Supporting Information

Palladium-catalyzed carbonylative C-C bond activation of cyclobutanones

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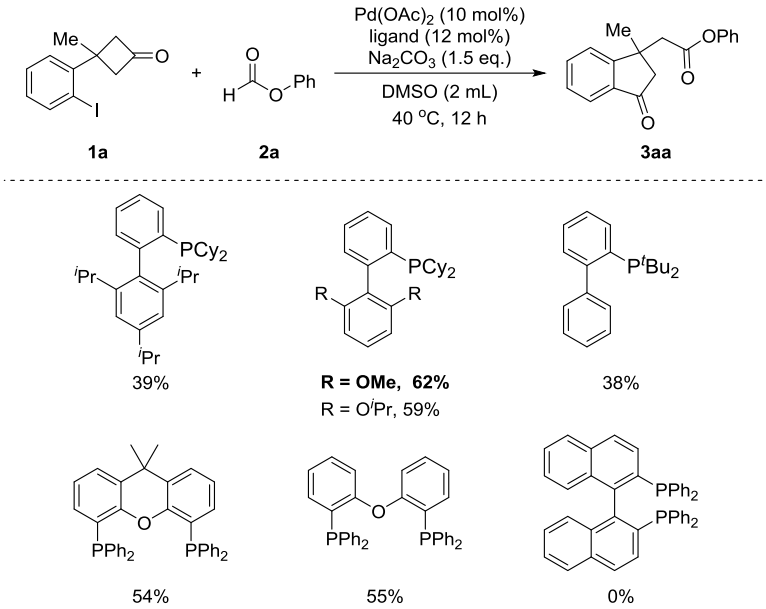
General information

Unless otherwise noted, all reactions were carried out under N_2 atmosphere. All reagents were from commercial sources and used as received without further purification. All solvents were dried by standard techniques and distilled prior to use. Column chromatography was performed on silica gel (200-300 meshes) using petroleum ether (bp. 60~90 °C) and ethyl acetate as eluent. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded on a Bruker Avance (400 MHz) spectrometer, using $CDCl_3$ as the solvent and TMS as internal standard; chemical shifts were quoted in parts per million and *J* values were given in hertz. The following abbreviations were used to describe peak splitting patterns when appropriate: s = singlet, d = doublet, dd = double doublet, ddd = double doublet of doublets, t = triplet, dt = double triplet, q = quatriplet, m = multiplet, br = broad. High resolution mass spectrometry (HRMS) was performed on a Waters Micromass GCT (ESI-TOF).

Optimization of Reaction Conditions

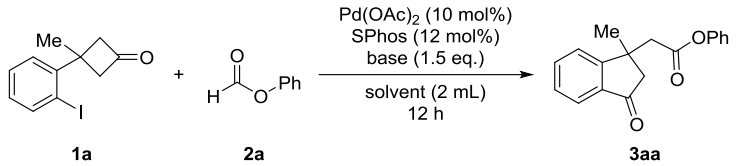
Reaction of cyclobutanones and phenyl formate.

Table S1: Optimization of ligands.[a]



[a]Unless otherwise noted, the reaction conditions were as follows: **1a** (0.2 mmol, 1.0 eq.), **2a** (0.3 mmol, 1.5 eq.), $Pd(OAc)_2$ (10 mol%), ligand (12 mol%), Na_2CO_3 (1.5 eq.), DMSO 2 mL, 40 °C for 12 h. Isolated yield.

Table S2: Optimization of solvents, temperature and bases.[a]

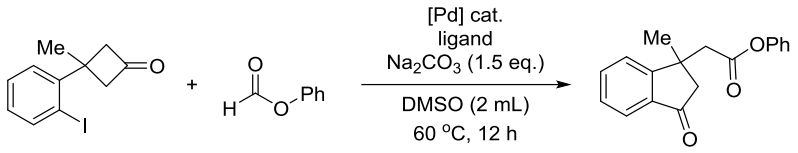


1a **2a** **3aa**

Entry	Solvent	Temp.(°C)	base	Yield(%)[b]
1	DMSO	40	Na_2CO_3	62
2	toluene	40	Na_2CO_3	trace
3	DCM	40	Na_2CO_3	trace
4	dioxane	40	Na_2CO_3	trace
5	CH_3CN	40	Na_2CO_3	trace
6	THF	40	Na_2CO_3	trace
7	DMSO	25	Na_2CO_3	27
8	**DMSO**	**60**	**Na_2CO_3**	**75**
9	DMSO	70	Na_2CO_3	68
10	DMSO	60	K_2CO_3	61
11	DMSO	60	Cs_2CO_3	24
12	DMSO	60	Ag_2CO_3	trace
13	DMSO	60	K_3PO_4	51

[a]Unless otherwise noted, the reaction conditions were as follows: **1a** (0.2 mmol, 1.0 eq.), **2a** (0.3 mmol, 1.5 eq.), $Pd(OAc)_2$ (10 mol%), SPhos (12 mol%), base (1.5 eq.), solvent 2 mL for 12 h. [b]Isolated yield.

Table S3: Optimization of catalysts and ligands.[a]



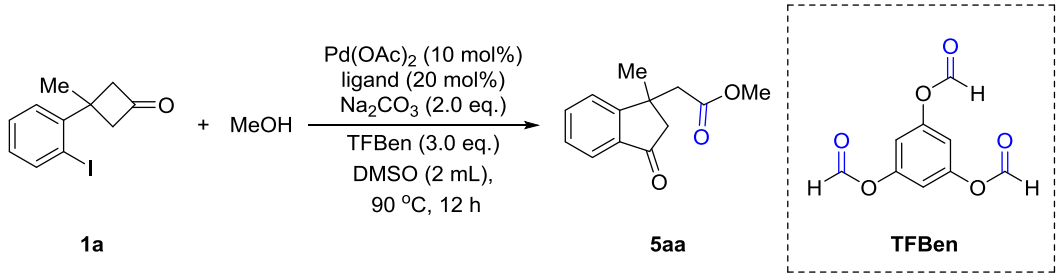
1a **2a** **3aa**

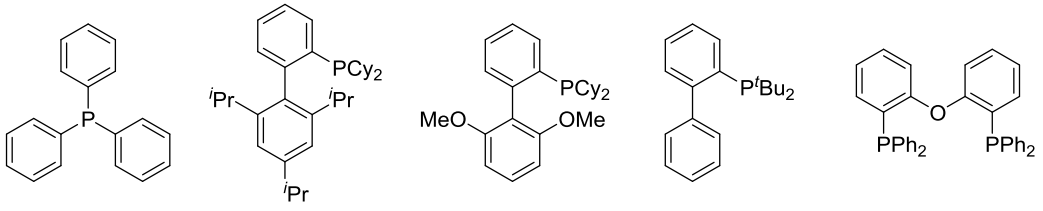
Entry	[Pd] cat.	Ligand	Yield(%)[b]
1	$PdCl_2$	SPhos	76
2	$Pd(TFA)_2$	SPhos	60
3	$Pd(dba)_2$	SPhos	67
4	$Pd(MeCN)_2Cl_2$	SPhos	75
5	$Pd(acac)_2$	SPhos	56
6	$Pd(dppb)Cl_2$	SPhos	80
7	$Pd(dppb)Cl_2$	/	75
8	$Pd(dtbpf)Cl_2$	SPhos	87
9	$Pd(dtbpf)Cl_2$	/	80
10	$PdCl_2$	dppf	88
11[c]	**$PdCl_2$**	**dppf**	**83**
12[d]	$PdCl_2$	dppf	67

[a]Unless otherwise noted, the reaction conditions were as follows: **1a** (0.2 mmol, 1.0 eq.), **2a** (0.3 mmol, 1.5 eq.), [Pd] cat. (10 mol%), ligand (12 mol%), Na_2CO_3 (1.5 eq.), DMSO 2 mL, 60 °C for 12 h. [b]Isolated yield. [c]$PdCl_2$ (5 mol%), dppf (6 mol%). [d]$PdCl_2$ (2.5 mol%), dppf (3 mol%).

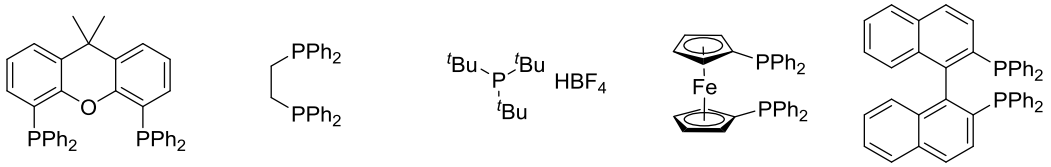
Reaction of cyclobutanones, MeOH and TFBen.

Table S4: Optimization of ligands.[a]





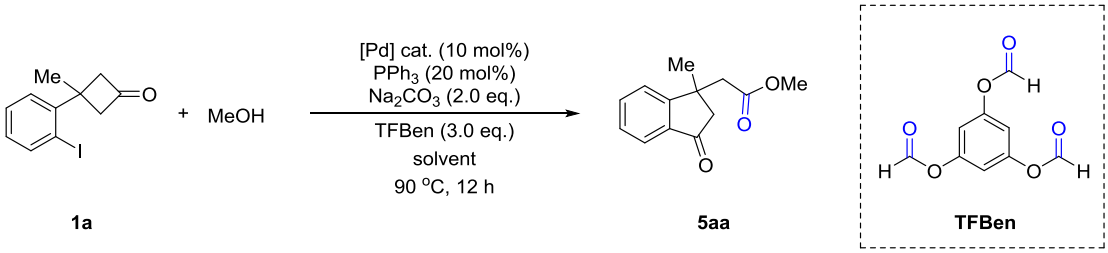
30% 15% 13% 15% 14%



21% 0% 12% 0% 0%

[a] Unless otherwise noted, the reaction conditions were as follows: **1a** (0.2 mmol, 1.0 eq.), **TFBen** (0.6 mmol, 3.0 eq.), **MeOH** (0.6 mmol, 3.0 eq.), $Pd(OAc)_2$ (10 mol%), ligand (20 mol%), Na_2CO_3 (2.0 eq.), DMSO 2 mL, 90 °C for 12 h. Isolated yield.

Table S5: Optimization of catalysts and solvents.[a]

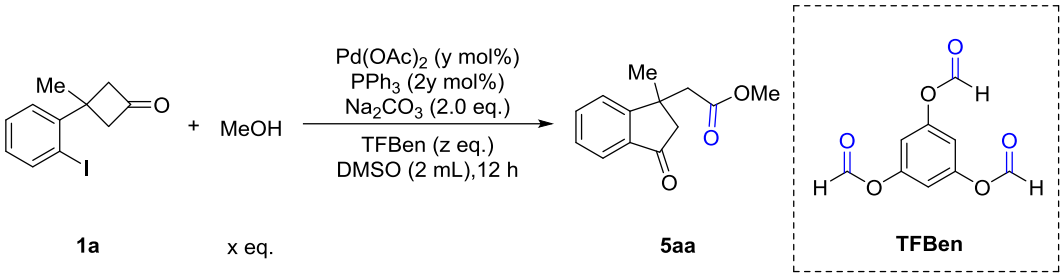


1a **5aa** **TFBen**

Entry	[Pd] cat.	Solvent	Yield(%)[b]
1	**$Pd(OAc)_2$**	**DMSO**	**30**
2	$Pd(CH_3CN)_2Cl_2$	DMSO	18
3	$Pd(PPh_3)_4$	DMSO	22
4	$Pd(TFA)_2$	DMSO	18
5	$[PdCl(allyl)]_2$	DMSO	15
6	$Pd_2(dba)_3$	DMSO	12
7	$Pd(cod)Cl_2$	DMSO	17
8	$PdBr_2$	DMSO	19
9	$PdCl_2$	DMSO	24
10	$Pd(OAc)_2$	CH_3CN	N.D.
11	$Pd(OAc)_2$	DMF	20
13	$Pd(OAc)_2$	DCE	N.D.
14	$Pd(OAc)_2$	THF	N.D.
15	$Pd(OAc)_2$	Toluene	N.D.
16	$Pd(OAc)_2$	Hexane	N.D.
17	$Pd(OAc)_2$	EtOAc	N.D.

[a] Unless otherwise noted, the reaction conditions were as follows: **1a** (0.2 mmol, 1.0 eq.), **TFBen** (0.6 mmol, 3.0 eq.), **MeOH** (0.6 mmol, 3.0 eq.), [Pd] cat. (10 mol%), PPh_3 (20 mol%), Na_2CO_3 (2.0 eq.), solvent 2 mL, 90 °C for 12 h. [b]Isolated yield. N.D. = Not determined.

Table S6: Optimization of temperature and the amount of methanol, catalyst/ligand and TFBen.[a]



1a x eq. **5aa** **TFBen**

Entry	MeOH (x eq.)	Temp.(°C)	$Pd(OAc)_2$ (y mol%)	TFBen (z eq.)	Yield(%)[b]
1	3	90	10	3	30
2	5	90	10	3	45
3	10	90	10	3	50
4	10	60	10	3	trace
5	10	100	10	3	75
6	10	110	10	3	84
7	10	120	10	3	86
8	10	130	10	3	86
9	10	120	5	3	85
10	10	120	2.5	3	86
11	**10**	**120**	**2.5**	**2**	**84**
12	10	120	2.5	1	76

[a]Unless otherwise noted, the reaction conditions were as follows: **1a** (0.2 mmol, 1.0 eq.), Na_2CO_3 (2.0 eq.), DMSO 2 mL, 12 h. [b]Isolated yield.

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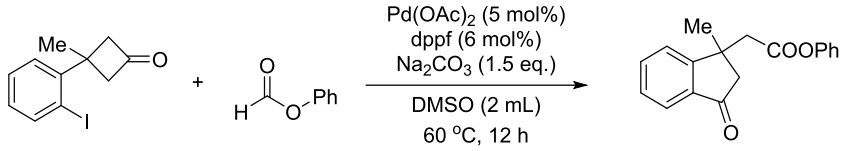
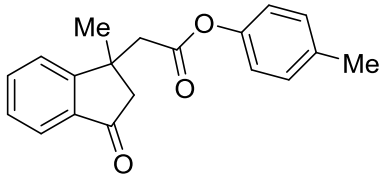
Typical procedure for the synthesis of esters 3



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

A vial was charged with 3-(2-iodophenyl)-3-methylcyclobutan-1-one **1a** (57.2 mg, 0.2 mmol), $PdCl_2$ (1.8 mg, 5 mol%), dppf (6.7 mg, 6 mol%), Na_2CO_3 (31.8 mg, 1.5 eq.) and evacuated under high vacuum and backfilled with N_2. DMSO (2 mL) and phenyl formate (32 uL, 1.5 eq.) were next added. The mixture was stirred at 60 °C in an oil bath for 12 h, and then cooled to room temperature. The reaction mixture was extracted with EA and dried over Na_2SO_4, concentrated under reduced pressure and then purified by silica column (PE-EtOAc, 20:1) to get the product **3aa**. The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (46.5 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 7.6 Hz, 1H), 7.56 (t, J = 7.6 Hz, 1H), 7.49 (d, J = 7.6 Hz, 1H), 7.33 (t, J = 7.2 Hz, 1H), 7.21 (t, J = 8.0 Hz, 2H), 7.08 (t, J = 7.6 Hz, 1H), 6.74 (d, J = 8.0 Hz, 2H), 3.08 (d, J = 19.2 Hz, 1H), 2.94 (d, J = 14.8 Hz, 1H), 2.84 (d, J = 14.8 Hz, 1H), 2.56 (d, J = 19.2 Hz, 1H), 1.49 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.7, 169.3, 160.4, 150.2, 136.0, 135.1, 129.4, 128.2, 126.0, 123.9, 123.6, 121.3, 50.3, 45.6, 40.6, 28.9. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{16}NaO_3$, 303.1005; found 303.1001.

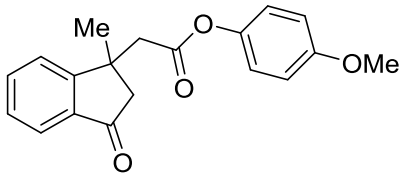


3ab

3-methyl-3-(2-oxo-2-(p-tolyl) ethyl)-2,3-dihydro-1H-inden-1-one

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (50.5 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 7.6 Hz, 1H), 7.69-7.62 (m, 1H), 7.58 (d, J = 7.6 Hz, 1H), 7.42 (t, J = 7.6 Hz, 1H), 7.09 (d, J = 7.6 Hz, 2H), 6.71 (d, J = 8.4 Hz, 2H), 3.17 (d, J = 18.8 Hz, 1H), 3.02 (d, J = 14.8 Hz, 1H), 2.92 (d, J = 14.8 Hz, 1H), 2.65 (d, J = 18.8 Hz, 1H), 2.29 (s, 3H), 1.58 (s, 3H). ^{13}C NMR (100 MHz,

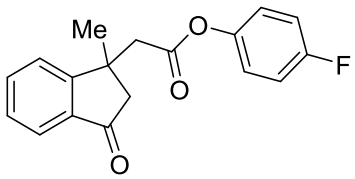
$CDCl_3$) δ 204.8, 169.6, 160.5, 148.0, 136.0, 135.7, 135.1, 130.0, 128.2, 124.0, 123.7, 121.0, 50.4, 45.7, 40.7, 28.9, 20.9. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{18}NaO_3$, 317.1148; found 317.1145.



3ac

4-methoxyphenyl 2-(1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

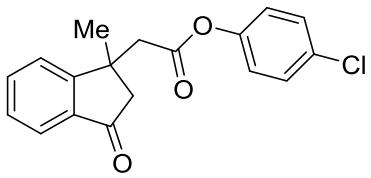
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (45.0 mg, 73%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 7.6 Hz, 1H), 7.69-7.62 (m, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.46-7.39 (m, 1H), 6.81 (d, J = 8.8 Hz, 1H), 6.74 (d, J = 8.8 Hz, 1H), 3.74 (s, 3H), 3.16 (d, J = 18.8Hz, 1H), 3.01 (d, J = 14.8 Hz, 1H), 2.91 (d, J = 14.8 Hz, 1H), 2.64 (d, J = 18.8 Hz, 1H), 1.58 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.8, 169.8, 160.5, 157.4, 143.7, 136.0, 135.1, 128.3, 124.0, 123.7, 122.1, 114.5, 55.6, 50.4, 45.7, 40.7, 28.9. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{18}NaO_4$, 333.1097; found 333.1090.



3ad

4-fluorophenyl 2-(1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

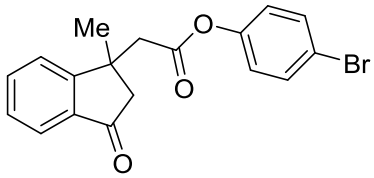
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (59.0 mg, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.6 Hz, 1H), 7.68-7.62 (m, 1H), 7.57 (d, J = 7.6 Hz, 1H), 7.45-7.37 (m, 1H), 7.00-6.92 (m, 2H), 6.80-6.74 (m, 2H), 3.14 (d, J = 19.2 Hz, 1H), 3.02 (d, J = 14.8 Hz, 1H), 2.92 (d, J = 14.8 Hz, 1H), 2.64 (d, J = 19.2 Hz, 1H), 1.58 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 204.6, 169.4, 160.28, 160.26 (d, J = 244.5 Hz), 146.0 (d, J = 2.9 Hz), 136.0, 135.2, 128.3, 123.9, 123.7, 122.7 (d, J = 8.3 Hz), 116.1 (d, J = 23.3 Hz), 50.4, 45.6, 40.6, 28.9. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{15}FNaO_3$, 321.0897; found 321.0898.



3ae

4-chlorophenyl 2-(1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

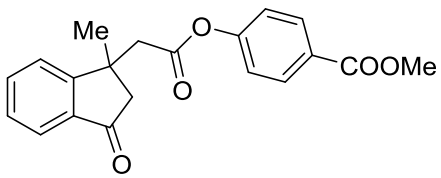
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (62.2 mg, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 7.6 Hz, 1H), 7.69-7.62 (m, 1H), 7.57 (d, J = 7.6 Hz, 1H), 7.43 (t, J = 7.2 Hz, 1H), 7.27-7.24 (m, 2H), 6.79-6.73 (m, 2H), 3.14 (d, J = 19.2 Hz, 1H), 3.02 (d, J = 14.8 Hz, 1H), 2.93 (d, J = 14.8 Hz, 1H), 2.65 (d, J = 19.2 Hz, 1H), 1.58 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.7, 168.2, 159.3, 147.7, 135.1, 134.2, 130.4, 128.6, 127.4, 122.9, 122.8, 121.8, 49.4, 44.7, 39.7, 27.9. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{15}ClNaO_3$, 337.0602; found 337.0594.



3af

4-bromophenyl 2-(1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

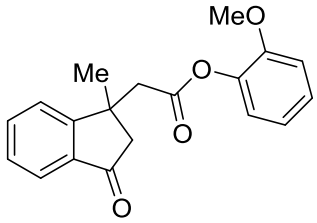
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (64.5 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 7.6 Hz, 1H), 7.70-7.63 (m, 1H), 7.58 (d, J = 7.6 Hz, 1H), 7.47-7.38 (m, 3H), 6.71 (d, J = 8.0 Hz, 2H), 3.14 (d, J = 18.8 Hz, 1H), 3.03 (d, J = 14.8 Hz, 1H), 2.93 (d, J = 14.8 Hz, 1H), 2.65 (d, J = 18.8 Hz, 1H), 1.59 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.6, 168.1, 159.2, 148.2, 135.0, 134.2, 131.5, 127.4, 122.9, 122.7, 122.2, 118.1, 49.4, 44.7, 39.7, 27.9. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{15}BrNaO_3$, 381.0097; found 381.0079.



3ag

methyl 4-(2-(1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetoxy) benzoate

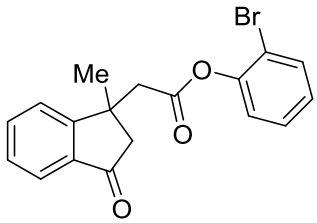
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (50.5 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, J = 8.8 Hz, 2H), 7.74 (d, J = 7.6 Hz, 1H), 7.69-7.62 (m, 1H), 7.57 (d, J = 7.6 Hz, 1H), 7.42 (t, J = 7.6 Hz, 1H), 6.89 (d, J = 8.7 Hz, 2H), 3.87 (s, 3H), 3.14 (d, J = 18.8 Hz, 1H), 3.04 (d, J = 14.8 Hz, 1H), 2.94 (d, J = 14.8 Hz, 1H), 2.65 (d, J = 18.8 Hz, 1H), 1.58 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 204.6, 168.8, 166.3, 160.2, 153.8, 136.0, 135.2, 131.2, 128.4, 127.9, 123.9, 123.8, 121.4, 52.3, 50.4, 45.8, 40.7, 28.9. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{18}NaO_5$, 361.1046; found 361.1056.



3ah

2-methoxyphenyl 2-(1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (49.3 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 7.6 Hz, 1H), 7.70-7.62 (m, 1H), 7.58 (d, J = 7.6 Hz, 1H), 7.44-7.36 (m, 1H), 7.19-7.12 (m, 1H), 6.94-6.79 (m, 3H), 3.74 (s, 3H), 3.22 (d, J = 19.2 Hz, 1H), 3.07 (d, J = 14.8 Hz, 1H), 2.95 (d, J = 14.8 Hz, 1H), 2.65 (d, J = 19.2 Hz, 1H), 1.59 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.1, 169.0, 161.0, 151.0, 139.4, 136.0, 135.1, 128.1, 127.1, 123.9, 123.6, 122.6, 120.8, 112.4, 55.7, 50.3, 45.3, 40.7, 28.9. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{18}NaO_4$, 333.1097; found 333.1107.



3ai

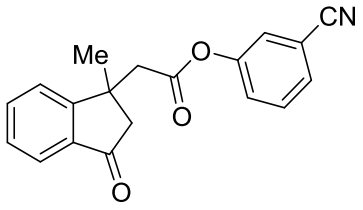
2-bromophenyl 2-(1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (70.2 mg, 98%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.6 Hz, 1H), 7.68-7.61 (m,

1H), 7.59 (d, J = 7.6 Hz, 1H), 7.54 (dd, J = 8.0, 1.6 Hz, 1H), 7.44-7.38 (m, 1H), 7.25 (td, J = 8.0, 1.6 Hz, 1H), 7.07 (td, J = 8.0, 1.6 Hz, 1H), 6.86 (dd, J = 8.0, 1.6 Hz, 1H), 3.18 (d, J = 18.8 Hz, 1H), 3.12 (d, J = 15.6 Hz, 1H), 3.01 (d, J = 15.6 Hz, 1H), 2.68 (d, J = 18.8 Hz, 1H), 1.60 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.7, 168.5, 160.4, 147.8, 135.9, 135.1, 133.3, 128.5, 128.2, 127.5, 123.8, 123.6, 123.5, 116.0, 50.3, 45.0, 40.3, 28.9. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{15}BrNaO_3$, 381.0097; found 381.0100.

A gram-scale procedure for the synthesis of 3ai:

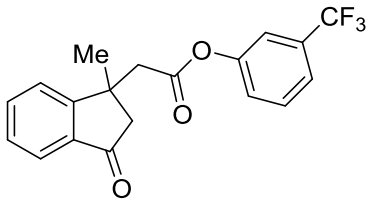
A vial was charged with 3-(2-iodophenyl)-3-methylcyclobutan-1-one **1a** (1.144 g, 4 mmol), $PdCl_2$ (36 mg, 5 mol%), dppf (134 mg, 6 mol%), Na_2CO_3 (636 mg, 1.5 eq.) and evacuated under high vacuum and backfilled with N_2. DMSO (40 mL) and phenyl formate (1.200 g, 1.5 eq.) was next added. The mixture was stirred at 60 °C in an oil bath for 12 h, and then cooled to room temperature. The reaction mixture was extracted with EA and dried over Na_2SO_4, concentrated under reduced pressure and then purified by silica column (PE-EtOAc, 20:1) to get the product **3ai** (1.250 g, 87%).



3aj

3-cyanophenyl 2-(1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

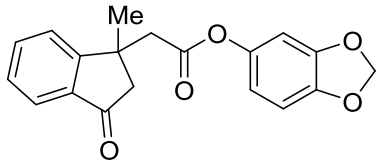
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (54.9 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.6 Hz, 1H), 7.69-7.63 (m, 1H), 7.58 (d, J = 7.6 Hz, 1H), 7.48-7.36 (m, 3H), 7.13-7.07 (m, 1H), 7.08-7.02 (m, 1H), 3.11 (d, J = 19.2 Hz, 1H), 3.05 (d, J = 14.8 Hz, 1H), 2.96 (d, J = 14.8 Hz, 1H), 2.64 (d, J = 19.2 Hz, 1H), 1.58 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.4, 168.8, 159.9, 150.2, 1366.0, 135.2, 130.4, 129.7, 128.4, 126.4, 125.1, 123.9, 123.7, 117.7, 113.4, 50.3, 45.5, 40.6, 28.9. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{15}NNaO_3$, 328.0944; found 328.0936.



3ak

3-(trifluoromethyl) phenyl 2-(1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

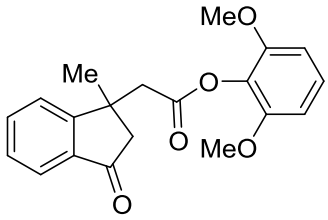
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (59.9 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 7.6 Hz, 1H), 7.70-7.63 (m, 1H), 7.59 (d, J = 7.6 Hz, 1H), 7.47-7.37 (m, 3H), 7.09-6.97 (m, 2H), 3.15 (d, J = 19.2 Hz, 1H), 3.05 (d, J = 14.8 Hz, 1H), 2.97 (d, J = 14.8 Hz, 1H), 2.66 (d, J = 19.2 Hz, 1H), 1.60 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.5, 169.0, 160.1, 150.3, 136.1, 135.2, 132.0 (q, J = 33.0 Hz), 130.1, 128.4, 125.1, 124.0, 123.8, 123.5 (q, J = 270.7 Hz), 122.9 (q, J = 3.8 Hz), 118.7 (q, J = 3.9 Hz), 50.4, 45.7, 40.7, 28.9. HRMS (ESI-TOF) m/z: [M + Na]$^{+}$ Calcd for $C_{19}H_{15}F_3NaO_5$, 371.0865; found 371.0875.



3al

benzo[d] [1,3] dioxol-5-yl 2-(1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

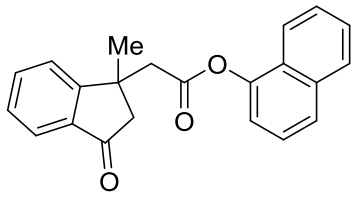
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (44.9 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.6 Hz, 1H), 7.68-7.62 (m, 1H), 7.57 (d, J = 7.6 Hz, 1H), 7.42 (t, J = 7.6 Hz, 1H), 6.68 (d, J = 8.4 Hz, 1H), 6.29 (d, J = 2.4 Hz, 1H), 6.25 (dd, J = 8.4, 2.4 Hz, 1H), 5.92 (s, 2H), 3.14 (d, J = 18.8 Hz, 1H), 2.99 (d, J = 14.8 Hz, 1H), 2.90 (d, J = 14.8 Hz, 1H), 2.63 (d, J = 18.8 Hz, 1H), 1.57 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.7, 169.7, 160.4, 148.0, 145.5, 144.5, 136.0, 135.1, 128.3, 123.9, 123.7, 113.7, 108.0, 103.5, 100.8, 50.4, 45.6, 40.6, 28.9. HRMS (ESI-TOF) m/z: [M + Na]$^{+}$ Calcd for $C_{19}H_{16}NaO_5$, 347.0890; found 347.0900.



3am

2,6-dimethoxyphenyl 2-(1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

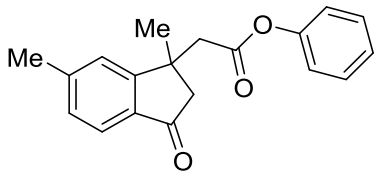
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (25.9 mg, 38%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 7.6 Hz, 1H), 7.64 (t, J = 7.2 Hz, 1H), 7.58 (d, J = 7.6 Hz, 1H), 7.40 (t, J = 7.2 Hz, 1H), 7.09 (t, J = 8.4 Hz, 1H), 6.56 (d, J = 8.4 Hz, 2H), 3.74 (s, 6H), 3.25 (d, J = 19.2 Hz, 1H), 3.11 (d, J = 14.4 Hz, 1H), 2.97 (d, J = 14.4 Hz, 1H), 2.65 (d, J = 19.2 Hz, 1H), 1.59 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.4, 168.6, 161.3, 152.2, 135.9, 135.0, 128.4, 128.0, 126.5, 123.9, 123.6, 104.8, 56.1, 50.3, 45.1, 40.8, 29.0. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{10}NaO_5$, 363.1203; found 363.1211.



3an

3-methyl-3-(2-(naphthalen-2-yl)-2-oxoethyl)-2,3-dihydro-1H-inden-1-one

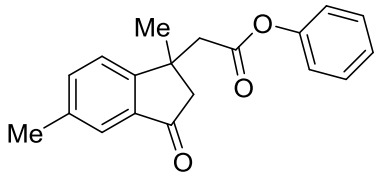
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (60.7 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 8.8 Hz, 1H), 7.68 (d, J = 7.6 Hz, 1H), 7.61-7.52 (m, 3H), 7.39-7.27 (m, 5H), 6.87 (d, J = 7.6 Hz, 1H), 3.16 (d, J = 18.8 Hz, 1H), 3.10 (d, J = 15.2 Hz, 1H), 3.03 (d, J = 15.2 Hz, 1H), 2.59 (d, J = 18.8 Hz, 1H), 1.53 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.7, 169.5, 160.4, 146.2, 136.1, 135.2, 134.6, 128.3, 128.0, 126.6, 126.47, 126.45, 126.2, 125.3, 123.9, 123.7, 120.9, 117.9, 50.3, 45.4, 40.6, 29.1. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{22}H_{18}NaO_3$, 353.1148; found 353.1142.



3ba

phenyl 2-(1,6-dimethyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

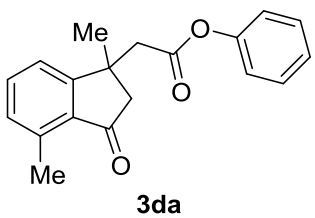
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (55.4 mg, 94%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, J = 7.6 Hz, 1H), 7.36 (s, 1H), 7.31 (t, J = 7.6 Hz, 2H), 7.23 (d, J = 7.6 Hz, 1H), 7.18 (t, J = 7.2 Hz, 1H), 6.86 (d, J = 8.0 Hz, 2H), 3.15 (d, J = 18.8 Hz, 1H), 3.02 (d, J = 14.8 Hz, 1H), 2.90 (d, J = 14.8 Hz, 1H), 2.64 (d, J = 18.8 Hz, 1H), 2.46 (s, 3H), 1.57 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.2, 169.4, 161.0, 150.2, 146.3, 133.7, 129.49, 129.46, 126.0, 124.2, 123.5, 121.4, 50.6, 45.7, 40.4, 28.8, 22.3. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{18}NaO_3$, 317.1148; found 317.1148.



3ca

phenyl 2-(1,5-dimethyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

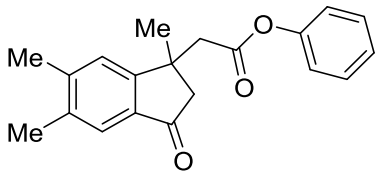
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (50.1 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.47 (s, 2H), 7.31 (t, J = 7.6 Hz, 2H), 7.18 (t, J = 7.2 Hz, 1H), 6.86 (d, J = 7.2 Hz, 2H), 3.16 (d, J = 18.8 Hz, 1H), 3.01 (d, J = 14.8 Hz, 1H), 2.91 (d, J = 14.8 Hz, 1H), 2.64 (d, J = 18.8 Hz, 1H), 2.41 (s, 3H), 1.57 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.9, 169.4, 157.9, 150.3, 138.3, 136.3, 136.1, 129.4, 126.0, 123.65, 123.62, 121.4, 50.7, 45.7, 40.3, 28.9, 21.1. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{18}NaO_3$, 317.1148; found 317.1147.



3da

phenyl 2-(1,4-dimethyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

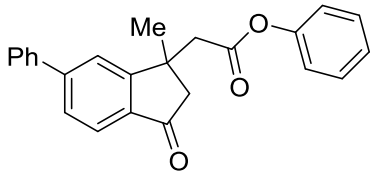
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (46.7 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (t, J = 7.6 Hz, 1H), 7.39 (d, J = 8.0 Hz, 1H), 7.32 (t, J = 8.0 Hz, 2H), 7.22-7.14 (m, 2H), 6.86 (d, J = 7.6 Hz, 2H), 3.14 (d, J = 18.8 Hz, 1H), 3.01 (d, J = 14.8 Hz, 1H), 2.90 (d, J = 14.8 Hz, 1H), 2.65 (s, 3H), 2.62 (d, J = 18.8 Hz, 1H), 1.57 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.7, 169.5, 161.3, 150.3, 138.8, 134.3, 133.3, 130.0, 129.4, 126.0, 121.4, 121.1, 50.8, 45.8, 39.8, 29.0, 18.5. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{18}NaO_3$, 317.1148; found 317.1138.



3ea

phenyl 2-(1,5,6-trimethyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. White solid. mp 79-81 ^{o}C. (59.7 mg, 97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.36-7.27 (m, 3H), 7.18 (t, J = 7.2 Hz, 1H), 6.88 (d, J = 7.6 Hz, 2H), 3.13 (d, J = 18.8 Hz, 1H), 3.01 (d, J = 14.8 Hz, 1H), 2.88 (d, J = 14.8 Hz, 1H), 2.62 (d, J = 18.8 Hz, 1H), 2.37 (s, 3H), 2.31 (s, 3H), 1.56 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.5, 169.4, 158.8, 150.3, 145.3, 137.2, 134.1, 129.4, 125.9, 124.6, 123.9, 121.4, 50.7, 45.7, 40.2, 28.8, 21.0, 19.8. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{20}NaO_3$, 331.1305; found 331.1309.

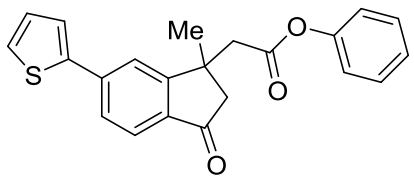


3fa

phenyl 2-(1-methyl-3-oxo-6-phenyl-2,3-dihydro-1H-inden-1-yl) acetate

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (61.1 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, J = 8.0 Hz, 1H), 7.78 (s, 1H), 7.70-7.62 (m, 3H), 7.49 (t, J = 6.8 Hz, 2H), 7.43 (t, J = 7.2 Hz, 1H), 7.31 (t, J = 7.6 Hz,

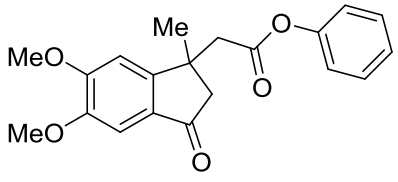
2H), 7.18 (t, *J* = 7.2 Hz, 1H), 6.87 (d, *J* = 7.6 Hz, 2H), 3.23 (d, *J* = 19.2 Hz, 1H), 3.09 (d, *J* = 14.8 Hz, 1H), 3.00 (d, *J* = 14.8 Hz, 1H), 2.72 (d, *J* = 19.2 Hz, 1H), 1.65 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.2, 169.4, 161.1, 150.2, 148.3, 140.2, 134.8, 129.4, 129.0, 128.5, 127.67, 127.60, 126.0, 124.1, 122.5, 121.4, 50.8, 45.7, 40.7, 28.9. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{24}H_{20}NaO_3$, 379.1305; found 379.1286.



3ga

phenyl 2-(1-methyl-3-oxo-6-(thiophen-2-yl)-2,3-dihydro-1H-inden-1-yl) acetate

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (53.8 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.0 Hz, 2H), 7.68 (dd, *J* = 8.0, 2.8 Hz, 1H), 7.47 (dd, *J* = 3.6, 0.8 Hz, 1H), 7.40 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.31 (t, *J* = 8.0 Hz, 2H), 7.18 (t, *J* = 7.6 Hz, 1H), 7.13 (dd, *J* = 5.2, 3.6 Hz, 1H), 6.91-6.87 (m, 2H), 3.19 (d, *J* = 19.2 Hz, 1H), 3.08 (d, *J* = 14.8 Hz, 1H), 2.97 (d, *J* = 14.8 Hz, 1H), 2.69 (d, *J* = 19.2 Hz, 1H), 1.63 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.8, 169.4, 161.4, 150.2, 143.0, 141.0, 134.8, 129.5, 128.5, 127.0, 126.2, 126.0, 125.3, 124.4, 121.4, 120.6, 50.7, 45.6, 40.6, 28.8. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{22}H_{18}NaO_3S$, 385.0869; found 385.0854.

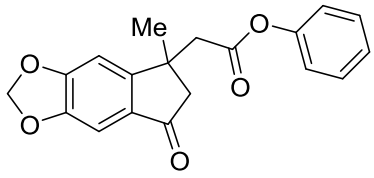


3ha

phenyl 2-(5,6-dimethoxy-1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (67.5 mg, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (t, *J* = 7.6 Hz, 2H), 7.19-7.12 (m, 2H), 6.94 (s, 1H), 6.86 (d, *J* = 7.6 Hz, 2H), 3.95 (s, 3H), 3.88 (s, 3H), 3.11 (d, *J* = 18.4 Hz, 1H), 2.98 (d, *J* = 14.8 Hz, 1H), 2.87 (d, *J* = 14.8 Hz, 1H), 2.61 (d, *J* = 18.8 Hz, 1H), 1.55 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.2, 169.4, 155.7, 155.6, 150.2, 149.9, 129.4, 128.8, 126.0, 121.3, 104.9, 104.0, 56.3, 56.1, 50.6, 45.7, 40.3, 28.6. HRMS (ESI-

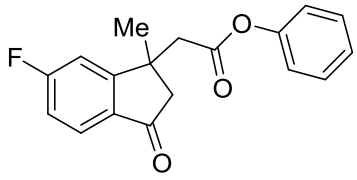
TOF) m/z: $[M + Na]^+$ Calcd for $C_{20}H_{20}NaO_5$, 363.1203; found 363.1194.



3ia

phenyl 2-(5-methyl-7-oxo-6,7-dihydro-5H-indeno[5,6-d][1,3]dioxol-5-yl) acetate

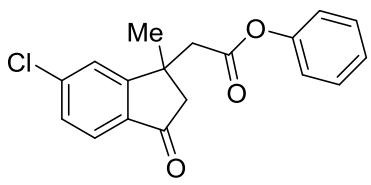
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. White solid. (46.8 mg, 73%). mp 139-141 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (t, J = 8.0 Hz, 2H), 7.19 (t, J = 7.6 Hz, 1H), 7.07 (s, 1H), 6.94-6.88 (m, 3H), 6.06 (d, J = 0.8 Hz, 1H), 6.05 (d, J = 0.8 Hz, 1H), 3.12 (d, J = 18.8 Hz, 1H), 2.96 (d, J = 14.8 Hz, 1H), 2.85 (d, J = 14.8 Hz, 1H), 2.62 (d, J = 18.8 Hz, 1H), 1.53 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.4, 169.3, 158.0, 154.5, 150.2, 148.8, 130.7, 129.5, 126.0, 121.4, 103.3, 102.5, 102.1, 50.6, 45.7, 40.4, 28.7. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{16}NaO_5$, 347.0890; found 347.0876.



3ja

5-fluoro-3-methyl-3-(2-oxo-2-phenylethyl)-2,3-dihydro-1H-inden-1-one

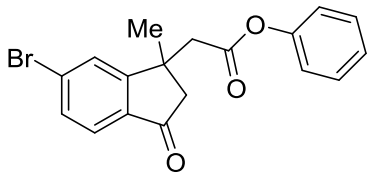
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (33.6 mg, 57%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (dd, J = 8.4, 5.2 Hz, 1H), 7.32 (t, J = 8.0 Hz, 2H), 7.25-7.17 (m, 2H), 7.12 (td, J = 8.4, 2.4 Hz, 1H), 6.88 (d, J = 7.6 Hz, 2H), 3.16 (d, J = 19.2 Hz, 1H), 3.02 (d, J = 15.2 Hz, 1H), 2.93 (d, J = 15.2 Hz, 1H), 2.67 (d, J = 19.2 Hz, 1H), 1.58 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.8, 169.2, 167.4 (d, J = 256.9 Hz), 163.5 (d, J = 8.8 Hz), 150.2, 132.5, 129.6, 126.23 (d, J = 9.1 Hz), 126.16, 121.4, 116.6 (d, J = 23.7 Hz), 110.9 (d, J = 22.5 Hz), 50.6, 45.5, 40.6, 28.8. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{15}FNaO_3$, 321.0897; found 321.0891.



3ka

5-chloro-3-methyl-3-(2-oxo-2-phenylethyl)-2,3-dihydro-1H-inden-1-one

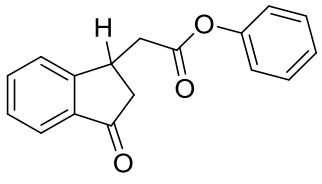
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (50.0 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 8.1Hz, 1H), 7.56 (d, J = 2.4 Hz, 1H), 7.39 (dd, J = 8.0 Hz, 1.6Hz, 1H), 7.37-7.28 (m, 2H), 7.19 (t, J = 7.2 Hz, 1H), 6.94-6.83 (m, 2H), 3.14 (d, J = 19.2 Hz, 1H), 3.02 (d, J = 15.6 Hz, 1H), 2.93 (d, J = 15.2 Hz, 1H), 2.65 (d, J = 19.2 Hz, 1H), 1.57 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.1, 169.1, 161.9, 150.1, 141.5, 134.5, 129.5, 129.0, 126.1, 124.9, 124.3, 121.3, 50.4, 45.3, 40.5, 28.8. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{15}ClNaO_3$, 337.0602; found 337.0593.



3la

5-bromo-3-methyl-3-(2-oxo-2-phenylethyl)-2,3-dihydro-1H-inden-1-one

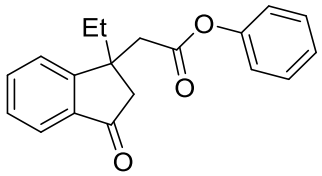
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (56.8 mg, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 1.6 Hz, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.55 (dd, J = 8.0, 1.6 Hz, 1H), 7.35-7.30 (m, 2H), 7.22-7.18 (m, 1H), 6.88 (d, J = 7.6 Hz, 2H), 3.14 (d, J = 18.8 Hz, 1H), 3.03 (d, J = 14.8 Hz, 1H), 2.93 (d, J = 14.8 Hz, 1H), 2.65 (d, J = 18.8 Hz, 1H), 1.57 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.4, 169.1, 162.1, 150.2, 134.9, 131.9, 130.4, 129.6, 127.5, 126.1, 125.1, 121.4, 50.4, 45.4, 40.6, 28.8. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{15}BrNaO_3$, 381.0097; found 381.0088.



3ma

3-(2-oxo-2-phenylethyl)-2,3-dihydro-1H-inden-1-one

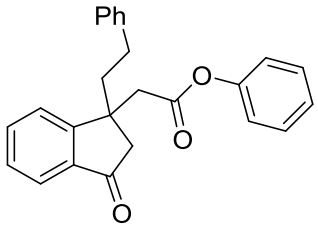
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (45.4 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 7.6 Hz, 1H), 7.58-7.48 (m, 1H), 7.50 (d, J = 7.6 Hz, 1H), 7.35 (t, J = 7.2 Hz, 1H), 7.29 (t, J = 8.0 Hz, 2H), 7.15 (t, J = 7.2 Hz, 1H), 6.96 (d, J = 7.6 Hz, 2H), 3.89-3.80 (m, 1H), 3.05 (dd, J = 16.4, 5.2 Hz, 1H), 2.97 (dd, J = 19.2, 7.6 Hz, 1H), 2.75 (dd, J = 16.0, 8.8 Hz, 1H), 2.48 (dd, J = 19.2, 3.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.0, 169.3, 155.3, 149.4, 135.9, 134.1, 128.6, 127.3, 125.1, 124.5, 122.9, 120.4, 42.3, 39.4, 33.6. HRMS (ESI-TOF) m/z: [M + Na]$^+$ Calcd for $C_{17}H_{14}NaO_3$, 289.0835; found 289.0835.



3na
400 MHz, $CDCl_3$

3-ethyl-3-(2-oxo-2-phenylethyl)-2,3-dihydro-1H-inden-1-one

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (48.0 mg, 82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 7.8 Hz, 1H), 7.69-7.62 (m, 1H), 7.55 (d, J = 7.6 Hz, 1H), 7.46-7.40 (m, 1H), 7.32-7.24 (m, 2H), 7.16 (t, J = 7.2 Hz, 1H), 6.76 (d, J = 7.6 Hz, 2H), 3.11-3.03 (m, 2H), 2.97 (d, J = 14.8 Hz, 1H), 2.72 (d, J = 19.2 Hz, 1H), 1.99 (dq, J = 14.8, 7.4 Hz, 1H), 1.87 (dq, J = 14.8, 7.4 Hz, 1H), 0.77 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.9, 169.5, 158.6, 150.2, 137.1, 134.9, 129.4, 128.2, 126.0, 124.3, 123.6, 121.3, 47.2, 44.6, 44.3, 33.9, 8.9. HRMS (ESI-TOF) m/z: [M + Na]$^+$ Calcd for $C_{19}H_{18}NaO_3$, 317.1148; found 317.1152.

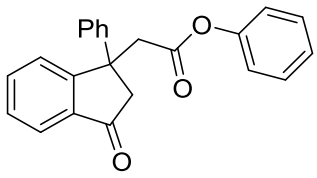


3oa

3-(2-oxo-2-phenylethyl)-3-phenethyl-2,3-dihydro-1H-inden-1-one

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil.

(62.7 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, J = 7.6 Hz, 1H), 7.67 (t, J = 7.2 Hz, 1H), 7.60 (d, J = 7.6 Hz, 1H), 7.45 (t, J = 7.6 Hz, 1H), 7.34-7.24 (m, 4H), 7.16 (t, J = 7.2 Hz, 2H), 7.07 (d, J = 7.2 Hz, 2H), 6.77 (d, J = 7.6 Hz, 2H), 3.20-3.10 (m, 2H), 3.02 (d, J = 15.2 Hz, 1H), 2.85 (d, J = 18.8 Hz, 1H), 2.59-2.50 (m, 1H), 2.34-2.21 (m, 2H), 2.17-2.08 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.5, 169.3, 158.4, 150.1, 141.1, 136.9, 135.1, 129.4, 128.5, 128.4, 128.2, 126.1, 125.9, 124.2, 123.6, 121.3, 47.6, 44.5, 44.2, 43.0, 31.0. HRMS (ESI-TOF) m/z: [M + Na]$^+$ Calcd for $C_{25}H_{22}NaO_3$, 393.1461; found 393.1471.

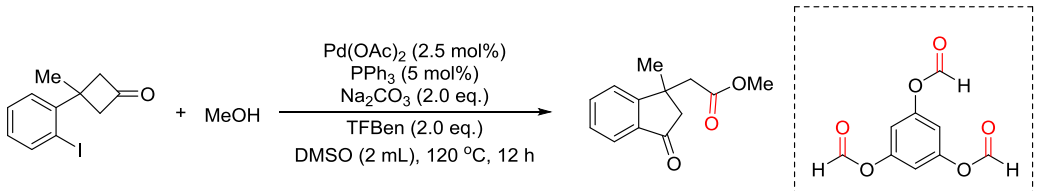


3pa

phenyl 2-(3-oxo-1-phenyl-2,3-dihydro-1H-inden-1-yl)acetate

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (56.8 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.6 Hz, 1H), 7.59-7.50 (m, 1H), 7.43-7.35 (m, 2H), 7.23 (t, J = 7.2 Hz, 2H), 7.19-7.09 (m, 5H), 7.05 (t, J = 7.6 Hz, 1H), 6.58 (d, J = 8.0 Hz, 2H), 3.57 (d, J = 15.2 Hz, 1H), 3.45 (d, J = 19.2 Hz, 1H), 3.31 (d, J = 15.2 Hz, 1H), 3.02 (d, J = 19.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.6, 169.2, 158.4, 150.1, 145.8, 136.9, 135.1, 129.4, 128.9, 128.6, 127.0, 126.3, 126.0, 123.7, 121.3, 52.9, 48.2, 44.2. HRMS (ESI-TOF) m/z: [M + Na]$^+$ Calcd for $C_{23}H_{18}NaO_3$, 365.1148; found 365.1158.

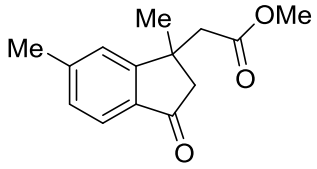
Typical procedure for the synthesis of esters 5.



1a **5aa** **TFBen**

A vial was charged with 3-(2-iodophenyl)-3-methylcyclobutan-1-one **1a** (57.2 mg, 0.2 mmol), $Pd(OAc)_2$ (1.2 mg, 2.5 mol%), PPh_3 (2.7 mg, 5 mol%), Na_2CO_3 (42.4 mg, 2.0 eq.), TFBen (84.0 mg, 2.0 eq.) and evacuated under high vacuum and backfilled with N_2. DMSO (2 mL) and methanol (81 uL, 10.0 eq.) was next added. The mixture was

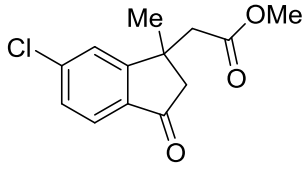
stirred at 120 °C for 12 h, and then cooled to room temperature. The reaction mixture was extracted with EA and dried over Na_2SO_4, concentrated under reduced pressure and then purified by silica column (PE-EtOAc, 20:1) to get the product **5aa**. The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (36.7 mg, 84%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, J = 7.6 Hz, 1H), 7.55 (t, J = 7.6 Hz, 1H), 7.42 (d, J = 7.6 Hz, 1H), 7.32 (t, J = 7.6 Hz, 1H), 3.48 (s, 3H), 2.97 (d, J = 19.2 Hz, 1H), 2.73 (d, J = 15.2 Hz, 1H), 2.59 (d, J = 15.2 Hz, 1H), 2.50 (d, J = 19.2 Hz, 1H), 1.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.0, 171.3, 160.8, 135.8, 135.0, 128.0, 123.7, 123.5, 51.5, 50.4, 45.4, 40.3, 28.6. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{13}H_{14}NaO_3$, 241.0835; found 241.0846.



5ba

methyl 2-(1,6-dimethyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. White solid. mp 67-69 ^{o}C. (41.9 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 8.0 Hz, 1H), 7.24 (s, 1H), 7.18 (d, J = 7.6 Hz, 1H), 3.55 (s, 3H), 3.00 (d, J = 18.8 Hz, 1H), 2.76 (d, J = 14.8 Hz, 1H), 2.62 (d, J = 14.8 Hz, 1H), 2.53 (d, J = 18.8 Hz, 1H), 2.43 (s, 3H), 1.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.6, 171.3, 161.4, 146.2, 133.6, 129.3, 124.0, 123.4, 51.6, 50.7, 45.5, 40.2, 28.5, 22.3. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{14}H_{16}NaO_3$, 255.0992; found 255.1000.

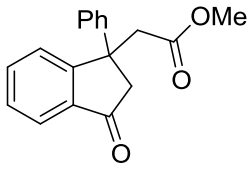


5ca

methyl 2-(6-chloro-1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. White solid. mp 80-82 ^{o}C. (46.5 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, J = 8.0 Hz, 1H), 7.44 (d, J = 1.6 Hz, 1H), 7.34 (dd, J = 8.0, 1.6 Hz, 1H), 3.55 (s, 3H), 3.01 (d, J = 18.8

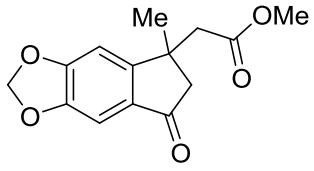
Hz, 1H), 2.76 (d, J = 15.2 Hz, 1H), 2.65 (d, J = 15.2 Hz, 1H), 2.55 (d, J = 18.8 Hz, 1H), 1.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.4, 171.0, 162.3, 141.4, 134.4, 128.8, 124.8, 124.2, 51.7, 50.5, 45.1, 40.3, 28.6. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{13}H_{13}ClNaO_3$, 275.0445; found 275.0453.



5ea

methyl 2-(3-oxo-1-phenyl-2,3-dihydro-1H-inden-1-yl) acetate

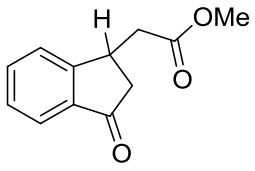
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. White solid. mp 81-83 ºC. (45.7 mg, 82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 7.6 Hz, 1H), 7.57 (td, J = 7.6, 1.2 Hz, 1H), 7.39 (t, J = 7.2 Hz, 1H), 7.33 (d, J = 8.0 Hz, 1H), 7.27-7.20 (m, 2H), 7.21-7.13 (m, 1H), 7.15-7.07 (m, 2H), 3.43 (s, 3H), 3.41 (d, J = 15.2 Hz, 1H), 3.37 (d, J = 19.2 Hz, 1H), 3.10 (d, J = 15.2 Hz, 1H), 3.00 (d, J = 19.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.9, 171.0, 158.8, 145.9, 136.7, 135.0, 128.8, 128.4, 126.8, 126.0, 126.0, 123.5, 53.1, 51.7, 48.0, 43.8. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{16}NaO_3$, 303.0992; found 303.1003.



5fa

methyl 2-(5-methyl-7-oxo-6,7-dihydro-5H-indeno[5,6-d] [1,3] dioxol-5-yl) acetate

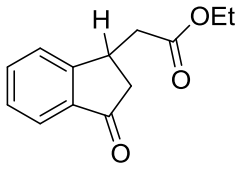
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. White solid. mp 76-78 ºC. (49.4 mg, 94%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.02 (s, 1H), 6.82 (s, 1H), 6.05 (s, 2H), 3.56 (s, 3H), 2.98 (d, J = 18.8 Hz, 1H), 2.71 (d, J = 14.8 Hz, 1H), 2.58 (d, J = 14.8 Hz, 1H), 2.52 (d, J = 18.8 Hz, 1H), 1.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 202.7, 171.2, 158.4, 154.4, 148.7, 130.6, 103.2, 102.4, 102.1, 51.7, 50.7, 45.5, 40.1, 28.5. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{14}H_{14}NaO_5$, 285.0733; found 285.0745



5da

methyl 2-(3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

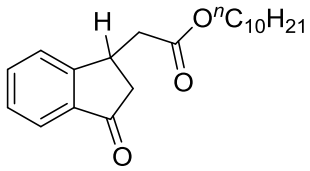
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (33.8 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 7.6 Hz, 1H), 7.60 (t, J = 7.6 Hz, 1H), 7.48 (d, J = 7.6 Hz, 1H), 7.39 (t, J = 7.6 Hz, 1H), 3.86-3.74 (m, 1H), 3.70 (s, 3H), 2.98 (dd, J = 19.2, 8.0 Hz, 1H), 2.88 (dd, J = 16.0, 5.2 Hz, 1H), 2.54 (dd, J = 16.0, 9.2 Hz, 1H), 2.42 (dd, J = 19.2, 3.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.4, 172.3, 156.7, 136.9, 135.0, 128.1, 125.5, 123.8, 52.0, 43.4, 40.2, 34.6. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{12}H_{12}NaO_3$, 227.0679; found 227.0667.



5db

ethyl 2-(3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

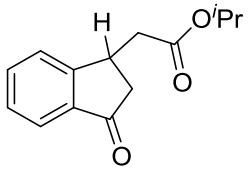
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (40.4 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 7.6 Hz, 1H), 7.60 (t, J = 7.6 Hz, 1H), 7.49 (d, J = 7.6 Hz, 1H), 7.39 (t, J = 7.6 Hz, 1H), 4.15 (q, J = 7.2 Hz, 2H), 3.86-3.74 (m, 1H), 2.98 (dd, J = 19.2, 7.6 Hz, 1H), 2.87 (dd, J = 16.0, 5.2 Hz, 1H), 2.53 (dd, J = 16.0, 9.2 Hz, 1H), 2.44 (dd, J = 19.2, 3.2 Hz, 1H), 1.23 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.4, 171.8, 156.7, 136.9, 135.0, 128.1, 125.5, 123.8, 60.9, 43.4, 40.5, 34.6, 14.3. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{13}H_{14}NaO_3$, 241.0835; found 241.0844.



5dc

decyl 2-(3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

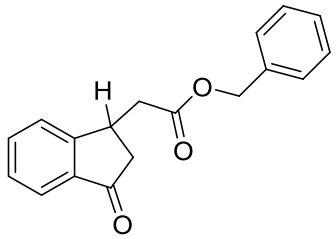
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (46.2 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 7.6 Hz, 1H), 7.66-7.57 (m, 1H), 7.51 (d, J = 7.6 Hz, 1H), 7.41 (t, J = 7.6 Hz, 1H), 4.10 (t, J = 6.8 Hz, 2H), 3.88-3.77 (m, 1H), 3.00 (dd, J = 19.2, 7.6 Hz, 1H), 2.89 (dd, J = 16.0, 5.2 Hz, 1H), 2.56 (dd, J = 16.0, 9.2 Hz, 1H), 2.46 (dd, J = 19.2, 3.6 Hz, 1H), 1.65-1.56 (m, 2H), 1.29-1.23 (m, 14H), 0.92-0.83 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.5, 172.0, 156.9, 137.0, 135.1, 128.2, 125.6, 123.9, 65.3, 43.5, 40.7, 34.8, 32.1, 29.7, 29.7, 29.5, 29.4, 28.8, 26.1, 22.9, 14.2. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{30}NaO_3$, 353.2087; found 353.2097.



5dd

isopropyl 2-(3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (23.1 mg, 47%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 7.6 Hz, 1H), 7.63-7.54 (m, 1H), 7.48 (d, J = 7.6 Hz, 1H), 7.37 (t, J = 7.6 Hz, 1H), 5.00 (hept, J = 6.2 Hz, 1H), 3.84-3.73 (m, 1H), 2.95 (dd, J = 19.2, 7.6 Hz, 1H), 2.83 (dd, J = 16.0, 4.8 Hz, 1H), 2.50 (dd, J = 16.0, 9.2 Hz, 1H), 2.44 (dd, J = 19.2, 3.6 Hz, 1H), 1.19 (d, J = 3.2 Hz, 3H), 1.18 (d, J = 3.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.4, 171.2, 156.8, 136.9, 134.9, 128.0, 125.5, 123.7, 68.3, 43.3, 40.7, 34.7, 21.84, 21.80. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{14}H_{16}NaO_3$, 255.0992; found 255.1002.

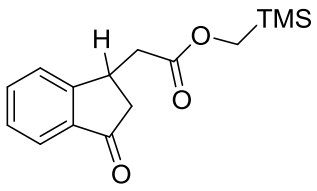


5de

benzyl 2-(3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (33.6 mg, 60%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.6 Hz, 1H), 7.63-7.54 (m,

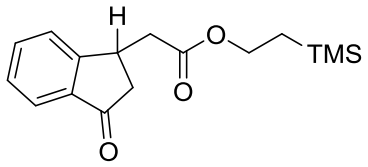
1H), 7.45 (d, J = 7.6 Hz, 1H), 7.44-7.34 (m, 1H), 7.40-7.30 (m, 5H), 5.20-5.11 (m, 2H), 4.10-3.62 (m, 1H), 3.13-2.76 (m, 2H), 2.61 (dd, J = 16.0, 9.2 Hz, 1H), 2.45 (dd, J = 19.2, 3.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.3, 171.6, 156.6, 136.9, 135.6, 135.0, 128.7, 128.51, 128.47, 128.1, 125.5, 123.8, 66.7, 43.3, 40.4, 34.6. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{18}H_{16}NaO_3$, 303.0992; found 303.1004.



5df

(trimethylsilyl)methyl 2-(3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Yellow oil. (42.1 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 7.6 Hz, 1H), 7.64-7.55 (m, 1H), 7.49 (d, J = 7.2 Hz, 1H), 7.38 (t, J = 7.6 Hz, 1H), 3.85-3.95 (m, 3H), 2.97 (dd, J = 19.2, 7.6 Hz, 1H), 2.88 (dd, J = 16.0, 5.2 Hz, 1H), 2.54 (dd, J = 15.6, 9.2 Hz, 1H), 2.42 (dd, J = 19.2, 3.6 Hz, 1H), 0.05 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.2, 172.4, 156.7, 136.7, 134.8, 127.9, 125.4, 123.6, 58.2, 43.3, 40.3, 34.6, -3.1. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{20}NaO_3Si$, 299.1074; found 299.1085.

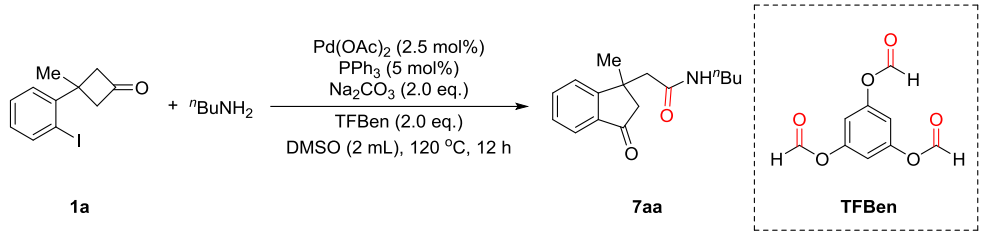


5dg

2-(trimethylsilyl) ethyl 2-(3-oxo-2,3-dihydro-1H-inden-1-yl) acetate

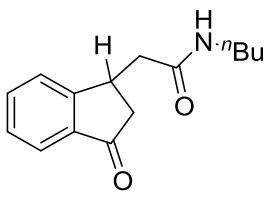
The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (49.8 mg, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.6 Hz, 1H), 7.65-7.56 (m, 1H), 7.50 (d, J = 7.6 Hz, 1H), 7.39 (t, J = 7.2 Hz, 1H), 4.24-4.14 (m, 2H), 3.87-3.75 (m, 1H), 2.99 (dd, J = 19.2, 7.6 Hz, 1H), 2.86 (dd, J = 16.0, 5.2 Hz, 1H), 2.51 (dd, J = 16.0, 9.2 Hz, 1H), 2.44 (dd, J = 19.2, 3.2 Hz, 1H), 1.01-0.92 (m, 2H), 0.03 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.3, 171.8, 156.7, 136.8, 134.9, 128.0, 125.4, 123.7, 63.1, 43.3, 40.6, 34.6, 17.4, -1.5. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{16}H_{22}NaO_3Si$, 313.1230; found 313.1241.

Typical procedure for the synthesis of amides 7.



1a **7aa** **TFBen**

A vial was charged with 3-(2-iodophenyl)-3-methylcyclobutan-1-one **1a** (57.2 mg, 0.2 mmol), $Pd(OAc)_2$ (1.2 mg, 2.5 mol%), PPh_3 (2.7 mg, 5 mol%), Na_2CO_3 (42.4 mg, 2.0 eq.), TFBen (84.0 mg, 2.0 eq.) and evacuated under high vacuum and backfilled with N_2. DMSO (2 mL) was next added and the reaction mixture was stirred for 20 min at 120 °C in an oil bath. n-Butylamine (20 uL, 0.2 mmol) was added and the reaction mixture was stirred for 5 min at 120 °C. Then the second batch of n-butylamine (20 uL, 0.2 mmol) was added. The mixture was stirred at 120 °C for 12 h, then cooled to room temperature. The reaction mixture was extracted with EA and dried over Na_2SO_4, concentrated under reduced pressure and then purified by silica column (PE-EtOAc, 5:1) to get the product **7aa**. The mobile phase for flash chromatography: hexane/ethyl acetate = 5:1. Colorless oil. (48.1 mg, 93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 7.6 Hz, 1H), 7.60 (t, J = 7.6 Hz, 1H), 7.49 (d, J = 7.6 Hz, 1H), 7.36 (t, J = 7.6 Hz, 1H), 5.67 (s, 1H), 3.20-2.97 (m, 3H), 2.57 (d, J = 14.0 Hz, 1H), 2.55-2.47 (m, 2H), 1.48 (s, 3H), 1.32-1.20 (m, 2H), 1.19-1.09 (m, 2H), 0.81 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.5, 170.0, 161.4, 136.0, 135.0, 128.0, 123.7, 123.6, 50.4, 47.9, 41.0, 39.2, 31.6, 28.7, 20.0, 13.8. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{16}H_{21}NNaO_2$, 282.1464; found 282.1455.

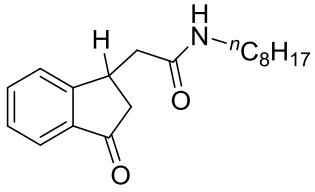


7ba

N-butyl-2-(3-oxo-2,3-dihydro-1H-inden-1-yl) acetamide

The mobile phase for flash chromatography: hexane/ethyl acetate = 5:1. White solid. (47.2 mg, 96%). mp 85-87 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 7.6 Hz, 1H),

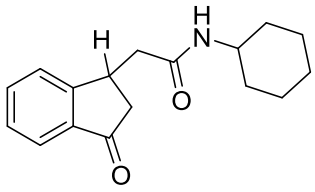
7.58 (t, J = 7.6 Hz, 1H), 7.50 (d, J = 7.6 Hz, 1H), 7.37 (t, J = 7.2 Hz, 1H), 5.75 (s, 1H), 3.92 (d, J = 7.6 Hz, 1H), 3.35-3.21 (m, 2H), 2.95 (dd, J = 19.2, 7.6 Hz, 1H), 2.66 (dd, J = 14.4, 6.0 Hz, 1H), 2.43-2.30 (m, 2H), 1.41-1.43 (m, 2H), 1.36-1.25 (m, 2H), 0.91 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.8, 170.8, 157.5, 136.8, 135.0, 128.1, 125.8, 123.8, 43.3, 43.1, 39.5, 35.1, 31.7, 20.2, 13.8. HRMS (ESI-TOF) m/z: [M + Na]$^+$ Calcd for $C_{15}H_{19}NNaO_2$, 268.1308; found 268.1319.



7bb

N-octyl-2-(3-oxo-2,3-dihydro-1H-inden-1-yl) acetamide

The mobile phase for flash chromatography: hexane/ethyl acetate = 10:1. White solid. mp 171-173 ^{o}C. (46.7 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 7.6 Hz, 1H), 7.58 (t, J = 6.8 Hz, 1H), 7.49 (d, J = 7.6 Hz, 1H), 7.37 (t, J = 7.6 Hz, 1H), 5.79 (t, J = 6.0 Hz, 1H), 3.97-3.86 (m, 1H), 3.25 (q, J = 6.8 Hz, 2H), 2.94 (dd, J = 19.6, 7.6 Hz, 1H), 2.65 (dd, J = 14.4, 6.0 Hz, 1H), 2.44-2.30 (m, 2H), 1.47-1.42 (m, 2H), 1.32-1.19 (m, 10H), 0.86 (t, J = 6.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.8, 170.8, 157.5, 136.8, 135.0, 128.0, 125.8, 123.8, 43.3, 43.1, 39.8, 35.1, 31.9, 29.7, 29.3, 29.3, 27.0, 22.7, 14.2. HRMS (ESI-TOF) m/z: [M + Na]$^+$ Calcd for $C_{19}H_{27}NNaO_2$, 324.1934; found 324.1945.

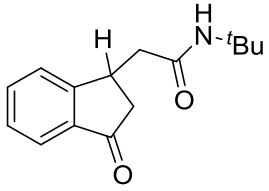


7bc

N-cyclohexyl-2-(3-oxo-2,3-dihydro-1H-inden-1-yl) acetamide

The mobile phase for flash chromatography: hexane/ethyl acetate = 10:1. White solid. mp 70-72 ^{o}C. (43.3 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 7.6 Hz, 1H), 7.61-7.52 (m, 1H), 7.48 (d, J = 7.6 Hz, 1H), 7.35 (t, J = 7.6 Hz, 1H), 5.74 (d, J = 8.4 Hz, 1H), 3.92-3.84 (m, 1H), 3.82-3.71 (m, 1H), 2.90 (dd, J = 19.2, 7.6 Hz, 1H), 2.60

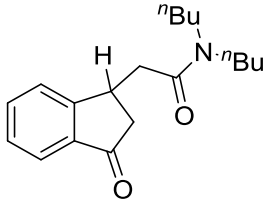
(dd, J = 14.4, 6.0 Hz, 1H), 2.41-2.27 (m, 2H), 1.95-1.80 (m, 2H), 1.72-1.52 (m, 3H) 1.41-1.26 (m, 2H), 1.17-1.05 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.8, 169.8, 157.5, 136.7, 135.0, 128.0, 125.8, 123.7, 48.5, 43.2, 43.1, 35.1, 33.23, 33.16, 25.5, 24.92, 24.90. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{17}H_{21}NaO_2$, 294.1464; found 294.1478.



7bd

N-(tert-butyl)-2-(3-oxo-2,3-dihydro-1H-inden-1-yl) acetamide

The mobile phase for flash chromatography: hexane/ethyl acetate = 10:1. White solid. mp 73-75 ºC. (39.4 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 7.6 Hz, 1H), 7.56 (t, J = 7.6 Hz, 1H), 7.48 (d, J = 7.6 Hz, 1H), 7.34 (t, J = 7.6 Hz, 1H), 5.56 (s, 1H), 3.93-3.81 (m, 1H), 2.91 (dd, J = 19.2, 7.6 Hz, 1H), 2.55 (dd, J = 14.0, 6.0 Hz, 1H), 2.35 (dd, J = 19.2, 2.8 Hz, 1H), 2.28 (dd, J = 14.4, 8.4 Hz, 1H), 1.32 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.9, 170.1, 157.6, 136.7, 134.9, 127.9, 125.8, 123.7, 51.5, 43.9, 43.1, 35.1, 28.8. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{19}NNaO_2$, 268.1308; found 268.1315.

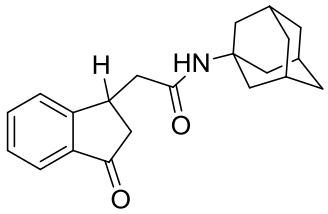


7be

N, N-dibutyl-2-(3-oxo-2,3-dihydro-1H-inden-1-yl) acetamide

The mobile phase for flash chromatography: hexane/ethyl acetate = 10:1. Colorless oil. (44.4 mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 7.6 Hz, 1H), 7.63-7.54 (m, 1H), 7.51 (d, J = 7.6 Hz, 1H), 7.38 (t, J = 7.6 Hz, 1H), 4.05-3.94 (m, 1H), 3.38-3.29 (m, 2H), 3.19-3.10 (m, 2H), 3.04 (dd, J = 19.2, 7.6 Hz, 1H), 2.80 (dd, J = 16.0, 5.6 Hz, 1H), 2.50 (dd, J = 16.0, 9.2 Hz, 1H), 2.31 (dd, J = 19.2, 3.2 Hz, 1H), 1.56-1.40 (m, 4H),

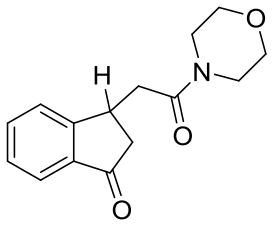
1.36-1.22 (m, 4H), 0.92 (t, J = 7.2 Hz, 3H), 0.87 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 206.2, 170.3, 158.0, 137.0, 134.9, 127.9, 125.8, 123.7, 47.8, 46.1, 44.2, 40.0, 35.0, 31.3, 30.0, 20.4, 20.1, 14.0, 13.9. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{19}H_{27}NNaO_2$, 324.1934; found 324.1949.



7bf

N-(adamantan-1-yl)-2-(3-oxo-2,3-dihydro-1H-inden-1-yl) acetamide

The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. White solid. mp 211-213 ^{o}C. (50.2 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, J = 7.6 Hz, 1H), 7.56 (t, J = 7.6 Hz, 1H), 7.49 (d, J = 7.6 Hz, 1H), 7.34 (t, J = 7.6 Hz, 1H), 5.37 (s, 1H), 3.95-3.77 (m, 1H), 2.91 (dd, J = 19.2, 7.6 Hz, 1H), 2.54 (dd, J = 14.4, 6.4 Hz, 1H), 2.39-2.26 (m, 2H), 2.06-2.02 (m, 3H), 1.96 (d, J = 2.8 Hz, 6H), 1.64 (t, J = 3.1 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.9, 169.8, 157.6, 136.7, 134.9, 127.9, 125.8, 123.6, 52.2, 43.9, 43.1, 41.6, 36.3, 35.1, 29.4. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{21}H_{25}NNaO_2$, 346.1777; found 346.1790.

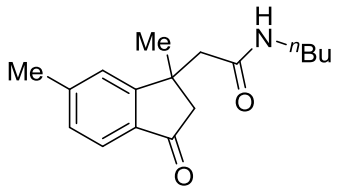


7bg

3-(2-morpholino-2-oxoethyl)-2,3-dihydro-1H-inden-1-one

The mobile phase for flash chromatography: hexane/ethyl acetate = 5:1. White solid. mp 81-83 ^{o}C. (46.8 mg, 90%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 7.6 Hz, 1H), 7.58 (t, J = 7.6 Hz, 1H), 7.50 (d, J = 7.6 Hz, 1H), 7.37 (t, J = 7.6 Hz, 1H), 4.00-3.89 (m, 1H), 3.74-3.55 (m, 6H), 3.43-3.37 (m, 2H), 3.05 (dd, J = 19.2, 7.6 Hz, 1H), 2.83 (dd, J = 16.4, 5.2 Hz, 1H), 2.52 (dd, J = 16.4, 9.2 Hz, 1H), 2.33 (dd, J = 19.2, 3.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.9, 169.6, 157.6, 137.0, 134.9, 128.0, 125.8, 123.8,

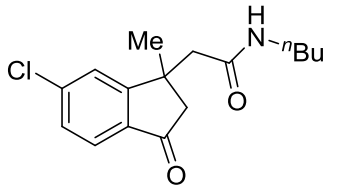
67.0, 66.6, 45.9, 44.2, 42.2, 39.9, 34.7. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{15}H_{17}NNaO_3$, 282.1100; found 282.1109.



7ca

N-butyl-2-(1,6-dimethyl-3-oxo-2,3-dihydro-1H-inden-1-yl)acetamide

The mobile phase for flash chromatography: hexane/ethyl acetate = 3:1. Colorless oil. (50.0 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.6 (d, J = 8.0 Hz, 1H), 7.3 (s, 1H), 7.2 (d, J = 7.6 Hz, 1H), 5.6 (s, 1H), 3.2-3.0 (m, 3H), 2.6-2.4 (m, 3H), 2.4 (s, 3H), 1.5 (s, 3H), 1.3-1.2 (m, 2H), 1.2-1.1 (m, 2H), 0.8 (t, J = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 205.0, 170.1, 162.0, 146.2, 133.7, 129.2, 124.1, 123.5, 50.7, 48.0, 40.8, 39.1, 31.6, 28.6, 22.3, 20.0, 13.8. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{17}H_{23}NNaO_2$, 296.1621; found 296.1615.

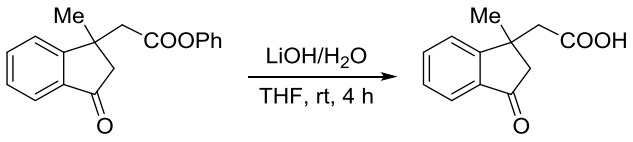


7da

N-butyl-2-(6-chloro-1-methyl-3-oxo-2,3-dihydro-1H-inden-1-yl)acetamide

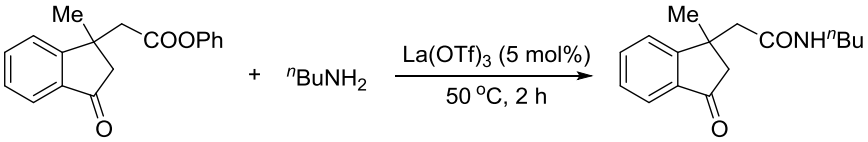
The mobile phase for flash chromatography: hexane/ethyl acetate = 3:1. Colorless oil. (50.1 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.6 (d, J = 8.4 Hz, 1H), 7.5 (d, J = 1.6 Hz, 1H), 7.3 (dd, J = 8.4, 1.6 Hz, 1H), 5.7 (s, 1H), 3.2 (d, J = 19.2 Hz, 1H), 3.2-3.0 (m, 2H), 2.6-2.5 (m, 3H), 1.5 (s, 3H), 1.3-1.3 (m, 2H), 1.2-1.1 (m, 2H), 0.8 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 203.9, 169.7, 162.8, 141.3, 134.5, 128.7, 124.8, 124.3, 50.6, 47.5, 41.0, 39.2, 31.6, 28.6, 20.0, 13.8. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{16}H_{20}ClNNaO_2$, 316.1075; found 316.1061.

Procedures for the synthesis of 7aa and 8.



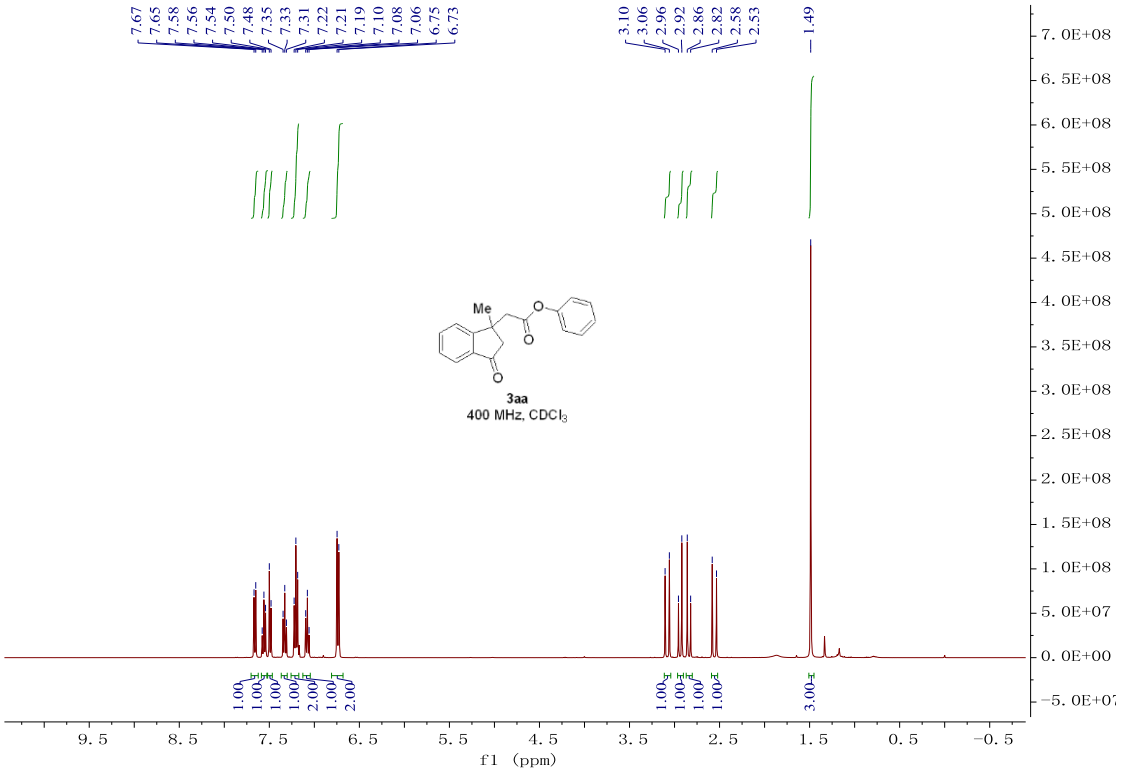
3aa **8,** 99% yield

To a solution of **3aa** (0.14 g, 0.50 mmol) in THF (3.0 mL) and water (0.50 mL) at 0 °C were added 30% H_2O_2 (0.29 mL) and LiOH (2.0 M, aqueous) (0.75 mL). The reaction mixture was stirred at 0 °C for 6 h, quenched with $Na_2S_2O_3$ (0.7 M) (3 mL) and $NaHCO_3$ (0.5 M) (6 mL), stirred for another 15 min, acidified with 20% HCl, extracted with EtOAc (3×5 mL), dried over Na_2SO_4, filtered, concentrated, and purified by flash chromatography (silica gel, eluent: petroleum ether/ethyl acetate = 5:1) to give acid **8** as a white solid (100.1 mg, 99% yield). The mobile phase for flash chromatography: hexane/ethyl acetate = 10:1. Colorless oil. (100.9 mg, 99%). mp 75-77 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.00 (s, 1H), 7.68 (d, J = 7.6 Hz, 1H), 7.64-7.57 (m, 1H), 7.47 (d, J = 7.6 Hz, 1H), 7.36 (t, J = 7.6 Hz, 1H), 3.03 (d, J = 19.2 Hz, 1H), 2.81 (d, J = 15.2 Hz, 1H), 2.66 (d, J = 15.2 Hz, 1H), 2.56 (d, J = 19.2 Hz, 1H), 1.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.8, 175.0, 160.0, 134.6, 134.3, 127.1, 122.68, 122.67, 49.3, 44.1, 39.2, 27.6. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{12}H_{12}NaO_3$, 227.0679; found 227.0688.



3aa **7aa,** 99% yield

To a solution of **3aa** (0.028 g, 0.1 mmol) in 1 mL ^{n}BuNH$_2$ was added La(OTf)$_3$ (3 mg, 5 mol%). The reaction mixture was stirred at 50 °C for 2 h, concentrated, and purified by flash chromatography (silica gel, eluent: petroleum ether/ethyl acetate = 5:1) to give amide **7aa** as a colorless oil (25.7 mg, 99% yield). The mobile phase for flash chromatography: hexane/ethyl acetate = 20:1. Colorless oil. (25.6 mg, 99%).


7.67
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7.58
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7.35
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7.31
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7.06
6.75
6.73
3.10
3.06
2.96
2.92
2.86
2.82
2.58
2.53
1.49
Me
O
O
O
3aa
400 MHz, CDCl3
1.00
1.00
1.00
1.00
2.00
1.00
2.00
1.00
1.00
1.00
1.00
3.00
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6.5
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4.5
3.5
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1.5
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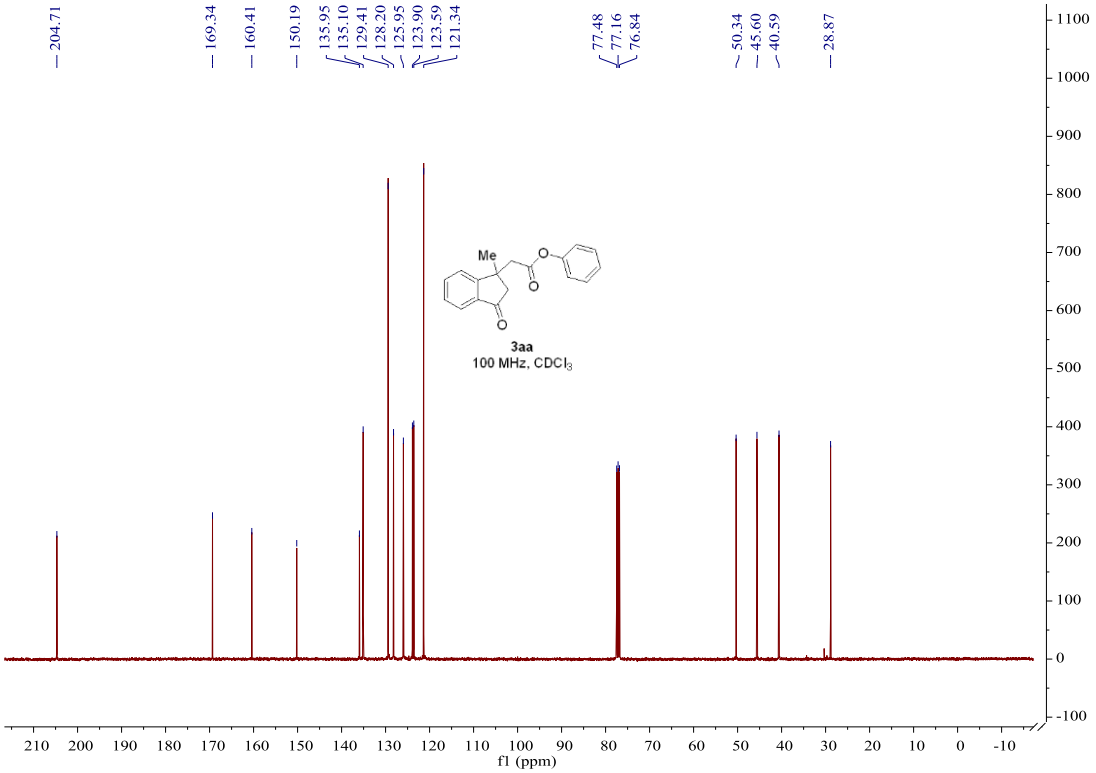
−0.5
f1 (ppm)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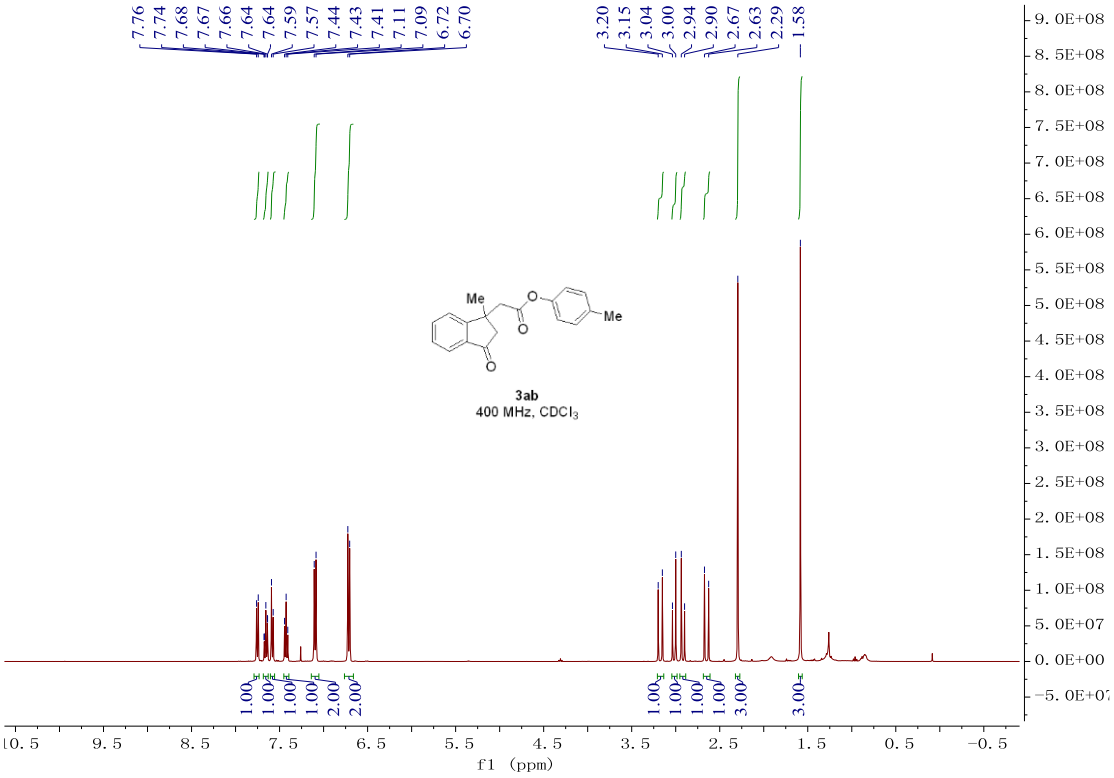
150.19
135.95
135.10
129.41
128.20
125.95
123.90
123.59
121.34
77.48
77.16
76.84
50.34
45.60
40.59
28.87
Me
O
O
O
3aa
100 MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.64
7.59
7.57
7.44
7.43
7.41
7.11
7.09
6.72
6.70
3.20
3.15
3.04
3.00
2.94
2.90
2.67
2.63
2.29
1.58
Me
O
Me
O
O
3ab
400 MHz, CDCl3
1.00
1.00
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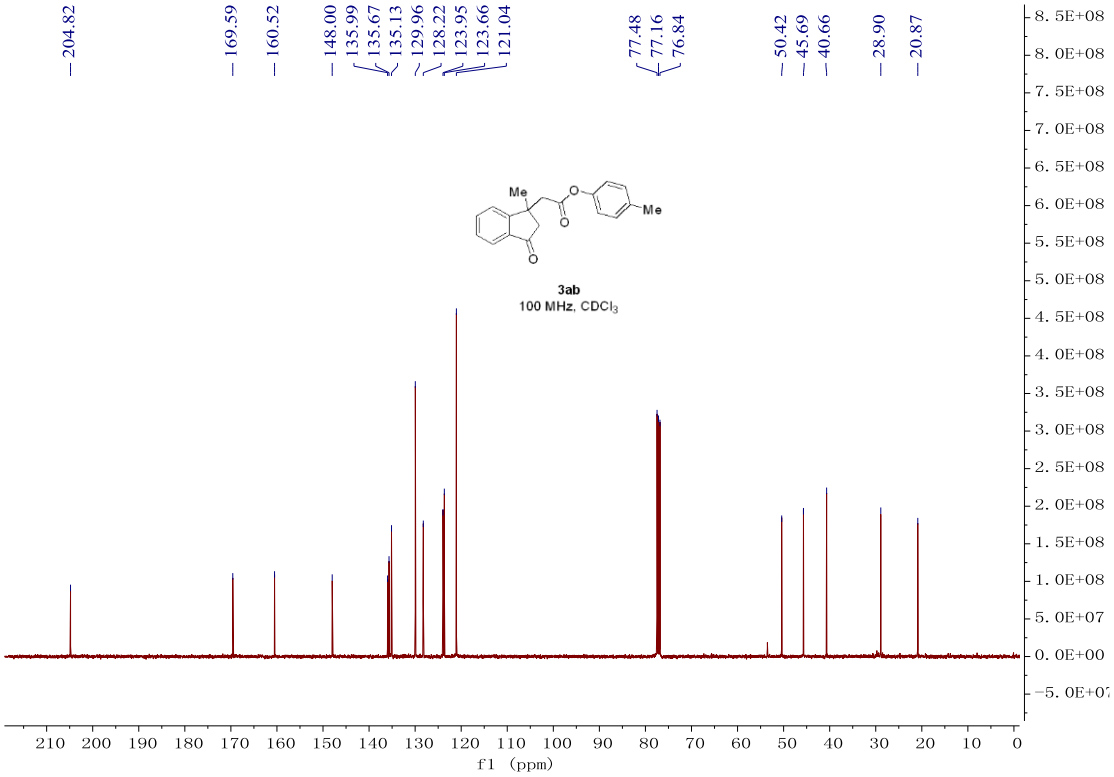
1.00
2.00
2.00
1.00
1.00
1.00
3.00
3.00
f1 (ppm)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135.13
129.96
128.22
123.95
123.66
121.04
77.48
77.16
76.84
50.42
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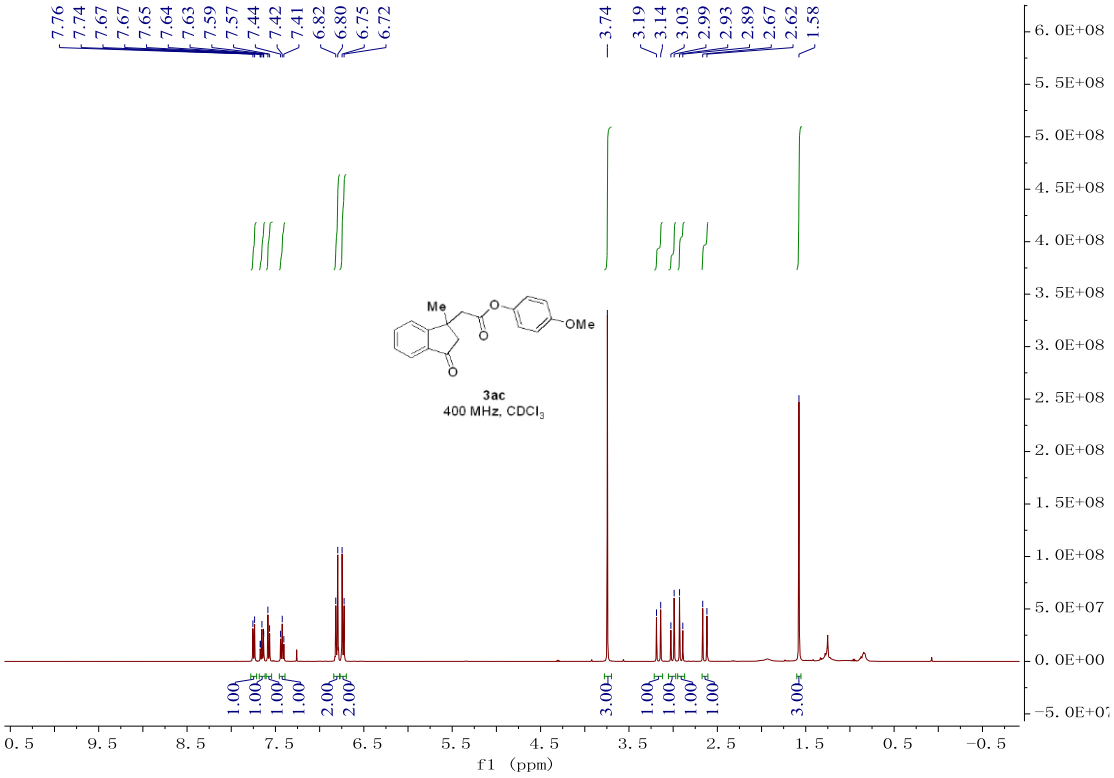
40.66
28.90
20.87
Me
O
Me
O
O
3ab
100 MHz, CDCl3
f1 (ppm)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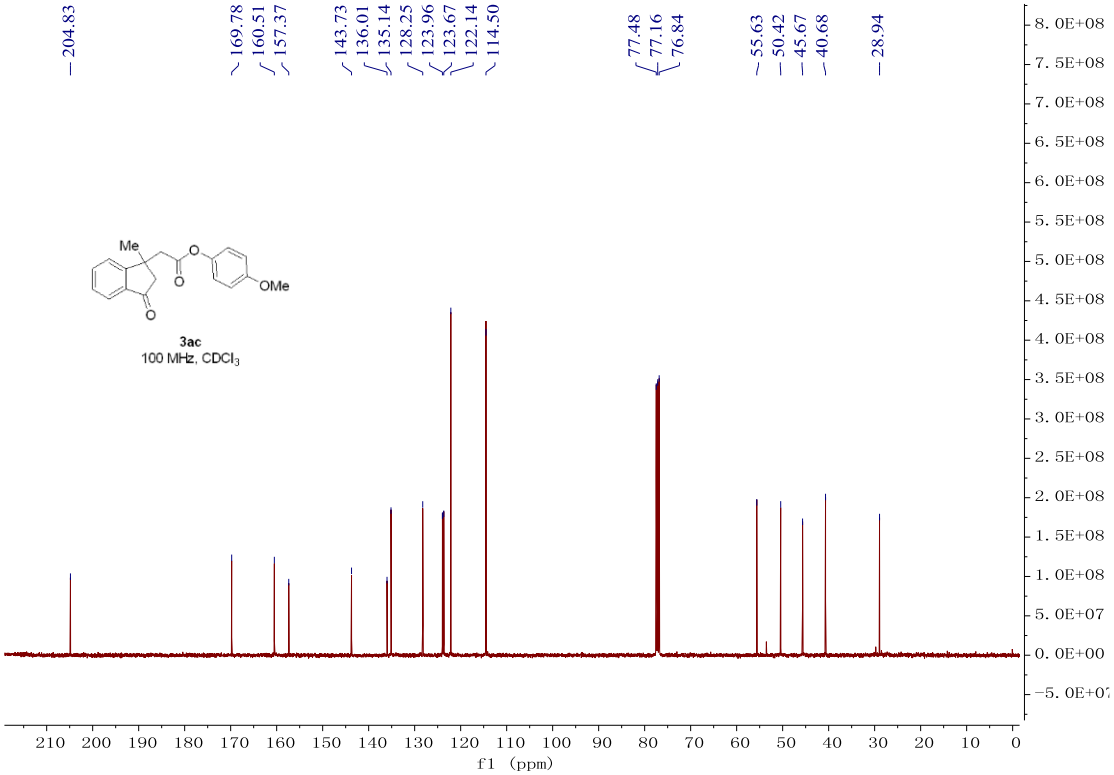
7.64
7.63
7.59
7.57
7.44
7.42
7.41
6.82
6.80
6.75
6.72
3.74
3.19
3.14
3.03
2.99
2.93
2.89
2.67
2.62
1.58
Me
O
O
OMe
O
3ac
400 MHz, CDCl3
1.00
1.00
1.00
1.00
2.00
2.00
3.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)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157.37
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135.14
128.25
123.96
123.67
122.14
114.50
77.48
77.16
76.84
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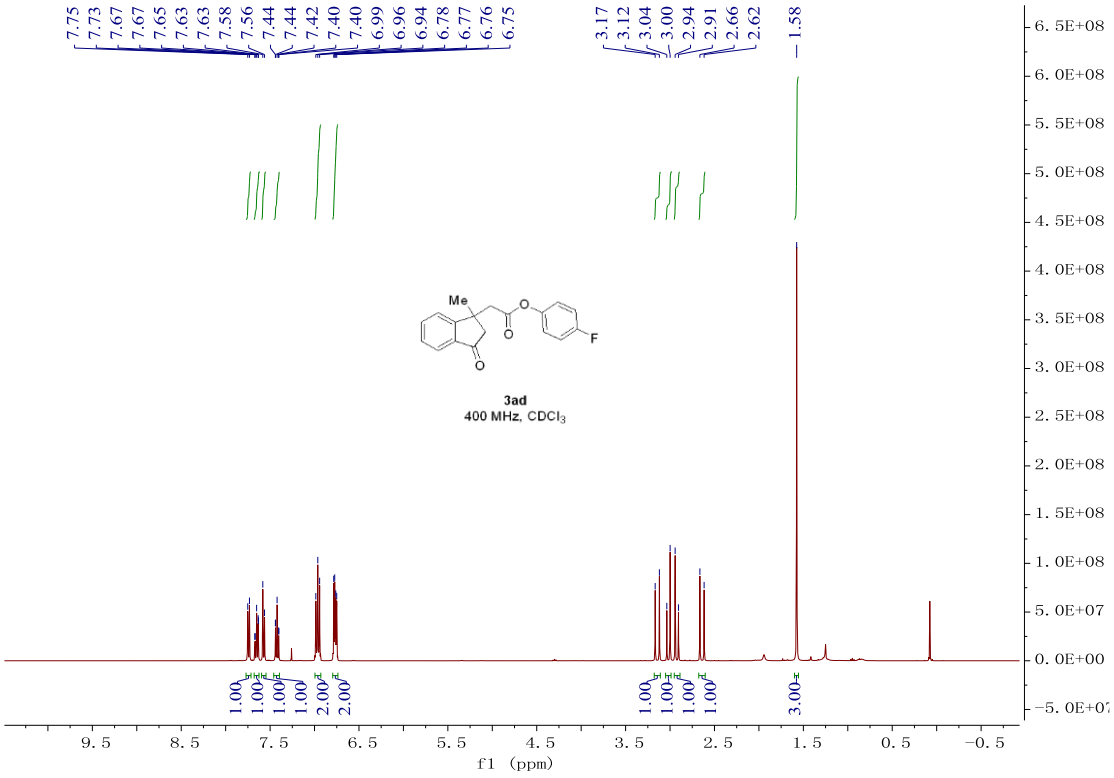
50.42
45.67
40.68
28.94
Me
O
O
OMe
O
3ac
100 MHz, CDCl3
f1 (ppm)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7.73
7.67
7.67
7.65
7.63
7.63
7.58
7.56
7.44
7.44
7.42
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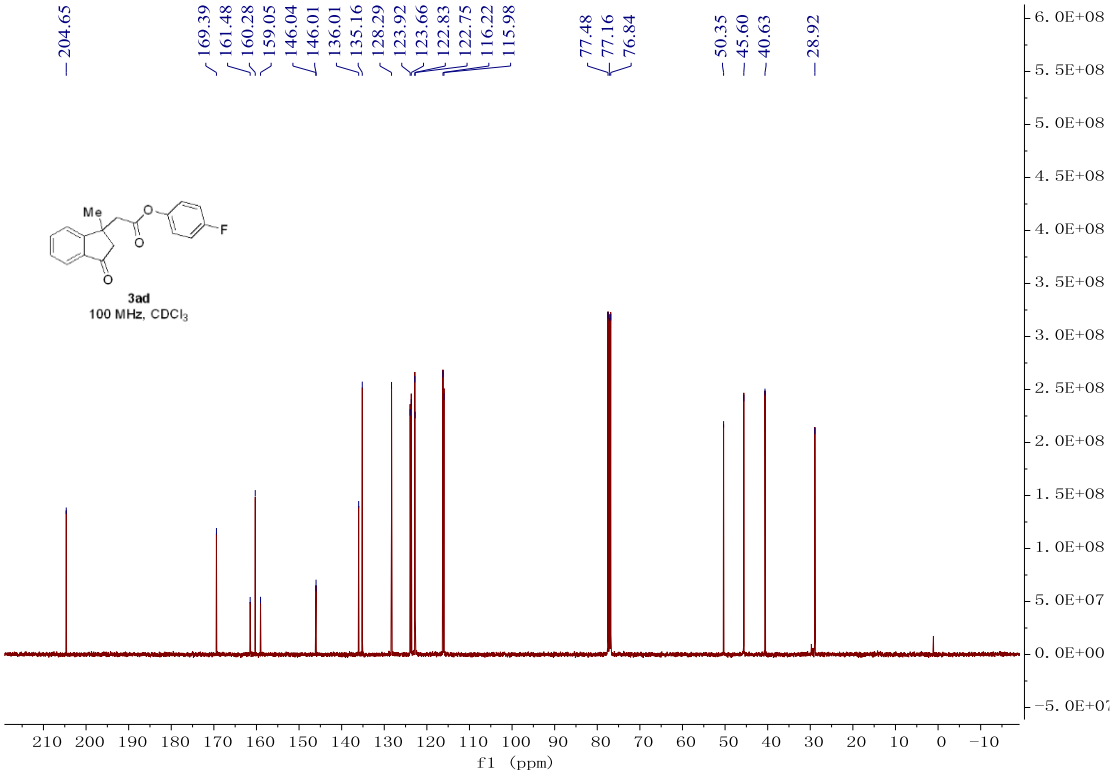
7.40
6.99
6.96
6.94
6.78
6.77
6.76
6.75
3.17
3.12
3.04
3.00
2.94
2.91
2.66
2.62
1.58
Me
O
O
F
O
3ad
400 MHz, CDCl3
1.00
1.00
1.00
1.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5
f1 (ppm)
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
−5.0E+07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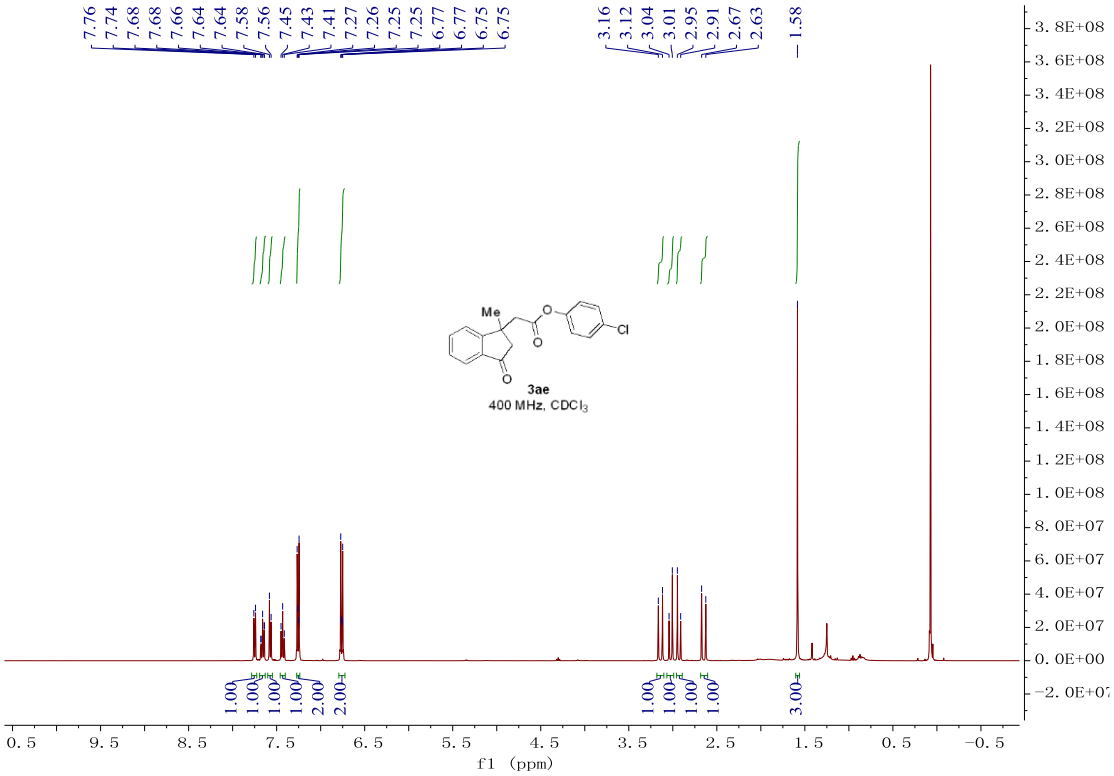
169.39
161.48
160.28
159.05
146.04
146.01
136.01
135.16
128.29
123.92
123.66
122.83
122.75
116.22
115.98
77.48
77.16
76.84
50.35
45.60
40.63
28.92
Me
O
O
F
O
3ad
100 MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
−5.0E+07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7.74
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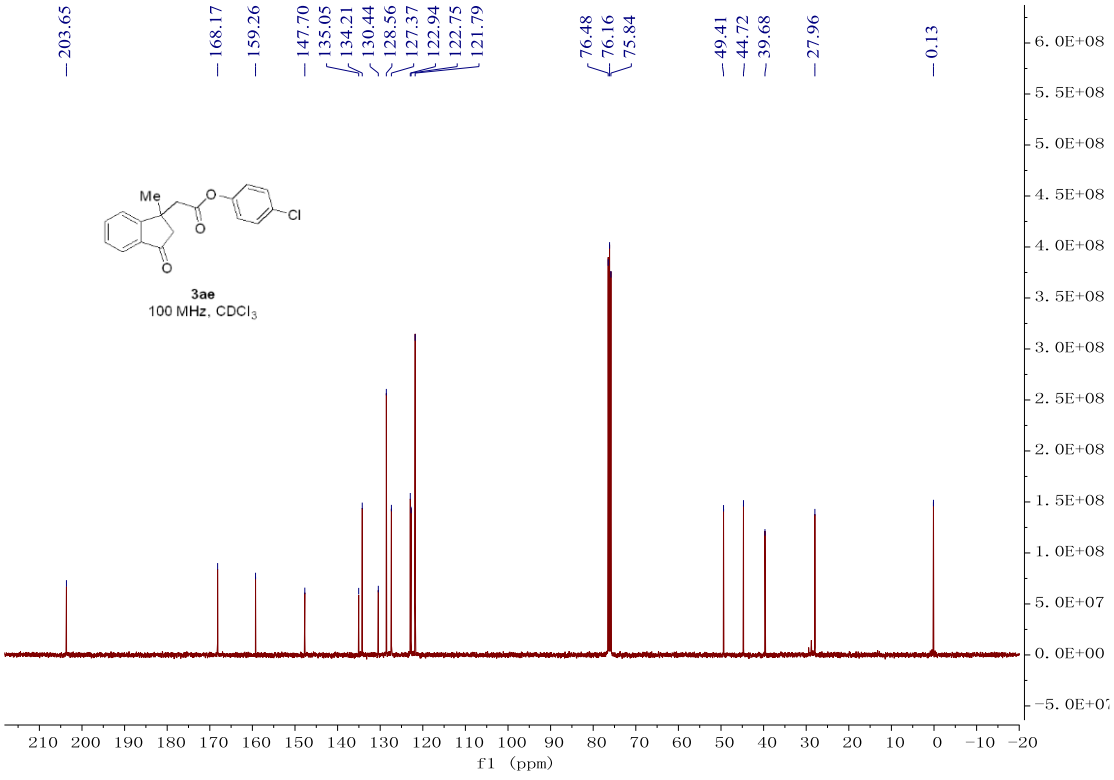
7.68
7.66
7.64
7.64
7.58
7.56
7.45
7.43
7.41
7.27
7.26
7.25
6.77
6.77
6.75
6.75
3.16
3.12
3.04
3.01
2.95
2.91
2.67
2.63
1.58
Me
O
O
O
Cl
3ae
400 MHz, CDCl3
1.00
1.00
1.00
1.00
2.00
2.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)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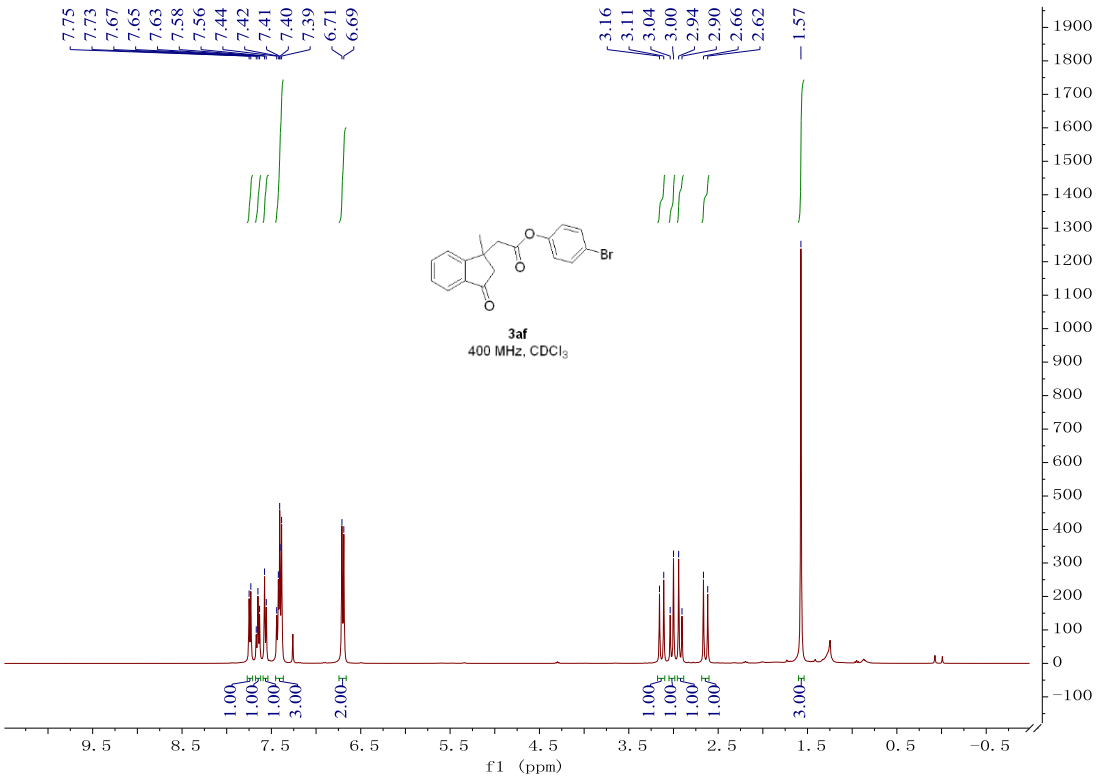
130.44
128.56
127.37
122.94
122.75
121.79
76.48
76.16
75.84
49.41
44.72
39.68
27.96
0.13
Me
O
O
O
Cl
3ae
100 MHz, CDCl3
f1 (ppm)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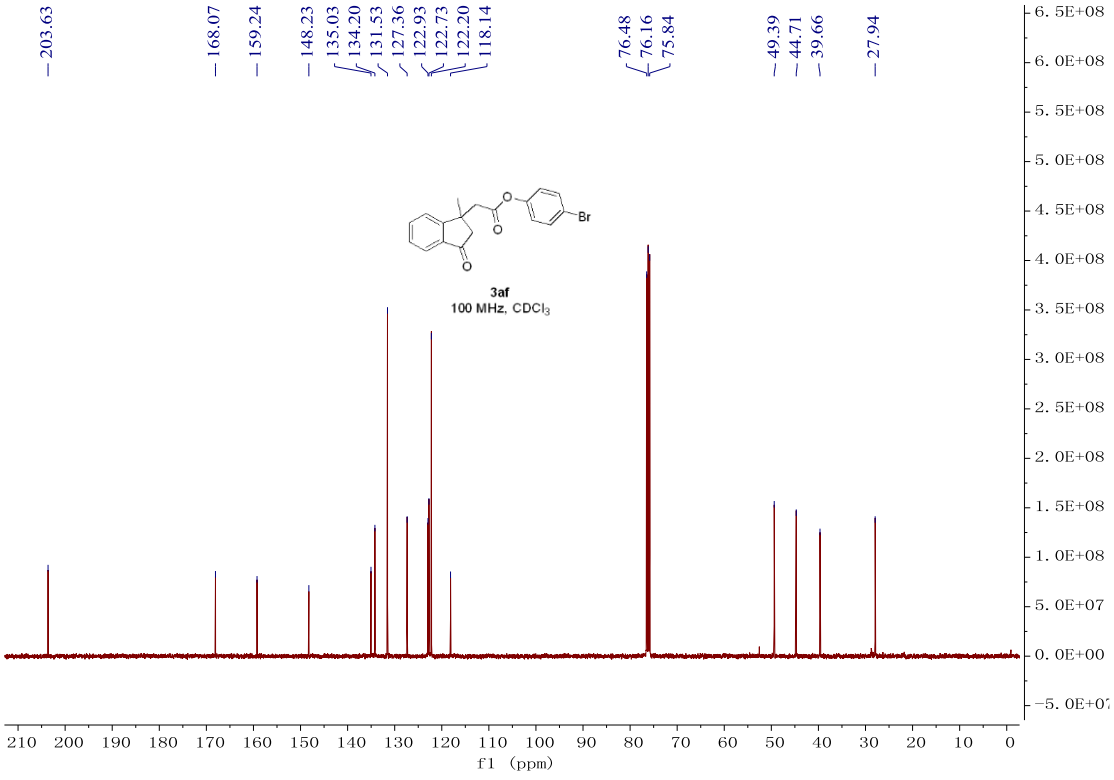
7.73
7.67
7.65
7.63
7.58
7.56
7.44
7.42
7.41
7.40
7.39
6.71
6.69
3.16
3.11
3.04
3.00
2.94
2.90
2.66
2.62
1.57
Br
O
O
O
3af
400 MHz, CDCl3
1.00
1.00
1.00
3.00
2.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)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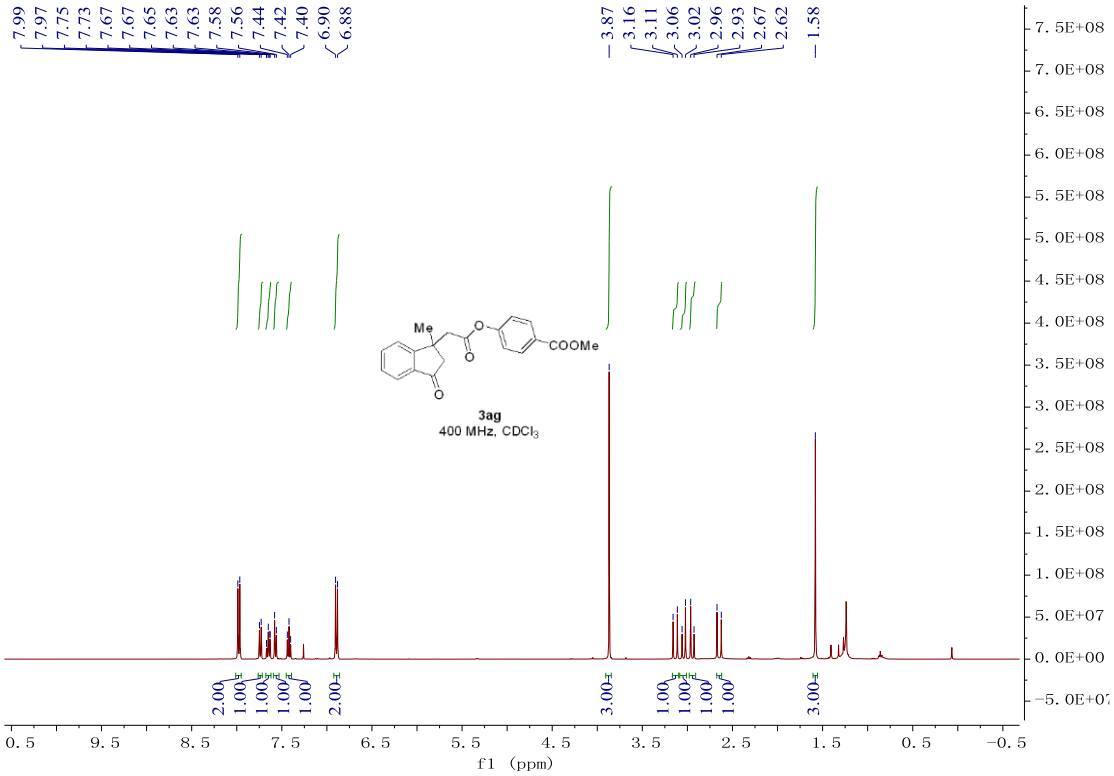
122.73
122.20
118.14
76.48
76.16
75.84
49.39
44.71
39.66
27.94
Br
O
O
O
3af
100 MHz, CDCl3
f1 (ppm)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7.58
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7.42
7.40
6.90
6.88
3.87
3.16
3.11
3.06
3.02
2.96
2.93
2.67
2.62
1.58
Me
O
O
O
COOMe
O
3ag
400 MHz, CDCl3
2.00
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1.00
2.00
3.00
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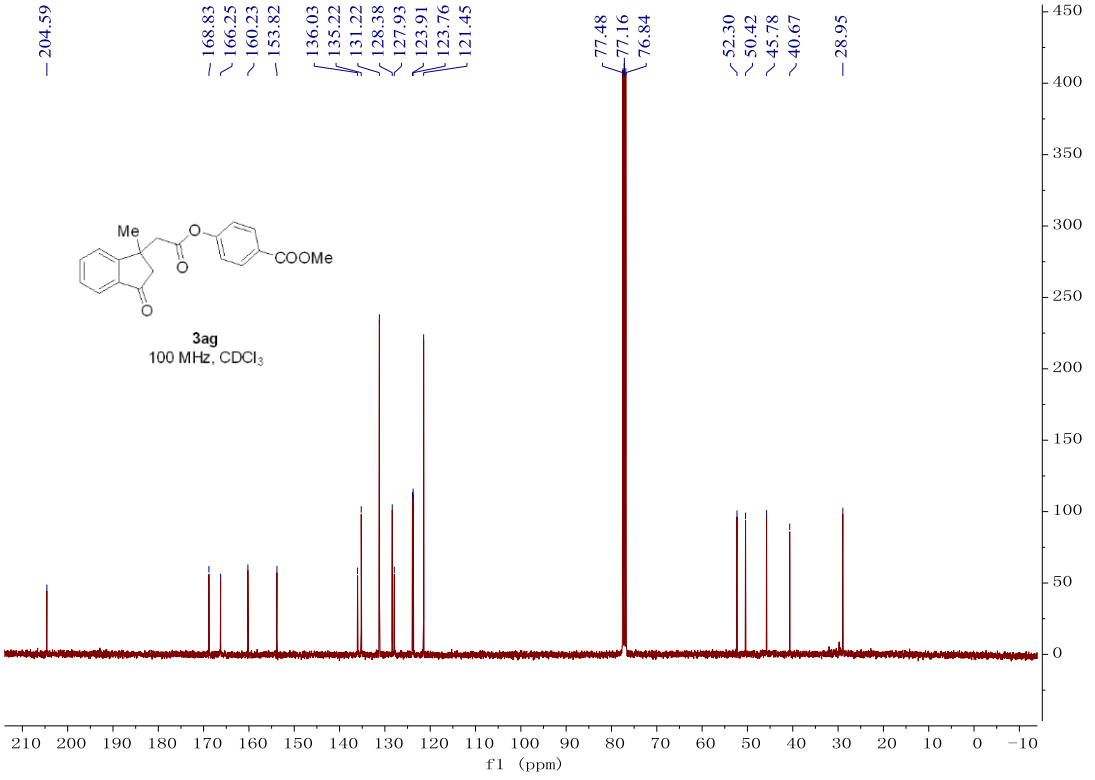
1.00
1.00
1.00
3.00
f1 (ppm)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123.91
123.76
121.45
77.48
77.16
76.84
52.30
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28.95
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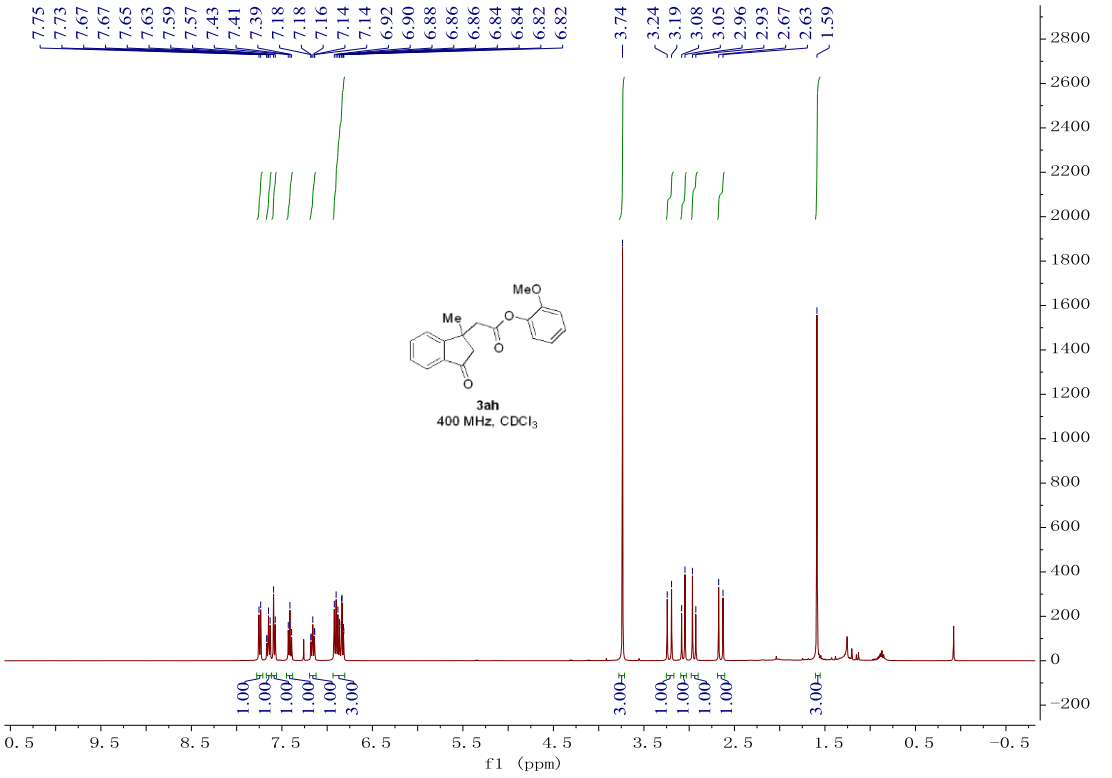
O
O
O
COOMe
O
3ag
100 MHz, CDCl3
f1 (ppm)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7.18
7.16
7.14
7.14
6.92
6.90
6.88
6.86
6.86
6.84
6.84
6.82
6.82
3.74
3.24
3.19
3.08
3.05
2.96
2.93
2.67
2.63
1.59
MeO
Me
O
O
O
3ah
400 MHz, CDCl3
1.00
1.00
1.00
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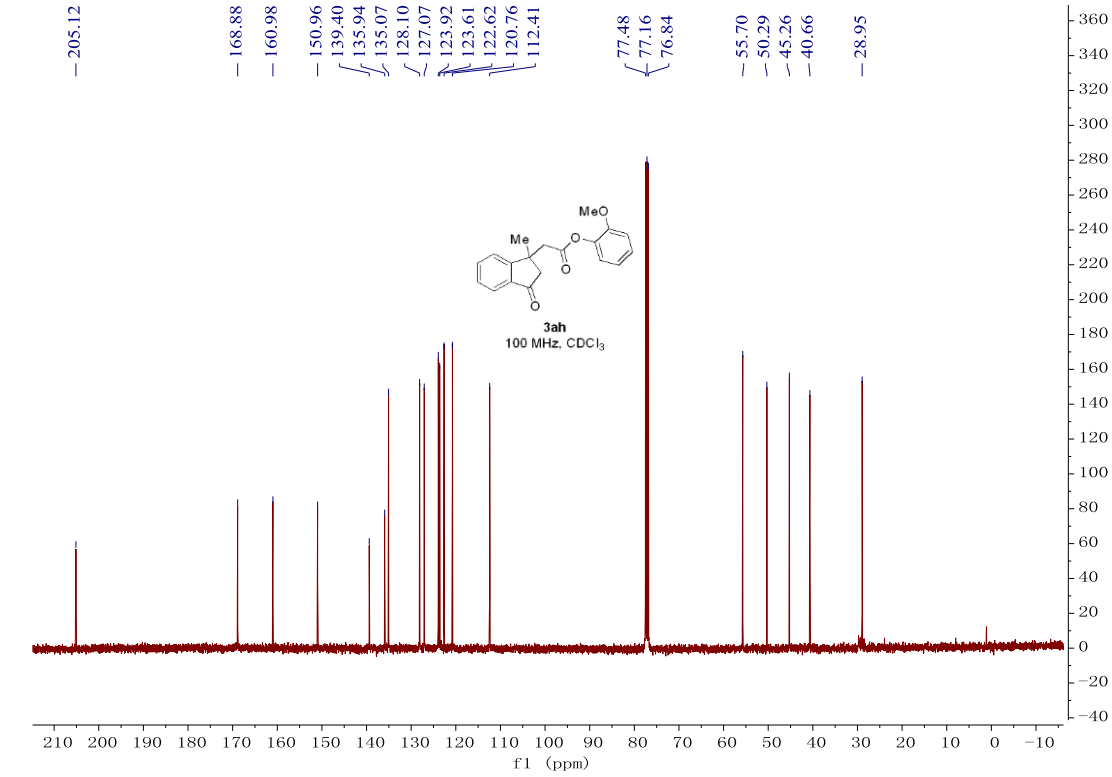
1.00
3.00
3.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)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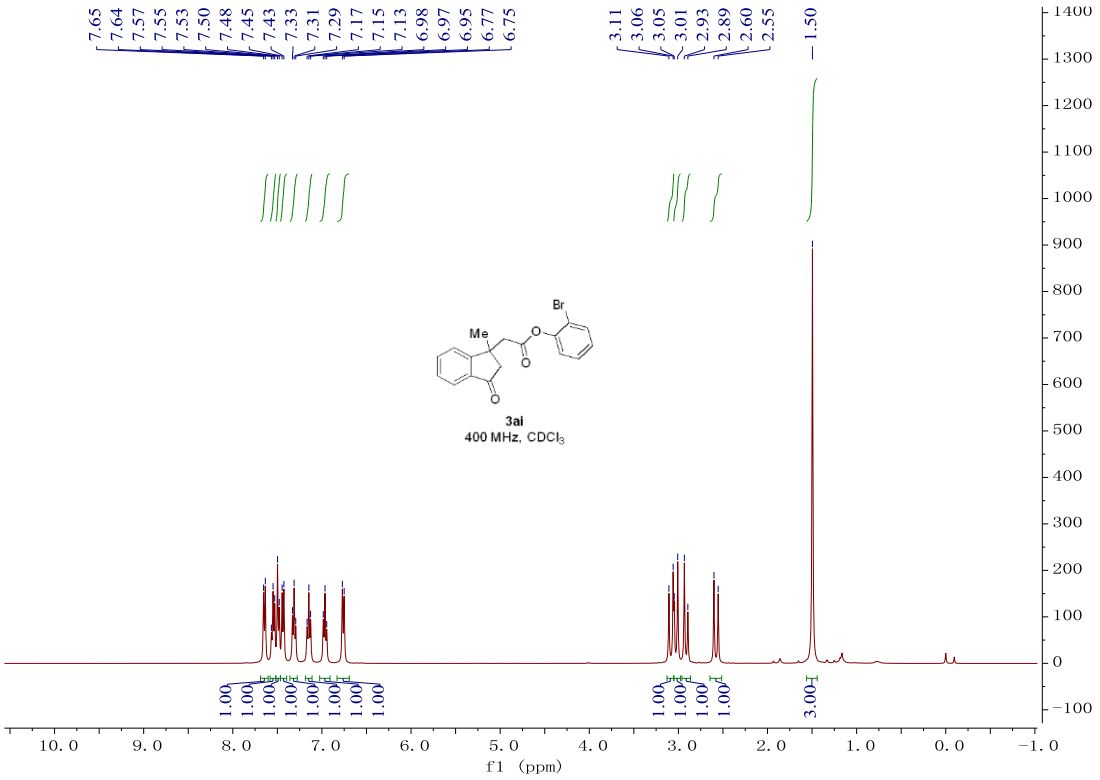
127.07
123.92
123.61
122.62
120.76
112.41
77.48
77.16
76.84
55.70
50.29
45.26
40.66
28.95
MeO
Me
O
O
O
3ah
100 MHz, CDCl3
f1 (ppm)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7.33
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7.17
7.15
7.13
6.98
6.97
6.95
6.77
6.75
3.11
3.06
3.05
3.01
2.93
2.89
2.60
2.55
1.50
Br
Me
O
O
O
3ai
400 MHz, CDCl3
1.00
1.00
1.00
1.00
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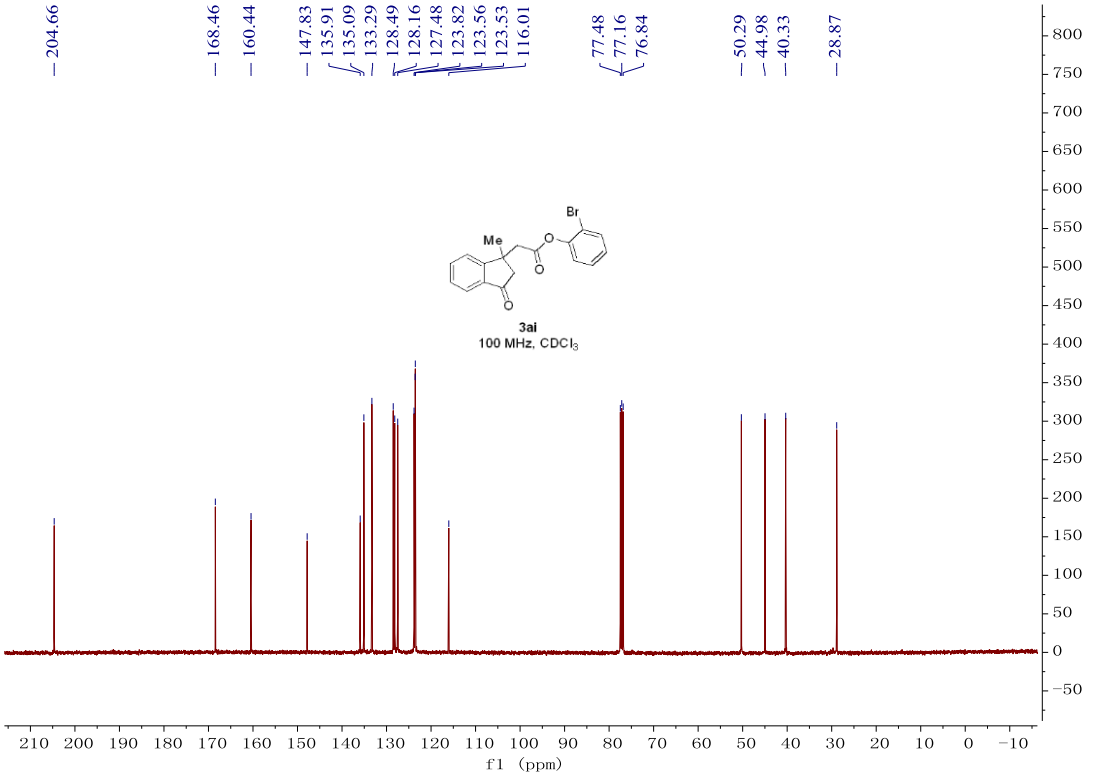
1.00
1.00
1.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)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128.49
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127.48
123.82
123.56
123.53
116.01
77.48
77.16
76.84
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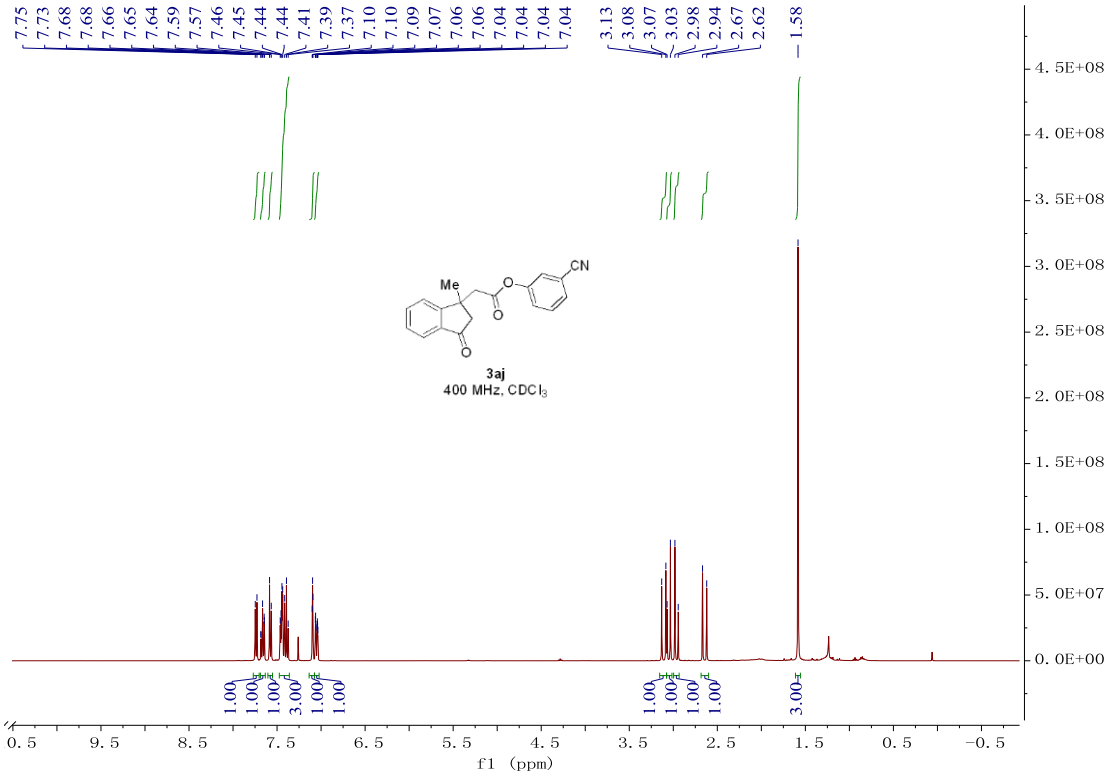
44.98
40.33
28.87
Br
Me
O
O
O
3ai
100 MHz, CDCl3
f1 (ppm)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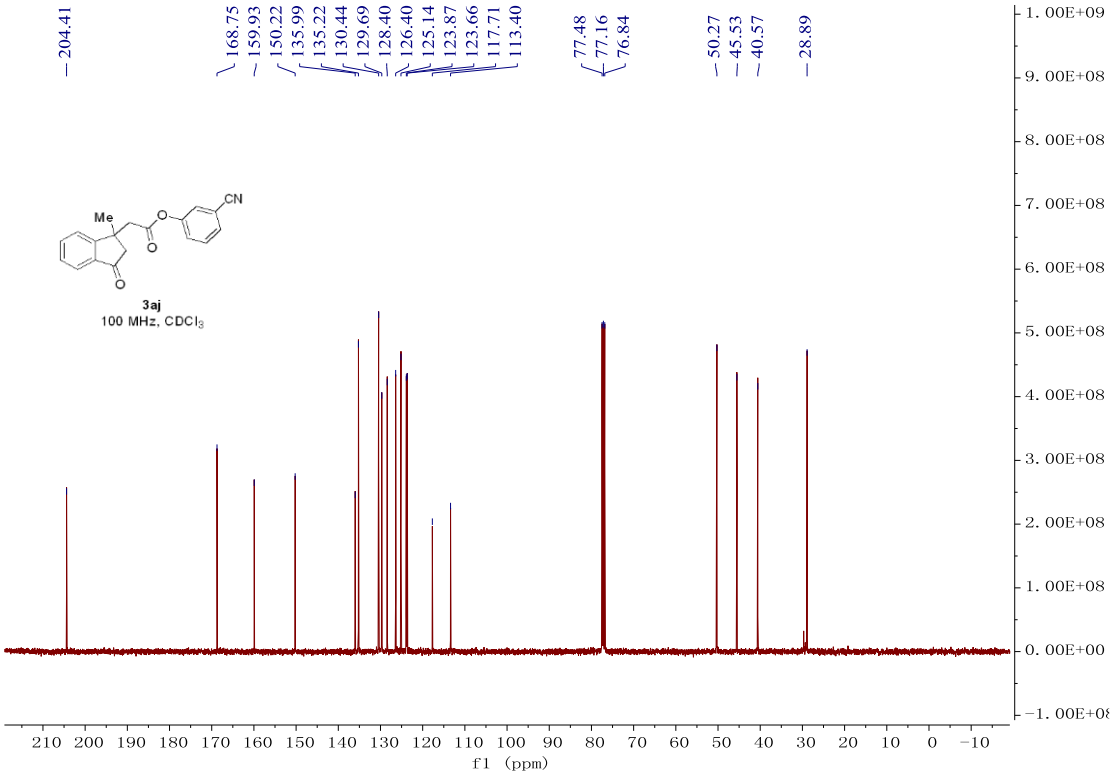
7.45
7.44
7.44
7.41
7.39
7.37
7.10
7.10
7.09
7.07
7.06
7.06
7.04
7.04
7.04
7.04
3.13
3.08
3.07
3.03
2.98
2.94
2.67
2.62
1.58
Me
O
O
O
CN
3aj
400 MHz, CDCl3
1.00
1.00
1.00
3.00
1.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)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126.40
125.14
123.87
123.66
117.71
113.40
77.48
77.16
76.84
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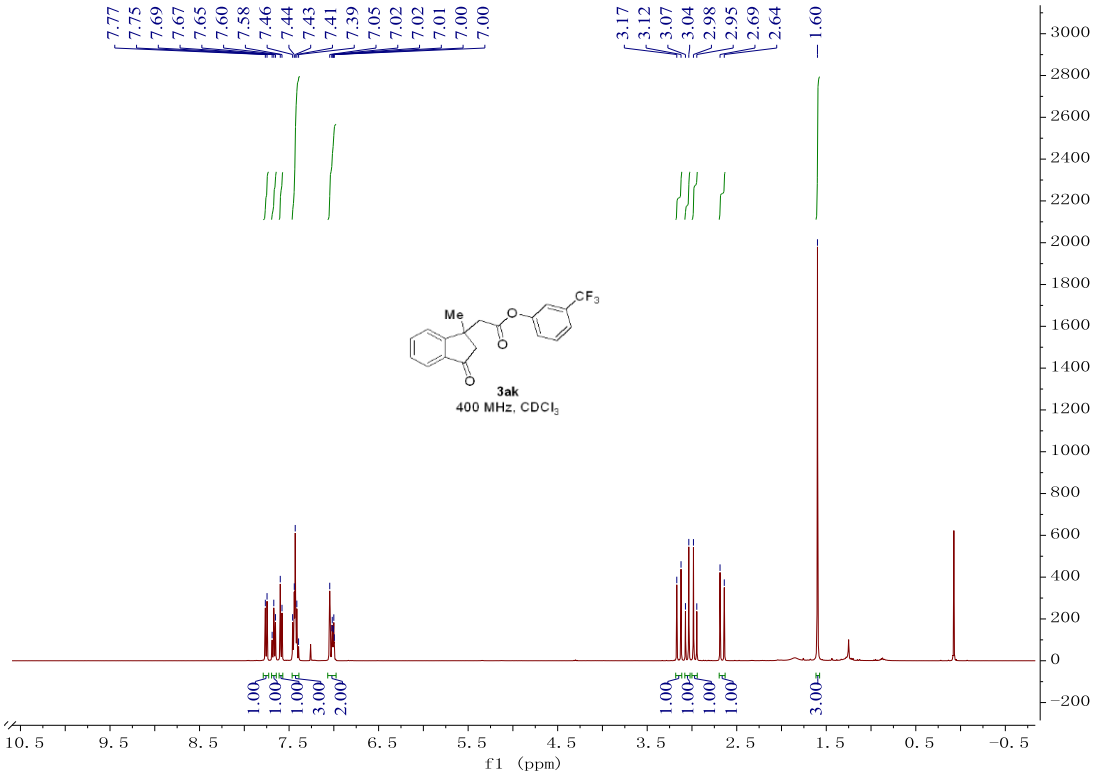
45.53
40.57
28.89
Me
O
O
O
CN
3aj
100 MHz, CDCl3
f1 (ppm)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7.43
7.41
7.39
7.05
7.02
7.02
7.01
7.00
7.00
3.17
3.12
3.07
3.04
2.98
2.95
2.69
2.64
1.60
Me
O
O
O
CF3
3ak
400 MHz, CDCl3
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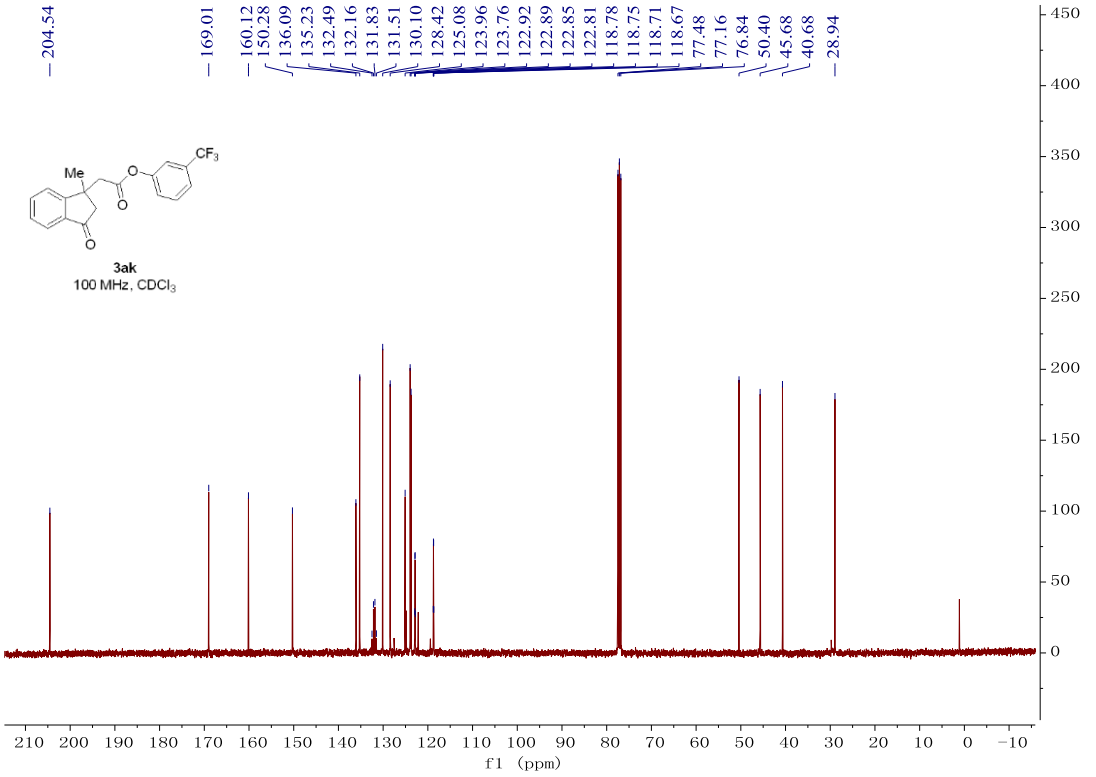
1.00
3.00
2.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)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132.49
132.16
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131.51
130.10
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125.08
123.96
123.76
122.92
122.89
122.85
122.81
118.78
118.75
118.71
118.67
77.48
77.16
76.84
50.40
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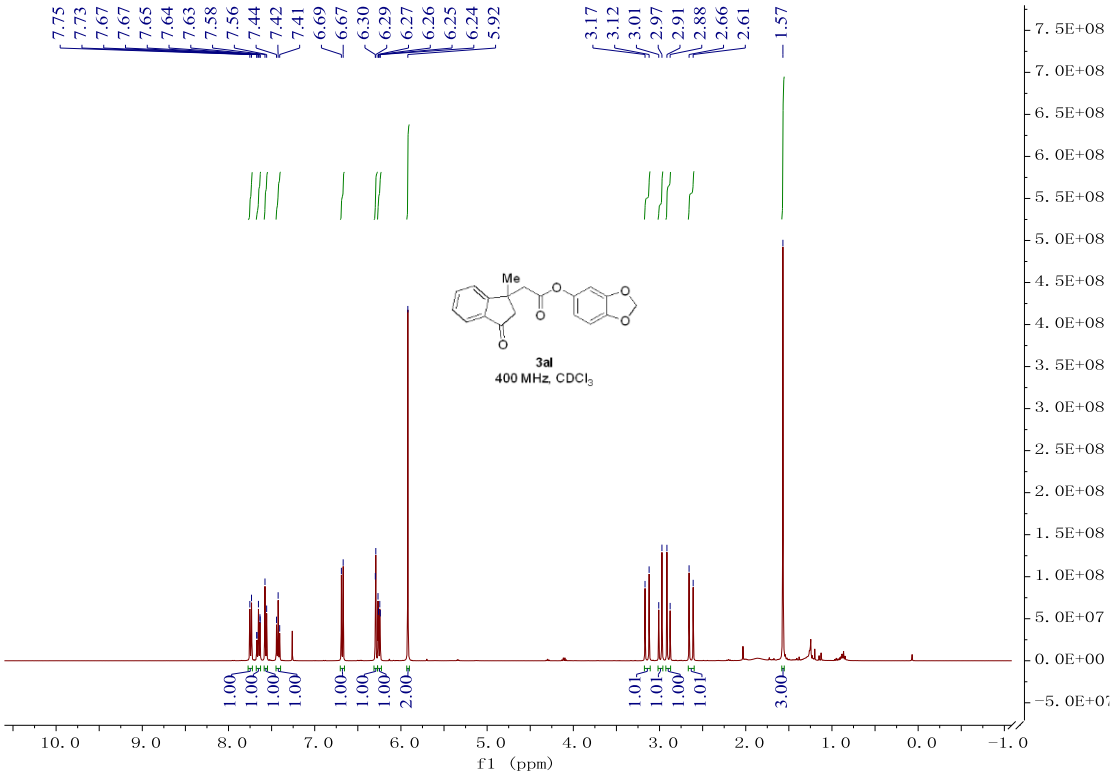
40.68
28.94
Me
O
O
O
CF3
3ak
100 MHz, CDCl3
f1 (ppm)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7.67
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7.63
7.58
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7.44
7.42
7.41
6.69
6.67
6.30
6.29
6.27
6.26
6.25
6.24
5.92
3.17
3.12
3.01
2.97
2.91
2.88
2.66
2.61
1.57
Me
3al
400 MHz, CDCl3
1.00
1.00
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1.00
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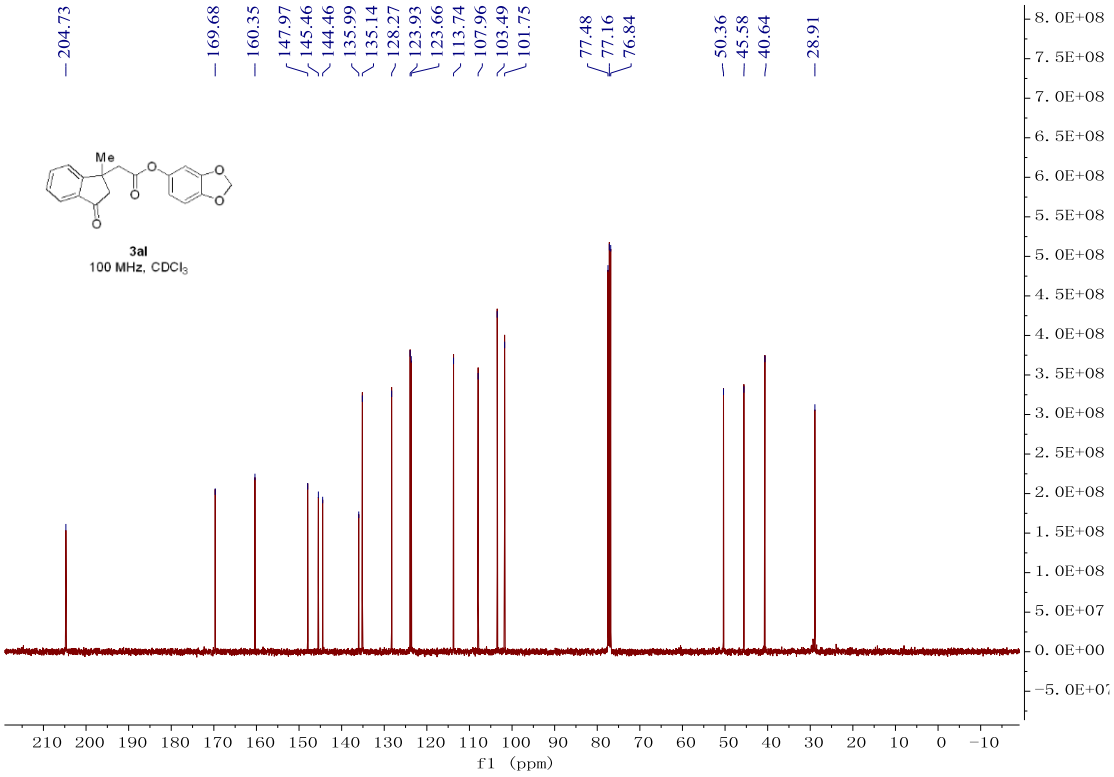
1.00
1.00
2.00
1.01
1.01
1.00
1.01
3.00
f1 (ppm)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144.46
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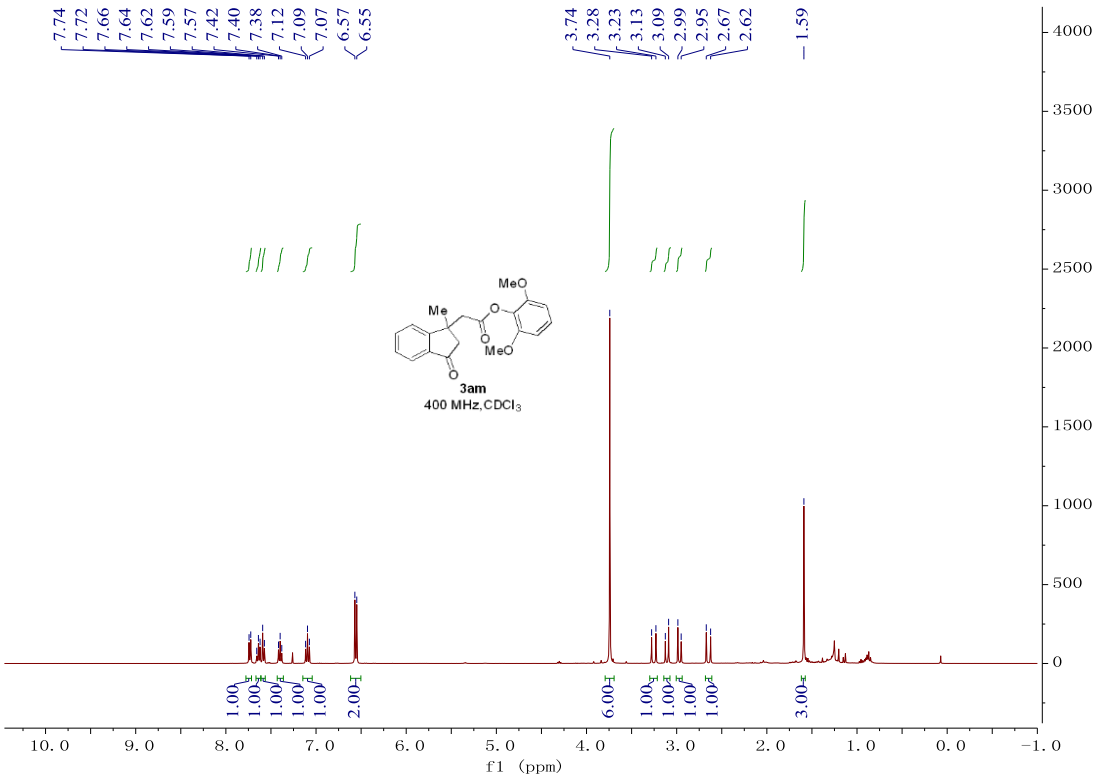
135.14
128.27
123.93
123.66
113.74
107.96
103.49
101.75
77.48
77.16
76.84
50.36
45.58
40.64
28.91
Me
3al
100 MHz, CDCl3
f1 (ppm)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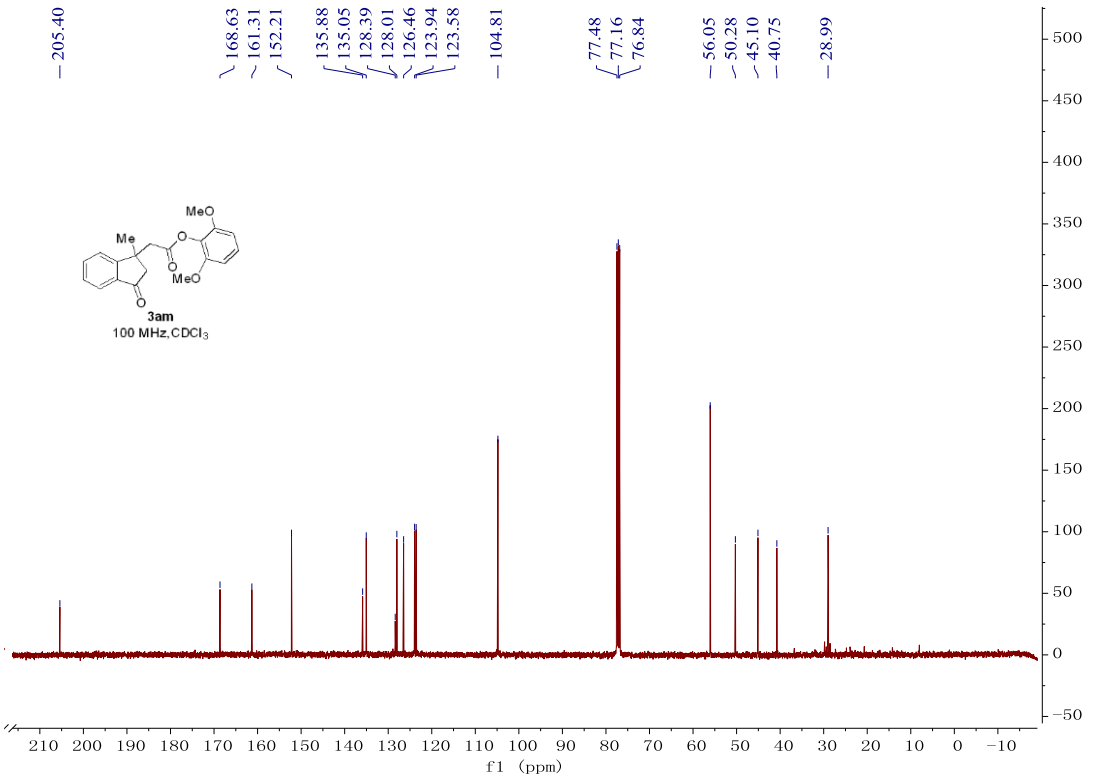
7.38
7.12
7.09
7.07
6.57
6.55
3.74
3.28
3.23
3.13
3.09
2.99
2.95
2.67
2.62
1.59
MeO
Me
O
MeO
O
3am
400 MHz,CDCl3
1.00
1.00
1.00
1.00
1.00
2.00
6.00
1.00
1.00
1.00
3.00
f1 (ppm)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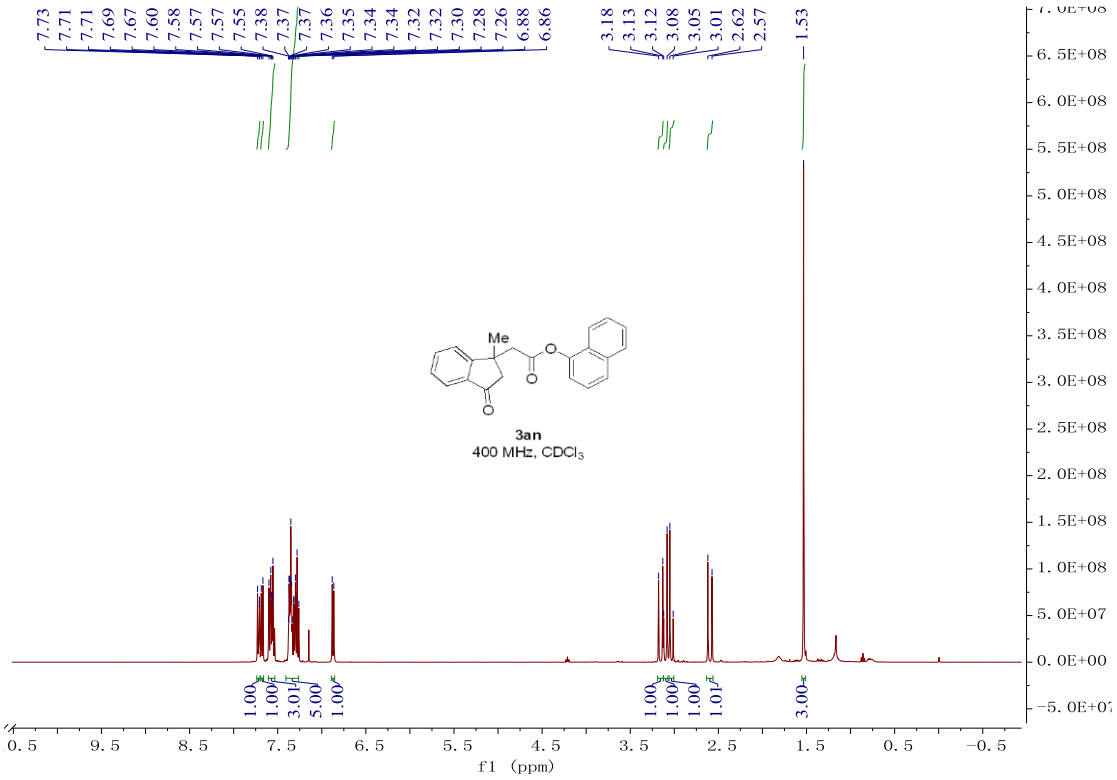
161.31
152.21
135.88
135.05
128.39
128.01
126.46
123.94
123.58
104.81
77.48
77.16
76.84
56.05
50.28
45.10
40.75
28.99
MeO
Me
O
MeO
O
3am
100 MHz,CDCl3
f1 (ppm)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7.57
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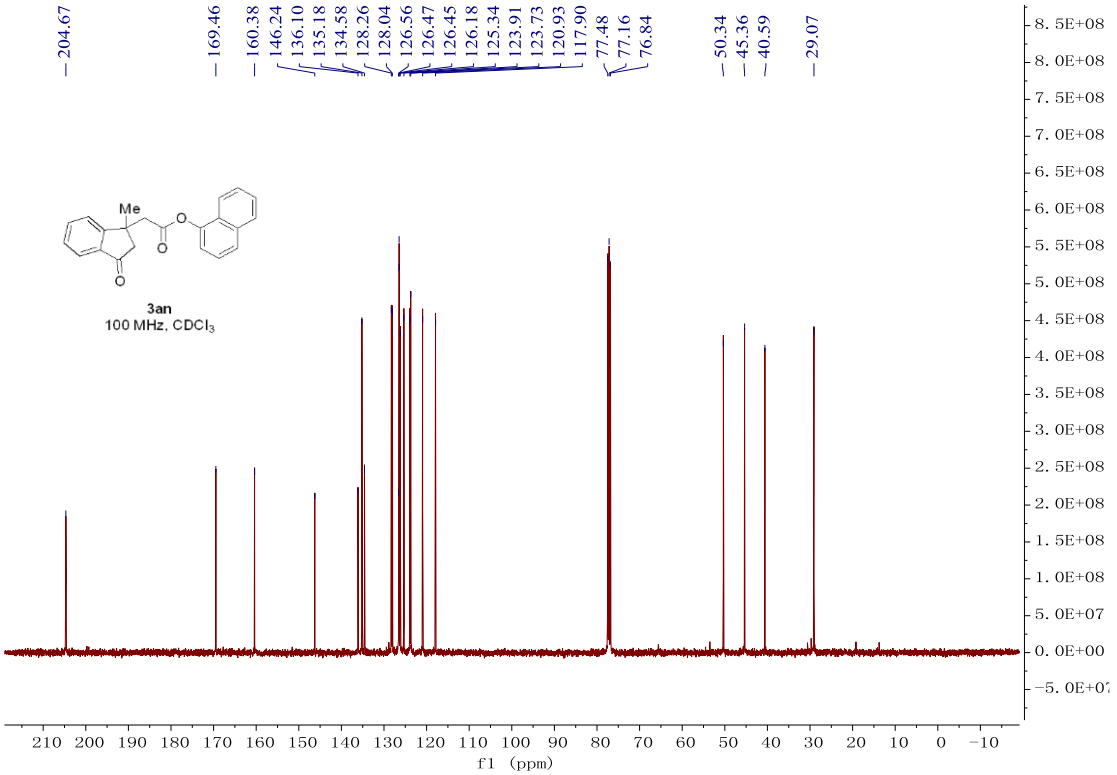
7.37
7.36
7.35
7.34
7.34
7.32
7.32
7.30
7.28
7.26
6.88
6.86
3.18
3.13
3.12
3.08
3.05
3.01
2.62
2.57
1.53
Me
O
O
O
3an
400 MHz, CDCl3
1.00
1.00
3.01
5.00
1.00
1.00
1.00
1.00
1.01
3.00
f1 (ppm)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126.56
126.47
126.45
126.18
125.34
123.91
123.73
120.93
117.90
77.48
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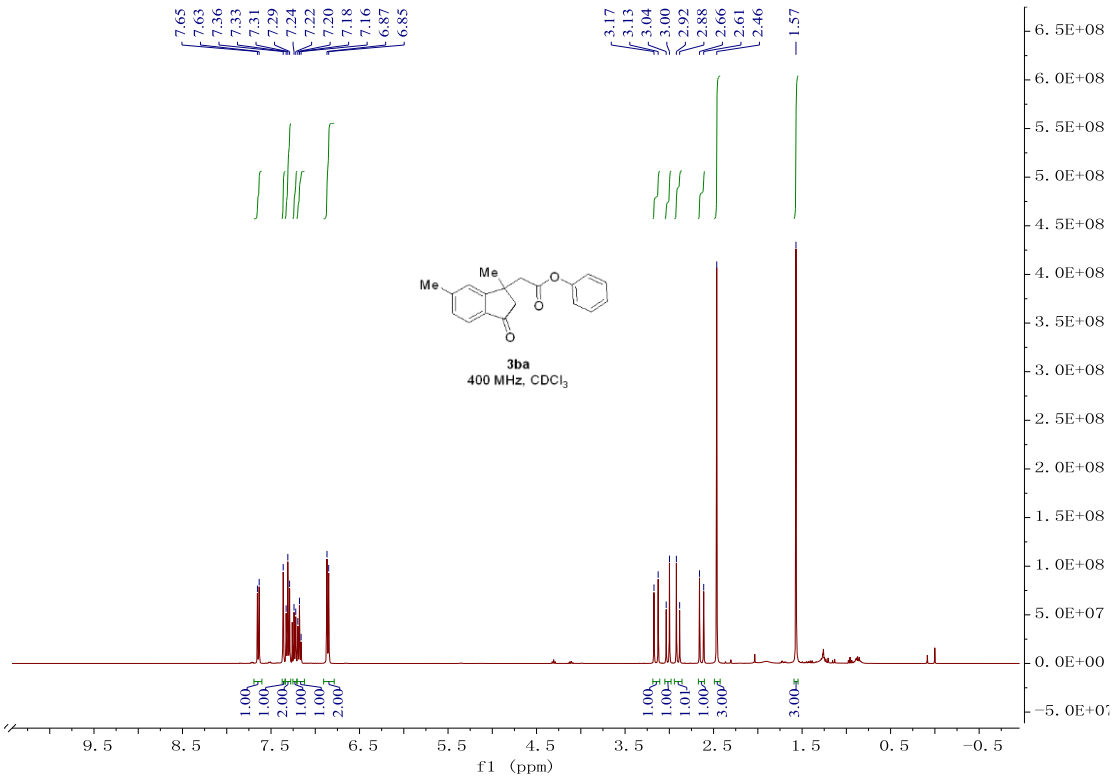
29.07
Me
O
O
O
3an
100 MHz, CDCl3
f1 (ppm)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7.63
7.36
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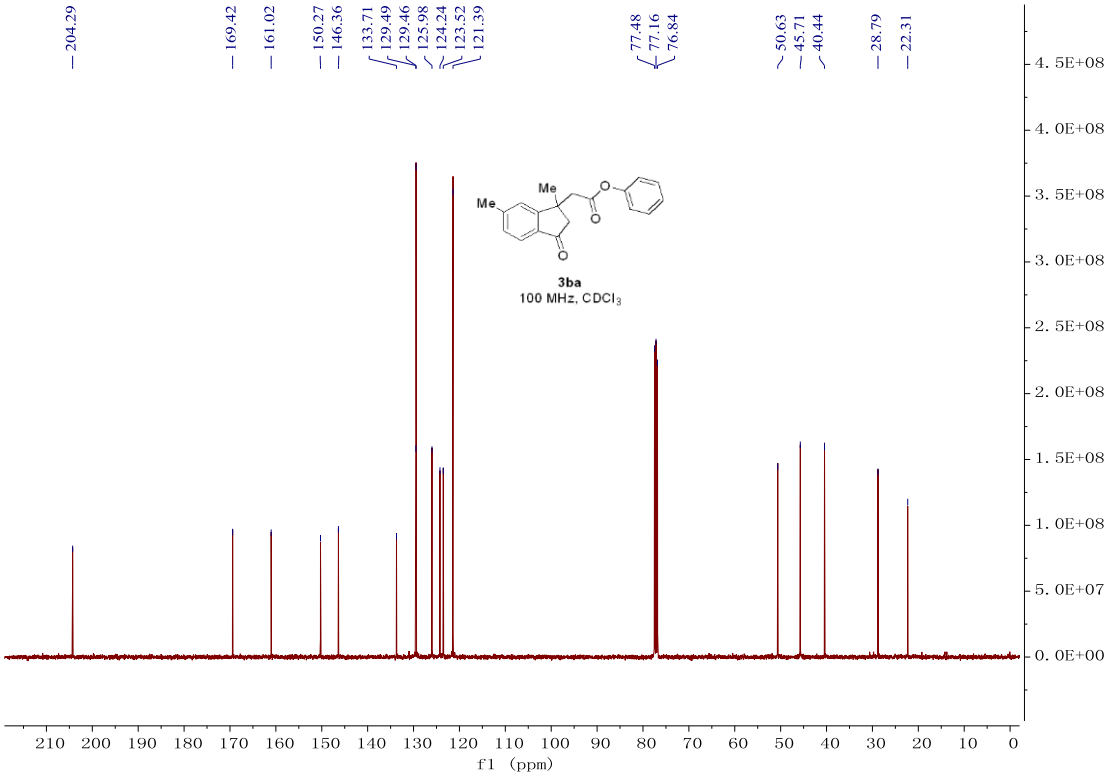
7.29
7.24
7.22
7.20
7.18
7.16
6.87
6.85
3.17
3.13
3.04
3.00
2.92
2.88
2.66
2.61
2.46
1.57
Me
Me
O
O
O
3ba
400 MHz, CDCl3
1.00
1.00
2.00
1.00
1.00
2.00
1.00
1.00
1.01
1.00
3.00
3.00
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5
f1 (ppm)
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
−5.0E+07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133.71
129.49
129.46
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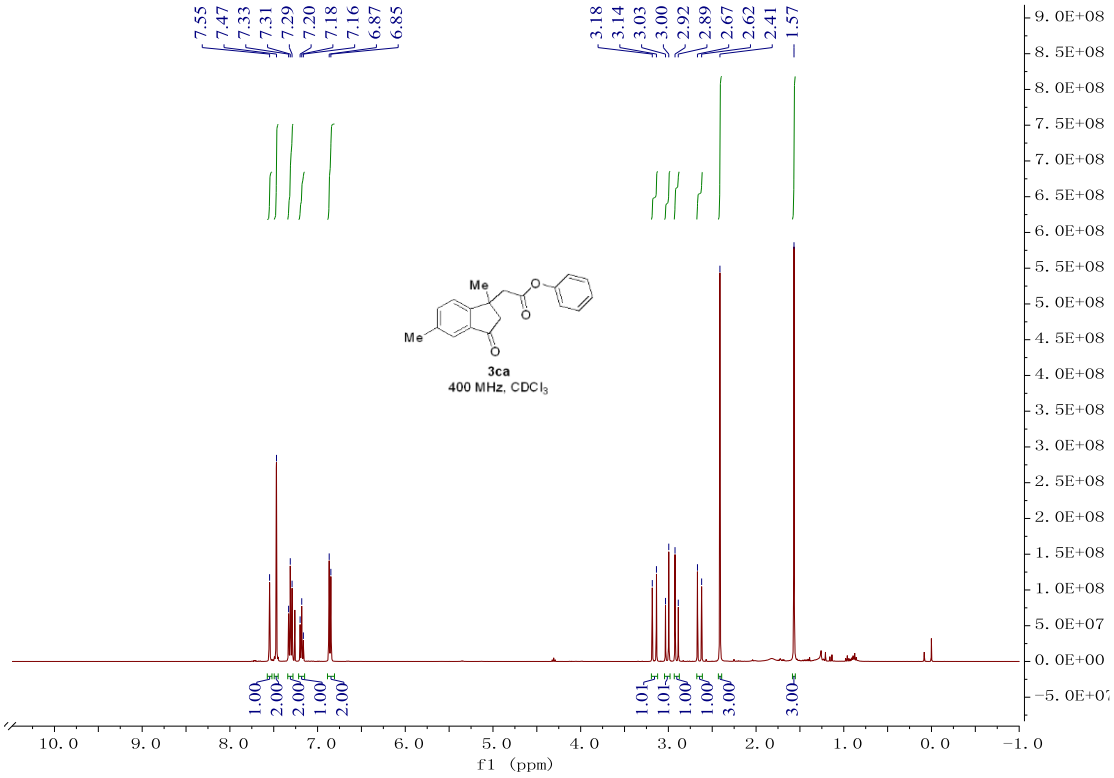
124.24
123.52
121.39
77.48
77.16
76.84
50.63
45.71
40.44
28.79
22.31
Me
Me
O
O
O
3ba
100 MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00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7.18
7.16
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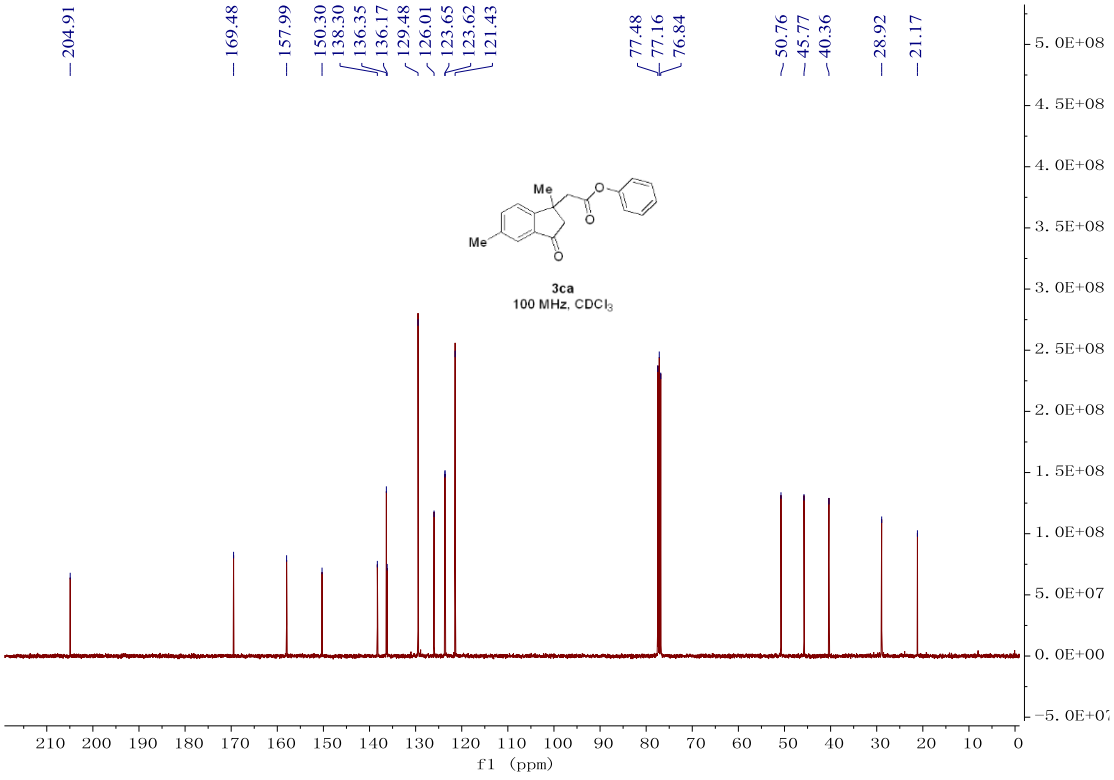
6.85
3.18
3.14
3.03
3.00
2.92
2.89
2.67
2.62
2.41
1.57
Me
Me
O
O
3ca
400 MHz, CDCl3
1.00
2.00
2.00
1.00
2.00
1.01
1.01
1.00
1.00
3.00
3.00
f1 (ppm)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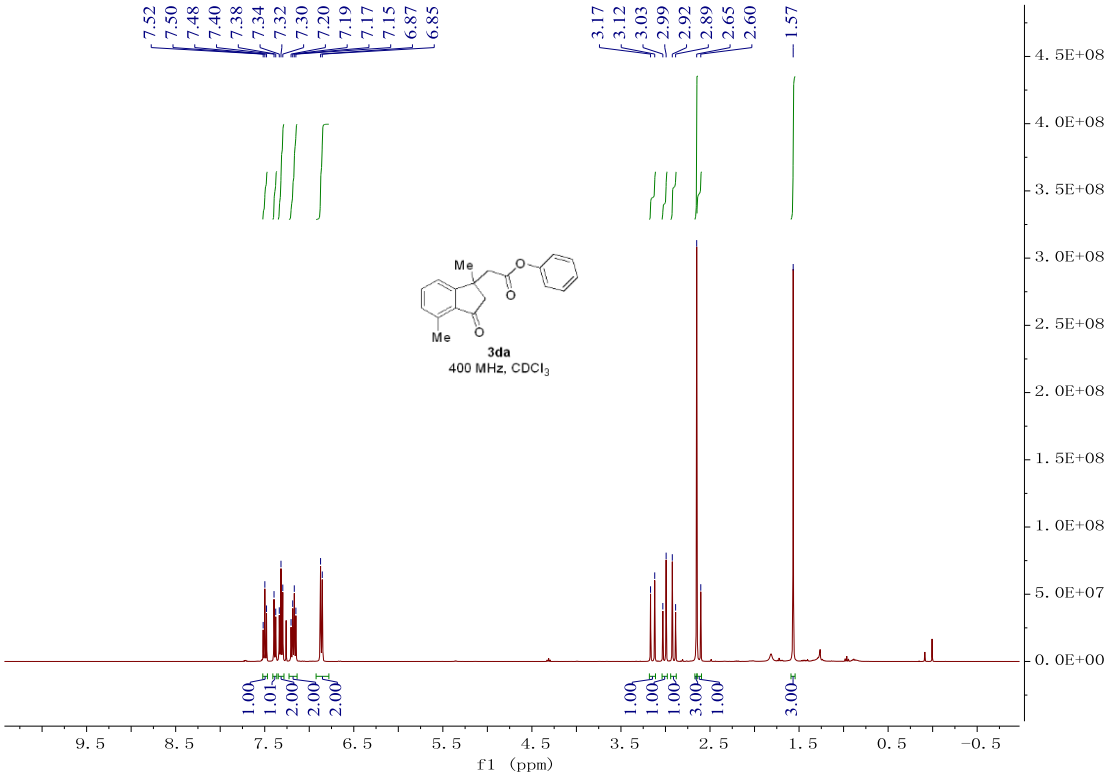
136.35
136.17
129.48
126.01
123.65
123.62
121.43
77.48
77.16
76.84
50.76
45.77
40.36
28.92
21.17
Me
Me
O
O
3ca
100 MHz, CDCl3
f1 (ppm)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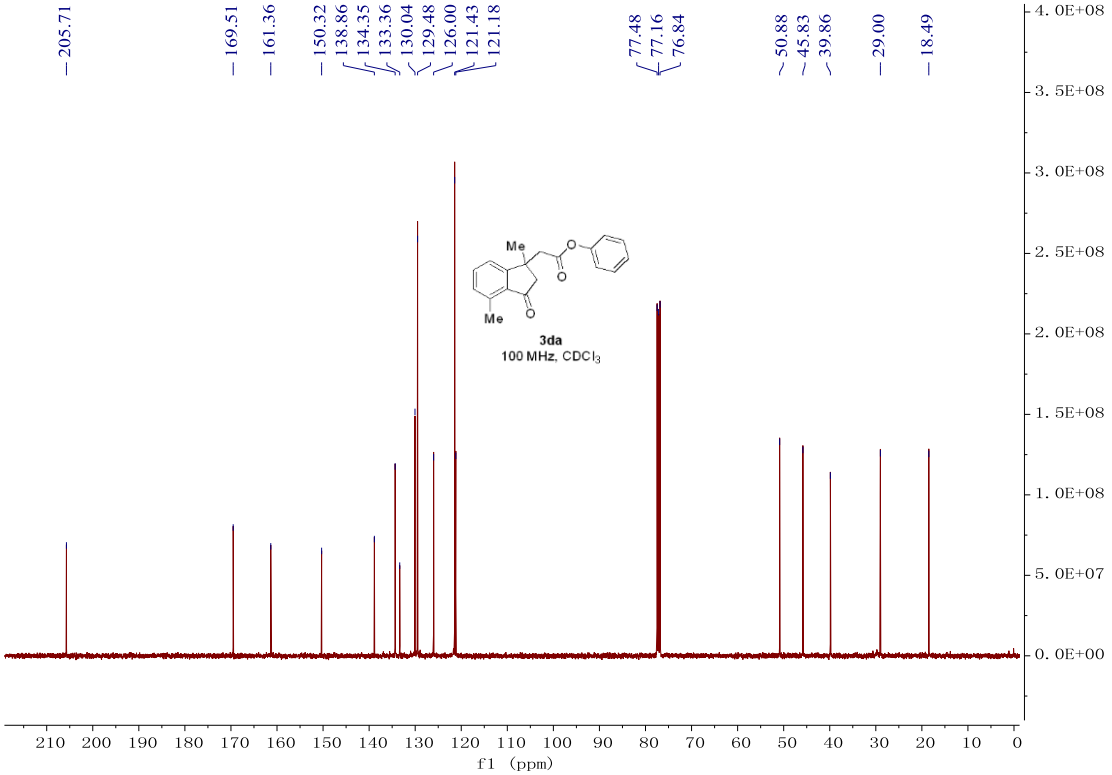
7.50
7.48
7.40
7.38
7.34
7.32
7.30
7.20
7.19
7.17
7.15
6.87
6.85
3.17
3.12
3.03
2.99
2.92
2.89
2.65
2.60
1.57
Me
O
O
Me
O
3da
400 MHz, CDCl3
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
1.00
1.01
2.00
2.00
2.00
1.00
1.00
1.00
3.00
1.00
3.00
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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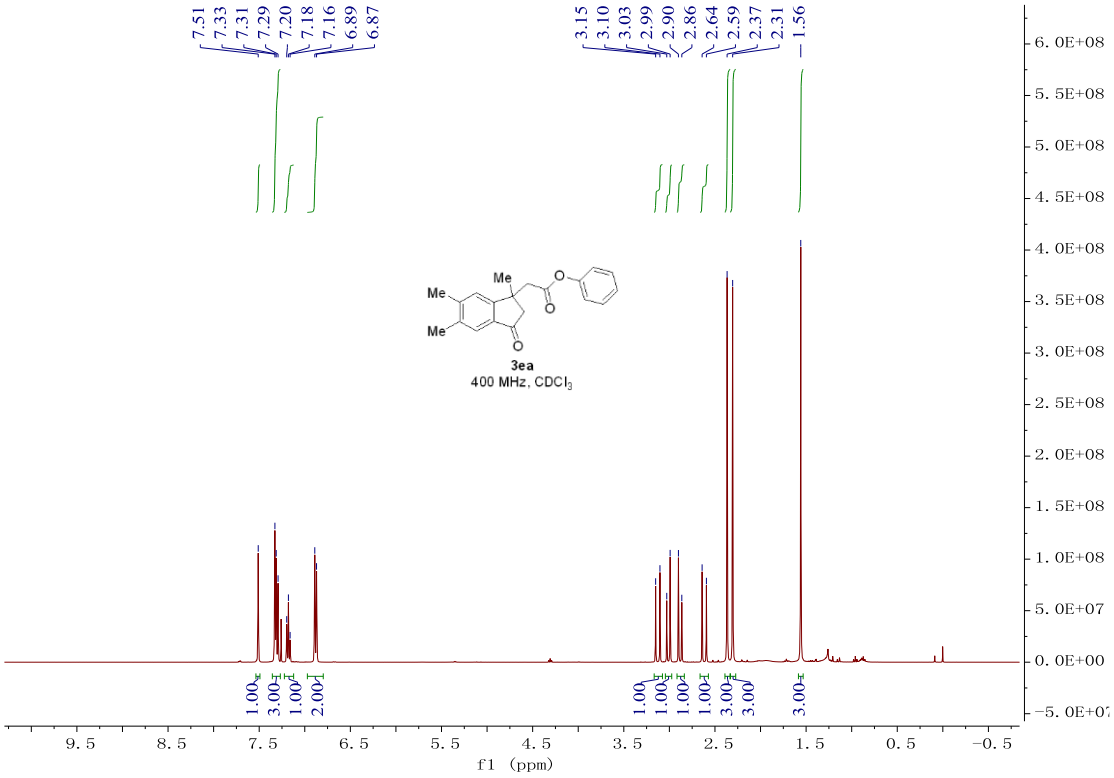
150.32
138.86
134.35
133.36
130.04
129.48
126.00
121.43
121.18
77.48
77.16
76.84
50.88
45.83
39.86
29.00
18.49
Me
O
O
Me
O
3da
100 MHz, CDCl3
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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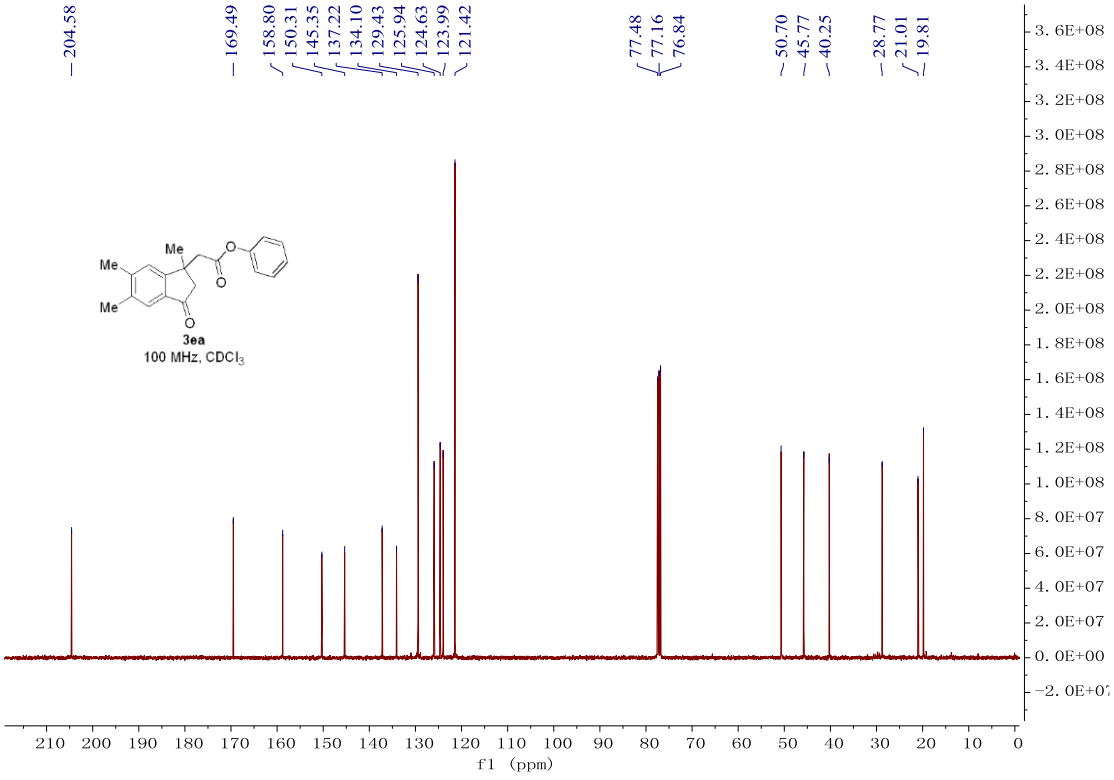
7.33
7.31
7.29
7.20
7.18
7.16
6.89
6.87
3.15
3.10
3.03
2.99
2.90
2.86
2.64
2.59
2.37
2.31
1.56
Me
Me
Me
O
O
O
3ea
400 MHz, CDCl3
1.00
3.00
1.00
2.00
1.00
1.00
1.00
1.00
3.00
3.00
3.00
f1 (ppm)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145.35
137.22
134.10
129.43
125.94
124.63
123.99
121.42
77.48
77.16
76.84
50.70
45.77
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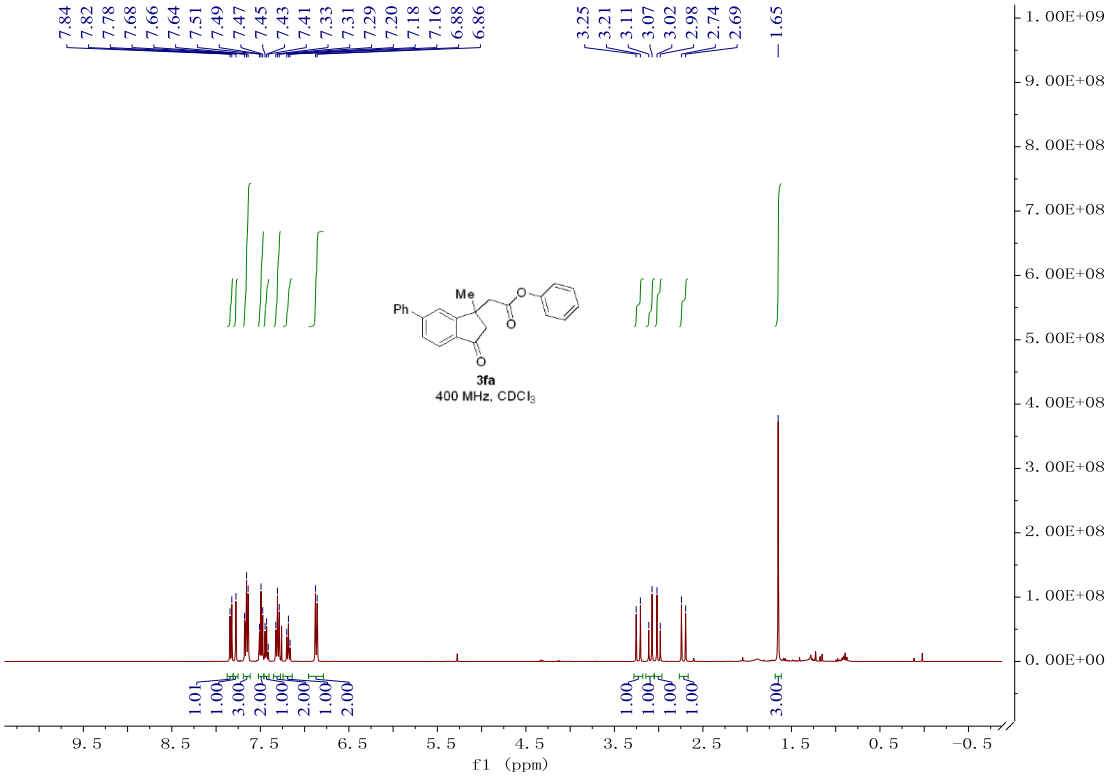
21.01
19.81
Me
Me
Me
O
O
O
3ea
100 MHz, CDCl3
f1 (ppm)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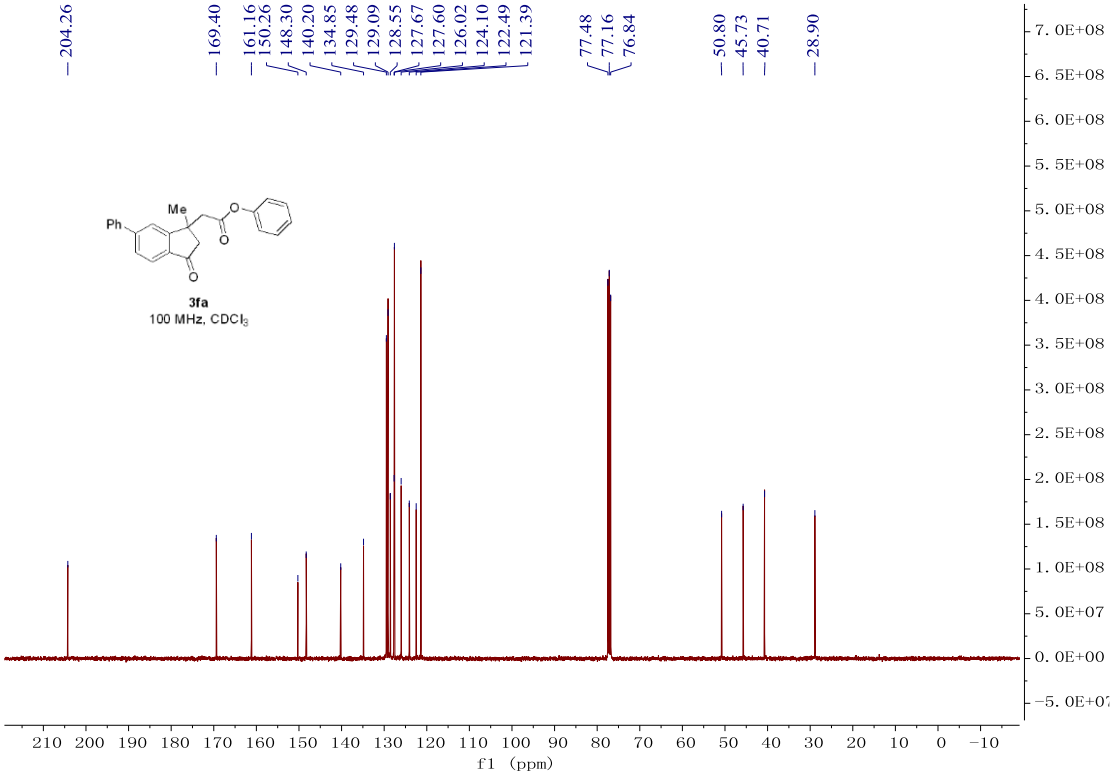
7.66
7.64
7.51
7.49
7.47
7.45
7.43
7.41
7.33
7.31
7.29
7.20
7.18
7.16
6.88
6.86
3.25
3.21
3.11
3.07
3.02
2.98
2.74
2.69
1.65
Me
Ph
O
O
O
3fa
400 MHz, CDCl3
1.01
1.00
3.00
2.00
1.00
2.00
1.00
2.00
1.00
1.00
1.00
1.00
3.00
1. 00E+09
9. 00E+08
8. 00E+08
7. 00E+08
6. 00E+08
5. 00E+08
4. 00E+08
3. 00E+08
2. 00E+08
1. 00E+08
0. 00E+00
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5
f1 (ppm)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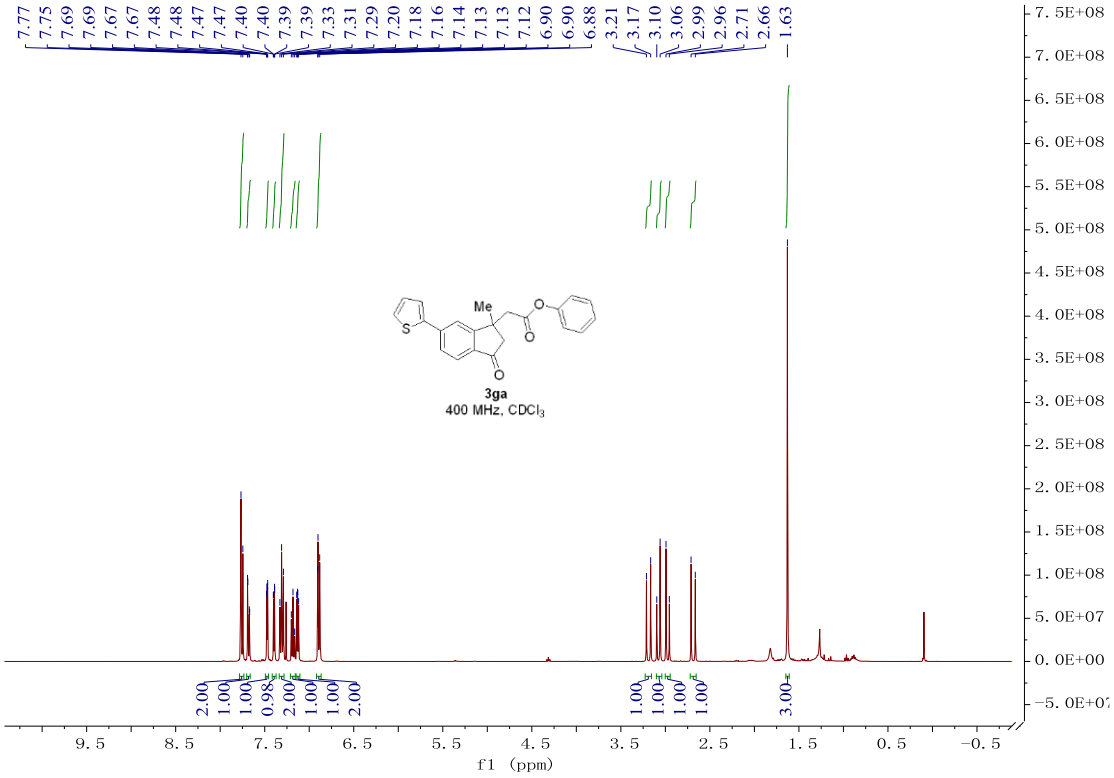
161.16
150.26
148.30
140.20
134.85
129.48
129.09
128.55
127.67
127.60
126.02
124.10
122.49
121.39
77.48
77.16
76.84
50.80
45.73
40.71
28.90
Me
Ph
O
O
O
3fa
100 MHz, CDCl3
7. 0E+08
6. 5E+08
6. 0E+08
5. 5E+08
5. 0E+08
4. 5E+08
4. 0E+08
3. 5E+08
3. 0E+08
2. 5E+08
2. 0E+08
1. 5E+08
1. 0E+08
5. 0E+07
0. 0E+00
−5. 0E+07
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)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7.69
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7.67
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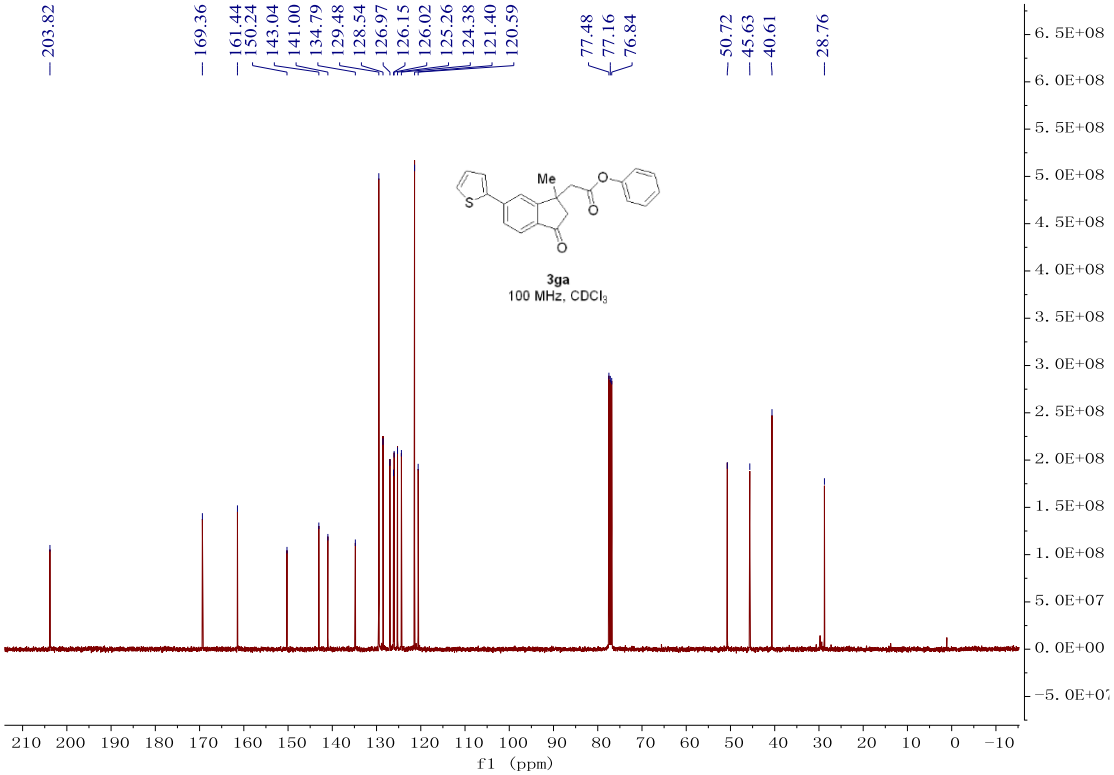
7.48
7.47
7.47
7.40
7.40
7.39
7.39
7.33
7.31
7.29
7.20
7.18
7.16
7.14
7.13
7.13
7.12
6.90
6.90
6.88
3.21
3.17
3.10
3.06
2.99
2.96
2.71
2.66
1.63
Me
S
O
O
O
3ga
400 MHz, CDCl3
2.00
1.00
1.00
0.98
2.00
1.00
1.00
2.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)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143.04
141.00
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129.48
128.54
126.97
126.15
126.02
125.26
124.38
121.40
120.59
77.48
77.16
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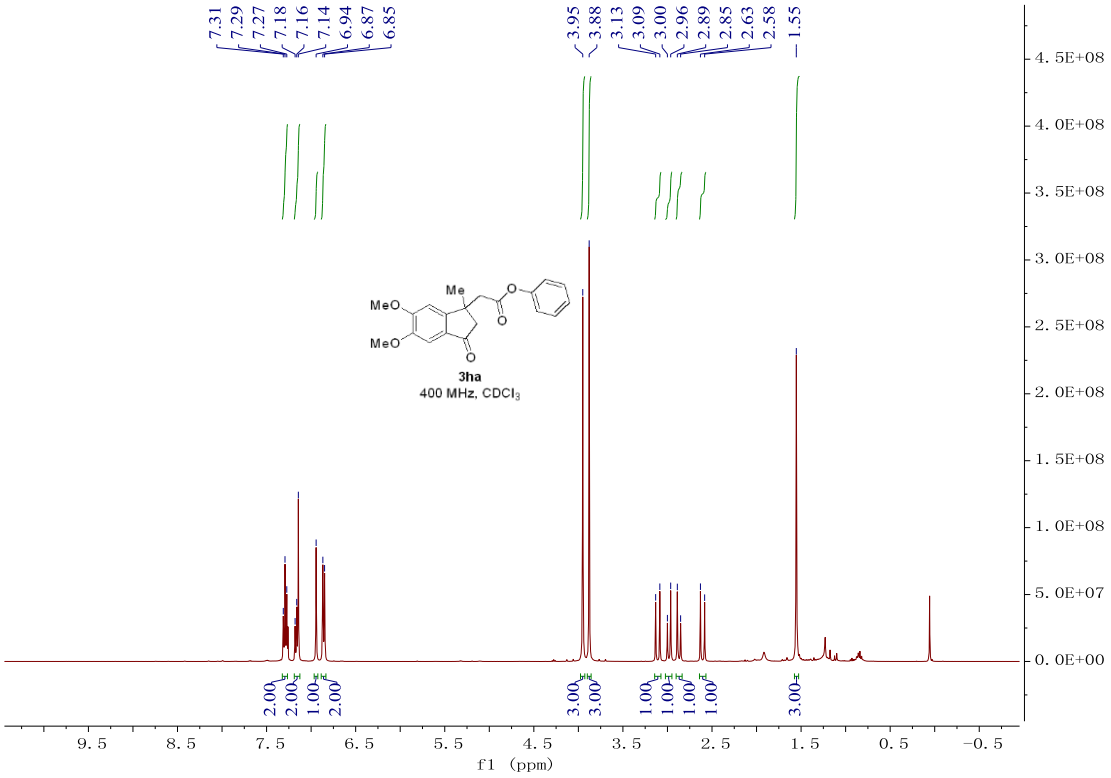
50.72
45.63
40.61
28.76
Me
S
O
O
O
3ga
100 MHz, CDCl3
f1 (ppm)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7.29
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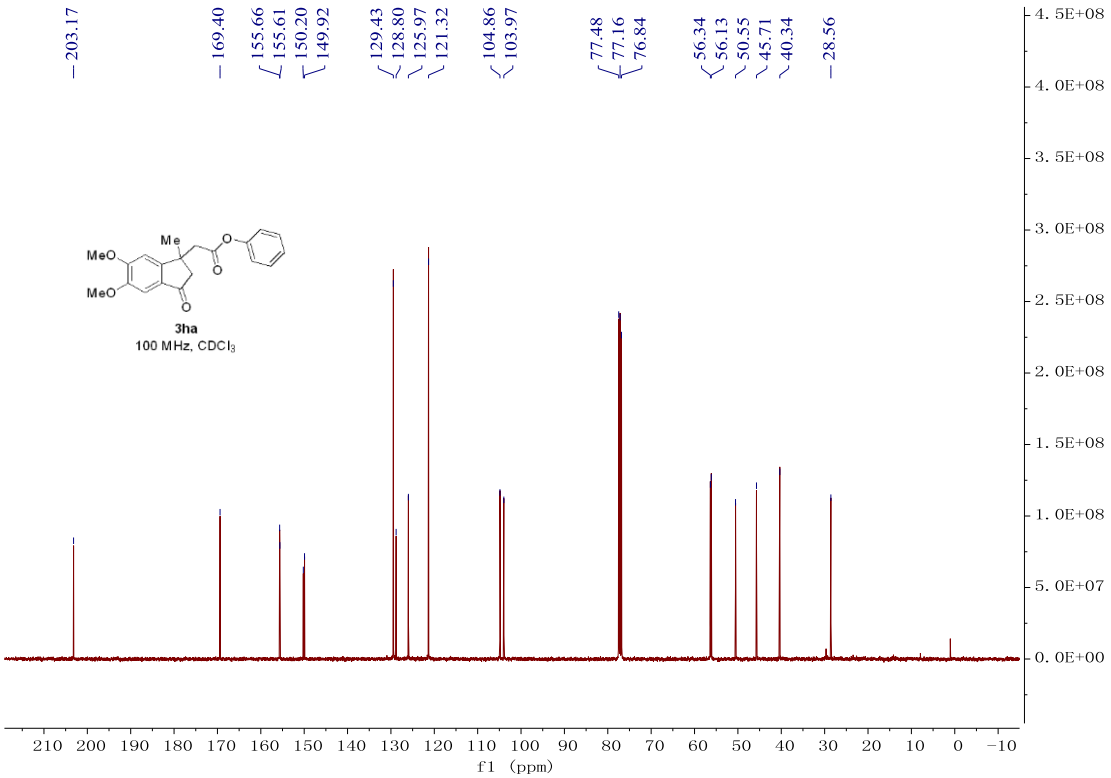
7.18
7.16
7.14
6.94
6.87
6.85
3.95
3.88
3.13
3.09
3.00
2.96
2.89
2.85
2.63
2.58
1.55
MeO
MeO
Me
O
O
O
3ha
400 MHz, CDCl3
2.00
2.00
1.00
2.00
3.00
3.00
1.00
1.00
1.00
3.00
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
−0.5
f1 (ppm)
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00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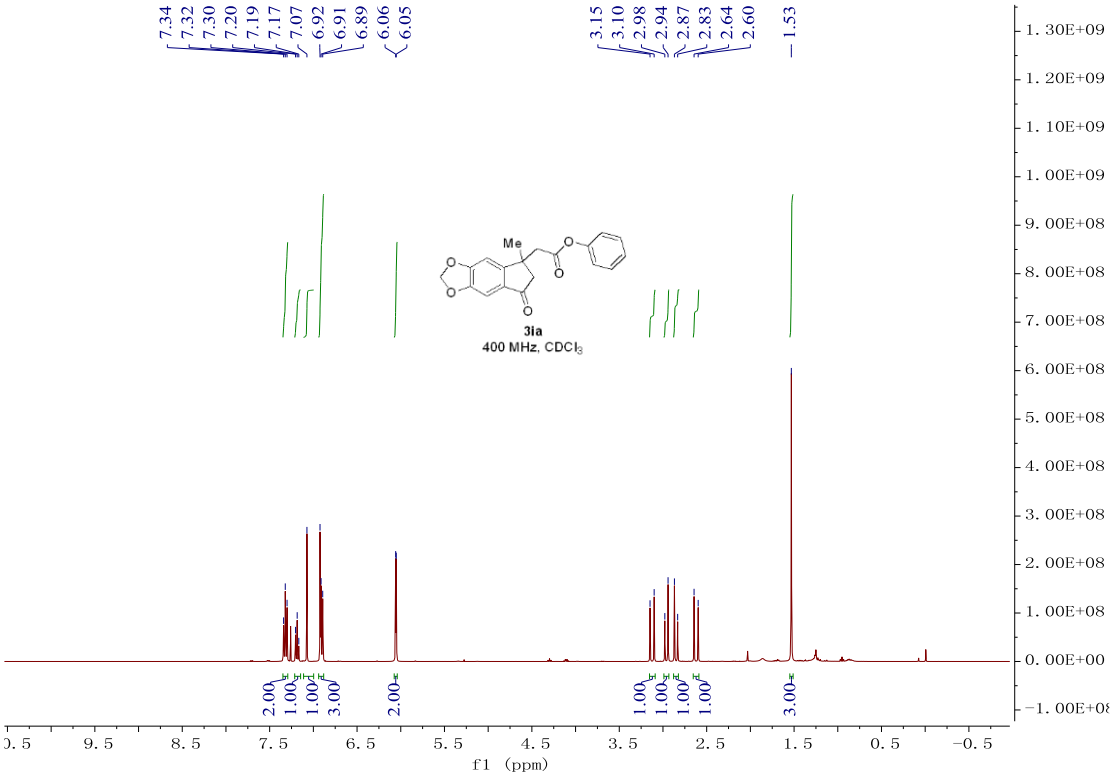
155.66
155.61
150.20
149.92
129.43
128.80
125.97
121.32
104.86
103.97
77.48
77.16
76.84
56.34
56.13
50.55
45.71
40.34
28.56
MeO
MeO
Me
O
O
O
3ha
100 MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00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7.32
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7.20
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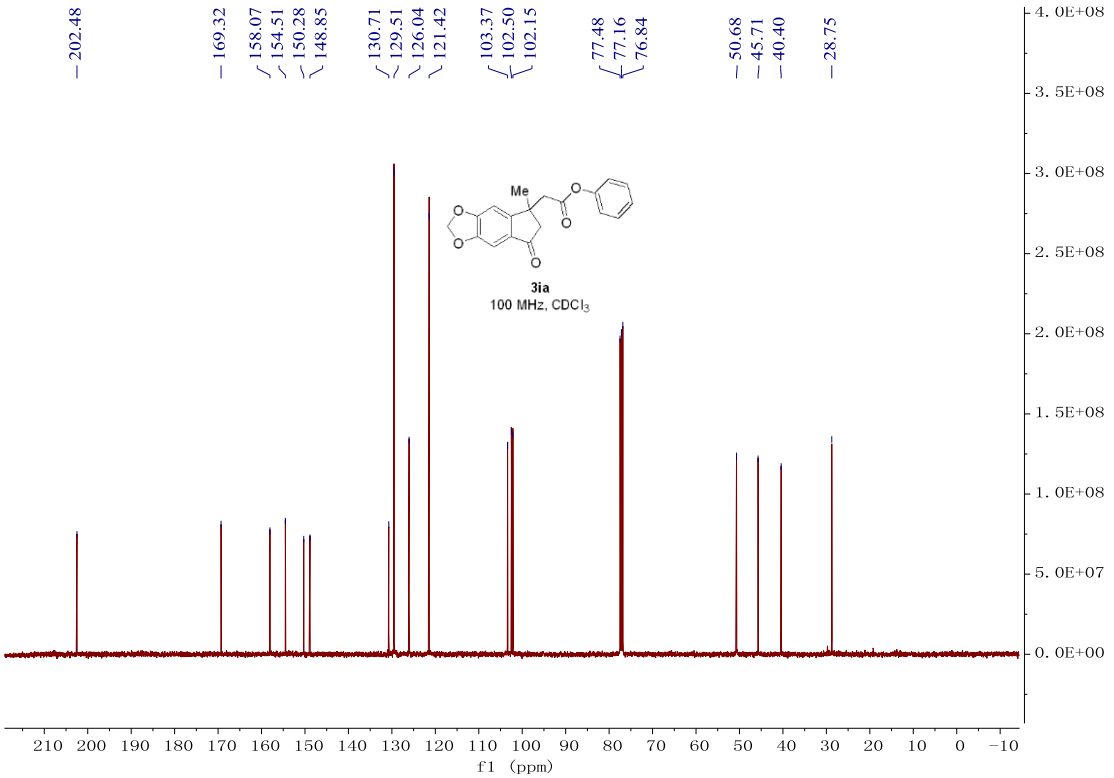
7.17
7.07
6.92
6.91
6.89
6.06
6.05
3.15
3.10
2.98
2.94
2.87
2.83
2.64
2.60
1.53
Me
3ia
400 MHz, CDCl3
2.00
1.00
1.00
3.00
2.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)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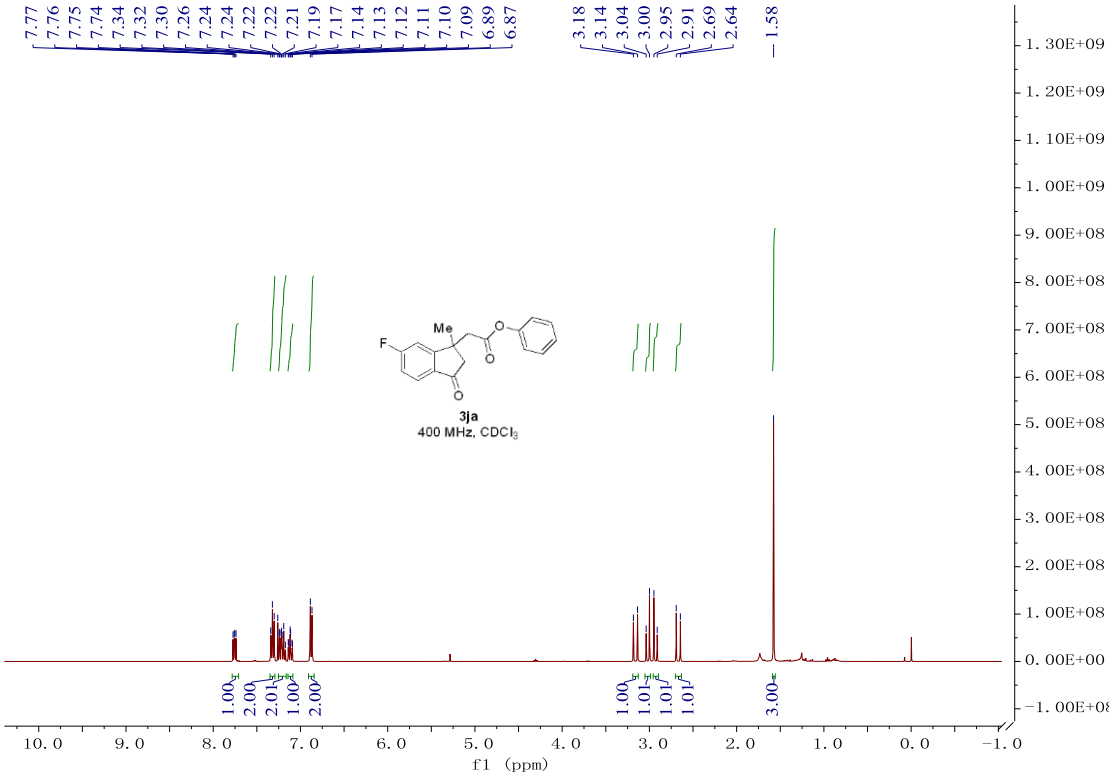
150.28
148.85
130.71
129.51
126.04
121.42
103.37
102.50
102.15
77.48
77.16
76.84
50.68
45.71
40.40
28.75
Me
3ia
100 MHz, CDCl3
f1 (ppm)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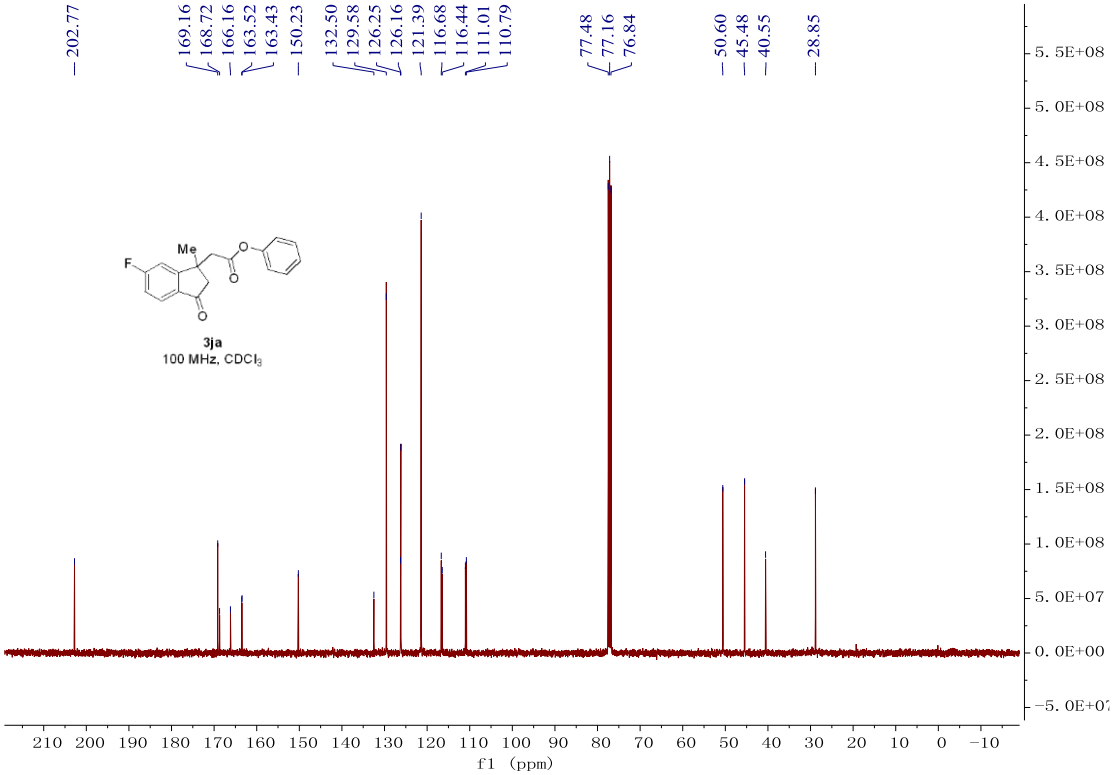
7.30
7.26
7.24
7.24
7.22
7.22
7.21
7.19
7.17
7.14
7.13
7.12
7.11
7.10
7.09
6.89
6.87
3.18
3.14
3.04
3.00
2.95
2.91
2.69
2.64
1.58
Me
F
O
O
O
3ja
400 MHz, CDCl3
1.00
2.00
2.01
1.00
2.00
1.00
1.01
1.01
1.01
3.00
f1 (ppm)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168.72
166.16
163.52
163.43
150.23
132.50
129.58
126.25
126.16
121.39
116.68
116.44
111.01
110.79
77.48
77.16
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40.55
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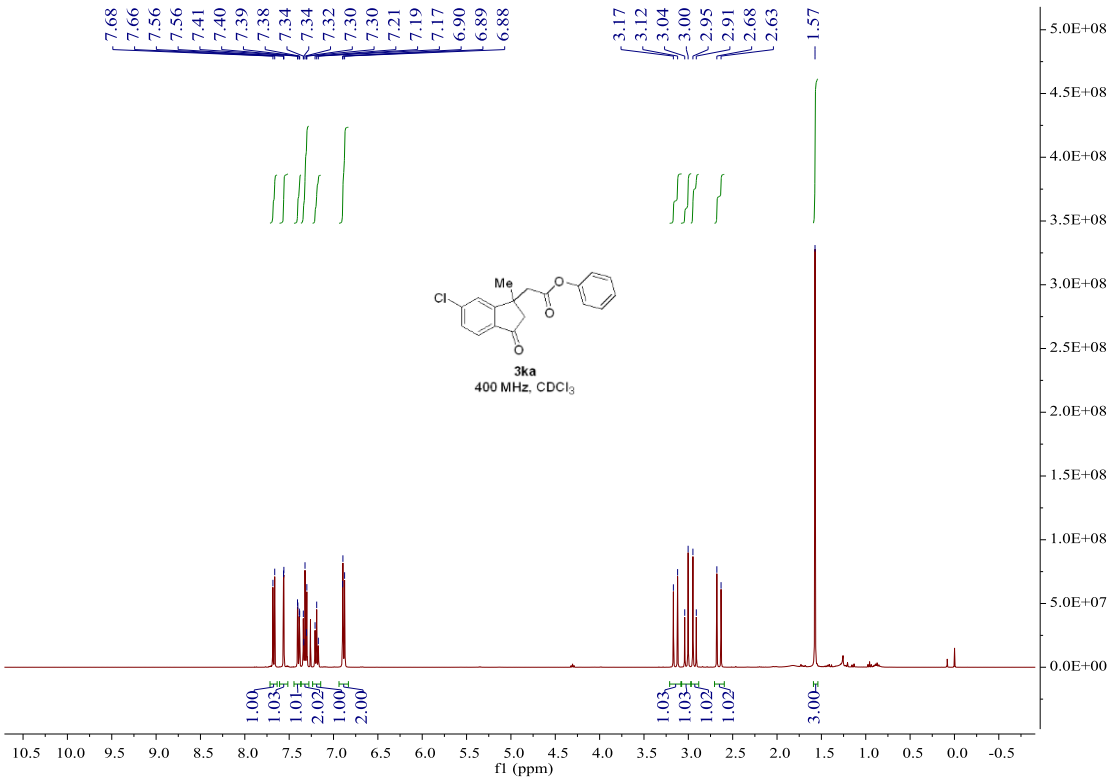
F
O
O
O
3ja
100 MHz, CDCl3
f1 (ppm)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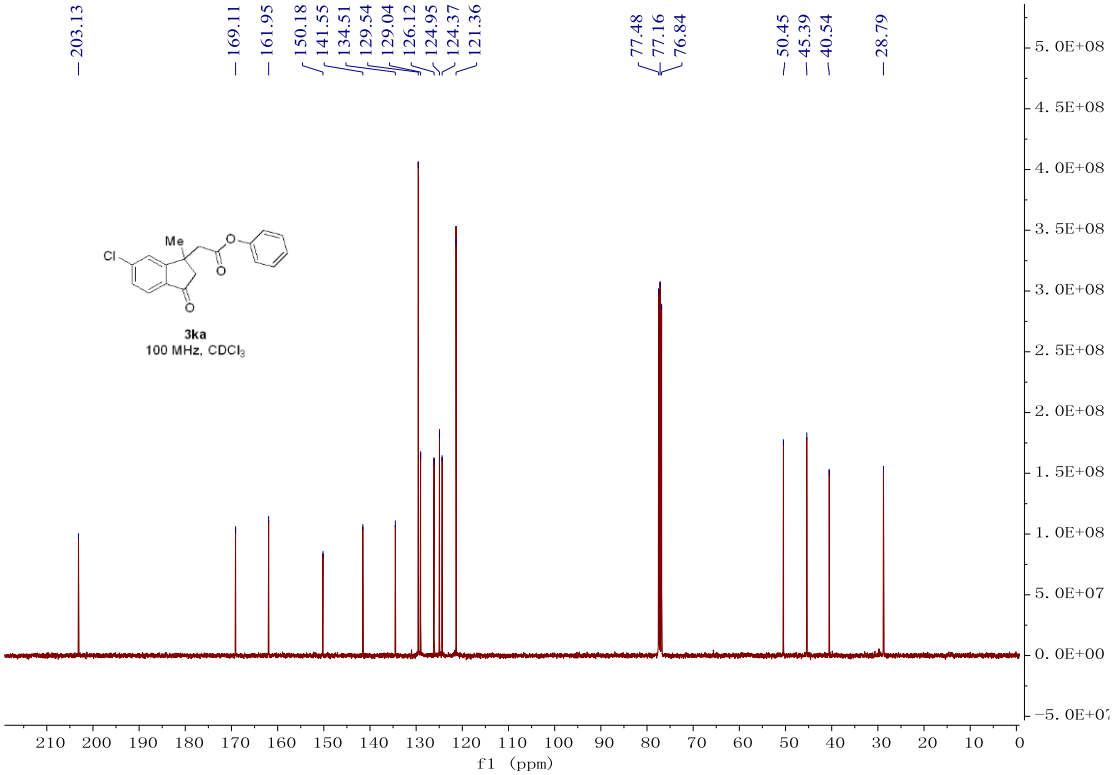
7.56
7.56
7.41
7.40
7.39
7.38
7.34
7.34
7.32
7.30
7.30
7.21
7.19
7.17
6.90
6.89
6.88
3.17
3.12
3.04
3.00
2.95
2.91
2.68
2.63
1.57
Me
Cl
O
O
O
3ka
400 MHz, CDCl3
1.00
1.03
1.01
2.02
1.00
2.00
1.03
1.03
1.02
1.02
3.00
f1 (ppm)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150.18
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134.51
129.54
129.04
126.12
124.95
124.37
121.36
77.48
77.16
76.84
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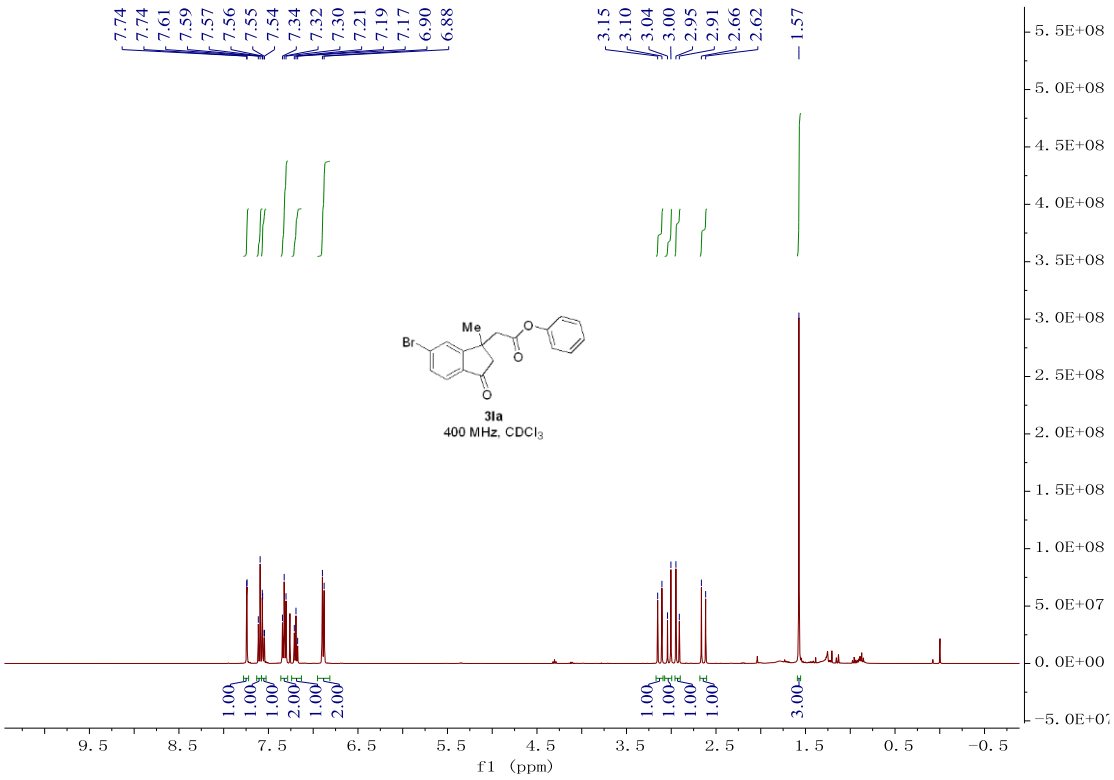
45.39
40.54
28.79
Me
Cl
O
O
O
3ka
100 MHz, CDCl3
f1 (ppm)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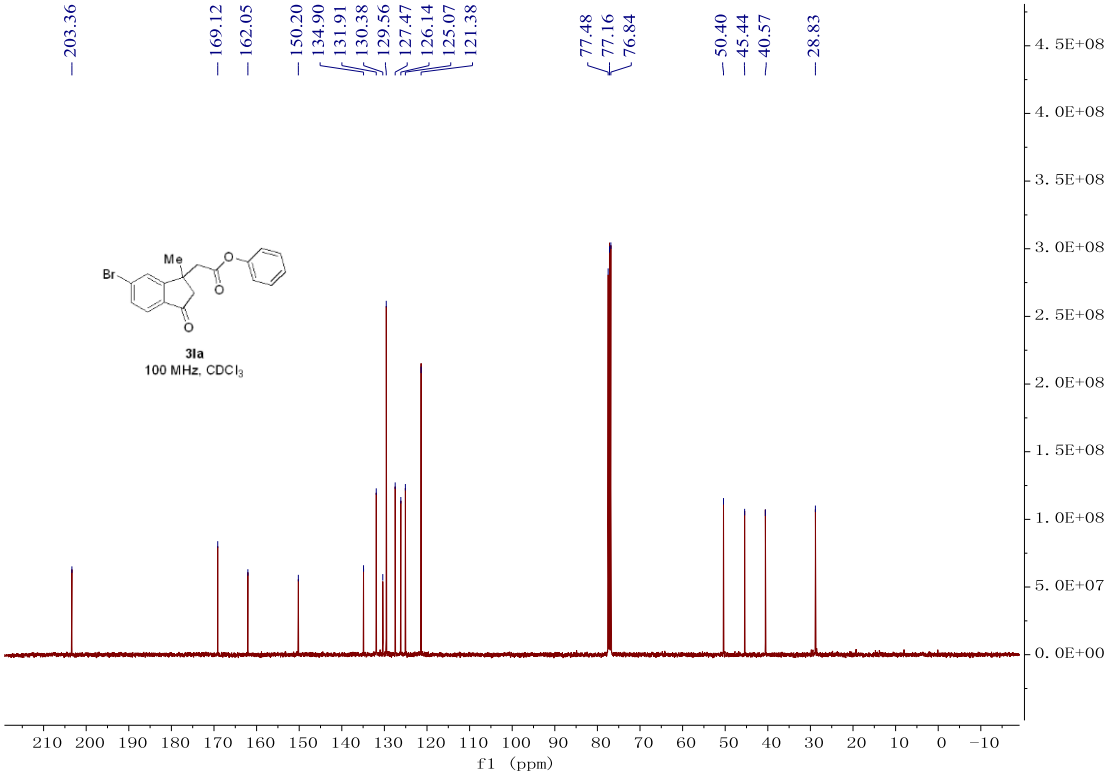
7.74
7.61
7.59
7.57
7.56
7.55
7.54
7.34
7.32
7.30
7.21
7.19
7.17
6.90
6.88
3.15
3.10
3.04
3.00
2.95
2.91
2.66
2.62
1.57
Me
Br
O
O
O
3la
400 MHz, CDCl3
1.00
1.00
1.00
2.00
1.00
2.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)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162.05
150.20
134.90
131.91
130.38
129.56
127.47
126.14
125.07
121.38
77.48
77.16
76.84
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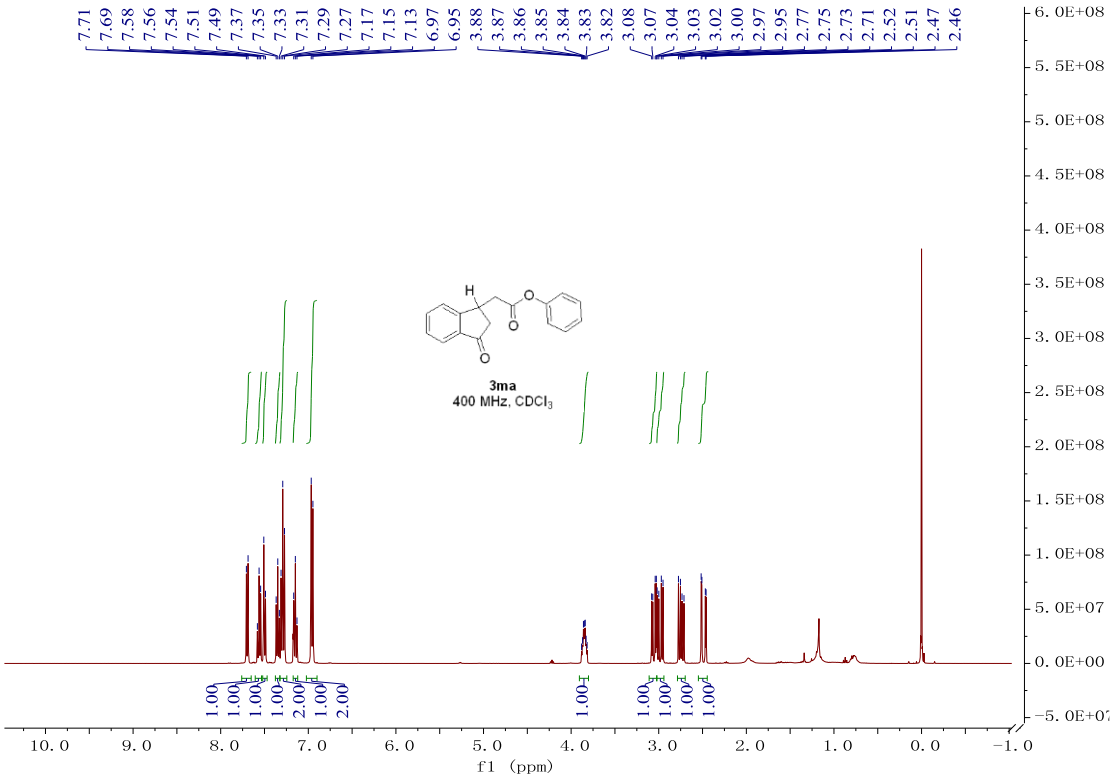
45.44
40.57
28.83
Me
Br
O
O
O
3la
100 MHz, CDCl3
f1 (ppm)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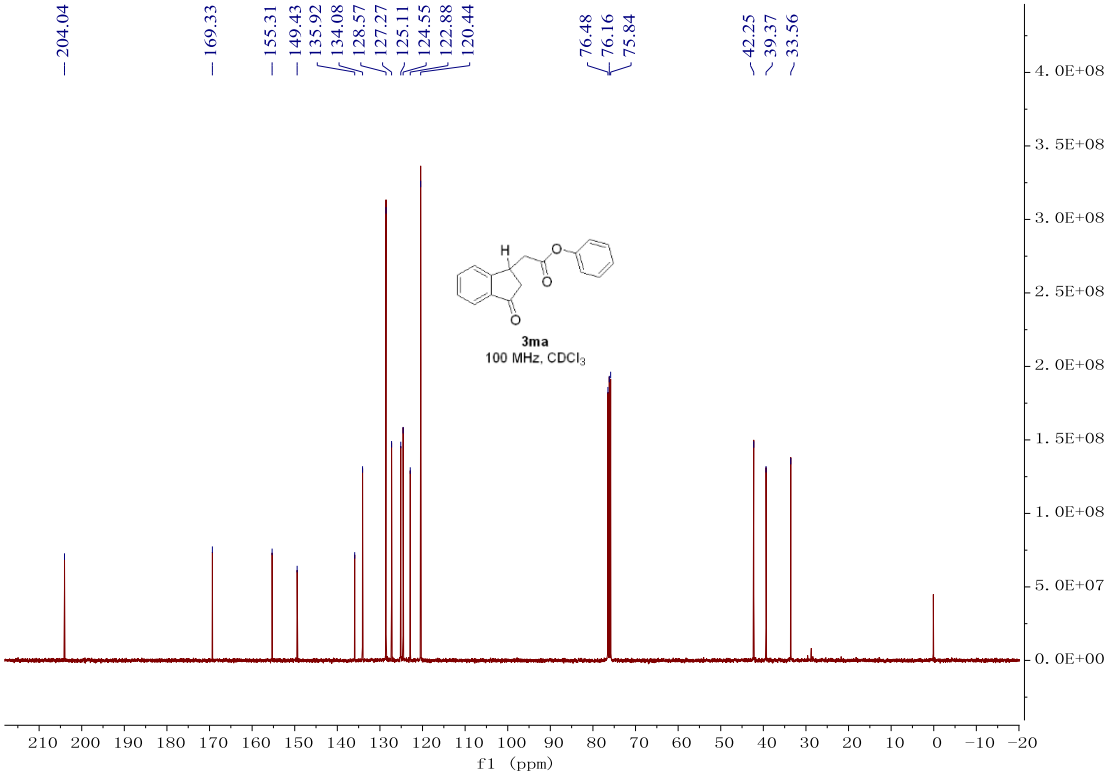
7.31
7.29
7.27
7.17
7.15
7.13
6.97
6.95
3.88
3.87
3.86
3.85
3.84
3.83
3.82
3.08
3.07
3.04
3.03
3.02
3.00
2.97
2.95
2.77
2.75
2.73
2.71
2.52
2.51
2.47
2.46
3ma
400 MHz, CDCl3
1.00
1.00
1.00
1.00
2.00
1.00
2.00
1.00
1.00
1.00
1.00
f1 (ppm)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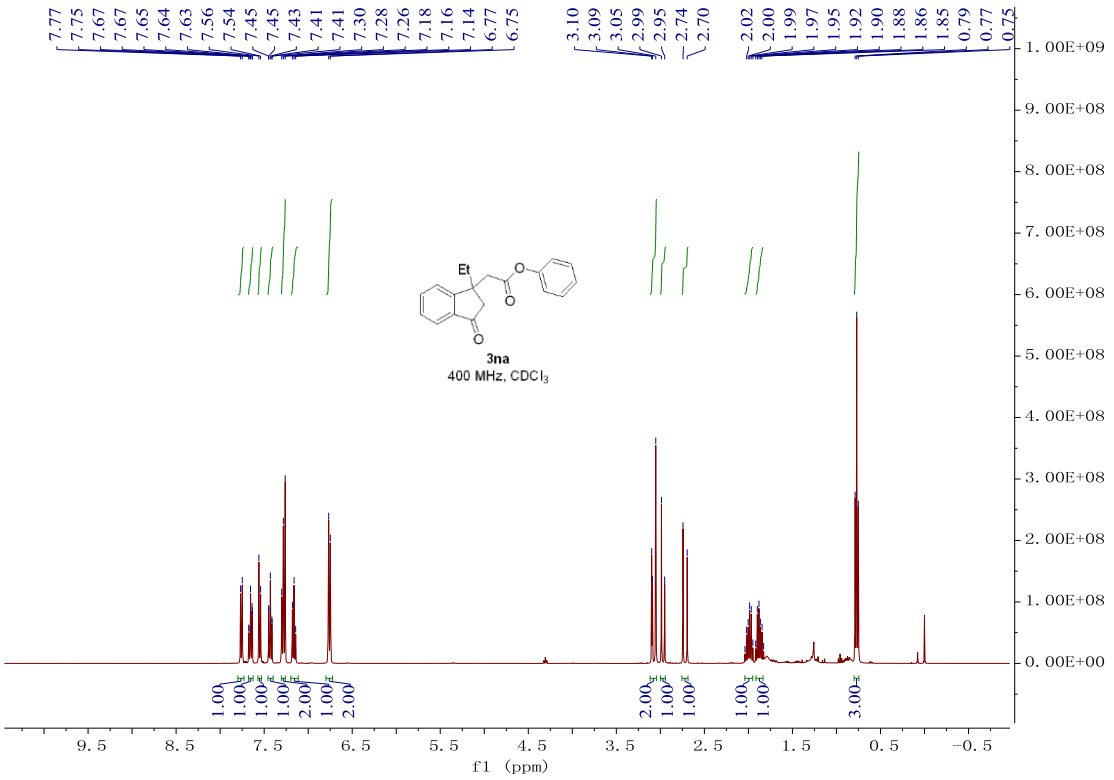
169.33
155.31
149.43
135.92
134.08
128.57
127.27
125.11
124.55
122.88
120.44
76.48
76.16
75.84
42.25
39.37
33.56
3ma
100 MHz, CDCl3
f1 (ppm)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7.75
7.67
7.67
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7.64
7.63
7.56
7.54
7.45
7.45
7.43
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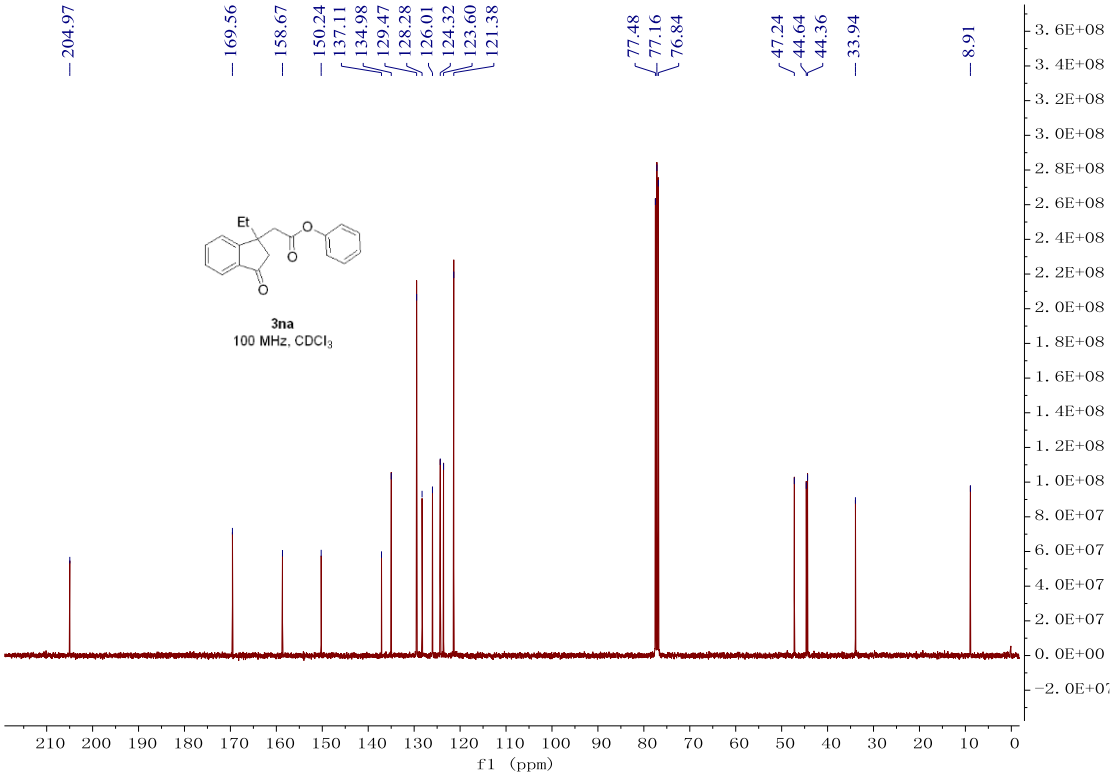
7.41
7.30
7.28
7.26
7.18
7.16
7.14
6.77
6.75
3.10
3.09
3.05
2.99
2.95
2.74
2.70
2.02
2.00
1.99
1.97
1.95
1.92
1.90
1.88
1.86
1.85
0.79
0.77
0.75
Et
O
O
O
3na
400 MHz, CDCl3
1.00
1.00
1.00
1.00
2.00
1.00
2.00
2.00
1.00
1.00
1.00
3.00
f1 (ppm)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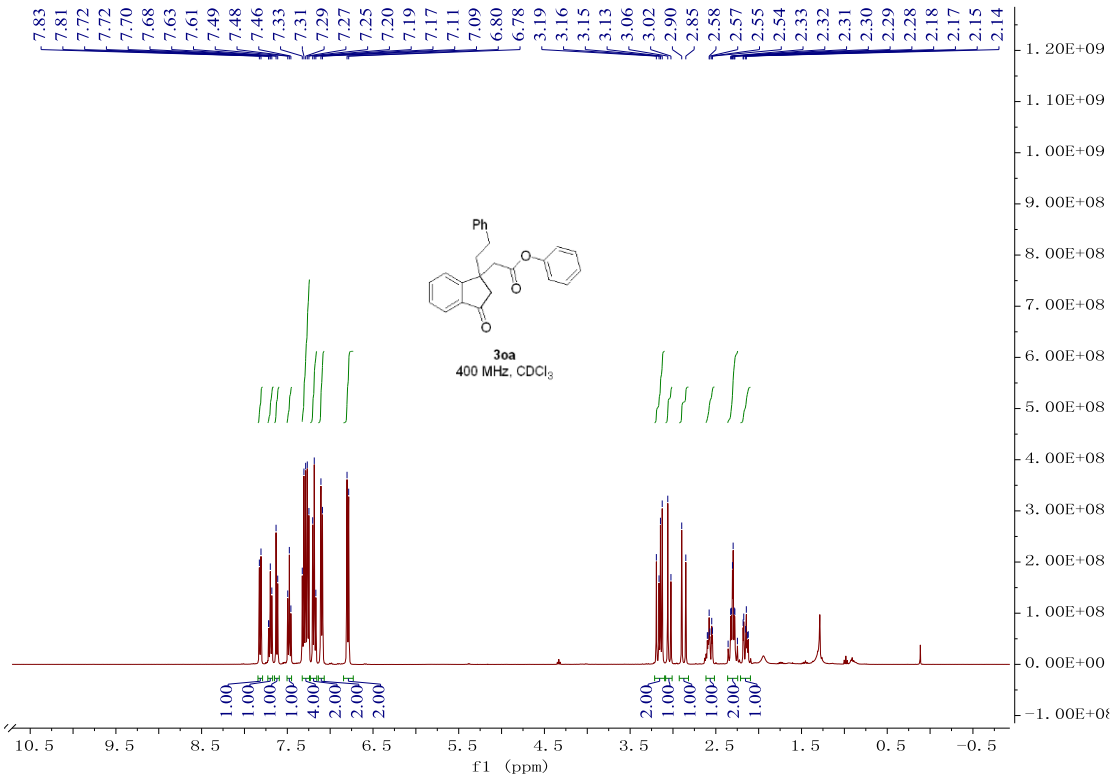
169.56
158.67
150.24
137.11
134.98
129.47
128.28
126.01
124.32
123.60
121.38
77.48
77.16
76.84
47.24
44.64
44.36
33.94
8.91
Et
O
O
O
3na
100 MHz, CDCl3
f1 (ppm)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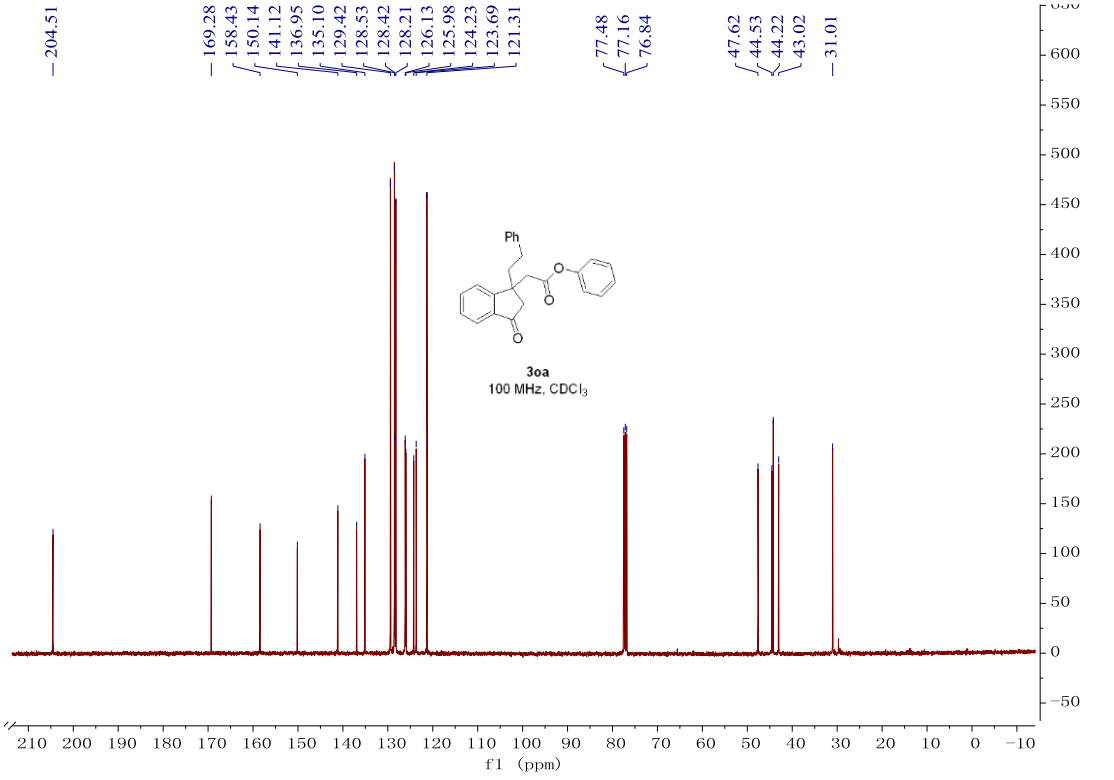
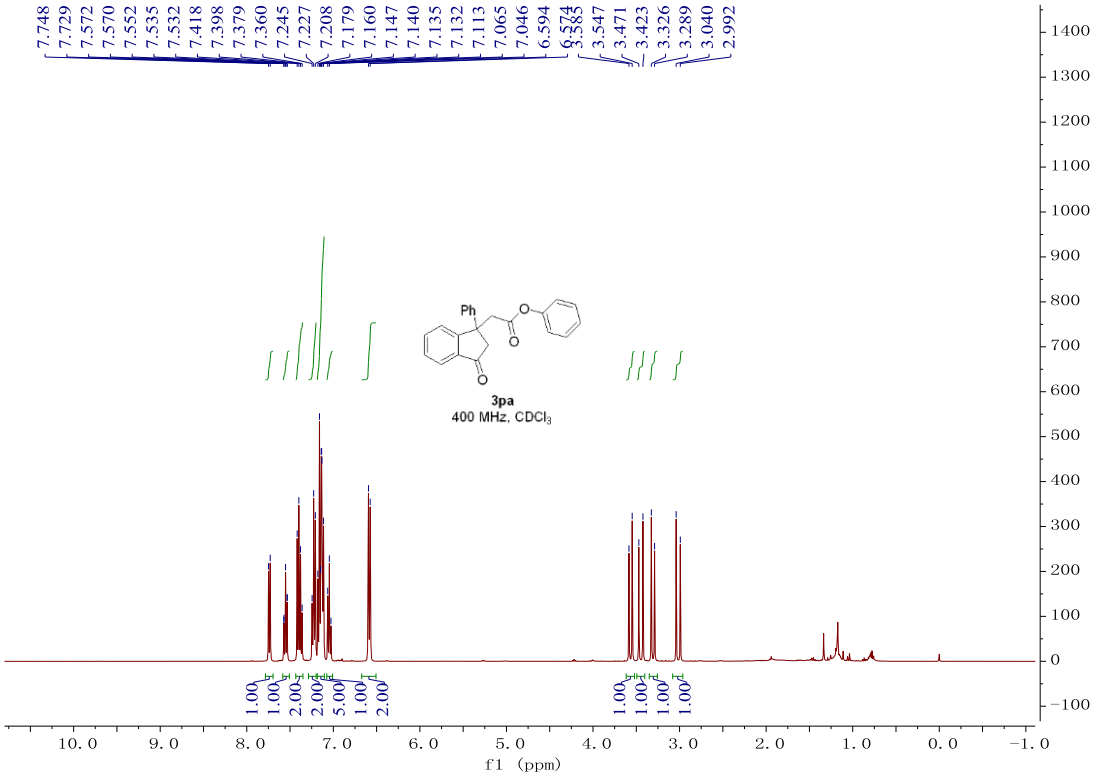
3.19 3.16 3.15 3.13 3.06 3.02 2.90 2.85 2.58 2.57 2.55 2.54 2.33 2.32 2.31 2.30 2.29 2.28 2.18 2.17 2.15 2.14
Ph
O
O
O
3oa
400 MHz, CDCl3
1.00 1.00 1.00 1.00 4.00 2.00 2.00 2.00 2.00 1.00 1.00 1.00 2.00 1.00
f1 (ppm)


204.51
169.28 158.43 150.14 141.12 136.95 135.10 129.42 128.53 128.42 128.21 126.13 125.98 124.23 123.69 121.31
77.48 77.16 76.84
47.62 44.53 44.22 43.02
31.01
Ph
O
O
O
3oa
100 MHz, CDCl3
f1 (ppm)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7.572
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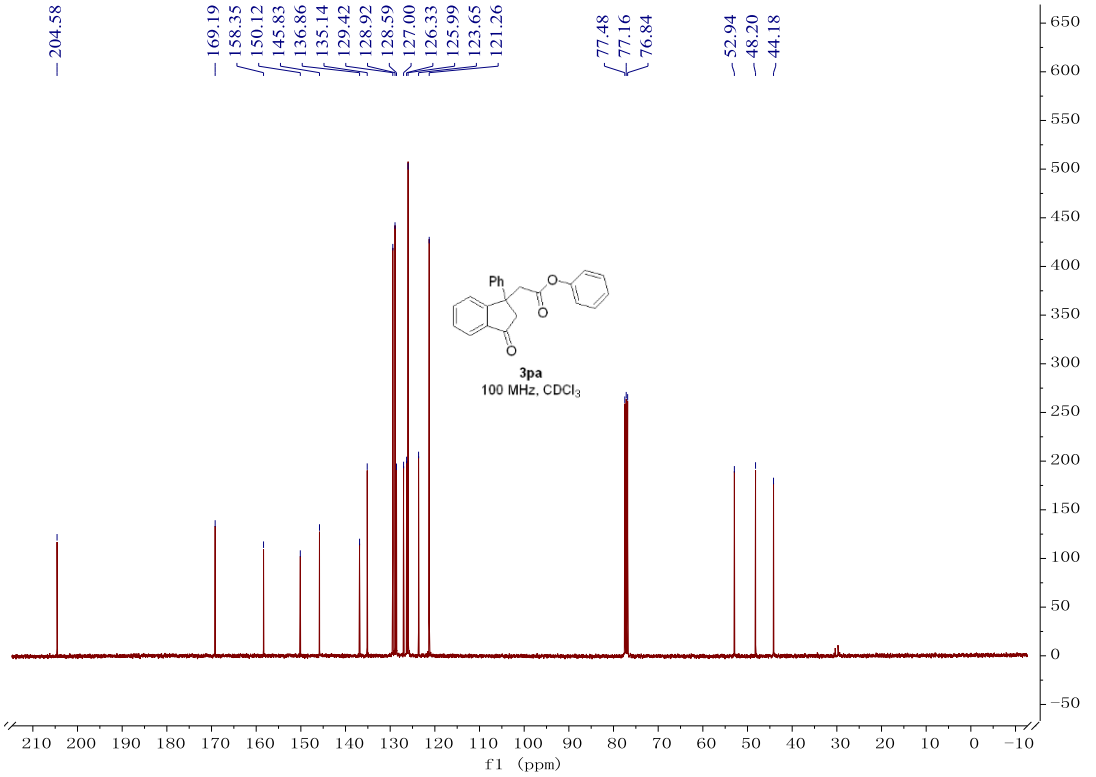
7.535
7.532
7.418
7.398
7.379
7.360
7.245
7.227
7.208
7.179
7.160
7.147
7.140
7.135
7.132
7.113
7.065
7.046
6.594
6.574
3.585
3.547
3.471
3.423
3.326
3.289
3.040
2.992
Ph
O
O
O
3pa
400 MHz, CDCl3
1.00
1.00
2.00
2.00
5.00
1.00
2.00
1.00
1.00
1.00
1.00
f1 (ppm)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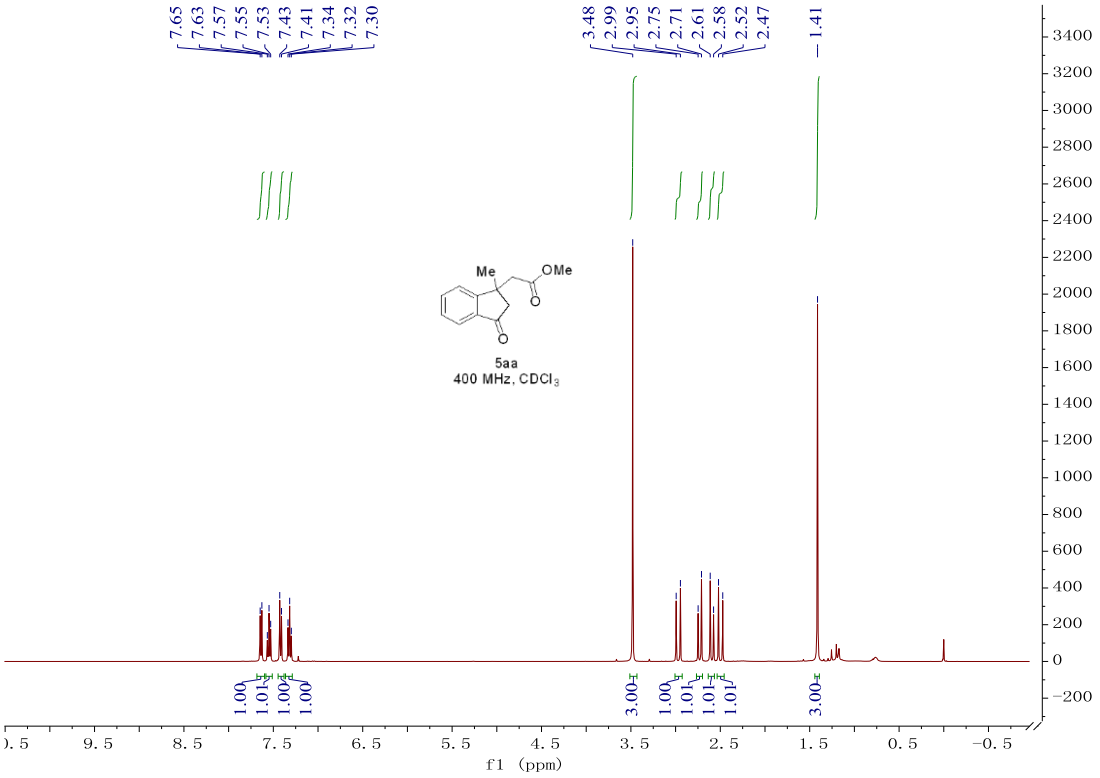
158.35
150.12
145.83
136.86
135.14
129.42
128.92
128.59
127.00
126.33
125.99
123.65
121.26
77.48
77.16
76.84
52.94
48.20
44.18
Ph
O
O
O
3pa
100 MHz, CDCl3
f1 (ppm)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7.63
7.57
7.55
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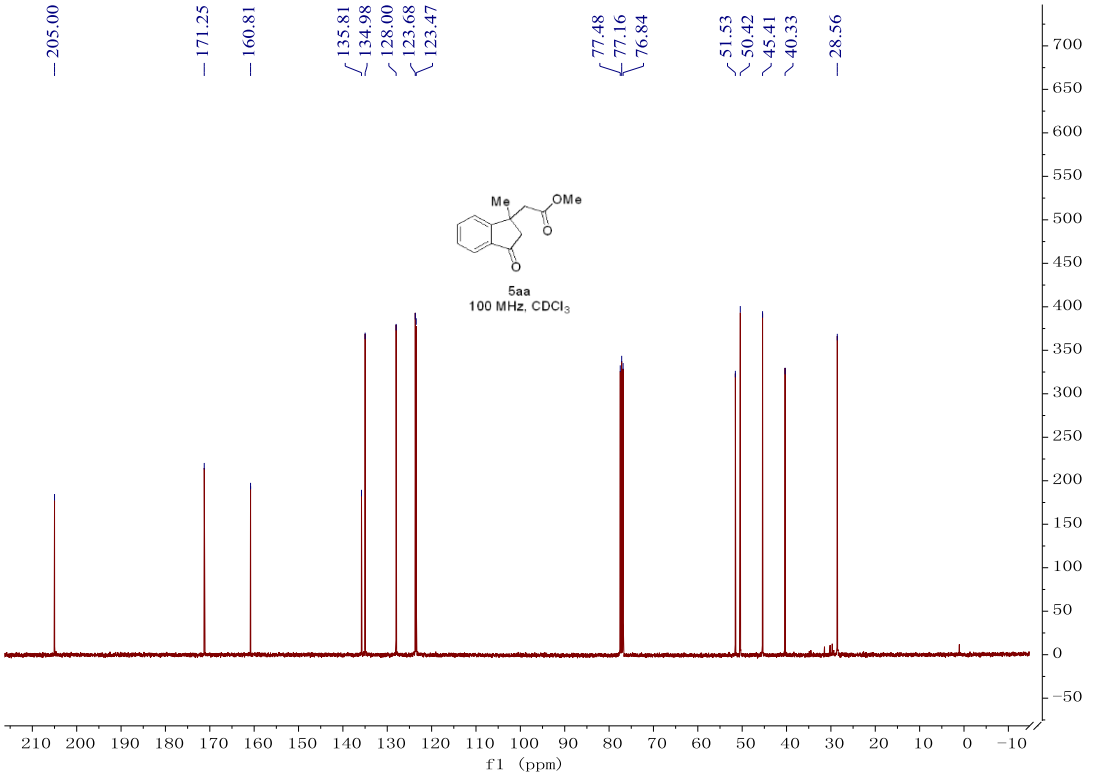
7.43
7.41
7.34
7.32
7.30
3.48
2.99
2.95
2.75
2.71
2.61
2.58
2.52
2.47
1.41
Me
OMe
O
O
5aa
400 MHz, CDCl3
1.00
1.01
1.00
1.00
3.00
1.00
1.01
1.01
1.01
3.00
f1 (ppm)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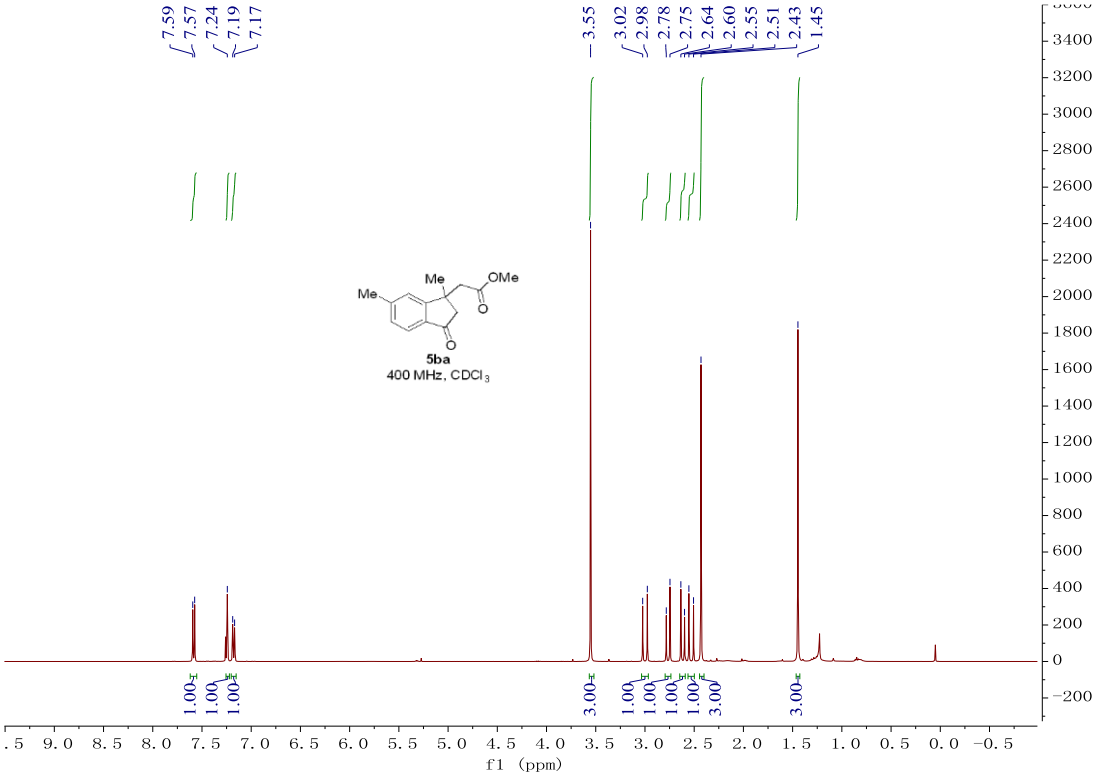
171.25
160.81
135.81
134.98
128.00
123.68
123.47
77.48
77.16
76.84
51.53
50.42
45.41
40.33
28.56
Me
OMe
O
O
5aa
100 MHz, CDCl3
f1 (ppm)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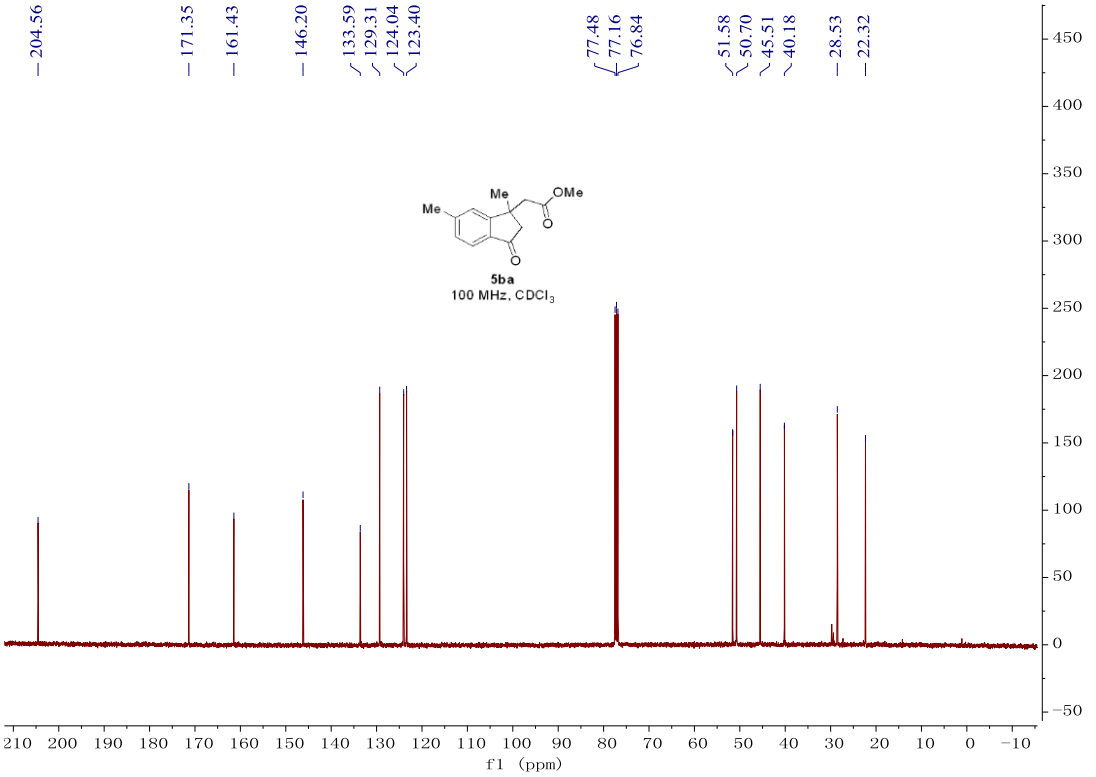
7.57
7.24
7.19
7.17
3.55
3.02
2.98
2.78
2.75
2.64
2.60
2.55
2.51
2.43
1.45
Me
OMe
Me
O
O
5ba
400 MHz, CDCl3
1.00
1.00
1.00
3.00
1.00
1.00
1.00
1.00
3.00
3.00
f1 (ppm)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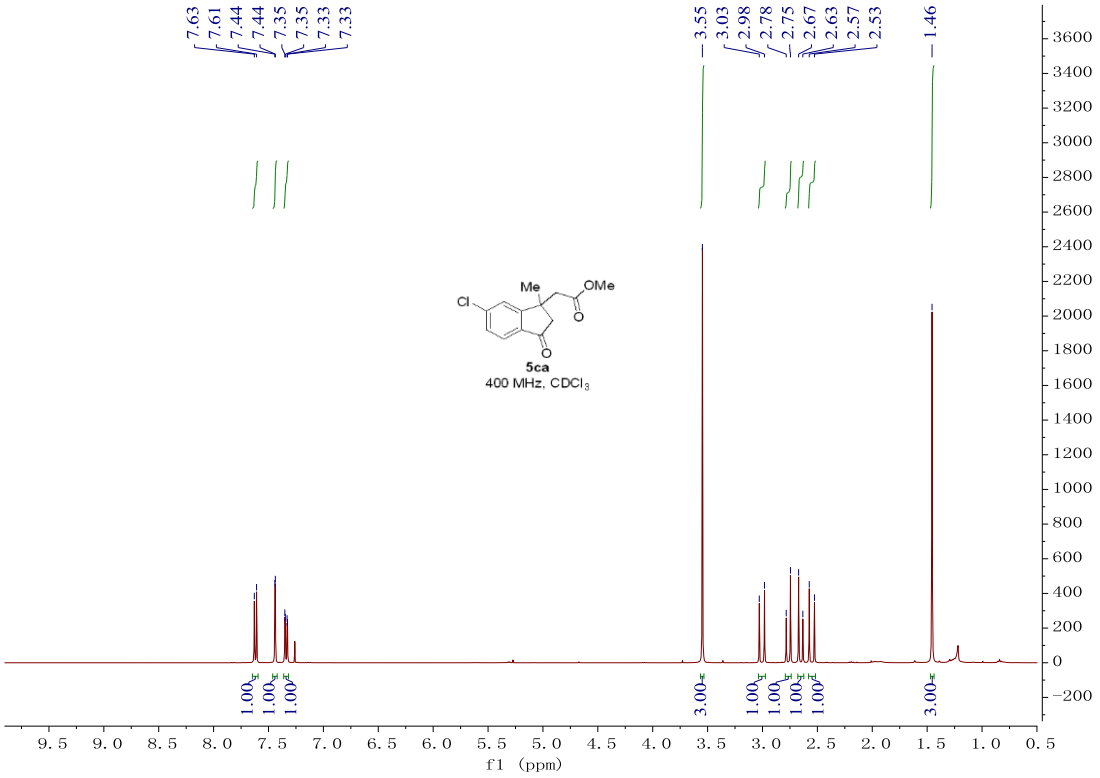
133.59
129.31
124.04
123.40
77.48
77.16
76.84
51.58
50.70
45.51
40.18
28.53
22.32
Me
OMe
Me
O
O
5ba
100 MHz, CDCl3
f1 (ppm)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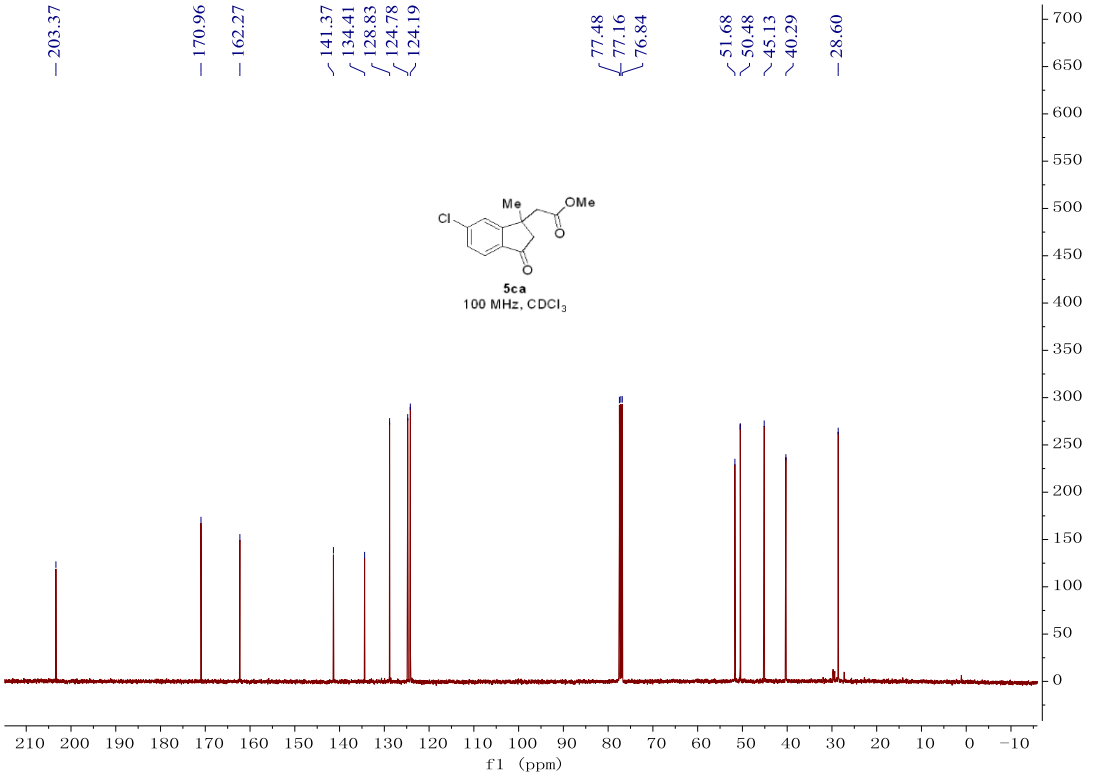
7.61
7.44
7.44
7.35
7.35
7.33
7.33
3.55
3.03
2.98
2.78
2.75
2.67
2.63
2.57
2.53
1.46
Me
OMe
Cl
O
O
5ca
400 MHz, CDCl3
1.00
1.00
1.00
3.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)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141.37
134.41
128.83
124.78
124.19
77.48
77.16
76.84
51.68
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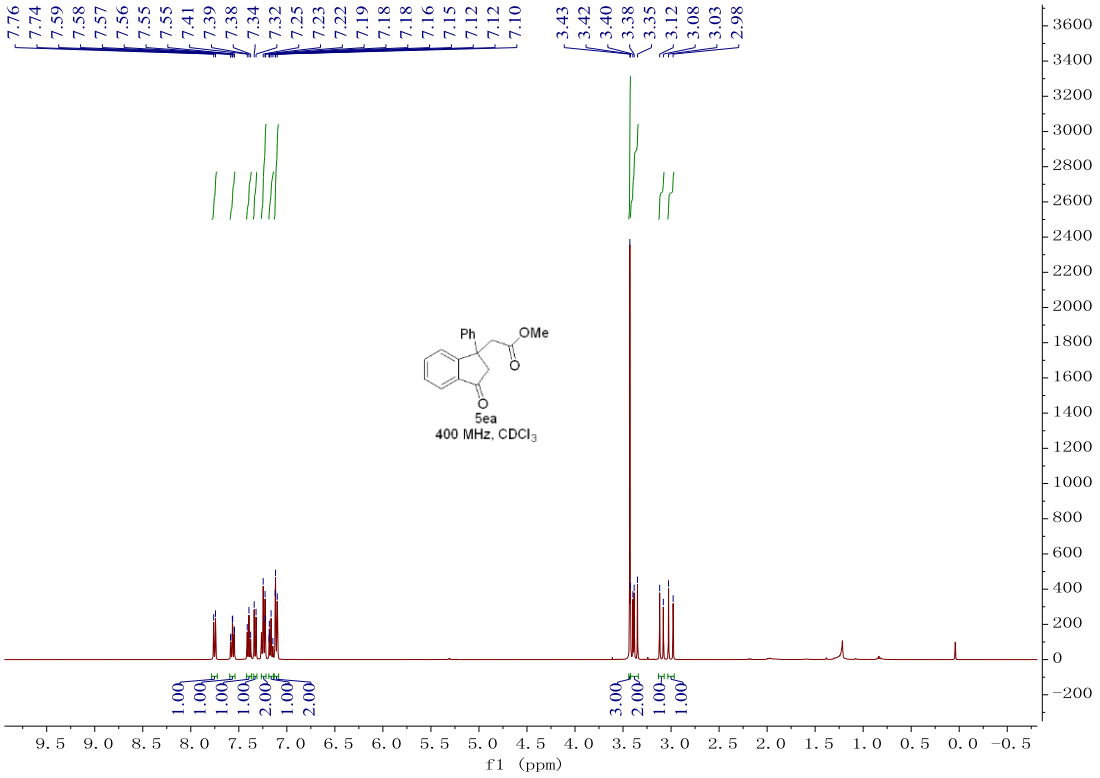
Cl
O
O
5ca
100 MHz, CDCl3
f1 (ppm)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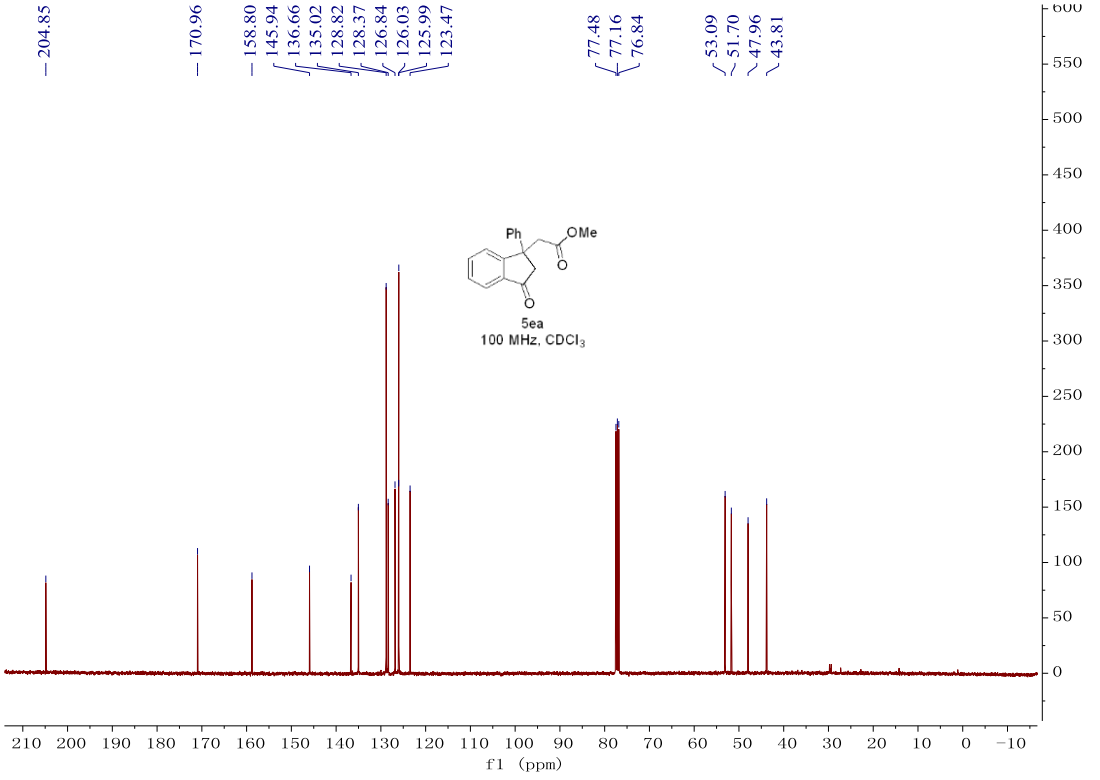
7.58
7.57
7.56
7.55
7.55
7.41
7.39
7.38
7.34
7.32
7.25
7.23
7.22
7.19
7.18
7.18
7.16
7.15
7.12
7.12
7.10
3.43
3.42
3.40
3.38
3.35
3.12
3.08
3.03
2.98
Ph
OMe
O
O
5ea
400 MHz, CDCl3
1.00
1.00
1.00
1.00
2.00
1.00
2.00
3.00
2.00
1.00
1.00
f1 (ppm)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145.94
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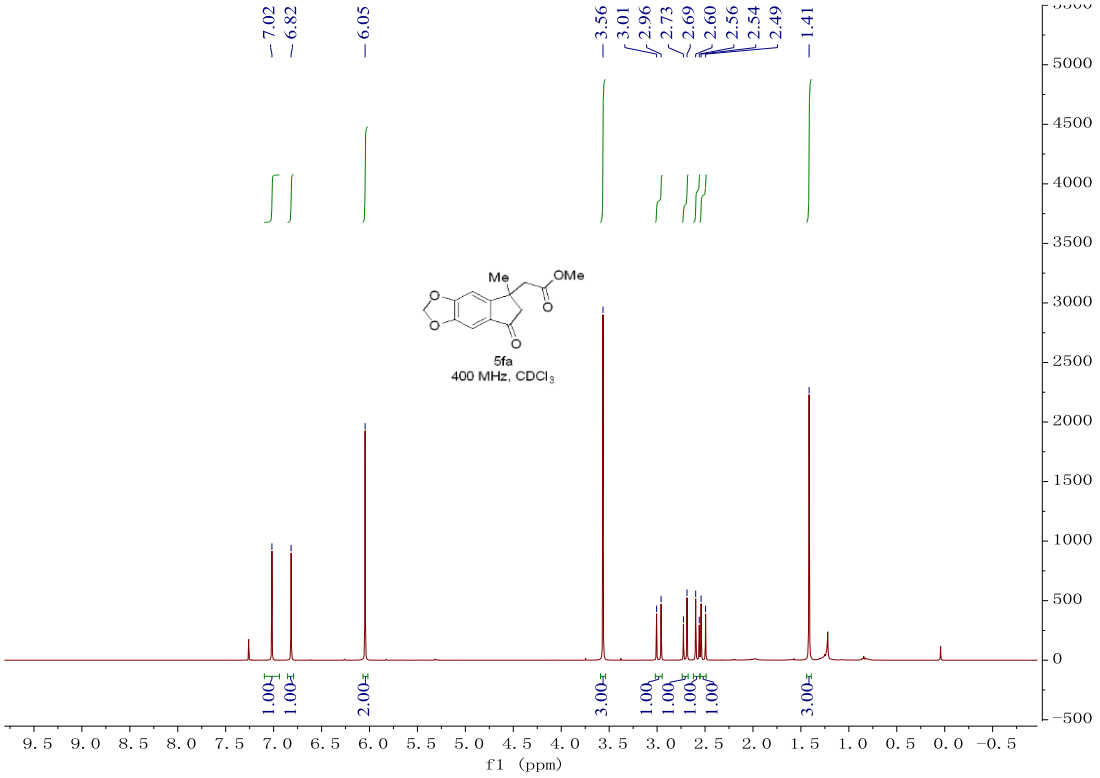
128.37
126.84
126.03
125.99
123.47
77.48
77.16
76.84
53.09
51.70
47.96
43.81
Ph
OMe
O
O
5ea
100 MHz, CDCl3
f1 (ppm)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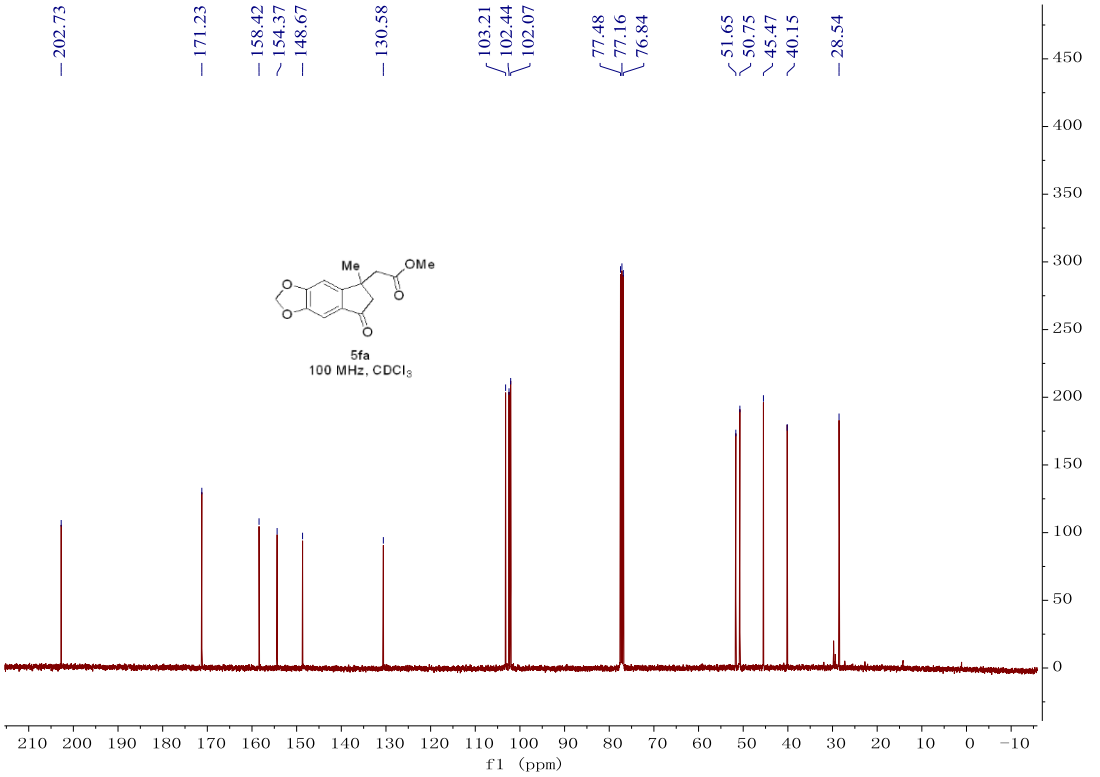
6.82
6.05
3.56
3.01
2.96
2.73
2.69
2.60
2.56
2.54
2.49
1.41
Me
OMe
5fa
400 MHz, CDCl3
1.00
1.00
2.00
3.00
1.00
1.00
1.00
1.00
3.00
f1 (ppm)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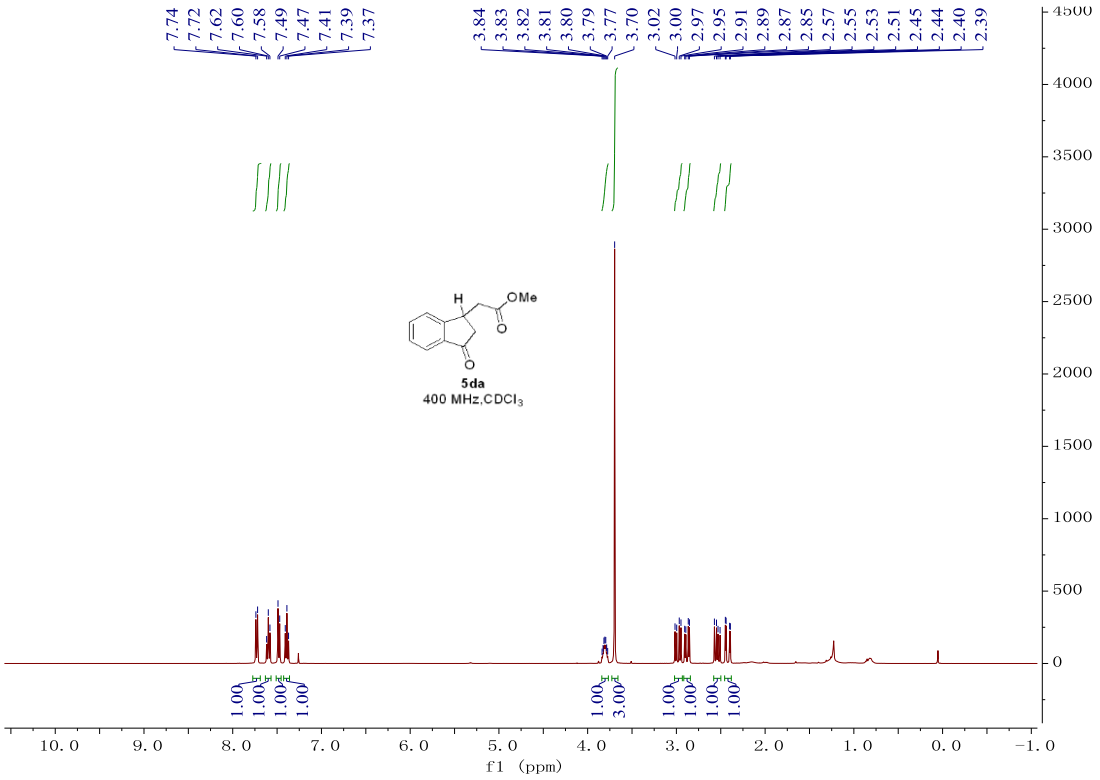
148.67
130.58
103.21
102.44
102.07
77.48
77.16
76.84
51.65
50.75
45.47
40.15
28.54
Me
OMe
5fa
100 MHz, CDCl3
f1 (ppm)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7.72
7.62
7.60
7.58
7.49
7.47
7.41
7.39
7.37
3.84
3.83
3.82
3.81
3.80
3.79
3.77
3.70
3.02
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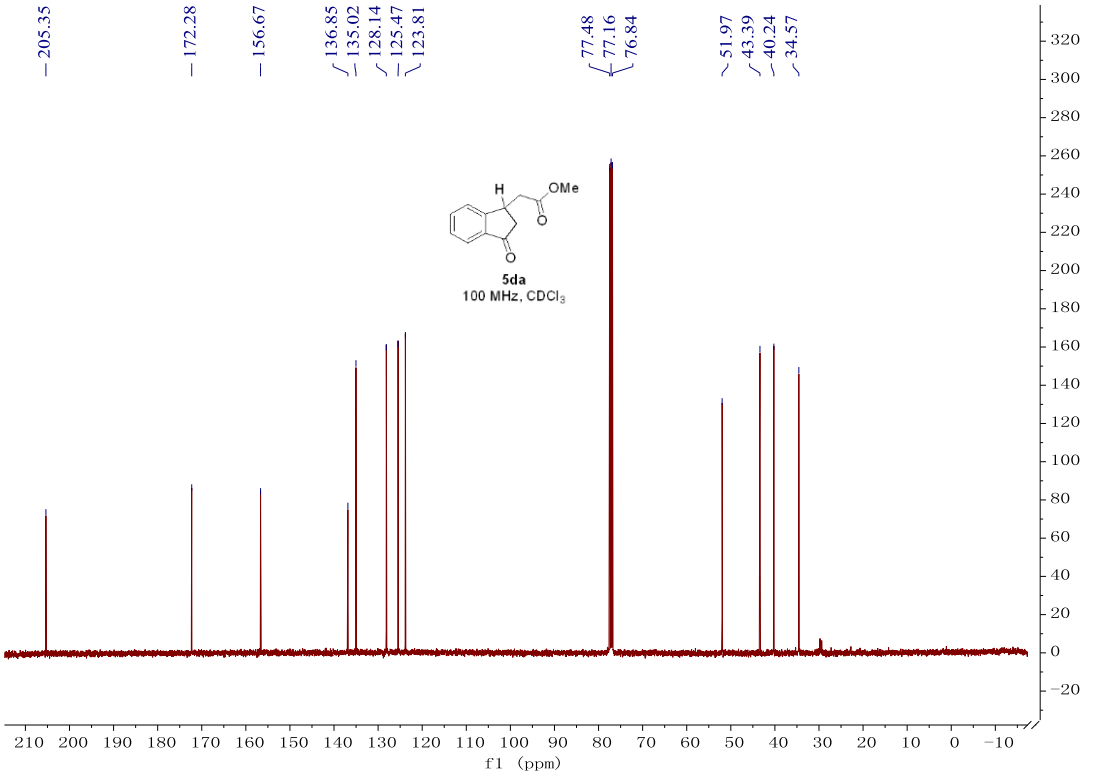
2.89
2.87
2.85
2.57
2.55
2.53
2.51
2.45
2.44
2.40
2.39
OMe
H
O
O
5da
400 MHz,CDCl3
1.00
1.00
1.00
1.00
1.00
3.00
1.00
1.00
1.00
1.00
f1 (ppm)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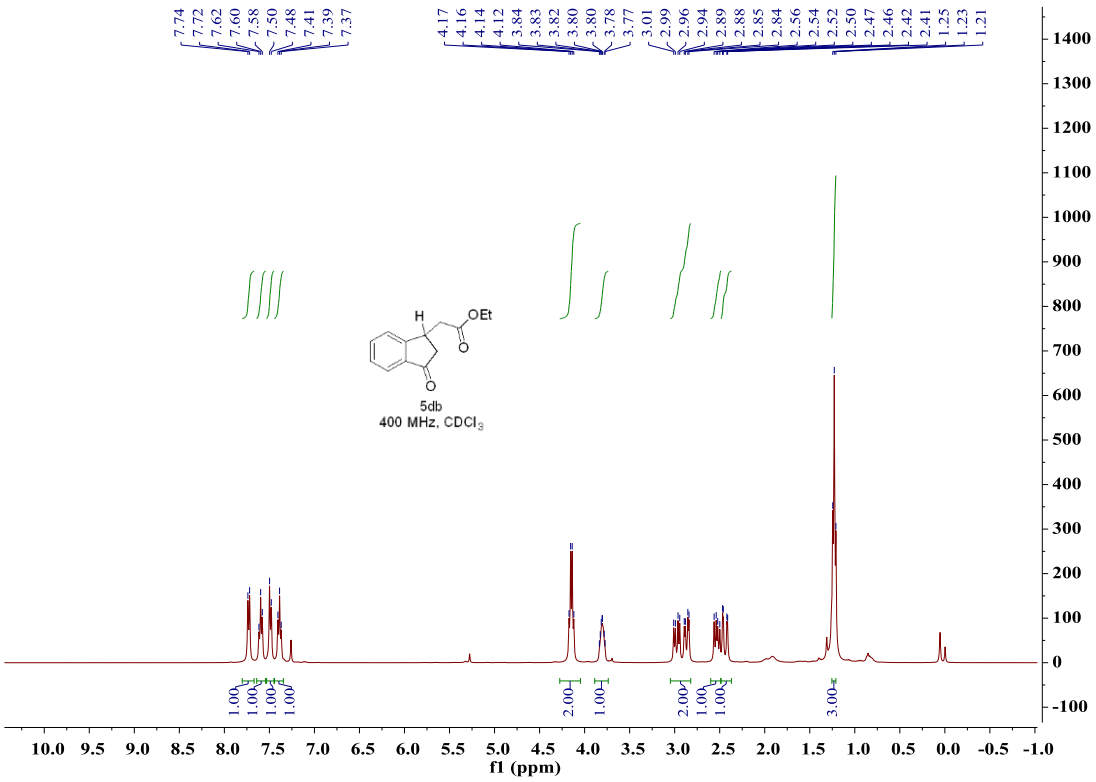
136.85
135.02
128.14
125.47
123.81
77.48
77.16
76.84
51.97
43.39
40.24
34.57
OMe
H
O
O
5da
100 MHz, CDCl3
f1 (ppm)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7.72
7.62
7.60
7.58
7.50
7.48
7.41
7.39
7.37
4.17
4.16
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4.12
3.84
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3.82
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3.80
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3.77
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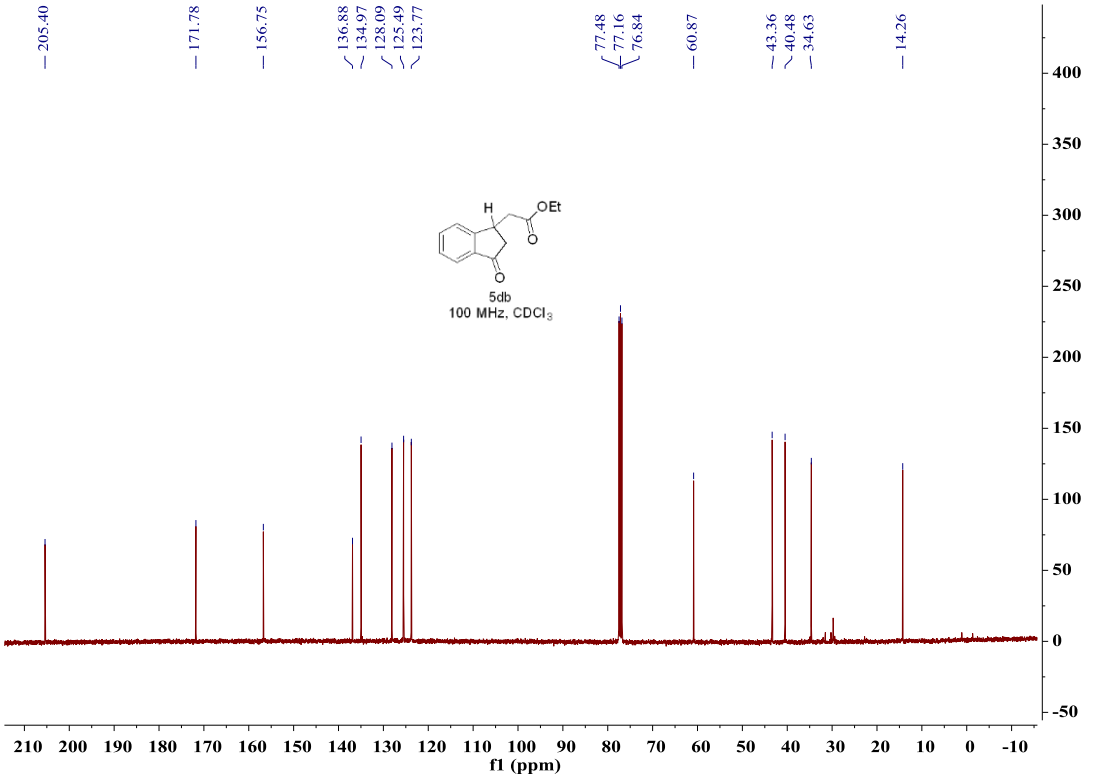
2.88
2.85
2.84
2.56
2.54
2.52
2.50
2.47
2.46
2.42
2.41
1.25
1.23
1.21
H
OEt
O
O
5db
400 MHz, CDCl3
1.00
1.00
1.00
1.00
2.00
1.00
2.00
1.00
1.00
3.00
f1 (ppm)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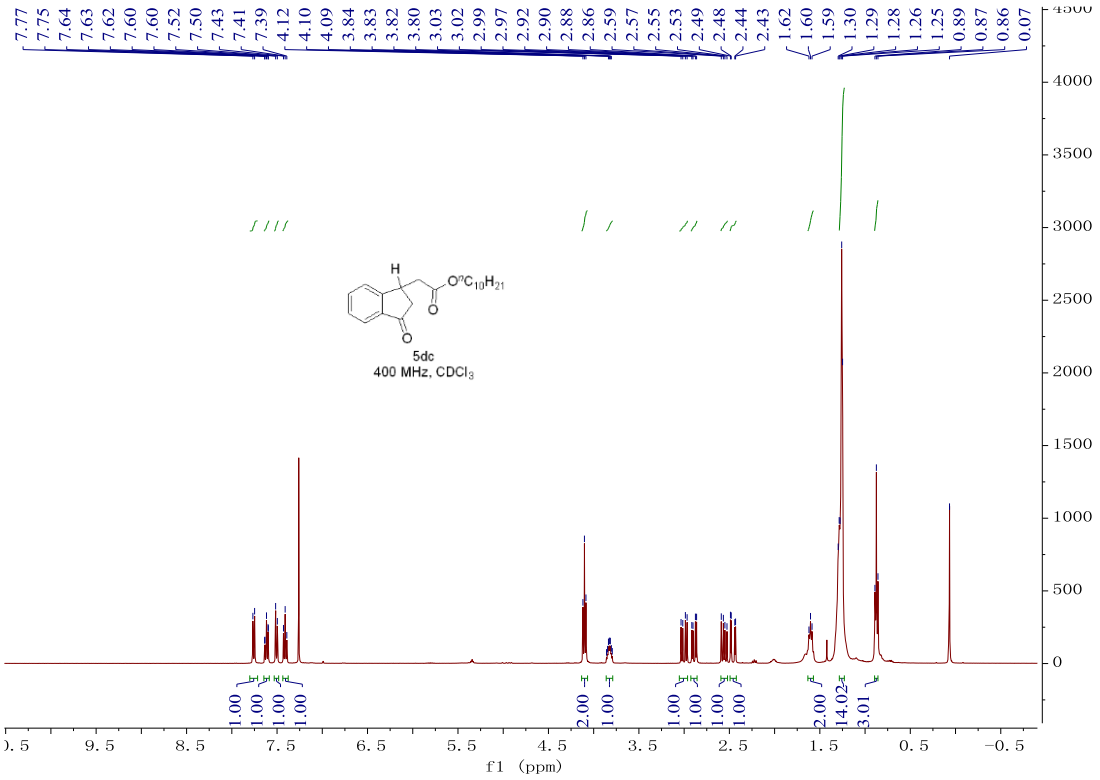
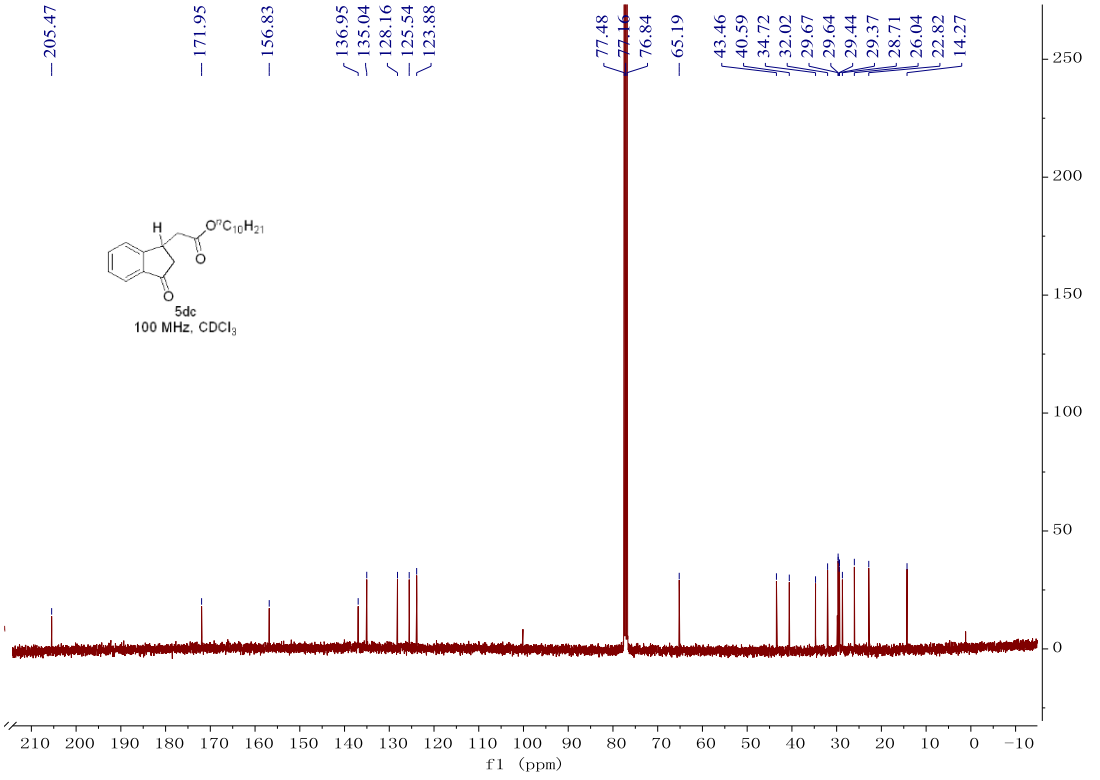
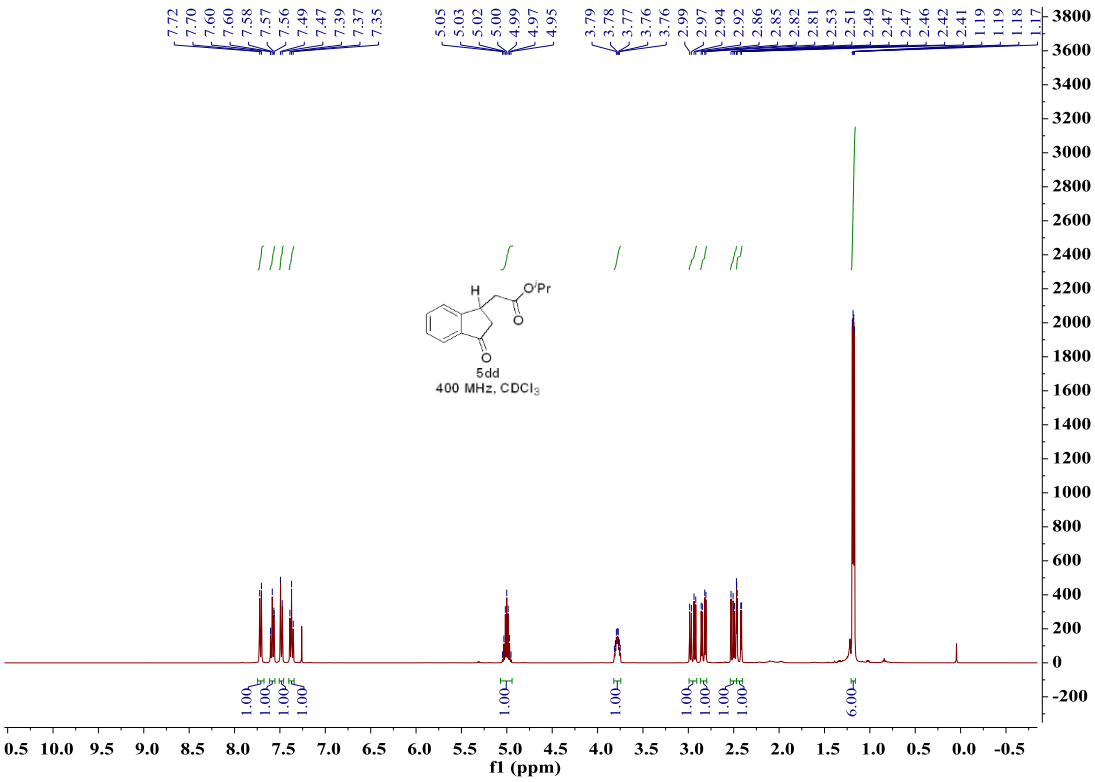
171.78
156.75
136.88
134.97
128.09
125.49
123.77
77.48
77.16
76.84
60.87
43.36
40.48
34.63
14.26
H
OEt
O
O
5db
100 MHz, CDCl3
f1 (ppm)


