

Regioselective Synthesis of Isocoumarins *via* Iridium(III)-Catalyzed Oxidative Cyclization of Aromatic Acids with Propargyl Alcohols

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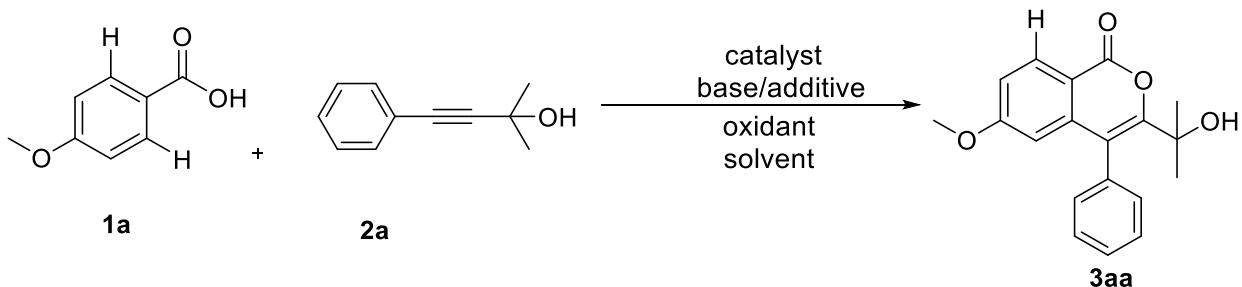
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Supporting Information (SI)

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Table S1. Optimization Studies



	Base /Additive	Solvent	Catalyst	Oxidant	Yield 3aa (%) ⁱ
1	NaOAc (1.5 equiv)	THF	[{Ru(CH ₃ CN) ₃ (<i>p</i> -cymene)}{SbF ₆ } ₂]	-	22% ^a
2	NaOAc (1.5 equiv)	DCE	[{Ru(CH ₃ CN) ₃ (<i>p</i> -cymene)}{SbF ₆ } ₂]	-	25% ^a
3	AgOAc (1.5 equiv)	DCE	[{Ru(CH ₃ CN) ₃ (<i>p</i> -cymene)}{SbF ₆ } ₂]	-	NR ^a
4	Cu(OAc) ₂ (1.5 equiv)	DCE	[{Ru(CH ₃ CN) ₃ (<i>p</i> -cymene)}{SbF ₆ } ₂]	-	NR ^a
5	LiOAc.2H ₂ O (1.5 equiv)	DCE	[{Ru(CH ₃ CN) ₃ (<i>p</i> -cymene)}{SbF ₆ } ₂]	-	22% ^a
5	K ₂ CO ₃ (2.0 equiv)	DCE	[{Ru(CH ₃ CN) ₃ (<i>p</i> -cymene)}{SbF ₆ } ₂]	-	25% ^a
7	NaOAc / Pivalic acid (2.0equiv)/ (1 equiv.)	THF	[{Ru(CH ₃ CN) ₃ (<i>p</i> -cymene)}{SbF ₆ } ₂]	-	NR ^a
8	LiOAc (1.0 equiv)	DCE	[{Ru(CH ₃ CN) ₃ (<i>p</i> -cymene)}{SbF ₆ } ₂]	Ag ₂ CO ₃ (1.2 equiv)	20% ^a
9	LiOAc (1.0 equiv)	DCE	[Ru (<i>p</i> -cymene)Cl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	19% ^a
10	AgOAc (1.0 equiv)	DCE	[Ru (<i>p</i> -cymene)Cl ₂] ₂	-	20% ^a
11	NaOAc (1.0 equiv)	DCE	[Ru (<i>p</i> -cymene)Cl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	22% ^a
12	NaOAc (0.50 equiv)	DCE	[{Rh(CH ₃ CN) ₃ (Cp*)}{SbF ₆ } ₂]	-	63% ^a
13	NaOAc (1.5 equiv)	DCE	[{Rh(CH ₃ CN) ₃ (Cp*)}{SbF ₆ } ₂]	-	42% ^a
14	AgOAc (0.50 equiv)	DCE	[{Rh(CH ₃ CN) ₃ (Cp*)}{SbF ₆ } ₂]	-	NR ^a
15	NaOAc (0.30 equiv)	DCE	[{Rh(CH ₃ CN) ₃ (Cp*)}{SbF ₆ } ₂]	-	52% ^b

16	NaOAc (0.50 equiv)	MeOH	$[\{Rh(CH_3CN)_3(Cp^*)\}\{SbF_6\}_2]$	-	40% ^a
17	NaOAc (0.50 equiv)	THF	$[\{Rh(CH_3CN)_3(Cp^*)\}\{SbF_6\}_2]$	-	58% ^a
18	NaOAc (0.50 equiv)	Toulene	$[\{Rh(CH_3CN)_3(Cp^*)\}\{SbF_6\}_2]$	-	NR ^a
19	NaOAc/ Acetic acid (0.50 equiv)/(1.5 equiv)	THF	$[\{Rh(CH_3CN)_3(Cp^*)\}\{SbF_6\}_2]$	-	45% ^c
20	NaOAc/ Pivalic acid (0.50equiv)/(1.5equiv.)	THF	$[\{Rh(CH_3CN)_3(Cp^*)\}\{SbF_6\}_2]$	-	56% ^c
21	NaOAc (0.50 equiv)	DCE	$[\{Rh(CH_3CN)_3(Cp^*)\}\{SbF_6\}_2]$	AgOAc (1.2 equiv)	74% ^c
22	LiOAc (1.0 equiv)	DCE	$[\{Rh(CH_3CN)_3(Cp^*)\}\{SbF_6\}_2]$	Ag ₂ CO ₃ (1.2 equiv)	76% ^c
23	K ₂ CO ₃ (1.0 equiv)	DCE	$[\{Rh(CH_3CN)_3(Cp^*)\}\{SbF_6\}_2]$	Ag ₂ CO ₃ (1.2 equiv)	NR ^a
24	K ₃ PO ₄ (1.0 equiv)	DCE	$[\{Rh(CH_3CN)_3(Cp^*)\}\{SbF_6\}_2]$	Ag ₂ CO ₃ (1.2 equiv)	NR ^c
25	WB	DCE	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	65% ^d
26	NaOAc (1 equiv)	DCE	[Cp*IrCl ₂] ₂	-	NR ^d
27	LiOAc.2H ₂ O (0.50 equiv)	DCE	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	81% ^d
28	CsOAc (0.50 equiv)	DCE	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	58% ^d
29	NaOAc (0.50 equiv)	DCE	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	79% ^d
30	Na ₂ CO ₃ (0.50 equiv)	DCE	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	48% ^d
31	LiOAc.2H ₂ O (0.50 equiv)	DCE	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	70% ^b
32	LiOAc.2H ₂ O (0.50 equiv)	THF	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	79% ^d
33	LiOAc.2H ₂ O (0.50 equiv)	Toulene	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	70% ^d
34	LiOAc.2H ₂ O (0.50 equiv)	CF ₃ CH ₂ OH	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	NR ^d
35	LiOAc.2H ₂ O (0.50 equiv)	DCE	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	84% ^e
36	LiOAc.2H ₂ O (1 equiv)	DCE	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	89% ^d
37	LiOAc.2H₂O (1 equiv)	DCE	[Cp*IrCl₂]₂	Ag₂CO₃ (1.2 equiv)	86% ^e

38	LiOAc.2H ₂ O (1 equiv)	DCE	[Cp*IrCl ₂] ₂	Ag ₂ O (1.2equiv)	75% ^e
39	LiOAc.2H ₂ O (1 equiv)	DCE	[Cp*IrCl ₂] ₂	AgOAc (1.2equiv)	82% ^e
40	NaOAc (1 equiv)	DCE	[Cp*IrCl ₂] ₂	-	NR ^d
41	LiOAc.2H ₂ O/ Pivalic acid (0.50 equiv)/(1.5 equiv)	DCE	[Cp*IrCl ₂] ₂	-	65% ^d
42	LiOAc.2H ₂ O (1 equiv)	DCE	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	75% ^f
43	LiOAc.2H ₂ O (1 equiv)	DCE	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	48% ^g
44	LiOAc.2H ₂ O (1 equiv)	DCE	[Cp*IrCl ₂] ₂	Ag ₂ CO ₃ (1.2 equiv)	84% ^h

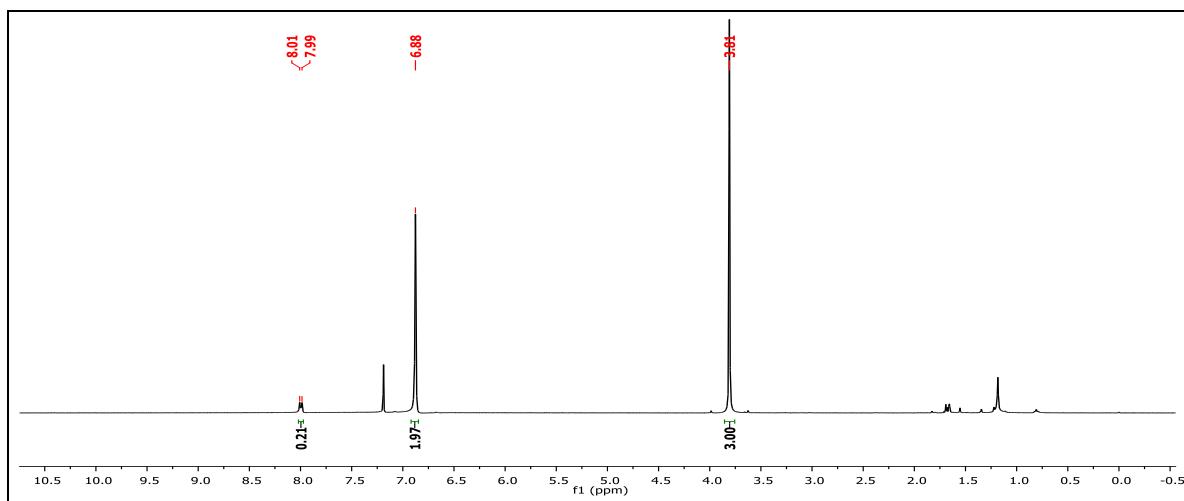
^a**1a** (1.2 equiv), **2a** (50 mg), catalyst (10 mol %) at 100 °C for 24 h. ^b**1a** (50 mg), **2a** (1.2 equiv), catalyst (10 mol %) at 100 °C for 24 h. ^c **1a** (1.2 equiv), **2a** (50 mg), catalyst (10 mol %) at 100 °C for 24 h and regioisomer product **3aa'** formed. ^d**1a** (1.2 equiv), **2a** (50 mg), catalyst (5 mol %) at 80 °C for 20 h. ^e**1a** (1.2 equiv), **2a** (50 mg), catalyst (3 mol %) at 80 °C for 20 h. ^f**1a** (1.2 equiv), **2a** (50 mg), catalyst (3 mol %) at 110°C for 20 h. ^g**1a** (1.2 equiv), **2a** (50 mg), catalyst (3 mol %) at 50 °C for 20 h. ^h**1a** (1.2 equiv), **2a** (50 mg), catalyst (3 mol %) at 80°C for 24 h.

ⁱIsolated yield.

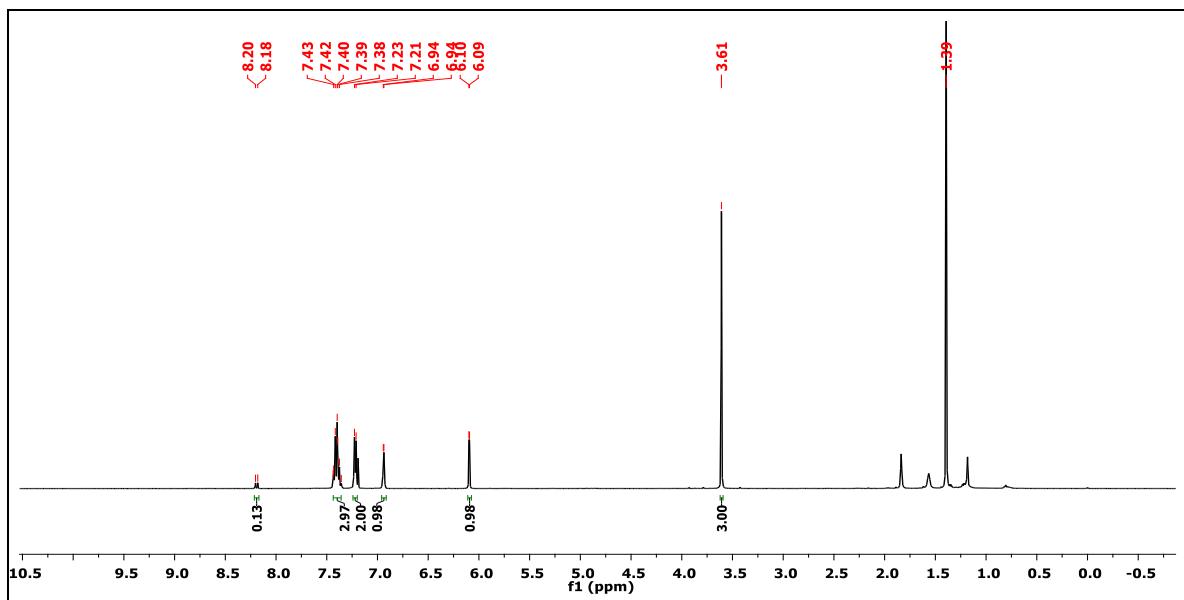
Spectra of Mechanistic Studies

Deutrium labelling studies

(i) ^1H -NMR of [D]-1a:



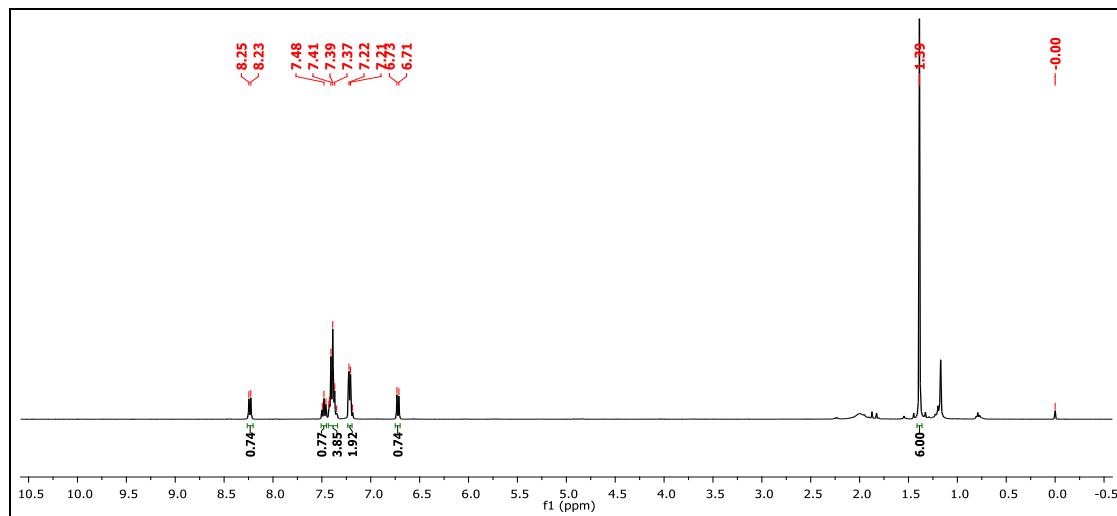
^1H -NMR of [D]-3aa:



(ii) KIE studies:

(a) For one pot reaction:

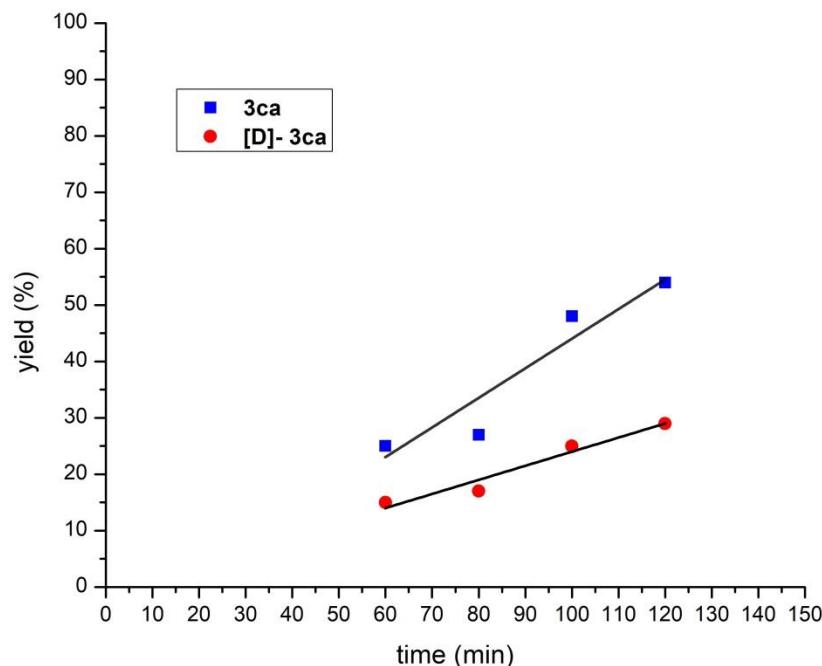
¹H-NMR of [D]-3ca:



(b) For independent reaction:

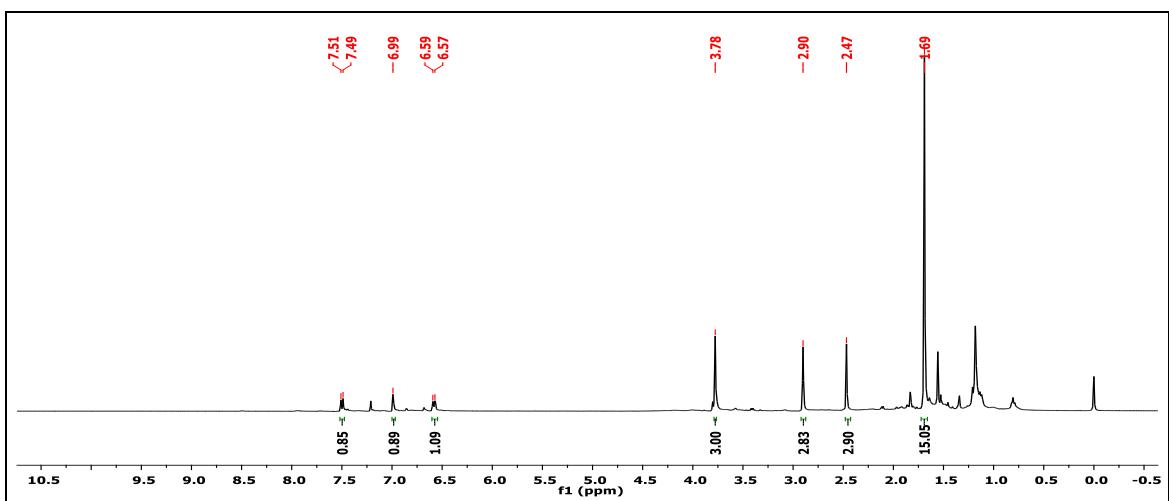
Table S2:

Time (min)	60	80	100	120
3ca (%)	26	27	48	54
[D]-3ca (%)	15	17	25	29

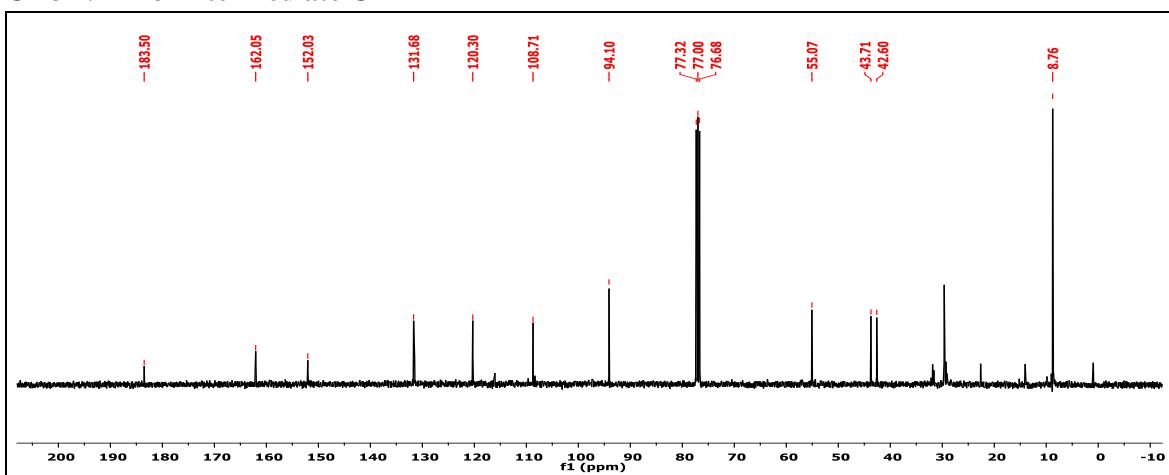


Intermediate Isolation

¹H-NMR of intermediate C:



C-13 NMR of intermediate C



Crystallographic Data of Compound 3ba and 4a:

Suitable single crystals for X-ray diffraction studies were obtained from the compound synthesized in this study. Single crystals were grown in a NMR tube at room temperature using CDCl_3 over a period of 3-4 weeks by slow evaporation of solvent.

X-ray data was collected with a Bruker AXS (Kappa Apex 2) CCD diffractometer equipped with graphite monochromatic Mo ($\text{K}\alpha$) ($\lambda = 0.7107 \text{ \AA}$) radiation source. The data were collected with 100% completeness for Θ up to 25° . ω and ϕ scans were employed to collect the data. The frame width for ω for was fixed to 0.5° for data collection. The crystal was solved by direct methods using Bruker SHELXS (Sheldrick, 1997). The Structure was refined using the Bruker SHELXTL (Version 6.12) software package. These data were deposited with Cambridge Crystallographic Data Center with the following numbers: CCDC 1875730 and CCDC 1875796.

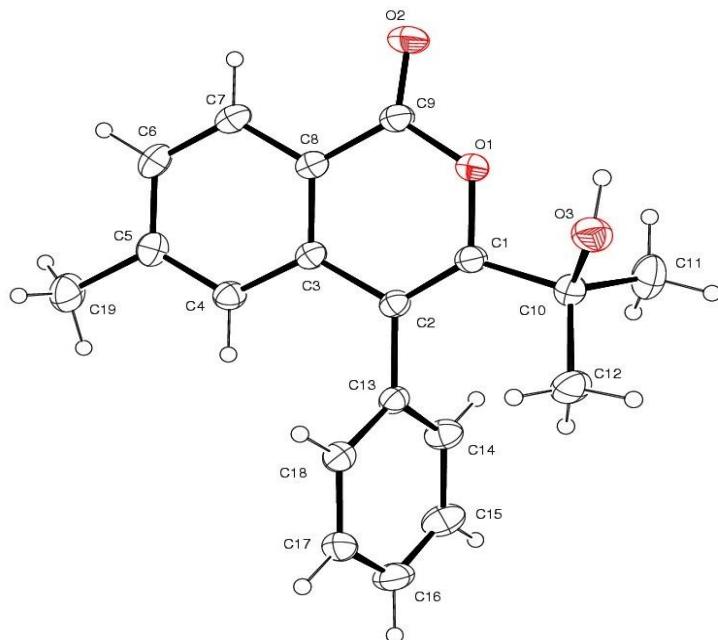


Figure S1: ORTEP representation of compound 3ba displaying thermal elliposoid at 50% probability

Table S3. Crystal data and structure refinement for 3ba.

Identification code	3ba
Empirical formula	$\text{C}_{19}\text{H}_{18}\text{O}_3$
Formula weight	294.35
Temperature/K	296.15
Crystal system	Triclinic
Space group	P-1
a/ \AA	8.9804(4)
b/ \AA	9.2764(4)
c/ \AA	10.1223(4)
$\alpha/^\circ$	75.653(2)

β/\circ	85.6189(19)
γ/\circ	69.2243(18)
Volume/ \AA^3	763.76(6)
Z	2
$\rho_{\text{calc}} \text{g/cm}^{-3}$	1.2798
μ/mm^{-1}	0.086
F(000)	312.2
Crystal size/mm ³	0.25 \times 0.22 \times ?
Radiation	Mo K α ($\lambda = 0.71073$)
2 Θ range for data collection/ \circ	4.16 to 50
Index ranges	-11 \leq h \leq 7, -12 \leq k \leq 11, -12 \leq l \leq 13
Reflections collected	12399
Independent reflections	2682 [R _{int} = 0.0217, R _{sigma} = 0.0208]
Data/restraints/parameters	2682/0/207
Goodness-of-fit on F ²	1.061
Final R indexes [I \geq 2 σ (I)]	R ₁ = 0.0369, wR ₂ = 0.1002
Final R indexes [all data]	R ₁ = 0.0443, wR ₂ = 0.1084
Largest diff. peak/hole / e \AA^{-3}	0.22/-0.15

CCDC **1875730**

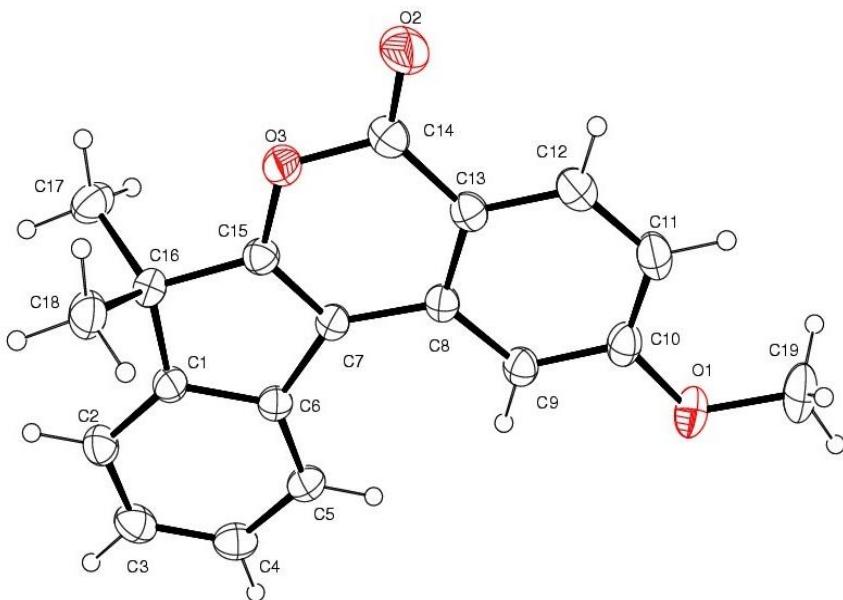


Figure S2: ORTEP representation of compound **4a** displaying thermal elliposoid at 50% probability

Table S4. Crystal data and structure refinement for 4a

Identification code	4a
Empirical formula	C ₁₉ H ₁₆ O ₃
Formula weight	292.32
Temperature/K	296(2)
Crystal system	Monoclinic
Space group	P2 ₁ /c
a/Å	8.6696(5)
b/Å	16.0188(11)
c/Å	11.0129(7)
α/°	90
β/°	106.132(3)
γ/°	90
Volume/Å ³	1469.21(16)
Z	4
ρ _{calcd} g/cm ⁻³	1.322
μ/mm ⁻¹	0.089
F(000)	616.0
Crystal size/mm ³	0.250 × 0.220 × 0.100
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.614 to 49.996
Index ranges	-10 ≤ h ≤ 8, -19 ≤ k ≤ 18, -12 ≤ l ≤ 13
Reflections collected	10463
Independent reflections	2592 [R _{int} = 0.0240, R _{sigma} = 0.0214]

Data/restraints/parameters 2592/0/203
Goodness-of-fit on F² 1.045
Final R indexes [I>=2σ (I)] R₁ = 0.0350, wR₂ = 0.0854
Final R indexes [all data] R₁ = 0.0453, wR₂ = 0.0937
Largest diff. peak/hole / e Å⁻³ 0.16/-0.15
CCDC **1875796**

Cartesian coordinates of all molecules

Benzoic acid:

Zero-point correction	=	0.115937 (Hartree/Particle)
Thermal correction to Energy	=	0.123029
Thermal correction to Enthalpy	=	0.123973
Thermal correction to Gibbs Free Energy	=	0.083943
Sum of electronic and zero-point Energies	=	-420.706212
Sum of electronic and thermal Energies	=	-420.699121
Sum of electronic and thermal Enthalpies	=	-420.698177
Sum of electronic and thermal Free Energies	=	-420.738206

C	-2.57076900	-0.04136900	0.00000100
C	-1.84368100	-1.23426500	-0.00001200
C	-0.45026100	-1.20387900	0.00000000
C	0.22024700	0.02740800	0.00001300
C	-0.51227000	1.22233900	0.00001000
C	-1.90400100	1.18699100	0.00001100
H	-3.65725000	-0.06894300	-0.00000400
H	-2.36304100	-2.18853300	-0.00003800
H	0.12075300	-2.12572700	-0.00003600
H	0.02812500	2.16324500	0.00000100
H	-2.46973500	2.11446200	0.00001600
C	1.70346600	0.12169700	-0.00001000
O	2.33674600	1.15879600	-0.00002600
O	2.31494300	-1.09203100	0.00001100
H	3.27126200	-0.90215700	0.00010400

Acetic acid:

Zero-point correction	=	0.062019 (Hartree/Particle)	
Thermal correction to Energy	=	0.066599	
Thermal correction to Enthalpy	=	0.067543	
Thermal correction to Gibbs Free Energy	=	0.034691	
Sum of electronic and zero-point Energies	=	-229.019769	
Sum of electronic and thermal Energies	=	-229.015188	
Sum of electronic and thermal Enthalpies	=	-229.014244	
Sum of electronic and thermal Free Energies	=	-229.047097	
C	-0.09223800	0.12593300	-0.00011200
O	-0.64487600	1.20241000	0.00002500
O	-0.77914500	-1.04655400	0.00000200
H	-1.72379300	-0.80231300	0.00014600
C	1.39717200	-0.11043400	0.00000000
H	1.68436400	-0.69134700	0.88256800
H	1.68430600	-0.69344200	-0.88118400
H	1.91768900	0.84726400	-0.00106900

AgOAc:

Zero-point correction	=	0.103493 (Hartree/Particle)	
Thermal correction to Energy	=	0.117046	
Thermal correction to Enthalpy	=	0.117991	
Thermal correction to Gibbs Free Energy	=	0.058161	
Sum of electronic and zero-point Energies	=	-748.499697	
Sum of electronic and thermal Energies	=	-748.486143	
Sum of electronic and thermal Enthalpies	=	-748.485199	
Sum of electronic and thermal Free Energies	=	-748.545028	
O	2.13808000	-1.13909100	-0.01352400
O	2.13808000	1.13909200	-0.01352400
C	2.69959100	0.00000000	-0.01731300
C	4.22045100	-0.00000100	0.01058600
H	4.54982300	-0.00002900	1.05658000
H	4.61308900	-0.89853200	-0.46955300
H	4.61309100	0.89855100	-0.46950900
Ag	0.00000000	-1.39802300	-0.00000200
Ag	0.00000000	1.39802400	-0.00000200
O	-2.13808000	1.13909100	0.01352700
O	-2.13808000	-1.13909200	0.01352700
C	-2.69959100	-0.00000100	0.01731700
C	-4.22045100	0.00000000	-0.01057700
H	-4.61308900	-0.89854500	0.46953500
H	-4.61308900	0.89853800	0.46954800
H	-4.54982600	0.00000700	-1.05657000

Propargyl alcohol:

Zero-point correction	=	0.199205 (Hartree/Particle)	
Thermal correction to Energy	=	0.211143	
Thermal correction to Enthalpy	=	0.212087	
Thermal correction to Gibbs Free Energy	=	0.159809	
Sum of electronic and zero-point Energies	=	-501.354884	
Sum of electronic and thermal Energies	=	-501.342945	
Sum of electronic and thermal Enthalpies	=	-501.342001	
Sum of electronic and thermal Free Energies	=	-501.394280	
C	3.43805400	1.21160100	0.06471000
C	2.04551400	1.21116100	0.04691700
C	1.33413700	-0.00243600	-0.01516300
C	2.05467700	-1.21148400	-0.06064600
C	3.44714800	-1.20248500	-0.04482500
C	4.14353500	0.00684600	0.01866300
H	3.97465800	2.15539300	0.11322600
H	1.49420200	2.14594800	0.08021000
H	1.50971100	-2.14909600	-0.11048300
H	3.99093300	-2.14265700	-0.08195200
H	5.23008500	0.01041100	0.03147100

C	-0.09533100	-0.00874900	-0.03118700
C	-1.30712500	-0.02368800	-0.05031100
C	-2.77845300	-0.01634100	-0.02511900
C	-3.28538500	-0.74240400	1.23713200
H	-4.38330700	-0.74499700	1.25084200
H	-2.93271700	-1.77729700	1.23918700
H	-2.93456200	-0.24783300	2.14852000
C	-3.29711800	1.43422200	-0.07706900
H	-2.95653400	1.91908000	-0.99591400
H	-4.39486800	1.43903600	-0.06285600
H	-2.94294900	2.01429600	0.78125000
O	-3.20901700	-0.72847300	-1.19926100
H	-4.18043200	-0.73196700	-1.17803600

Ir Catalyst 5 :

Zero-point correction	=	0.327376 (Hartree/Particle)
Thermal correction to Energy	=	0.351454
Thermal correction to Enthalpy	=	0.352398
Thermal correction to Gibbs Free Energy	=	0.272659
Sum of electronic and zero-point Energies	=	-951.181150
Sum of electronic and thermal Energies	=	-951.157071
Sum of electronic and thermal Enthalpies	=	-951.156127
Sum of electronic and thermal Free Energies	=	-951.235867

C	1.98822700	-0.44833900	0.95094200
C	1.64129500	0.96694800	1.03993000
C	1.57243300	1.48347400	-0.31398100
C	1.80244800	0.39411700	-1.22333700
C	2.08351100	-0.80910800	-0.43567800
C	1.24406200	2.90305800	-0.66659800
H	0.27633700	3.18492700	-0.23907400
H	1.18500500	3.04466200	-1.74836000
H	2.01282000	3.58147100	-0.27677700
C	1.52765600	1.78026500	2.29515600
H	2.50254500	2.20032500	2.57953900
H	1.16715800	1.17414500	3.13119300
H	0.82804900	2.60967400	2.16079600
C	2.20560200	-1.35422000	2.12529200
H	1.52083000	-1.11121500	2.94241300
H	3.23263400	-1.25026200	2.49998000
H	2.04482500	-2.40188000	1.85972600
C	2.47051200	-2.14408500	-0.99986000
H	2.28790600	-2.94882000	-0.28277900
H	3.53767000	-2.16143400	-1.25983400

H	1.90026000	-2.37262900	-1.90486900
C	1.82790100	0.46592900	-2.72105900
H	1.43894900	-0.45437100	-3.16572000
H	2.85558400	0.60794100	-3.08198900
H	1.21921300	1.29441600	-3.09146000
Ir	0.06602500	-0.07859800	-0.00093400
C	-2.77050800	1.21410700	-0.01718500
O	-3.40888500	0.16936100	0.00216600
O	-1.46144800	1.34922100	-0.03219400
C	-1.70747900	-1.92113800	0.00385700
O	-1.20311600	-1.46506500	1.08677000
O	-1.20612000	-1.49386300	-1.08829600
C	-3.47378200	2.57193300	-0.02578800
H	-3.18398700	3.15252400	0.85722600
H	-3.17536200	3.14826900	-0.90839500
H	-4.55610900	2.42853900	-0.02955100
C	-2.83840500	-2.90108100	0.02206100
H	-3.76428700	-2.31752900	0.02495900
H	-2.81634500	-3.53052400	-0.87096500
H	-2.80186400	-3.51456600	0.92577100

int-6:

Zero-point correction	=	0.381308 (Hartree/Particle)
Thermal correction to Energy	=	0.408111
Thermal correction to Enthalpy	=	0.409056
Thermal correction to Gibbs Free Energy	=	0.322818
Sum of electronic and zero-point Energies	=	-1142.872841
Sum of electronic and thermal Energies	=	-1142.846038
Sum of electronic and thermal Enthalpies	=	-1142.845094
Sum of electronic and thermal Free Energies	=	-1142.931332

C	-2.91526500	-0.22722300	0.64334400
C	-1.97620700	-1.05746200	1.40148800
C	-1.29351300	-1.91877100	0.46646500
C	-1.73902200	-1.58655400	-0.86586200
C	-2.76492200	-0.54945700	-0.74364400
C	-0.30864500	-2.99525500	0.80972700
H	0.14090600	-2.82950900	1.79241400
H	0.49296400	-3.03734400	0.07022700
H	-0.82206500	-3.96621600	0.83579800
C	-1.85091200	-1.08492400	2.89588900
H	-2.58483900	-1.77582200	3.33316400
H	-2.02425400	-0.09465900	3.32651000
H	-0.85454100	-1.41095800	3.20476400
C	-3.86928200	0.76216300	1.24342000

H	-3.41331300	1.29267400	2.08405000
H	-4.76846100	0.25146700	1.61343900
H	-4.18406200	1.51030500	0.51154700
C	-3.52073300	0.04690000	-1.89305900
H	-3.97038500	1.00597600	-1.62421200
H	-4.32552000	-0.62854700	-2.21203100
H	-2.86206900	0.21651000	-2.74936600
C	-1.31861800	-2.27356900	-2.12979300
H	-1.55709200	-1.66506200	-3.00654900
H	-1.83926100	-3.23549100	-2.23569500
H	-0.24017400	-2.44283900	-2.12328000
Ir	-0.86340000	0.18911300	0.02723500
C	-0.28063100	2.65514400	-0.42266300
O	-0.57640500	2.25456400	0.75024500
O	-0.39732000	1.82013300	-1.37860700
C	0.22749400	4.04836000	-0.66592800
H	1.32130200	4.03917200	-0.59277100
H	-0.04453000	4.38568200	-1.66892100
H	-0.16232800	4.73562700	0.08855300
C	6.19758700	0.03578800	0.43122100
C	5.24980300	0.81787800	1.09640300
C	3.88995700	0.64058000	0.83965300
C	3.46762300	-0.32367700	-0.08577500
C	4.42265100	-1.10624600	-0.74818700
C	5.78110400	-0.92693400	-0.49238800
H	7.25695100	0.17582000	0.63182200
H	5.57114400	1.56671600	1.81607700
H	3.14507200	1.24111100	1.35054200
H	4.07591000	-1.84767100	-1.46034700
H	6.51581200	-1.53691500	-1.01197900
C	2.00787700	-0.55477100	-0.39011600
O	1.66754400	-1.43445900	-1.18646400
O	1.20325300	0.24431700	0.26332200

TS-1

Zero-point correction	=	0.375853 (Hartree/Particle)
Thermal correction to Energy	=	0.402006
Thermal correction to Enthalpy	=	0.402950
Thermal correction to Gibbs Free Energy	=	0.319781
Sum of electronic and zero-point Energies	=	-1142.828323
Sum of electronic and thermal Energies	=	-1142.802169
Sum of electronic and thermal Enthalpies	=	-1142.801225
Sum of electronic and thermal Free Energies	=	-1142.884395

C 2.33746200 -0.60972900 -0.81805700

C	1.27310300	-1.40626000	-1.35043300
C	0.62658900	-2.09668200	-0.23176700
C	1.33172100	-1.73024000	0.97117500
C	2.37509000	-0.78991900	0.62686400
C	-0.45728500	-3.12823100	-0.35076000
H	-1.14640100	-2.88982000	-1.16461000
H	-1.04701800	-3.19639600	0.56702200
H	-0.02643000	-4.11885700	-0.55004300
C	0.96005200	-1.61983200	-2.80250500
H	1.53159800	-2.47299900	-3.19339600
H	1.21584700	-0.74317100	-3.40413200
H	-0.10040500	-1.83229600	-2.95511800
C	3.28458900	0.25494600	-1.59504100
H	2.90276200	0.46963000	-2.59634300
H	4.25581600	-0.24568300	-1.70328500
H	3.45031000	1.20936000	-1.08737900
C	3.37880500	-0.19564500	1.57035100
H	3.72269400	0.78108900	1.21887100
H	4.25869500	-0.84658200	1.67051300
H	2.94767000	-0.05575800	2.56549000
C	1.03289500	-2.20176500	2.36267000
H	1.80515100	-2.90790600	2.69429500
H	0.06580000	-2.70630300	2.41892900
H	1.00783500	-1.36184000	3.06281100
Ir	0.42498900	0.06759700	0.07371000
C	-3.52325000	-0.71638000	-1.91528400
C	-2.24834700	-0.15455200	-1.84321900
C	-1.69479400	0.22984400	-0.60325800
C	-2.48034200	0.03826800	0.55814600
C	-3.75970000	-0.50907400	0.48990000
C	-4.27768300	-0.89568600	-0.74840100
H	-3.94114100	-0.99834800	-2.87876800
H	-1.69015800	0.03183100	-2.75817300
H	-4.32533700	-0.62946900	1.40940100
H	-5.27320900	-1.32821900	-0.80967100
C	-1.86573300	0.41932900	1.88133400
O	-2.52454900	0.49325100	2.90864400
O	-0.56559400	0.65532900	1.81903600
C	0.13444700	3.02487200	-0.42035700
O	0.95649900	2.13415600	-0.02158000
O	-1.02866200	2.77540200	-0.84348500
H	-1.20465500	1.43076200	-0.71781000
C	0.58908900	4.46590600	-0.35105100
H	0.13258900	5.04570500	-1.15640200
H	0.25405800	4.88689500	0.60410300
H	1.67800300	4.53330800	-0.39471300

int-7:

Zero-point correction	=	0.381032 (Hartree/Particle)
Thermal correction to Energy	=	0.407808
Thermal correction to Enthalpy	=	0.408752
Thermal correction to Gibbs Free Energy	=	0.323765
Sum of electronic and zero-point Energies	=	-1142.847241
Sum of electronic and thermal Energies	=	-1142.820466
Sum of electronic and thermal Enthalpies	=	-1142.819522
Sum of electronic and thermal Free Energies	=	-1142.904509

C 2.18665000 -0.19250900 -1.24867900
C 1.59049800 -1.46820400 -0.98545800
C 1.59417500 -1.66521600 0.45995800
C 2.36210300 -0.55742300 1.05245000
C 2.70405700 0.34002400 0.02091600
C 1.18357600 -2.91103000 1.19079400
H 0.36347300 -3.42009200 0.67725500
H 0.84548900 -2.67735200 2.20431300
H 2.02415100 -3.61496700 1.26801400
C 1.13124300 -2.47302200 -1.99965500
H 1.92772300 -3.20723700 -2.18278300
H 0.88822700 -2.00167000 -2.95583400
H 0.24492100 -3.01426400 -1.65953100
C 2.44469000 0.41914400 -2.59567200
H 1.72809100 0.06258100 -3.34075000
H 3.45343800 0.16943000 -2.95382600
H 2.36801000 1.50989600 -2.55669100
C 3.42831800 1.64826500 0.14496600
H 2.87171800 2.45412400 -0.34579200
H 4.41823500 1.59242400 -0.32695100
H 3.56992500 1.93283000 1.19047300
C 2.61360500 -0.41465900 2.52434700
H 3.12904300 0.52036000 2.75767000
H 3.23121500 -1.24294600 2.89393500
H 1.66756300 -0.42079200 3.07720400
Ir 0.39286400 0.04460000 0.04533700
C -3.26386500 -1.46814400 -1.92990900
C -1.95786900 -0.99102300 -1.77182500
C -1.48416800 -0.59314700 -0.50754200
C -2.38766400 -0.66833500 0.57720800
C -3.69258800 -1.14670800 0.42349800
C -4.13165900 -1.55594800 -0.83454500
H -3.60828900 -1.77039800 -2.91675500
H -1.30827200 -0.92787100 -2.64201300
H -4.33680300 -1.18232000 1.29805400
H -5.14343300 -1.92930800 -0.96906700

C	-1.88195400	-0.15851600	1.89714100
O	-2.54269700	-0.18203000	2.92551000
O	-0.65924900	0.35284800	1.81952200
C	-1.09763000	2.87082200	-0.39126200
O	-0.04672900	2.22280600	-0.32970500
O	-2.29979000	2.33516200	-0.47775400
H	-2.22883300	1.34848400	-0.44826500
C	-1.10857800	4.37363600	-0.36524700
H	-1.80529100	4.76343100	-1.11236100
H	-1.45758600	4.70402400	0.62002200
H	-0.10317800	4.75907700	-0.53678900

int-8a

Zero-point correction	=	0.518779 (Hartree/Particle)
Thermal correction to Energy	=	0.552918
Thermal correction to Enthalpy	=	0.553862
Thermal correction to Gibbs Free Energy	=	0.451184
Sum of electronic and zero-point Energies	=	-1415.175683
Sum of electronic and thermal Energies	=	-1415.141544
Sum of electronic and thermal Enthalpies	=	-1415.140600
Sum of electronic and thermal Free Energies	=	-1415.243279

C	-0.11685300	-2.26788400	-0.56780800
C	-0.76628900	-1.68918100	-1.70341600
C	-2.18745100	-1.59286100	-1.38851600
C	-2.40531100	-2.29625000	-0.11181000
C	-1.15085100	-2.68835000	0.39099800
C	-3.27476700	-1.15851400	-2.32819800
H	-2.92502900	-0.37012400	-3.00013400
H	-4.13689200	-0.76821400	-1.77985900
H	-3.61945400	-2.00188000	-2.94339300
C	-0.14121600	-1.34124000	-3.02122200
H	-0.28448000	-2.16859500	-3.72992200
H	0.93427700	-1.16874800	-2.92671800
H	-0.58772600	-0.44365500	-3.45628900
C	1.34034000	-2.60554800	-0.44156900
H	1.95756700	-1.97463800	-1.08562800
H	1.51930200	-3.65334600	-0.72210100
H	1.69312400	-2.46732200	0.58401800
C	-0.85681700	-3.38685500	1.68582400
H	-0.06301700	-2.87448600	2.23938300
H	-0.52258100	-4.41738300	1.50519800
H	-1.73752400	-3.43012000	2.33171900
C	-3.75037900	-2.45950600	0.53056800
H	-3.66801000	-2.83596900	1.55336000
H	-4.36888500	-3.16394600	-0.04082900
H	-4.27902100	-1.50158100	0.57191000
Ir	-1.14434900	-0.38165900	0.00833400
C	0.36514500	3.10979900	-2.22461200
C	0.28094600	1.80643600	-1.72019100

