Supporting Information

Merging Base-promoted C-C Bond Cleavage and Iron-catalyzed Skeletal Rearrangement Involving C-C/C-H Bond Activation: Synthesis of Highly Functionalized Carbozoles

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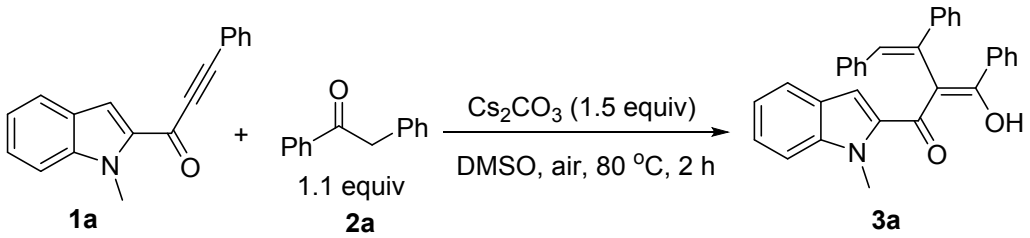
1. General Details.

All reactions under N_2 were performed in flame-dried glassware under an atmosphere of dry nitrogen, unless otherwise noted. Column chromatographic purification of products was carried out using silica gel (200~300 mesh or 300~400 mesh). The reagents were used without further purification. ^{1}H NMR spectra was recorded at 400 MHz, ^{13}C NMR spectra was recorded at 100 MHz, and in $CDCl_3$ (containing 0.03% TMS) solutions. ^{1}H NMR spectra was recorded with tetramethylsilane (δ = 0.00 ppm) as internal reference; ^{13}C NMR spectra was recorded with $CDCl_3$ (δ = 77.00 ppm) as internal reference. High-resolution mass spectra were performed on a mass spectrometer with a TOF (for EI or ESI) or FT-ICR (for MALDI) analyzer. Single crystal X-raydiffraction data was collected in Bruker SMARTAPEX diffractiometers with molybdenum cathodes.

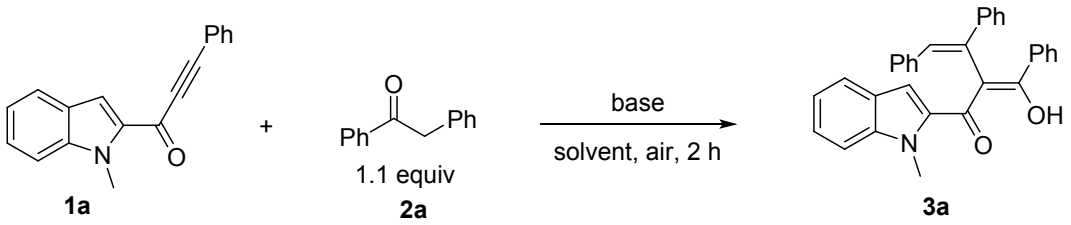
2. Synthesis of 3a.



In a schlenk tube, indolyl alkynyl ketones **1a** (0.20 mmol, 51.9 mg), 2-phenylacetophenone **2a** (0.22 mmol, 43.2 mg), Cs_2CO_3 (0.3 mmol, 97.7 mg) and DMSO (2.0 mL) were stirred at 80 °C. After the reaction was completed as monitored by thin-layer chromatography, the reaction mixture was then quenched by water, and the water layers were extracted with ethyl acetate (10 mL × 3). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. Purification by chromatography on silica gel (petroleum ether/ethyl acetate = 100:1) afforded desired compound **3a** (yellow solid, 74.4 mg, 82%).

(2*Z*,3*Z*)-2-(Hydroxy(phenyl)methylene)-1-(1-methyl-1*H*-indol-2-yl)-3,4-diphenylbut-3-en-1-one (**3a**, yellow solid, 74.4 mg, 82%). mp 179-181 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.57 (s, 3H), 6.77 (s, 1H), 6.99-7.23 (m, 15H), 7.35-7.38 (m, 2H), 7.43-7.52 (m, 3H), 17.87 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.42, 109.09, 109.93, 111.51, 120.22, 122.47, 124.72, 126.52, 126.81, 127.21, 127.46, 127.67, 127.75, 128.49, 128.65, 128.74, 130.43, 132.45, 134.58, 136.69, 137.56, 137.99, 139.54, 142.95, 185.94, 186.16. HRMS (ESI) calcd for $C_{32}H_{25}NNaO_2$ $[M+Na]^+$: 478.1778, found: 478.1788.

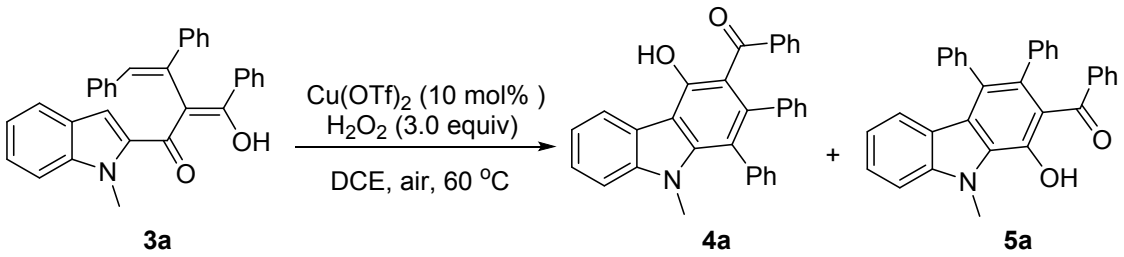
Table S1. Optimization studies for the formation of 3a.



Entry	Base (equiv)	Solvent	Temp (°C)	Yield (%)[a]
1[b]	Cs_2CO_3 (1.5)	DMSO	60	70
2	**Cs_2CO_3 (1.5)**	**DMSO**	**80**	**82**
3[c]	Cs_2CO_3 (1.5)	DMSO	100	70
4	NaO^tBu (1.5)	DMSO	80	46
5	NaOH (1.5)	DMSO	80	32
6	KOH (1.5)	DMSO	80	56
7	K_2CO_3 (1.5)	DMSO	80	65
8	KOAc (1.5)	DMSO	80	trace
9	DBU (1.5)	DMSO	80	trace
10[d]	Cs_2CO_3 (1.0)	DMSO	80	79
11[e]	Cs_2CO_3 (2.0)	DMSO	80	82
12	Cs_2CO_3 (1.5)	DMAc	80	43
13	Cs_2CO_3 (1.5)	DMF	80	39
14	Cs_2CO_3 (1.5)	toluene	80	trace
15	Cs_2CO_3 (1.5)	1,4-dioxane	80	trace

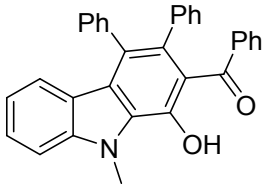
[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.22 mmol), Cs_2CO_3 (0.3 mmol), solvent (2.0 mL), 80 °C, isolated yields. [b]60 °C. [c]100 °C. [d]Cs_2CO_3 (0.2 mmol). [e]Cs_2CO_3 (0.4 mmol).

3. Synthesis of 5a.



3a **4a** **5a**

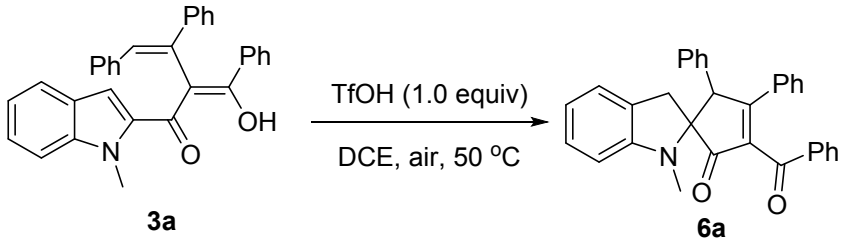
Indole derivative **3a** (0.2 mmol, 91.1 mg), $Cu(OTf)_2$ (0.02 mmol, 7.2 mg) and DCE (2 mL) were placed in a schlenk tube, then H_2O_2 (0.6 mmol, 60 uL, 30% in water) was added. After the completion of the addition, the reaction mixture was allowed to react at 60 °C for 5 h. Then, the reaction mixture was cooled to room temperature and was treated with H_2O, then extracted with EA and dried over anhydrous Na_2SO_4. After removal of the EA, the residue was purified by chromatography on basic silica gel (PE : EA = 100 : 1) to afford **4a** and **5a** (**4a**:**5a** = 1 : 6, yellow solid, 52.1 mg, 58%).



5a

(1-Hydroxy-9-methyl-3,4-diphenyl-9*H*-carbazol-2-yl)(phenyl)methanon (**5a**, yellow solid). mp 251-253 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 4.33 (s, 3H), 6.71-6.77 (m, 6H), 6.87-6.92 (m, 1H), 7.01-7.06 (m, 2H), 7.13-7.19 (m, 3H), 7.24-7.31 (m, 5H), 7.42-7.44 (m, 2H), 10.36 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.95, 108.98, 119.32, 119.74, 122.86, 123.13, 125.88, 126.08, 126.92, 127.14, 127.55, 128.20, 128.27, 128.70, 129.04, 131.11, 131.40, 132.58, 132.66, 139.37, 139.95, 141.29, 143.27, 147.54, 203.88. HRMS (ESI) calcd for $C_{32}H_{24}NO_2$ $[M+H]^+$: 454.1802, found: 454.1804.

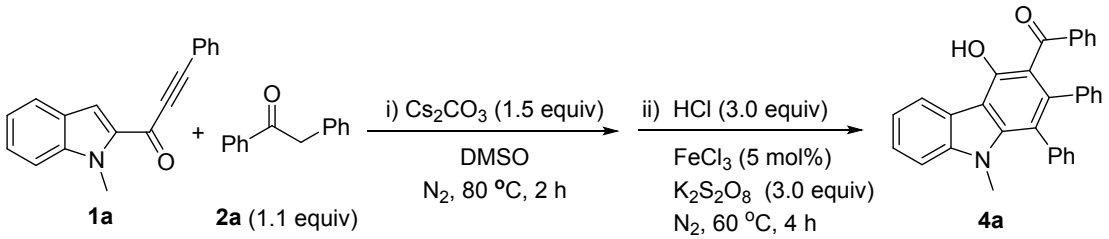
4. Synthesis of 6a.



Indole derivative **3a** (1.0 mmol, 455.6 mg), DCE (10 mL) and TfOH (1.0 mmol, 88uL) and were placed in a schlenk tube, then the reaction mixture was allowed to react at 50 °C for 6 h. Then, the reaction mixture was cooled to room temperature and was treated with saturated $NaHCO_3$, then extracted with DCM and dried over anhydrous Na_2SO_4. After removal of the DCM, the residue was purified by chromatography on basic silica gel (PE : EA = 10 : 1) to afford **6a** (red solid, 354.1 mg, 78%).

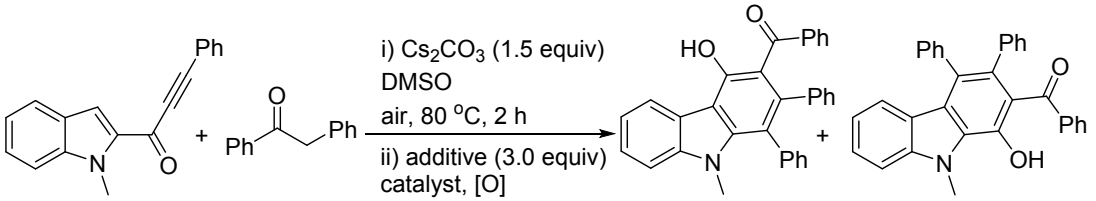
3-Benzoyl-1'-methyl-4,5-diphenylspiro[cyclopentane-1,2'-indolin]-3-en-2-one (**6a**, red solid, 78%). mp 110-112 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.56 (d, *J* = 16.4 Hz, 1H), 2.95 (s, 3H), 3.06 (d, *J* = 16.0 Hz, 1H), 4.95 (s, 1H), 6.42 (d, *J* = 7.6 Hz, 1H), 6.56-6.60 (m, 1H), 6.75-6.77 (m, 1H), 7.03-7.06 (m, 3H), 7.14-7.25 (m, 6H), 7.35-7.38 (m, 2H), 7.41-7.46 (m, 2H), 7.54-7.58 (m, 1H), 7.88-7.90 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 30.10, 36.51, 54.84, 79.38, 106.03, 118.29, 123.74, 127.02, 127.60, 127.69, 128.98, 129.08, 129.21, 129.48, 129.56, 131.38, 133.07, 134.34, 136.28, 138.12, 140.45, 151.42, 170.24, 194.77, 204.40. HRMS (ESI) calcd for $C_{32}H_{25}NNaO_2$ $[M+Na]^+$: 478.1778, found: 478.1788.

5. Synthesis of 4.



In a schlenk tube, indolyl alkynyl ketones **1a** (0.20 mmol, 51.9 mg), 2-phenylacetophenone **2a** (0.22 mmol, 43.2 mg), Cs_2CO_3 (0.3 mmol, 97.7 mg) and DMSO (2.0 mL) were stirred at 80 °C under N_2. After 2 h, the reaction mixture was then quenched by HCl (0.6 mmol, 100 uL, 6M), then $FeCl_3$ (0.01 mmol, 1.6 mg) and $K_2S_2O_8$ (0.6 mmol, 162.2 mg) were added. After the completion of the addition, the reaction mixture was allowed to react at 60 °C for 4 h. Then, the reaction mixture was cooled to room temperature and was treated with H_2O, then extracted with EA and dried over anhydrous Na_2SO_4. After removal of the EA, the residue was purified by chromatography on basic silica gel (PE : EA = 100 : 1) to afford **4a** (yellow solid, 75.7 mg, 83%).

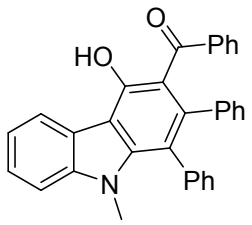
Table S2. Optimization studies for the formation of 4a.



1a **2a** (1.1 equiv) **4a** **5a**

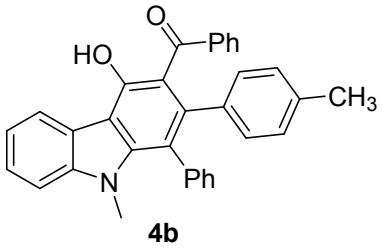
Entry	Additive	Catalyst (5 mol%)	[O] (equiv)	Temp (°C)	Yields (%)[a] of **4a** + **5a**
1	HCl	$FeBr_2$	-	60	trace
2	HCl	-	$K_2S_2O_8$ (3)	60	60 (6:1)
3	HCl	$FeBr_2$	$K_2S_2O_8$ (3)	60	75 (1:0)
4	HCl	$FeCl_3$	$K_2S_2O_8$ (3)	60	77 (1:0)
5	-	$FeBr_2$	$K_2S_2O_8$ (3)	60	–[e]
6	HCl	$CuCl_2$	$K_2S_2O_8$ (3)	60	70 (5:1)
7	HCl	CuI	$K_2S_2O_8$ (3)	60	51 (6:1)
8	HCl	$FeCl_3$	$(NH_4)_2S_2O_8$ (3)	60	43 (1:0)
9	HCl	$FeCl_3$	TBHP (3)	60	trace
10	HCl	$FeCl_3$	DTBP (3)	60	–[e]
11	HCl	$FeCl_3$	H_2O_2 (3)	60	–[e]
12	HCl	$FeCl_3$	$K_2S_2O_8$ (2)	60	70 (30:1)
13	HCl	$FeCl_3$	$K_2S_2O_8$ (4)	60	57 (1:0)
14	HCl	$FeCl_3$	$K_2S_2O_8$ (3)	80	52 (1:0)
15[b]	HCl	$FeCl_3$	$K_2S_2O_8$ (3)	60	81 (1:0)
16[b,c]	**HCl**	**$FeCl_3$**	**$K_2S_2O_8$ (3)**	**60**	**83 (1:0)**
17[b,d]	HCl	$FeCl_3$	$K_2S_2O_8$ (3)	60	81 (1:0)

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.22 mmol), Cs_2CO_3 (0.3 mmol), solvent (2.0 mL), 80 °C, HCl (0.6 mmol, 12M), catalyst (5 mol%), [O], 60 °C, isolated yields. The ratio of **4a**:**5a** was shown in parentheses. [b]Under nitrogen. [c]HCl (0.6 mmol, 6M). [d]HCl (0.6 mmol, 3M). [e]Complicated reaction mixture.



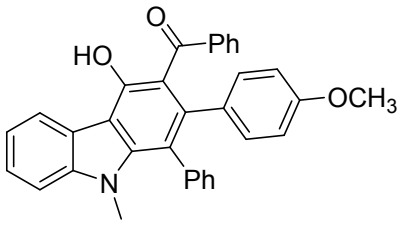
4a

(4-Hydroxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)(phenyl)methanone (**4a**, yellow solid, 75.7 mg, 83%). mp 245-247 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.18 (s, 3H), 6.68-6.72 (m, 5H), 6.98-7.02 (m, 2H), 7.09-7.21 (m, 8H), 7.31-7.38 (m, 2H), 7.45-7.50 (m, 1H), 8.54 (d, *J* = 7.6 Hz, 1H), 11.29 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.92, 108.83, 110.71, 114.83, 118.58, 120.93, 122.52, 123.48, 125.64, 126.07, 126.67, 127.34, 127.45, 127.64, 128.63, 130.67, 132.40, 132.59, 137.67, 140.05, 141.56, 141.99, 142.16, 142.41, 157.71, 203.35. HRMS (ESI) calcd for $C_{32}H_{24}NO_2$ $[M+H]^+$: 454.1802, found: 454.1810.



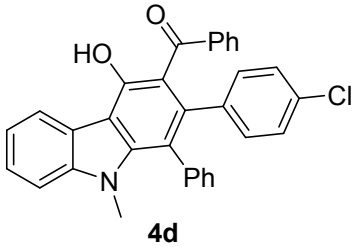
4b

(4-Hydroxy-9-methyl-1-phenyl-2-(p-tolyl)-9*H*-carbazol-3-yl)(phenyl)methanone (**4b**, yellow solid, 113.5 mg, 81%). mp 273-275 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.98 (s, 3H), 3.17 (s, 3H), 6.45-6.48 (m, 2H), 6.56-6.59 (m, 2H), 6.97-7.02 (m, 2H), 7.09-7.21 (m, 8H), 7.30-7.37 (m, 2H), 7.45-7.49 (m, 1H), 8.53 (d, *J* = 7.6 Hz, 1H), 11.28 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.52, 31.90, 108.79, 110.55, 115.07, 118.46, 120.87, 122.53, 123.43, 125.55, 127.25, 127.29, 127.40, 127.65, 128.55, 130.44, 132.30, 132.59, 135.64, 137.06, 137.78, 141.70, 141.96, 142.23, 142.46, 157.61, 203.49. HRMS (ESI) calcd for $C_{33}H_{26}NO_2$ $[M+H]^+$: 468.1958, found: 468.1966.



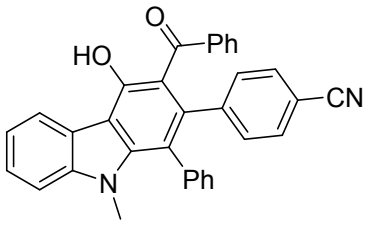
4c

(4-Hydroxy-2-(4-methoxyphenyl)-9-methyl-1-phenyl-9*H*-carbazol-3-yl)(phenyl)methanone (**4c**, yellow solid, 108.8 mg, 75%). mp 239-241 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.18 (s, 3H), 3.55 (s, 3H), 6.20-6.23 (m, 2H), 6.59-6.62 (m, 2H), 7.00-7.04 (m, 2H), 7.10-7.21 (m, 8H), 7.30-7.37 (m, 2H), 7.45-7.49 (m, 1H), 8.53 (d, *J* = 7.6 Hz, 1H), 11.29 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.91, 54.88, 108.79, 110.53, 112.26, 115.10, 118.59, 120.87, 122.53, 123.41, 125.56, 127.32, 127.41, 127.71, 128.46, 130.57, 132.57, 132.67, 133.49, 137.77, 141.31, 141.96, 142.27, 142.48, 157.61, 157.90, 203.40. HRMS (ESI) calcd for $C_{33}H_{26}NO_3$ $[M+H]^+$: 484.1907, found: 484.1904.



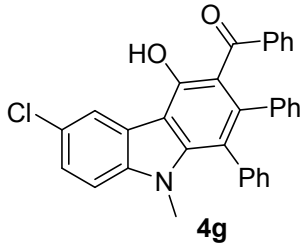
4d

(2-(4-Chlorophenyl)-4-hydroxy-9-methyl-1-phenyl-9*H*-carbazol-3-yl)(phenyl)methanone (**4d**, yellow solid, 110.3 mg, 75%). mp 275-277 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.18 (s, 3H), 6.61-6.67 (m, 4H), 7.02-7.07 (m, 2H), 7.13-7.22 (m, 8H), 7.32-7.39 (m, 2H), 7.47-7.51 (m, 1H), 8.54 (d, *J* = 8.0 Hz, 1H), 11.38 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.91, 108.90, 110.90, 114.65, 118.61, 121.06, 122.43, 123.53, 125.79, 126.82, 127.59, 127.86, 128.46, 130.84, 132.19, 132.46, 133.48, 137.31, 138.65, 140.15, 141.96, 142.21, 157.95, 203.21. HRMS (ESI) calcd for $C_{32}H_{23}ClNO_2$ $[M+H]^+$: 488.1412, found: 488.1418.



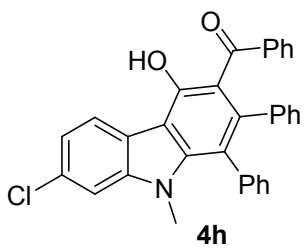
4e

4-(3-Benzoyl-4-hydroxy-9-methyl-1-phenyl-9*H*-carbazol-2-yl)benzonitrile (**4e**, yellow solid, 110.7 mg, 77%). mp 234-236 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.20 (s, 3H), 6.81-6.84 (m, 2H), 6.95-6.98 (m, 2H), 7.02-7.07 (m, 2H), 7.10-7.24 (m, 8H), 7.33-7.40 (m, 2H), 7.48-7.53 (m, 1H), 8.55 (d, *J* = 7.6 Hz, 1H), 11.48 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.93, 109.00, 109.52, 111.31, 113.99, 118.62, 118.91, 121.26, 122.31, 123.62, 126.05, 127.80, 127.88, 127.98, 128.55, 130.31, 131.19, 132.36, 132.82, 136.83, 139.29, 141.97, 142.01, 142.20, 145.33, 158.33, 202.69. HRMS (ESI) calcd for $C_{33}H_{23}N_2O_2$ $[M+H]^+$: 479.1754, found: 479.1762.



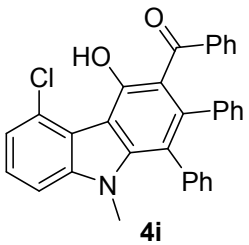
4g

(6-Chloro-4-hydroxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)(phenyl)methanone (**4g**, yellow solid, 115.2 mg, 79%). mp 210-212 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.16 (s, 3H), 6.69 (br s, 5H), 6.99-7.03 (m, 2H), 7.10-7.23 (m, 9H), 7.39-7.42 (m, 1H), 8.50 (d, *J* = 0.8 Hz, 1H), 11.26 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.09, 109.80, 110.04, 114.94, 118.66, 122.96, 123.53, 125.72, 126.22, 126.30, 126.75, 127.49, 127.72, 128.64, 130.82, 132.32, 132.53, 137.27, 139.81, 140.34, 141.91, 142.18, 142.73, 157.67, 203.23. HRMS (ESI) calcd for $C_{32}H_{23}ClNO_2$ $[M+H]^+$: 488.1412, found: 488.1425.



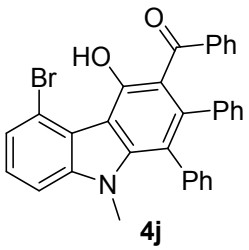
4h

(7-Chloro-4-hydroxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)(phenyl)methanone (**4h**, yellow solid, 127.7 mg, 87%). mp 239-241 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.14 (s, 3H), 6.69 (br s, 5H), 6.98-7.03 (m, 2H), 7.10-7.20 (m, 8H), 7.29-7.32 (m, 2H), 8.42 (d, *J* = 8.8 Hz, 1H), 11.17 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.06, 109.10, 110.42, 115.20, 118.67, 121.05, 121.33, 124.24, 126.21, 126.74, 127.49, 127.73, 128.64, 130.85, 131.57, 132.33, 132.51, 137.28, 139.82, 141.89, 142.64, 157.28, 203.29. HRMS (ESI) calcd for $C_{32}H_{23}ClNO_2$ $[M+H]^+$: 488.1412, found: 488.1420.



