Supplementary Information

Decarboxylative [4+2] Annulation of Arylglyoxylic Acids with Internal Alkynes using the Anodic Ruthenium Catalysis

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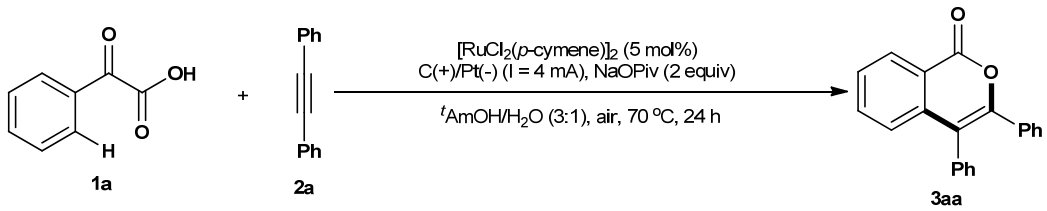
(A) Typical Experimental Procedure

(a) General

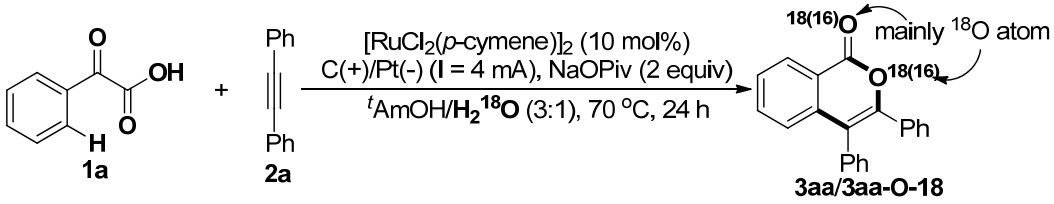
The ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ solvent on a NMR spectrometer using TMS as internal standard. HRMS was measured on an electrospray ionization (ESI) apparatus using time-of-flight (TOF) mass spectrometry. Melting points are uncorrected. The instrument for electrolysis is DC power source (PM3005B) (made in China). Cyclic voltammograms were obtained on a CHI 605E potentiostat. The anode electrode is graphite rod (Φ 6mm×80mm) and cathode electrode is platinum electrodes (1.0×1.0 cm^2).

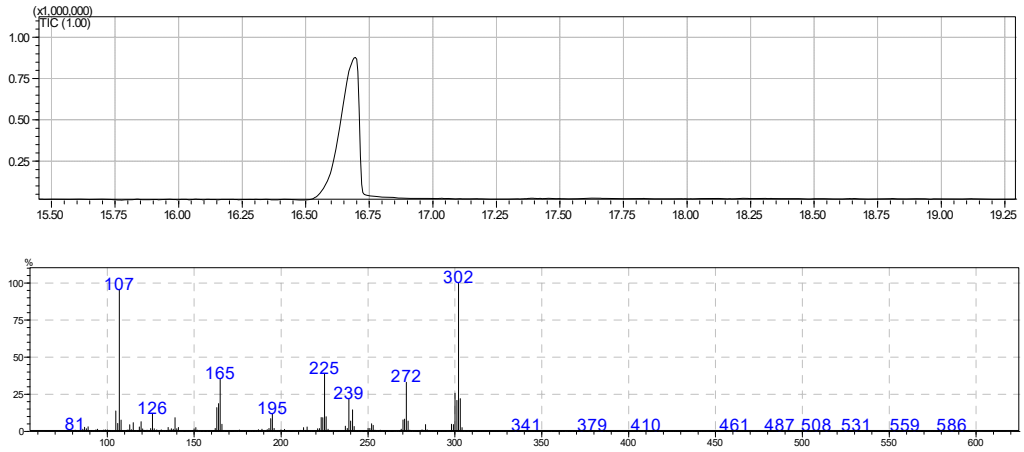
(b) General procedure for the synthesis of compound 3.



To an undivided three-necked bottle (10 mL) were added phenylglyoxylic acid **1a** (0.3 mmol), diphenylacetylene **2a** (0.2 mmol), NaOPiv (2 equiv), $[RuCl_2(p\text{-cymene})]_2$ (5 mol%), and $^{t}AmOH/H_2O$ (3:1; 6 mL). The bottle was equipped with platinum electrodes (1.0×1.0 cm^2) as cathode and graphite rod electrode as anode under air. The reaction mixture was stirred and electrolyzed at a constant current of 4 mA at 70 °C for 24 h until complete consumption of starting material as monitored by TLC and/or GC-MS analysis. After the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered and concentrated in vacuum. The resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the desired product **3aa**.

(c) $H_2{}^{18}O$ experiments.





[MS Spectrum]

# of Peaks 518

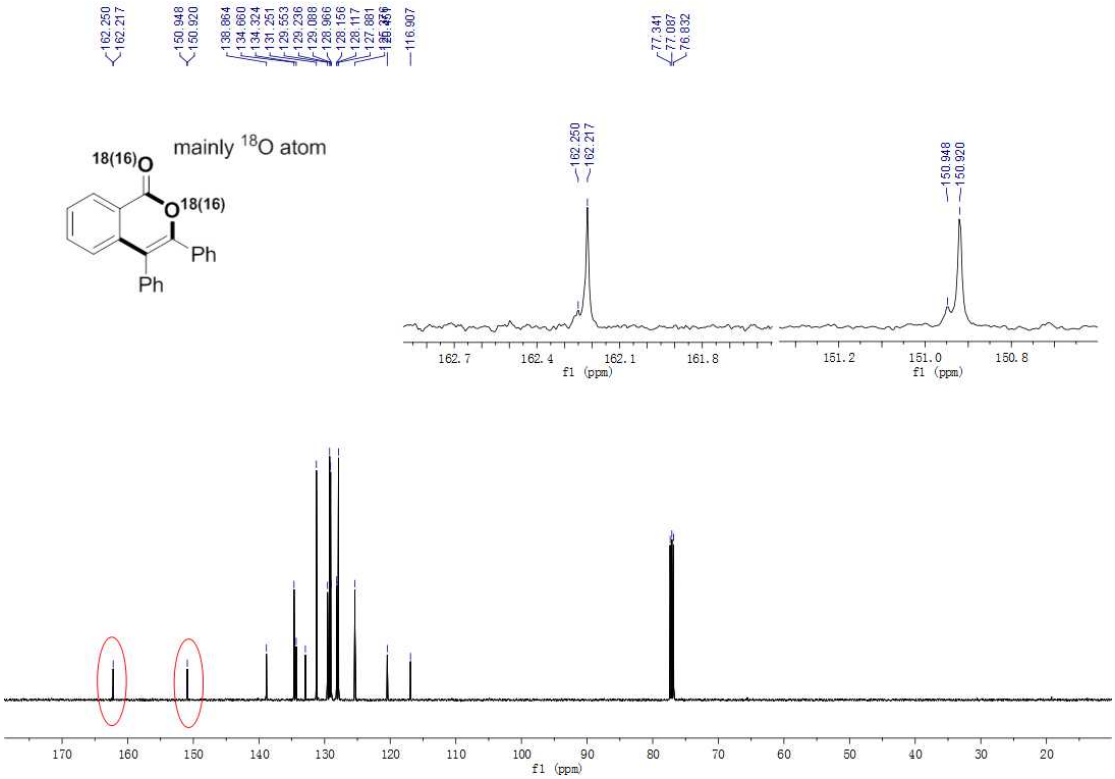
Raw Spectrum 16.695 (scan : 2540)

Background No Background Spectrum

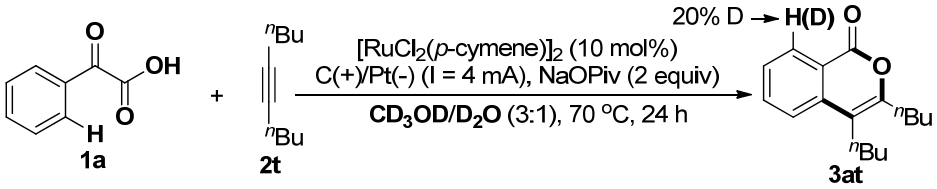
Base Peak m/z 302.15 (Inten : 118,160)

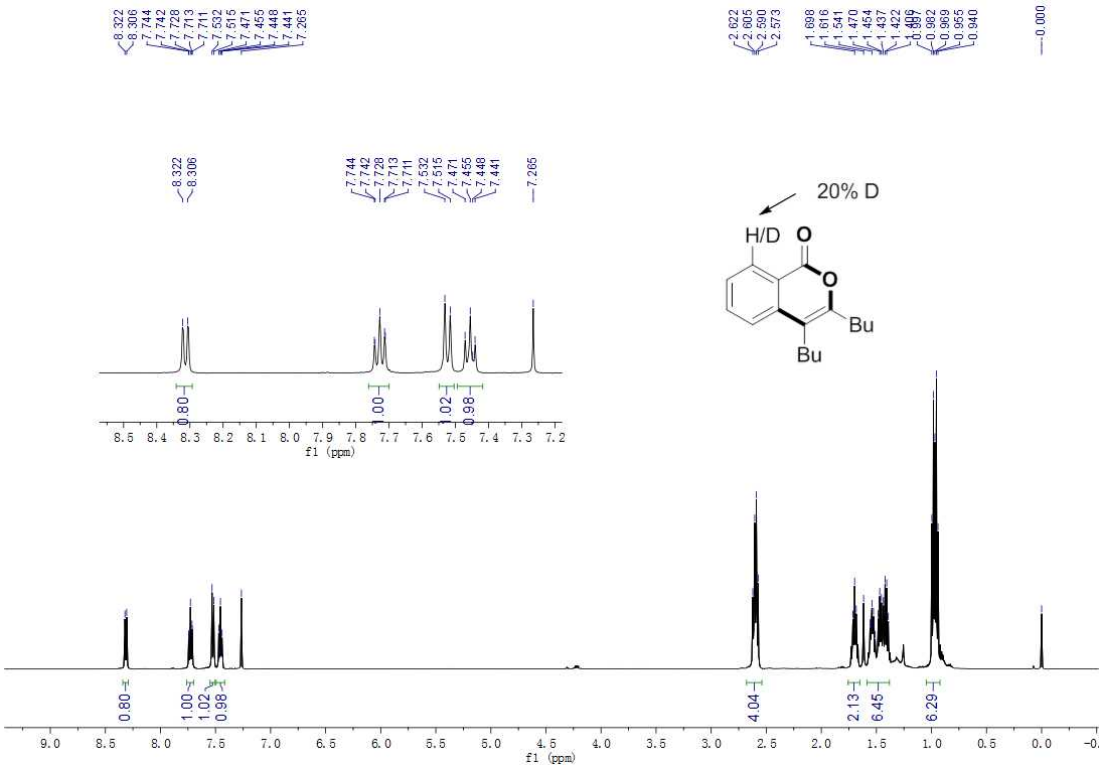
Event# 1

m/z	Absolute Intensity	Relative Intensit						
291.10	34	0.03	297.15	718	0.61	303.15	26066	22.06
292.10	49	0.04	**298.10**	**5735**	**4.85**	304.10	2988	2.53
293.10	57	0.05	299.15	5412	4.58	305.10	250	0.21
294.10	36	0.03	**300.15**	**30334**	**25.67**	1		
295.10	62	0.05	301.15	24604	20.82			
296.10	65	0.06	**302.15**	**118160**	**100.00**			

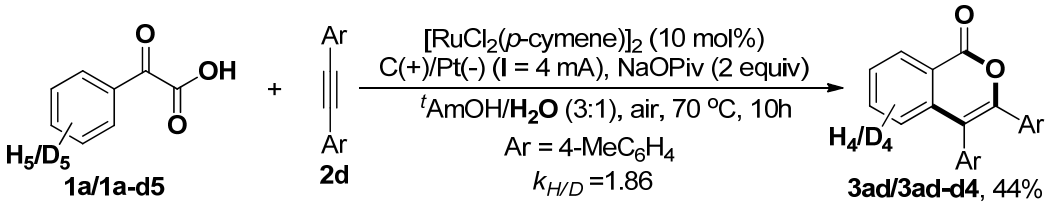


(d) H/D Exchange Experiment.

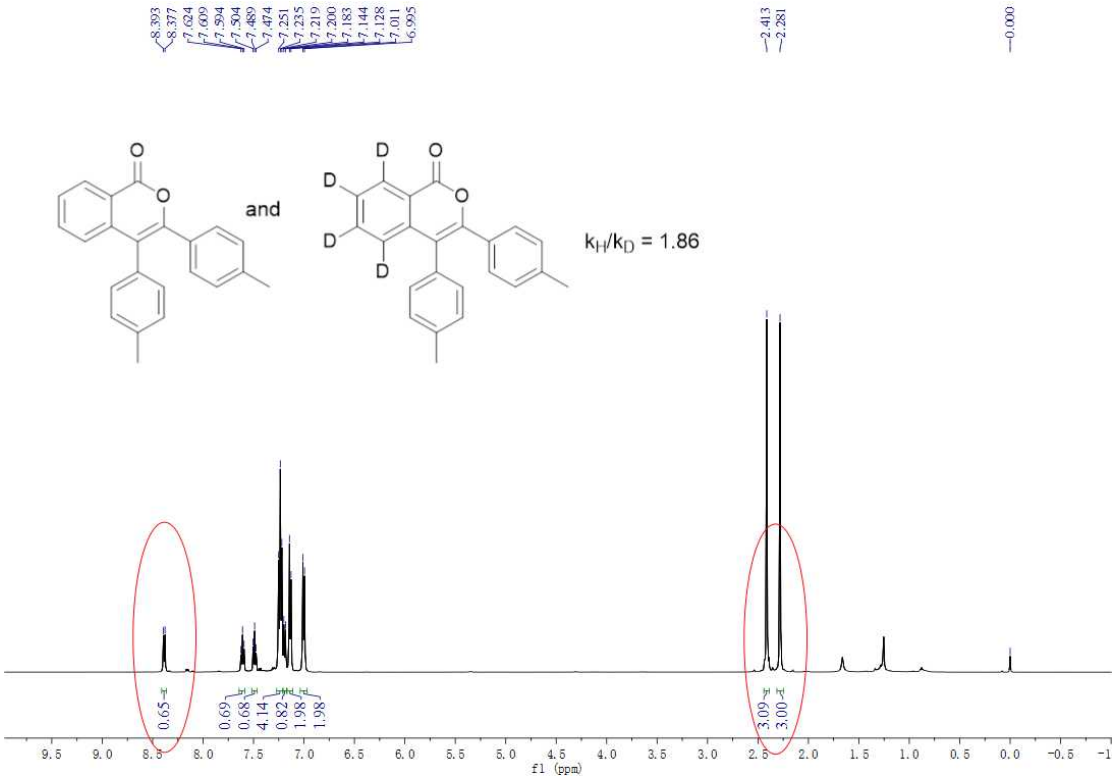




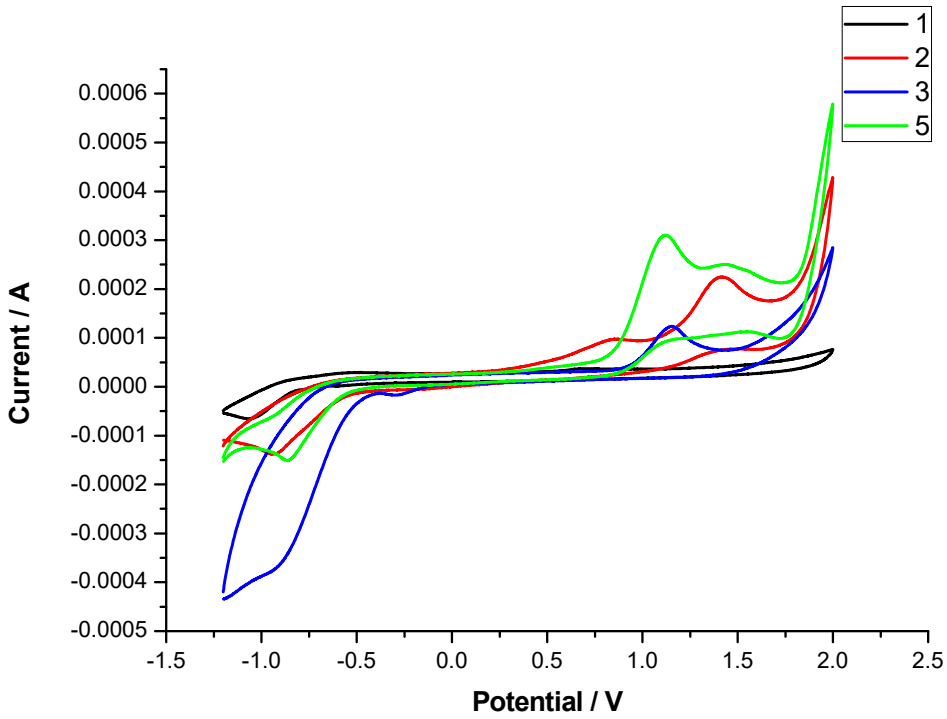
(e) Kinetic experiment

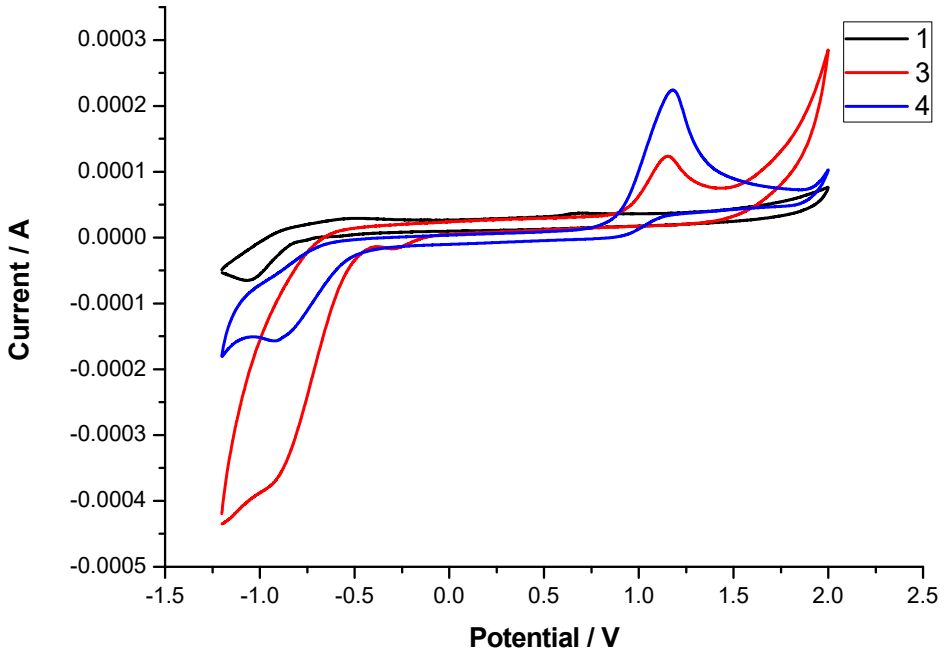


To an undivided three-necked bottle (10 mL) were added phenylglyoxylic acid **1a** (0.15 mmol), **[D_5]-1a** (0.15 mmol), Diphenylacetylene **2b** (0.6 mmol, 2 equiv), NaOPiv (2 equiv), [$RuCl_2$(*p*-cymene)]$_2$ (10 mmol%), and ^{t}AmOH/H_2O = 3:1 (6 mL). The bottle was equipped with platinum electrodes (1.0×1.0 cm^2) as cathode and graphite rod electrode as anode under air. The reaction mixture was stirred and electrolyzed at a constant current of 4 mA at 70 °C for 10 h. After the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered and concentrated in vacuum. The resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the desired products **3ad/3ad-d4**.



(f) Cyclic Voltammogram Curves (Figure S1)





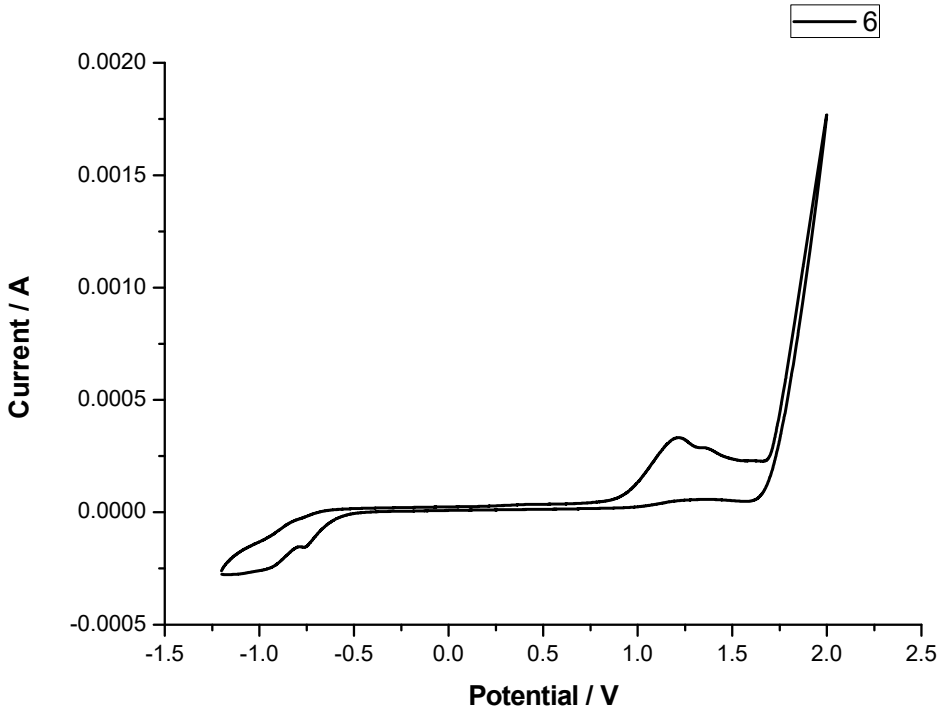
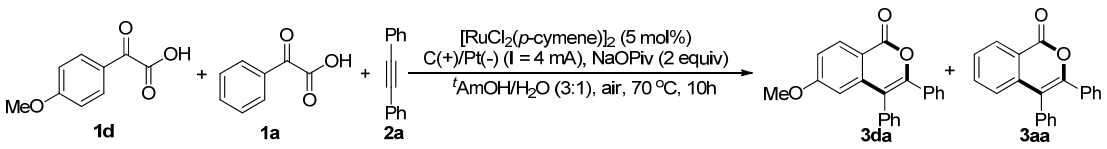


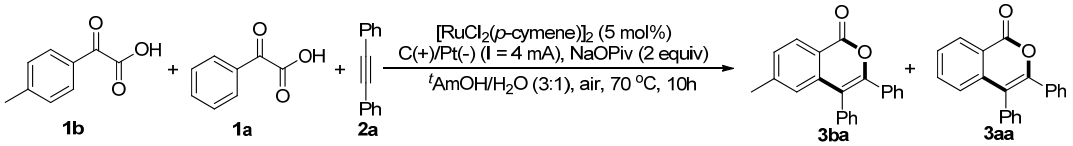
Figure S1. Cyclic voltammogram curves. using GC disk as working electrode, Pt slice, and Ag/AgCl as counter and reference electrode at 100 mV/s scan rate: (1) (black) $^{n}Bu_4NPF_6$ (0.1 M) and MeCN (10 mL); (2) $[RuCl_2(p\text{-cymene})]_2$ (0.005 M), NaOPiv (0.1 M), $^{n}Bu_4NPF_6$ (0.1 M) and MeCN (10 mL); (3) 1a (0.05 M), $^{n}Bu_4NPF_6$ (0.1 M) and MeCN (10 mL); (4) 1a (0.05 M), NaOPiv (0.1 M), $^{n}Bu_4NPF_6$ (0.1 M), and MeCN (10 mL); (5) 1a (0.05 M), $[RuCl_2(p\text{-cymene})]_2$ (0.005 M), NaOPiv (0.1 M), $^{n}Bu_4NPF_6$ (0.1 M), and MeCN (10 mL); (6) 1a (0.05 M), 2a (0.1 M), $[RuCl_2(p\text{-cymene})]_2$ (0.005 M), NaOPiv (0.1 M), $^{n}Bu_4NPF_6$ (0.1 M), and MeCN (10 mL);

(g) Hammett Competition Experiments and Analysis[7]

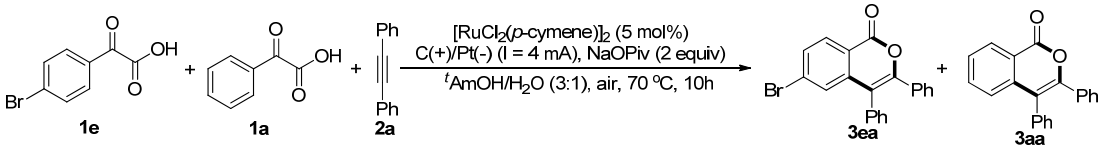


To an undivided three-necked bottle (10 mL) were added phenylglyoxylic acid **1d** (0.15 mmol), **1a** (0.15 mmol), Diphenylacetylene **2a** (0.2 mmol), NaOPiv (2 equiv), $[RuCl_2(p\text{-cymene})]_2$ (5 mmol%), and $^{t}AmOH/H_2O$ = 3:1 (6 mL). The bottle was

equipped with platinum electrodes (1.0×1.0 cm^2) as cathode and graphite rod electrode as anode under air. The reaction mixture was stirred and electrolyzed at a constant current of 4 mA at 70 °C for 10 h. After the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered and concentrated in vacuum. The resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the desired products **3da** (13.8 mg, 42% yield) and **3aa** (7.7 mg, 26% yield).

