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Supplementary information

Facile Access to 2,2-Diaryl 2H-Chromenes through a Palladium-Catalyzed Cascade Reaction of *ortho*-Vinyl Bromobenzenes with *N*-Tosylhydrazones

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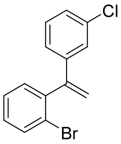
General information

Unless otherwise indicated, all glassware was oven dried by a heat gun before use and all reactions were performed under an atmosphere of Argon. All solvents were distilled from appropriate drying agents prior to use. All reagents were used as received from commercial suppliers unless otherwise stated. *N*-tosylhydrazones were prepared according to the procedures reported in the literature.[1,2] Reaction progress was monitored by thin layer chromatography (TLC). Visualization was achieved by ultraviolet light (254 nm). Pressed KBr Disks for infra-red spectra were recorded using a Bruker-VERTEX 70 FT-IR spectrometer. Wavelengths (ν) are reported in cm^{-1}. All ^{1}H NMR, ^{13}C NMR spectra were recorded on Bruker AV-III 400 in $CDCl_3$. Chemical shifts were given in parts per million (ppm, δ), referenced to the peak of tetramethylsilane, defined at $\delta = 0.00$ (^{1}H NMR), or the solvent peak of $CDCl_3$, defined at $\delta = 77.0$ (^{13}C NMR); the peak of DMSO-d_6, defined at $\delta = 2.50$ (^{1}H NMR), defined at $\delta = 40.0$ (^{13}C NMR). Coupling constants were quoted in Hz (*J*). ^{1}H NMR Spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t), quartet (q), pentet (p), septet (se), octet (o). Splitting patterns that could not be interpreted or easily visualized were designated as multiplet (m) or broad (br). High resolution mass spectra were measured on Thermo Scientific LTQ Orbitrap XL or Waters Micromass GCT Premier.

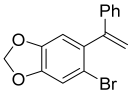
Preparation of *ortho*-vinyl bromobenzenes

Ortho-vinyl bromobenzenes were prepared according to the known procedure.[3,4,5] The data of new compounds are described below.



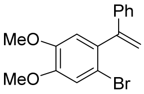
1-bromo-2-(1-(3-chlorophenyl)vinyl)benzene (1g)

Compound **1g** was obtained as a colorless oil; R_f = 0.45 (petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.57 (d, *J* = 8.0 Hz, 1H), 7.34-7.17 (m, 6H), 7.10 (d, *J* = 7.6 Hz, 1H), 5.81 (s, 1H), 5.29 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.8, 141.9, 141.5, 134.3, 133.0, 131.5, 129.5, 129.3, 127.7, 127.4, 126.6, 124.8, 123.2, 117.3; IR (KBr) ν 3090, 3062, 1594, 1564, 1474, 1317, 1025 cm^{-1}; HRMS (EI): m/z Exact mass calcd for $C_{14}H_{10}BrCl$ $[M]^+$: 291.9654, found: 291.9662.



5-bromo-6-(1-phenylvinyl)benzo[*d*][1,3]dioxole (1n)

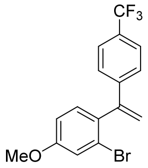
Compound **1n** was obtained as a white solid; R_f = 0.55 (petroleum ether : dichloromethane = 20 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.28-7.23 (m, 5H), 7.04 (s, 1H), 6.78 (s, 1H), 5.99 (s, 2H), 5.80 (s, 1H), 5.23 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.6, 147.8, 147.2, 139.6, 135.7, 128.3, 127.7, 126.5, 116.2, 113.8, 112.9, 111.2, 101.8; IR (KBr) ν 1497, 1472, 1223, 1038, 871, 784 cm^{-1}; HRMS (EI): m/z Exact mass calcd for $C_{15}H_{11}BrO_2$ $[M]^+$: 301.9942, found: 301.9937.



1-bromo-4,5-dimethoxy-2-(1-phenylvinyl)benzene (1o)

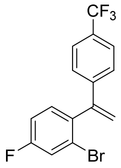
Compound **1o** was obtained as a white solid; R_f = 0.51 (petroleum ether : dichloromethane = 20 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.29-7.26 (m, 5H), 7.06

(s, 1H), 6.80 (s, 1H), 5.83 (s, 1H), 5.26 (s, 1H), 3.89 (s, 3H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.8, 148.6, 148.1, 139.6, 134.6, 128.3, 127.7, 126.5, 116.0, 115.5, 114.0, 113.3, 56.1, 56.0; IR (KBr) ν 3072, 1592, 1500 1438, 1206, 780 cm^{-1}; HRMS (EI): m/z Exact mass calcd for $C_{16}H_{15}BrO$ [M]$^+$: 318.0255, found: 318.0261.



2-bromo-4-methoxy-1-(1-(4-(trifluoromethyl)phenyl)vinyl)benzene (1p)

Compound **1p** was obtained as a colorless oil; R_f = 0.65 (petroleum ether : dichloromethane = 50 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 1H), 7.15 (d, *J* = 2.4 Hz, 1H), 6.90 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 5.85 (s, 1H), 5.36 (s, 1H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 147.6, 143.6, 134.0, 132.0, 129.5 (q, *J* = 32.8 Hz), 126.8, 125.2 (q, *J* = 3.75 Hz), 124.2 (q, *J* = 270 Hz), 123.5, 118.23, 118.18, 113.5, 55.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.39 (s); IR (KBr) ν 1599, 1492, 1325, 1225, 1120 cm^{-1}; HRMS (EI): m/z Exact mass calcd for $C_{16}H_{12}BrF_3O$ [M]$^+$: 356.0024, found: 318.0018.

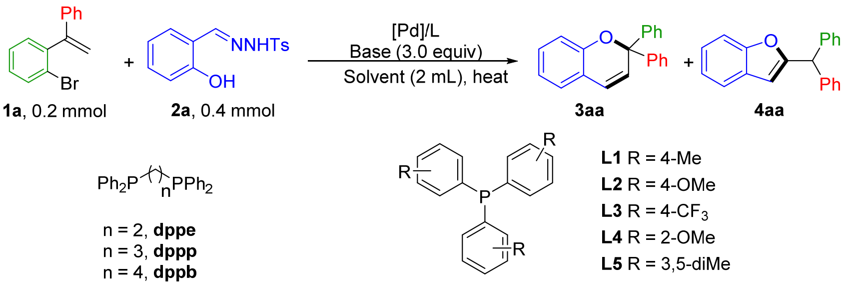


2-bromo-4-fluoro-1-(1-(4-(trifluoromethyl)phenyl)vinyl)benzene (1q)

Compound **1q** was obtained as a colorless oil; R_f = 0.35 (petroleum ether); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.55 (d, *J* = 8.4 Hz, 2H), 7.36-7.27 (m, 4H), 7.08 (td, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 5.89 (s, 1H), 5.37 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.0 (d, *J* = 249.9 Hz), 147.1, 143.0, 138.0 (d, *J* = 3.6 Hz), 132.4 (d, *J* = 8.3 Hz), 129.8 (q, *J* = 32.2

Hz), 126.8, 125.4 (q, *J* = 3.7 Hz), 124.2 (q, *J* = 270.4 Hz), 123.4 (d, *J* = 9.5 Hz), 123.5, 120.4 (d, *J* = 24.3 Hz), 114.7 (d, *J* = 20.8 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.50 (s), -112.1-112.2 (m); IR (KBr) ν 1675, 1592, 1328, 1325, 1067, 935, 855 cm^{-1}; HRMS (EI): m/z Exact mass calcd for $C_{15}H_9F_4$ $[M]^+$: 343.9824, found: 343.9831.

Optimization of reaction conditions for 2*H*-chromene synthesis[a]



1a, 0.2 mmol + **2a**, 0.4 mmol → **3aa** + **4aa**

n = 2, **dppe**
n = 3, **dppp**
n = 4, **dppb**

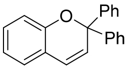
L1 R = 4-Me
L2 R = 4-OMe
L3 R = 4-CF_3
L4 R = 2-OMe
L5 R = 3,5-diMe

Entry	[Pd]/L	T/°C	Solvent	Base	[%][b]		
					1a	**3aa**	**4aa**
1	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **dppb**	110	THF	K_2CO_3	16	51(46)[c]	3
2	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **dppe**	110	THF	K_2CO_3	21	25	1
3	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **dppp**	110	THF	K_2CO_3	43	15	<1
4	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **PPh_3**	110	THF	K_2CO_3	34	29	<1
5	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **L1**	110	THF	K_2CO_3	32	35	<1
6	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **L2**	110	THF	K_2CO_3	23	38	<1
7	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **L3**	110	THF	K_2CO_3	39	27	<1
8	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **L4**	110	THF	K_2CO_3	79	4	<1
9	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **L5**	110	THF	K_2CO_3	71	32	<1
10	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **dppb**	100	THF	K_2CO_3	27	50	3
11	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **dppb**	100	dioxane	K_2CO_3	13	36	<1
12	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **dppb**	100	toluene	K_2CO_3	79	8	<1
13	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **dppb**	100	2-MeTHF	K_2CO_3	35	52	3
14[d]	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **dppb**	100	2-MeTHF	K_2CO_3	11	43	3
15	5 mol% $[Pd(allyl)Cl]_2$/15 mol% **dppb**	100	2-MeTHF	K_2CO_3	0	87(79)[c,e]	8
16	5 mol% $[Pd(allyl)Cl]_2$/15 mol% **dppb**	100	2-MeTHF	Na_2CO_3	62	6	<1
17	5 mol% $[Pd(allyl)Cl]_2$/15 mol% **dppb**	100	2-MeTHF	^tBuOLi	0	0	0
18	5 mol% $[Pd(allyl)Cl]_2$/15 mol% **dppb**	100	2-MeTHF	CsF	16	36	<1
19	5 mol% $[Pd(allyl)Cl]_2$/15 mol% **dppb**	100	2-MeTHF	K_3PO_4	0	68	<1
20	10 mol% $Pd(OAc)_2$/15 mol% **dppb**	100	2-MeTHF	K_2CO_3	0	59	2
21	10 mol% $Pd(MeCN)_2Cl_2$/15 mol% **dppb**	100	2-MeTHF	K_2CO_3	0	57	2
22	5 mol% $Pd_2dba_3{\cdot}CHCl_3$/15 mol% **dppb**	100	2-MeTHF	K_2CO_3	61	21	<1
23	5 mol% $[Pd(cinnamyl)Cl]_2$/15 mol% **dppb**	100	2-MeTHF	K_2CO_3	0	79(78)[c,e]	2
24[f]	5 mol% $[Pd(allyl)Cl]_2$/15 mol% **dppb**	100	2-MeTHF	K_2CO_3	0	19[c]	<1
25	15 mol% **dppb**	100	2-MeTHF	K_2CO_3		0	0
26	5 mol% $[Pd(allyl)Cl]_2$	100	2-MeTHF	K_2CO_3		0	0
27	5 mol% $[Pd(allyl)Cl]_2$/15 mol% **dppb**	100	2-MeTHF			0	0

[a] The reaction was carried out for 20 h. [b] Yields were determined by ^{1}H NMR using *N*,*N*-dimethylpyridin-4-amine as an internal standard. [c] yield of isolated product. [d] TBAB (0.02 mmol) was added. [e] The reaction was complete in 6 h. [f] Replaced bromine with iodine.

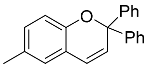
General procedure for the synthesis of 2,2-disubstituted 2*H*-Chromenes

An oven-dried Schlenk tube under argon atmosphere was charged with *ortho*-vinyl bromobenzenes **1** (0.2 mmol, 1.0 equiv), *N*-tosylhydrazones **2** (0.4 mmol, 2.0 equiv), $[Pd(allyl)Cl]_2$ or $[Pd(cinnamyl)Cl]_2$ (5.0 mol% or 10.0 mol%), dppb (15 mol% or 30 mol%), K_2CO_3 (0.60 mmol, 3.0 equiv), and 2-MeTHF (2 mL). The mixture was stirred at 100 °C and the progress of the reaction was monitored by TLC. Upon completion, the resulting mixture was cooled to room temperature and filtered through Celite with EtOAc as the eluent. The solvents were evaporated under reduced pressure and the residue was purified by column chromatography on silica gel to afford the products.



2,2-diphenyl-2*H*-chromene (3aa)

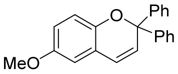
Compound **3aa** was obtained as a white solid, 45.0 mg, in 79% yield; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.42 (d, *J* = 7.8 Hz, 4H), 7.30 (t, *J* = 7.2 Hz, 4H), 7.25-7.21 (m, 2H), 6.98 (d, *J* = 7.2 Hz, 1H), 6.91 (d, *J* = 8.0 Hz, 1H), 6.82 (t, *J* = 7.8 Hz, 1H), 6.59 (d, *J* = 10.0 Hz, 1H), 6.15 (d, *J* = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 144.9, 129.5, 128.8, 128.1, 127.5, 127.0, 126.5, 123.3, 121.1, 121.0, 116.5, 82.5. Spectroscopic data were in accordance with literature values.[6]



6-methyl-2,2-diphenyl-2*H*-chromene (3ab)

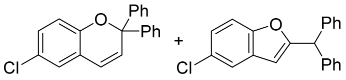
Compound **3ab** was obtained as a yellow solid, 39.0 mg, in 65% yield; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.43-7.41 (m, 4H), 7.30 (t, *J* = 7.2 Hz, 4H), 7.25-7.21 (m, 2H), 6.91 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 6.82-6.79 (m, 2H), 6.56 (d, *J* = 9.6 Hz, 1H), 6.14

(d, J = 10.0 Hz, 1H), 2.20 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.3, 145.0, 130.3, 130.0, 128.9, 128.1, 127.4, 127.0, 123.5, 120.8, 116.2, 82.4, 20.5 (the peak of the quaternary carbon does not appear). Spectroscopic data were in accordance with literature values.[7]



6-methoxy-2,2-diphenyl-2*H*-chromene (3ac)

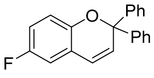
Compound **3ac** was obtained as a white solid, 46.0 mg, in 73% yield; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.42 (d, J = 7.2 Hz, 4H), 7.30 (t, J = 7.6 Hz, 4H), 7.25-7.22 (m, 2H), 6.85 (d, J = 8.8 Hz, 1H), 6.66 (dd, J_1 = 8.8 Hz, J_2 = 2.8 Hz, 1H), 6.58-6.55 (m, 2H), 6.20 (d, J = 9.6 Hz, 1H), 3.70 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.9, 146.4, 144.8, 129.9, 128.1, 127.4, 127.0, 123.5, 121.7, 117.1, 114.7, 111.5, 82.3, 55.6. Spectroscopic data were in accordance with literature values.[6]



3ad 4ad

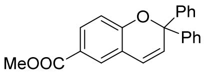
6-chloro-2,2-diphenyl-2*H*-chromene (3ad) and 2-benzhydryl-5-chlorobenzofuran (4ad)

The mixture of **3ad** and **4ad** (97/3) was obtained as a yellow solid, 40.9 mg, in 64% yield; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.41-7.38 (m, 4H), 7.32 (t, J = 7.2 Hz, 4H), 7.28-7.25 (m, 2H), 7.05 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 6.98 (d, J = 2.4 Hz, 1H), 6.84 (d, J = 8.4 Hz, 1H), 6.55 (d, J = 9.6 Hz, 1H), 6.21 (d, J = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.0, 144.3, 130.2, 129.1, 128.2, 127.7, 126.9, 126.1, 125.9, 122.8, 122.41, 117.8, 82.8. Spectroscopic data were in accordance with literature values.[6]



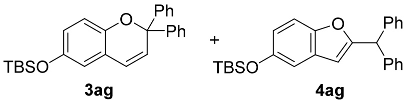
6-fluoro-2,2-diphenyl-2*H*-chromene (3ae)

Compound **3ae** was obtained as a light yellow solid, 33.0 mg, in 55% yield; ^{1}H NMR (400 MHz, CDCl$_3$, TMS) δ 7.40 (d, *J* = 7.2 Hz, 4H), 7.31 (t, *J* = 7.2 Hz, 4H), 7.27-7.23 (m, 2H), 6.86-6.76 (m, 2H), 6.71 (dd, J_1 = 8.4 Hz, J_2 = 2.8 Hz, 1H), 6.55 (d, *J* = 10.0 Hz, 1H), 6.22 (d, *J* = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 157.3 (d, *J* = 236.8 Hz), 148.3 (d, *J* = 2.1 Hz), 144.4, 130.4, 128.1, 127.6, 127.0, 122.8 (d, *J* = 2.1 Hz), 122.0 (d, *J* = 8.4 Hz), 117.4 (d, *J* = 8.1 Hz), 115.6 (d, *J* = 23.2 Hz), 112.6 (d, *J* = 23.7 Hz), 82.6; ^{19}F NMR (376 MHz, CDCl$_3$) δ -123.0. Spectroscopic data were in accordance with literature values.[8]



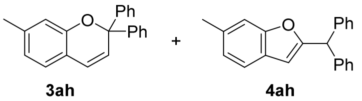
methyl 2,2-diphenyl-2*H*-chromene-6-carboxylate (3af)

Compound **3af** was obtained as a white solid, 32.5 mg, in 48% yield; R$_f$ = 0.62 (petroleum ether : ethyl acetate = 5 : 1) ; ^{1}H NMR (400 MHz, CDCl$_3$, TMS) δ 7.83 (dd, J_1 = 8.8 Hz, J_2 = 2.0 Hz, 1H), 7.72 (d, *J* = 2.0 Hz, 1H), 7.41-7.39 (m, 4H), 7.34-7.31 (m, 4H), 7.28-7.25 (m, 2H), 6.93 (d, *J* = 8.4 Hz, 1H), 6.64 (d, *J* = 10.0 Hz, 1H), 6.20 (d, *J* = 10.0 Hz, 1H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 166.6, 156.5, 144.3, 131.4, 129.2, 128.3, 128.2, 127.7, 126.9, 123.1, 122.7, 120.5, 116.4, 83.5, 51.9; IR (KBr) ν 1706, 1494, 1365, 1300, 986, 774 cm^{-1}; HRMS-(ESI) (m/z): [M+H]$^+$ calcd for $C_{23}H_{19}O_3$, 343.13287; found 343.13297.



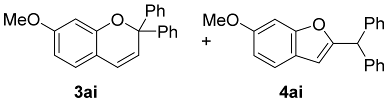
tert-butyl((2,2-diphenyl-2*H*-chromen-6-yl)oxy)dimethylsilane (3ag)

The mixture of **3ag** and **4ag** (95/5) was obtained as a white solid, 42.0 mg, in 51% yield;; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.27 (d, *J* = 7.6 Hz, 4H), 7.15 (t, *J* = 7.6 Hz, 4H), 7.11-7.07 (m, 2H), 6.63 (d, *J* = 8.8 Hz, 1H), 6.44 (dd, J_1 = 8.4 Hz, J_2 = 2.8 Hz, 1H), 6.38 (d, *J* = 9.6 Hz, 1H), 6.35 (d, *J* = 2.8 Hz, 1H), 6.02 (d, *J* = 10.0 Hz, 1H), 0.81 (s, 9H), 0.00 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.5, 146.8, 144.9, 129.5, 128.0, 127.4, 127.0, 123.5, 121.6, 120.6, 117.5, 117.0, 82.3, 25.7, 18.1, -4.5. Spectroscopic data were in accordance with literature values.[9]



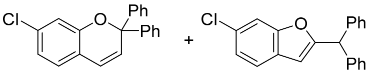
7-methyl-2,2-diphenyl-2*H*-chromene (3ah) and 2-benzhydryl-6-methylbenzofuran (4ah)

The mixture of **3ah** and **4ah** (96/4) was obtained as a light yellow solid, 35.0 mg, in 58% yield; R_f = 0.64 (petroleum ether : ethyl acetate = 100 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.42 (d, *J* = 7.2 Hz, 4H), 7.30 (t, *J* = 7.2 Hz, 4H), 7.25-7.20 (m, 2H), 6.87 (d, *J* = 7.8 Hz, 1H), 6.74 (s, 1H), 6.63 (d, *J* = 7.8 Hz, 1H), 6.57 (d, *J* = 9.6 Hz, 1H), 6.07 (d, *J* = 10.0 Hz, 1H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 145.1, 139.9, 128.1, 127.6, 127.4, 127.0, 126.3, 123.2, 121.9, 118.4, 117.0, 82.5, 21.5; IR (KBr) ν 1488, 1441, 1229, 985, 755, 703 cm^{-1}; HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{22}H_{19}O$, 299.14304; found 299.14343.



7-methoxy-2,2-diphenyl-2*H*-chromene (3ai) and 2-benzhydryl-6-methoxybenzofuran (4ai)

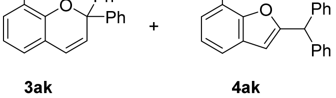
The mixture of **3ai** and **4ai** (90/10) was obtained as a white solid, 31.0 mg, in 50% yield; ^{1}H NMR (400 MHz, CDCl$_3$, TMS) δ 7.43-7.41 (m, 4H), 7.33-7.29 (m, 4H), 7.26-7.21 (m, 2H), 6.90 (d, *J* = 8.4 Hz, 1H), 6.55 (d, *J* = 10.0 Hz, 1H), 6.50 (d, *J* = 2.4 Hz, 1H), 6.39 (dd, J_1 = 8.0 Hz, J_2 = 2.4 Hz, 1H), 6.01 (d, *J* = 10.0 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 160.9, 153.7, 145.0, 128.1, 127.4, 127.2, 127.0, 125.9, 123.0, 114.4, 107.1, 102.1, 82.8, 55.3. Spectroscopic data were in accordance with literature values.[10]



3aj **4aj**

7-chloro-2,2-diphenyl-2*H*-chromene (3aj) and 2-benzhydryl-6-chlorobenzofuran (4aj)

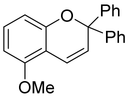
The mixture of **3aj** and **4aj** (92/8) was obtained as a yellow solid, 32.0 mg, in 50% yield; R_f = 0.66 (petroleum ether : ethyl acetate = 100 : 1); ^{1}H NMR (400 MHz, CDCl$_3$, TMS) δ 7.39 (d, *J* = 7.6 Hz, 4H), 7.31 (t, *J* = 7.2 Hz, 4H), 7.25 (t, *J* = 7.2 Hz, 2H), 6.92-6.89 (m, 2H), 6.80 (dd, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 6.56 (d, *J* = 10.0 Hz, 1H), 6.14 (d, *J* = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 153.1, 144.4, 134.3, 128.9, 128.8, 127.7, 127.2, 126.9, 122.5, 121.4, 119.6, 116.9, 83.0; IR (KBr) ν 1597, 1559, 1484, 1048, 988, 694 cm^{-1}; HRMS (EI): m/z Exact mass calcd for $C_{21}H_{15}ClO$ $[M]^+$: 318.0811, found: 318.0810.



3ak **4ak**

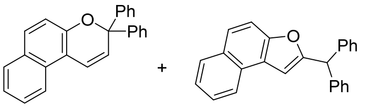
8-methyl-2,2-diphenyl-2*H*-chromene (3ak) and 2-benzhydryl-7-methylbenzofuran (4ak)

The mixture of **3ak** and **4ak** (94/6) was obtained as a light yellow oil, 34.0 mg, in 57% yield; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.44 (d, *J* = 7.6 Hz, 4H), 7.29 (t, *J* = 7.6 Hz, 4H), 7.22 (t, *J* = 6.8 Hz, 2H), 6.96 (d, *J* = 7.6 Hz, 1H), 6.84 (d, *J* = 7.2 Hz, 1H), 6.72 (t, *J* = 7.6 Hz, 1H), 6.59 (d, *J* = 10.0 Hz, 1H), 6.11 (d, *J* = 9.6 Hz, 1H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.4, 145.4, 130.9, 128.3, 128.0, 127.3, 126.8, 125.3, 124.2, 123.8, 120.60, 120.55, 82.4, 15.8. Spectroscopic data were in accordance with literature values.[6]



5-methoxy-2,2-diphenyl-2*H*-chromene (3al)

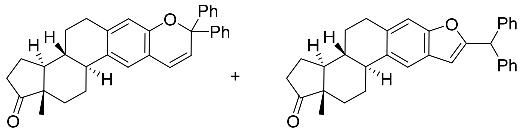
Compound **3al** was obtained as a white solid, 31.0 mg, in 50% yield; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.47-7.45 (m, 4H), 7.32-7.28 (m, 4H), 7.25-7.22 (m, 2H), 7.77-7.78 (m, 2H), 6.65-6.62 (m, 1H), 6.59 (d, *J* = 10.0 Hz, 1H), 6.23 (d, *J* = 10.0 Hz, 1H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.3, 144.7, 141.6, 129.4, 128.0, 127.4, 127.0, 123.4, 122.1, 120.9, 118.8, 112.9, 82.5, 56.3. Spectroscopic data were in accordance with literature values.[11]



3am **4am**

3,3-diphenyl-3*H*-benzo[*f*]chromene and 2-benzhydrylnaphtho[2,1-*b*]furan (3am) and 2-benzhydrylnaphtho[2,1-*b*]furan (4am)

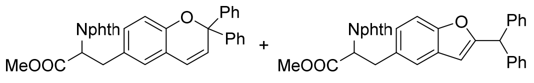
The mixture of **3am** and **4am** (1/2) was obtained as a yellow solid, 40.0 mg, in 60% yield. Spectroscopic data were in accordance with literature values.[12]



3an **4an**

(3aS,3bR,11bS,13aS)-13a-methyl-8,8-diphenyl-3,3a,3b,4,5,8,11b,12,13,13a-decahydrocyclopenta[5,6]naphtho[1,2-*g*]chromen-1(2*H*)-one (3an) and (3aS,3bR,10bS,12aS)-8-benzhydryl-12a-methyl-2,3,3a,3b,4,5,10b,11,12,12a-decahydro-1*H*-cyclopenta[7,8]phenanthro[2,3-*b*]furan-1-one (4an)

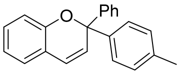
The mixture of **3an** and **4an** (96/4) was obtained as a white solid, 64.0 mg, in 70% yield; $R_f = 0.42$ (petroleum ether : ethyl acetate = 30 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.41 (d, $J = 7.6$ Hz, 4H), 7.30 (d, $J = 6.8$ Hz, 4H), 7.25-7.21 (m, 2H), 6.90 (s, 1H), 6.65 (s, 1H), 6.56 (d, $J = 10.0$ Hz, 1H), 6.08 (d, $J = 10.0$ Hz, 1H), 2.81 (dd, $J_1 = 8.4$ Hz, $J_2 = 3.6$ Hz, 2H), 2.47 (dd, $J_1 = 19.6$ Hz, $J_2 = 8.8$ Hz, 1H), 2.34-2.31 (m, 1H), 2.16-1.91 (m, 5H), 1.63-1.34 (m, 6H), 0.87 (t, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.3, 145.2, 145.1, 138.2, 132.4, 128.0, 127.9, 127.4, 127.3, 127.0, 126.9, 123.4, 123.3, 118.7, 116.2, 82.4, 50.3, 47.9, 43.8, 38.2, 35.8, 31.4, 29.5, 26.4, 25.8, 21.5, 13.8; IR (KBr) ν 2928, 1739, 1494, 1225, 699 cm^{-1}; HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{33}H_{33}O_2$, 461.24751; found 461.24780.



3ao **4ao**

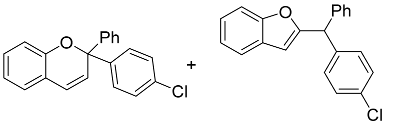
methyl 2-(1,3-dioxoisoindolin-2-yl)-3-(2,2-diphenyl-2*H*-chromen-6-yl)propanoate (3ao) and methyl 3-(2-benzhydrylbenzofuran-5-yl)-2-(isoindolin-2-yl)propanoate (4ao)

The mixture of **3ao** and **4ao** (96/4) was obtained as a white solid, 64.0 mg, in 62% yield; $R_f = 0.43$ (petroleum ether : dichloromethane = 1 : 1); ^{1}H NMR (400 MHz, DMSO, TMS) δ 7.75-7.73 (m, 2H), 7.67-7.65 (m, 2H), 7.34 (d, *J* = 7.2 Hz, 4H), 7.28-7.20 (m, 6H), 6.91 (d, *J* = 8.4 Hz, 1H), 6.80 (s, 1H), 6.73 (d, *J* = 8.4 Hz, 1H), 6.46 (d, *J* = 10.0 Hz, 1H), 6.09 (d, *J* = 10.0 Hz, 1H), 5.11-5.08 (m, 1H), 3.75 (s, 3H), 3.49-3.38 (m, 2H); ^{13}C NMR (100 MHz, DMSO) δ 169.4, 167.5, 151.3, 144.7, 134.0, 131.5, 129.8, 129.2, 128.9, 128.0, 127.41, 127.35, 126.9, 126.8, 123.4, 123.2, 121.0, 116.5, 82.5, 53.1, 52.8, 33.8; IR (KBr) ν 3648, 1724, 1390, 1243, 719 cm^{-1}; HRMS-(ESI) (m/z): [M+H]$^+$ calcd for $C_{25}H_{22}O_3$, 516.18055; found 516.18054.



2-phenyl-2-(p-tolyl)-2*H*-chromene (3ba)

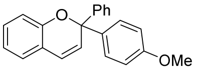
Compound **3ba** was obtained as a white solid, 40.0 mg, in 68% yield; R_f = 0.62 (petroleum ether : ethyl acetate = 100 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.42 (d, *J* = 7.8 Hz, 2H), 7.29 (t, *J* = 8.0 Hz, 4H), 7.24-7.19 (m, 1H), 7.12-7.07 (m, 3H), 6.97 (d, *J* = 6.4 Hz, 1H), 6.90 (d, *J* = 8.0 Hz, 1H), 6.80 (t, *J* = 7.2 Hz, 1H), 6.57 (d, *J* = 9.6 Hz, 1H), 6.13 (d, *J* = 9.6 Hz, 1H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 145.1, 142.0, 137.2, 129.4, 128.9, 128.8, 128.1, 127.4, 127.0, 126.9, 126.5, 123.2, 121.1, 121.0, 116.4, 82.4, 21.0; IR (KBr) 2360, 1579, 1484, 1240, 757 cm^{-1}; HRMS-(ESI) (m/z): [M+H]$^+$ calcd for $C_{22}H_{19}O$, 299.14304; found 299.14343.



3ca **4ca**

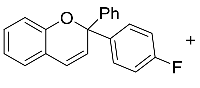
2-(4-chlorophenyl)-2-phenyl-2*H*-chromene (3ca) and 2-((4-chlorophenyl)(phenyl)methyl)benzofuran (4ca)

The mixture of **3ca** and **4ca** (98/2) was obtained as a white solid, 46.0 mg, in 72% yield; R_f = 0.65 (petroleum ether : ethyl acetate = 100 : 1) ; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.41-7.24 (m, 9H), 7.12 (td, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 7.00 (td, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 6.90 (d, J = 8.0 Hz, 1H), 6.84 (td, J_1 = 7.6 Hz, J_2 = 0.8 Hz, 1H), 6.62 (d, J = 9.6 Hz, 1H), 6.10 (d, J = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 144.5, 143.4, 133.4, 129.7, 128.5, 128.31, 128.26, 128.2, 127.6, 126.9, 126.6, 123.7, 121.4, 121.0, 116.5, 82.1; IR (KBr) ν 1597, 1487, 1239, 993, 757 cm^{-1}; HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{21}H_{16}ClO$, 319.08842; found 319.08865.

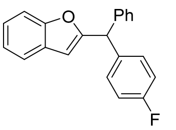


2-(4-methoxyphenyl)-2-phenyl-2*H*-chromene (3da)

Compound **3da** was obtained as a white solid, 46.0 mg, in 74% yield; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.43-7.41 (m, 2H), 7.34-7.28 (m, 4H), 7.25-7.21 (m, 1H), 7.09 (td, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 6.98 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1H), 6.89 (d, J = 8.4 Hz, 1H), 6.81-6.79 (m 3H), 6.57 (d, J = 10.0 Hz, 1H), 6.11 (d, J = 9.6 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 152.5, 145.1, 137.0, 129.5, 129.0, 128.4, 128.0, 127.3, 126.8, 126.5, 123.1, 121.1, 121.0, 116.4, 113.4, 82.3, 55.2. Spectroscopic data were in accordance with literature values.[11]



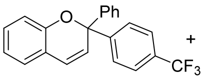
3ea



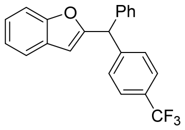
4ea

2-(4-fluorophenyl)-2-phenyl-2*H*-chromene (3ea) and 2-((4-fluorophenyl)(phenyl)methyl)benzofuran (4ea)

The mixture of **3ea** and **4ea** (95/5) was obtained as a light yellow solid, 43.0 mg, in 71% yield; $R_f = 0.65$ (petroleum ether : ethyl acetate = 100 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.41-7.36 (m, 4H), 7.30 (td, J_1 = 6.8 Hz, J_2 = 1.2 Hz, 1H), 7.25-7.22 (m, 1H), 7.10 (t, J = 7.8 Hz, 1H), 6.99-6.95 (m, 3H), 6.89 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 6.82 (t, J = 7.2 Hz, 1H), 6.59 (d, J = 10.0 Hz, 1H), 6.09 (d, J = 9.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.0 (d, J = 245 Hz), 152.3, 144.7, 140.66 (d, J = 3.0 Hz), 129.6, 128.9 (d, J = 8.2 Hz), 128.6, 128.2, 127.5, 126.8, 126.6, 123.5, 121.3 , 116.4, 115.0, 114.9 (d, J = 21.3 Hz), 82.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.77 - -114.84 (m); IR (KBr) ν 1599, 1507, 1233, 1218, 757, 702 cm^{-1}; HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{21}H_{16}FO$, 303.11797; found 303.11823.



3fa

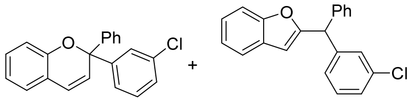


4fa

2-phenyl-2-(4-(trifluoromethyl)phenyl)-2*H*-chromene (3fa) and 2-(phenyl(4-(trifluoromethyl)phenyl)methyl)benzofuran (4fa)

The mixture of **3fa** and **4fa** (92/8) was obtained as a light yellow oil, 49 mg, in 70% yield; $R_f = 0.54$ (petroleum ether : ethyl acetate = 100 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.59-7.56 (m, 4H), 7.41 (d, J = 7.6 Hz, 2H), 7.34-7.28 (m, 3H), 7.13 (t, J = 7.6 Hz, 1H), 7.01 (d, J = 7.2 Hz, 1H), 6.92 (d, J = 8.0 Hz, 1H), 6.85 (t, J = 7.6 Hz, 1H), 6.64 (d, J = 9.6 Hz, 1H), 6.13 (d, J = 9.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 148.8, 144.2, 129.8, 129.6 (q, J = 32.4 Hz), 128.3, 128.0, 127.8, 127.3, 126.9, 126.7, 125.1 (q, J = 3.8 Hz), 124.1 (q, J = 270.5 Hz), 124.0, 121.5, 120.9, 116.5, 82.1; ^{19}F NMR (376 MHz,

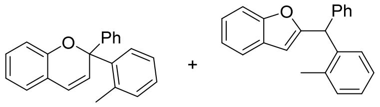
$CDCl_3$) δ -62.5 (s); IR (KBr) ν 1512, 1318, 1240, 1185, 759 cm^{-1}; HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{22}H_{16}F_3O$, 353.11478; found 353.11496.



3ga **4ga**

2-(3-chlorophenyl)-2-phenyl-2*H*-chromene (3ga) and 2-((3-chlorophenyl)(phenyl)methyl)benzofuran (4ga)

The mixture of **3ga** and **4ga** (90/10) was obtained as a yellow oil, 47.0 mg, in 73% yield; $R_f = 0.65$ (petroleum ether : ethyl acetate = 100 : 1); ^1H NMR (400 MHz, $CDCl_3$, TMS) δ 7.45 (s, 1H), 7.40 (d, *J* = 7.2 Hz, 2H), 7.32-7.21 (m, 6H), 7.14-7.09 (m, 1H), 6.99 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 6.91 (d, *J* = 8.0 Hz, 1H), 6.83 (t, *J* = 7.2 Hz, 1H), 6.61 (d, *J* = 10.0 Hz, 1H), 6.09 (d, *J* = 9.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 147.0, 144.3, 134.1, 129.7, 129.4, 128.2, 128.1, 127.7, 127.6, 127.2, 126.9, 126.7, 125.2, 123.8, 121.4, 120.9, 116.5, 82.0; IR (KBr) ν 1480, 1233, 991, 781, 697 cm^{-1}; HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{21}H_{16}ClO$, 319.08842; found 319.08862.

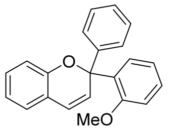


3ha **4ha**

2-phenyl-2-(*o*-tolyl)-2*H*-chromene (3ha) and 2-(phenyl(*o*-tolyl)methyl)benzofuran (4ha)

The mixture of **3ha** and **4ha** (75/25) was obtained as a colorless oil, 41.0 mg, in 69% yield; $R_f = 0.61$ (petroleum ether : ethyl acetate = 100 : 1); ^1H NMR of **3ga** (400 MHz, $CDCl_3$, TMS) δ 7.45-7.06 (m, 10H), 7.00-7.95 (m, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 6.81 (t, *J* = 7.2 Hz, 1H), 6.58 (d, *J* = 10.0 Hz, 1H), 6.01 (d, *J* = 10.0 Hz, 1H), 2.20 (s, 3H); ^{13}C

NMR of **3ga** and **4ga** (100 MHz, CDCl$_3$) δ 159.9, 155.1, 152.7, 145.1, 141.5, 140.3, 139.2, 137.6, 136.4, 132.4, 130.6, 129.4, 129.1, 129.0, 128.7, 128.52, 128.45, 128.3, 128.2, 128.0, 127.1, 127.0, 129.9, 126.53, 126.48, 126.1, 125.0, 123.7, 123.0, 122.6, 121.2, 121.1, 120.6, 116.2, 111.1, 106.0, 83.5, 47.9, 21.5, 19.6; IR (KBr) ν 1597, 1487, 1455, 1243, 752, 704 cm^{-1}; HRMS-(ESI) (m/z): [M+H]$^+$ calcd for $C_{22}H_{19}O$, 299.14304; found 199.14313.



3ia

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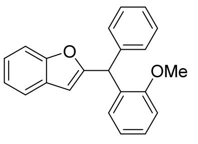
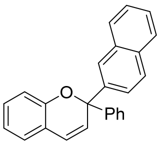


4ia

2-(2-methoxyphenyl)-2-phenyl-2*H*-chromene (3ia) and 2-((2-methoxyphenyl)(phenyl)methyl)benzofuran (4ia)

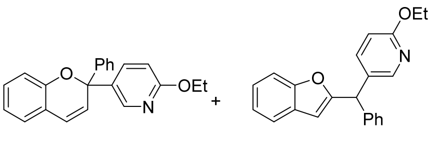
Compound **3ia** was obtained as a colorless oil, 34.0 mg, in 54% yield; R$_f$ = 0.36 (petroleum ether : ethyl acetate = 100 : 1); ^{1}H NMR (400 MHz, CDCl$_3$, TMS) δ 7.74 (dd, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.37 (d, J = 7.6 Hz, 2H), 7.28-7.19 (m, 4H), 7.09 (t, J = 7.6 Hz, 1H), 7.00-6.96 (m, 2H), 6.89 (d, J = 8.0 Hz, 1H), 6.85 (d, J = 8.0 Hz, 1H), 6.81 (t, J = 7.2 Hz, 1H), 6.54 (d, J = 10.0 Hz, 1H), 6.46 (d, J = 10.0 Hz, 1H), 3.50 (s, 3H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 155.6, 152.4, 144.5, 132.6, 129.2, 128.9, 127.8, 127.6, 127.4, 127.3, 126.9, 126.4, 122.7, 121.02, 121.00, 120.6, 116.2, 112.3, 82.1, 55.4; IR (KBr) ν 1487, 1450, 1228, 983, 754 cm^{-1}; HRMS-(ESI) (m/z): [M+H]$^+$ calcd for $C_{22}H_{19}O_2$, 315.13796; 315.13766. Compound **4ia** was obtained as a light yellow oil, 10 mg, in 16% yield; R$_f$ = 0.37 (petroleum ether : ethyl acetate = 100 : 1); ^{1}H NMR (400 MHz, CDCl$_3$, TMS) δ 7.45-7.43 (m, 1H), 7.40 (d, J = 8.0 Hz, 1H), 7.32-7.15 (m, 8H), 7.03 (d, J = 6.4 Hz, 1H), 6.89 (t, J = 7.2 Hz, 2H), 6.21 (s, 1H), 6.02 (s, 1H), 3.77 (s, 3H); ^{13}C NMR (100 MHz,

$CDCl_3$) δ 160.2, 156.8, 155.1, 140.9, 129.6, 129.5, 128.9, 128.6, 128.3, 128.2, 126.7, 123.5, 122.5, 120.5, 111.1, 110.7, 105.4, 55.6, 44.0 (one aryl carbon overlapped); IR (KBr) ν 1492, 1495, 1245, 1028, 757 cm^{-1}; HRMS (EI): m/z Exact mass calcd for $C_{22}H_{18}O_2$ $[M]^+$: 314.1307, found: 314.1306.



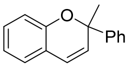
2-(naphthalen-2-yl)-2-phenyl-2*H*-chromene (3ja)

Compound **3ja** was obtained as a white solid, 42.0 mg, in 63% yield; R_f = 0.66 (petroleum ether : ethyl acetate = 100 : 1); ^1H NMR (400 MHz, $CDCl_3$, TMS) $δ^1H$ NMR (400 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.80-7.75 (m, 3H), 7.51-7.42 (m, 5H), 7.31 (t, *J* = 8.0 Hz, 2H), 7.26-7.23 (m, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.99 (d, *J* = 7.2 Hz, 1H), 6.94 (d, *J* = 8.0 Hz, 1H), 6.81 (t, *J* = 7.2 Hz, 1H), 6.65 (d, *J* = 10.0 Hz, 1H), 6.22 (d, *J* = 9.6 Hz, 1H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 144.8, 142.0, 132.8, 132.7, 129.6, 128.7, 128.3, 128.2, 128.0. 127.5, 127.0, 126.6, 126.2, 126.1, 126.0, 125.3, 123.6, 121.2, 121.1, 116.5, 82.7 (one aryl carbon overlapped); IR (KBr) ν 1602, 1484, 1238, 749, 697 cm^{-1}; HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{25}H_{19}O$, 335.14304; found 335.14301.



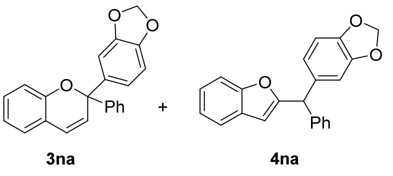
2-ethoxy-5-(2-phenyl-2*H*-chromen-2-yl)pyridine (3ka) and 5-(benzofuran-2-yl(phenyl)methyl)-2-ethoxypyridine (4ka)

The mixture of **3ka** and **4ka** (87/13) was obtained as a colorless solid, 45.0 mg, in 68% yield; R_f = 0.65 (petroleum ether : ethyl acetate = 3 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.17 (d, *J* = 2.4 Hz, 1H), 7.60 (dd, J_1 = 8.8 Hz, J_2 = 2.4 Hz, 1H), 7.42 (d, *J* = 7.2 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 2H), 7.27-7.22 (m, 2H), 7.10 (td, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 6.83 (t, *J* = 7.2 Hz, 1H), 6.65 (d, *J* = 10.4 Hz, 1H), 6.61 (d, *J* = 9.6 Hz, 1H), , 6.08 (d, *J* = 9.6 Hz, 1H), 4.31 (q, *J* = 7.2 Hz, 2H), 1.35 (t, *J* = 7.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.2, 152.2, 145.8, 144.4, 138.0, 132.9, 129.7, 128.2, 128.1, 127.6, 126.7, 126.6, 123.9, 121.4, 121.0, 116.5, 110.6, 81.1, 61.7, 14.6; IR (KBr) ν 1607, 1489, 1290, 1237, 757 cm^{-1}; HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{22}H_{20}NO_2$, 330.14886; found 330.14899.



2-methyl-2-phenyl-2*H*-chromene (3la)

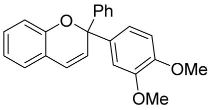
Compound **3la** was obtained as a colorless oil, 11.8 mg, in 27% yield; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.6 Hz, 2H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.23-7.20 (m, 1H), 7.10 (td, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 6.95 (dd, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 6.81 (td, J_1 = 7.6 Hz, J_2 = 0.8 Hz, 1H), 6.43 (d, *J* = 10.0 Hz, 1H), 5.91 (d, *J* = 9.6 Hz, 1H), 1.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 145.8, 129.6, 129.3, 128.2, 127.2, 126.5, 125.1, 122.7, 121.1, 120.9, 116.3, 78.6, 29.3. Spectroscopic data were in accordance with literature values.[12]



3na **4na**

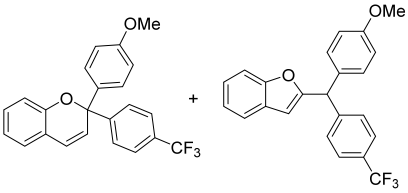
2-(benzo[*d*][1,3]dioxol-5-yl)-2-phenyl-2*H*-chromene (3na) and 5-(benzofuran-2-yl(phenyl)methyl)benzo[*d*][1,3]dioxole (4na)

The mixture of **3na** and **4na** (95/5) was obtained as a colorless oil, 44.0 mg, in 67% yield; R_f = 0.34 (petroleum ether : dichloromethane = 20 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.42 (d, *J* = 7.6 Hz, 2H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.25-7.20 (m, 1H), 7.10 (td, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 6.99 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1H), 6.91-6.87 (m, 3H), 6.82 (t, *J* = 7.8 Hz, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 6.58 (d, *J* = 9.6 Hz, 1H), 6.09 (d, *J* = 10.0 Hz, 1H), 5.89 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 147.5, 146.9, 145.0, 138.9, 129.5, 128.8, 128.1, 127.4, 126.8, 126.5, 123.3, 121.2, 121.0, 120.8, 116.5, 108.1, 107.6, 101.1, 82.4; IR (KBr) ν 1487, 1240, 1113, 1036, 752 cm^{-1}; HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{22}H_{17}O_3$, 329.11722; found 329.11749.