4i

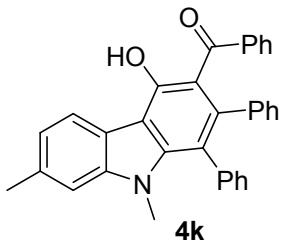
(5-Chloro-4-hydroxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)(phenyl)methanone (**4i**, yellow solid, 130.3 mg, 89%). mp 236-237 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.20 (s, 3H), 6.83 (br s, 5H), 7.17-7.30 (m, 9H), 7.33-7.41 (m, 2H), 7.60 (d, *J* = 7.6 Hz, 2H), 9.36 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.92, 108.21, 108.96, 117.84, 118.74, 119.97, 121.78, 125.52, 126.36, 126.42, 126.91, 127.28, 127.70, 128.07, 129.32, 131.29, 132.26, 132.45, 137.77, 138.63, 139.91, 141.36, 141.53, 144.14, 150.38, 199.71. HRMS (ESI) calcd for $C_{32}H_{23}ClNO_2$ $[M+H]^+$: 488.1412, found: 488.1414.



4j

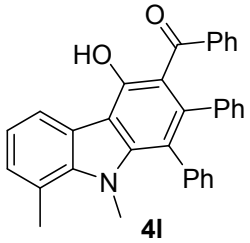
(5-Bromo-4-hydroxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)(phenyl)methanone (**4j**, yellow solid, 140.7 mg, 88%). mp 238-240 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.18 (s, 3H), 6.81 (br s, 5H), 7.17-7.22 (m, 7H), 7.28-7.32 (m, 3H), 7.50-7.56 (m, 3H), 9.67 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.92, 108.58,

109.11, 114.24, 117.81, 118.51, 122.26, 125.79, 126.38, 126.53, 126.88, 127.28, 127.72, 127.98, 129.23, 131.39, 132.07, 132.47, 137.81, 138.76, 140.22, 141.47, 141.78, 144.22, 151.44, 200.26. HRMS (ESI) calcd for $C_{32}H_{23}BrNO_2$ $[M+H]^+$: 532.0907, found: 532.0913.



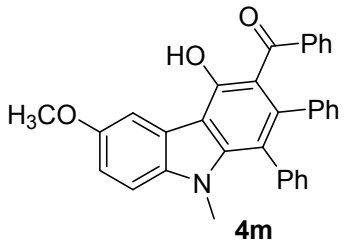
4k

(4-Hydroxy-7,9-dimethyl-1,2-diphenyl-9*H*-carbazol-3-yl)(phenyl)methanone (**4k**, yellow solid, 114.1 mg, 81%). mp 221-223 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.57 (s, 3H), 3.15 (s, 3H), 6.67-6.70 (m, 5H), 6.97-7.02 (m, 2H), 7.09-7.21 (m, 10H), 8.39 (d, J = 8.0 Hz, 1H), 11.25 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.03, 31.84, 109.09, 110.74, 114.80, 118.57, 120.17, 122.46, 123.08, 126.00, 126.64, 127.28, 127.42, 127.61, 128.64, 130.62, 132.43, 132.57, 135.86, 137.77, 140.11, 141.07, 142.20, 142.41, 157.35, 203.37. HRMS (ESI) calcd for $C_{33}H_{26}NO_2$ $[M+H]^+$: 468.1958, found: 468.1969.



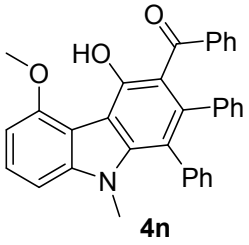
4l

(4-Hydroxy-8,9-dimethyl-1,2-diphenyl-9*H*-carbazol-3-yl)(phenyl)methanone (**4l**, yellow solid, 103.8 mg, 74%). mp 227-229 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.74 (s, 3H), 3.44 (s, 3H), 6.68 (br s, 5H), 6.97-7.02 (m, 2H), 7.09-7.23 (m, 10H), 8.43 (d, J = 7.2 Hz, 1H), 11.18 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.59, 35.64, 111.30, 115.16, 118.64, 120.75, 121.19, 121.61, 123.65, 126.04, 126.64, 127.07, 127.44, 127.70, 128.56, 129.37, 130.66, 132.42, 132.46, 138.11, 140.10, 141.48, 141.50, 142.18, 143.85, 157.31, 203.40. HRMS (ESI) calcd for $C_{33}H_{26}NO_2$ $[M+H]^+$: 468.1958, found: 468.1957.



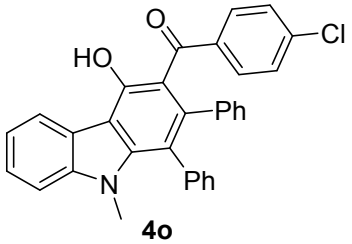
4m

(4-Hydroxy-6-methoxy-9-methyl-1,2-diphenyl-9H-carbazol-3-yl)(phenyl)methanone (**4m**, yellow solid, 117.8 mg, 81%). mp 189-190 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.15 (s, 3H), 3.99 (s, 3H), 6.68-6.72 (m, 5H), 6.98-7.02 (m, 2H), 7.09-7.24 (m, 10H), 8.05 (d, *J* = 2.4 Hz, 1H), 11.50 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.98, 55.95, 105.67, 109.62, 110.50, 114.30, 115.06, 118.67, 122.97, 126.03, 126.65, 127.32, 127.44, 127.63, 128.59, 130.58, 132.40, 132.57, 136.81, 137.64, 140.09, 141.42, 142.24, 142.71, 155.12, 158.09, 203.31. HRMS (ESI) calcd for $C_{33}H_{26}NO_3$ $[M+H]^+$: 484.1907, found: 484.1918.



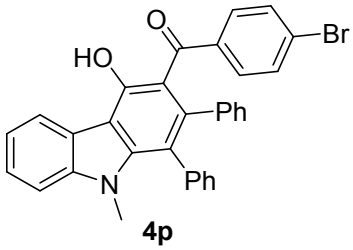
4n

(4-Hydroxy-5-methoxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)(phenyl)methanone (**4n**, yellow solid, 105.3 mg, 73%). mp 275-277 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.18 (s, 3H), 4.09 (s, 3H), 6.75 (d, *J* = 8.0 Hz, 1H), 6.86-6.91 (m, 5H), 7.02 (d, *J* = 8.4 Hz, 1H), 7.17-7.18 (m, 5H), 7.26-7.31 (m, 2H), 7.38-7.43 (m, 2H), 7.75 (d, *J* = 7.6 Hz, 2H), 9.89 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.61, 56.26, 101.03, 103.64, 109.79, 110.86, 117.15, 118.83, 126.26, 126.63, 126.88, 127.00, 127.53, 128.18, 129.66, 131.17, 132.49, 132.63, 138.00, 138.73, 139.23, 139.69, 140.03, 143.84, 148.05, 152.20, 198.59. HRMS (ESI) calcd for $C_{33}H_{26}NO_3$ $[M+H]^+$: 484.1907, found: 484.1911.



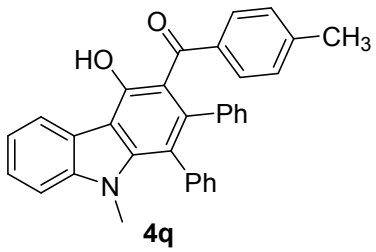
4o

(4-Chlorophenyl)(4-hydroxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)methanone (**4o**, yellow solid, 116.2 mg, 79%). mp 266-268 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.19 (s, 3H), 6.71-6.75 (m, 5H), 6.96-6.98 (m, 2H), 7.11-7.20 (m, 7H), 7.32-7.38 (m, 2H), 7.46-7.51 (m, 1H), 8.53 (d, *J* = 7.6 Hz, 1H), 11.27 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.94, 108.89, 110.73, 114.58, 118.74, 121.04, 122.45, 123.48, 125.74, 126.35, 126.81, 127.45, 127.68, 127.70, 129.95, 132.40, 132.53, 136.68, 137.50, 139.97, 140.50, 141.37, 141.98, 142.52, 157.84, 201.95. HRMS (ESI) calcd for $C_{32}H_{23}ClNO_2$ $[M+H]^+$: 488.1412, found: 488.1416.



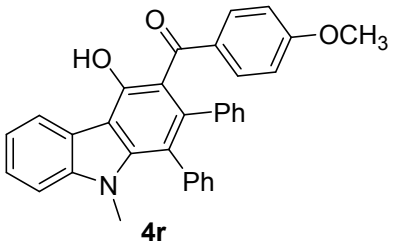
4p

(4-Bromophenyl)(4-hydroxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)methanone (**4p**, yellow solid, 116.9 mg, 73%). mp 271-273 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.19 (s, 3H), 6.69-6.77 (m, 5H), 7.03-7.06 (m, 2H), 7.12-7.20 (m, 7H), 7.32-7.39 (m, 2H), 7.46-7.51 (m, 1H), 8.53 (d, *J* = 7.6 Hz, 1H), 11.30 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.94, 108.90, 110.72, 114.56, 118.77, 121.06, 122.45, 123.49, 125.15, 125.75, 126.37, 126.82, 127.46, 127.71, 130.06, 130.65, 132.41, 132.53, 137.48, 139.96, 140.97, 141.40, 141.97, 142.54, 157.90, 202.10. HRMS (EI^+) calcd for $C_{32}H_{22}BrNO_2$ $[M^+]$: 531.0834, found: 531.0833.



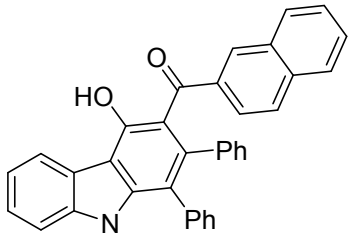
4q

(4-Hydroxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)(p-tolyl)methanone (**4q**, yellow solid, 118.1 mg, 84%). mp 279-281 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.18 (s, 3H), 3.18 (s, 3H), 6.69-6.72 (m, 5H), 6.79-6.82 (m, 2H), 7.12-7.18 (m, 7H), 7.30-7.37 (m, 2H), 7.45-7.50 (m, 1H), 8.53 (d, *J* = 7.2 Hz, 1H), 11.10 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.07, 31.93, 108.78, 110.70, 115.06, 118.43, 120.83, 122.49, 123.47, 125.59, 125.99, 126.56, 127.31, 127.61, 128.11, 128.97, 132.37, 132.62, 137.75, 139.26, 140.11, 141.31, 141.43, 141.98, 142.25, 157.26, 202.98. HRMS (ESI) calcd for $C_{33}H_{25}NNaO_2$ $[M+Na]^+$: 490.1777, found: 490.1779.



4r

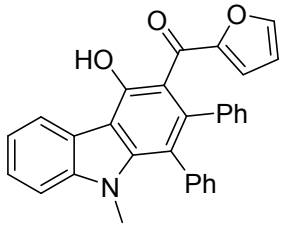
(4-Hydroxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)(4-methoxyphenyl)methanone (**4r**, yellow solid, 114.7 mg, 79%). mp 255-257 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.19 (s, 3H), 3.69 (s, 3H), 6.52 (d, *J* = 8.8 Hz, 2H), 6.71-6.78 (m, 5H), 7.17-7.20 (m, 5H), 7.26-7.36 (m, 4H), 7.45-7.50 (m, 1H), 8.53 (d, *J* = 7.6 Hz, 1H), 10.84 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.95, 55.14, 108.75, 110.78, 112.74, 115.09, 118.32, 120.77, 122.46, 123.48, 125.59, 126.09, 126.69, 127.31, 127.62, 131.38, 132.29, 132.65, 134.37, 137.80, 140.14, 141.11, 142.01, 142.12, 156.81, 162.14, 201.58. HRMS (ESI) calcd for $C_{33}H_{26}NO_3$ $[M+H]^+$: 484.1907, found: 484.1913.



4s

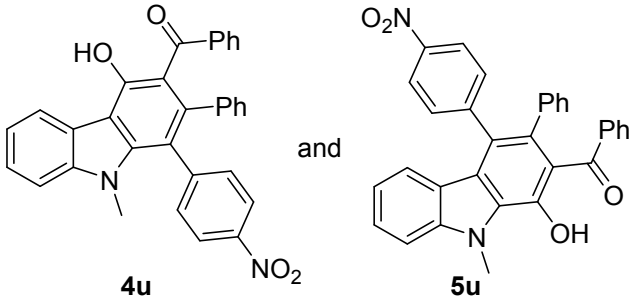
(4-Hydroxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)(naphthalen-2-yl)methanone (**4s**, yellow solid, 117.7 mg, 78%). mp 206-208 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.21 (s, 3H), 6.46-6.48 (m, 3H), 6.69-6.72 (m, 2H), 7.17 (br s, 5H),

7.33-7.52 (m, 7H), 7.63-7.67 (m, 3H), 8.57 (d, *J* = 8.0 Hz, 1H), 11.38 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.96, 108.84, 110.78, 114.98, 118.60, 120.96, 122.53, 123.52, 124.89, 125.67, 125.90, 126.33, 126.52, 127.33, 127.48, 127.64, 128.90, 130.06, 131.84, 132.10, 132.58, 134.26, 137.68, 139.13, 140.24, 141.68, 142.01, 142.47, 157.85, 164.48, 203.09. HRMS (ESI) calcd for $C_{36}H_{25}NNaO_2$ $[M+Na]^+$: 526.1777, found: 526.1776.



4t

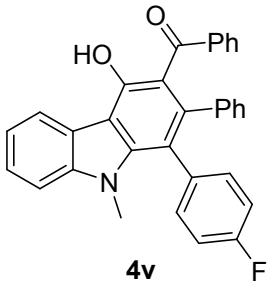
Furan-2-yl(4-hydroxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)methanone (**4t**, yellow solid, 90.7 mg, 68%). mp 224-226 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.17 (s, 3H), 6.11 (d, *J* = 1.6 Hz, 1H), 6.66 (d, *J* = 3.2 Hz, 1H), 6.83-6.87 (m, 3H), 6.95-6.98 (m, 2H), 7.17-7.24 (m, 6H), 7.29-7.36 (m, 2H), 7.44-7.49 (m, 1H), 8.50 (d, *J* = 7.6 Hz, 1H), 10.63 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.97, 108.78, 110.80, 111.90, 114.34, 118.45, 118.64, 120.86, 122.41, 123.52, 125.66, 126.18, 126.71, 127.41, 127.69, 131.94, 132.70, 137.76, 140.00, 140.75, 142.03, 142.44, 145.61, 153.41, 156.86, 187.97. HRMS (ESI) calcd for $C_{30}H_{21}NNaO_3$ $[M+Na]^+$: 466.1414, found: 466.1417.



4u **5u**

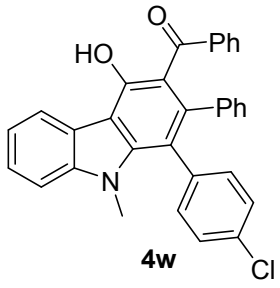
(4-Hydroxy-9-methyl-1-(4-nitrophenyl)-2-phenyl-9*H*-carbazol-3-yl)(phenyl)methanone (4u) and (1-hydroxy-9-methyl-4-(4-nitrophenyl)-3-phenyl-9*H*-carbazol- 2-yl)(phen- yl)methanone (5u) (yellow solid, 121.8 mg, 81%). mp 241-243 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.21 (s, 3H), 6.65-6.74 (m, 5H), 6.99-7.07 (m, 2H), 7.11-7.20 (m, 3H), 7.34-7.40 (m, 4H), 7.47-7.53 (m, 1H), 8.04-8.07 (m, 2H),

8.54 (d, J = 7.6 Hz, 1H), 11.22 (s, 1H); isomer: 4.35 (s, 3H), 7.28 (d, J = 7.6 Hz, 2H), 8.15 (d, J = 8.4 Hz, 2H); other peaks are overlapped with the signals of the other isomer; ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.48, 108.95, 111.18, 115.02, 115.98, 121.32, 122.34, 122.70, 123.61, 126.07, 126.69, 127.11, 127.56, 128.53, 130.96, 132.19, 133.50, 139.17, 141.45, 141.71, 141.85, 141.89, 145.70, 147.13, 158.04, 203.21; isomer: 32.03, 119.66, 123.47, 127.31, 127.65, 128.94, 132.33, 132.38. HRMS (ESI) calcd for $C_{32}H_{22}N_2NaO_4$ $[M+Na]^+$: 521.1472, found: 521.1481.



4v

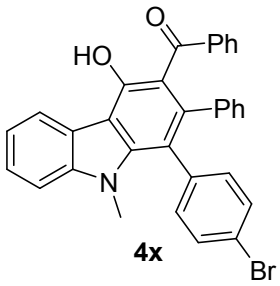
(1-(4-Fluorophenyl)-4-hydroxy-9-methyl-2-phenyl-9*H*-carbazol-3-yl)(phenyl)methanone (**4v**, yellow solid, 112.8 mg, 80%). mp 273-275 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.21 (s, 3H), 6.69-6.70 (m, 5H), 6.86-6.92 (m, 2H), 6.98-7.03 (m, 2H), 7.09-7.14 (m, 3H), 7.17-7.20 (m, 2H), 7.32-7.38 (m, 2H), 7.46-7.51 (m, 1H), 8.54 (d, J = 7.6 Hz, 1H), 11.28 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.07, 108.84, 110.82, 114.53, 114.75, 114.88, 117.31, 121.03, 122.47, 123.51, 125.75, 126.20, 126.83, 127.48, 128.59, 130.75, 132.33, 133.61 ($J_{C\text{-}F}$ = 3.9 Hz), 134.02 ($J_{C\text{-}F}$ = 8.3 Hz), 139.88, 141.91 ($J_{C\text{-}F}$ = 3.8 Hz), 142.09, 142.44, 157.79, 162.32 ($J_{C\text{-}F}$ = 246.5 Hz), 203.32. HRMS (ESI) calcd for $C_{32}H_{22}FNNaO_2$ $[M+Na]^+$: 494.1527, found: 494.1530.



4w

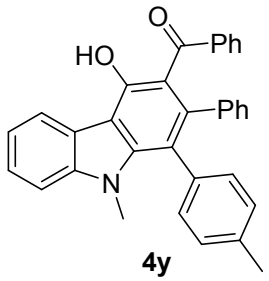
(4-Hydroxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)(4-methoxyphenyl)methanone (**4w**, yellow solid, 114.1 mg, 78%). mp 287-289 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.22 (s, 3H), 6.69-6.72 (m, 5H), 6.98-7.03 (m, 2H), 7.08-7.20 (m, 7H), 7.32-7.39 (m, 2H), 7.47-7.51 (m, 1H), 8.54 (d, J = 8.0 Hz, 1H), 11.25 (s,

1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.19, 108.86, 110.87, 114.93, 117.08, 121.07, 122.44, 123.52, 125.80, 126.30, 126.90, 127.49, 127.91, 128.58, 130.78, 132.31, 133.45, 133.82, 136.33, 139.72, 141.69, 141.93, 142.05, 142.27, 157.80, 203.30. HRMS (ESI) calcd for $C_{32}H_{23}ClNO_2$ $[M+H]^+$: 488.1412, found: 488.1430.



4x

(1-(4-Bromophenyl)-4-hydroxy-9-methyl-2-phenyl-9*H*-carbazol-3-yl)(phenyl)methanone (**4x**, yellow solid, 131.4 mg, 82%). mp 287-289 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.22 (s, 3H), 6.69-6.73 (m, 5H), 6.98-7.05 (m, 4H), 7.10-7.15 (m, 1H), 7.17-7.20 (m, 2H), 7.31-7.39 (m, 4H), 7.47-7.51 (m, 1H), 8.53 (d, *J* = 8.0 Hz, 1H), 11.25 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 32.22, 108.87, 110.87, 114.92, 117.04, 121.07, 121.55, 122.43, 123.52, 125.80, 126.33, 126.92, 127.49, 128.57, 130.78, 130.86, 132.31, 134.16, 136.83, 139.69, 141.60, 141.92, 142.03, 142.20, 157.79, 203.29. HRMS (ESI) calcd for $C_{32}H_{22}BrNNaO_2$ $[M+Na]^+$: 554.0726, found: 554.0730.

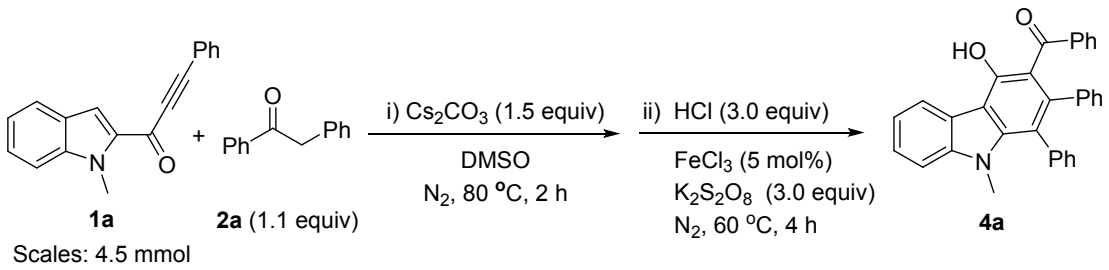


4y

(4-Hydroxy-9-methyl-2-phenyl-1-(p-tolyl)-9*H*-carbazol-3-yl)(phenyl)methanone (**4y**, yellow solid, 97.8 mg, 70%). mp 257-259 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.28 (s, 3H), 3.19 (s, 3H), 6.69-6.73 (m, 5H), 6.97-7.04 (m, 6H), 7.09-7.14 (m, 1H), 7.18-7.21 (m, 2H), 7.31-7.37 (m, 2H), 7.45-7.50 (m, 1H), 8.54 (d, *J* = 8.0 Hz, 1H), 11.28 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.95, 31.92, 108.82, 110.63, 114.87, 118.60, 120.87, 122.53, 123.45, 125.57, 126.00, 126.66, 127.43, 128.37, 128.63, 130.64, 132.36, 132.44, 134.41, 136.99, 140.19, 141.63, 141.98, 142.19, 142.63, 157.62,