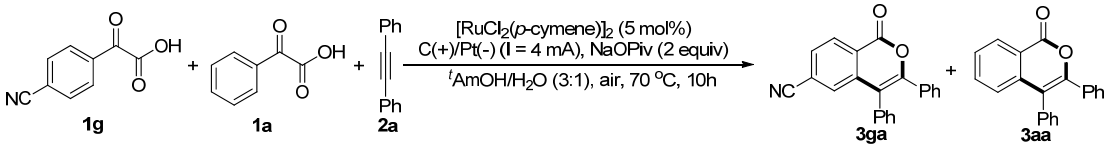


To an undivided three-necked bottle (10 mL) were added phenylglyoxylic acid **1b** (0.15 mmol), **1a** (0.15 mmol), Diphenylacetylene **2a** (0.2 mmol), NaOPiv (2 equiv), $[RuCl_2(p\text{-cymene})]_2$ (5 mmol%), and ^{t}AmOH/H_2O = 3:1 (6 mL). The bottle was equipped with platinum electrodes (1.0×1.0 cm^2) as cathode and graphite rod electrode as anode under air. The reaction mixture was stirred and electrolyzed at a constant current of 4 mA at 70 °C for 10 h. After the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered and concentrated in vacuum. The resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the desired products **3ba** (11.9 mg, 38% yield) and **3aa** (8.9 mg, 30% yield).



To an undivided three-necked bottle (10 mL) were added phenylglyoxylic acid **1e** (0.15 mmol), **1a** (0.15 mmol), Diphenylacetylene **2a** (0.2 mmol), NaOPiv (2 equiv), $[RuCl_2(p\text{-cymene})]_2$ (5 mmol%), and ^{t}AmOH/H_2O = 3:1 (6 mL). The bottle was equipped with platinum electrodes (1.0×1.0 cm^2) as cathode and graphite rod electrode as anode under air. The reaction mixture was stirred and electrolyzed at a constant current of 4 mA at 70 °C for 10 h. After the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried

with Na_2SO_4, filtered and concentrated in vacuum. The resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the desired products **3ea** (9.8 mg, 26% yield) and **3aa** (11.6 mg, 39% yield).



To an undivided three-necked bottle (10 mL) were added phenylglyoxylic acid **1g** (0.15 mmol), **1a** (0.15 mmol), Diphenylacetylene **2a** (0.2 mmol), NaOPiv (2 equiv), $[RuCl_2(p\text{-cymene})]_2$ (5 mmol%), and ^{t}AmOH/H_2O = 3:1 (6 mL). The bottle was equipped with platinum electrodes (1.0×1.0 cm^2) as cathode and graphite rod electrode as anode under air. The reaction mixture was stirred and electrolyzed at a constant current of 4 mA at 70 °C for 10 h. After the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered and concentrated in vacuum. The resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the desired products **3ga** (6.1mg, 19% yield) and **3aa** (12.8mg, 43% yield).

entry	R	[1]/M	[2]/M	$\log(k/k_0)$	σ_{para}
1	OMe	0.025	0.033	0.21	-0.27
2	Me	0.025	0.033	0.10	-0.07
3	H	0.025	0.033	0	0
4	Br	0.025	0.033	-0.18	0.39
5	CN	0.025	0.033	-0.35	0.56

σ_{para} values taken from ref. 7

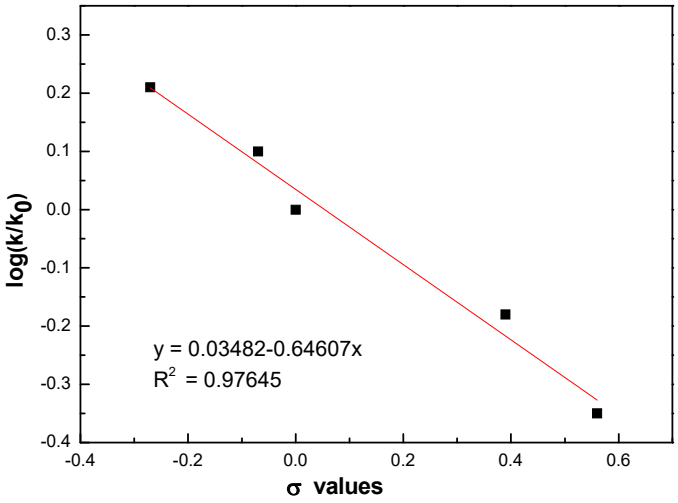
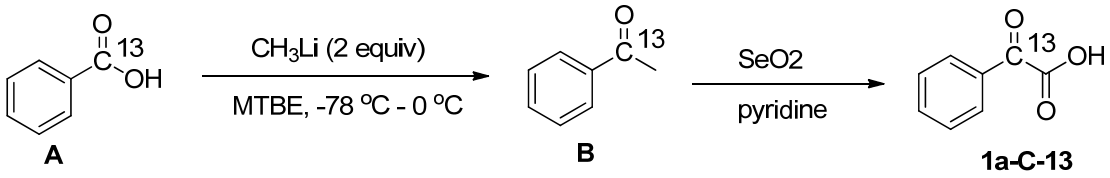
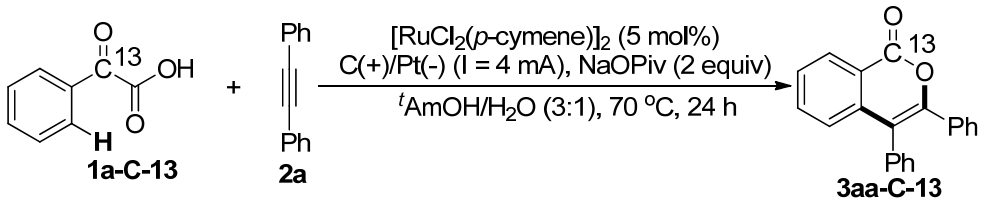


Figure S2. Intermolecular Hammett analysis.

(h) ^{13}C labeling experiment

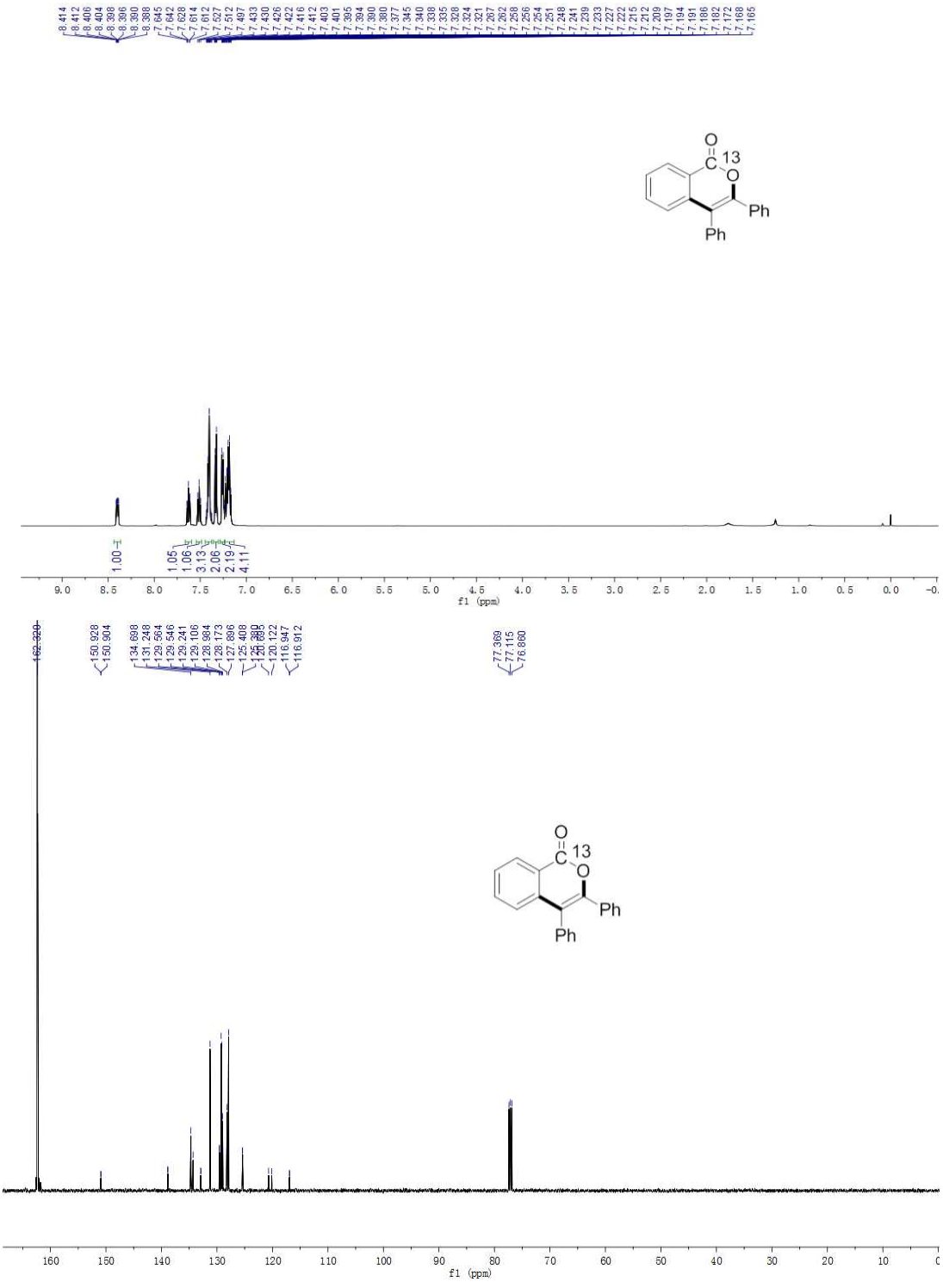


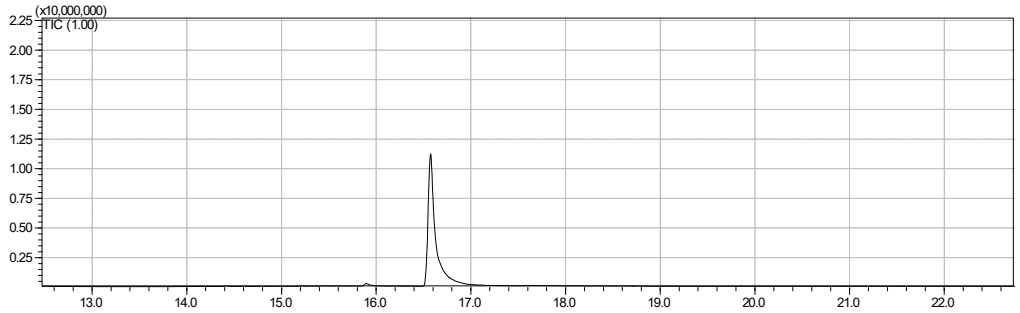
The synthesis of compound **1a-C-13** is based on the known methods.[8,9]

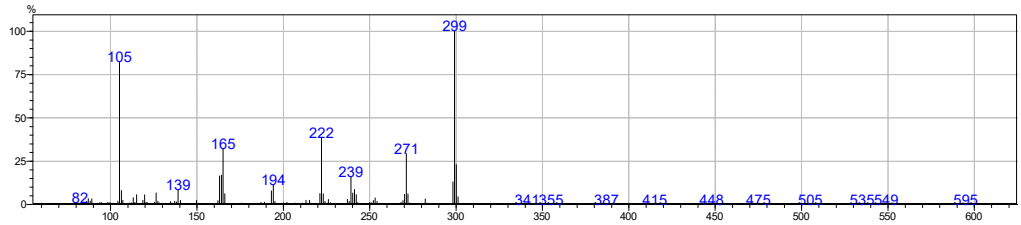


To an undivided three-necked bottle (10 mL) were added phenylglyoxylic acid **1a-C-13** (0.3 mmol), Diphenylacetylene **2a** (0.2 mmol), NaOPiv (2 equiv), $[RuCl_2(p\text{-cymene})]_2$ (5 mmol%), and ^{t}AmOH/H_2O = 3:1 (6 mL). The bottle was equipped with platinum electrodes (1.0×1.0 cm^2) as cathode and graphite rod electrode as anode under air. The reaction mixture was stirred and electrolyzed at a constant current of 4 mA at 70 °C for 24 h. After the reaction was finished, the

solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered and concentrated in vacuum. The resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the desired products **3aa-C-13** (81% yield).





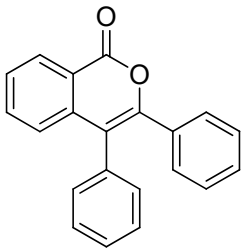


[MS Spectrum]
# of Peaks 517
Raw Spectrum 16.585 (scan : 2518)
Background No Background Spectrum
Base Peak m/z 299.10 (Inten : 1,731,023)
Event# 1

m/z	Absolute Intensity	Relative Intensity	m/z	Absolute Intensity	Relative Intensity	m/z	Absolute Intensity	Relative Intensity
270.15	100833	5.83	281.15	9133	0.53	292.10	97	0.01
271.15	508286	29.36	282.10	55697	3.22	293.10	262	0.02
272.15	105405	6.09	283.10	13697	0.79	294.10	225	0.01
273.10	14903	0.86	284.10	7649	0.44	295.05	622	0.04
274.10	1530	0.09	285.10	1634	0.09	296.15	2707	0.16
275.05	337	0.02	286.05	439	0.03	297.15	10670	0.62
276.10	57	0.00	287.10	95	0.01	**298.15**	**226379**	**13.08**
277.10	84	0.00	288.10	102	0.01	**299.10**	**1731023**	**100.00**
278.10	30	0.00	289.10	29	0.00	300.10	399118	23.06
279.10	236	0.01	290.10	68	0.00	301.10	77814	4.50
280.15	3411	0.20	291.10	78	0.00	302.10	10882	0.63

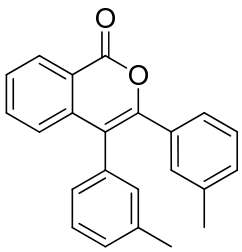
(B) Analytical data

3,4-Diphenyl-1*H*-isochromen-1-one (3aa):[1]



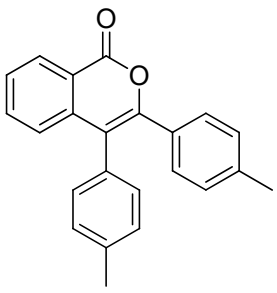
White solid; mp 171.5-172.9 °C (lit.[1] 172-174 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.42-8.40 (m, 1H), 7.65-7.62 (m, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.44-7.39 (m, 3H), 7.35-7.32 (m, 2H), 7.27-7.25 (m, 2H), 7.24-7.17 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.3, 150.9, 138.9, 134.7, 134.3, 132.9, 131.3, 129.6, 129.2, 129.1, 129.0, 128.2, 128.1, 127.9, 125.4, 120.4, 116.9; LRMS (EI, 70 eV) *m/z* (%): 298 (M^+, 100), 270 (22), 221 (35), 165 (28), 105 (86). The analytical data are in accordance with those reported in the literature.[1]

3,4-Di-*m*-tolyl-1*H*-isochromen-1-one (3ac):[2]



White solid; mp 121.3-124.1 °C (lit.[2] 115-145 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41-8.39 (m, 1H), 7.65-7.62 (m, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.32-7.26 (m, 2H), 7.22-7.20 (m, 2H), 7.08-7.04 (m, 5H), 2.35 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ) δ 162.5, 150.9, 139.1, 138.7, 137.5, 134.6, 134.3, 132.8, 131.7, 129.7 (2C), 129.5, 1289, 128.8, 128.3, 128.0, 127.6, 126.4, 125.5, 120.4, 116.9, 21.5, 21.4; LRMS (EI, 70 eV) *m/z* (%): 326 (M^+, 99), 298 (41), 235 (35), 178 (27), 119 (100). The analytical data are in accordance with those reported in the literature.[2]

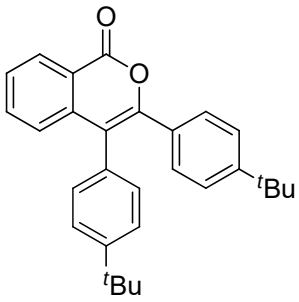
3,4-Di-*p*-tolyl-1*H*-isochromen-1-one (3ad):[2]



Light yellow solid; mp 153.3-156.1 °C (lit.[2] 153-155 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40-8.38 (m, 1H), 7.63-7.60 (m, 1H), 7.51-7.48 (m, 1H), 7.26-7.19 (m, 5H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.01 (d, *J* = 8.0 Hz, 2H), 2.42 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) 162.5, 151.0, 139.3, 139.0, 137.8,

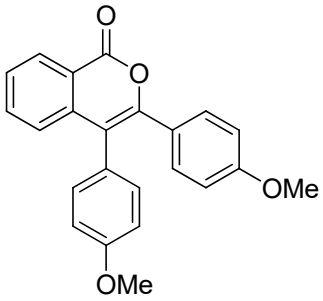
134.6, 131.4, 131.0, 130.2, 129.9, 129.5, 129.1, 128.6, 127.8, 125.4, 120.3, 116.3, 21.4, 21.3; LRMS (EI, 70 eV) *m/z* (%): 326 (M^+, 100), 298 (46), 235 (23), 178 (18), 119 (50). The analytical data are in accordance with those reported in the literature.[2]

3,4-Bis(4-(*tert*-butyl)phenyl)-1*H*-isochromen-1-one (3ae):



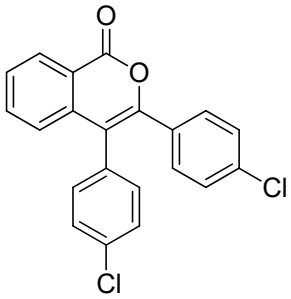
Light yellow solid, mp 164.8-166.1 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40-8.38 (m, 1H), 7.64-7.60 (m, 1H), 7.51-7.48 (m, 1H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.28-7.26 (m, 2H), 7.21-7.18 (m, 5H), 1.38 (s, 9H), 1.26 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.5, 152.0, 151.2, 150.7, 139.4, 134.5, 131.4, 130.8, 130.1, 129.4, 128.8, 127.8, 126.0, 125.5, 124.8, 120.3, 116.4, 34.7 (2C), 31.4, 31.1; LRMS (EI, 70 eV) *m/z* (%): 410 (M^+, 99), 354 (100), 297 (15), 221 (18), 161 (37); HRMS *m/z* (ESI) calcd for $C_{29}H_{31}O_2$ $[M+H]^+$ 411.2324, found 411.2346.

3,4-Bis(4-methoxyphenyl)-1*H*-isochromen-1-one (3af):[3]



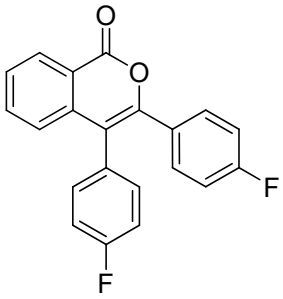
Light yellow solid; mp 157.1-158.8 °C (lit.[3] 158.4-159.7 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, *J* = 7.5 Hz, 1H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.30-7.26 (m, 2H), 7.21-7.16 (m, 3H), 6.96 (d, *J* = 8.5 Hz, 2H), 6.72 (d, *J* = 9.0 Hz, 2H), 3.86 (s, 3H), 3.75 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.5, 159.9, 159.3, 150.9, 139.5, 134.6, 132.3, 130.7, 129.4, 127.7, 126.6, 125.4, 125.2, 120.2, 115.4, 114.6, 113.3, 55.3, 55.2; LRMS (EI, 70 eV) *m/z* (%): 358 (M^+, 100), 330 (94), 315 (157), 135 (56). The analytical data are in accordance with those reported in the literature.[3]

3,4-Bis(4-chlorophenyl)-1*H*-isochromen-1-one (3ag):[3]



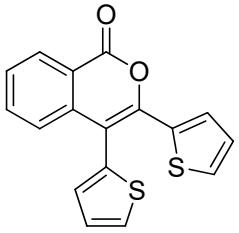
Light yellow solid; mp 171.8-173.3 °C (lit.[3] 172.6-173.6 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, *J* = 7.5 Hz, 1H), 7.67 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 8.5 Hz, 2H), 7.21-7.16 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.8, 150.0, 138.2, 135.3, 134.9, 134.5, 132.5 (2C), 131.1, 130.5, 129.8, 129.6, 128.5, 128.4, 125.1, 120.4, 116.1; LRMS (EI, 70 eV) *m/z* (%): 366 (M^+, 100), 338 (56), 303 (37), 239 (41), 139 (78). The analytical data are in accordance with those reported in the literature.[3]

3,4-Bis(4-fluorophenyl)-1*H*-isochromen-1-one (3ah):[2]



White solid; mp 151.8-153.9 °C (lit.[2] 150-152 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.0 Hz, 1H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.32-7.29 (m, 2H), 7.25-7.23 (m, 2H), 7.18-7.12 (m, 3H), 6.91-6.88 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.8, 163.6, 161.9, 161.8, 161.6, 150.3, 138.6, 134.8, 133.0, 132.9, 131.3, 131.2, 130.1, 130.0, 129.7, 128.9 (2C), 128.3, 125.1, 120.4, 116.5, 116.3, 115.8, 115.24, 115.1; ^{19}F NMR (471 MHz, $CDCl_3$) δ -110.75, -112.82; LRMS (EI, 70 eV) *m/z* (%): 334 (M^+, 100), 306 (71), 123 (72), 95 (61). The analytical data are in accordance with those reported in the literature.[2]

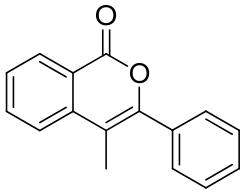
3,4-Di(thiophen-2-yl)-1*H*-isochromen-1-one (3ai):[1]



Yellow solid, mp 184.7-185.4 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (d, *J* = 7.5 Hz, 1H), 7.66-7.63 (m, 2H), 7.48 (t, *J* = 7.5 Hz, 1H), 7.41 (d, *J* = 3.5 Hz, 1H), 7.32 (d, *J* = 4.5 Hz, 1H), 7.28-7.26 (m, 1H), 7.15-7.12 (m, 2H), 6.97 (t, *J* = 4.0 Hz 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.2, 148.2, 139.7, 135.0, 134.6, 133.7, 130.8, 130.0, 129.5

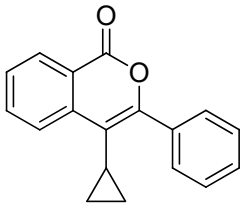
(2C), 129.0, 128.4, 128.0, 127.0, 125.2, 119.7, 107.2; LRMS (EI, 70 eV) *m/z* (%): 310 (M^+, 81), 282 (100), 253 (63), 221 (28), 111 (31). The analytical data are in accordance with those reported in the literature.[1]

4-Methyl-3-phenyl-1*H*-isochromen-1-one (3aj):[2]



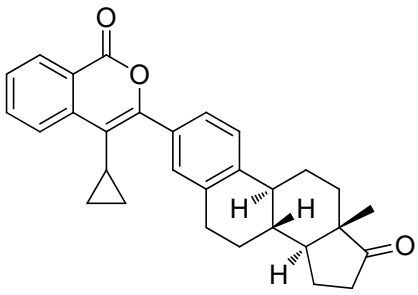
White solid; mp 90.8-92.1 °C (lit.[2] 92-94 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (d, *J* = 7.5 Hz, 1H), 7.82-7.79 (m, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 6.5 Hz, 2H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.49-7.42 (m, 3H), 2.32 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.6, 151.2, 138.8, 134.8, 133.3, 129.8, 129.5, 129.4, 128.3, 128.0, 123.4, 120.8, 109.2, 13.6; LRMS (EI, 70 eV) *m/z* (%): 236 (M^+, 94), 208 (100), 178 (21), 105 (36), 77 (54). The analytical data are in accordance with those reported in the literature.[2]

4-Cyclopropyl-3-phenyl-1*H*-isochromen-1-one (3ak):[4]



