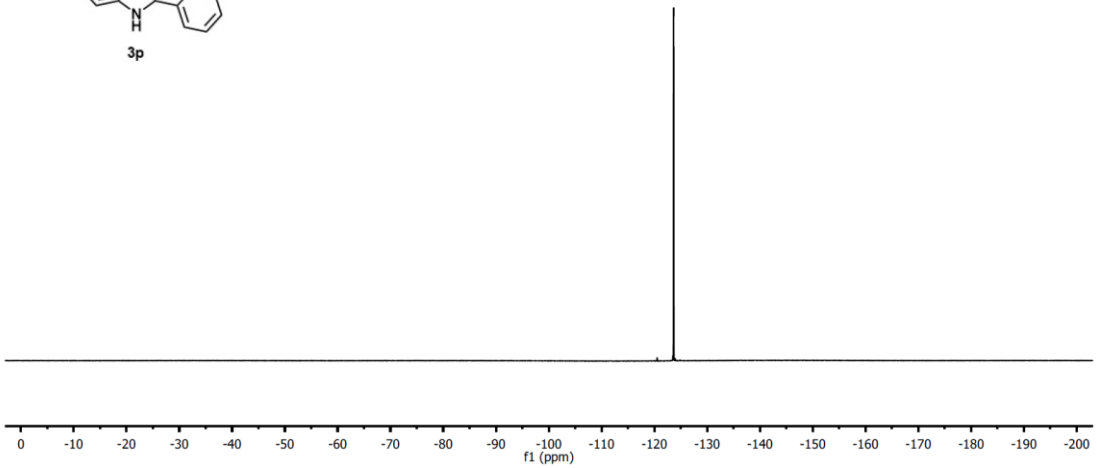

PROTON_01
r/Wang_CMW-379
12.2776
9.6450
8.7010
8.6872
8.5969
8.5823
8.5247
8.5235
8.5114
8.1535
7.7492
7.7484
7.7366
7.7248
7.7234
7.6950
7.6931
7.6913
7.6696
7.6617
7.6550
7.6471
7.3303
7.3264
7.3159
7.3120
7.2592
7.2552
7.2441
7.2403
7.2292
7.2252
OH
F
N
H
3p
1.00
1.01
0.98
0.98
0.96
0.98
0.99
0.96
1.93
1.00
1.00
13.5 12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

