A facile synthesis of CF3-containing iminoisobenzofurans via copper-catalyzed oxygen trifluoromethylation– cyclization of o-Vinyl-N-alkylamide

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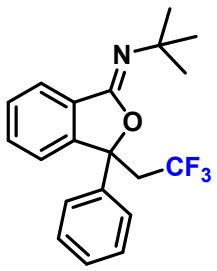
^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded on a Bruker AVANCE 400 MHz spectrometer, with $CDCl_3$ as a solvent and tetramethylsilane as an internal standard. All reactions were carried out under an air atmosphere. Thin-layer chromatography (TLC) was conducted on silica gel 60 F254 plates (Yinlong) and column chromatography was performed over silica gel (mesh 300-400). Highresolution mass spectra were obtained on a Q-TOF6510 spectrograph (Agilent). Single-distilled water was used throughout all experiments; other reagents were commercially available and were used without further purification.



3a

(E)-N-(tert-butyl)-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

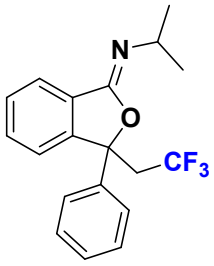
3a was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (91% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 - 7.76 (m, 1H), 7.54 - 7.44 (m, 3H), 7.43 - 7.34 (m, 4H), 7.34 - 7.28 (m, 1H), 3.33 - 3.21 (m, 1H), 3.15 - 3.01 (m, 1H), 1.48 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) 153.5, 146.2, 141.2, 131.2, 131.1, 129.1, 128.8, 128.2, 124.5, 124.4 (q, *J*= 274.7Hz,1C), 124.1, 123.0, 121.8, 53.9, 43.5 (q, *J* = 22.22Hz, 1C), 30.2.

^{19}F NMR (376 MHz, $CDCl_3$) δ - 60.1.

HRMS (ESI) m/z calcd for $C_{20}H_{20}F_3NO$ $[M+H]^+$: 348.1570, found:348.1569.



3ba

(Z)-N-isopropyl-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

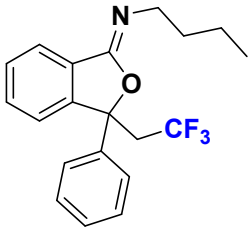
3ba was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (82% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dt, *J* = 7.6, 1.1 Hz, 1H), 7.50 - 7.29 (m, 8H), 4.34 - 4.25 (m, 1H), 3.31 - 3.17 (m, 1H), 3.11 - 3.00 (m, 1H), 1.29 (ddd, *J* = 10.9, 6.4, 1.0 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.8, 147.0, 141.2, 131.5, 129.9, 129.3, 129.0, 128.4, 124.7 (q, *J* = 279.8 Hz, 1C), 124.5, 123.9, 122.1, 86.1, 47.8, 43.5 (q, *J* = 27.3Hz, 1C), 24.2, 23.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ - 60.2.

HRMS (ESI) m/z calcd for $C_{19}H_{18}F_3NO$ $[M+H]^+$: 334.1413, found: 334.1408.



3ca

(Z)-N-butyl-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

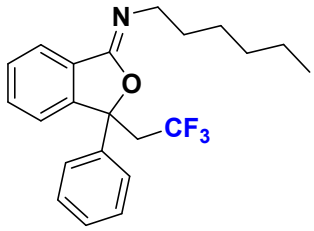
3ca was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (85% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.5 Hz, 1H), 7.57 - 7.33 (m, 7H), 7.29 (t, *J* = 7.2 Hz, 1H), 3.76 - 3.55 (m, 2H), 3.16 (ddq, *J* = 76.6, 15.6, 10.0 Hz, 2H), 1.81 - 1.65 (m, 2H), 1.53 - 1.39 (m, 2H), 0.98 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.9, 147.1, 141.1, 131.4, 129.8, 129.2, 128.9, 128.3, 124.7 (q, *J* = 279.8 Hz, 1C), 124.4, 123.6, 122.0, 120.5, 86.1, 86.0, 47.4, 43.5 (q, *J* = 27.3 Hz, 1C), 33.0, 20.8, 14.0.

^{19}F NMR (377 MHz, $CDCl_3$) δ - 60.3.

HRMS (ESI) m/z calcd for $C_{20}H_{20}F_3NO$ $[M+H]^+$: 348.1570, found:348.1567.



3da

(Z)-N-hexyl-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine.

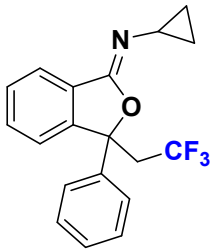
3da was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (80% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (dt, *J* = 7.4, 1.1 Hz, 1H), 7.52 - 7.33 (m, 7H), 7.33 - 7.27 (m, 1H), 3.65 (td, *J* = 7.2, 3.7 Hz, 2H), 3.36 - 3.18 (m, 1H), 3.15 - 2.97 (m, 1H), 1.73 (p, *J* = 7.3 Hz, 2H), 1.54 - 1.28 (m, 6H), 0.96 - 0.83 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.9, 147.0, 141.1, 131.4, 129.8, 129.2, 128.9, 128.3, 124.7 (q, J = 279.8Hz,1C), 124.4, 123.6, 122.0, 86.1, 86.0, 86.0, 47.8, 43.5 (q, J = 27.3 Hz, 1C), 31.8, 30.9, 27.4, 22.7, 14.1.

^{19}F NMR (377 MHz, $CDCl_3$) δ - 60.3.

HRMS (ESI) m/z calcd for $C_{22}H_{24}F_3NO$ $[M+H]^+$: 376.1883, found:376.1881.



3ea

(Z)-N-cyclopropyl-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

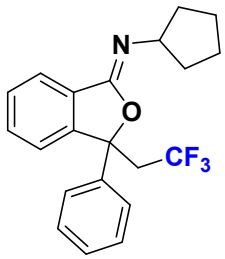
3ea was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). White solid (95% yield), mp 132-136 °C.

^{1}H NMR (400 MHz, $CDCl_3$)δ 7.74 (dq, *J* = 7.6, 1.2 Hz, 1H), 7.56 - 7.50 (m, 2H), 7.48 - 7.35 (m, 5H), 7.34 - 7.28 (m, 1H), 3.62 - 3.46 (m, 1H), 3.28 (dq, *J* = 15.5, 10.0 Hz, 1H), 3.08 (dq, *J* = 15.5, 9.8 Hz, 1H), 0.93 - 0.75 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.0, 146.8, 141.1, 131.3, 129.8, 129.3, 128.9, 128.4, 124.5, 123.4, 122.1, 86.3, 43.6 (q, J=27.3Hz), 29.9, 8.1, 8.0.

^{19}F NMR (376 MHz, $CDCl_3$) δ - 60.13.

HRMS (ESI) m/z calcd for $C_{19}H_{16}F_3NO$ $[M+H]^+$: 332.1257, found:332.1252.



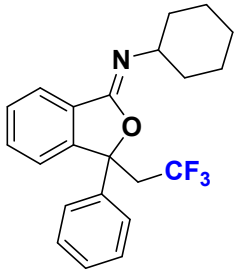
3fa

(Z)-N-cyclopentyl-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

3fa was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (73% yield).

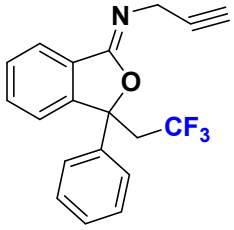
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 - 7.79 (m, 1H), 7.52 - 7.34 (m, 7H), 7.33 - 7.26 (m, 1H), 4.40 (t, *J* = 7.1 Hz, 1H), 3.33 - 3.15 (m, 1H), 3.15 - 2.97 (m, 1H), 2.08 (dt, *J* = 7.7, 4.2 Hz, 2H), 1.83 (ddt, *J* = 8.7, 5.3, 2.7 Hz, 2H), 1.72 - 1.58 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.3, 147.0, 141.2, 131.33, 129.9, 129.1, 129.1, 129.1, 128.9, 128.3, 124.7 (q, *J* = 280.8Hz,1C), 124.4, 123.8, 121.9, 120.5, 86.0, 86.0, 58.0, 43.5(q, *J*=27.3Hz,1C), 34.5, 34.2, 24.6, 24.5.
^{19}F NMR (377 MHz, $CDCl_3$) δ - 60.3.
HRMS (ESI) m/z calcd for $C_{21}H_{20}F_3NO$ $[M+H]^+$: 360.1570, found:360.1567.



3ga

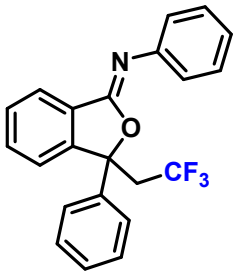
(Z)-N-cyclohexyl-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine
3ga was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (70% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.5 Hz, 1H), 7.49 - 7.37 (m, 7H), 7.32 - 7.29 (m, 1H), 3.92 (tt, *J* = 10.4, 4.1 Hz, 1H), 3.30 - 3.21 (m, 1H), 3.14 - 3.03 (m, 1H), 1.97 - 1.88 (m, 2H), 1.85 - 1.76 (m, 2H), 1.71 - 1.64 (m, 1H), 1.52 - 1.36 (m, 4H), 1.25 (q, *J* = 4.8 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 155.7, 147.0, 141.3, 134.5, 131.4, 130.0, 129.2, 129.2, 129.0, 128.4, 124.8 (q, *J* = 279.8Hz,1C), 124.7, 124.5, 123.9, 122.0, 86.0, 56.0, 43.4 (q, *J* = 27.3Hz), 34.3, 33.8, 26.0, 25.3, 25.3.
^{19}F NMR (376 MHz, $CDCl_3$) δ - 60.2.
HRMS (ESI) m/z calcd for $C_{22}H_{22}F_3NO$ $[M+H]^+$: 374.1726, found:374.1726.



3ha

(Z)-3-phenyl-N-(prop-2-yn-1-yl)-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine
3ha was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). White solid (64% yield), mp 129-133 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dt, *J* = 7.5, 1.1 Hz, 1H), 7.56 - 7.29 (m, 8H), 4.50 - 4.35 (m, 2H), 3.29 (dq, *J* = 15.6, 10.0 Hz, 1H), 3.10 (dq, *J* = 15.6, 9.8 Hz, 1H), 2.29 (d, *J* = 5.2 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 159.6, 147.3, 140.4, 132.1, 129.5, 129.2, 129.0, 128.8, 128.6, 124.6 (q, *J* = 280.8 Hz, 1C), 124.5, 124.1, 122.1, 87.3, 82.2, 70.3, 43.5 (q, *J* = 28.3 Hz, 1C), 36.9.
^{19}F NMR(376 MHz, $CDCl_3$) δ - 60.2.

HRMS (ESI) m/z calcd for $C_{19}H_{14}F_3NO[M+H]^+$: 330.1100, found:330.1098.



3ia

(Z)-N,3-diphenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

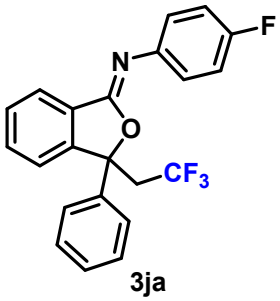
3ia was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (86% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 - 7.93 (m, 1H), 7.61 - 7.48 (m, 3H), 7.48 - 7.27 (m, 9H), 7.16 (dd, *J* = 6.8, 1.8 Hz, 1H), 3.21 (ddq, *J* = 54.3, 15.6, 9.9 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.2, 146.9, 146.3, 140.5, 132.2, 130.3, 129.6, 129.0, 129.0, 128.8, 124.7 (q, *J* = 279.8 Hz, 1C), 124.5, 123.7, 123.6, 122.3, 87.6, 43.4 (q, *J* = 28.3 Hz, 1C).

^{19}F NMR (376 MHz, $CDCl_3$) δ - 60.3.

HRMS (ESI) m/z calcd for $C_{22}H_{16}F_3NO$ $[M+H]^+$: 368.1257, found: 368.1254.



3ja

(Z)-N-(4-fluorophenyl)-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

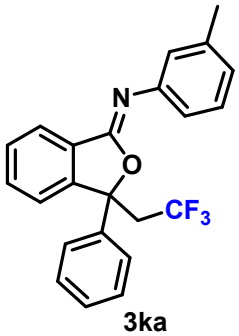
3ja was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). White solid (71% yield), mp 114-118 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 - 7.93 (m, 1H), 7.59 - 7.27 (m, 10H), 7.10 - 6.99 (m, 2H), 3.30 (dq, *J* = 15.7, 9.9 Hz, 1H), 3.14 (dq, *J* = 15.6, 9.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.5 (d, *J* = 242.4 Hz, 1C), 156.3, 146.8, 142.1, 140.3, 132.3, 130.2, 129.7, 129.1, 128.7, 125.4 (d, J = 9.1 Hz, 1C), 124.6 (q, *J* = 279.8 Hz, 1C), 124.5, 124.4, 122.3, 115.5 (d, *J* = 22.2Hz, 1C), 87.8, 43.4 (q, *J* = 27.8 Hz,1C).

^{19}F NMR(376 MHz, $CDCl_3$) δ - 60.3, - 118.6.

HRMS (ESI) m/z calcd for $C_{22}H_{15}F_4NO$ $[M+H]^+$: 386.1163, found: 386.1162.



3ka

(Z)-3-phenyl-N-(m-tolyl)-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

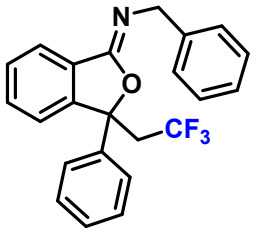
3ka was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). White solid (78% yield), mp 121-125 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 - 7.95 (m, 1H), 7.59 - 7.44 (m, 5H), 7.38 - 7.27 (m, 4H), 7.25 - 7.21 (m, 2H), 6.98 (dtd, *J* = 7.1, 1.6, 0.8 Hz, 1H), 3.29 (dq, *J* = 15.6, 10.0 Hz, 1H), 3.20 - 3.10 (m, 1H), 2.39 (d, *J* = 0.7 Hz, 3H).

^{13}C NMR[1] (101 MHz, $CDCl_3$) δ 156.1, 147.0, 146.1, 140.5, 138.5, 132.2, 130.3, 129.6, 129.0, 128.6, 128.6, 125.2, 124.7 (q, *J* = 280.8 Hz, 1C) 124.6, 124.5, 122.2, 120.5, 87.6, 43.4(q, *J* = 28.3 Hz, 1C), 21.6.

^{19}F NMR(376 MHz, $CDCl_3$) δ - 60.2.

HRMS (ESI) m/z calcd for $C_{23}H_{18}F_3NO$ $[M+H]^+$: 382.1413, found: 382.1416.



3la

(Z)-N-benzyl-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

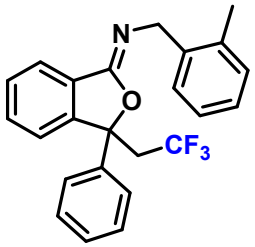
3la was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (89% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 - 7.85 (m, 1H), 7.52 - 7.26 (m, 13H), 4.88 (d, *J* = 3.1 Hz, 2H), 3.29 (dq, *J* = 15.6, 10.0 Hz, 1H), 3.11 (qd, *J* = 9.9, 5.4 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 147.3, 140.8, 140.7, 131.8, 129.7, 129.4, 129.0, 128.5, 128.1, 126.7, 124.7 (q, *J* = 279.8 Hz, 1C) 124.5, 124.0, 122.1, 86.7, 51.5, 43.6 (q, *J* = 27.7 Hz, 1C).

^{19}F NMR (376 MHz, $CDCl_3$) δ - 60.1.

HRMS (ESI) m/z calcd for $C_{23}H_{18}F_3NO$ $[M+H]^+$: 382.1413, found: 382.1415



3ma

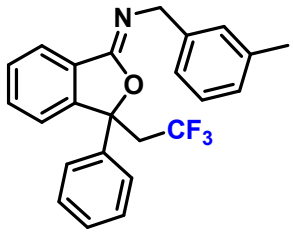
(E)-N-(2-methylbenzyl)-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine **3ma** was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (82% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (dt, *J* = 7.6, 1.1 Hz, 1H), 7.56 - 7.43 (m, 6H), 7.39 - 7.32 (m, 3H), 7.24 - 7.18 (m, 3H), 4.86 (s, 2H), 3.37 - 3.26 (m, 1H), 3.18 - 3.08 (m, 1H), 2.44 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.7, 147.3, 140.9, 138.8, 136.4, 134.5, 131.7, 130.1, 129.4, 129.2, 129.0, 128.5, 128.4, 126.8, 126.3, 126.0, 124.7 (q, *J* = 280.8 Hz, 1C), 124.7, 124.5, 124.0, 122.1, 86.6, 49.5, 43.6(q, *J* = 27.3 Hz,1C), 19.4.

^{19}F NMR (376 MHz, $CDCl_3$) δ -60.1.

HRMS (ESI) m/z calcd for $C_{24}H_{20}F_3NO$ $[M+H]^+$: 396.1570, found: 396.1569.



3na

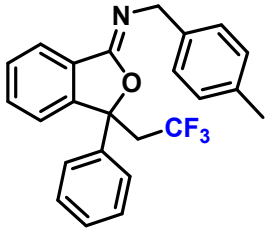
(E)-N-(3-methylbenzyl)-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine **3na** was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (80% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (dt, *J* = 7.5, 1.0 Hz, 1H), 7.55 - 7.44 (m, 6H), 7.39 - 7.30 (m, 5H), 7.11 - 7.06 (m, 1H), 4.86 (s, 2H), 3.35 - 3.27 (m, 1H), 3.15 - 3.07 (m, 1H), 2.36 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 147.2, 140.9, 140.5, 138.1, 134.5, 131.8, 130.0, 129.4, 129.2, 129.0, 128.5, 128.4, 127.4, 125.2, 124.7 (q, *J* = 279.8Hz, 1C), 124.7, 124.5, 124.0, 122.1, 86.6, 51.6, 43.6 (q, *J* = 27.27 Hz, 1C) 21.6.

^{19}F NMR NMR (376 MHz, $CDCl_3$) δ - 60.1.

HRMS (ESI) m/z calcd for $C_{24}H_{20}F_3NO$ $[M+H]^+$: 396.1570, found: 396.1566.



3oa

(Z)-N-(4-methylbenzyl)-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

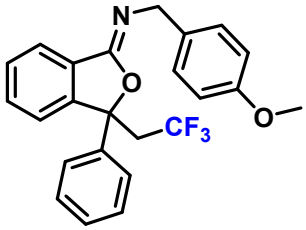
3oa was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (85% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dt, *J* = 7.4, 1.0 Hz, 1H), 7.56 - 7.44 (m, 5H), 7.41 - 7.32 (m, 5H), 7.18 (d, *J* = 7.7 Hz, 2H), 4.85 (d, *J* = 3.6 Hz, 2H), 3.35 - 3.26 (m, 1H), 3.19 - 3.06 (m, 1H), 2.36 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.7, 147.2, 140.9, 137.7, 136.2, 134.5, 131.7, 129.8, 129.4, 129.2, 129.0, 128.9, 128.5, 128.1, 126.3, 124.7 (q, *J* = 279.8 Hz, 1C), 124.7, 124.5, 124.0, 122.1, 86.6, 51.3, 43.6 (q, *J* = 28.3 Hz,1C), 21.2.

^{19}F NMR (376 MHz, $CDCl_3$) δ - 60.1.

HRMS (ESI) m/z calcd for $C_{24}H_{20}F_3NO$ $[M+H]^+$: 396.1570, found: 396.1574.



3pa

(Z)-N-(4-methoxybenzyl)-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

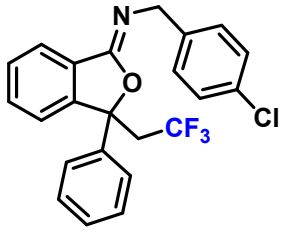
3pa was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (77% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 - 7.83 (m, 1H), 7.53 - 7.30 (m, 10H), 6.91 (dq, *J* = 8.6, 2.4 Hz, 2H), 4.99 - 4.67 (m, 2H), 3.82 (s, 3H), 3.30 (dtd, *J* = 15.9, 10.9, 9.4 Hz, 1H), 3.10 (dq, *J* = 15.5, 9.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.5, 157.7, 147.2, 140.9, 132.9, 131.7, 129.8, 129.4, 129.3, 128.9, 128.5, 124.7 (q, *J* = 279.8Hz, 1C), 124.5, 124.0, 122.1, 113.9, 86.6, 55.4, 51.0,43.6 (q, *J* = 27.3 Hz,1C).

^{19}F NMR(376 MHz, $CDCl_3$) δ - 60.1.

HRMS (ESI) m/z calcd for $C_{24}H_{20}F_3NO_2$ $[M+H]^+$: 12.1519, found: 412.1520.



3qa

(Z)-N-(4-chlorobenzyl)-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

3qa was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). White solid (79% yield), mp 136-140 °C.

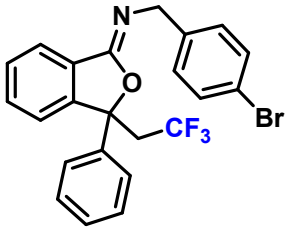
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (dt, *J* = 7.6, 1.1 Hz, 1H), 7.52 - 7.30 (m, 12H), 4.90 - 4.73 (m, 2H), 3.29 (dq, *J* = 15.6, 9.9 Hz, 1H), 3.17 - 3.05 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.2, 147.2, 140.7, 139.2, 132.3, 131.9, 129.6, 129.5, 129.4, 129.0, 128.6, 128.5, 124.7 (q, *J* = 279.8 Hz, 1C), 124.5, 124.0, 122.2, 86.8,

50.8, 43.6 (q, J = 27.3Hz, 1C).

^{19}F NMR(376 MHz, $CDCl_3$) δ - 60.2.

HRMS (ESI) m/z calcd for $C_{23}H_{17}ClF_3NO$ $[M+H]^+$: 416.1024, found: 416.1020.



3ra

(E)-N-(4-bromobenzyl)-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

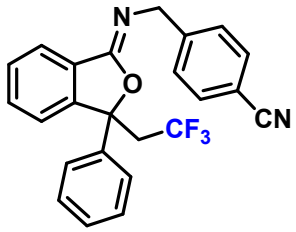
3ra was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). White solid (75% yield), mp 142-145 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (dt, J = 7.6, 1.0 Hz, 1H), 7.55 - 7.45 (m, 6H), 7.42 - 7.35 (m, 6H), 4.87 - 4.76 (m, 2H), 3.35 - 3.26 (m, 1H), 3.18 - 3.08 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3, 147.2, 140.7, 139.8, 134.5, 131.9, 131.5, 130.0, 129.8, 129.5, 129.2, 129.0, 126.3, 124.7, 124.7 (q, J = 279.8 Hz, 1C), 124.5, 123.9, 122.9, 122.2, 120.4, 86.8, 50.8, 43.5 (q,J = 27.3Hz,1C).

^{19}F NMR (376 MHz, $CDCl_3$) δ - 60.2.

HRMS (ESI) m/z calcd for $C_{23}H_{17}BrF_3NO$ $[M+H]^+$: 460.0518, found: 460.0517.



