Supporting Information

Cobalt(III)-Catalyzed Annulation of Esters and Alkynes: A Facile Route to Indenones

Wenlong Yu,[a] Wei Zhang,[a] Zhanxiang Liu,[a] Yuhong Zhang*[,a,b]

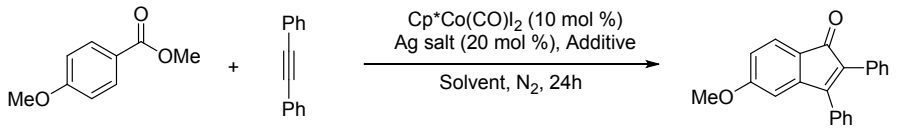
[a]*Department of Chemistry, Zhejiang University, Hangzhou 310027, China*

[b]*State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou 730000, China*

E-mail: *yhzhang@zju.edu.cn*

General All reactions were performed under nitrogen in a flame-dried reaction flask. The esters were purchased from commercial resources. The Cp*Co(CO)I_2[1], d_5-methyl benzoate[2] and (*E*)-methyl-2-(1,2-diphenylvinyl)benzoate (**4a**)[3] were prepared according the previous reports. ^{1}H NMR spectra were recorded at 400 MHz using TMS as internal standard. ^{13}C NMR spectra were recorded at 100 MHz using TMS as internal standard. The multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), multiplet (m), and broad resonances (br). Mass spectroscopy data of the products were collected on an HRMS-TOF instrument. GC-MS spectra were recorded using a HP6890 gas chromatograph with a HP5973 mass spectrometric detector equipped with an electron ionization source and a single-stage quadrupole. MALDI-TOF analysis was carried out on an ultrafleXtreme MALDI-TOF/TOF Mass Spectrometer (Bruker Daltonics, USA).

The Optimization of the reaction conditions[a,b]



1a **2a** **3aa**

entry	catalyst (mol %)	Ag salt	additive1 (mol %)	additive2 (mol %)	solvent	Temp	yield (%)[b]
1	Cp*Co(CO)I_2	$AgSbF_6$	$Cu(OAc)_2$ (20)	-	DCE	130 °C	32
2	Cp*Co(CO)I_2	$AgSbF_6$	AgOAc (20)	-	DCE	130 °C	25
3	Cp*Co(CO)I_2	$AgSbF_6$	AgOPiv (20)	-	DCE	130 °C	40
4	Cp*Co(CO)I_2	$AgSbF_6$	HOAc(20)	-	DCE	130 °C	22
5	Cp*Co(CO)I_2	$AgSbF_6$	HOAc (200)	-	DCE	130 °C	Trace
6	Cp*Co(CO)I_2	$AgSbF_6$	NaOAc (20)	-	DCE	130 °C	54
7	Cp*Co(CO)I_2	$AgSbF_6$	KOAc (20)	-	DCE	130 °C	70
8	Cp*Co(CO)I_2	$AgSbF_6$	KOPiv (20)	-	DCE	130 °C	65
9	Cp*Co(CO)I_2	$AgSbF_6$	AdCOOK (20)	-	DCE	130 °C	Trace
10	Cp*Co(CO)I_2	$AgSbF_6$	MesCOOK (20)	-	DCE	130 °C	40
11	Cp*Co(CO)I_2	$AgSbF_6$	PhCOOK (20)	-	DCE	130 °C	Trace
12	Cp*Co(CO)I_2	AgOTf	KOAc (20)	-	DCE	130 °C	NR
13	Cp*Co(CO)I_2	$AgBF_4$	KOAc (20)	-	DCE	130 °C	NR
14	Cp*Co(CO)I_2	$AgPF_6$	KOAc (20)	-	DCE	130 °C	NR
15	Cp*Co(CO)I_2	$AgNTf_2$	KOAc (20)	-	DCE	130 °C	50
16	Cp*Co(CO)I_2	$AgSbF_6$	KOAc (20)	$AgNTf_2$ (20)	DCE	130 °C	44
17	Cp*Co(CO)I_2	$AgSbF_6$	KOAc (20)	AgOTf (20)	DCE	130 °C	NR
18	Cp*Co(CO)I_2	$AgSbF_6$	KOAc (20)	$AgBF_4$ (20)	DCE	130 °C	15
19	Cp*Co(CO)I_2	$AgSbF_6$	KOAc (20)	$Zn(OTf)_2$ (20)	DCE	130 °C	NR
20	Cp*Co(CO)I_2	$AgSbF_6$	KOAc (20)	$ZnBr_2$ (20)	DCE	130 °C	NR
21	Cp*Co(CO)I_2	$AgSbF_6$	KOAc (20)	$Cu(OTf)_2$ (20)	DCE	130 °C	NR
22	Cp*Co(CO)I_2	$AgSbF_6$	KOAc (20)	$Sc(OTf)_3$ (20)	DCE	130 °C	NR
23	Cp*Co(CO)I_2	$AgSbF_6$	KOAc (20)	BPh_3 (100)	DCE	130 °C	65
24	Cp*Co(CO)I_2	$AgSbF_6$	KOAc (20)	$BF_3{\cdot}OEt_2$ (20)	DCE	130 °C	NR

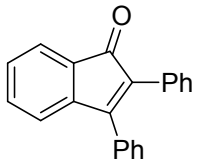
25	$Cp^*Co(CO)I_2$	$AgSbF_6$	-	$Zn(OTf)_2$ (20)	DCE	130 °C	NR
26	$Cp^*Co(CO)I_2$	$AgSbF_6$	-	$Cu(OTf)_2$ (20)	DCE	130 °C	NR
27	$Cp^*Co(CO)I_2$	$AgSbF_6$	-	$Sc(OTf)_3$ (20)	DCE	130 °C	NR
28	$Cp^*Co(CO)I_2$	$AgSbF_6$	KOAc (20)	-	PhMe	130 °C	NR
29	$Cp^*Co(CO)I_2$	$AgSbF_6$	KOAc (20)	-	$PhCF_3$	130 °C	63
30	$Cp^*Co(CO)I_2$	$AgSbF_6$	KOAc (20)	-	PhCl	130 °C	59
31	$Cp^*Co(CO)I_2$	$AgSbF_6$	KOAc (20)	-	PhF	130 °C	NR
32	$Cp^*Co(CO)I_2$	$AgSbF_6$	KOAc (20)	-	*o*-DCB	130 °C	55
33	$Cp^*Co(CO)I_2$	$AgSbF_6$	KOAc (20)	-	t-AmOH	130 °C	NR
34	$Cp^*Co(CO)I_2$	$AgSbF_6$	KOAc (20)	-	TFE	130 °C	Trace
35	$Cp^*Co(CO)I_2$	$AgSbF_6$	KOAc (20)	-	DCE	120 °C	65
36	$Cp^*Co(CO)I_2$	$AgSbF_6$	KOAc (20)	-	DCE	140 °C	69
37	$Cp^*Co(CO)I_2$	none	KOAc (20)	-	DCE	130 °C	NR
38	$Cp^*Co(CO)I_2$	$AgSbF_6$	none	-	DCE	130 °C	NR
39	$[Cp^*RhCl_2]_2$	$AgSbF_6$	KOAc (20)	-	DCE	130 °C	Trace
40[c]	$[Cp^*RhCl_2]_2$	$AgSbF_6$	$Cu(OAc)_2$ (20)	-	DCE	130 °C	6
41	none	$AgSbF_6$	KOAc (20)	-	DCE	130 °C	NR
42	$Co(OAc)_2$	$AgSbF_6$	KOAc (20)	-	DCE	130 °C	NR
43	$CoCl_2$	$AgSbF_6$	KOAc (20)	-	DCE	130 °C	NR

[a]Reaction conditions: substrate **1a** (0.1 mmol), diphenylacetylene **2a** (0.15 mmol), $Cp^*Co(CO)I_2$ (10 mol%), Ag salts (20 mol%), additive **1** (20 mol%), solvent (1 mL), 130 °C, N_2, 24 h. [b]Isolated yields. [c]determined by GC-MS. TFE = CF_3CH_2OH, *o*-DCB = *o*-dichlorobenzene

Typical Procedure for the Product

The methyl 4-methoxybenzoate (0.1 mmol) and diphenylacetylene (0.15 mmol) were dissolved in 1mL DCE in a sealed tube. 5 mg (10 mol%) $Cp^*Co(CO)I_2$, 7 mg (20 mol%) $AgSbF_6$ and 2 mg (20 mol%) KOAc were added. The tube was stirred at 130 °C for 24 h under N_2. The solvent was removed in vacuum and the product was isolated through column chromatography to afford the corresponding indenones.

2,3-diphenyl-1H-inden-1-one (eluent: petroleum ether(**PE**)→ethyl acetate(**EA**):petroleum ether(**PE**) = 1:200)

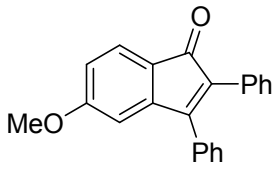


3ba

Yield: 74%; Red solid; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.59 (d, *J* = 8 Hz, 1H), 7.35-7.42 (m, 6H), 7.25-7.31 (m, 6H), 7.15 (d, *J* = 8 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 196.6, 155.4, 145.3, 133.5, 132.7, 132.4, 130.8, 130.8, 130.0, 129.3, 129.0, 128.8,

128.5, 128.1, 127.8, 123.0, 121.3. HRMS (EI-TOF) calcd for $C_{21}H_{14}O$ (M^+): 282.1045, found: 282.1045.

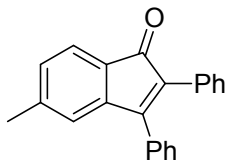
5-methoxy-2,3-diphenyl-1H-inden-1-one (eluent: PE→PE/EA = 100/1)



3aa

Yield: 70%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.55 (d, *J* = 8 Hz, 1H), 7.34-7.41 (m, 5H), 7.26 (s, 5H), 6.66-6.70 (m, 2H), 3.84 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 195.2, 164.5, 153.1, 147.9, 133.9, 132.7, 130.9, 130.0, 129.2, 128.8, 128.6, 128.1, 127.8, 124.9, 123.5, 110.5, 110.3, 55.8. HRMS (EI-TOF) calcd for $C_{22}H_{16}O_2$ (M^+): 312.1150, found: 312.1153.

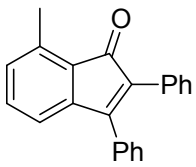
5-methyl-2,3-diphenyl-1H-inden-1-one (eluent: PE→PE/EA = 200/1)



3ca

Yield: 71%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.48 (d, *J* = 8 Hz, 1H), 7.36-7.43 (m, 5H), 7.26 (s, 5H), 7.08 (d, *J* = 8 Hz, 1H), 6.94 (s, 1H), 2.35 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 196.3, 155.0, 145.7, 144.5, 132.9, 132.8, 130.9, 130.0, 129.2, 129.0, 128.8, 128.5, 128.4, 128.1, 127.7, 123.1, 122.6, 22.1. HRMS (EI-TOF) calcd for $C_{22}H_{16}O$ (M^+): 296.1201, found: 296.1201.

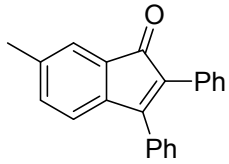
7-methyl-2,3-diphenyl-1H-inden-1-one (eluent: PE→PE/EA = 200/1)



3da

Yield: 60%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.34-7.40 (m, 5H), 7.21-7.26 (m, 6H), 7.06 (d, *J* = 8 Hz, 1H), 6.97 (d, *J* = 8 Hz, 1H), 2.61 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 197.7, 154.3, 145.7, 138.0, 132.9, 132.6, 132.4, 132.2, 130.9, 130.1, 129.1, 128.7, 128.6, 128.0, 127.6, 127.1, 119.3, 17.4. HRMS (EI-TOF) calcd for $C_{22}H_{16}O$ (M^+): 296.1201, found: 296.1204.

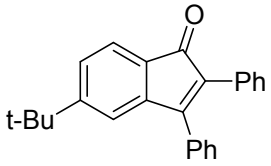
6-methyl-2,3-diphenyl-1H-inden-1-one(eluent: PE→PE/EA = 200/1)



3ea

Yield: 64%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.37-7.41 (m, 6H), 7.24-7.26 (m, 5H), 7.15 (d, *J* = 8 Hz, 1H), 7.02 (d, *J* = 8 Hz, 1H), 2.38 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 196.8, 155.6, 142.4, 139.3, 133.3, 132.9, 131.9, 131.1, 130.9, 130.0, 129.3, 128.8, 128.5, 128.1, 127.6, 124.1, 121.2, 21.4. HRMS (EI-TOF) calcd for $C_{22}H_{16}O$ (M^+): 296.1201, found: 296.1203.

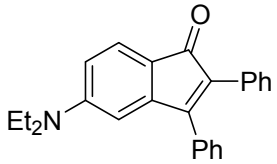
5-(tert-butyl)-2,3-diphenyl-1H-inden-1-one (eluent: PE→PE/EA = 200/1)



3fa

Yield: 68%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.52 (d, *J* = 8 Hz, 1H), 7.37-7.43 (m, 5H), 7.29 (d, *J* = 8 Hz, 1H), 7.24 (d, 5H), 7.17 (s, 1H), 1.31 (s, 9H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 198.2, 157.7, 155.2, 145.4, 133.0, 132.9, 131.0, 130.0, 129.2, 128.8, 129.2, 128.8, 128.6, 128.4, 128.1, 127.7, 125.3, 122.9, 119.0, 35.5, 31.1. HRMS (EI-TOF) calcd for $C_{25}H_{22}O$ (M^+): 338.1671, found: 338.1671.

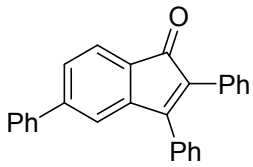
5-(diethylamino)-2,3-diphenyl-1H-inden-1-one (eluent: PE→PE/EA = 100/1)



3ga

Yield: 25%; Purple solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.48 (d, J = 8 Hz, 1H), 7.33-7.40 (m, 5H), 7.22-7.26 (m, 5H), 6.43 (d, J = 2.4 Hz, 1H), 6.34 (dd, J = 8 Hz, 1H), 3.40 (q, J = 8 Hz, 4H), 1.18 (t, J = 8 Hz, 6Hz). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 194.5, 152.1, 151.7, 148.6, 134.4, 133.3, 131.5, 130.1, 128.7, 128.7, 127.9, 127.4, 125.7, 117.1, 107.5, 106.3, 45.0, 12.6. HRMS (EI-TOF) calcd for $C_{25}H_{23}NO$ (M^+): 353.1780, found: 353.1781.

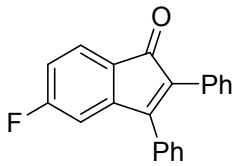
2,3,5-triphenyl-1H-inden-1-one(eluent: PE→PE/EA = 200/1)



3ha

Yield: 75%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.66 (d, J = 8 Hz, 1H), 7.56 (d, J = 8 Hz, 2H), 7.49 (dd, J = 8 Hz, 1H), 7.35-7.45 (m, 9H), 7.25-7.27 (m, 5H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 196.2, 154.9, 146.8, 146.1, 140.4, 133.2, 132.7, 130.8, 130.0, 129.5, 129.3, 128.9, 128.6, 128.3, 128.1, 127.8, 127.6, 127.2, 123.5, 120.5. HRMS (EI-TOF) calcd for $C_{27}H_{18}O$ (M^+): 358.1358, found: 358.1360.

5-fluoro-2,3-diphenyl-1H-inden-1-one(eluent: PE→PE/EA = 200/1)

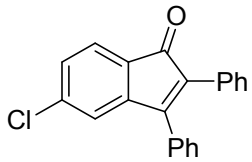


3ia

Yield: 50%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.57 (q, J = 8 Hz, 1H), 7.42-7.43 (m, 3H), 7.35-7.37 (m, 2H), 6.92 (t, J = 8 Hz, 1H), 6.86 (dd, J = 8 Hz). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 194.8, 167.7, 165.2 (d, $J_{C\text{-}F}$ = 252 Hz), 153.2 (d, $J_{C\text{-}F}$ = 2 Hz), 148.7, 148.6 (d, $J_{C\text{-}F}$ = 9 Hz), 133.7, 132.2, 130.4, 130.0, 129.5, 129.0, 128.4, 128.2, 128.1, 126.6, 126.5 (d, $J_{C\text{-}F}$ = 4 Hz), 124.9, 124.8 (d, $J_{C\text{-}F}$ = 9 Hz), 114.6, 114.3 (d, $J_{C\text{-}$

$_F$ = 22 Hz), 110.3, 110.1. HRMS (EI-TOF) calcd for $C_{21}H_{13}FO$ (M^+): 300.0950, found: 300.0955.

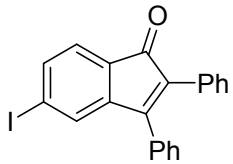
5-chloro-2,3-diphenyl-1H-inden-1-one (eluent: PE→PE/EA = 200/1)



3ja

Yield: 46%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.51 (d, *J* = 8 Hz, 1H), 7.42-7.44 (m, 3H), 7.35-7.37 (m, 2H), 7.62-7.28 (m, 6H), 7.12 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 195.1, 154.1, 147.3, 139.8, 133.5, 132.1, 130.3, 130.0, 129.6, 129.0, 128.9, 128.6, 128.4, 128.2, 128.1, 123.9, 122.0. HRMS (EI-TOF) calcd for $C_{21}H_{13}ClO$ (M^+): 316.0655, found: 316.0656.

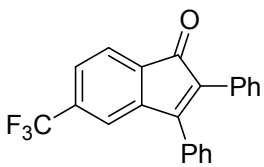
5-iodo-2,3-diphenyl-1H-inden-1-one(eluent: PE→PE/EA = 200/1)



3ka

Yield: 40%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.70 (dd, *J* = 8 Hz, 1H), 7.47-7.47 (m, 1H), 7.43-7.44 (m, 3H), 7.34-7.36 (m, 3H), 7.33 (d, *J* = 24 Hz, 1H), 7.26 (s, 5H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 195.6, 154.4, 146.9, 138.0, 133.1, 132.2, 130.2, 130.0, 129.6, 129.0, 128.4, 128.2, 128.1, 124.2, 100.9. HRMS (EI-TOF) calcd for $C_{21}H_{13}IO$ (M^+): 408.0011, found: 408.0014.

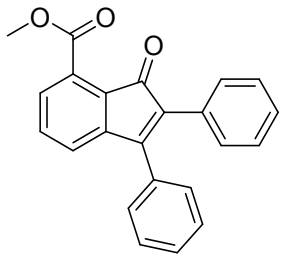
2,3-diphenyl-5-(trifluoromethyl)-1H-inden-1-one (eluent: PE→PE/EA = 200/1)



3la

Yield: 33%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.69 (d, J = 8 Hz, 1H), 7.61 (d, J = 8 Hz, 1H), 7.45-7.47 (m, 3H), 7.36-7.40 (m, 4H), 7.28 (s, 5H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 195.1, 154.7, 146.1, 135.2, 135.0, 133.6, 133.4, 132.0, 131.6, 130.1, 130.0, 129.1, 228.4, 128.2, 126.5 (q, J_{CF3-C} =5 Hz), 122.8, 117.7 (q, J_{C-F} = 4 Hz). HRMS (EI-TOF) calcd for $C_{22}H_{13}F_3O$ (M^+): 350.0918, found: 350.0922.

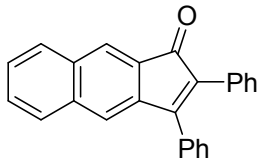
methyl 1-oxo-2,3-diphenyl-1H-indene-7-carboxylate (eluent: PE→PE/EA = 100/1)



3ma

Yield: 21%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.36-7.44 (m, 7H), 7.25-7.27 (m, 6H), 3.99 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 193.9, 167.5, 154.3, 145.9, 133.3, 132.7, 132.3, 130.3, 130.0, 129.5, 128.9, 128.4, 128.1, 128.0, 128.0, 123.2, 52.8. HRMS (EI-TOF) calcd for $C_{23}H_{16}O_3$ (M^+): 340.1099, found: 340.1103.

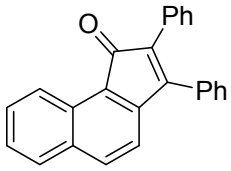
2,3-diphenyl-1H-cyclopenta[b]naphthalen-1-one(eluent: PE→PE/EA = 100/1)



3na

Yield: 48%; Yellow solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.04 (s, 1H), 7.87 (d, J = 8 Hz, 1H), 7.71 (d, J = 8 Hz, 1H), 7.45-7.51 (m, 7H), 7.41 (s, 1H), 7.25-7.32 (m, 5H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 194.8, 156.5, 140.0, 136.6, 136.2, 133.7, 132.9, 130.9, 130.7, 130.3, 130.0, 129.4, 129.2, 128.9, 128.8, 128.7, 128.1, 127.9, 127.2, 124.4, 121.0. HRMS (EI-TOF) calcd for $C_{25}H_{16}O$ (M^+): 332.1201, found: 332.1202.