203.36. HRMS (ESI) calcd for $C_{33}H_{26}NO_2$ $[M+H]^+$: 468.1958, found: 468.1963.

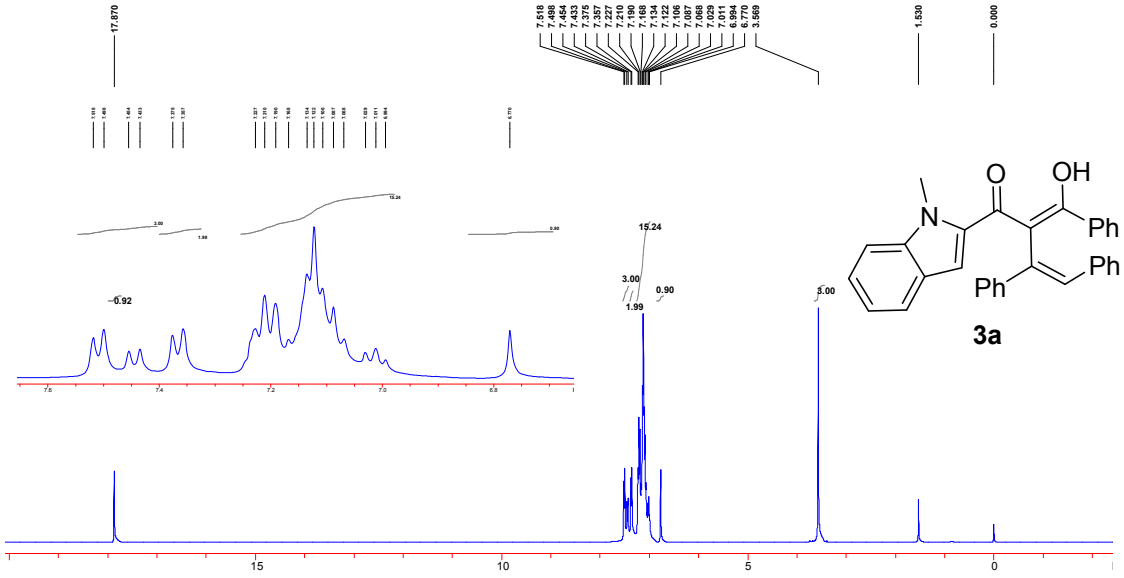
6. Gram Scale

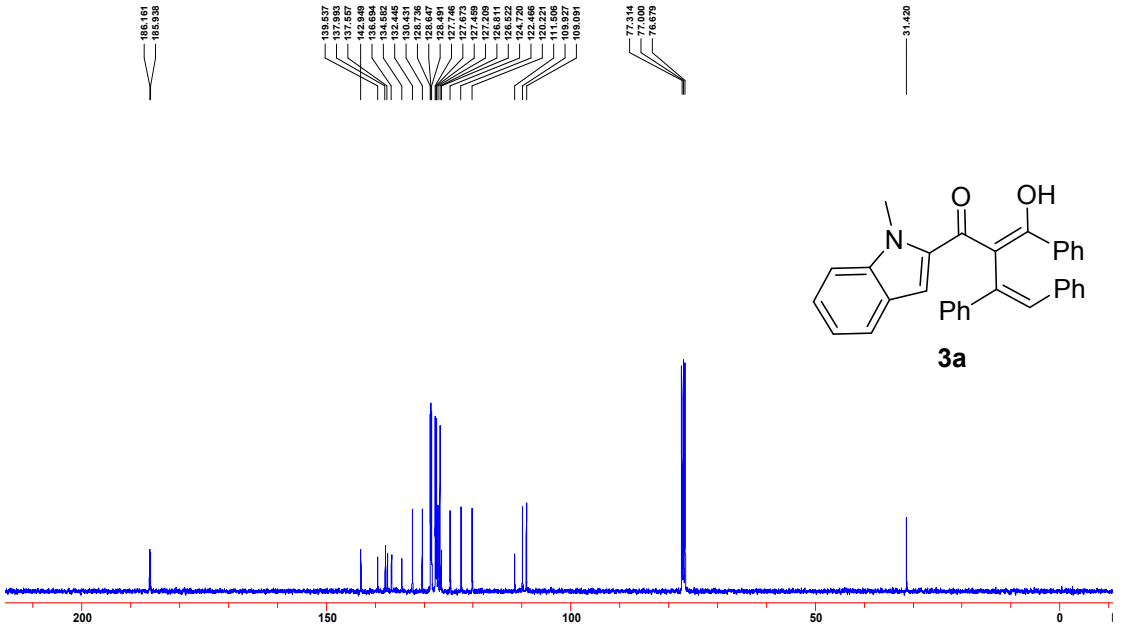


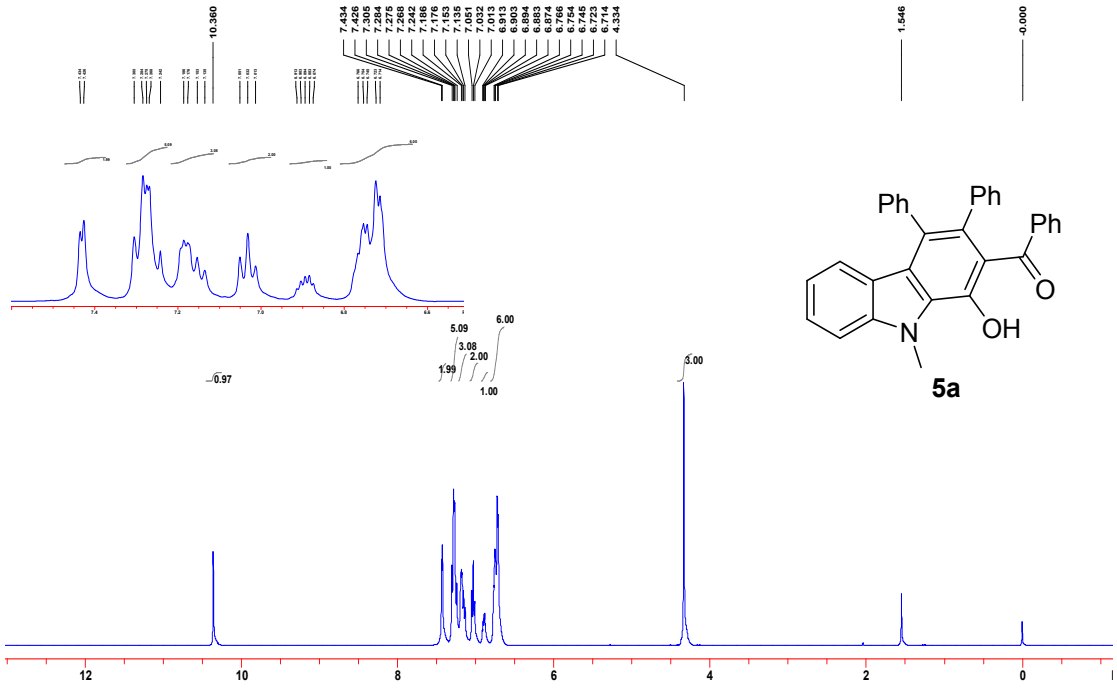
Scales: 4.5 mmol

In a schlenk tube, indolyl alkynyl ketones **1a** (4.5 mmol, 1.17 g), 2-phenylacetophenone **2a** (4.95 mmol, 0.97 g), Cs_2CO_3 (6.75 mmol, 2.20 g) and DMSO (45 mL) were stirred at 80 °C under N_2. After 2 h, the reaction mixture was then quenched by HCl (13.5 mmol, 2.25 mL, 6M), then $FeCl_3$ (0.225 mmol, 36.5 mg) and $K_2S_2O_8$ (13.5 mmol, 3.65 g) were added. After the completion of the addition, the reaction mixture was allowed to react at 60 °C for 4 h. Then, the reaction mixture was cooled to room temperature and was treated with H_2O, then extracted with EA. The combined organic layers were washed with brine, and dried over anhydrous Na_2SO_4. After removal of the EA, the residue was purified by chromatography on basic silica gel (PE : EA = 100 : 1) to afford **4a** (yellow solid, 1.37 g, 67%).

7. Copies of Spectra of New Products



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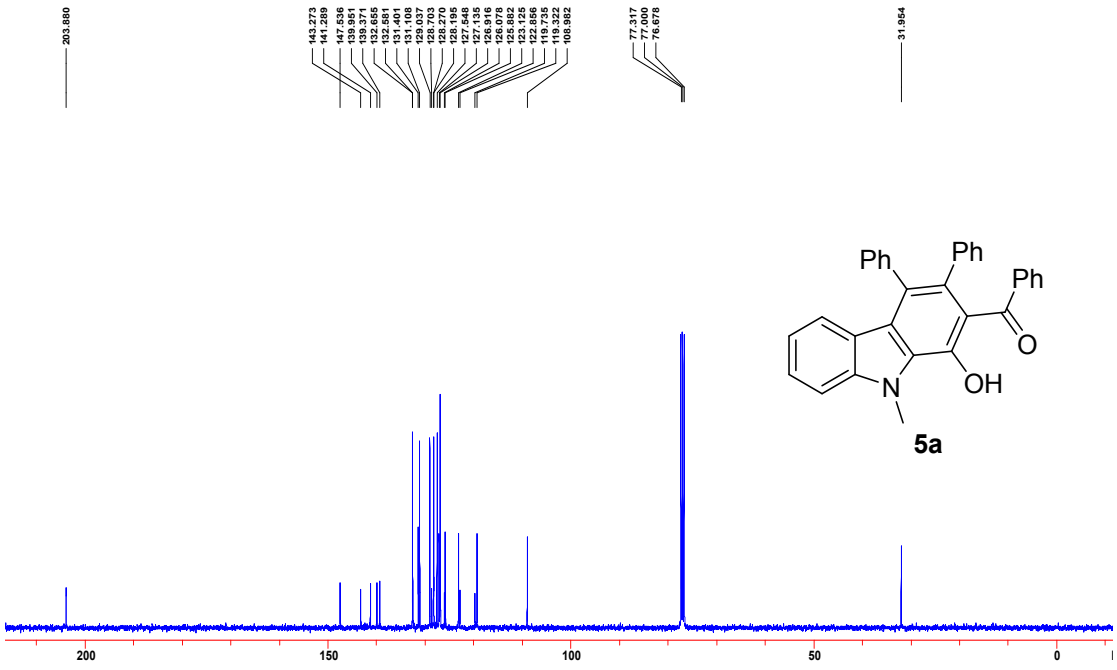
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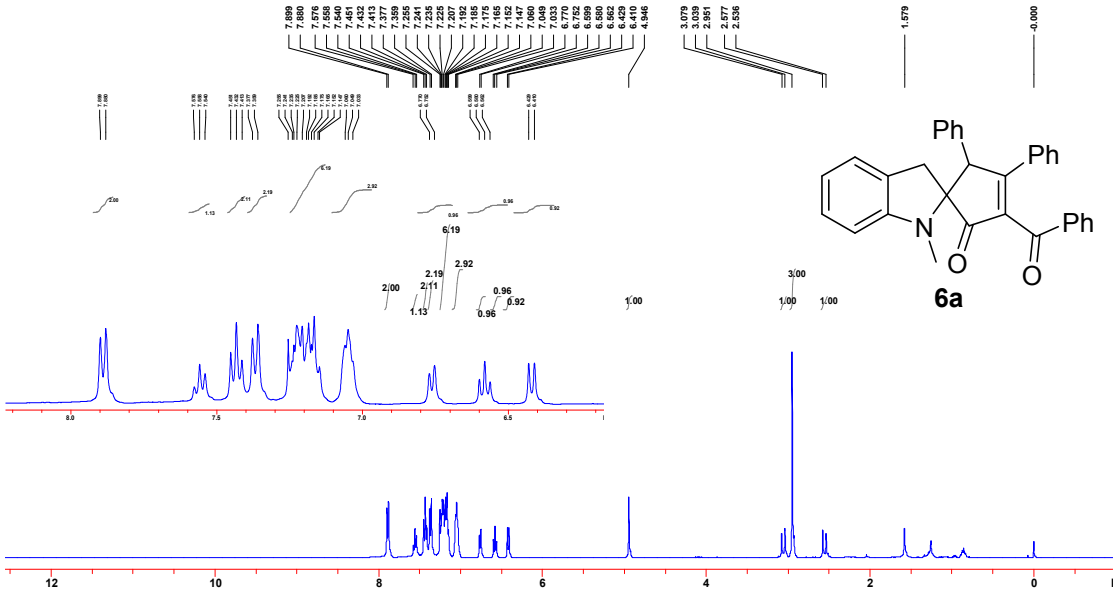
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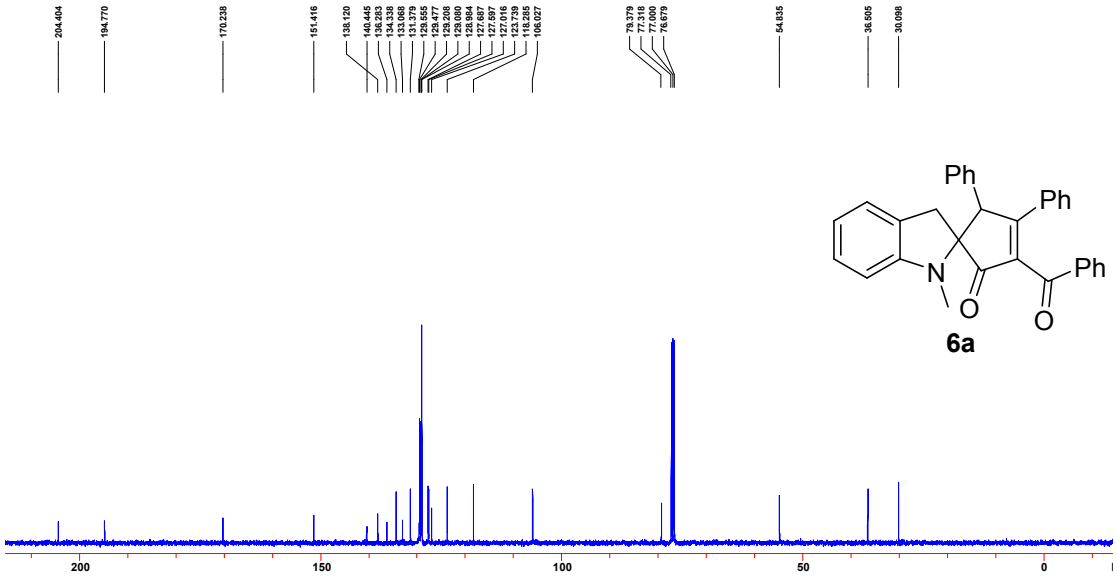
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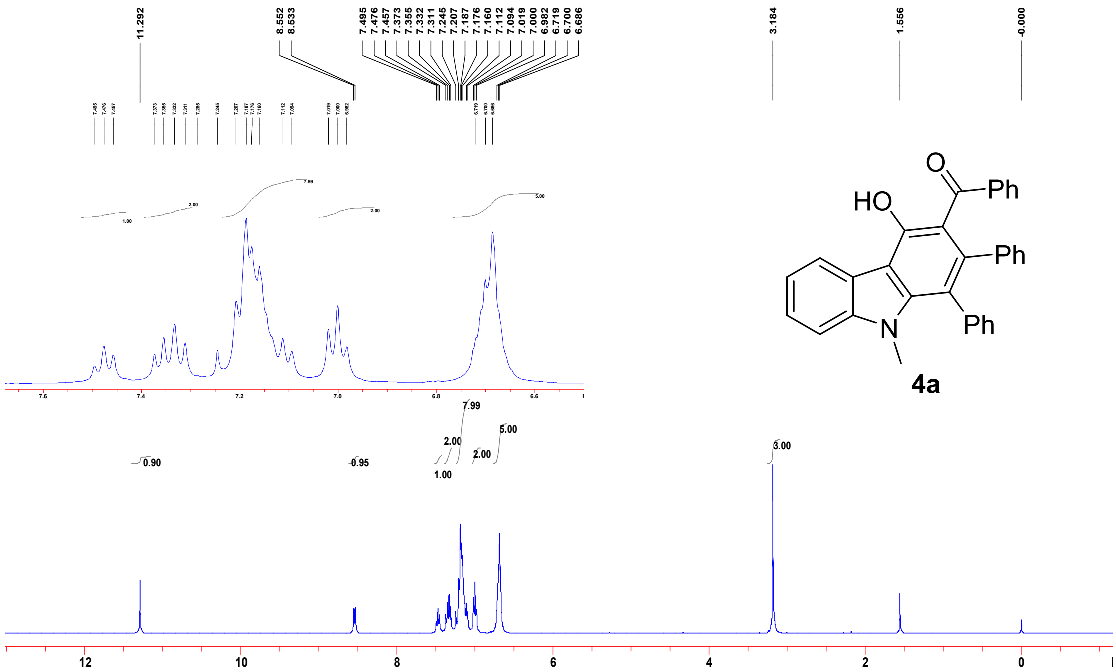