3sa

(E)-4-(((3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H) ylidene)amino)methyl)benzonitrile

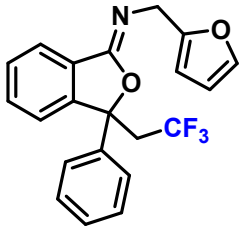
3sa was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). White solid (78% yield), mp 133-137 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (dt, J = 7.5, 1.1 Hz, 1H), 7.66 - 7.33 (m, 12H), 4.96 - 4.85 (m, 2H), 3.35 - 3.25 (m, 1H), 3.12 (dq, J = 15.6, 9.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.7, 147.2, 146.4, 140.5, 132.3, 132.1, 129.6, 129.4, 129.0, 128.7, 128.6, 124. 7(q, J = 279.8Hz,1C), 124.4, 123.9, 123.3, 122.3, 119.4, 110.3, 87.1, 87.1, 51.0, 43.5(q, J = 28.3Hz,1C).

^{19}F NMR (376 MHz, $CDCl_3$) δ - 60.2.

HRMS (ESI) m/z calcd for $C_{24}H_{17}F_3N_2O$ $[M+H]^+$: 407.1366, found: 407.1366.



3ta

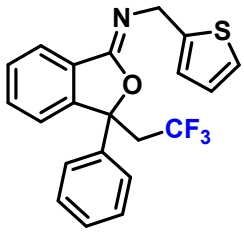
(Z)-N-(furan-2-ylmethyl)-3-phenyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine **3ta** was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Yellow oil (72% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 - 7.83 (m, 1H), 7.52 - 7.42 (m, 5H), 7.40 - 7.31 (m, 4H), 6.46 - 6.16 (m, 2H), 4.89 - 4.75 (m, 2H), 3.34 - 3.23 (m, 1H), 3.15 - 3.05 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.9, 153.9, 147.3, 141.9, 140.6, 132.0, 129.4, 129.0, 128.6, 124.7 (q, J = 280.8 Hz, 1C), 124.5, 124.2, 122.1, 110.4, 106.7, 87.0, 44.7, 43.5 (q, J = 27.3 Hz, 1C).

^{19}F NMR(376 MHz, $CDCl_3$) δ - 60.2.

HRMS (ESI) m/z calcd for $C_{21}H_{16}F_3NO_2$ $[M+H]^+$: 372.1206, found: 372.1204.



3ua

(Z)-3-phenyl-N-(thiophen-2-ylmethyl)-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

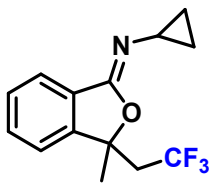
3ua was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Yellow oil (70% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (dt, J = 7.6, 1.0 Hz, 1H), 7.53 - 7.42 (m, 5H), 7.38 - 7.29 (m, 3H), 7.21 (dd, J = 5.1, 1.2 Hz, 1H), 7.06 (dq, J = 3.4, 1.1 Hz, 1H), 6.98 (dd, J = 5.1, 3.4 Hz, 1H), 5.11 - 4.96 (m, 2H), 3.35 - 3.24 (m, 1H), 3.09 (dq, J = 15.6, 9.9 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 158.3, 147.3, 144.0, 140.6, 131.9, 129.5, 129.5, 129.2, 129.0, 128.6, 126.8, 124.7,124.7 (q, J = 124.7 Hz,1C), 124.7, 124.5, 124.2, 124.1, 122.1, 87.0, 46.6, 43.6 (q, J = 27.3 Hz, 1C).

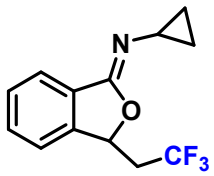
^{19}F NMR (376 MHz, $CDCl_3$) δ - 60.1.

HRMS (ESI) m/z calcd for $C_{21}H_{16}SF_3NO$ $[M+H]^+$: 388.0977, found: 388.0977.



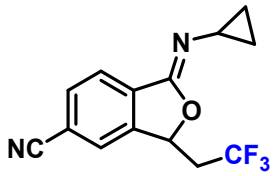
3ab

(Z)-N-cyclopropyl-3-methyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine
3ab was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (72% yield).
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.8 Hz, 1H), 7.48 (td, *J* = 7.5, 1.2 Hz, 1H), 7.42 (td, *J* = 7.5, 1.1 Hz, 1H), 7.29 (d, *J* = 7.6 Hz, 1H), 3.37 (tt, *J* = 7.2, 3.7 Hz, 1H), 2.78 (dq, *J* = 15.5, 10.4 Hz, 1H), 2.71 - 2.62 (m, 1H), 1.72 (s, 3H), 0.84 - 0.79 (m, 2H), 0.78 - 0.73 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 147.9, 131.2, 130.0, 129.1, 125.0 (q, *J* = 224.2 Hz, 1C), 123.2, 120.7, 84.0 (q, *J* = 2.0 Hz, 1C) 43.8 (q, *J* = 21.21Hz, 1C), 29.6, 26.7, 26.7, 8.0, 7.9.
^{19}F NMR (377 MHz, $CDCl_3$) δ - 60.9.
HRMS (ESI) m/z calcd for $C_{14}H_{14}F_3NO$ $[M+H]^+$: 270.1100, found: 270.1100.



3ac

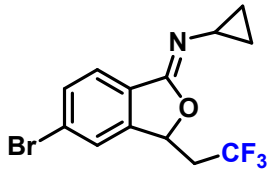
(Z)-N-cyclopropyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine
3ac was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (68% yield).
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.8 Hz, 1H), 7.50 (td, *J* = 7.5, 1.2 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.37 - 7.31 (m, 1H), 5.74 (dd, *J* = 8.8, 3.3 Hz, 1H), 3.41 (tt, *J* = 7.2, 3.7 Hz, 1H), 2.71 (dqd, *J* = 15.6, 10.6, 3.4 Hz, 1H), 2.57 (dqd, *J* = 15.4, 10.2, 8.7 Hz, 1H), 0.86 - 0.80 (m, 2H), 0.76 (tdd, *J* = 8.5, 7.3, 4.5 Hz, 2H).
^{13}C NMR (126MHz,$CDCl_3$)δ 158.5, 143.6, 131.3, 130.5, 129.3, 125.4 (q, *J* = 223.2 Hz, 1C), 123.3, 121.2, 76.4 (q, *J* = 3.0 Hz,1C), 40.6 (q, *J* = 8.1Hz, 1C), 29.6, 8.1, 7.9.
^{19}F NMR (377 MHz, $CDCl_3$) δ - 63.7.
HRMS (ESI) m/z calcd for $C_{13}H_{12}F_3NO$ $[M+H]^+$: 256.0944, found: 256.0943.



3ad

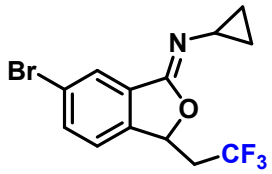
(Z)-1-(cyclopropylimino)-3-(2,2,2-trifluoroethyl)-1,3-dihydroisobenzofuran-5-carbonitrile
3ad was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). White solid (74% yield), mp 113-116 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.66 (s, 1H), 5.78 (dd, *J* = 8.1, 4.0 Hz, 1H), 3.39 (tt, *J* = 7.1, 3.5 Hz, 1H), 2.79 - 2.57 (m, 2H), 0.87 (td, *J* = 6.6, 2.1 Hz, 2H), 0.82 - 0.73 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 156.3, 144.0, 134.8, 133.3, 125.6, 125.0 (q, *J* = 279.8 Hz, 1C), 124.2, 117.9, 114.8, 76.2, 40.1(q, *J* = 29.3 Hz, 1C), 30.1, 8.6, 8.5.
^{19}F NMR (377 MHz, $CDCl_3$) δ - 63.5.
HRMS (ESI) m/z calcd for $C_{14}H_{11}F_3N_2O$ $[M+H]^+$: 281.0896, found: 281.0898.



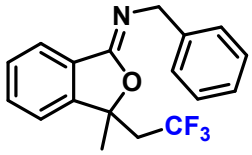
3ae

(Z)-5-bromo-N-cyclopropyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine
3ae was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). White solid (78% yield), mp 119-123 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.2 Hz, 1H), 7.57 (dd, *J* = 8.2, 1.6 Hz, 1H), 7.50 (s, 1H), 5.71 (dd, *J* = 8.5, 3.5 Hz, 1H), 3.37 (tt, *J* = 7.3, 3.6 Hz, 1H), 2.76 - 2.51 (m, 2H), 0.91 - 0.80 (m, 2H), 0.80 - 0.67 (m, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 157.3, 145.4, 132.8, 129.6, 125.6, 125.2 (q, *J* = 278.8 Hz, 1C), 124.7, 124.6, 75.8, 40.3 (q, *J* = 28.3 Hz, 1C), 29.7, 8.2, 8.0.
^{19}F NMR (377 MHz, $CDCl_3$) δ - 63.7.
HRMS (ESI) m/z calcd for $C_{13}H_{11}BrF_3NO$ $[M+H]^+$: 334.0049, found: 334.0048.



3af

(Z)-6-bromo-N-cyclopropyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine
3af was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). White solid (77% yield), mp 123-126 °C.
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (d, *J* = 1.8 Hz, 1H), 7.61 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.22 (d, *J* = 8.1 Hz, 1H), 5.69 (dd, *J* = 8.4, 3.7 Hz, 1H), 3.37 (tt, *J* = 7.2, 3.6 Hz, 1H), 2.75 - 2.52 (m, 2H), 0.87 - 0.80 (m, 2H), 0.75 (dtdt, *J* = 7.9, 4.8, 3.7, 1.4 Hz, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 156.8, 142.2, 134.3, 132.7, 126.3, 125.3 (q, *J* = 223.21 Hz, 1C), 123.6, 122.8, 76.3 (q, *J* = 2.02Hz, 1C), 40.19 (q, *J* = 23.23 Hz, 1C), 29.73, 8.28, 8.12.
^{19}F NMR (377 MHz, $CDCl_3$) δ - 63.6.
HRMS (ESI) m/z calcd for $C_{13}H_{11}BrF_3NO$ $[M+H]^+$: 334.0049, found: 334.0048.



3ag

(E)-N-benzyl-3-methyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

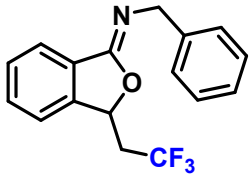
3ag was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (75% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.5 Hz, 1H), 7.48 - 7.27 (m, 5H), 7.25 - 7.13 (m, 3H), 4.66 (s, 2H), 2.77 - 2.68 (m, 1H), 2.65 - 2.54 (m, 1H), 1.64 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1, 147.3, 139.5, 130.7, 128.8, 128.2, 127.3, 126.9, 125.5, 123.9 (q, *J* = 278.76 Hz, 1C), 122.8, 119.7, 83.4, 83.4, 50.1, 42.6 (q, *J* = 27.3 Hz, 1C), 25.8.

^{19}F NMR (376 MHz, $CDCl_3$) δ - 60.9.

HRMS (ESI) m/z calcd for $C_{18}H_{16}F_3NO$ $[M+H]^+$: 320.1257, found: 320.1256.



3ah

(E)-N-benzyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

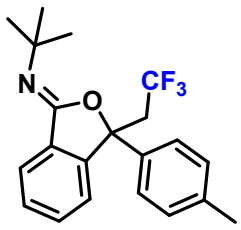
3ah was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (66% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.6 Hz, 1H), 7.47 (td, *J* = 7.4, 1.3 Hz, 1H), 7.42 (d, *J* = 7.4 Hz, 1H), 7.37 (d, *J* = 7.5 Hz, 2H), 7.30 - 7.23 (m, 3H), 7.18 - 7.13 (m, 1H), 5.68 (dd, *J* = 8.8, 3.3 Hz, 1H), 4.67 (s, 2H), 2.73 - 2.59 (m, 1H), 2.54 - 2.41 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6, 143.1, 139.4, 130.7, 129.3, 128.5, 127.3, 127.0, 125.6,124.3(q, J = 278.76 Hz, 1C), 122.9, 120.2, 50.2, 39.2(q, J = 29.3Hz), 28.7.

^{19}F NMR (376 MHz, $CDCl_3$) δ - 63.6.

HRMS (ESI) m/z calcd for $C_{17}H_{14}F_3NO$ $[M+H]^+$: 306.1100, found: 306.1099.

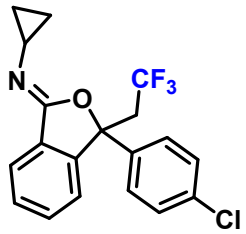


3ai

(E)-N-(tert-butyl)-3-(p-tolyl)-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

3ai was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). Colorless oil (76% yield).

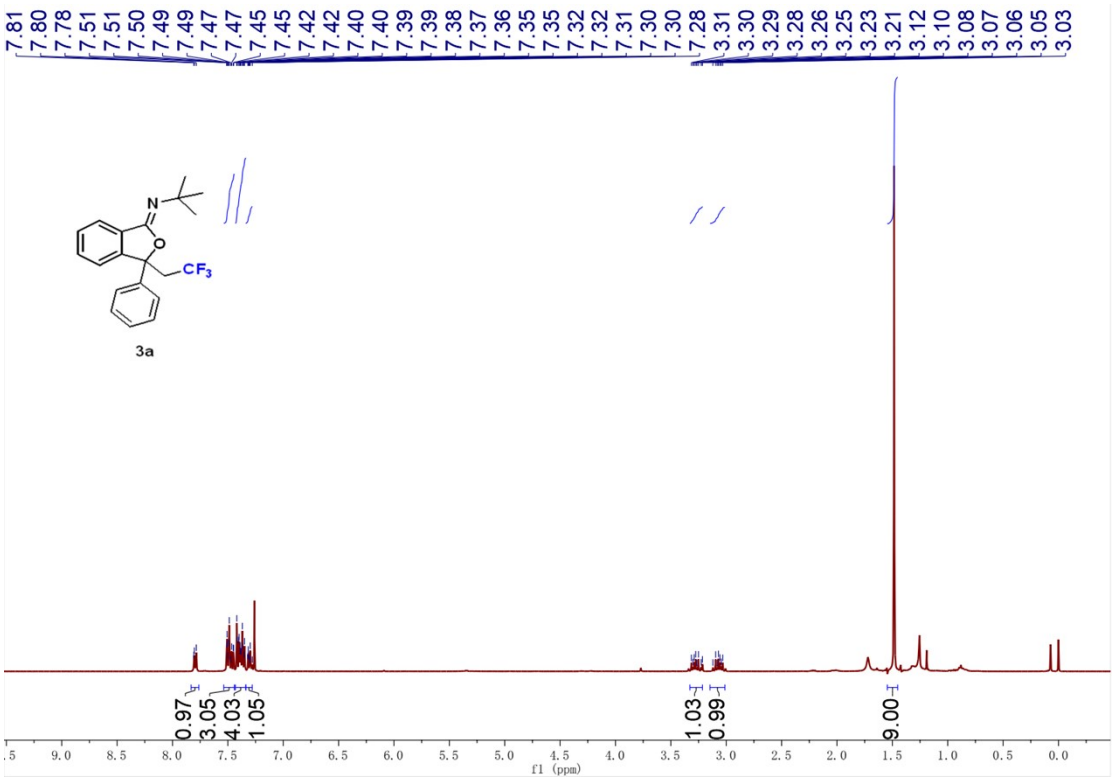
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.6 Hz, 1H), 7.40 - 7.35 (m, 1H), 7.33 - 7.26 (m, 4H), 7.09 (d, *J* = 8.1 Hz, 2H), 3.19 (dq, *J* = 15.6, 10.0 Hz, 1H), 2.97 (dq, *J* = 15.6, 9.9 Hz, 1H), 2.23 (s, 3H), 1.40 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 152.9, 145.3, 137.2, 137.1, 130.2, 130.0, 128.4, 128.0, 123.6 (q, *J* = 279.8 Hz, 1C), 123.4, 123.1, 120.7, 85.8, 52.8, 42.3 (q, *J* = 28.3 Hz, 1C), 29.1, 19.9.
^{19}F NMR (376 MHz, $CDCl_3$) δ - 60.1.
HRMS (ESI) m/z calcd for $C_{21}H_{22}F_3NO$ $[M+H]^+$: 362.1726, found: 362.1726.

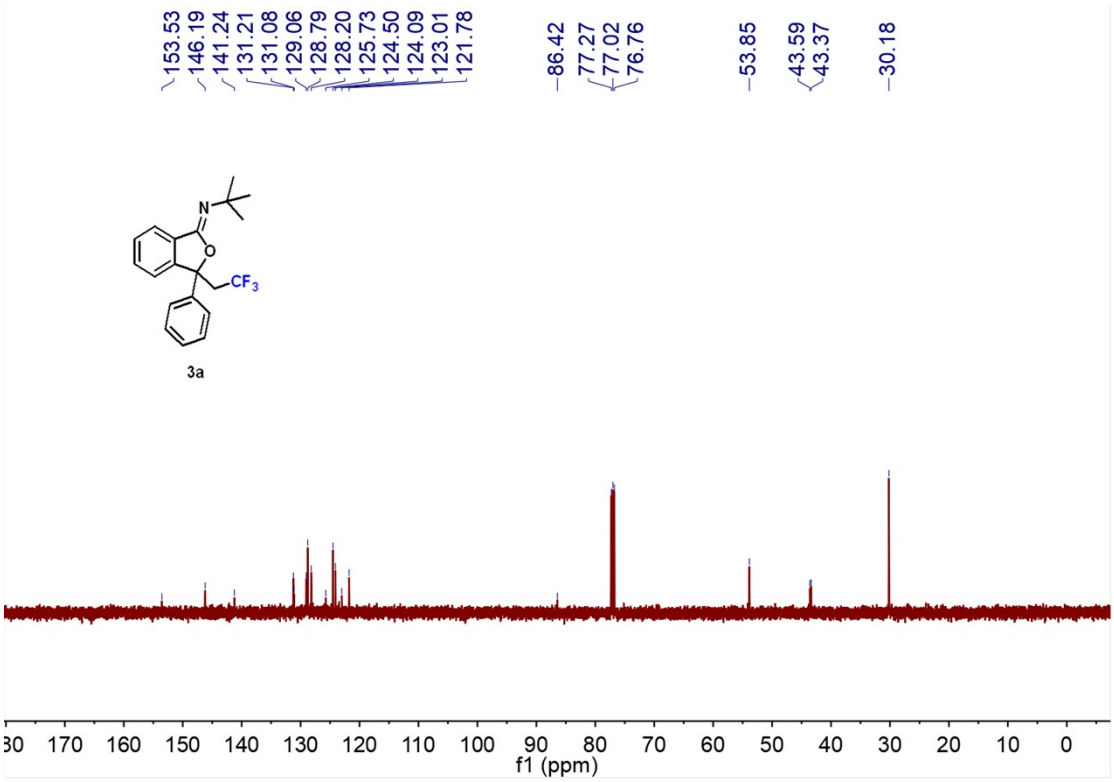


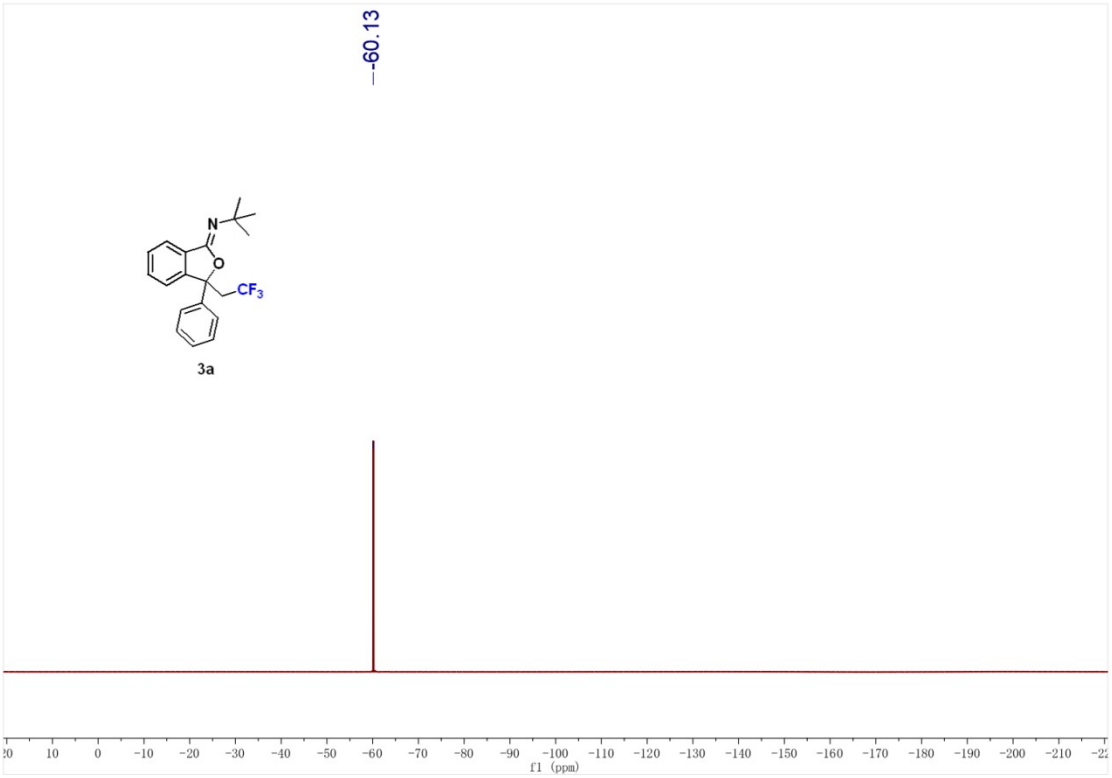
3aj

(Z)-3-(4-chlorophenyl)-N-cyclopropyl-3-(2,2,2-trifluoroethyl)isobenzofuran-1(3H)-imine

3aj was obtained according the general procedure and purified by neutral alumina column (petroleum ether/ethyl acetate =15:1 to 10:1). White solid (81% yield), mp 145-149 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.48 - 7.32 (m, 7H), 3.50 (tt, *J* = 7.0, 3.7 Hz, 1H), 3.24 (dq, *J* = 15.6, 9.9 Hz, 1H), 3.02 (dq, *J* = 15.5, 9.8 Hz, 1H), 0.90 - 0.84 (m, 2H), 0.84 - 0.77 (m, 2H).
^{13}C NMR (101 MHz, $CDCL_3$) δ 157.6, 146.4, 139.5, 134.5, 131.5, 129.5, 129.1, 126.1, 124.6 (q, *J* = 279.78Hz, 1C), 123.5, 121.9, 85.8 ,43.6 (q, *J* = 27.3 Hz, 1C), 29.9, 8.1, 8.1.
^{19}F NMR (376 MHz, $CDCl_3$) δ - 60.1.
HRMS (ESI) m/z calcd for $C_{19}H_{15}ClF_3NO$ $[M+H]^+$: 366.0867, found: 366.0865.