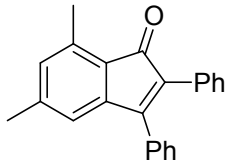
2,3-diphenyl-1H-cyclopenta[a]naphthalen-1-one(eluent: PE→PE/EA = 100/1)



3oa

Yield: 56%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.81 (d, *J* = 8 Hz, 1H), 7.87 (d, *J* = 8 Hz, 1H), 7.74 (d, *J* = 8 Hz, 1H), 7.54 (t, *J* = 8 Hz, 1H), 7.43 (s, 5H), 7.37 (t, *J* = 8 Hz, 1H), 7.25-7.33 (m, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 198.6, 153.8, 146.7, 134.7, 134.2, 132.8, 131.2, 130.8, 130.1, 129.4, 129.4, 129.2, 128.9, 128.6, 128.5, 128.1, 127.7, 126.0, 123.9, 122.3, 119.3. HRMS (EI-TOF) calcd for $C_{25}H_{16}O$ (M^+): 332.1201, found: 332.1201.

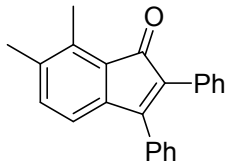
5,7-dimethyl-2,3-diphenyl-1H-inden-1-one(eluent: PE→PE/EA = 200/1)



3pa

Yield: 60%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.33-7.41 (m, 5H), 7.24 (s, 5H), 6.85 (s, 1H), 6.76 (s, 1H), 2.57 (s, 3H), 2.30 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 197.3, 153.9, 146.2, 143.4, 138.0, 133.1, 132.8, 132.1, 131.1, 130.1, 128.9, 128.7, 128.6, 128.0, 127.5, 124.8, 120.6, 21.9, 17.3. HRMS (EI-TOF) calcd for $C_{23}H_{18}O$ (M^+): 310.1358, found: 310.1358.

6,7-dimethyl-2,3-diphenyl-1H-inden-1-one(eluent: PE→PE/EA = 200/1)

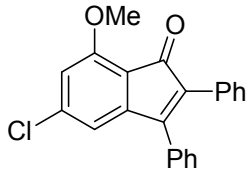


3qa

Yield: 62%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.34-7.40 (m, 5H), 7.24 (s, 5H), 7.09 (d, *J* = 8 Hz, 1H), 6.86 (d, *J* = 8 Hz, 1H), 2.58 (s, 3H), 2.29 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 198.0, 154.4, 143.4, 139.7, 137.7, 133.1, 132.0, 131.2, 130.0, 129.0, 128.7, 128.6, 128.0, 127.4, 127.3, 119.0, 19.4, 13.0. HRMS (EI-TOF) calcd for

$C_{23}H_{18}O$ (M^+): 310.1358, found: 310.1360.

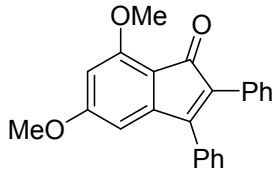
5-chloro-7-methoxy-2,3-diphenyl-1H-inden-1-one(eluent: PE→PE/EA = 100/1)



3ra

Yield: 54%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.40-7.42 (m, 3H), 7.31-7.33 (m, 2H), 7.24 (s, 5H), 6.89 (d, *J* = 0.8 Hz, 1H), 6.73 (d, *J* = 0.8 Hz, 1H), 3.99 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 192.8, 156.5, 151.4, 148.8, 140.8, 133.0, 131.8, 129.9, 129.7, 128.7, 128.4, 128.1, 127.5, 127.4, 115.1, 113.7, 113.3, 56.0. HRMS (EI-TOF) calcd for $C_{22}H_{15}ClO_2$ (M^+): 346.0761, found: 346.0765.

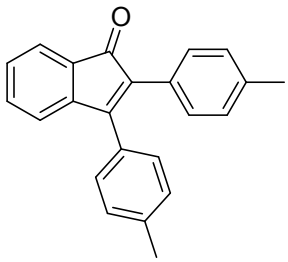
5,7-dimethoxy-2,3-diphenyl-1H-inden-1-one(eluent: PE→PE/EA = 100/1)



3sa

Yield: 65%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.38-7.39 (m, 3H), 7.31-7.33 (m, 2H), 7.21-7.26 (m, 5H), 6.34 (d, *J* = 4 Hz, 1H), 6.23 (d, *J* = 4 Hz, 1H), 4.00 (s, 3H), 3.83 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 192.9, 166.3, 158.7, 151.0, 149.8, 134.0, 133.0, 131.0, 130.2, 128.8, 128.7, 127.9, 127.6, 108.9, 103.8, 97.1, 56.2, 55.8. HRMS (EI-TOF) calcd for $C_{23}H_{18}O_3$ (M^+): 342.1256, found: 342.1258.

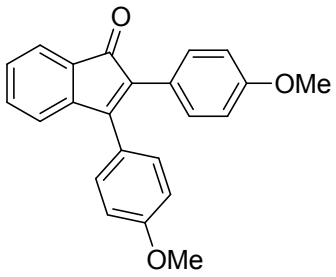
2,3-di-p-tolyl-1H-inden-1-one (eluent: PE→PE/EA = 200/1)



3ab

Yield: 72%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.56 (d, *J* = 8 Hz, 1H), 7.36 (t, *J* = 8 Hz, 1H), 7.14-7.30 (m, 8H), 7.08 (d, *J* = 8 Hz, 2H), 2.40 (s, 3H), 2.32 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 196.8, 154.8, 145.4, 139.4, 137.6, 133.3, 132.1, 130.9, 129.9, 129.5, 128.9, 128.7, 128.5, 128.0, 122.8, 121.2, 21.6, 21.4. HRMS (EI-TOF) calcd for $C_{23}H_{18}O$ (M^+): 310.1358, found: 310.1359.

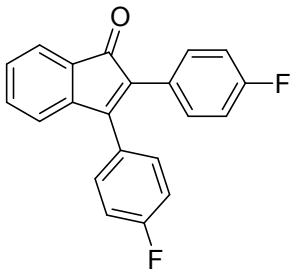
2,3-bis(4-methoxyphenyl)-1H-inden-1-one(eluent: PE→PE/EA = 100/1)



3ac

Yield: 44%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.55 (d, *J* = 8 Hz, 1H), 7.34-7.37 (m, 3H), 7.23-7.26 (m, 3H), 7.17 (d, *J* = 8 Hz, 1H), 6.94 (d, *J* = 8 Hz, 2H), 6.82 (d, *J* = 8 Hz, 2H), 3.86 (s, 3H), 3.80 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 197.0, 160.3, 159.1, 153.8, 145.5, 133.3, 131.3, 131.0, 130.2, 128.6, 125.1, 123.4, 122.7, 121.0, 114.2, 113.7, 55.3, 55.2. HRMS (EI-TOF) calcd for $C_{23}H_{18}O_3$ (M^+): 342.1256, found: 342.1258.

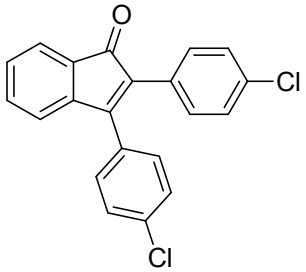
2,3-bis(4-fluorophenyl)-1H-inden-1-one (eluent: PE→PE/EA = 200/1)



3ad

Yield: 56%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.58 (d, J = 8 Hz, 1H), 7.35-7.41 (m, 3H), 7.30 (t, J = 8 Hz, 1H), 7.21-7.26 (m, 2H), 7.13 (t, J = 8 Hz, 3H), 6.97 (t, J = 8 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 196.2, 163.2 (d, J_{C-F} = 249 Hz), 162.5 (d, J_{C-F} = 267 Hz), 154.2, 144.9, 133.6, 131.7 (d, J_{C-F} = 8 Hz), 131.5, 130.5 (d, J_{C-F} = 8 Hz), 130.5, 129.2, 128.5 (d, J_{C-F} = 3 Hz), 126.5 (d, J_{C-F} = 4 Hz), 123.2, 121.1, 116.2 (d, J_{C-F} = 21 Hz), 115.4 (d, J_{C-F} = 21 Hz). HRMS (EI-TOF) calcd for $C_{21}H_{12}F_2O$ (M^+): 318.0856, found: 318.0851.

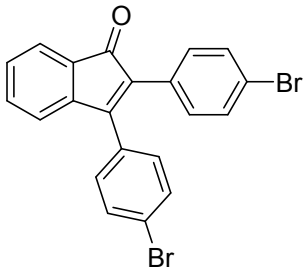
2,3-bis(4-chlorophenyl)-1H-inden-1-one(eluent: PE→PE/EA = 200/1)



3ae

Yield: 58%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.59 (d, J = 8 Hz, 1H), 7.38-7.43 (m, 3H), 7.30-7.33 (m, 3H), 7.25-7.27 (m, 2H), 7.18-7.20 (m, 2H), 7.11 (d, J = 8 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 195.9, 154.3, 144.7, 135.5, 134.0, 133.7, 131.5, 131.2, 130.7, 130.4, 129.9, 129.4, 128.8, 128.5, 123.3, 121.1. HRMS (EI-TOF) calcd for $C_{21}H_{12}Cl_2O$ (M^+): 350.0265, found: 350.0269.

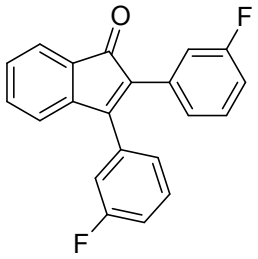
2,3-bis(4-bromophenyl)-1H-inden-1-one(eluent: PE→PE/EA = 200/1)



3af

Yield: 63%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.56-7.58 (m, 3H), 7.37-7.42 (m, 3H), 7.31 (t, *J* = 8 Hz, 1H), 7.25 (d, *J* = 8 Hz, 2H), 7.10-7.13 (m, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 195.7, 154.4, 144.6, 133.7, 132.3, 131.5, 131.5, 131.3, 130.5, 130.1, 129.4, 129.3, 123.8, 123.3, 122.4, 121.2. HRMS (EI-TOF) calcd for $C_{21}H_{12}Br_2O$ (M^+): 437.9255, found: 437.9255.

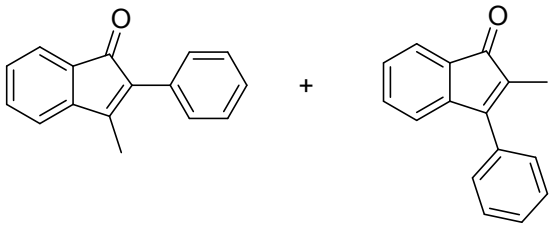
2,3-bis(3-fluorophenyl)-1H-inden-1-one (eluent: PE→PE/EA = 200/1)



3ag

Yield: 54%; Red solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.53 (d, *J* = 8 Hz, 1H), 7.33 (t, *J* = 8 Hz, 2H), 7.25 (t, *J* = 8 Hz, 2H), 7.12-7.18 (m, 1H), 7.03-7.08 (m, 4H), 6.89-6.95 (m, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 195.7, 162.9 (d, $J_{C\text{-}F}$ = 246 Hz), 162.5 (d, $J_{C\text{-}F}$ = 244 Hz), 154.7, 144.6, 134.5 (d, $J_{C\text{-}F}$ = 8 Hz), 133.8, 132.4 (d, $J_{C\text{-}F}$ = 8 Hz), 131.7 (d, $J_{C\text{-}F}$ = 3 Hz), 130.8 (d, $J_{C\text{-}F}$ = 8 Hz), 130.4, 129.7 (d, $J_{C\text{-}F}$ = 8 Hz), 129.5, 125.7 (d, $J_{C\text{-}F}$ = 3 Hz), 124.3 (d, $J_{C\text{-}F}$ = 3 Hz), 123.4, 121.4, 116.8 (d, $J_{C\text{-}F}$ = 17 Hz), 116.6 (d, $J_{C\text{-}F}$ = 17 Hz), 115.3 (d, $J_{C\text{-}F}$ = 33 Hz), 115.2 (d, $J_{C\text{-}F}$ = 33 Hz). HRMS (EI-TOF) calcd for $C_{21}H_{12}F_2O$ (M^+): 318.0856, found: 318.0860.

The mixture of **3ah** and **3ah'** (eluent: PE→PE/EA = 200/1)

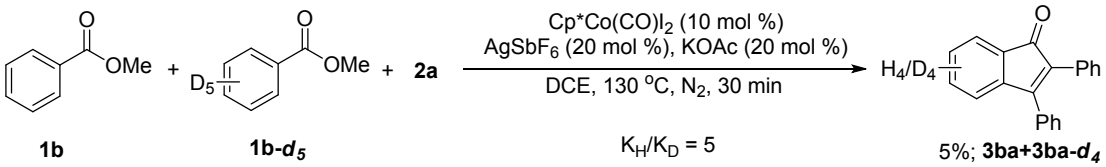


3ah **3ah'**

Yield: 44%; Red oil liquid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.156-7.50 (m, 14 H), 7.06 (d, *J* = 8 Hz, 0.56 H), 2.32 (s, 3H), 1.93 (s, 1.66 H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 198.4, 196.5, 154.7, 154.7, 145.9, 145.7, 133.6, 133.4, 133.2, 132.8, 131.2, 131.2, 131.1, 130.4, 129.6, 129.2, 128.9, 128.7, 128.3, 128.1, 128.1, 127.7, 122.5, 122.2, 120.4, 119.5, 12.6, 8.7. HRMS (EI-TOF) calcd for $C_{16}H_{12}O$ (M^+): 220.0888, found: 220.0888.

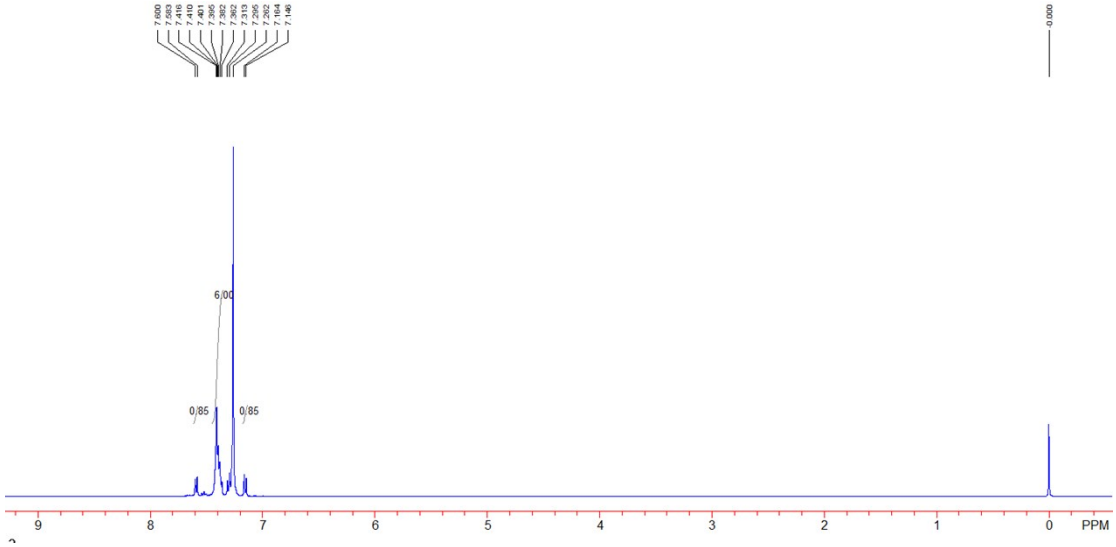
Mechanism experiments

1.

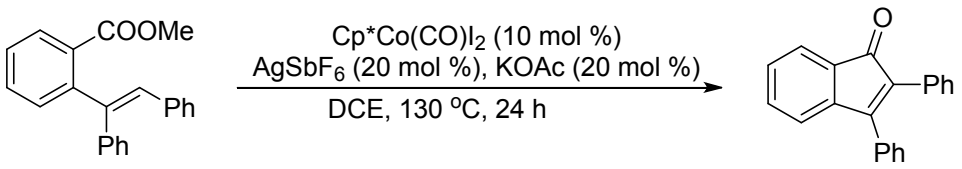


1b **1b-*d*$_5$** K_H/K_D = 5 5%; **3ba+3ba-*d*$_4$**

7 mg (0.05 mmol) of the methyl benzoate, 7 mg (0.05 mmol) of the deuterated methyl benzoate and 27 mg (0.15 mmol) diphenylacetylene were dissolved in 1mL DCE in a sealed tube. 5 mg (10 mol%) Cp*Co(CO)I_2, 7 mg (20 mol%) $AgSbF_6$ and 2 mg (20 mol%) KOAc were added. The tube was stirred at 130 °C for 30 min under N_2. The solvent was removed in vacuum and the product was separated by a preparative TLC to furnish 1.5 mg (5%) of the product mixture as red solid. The KIE value (K_H/K_D = 5) was determined from the ^{1}H-NMR.

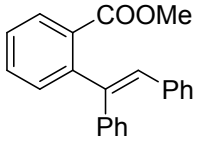


2.

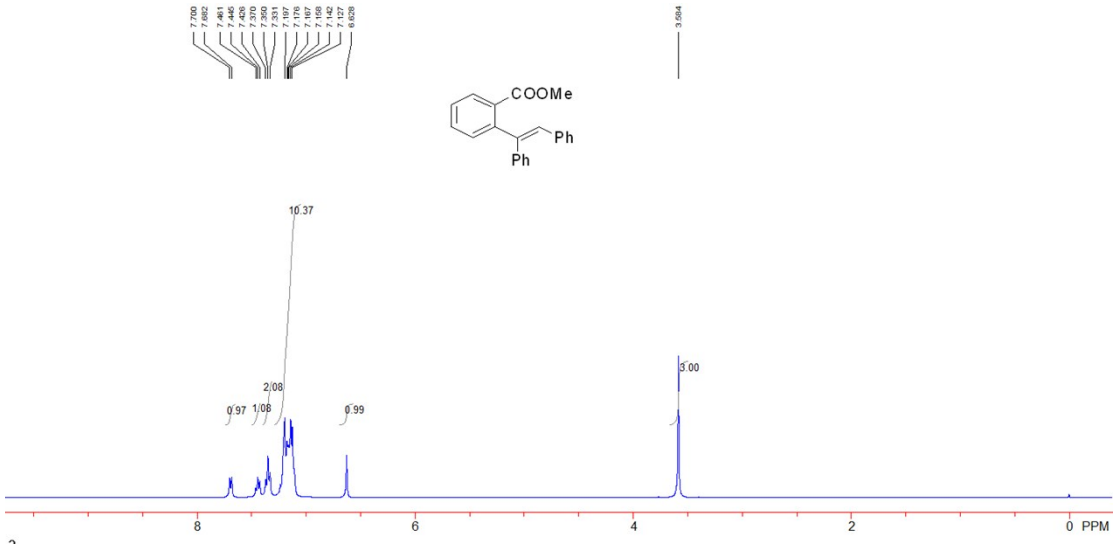


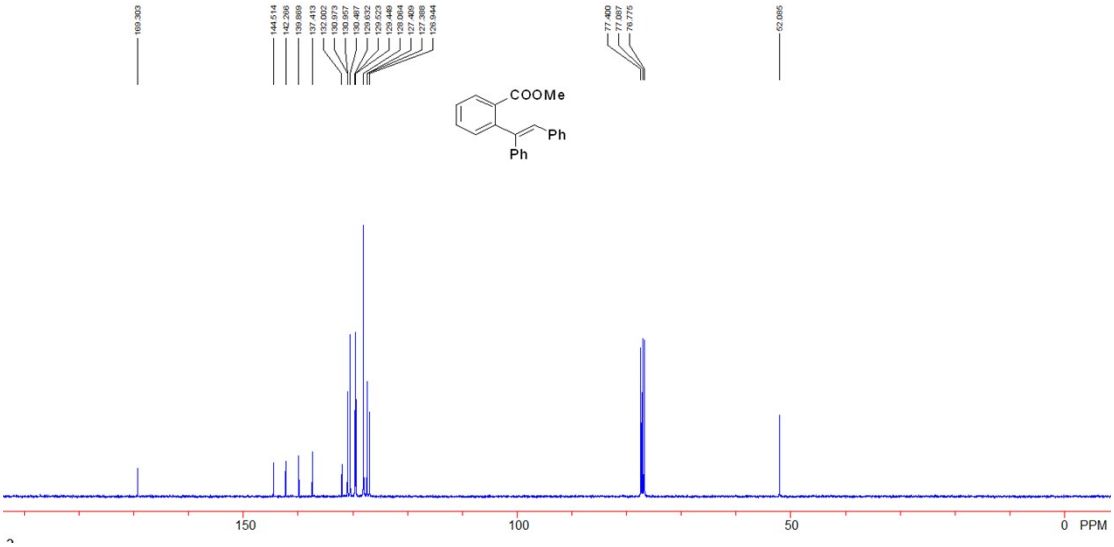
31 mg (0.1 mmol) of the **4a** were dissolved in 1mL DCE in a sealed tube. 5 mg (10 mol%) Cp*Co(CO)I_2, 7 mg (20 mol%) $AgSbF_6$ and 2 mg (20 mol%) KOAc were added. The tube was stirred at 130 °C for 24 h under N_2. The desired product was not observed.