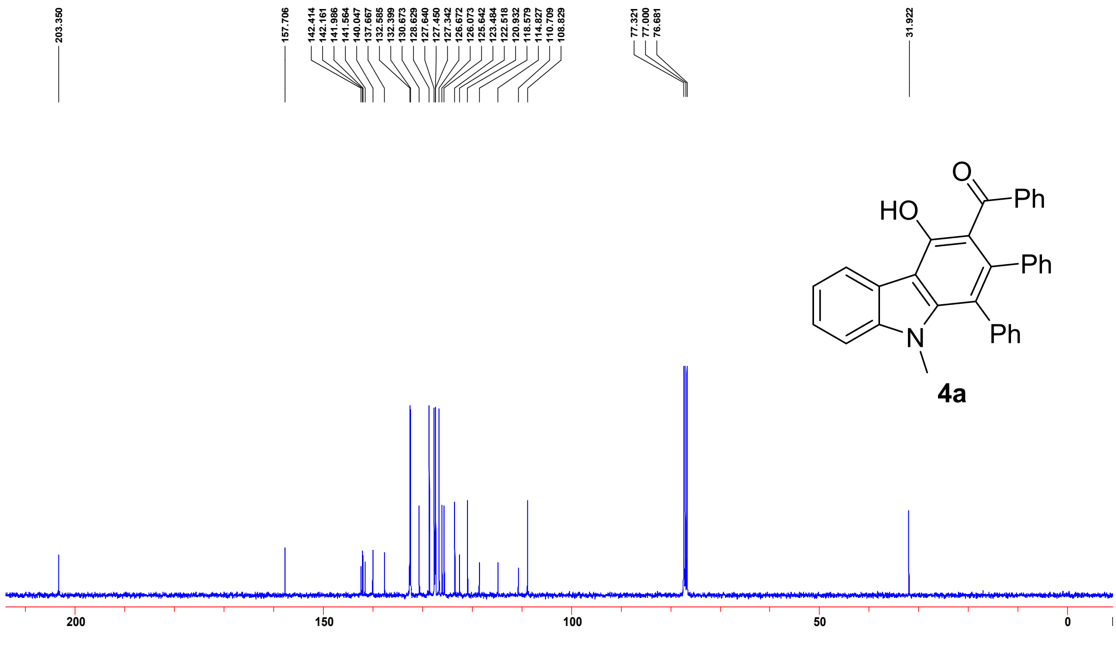

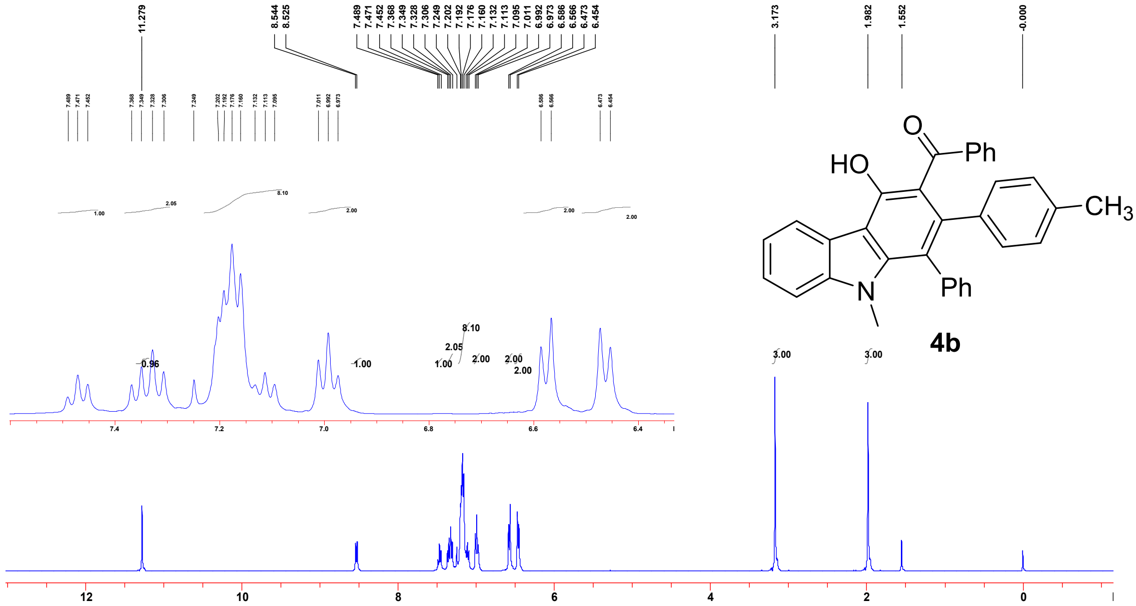

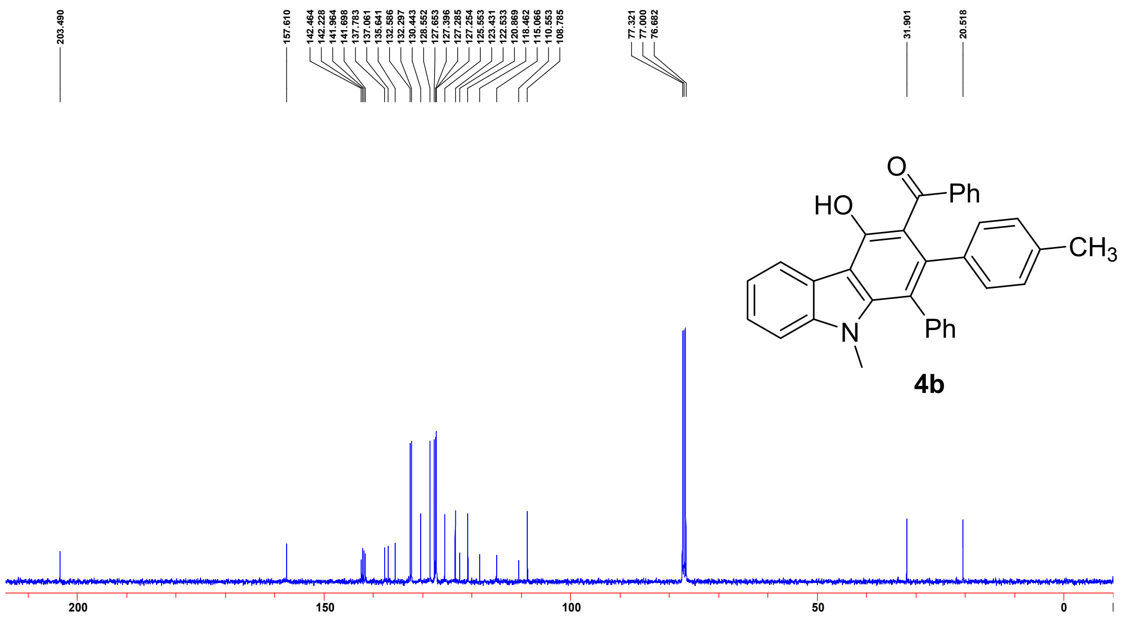

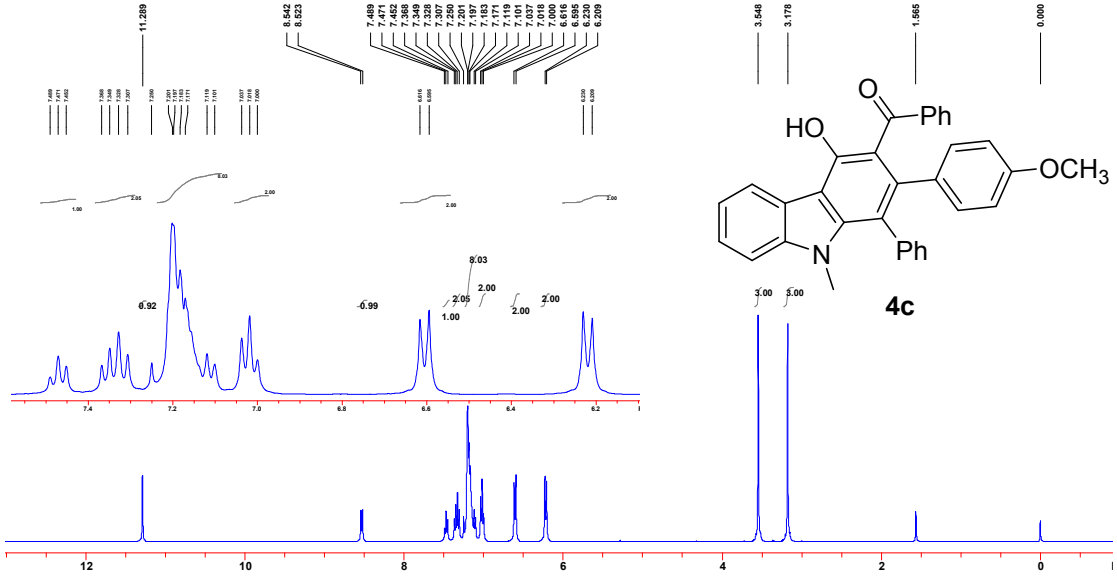
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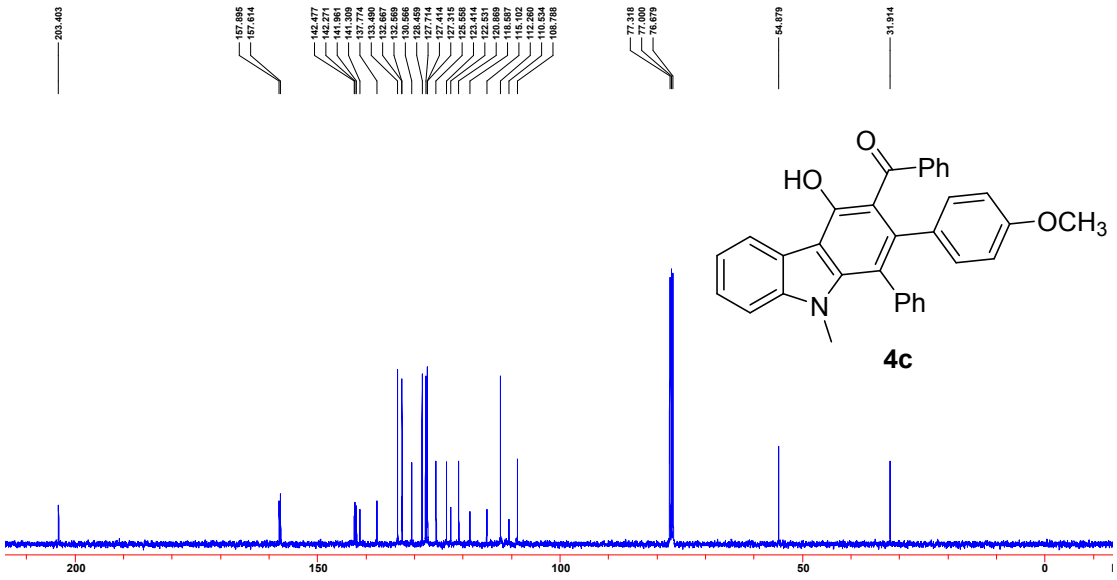
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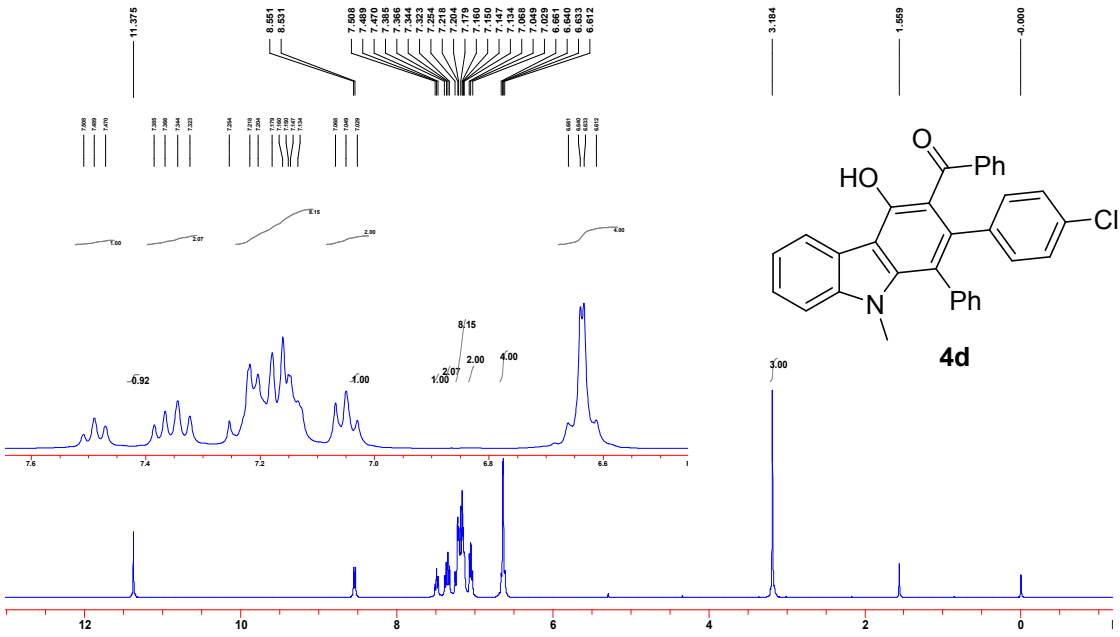
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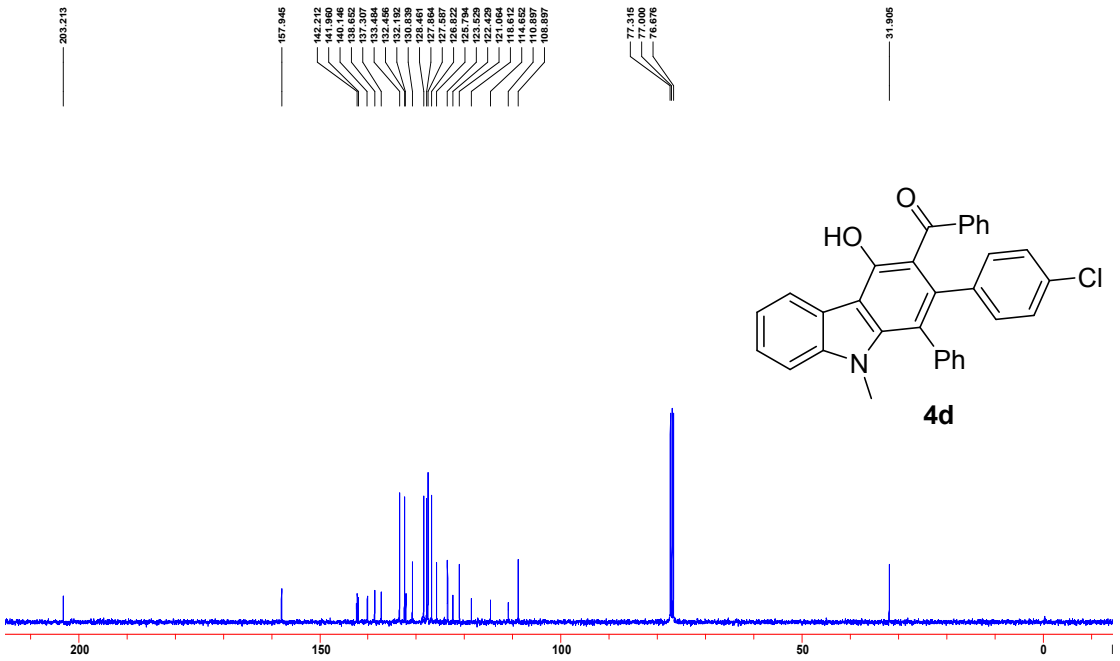
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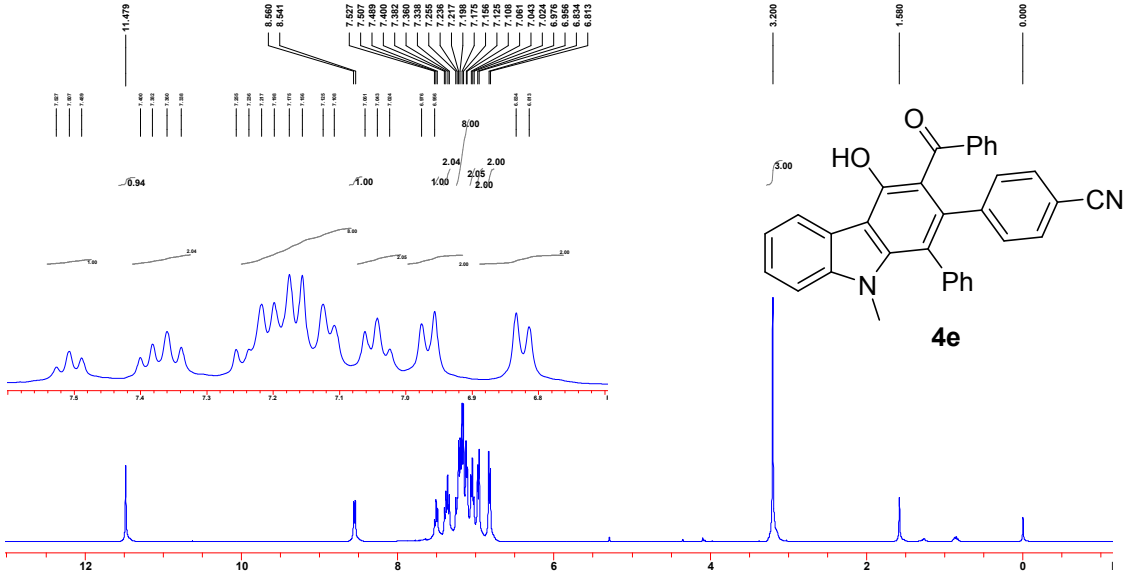
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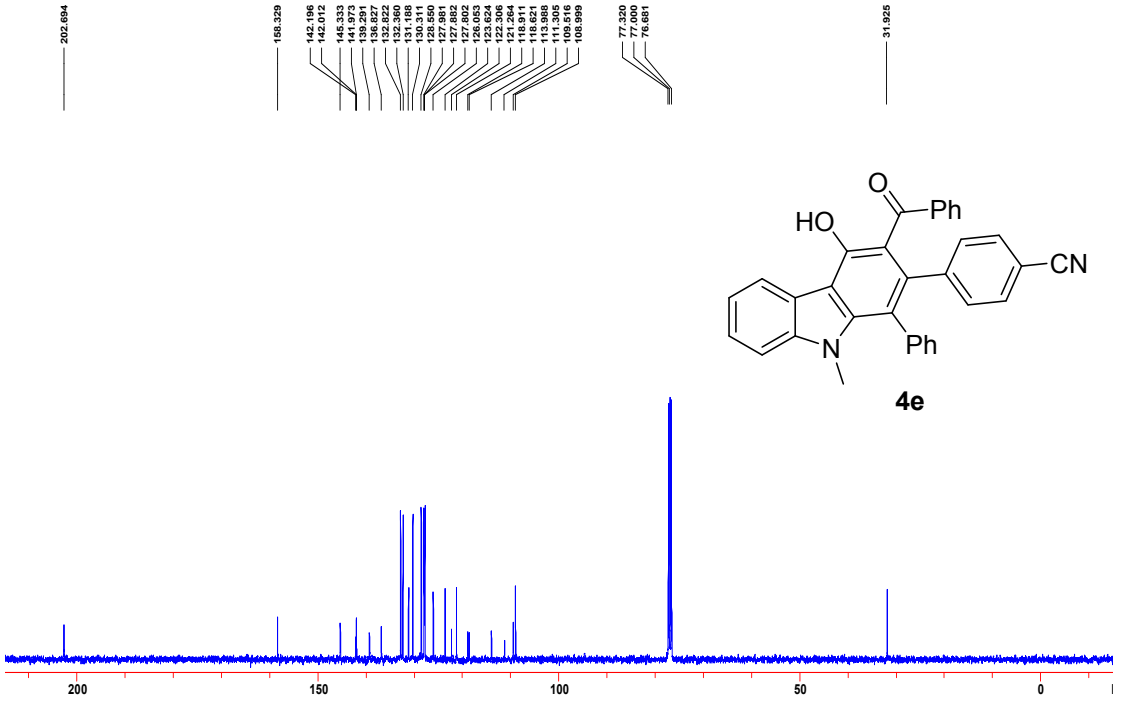
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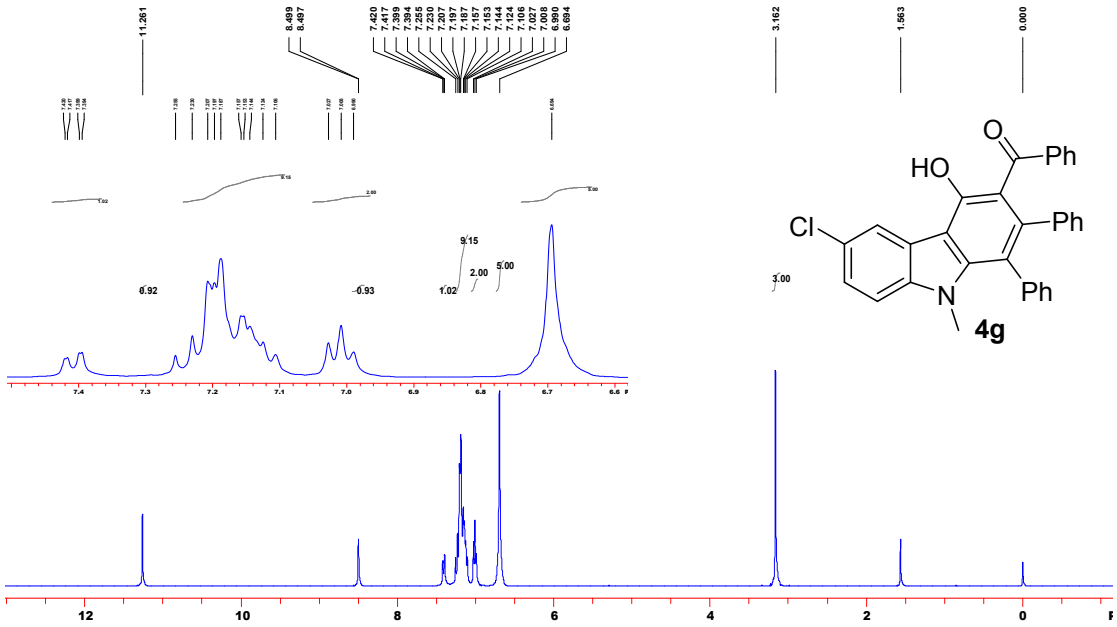
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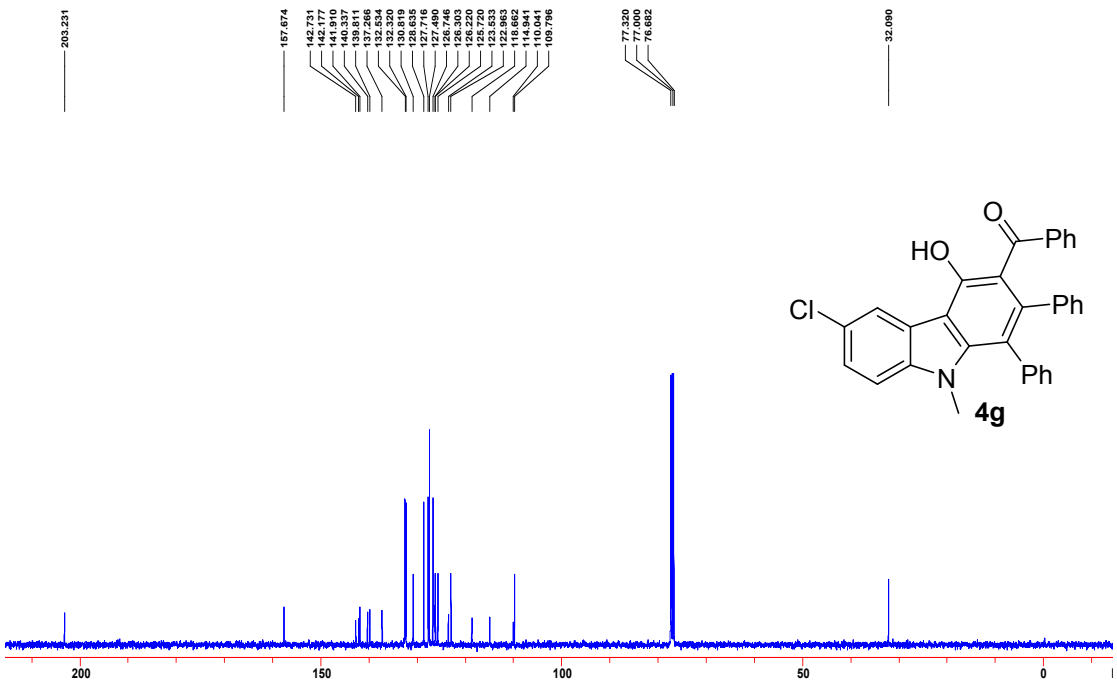
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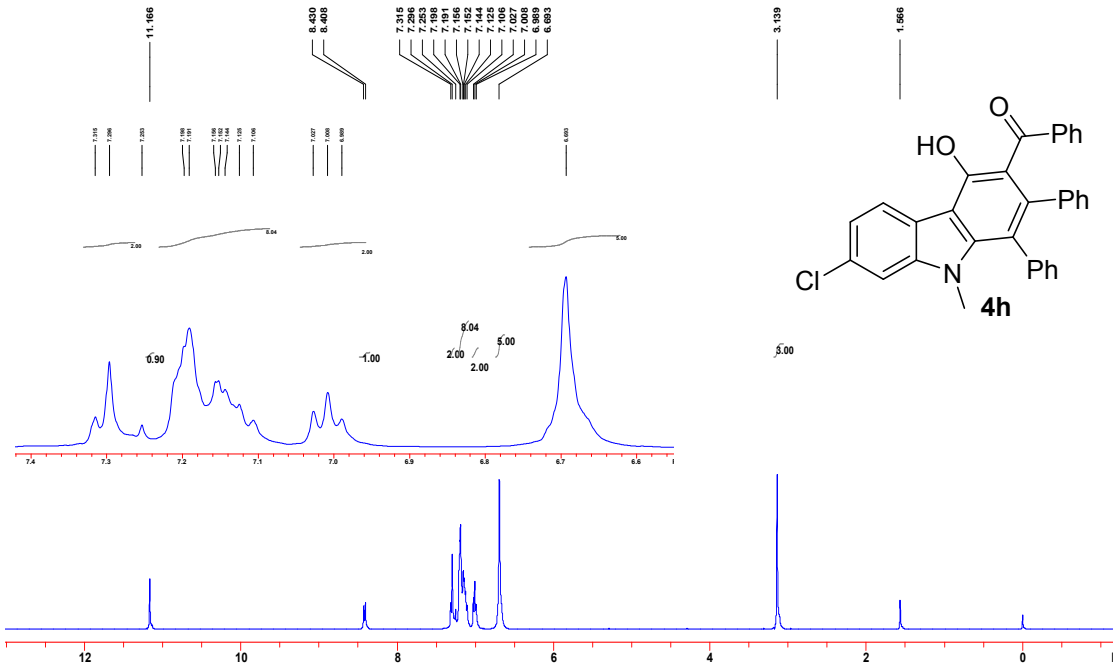
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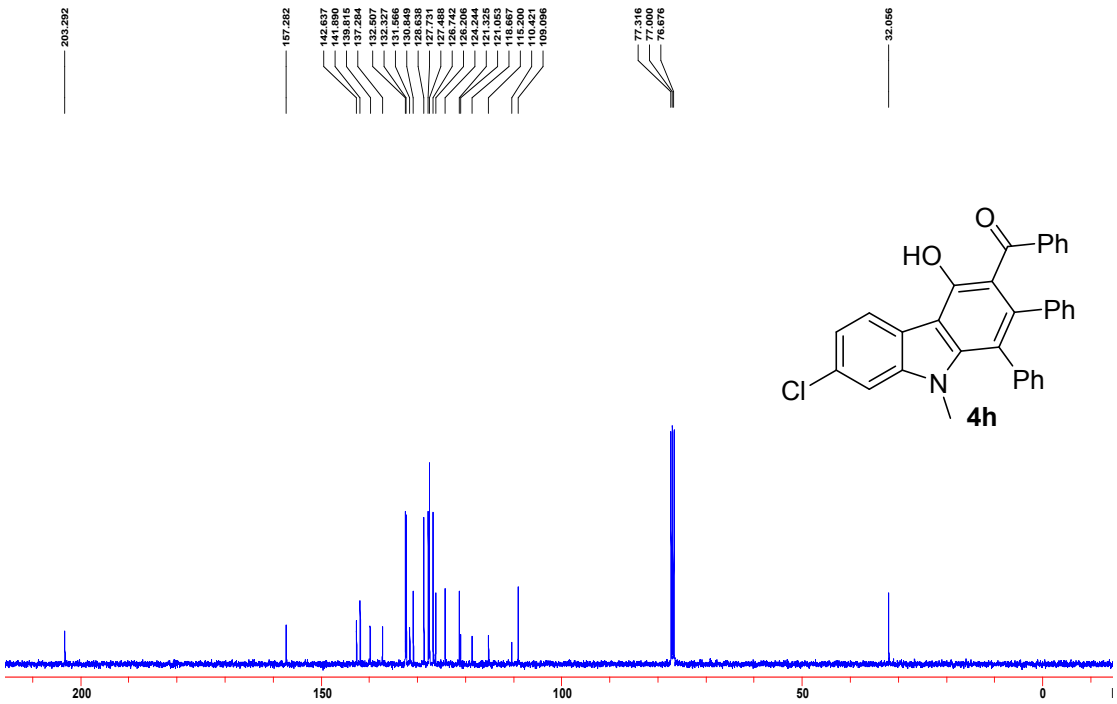
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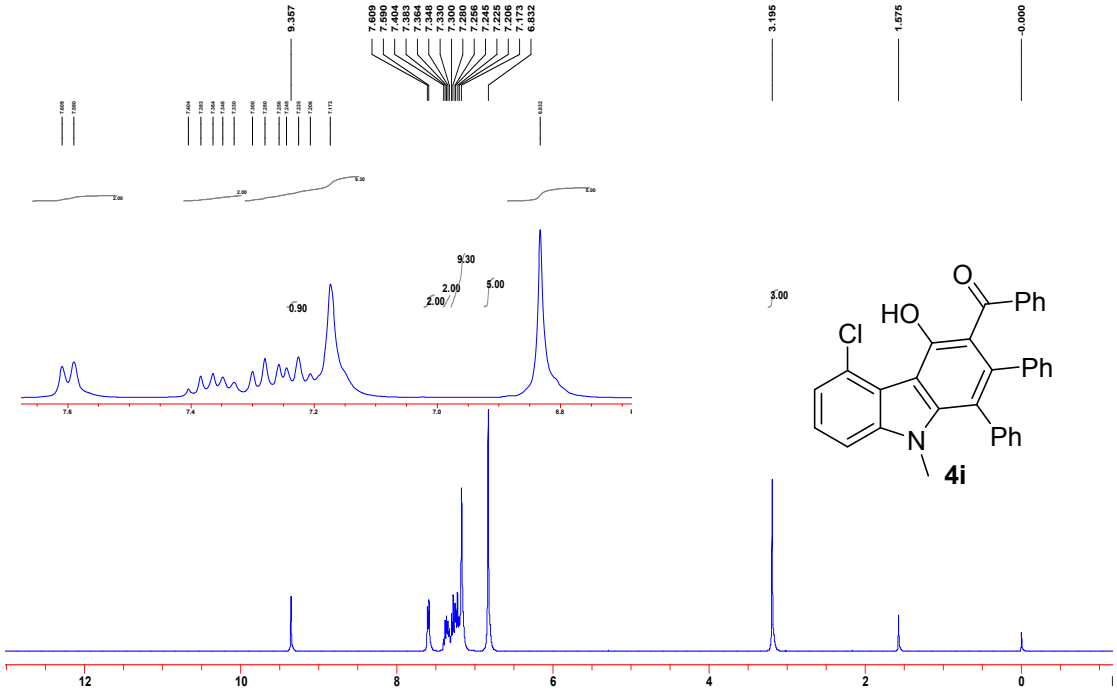