7.81 7.80 7.78 7.51 7.51 7.50 7.49 7.49 7.47 7.47 7.45 7.45 7.42 7.42 7.40 7.40 7.39 7.39 7.38 7.37 7.36 7.35 7.35 7.32 7.32 7.31 7.30 7.30 7.28 3.31 3.30 3.29 3.28 3.26 3.25 3.23 3.21 3.12 3.10 3.08 3.07 3.06 3.05 3.03
N
O
CF3
3a
0.97
3.05
4.03
1.05
1.03
0.99
9.00
f1 (ppm)


153.53 146.19 141.24 131.21 131.08 129.06 128.79 128.20 125.73 124.50 124.09 123.01 121.78
86.42 77.27 77.02 76.76
53.85
43.59 43.37
30.18
N
O
CF3
3a
f1 (ppm)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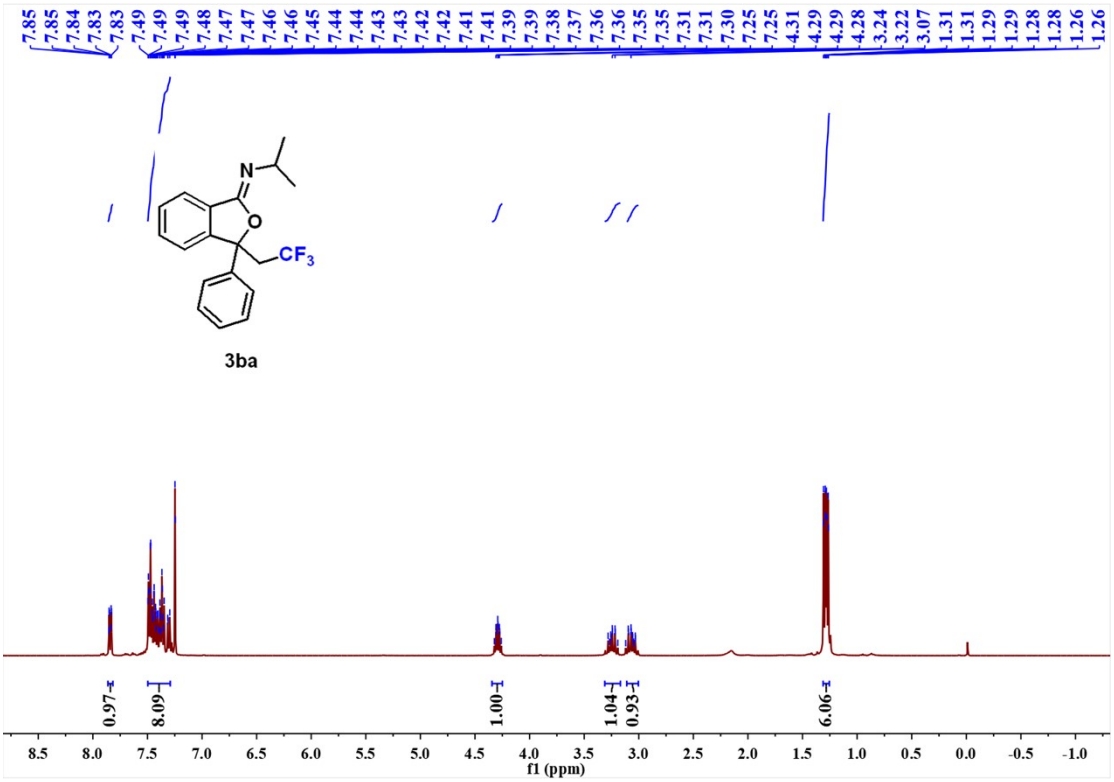
N
O
CF3
3a
f1 (ppm)


7.85 7.85 7.84 7.83 7.83 7.49 7.49 7.49 7.48 7.47 7.47 7.46 7.46 7.45 7.44 7.44 7.43 7.43 7.42 7.42 7.41 7.41 7.39 7.39 7.38 7.37 7.36 7.36 7.35 7.35 7.31 7.31 7.30 7.25 7.25 4.31 4.29 4.29 4.28 3.24 3.22 3.07 1.31 1.31 1.29 1.29 1.28 1.28 1.26 1.26
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O
CF3
3ba
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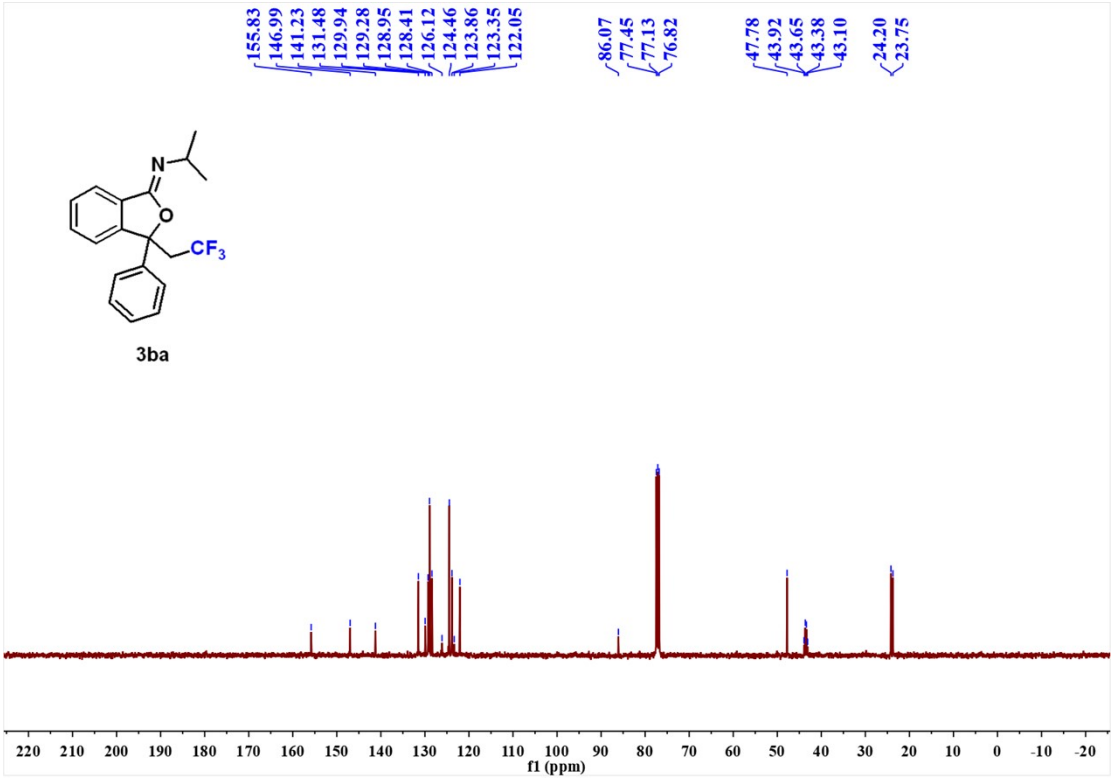
1.00
1.04
0.93
6.06
f1 (ppm)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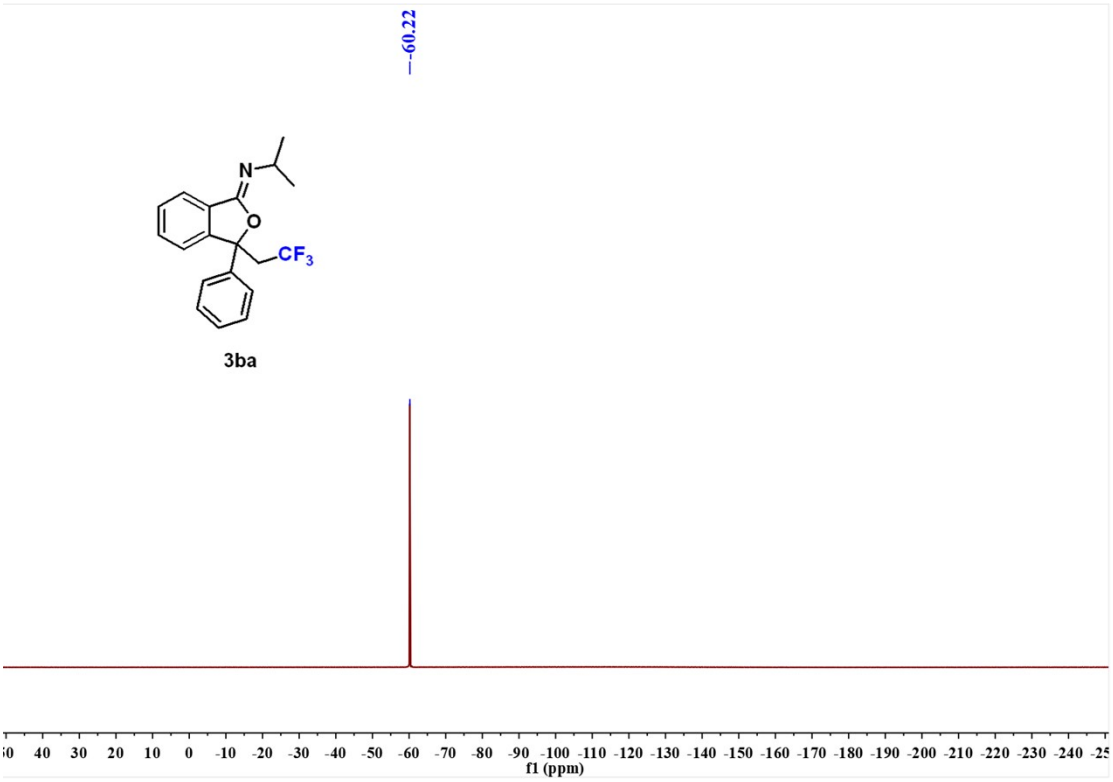
146.99
141.23
131.48
129.94
129.28
128.95
128.41
126.12
124.46
123.86
123.35
122.05
86.07
77.45
77.13
76.82
47.78
43.92
43.65
43.38
43.10
24.20
23.75
N
O
CF3
3ba
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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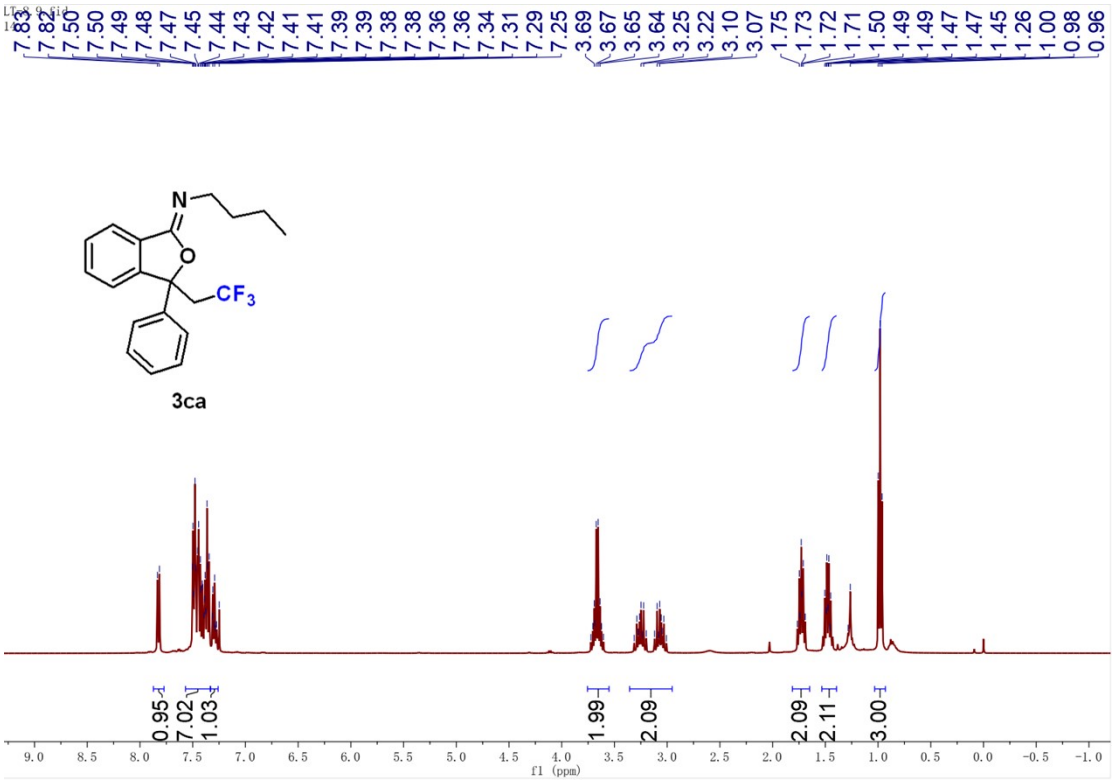
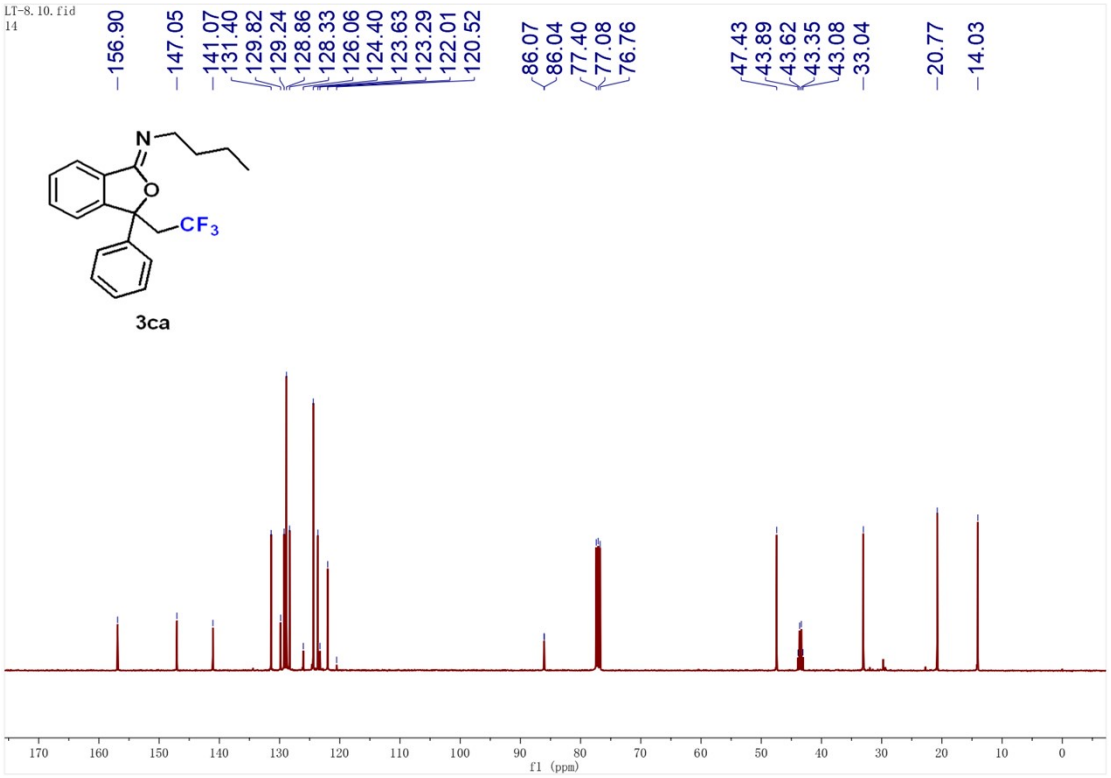
N
O
CF3
3ba
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)


7.83
7.82
7.50
7.50
7.49
7.48
7.47
7.45
7.44
7.43
7.42
7.41
7.41
7.39
7.39
7.38
7.38
7.36
7.36
7.34
7.31
7.29
7.25
3.69
3.67
3.65
3.64
3.25
3.22
3.10
3.07
1.75
1.73
1.72
1.71
1.50
1.49
1.49
1.47
1.47
1.45
1.26
1.00
0.98
0.96
N
O
CF3
3ca
0.95
7.02
1.03
1.99
2.09
2.09
2.11
3.00
f1 (ppm)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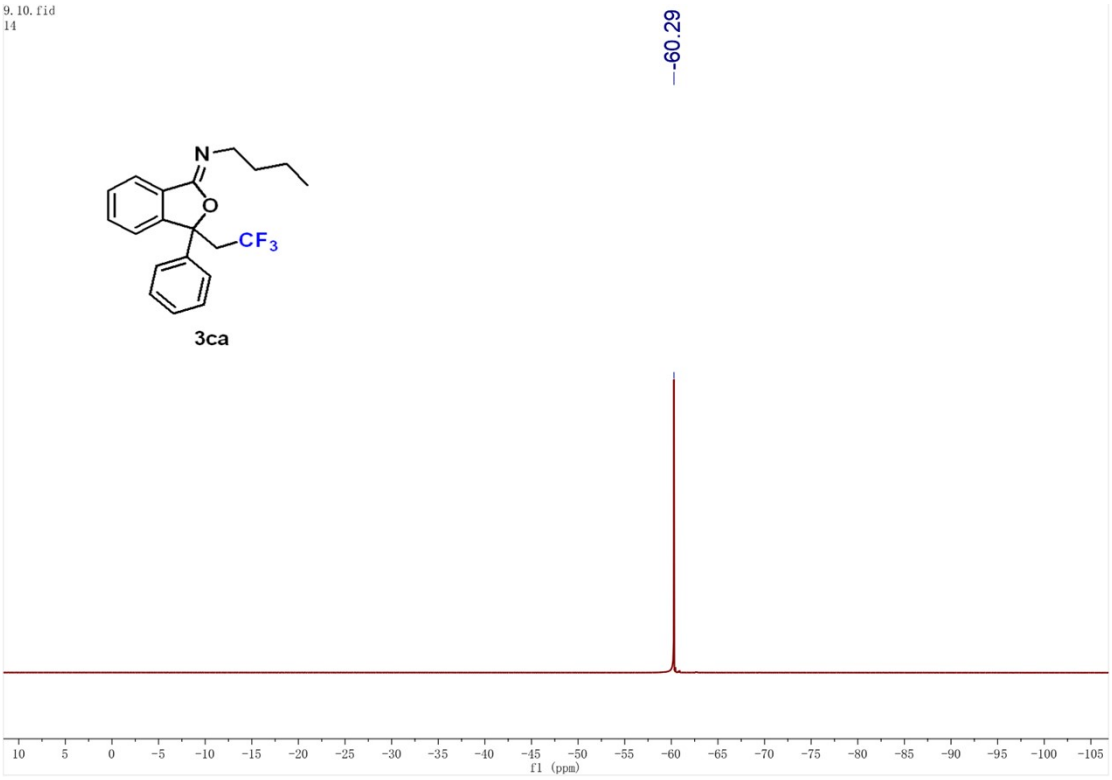
156.90
147.05
141.07
131.40
129.82
129.24
128.86
128.33
126.06
124.40
123.63
123.29
122.01
120.52
86.07
86.04
77.40
77.08
76.76
47.43
43.89
43.62
43.35
43.08
33.04
20.77
14.03
N
O
CF3
3ca
f1 (ppm)

9. 10. fid
14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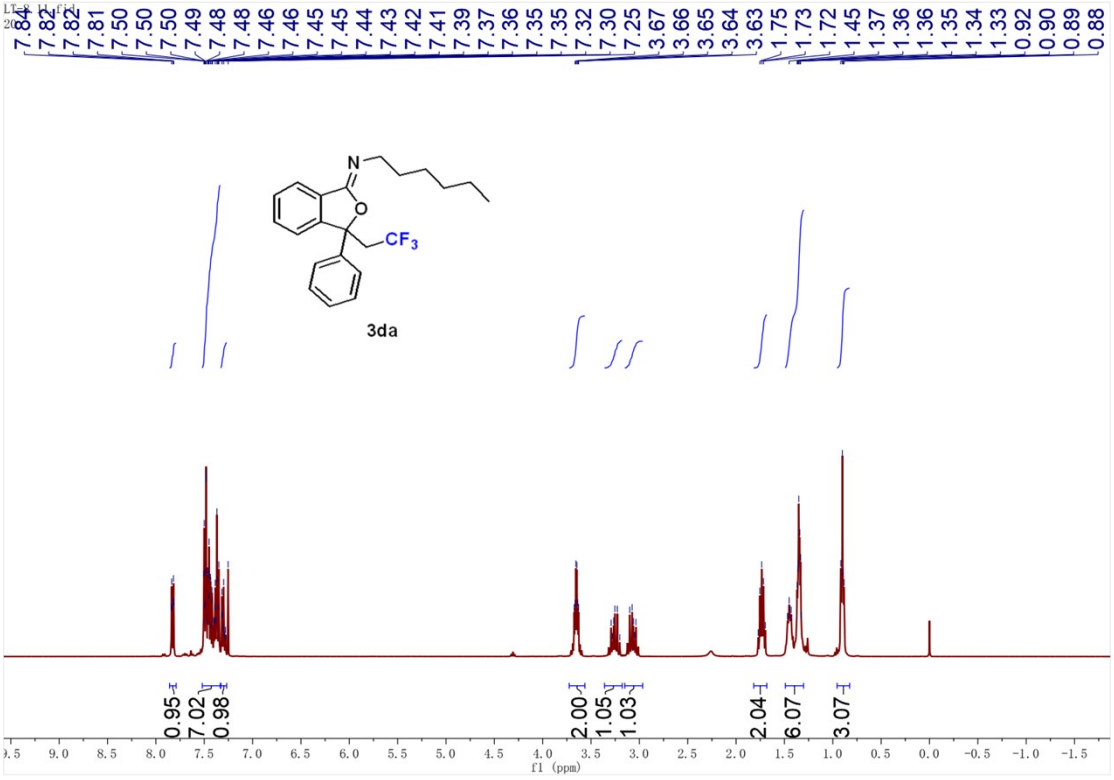
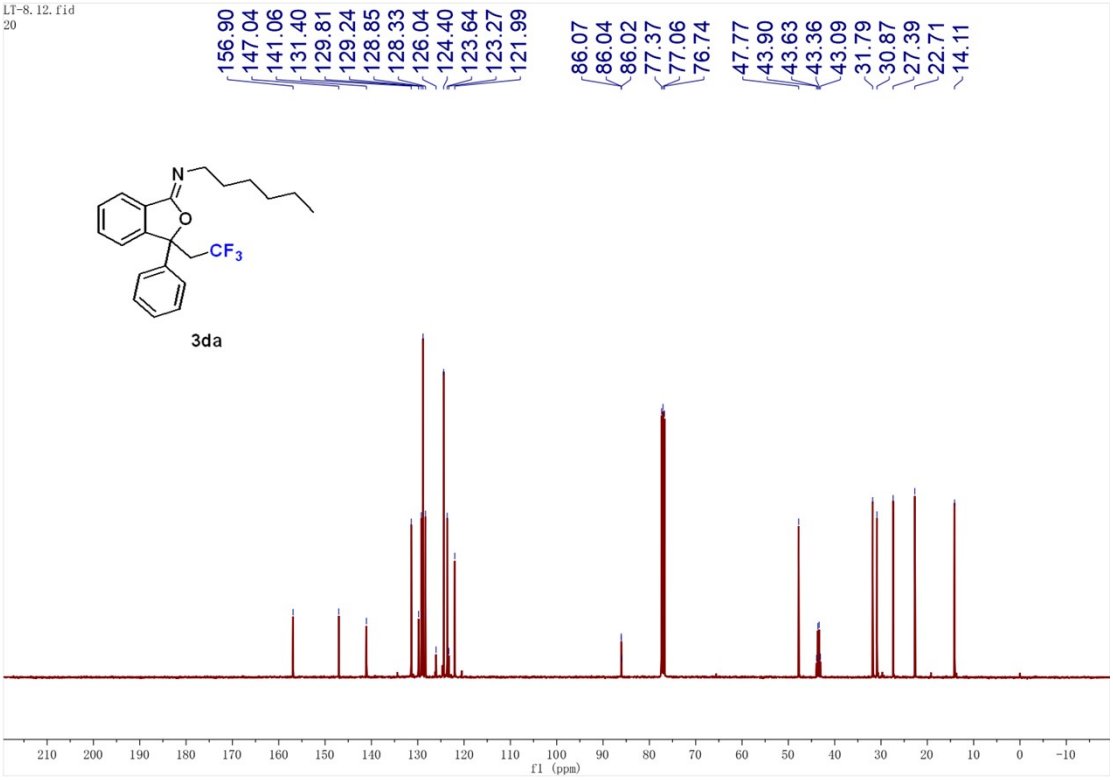
N
O
CF3
3ca
10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105
f1 (ppm)