(E)-methyl-2-(1,2-diphenylvinyl)benzoate[3]

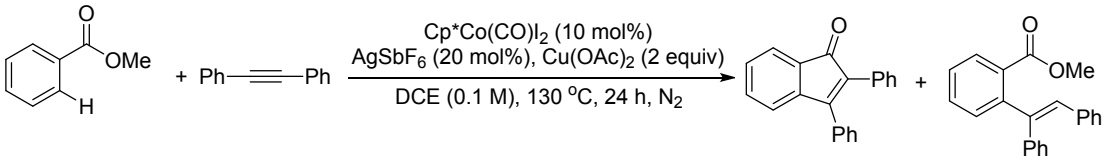


White solid; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.69 (d, J = 8 Hz, 1H), 7.44 (t, J = 8 Hz, 1H), 7.35 (t, J = 8 Hz, 2H), 7.13-7.20 (m, 10 H), 3.58 (s, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.3, 144.5, 142.3, 139.9, 137.4, 132.0, 132.0, 132.0, 130.5, 129.6, 129.5, 129.4, 128.1, 127.4, 127.4, 126.9, 52.1. HRMS (EI-TOF) calcd for $C_{22}H_{18}O_2$ (M^+): 314.1307, found: 314.1309.

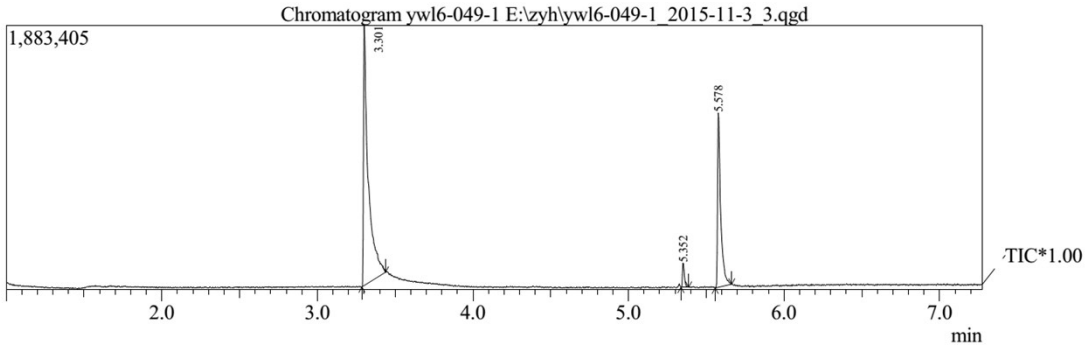




GC-MS

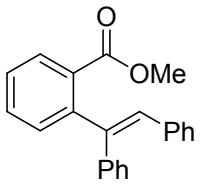


1b **2a** **3ba** **4, by GC-Ms**

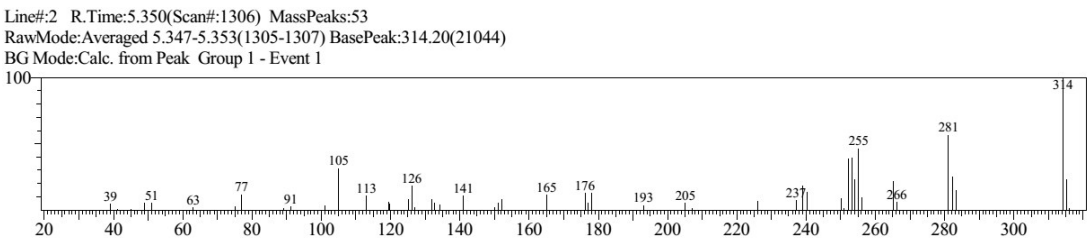


Peak Report TIC

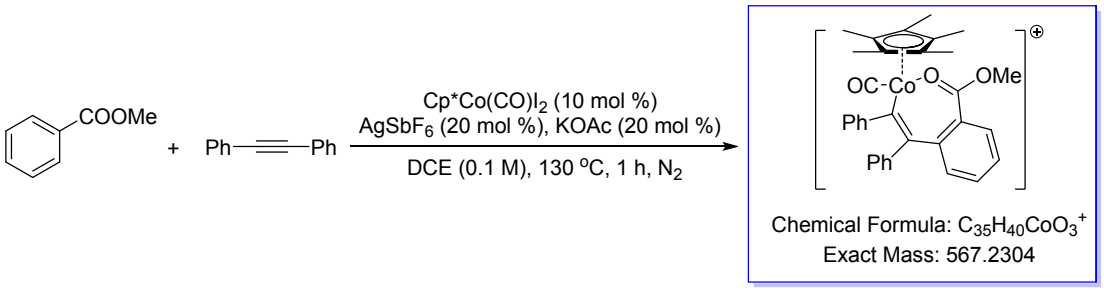
Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Nar
1	3.301	3.287	3.437	3991762	68.14	1851494	56.73	2.16		Phe
2	5.352	5.337	5.387	144868	2.47	170914	5.24	0.85		Eth
3	5.578	5.557	5.663	1721860	29.39	1241418	38.04	1.39		9-C
				5858490	100.00	3263826	100.00			

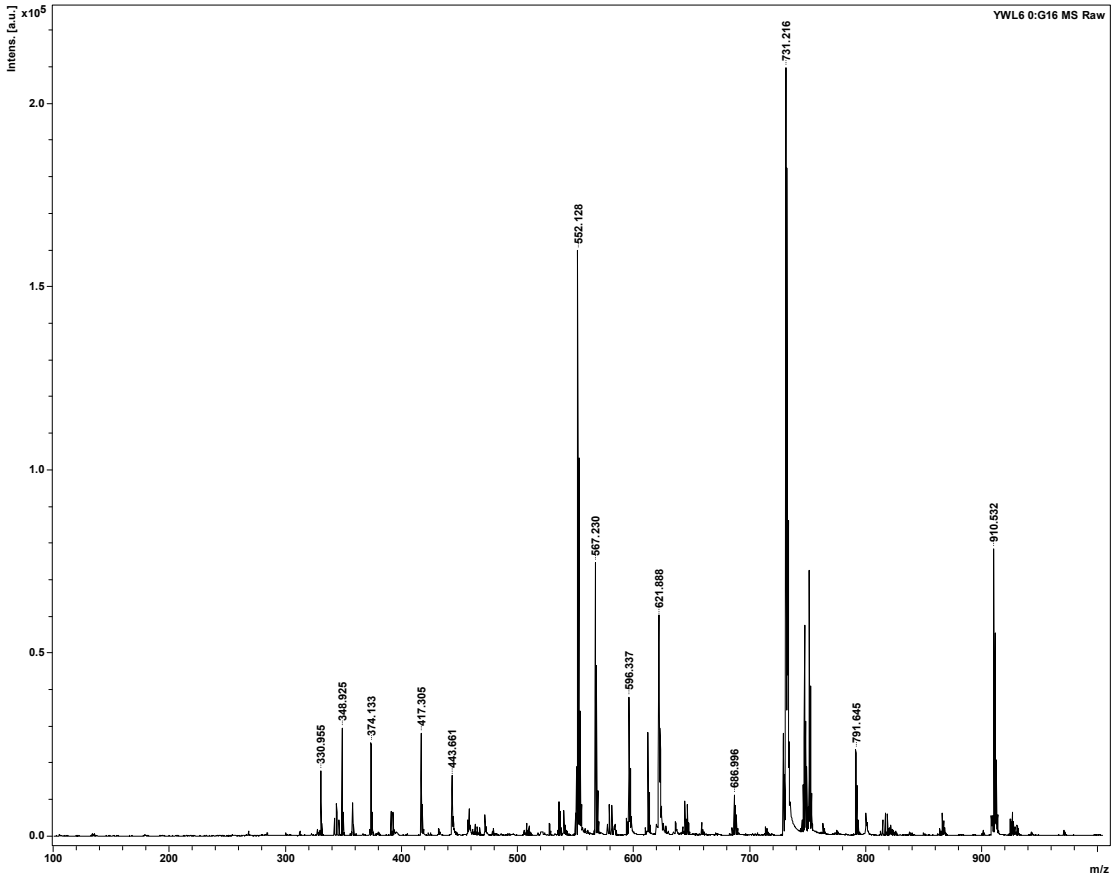


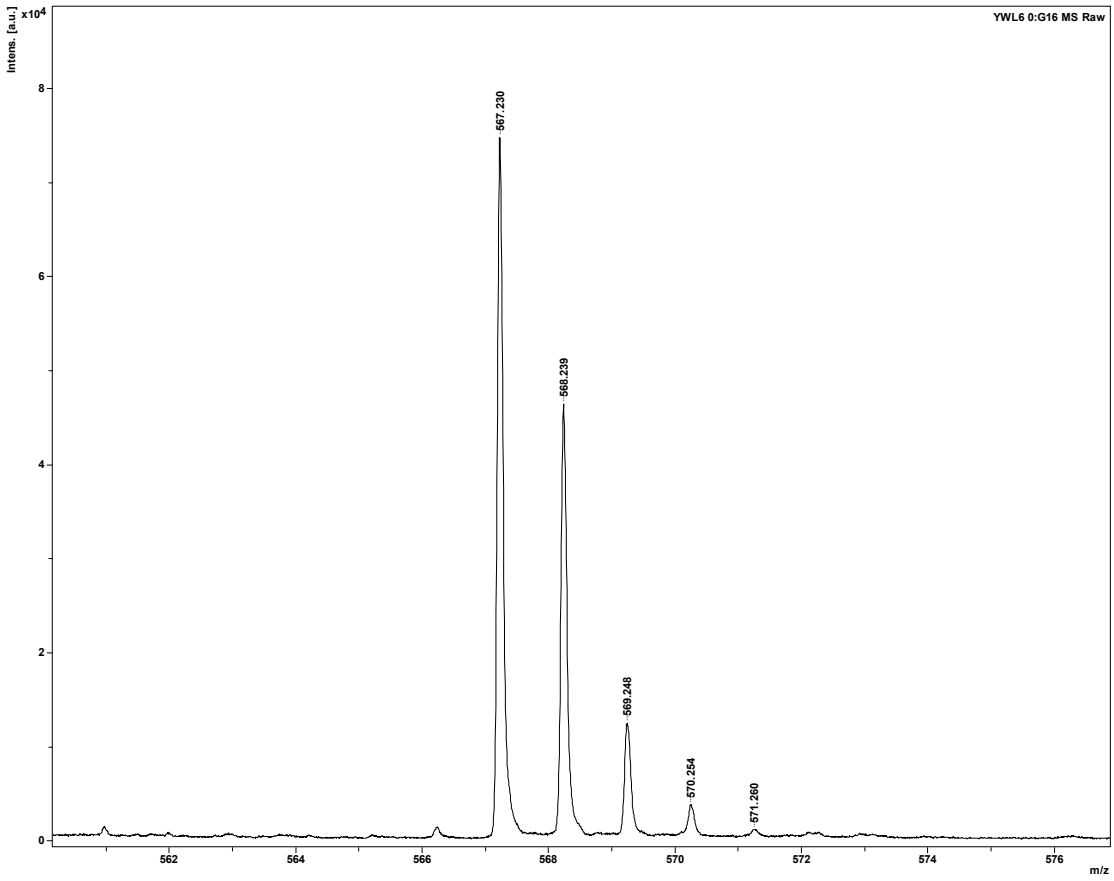
Chemical Formula: $C_{22}H_{18}O_2$
Exact Mass: 314.1307


Line#:2 R.Time:5.350(Scan#:1306) MassPeaks:53
RawMode:Averaged 5.347-5.353(1305-1307) BasePeak:314.20(21044)
BG Mode:Calc. from Peak Group 1 - Event 1
100
314
281
255
105
126
39
51
63
77
91
113
141
165
176
193
205
237
266
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300

MALDI-TOF


COOMe
+
Ph
Ph
Cp*Co(CO)I2 (10 mol %)
AgSbF6 (20 mol %), KOAc (20 mol %)
DCE (0.1 M), 130 °C, 1 h, N2
OC-Co
O
OMe
Ph
Ph
Chemical Formula: C35H40CoO3+
Exact Mass: 567.2304


YWL6 0:G16 MS Raw
Intens. [a.u.]
x10^5
2.0
1.5
1.0
0.5
0.0
731.216
552.128
567.230
621.888
596.337
910.532
348.925
374.133
417.305
330.955
443.661
686.996
791.645
100
200
300
400
500
600
700
800
900
m/z

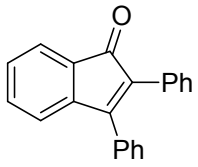


References

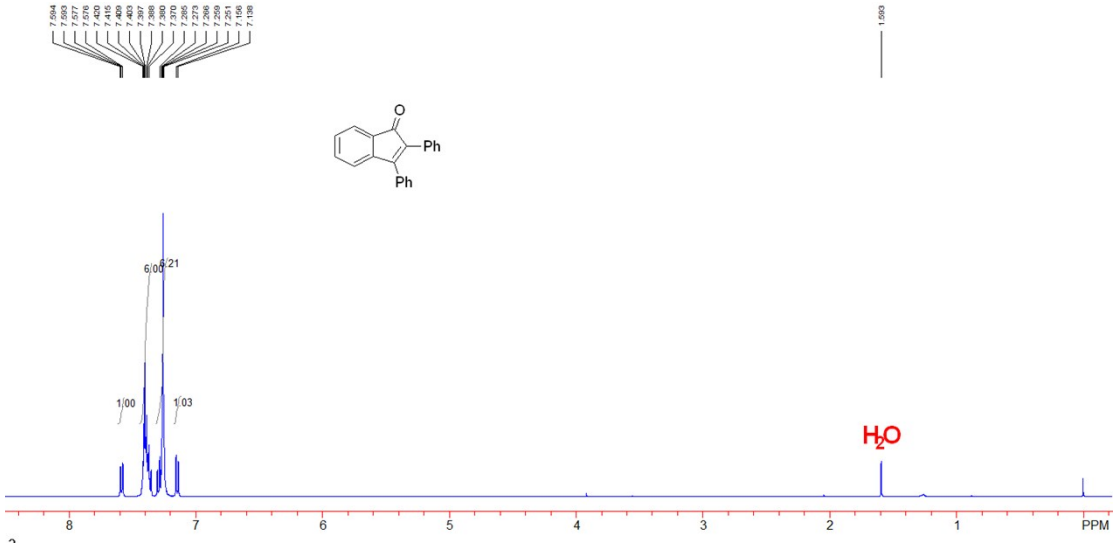
1 B. Sun, T. Yoshino, S. Matsunaga and M. Kanai, *Adv. Synth. Catal*., 2014, **356**, 1491.

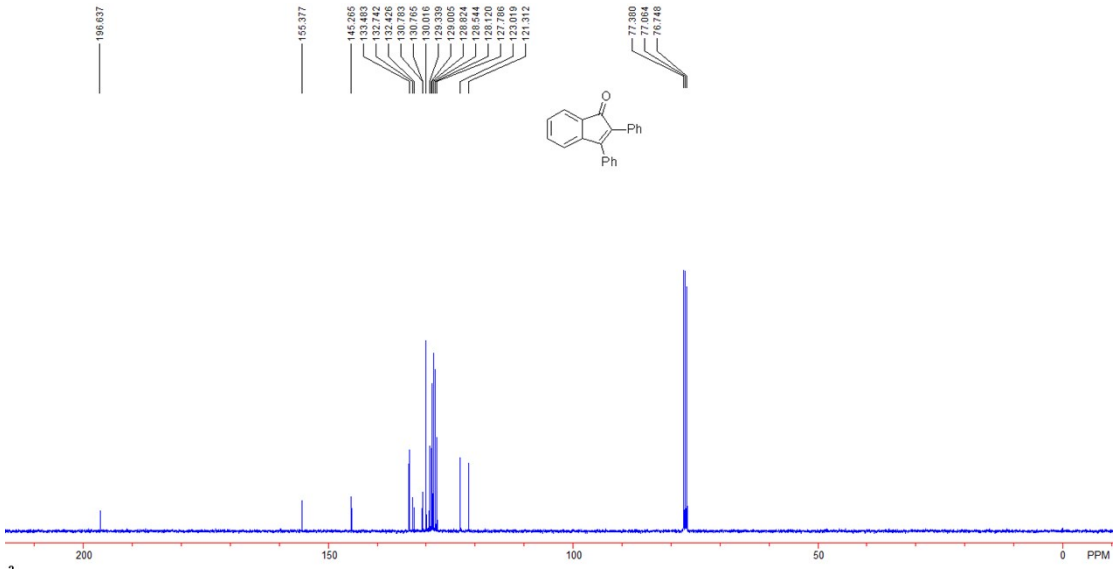
2 K. Graczyk, W. Ma and L. Ackermann, *Org. Lett*., 2012, **14**, 4110.

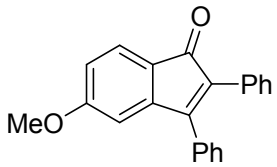
3 N. Guimond, C. Gouliaras and K. Fagnou, *J. Am. Chem. Soc*., 2010, **132**, 6908.


O
Ph
Ph

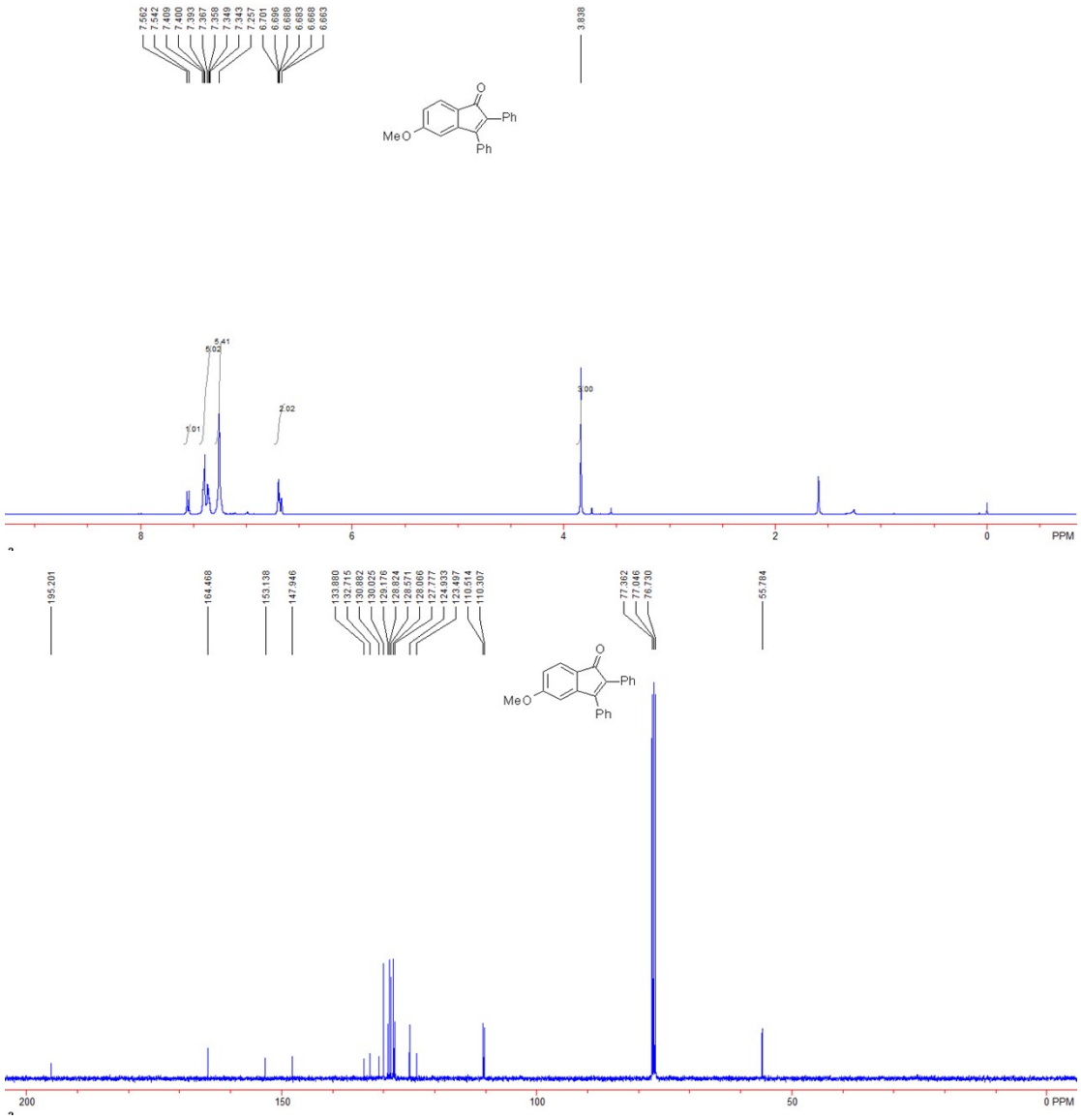
3ba

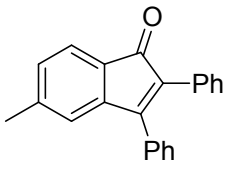

7.594
7.593
7.577
7.576
7.495
7.415
7.409
7.403
7.397
7.388
7.380
7.370
7.285
7.273
7.266
7.259
7.251
7.196
7.188
1.593
O
Ph
Ph
6.00
6.21
1.00
1.03
H2O
8
7
6
5
4
3
2
1
PPM


196.637
155.377
145.265
133.463
132.742
132.426
130.783
130.765
130.016
129.339
129.005
128.824
128.144
128.070
127.766
123.019
121.312
77.380
77.064
76.748
O
Ph
Ph
200
150
100
50
0
PPM

