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Supporting Information

for

Ortho-ester-substituted diaryliodonium salts enabled regioselective arylocyclization of naphthols toward 3,4-benzocoumarins

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Experimental procedures, LC–MS spectra and characterization data of all products, copies of ^{1}H, ^{13}C, ^{19}F NMR spectra of all compounds

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Part 1. General information

a. Methods:

NMR spectrum: ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 (with tetramethylsilane as an internal standard) on a Bruker AVANCE 400 spectrometer at ambient temperature, operating at 400 MHz, 101 MHz, and 376 MHz, respectively. Data were reported as follows: Chemical shifts (δ) are reported in ppm, and coupling constants (J) are in Hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad.

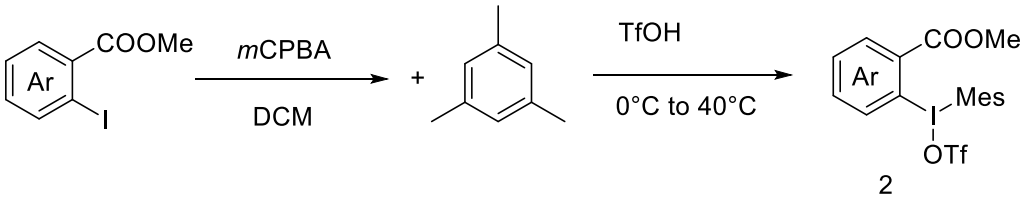
Mass spectroscopy: Mass spectra were in general recorded on a Waters LCT Premier XE spectrometer or EI Mass spectra were measured on HP HP5989A, Aglient HP5873 or Waters Micromass GCT mass spectrometer. ESI-MS analyses were performed in positive ionization mode on an Agilent 1100-MSD or Bruker Daltonics FTMS-7 mass spectrometer.

Chromatography: Column chromatography was performed with silica gel (200-300 mesh ASTM).

b. Materials:

All solvents were purchased from Adamas-beta and dried and/or distilled by standard methods. All reagents were purchased from commercial sources (Adamas-beta; Sinopharma reagents; TCI; Acros) and used without further purification. Reactions were monitored by TLC (detection with UV light). The preparation of all other materials is described in detail below.

Part 2. Synthesis and characterization of *ortho*-ester-substituted diaryliodonium salts



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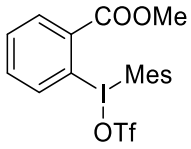
General procedure 1: To a solution of methyl 2-iodobenzoate (10 mmol) in CH_2Cl_2 (40 mL) was slowly added *m*CPBA (2.5 g, 11mmol) at room temperature. After stirring for 5 minutes, mesitylene (2.0ml,12mmol) was added. Then trifluoromethanesulfonic acid (1.2 mL,15 mmol) was added dropwise over 2 minutes at 0 °C and the solution was stirred at 4 0°C for 2–3 hours until TLC indicated that the methyl 2-iodobenzoate was completely consumed. The solvent was removed in vacuo and Et_2O (50 mL) was added in the mixture. The mixture was stirred vigorously until the solid precipitated. The solids were washed with Et_2O (2 × 10 mL) and filtrated under reduced pressure to give the *ortho*-ester-substituted diaryliodonium Salts (**2a–j**) in a pure form [1].

Methyl 2-(mesityl(((trifluoromethyl)sulfonyl)oxy)-λ^3-iodaneyl)benzoate (2a)

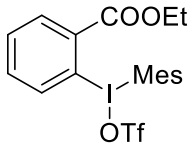


Prepared according to the ***General procedure 1*** on 10 mmol scale. The desired product of *ortho*-ester-substituted diaryliodonium salts (**2a**) was obtained as white solid (4.24 g, 81%).

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 8.34 (d, *J* = 7.3 Hz, 1H), 7.83 – 7.73 (m, 2H), 7.42 (s, 2H), 6.90 (d, *J* = 7.7 Hz, 1H), 4.07 (s, 3H), 2.53 (s, 6H), 2.43 (s, 3H).

Analytical data are consistent with the reported ones [2].

Ethyl 2-(mesityl(((trifluoromethyl)sulfonyl)oxy)- λ^3-iodaneyl)benzoate (2b)



Prepared according to the ***General procedure 1*** on 1 mmol scale. The desired product of *ortho*-ester-substituted diaryliodonium salts (**2b**) was obtained as white solid (462 mg, 85%).

M.P.: 186-189 ℃.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 8.33 (dd, *J* = 7.5, 1.8 Hz, 1H), 7.80 (d, *J* = 1.0 Hz, 2H), 7.41 (s, 2H), 6.87 (dd, *J* = 8.0, 0.9 Hz, 1H), 4.52 (d, *J* = 7.1 Hz, 2H), 3.36(water, the same as below), 2.51 (s, 6H), 2.42 (s, 3H), 1.42 (t, *J* = 7.1 Hz, 3H).

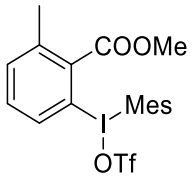
^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 167.44 (s), 144.59 (s), 143.30 (s), 137.37 (s), 132.97 (s), 131.43 (s), 130.17 (s), 128.57 (s), 127.65 (s), 120.72(q, J_{C-F} = 323.2Hz), 117.87 (s), 113.65 (s), 63.82 (s), 26.13 (s), 20.83 (s), 13.95 (s).

^{19}F NMR (376 MHz, DMSO-*d*$_6$) δ -77.77.

The peak at 3.36 ppm is the water peak from DMSO-d6, which cannot be removed, and is similar to the following

HRMS m/z (ESI-TOF): calculated for $C_{18}H_{20}O_2I^+$ $[M\text{-}OTf]^+$ 395.0508, found 395.0486.

Methyl 2-(mesityl(((trifluoromethyl)sulfonyl)oxy)- λ^3-iodaneyl)-6-methylbenzoate (2c)



Prepared according to the ***General procedure 1*** on 1 mmol scale. The desired product of *ortho*-ester-substituted diaryliodonium salts (**2c**) was obtained as white solid (450 mg, 80%).

M.P.: 175-178 ℃.

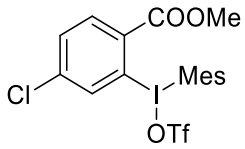
^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 7.65 (d, *J* = 7.5 Hz, 1H), 7.56 (t, *J* = 7.9 Hz, 1H), 7.37 (s, 2H), 6.92 (d, *J* = 8.0 Hz, 1H), 4.04 (s, 3H), 2.64 (s, 3H), 2.51 (s, 6H), 2.40 (s, 3H).

^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 169.41, 144.37, 144.35, 143.05, 135.65, 135.03, 130.07, 127.70, 127.63, 120.69(q, $J_{C\text{-}F}$ = 323.2Hz), 119.38, 115.59, 54.32, 39.52, 26.04, 22.90, 20.75.

^{19}F NMR (376 MHz, DMSO-*d*$_6$) δ -77.77.

HRMS m/z (ESI-TOF): calculated for $C_{18}H_{20}O_2I^+$ $[M\text{-}OTf]^+$ 395.0508, found 395.0489.

Methyl 4-chloro-2-(mesityl(((trifluoromethyl)sulfonyl)oxy)- λ^3-iodaneyl)benzoate (2d)



Prepared according to the ***General procedure 1*** on 1 mmol scale. The desired product of *ortho*-ester-substituted diaryliodonium salts (**2d**) was obtained as white solid (423 mg, 75%).

M.P.: 157-160 ℃.

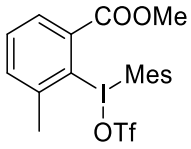
^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 8.29 (d, *J* = 8.4 Hz, 1H), 7.90 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.43 (s, 2H), 6.64 (d, *J* = 1.5 Hz, 1H), 4.06 (s, 3H), 2.54 (s, 6H), 2.44 (s, 3H).

^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 167.34, 144.96, 143.32, 141.45, 133.88, 131.58, 130.28, 127.91, 126.88, 120.69(q, $J_{C\text{-}F}$ = 323.2Hz), 118.34, 115.40, 54.63, 39.52, 26.09, 20.82.

^{19}F NMR (376 MHz, DMSO-*d*$_6$) δ -77.76.

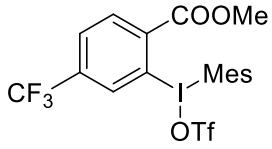
HRMS m/z (ESI-TOF): calculated for $C_{17}H_{17}ClO_2I^+$ $[M\text{-}OTf]^+$ 414.9962, found 414.9986.

Methyl 2-(mesityl(((trifluoromethyl)sulfonyl)oxy)- λ^3-iodaneyl)-3-methylbenzoate (2e)



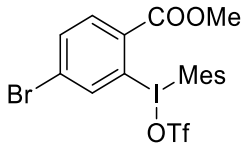
Prepared according to the ***General procedure 1*** on 1 mmol scale. The desired product of *ortho*-ester-substituted diaryliodonium salts (**2e**) was obtained as white solid (425 mg, 78%).
M.P.: 159-162 ℃.
^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 7.82 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.77 (d, *J* = 6.3 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.18 (s, 2H), 3.77 (s, 3H), 2.53 (s, 3H), 2.39 (s, 6H), 2.29 (s, 3H).
^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 166.19, 143.54, 143.00, 142.11, 135.95, 133.21, 132.44, 130.20, 129.85, 120.69(q, J_{C-F} = 324.2Hz), 120.62, 119.09, 117.44, 53.38, 39.52, 25.37, 25.23, 20.38.
^{19}F NMR (376 MHz, DMSO-*d*$_6$) δ -77.77.
HRMS m/z (ESI-TOF): calculated for $C_{18}H_{20}O_2I^+$ [M-OTf]$^+$ 395.0508, found 395.0488.

Methyl 2-(mesityl(((trifluoromethyl)sulfonyl)oxy)-λ^3-iodaneyl)-4-(trifluoromethyl)benzoate (2f)



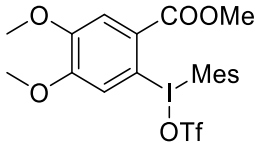
Prepared according to the ***General procedure 1*** on 1 mmol scale. The desired product of *ortho*-ester-substituted diaryliodonium salts (**2f**) was obtained as white solid (425 mg, 71%).
M.P.: 175-178 ℃.
^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 8.48 (d, *J* = 8.0 Hz, 1H), 8.20 (d, *J* = 8.1 Hz, 1H), 7.45 (s, 2H), 6.89 (s, 1H), 4.10 (s, 3H), 2.53 (s, 6H), 2.44 (s, 3H).
^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 167.03, 145.05, 143.30, 135.41, 135.08, 133.59, 131.87, 130.20, 126.71(dd, J_{C-F} = 394.9, 4.0Hz), 122.29(q, J_{C-F} = 274.7Hz), 120.68(q, J_{C-F} = 323.2Hz), 118.44, 115.14, 54.86, 39.52, 26.00, 20.76.
^{19}F NMR (376 MHz, DMSO-*d*$_6$) δ -62.28, -77.80.
HRMS m/z (ESI-TOF): calculated for $C_{18}H_{17}F_3O_2I^+$ [M-OTf]$^+$ 449.0225, found 449.0206.

Methyl 4-bromo-2-(mesityl(((trifluoromethyl)sulfonyl)oxy)- λ^3-iodaneyl)benzoate (2g)



Prepared according to the ***General procedure 1*** on 1 mmol scale. The desired product of *ortho*-ester-substituted diaryliodonium salts (**2g**) was obtained as white solid (487 mg, 80%).
M.P.: 187-190 ℃.
^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 8.20 (d, *J* = 8.3 Hz, 1H), 8.03 (d, *J* = 1.7 Hz, 1H), 7.44 (s, 2H), 6.77 (d, *J* = 1.7 Hz, 1H), 4.05 (s, 3H), 2.53 (s, 6H), 2.44 (s, 3H).
^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 167.49, 144.94, 143.30, 134.50, 134.00, 130.63, 130.49, 130.26, 127.16, 120.69(q, J_{C-F} = 324.2Hz), 118.32, 115.47, 54.62, 39.52, 26.08, 20.82.
^{19}F NMR (376 MHz, DMSO-*d*$_6$) δ -77.76.
HRMS m/z (ESI-TOF): calculated for $C_{17}H_{17}BrO_2I^+$ [M-OTf]$^+$ 458.9457, found 458.9435.

Methyl 2-(mesityl(((trifluoromethyl)sulfonyl)oxy)- λ^3-iodaneyl)-4,5-dimethoxybenzoate (2h)



Prepared according to the ***General procedure 1*** on 1 mmol scale. The desired product of *ortho*-ester-substituted diaryliodonium salts (**2h**) was obtained as white solid (442 mg, 75%).

M.P.: 190-193 ℃.

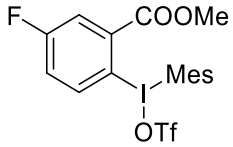
^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 7.73 (s, 1H), 7.41 (s, 2H), 6.11 (s, 1H), 4.04 (s, 3H), 3.88 (s, 3H), 2.52 (d, *J* = 7.5 Hz, 6H), 2.41 (s, 3H).

^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 167.77, 155.12, 150.35, 144.65, 143.22, 129.97, 120.69(q, J_{C-F} = 324.2Hz), 119.74, 118.50, 114.04, 110.35, 104.53, 56.30, 55.56, 54.30, 39.52, 26.12, 20.75.

^{19}F NMR (376 MHz, DMSO-*d*$_6$) δ -77.77.

HRMS m/z (ESI-TOF): calculated for $C_{19}H_{22}O_4I^+$ $[M\text{-}OTf]^+$ 441.0563, found 441.0541.

Methyl 5-fluoro-2-(mesityl(((trifluoromethyl)sulfonyl)oxy)- λ^3-iodaneyl)benzoate (2i)



Prepared according to the ***General procedure 1*** on 1 mmol scale. The desired product of *ortho*-ester-substituted diaryliodonium salts (**2i**) was obtained as white solid (438 mg, 80%).

M.P.: 186-189 ℃.

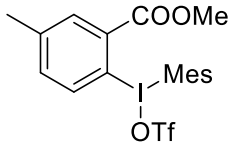
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.03 (dd, *J* = 8.1, 2.9 Hz, 1H), 7.30 (ddd, *J* = 10.0, 7.3, 2.9 Hz, 1H), 7.20 (s, 2H), 6.79 (dd, *J* = 9.0, 4.6 Hz, 1H), 4.13 (s, 3H), 2.55 (s, 6H), 2.42 (s, 3H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 166.81, 162.99, 145.57, 143.91, 130.61(d, J_{C-F} = 8.1Hz), 129.56(d, J_{C-F} = 8.1Hz), 124.40(d, J_{C-F} = 23.2Hz), 120.79(d, J_{C-F} = 23.2Hz), 120.42(q, J_{C-F} = 321.2Hz), 117.53(d, J_{C-F} = 263.6Hz), 117.40, 116.22, 105.91(d, J_{C-F} = 3.0Hz), 77.16, 55.21, 26.94, 26.84, 21.43.

^{19}F NMR (376 MHz, CDCl$_3$) δ -77.23, -109.22.

HRMS m/z (ESI-TOF): calculated for $C_{17}H_{17}FO_2I^+$ $[M\text{-}OTF]^+$ 399.0257, found 399.0240.

Methyl 2-(mesityl(((trifluoromethyl)sulfonyl)oxy)-λ^3-iodaneyl)-5-methylbenzoate (2j)



Prepared according to the ***General procedure 1*** on 1 mmol scale. The desired product of *ortho*-ester-substituted diaryliodonium salts (**2j**) was obtained as white solid (478 mg, 88%).

M.P.: 176-179 ℃.

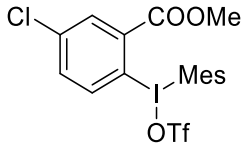
^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 8.76 (d, *J* = 1.6 Hz, 1H), 8.04 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.90 (s, 2H), 7.34 (d, *J* = 8.5 Hz, 1H), 4.65 (s, 3H), 3.06 (s, 6H), 3.00 (s, 6H).

^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 167.93, 144.51, 143.18, 141.86, 137.91, 133.36, 130.12, 128.43, 127.33, 120.68(q, J_{C-F} = 324.2Hz), 117.83, 109.87, 54.38, 39.52, 26.09, 20.78, 20.09.

^{19}F NMR (377 MHz, DMSO-*d*$_6$) δ -77.76.

HRMS m/z (ESI-TOF): calculated for $C_{18}H_{20}O_2I^+$ [M-OTF]$^+$ 395.0508, found 395.0496.

Methyl 5-chloro-2-(mesityl(((trifluoromethyl)sulfonyl)oxy)- λ^3-iodaneyl)benzoate (2k)



Prepared according to the ***General procedure 1*** on 1 mmol scale. The desired product of *ortho*-ester-substituted diaryliodonium salts (**2k**) was obtained as white solid (456 mg, 81%).

M.P.: 179-182℃.

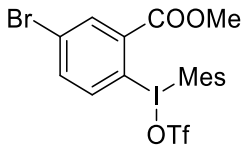
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.29 (d, *J* = 2.4 Hz, 1H), 7.51 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.20 (s, 2H), 6.74 (d, *J* = 8.7 Hz, 1H), 4.14 (s, 3H), 2.55 (s, 6H), 2.43 (s, 3H).

^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 166.87, 144.73, 143.27, 136.66, 136.42, 132.15, 130.40, 130.23, 129.58, 120.68(q, J_{C-F} = 324.2Hz), 118.06, 111.93, 54.66, 39.52, 26.11, 20.78.

^{19}F NMR (377 MHz, DMSO-*d*$_6$) δ -77.76.

HRMS m/z (ESI-TOF): calculated for $C_{17}H_{17}ClO_2I^+$ [M-OTF]$^+$ 414.9962, found 414.9946.

Methyl 5-bromo-2-(mesityl(((trifluoromethyl)sulfonyl)oxy)- λ^3-iodaneyl)benzoate (2l)



Prepared according to the ***General procedure 1*** on 1 mmol scale. The desired product of *ortho*-ester-substituted diaryliodonium salts (**2l**) was obtained as white solid (510 mg, 84%).

M.P.: 170-173℃.

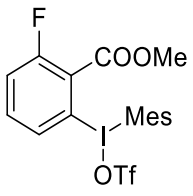
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.43 (d, *J* = 2.3 Hz, 1H), 7.65 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.20 (s, 2H), 6.66 (d, *J* = 8.7 Hz, 1H), 4.14 (s, 3H), 2.55 (s, 6H), 2.43 (s, 3H).

^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 166.84, 144.76, 143.31, 139.62, 135.00, 130.53, 130.26, 129.68, 124.79, 120.70(q, J_{C-F} = 324.2Hz), 118.01, 112.75, 54.69, 39.52, 26.14, 20.82.

^{19}F NMR (377 MHz, DMSO-*d*$_6$) δ -77.76.

HRMS m/z (ESI-TOF): calculated for $C_{17}H_{17}BrO_2I^+$ [M-OTF]$^+$ 458.9457, found 458.9445.

Methyl 2-fluoro-6-(mesityl(((trifluoromethyl)sulfonyl)oxy)- λ^3-iodaneyl)benzoate (2m)



Prepared according to the ***General procedure 1*** on 1 mmol scale. The desired product of *ortho*-ester-substituted diaryliodonium salts (**2m**) was obtained as white solid (427 mg, 78%).

M.P.: 140-143℃.

^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 7.78 – 7.67 (m, 2H), 7.39 (s, 2H), 6.79 (d, *J* = 7.3 Hz, 1H), 4.06 (s, 3H), 2.52 (s, 6H), 2.41 (s, 3H).

^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 166.78, 164.33, 161.69, 144.68, 143.23, 138.30, 138.20, 130.19, 125.39(d, J_{C-F} = 3.0Hz), 120.71(q, J_{C-F} = 322.2Hz), 120.36(d, J_{C-F} = 24.2Hz), 116.88(d, J_{C-F} = 7.1Hz), 116.04, 54.79, 39.52, 26.08, 20.80.

^{19}F NMR (376 MHz, DMSO-*d*$_6$) δ -77.77, -100.41.

HRMS m/z (ESI-TOF): calculated for $C_{17}H_{17}FO_2I^+$ [M-OTF]$^+$ 399.0257, found 399.0240.

Part 3. Table of recation condition optimization

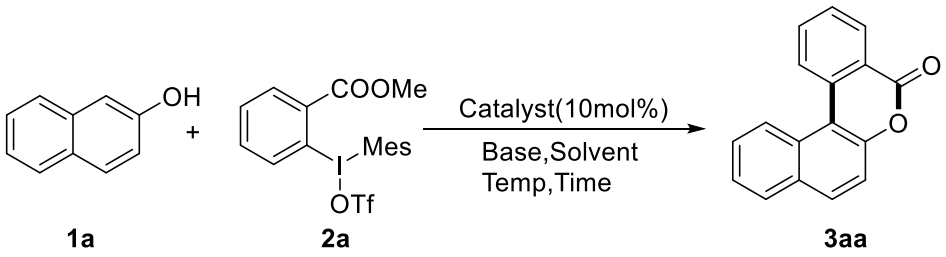


Table S1: Base optimization

Entry	Base	Yield
1	K_2CO_3	27%
2	Na_2CO_3	25%
3	Cs_2CO_3	16%
4	KOH	24%
5	KH_2PO_4	10%
6	/	50%
7	DMAP	26%
8	NaO*t*-Bu	35%
9	LiHMDS	30%
10	NaHMDS	20%
11	HNa	0%

Reaction conditions unless specifically noted: **1a** (43.2 mg, 0.3 mmol, 1.0 equiv), **2a** (174.9 mg, 0.33 mmol, 1.1 equiv), base (0.3 mmol, 1.0 equiv), and catalyst $Cu(OTf)_2$ (10.8 mg, 0.03 mmol, 10 mol %) in solvent DCE (2 mL) at 80 ℃ for 3 h. Isolated yields were obtained after purification with column chromatography.

Table S2: Solvent optimization

Entry	Solvent	Yield
1	DCE	50%
2	DMSO	45%
3	DMF	23%
4	NMP	0%
5	Toluene	10%

6	AcOH	0%
7	MeCN	36%
8	DMA	35%
9	EA	17%
10	H_2O	0%
11	Ethanol	28%
12	DCE/H_2O (1/1)	0%
13	Cyclohexane	30%
14	Cyclohexane/ Ethyl ether (1/1)	0%
15	DMSO (110 ℃)	40%
16	DMSO (130 ℃)	37%
17	DCE (12 h)	48%

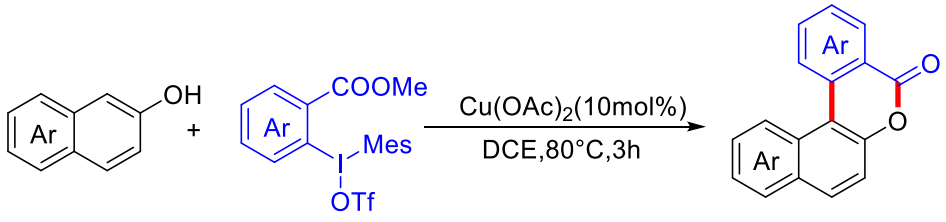
Reaction conditions unless specifically noted: **1a** (43.2 mg, 0.3 mmol, 1.0 equiv), **2a** (174.9 mg, 0.33 mmol, 1.1 equiv), and catalyst $Cu(OTf)_2$ (10.8 mg, 0.03 mmol, 10 mol %) in solvent (2 mL) at 80 ℃ for 3 h. Isolated yields were obtained after purification with column chromatography.

Table S3: Catalyst optimization

Entry	Catalyst	Yield
1	$Cu(OAc)_2$	61%
2[a]	$Cu(OTf)_2$	50%(48%)
3	$Pd(OAc)_2$	22%
4	$Cu(CF_3SO_3)_2$	32%
5	$Pd(PPh_3)_4$	20%
6	/	0%
7	$PdCl_2$	40%
8	$Pd(acac)_2$	24%
9	$FeCl_3$	21%
10	AgOAc	20%

Reaction conditions unless specifically noted: **1a** (43.2 mg, 0.3 mmol, 1.0 equiv), **2a** (174.9 mg, 0.33 mmol, 1.1 equiv), and catalyst (0.03 mmol, 10 mol %) in solvent DCE (2 mL) at 80 ℃ for 3 h. Isolated yields were obtained after purification with column chromatography. [a]The reaction time was 12 hours.

Part 4. Synthesis and characterization of 3,4-benzocoumarins

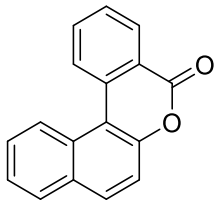


1 **2** **3**

General procedure 2: To an oven-dried Schlenk tube was added 2-Naphthol **1** (0.3 mmol, 1.0 equiv) *ortho*-ester-substituted diaryliodonium salt **2** (0.33 mmol, 1.1 equiv) $Cu(OAc)_2$ (0.03 mmol, 10% equiv) and DCE (2 mL). The mixture was stirred at 80 ℃ in an oil bath until TLC indicated that the 2-naphthol was completely consumed. The solvent was evaporated under vacuum. The crude products were purified using flash column chromatography (eluent: petroleum ether: EtOAc) on silica gel to afford the desired product **3**.

The compounds are difficult to purify by chromatography due to their high lipophilicity and the yields may deviate slightly. The impurity in the NMR spectra mainly arise from solvent impurities.

5*H*-Dibenzo[*c,f*]chromen-5-one (3aa)



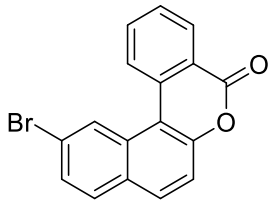
The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 61% (45 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, *J* = 8.6 Hz, 1H), 8.66 (d, *J* = 8.3 Hz, 1H), 8.51 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.99 – 7.86 (m, 3H), 7.72 – 7.61 (m, 2H), 7.56 (ddd, *J* = 8.0, 6.9, 1.0 Hz, 1H), 7.49 (d, *J* = 8.9 Hz, 1H).

Analytical data are consistent with the reported ones [3].

The peak at 1.58 ppm is the water peak from $CDCl_3$, which cannot be removed, and is similar to the following

11-Bromo-5*H*-dibenzo[*c,f*]chromen-5-one (3ab)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 63% (61 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

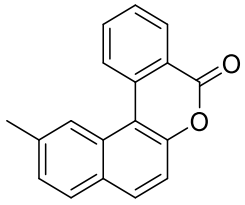
M.P.: 131-134℃.

^{1}H NMR (400 MHz, $CDCl_3$)δ 8.50 (dd, *J* = 7.9, 1.1 Hz, 1H), 8.42 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.97 – 7.91 (m, 1H), 7.88 (d, *J* = 8.9 Hz, 1H), 7.80 (d, *J* = 8.7 Hz, 1H), 7.59 – 7.56 (m, 2H), 7.51 – 7.46 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.08, 150.82, 134.87, 134.83, 131.40, 130.96, 130.87, 130.71, 130.13, 128.89, 128.66, 127.46, 126.10, 122.73, 122.37, 118.18, 111.98, 77.16.

HRMS m/z (EI-TOF): calculated for $C_{17}H_9BrO_2$ $[M]^+$ 323.9786, found 323.9787.

11-Methyl-5*H*-dibenzo[*c,f*]chromen-5-one (3ac)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 80% (62 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

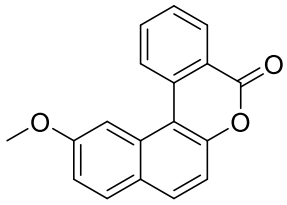
M.P.: 133-136℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (d, *J* = 8.3 Hz, 1H), 8.54 (s, 1H), 8.50 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.88 (ddd, *J* = 20.2, 9.4, 4.9 Hz, 3H), 7.66 – 7.59 (m, 1H), 7.40 (dd, *J* = 13.0, 5.0 Hz, 2H), 2.62 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.57, 150.56, 137.97, 135.70, 134.43, 131.42, 130.80, 129.94, 129.92, 129.29, 128.15, 127.56, 126.47, 124.47, 122.40, 116.73, 112.15, 77.16, 22.51.

HRMS m/z (EI-TOF): calculated for $C_{18}H_{12}O_2$ $[M]^+$ 260.0837, found 260.0840.

11-Methoxy-5*H*-dibenzo[*c*,*f*]chromen-5-one (3ad)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 77% (64 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

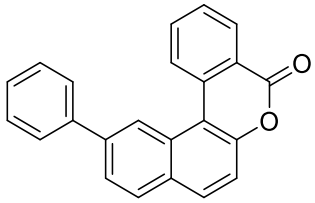
M.P.: 129-132℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 8.3 Hz, 1H), 8.51 (dd, *J* = 7.9, 1.2 Hz, 1H), 8.15 (d, *J* = 2.2 Hz, 1H), 7.92 – 7.83 (m, 3H), 7.65 – 7.59 (m, 1H), 7.35 (d, *J* = 8.8 Hz, 1H), 7.23 (dd, *J* = 8.9, 2.4 Hz, 1H), 4.00 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.56, 159.63, 151.14, 135.89, 134.47, 131.46, 131.14, 131.01, 130.96, 128.10, 127.00, 125.71, 122.39, 116.59, 115.29, 111.86, 105.95, 77.16, 55.69.

HRMS m/z (EI-TOF): calculated for $C_{18}H_{12}O_3$ $[M]^+$ 276.0786, found 276.0791.

11-Phenyl-5*H*-dibenzo[*c*,*f*]chromen-5-one (3ae)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 26% (26 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

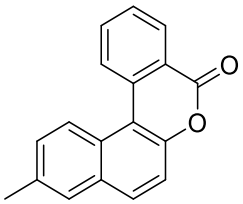
M.P.: 139-142℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 – 8.94 (m, 1H), 8.86 (d, *J* = 0.6 Hz, 1H), 8.62 (d, *J* = 8.3 Hz, 1H), 8.49 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.91 – 7.83 (m, 2H), 7.76 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.71 (dd, *J* = 5.2, 3.4 Hz, 2H), 7.64 – 7.58 (m, 1H), 7.53 (dd, *J* = 10.3, 4.8 Hz, 2H), 7.44 (dt, *J* = 7.3, 2.9 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.35, 150.67, 141.06, 140.69, 135.45, 134.54, 131.29, 130.85, 130.77, 129.94, 129.87, 129.19, 128.29, 127.93, 127.67, 126.37, 125.16, 123.31, 122.43, 117.63, 112.83, 77.16.

HRMS m/z (EI-TOF): calculated for $C_{23}H_{14}O_2$ $[M]^+$ 322.0994, found 322.0990.

10-Methyl-5*H*-dibenzo[*c,f*]chromen-5-one (3af)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 31% (25 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

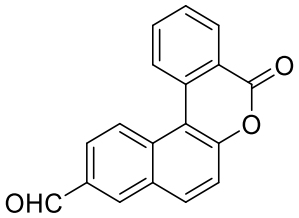
M.P.:141-144℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 – 8.59 (m, 2H), 8.49 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.90 – 7.85 (m, 1H), 7.82 (d, *J* = 8.9 Hz, 1H), 7.70 (s, 1H), 7.64 – 7.59 (m, 1H), 7.48 (dd, *J* = 8.8, 1.7 Hz, 1H), 7.44 (d, *J* = 8.9 Hz, 1H), 2.55 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.56, 149.91, 135.65, 135.23, 134.43, 132.04, 131.11, 130.81, 130.01, 128.62, 128.21, 127.69, 126.47, 124.97, 122.44, 117.67, 112.60, 77.16, 21.35.

HRMS m/z (EI-TOF): calculated for $C_{18}H_{12}O_2$ $[M]^+$ 260.0837, found 260.0841.

5-Oxo-5*H*-dibenzo[*c,f*]chromene-10-carbaldehyde (3ag)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 28% (23 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

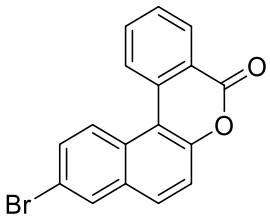
M.P.:145-148℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.22 (s, 1H), 8.89 (d, *J* = 8.9 Hz, 1H), 8.62 (d, *J* = 8.2 Hz, 1H), 8.53 (d, *J* = 7.8 Hz, 1H), 8.46 (s, 1H), 8.15 (dd, *J* = 8.9, 1.5 Hz, 1H), 8.10 (d, *J* = 8.8 Hz, 1H), 7.95 (t, *J* = 7.7 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.62 (d, *J* = 8.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 191.66, 160.91, 152.23, 134.86, 134.83, 134.79, 133.50, 132.81, 131.16, 131.06, 129.01, 126.61, 126.26, 125.14, 122.60, 119.16, 113.43, 111.88, 77.16.

HRMS m/z (EI-TOF): calculated for $C_{18}H_{10}O_3$ $[M]^+$ 274.0630, found 274.0633.

10-Bromo-5*H*-dibenzo[*c,f*]chromen-5-one (3ah)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 54% (52 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

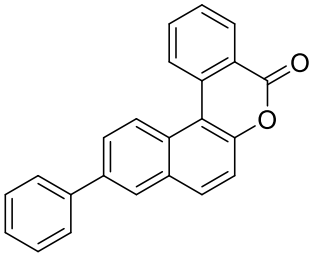
M.P.:201-204℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, *J* = 9.2 Hz, 1H), 8.56 – 8.47 (m, 2H), 8.08 (d, *J* = 2.1 Hz, 1H), 7.93 – 7.87 (m, 1H), 7.81 (d, *J* = 8.9 Hz, 1H), 7.71 (dd, *J* = 9.2, 2.1 Hz, 1H), 7.68 – 7.63 (m, 1H), 7.50 (d, *J* = 8.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.13, 150.39, 134.99, 134.65, 133.02, 131.37, 131.02, 130.98, 130.55, 128.72, 128.20, 126.84, 126.35, 122.56, 119.36, 118.95, 113.01, 77.16.

HRMS m/z (EI-TOF): calculated for $C_{17}H_9BrO_2$ $[M]^+$ 323.9786, found 323.9790.

10-Phenyl-5*H*-dibenzo[*c,f*]chromen-5-one (3ai)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 25% (24 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

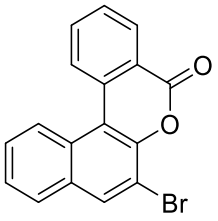
M.P.:149-152℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, *J* = 8.9 Hz, 1H), 8.67 (d, *J* = 8.2 Hz, 1H), 8.51 (dd, *J* = 7.9, 1.2 Hz, 1H), 8.13 (d, *J* = 1.8 Hz, 1H), 7.97 (d, *J* = 8.9 Hz, 1H), 7.94 – 7.88 (m, 2H), 7.76 (d, *J* = 7.3 Hz, 2H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.55 – 7.49 (m, 3H), 7.43 (t, *J* = 7.3 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.42, 150.42, 140.16, 138.15, 135.49, 134.55, 132.15, 131.91, 130.89, 129.17, 128.77, 128.41, 127.88, 127.38, 127.32, 127.10, 126.49, 125.72, 122.51, 118.17, 112.71, 77.16.

HRMS m/z (EI-TOF): calculated for $C_{23}H_{14}O_2$ $[M]^+$ 322.0994, found 322.0998.

7-Bromo-5*H*-dibenzo[*c,f*]chromen-5-one (3aj)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 22% (20 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

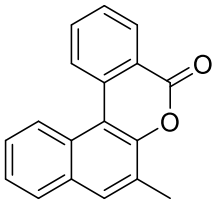
M.P.:154-157℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 8.6 Hz, 1H), 8.62 (d, *J* = 8.3 Hz, 1H), 8.52 (dd, *J* = 7.9, 1.2 Hz, 1H), 8.22 (s, 1H), 7.94 – 7.89 (m, 1H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.67 (dd, *J* = 11.3, 4.1 Hz, 2H), 7.61 – 7.55 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.46, 146.54, 135.02, 134.63, 134.19, 131.97, 130.92, 129.01, 128.72, 128.52, 128.08, 126.97, 126.35, 125.35, 122.54, 114.48, 111.04, 77.16.

HRMS m/z (EI-TOF): calculated for $C_{17}H_9BrO_2$ $[M]^+$ 323.9786, found 323.9790.

7-Methyl-5*H*-dibenzo[*c,f*]chromen-5-one (3ak)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 49% (38 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

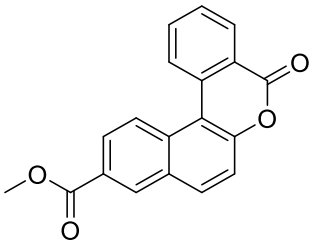
M.P.:127-130℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 8.5 Hz, 1H), 8.60 (d, *J* = 8.3 Hz, 1H), 8.49 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.86 (ddd, *J* = 8.9, 5.3, 1.6 Hz, 2H), 7.73 (s, 1H), 7.59 (ddd, *J* = 10.0, 8.2, 1.2 Hz, 2H), 7.53 – 7.47 (m, 1H), 2.60 (d, *J* = 0.8 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.44, 149.61, 135.71, 134.32, 131.43, 131.36, 130.63, 128.58, 128.42, 128.16, 126.85, 126.72, 126.60, 125.44, 124.99, 122.25, 112.47, 77.16, 16.92.

HRMS m/z (EI-TOF): calculated for $C_{18}H_{12}O_2$ $[M]^+$ 260.0837, found 260.0845.

Methyl 5-oxo-5*H*-dibenzo[*c,f*]chromene-10-carboxylate (3al)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 48% (44 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

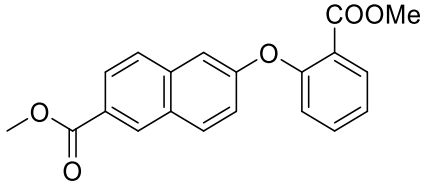
M.P.:150-153℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (d, *J* = 9.0 Hz, 1H), 8.68 (d, *J* = 1.6 Hz, 1H), 8.62 (d, *J* = 8.3 Hz, 1H), 8.52 (dd, *J* = 7.9, 1.1 Hz, 1H), 8.24 (dd, *J* = 9.0, 1.8 Hz, 1H), 8.03 (d, *J* = 8.9 Hz, 1H), 7.96 – 7.90 (m, 1H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.56 (d, *J* = 8.9 Hz, 1H), 4.02 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.80, 161.07, 151.76, 135.06, 134.73, 132.74, 132.19, 132.07, 131.01, 130.98, 128.77, 127.36, 127.09, 126.51, 125.40, 122.51, 118.73, 112.98, 77.16, 52.56.

HRMS m/z (EI-TOF): calculated for $C_{19}H_{12}O_4$ $[M]^+$ 304.0736, found 304.0741.

Methyl 6-(2-(methoxycarbonyl)phenoxy)-2-naphthoate (3al')



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 20% (20 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

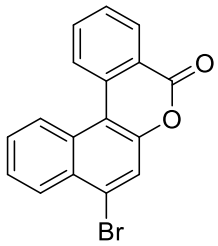
M.P.:125-128℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 8.00 (dd, *J* = 8.3, 1.5 Hz, 2H), 7.93 (d, *J* = 8.9 Hz, 1H), 7.66 (d, *J* = 8.7 Hz, 1H), 7.58 – 7.51 (m, 1H), 7.34 – 7.26 (m, 2H), 7.12 (dd, *J* = 6.0, 1.8 Hz, 2H), 3.96 (s, 3H), 3.75 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 129.66, 128.21, 120.53, 117.54, 99.15, 96.37, 94.62, 93.87, 93.32, 91.25, 89.65, 88.52, 88.44, 87.05, 86.19, 84.69, 82.34, 74.16, 39.52, 14.67, 14.62.

HRMS m/z (EI-TOF): calculated for $C_{20}H_{16}O_5$ $[M]^+$ 336.0998, found 336.1002.

8-Bromo-5*H*-dibenzo[*c,f*]chromen-5-one (3am)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 83% (81 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

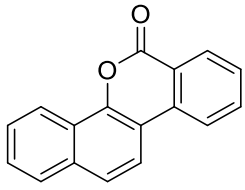
M.P.:151-154℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 8.5 Hz, 1H), 8.58 (d, *J* = 8.3 Hz, 1H), 8.50 (dd, *J* = 7.9, 1.1 Hz, 1H), 8.40 (dd, *J* = 8.3, 1.0 Hz, 1H), 7.93 – 7.86 (m, 1H), 7.84 (s, 1H), 7.72 (ddd, *J* = 8.5, 6.9, 1.4 Hz, 1H), 7.66 (dd, *J* = 8.0, 7.1 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.90, 149.37, 134.95, 134.67, 131.02, 130.30, 130.19, 128.69, 128.60, 126.76, 126.69, 125.68, 125.55, 122.53, 121.75, 112.76, 77.16.

HRMS m/z (EI-TOF): calculated for $C_{17}H_9BrO_2$ $[M]^+$ 323.9786, found 323.9795.

6*H*-Dibenzo[*c,h*]chromen-6-one (3an)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 49% (36 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

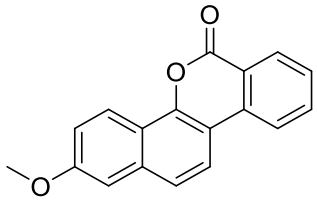
M.P.:171-174℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 7.9 Hz, 1H), 8.46 (d, *J* = 7.9 Hz, 1H), 8.18 (d, *J* = 8.1 Hz, 1H), 8.04 (d, *J* = 8.7 Hz, 1H), 7.86 (t, *J* = 7.2 Hz, 2H), 7.75 (d, *J* = 8.7 Hz, 1H), 7.65 – 7.58 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.38, 147.35, 135.50, 135.10, 134.36, 130.76, 128.74, 128.01, 127.77, 127.24, 124.62, 123.98, 122.44, 122.15, 121.27, 119.27, 113.14, 77.16.

HRMS m/z (EI-TOF): calculated for $C_{17}H_{10}O_2$ $[M]^+$ 246.0681, found 246.0685.

2-Methoxy-6*H*-dibenzo[*c*,*h*]chromen-6-one (3ao)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 40% (33 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

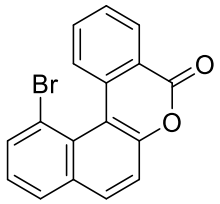
M.P.:155-158℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 – 8.40 (m, 2H), 8.13 (d, *J* = 8.0 Hz, 1H), 8.00 (d, *J* = 8.8 Hz, 1H), 7.87 – 7.80 (m, 1H), 7.63 (d, *J* = 8.7 Hz, 1H), 7.58 – 7.52 (m, 1H), 7.27 – 7.23 (m, 2H), 7.15 (d, *J* = 2.5 Hz, 1H), 3.95 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.52, 159.41, 147.62, 136.08, 135.77, 135.04, 130.70, 128.23, 124.15, 123.51, 121.81, 120.78, 120.02, 119.43, 118.93, 111.36, 106.36, 77.16, 55.49.

HRMS m/z (EI-TOF): calculated for $C_{18}H_{12}O_3$ $[M]^+$ 276.0786, found 276.0790.

12-Bromo-5*H*-dibenzo[*c*,*f*]chromen-5-one (3ap)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 25% (24 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

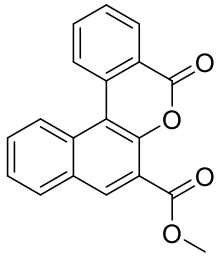
M.P.:152-155℃.

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.35 (d, *J* = 9.1 Hz, 1H), 8.15 (td, *J* = 8.3, 1.1 Hz, 2H), 8.06 (dd, *J* = 7.6, 1.1 Hz, 1H), 7.87 (ddd, *J* = 8.7, 7.2, 1.7 Hz, 1H), 7.74 (t, *J* = 9.1 Hz, 2H), 7.56 (ddd, *J* = 11.5, 9.5, 4.4 Hz, 2H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 174.24, 158.03, 153.68, 136.38, 135.30, 134.33, 132.66, 128.84, 128.23, 127.15, 125.76, 125.12, 124.30, 120.31, 118.92, 117.55, 115.89, 39.52.

HRMS m/z (EI-TOF): calculated for $C_{17}H_9BrO_2$ $[M]^+$ 323.9786, found 323.9788.

Methyl 5-oxo-5*H*-dibenzo[*c,f*]chromene-7-carboxylate (3aq)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 43% (39 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

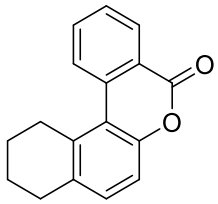
M.P.:145-148℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.01 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.93 (d, *J* = 8.1 Hz, 1H), 7.69 (d, *J* = 8.2 Hz, 1H), 7.58 – 7.53 (m, 1H), 7.52 – 7.44 (m, 2H), 7.26 – 7.21 (m, 1H), 6.99 (d, *J* = 8.2 Hz, 1H), 3.90 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.21, 156.77, 156.51, 153.13, 135.88, 133.73, 133.62, 132.14, 129.30, 128.91, 128.68, 126.97, 125.74, 123.47, 122.86, 122.70, 120.11, 115.99, 77.16, 52.43.

HRMS m/z (EI-TOF): calculated for $C_{19}H_{12}O_4$ $[M]^+$ 304.0736, found 304.0741.

9,10,11,12-Tetrahydro-5*H*-dibenzo[*c,f*]chromen-5-one (3ar)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 45% (34 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

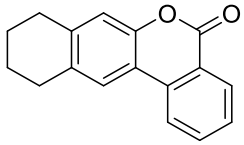
M.P.:144-147℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.0 Hz, 1H), 7.64 (dd, *J* = 8.3, 7.1 Hz, 1H), 7.42 – 7.28 (m, 3H), 7.20 (d, *J* = 8.5 Hz, 1H), 3.52 (t, *J* = 5.5 Hz, 2H), 2.81 (s, 2H), 1.87 – 1.76 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 179.28, 156.28, 155.24, 140.73, 135.94, 134.16, 133.23, 126.92, 123.61, 123.26, 119.87, 117.41, 115.41, 77.16, 30.35, 29.40, 23.30, 22.26.

HRMS m/z (EI-TOF): calculated for $C_{17}H_{14}O_2$ $[M]^+$ 250.0994, found 250.0998.

8,9,10,11-Tetrahydro-5*H*-dibenzo[*c,g*]chromen-5-one (3as)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 10% (7.5 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

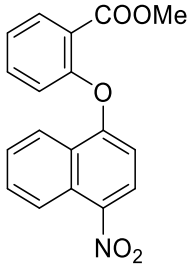
M.P.:142-145℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.02 (s, 1H), 7.69 (ddd, *J* = 8.7, 7.1, 1.7 Hz, 1H), 7.48 – 7.43 (m, 1H), 7.37 – 7.31 (m, 1H), 7.19 (s, 1H), 2.91 (dd, *J* = 6.0, 3.3 Hz, 4H), 1.88 – 1.82 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 177.36, 156.38, 154.32, 146.13, 134.58, 133.80, 126.85, 126.29, 123.63, 121.96, 119.85, 118.02, 117.30, 77.16, 30.27, 28.95, 23.13, 22.78.

HRMS m/z (EI-TOF): calculated for $C_{17}H_{14}O_2$ $[M]^+$ 250.0994, found 250.0998.

Methyl 2-((4-nitronaphthalen-1-yl)oxy)benzoate (3at)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 51% (49 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

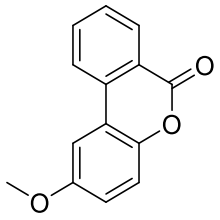
M.P.:133-136℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, *J* = 8.8 Hz, 1H), 8.58 (d, *J* = 8.1 Hz, 1H), 8.24 (d, *J* = 8.7 Hz, 1H), 8.09 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.81 (ddd, *J* = 8.6, 6.9, 1.3 Hz, 1H), 7.67 (ddd, *J* = 17.3, 8.1, 1.3 Hz, 2H), 7.41 (td, *J* = 7.8, 1.0 Hz, 1H), 7.22 (d, *J* = 8.1 Hz, 1H), 6.51 (d, *J* = 8.7 Hz, 1H), 3.61 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.26, 160.01, 153.99, 134.52, 132.83, 130.56, 130.51, 127.29, 127.24, 126.48, 126.09, 125.88, 124.13, 123.67, 123.39, 123.05, 106.49, 77.16, 52.40.

HRMS m/z (EI-TOF): calculated for $C_{18}H_{13}NO_5$ $[M]^+$ 323.0794, found 323.0799.

2-Methoxy-6*H*-benzo[*c*]chromen-6-one (3au)



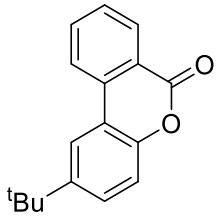
The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 34% (23 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

M.P.:140-143℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.75 – 7.70 (m, 2H), 7.50 (d, *J* = 8.5 Hz, 1H), 7.45 (d, *J* = 9.1 Hz, 1H), 7.40 – 7.36 (m, 1H), 7.34 (dd, *J* = 9.1, 3.1 Hz, 1H), 3.93 (s, 3H).

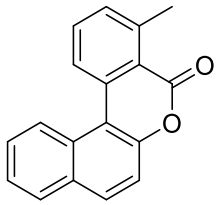
^{13}C NMR (101 MHz, $CDCl_3$) δ 177.27, 156.14, 151.16, 134.75, 126.84, 125.09, 123.87, 120.44, 119.58, 119.20, 118.12, 114.98, 105.96, 77.16, 56.09.
HRMS m/z (EI-TOF): calculated for $C_{14}H_{10}O_3$ $[M]^+$ 226.0630, found 226.0638.

2-(*tert*-Butyl)-6*H*-benzo[*c*]chromen-6-one (3av)



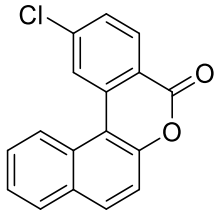
The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 39% (29 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.
M.P.:135-138℃.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, *J* = 8.0, 1.5 Hz, 1H), 8.32 (d, *J* = 2.5 Hz, 1H), 7.79 – 7.76 (m, 1H), 7.69 (ddd, *J* = 8.7, 7.1, 1.7 Hz, 1H), 7.46 (dd, *J* = 8.4, 0.5 Hz, 1H), 7.42 (d, *J* = 8.8 Hz, 1H), 7.37 – 7.32 (m, 1H), 1.40 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 177.54, 156.24, 154.41, 147.15, 141.40, 134.69, 132.86, 131.02, 126.83, 123.79, 122.50, 118.00, 117.69, 77.16, 34.84, 31.45.
HRMS m/z (EI-TOF): calculated for $C_{17}H_{16}O_2$ $[M]^+$ 252.1150, found 252.1145.

4-Methyl-5*H*-dibenzo[*c,f*]chromen-5-one (3ca)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 32% (25 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.
M.P.:122-125℃.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 8.6 Hz, 1H), 8.44 (d, *J* = 8.2 Hz, 1H), 7.91 (dd, *J* = 15.5, 8.4 Hz, 2H), 7.72 (t, *J* = 7.9 Hz, 1H), 7.64 (ddd, *J* = 8.5, 6.9, 1.4 Hz, 1H), 7.56 – 7.51 (m, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 2.92 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 160.68, 149.98, 143.92, 136.80, 133.44, 131.68, 131.45, 131.44, 129.66, 129.36, 127.65, 125.30, 125.21, 124.89, 121.13, 117.26, 113.17, 77.16, 23.81.
HRMS m/z (EI-TOF): calculated for $C_{18}H_{12}O_2$ $[M]^+$ 260.0837, found 260.0838.

2-Chloro-5*H*-dibenzo[*c,f*]chromen-5-one (3da)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 50% (42 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

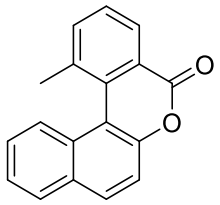
M.P.:132-135℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 8.7 Hz, 1H), 8.61 (d, *J* = 1.7 Hz, 1H), 8.42 (d, *J* = 8.5 Hz, 1H), 7.97 – 7.93 (m, 2H), 7.71 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H), 7.61 – 7.55 (m, 2H), 7.47 (d, *J* = 8.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.71, 150.97, 141.46, 136.90, 132.52, 132.40, 131.70, 129.63, 129.41, 128.68, 128.43, 126.28, 125.78, 124.62, 120.71, 117.65, 111.60, 77.16.