2-(3,4-dimethoxyphenyl)-2-phenyl-2*H*-chromene (3oa)

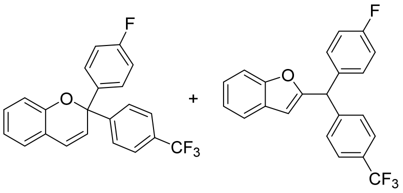
Compound **3oa** was obtained as a colorless oil, 44.0 mg, in 64% yield; R_f = 0.28 (petroleum ether : dichloromethane = 20 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.43 (d, *J* = 8.0 Hz, 2H), 7.31 (t, *J* = 7.2 Hz, 2H), 7.25 (d, *J* = 7.2 Hz, 1H), 7.12-7.08 (m, 1H), 7.00-6.98 (m, 2H), 6.92-6.89 (m, 2H), 6.82 (t, *J* = 7.8 Hz, 2H), 6.77 (d, *J* = 8.4 Hz, 1H), 6.59 (d, *J* = 10.0 Hz, 1H), 6.14-6.11 (m, 1H), 3.83 (d, *J* = 8.0 Hz, 3H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 148.6, 148.4, 144.9, 137.3, 129.5, 129.0, 128.0, 127.4, 126.9, 126.5, 123.2, 121.15, 121.10, 119.7, 116.4, 110.6, 110.3, 82.5, 55.77, 55.75; IR (KBr) ν 1512, 1260, 1238, 1138, 1026, 759 cm^{-1}; HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{23}H_{21}O_3$, 345.14852; found 345.14868.



3pa **4pa**

2-(4-methoxyphenyl)-2-(4-(trifluoromethyl)phenyl)-2*H*-chromene (3pa) and 2-((4-methoxyphenyl)(4-(trifluoromethyl)phenyl)methyl)benzofuran (4pa)

The mixture of **3pa** and **4pa** (93/7) was obtained as a colorless oil, 46.0 mg, in 61% yield; R_f = 0.55 (petroleum ether : ethyl acetate = 10 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.63-7.54 (m, 4H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.12 (t, *J* = 7.6 Hz, 1H), 7.00 (d, *J* = 7.2 Hz, 1H), 6.90 (d, *J* = 8.0 Hz, 1H), 6.86-6.83 (m, 3H), 6.62 (d, *J* = 9.6 Hz, 1H), 6.09 (d, *J* = 9.6 Hz, 1H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 152.2, 149.1, 136.2, 130.0, 129.5 (q, *J* = 32.3 Hz), 128.4, 128.1, 127.1, 126.7, 125.1 (q, *J* = 3.8 Hz), 122.6 (q, *J* = 270.4 Hz), 121.4, 120.9, 120.0, 116.5, 113.6, 82.0, 55.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.44; IR (KBr) ν 1587, 1325, 1170, 1068, 828 cm^{-1}; HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{23}H_{18}F_3O_2$, 383.12534; found 383.12579.

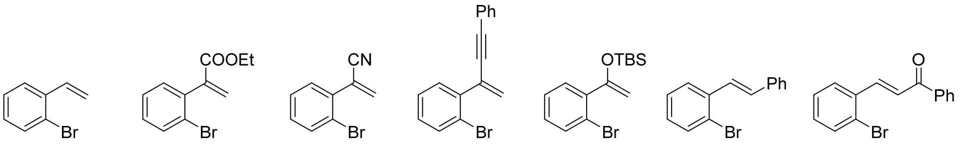


3qa **4qa**

2-(4-fluorophenyl)-2-(4-(trifluoromethyl)phenyl)-2*H*-chromene (3qa) and 2-((4-fluorophenyl)(4-(trifluoromethyl)phenyl)methyl)benzofuran (4qa)

The mixture of **3qa** and **4qa** (86/14) was obtained as a yellow oil, 48.0 mg, in 65% yield; $R_f = 0.43$ (petroleum ether : dichloromethane = 50 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.59-7.53 (m, 4H), 7.39-7.35 (m, 2H), 7.13 (td, $J_1 = 8.0$ Hz, $J_2 = 1.2$ Hz, 1H), 7.02-6.97 (m, 3H), 6.90 (d, $J = 8.0$ Hz, 1H), 6.858 (td, $J_1 = 7.6$ Hz, $J_2 = 0.8$ Hz, 1H), 6.65 (d, $J = 9.6$ Hz, 1H), 6.08 (d, $J = 10.0$ Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2 (d, $J = 245.8$ Hz), 152.0, 148.6, 139.9 (d, $J = 3.1$ Hz), 129.9, 129.7 (q, $J = 32.3$ Hz), 128.9 (d, $J = 8.2$ Hz), 127.7, 127.2, 126.8, 125.2 (q, $J = 3.7$ Hz), 124.0 (q, $J = 270.6$ Hz), 124.3, 121.7, 120.9, 116.5, 115.1 (d, $J = 21.4$ Hz), 81.7; IR (KBr) ν 1509, 1327, 1230, 1168, 1125, 1070, 839 cm^{-1}; HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{22}H_{15}F_4O$, 371.10535; found 371.10590.

Unsuccessful substrates

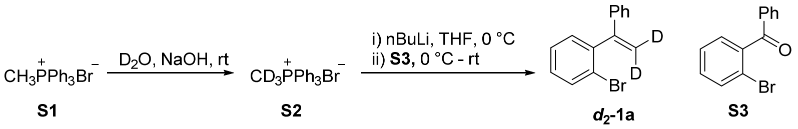


Procedure for one-pot gram scale experiment

A 150 mL oven-dried Schlenk bottle under argon atmosphere charged with salicylaldehyde (10 mmol, 1.22 g), 4-methylbenzenesulfonohydrazide (10 mmol, 1.86 g) and 2-MeTHF (30 mL) was stirred at room temperature for 2 h. Then 1-bromo-2-(1-phenylvinyl)benzene **1a** (5 mmol, 1.29 g), $[Pd(allyl)Cl]_2$ (90 mg, 5 mol%), dppb (320 mg, 15 mol%), K_2CO_3 (15 mmol, 2.07 g, 3.0 equiv), and 2-MeTHF (20 mL) were added sequentially to the resulting mixture. The bottle was heated in an oil bath at 100 °C for 20 h. The resulting mixture was cooled to room temperature and filtered through Celite with EtOAc as the eluent. The solvents were evaporated under reduced pressure and the residue was purified by column chromatography on silica gel using petroleum ether: dichloromethane (200: 1) as eluent to afford **3aa,** 0.91 g, in 64% yield.

Deuterium labeling experiments

Preparation of 1-bromo-2-(1-phenylvinyl-2,2-*d*2)benzene (*d*$_2$-1a)[13]

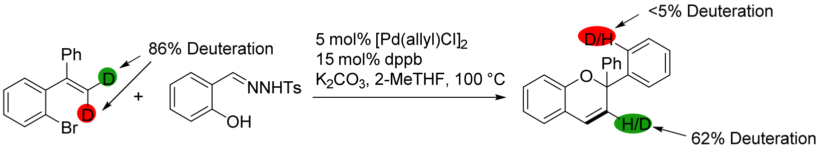


Step 1: To a flask with a magnetic stir bar was added **S1** (1060 mg, 3.0 mmol, 1.0 equiv), D_2O (4 mL), and NaOH (60 mg, 1.50 mmol, 0.5 equiv). The reaction mixture was stirred under argon atmosphere, and after 24 h, CH_2Cl_2 (10 mL) was added to the solution and organic layer was collected and dried with $MgSO_4$. Then added hexanes (20 mL) to the resulting solution and stored at fridge for 24 h to afford colorless crystals **S2** 900 mg used directly for the next step.

Step 2: An oven dried flask charged with **S2** (1.5 mmol, 534 mg, 1.0 equiv) and THF (5 mL) was cooled to 0 °C. Then 2.6M n-BuLi (1.8 mmol, 0.7 mL, 1.2 equiv) was added dropwise and the resulting yellow suspension was stirred for 60 minutes. To this suspension, a solution of (2-bromophenyl)(phenyl)methanone **S3** (1.5 mmol, 390 mg, 1.0 equiv.) was added in one portion and the resulting mixture was warmed to room temperature and further stirred at room temperature for 2 h. Water and EA were added to the reaction mixture, separated and the aqueous phase was extracted with EA (3 x 20 mL). The combined organic phases were washed with brine, dried over Na_2SO_4 and the solvent removed under reduced pressure. The reaction mixture was purified by column chromatography using hexanes as eluent to obtain the product ***d*$_2$-1a** as a colorless oil, 296 mg, 74% (two steps), 86%D; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.58 (d, *J* = 8.0

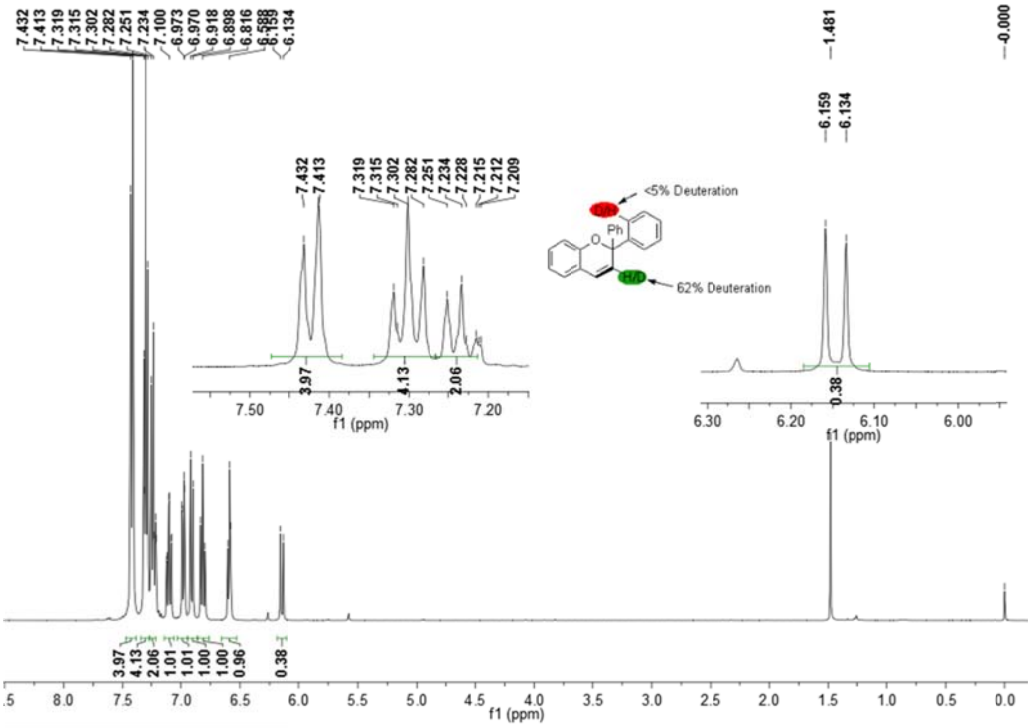
Hz, 1H), 7.35-7.25 (m, 7H), 7.21-7.16 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 142.6, 139.5, 132.9, 131.6, 129.0, 128.3, 127.7, 127.2, 126.5, 123.3, 112.0-115.2 (m, 1C).

Deuterium labeling experiment 1



***d*$_2$-1a** **2a**

An oven-dried Schlenk tube under argon atmosphere was charged with 1-bromo-2-(1-phenylvinyl-2,2-*d*2)benzene **(*d*$_2$-1a)** (0.2 mmol, 1.0 equiv), *N*-tosylhydrazones **2a** (0.4 mmol, 2.0 equiv)**,** $[Pd(allyl)Cl]_2$ (3.6 mg, 5 mol%), dppb (12.8 mg, 15 mol%), K_2CO_3 (0.6 mmol, 82 mg, 3.0 equiv) and 2-MeTHF (2 mL) was stirred at 100 °C for 20 h . After work-up and purification, the product was obtained, 38 mg, 67%; ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.42 (d, $J = 7.2$ Hz, 4H), 7.32-7.28 (m, 4H), 7.25-7.21 (m 2H), 7.10 (td, $J_1 = 7.6$ Hz, $J_2 = 1.6$ Hz, 1H), 6.98 (dd, $J_1 = 7.6$ Hz, $J_2 = 1.6$ Hz, 1H), 6.91 (d, $J = 8.0$ Hz, 1H), 6.82 (t, $J = 7.6$ Hz, 1H), 6.59 (t, $J = 4.8$ Hz, 1H), 6.15 (d, $J = 10.0$ Hz, 0.38 H).; ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 144.9, 129.5, 128.8, 128.1, 127.4, 127.0, 126.5, 123.2(d, 1C), 121.1, 121.0 (d, 1C), 116.5, 82.51 (d, 1C).



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6.816
6.588
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-0.000
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7.302
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7.212
7.209
3.97
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7.30
7.20
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D/H
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O
Ph
H/D
62% Deuteration
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6.00
f1 (ppm)
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1.01
1.00
1.00
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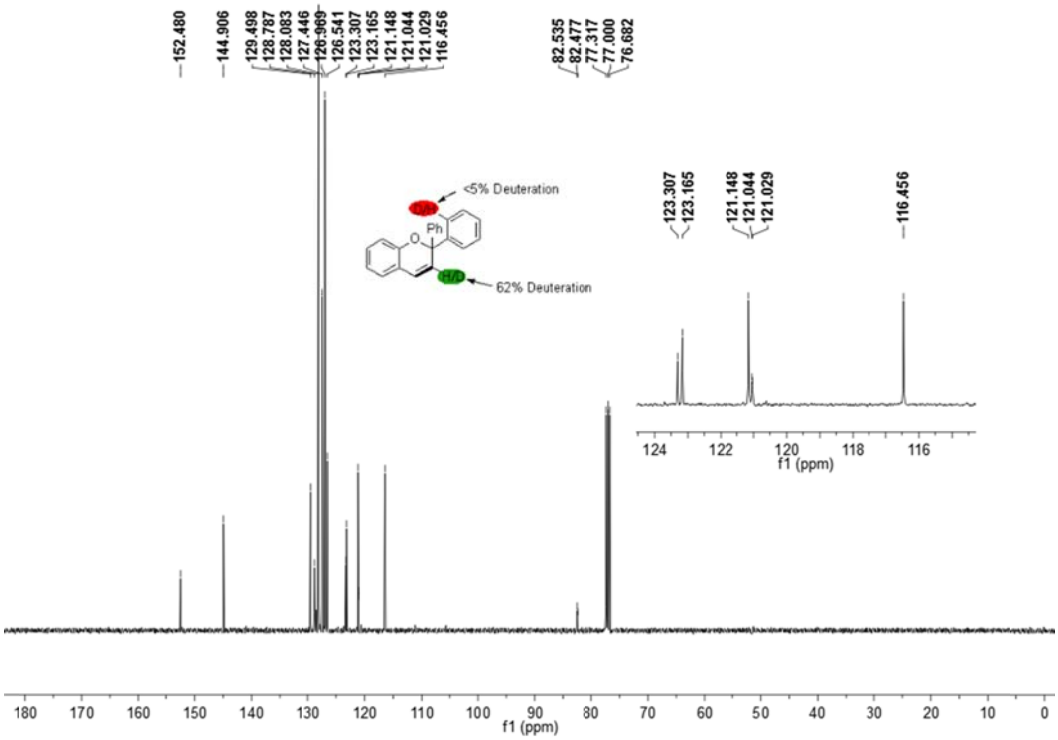
f1 (ppm)



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D/H
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O
Ph
H/D
62% Deuteration
123.307
123.165
121.148
121.044
121.029
116.456
124
122
120
118
116
f1 (ppm)
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160
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140
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20
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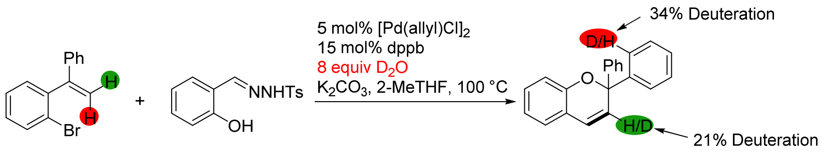
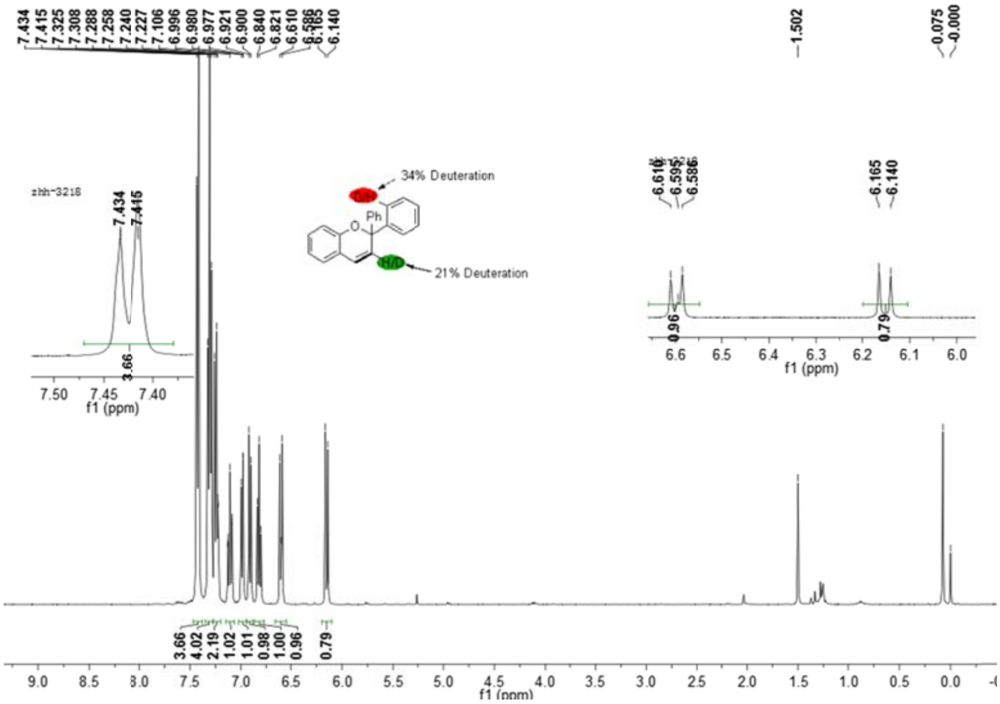
f1 (ppm)

Deuterium labeling experiment 2



1a **2a**

An oven-dried Schlenk tube under argon atmosphere was charged with 1-bromo-2-(1-phenylvinyl)benzene **(1a)** (0.2 mmol, 1.0 equiv), *N*-tosylhydrazones **2a** (0.4 mmol, 2.0 equiv)**,** [Pd(allyl)Cl]$_2$ (3.6 mg, 5 mol%), dppb (12.8 mg, 15 mol%), K$_2$CO$_3$ (0.6 mmol, 82 mg, 3.0 equiv), D$_2$O (32 mg, 8.0 equiv) and 2-MeTHF (2 mL) was stirred at 100 °C for 20 h . After work-up and purification, the product was obtained, 24 mg, 42%; ^{1}H NMR (400 MHz, CDCl$_3$) δ 7.42 (d, J = 7.56 Hz, 3.66H), 7.31 (t, J = 7.6 Hz, 4H), 7.26-7.22 (m, 1H), 7.11 (td, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 6.99 (dd, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 6.91 (d, J = 8.0 Hz, 1H), 6.82 (t, J = 7.6 Hz, 1H), 6.61-6.59 (m, 1H), 6.15 (d, J = 10.0 Hz, 0.79H); ^{13}C NMR (101 MHz, CDCl$_3$) δ 152.5, 144.9, 129.5, 128.8, 128.0 (d, 1C), 127.5, 127.0, 126.6, 123.2 (d, 1C), 121.2, 121.0, 116.5, 82.5.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6.821
6.610
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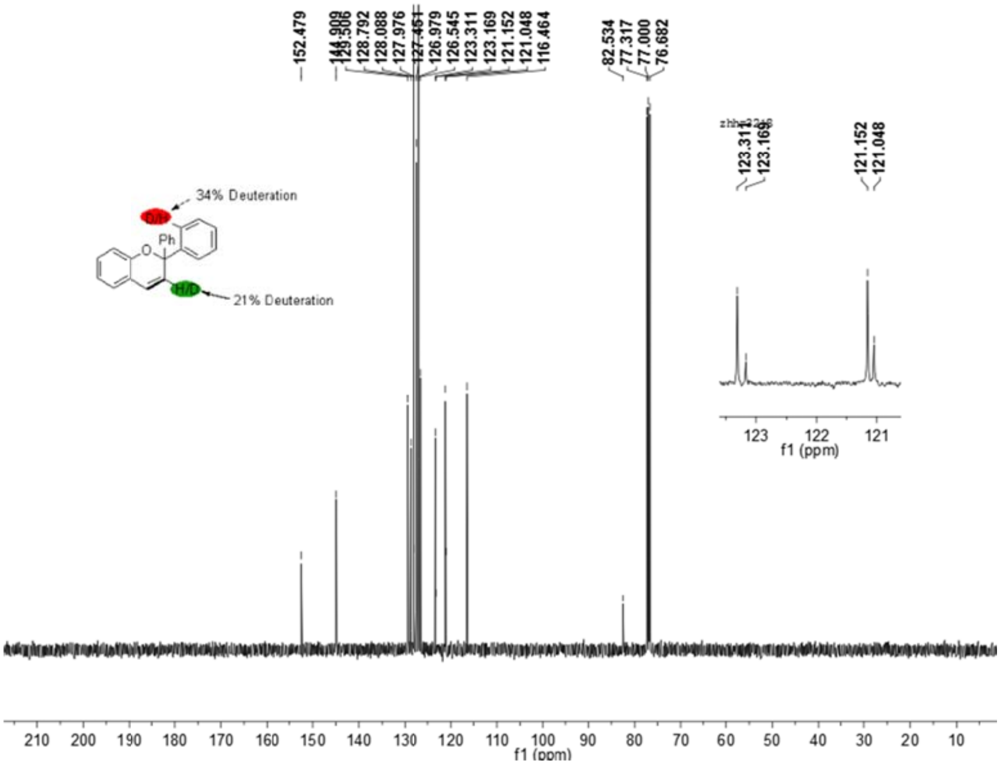
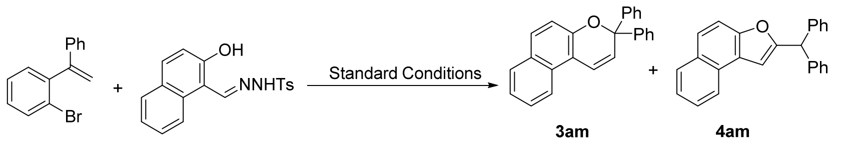
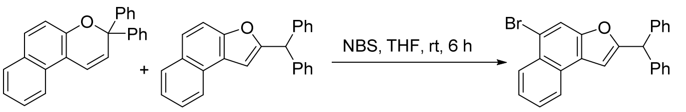
zhh-3218
34% Deuteration
D/H
Ph
O
H/D
21% Deuteration
3.66
4.02
2.19
1.02
1.01
0.98
1.00
0.96
0.79
f1 (ppm)


152.479
144.909
129.506
128.792
128.088
127.976
127.451
126.979
126.545
123.311
123.169
121.152
121.048
116.464
82.534
77.317
77.000
76.682
34% Deuteration
D/H
Ph
O
H/D
21% Deuteration
f1 (ppm)

Structure conformation of the other isomer



3am **4am**

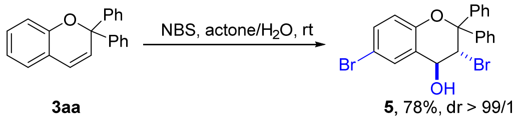


3am/4am = 1/2 **4am' (major product)**

The mixture of **3am** and **4am** was synthesized first. Then to the mixture (0.7 mmol, 234 mg) in THF (14 mL) was added NBS (1.4 mmol, 247 mg) and the result solution was stirred at room temperature for 6 h.. Diluted with EA (50 mL) and washed with brine (30 mL). The solvent was removed under reduced pressure and the residual mass was purified by silica gel column chromatography using PE/DCM=100 as eluent to afford the pure product **4am’** (91 mg) as major product as a yellow solid; R_f = 0.61 (petroleum ether : ethyl acetate = 100 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 8.32-8.30 (m, 1H), 8.00-7.98 (m, 1H), 7.93 (s, 1H), 7.56-7.53 (m, 2H), 7.35 (t, *J* = 7.6 Hz, 4H), 7.29 (d, *J* = 7.2 Hz, 2H), 7.25 (d, *J* = 7.6 Hz, 4H), 6.73 (s, 1H), 5.66 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) 159.7, 151.6, 140.9, 128.8, 128.7, 128.4, 128.0, 127.8, 127.1, 126.9, 125.6, 123.8, 123.6, 118.2, 116.7, 104.7, 51.4; IR (KBr) ν 1493, 1448, 1351, 1010, 765, 701 cm^{-1}; HRMS (EI): m/z Exact mass calcd for $C_{25}H_{17}BrO$ $[M]^+$: 412.0463, found: 412.0461. The structure of **4am’** was further established by X-ray diffraction.

Transformations of the products

b)



3,6-dibromo-2,2-diphenylchroman-4-ol (5)[15]

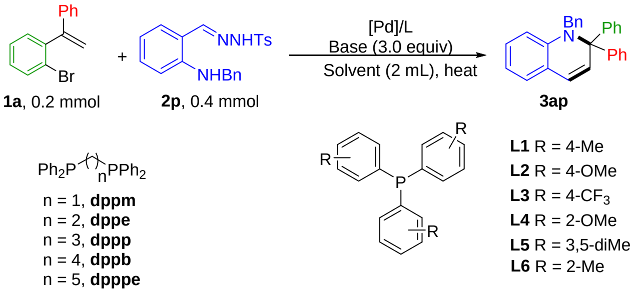
To an oven-dried tube charged with **3aa** (0.2 mmol, 57 mg), acetone (2 mL) and H_2O (400 uL) was added NBS (0.6 mmol, 106 mg). The mixture was stirred at room temperature for 16 hours. Then the reaction mixture was diluted with EA (50 mL) and washed with brine (30 mL). The solvent was removed under reduced pressure and the residual mass was purified to afford the product **5** (72 mg, 87%) as a white solid; R_f = 0.35 (petroleum ether : ethyl acetate = 10 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.74 (d, J = 7.6 Hz, 2H), 7.47 (d, J = 2.0 Hz, 1H), 7.43-7.40 (m, 3H), 7.35 (t, J = 7.6 Hz, 2H), 7.28-7.19 (m, 4H), 7.09 (d, J = 8.8 Hz, 1H), 5.34 (d, J = 4.8 Hz, 1H), 5.05 (t, J = 4.0 Hz, 1H), 1.84 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.1, 142.1, 140.6, 133.2, 132.6, 128.6, 128.3, 128.2, 127.8, 126.9, 125.9, 124.0, 119.4, 114.0, 83.3, 69.8, 57.0; IR (KBr) ν 1739, 1475, 1235, 983, 754, 699 cm^{-1}; EI-MS m/z (%): 458, 460 (M^+, M^++2); HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{21}H_{17}Br_2O_2$, 458.95898; found 440.9478 (- H_2O).

c)

2,2-diphenyl-3-(*p*-tolylthio)chroman-4-ol (6)

In an ice-bath, to an oven-dried tube charged with methylbenzenethiol (53 mg, 0.4 mmol) and DCM (2 mL) was added NCS (0.4 mmol, 50 mg) in DCM (1 mL) slowly at 0 °C and the resulting yellow solution was stirred at this temperature for 30 minutes, followed by the addition of **3aa** (0.2 mmol, 57 mg). The resulting mixture was stirred at room temperature for 2 h. The reaction mixture was diluted with EA (50 mL) and washed with brine (30 mL). The solvent was removed under reduced pressure and the residual mass was purified by silica gel column chromatography using PE/EA=50 as eluent to afford the pure product **6** (67 mg, 79%) as a white solid; R_f = 0.42 (petroleum ether : ethyl acetate = 10 : 1); ^{1}H NMR (400 MHz, $CDCl_3$, TMS) δ 7.73 (d, *J* = 7.6 Hz, 2H), 7.37-7.31 (m, 5H), 7.26-7.15 (m, 5H), 7.09 (d, *J* = 8.0 Hz, 1H), 7.00-6.92 (m, 5H), 4.87 (t, *J* = 6.8 Hz, 1H), 4.23 (d, *J* = 7.2 Hz, 1H), 2.43 (d, *J* = 6.8 Hz, 1H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 142.6, 141.7, 137.6, 132.5, 131.6, 129.7, 129.6, 129.2, 128.3, 128.0, 127.7, 127.6, 127.4, 126.8, 123.7, 121.5, 117.4, 85.0, 68.8, 62.3, 21.0; IR (KBr) ν 1587, 1489, 1457, 1230, 754, 694 cm^{-1}; EI-MS m/z (%): 424 (M^+); HRMS-(ESI) (m/z): $[M+Na]^+$ $C_{28}H_{24}NaO_2S$, 447.1389; found 447.1382.

Optimization of reaction conditions for 1,2-dihydroquinoline synthesis[a]



1a, 0.2 mmol + **2p**, 0.4 mmol → **3ap**

n = 1, **dppm**
n = 2, **dppe**
n = 3, **dppp**
n = 4, **dppb**
n = 5, **dpppe**

L1 R = 4-Me
L2 R = 4-OMe
L3 R = 4-CF_3
L4 R = 2-OMe
L5 R = 3,5-diMe
L6 R = 2-Me

Entry	[Pd]/L	T/°C	Solvent	Base	**3ap** [%][b]
1	5 mol% $[Pd(allyl)Cl]_2$/15 mol% **dppb**	100	2-MeTHF	K_2CO_3	0
2	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **PPh_3**	90	THF	K_2CO_3	20
3	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **PPh_3**	90	2-MeTHF	K_2CO_3	18
4	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **PPh_3**	90	dioxane	K_2CO_3	12
5	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **PPh_3**	90	toluene	K_2CO_3	trace
6	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **PPh_3**	100	dioxane	K_2CO_3	24
7	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **L1**	100	dioxane	K_2CO_3	21
8	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **L2**	100	dioxane	K_2CO_3	20
9	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **L3**	100	dioxane	K_2CO_3	26
10	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **L4**	100	dioxane	K_2CO_3	0
11	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **L5**	100	dioxane	K_2CO_3	22
12	2.5 mol% $[Pd(allyl)Cl]_2$/15 mol% **L6**	100	dioxane	K_2CO_3	trace
13	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **dppm**	100	dioxane	K_2CO_3	trace
14	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **dppe**	100	dioxane	K_2CO_3	trace
15	2.5 mol% $[Pd(allyl)Cl]_2$/7.5mol% **dppp**	100	dioxane	K_2CO_3	13
16	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **dppb**	100	dioxane	K_2CO_3	15
17	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **dpppe**	100	dioxane	K_2CO_3	8
18	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **DPEphos**	100	dioxane	K_2CO_3	23
19	2.5 mol% $[Pd(allyl)Cl]_2$/7.5mol% **Xantphos**	100	dioxane	K_2CO_3	18
20	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **BINAP**	100	dioxane	K_2CO_3	17
21	2.5 mol% $[Pd(allyl)Cl]_2$/7.5 mol% **Johnphos**	100	dioxane	K_2CO_3	0
22	5 mol% $Pd(OAc)_2$/15 mol% **PPh_3**	100	dioxane	K_2CO_3	19
23	5 mol% $Pd(MeCN)_2Cl_2$/15 mol% **PPh_3**	100	dioxane	K_2CO_3	28
24	2.5 mol% $Pd_2dba_3\cdot CHCl_3$/15 mol% **PPh_3**	100	dioxane	K_2CO_3	22
25	5 mol% $Pd(PPh_3)_2Cl_2$	100	dioxane	K_2CO_3	28 (25)[c]
26	5 mol% $Pd(PPh_3)_4$	100	dioxane	K_2CO_3	23
27	5 mol% $Pd(PPh_3)_2Cl_2$	80	dioxane	K_2CO_3	6
28	5 mol% $Pd(PPh_3)_2Cl_2$	120	dioxane	K_2CO_3	17

[a]The reaction was carried out for 10 h. [b]Yields were determined by ^1H NMR using *N*,*N*-dimethylpyridin-4-amine as an internal standard. [c]yield of isolated product.

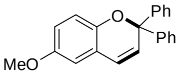
1-benzyl-2,2-diphenyl-1,2-dihydroquinoline (3ap): R_f = 0.55 (petroleum ether : ethyl acetate = 100 : 1); ^1H NMR (400 MHz, $CDCl_3$, TMS) δ 7.43 (d, *J* = 7.2 Hz, 4H), 7.26 (t, *J* = 7.6 Hz, 4H), 7.17 (t, *J* = 7.2 Hz, 2H), 7.04-6.92 (m, 5H), 6.85-6.83 (m, 2H), 6.58 (t, *J*

= 7.2 Hz, 1H), 6.44 (d, *J* = 9.6 Hz, 1H), 6.35 (d, *J* = 8.0 Hz, 1H), 5.81 (d, *J* = 9.6 Hz, 1H), 4.61 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.0, 143.1, 137.8, 130.1, 129.4, 128.6, 128.1, 127.7, 127.1, 127.0, 125.9, 122.7, 120.2, 116.6, 111.1, 72.0, 50.9 (one aryl carbon overlapped); IR (KBr) ν 1636, 1395, 1286, 1122, 782 cm^{-1}; HRMS-(ESI) (m/z): $[M+H]^+$ calcd for $C_{28}H_{24}N$, 374.19033; found 374.19073.

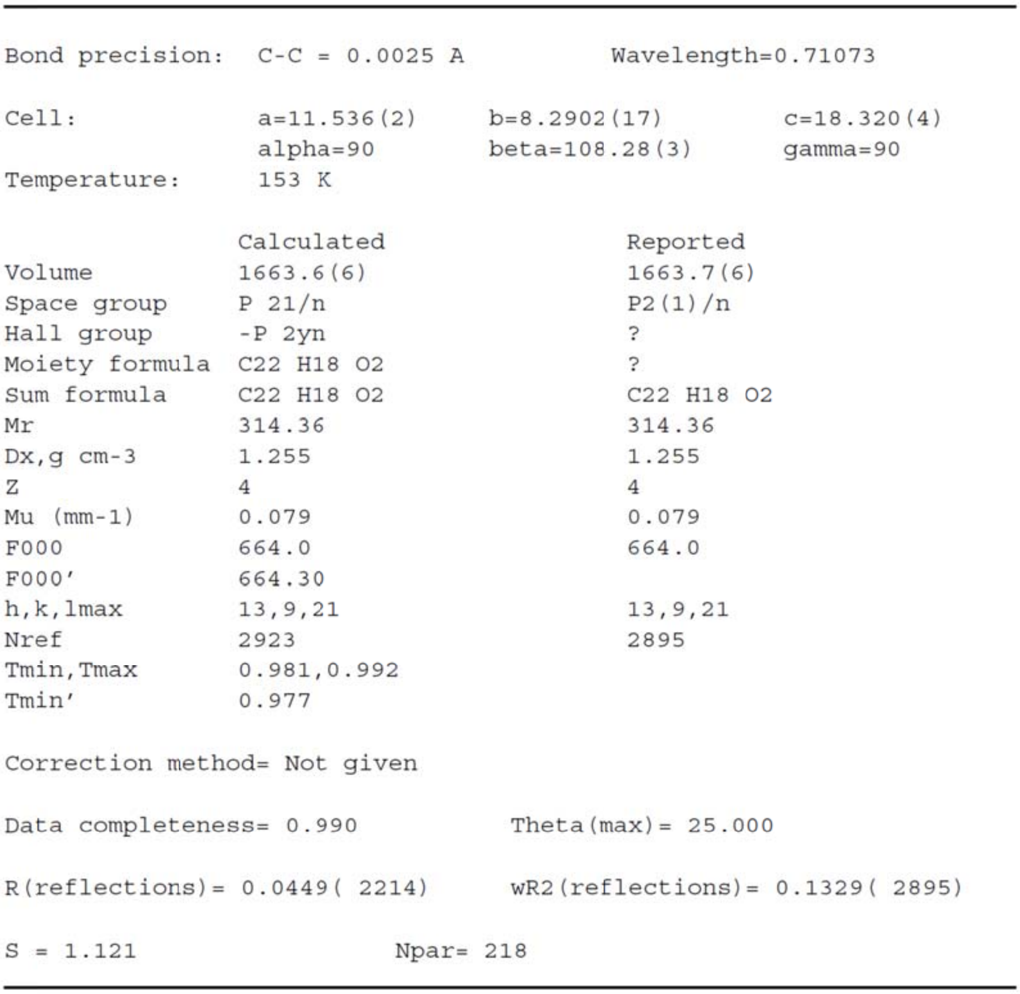
Crystal structure

Procedure for preparation of the crystals: The product (20 mg) was dissolved in DCM and filtered through a pad of filter paper. The filtrate was then transferred into several test-tubes by different volumes. Then to these solutions was added hexane in dropwise. These samples were allowed to be evaporated slowly at room temperature, which would eventually give crystals on the surface of the tubes.

Crystal data of product 3ac (CCDC 1975385)



3ac



```
Bond precision:   C-C = 0.0025 A          Wavelength=0.71073

Cell:             a=11.536(2)     b=8.2902(17)        c=18.320(4)
                  alpha=90        beta=108.28(3)      gamma=90
Temperature:      153 K

                Calculated                  Reported
Volume          1663.6(6)                   1663.7(6)
Space group     P 21/n                      P2(1)/n
Hall group      -P 2yn                      ?
Moiety formula  C22 H18 O2                  ?
Sum formula     C22 H18 O2                  C22 H18 O2
Mr              314.36                      314.36
Dx,g cm-3       1.255                       1.255
Z               4                           4
Mu (mm-1)       0.079                       0.079
F000            664.0                       664.0
F000'           664.30
h,k,lmax        13,9,21                     13,9,21
Nref            2923                        2895
Tmin,Tmax       0.981,0.992
Tmin'           0.977

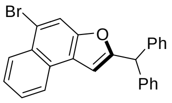
Correction method= Not given

Data completeness= 0.990          Theta(max)= 25.000

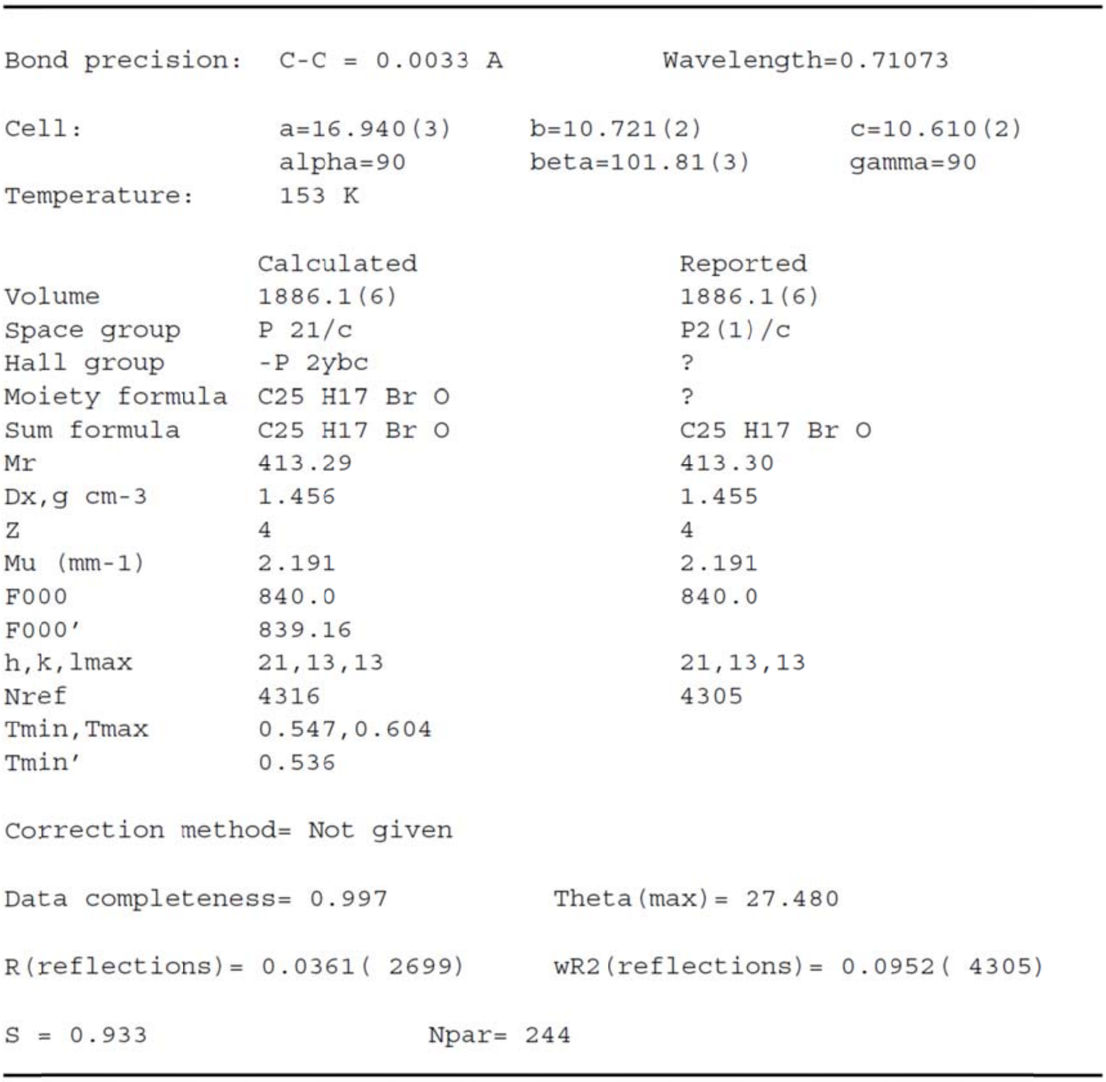
R(reflections)= 0.0449( 2214)     wR2(reflections)= 0.1329( 2895)

S = 1.121                 Npar= 218
```

Crystal data of product 4am’ (CCDC 1975387)



4am'



```
Bond precision:   C-C = 0.0033 A          Wavelength=0.71073

Cell:             a=16.940(3)     b=10.721(2)        c=10.610(2)
                  alpha=90        beta=101.81(3)     gamma=90
Temperature:      153 K

                Calculated                 Reported
Volume          1886.1(6)                  1886.1(6)
Space group     P 21/c                     P2(1)/c
Hall group      -P 2ybc                    ?
Moiety formula  C25 H17 Br O               ?
Sum formula     C25 H17 Br O               C25 H17 Br O
Mr              413.29                     413.30
Dx,g cm-3       1.456                      1.455
Z               4                          4
Mu (mm-1)       2.191                      2.191
F000            840.0                      840.0
F000’           839.16
h,k,lmax        21,13,13                   21,13,13
Nref            4316                       4305
Tmin,Tmax       0.547,0.604
Tmin’           0.536

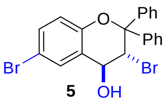
Correction method= Not given

Data completeness= 0.997            Theta(max)= 27.480

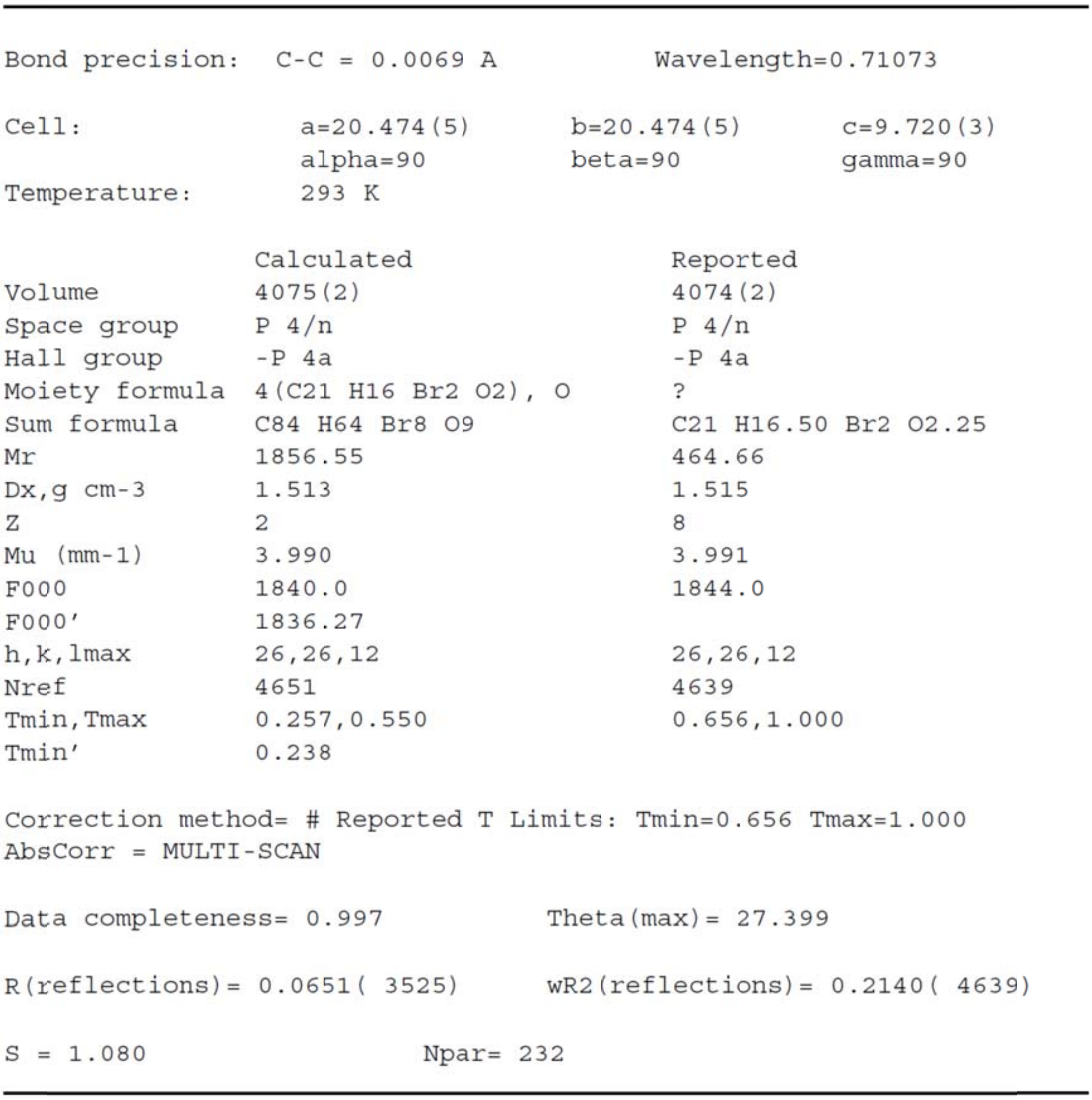
R(reflections)= 0.0361( 2699)      wR2(reflections)= 0.0952( 4305)

S = 0.933                   Npar= 244
```