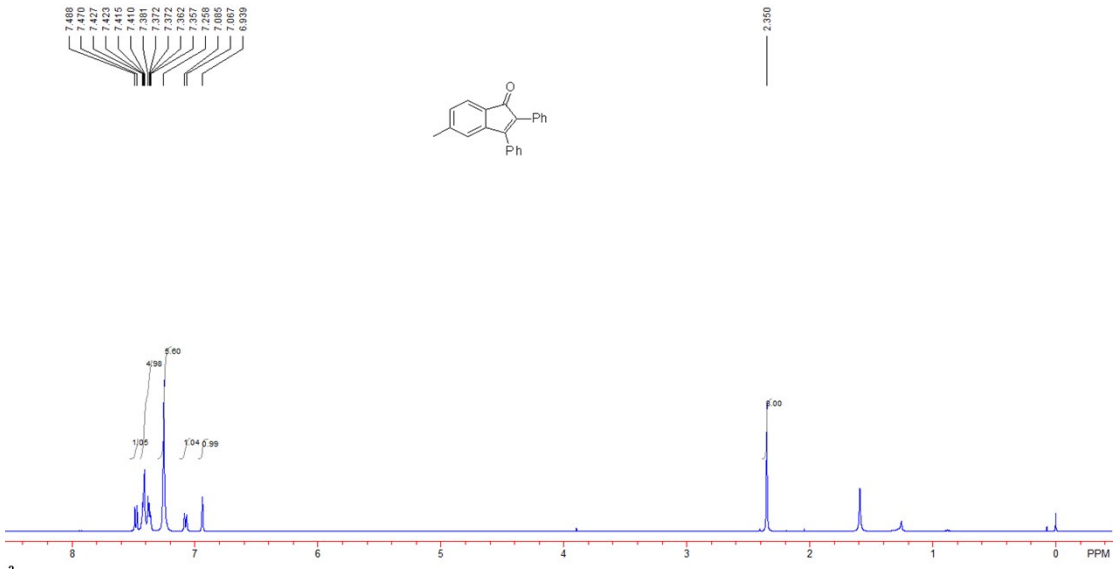

O
Ph
MeO
Ph

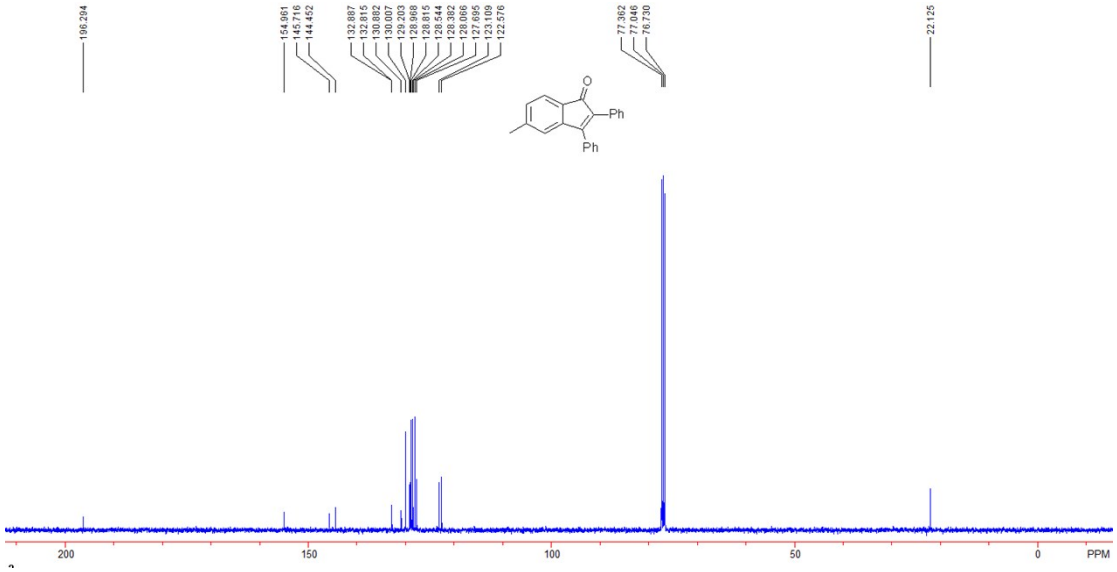
3aa

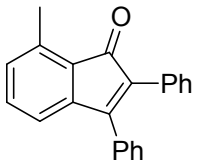

7.562
7.542
7.409
7.400
7.393
7.367
7.358
7.349
7.343
7.257
6.701
6.696
6.688
6.683
6.668
6.663
3.838
MeO
Ph
Ph
O
5.41
5.02
1.01
2.02
3.00
8
6
4
2
0
PPM
195.201
164.468
153.138
147.946
133.880
132.715
130.882
130.025
129.176
128.824
128.571
128.066
127.777
124.933
123.497
110.514
110.307
77.362
77.046
76.730
55.784
200
150
100
50
0 PPM


O
Ph
Ph

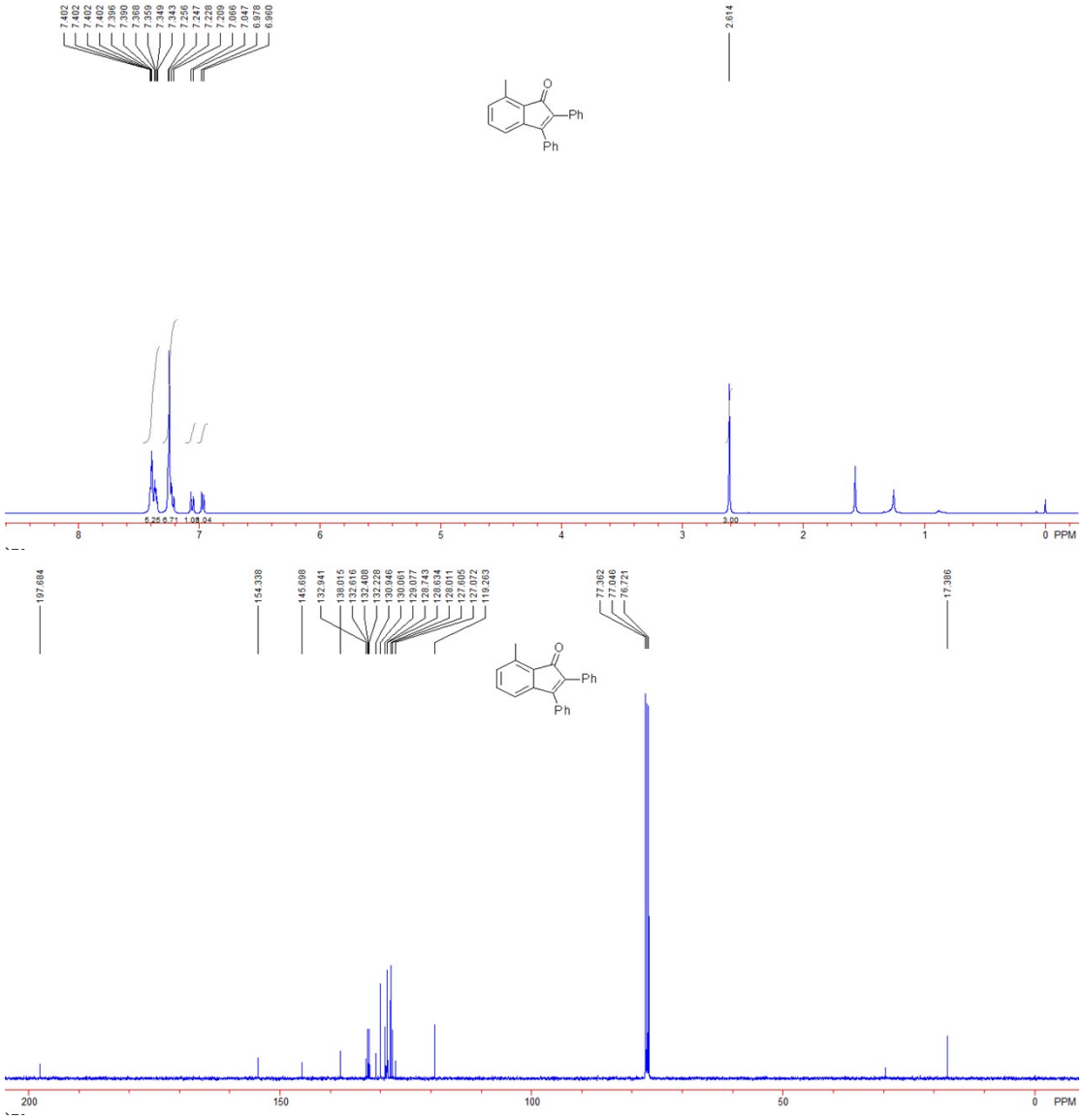
3ca

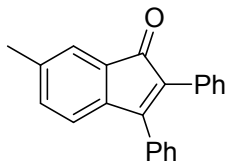

7.488
7.470
7.427
7.423
7.415
7.410
7.381
7.372
7.372
7.362
7.357
7.258
7.085
7.067
6.939
2.350
O
Ph
Ph
5.60
4.98
1.05
1.04
0.99
5.00
8
7
6
5
4
3
2
1
0
PPM


196.294
154.961
145.716
144.452
132.887
132.815
130.852
130.007
129.203
128.968
128.815
128.544
128.382
128.066
127.695
127.169
122.576
77.362
77.046
76.730
22.125
O
Ph
Ph
200
150
100
50
0
PPM

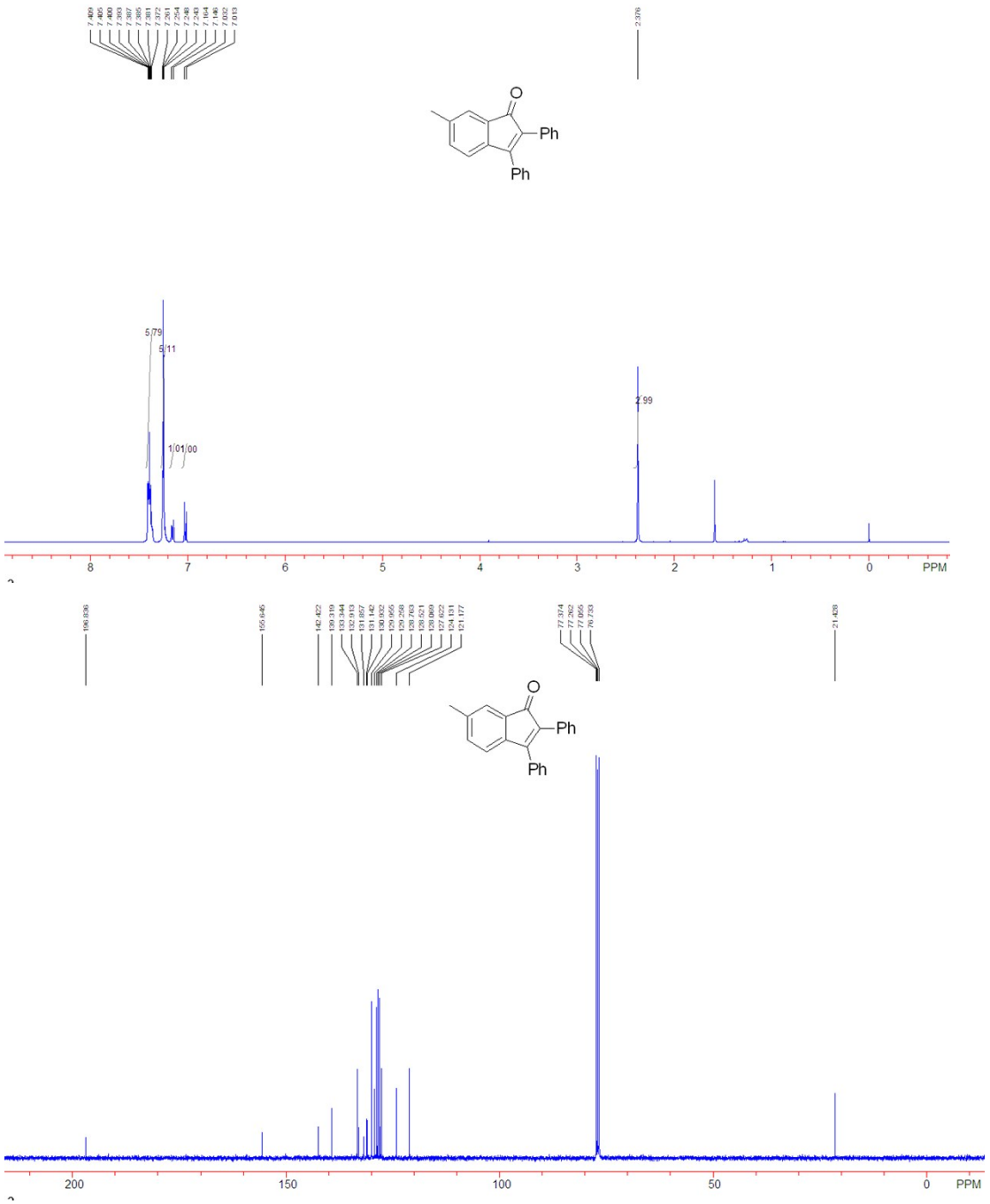

O
Ph
Ph

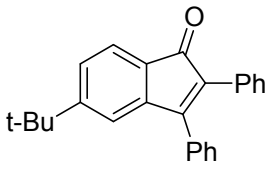
3da


7.402
7.402
7.402
7.402
7.396
7.390
7.368
7.359
7.349
7.343
7.256
7.247
7.228
7.209
7.066
7.047
6.978
6.960
2.614
O
Ph
Ph
5.25
6.71
1.08
4.04
3.00
8
7
6
5
4
3
2
1
0 PPM
197.684
154.338
145.698
132.941
130.015
129.616
129.466
128.228
130.946
130.061
129.077
128.743
128.634
128.011
127.605
127.072
119.263
77.362
77.046
76.721
17.386
O
Ph
Ph
200
150
100
50
0 PPM

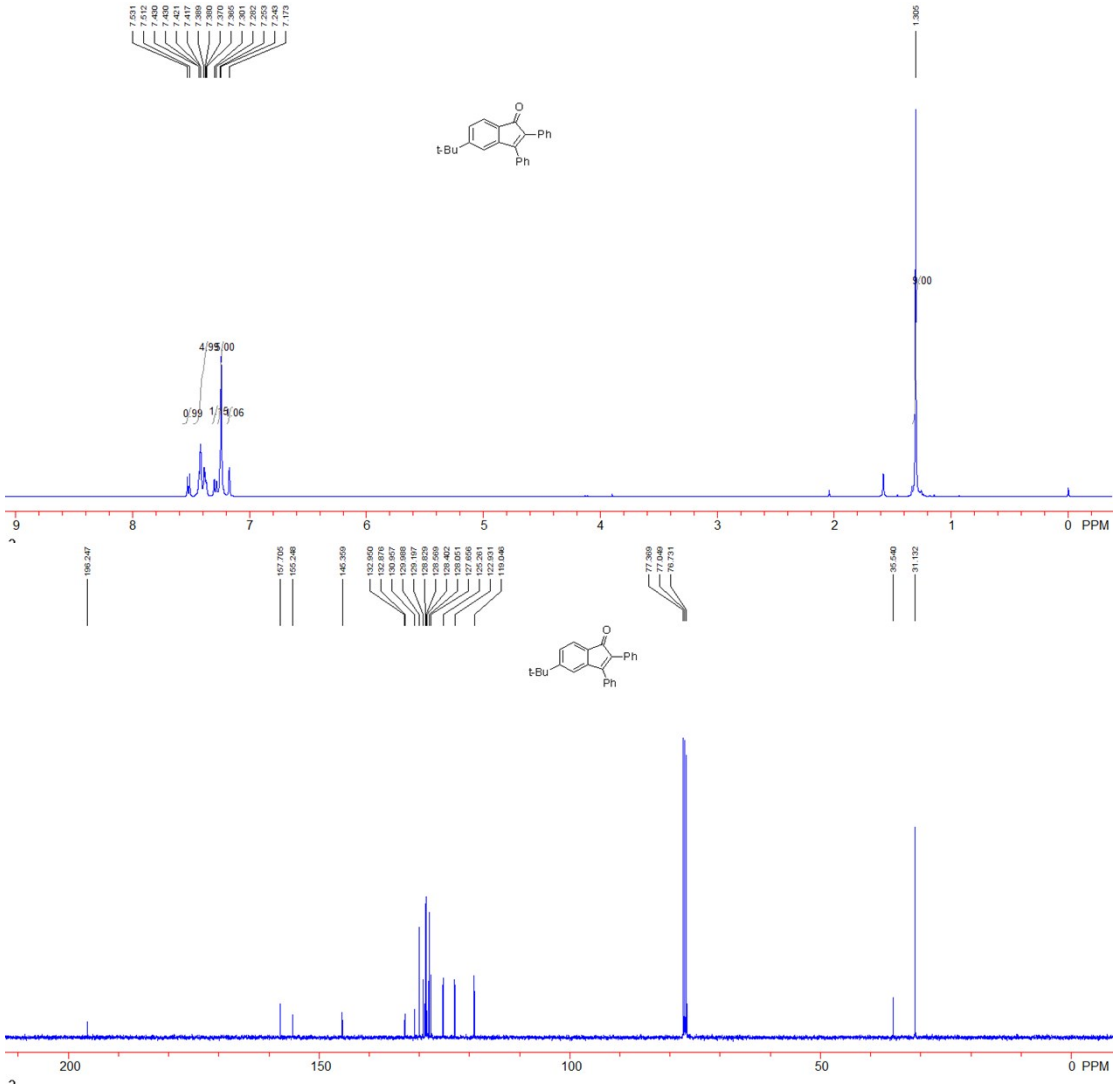

O
Ph
Ph

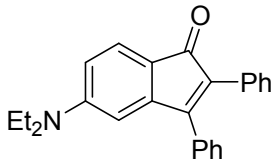
3ea


5.79
5.11
1.01
1.00
2.99
PPM
O
Ph
Ph
77.374
77.262
77.055
76.733
21.458
200
150
100
50
0
PPM

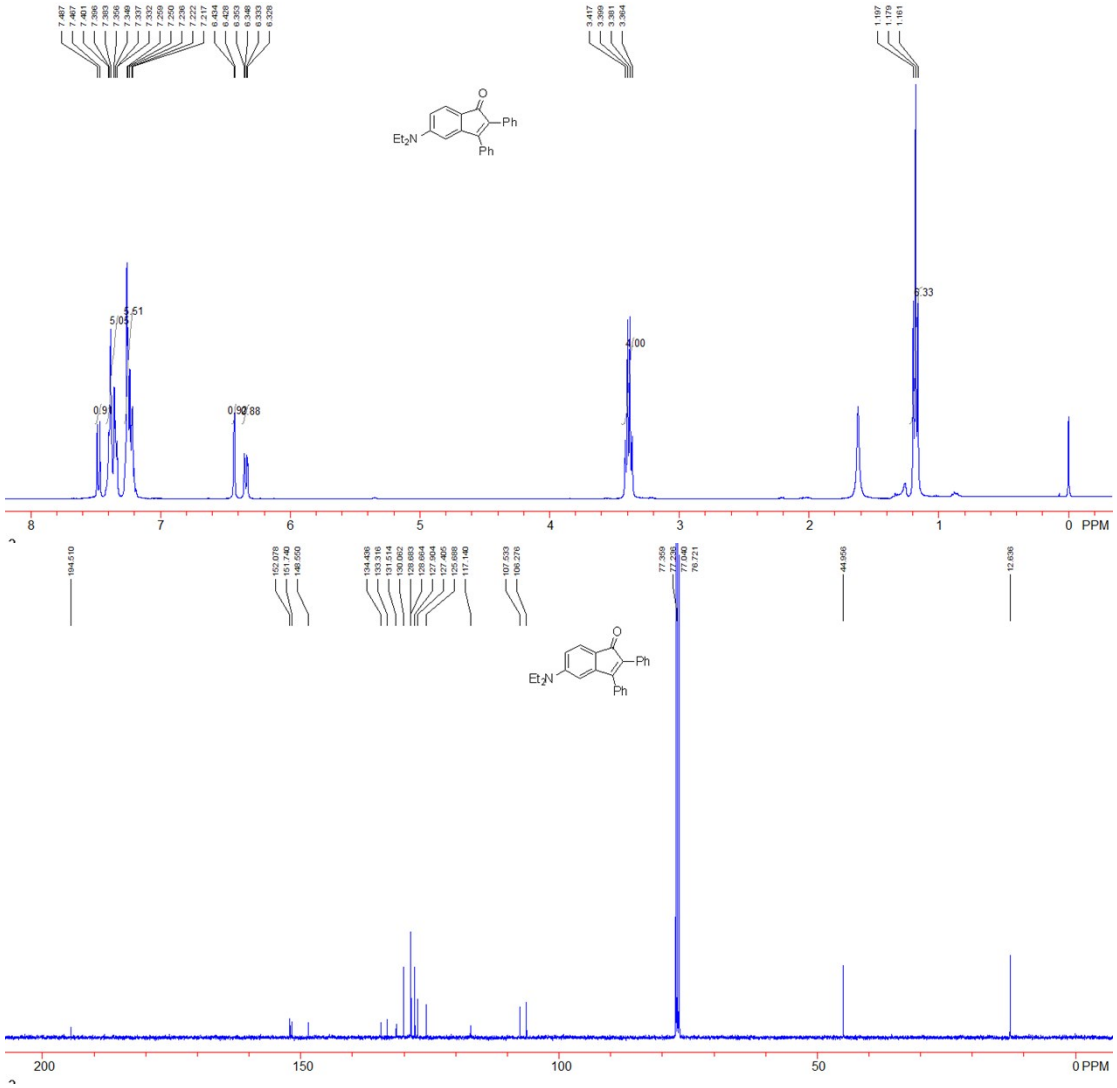

O
Ph
t-Bu
Ph

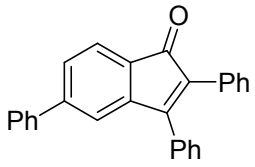
3fa


7.531
7.512
7.490
7.466
7.421
7.417
7.389
7.369
7.370
7.365
7.361
7.292
7.253
7.243
7.173
1.305
9.00
4.95
5.00
0.99
1.19
3.06
t-Bu
Ph
Ph
O
9
8
7
6
5
4
3
2
1
0 PPM
199.247
157.705
155.248
140.359
132.950
132.876
130.957
130.668
129.197
128.829
128.569
128.451
128.051
127.656
125.261
123.931
110.046
77.369
77.049
76.731
35.640
31.132
200
150
100
50
0 PPM