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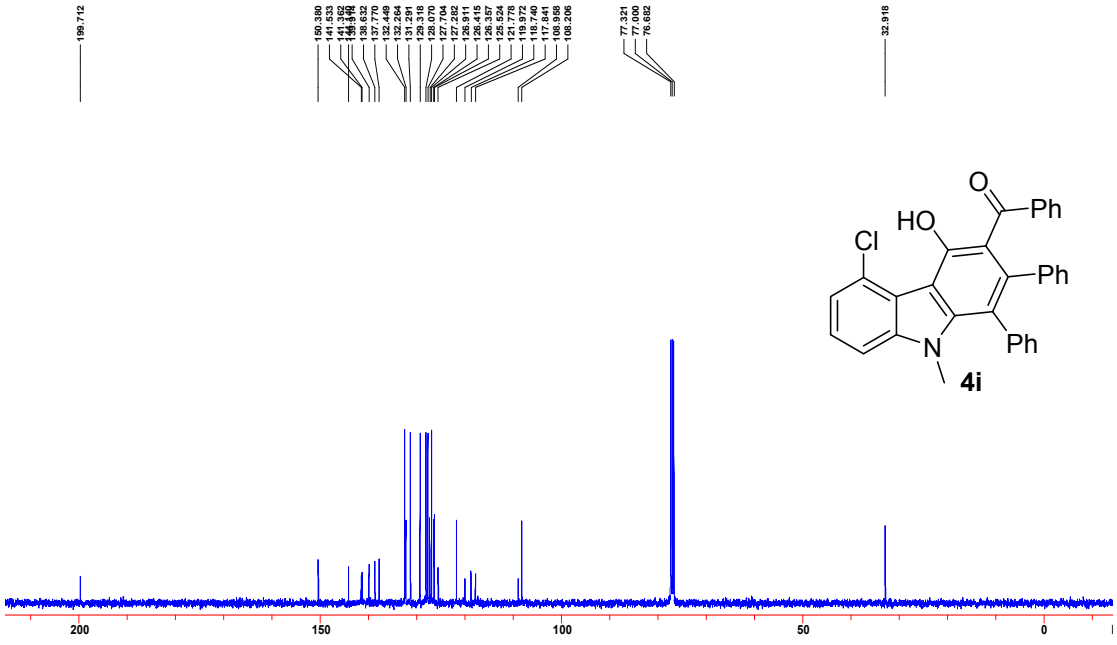
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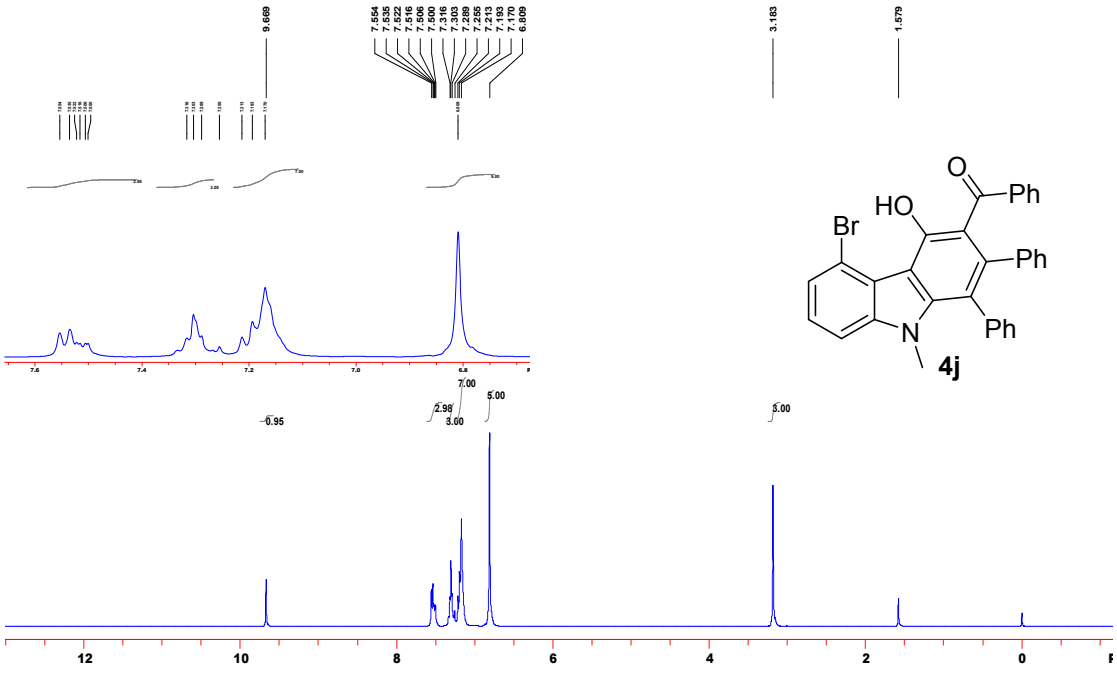
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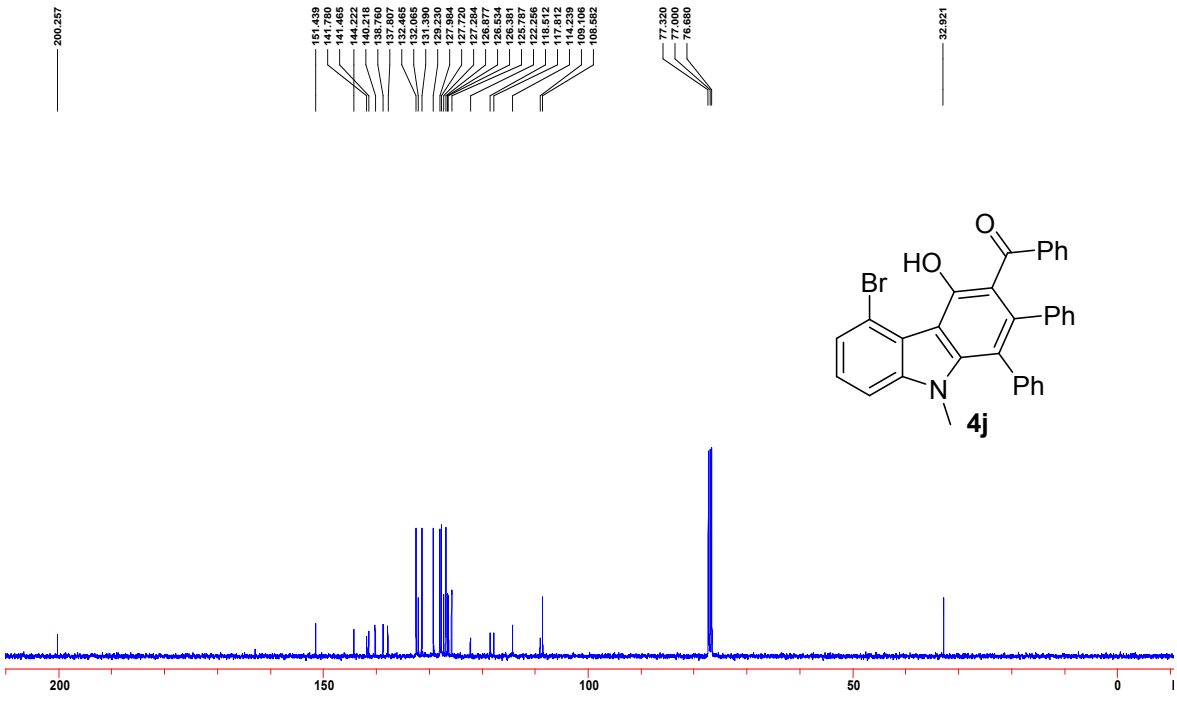
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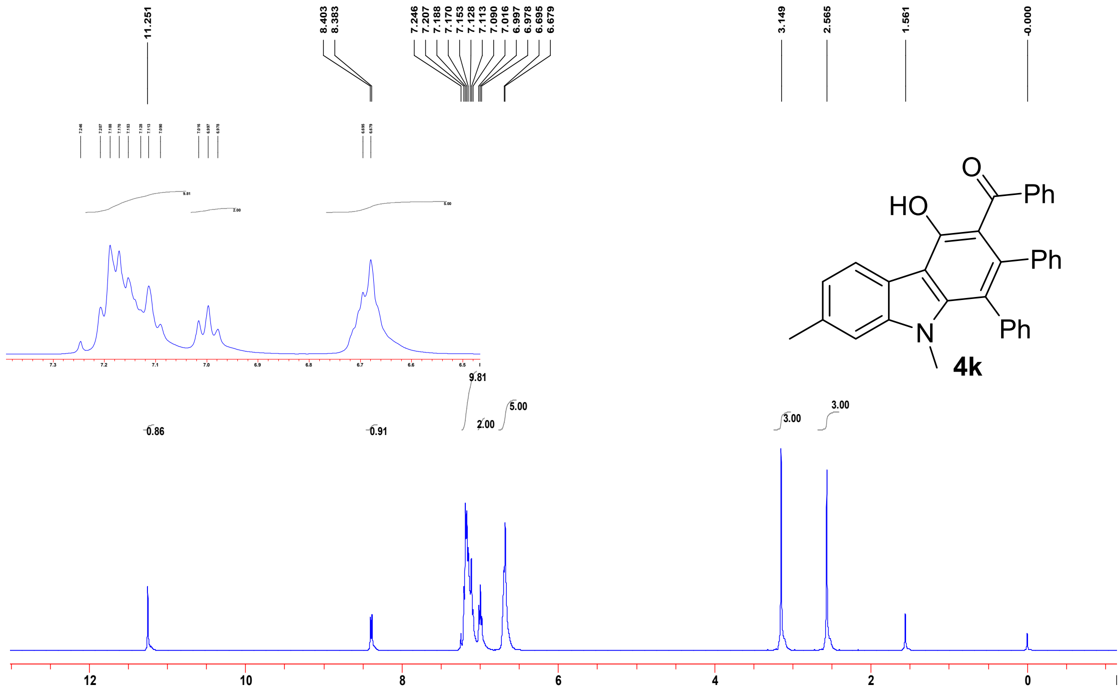
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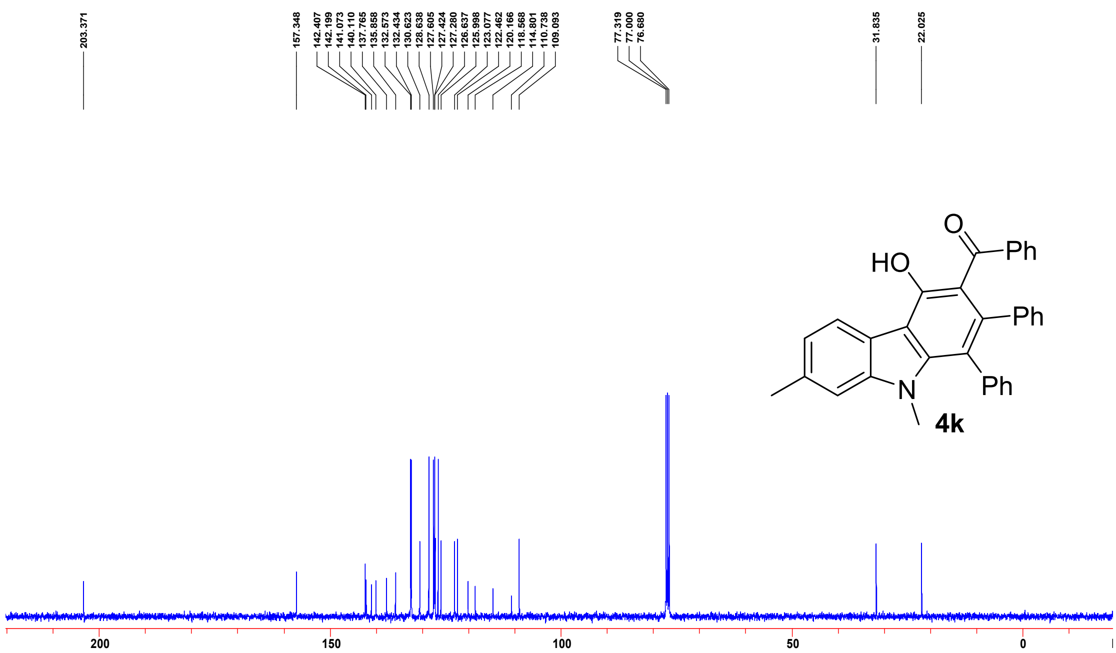
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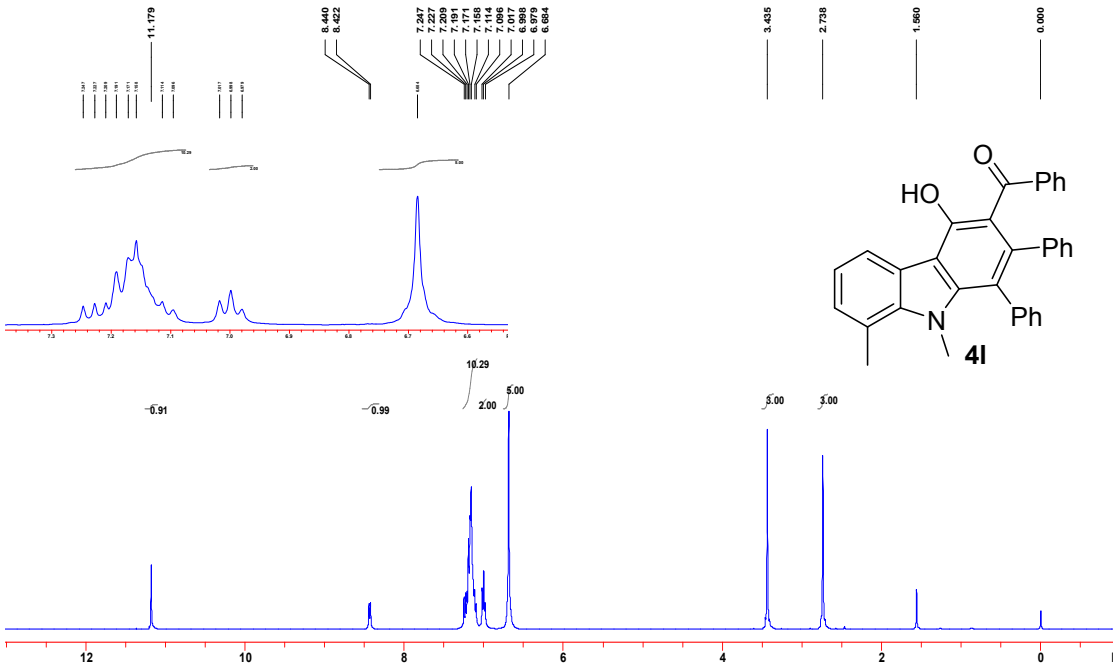
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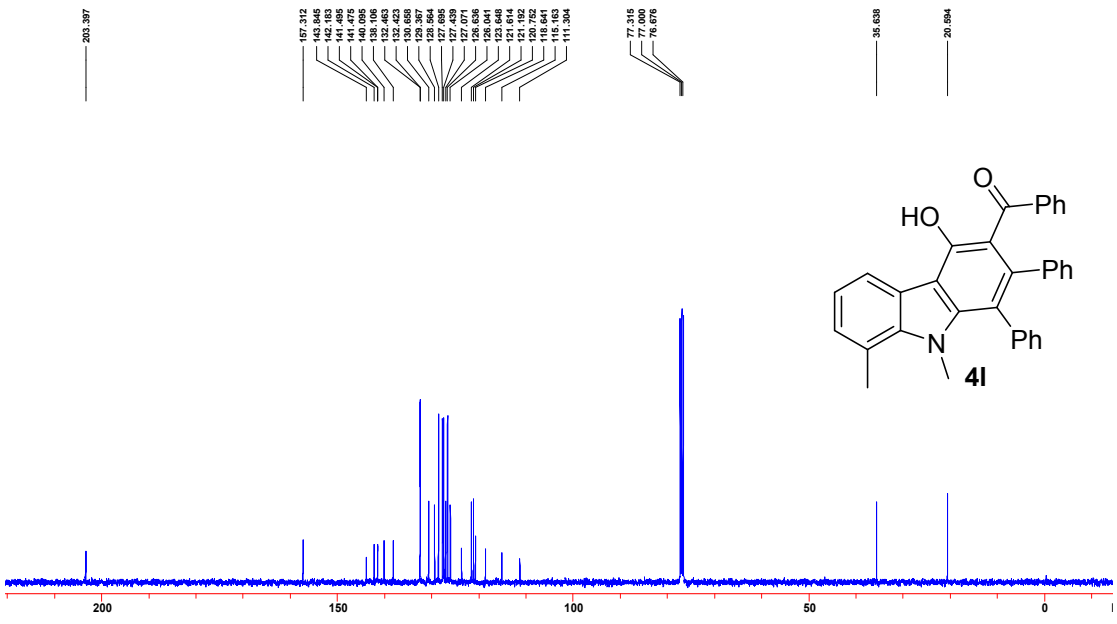
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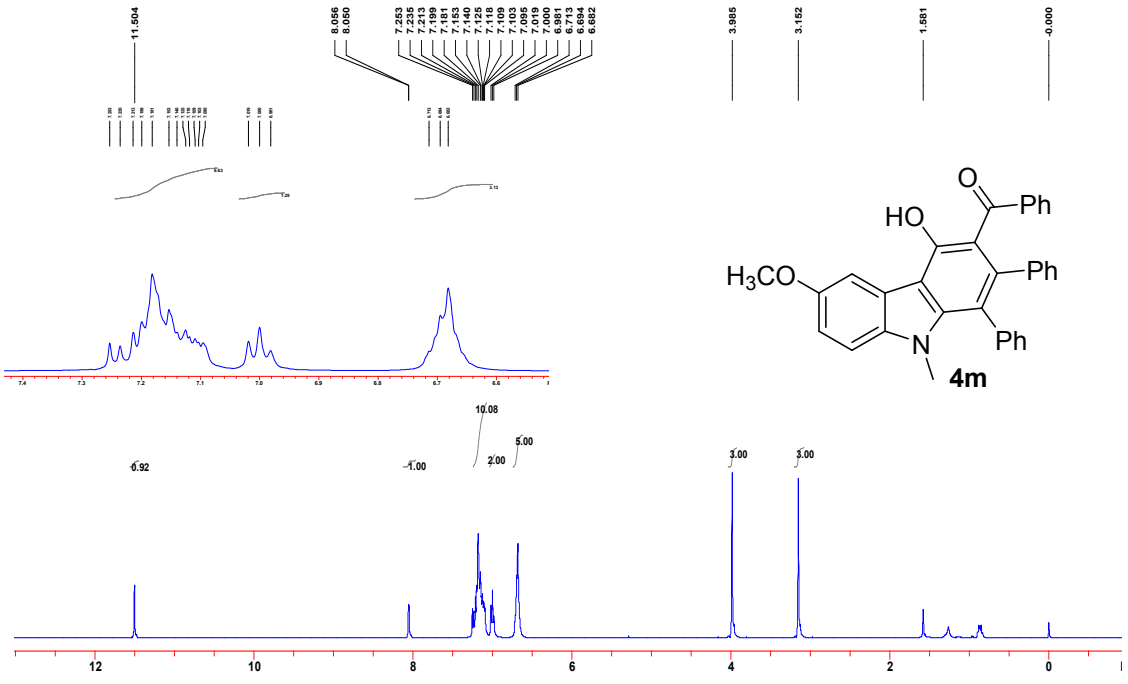
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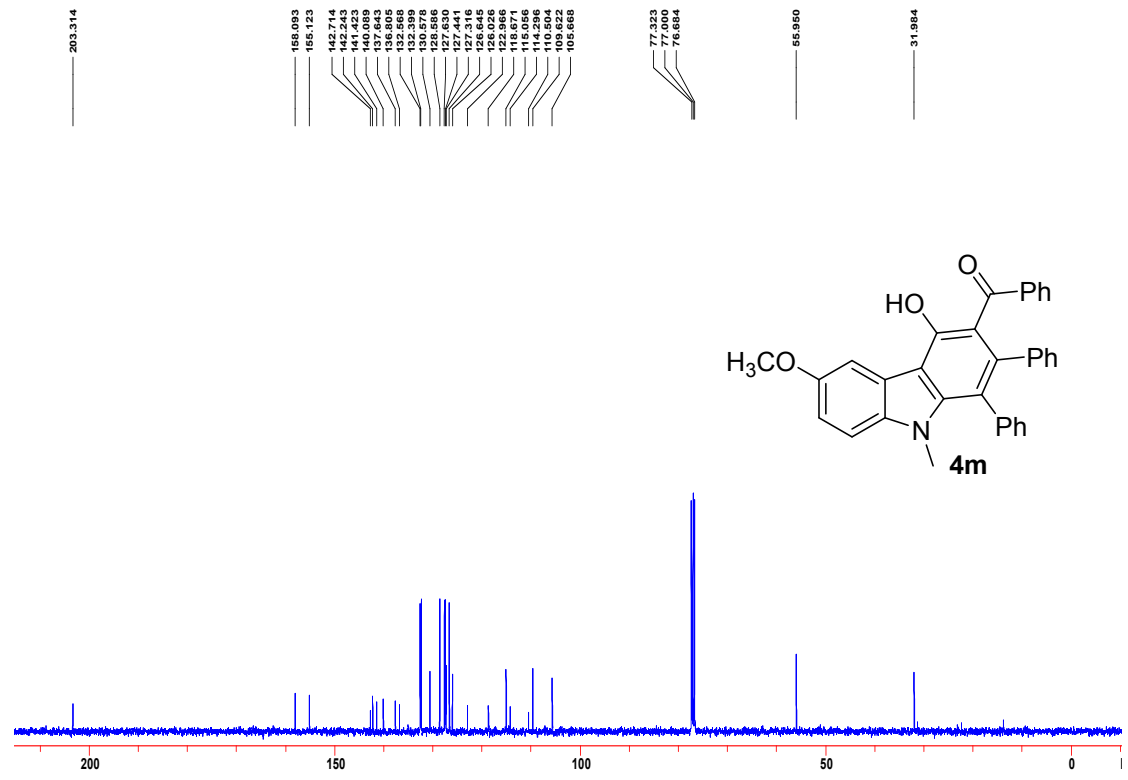
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114.296
110.504
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Ph
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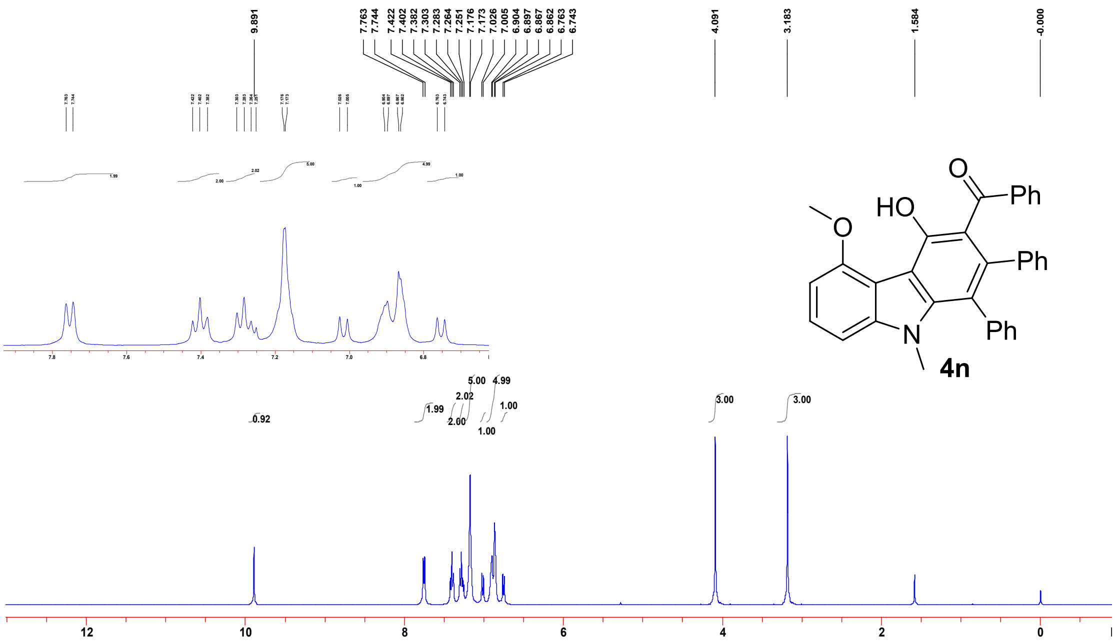
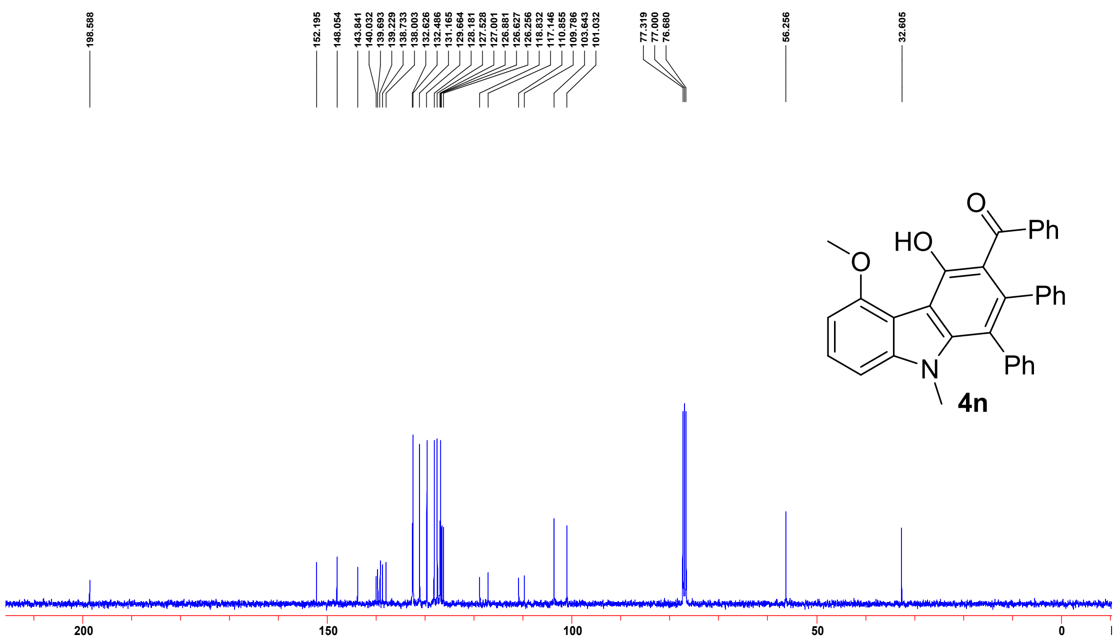
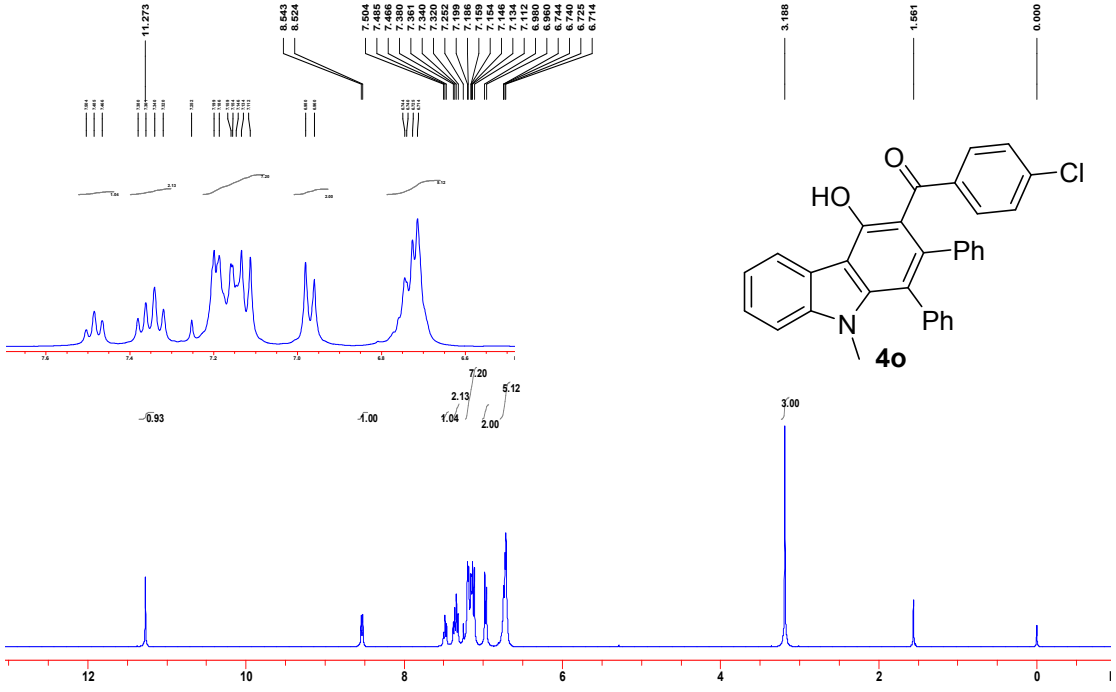
100
50
0