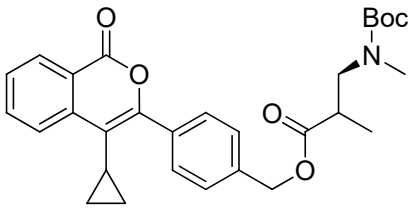
Light yellow solid; mp 116.5-117.4 °C (lit.[4] 115-117 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.0 Hz, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 7.82-7.78 (m, 1H), 7.75-7.73 (m, 2H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.46-7.43 (m, 3H), 1.94-1.89 (m, 1H), 0.96-0.93 (m, 2H), 0.20-0.17 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.5, 153.5, 139.7, 134.5, 133.2, 129.5 (2C), 129.4, 127.9, 124.6, 120.6, 114.6, 10.0, 9.1; LRMS (EI, 70 eV) *m/z* (%): 262 (M^+, 77), 233 (22), 217 (54), 185 (64), 105 (100). The analytical data are in accordance with those reported in the literature.[4]

4-Cyclopropyl-3-((8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[a]phenanthren-3-yl)-1*H*-isochromen-1-one (3al):[1b]



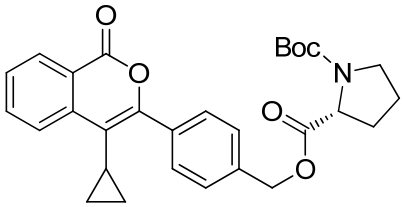
White solid; mp 220.2-221.9 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.0 Hz, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 7.80 (t, *J* = 8.0 Hz, 1H), 7.55-7.51 (m, 3H), 7.35 (d, *J* = 8.0 Hz, 1H), 2.99-2.97 (m, 2H), 2.56- 2.46 (m, 2H), 2.40-2.35 (m, 1H), 2.21-2.06 (m, 3H), 2.01 (d, *J* = 12.5 Hz, 1H), 1.94-1.91 (m, 1H), 1.71-1.60 (m, 2H), 1.59-1.49 (m, 4H), 1.02-0.88 (m, 5H), 0.27-0.21 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 221.0, 162.6, 153.6, 141.2, 139.9, 136.1, 134.5, 130.6, 129.8, 129.5, 127.7, 127.1, 124.7, 124.5, 120.5, 114.2, 50.6, 48.0, 44.6, 38.0, 35.9, 31.6, 29.4, 26.5, 25.6, 21.6, 13.9, 10.2, 10.1, 9.2. The analytical data are in accordance with those reported in the literature.[1b]

4-(4-Cyclopropyl-1-oxo-1*H*-isochromen-3-yl)benzyl-3-((tert-butoxycarbonyl)(methyl)amino)-2-methylpropanoate (3am):[1b]



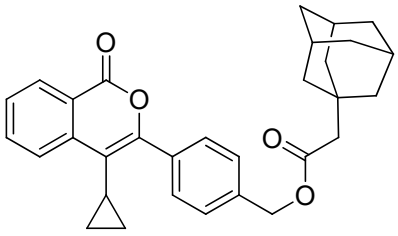
Light yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (t, *J* = 7.0 Hz,, 1H), 8.12 (d, *J* = 8.5 Hz, 1H), 7.83-7.79 (m, 1H), 7.75 (d, *J* = 5.0 Hz, 2H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.42 (d, *J* = 7.5 Hz, 2H), 5.23 (s, 2H), 4.94-4.90 (m, 0.5H), 4.56-4.52 (m, 0.5H), 2.89-2.82 (m, 3H), 1.94-1.91 (m, 1H), 1.48-1.42 (m, 12H), 0.97-0.95 (m, 2H), 0.21-0.18 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.3, 162.3, 156.0, 152.9, 139.6, 136.8, 134.6, 133.0, 129.7, 129.5, 127.9, 127.3, 127.2, 124.6, 120.6, 114.9, 80.4, 80.1, 66.2, 55.2, 53.7, 30.6, 28.4, 15.3, 14.8, 10.0, 9.0. The analytical data are in accordance with those reported in the literature.[1b]

(R)-1-*tert*-Butyl 2-(4-(4-cyclopropyl-1-oxo-1*H*-isochromen-3-yl)benzyl) pyrrolidine-1,2-dicarboxylate (3an):[1b]



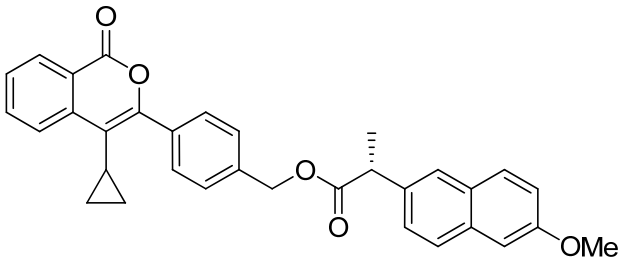
Light yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.0 Hz, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.81 (t, *J* = 7.5 Hz, 1H), 7.78-7.73 (m, 2H), 7.54 (t, *J* = 7.5 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 2H), 5.34-5.18 (m, 2H), 4.44-4.31 (m, 1H), 3.61-3.43 (m, 2H), 2.29-2.20 (m, 1H), 2.01-1.86 (m, 4H), 1.49-1.47 (m, 4H), 1.39-1.37 (m, 5H), 0.98-0.96 (m, 2H), 0.21-0.18 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.1, 172.8, 162.3, 153.8, 152.9, 139.6, 137.2, 136.9, 134.6, 133.2, 129.8, 129.7, 129.5, 128.0, 127.9, 127.5, 127.2, 124.6, 120.6, 114.9, 114.8, 80.0, 79.9, 66.1, 66.1, 59.2, 58.9, 46.6, 46.4, 30.9, 30.0, 28.5, 28.3, 24.4, 23.7, 10.0, 9.0. The analytical data are in accordance with those reported in the literature.[1b]

4-(4-Cyclopropyl-1-oxo-1*H*-isochromen-3-yl)benzyl-2-((3r,5r,7r)-adamantan-1-yl)acetate (3ao):[1b]



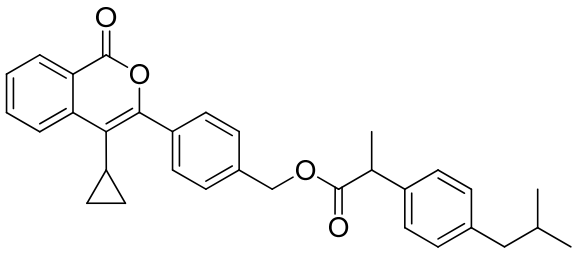
White solid; mp 135.1-136.6 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (t, *J* = 7.0 Hz, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 7.82-7.79 (m, 1H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 2H), 5.17 (s, 2H), 2.16 (s, 2H), 1.99-1.96 (m, 3H), 1.94-1.91 (m, 1H), 1.72-1.70 (m, 3H), 1.65-1.62 (m, 9H), 0.97-0.95 (m, 2H), 0.21-0.18 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.6, 162.4, 153.0, 139.7, 137.5, 134.6, 132.9, 129.7, 129.5, 127.9, 127.6, 124.6, 120.6, 114.8, 65.4, 48.9, 42.4, 36.7, 33.0, 28.6, 10.0, 9.1; LRMS (EI, 70 eV) *m/z* (%): 468 (M^+, 8), 450 (9), 292 (18), 274 (100), 246 (30). The analytical data are in accordance with those reported in the literature.[1b]

(R)-4-(4-Cyclopropyl-1-oxo-1*H*-isochromen-3-yl)benzyl-2-(6-methoxynaphthalen-2-yl)propanoate (3ap):



Light yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.0 Hz, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 7.76 (t, *J* = 8.5 Hz, 1H), 7.70-7.67 (m, 3H), 7.63 (d, *J* = 8.5 Hz, 2H), 7.48 (t, *J* = 8.0 Hz, 1H), 7.42-7.40 (m, 1H), 7.27 (d, *J* = 8.5 Hz, 2H), 7.24 (s, 1H), 7.14-7.10 (m, 2H), 5.17 (s, 2H), 3.94 (q, *J* = 7.0 Hz, 1H), 3.88 (s, 3H), 1.85-1.79 (m, 1H), 1.62 (d, *J* = 7.0 Hz, 3H), 0.89-0.85 (m, 2H), 0.13-0.10 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 174.4, 162.3, 157.7, 153.0, 139.6, 137.3, 135.5, 134.5, 133.8, 132.9, 129.6, 129.4, 129.3, 128.9, 127.9, 127.2, 127.1, 126.3, 126.1, 124.6, 120.6, 119.1, 114.8, 105.7, 77.4, 65.9, 55.3, 45.5, 18.5, 10.0, 9.0; HRMS *m/z* (ESI) calcd for $C_{33}H_{29}O_5$ $[M+H]^+$ 505.2015, found 505.2027.

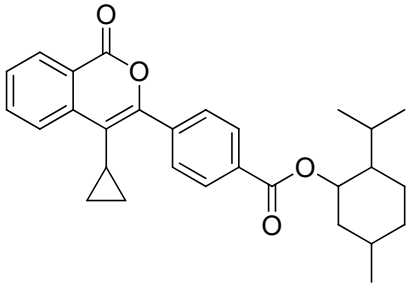
4-(4-Cyclopropyl-1-oxo-1*H*-isochromen-3-yl)benzyl-2-(4-isobutylphenyl)propanoate (3aq):



Light yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.0 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 7.78 (t, *J* = 8.5 Hz, 1H), 7.68 (d, *J* = 8.5 Hz, 2H), 7.50 (t, *J* = 8.0 Hz, 1H), 7.28 (d, *J* = 8.5 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 5.17 (d, *J* = 3.0 Hz, 2H), 3.79 (q, *J* = 7.0 Hz, 1H), 2.45 (d, *J* = 7.0 Hz, 2H), 1.91-1.82 (m, 2H), 1.54 (d, *J* = 7.0 Hz, 3H), 0.95-0.91 (m, 2H), 0.90 (d, *J* = 6.5 Hz, 6H), 0.18-0.15 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 174.5, 162.3, 153.0, 140.7, 139.7, 137.7, 137.4, 134.5, 132.8, 129.6, 129.5, 129.4, 127.9, 127.3, 127.0, 124.6,

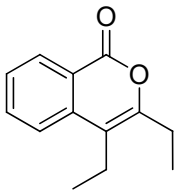
120.6, 114.7, 65.8, 45.2, 45.1, 30.2, 22.4, 18.4, 10.1, 9.1; HRMS *m/z* (ESI) calcd for $C_{32}H_{33}O_4$ $[M+H]^+$ 481.2379, found 481.2361.

2-Isopropyl-5-methylcyclohexyl-4-(4-cyclopropyl-1-oxo-1*H*-isochromen-3-yl)benzoate (3ar):[1b]



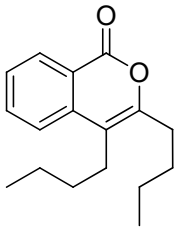
Light yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.35-8.33 (m, 1H), 8.12-8.11 (m, 3H), 7.85-7.81 (m, 3H), 7.57-7.54 (m, 1H), 5.00-4.95 (m, 1H), 2.19-2.16 (m, 1H), 2.01-1.93 (m, 2H), 1.76 (t, *J* = 2.5 Hz, 2H), 1.62-1.57 (m, 2H), 1.18-1.11 (m, 2H), 1.00-0.94 (m, 9H), 0.84-0.81 (m, 3H), 0.21-0.19 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.7, 162.1, 152.3, 139.4, 137.2, 134.7, 131.3, 129.6, 129.5, 129.0, 128.3, 124.7, 120.7, 115.9, 75.2, 47.2, 41.0, 34.3, 31.5, 26.5, 23.6, 22.1, 20.8, 16.6, 10.2, 10.1, 9.1; LRMS (EI, 70 eV) *m/z* (%): 444 (M^+, 8), 307 (48), 289 (100), 261 (35), 138 (35). The analytical data are in accordance with those reported in the literature.[1b]

3,4-diethyl-1*H*-isochromen-1-one (3as):[5]



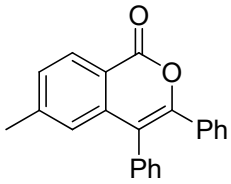
White solid; mp 58.3-60.1 °C (lit.[5] 59-64 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 (d, *J* = 7.0 Hz, 1H), 7.76-7.72 (m, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 2.68-2.60 (m, 4H), 1.29 (t, *J* = 8.0 Hz, 3H), 1.21 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.0, 155.0, 137.8, 134.6, 129.9, 127.1, 122.5, 120.9, 113.1, 24.1, 19.3, 14.4, 12.6; LRMS (EI, 70 eV) *m/z* (%): 202 (M^+, 100), 187 (94), 259 (32), 131 (87), 115 (44). The analytical data are in accordance with those reported in the literature.[5]

3,4-Dibutyl-1*H*-isochromen-1-one (3at):[2]



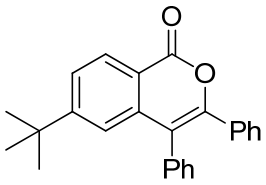
Colourless oil; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32-8.30 (m, 1H), 7.75-7.71 (m, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.47-7.44 (m, 1H), 2.62-2.57 (m, 4H), 1.73-1.67 (m, 2H), 1.57-1.38 (m, 6H), 1.10-0.94 (m, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.0, 154.2, 138.0, 134.6, 129.8, 127.0, 122.6, 120.8, 112.3, 31.9, 30.6, 30.0, 25.9, 22.9, 22.5, 14.0, 13.9; LRMS (EI, 70 eV) *m/z* (%): 258 (M^+, 44), 215 (48), 173 (100), 145 (23), 131 (21). The analytical data are in accordance with those reported in the literature.[2]

6-Methyl-3,4-diphenyl-1*H*-isochromen-1-one (3ba):[1]



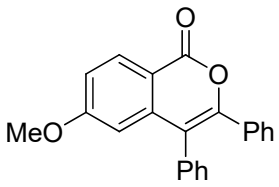
White solid; mp 187.1-188.7 ºC (lit.[1]186-188 ºC); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (d, *J* = 8.0 Hz, 1H), 7.44-7.40 (m, 3H), 7.34-7.30 (m, 3H), 7.26-7.24 (m, 2H), 7.22-7.16 (m, 3H), 6.97 (s, 1H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.4, 151.0, 145.8, 138.9, 134.4, 133.1, 131.3, 129.6, 129.5, 129.3, 129.1, 128.9, 128.1, 127.9, 125.3, 118.1, 116.9, 22.3; LRMS (EI, 70 eV) *m/z* (%): 312 (M^+, 100), 284 (31), 235 (28), 178 (17), 105 (51). The analytical data are in accordance with those reported in the literature.[1]

6-(*tert*-Butyl)-3,4-diphenyl-1*H*-isochromen-1-one (3ca):[2]



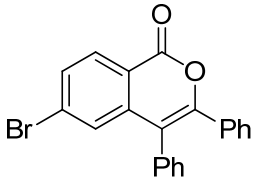
White solid; mp 158.2-162.4 ºC (lit.[2] 161-163 ºC); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.5 Hz, 1H), 7.58-7.56 (m, 1H), 7.43-7.41 (m, 3H), 7.34-7.32 (m, 2H), 7.28-7.26 (m, 2H), 7.22-7.15 (m, 4H), 1.23 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.2, 158.6, 150.9, 138.7, 134.5, 133.2, 131.3, 129.4, 129.3, 129.0, 128.8, 128.1, 127.9, 126.0, 121.8, 118.1, 117.3, 35.5, 30.9; LRMS (EI, 70 eV) *m/z* (%): 354 (M^+, 100), 326 (13), 298 (36), 105 (69). The analytical data are in accordance with those reported in the literature.[2]

6-Methoxy-3,4-diphenyl-1*H*-isochromen-1-one (3da):[1]



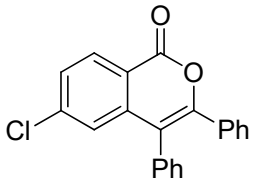
White solid; mp 176.8-178.1 °C (lit.[1] 178-180 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (d, *J* = 9.0 Hz, 1H), 7.43-7.37 (m, 3H), 7.33-7.31 (m, 2H), 7.28-7.25 (m, 2H), 7.24-7.17 (m, 3H), 7.07-7.05 (m, 1H), 6.58 (d, *J* = 2.5 Hz, 1H), 3.75 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.7, 162.1, 151.5, 141.2, 134.4, 133.0, 131.9, 131.2, 129.3, 129.1, 129.0, 128.2, 127.8, 116.8, 115.7, 113.7, 108.5, 55.5; LRMS (EI, 70 eV) *m/z* (%): 328 (M^+, 100), 300 (20), 251 (33), 152 (26), 105 (61). The analytical data are in accordance with those reported in the literature.[1]

6-Bromo-3,4-diphenyl-1*H*-isochromen-1-one (3ea):[1]



White solid; mp 199.7-201.4 °C (lit.[1] 198-200 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.5 Hz, 1H), 7.64-7.62 (m, 1H), 7.45-7.43 (m, 3H), 7.33-7.30 (m, 3H), 7.25-7.23 (m, 3H), 7.20-7.18 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.7, 152.2, 140.4, 133.6, 132.6, 131.5, 131.2, 131.1, 130.5, 129.3 (3C), 128.5, 128.1, 128.0, 119.1, 116.0; LRMS (EI, 70 eV) *m/z* (%): 378 (M^{2+}, 38), 376 (M^+, 41), 348 (6), 299 (20), 163 (38), 105 (100). The analytical data are in accordance with those reported in the literature.[1]

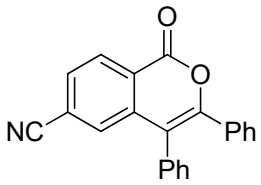
6-Chloro-3,4-diphenyl-1*H*-isochromen-1-one (3fa):[6]



White solid; mp 169.4-172.1 °C (lit.[6] 168-170 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.5 Hz, 1H), 7.48-7.43 (m, 4H), 7.32-7.31 (m, 2H), 7.26-7.24 (m, 3H), 7.21-7.16 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.5, 152.2, 141.7, 140.4, 133.6, 132.6, 131.3, 131.1, 129.3 (3C), 128.6, 128.5, 128.0, 125.0, 118.7, 116.1; LRMS (EI, 70 eV) *m/z* (%): 332

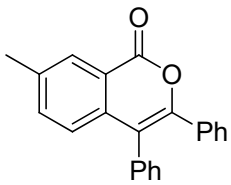
(M^+, 94), 304 (21), 255 (30), 163 (24), 105 (100). The analytical data are in accordance with those reported in the literature.[6]

1-Oxo-3,4-diphenyl-1*H*-isochromene-6-carbonitrile (3ga):[1]



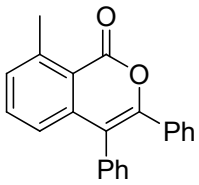
Light yellow solid; mp 176.8-178.5 °C (lit.[1] 176-178 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.0 Hz, 1H), 7.74-7.72 (m, 1H), 7.50-7.45 (m, 4H), 7.34-7.32 (m, 2H), 7.29-7.20 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.7, 152.8, 139.5, 132.9, 132.1, 131.0, 130.5, 130.2, 129.7 (2C), 129.6, 129.3, 128.9, 128.1, 123.0, 118.2, 117.7, 115.7; LRMS (EI, 70 eV) *m/z* (%): 323 (M^+, 100), 295 (28), 246 (27), 105 (78). The analytical data are in accordance with those reported in the literature.[1]

7-Methyl-3,4-diphenyl-1*H*-isochromen-1-one (3ha):[1]



White solid; mp 169.1-172.5 °C (lit.[1] 171-173 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.45-7.38 (m, 4H), 7.33-7.31 (m, 2H), 7.25-7.22 (m, 2H), 7.22-7.14 (m, 3H), 7.09 (d, *J* = 8.0 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.5, 150.1, 138.5, 136.4, 136.0, 134.5, 133.0, 131.2, 129.3, 129.2, 129.1, 128.8, 128.1, 127.9, 125.4, 120.43, 116.9, 21.3; LRMS (EI, 70 eV) *m/z* (%): 312 (M^+, 100), 284 (23), 235 (39), 178 (21), 105 (78). The analytical data are in accordance with those reported in the literature.[1]

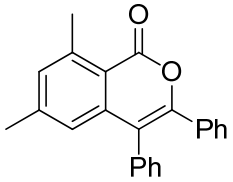
8-Methyl-3,4-diphenyl-1*H*-isochromen-1-one (3ia):[1]



White solid; mp 142.5-143.9 °C (lit.[1] 143-144 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (t, *J* = 7.5 Hz, 1H), 7.42-7.38 (m, 3H), 7.32-7.29 (m, 2H), 7.25-7.20 (m, 3H), 7.19-7.16 (m, 2H), 7.00 (d, *J* = 8.0 Hz, 1H), 2.91 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.6, 150.6, 143.5, 140.5, 135.0, 133.7, 133.0, 131.4, 131.1, 129.1 (2C), 128.8, 128.0, 127.8, 123.7, 118.9, 117.0,

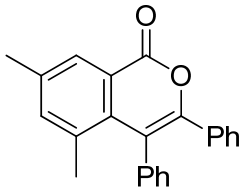
23.60; LRMS (EI, 70 eV) *m/z* (%): 312 (M^+, 100), 284 (29), 235 (21), 178 (26), 105 (82). The analytical data are in accordance with those reported in the literature.[1]

6,8-Dimethyl-3,4-diphenyl-1*H*-isochromen-1-one (3ja):[1]



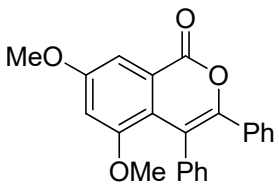
White solid; mp 157.4-159.1 °C (lit.[1] 158-160 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40-7.38 (m, 3H), 7.30-7.28 (m, 2H), 7.24-7.22 (m, 2H), 7.21-7.14 (m, 3H), 7.12 (s, 1H), 6.78 (s, 1H), 2.87 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.6, 150.7, 144.6, 143.4, 140.6, 135.1, 133.2, 132.4, 131.4, 129.1, 129.0, 128.7, 128.0, 127.8, 123.7, 116.9, 116.6, 23.4, 21.9; LRMS (EI, 70 eV) *m/z* (%): 326 (M^+, 100), 298 (24), 193 (27), 105 (80). The analytical data are in accordance with those reported in the literature.[1]

5,7-Dimethyl-3,4-diphenyl-1*H*-isochromen-1-one (3ka):[5]



White solid; mp 168.5-169.9 °C (lit.[5] 165-166 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 (s, 1H), 7.30-7.27 (m, 4H), 7.23-7.19 (m, 3H), 7.19-7.14 (m, 4H), 2.43 (s, 3H), 1.72 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.0, 150.7, 140.4, 138.2, 137.3, 135.5, 133.8, 133.5, 131.8, 129.5, 128.4, 128.2, 127.9, 127.6, 121.6, 117.3, 23.2, 21.0; LRMS (EI, 70 eV) *m/z* (%): 326 (M^+, 100), 298 (23), 193 (37), 105 (98). The analytical data are in accordance with those reported in the literature.[5]

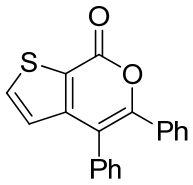
5,7-Dimethoxy-3,4-diphenyl-1*H*-isochromen-1-one (3la):[6]



White solid; mp 158.4-159.8 °C (lit.[6] 159-161 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (d, *J* = 2.5 Hz, 1H), 7.24-7.21 (m, 5H), 7.18-7.11 (m, 5H), 6.68 (d, *J* = 2.6 Hz, 1H), 3.93 (s, 3H), 3.32 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.5, 160.3, 157.6, 149.0, 137.6, 133.6, 130.7, 129.5, 128.3, 127.6, 127.4, 126.7, 122.9, 122.1, 115.5, 106.9, 102.1, 55.9, 55.8;

LRMS (EI, 70 eV) *m/z* (%): 358 (M^+, 100), 315 (14), 253 (71), 105 (52). The analytical data are in accordance with those reported in the literature.[6]

4,5-Diphenyl-7*H*-thieno[2,3-c]pyran-7-one (3ma):[2]



Light yellow solid; mp 147.5-149.6 °C (lit.[2] 146-148 °C); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 5.0 Hz, 1H), 7.41-7.34 (m, 5H), 7.28-7.25 (m, 3H), 7.22-7.19 (m, 2H), 6.96 (d, *J* = 5.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.2, 153.4, 149.5, 136.3, 134.9, 132.4, 130.3, 129.3, 129.2, 129.1, 128.2, 128.0, 125.2, 122.8, 115.9; LRMS (EI, 70 eV) *m/z* (%): 304 (M^+, 100), 276 (17), 227 (40), 171 (20), 105 (52). The analytical data are in accordance with those reported in the literature.[2]

(C) References

(1) (a) Qiu, Y.; Tian, C.; Massignan, L.; Rogge, T.; Ackermann. L. *Angew. Chem., Int. Ed.* **2018**, *130*, 5920. (b) Luo, M.-J.; Hu, M.; Song, R.-J.; He, D.-L.; Li, J.-H. *Chem. Commun.* **2019**, *55*, 1124.

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(6) Ueura, K.; Satoh, T.; Miura, M. *Org. Lett.* **2007**, *9,* 1407.