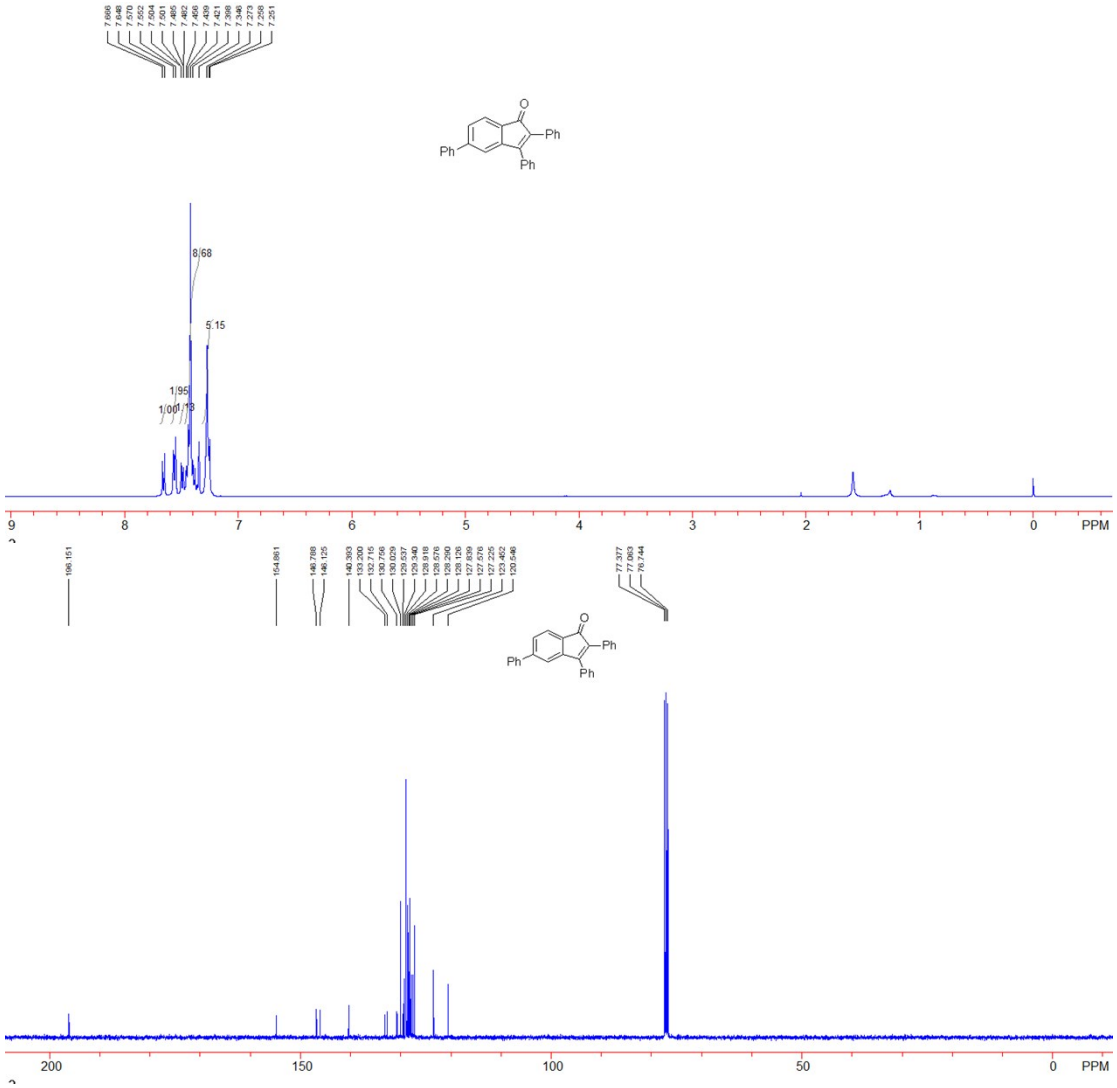

O
Ph
Et2N
Ph

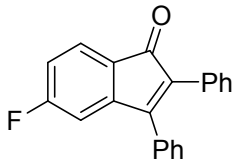
3ga



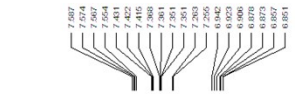


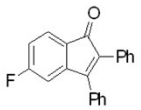
3ha

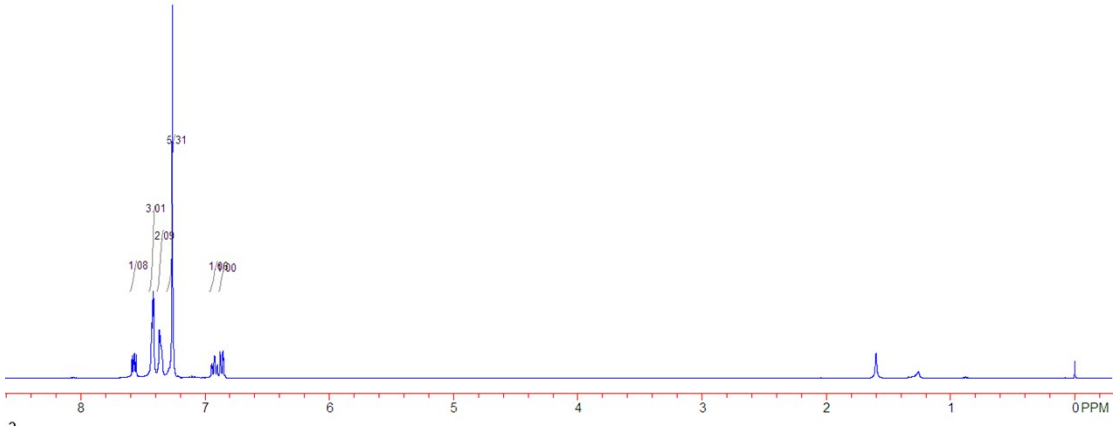

7.666
7.648
7.570
7.552
7.504
7.501
7.485
7.482
7.466
7.439
7.421
7.398
7.346
7.273
7.258
7.251
O
Ph
Ph
Ph
8.68
5.15
1.95
1.00
1.13
9
8
7
6
5
4
3
2
1
0
PPM
196.151
154.861
140.788
140.125
140.393
133.200
132.715
130.756
130.029
129.937
129.340
129.016
128.576
128.290
128.135
127.839
127.576
127.225
120.463
120.546
77.377
77.063
76.744
O
Ph
Ph
Ph
200
150
100
50
0
PPM

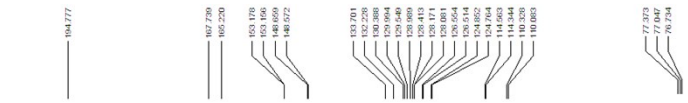

O
Ph
F
Ph

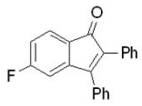
3ia

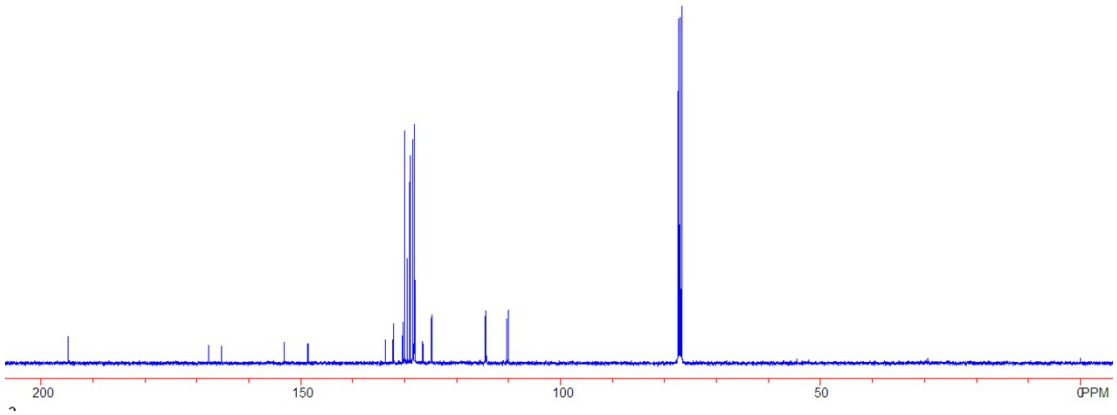


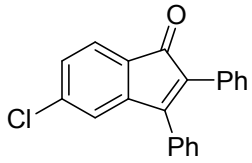

O
Ph
F
Ph


5.31
3.01
2.09
1.08
1.00
8
7
6
5
4
3
2
1
0PPM

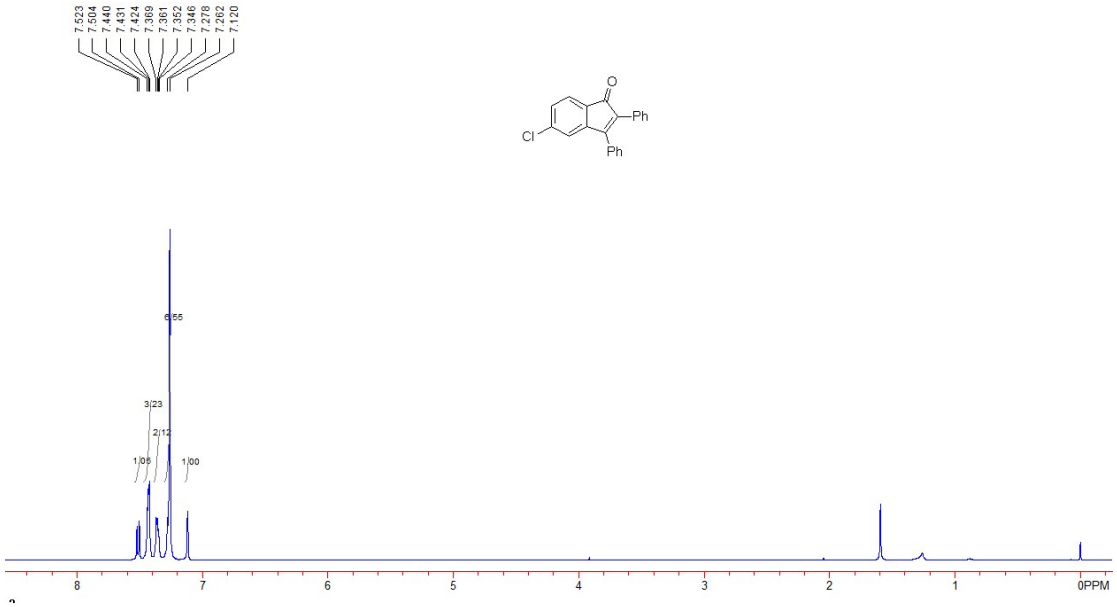


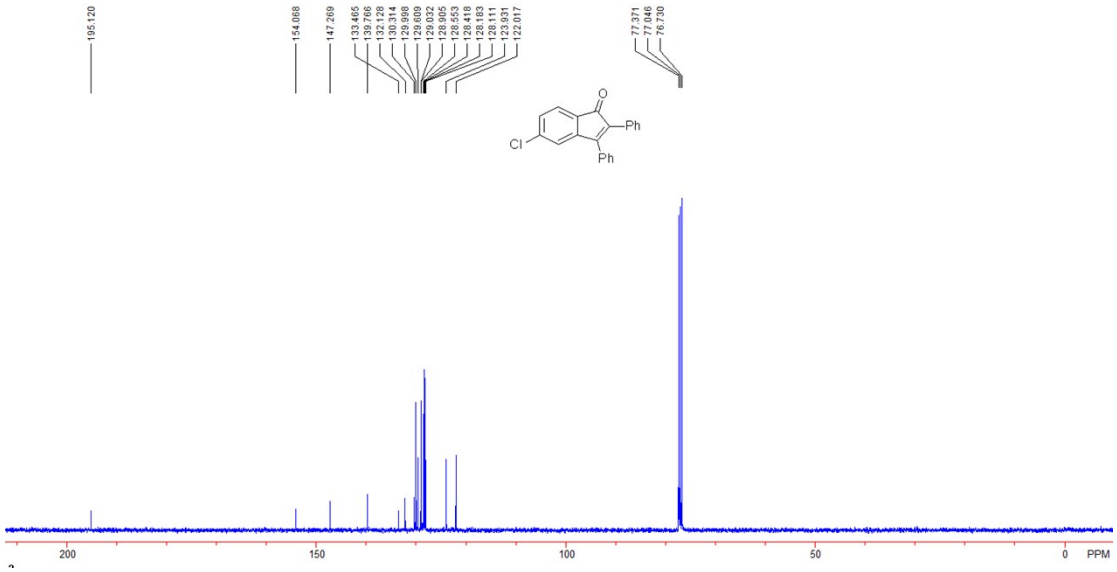

O
Ph
F
Ph

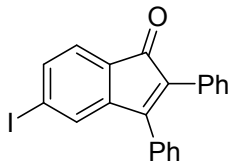

200
150
100
50
0PPM


O
Ph
Cl
Ph

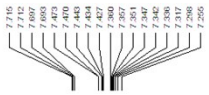
3ja

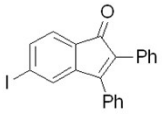

7.523
7.504
7.440
7.431
7.424
7.369
7.361
7.352
7.346
7.278
7.262
7.120
O
Ph
Cl
Ph
6.65
3.23
2.12
1.05
1.00
8
7
6
5
4
3
2
1
0PPM

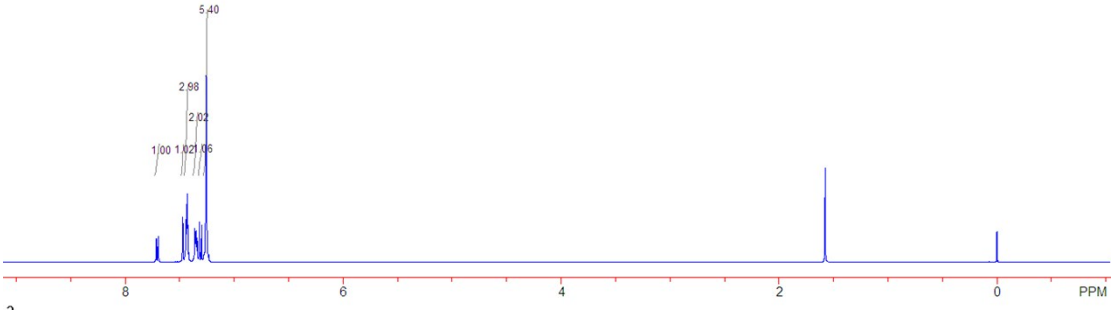

195.120
154.068
147.269
133.465
139.766
132.128
130.314
129.966
129.609
129.032
128.905
128.553
128.418
128.183
128.111
123.931
122.017
77.371
77.046
76.730
O
Ph
Cl
Ph
200
150
100
50
0
PPM

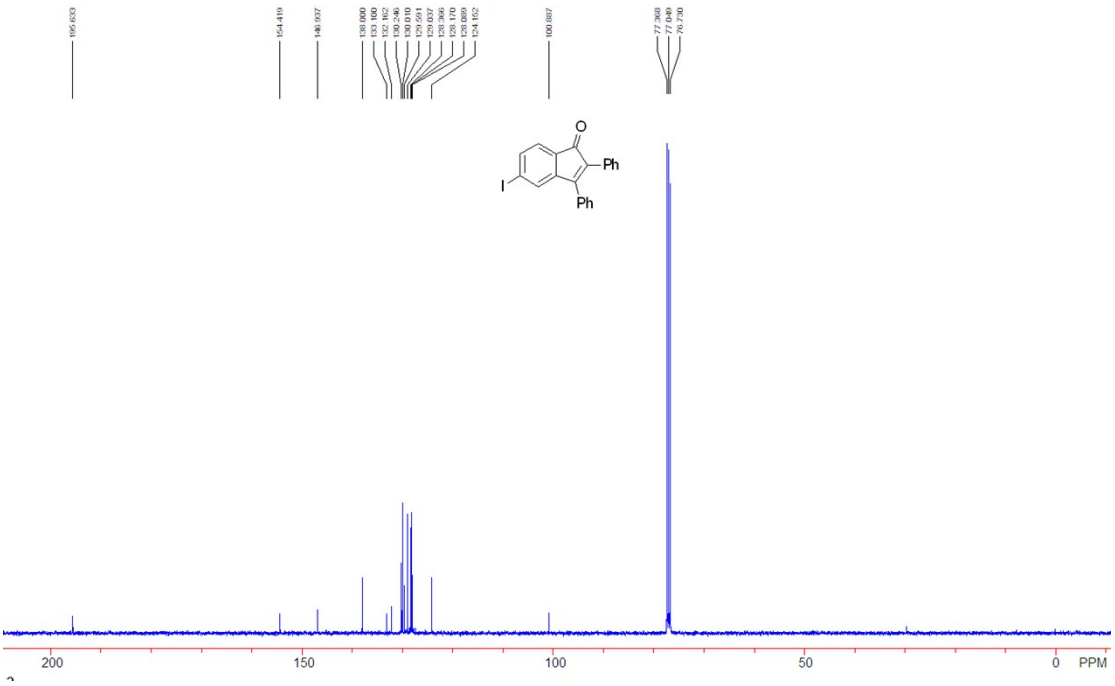

O
Ph
I
Ph

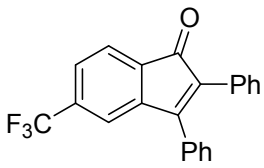
3ka


7.715
7.712
7.697
7.693
7.473
7.469
7.443
7.434
7.427
7.360
7.357
7.351
7.347
7.342
7.306
7.301
7.298
7.295

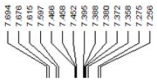

O
Ph
I
Ph

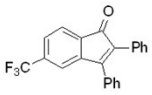

5.40
2.98
2.02
1.00
1.02
1.06
8
6
4
2
0
PPM

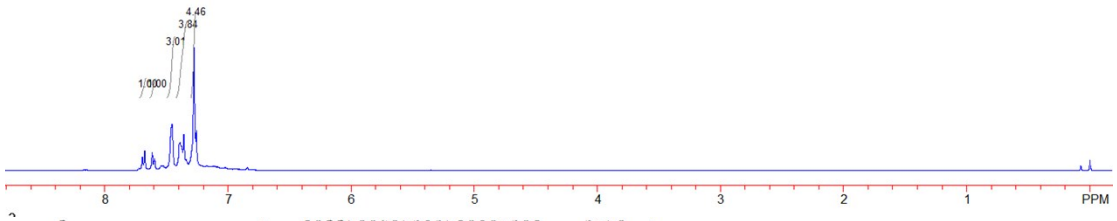

195.633
154.419
140.957
130.000
132.162
130.246
130.010
129.591
129.057
128.366
128.170
126.089
124.152
100.887
77.368
77.049
76.730
O
Ph
I
Ph
200
150
100
50
0
PPM