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Ph
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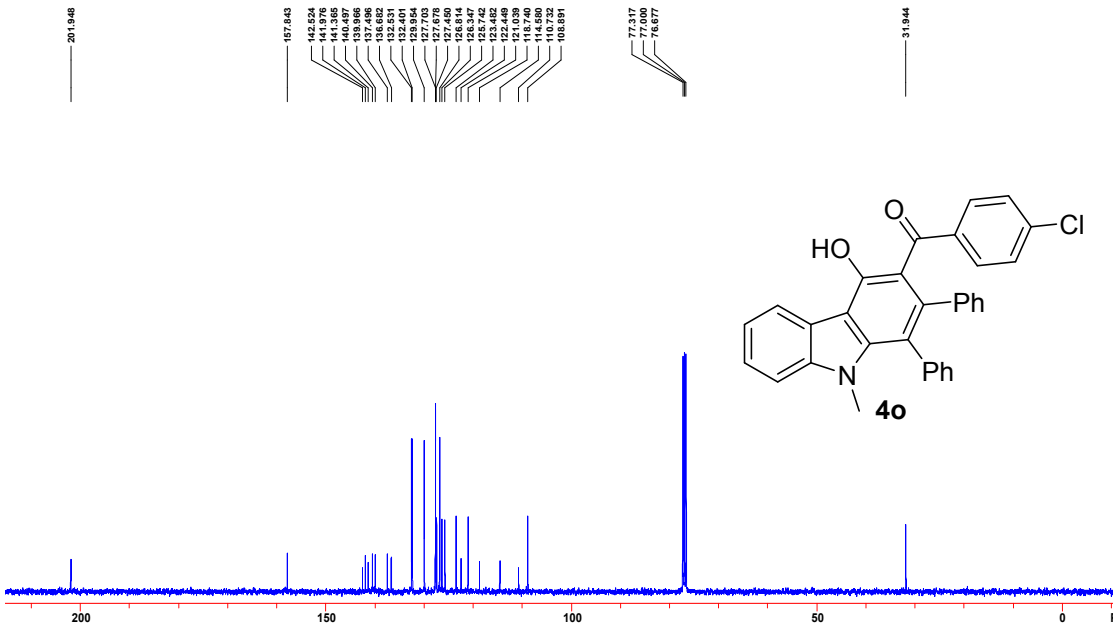
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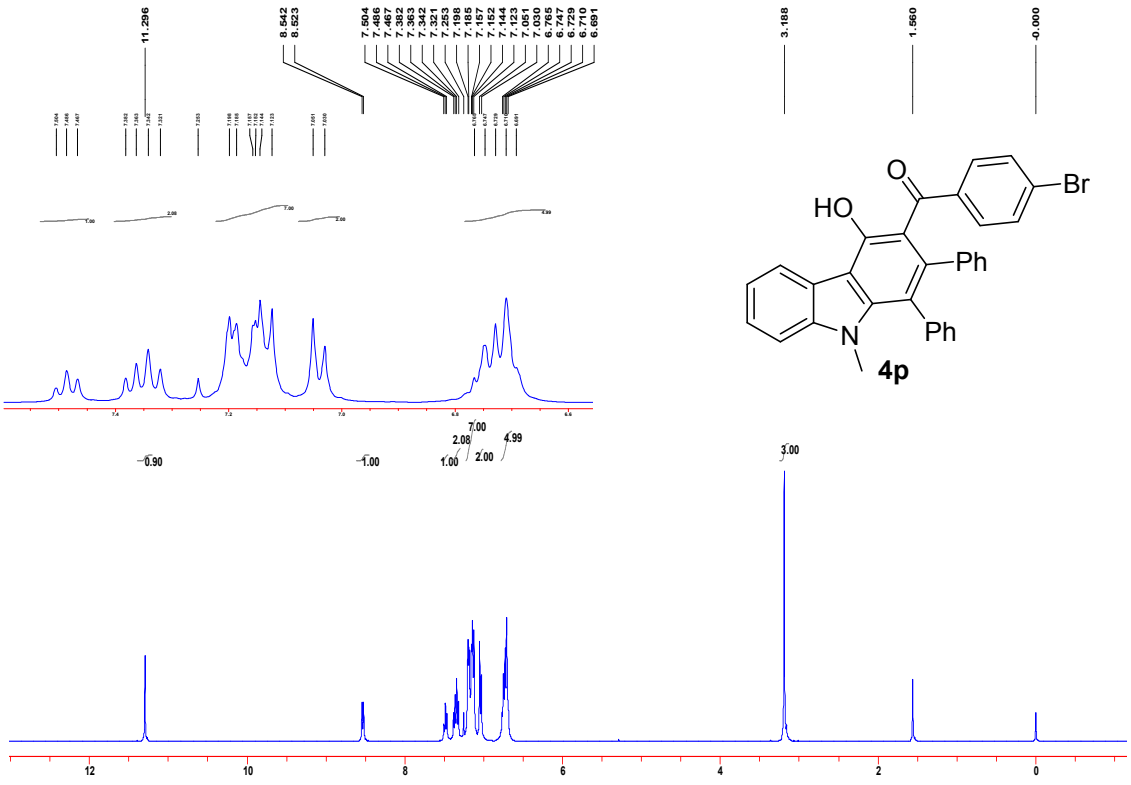
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Ph
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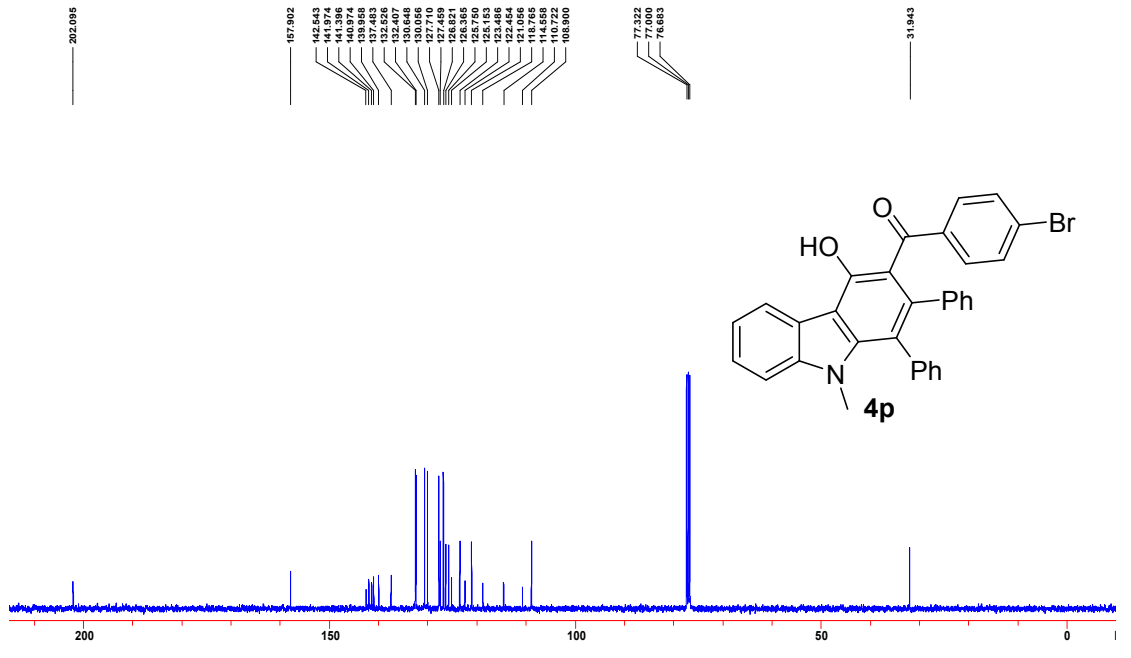
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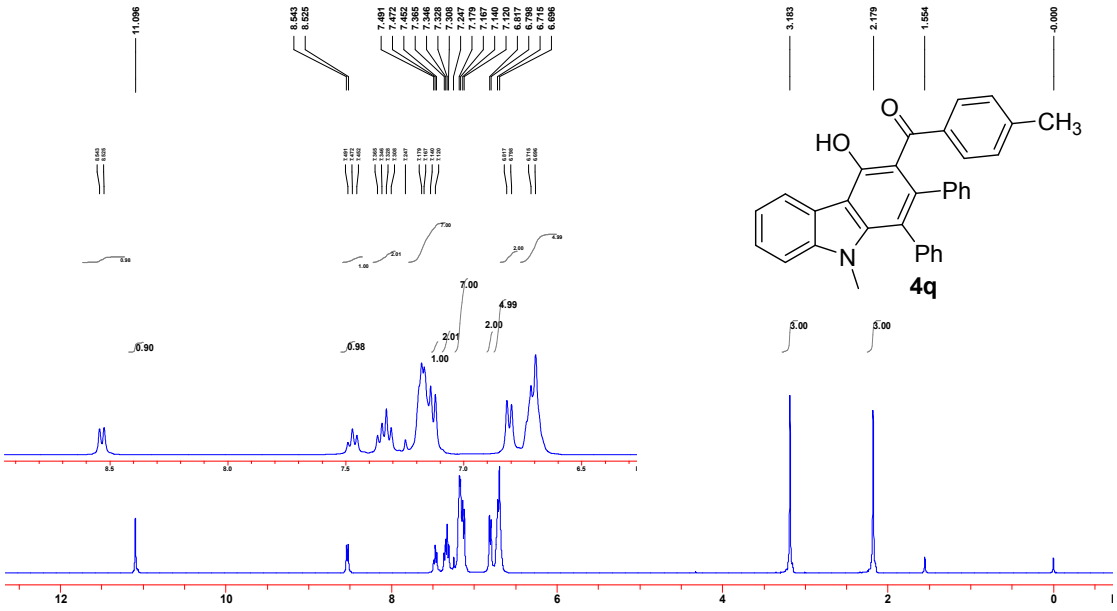
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CH3
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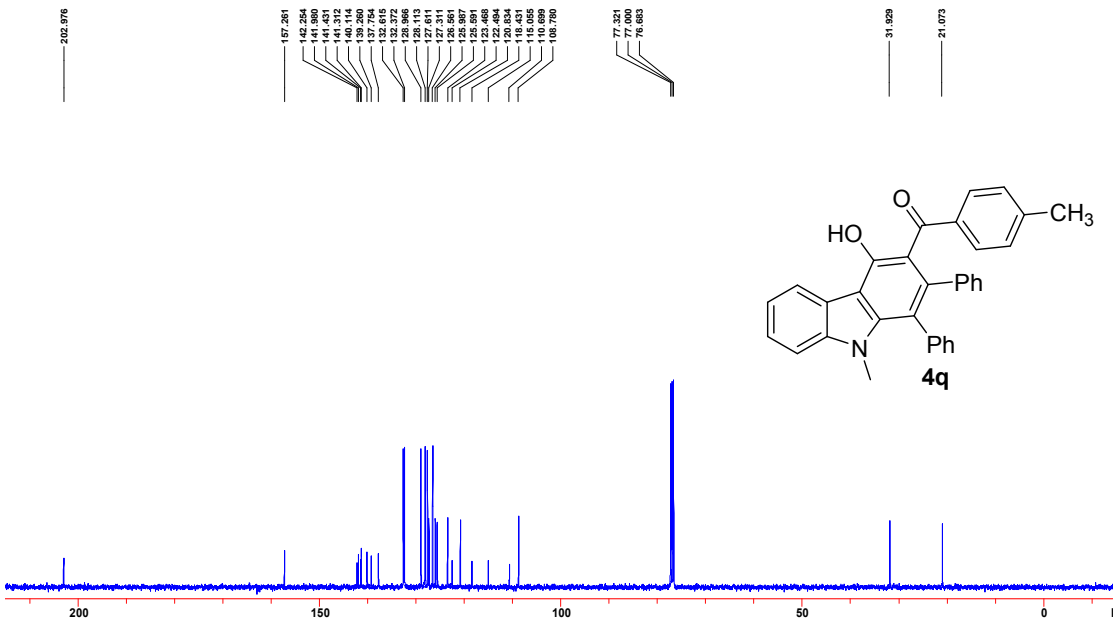
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123.468
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115.055
110.699
108.780
77.321
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Ph
N
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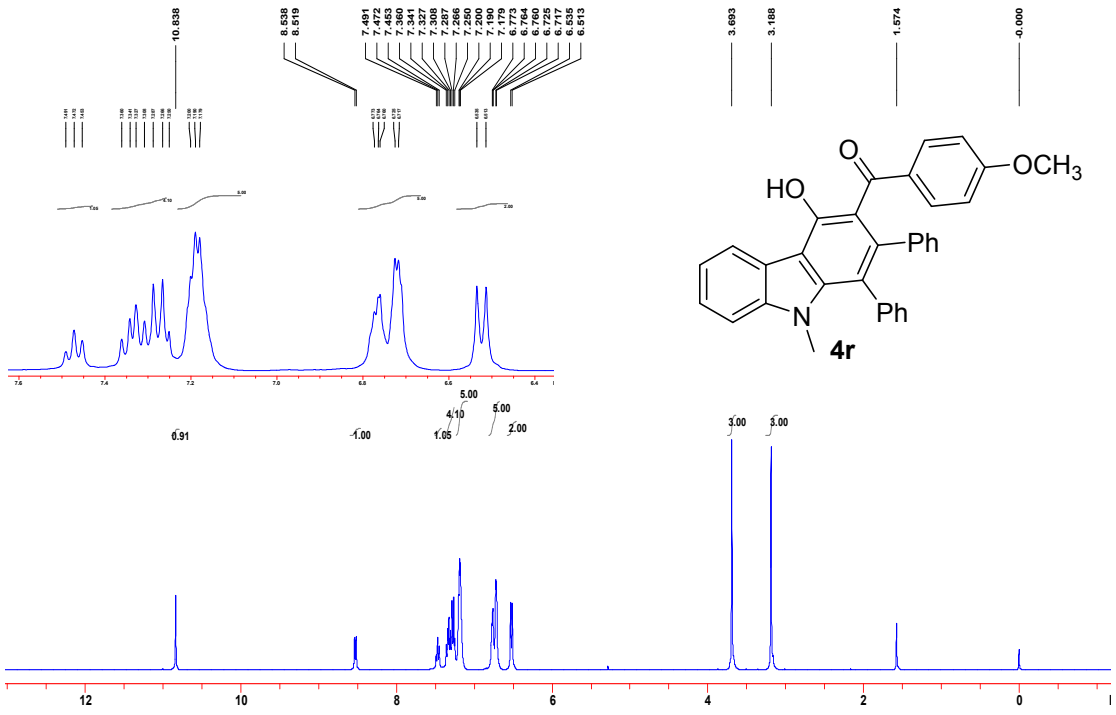
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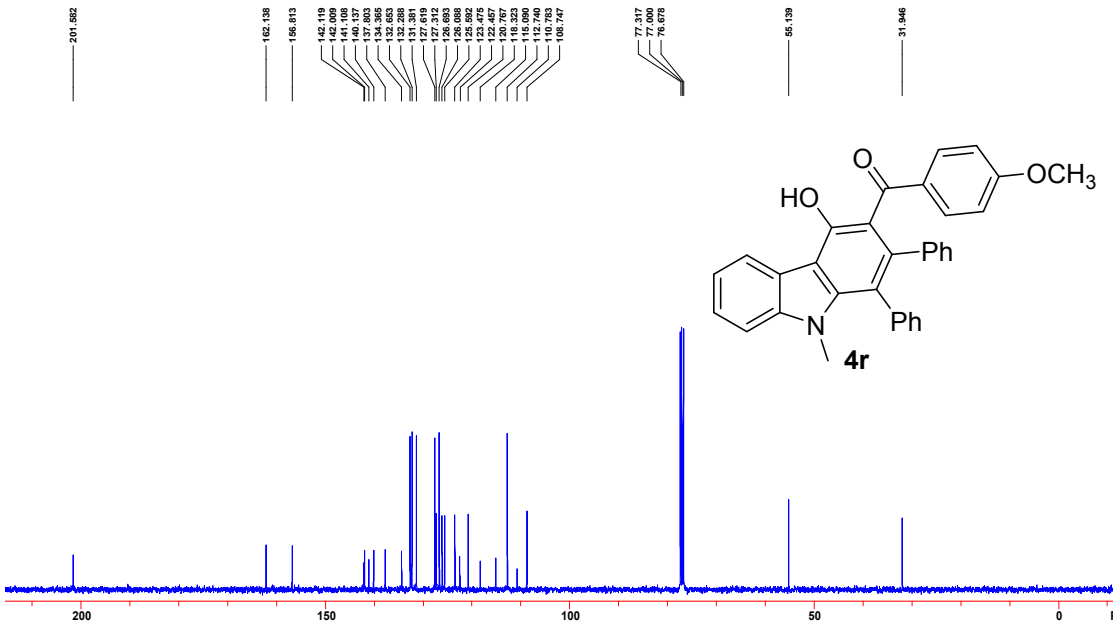
3.00
3.00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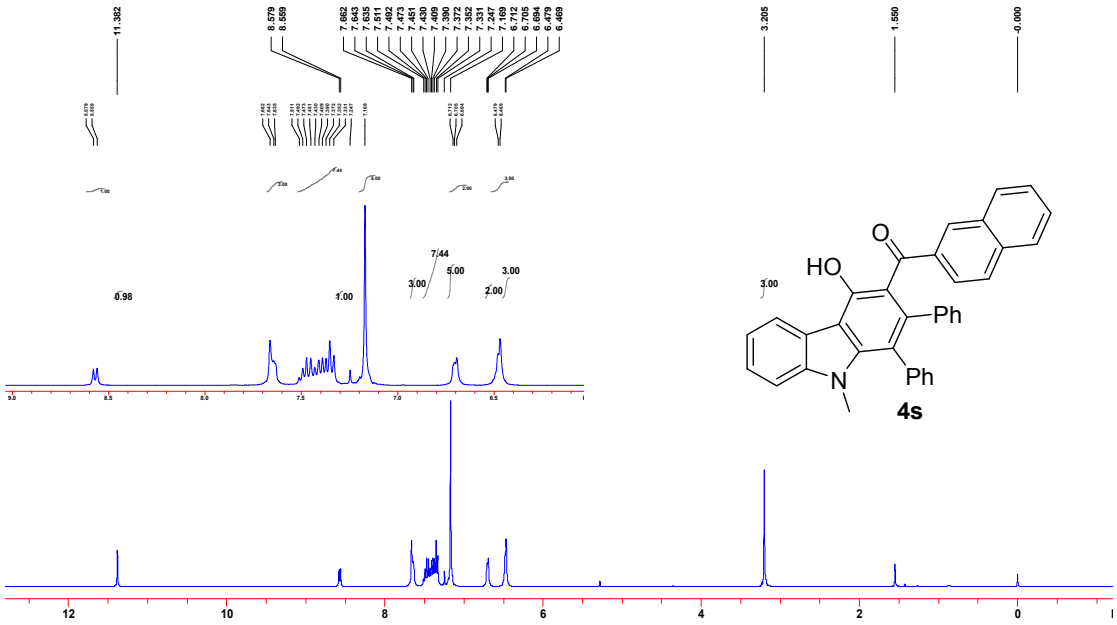
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7.247
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6.694
6.479
6.469
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3.00
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Ph
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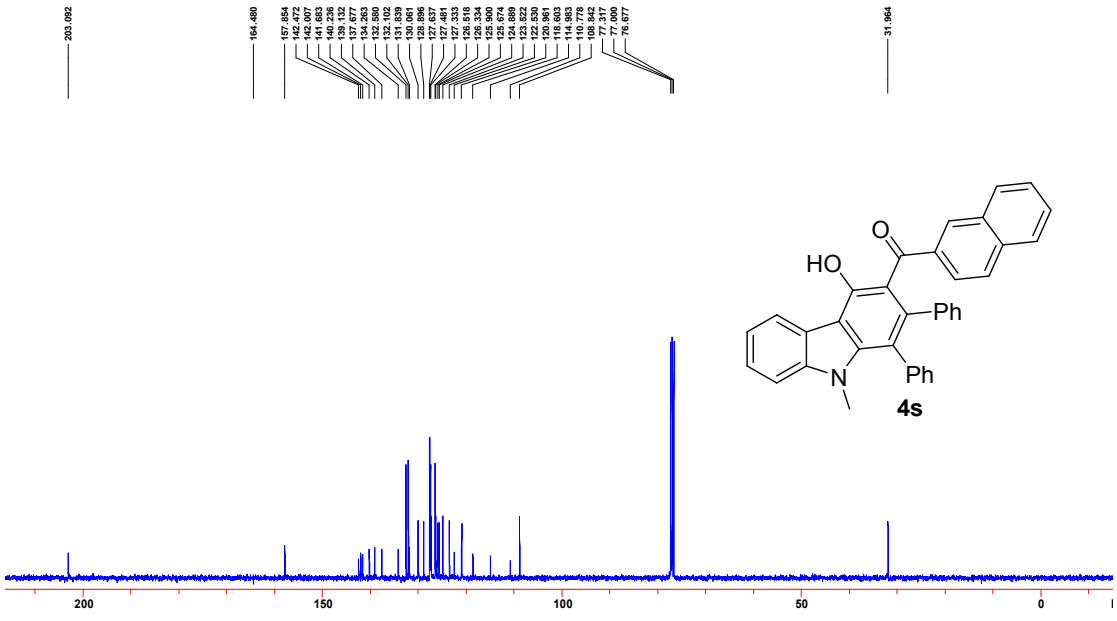
4s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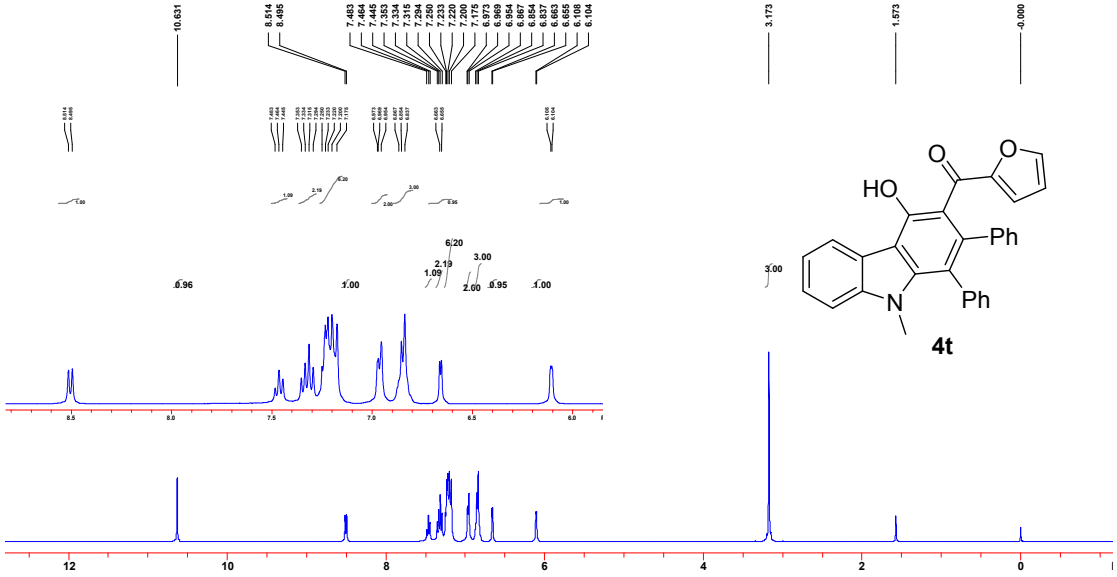
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Ph
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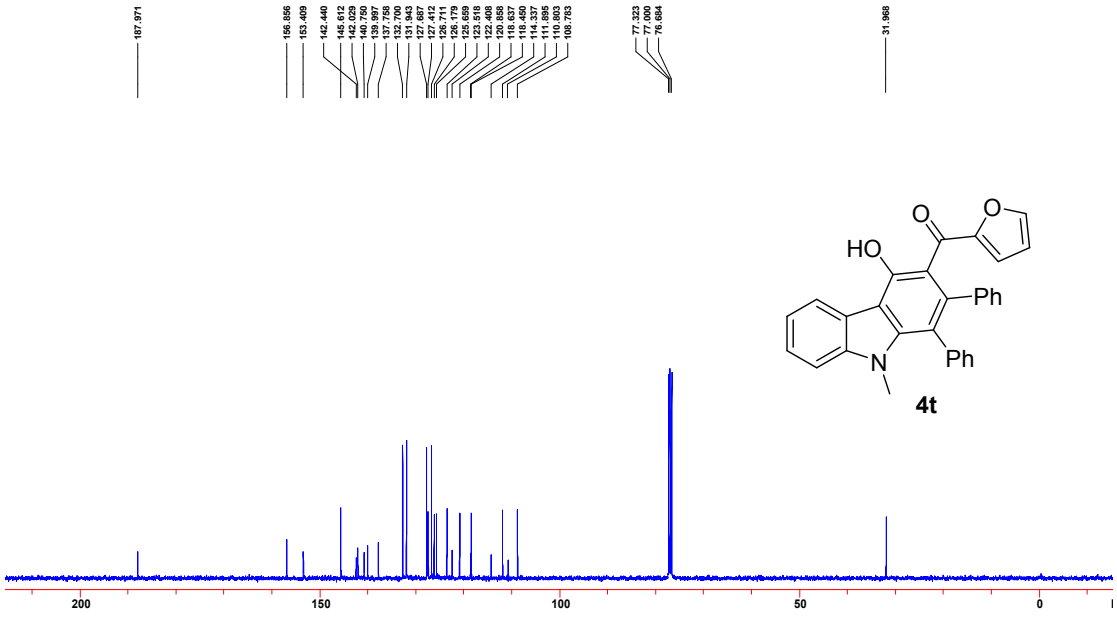
4t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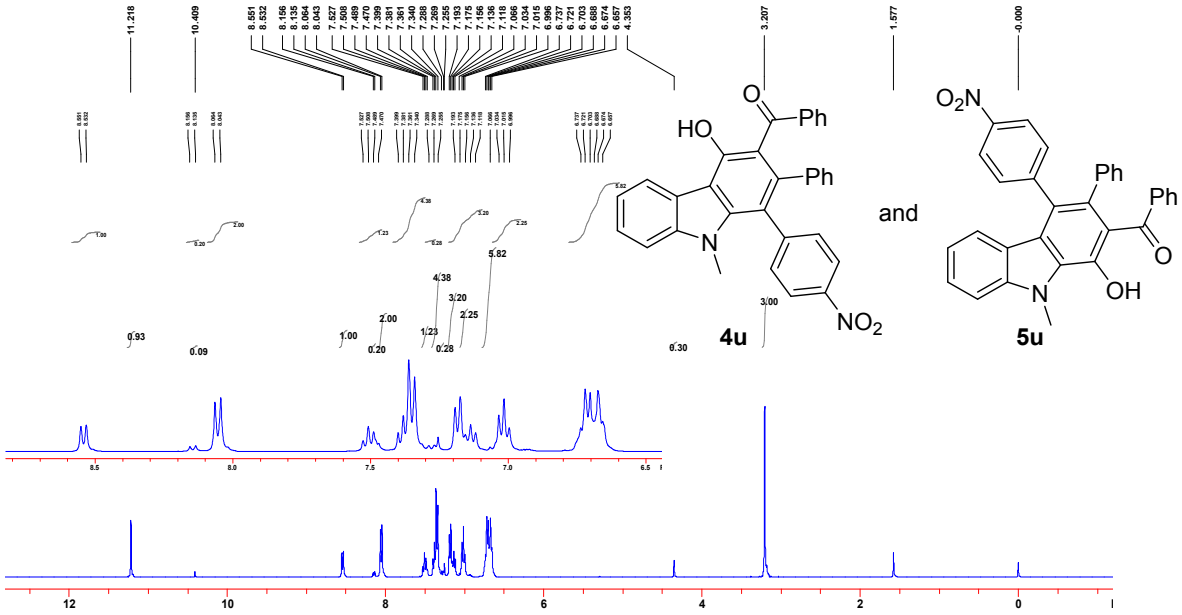
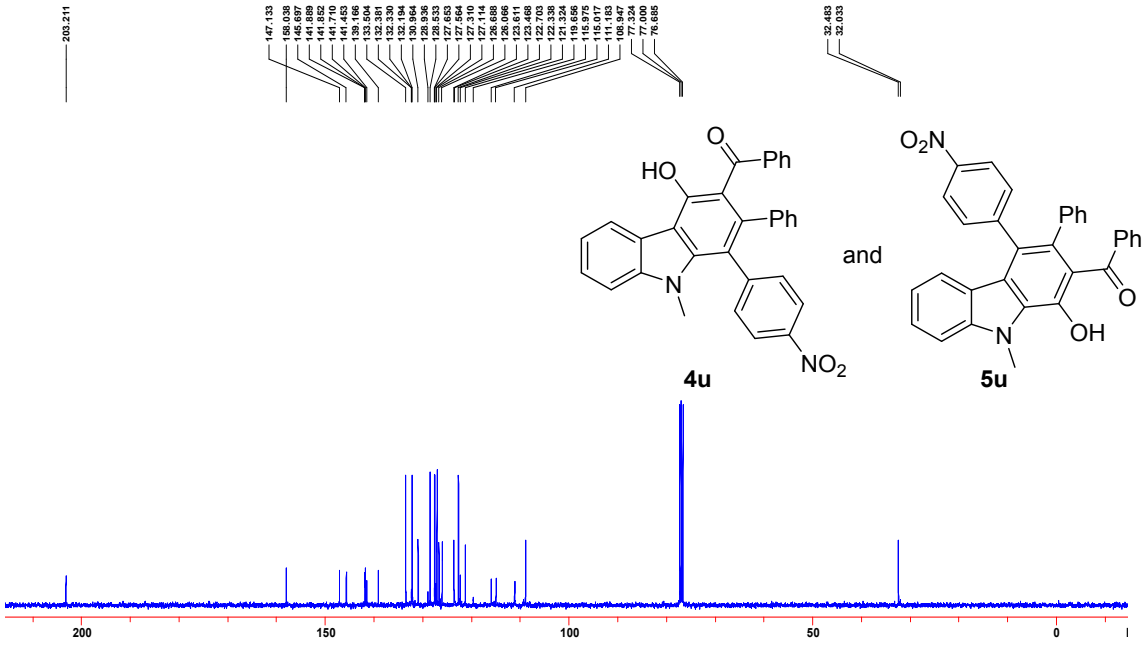
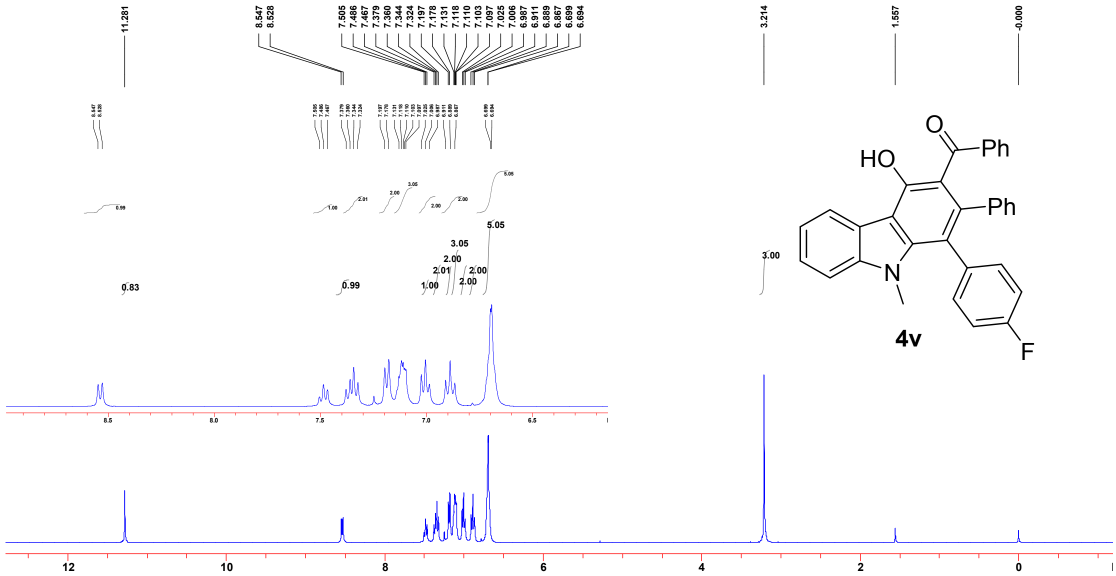
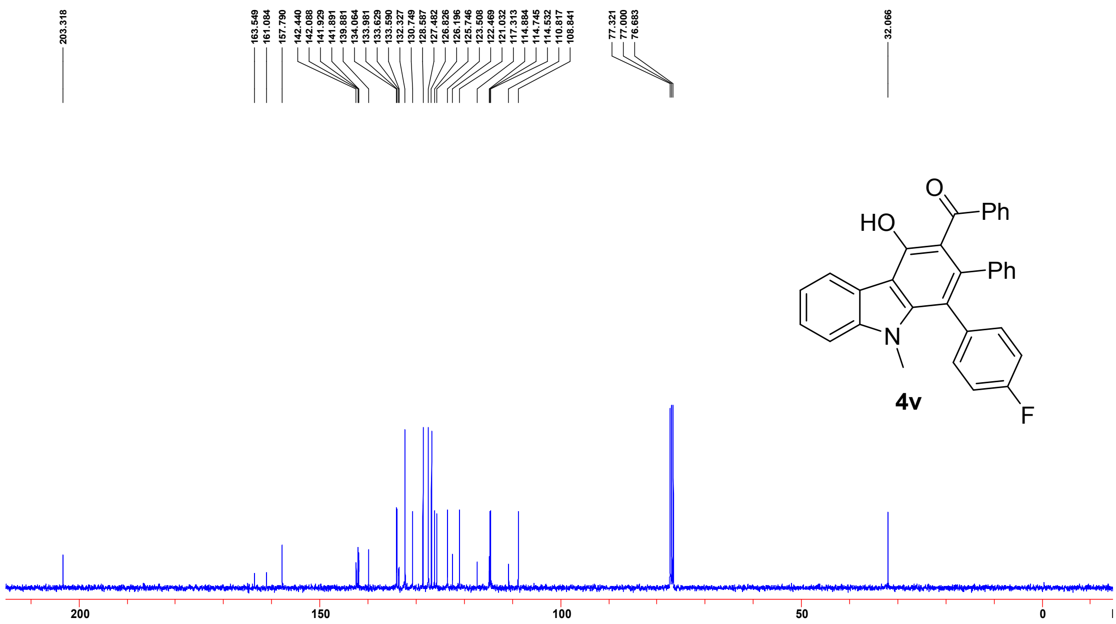
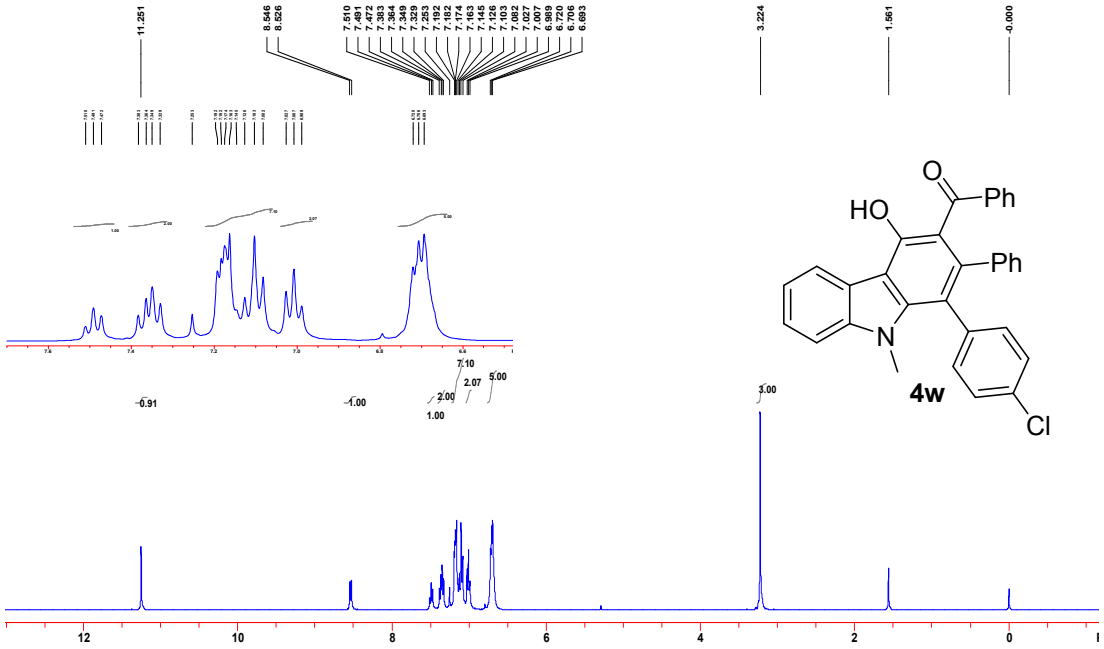
N
4t