7.77 7.75 7.64 7.63 7.62 7.60 7.60 7.52 7.50 7.43 7.41 7.39 4.12 4.10 4.09 3.84 3.83 3.82 3.80 3.03 3.02 2.99 2.97 2.92 2.90 2.88 2.86 2.59 2.57 2.55 2.53 2.49 2.48 2.44 2.43 1.62 1.60 1.59 1.30 1.29 1.28 1.26 1.25 0.89 0.87 0.86 0.07
5dc
400 MHz, CDCl3
1.00 1.00 1.00 1.00 2.00 1.00 1.00 1.00 1.00 1.00 2.00 14.02 3.01
f1 (ppm)


205.47 171.95 156.83 136.95 135.04 128.16 125.54 123.88 77.48 77.16 76.84 65.19 43.46 40.59 34.72 32.02 29.67 29.64 29.44 29.37 28.71 26.04 22.82 14.27
5dc
100 MHz, CDCl3
f1 (ppm)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7.60
7.60
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7.57
7.56
7.49
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7.39
7.37
7.35
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5.03
5.02
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3.77
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3.76
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2.94
2.92
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2.85
2.82
2.81
2.53
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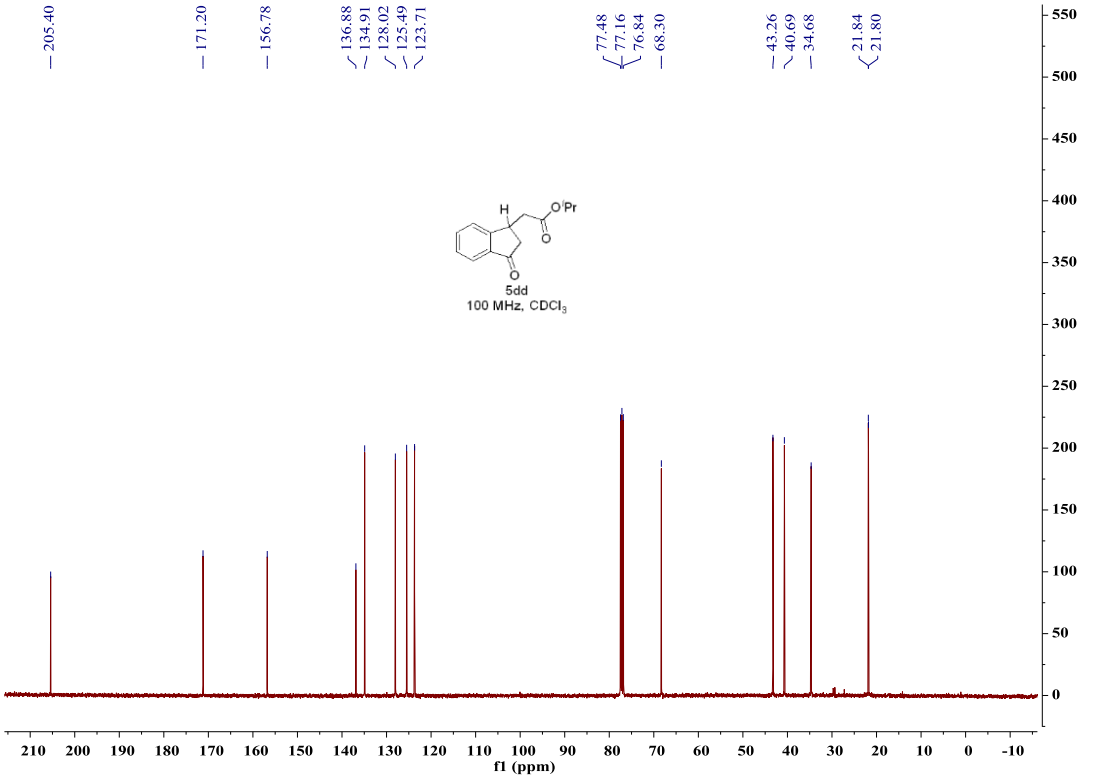
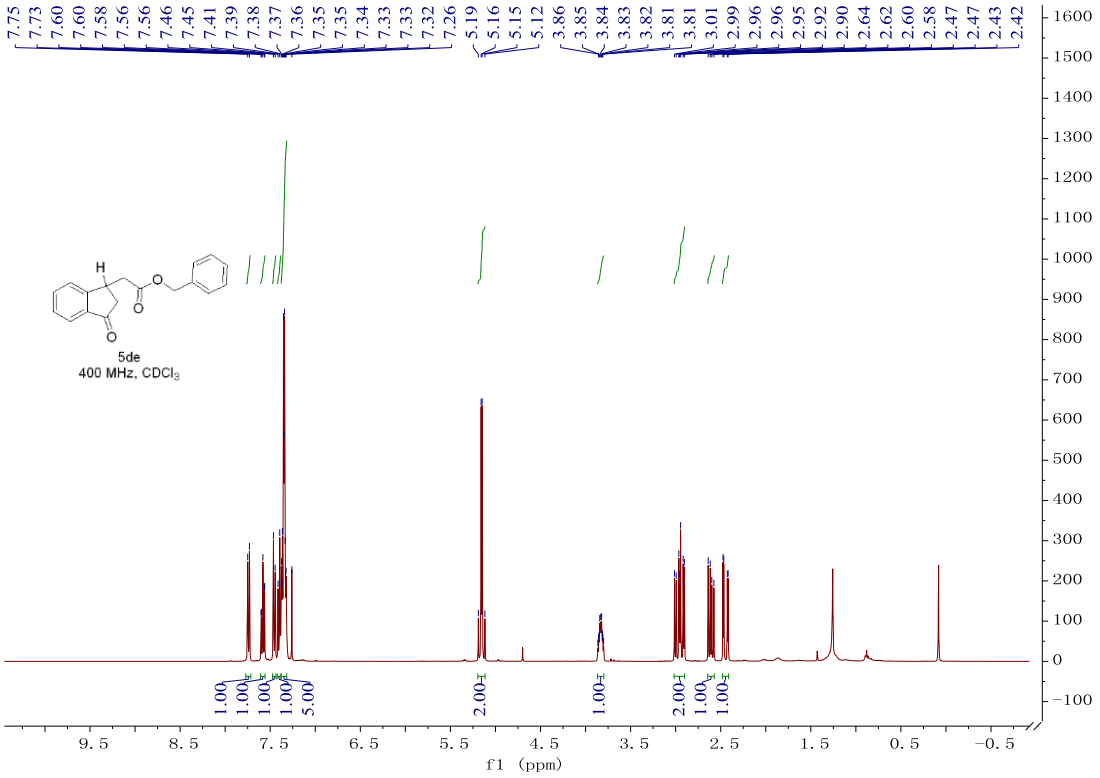
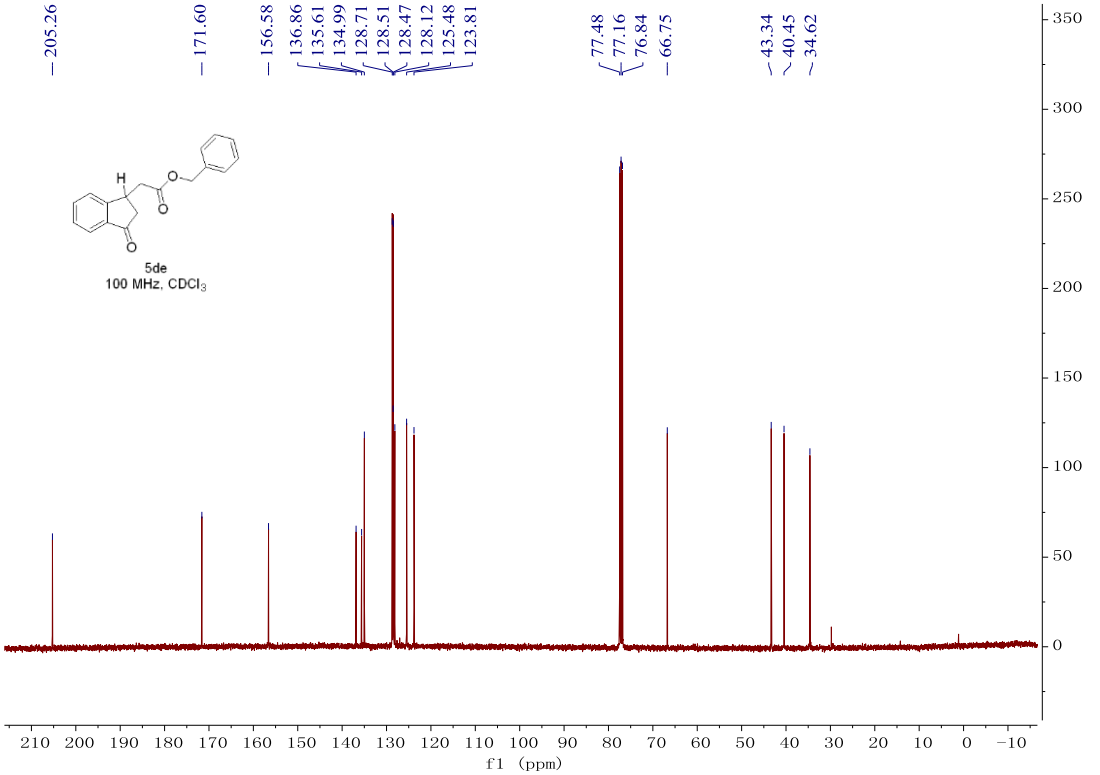
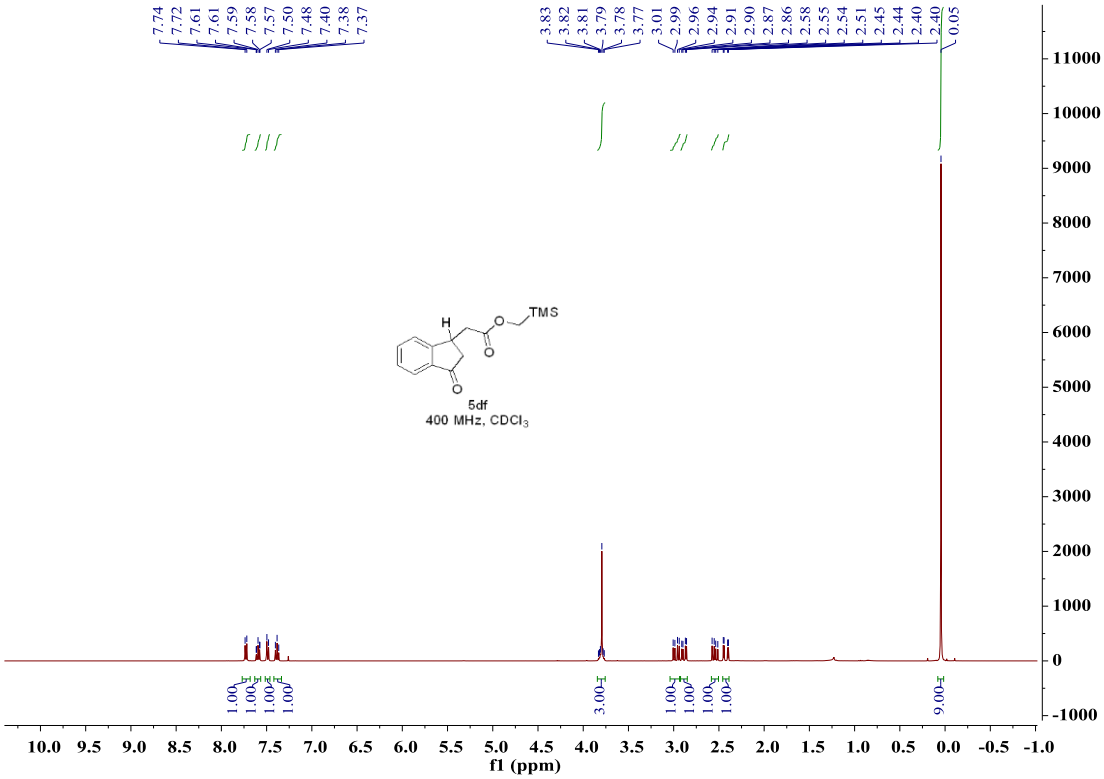
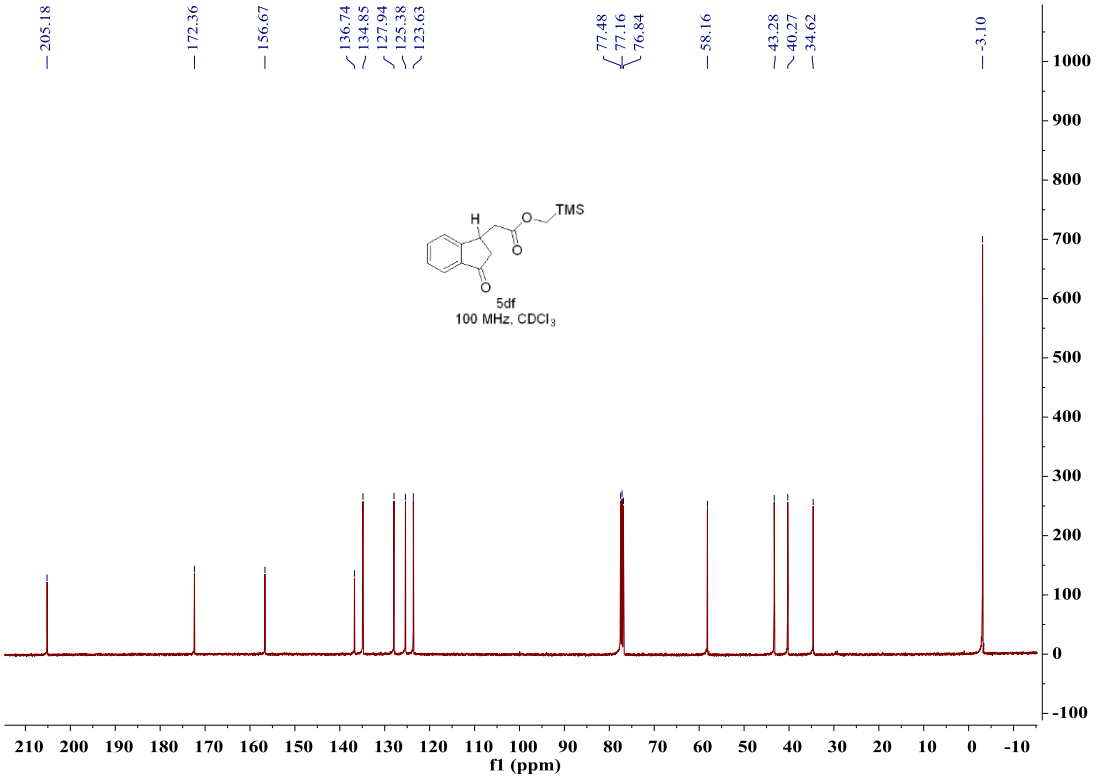
2.47
2.46
2.42
2.41
1.19
1.19
1.18
1.17
O^{i}Pr
H
O
O
5dd
400 MHz, CDCl$_3$
1.00
1.00
1.00
1.00
1.00
1.00
1.00
1.00
1.00
1.00
6.00
f1 (ppm)