Crystal data of product 5 (CCDC 1978345)



5



```
Bond precision:   C-C = 0.0069 A          Wavelength=0.71073

Cell:              a=20.474(5)      b=20.474(5)      c=9.720(3)
                   alpha=90         beta=90          gamma=90
Temperature:       293 K

                Calculated                 Reported
Volume          4075(2)                    4074(2)
Space group     P 4/n                      P 4/n
Hall group      -P 4a                      -P 4a
Moiety formula  4(C21 H16 Br2 O2), O       ?
Sum formula     C84 H64 Br8 O9             C21 H16.50 Br2 O2.25
Mr              1856.55                    464.66
Dx,g cm-3       1.513                      1.515
Z               2                          8
Mu (mm-1)       3.990                      3.991
F000            1840.0                     1844.0
F000'           1836.27
h,k,lmax        26,26,12                   26,26,12
Nref            4651                       4639
Tmin,Tmax       0.257,0.550                0.656,1.000
Tmin'           0.238

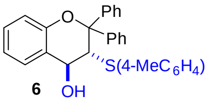
Correction method= # Reported T Limits: Tmin=0.656 Tmax=1.000
AbsCorr = MULTI-SCAN

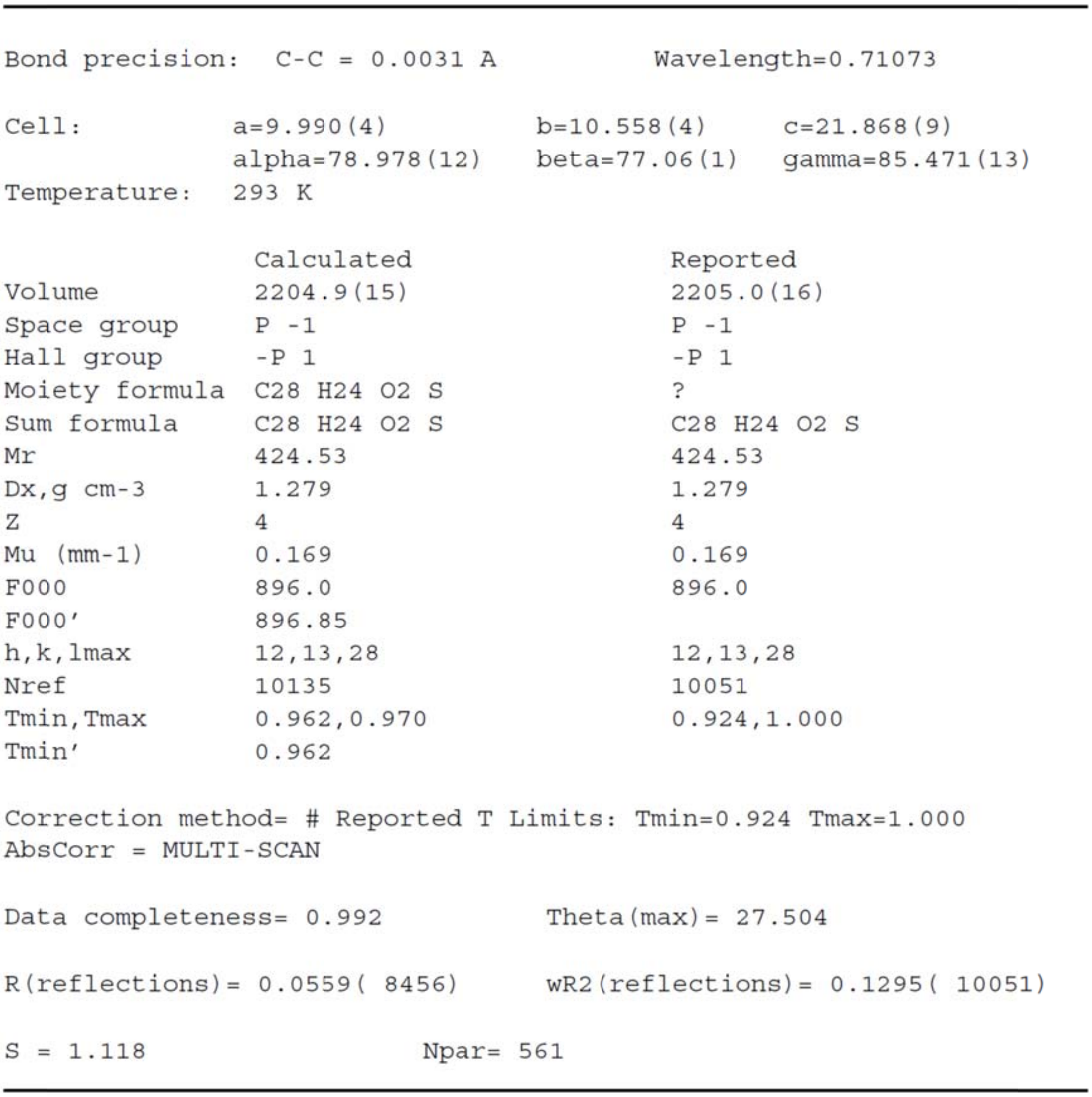
Data completeness= 0.997          Theta(max)= 27.399

R(reflections)= 0.0651( 3525)     wR2(reflections)= 0.2140( 4639)

S = 1.080                   Npar= 232
```

Crystal data of product 6 (CCDC 1978346)


6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Bond precision:   C-C = 0.0031 A          Wavelength=0.71073

Cell:           a=9.990(4)          b=10.558(4)     c=21.868(9)
                alpha=78.978(12)    beta=77.06(1)   gamma=85.471(13)
Temperature:    293 K

                  Calculated                Reported
Volume            2204.9(15)                2205.0(16)
Space group       P -1                      P -1
Hall group        -P 1                      -P 1
Moiety formula    C28 H24 O2 S              ?
Sum formula       C28 H24 O2 S              C28 H24 O2 S
Mr                424.53                    424.53
Dx,g cm-3         1.279                     1.279
Z                 4                         4
Mu (mm-1)         0.169                     0.169
F000              896.0                     896.0
F000'             896.85
h,k,lmax          12,13,28                  12,13,28
Nref              10135                     10051
Tmin,Tmax         0.962,0.970               0.924,1.000
Tmin'             0.962

Correction method= # Reported T Limits: Tmin=0.924 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992           Theta(max)= 27.504

R(reflections)= 0.0559( 8456)      wR2(reflections)= 0.1295( 10051)