HRMS m/z (EI-TOF): calculated for $C_{17}H_9ClO_2$ $[M]^+$ 280.0291, found 280.0298.

1-Methyl-5*H*-dibenzo[*c,f*]chromen-5-one (3ea)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 46% (36 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

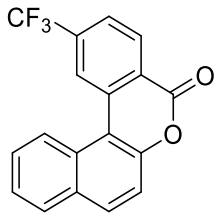
M.P.:135-138℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 7.7 Hz, 1H), 7.94 (dd, *J* = 13.5, 8.3 Hz, 2H), 7.76 (dd, *J* = 15.4, 8.1 Hz, 2H), 7.60 – 7.47 (m, 4H), 2.35 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 162.26, 149.87, 137.84, 135.67, 134.31, 131.16, 131.03, 129.39, 128.44, 128.11, 127.99, 127.04, 126.38, 125.29, 124.57, 117.16, 113.57, 77.16, 23.84.

HRMS m/z (EI-TOF): calculated for $C_{18}H_{12}O_2$ $[M]^+$ 260.0837, found 260.0838.

2-(Trifluoromethyl)-5*H*-dibenzo[*c,f*]chromen-5-one (3fa)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 49% (46 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

M.P.:140-143℃.

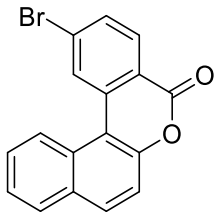
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (s, 1H), 8.66 (d, *J* = 8.6 Hz, 1H), 8.61 (d, *J* = 8.2 Hz, 1H), 7.98 (d, *J* = 9.1 Hz, 2H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.74 (ddd, *J* = 8.4, 7.0, 1.3 Hz, 1H), 7.61 (dd, *J* = 11.2, 3.9 Hz, 1H), 7.50 (d, *J* = 8.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.31, 150.90, 136.01, 135.94 (q, J_{C-F} = 33.3Hz), 132.80, 131.80, 131.72, 129.73, 129.35, 128.70, 125.95, 124.57(q, J_{C-F} = 4Hz), 124.41, 123.62 (q, J_{C-F} = 274.7Hz), 123.56 (q, J_{C-F} = 4 Hz), 117.56, 114.34, 111.76, 77.16.

^{19}F NMR (376 MHz, $CDCl_3$) δ -63.16.

HRMS m/z (EI-TOF): calculated for $C_{18}H_9F_3O_2$ $[M]^+$ 314.0555, found 314.0558.

2-Bromo-5*H*-dibenzo[*c*,*f*]chromen-5-one (3ga)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 55% (53 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

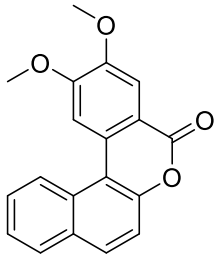
M.P.:136-139℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, *J* = 9.8 Hz, 1H), 8.65 (d, *J* = 8.6 Hz, 1H), 8.32 (d, *J* = 8.4 Hz, 1H), 7.94 (dd, *J* = 8.4, 3.1 Hz, 2H), 7.72 (ddd, *J* = 12.8, 8.4, 1.4 Hz, 2H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.46 (d, *J* = 8.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.82, 150.94, 136.95, 132.51, 132.33, 131.69, 131.55, 130.21, 129.62, 129.37, 129.27, 128.46, 125.78, 124.58, 121.07, 117.63, 111.47, 77.16.

HRMS m/z (EI-TOF): calculated for $C_{17}H_9BrO_2$ $[M]^+$ 323.9786, found 323.9791.

2,3-Dimethoxy-5*H*-dibenzo[*c*,*f*]chromen-5-one (3ha)

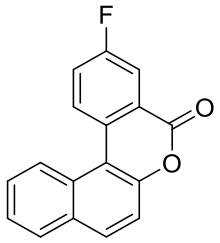


The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 43% (39 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

M.P.:129-132℃.

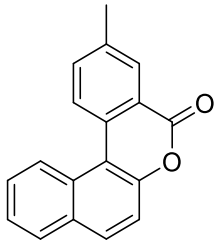
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (d, *J* = 8.6 Hz, 1H), 8.08 (s, 1H), 7.96 (d, *J* = 7.7 Hz, 1H), 7.89 (d, *J* = 8.3 Hz, 2H), 7.67 (ddd, *J* = 8.5, 6.9, 1.3 Hz, 1H), 7.58 – 7.53 (m, 1H), 7.49 (d, *J* = 8.9 Hz, 1H), 4.11 (s, 3H), 4.05 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 161.31, 154.55, 150.07, 149.54, 131.80, 130.80, 130.76, 129.66, 129.47, 127.69, 125.37, 124.58, 117.85, 115.88, 112.72, 110.93, 108.12, 77.16, 56.52, 56.47.
HRMS m/z (EI-TOF): calculated for $C_{19}H_{14}O_4$ $[M]^+$ 306.0892, found 306.0895.

3-Fluoro-5*H*-dibenzo[*c,f*]chromen-5-one (3ia)



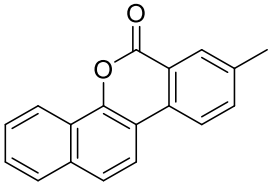
The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 21% (17 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.
M.P.:130-133℃.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 – 8.62 (m, 2H), 8.15 (dd, *J* = 8.4, 2.9 Hz, 1H), 7.93 (dd, *J* = 13.6, 8.2 Hz, 2H), 7.68 (ddd, *J* = 8.5, 6.9, 1.4 Hz, 1H), 7.63 – 7.53 (m, 2H), 7.48 (d, *J* = 8.9 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 160.56, 149.93, 132.08(d, J_{C-F} = 3.0Hz), 131.95, 131.81, 131.63, 129.57, 129.37, 128.93(d, J_{C-F} = 8.1Hz),127.89, 126.88(d, J_{C-F} = 243.4Hz), 124.85, 124.46(d, J_{C-F} = 8.1Hz), 122.53(d, J_{C-F} = 22.2Hz), 117.63, 116.50(d, J_{C-F} = 23.2Hz), 112.13, 77.16.
^{19}F NMR (376 MHz, $CDCl_3$) δ -110.76.
HRMS m/z (EI-TOF): calculated for $C_{17}H_9FO_2$ $[M]^+$ 264.0587, found 264.0580.

3-Methyl-5*H*-dibenzo[*c,f*]chromen-5-one (3ja)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 59% (46 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.
M.P.:154-157℃.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 8.6 Hz, 1H), 8.53 (d, *J* = 8.4 Hz, 1H), 8.29 (d, *J* = 0.8 Hz, 1H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.88 (d, *J* = 8.9 Hz, 1H), 7.71 – 7.62 (m, 2H), 7.57 – 7.51 (m, 1H), 7.46 (d, *J* = 8.9 Hz, 1H), 2.54 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 161.62, 149.98, 138.66, 135.64, 132.96, 131.72, 131.10, 130.65, 129.61, 129.41, 127.73, 126.45, 125.40, 125.16, 122.30, 117.69, 112.78, 77.16, 21.29.
HRMS m/z (EI-TOF): calculated for $C_{18}H_{12}O_2$ $[M]^+$ 260.0837, found 260.0831.

8-Methyl-6*H*-dibenzo[*c*,*h*]chromen-6-one (3jb)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 28% (22 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

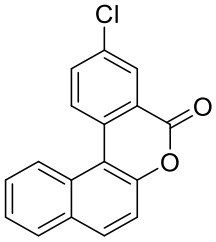
M.P.:150-153℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 8.0 Hz, 1H), 8.26 (s, 1H), 8.05 (dd, *J* = 16.5, 8.5 Hz, 2H), 7.86 (d, *J* = 7.4 Hz, 1H), 7.75 (d, *J* = 8.8 Hz, 1H), 7.66 (dd, *J* = 8.2, 1.4 Hz, 1H), 7.61 (ddd, *J* = 9.1, 7.7, 1.1 Hz, 2H), 2.51 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.57, 146.86, 139.09, 136.31, 134.10, 132.94, 130.51, 130.48, 127.75, 127.15, 124.52, 123.97, 122.32, 122.12, 121.08, 119.26, 113.29, 77.16, 21.40.

HRMS m/z (EI-TOF): calculated for $C_{18}H_{12}O_2$ $[M]^+$ 260.0837, found 260.0840.

3-Chloro-5*H*-dibenzo[*c*,*f*]chromen-5-one (3ka)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 37% (31 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

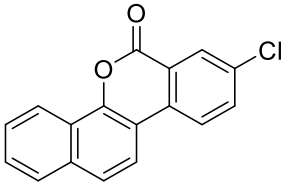
M.P.:140-143℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 8.6 Hz, 1H), 8.60 (d, *J* = 8.8 Hz, 1H), 8.46 (d, *J* = 2.4 Hz, 1H), 7.95 (t, *J* = 7.8 Hz, 2H), 7.83 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.69 (ddd, *J* = 8.5, 7.0, 1.3 Hz, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.48 (d, *J* = 8.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.30, 150.35, 134.66, 134.31, 133.93, 132.05, 131.77, 130.25, 129.60, 129.40, 128.19, 128.01, 125.74, 124.82, 123.77, 117.62, 112.00, 77.16.

HRMS m/z (EI-TOF): calculated for $C_{17}H_9ClO_2$ $[M]^+$ 280.0291, found 280.0290.

8-Chloro-6*H*-dibenzo[*c*,*h*]chromen-6-one (3kb)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 45% (37 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

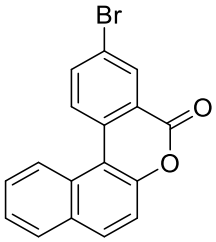
M.P.:142-145℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 – 8.53 (m, 1H), 8.42 (d, *J* = 2.3 Hz, 1H), 8.12 (d, *J* = 8.6 Hz, 1H), 8.00 (d, *J* = 8.8 Hz, 1H), 7.88 (dd, *J* = 6.7, 2.4 Hz, 1H), 7.82 – 7.76 (m, 2H), 7.66 – 7.60 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.27, 147.31, 135.41, 134.82, 134.48, 133.98, 130.24, 130.20, 128.28, 127.85, 127.48, 124.96, 123.88, 122.52, 122.42, 119.04, 112.44, 77.16.

HRMS m/z (EI-TOF): calculated for $C_{17}H_9ClO_2$ $[M]^+$ 280.0291, found 280.0295.

3-Bromo-5*H*-dibenzo[*c,f*]chromen-5-one (3la)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 35% (34 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

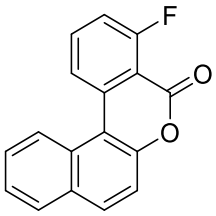
M.P.:140-143℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 8.6 Hz, 1H), 8.59 (d, *J* = 2.2 Hz, 1H), 8.49 (d, *J* = 8.8 Hz, 1H), 7.94 (dt, *J* = 15.6, 5.6 Hz, 3H), 7.67 (ddd, *J* = 8.5, 6.9, 1.3 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.45 (d, *J* = 8.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.15, 150.40, 137.48, 134.30, 133.31, 132.13, 131.78, 129.61, 129.37, 128.21, 128.08, 125.75, 124.81, 123.90, 122.08, 117.63, 112.04, 77.16.

HRMS m/z (EI-TOF): calculated for $C_{17}H_9BrO_2$ $[M]^+$ 323.9786, found 323.9791.

4-Fluoro-5*H*-dibenzo[*c,f*]chromen-5-one (3ma)



The preparation was according to the ***general procedure 2*** on 0.3 mmol scale, and obtained an isolated yield of 50% (40 mg) as yellow solid after column chromatography (petroleum ether: EtOAc = 8:1) on silica gel.

M.P.:147-150℃.

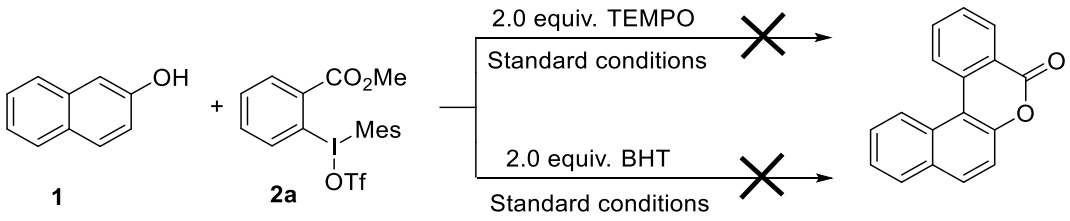
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 8.6 Hz, 1H), 8.40 (d, *J* = 8.3 Hz, 1H), 7.94 (dd, *J* = 8.5, 4.9 Hz, 2H), 7.84 (td, *J* = 8.3, 5.4 Hz, 1H), 7.70 – 7.63 (m, 1H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.44 (d, *J* = 8.9 Hz, 1H), 7.31 (dd, *J* = 10.0, 8.6 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 164.79, 162.13, 156.96, 156.91, 150.66, 137.98, 135.79(d, J_{C-F} = 10.1Hz), 132.46, 130.63(d, J_{C-F} = 226.1Hz), 129.55, 128.14, 125.69, 124.95, 122.50(d, J_{C-F} = 4.1Hz), 117.41, 115.79(d, J_{C-F} = 21.2Hz), 111.91(d, J_{C-F} = 22.1Hz), 111.40(d, J_{C-F} = 10.0Hz), 77.16.

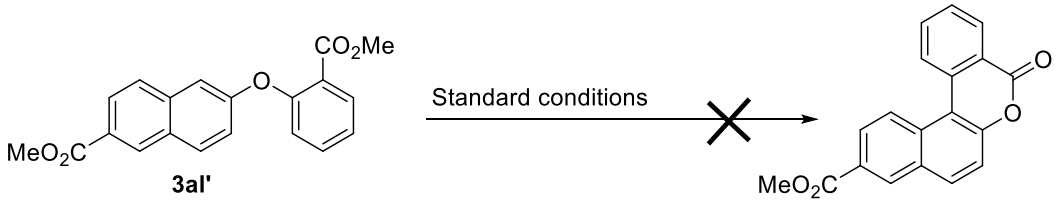
^{19}F NMR (377 MHz, $CDCl_3$) δ -106.47.

HRMS m/z (EI-TOF): calculated for $C_{17}H_9FO_2$ $[M]^+$ 264.0587, found 264.0590.

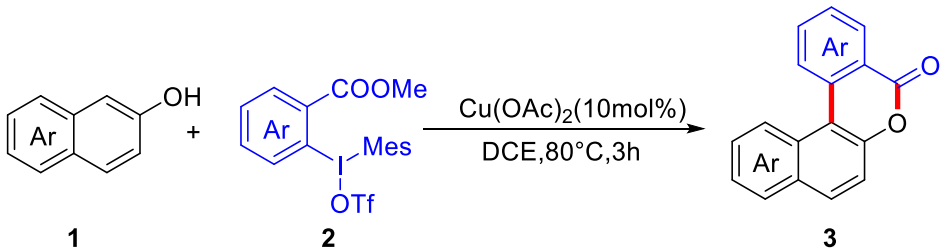
Part 5. Mechanism study



To an oven-dried Schlenk tube was added 2-Naphthol **1** (0.3 mmol, 1.0 equiv) *ortho*-ester-substituted diaryliodonium salt **2** (0.33 mmol, 1.1 equiv) $Cu(OAc)_2$ (0.03 mmol, 10% equiv) and DCE (2 mL). BHT or TEMPO (2.0 equiv) was added. The mixture was stirred at 80 ℃ in an oil bath until TLC indicated that the 2-naphthol was completely consumed. TEMPO = 2,2,6,6-tetramethylpiperidine-1-oxyl. BHT = butylated hydroxytoluene.



To an oven-dried Schlenk tube was added **3al'** (0.3 mmol, 1.0 equiv) $Cu(OAc)_2$ (0.03 mmol, 10% equiv) and DCE (2 mL). The mixture was stirred at 80 ℃ in an oil bath.



To an oven-dried Schlenk tube was added 2-naphthol **1** (0.3 mmol, 1.0 equiv.) *ortho*-ester-substituted diaryliodonium salt **2** (0.33 mmol, 1.1 equiv) $Cu(OAc)_2$ (0.03mmol, 10% equiv) and DCE (2 mL). The mixture was stirred at 80 ℃ in an oil bath. After 1 hours, a drop of the reaction mixture was delivered to LC-MS analysis.

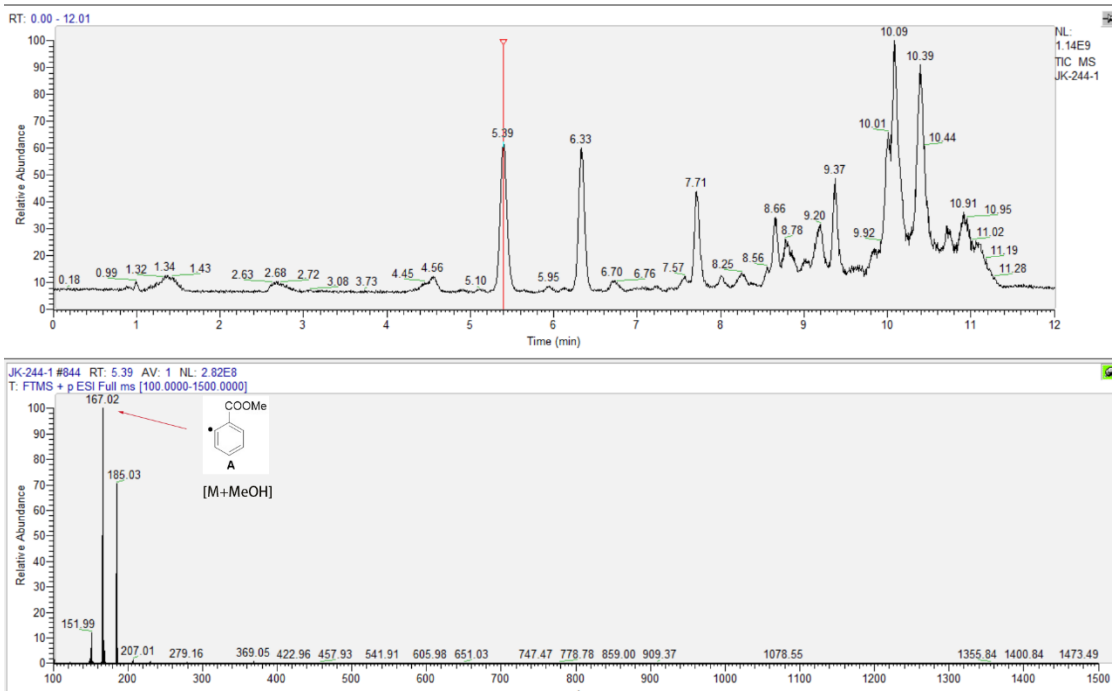


Figure S1. LC-MS spectra of reaction mixture

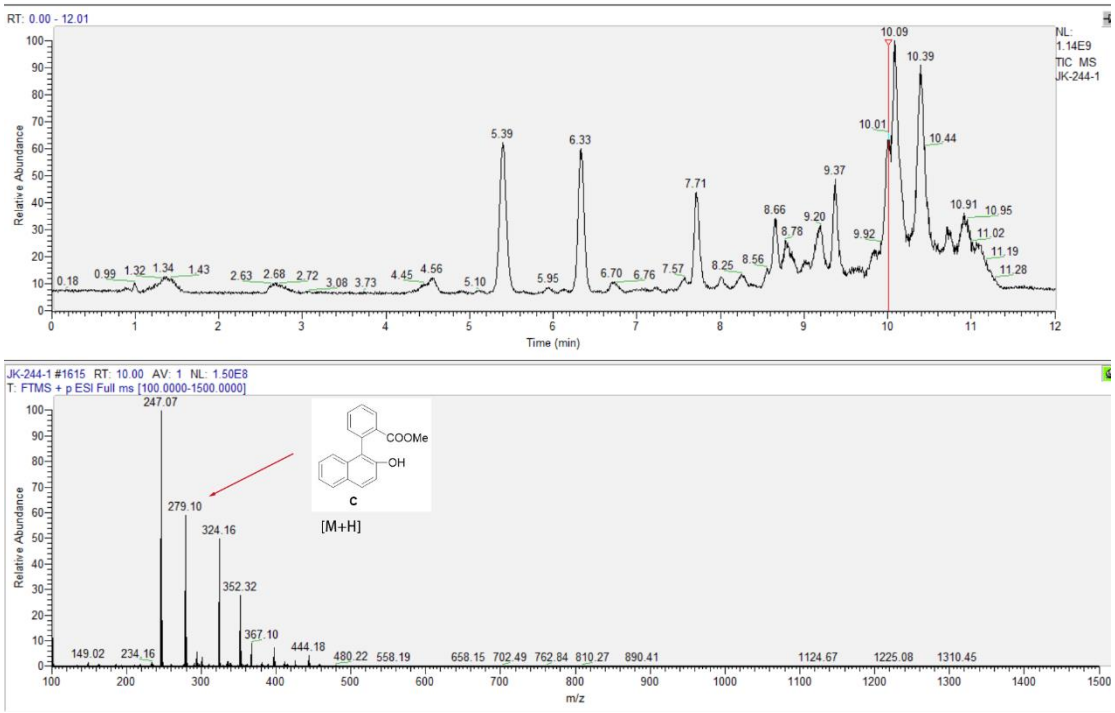


Figure S2. LC-MS spectra of reaction mixture

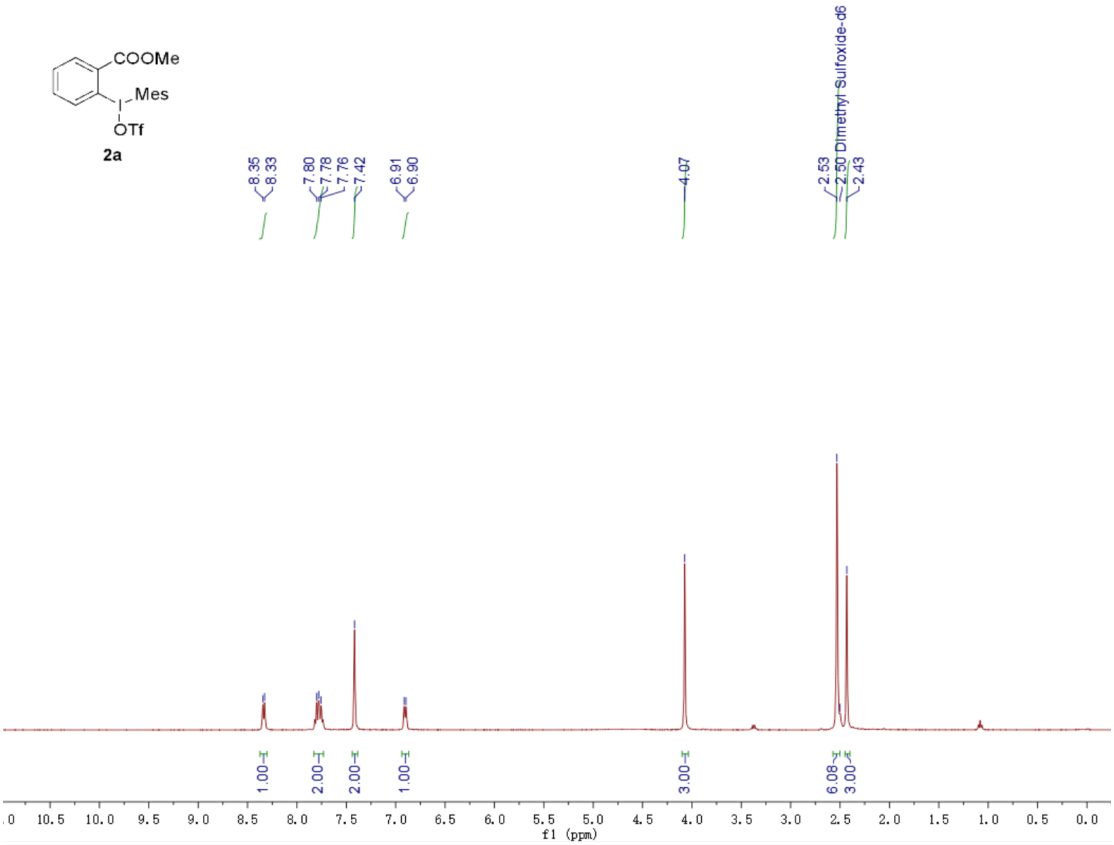
Part 6. References

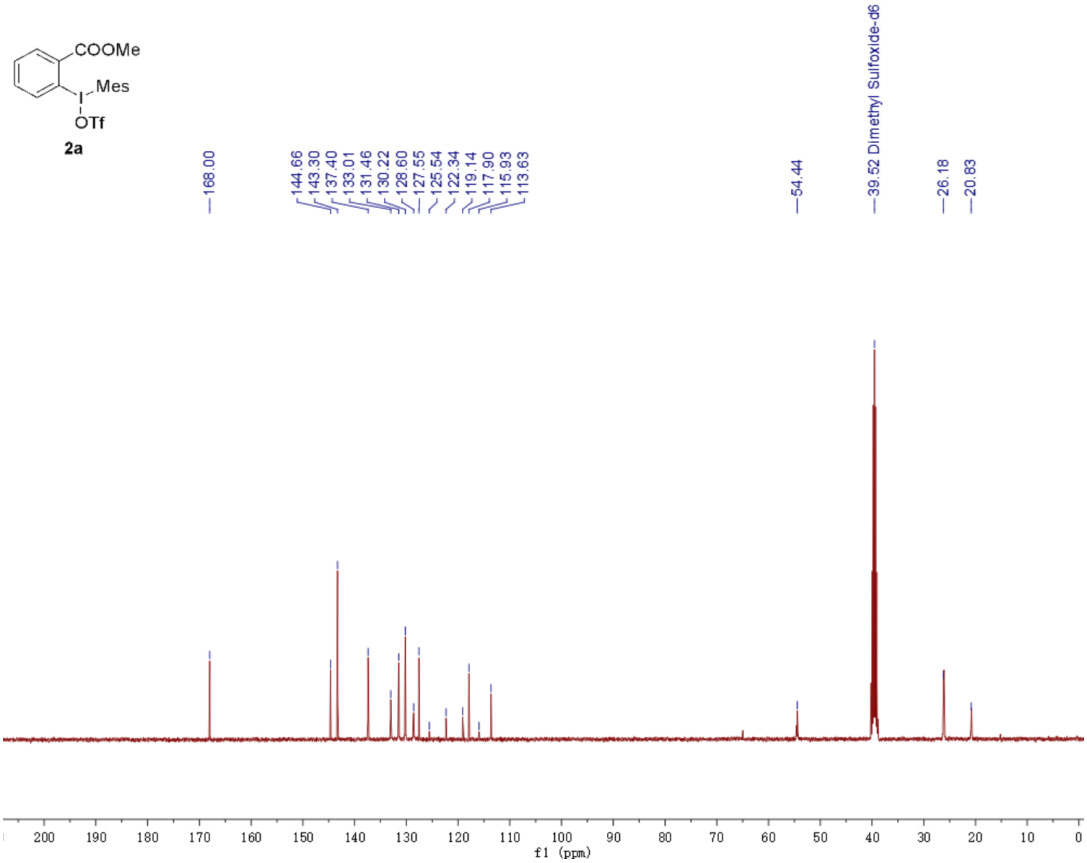
[1] Yang, J.; Xu, X.; Qing, F. *J. Fluorine Chem*. **2015**, 180,175-180.

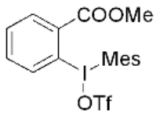
[2] Saravanan, P.; Anbarasan, P.; *Adv. Synth. Catal*. **2015**, *357*, 3521-3528.

[3] Beugelmans, R.; Bois-Choussy, M.; Chastanet, J.; *Heterocycl*. **1993**, *36*, 2723-2732.

Part 7. ^{1}H, ^{13}C, and ^{19}F NMR spectra of products



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Mes
I
OTf

2a

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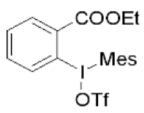
f1 (ppm)


COOEt
Mes
I
OTf

2b

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7.79
7.41
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6.88
6.87
6.86
4.53
4.51
2.51
2.50
Dimethyl Sulfoxide-d6
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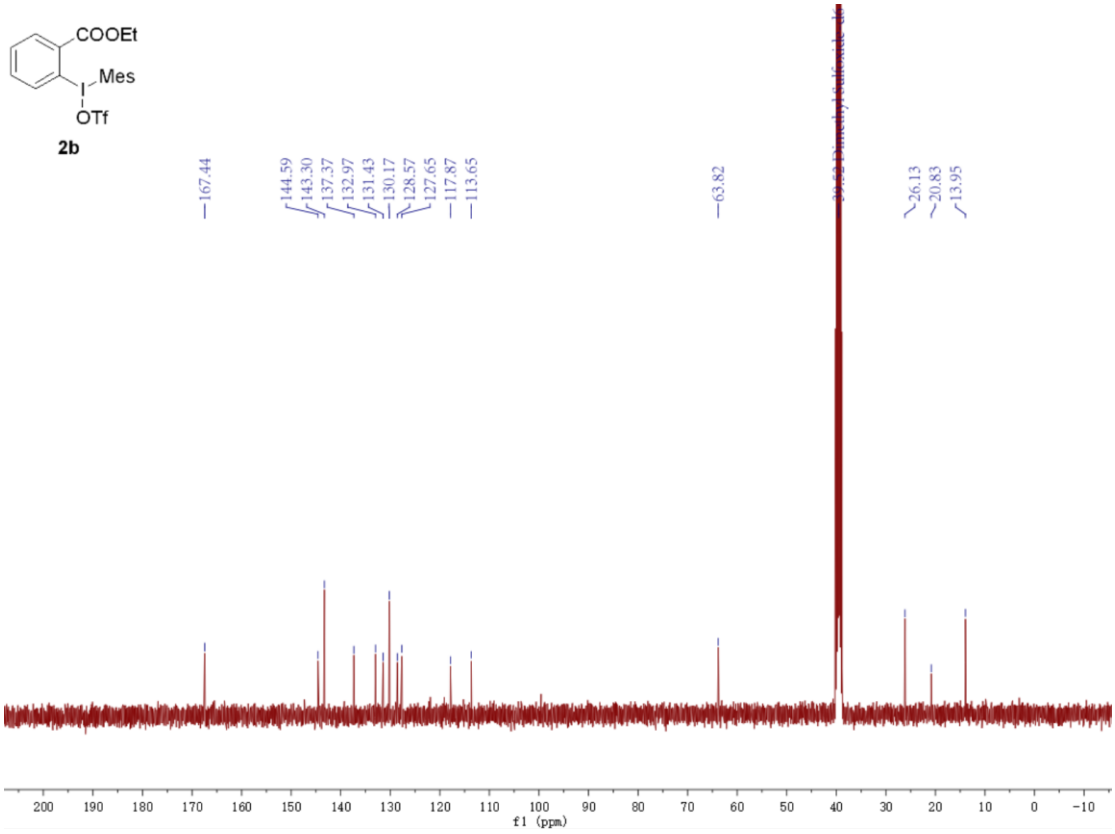
1.44
1.42
1.40
1.00
2.00
1.99
1.00
2.01
5.93
2.99
2.97
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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Mes
OTf
2b
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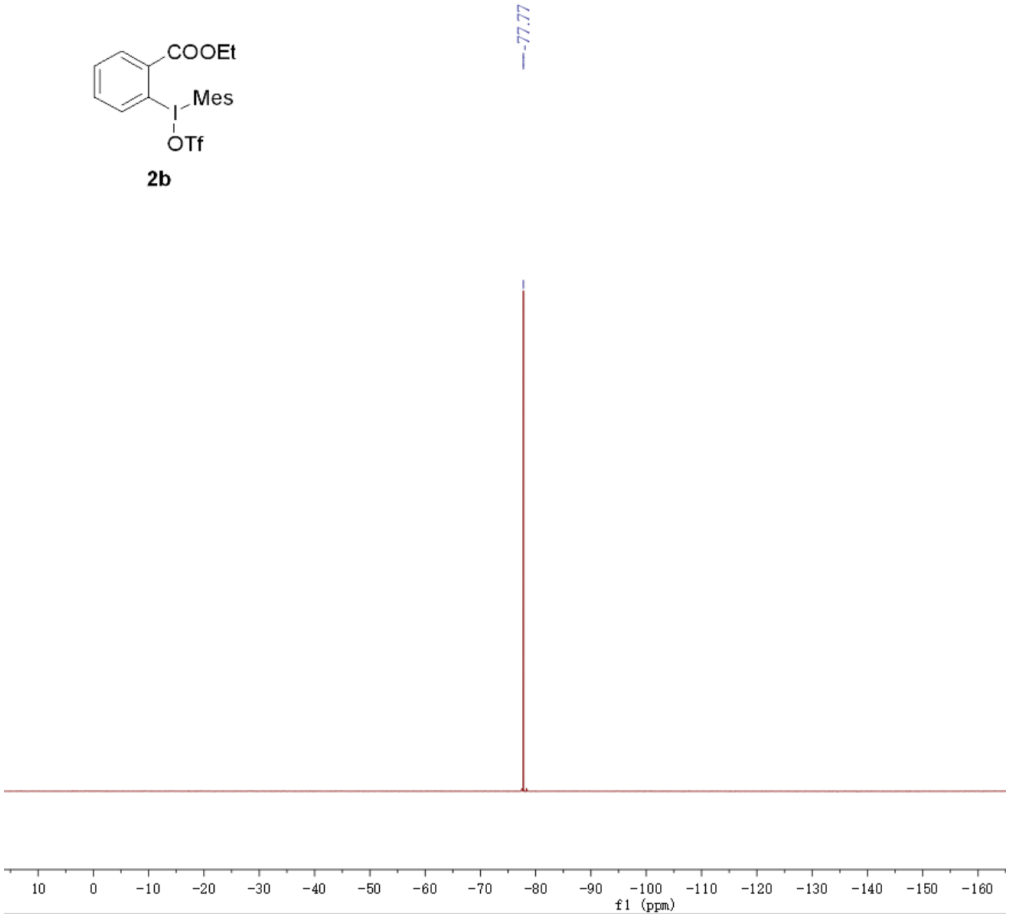
13.95
f1 (ppm)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Mes
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2b
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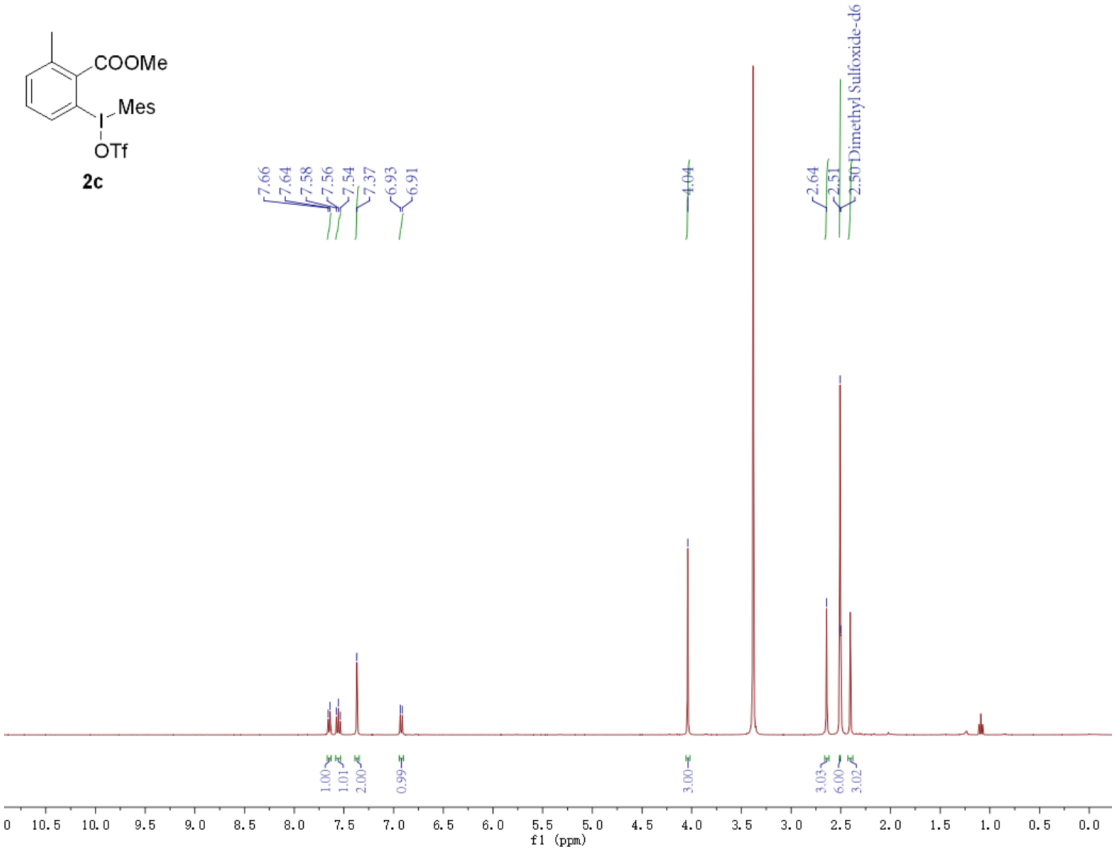
f1 (ppm)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Mes
OTf
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7.54
7.37
6.93
6.91
4.04
2.64
2.51
2.50 Dimethyl Sulfoxide-d6
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3.03
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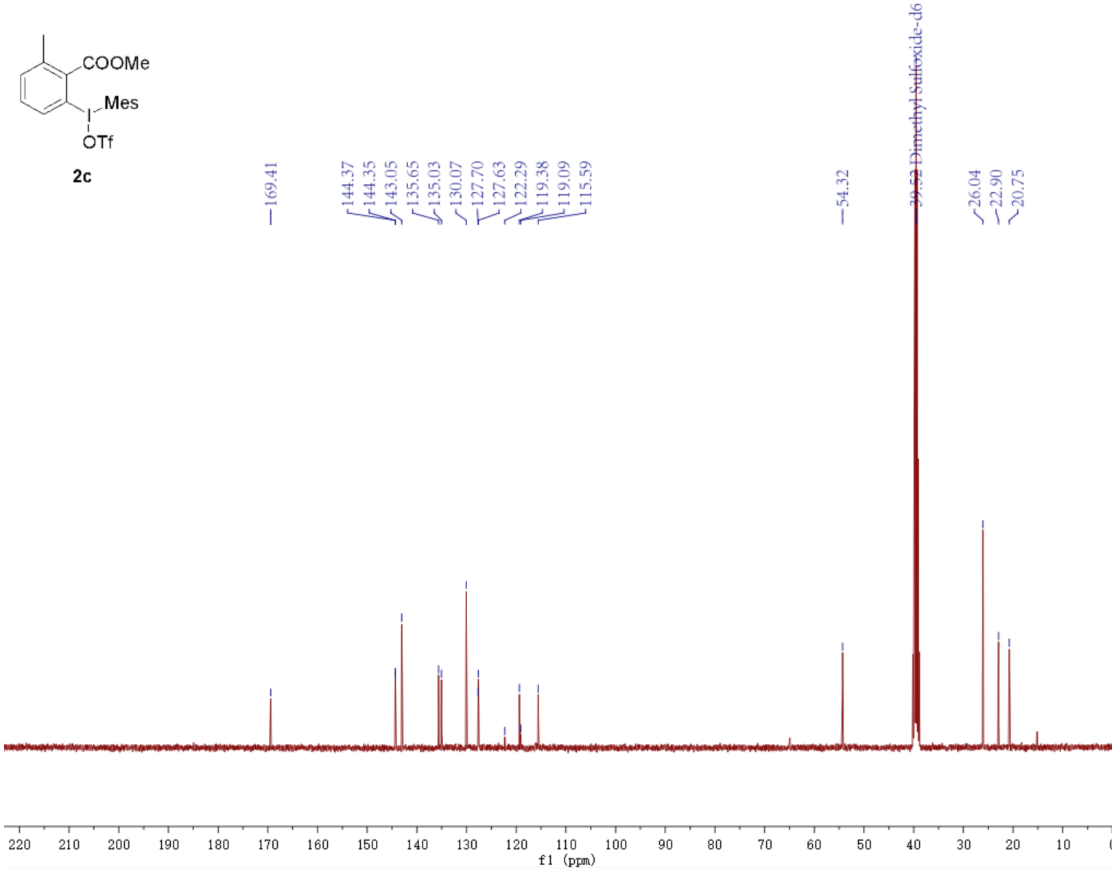
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39.52 Dimethyl Sulfoxide-d6
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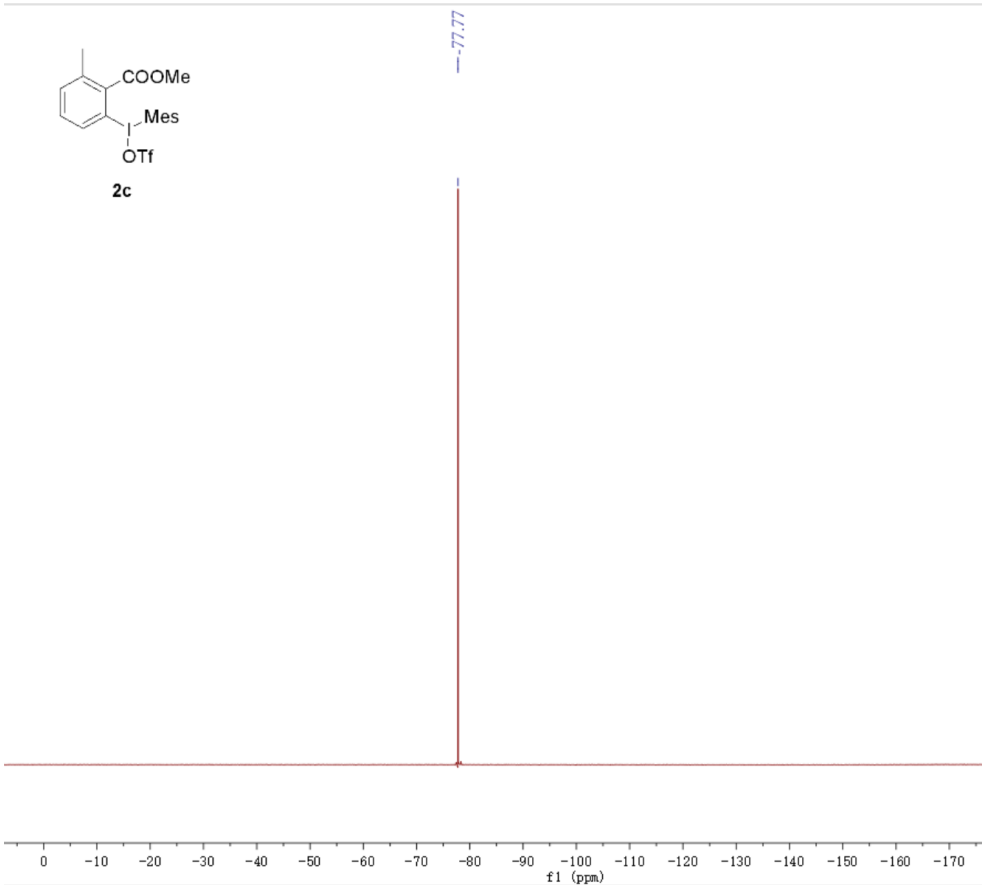
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2c
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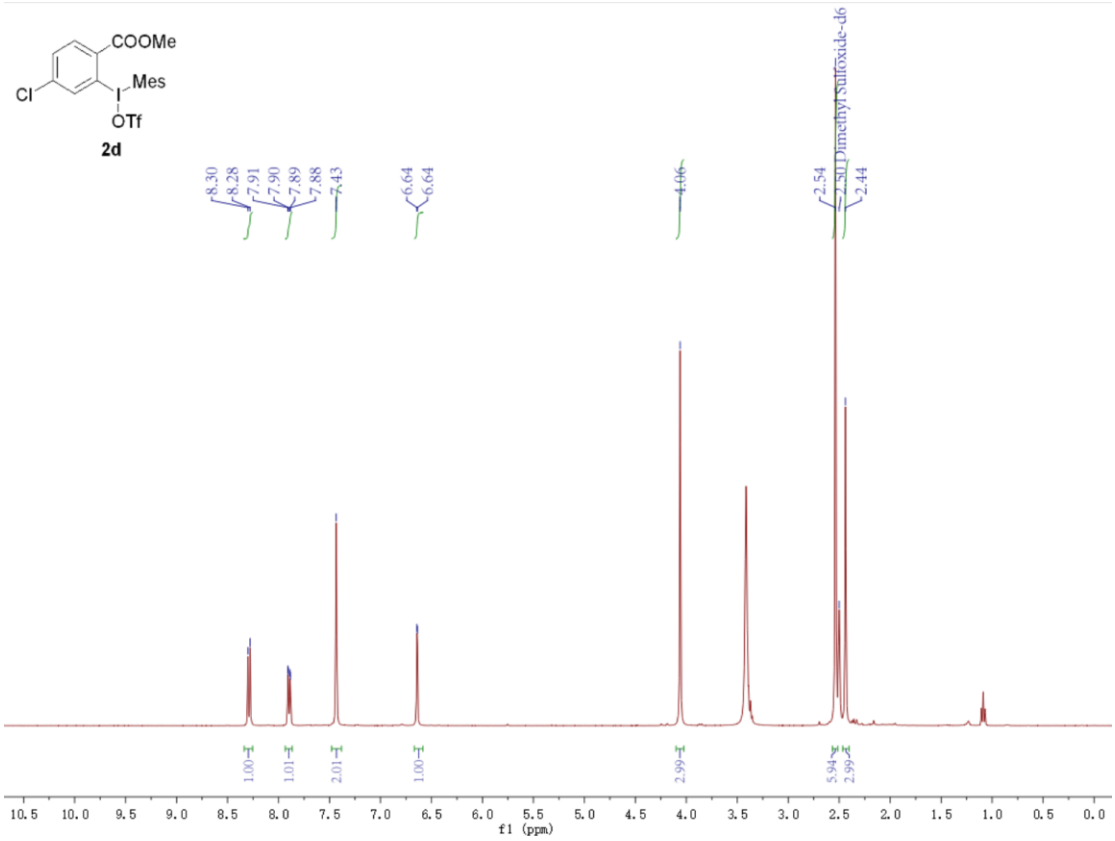
f1 (ppm)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OTf
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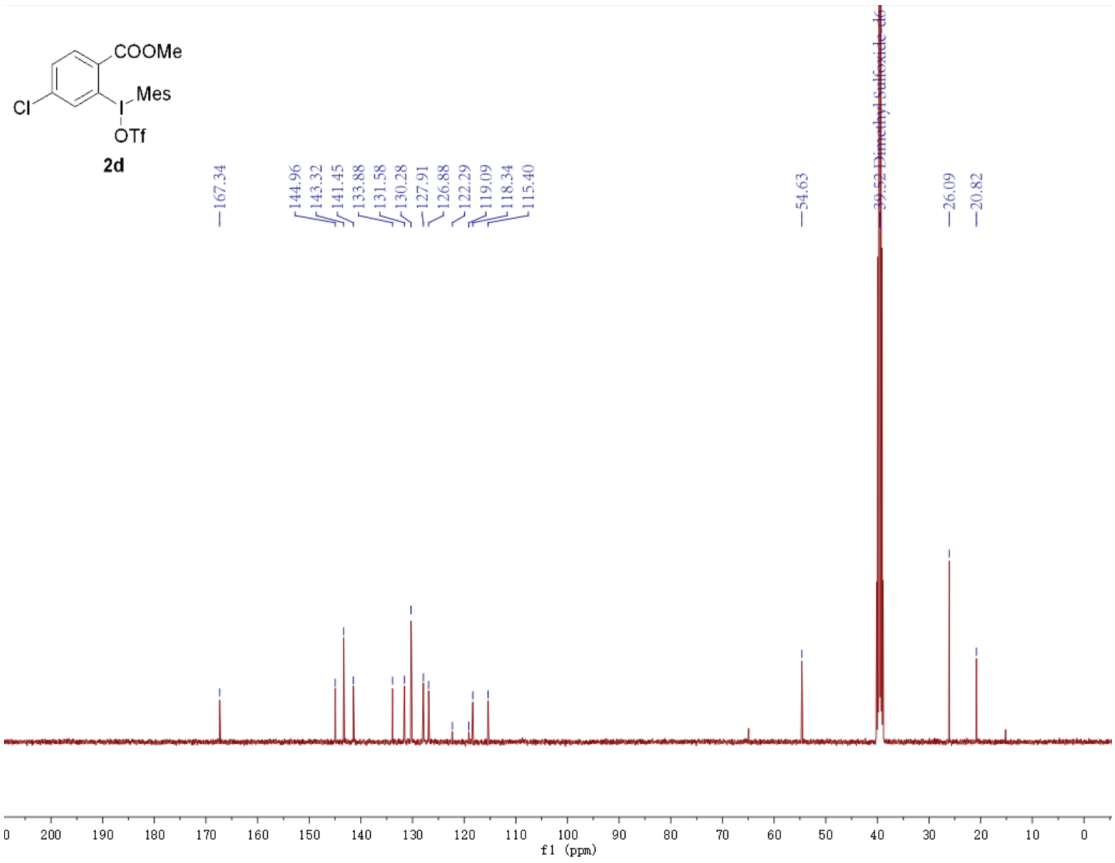
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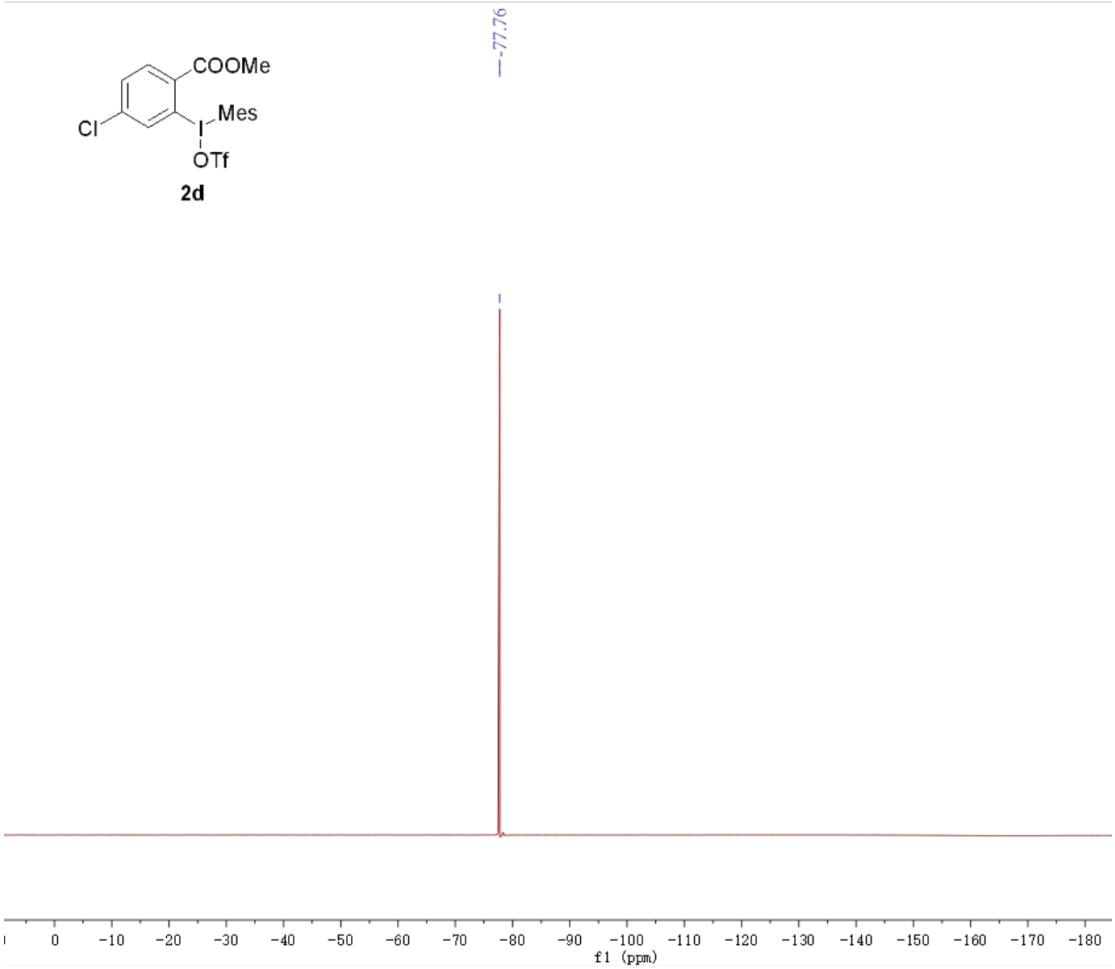
f1 (ppm)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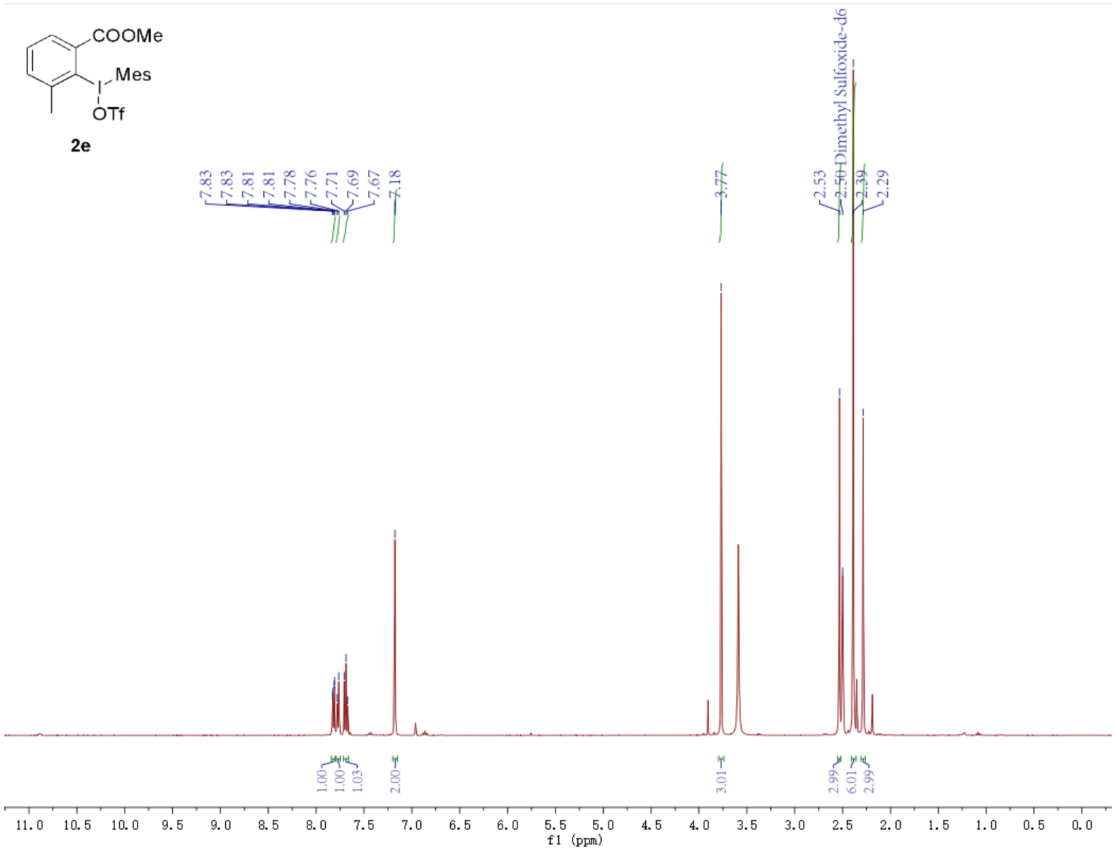
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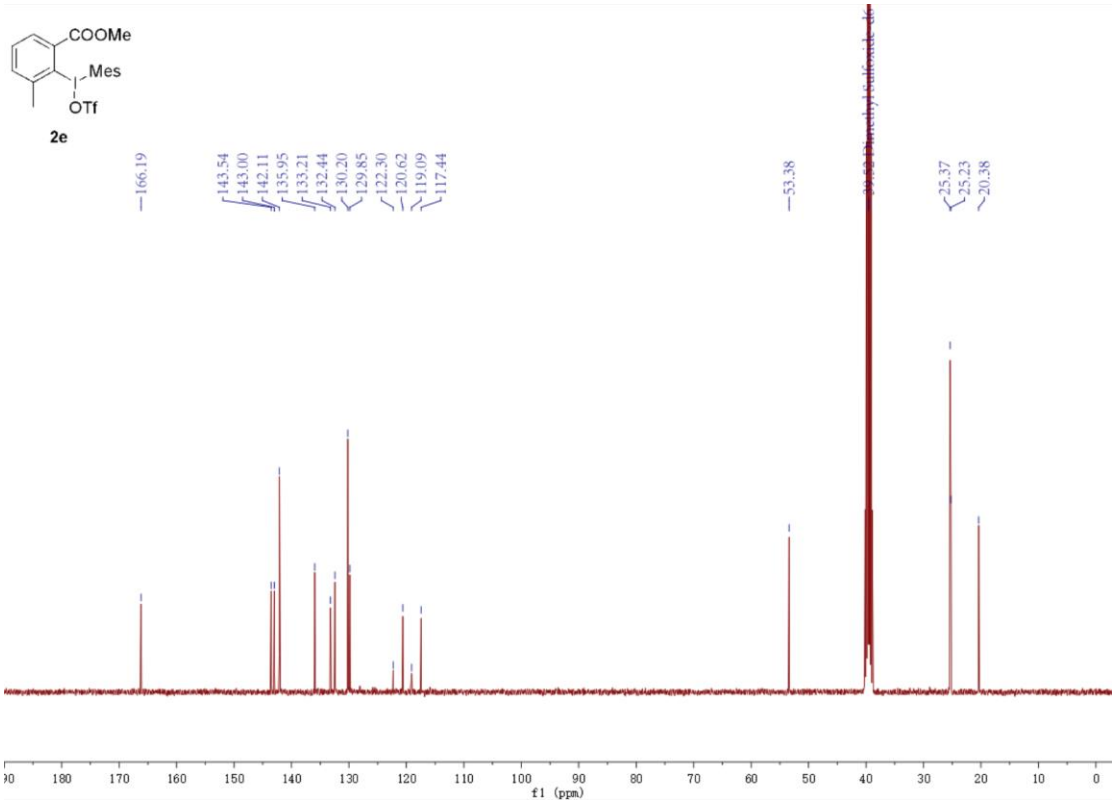
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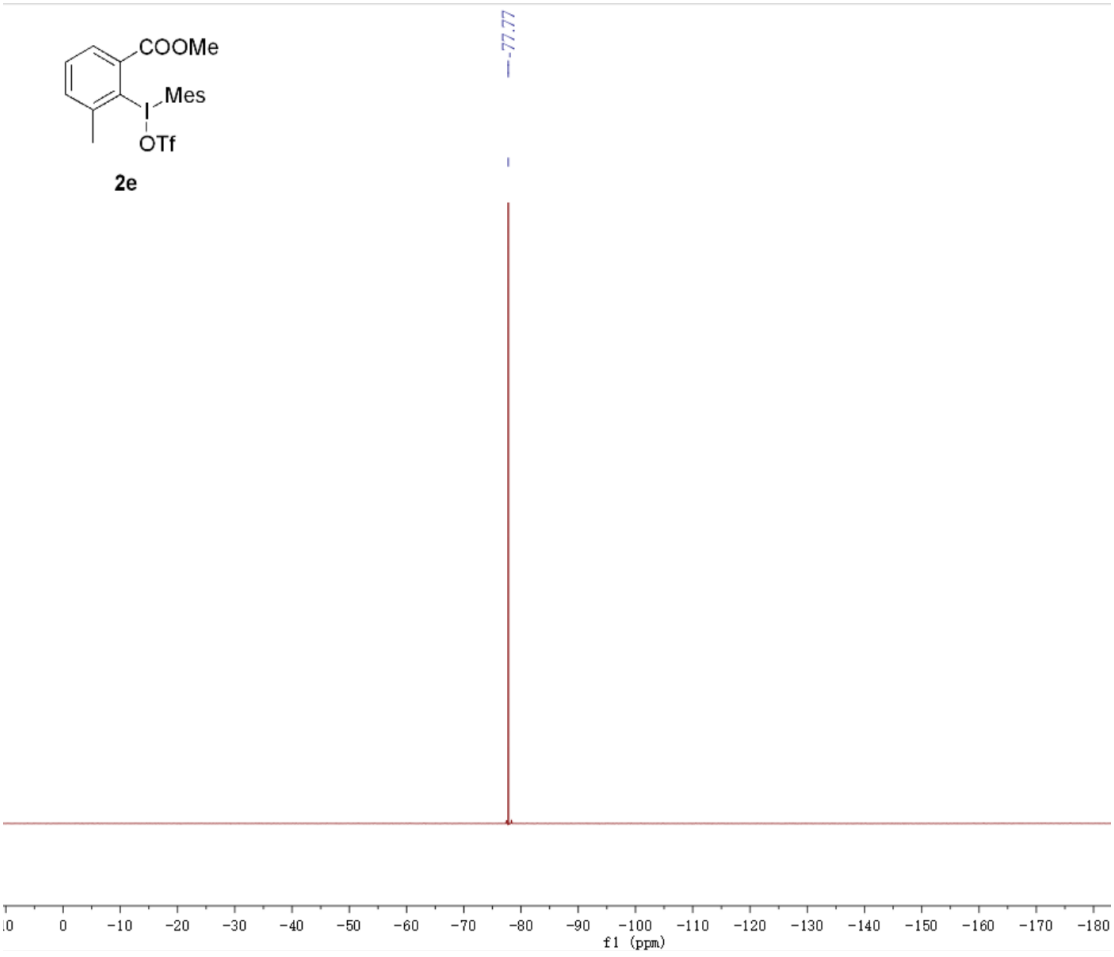
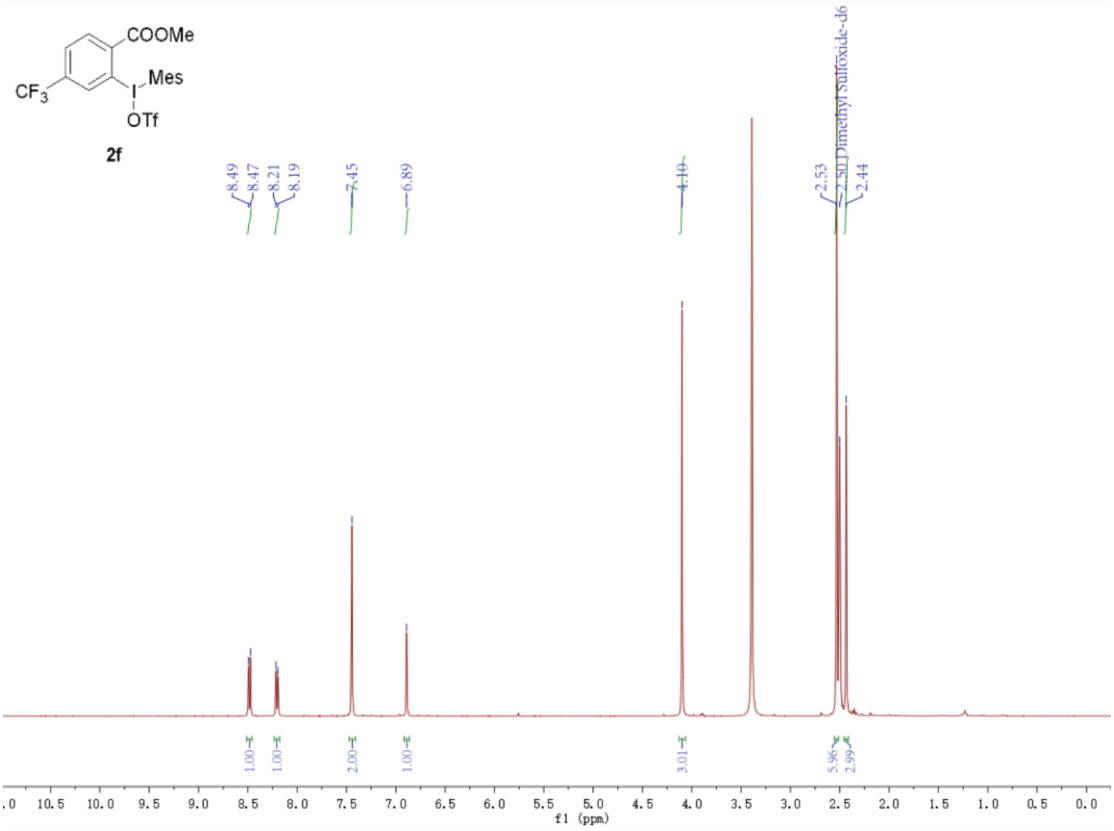
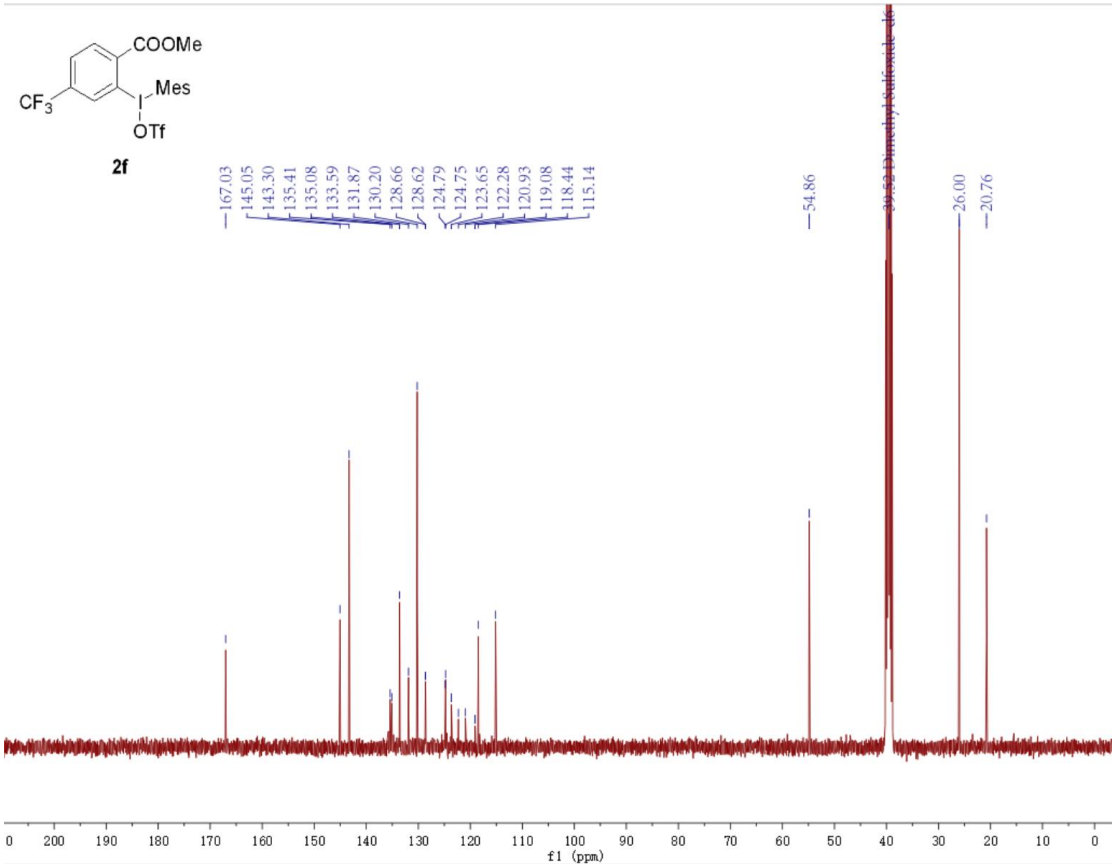
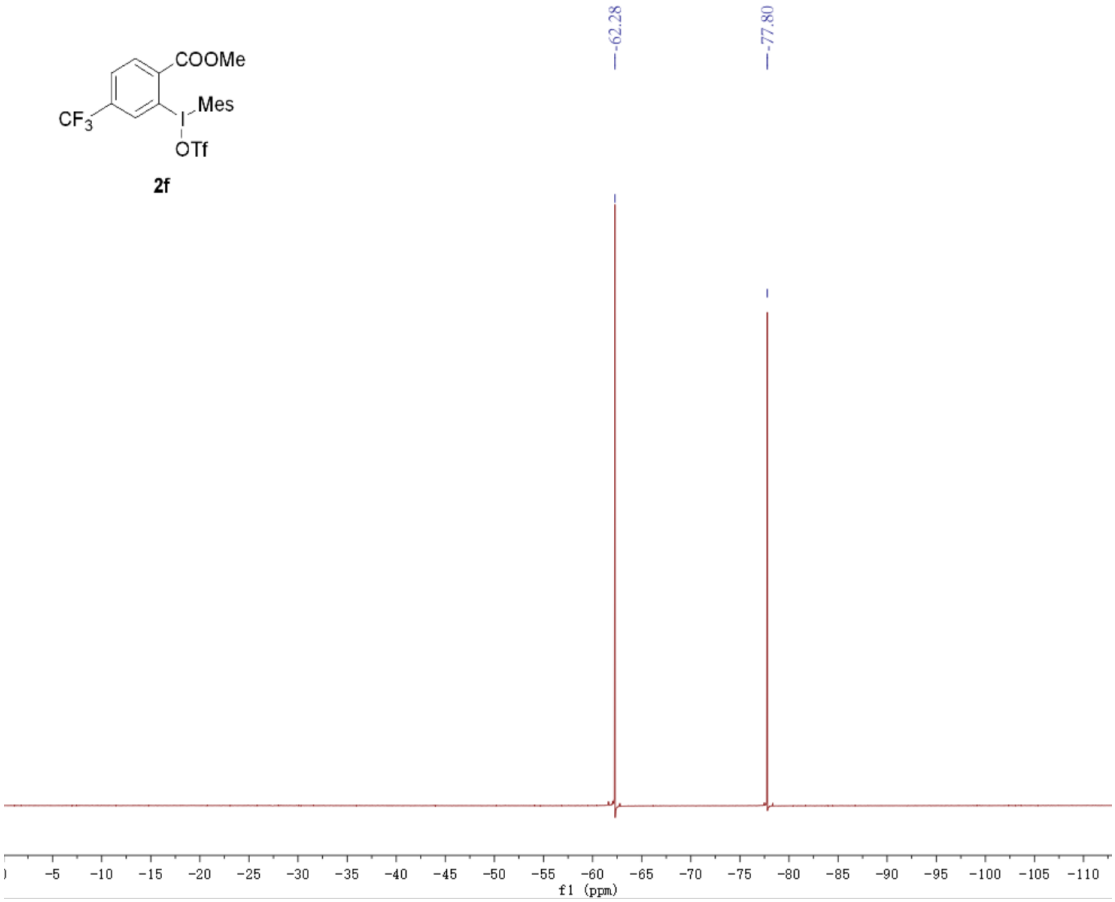
122.30
120.62
119.09
117.44
53.38
39.52 Dimethyl sulfoxide-d6
25.37
25.23
20.38
f1 (ppm)