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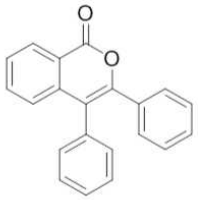
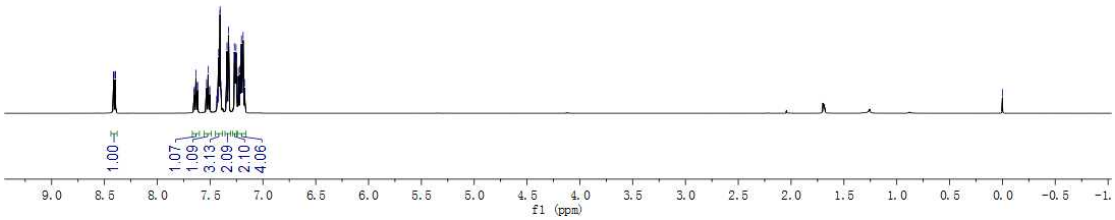
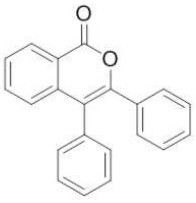
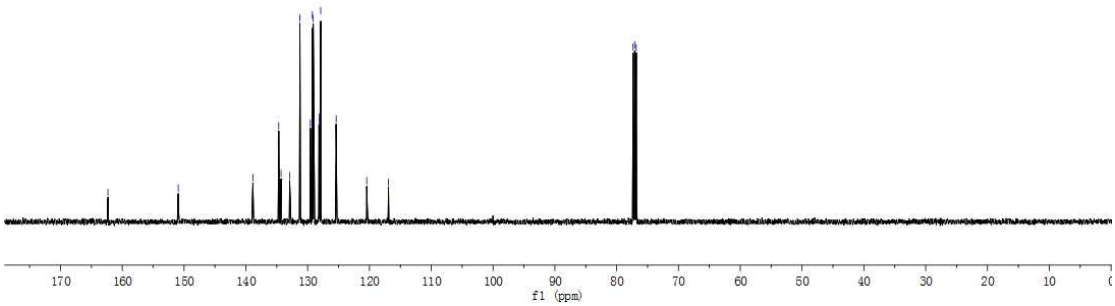
(D) Spectra

3,4-Diphenyl-1*H*-isochromen-1-one (3aa):

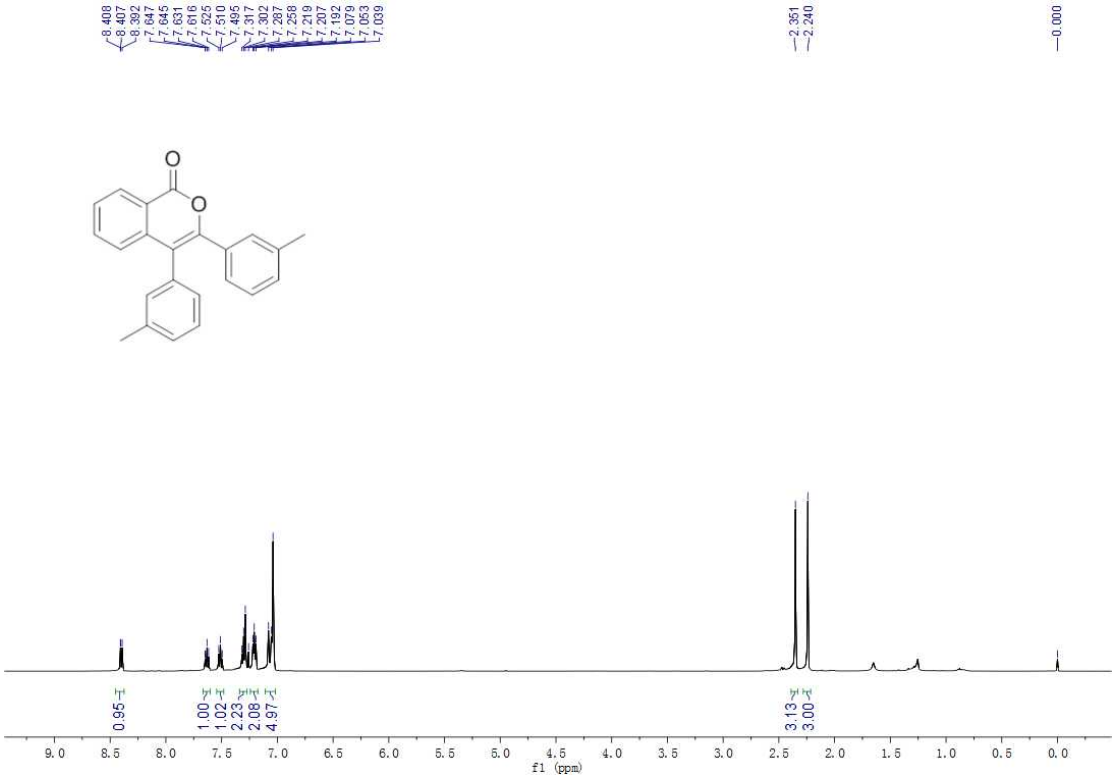


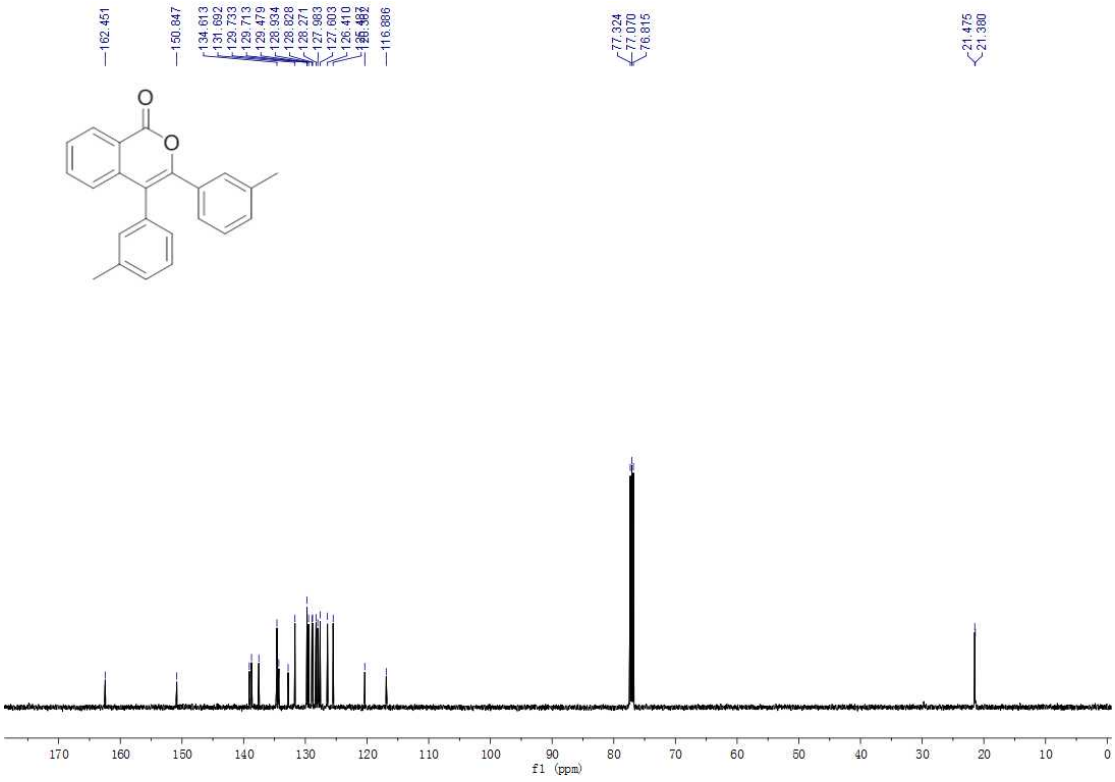




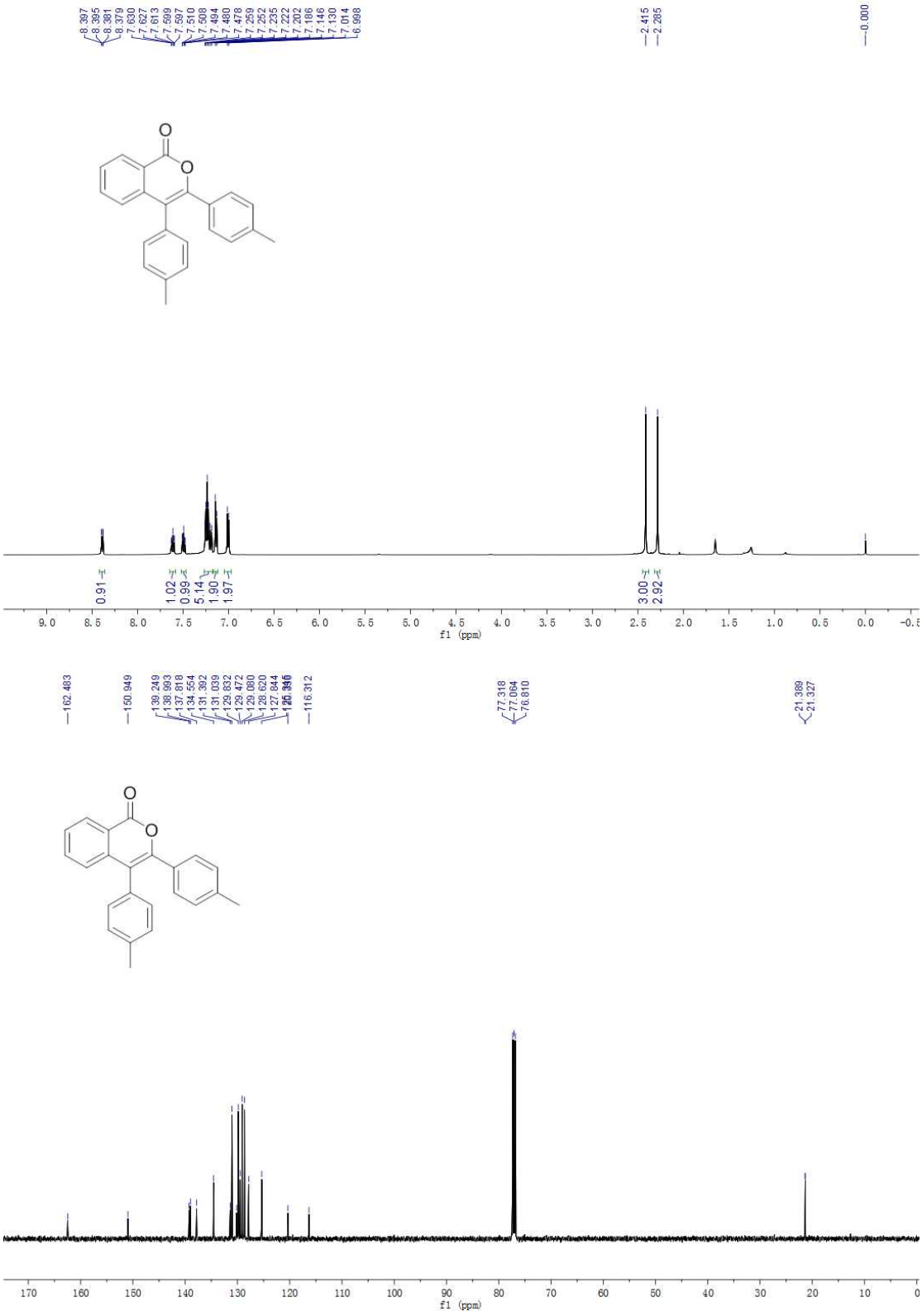


3,4-Di-*m*-tolyl-1*H*-isochromen-1-one (3ac):

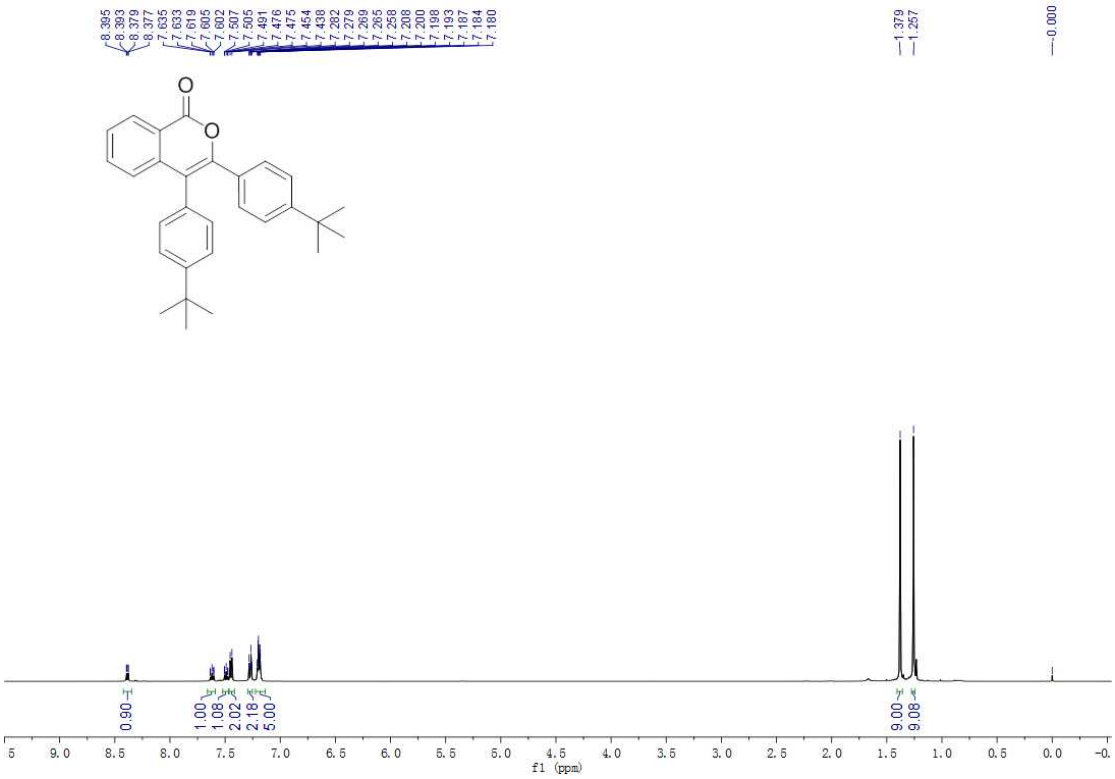


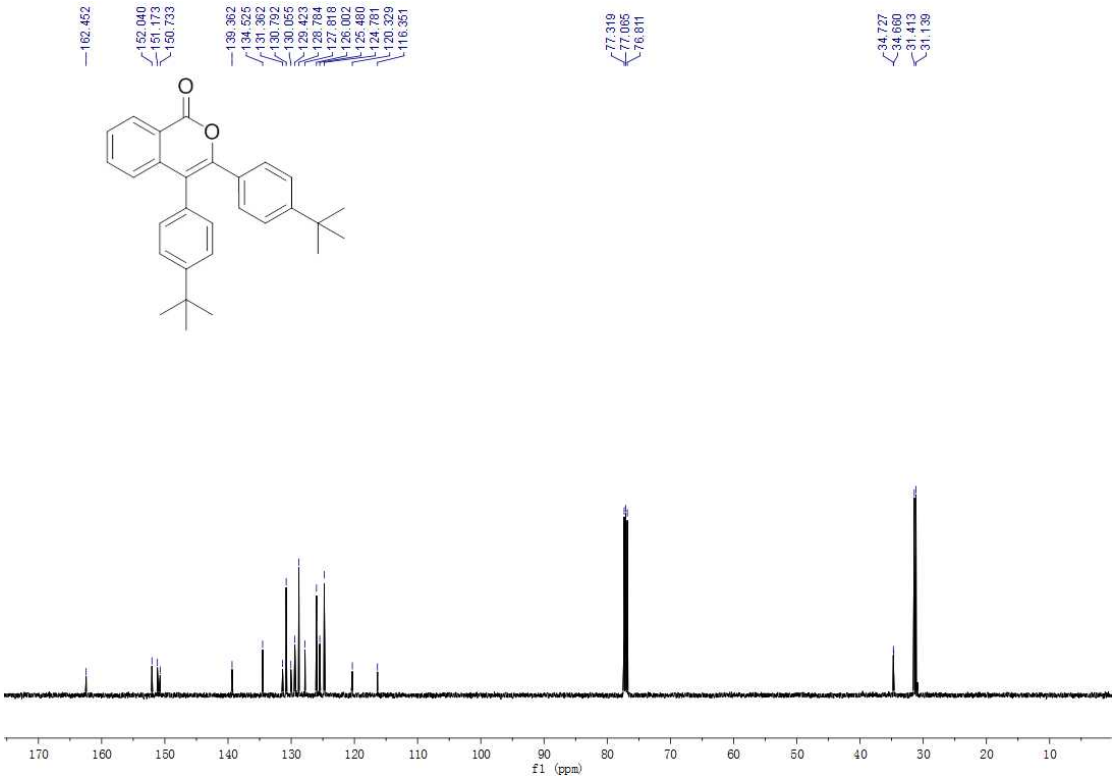


3,4-Di-*p*-tolyl-1*H*-isochromen-1-one (3ad):

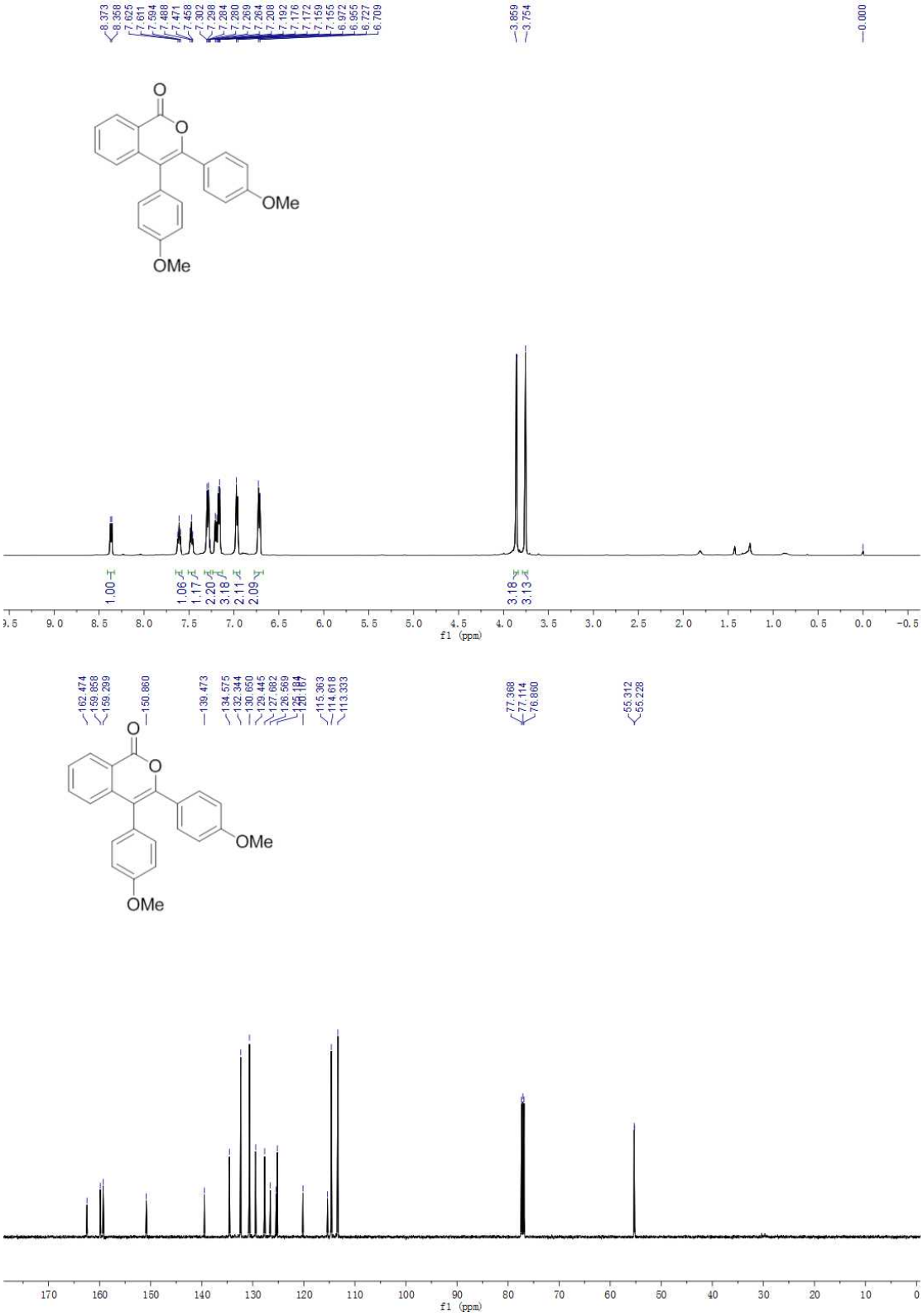


3,4-Bis(4-(*tert*-butyl)phenyl)-1*H*-isochromen-1-one (3ae):