S = 1.118                    Npar= 561
```

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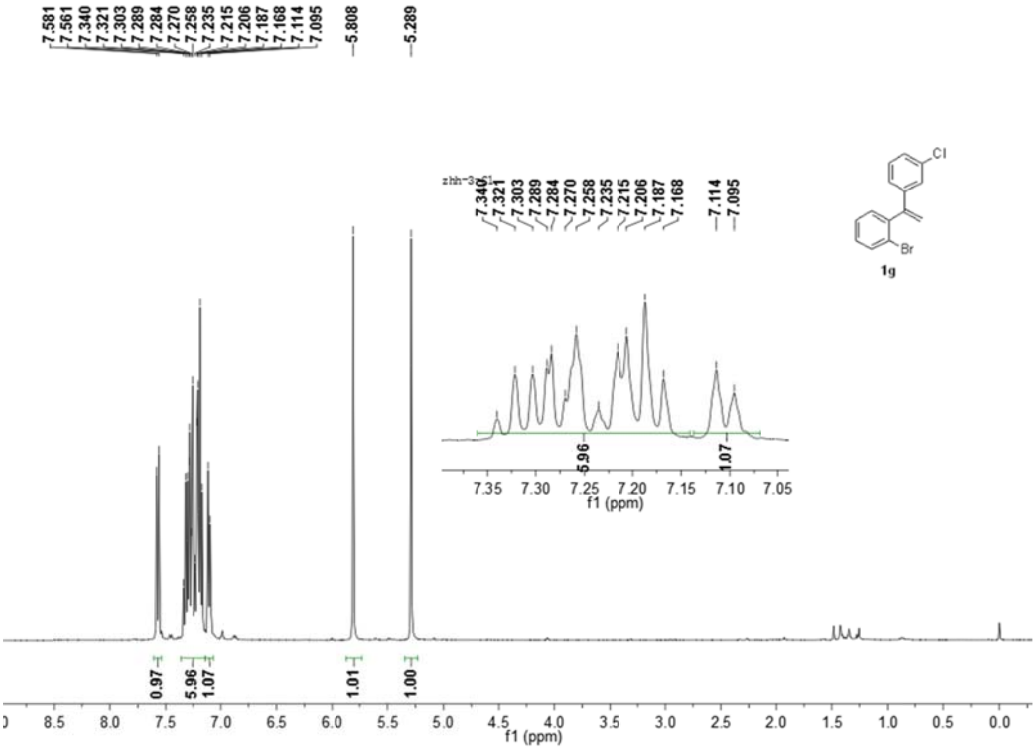
NMR Spectra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7.340
7.321
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7.284
7.270
7.258
7.235
7.215
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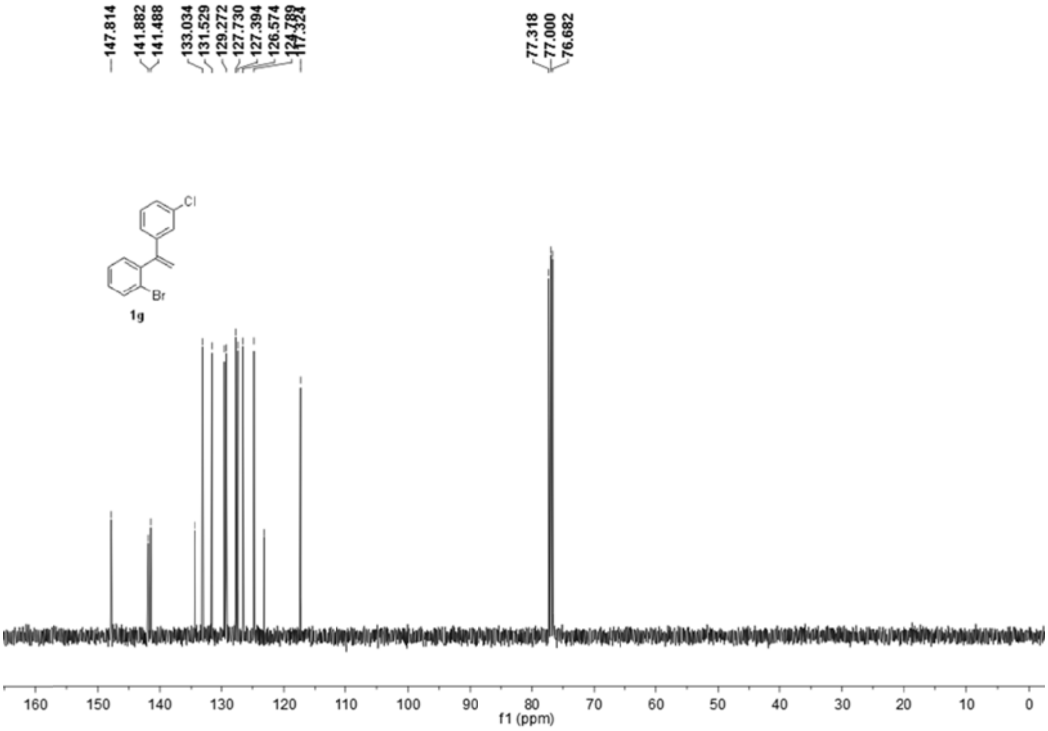
7.187
7.168
7.114
7.095
5.808
5.289
zhh-3-51
Cl
Br
1g
5.96
1.07
7.35 7.30 7.25 7.20 7.15 7.10 7.05
f1 (ppm)
0.97
5.96
1.07
1.01
1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


147.814
141.882
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129.272
127.730
127.394
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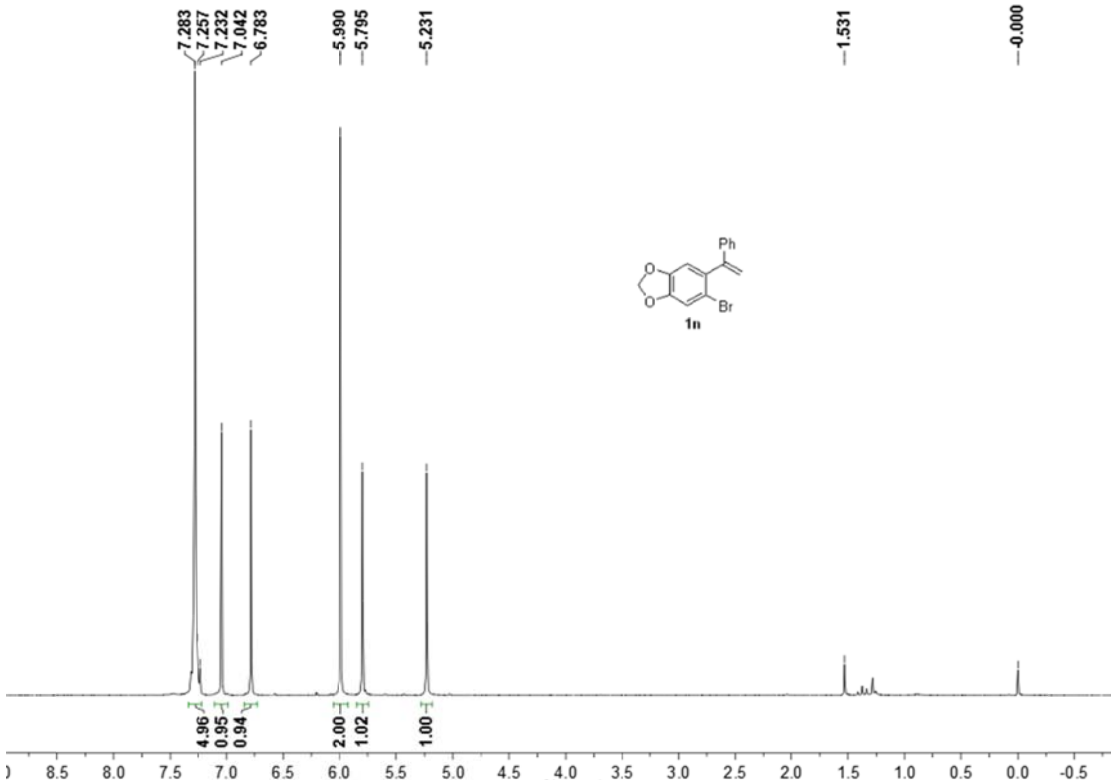
77.000
76.682
Cl
Br
1g
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.283
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7.232
7.042
6.783
5.990
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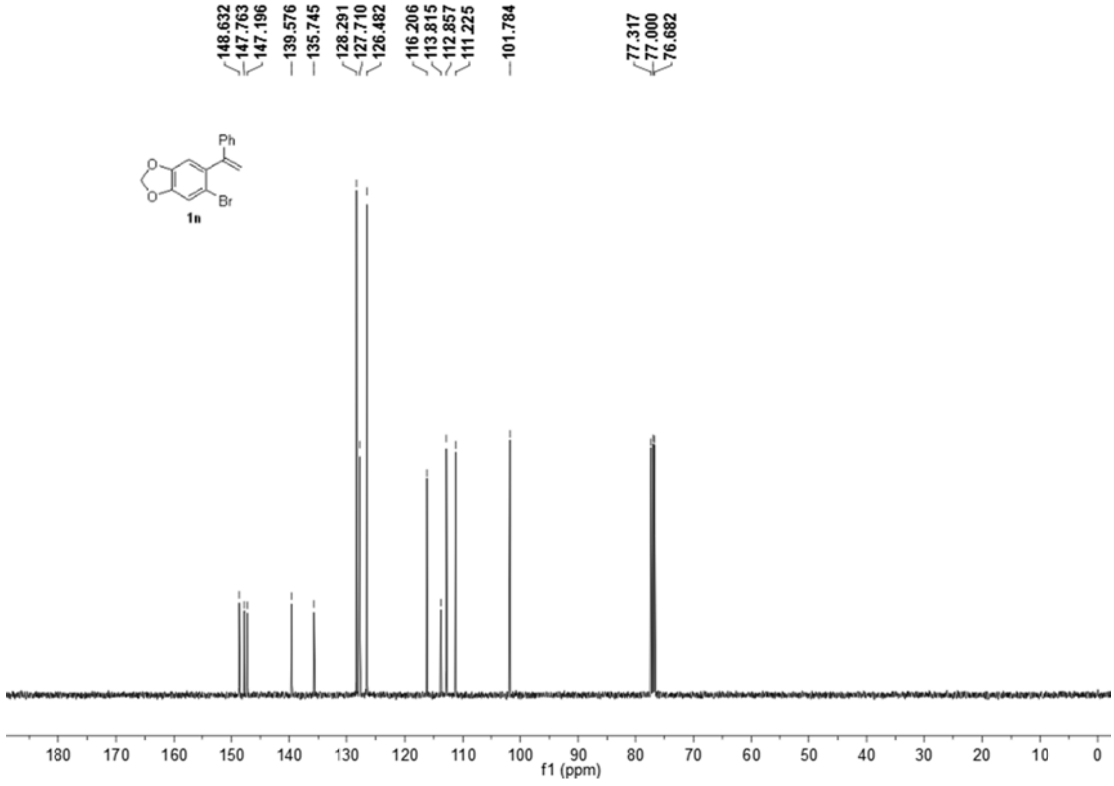
5.231
1.531
0.000
Ph
O
O
Br
1n
4.96
0.95
0.94
2.00
1.02
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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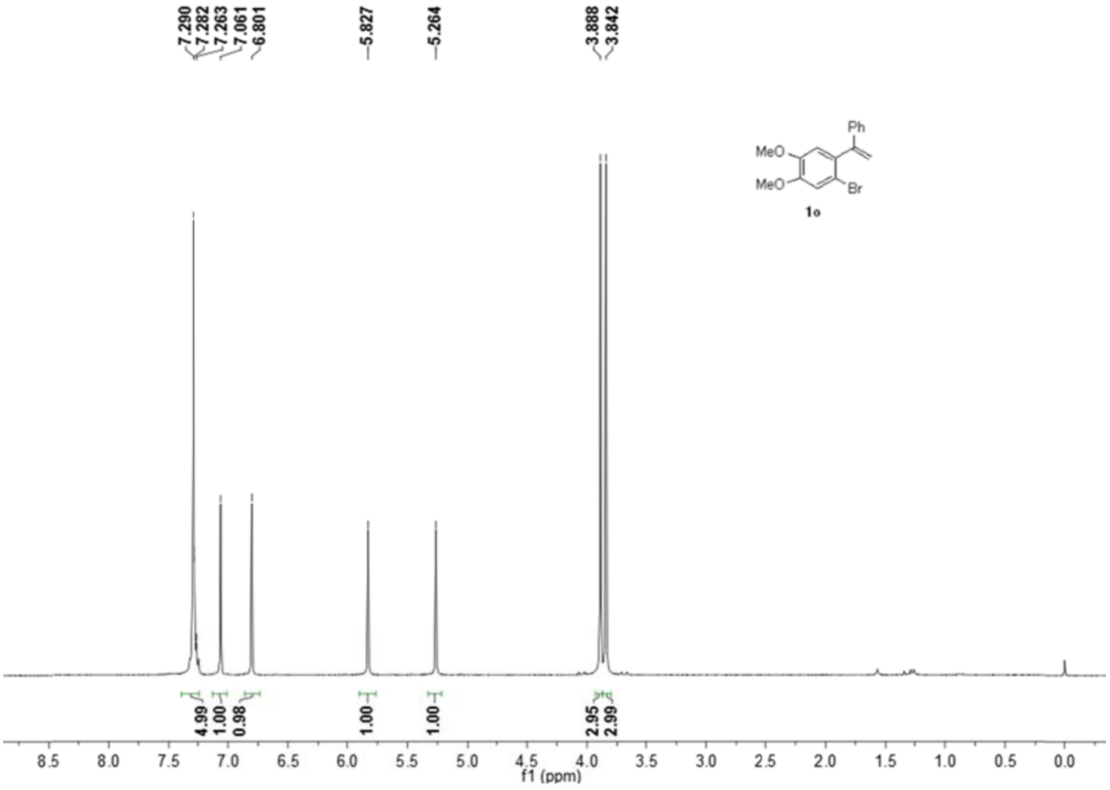
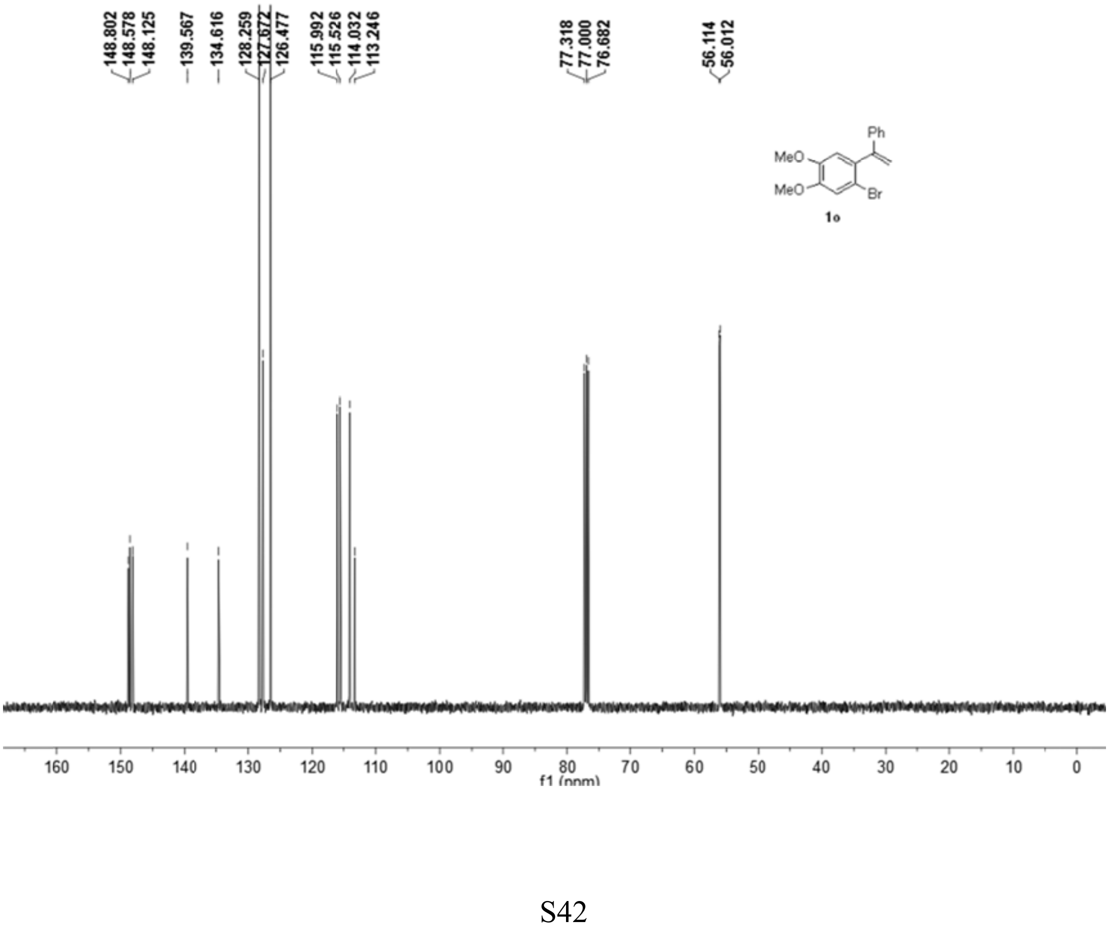
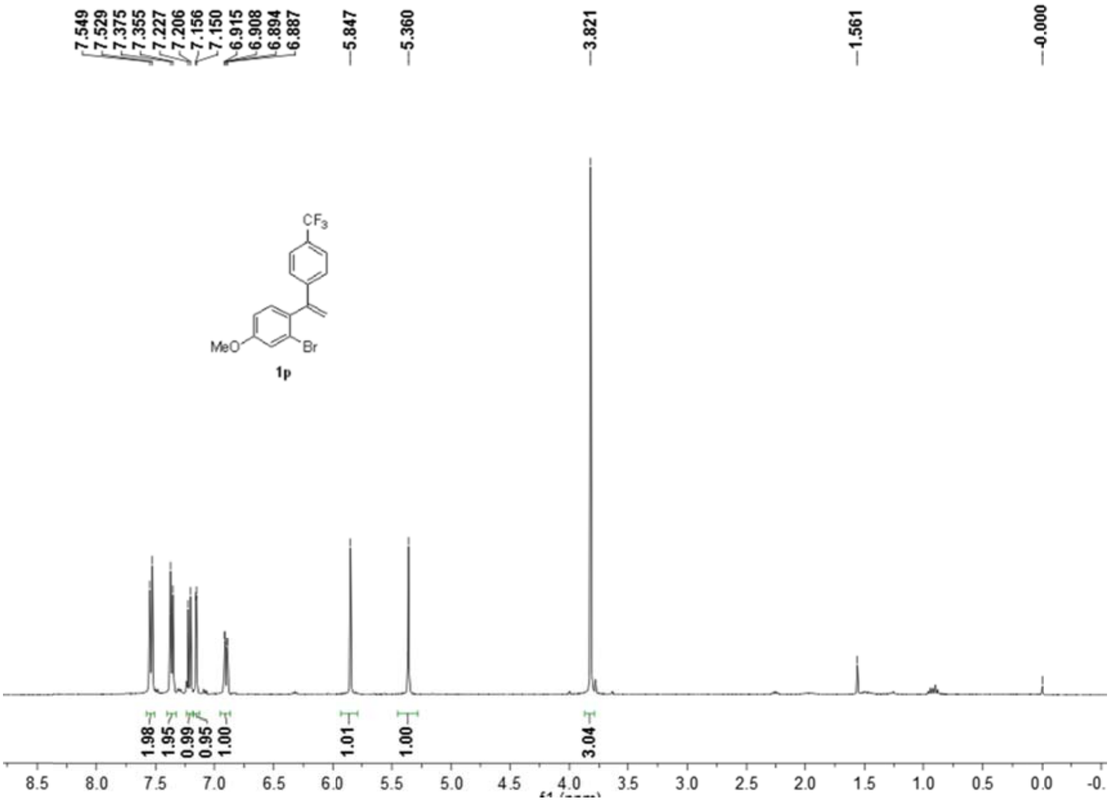
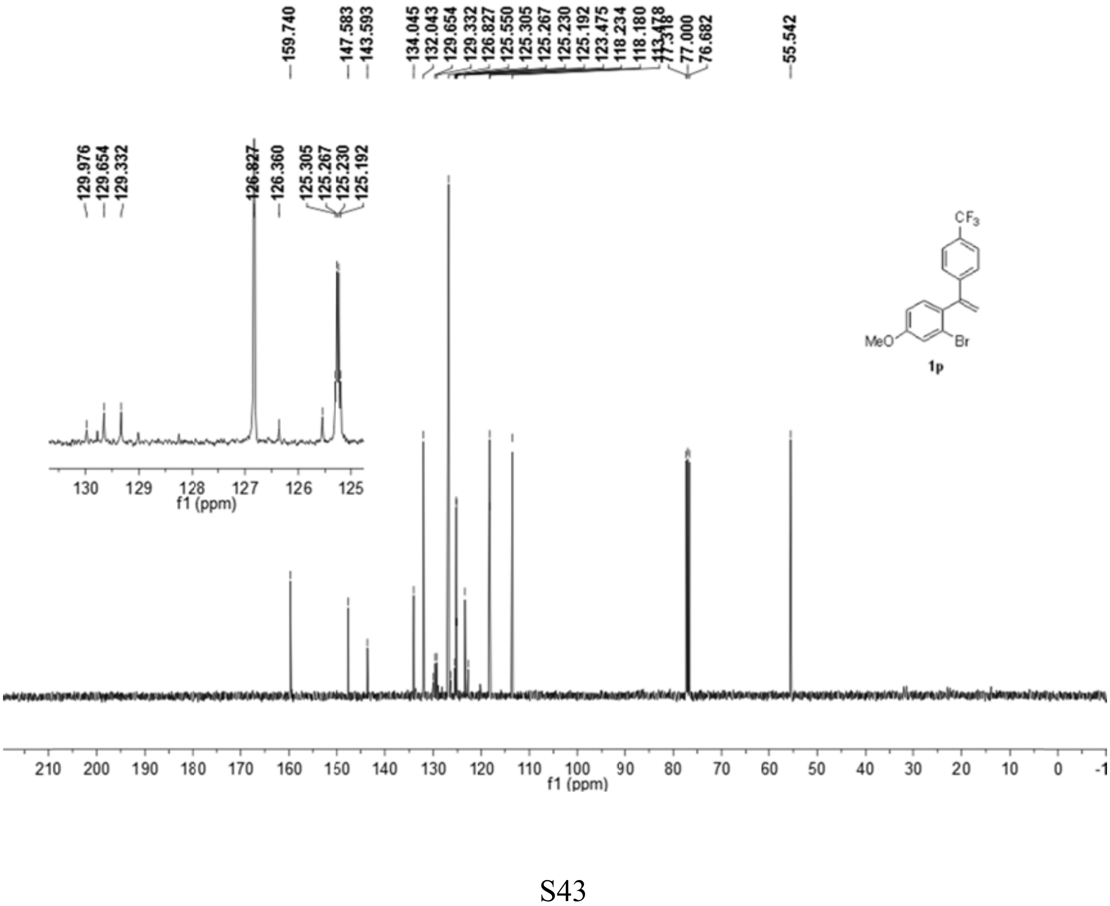
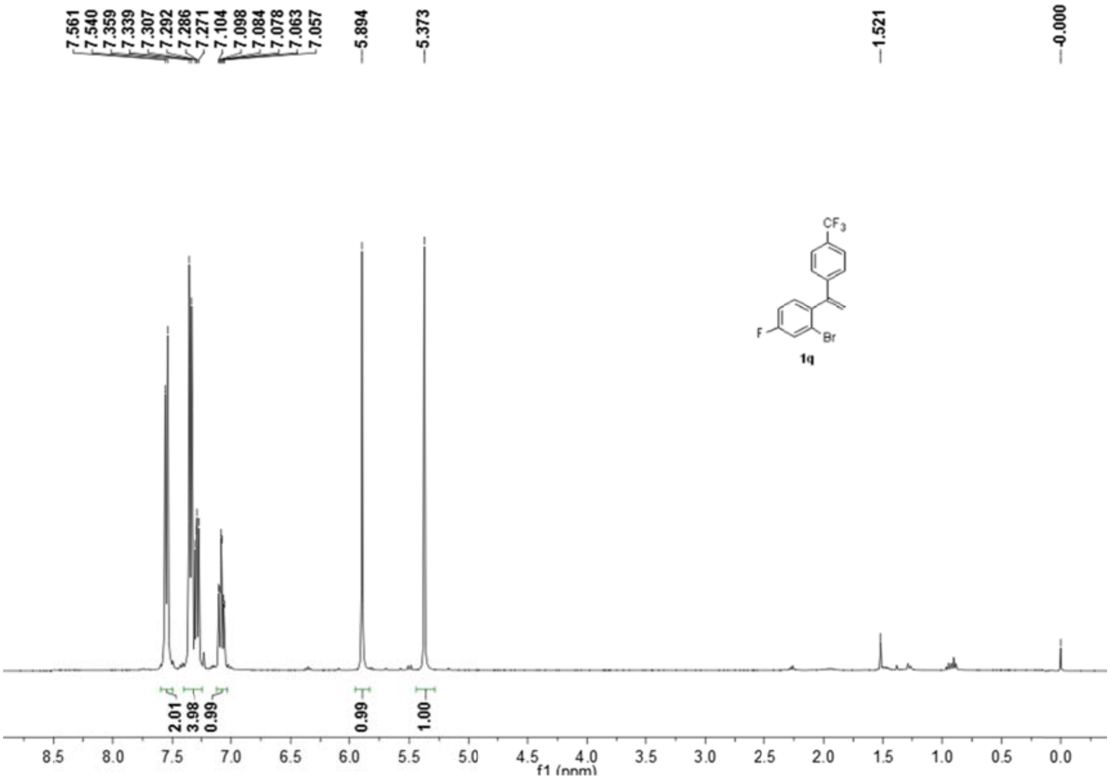
147.763
147.196
139.576
135.745
128.291
127.710
126.482
116.206
113.815
112.857
111.225
101.784
77.317
77.000
76.682
Ph
O
O
Br
1n
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

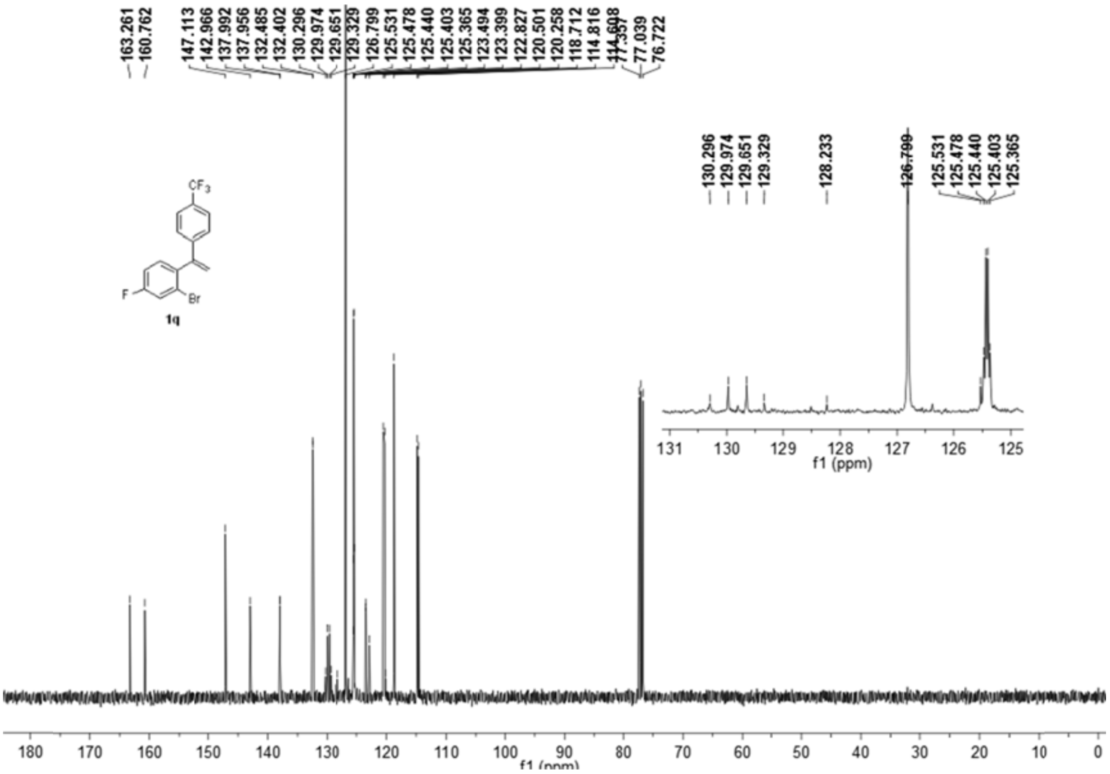

7.290
7.282
7.263
7.061
6.801
5.827
5.264
3.888
3.842
Ph
MeO
MeO
Br
1o
4.99
1.00
0.98
1.00
1.00
2.95
2.99
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

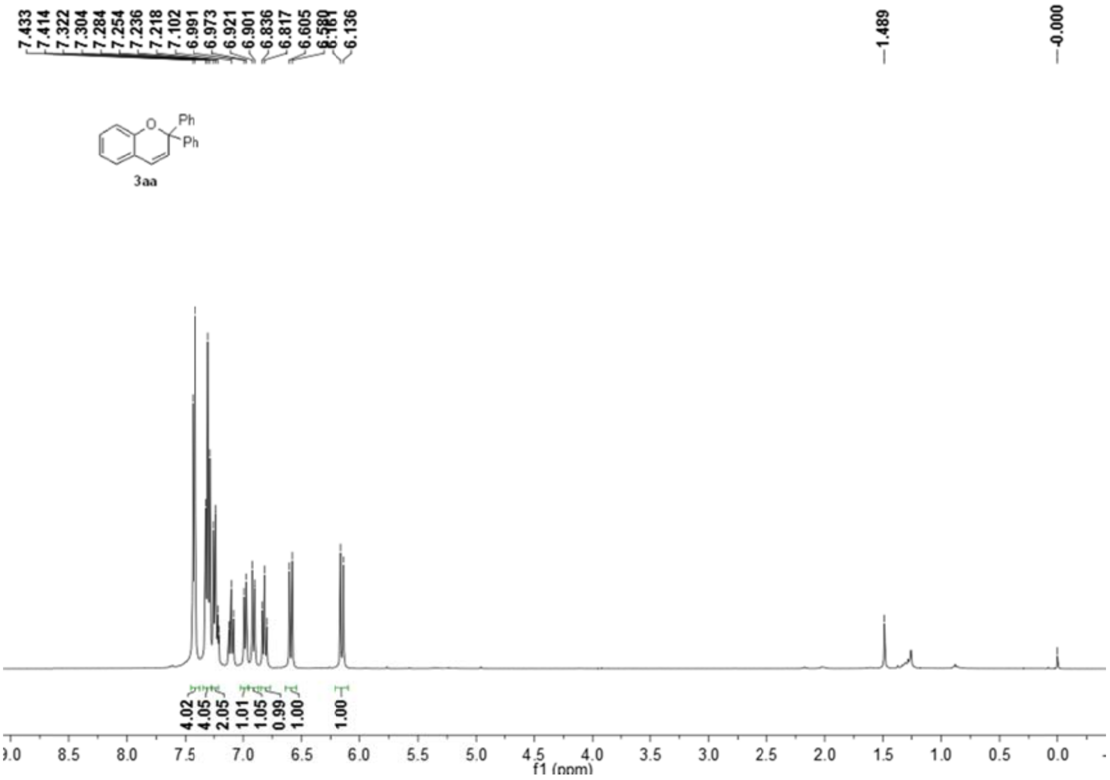

148.802
148.578
148.125
139.567
134.616
128.259
127.672
126.477
115.992
115.526
114.032
113.246
77.318
77.000
76.682
56.114
56.012
Ph
MeO
MeO
Br
1o
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

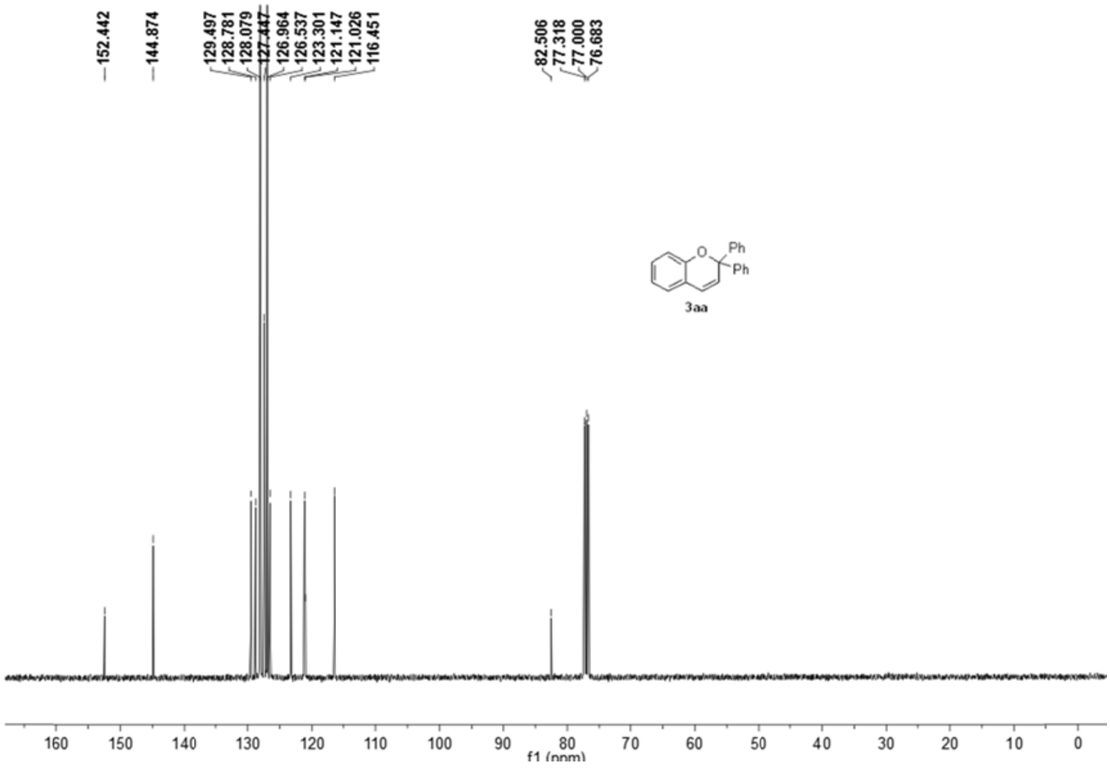

7.549
7.529
7.375
7.355
7.227
7.206
7.156
7.150
6.915
6.908
6.894
6.887
5.847
5.360
3.821
1.561
0.000
CF3
MeO
Br
1p
1.98
1.95
0.99
0.95
1.00
1.01
1.00
3.04
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

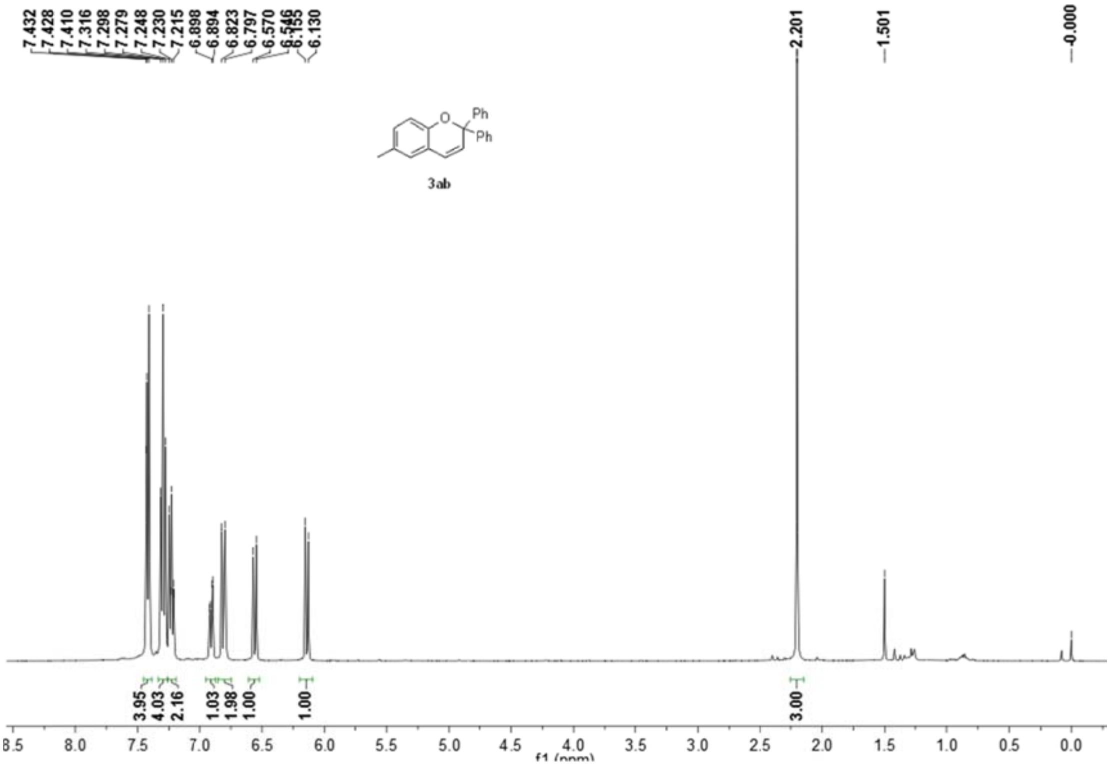

159.740
147.583
143.593
134.045
132.043
129.654
129.332
126.827
125.550
125.305
125.267
125.230
125.192
123.475
118.234
118.180
113.478
77.318
77.000
76.682
55.542
129.976
129.654
129.332
126.827
126.360
125.305
125.267
125.230
125.192
130 129 128 127 126 125
f1 (ppm)
CF3
MeO
Br
1p
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

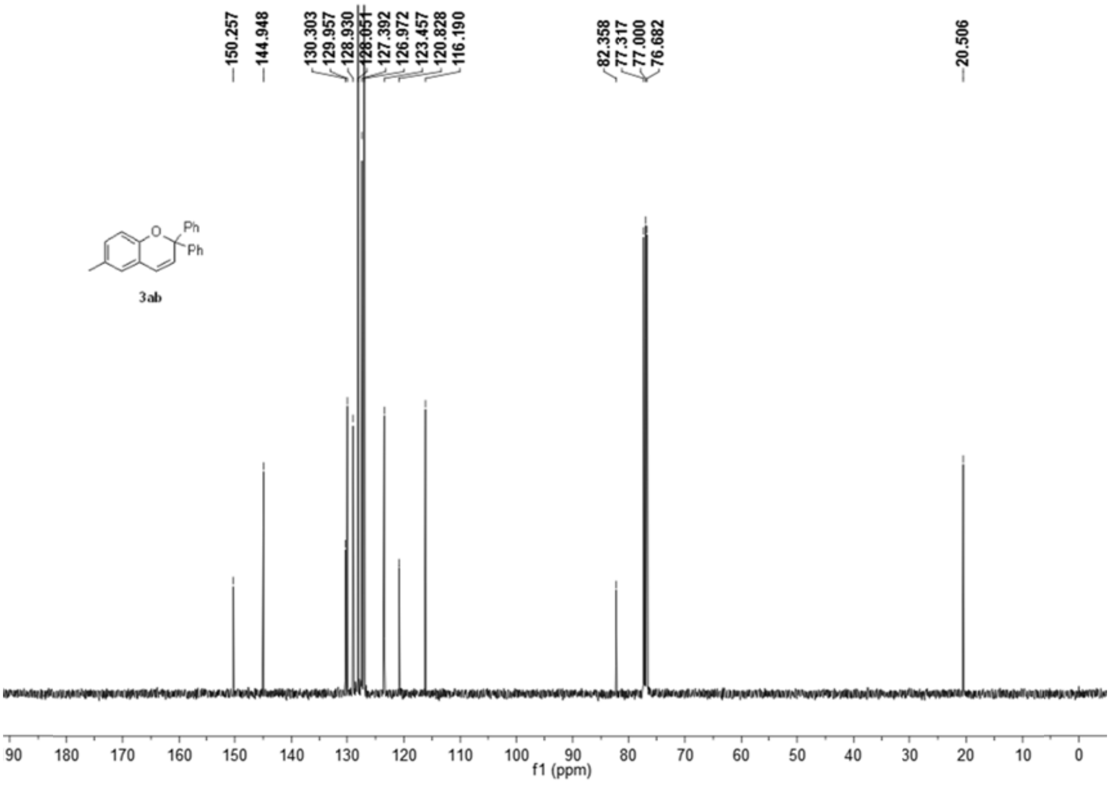

7.561
7.540
7.359
7.339
7.307
7.292
7.286
7.271
7.104
7.098
7.084
7.078
7.063
7.057
5.894
5.373
1.521
-0.000
CF3
F
Br
1q
2.01
3.98
0.99
0.99
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

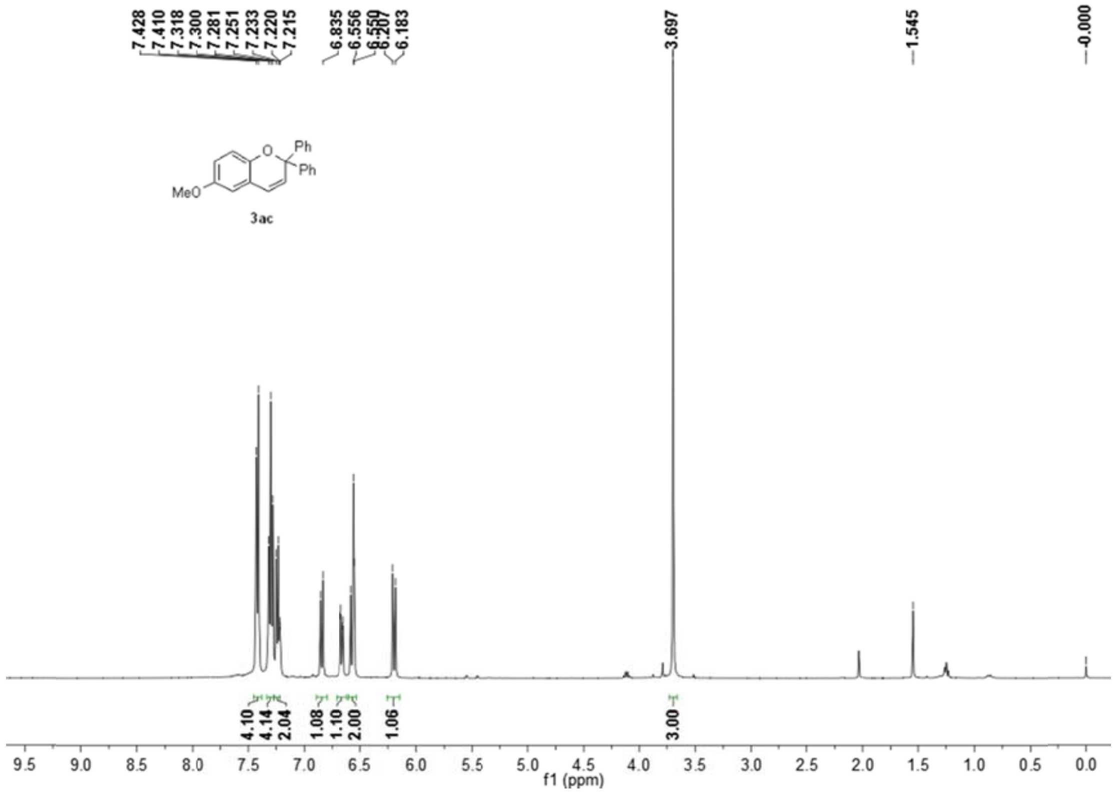

163.261
160.762
147.113
142.966
137.992
137.956
132.485
132.402
130.296
129.974
129.651
129.329
126.799
125.531
125.478
125.440
125.403
125.365
123.494
123.399
122.827
120.501
120.258
118.712
114.816
114.608
77.357
77.039
76.722
CF3
F
Br
1q
130.296
129.974
129.651
129.329
128.233
126.799
125.531
125.478
125.440
125.403
125.365
131
130
129
128
127
126
125
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

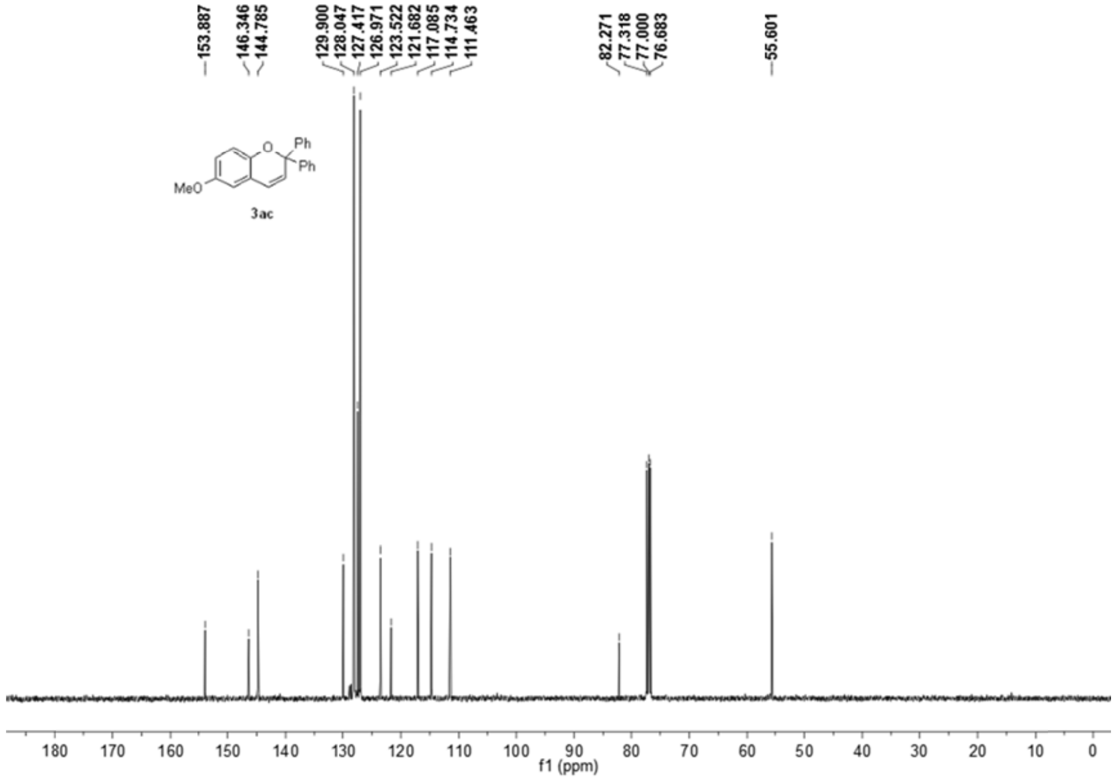

7.433
7.414
7.322
7.304
7.284
7.254
7.236
7.218
7.102
6.991
6.973
6.921
6.901
6.836
6.817
6.605
6.580
6.161
6.136
1.489
-0.000
O
Ph
Ph
3aa
4.02
4.05
2.05
1.01
1.05
0.99
1.00
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

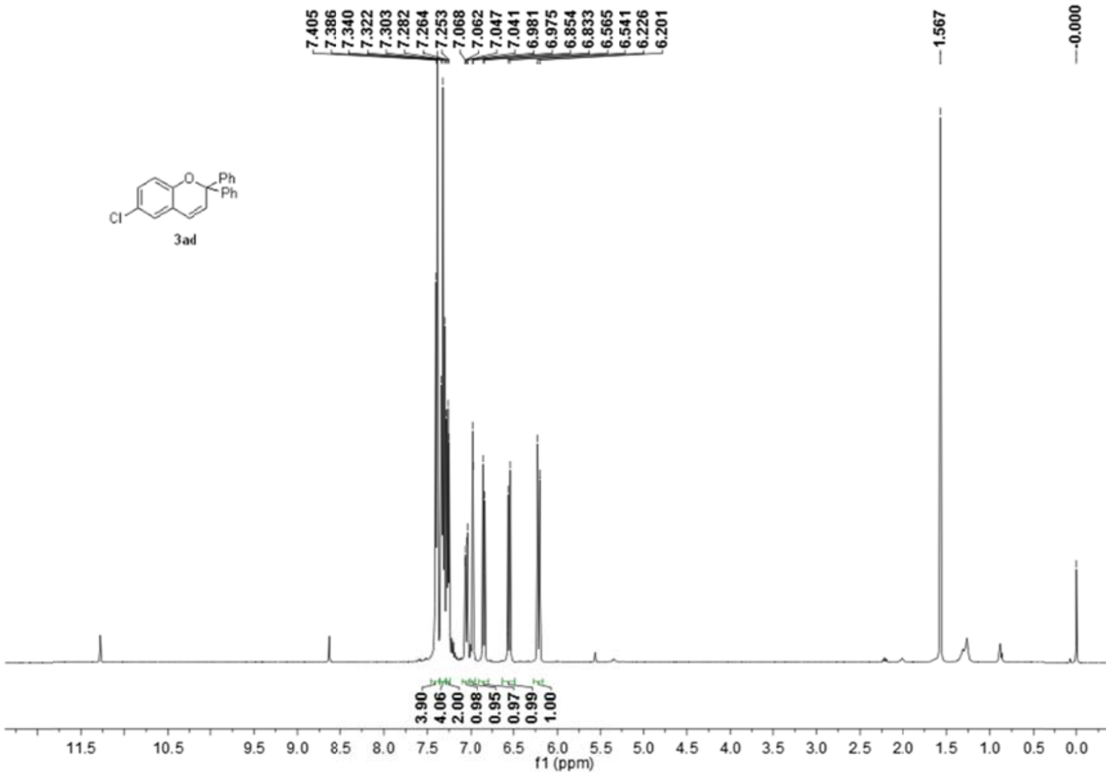

152.442
144.874
129.497
128.781
128.079
127.447
126.964
126.537
123.301
121.147
121.026
116.451
82.506
77.318
77.000
76.683
O
Ph
Ph
3aa
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

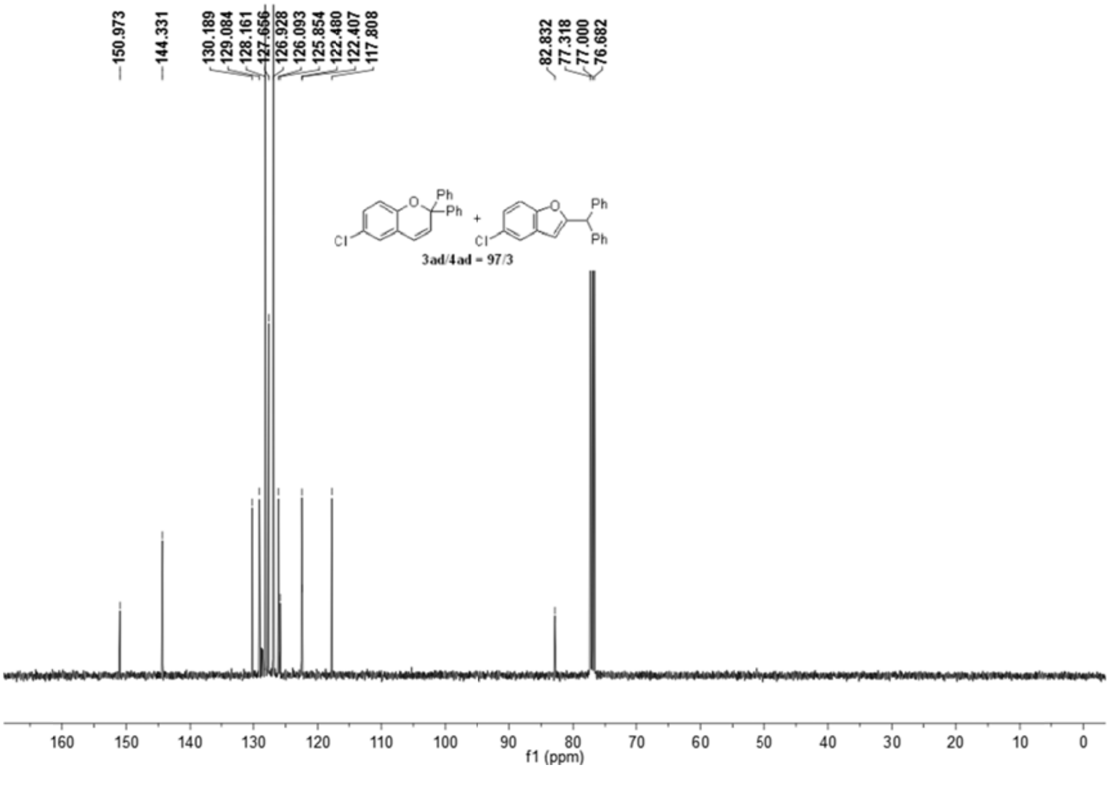

7.432
7.428
7.410
7.316
7.298
7.279
7.248
7.230
7.215
6.898
6.894
6.823
6.797
6.570
6.546
6.155
6.130
2.201
1.501
0.000
Ph
Ph
O
3ab
3.95
4.03
2.16
1.03
1.98
1.00
1.00
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

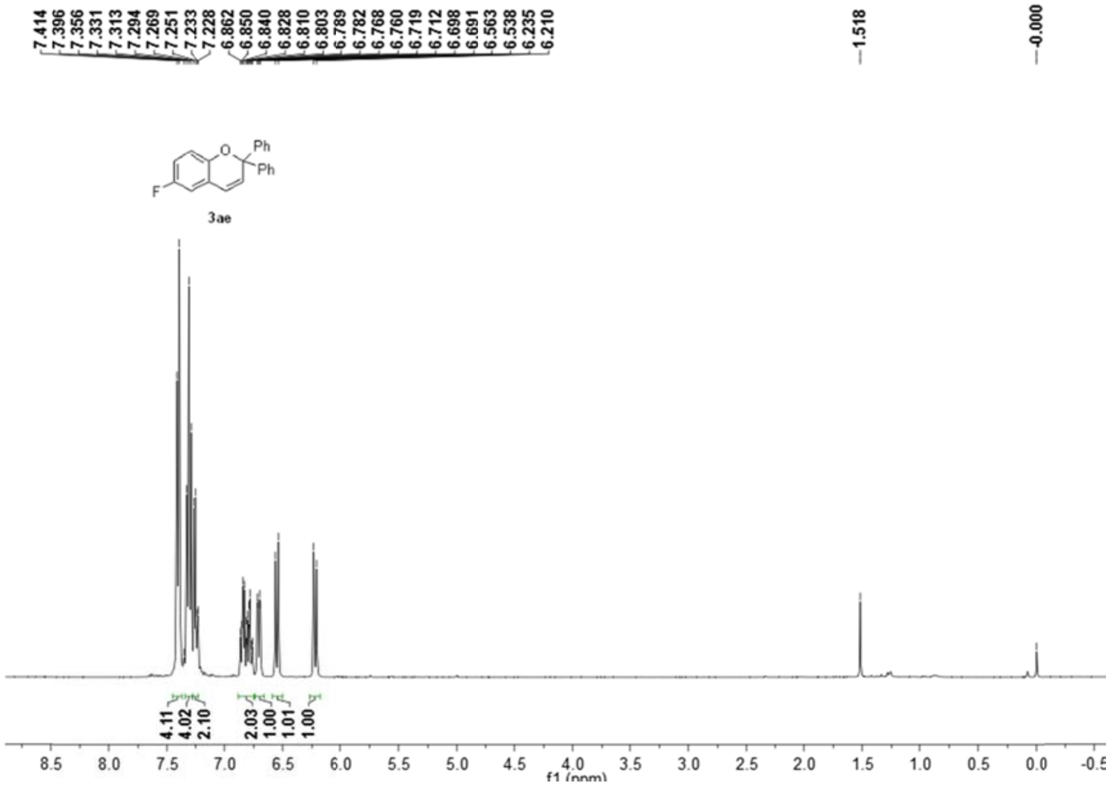

150.257
144.948
130.303
129.957
128.930
128.051
127.392
126.972
123.457
120.828
116.190
82.358
77.317
77.000
76.682
20.506
Ph
Ph
O
3ab
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

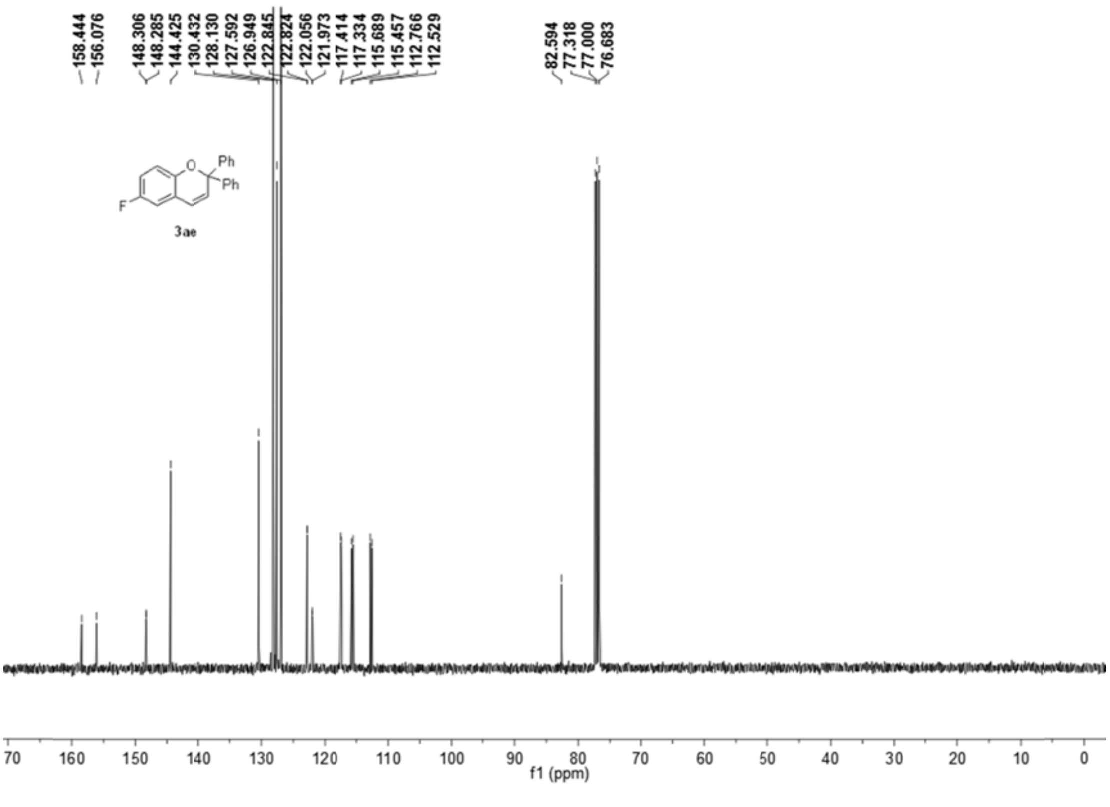

7.428
7.410
7.318
7.300
7.281
7.251
7.233
7.220
7.215
6.835
6.556
6.550
6.207
6.183
3.697
1.545
-0.000
O
Ph
Ph
MeO
3ac
4.10
4.14
2.04
1.08
1.10
2.00
1.06
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

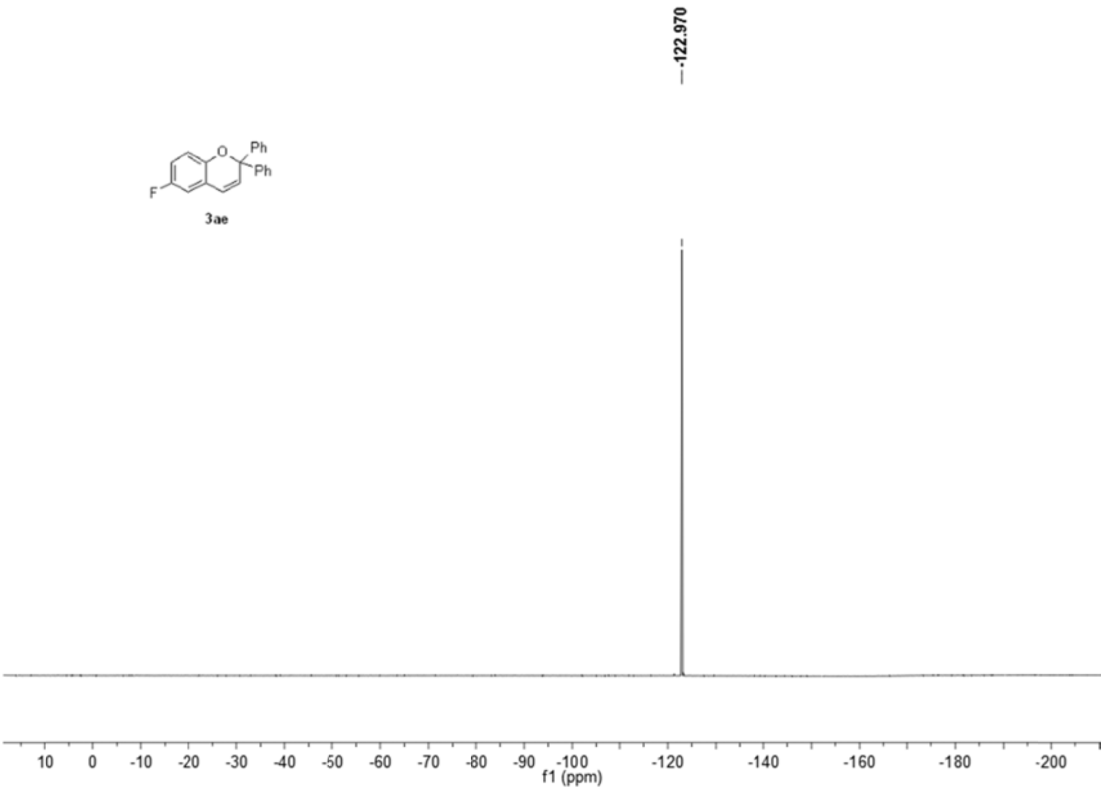

153.887
146.346
144.785
129.900
128.047
127.417
126.971
123.522
121.682
117.085
114.734
111.463
82.271
77.318
77.000
76.683
55.601
O
Ph
Ph
MeO
3ac
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.405
7.386
7.340
7.322
7.303
7.282
7.264
7.253
7.068
7.062
7.047
7.041
6.981
6.975
6.854
6.833
6.565
6.541
6.226
6.201
1.567
-0.000
O
Ph
Ph
Cl
3ad
3.90
4.06
2.00
0.98
0.95
0.97
0.99
1.00
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)


150.973
144.331
130.189
129.084
128.161
127.656
126.928
126.093
125.854
122.480
122.407
117.808
82.832
77.318
77.000
76.682
O
Ph
Ph
Cl
+
O
Ph
Ph
Cl
3ad/4ad = 97/3