COOMe
Mes
I
OTf
2e
-77.77
f1 (ppm)


COOMe
Mes
CF3
I
OTf
2f
8.49
8.47
8.21
8.19
7.45
6.89
4.10
2.53
2.50 Dimethyl Sulfoxide-d6
2.44
1.00
1.00
2.00
1.00
3.01
5.96
2.99
f1 (ppm)


COOMe
Mes
CF3
OTf
2f
167.03
145.05
143.30
135.41
135.08
133.59
131.87
130.20
128.66
128.62
124.79
124.75
123.65
122.28
120.93
119.08
118.44
115.14
54.86
39.52 Dimethyl sulfoxide-d6
26.00
20.76
f1 (ppm)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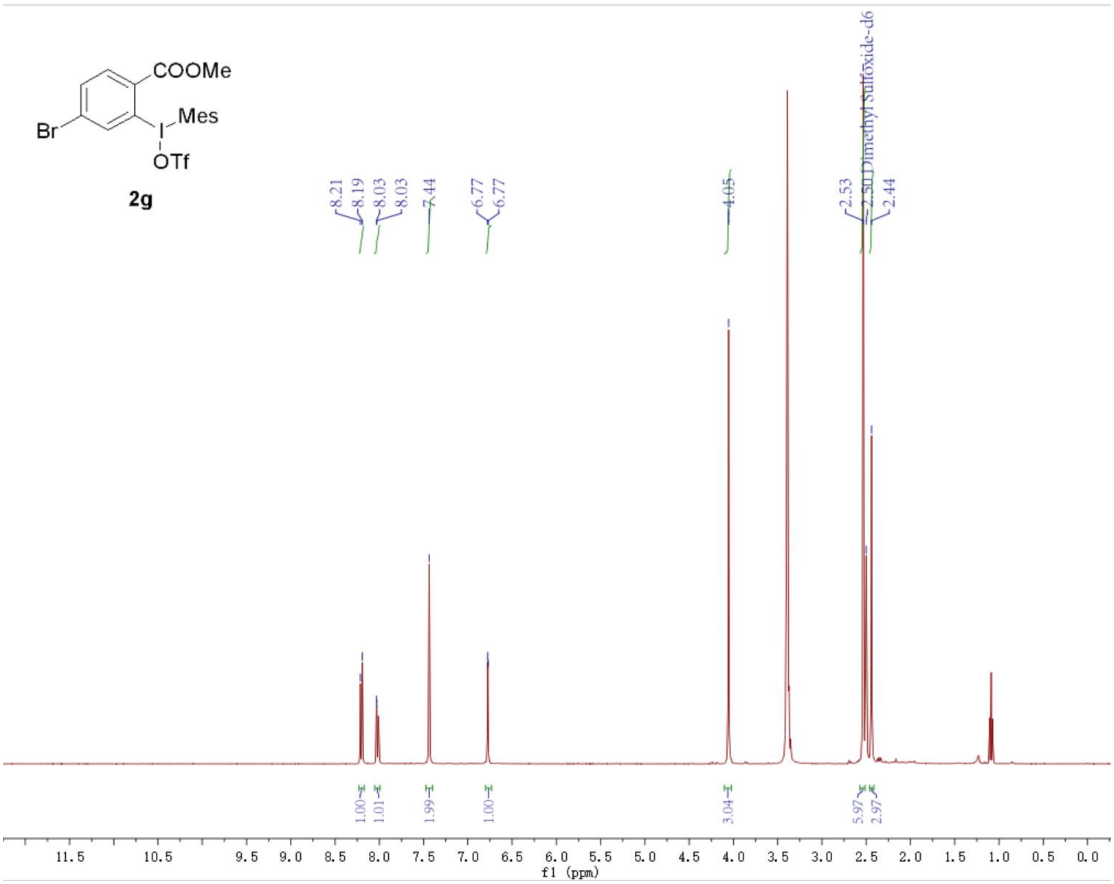
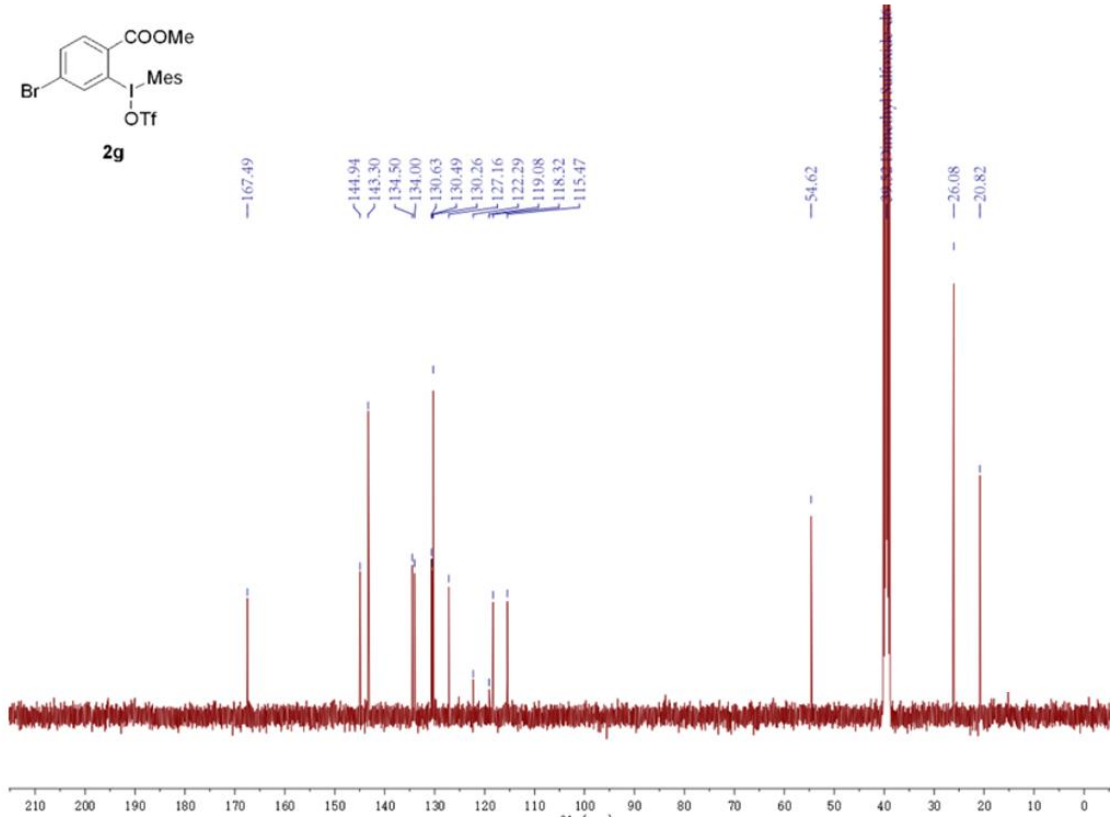
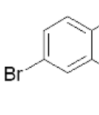
Mes
CF3
OTf
2f
-62.28
-77.80
f1 (ppm)


COOMe
Br
Mes
I
OTf
2g
8.21
8.19
8.03
8.03
7.44
6.77
6.77
4.05
2.53
2.50 Dimethyl Sulfoxide-d6
2.44
1.00
1.01
1.99
1.00
3.04
5.97
2.97
f1 (ppm)


COOMe
Br
Mes
I
OTf
2g
167.49
144.94
143.30
134.50
134.00
130.63
130.49
130.26
127.16
122.29
119.08
118.32
115.47
54.62
39.52 Dimethyl Sulfoxide-d6
26.08
20.82


COOMe
Br
Mes
I
OTf

2g

-77.76
0
-10
-20
-30
-40
-50
-60
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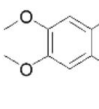
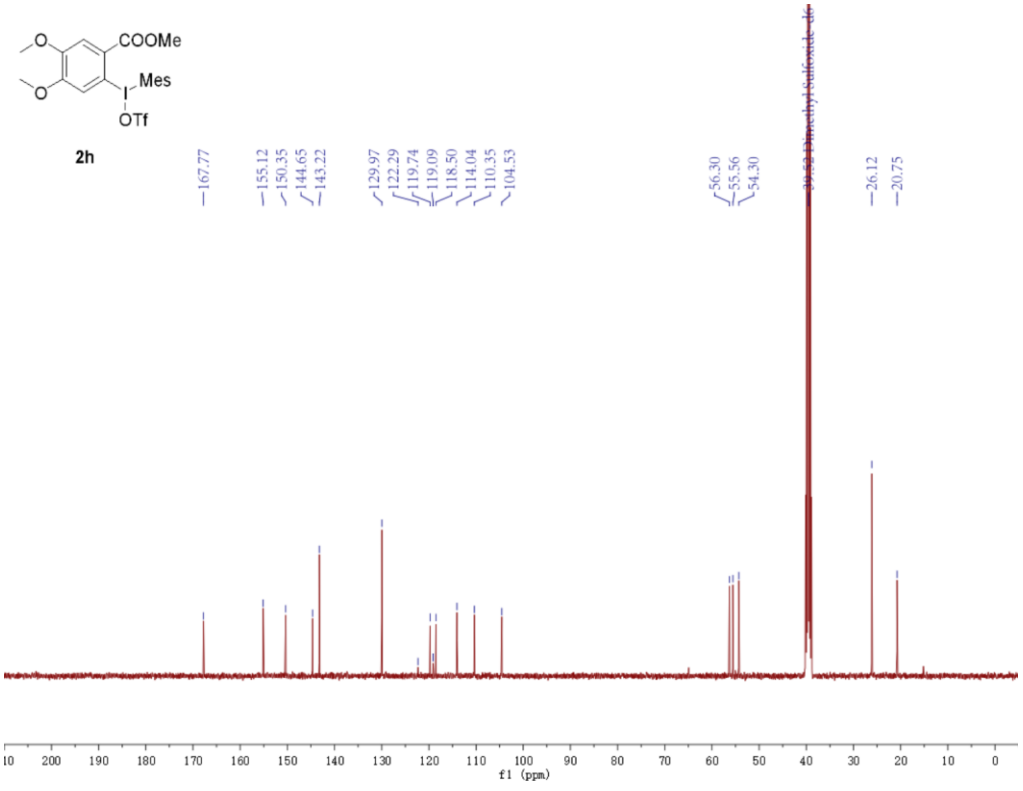
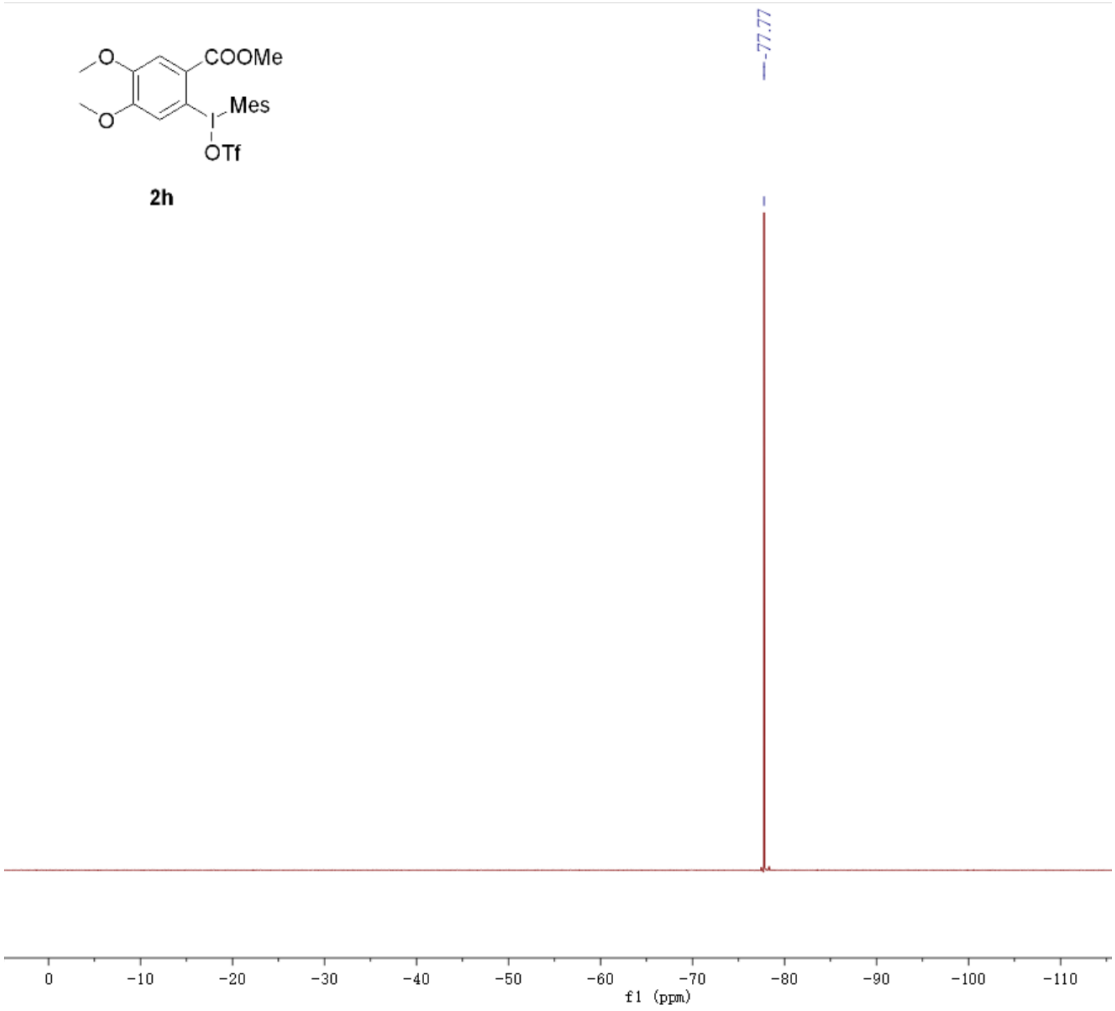
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
f1 (ppm)

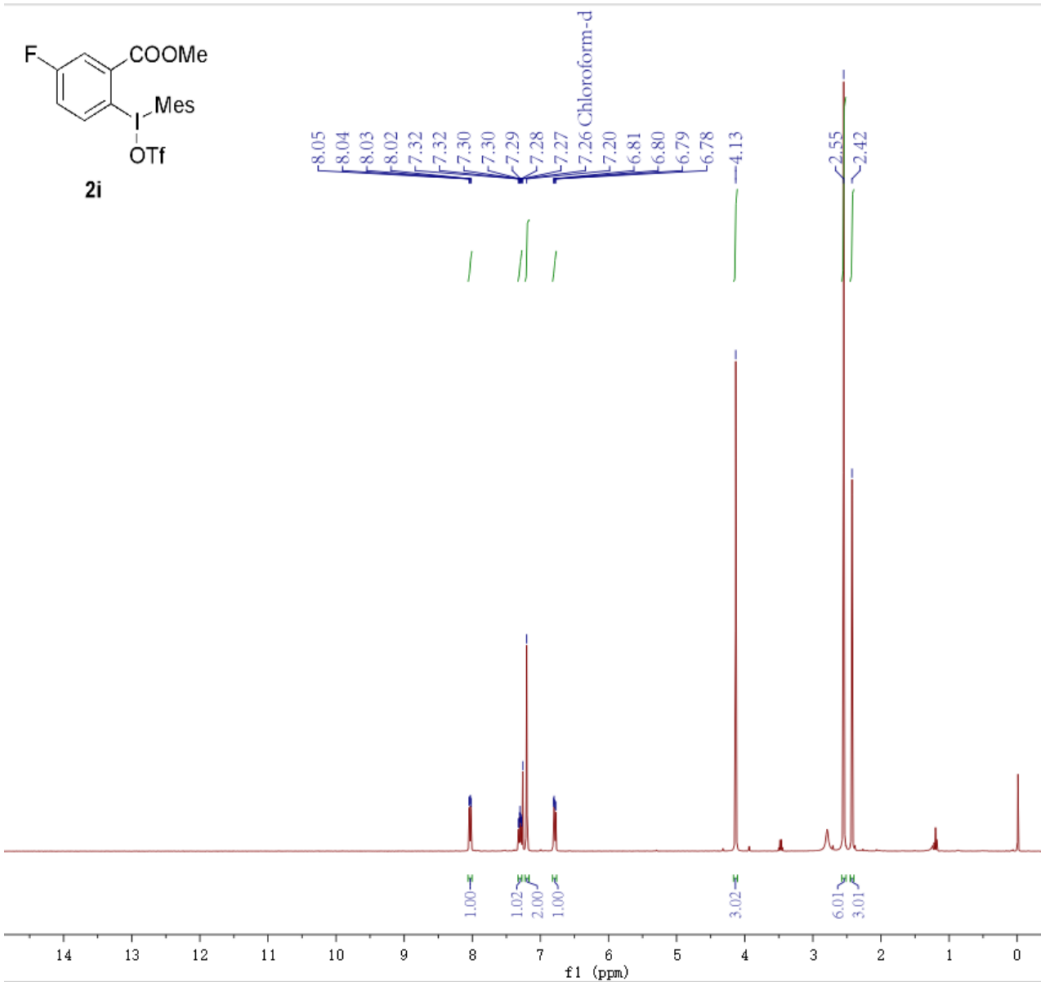

COOMe
O
O
Mes
I
OTf

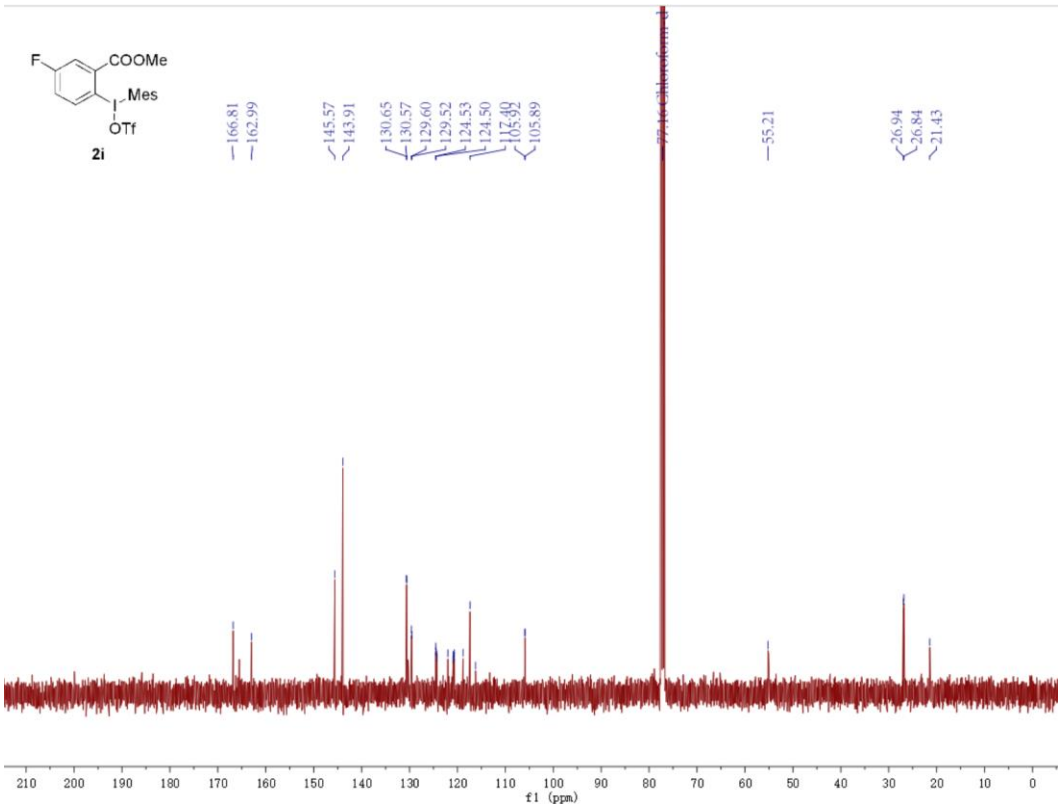
2h

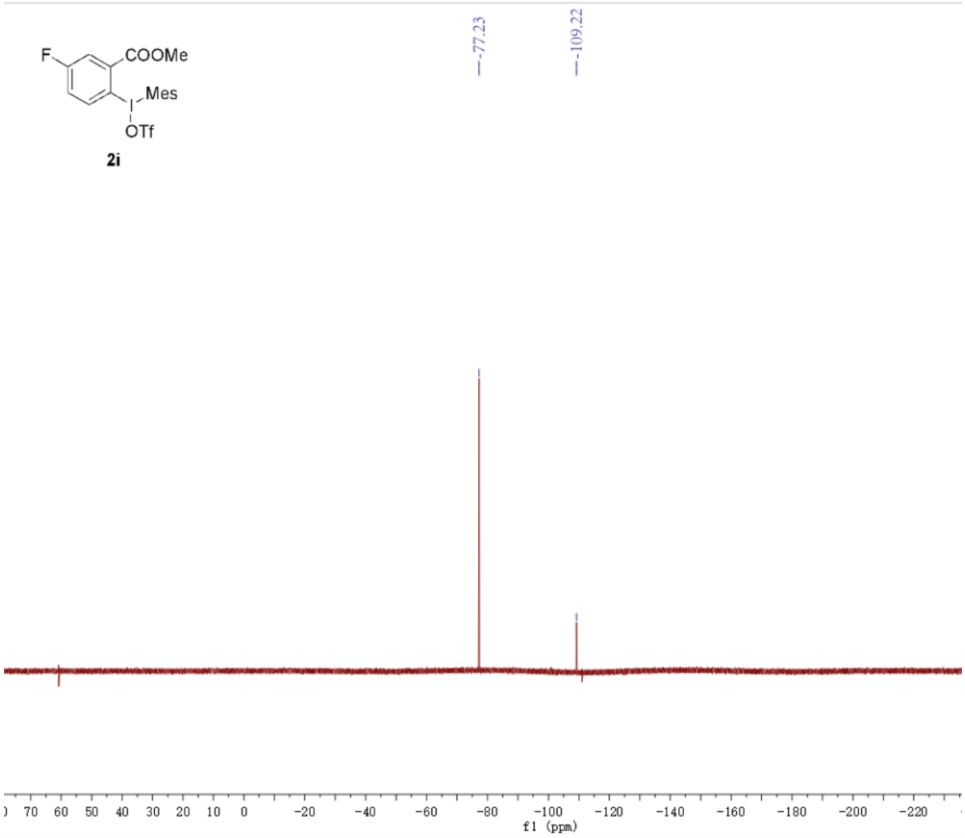
7.73
7.41
6.11
4.04
3.88
2.53
2.50 Dimethyl Sulfoxide-d6
2.41
1.00
1.99
0.98
3.02
3.01
5.92
2.94
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

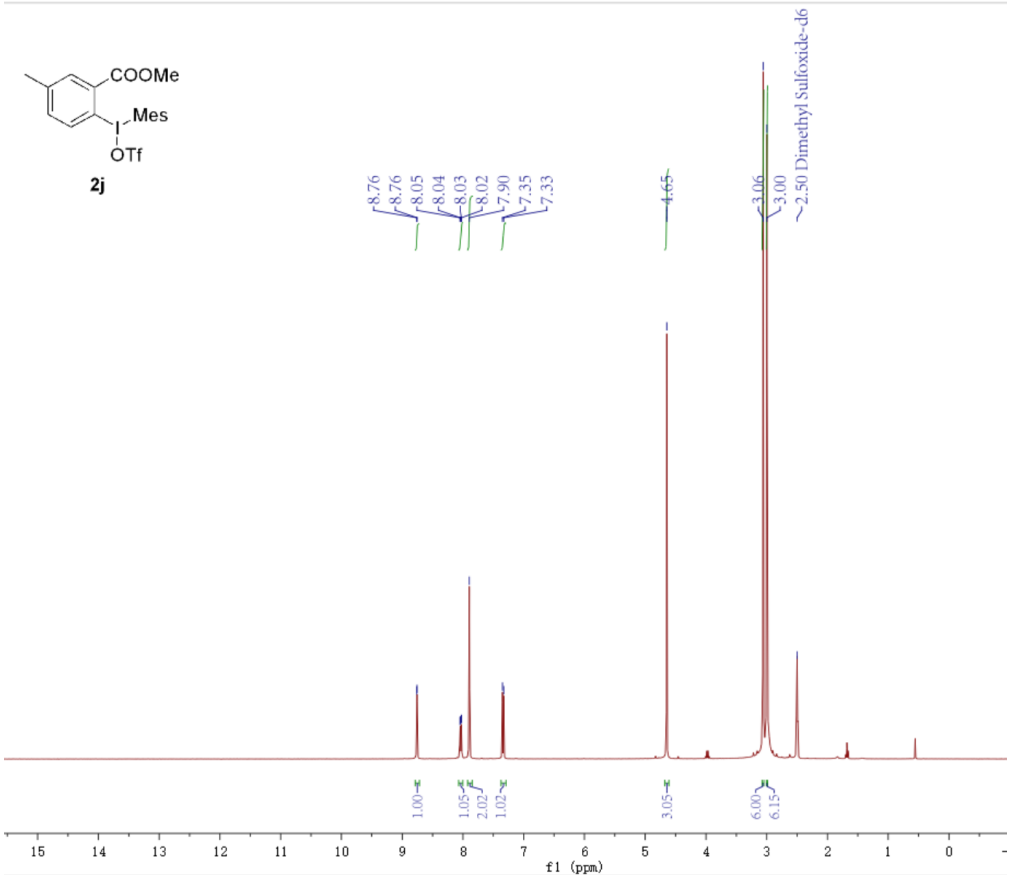

COOMe
Mes
OTf
2h
167.77
155.12
150.35
144.65
143.22
129.97
122.29
119.74
119.09
118.50
114.04
110.35
104.53
56.30
55.56
54.30
39.62 Dimethyl sulfoxide-d6
26.12
20.75
f1 (ppm)

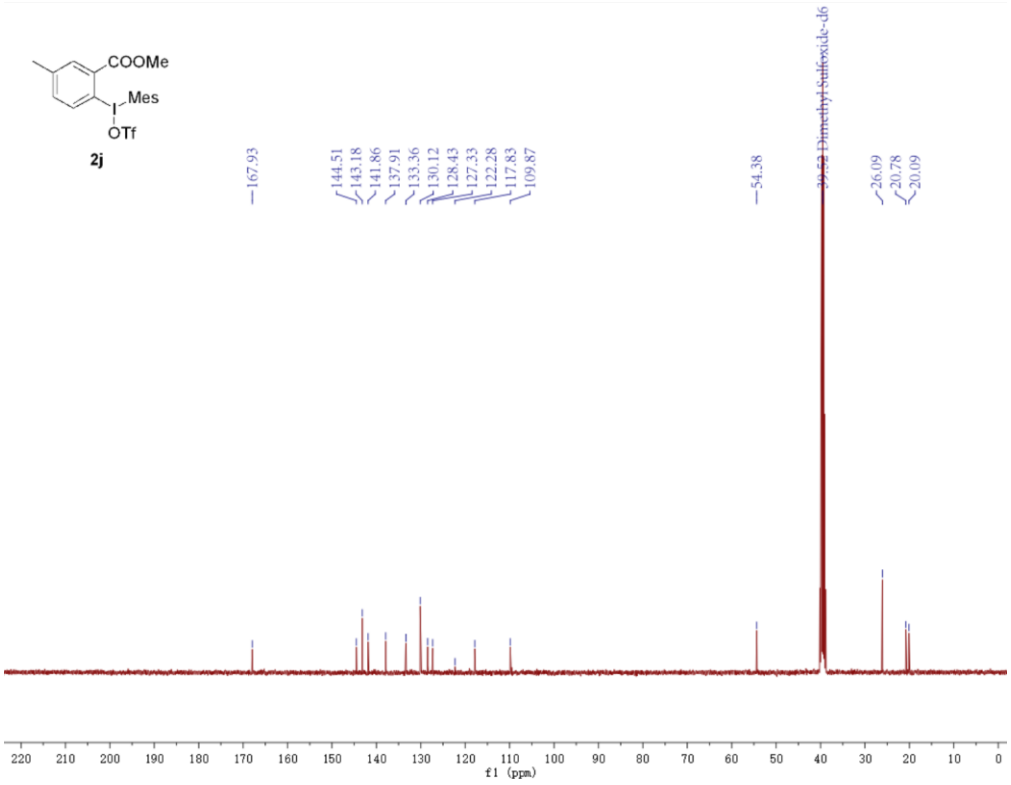

COOMe
Mes
OTf
2h
-77.77
f1 (ppm)

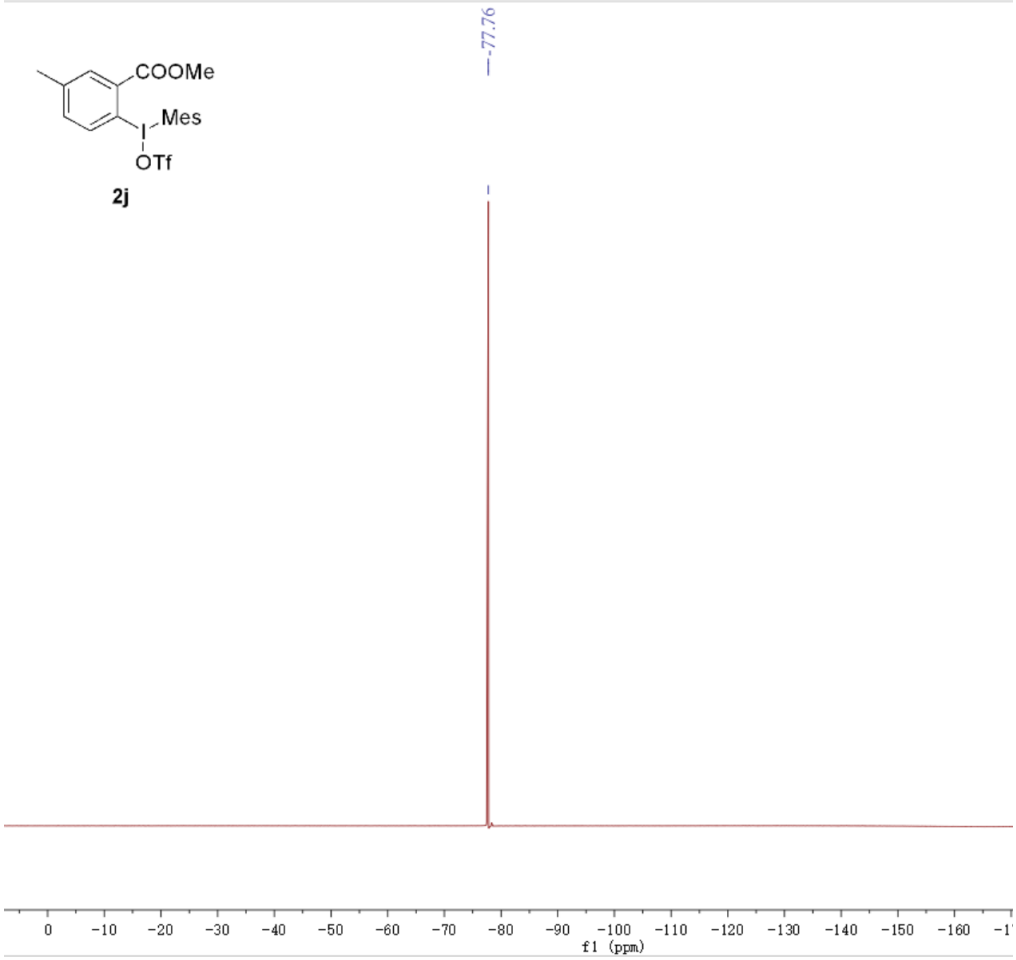

F
COOMe
Mes
I
OTf
2i
8.05
8.04
8.03
8.02
7.32
7.32
7.30
7.30
7.29
7.28
7.27
7.26 Chloroform-d
7.20
6.81
6.80
6.79
6.78
4.13
2.55
2.42
1.00
1.02
2.00
1.00
3.02
6.01
3.01
f1 (ppm)