7.84 7.82 7.82 7.81 7.50 7.50 7.50 7.49 7.48 7.48 7.46 7.46 7.45 7.45 7.44 7.43 7.42 7.41 7.39 7.37 7.36 7.35 7.35 7.32 7.30 7.25 3.67 3.66 3.65 3.64 3.63 1.75 1.73 1.72 1.45 1.37 1.36 1.36 1.35 1.34 1.33 0.92 0.90 0.89 0.88
N
O
CF3
3da
0.95 7.02 0.98 2.00 1.05 1.03 2.04 6.07 3.07
f1 (ppm)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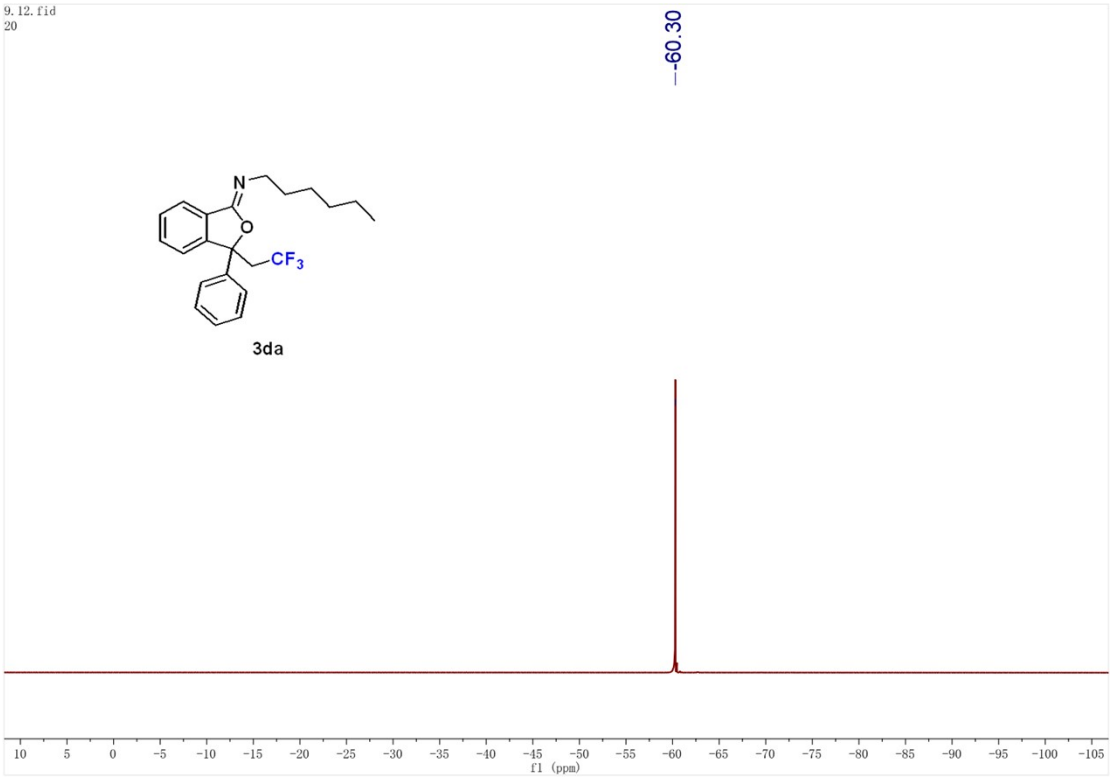
147.04
141.06
131.40
129.81
129.24
128.85
128.33
126.04
124.40
123.64
123.27
121.99
86.07
86.04
86.02
77.37
77.06
76.74
47.77
43.90
43.63
43.36
43.09
31.79
30.87
27.39
22.71
14.11
N
O
CF3
3da
f1 (ppm)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-60.30
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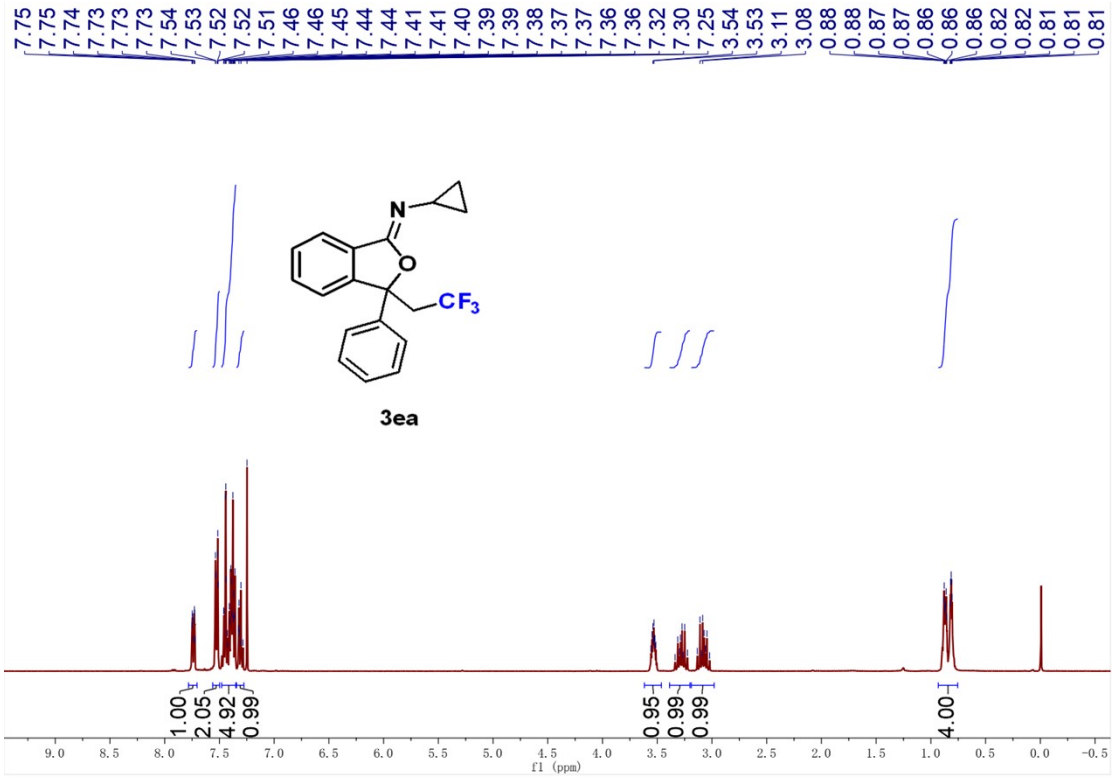
O
CF3
3da
f1 (ppm)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7.75
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7.73
7.54
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7.52
7.52
7.51
7.46
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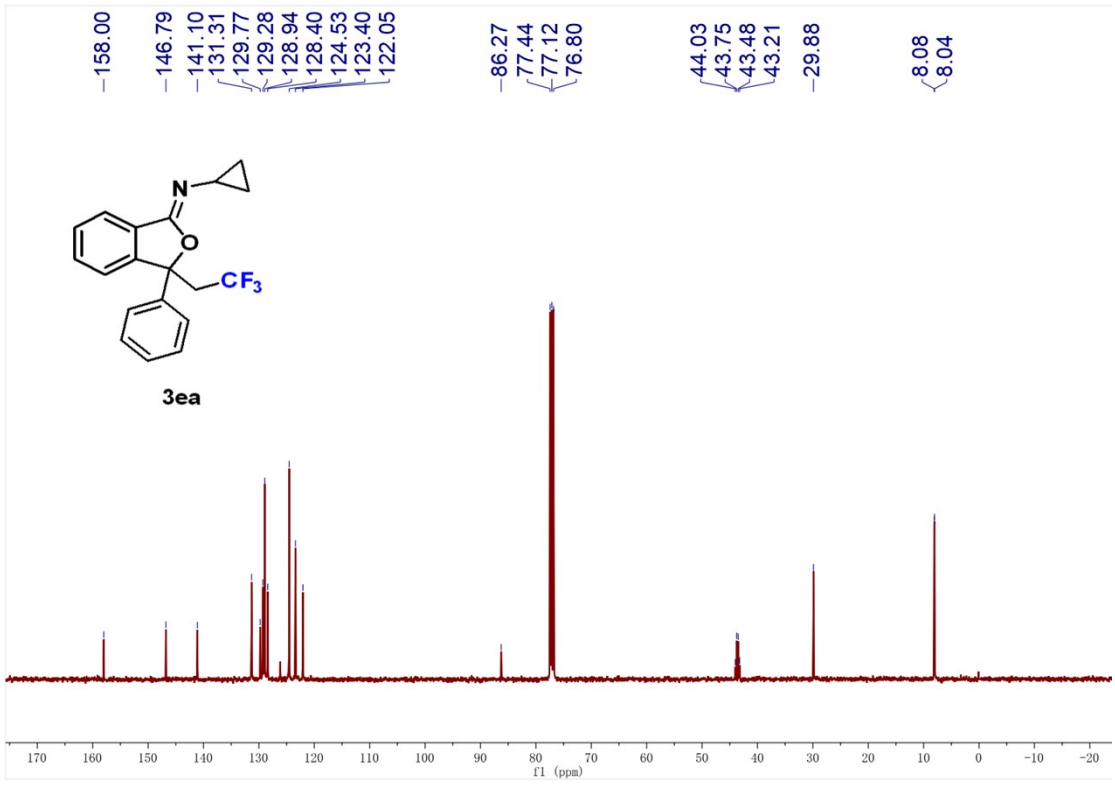
7.45
7.44
7.44
7.41
7.41
7.40
7.39
7.39
7.38
7.37
7.37
7.36
7.36
7.32
7.30
7.25
3.54
3.53
3.11
3.08
0.88
0.88
0.87
0.87
0.86
0.86
0.86
0.82
0.82
0.81
0.81
0.81
N
O
CF3
3ea
1.00
2.05
4.92
0.99
0.95
0.99
0.99
4.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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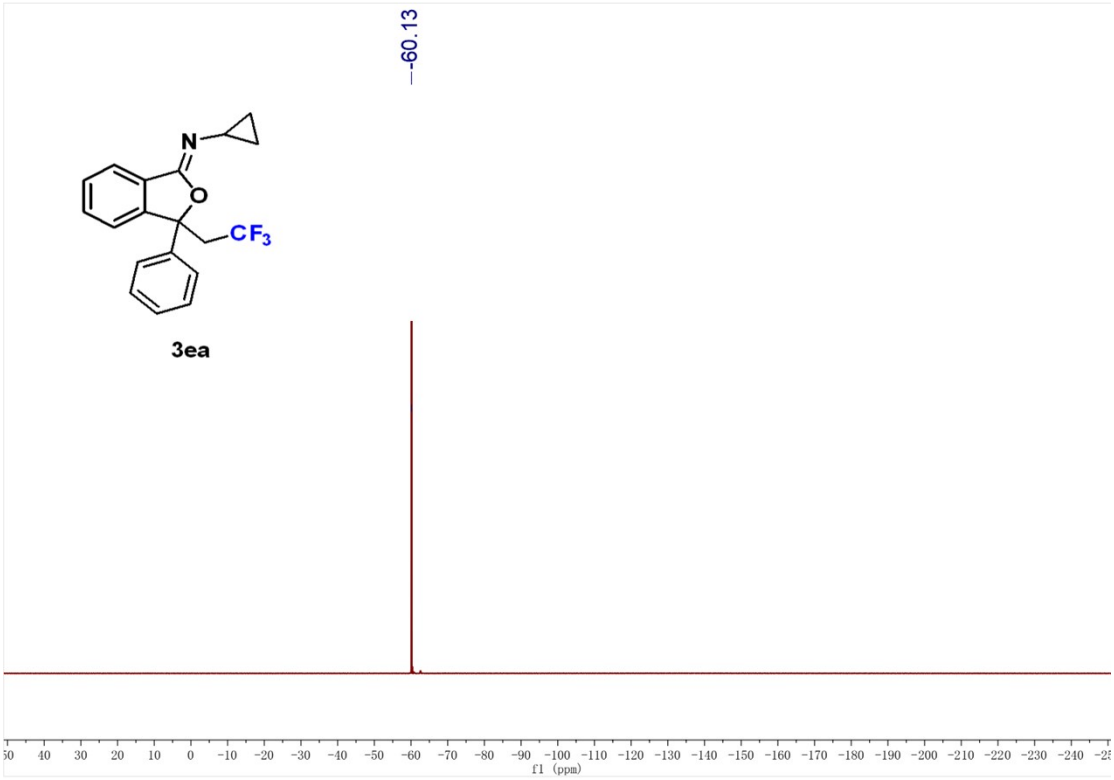
146.79
141.10
131.31
129.77
129.28
128.94
128.40
124.53
123.40
122.05
86.27
77.44
77.12
76.80
44.03
43.75
43.48
43.21
29.88
8.08
8.04
N
O
CF3
3ea
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)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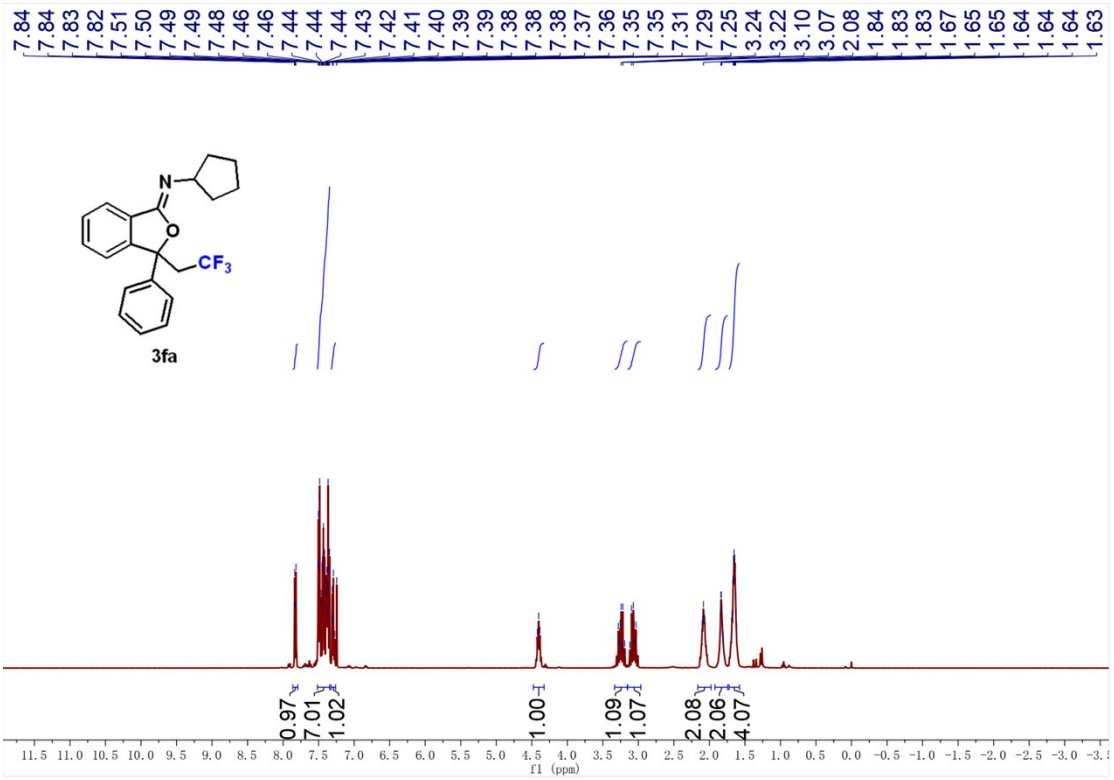
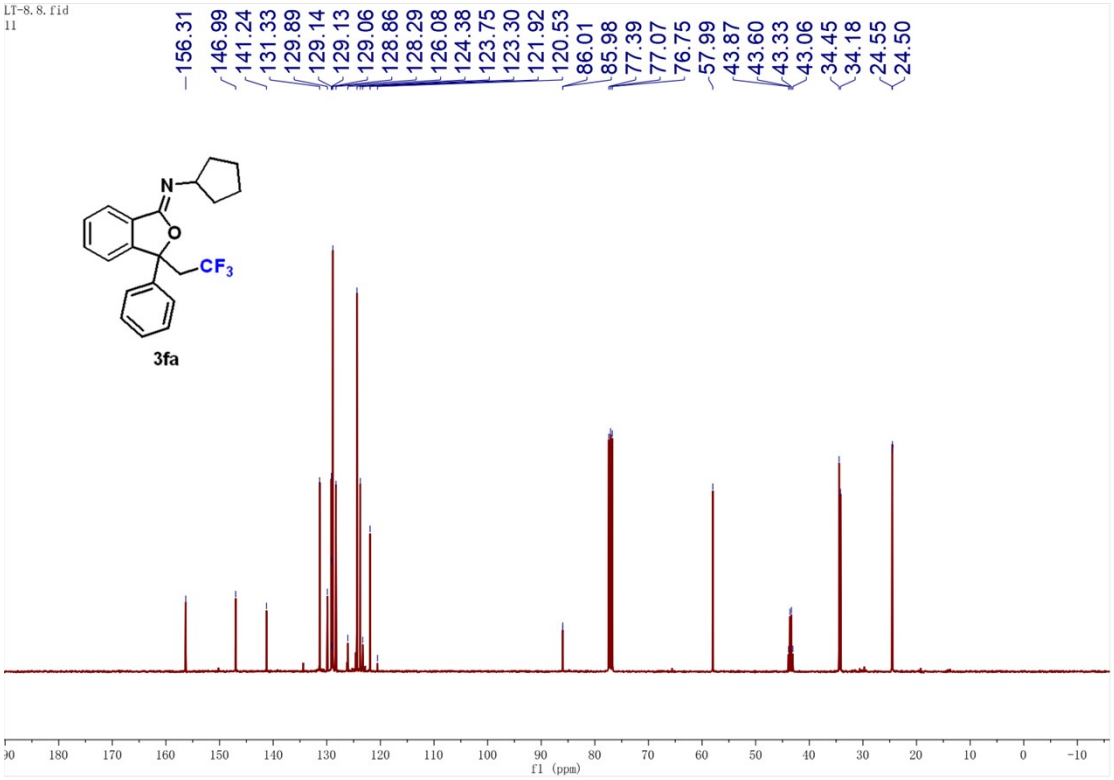
N
O
CF3
3ea
f1 (ppm)


7.84 7.84 7.83 7.82 7.51 7.50 7.49 7.49 7.48 7.46 7.46 7.44 7.44 7.44 7.43 7.42 7.41 7.40 7.39 7.39 7.38 7.38 7.38 7.37 7.36 7.35 7.35 7.31 7.29 7.25 3.24 3.22 3.10 3.07 2.08 1.84 1.83 1.83 1.67 1.65 1.65 1.64 1.64 1.64 1.63
N
O
CF3
3fa
0.97 7.01 1.02 1.00 1.09 1.07 2.08 2.06 4.07
f1 (ppm)


LT-8. 8. fid
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141.24
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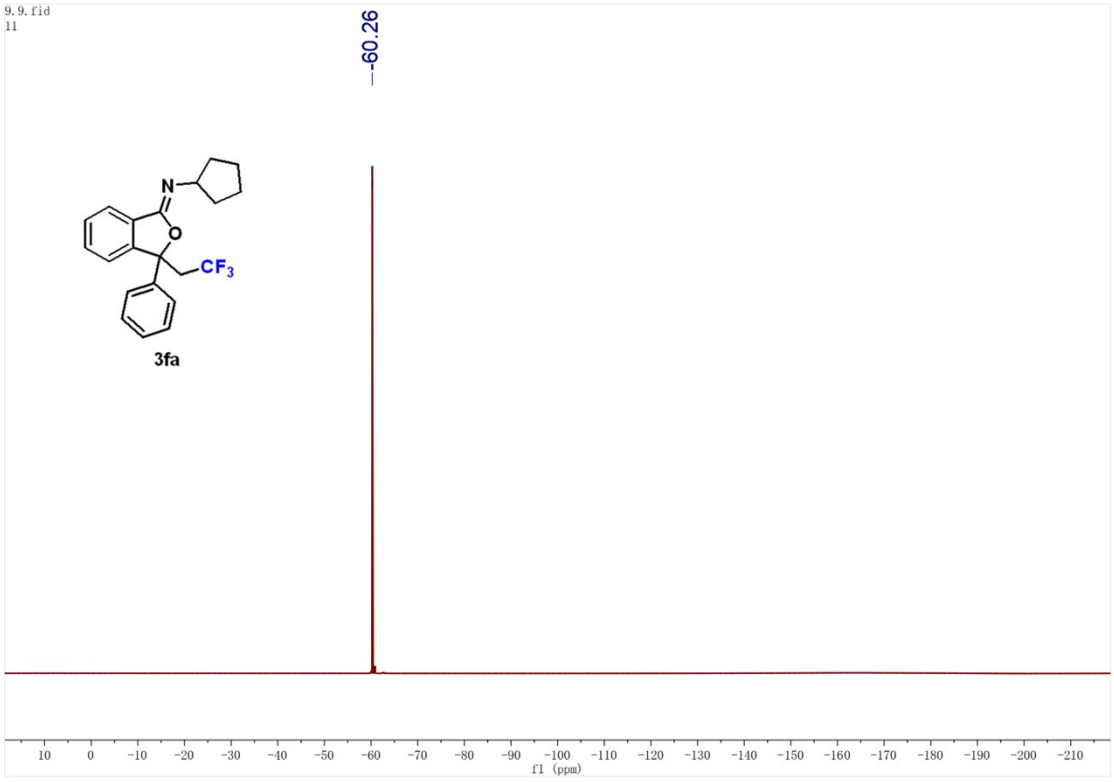
129.89
129.14
129.13
129.06
128.86
128.29
126.08
124.38
123.75
123.30
121.92
120.53
86.01
85.98
77.39
77.07
76.75
57.99
43.87
43.60
43.33
43.06
34.45
34.18
24.55
24.50
N
O
CF3
3fa
f1 (ppm)


9. 9. fid
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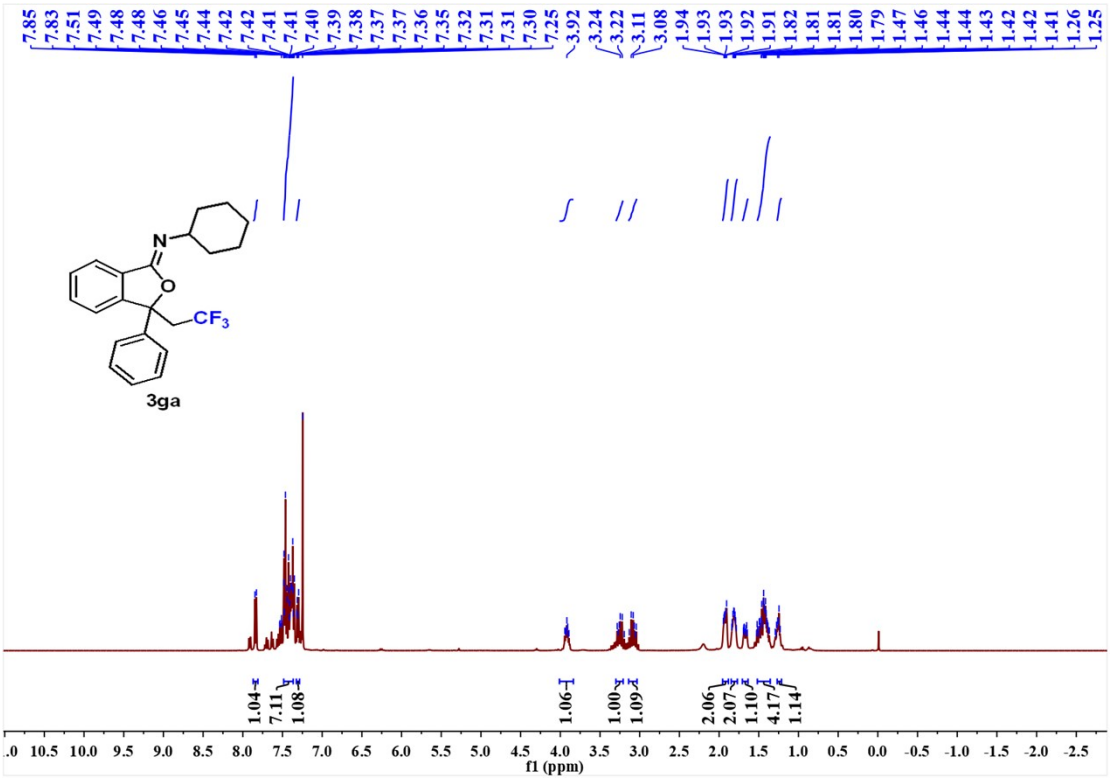
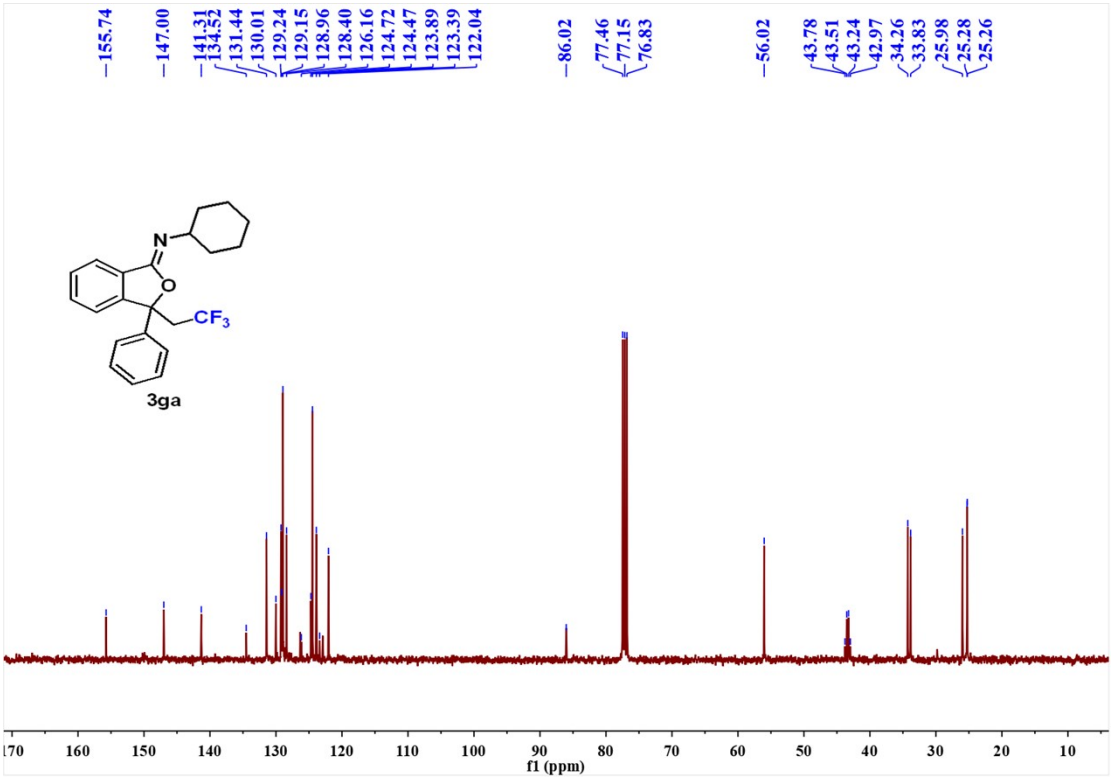
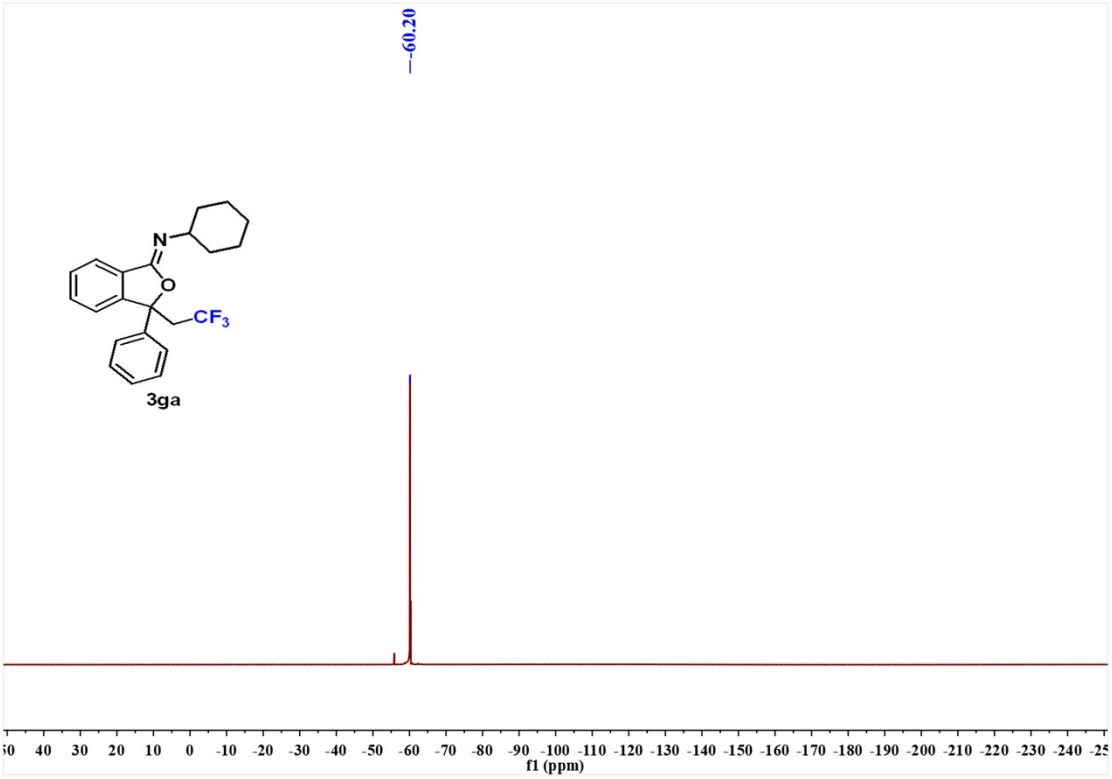
N
O
CF3
3fa
f1 (ppm)


7.85 7.83 7.51 7.49 7.48 7.48 7.46 7.45 7.44 7.42 7.42 7.41 7.41 7.40 7.39 7.38 7.37 7.37 7.36 7.35 7.32 7.31 7.31 7.30 7.25 3.92 3.24 3.22 3.11 3.08 1.94 1.93 1.93 1.92 1.91 1.82 1.81 1.81 1.80 1.79 1.47 1.46 1.44 1.44 1.43 1.42 1.42 1.41 1.26 1.25
N
O
CF3
3ga
1.04 7.11 1.08 1.06 1.00 1.09 2.06 2.07 1.10 4.17 1.14
f1 (ppm)


155.74 147.00 141.31 134.52 131.44 130.01 129.24 129.15 128.96 128.40 126.16 124.72 124.47 123.89 123.39 122.04 86.02 77.46 77.15 76.83 56.02 43.78 43.51 43.24 42.97 34.26 33.83 25.98 25.28 25.26
N
O
CF3
3ga
f1 (ppm)


-60.20
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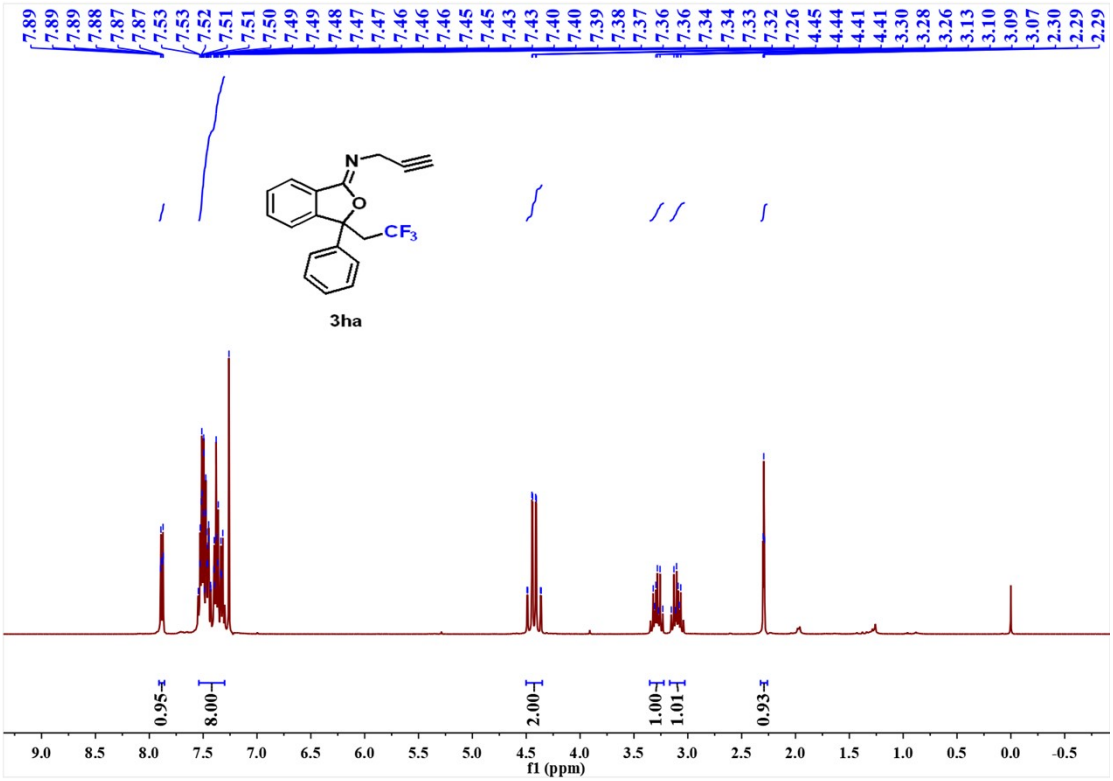
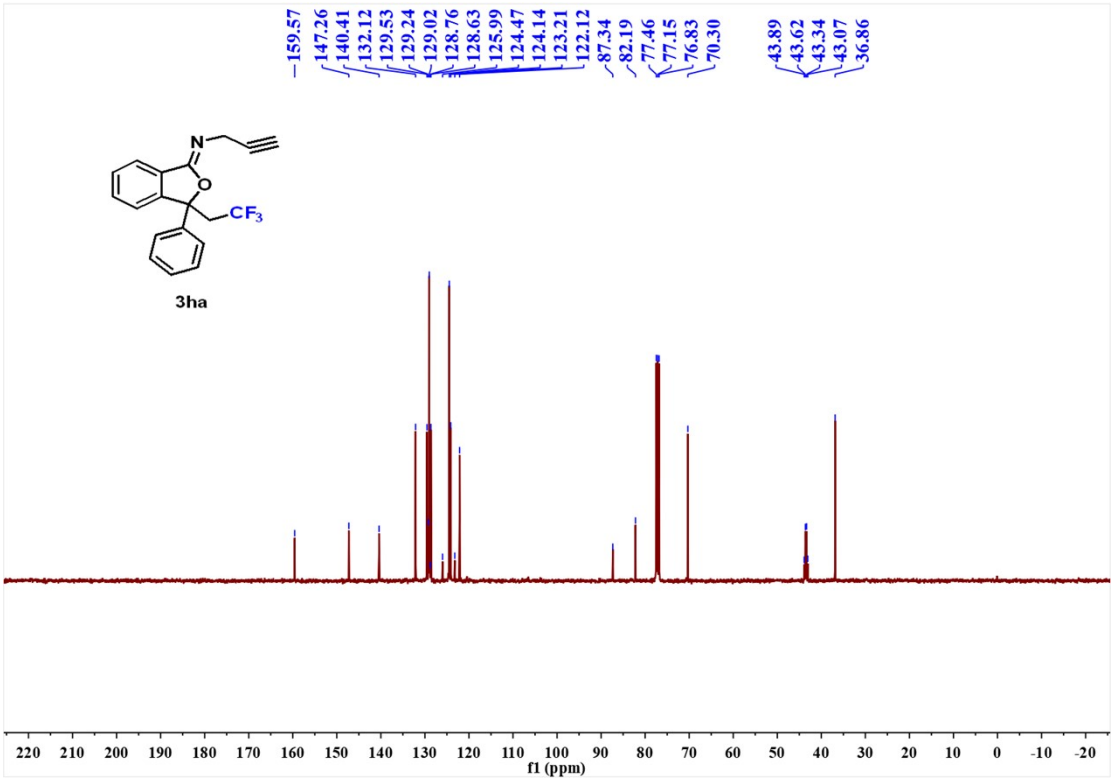
O
CF3
3ga
60 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -25
f1 (ppm)


7.89 7.89 7.89 7.88 7.87 7.87 7.53 7.53 7.52 7.51 7.51 7.50 7.49 7.49 7.48 7.47 7.47 7.46 7.46 7.46 7.45 7.45 7.43 7.43 7.40 7.40 7.39 7.38 7.37 7.36 7.36 7.34 7.34 7.33 7.32 7.26 4.45 4.44 4.41 4.41 3.30 3.28 3.26 3.13 3.10 3.09 3.07 2.30 2.29 2.29
N
O
CF3
3ha
0.95
8.00
2.00
1.00
1.01
0.93
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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129.24
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128.63
125.99
124.47
124.14
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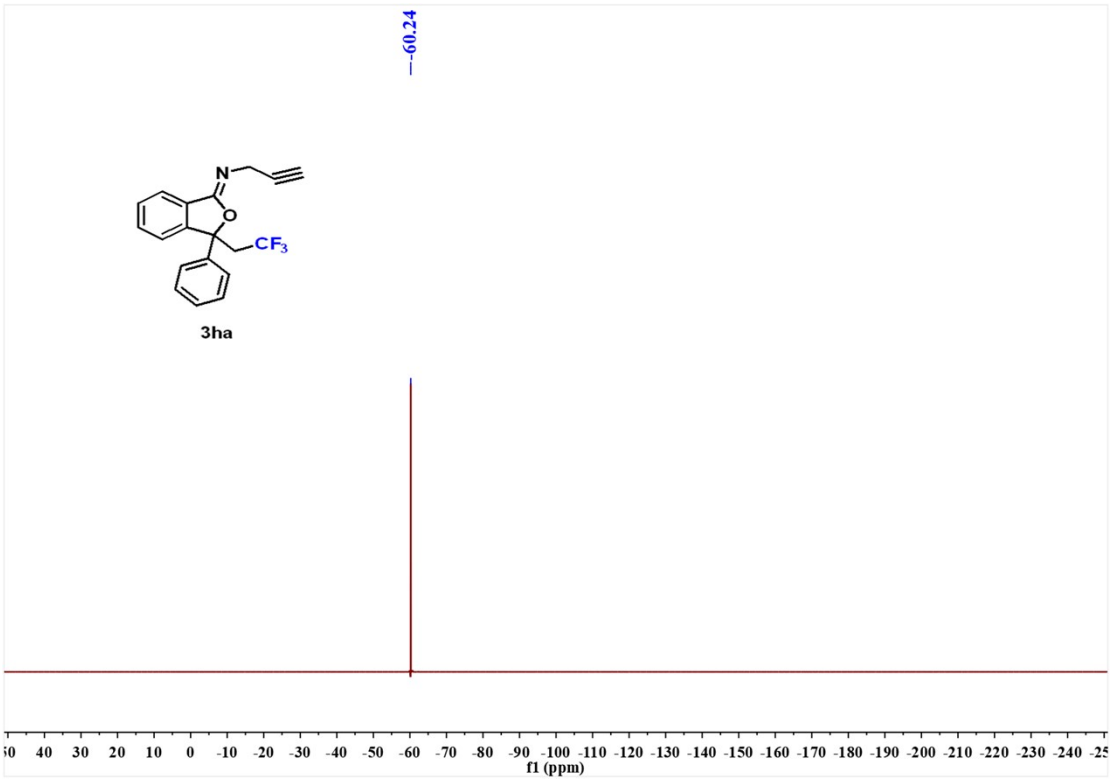
122.12
87.34
82.19
77.46
77.15
76.83
70.30
43.89
43.62
43.34
43.07
36.86
N
O
CF3
3ha
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


-60.24
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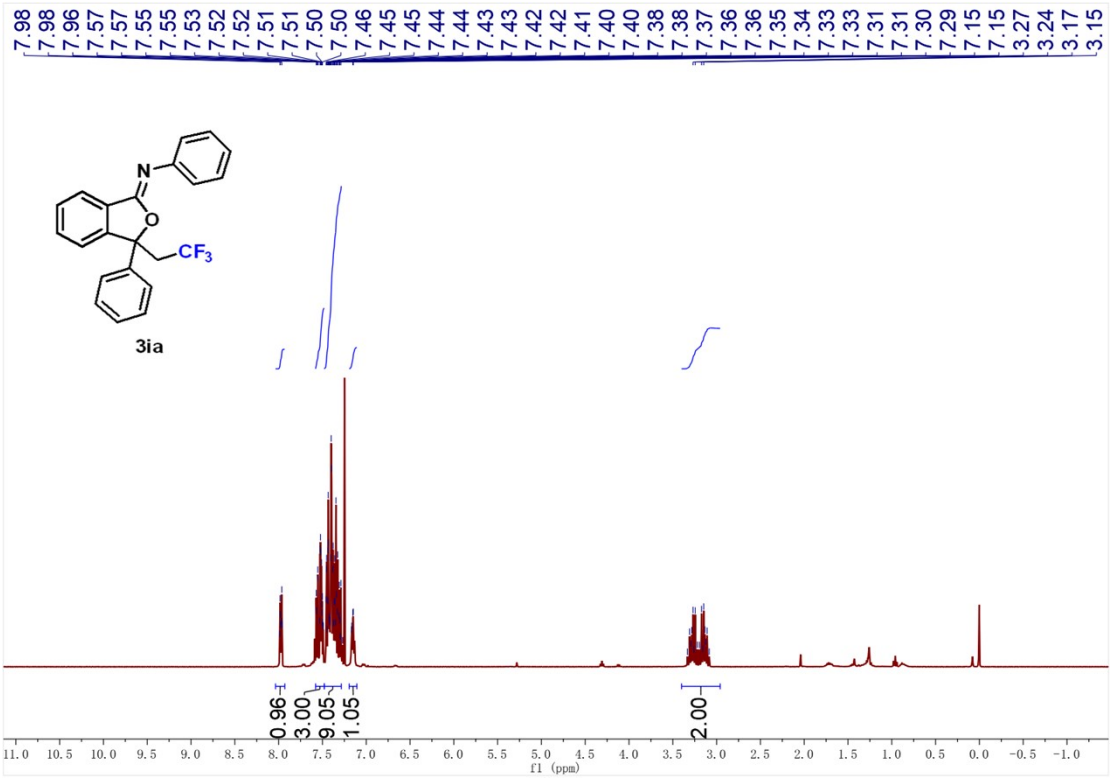
O
CF3
3ha
60 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -25
f1 (ppm)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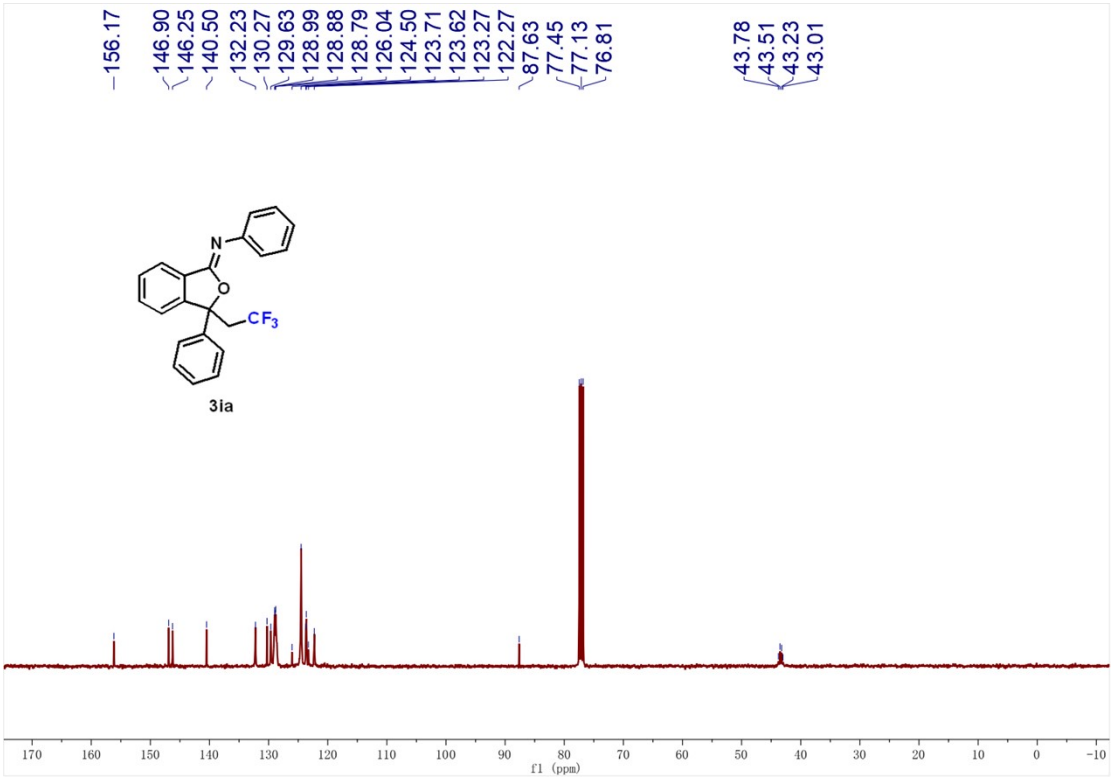
N
O
CF3
3ia
0.96
3.00
9.05
1.05
2.00
f1 (ppm)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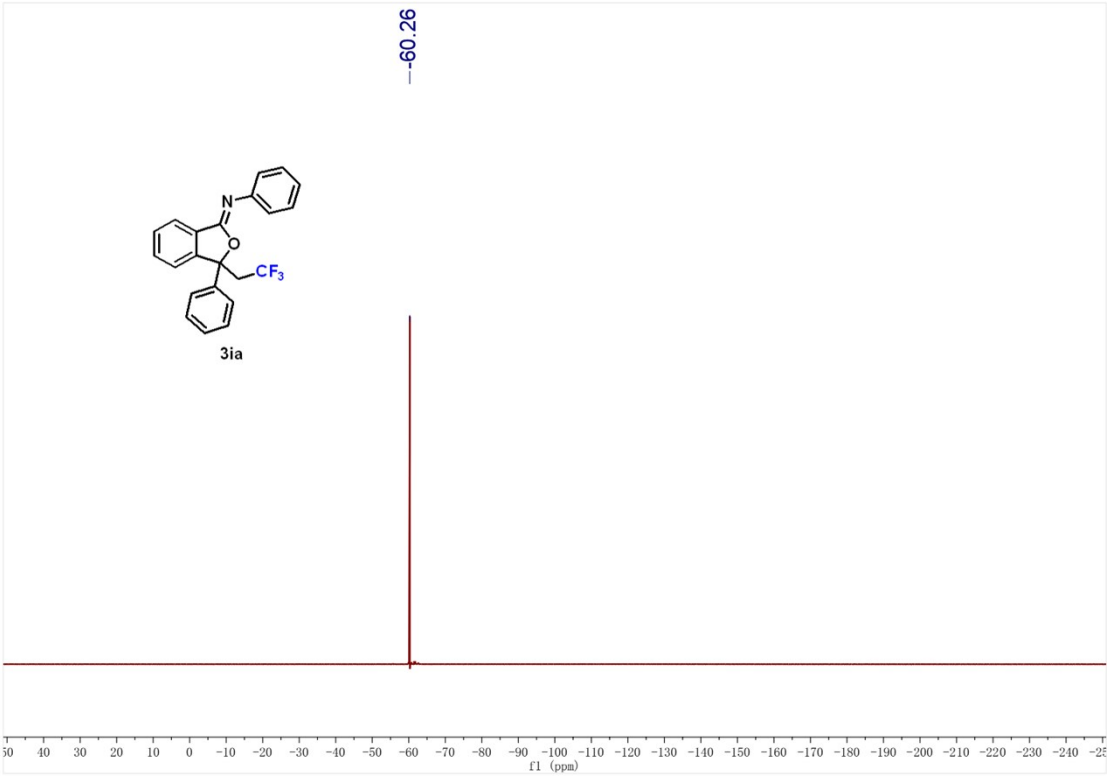
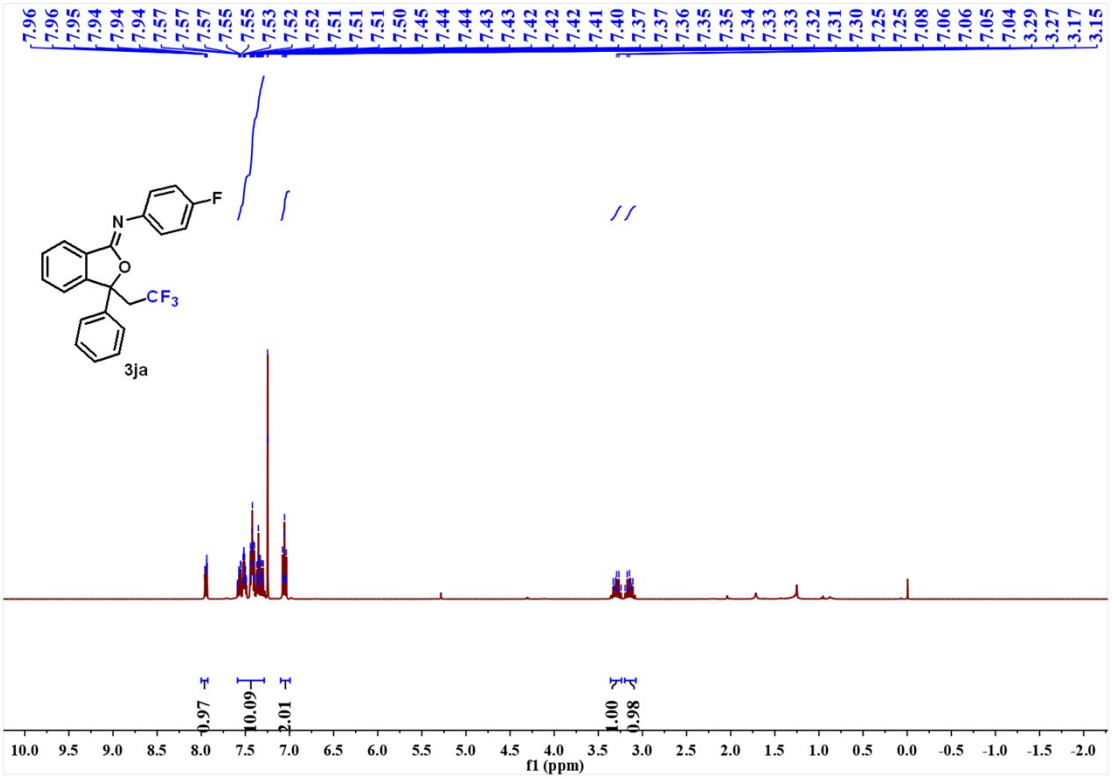
140.50
132.23
130.27
129.63
128.99
128.88
128.79
126.04
124.50
123.71
123.62
123.27
122.27
87.63
77.45
77.13
76.81
43.78
43.51
43.23
43.01
N
O
CF3
3ia
f1 (ppm)


-60.26
N
O
CF3
3ia
f1 (ppm)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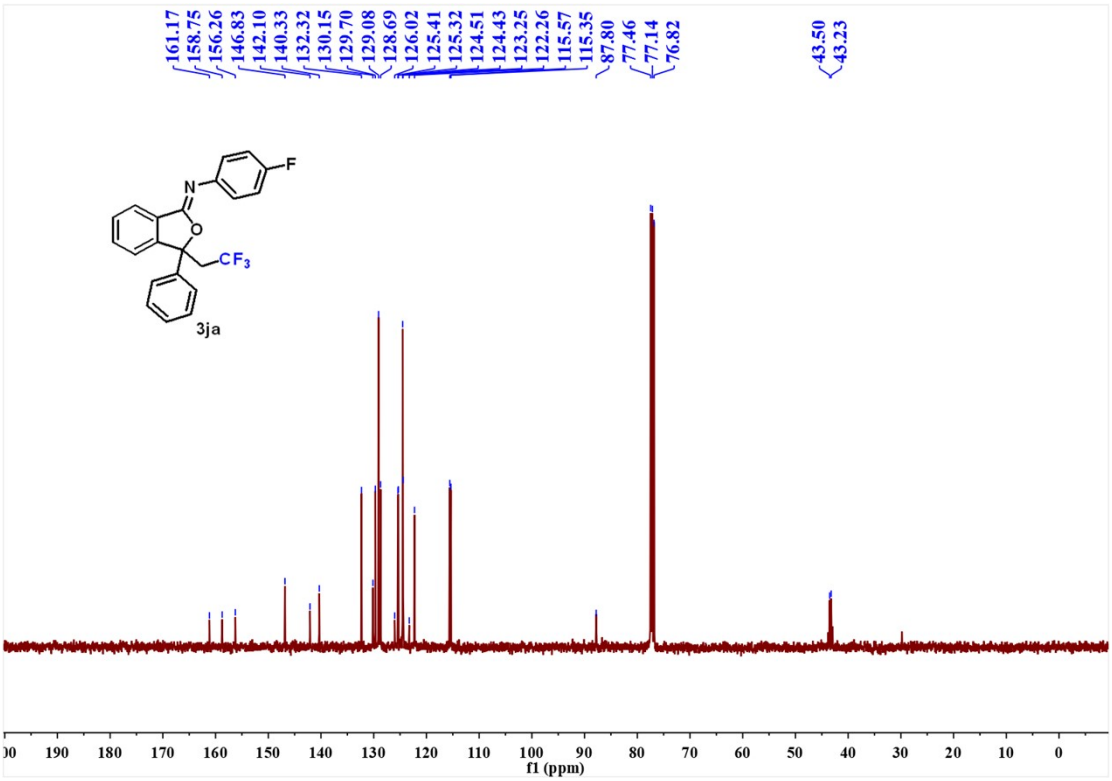
F
N
O
CF3
3ja
0.97
10.09
2.01
1.00
0.98
f1 (ppm)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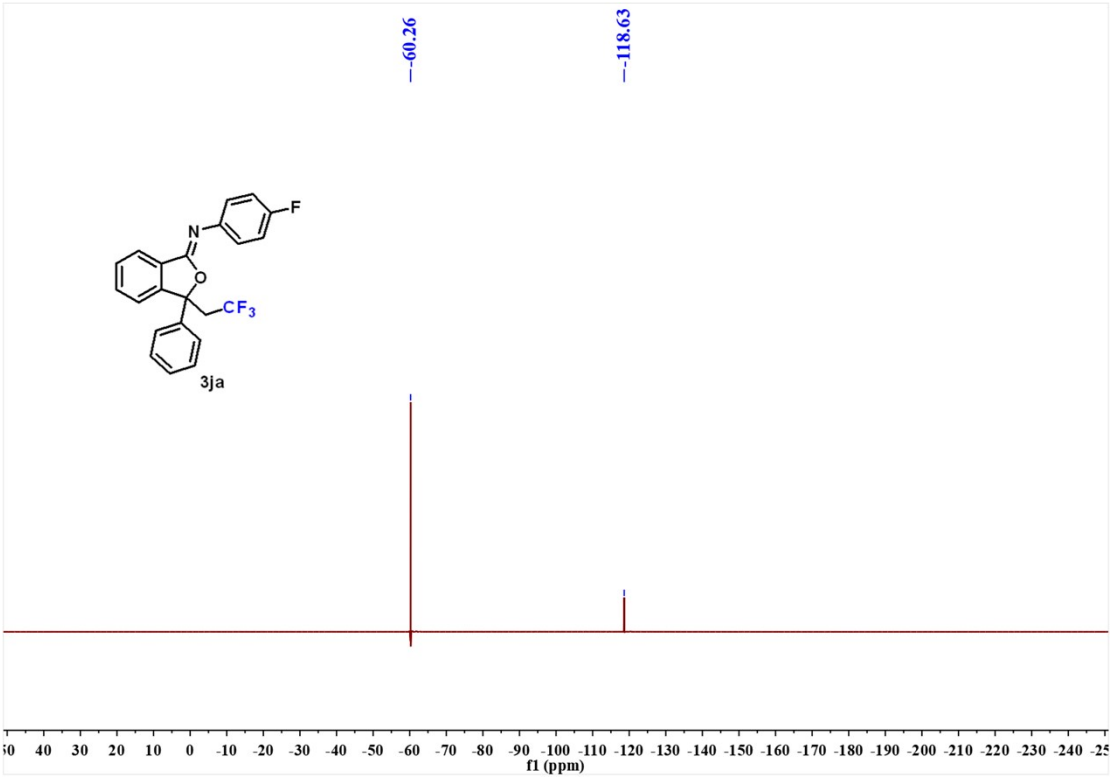
158.75
156.26
146.83
142.10
140.33
132.32
130.15
129.70
129.08
128.69
126.02
125.41
125.32
124.51
124.43
123.25
122.26
115.57
115.35
87.80
77.46
77.14
76.82
43.50
43.23
F
N
O
CF3
3ja
f1 (ppm)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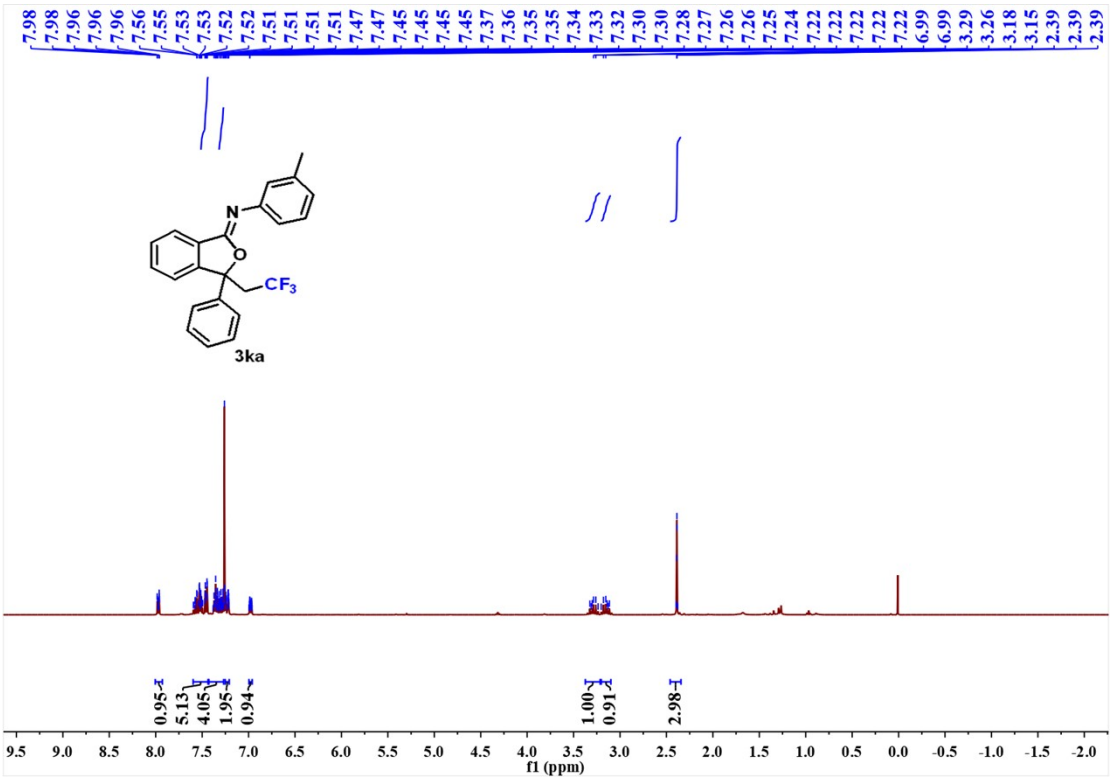
3ja
f1 (ppm)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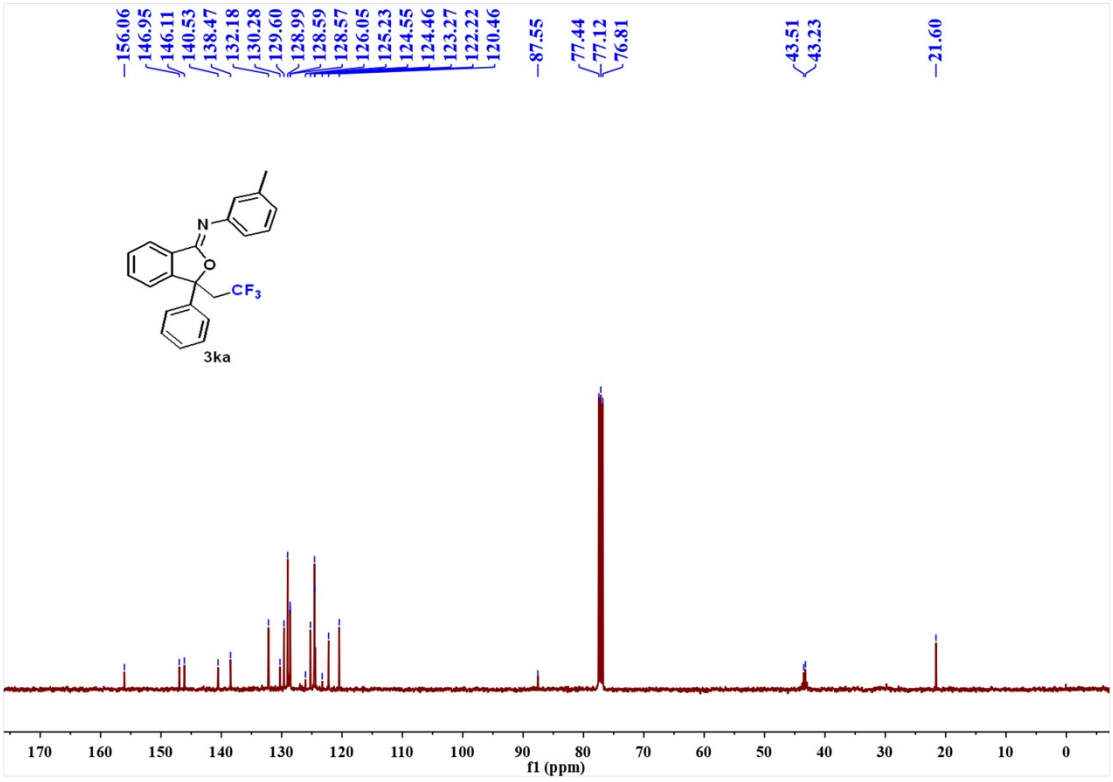
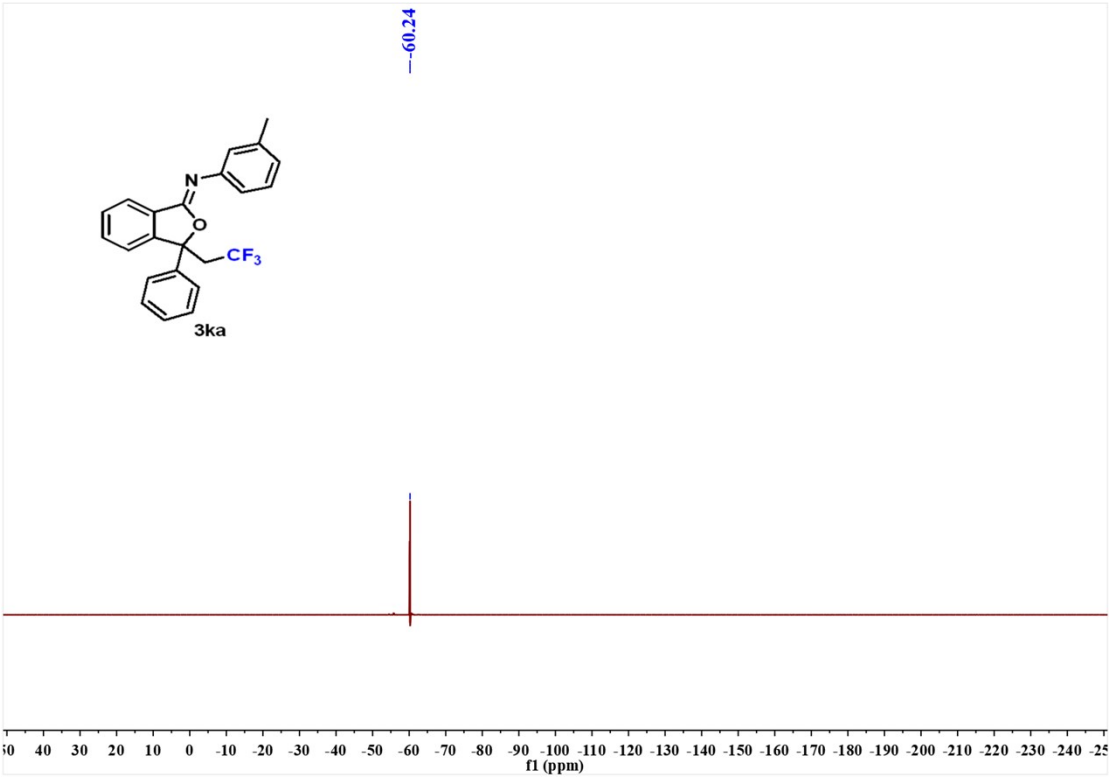
N
O
CF3
3ka
0.95 5.13 4.05 1.95 0.94 1.00 0.91 2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)


156.06 146.95 146.11 140.53 138.47 132.18 130.28 129.60 128.99 128.59 128.57 126.05 125.23 124.55 124.46 123.27 122.22 120.46 87.55 77.44 77.12 76.81 43.51 43.23 21.60
N
O
CF3
3ka
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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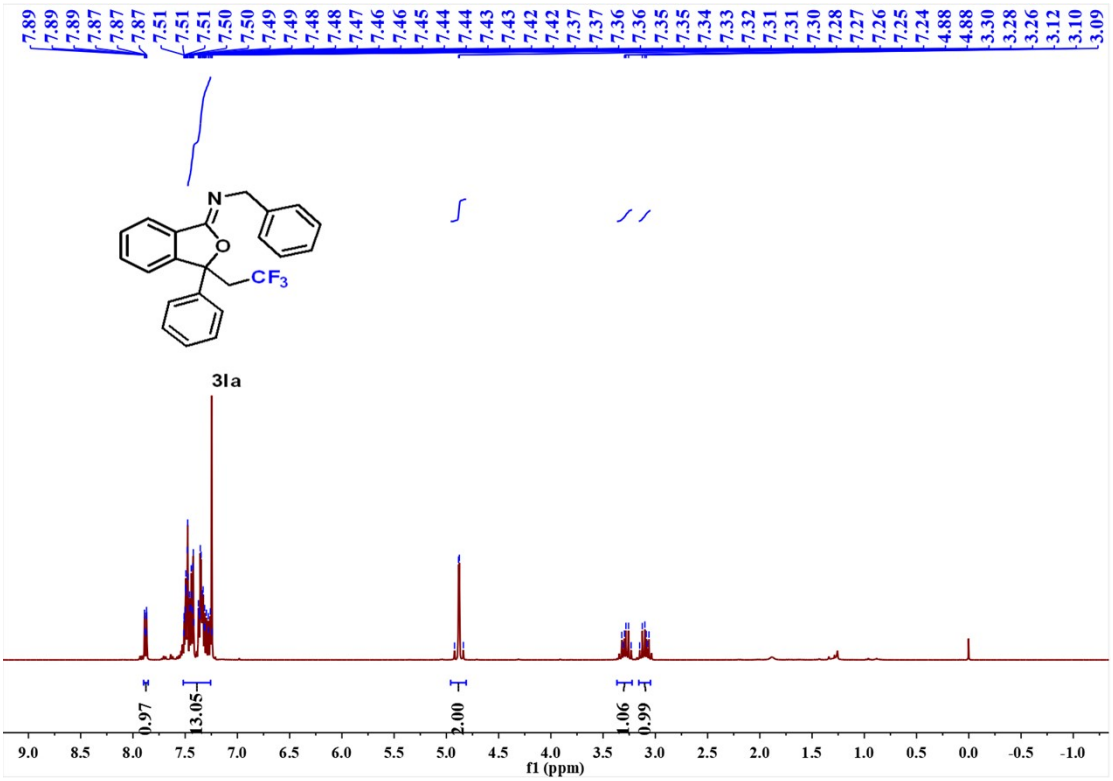
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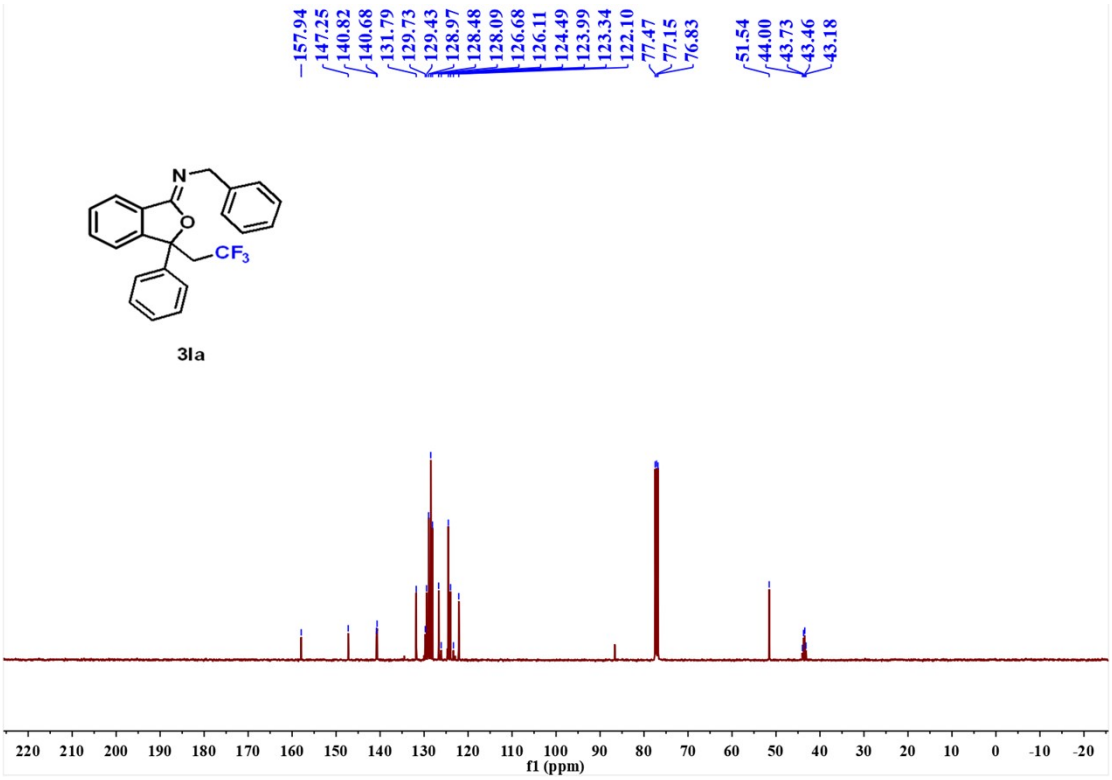
N
O
CF3
3la
0.97
13.05
2.00
1.06
0.99
f1 (ppm)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140.68
131.79
129.73
129.43
128.97
128.48
128.09
126.68
126.11
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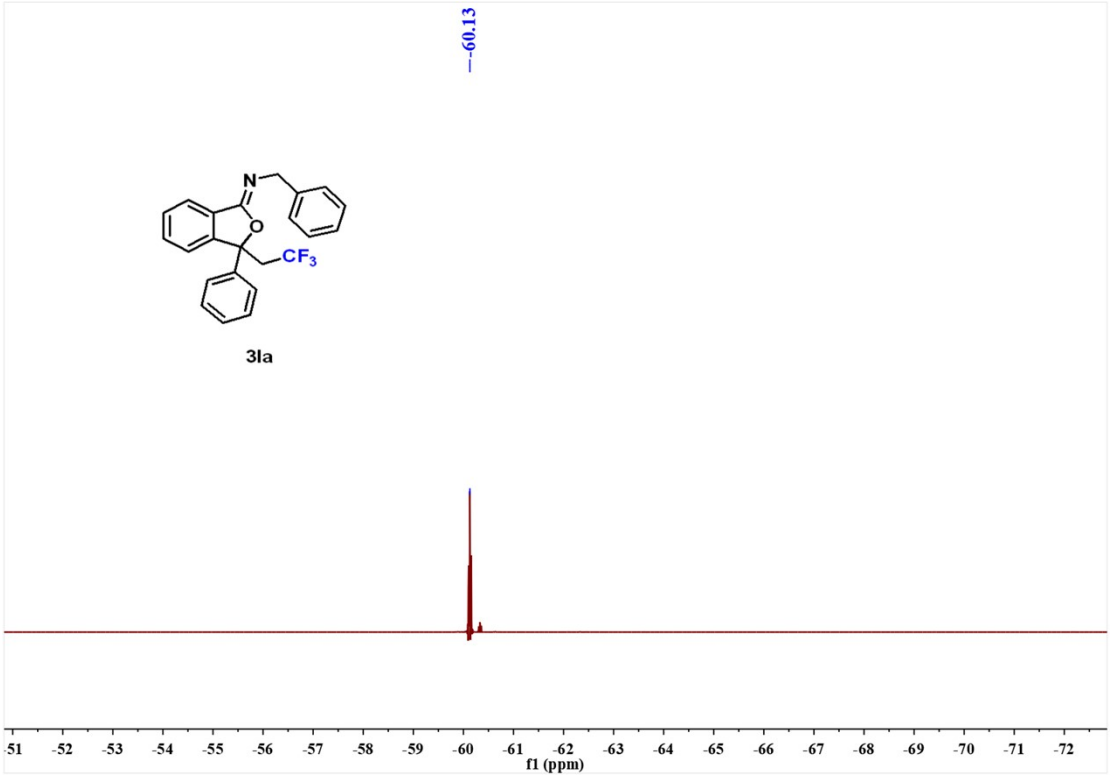
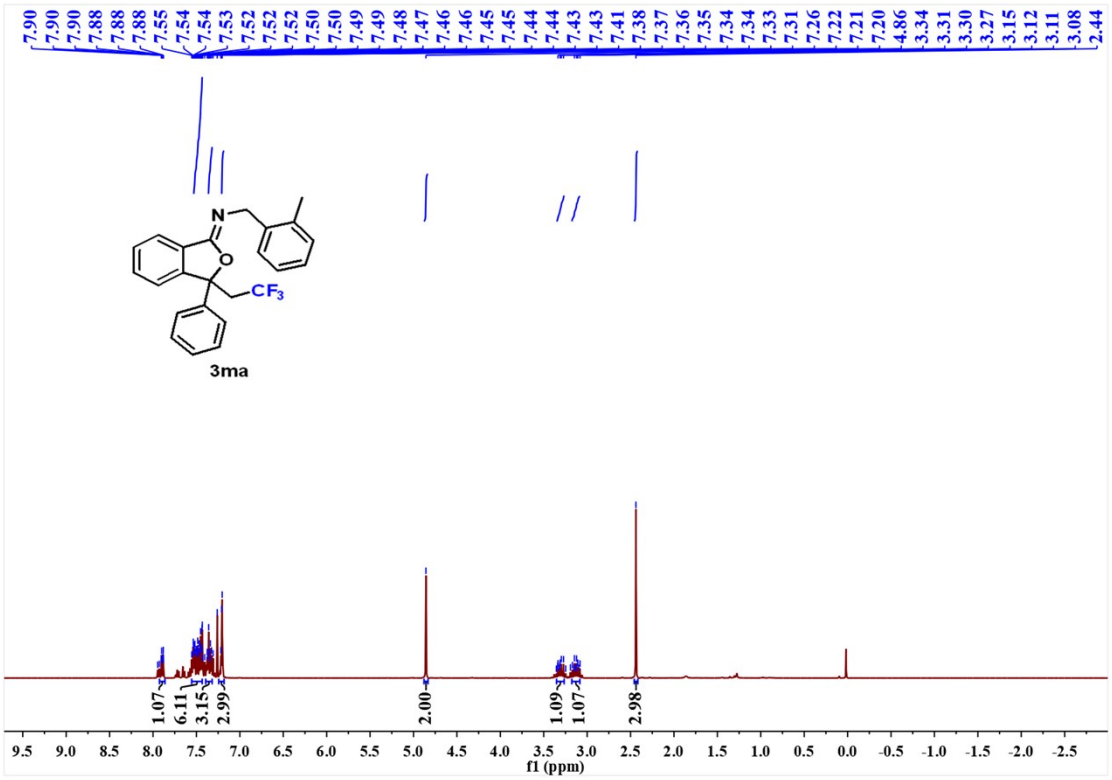
123.99
123.34
122.10
77.47
77.15
76.83
51.54
44.00
43.73
43.46
43.18
N
O
CF3
3la
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


-60.13
N
O
CF3
3la
-51 -52 -53 -54 -55 -56 -57 -58 -59 -60 -61 -62 -63 -64 -65 -66 -67 -68 -69 -70 -71 -72
f1 (ppm)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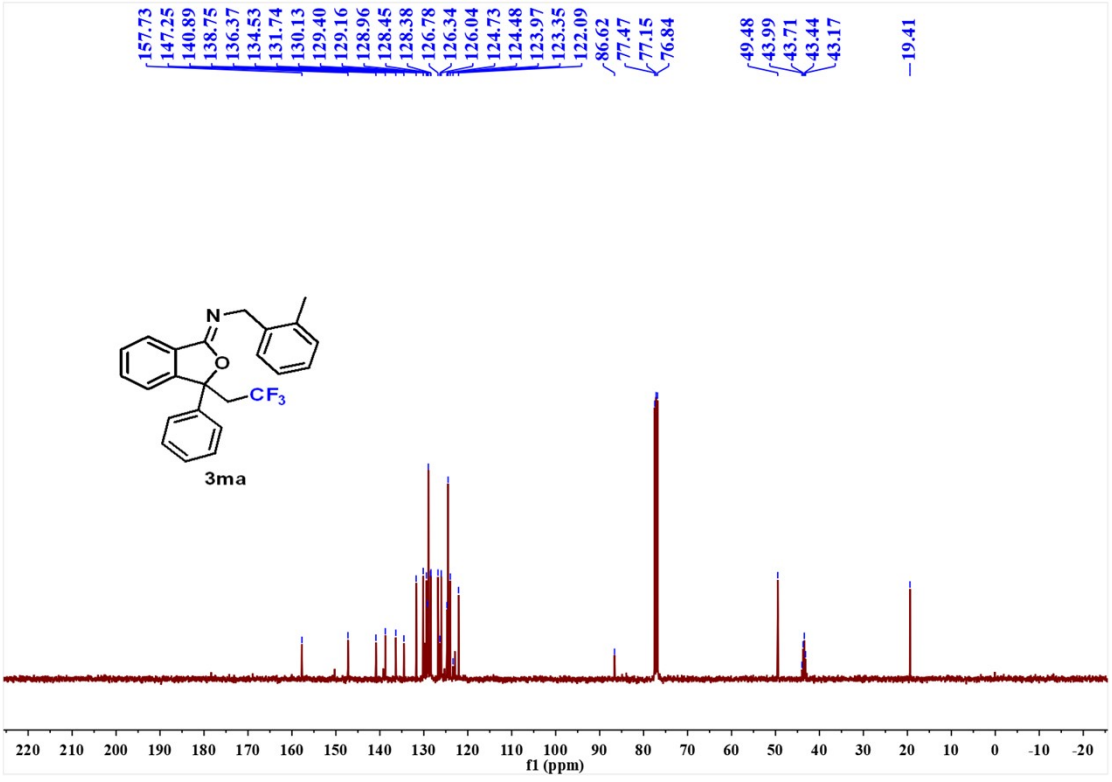
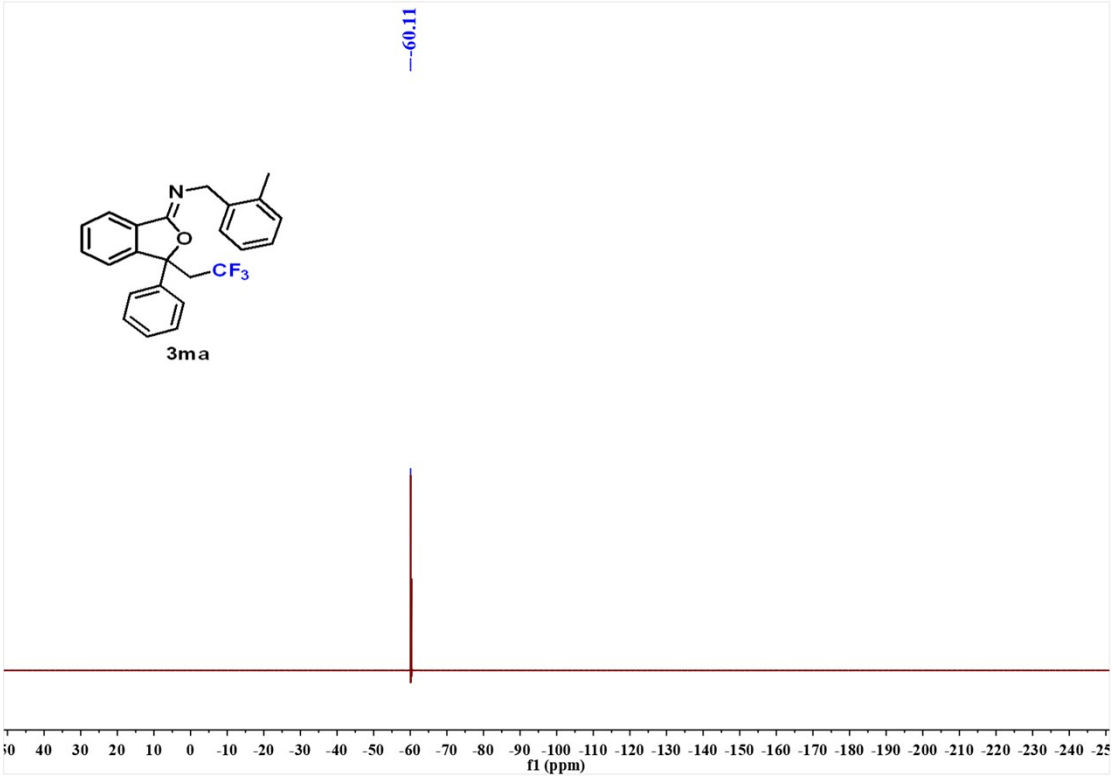
N
O
CF3
3ma
1.07 6.11 3.15 2.99 2.00 1.09 1.07 2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5
f1 (ppm)


157.73 147.25 140.89 138.75 136.37 134.53 131.74 130.13 129.40 129.16 128.96 128.45 128.38 126.78 126.34 126.04 124.73 124.48 123.97 123.35 122.09 86.62 77.47 77.15 76.84 49.48 43.99 43.71 43.44 43.17 19.41
N
O
CF3
3ma
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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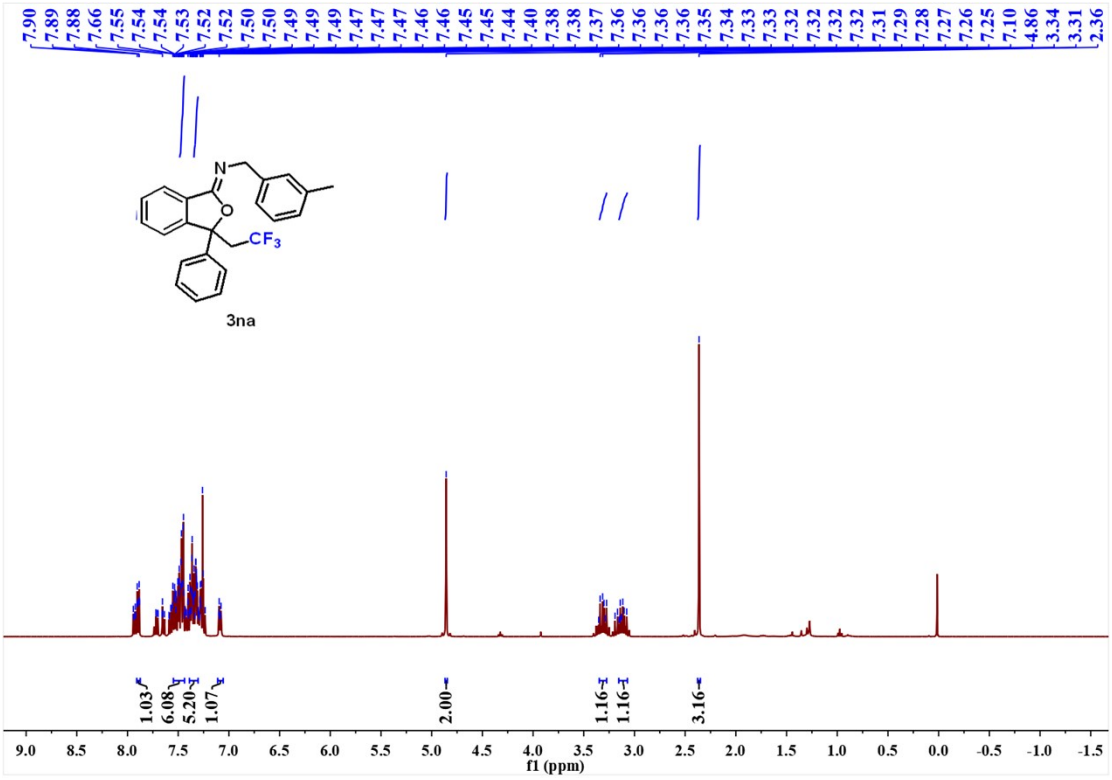
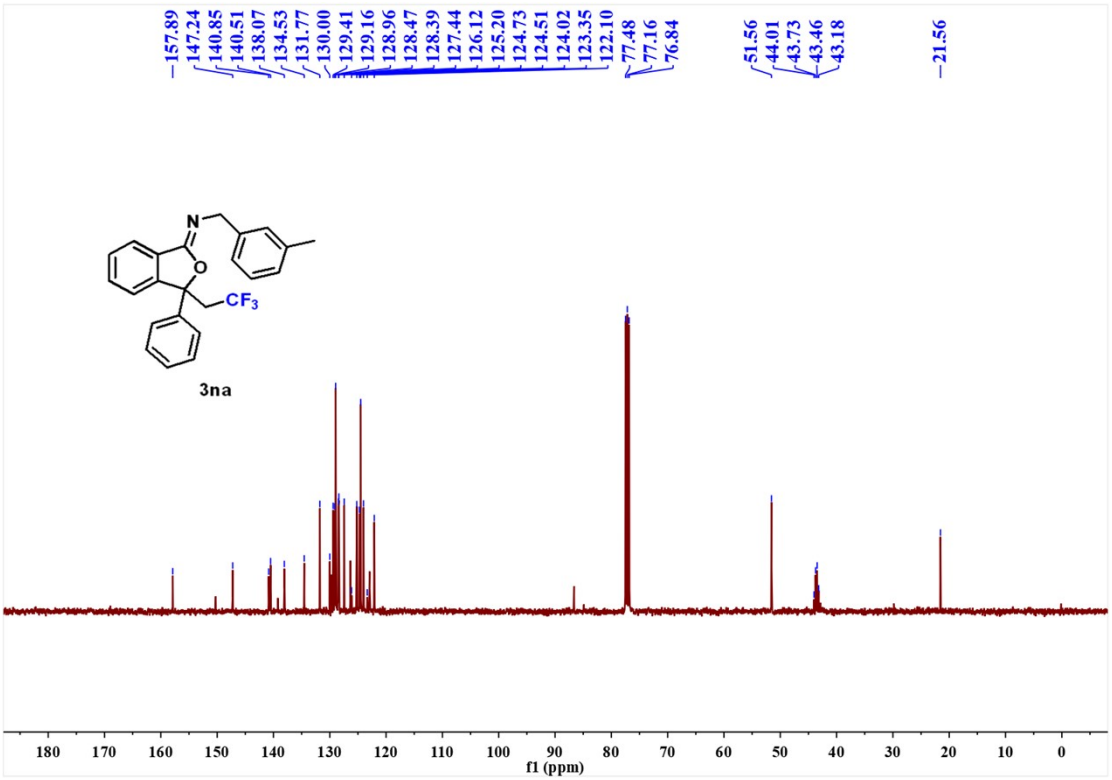
O
CF3
3ma
f1 (ppm)