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

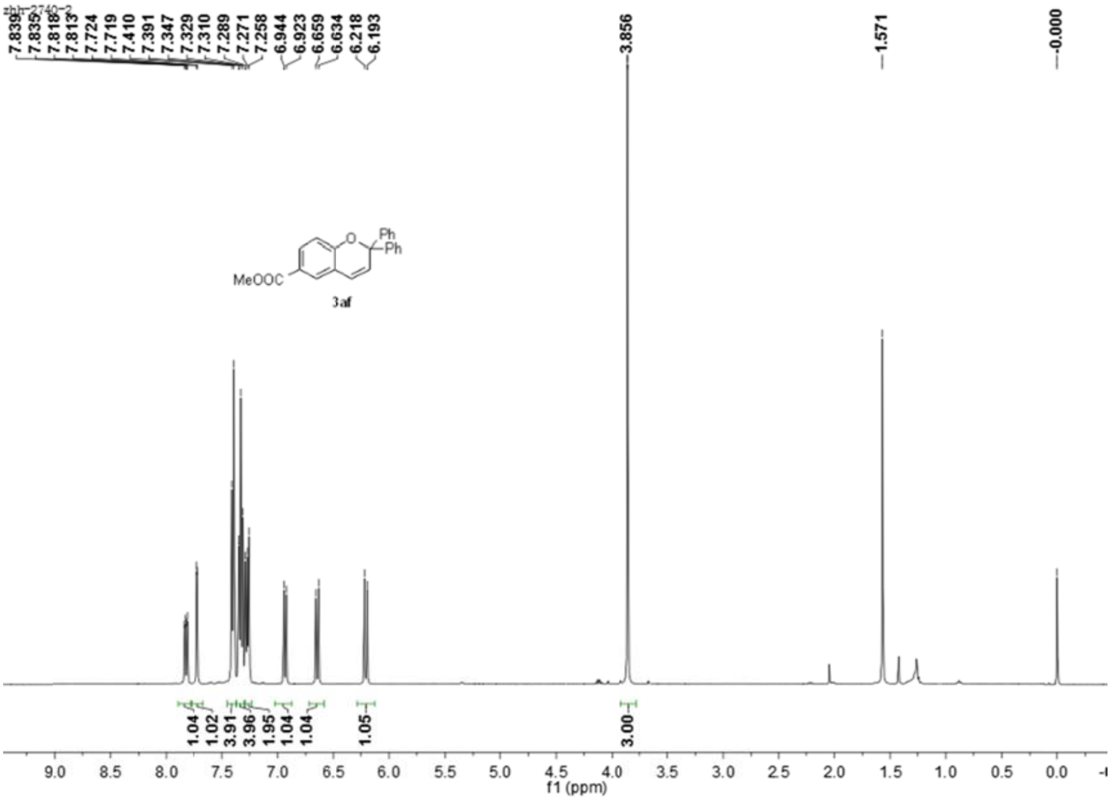

7.414
7.396
7.356
7.331
7.313
7.294
7.269
7.251
7.233
7.228
6.862
6.850
6.840
6.828
6.810
6.803
6.789
6.782
6.768
6.760
6.719
6.712
6.698
6.691
6.563
6.538
6.235
6.210
1.518
0.000
O
Ph
Ph
F
3ae
4.11
4.02
2.10
2.03
1.00
1.01
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

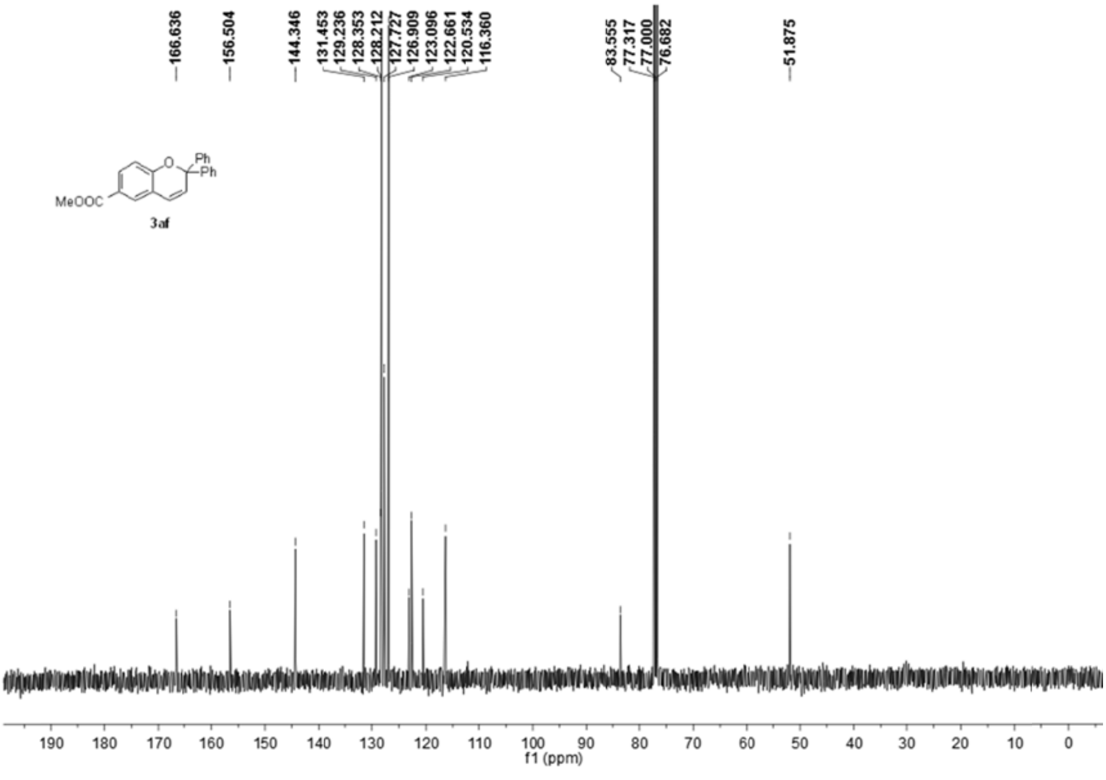

158.444
156.076
148.306
148.285
144.425
130.432
128.130
127.592
126.949
122.845
122.824
122.056
121.973
117.414
117.334
115.689
115.457
112.766
112.529
82.594
77.318
77.000
76.683
O
Ph
Ph
F
3ae
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

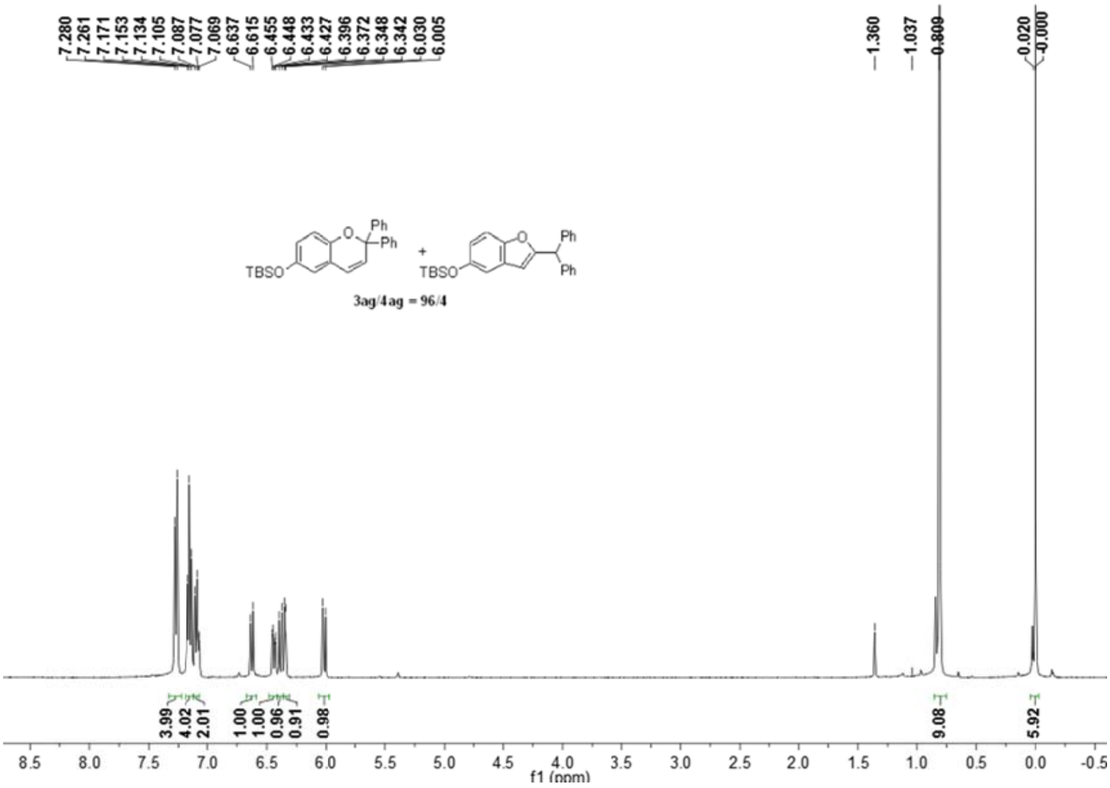


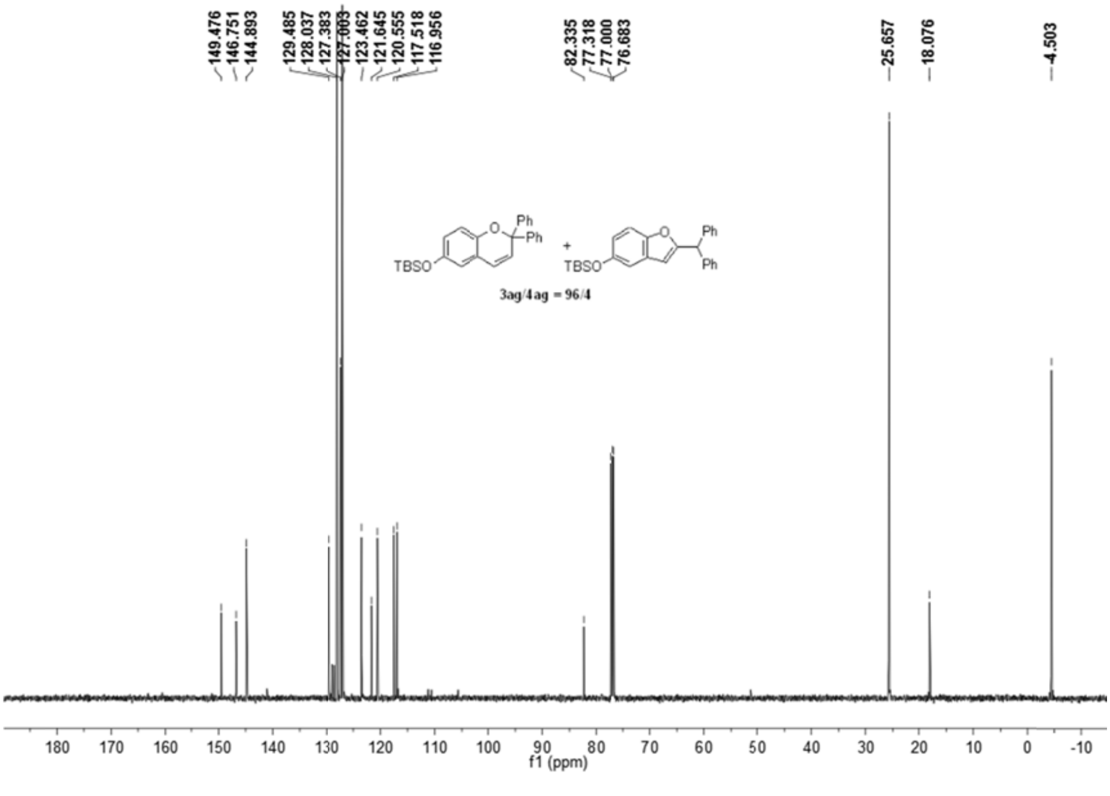
3ae

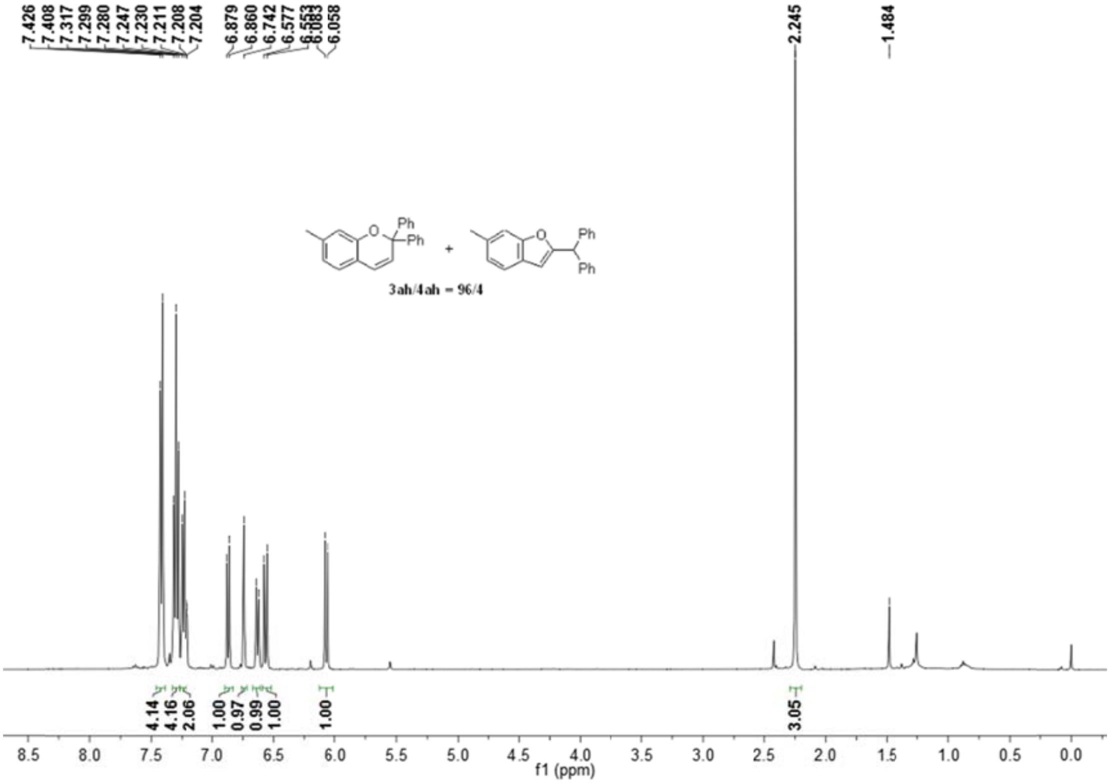
-122.970
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)


zhh-2740-2
7.839
7.835
7.818
7.813
7.724
7.719
7.410
7.391
7.347
7.329
7.310
7.289
7.271
7.258
6.944
6.923
6.659
6.634
6.218
6.193
3.856
1.571
0.000
MeOOC
O
Ph
Ph
3af
1.04
1.02
3.91
3.96
1.95
1.04
1.04
1.05
3.00
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)

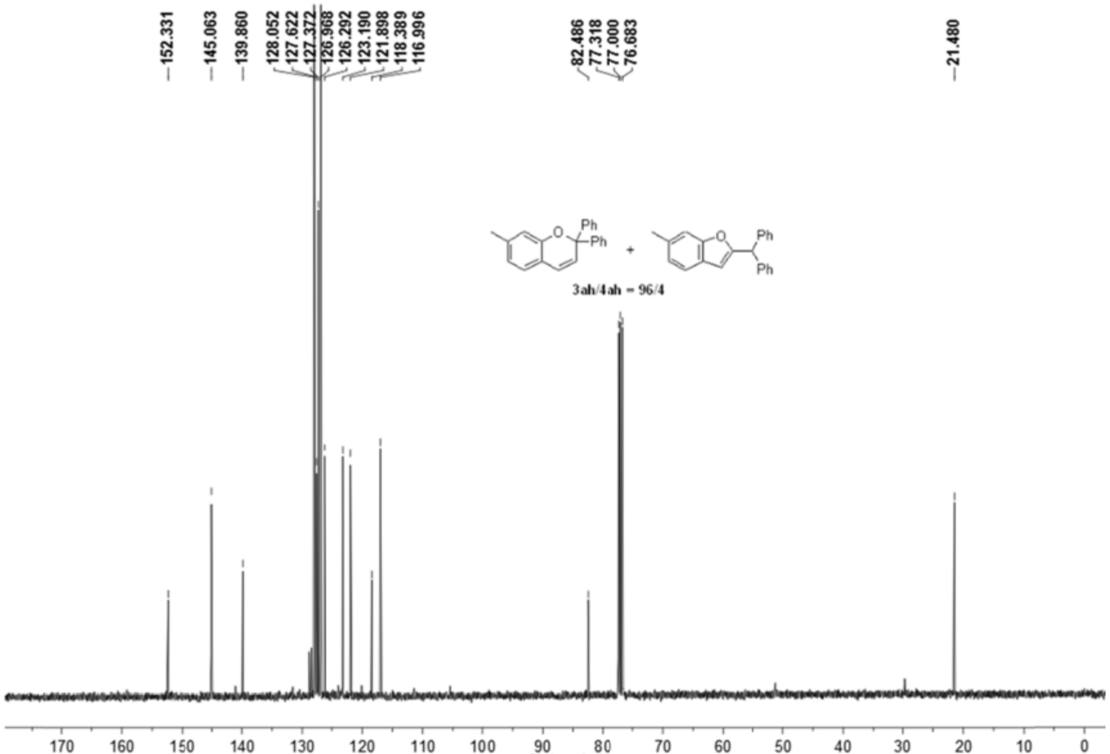

166.636
156.504
144.346
131.453
129.236
128.353
128.212
127.727
126.909
123.096
122.661
120.534
116.360
83.555
77.317
77.000
76.682
51.875
MeOOC
O
Ph
Ph
3af
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.280
7.261
7.171
7.153
7.134
7.105
7.087
7.077
7.069
6.637
6.615
6.455
6.448
6.433
6.427
6.396
6.372
6.348
6.342
6.030
6.005
1.360
1.037
0.809
0.020
0.000
Ph
Ph
TBSO
+
Ph
TBSO
Ph
3ag/4ag = 96/4
3.99
4.02
2.01
1.00
1.00
0.96
0.91
0.98
9.08
5.92
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 -0.5
f1 (ppm)

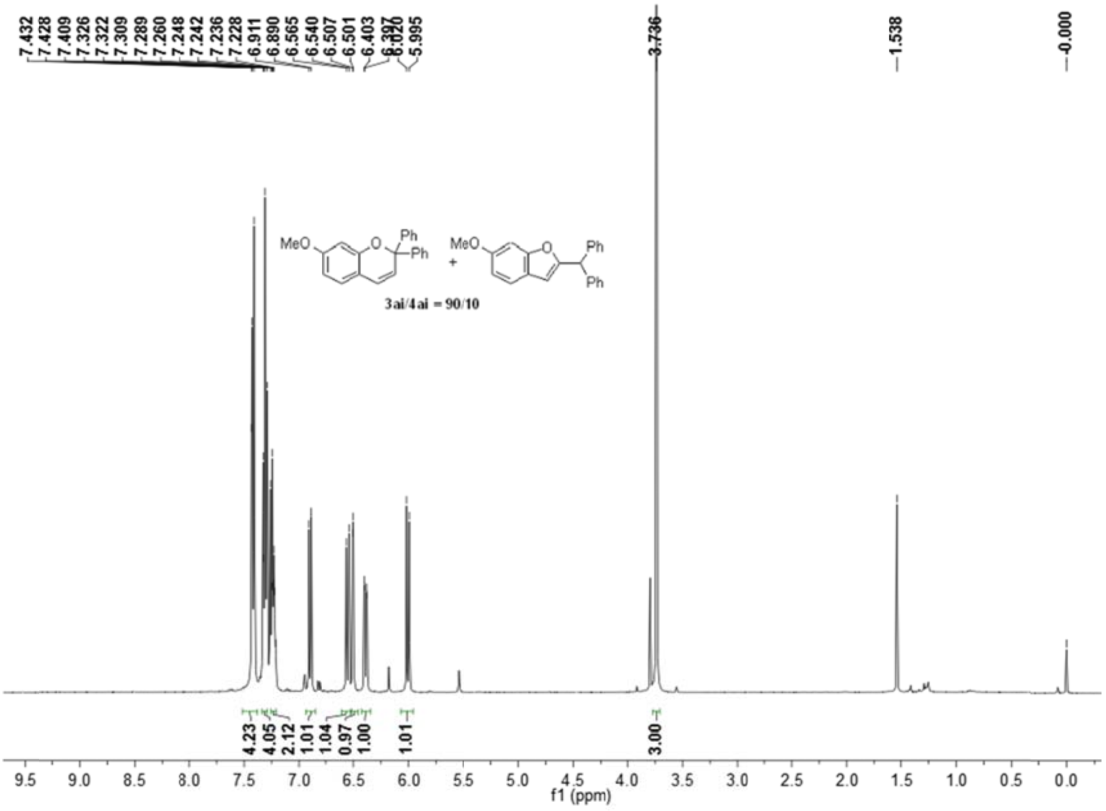

149.476
146.751
144.893
129.485
128.037
127.383
127.003
123.462
121.645
120.555
117.518
116.956
82.335
77.318
77.000
76.683
25.657
18.076
-4.503
Ph
Ph
TBSO
+
Ph
TBSO
Ph
3ag/4ag = 96/4
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

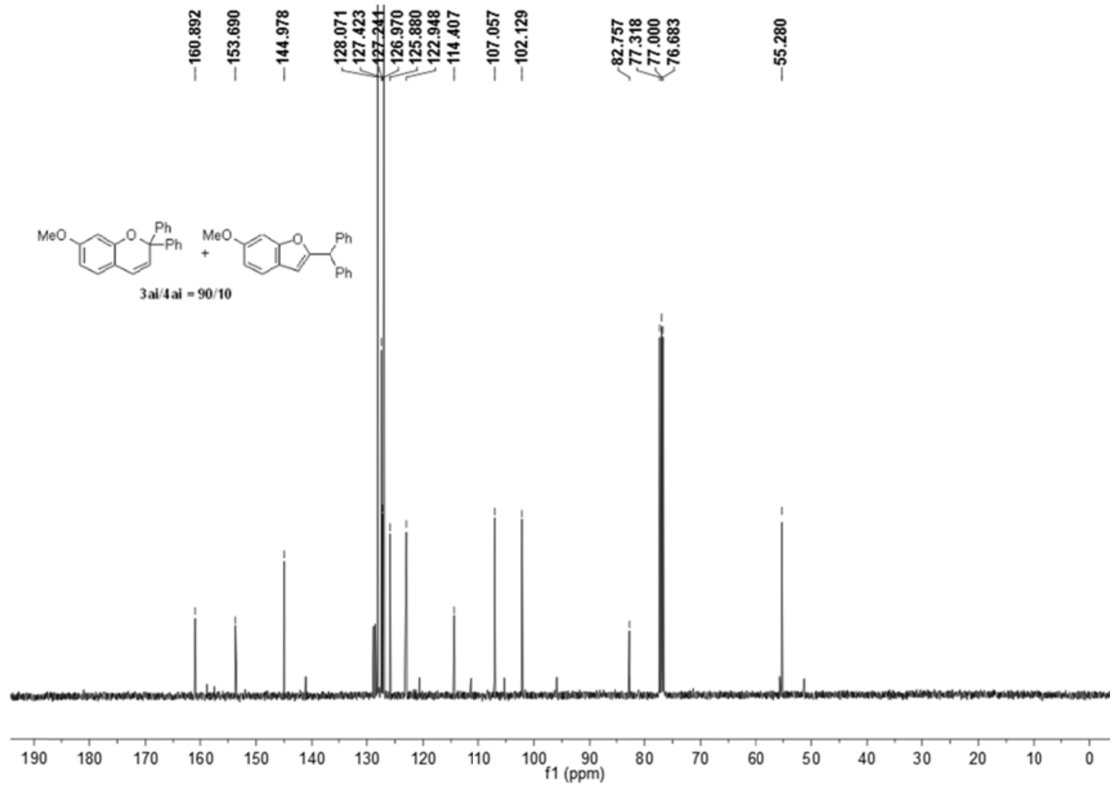


7.426
7.408
7.317
7.299
7.280
7.247
7.230
7.211
7.208
7.204
6.879
6.860
6.742
6.577
6.553
6.083
6.058
2.245
1.484
Ph
Ph
O
+
O
Ph
Ph
3ah/4ah = 96/4
4.14
4.16
2.06
1.00
0.97
0.99
1.00
1.00
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



152.331
145.063
139.860
128.052
127.622
127.372
126.968
126.292
123.190
121.898
118.389
116.996
82.486
77.318
77.000
76.683
21.480
Ph
Ph
O
+
O
Ph
Ph
3ah/4ah = 96/4
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.432
7.428
7.409
7.326
7.322
7.309
7.289
7.260
7.248
7.242
7.236
7.228
6.911
6.890
6.565
6.540
6.507
6.501
6.403
6.397
6.020
5.995
3.736
1.538
-0.000
MeO
O
Ph
Ph
+
MeO
O
Ph
Ph
3ai/4ai = 90/10
4.23
4.05
2.12
1.01
1.04
0.97
1.00
1.01
3.00
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)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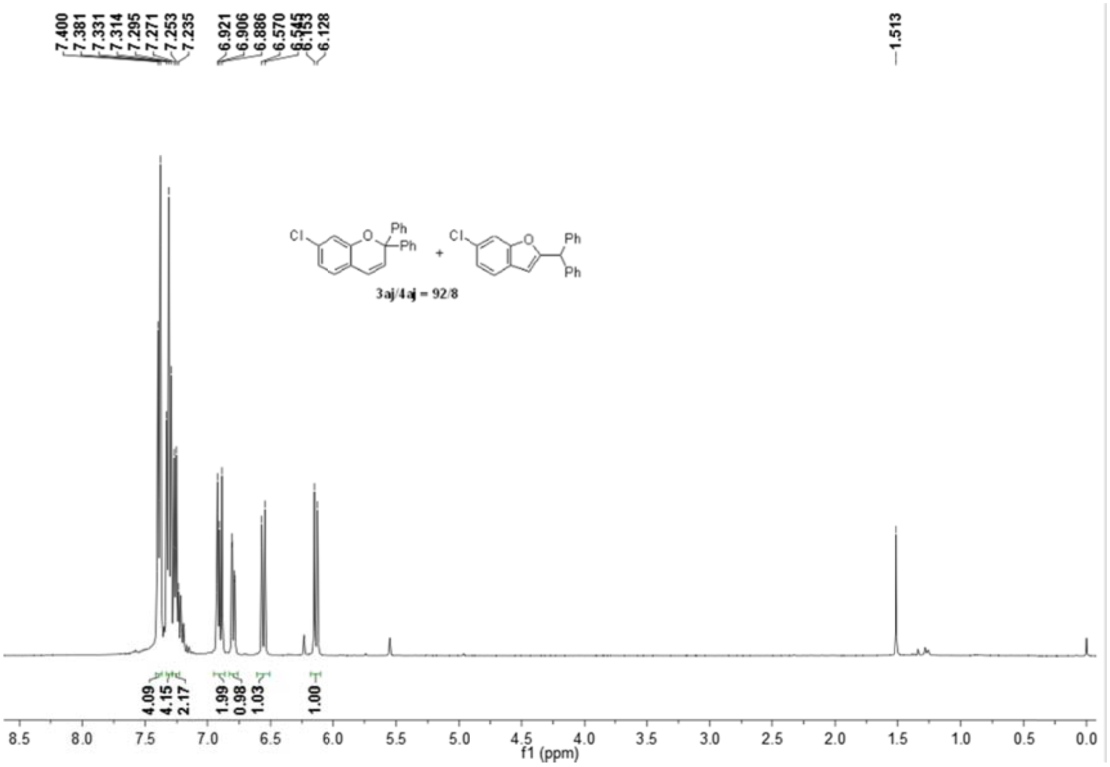
153.690
144.978
128.071
127.423
127.241
126.970
125.880
122.948
114.407
107.057
102.129
82.757
77.318
77.000
76.683
55.280
MeO
O
Ph
Ph
+
MeO
O
Ph
Ph
3ai/4ai = 90/10
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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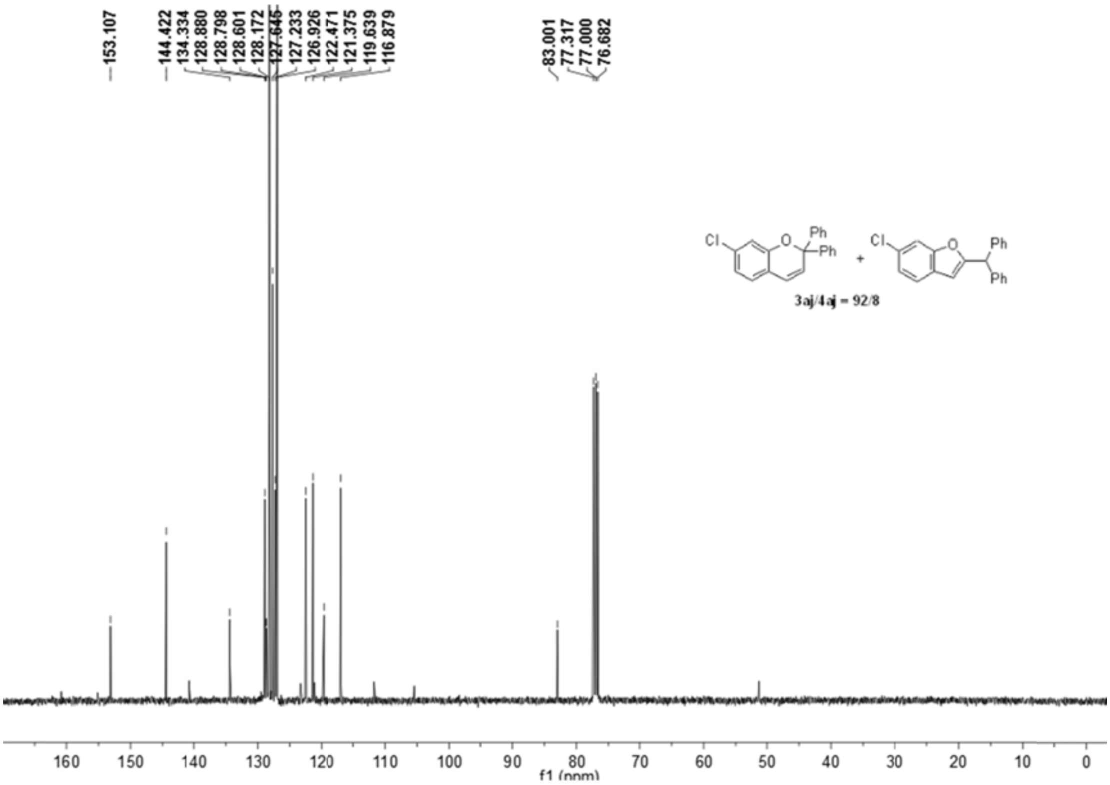
7.381
7.331
7.314
7.295
7.271
7.253
7.235
6.921
6.906
6.886
6.570
6.545
6.153
6.128
1.513
Cl
O
Ph
Ph
+
Cl
O
Ph
Ph
3aj/4aj = 92/8
4.09
4.15
2.17
1.99
0.98
1.03
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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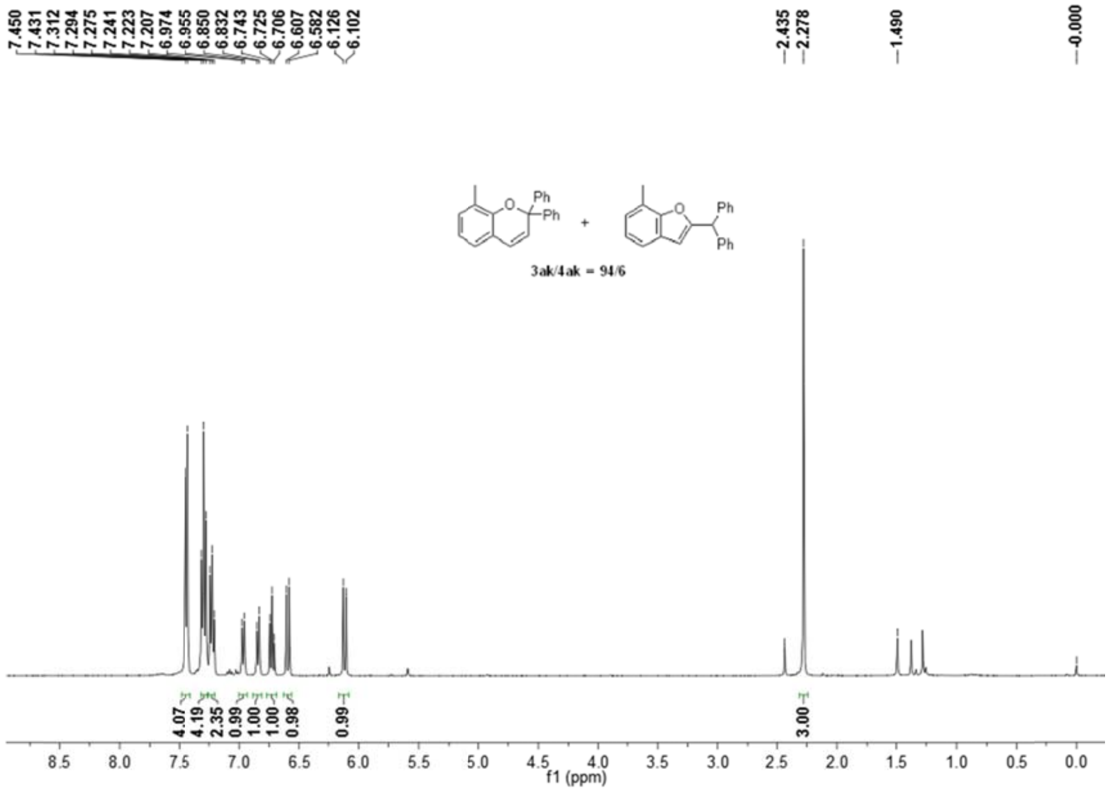
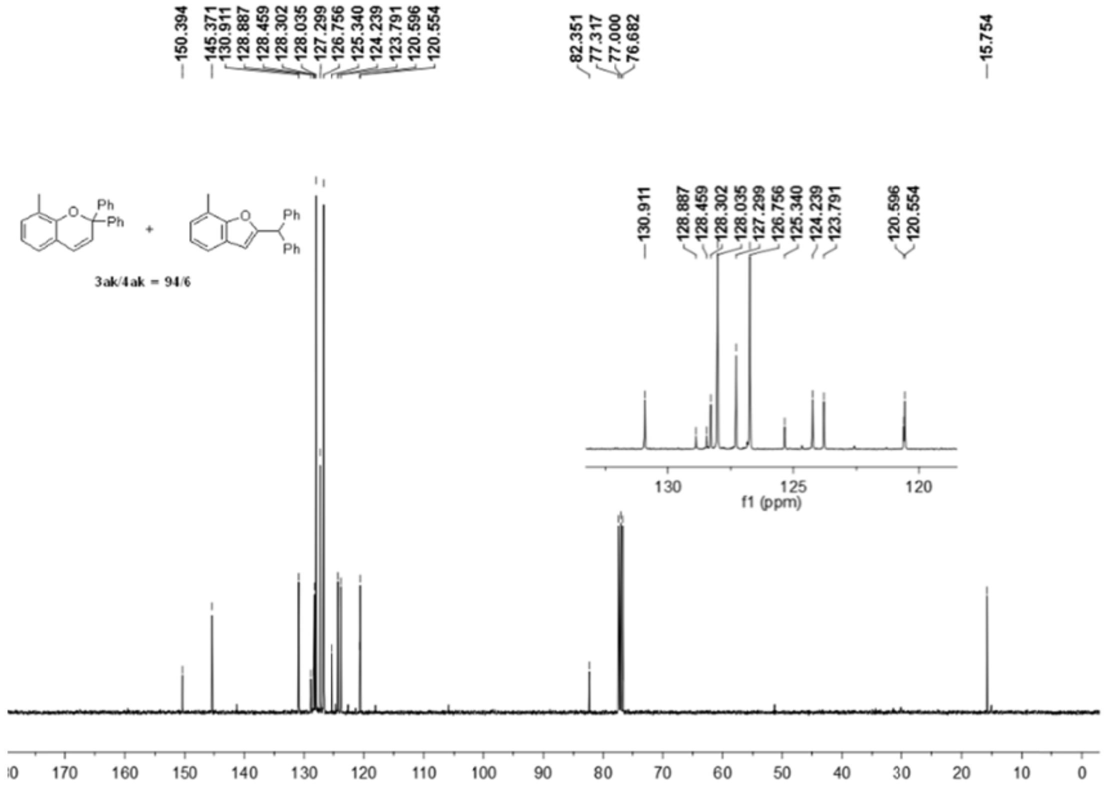
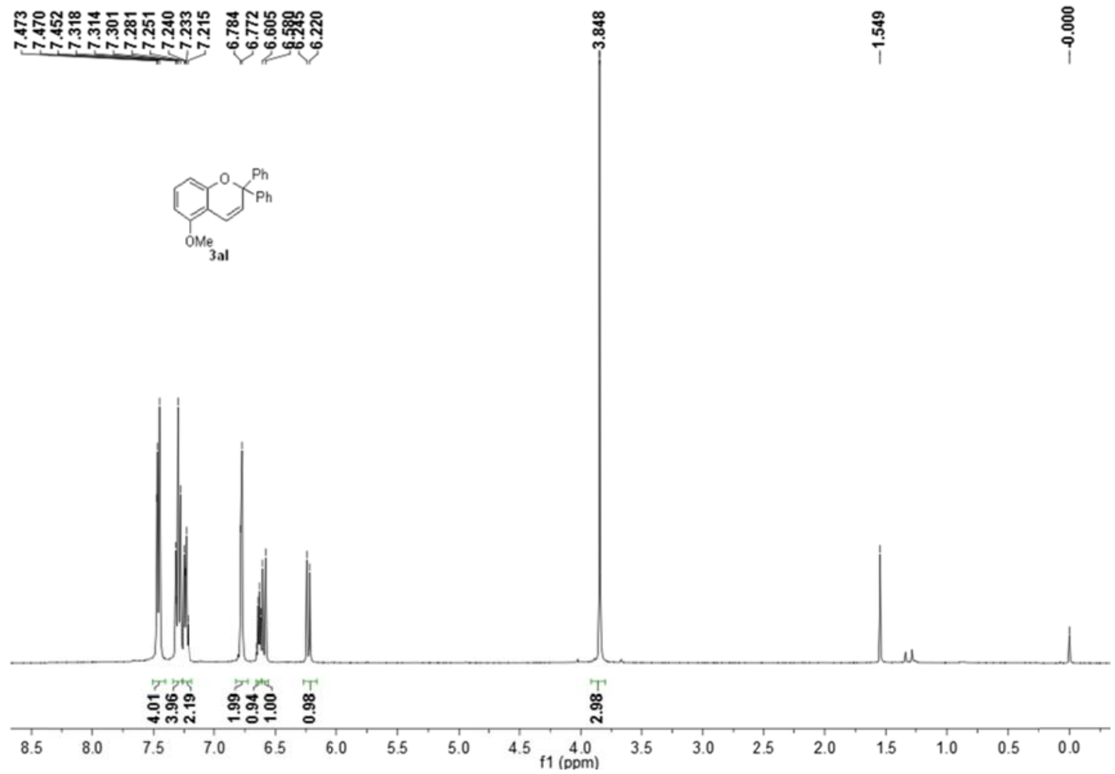
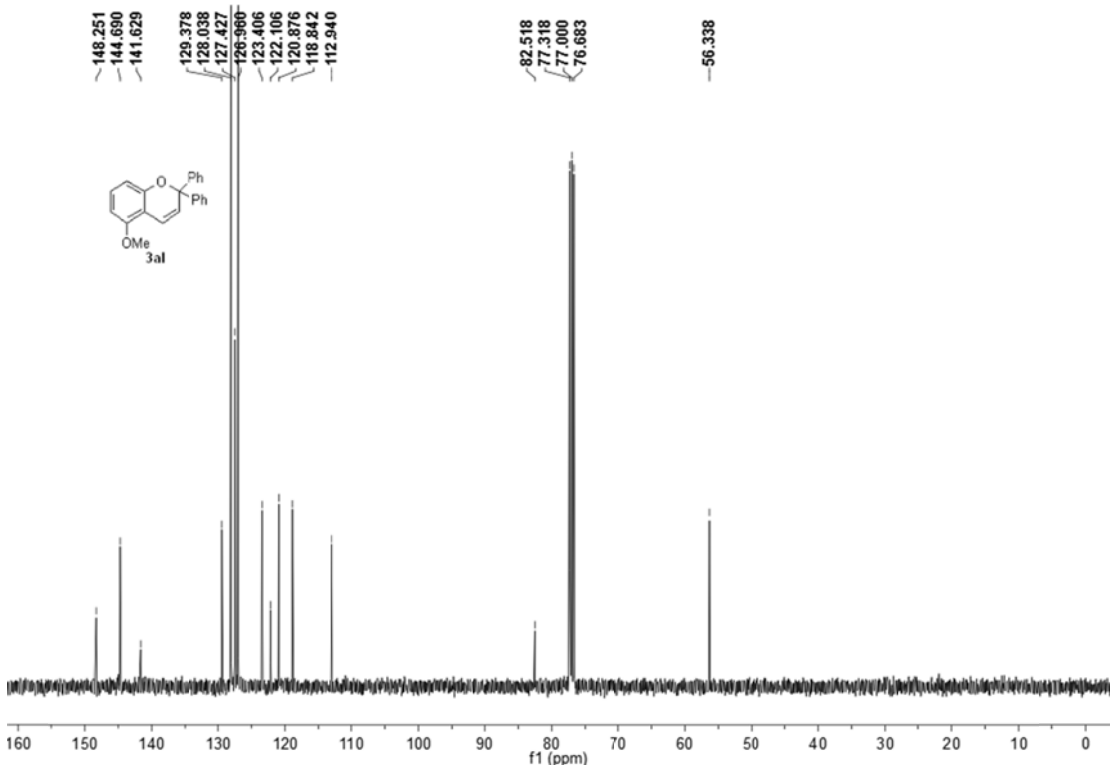
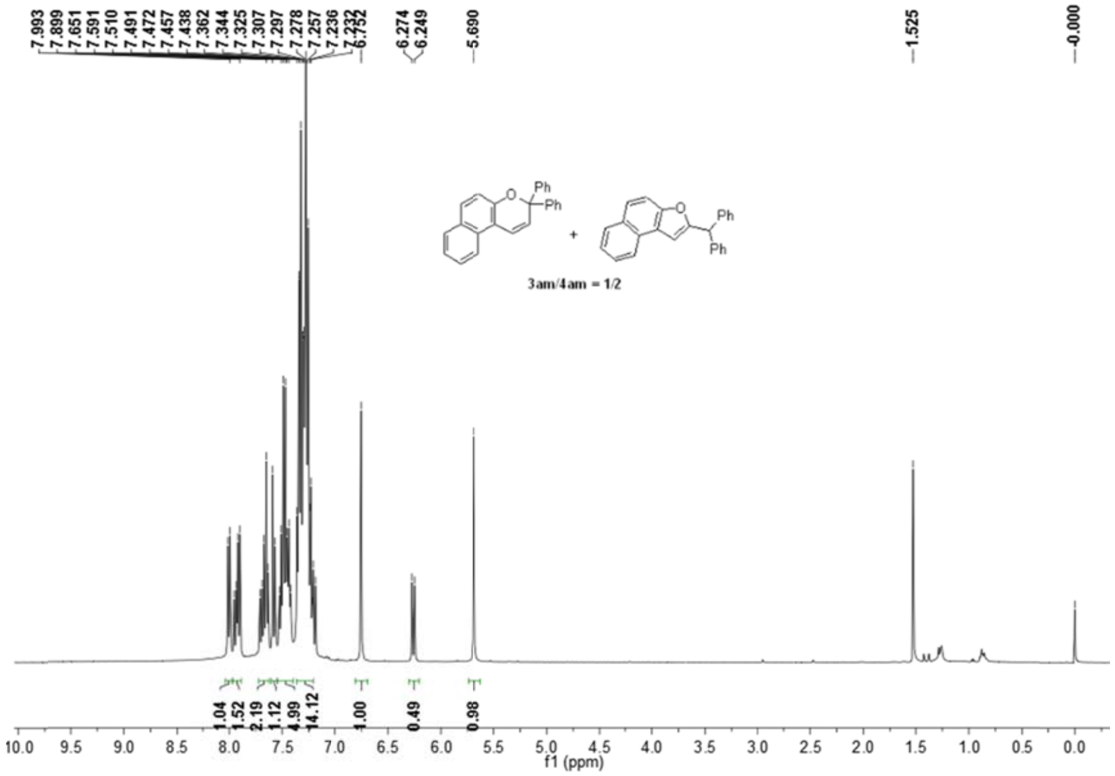
144.422
134.334
128.880
128.798
128.601
128.172
127.646
127.233
126.926
122.471
121.375
119.639
116.879
83.001
77.317
77.000
76.682
Cl
O
Ph
Ph
+
Cl
O
Ph
Ph
3aj/4aj = 92/8
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

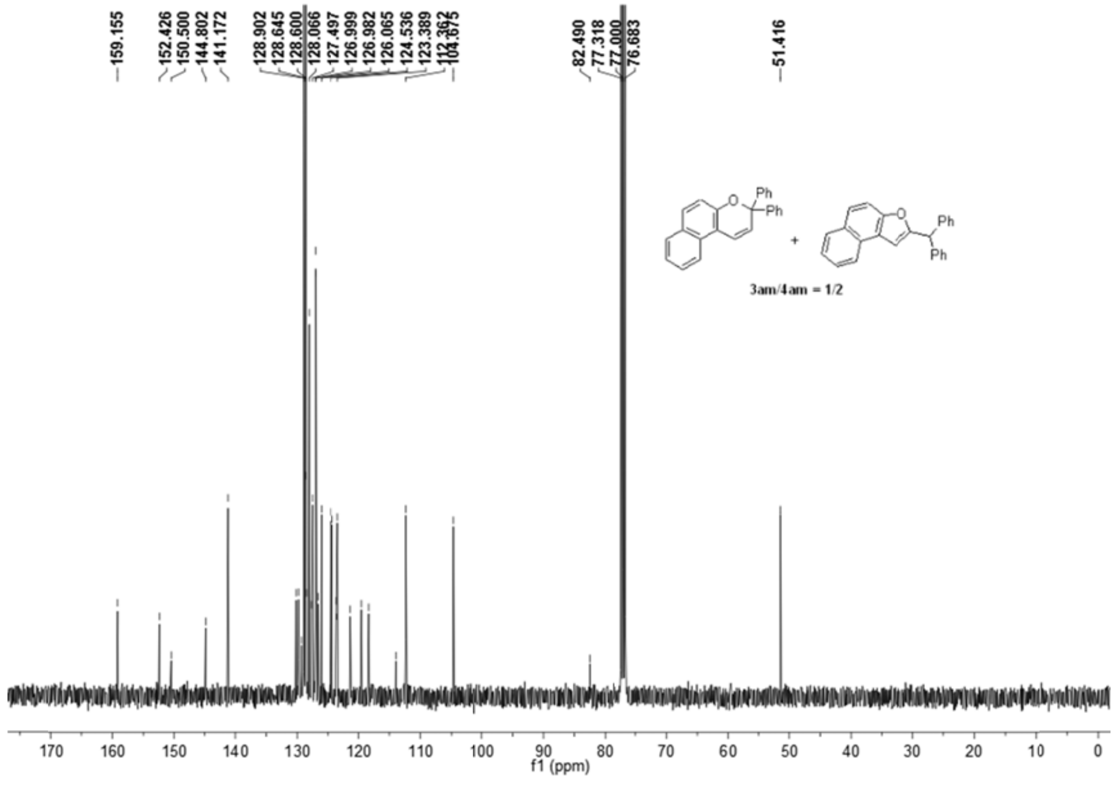

7.450
7.431
7.312
7.294
7.275
7.241
7.223
7.207
6.974
6.955
6.850
6.832
6.743
6.725
6.706
6.607
6.582
6.126
6.102
2.435
2.278
1.490
0.000
Ph
Ph
+
Ph
Ph
3ak/4ak = 94/6
4.07
4.19
2.35
0.99
1.00
1.00
0.98
0.99
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

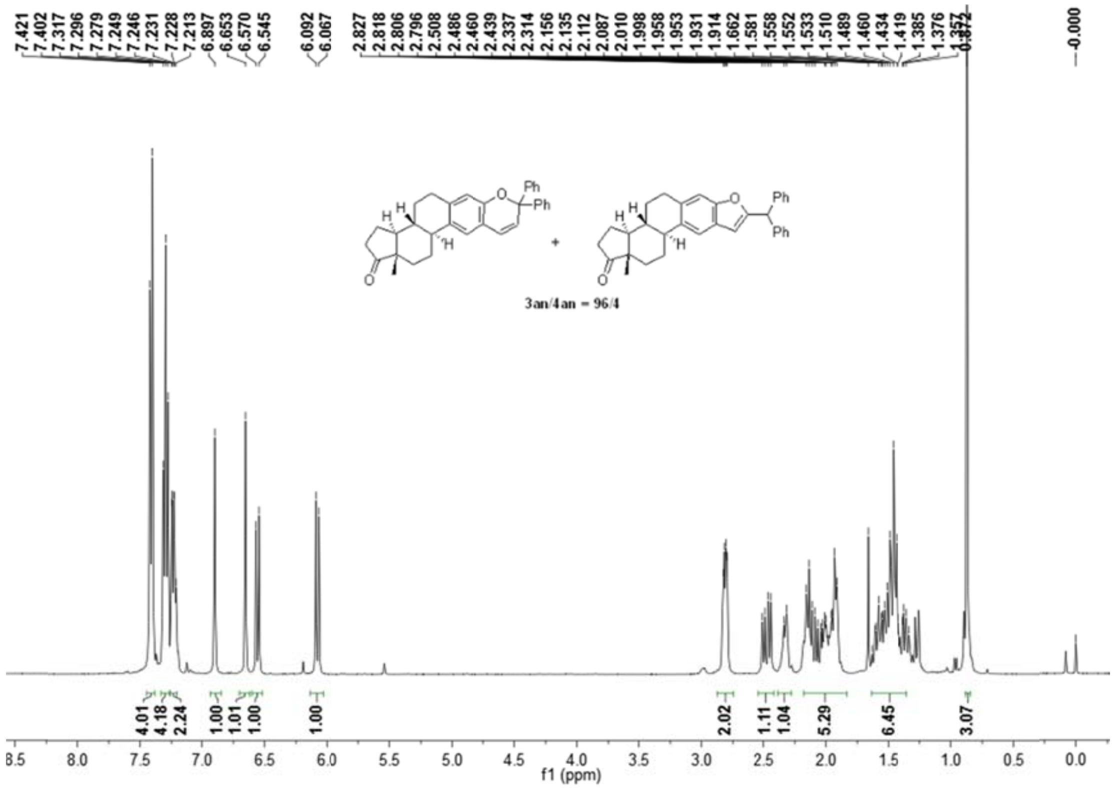

150.394
145.371
130.911
128.887
128.459
128.302
128.035
127.299
126.756
125.340
124.239
123.791
120.596
120.554
82.351
77.317
77.000
76.682
15.754
Ph
Ph
+
Ph
Ph
3ak/4ak = 94/6
130.911
128.887
128.459
128.302
128.035
127.299
126.756
125.340
124.239
123.791
120.596
120.554
130
125
120
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

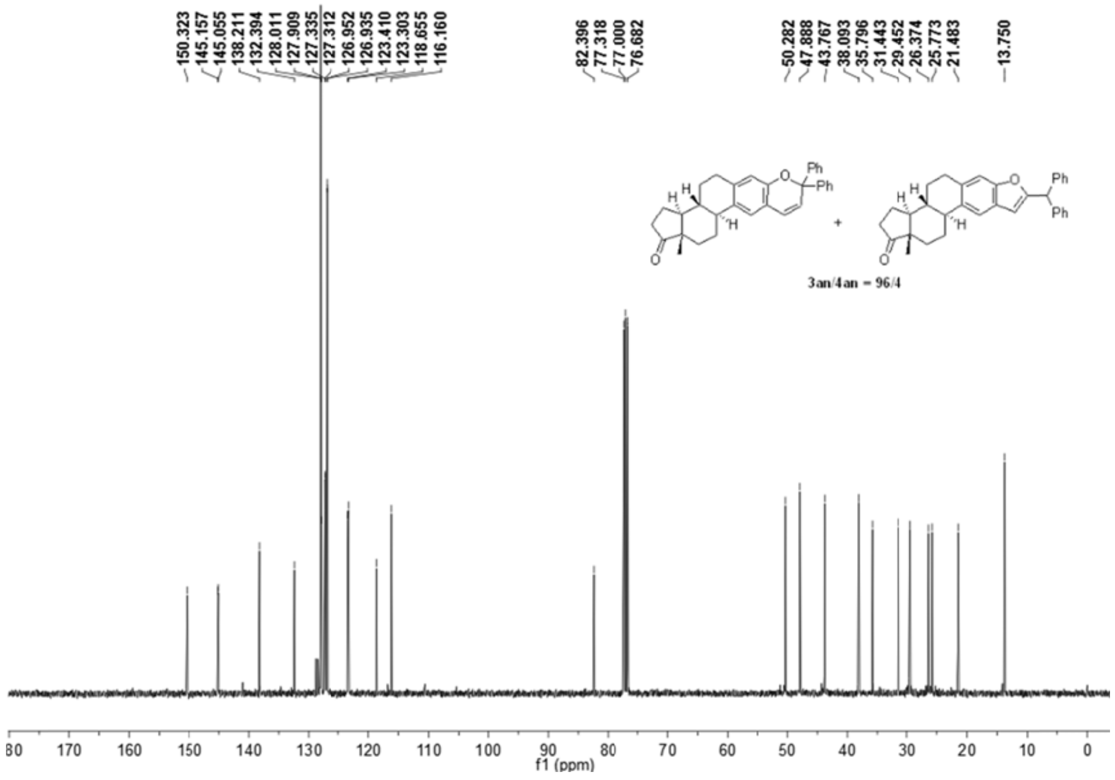

7.473
7.470
7.452
7.318
7.314
7.301
7.281
7.251
7.240
7.233
7.215
6.784
6.772
6.605
6.580
6.245
6.220
3.848
1.549
-0.000
O
Ph
Ph
OMe
3al
4.01
3.96
2.19
1.99
0.94
1.00
0.98
2.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


148.251
144.690
141.629
129.378
128.038
127.427
126.960
123.406
122.106
120.876
118.842
112.940
82.518
77.318
77.000
76.683
56.338
O
Ph
Ph
OMe
3al
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.993
7.899
7.651
7.591
7.510
7.491
7.472
7.457
7.438
7.362
7.344
7.325
7.307
7.297
7.278
7.257
7.236
7.232
6.752
6.274
6.249
5.690
1.525
-0.000
Ph
Ph
+
Ph
Ph
3am/4am = 1/2
1.04
1.52
2.19
1.12
4.99
14.12
1.00
0.49
0.98
10.0