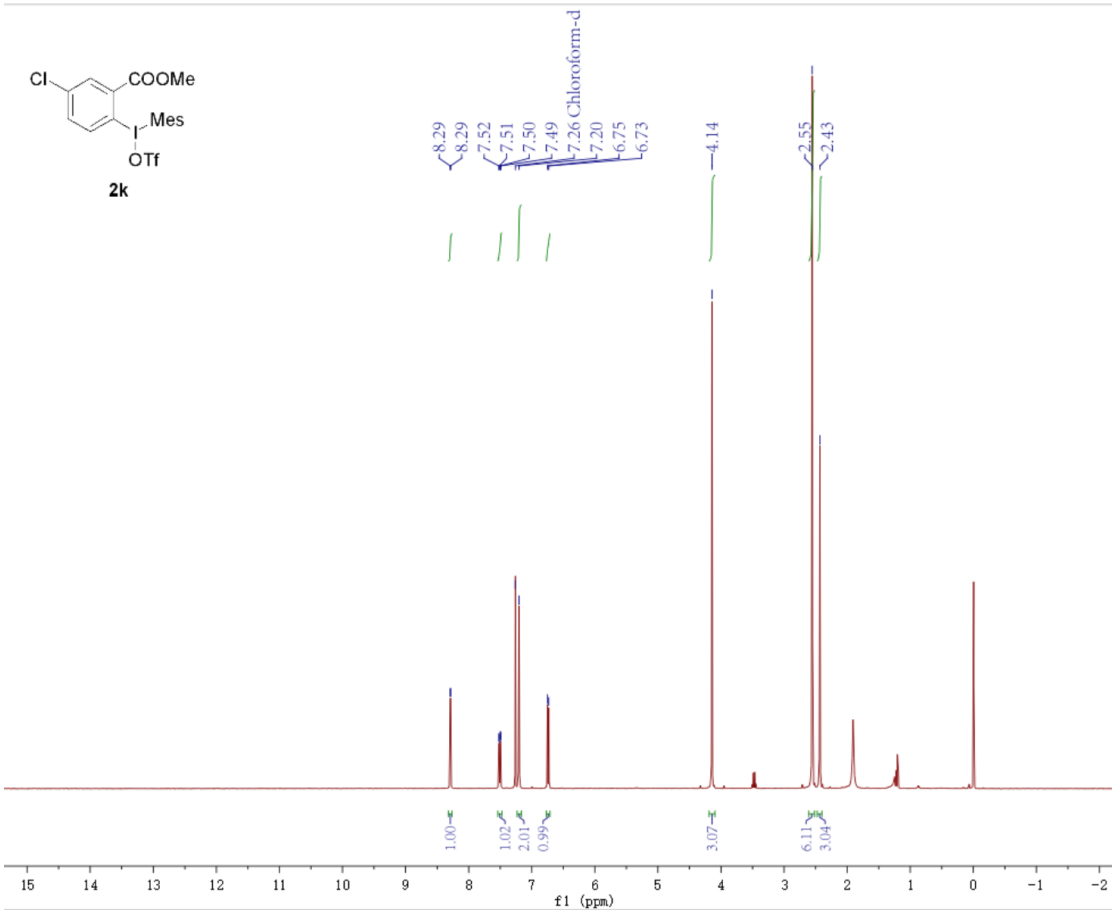

F
COOMe
Mes
I
OTf
2i
166.81
162.99
145.57
143.91
130.65
130.57
129.60
129.52
124.53
124.50
117.40
105.92
105.89
77.16 Chloroform-d
55.21
26.94
26.84
21.43
f1 (ppm)

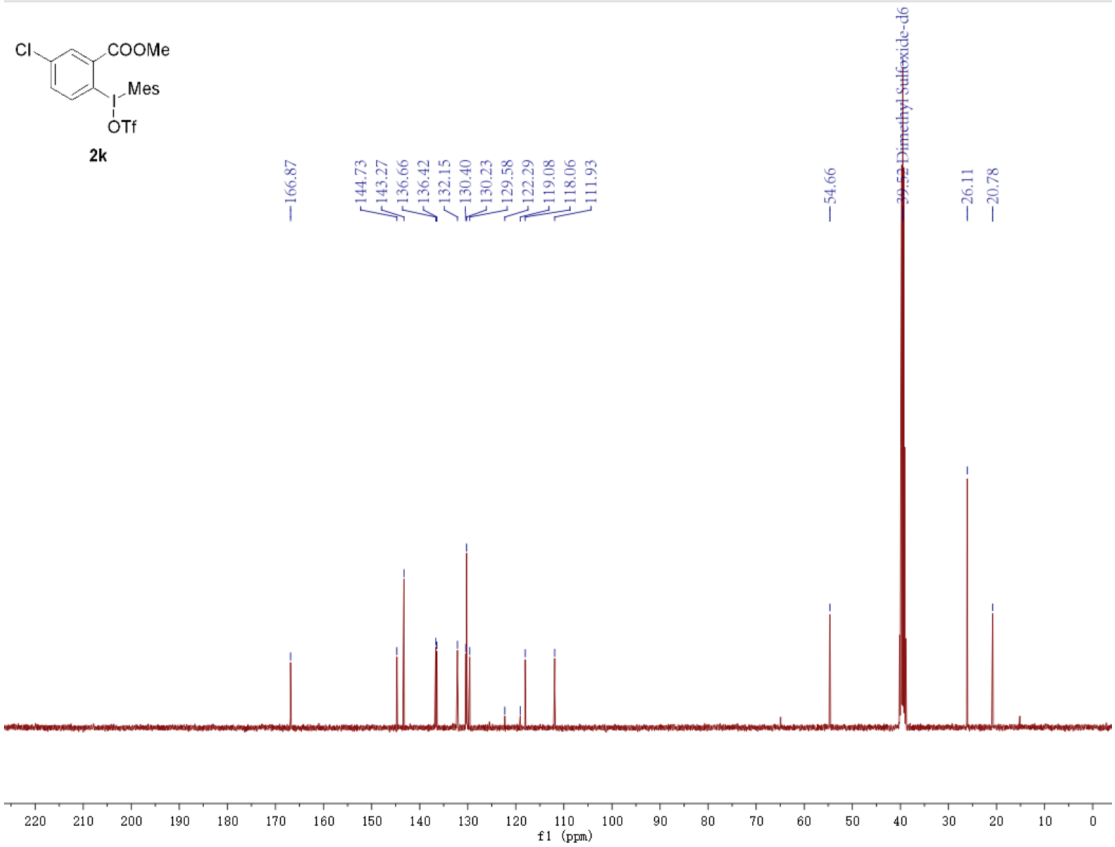

F
COOMe
Mes
I
OTf
2i
-77.23
-109.22
70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220
f1 (ppm)

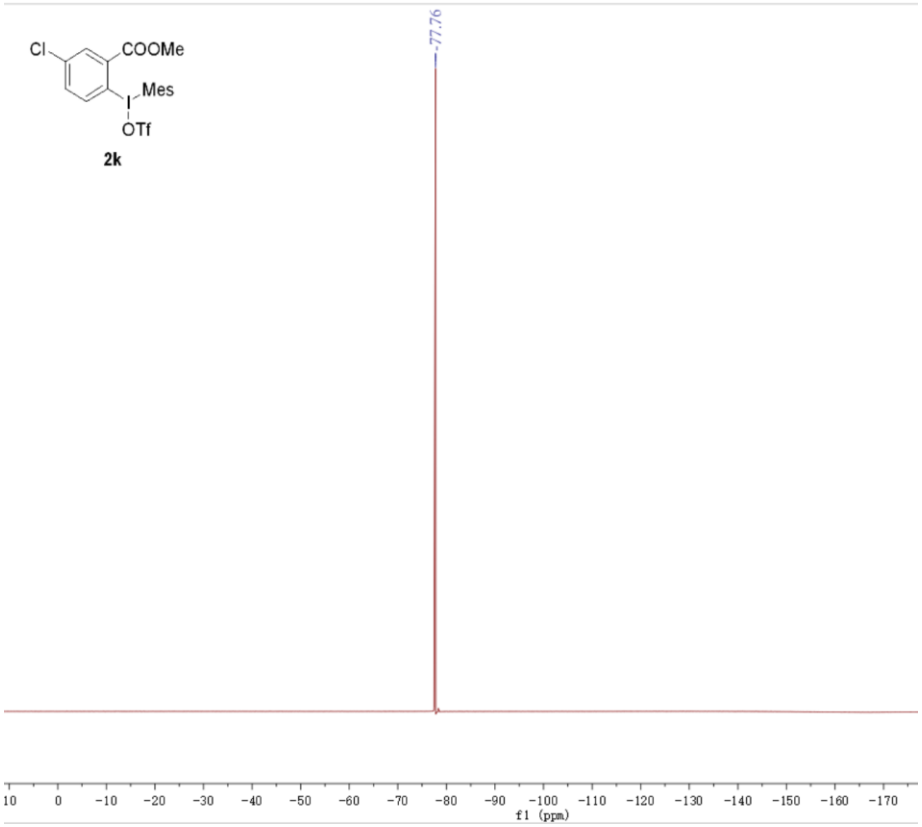

COOMe
Mes
I
OTf
2j
8.76
8.76
8.05
8.04
8.03
8.02
7.90
7.35
7.33
4.65
3.06
3.00
2.50 Dimethyl Sulfoxide-d6
1.00
1.05
2.02
1.02
3.05
6.00
6.15
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


COOMe
Mes
OTf
2j
167.93
144.51
143.18
141.86
137.91
133.36
130.12
128.43
127.33
122.28
117.83
109.87
54.38
39.52 Dimethyl sulfoxide-d6
26.09
20.78
20.09
f1 (ppm)

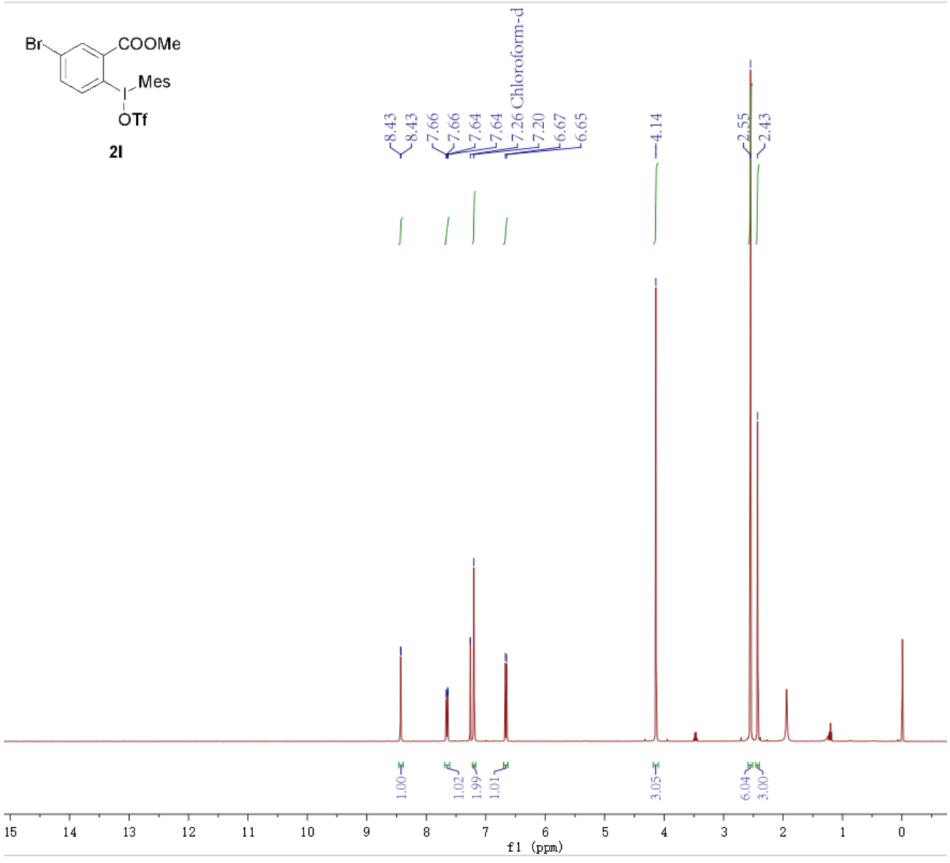

COOMe
Mes
OTf
2j
-77.76
f1 (ppm)


Cl
COOMe
Mes
I
OTf
2k
8.29
8.29
7.52
7.51
7.50
7.49
7.26 Chloroform-d
7.20
6.75
6.73
4.14
2.55
2.43
1.00
1.02
2.01
0.99
3.07
6.11
3.04
f1 (ppm)

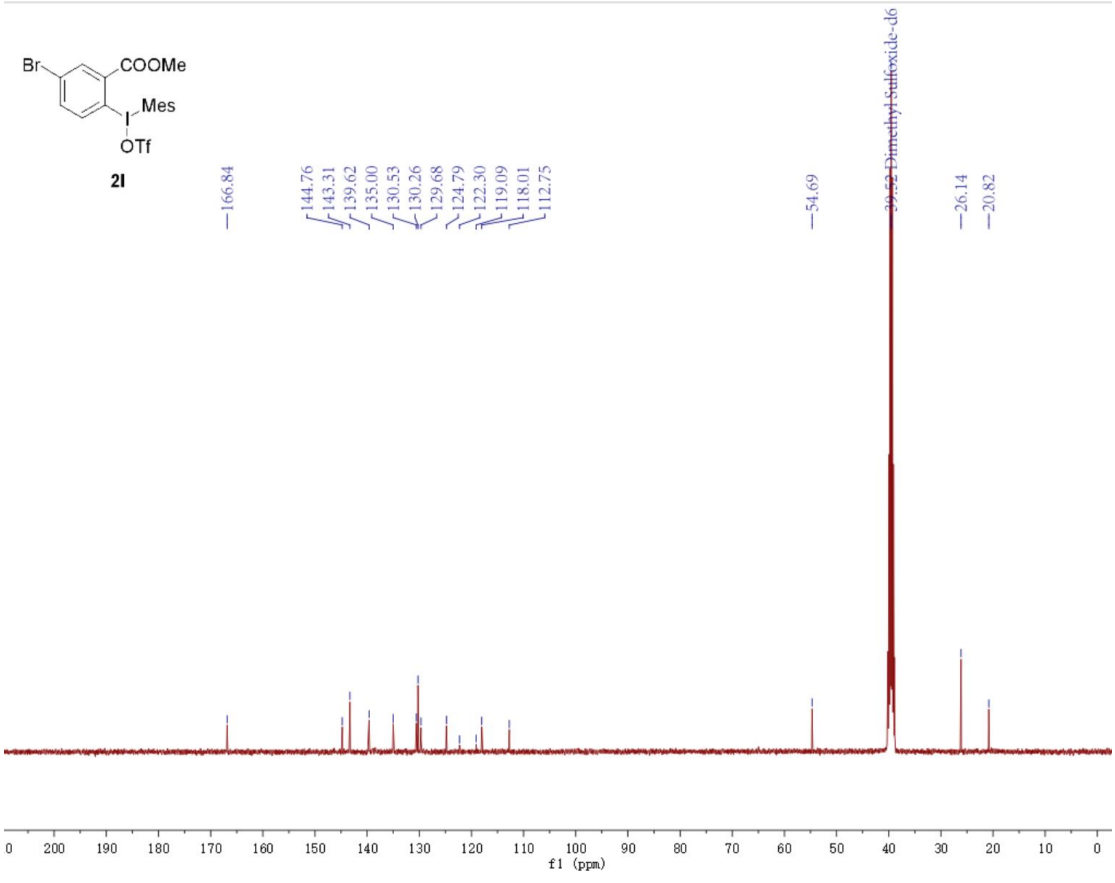

Cl
COOMe
Mes
I
OTf
2k
166.87
144.73
143.27
136.66
136.42
132.15
130.40
130.23
129.58
122.29
119.08
118.06
111.93
54.66
39.52 Dimethyl Sulfoxide-d6
26.11
20.78
f1 (ppm)

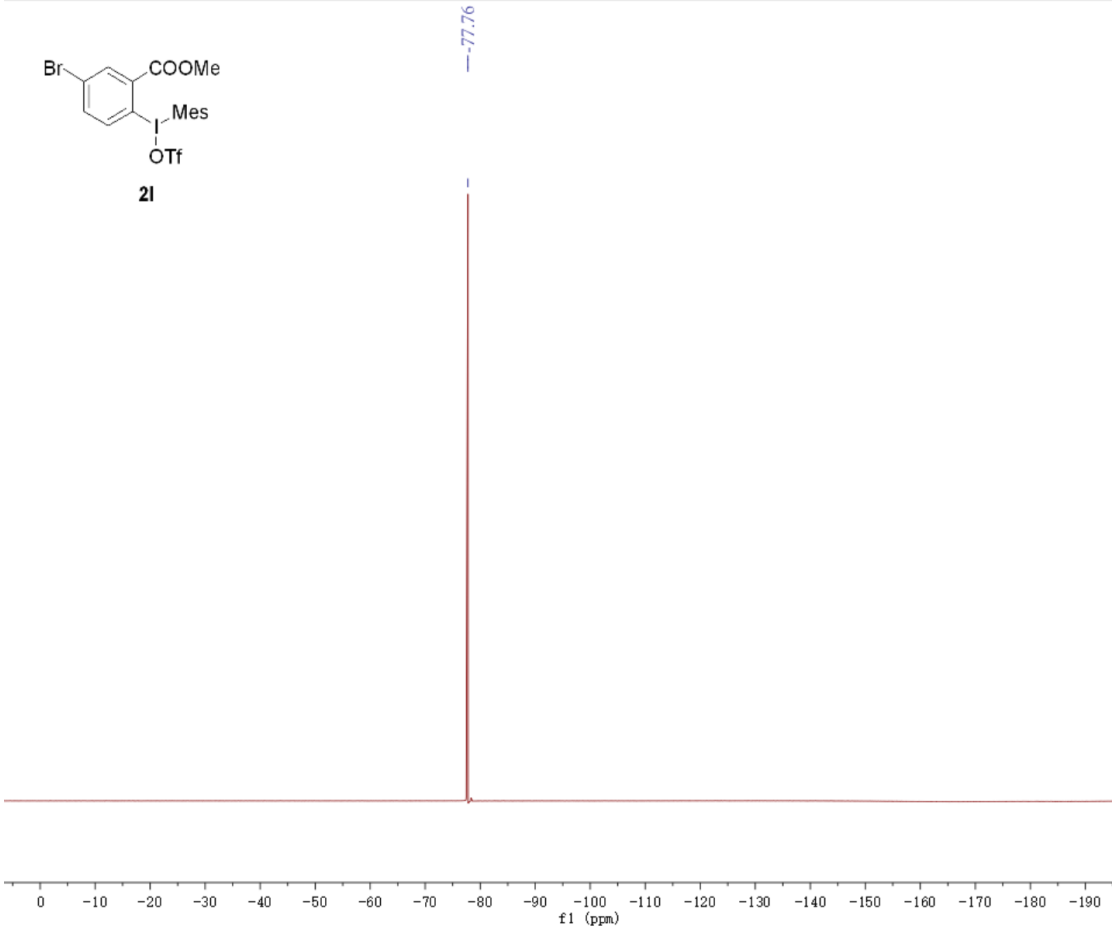

Cl
COOMe
Mes
I
OTf
-77.76
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170
f1 (ppm)

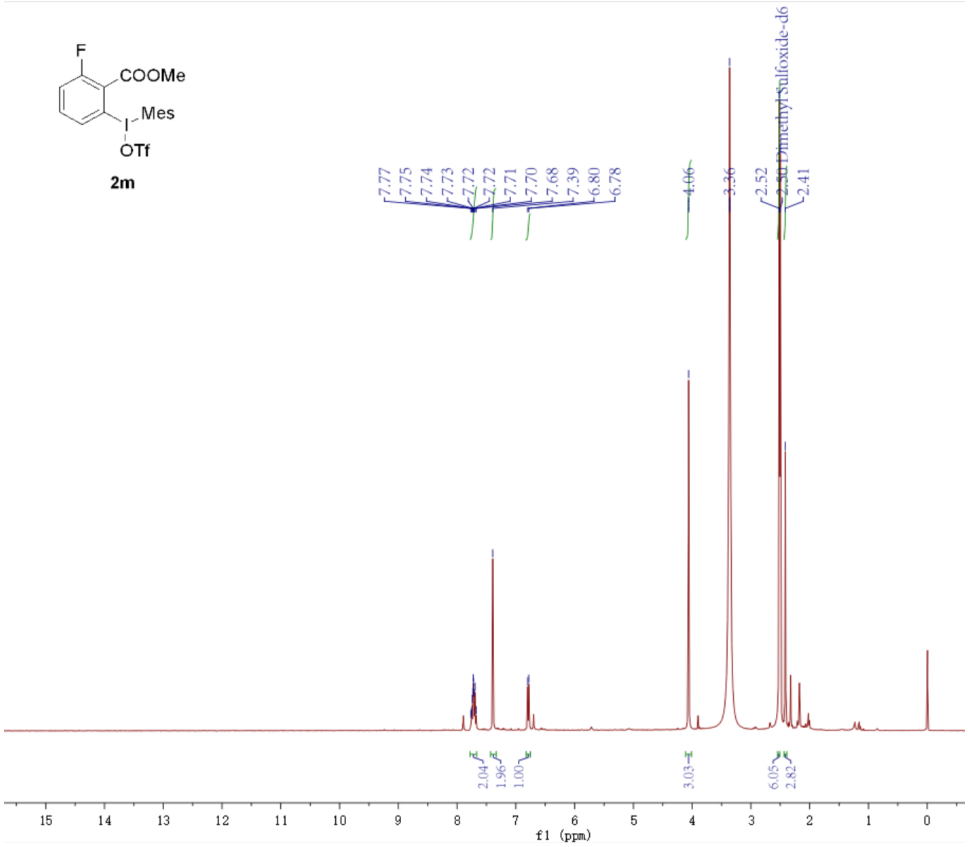
2k


Br
COOMe
Mes
I
OTf
8.43
8.43
7.66
7.66
7.64
7.64
7.26 Chloroform-d
7.20
6.67
6.65
4.14
2.55
2.43
1.00
1.02
1.99
1.01
3.05
6.04
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

2l


Br
COOMe
Mes
I
OTf
2l
166.84
144.76
143.31
139.62
135.00
130.53
130.26
129.68
124.79
122.30
119.09
118.01
112.75
54.69
39.52 Dimethyl Sulfoxide-d6
26.14
20.82
f1 (ppm)


Br
COOMe
Mes
I
OTf
2l
-77.76
f1 (ppm)


F
COOMe
Mes
I
OTf
2m
7.77
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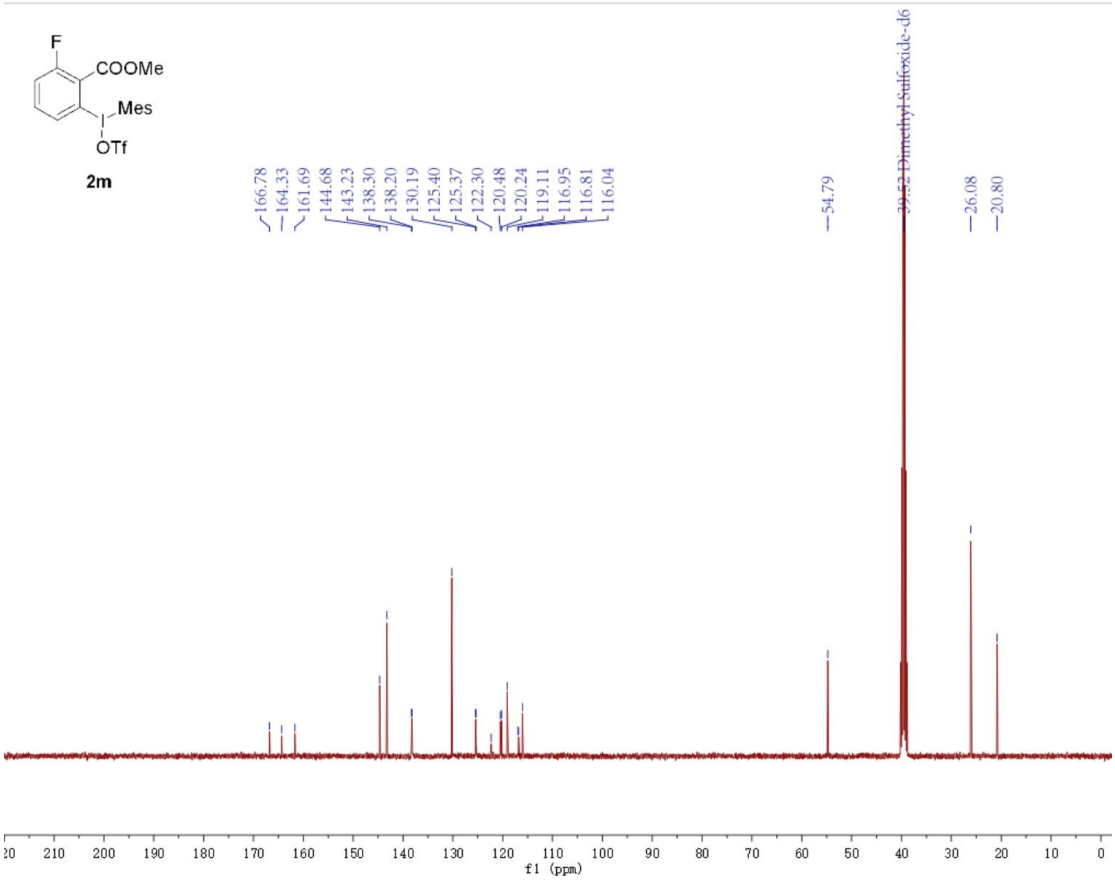
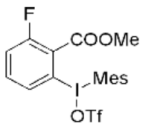
7.74
7.73
7.72
7.72
7.71
7.70
7.68
7.39
6.80
6.78
4.06
3.36
2.52
2.50 Dimethyl Sulfoxide-d6
2.41
2.04
1.96
1.00
3.03
6.05
2.82
f1 (ppm)

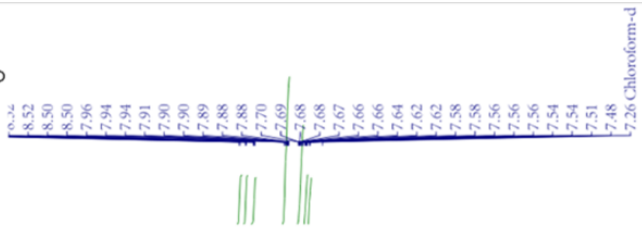

F
COOMe
Mes
I
OTf
2m
166.78
164.33
161.69
144.68
143.23
138.30
138.20
130.19
125.40
125.37
122.30
120.48
120.24
119.11
116.95
116.81
116.04
54.79
39.52 Dimethyl Sulfoxide-d6
26.08
20.80
f1 (ppm)


F
COOMe
Mes
I
OTf

2m

-77.77
-100.41
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
f1 (ppm)

3aa


8.52
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8.50
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7.94
7.91
7.90
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7.89
7.88
7.88
7.70
7.69
7.68
7.68
7.67
7.66
7.66
7.64
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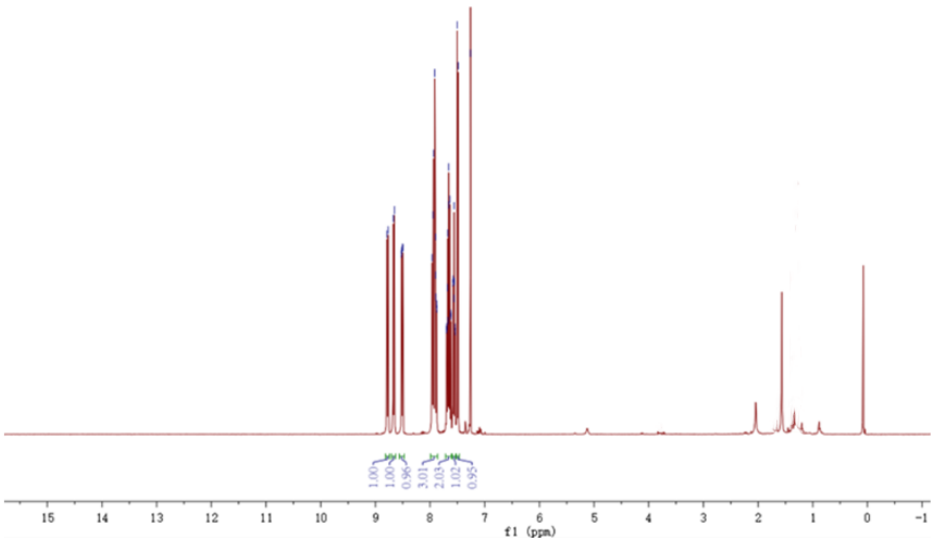
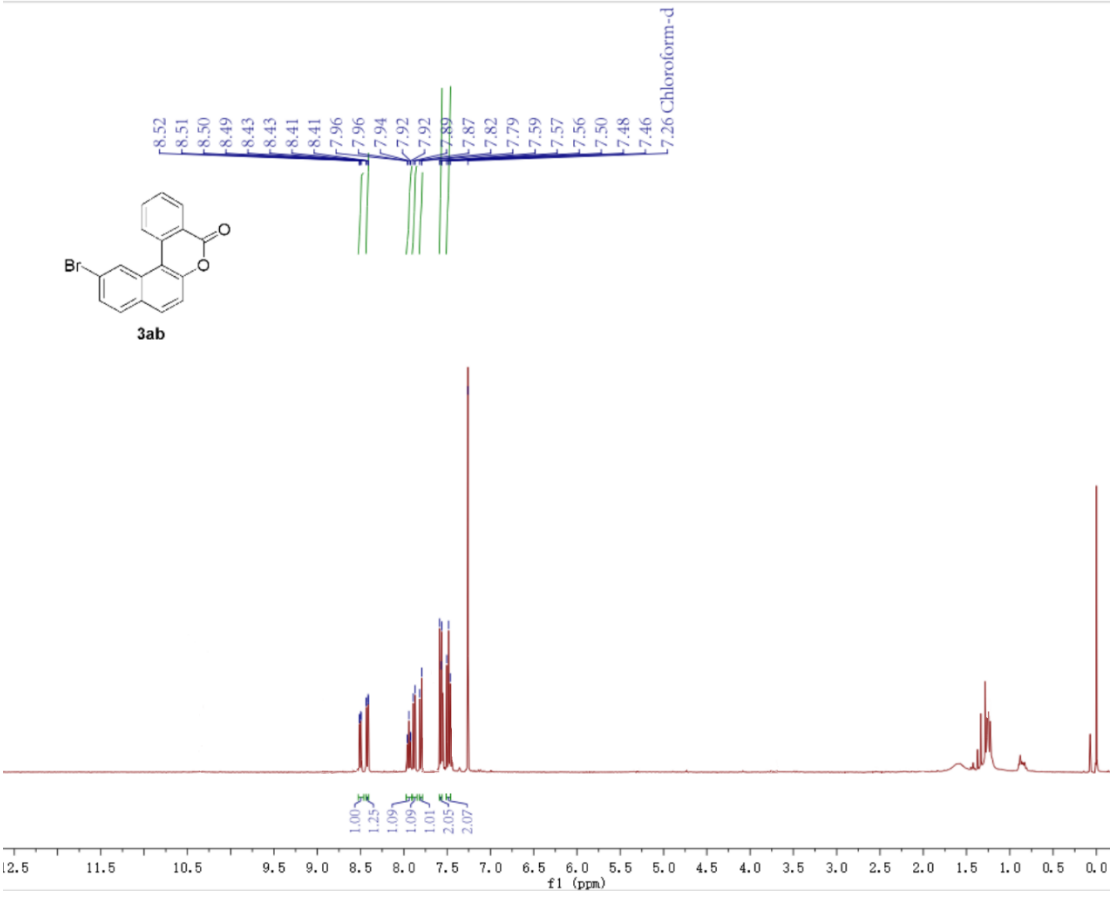
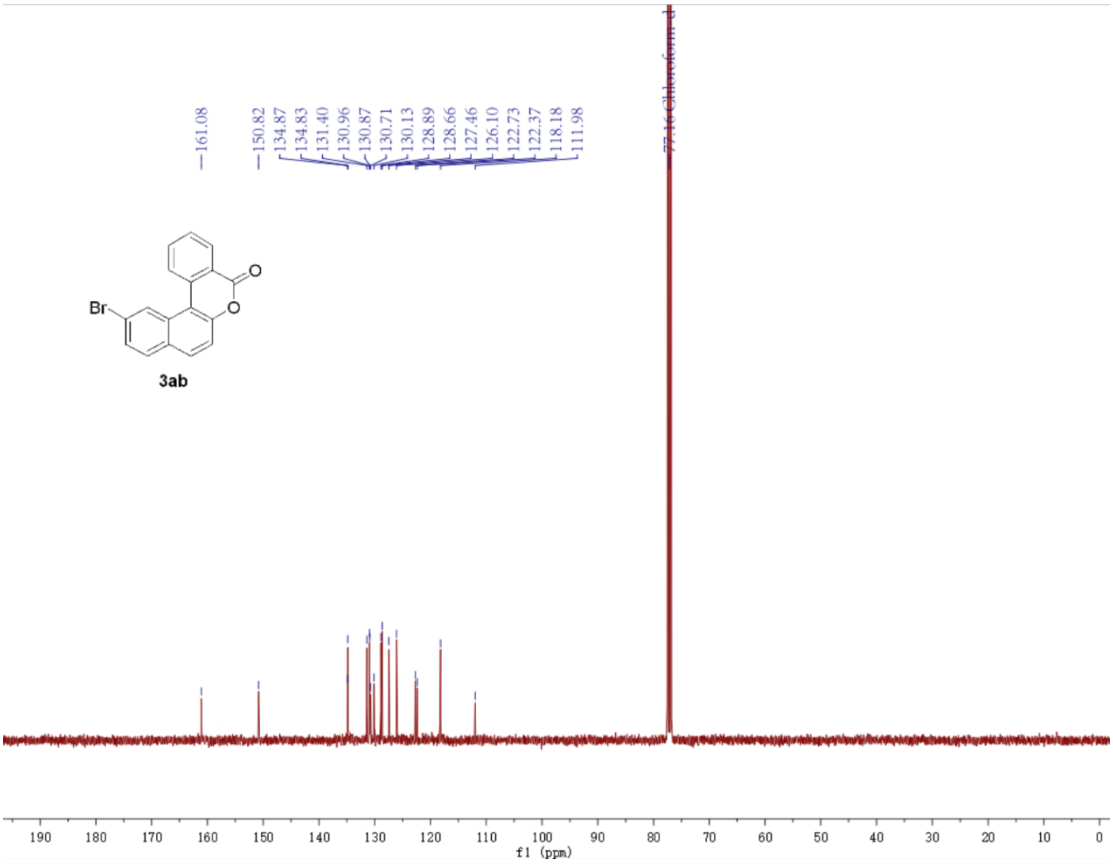
7.54
7.54
7.51
7.48
7.26 Chloroform-d


1.00
1.00
0.96
3.01
2.03
1.02
0.95
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)


8.52
8.51
8.50
8.49
8.43
8.43
8.41
8.41
7.96
7.96
7.94
7.92
7.92
7.89
7.87
7.82
7.79
7.59
7.57
7.56
7.50
7.48
7.46
7.26 Chloroform-d
Br
O
O
3ab
1.00
1.25
1.09
1.09
1.01
2.05
2.07
f1 (ppm)


161.08
150.82
134.87
134.83
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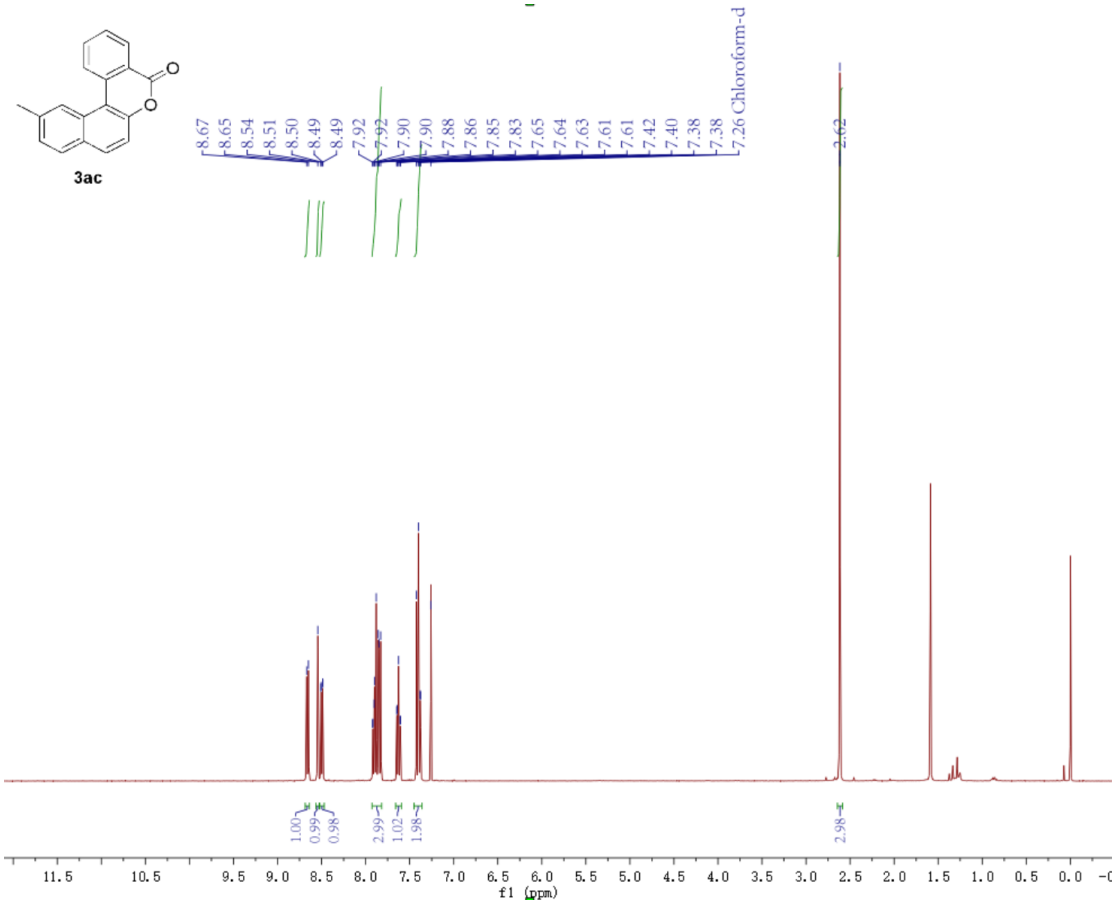
130.96
130.87
130.71
130.13
128.89
128.66
127.46
126.10
122.73
122.37
118.18
111.98
77.16 Chloroform-d
Br
O
O
3ab
f1 (ppm)


3ac
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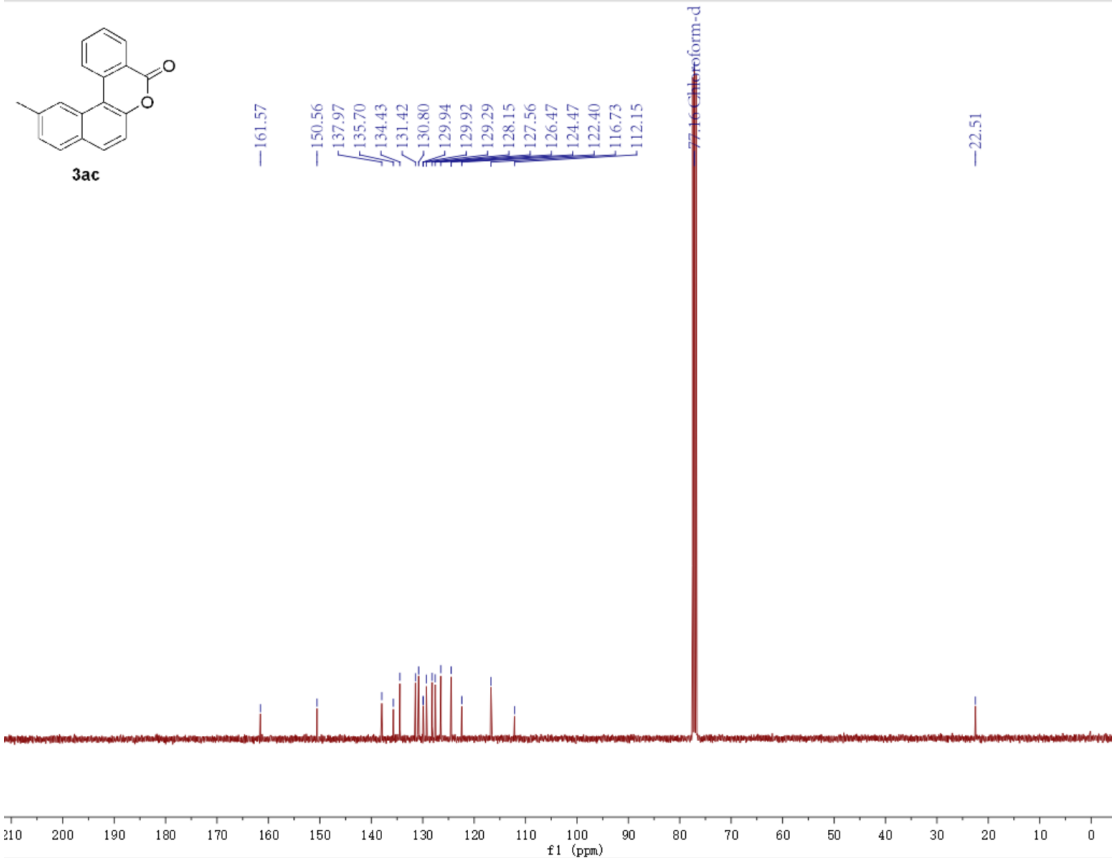
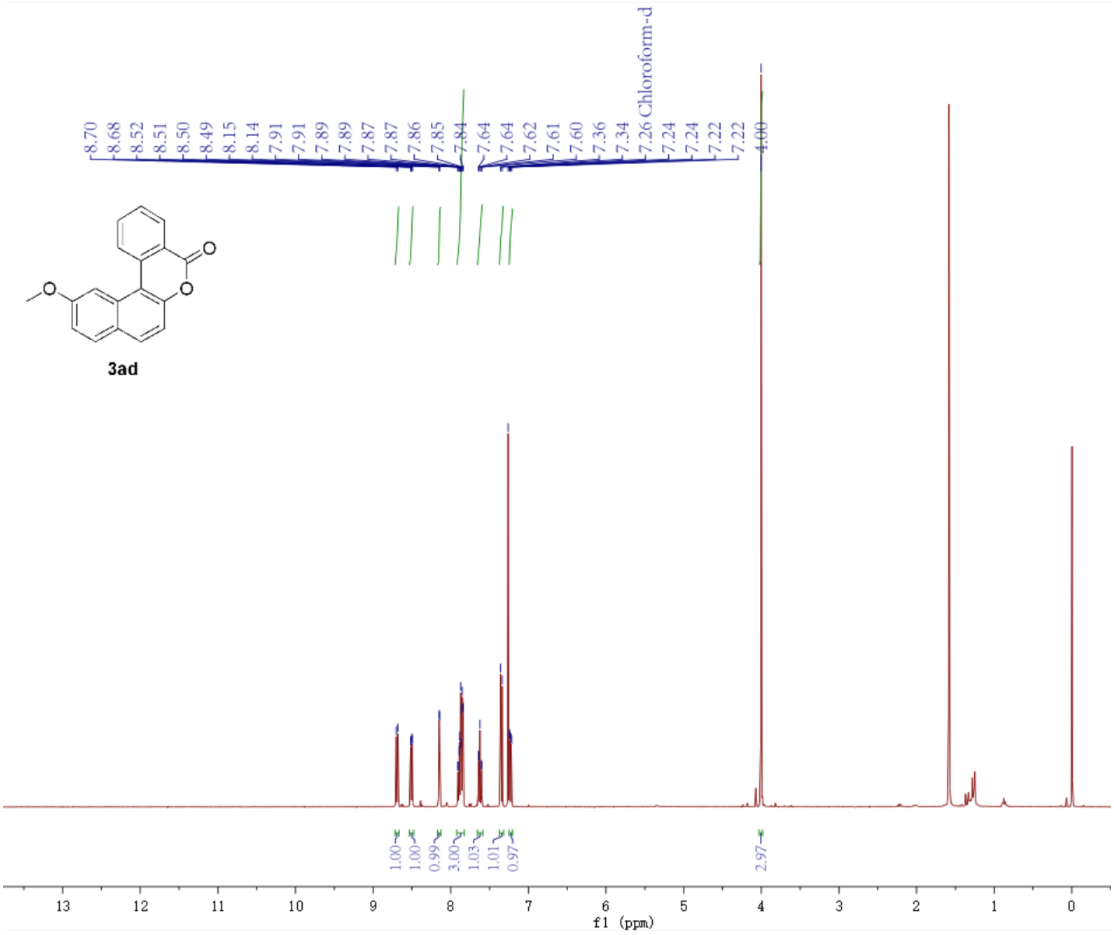
8.54
8.51
8.50
8.49
8.49
7.92
7.92
7.90
7.90
7.88
7.86
7.85
7.83
7.65
7.64
7.63
7.61
7.61
7.42
7.40
7.38
7.38
7.26 Chloroform-d
2.62
1.00
0.99
0.98
2.99
1.02
1.98
2.98
f1 (ppm)


3ac
161.57
150.56
137.97
135.70
134.43
131.42
130.80
129.94
129.92
129.29
128.15
127.56
126.47
124.47
122.40
116.73
112.15
77.16 Chloroform-d
22.51
f1 (ppm)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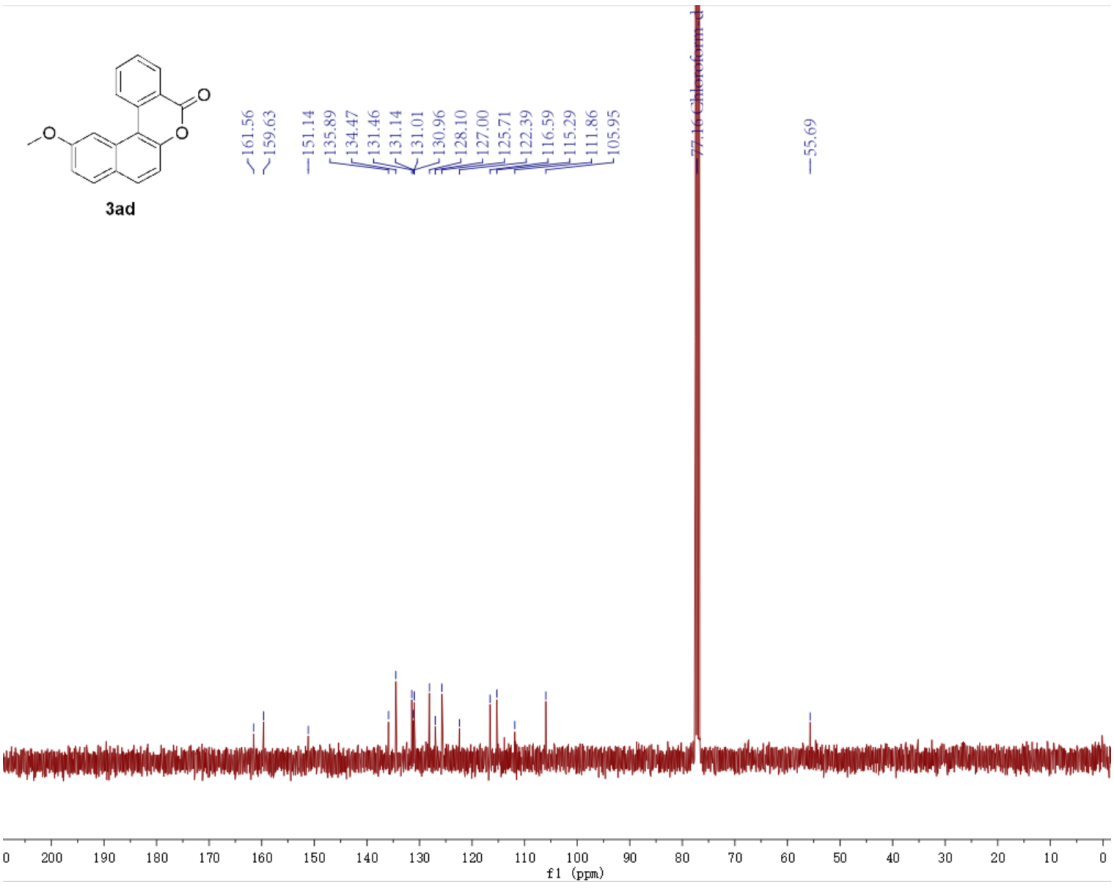
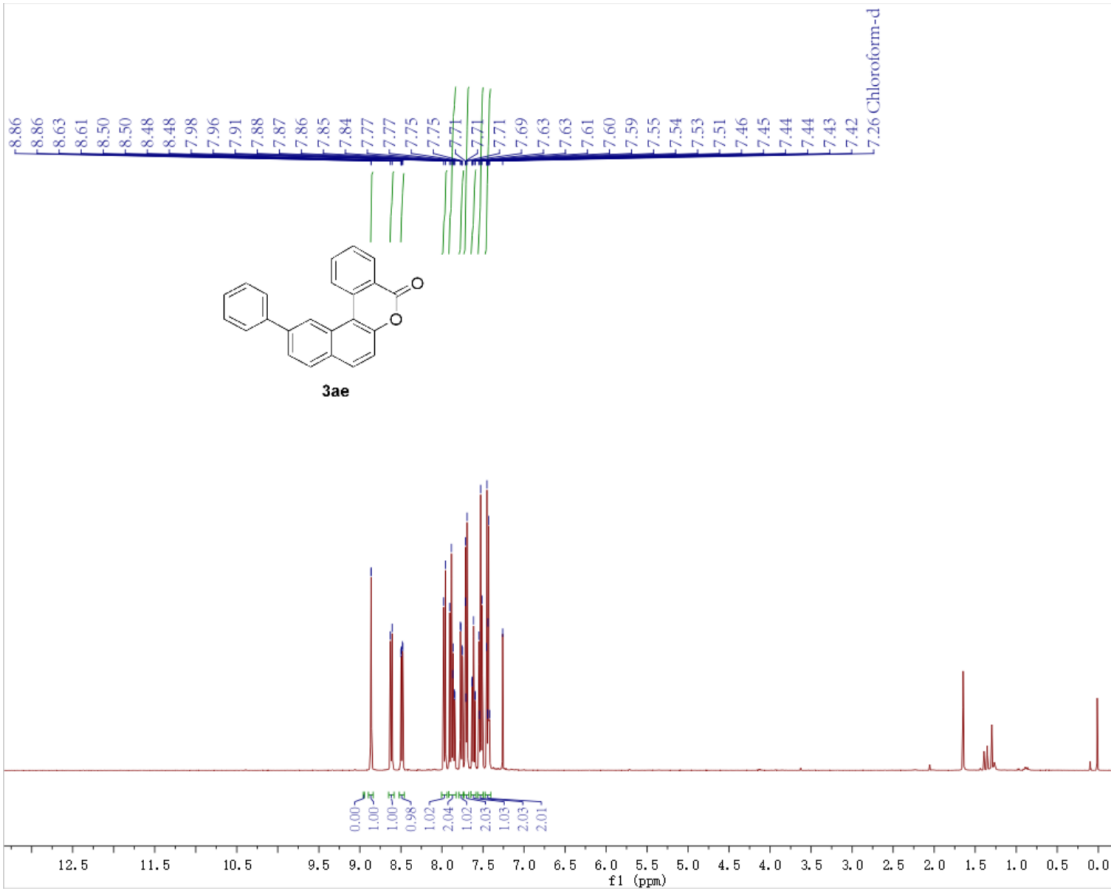
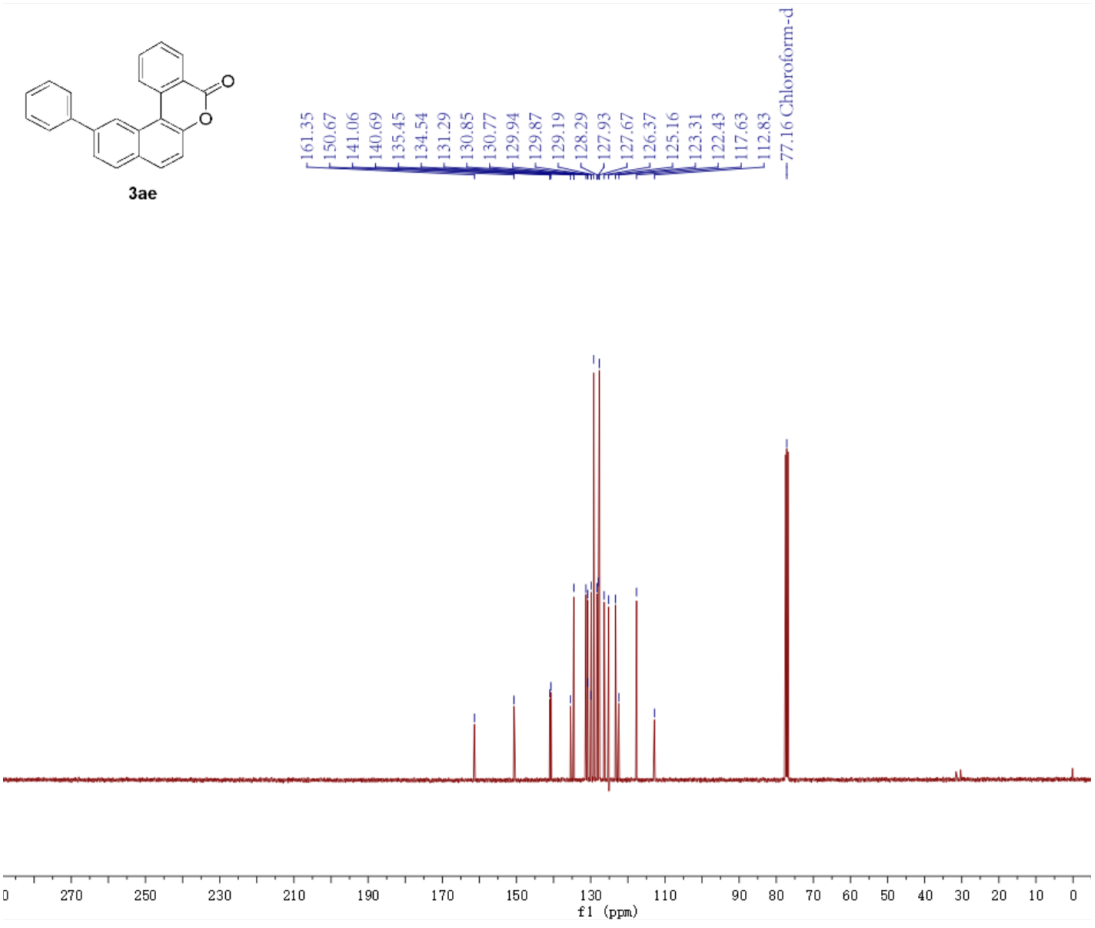
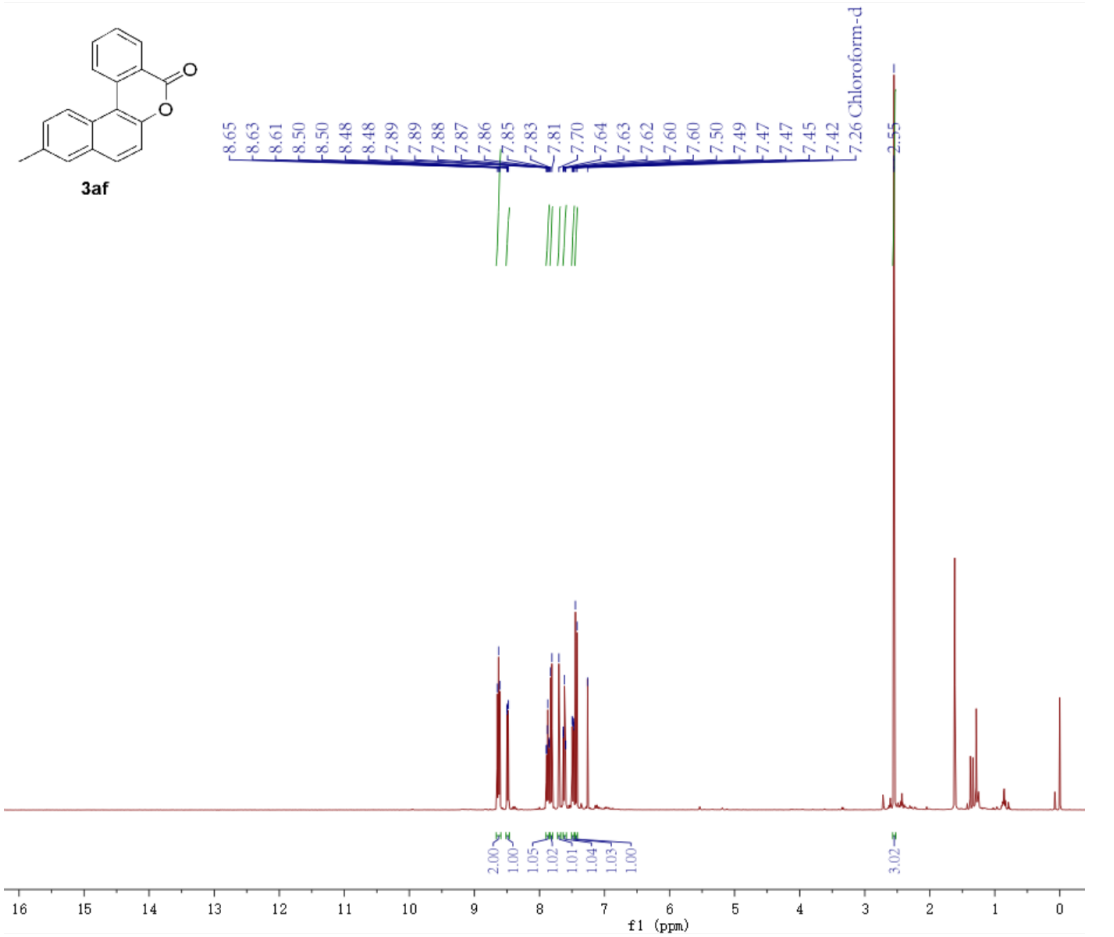
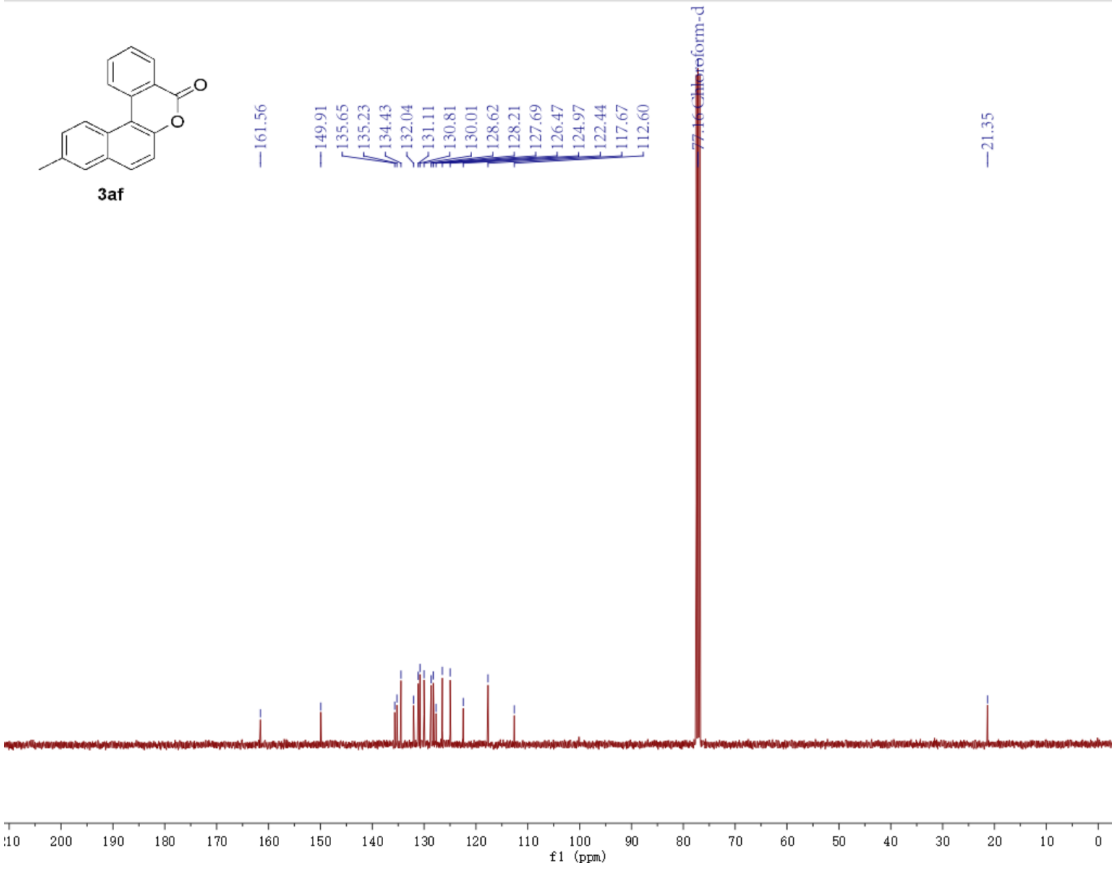
8.68
8.52
8.51
8.50
8.49
8.15
8.14
7.91
7.91
7.89
7.89
7.87
7.87
7.86
7.85
7.84
7.64
7.64
7.62
7.61
7.60
7.36
7.34
7.26 Chloroform-d
7.24
7.24
7.22
7.22
4.00
3ad
1.00
1.00
0.99
3.00
1.03
1.01
0.97
2.97
f1 (ppm)