C	-0.74346800	1.44531100	-0.83046200
C	-1.65876100	2.44984500	-0.45295300
C	-1.58159100	3.75176000	-0.95496300
C	-0.56803000	4.08424800	-1.85275800
H	1.16760700	3.36733600	-2.91349700
H	1.03024100	1.07692400	-2.01710900
H	-2.31566300	4.48119300	-0.62254800
H	-0.49648300	5.09189700	-2.25398100
C	-2.66795100	2.07659100	0.58463900
O	-3.50674800	2.84090300	1.03540200
O	-2.52652400	0.81813000	1.02375300
C	5.69209600	0.52764300	-1.63598400
C	4.54739100	0.79905800	-0.89006300
C	4.28537700	0.08337800	0.29531500
C	5.19763000	-0.90550500	0.71185900
C	6.34017600	-1.17008100	-0.03984600
C	6.59109700	-0.45577200	-1.21430300
H	5.88502700	1.08696700	-2.54739700
H	3.84633900	1.56468200	-1.20828800
H	5.00046900	-1.45630800	1.62661700
H	7.03773600	-1.93414000	0.29231600
H	7.48407800	-0.66321900	-1.79749900
C	3.11318900	0.36740500	1.06221500
C	2.10648000	0.62484000	1.68757000
C	0.95666600	1.01915300	2.50718300
C	1.19361400	0.63905900	3.98001300
H	0.31780800	0.91147100	4.57958300
H	1.36213500	-0.43732100	4.07224400
H	2.06583600	1.16804000	4.37736500
C	0.67751200	2.52418800	2.35883500
H	0.49098800	2.78428500	1.31573400
H	-0.19861600	2.80429100	2.95675900
H	1.53492500	3.09950000	2.72174600
O	-0.20224500	0.24342800	2.05177900
H	-1.03264800	0.71545500	2.28996800

int-8b

Zero-point correction	=	0.519532 (Hartree/Particle)
Thermal correction to Energy	=	0.553094
Thermal correction to Enthalpy	=	0.554039
Thermal correction to Gibbs Free Energy	=	0.455406
Sum of electronic and zero-point Energies	=	-1415.191492
Sum of electronic and thermal Energies	=	-1415.157930
Sum of electronic and thermal Enthalpies	=	-1415.156986
Sum of electronic and thermal Free Energies	=	-1415.255618

C	-0.84270500	-1.28506700	-2.08062200
C	-0.95131200	0.10338300	-2.44925200
C	-2.09313200	0.65360800	-1.74910000

C	-2.73023300	-0.44385400	-1.02858900
C	-1.97643300	-1.62798200	-1.23860200
C	-2.67247600	2.02918600	-1.91872400
H	-1.89605300	2.76321700	-2.14974700
H	-3.17693400	2.35845300	-1.00564900
H	-3.40911300	2.04714100	-2.73390600
C	-0.14726700	0.80114300	-3.50613700
H	-0.63907500	0.68824300	-4.48234600
H	0.85929000	0.38249100	-3.59376300
H	-0.05105400	1.87002200	-3.30224700
C	0.14888800	-2.26178700	-2.64085100
H	1.10575400	-1.78268900	-2.86332500
H	-0.23251200	-2.70439600	-3.57127500
H	0.34097400	-3.08001300	-1.94185500
C	-2.31400900	-2.99390300	-0.71411400
H	-1.43775900	-3.64793400	-0.71417100
H	-3.07885000	-3.47143300	-1.34145200
H	-2.68732300	-2.94159800	0.31167100
C	-3.97403400	-0.30579000	-0.20370900
H	-4.16261300	-1.20277600	0.39016100
H	-4.84392900	-0.13252700	-0.85074900
H	-3.89073100	0.54141400	0.48449100
Ir	-0.61008600	0.03679100	-0.23291000
C	2.12520100	3.47473100	-0.65375000
C	1.50972300	2.24176700	-0.90141800
C	0.49997200	1.76496700	-0.05329700
C	0.15207000	2.55553900	1.05745800
C	0.77431700	3.78023100	1.31764100
C	1.76249900	4.24835300	0.45417300
H	2.90362800	3.82663600	-1.32776800

H	1.84230800	1.65129800	-1.75016600
H	0.46452900	4.34128400	2.19541300
H	2.25046900	5.20141600	0.64011800
C	-0.91123800	2.02261900	1.95042400
O	-1.29684600	2.55346700	2.98028600
O	-1.42413100	0.86910000	1.50832500
C	4.86849000	-0.03620200	0.04892700
C	3.53049600	0.03485900	0.43352200
C	2.65314200	-1.03000000	0.15045000
C	3.15656800	-2.16410200	-0.51852800
C	4.49582800	-2.22716100	-0.89786500
C	5.35561500	-1.16175900	-0.61960300
H	5.53403200	0.79172100	0.27756100
H	3.15671800	0.90637900	0.95749900
H	2.49167100	-2.99700000	-0.72394400
H	4.86900400	-3.11140300	-1.40773800
H	6.39978500	-1.21170100	-0.91609700
C	1.27251400	-1.00158200	0.57682800
C	0.25969000	-1.27907300	1.26874000
C	-0.39509100	-1.85329200	2.50500100
C	-0.15554900	-3.36993100	2.55082600
H	-0.64346000	-3.77931400	3.44161300
H	-0.58106000	-3.85692100	1.66906900
H	0.91452800	-3.59524100	2.59775900
C	0.20898200	-1.17303600	3.75182800
H	-0.00187100	-0.10000500	3.74550100
H	-0.24583700	-1.60987600	4.64766300
H	1.29410300	-1.31725600	3.79737000
O	-1.80363500	-1.66469600	2.47923800
H	-1.93817300	-0.69869500	2.36169800

int-8b'

Zero-point correction	=	0.519650 (Hartree/Particle)
Thermal correction to Energy	=	0.553140
Thermal correction to Enthalpy	=	0.554084
Thermal correction to Gibbs Free Energy	=	0.456091
Sum of electronic and zero-point Energies	=	-1415.185208
Sum of electronic and thermal Energies	=	-1415.151718
Sum of electronic and thermal Enthalpies	=	-1415.150774
Sum of electronic and thermal Free Energies	=	-1415.248767
C	-0.35129200	1.82604600
C	1.04227600	2.01753000
C	1.13113000	2.52637500
C	-0.21928400	2.71247700
C	-1.13269500	2.29109500
C	2.37671200	2.98705700
H	3.24009000	2.37683800
H	2.26399400	2.92116900
H	2.60326200	4.03216200
C	2.16236100	1.93636100
H	2.16058000	2.83265000
H	2.06368700	1.06475600
H	3.13643700	1.88762700
C	-0.90514900	1.38511100
H	-0.20770200	0.72358600
H	-1.09696800	2.25397500
H	-1.84933800	0.84663700
C	-2.62937900	2.38989500
H	-3.10713900	1.67832200
H	-2.95793000	3.39722800
H	-3.01101700	2.18533700
C	-0.57112800	3.22424700
H	-1.65259100	3.31552900
H	-0.12476700	4.21119000
H	-0.20196400	2.54115600
Ir	0.25586800	0.47387600
C	4.29518800	-1.37476300
C	3.16280900	-0.68921800
C	2.04017100	-0.51320300

C	2.11084400	-1.02849200	1.69335900
C	3.23400100	-1.71719200	2.15850100
C	4.33255200	-1.90031300	1.31974200
H	5.15135600	-1.49631800	-0.63477500
H	3.18133700	-0.27794700	-1.44290700
H	3.22001600	-2.09200200	3.17865000
H	5.21081700	-2.43632400	1.66901200
C	0.93880400	-0.76886900	2.57729600
O	0.85183600	-1.14187900	3.73810000
O	-0.01113700	-0.05598300	1.97902100
C	-5.13589100	-1.26523500	-0.12115100
C	-3.82177900	-1.26459300	-0.58579400
C	-2.75619300	-0.96318600	0.28746000
C	-3.03879000	-0.65493300	1.63257200
C	-4.35776000	-0.65448300	2.08358700
C	-5.40913300	-0.95841500	1.21402200
H	-5.94698700	-1.50406500	-0.80411500
H	-3.60868000	-1.50045300	-1.62458000
H	-2.21254600	-0.42944500	2.29808100
H	-4.56402600	-0.42226400	3.12504000
H	-6.43426100	-0.95888700	1.57455600
C	-1.40422200	-0.99046900	-0.22384500
C	-0.41844100	-1.41126500	-0.89191000
C	0.17042000	-2.52245800	-1.72540100
C	0.64950400	-3.66710500	-0.81148000
H	1.06552500	-4.46908300	-1.43167400
H	1.42242500	-3.31903600	-0.11997700
H	-0.17831700	-4.06886200	-0.21834800
C	-0.90181400	-3.02561000	-2.70411600
H	-1.21758400	-2.21799100	-3.37156800
H	-0.48297600	-3.83404500	-3.31222800
H	-1.77500500	-3.40293500	-2.16331800
O	1.24349200	-2.05910400	-2.54343200
H	1.97196900	-1.82955100	-1.94094700

TS-2

Zero-point correction	=	0.518470 (Hartree/Particle)
Thermal correction to Energy	=	0.551236
Thermal correction to Enthalpy	=	0.552180
Thermal correction to Gibbs Free Energy	=	0.455777
Sum of electronic and zero-point Energies	=	-1415.153325
Sum of electronic and thermal Energies	=	-1415.120559
Sum of electronic and thermal Enthalpies	=	-1415.119615
Sum of electronic and thermal Free Energies	=	-1415.216018

C 1.70638800 -0.09271000 -2.13712100
C 2.26196000 -1.18746100 -1.37295700
C 2.97589100 -0.63029100 -0.26084400
C 2.94267700 0.83252400 -0.40002500
C 2.20382200 1.15299200 -1.56802800
C 3.77855200 -1.38448300 0.75895700
H 3.32447500 -2.35162400 0.98629900
H 3.84389800 -0.82630900 1.69704200
H 4.80317300 -1.55436400 0.39903400
C 2.18228200 -2.64074600 -1.73478100
H 2.98514300 -2.89807800 -2.43983600
H 1.23120400 -2.88930300 -2.21486800
H 2.29594800 -3.27663000 -0.85400200
C 0.97526800 -0.21541900 -3.44404800
H 0.36653500 -1.12338500 -3.48149800
H 1.68315600 -0.25452800 -4.28409700
H 0.31268400 0.63827500 -3.61321200
C 1.95980500 2.51760300 -2.14062200
H 0.91337800 2.65568100 -2.43046000
H 2.57717400 2.67461000 -3.03542900
H 2.20649300 3.30491500 -1.42375900
C 3.62208100 1.78418100 0.54012100
H 4.70879700 1.77617200 0.38284100
H 3.42887300 1.50811300 1.58118400
H 3.26804600 2.80858600 0.39913800
Ir 0.86067600 0.01143400 -0.06897100
C -1.94850700 3.92414200 0.48136100
C -1.37983300 3.23731400 1.55657100
C -0.81289400 1.97822800 1.36238500
C -0.84956800 1.34767300 0.09391400
C -1.42432400 2.06114700 -0.98053700
C -1.95156900 3.33716600 -0.79030100
H -2.37895700 4.91098700 0.62807500
H -1.33601700 3.66956200 2.55240800
H -1.49083300 1.59234200 -1.95920400
H -2.38478300 3.86990700 -1.63351200
C -0.05886800 1.30083800 2.46917700
C -4.39951100 -1.72570700 -1.82853600
C -3.09849700 -1.56176800 -1.35132400
C -2.79713700 -0.54626500 -0.42642300
C -3.82962100 0.30441900 0.00692800
C -5.12906500 0.13101000 -0.46351300

C	-5.41776700	-0.88046800	-1.38500300
H	-4.61595800	-2.51342400	-2.54528300
H	-2.30269500	-2.21809900	-1.69093900
H	-3.60776400	1.08841800	0.72358200
H	-5.92053000	0.78555600	-0.10870000
H	-6.43192500	-1.00808200	-1.75393400
C	-1.43798700	-0.45869000	0.13211200
C	-0.56446400	-1.30244700	0.60668800
C	-0.46637800	-2.52639300	1.48375700
C	-0.55674700	-3.82989100	0.67814100
H	-0.40187500	-4.67815700	1.35378000
H	-1.54127700	-3.92909100	0.21024500
H	0.21043300	-3.86545700	-0.09876900
C	-1.58589100	-2.47407500	2.54445900
H	-1.50634700	-3.35150800	3.19514000
H	-1.48602100	-1.57485200	3.15982700
H	-2.57695700	-2.466666300	2.07698600
O	0.80723600	-2.53683000	2.13309900
H	0.96733900	-1.61627200	2.42638900
O	0.79722000	0.38761000	2.03406300
O	-0.20663200	1.58893400	3.64824400

TS-2'

Zero-point correction	=	0.518026 (Hartree/Particle)
Thermal correction to Energy	=	0.550999
Thermal correction to Enthalpy	=	0.551943
Thermal correction to Gibbs Free Energy	=	0.455541
Sum of electronic and zero-point Energies	=	-1415.142138
Sum of electronic and thermal Energies	=	-1415.109165
Sum of electronic and thermal Enthalpies	=	-1415.108221
Sum of electronic and thermal Free Energies	=	-1415.204623

C	0.48313300	-2.07606900	-1.70233300
C	-0.86068000	-2.25679800	-1.20250300
C	-0.77288300	-2.66349800	0.17257300
C	0.64945900	-2.81228200	0.49659100
C	1.41201300	-2.48805000	-0.65929700
C	-1.91010300	-3.03358200	1.07979000
H	-2.82200800	-2.48904900	0.81934200
H	-1.67245000	-2.79751000	2.12081800
H	-2.12911300	-4.10913700	1.01935600
C	-2.12476300	-2.12071600	-1.99888100
H	-2.41790100	-3.09488400	-2.41370700
H	-2.00088600	-1.42992500	-2.83805800
H	-2.95269400	-1.75547200	-1.38553100
C	0.86451400	-1.77225200	-3.12350000

H	0.11970500	-1.14022100	-3.61618100
H	0.95109600	-2.69802400	-3.70978100
H	1.82847300	-1.25835100	-3.17779100
C	2.90297900	-2.55080200	-0.81068000
H	3.30096000	-1.63948600	-1.26902700
H	3.19279900	-3.39928600	-1.44500900
H	3.39842700	-2.67232000	0.15580800
C	1.15956800	-3.25589400	1.83584000
H	0.92246600	-4.31379600	2.00882100
H	0.70099000	-2.66638700	2.63593100
H	2.24285600	-3.13559100	1.91547700
Ir	0.16741300	-0.66528100	0.01434000
C	4.24531300	1.85603900	0.68158100
C	3.28850200	1.68544700	1.68564300
C	2.02746400	1.18658800	1.36671900
C	1.67566100	0.88598300	0.03057100
C	2.65087500	1.06399600	-0.97194700
C	3.92612200	1.52926200	-0.64138100
H	5.23500700	2.23221000	0.92676900
H	3.50631200	1.90115400	2.72802300
H	2.40480100	0.87020800	-2.00942100
H	4.66937000	1.65325600	-1.42549100
C	1.04714800	0.82105000	2.44275000
C	-4.35963400	0.99674000	1.79004000
C	-2.99636600	0.96103800	1.50018900
C	-2.55583100	0.99205300	0.16281500
C	-3.51278700	1.03062200	-0.86692300
C	-4.87606500	1.05454300	-0.56773600
C	-5.30439900	1.04294600	0.76083300
H	-4.68493100	0.98311500	2.82695200
H	-2.25631100	0.89864000	2.29171000
H	-3.18624200	1.04263400	-1.90302300
H	-5.60235800	1.08746900	-1.37583700
H	-6.36576800	1.06730500	0.99251200
C	-1.12066000	0.94877300	-0.11026000
C	-0.09620700	1.65611700	-0.46377500
C	0.15609600	2.99171900	-1.17385100
C	1.10514500	3.93012400	-0.42492900
H	1.16793100	4.87530600	-0.97431500

H	0.72376600	4.13161400	0.58034600
H	2.10877500	3.51565300	-0.34428900
C	-1.20900100	3.68855400	-1.34472500
H	-1.04746500	4.64312300	-1.85535600
H	-1.89383400	3.08500800	-1.94841800
H	-1.69025400	3.87947600	-0.38118700
O	0.73573200	2.77631800	-2.46649500
H	0.08836600	2.27183400	-2.98612300
O	0.12812700	-0.03764300	2.04005600
O	1.12384400	1.25359800	3.58559200

int-9:

Zero-point correction	=	0.521093 (Hartree/Particle)
Thermal correction to Energy	=	0.553798
Thermal correction to Enthalpy	=	0.554742
Thermal correction to Gibbs Free Energy	=	0.458575
Sum of electronic and zero-point Energies	=	-1415.200463
Sum of electronic and thermal Energies	=	-1415.167759
Sum of electronic and thermal Enthalpies	=	-1415.166815
Sum of electronic and thermal Free Energies	=	-1415.262981

C	-1.90716400	-0.14256500	1.82265000
C	-2.67641300	-1.16871700	1.18017600
C	-3.50422600	-0.53515500	0.14233300
C	-3.20386100	0.83616100	0.11141400
C	-2.15363400	1.09840900	1.10556300
C	-4.47302900	-1.28493900	-0.72418700
H	-4.03122900	-2.21417800	-1.09916200
H	-4.78731200	-0.69332800	-1.58777900
H	-5.37388000	-1.55457600	-0.15642600
C	-2.83840900	-2.59237300	1.62925000
H	-3.77369700	-2.71170700	2.19405400
H	-2.01964900	-2.90499500	2.28264100
H	-2.87567000	-3.28275400	0.78071300
C	-1.05652500	-0.28686200	3.04983000
H	-0.67185300	-1.30508500	3.15389600
H	-1.64168700	-0.05214600	3.94957600
H	-0.19948400	0.39068900	3.01764300
C	-1.71266600	2.46534900	1.53652900
H	-0.72425000	2.44513200	2.00052500
H	-2.42495100	2.87984500	2.26473100
H	-1.66000700	3.15288300	0.68959400
C	-3.76725800	1.88002200	-0.80618400

H	-2.96803000	2.46203200	-1.27616900
H	-4.40793000	2.57870500	-0.25210300
H	-4.36655800	1.43689400	-1.60561700
Ir	-1.20351800	-0.31212800	-0.23175300
C	1.46599600	4.26401800	0.51760800
C	0.95063800	3.59092100	-0.58900200
C	0.99292700	2.19157300	-0.67305100
C	1.62297400	1.45370100	0.35675500
C	2.17363900	2.15166700	1.44489200
C	2.07842700	3.53935200	1.54291600
H	1.41133900	5.34836000	0.56827700
H	0.52380700	4.14666200	-1.41889600
H	2.69625200	1.58941100	2.21474500
H	2.50055100	4.05326400	2.40281700
C	0.47508100	1.58007800	-1.96847900
C	4.93612400	-1.97275900	1.23705300
C	3.61173900	-1.53467900	1.16048800
C	3.24393300	-0.48610500	0.30046600
C	4.25402500	0.13484900	-0.45772700
C	5.57453900	-0.30427700	-0.38514900
C	5.92180700	-1.36242500	0.46042500
H	5.19766700	-2.78380100	1.91226100
H	2.85222500	-1.99300500	1.78791300
H	3.99139800	0.95696600	-1.11787700
H	6.33598400	0.18042400	-0.99084800
H	6.95303200	-1.70031900	0.51935700
C	1.82566800	-0.02079100	0.21109200
C	0.77644000	-0.82168700	-0.07517800
C	0.77944500	-2.16462500	-0.80043300
C	0.58888300	-3.39404800	0.08269800
H	0.36368600	-4.27268000	-0.53215800
H	1.50844900	-3.58752200	0.64259400
H	-0.22710300	-3.24236200	0.79237700
C	1.87241800	-2.39285000	-1.84438200
H	1.60557000	-3.25239200	-2.47066300
H	2.00056600	-1.51213900	-2.48227300
H	2.83081500	-2.60074600	-1.36399400
O	-0.52764000	-2.01675300	-1.55175700
H	-0.33972400	-1.444801400	-2.33047500
O	-0.47815200	0.66520400	-1.92583700
O	0.91622300	2.00115500	-3.02921000

int-10a:

Zero-point correction	=	0.521948 (Hartree/Particle)
Thermal correction to Energy	=	0.554039

Thermal correction to Enthalpy	=	0.554984
Thermal correction to Gibbs Free Energy	=	0.462211
Sum of electronic and zero-point Energies	=	-1415.196513
Sum of electronic and thermal Energies	=	-1415.164422
Sum of electronic and thermal Enthalpies	=	-1415.163477
Sum of electronic and thermal Free Energies	=	-1415.256250

C 2.84719800 -0.11671800 -0.68969800
C 2.16643300 0.45617200 -1.83480400
C 1.26882600 -0.52538400 -2.34557600
C 1.36534700 -1.70302900 -1.50551000
C 2.37806600 -1.45913700 -0.49587800
C 0.44690200 -0.41282100 -3.59711200
H 0.18304900 0.62642100 -3.81649200
H -0.48144100 -0.98752000 -3.52656800
H 1.00343700 -0.79767800 -4.46357600
C 2.42150500 1.82165800 -2.40571600
H 3.27888300 1.81154100 -3.09352300
H 2.63715700 2.55158500 -1.61973700
H 1.55499500 2.18945300 -2.96369300
C 3.95902100 0.54823900 0.06836900
H 3.76817600 1.61577900 0.21205500
H 4.90524000 0.44977300 -0.48131700
H 4.09829200 0.09712300 1.05451200
C 2.92155100 -2.48344700 0.45889700
H 3.35752100 -2.01330600 1.34502100
H 3.70644800 -3.08726400 -0.01994300
H 2.12880400 -3.15315700 0.79955400
C 0.78766600 -3.05551100 -1.81136900
H 0.47050000 -3.56261400 -0.89767300
H 1.54440700 -3.67827400 -2.30977300
H -0.07292900 -2.98944600 -2.48306200
Ir 0.65539400 -0.08317500 -0.12195500
C -0.65921100 2.89040800 0.13805600
C -0.51506500 1.58719900 0.73903900
C 0.61302500 1.33703100 1.63738500
C 1.58150500 2.39847100 1.80120500
C 1.44208300 3.59292400 1.15690600
C 0.29354700 3.84806100 0.33580600
H -1.53911600 3.09123800 -0.46476300
H 2.38384400 2.23383100 2.51308000
H 2.17204300 4.38381000 1.30789400
H 0.17486200 4.82831500 -0.11877600
C 0.41538600 0.43236500 2.80773200
O 0.98473500 0.53957600 3.87283900

O	-0.51583200	-0.52240000	2.60140500
C	-1.36041200	0.43751200	0.47696500
C	-0.86718400	-0.74199100	1.21074800
C	-2.64460000	0.61121200	-0.26641500
C	-2.70335000	0.71489400	-1.66242700
C	-3.83760300	0.73942000	0.46553200
C	-3.92170200	0.91846300	-2.31370100
H	-1.78372400	0.62438100	-2.23085200
C	-5.05618000	0.93917300	-0.18402100
H	-3.80436500	0.68791000	1.55070300
C	-5.10293300	1.02600800	-1.57754600
H	-3.94728100	0.99055600	-3.39810900
H	-5.96840500	1.03220800	0.39951500
H	-6.05180300	1.18042100	-2.08412000
C	-1.52244100	-2.13342500	1.16380000
C	-2.22861400	-2.45724600	-0.16167100
H	-3.19590400	-1.95740800	-0.24591400
H	-1.61600900	-2.17834600	-1.01908100
H	-2.40316900	-3.53909800	-0.20107200
C	-2.52013300	-2.32504300	2.32442500
H	-3.34118500	-1.60394500	2.26279300
H	-2.96314700	-3.32883400	2.26516800
H	-2.02409100	-2.20874300	3.28907200
O	-0.42540800	-3.05988800	1.34053300
H	-0.80017700	-3.87532200	1.71045400

int-10b:

Zero-point correction	=	0.574315 (Hartree/Particle)
Thermal correction to Energy	=	0.612058
Thermal correction to Enthalpy	=	0.613002
Thermal correction to Gibbs Free Energy	=	0.505727
Sum of electronic and zero-point Energies	=	-1643.618608
Sum of electronic and thermal Energies	=	-1643.580865
Sum of electronic and thermal Enthalpies	=	-1643.579921
Sum of electronic and thermal Free Energies	=	-1643.687195

Ir	-0.84600500	-0.32485500	-0.03620900
O	1.01145900	-0.53530200	2.21303800
O	2.26914100	-2.24422000	2.84300200
C	2.03014700	-1.42574400	1.98413400
C	2.75654000	-1.27747500	0.71248400
C	2.32923100	-0.34951500	-0.25800000
C	3.86012300	-2.11013100	0.48597500
C	3.02095800	-0.32051800	-1.48202200

C	4.54092700	-2.05301400	-0.72438600
C	4.10523800	-1.16191800	-1.71228100
C	1.22494500	0.61311600	0.04719600
C	0.62793700	0.52778800	1.35685600
C	0.26849200	1.67054000	2.34828100
H	4.15082300	-2.79964200	1.27176700
H	2.70797800	0.37035100	-2.25609800
H	5.39504500	-2.69939500	-0.90473700
H	4.61841100	-1.11838800	-2.66916300
C	-2.76579400	-1.24548500	-0.69193500
C	-3.01582900	-0.65533200	0.60358300
C	-2.89286700	0.76735500	0.46449000
C	-2.55880000	1.06169100	-0.90321500
C	-2.51550900	-0.18036100	-1.63477200
C	-2.95736700	-2.69602200	-1.03020900
C	-3.43959200	-1.37731800	1.84711600
C	-3.34403000	1.75177400	1.50454900
C	-2.58202400	2.43621500	-1.51058400
C	-2.31898200	-0.36070000	-3.10996400
H	-4.01948300	-2.89682400	-1.22680000
H	-2.38141700	-2.97810000	-1.91245500
H	-2.64569800	-3.34074000	-0.20334700
H	-3.02054200	-2.38668400	1.88741500
H	-3.11446500	-0.83984300	2.74227200
H	-4.53480800	-1.47028000	1.89023900
H	-2.81493500	1.61386100	2.44932800
H	-3.20100200	2.78418700	1.17834700
H	-4.41932200	1.61076800	1.68255000
H	-3.61842600	2.79762400	-1.56467100
H	-2.00937000	3.16449600	-0.93089400
H	-2.18387200	2.43832300	-2.52729200
H	-1.90445700	0.53860500	-3.57490800
H	-1.63174200	-1.18810300	-3.30340200
H	-3.27734900	-0.57489400	-3.60452800
O	0.03891900	-2.44066200	-2.19825600
C	0.31400000	-2.83788400	-1.06656300
C	0.93681300	-4.20447800	-0.82042700
O	0.12896500	-2.15364600	0.04012900
H	0.83393000	-4.82462600	-1.71329700
H	0.47458600	-4.69580200	0.04075700
H	2.00142400	-4.08018200	-0.59456200
C	1.42333700	1.92713200	-0.68365500
C	2.45630600	2.78895700	-0.27317400
C	0.72607100	2.25144100	-1.85145000
C	2.73617800	3.96349800	-0.97020000

H	3.05754500	2.52843600	0.59285200
C	1.00853000	3.42333800	-2.55971300
H	-0.03011300	1.56260000	-2.20820600
C	2.00588000	4.29058800	-2.11574000
H	3.53202300	4.61767500	-0.62380800
H	0.45137800	3.65148200	-3.46494300
H	2.22441000	5.20337500	-2.66327500
O	-0.75501500	1.17608900	3.22768600
H	-0.45035000	0.30284500	3.52974300
C	1.50254500	2.01522100	3.21559000
H	1.84765100	1.14367300	3.77753100
H	2.33428800	2.39226500	2.61251900
H	1.21656600	2.79400400	3.92993200
C	-0.27549500	2.95555100	1.72542600
H	-0.81756000	3.50095000	2.50433500
H	0.53079700	3.59031400	1.35607300
H	-0.95478300	2.75360700	0.89972600

Ir-acetate complex

Zero-point correction	=	0.273927 (Hartree/Particle)
Thermal correction to Energy	=	0.292385
Thermal correction to Enthalpy	=	0.293329
Thermal correction to Gibbs Free Energy	=	0.226144
Sum of electronic and zero-point Energies	=	-722.718662
Sum of electronic and thermal Energies	=	-722.700204
Sum of electronic and thermal Enthalpies	=	-722.699259
Sum of electronic and thermal Free Energies	=	-722.766445

Ir	-0.33210300	-0.00107300	-0.01234200
C	1.58684800	-0.08273400	1.23672100
C	1.49715200	1.13065700	0.46650100
C	1.51753200	0.78844900	-0.94877400
C	1.53417700	-0.64375600	-1.05156100
C	1.49813500	-1.17796100	0.30021800
C	1.71952000	-0.19053300	2.72593100
H	2.77775000	-0.22844100	3.02582100
H	1.23860100	-1.09565900	3.10909400
H	1.26552700	0.66551200	3.23423000
C	1.54213700	2.52602700	1.01994000

H	1.06776500	2.58047800	2.00427100
H	1.02368500	3.23165200	0.36449900
H	2.57999500	2.87119100	1.12733200
C	1.59510000	1.76635200	-2.08434700
H	1.05191400	2.68781900	-1.85499800
H	1.16609800	1.35061900	-3.00092500
H	2.63862200	2.04049700	-2.29756600
C	1.63654300	-1.44953300	-2.31278700
H	2.68651000	-1.67742700	-2.54881300
H	1.21376200	-0.91315300	-3.16744100
H	1.10542300	-2.40190800	-2.22515900
C	1.54297800	-2.63609700	0.65715600
H	1.03275800	-3.24574200	-0.09407300
H	1.05769600	-2.82471400	1.61939100
H	2.58053300	-2.99124100	0.72846300
O	-2.20179400	-1.09351100	0.03281900
C	-2.87009200	-0.00428000	0.04067600
C	-4.37129500	-0.00738000	0.01427600
H	-4.75752700	-0.89576900	0.51956200
H	-4.76161100	0.89973200	0.48126500
H	-4.71251600	-0.03186700	-1.02797100
O	-2.20514300	1.08673000	0.03838500

3aa:

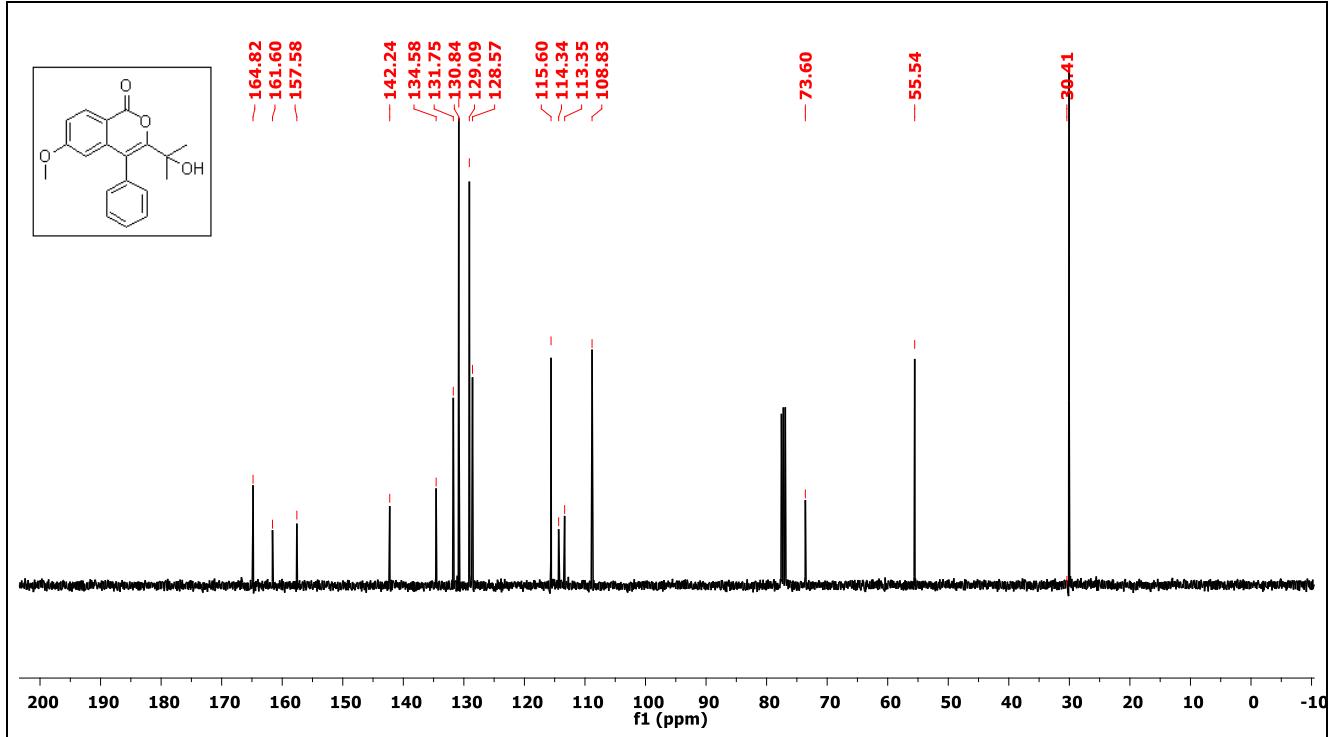
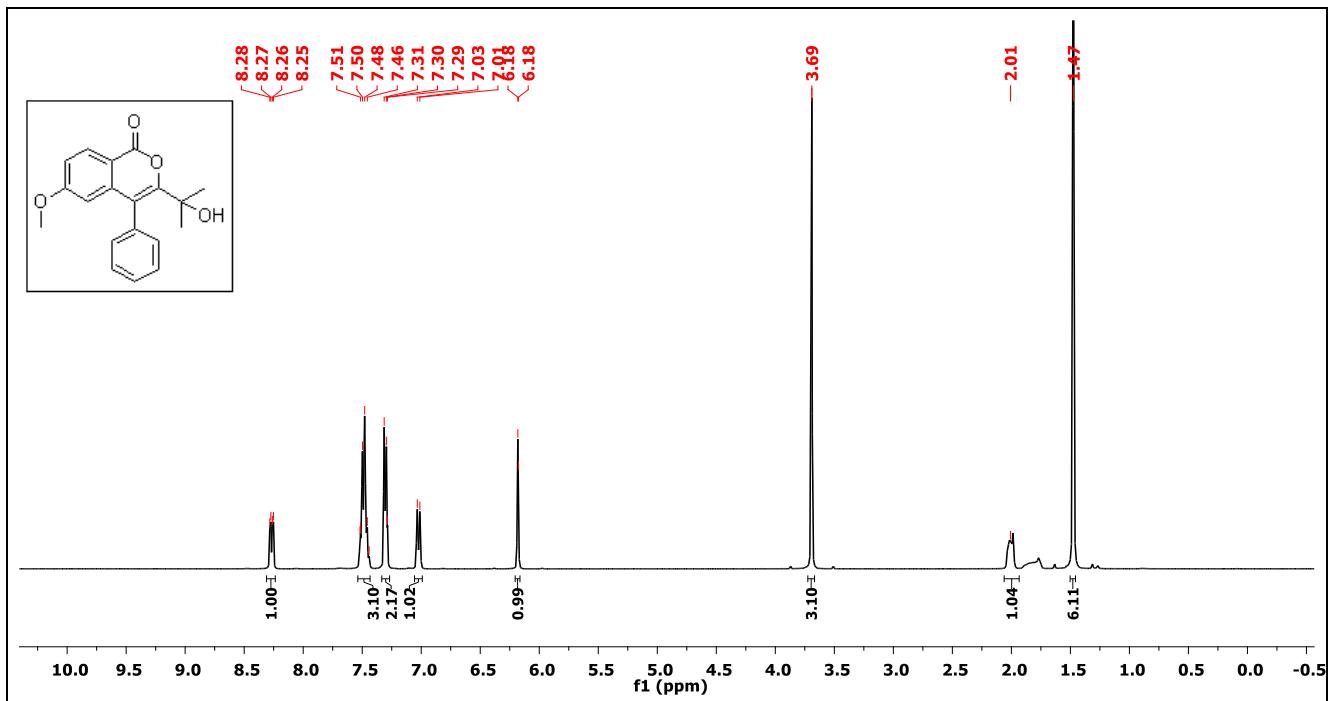
Zero-point correction	=	0.297091 (Hartree/Particle)	
Thermal correction to Energy	=	0.315166	
Thermal correction to Enthalpy	=	0.316110	
Thermal correction to Gibbs Free Energy	=	0.250290	
Sum of electronic and zero-point Energies	=	-920.925575	
Sum of electronic and thermal Energies	=	-920.907500	
Sum of electronic and thermal Enthalpies	=	-920.906556	
Sum of electronic and thermal Free Energies	=	-920.972376	
C	-0.95630800	-2.38085400	-0.02488500
C	-1.08325500	-0.97602500	-0.01417200

C	-2.38803200	-0.43576700	0.00739700
C	-3.51964200	-1.26460300	0.01462400
C	-3.37072800	-2.64311900	0.00302800
C	-2.08140700	-3.19513900	-0.01661500
H	0.03079700	-2.82810200	-0.03864000
H	-4.49784600	-0.79551900	0.03051300
H	-4.24333400	-3.28971300	0.00998500
H	-1.95646800	-4.27480800	-0.02472000
C	-2.58169000	1.01476200	0.01756800
O	-3.63971900	1.60167500	0.02335900
O	-1.42362100	1.76639400	0.01231200
C	0.07618500	-0.07649100	-0.01830400
C	-0.14625600	1.26416300	-0.00726100
C	1.42955600	-0.71659700	-0.01128500
C	2.04566400	-1.10448100	-1.20964400
C	2.06532900	-1.01912900	1.20179500
C	3.28236900	-1.75186700	-1.19797000
H	1.55241200	-0.89187000	-2.15470900
C	3.30168600	-1.66676000	1.21473900
H	1.58895100	-0.73404900	2.13593800
C	3.91498900	-2.03175400	0.01459300
H	3.75010400	-2.03828200	-2.13622700
H	3.78513400	-1.88610800	2.16301900
H	4.87780000	-2.53545200	0.02458400
C	0.81260400	2.46467100	0.01116600
C	0.38820000	3.46578300	-1.08442100
H	0.49475400	3.02828500	-2.08335000
H	-0.64722600	3.77982200	-0.94631500
H	1.03897200	4.34840800	-1.03960200
C	2.30582200	2.15215100	-0.14548500

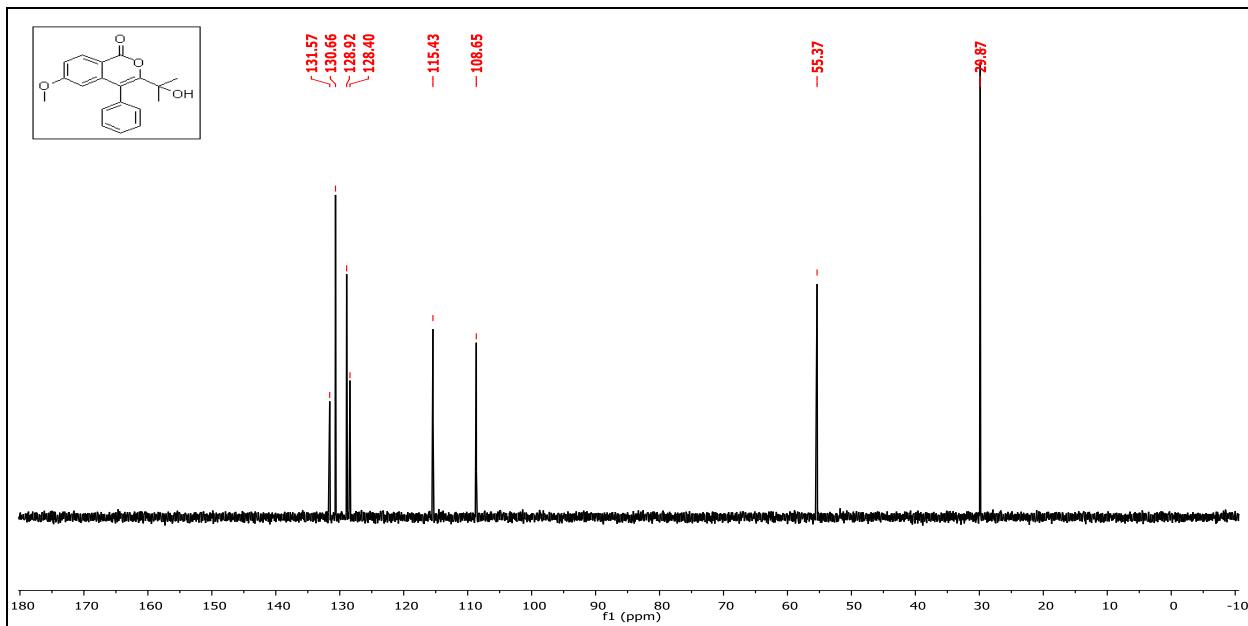
H	2.53753100	1.66130400	-1.09466100
H	2.84951700	3.10451700	-0.11866100
H	2.67424200	1.53192200	0.67137700
O	0.59727500	3.04084600	1.31355900
H	0.92266600	3.95465900	1.2784260

Copies of H¹, C¹³ and DEPT135

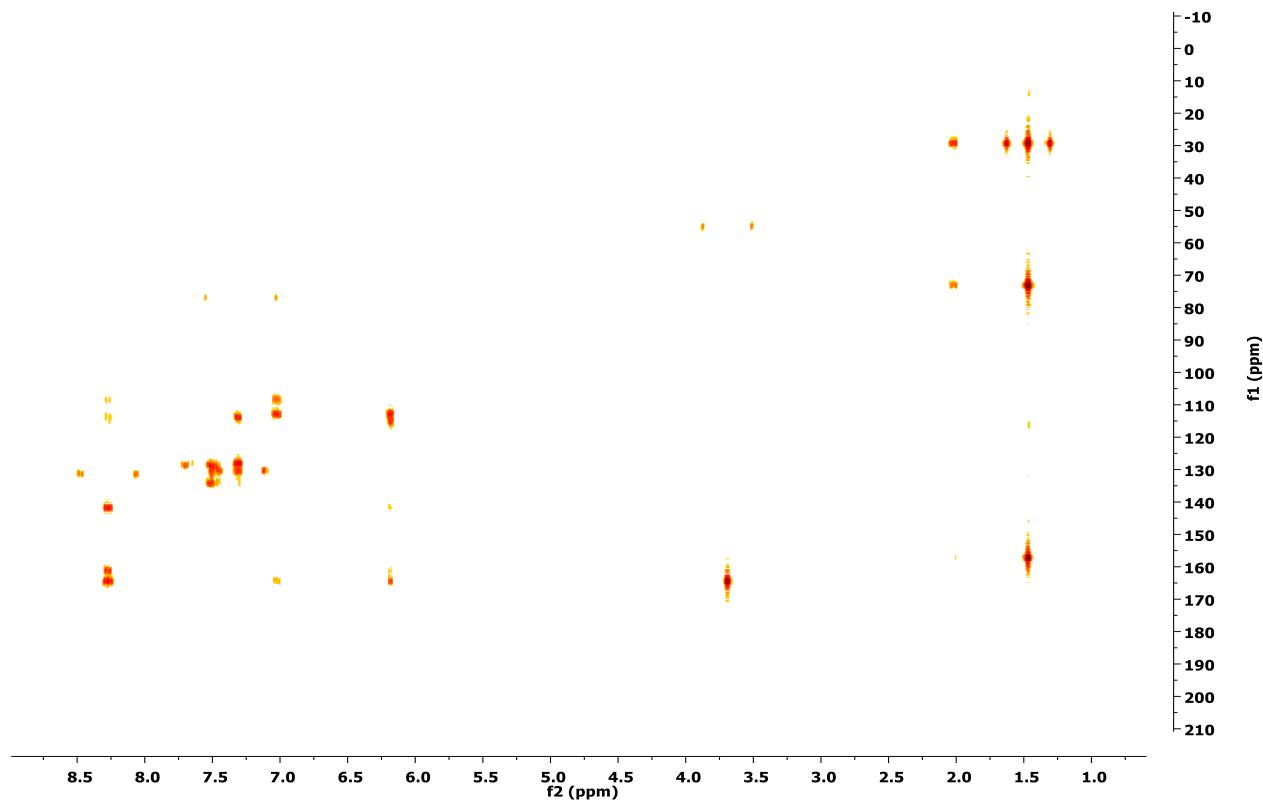
¹H and ¹³C spectra of compound 3aa:



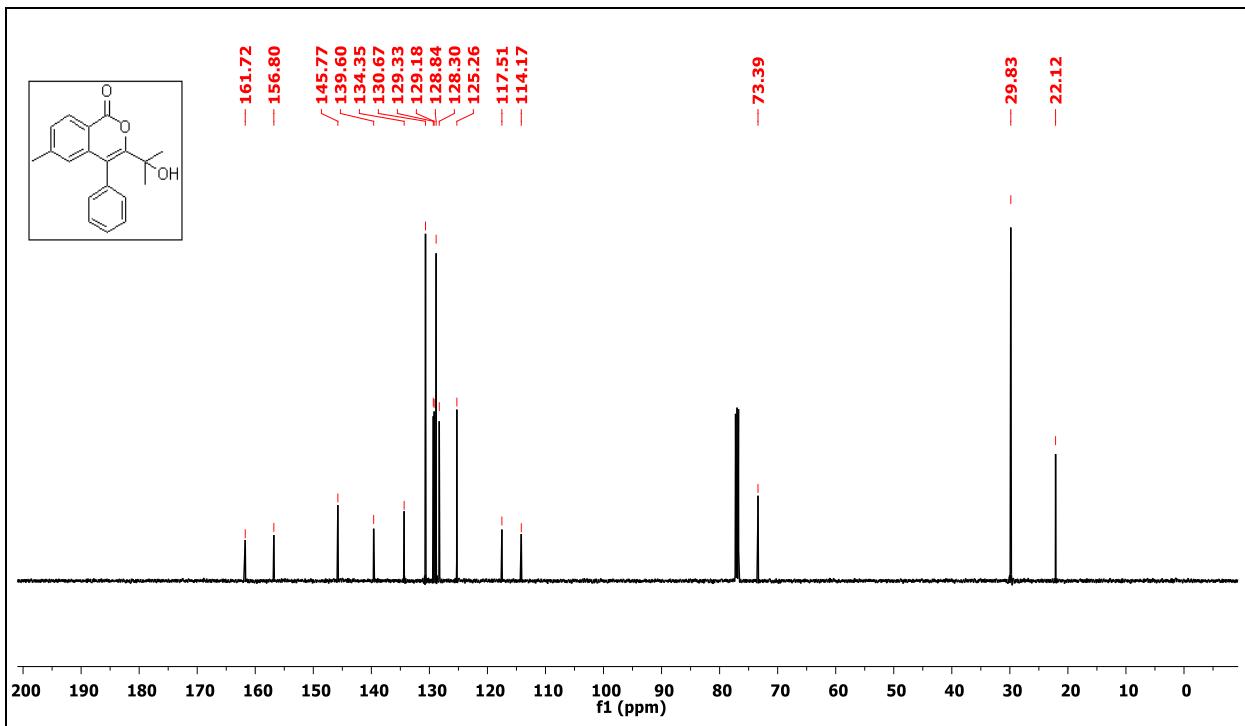
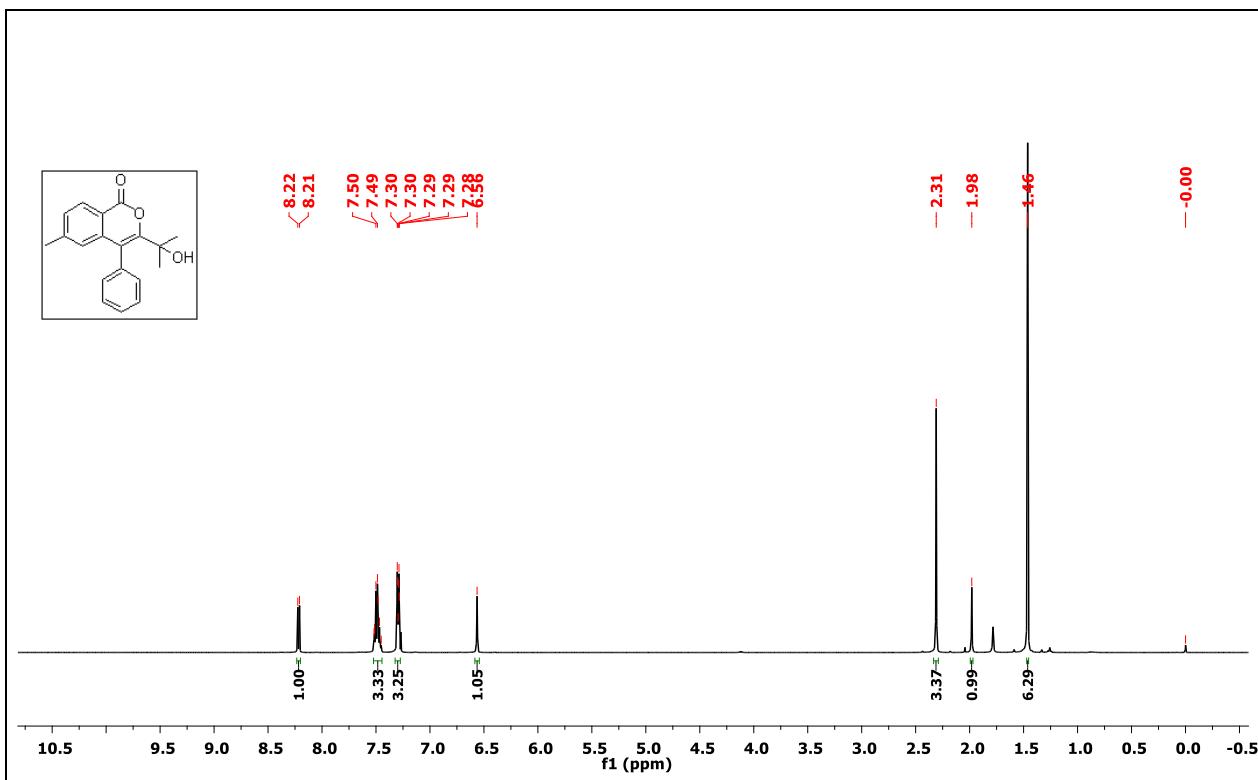
DEPT spectra of compound 3aa:



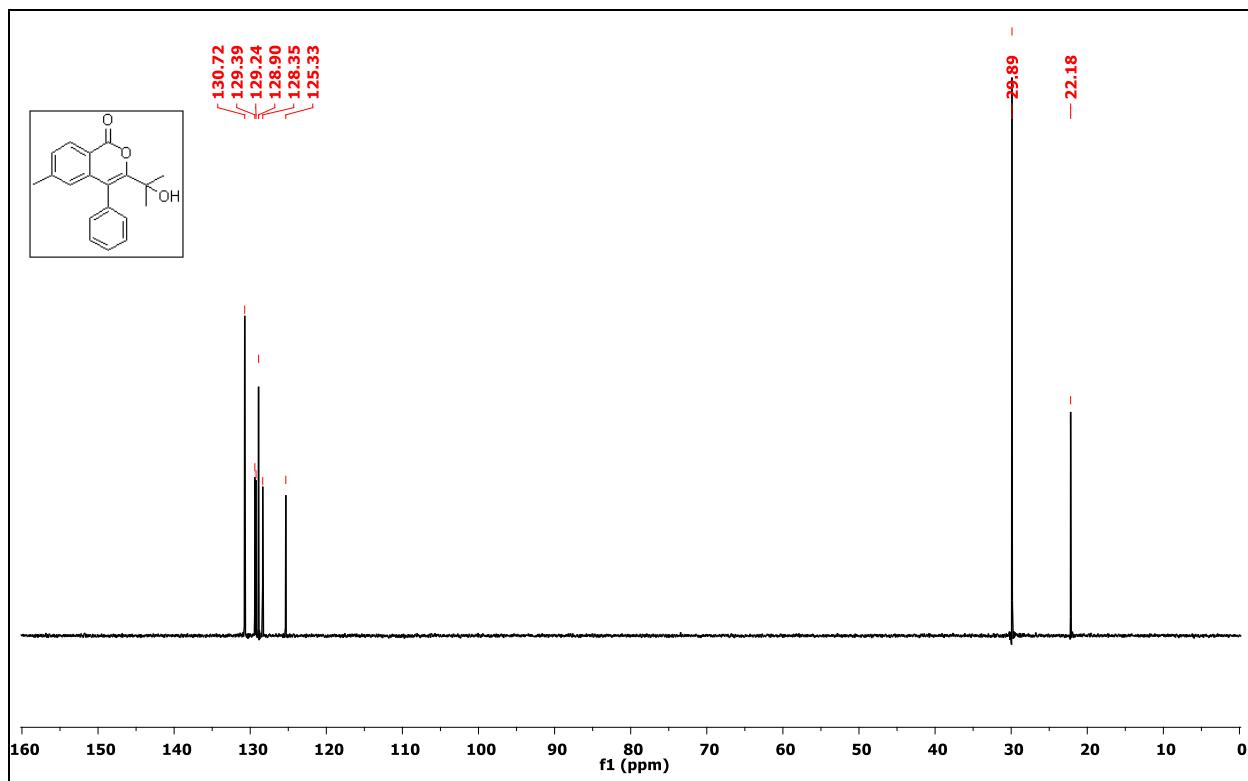
HMBC spectra of compound 3aa:



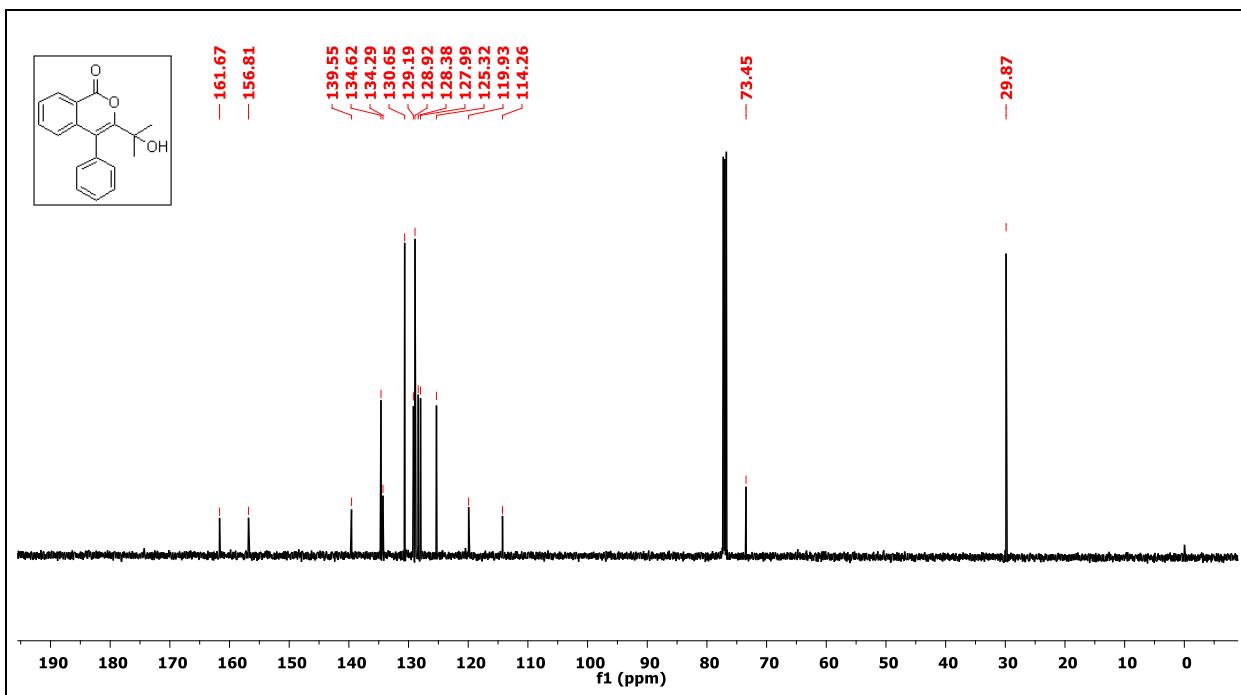
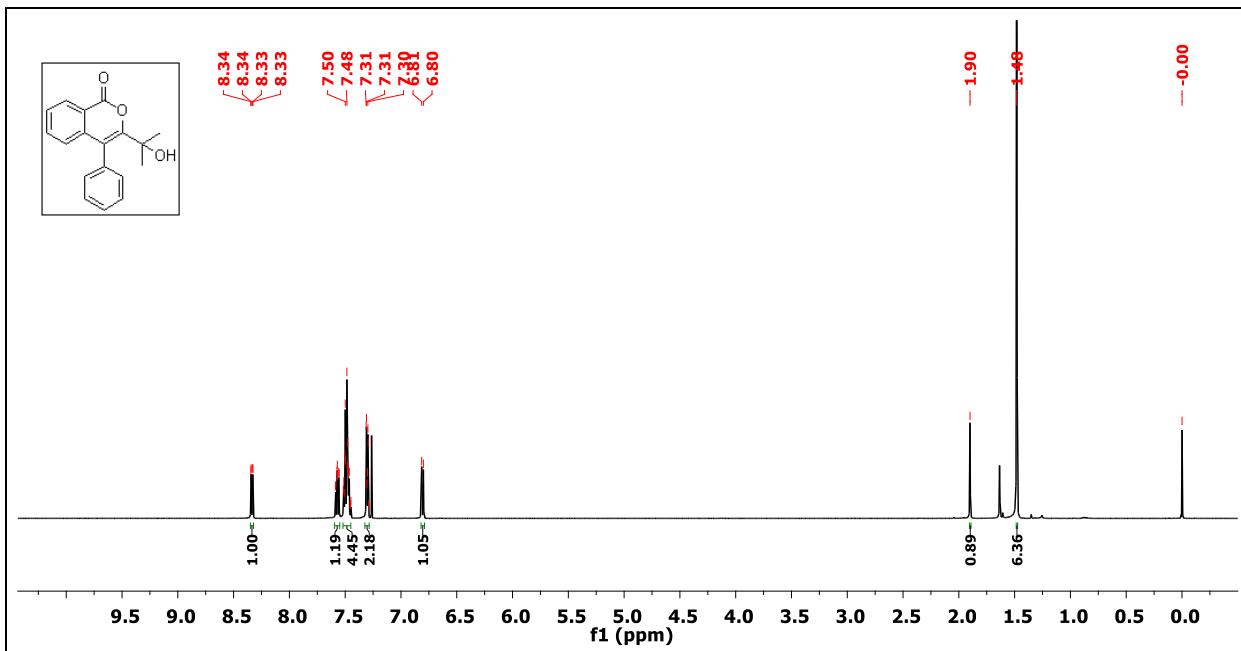
¹H and ¹³C spectra of compound 3ba:



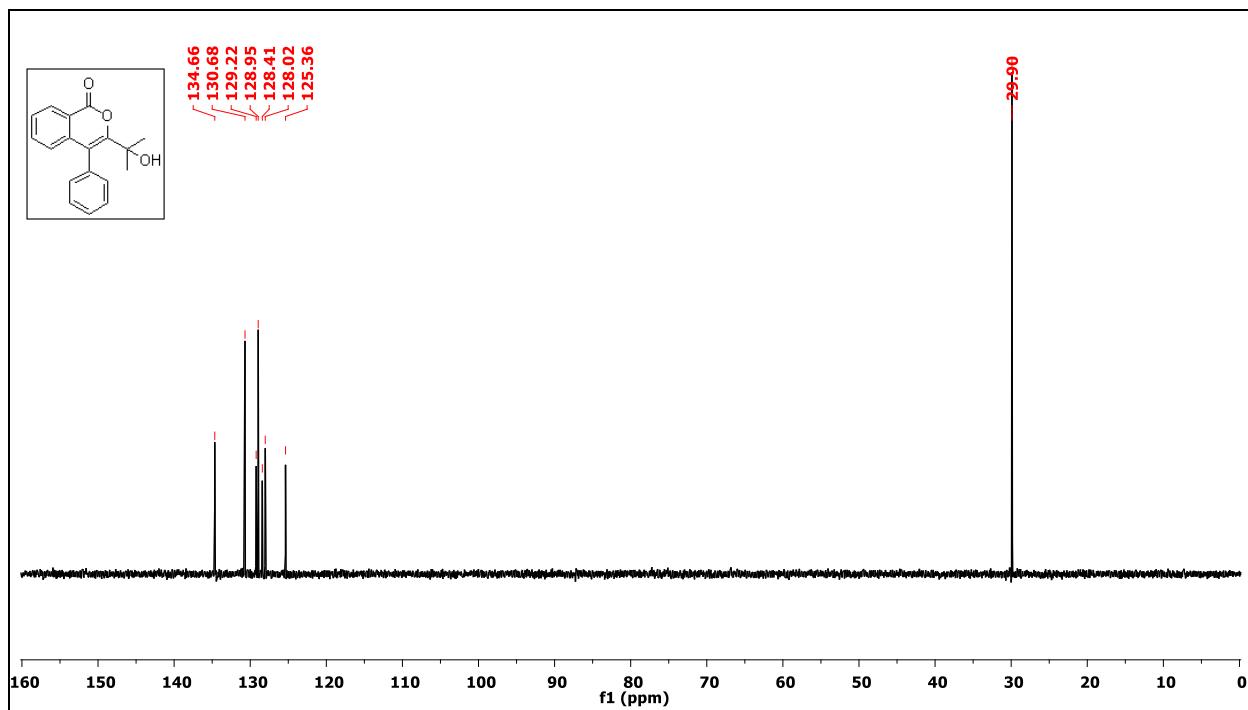
DEPT spectra of compound 3ba:



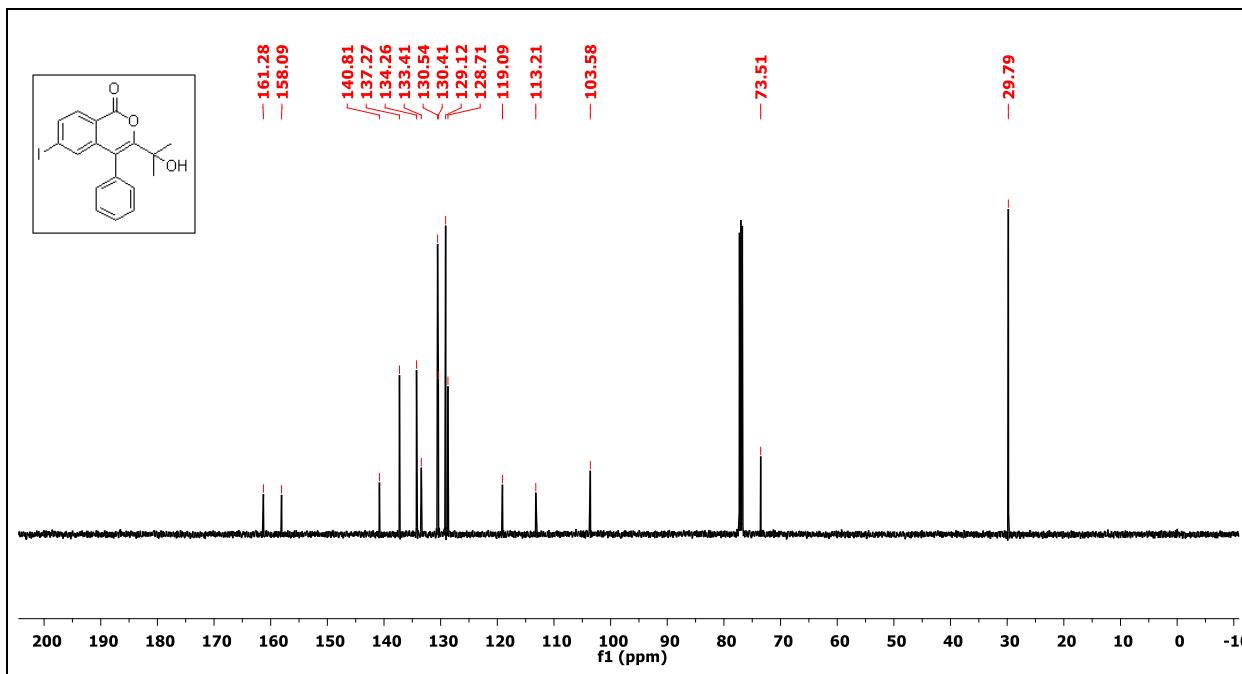
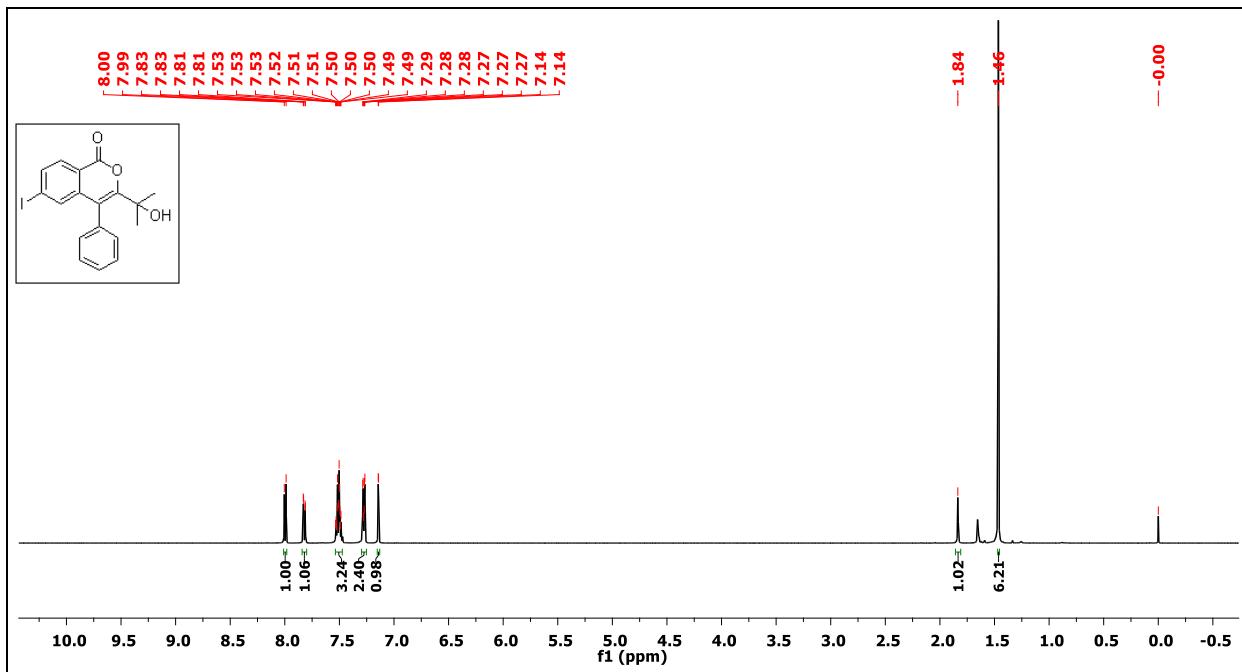
¹H and ¹³C spectra of compound 3ca:



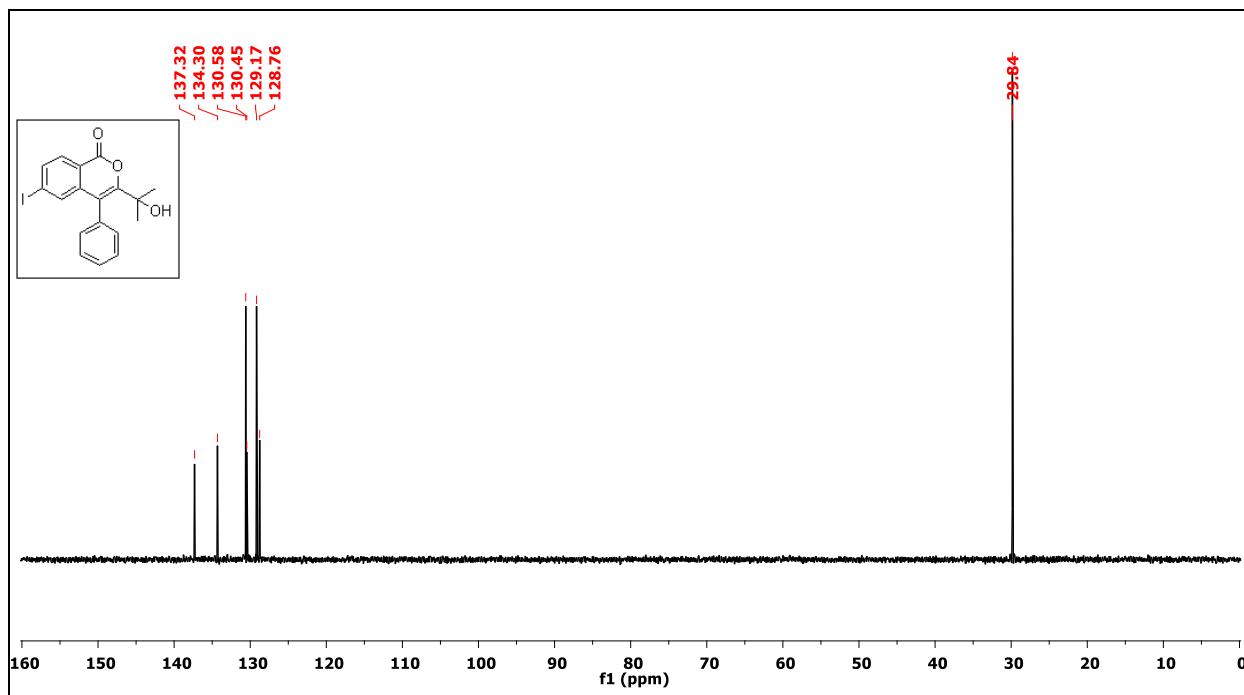
DEPT spectra of compound 3ca:



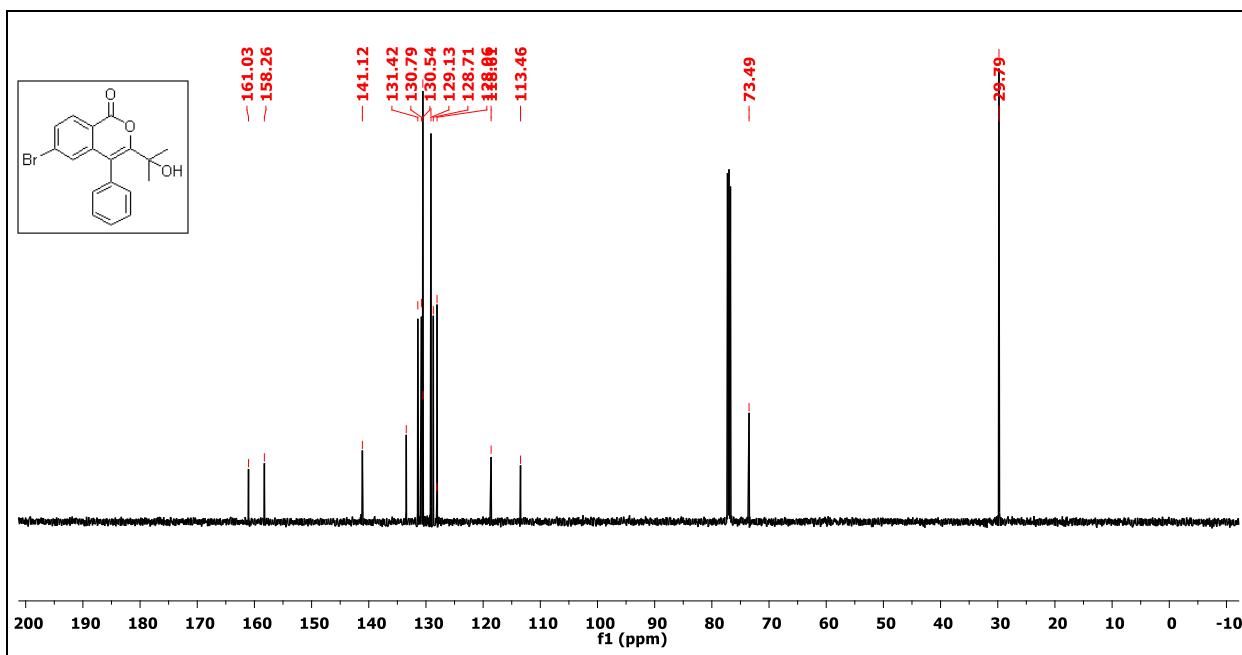
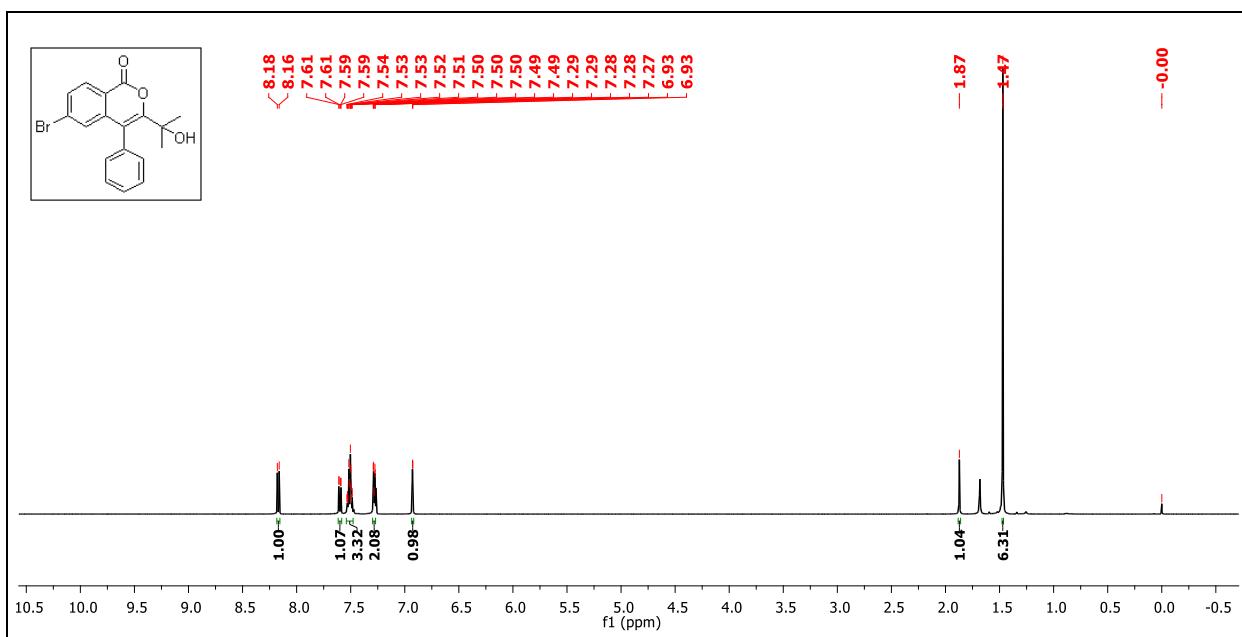
¹H and ¹³C spectra of compound 3da:



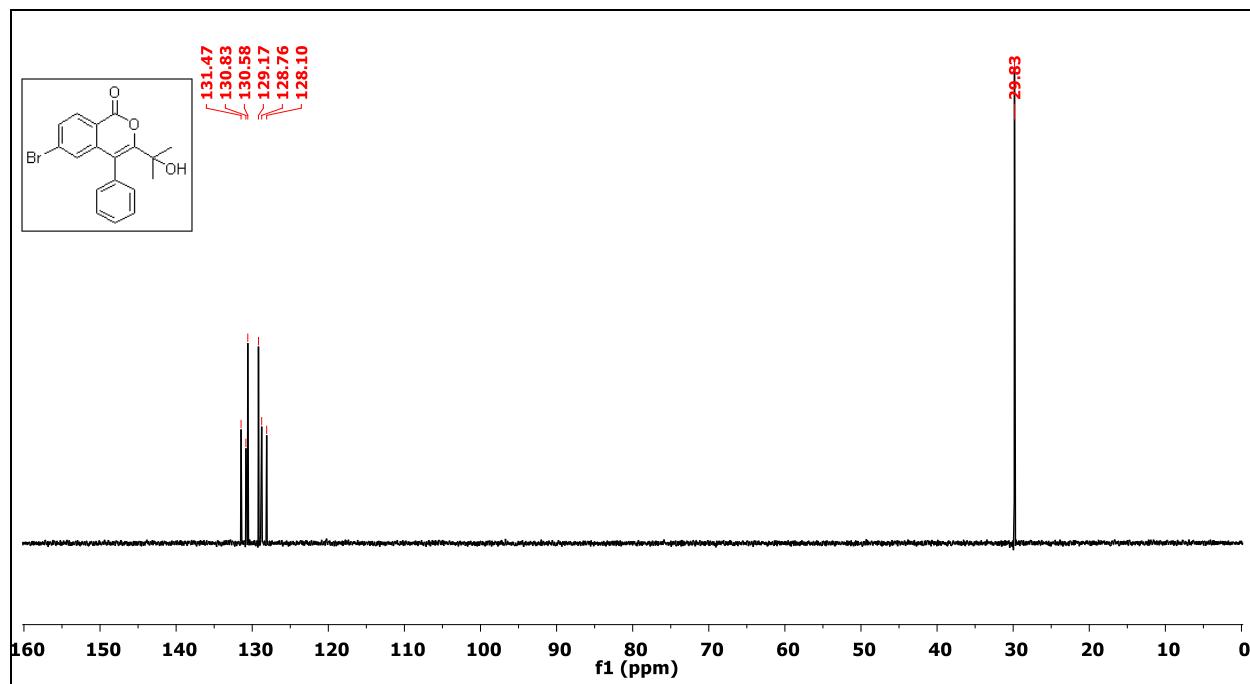
DEPT spectra of compound 3da:



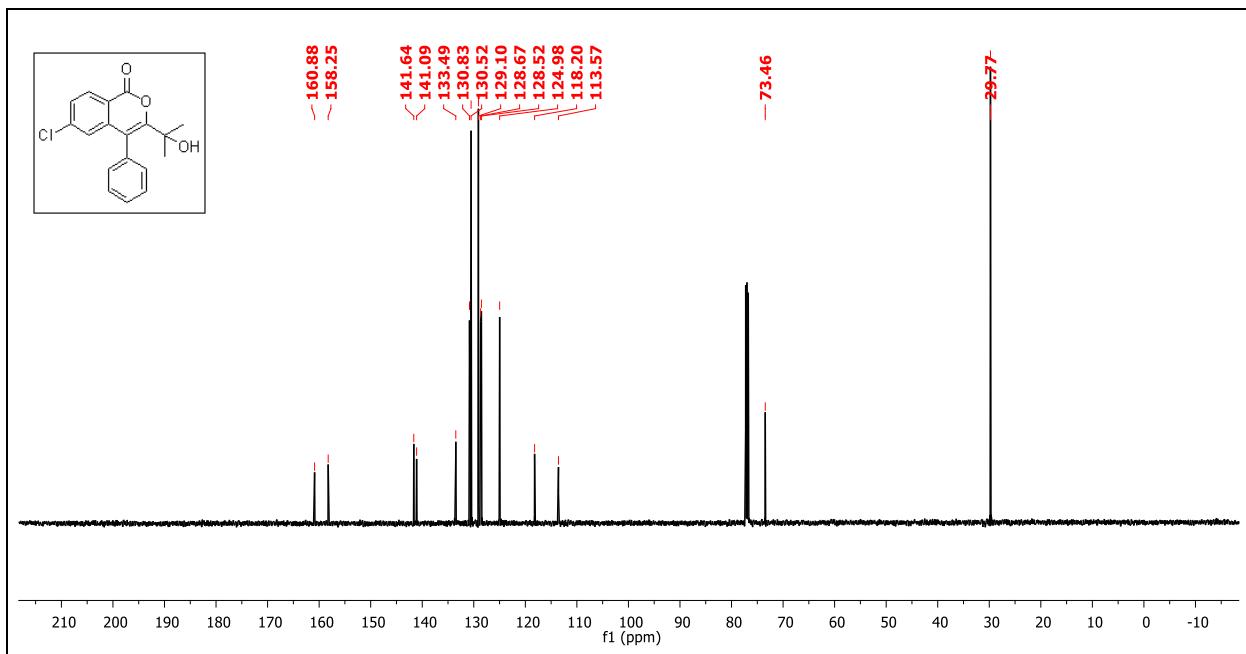
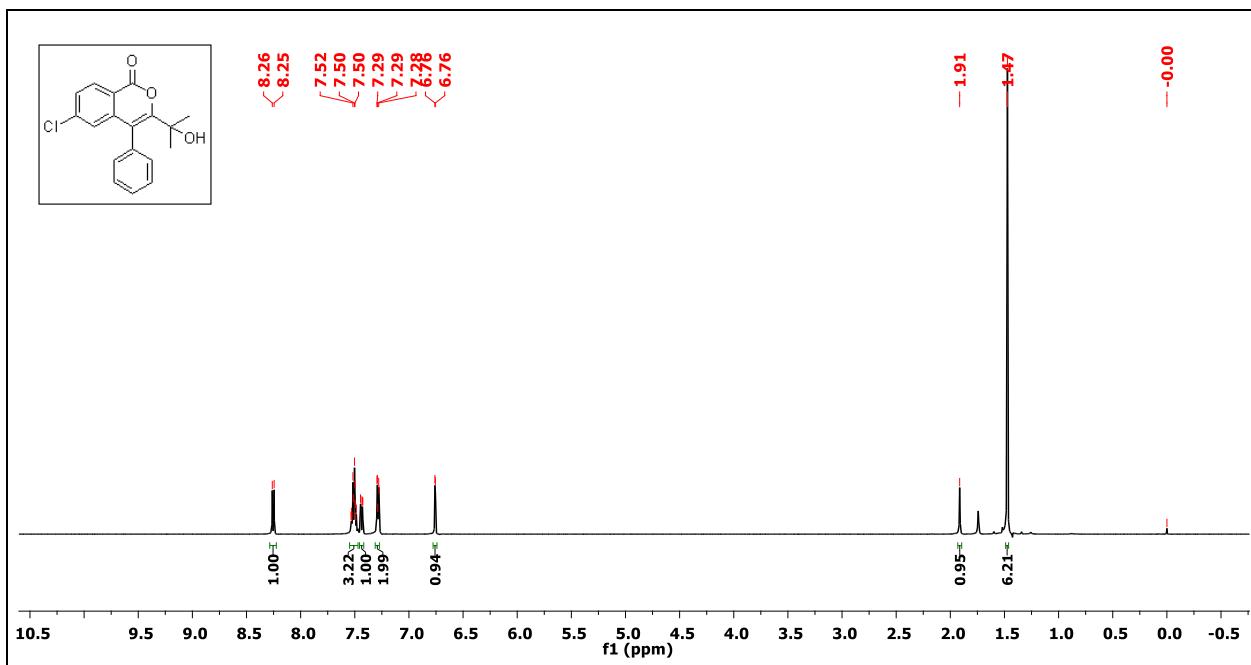
¹H and ¹³C spectra of compound 3ea:



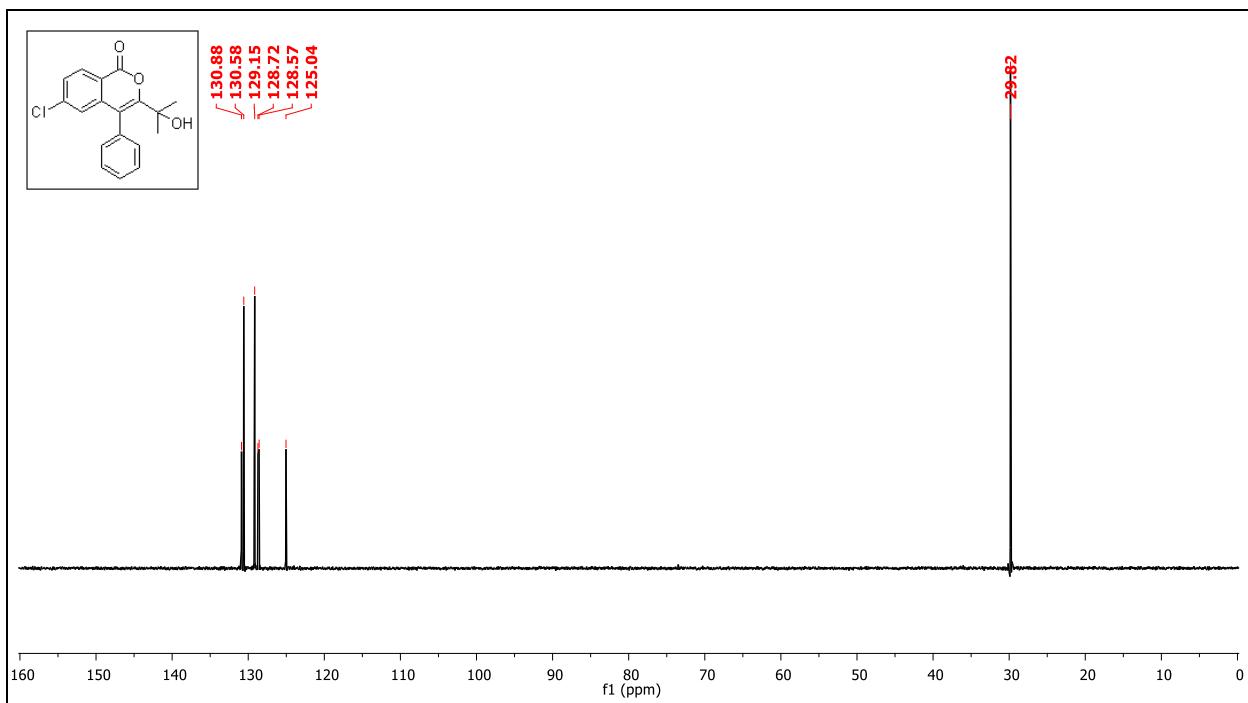
DEPT spectra of compound 3ea:



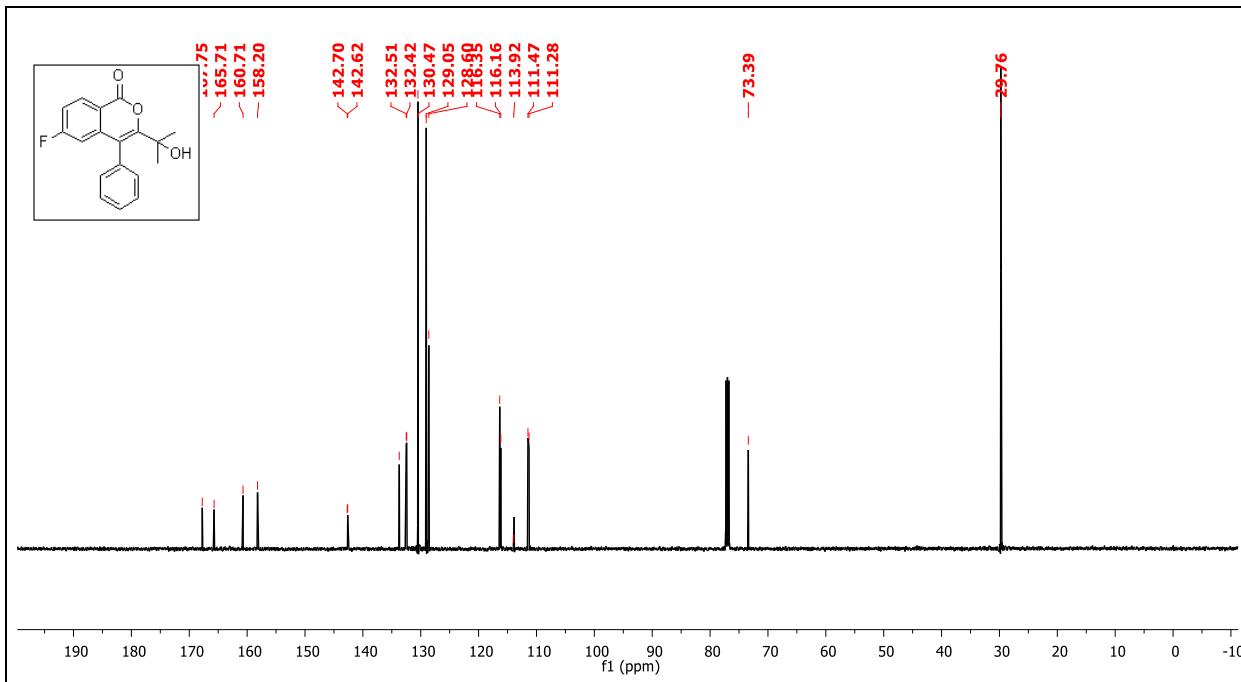
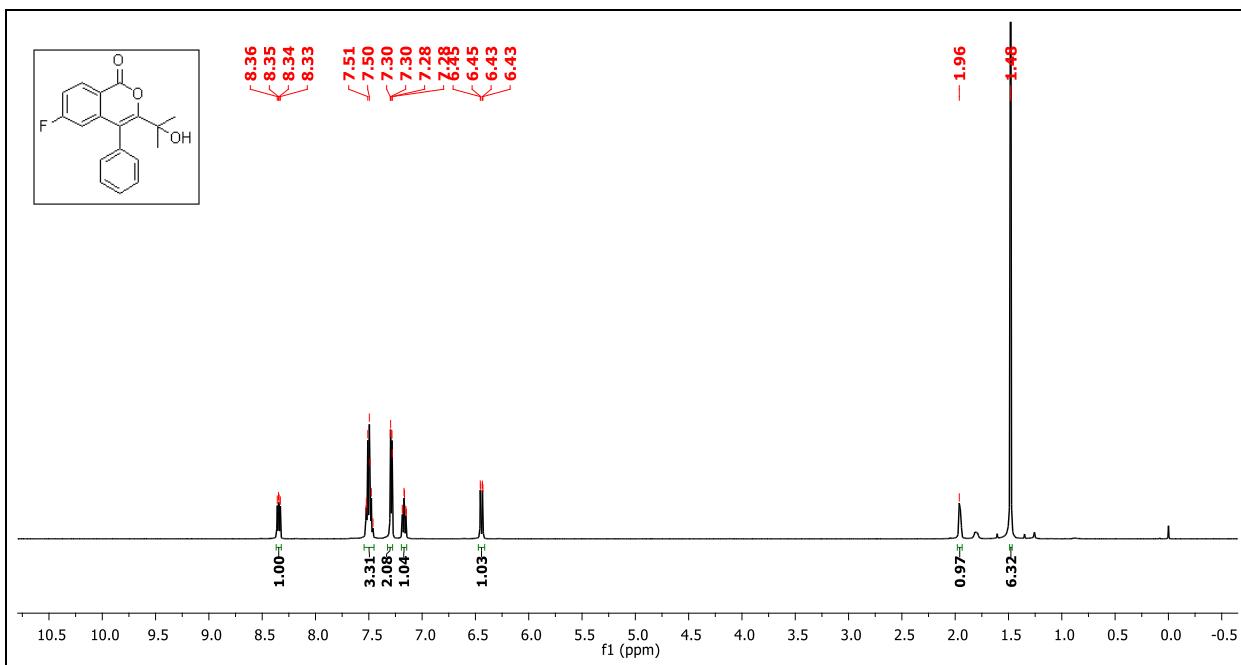
¹H and ¹³C spectra of compound 3fa:



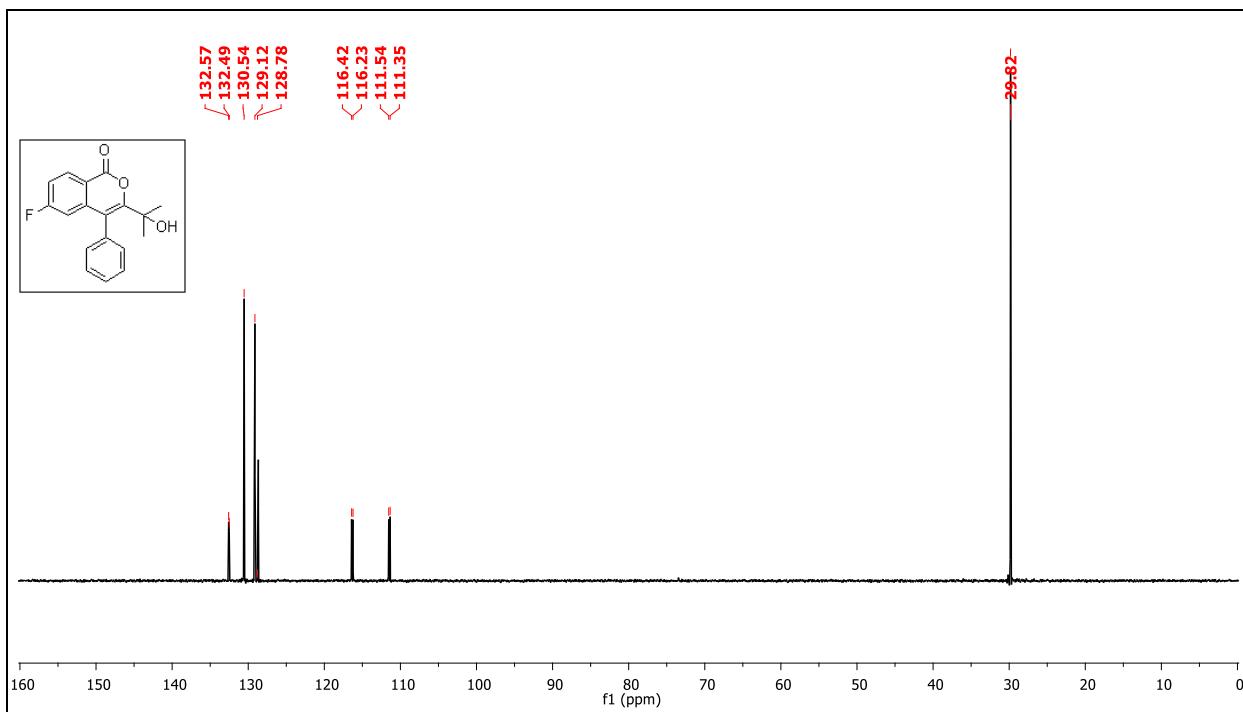
DEPT spectra of compound 3fa:



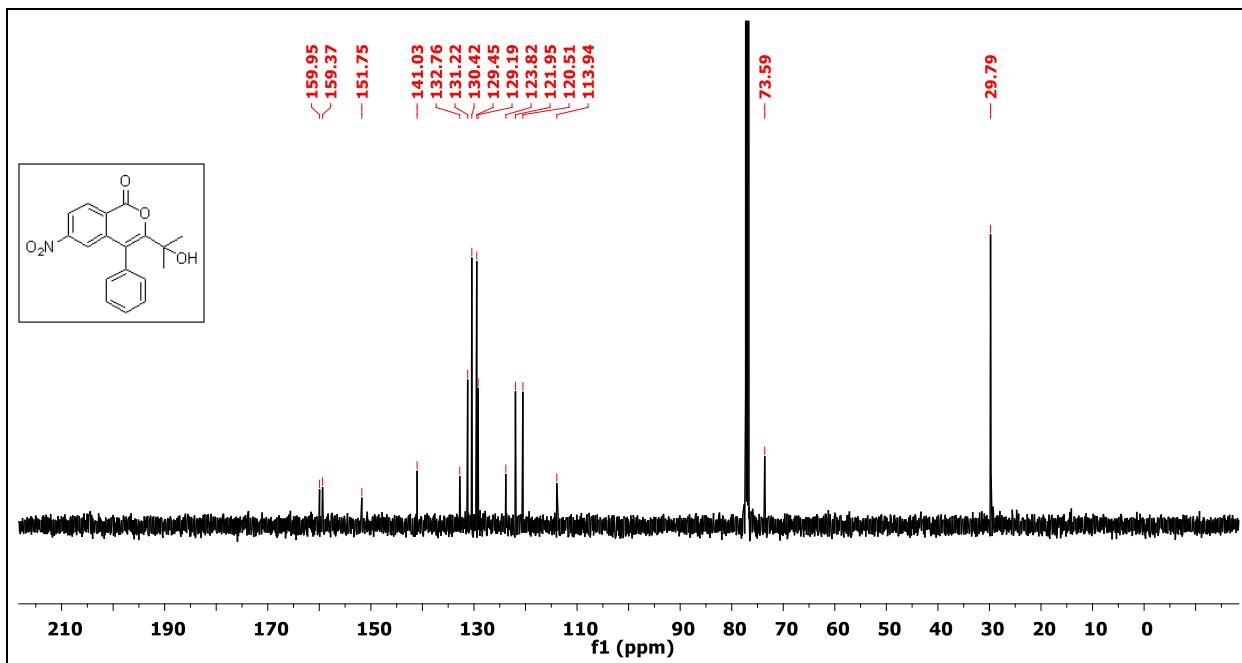
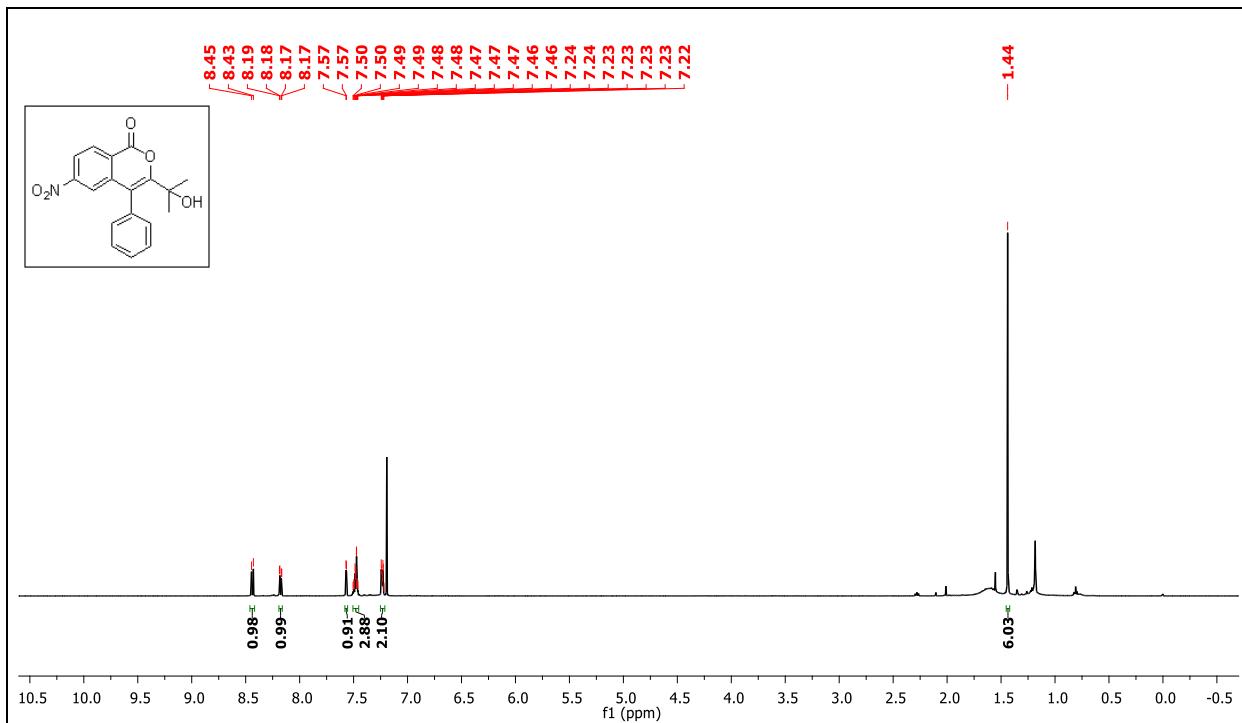
¹H and ¹³C spectra of compound 3ga:



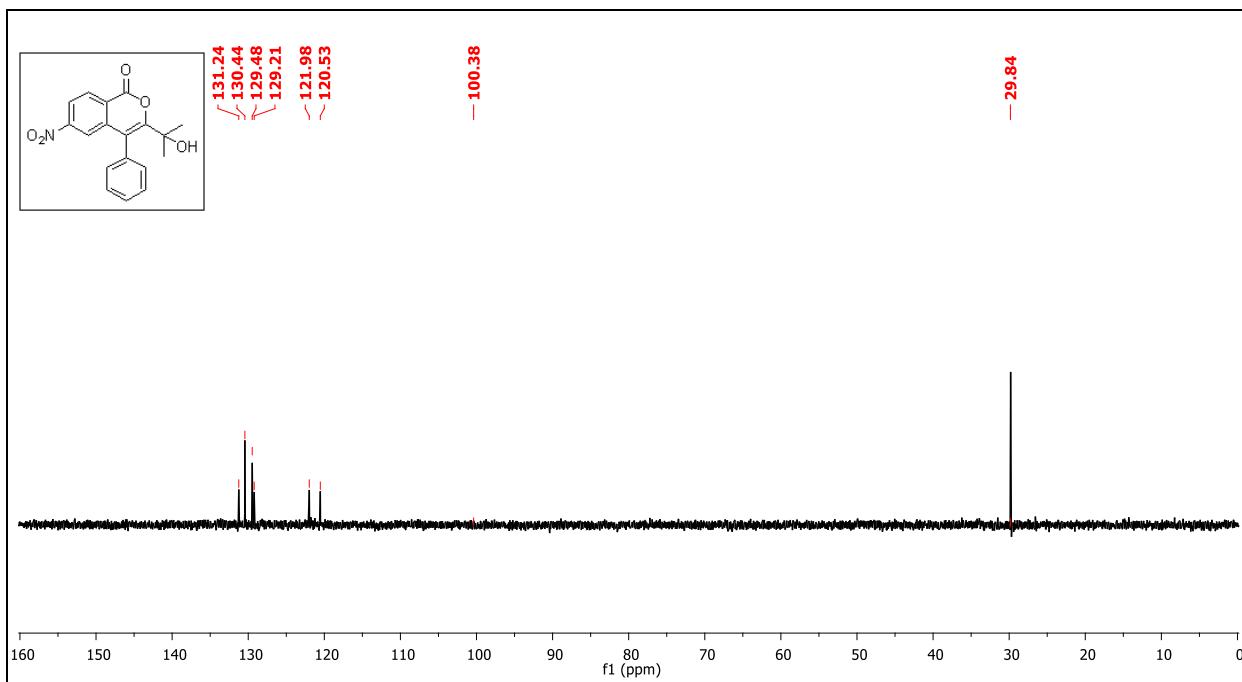
DEPT spectra of compound 3ga:



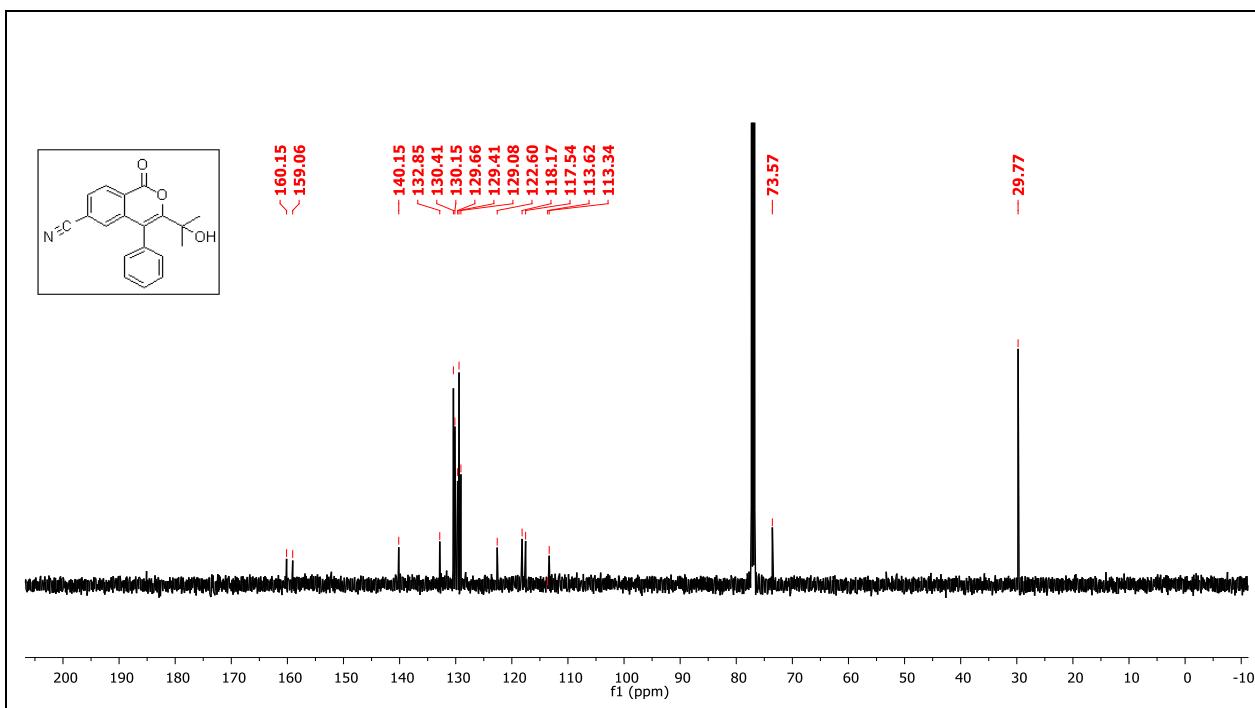
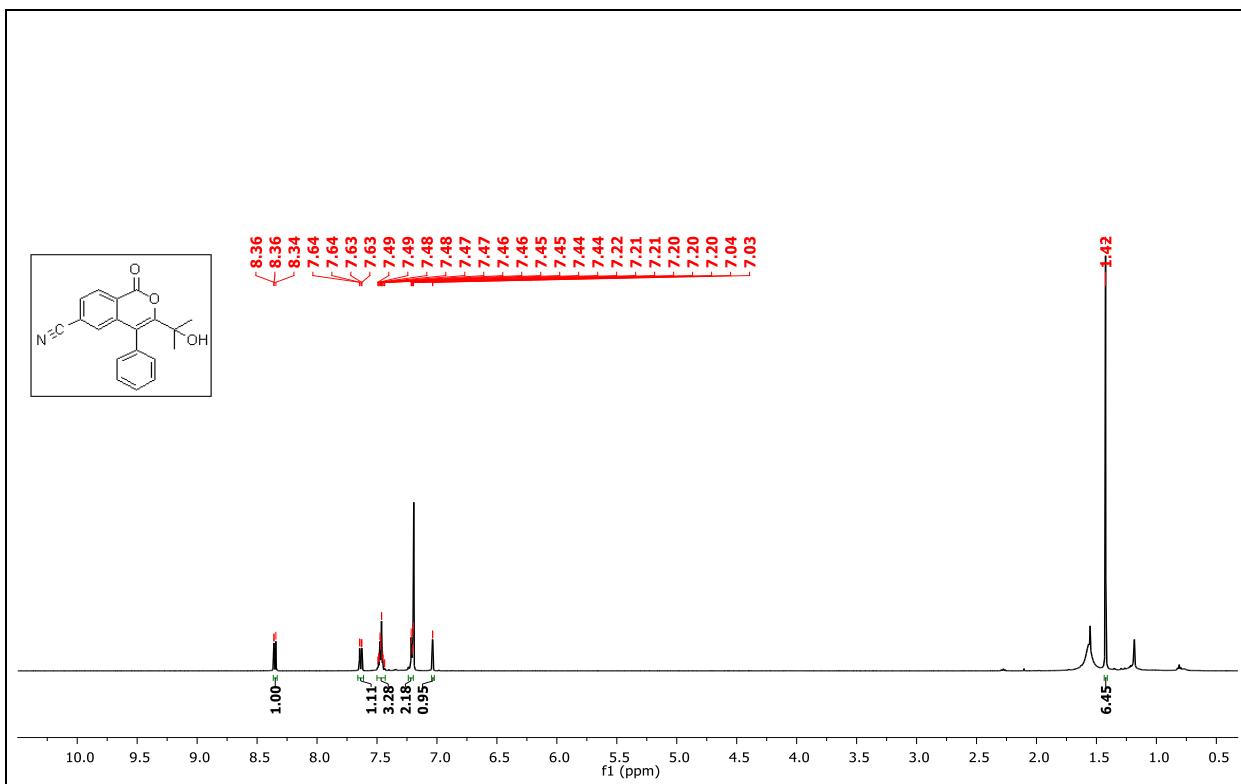
¹H and ¹³C spectra of compound 3ha:



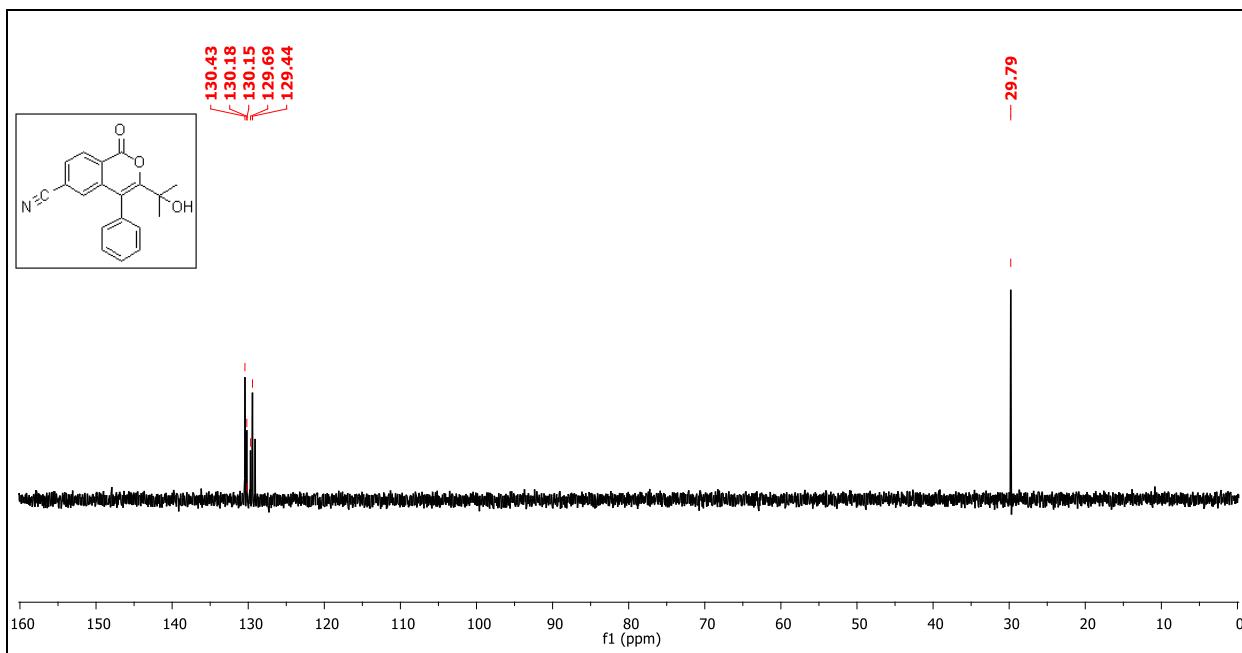
DEPT spectra of compound 3ha:



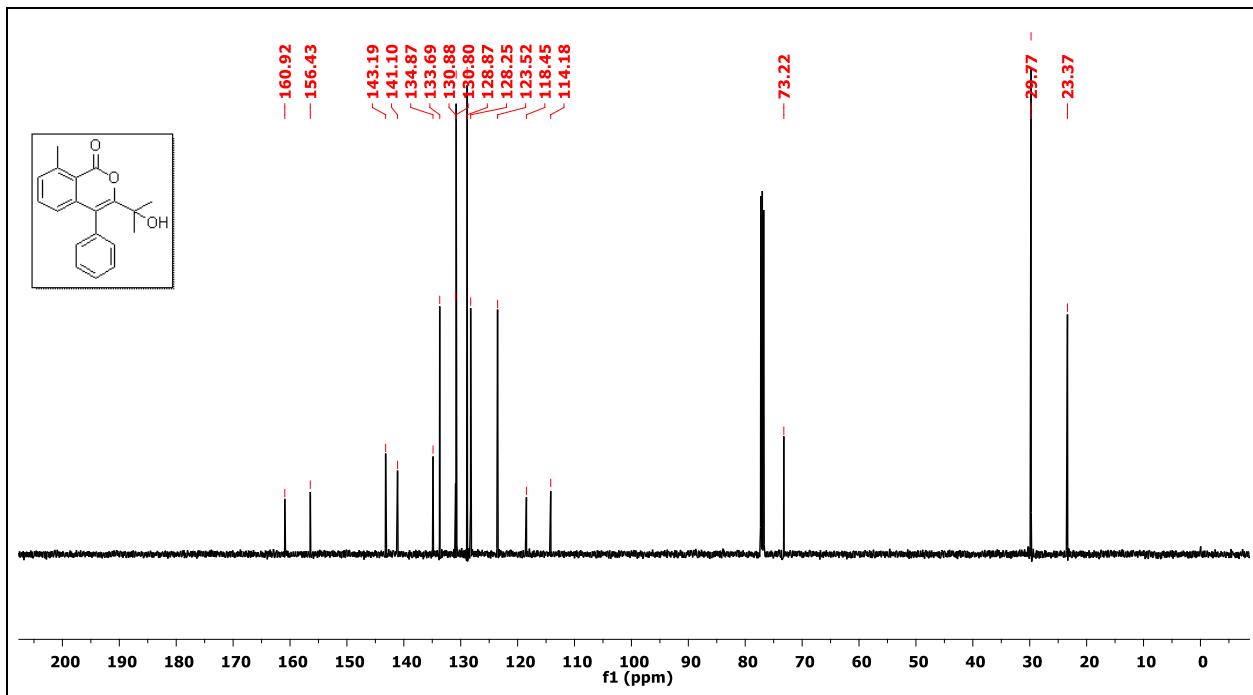
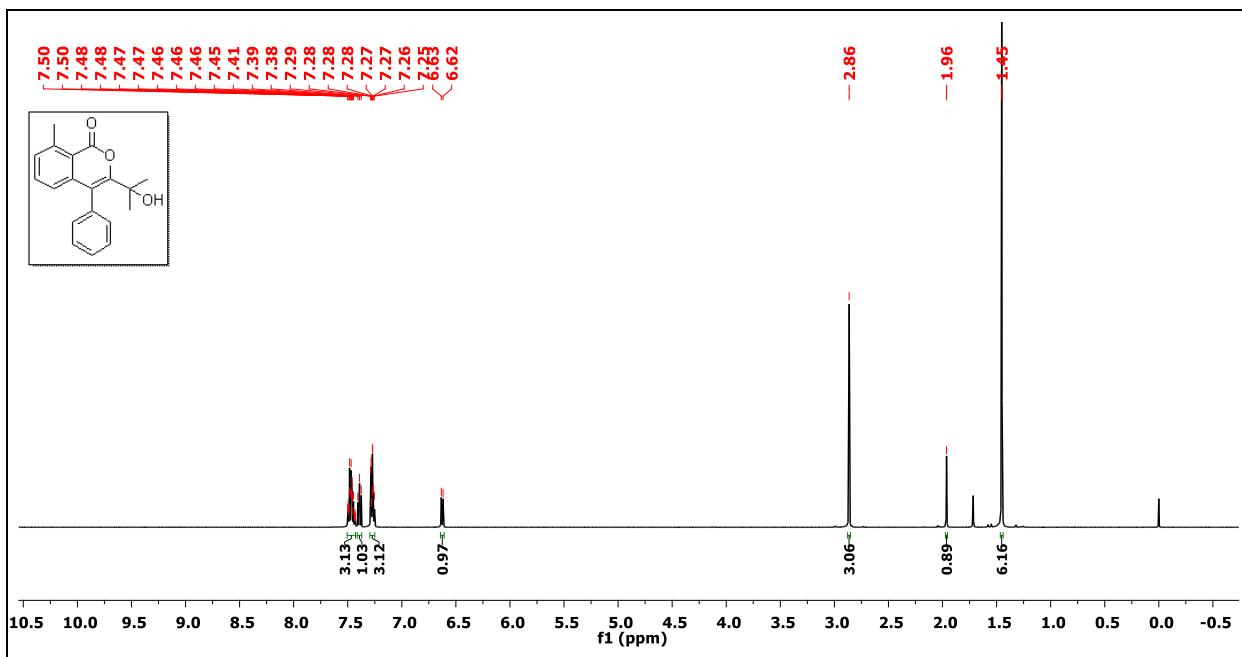
¹H and ¹³C spectra of compound 3ia:



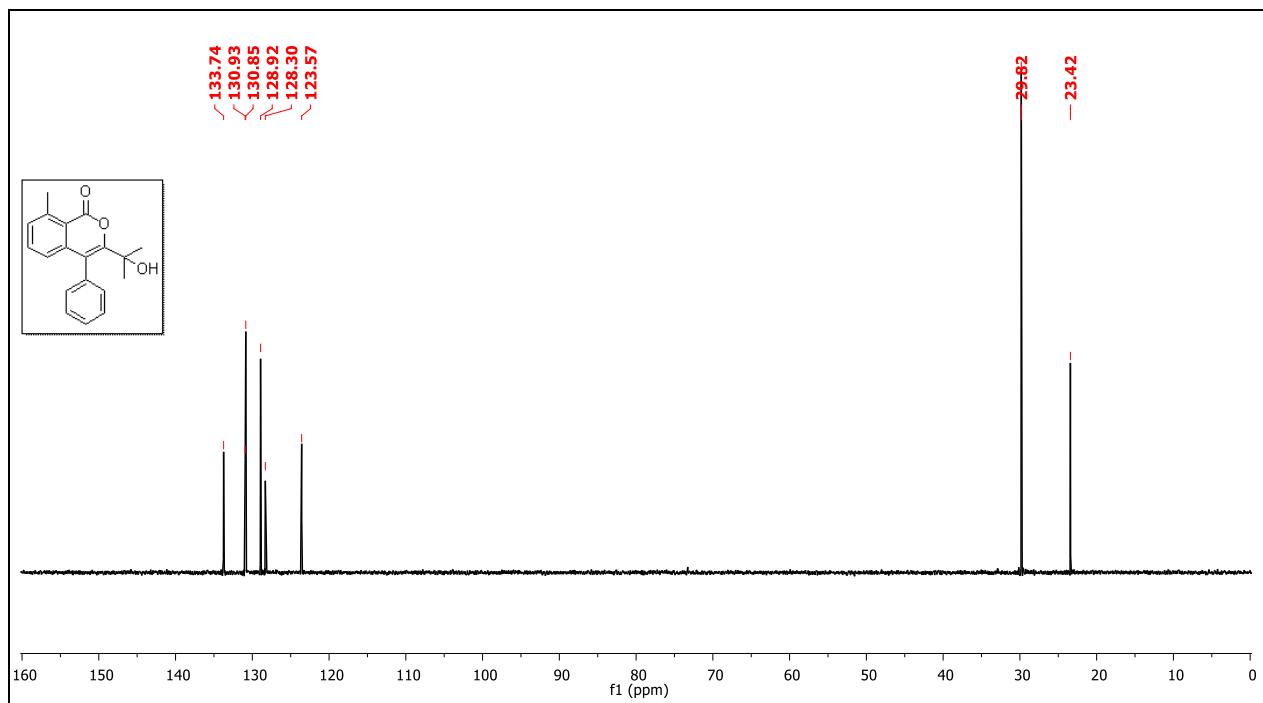
DEPT spectra of compound 3ia:



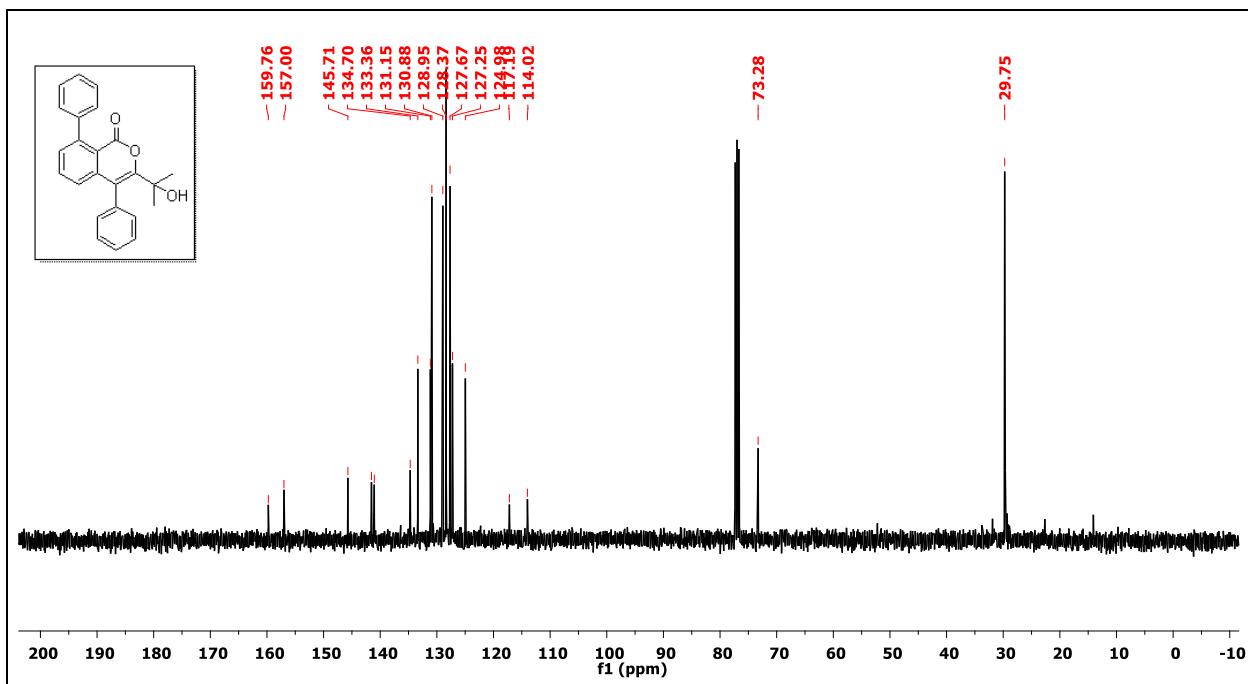
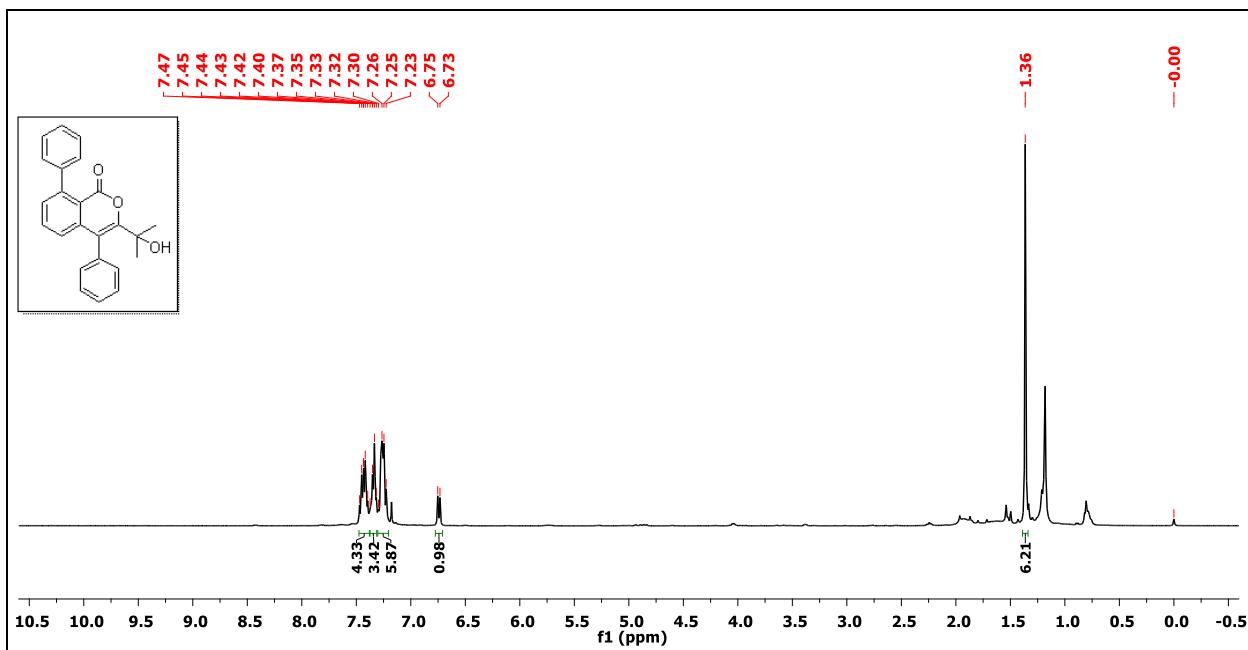
¹H and ¹³C spectra of compound 3ja:



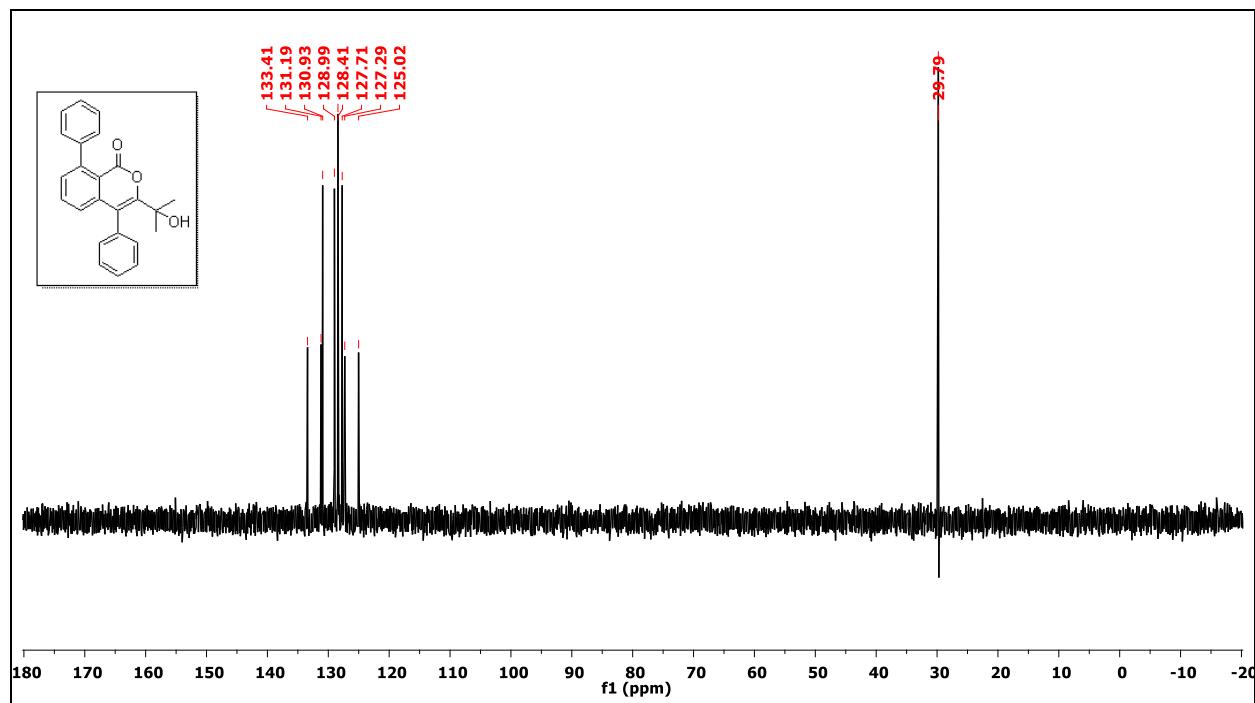
DEPT spectra of compound 3ja:



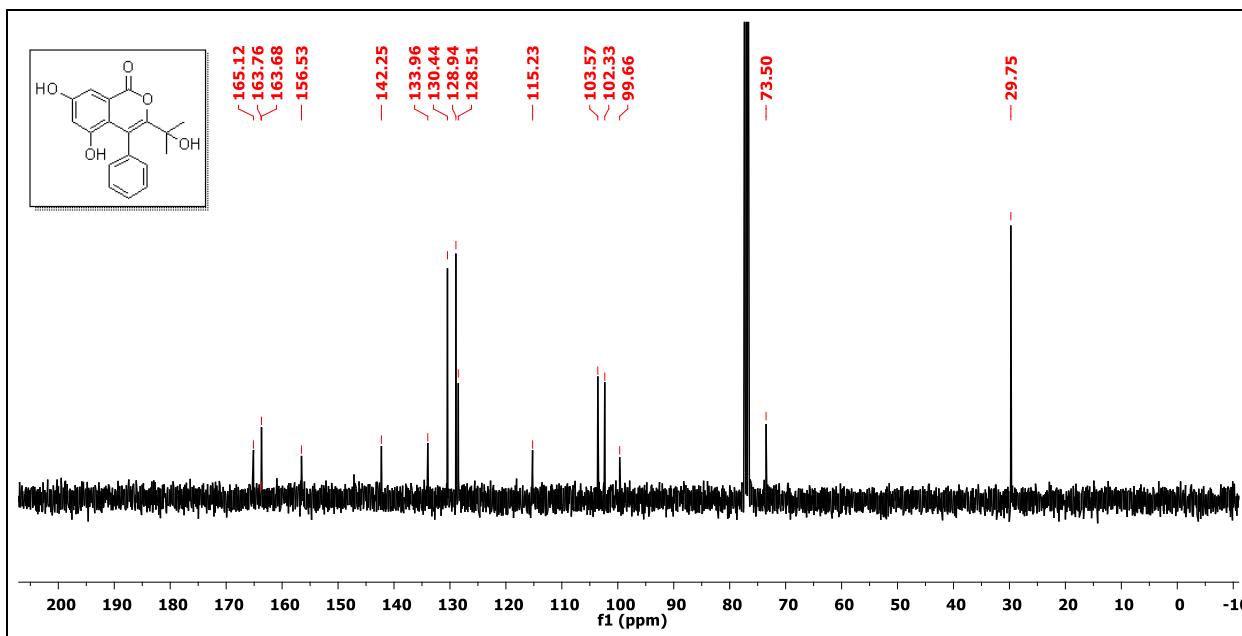
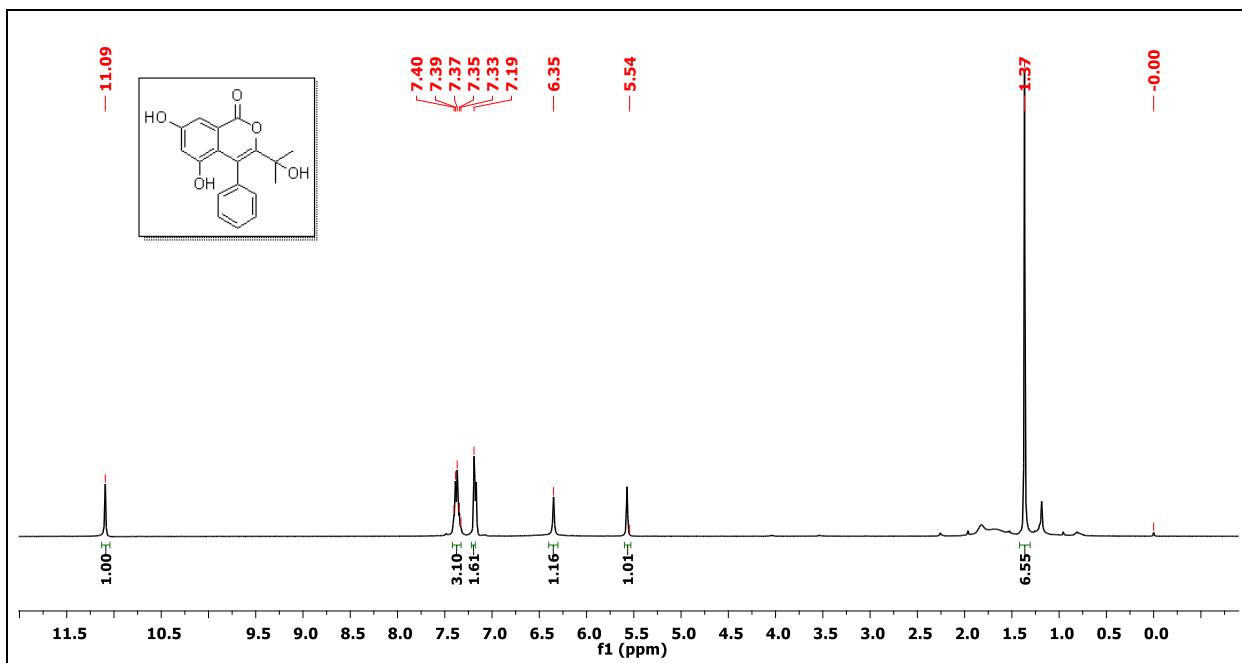
¹H and ¹³C spectra of compound 3ka:



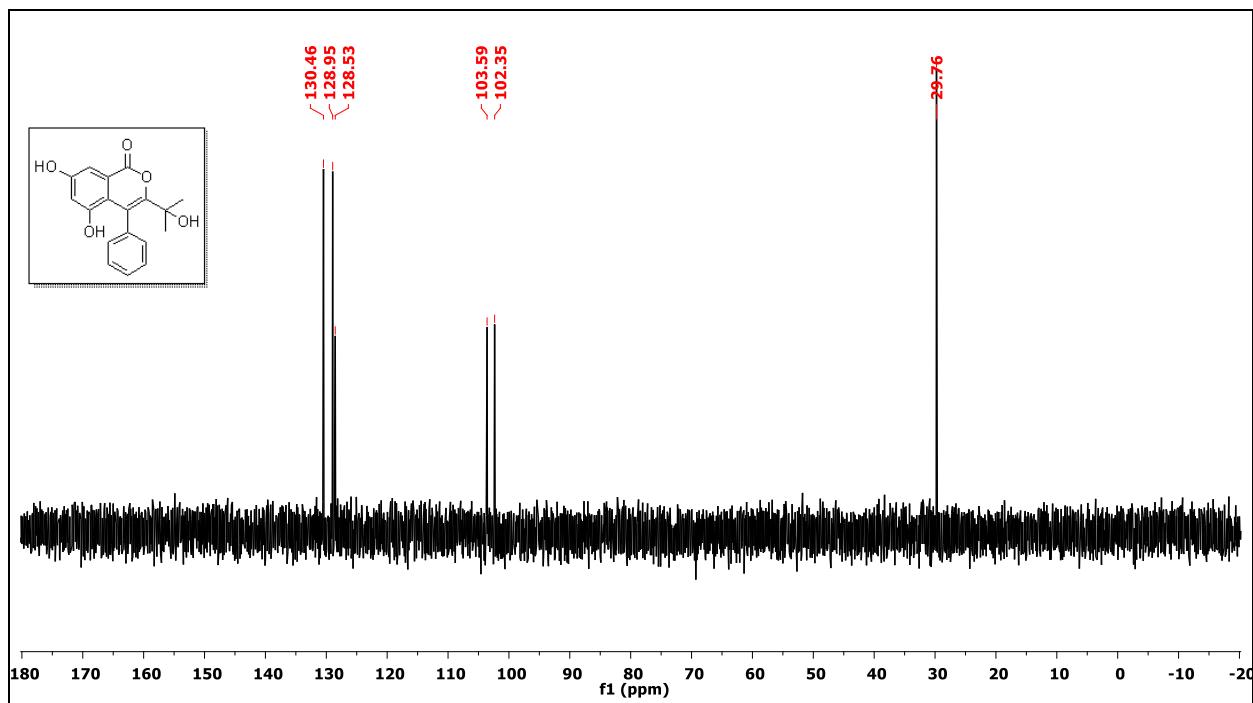
DEPT spectra of compound 3ka:



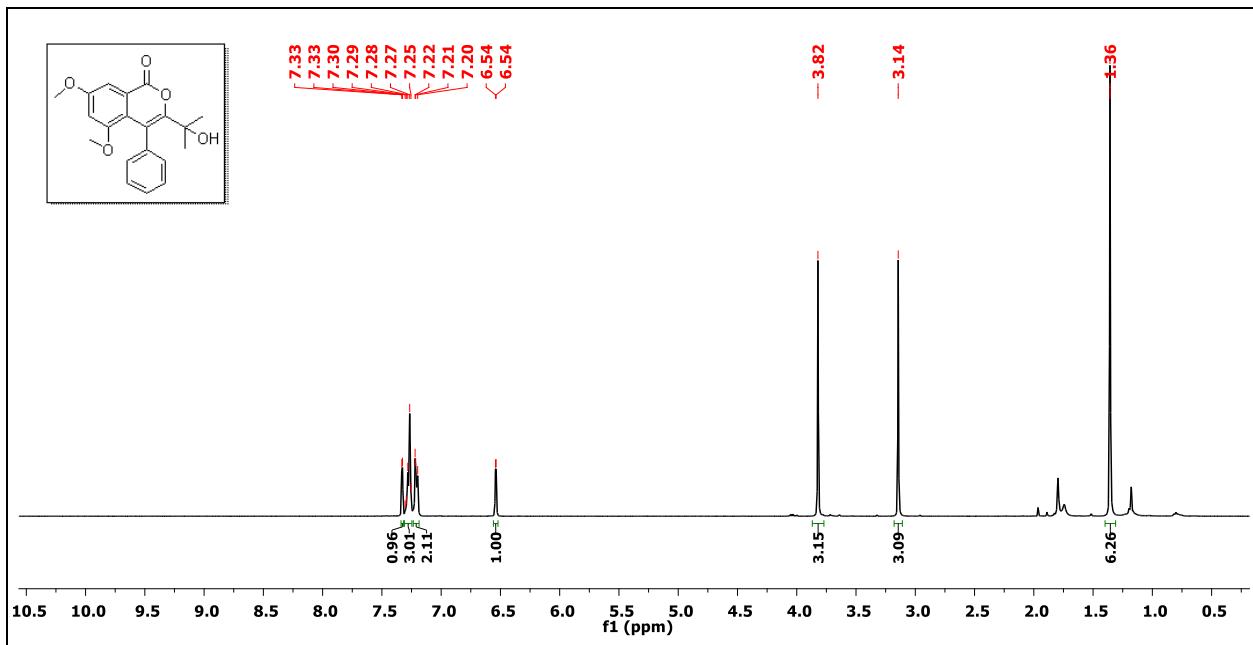
¹H and ¹³C spectra of compound 3la:



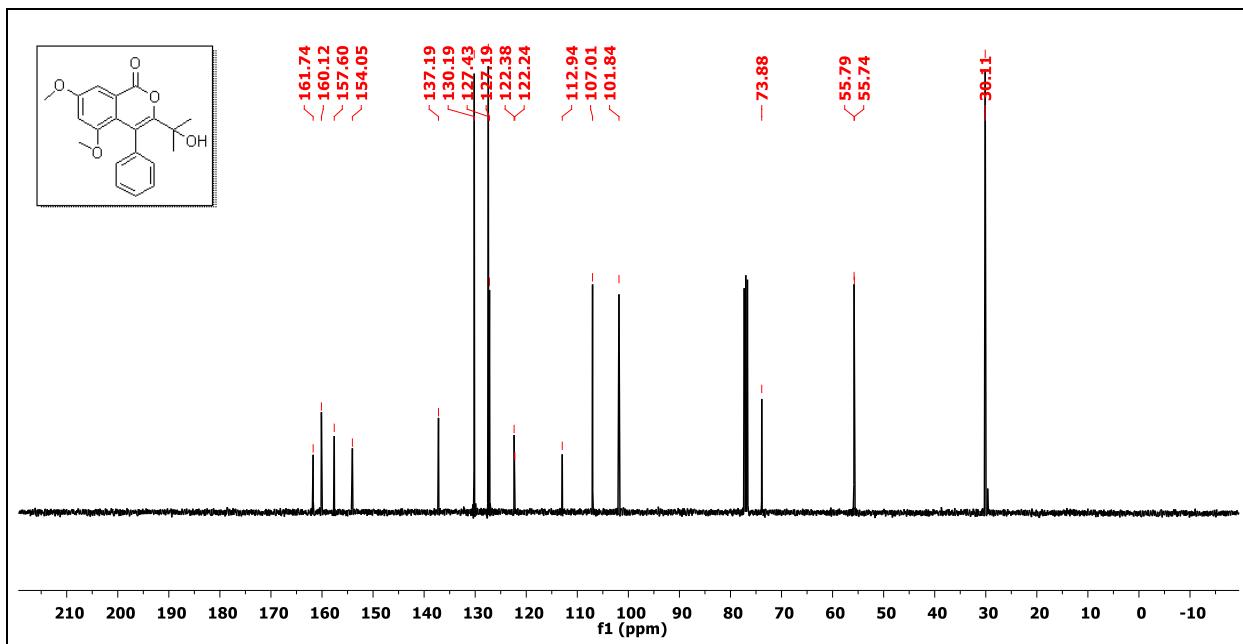
DEPT spectra of compound 3la:



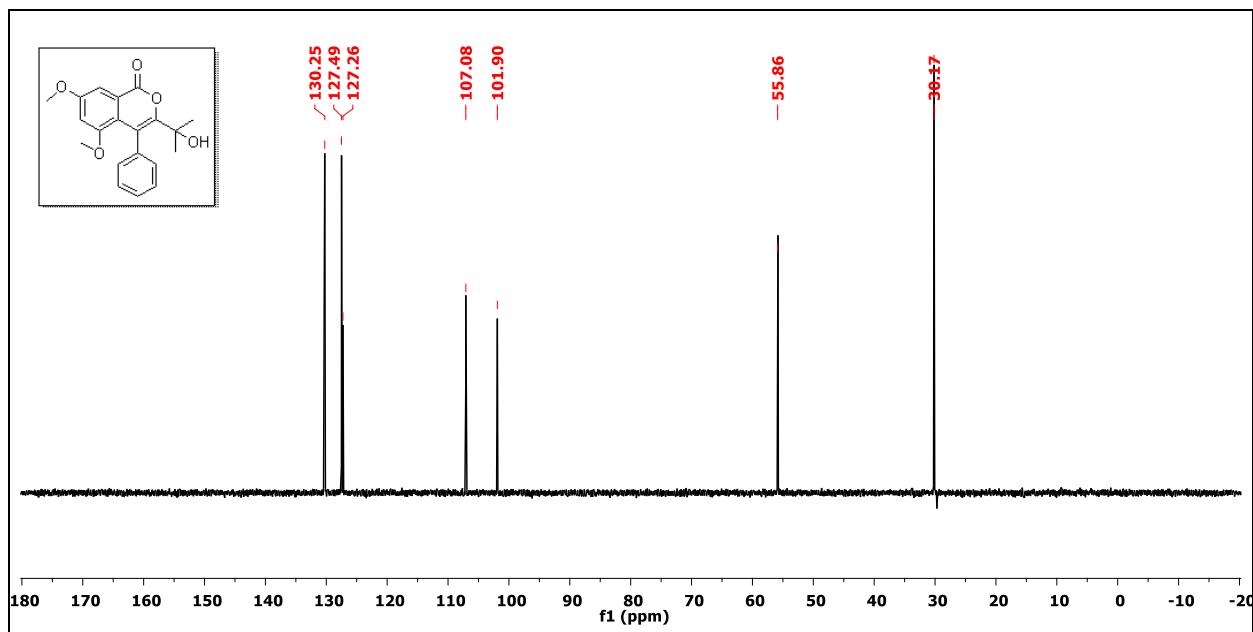
¹H and ¹³C spectra of compound 3ma



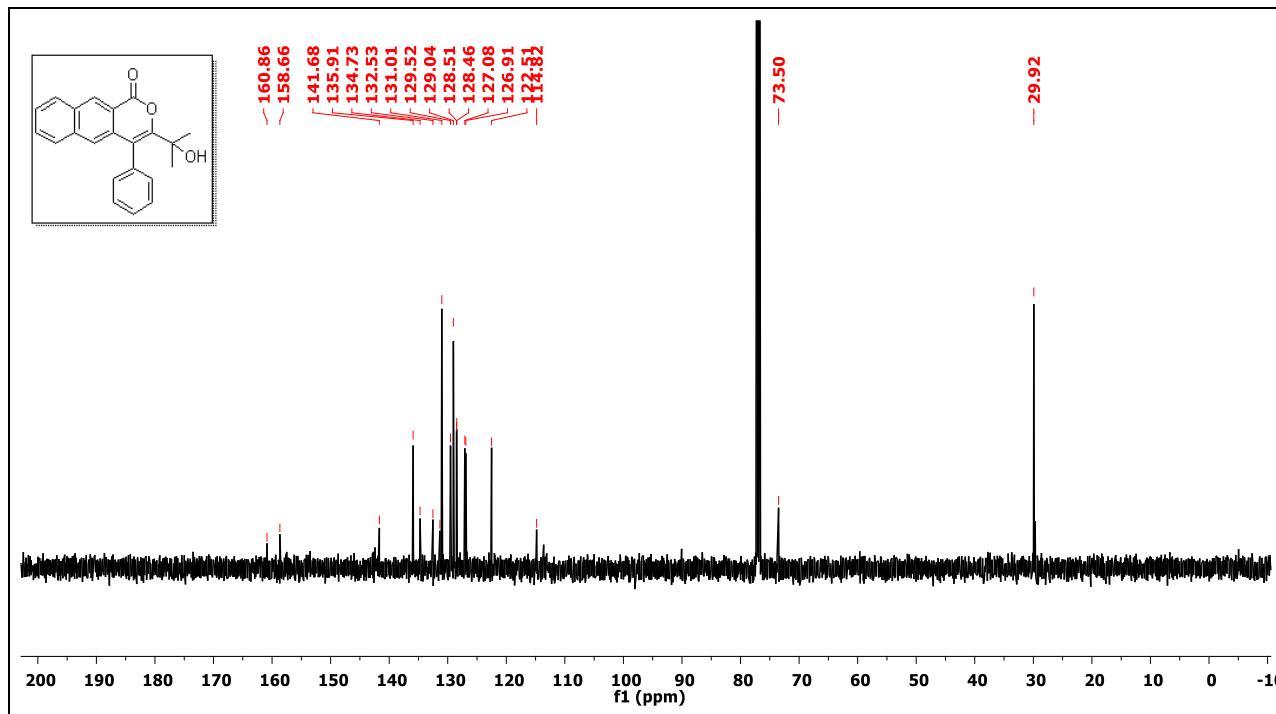
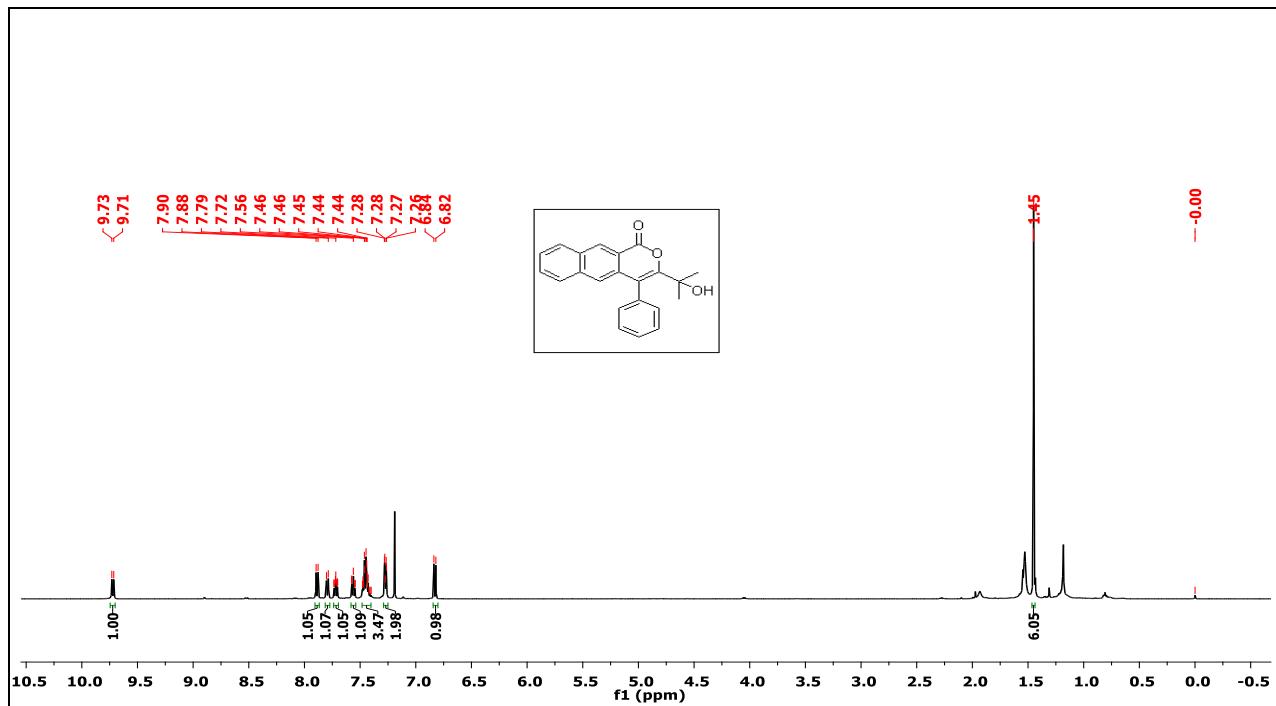
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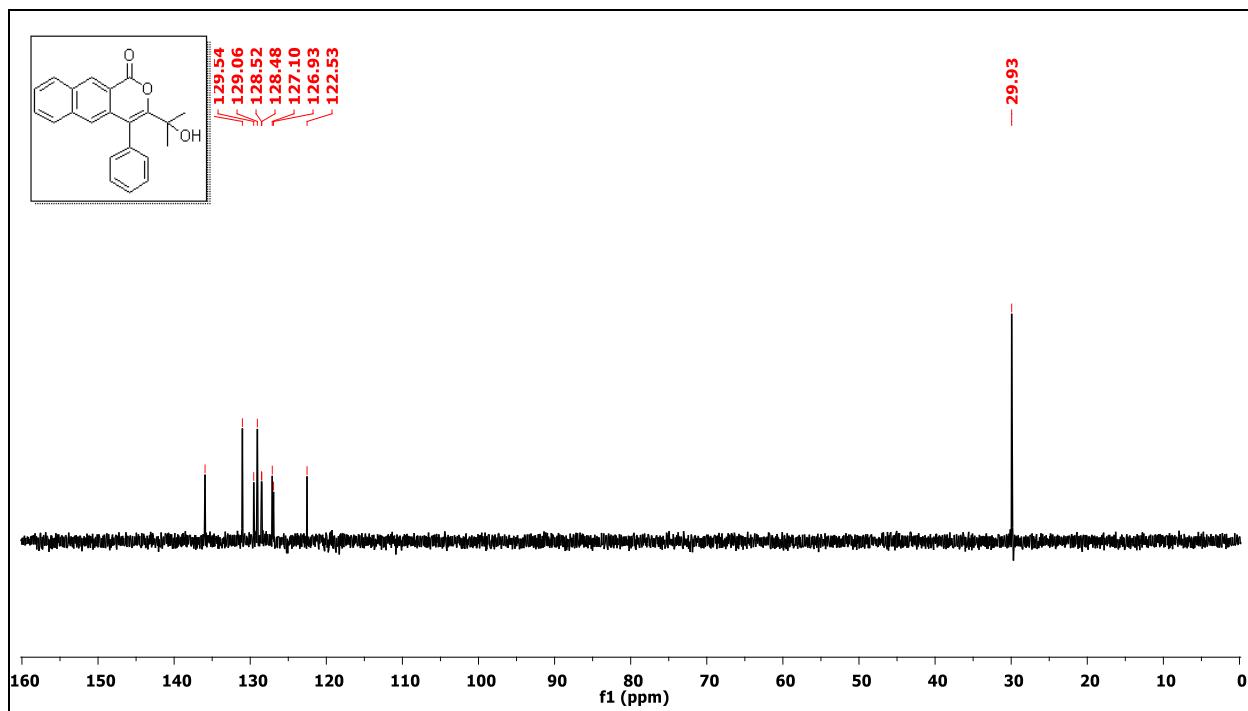
DEPT spectra of compound 3ma:



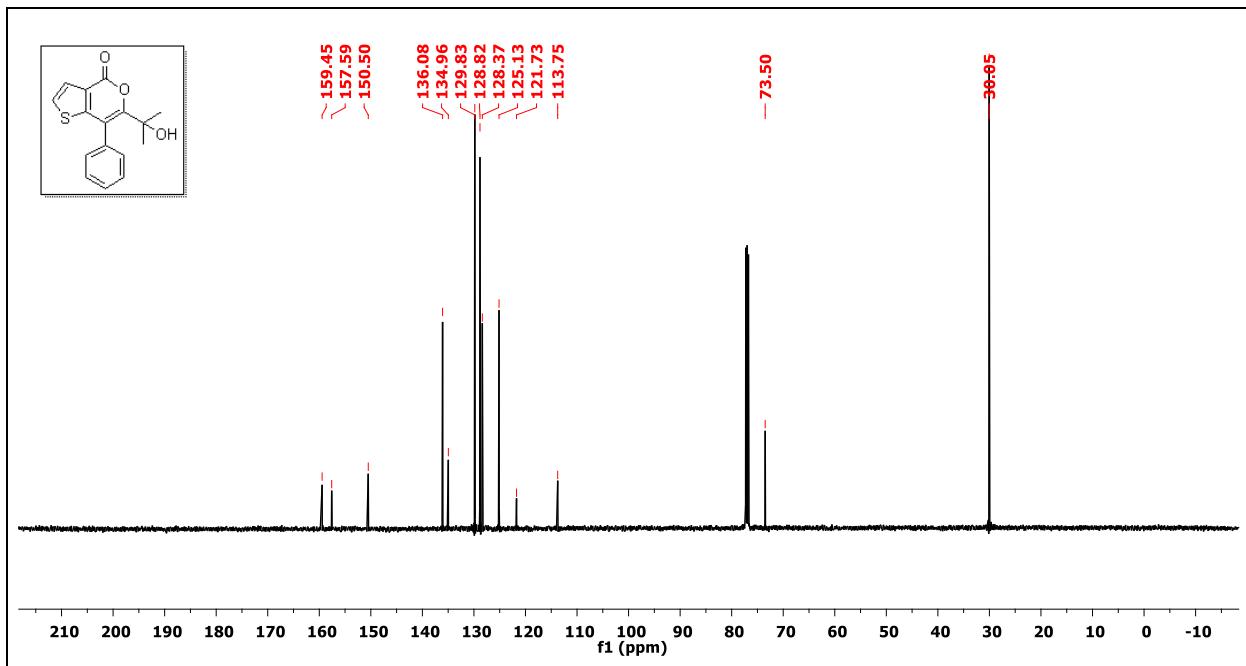
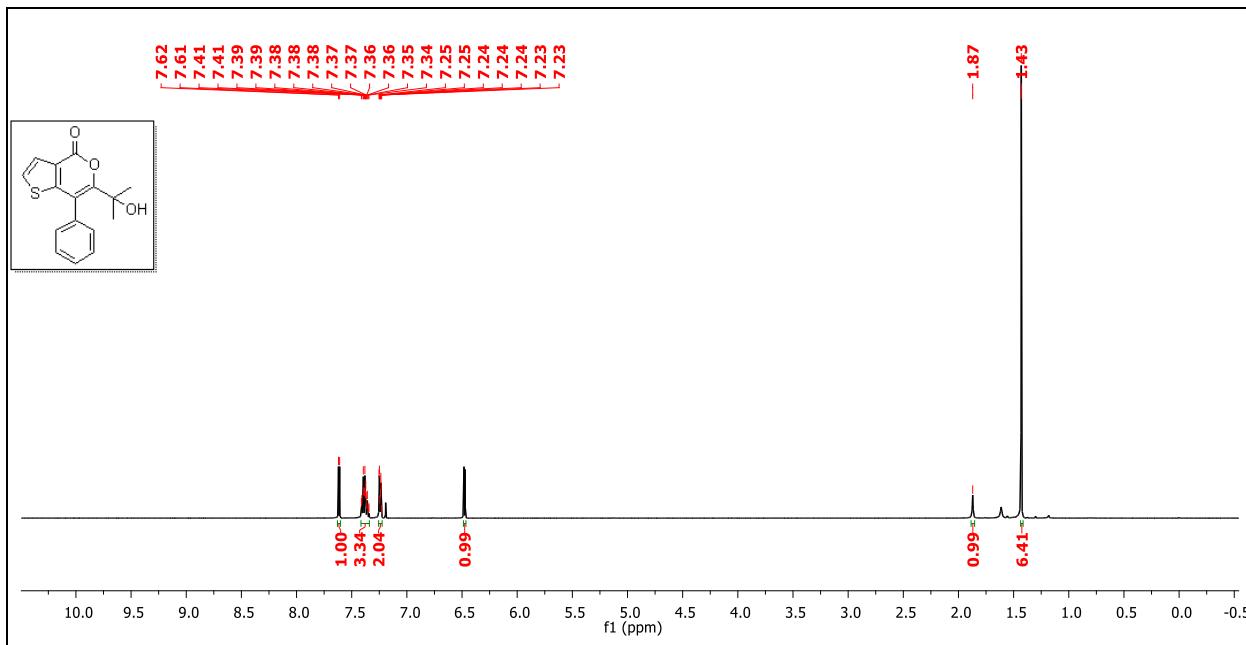
¹H and ¹³C spectra of compound 3na:



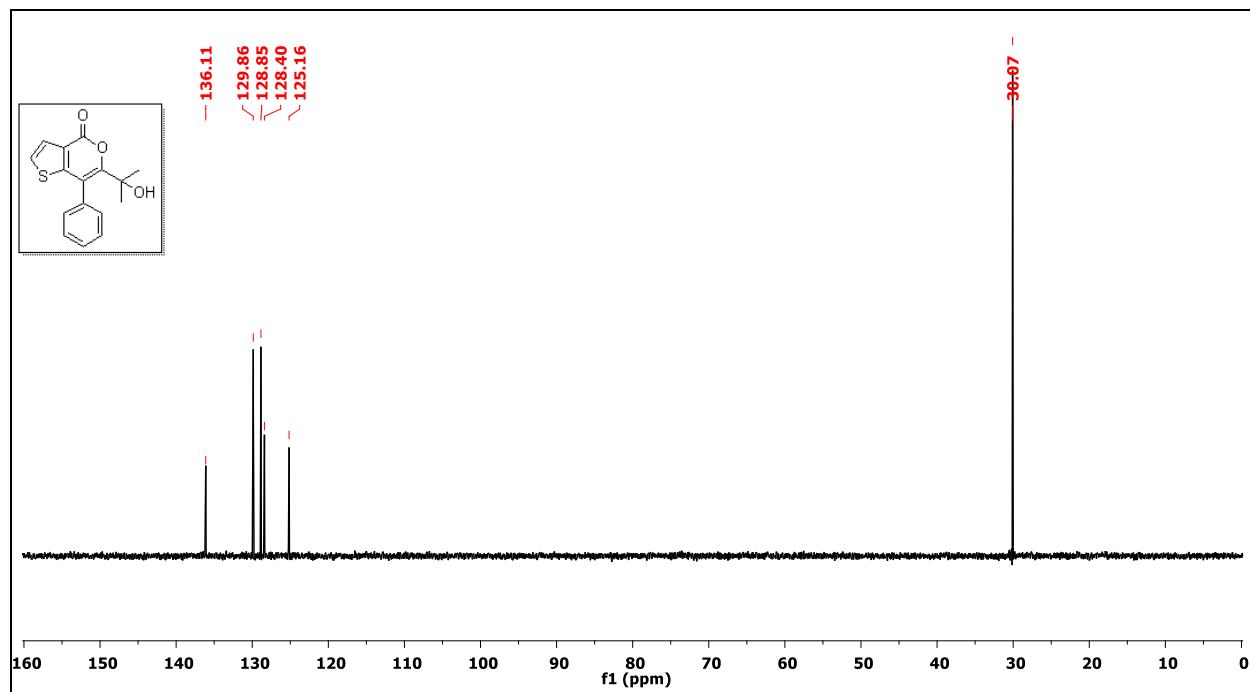
DEPT spectra of compound 3na:



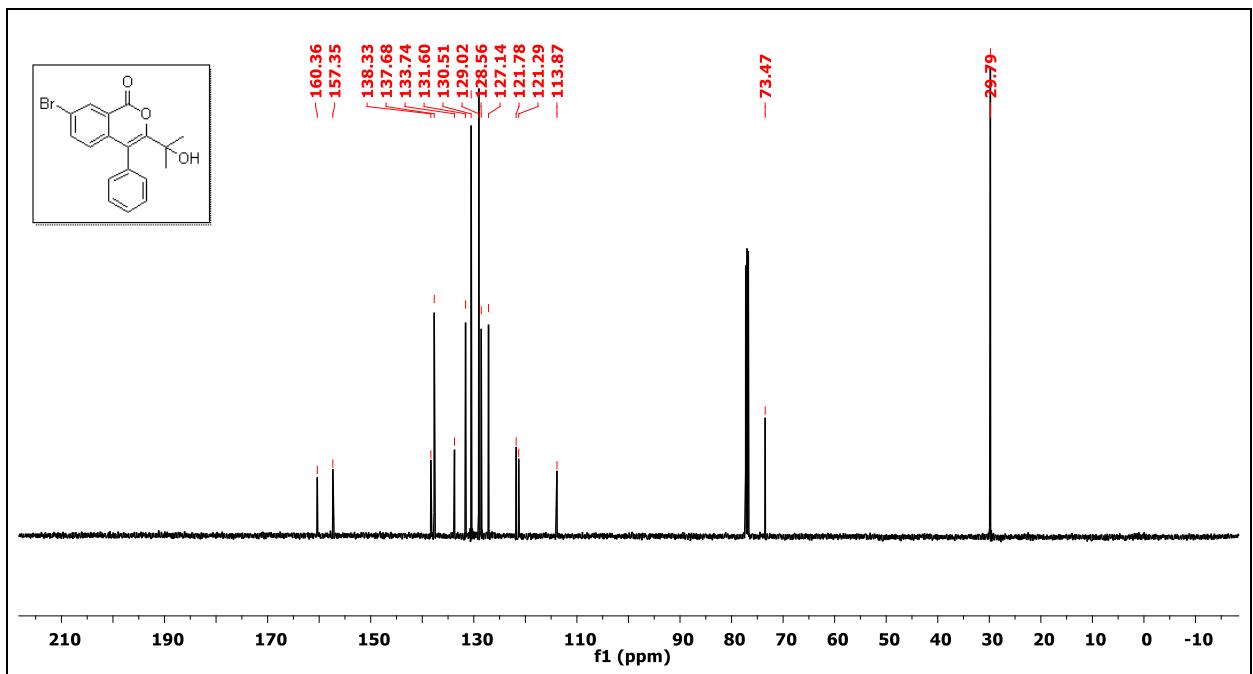
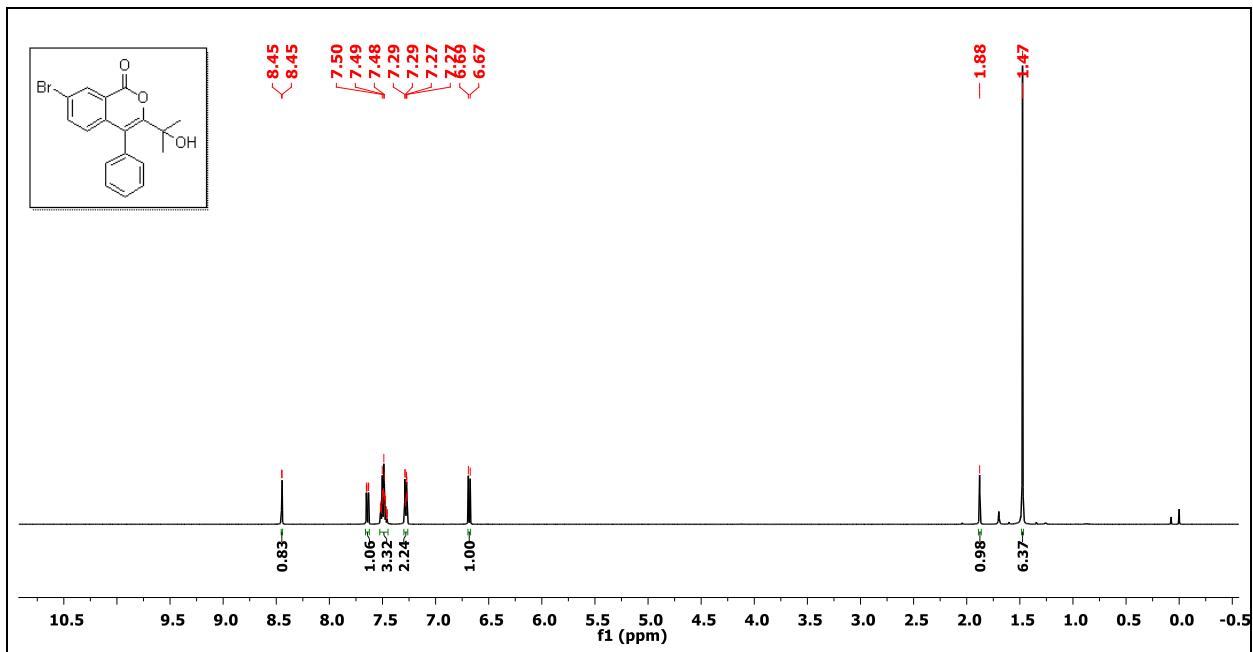
¹H and ¹³C spectra of compound 3oa:



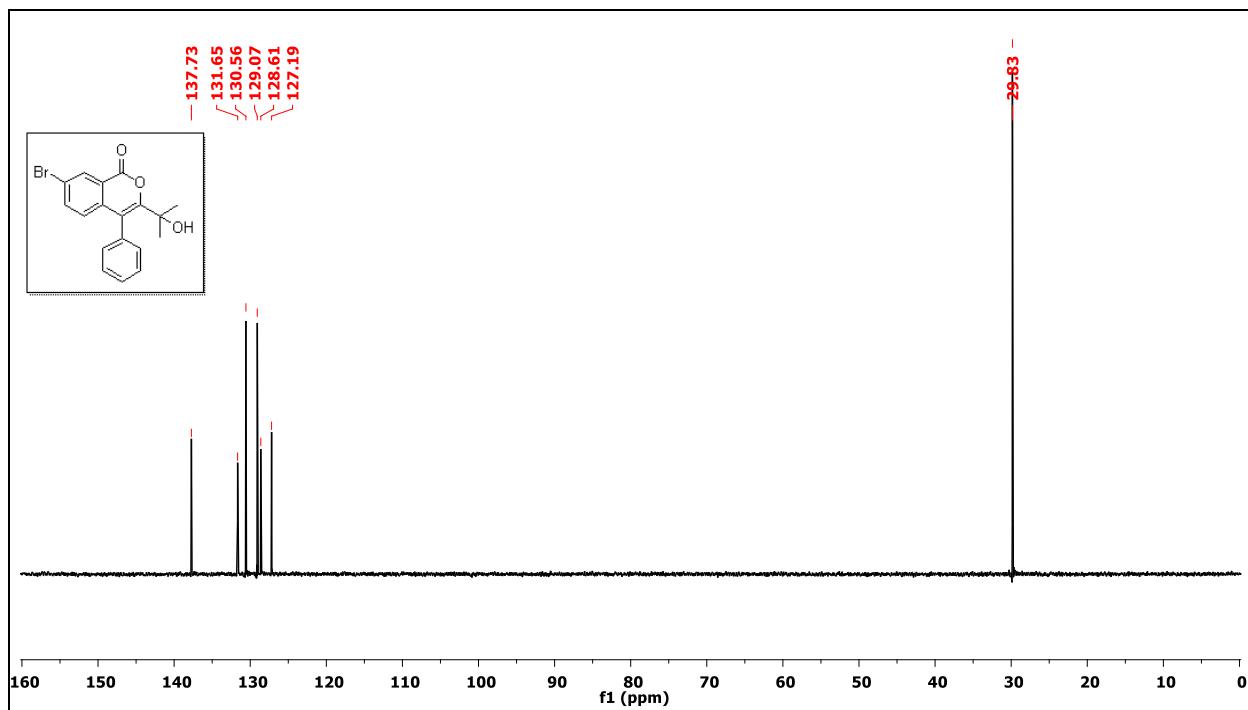
DEPT spectra of compound 3oa:



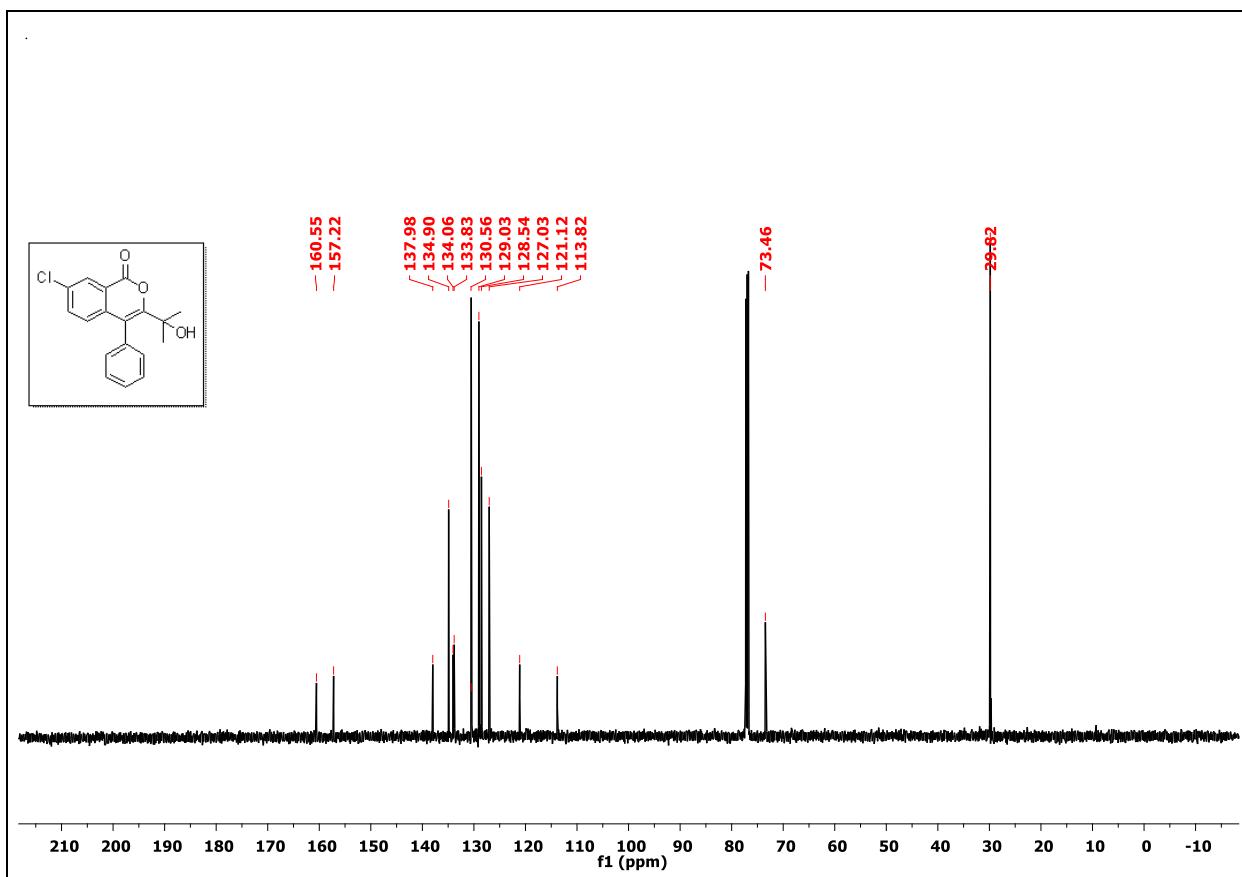
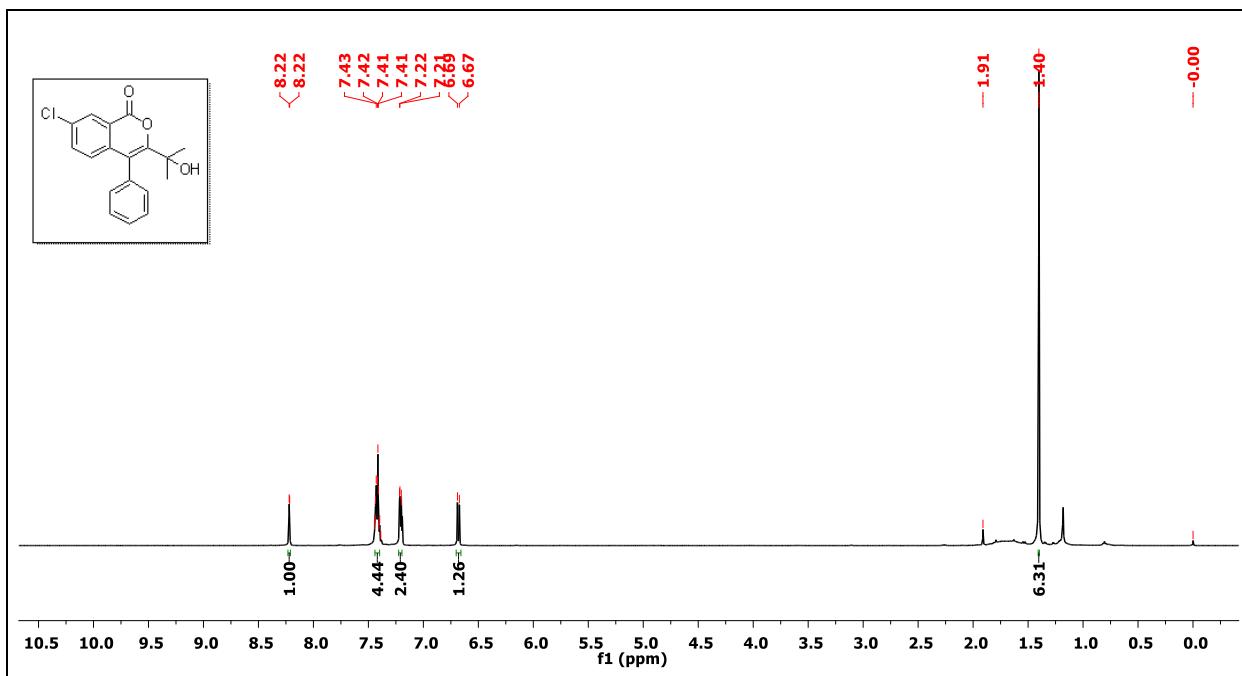
¹H and ¹³C spectra of compound 3ma:



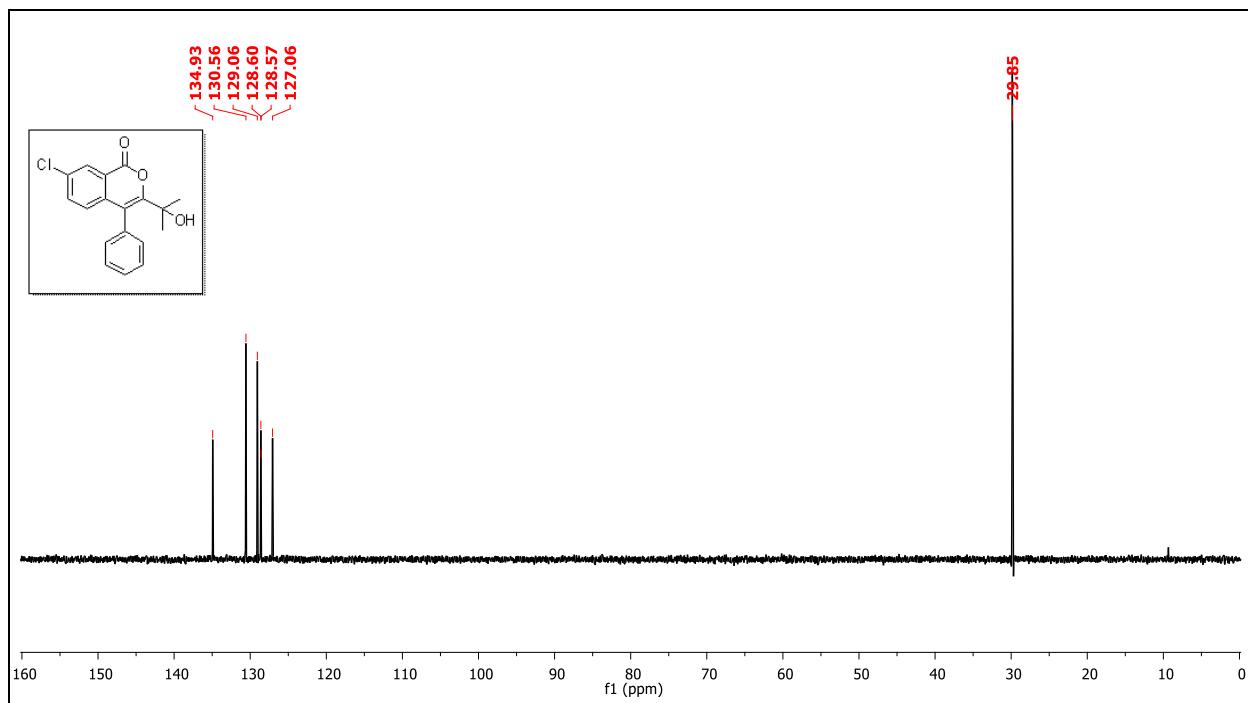
DEPT spectra of compound 3ma:



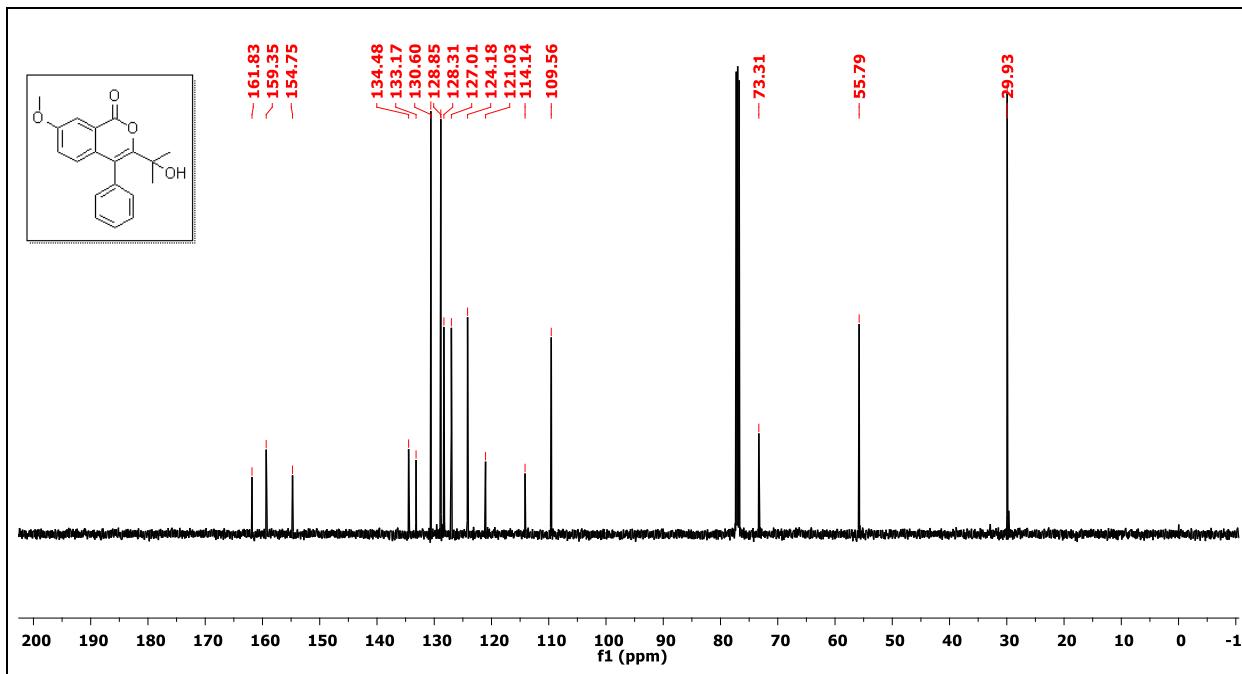
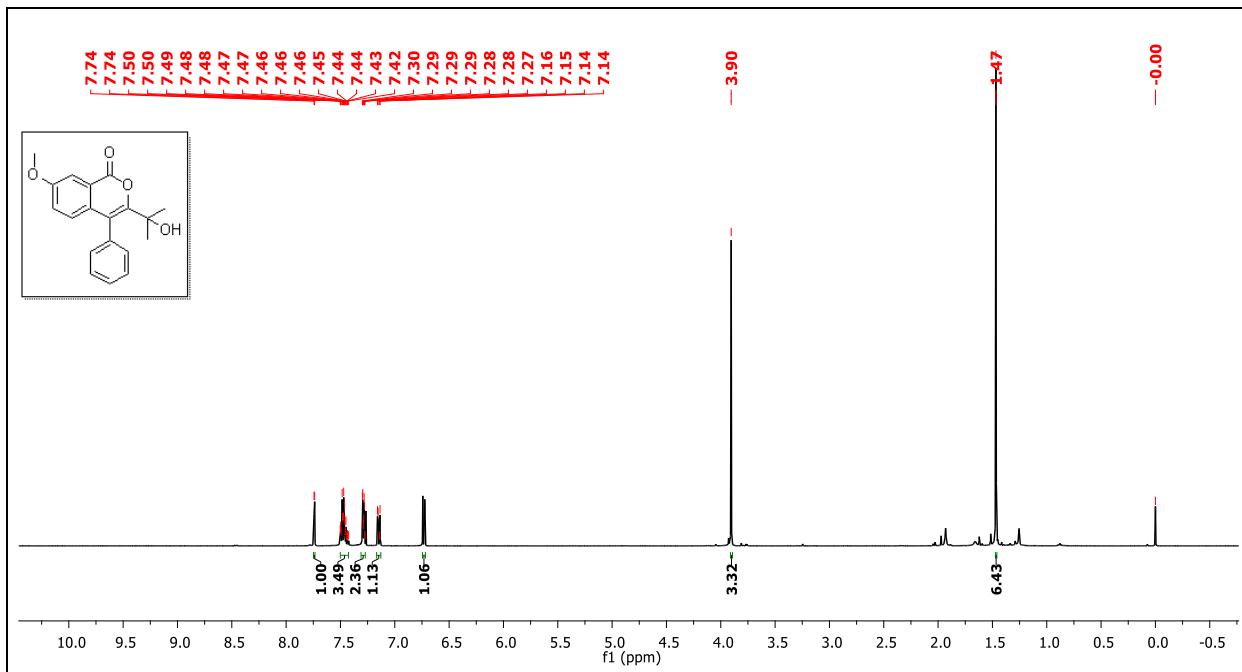
¹H and ¹³C spectra of compound 3na:



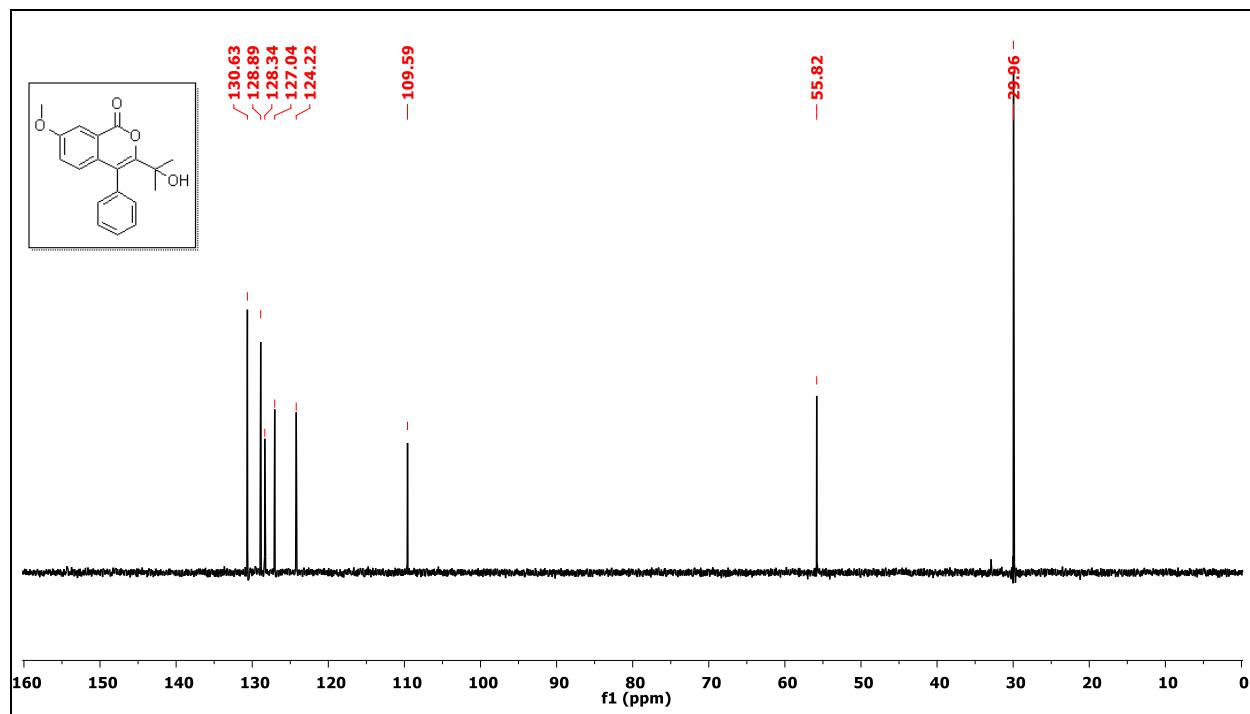
DEPT spectra of compound 3ma:



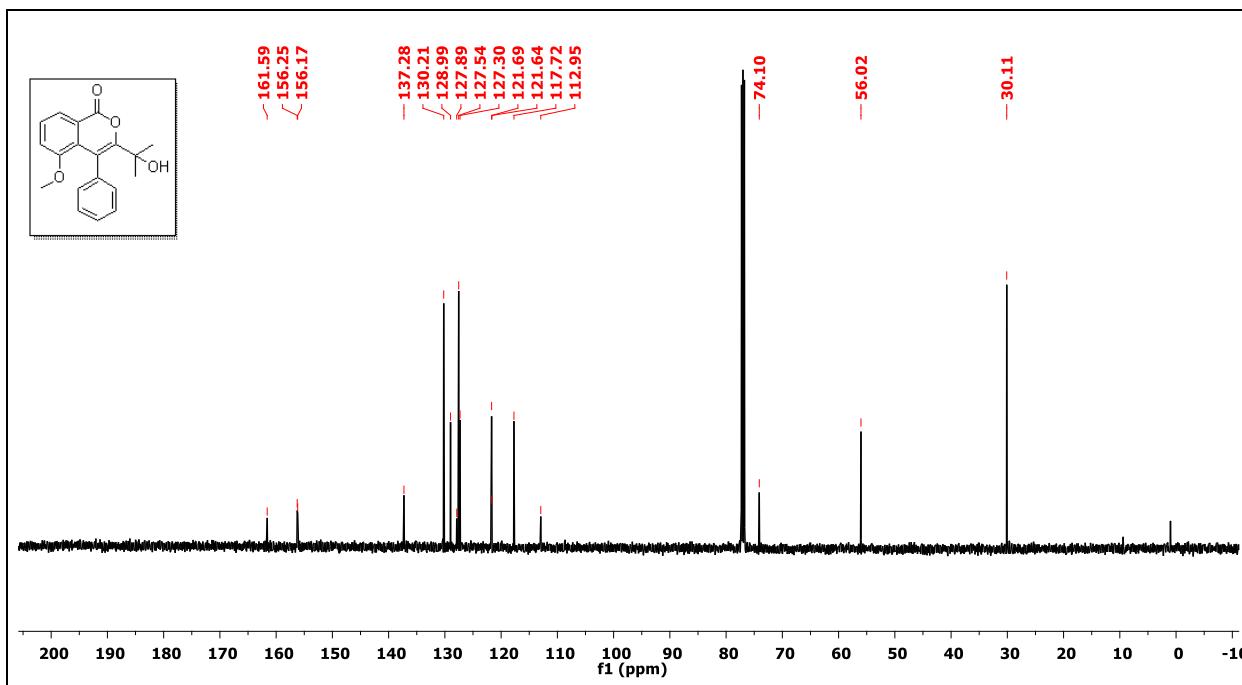
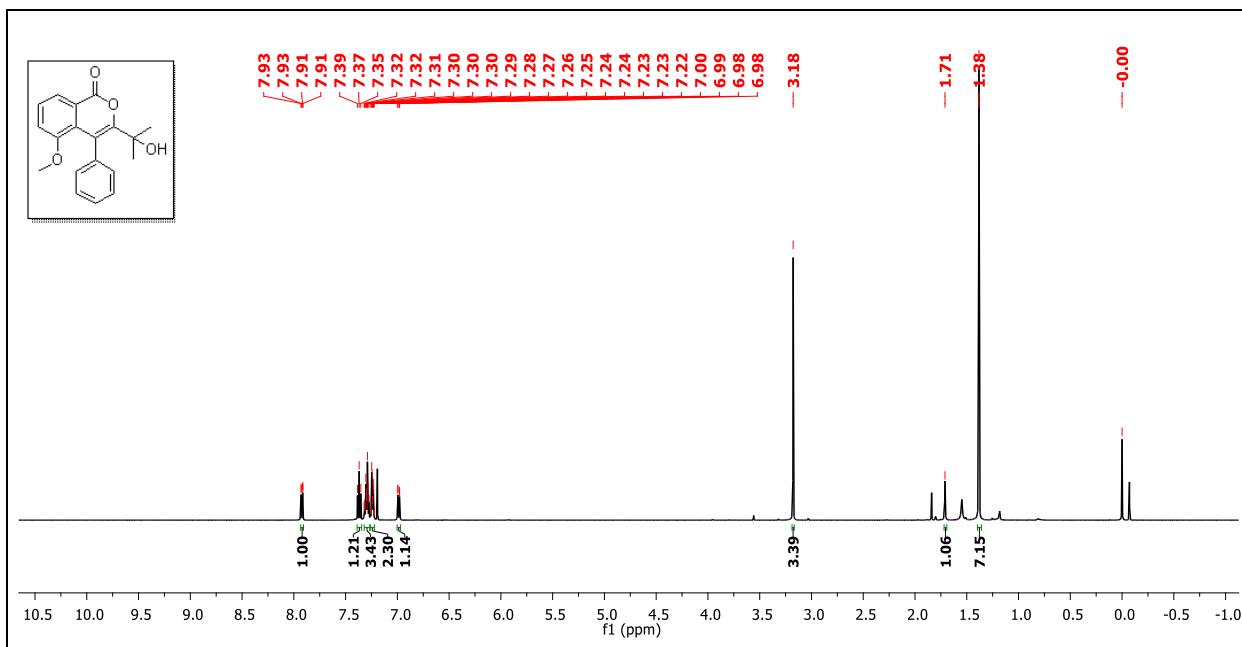
¹H and ¹³C spectra of compound 3ra:



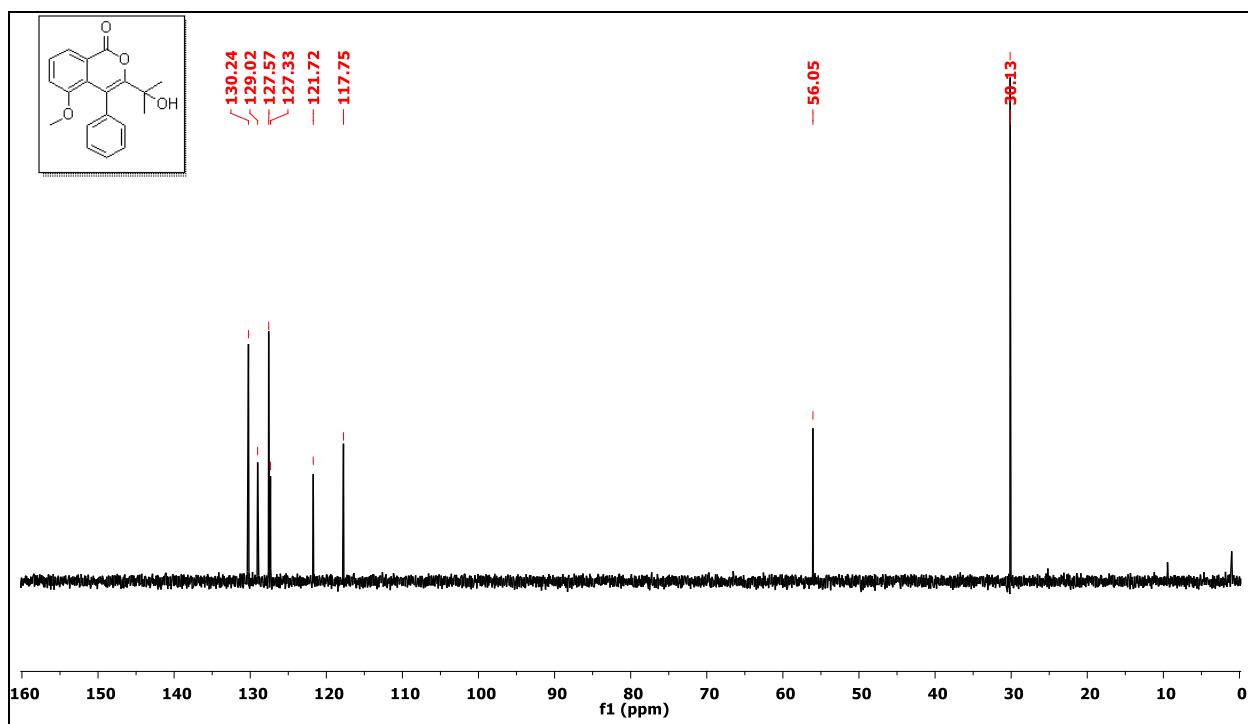
DEPT spectra of compound 3ra:



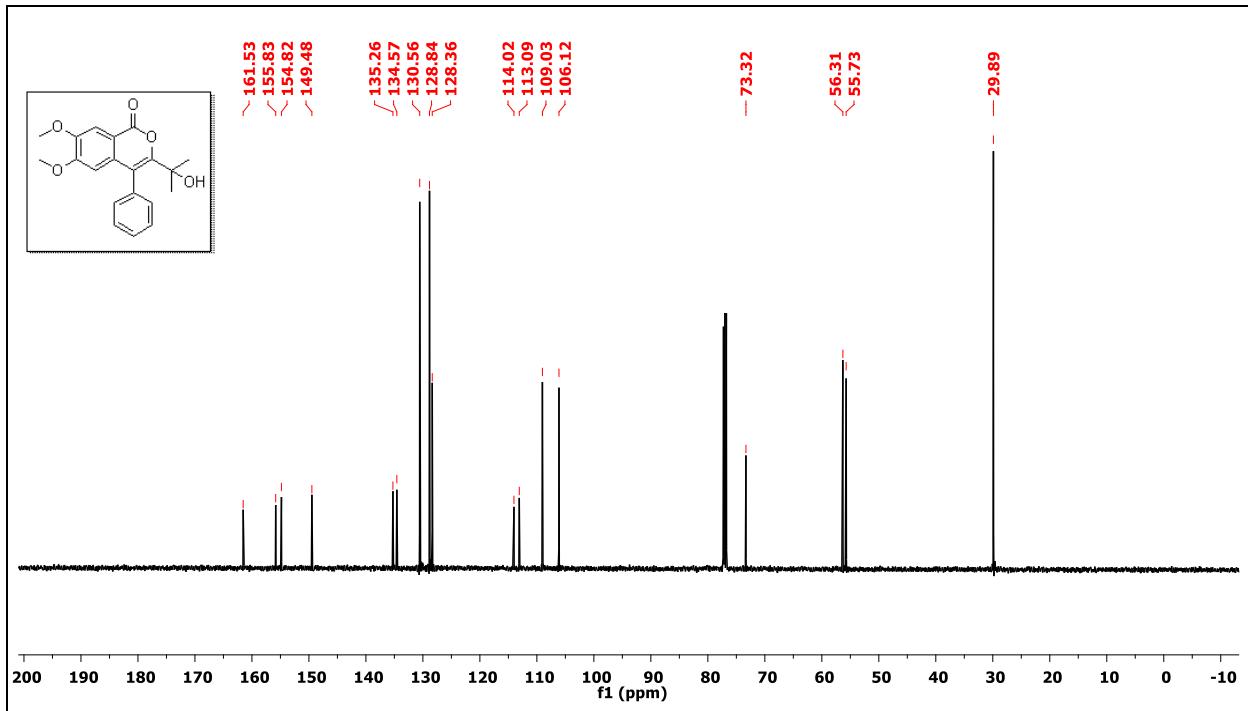
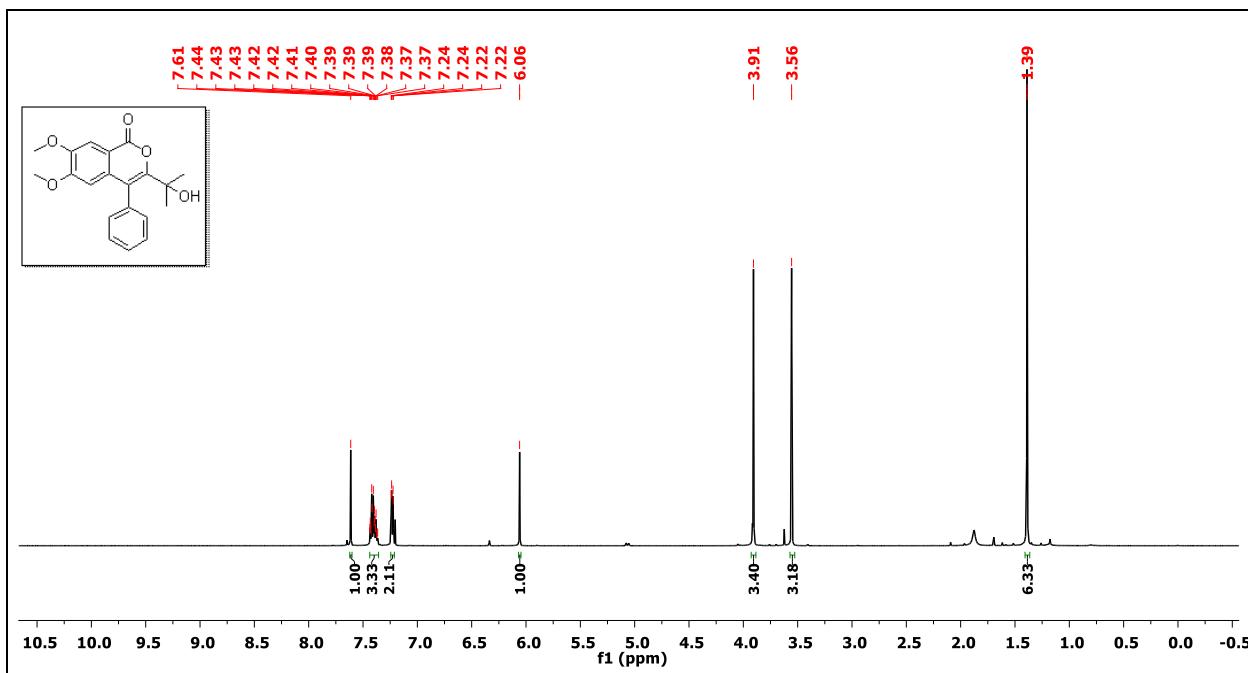
¹H and ¹³C spectra of compound 3ra':



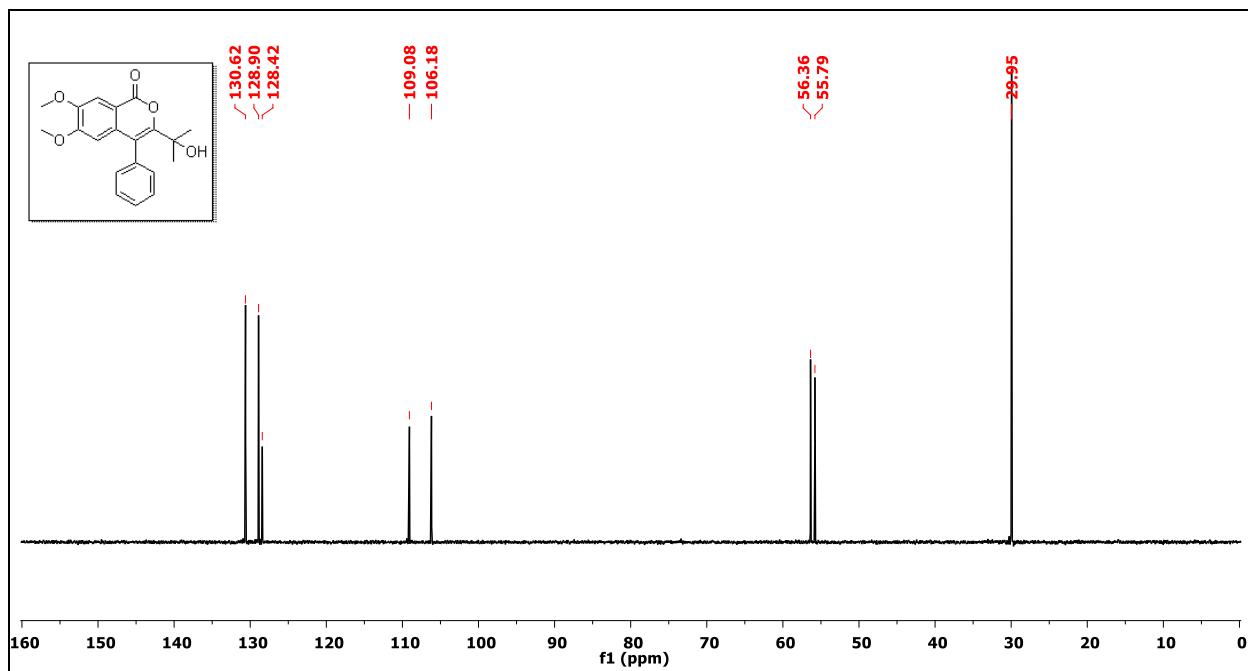
DEPT spectra of compound 3ra':



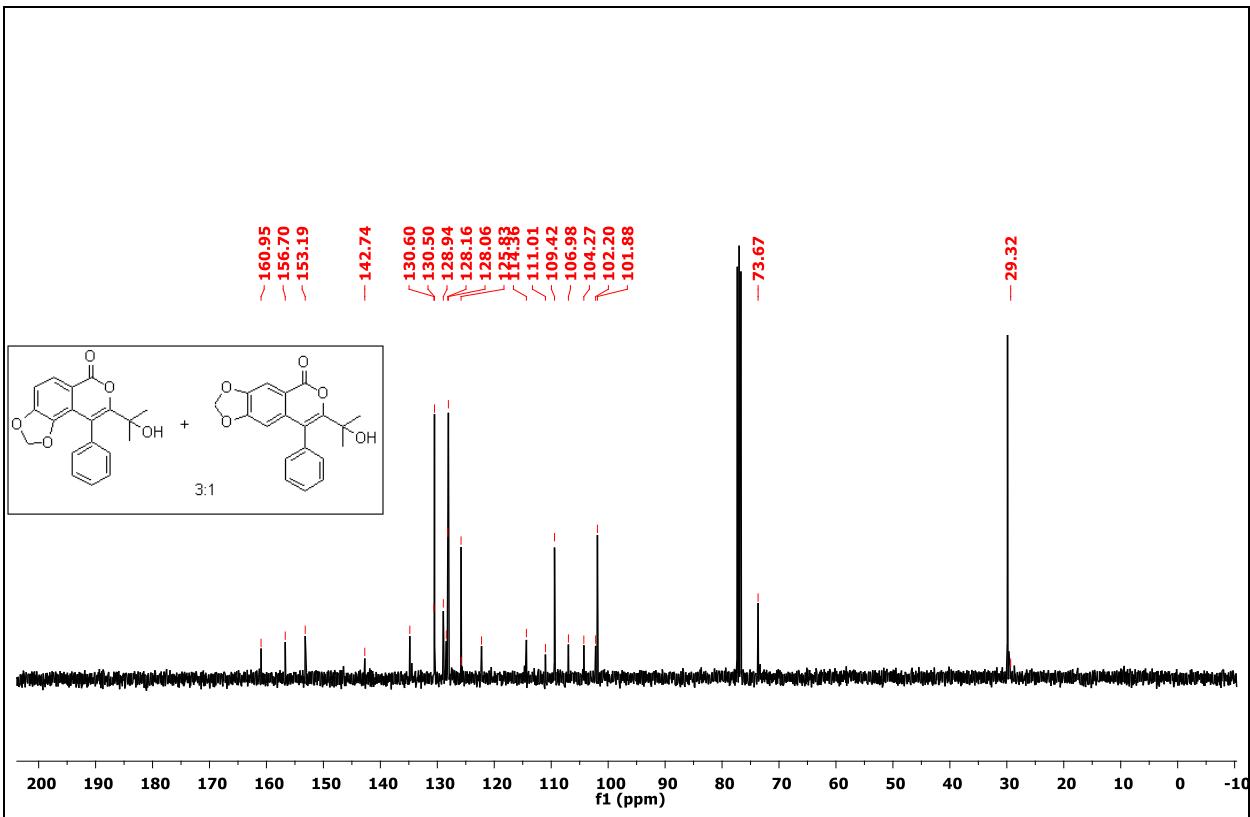
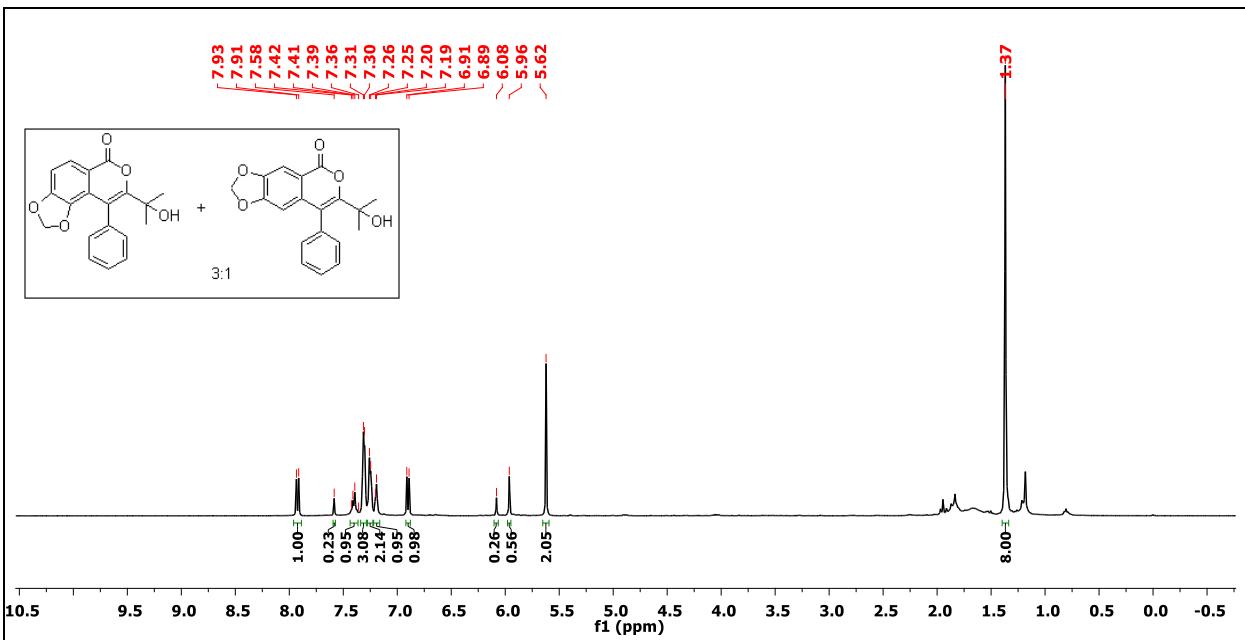
¹H and ¹³C spectra of compound 3sa:



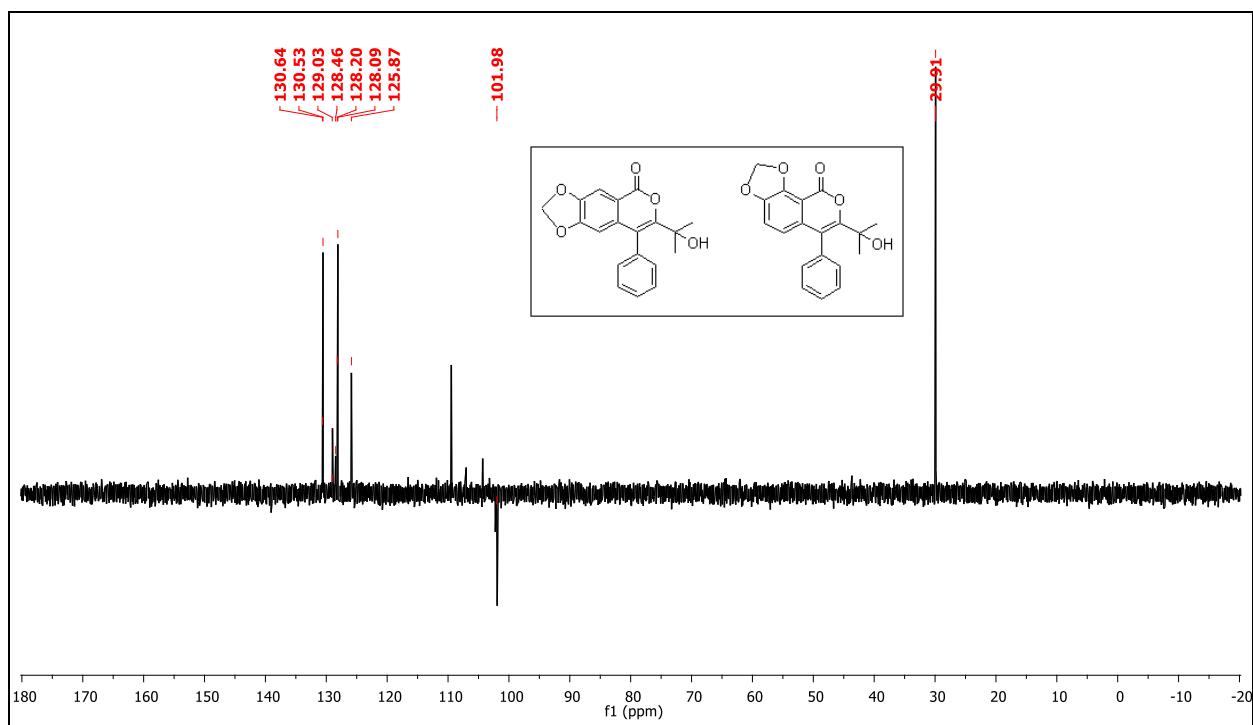
DEPT spectra of compound 3sa:



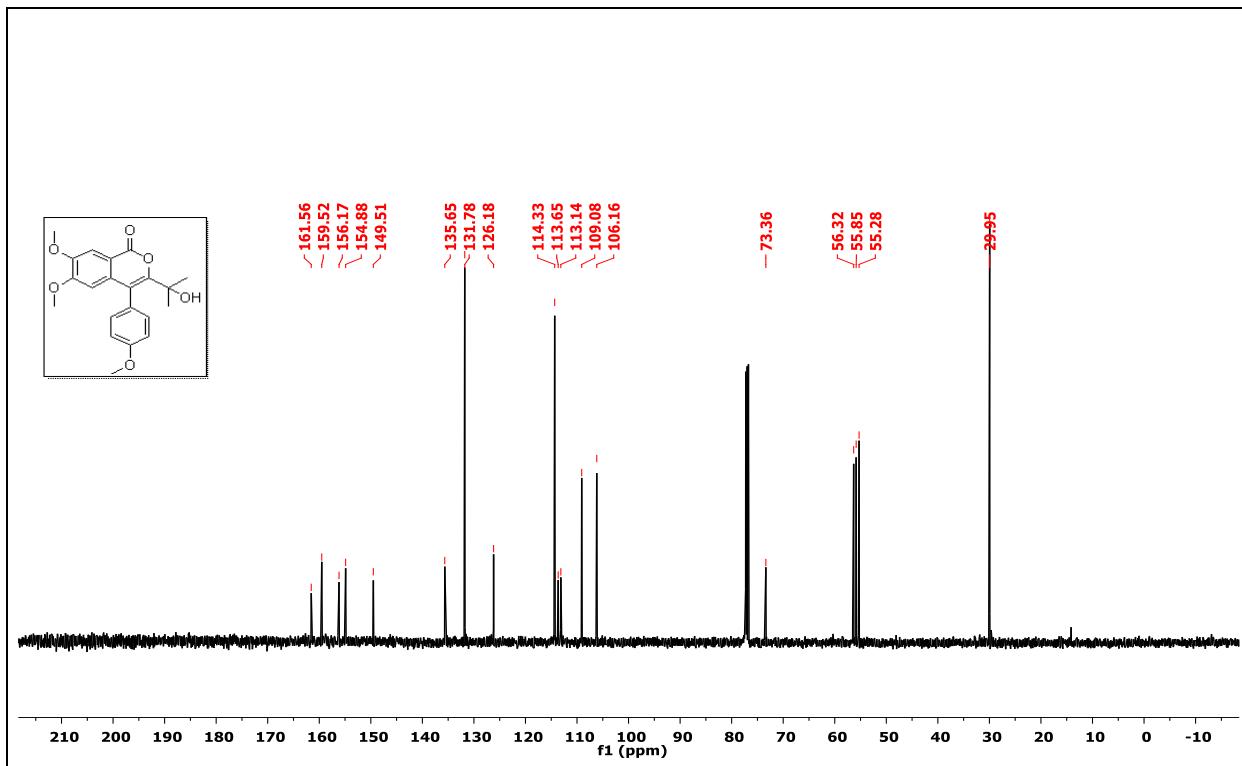
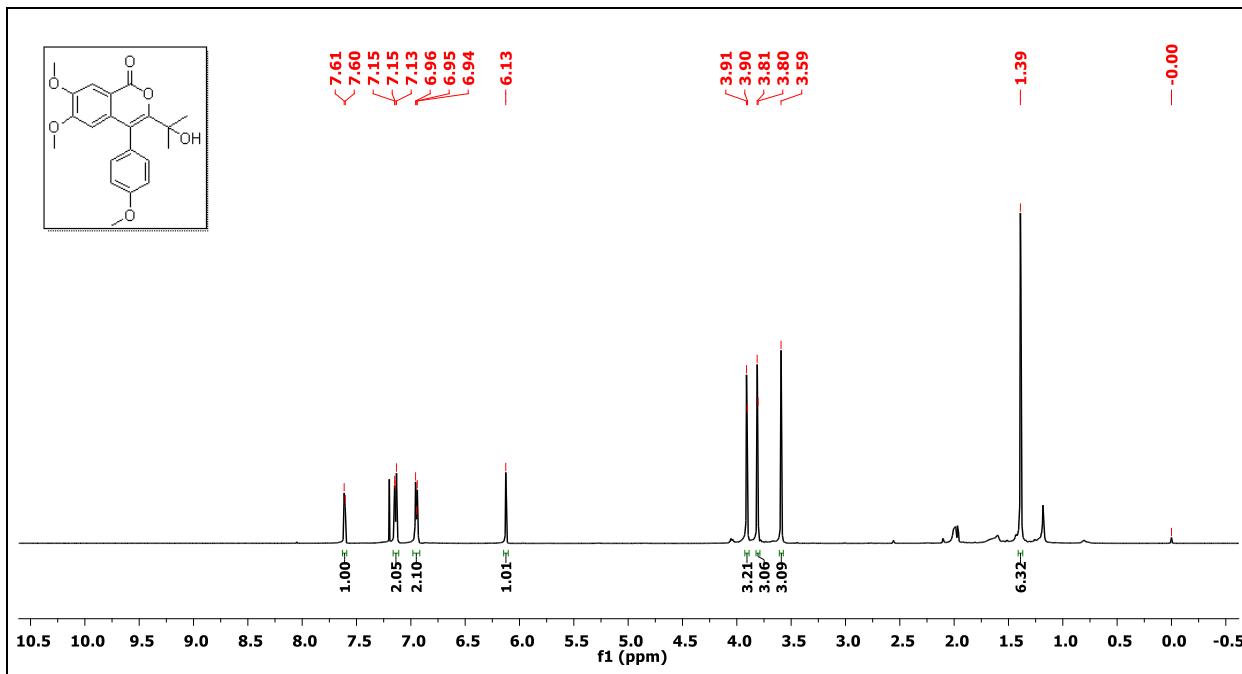
¹H and ¹³C spectra of compound 3ta:



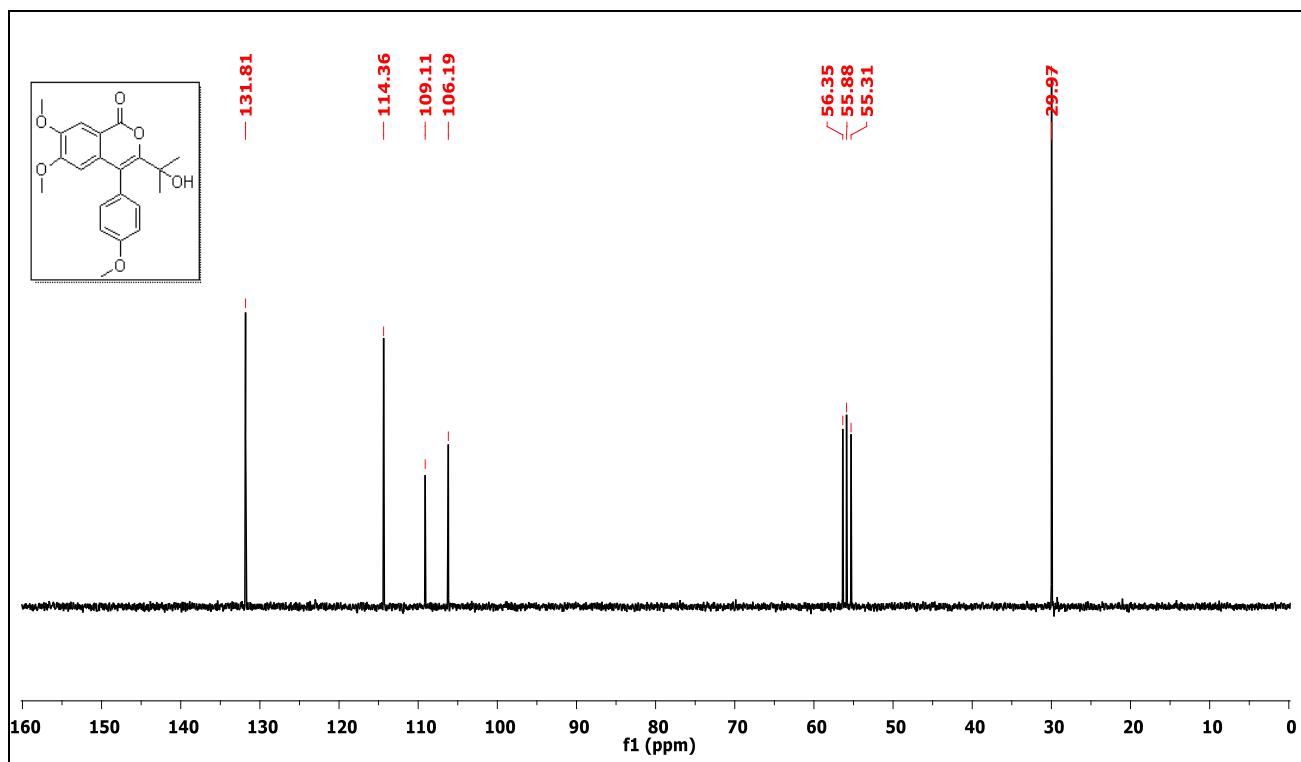
DEPT spectra of compound 3ta:



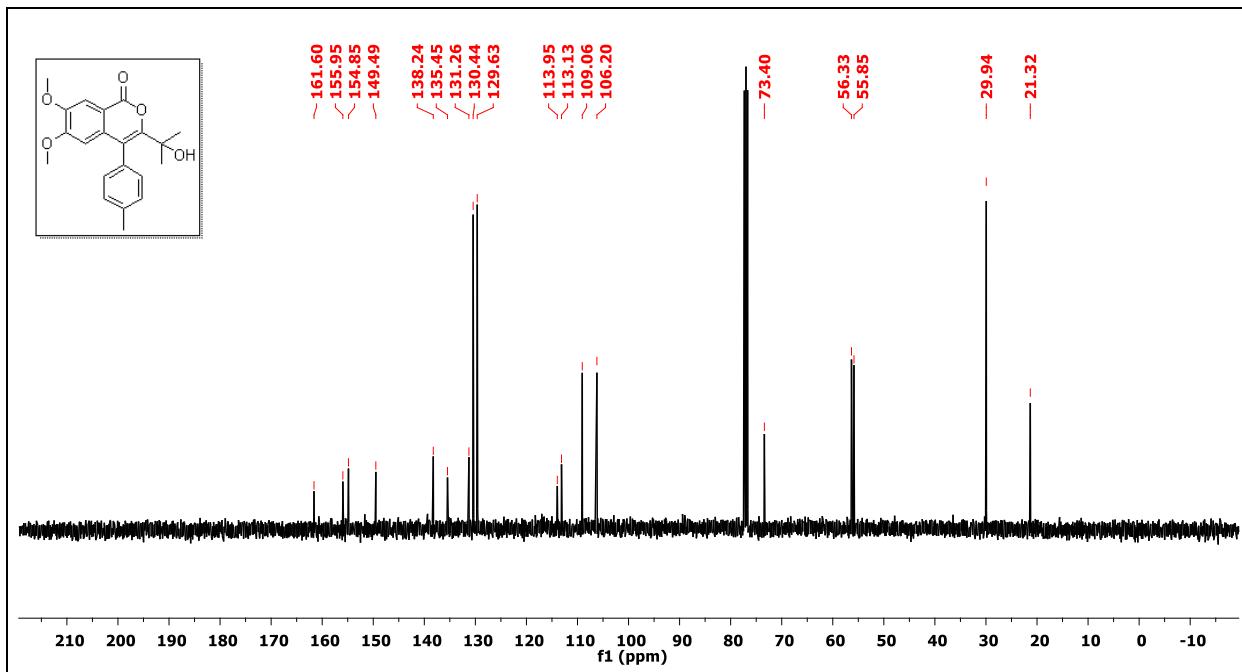
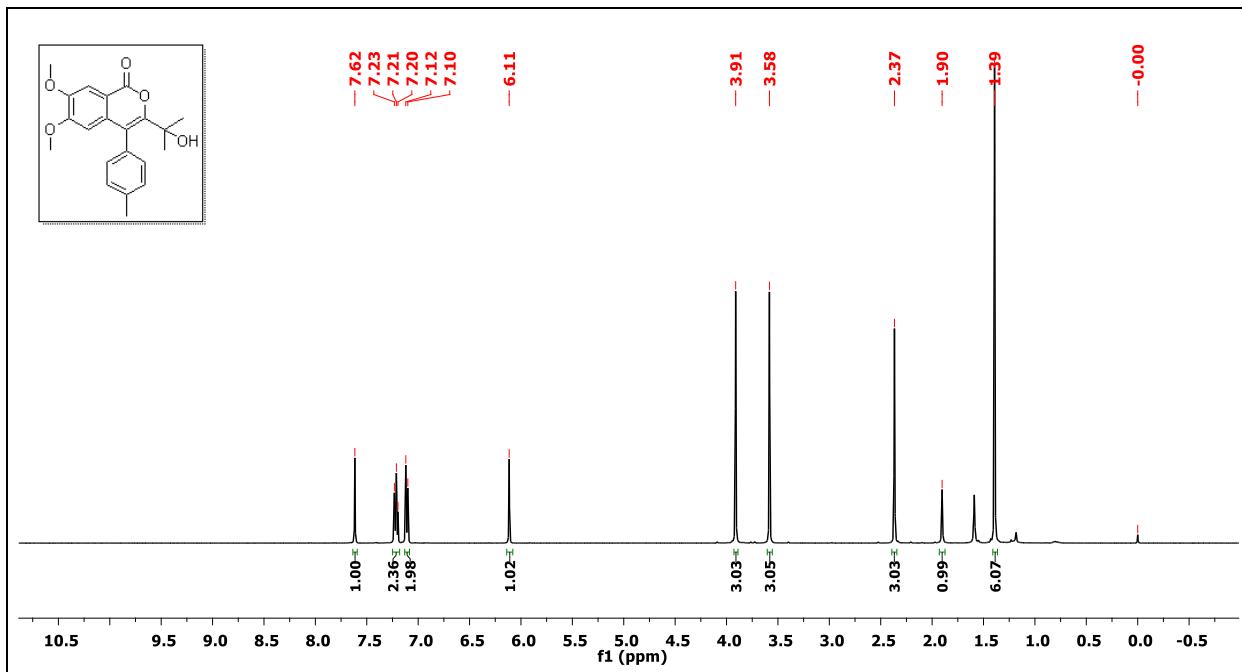
¹H and ¹³C spectra of compound 3sb:



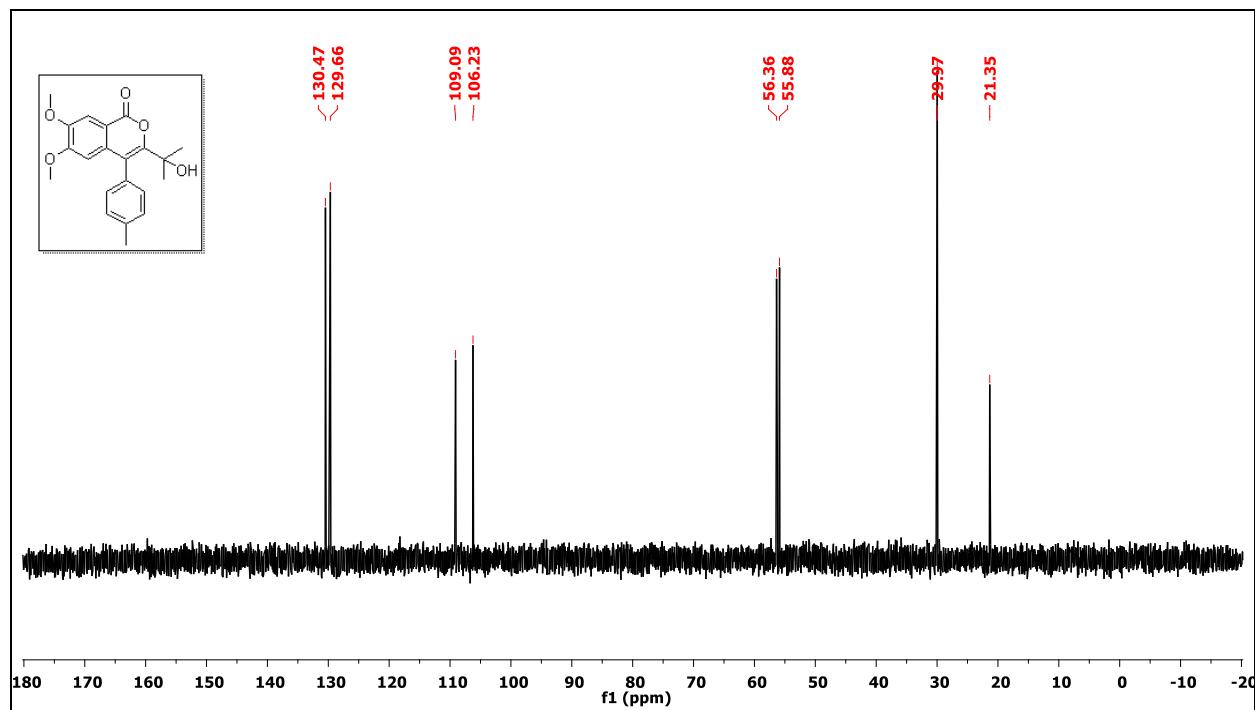
DEPT spectra of compound 3sb:



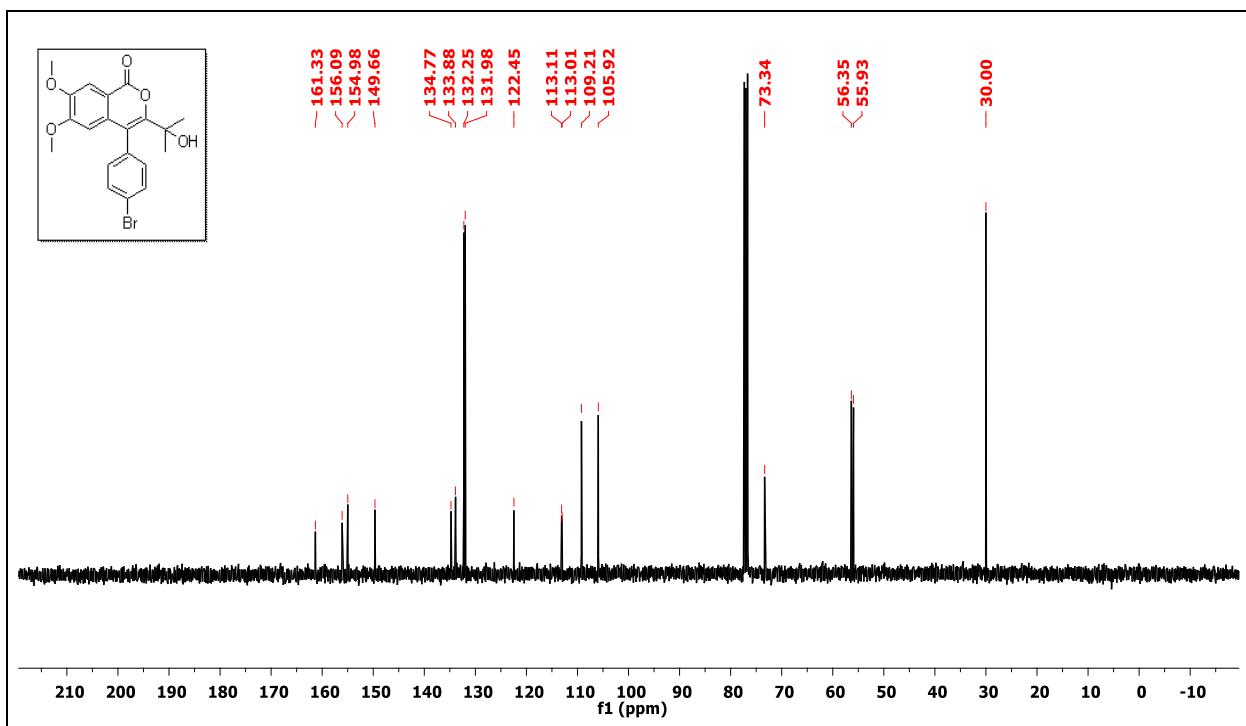
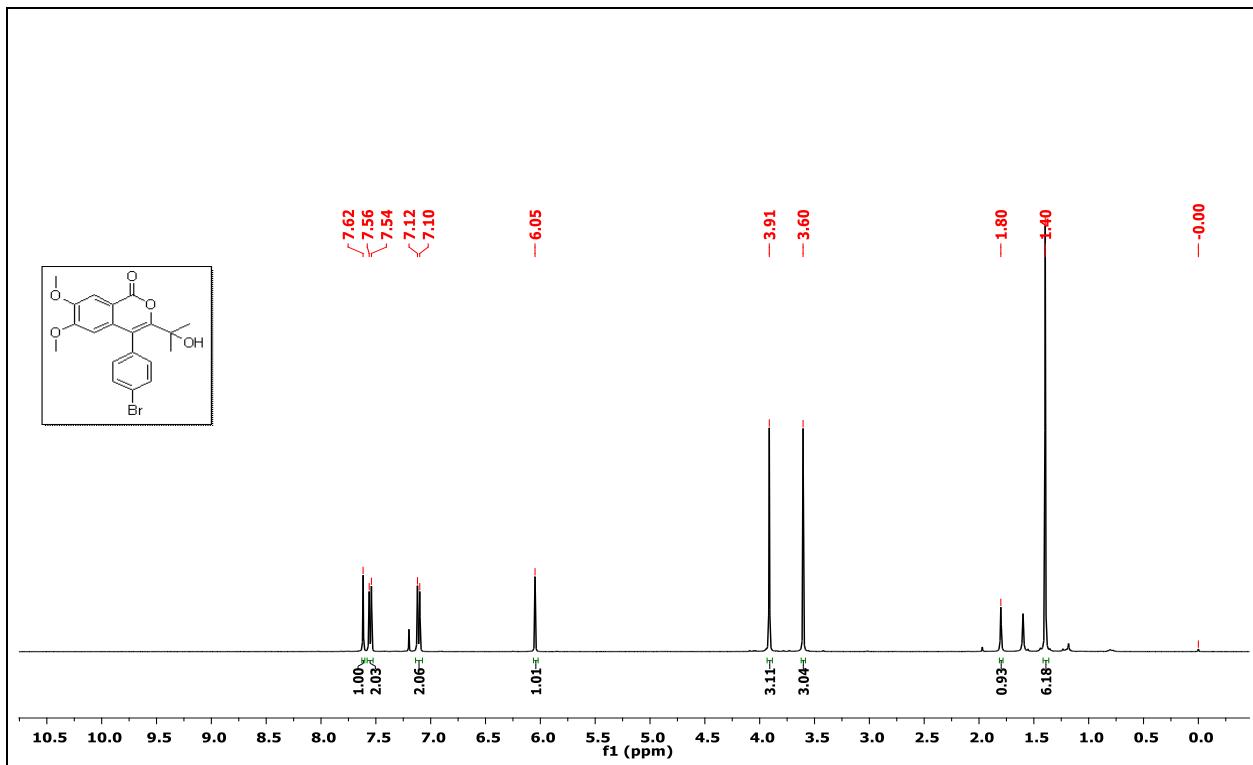
¹H and ¹³C spectra of compound 3sc:



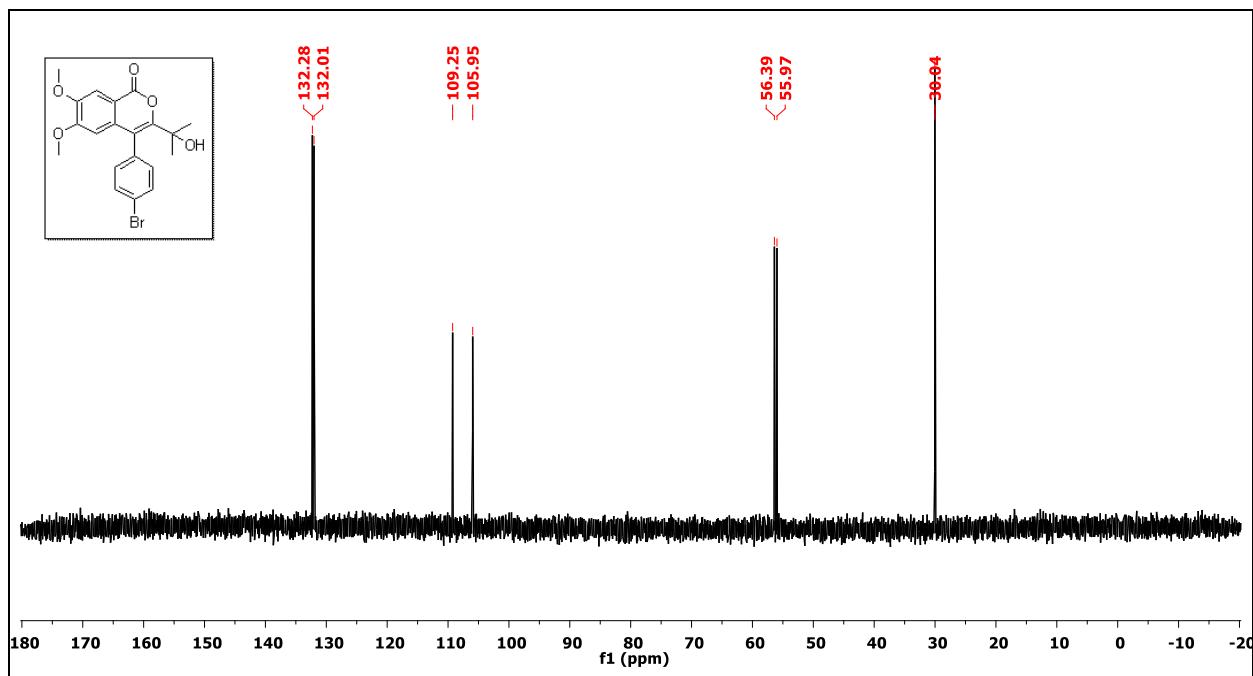
DEPT spectra of compound 3sc:



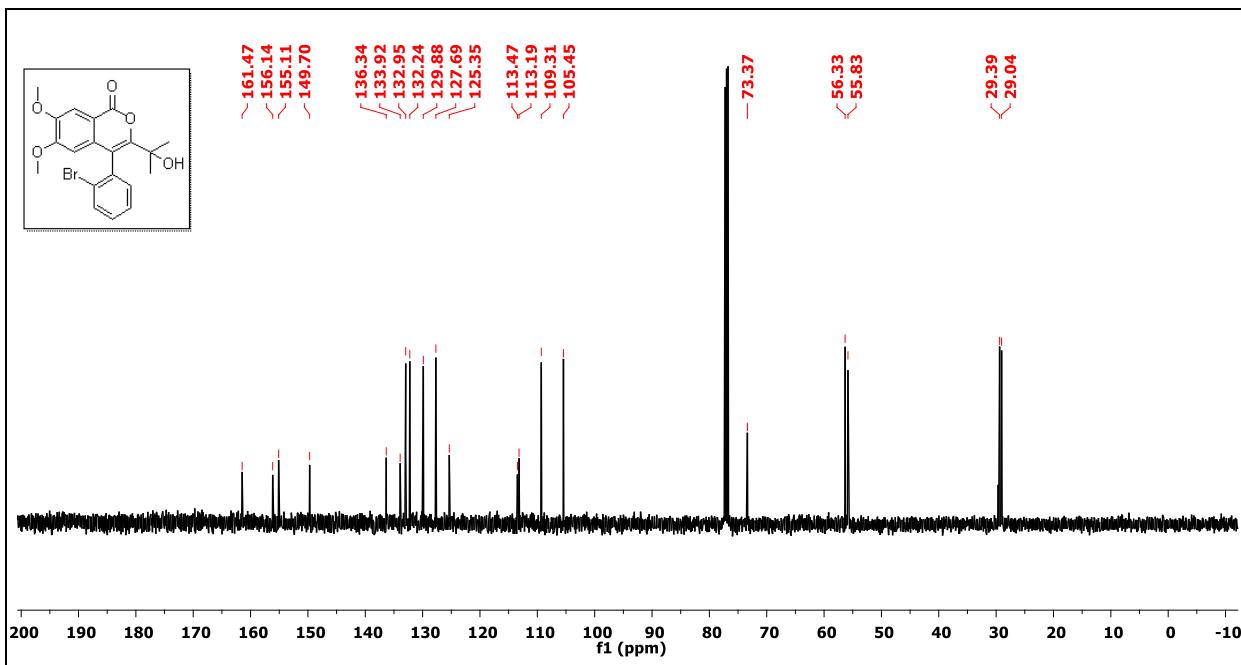
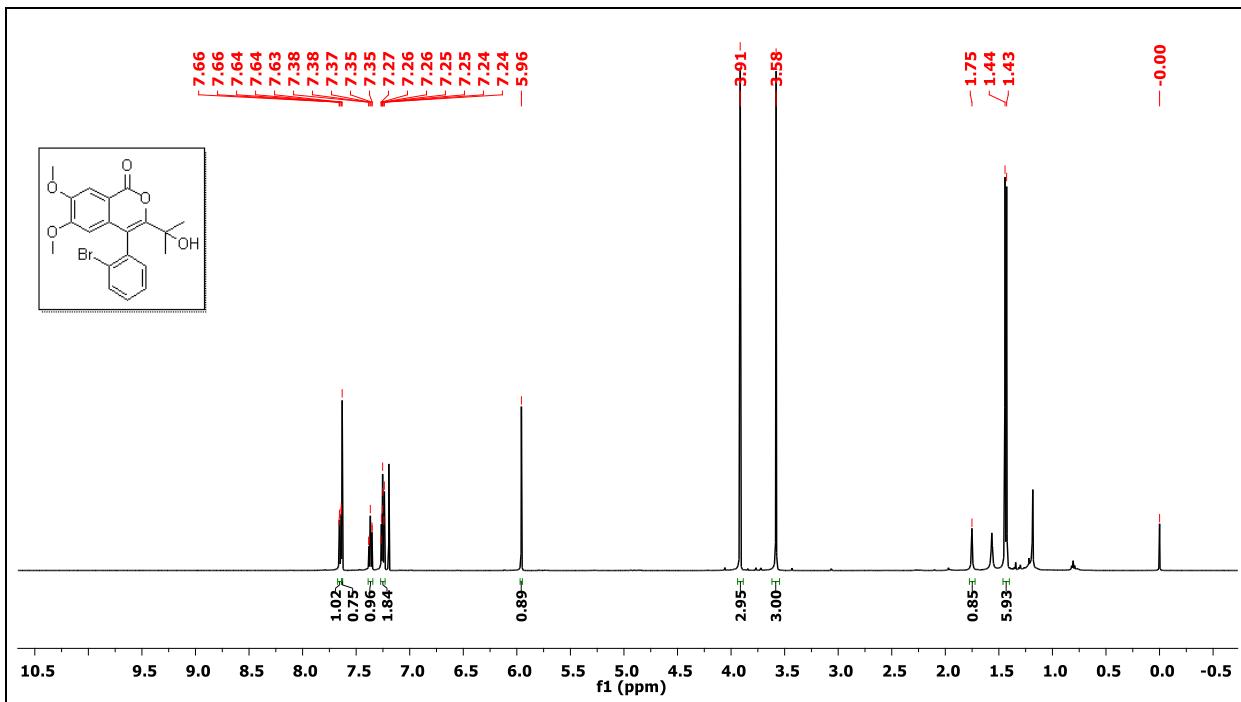
¹H and ¹³C spectra of compound 3sd:



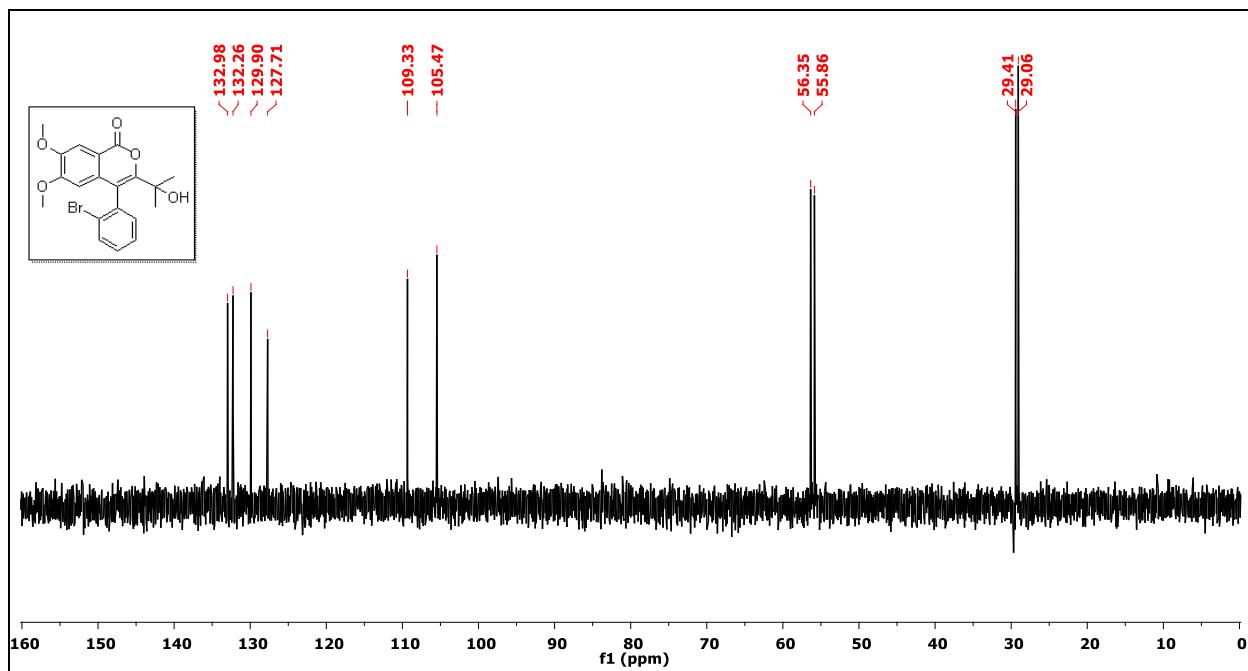
DEPT spectra of compound 3sd:



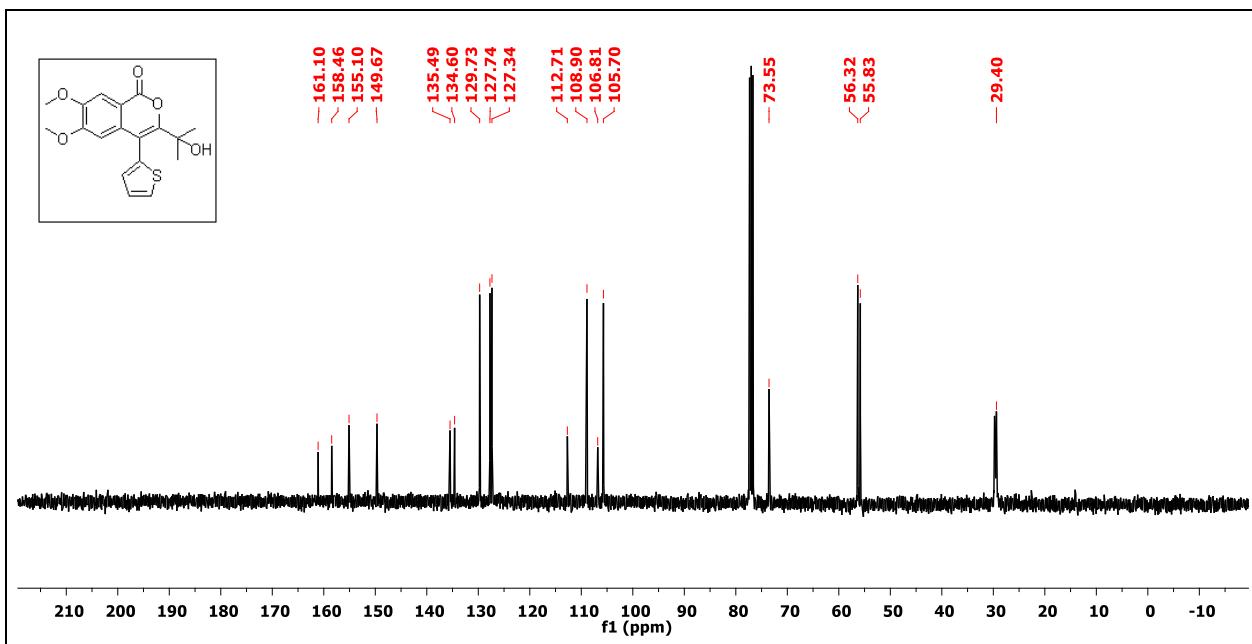
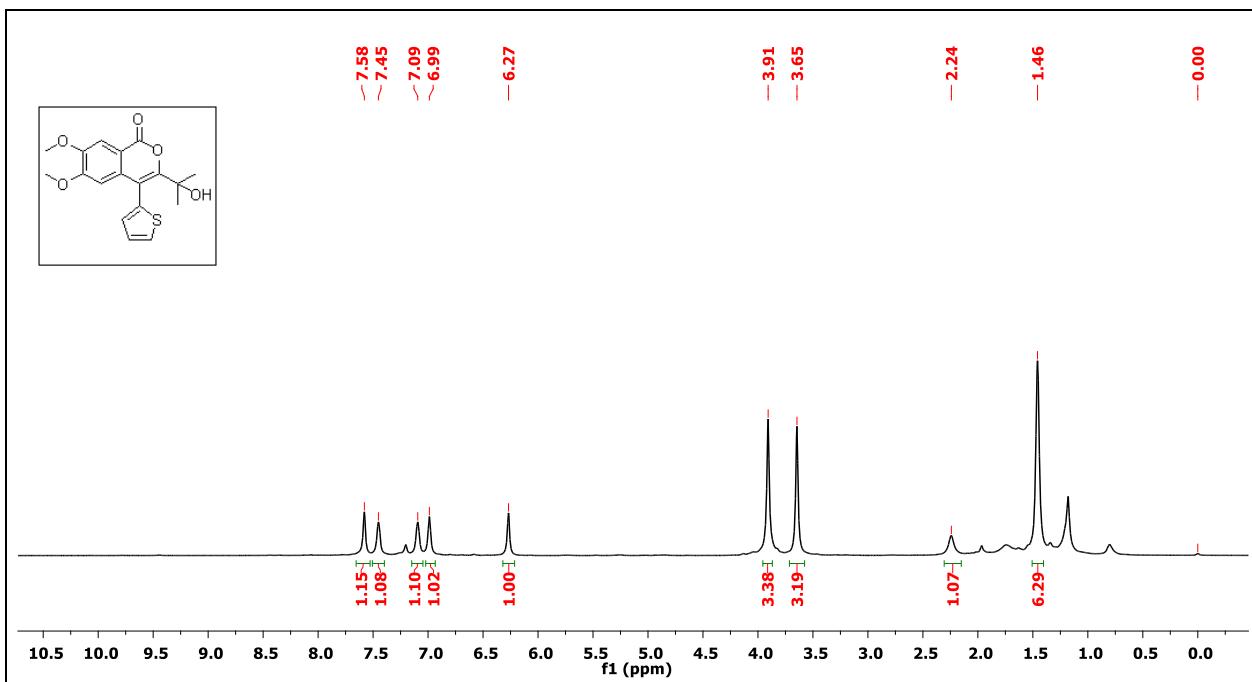
¹H and ¹³C spectra of compound 3se:



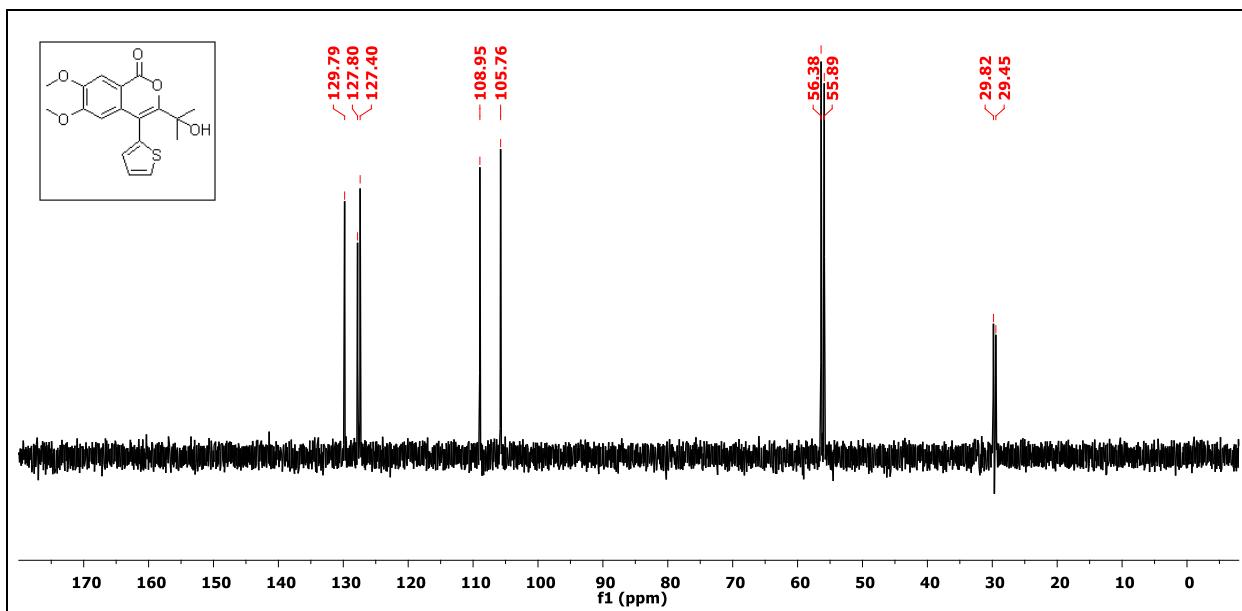
DEPT spectra of compound 3se:



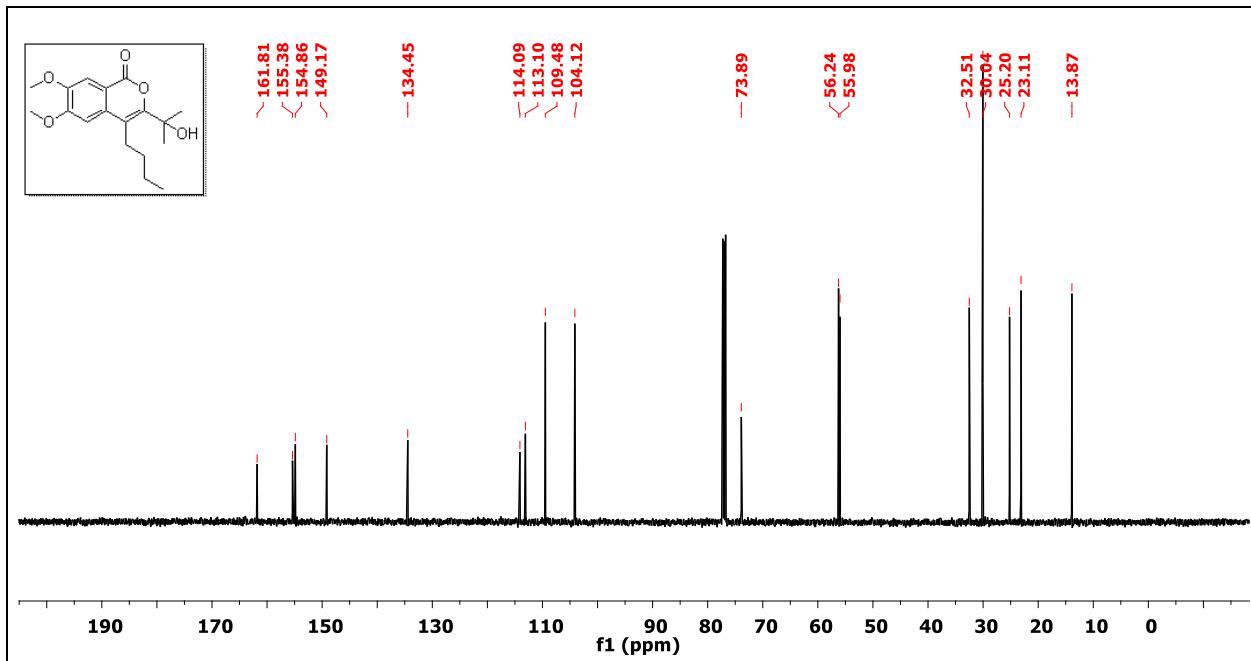
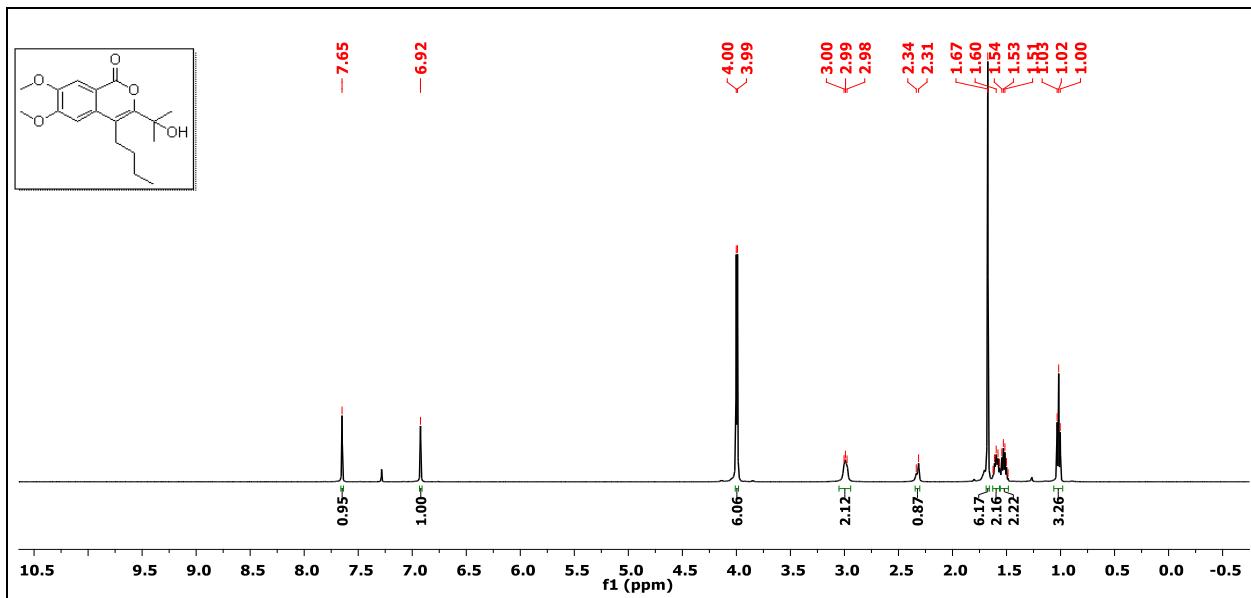
¹H and ¹³C spectra of compound 3sf:



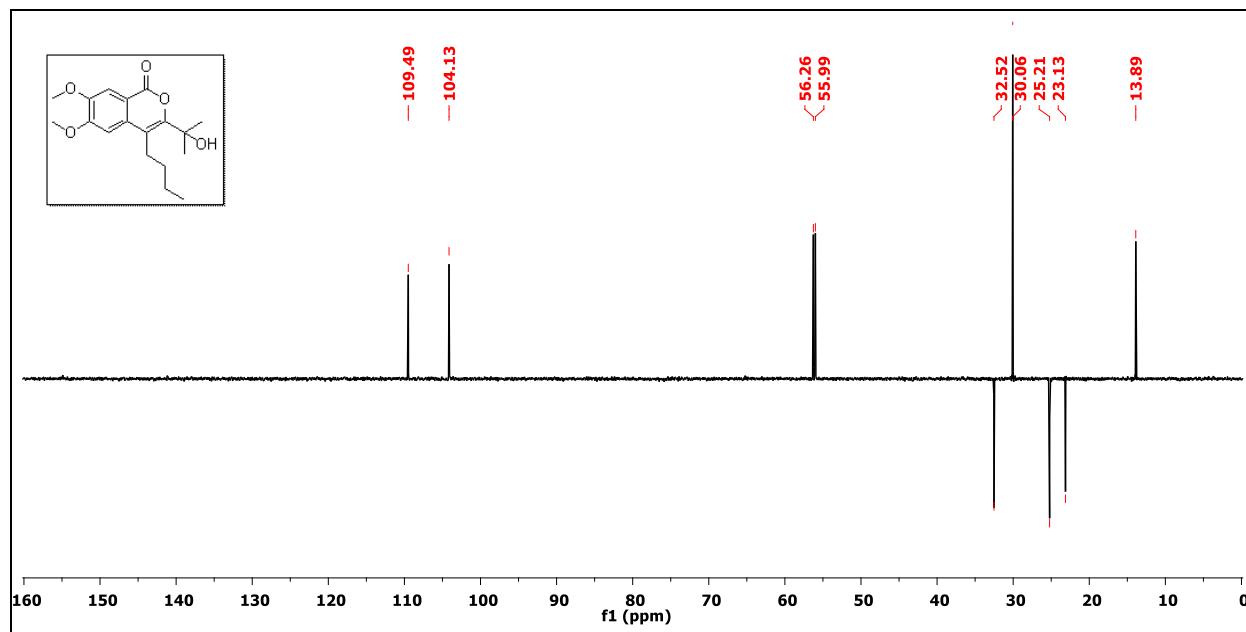
DEPT spectra of compound 3sf:



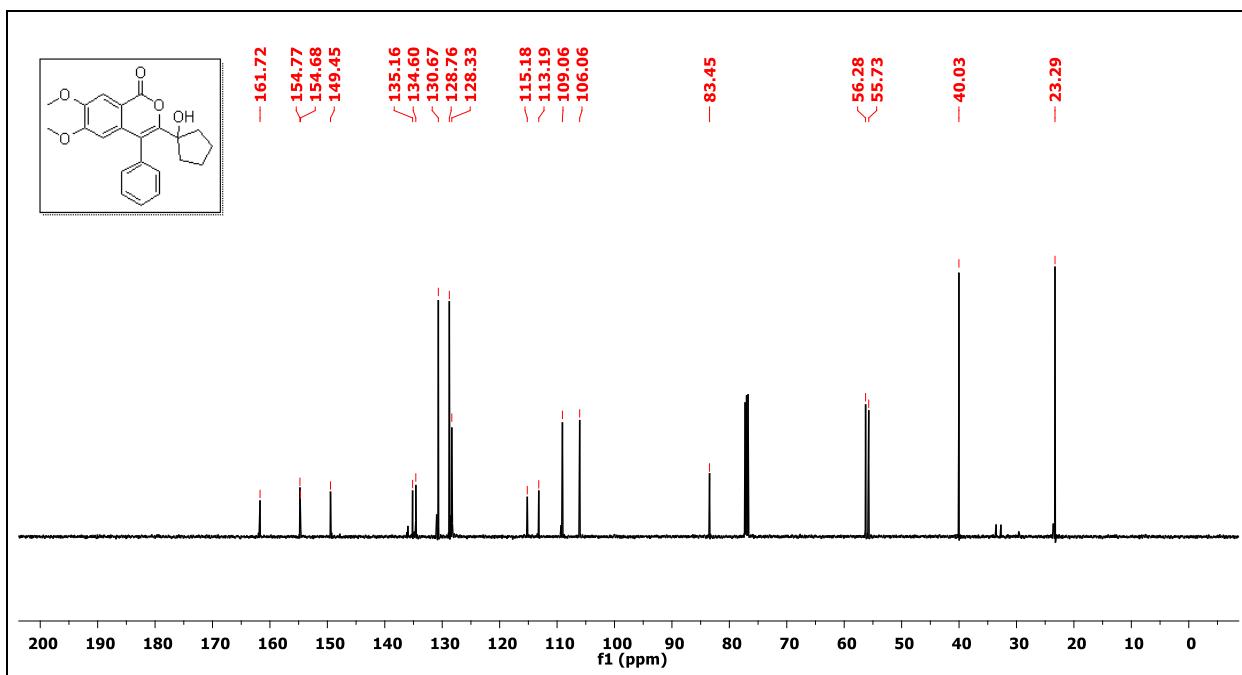
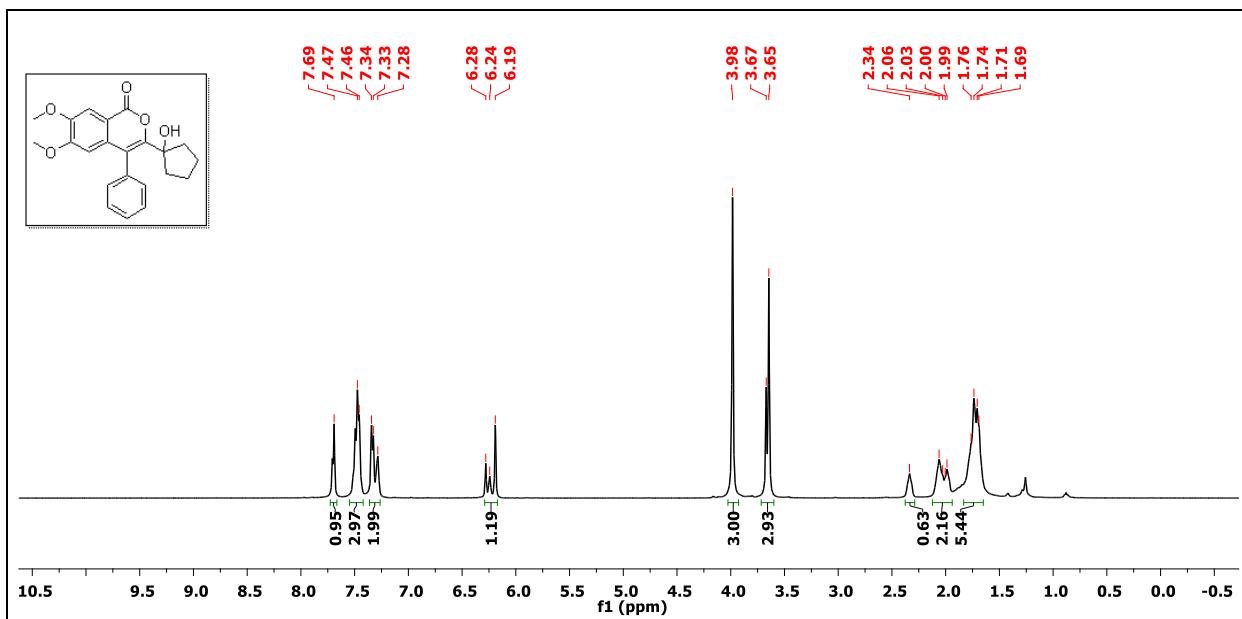
¹H and ¹³C spectra of compound 3sg:



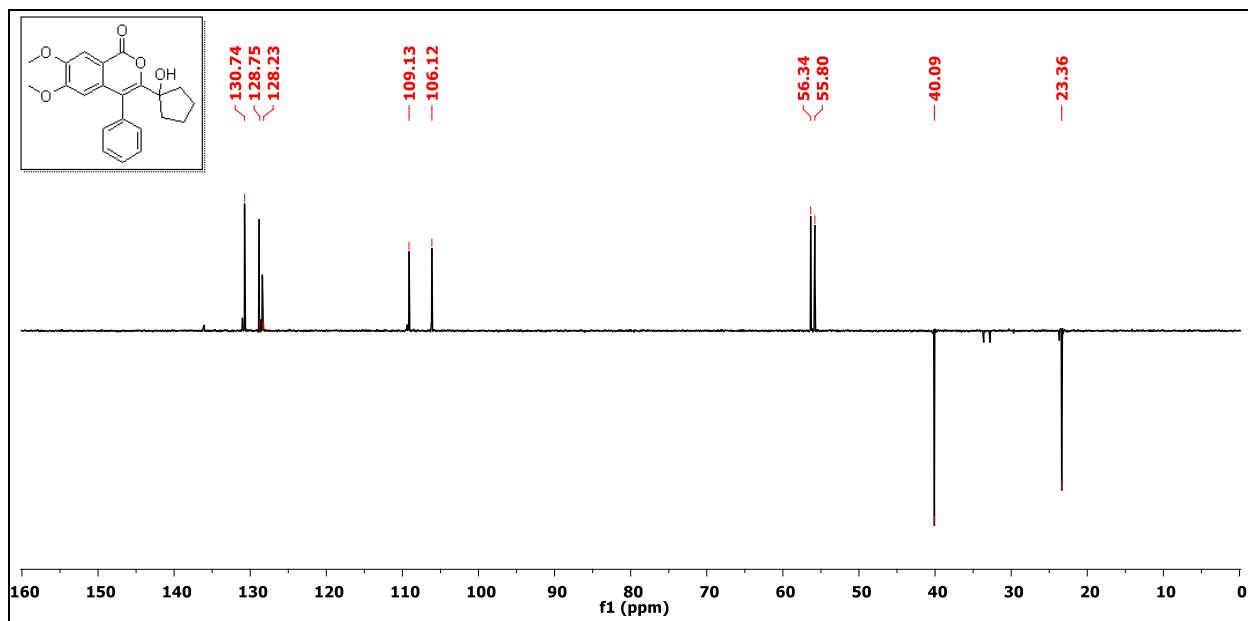
DEPT spectra of compound 3sg:



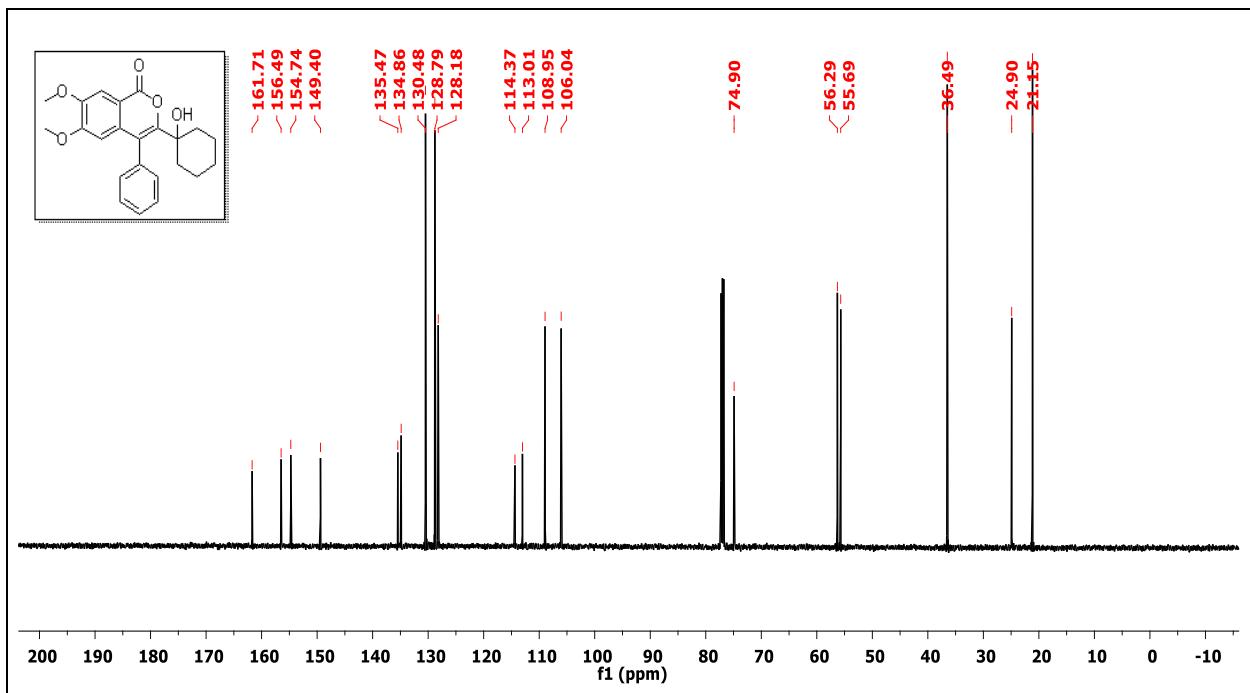
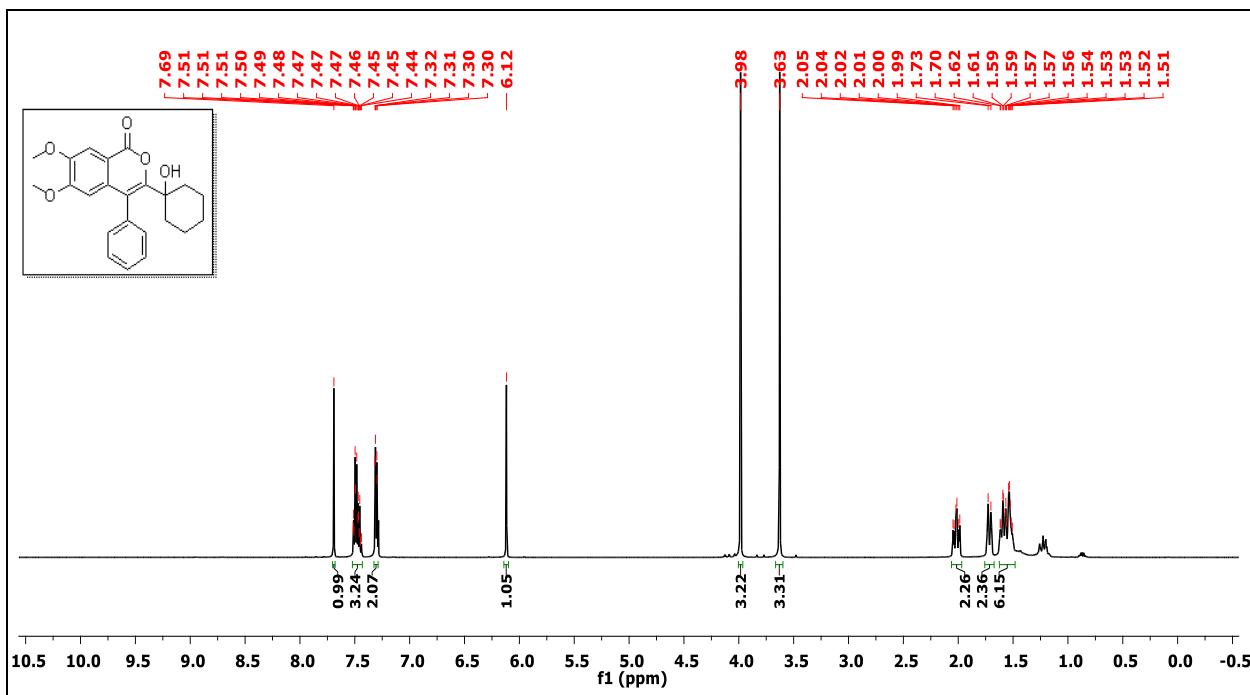
¹H and ¹³C spectra of compound 3sh:



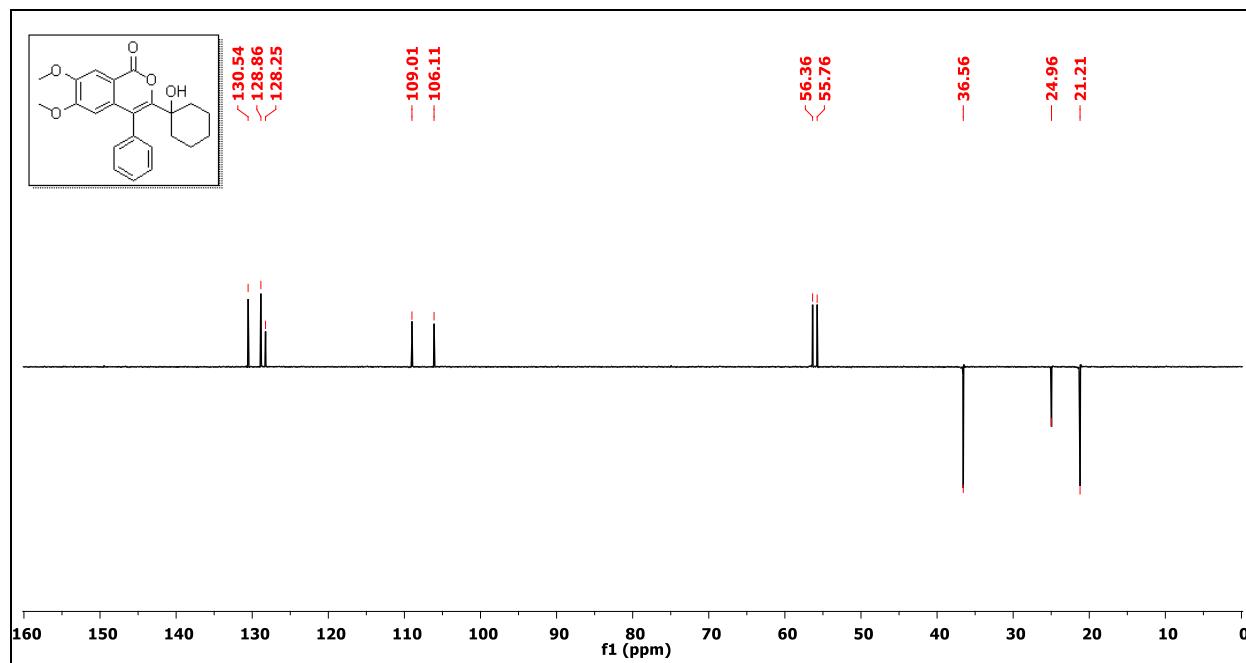
DEPT spectra of compound 3sh:



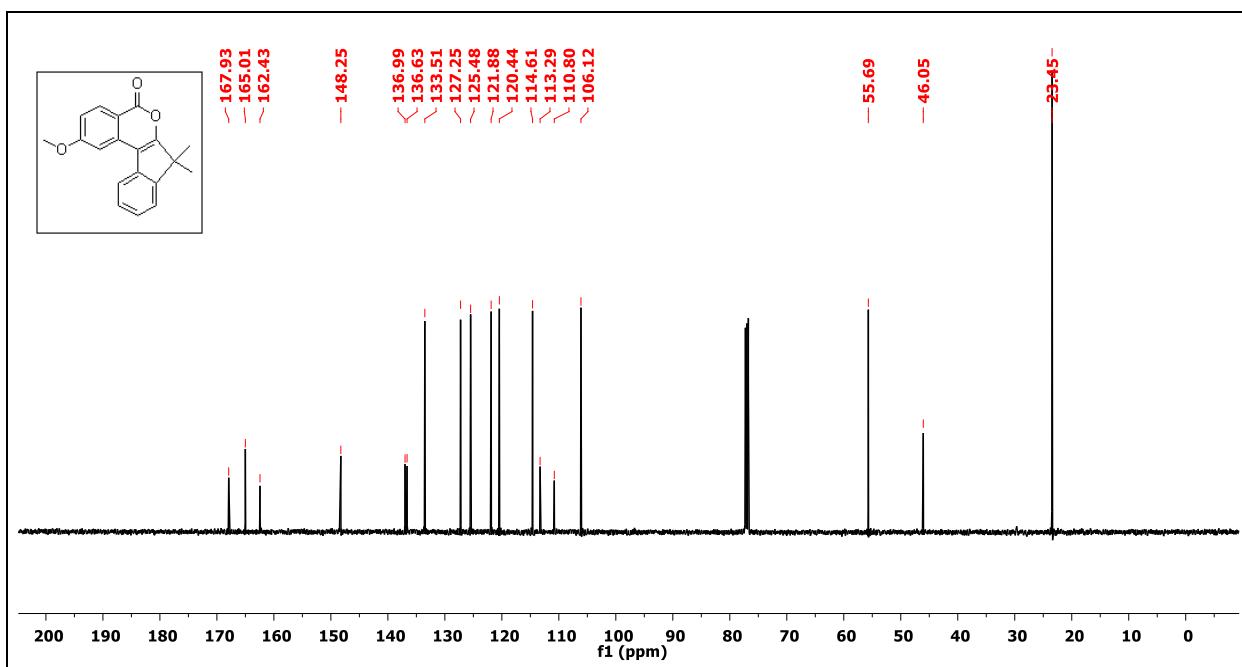
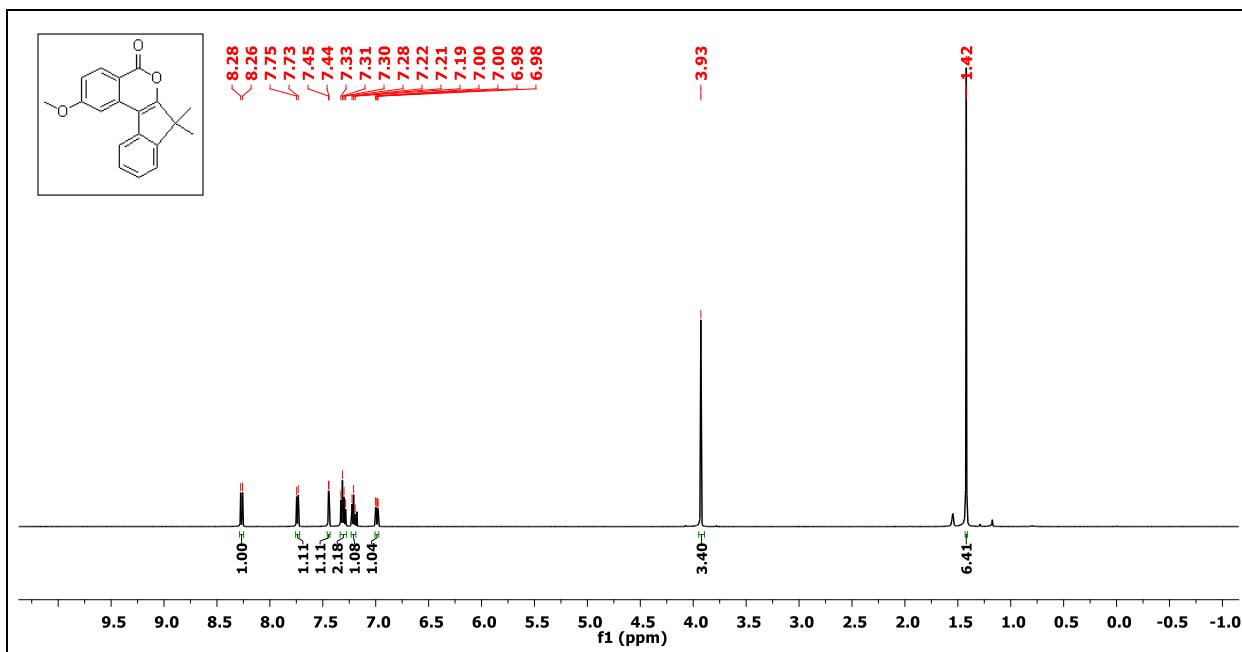
¹H and ¹³C spectra of compound 3si:



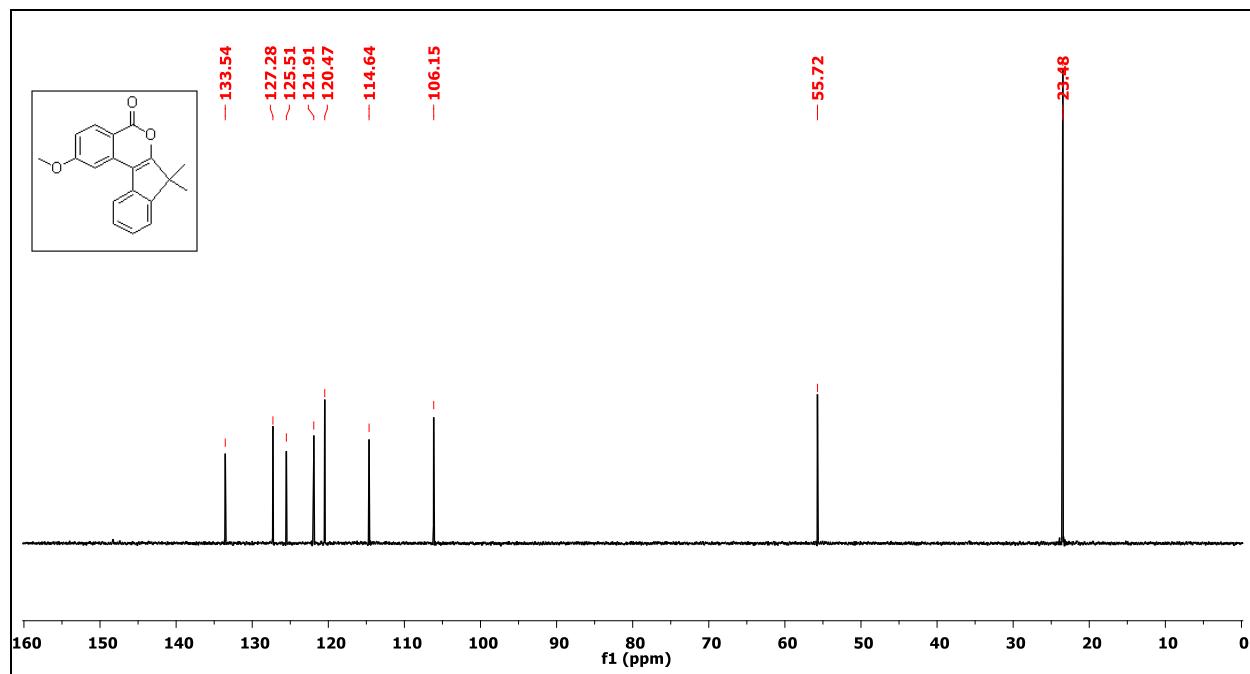
DEPT spectra of compound 3si:



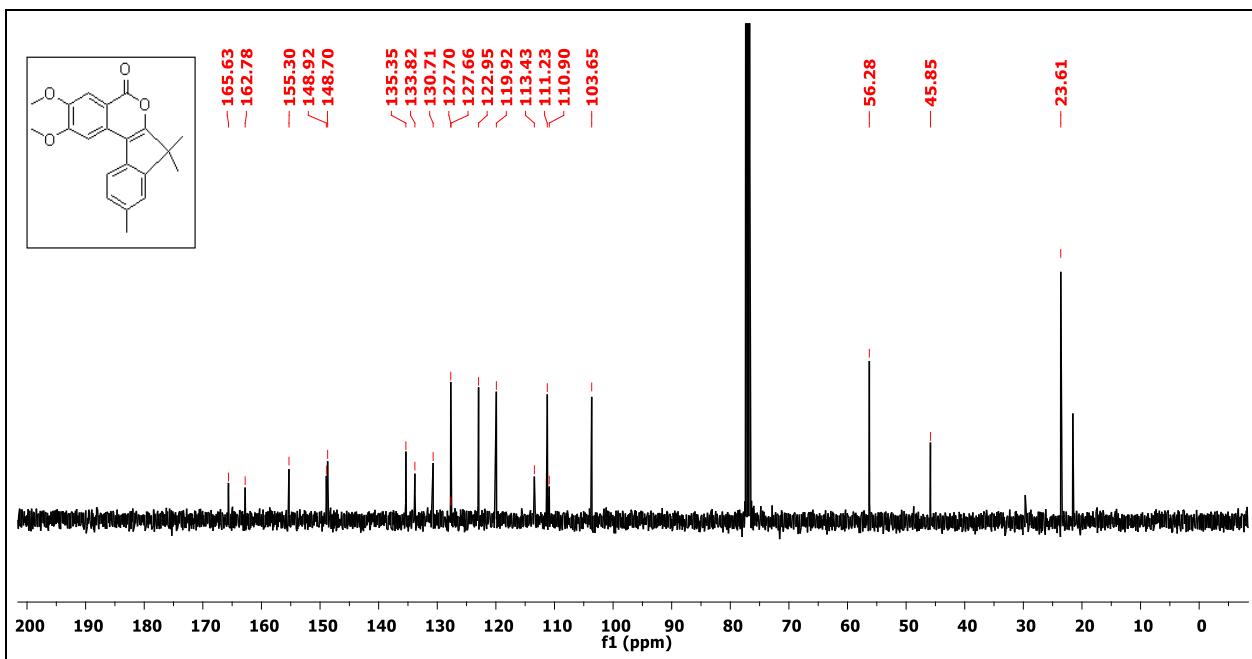
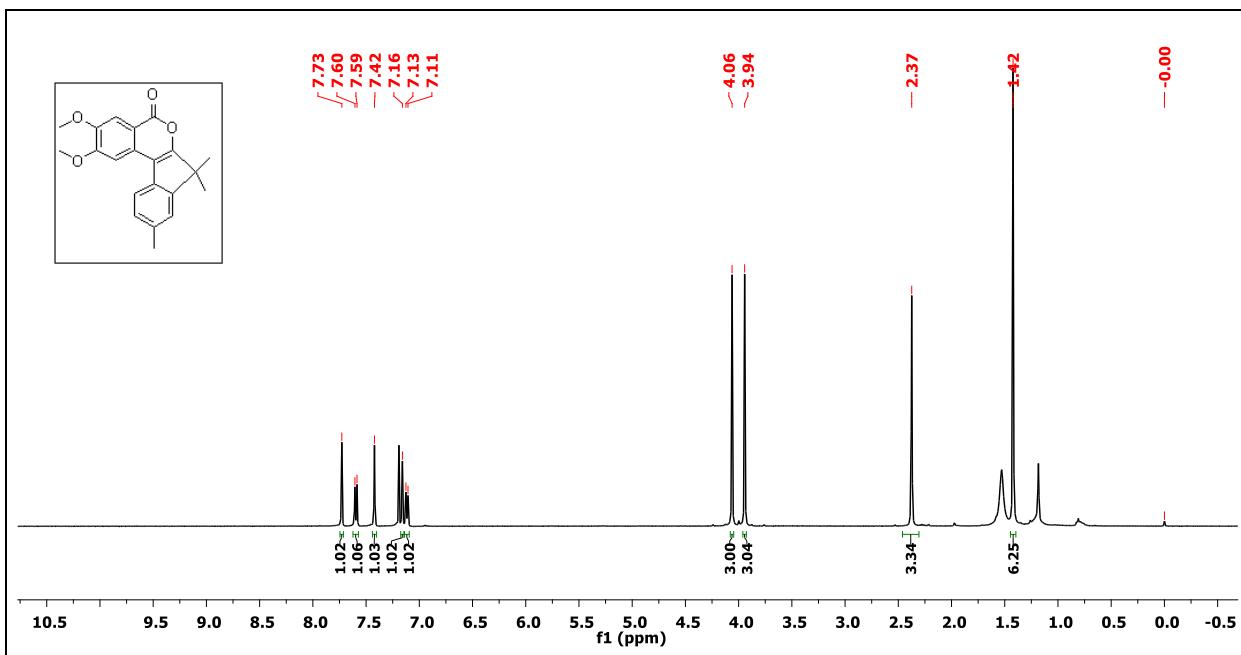
¹H and ¹³C spectra of compound 4a:



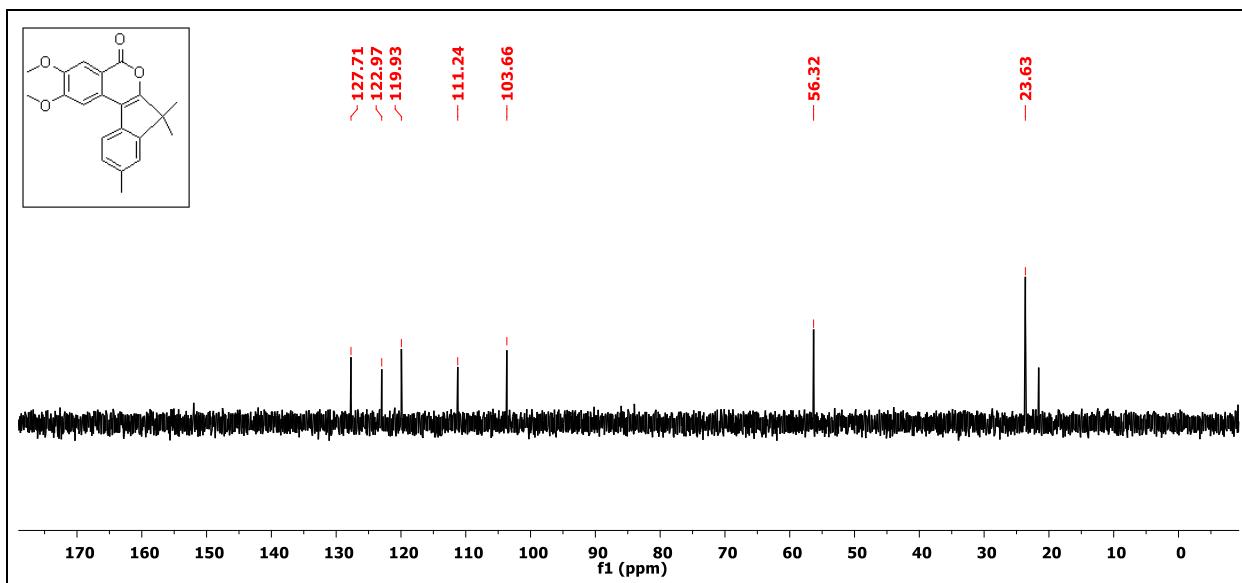
DEPT spectra of compound 4a:



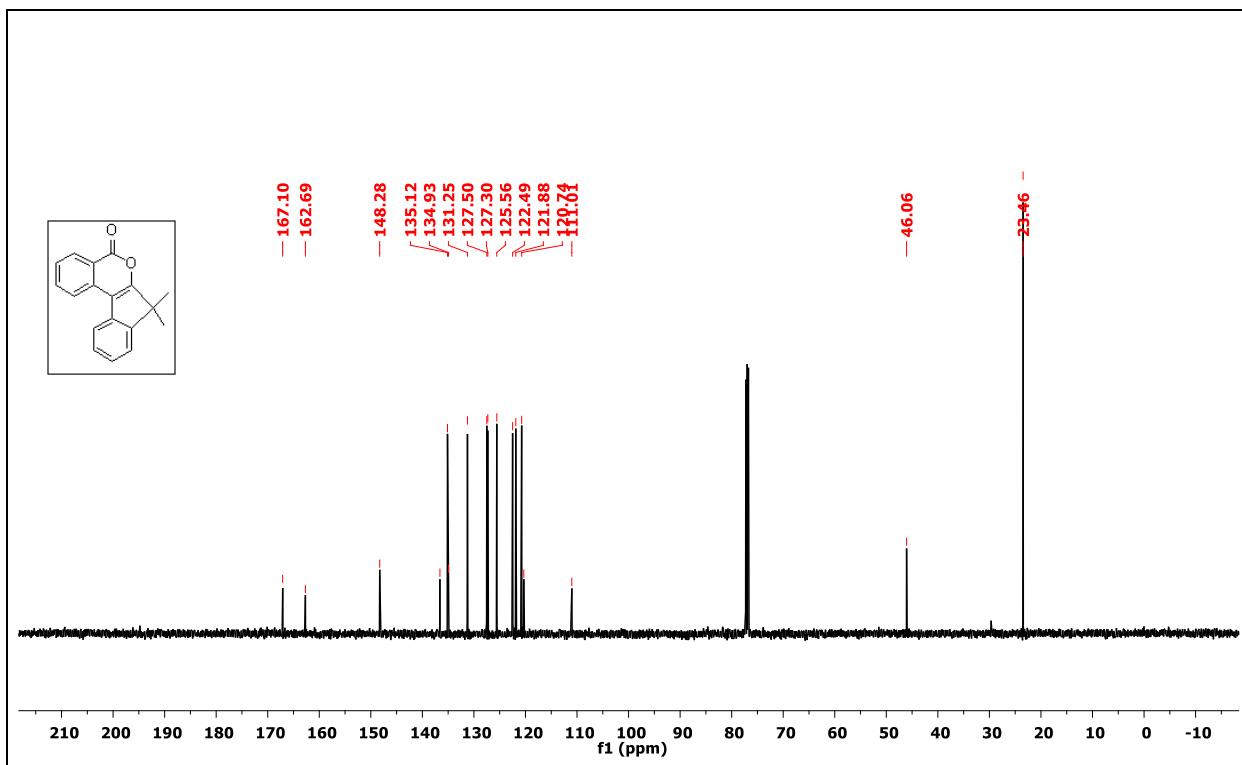
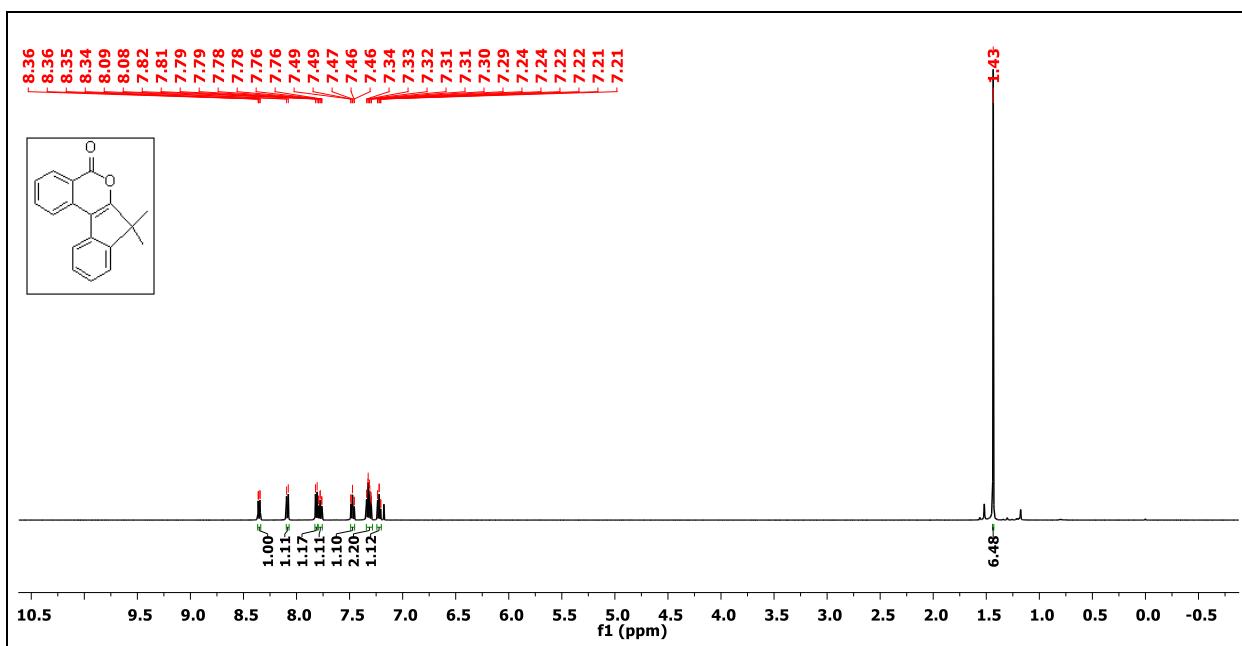
¹H and ¹³C spectra of compound 4b:



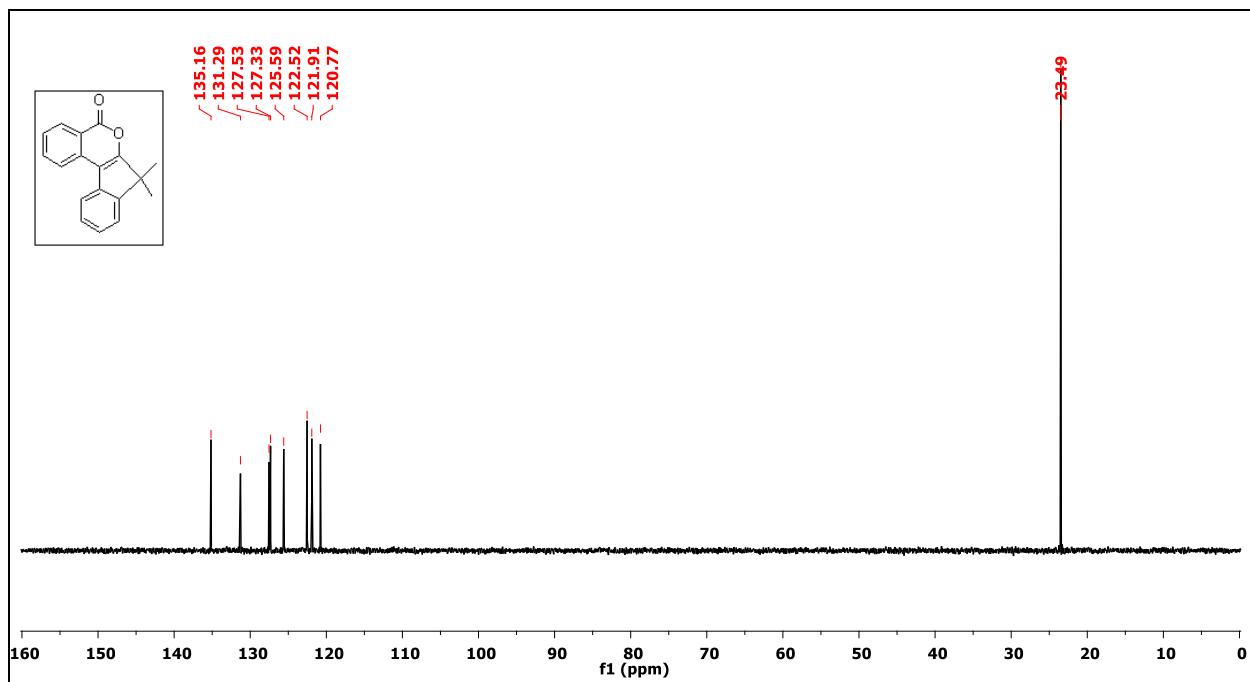
DEPT spectra of compound 4b:



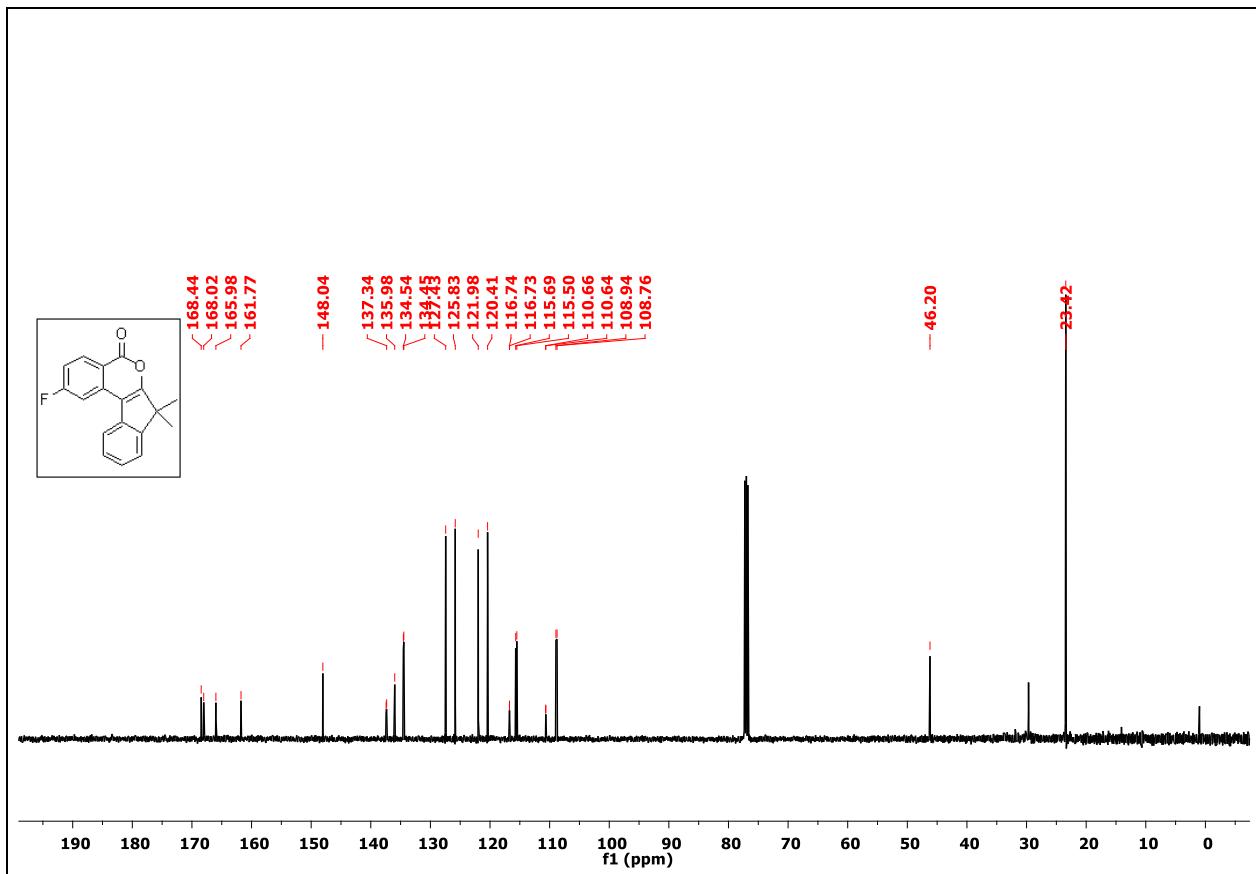
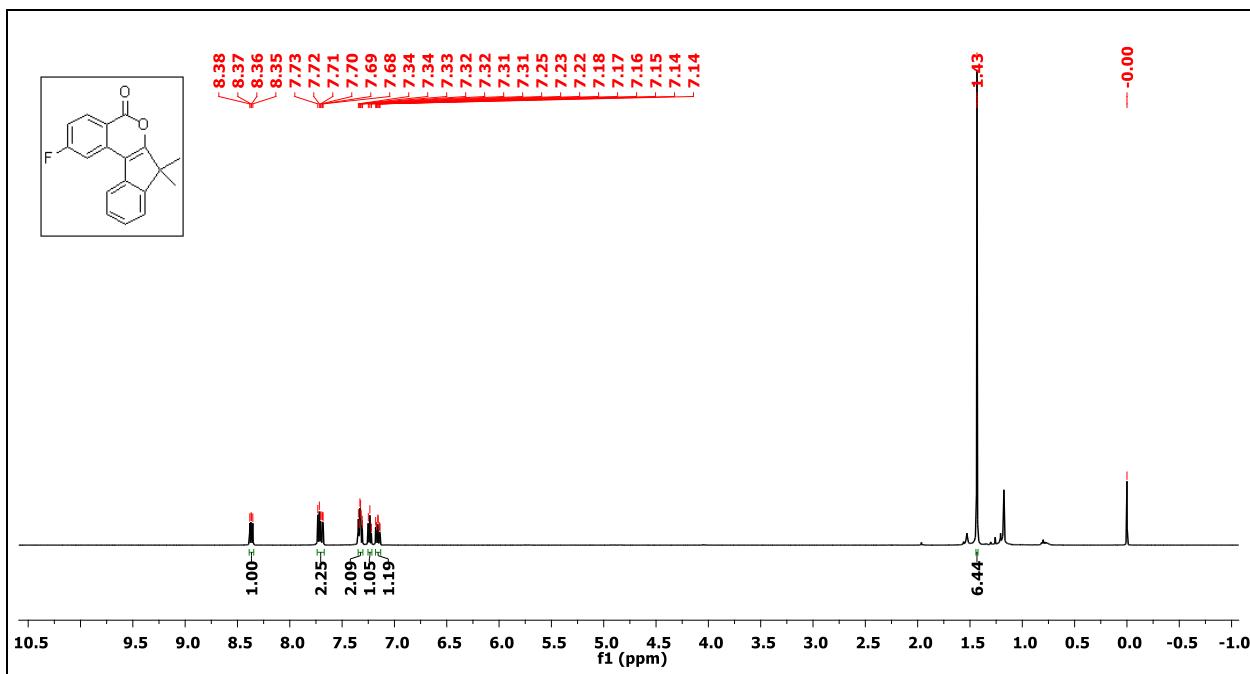
¹H and ¹³C spectra of compound 4c:



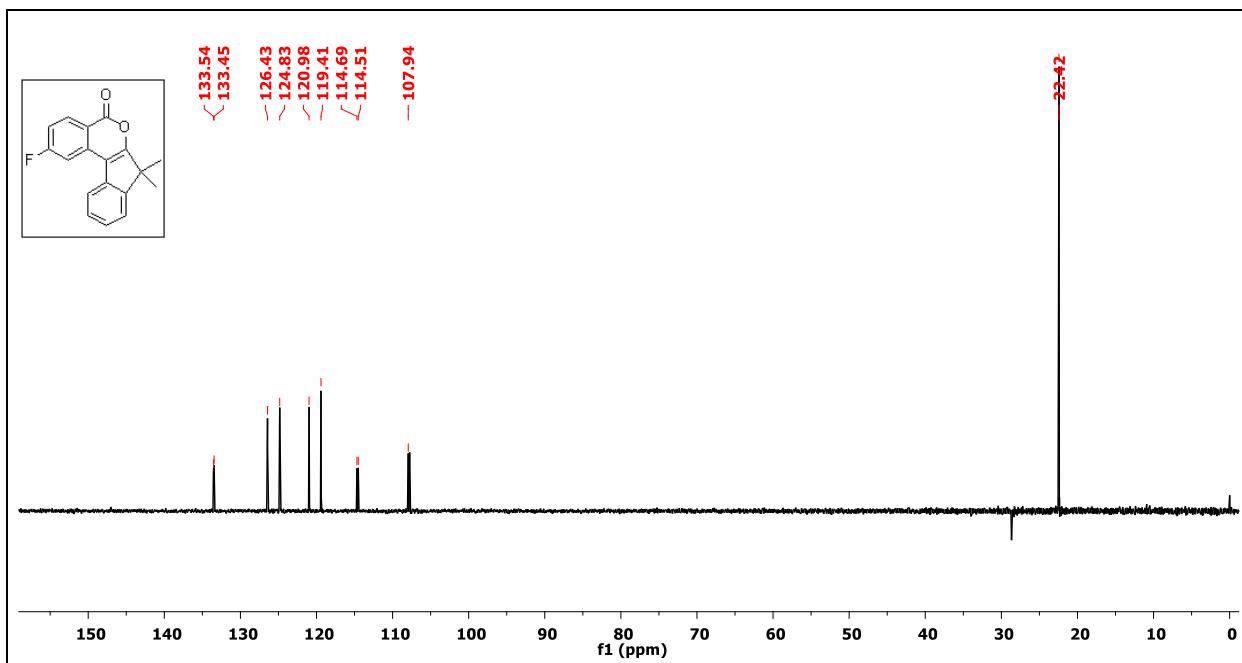
DEPT spectra of compound 4c:



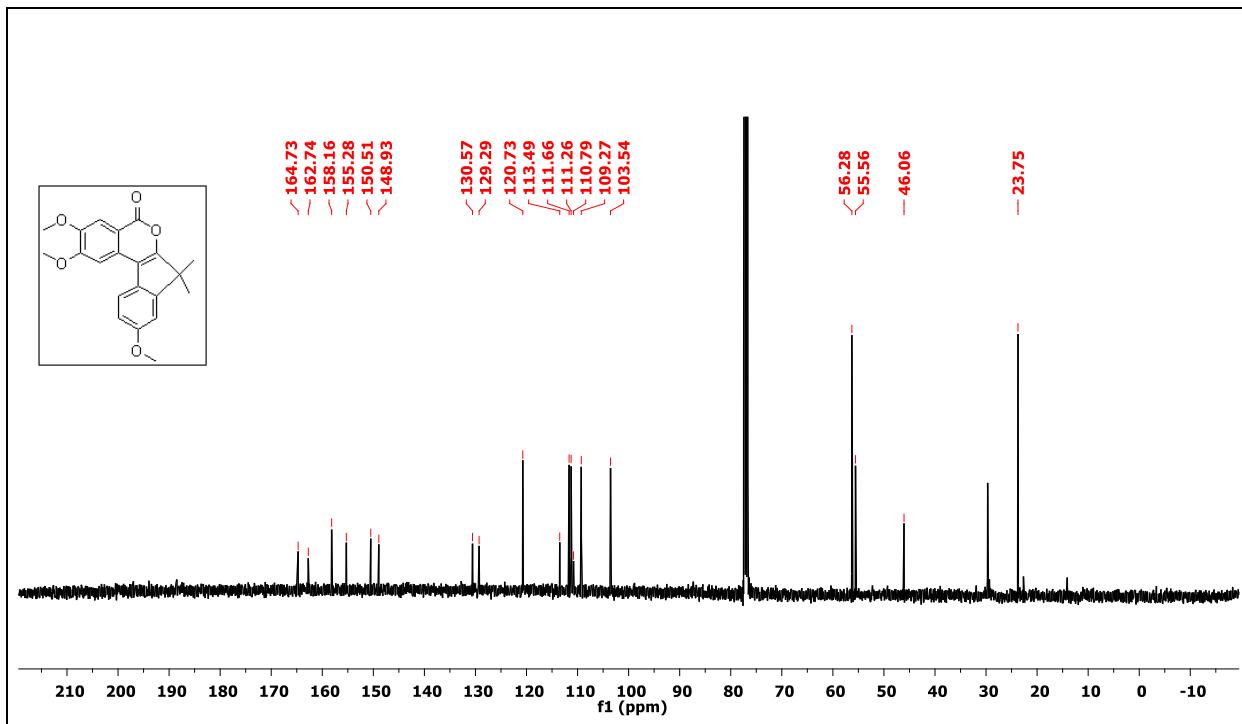
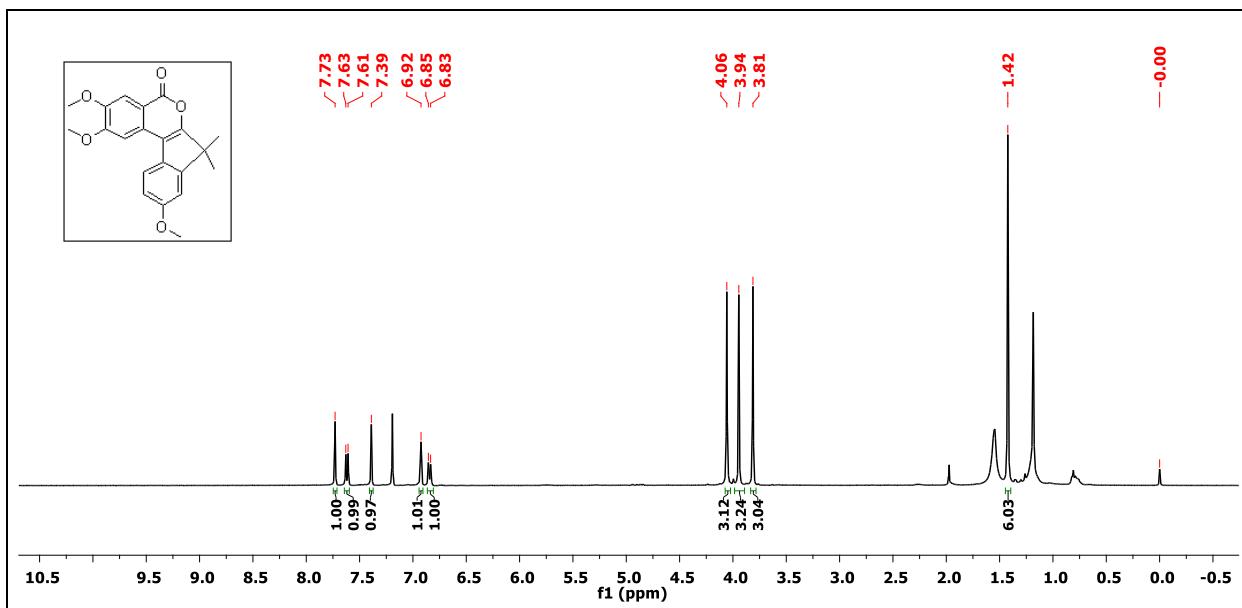
¹H and ¹³C spectra of compound 4d:



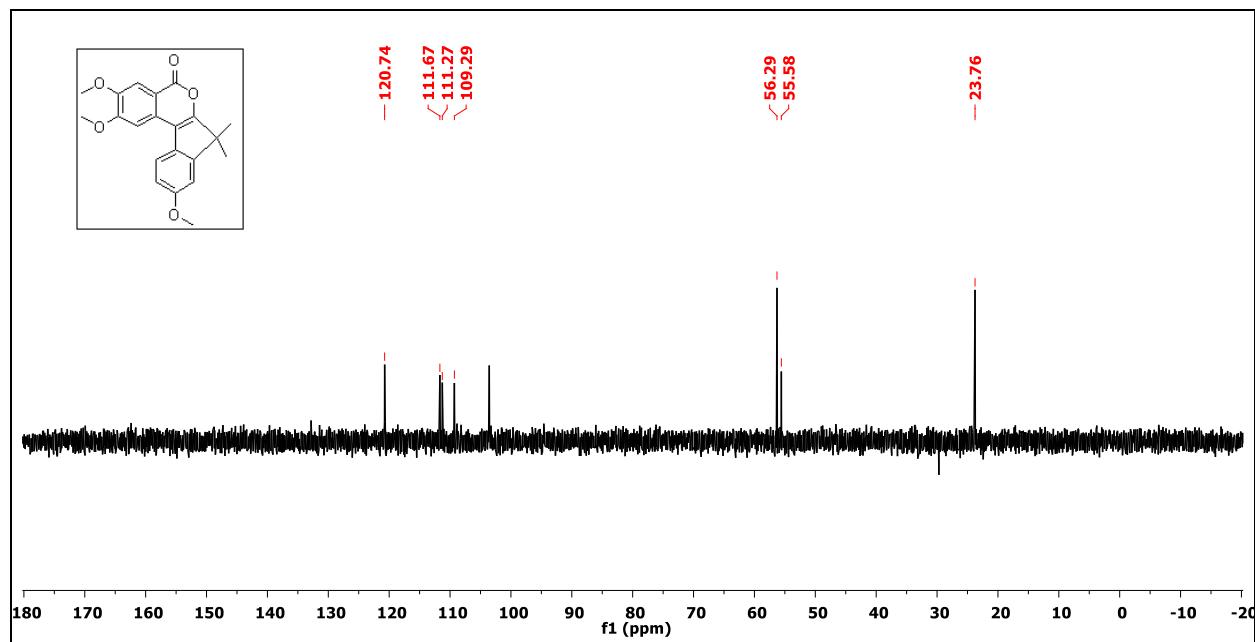
DEPT spectra of compound 4d:



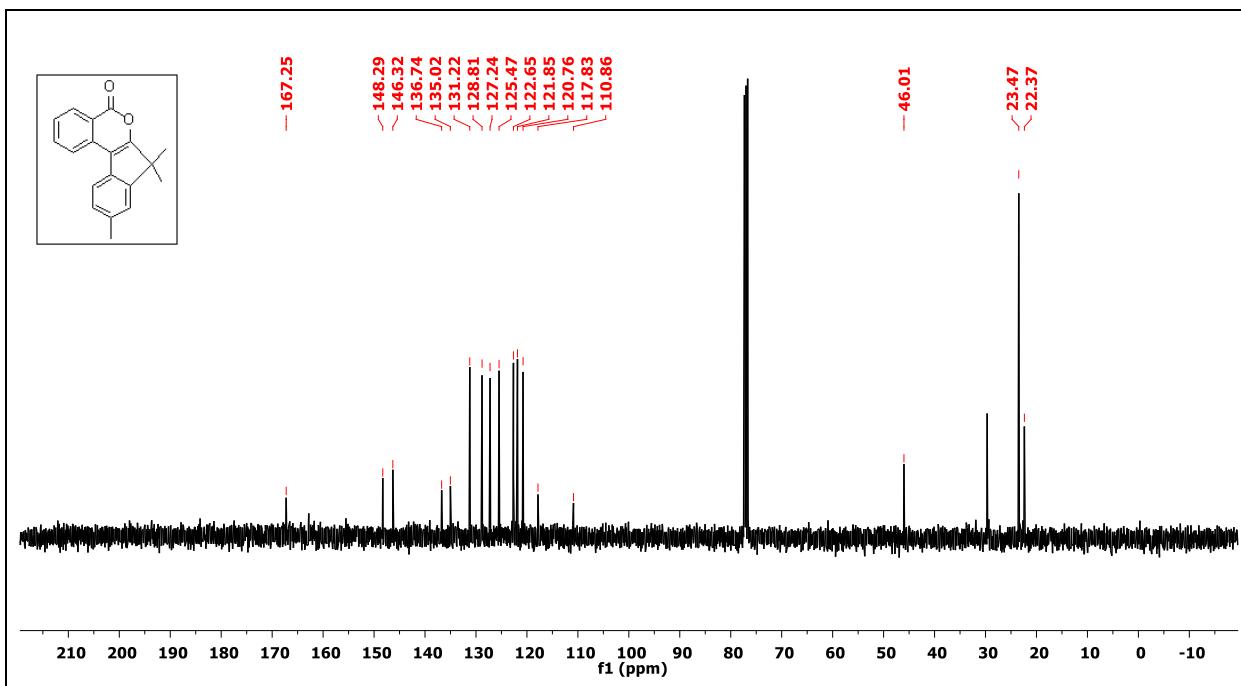
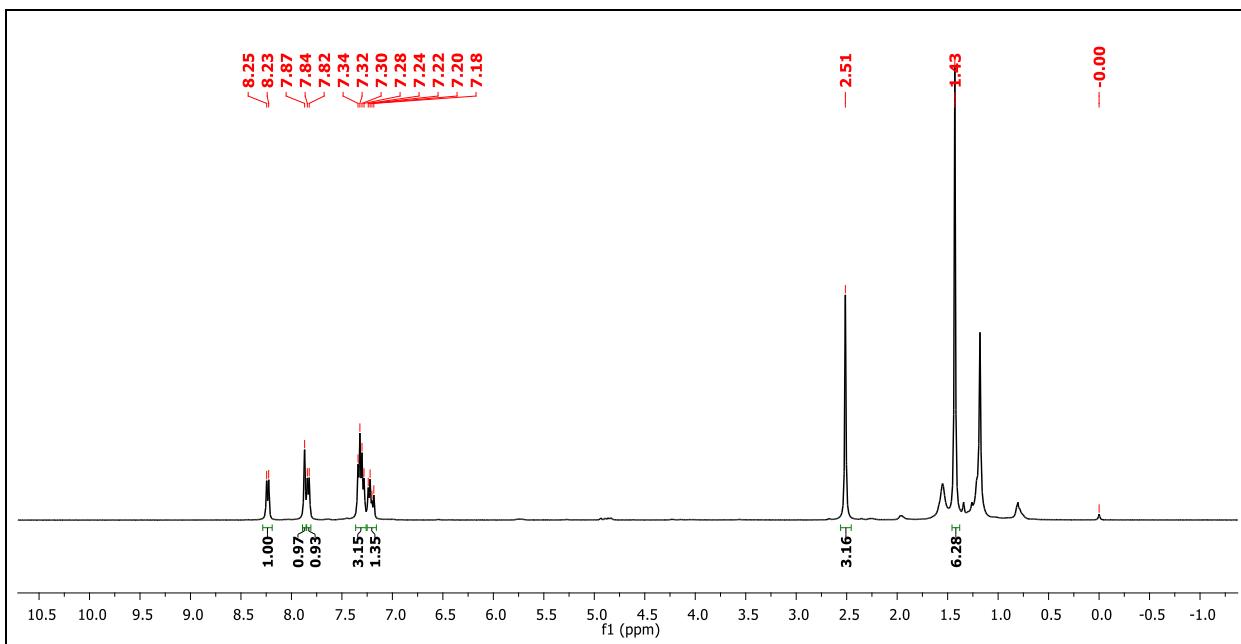
¹H and ¹³C spectra of compound 4e:



DEPT spectra of compound 4e:



¹H and ¹³C spectra of compound 4f:



DEPT spectra of compound 4f:

