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Electronic Supplementary Information

Study on the ArI-catalyzed Intramolecular Oxy-Cyclization of 2-Alkenylbenzamides to Benzoiminolactones

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Contents

General information

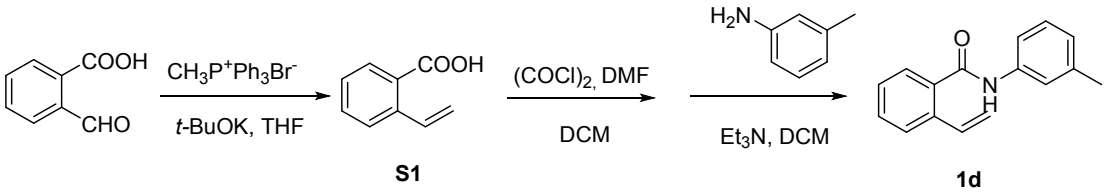
All commercially available reagents and solvents, unless otherwise notes, were used without further purification. Thin layer chromatography (TLC) was used to monitor reaction progress performed on GF-254 silica gel plates (0.2 mm). Flash column chromatography (200-300 mesh silica gel purchased from Yantai, China and 200-300 mesh Alumina-B purchased from Greagent) eluted with the gradient of petroleum ether (PE) and ethyl acetate (EtOAc) was used to isolate and purify products. Nuclear magnetic resonance (NMR) spectra were recorded on Bruker ADVANCE III 400 MHz (or Bruker ADVANCE III 600 MHz) using $CDCl_3$ as solvent ($CDCl_3$, δ = 7.26 ppm for ^1H NMR, δ = 77.0 ppm for ^{13}C NMR). ^1H NMR experiments used CD_3CN as solvent (CD_3CN, δ = 1.94 ppm). Chemical shift are presented as: multiplicities (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad). Coupling constant (Hz) were given as a *J* value. MS was recorded on Agilent 6260C Liquid Chromatograph Mass Spectrometer. HRMS was performed on Waters I-Class VION IMS Q-Tof Mass Spectrometer of Instrument Analysis Center of Xi'an Jiaotong University.

1. Synthesis of iodine reagents and substrates

Iodine reagents **I1-I6**, **PIDA** were all commercially available. **I7**,[1] **I8**[1] and **I6(OAc)$_2$**[2] are known compounds and were synthesized according to the methods of reported literature. Substrates **1a-1r**,[3] **1s-1ab**,[3,4] **1ac-1ag**,[3,5] **1ah**,[3] **1ai-1aj**[3,6] and **1ak**[3,7] were synthesized according to the methods of reported literature and typical procedures for their synthesis were described below. Among them, **1d**, **1i**, **1j**, **1q** and **1v-1ab** are new compounds and were characterized by ^{1}H NMR, ^{13}C NMR and HRMS.

2.1 Typical procedures for the synthesis of substrates 1a-1r, 1ah-1ak

Take the synthesis of **1d** as an example.



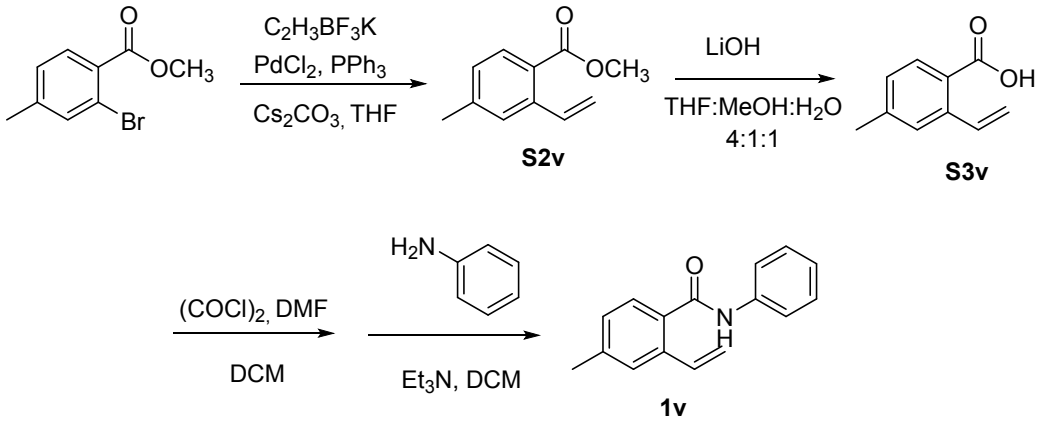
A 250 mL three necked bottle charged with methyl triphenylphosphonium bromide (7.2 g, 20.0 mmol) and *t*-BuOK (3.4 g, 30.0 mmol) was added anhydrous THF (50.0 mL) under argon protection and stirred. After 1 h, a solution of 2-carboxybenzaldehyde (1.5 g, 10.0 mmol) in dry THF (10.0 mL) was added through syringe and refluxed overnight. The reaction solution was detected by TLC until completely finished. After cooling down, the mixture quenched with saturated NH_4Cl solution (20 mL), extracted with EtOAc (30 mL × 3), the organic layer was separated and concentrated *in vacuo*. The residue was purified by flash chromatography on silica gel (PE:EtOAc = 5:1) to give the compound **S1** (1.3 g, 89%) as a white solid.

To a stirring solution of **S1** (740 mg, 5 mmol) in dry DCM (10 mL) was added $(COCl)_2$ (2.1 mL, 25 mmol) and a drop of DMF. The resulting mixture was stirred for 1 h. Then, the above mixture was slowly added to a solution of *m*-toluidine (642 mg, 6 mmol) and Et_3N (1.4 mL, 10 mmol) in DCM (10 mL) through syringe at 0 ^{o}C. After been stirred at room temperature for 3 h, the reaction mixture was quenched with H_2O (20 mL) and aqueous solution was acidified to pH = 1 with 2 N HCl solution. The

organic layer was separated and the aqueous layer was extracted with DCM (20 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by flash column chromatography on silica gel (PE:EtOAc = 5:1) to afford desired product **1d** (749 mg, 79%) as a white solid.

2.2 Typical procedures for the synthesis of substrates 1s-1ab

Take the synthesis of **1v** as an example.



A 250 mL three necked bottle was charged with methyl 2-bromo-4-methylbenzoate (1.1 g, 5 mmol), cesium carbonate (4.6 g, 7.0 mmol), triphenylphosphine (136 mg, 5.2 mmol), potassium vinyltrifluoroborate (700 mg, 5.2 mmol), palladium (II) chloride (36 mg 1 mmol), THF (18 mL) and degassed water (2 mL). The reaction mixture was stirred at 70 °C under argon protection for 40 h, which was detected by TLC until completely finished. After cooling down, the reaction mixture was diluted with DCM (50 mL) and filtered over celite. The organic layer was separated and concentrated *in vacuo*. The residue was purified by flash chromatography on silica gel (PE:EtOAc = 8:1) to give the compound **S2v** (730 mg, 86%) as a colorless oil.

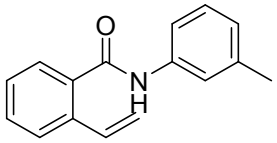
To a solution of **S2v** (730 mg, 4.1 mmol) in a mixed solvent (30 mL, THF: MeOH: H_2O = 4:1:1) was added lithium hydroxide (196 mg, 8.2 mmol). The reaction mixture was heated at 70 ºC for 5 h, which was detected by TLC until completely finished. After cooling down, the reaction mixture was concentrated *in vacuo* to remove THF and then adjusted to pH = 1 using 2 N HCl solution. The mixture was extracted with

DCM (20 mL × 2). The combined organic layer was dried over Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by flash column chromatography on silica gel (PE:EtOAc = 5:1-3:1) to yield the compound **S3v** (680 mg, 99%) as a white solid.

To a stirring solution of **S3v** (650 mg, 4 mmol) in dry DCM (10 mL) was added $(COCl)_2$ (2.1 mL, 25 mmol) and a drop of DMF. The resulting mixture was stirred for 1 h. Then, the above mixture was slowly added to a solution of aniline (558 mg, 6 mmol) and Et_3N (1.4 mL, 10 mmol) in DCM (10 mL) through syringe at 0 °C. After been stirred at room temperature for 3 h, the reaction mixture was quenched with H_2O (20 mL) and aqueous solution was acidified to pH = 1 with 2 N HCl solution. The organic layer was separated and the aqueous layer was extracted with DCM (20 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by flash column chromatography on silica gel (PE:EtOAc = 5:1) to afford desired product **1v** (635 mg, 67%) as a white solid.

2.3 Characterization data of the new substrates

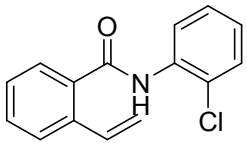
***N*-(*m*-tolyl)-2-vinylbenzamide (1d):**



1d

White solid (749 mg, 79%); m.p. 117.9–118.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (t, *J* = 8.0 Hz, 2H), 7.52-7.41 (m, 3H), 7.36 (q, *J* = 7.6, 7.2 Hz, 2H), 7.25 (t, *J* = 8.0 Hz, 1H), 7.11 (dd, *J* = 17.6, 11.2 Hz, 1H), 6.98 (d, *J* = 7.6 Hz, 1H), 5.77 (dd, *J* = 17.6, 1.2 Hz, 1H), 5.40 (dd, *J* = 11.2, 1.2 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 139.1, 137.8, 136.0, 135.4, 134.5, 130.6, 128.9, 127.9, 127.6, 126.6, 125.5, 120.4, 117.3, 116.7, 21.5; HRMS: $[M+H]^+$ calcd for $C_{16}H_{15}NO$ 238.1226, found 238.1224.

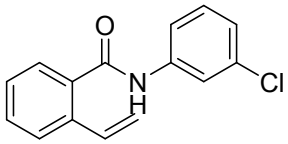
***N*-(2-chlorophenyl)-2-vinylbenzamide (1i)**:



1i

White solid (874 mg, 85%); m.p. 114.5–115.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (d, *J* = 8.4 Hz, 1H), 8.07 (s, 1H), 7.64 (t, *J* = 8.0 Hz, 2H), 7.52 – 7.46 (m, 1H), 7.45 – 7.37 (m, 2H), 7.37 – 7.29 (m, 1H), 7.17 (dd, *J* = 17.6, 11.2 Hz, 1H), 7.13 – 7.03 (m, 1H), 5.79 (dd, *J* = 17.6, 1.2 Hz, 1H), 5.43 (dd, *J* = 10.8, 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.2, 136.5, 134.8, 134.7, 134.4, 131.0, 129.1, 128.0, 127.8, 127.7, 126.9, 124.9, 123.1, 121.6, 117.8; HRMS: $[M+H]^+$ calcd for $C_{15}H_{12}ClNO$ 258.0680, found 258.0680.

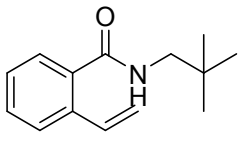
***N*-(3-chlorophenyl)-2-vinylbenzamide (1j)**:



1j

White solid (894 mg, 87%); m.p. 113.3–115.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (t, *J* = 2.0 Hz, 1H), 7.69 (s, 1H), 7.61 – 7.48 (m, 2H), 7.48 – 7.38 (m, 2H), 7.36 – 7.20 (m, 2H), 7.15 – 6.98 (m, 2H), 5.75 (dd, *J* = 17.6, 1.2 Hz, 1H), 5.39 (dd, *J* = 11.2, 1.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.7, 139.1, 136.0, 134.7, 134.7, 134.2, 130.8, 130.0, 127.8, 127.5, 126.6, 124.6, 120.0, 118.0, 117.4; HRMS: $[M+H]^+$ calcd for $C_{15}H_{12}ClNO$ 258.0680, found 258.0680.

***N*-neopentyl-2-vinylbenzamide (1q)**:

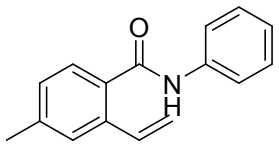


1q

White solid (739 mg, 91%); m.p. 110.2–112.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.0 Hz, 1H), 7.48 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.44 – 7.37 (m, 1H), 7.35 – 7.28 (m, 1H), 7.07 (dd, *J* = 17.6, 11.2 Hz, 1H), 5.81 (s, 1H), 5.73 (dd, *J* = 17.6, 1.2 Hz, 1H), 5.37 (dd, *J* = 11.2, 1.2 Hz, 1H), 3.27 (d, *J* = 6.4 Hz, 2H), 0.98 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 135.9, 135.8, 134.8, 130.1, 127.8, 127.4,

126.3, 116.8, 51.1, 32.0, 27.3 (3C); HRMS: $[M+H]^+$ calcd for $C_{14}H_{19}NO$ 218.1539, found 218.1539.

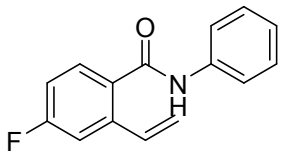
4-Methyl-*N*-phenyl-2-vinylbenzamide (1v):



1v

White solid (635 mg, 67%); m.p. 114.5–115.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, J = 8.0 Hz, 2H), 7.56 – 7.44 (m, 2H), 7.37 (dd, J = 14.0, 6.4 Hz, 3H), 7.16 (dd, J = 7.6, 4.0 Hz, 2H), 7.14 – 7.04 (m, 1H), 5.75 (d, J = 18.4 Hz, 1H), 5.38 (d, J = 11.6 Hz, 1H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.3, 140.9, 138.0, 136.1, 134.7, 132.5, 129.1 (2C), 128.7, 127.8 (2C), 127.4, 124.5, 119.7, 117.1, 21.5; HRMS: $[M+H]^+$ calcd for $C_{16}H_{15}NO$ 238.1226, found 238.1225.

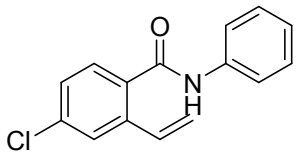
4-Fluoro-*N*-phenyl-2-vinylbenzamide (1w):



1w

White solid (858 mg, 89%); m.p. 109.5–110.9 °C; m.p. 109.5–110.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 – 7.54 (m, 4H), 7.36 (t, J = 8.0 Hz, 2H), 7.30 – 7.23 (m, 1H), 7.16 (t, J = 7.2 Hz, 1H), 7.12 – 6.96 (m, 2H), 5.76 (d, J = 17.6 Hz, 1H), 5.44 (d, J = 10.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 165.1, 162.59, 138.9 (d, J_{CF} = 8.2 Hz), 137.8, 133.5 (d, J_{CF} = 2.2 Hz), 131.5, 129.9 (d, J_{CF} = 8.9 Hz), 129.1, 124.8, 119.9, 118.4, 114.9 (d, J_{CF} = 21.8 Hz), 113.2 (d, J_{CF} = 22.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -109.4; HRMS: $[M+H]^+$ calcd for $C_{15}H_{12}FNO$ 242.0975, found 242.0973.

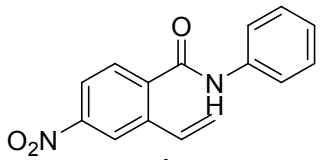
4-Chloro-*N*-phenyl-2-vinylbenzamide (1x):



1x

White solid (853 mg, 83%); m.p. 118.5–119.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.48 (m, 5H), 7.42 – 7.28 (m, 3H), 7.17 (t, *J* = 7.6 Hz, 1H), 7.05 (dd, *J* = 17.6, 10.8 Hz, 1H), 5.78 (d, *J* = 17.6 Hz, 1H), 5.45 (d, *J* = 10.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 137.9, 137.7, 136.8, 133.4, 129.2 (2C), 129.1, 127.9, 126.7, 124.9, 120.1, 119.9, 119.8, 118.6; HRMS: $[M+H]^+$ calcd for $C_{15}H_{12}ClNO$ 258.0680, found 258.0679.

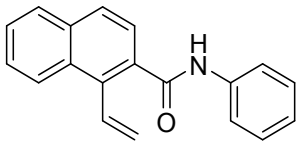
4-Nitro-*N*-phenyl-2-vinylbenzamide (1y):



1y

White solid (911 mg, 85%); m.p. 120.8–123.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (t, *J* = 2.8 Hz, 1H), 8.16 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.61 (d, *J* = 7.6 Hz, 3H), 7.44 – 7.35 (m, 2H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.11 – 7.01 (m, 1H), 5.95 (d, *J* = 17.6 Hz, 1H), 5.58 (d, *J* = 11.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 148.9, 140.4, 137.6, 137.2, 132.3, 129.3(2C), 128.8, 125.3, 122.4, 121.4, 120.2, 120.1 (2C); HRMS: $[M+H]^+$ calcd for $C_{15}H_{12}N_2O_3$ 269.0921, found 269.0918.

***N*-phenyl-1-vinyl-2-naphthamide (1z)**:

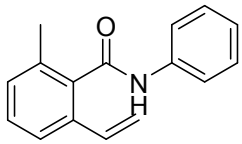


1z

White solid (699 mg, 64%); m.p. 121.0–122.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 – 8.17 (m, 1H), 7.91 – 7.80 (m, 2H), 7.70 (dd, *J* = 8.4, 3.6 Hz, 1H), 7.67 – 7.51 (m, 5H), 7.37 (t, *J* = 8.0 Hz, 2H), 7.34 – 7.26 (m, 1H), 7.16 (t, *J* = 7.6 Hz, 1H), 5.81 (d, *J* = 11.6 Hz, 1H), 5.68 (d, *J* = 17.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 138.1, 134.2, 133.1, 132.7, 131.2, 129.4, 129.1 (2C), 128.3,

128.1, 127.1, 126.9, 126.0, 124.7, 124.6, 123.8, 122.8, 119.8; HRMS: $[M+H]^+$ calcd for $C_{19}H_{15}NO$ 274.1226, found 274.1222.

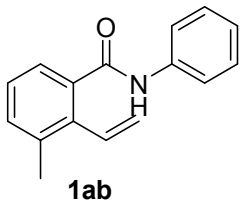
2-Methyl-*N*-phenyl-6-vinylbenzamide (1aa):



1aa

White solid (597 mg, 63%); m.p. 101.2–102.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.41 – 7.34 (m, 3H), 7.30 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 2H), 6.86 (dd, *J* = 17.2, 11.2 Hz, 1H), 5.77 (dd, *J* = 17.2, 1.2 Hz, 1H), 5.32 (dd, *J* = 10.8, 1.2 Hz, 1H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9, 137.7, 136.2, 135.0, 134.7, 133.9, 129.7, 129.3, 129.2 (2C), 124.8, 122.9, 119.9 (2C), 116.9, 19.2; HRMS: $[M+H]^+$ calcd for $C_{16}H_{15}NO$ 238.1226, found 238.1225.

2-Methyl-*N*-phenyl-6-vinylbenzamide (1ab):

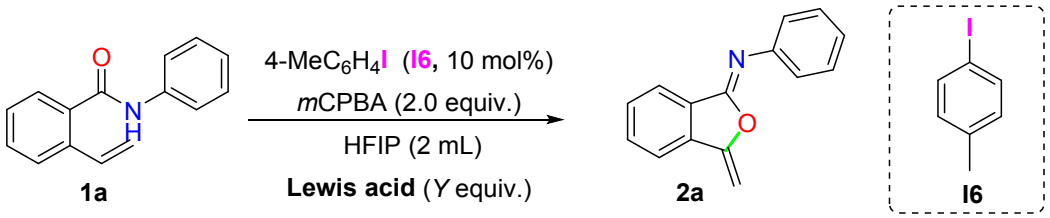


1ab

White solid (683 mg, 73%); m.p. 111.0–112.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.35 (t, *J* = 8.0 Hz, 2H), 7.31 – 7.20 (m, 3H), 7.14 (t, *J* = 7.6 Hz, 1H), 6.91 (dd, *J* = 18.0, 11.6 Hz, 1H), 5.55 (d, *J* = 11.2 Hz, 1H), 5.48 (d, *J* = 18.0 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.3, 138.1, 136.8, 136.3, 135.4, 133.8, 132.1, 129.1 (2C), 127.3, 125.7, 124.5, 120.9, 119.7 (2C), 20.6; HRMS: $[M+H]^+$ calcd for $C_{16}H_{15}NO$ 238.1226, found 238.1226.

2. Optimization of the reaction conditions

Table S1. Influence of Lewis acid screening on the reaction.

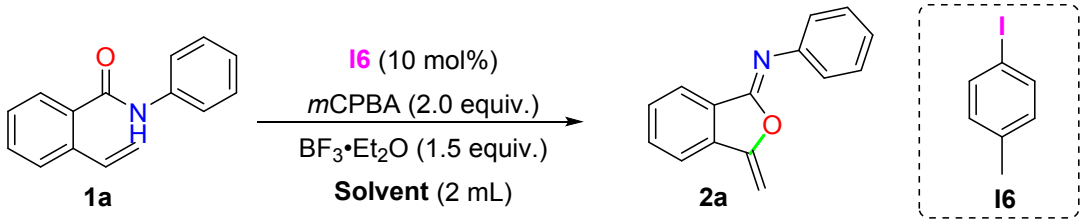


Entry[a]	Lewis acid	Equiv (*Y*)	Time	Temp. (°C)	Yield[b] (%)
1	CF_3COOH	2.0	60 min	25	15
2	CH_3SO_3H	2.0	60 min	25	23
3	$C_7H_7SO_3H$	2.0	60 min	25	-
4	CF_3SO_3H	2.0	60 min	25	-
5	CH_3COOH	2.0	60 min	25	-
6	$BF_3{\cdot}Et_2O$	2.0	30 min	25	55
7	$BF_3{\cdot}Et_2O$	1.0	30 min	25	36
8	$BF_3{\cdot}Et_2O$	1.2	30 min	25	46
9	$BF_3{\cdot}Et_2O$	1.5	30 min	25	58
10	$BF_3{\cdot}Et_2O$	0	60 min	25	trace

[a] Reaction conditions: **1a** (0.2 mmol), **I6** (10 mol%), *m*CPBA (0.4 mmol, 2.0 equiv.), **Lewis acid** (*Y* equiv.), HFIP (2 mL), air atmosphere; [b] Isolated yield.

Experimental Procedure: *m*CPBA (86.3 mg, 80%, 0.4 mmol) and **I6** (4.4 mg 0.02 mmol) were weighted into an oven-dried 10 mL Pyrex tube equipped with a magnetic stir bar. HFIP (2.0 mL) was added and the reaction mixture was stirred vigorously for 5 min. Then, **1a** (44.6 mg, 0.2 mmol) and **Lewis acid** was added in turn. The reaction mixture was stirred at room temperature, which was detected by TLC until completely finished. Then, the mixture was directly purified by flash chromatography (mixture of one tenth Alumina-B and nine tenth silica gel) with an eluent of PE:EtOAc = 30:1 to afford the desired product.

Table S2. Influence of solvent on the reaction.

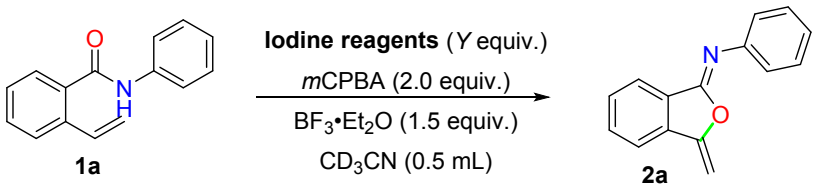


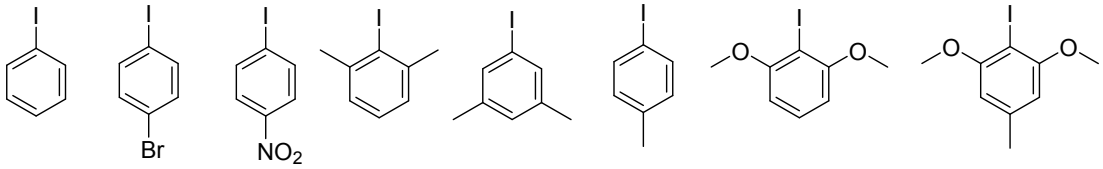
Entry[a]	Solvent	Time	Temp. (°C)	Yield[b] (%)
1	HFIP	30 min	25	58
2	DCM	60 min	25	46
3	DCE	1 h	25	34
4	THF	8 h	25	-
5	MeCN	30 min	25	88
6	DMF	1 h	25	23
7	*i*-PrOH	8 h	25	-
8	CF_3CH_2OH	8 h	25	-
9	*n*-Hexane	8 h	25	-
10	$C_7H_5F_3$	8 h	25	-

[a] Reaction conditions: **1a** (0.2 mmol), **I6** (10 mol%), *m*CPBA (0.4 mmol, 2.0 equiv.), $BF_3 \cdot Et_2O$ (0.3 mmol, 1.5 equiv.), **Solvent** (2 mL), air atmosphere; [b] Isolated yield.

Experimental Procedure: *m*CPBA (86.3 mg, 80%, 0.2 mmol) and **I6** (4.4 mg 0.02 mmol) were weighted into an oven-dried 10 mL Pyrex tube equipped with a magnetic stir bar. **Solvent** (2.0 mL) was added and the reaction mixture was stirred vigorously for 5 min. Then, **1a** (44.6 mg, 0.2 mmol) and $BF_3 \cdot Et_2O$ (38 μL, 0.3 mmol) was added in turn. The reaction mixture was stirred at room temperature, which was detected by TLC until completely finished. Then, the mixture was directly purified by flash chromatography (mixture of one tenth Alumina-B and nine tenth silica gel) with an eluent of PE:EtOAc = 30:1 to afford the desired product.

Table S3. Influence of iodine reagentson the reaction.





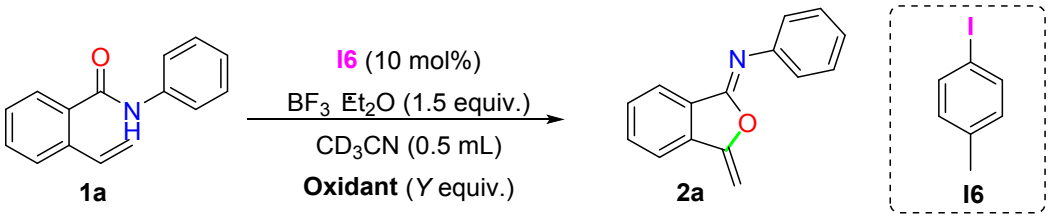
I1 **I2** **I3** **I4** **I5** **I6** **I7** **I8**

Entry[a]	**ArI reagents**	Equiv (*Y*)	Time	Yield[b] (%)
1	**I1**	0.1	30 min	91
2	**I2**	0.1	30 min	81
3	**I3**	0.1	30 min	85
4	**I4**	0.1	30 min	88
5	**I5**	0.1	30 min	89
6	**I6**	0.1	30 min	95
7	**I7**	0.1	30 min	93
8	**I8**	0.1	30 min	95(89)
9	PIDA	1.0	30 min	86(79)
10	I_2	0.1	3 h	87(78)
11	KI	0.2	3 h	89(83)
12	**I6**	0	30 min	trace
13	**I6**	0.05	1 h	90(85)
14	**I6**	0.15	30 min	92
15	**I6**	0.2	30 min	91

[a] Reaction conditions: **1a** (0.05 mmol), **ArI reagents**, $BF_3 \cdot Et_2O$ (0.075 mmol, 1.5 equiv.), *m*CPBA (0.1 mmol, 2.0 equiv.), CD_3CN (0.5 mL), r.t., air atmosphere; [b] ^1H NMR yield; Isolated yield was given in parentheses.

Experimental Procedure: *m*CPBA (21.6 mg, 80%, 0.075 mmol), **ArI reagents** and **1a** (11.2 mg, 0.05 mmol) were weighted into an oven-dried septum-capped NMR tube. CD_3CN (0.5 mL, with 0.5 μL CH_2Br_2/mL) and $BF_3 \cdot Et_2O$ (10 μL, 0.075 mmol) were added in turn. The reaction mixture was shocked for 5 min. Then, the mixture was placing 25 minutes for ^1H NMR spectroscopic analyses. Some experiments with low yields will be detected for a prolonged reaction time.

Table S4. Influence of oxidant on the reaction.



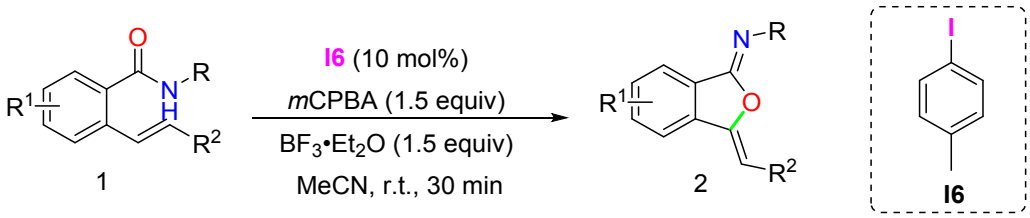
Entry[a]	Oxidant	Equiv (*Y*)	Time	Yield[b] (%)
1	*m*CPBA	2	30 min	90
2	H_2O_2	2	3 h	trace
3	DTBP	2	3 h	trace
4	TBHP	2	3 h	trace
5	TBPB	2	3 h	trace
6	CHP	2	3 h	trace
7	Oxone	2	3 h	25(22)
8	*m*CPBA	0	3 h	-
9	*m*CPBA	1.0	30 min	35
10	*m*CPBA	1.2	30 min	65
11	*m*CPBA	1.5	30 min	95(90)
12	*m*CPBA	3.0	30 min	70

[a] Reaction conditions: **1a** (0.05 mmol), **I6** (10 mol%), ***Oxidant*** (*Y* equiv.), $BF_3{\cdot}Et_2O$ (0.075 mmol, 1.5 equiv.), CD_3CN (0.5 mL), r.t., air atmosphere; [b] ^1H NMR yield; Isolated yield was given in parentheses.

Experimental Procedure: Oxidant, **I6** (1.1 mg 0.005 mmol) and **1a** (11.2 mg, 0.05 mmol) were weighted into an oven-dried septum-capped NMR tube. CD_3CN (0.5 mL, with 0.5 μL CH_2Br_2/mL) and $BF_3{\cdot}Et_2O$ (10 μL, 0.075 mmol) were added in turn. The reaction mixture was shocked for 5 min. Then, the mixture was placing for 25 minutes, for ^1H NMR spectroscopic analyses. Some experiments with low yields will be detected for a prolonged reaction time.

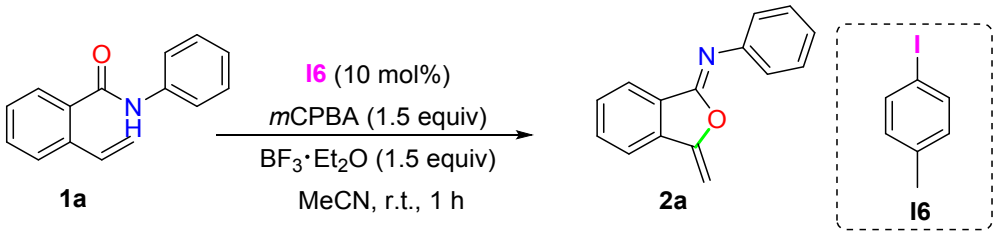
3. General procedure for the reaction of 2-alkenylbenzamides

4.1 General procedure for the reaction of 1a-1ah (Table 2)



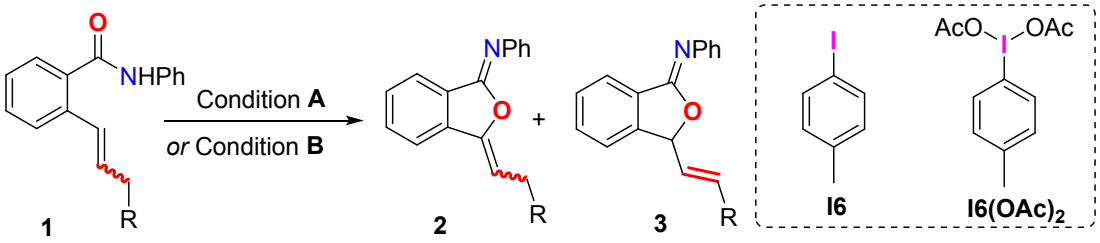
Experimental Procedure: *m*CPBA (64.8 mg, 80%, 0.3 mmol) and **I6** (4.4 mg 0.02 mmol) were weighted into an oven-dried 10 mL Pyrex tube equipped with a magnetic stir bar. Dry CH_3CN (2.0 mL) was added and the reaction mixture was stirred vigorously for 5 min. Then, 2-Alkenylbenzamides **1** (0.2 mmol) and $BF_3 \cdot Et_2O$ (38 μL, 0.3 mmol) was added in turn. The reaction mixture was stirred at room temperature, which was detected by TLC until completely finished. Then, the mixture was directly purified by flash chromatography (mixture of one tenth Alumina-B and nine tenth silica gel) with an eluent of PE:EtOAc = 30:1 to afford the desired product **2**.

4.2 1.0 mmol scale-up reaction of 1a



Experimental Procedure: *m*CPBA (324 mg, 80%, 1.5 mmol) and **I6** (22 mg 0.1 mmol) were weighted into an oven-dried 100 mL Pyrex tube equipped with a magnetic stir bar. Dry CH_3CN (10.0 mL) was added and the reaction mixture stirred vigorously for 5 min. Then, **1a** (223 mg, 1 mmol) and $BF_3 \cdot Et_2O$ (189 μL, 1.5 mmol) were added in turn. The reaction mixture was stirred at room temperature, which was detected by TLC until completely finished. Then, the mixture was evaporated to remove the most of the solvent and the residue was purified by flash chromatography (mixture of one tenth Alumina-B and nine tenth silica gel) with an eluent of PE:EtOAc = 30:1 to afford the desired product **2a** as a colorless oil with 82% yield.

4.3 General procedure for the reaction of 1ai-1ak (Scheme 2)



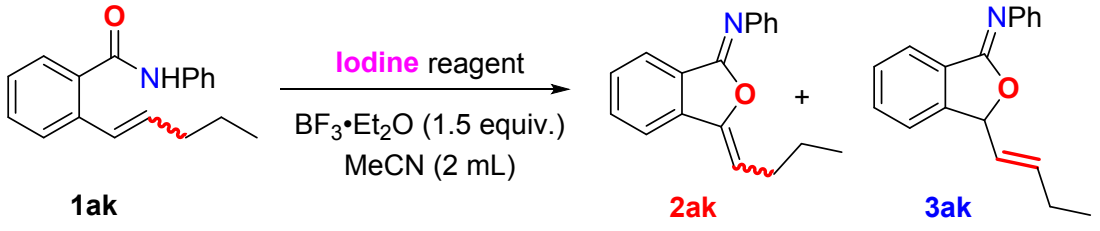
Conditions A:

Experimental Procedure: *m*CPBA (64.8 mg, 80%, 0.3 mmol) and **I6** (4.4 mg 0.02 mmol) were weighted into an oven-dried 10 mL Pyrex tube equipped with a magnetic stir bar. Dry CH_3CN (2.0 mL) was added and the reaction mixture was stirred vigorously for 5 min. Then, 2-alkenylbenzamides **1** (0.2 mmol) and $BF_3{\cdot}Et_2O$ (38 μL, 0.3 mmol) were added in turn. The reaction mixture was stirred at room temperature, which was detected by TLC until completely finished. Then, the mixture was directly purified by flash chromatography (mixture of one tenth Alumina-B and nine tenth silica gel) with an eluent of PE:EtOAc = 30:1 to afford the desired product.

Conditions B:

Experimental Procedure: $I6(OAc)_2$ (80.7 mg 0.24 mmol) were weighted into an oven-dried 10 mL Pyrex tube equipped with a magnetic stir bar. Then, 2-alkenylbenzamides **1** (0.2 mmol), $BF_3{\cdot}Et_2O$ (38 μL, 0.3 mmol) and dry CH_3CN (2.0 mL) were added in turn. The reaction mixture was stirred at room temperature, which was detected by TLC until completely finished. Then, the mixture was directly purified by flash chromatography (mixture of one tenth Alumina-B and nine tenth silica gel) with an eluent of PE:EtOAc = 30:1 to afford the desired product.

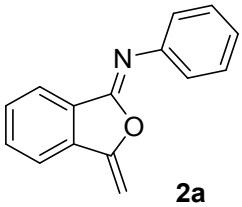
4.4 General procedure for the reaction of 1ak (Scheme 3)



Experimental Procedure: An oven-dried 10 mL Pyrex tube equipped with a magnetic stir bar was added the corresponding **iodine reagent** and ***m*CPBA**, then added CH_3CN (2.0 mL). After that, 2-alkenylbenzamides **1ak** (53 mg, 0.2 mmol) and $BF_3 \cdot Et_2O$ (38 μL, 0.3 mmol) was added in turn, and the reaction mixture was stirred at room temperature. The reaction solution was detected by TLC until completely finished. Then, the mixture was directly purified by flash chromatography (mixture of one tenth Alumina-B and nine tenth silica gel) with an eluent of PE:EtOAc = 30:1 to afford the desired product

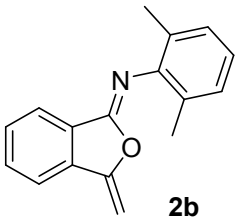
4.5 Characterization data of products

(*Z*)-3-methylene-*N*-phenylisobenzofuran-1(3*H*)-imine (2a):



2a Colorless oil (39.8 mg, 90%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.68 – 7.58 (m, 1H), 7.58 – 7.48 (m, 1H), 7.45 – 7.31 (m, 3H), 7.16 (tt, *J* = 6.8, 2.0 Hz, 1H), 5.00 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 153.9, 145.7, 136.2, 132.2, 130.8, 130.2, 128.8 (2C), 124.7, 123.7 (2C), 123.6, 120.3, 87.2; HRMS: $[M+H]^+$ calcd for $C_{15}H_{11}NO$ 222.0913, found 222.0912.

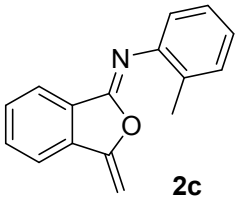
(*Z*)-*N*-(2,6-dimethylphenyl)-3-methyleneisobenzofuran-1(3*H*)-imine (2b):



2b Colorless oil (41.5 mg, 83%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.02 (m, 1H), 7.63 (t, *J* = 8.0 Hz, 2H), 7.60 – 7.53 (m, 1H), 7.08 (d, *J* = 7.4 Hz, 2H), 6.97 (t, *J* = 7.4 Hz, 1H), 4.97 – 4.89 (m, 2H), 2.17 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.8, 153.1, 144.6, 136.8, 135.2, 134.5, 132.3, (130.3, 130.2) (1C), (129.7,

129.8) (1C), (128.2, 127.9) (1C), 127.7 (2C), (123.7, 123.5) (1C) 120.36, 87.11, 18.37 (2C); HRMS: $[M+H]^+$ calcd for $C_{17}H_{15}NO$ 250.1226, found 250.1227.

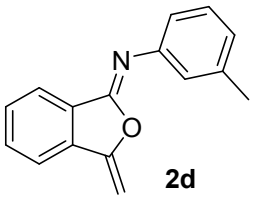
(*Z*)-3-methylene-*N*-(*o*-tolyl)isobenzofuran-1(3*H*)-imine (2c):



2c

Colorless oil (37.2 mg, 79%); ^1H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 7.6 Hz, 1H), 7.70 – 7.49 (m, 3H), 7.24 – 7.15 (m, 3H), 7.06 (t, *J* = 7.2 Hz, 1H), 4.96 (q, *J* = 2.8 Hz, 2H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 153.3, 144.9, 136.5, 132.2, 130.6, 130.4, 130.3, 130.2, 126.1, 124.2, 123.6, 121.7, 120.3, 87.1, 18.2; HRMS: $[M+H]^+$ calcd for $C_{16}H_{13}NO$ 236.1070, found 236.1072.

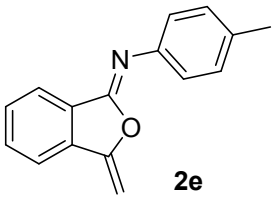
(*Z*)-3-methylene-*N*-(*m*-tolyl)isobenzofuran-1(3*H*)-imine (2d):



2d

Colorless oil (37.1 mg, 79%); ^1H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.6 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.61 – 7.51 (m, 2H), 7.31 – 7.23 (m, 1H), 7.17 (d, *J* = 7.6 Hz, 2H), 6.98 (d, *J* = 7.6 Hz, 1H), 4.99 (t, *J* = 2.4 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 153.7, 145.6, 138.5, 136.2, 132.1, 130.8, 130.1, 128.5, 125.5, 124.2, 123.5, 120.5, 120.2, 87.1, 21.5; HRMS: $[M+H]^+$ calcd for $C_{16}H_{13}NO$ 236.1070, found 236.1071.

(*Z*)-3-methylene-*N*-(*p*-tolyl)isobenzofuran-1(3*H*)-imine (2e):

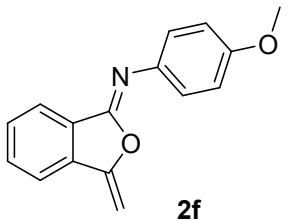


2e

Colorless oil (38.1 mg, 81%); ^1H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.6 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.62 – 7.49 (m, 2H), 7.34 – 7.23 (m,

2H), 7.19 (d, J = 8.0 Hz, 2H), 5.00 (q, J = 3.2 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.2, 153.5, 142.9, 136.1, 134.4, 132.0, 130.9, 130.1, 129.4 (2C), 123.8 (2C), 123.5, 120.2, 86.9, 21.1; HRMS: $[M+H]^+$ calcd for $C_{16}H_{13}NO$ 236.1070, found 236.1070.

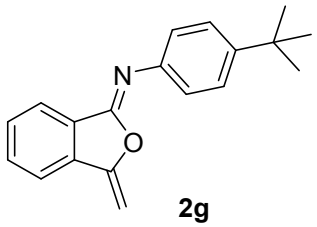
(*Z*)-*N*-(4-methoxyphenyl)-3-methyleneisobenzofuran-1(3*H*)-imine (2f):



2f

White solid (39.2 mg, 78%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (dt, J = 7.2, 1.2 Hz, 1H), 7.65 (dt, J = 8.0, 1.2 Hz, 1H), 7.62 – 7.49 (m, 2H), 7.50 – 7.41 (m, 2H), 6.96 – 6.90 (m, 2H), 5.06 – 4.97 (m, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.0, 155.2, 152.8, 138.5, 135.9, 131.8, 131.2, 130.1, 125.7 (2C), 123.4, 120.2, 114.0 (2C), 86.6, 55.4; HRMS: $[M+H]^+$ calcd for $C_{16}H_{13}NO_2$ 252.1019, found 252.1020.

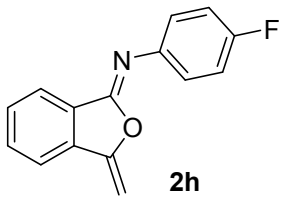
(*Z*)-*N*-(4-(*tert*-butyl)phenyl)-3-methyleneisobenzofuran-1(3*H*)-imine (2g):



2g

White solid (44.0 mg, 79%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (dt, J = 7.6, 1.2 Hz, 1H), 7.65 (dt, J = 7.6, 1.2 Hz, 1H), 7.62 – 7.48 (m, 2H), 7.44 – 7.32 (m, 1H), 5.04 – 4.97 (m, 2H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.2, 153.4, 147.7, 142.8, 136.1, 132.0, 131.0, 130.1, 125.6 (2C), 123.7 (2C), 123.5, 120.2, 86.9, 34.5, 31.5 (3C); HRMS: $[M+H]^+$ calcd for $C_{19}H_{19}NO$ 278.1539, found 278.1537.

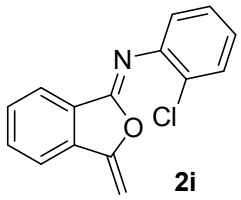
(*Z*)-*N*-(4-fluorophenyl)-3-methyleneisobenzofuran-1(3*H*)-imine (2h):



2h

Colorless oil (39.2 mg, 82%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 7.6 Hz, 1H), 7.65 (d, J = 7.6 Hz, 1H), 7.62 – 7.49 (m, 2H), 7.39 (dd, J = 8.8, 5.2 Hz, 2H), 7.06 (t, J = 8.8 Hz, 2H), 5.02 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 158.9, 155.1, 153.8 (d, J_{CF} = 1.6 Hz), 141.5 (d, J_{CF} = 3.0 Hz), 136.1, 132.2, 130.7, 130.2, 125.5 (d, J_{CF} = 8.0 Hz), 123.5, 120.3, 115.5, 115.3, 87.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.1; HRMS: $[M+H]^+$ calcd for $C_{15}H_{10}FNO$ 240.0819, found 240.0823.

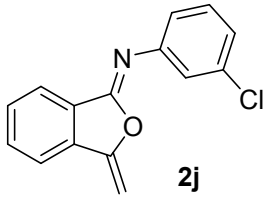
(*Z*)-*N*-(2-chlorophenyl)-3-methyleneisobenzofuran-1(3*H*)-imine (2i):



2i

Colorless oil (42.3 mg, 83%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 7.6 Hz, 1H), 7.65 (q, J = 8.0 Hz, 2H), 7.58 (t, J = 7.6 Hz, 1H), 7.44 (d, J = 8.0 Hz, 1H), 7.26 (d, J = 3.6 Hz, 2H), 7.13 – 7.03 (m, 1H), 5.05 – 4.97 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.2, 154.9, 143.8, 136.6, 132.6, 130.3, 130.0, 129.7, 127.0, 127.0, 125.0, 123.9, 123.5, 120.3, 87.8; HRMS: $[M+H]^+$ calcd for $C_{15}H_{10}ClNO$ 256.0524, found 256.0521.

(*Z*)-*N*-(3-chlorophenyl)-3-methyleneisobenzofuran-1(3*H*)-imine (2j):

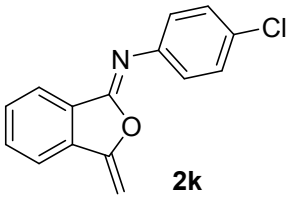


2j

Colorless oil (42.3 mg, 83%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 7.6 Hz, 1H), 7.69 – 7.51 (m, 3H), 7.37 (t, J = 2.0 Hz, 1H), 7.29 (t, J = 8.0 Hz, 1H), 7.22 (dt, J = 8.0, 1.2 Hz, 1H), 7.13 (dt, J = 8.0, 1.6 Hz, 1H), 5.05 (d, J = 3.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 154.6, 147.0, 136.3, 134.2, 132.5,

130.4, 130.3, 129.7, 124.7, 123.8, 123.6, 122.0, 120.3, 87.8; HRMS: $[M+H]^+$ calcd for $C_{15}H_{10}ClNO$ 256.0524, found 256.0523.

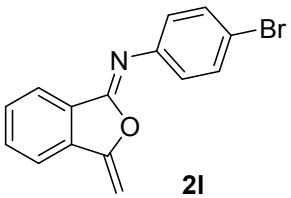
(*Z*)-*N*-(4-chlorophenyl)-3-methyleneisobenzofuran-1(3*H*)-imine (2k):



2k

White solid (44.9 mg, 88%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.6, 1H), 7.67 – 7.49 (m, 3H), 7.32 (s, 4H), 5.02 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 154.2, 144.2, 136.2, 132.3, 130.6, 130.3, 130.0, 128.8 (2C), 125.3 (2C), 123.6, 120.3, 87.5; HRMS: $[M+H]^+$ calcd for $C_{15}H_{10}ClNO$ 256.0524, found 256.0524.

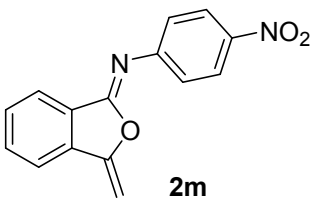
(*Z*)-*N*-(4-bromophenyl)-3-methyleneisobenzofuran-1(3*H*)-imine (2l):



2l

White solid (50.7 mg, 85%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.6 Hz, 1H), 7.62 – 7.51 (m, 2H), 7.48 (td, *J* = 7.6, 1.2 Hz, 1H), 7.45 – 7.37 (m, 2H), 7.21 – 7.15 (m, 2H), 4.96 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 154.3, 144.7, 136.2, 132.4 (2C), 130.3, 129.7, 127.7, 125.6 (2C), 123.6, 120.3, 117.8, 87.6; HRMS: $[M+H]^+$ calcd for $C_{15}H_{10}BrNO$ 300.0019, found 300.0017.

(*Z*)-3-methylene-*N*-(4-nitrophenyl)isobenzofuran-1(3*H*)-imine (2m):

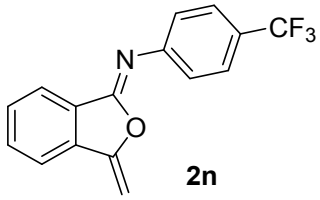


2m

Light yellow solid (47.4 mg, 88%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.8 Hz, 2H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.68 (q, *J* = 8.0 Hz, 2H),

7.59 (t, J = 7.6 Hz, 1H), 7.38 (d, J = 8.8 Hz, 2H), 5.14 – 5.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 154.8, 152.4, 144.3, 136.4, 133.0 (2C), 130.5, 129.9, 124.7 (2C), 123.9, 123.8, 120.5, 88.7; HRMS: $[M+H]^+$ calcd for $C_{15}H_{10}N_2O_3$ 267.0764, found 267.0762.

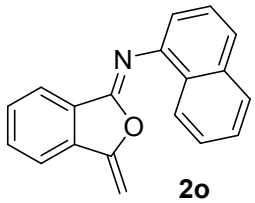
(*Z*)-3-methylene-*N*-(4-(trifluoromethyl)phenyl)isobenzofuran-1(3*H*)-imine (2n):



2n

White solid (52.0 mg, 90%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, J = 7.6 Hz, 1H), 7.64 (dd, J = 12.4, 6.4 Hz, 4H), 7.59 – 7.55 (m, 1H), 7.38 (d, J = 8.4 Hz, 2H), 5.08 – 5.00 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9(d, J_{CF} = 5.9 Hz), 149.1, 136.4, 132.6, 130.3 (d, J_{CF} = 8.9 Hz), 126.3 (q, J_{CF} = 271.1 Hz), 125.9 (q, J_{CF} = 29.6 Hz), 123.7, 123.5, 120.4, 88.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.21; HRMS: $[M+H]^+$ *calcd* for $C_{16}H_{10}F_3NO$ 290.0787, *found* 290.7881.

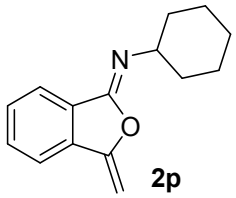
(*Z*)-3-methylene-*N*-(naphthalen-1-yl)isobenzofuran-1(3*H*)-imine (2o):



2o

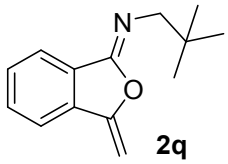
White solid (47.7 mg, 88%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 – 8.23 (m, 1H), 8.13 (d, J = 7.2 Hz, 1H), 7.74 – 7.54 (m, 5H), 7.47 (dq, J = 12.0, 7.6, 6.4 Hz, 4H), 5.05 – 4.87 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 154.3, 142.2, 136.5, 134.2, 132.3, 130.7, 130.2, 128.7, 127.8, 126.0, 125.8, 125.5, 124.5, 124.1, 123.7, 120.3, 117.7, 87.4; HRMS: $[M+H]^+$ calcd for $C_{19}H_{13}NO$ 272.1070, found 272.1067.

(*Z*)-*N*-cyclohexyl-3-methyleneisobenzofuran-1(3*H*)-imine (2p):



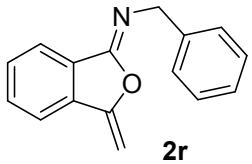
2p Colorless oil (35.4 mg, 78%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.2 Hz, 1H), 7.63 – 7.44 (m, 1H), 7.44 (d, *J* = 1.2 Hz, 2H), 4.95 – 4.86 (m, 2H), 3.90 (tt, *J* = 10.4, 4.0 Hz, 1H), 1.90 – 1.76 (m, 3H), 1.73 – 1.63 (m, 1H), 1.54 – 1.33 (m, 5H), 1.26 (ddt, *J* = 12.8, 7.6, 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 153.3, 136.4, 131.3, 130.7, 129.8, 123.1, 120.1, 84.8, 56.2, 34.0 (2C), 25.8, 25.0 (2C); HRMS: $[M+H]^+$ calcd for $C_{15}H_{17}NO$ 228.1383, found 228.1382.

(*Z*)-3-methylene-*N*-neopentylisobenzofuran-1(3*H*)-imine (2q):



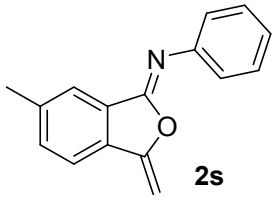
2q Colorless oil (32.3 mg, 75%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.59 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.55 – 7.43 (m, 2H), 5.00 – 4.78 (m, 2H), 3.39 (s, 2H), 1.01 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 154.0, 136.4, 131.2, 130.8, 129.8, 123.0, 120.1, 84.7, 59.6, 32.3, 27.8 (3C); HRMS: $[M+H]^+$ calcd for $C_{14}H_{17}NO$ 216.1383, found 216.1385.

(*Z*)-*N*-benzyl-3-methyleneisobenzofuran-1(3*H*)-imine (2r).



2r White solid (37.6 mg, 78%); ^{1}H NMR (400 MHz, $CDCl_3$); δ 7.93 (d, *J* = 7.6 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.54 – 7.46 (m, 3H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.32 – 7.28 (m, 1H), 5.06 – 4.96 (m, 2H), 4.90 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.4, 155.0, 140.2, 136.5, 131.6, 130.5, 130.0, 128.4 (2C), 127.9 (2C), 126.7, 123.2, 120.2, 85.7, 51.7; HRMS: $[M+H]^+$ calcd for $C_{16}H_{13}NO$ 236.1070, found 236.1077.

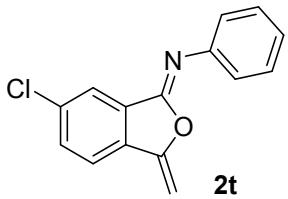
(*Z*)-6-methyl-3-methylene-*N*-phenylisobenzofuran-1(3*H*)-imine (2s):



2s

Colorless oil (37.6 mg, 80%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 5.6 Hz, 5H), 7.15 (tt, *J* = 6.4, 2.4 Hz, 1H), 4.93 (q, *J* = 2.8 Hz, 2H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.2, 154.0, 145.7, 140.7, 133.8, 133.4, 131.1, 128.7(2C), 124.6, 123.7 (2C), 123.6, 120.1, 86.3, 21.6; HRMS: $[M+H]^+$ calcd for $C_{16}H_{13}NO$ 236.1070, found 236.1071.

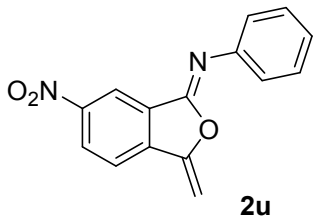
(*Z*)-6-chloro-3-methylene-*N*-phenylisobenzofuran-1(3*H*)-imine (2t):



2t

White solid (45.4 mg, 89%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 1.6 Hz, 1H), 7.53 (s, 2H), 7.37 (d, *J* = 4.4 Hz, 4H), 7.17 (tt, *J* = 5.4, 3.6 Hz, 1H), 5.01 (d, *J* = 3.2 Hz, 1H), 4.97 (d, *J* = 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.4, 152.3, 145.1, 136.4, 134.5, 132.5, 132.5, 128.8 (2C), 125.1, 123.9 (2C), 123.6, 121.5, 87.8; HRMS: $[M+H]^+$ calcd for $C_{15}H_{10}ClNO$ 256.0524, found 256.0523.

(*Z*)-3-methylene-6-nitro-*N*-phenylisobenzofuran-1(3*H*)-imine (2u):

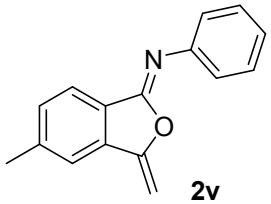


2u

Light yellow solid (47.9 mg, 90%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 2.0 Hz, 1H), 8.39 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.34 (d, *J* = 4.8 Hz, 4H), 7.15 (ddd, *J* = 8.4, 5.2, 3.6 Hz, 1H), 5.20 – 5.12 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.7, 151.1, 149.4, 144.5, 140.7, 132.4, 128.9 (2C), 127.1, 125.6, 124.0 (2C), 121.4, 119.6, 91.2; HRMS: $[M+H]^+$ calcd for $C_{15}H_{10}N_2O_3$

267.0764, found 267.0764.

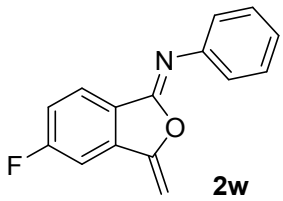
(*Z*)-5-methyl-3-methylene-*N*-phenylisobenzofuran-1(3*H*)-imine (2v):



2v

Colorless oil (38.0 mg, 81%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 1H), 7.44 (s, 1H), 7.42 – 7.31 (m, 5H), 7.15 (td, *J* = 6.8, 2.0 Hz, 1H), 4.97 (s, 2H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 154.0, 145.8, 143.0, 136.6, 131.5, 128.7 (2C), 128.3, 124.5 (2C), 123.7, 123.3, 120.4, 86.8, 21.9; HRMS: $[M+H]^+$ calcd for $C_{16}H_{13}NO$ 236.1070, found 236.1071.

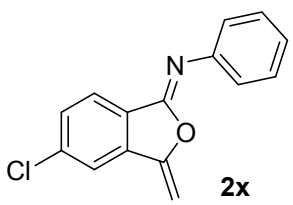
(*Z*)-5-fluoro-3-methylene-N-phenylisobenzofuran-1(3*H*)-imine (2w):



2w

Colorless oil (41.1 mg, 87%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 8.4, 4.8 Hz, 1H), 7.42 – 7.31 (m, 4H), 7.26 (ddd, *J* = 10.8, 6.8, 2.4 Hz, 3H), 7.16 (t, *J* = 6.8 Hz, 1H), 5.04 (d, *J* = 3.2 Hz, 1H), 4.98 (d, *J* = 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 164.2, 154.1 (d, J_{CF} = 4.4 Hz), 152.7, 145.4, 138.4 (d, J_{CF} = 10.3 Hz), 128.8 (2C), 125.9 (d, J_{CF} = 9.8 Hz), 124.8, 123.7 (2C), 118.5(d, J_{CF} = 24.2 Hz), 107.0 (d, J_{CF} = 24.6 Hz), 88.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -106.2; HRMS: $[M+H]^+$ calcd for $C_{15}H_{10}FNO$ 240.0819, found 240.0819.

(*Z*)-5-chloro-3-methylene-*N*-phenylisobenzofuran-1(3*H*)-imine (2x).

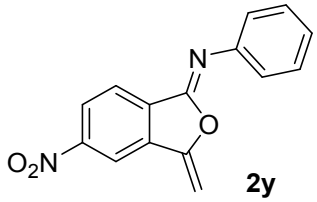


2x

White solid (45.4 mg, 89%); ^{1}H NMR (400 MHz, $CDCl_3$) δ

7.88 (d, J = 8.4 Hz, 1H), 7.59 (s, 1H), 7.48 (d, J = 8.0, 1H), 7.37 (d, J = 6.4 Hz, 4H), 7.16 (tq, J = 6.4, 4.0, 3.2 Hz, 1H), 5.03 (d, J = 3.2 Hz, 1H), 4.98 (d, J = 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.9, 152.7, 145.3, 138.6, 137.7, 130.7, 129.3, 128.8 (2C), 125.0, 124.8, 123.8 (2C), 120.5, 88.4; HRMS: $[M+H]^+$ calcd for $C_{15}H_{10}ClNO$ 256.0524, found 256.0524.

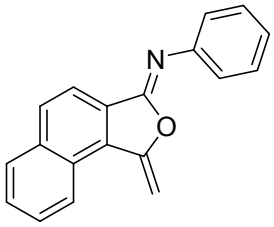
(*Z*)-3-methylene-5-nitro-*N*-phenylisobenzofuran-1(3*H*)-imine (2y):



2y

Light yellow solid (47.3 mg, 89%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, J = 2.0 Hz, 1H), 8.39 (dd, J = 8.4, 2.0 Hz, 1H), 8.13 (d, J = 8.4 Hz, 1H), 7.46 – 7.36 (m, 4H), 7.22 (tt, J = 6.0, 2.4 Hz, 1H), 5.19 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 151.3, 150.6, 144.6, 137.0, 135.8, 128.9 (2C), 125.7, 125.2, 124.9, 124.1 (2C), 116.1, 89.8; HRMS: $[M+H]^+$ calcd for $C_{15}H_{10}N_2O_3$ 267.0764, found 267.0763.

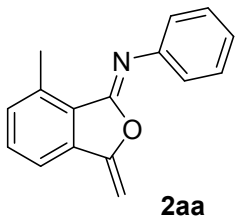
(*Z*)-1-methylene-*N*-phenylnaphtho[1,2-*c*]furan-3(1*H*)-imine (2z):



2z

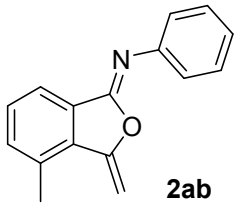
White solid (47.7 mg, 88%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, J = 8.0 Hz, 1H), 8.03 – 7.95 (m, 3H), 7.72 – 7.57 (m, 2H), 7.47 – 7.35 (m, 4H), 7.22-7.13 (m, 1H), 5.45 (d, J = 3.2 Hz, 1H), 5.32 (d, J = 3.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 154.1, 145.8, 135.7, 132.1, 131.8, 130.8, 129.7, 128.8 (2C), 128.3, 127.8, 127.0, 124.7, 124.0 (2C), 123.7, 119.5, 92.2; HRMS: $[M+H]^+$ calcd for $C_{19}H_{13}NO$ 272.1070, found 272.1271.

(*Z*)-7-methyl-3-methylene-*N*-phenylisobenzofuran-1(3*H*)-imine (2aa):



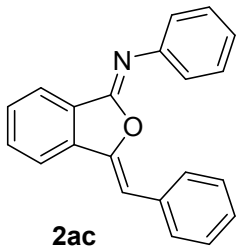
2aa Colorless oil (32.0 mg, 68%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (q, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 7.2 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 3H), 7.14 (t, *J* = 7.2 Hz, 1H), 4.95 – 4.90 (m, 2H), 2.78 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 154.2, 146.3, 137.8, 136.7, 132.0, 131.6, 128.7 (2C), 127.9, 124.3, 123.4 (2C), 117.6, 86.1, 18.6; HRMS: $[M+H]^+$ calcd for $C_{16}H_{13}NO$ 236.1070, found 236.1071.

(*Z*)-4-methyl-3-methylene-*N*-phenylisobenzofuran-1(3*H*)-imine (2ab):



2ab Colorless oil (37.6 mg, 80%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.6 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 5.6 Hz, 5H), 7.15 (tt, *J* = 6.0, 2.8 Hz, 1H), 5.12 (d, *J* = 3.2 Hz, 1H), 4.97 (d, *J* = 3.2 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.7, 154.1, 145.9, 134.1, 133.8, 133.5, 131.6, 130.0, 128.7 (2C), 124.5, 123.7 (2C), 121.4, 91.3, 20.0; HRMS: $[M+H]^+$ calcd for $C_{16}H_{13}NO$ 236.1070, found 236.1072.

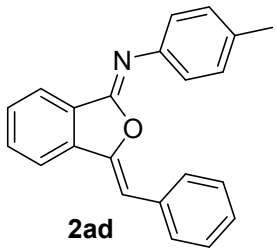
(*Z*)-3-((*Z*)-benzylidene)-*N*-phenylisobenzofuran-1(3*H*)-imine (2ac):



2ac White solid (35.6 mg, 60%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.0 Hz, 1H), 7.63 – 7.50 (m, 3H), 7.42 (q, *J* = 8.8, 7.6 Hz, 3H), 7.34 (d, *J* = 6.4 Hz, 4H), 7.26 (s, 2H), 7.14 (q, *J* = 7.6 Hz, 1H), 6.73 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 149.8, 146.8, 134.0, 132.5, 132.4, 129.5, 128.8 (2C), 128.7 (2C), 128.2, 127.5, 125.7, 124.6 (2C), 123.7, 123.6, 122.4 (2C), 100.9; HRMS:

$[M+H]^+$ calcd for $C_{21}H_{15}NO$ 298.1226, found 298.1228.

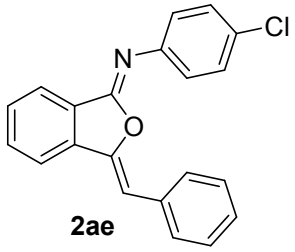
(*Z*)-3-((*Z*)-benzylidene)-*N*-(*p*-tolyl)isobenzofuran-1(3*H*)-imine (2ad):



2ad

White solid (39.8 mg, 64%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 8.0 Hz, 1H), 7.63 (dd, *J* = 6.8, 3.2 Hz, 2H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.46 – 7.39 (m, 1H), 7.39 – 7.29 (m, 4H), 7.20 (s, 4H), 6.72 (s, 1H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 149.4, 143.8, 133.9, 133.1, 132.5, 132.3, 129.4, 129.3 (2C), 128.7 (2C), 128.1, 127.5, 125.6, 124.7 (2C), 124.0, 122.6 (2C), 100.9, 21.1; HRMS: $[M+H]^+$ calcd for $C_{22}H_{17}NO$ 312.1383, found 312.1379.

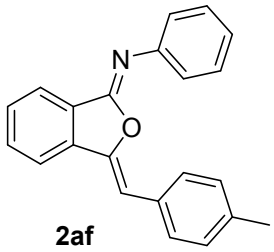
(*Z*)-3-((*Z*)-benzylidene)-*N*-(4-chlorophenyl)isobenzofuran-1(3*H*)-imine (2ae):



2ae

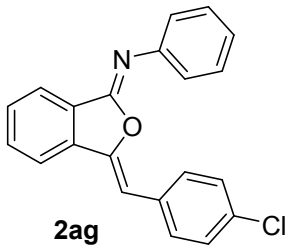
White solid (43.7 mg, 66%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 8.0 Hz, 1H), 7.62 – 7.55 (m, 3H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.2 Hz, 6H), 7.20 (d, *J* = 8.6 Hz, 2H), 6.75 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 150.2, 145.3, 134.0, 132.7, 132.2, 129.6, 128.8 (2C), 128.8 (2C), 128.6, 128.3, 127.5, 125.7, 124.6 (2C), 123.9 (2C), 123.5, 101.1; HRMS: $[M+H]^+$ calcd for $C_{21}H_{14}ClNO$: 332.0837, found 332.0838.

(*Z*)-3-((*Z*)-4-methylbenzylidene)-*N*-phenylisobenzofuran-1(3*H*)-imine (2af):



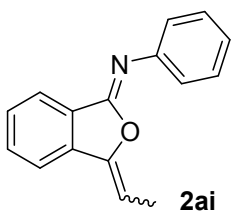
2af White solid (40.4 mg, 65%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.43 – 7.35 (m, 4H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.24 (s, 1H), 7.14 (d, *J* = 8.0 Hz, 3H), 6.67 (s, 1H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.9, 149.9, 146.9, 139.7, 134.2, 132.4, 129.6, 129.4 (2C), 128.7 (2C), 128.0, 127.5, 125.5, 124.6 (2C), 123.6 (2C), 122.5 (2C), 100.1, 21.3; HRMS: $[M+H]^+$ calcd for $C_{22}H_{17}NO$ 312.1383, found 312.1378.

(*Z*)-3-((*Z*)-4-chlorobenzylidene)-*N*-phenylisobenzofuran-1(3*H*)-imine (2ag):



2ag White solid (46.3 mg, 70%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.0 Hz, 1H), 7.55 (t, *J* = 7.2, 1H), 7.49 (d, *J* = 8.8 Hz, 2H), 7.41 (dt, *J* = 15.6, 8.0 Hz, 3H), 7.31 (t, *J* = 9.6 Hz, 3H), 7.22 (d, *J* = 7.6 Hz, 2H), 7.14 (t, *J* = 7.6 Hz, 1H), 6.69 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.6, 149.5, 146.7, 135.4, 133.7, 132.5, 130.8, 129.5, 128.9 (2C), 128.8 (2C), 128.4, 127.6, 125.9 (2C), 125.7, 123.7, 122.3 (2C), 101.2; HRMS: $[M+H]^+$ calcd for $C_{21}H_{14}ClNO$ 332.0837, found 332.0838.

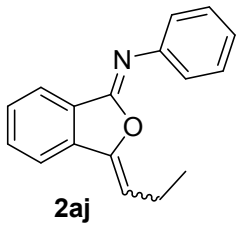
(1*Z*)-3-ethylidene-N-phenylisobenzofuran-1(3*H*)-imine (2ai):



2ai A mixture of inseparable *cis-trans* isomerism (*Z:E* ≈ 5.8:1);

Colorless oil; Major isomer shown: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.6 Hz, 1H), 7.52 (d, *J* = 3.2 Hz, 2H), 7.46 (d, *J* = 8.0 Hz, 3H), 7.39 (d, *J* = 7.6 Hz, 2H), 7.15 (t, *J* = 7.6 Hz, 1H), 5.43 (q, *J* = 7.2 Hz, 1H) , 1.92 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 149.6, 145.8, 136.6, 132.0, 130.2, 129.1, 128.7 (2C), 124.6, 124.2 (2C), 123.8, 119.2, 99.6, 11.1; HRMS: $[M+H]^+$ calcd for $C_{16}H_{13}NO$ 236.1070, found 236.1071.

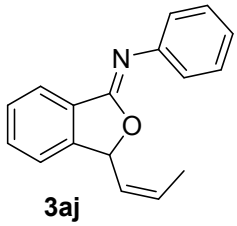
(*1Z,3Z*)-*N*-phenyl-3-propylideneisobenzofuran-1(*3H*)-imine (2aj):



2aj

A mixture of inseparable *cis-trans* isomerism (*Z:E* ≈ 6.3:1); Colorless oil; Major isomer shown: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 5.6 Hz, 2H), 7.47 (dd, *J* = 15.2, 7.6 Hz, 3H), 7.41 – 7.36 (m, 2H), 7.16 (t, *J* = 7.2 Hz, 1H), 5.41 (d, *J* = 7.6 Hz, 1H), 2.41 (p, *J* = 7.6 Hz, 2H), 1.12 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.2, 148.4, 145.7, 136.7, 132.0, 130.2, 129.1, 128.7 (2C), 124.5, 124.2 (2C), 123.6, 119.3, 106.7, 19.2, 14.1; HRMS: $[M+H]^+$ calcd for $C_{17}H_{15}NO$ 250.1226, found 250.1226.

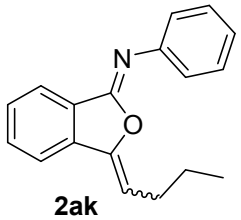
(*Z*)-N-phenyl-3-((*Z*)-prop-1-en-1-yl)isobenzofuran-1(*3H*)-imine (3aj):



3aj

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.6 Hz, 1H), 7.59 – 7.45 (m, 2H), 7.33 (d, *J* = 7.2 Hz, 5H), 7.10 (dq, *J* = 6.4, 4.0, 3.2 Hz, 1H), 6.04 – 5.94 (m, 1H), 5.86 (d, *J* = 8.4 Hz, 1H), 5.47 (ddd, *J* = 15.6, 8.8, 2.0 Hz, 1H), 1.84 – 1.63 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 146.6, 145.8, 132.0, 131.9, 130.8, 128.9, 128.7 (2C), 127.6, 124.0, 123.9, 123.5 (2C), 122.1, 85.5, 17.9; HRMS: $[M+H]^+$ calcd for $C_{17}H_{15}NO$ 250.1226, found 250.1231.

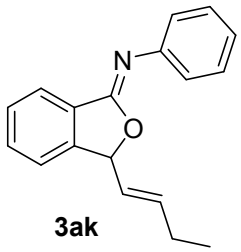
(*1Z,3Z*)-3-butylidene-*N*-phenylisobenzofuran-1(*3H*)-imine (2ak):



2ak

A mixture of inseparable *cis-trans* isomerism (*Z:E* ≈ 6.7:1); Colorless oil; Major isomer shown: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.6 Hz, 1H), 7.59 – 7.55 (m, 2H), 7.49 – 7.42 (m, 3H), 7.42 – 7.34 (m, 2H), 7.19 – 7.10 (m, 1H), 5.43 (t, *J* = 7.6 Hz, 1H), 2.37 (q, *J* = 7.6 Hz, 2H), 1.52 (dt, *J* = 14.8, 7.2 Hz, 2H), 0.97 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.2, 148.4, 145.8, 136.7, 132.0, 130.3, 129.1, 128.7 (2C), 124.6, 124.2 (2C), 123.6, 119.3, 106.7, 29.7, 19.2, 14.1. HRMS: $[M+H]^+$ calcd for $C_{18}H_{17}NO$ 264.1383, found 264.1384.

(*Z*)-3-((*Z*)-but-1-en-1-yl)-*N*-phenylisobenzofuran-1(*3H*)-imine (3ak).

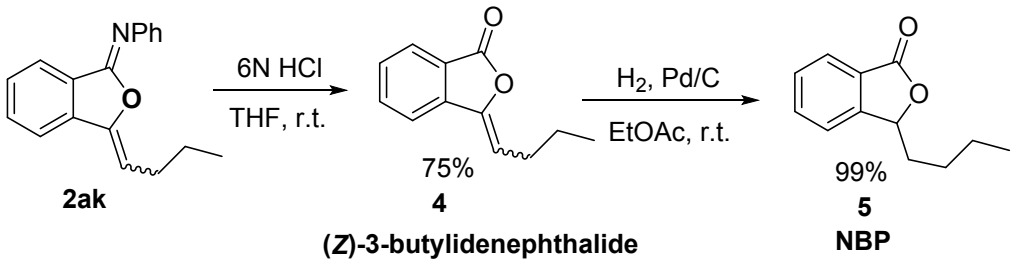


3ak

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.6 Hz, 1H), 7.59 – 7.44 (m, 2H), 7.39 – 7.26 (m, 5H), 7.09 (tt, *J* = 6.0, 2.8 Hz, 1H), 6.02 (dt, *J* = 15.2, 6.4 Hz, 1H), 5.87 (d, *J* = 8.0 Hz, 1H), 5.47 – 5.41 (m, 1H), 2.14 – 2.10 (m, 2H), 1.02 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 146.6, 145.9, 138.6, 131.9, 130.8, 128.9, 128.7 (2C), 125.4, 123.9 (2C), 123.5 (2C), 122.1, 85.6, 25.3, 13.0; HRMS: $[M+H]^+$ calcd for $C_{18}H_{17}NO$ 264.1383, found 264.1385.

4. Transformation of the products

5.1 Synthesis of NBP (Scheme 4)

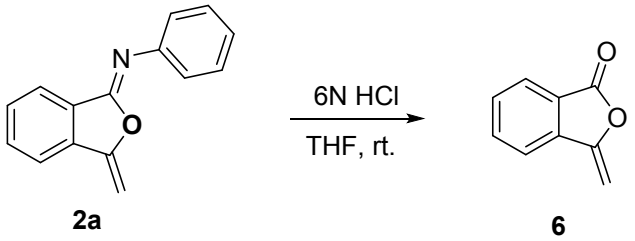


Compound **4** was synthesized according to the methods of reported literature[8]: the obtained product **2ak** (60 mg, 2.3 mmol) was dissolved in THF (2 mL). 6N HCl (0.5 mL) was added and the reaction mixture stirred at room temperature. After 3h, the reaction mixture was quenched with saturated aqueous $NaHCO_3$ and extracted by EtOAc (10 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by flash column chromatography on silica gel (PE:EtOAc = 8:1) to afford desired product **4** (*Z*/*E* = 25:1) (32.5 mg, 75%) as a light yellow oil. Major isomer shown: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (dt, *J* = 8.0, 1.2 Hz, 1H), 7.74 – 7.62 (m, 2H), 7.51 (ddd, *J* = 8.0, 6.8, 1.6 Hz, 1H), 5.66 (t, *J* = 8.0 Hz, 1H), 2.47 (q, *J* = 8.0 Hz, 2H), 1.56 (q, *J* = 7.6 Hz, 2H), 1.00 (t, *J* = 7.6 Hz, 3H). The spectroscopic date was in agreement with literature report.[8,9]

Compound **5** was synthesized according to the methods of reported literature[9]: to a solution of product **4** (30 mg, 1.6 mmol) in EtOAc (3 mL) was added Pd/C (5 %, 60 mg). The reaction mixture was allowed to stir under H_2 protection at room temperature. After 16 h, the reaction mixture was diluted with EtOAc (10 mL) and filtered over celite. The organic layer was separated and concentrated *in vacuo*. The residue was purified by flash chromatography on silica gel (PE:EtOAc = 8:1) to give the compound **NBP** (30 mg, 1.6 mmol, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.6 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.46 (d, *J* = 7.6 Hz, 1H), 5.49 (dd, *J* = 8.0, 4.0 Hz, 1H), 2.14 – 1.98 (m, 1H), 1.84 – 1.70 (m, 1H), 1.57 – 1.18 (m, 4H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.7, 150.1,

133.9, 129.0, 126.1, 125.6, 121.7, 81.4, 34.4, 26.9, 22.4, 13.9. The spectroscopic data were in agreement with literature report.[9]

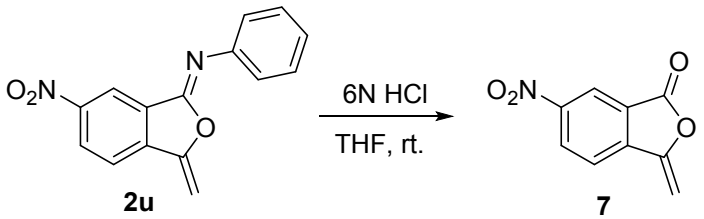
5.2 Transformation of the product 2a



2a **6**

Compound **6** was synthesized according to the methods of reported literature[8]: the obtained product **2a** (88 mg, 4 mmol) was dissolved in THF (2 mL). 6N HCl (1 mL) was added and the reaction mixture was stirred at room temperature. After 3 h, the reaction mixture was quenched with saturated aqueous $NaHCO_3$ and extracted by EtOAc (10 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by flash column chromatography on silica gel (PE:EtOAc = 8:1) to afford desired product **6** (46 mg, 78%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.6 Hz, 1H), 7.73 (d, *J* = 4.4 Hz, 2H), 7.60 (dq, *J* = 8.0, 4.4 Hz, 1H), 5.24 (t, *J* = 2.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9, 151.8, 139.0, 134.5, 130.5, 125.3, 125.1, 120.6, 91.3. The spectroscopic date of **6** were in agreement with literature report.[9]

5.3 Transformation of the product 2u



2u **7**

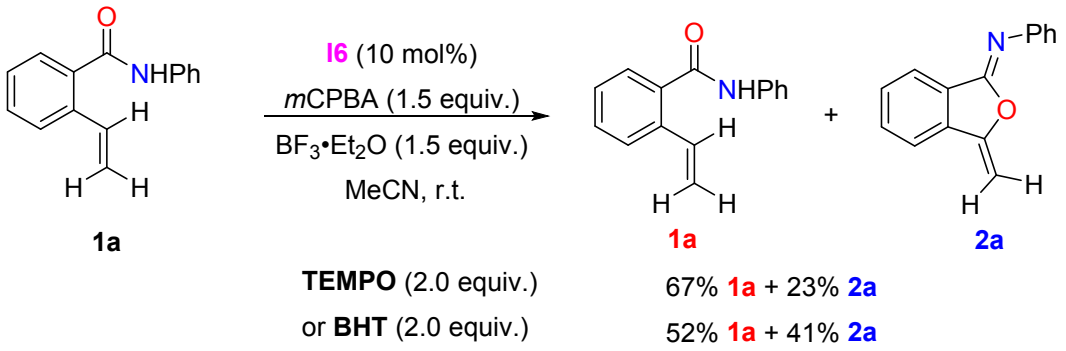
Compound **7** was synthesized according to the methods of reported literature[8]: The obtained product **2u** (106 mg, 4 mmol) was dissolved in THF (2 mL). 6N HCl (1 mL) was added and the reaction mixture was stirred at room temperature. After 3h, the reaction mixture was quenched with saturated aqueous $NaHCO_3$ and extracted by

EtOAc (10 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by flash column chromatography on silica gel (PE:EtOAc = 8:1) to afford desired product **7** (61 mg, 80%) as white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (dd, *J* = 2.0, 0.8 Hz, 1H), 8.61 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.94 (dd, *J* = 8.4, 0.8 Hz, 1H), 5.54 – 5.47 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ164.4, 150.4, 149.4, 143.3, 129.4, 126.4, 122.0, 121.3, 95.8; HRMS: $[M+H]^+$ calcd for $C_9H_5NO_4$ 192.0291, found 192.0280.

5. Control experiments

6.1 Free radical inhabitation test

Scheme S1 Free radical inhabitation test.

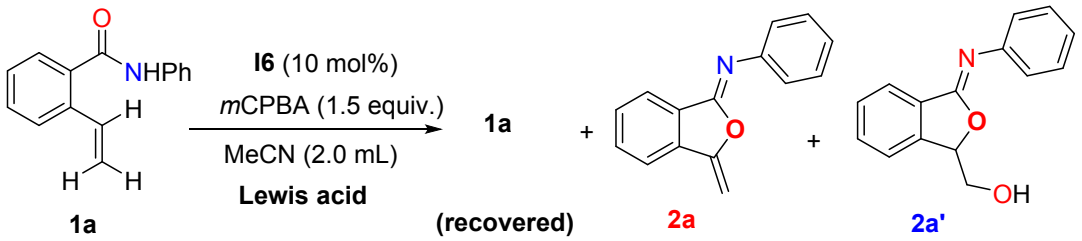


[a] Reaction conditions: **61a** (0.2 mmol), **I6** (0.02 mmol), *m*CPBA (0.3 mmol, 1.5 equiv.), $BF_3{\cdot}Et_2O$ (0.3 mmol, 1.5 equiv.), MeCN (2 mL), r.t., air atmosphere, 30 min. [b] Isolated yield.

Experimental Procedure: *m*CPBA (64.8 mg, 80%, 0.3 mmol) and **I6** (4.4 mg 0.02 mmol) were weighted into an oven-dried 10 mL Pyrex tube equipped with a magnetic stir bar. CH_3CN (2.0 mL) was added and the reaction mixture was stirred vigorously for 5 min. Then, **1a** (44.6 mg, 0.2 mmol), **TEMPO/BHT (0.4 mmol, 2.0 equiv.)** and $BF_3{\cdot}Et_2O$ (38 μL, 0.3 mmol) were added in turn. The reaction mixture was stirred at room temperature, which was detected by TLC until completely finished. Then, the mixture was directly purified by flash chromatography (mixture of one tenth Alumina-B and nine tenth silica gel) with an eluent of PE:EtOAc = 30:1 to afford the desired product. For 2.0 equiv. TEMPO, 67 % **1a** was recovered and 23 % **2a** was isolated. For 2 equiv. BHT, 52 % **1a** was recovered and 41 % **2a** was isolated.

6.2 Further Lewis acid comparative experiments (Scheme 5a)

Scheme S2 Further Lewis acid effect experiments[a,b]



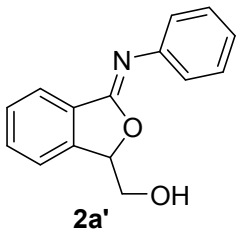
MsOH (2.0 equiv.)	50% **1a** + 10% **2a** + 23% **2a'**
TFA (2.0 equiv.)	20% **1a** + 9% **2a** + 45% **2a'**
TsOH (2.0 equiv.)	5% **1a** + 12% **2a** + 73% **2a'**
BF_3•Et_2O (1.2 equiv.)	10% **1a** + 78% **2a**
BF_3•Et_2O (1.5 equiv.)	90% **2a**
BF_3•Et_2O (2.0 equiv.)	85% **2a**

[a] Reaction conditions: **1a** (0.2 mmol), **I6** (0.02 mmol), *m*CPBA (0.3 mmol, 1.5 equiv.), **Lewis acid**, MeCN (2 mL), r.t., air atmosphere, 30 min. [b] Isolated yield.

Experimental Procedure: *m*CPBA (64.8 mg, 80%, 0.3 mmol) and **I6** (4.4 mg 0.02 mmol) were weighted into an oven-dried 10 mL Pyrex tube equipped with a magnetic stir bar. Dry CH_3CN (2.0 mL) was added and the reaction mixture was stirred vigorously for 5 min. Then, **1a** (44.6 mg, 0.2 mmol) and **Lewis acid** were added in turn. The reaction mixture was stirred at room temperature, which was detected by TLC until completely finished. Then, the mixture was directly purified by flash chromatography (mixture of one tenth Alumina-B and nine tenth silica gel) with an eluent of PE:EtOAc = 30:1 to afford the desired product.

Characterization data of 2a':

(*Z*)-(3-(phenylimino)-1,3-dihydroisobenzofuran-1-yl)methanol (2a'):



2a'

Colorless oil (37.3 mg, 78%); ^{1}H NMR (600 MHz, $CDCl_3$) ^{1}H NMR (600 MHz,) δ 7.91 (d, J = 7.6 Hz, 1H), 7.51 (t, J = 7.6 Hz, 1H), 7.43 (t, J = 7.6 Hz, 1H), 7.37 – 7.32 (m, 1H), 7.32 – 7.22 (m, 4H), 7.11 – 7.04 (m, 1H), 5.52 (t, J = 4.4 Hz, 1H), 3.97 – 3.90 (m, 1H), 3.81 – 3.74 (m, 1H), 3.30 (br, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.8, 146.2, 143.4, 132.1, 131.3, 129.3, 128.7 (2C), 124.2, 124.1, 123.5 (2C), 121.6, 84.9, 64.2; HRMS: $[M+H]^+$ calcd for $C_{15}H_{13}NO_2$ 240.1019, found 240.1013.

6.3 ^{1}H NMR experiments

6.3.1 Characterization of product 2a

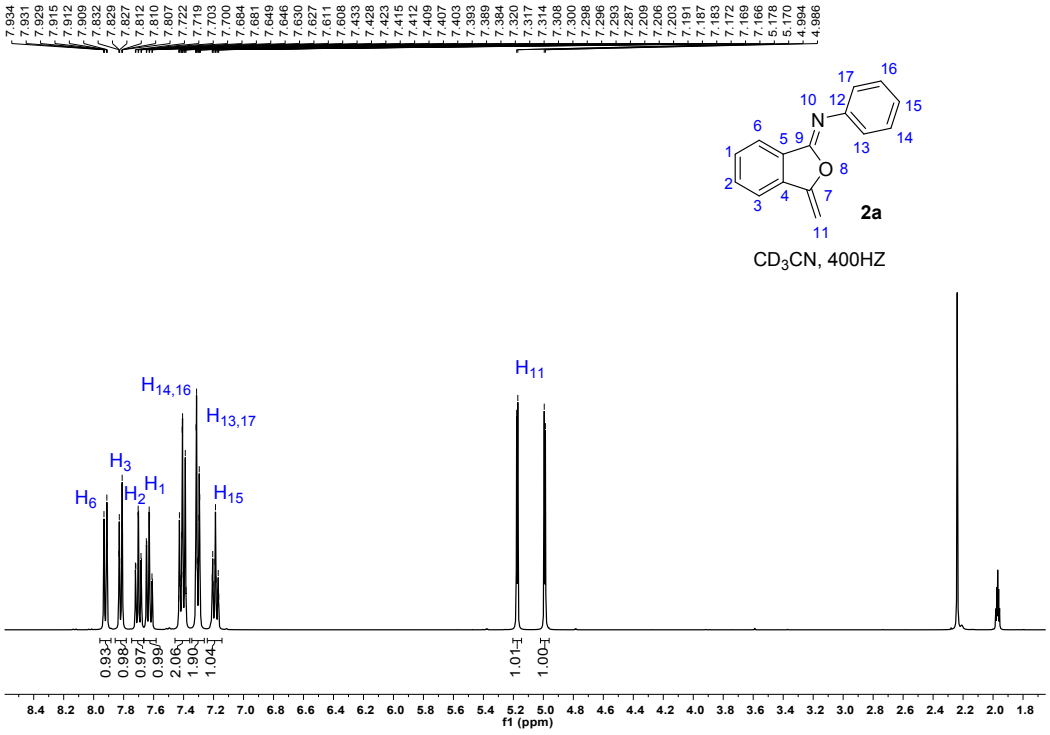


Figure S1 ^{1}H NMR spectrum for **2a** in CD_3CN

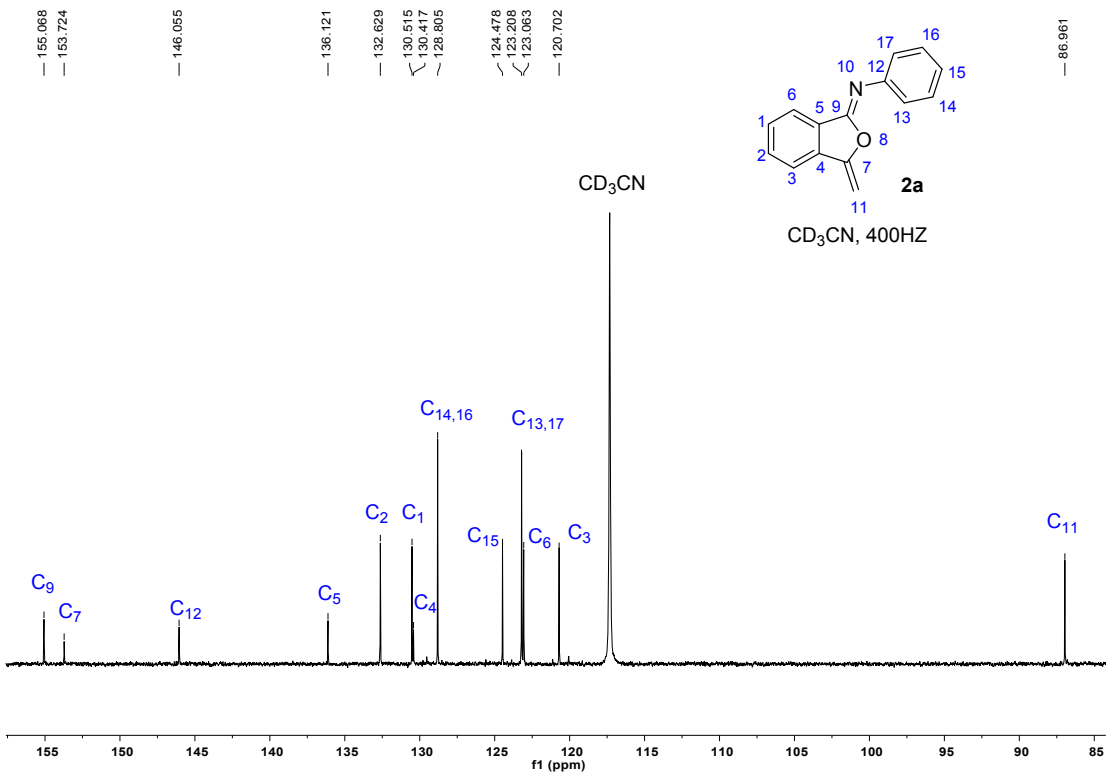


Figure S2 ^{13}C NMR spectrum for **2a** in CD_3CN

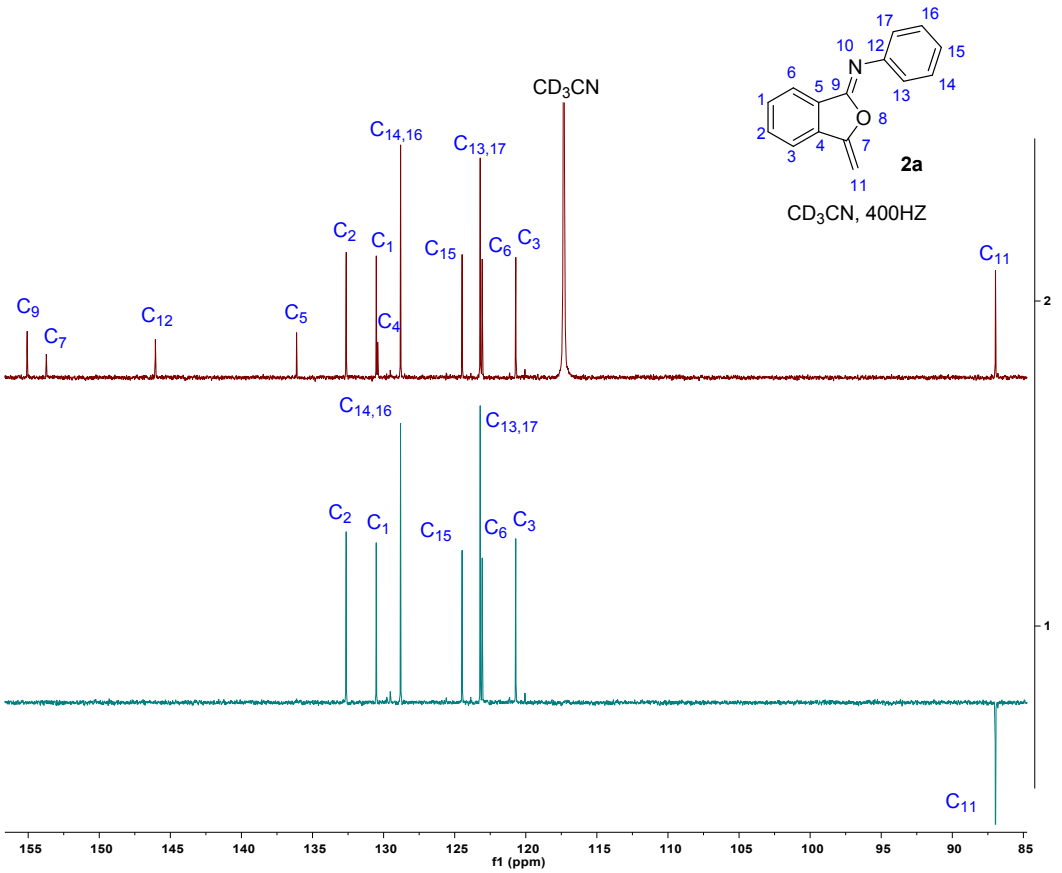


Figure S3 DEPT 135° spectrum for **2a** in CD_3CN

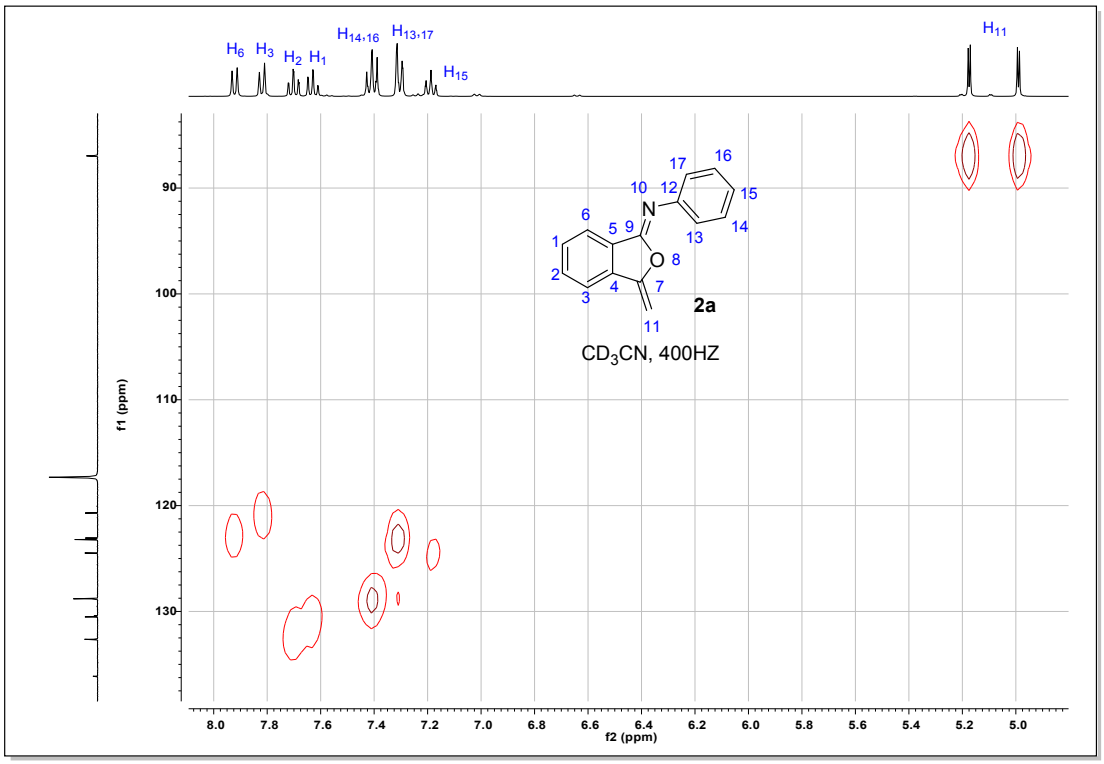
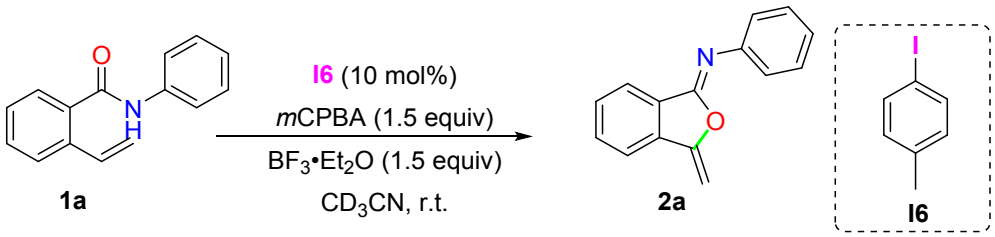


Figure S4 HSQC spectrum for **2a** in CD_3CN

6.3.2 Dynamic ^{1}H NMR analysis (Scheme 5b)



Experimental Procedure: *m*CPBA (21.6 mg, 80%, 0.075 mmol), **I6** (1.1 mg 0.005 mmol) and **1a** (11.2 mg, 0.05 mmol) were weighted into an oven-dried septum-capped NMR tube. CD_3CN (0.5 mL, with 0.5 μL CH_2Br_2/mL) was added the for the first ^{1}H NMR spectroscopic analyses. Then $BF_3{\cdot}Et_2O$ (10 μL, 0.075 mmol) was added to the NMR tube and the ^{1}H NMR spectrum was detected continuously until completed.

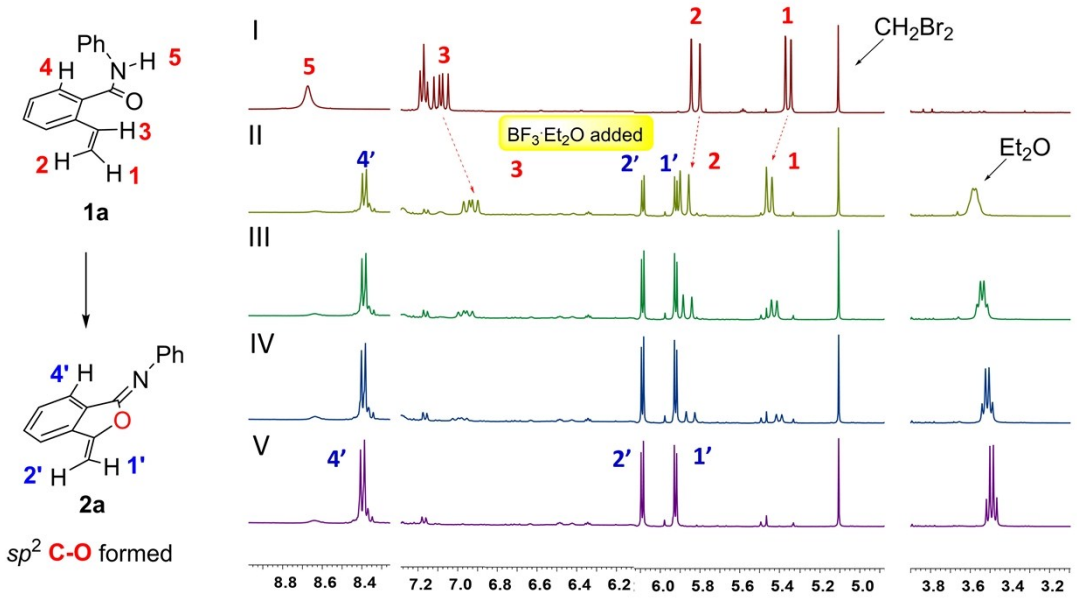
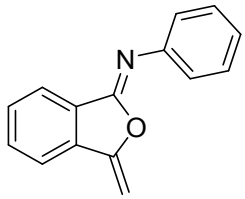
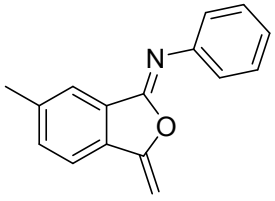


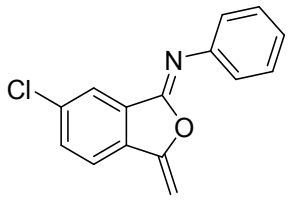
Figure S5 [a] **I**: ^{1}H NMR (400 MHZ) spectra of reaction mixture of **1a** (0.05 mmol), **I6** (10 mol%), and *m*CPBA (0.075 mmol) in CD_3CN (0.5 mL) with CH_2Br_2 (2.5 μL) as internal standard. **II**: $BF_3{\cdot}Et_2O$ (0.075 mmol) was added to the NMR tube; **III**: for 12 min; **IV**: for 22 min; **V**: for 30 min.

Discussion:

The reaction progress was conveniently showed by chemical shifts and intensity changes in hydrogen resonances obtained from ^{1}H NMR spectroscopy As shown, no obvious signal changes were observed during the oxidation of **1a** with *m*CPBA (Figure S5, I). Upon adding $BF_3{\cdot}Et_2O$, signals of substrate (**H1**, **H2** and **H3**) decreased and new signals of product (**H1'**, **H2'**, and **H4'**) appeared (Figure S5, II). And the gradual appearance of free Et_2O (–CH_2 signals) confirmed liberation of the BF_3 unit (Figure S5, II–V). These outcomes confirmed the significant role of $BF_3{\cdot}Et_2O$ in triggering and accelerating the reaction process. Elongated reaction times (30 min) enabled the formation of **2a** in 95% ^{1}H NMR yield as the main product (Figure S5, V).

6. Comparison of the structure data of 2a, 2s and 2t with the reported[10]

	**4a** reported by Liu group[10]	Blue solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 - 7.90 (m, 1H), 7.79 - 7.73 (m, 1H), 7.67 - 7.61 (m, 1H), 7.59 - 7.48 (m, 3H), 7.44 - 7.34 (m, 3H), 5.24 - 7.21 (m, 1H), 4.82 - 4.78 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 143.1, 136.2, 134.5, 132.3, 129.8, 129.3, 128.9, 128.1, 128.0, 123.6, 120.0, 90.5; HRMS: $[M+H]^+$ calcd for $C_{15}H_{11}NO$ 222.0913, found 222.0912.
	2a reported by our group	Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.68 – 7.58 (m, 1H), 7.58 – 7.48 (m, 1H), 7.45 – 7.31 (m, 3H), 7.16 (tt, *J* = 6.8, 2.0 Hz, 1H), 5.00 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 153.9, 145.7, 136.2, 132.2, 130.8, 130.2, 128.8 (2C), 124.7, 123.7 (2C), 123.6, 120.3, 87.2; HRMS: $[M+H]^+$ calcd for $C_{15}H_{11}NO$ 222.0913, found 222.0912.
	**4b** reported by Liu group[10]	Blue solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.47 - 7.41 (m, 2H), 7.38 (t, *J* = 7.8 Hz, 2H), 5.16 (d, *J* = 1.9 Hz, 1H), 4.75 (d, *J* = 1.9 Hz, 1H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 143.1, 140.2, 134.6, 133.7, 133.3, 129.3, 128.1, 127.9, 126.5, 123.7, 119.9, 89.7, 21.6; HRMS (ESI) calcd for $C_{16}H_{14}NO^+$: 236.1070 (M^++H), found: 236.1076.
	2s reported by our group	Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.37 (d, *J* = 5.6 Hz, 5H), 7.15 (tt, *J* = 6.4, 2.4 Hz, 1H), 4.93 (q, *J* = 2.8 Hz, 2H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.2, 154.0, 145.7, 140.7, 133.8, 133.4, 131.1, 128.7(2C), 124.6, 123.7 (2C), 123.6, 120.1, 86.3, 21.6; HRMS: $[M+H]^+$ calcd for $C_{16}H_{13}NO$ 236.1070, found 236.1071.

	**4e** reported by Liu group[10]	Blue solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 2H), 7.47 - 7.41 (m, 2H), 7.38 (t, *J* = 7.8 Hz, 2H), 5.16 (d, *J* = 1.9 Hz, 1H), 4.75 (d, *J* = 1.9 Hz, 1H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 143.1, 140.2, 134.6, 133.7, 133.3, 129.3, 128.1, 127.9, 126.5, 123.7, 119.9, 89.7, 21.6; HRMS (ESI) calcd for $C_{16}H_{14}NO^+$: 236.1070 (M^++H), found: 236.1076.
	2t reported by our group	White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 1.6 Hz, 1H), 7.53 (s, 2H), 7.37 (d, *J* = 4.4 Hz, 4H), 7.17 (tt, *J* = 5.4, 3.6 Hz, 1H), 5.01 (d, *J* = 3.2 Hz, 1H), 4.97 (d, *J* = 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.4, 152.3, 145.1, 136.4, 134.5, 132.5, 132.5, 128.8 (2C), 125.1, 123.9 (2C), 123.6, 121.5, 87.8; HRMS: $[M+H]^+$ calcd for $C_{15}H_{10}ClNO$ 256.0524, found 256.0523.

7. Reference

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9. X. He and F. Xue, *Tetrahedron Lett.*, 2014, **55**, 1956.

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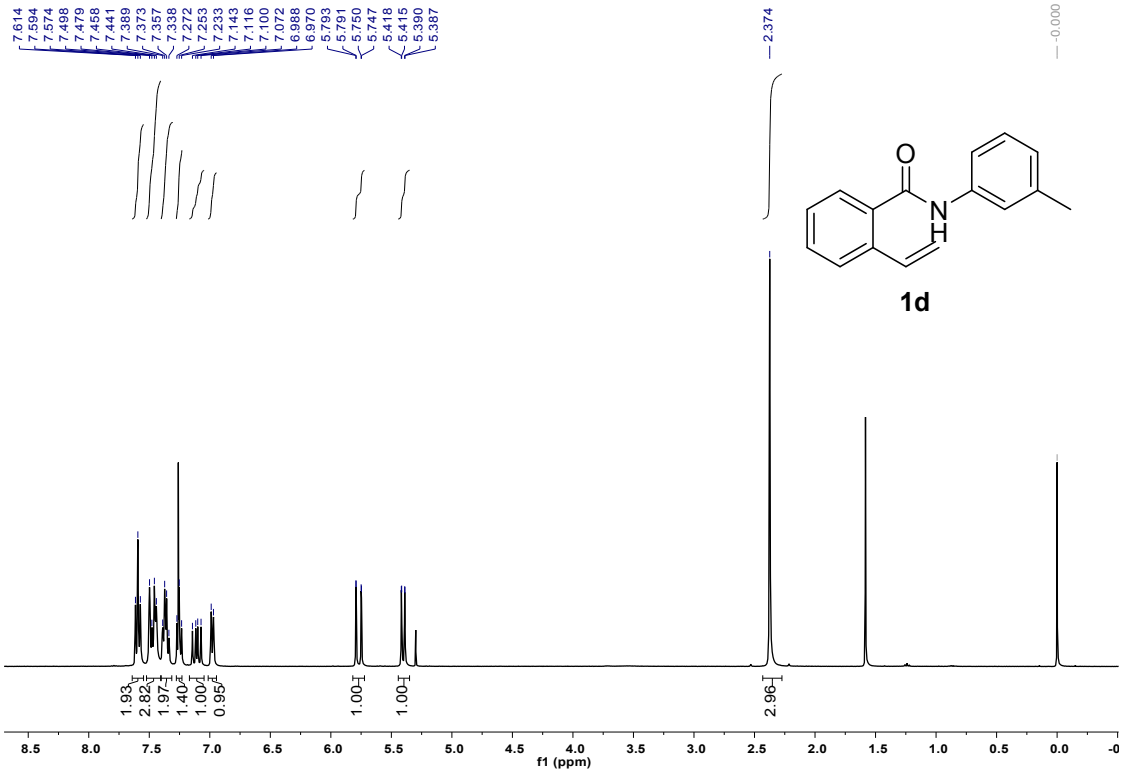
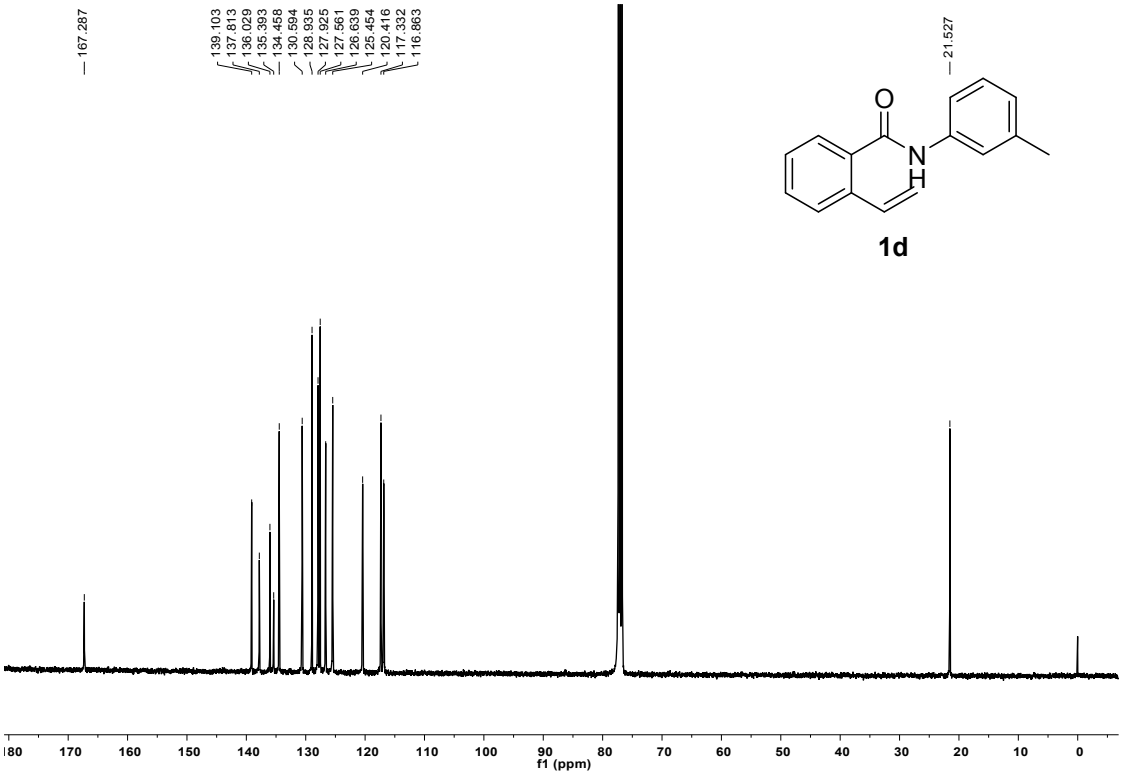
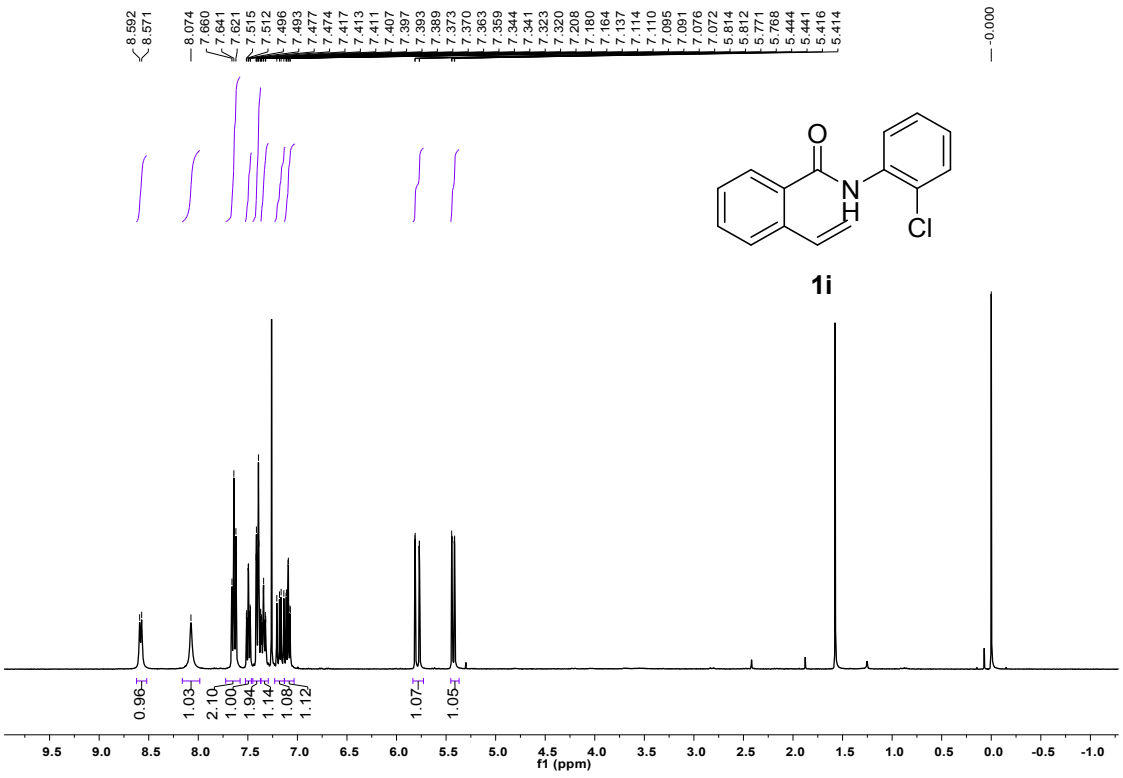
8. ^{1}H, ^{13}C and ^{19}F NMR spectra



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5.771
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N
H
Cl
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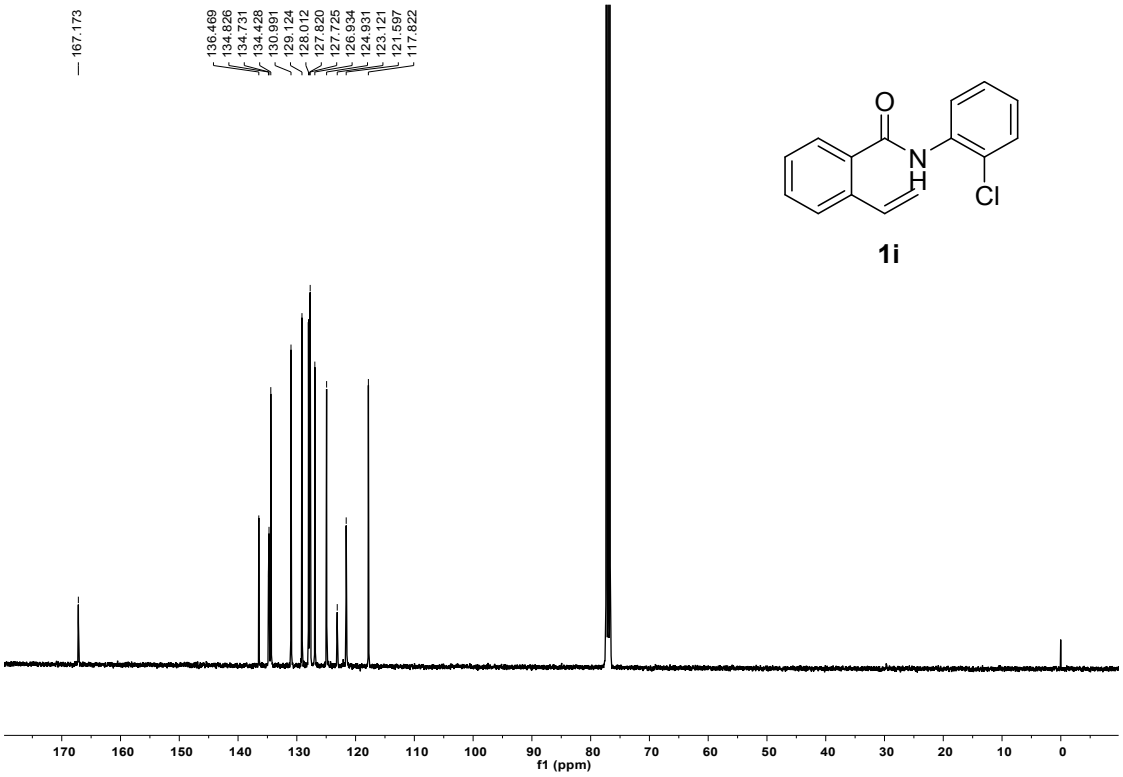
1.05
f1 (ppm)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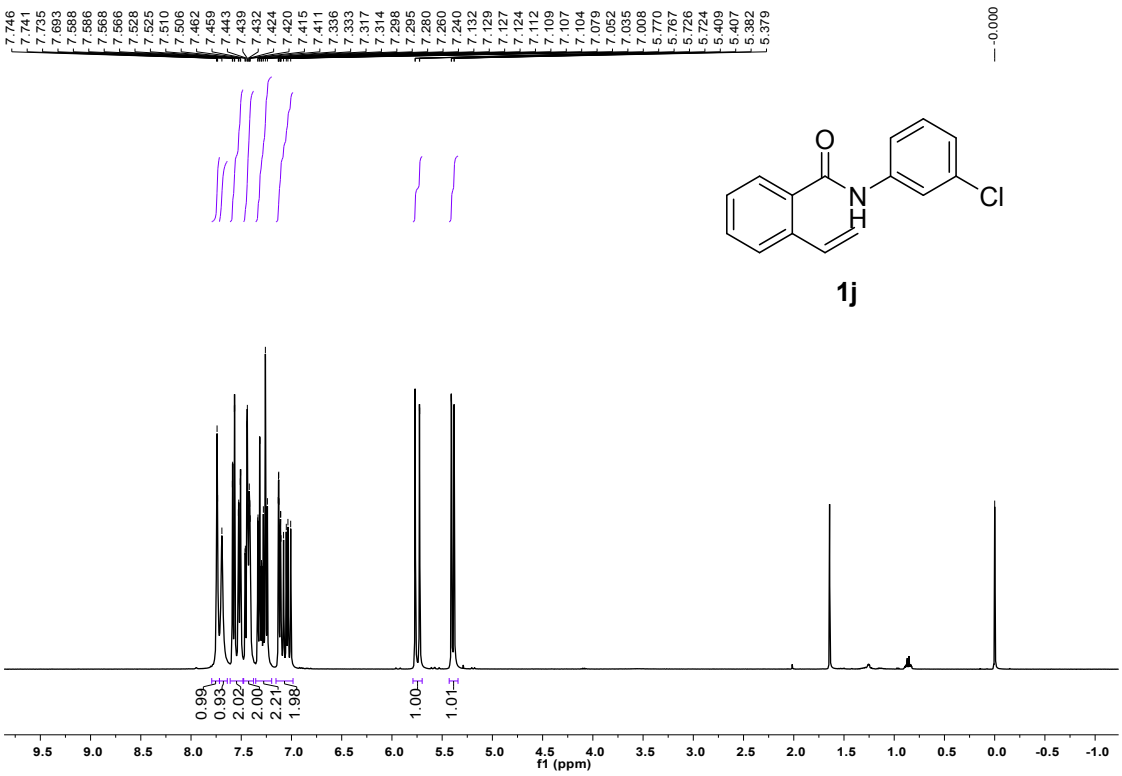
H
Cl
1i
f1 (ppm)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2.00
2.21
1.98
1.00
1.01
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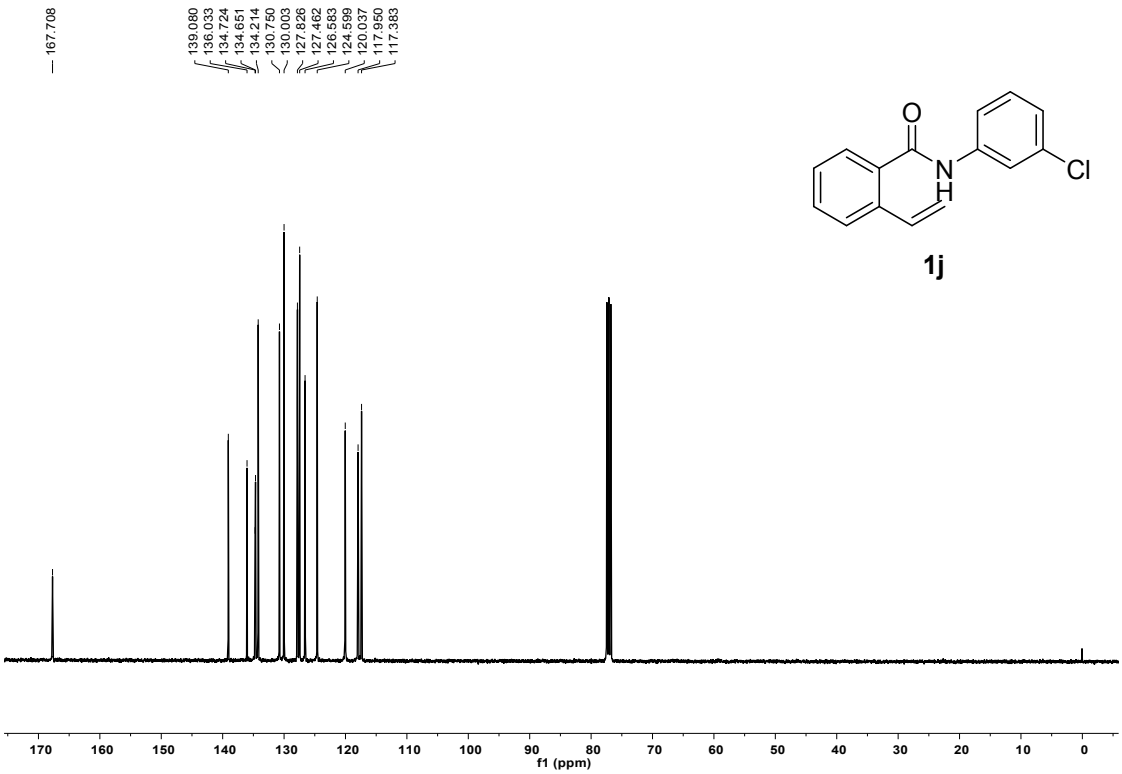
f1 (ppm)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Cl
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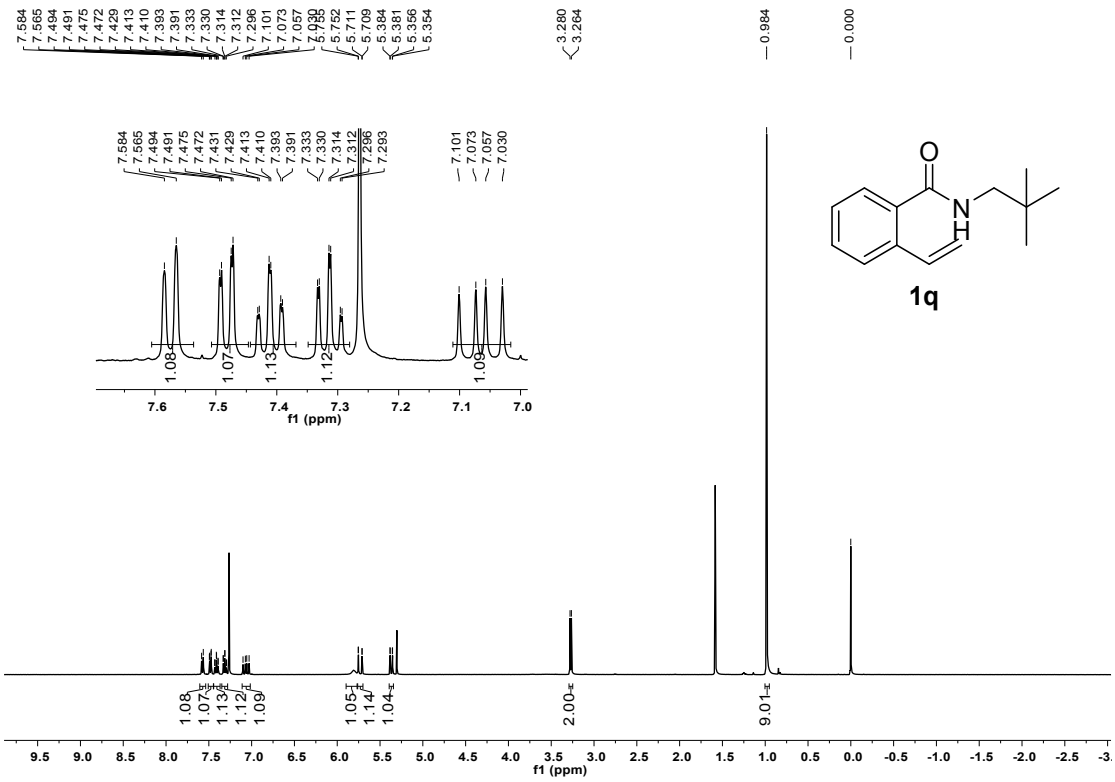
f1 (ppm)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1.07
1.13
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1.09
f1 (ppm)
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N
H
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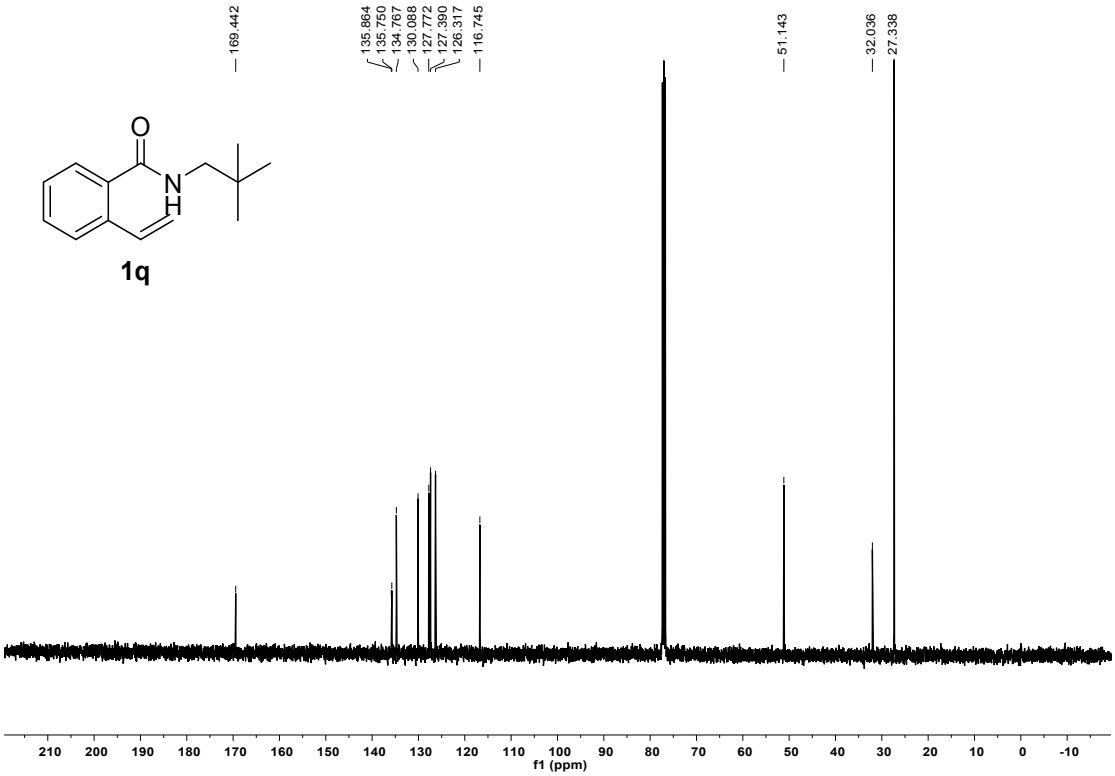
f1 (ppm)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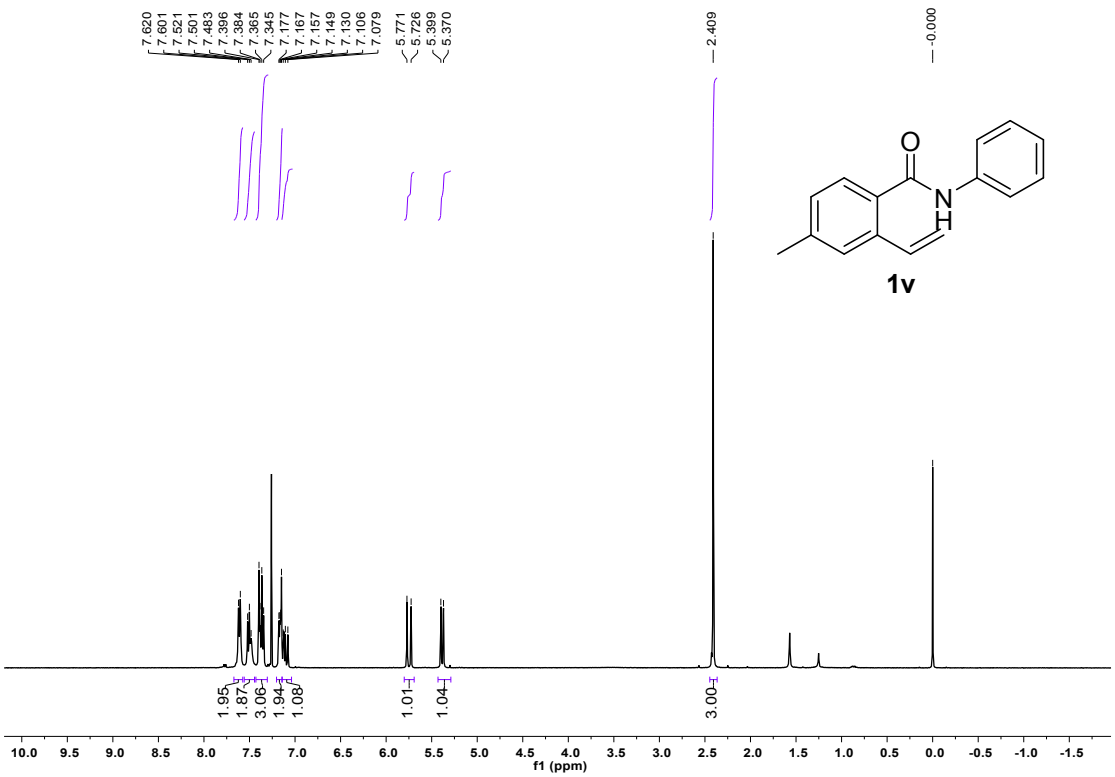
f1 (ppm)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7.130
7.106
7.079
5.771
5.726
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5.370
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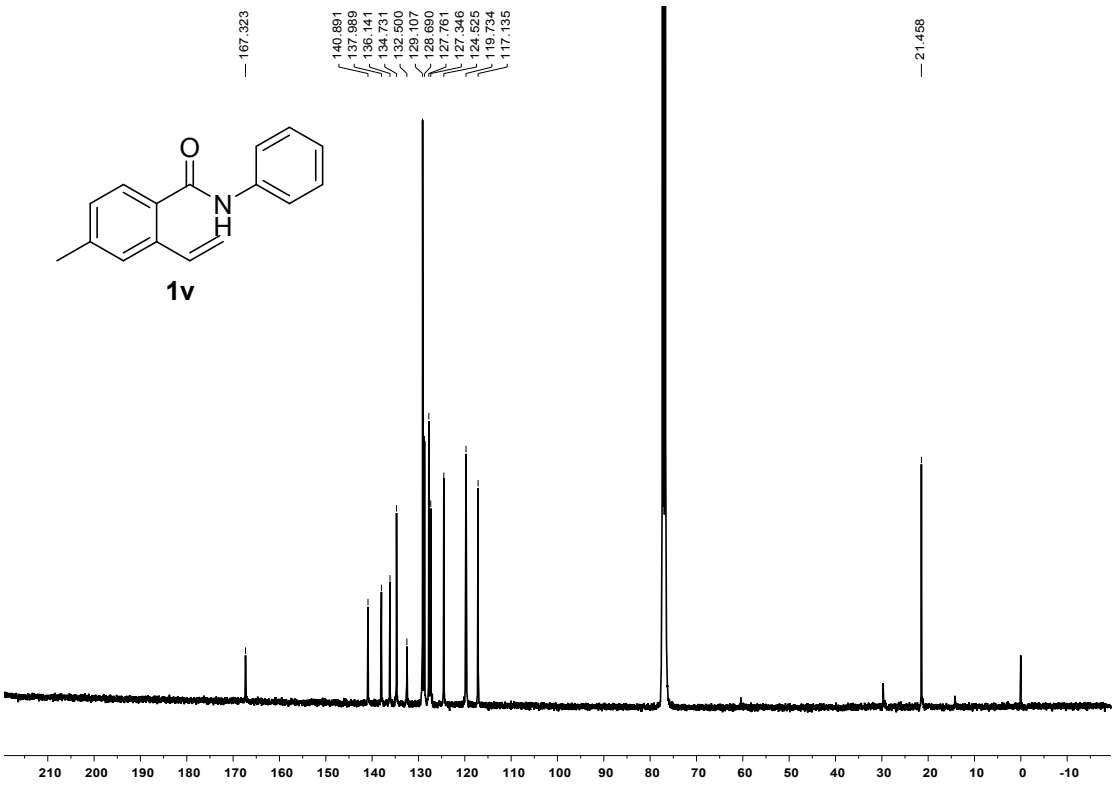
f1 (ppm)
1v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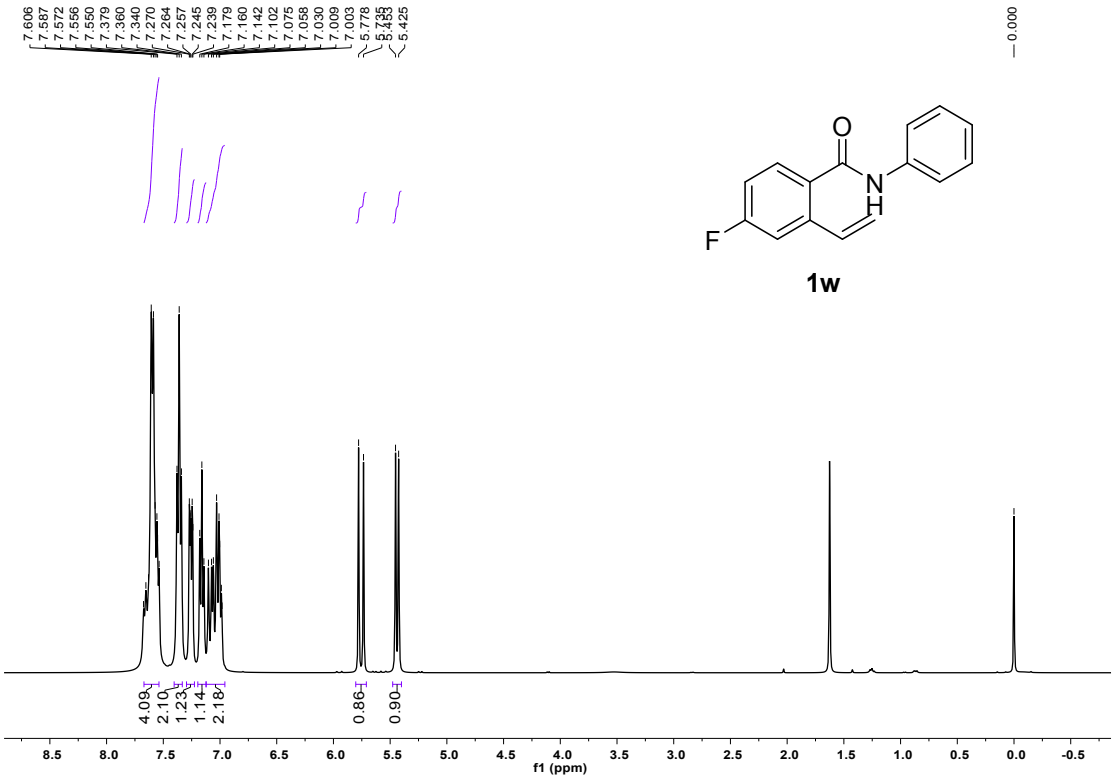
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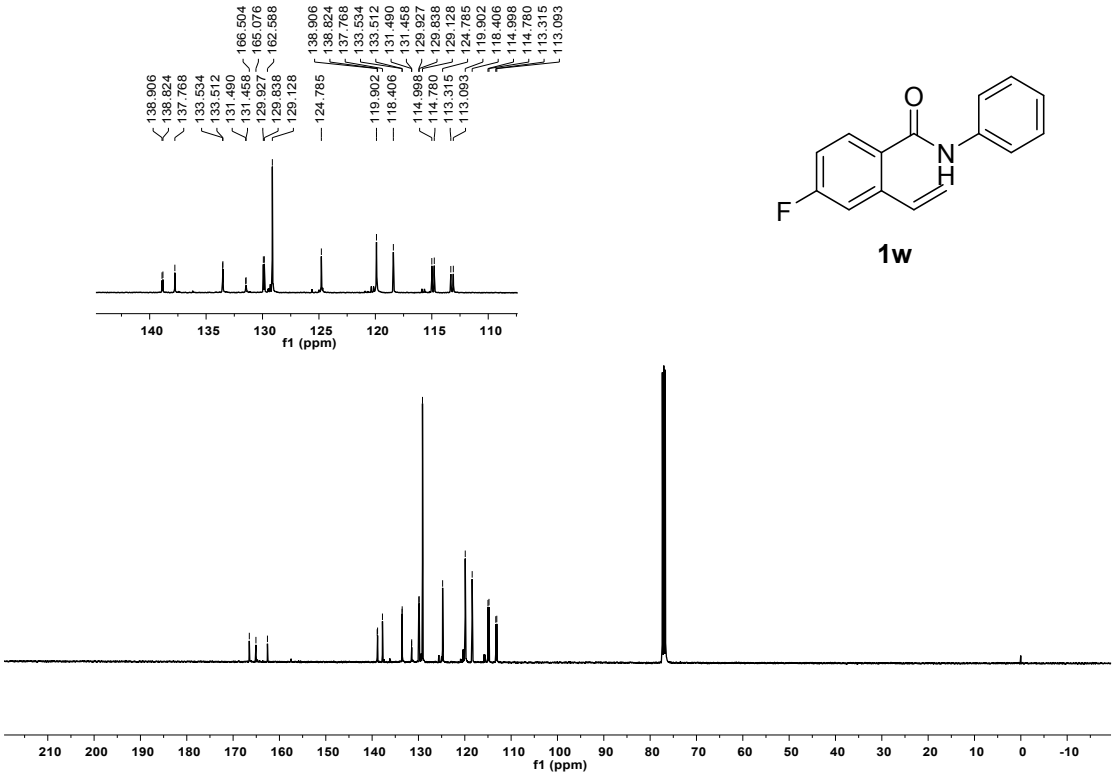
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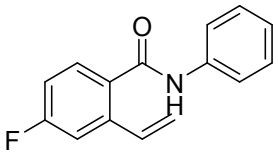
f1 (ppm)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F

1w

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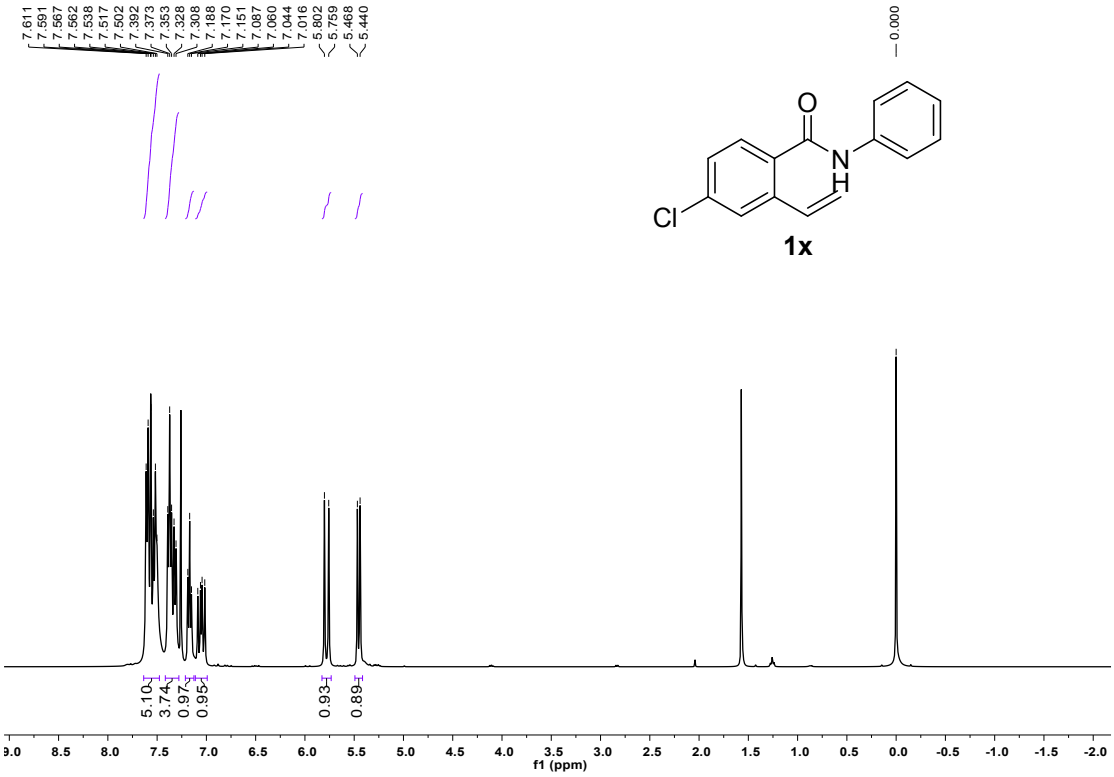
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7.044
7.016
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5.440
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0.95
0.93
0.89
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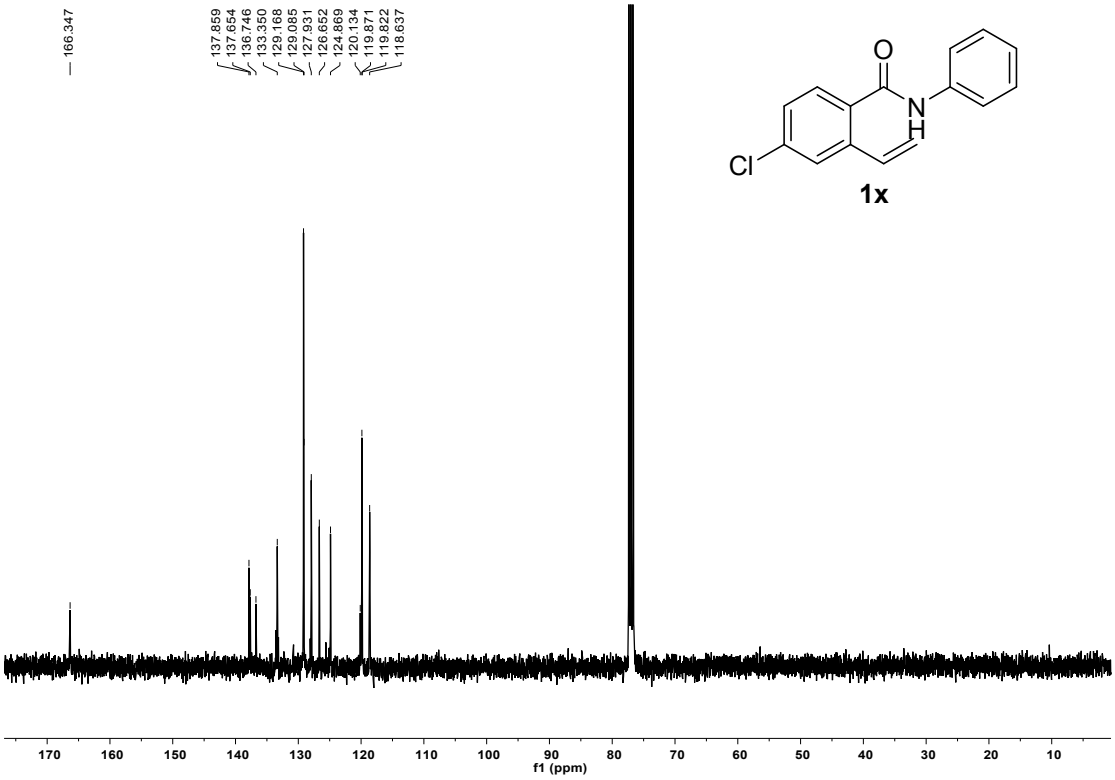
N
H
Cl

1x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O
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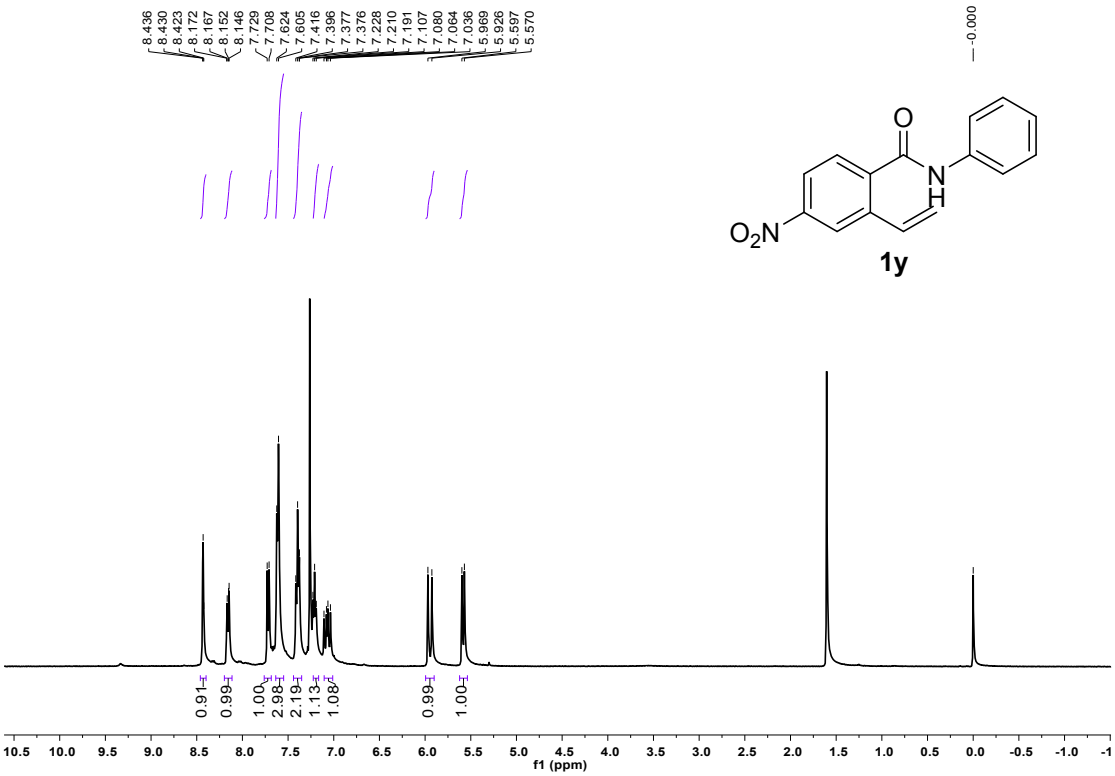
H
Cl
1x
f1 (ppm)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7.064
7.036
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5.926
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5.570
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N
H
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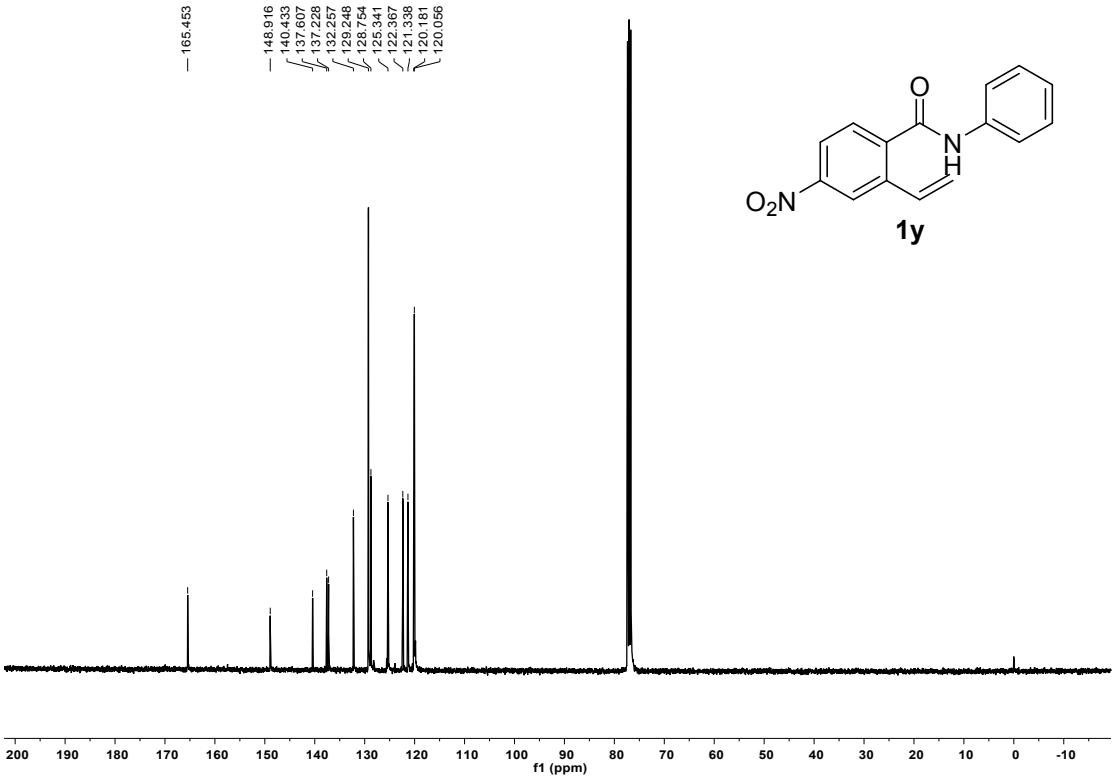
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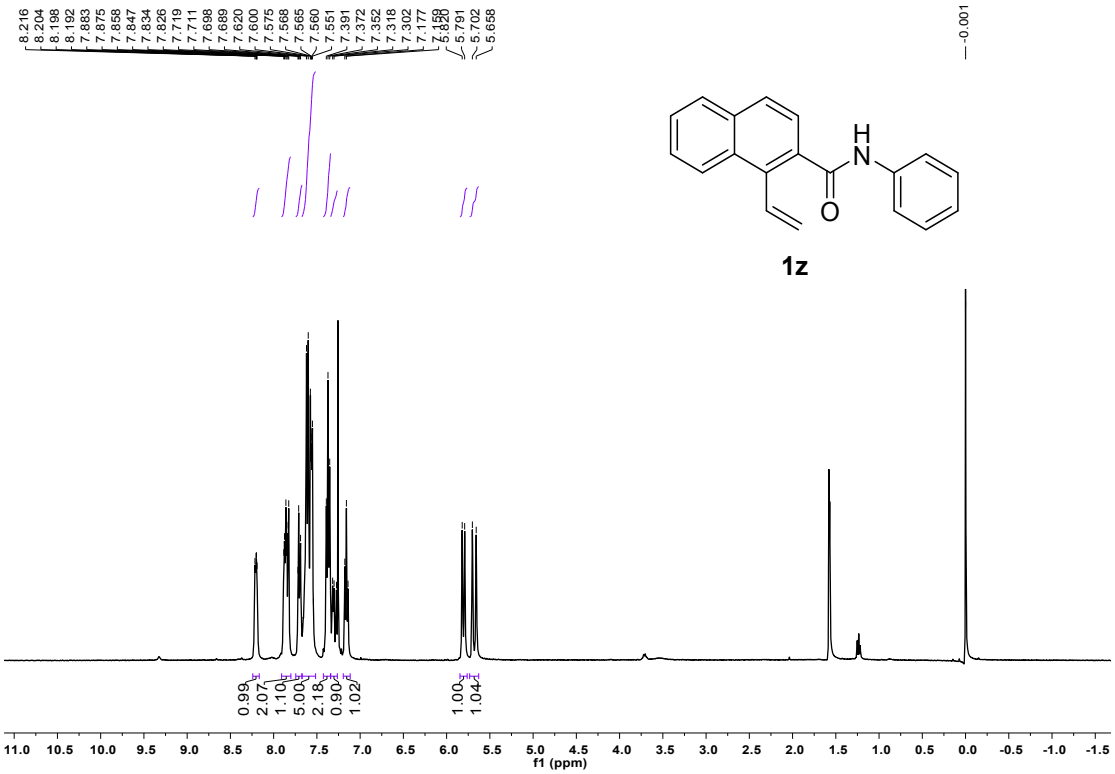
N
H
O2N
1y
f1 (ppm)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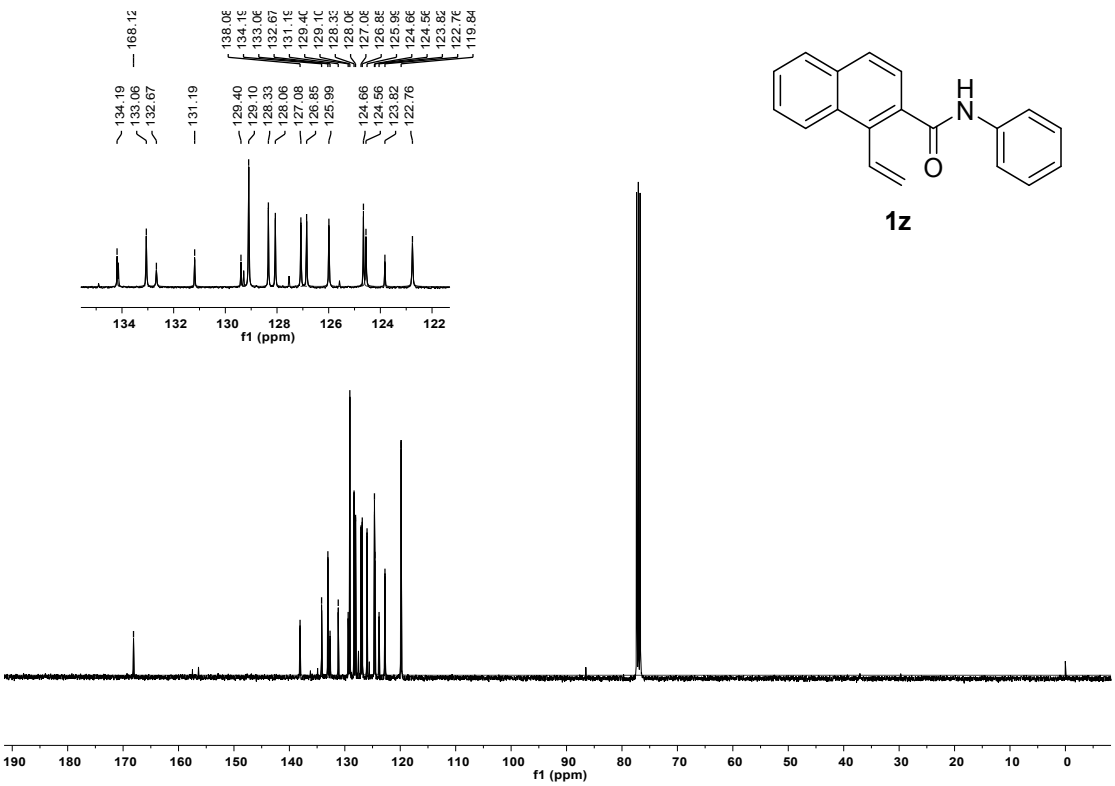
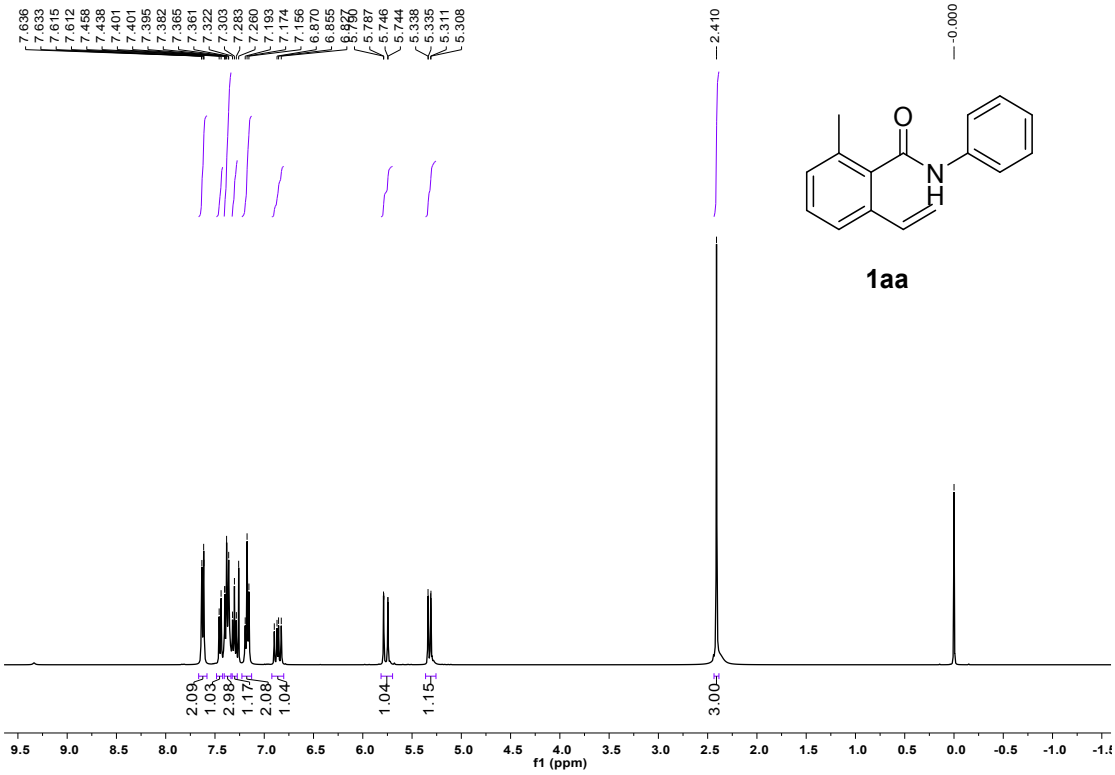
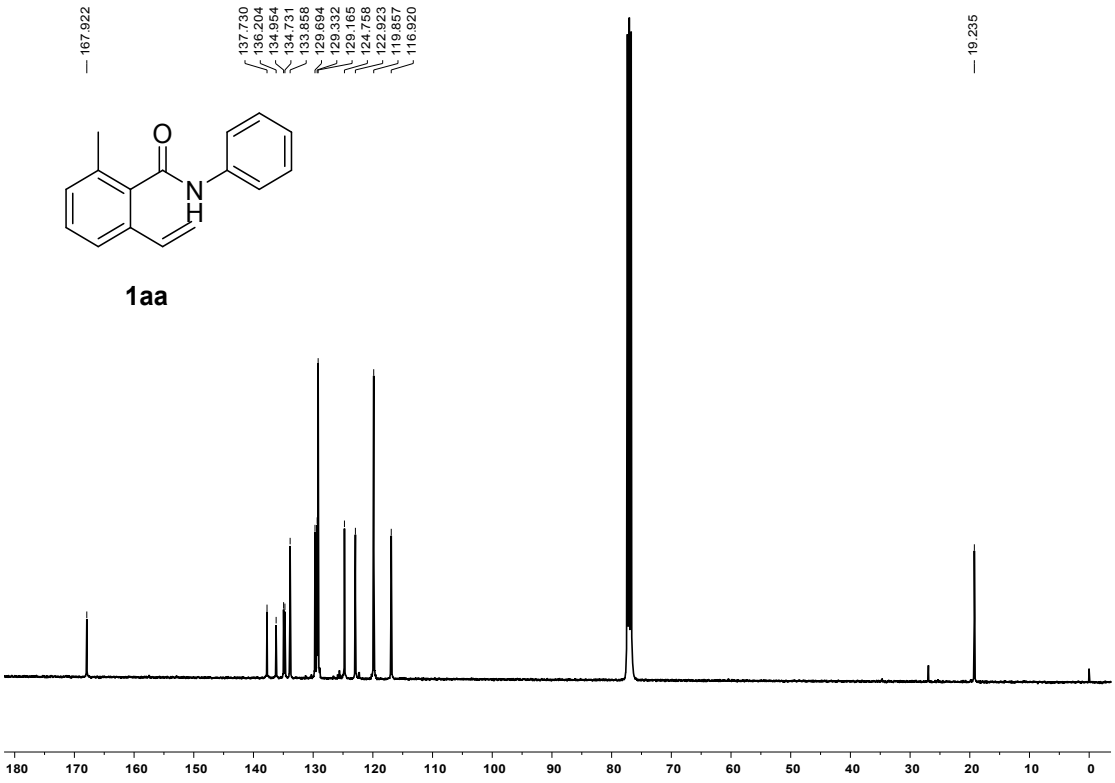
7.698
7.689
7.620
7.600
7.575
7.568
7.565
7.560
7.551
7.391
7.372
7.352
7.318
7.302
7.177
5.791
5.702
5.658
-0.001
H
N
O
1z
0.99
2.07
1.10
5.00
2.18
0.90
1.02
1.00
1.04
f1 (ppm)

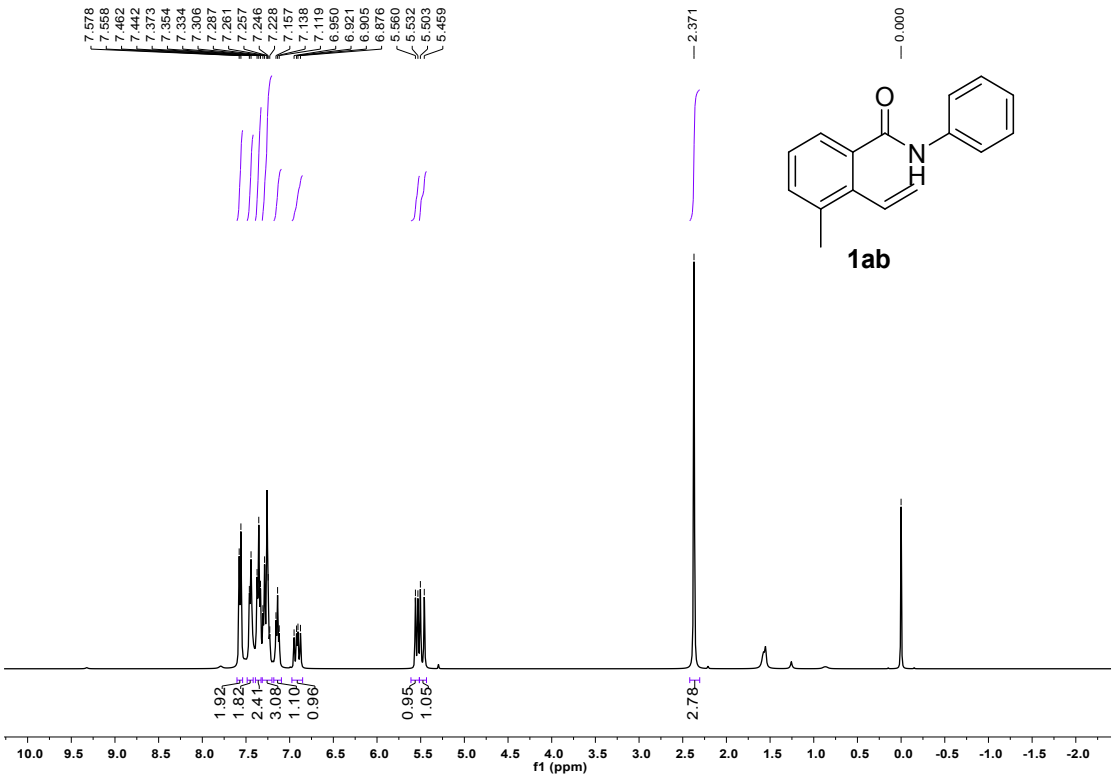

134.19
133.06
132.67
131.19
129.40
129.10
128.33
128.06
127.08
126.85
125.99
124.66
124.56
123.82
122.76
f1 (ppm)
f1 (ppm)

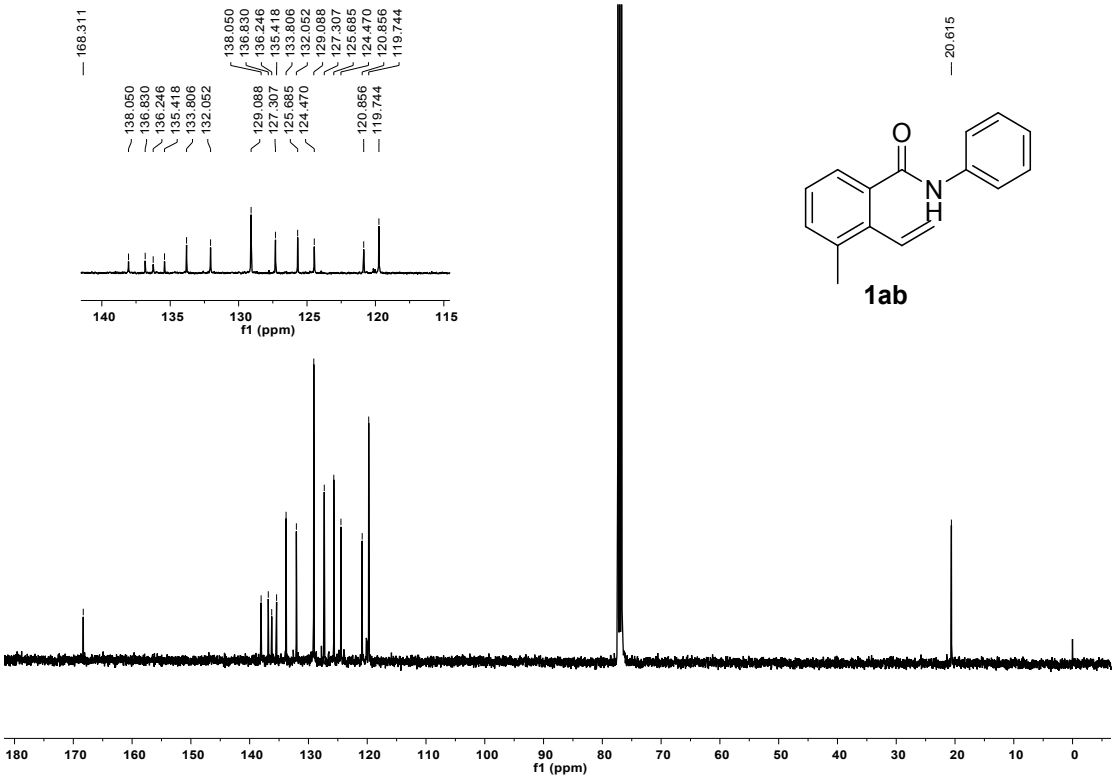
1z

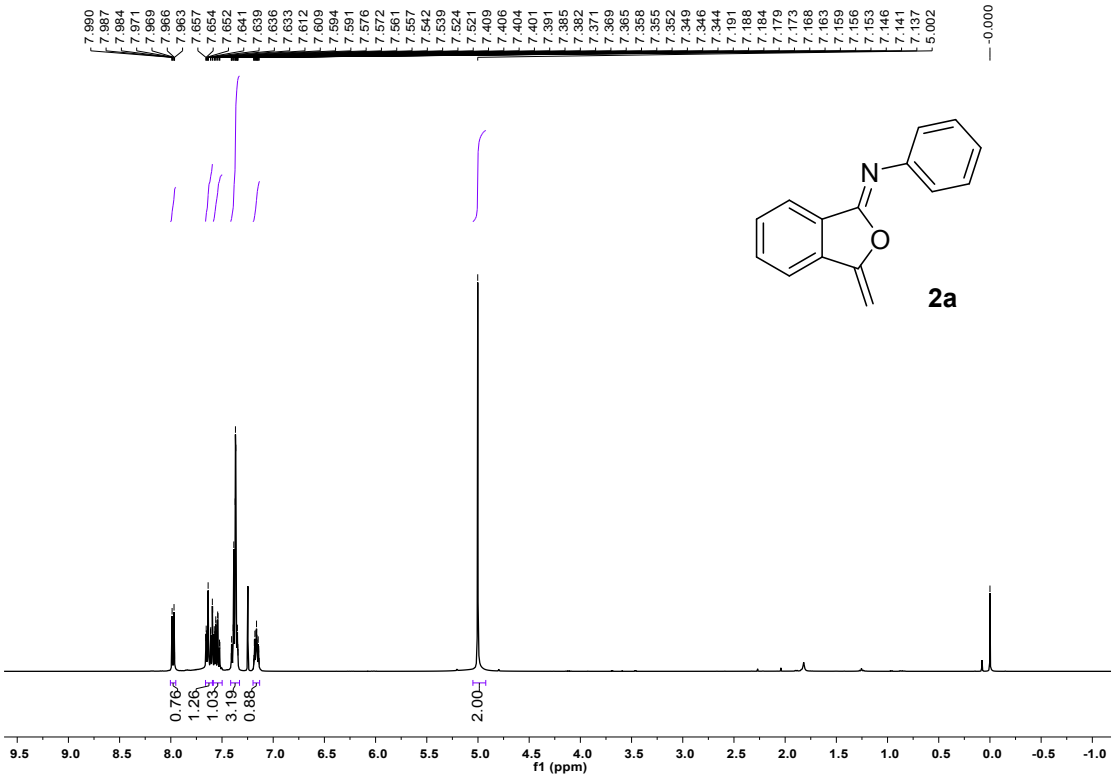

7.636
7.633
7.615
7.612
7.458
7.438
7.401
7.401
7.395
7.382
7.365
7.361
7.322
7.303
7.283
7.260
7.193
7.174
7.156
6.870
6.855
5.790
5.787
5.746
5.744
5.338
5.335
5.311
5.308
2.410
-0.000
2.09
1.03
2.98
1.17
2.08
1.04
1.04
1.15
3.00
f1 (ppm)

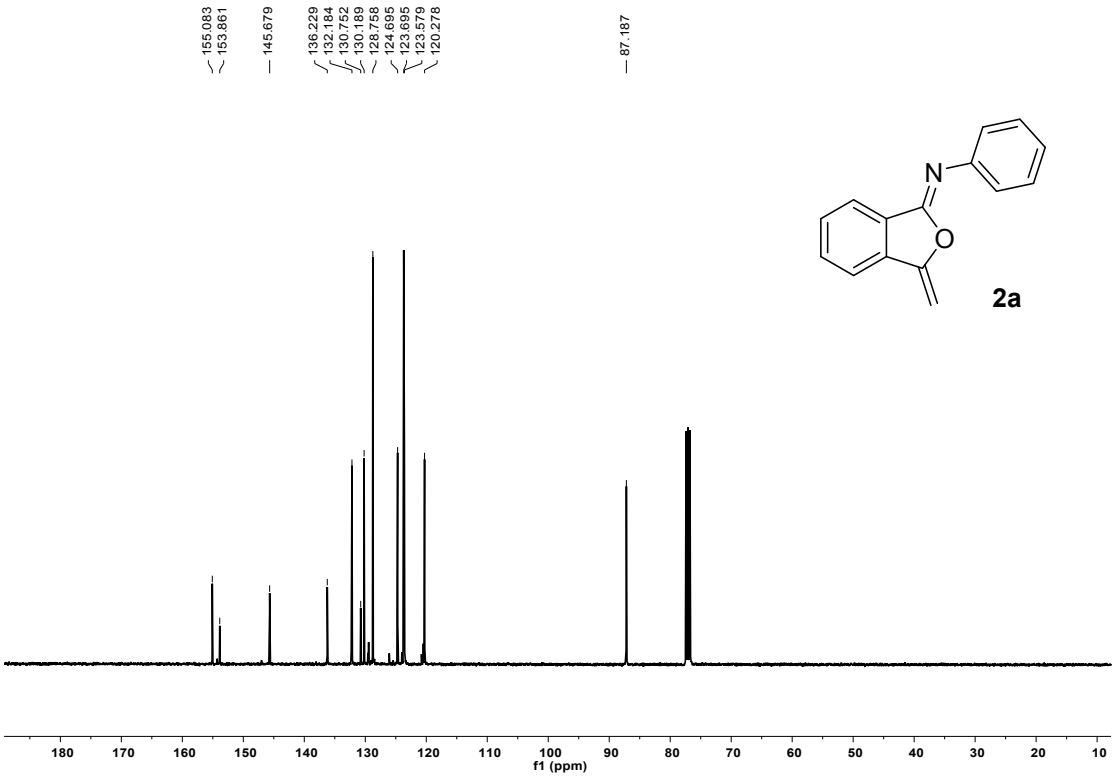
1aa


167.922
137.730
136.204
134.954
134.731
133.858
129.694
129.332
129.165
124.758
122.923
119.857
116.920
19.235
O
N
H
1aa


7.578
7.558
7.462
7.442
7.373
7.354
7.334
7.306
7.287
7.261
7.257
7.246
7.228
7.157
7.138
7.119
6.950
6.921
6.905
6.876
5.560
5.532
5.503
5.459
2.371
0.000
O
N
H
1ab
1.92
1.82
2.41
3.08
1.10
0.96
0.95
1.05
2.78
f1 (ppm)


168.311
138.050
136.830
136.246
135.418
133.806
132.052
129.088
127.307
125.685
124.470
120.856
119.744
20.615
O
N
H
1ab
f1 (ppm)


7.990
7.987
7.984
7.971
7.969
7.966
7.963
7.657
7.654
7.652
7.641
7.639
7.636
7.633
7.612
7.609
7.594
7.591
7.576
7.572
7.561
7.557
7.542
7.539
7.524
7.521
7.409
7.406
7.404
7.401
7.391
7.385
7.382
7.371
7.369
7.365
7.358
7.355
7.352
7.349
7.346
7.344
7.191
7.188
7.184
7.179
7.173
7.168
7.163
7.159
7.156
7.153
7.146
7.141
7.137
5.002
-0.000
N
O
2a
0.76
1.26
1.03
3.19
0.88
2.00
f1 (ppm)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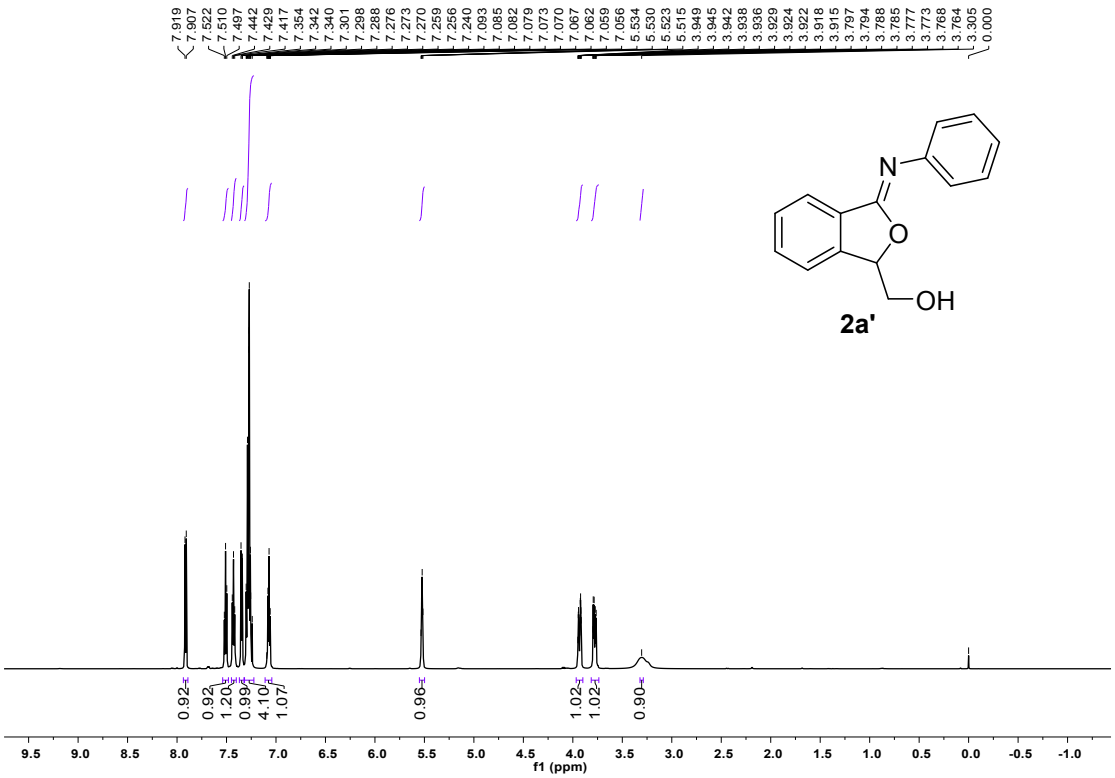
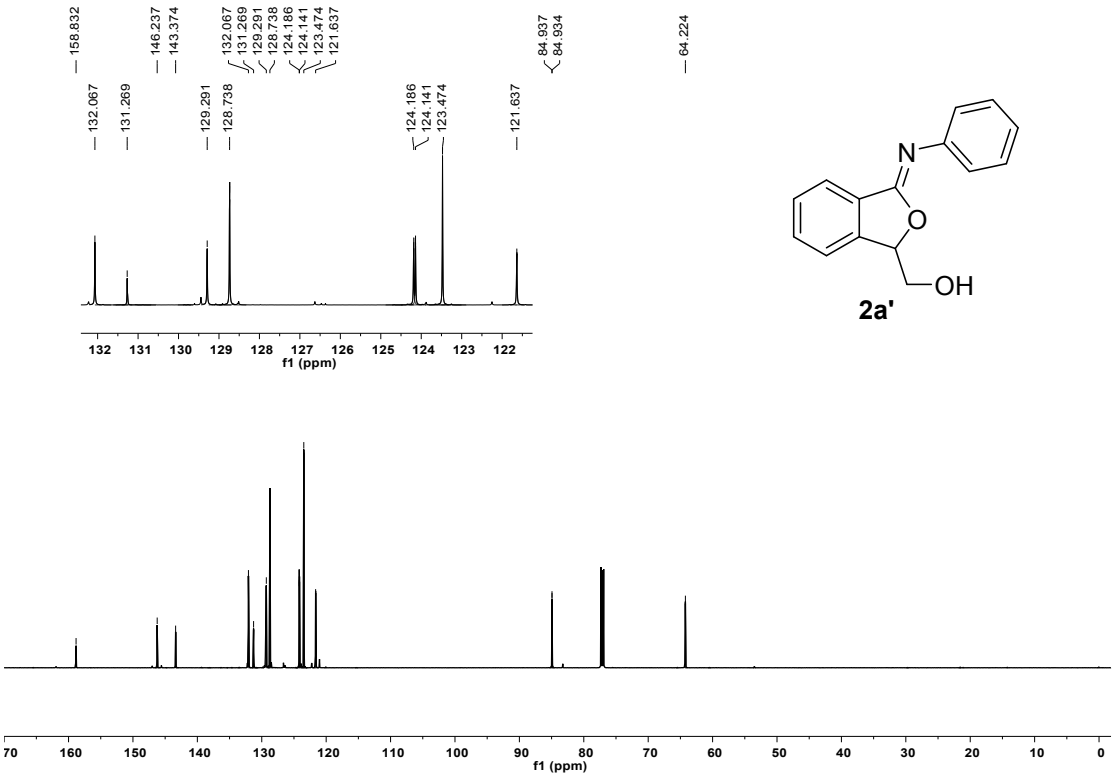
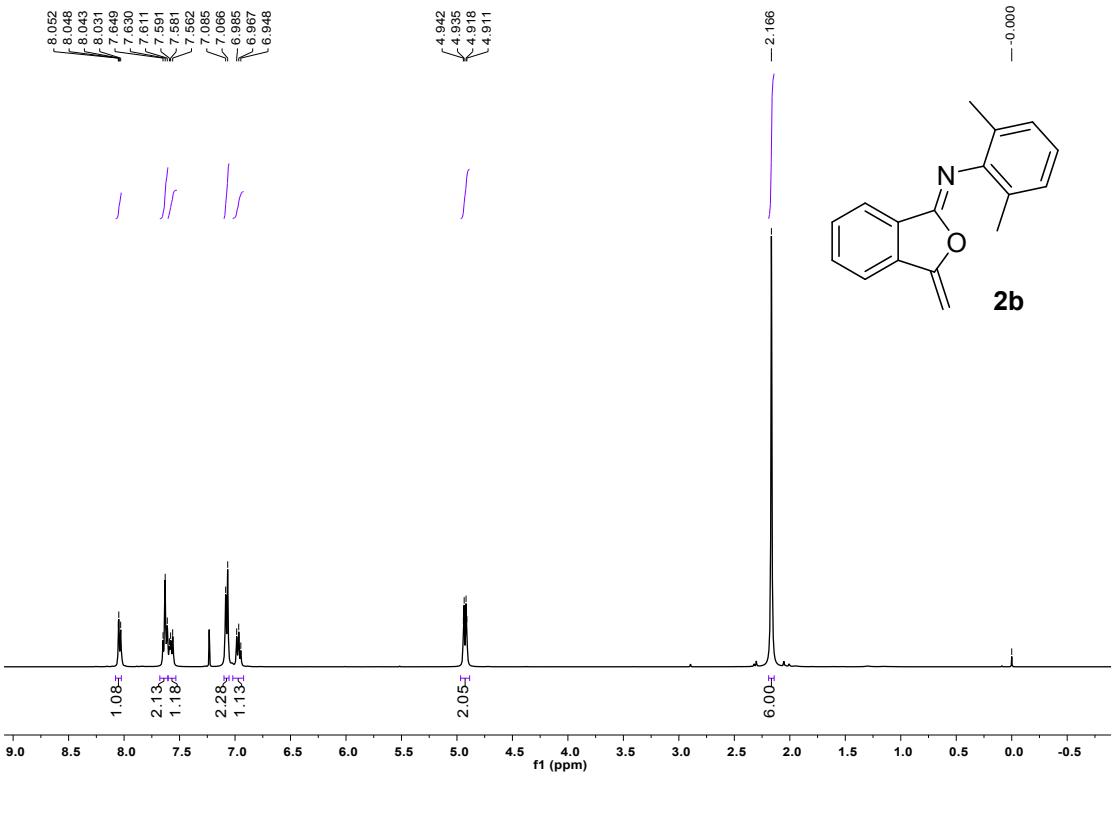
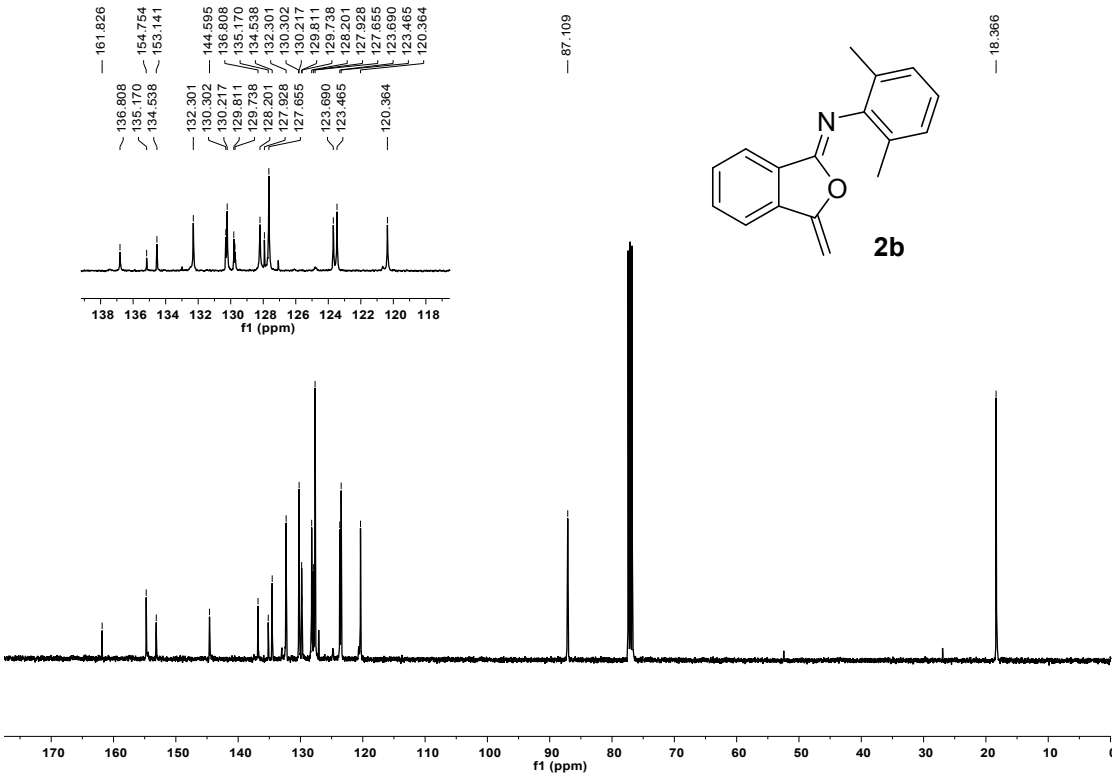
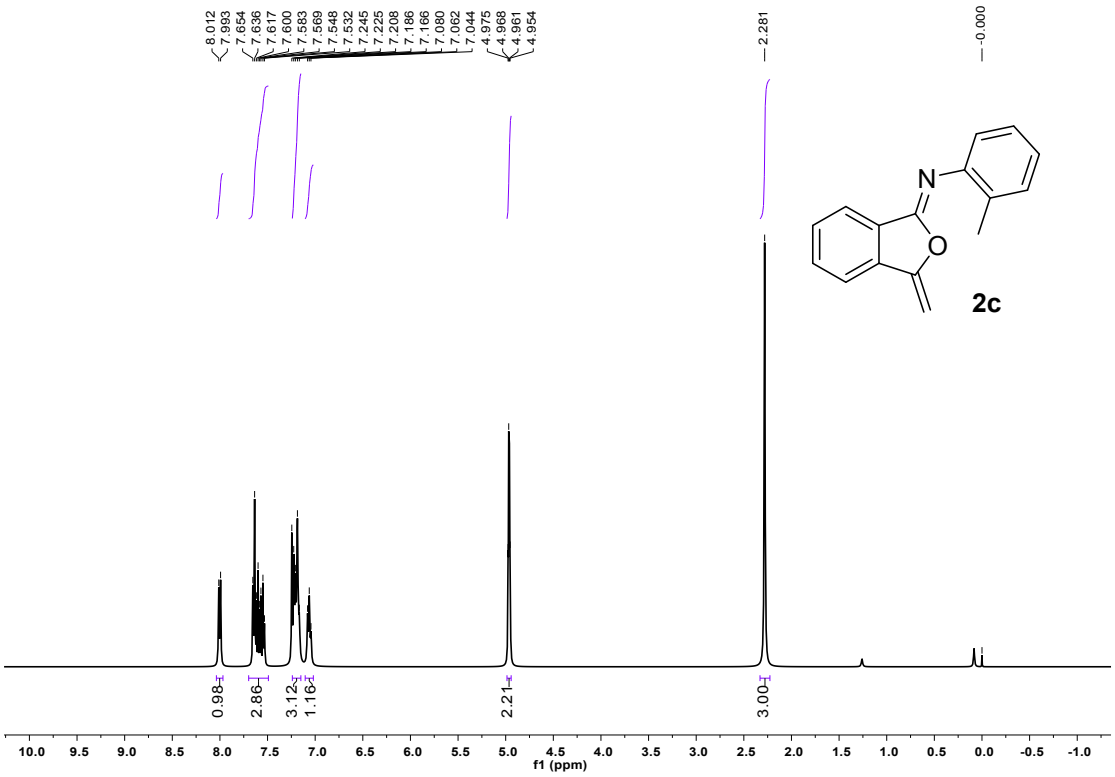
153.861
145.679
136.229
132.184
130.752
130.189
128.758
124.695
123.695
123.579
120.278
87.187
N
O
2a
f1 (ppm)

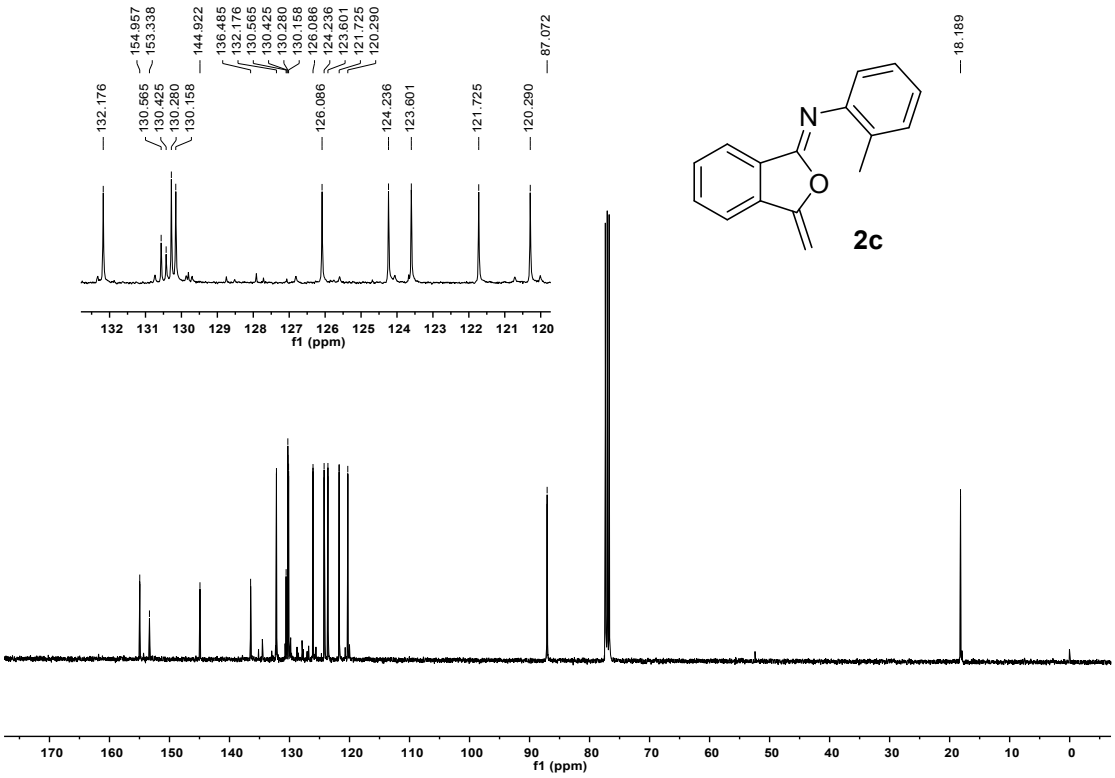

7.919
7.907
7.522
7.510
7.497
7.442
7.429
7.417
7.354
7.342
7.340
7.301
7.298
7.288
7.276
7.273
7.270
7.259
7.256
7.240
7.093
7.085
7.082
7.079
7.073
7.070
7.067
7.062
7.059
7.056
5.534
5.530
5.523
5.515
3.949
3.945
3.942
3.938
3.936
3.929
3.924
3.922
3.918
3.915
3.797
3.794
3.788
3.785
3.777
3.773
3.768
3.764
3.305
0.000
N
O
OH
2a'
0.92
0.92
1.20
0.99
4.10
1.07
0.96
1.02
1.02
0.90
f1 (ppm)


158.832
146.237
143.374
132.067
131.269
129.291
128.738
124.186
124.141
123.474
121.637
84.937
84.934
64.224
f1 (ppm)
N
O
OH
2a'


8.052
8.048
8.043
8.031
7.649
7.630
7.611
7.591
7.581
7.562
7.085
7.066
6.985
6.967
6.948
4.942
4.935
4.918
4.911
2.166
-0.000
1.08
2.13
1.18
2.28
1.13
2.05
6.00
f1 (ppm)
N
O
2b


161.826
154.754
153.141
144.595
136.808
135.170
134.538
132.301
130.302
130.217
129.811
129.738
128.201
127.928
127.655
123.690
123.465
120.364
87.109
18.366
N
O
2b
f1 (ppm)


8.012
7.993
7.654
7.636
7.617
7.600
7.583
7.569
7.548
7.532
7.245
7.225
7.208
7.186
7.166
7.080
7.062
7.044
4.975
4.968
4.961
4.954
2.281
-0.000
N
O
2c
0.98
2.86
3.12
1.16
2.21
3.00
f1 (ppm)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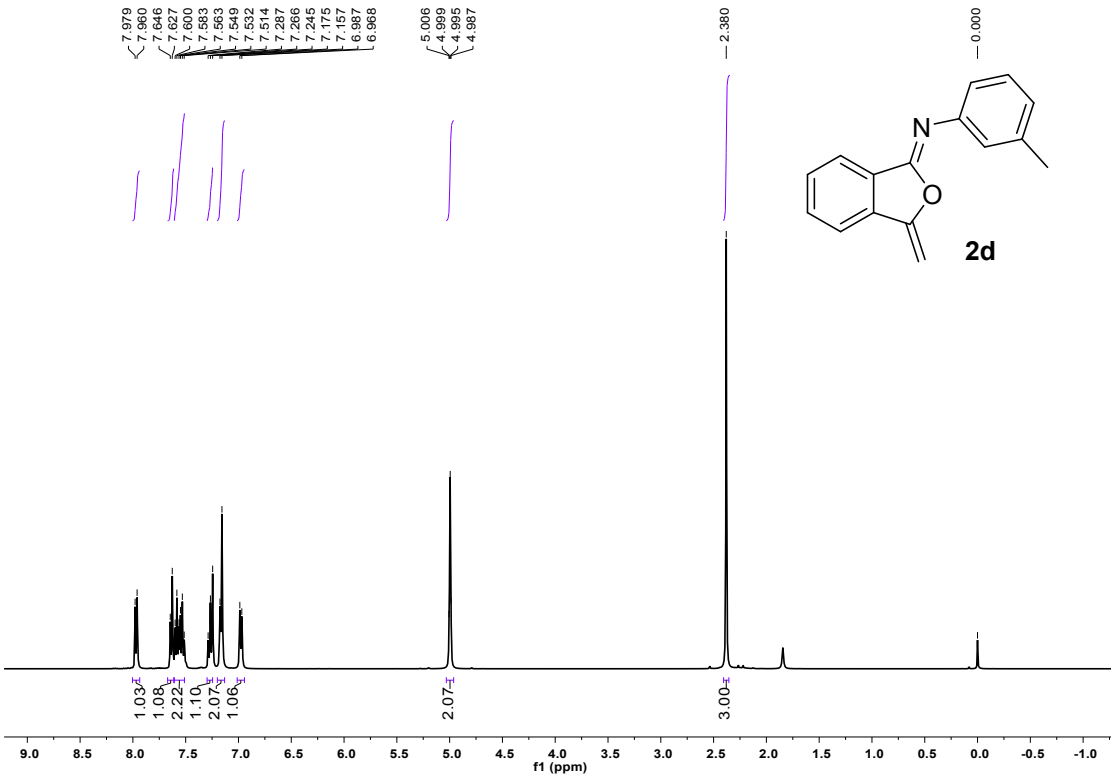
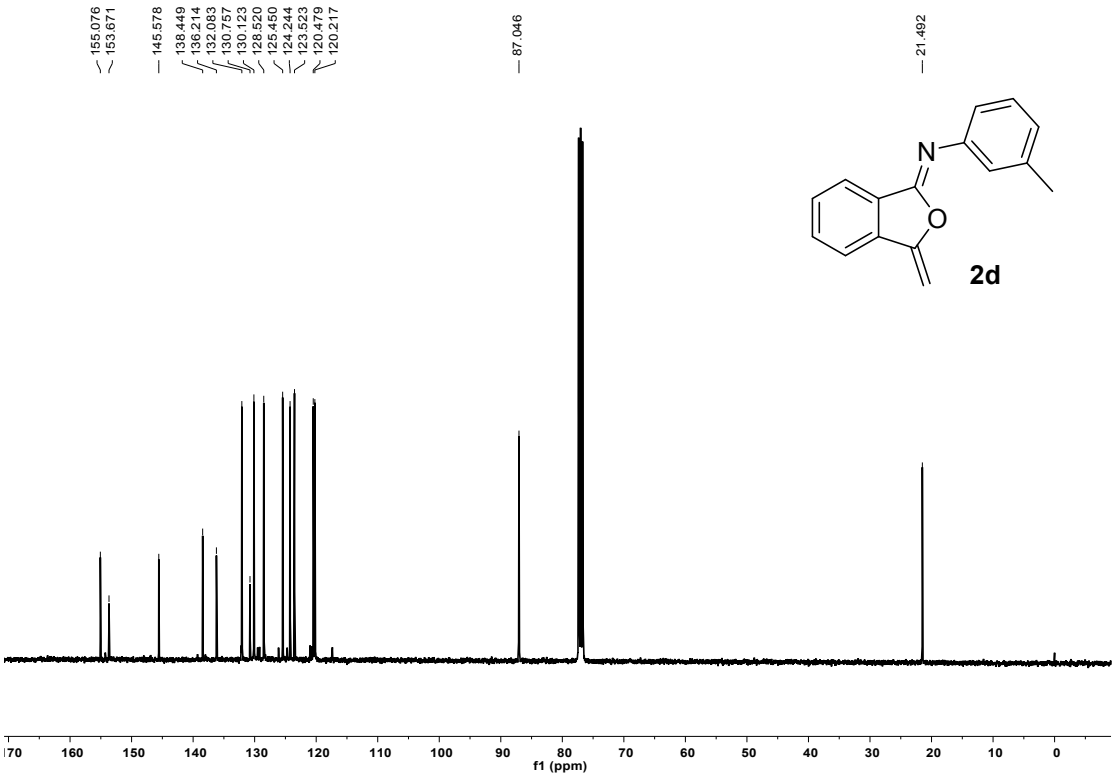
153.338
144.922
136.485
132.176
130.565
130.425
130.280
130.158
126.086
124.236
123.601
121.725
120.290
87.072
18.189
N
O
2c
f1 (ppm)


7.979
7.960
7.646
7.627
7.600
7.583
7.563
7.549
7.532
7.514
7.287
7.266
7.245
7.175
7.157
6.987
6.968
5.006
4.999
4.995
4.987
2.380
0.000
N
O
2d
1.03
1.08
2.22
1.10
2.07
1.06
2.07
3.00
f1 (ppm)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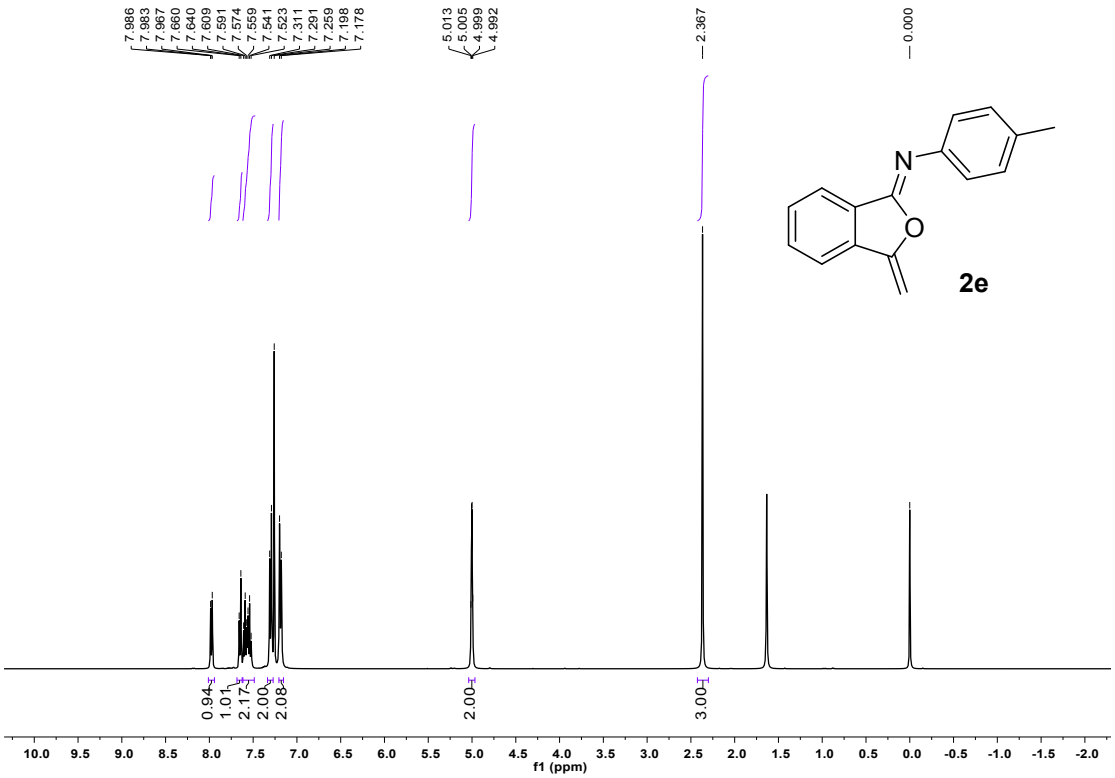
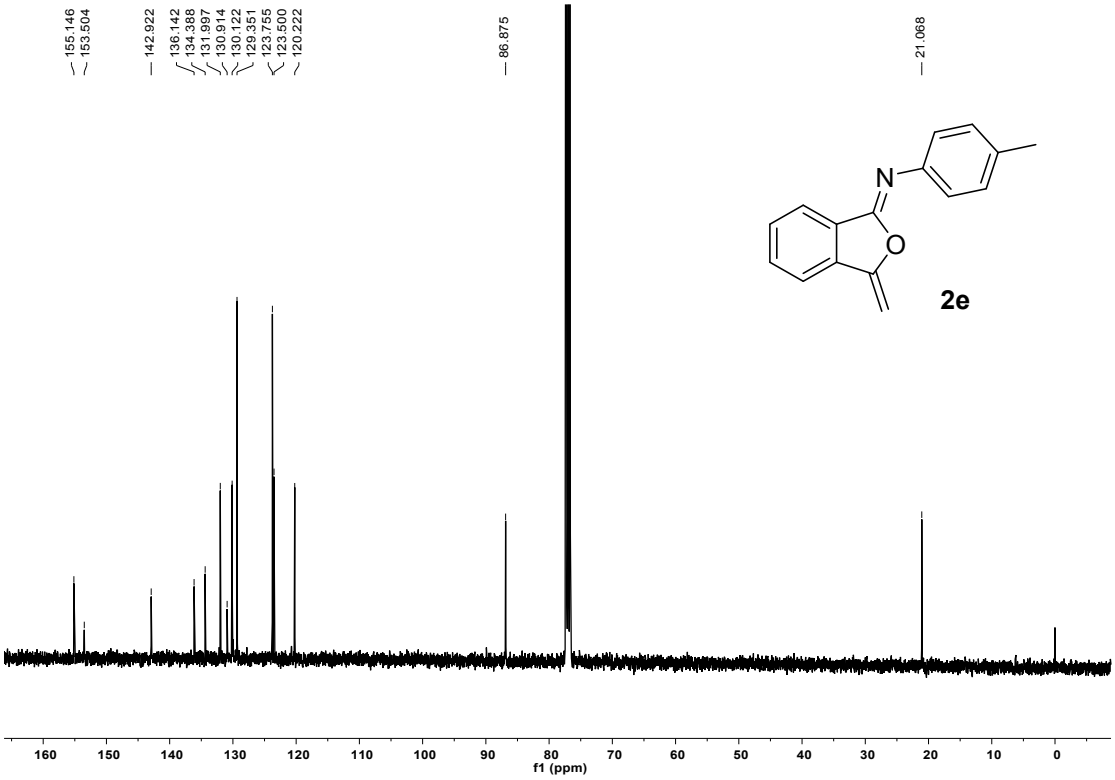
153.671
145.578
138.449
136.214
132.083
130.757
130.123
128.520
125.450
124.244
123.523
120.479
120.217
87.046
21.492
N
O
2d
f1 (ppm)


7.986
7.983
7.967
7.660
7.640
7.609
7.591
7.574
7.559
7.541
7.523
7.311
7.291
7.259
7.198
7.178
5.013
5.005
4.999
4.992
2.367
0.000
N
O
2e
0.94
1.01
2.17
2.00
2.08
2.00
3.00
f1 (ppm)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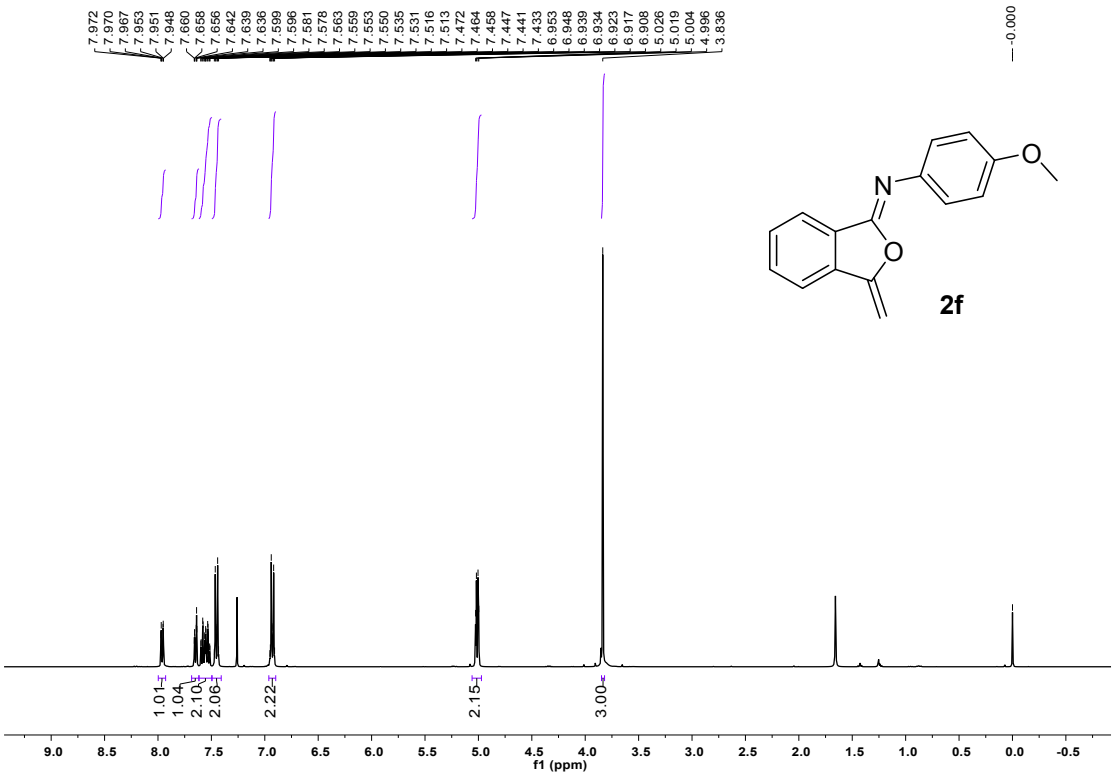
153.504
142.922
136.142
134.388
131.997
130.914
130.122
129.351
123.755
123.500
120.222
86.875
21.068
N
O
2e
f1 (ppm)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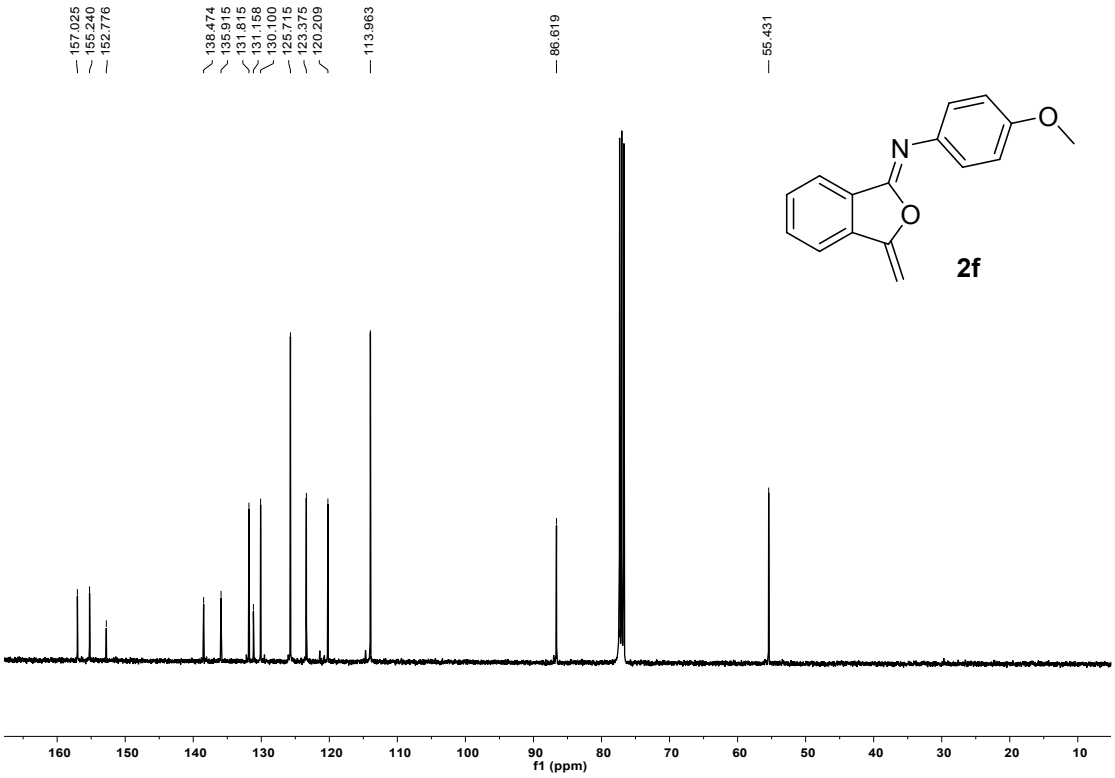
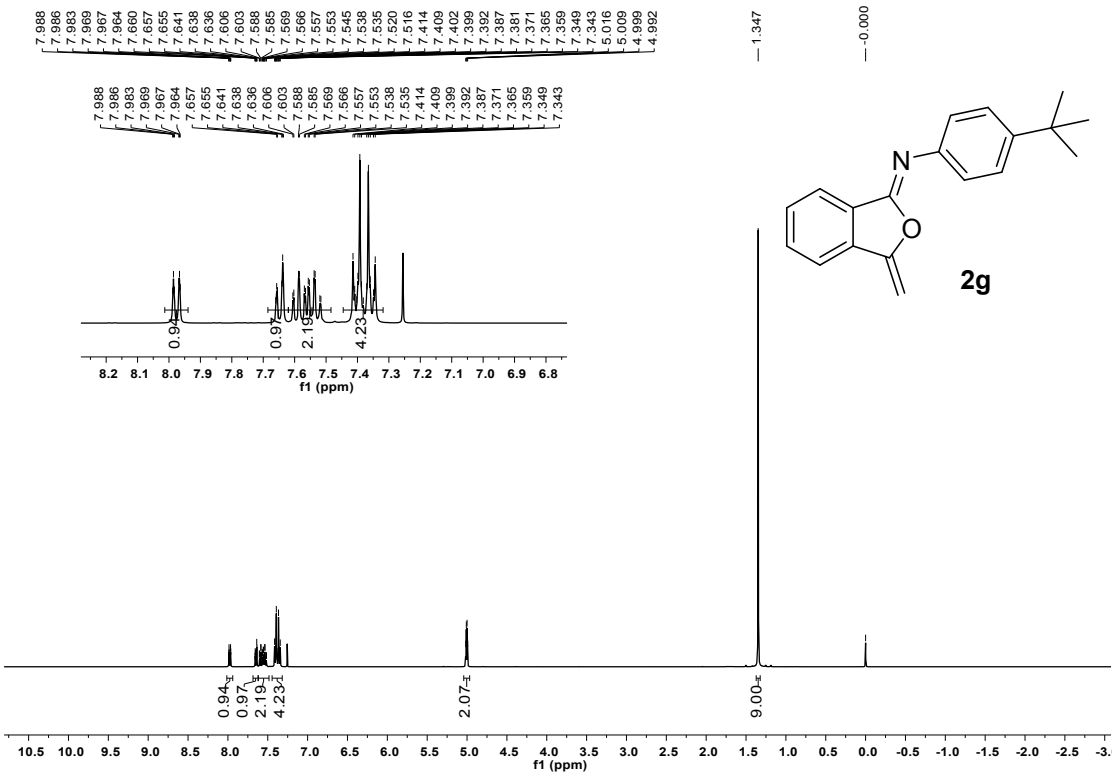
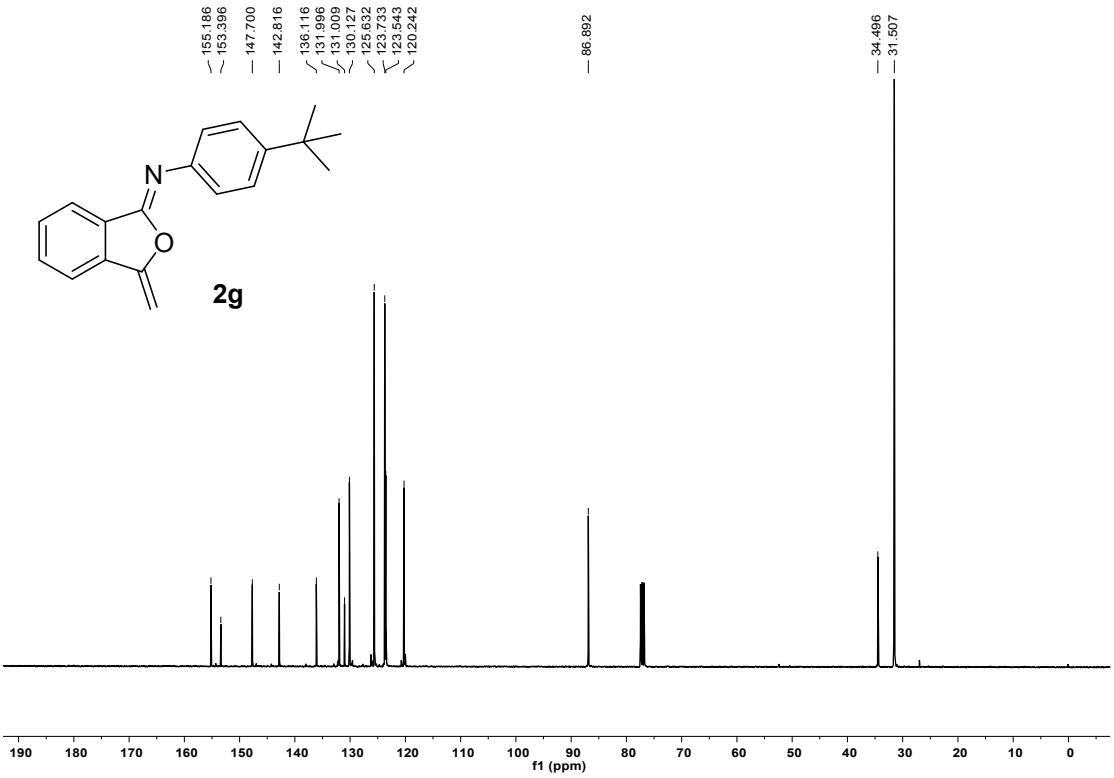
7.967
7.953
7.951
7.948
7.660
7.658
7.656
7.642
7.639
7.636
7.599
7.596
7.581
7.578
7.563
7.559
7.553
7.550
7.535
7.531
7.516
7.513
7.472
7.464
7.458
7.447
7.441
7.433
6.953
6.948
6.939
6.934
6.923
6.917
6.908
5.026
5.019
5.004
4.996
3.836
-0.000
N
O
O
2f
1.01
1.04
2.10
2.06
2.22
2.15
3.00
f1 (ppm)


157.025
155.240
152.776
138.474
135.915
131.815
131.158
130.100
125.715
123.375
120.209
113.963
86.619
55.431
2f
f1 (ppm)


1.347
-0.000
2g
0.94
0.97
2.19
4.23
2.07
9.00
f1 (ppm)


155.186
153.396
147.700
142.816
136.116
131.996
131.009
130.127
125.632
123.733
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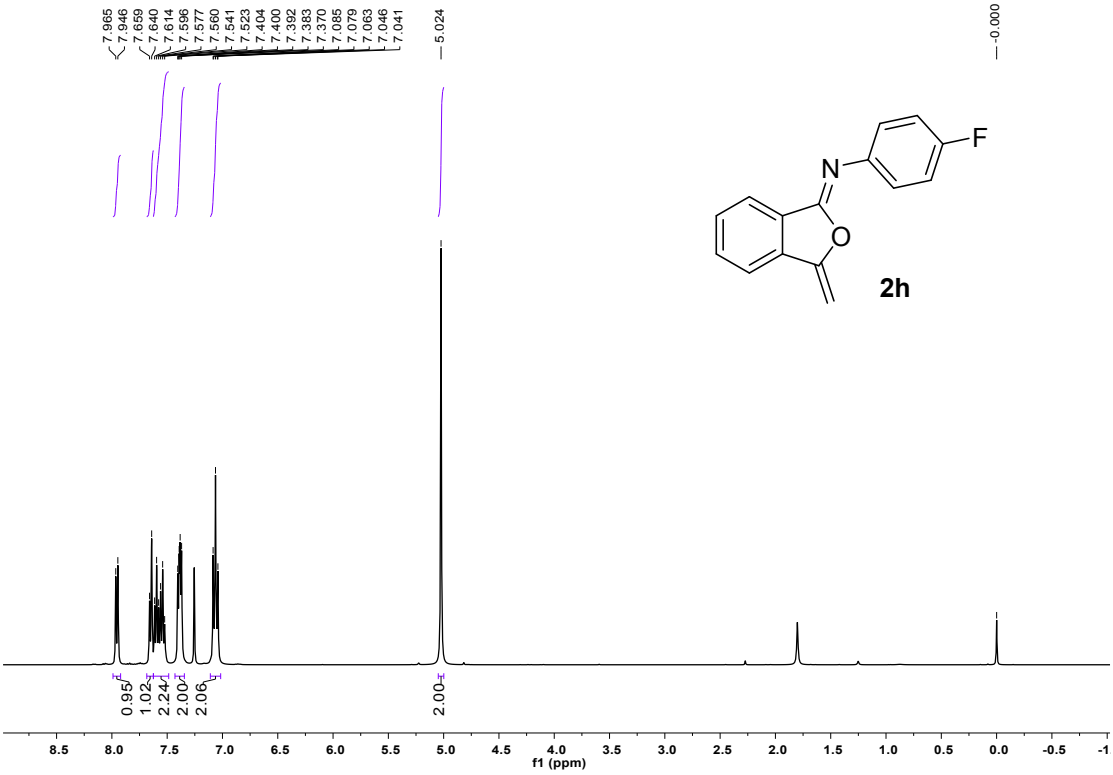
120.242
86.892
34.496
31.507
N
O
2g
f1 (ppm)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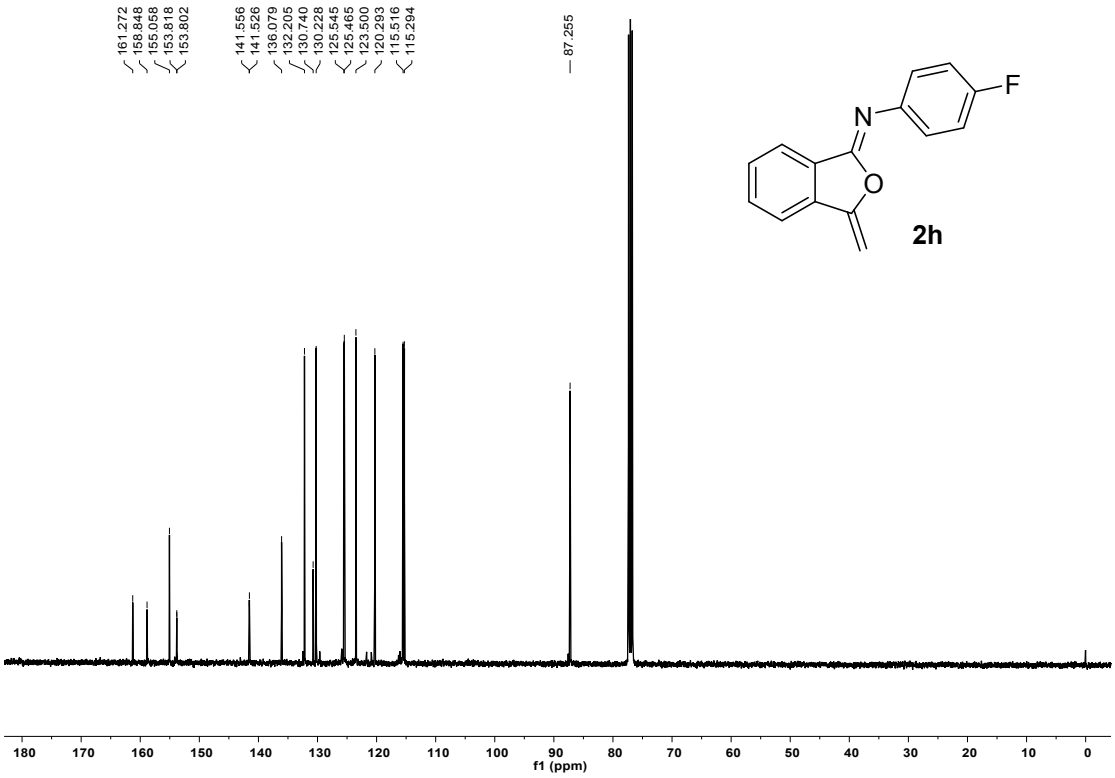
7.659
7.640
7.614
7.596
7.577
7.560
7.541
7.523
7.404
7.400
7.392
7.383
7.370
7.085
7.079
7.063
7.046
7.041
5.024
-0.000
F
N
O
2h
0.95
1.02
2.24
2.00
2.06
2.00
f1 (ppm)


161.272
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153.818
153.802
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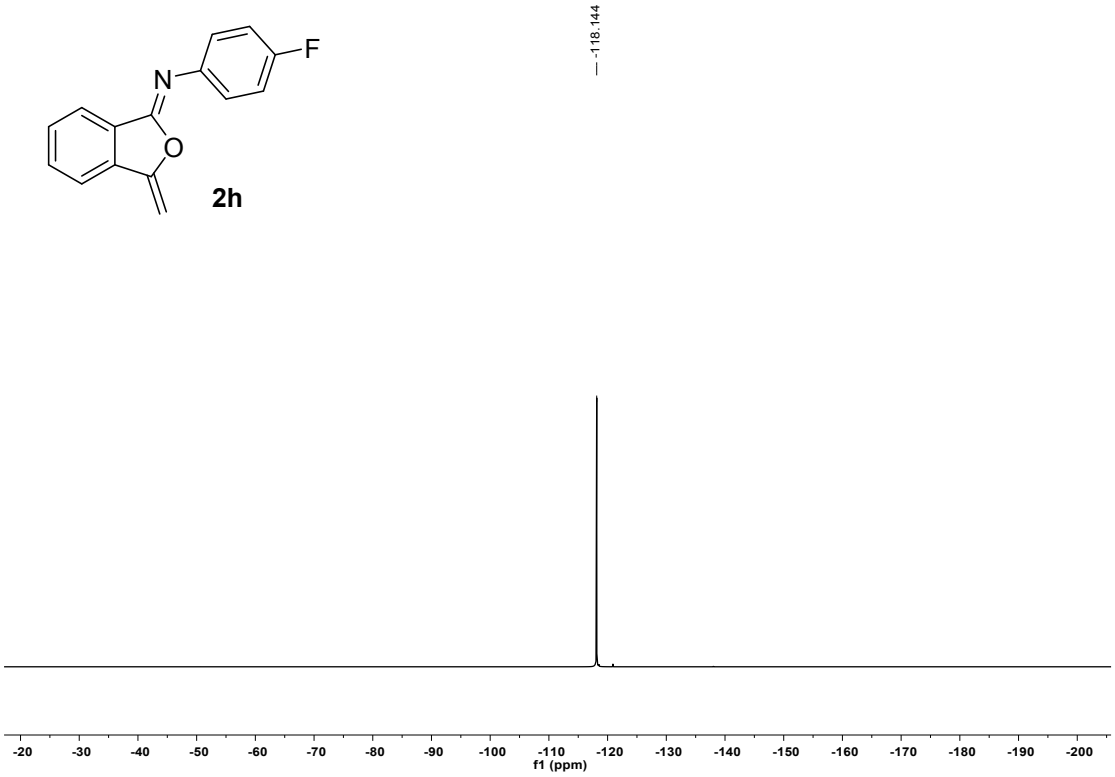
141.526
136.079
132.205
130.740
130.228
125.545
125.465
123.500
120.293
115.516
115.294
87.255
F
N
O
2h
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


-118.144
F
N
O
2h
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
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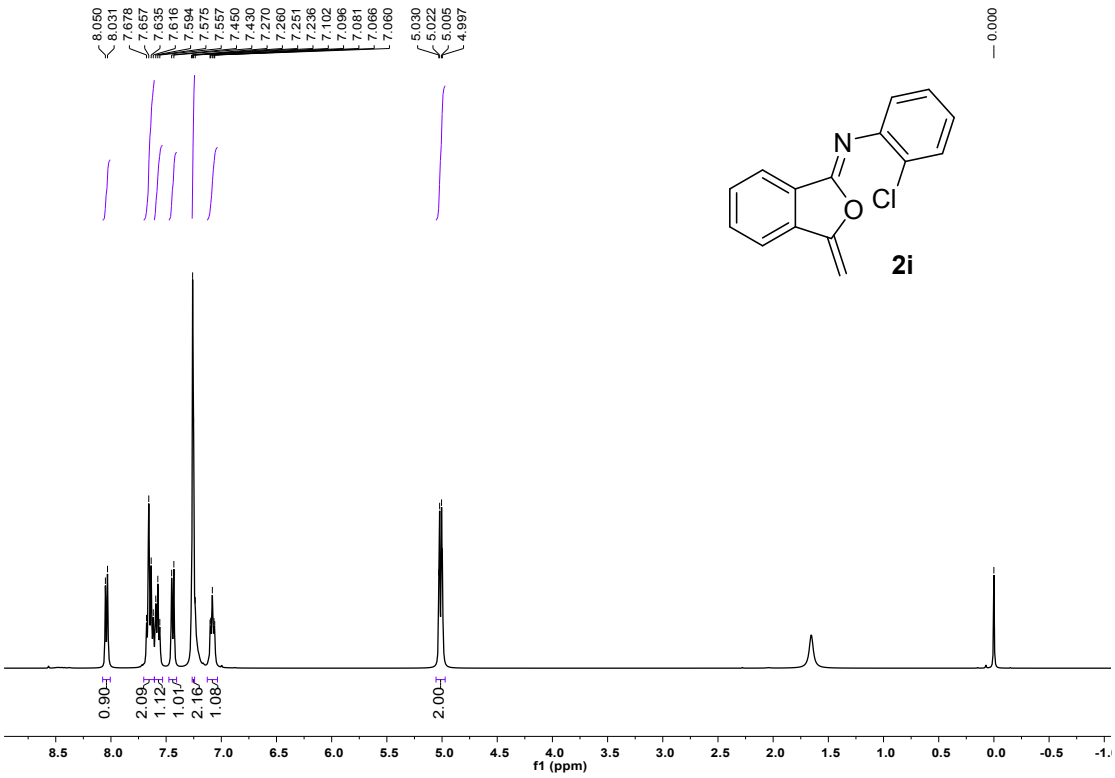
-130
-140
-150
-160
-170
-180
-190
-200
f1 (ppm)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8.031
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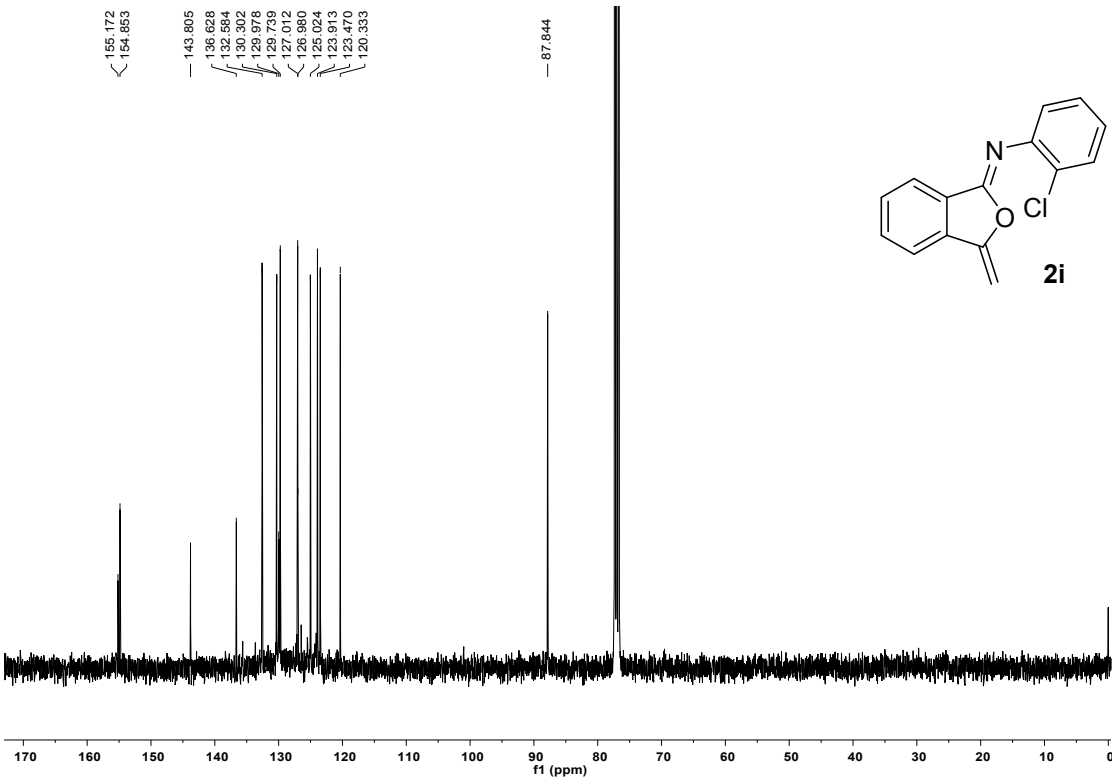
7.657
7.635
7.616
7.594
7.575
7.557
7.450
7.430
7.270
7.260
7.251
7.236
7.102
7.096
7.081
7.066
7.060
5.030
5.022
5.005
4.997
0.000
N
O
Cl
2i
0.90
2.09
1.12
1.01
2.16
1.08
2.00
f1 (ppm)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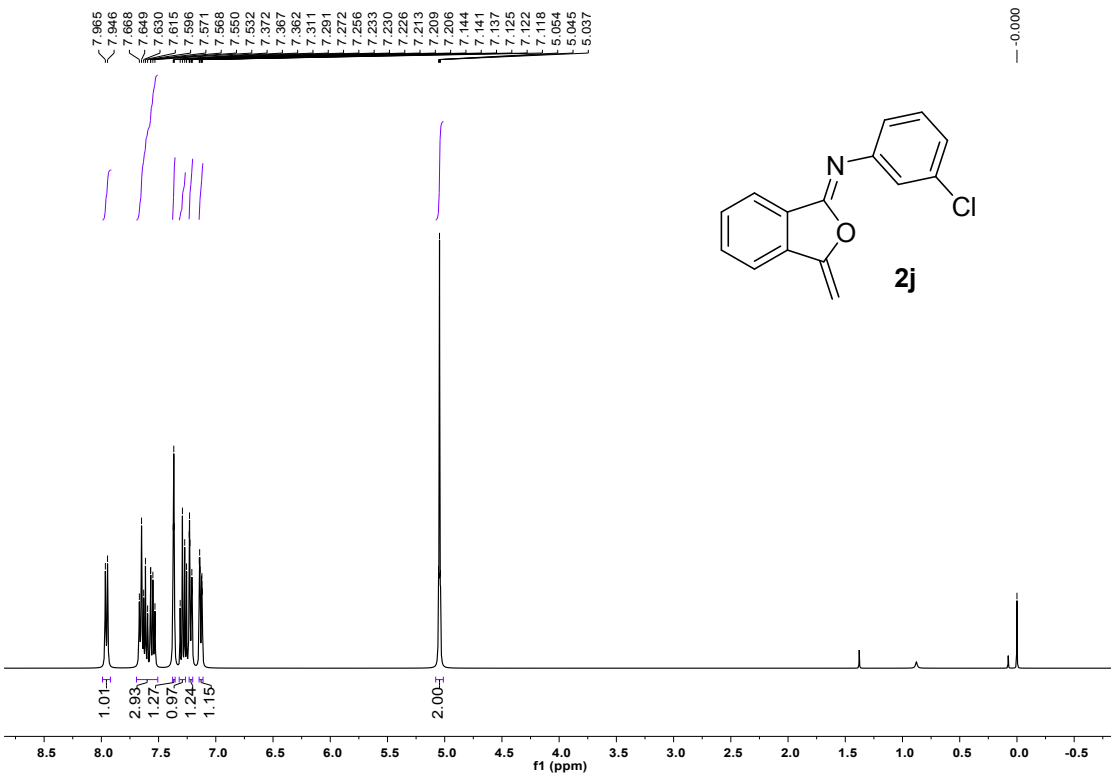
154.853
143.805
136.628
132.584
130.302
129.978
129.739
127.012
126.980
125.024
123.913
123.470
120.333
87.844
N
O
Cl
2i
f1 (ppm)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7.946
7.668
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7.550
7.532
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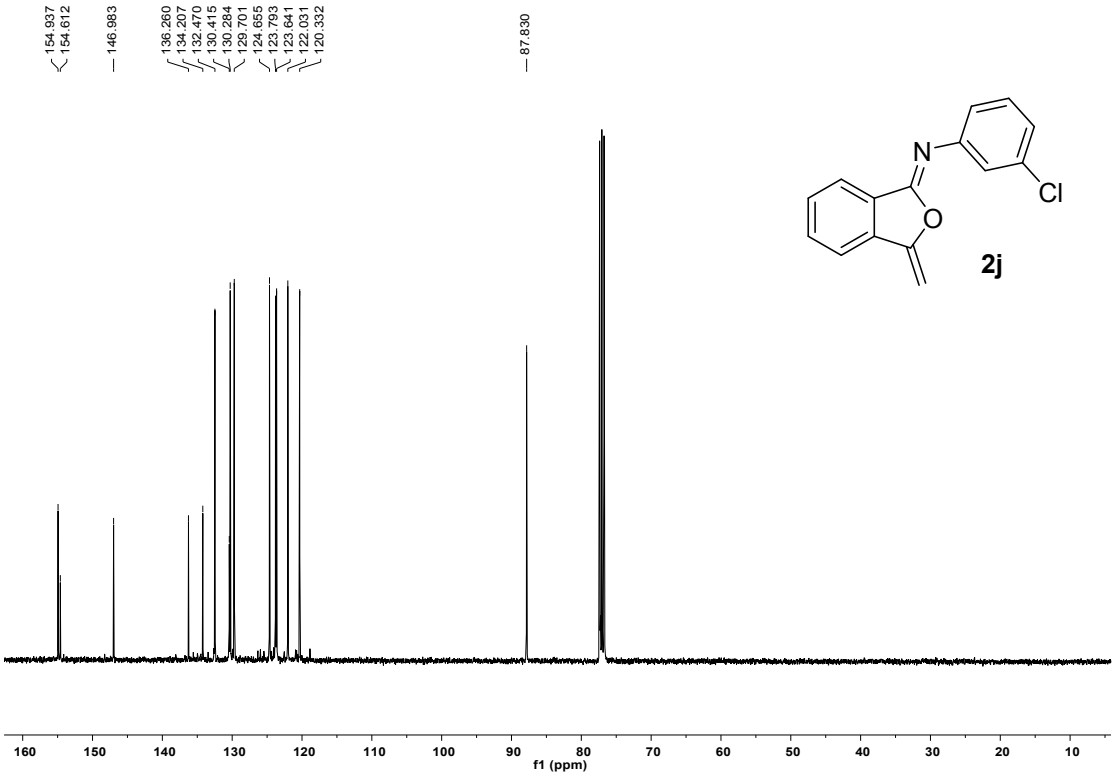
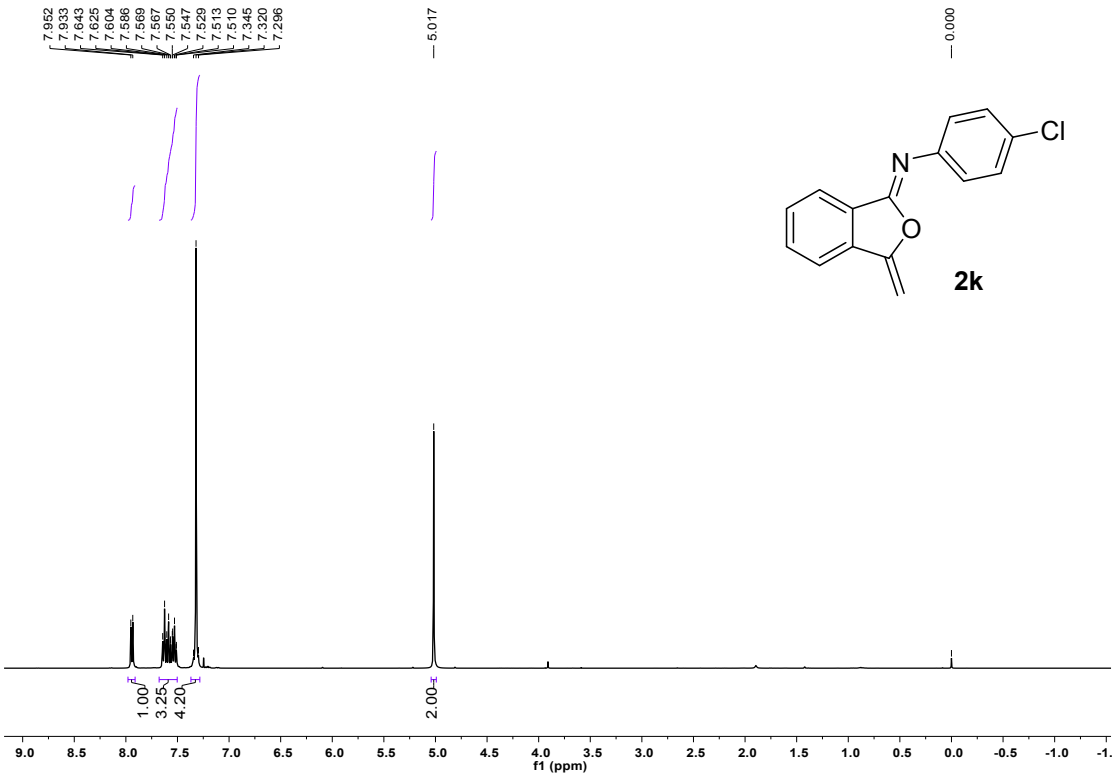
7.367
7.362
7.311
7.291
7.272
7.256
7.233
7.230
7.226
7.213
7.209
7.206
7.144
7.141
7.137
7.125
7.122
7.118
5.054
5.045
5.037
-0.000
1.01
2.93
1.27
0.97
1.24
1.15
2.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
N
Cl
O
2j


154.937
154.612
146.983
136.260
134.207
132.470
130.415
130.284
129.701
124.655
123.793
123.641
122.031
120.332
87.830
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)
N
Cl
O
2j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7.643
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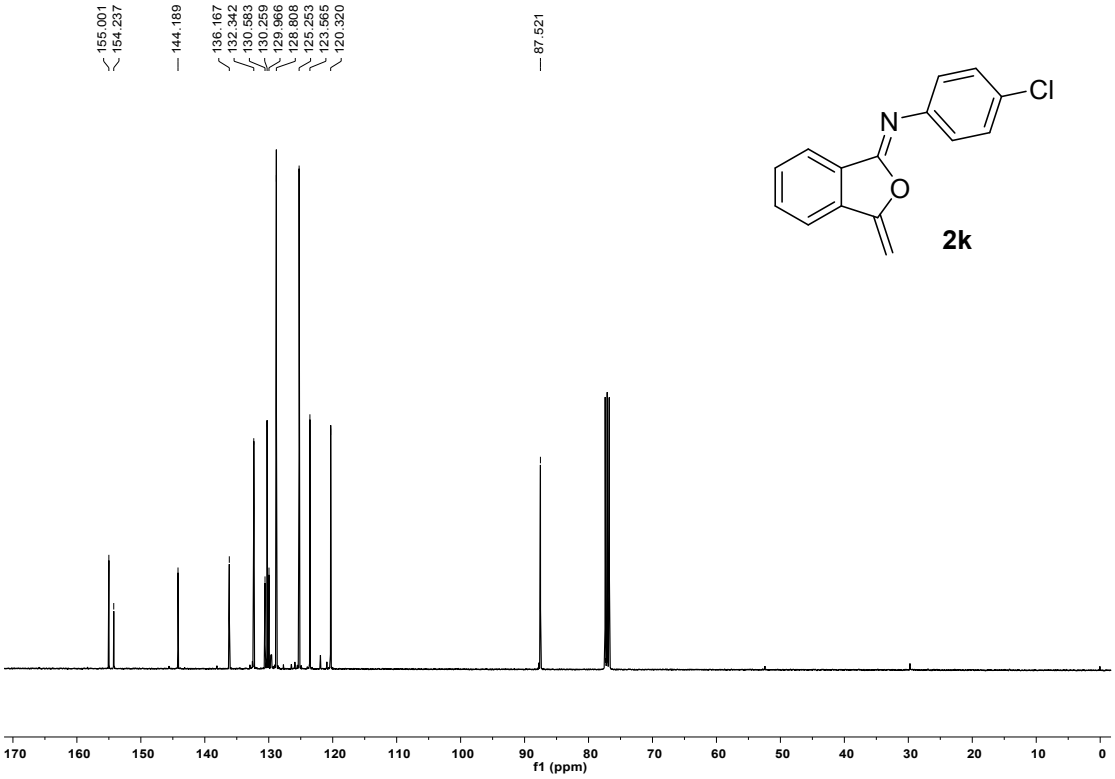
7.604
7.586
7.569
7.567
7.550
7.547
7.529
7.513
7.510
7.345
7.320
7.296
5.017
0.000
Cl
N
O
2k
1.00
3.25
4.20
2.00
f1 (ppm)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154.237
144.189
136.167
132.342
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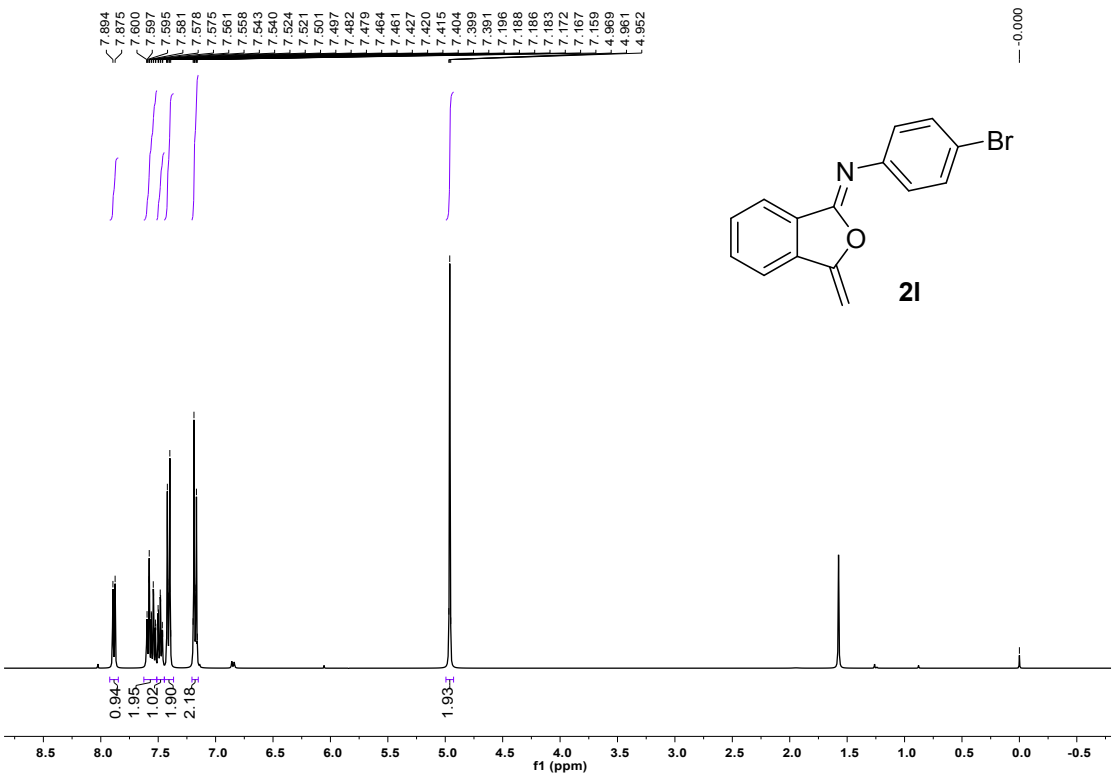
130.259
129.966
128.808
125.253
123.565
120.320
87.521
Cl
N
O
2k
f1 (ppm)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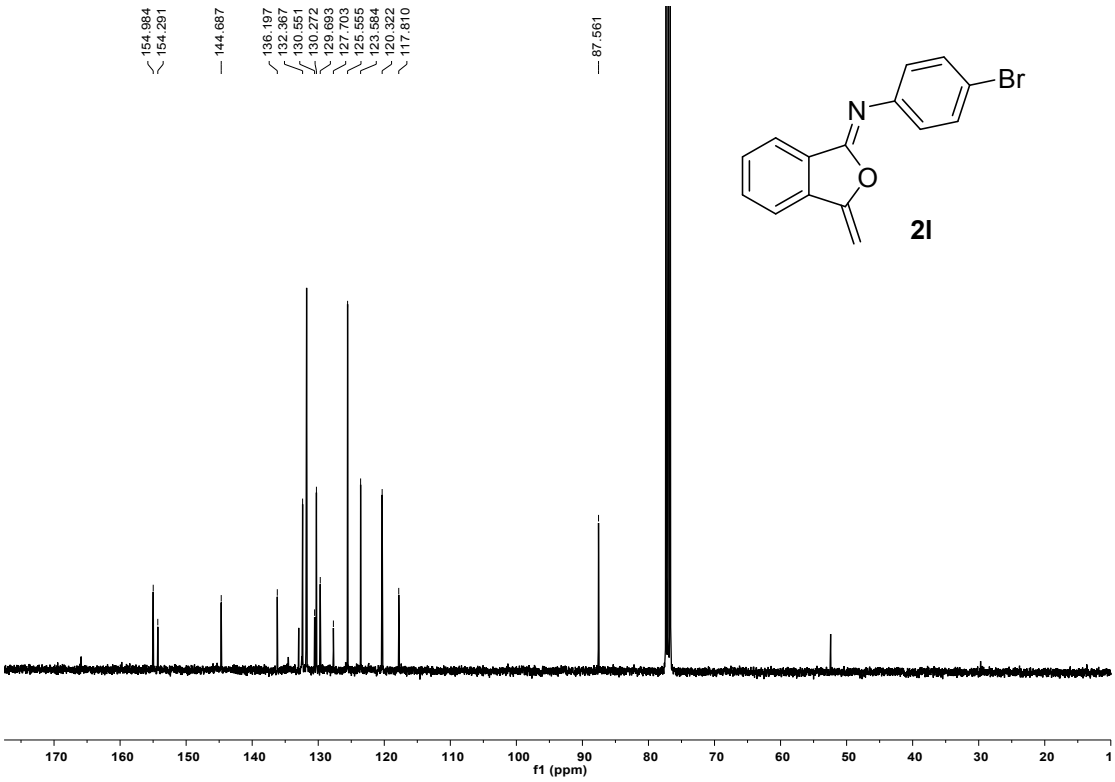
7.875
7.600
7.597
7.595
7.581
7.578
7.575
7.561
7.558
7.543
7.540
7.524
7.521
7.501
7.497
7.482
7.479
7.464
7.461
7.427
7.420
7.415
7.404
7.399
7.391
7.196
7.188
7.186
7.183
7.172
7.167
7.159
4.969
4.961
4.952
-0.000
Br
N
O
2l
0.94
1.95
1.02
1.90
2.18
1.93
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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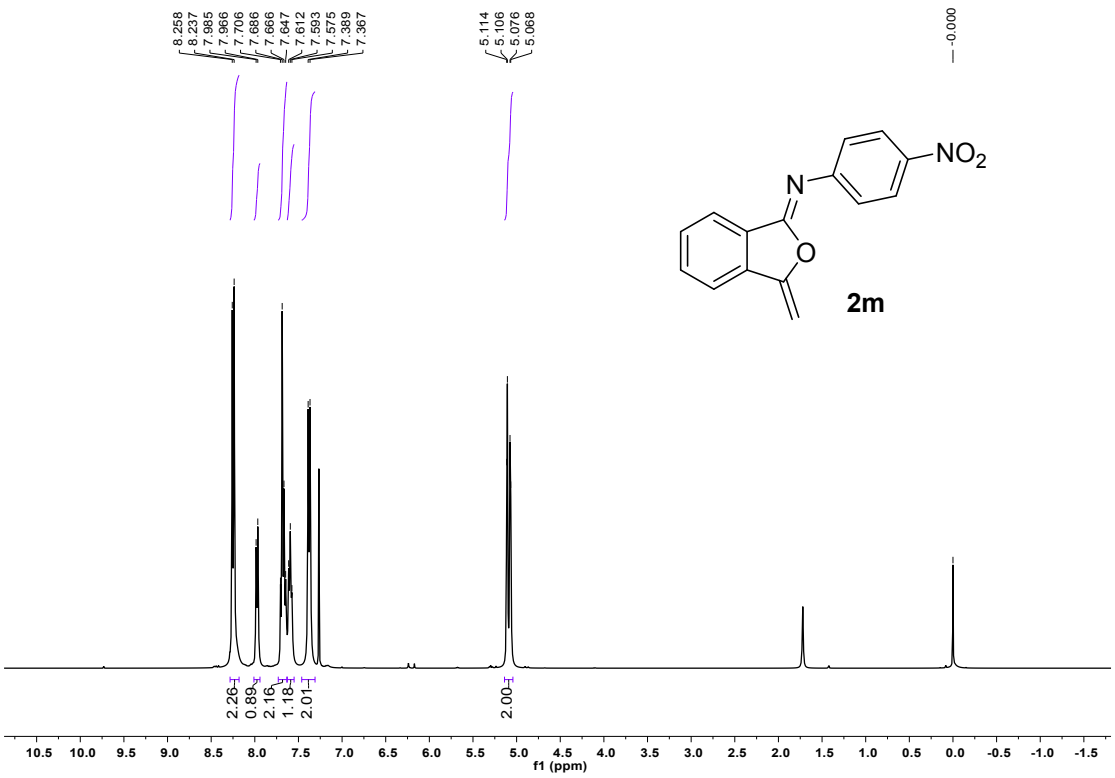
154.291
144.687
136.197
132.367
130.551
130.272
129.693
127.703
125.555
123.584
120.322
117.810
87.561
Br
N
O
2l
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
1
f1 (ppm)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8.237
7.985
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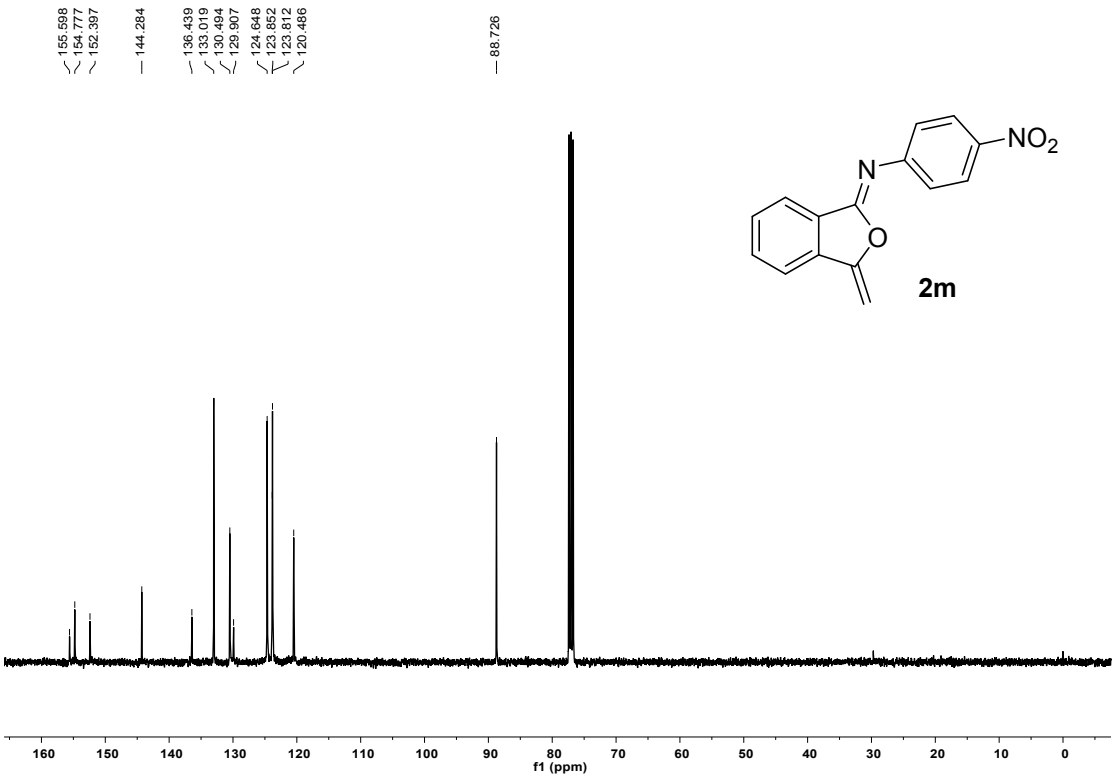
7.706
7.686
7.666
7.647
7.612
7.593
7.575
7.389
7.367
5.114
5.106
5.076
5.068
-0.000
2.26
0.89
2.16
1.18
2.01
2.00
f1 (ppm)
NO2
N
O
2m


155.598
154.777
152.397
144.284
136.439
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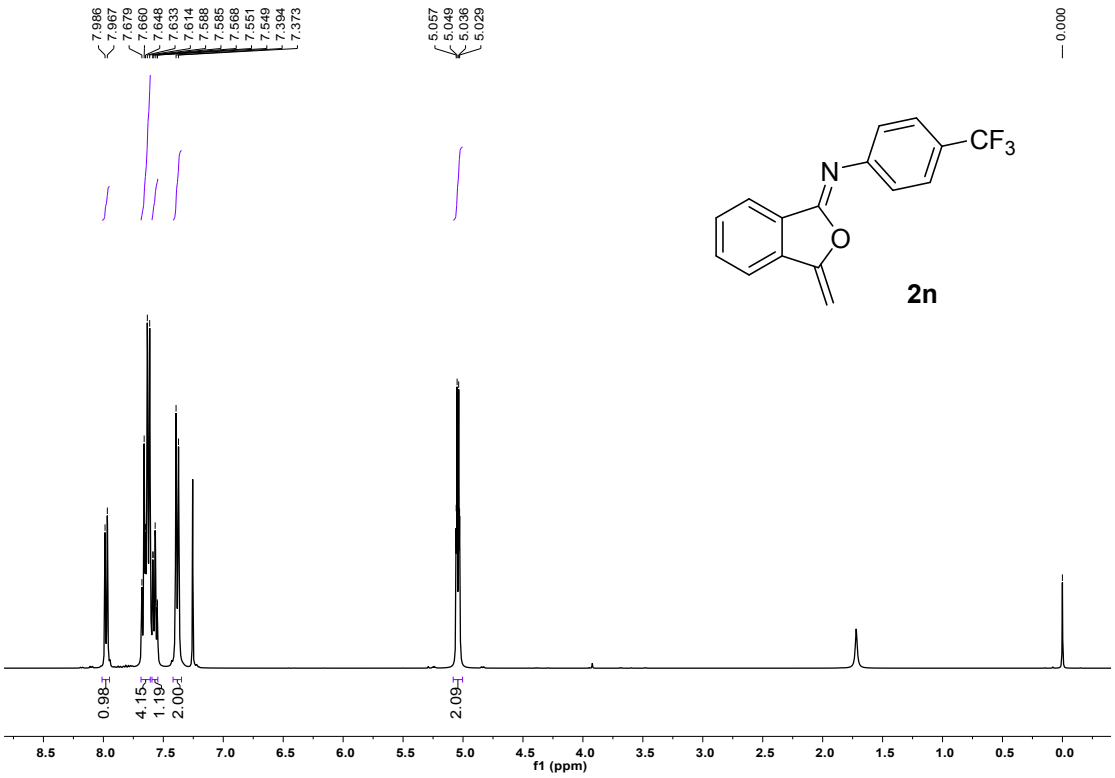
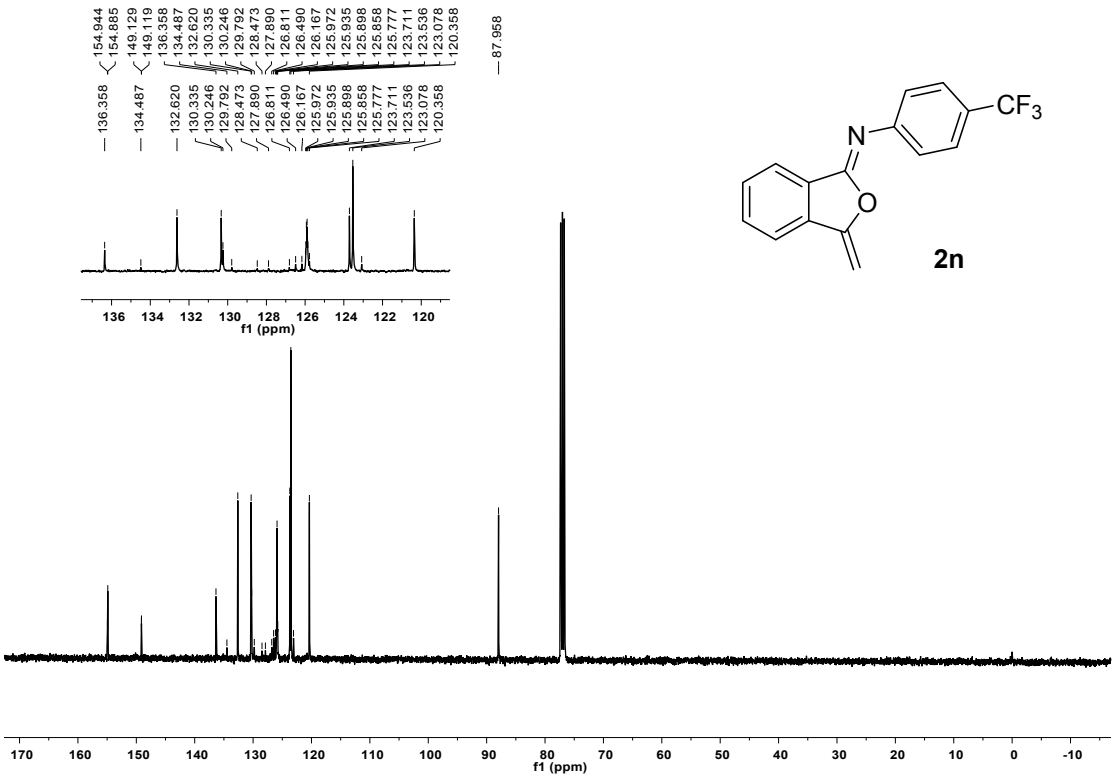
130.494
129.907
124.648
123.852
123.812
120.486
88.726
f1 (ppm)
NO2
N
O
2m


7.986
7.967
7.679
7.660
7.648
7.633
7.614
7.588
7.585
7.568
7.551
7.549
7.394
7.373
5.057
5.049
5.036
5.029
0.000
0.98
4.15
1.19
2.00
2.09
f1 (ppm)
CF3
N
O
2n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154.885
149.129
149.119
136.358
134.487
132.620
130.335
130.246
129.792
128.473
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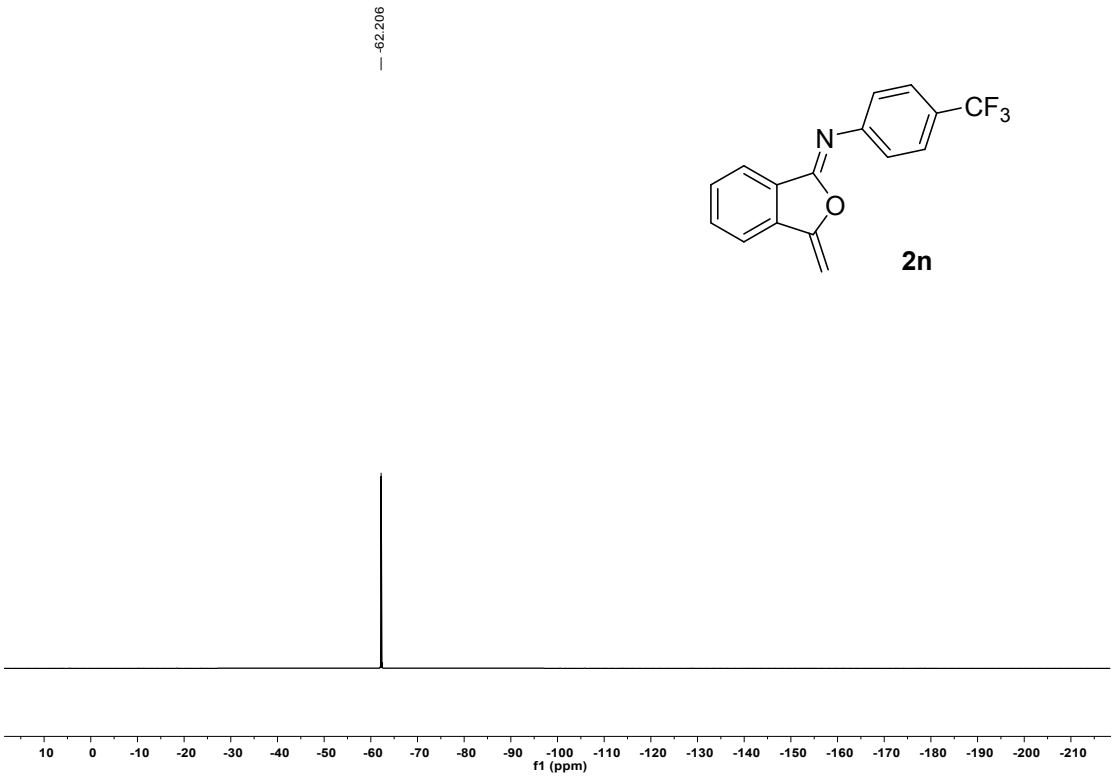
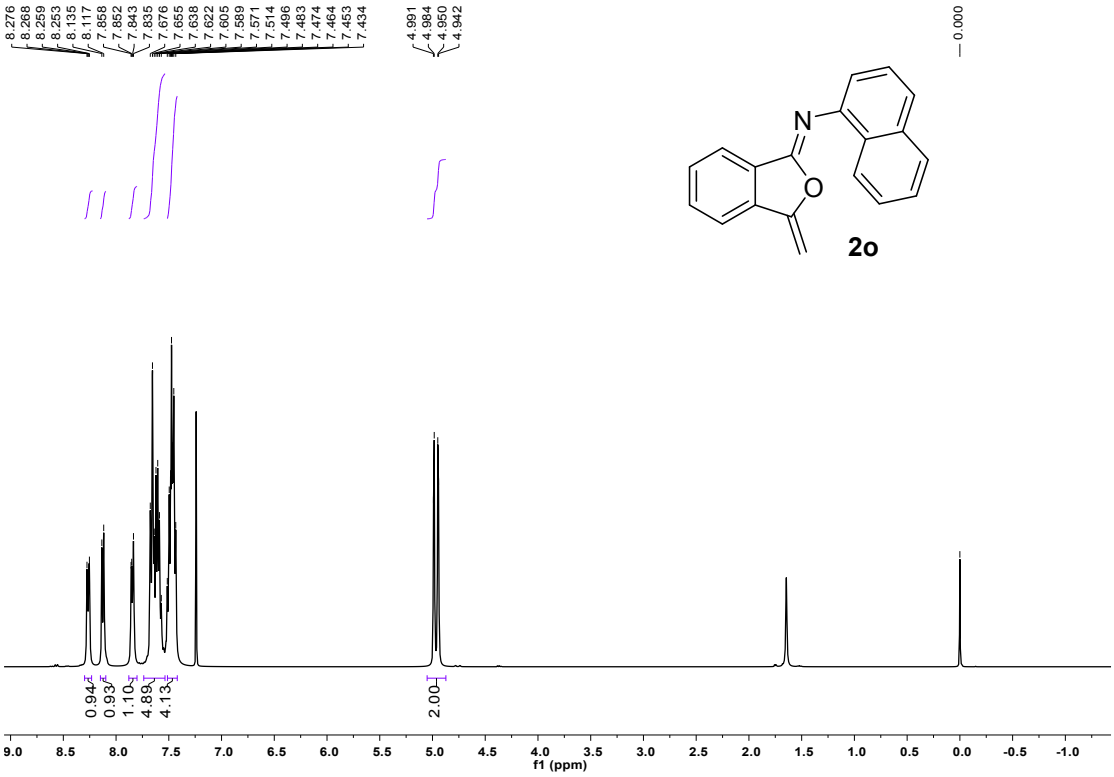
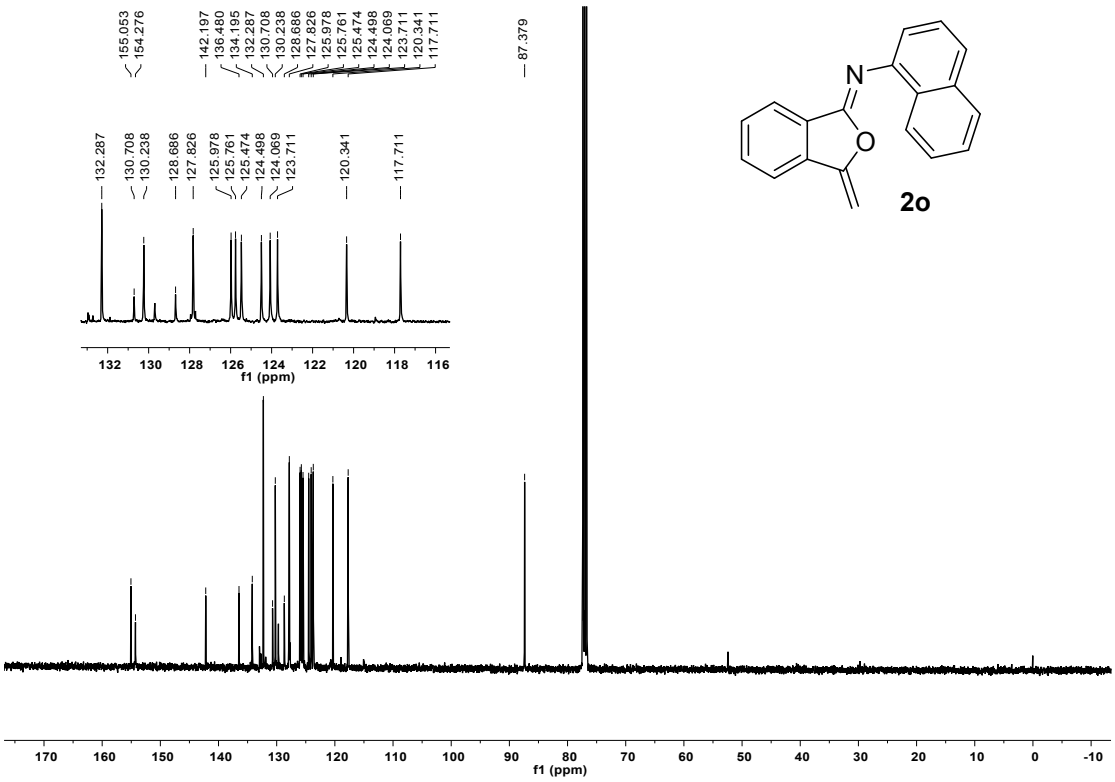
126.811
126.490
126.167
125.972
125.935
125.898
125.858
125.777
123.711
123.536
123.078
120.358
87.958
f1 (ppm)
CF3
N
O
2n


-62.206
CF3
N
O
2n
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


8.276
8.268
8.259
8.253
8.135
8.117
7.858
7.852
7.843
7.835
7.676
7.655
7.638
7.622
7.605
7.589
7.571
7.514
7.496
7.483
7.474
7.464
7.453
7.434
4.991
4.984
4.950
4.942
0.000
N
O
2o
0.94
0.93
1.10
4.89
4.13
2.00
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 -1.0
f1 (ppm)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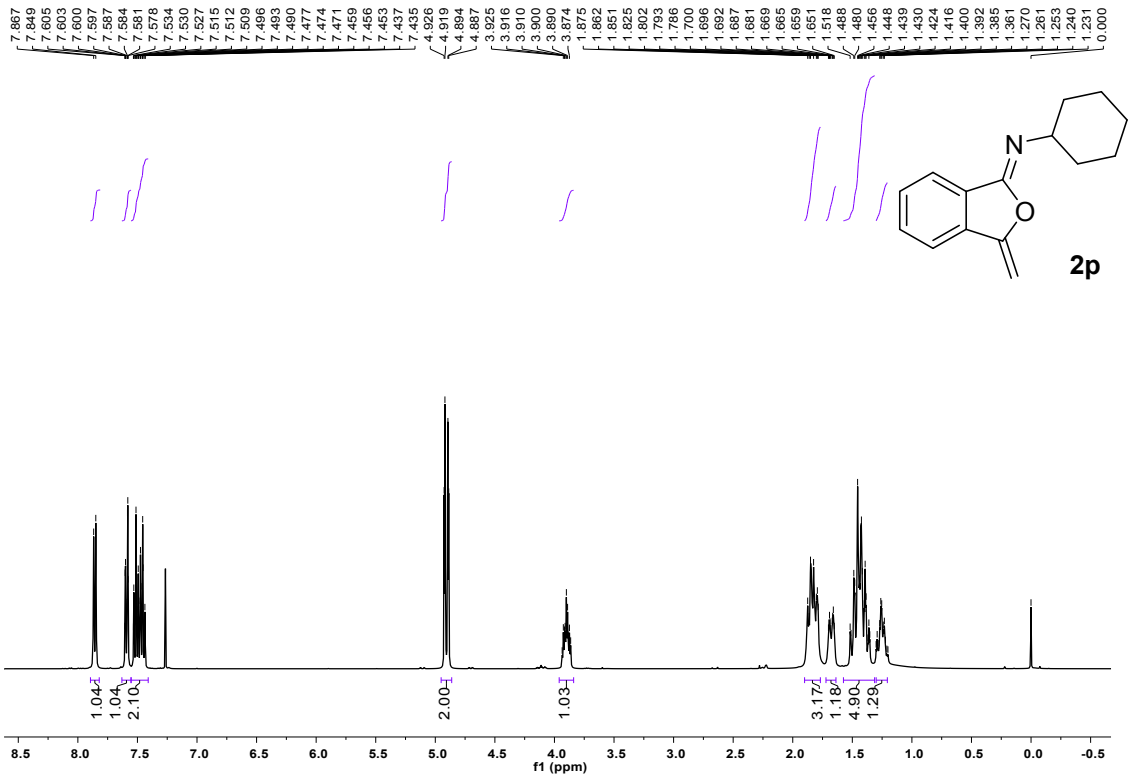
154.276
142.197
136.480
134.195
132.287
130.708
130.238
128.686
127.826
125.978
125.761
125.474
124.498
124.069
123.711
120.341
117.711
87.379
132.287
130.708
130.238
128.686
127.826
125.978
125.761
125.474
124.498
124.069
123.711
120.341
117.711
132 130 128 126 124 122 120 118 116
f1 (ppm)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
N
O
2o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7.603
7.600
7.597
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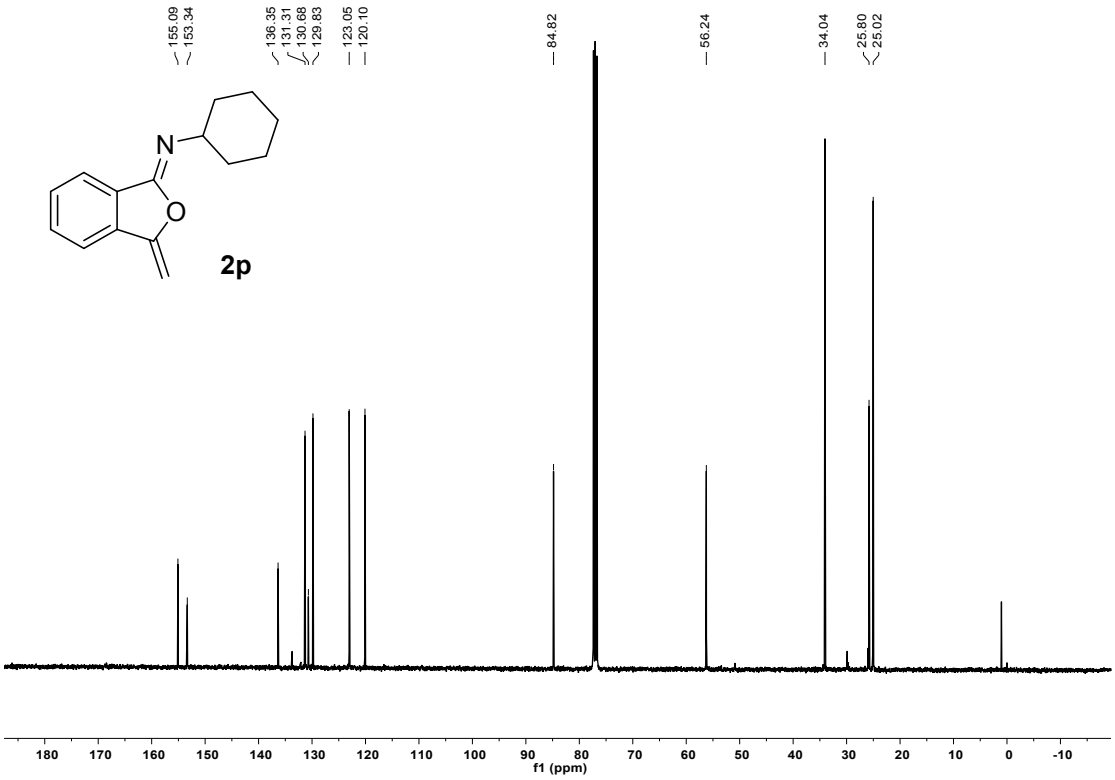
7.584
7.581
7.578
7.534
7.530
7.527
7.515
7.512
7.509
7.496
7.493
7.490
7.477
7.474
7.471
7.459
7.456
7.453
7.437
7.435
4.926
4.919
4.894
4.887
3.925
3.916
3.910
3.900
3.890
3.874
1.875
1.862
1.851
1.825
1.802
1.793
1.786
1.700
1.696
1.692
1.687
1.681
1.669
1.665
1.659
1.651
1.518
1.488
1.480
1.456
1.448
1.439
1.430
1.424
1.416
1.400
1.392
1.385
1.361
1.270
1.261
1.253
1.240
1.231
0.000
1.04
1.04
2.10
2.00
1.03
3.17
1.18
4.90
1.29
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
f1 (ppm)
N
O
2p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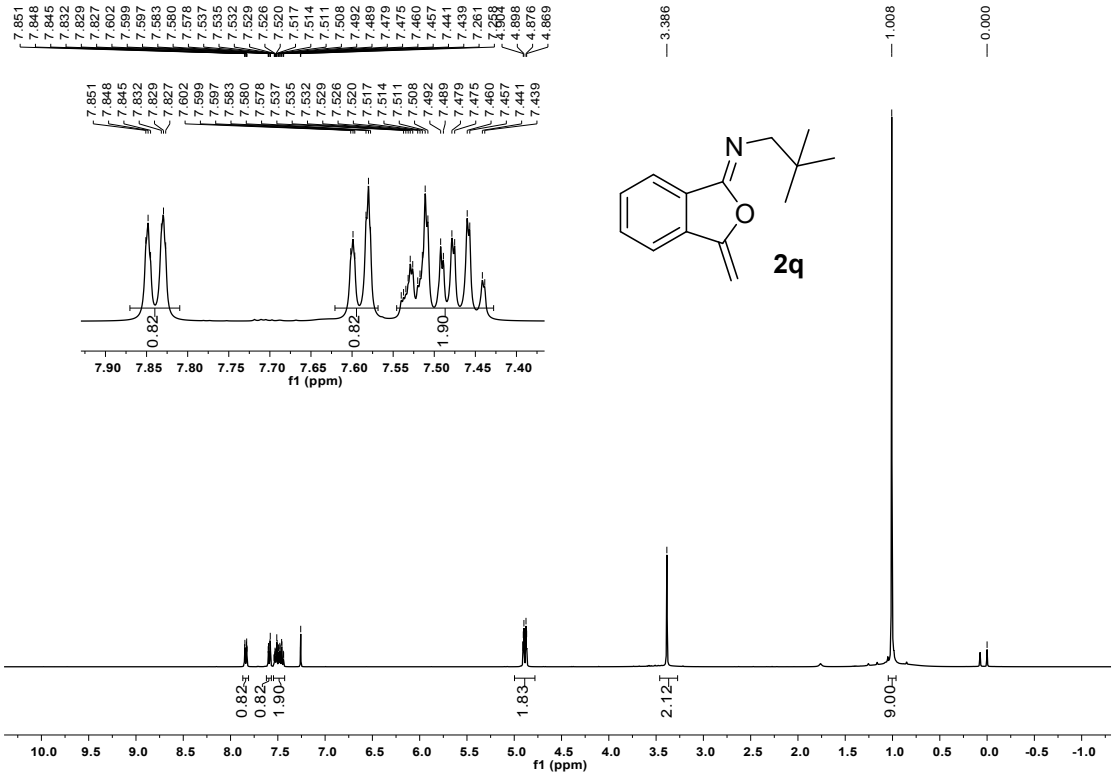
153.34
136.35
131.31
130.68
129.83
123.05
120.10
84.82
56.24
34.04
25.80
25.02
N
O
2p
f1 (ppm)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7.845
7.832
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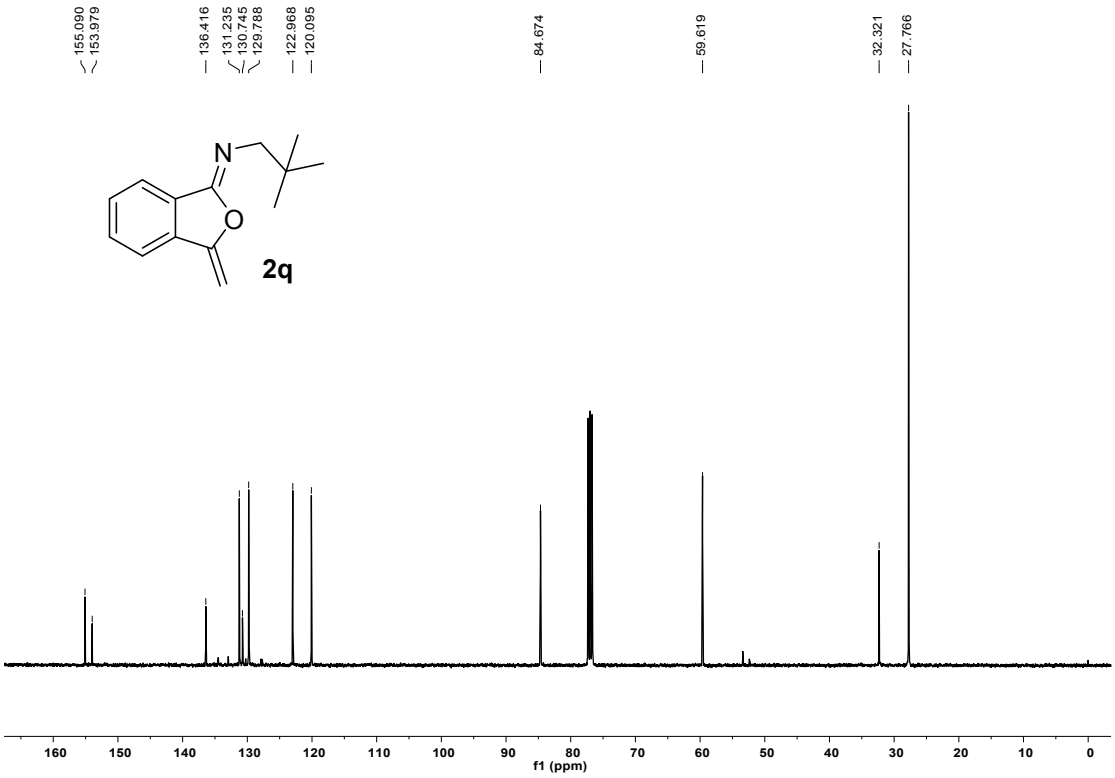
7.827
7.602
7.599
7.597
7.583
7.580
7.578
7.537
7.535
7.532
7.529
7.526
7.520
7.517
7.514
7.511
7.508
7.492
7.489
7.479
7.475
7.460
7.457
7.441
7.439
4.898
4.876
4.869
3.386
1.008
0.000
N
O
2q
0.82
0.82
1.90
1.83
2.12
9.00
f1 (ppm)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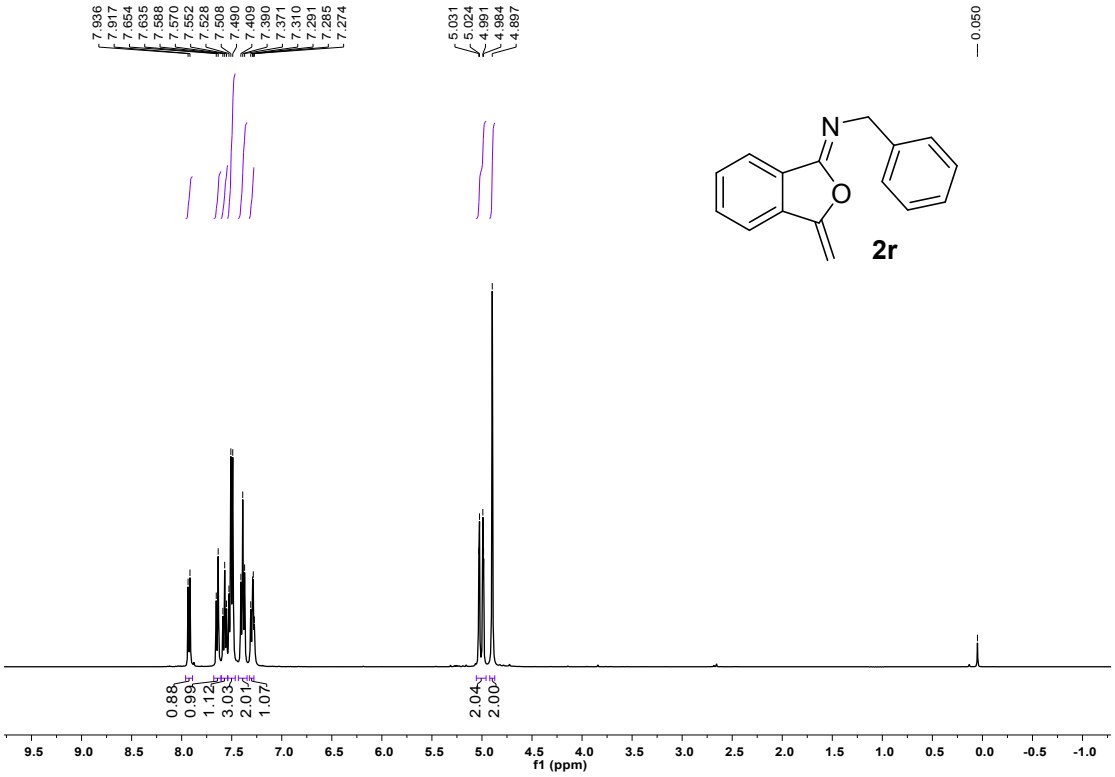
153.979
136.416
131.235
130.745
129.788
122.968
120.095
84.674
59.619
32.321
27.766
N
O
2q
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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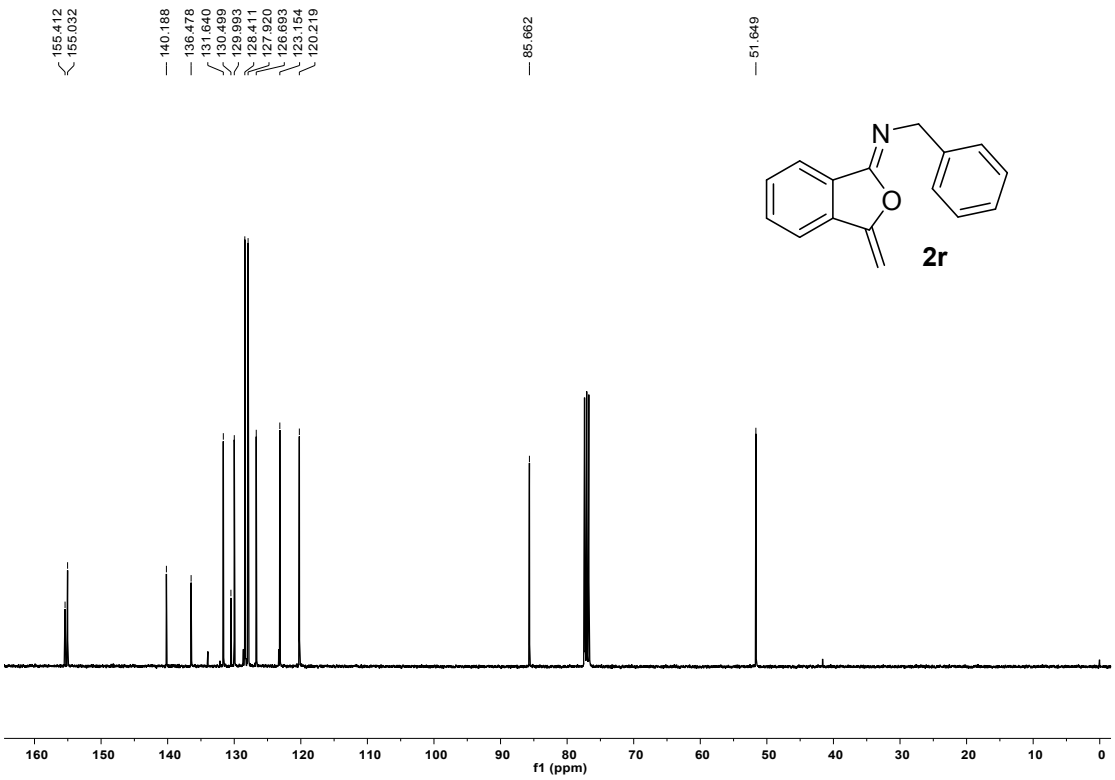
7.917
7.654
7.635
7.588
7.570
7.552
7.528
7.508
7.490
7.409
7.390
7.371
7.310
7.291
7.285
7.274
5.031
5.024
4.991
4.984
4.897
0.050
N
O
2r
0.88
0.99
1.12
3.03
2.01
1.07
2.04
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)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155.032
140.188
136.478
131.640
130.499
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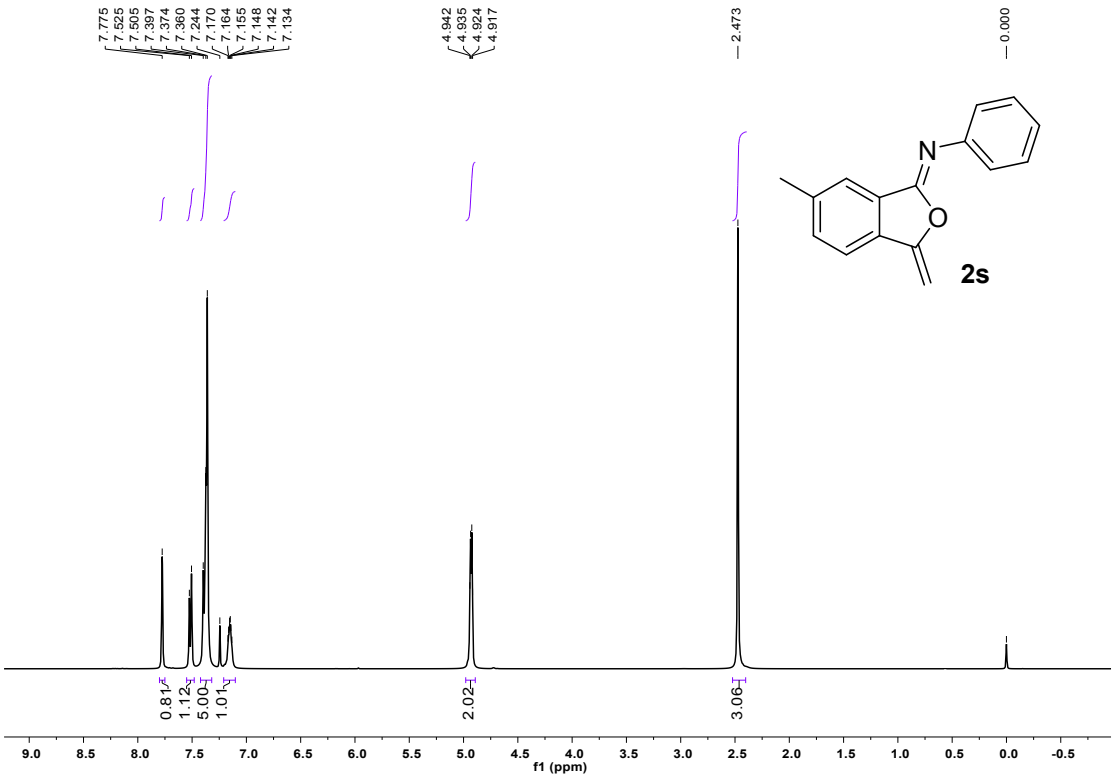
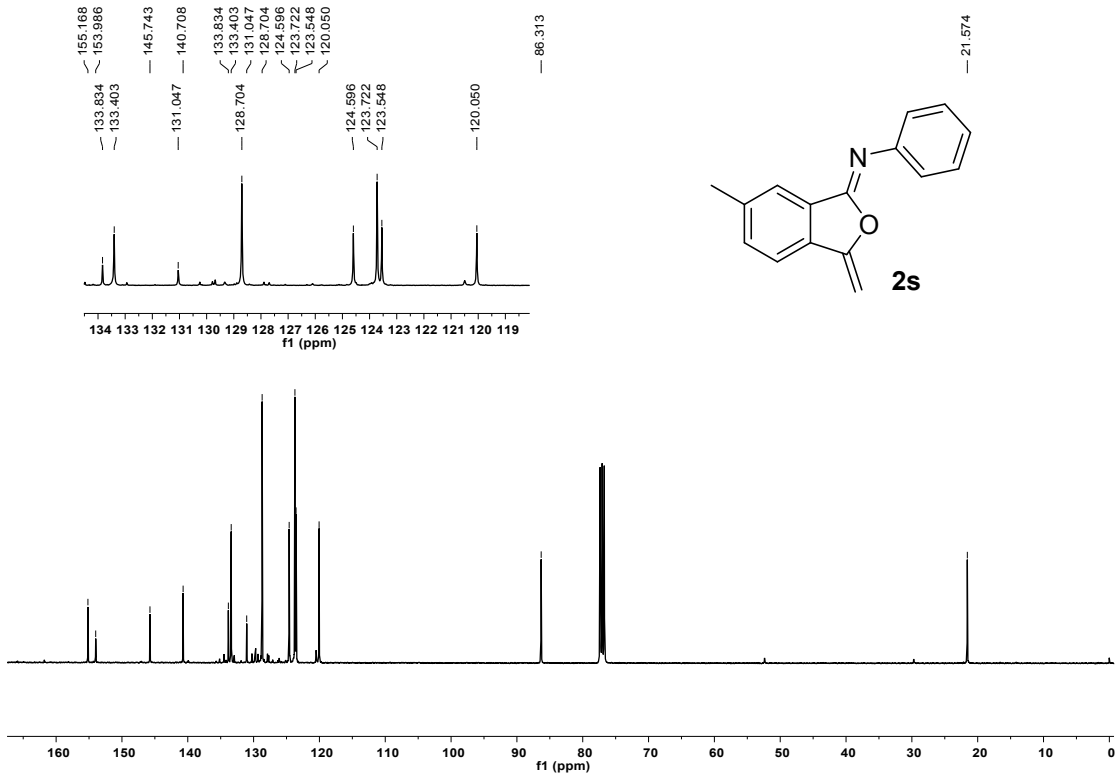
128.411
127.920
126.693
123.154
120.219
85.662
51.649
N
O
2r
f1 (ppm)


7.775
7.525
7.505
7.397
7.374
7.360
7.244
7.170
7.164
7.155
7.148
7.142
7.134
4.942
4.935
4.924
4.917
2.473
0.000
N
O
2s
0.81
1.12
5.00
1.01
2.02
3.08
f1 (ppm)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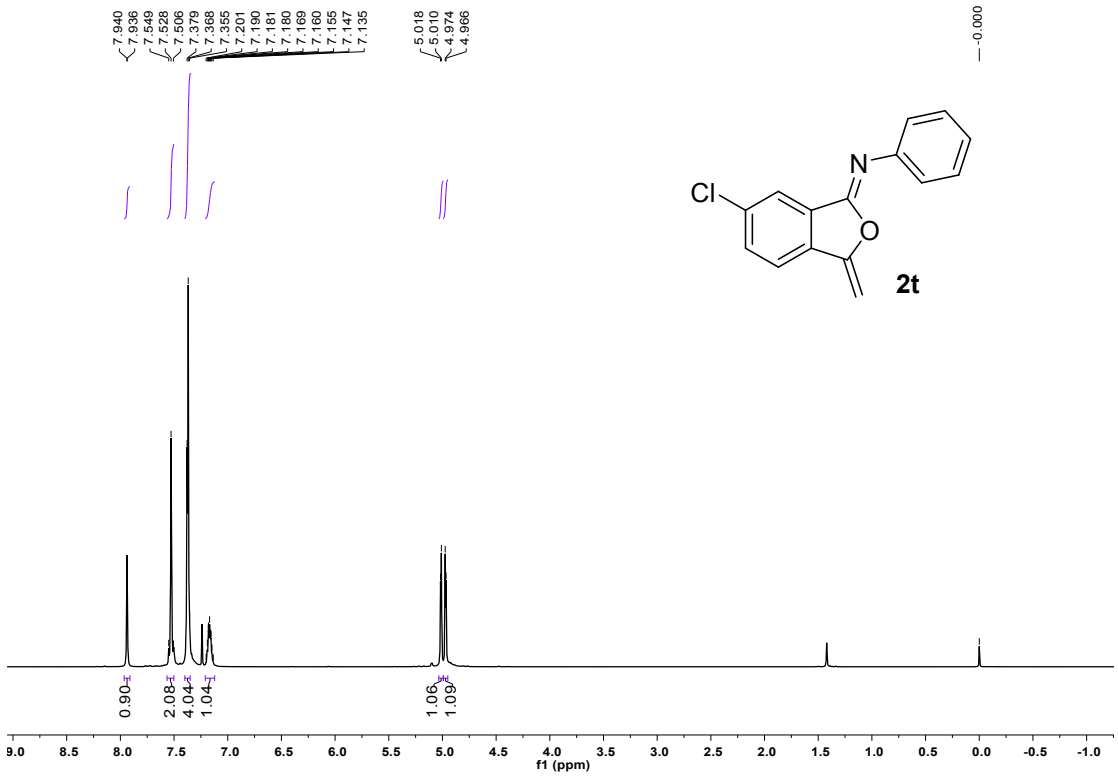
145.743
140.708
133.834
133.403
131.047
128.704
124.596
123.722
123.548
120.050
86.313
21.574
N
O
2s
f1 (ppm)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7.528
7.506
7.379
7.368
7.355
7.201
7.190
7.181
7.180
7.169
7.160
7.155
7.147
7.135
5.018
5.010
4.974
4.966
-0.000
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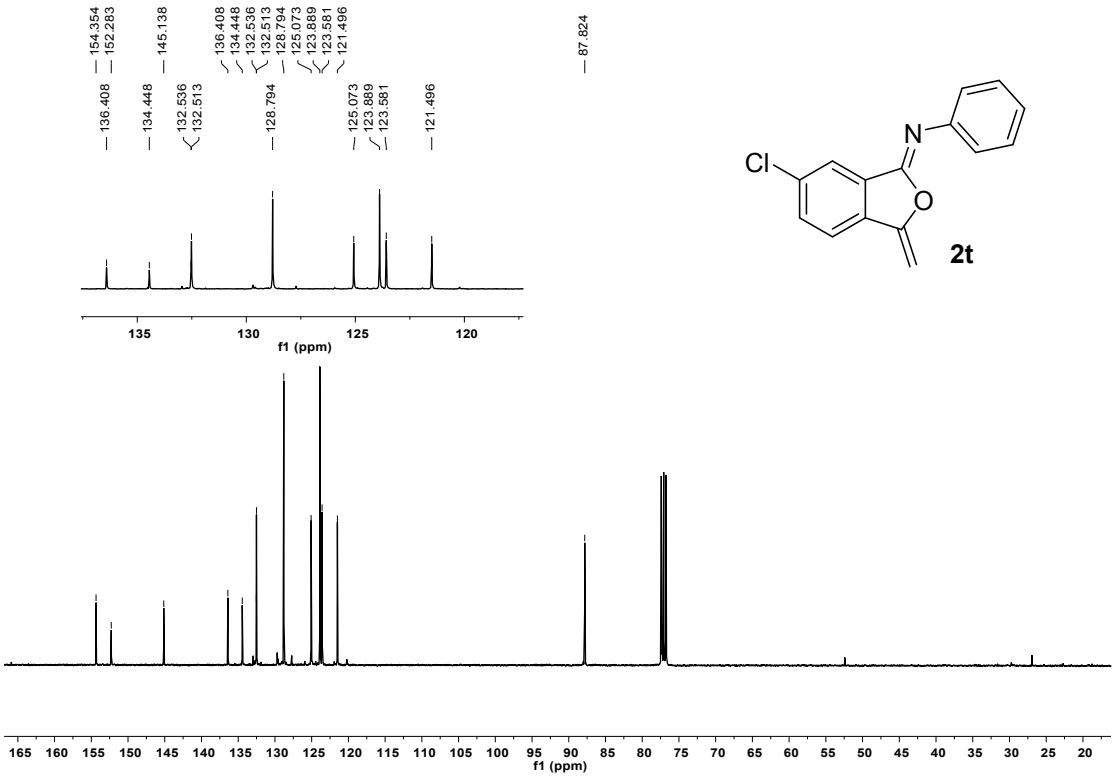
Cl
O
2t
0.90
2.08
4.04
1.04
1.06
1.09
f1 (ppm)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145.138
136.408
134.448
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132.513
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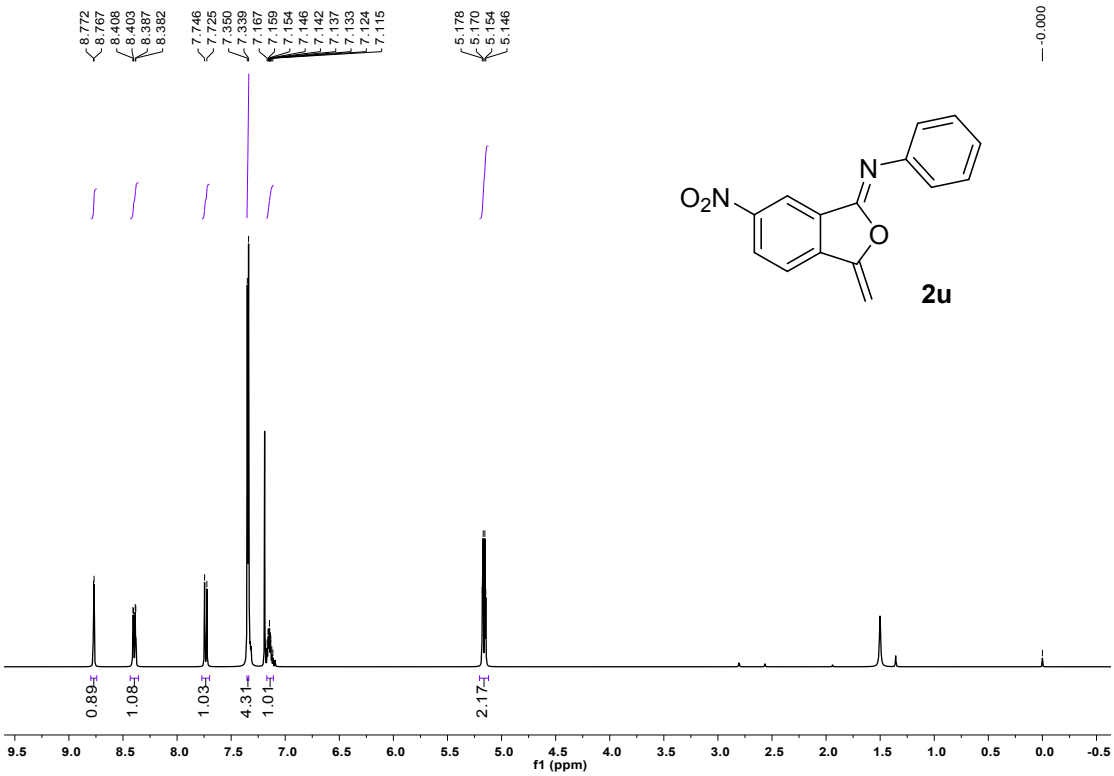
123.889
123.581
121.496
87.824
Cl
N
O
2t
f1 (ppm)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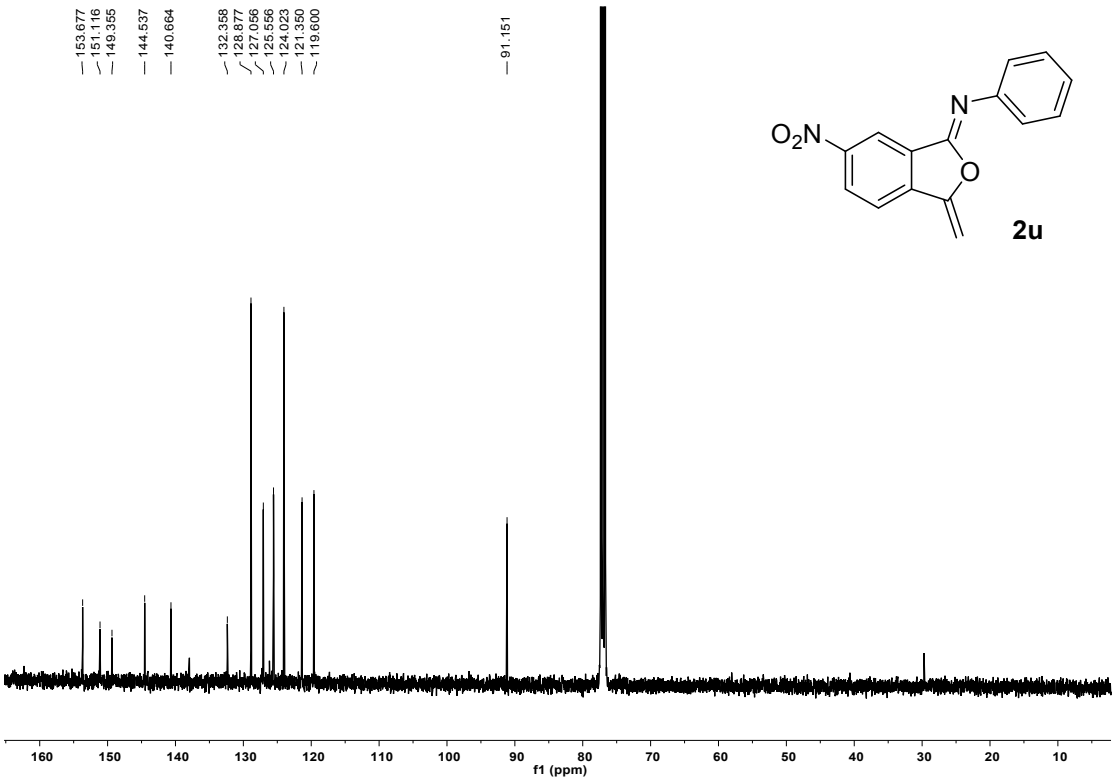
8.387
8.382
7.746
7.725
7.350
7.339
7.167
7.159
7.154
7.146
7.142
7.137
7.133
7.124
7.115
5.178
5.170
5.154
5.146
-0.000
O2N
N
O
2u
0.89
1.08
1.03
4.31
1.01
2.17
f1 (ppm)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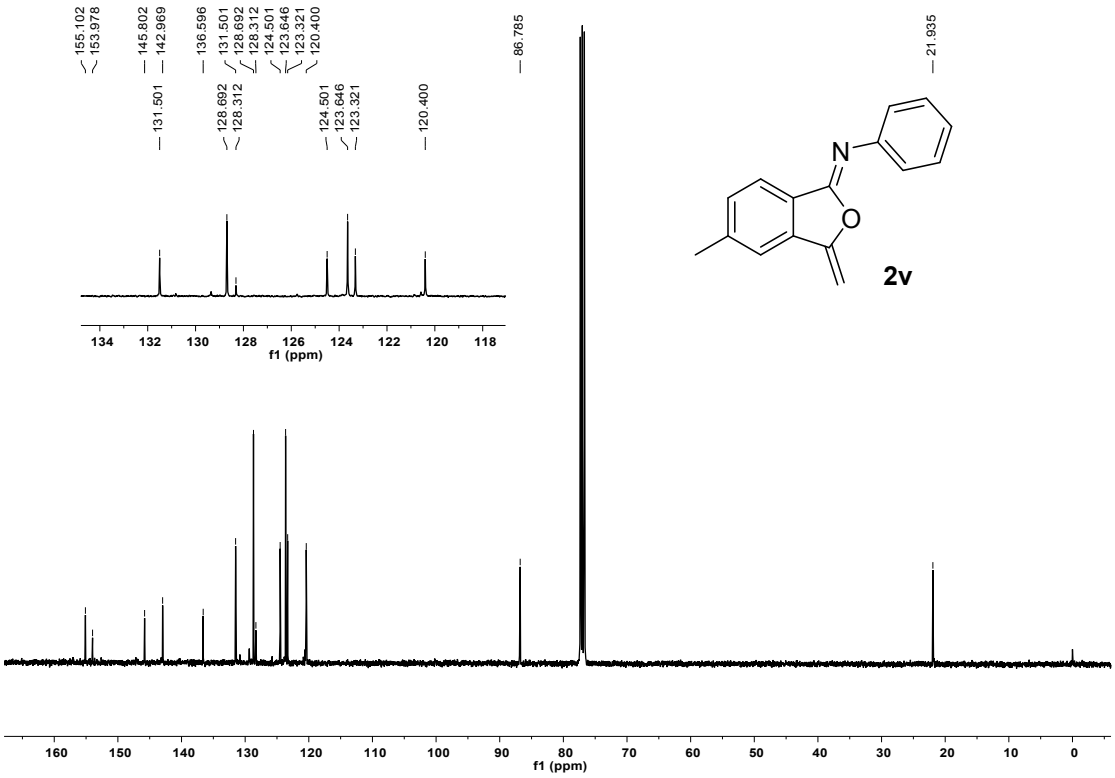
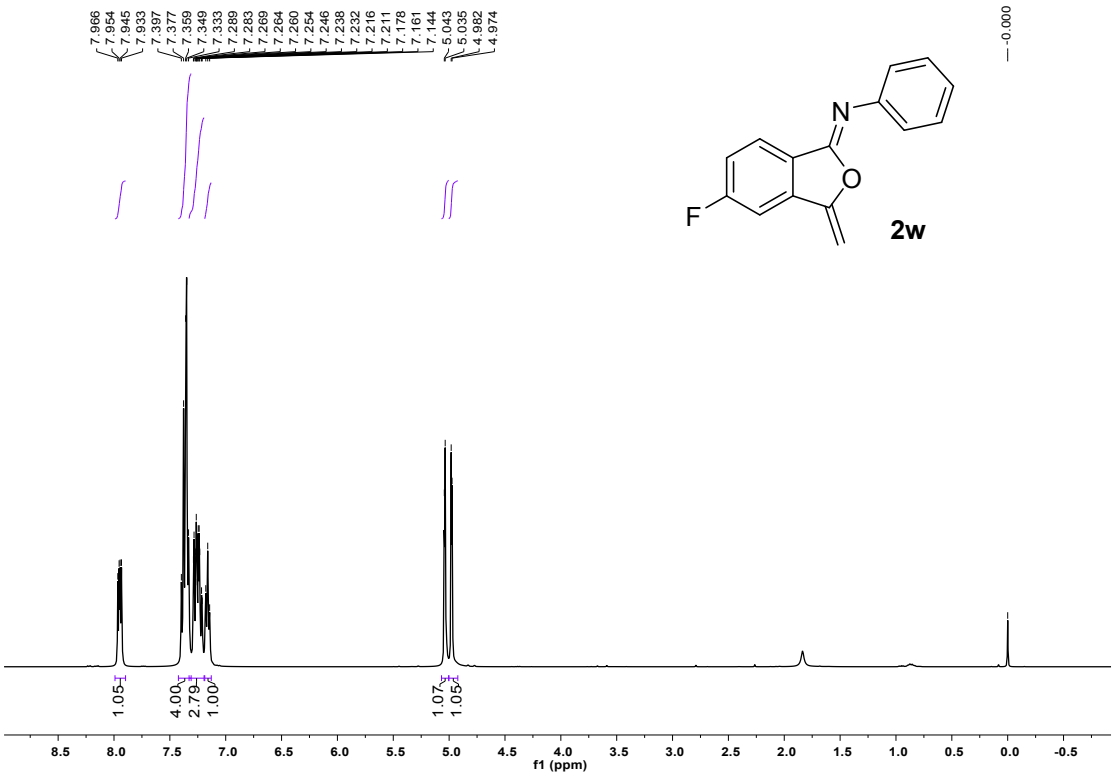
144.537
140.664
132.358
128.877
127.056
125.556
124.023
121.350
119.600
91.151
O_2N
N
O
2u
f1 (ppm)


7.868
7.848
7.442
7.395
7.374
7.357
7.351
7.334
7.172
7.167
7.155
7.149
7.139
7.133
4.967
2.495
0.000
0.96
1.15
5.24
1.11
2.00
2.90
N
O
2v
f1 (ppm)


155.102
153.978
145.802
142.969
136.596
131.501
128.692
128.312
124.501
123.646
123.321
120.400
86.785
21.935
N
O
2v
f1 (ppm)
f1 (ppm)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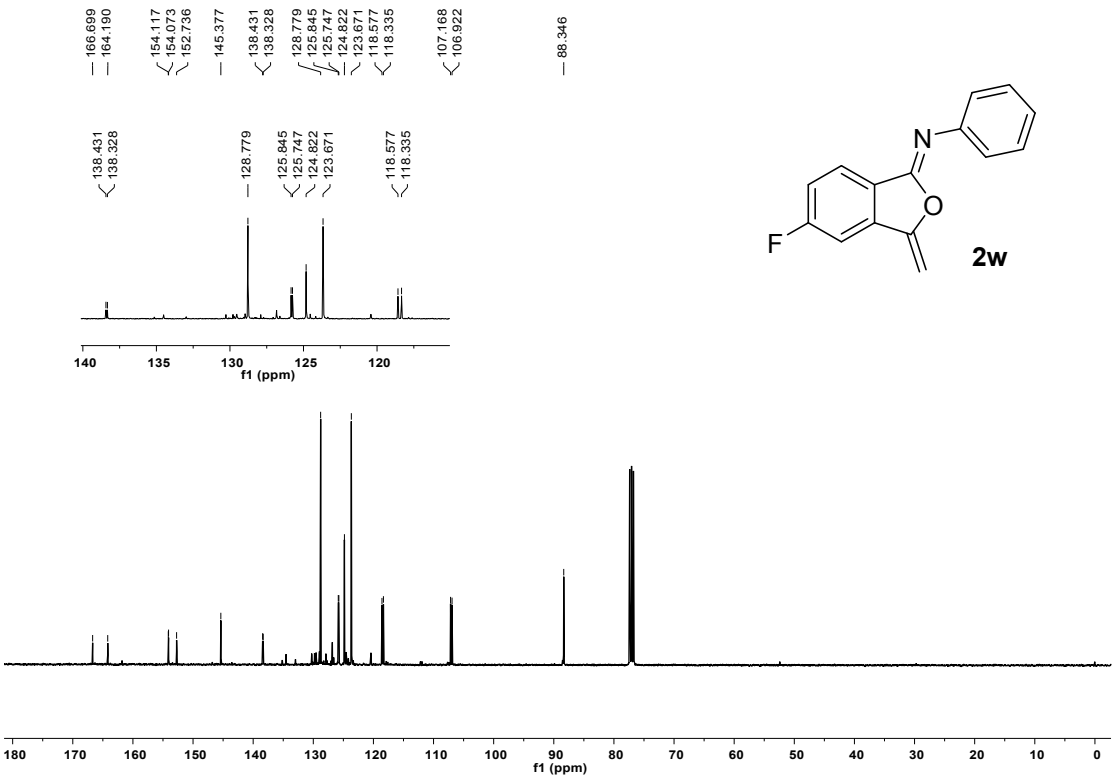
7.954
7.945
7.933
7.397
7.377
7.359
7.349
7.333
7.289
7.283
7.269
7.264
7.260
7.254
7.246
7.238
7.232
7.216
7.211
7.178
7.161
7.144
5.043
5.035
4.982
4.974
-0.000
N
O
F
2w
1.05
4.00
2.79
1.00
1.07
1.05
f1 (ppm)


166.699
164.190
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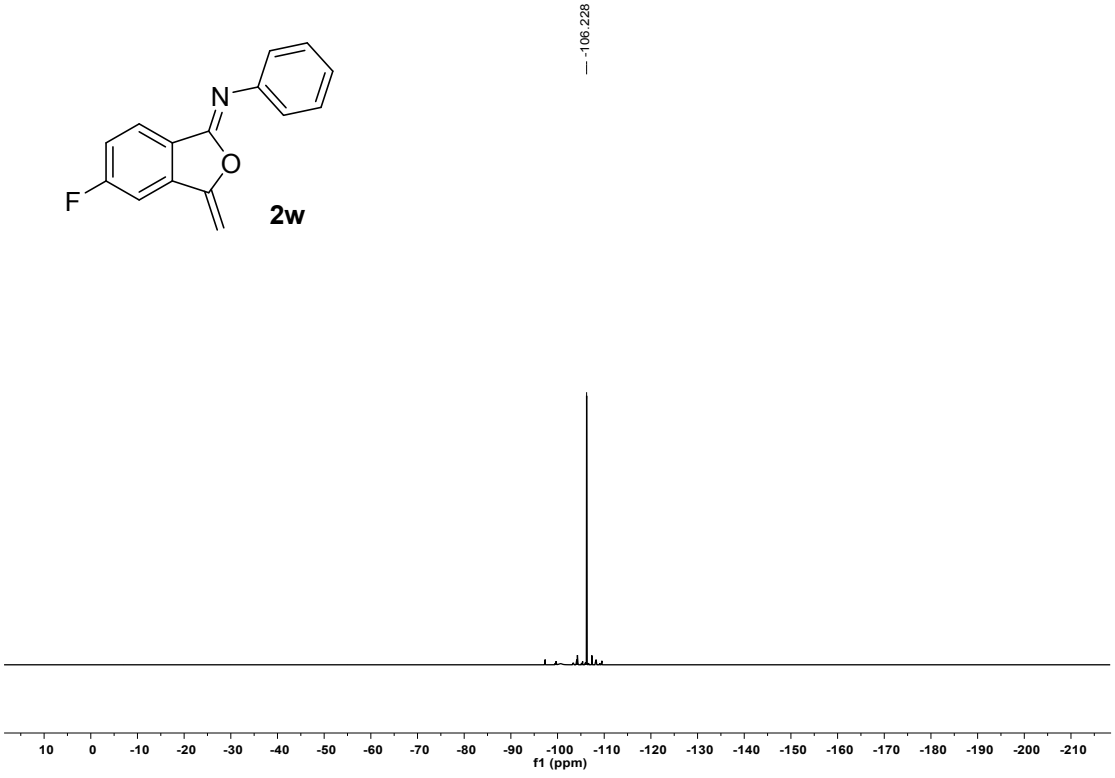
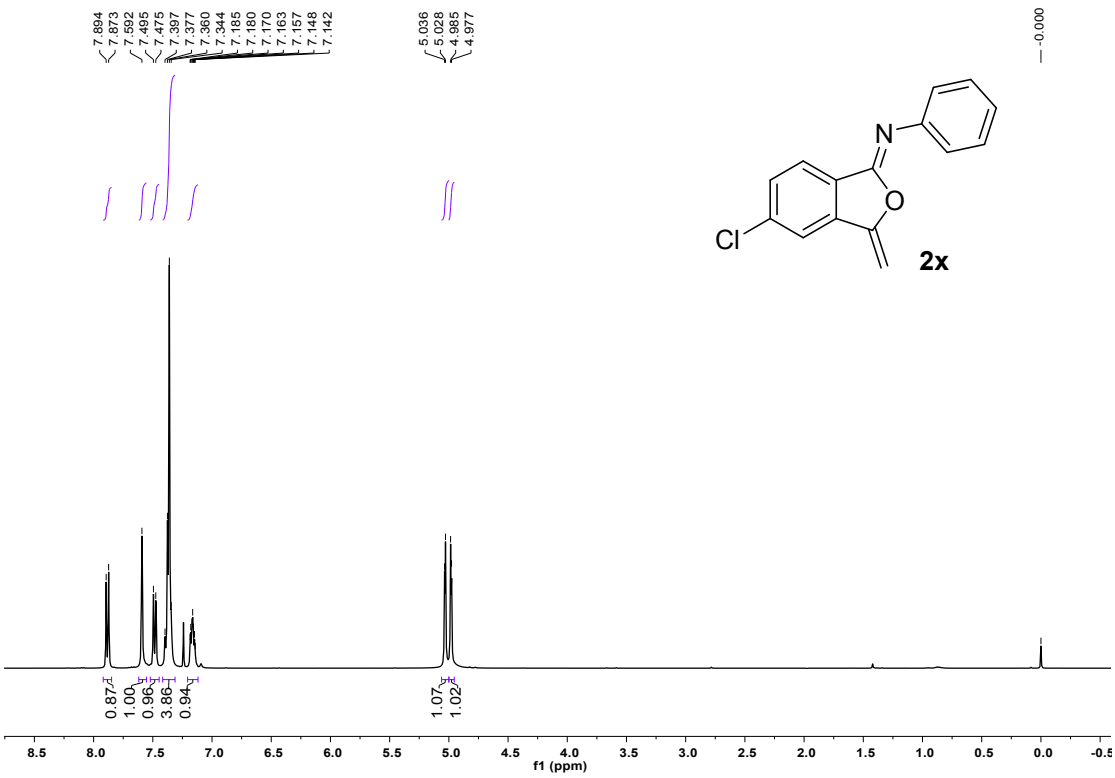
154.073
152.736
145.377
138.431
138.328
128.779
125.845
125.747
124.822
123.671
118.577
118.335
107.168
106.922
88.346
f1 (ppm)
N
O
F
2w


-106.228
N
O
F
2w
f1 (ppm)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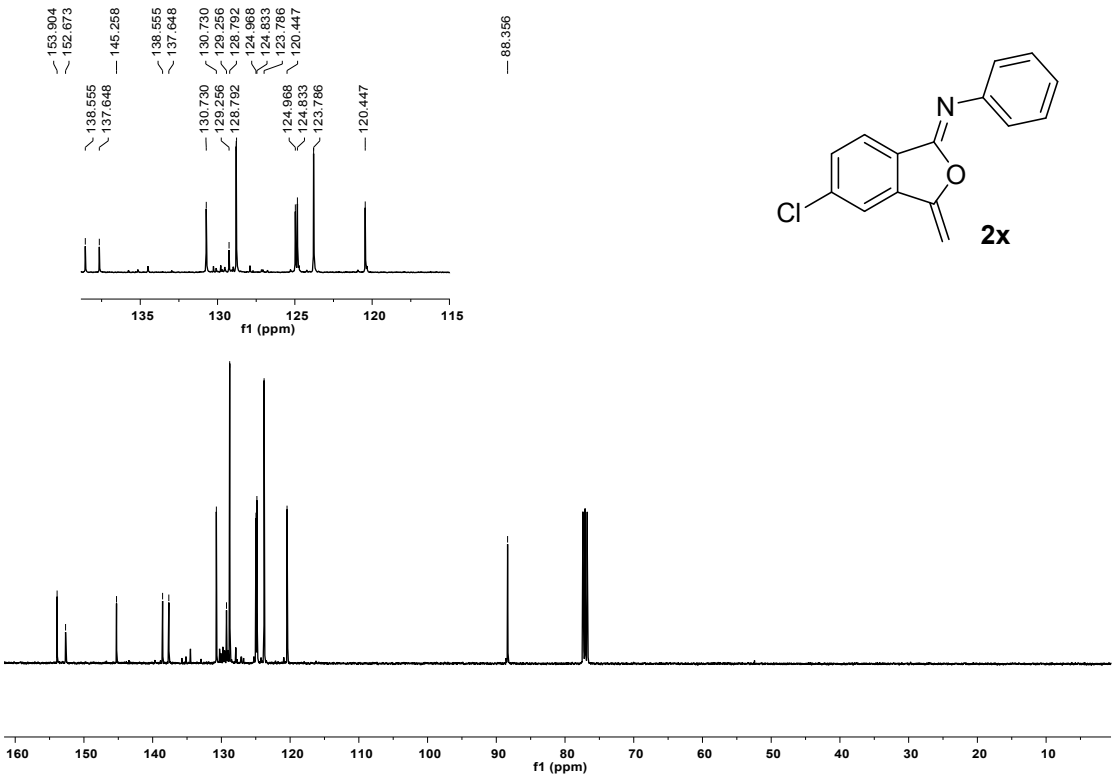
7.873
7.592
7.495
7.475
7.397
7.377
7.360
7.344
7.185
7.180
7.170
7.163
7.157
7.148
7.142
5.036
5.028
4.985
4.977
-0.000
0.87
1.00
0.96
3.86
0.94
1.07
1.02
f1 (ppm)
N
O
Cl
2x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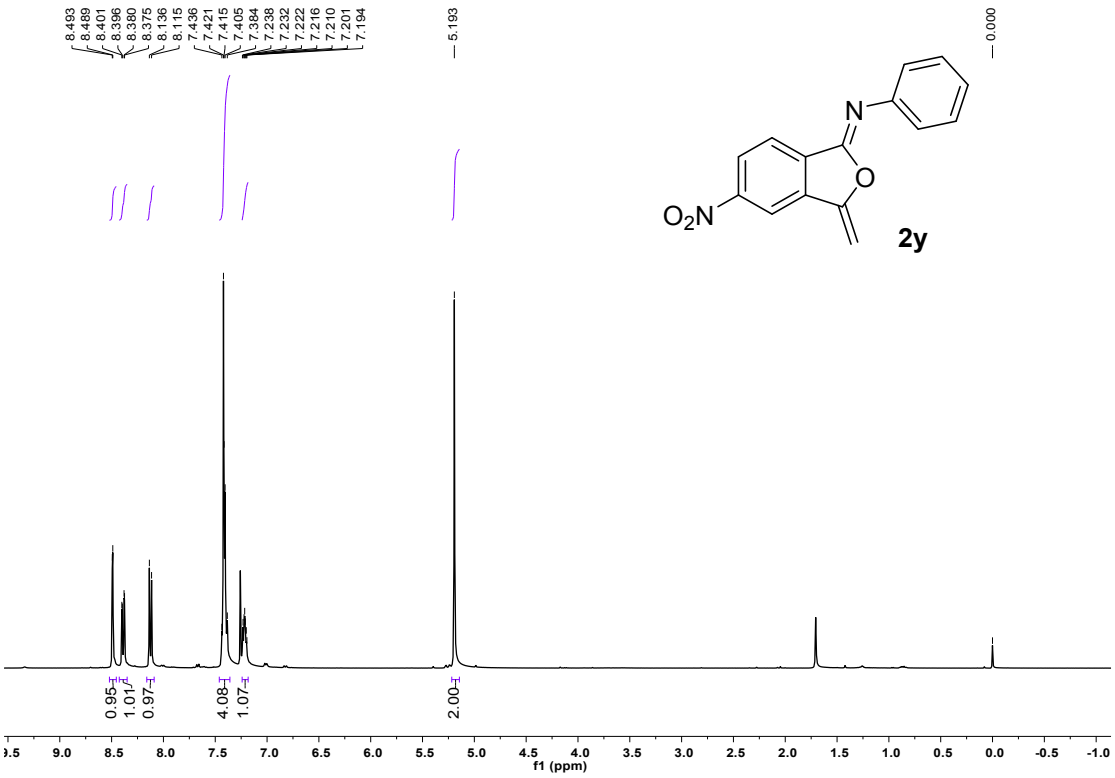
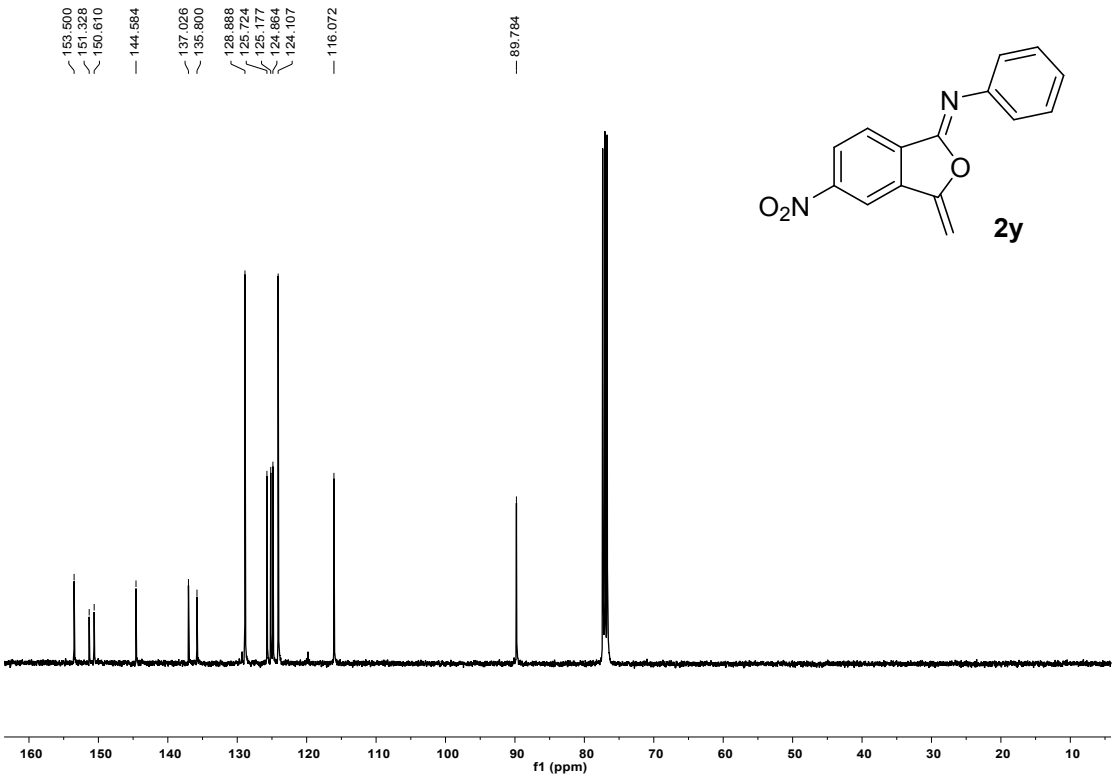
152.673
145.258
138.555
137.648
130.730
129.256
128.792
124.968
124.833
123.786
120.447
88.356
f1 (ppm)
N
O
Cl
2x


8.493
8.489
8.401
8.396
8.380
8.375
8.136
8.115
7.436
7.421
7.415
7.405
7.384
7.238
7.232
7.222
7.216
7.210
7.201
7.194
5.193
0.000
0.95
1.01
0.97
4.08
1.07
2.00
f1 (ppm)
N
O
O2N
2y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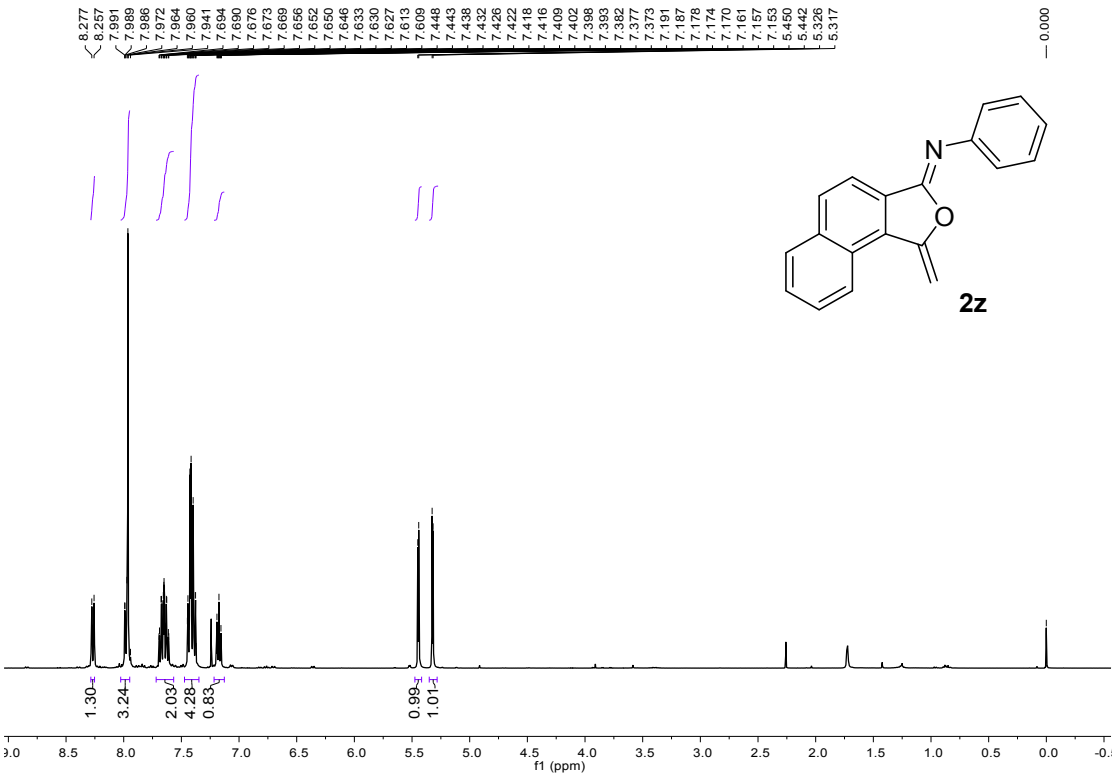
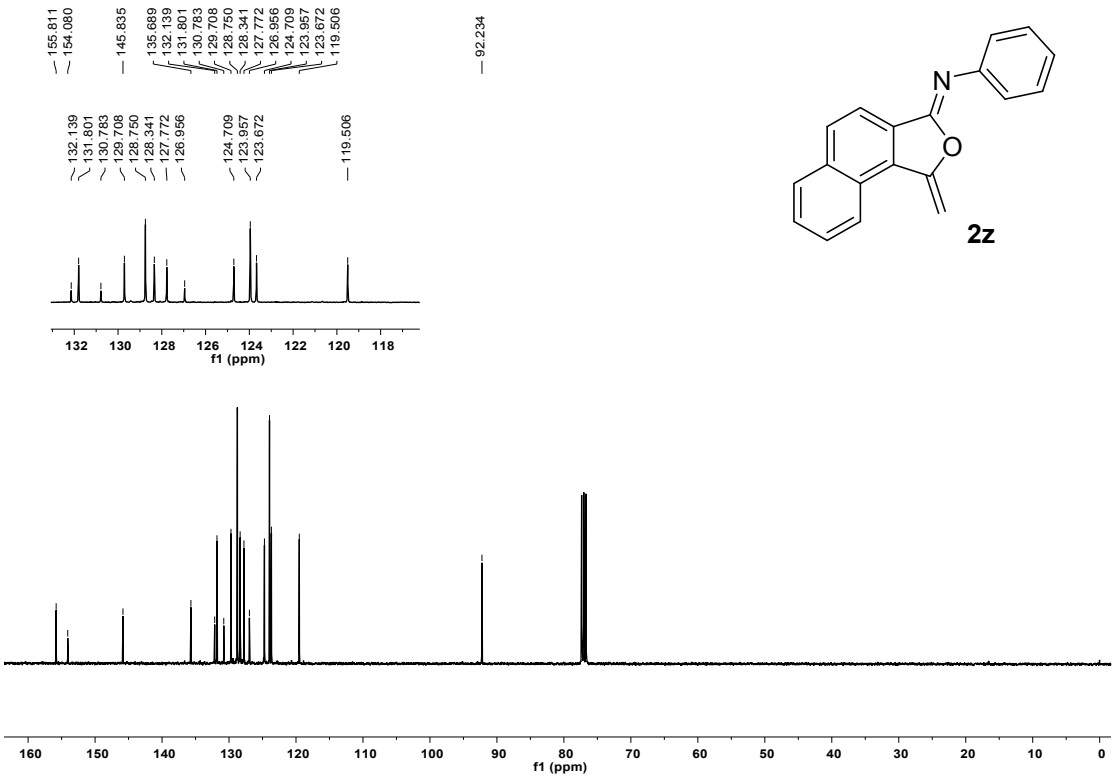
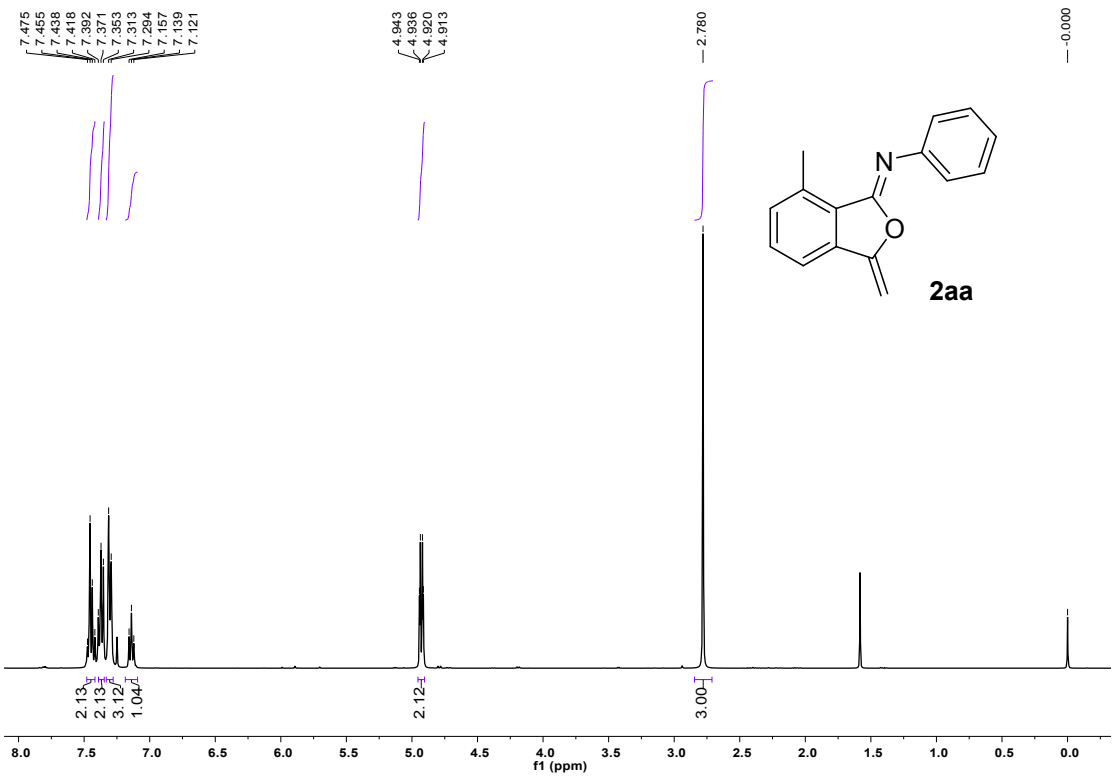
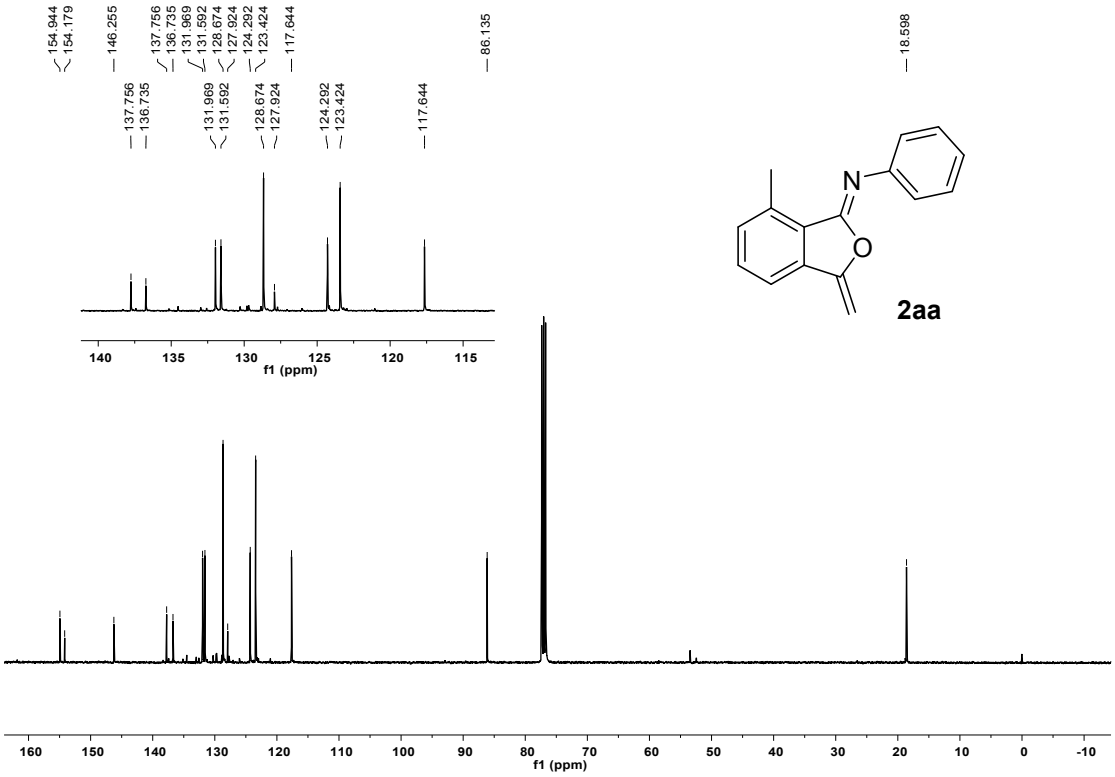
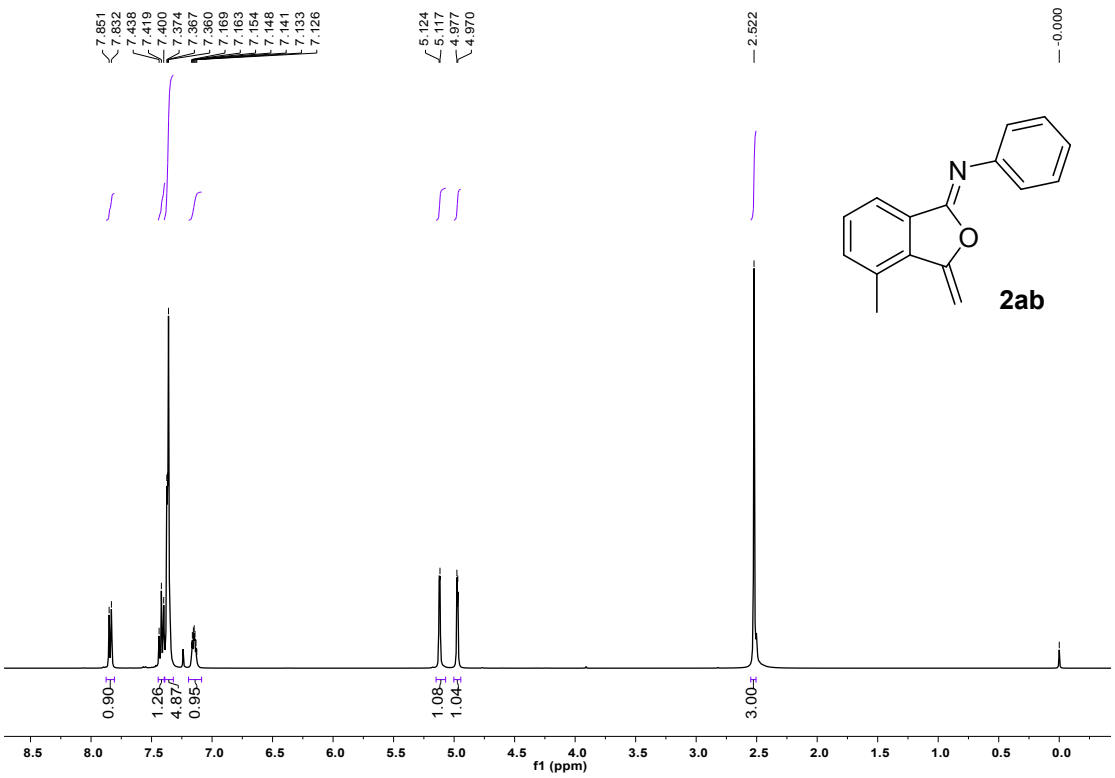
151.328
150.610
144.584
137.026
135.800
128.888
125.724
125.177
124.864
124.107
116.072
89.784
f1 (ppm)
N
O
O2N
2y

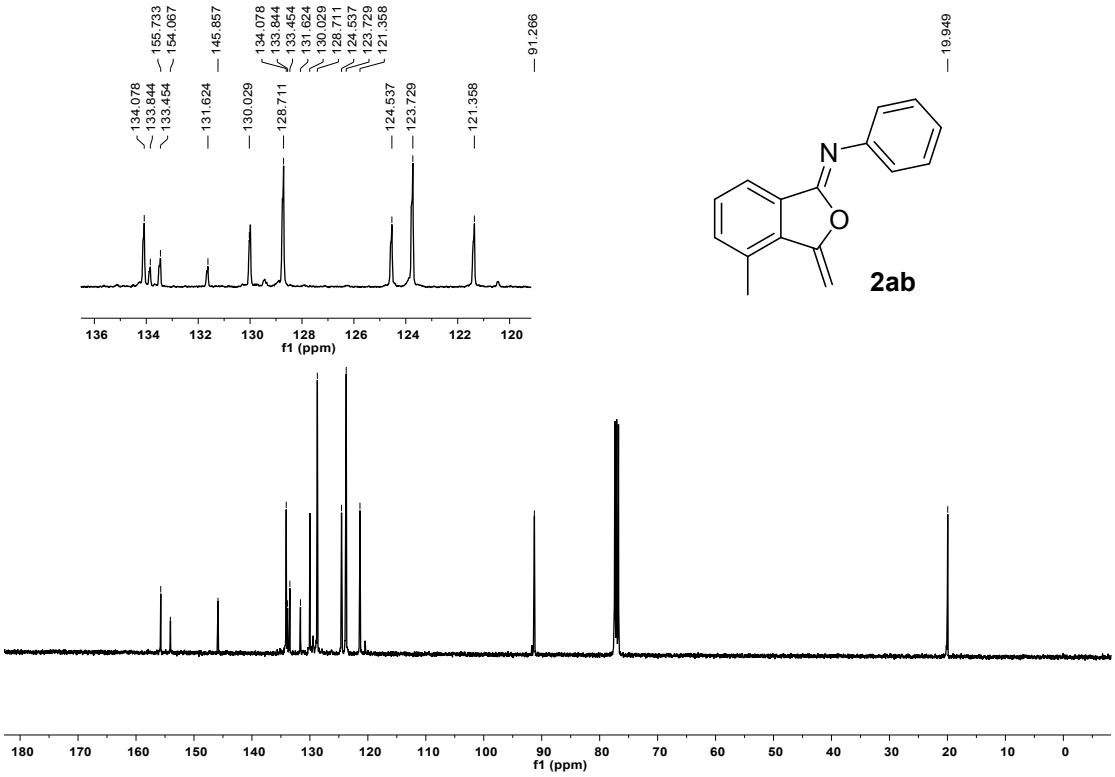

8.277
8.257
7.991
7.989
7.986
7.972
7.964
7.960
7.941
7.694
7.690
7.676
7.673
7.669
7.656
7.652
7.650
7.646
7.633
7.630
7.627
7.613
7.609
7.448
7.443
7.438
7.432
7.426
7.422
7.418
7.416
7.409
7.402
7.398
7.393
7.382
7.377
7.373
7.191
7.187
7.178
7.174
7.170
7.161
7.157
7.153
5.450
5.442
5.326
5.317
0.000
1.30
3.24
2.03
4.28
0.83
0.99
1.01
f1 (ppm)
N
O
2z

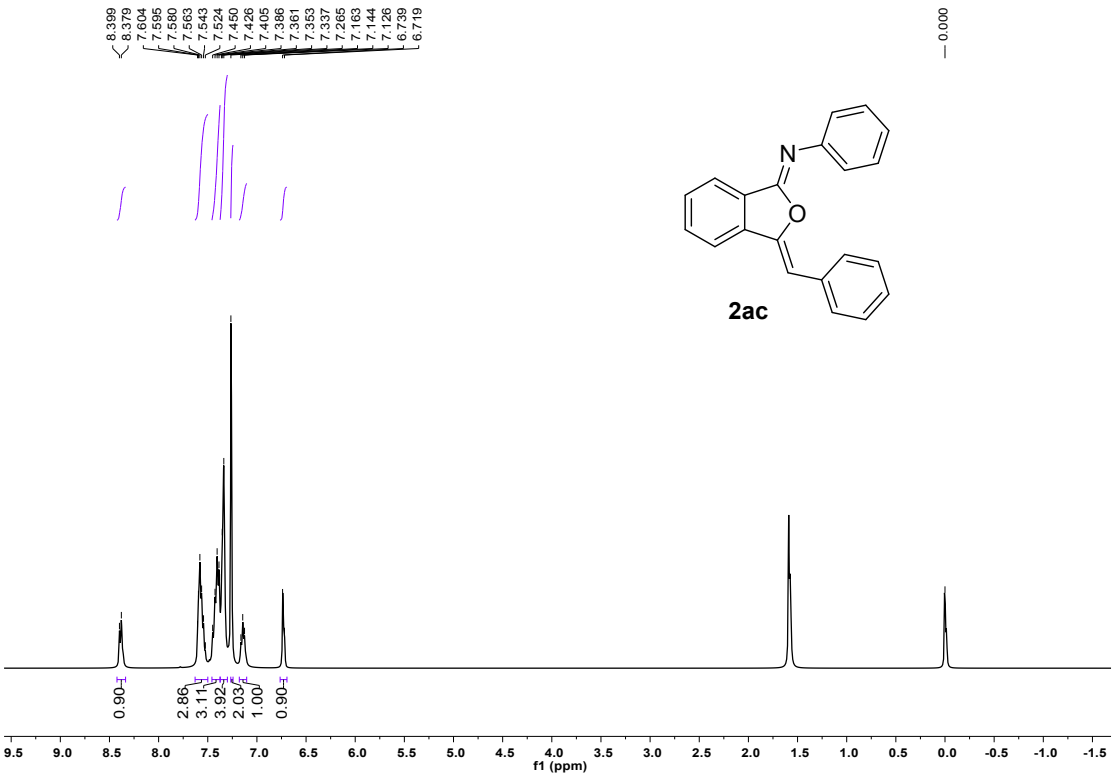

155.811
154.080
145.835
135.689
132.139
131.801
130.783
129.708
128.750
128.341
127.772
126.956
124.709
123.957
123.672
119.506
92.234
f1 (ppm)
N
O
2z

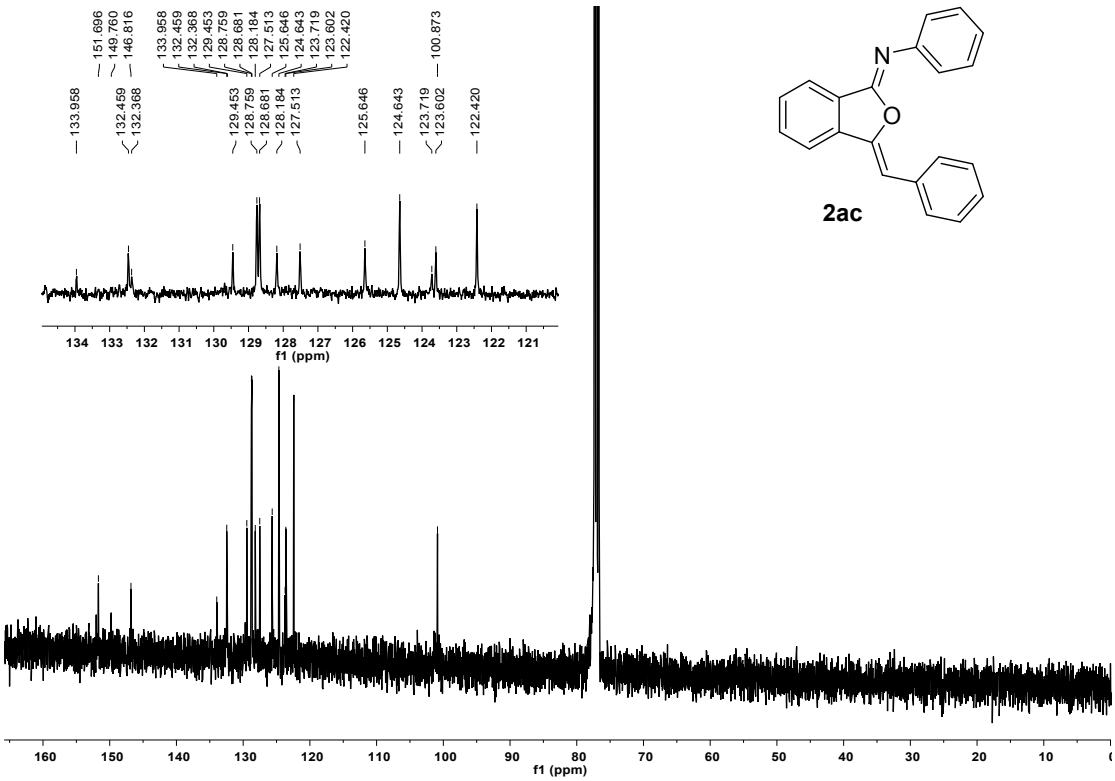

7.475
7.455
7.438
7.418
7.392
7.371
7.353
7.313
7.294
7.157
7.139
7.121
4.943
4.936
4.920
4.913
2.780
-0.000
2.13
2.13
3.12
1.04
2.12
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
N
O
2aa

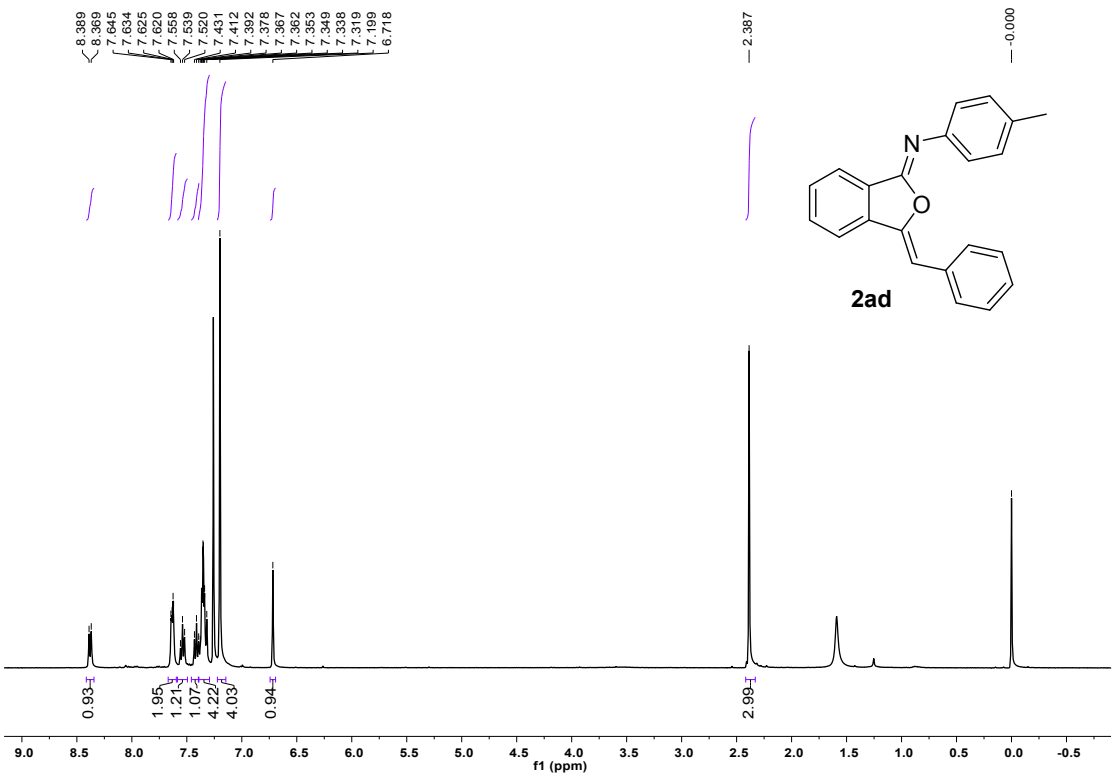

154.944
154.179
146.255
137.756
136.735
131.969
131.592
128.674
127.924
124.292
123.424
117.644
86.135
18.598
140
135
130
125
120
115
f1 (ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
N
O
2aa

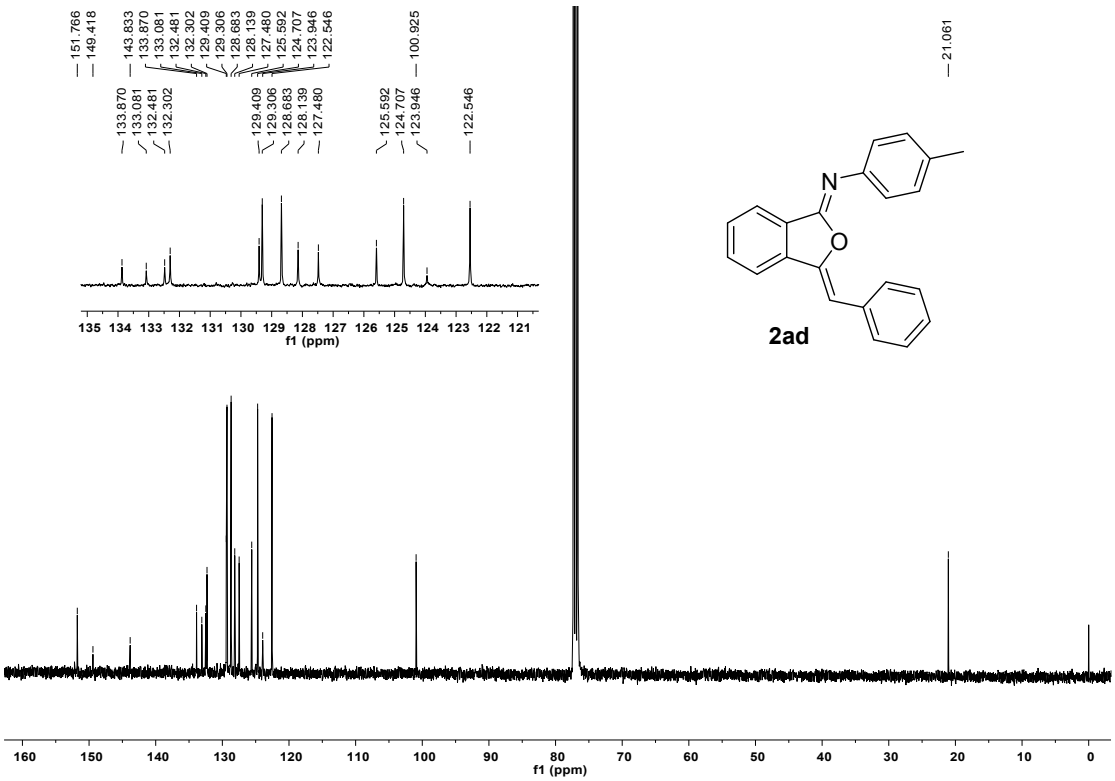

7.851
7.832
7.438
7.419
7.400
7.374
7.367
7.360
7.169
7.163
7.154
7.148
7.141
7.133
7.126
5.124
5.117
4.977
4.970
2.522
-0.000
0.90
1.26
4.87
0.95
1.08
1.04
3.00
f1 (ppm)
2ab


155.733
154.067
145.857
134.078
133.844
133.454
131.624
130.029
128.711
124.537
123.729
121.358
91.266
19.949
f1 (ppm)
2ab


8.399
8.379
7.604
7.595
7.580
7.563
7.543
7.524
7.450
7.426
7.405
7.386
7.361
7.353
7.337
7.265
7.163
7.144
7.126
6.739
6.719
0.000
N
O
2ac
0.90
2.86
3.11
3.92
2.03
1.00
0.90
f1 (ppm)


151.696
149.760
146.816
133.958
132.459
132.368
129.453
128.759
128.681
128.184
127.513
125.646
124.643
123.719
123.602
122.420
100.873
N
O
2ac
f1 (ppm)


8.389
8.369
7.645
7.634
7.625
7.620
7.558
7.539
7.520
7.431
7.412
7.392
7.378
7.367
7.362
7.353
7.349
7.338
7.319
7.199
6.718
2.387
-0.000
N
O
2ad
0.93
1.95
1.21
1.07
4.22
4.03
0.94
2.99
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
f1 (ppm)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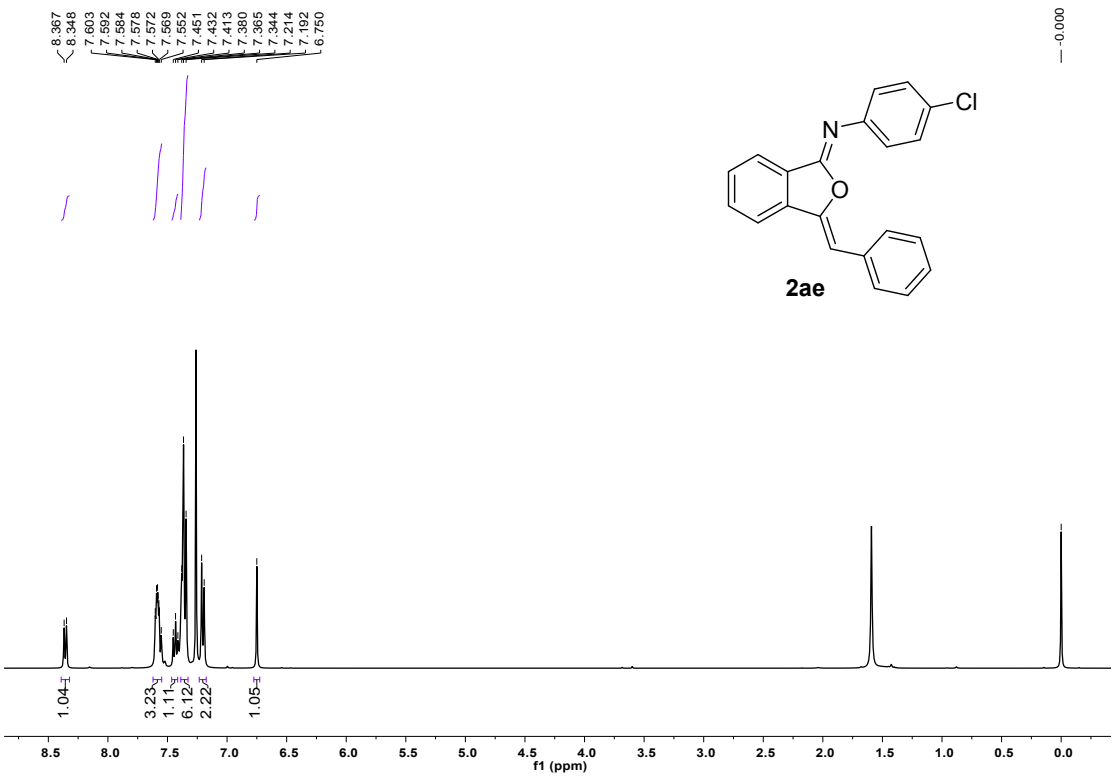
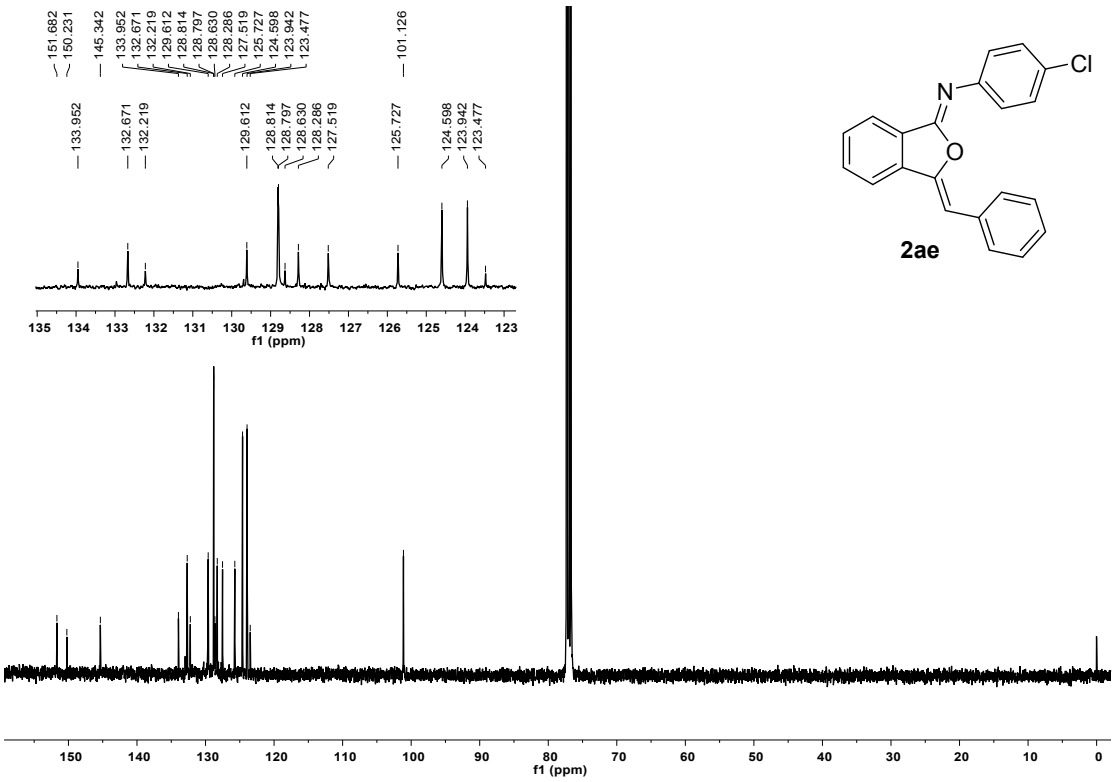
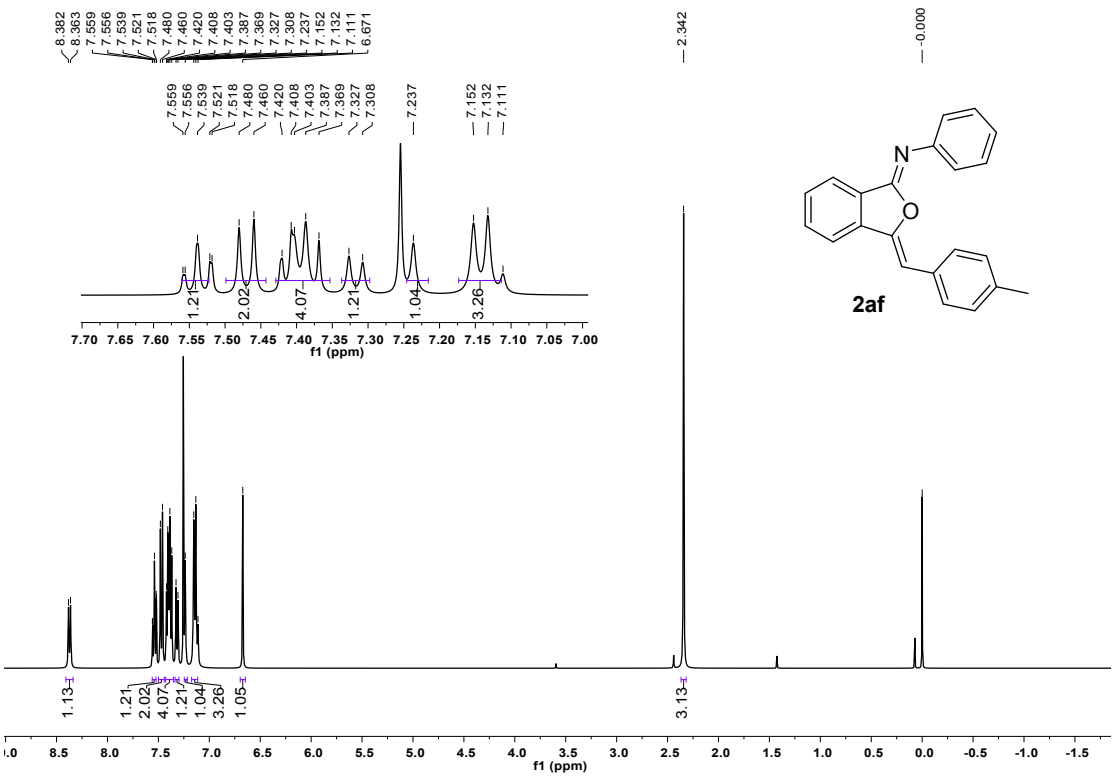
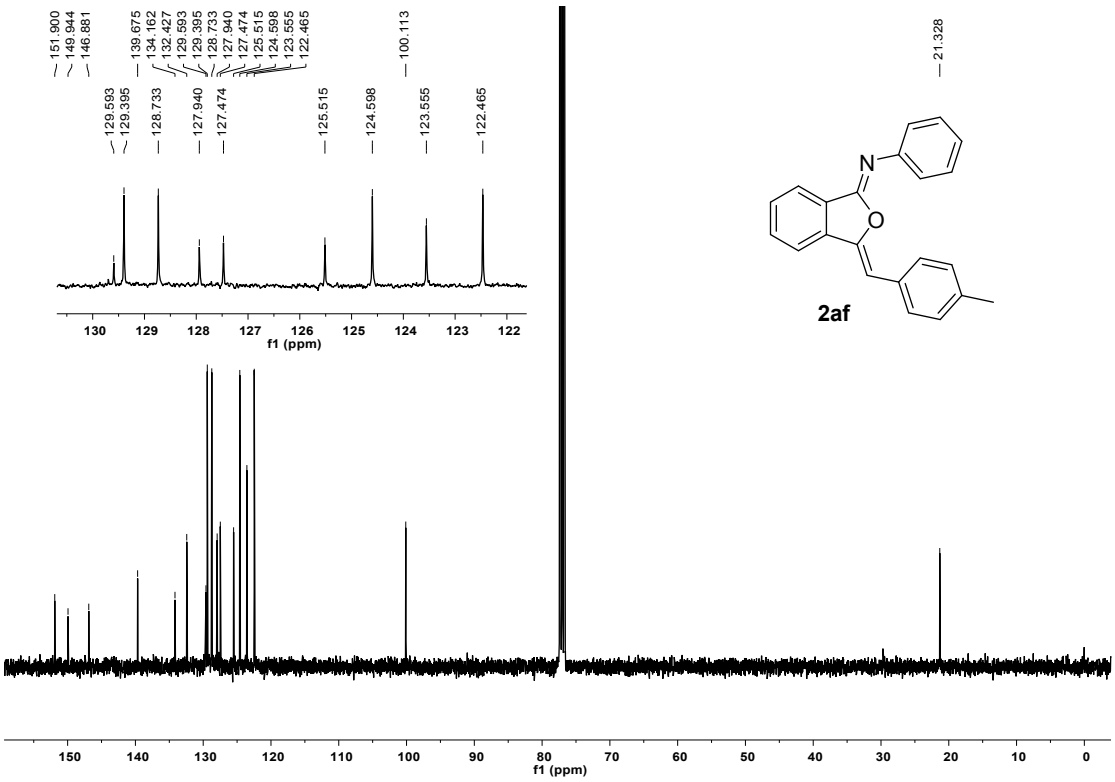
143.833
133.870
133.081
132.481
132.302
129.409
129.306
128.683
128.139
127.480
125.592
124.707
123.946
122.546
100.925
21.061
N
O
2ad
135 134 133 132 131 130 129 128 127 126 125 124 123 122 121
f1 (ppm)
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.367
8.348
7.603
7.592
7.584
7.578
7.572
7.569
7.552
7.451
7.432
7.413
7.380
7.365
7.344
7.214
7.192
6.750
-0.000
Cl
N
O
2ae
1.04
3.23
1.11
6.12
2.22
1.05
f1 (ppm)


151.682
150.231
145.342
133.952
132.671
132.219
129.612
128.814
128.797
128.630
128.286
127.519
125.727
124.598
123.942
123.477
101.126
Cl
N
O
2ae
f1 (ppm)


8.382
8.363
7.559
7.556
7.539
7.521
7.518
7.480
7.460
7.420
7.408
7.403
7.387
7.369
7.327
7.308
7.237
7.152
7.132
7.111
6.671
2.342
-0.000
1.21
2.02
4.07
1.21
1.04
3.26
1.13
1.21
2.02
4.07
1.21
1.04
3.26
1.05
3.13
N
O
2af
f1 (ppm)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139.675
134.162
132.427
129.593
129.395
128.733
127.940
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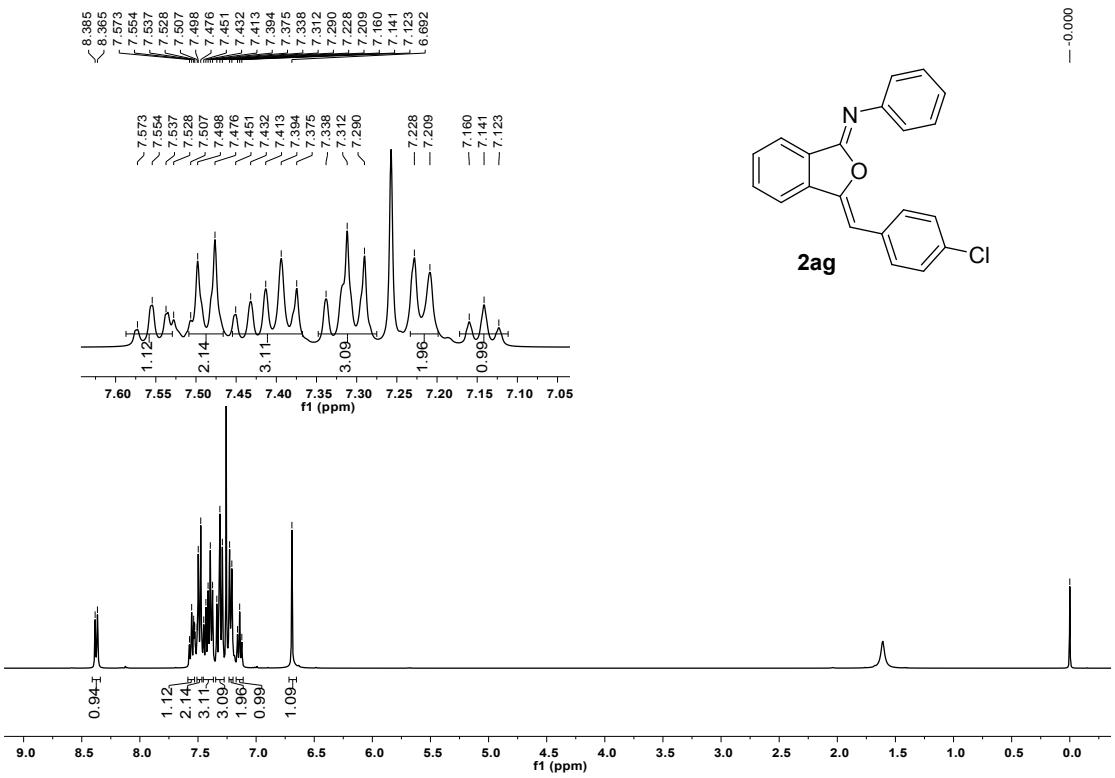
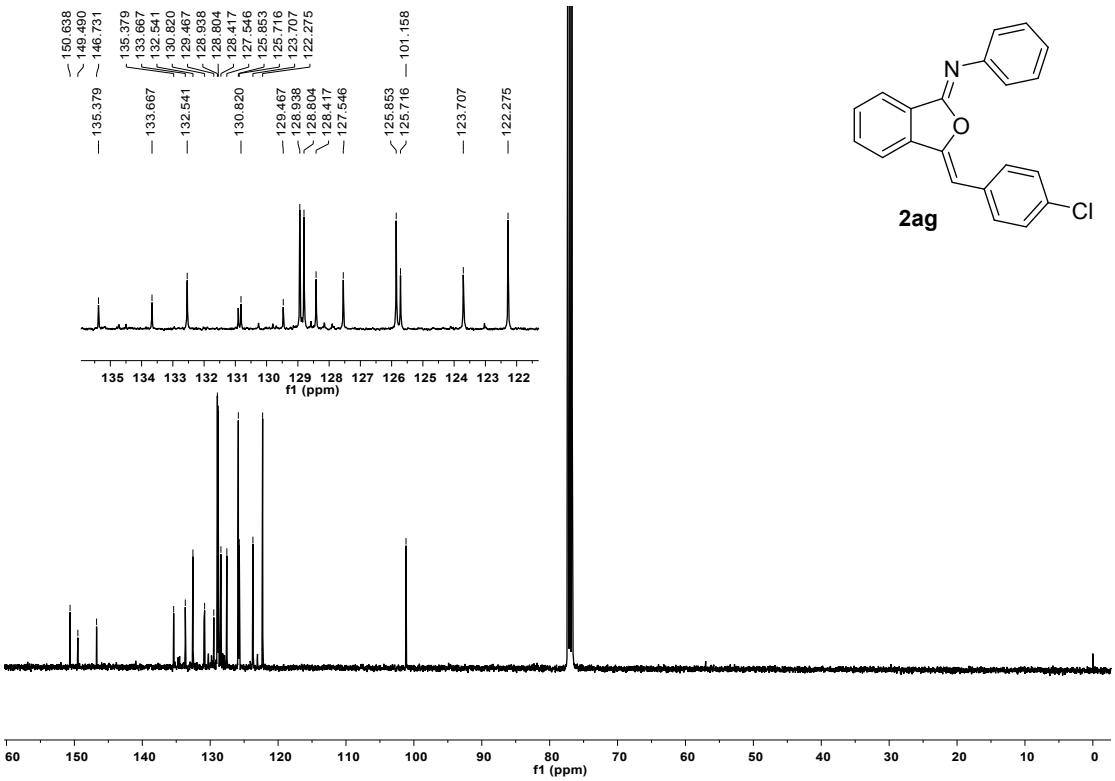
125.515
124.598
123.555
122.465
100.113
21.328
N
O
2af
f1 (ppm)