FLUORINE_01
r/Wang_CMW-379

123.6216
123.6300
123.6390
123.6466
123.6555
123.6639

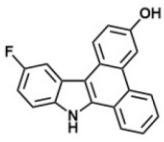


3p

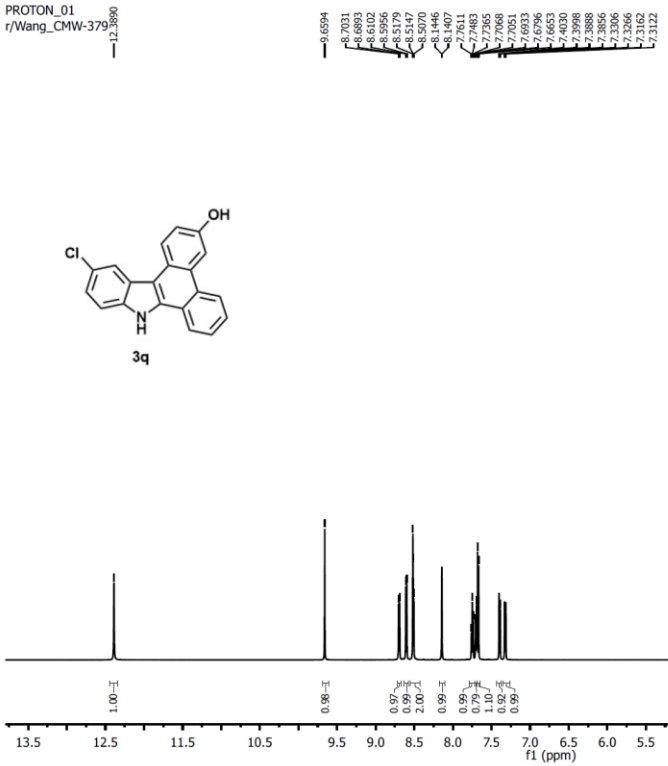


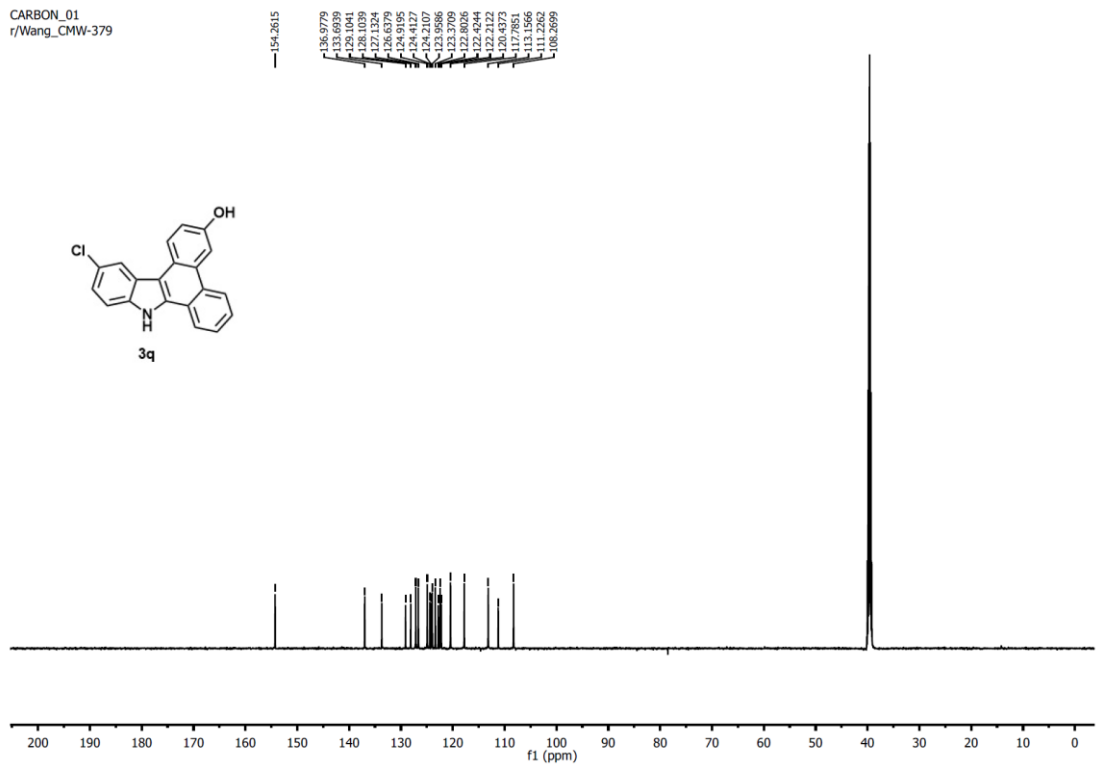
CARBON_01
r/Wang_CMW-379

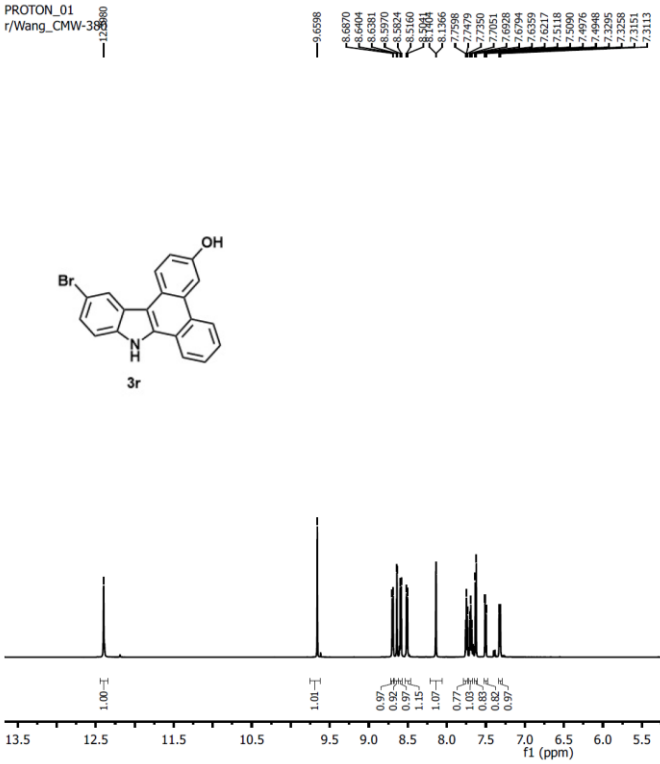
158.0329
156.4950
154.1330
135.1346
134.0706
129.0565
127.9490
127.0495
126.4903
124.7601
124.2053
123.4249
123.3590
122.9756
122.3818
117.6802
115.7440
112.5661
112.5019
111.7979
111.7683
111.4579
111.2928
108.2661
106.5329
106.3717