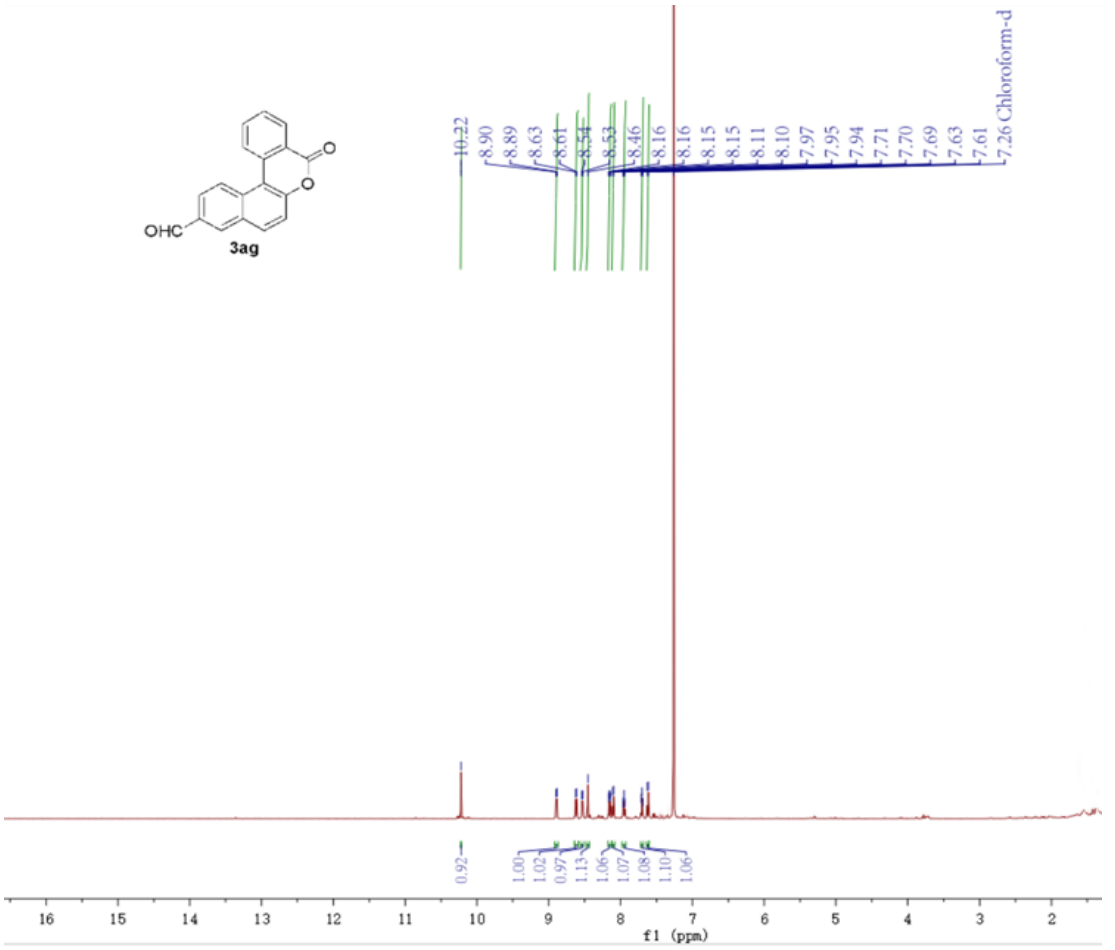

161.56
159.63
151.14
135.89
134.47
131.46
131.14
131.01
130.96
128.10
127.00
125.71
122.39
116.59
115.29
111.86
105.95
77.16 Chloroform-d
55.69
3ad
f1 (ppm)

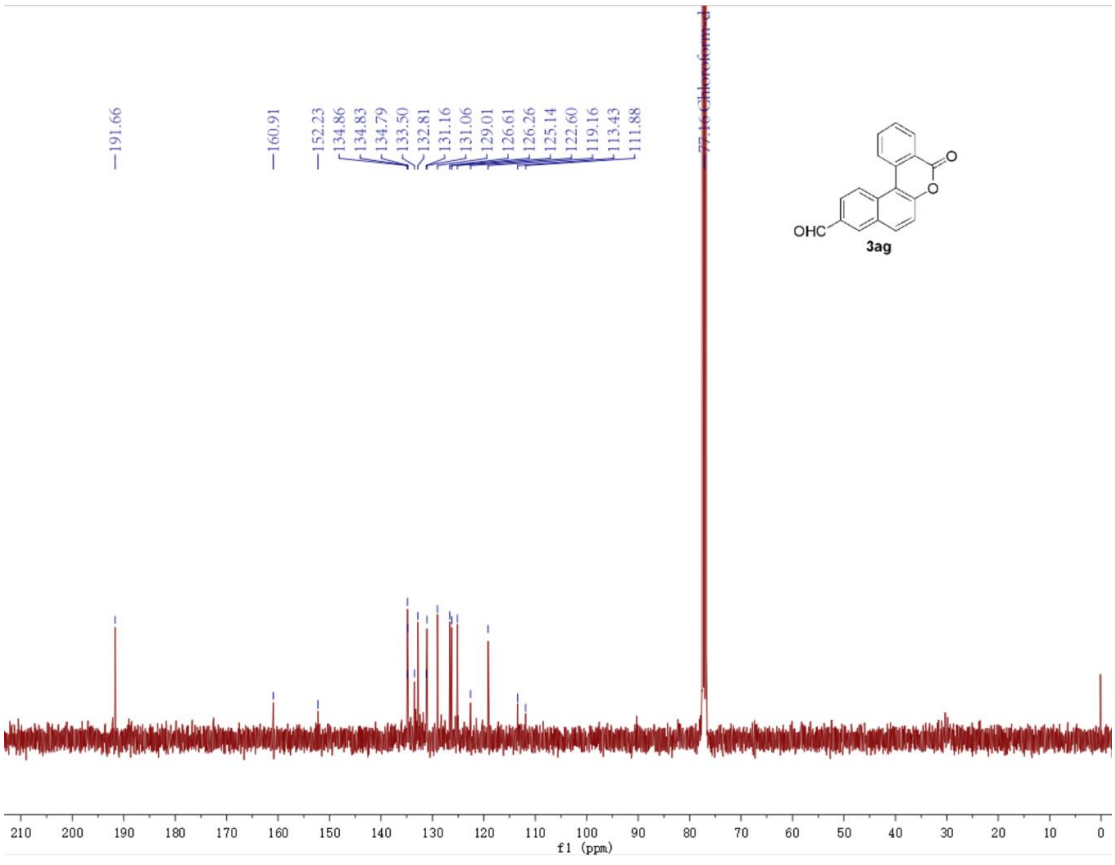

8.86
8.86
8.63
8.61
8.50
8.50
8.48
8.48
7.98
7.96
7.91
7.88
7.87
7.86
7.85
7.84
7.77
7.77
7.75
7.75
7.71
7.71
7.71
7.69
7.63
7.63
7.61
7.60
7.59
7.55
7.54
7.53
7.51
7.46
7.45
7.44
7.44
7.43
7.42
7.26 Chloroform-d
O
O
3ae
0.00
1.00
1.00
0.98
1.02
2.04
1.02
2.03
1.03
2.03
2.01
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

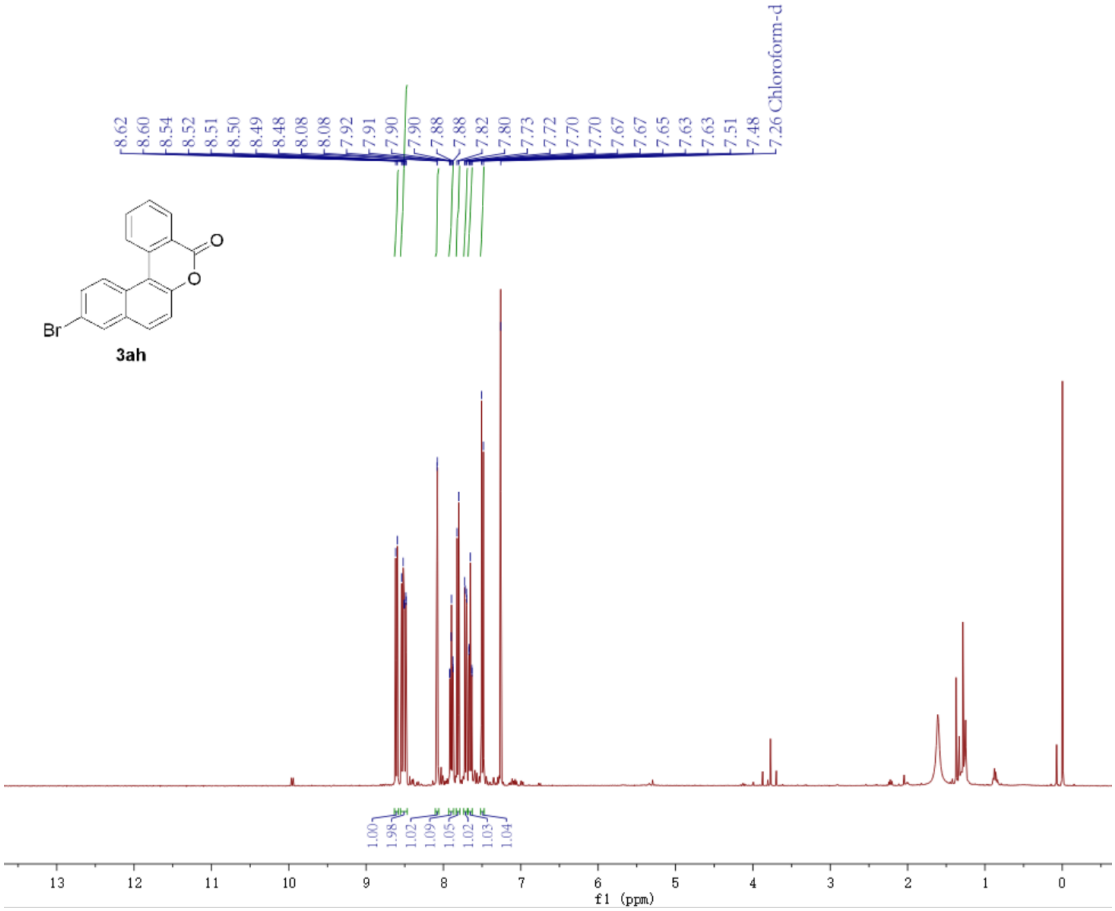

O
O
3ae
161.35
150.67
141.06
140.69
135.45
134.54
131.29
130.85
130.77
129.94
129.87
129.19
128.29
127.93
127.67
126.37
125.16
123.31
122.43
117.63
112.83
77.16 Chloroform-d
270
250
230
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

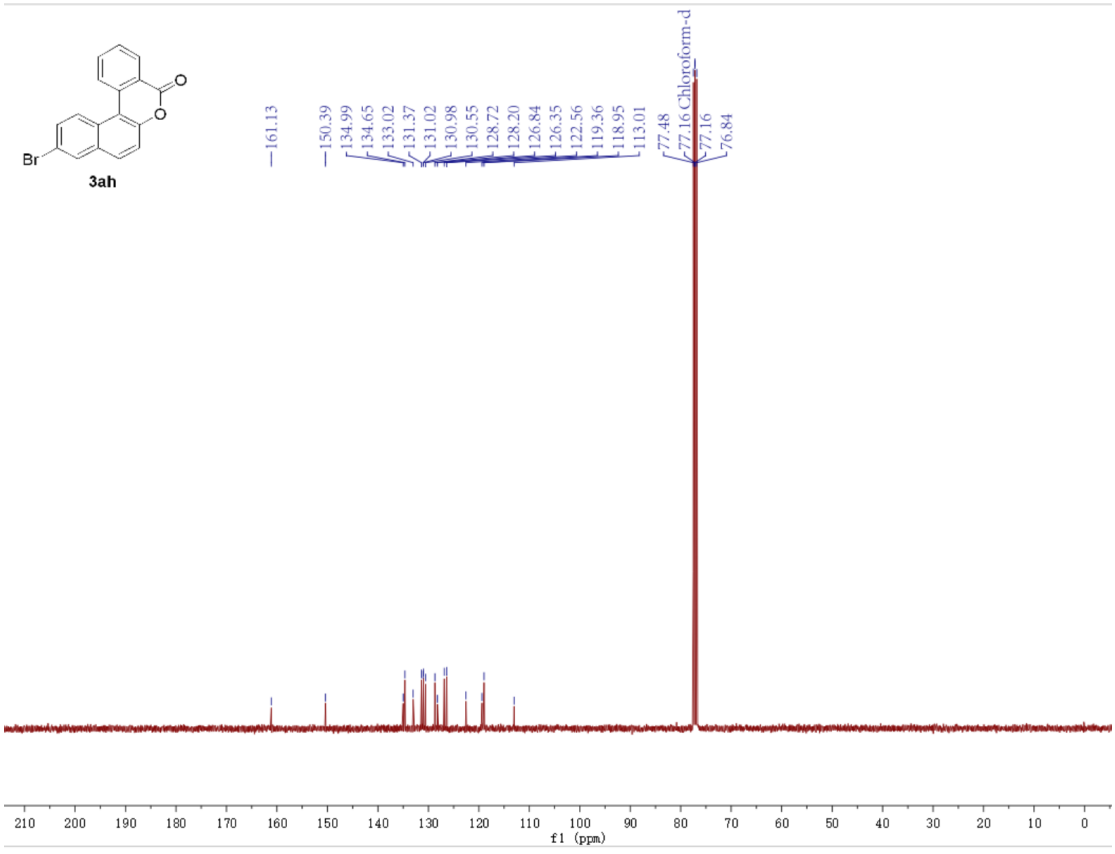

3af
8.65
8.63
8.61
8.50
8.50
8.48
8.48
7.89
7.89
7.88
7.87
7.86
7.85
7.83
7.81
7.70
7.64
7.63
7.62
7.60
7.60
7.50
7.49
7.47
7.47
7.45
7.42
7.26 Chloroform-d
2.55
2.00
1.00
1.05
1.02
1.01
1.04
1.03
1.00
3.02
f1 (ppm)

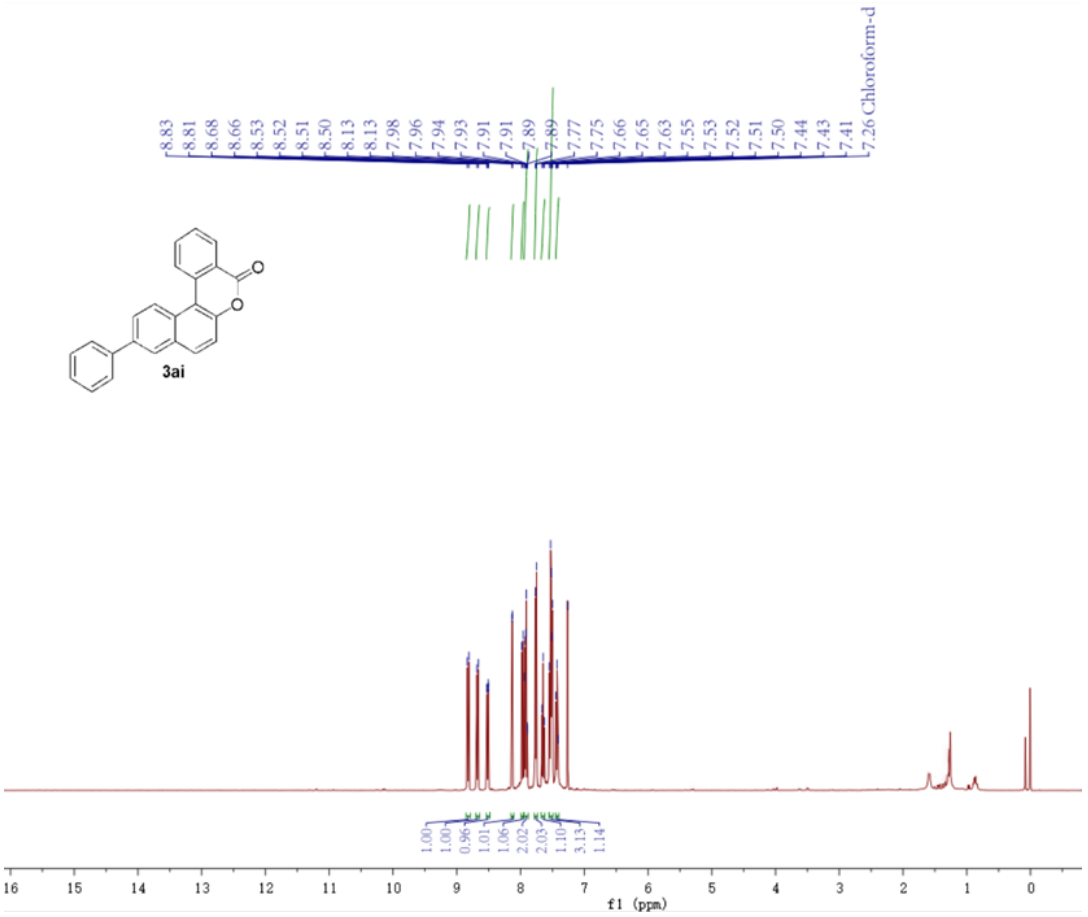

3af
161.56
149.91
135.65
135.23
134.43
132.04
131.11
130.81
130.01
128.62
128.21
127.69
126.47
124.97
122.44
117.67
112.60
77.16 Chloroform-d
21.35
f1 (ppm)

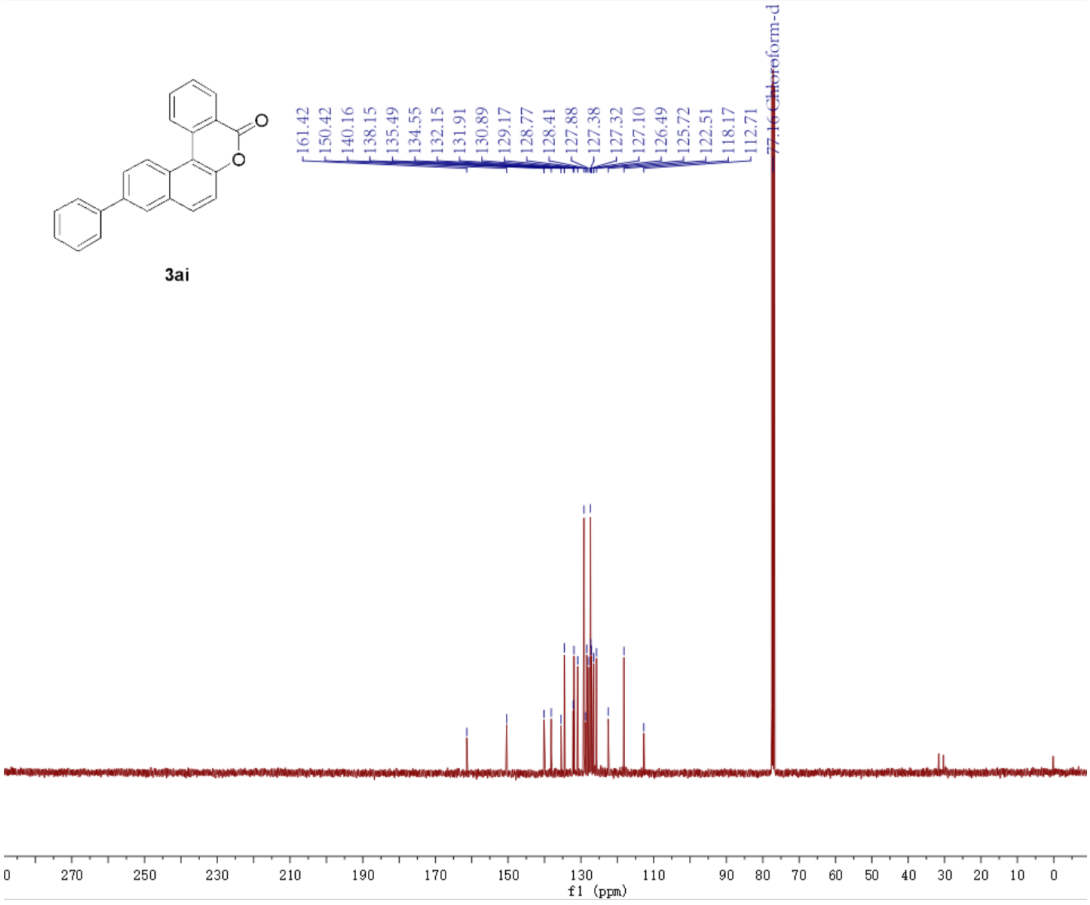

OHC
3ag
10.22
8.90
8.89
8.63
8.61
8.54
8.53
8.46
8.16
8.16
8.15
8.15
8.11
8.10
7.97
7.95
7.94
7.71
7.70
7.69
7.63
7.61
7.26 Chloroform-d
0.92
1.00
1.02
0.97
1.13
1.06
1.07
1.08
1.10
1.06
f1 (ppm)

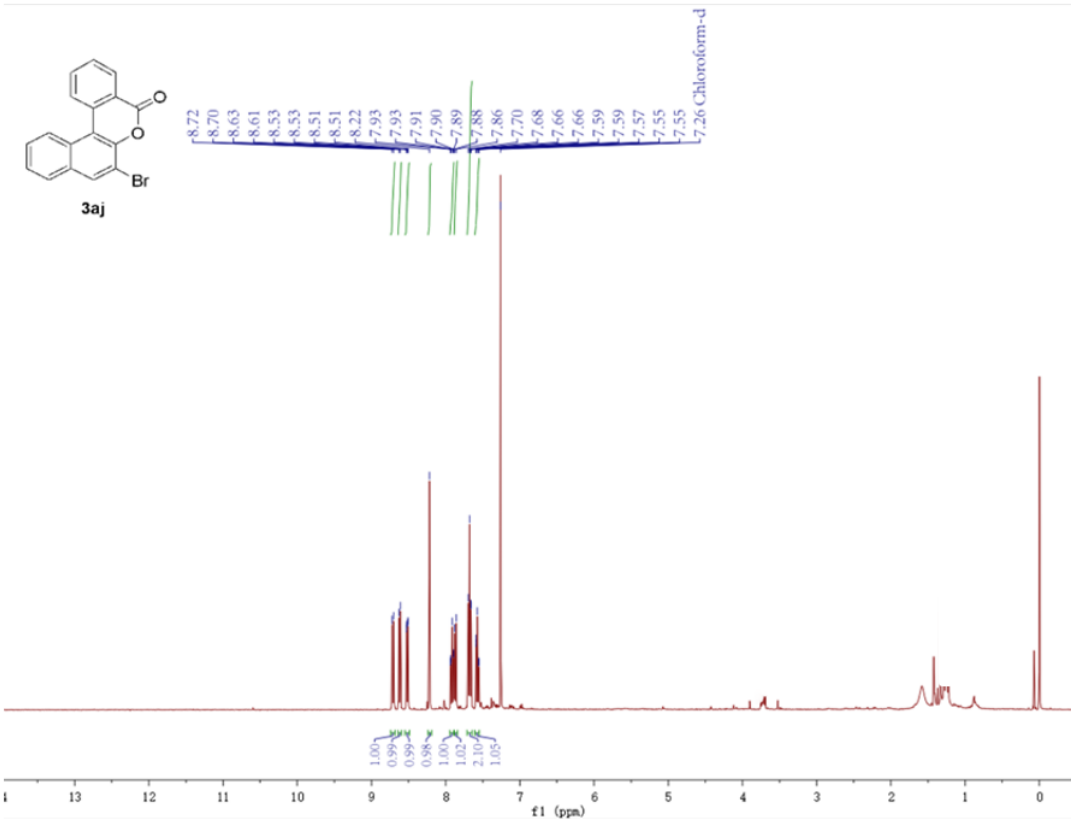

191.66
160.91
152.23
134.86
134.83
134.79
133.50
132.81
131.16
131.06
129.01
126.61
126.26
125.14
122.60
119.16
113.43
111.88
77.16 Chloroform-d
OHC
3ag
f1 (ppm)

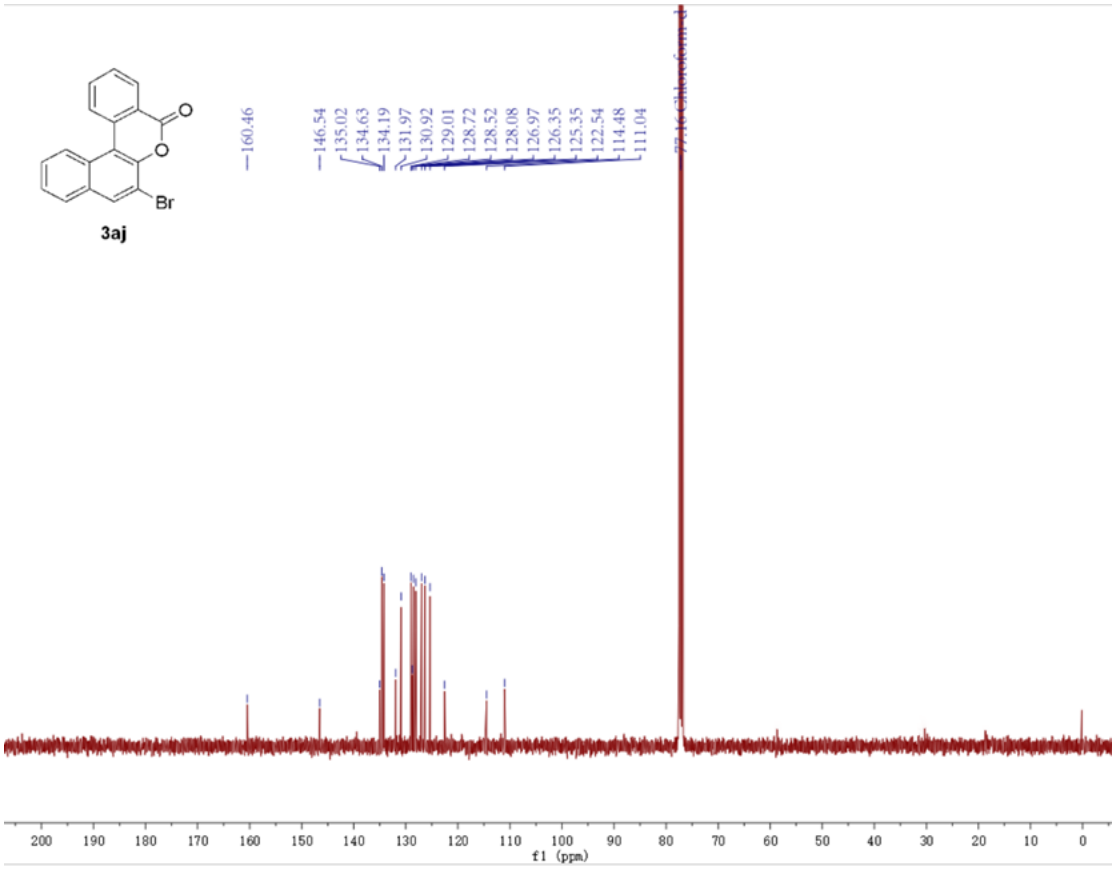

8.62
8.60
8.54
8.52
8.51
8.50
8.49
8.48
8.08
8.08
7.92
7.91
7.90
7.90
7.88
7.88
7.82
7.80
7.73
7.72
7.70
7.70
7.67
7.67
7.65
7.63
7.63
7.51
7.48
7.26 Chloroform-d
O
O
Br
3ah
1.00
1.98
1.02
1.09
1.05
1.02
1.03
1.04
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

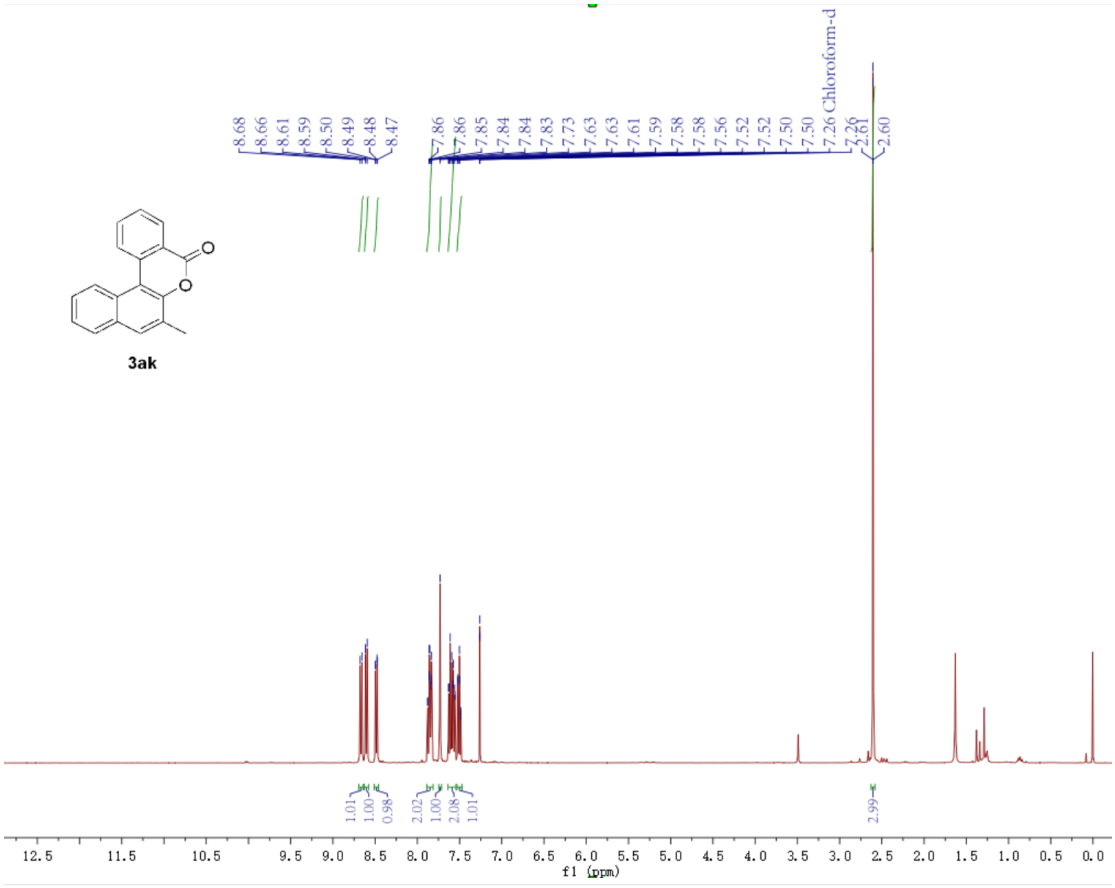

O
O
Br
3ah
161.13
150.39
134.99
134.65
133.02
131.37
131.02
130.98
130.55
128.72
128.20
126.84
126.35
122.56
119.36
118.95
113.01
77.48
77.16 Chloroform-d
77.16
76.84
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.83
8.81
8.68
8.66
8.53
8.52
8.51
8.50
8.13
8.13
7.98
7.96
7.94
7.93
7.91
7.91
7.89
7.89
7.77
7.75
7.66
7.65
7.63
7.55
7.53
7.52
7.51
7.50
7.44
7.43
7.41
7.26 Chloroform-d
3ai
1.00
1.00
0.96
1.01
1.06
2.02
2.03
1.10
3.13
1.14
f1 (ppm)

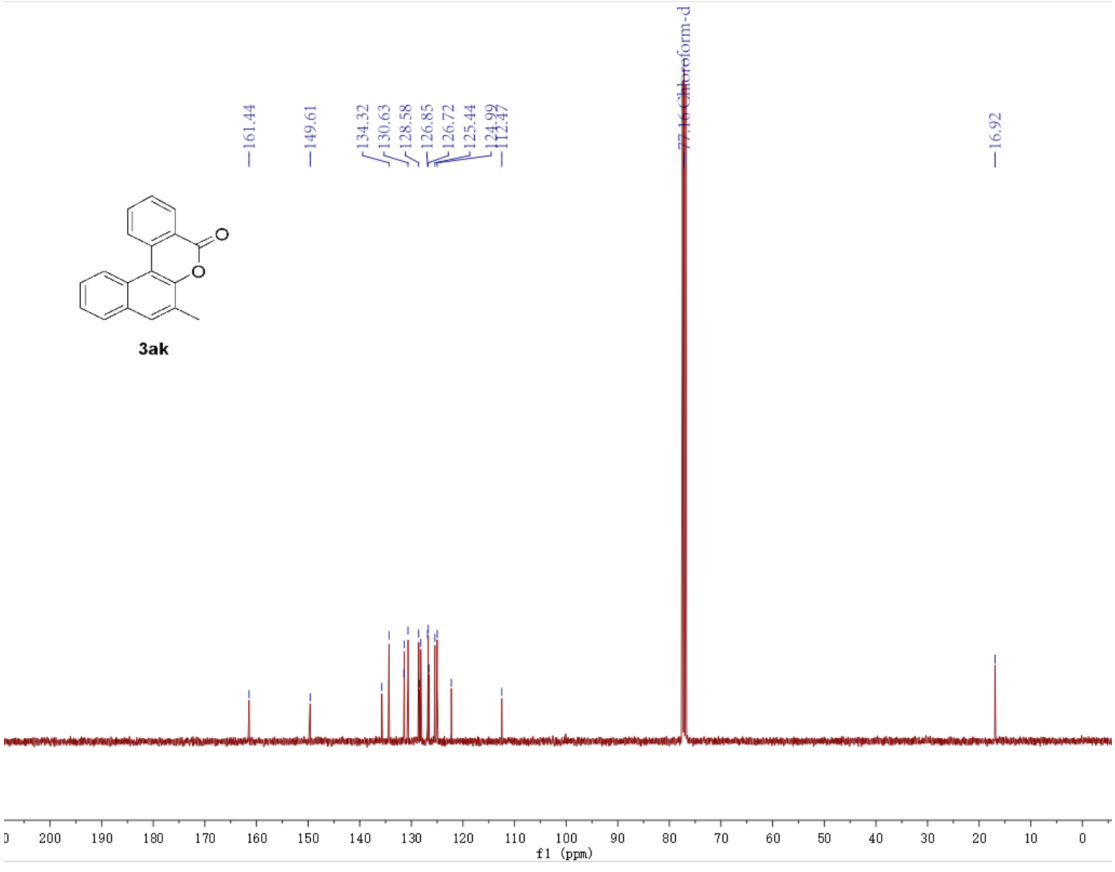

161.42
150.42
140.16
138.15
135.49
134.55
132.15
131.91
130.89
129.17
128.77
128.41
127.88
127.38
127.32
127.10
126.49
125.72
122.51
118.17
112.71
77.16 Chloroform-d
3ai
f1 (ppm)


3aj
8.72
8.70
8.63
8.61
8.53
8.53
8.51
8.51
8.22
7.93
7.93
7.91
7.90
7.89
7.88
7.86
7.70
7.68
7.66
7.66
7.59
7.59
7.57
7.55
7.55
7.26 Chloroform-d
1.00
0.99
0.99
0.98
1.00
1.02
2.10
1.05
f1 (ppm)

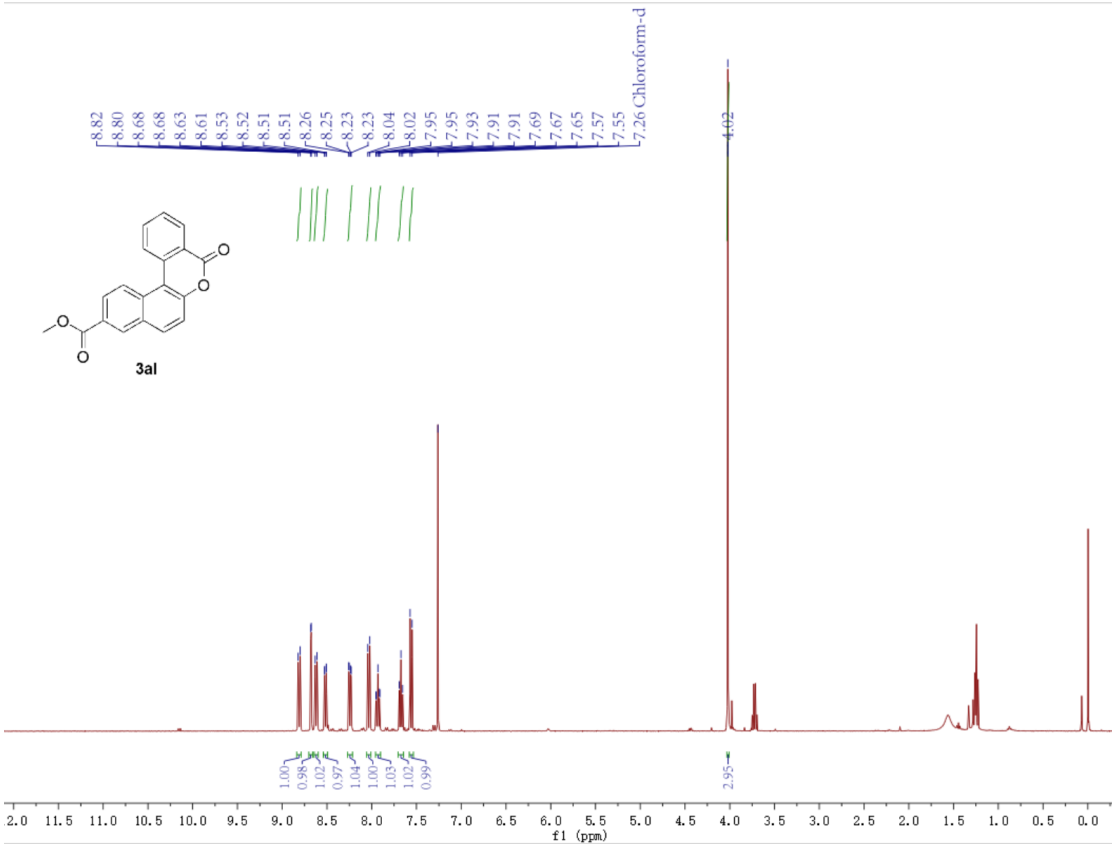

3aj
160.46
146.54
135.02
134.63
134.19
131.97
130.92
129.01
128.72
128.52
128.08
126.97
126.35
125.35
122.54
114.48
111.04
77.16 Chloroform-d
f1 (ppm)

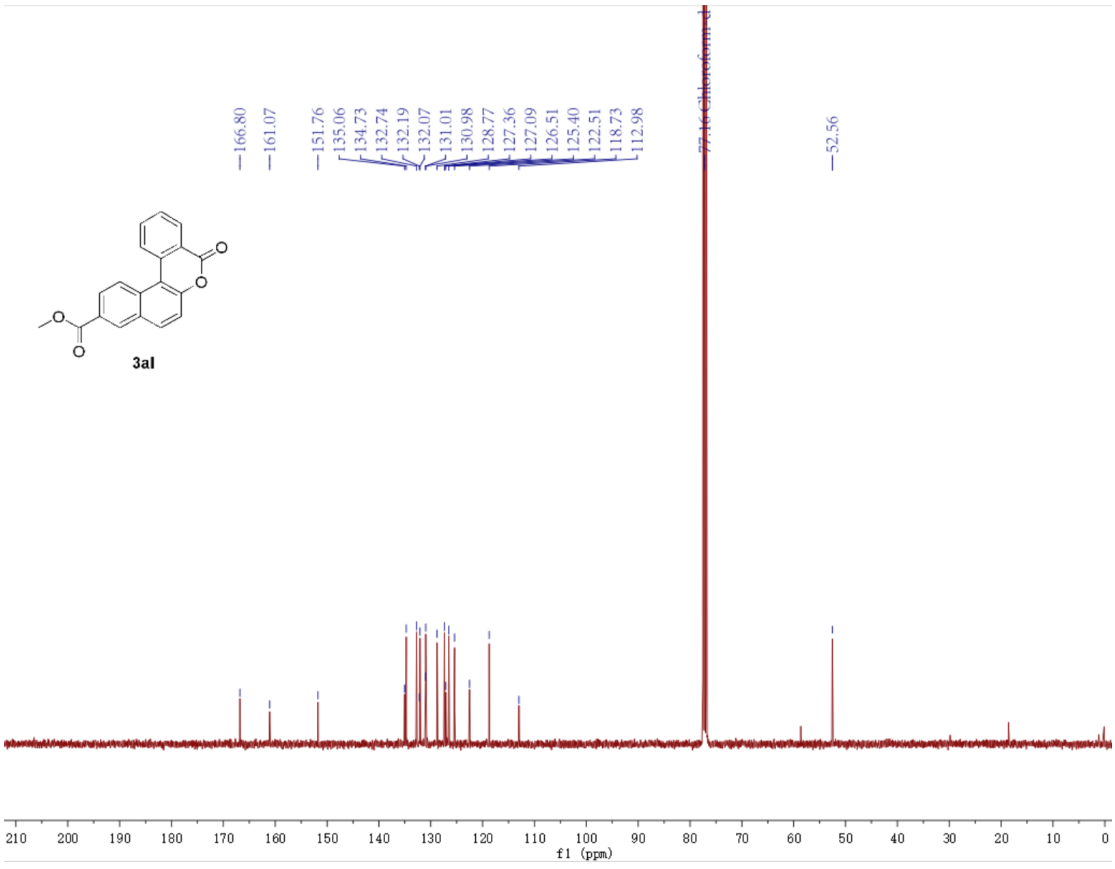

8.68
8.66
8.61
8.59
8.50
8.49
8.48
8.47
7.86
7.86
7.85
7.84
7.84
7.83
7.73
7.63
7.63
7.61
7.59
7.58
7.58
7.56
7.52
7.52
7.50
7.50
7.26 Chloroform-d
2.61
2.60
1.01
1.00
0.98
2.02
1.00
2.08
1.01
2.99
f1 (ppm)

3ak


161.44
149.61
134.32
130.63
128.58
126.85
126.72
125.44
77.16 Chloroform-d
16.92
f1 (ppm)

3ak


8.82
8.80
8.68
8.68
8.63
8.61
8.53
8.52
8.51
8.51
8.26
8.25
8.23
8.23
8.04
8.02
7.95
7.95
7.93
7.91
7.91
7.69
7.67
7.65
7.57
7.55
7.26 Chloroform-d
4.02
3al
1.00
0.98
1.02
0.97
1.04
1.00
1.03
1.02
0.99
2.95
f1 (ppm)