8.385
8.365
7.573
7.554
7.537
7.528
7.507
7.498
7.476
7.451
7.432
7.413
7.394
7.375
7.338
7.312
7.290
7.228
7.209
7.160
7.141
7.123
6.692
-0.000
N
O
Cl
2ag
1.12
2.14
3.11
3.09
1.96
0.99
0.94
1.09
f1 (ppm)


150.638
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135.379
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130.820
129.467
128.938
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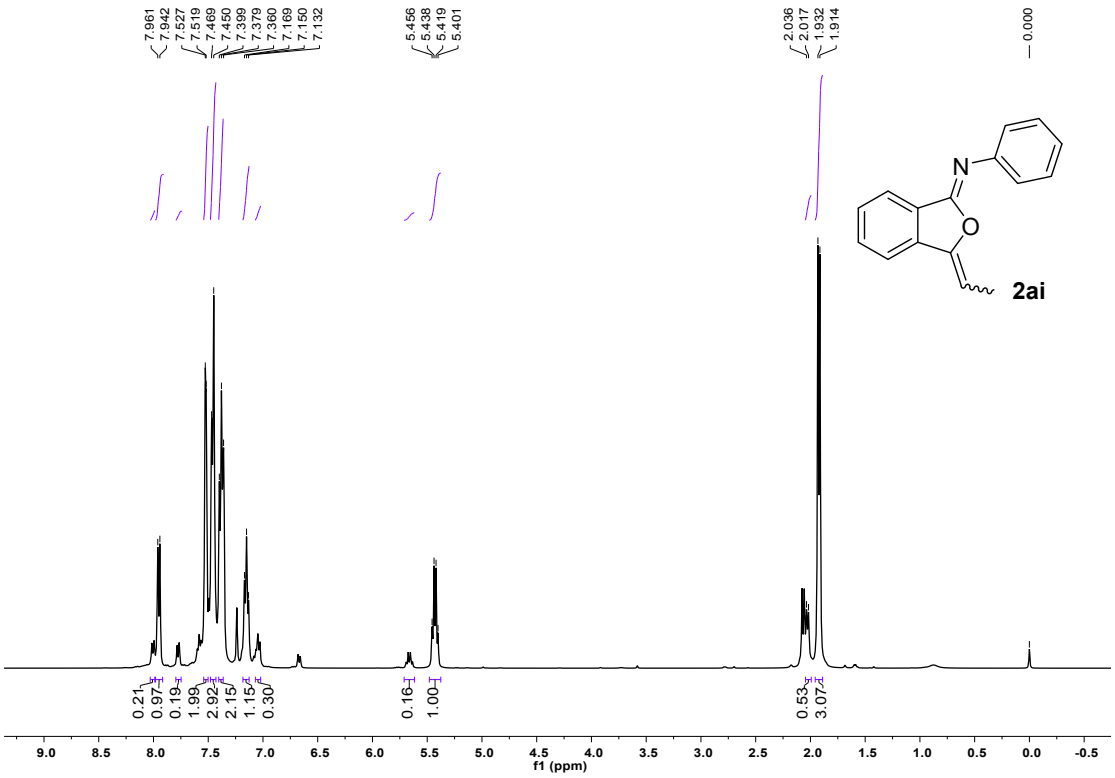
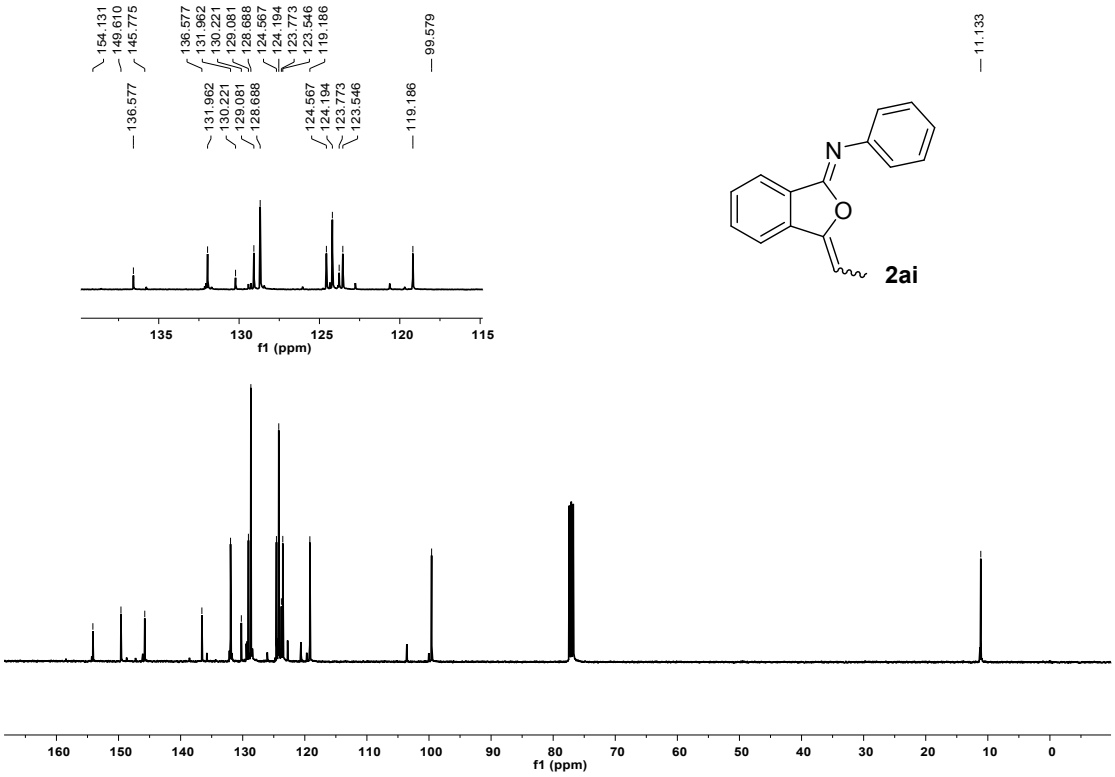
128.417
127.546
125.853
125.716
123.707
122.275
101.158
N
O
Cl
2ag
f1 (ppm)


7.961
7.942
7.527
7.519
7.469
7.450
7.399
7.379
7.360
7.169
7.150
7.132
5.456
5.438
5.419
5.401
2.036
2.017
1.932
1.914
0.000
0.21
0.97
0.19
1.99
2.92
2.15
1.15
0.30
0.16
1.00
0.53
3.07
f1 (ppm)
N
O
2ai


154.131
149.610
145.775
136.577
131.962
130.221
129.081
128.688
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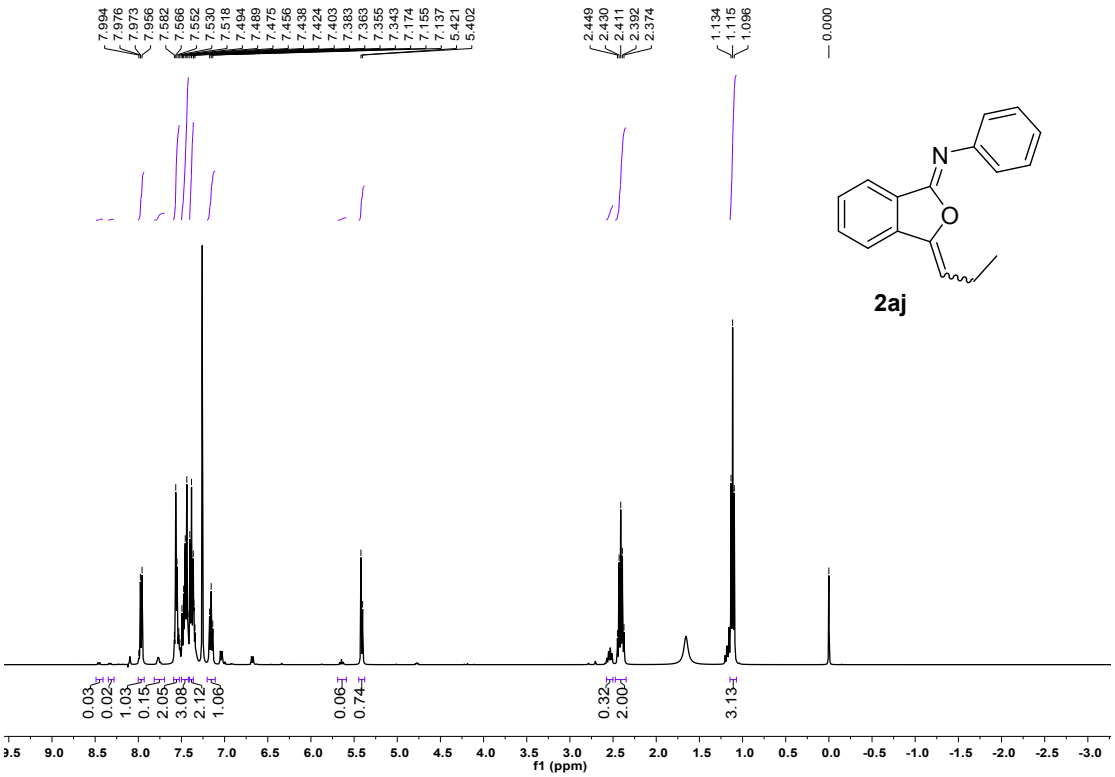
124.194
123.773
123.546
119.186
99.579
11.133
f1 (ppm)
N
O
2ai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7.973
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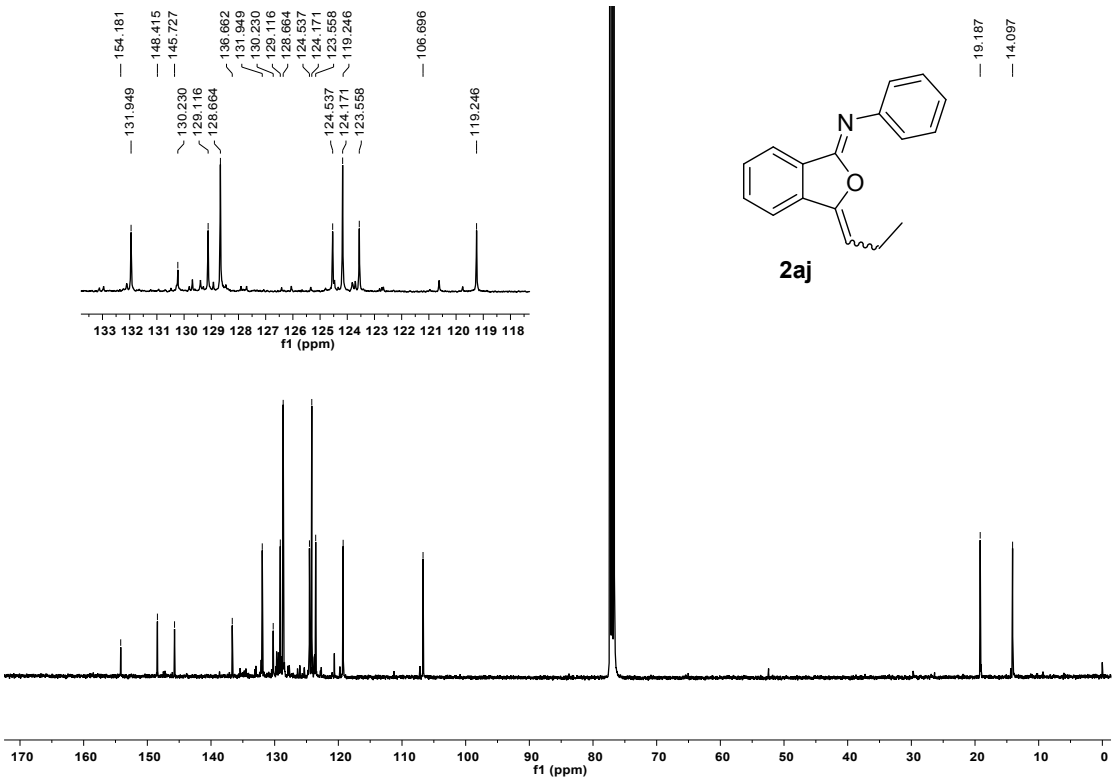
7.552
7.530
7.518
7.494
7.489
7.475
7.456
7.438
7.424
7.403
7.383
7.363
7.355
7.343
7.174
7.155
7.137
5.421
5.402
2.449
2.430
2.411
2.392
2.374
1.134
1.115
1.096
0.000
N
O
2aj
0.03
0.02
1.03
0.15
2.05
3.08
2.12
1.06
0.06
0.74
0.32
2.00
3.13
f1 (ppm)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145.727
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130.230
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128.664
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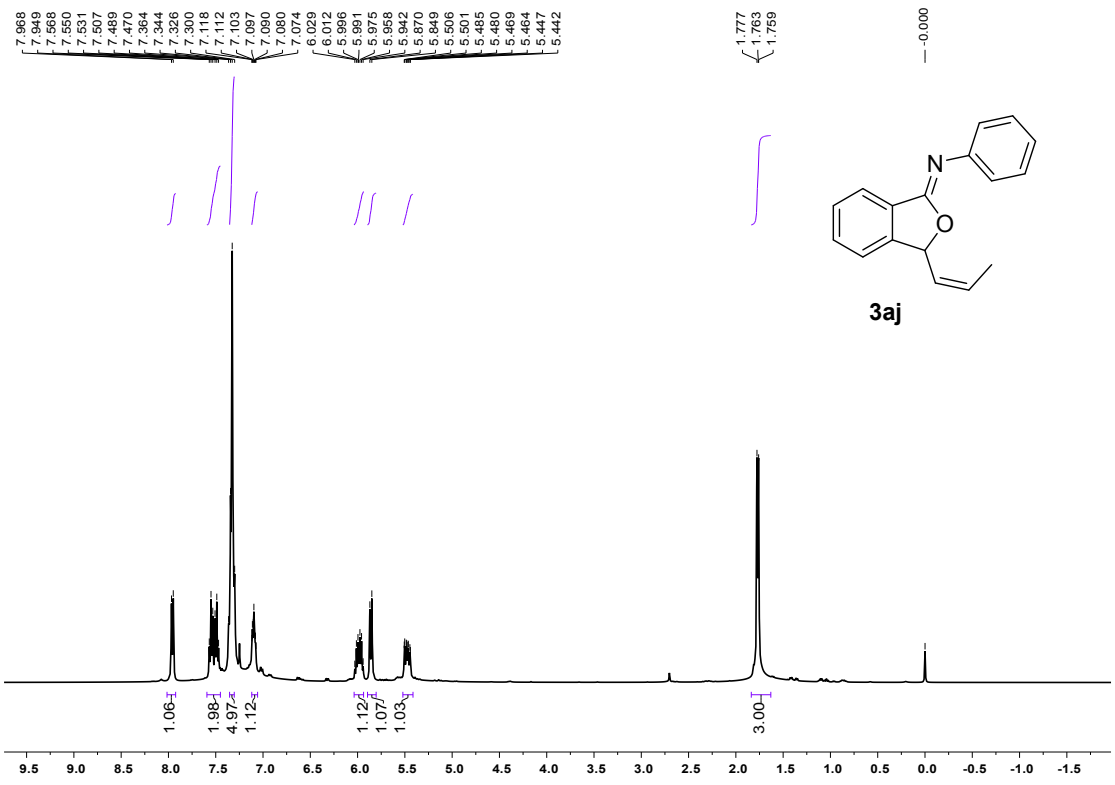
124.171
123.558
119.246
106.696
19.187
14.097
N
O
2aj
f1 (ppm)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7.531
7.507
7.489
7.470
7.364
7.344
7.326
7.300
7.118
7.112
7.103
7.097
7.090
7.080
7.074
6.029
6.012
5.996
5.991
5.975
5.958
5.942
5.870
5.849
5.506
5.501
5.485
5.480
5.469
5.464
5.447
5.442
1.777
1.763
1.759
0.000
N
O
3aj
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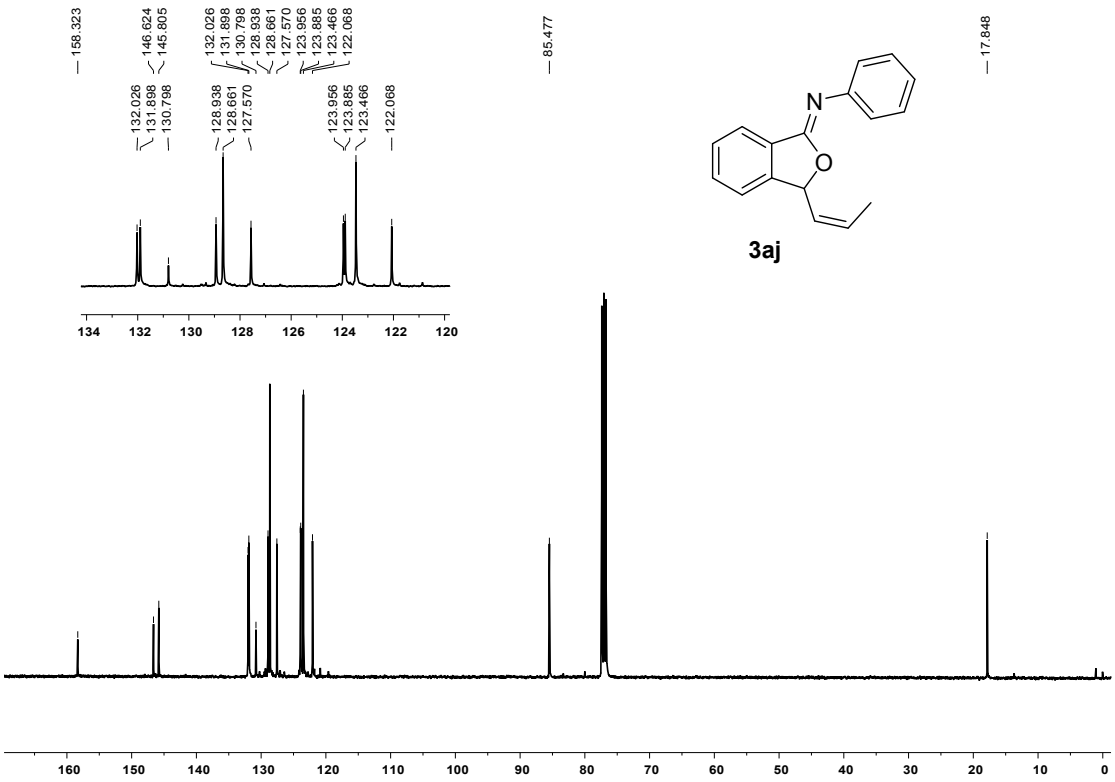
1.98
4.97
1.12
1.12
1.07
1.03
3.00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146.624
145.805
132.026
131.898
130.798
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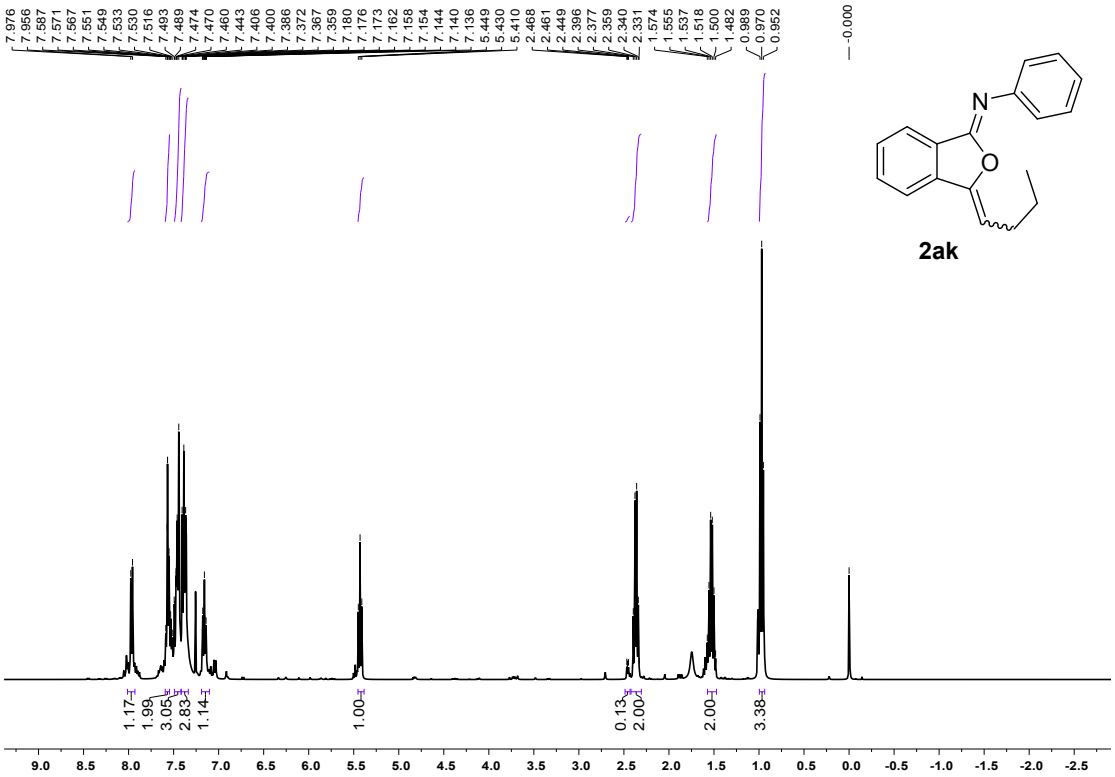
128.661
127.570
123.956
123.885
123.466
122.068
85.477
17.848
N
O
3aj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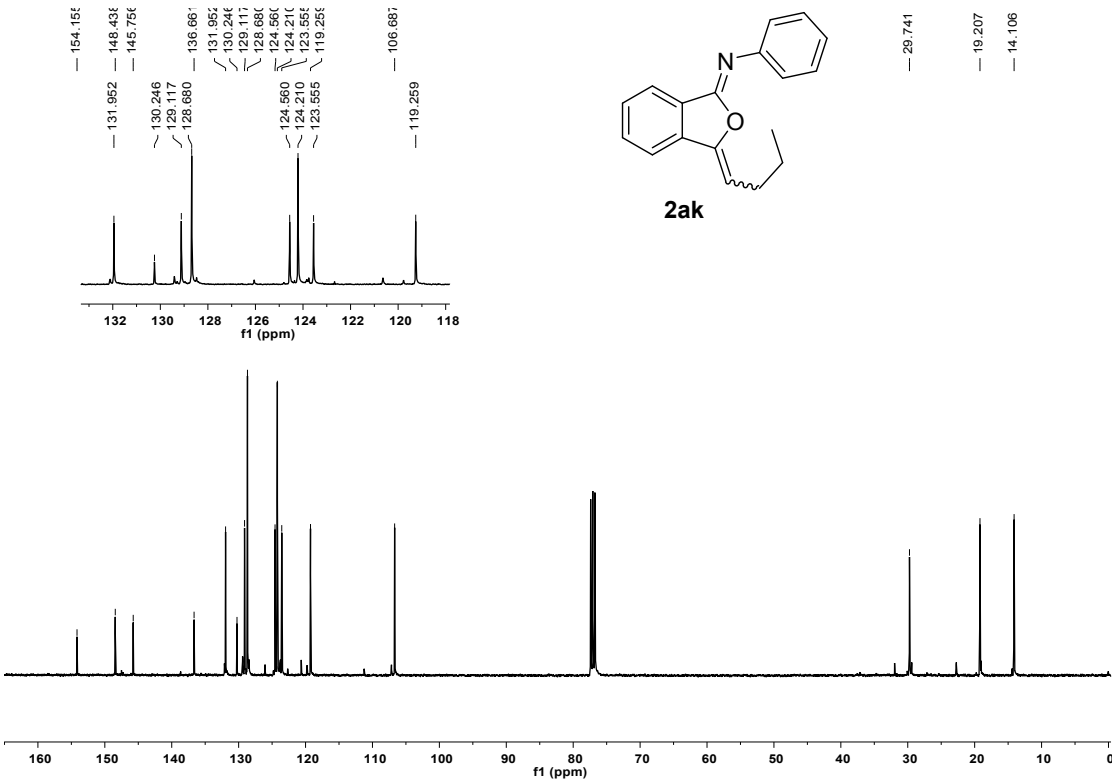
7.956
7.587
7.571
7.567
7.551
7.549
7.533
7.530
7.516
7.493
7.489
7.474
7.470
7.460
7.443
7.406
7.400
7.386
7.372
7.367
7.359
7.180
7.176
7.173
7.162
7.158
7.154
7.144
7.140
7.136
5.449
5.430
5.410
2.468
2.461
2.449
2.396
2.377
2.359
2.340
2.331
1.574
1.555
1.537
1.518
1.500
1.482
0.989
0.970
0.952
-0.000
N
O
2ak
1.17
1.99
3.05
2.83
1.14
1.00
0.13
2.00
2.00
3.38
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 -1.0 -1.5 -2.0 -2.5


154.15
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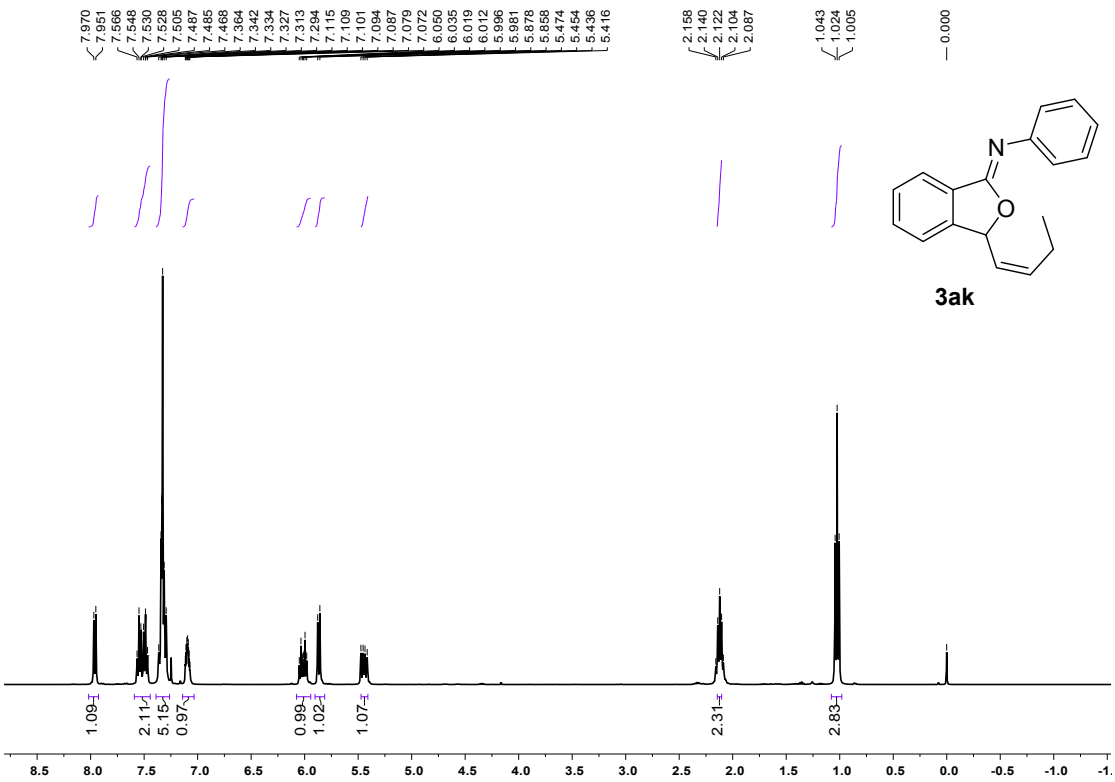
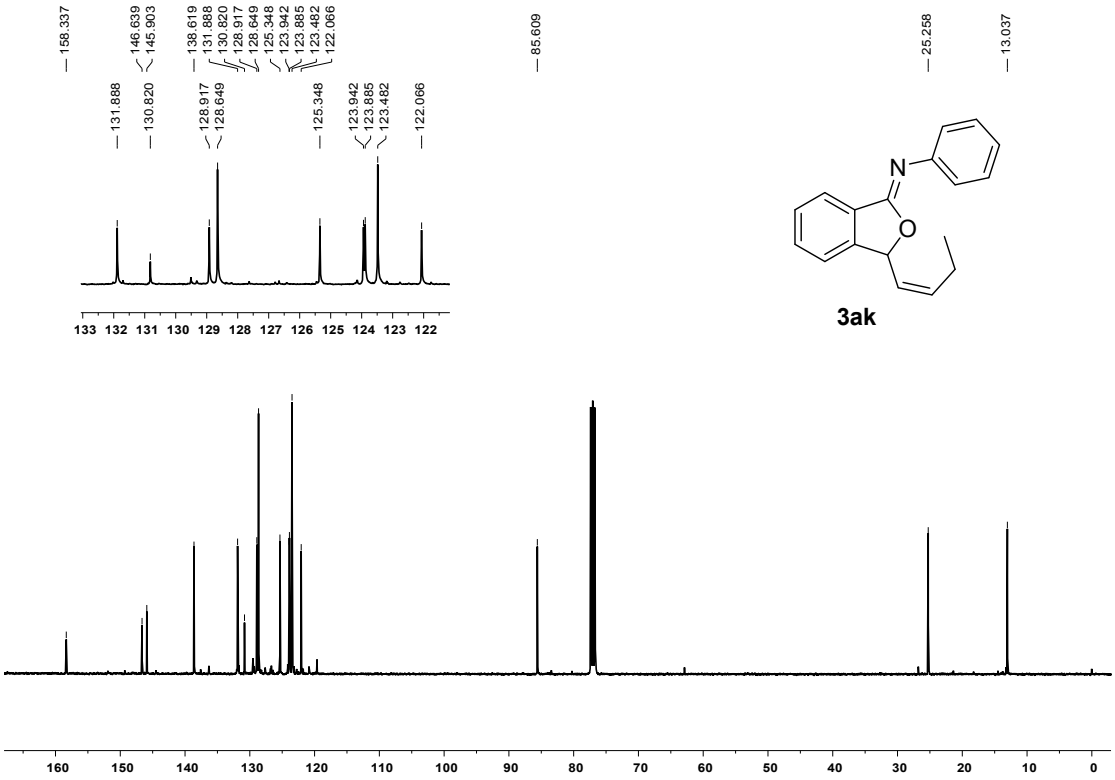
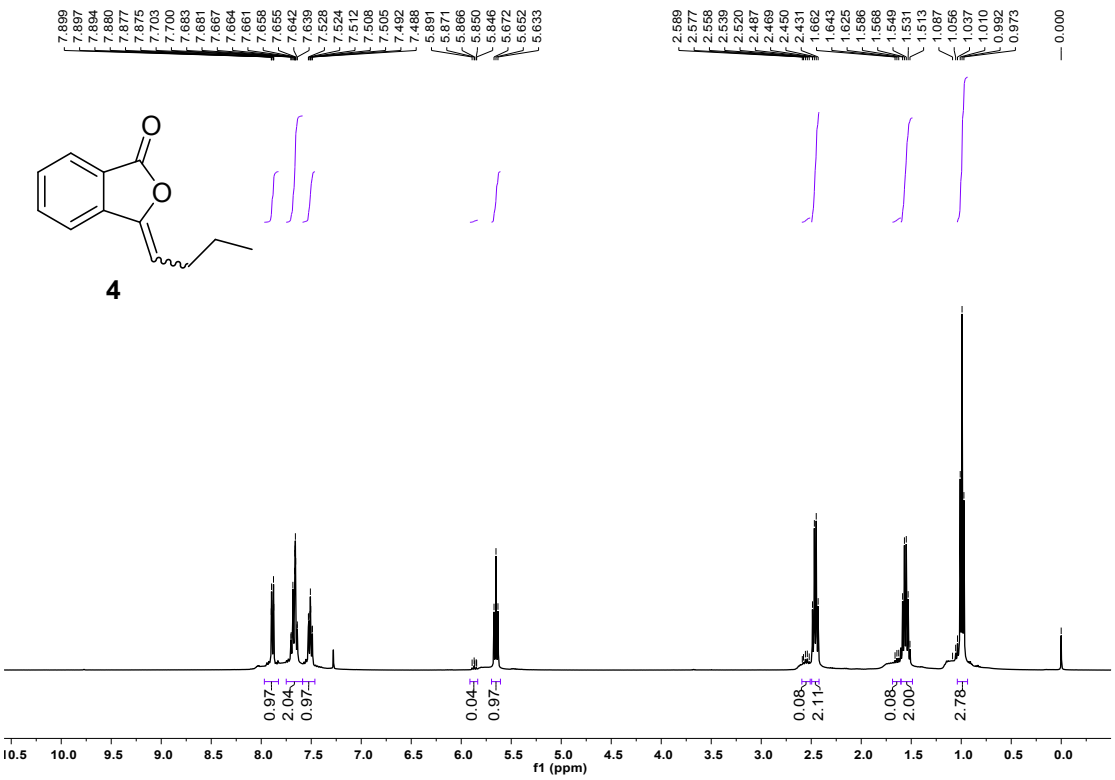
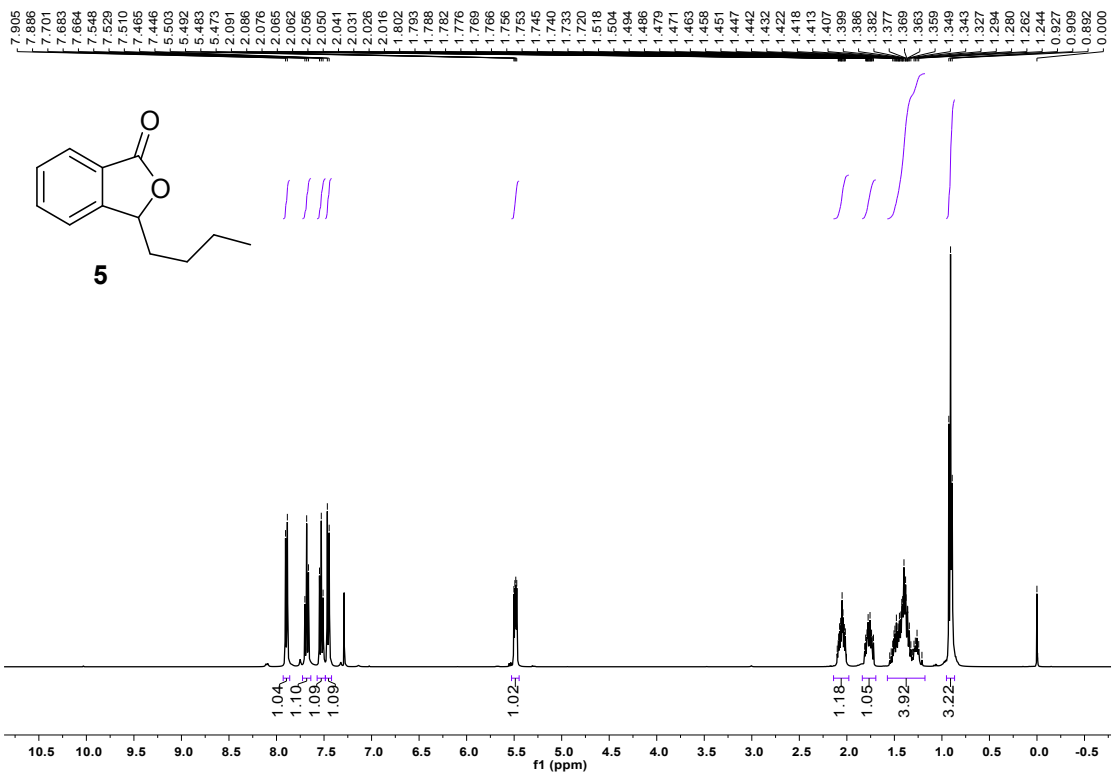
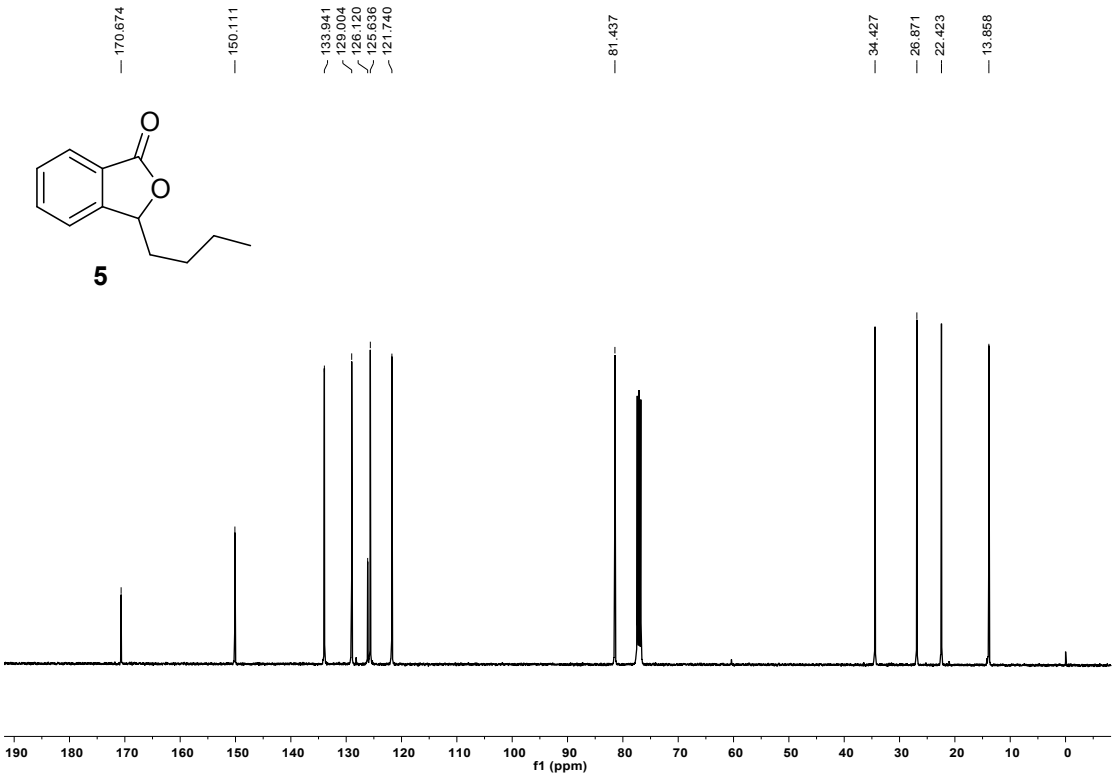
131.95
130.24
129.11
128.68
124.56
124.21
123.55
119.25
106.68
131.952
130.246
129.117
128.680
124.560
124.210
123.555
119.259
132 130 128 126 124 122 120 118
f1 (ppm)
N
O
2ak
29.741
19.207
14.106
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

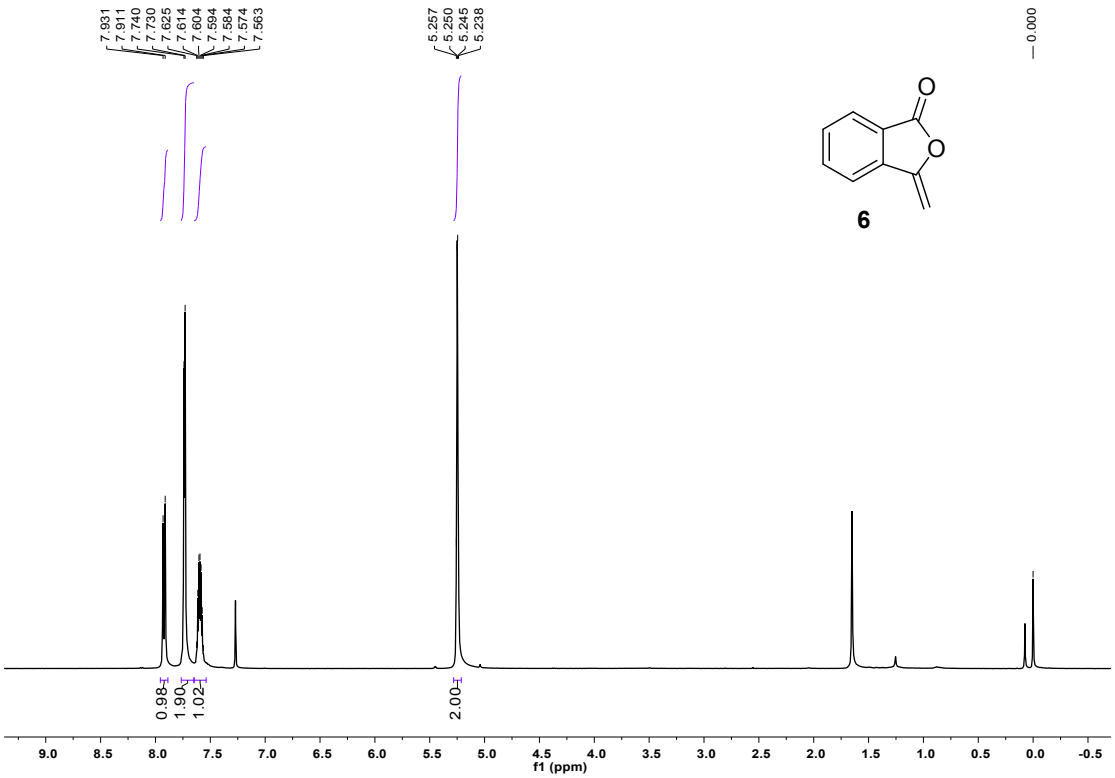

7.970
7.951
7.566
7.548
7.530
7.528
7.505
7.487
7.485
7.468
7.364
7.342
7.334
7.327
7.313
7.294
7.115
7.109
7.101
7.094
7.087
7.079
7.072
6.050
6.035
6.019
6.012
5.996
5.981
5.878
5.858
5.474
5.454
5.436
5.416
2.158
2.140
2.122
2.104
2.087
1.043
1.024
1.005
0.000
N
O
3ak
1.09
2.11
5.15
0.97
0.99
1.02
1.07
2.31
2.83
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 -1.0

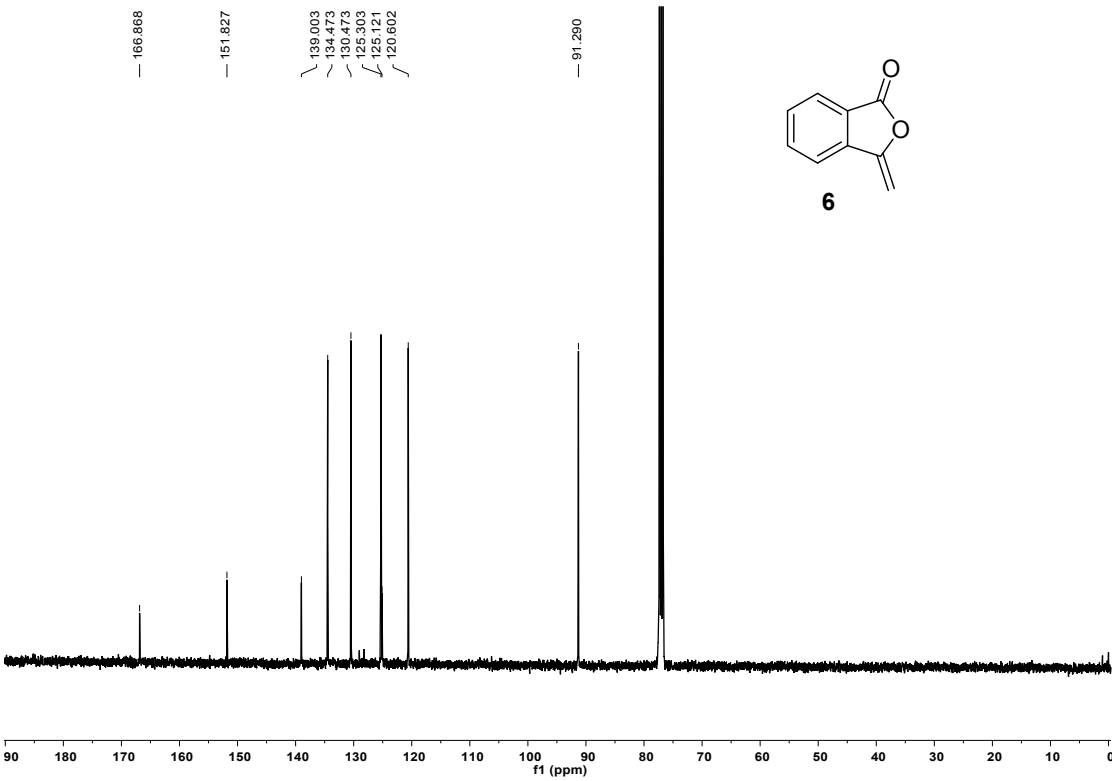

158.337
146.639
145.903
138.619
131.888
130.820
128.917
128.649
125.348
123.942
123.885
123.482
122.066
85.609
25.258
13.037
131.888
130.820
128.917
128.649
125.348
123.942
123.885
123.482
122.066
N
O
3ak
133 132 131 130 129 128 127 126 125 124 123 122
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

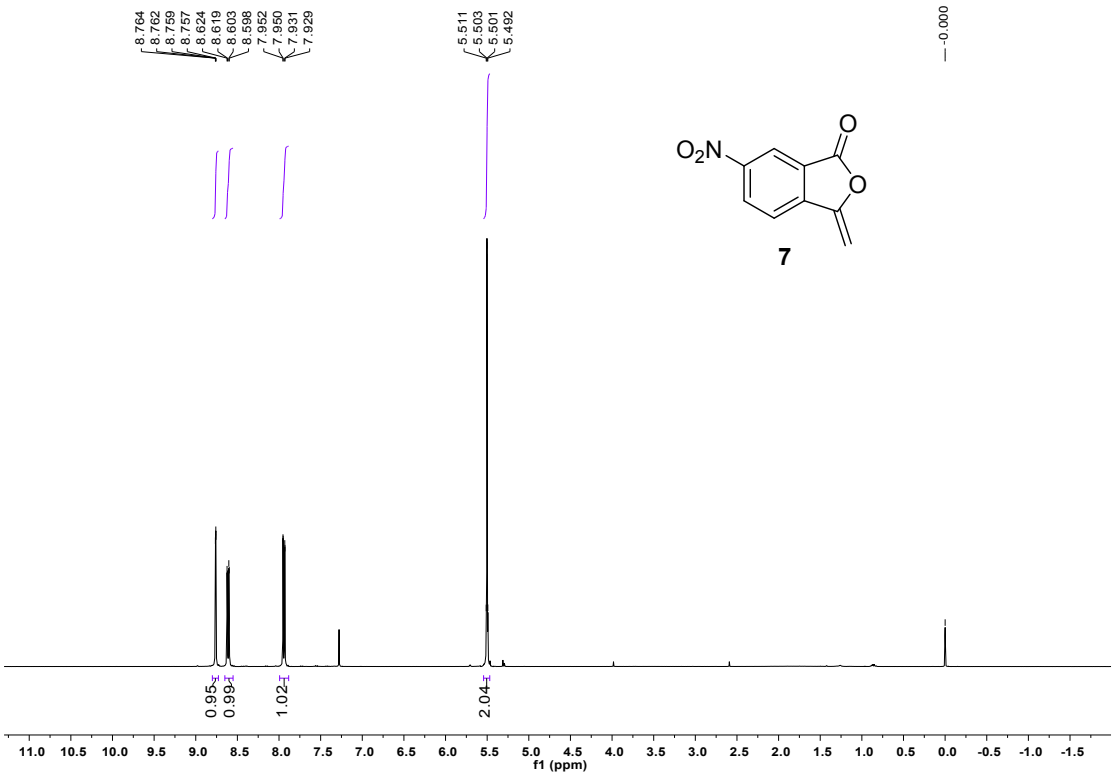

4
f1 (ppm)

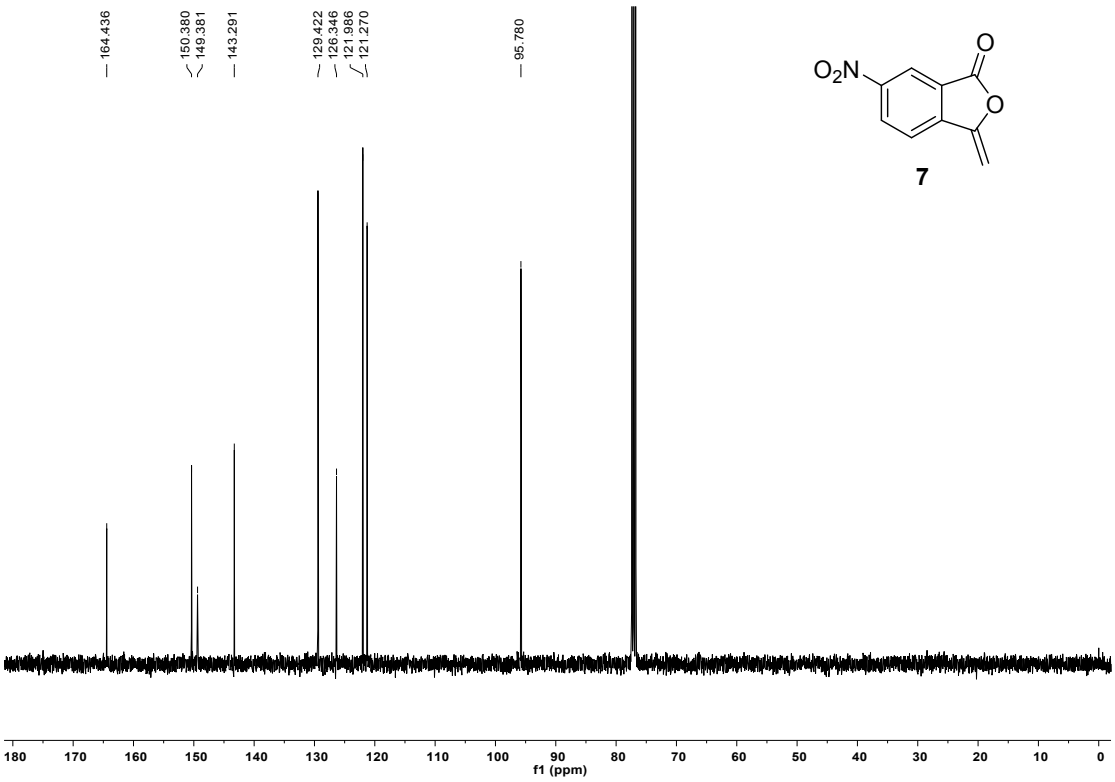

5
f1 (ppm)


170.674
150.111
133.941
129.004
126.120
125.636
121.740
81.437
34.427
26.871
22.423
13.858
O
O
5
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.931
7.911
7.740
7.730
7.625
7.614
7.604
7.594
7.584
7.574
7.563
5.257
5.250
5.245
5.238
0.000
O
O
6
0.98
1.90
1.02
2.00
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
f1 (ppm)


166.868
151.827
139.003
134.473
130.473
125.303
125.121
120.602
91.290
O
O
6
f1 (ppm)


8.764
8.762
8.759
8.757
8.624
8.619
8.603
8.598
7.952
7.950
7.931
7.929
5.511
5.503
5.501
5.492
-0.000
O2N
O
O
7
0.95
0.99
1.02
2.04
f1 (ppm)


164.436
150.380
149.381
143.291
129.422
126.346
121.986
121.270
95.780
O2N
O
O
7
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)