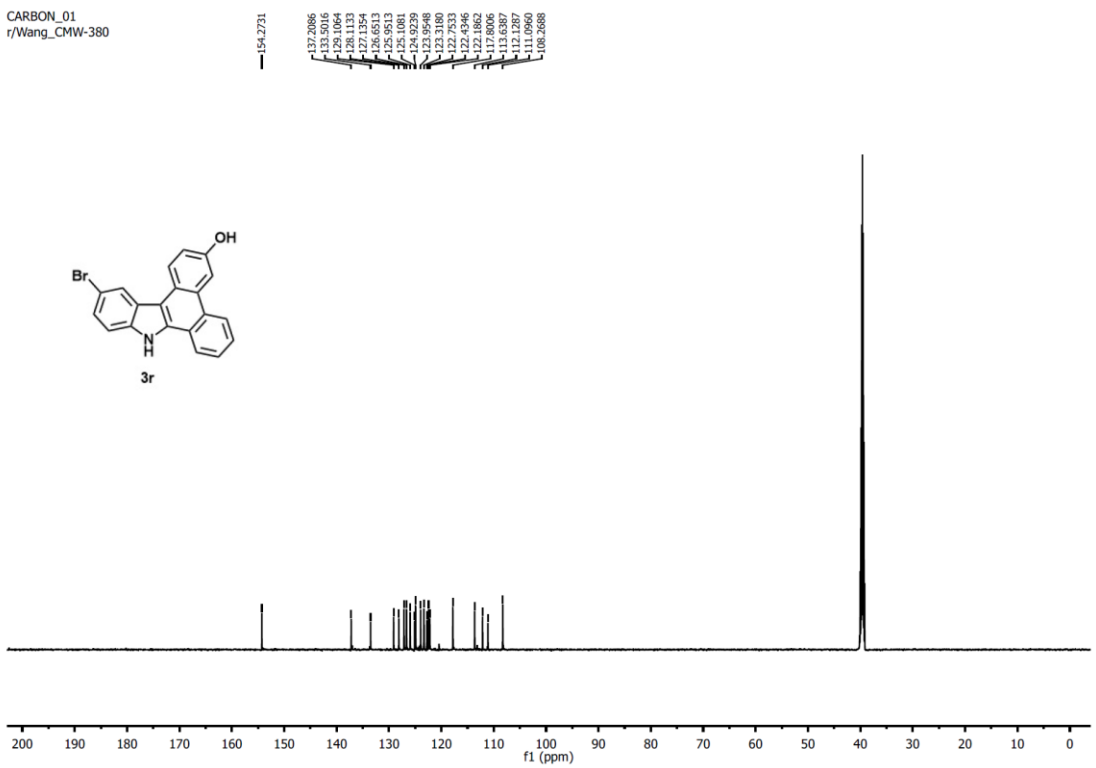


3p


PROTON_01
r/Wang_CMW-379
12.3890
9.6594
8.7031
8.6893
8.6102
8.5956
8.5179
8.5147
8.5070
8.1446
8.1407
7.7611
7.7483
7.7365
7.7068
7.7051
7.6933
7.6796
7.6653
7.4030
7.3998
7.3888
7.3856
7.3306
7.3266
7.3162
7.3122
OH
Cl
N
H
3q
1.00
0.98
0.97
0.99
2.00
0.99
0.99
0.79
1.10
0.92
0.99
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


CARBON_01
r/Wang_CMW-379
154.2615
136.9779
133.6939
129.1041
128.1039
127.1324
126.6779
124.9195
124.4127
124.2107
123.9586
123.3709
122.8026
122.4244
122.2122
120.4373
117.7851
117.3556
111.2262
108.2699
OH
Cl
N
H
3q
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


PROTON_01
r/Wang_CMW-380
12.5080
9.6598
8.6870
8.6404
8.6381
8.5970
8.5924
8.5160
8.5041
8.1404
8.1366
7.7598
7.7479
7.7030
7.7051
7.6928
7.6794
7.6359
7.6217
7.5118
7.5090
7.4976
7.4948
7.3295
7.3258
7.3151
7.3113
OH
Br
N
H
3r
1.00
1.01
0.97
0.92
0.97
1.15
1.07
0.77
1.03
0.83
0.82
0.97
13.5
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


CARBON_01
r/Wang_CMW-380
154.2731
137.2086
133.5016
129.1064
128.1133
127.1354
126.6513
125.9513
125.1081
124.9239
123.3948
123.3180
122.7353
122.4346
122.1862
117.8006
113.6387
112.1287
111.0960
108.2688
OH
Br
N
H
3r
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)