166.80
161.07
151.76
135.06
134.73
132.74
132.19
132.07
131.01
130.98
128.77
127.36
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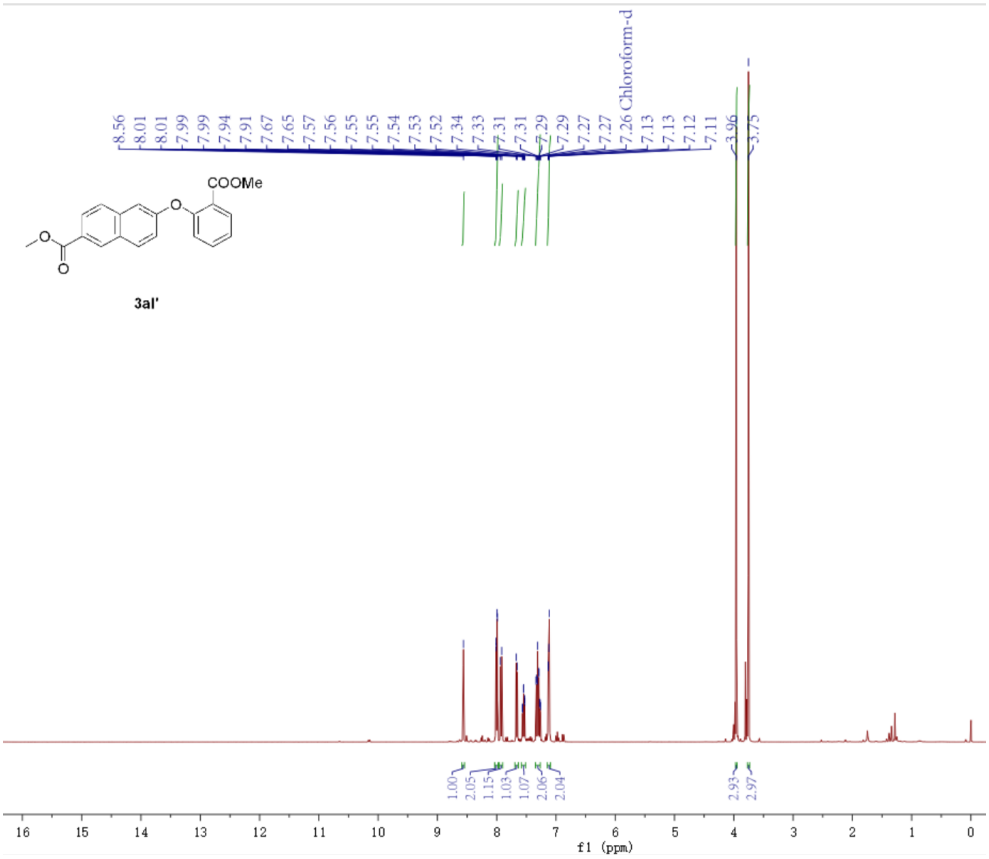
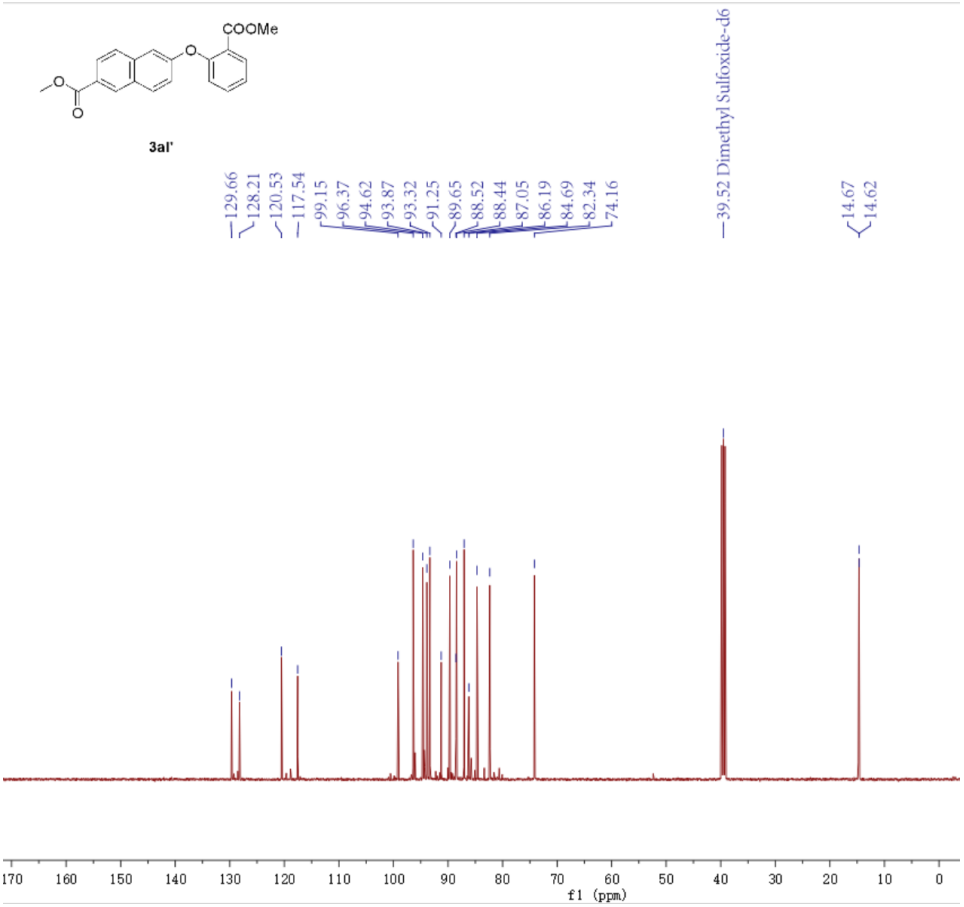
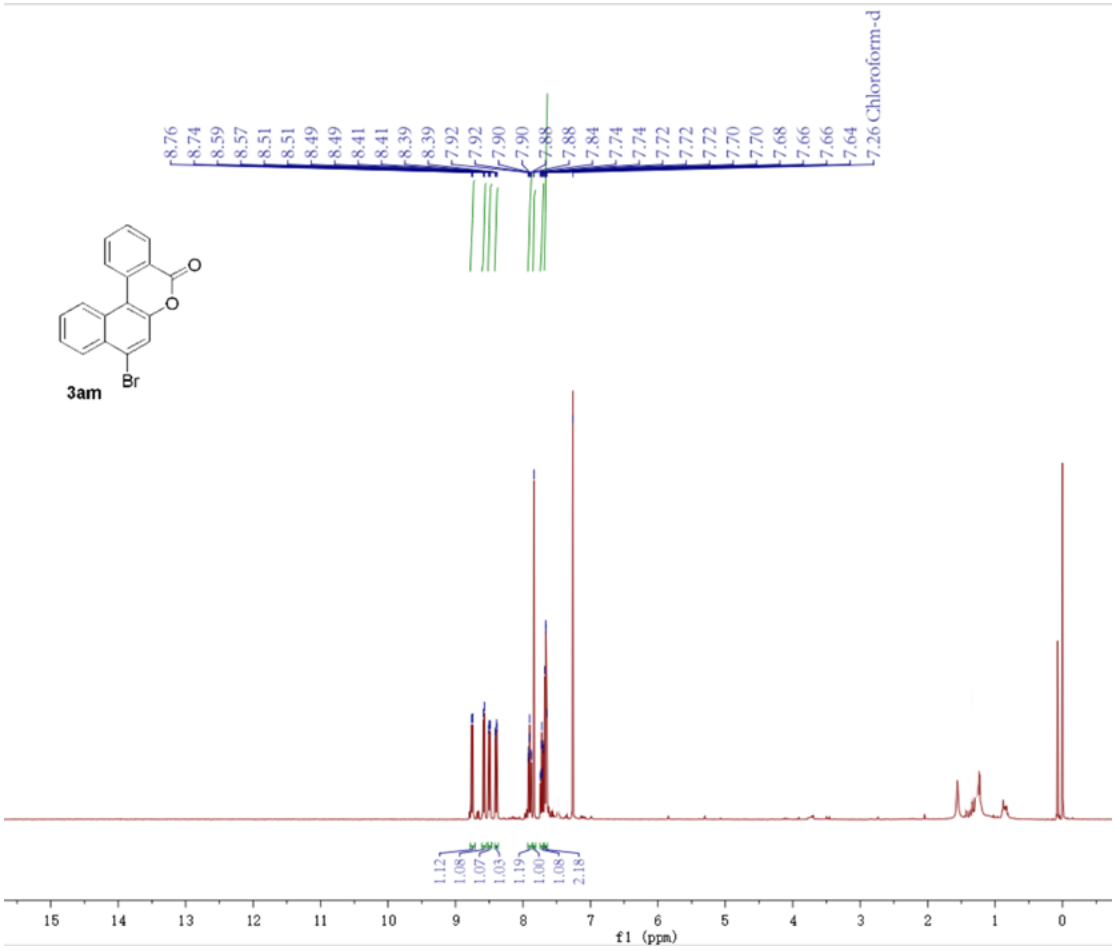
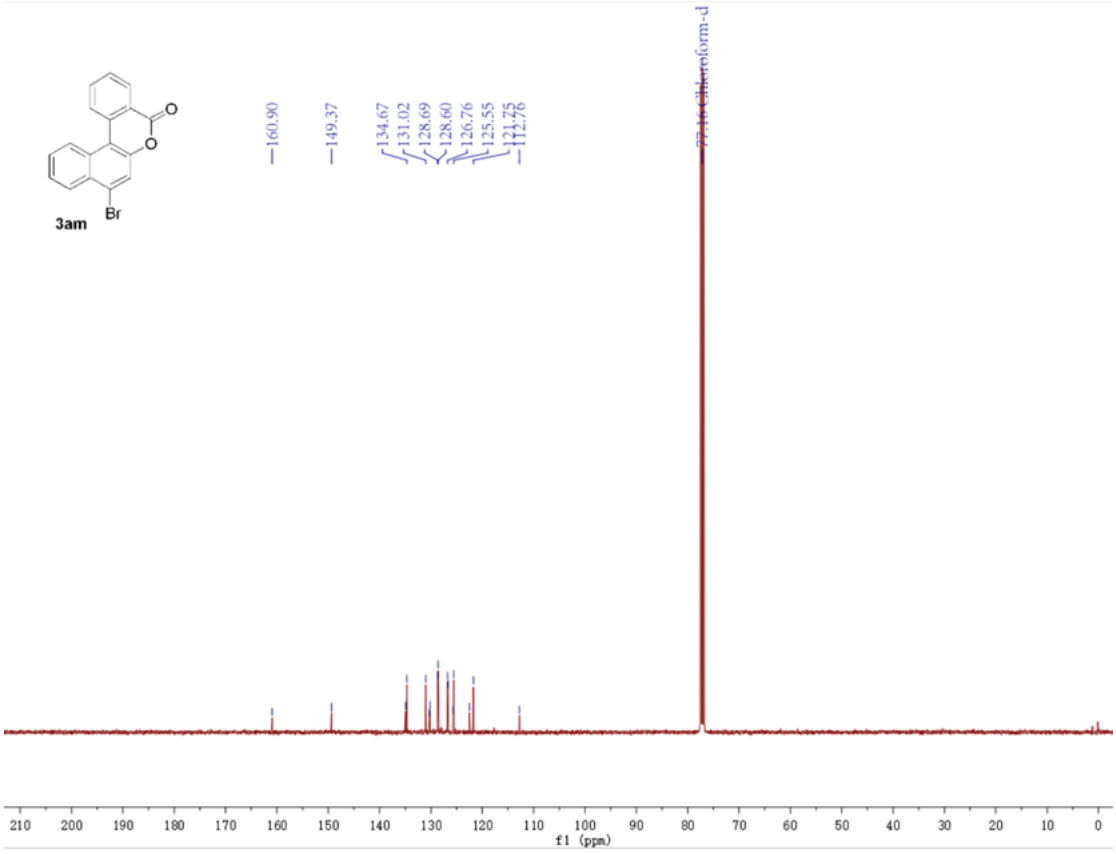
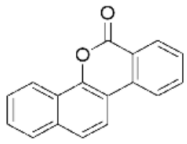
126.51
125.40
122.51
118.73
112.98
77.16 Chloroform-d
52.56
3al
f1 (ppm)


8.56
8.01
8.01
7.99
7.99
7.94
7.91
7.67
7.65
7.57
7.56
7.55
7.55
7.54
7.53
7.52
7.34
7.33
7.31
7.31
7.29
7.29
7.27
7.27
7.26 Chloroform-d
7.13
7.12
7.11
3.96
3.75
COOMe
3al'
1.00
2.05
1.15
1.03
1.07
2.06
2.04
2.93
2.97
f1 (ppm)

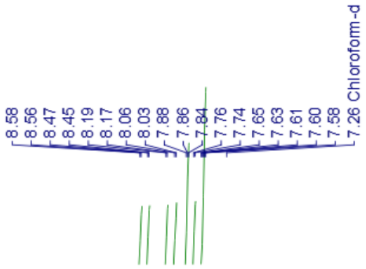

COOMe
3al'
129.66
128.21
120.53
117.54
99.15
96.37
94.62
93.87
93.32
91.25
89.65
88.52
88.44
87.05
86.19
84.69
82.34
74.16
39.52 Dimethyl Sulfoxide-d6
14.67
14.62
f1 (ppm)

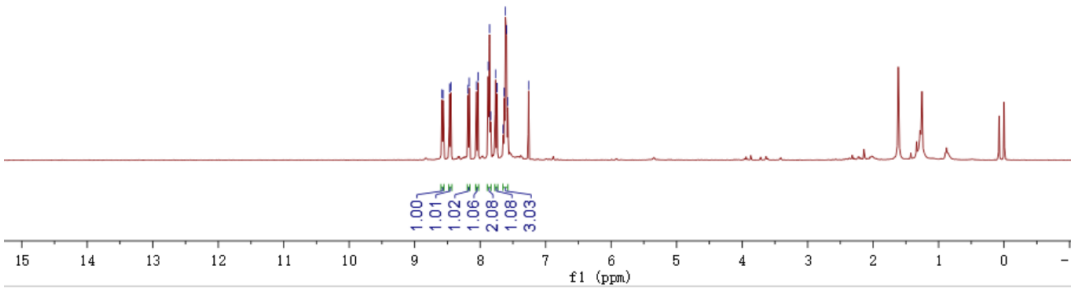

8.76
8.74
8.59
8.57
8.51
8.51
8.49
8.49
8.41
8.41
8.39
8.39
7.92
7.92
7.90
7.90
7.88
7.88
7.84
7.74
7.74
7.72
7.72
7.72
7.70
7.70
7.68
7.66
7.66
7.64
7.26 Chloroform-d
O
O
Br
3am
1.12
1.08
1.07
1.03
1.19
1.00
1.08
2.18
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

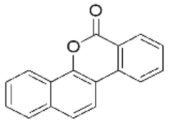

O
O
Br
3am
160.90
149.37
134.67
131.02
128.69
128.60
126.76
125.55
121.75
112.76
77.16 Chloroform-d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



3an

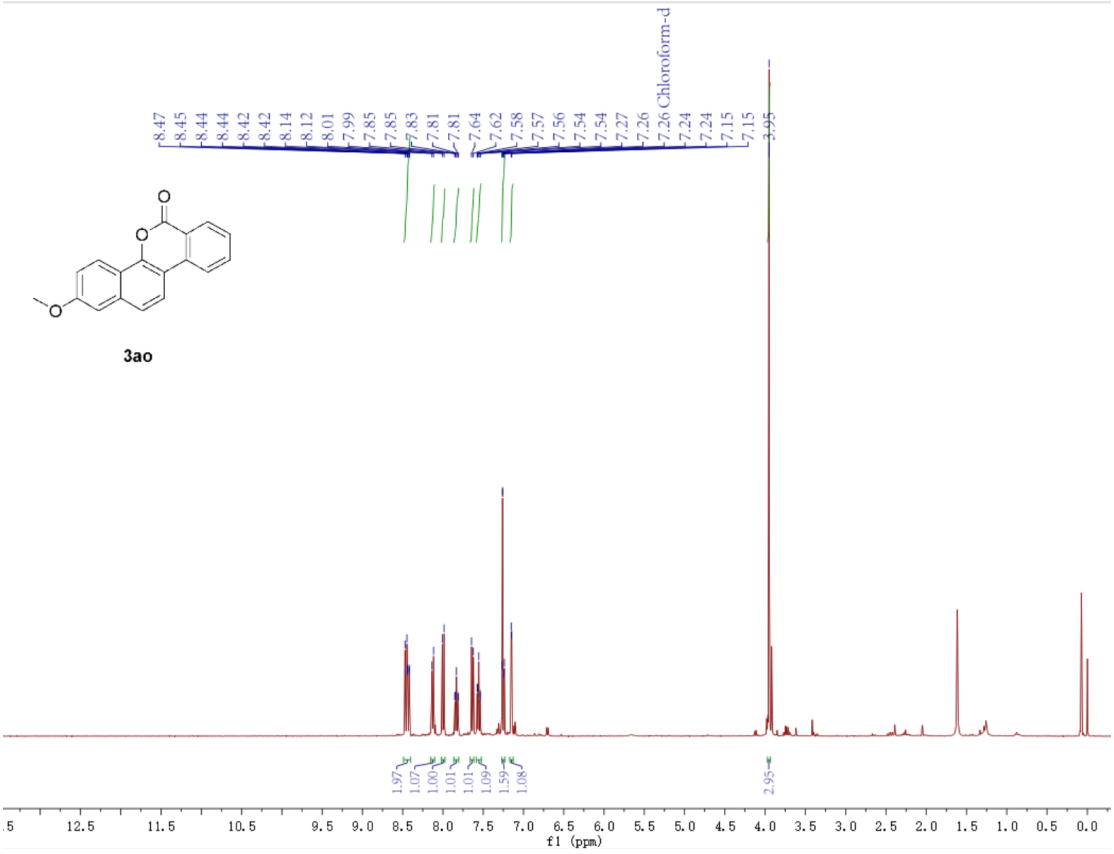

8.58
8.56
8.47
8.45
8.19
8.17
8.06
8.03
7.88
7.86
7.84
7.76
7.74
7.65
7.63
7.61
7.60
7.58
7.26 Chloroform-d

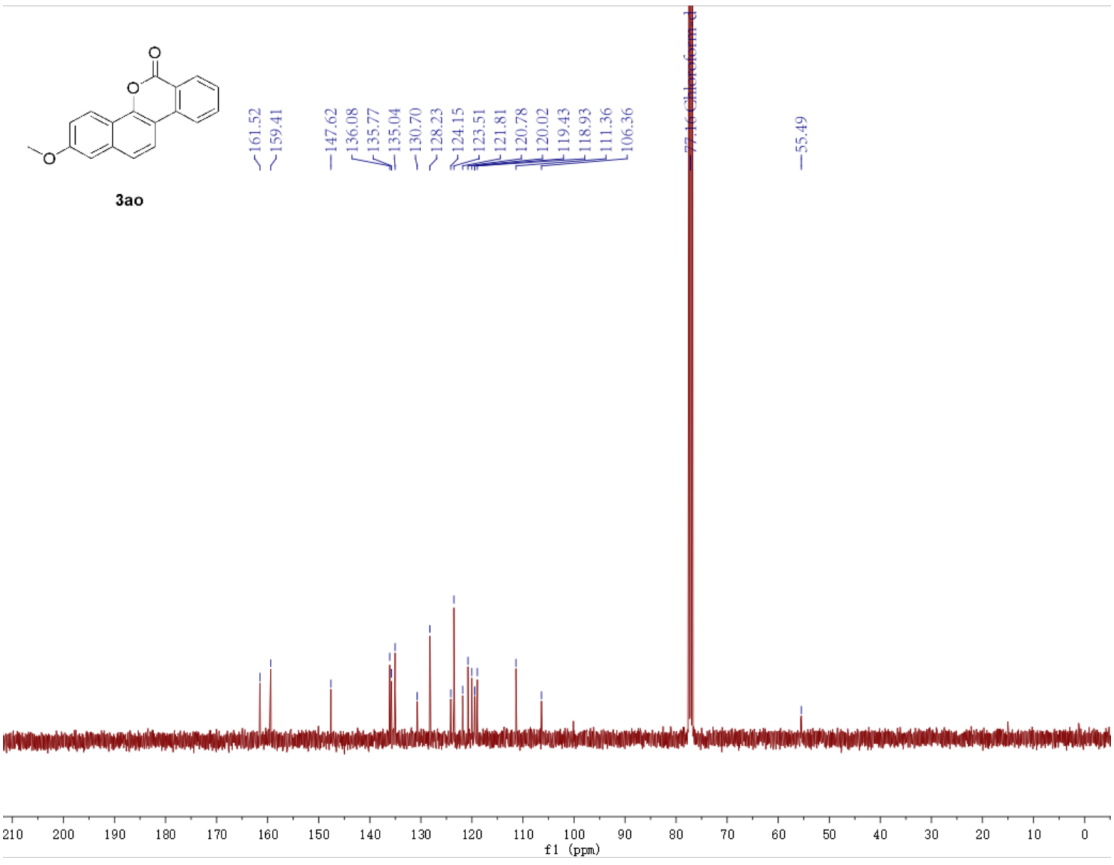

1.00
1.01
1.02
1.06
2.08
1.08
3.03
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

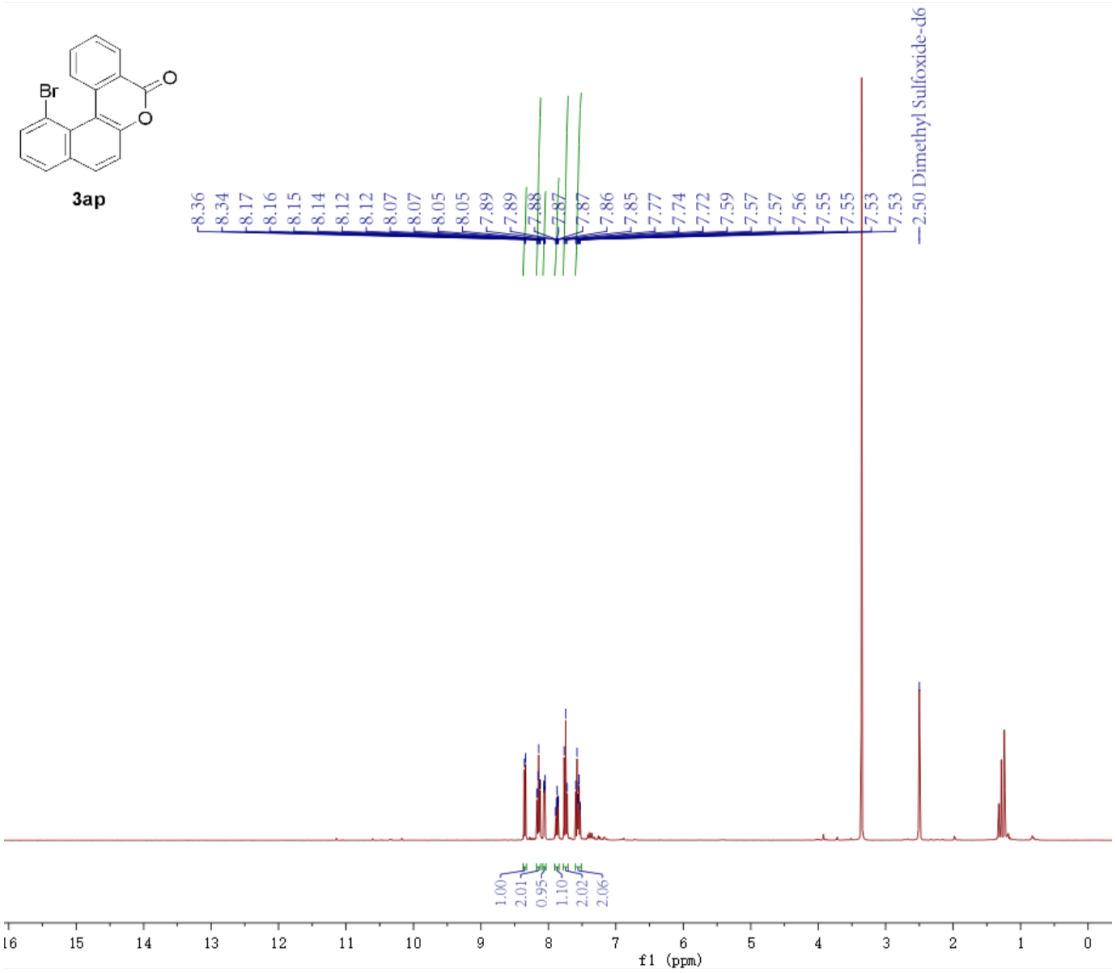


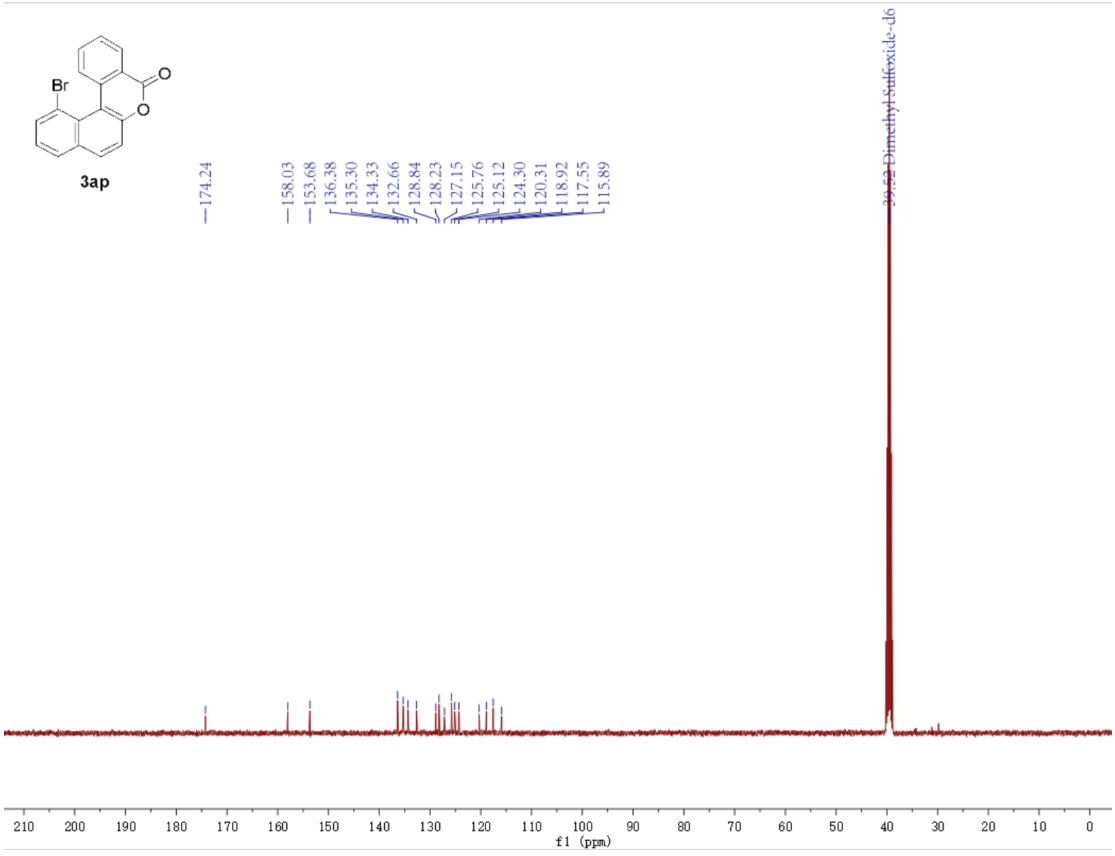
3an

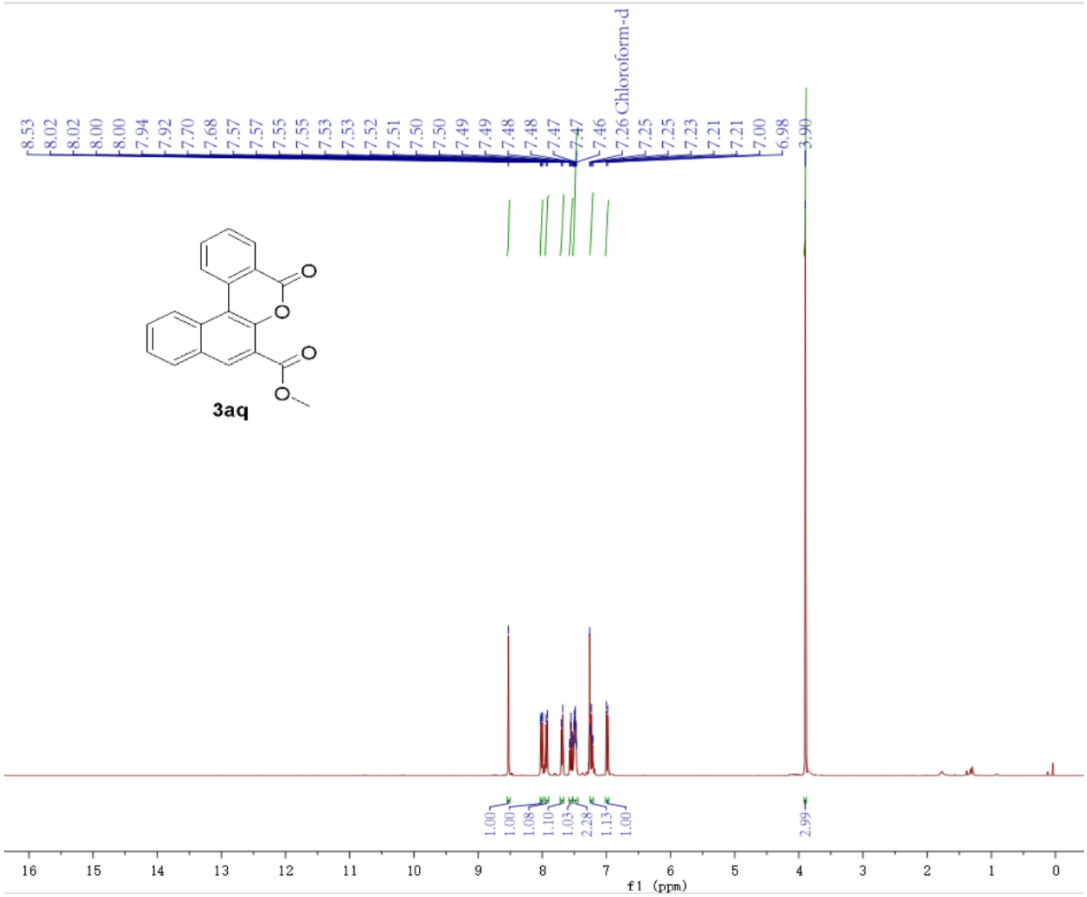
161.38
147.35
135.50
135.10
134.36
130.76
128.74
128.01
127.77
127.24
124.62
123.98
122.44
122.15
121.27
119.27
113.14
77.16 Chloroform-d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.47
8.45
8.44
8.44
8.42
8.42
8.14
8.12
8.01
7.99
7.85
7.85
7.83
7.81
7.81
7.64
7.62
7.58
7.57
7.56
7.54
7.54
7.27
7.26
7.26 Chloroform-d
7.24
7.24
7.15
7.15
3.95
3ao
1.97
1.07
1.00
1.01
1.01
1.09
1.59
1.08
2.95
f1 (ppm)


161.52
159.41
147.62
136.08
135.77
135.04
130.70
128.23
124.15
123.51
121.81
120.78
120.02
119.43
118.93
111.36
106.36
77.16 Chloroform-d
55.49
3ao
f1 (ppm)


Br
O
O
3ap
8.36
8.34
8.17
8.16
8.15
8.14
8.12
8.12
8.07
8.07
8.05
8.05
7.89
7.89
7.88
7.87
7.87
7.86
7.85
7.77
7.74
7.72
7.59
7.57
7.57
7.56
7.55
7.55
7.53
7.53
2.50 Dimethyl Sulfoxide-d6
1.00
2.01
0.95
1.10
2.02
2.06
f1 (ppm)


Br
O
O
3ap
174.24
158.03
153.68
136.38
135.30
134.33
132.66
128.84
128.23
127.15
125.76
125.12
124.30
120.31
118.92
117.55
115.89
39.52 Dimethyl Sulfoxide-d6
f1 (ppm)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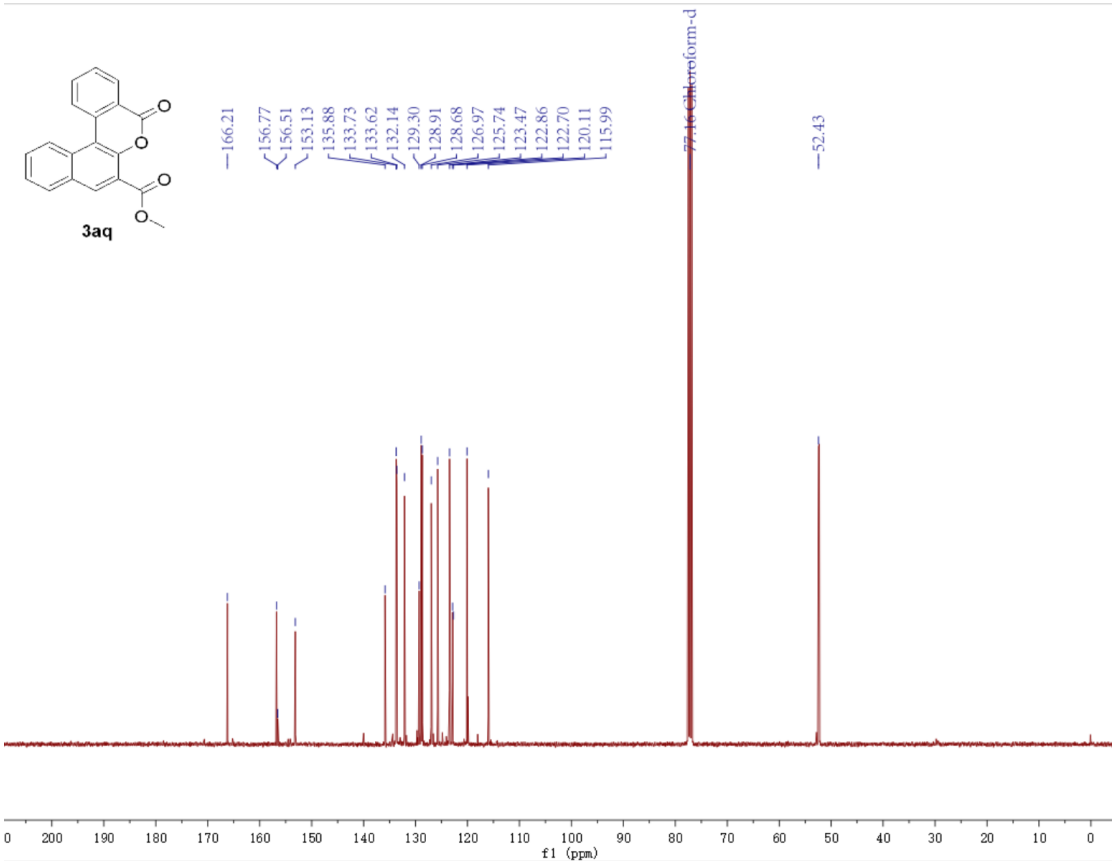
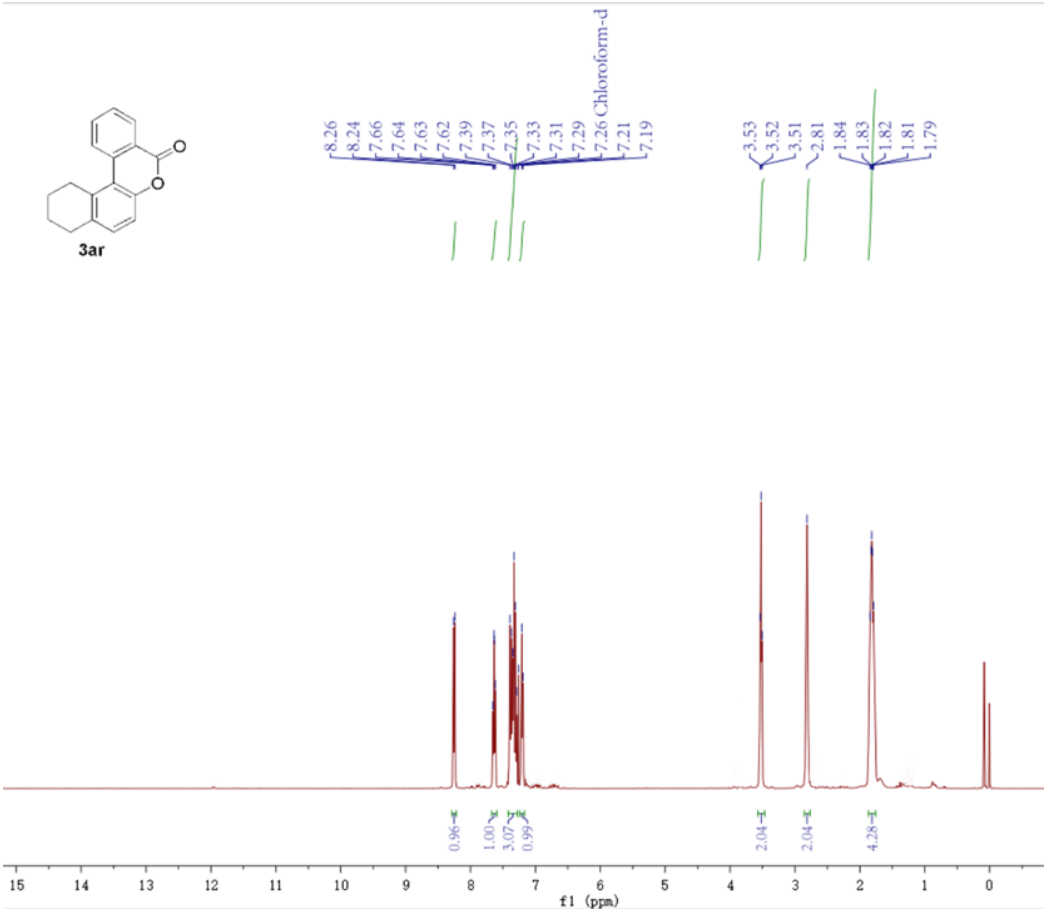
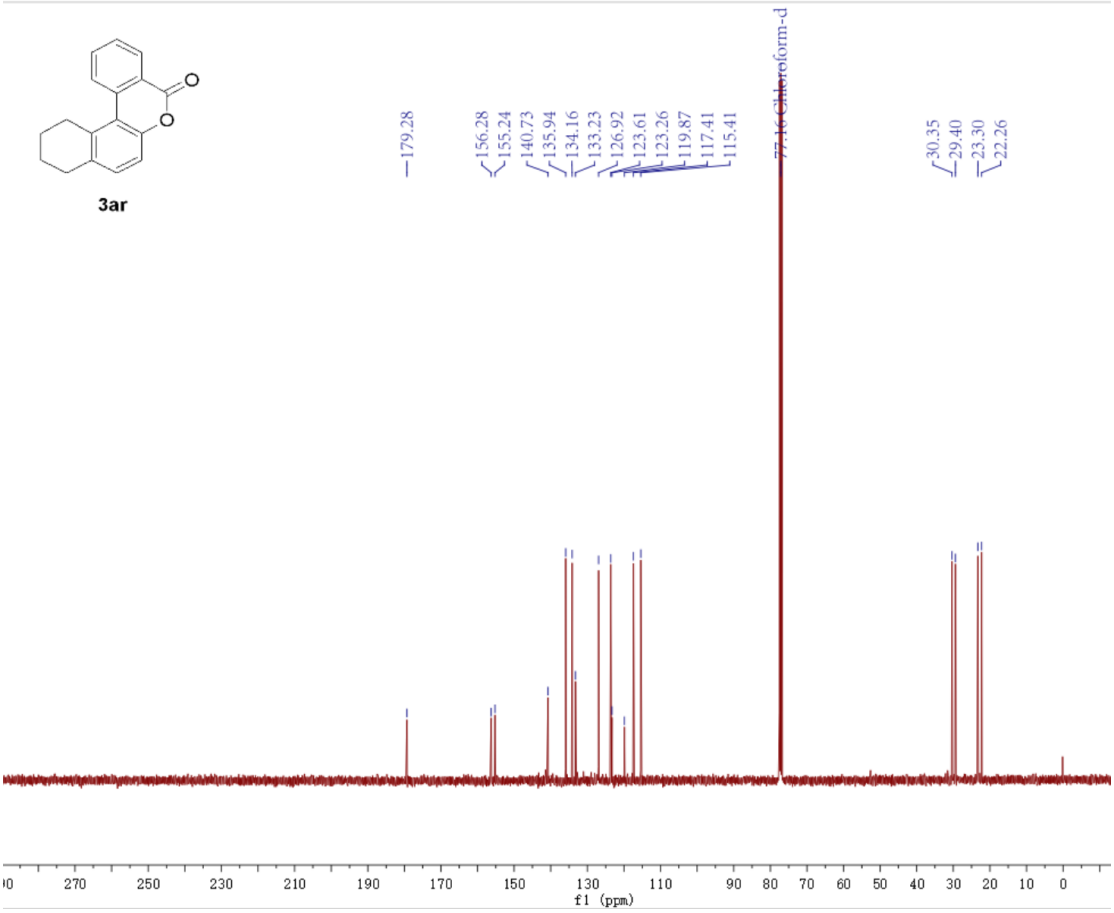
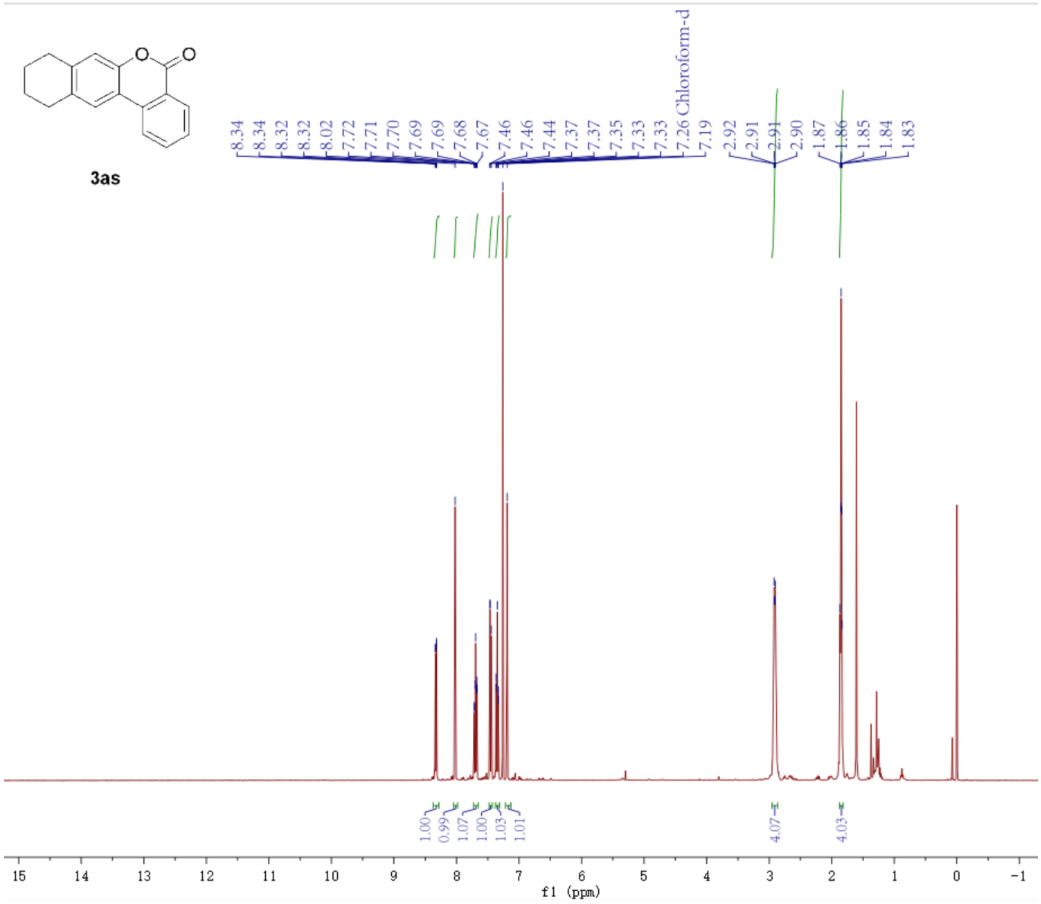
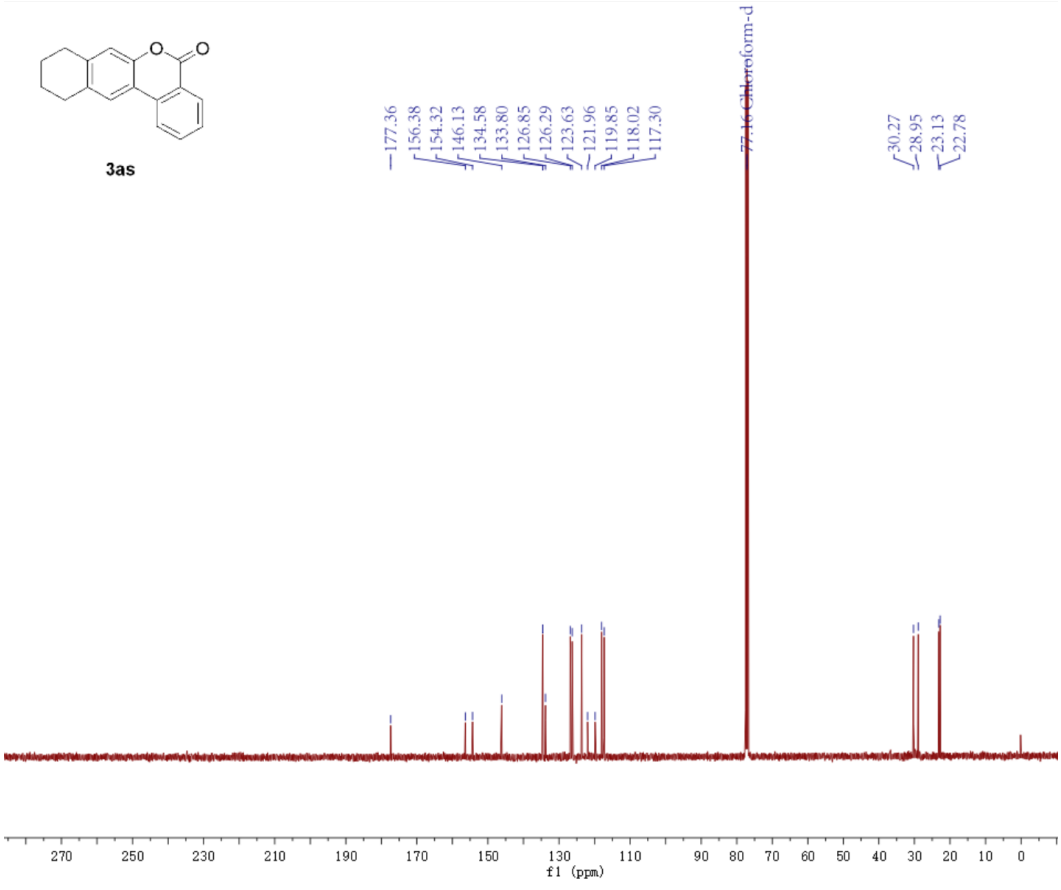
8.02
8.02
8.00
8.00
7.94
7.92
7.70
7.68
7.57
7.57
7.55
7.55
7.53
7.53
7.52
7.51
7.50
7.50
7.49
7.49
7.48
7.48
7.47
7.47
7.46
7.26 Chloroform-d
7.25
7.25
7.23
7.21
7.21
7.00
6.98
3.90
3aq
1.00
1.00
1.08
1.10
1.03
2.28
1.13
1.00
2.99
f1 (ppm)

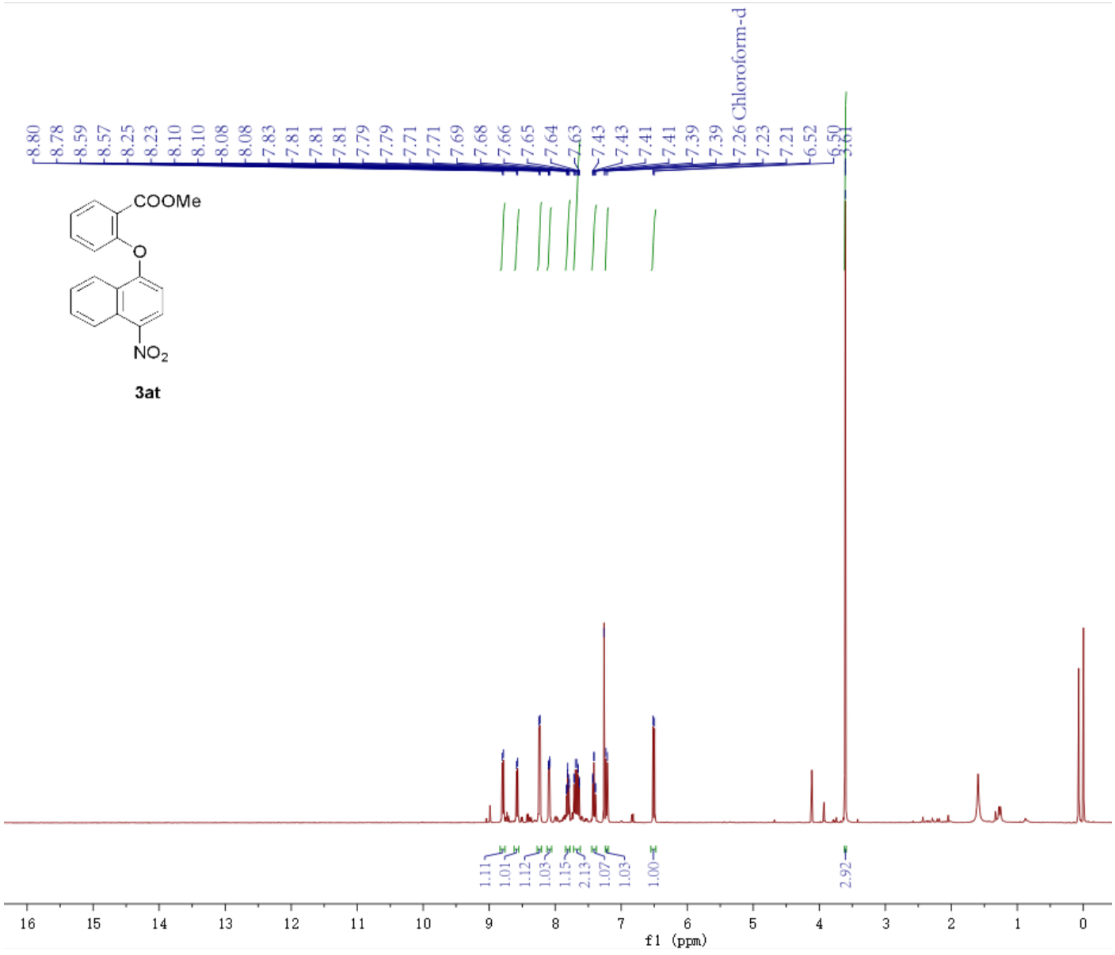

3aq
166.21
156.77
156.51
153.13
135.88
133.73
133.62
132.14
129.30
128.91
128.68
126.97
125.74
123.47
122.86
122.70
120.11
115.99
77.16 Chloroform-d
52.43
f1 (ppm)


3ar
8.26
8.24
7.66
7.64
7.63
7.62
7.39
7.37
7.35
7.33
7.31
7.29
7.26 Chloroform-d
7.21
7.19
3.53
3.52
3.51
2.81
1.84
1.83
1.82
1.81
1.79
0.96
1.00
3.07
0.99
2.04
2.04
4.28
f1 (ppm)


3ar
179.28
156.28
155.24
140.73
135.94
134.16
133.23
126.92
123.61
123.26
119.87
117.41
115.41
77.16 Chloroform-d
30.35
29.40
23.30
22.26
f1 (ppm)


3as
8.34
8.34
8.32
8.32
8.02
7.72
7.71
7.70
7.69
7.69
7.68
7.67
7.46
7.46
7.44
7.37
7.37
7.35
7.33
7.33
7.26 Chloroform-d
7.19
2.92
2.91
2.91
2.90
1.87
1.86
1.85
1.84
1.83
1.00
0.99
1.07
1.00
1.03
1.01
4.07
4.03
f1 (ppm)