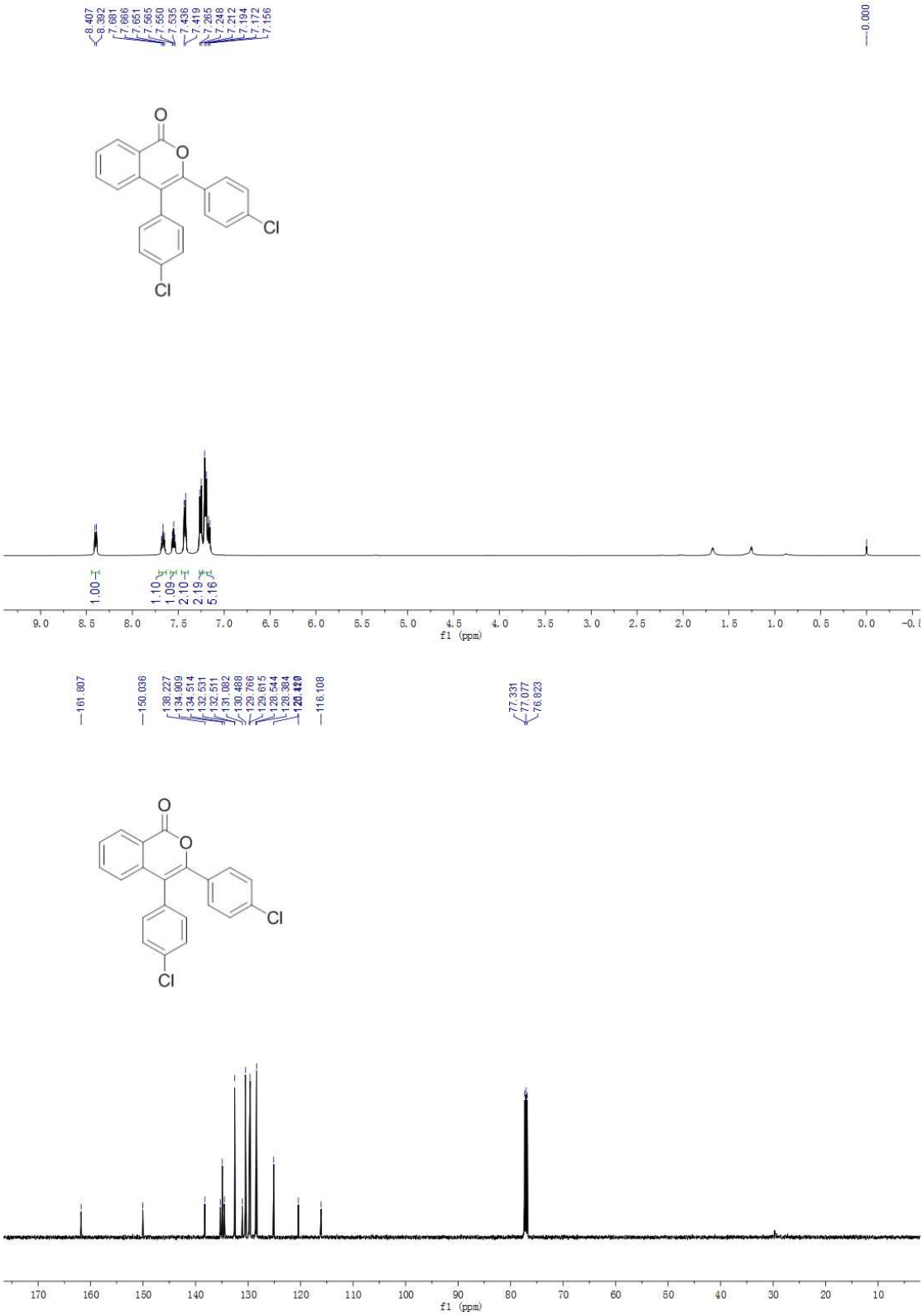




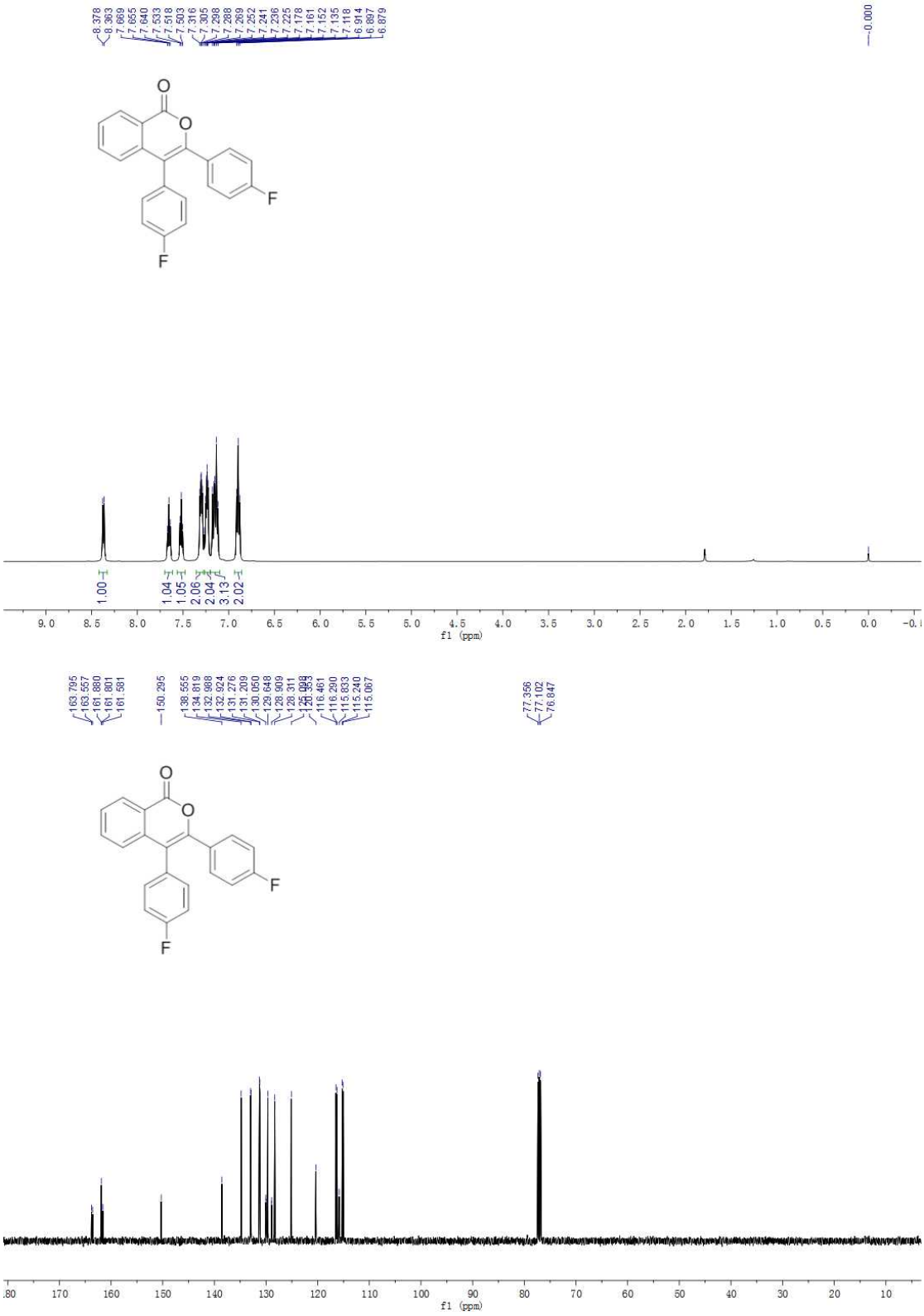
3,4-Bis(4-methoxyphenyl)-1*H*-isochromen-1-one (3af):

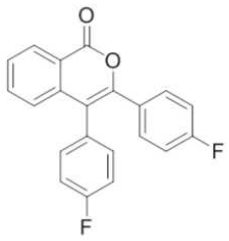


3,4-Bis(4-chlorophenyl)-1*H*-isochromen-1-one (3ag):



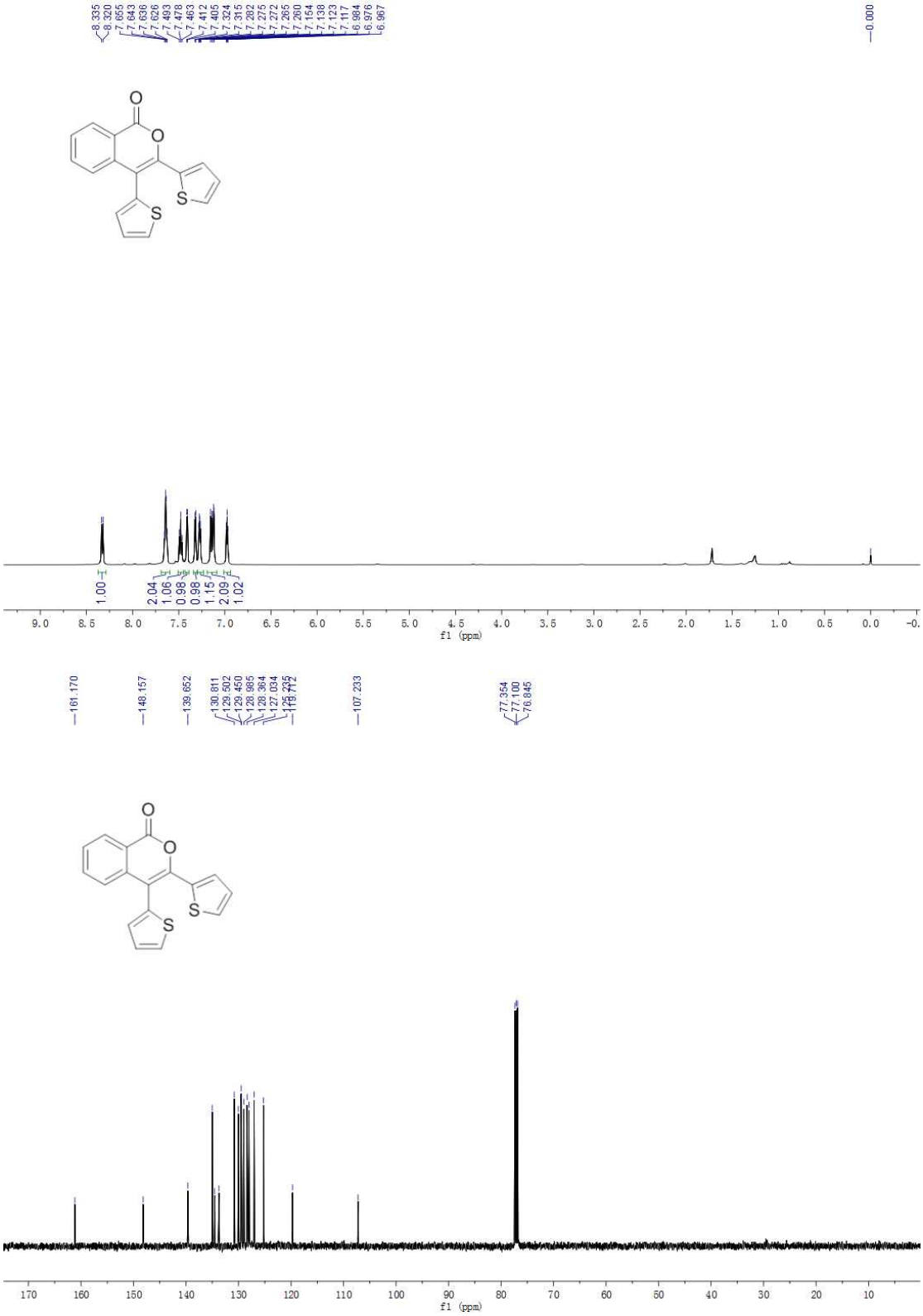
3,4-Bis(4-fluorophenyl)-1*H*-isochromen-1-one (3ah):



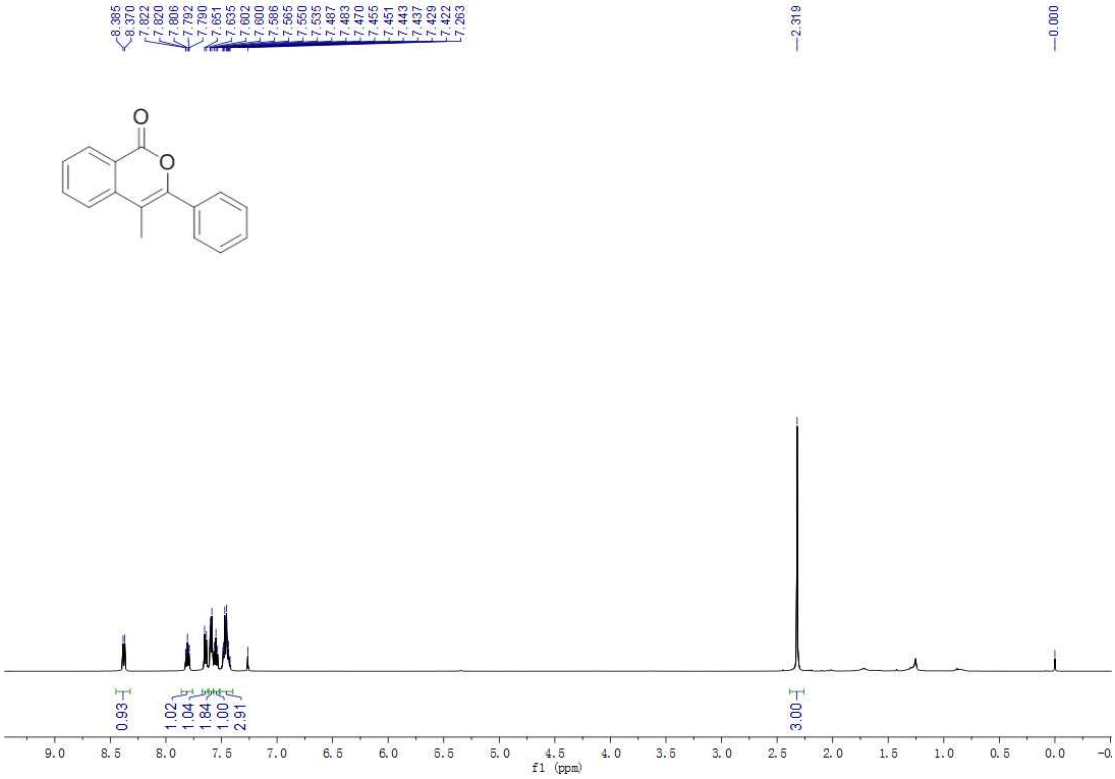

O
O
F
F

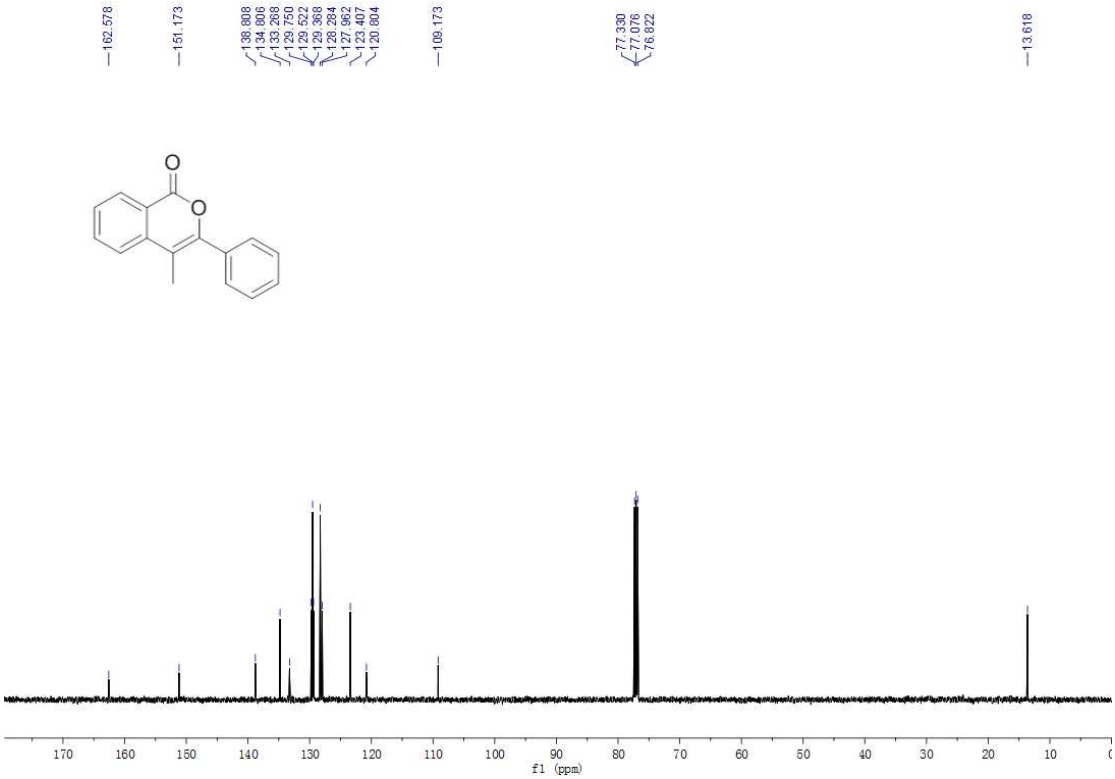
-110.745
-112.819
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
-115
-120
-125
-130
-135
-140
-145
-150
-155
-160
f1 (ppm)

3,4-Di(thiophen-2-yl)-1*H*-isochromen-1-one (3ai):

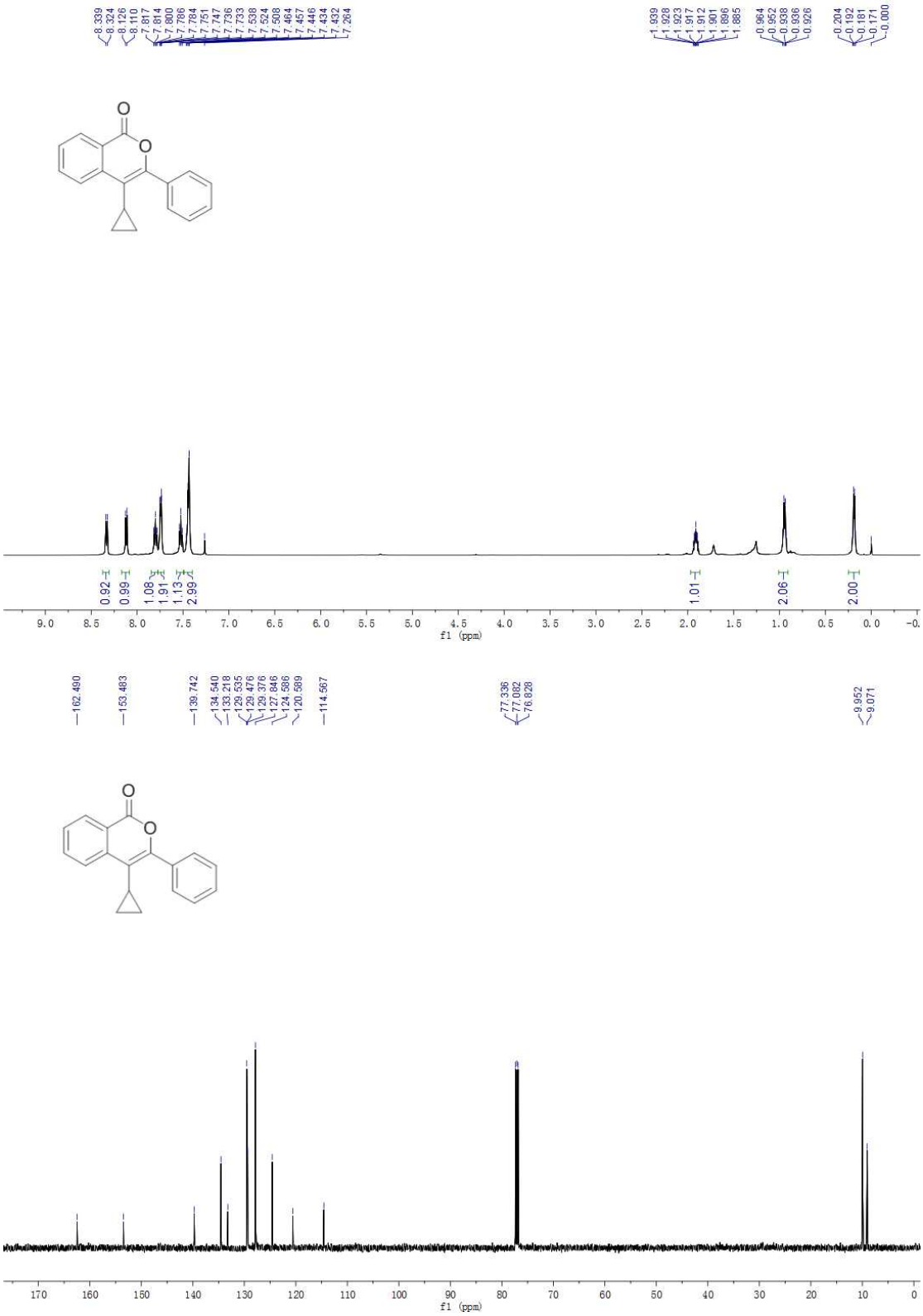


4-Methyl-3-phenyl-1*H*-isochromen-1-one (3aj):

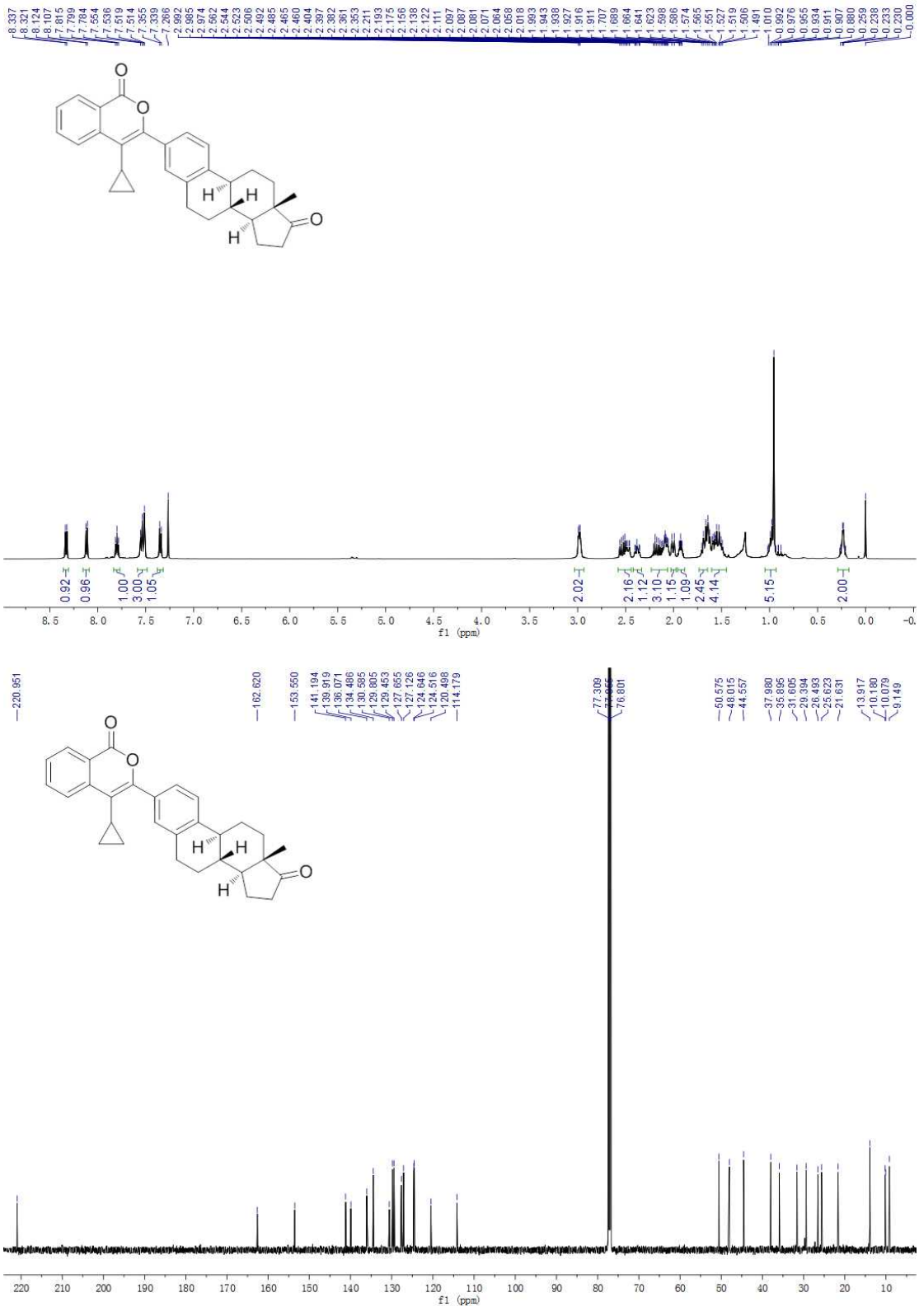




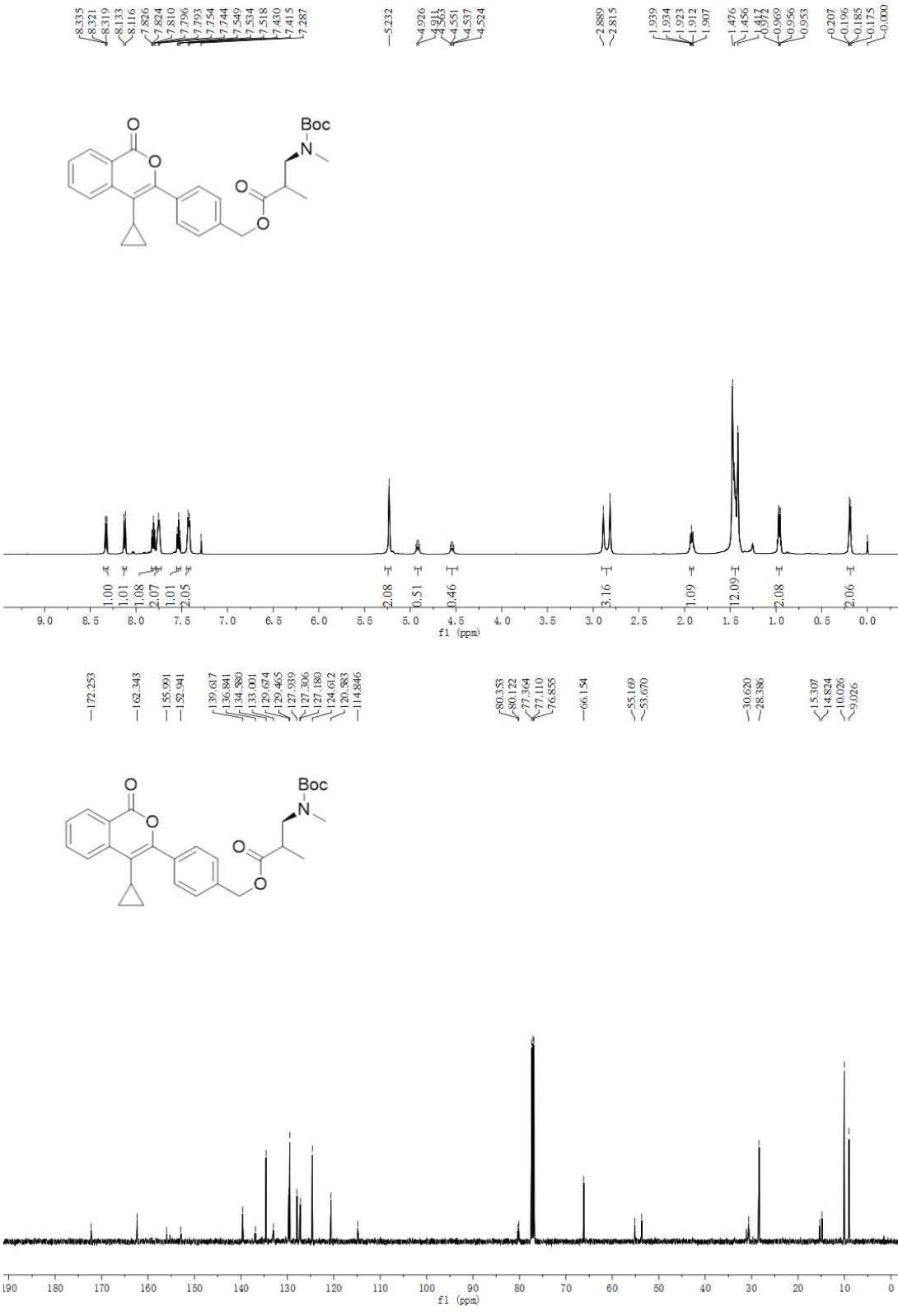
4-Cyclopropyl-3-phenyl-1*H*-isochromen-1-one (3ak):