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)


159.155
152.426
150.500
144.802
141.172
128.902
128.645
128.600
128.066
127.497
126.999
126.982
126.065
124.536
123.389
112.362
104.675
82.490
77.318
77.000
76.683
51.416
Ph
Ph
+
Ph
Ph
3am/4am = 1/2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.421
7.402
7.317
7.296
7.279
7.249
7.246
7.231
7.228
7.213
6.897
6.653
6.570
6.545
6.092
6.067
2.827
2.818
2.806
2.796
2.508
2.486
2.460
2.439
2.337
2.314
2.156
2.135
2.112
2.087
2.010
1.998
1.958
1.953
1.931
1.914
1.662
1.581
1.558
1.552
1.533
1.510
1.489
1.460
1.434
1.419
1.385
1.376
1.357
0.872
-0.000
H
H
O
Ph
Ph
H
+
H
H
O
Ph
Ph
O
H
3an/4an = 96/4
4.01
4.18
2.24
1.00
1.01
1.00
1.00
2.02
1.11
1.04
5.29
6.45
3.07
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)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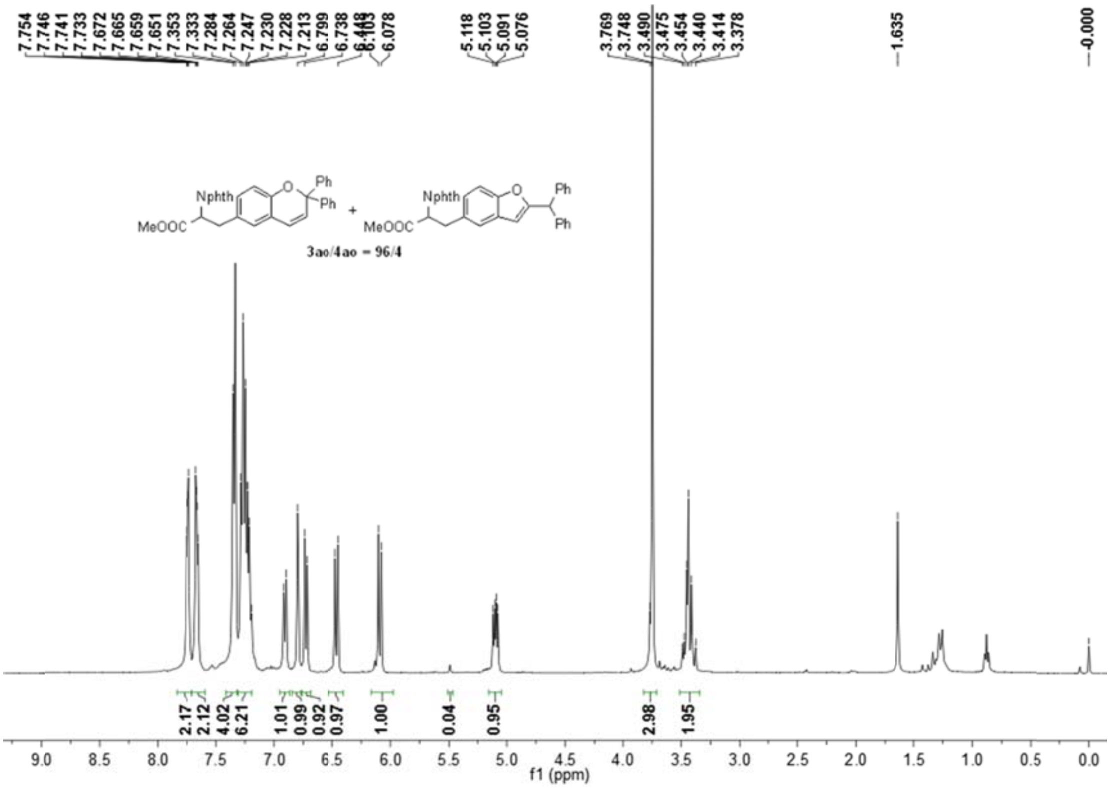
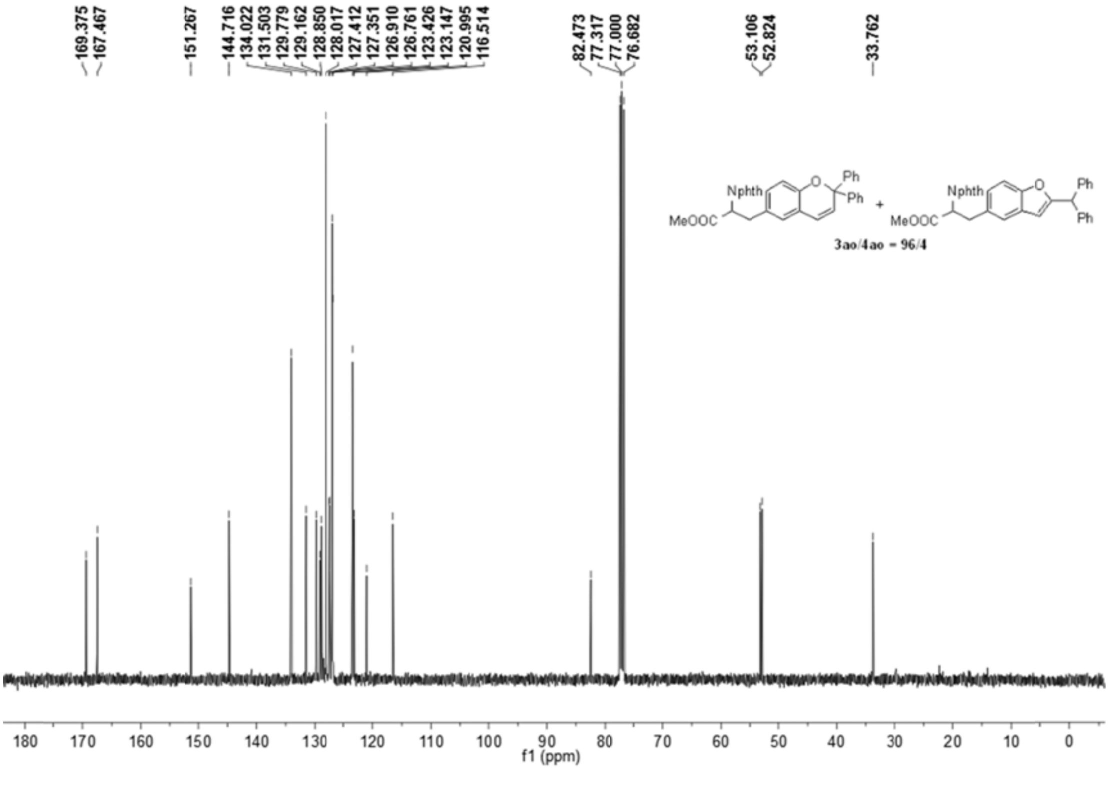
145.157
145.055
138.211
132.394
128.011
127.909
127.335
127.312
126.952
126.935
123.410
123.303
118.655
116.160
82.396
77.318
77.000
76.682
50.282
47.888
43.767
38.093
35.796
31.443
29.452
26.374
25.773
21.483
13.750
H
H
O
Ph
Ph
H
+
H
H
O
Ph
Ph
O
H
3an/4an = 96/4
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.754
7.746
7.741
7.733
7.672
7.665
7.659
7.651
7.353
7.333
7.284
7.264
7.247
7.230
7.228
7.213
6.799
6.738
6.448
6.103
6.078
5.118
5.103
5.091
5.076
3.769
3.748
3.490
3.475
3.454
3.440
3.414
3.378
1.635
-0.000
Nphth
MeOOC
O
Ph
Ph
+
Nphth
MeOOC
O
Ph
Ph
3ao/4ao = 96/4
2.17
2.12
4.02
6.21
1.01
0.99
0.92
0.97
1.00
0.04
0.95
2.98
1.95
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)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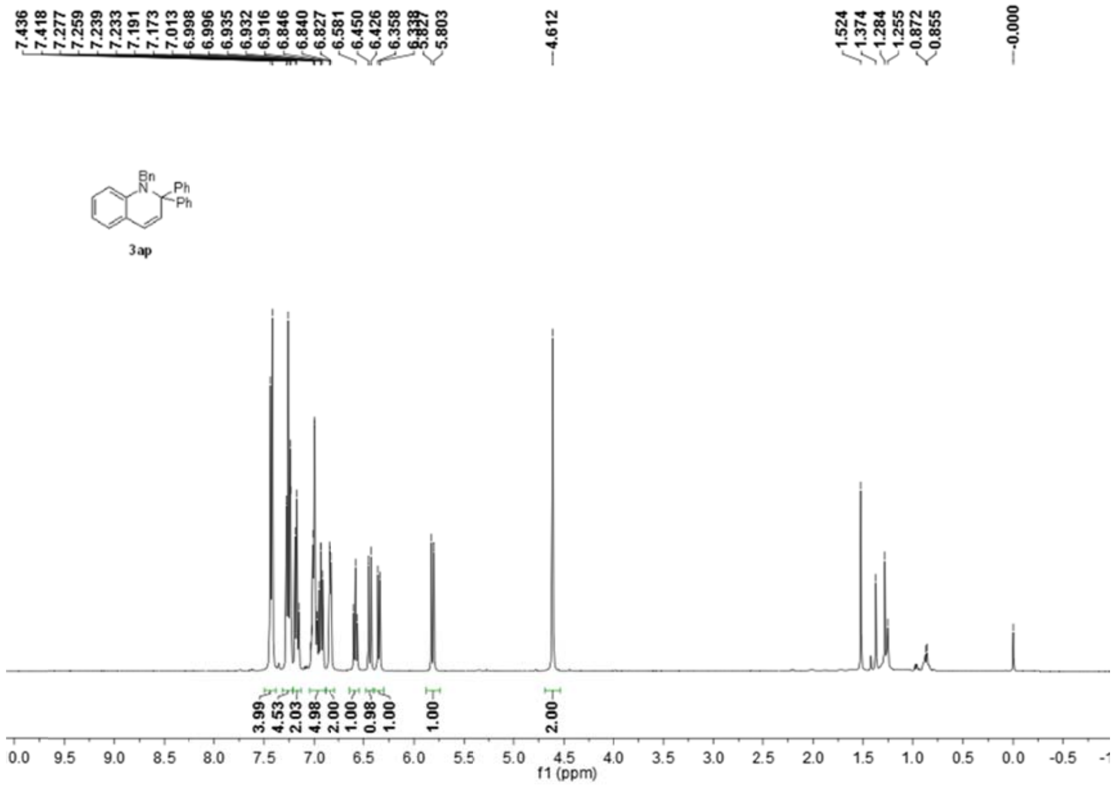
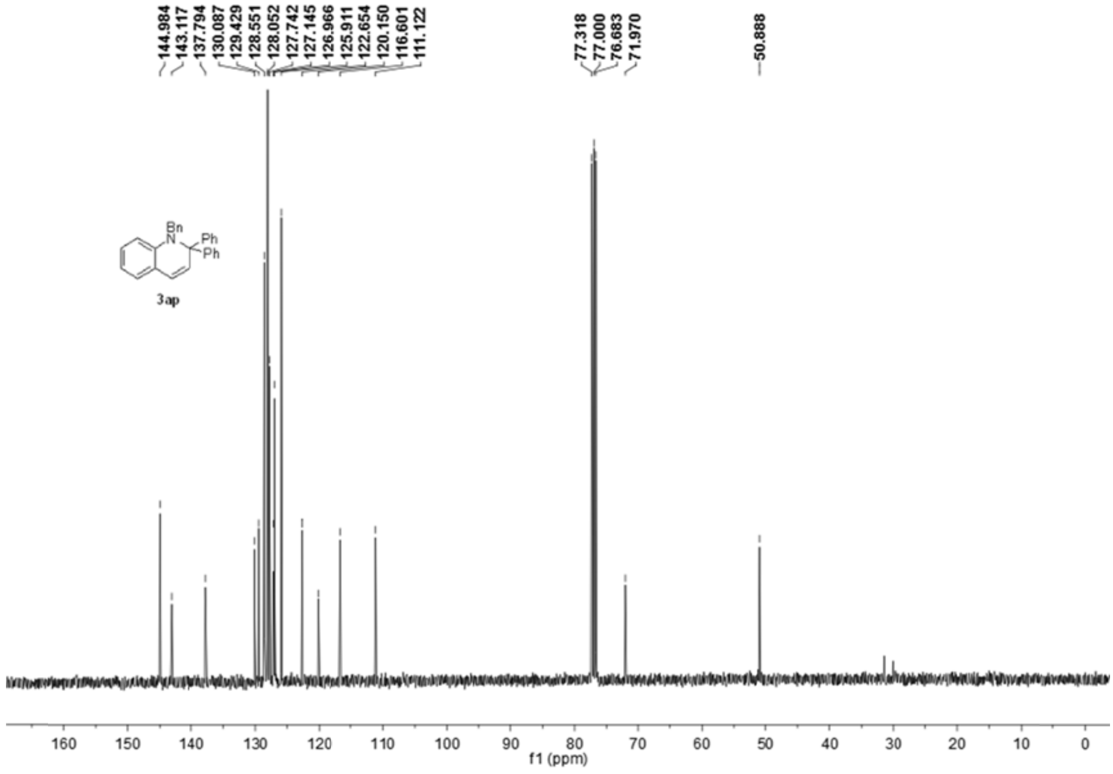
167.467
151.267
144.716
134.022
131.503
129.779
129.162
128.850
128.017
127.412
127.351
126.910
126.761
123.426
123.147
120.995
116.514
82.473
77.317
77.000
76.682
53.106
52.824
33.762
Nphth
MeOOC
O
Ph
Ph
+
Nphth
MeOOC
O
Ph
Ph
3ao/4ao = 96/4
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.436
7.418
7.277
7.259
7.239
7.233
7.191
7.173
7.013
6.998
6.996
6.935
6.932
6.916
6.846
6.840
6.827
6.581
6.450
6.426
6.358
6.338
5.827
5.803
4.612
1.524
1.374
1.284
1.255
0.872
0.855
-0.000
Bn
N
Ph
Ph
3ap
3.99
4.53
2.03
4.98
2.00
1.00
0.98
1.00
1.00
2.00
0.0 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 -0.5
f1 (ppm)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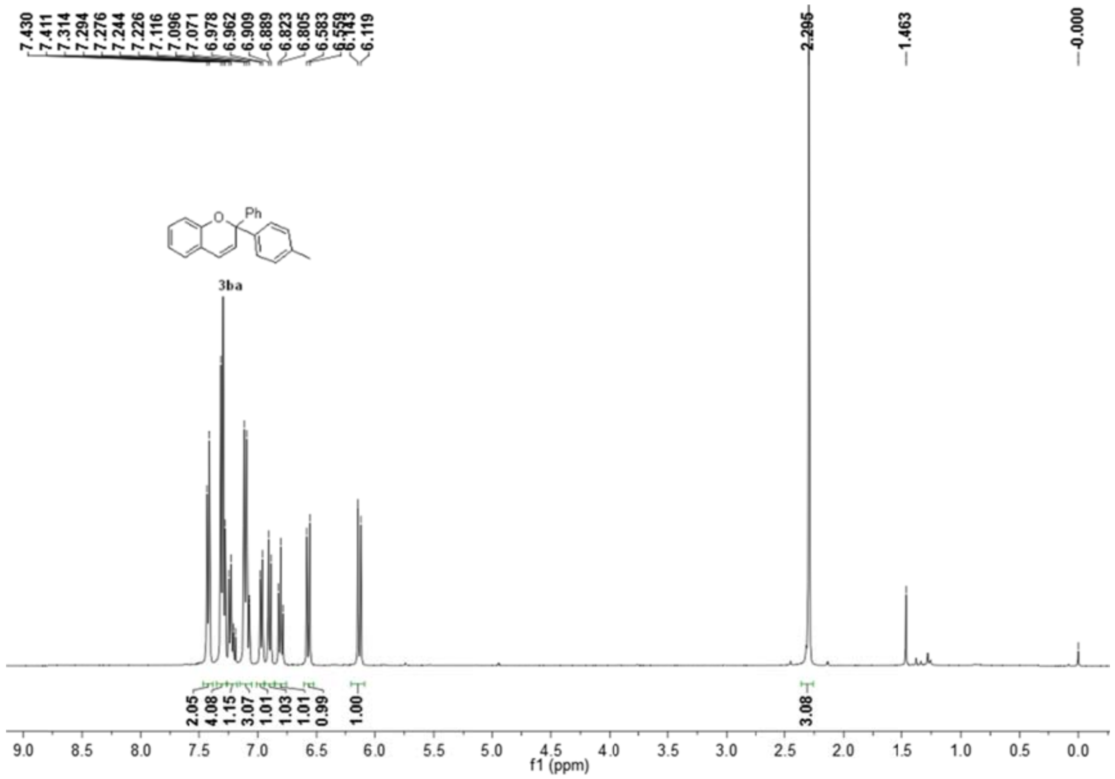
143.117
137.794
130.087
129.429
128.551
128.052
127.742
127.145
126.966
125.911
122.654
120.150
116.601
111.122
77.318
77.000
76.683
71.970
50.888
Bn
N
Ph
Ph
3ap
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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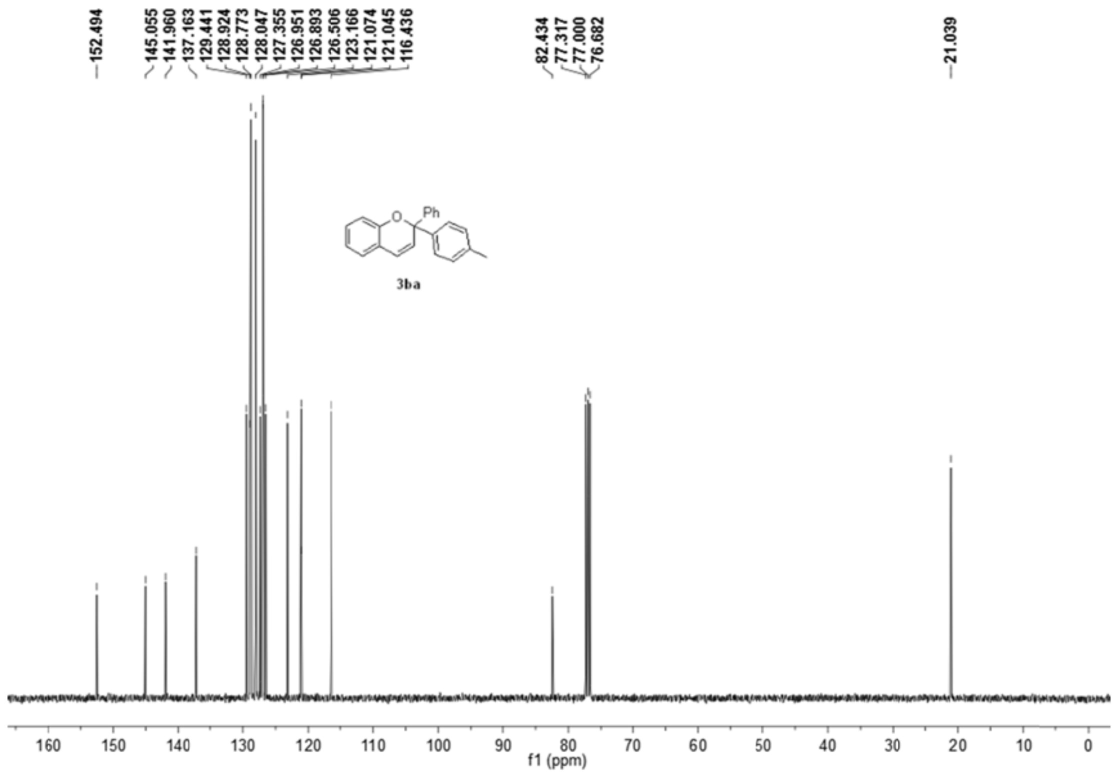
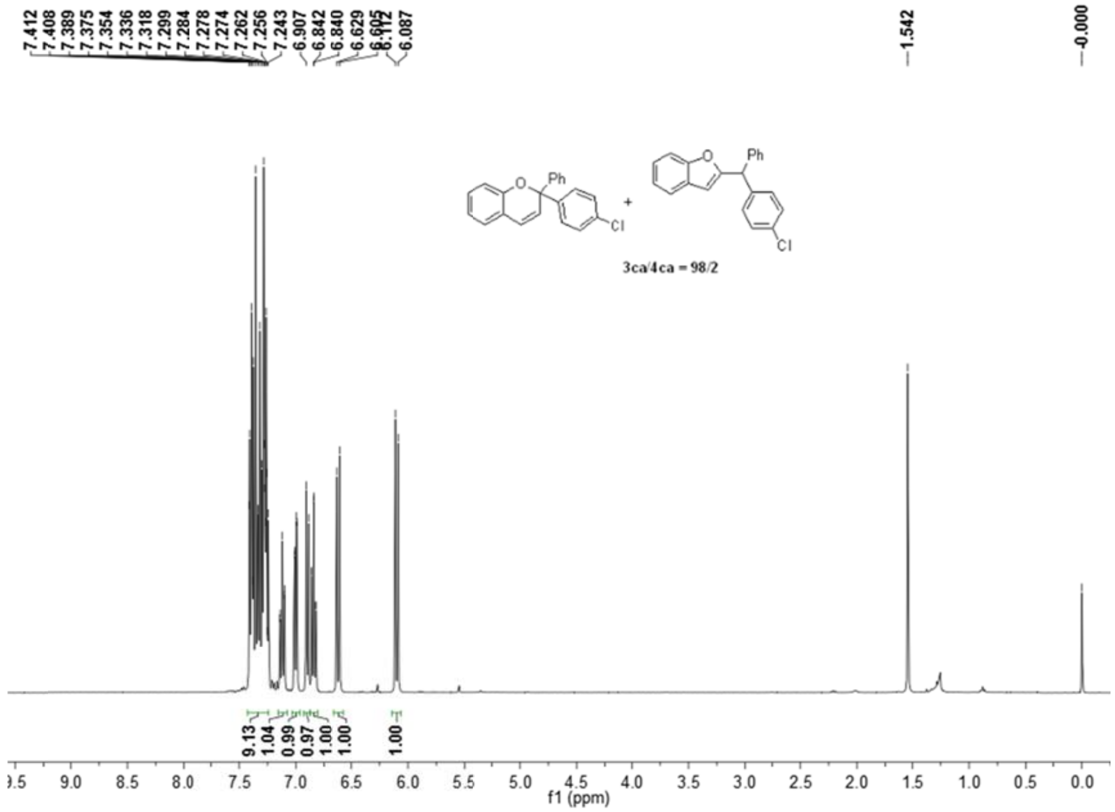
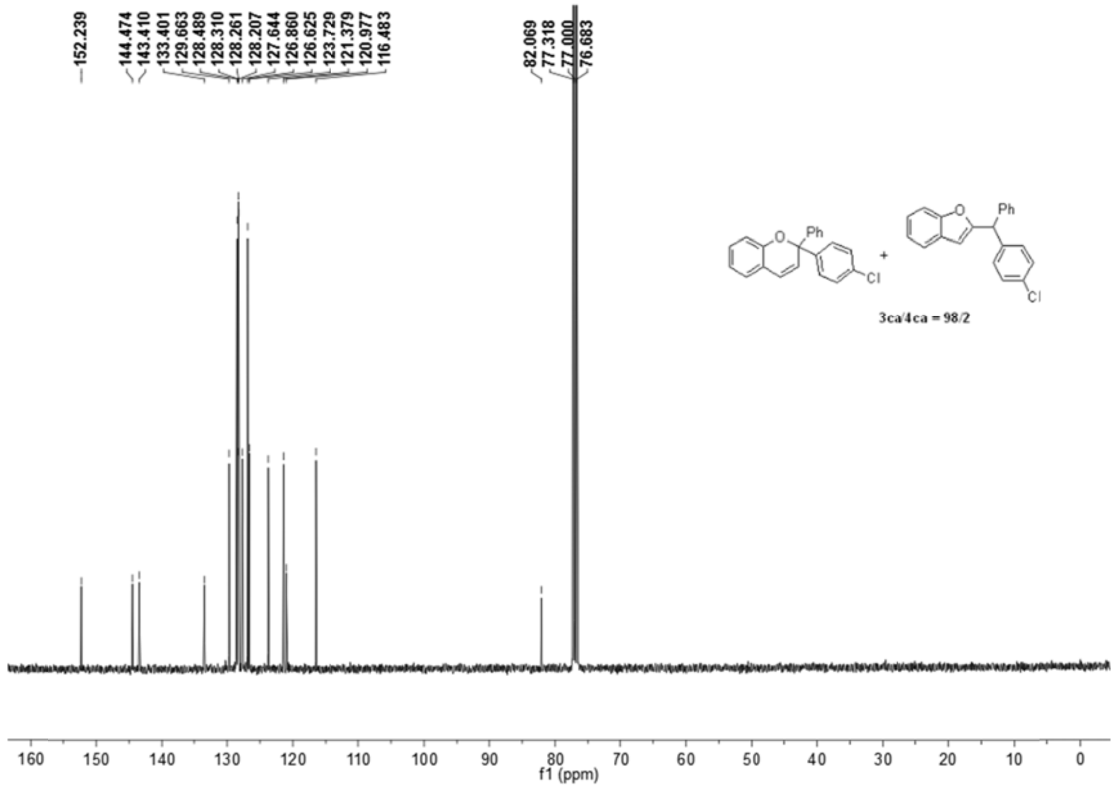
7.411
7.314
7.294
7.276
7.244
7.226
7.116
7.096
7.071
6.978
6.962
6.909
6.889
6.823
6.805
6.583
6.559
6.143
6.119
2.295
1.463
-0.000
O
Ph
3ba
2.05
4.08
1.15
3.07
1.01
1.03
1.01
0.99
1.00
3.08
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


152.494
145.055
141.960
137.163
129.441
128.924
128.773
128.047
127.355
126.951
126.893
126.506
123.166
121.074
121.045
116.436
82.434
77.317
77.000
76.682
21.039
O
Ph
3ba
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.412
7.408
7.389
7.375
7.354
7.336
7.318
7.299
7.284
7.278
7.274
7.262
7.256
7.243
6.907
6.842
6.840
6.629
6.605
6.112
6.087
1.542
-0.000
O
Ph
Cl
+
O
Ph
Cl
3ca/4ca = 98/2
9.13
1.04
0.99
0.97
1.00
1.00
1.00
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)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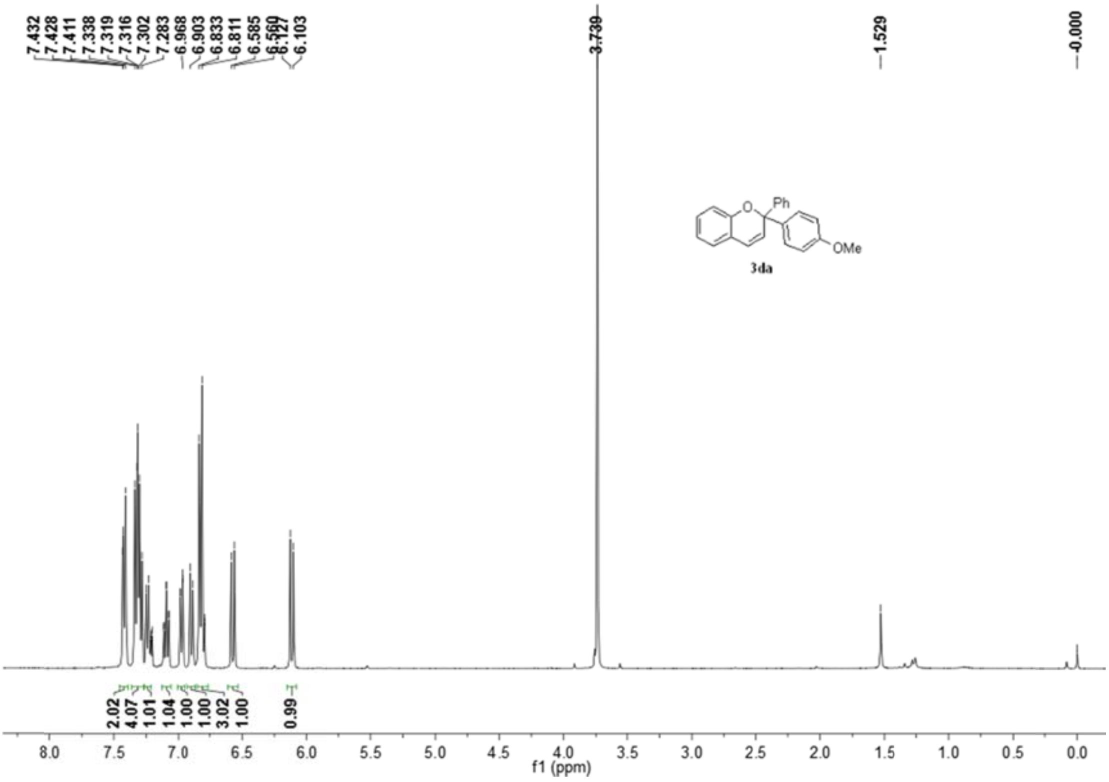
144.474
143.410
133.401
129.663
128.489
128.310
128.261
128.207
127.644
126.860
126.625
123.729
121.379
120.977
116.483
82.069
77.318
77.000
76.683
O
Ph
Cl
+
O
Ph
Cl
3ca/4ca = 98/2
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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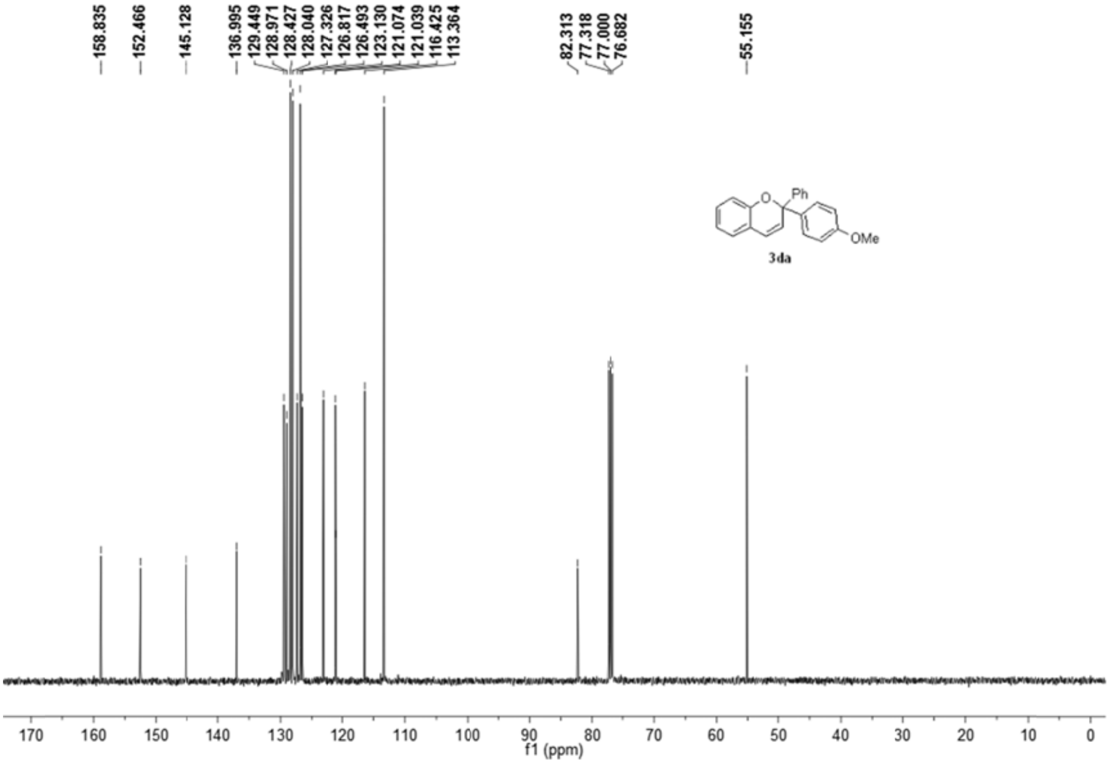
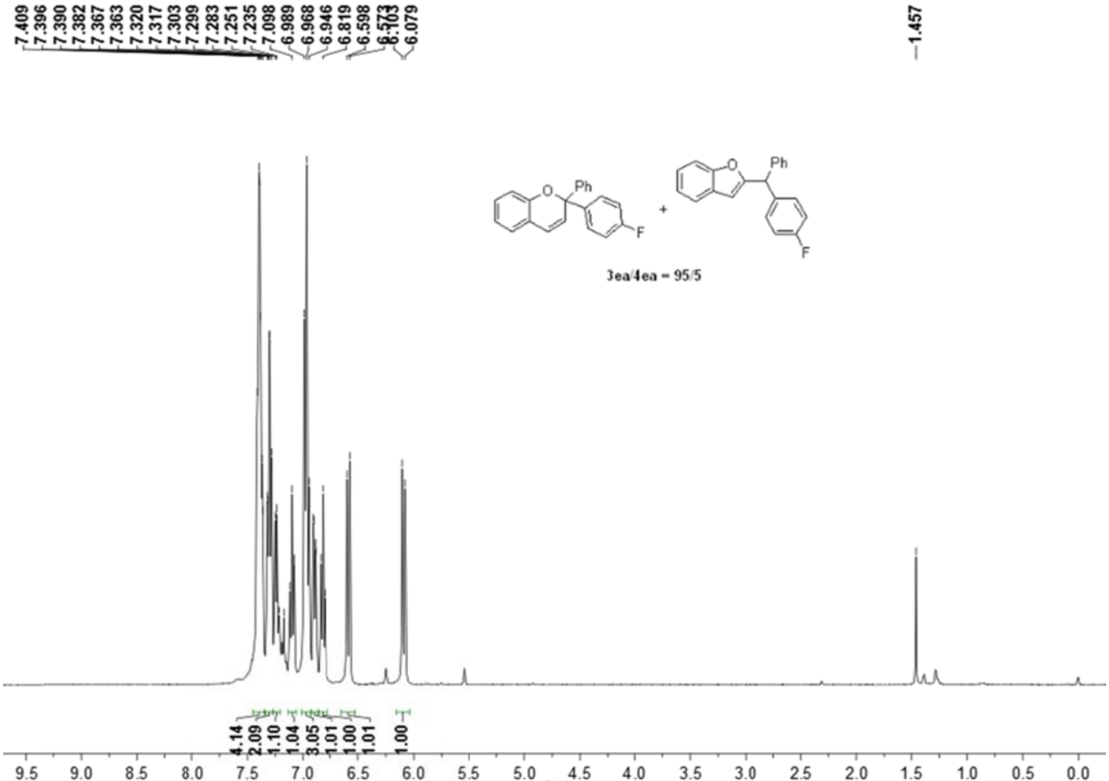
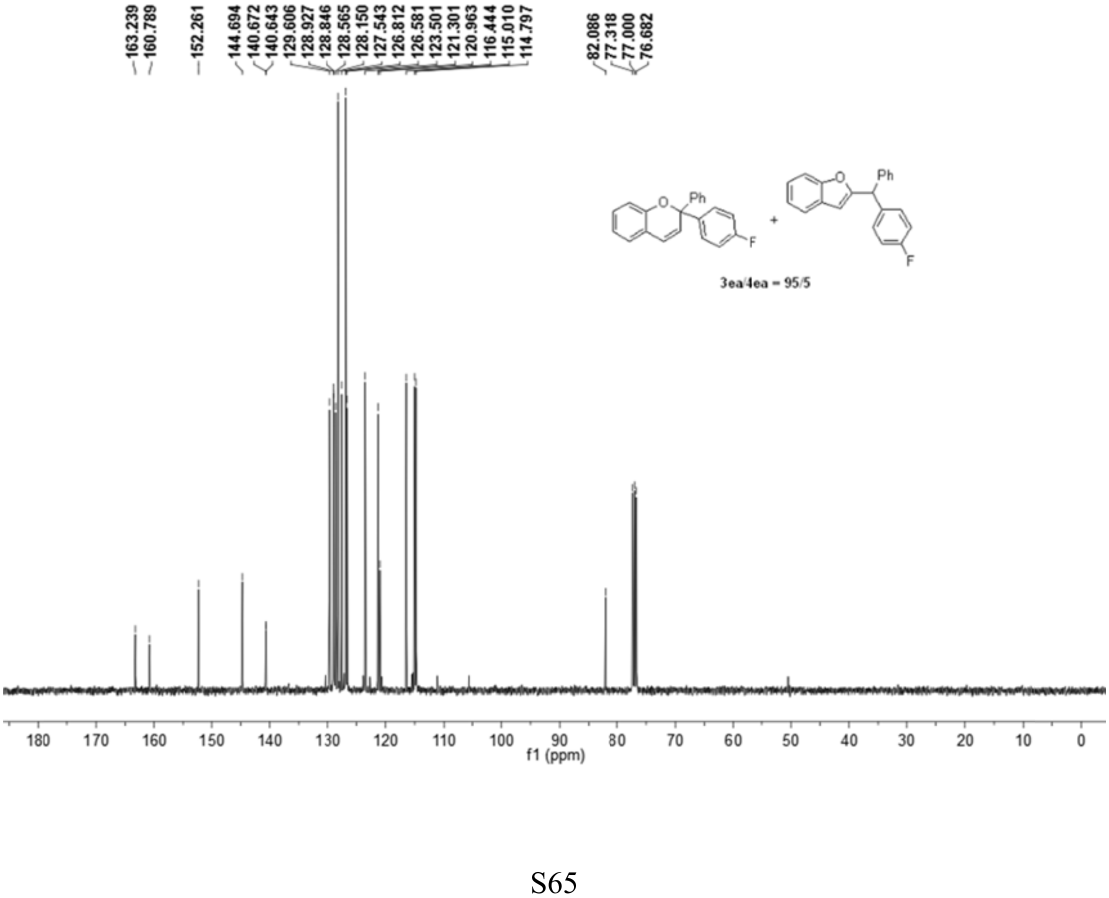
7.411
7.338
7.319
7.316
7.302
7.283
6.968
6.903
6.833
6.811
6.585
6.560
6.127
6.103
3.739
1.529
-0.000
Ph
O
OMe
3da
2.02
4.07
1.01
1.04
1.00
1.00
1.00
3.02
1.00
0.99
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


158.835
152.466
145.128
136.995
129.449
128.971
128.427
128.040
127.326
126.817
126.493
123.130
121.074
121.039
116.425
113.364
82.313
77.318
77.000
76.682
55.155
Ph
O
OMe
3da
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.409
7.396
7.390
7.382
7.367
7.363
7.320
7.317
7.303
7.299
7.283
7.251
7.235
7.098
6.989
6.968
6.946
6.819
6.598
6.573
6.103
6.079
1.457
Ph
F
+
Ph
F
3ea/4ea = 95/5
4.14
2.09
1.10
1.04
3.05
1.01
1.00
1.01
1.00
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)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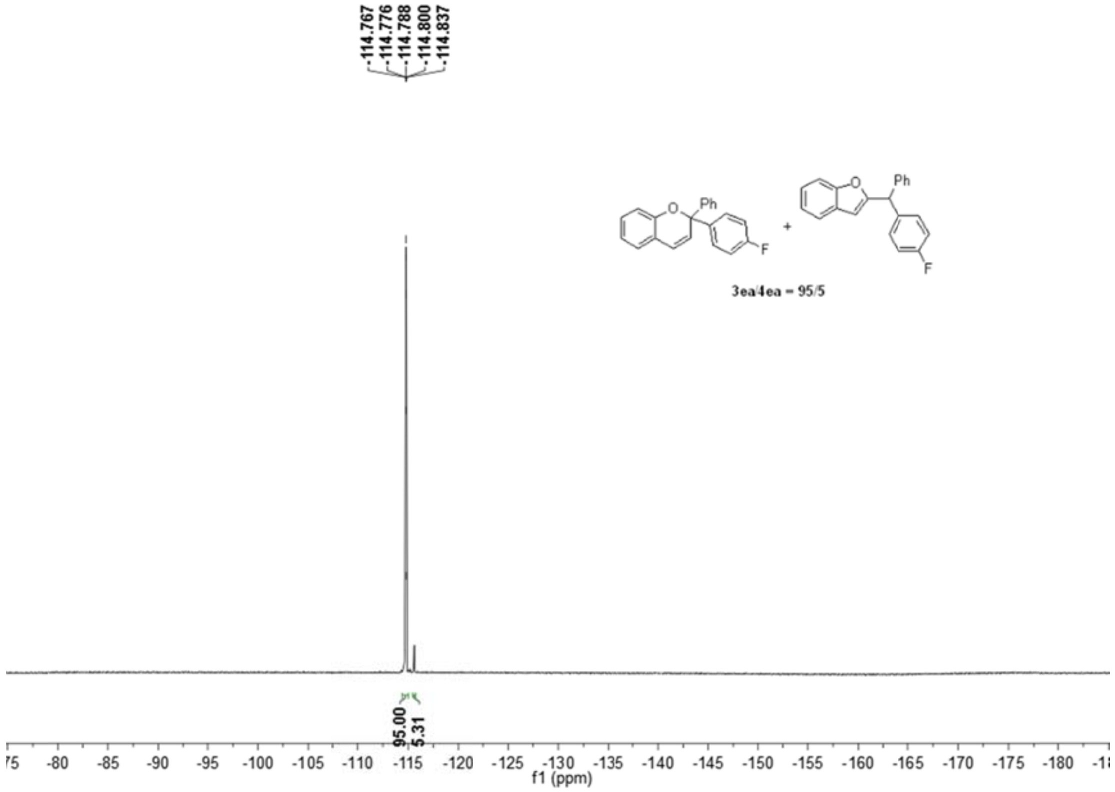
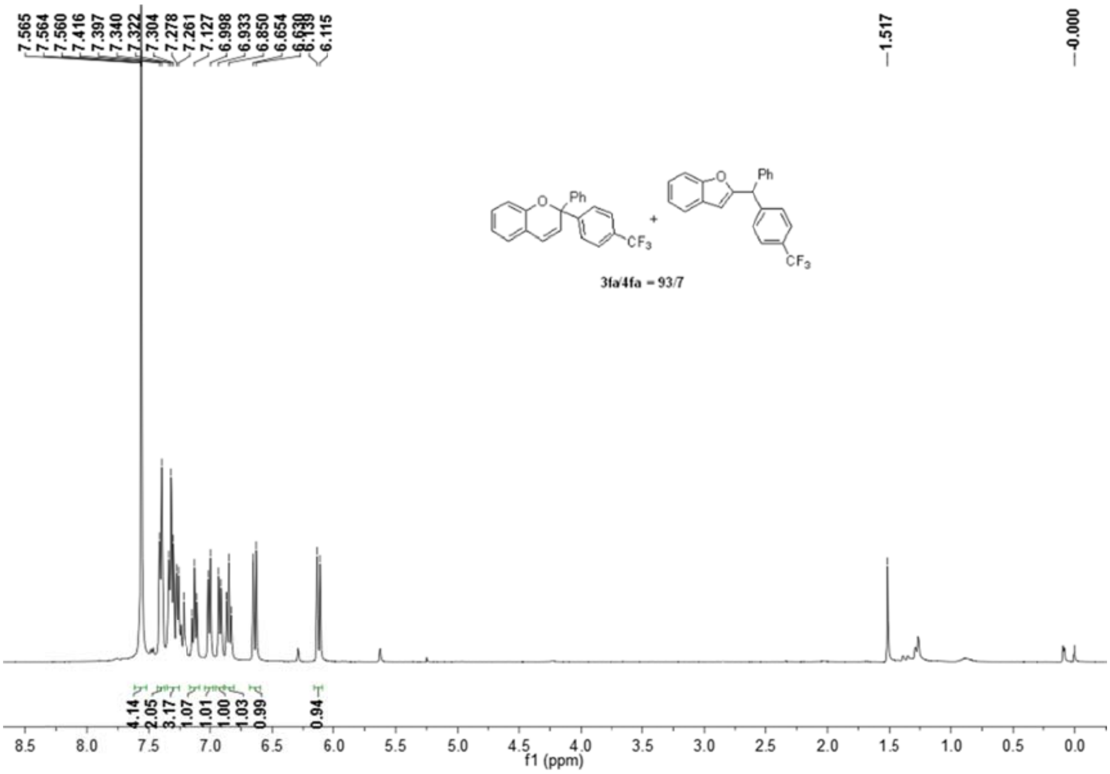
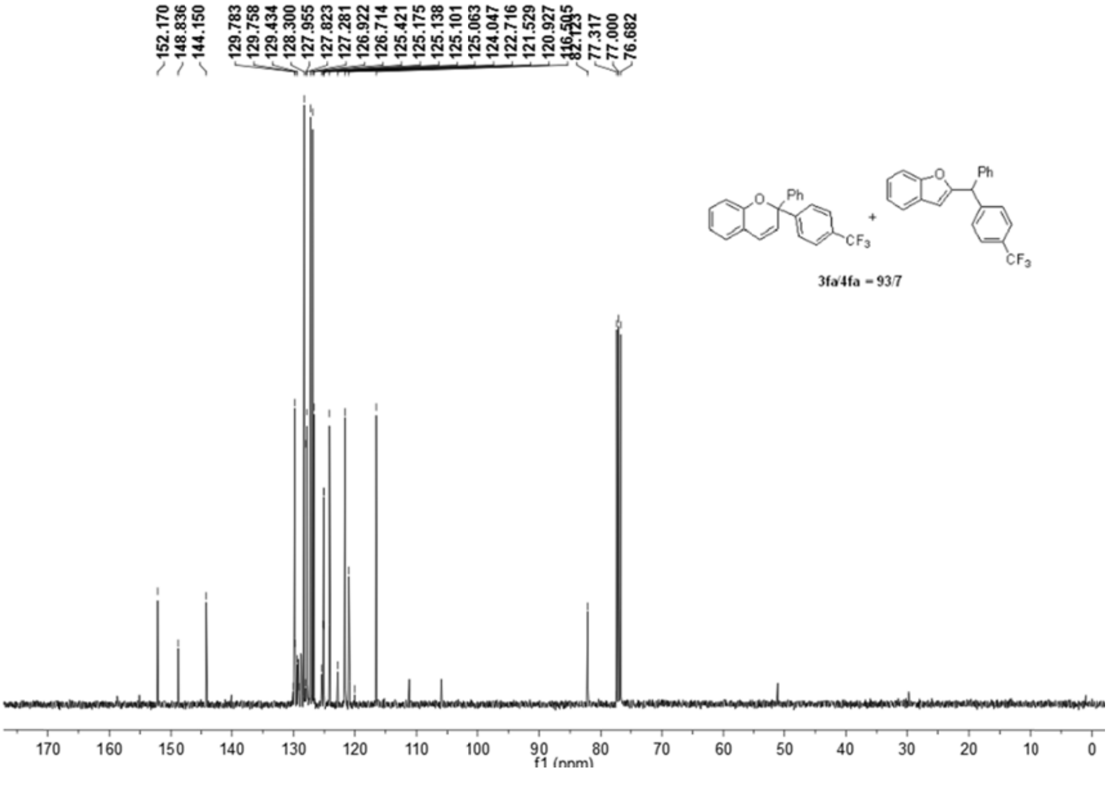
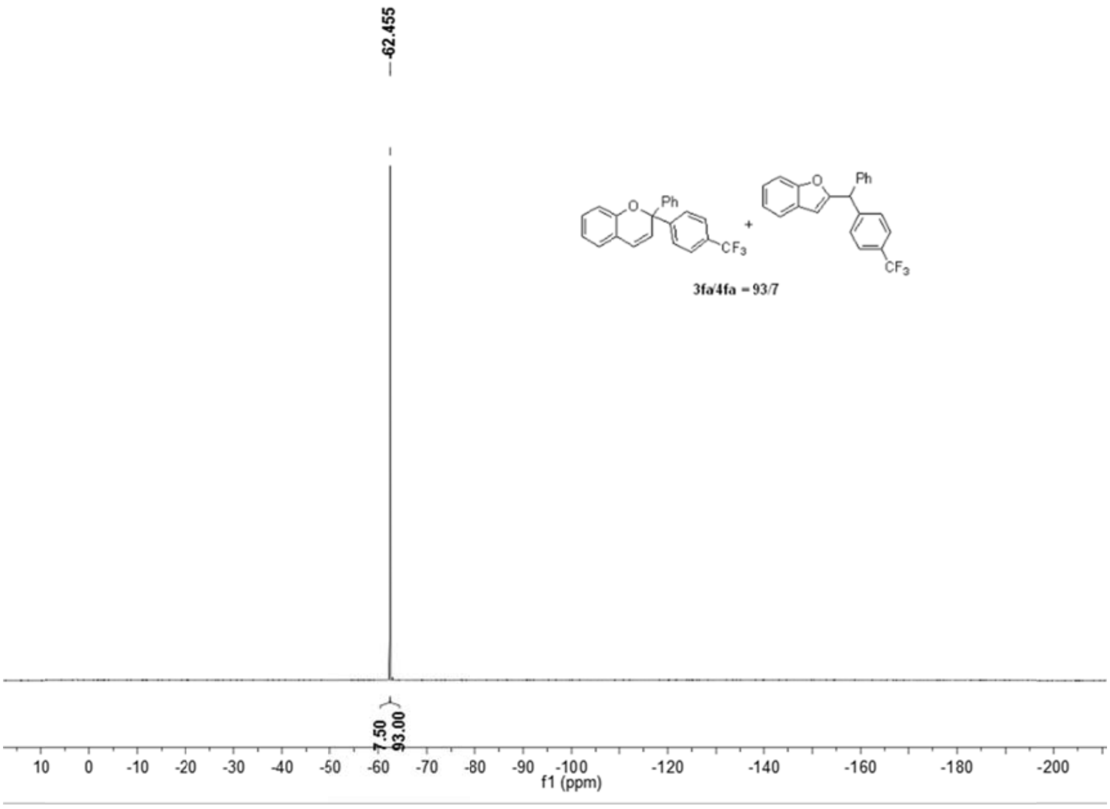
144.694
140.672
140.643
129.606
128.927
128.846
128.565
128.150
127.543
126.812
126.581
123.501
121.301
120.963
116.444
115.010
114.797
82.086
77.318
77.000
76.682
Ph
F
+
Ph
F
3ea/4ea = 95/5
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-114.767
-114.776
-114.788
-114.800
-114.837
Ph
O
F
+
95.00
5.31
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
-165
-170
-175
-180
f1 (ppm)

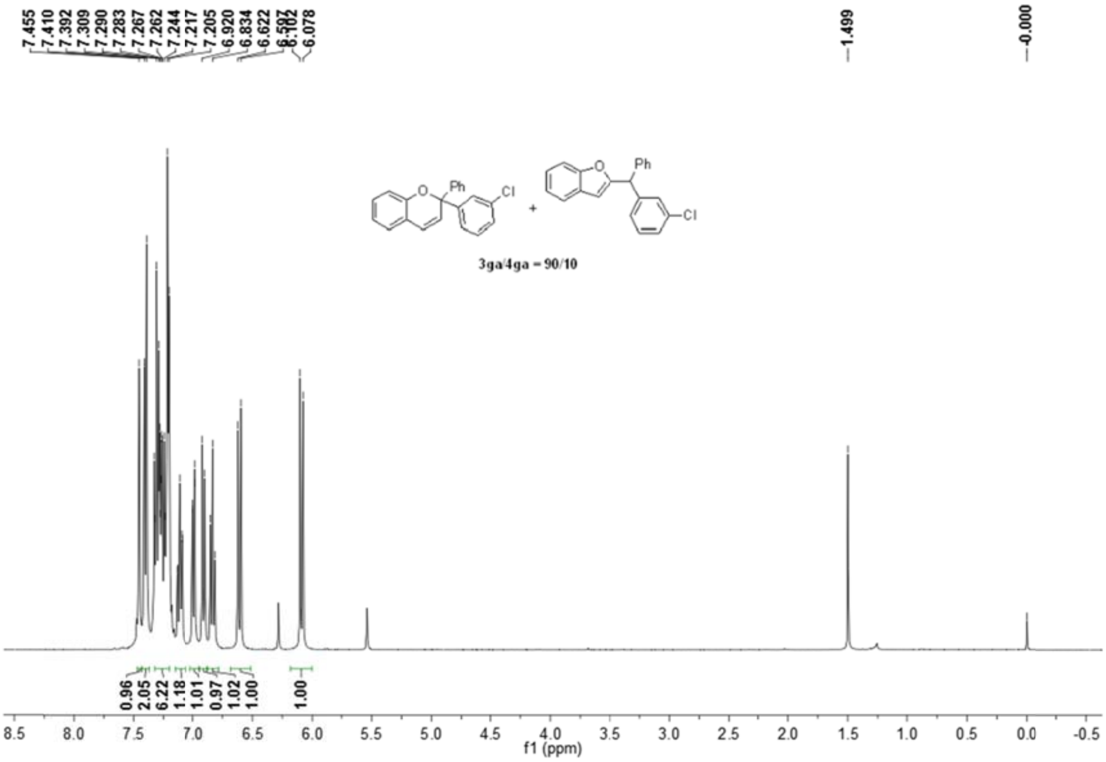
3ea/4ea = 95/5

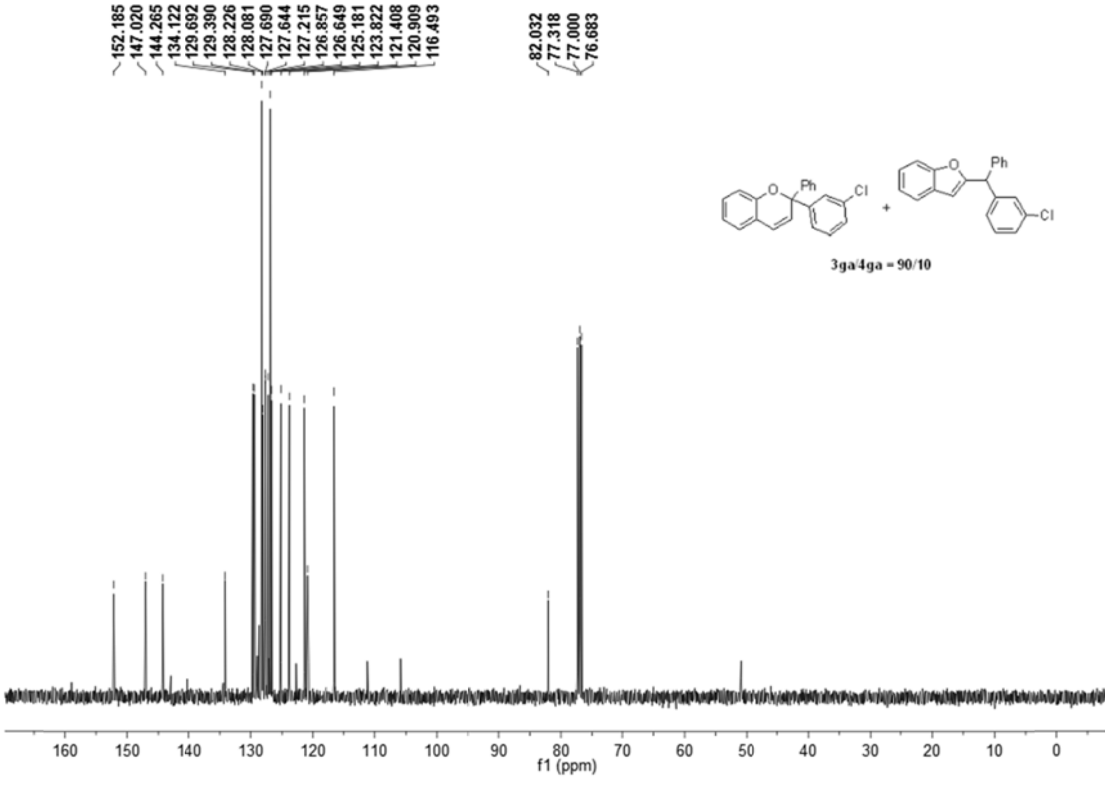

7.565
7.564
7.560
7.416
7.397
7.340
7.322
7.304
7.278
7.261
7.127
6.998
6.933
6.850
6.654
6.630
6.139
6.115
1.517
-0.000
Ph
O
CF3
+
Ph
O
CF3
3fa/4fa = 93/7
4.14
2.05
3.17
1.07
1.01
1.00
1.03
0.99
0.94
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

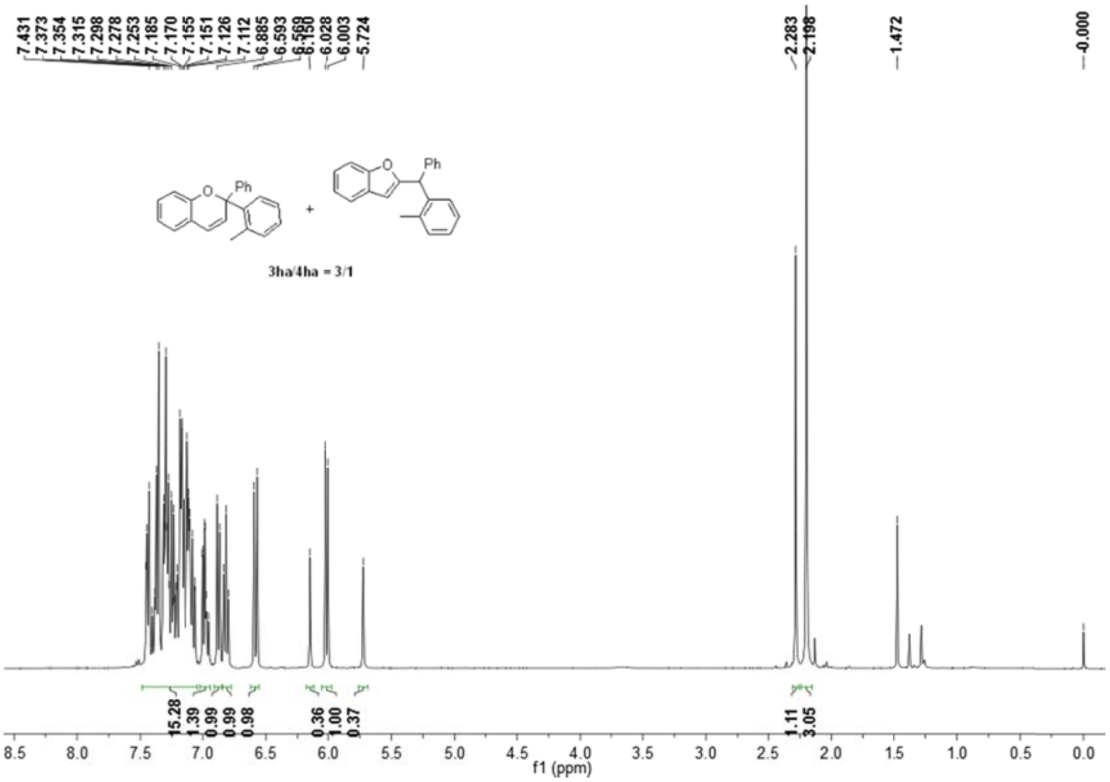

152.170
148.836
144.150
129.783
129.758
129.434
128.300
127.955
127.823
127.281
126.922
126.714
125.421
125.175
125.138
125.101
125.063
124.047
122.716
121.529
120.927
116.505
82.123
77.317
77.000
76.682
Ph
O
CF3
+
Ph
O
CF3
3fa/4fa = 93/7
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

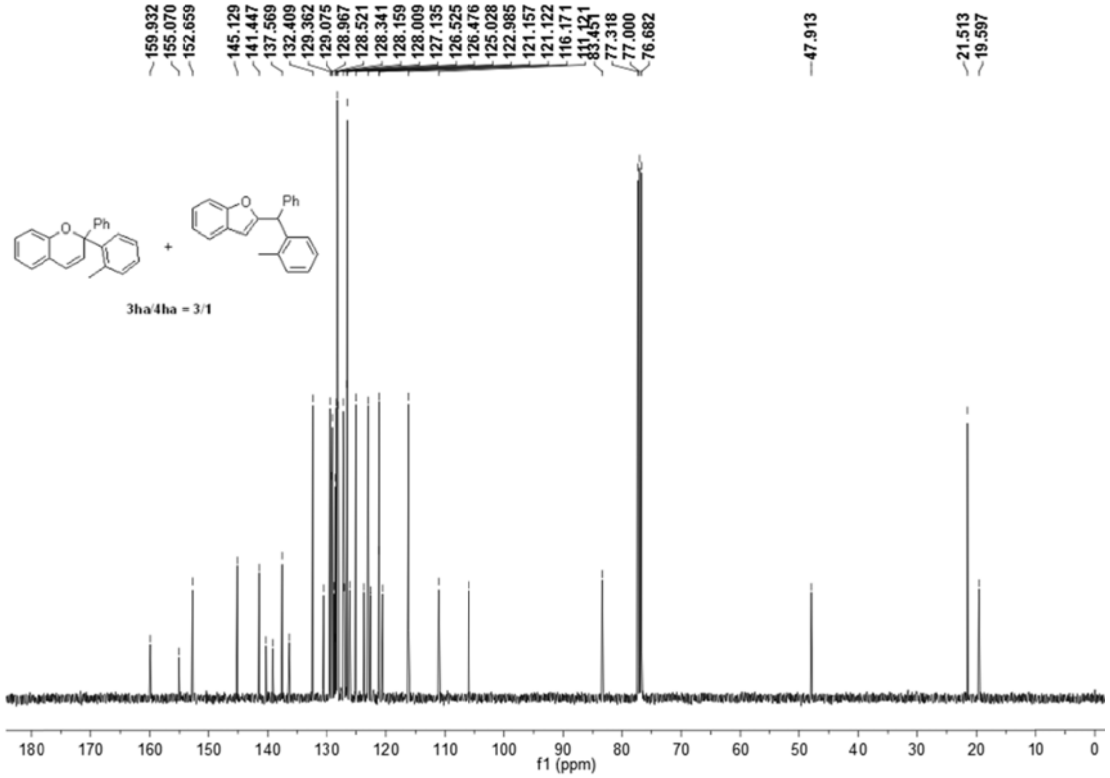


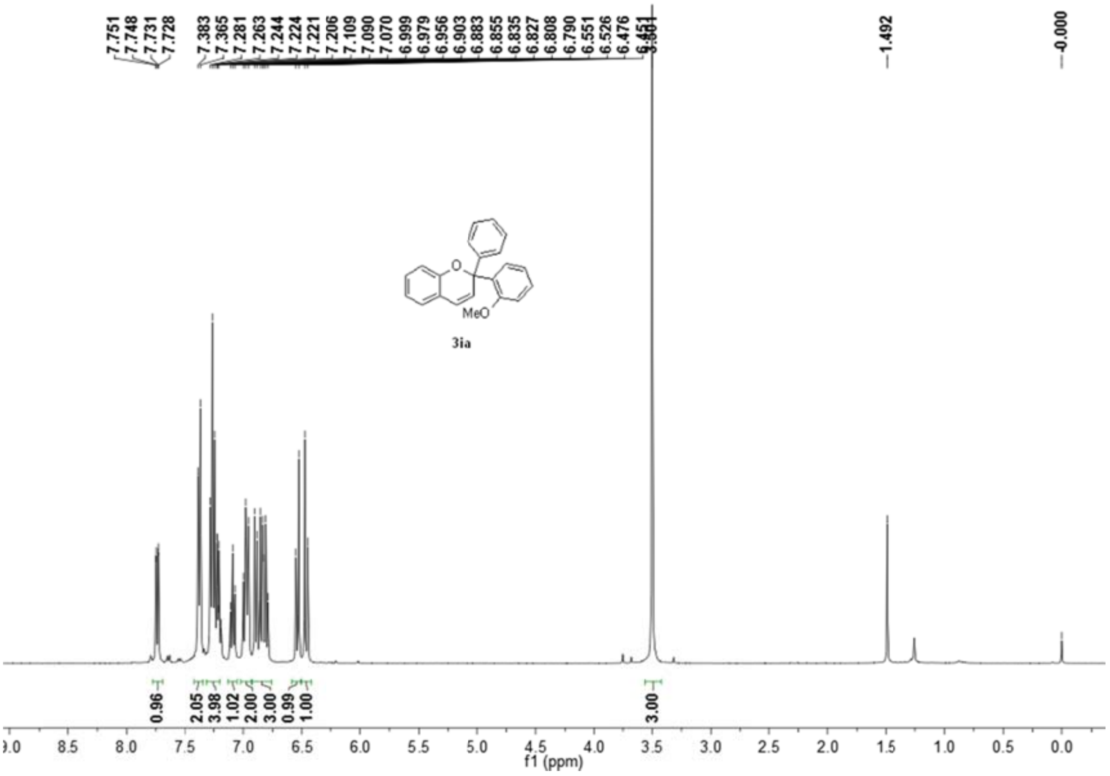
-62.455
Ph
CF3
+
Ph
CF3
3fa/4fa = 93/7
7.50
93.00
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)

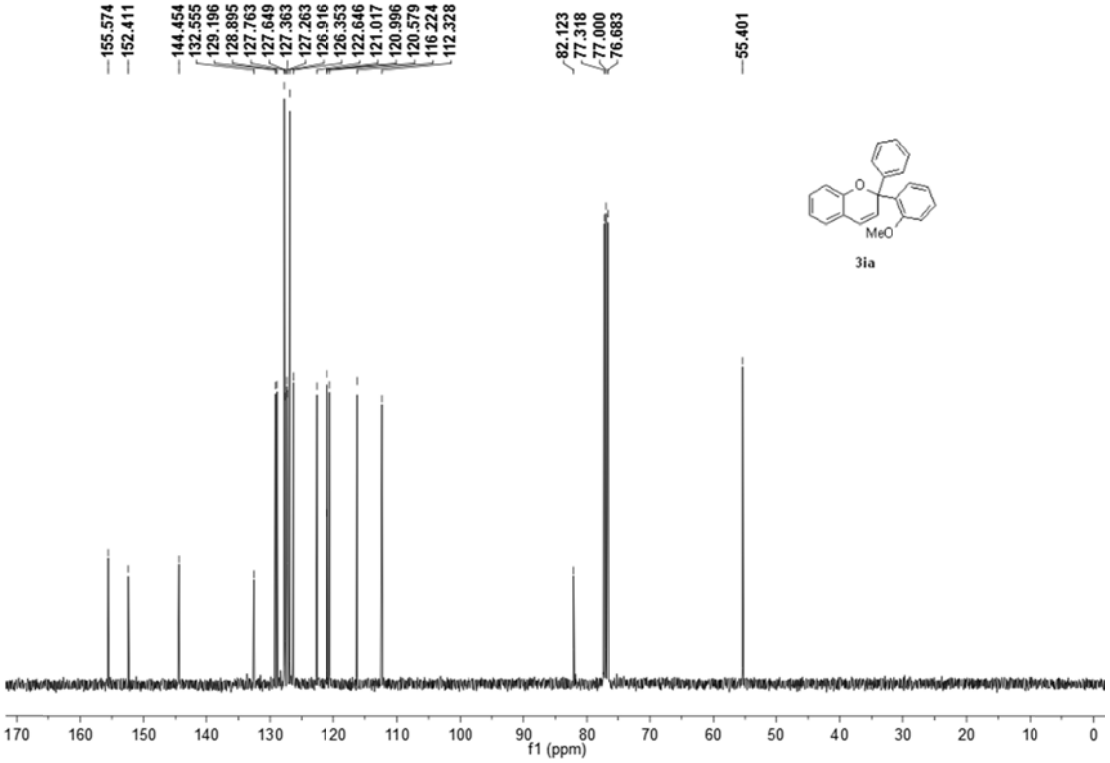

7.455
7.410
7.392
7.309
7.290
7.283
7.267
7.262
7.244
7.217
7.205
6.920
6.834
6.622
6.597
6.102
6.078
1.499
0.000
Ph
Cl
+
O
Ph
Cl
3ga/4ga = 90/10
0.96
2.05
6.22
1.18
1.01
0.97
1.02
1.00
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

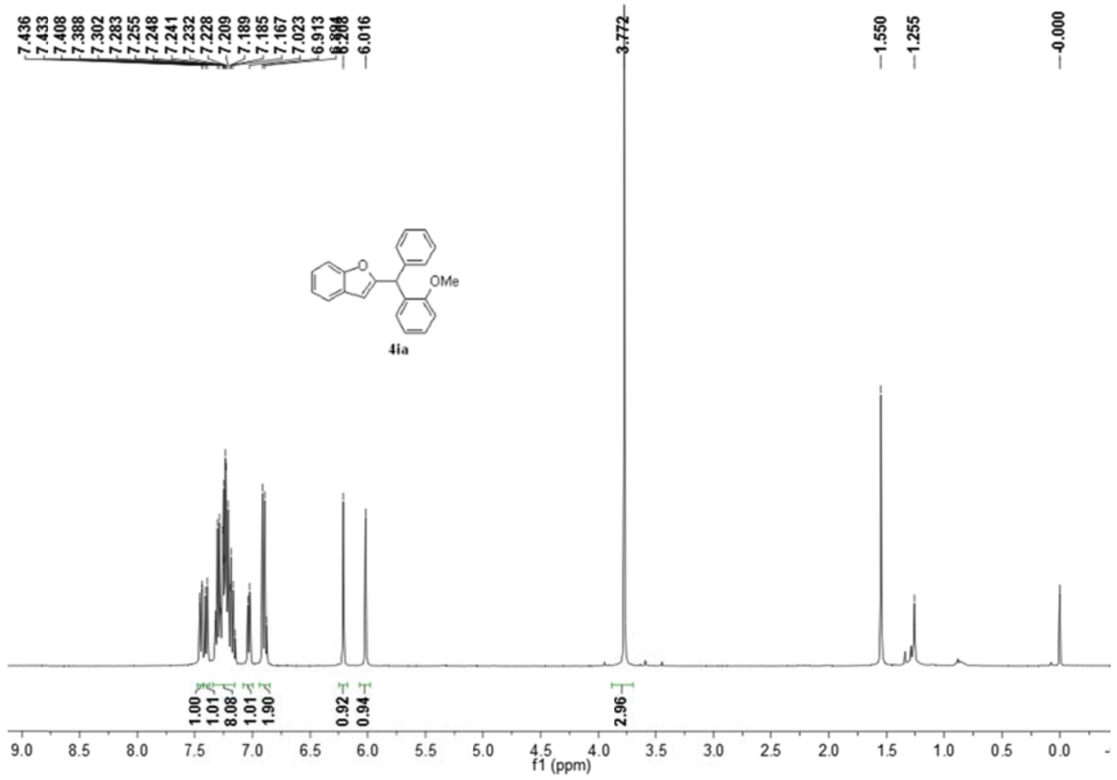

152.185
147.020
144.265
134.122
129.692
129.390
128.226
128.081
127.690
127.644
127.215
126.857
126.649
125.181
123.822
121.408
120.909
116.493
82.032
77.318
77.000
76.683
Ph
Cl
+
O
Ph
Cl
3ga/4ga = 90/10
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

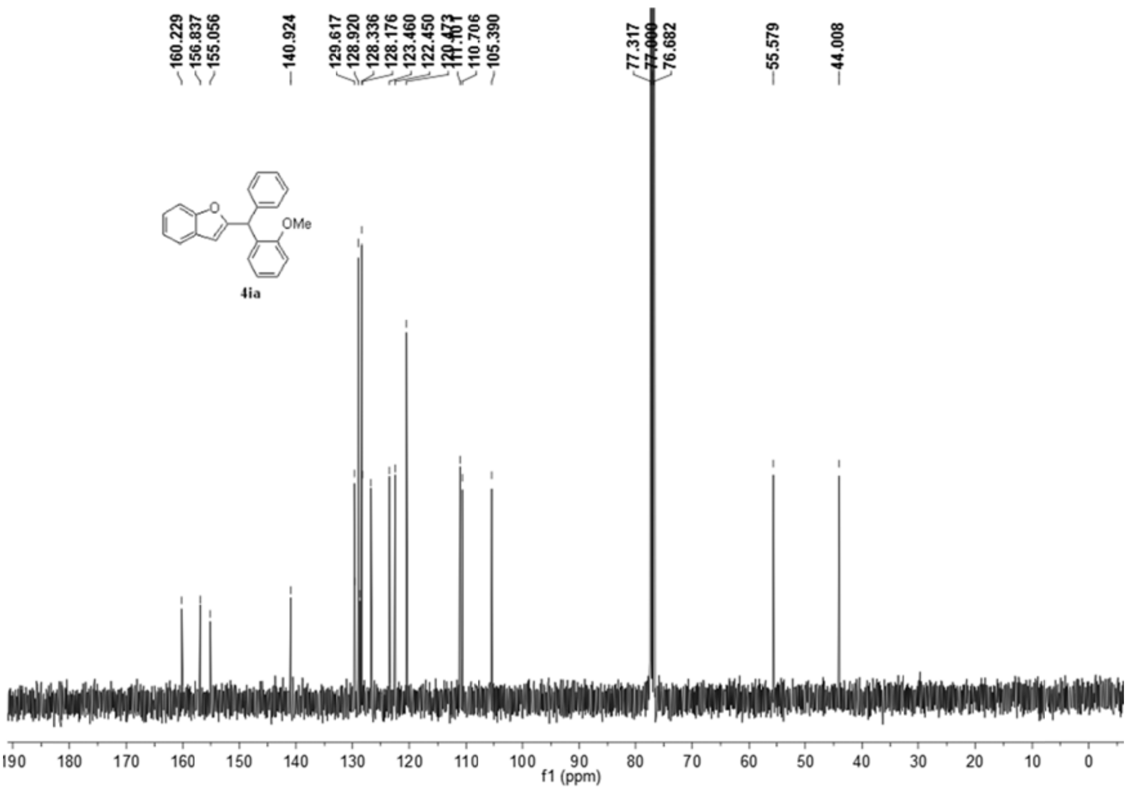

7.431
7.373
7.354
7.315
7.298
7.278
7.253
7.185
7.170
7.155
7.151
7.126
7.112
6.885
6.593
6.569
6.150
6.028
6.003
5.724
2.283
2.198
1.472
0.000
Ph
+
Ph
3ha/4ha = 3/1
15.28
1.39
0.99
0.99
0.98
0.36
1.00
0.37
1.11
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

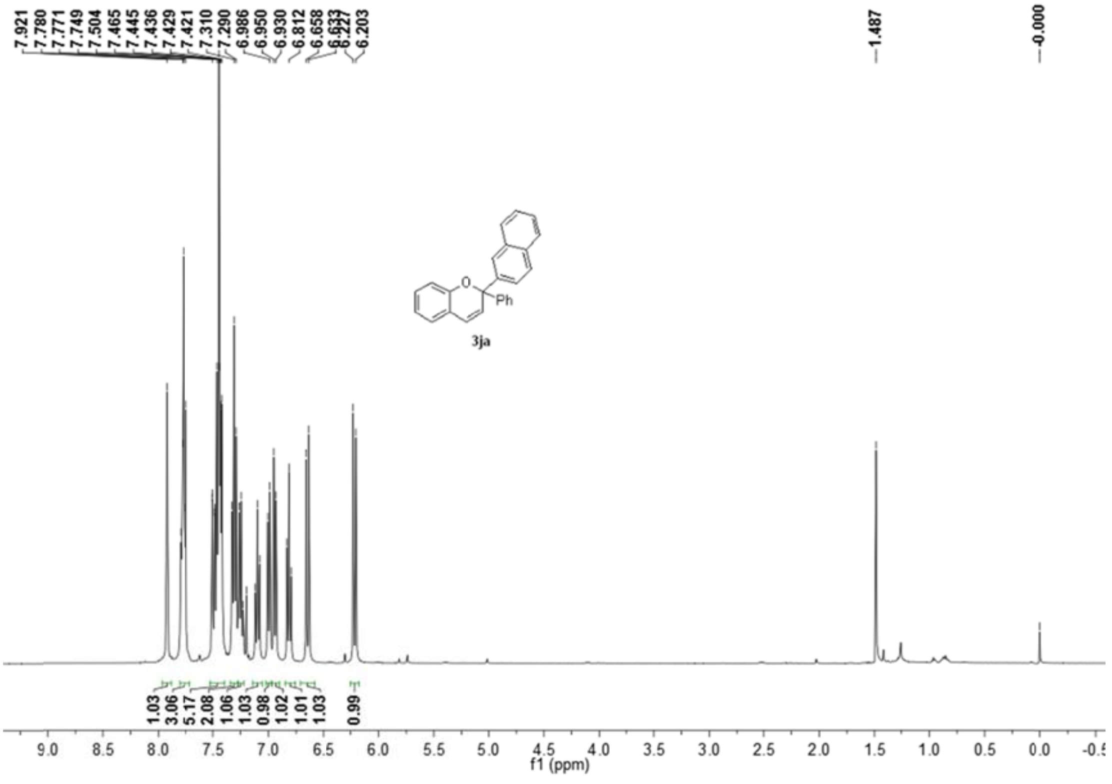

159.932
155.070
152.659
145.129
141.447
137.569
132.409
129.362
129.075
128.967
128.521
128.341
128.159
128.009
127.135
126.525
126.476
125.028
122.985
121.157
121.122
116.171
111.121
83.451
77.318
77.000
76.682
47.913
21.513
19.597
Ph
+
Ph
3ha/4ha = 3/1
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

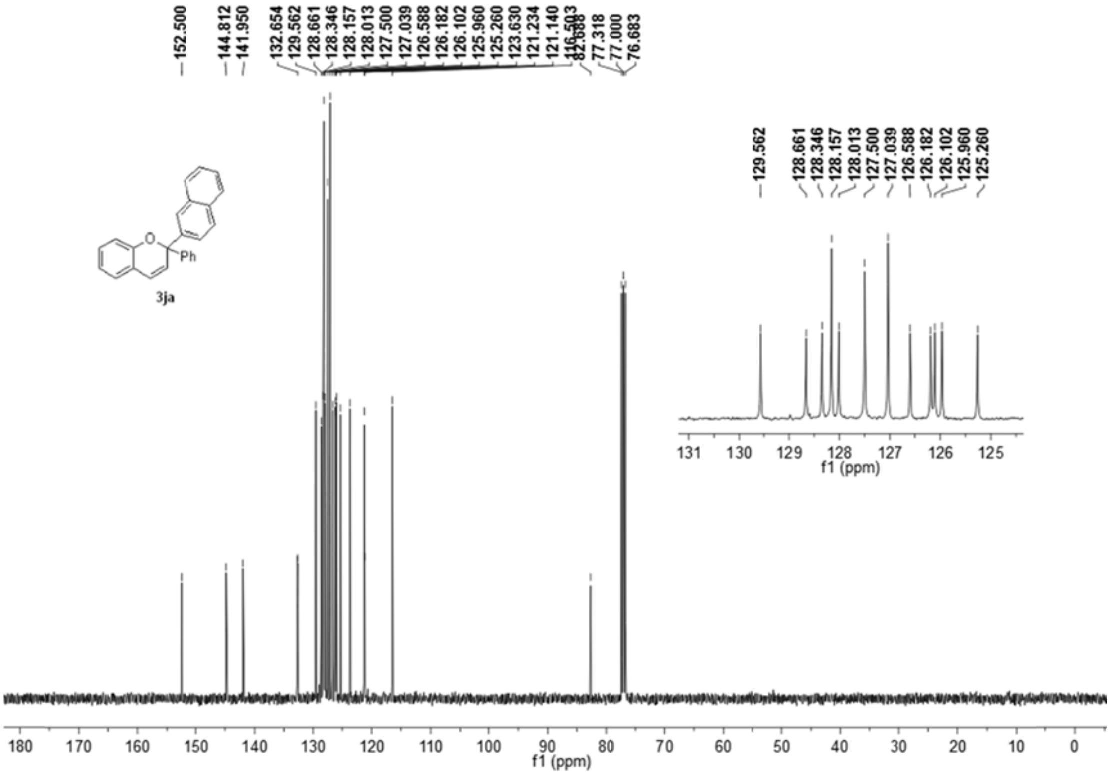

7.751
7.748
7.731
7.728
7.383
7.365
7.281
7.263
7.244
7.224
7.221
7.206
7.109
7.090
7.070
6.999
6.979
6.956
6.903
6.883
6.855
6.835
6.827
6.808
6.790
6.551
6.526
6.476
6.451
3.501
1.492
-0.000
O
MeO
3ia
0.96
2.05
3.98
1.02
2.00
3.00
0.99
1.00
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

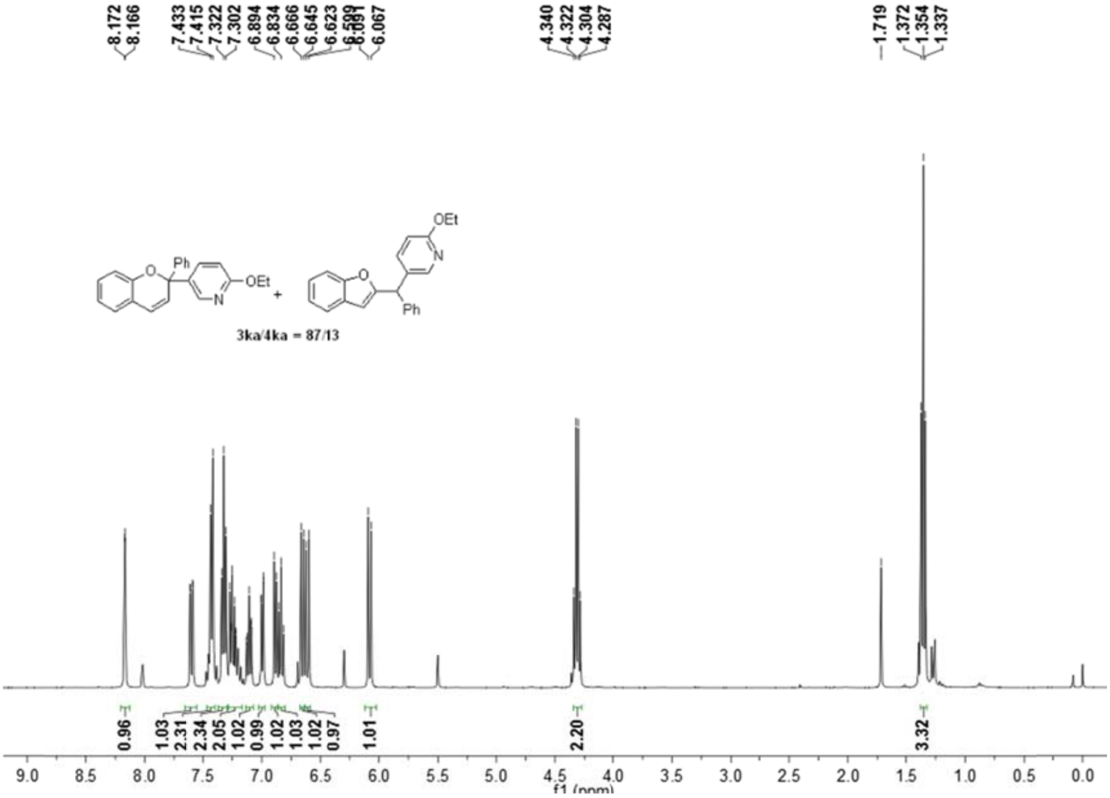

155.574
152.411
144.454
132.555
129.196
128.895
127.763
127.649
127.363
127.263
126.916
126.353
122.646
121.017
120.996
120.579
116.224
112.328
82.123
77.318
77.000
76.683
55.401
O
MeO
3ia
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

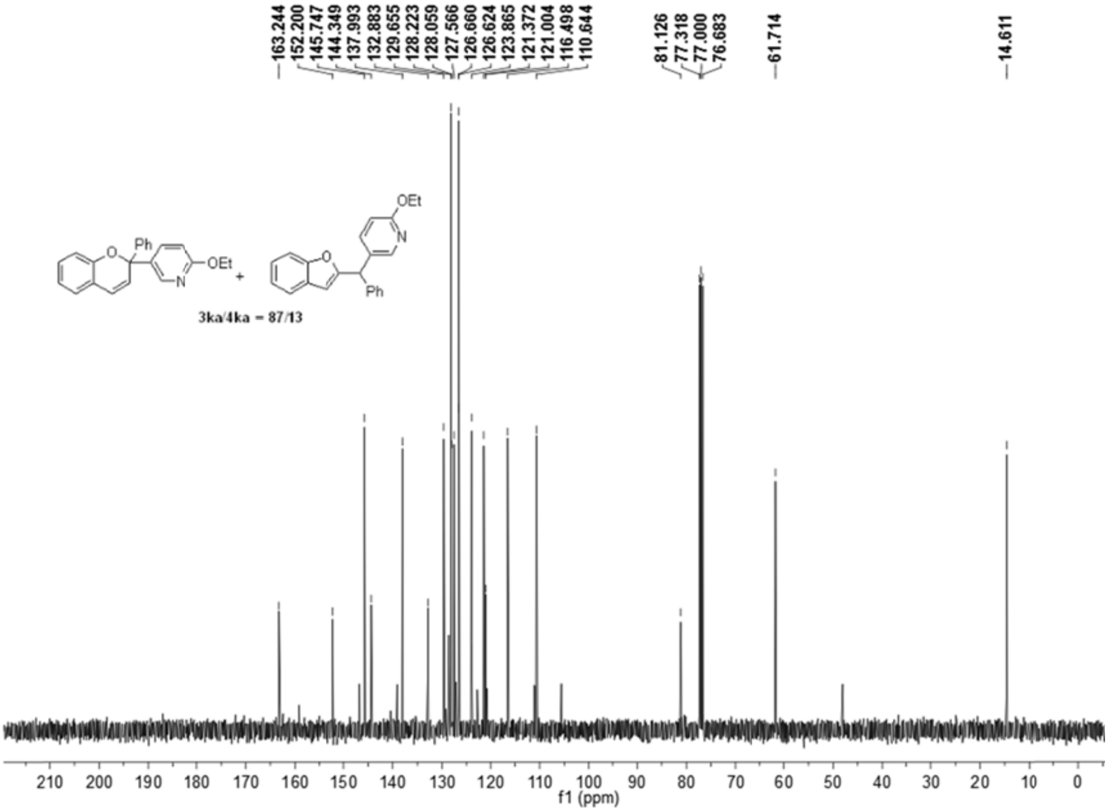

7.436
7.433
7.408
7.388
7.302
7.283
7.255
7.248
7.241
7.232
7.228
7.209
7.189
7.185
7.167
7.023
6.913
6.894
6.208
6.016
3.772
1.550
1.255
-0.000
OMe
4ia
1.00
1.01
8.08
1.01
1.90
0.92
0.94
2.96
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

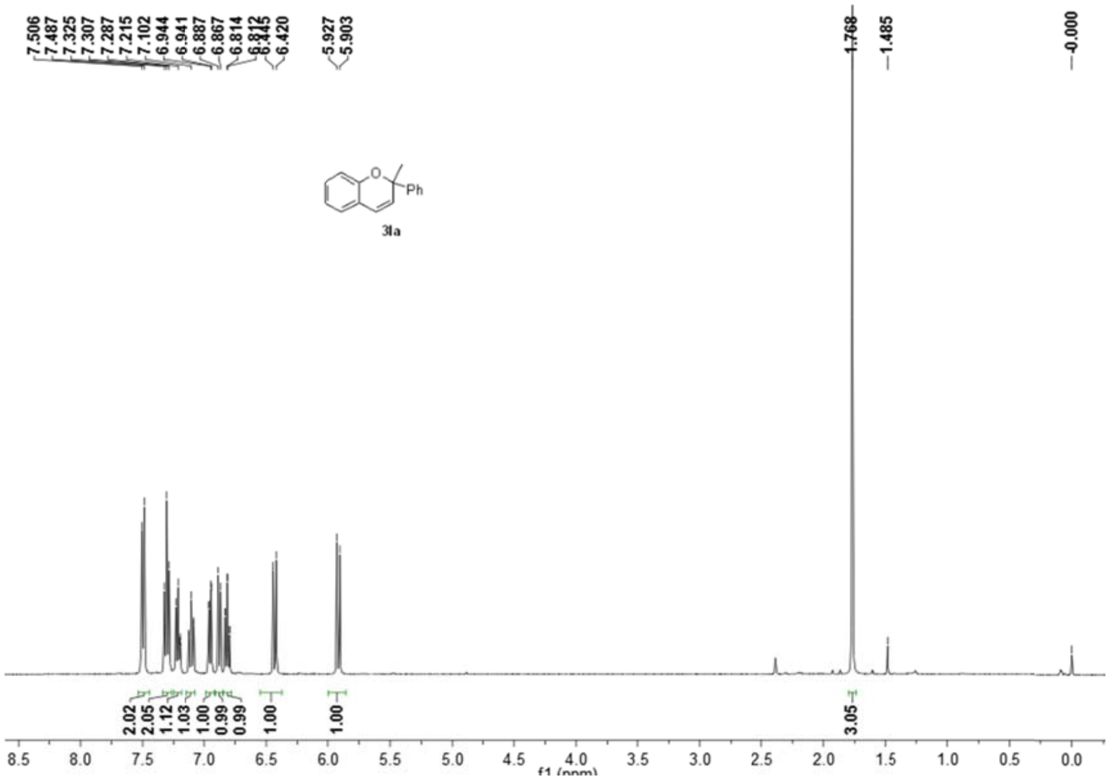

160.229
156.837
155.056
140.924
129.617
128.920
128.336
128.176
123.460
122.450
120.473
111.101
110.706
105.390
77.317
77.000
76.682
55.579
44.008
OMe
4ia
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

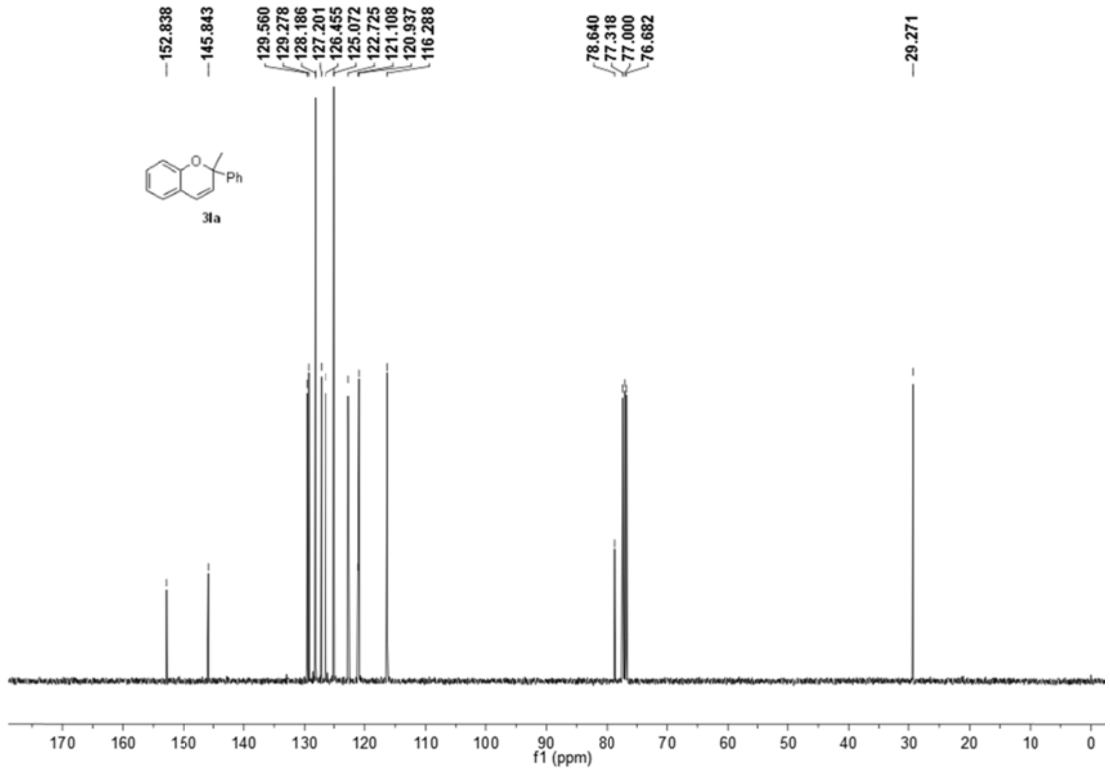

7.921
7.780
7.771
7.749
7.504
7.465
7.445
7.436
7.429
7.421
7.310
7.290
6.986
6.950
6.930
6.812
6.658
6.633
6.227
6.203
1.487
-0.000
Ph
3ja
1.03
3.06
5.17
2.08
1.06
1.03
0.98
1.02
1.01
1.03
0.99
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

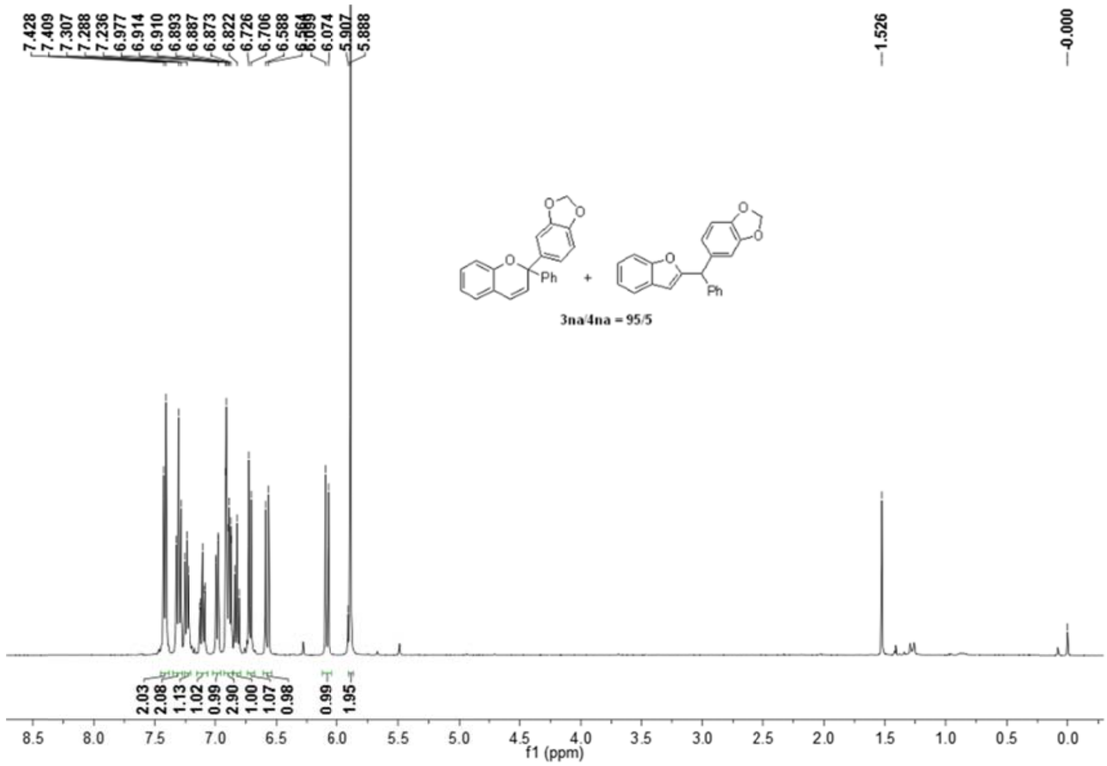

152.500
144.812
141.950
132.654
129.562
128.661
128.346
128.157
128.013
127.500
127.039
126.588
126.182
126.102
125.960
125.260
123.630
121.234
121.140
116.503
82.688
77.318
77.000
76.683
Ph
3ja
129.562
128.661
128.346
128.157
128.013
127.500
127.039
126.588
126.182
126.102
125.960
125.260
131
130
129
128
127
126
125
f1 (ppm)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

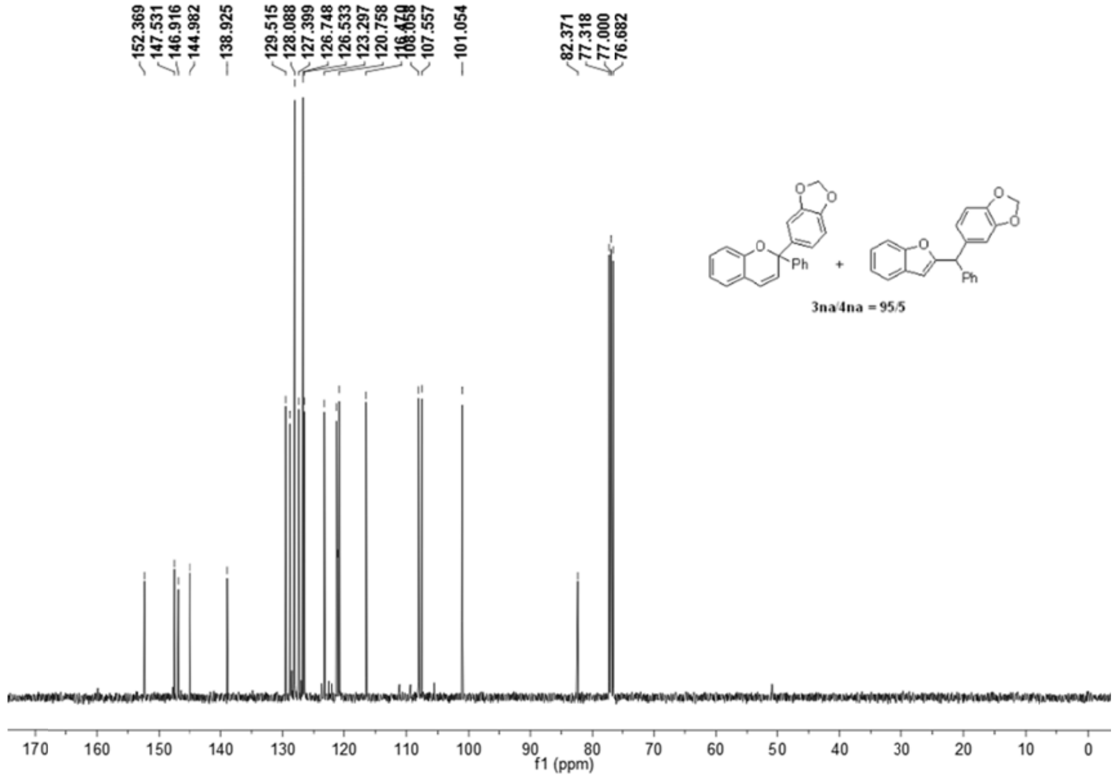

8.172
8.166
7.433
7.415
7.322
7.302
6.894
6.834
6.666
6.645
6.623
6.599
6.091
6.067
4.340
4.322
4.304
4.287
1.719
1.372
1.354
1.337
Ph
O
OEt
N
+
OEt
N
O
Ph
3ka/4ka = 87/13
0.96
1.03
2.31
2.34
2.05
1.02
0.99
1.02
1.03
1.02
0.97
1.01
2.20
3.32
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

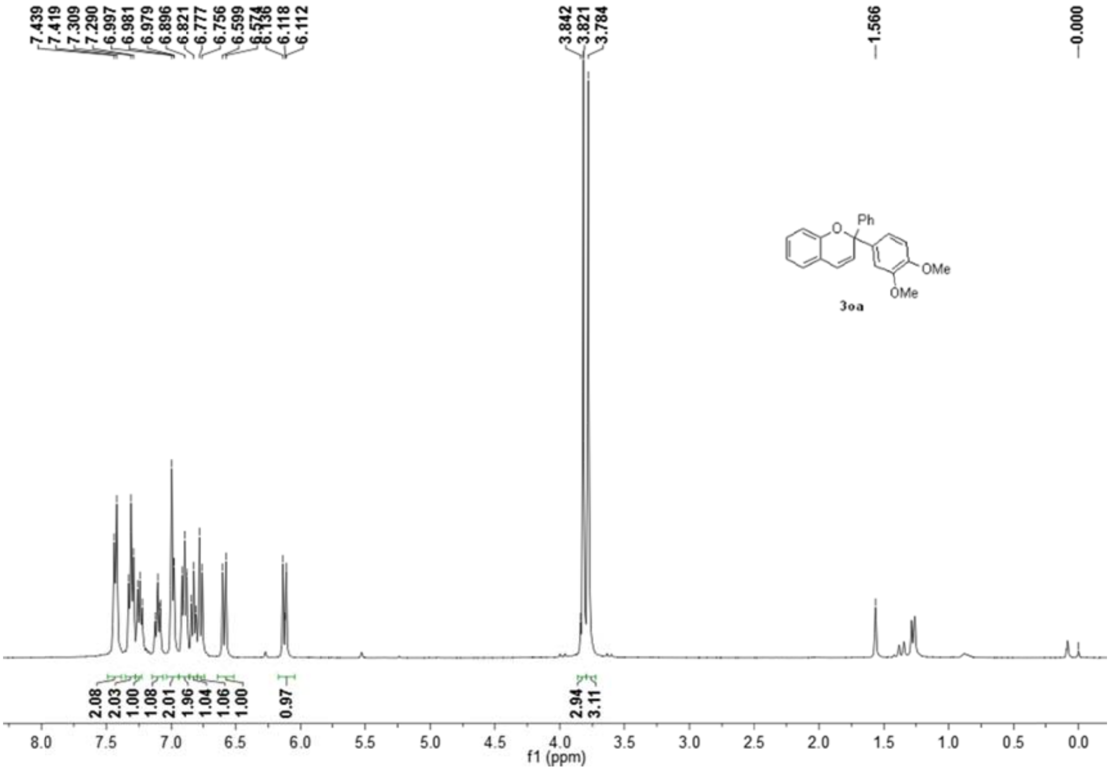

163.244
152.200
145.747
144.349
137.993
132.883
129.655
128.223
128.059
127.566
126.660
126.624
123.865
121.372
121.004
116.498
110.644
81.126
77.318
77.000
76.683
61.714
14.611
Ph
O
OEt
N
+
OEt
N
O
Ph
3ka/4ka = 87/13
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

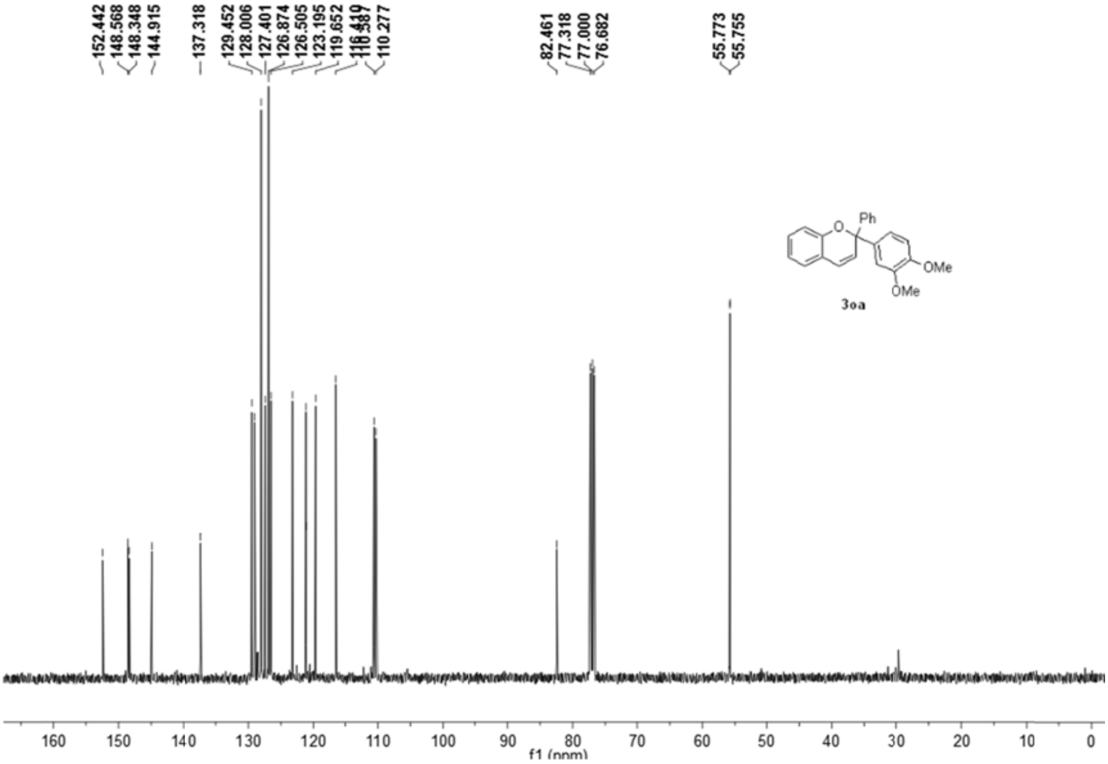

7.506
7.487
7.325
7.307
7.287
7.215
7.102
6.944
6.941
6.887
6.867
6.814
6.812
6.445
6.420
5.927
5.903
1.768
1.485
-0.000
O
Ph
3la
2.02
2.05
1.12
1.03
1.00
0.99
0.99
1.00
1.00
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

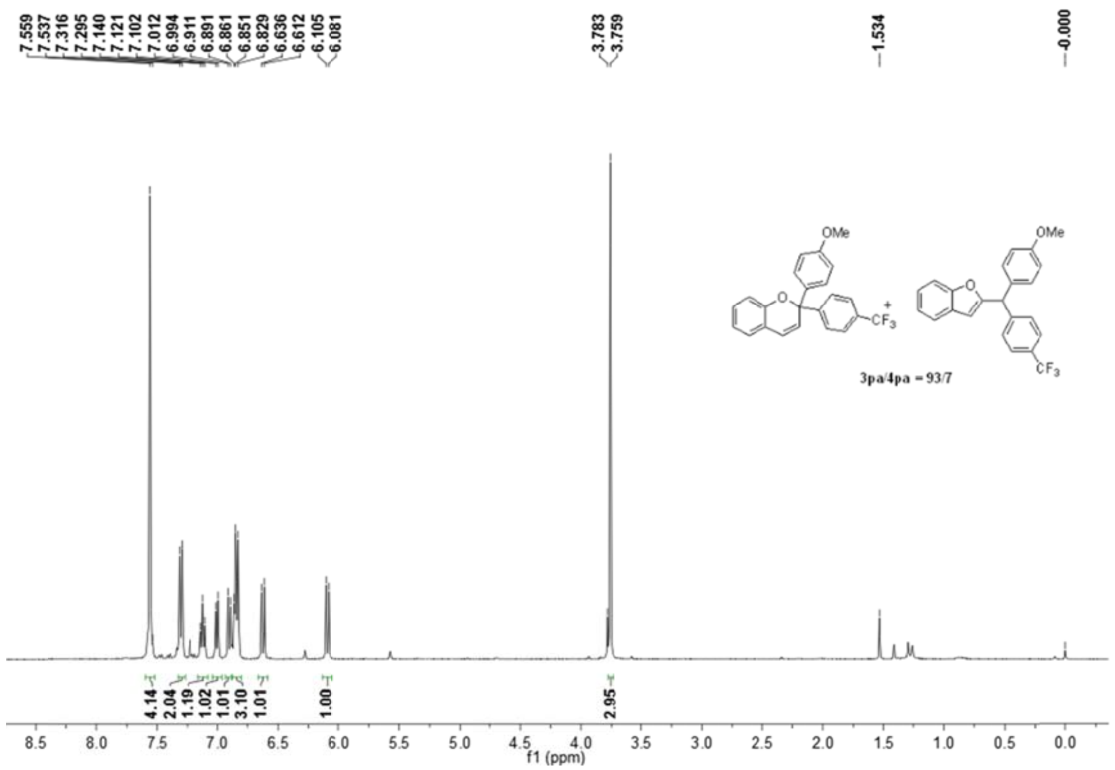

152.838
145.843
129.560
129.278
128.186
127.201
126.455
125.072
122.725
121.108
120.937
116.288
78.640