3as
177.36
156.38
154.32
146.13
134.58
133.80
126.85
126.29
123.63
121.96
119.85
118.02
117.30
77.16 Chloroform-d
30.27
28.95
23.13
22.78
f1 (ppm)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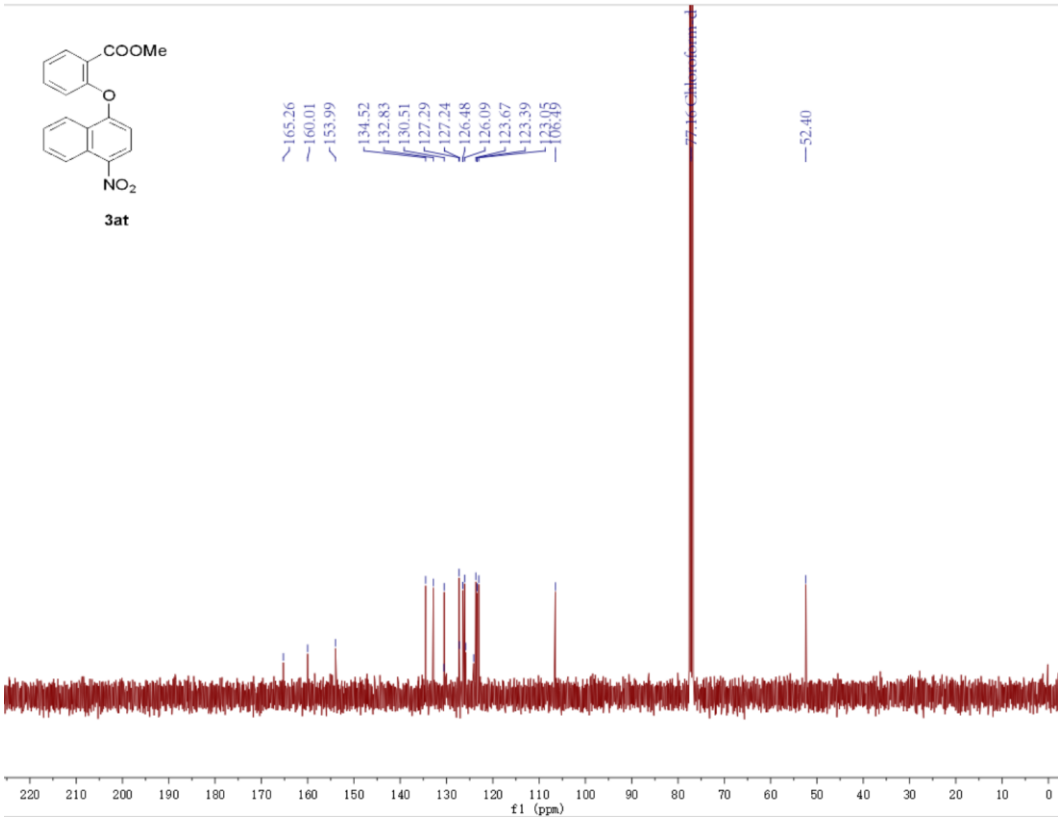
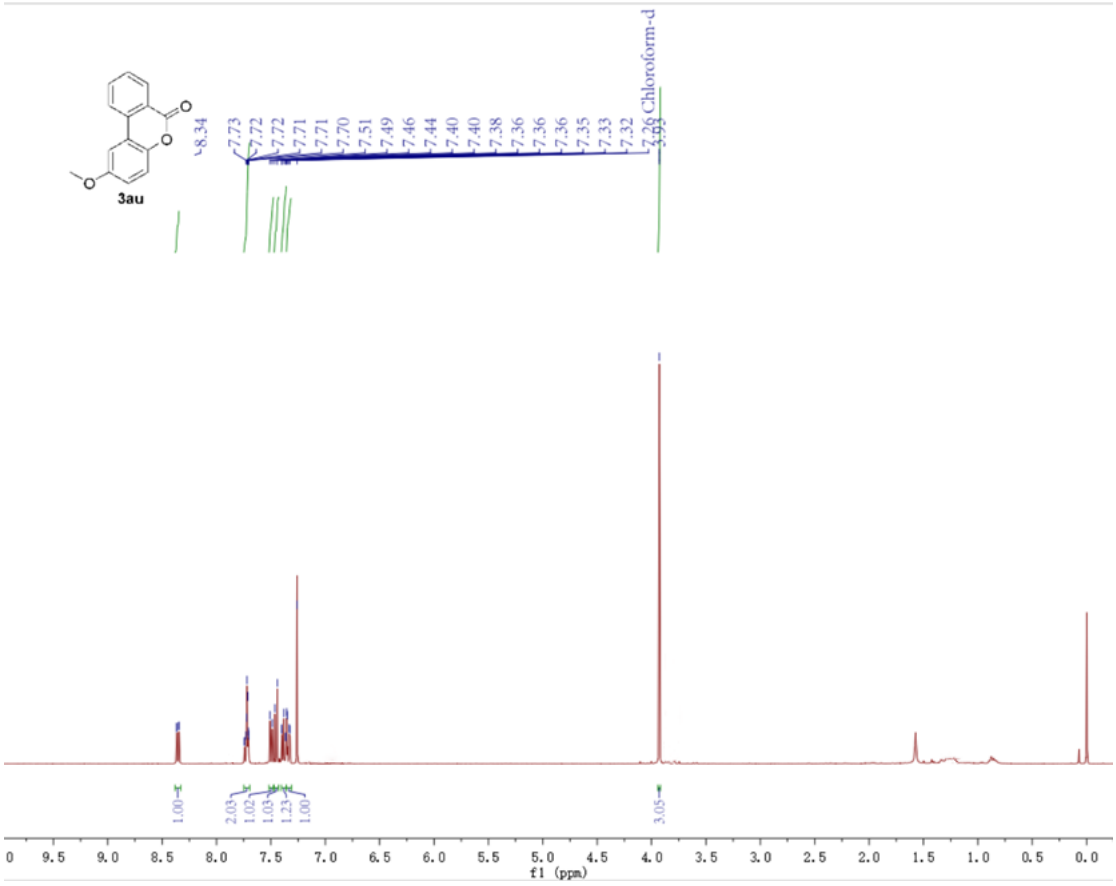
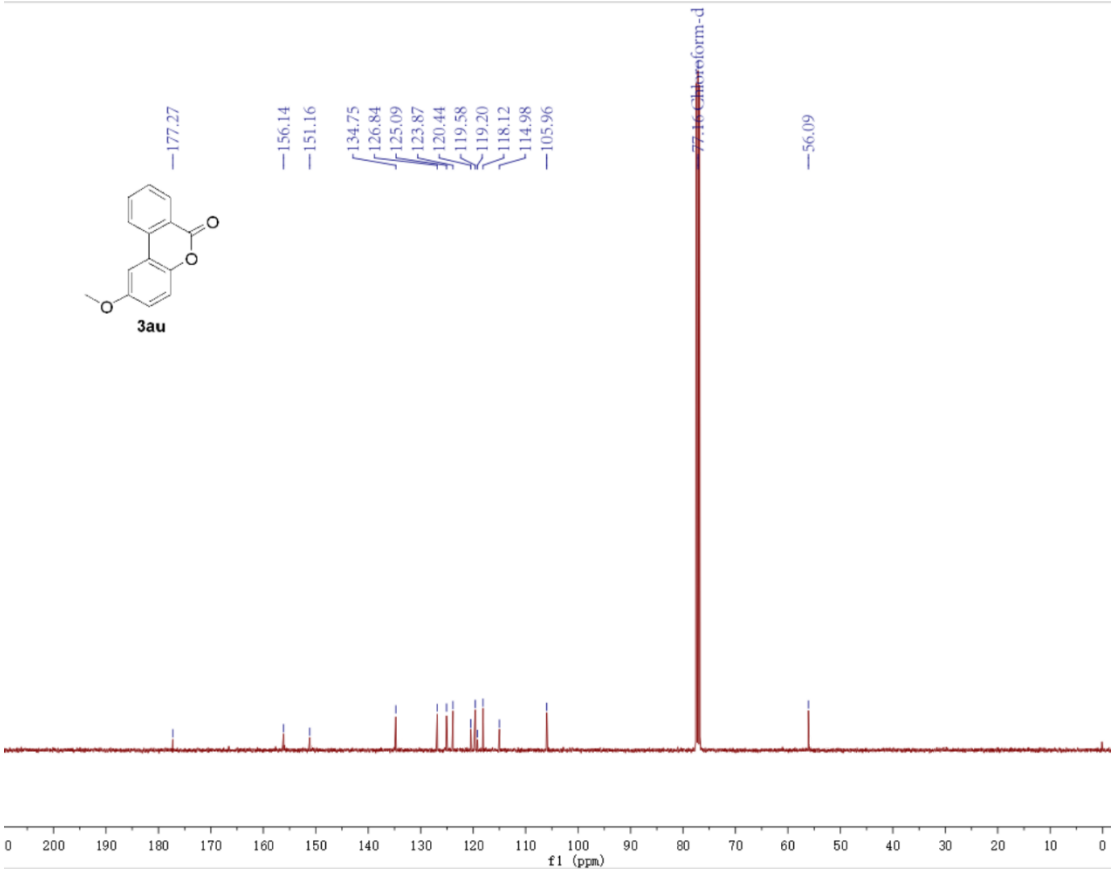
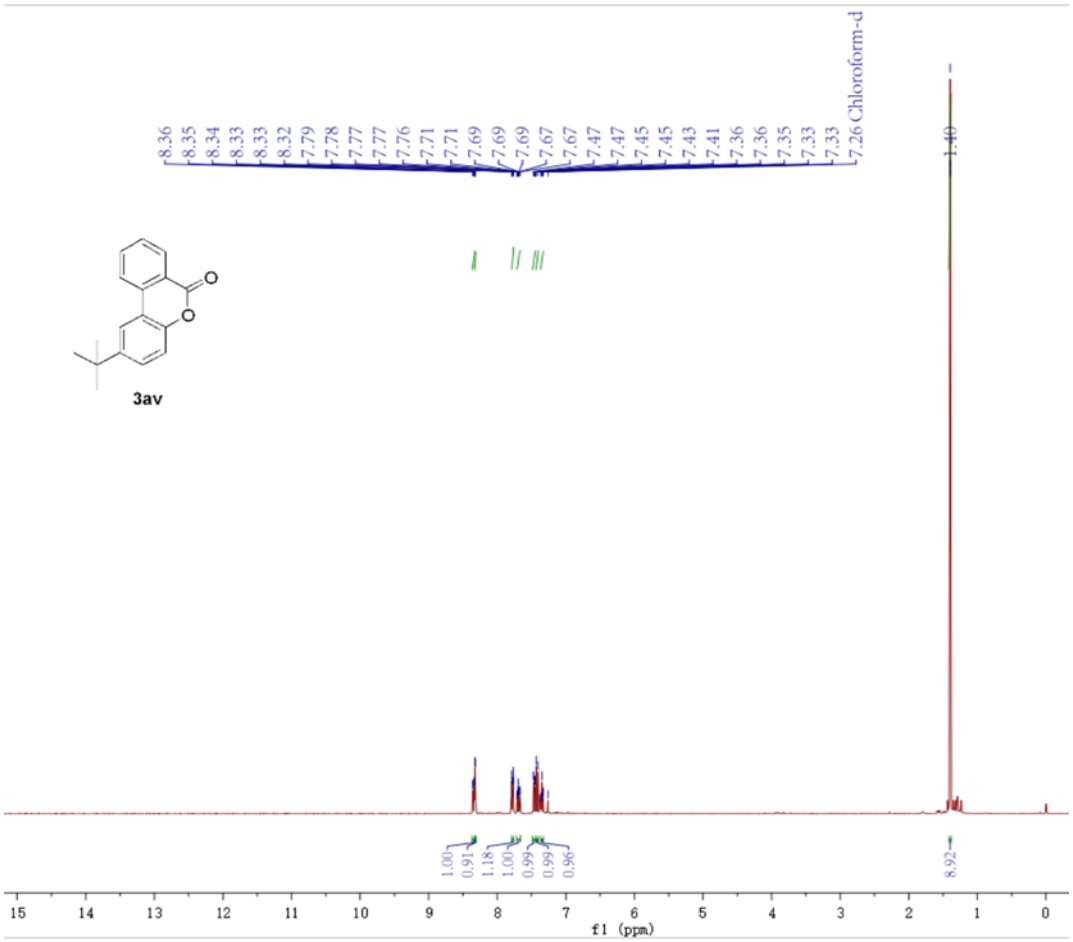
8.78
8.59
8.57
8.25
8.23
8.10
8.10
8.08
8.08
7.83
7.81
7.81
7.81
7.79
7.79
7.71
7.71
7.69
7.68
7.66
7.65
7.64
7.63
7.43
7.43
7.41
7.41
7.39
7.39
7.26 Chloroform-d
7.23
7.21
6.52
6.50
3.61
COOMe
O
NO2
3at
1.11
1.01
1.12
1.03
1.15
2.13
1.07
1.03
1.00
2.92
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


COOMe
O
NO2
3at
165.26
160.01
153.99
134.52
132.83
130.51
127.29
127.24
126.48
126.09
123.67
123.39
123.05
106.48
77.16 Chloroform-d
52.40
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


3au
8.34
7.73
7.72
7.72
7.71
7.71
7.70
7.51
7.49
7.46
7.44
7.40
7.40
7.38
7.36
7.36
7.36
7.35
7.33
7.32
7.26 Chloroform-d
3.93
1.00
2.03
1.02
1.03
1.23
1.00
3.05
f1 (ppm)


177.27
156.14
151.16
134.75
126.84
125.09
123.87
120.44
119.58
119.20
118.12
114.98
105.96
77.16 Chloroform-d
56.09
3au
f1 (ppm)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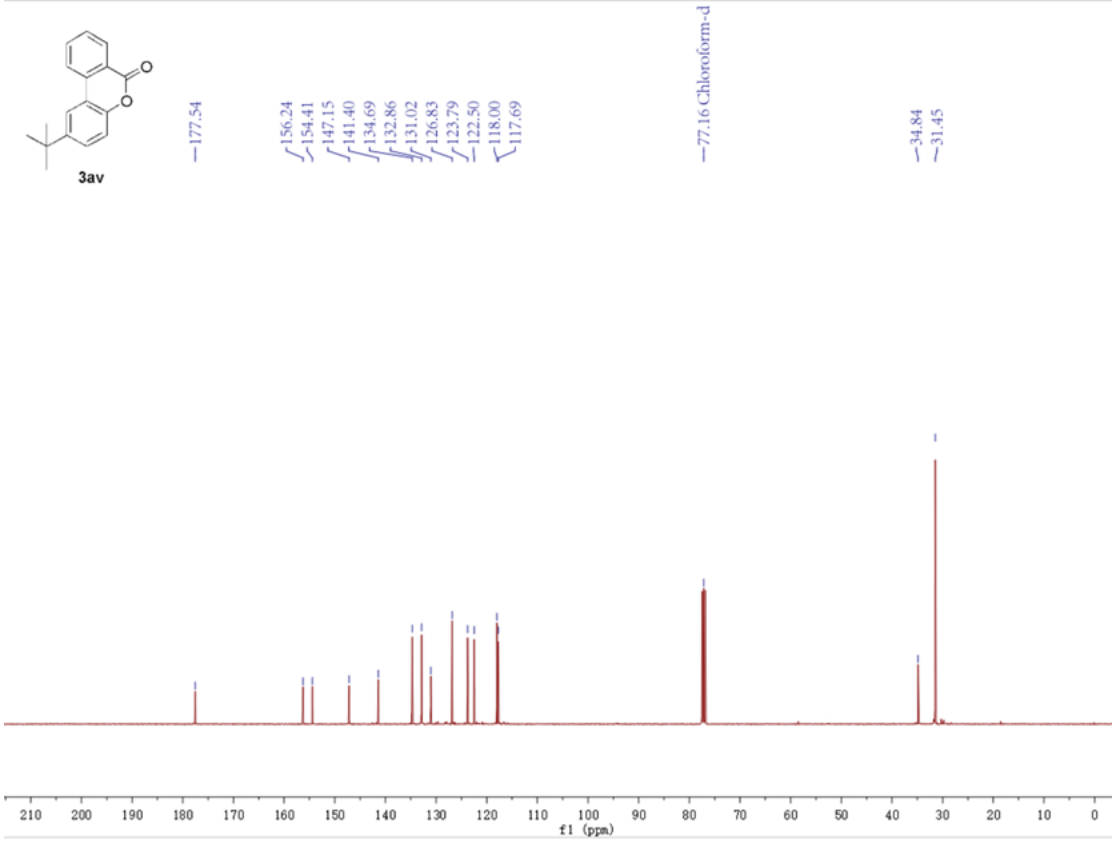
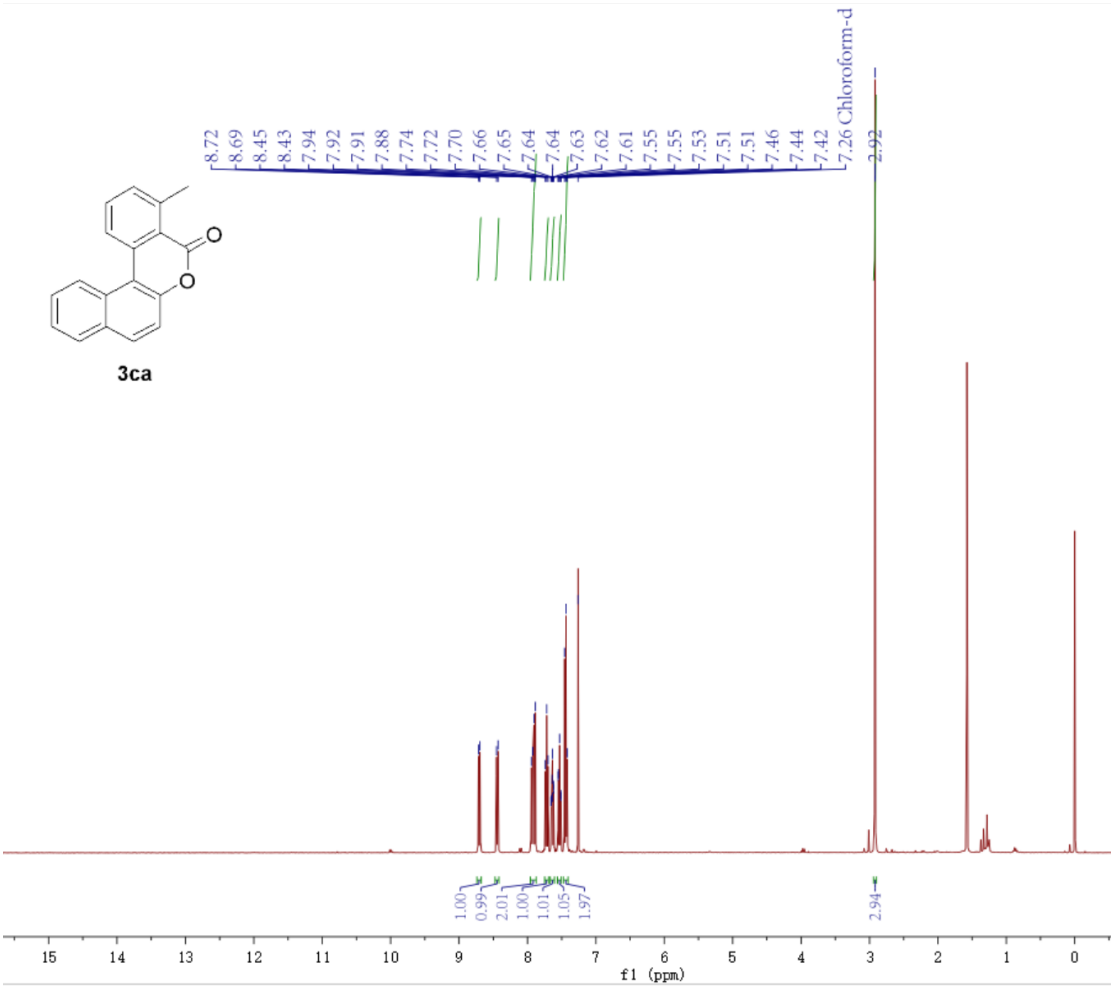
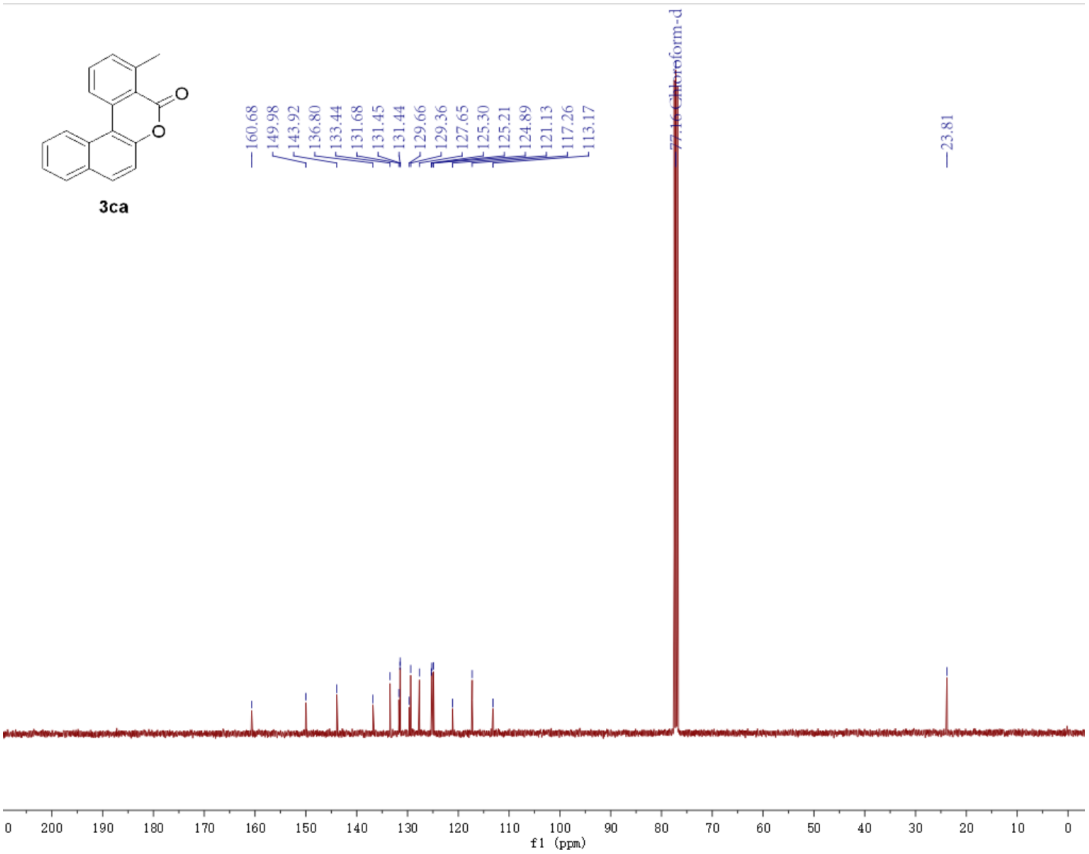
8.35
8.34
8.33
8.33
8.32
7.79
7.78
7.77
7.77
7.76
7.71
7.71
7.69
7.69
7.69
7.67
7.67
7.47
7.47
7.45
7.45
7.43
7.41
7.36
7.36
7.35
7.33
7.26 Chloroform-d
1.40
3av
1.00
0.91
1.18
1.00
0.99
0.99
0.96
8.92
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


3av
177.54
156.24
154.41
147.15
141.40
134.69
132.86
131.02
126.83
123.79
122.50
118.00
117.69
77.16 Chloroform-d
34.84
31.45
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.72
8.69
8.45
8.43
7.94
7.92
7.91
7.88
7.74
7.72
7.70
7.66
7.65
7.64
7.64
7.63
7.62
7.61
7.55
7.55
7.53
7.51
7.51
7.46
7.44
7.42
7.26 Chloroform-d
2.92
3ca
1.00
0.99
2.01
1.00
1.01
1.05
1.97
2.94
f1 (ppm)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149.98
143.92
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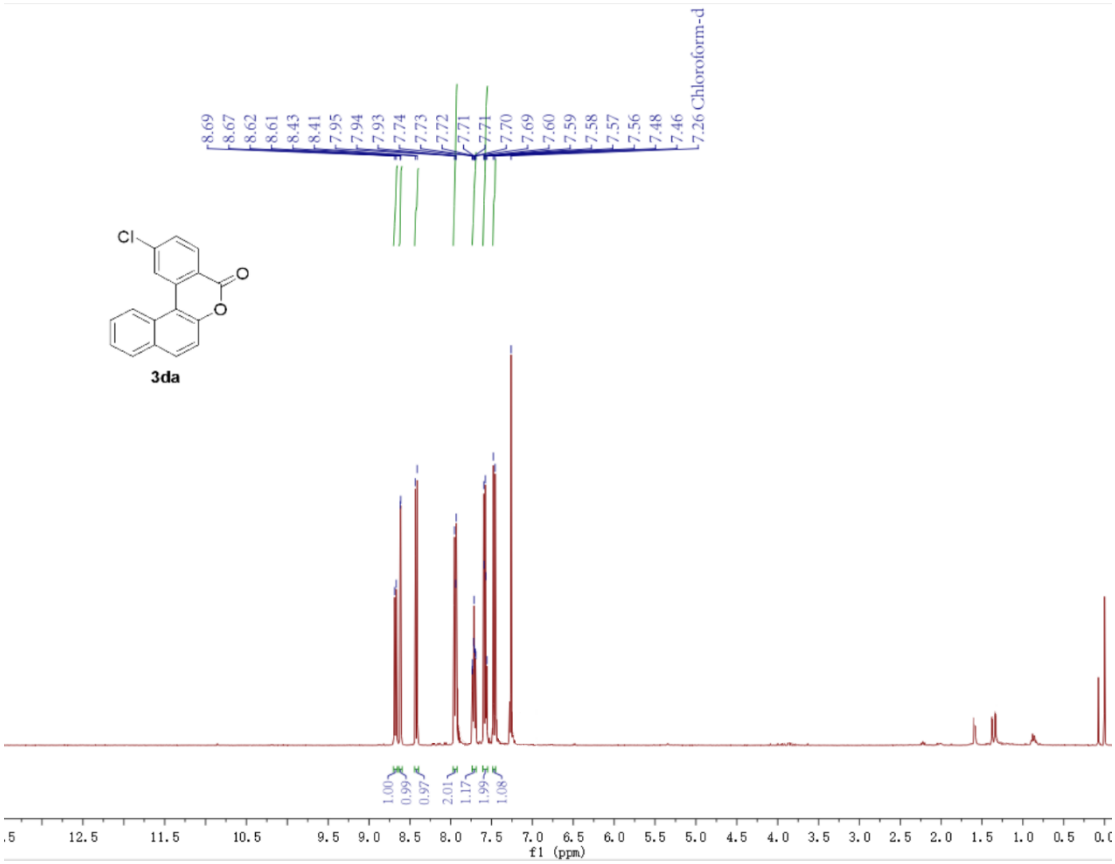
133.44
131.68
131.45
131.44
129.66
129.36
127.65
125.30
125.21
124.89
121.13
117.26
113.17
77.16 Chloroform-d
23.81
3ca
f1 (ppm)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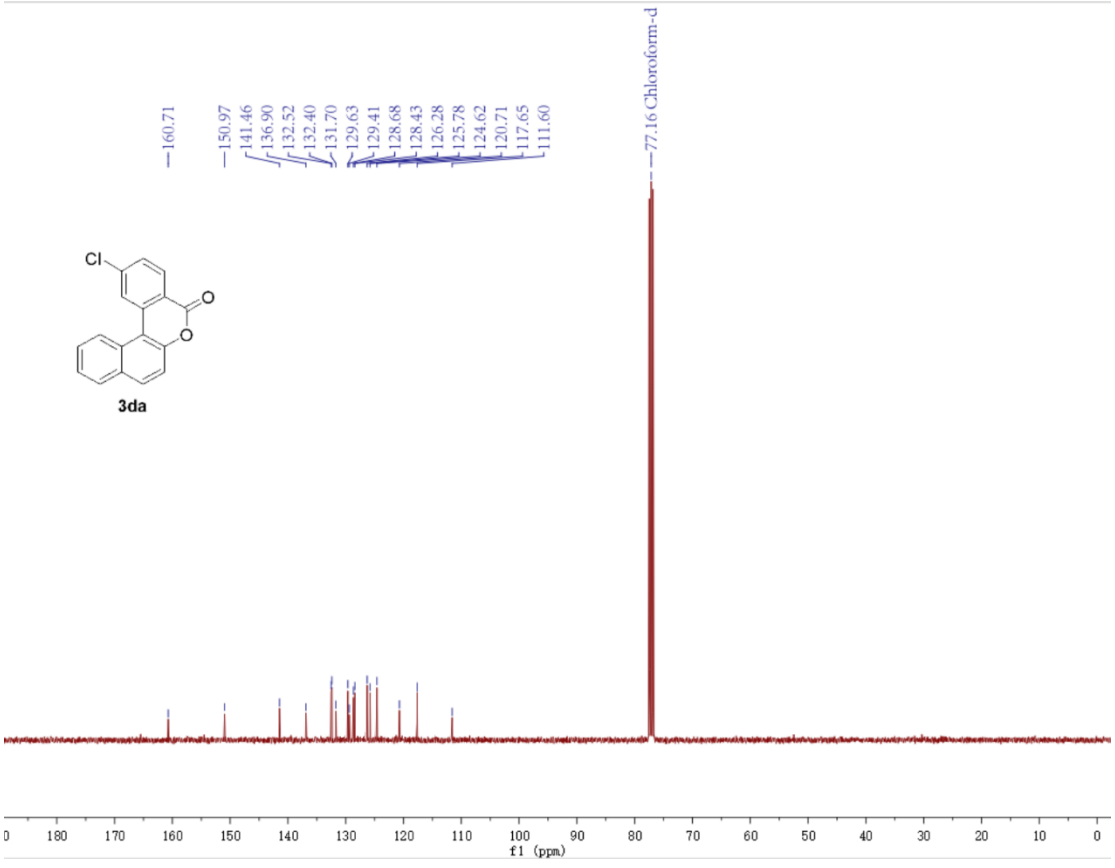
8.67
8.62
8.61
8.43
8.41
7.95
7.94
7.93
7.74
7.73
7.72
7.71
7.71
7.70
7.69
7.60
7.59
7.58
7.57
7.56
7.48
7.46
7.26 Chloroform-d
Cl
O
O
3da
1.00
0.99
0.97
2.01
1.17
1.99
1.08
f1 (ppm)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150.97
141.46
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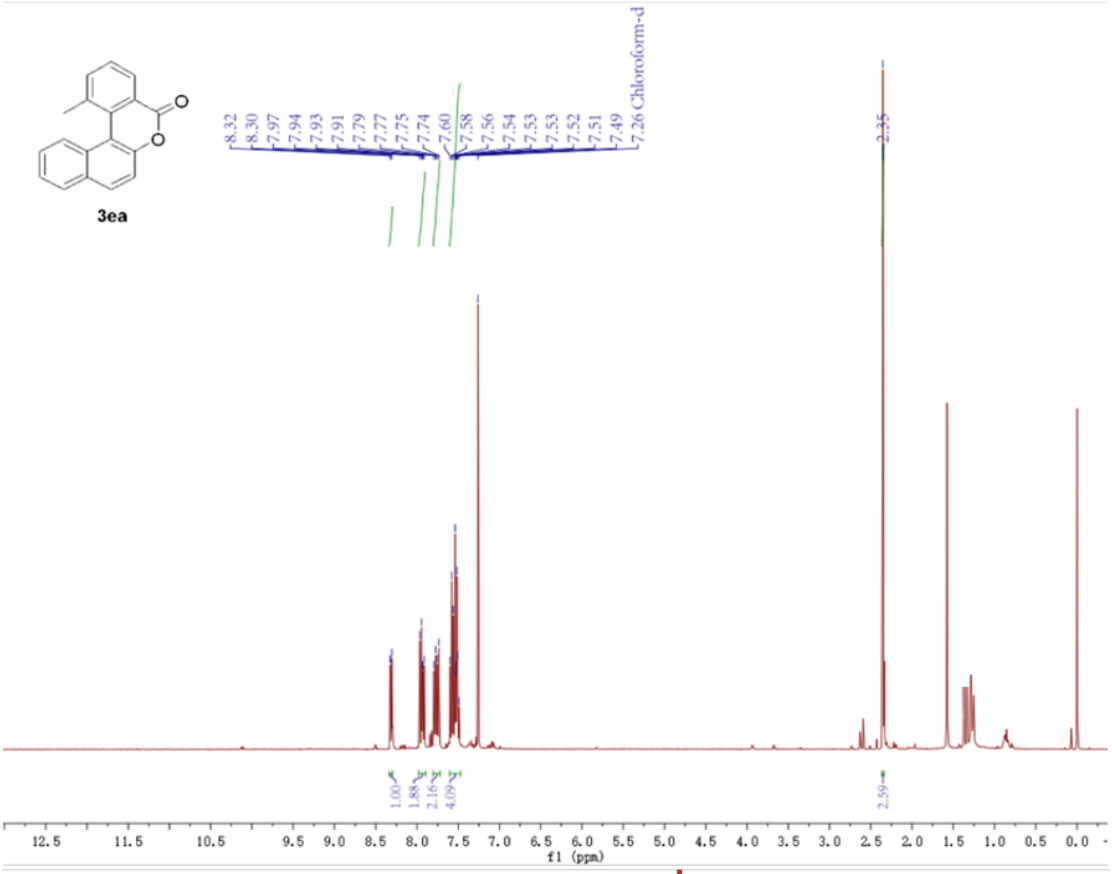
132.52
132.40
131.70
129.63
129.41
128.68
128.43
126.28
125.78
124.62
120.71
117.65
111.60
77.16 Chloroform-d
Cl
O
O
3da
f1 (ppm)


3ea
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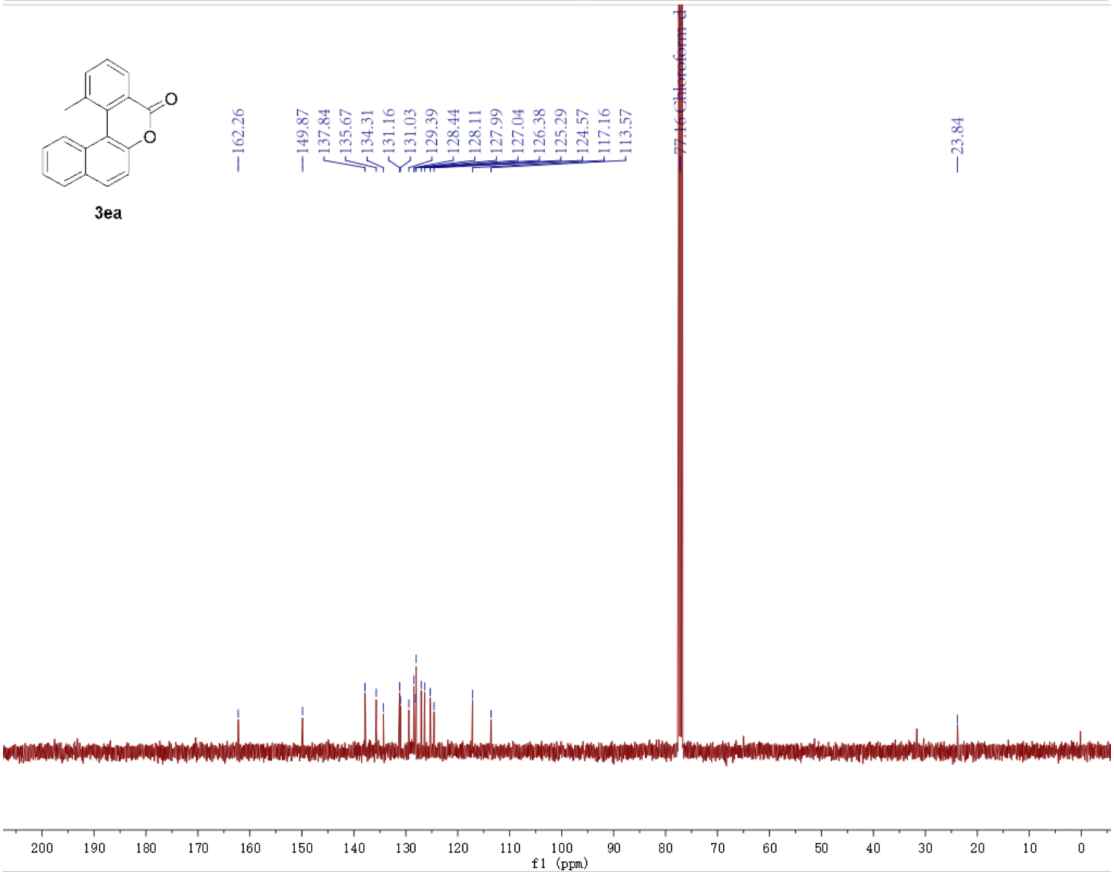
8.30
7.97
7.94
7.93
7.91
7.79
7.77
7.75
7.74
7.60
7.58
7.56
7.54
7.53
7.53
7.52
7.51
7.49
7.26 Chloroform-d
2.35
1.00
1.88
2.16
4.09
2.59
f1 (ppm)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134.31
131.16
131.03
129.39
128.44
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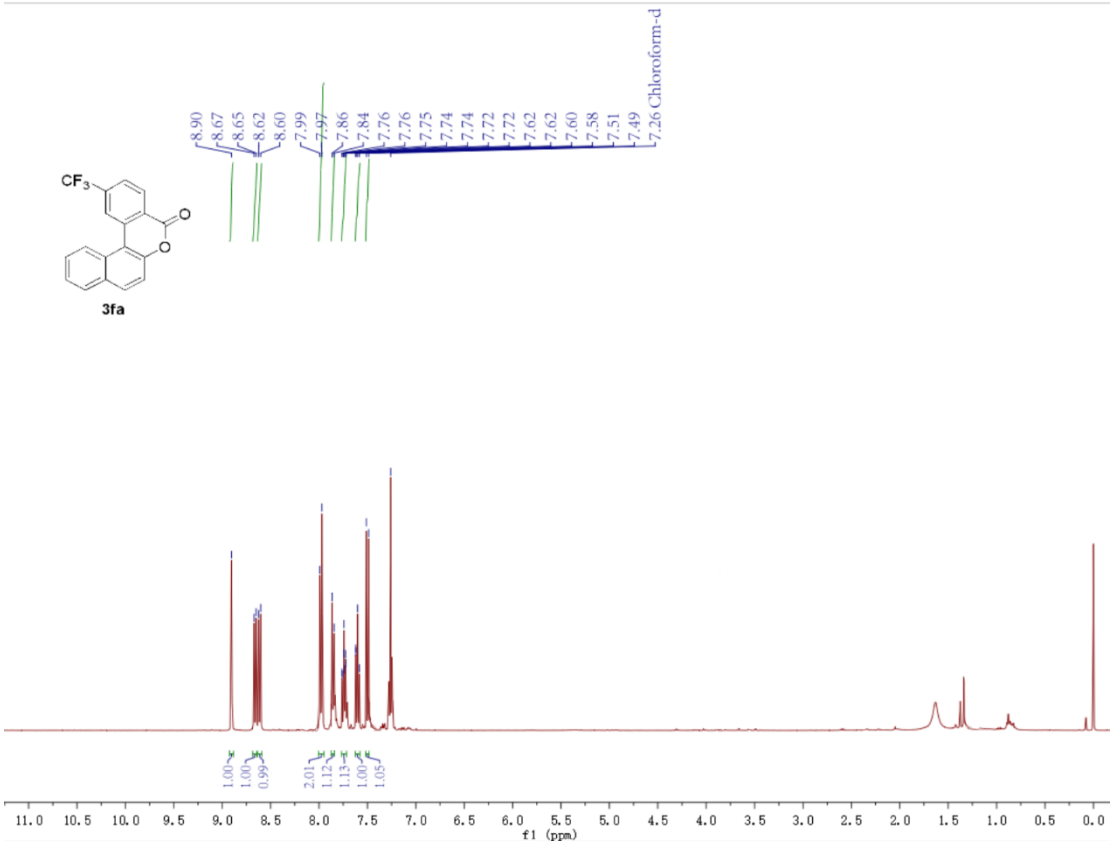
127.04
126.38
125.29
124.57
117.16
113.57
77.16 Chloroform-d
23.84
f1 (ppm)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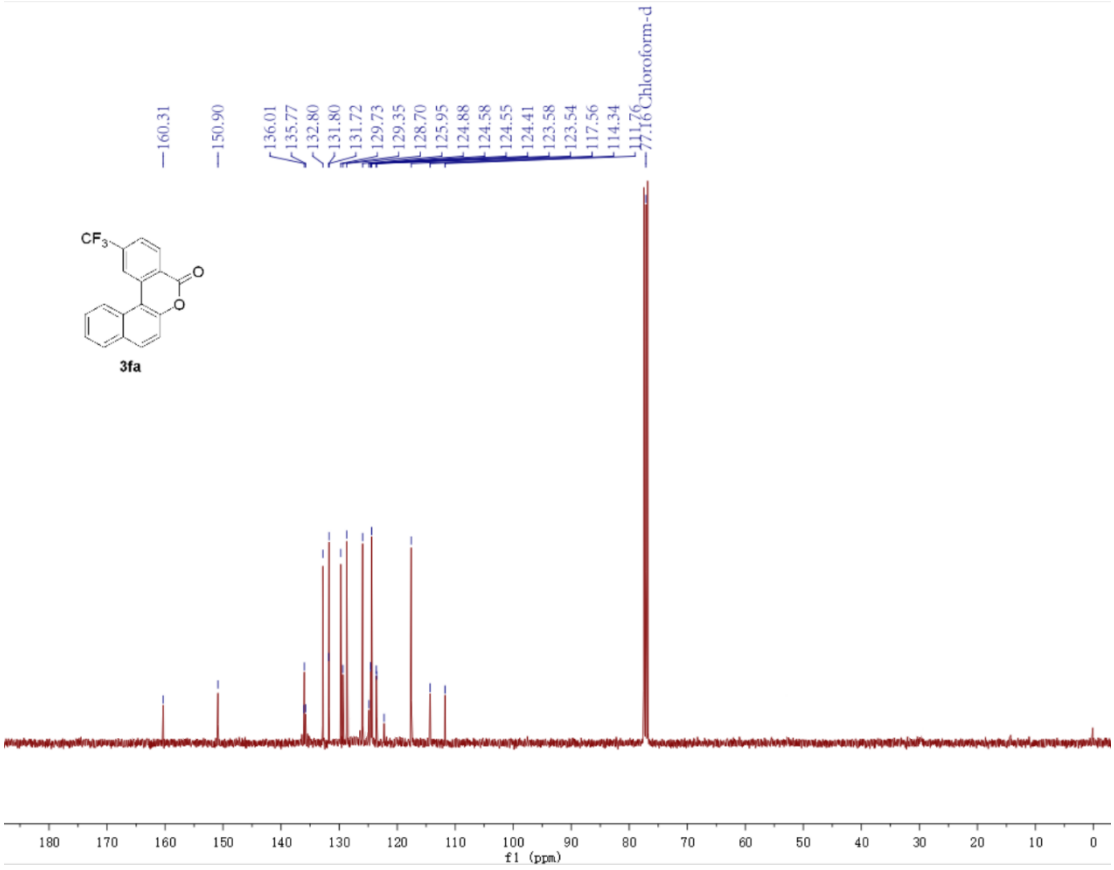
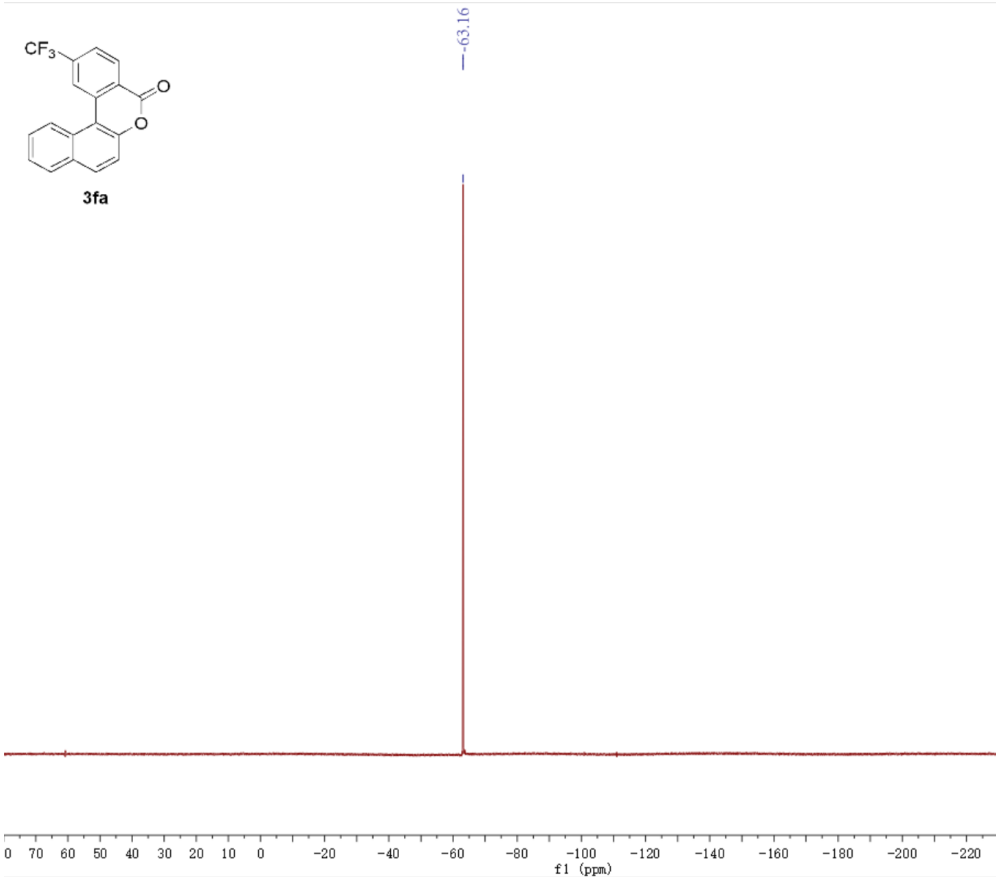
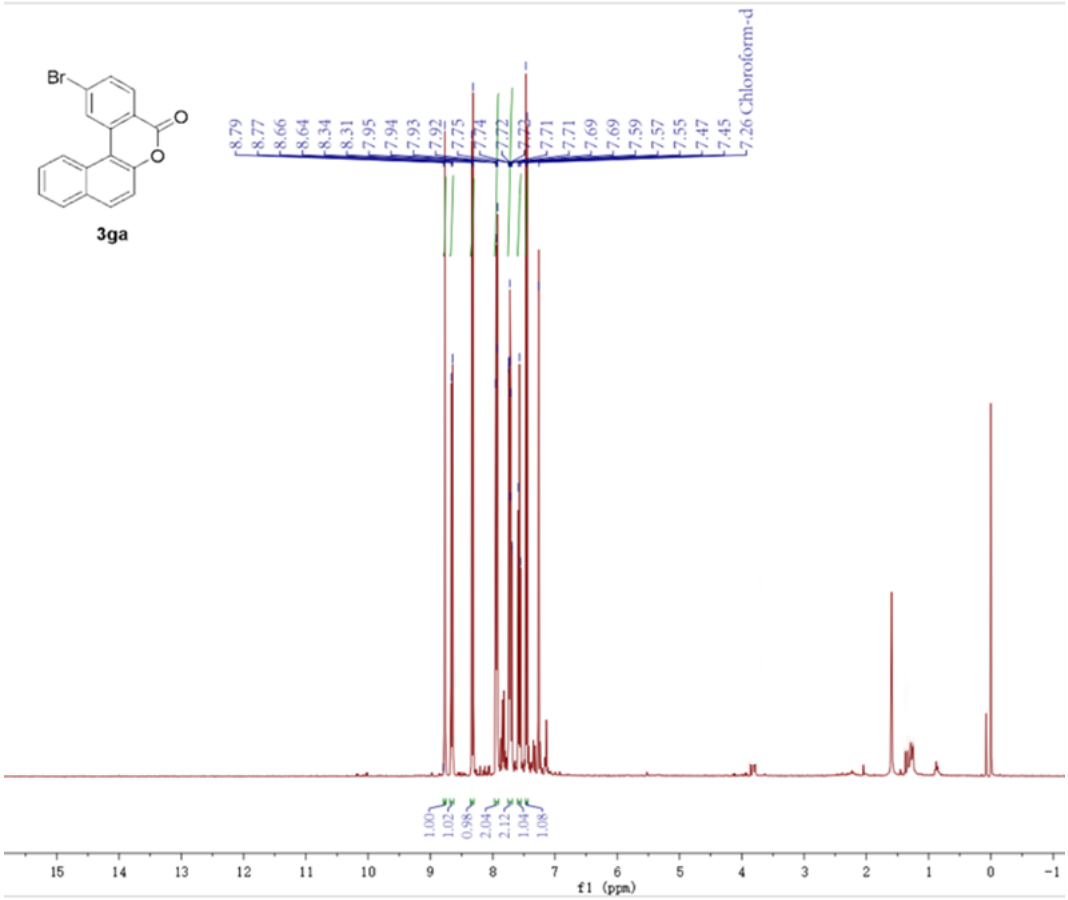
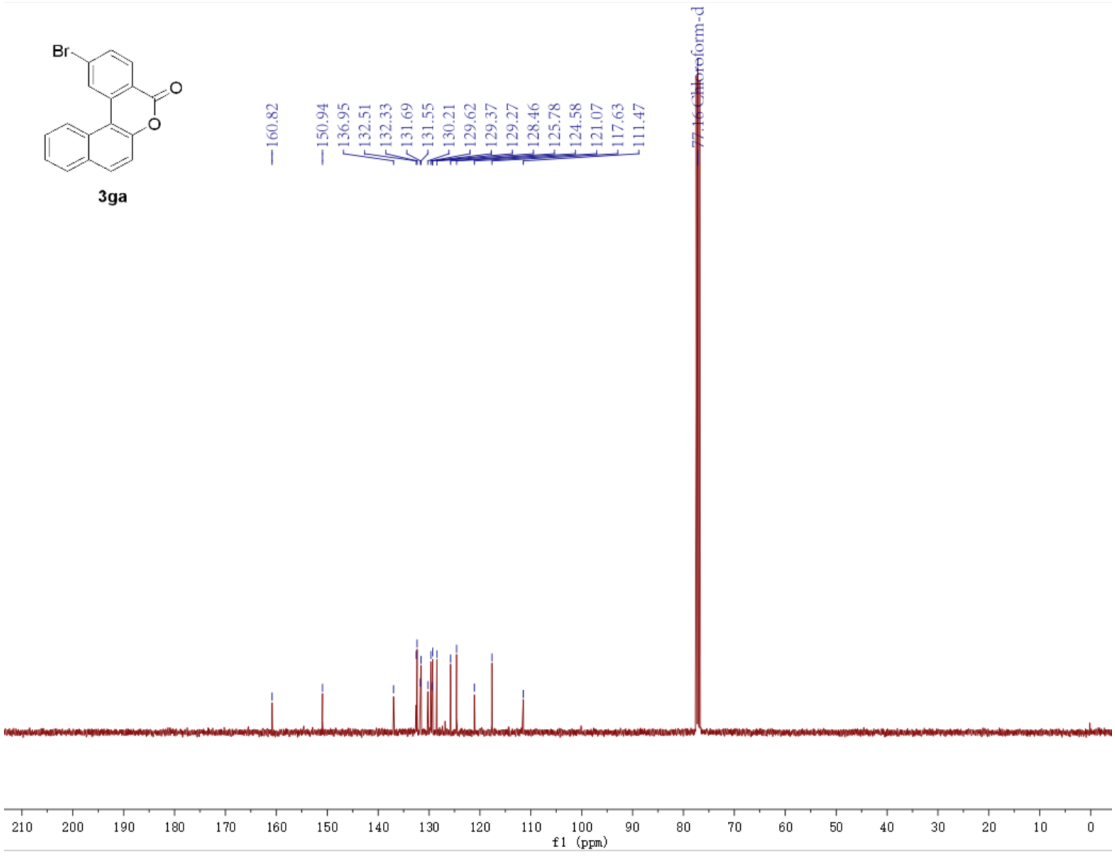
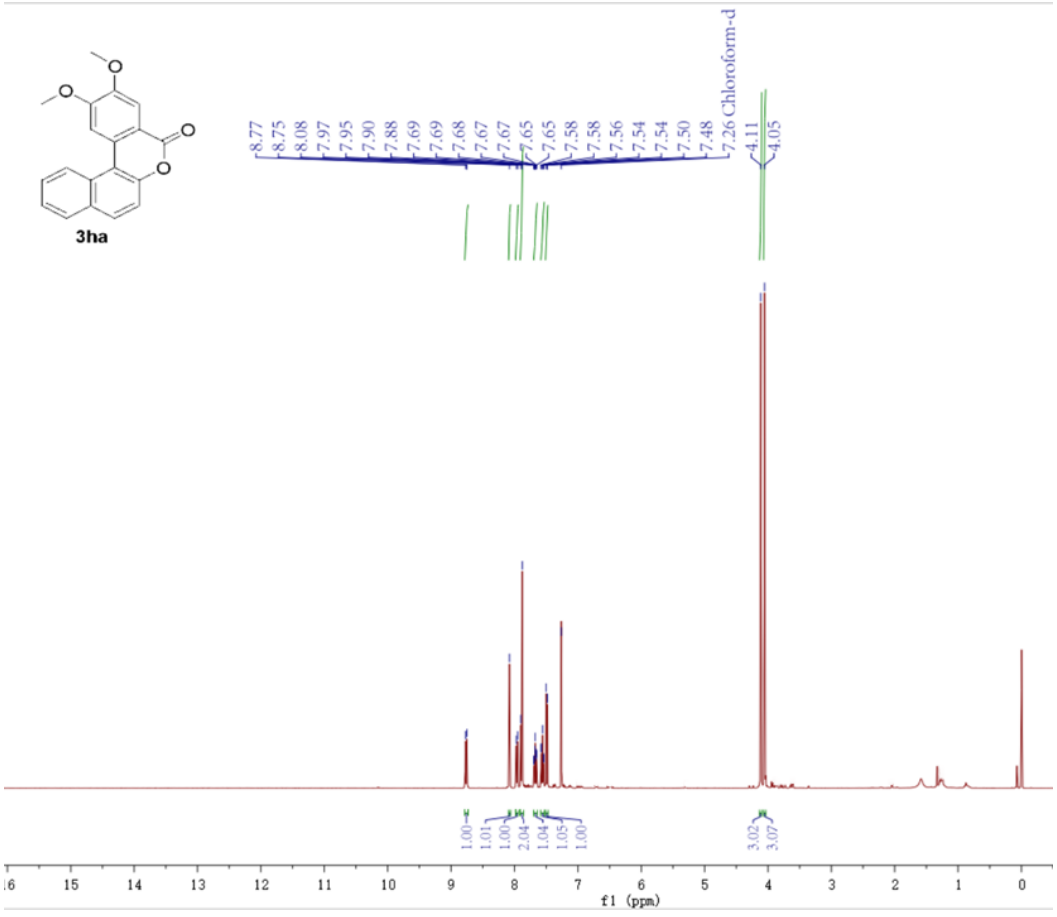
8.67
8.65
8.62
8.60
7.99
7.97
7.86
7.84
7.76
7.76
7.75
7.74
7.74
7.72
7.72
7.62
7.62
7.60
7.58
7.51
7.49
7.26 Chloroform-d
CF3
O
O
3fa
1.00
1.00
0.99
2.01
1.12
1.13
1.00
1.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


160.31
150.90
136.01
135.77
132.80
131.80
131.72
129.73
129.35
128.70
125.95
124.88
124.58
124.55
124.41
123.58
123.54
117.56
114.34
111.76
77.16 Chloroform-d
CF3
O
O
3fa
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


CF3
O
O
3fa
-63.16
0 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220
f1 (ppm)


Br
O
O
3ga
8.79
8.77
8.66
8.64
8.34
8.31
7.95
7.94
7.93
7.92
7.75
7.74
7.72
7.71
7.71
7.69
7.69
7.59
7.57
7.55
7.47
7.45
7.26 Chloroform-d
1.00
1.02
0.98
2.04
2.12
1.04
1.08
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


Br
O
O
3ga
160.82
150.94
136.95
132.51
132.33
131.69
131.55
130.21
129.62
129.37
129.27
128.46
125.78
124.58
121.07
117.63
111.47
77.16 Chloroform-d
f1 (ppm)


O
O
O
3ha
8.77
8.75
8.08
7.97
7.95
7.90
7.88
7.69
7.69
7.68
7.67
7.67
7.65
7.65
7.58
7.58
7.56
7.54
7.54
7.50
7.48
7.26 Chloroform-d
4.11
4.05
1.00
1.01
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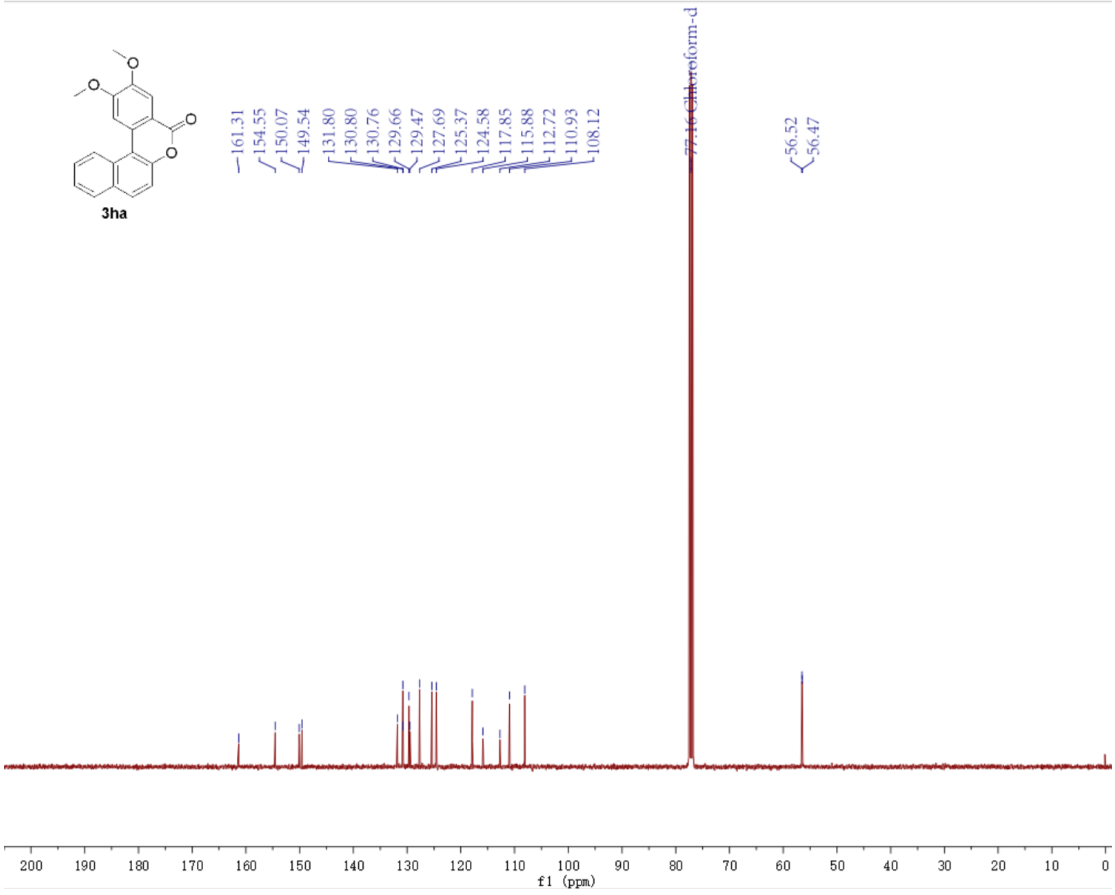
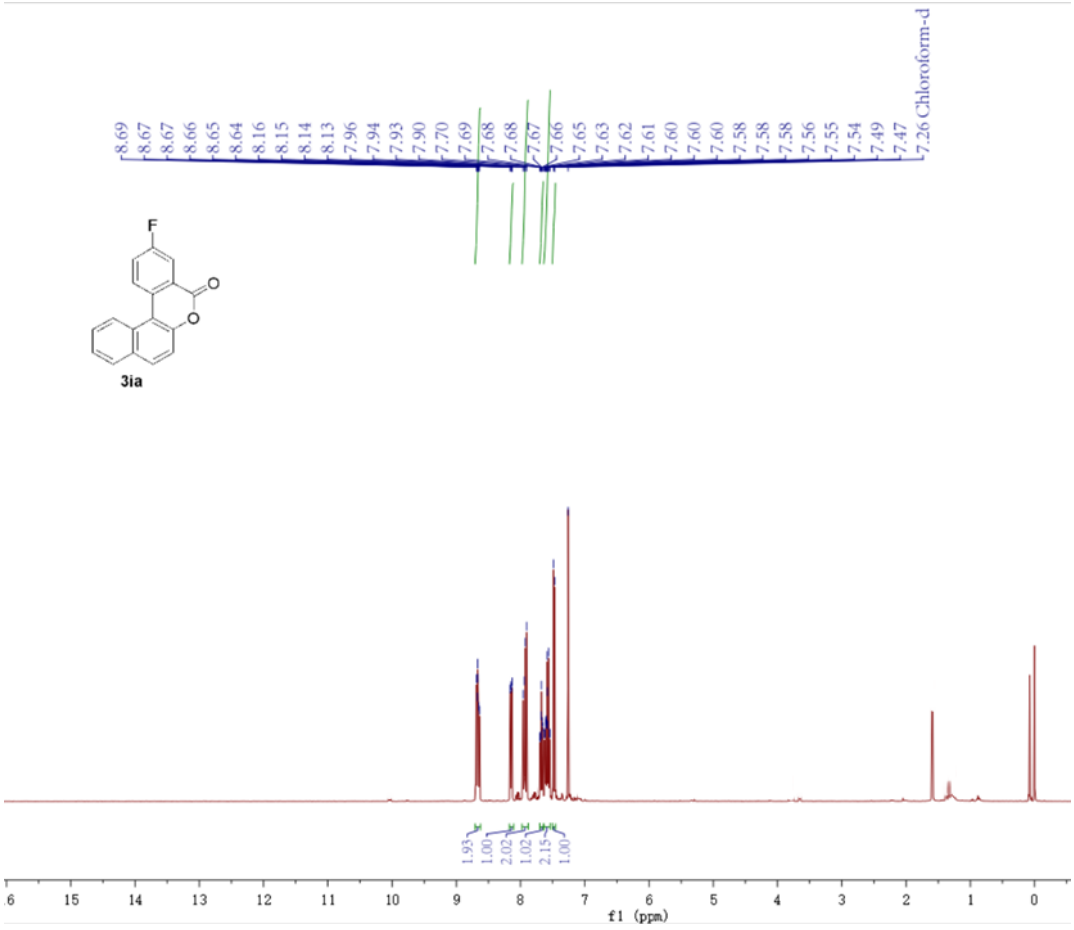
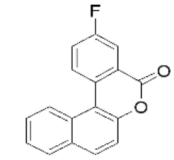
1.04
1.05
1.00
3.02
3.07
f1 (ppm)

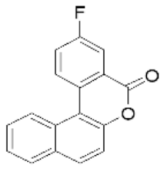

3ha
161.31
154.55
150.07
149.54
131.80
130.80
130.76
129.66
129.47
127.69
125.37
124.58
117.85
115.88
112.72
110.93
108.12
77.16 Chloroform-d
56.52
56.47
f1 (ppm)


3ia
F
8.69
8.67
8.67
8.66
8.65
8.64
8.16
8.15
8.14
8.13
7.96
7.94
7.93
7.90
7.70
7.69
7.68
7.68
7.67
7.66
7.65
7.63
7.62
7.61
7.60
7.60
7.60
7.58
7.58
7.58
7.56
7.55
7.54
7.49
7.47
7.26 Chloroform-d
1.93
1.00
2.02
1.02
2.15
1.00
f1 (ppm)


F
O
O

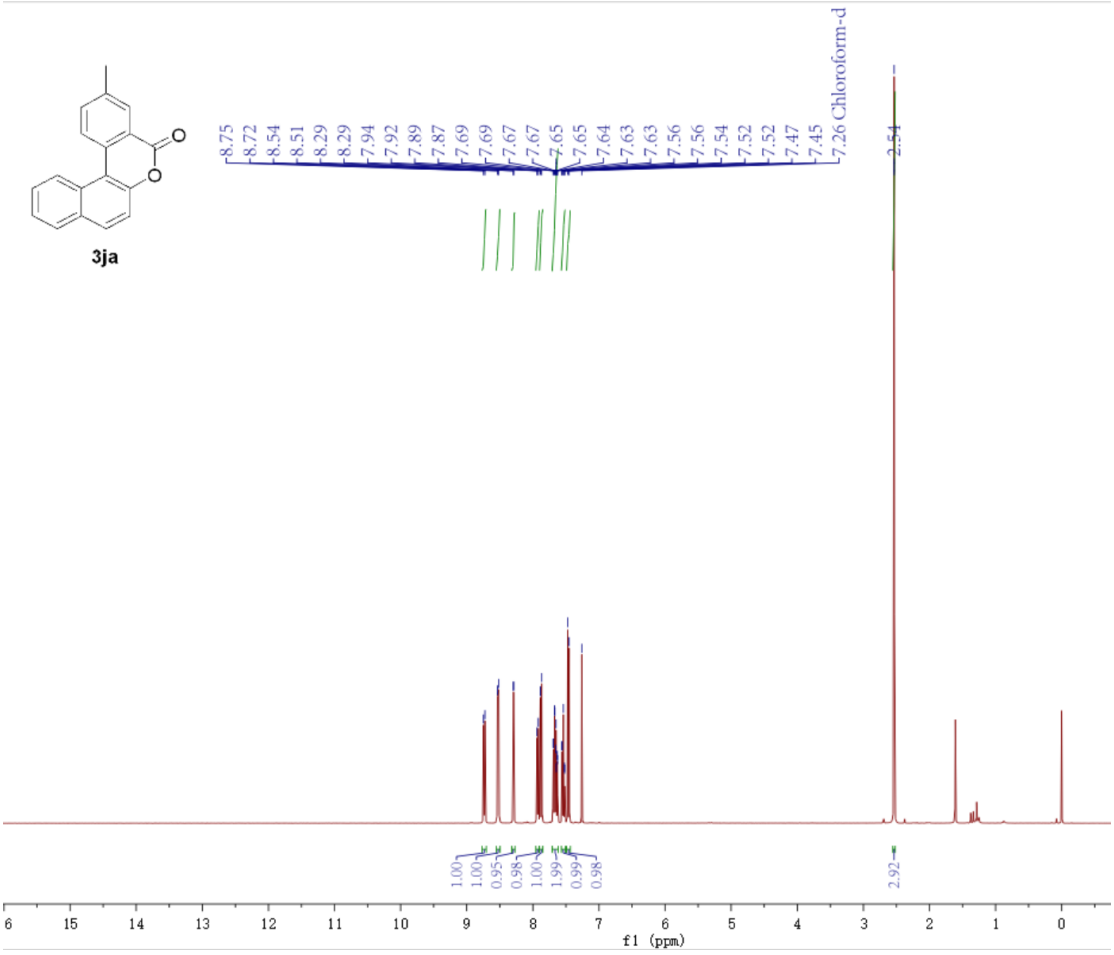
3ia

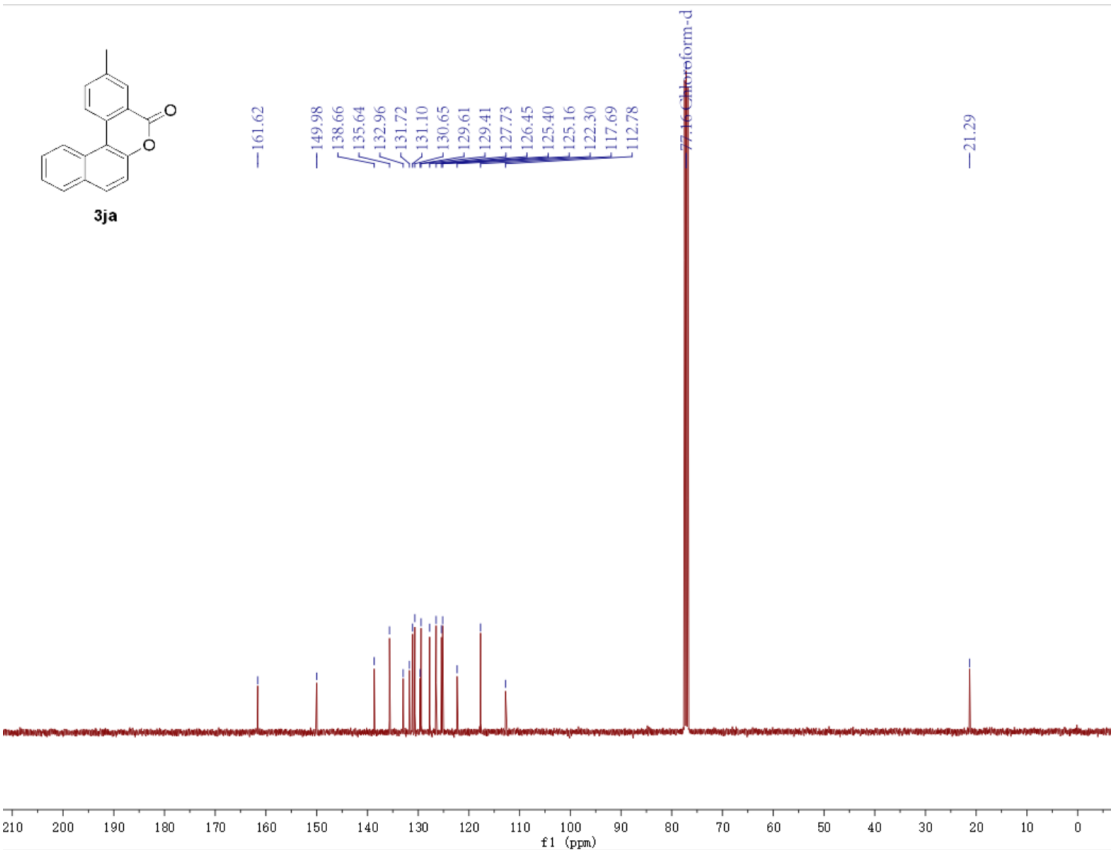
160.56
149.93
131.81
131.63
129.57
129.37
128.97
128.89
128.09
125.68
124.85
124.42
122.64
122.42
117.63
116.61
116.38
112.13
77.16 Chloroform-d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

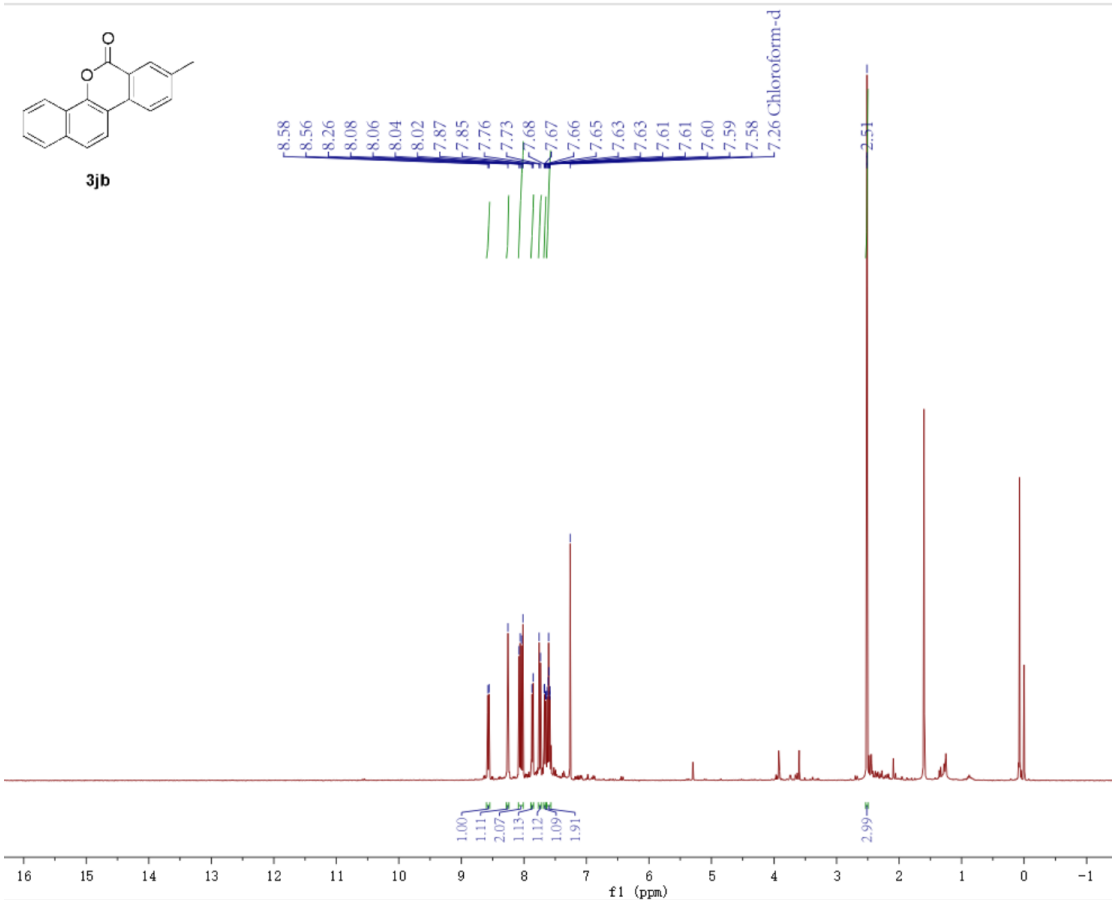

F
O
O

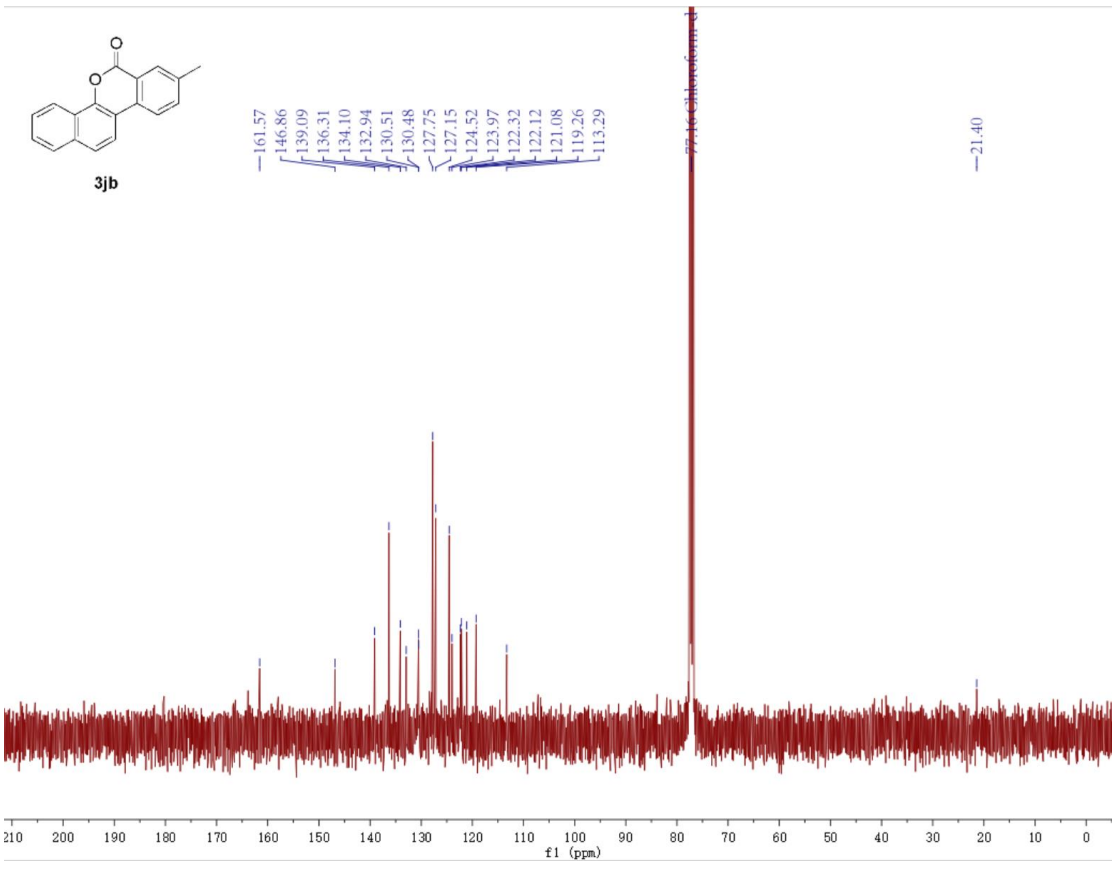
3ia

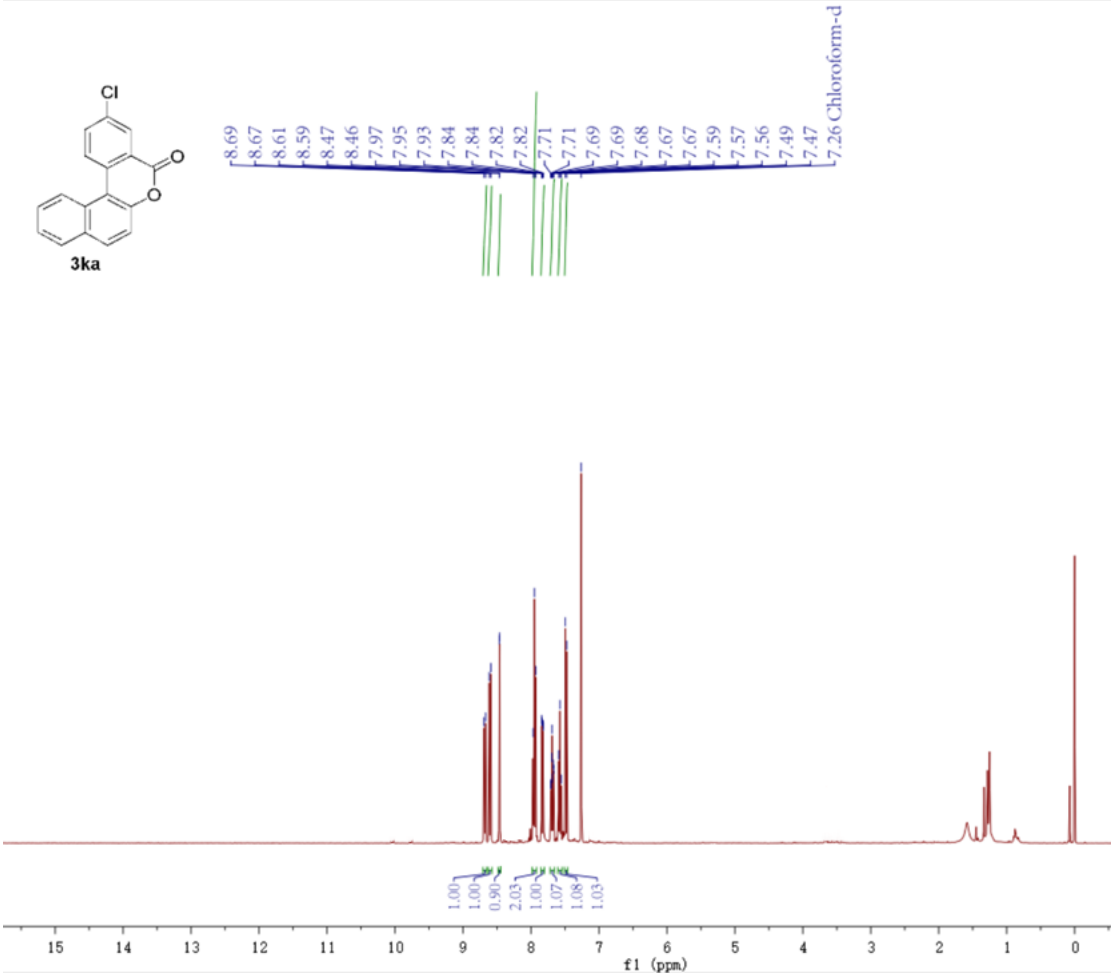
-110.76
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)

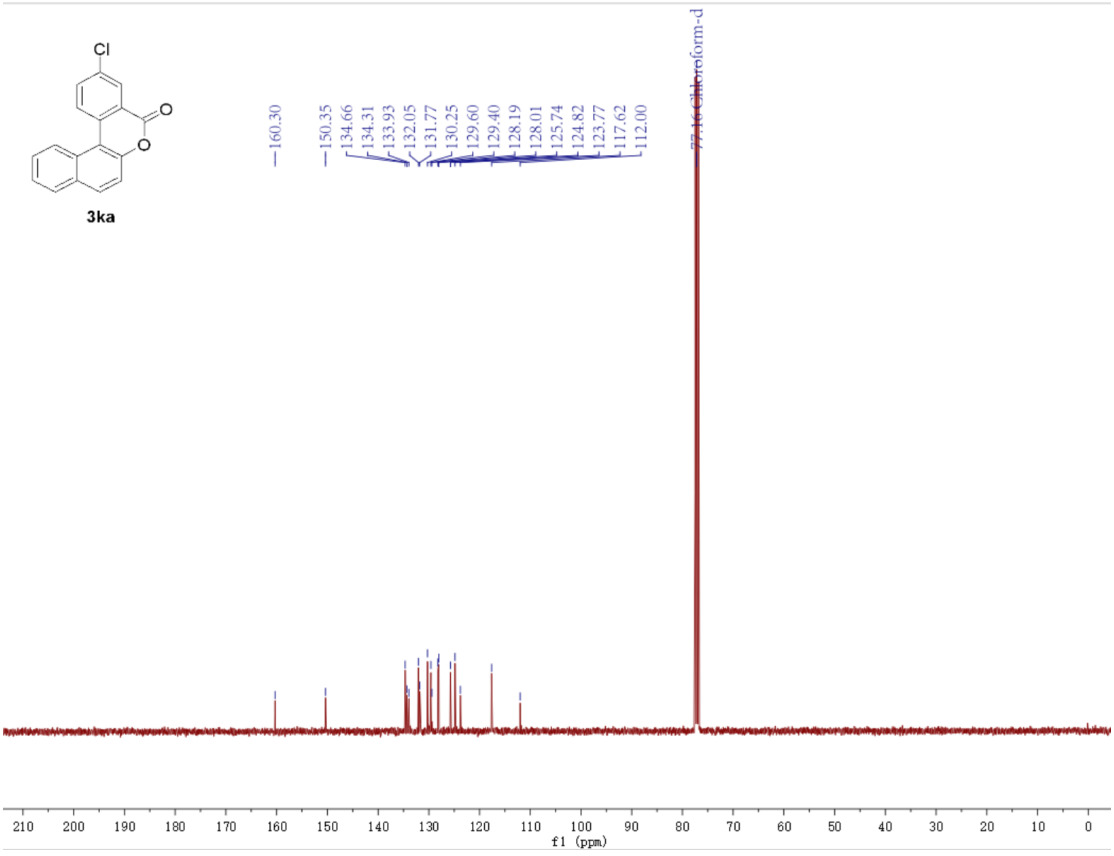

3ja
8.75
8.72
8.54
8.51
8.29
8.29
7.94
7.92
7.89
7.87
7.69
7.69
7.67
7.67
7.65
7.65
7.64
7.63
7.63
7.56
7.56
7.54
7.52
7.52
7.47
7.45
7.26 Chloroform-d
2.54
1.00
1.00
0.95
0.98
1.00
1.99
0.99
0.98
2.92
f1 (ppm)

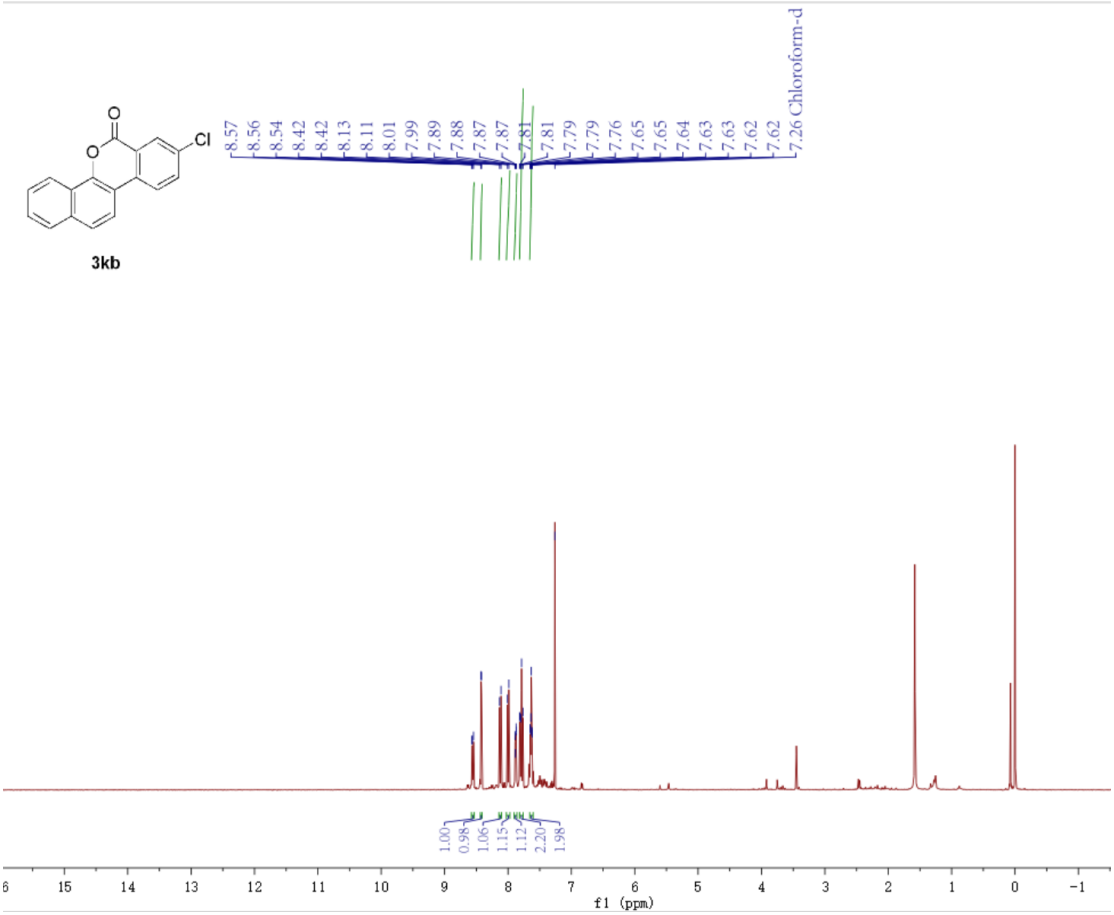

3ja
161.62
149.98
138.66
135.64
132.96
131.72
131.10
130.65
129.61
129.41
127.73
126.45
125.40
125.16
122.30
117.69
112.78
77.16 Chloroform-d
21.29
f1 (ppm)


3jb
8.58
8.56
8.26
8.08
8.06
8.04
8.02
7.87
7.85
7.76
7.73
7.68
7.67
7.66
7.65
7.63
7.63
7.61
7.61
7.60
7.59
7.58
7.26 Chloroform-d
2.51
1.00
1.11
2.07
1.13
1.12
1.09
1.91
2.99
f1 (ppm)


3jb
161.57
146.86
139.09
136.31
134.10
132.94
130.51
130.48
127.75
127.15
124.52
123.97
122.32
122.12
121.08
119.26
113.29
77.16 Chloroform-d
21.40
f1 (ppm)


Cl
O
O
3ka
8.69
8.67
8.61
8.59
8.47
8.46
7.97
7.95
7.93
7.84
7.84
7.82
7.82
7.71
7.71
7.69
7.69
7.68
7.67
7.67
7.59
7.57
7.56
7.49
7.47
7.26 Chloroform-d
1.00
1.00
0.90
2.03
1.00
1.07
1.08
1.03
f1 (ppm)


Cl
O
O
3ka
160.30
150.35
134.66
134.31
133.93
132.05
131.77
130.25
129.60
129.40
128.19
128.01
125.74
124.82
123.77
117.62
112.00
77.16 Chloroform-d
f1 (ppm)


3kb
8.57
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8.42
8.42
8.13
8.11
8.01
7.99
7.89
7.88
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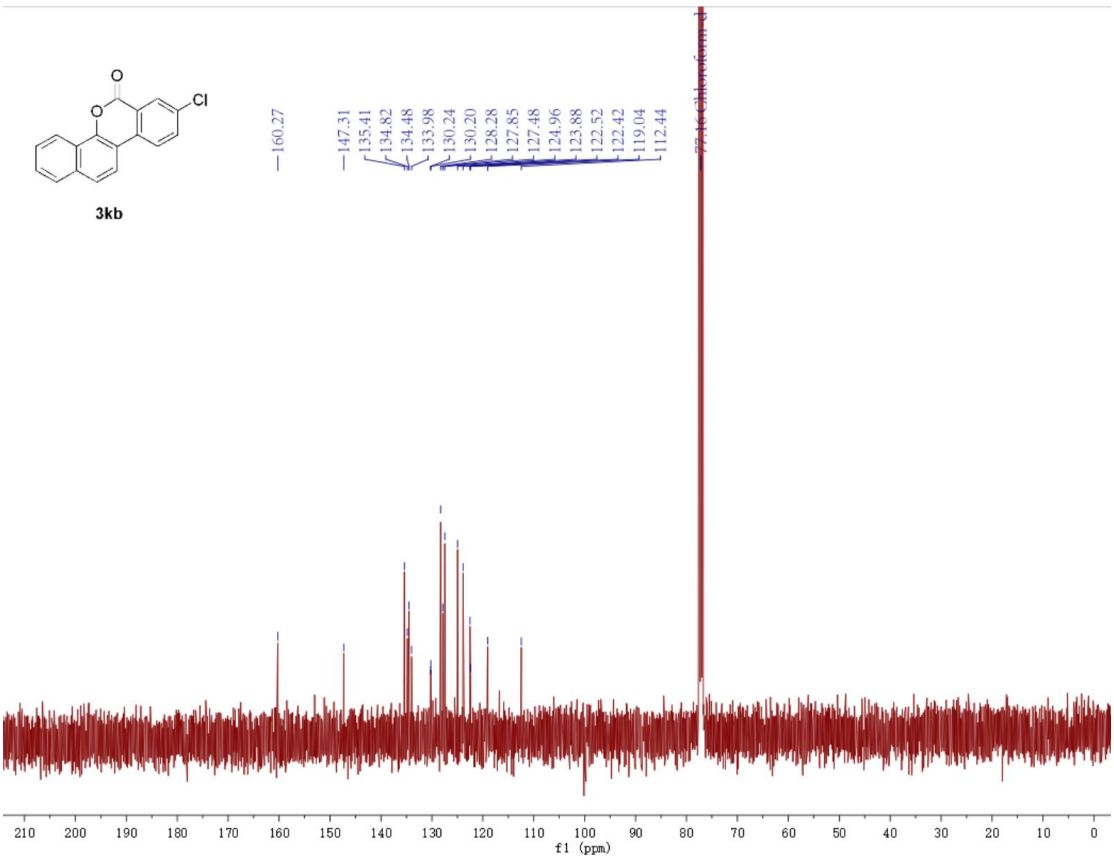
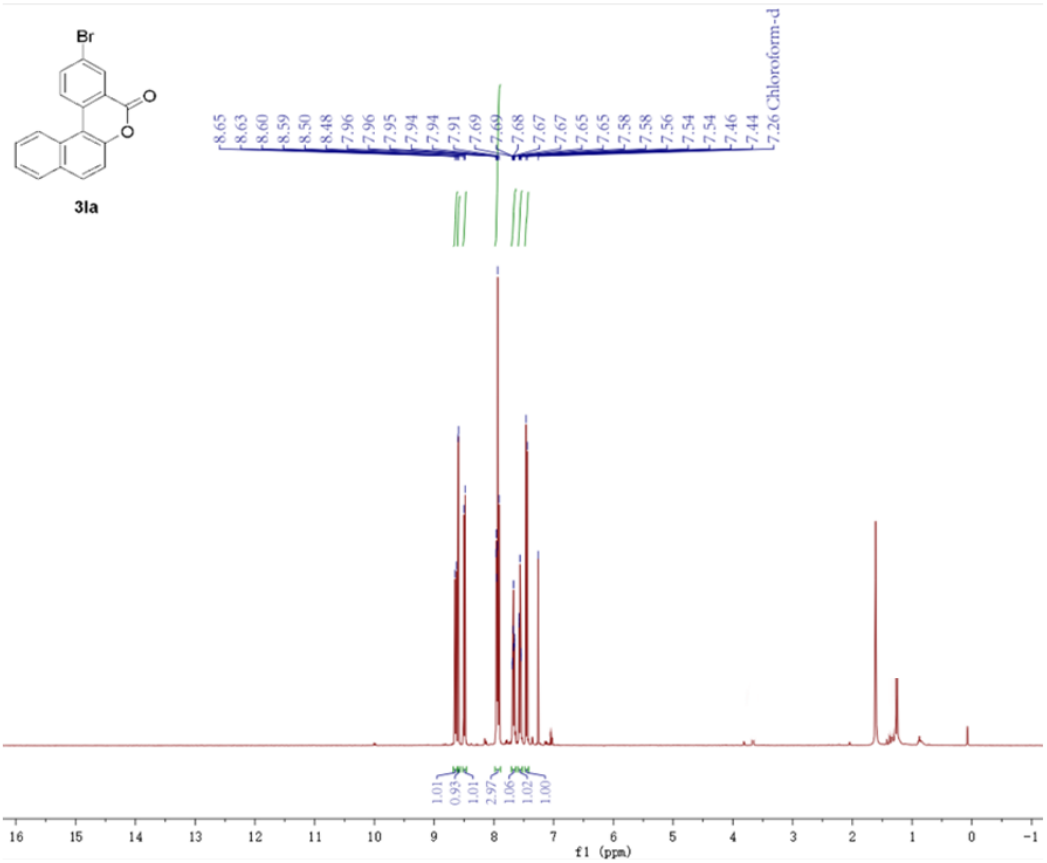
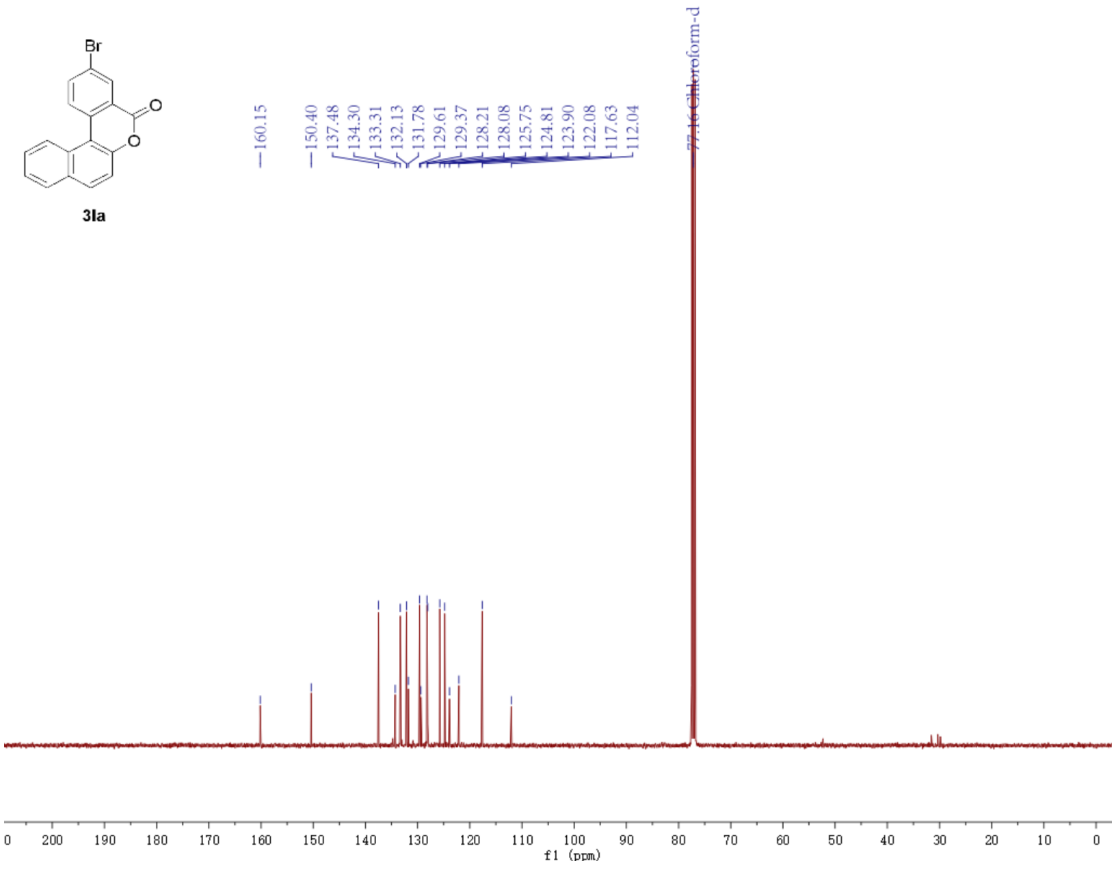
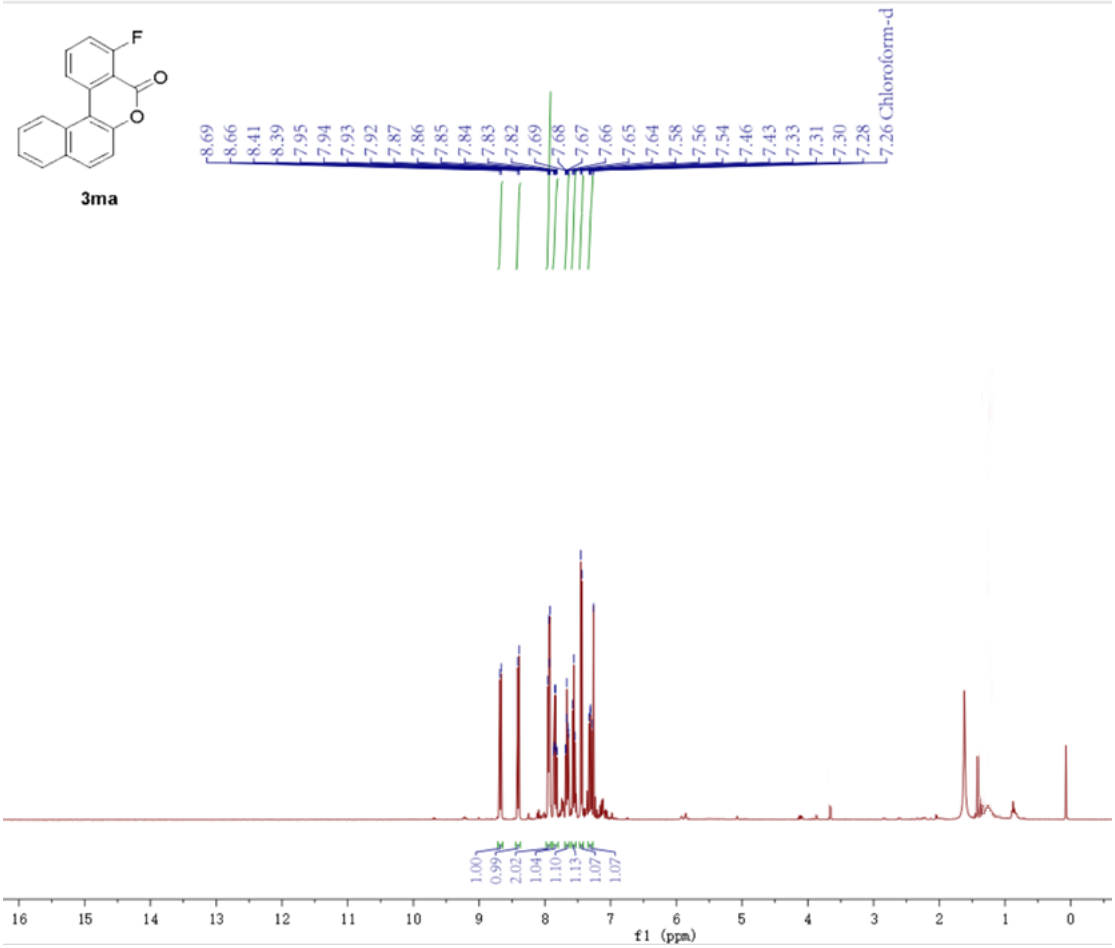
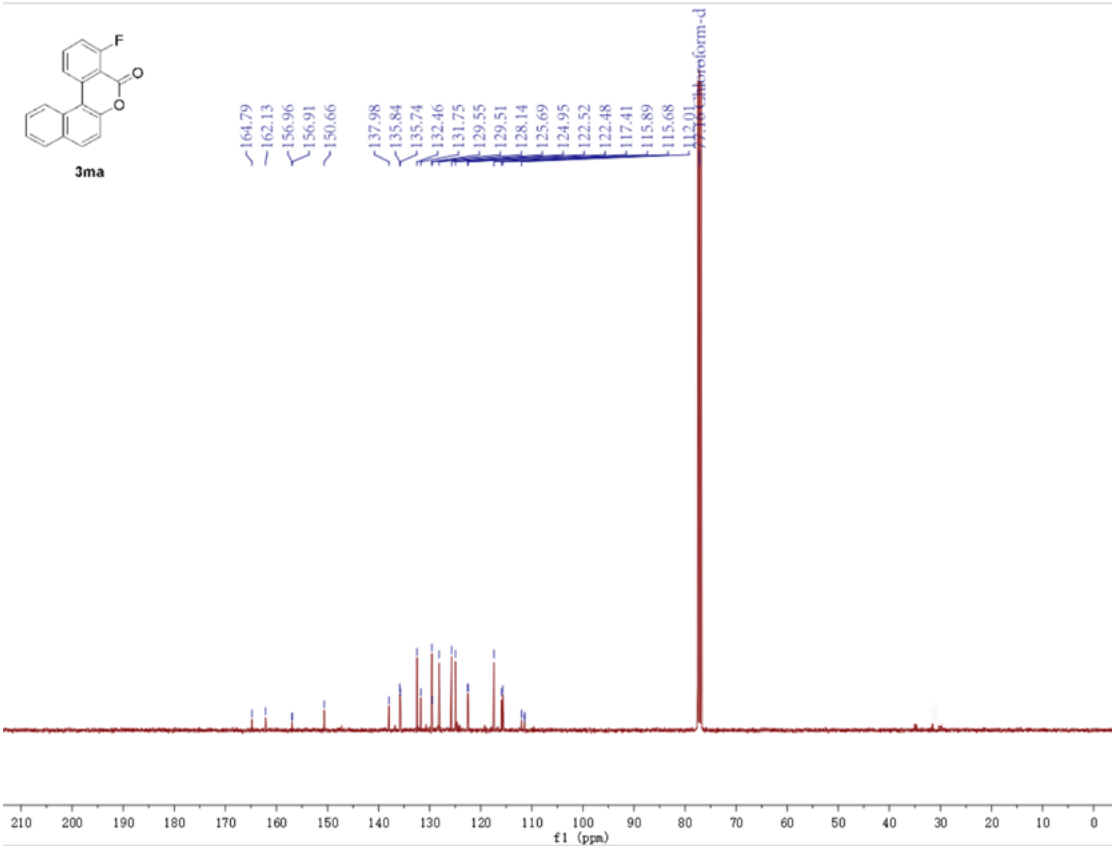
7.87
7.81
7.81
7.79
7.79
7.76
7.65
7.65
7.64
7.63
7.63
7.62
7.62
7.26 Chloroform-d
1.00
0.98
1.06
1.15
1.12
2.20
1.98
f1 (ppm)

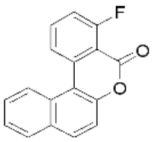

3kb
160.27
147.31
135.41
134.82
134.48
133.98
130.24
130.20
128.28
127.85
127.48
124.96
123.88
122.52
122.42
119.04
112.44
77.16 Chloroform-d
f1 (ppm)


Br
O
O
3la
8.65
8.63
8.60
8.59
8.50
8.48
7.96
7.96
7.95
7.94
7.94
7.91
7.69
7.69
7.68
7.67
7.67
7.65
7.65
7.58
7.58
7.56
7.54
7.54
7.46
7.44
7.26 Chloroform-d
1.01
0.93
1.01
2.97
1.06
1.02
1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


Br
O
O
3la
160.15
150.40
137.48
134.30
133.31
132.13
131.78
129.61
129.37
128.21
128.08
125.75
124.81
123.90
122.08
117.63
112.04
77.16 Chloroform-d
0 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


F
O
O
3ma
8.69
8.66
8.41
8.39
7.95
7.94
7.93
7.92
7.87
7.86
7.85
7.84
7.83
7.82
7.69
7.68
7.67
7.66
7.65
7.64
7.58
7.56
7.54
7.46
7.43
7.33
7.31
7.30
7.28
7.26 Chloroform-d
1.00
0.99
2.02
1.04
1.10
1.13
1.07
1.07
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


F
O
O
3ma
164.79
162.13
156.96
156.91
150.66
137.98
135.84
135.74
132.46
131.75
129.55
129.51
128.14
125.69
124.95
122.52
122.48
117.41
115.89
115.68
112.01
77.16 Chloroform-d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


F
O
O

3ma

-106.47
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200
f1 (ppm)