4u
and
5u


4u
and
5u



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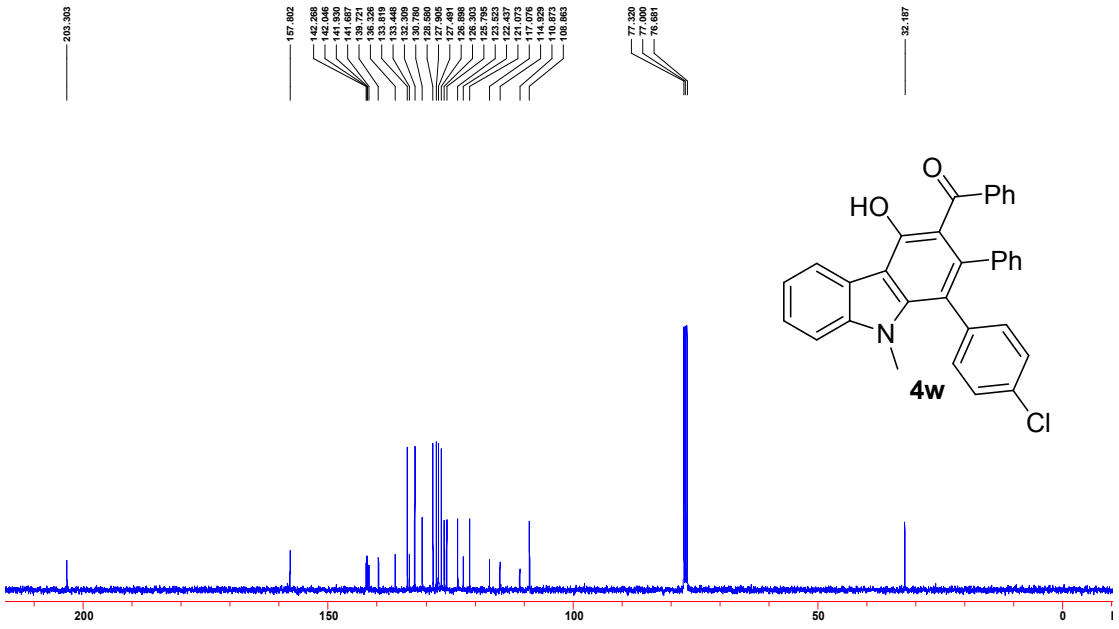
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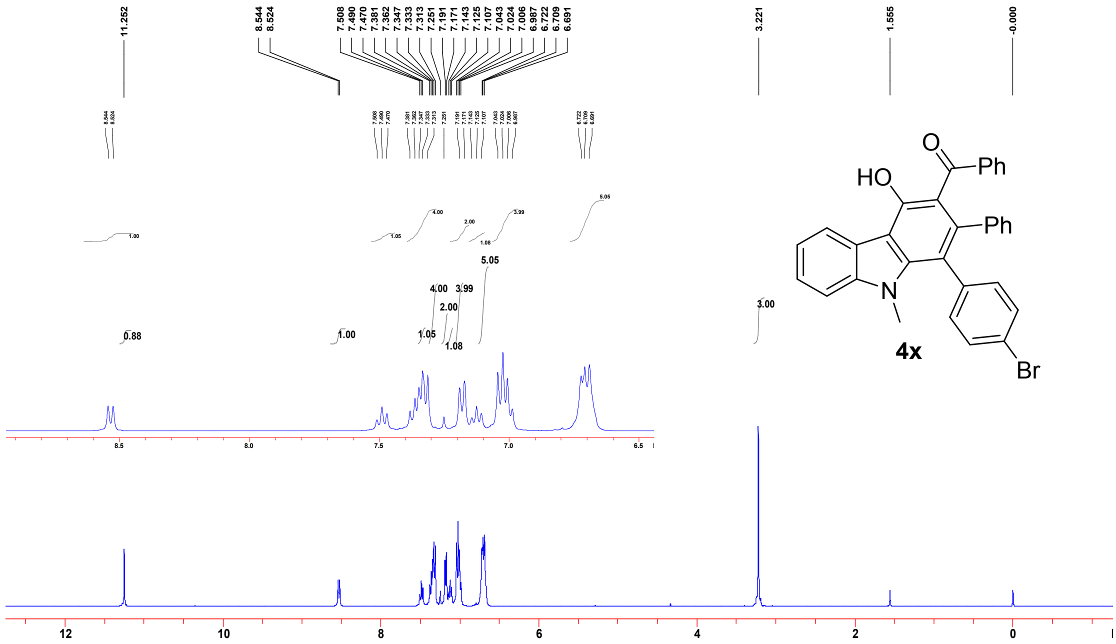

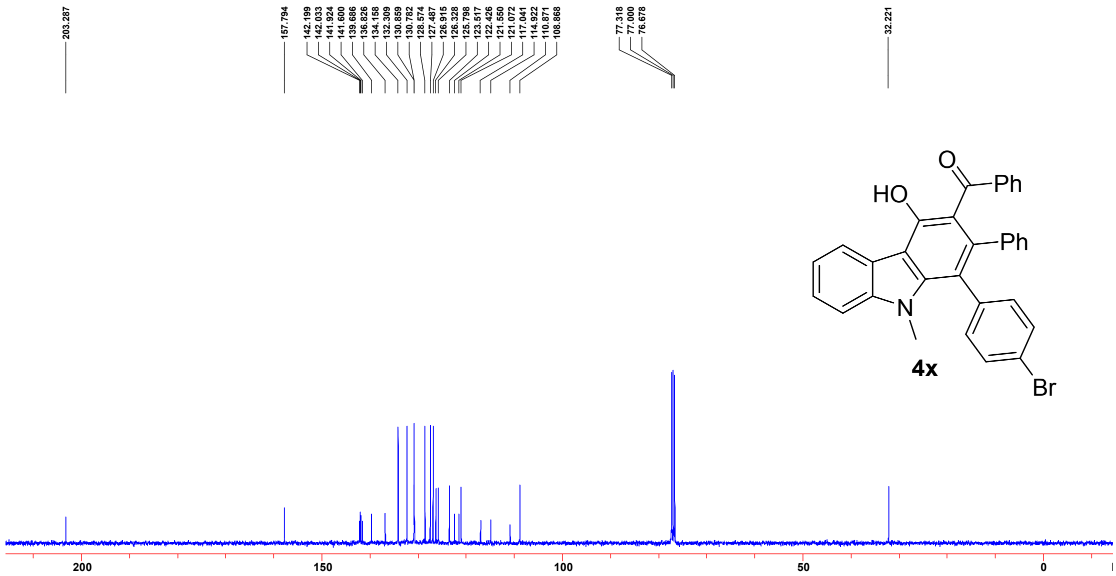

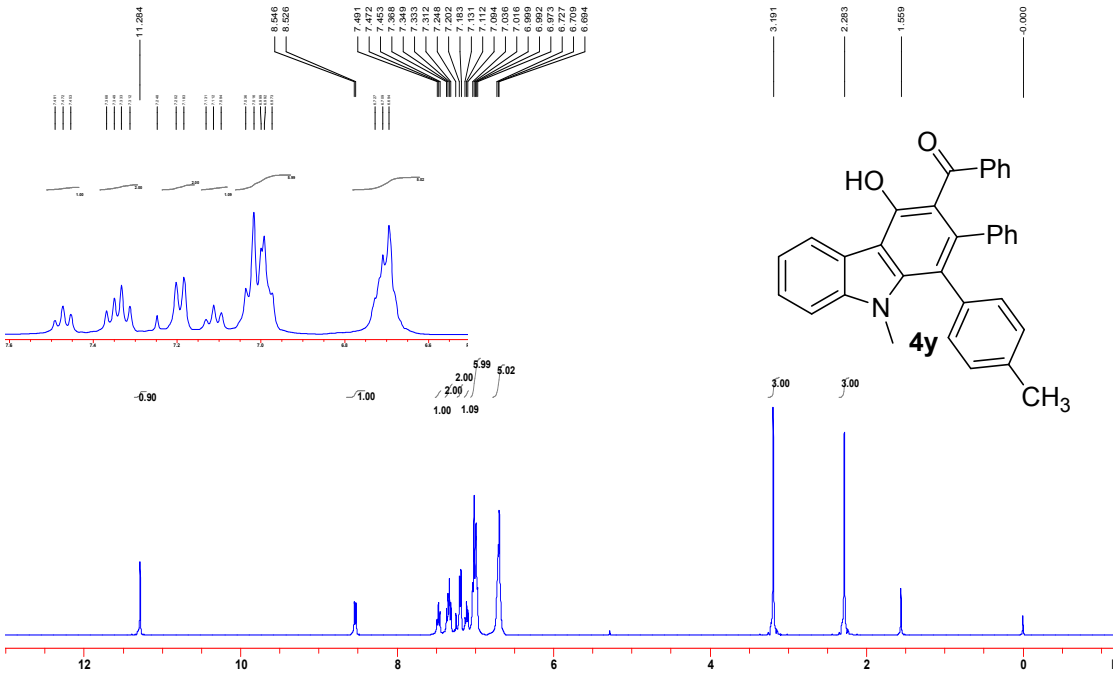
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6.694
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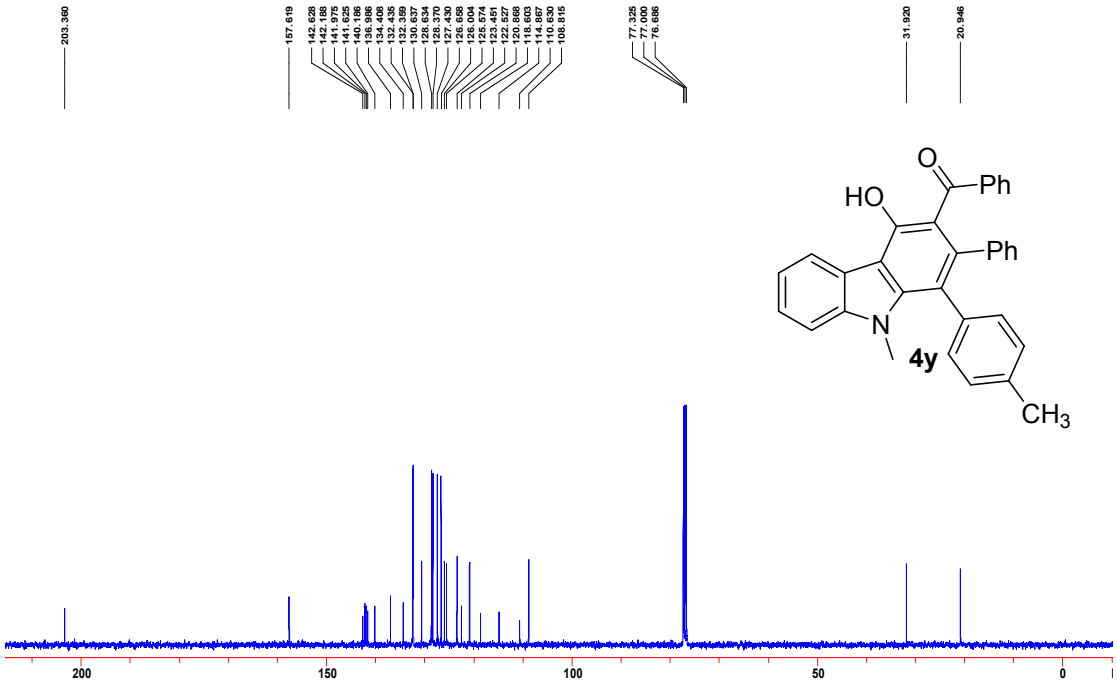
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123.451
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118.603
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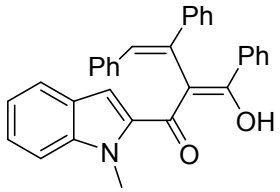
110.630
108.815
77.325
77.000
76.686
31.920
20.946
O
Ph
HO
Ph
N
4y
CH3
200
150
100
50
0

8. X-ray crystallography of compounds 3a

(2*Z*,3*Z*)-2-(Hydroxy(phenyl)methylene)-1-(1-methyl-1*H*-indol-2-yl)-3,4-diphenylbut-3-en-1-one (3a, d8v17780)

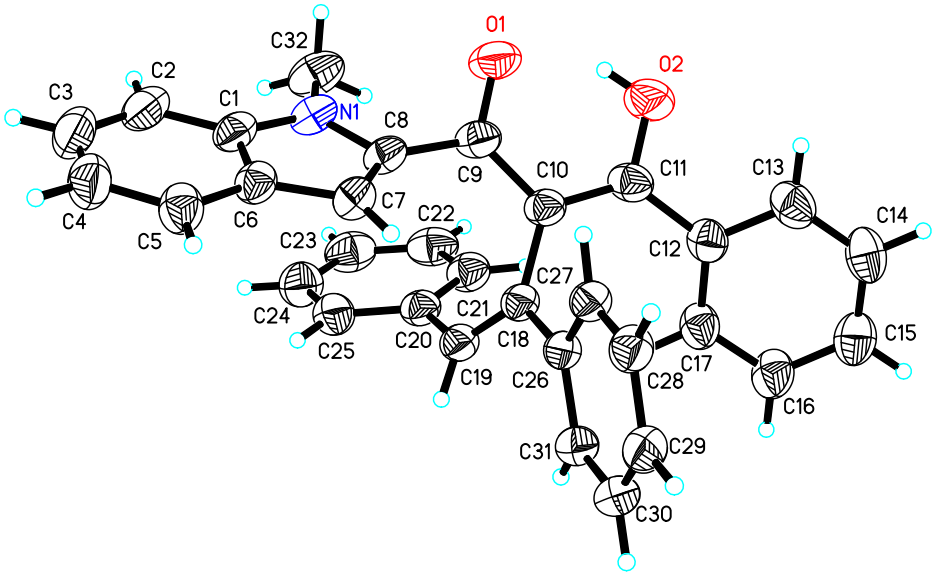
(Ortep ellipsoids are depicted at the 50% level)