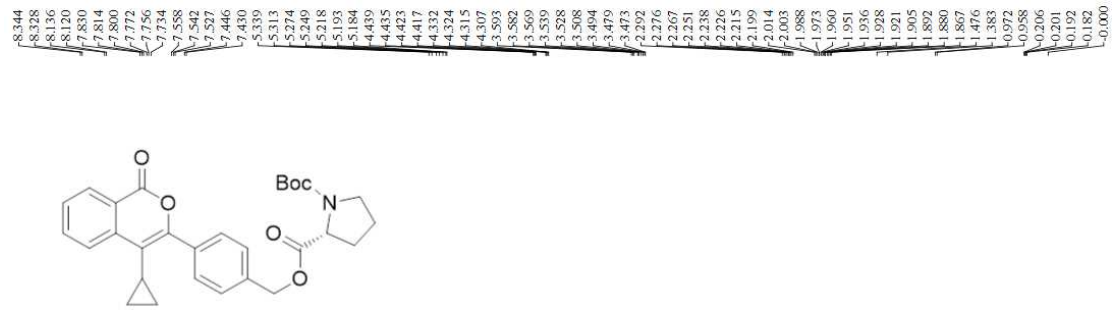
4-Cyclopropyl-3-((8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[a]phenanthren-3-yl)-1*H*-isochromen-1-one (3al):

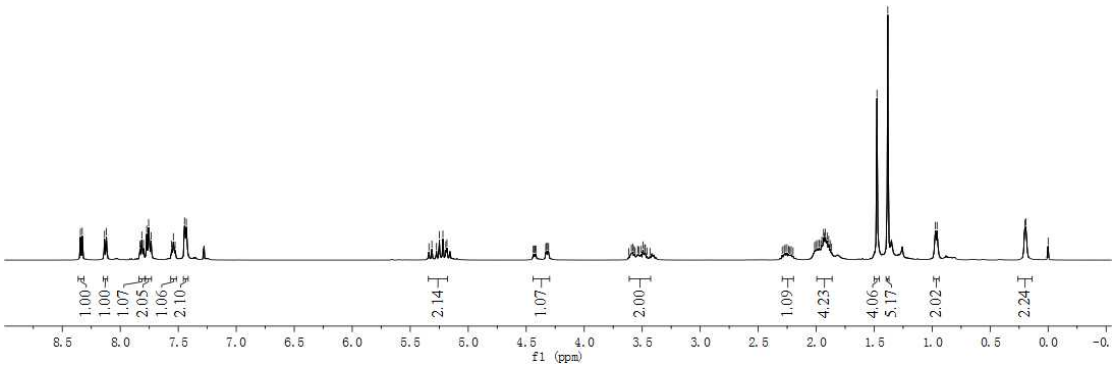


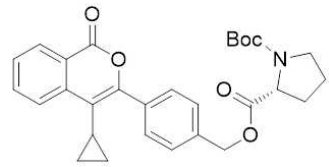
4-(4-Cyclopropyl-1-oxo-1*H*-isochromen-3-yl)benzyl-3-((tert-butoxycarbonyl)(methyl)amino)-2-methylpropanoate (3am):

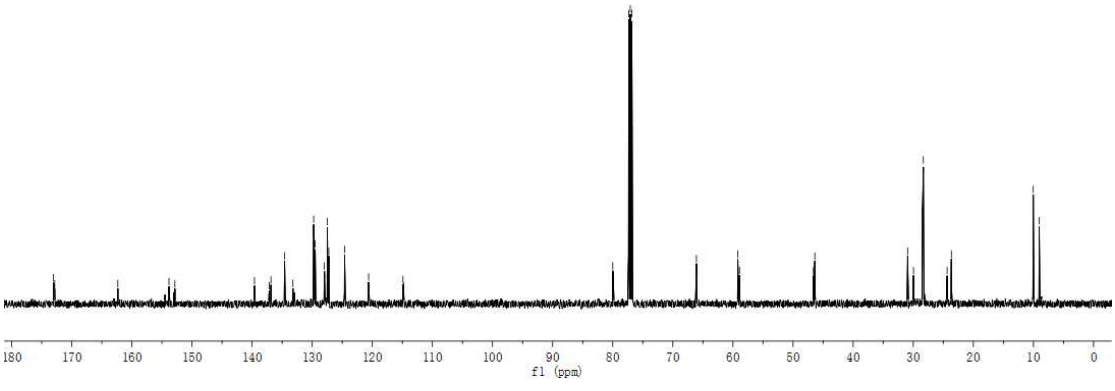


(R)-1-*tert*-Butyl 2-(4-(4-cyclopropyl-1-oxo-1*H*-isochromen-3-yl)benzyl) pyrrolidine-1,2-dicarboxylate (3an):

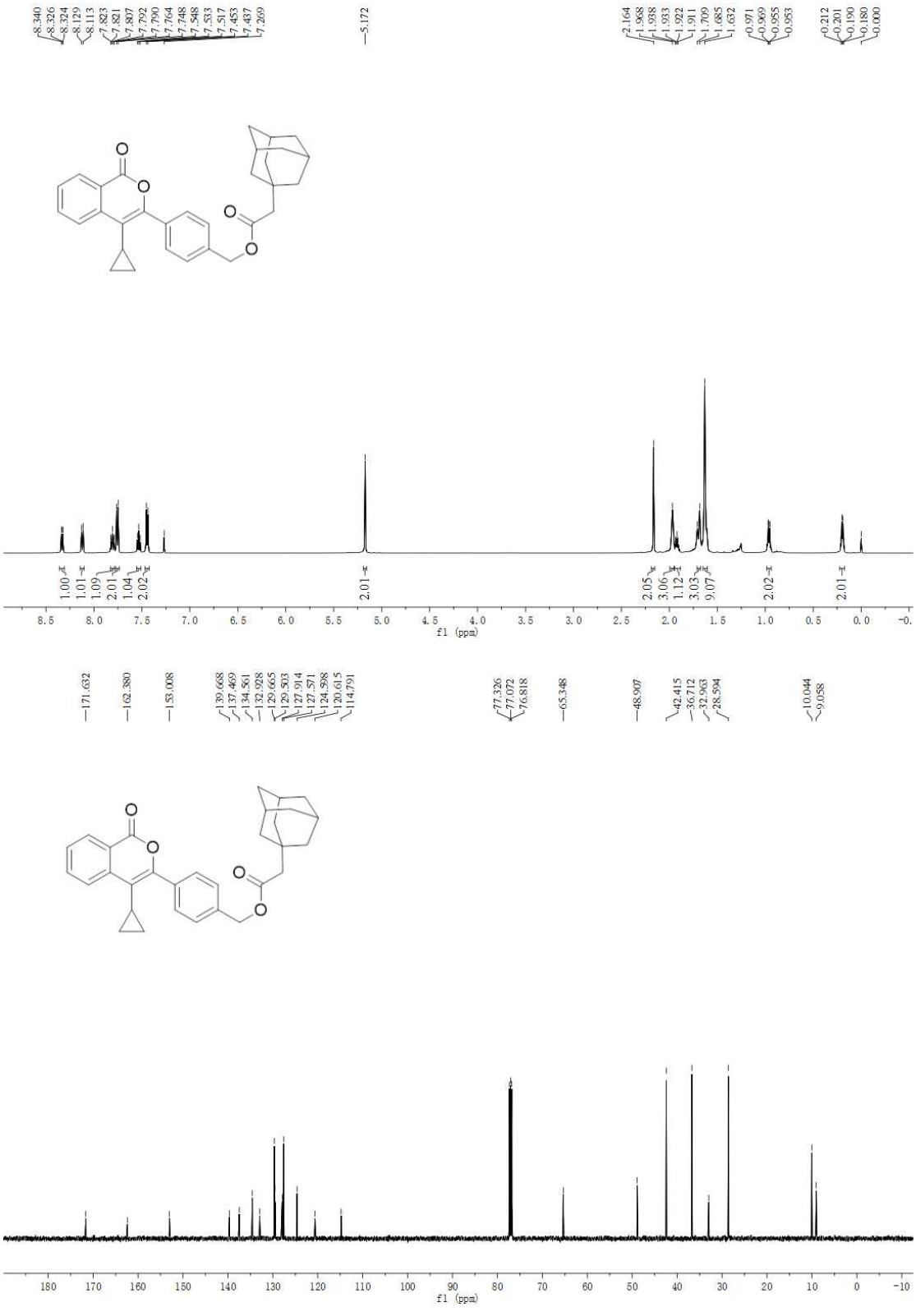




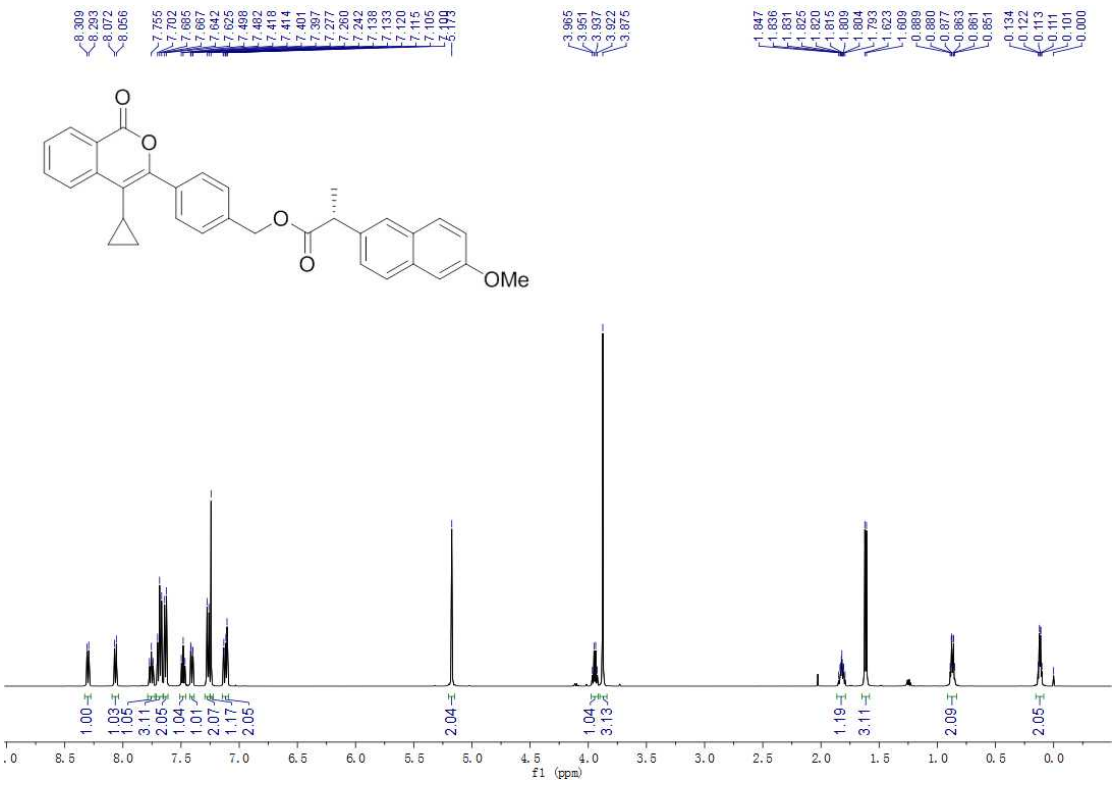


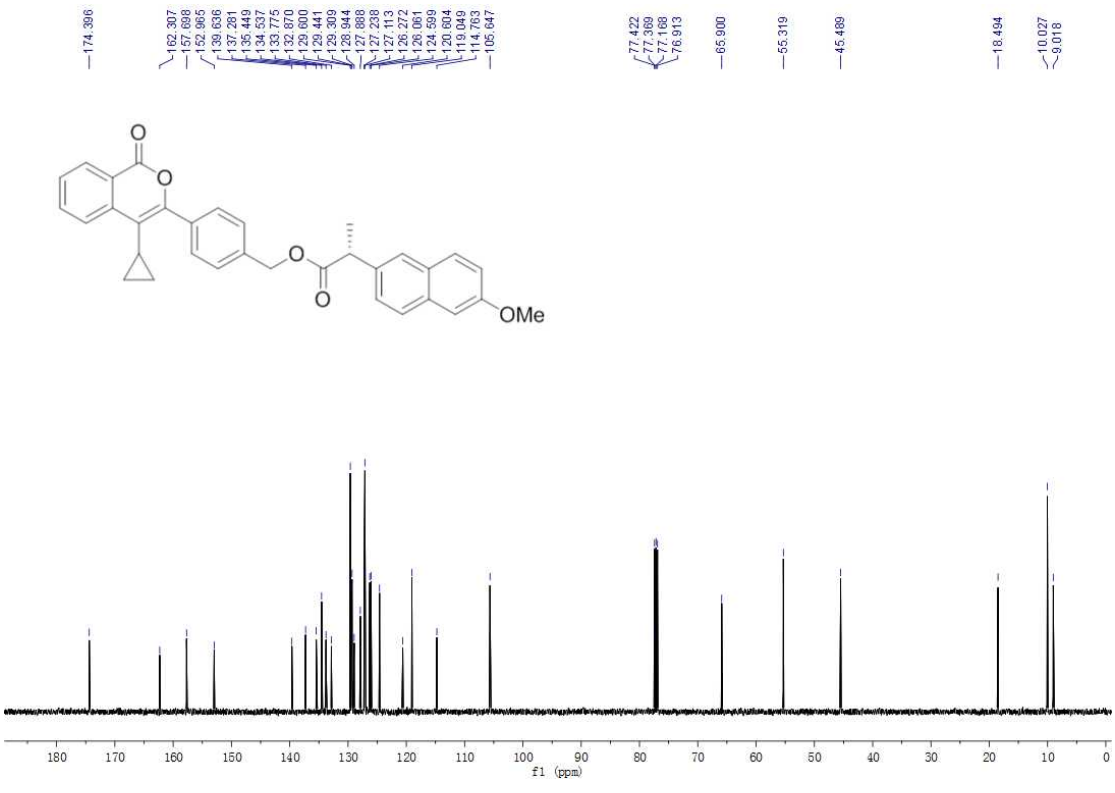


4-(4-Cyclopropyl-1-oxo-1H-isochromen-3-yl)benzyl-2-((3r,5r,7r)-adamantan-1-yl)acetate (3ao):

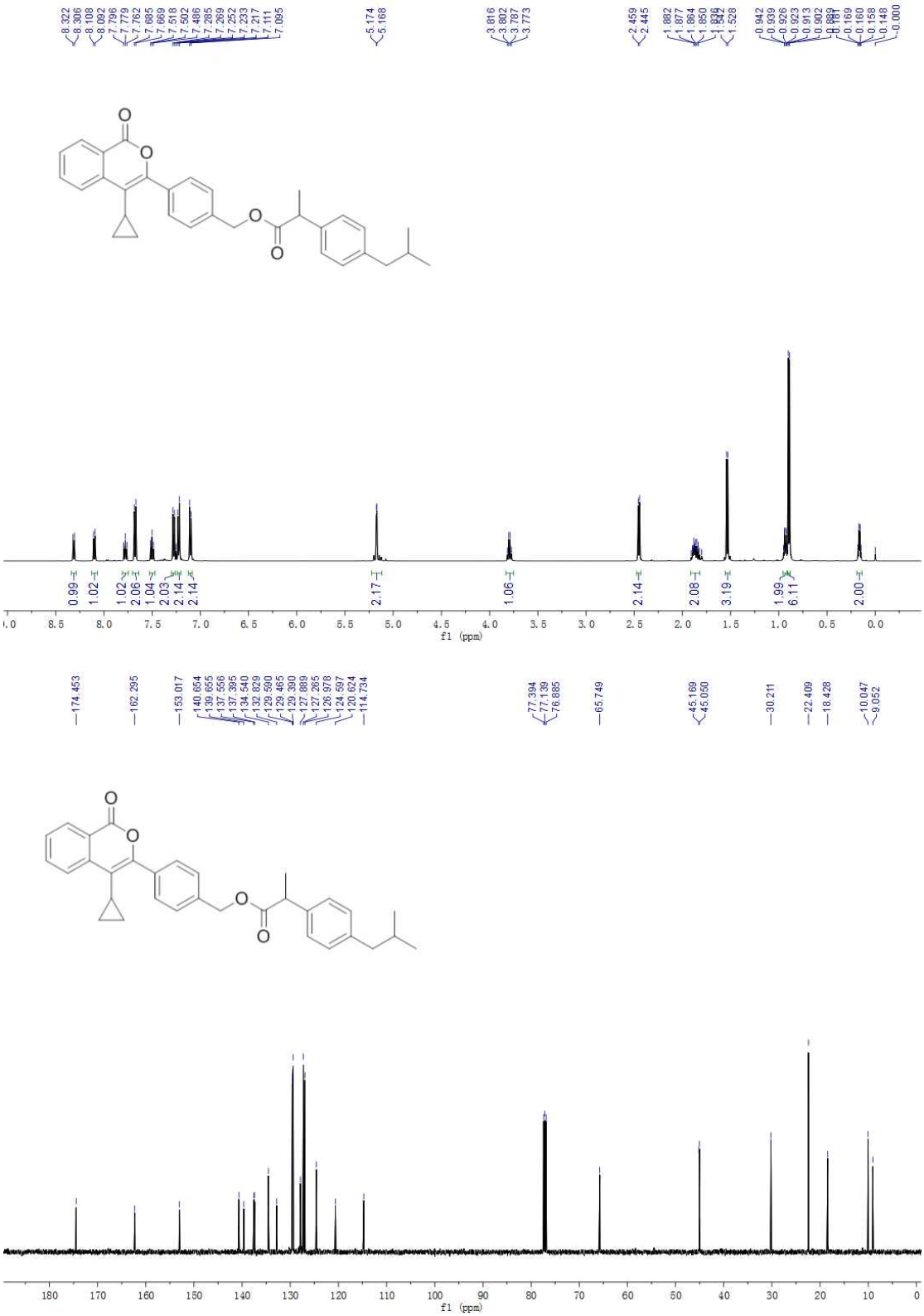


(R)-4-(4-cyclopropyl-1-oxo-1*H*-isochromen-3-yl)benzyl-2-(6-methoxynaphthalen-2-yl)propanoate (3ap):



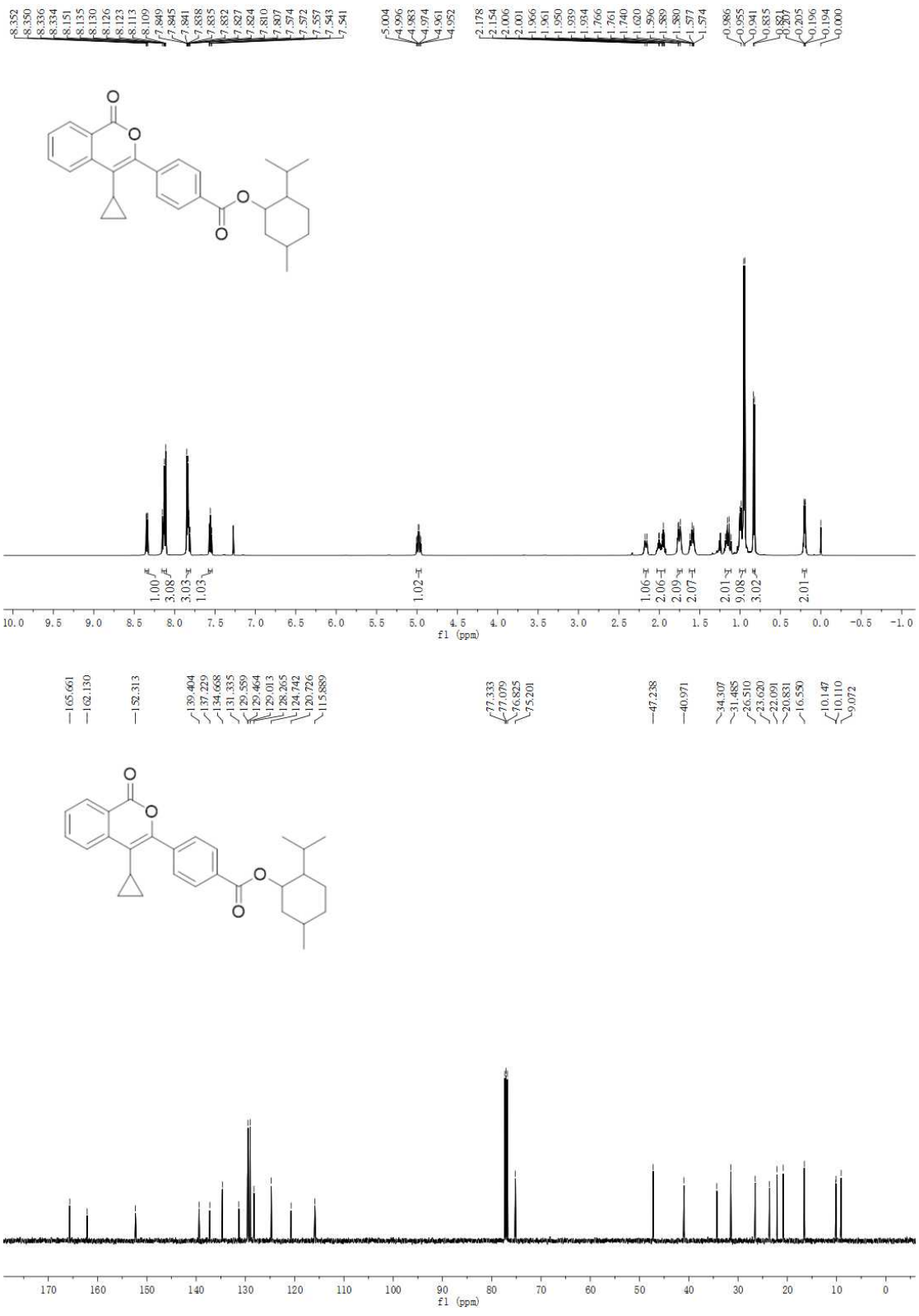


4-(4-Cyclopropyl-1-oxo-1*H*-isochromen-3-yl)benzyl-2-(4-isobutylphenyl)propano ate (3aq):