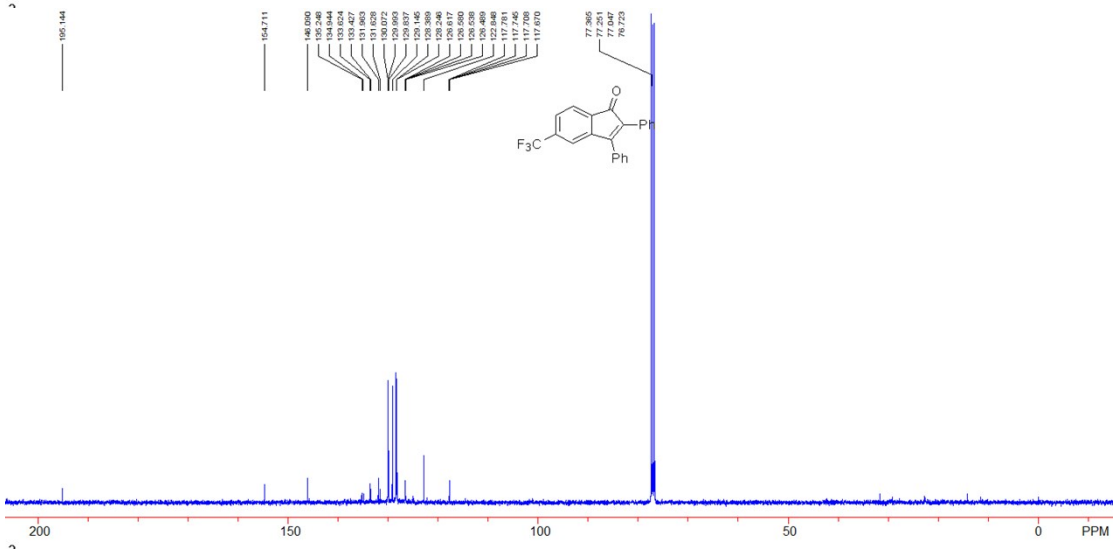

O
Ph
F3C
Ph

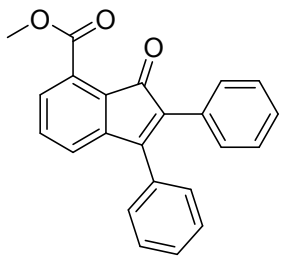
3la


7.694
7.676
7.615
7.597
7.466
7.458
7.402
7.396
7.380
7.372
7.356
7.334
7.256

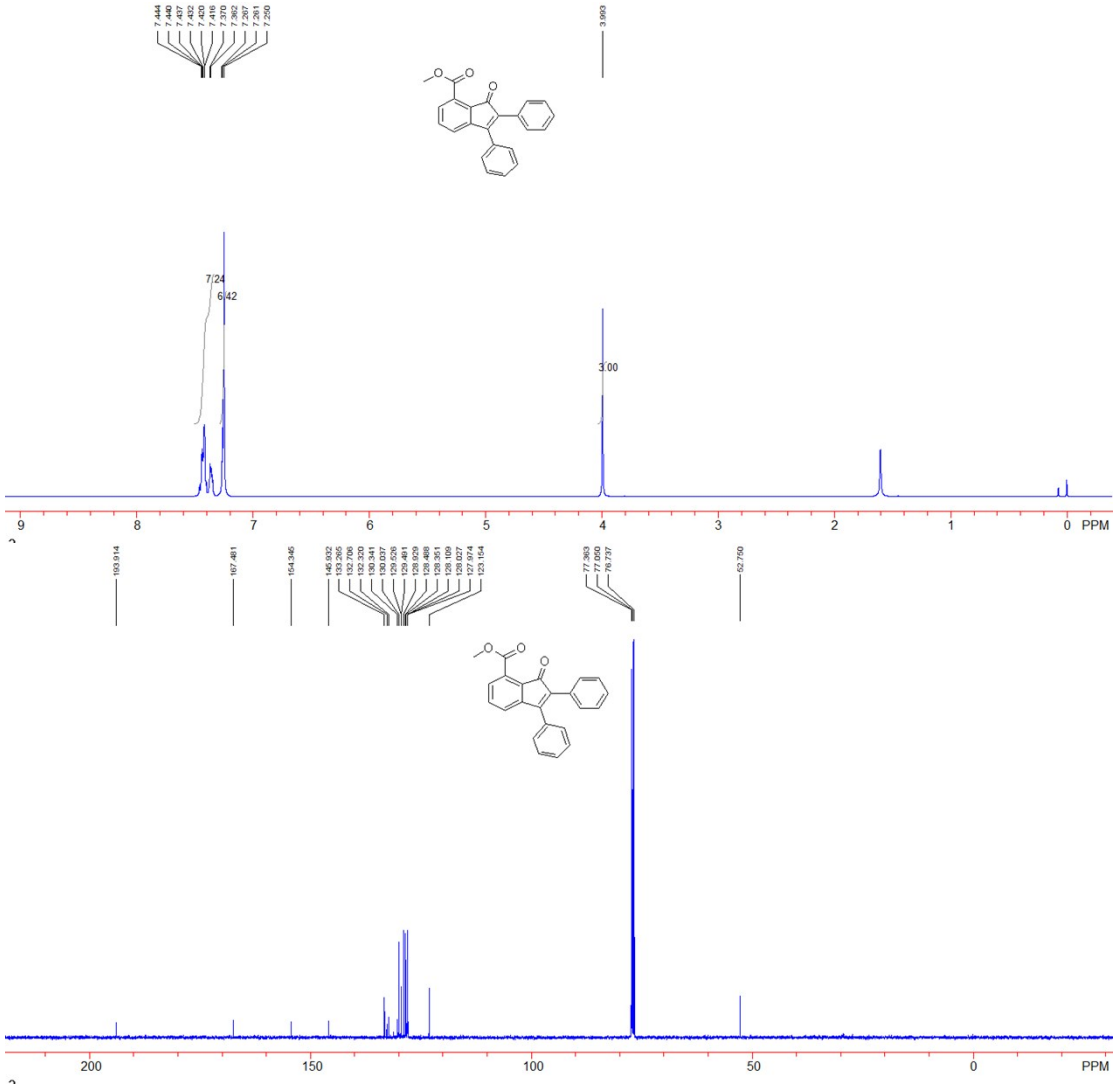

O
Ph
F3C
Ph

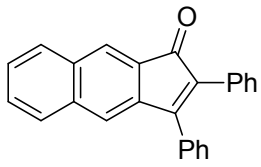

4.46
3.84
3.01
1.0000
8
7
6
5
4
3
2
1
PPM


195.144
154.711
140.090
135.246
134.944
133.824
133.427
131.965
131.628
130.072
129.993
129.837
129.646
129.389
129.246
129.017
128.660
126.539
126.489
122.848
117.781
117.746
117.708
117.670
77.365
77.251
77.047
76.723
O
Ph
F3C
Ph
200
150
100
50
0
PPM

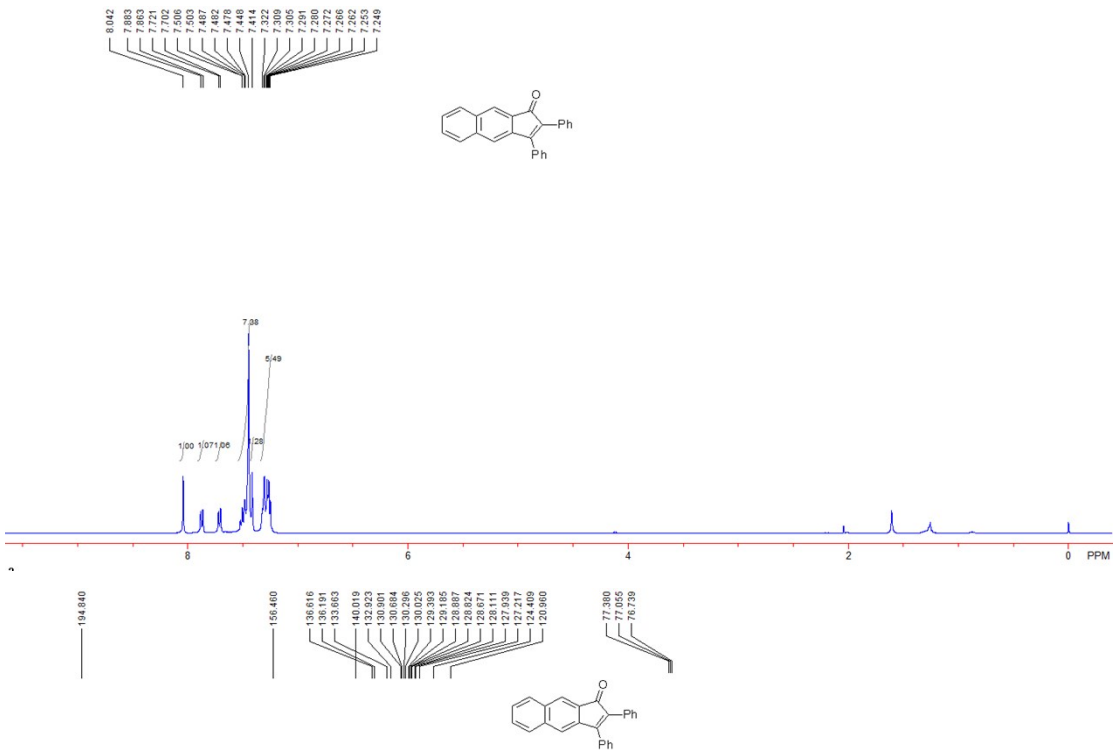

O
O
O

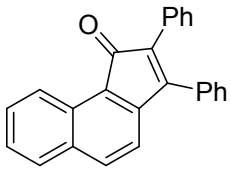
3ma


7.444
7.440
7.437
7.432
7.420
7.416
7.393
7.392
7.287
7.261
7.250
3.993
7.24
6.42
3.00
9
8
7
6
5
4
3
2
1
0 PPM
193.914
167.481
154.345
146.932
133.295
132.706
132.333
130.341
130.037
129.526
129.441
128.929
128.488
128.351
128.109
127.977
127.974
123.154
77.363
77.050
76.737
52.750
200
150
100
50
0
PPM

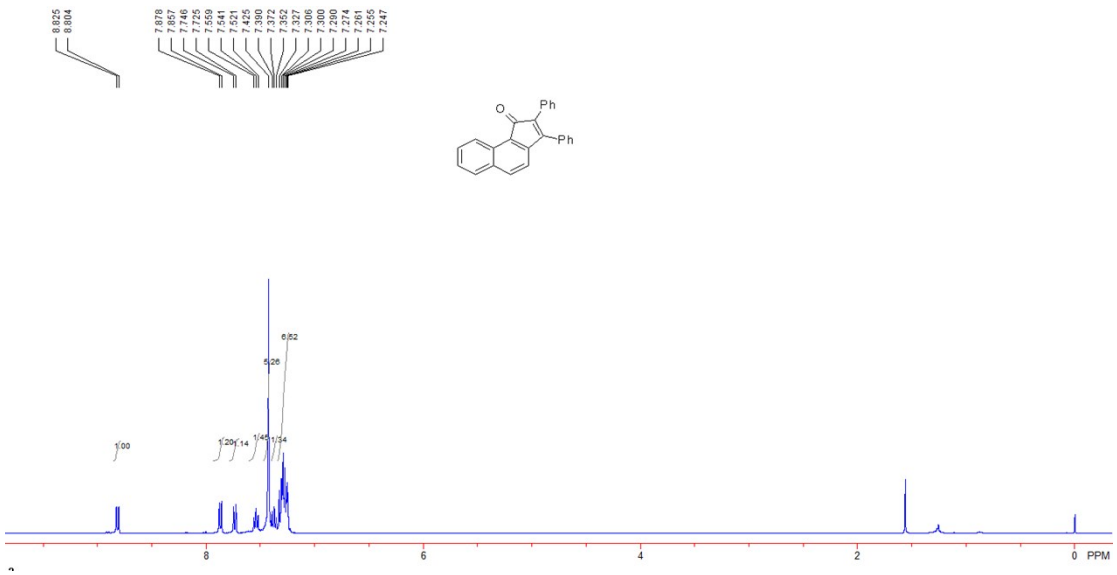

O
Ph
Ph

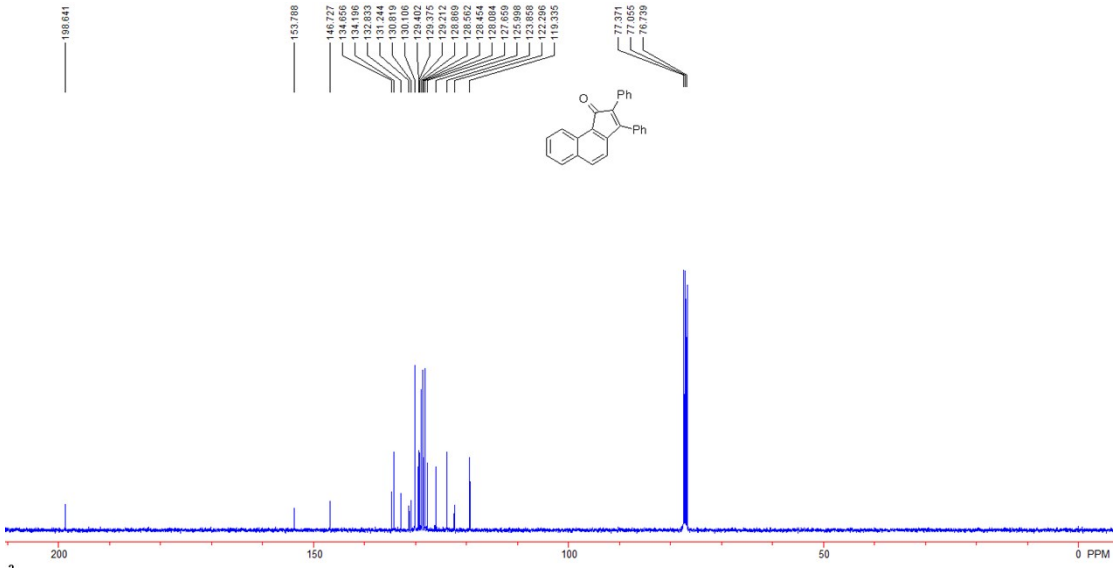
3na

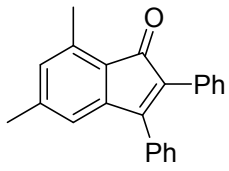

8.042
7.883
7.863
7.721
7.702
7.506
7.503
7.487
7.482
7.478
7.448
7.414
7.332
7.309
7.305
7.291
7.280
7.272
7.266
7.262
7.253
7.249
O
Ph
Ph
7.88
5.49
1.00
1.071.06
1.28
8
6
4
2
0
PPM
194.840
156.460
136.616
136.191
133.663
140.019
132.923
130.901
130.684
130.286
130.055
129.393
129.185
128.887
128.824
128.671
128.111
127.939
127.217
124.499
120.960
77.380
77.055
76.739
O
Ph
Ph
200
150
100
50
0
PPM


O
Ph
Ph

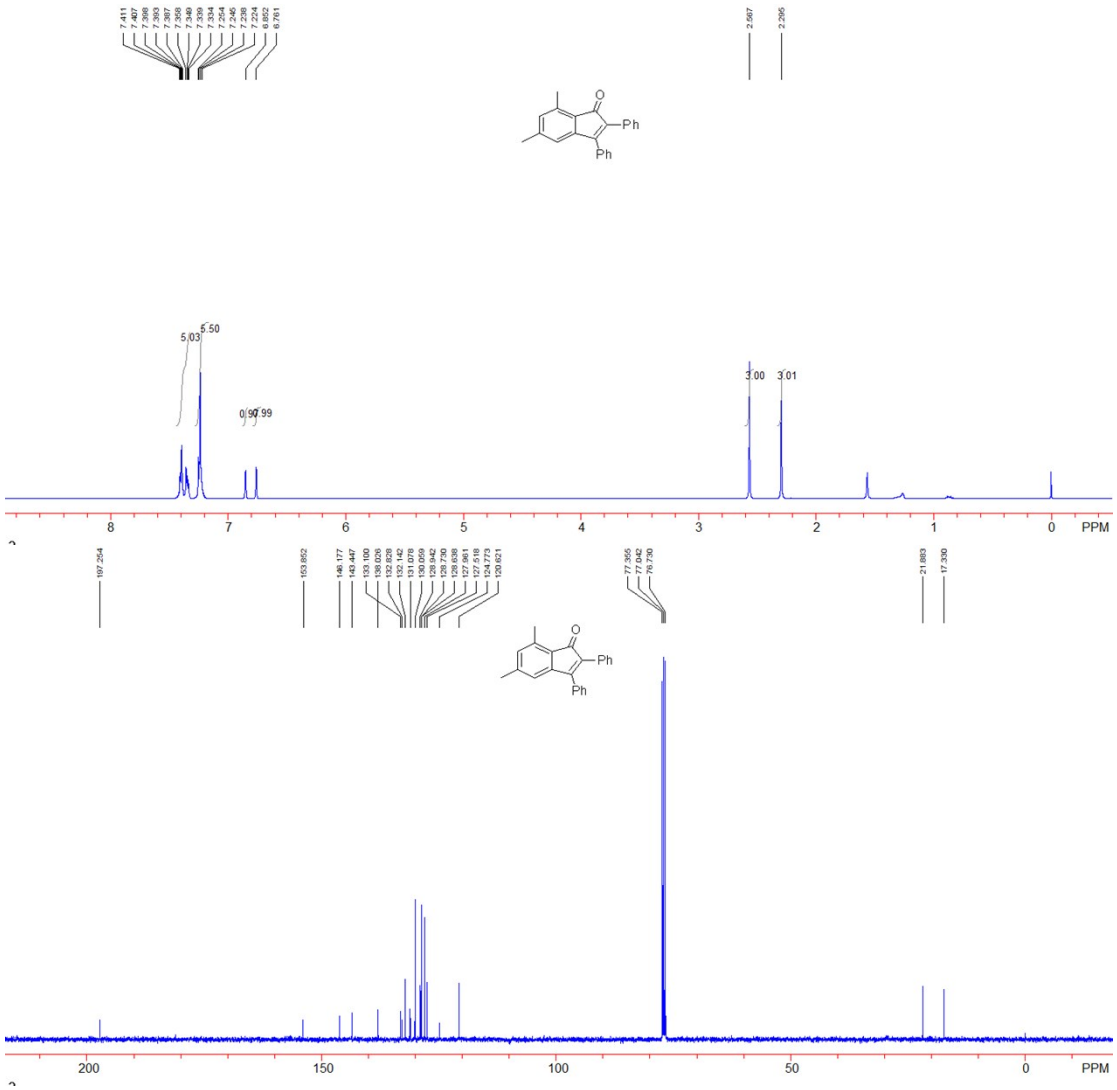
3oa

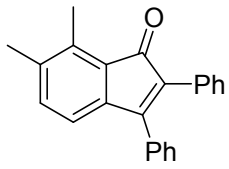

8.825
8.804
7.878
7.857
7.746
7.725
7.659
7.541
7.521
7.425
7.390
7.372
7.352
7.327
7.306
7.300
7.290
7.274
7.261
7.255
7.247
O
Ph
Ph
6.52
5.26
1.00
1.20
1.14
1.45
1.34
8
6
4
2
0 PPM


198.641
153.788
146.727
134.656
134.196
132.833
131.244
130.819
130.186
129.402
129.375
129.212
128.869
128.562
128.454
128.084
127.659
127.498
123.858
122.296
119.335
77.371
77.055
76.739
O
Ph
Ph
200
150
100
50
0 PPM

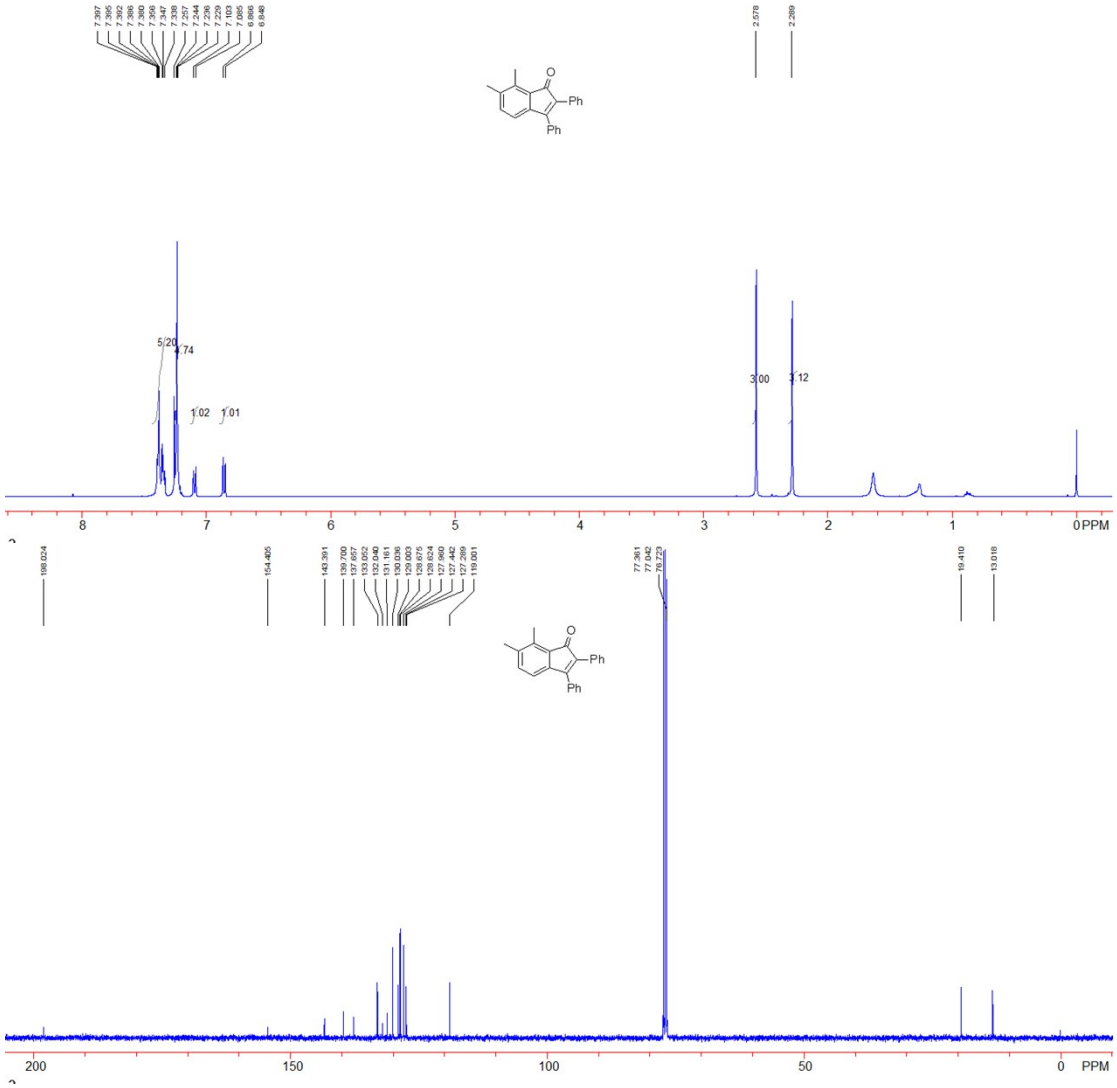

O
Ph
Ph

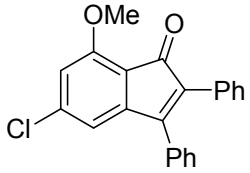
3pa


7.411
7.407
7.398
7.393
7.387
7.385
7.349
7.339
7.334
7.254
7.245
7.238
7.224
6.955
6.761
2.567
2.295
O
Ph
Ph
5.03
5.50
0.99
0.99
3.00
3.01
8
7
6
5
4
3
2
1
0
PPM
197.254
153.852
148.177
143.447
133.100
132.626
132.142
131.078
130.059
129.740
128.838
127.961
127.516
124.721
120.621
77.355
77.042
76.730
21.863
17.330
200
150
100
50
0
PPM