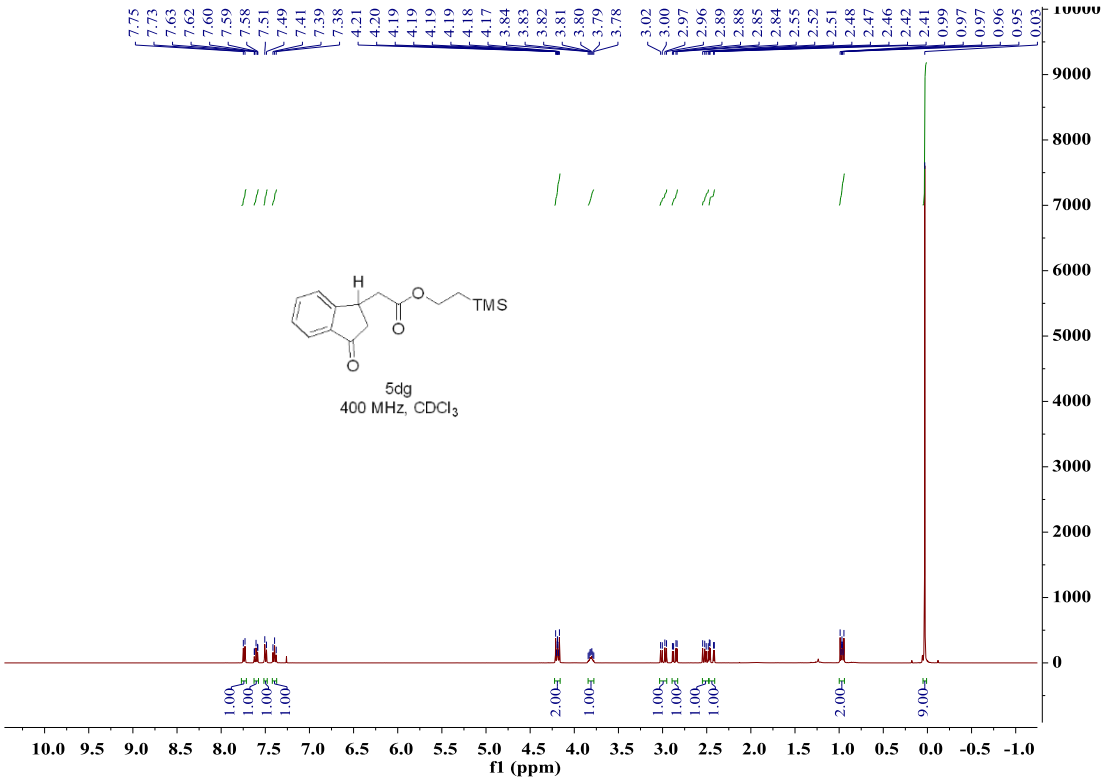

205.40
171.20
156.78
136.88
134.91
128.02
125.49
123.71
77.48
77.16
76.84
68.30
43.26
40.69
34.68
21.84
21.80
O^{i}Pr
H
O
O
5dd
100 MHz, CDCl$_3$
f1 (ppm)

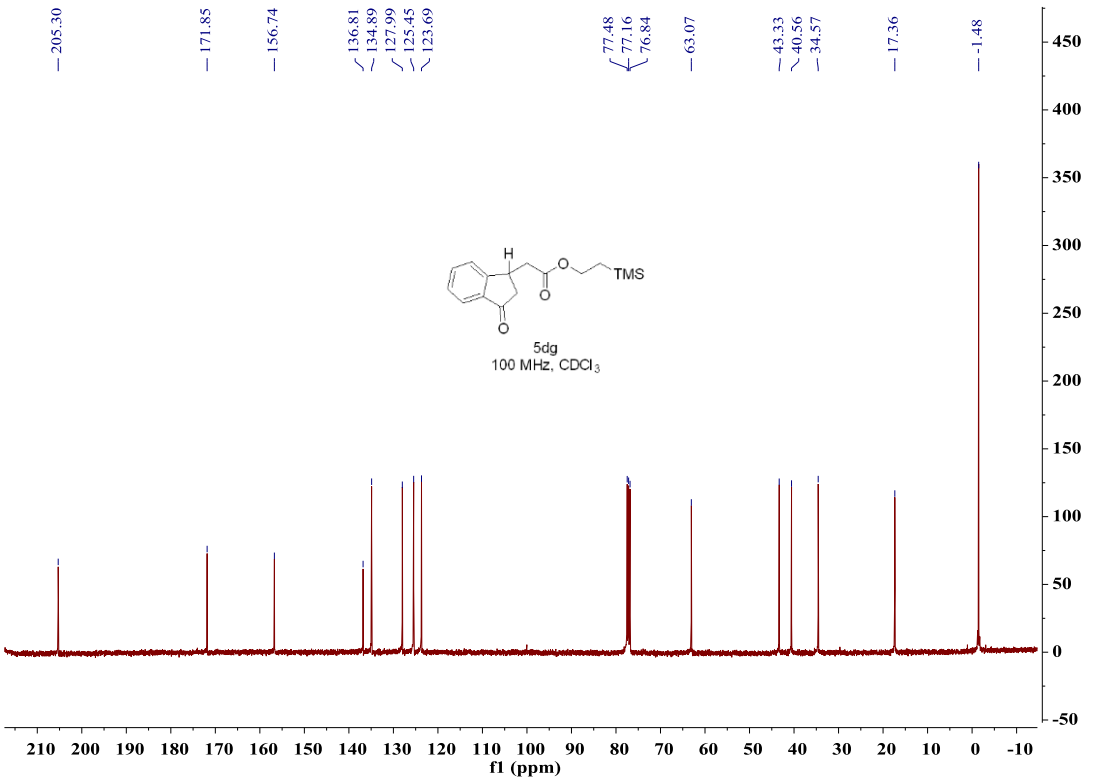

7.75 7.73 7.60 7.60 7.58 7.56 7.56 7.46 7.45 7.41 7.39 7.38 7.37 7.36 7.35 7.35 7.34 7.33 7.33 7.32 7.26 5.19 5.16 5.15 5.12 3.86 3.85 3.84 3.83 3.82 3.81 3.81 3.01 2.99 2.96 2.96 2.95 2.92 2.90 2.64 2.62 2.60 2.58 2.47 2.47 2.43 2.42
5de
400 MHz, CDCl3
1.00 1.00 1.00 1.00 5.00 2.00 1.00 2.00 1.00 1.00
f1 (ppm)


205.26 171.60 156.58 136.86 135.61 134.99 128.71 128.51 128.47 128.12 125.48 123.81 77.48 77.16 76.84 66.75 43.34 40.45 34.62
5de
100 MHz, CDCl3
f1 (ppm)


7.74
7.72
7.61
7.61
7.59
7.58
7.57
7.50
7.48
7.40
7.38
7.37
3.83
3.82
3.81
3.79
3.78
3.77
3.01
2.99
2.96
2.94
2.91
2.90
2.87
2.86
2.58
2.55
2.54
2.51
2.45
2.44
2.40
2.40
0.05
TMS
5df
400 MHz, CDCl3
1.00
1.00
1.00
1.00
3.00
1.00
1.00
1.00
1.00
9.00
f1 (ppm)


205.18
172.36
156.67
136.74
134.85
127.94
125.38
123.63
77.48
77.16
76.84
58.16
43.28
40.27
34.62
3.10
TMS
5df
100 MHz, CDCl3
f1 (ppm)


7.75 7.73 7.63 7.62 7.60 7.59 7.58 7.51 7.49 7.41 7.39 7.38 4.21 4.20 4.19 4.19 4.19 4.19 4.18 4.17 3.84 3.83 3.82 3.81 3.80 3.79 3.78 3.02 3.00 2.97 2.96 2.89 2.88 2.85 2.84 2.55 2.52 2.51 2.48 2.47 2.46 2.42 2.41 0.99 0.97 0.97 0.96 0.95 0.03
H
O
O
TMS
O
5dg
400 MHz, CDCl3
1.00 1.00 1.00 1.00 2.00 1.00 1.00 1.00 1.00 1.00 2.00 9.00
f1 (ppm)


205.30 171.85 156.74 136.81 134.89 127.99 125.45 123.69 77.48 77.16 76.84 63.07 43.33 40.56 34.57 17.36 -1.48
H
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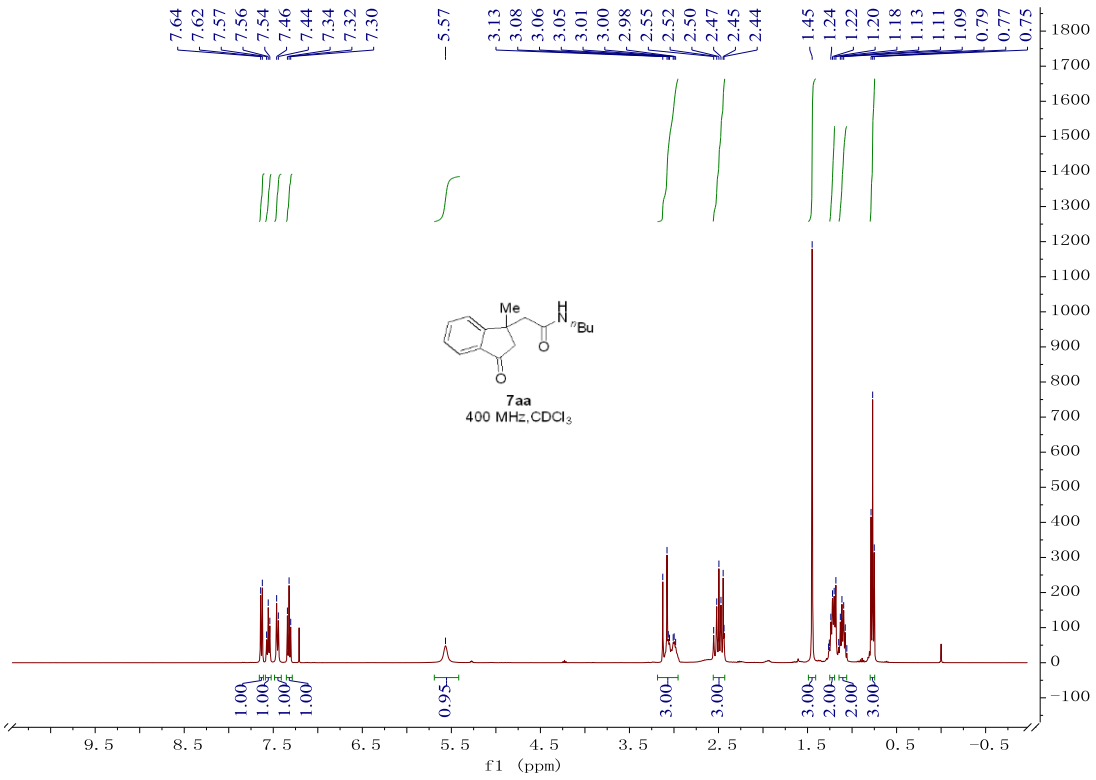
O
TMS
O
5dg
100 MHz, CDCl3
f1 (ppm)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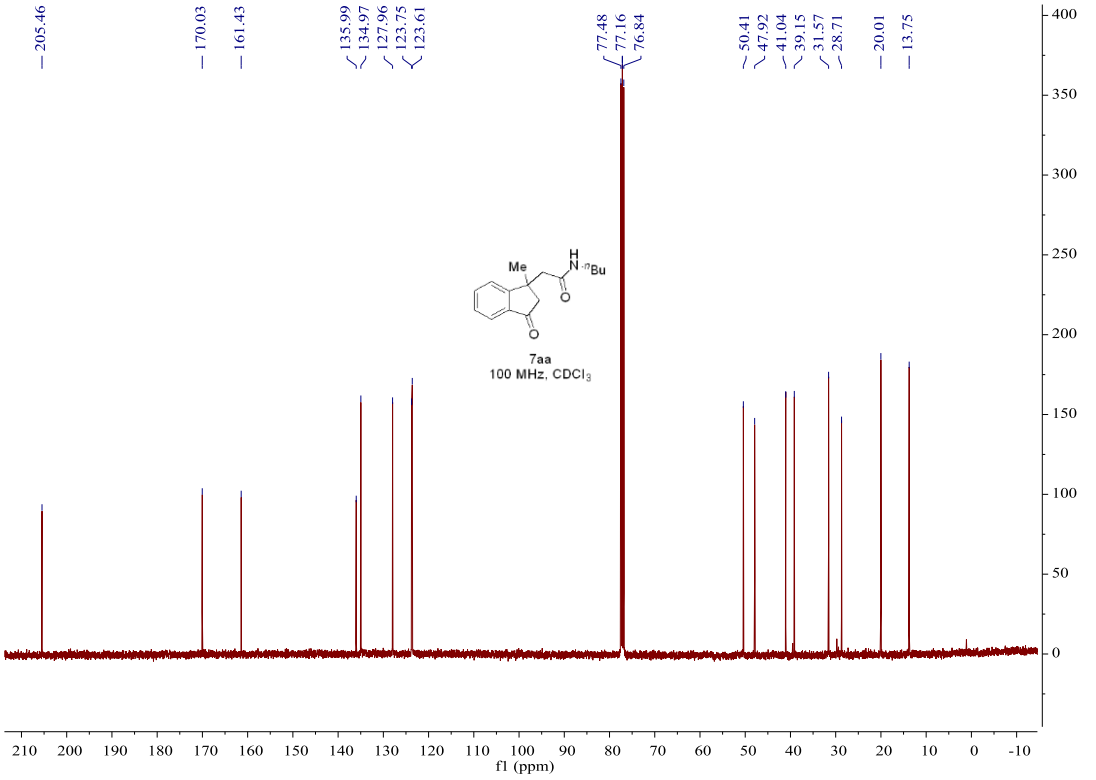
7.62
7.57
7.56
7.54
7.46
7.44
7.34
7.32
7.30
5.57
3.13
3.08
3.06
3.05
3.01
3.00
2.98
2.55
2.52
2.50
2.47
2.45
2.44
1.45
1.24
1.22
1.20
1.18
1.13
1.11
1.09
0.79
0.77
0.75
Me
H
N
nBu
O
O
7aa
400 MHz, CDCl3
1.00
1.00
1.00
1.00
0.95
3.00
3.00
3.00
2.00
2.00
3.00
f1 (ppm)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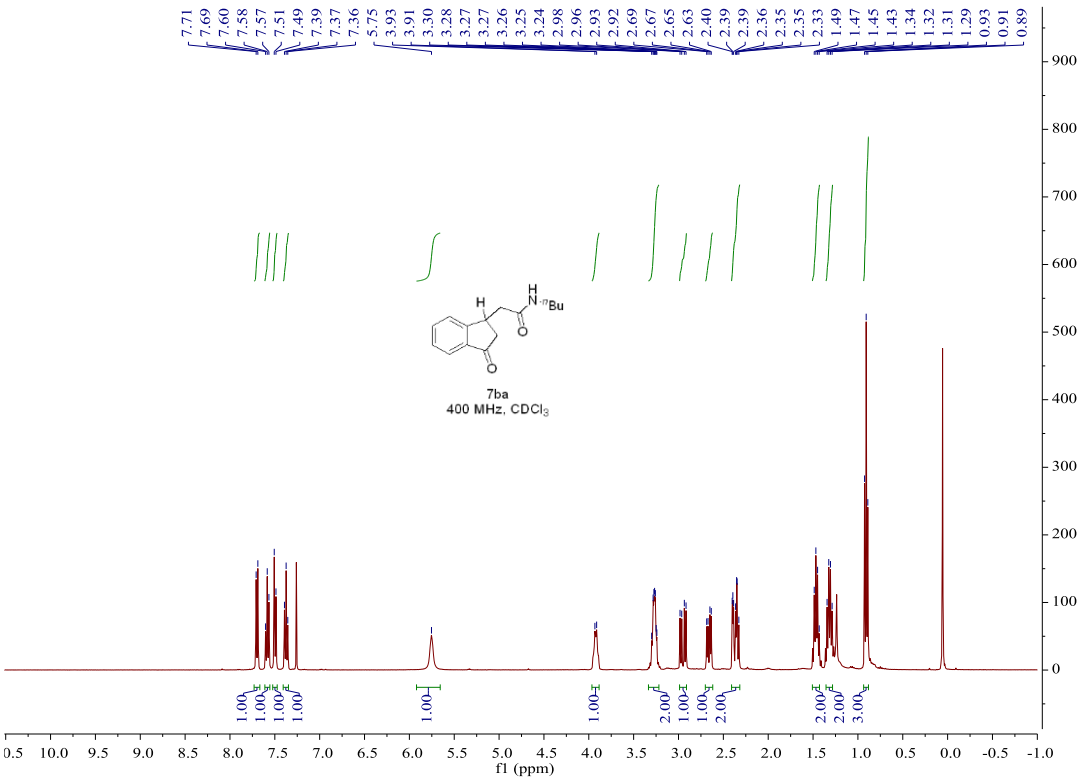
170.03
161.43
135.99
134.97
127.96
123.75
123.61
77.48
77.16
76.84
50.41
47.92
41.04
39.15
31.57
28.71
20.01
13.75
Me
H
N
nBu
O
O
7aa
100 MHz, CDCl3
f1 (ppm)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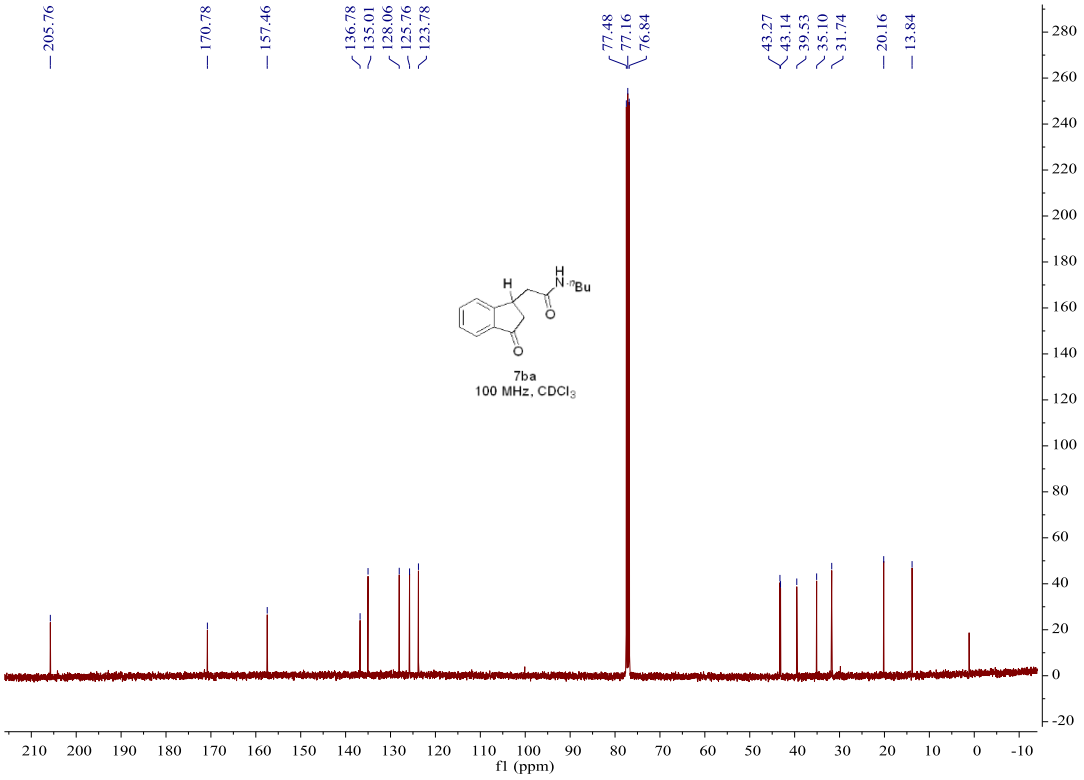
7.69
7.60
7.58
7.57
7.51
7.49
7.39
7.37
7.36
5.75
3.93
3.91
3.30
3.28
3.27
3.27
3.26
3.25
3.24
2.98
2.96
2.93
2.92
2.69
2.67
2.65
2.63
2.40
2.39
2.39
2.36
2.35
2.35
2.33
1.49
1.47
1.45
1.43
1.34
1.32
1.31
1.29
0.93
0.91
0.89
7ba
400 MHz, CDCl3
1.00
1.00
1.00
1.00
1.00
1.00
2.00
1.00
1.00
2.00
2.00
2.00
3.00
f1 (ppm)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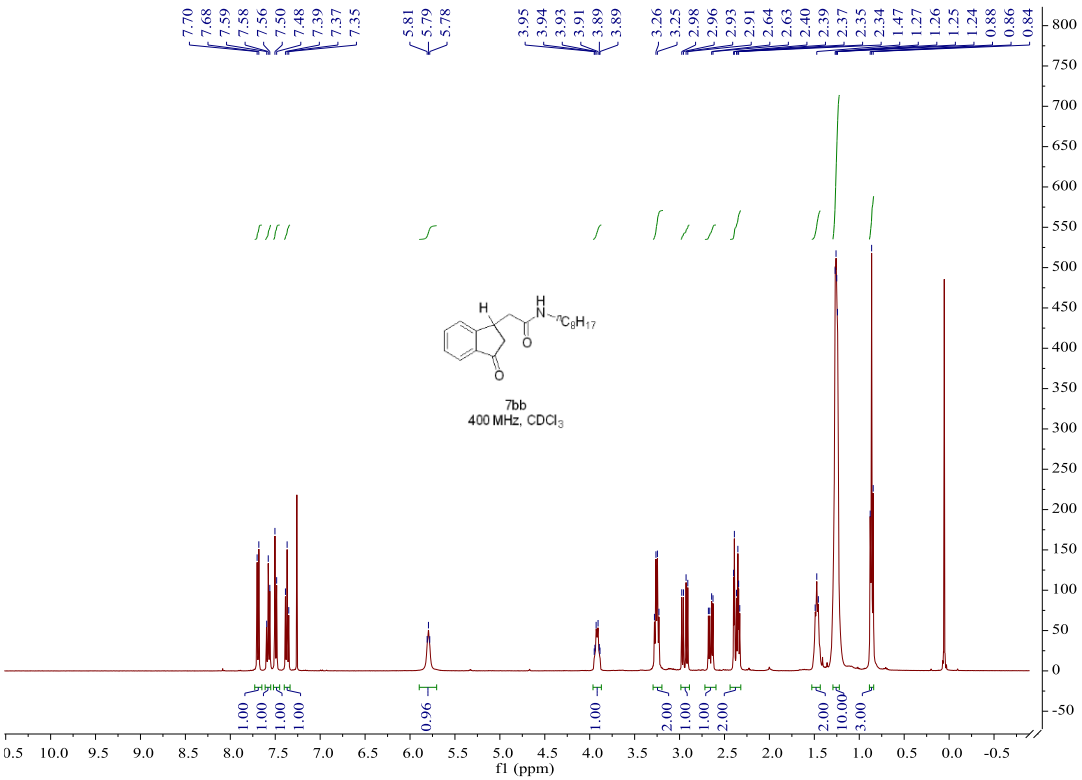
170.78
157.46
136.78
135.01
128.06
125.76
123.78
77.48
77.16
76.84
43.27
43.14
39.53
35.10
31.74
20.16
13.84
7ba
100 MHz, CDCl3
f1 (ppm)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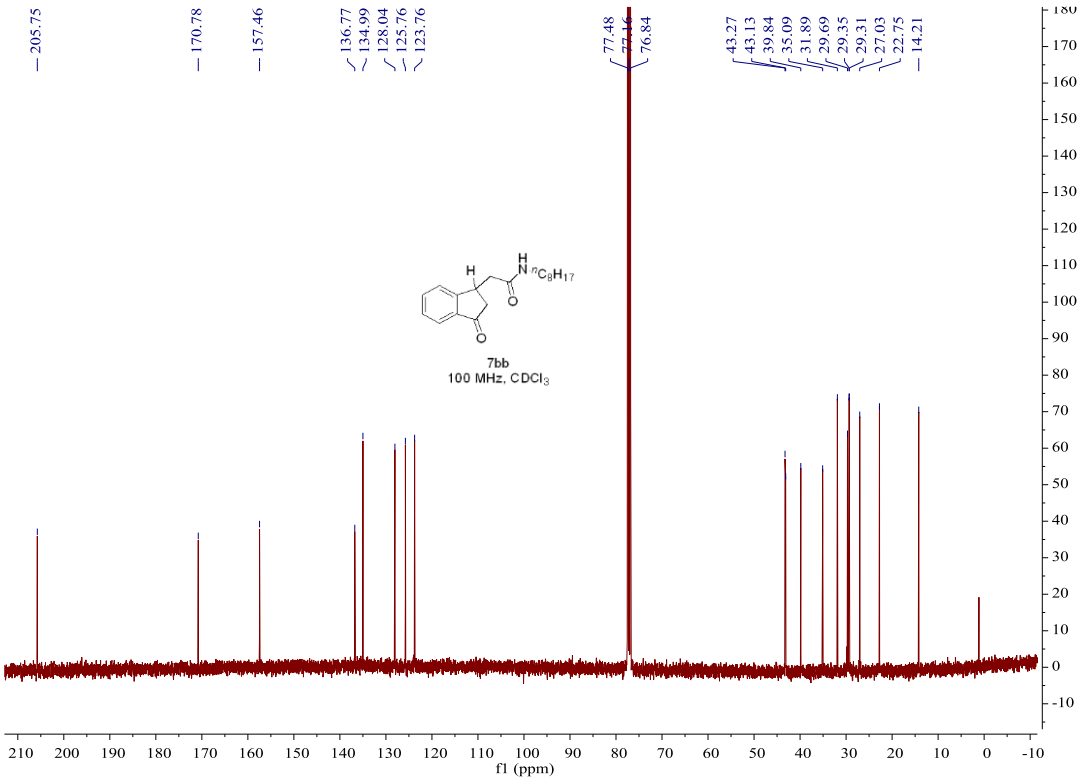
7.59
7.58
7.56
7.50
7.48
7.39
7.37
7.35
5.81
5.79
5.78
3.95
3.94
3.93
3.91
3.89
3.89
3.26
3.25
2.98
2.96
2.93
2.91
2.64
2.63
2.40
2.39
2.37
2.35
2.34
1.47
1.27
1.26
1.25
1.24
0.88
0.86
0.84
7bb
400 MHz, CDCl3
1.00
1.00
1.00
1.00
0.96
1.00
2.00
1.00
1.00
2.00
2.00
10.00
3.00
f1 (ppm)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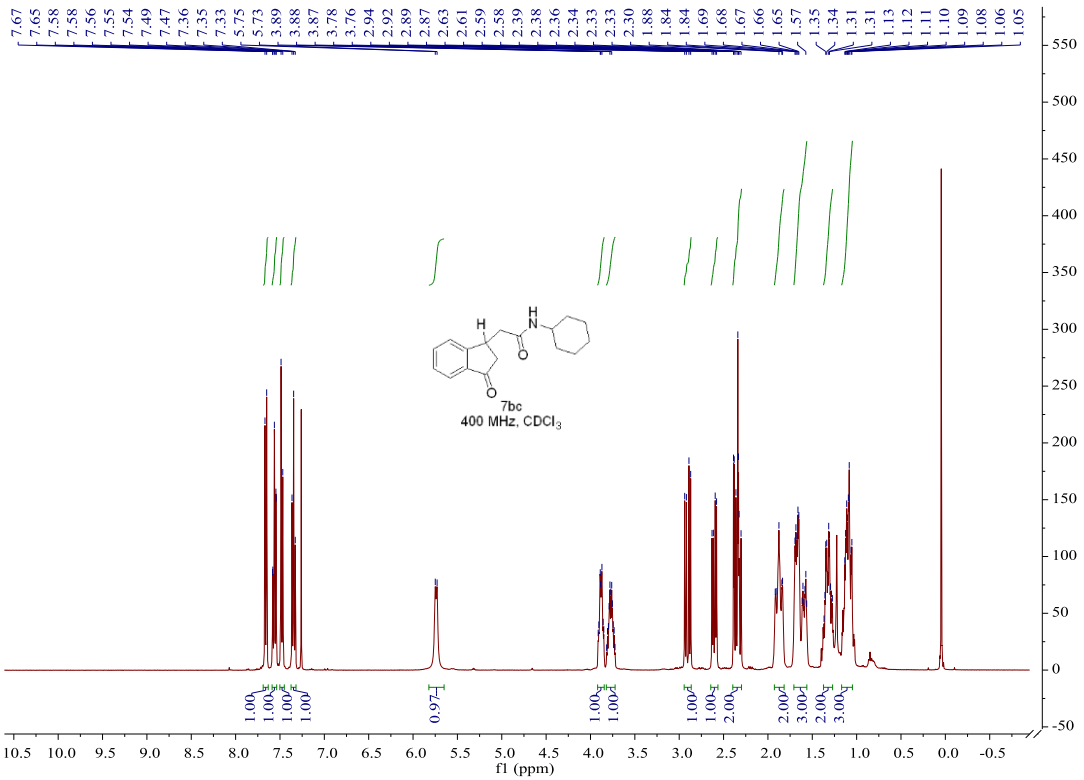
128.04
125.76
123.76
77.48
77.16
76.84
43.27
43.13
39.84
35.09
31.89
29.69
29.35
29.31
27.03
22.75
14.21
7bb
100 MHz, CDCl3
f1 (ppm)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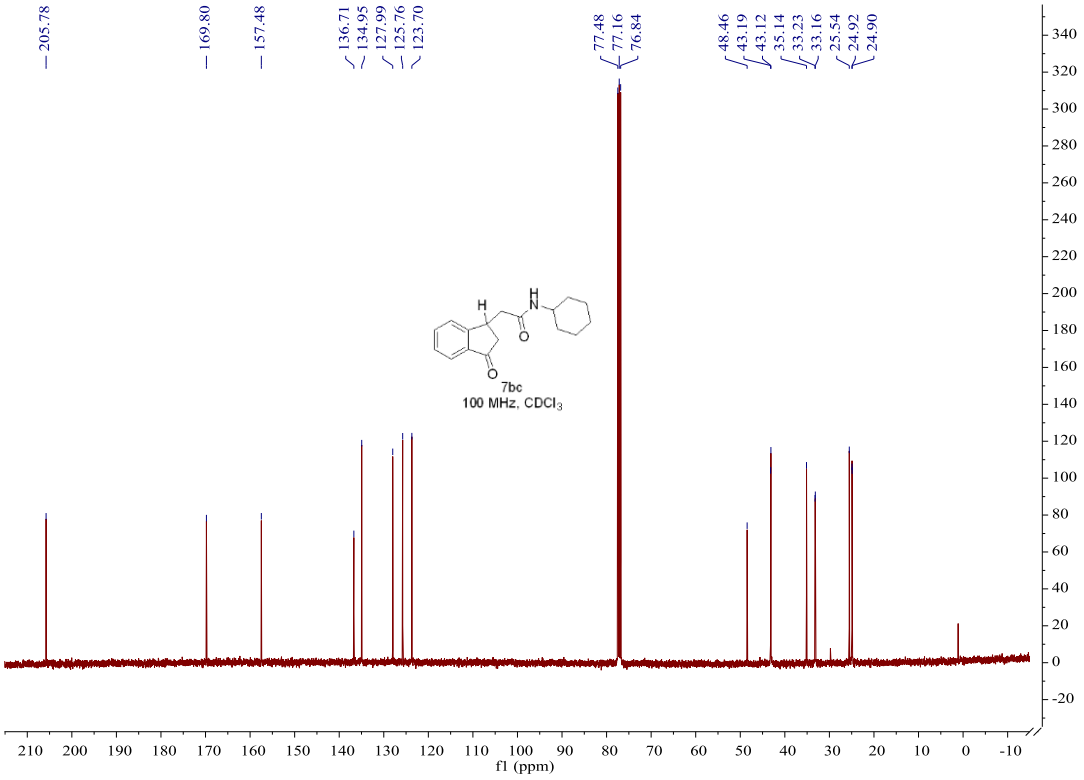
7.65
7.58
7.58
7.56
7.55
7.54
7.49
7.47
7.36
7.35
7.33
5.75
5.73
3.89
3.88
3.87
3.78
3.76
2.94
2.92
2.89
2.87
2.63
2.61
2.59
2.58
2.39
2.38
2.36
2.34
2.33
2.33
2.30
1.88
1.84
1.84
1.69
1.68
1.67
1.66
1.65
1.57
1.35
1.34
1.31
1.31
1.13
1.12
1.11
1.10
1.09
1.08
1.06
1.05
7bc
400 MHz, CDCl3
1.00
1.00
1.00
1.00
0.97
1.00
1.00
1.00
1.00
2.00
2.00
3.00
2.00
3.00
f1 (ppm)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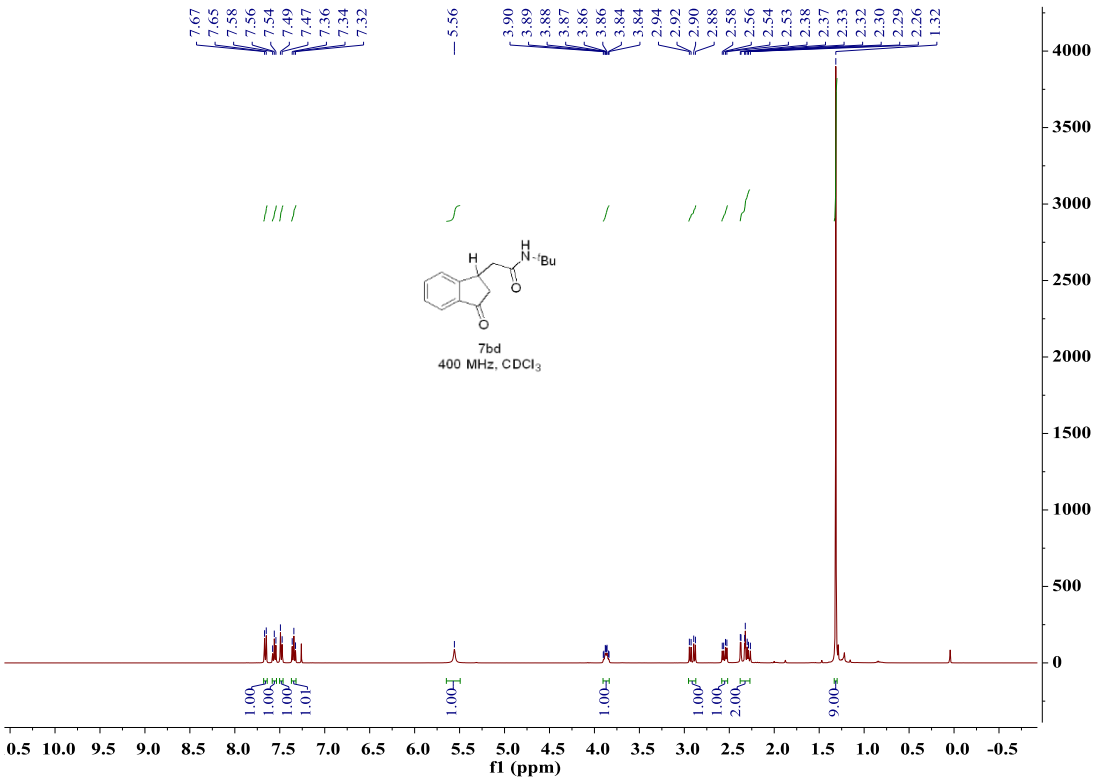
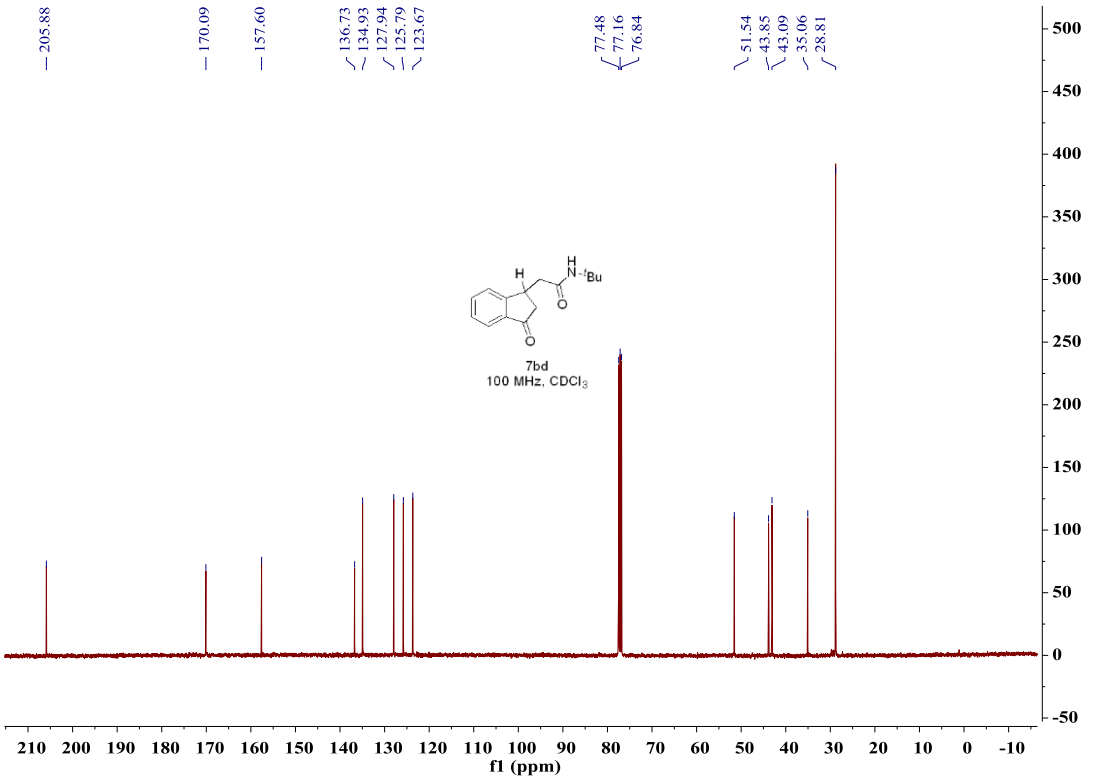
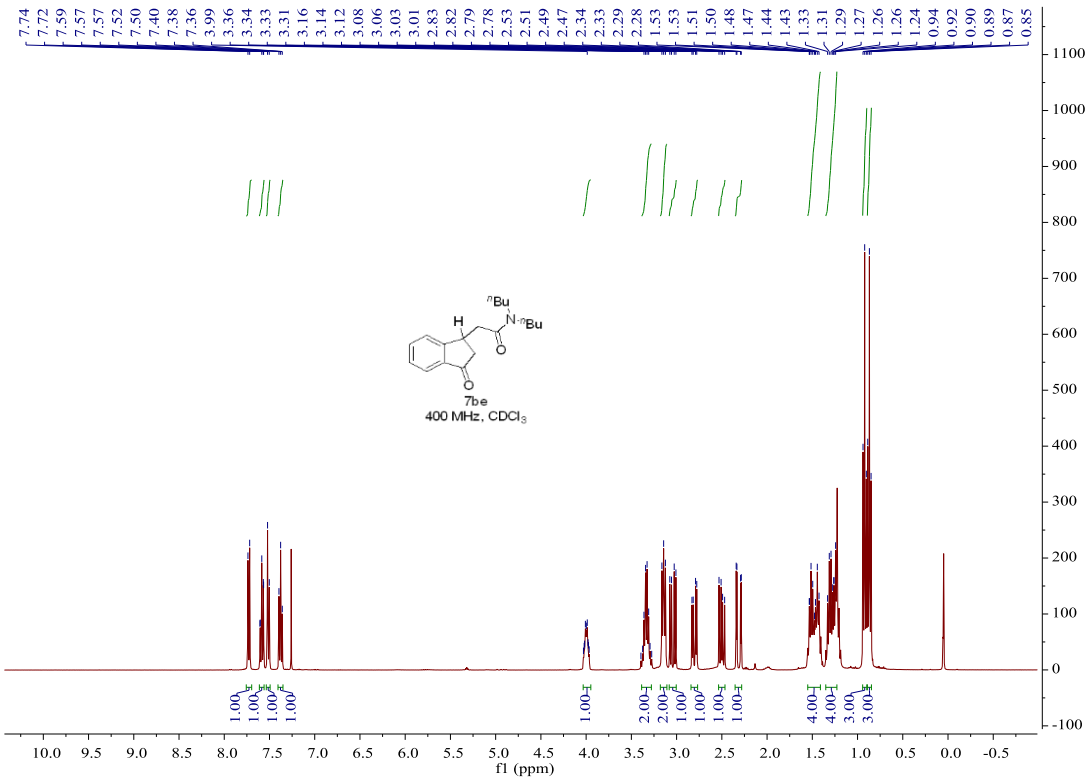
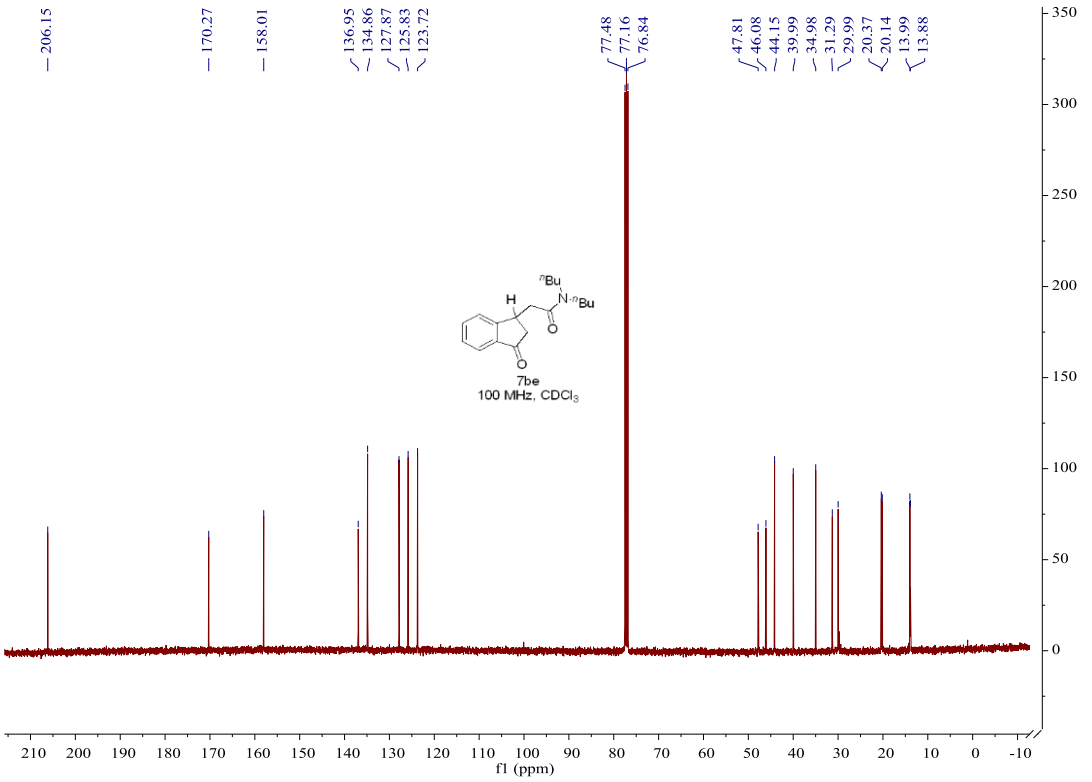
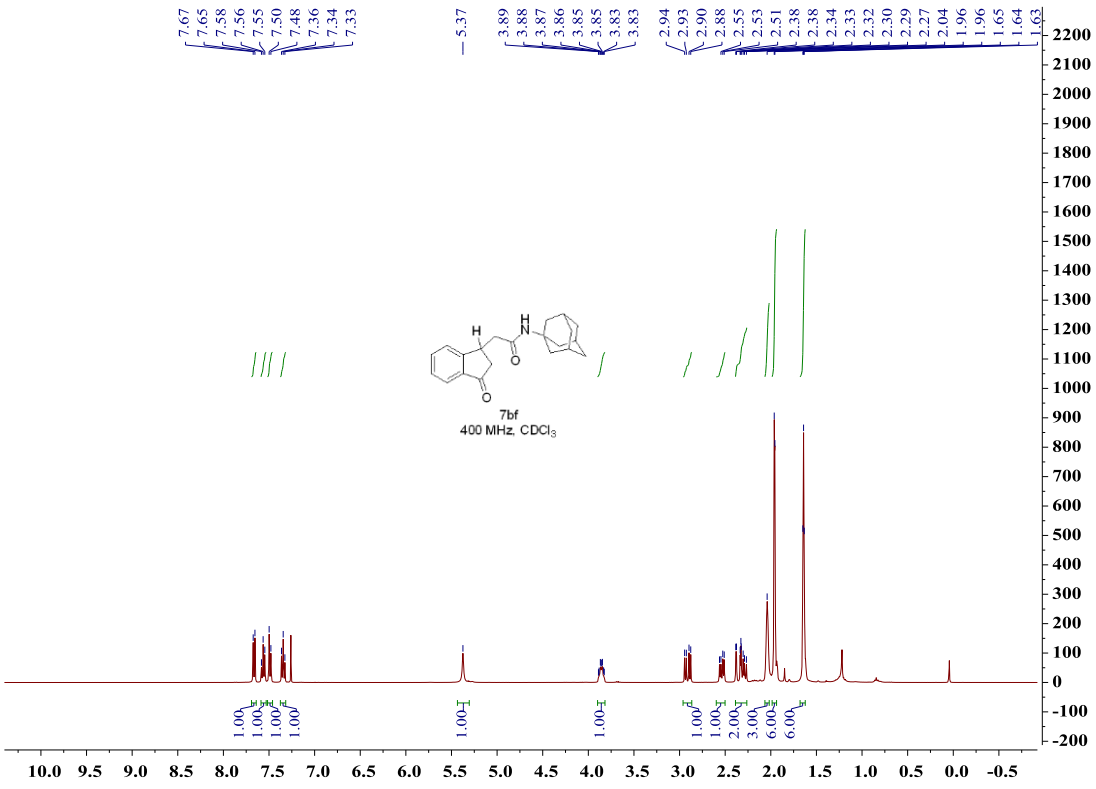
169.80
157.48
136.71
134.95
127.99
125.76
123.70
77.48
77.16
76.84
48.46
43.19
43.12
35.14
33.23
33.16
25.54
24.92
24.90
7bc
100 MHz, CDCl3
f1 (ppm)