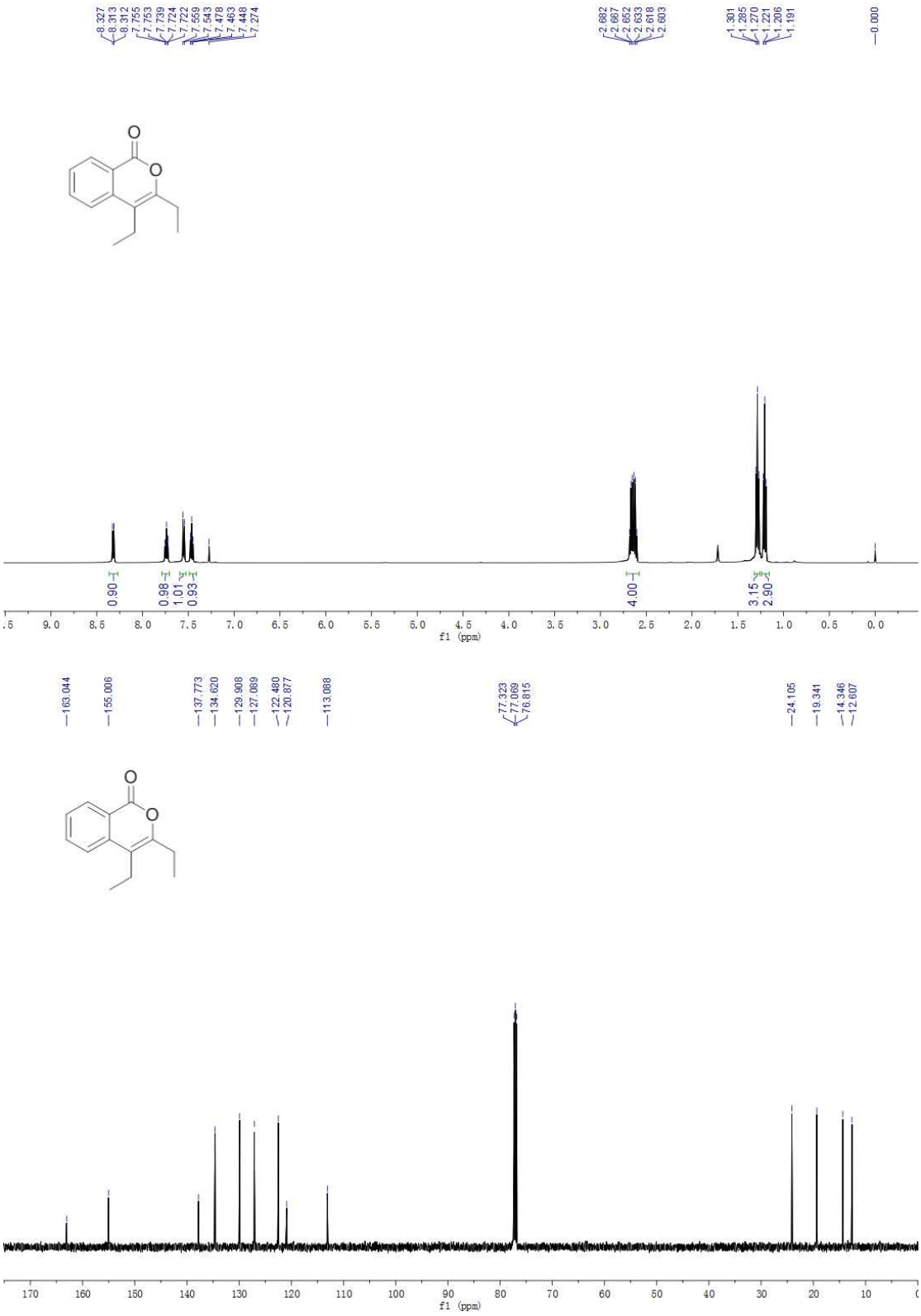


2-Isopropyl-5-methylcyclohexyl-4-(4-cyclopropyl-1-oxo-1*H*-isochromen-3-yl)ben

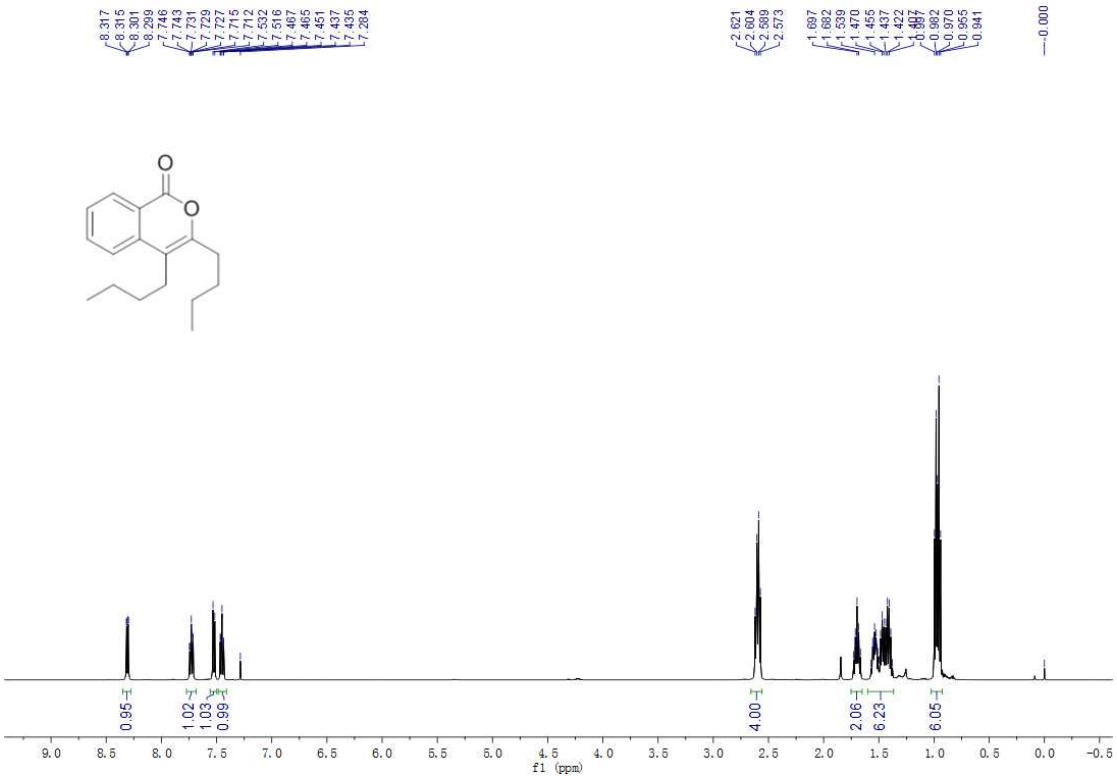
zoate (3ar):

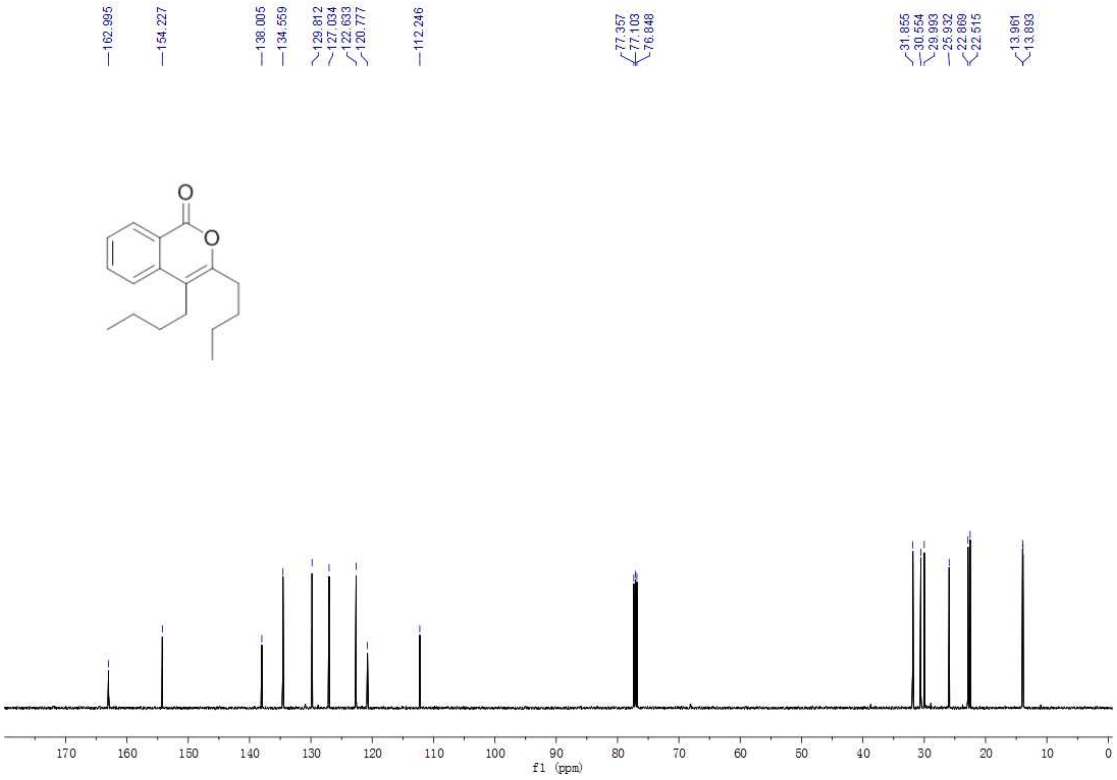


3,4-Diethyl-1*H*-isochromen-1-one (3as):

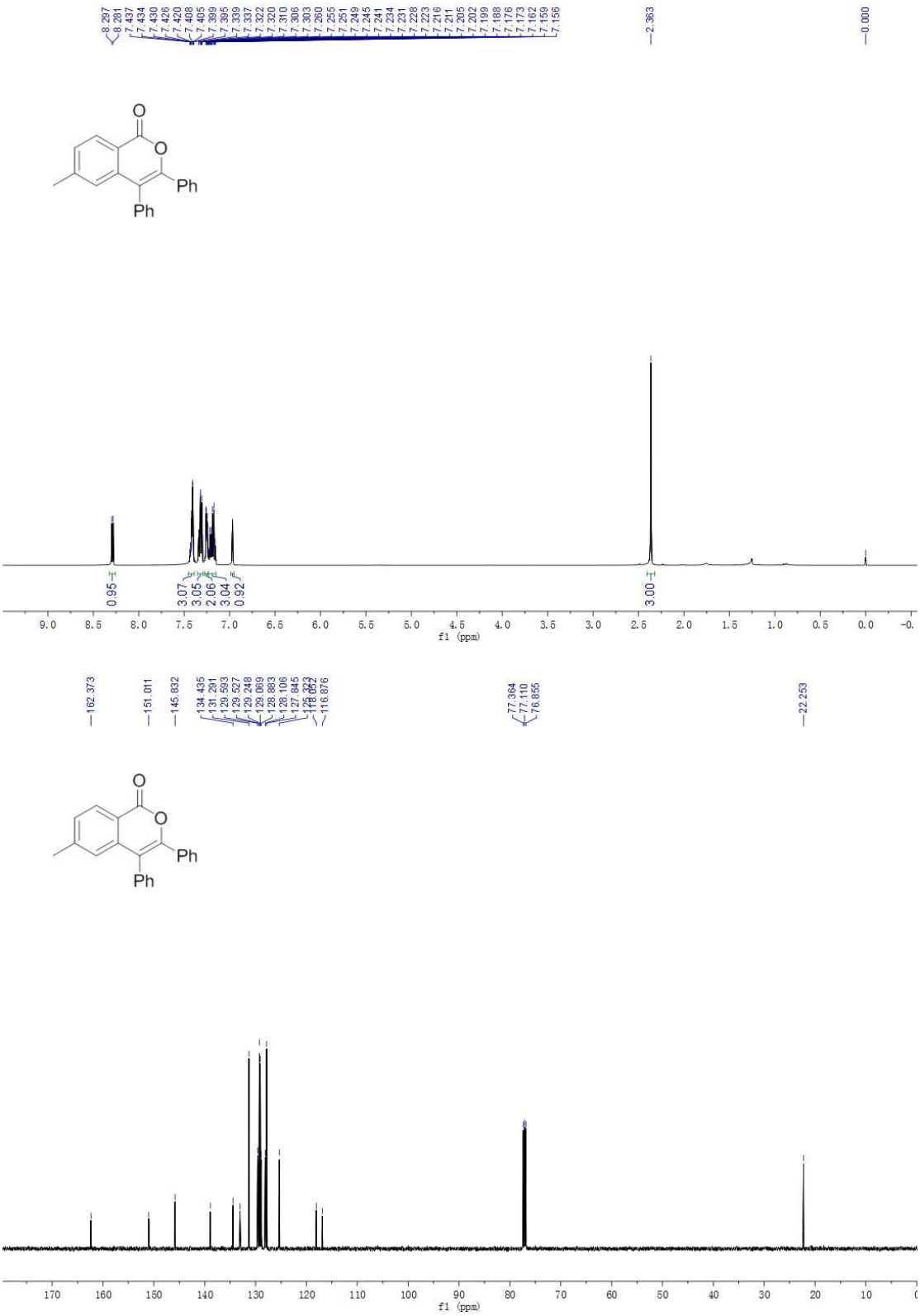


3,4-Dibutyl-1*H*-isochromen-1-one (3at):

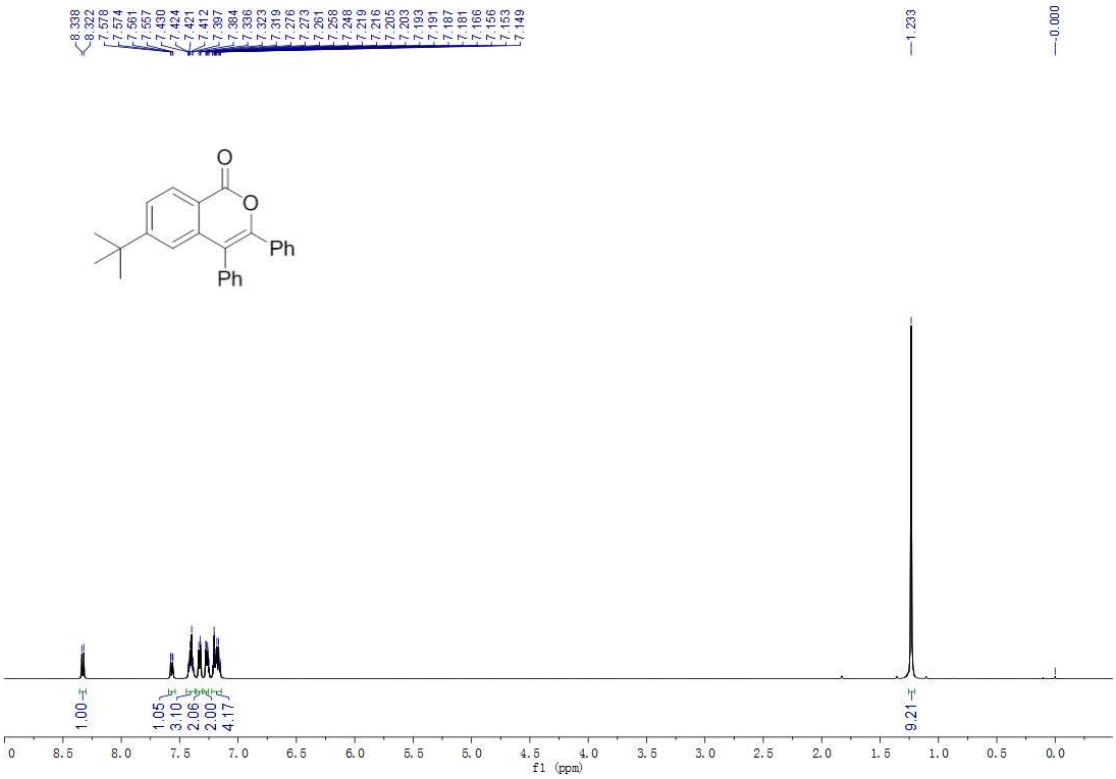


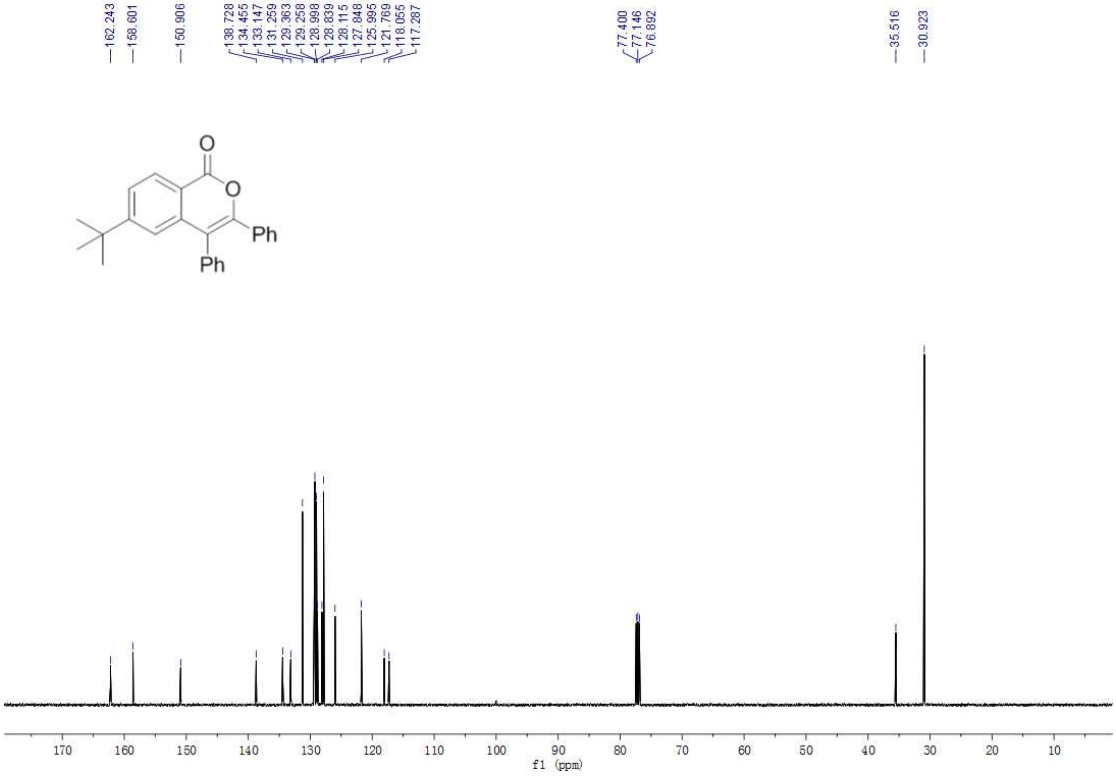


6-Methyl-3,4-diphenyl-1*H*-isochromen-1-one (3ba):

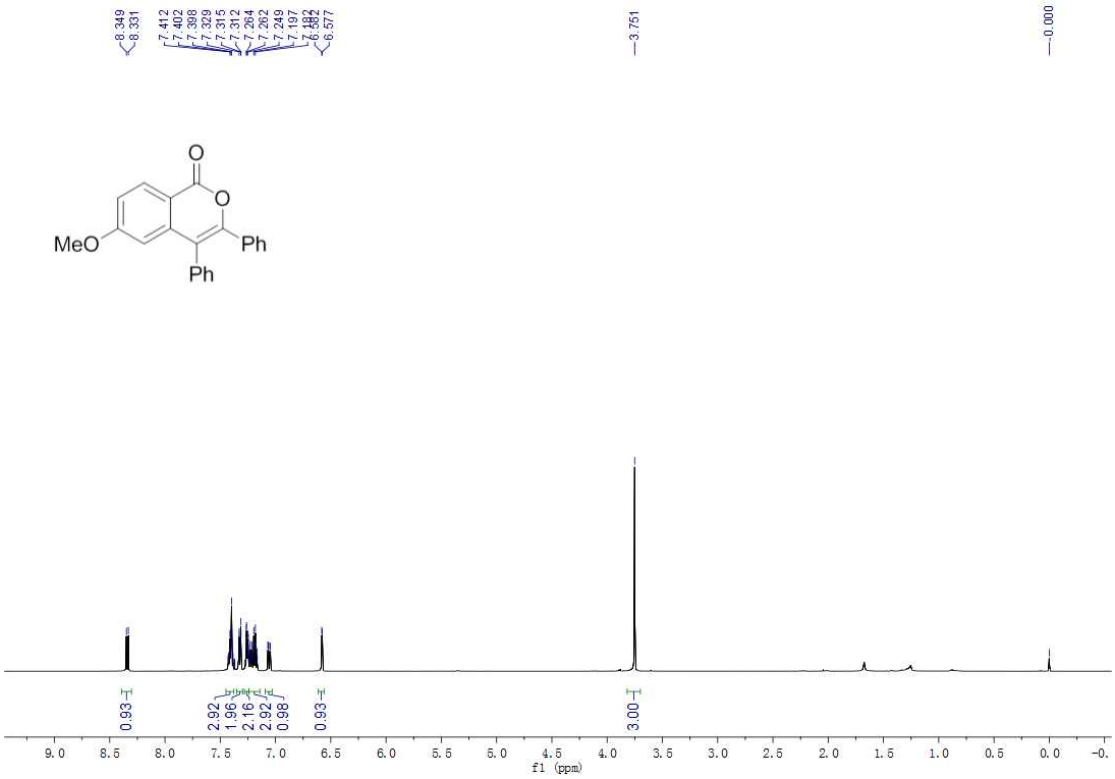


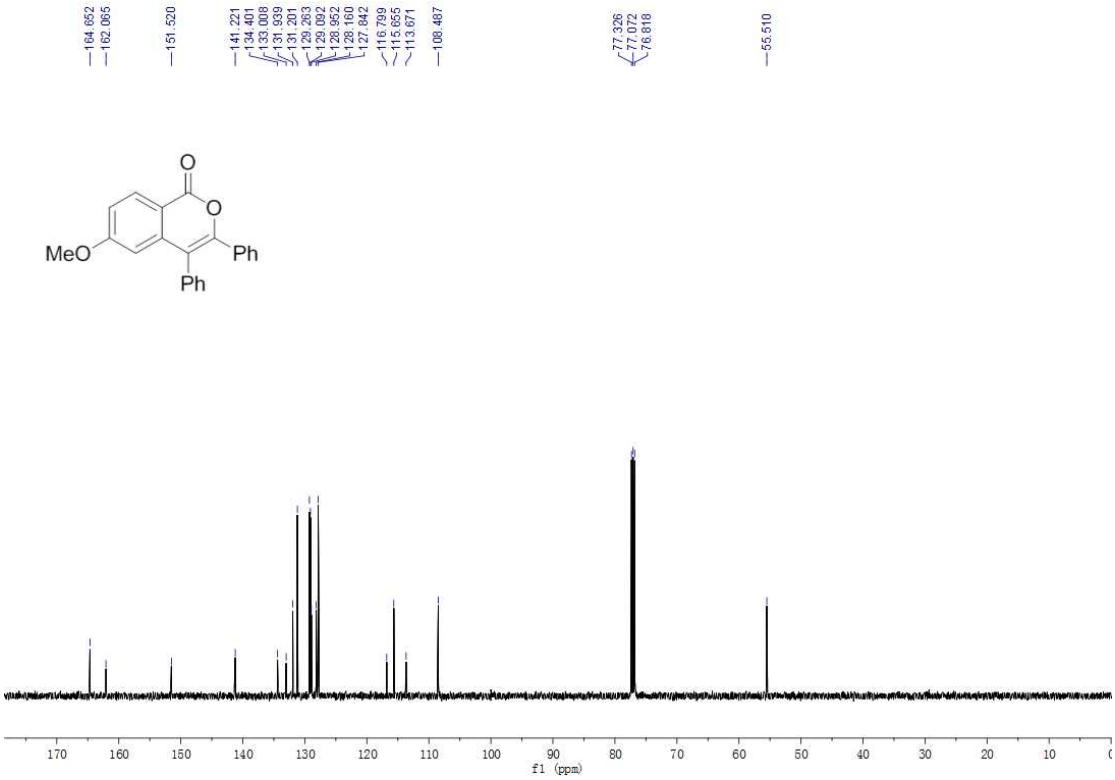
6-(*tert*-Butyl)-3,4-diphenyl-1*H*-isochromen-1-one (3ca):



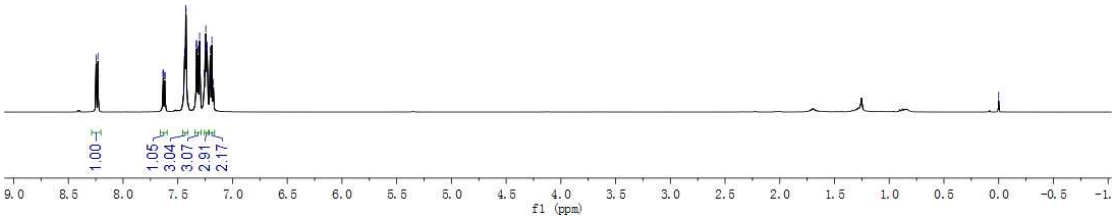


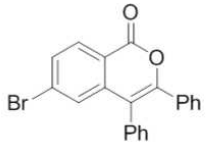
6-Methoxy-3,4-diphenyl-1*H*-isochromen-1-one (3da):

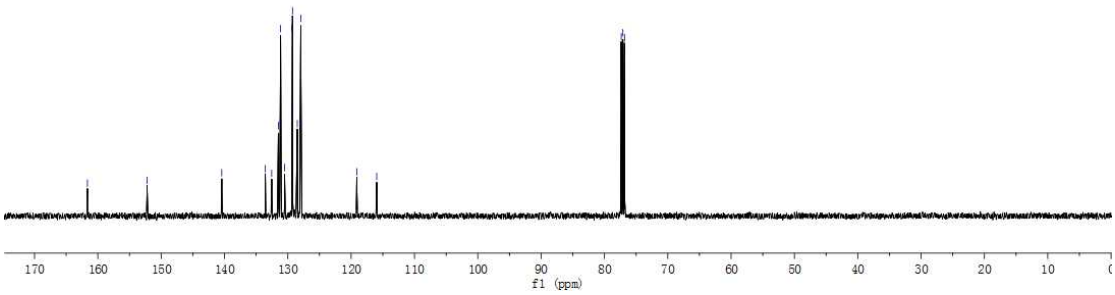




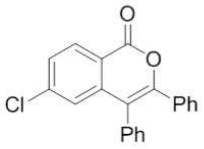
6-Bromo-3,4-diphenyl-1*H*-isochromen-1-one (3ea):