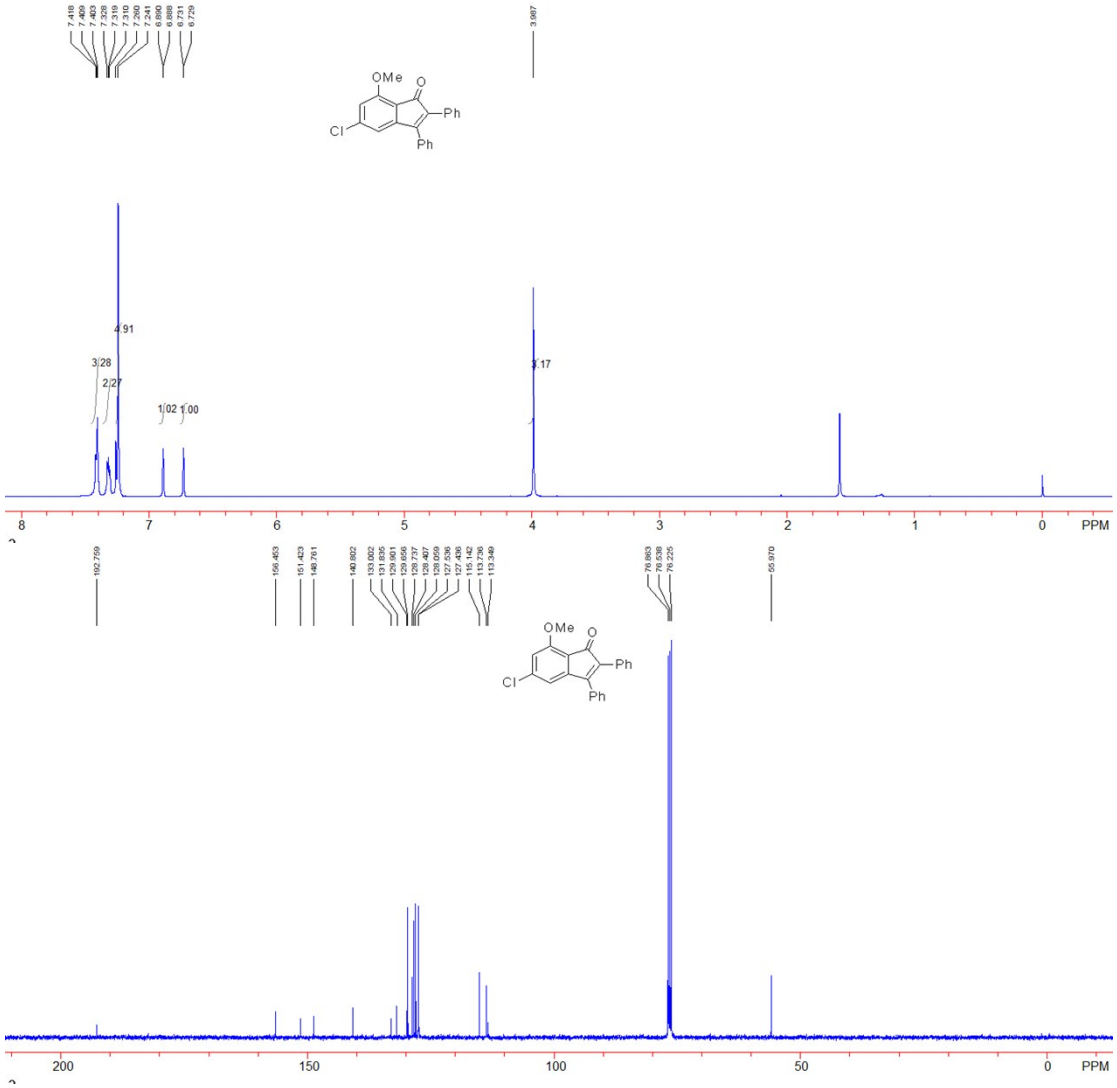

O
Ph
Ph

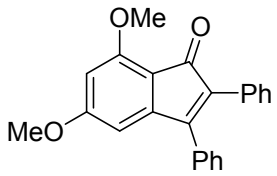
3qa


7.397
7.395
7.392
7.386
7.380
7.369
7.347
7.338
7.257
7.244
7.236
7.229
7.103
7.085
6.868
6.848
2.578
2.289
O
Ph
Ph
5.20
4.74
1.02
1.01
3.00
3.12
8
7
6
5
4
3
2
1
0 PPM
198.024
154.405
143.391
139.700
137.657
133.052
131.049
131.181
130.036
129.003
128.614
128.524
127.960
127.442
127.269
119.001
77.361
77.042
76.723
19.410
13.016
O
Ph
Ph
200
150
100
50
0 PPM

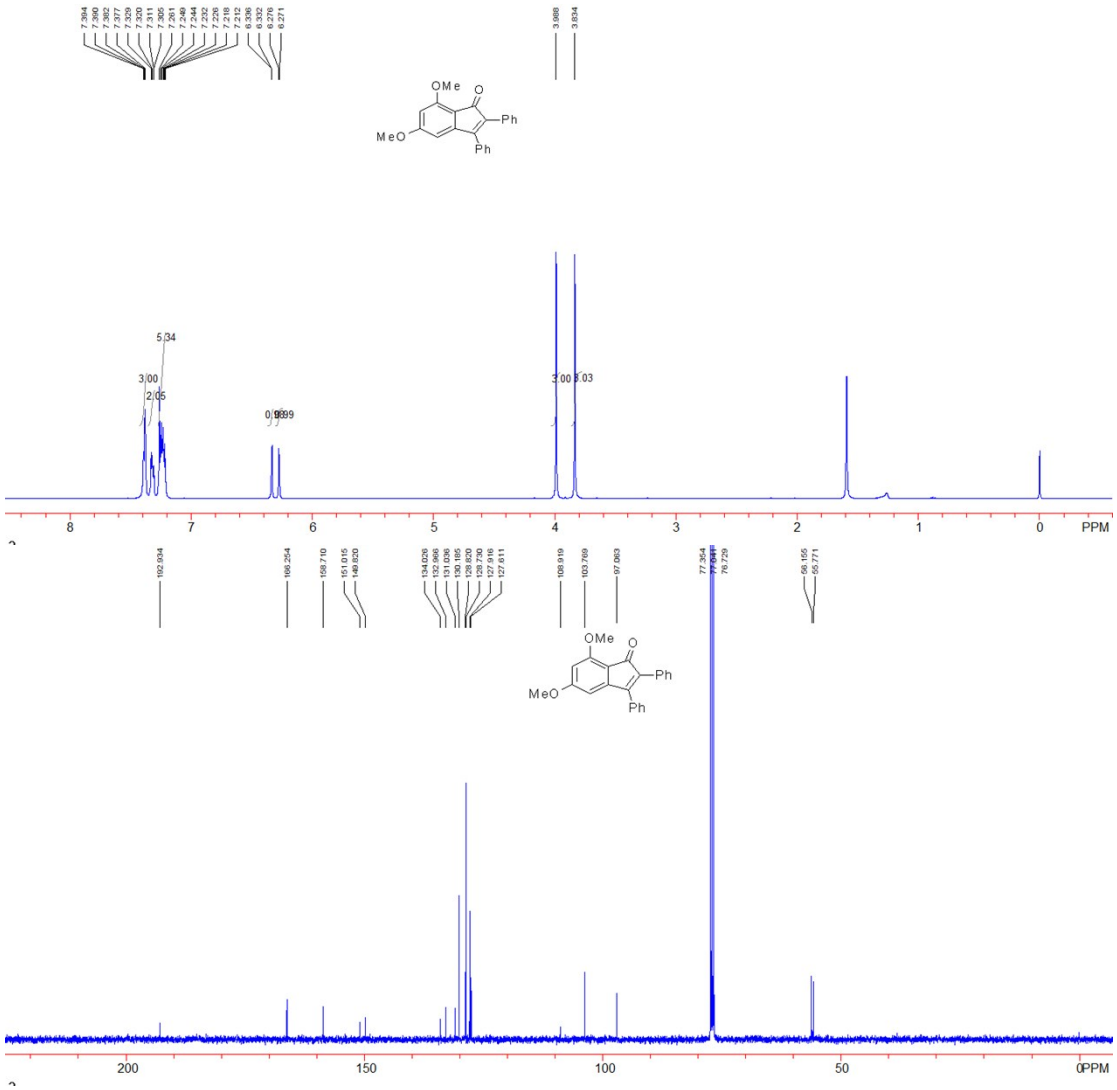

OMe
O
Ph
Cl
Ph

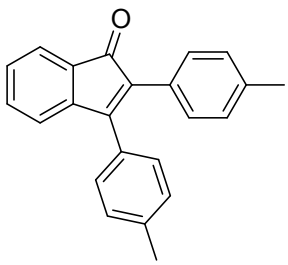
3ra


7.418
7.403
7.328
7.319
7.310
7.290
7.241
6.890
6.888
6.731
6.729
3.997
OMe
O
Cl
Ph
Ph
4.91
3.28
2.27
1.02
1.00
3.17
8
7
6
5
4
3
2
1
0
PPM
162.759
159.453
151.423
149.761
140.882
133.002
131.835
129.901
129.645
129.737
129.407
129.059
127.656
127.435
115.142
113.736
113.349
79.863
79.538
79.225
55.970
OMe
O
Cl
Ph
Ph
200
150
100
50
0
PPM

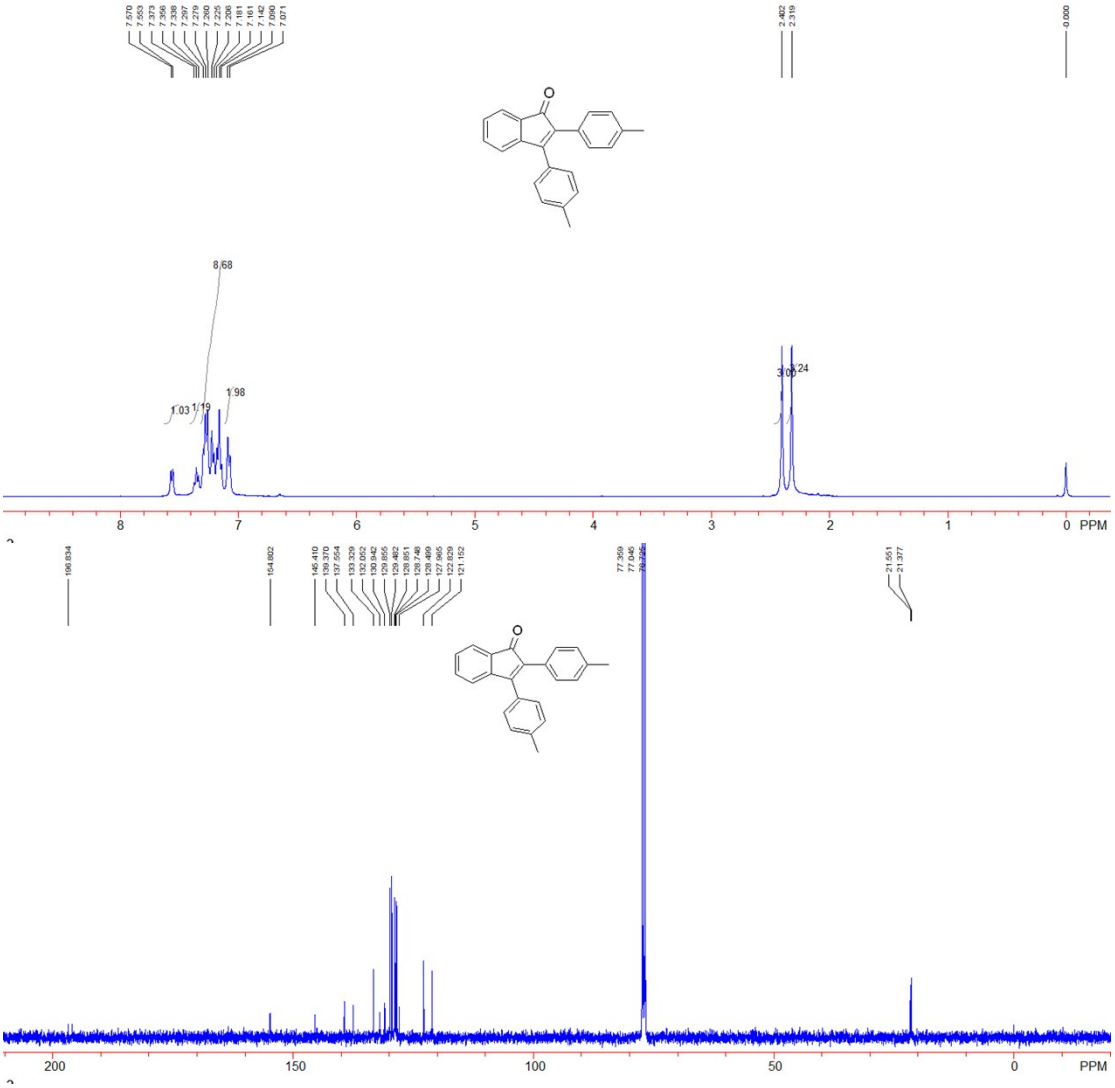

OMe
O
Ph
MeO
Ph

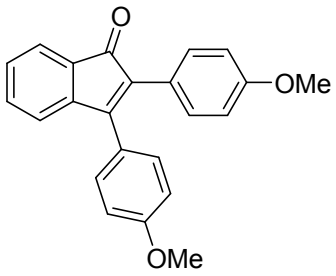
3sa


OMe
O
Ph
MeO
Ph
5.34
3.00
2.05
3.00
3.03
PPM
OMe
O
Ph
MeO
Ph
200
150
100
50
0PPM

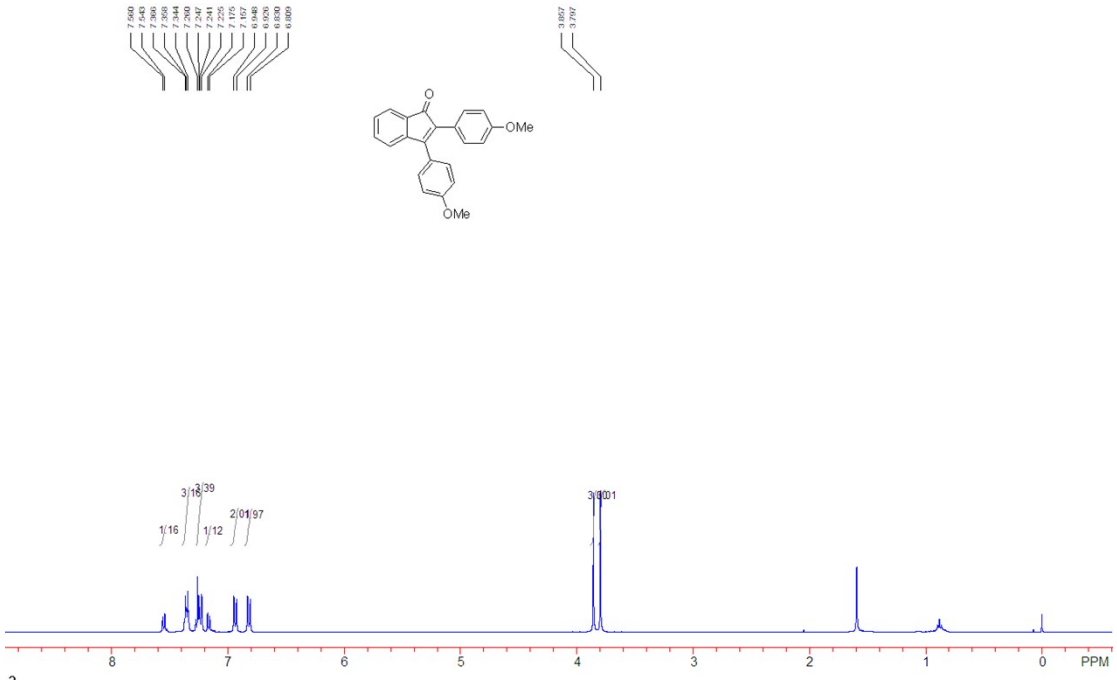

O

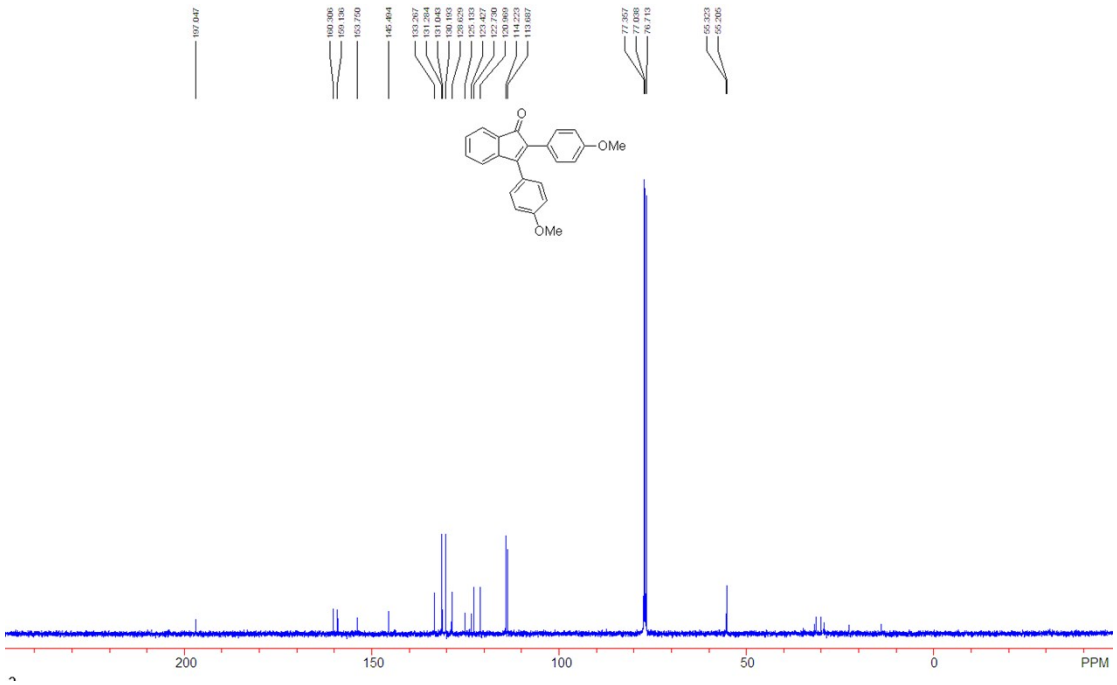
3ab

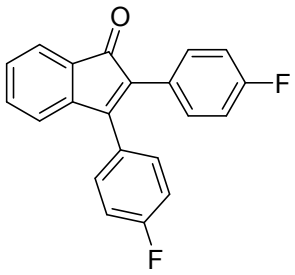




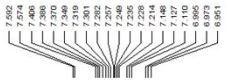
3ac

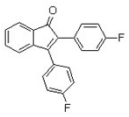

7.560
7.543
7.396
7.395
7.344
7.260
7.247
7.244
7.235
7.175
7.167
6.948
6.936
6.930
6.809
3.897
3.797
O
OMe
OMe
1.16
3.18
3.39
1.12
2.01
2.97
3.00
3.01
8
7
6
5
4
3
2
1
0
PPM