77.318
77.000
76.682
29.271
O
Ph
3la
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

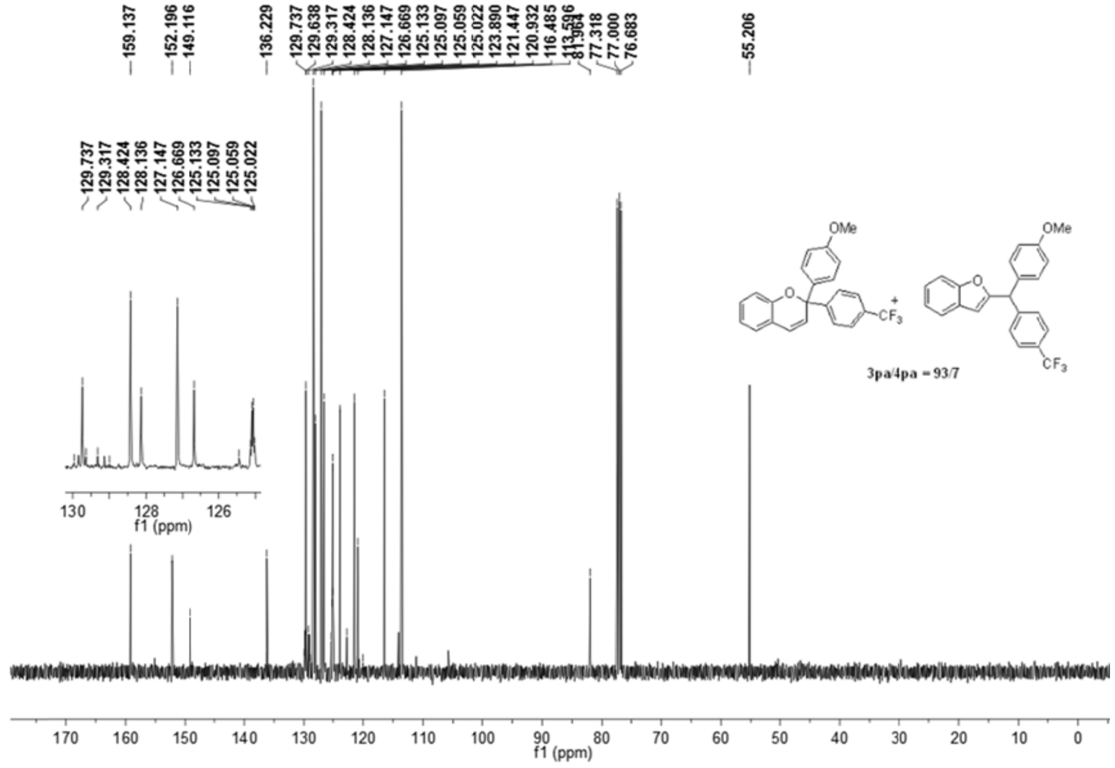

7.428
7.409
7.307
7.288
7.236
6.977
6.914
6.910
6.893
6.887
6.873
6.822
6.726
6.706
6.588
6.564
6.099
6.074
5.907
5.888
1.526
0.000
Ph
Ph
+
3na/4na = 95/5
2.03
2.08
1.13
1.02
0.99
2.90
1.00
1.07
0.98
0.99
1.95
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

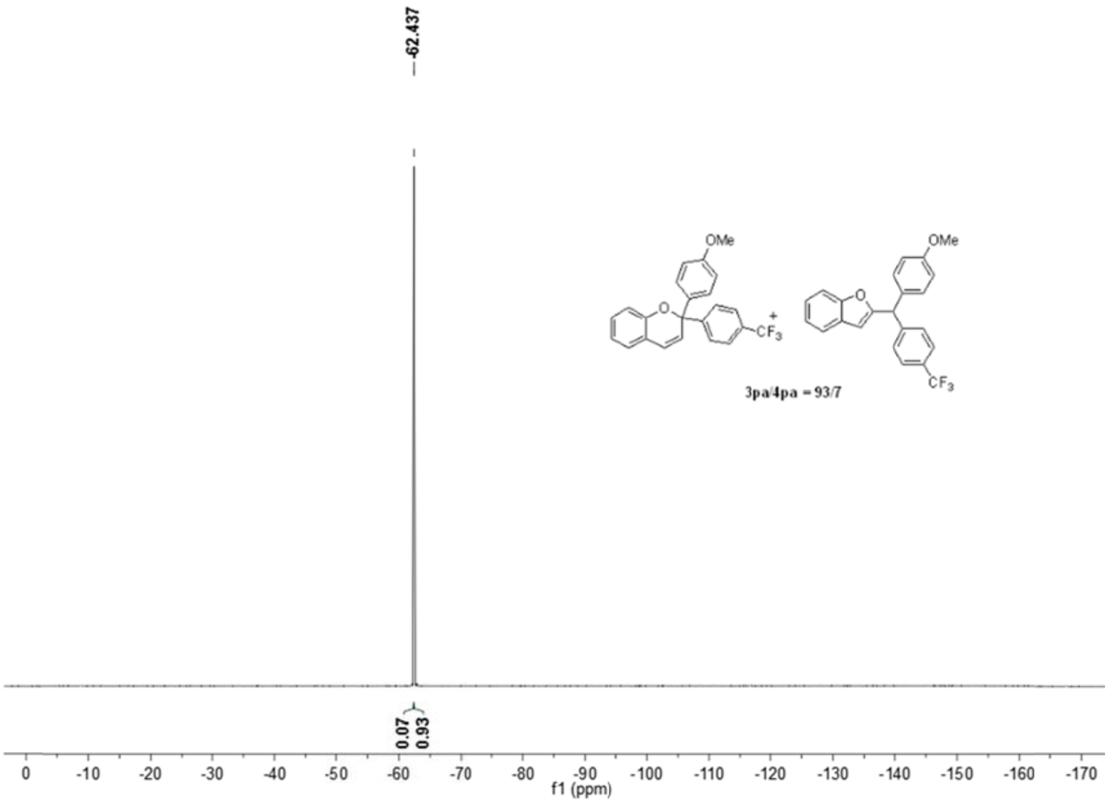

152.369
147.531
146.916
144.982
138.925
129.515
128.088
127.399
126.748
126.533
123.297
120.758
116.470
108.058
107.557
101.054
82.371
77.318
77.000
76.682
Ph
Ph
+
3na/4na = 95/5
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

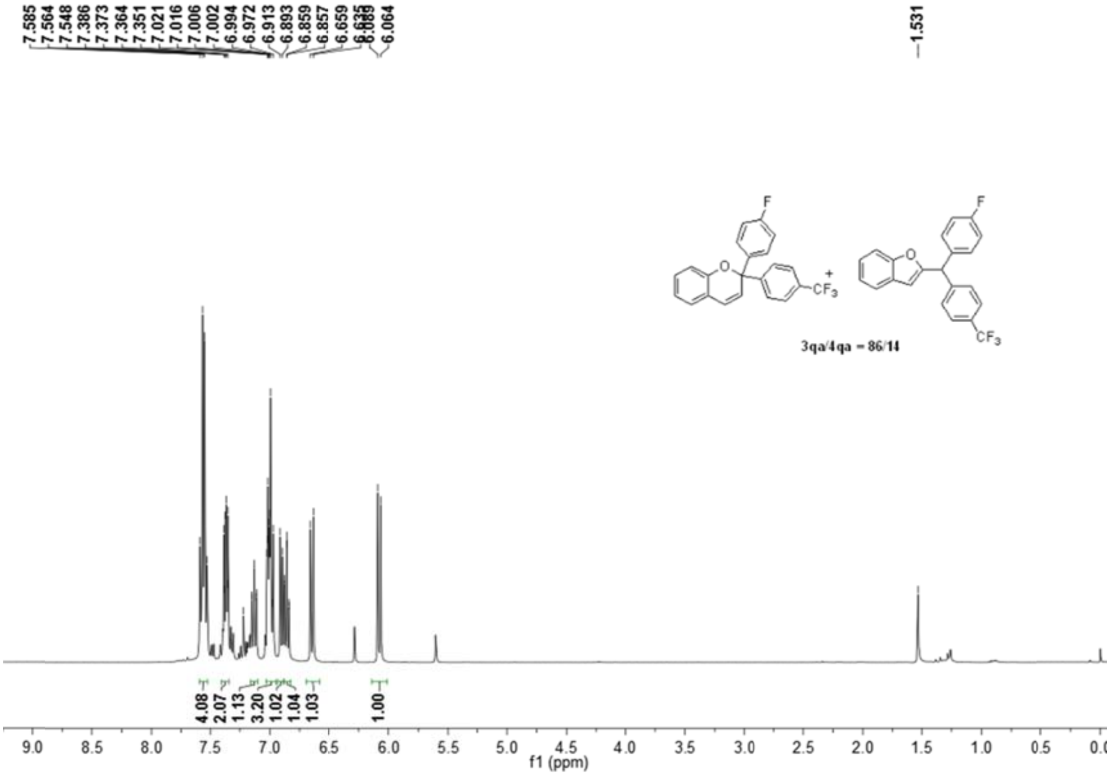

7.439
7.419
7.309
7.290
6.997
6.981
6.979
6.896
6.821
6.777
6.756
6.599
6.574
6.136
6.118
6.112
3.842
3.821
3.784
1.566
0.000
Ph
O
OMe
OMe
3oa
2.08
2.03
1.00
1.08
2.01
1.96
1.04
1.06
1.00
0.97
2.94
3.11
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

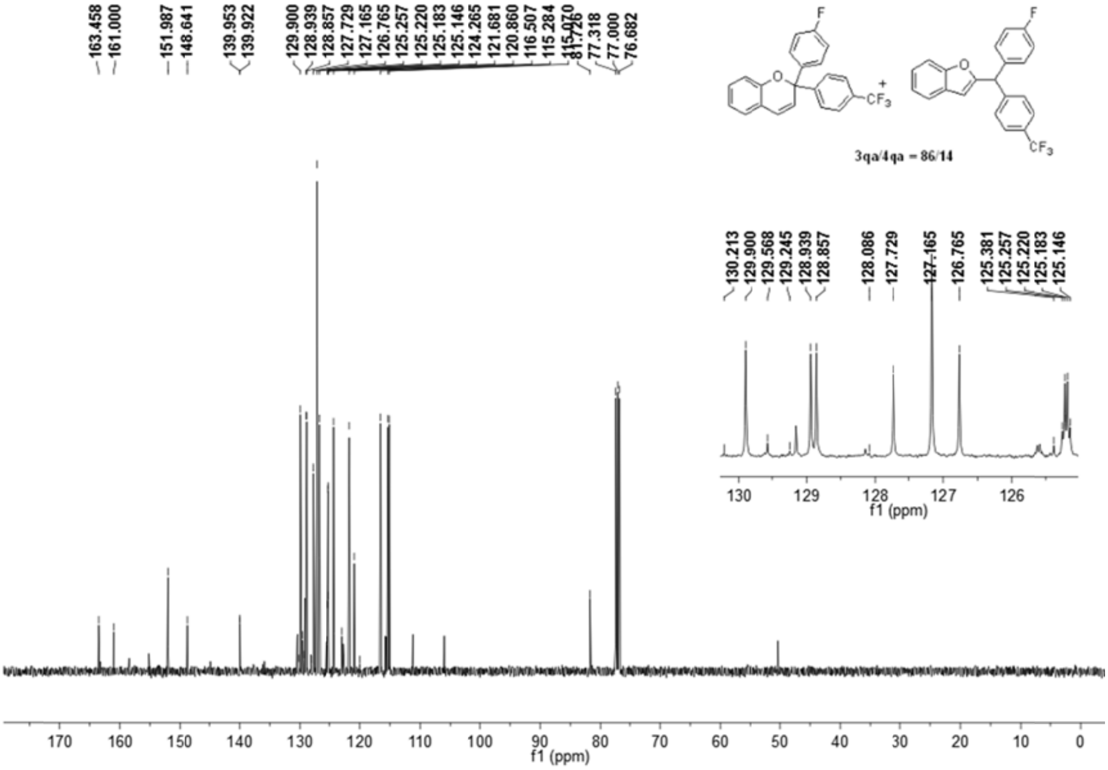

152.442
148.568
148.348
144.915
137.318
129.452
128.006
127.401
126.874
126.505
123.195
119.652
116.419
110.587
110.277
82.461
77.318
77.000
76.682
55.773
55.755
Ph
O
OMe
OMe
3oa
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

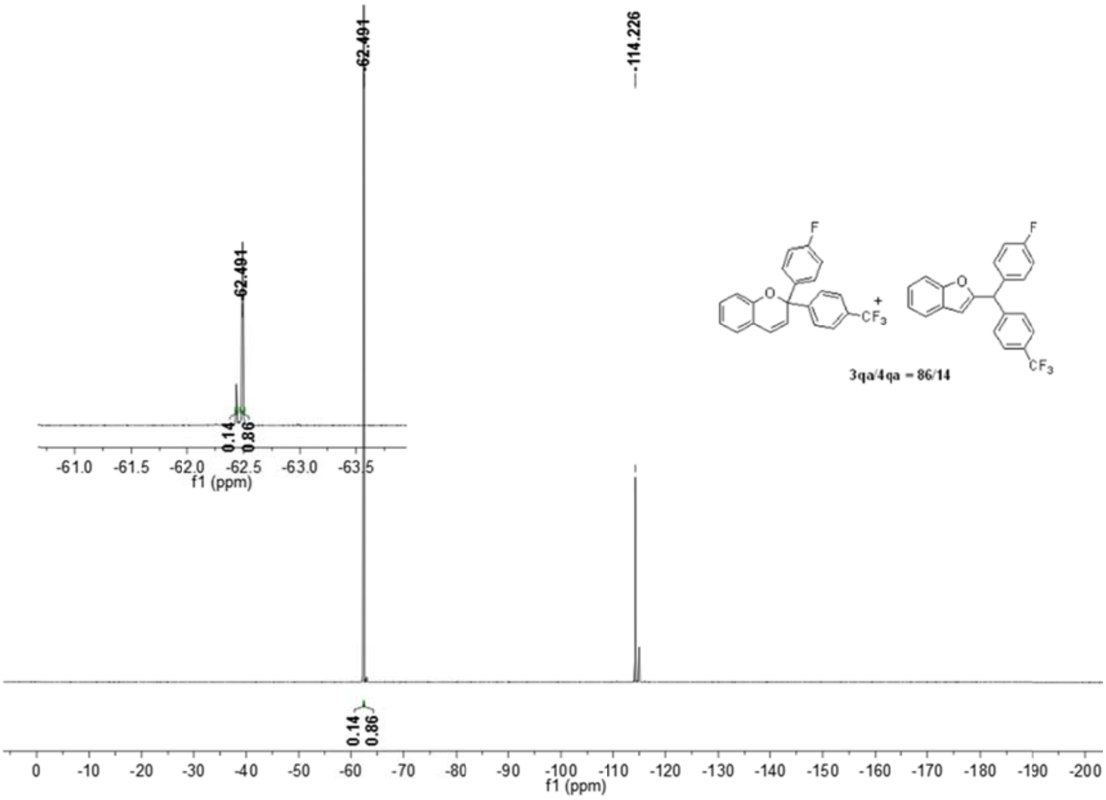

7.559
7.537
7.316
7.295
7.140
7.121
7.102
7.012
6.994
6.911
6.891
6.861
6.851
6.829
6.636
6.612
6.105
6.081
3.783
3.759
1.534
-0.000
OMe
O
CF3
+
3pa/4pa = 93/7
4.14
2.04
1.19
1.02
1.01
3.10
1.01
1.00
2.95
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

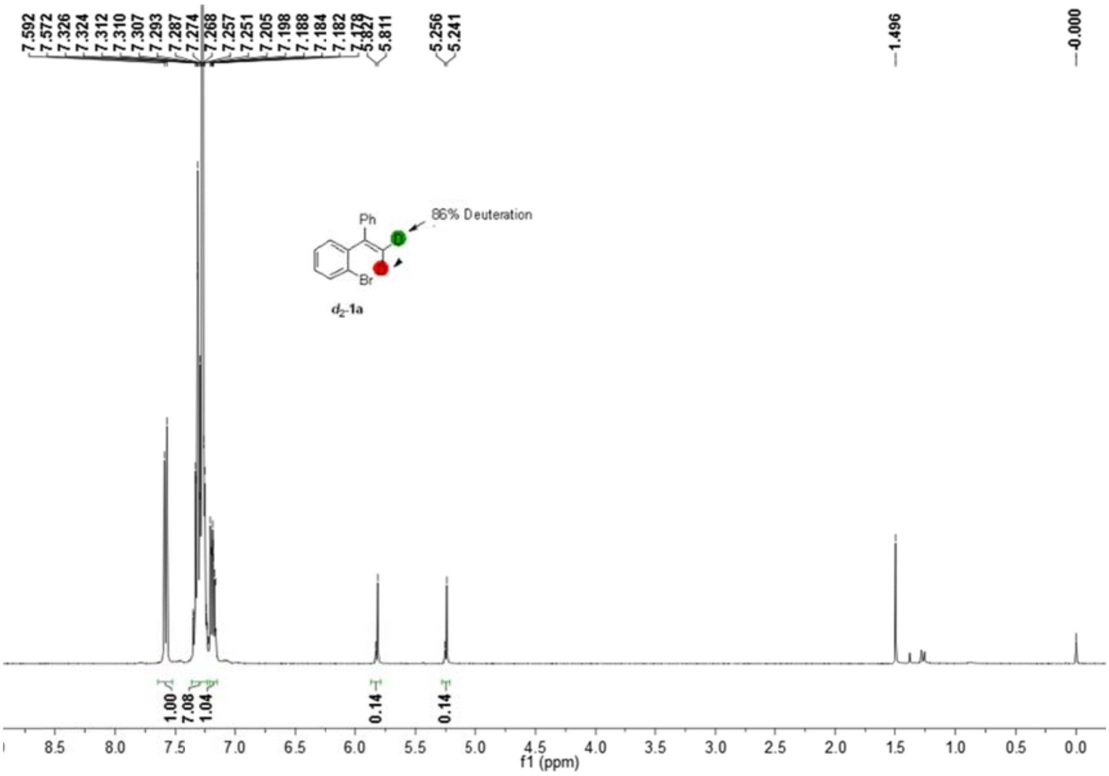

159.137
152.196
149.116
136.229
129.737
129.638
129.317
128.424
128.136
127.147
126.669
125.133
125.097
125.059
125.022
123.890
121.447
120.932
116.485
113.596
81.964
77.318
77.000
76.683
55.206
129.737
129.317
128.424
128.136
127.147
126.669
125.133
125.097
125.059
125.022
130
128
126
f1 (ppm)
OMe
O
CF3
+
3pa/4pa = 93/7
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

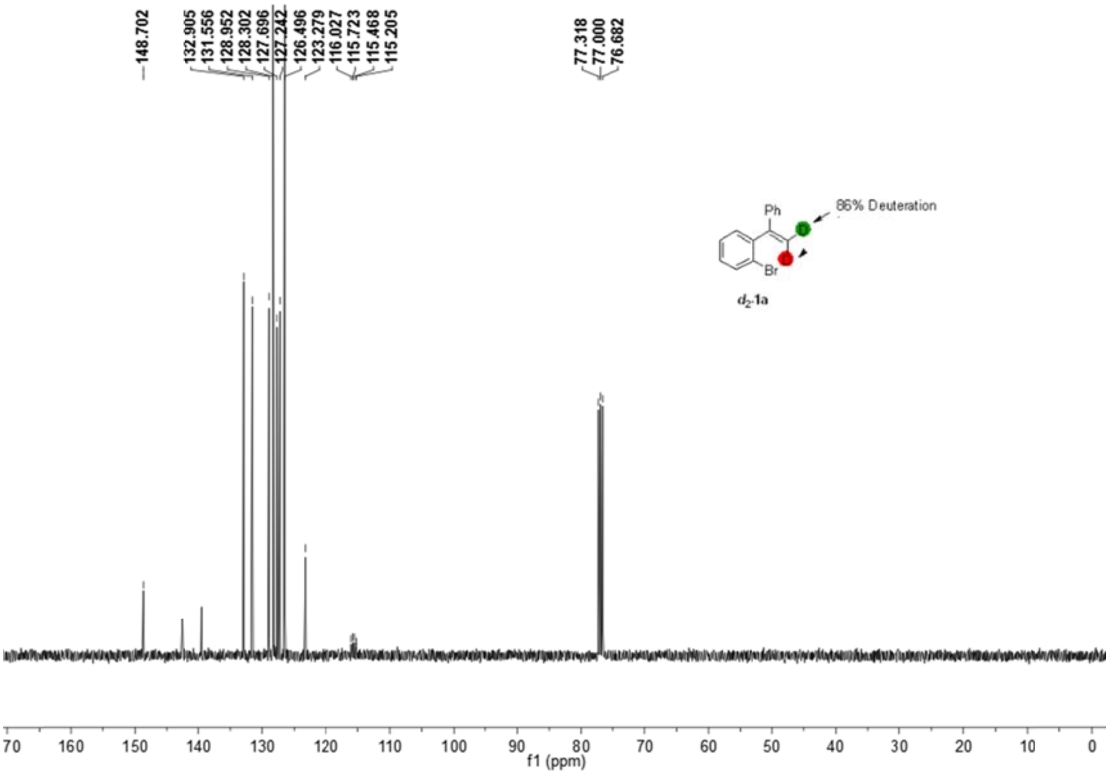

-62.437
OMe
CF3
+
OMe
CF3
3pa/4pa = 93/7
0.07
0.93
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
f1 (ppm)

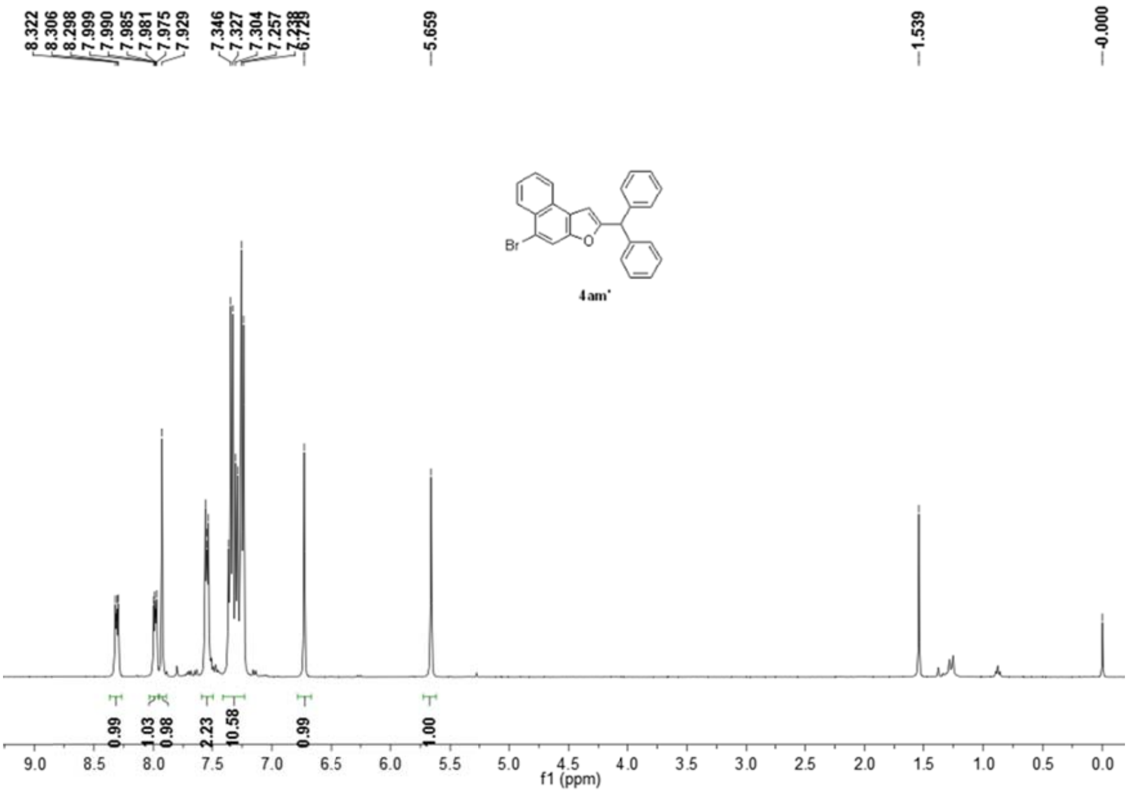

7.585
7.564
7.548
7.386
7.373
7.364
7.351
7.021
7.016
7.006
7.002
6.994
6.972
6.913
6.893
6.859
6.857
6.659
6.635
6.089
6.064
1.531
F
O
CF3
+
F
O
CF3
3qa/4qa = 86/14
4.08
2.07
1.13
3.20
1.02
1.04
1.03
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


163.458
161.000
151.987
148.641
139.953
139.922
129.900
128.939
128.857
127.729
127.165
126.765
125.257
125.220
125.183
125.146
124.265
121.681
120.860
116.507
115.284
115.070
81.726
77.318
77.000
76.682
F
O
CF3
+
F
O
CF3
3qa/4qa = 86/14
130.213
129.900
129.568
129.245
128.939
128.857
128.086
127.729
127.165
126.765
125.381
125.257
125.220
125.183
125.146
130
129
128
127
126
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

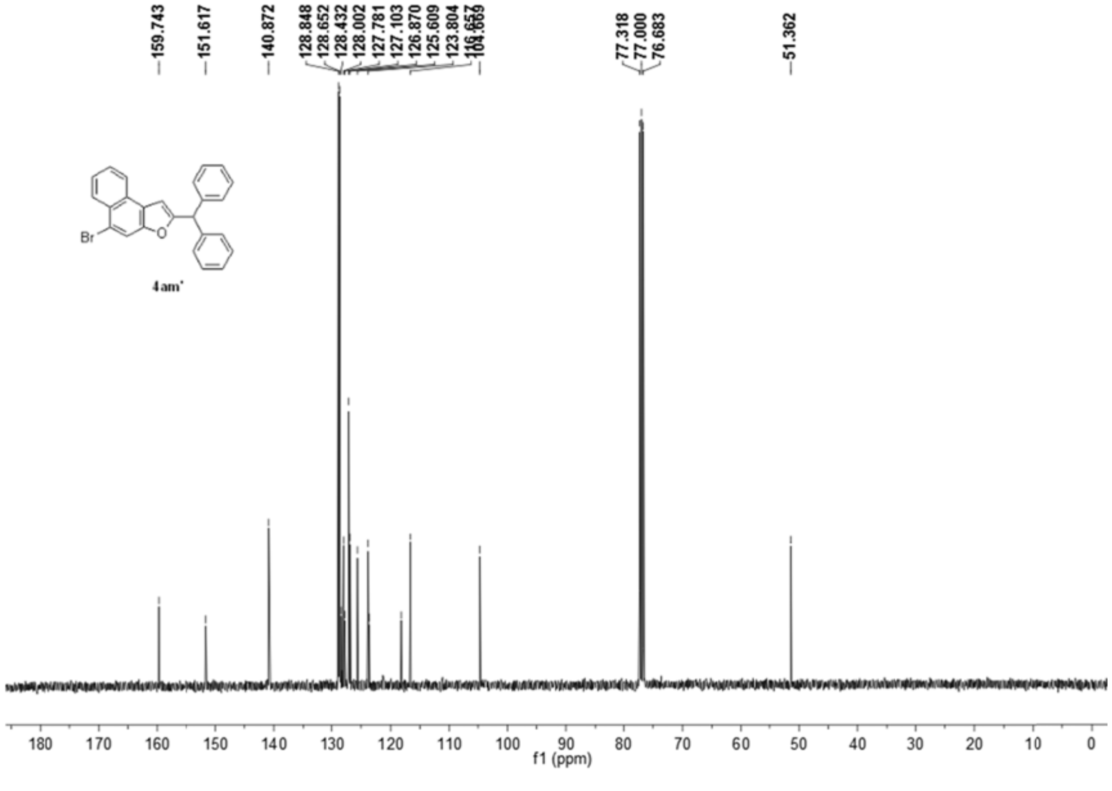

-62.491
-114.226
-62.491
0.14
0.86
-61.0 -61.5 -62.0 -62.5 -63.0 -63.5
f1 (ppm)
F
O
CF3
+
F
O
CF3
3qa/4qa = 86/14
0.14
0.86
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


7.592
7.572
7.326
7.324
7.312
7.310
7.307
7.293
7.287
7.274
7.268
7.257
7.251
7.205
7.198
7.188
7.184
7.182
7.178
5.827
5.811
5.256
5.241
1.496
-0.000
Ph
D
86% Deuteration
Br
d2-1a
1.00
7.08
1.04
0.14
0.14
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)

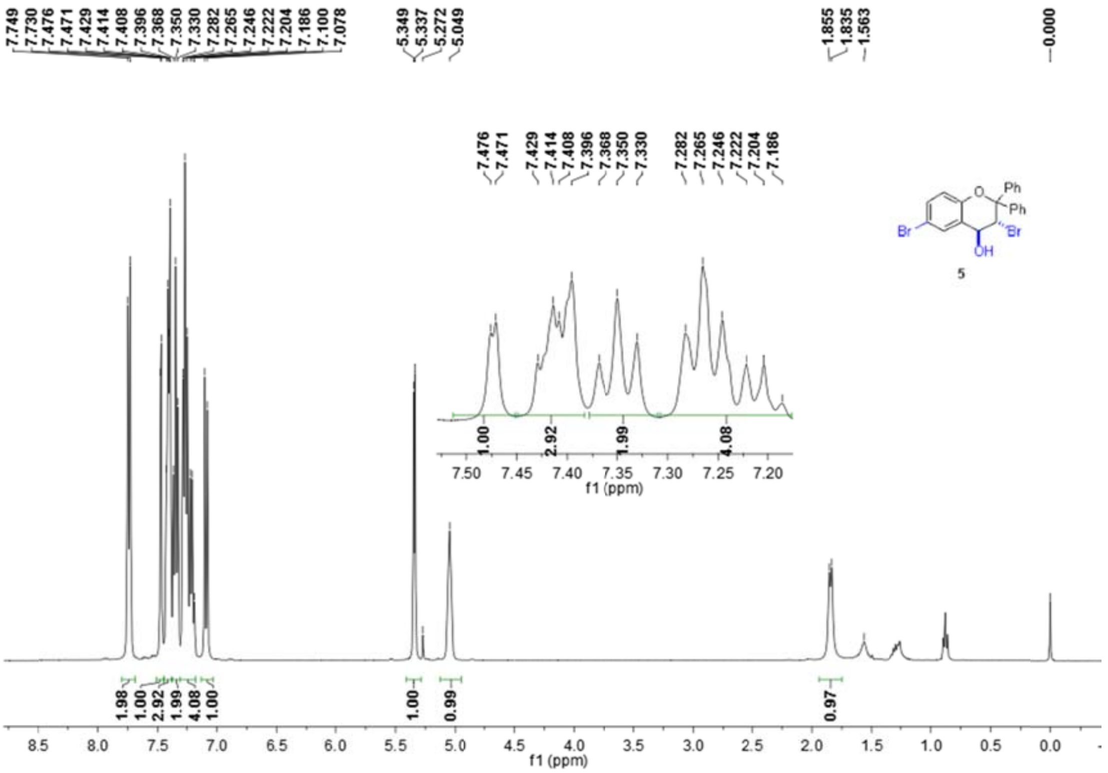

148.702
132.905
131.556
128.952
128.302
127.696
127.242
126.496
123.279
116.027
115.723
115.468
115.205
77.318
77.000
76.682
Ph
D
86% Deuteration
Br
d2-1a
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

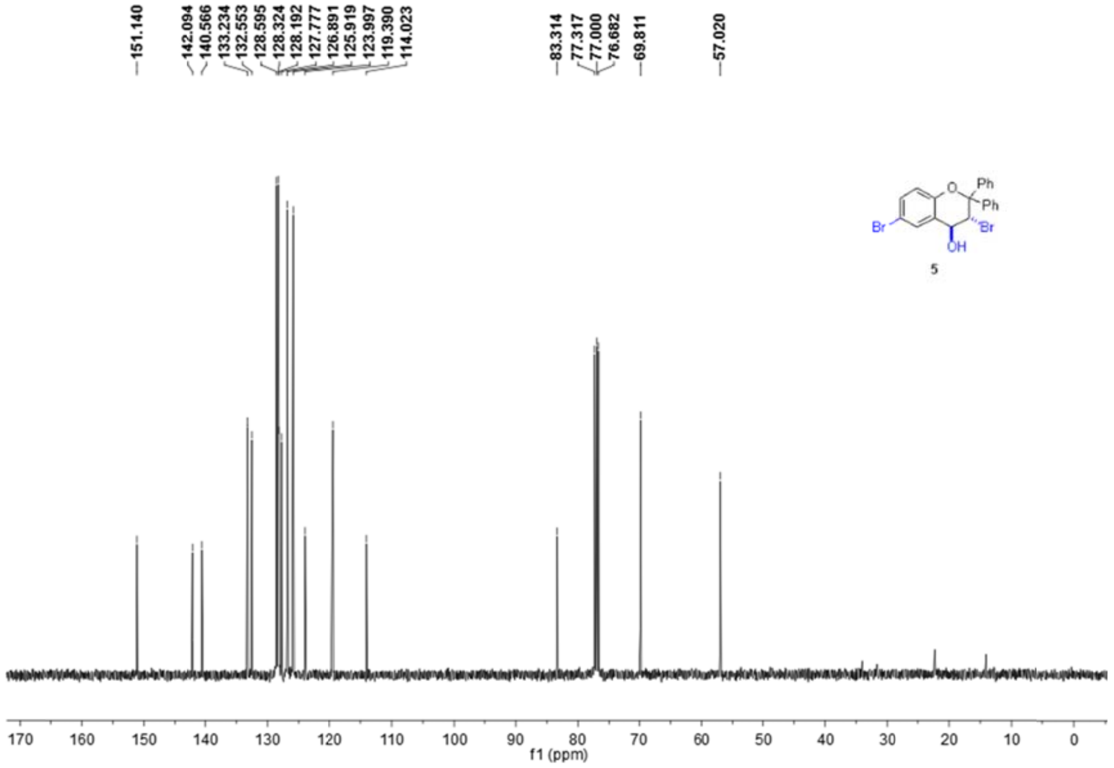

8.322
8.306
8.298
7.999
7.990
7.985
7.981
7.975
7.929
7.346
7.327
7.304
7.257
7.238
6.729
5.659
1.539
0.000
Br
O
0.99
1.03
0.98
2.23
10.58
0.99
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

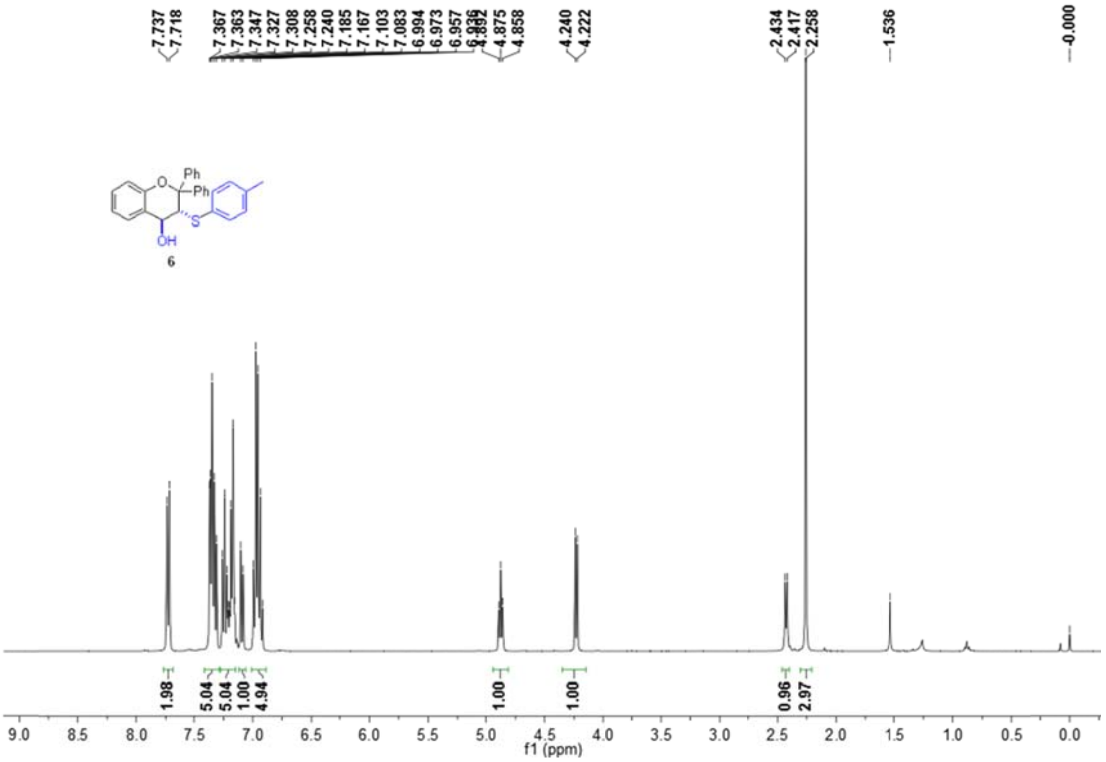
4am'

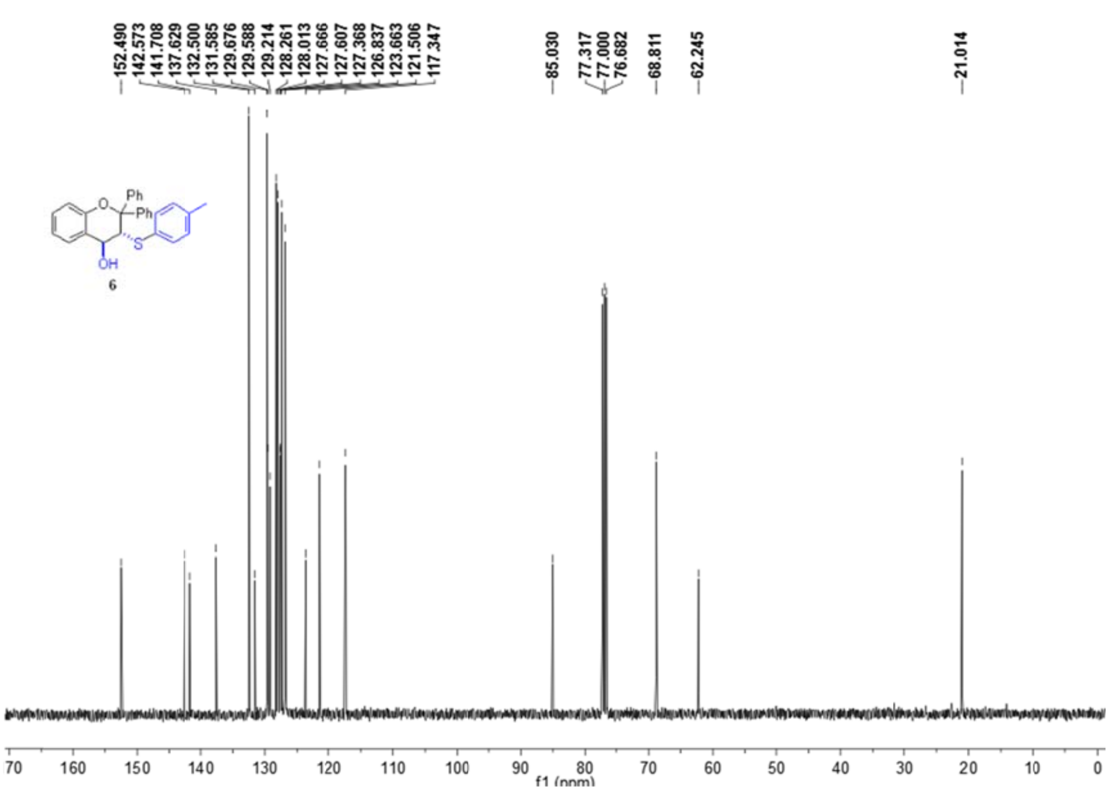

159.743
151.617
140.872
128.848
128.652
128.432
128.002
127.781
127.103
126.870
125.609
123.804
116.657
104.669
77.318
77.000
76.683
51.362
Br
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

4am'


7.749
7.730
7.476
7.471
7.429
7.414
7.408
7.396
7.368
7.350
7.330
7.282
7.265
7.246
7.222
7.204
7.186
7.100
7.078
5.349
5.337
5.272
5.049
1.855
1.835
1.563
0.000
1.00
2.92
1.99
4.08
7.50 7.45 7.40 7.35 7.30 7.25 7.20
f1 (ppm)
Br
O
Ph
Ph
Br
OH
5
1.98
1.00
2.92
1.99
4.08
1.00
1.00
0.99
0.97
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)


151.140
142.094
140.566
133.234
132.553
128.595
128.324
128.192
127.777
126.891
125.919
123.997
119.390
114.023
83.314
77.317
77.000
76.682
69.811
57.020
Br
O
Ph
Ph
Br
OH
5
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.737
7.718
7.367
7.363
7.347
7.327
7.308
7.258
7.240
7.185
7.167
7.103
7.083
6.994
6.973
6.957
6.936
4.892
4.875
4.858
4.240
4.222
2.434
2.417
2.258
1.536
-0.000
Ph
O
Ph
S
OH
6
1.98
5.04
5.04
1.00
4.94
1.00
1.00
0.96
2.97
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)


152.490
142.573
141.708
137.629
132.500
131.585
129.676
129.588
129.214
128.261
128.013
127.666
127.607
127.368
126.837
123.663
121.506
117.347
85.030
77.317
77.000
76.682
68.811
62.245
21.014
Ph
O
Ph
S
OH
6
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)