3a

Table 1. Crystal data and structure refinement for **3a**

Identification code	**3a**
Empirical formula	$C_{32}H_{25}NO_2$
Formula weight	455.53
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 12.5424(4) Å α= 90°. b = 9.1677(3) Å β= 104.0200(10)°. c = 22.0679(8) Å γ = 90°.
Volume	2461.89(14) $Å^3$
Z, Calculated density	4, 1.229 Mg/m^3
Absorption coefficient	0.076 mm^{-1}
F(000)	960
Crystal size	0.180 x 0.150 x 0.120 mm^3
Theta range for data collection	2.806 to 26.000°.
Index ranges	-15<=h<=15, -11<=k<=11, -27<=l<=27
Reflections collected / Independent reflections	34826/4819 [R(int) = 0.0496]
Completeness to theta = 25.242°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6920
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4819 / 0 / 319
Goodness-of-fit on F^2	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0469, wR2 = 0.1130
R indices (all data)	R1 = 0.0710, wR2 = 0.1329
Extinction coefficient	0.054(4)
Largest diff. peak and hole	0.155 and -0.155 $e.Å^{-3}$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O2
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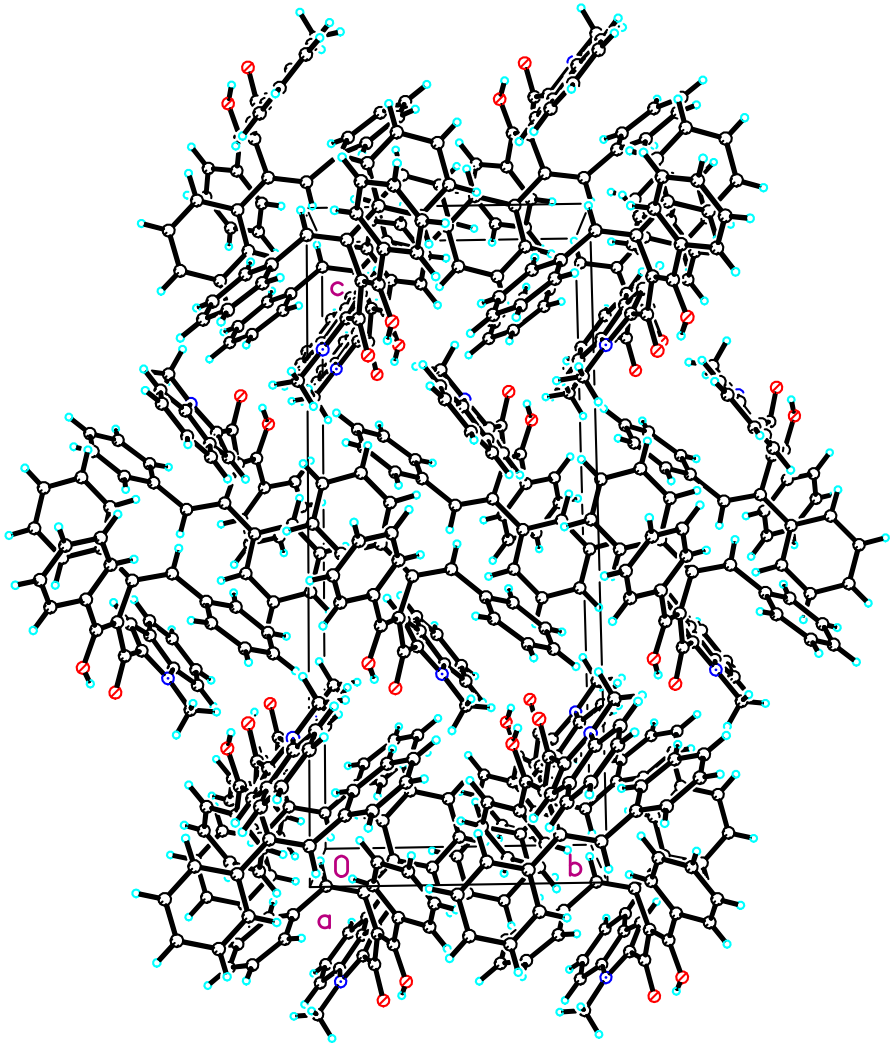
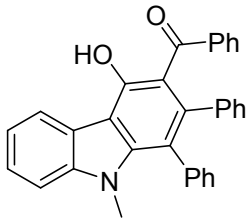
C2
C3
C1
N1
C8
C9
C10
C11
C13
C14
C4
C5
C6
C7
C22
C23
C12
C27
C24
C21
C18
C15
C25
C20
C19
C26
C28
C17
C16
C31
C29
C30


c
0
b
a

9. X-ray crystallography of compounds 4a

(4-Hydroxy-9-methyl-1,2-diphenyl-9*H*-carbazol-3-yl)(phenyl)methanone (4a, dm17402)

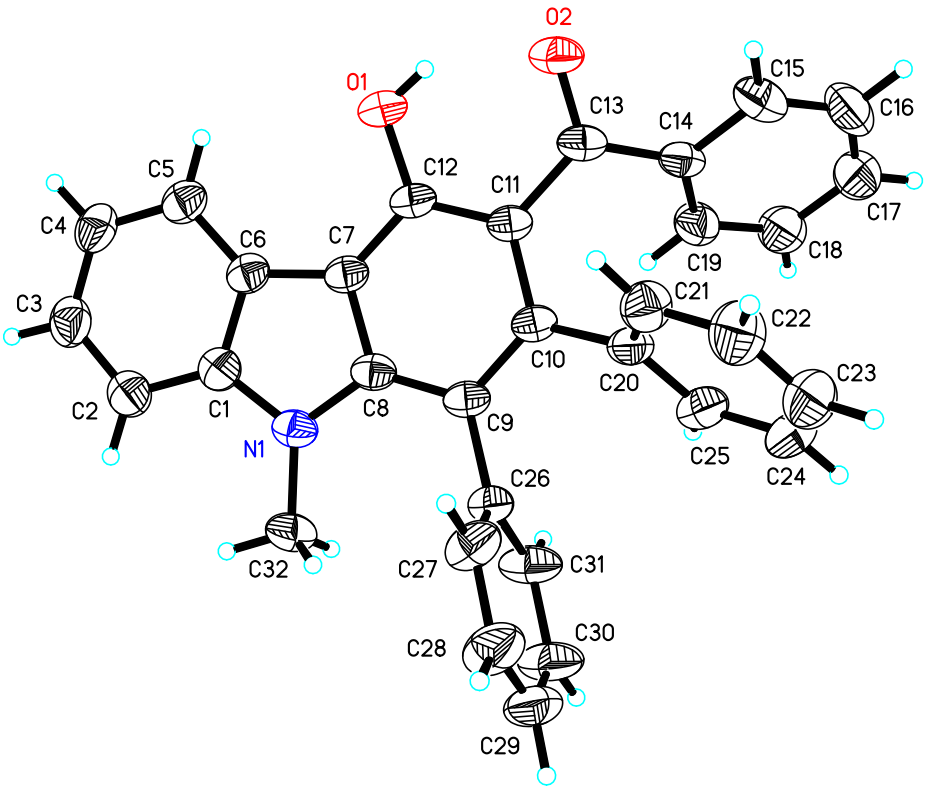
(Ortep ellipsoids are depicted at the 50% level)

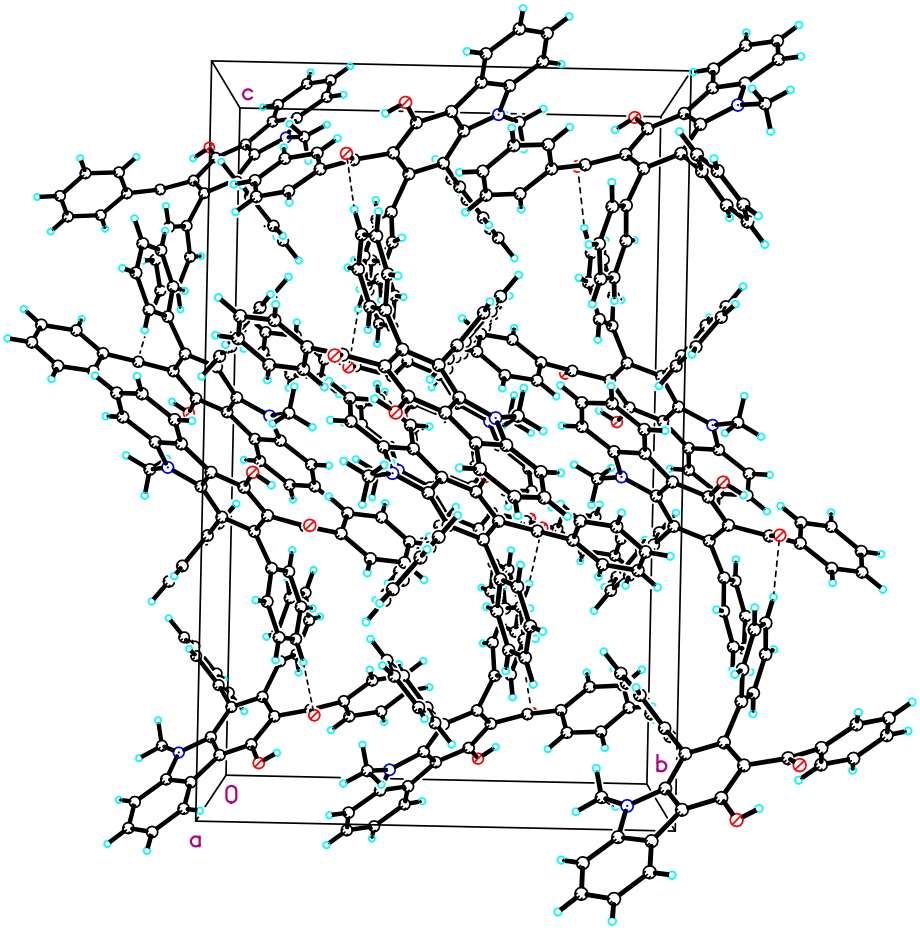


4a

Table 1. Crystal data and structure refinement for **4a**

Identification code	**4a**
Empirical formula	$C_{32}H_{23}NO_2$
Formula weight	453.51
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P b c a
Unit cell dimensions	a = 12.2322(13) Å α= 90°. b = 15.6754(16) Å β= 90°. c = 24.857(3) Å γ = 90°.
Volume	4766.3(9) $Å^3$
Z, Calculated density	8, 1.264 Mg/m^3
Absorption coefficient	0.078 mm^{-1}
F(000)	1904
Crystal size	0.200 x 0.160 x 0.120 mm^3
Theta range for data collection	1.638 to 25.500°.
Index ranges	-14<=h<=13, -18<=k<=18, -30<=l<=25
Reflections collected / Independent reflections	31644/4435 [R(int) = 0.0459]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6302
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4435 / 0 / 319
Goodness-of-fit on F^2	1.085
Final R indices [I>2sigma(I)]	R1 = 0.0428, wR2 = 0.1055
R indices (all data)	R1 = 0.0840, wR2 = 0.1384
Extinction coefficient	0.0017(4)
Largest diff. peak and hole	0.149 and -0.127 $e.Å^{-3}$

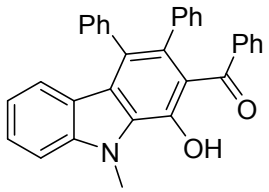

O2
O1
C13
C15
C16
C14
C5
C12
C11
C17
C4
C6
C7
C19
C18
C21
C3
C22
C10
C20
C23
C2
C1
C8
C9
N1
C25
C24
C26
C32
C27
C31
C28
C30
C29


c
b
0
a

10. X-ray crystallography of compounds 5a

(1-Hydroxy-9-methyl-3,4-diphenyl-9*H*-carbazol-2-yl)(phenyl)methanone (5a, cd17369)

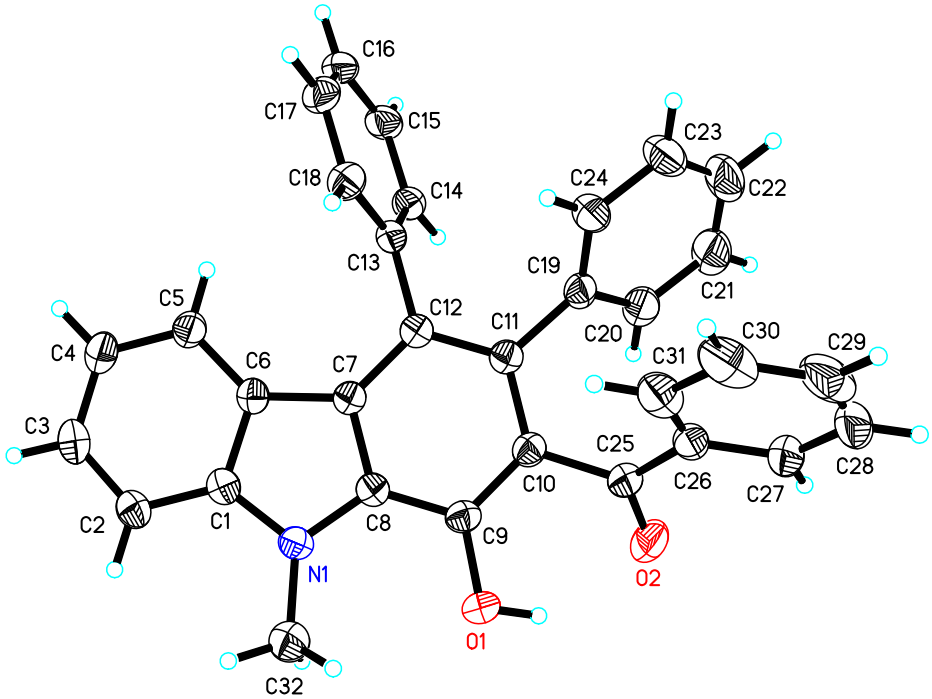
(Ortep ellipsoids are depicted at the 50% level)



5a

Table 1. Crystal data and structure refinement for **5a**

Identification code	**5a**
Empirical formula	$C_{32}H_{23}NO_2$
Formula weight	453.51
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 12.3437(14) Å α= 90°. b = 8.8269(10) Å β= 90.191(3)°. c = 21.695(2) Å γ = 90°.
Volume	2363.9(5) $Å^3$
Z, Calculated density	4, 1.274 Mg/m^3
Absorption coefficient	0.079 mm^{-1}
F(000)	952
Crystal size	0.200 x 0.160 x 0.130 mm^3
Theta range for data collection	1.877 to 25.499°.
Index ranges	-14<=h<=14, -9<=k<=10, -23<=l<=26
Reflections collected / Independent reflections	13191/4395 [R(int) = 0.0361]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6622
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4395 / 0 / 321
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0447, wR2 = 0.1131
R indices (all data)	R1 = 0.0655, wR2 = 0.1259
Extinction coefficient	n/a
Largest diff. peak and hole	0.171 and -0.174 $e.Å^{-3}$


C16
C17
C15
C18
C14
C13
C12
C11
C19
C20
C21
C22
C23
C24
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C4
C6
C7
C3
C2
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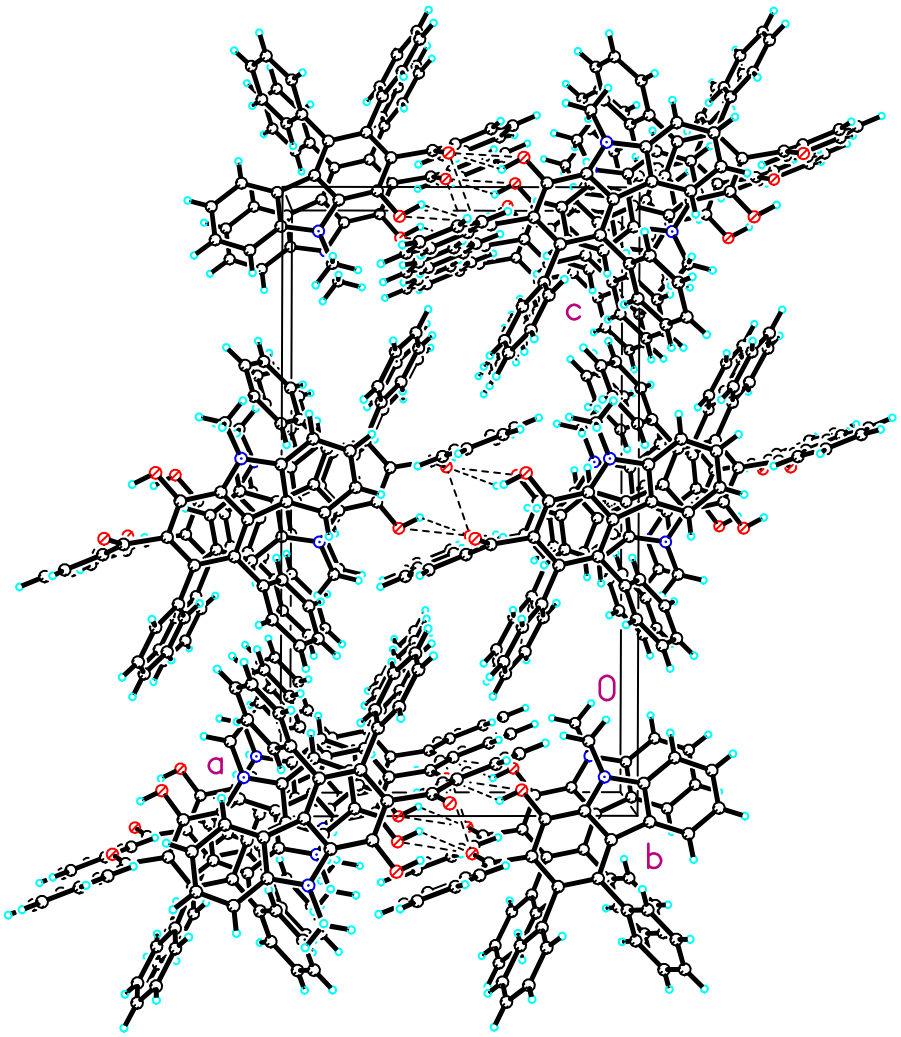
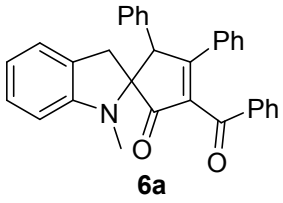
C28
C29
C30
C31
N1
O1
O2
C32


c
0
a
b

11. X-ray crystallography of compounds 6a

3-Benzoyl-1'-methyl-4,5-diphenylspiro[cyclopentane-1,2'-indolin]-3-en-2-one (6a, d8v17687)

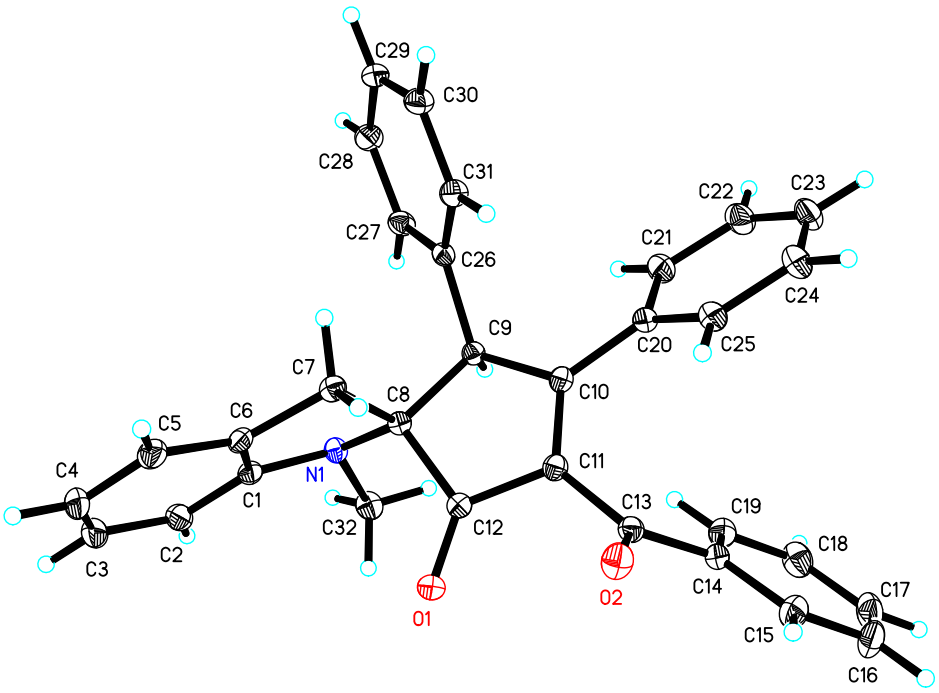
(Ortep ellipsoids are depicted at the 50% level)



6a

Table 1. Crystal data and structure refinement for **6a**

Identification code	**6a**
Empirical formula	$C_{32}H_{25}NO_2$
Formula weight	455.53
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 13.1322(4) Å α= 90°. b = 18.0792(5) Å β= 102.6540(10)°. c = 11.7504(3) Å γ = 90°.
Volume	2722.01(13) $Å^3$
Z, Calculated density	4, 1.112 Mg/m^3
Absorption coefficient	0.069 mm^{-1}
F(000)	960
Crystal size	0.200 x 0.170 x 0.130 mm^3
Theta range for data collection	2.103 to 25.999°.
Index ranges	-16<=h<=16, -22<=k<=22, -13<=l<=14
Reflections collected / Independent reflections	43554/5345 [R(int) = 0.0455]
Completeness to theta = 25.242°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6554
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5345 / 0 / 318
Goodness-of-fit on F^2	1.061
Final R indices [I>2sigma(I)]	R1 = 0.0577, wR2 = 0.1729
R indices (all data)	R1 = 0.0668, wR2 = 0.1802
Extinction coefficient	0.015(2)
Largest diff. peak and hole	0.466 and -0.294 e.$Å^{-3}$


C29
C30
C28
C31
C27
C26
C22
C23
C21
C24
C9
C20
C25
C7
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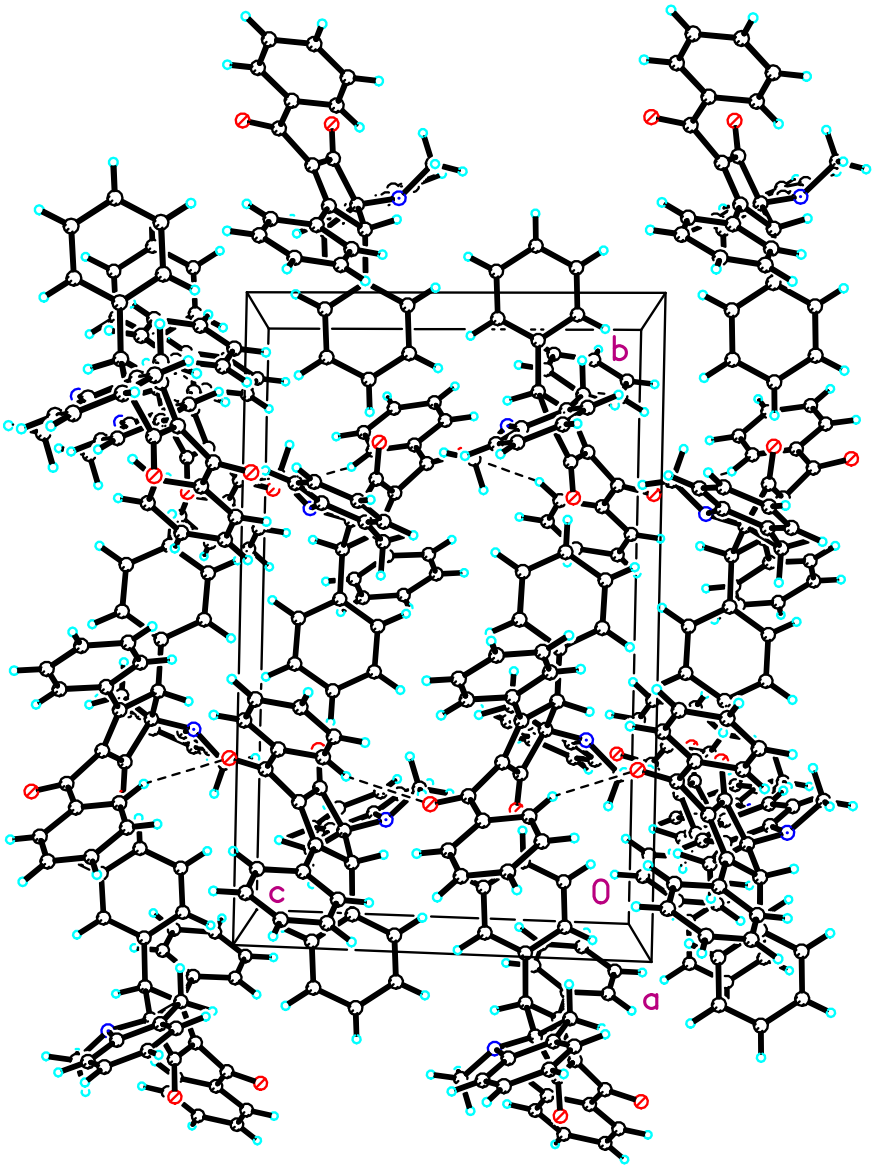
C10
C5
C6
C4
N1
C11
C1
C32
C12
C13
C19
C18
C2
C3
O1
O2
C14
C17
C15
C16


b
c
0
a