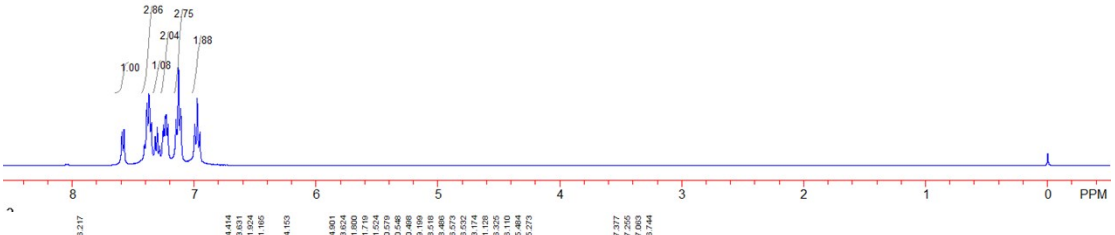

197.047
160.306
159.136
153.750
145.494
133.267
131.264
131.043
130.193
129.659
125.133
123.427
122.730
120.969
114.127
113.687
77.357
77.038
76.713
55.323
55.205
O
OMe
OMe
200
150
100
50
0
PPM

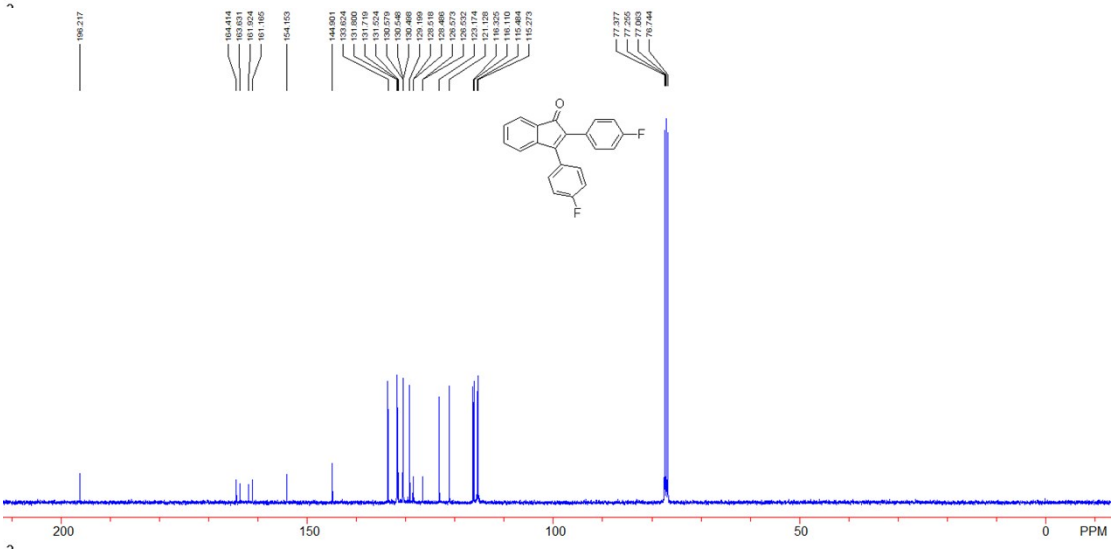

O
F
F

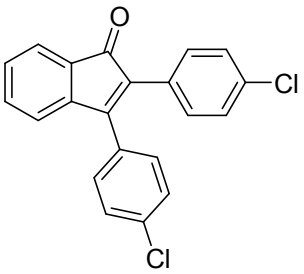
3ad



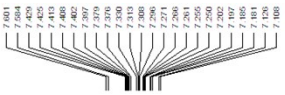


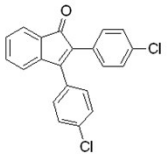


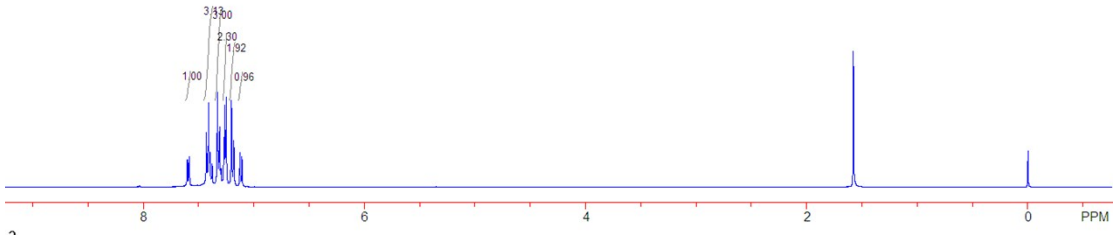


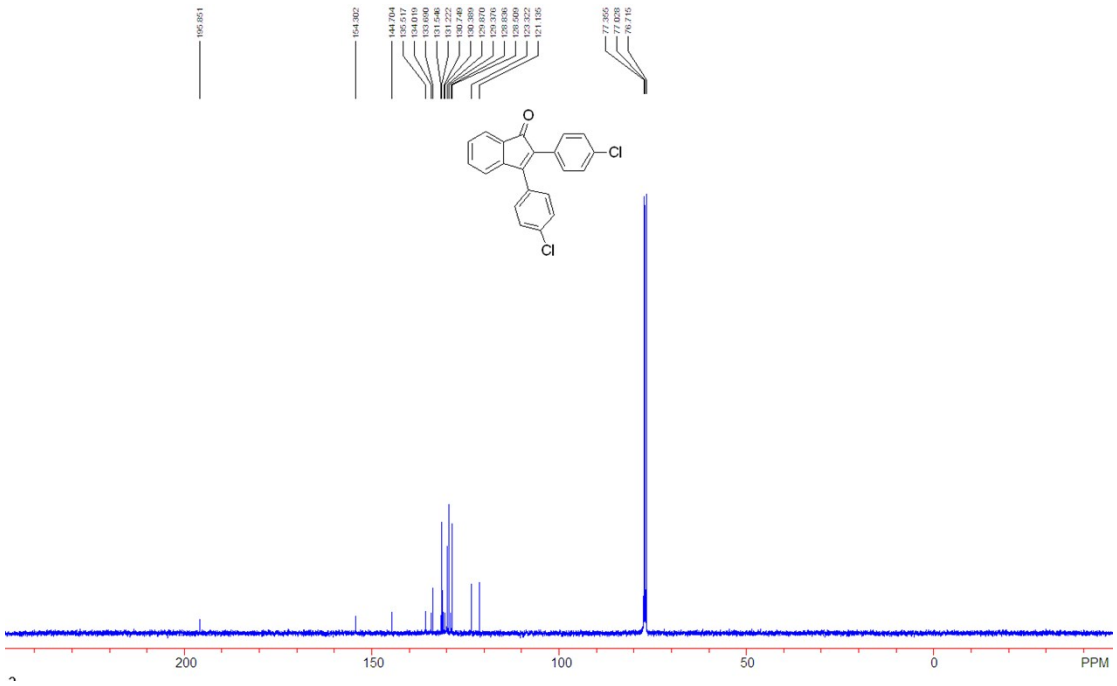


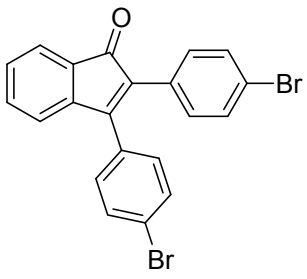
3ae



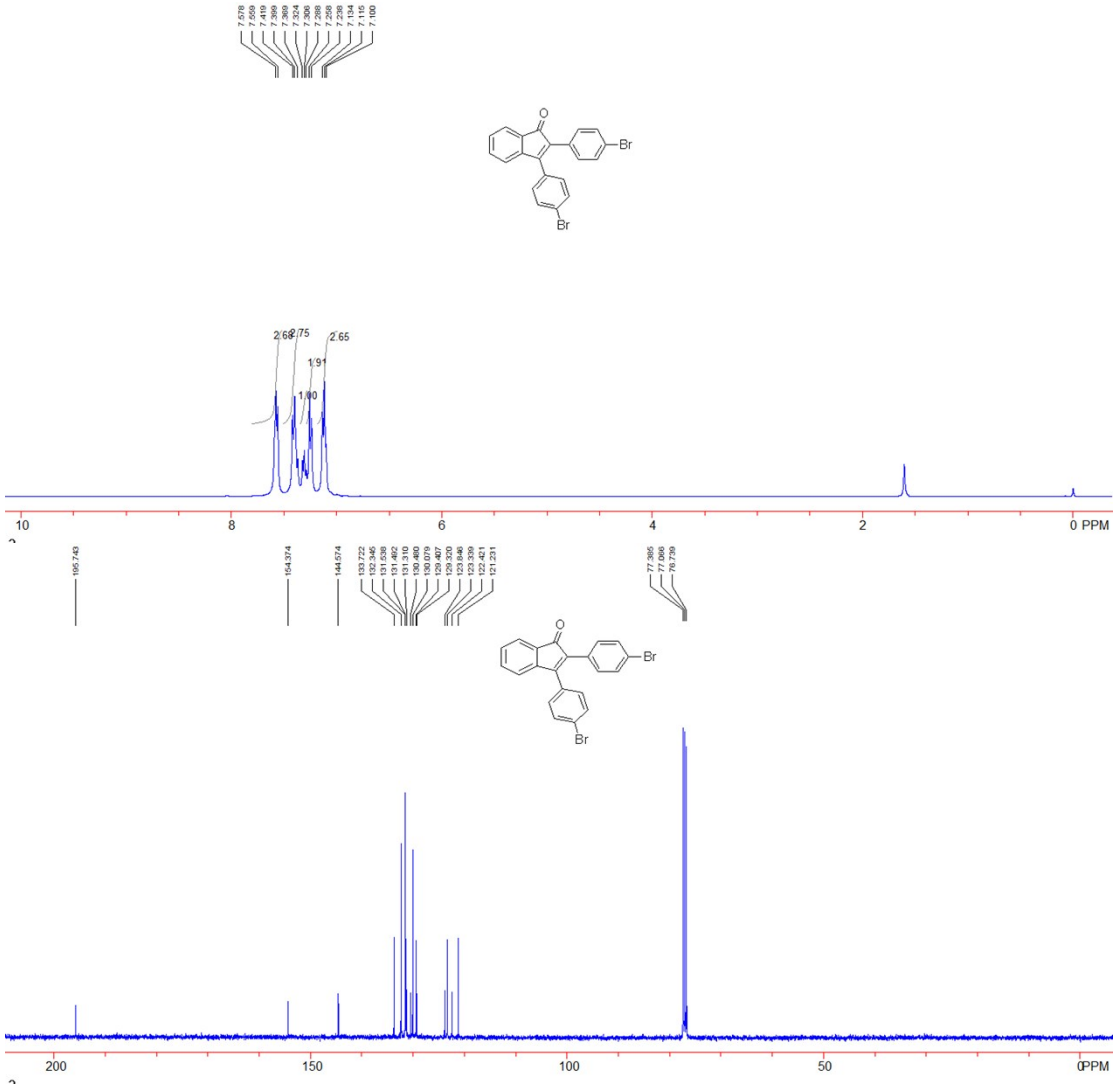

O
Cl
Cl

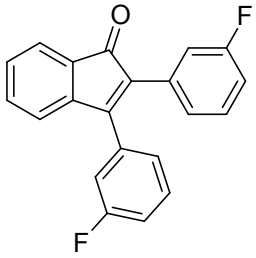

3.13
3.00
2.00
1.92
1.00
0.96
8
6
4
2
0
PPM


196.851
154.302
144.764
135.517
134.019
133.690
131.546
131.222
130.744
130.389
129.870
129.376
128.836
128.564
123.322
121.135
77.355
77.028
76.715
O
Cl
Cl
200
150
100
50
0
PPM

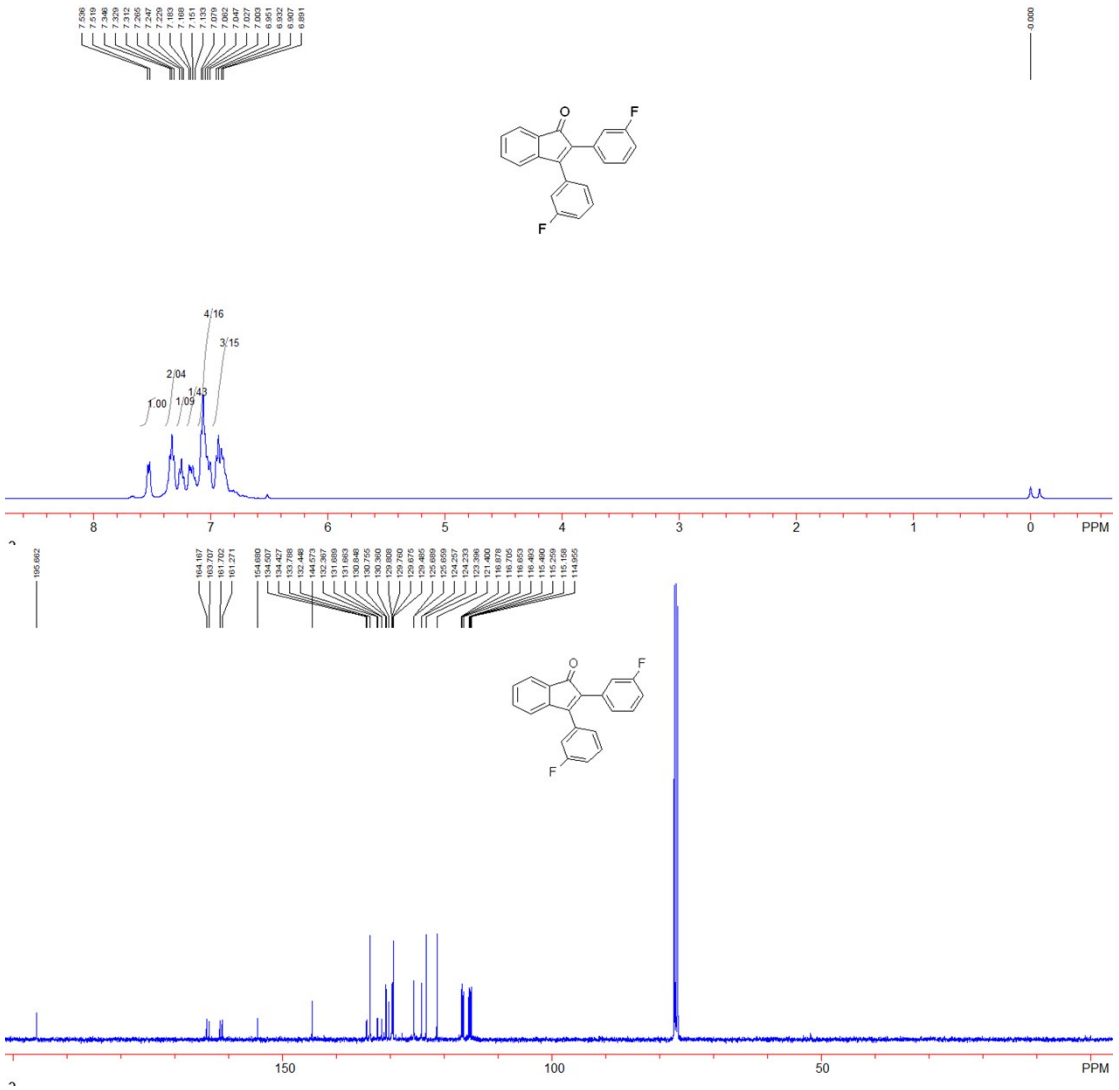

O
Br
Br

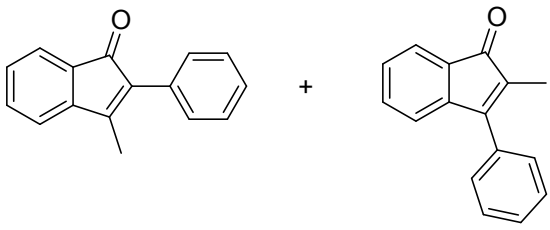
3af


7.578
7.459
7.449
7.399
7.369
7.324
7.306
7.298
7.259
7.238
7.134
7.115
7.100
O
Br
Br
2.68
2.75
2.65
1.91
1.00
10
8
6
4
2
0 PPM
195.743
154.374
144.574
133.722
132.345
131.538
131.492
131.310
130.480
130.079
129.407
129.320
123.466
123.339
122.421
121.231
77.385
77.066
76.739
O
Br
Br
200
150
100
50
0PPM


O
F
F

3ag

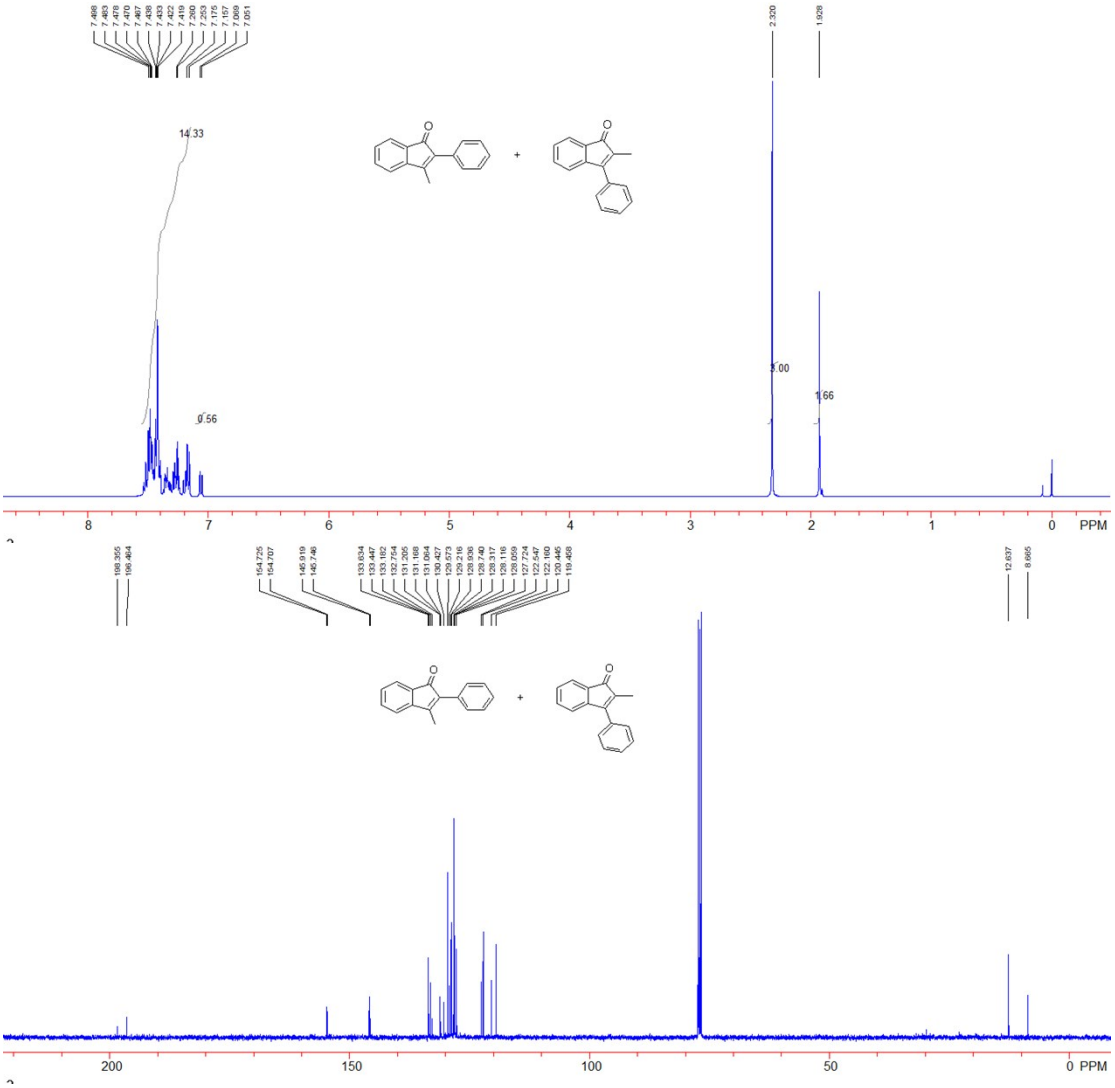

7.536
7.519
7.346
7.329
7.312
7.266
7.247
7.229
7.183
7.166
7.151
7.133
7.079
7.062
7.047
7.027
7.003
6.951
6.932
6.907
6.891
0.000
O
F
F
4/16
3/15
2.04
1.43
1.00
1.09
8
7
6
5
4
3
2
1
0
PPM
195.662
164.167
161.707
161.271
154.880
134.507
133.788
132.446
144.573
132.367
131.663
130.846
130.755
130.360
129.988
129.760
129.675
129.485
125.659
124.257
124.233
123.396
123.446
118.878
118.705
116.653
116.460
115.400
115.259
115.158
114.955
150
100
50
PPM


O

+

O

3ah **3ah'**


7.498
7.483
7.478
7.470
7.467
7.466
7.433
7.422
7.419
7.393
7.253
7.175
7.157
7.089
7.051
14.33
0.56
2.300
1.928
3.00
1.66
8
7
6
5
4
3
2
1
0
PPM
199.355
199.464
154.725
154.707
145.919
145.746
133.834
133.447
133.182
132.754
131.205
131.168
131.084
130.427
129.573
129.316
129.036
128.740
128.317
128.116
127.724
122.547
122.160
120.445
119.466
12.637
8.865
200
150
100
50
0
PPM