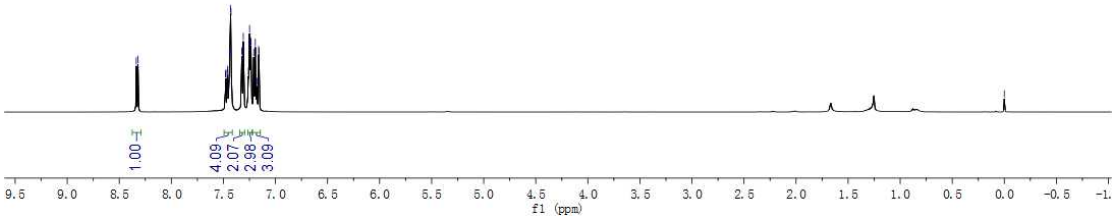


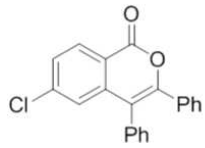


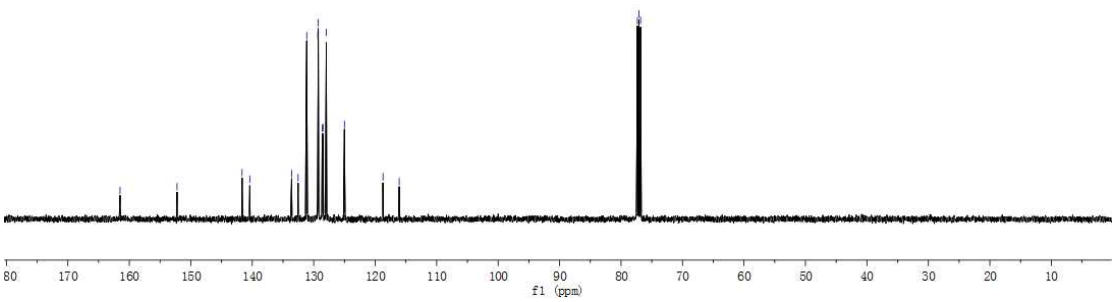


6-Chloro-3,4-diphenyl-1*H*-isochromen-1-one (3fa):

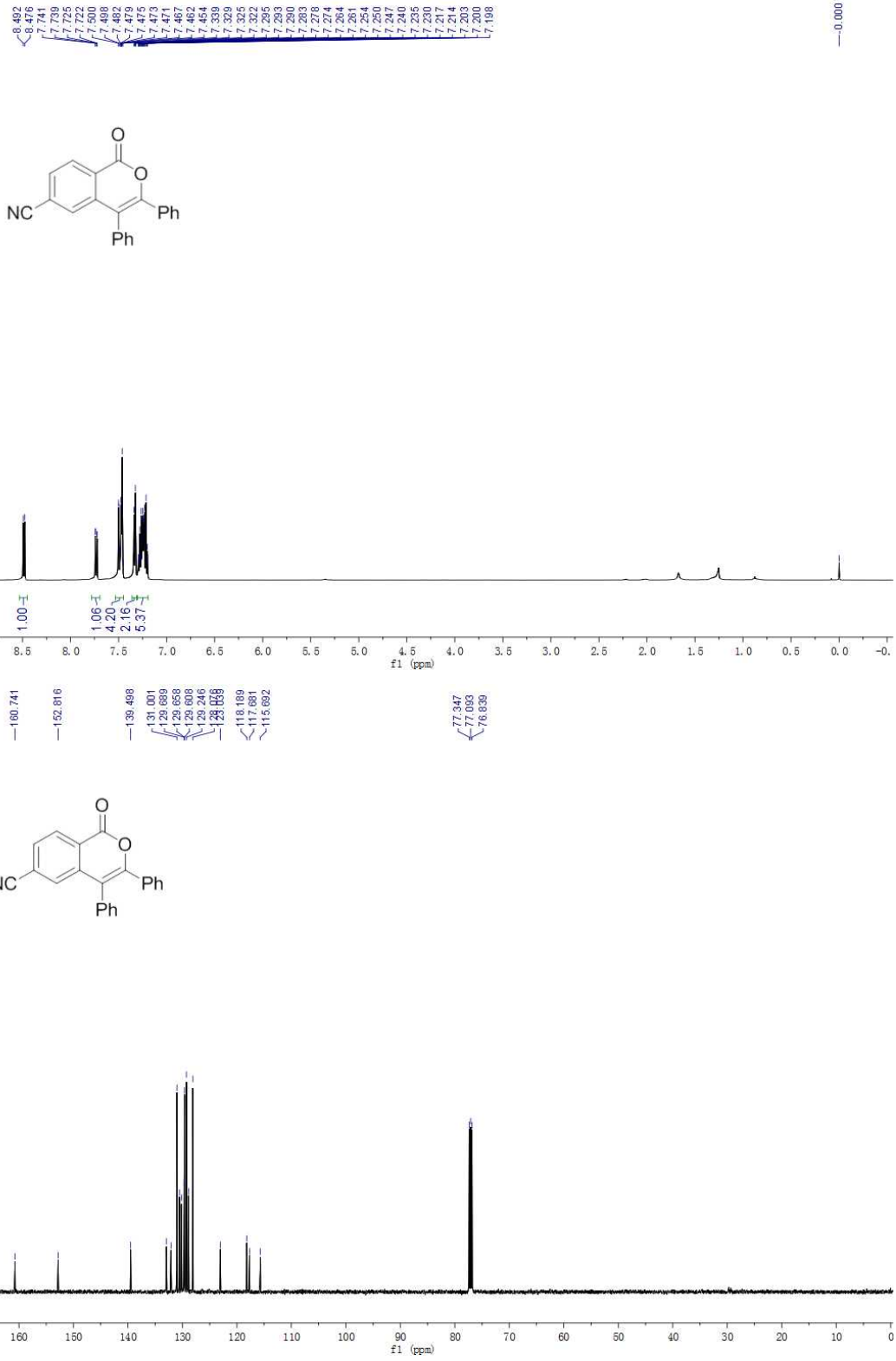




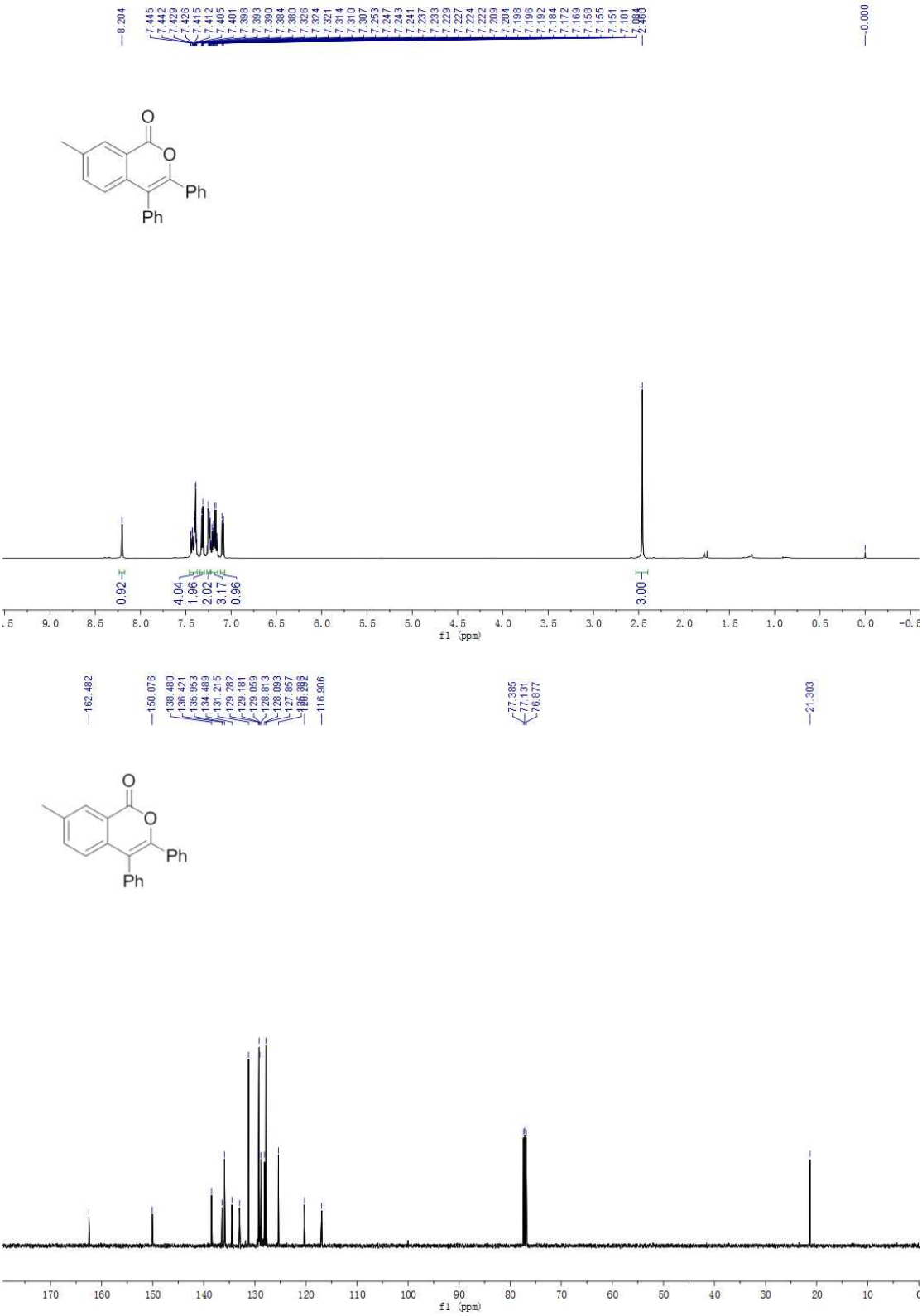




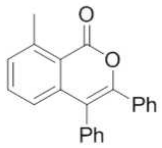
1-Oxo-3,4-diphenyl-1*H*-isochromene-6-carbonitrile (3ga):

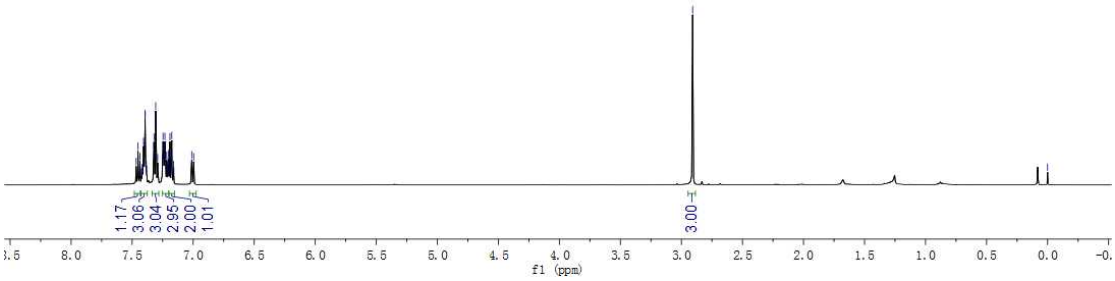


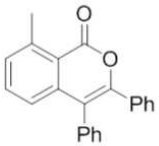
7-Methyl-3,4-diphenyl-1*H*-isochromen-1-one (3ha):

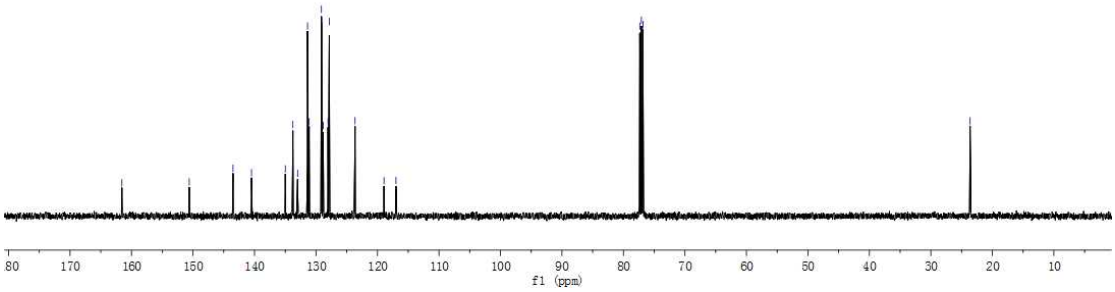


8-Methyl-3,4-diphenyl-1*H*-isochromen-1-one (3ia):

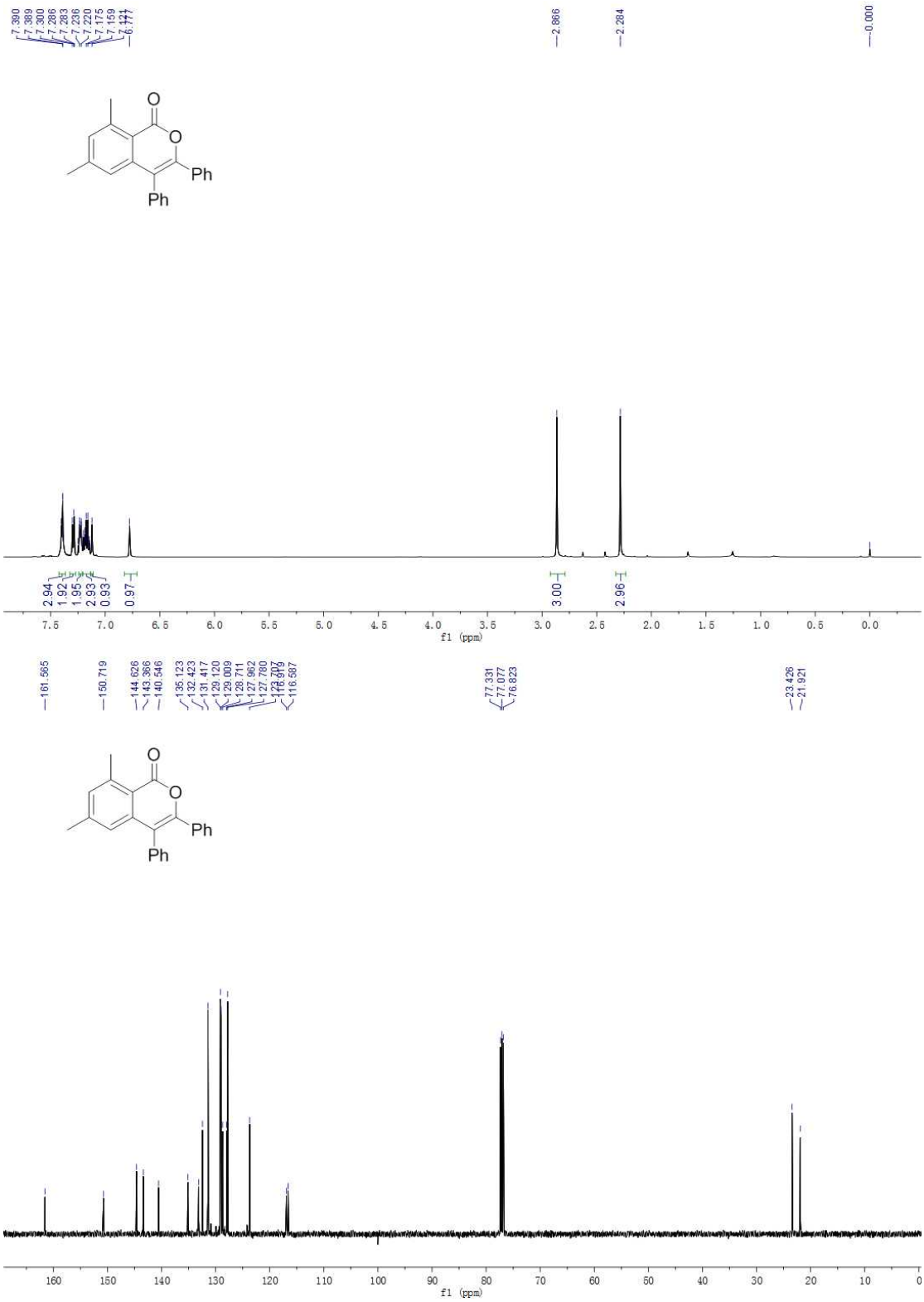




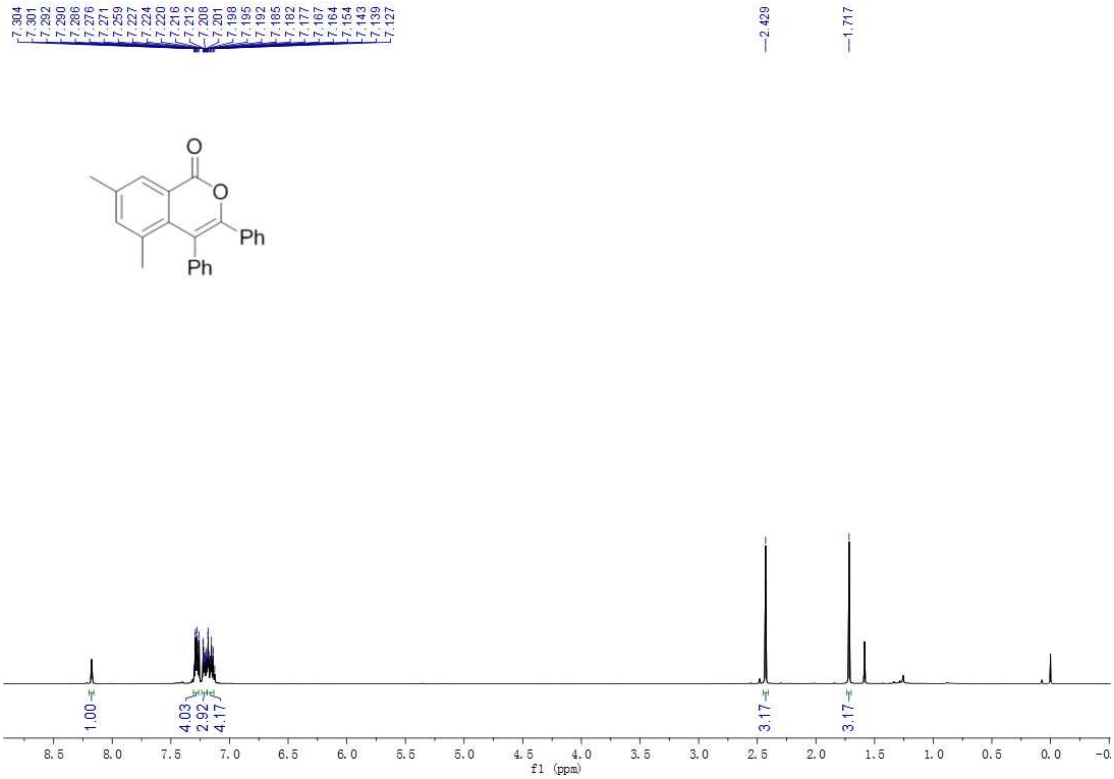


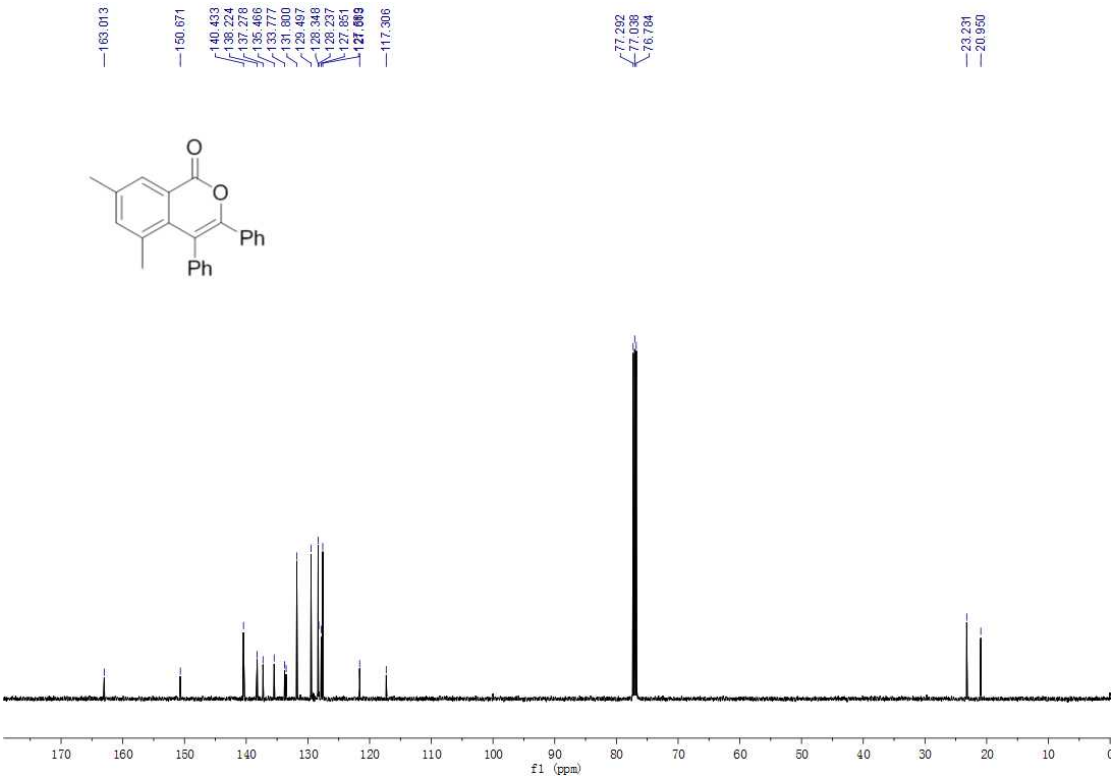


6,8-Dimethyl-3,4-diphenyl-1*H*-isochromen-1-one (3ja):

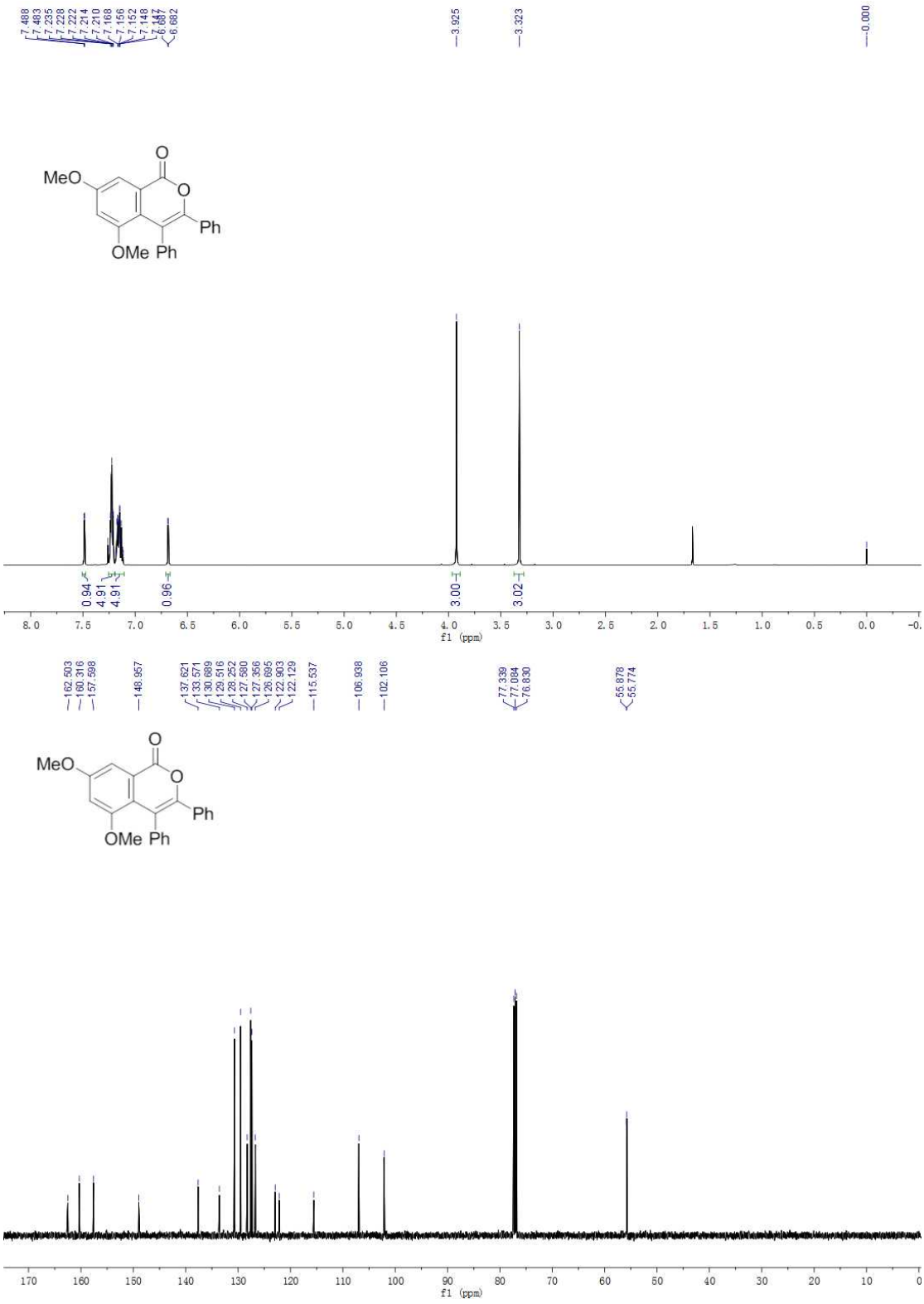


5,7-Dimethyl-3,4-diphenyl-1*H*-isochromen-1-one (3ka):





5,7-Dimethoxy-3,4-diphenyl-1*H*-isochromen-1-one (3la):



4,5-Diphenyl-7*H*-thieno[2,3-c]pyran-7-one (3ma):