7.67
7.65
7.58
7.56
7.54
7.49
7.47
7.36
7.34
7.32
5.56
3.90
3.89
3.88
3.87
3.86
3.86
3.84
3.84
2.94
2.92
2.90
2.88
2.58
2.56
2.54
2.53
2.38
2.37
2.33
2.32
2.30
2.29
2.26
1.32
7bd
400 MHz, CDCl3
1.00
1.00
1.00
1.01
1.00
1.00
1.00
1.00
2.00
9.00
f1 (ppm)


205.88
170.09
157.60
136.73
134.93
127.94
125.79
123.67
77.48
77.16
76.84
51.54
43.85
43.09
35.06
28.81
7bd
100 MHz, CDCl3
f1 (ppm)


7.74 7.72 7.59 7.57 7.57 7.52 7.50 7.40 7.38 7.36 3.99 3.36 3.34 3.33 3.31 3.16 3.14 3.12 3.08 3.06 3.03 3.01 2.83 2.82 2.79 2.78 2.53 2.51 2.49 2.47 2.34 2.33 2.29 2.28 1.53 1.53 1.51 1.50 1.48 1.47 1.44 1.43 1.33 1.31 1.29 1.27 1.26 1.26 1.24 0.94 0.92 0.90 0.89 0.87 0.85
nBu
H
N
nBu
O
O
7be
400 MHz, CDCl3
1.00 1.00 1.00 1.00 1.00 2.00 2.00 1.00 1.00 1.00 1.00 4.00 4.00 3.00 3.00
f1 (ppm)


206.15 170.27 158.01 136.95 134.86 127.87 125.83 123.72 77.48 77.16 76.84 47.81 46.08 44.15 39.99 34.98 31.29 29.99 20.37 20.14 13.99 13.88
nBu
H
N
nBu
O
O
7be
100 MHz, CDCl3
f1 (ppm)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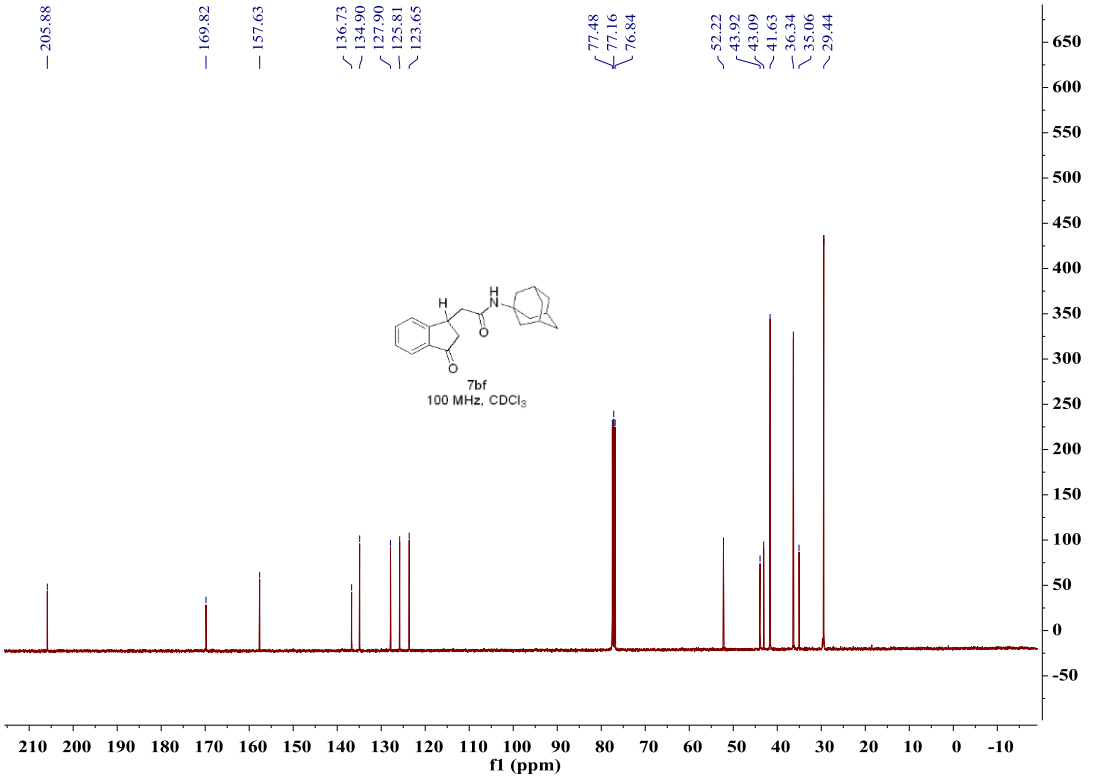
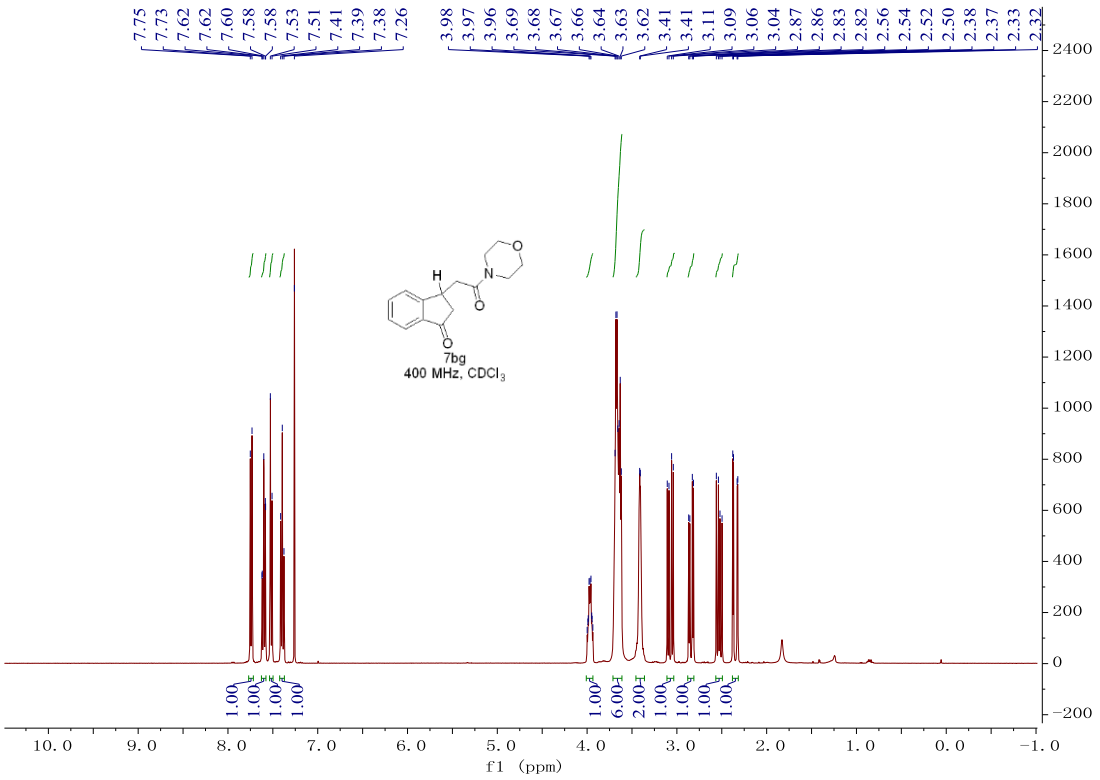
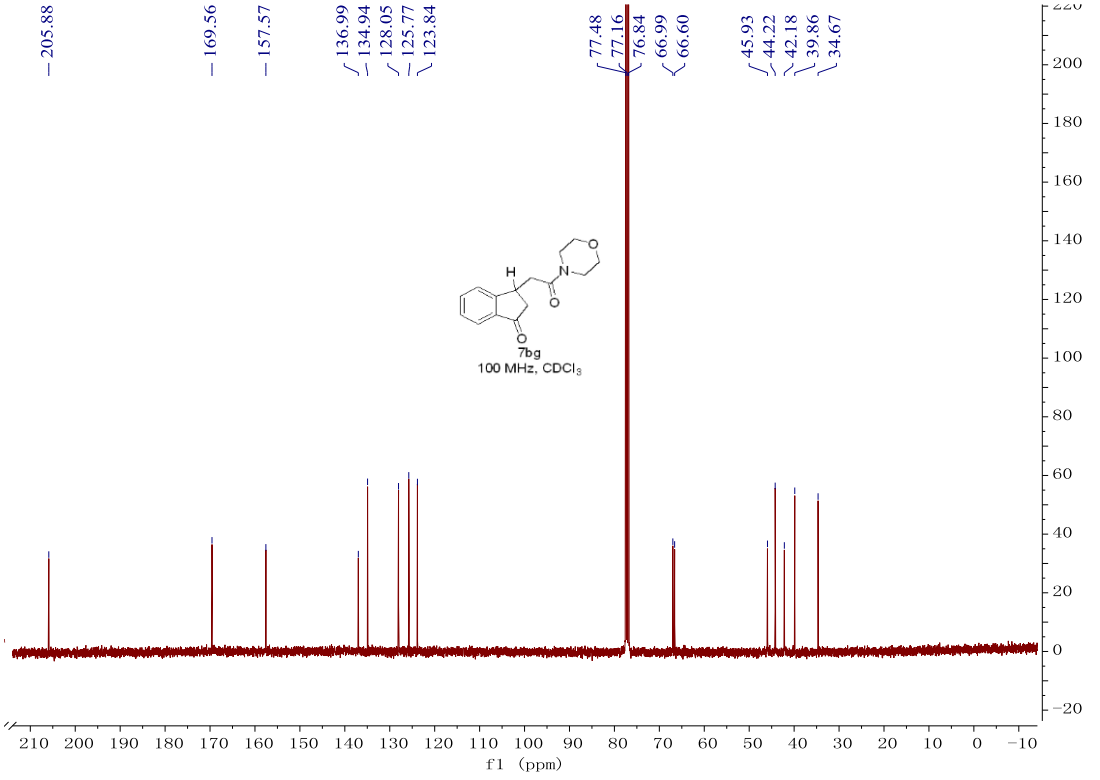
7.65
7.58
7.56
7.55
7.50
7.48
7.36
7.34
7.33
5.37
3.89
3.88
3.87
3.86
3.85
3.85
3.83
3.83
2.94
2.93
2.90
2.88
2.55
2.53
2.51
2.38
2.38
2.34
2.33
2.32
2.30
2.29
2.27
2.04
1.96
1.96
1.65
1.64
1.63
H
N
O
O
7bf
400 MHz, CDCl3
1.00
1.00
1.00
1.00
1.00
1.00
1.00
2.00
3.00
6.00
6.00
10.0 9.5 9.0 8.5 8.0 7.5 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 -0.5


205.88
169.82
157.63
136.73
134.90
127.90
125.81
123.65
77.48
77.16
76.84
52.22
43.92
43.09
41.63
36.34
35.06
29.44
H
N
O
O
7bf
100 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.75
7.73
7.62
7.62
7.60
7.58
7.58
7.53
7.51
7.41
7.39
7.38
7.26
3.98
3.97
3.96
3.69
3.68
3.67
3.66
3.64
3.63
3.62
3.41
3.41
3.11
3.09
3.06
3.04
2.87
2.86
2.83
2.82
2.56
2.54
2.52
2.50
2.38
2.37
2.33
2.32
7bg
400 MHz, CDCl3
1.00
1.00
1.00
1.00
1.00
6.00
2.00
1.00
1.00
1.00
1.00
f1 (ppm)


205.88
169.56
157.57
136.99
134.94
128.05
125.77
123.84
77.48
77.16
76.84
66.99
66.60
45.93
44.22
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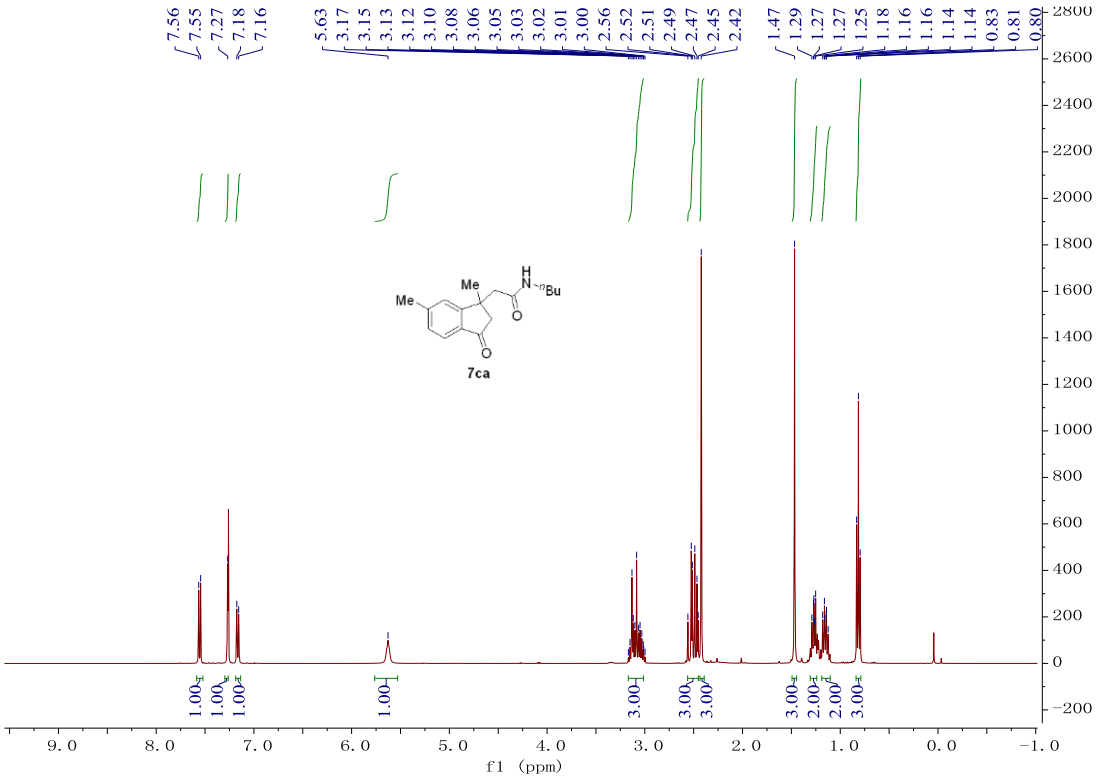
39.86
34.67
7bg
100 MHz, CDCl3
f1 (ppm)


7.56
7.55
7.27
7.18
7.16
5.63
3.17
3.15
3.13
3.12
3.10
3.08
3.06
3.05
3.03
3.02
3.01
3.00
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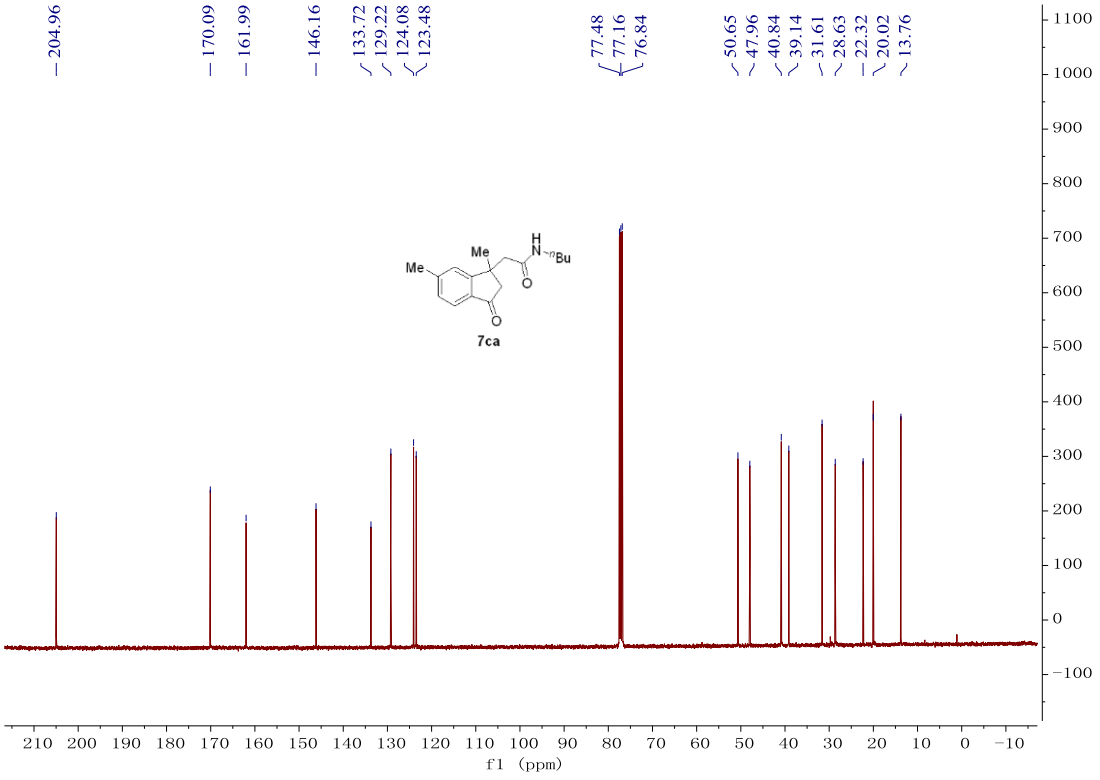
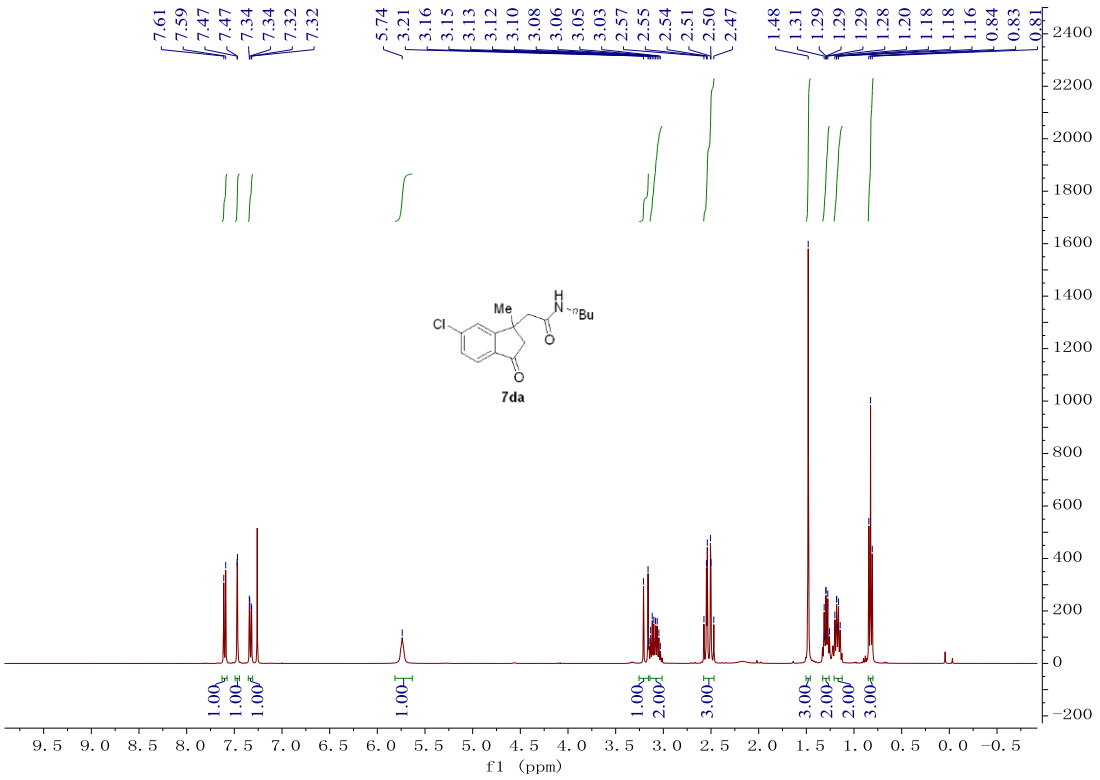
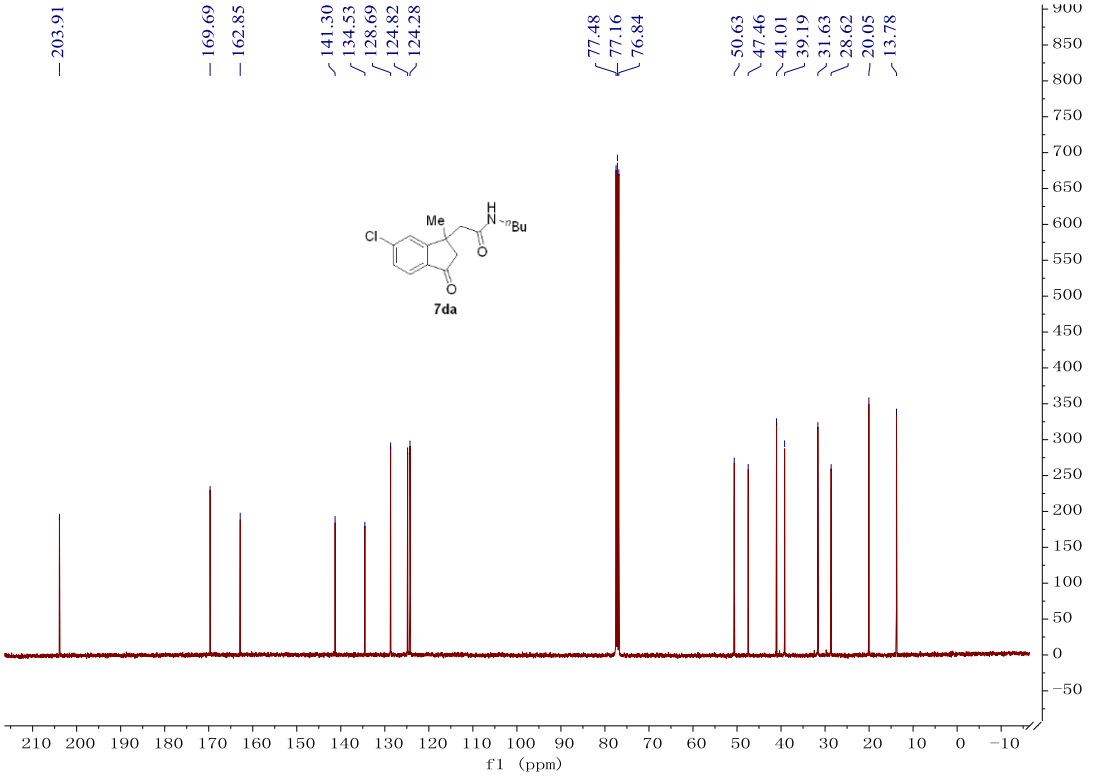
2.51
2.49
2.47
2.45
2.42
1.47
1.29
1.27
1.27
1.25
1.18
1.16
1.16
1.14
1.14
0.83
0.81
0.80
Me
Me
H
N
nBu
O
O
7ca
1.00
1.00
1.00
1.00
3.00
3.00
3.00
3.00
2.00
2.00
3.00
f1 (ppm)


204.96
170.09
161.99
146.16
133.72
129.22
124.08
123.48
77.48
77.16
76.84
50.65
47.96
40.84
39.14
31.61
28.63
22.32
20.02
13.76
Me
Me
H
N
nBu
O
O
7ca
f1 (ppm)


7.61
7.59
7.47
7.47
7.34
7.34
7.32
7.32
5.74
3.21
3.16
3.15
3.13
3.12
3.10
3.08
3.06
3.05
3.03
2.57
2.55
2.54
2.51
2.50
2.47
1.48
1.31
1.29
1.29
1.29
1.28
1.20
1.18
1.18
1.16
0.84
0.83
0.81
Me
Cl
H
N
nBu
O
O
7da
1.00
1.00
1.00
1.00
1.00
2.00
3.00
3.00
2.00
2.00
3.00
f1 (ppm)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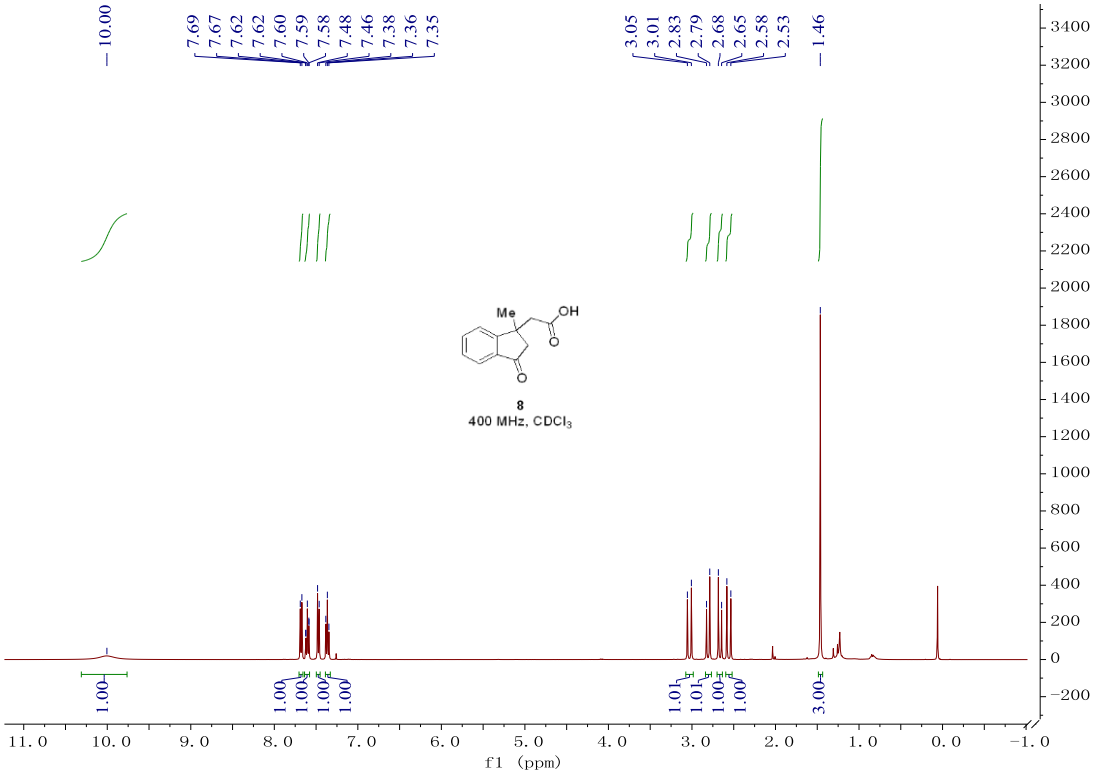
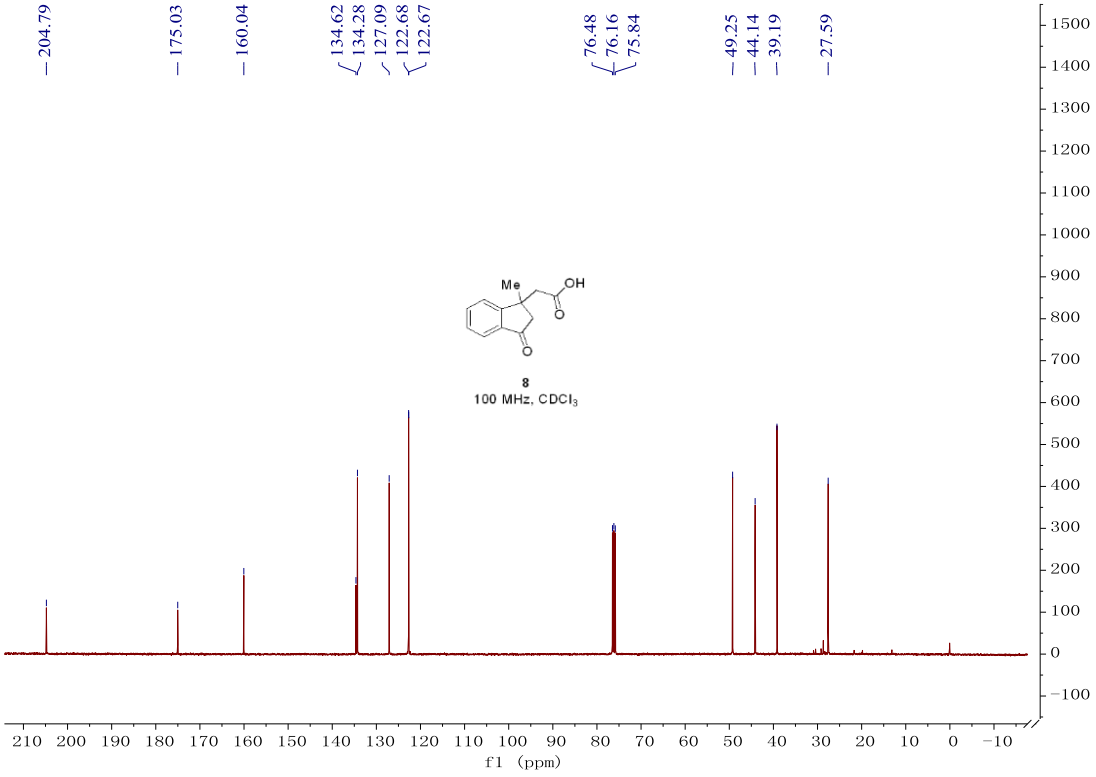
169.69
162.85
141.30
134.53
128.69
124.82
124.28
77.48
77.16
76.84
50.63
47.46
41.01
39.19
31.63
28.62
20.05
13.78
Me
Cl
H
N
nBu
O
O
7da
f1 (ppm)


10.00
7.69
7.67
7.62
7.62
7.60
7.59
7.58
7.48
7.46
7.38
7.36
7.35
3.05
3.01
2.83
2.79
2.68
2.65
2.58
2.53
1.46
Me
OH
O
O
8
400 MHz, CDCl3
1.00
1.00
1.00
1.00
1.01
1.01
1.00
1.00
3.00
f1 (ppm)


204.79
175.03
160.04
134.62
134.28
127.09
122.68
122.67
76.48
76.16
75.84
49.25
44.14
39.19
27.59
Me
OH
O
O
8
100 MHz, CDCl3
f1 (ppm)

Crystallographic data for 7bf (CCDC 2061060)

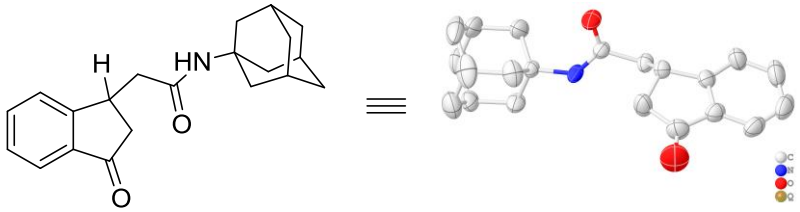


Table 1 Crystal data and structure refinement for mo210106a.

Identification code	mo210106a
Empirical formula	C21H25NO2
Formula weight	323.42
Temperature/K	294.55
Crystal system	monoclinic
Space group	Cc
a/Å	15.542(3)
b/Å	11.666(3)
c/Å	20.268(4)
α/°	90
β/°	107.742(7)
γ/°	90
Volume/Å3	3500.3(13)
Z	8
ρcalcg/cm3	1.227
μ/mm 1	0.078
F(000)	1392.0
Crystal size/mm3	0.15 × 0.15 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.22 to 61.106
Index ranges	-20 ≤ h ≤ 21, -16 ≤ k ≤ 16, -26 ≤ l ≤ 27
Reflections collected	16760
Independent reflections	8300 [Rint = 0.0406, Rsigma = 0.0617]
Data/restraints/parameters	8300/2/433
Goodness-of-fit on F2	1.013
Final R indexes [I>=2σ (I)]	R1 = 0.0515, wR2 = 0.1012
Final R indexes [all data]	R1 = 0.1013, wR2 = 0.1224
Largest diff. peak/hole / e Å-3	0.15/-0.17
Flack parameter	-0.3(9)