7.90 7.89 7.88 7.66 7.55 7.54 7.54 7.53 7.52 7.52 7.50 7.50 7.49 7.49 7.49 7.47 7.47 7.47 7.46 7.46 7.45 7.45 7.44 7.40 7.38 7.38 7.37 7.36 7.36 7.36 7.36 7.35 7.34 7.33 7.33 7.32 7.32 7.32 7.31 7.29 7.28 7.27 7.26 7.25 7.10 4.86 3.34 3.31 2.36
N
O
CF3
3na
1.03 6.08 5.20 1.07 2.00 1.16 1.16 3.16
f1 (ppm)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138.07
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131.77
130.00
129.41
129.16
128.96
128.47
128.39
127.44
126.12
125.20
124.73
124.51
124.02
123.35
122.10
77.48
77.16
76.84
51.56
44.01
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21.56
N
O
CF3
3na
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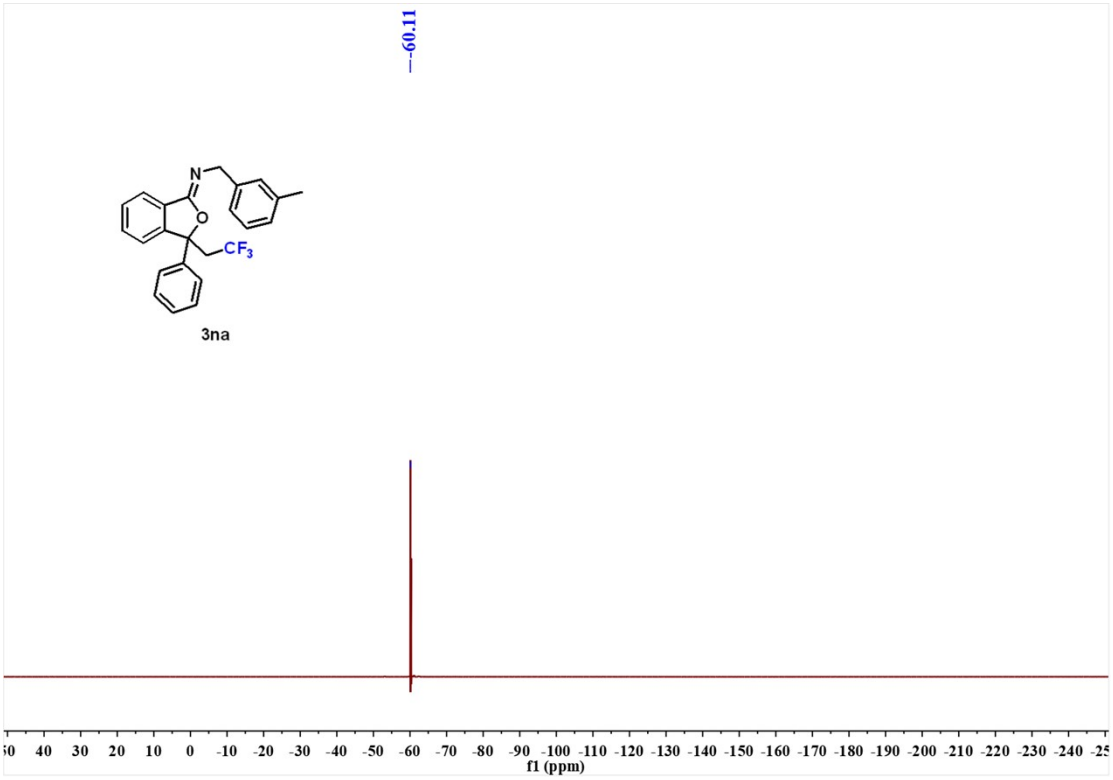
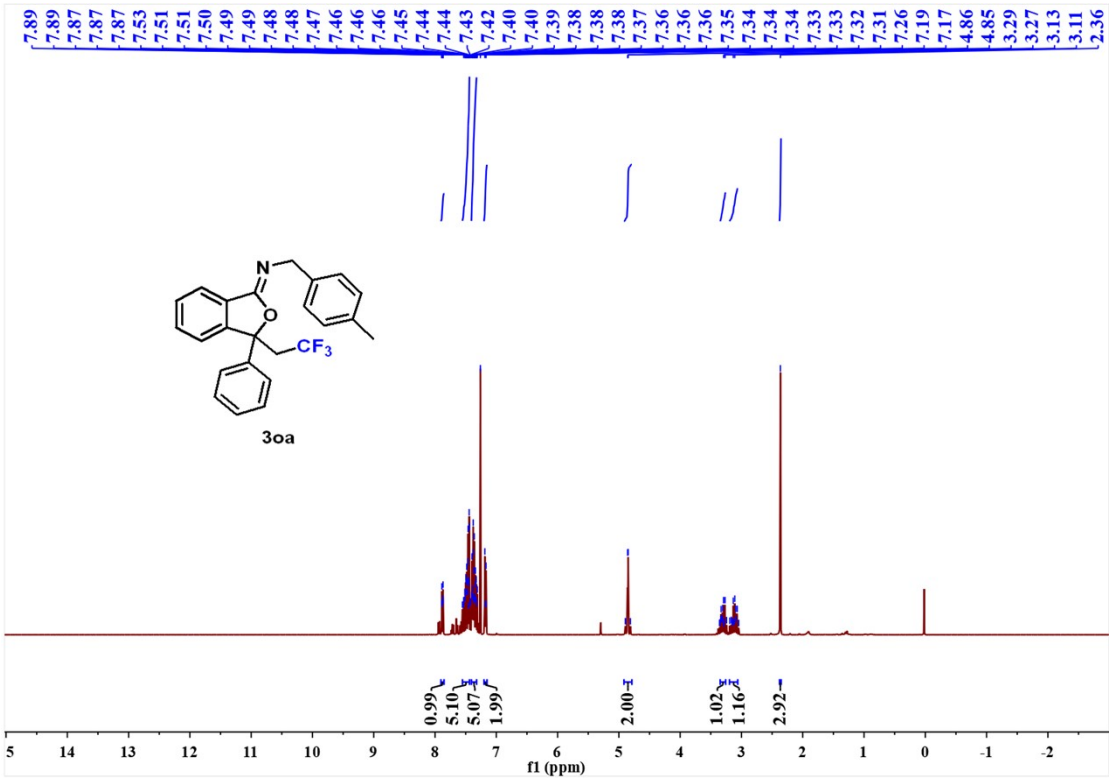
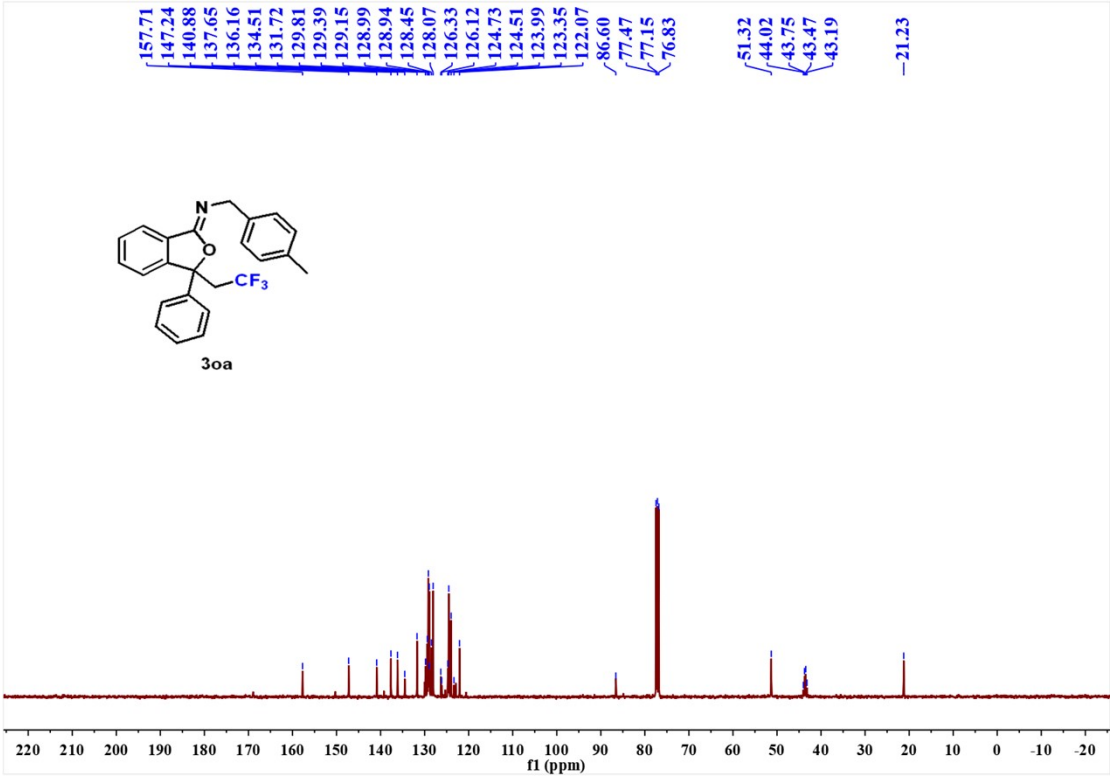
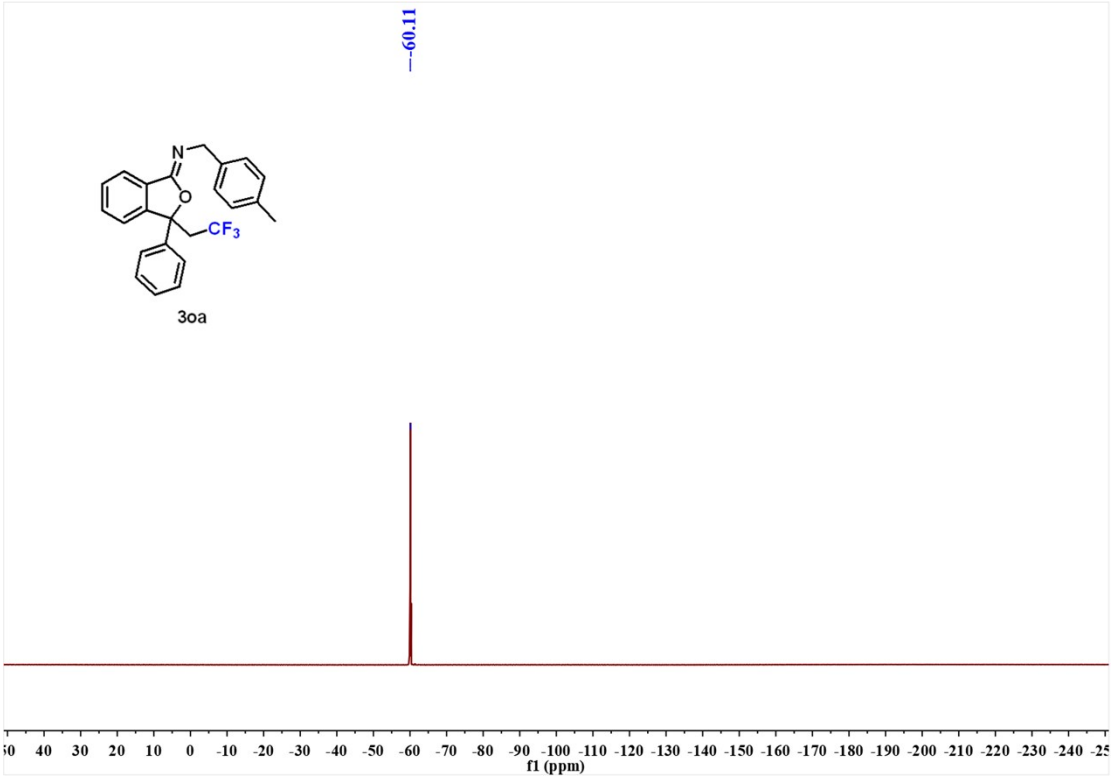
f1 (ppm)


-60.11
N
O
CF3
3na
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)


7.89 7.89 7.87 7.87 7.87 7.53 7.51 7.51 7.50 7.49 7.49 7.48 7.48 7.47 7.46 7.46 7.46 7.45 7.44 7.44 7.43 7.42 7.40 7.40 7.39 7.38 7.38 7.38 7.37 7.36 7.36 7.36 7.35 7.34 7.34 7.34 7.33 7.33 7.32 7.31 7.26 7.19 7.17 4.86 4.85 3.29 3.27 3.13 3.11 2.36
N
O
CF3
3oa
0.99 5.10 5.07 1.99 2.00 1.02 1.16 2.92
5 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)


157.71 147.24 140.88 137.65 136.16 134.51 131.72 129.81 129.39 129.15 128.99 128.94 128.45 128.07 126.33 126.12 124.73 124.51 123.99 123.35 122.07 86.60 77.47 77.15 76.83 51.32 44.02 43.75 43.47 43.19 21.23
N
O
CF3
3oa
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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N
O
CF3
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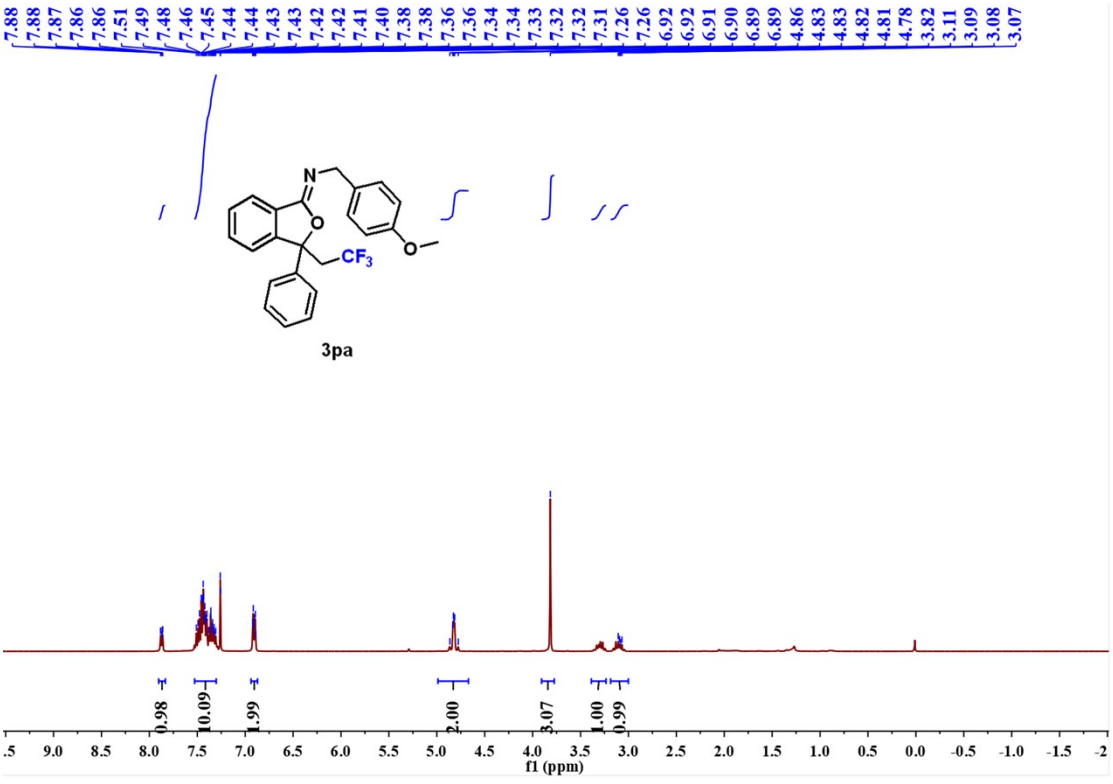
60 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -25
f1 (ppm)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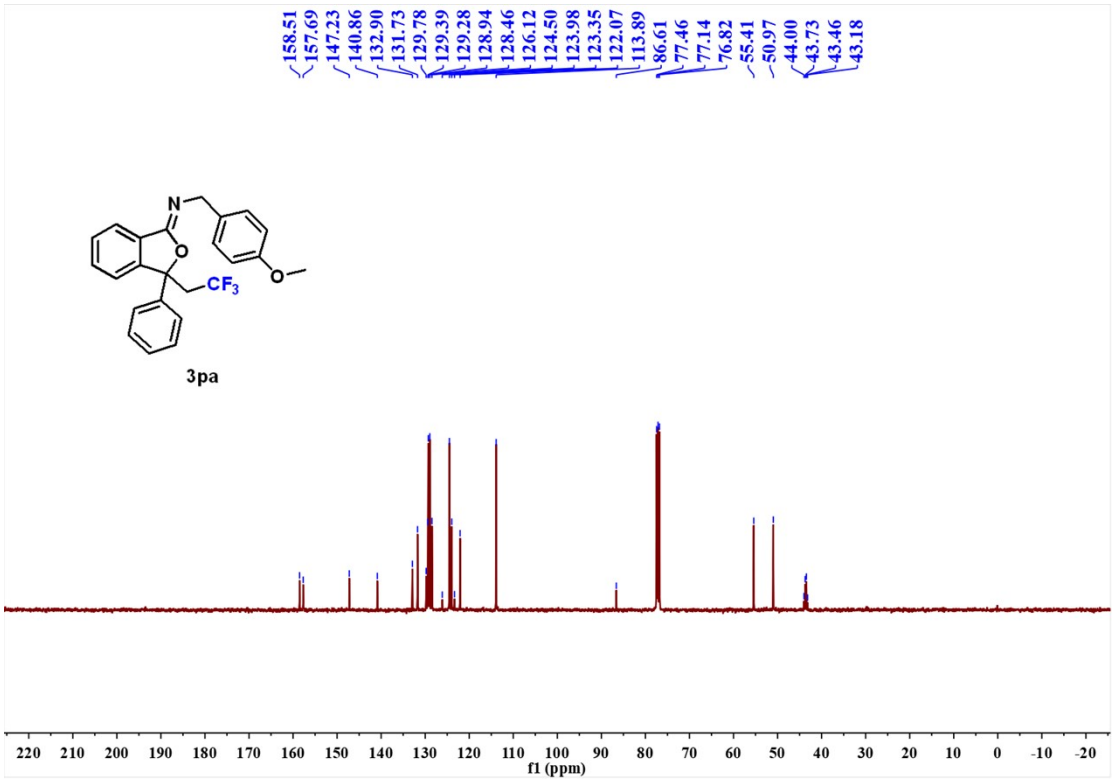
N
O
CF3
O
3pa
0.98 10.09 1.99 2.00 3.07 1.00 0.99
.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2
f1 (ppm)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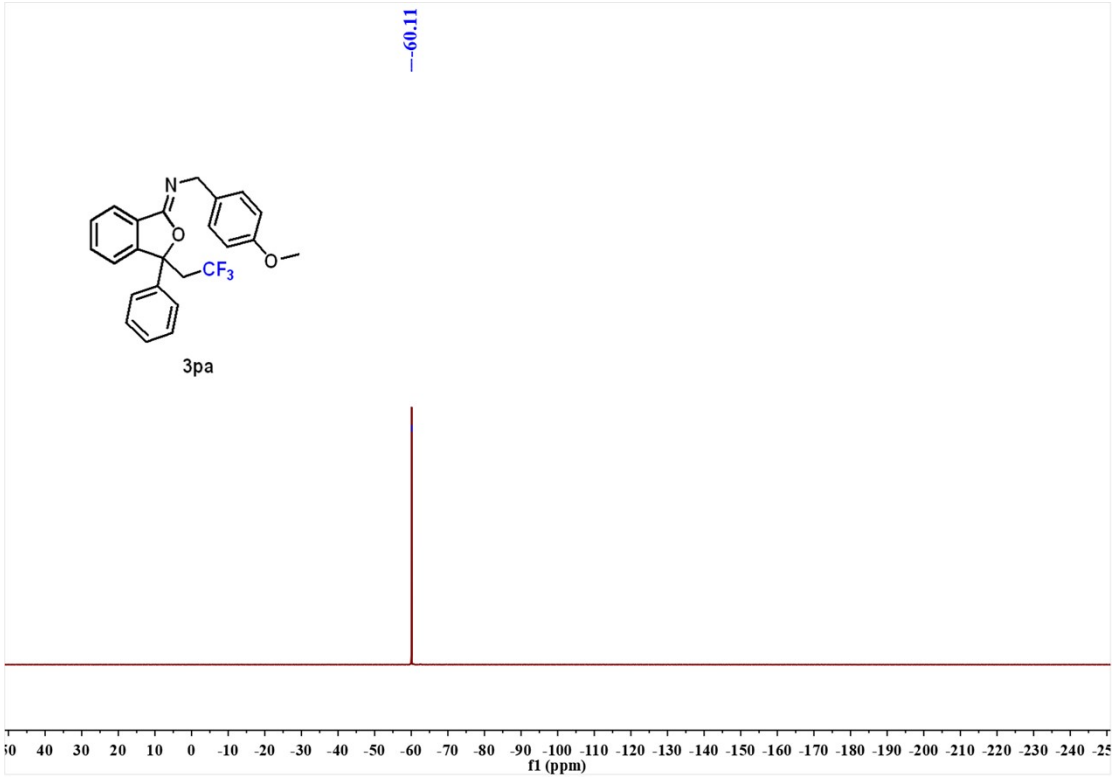
128.94
128.46
126.12
124.50
123.98
123.35
122.07
113.89
86.61
77.46
77.14
76.82
55.41
50.97
44.00
43.73
43.46
43.18
N
O
O
CF3
3pa
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


-60.11
N
O
O
CF3
3pa
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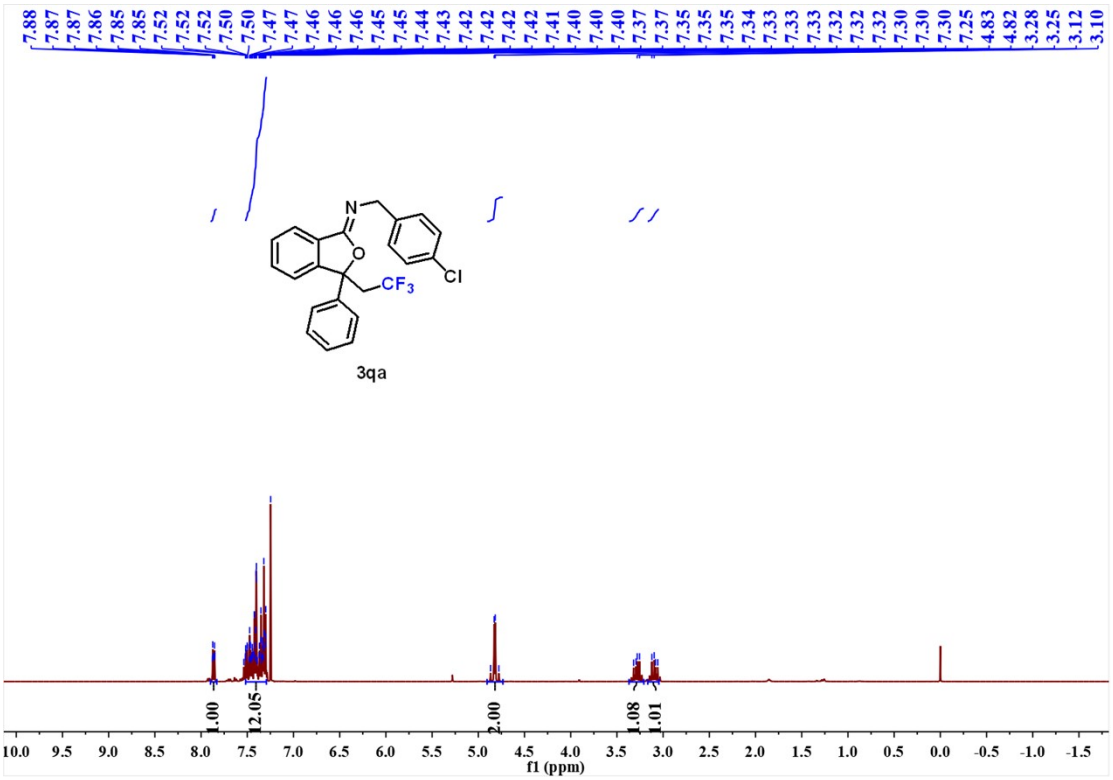
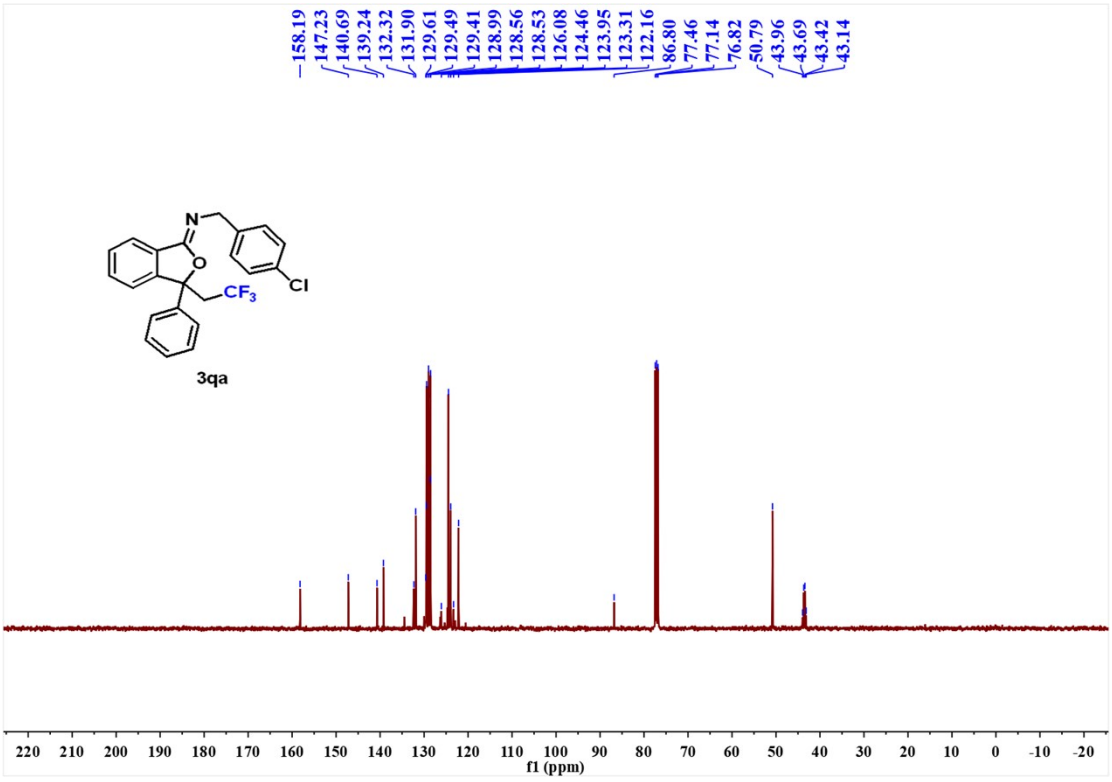
f1 (ppm)


7.88 7.87 7.87 7.86 7.85 7.85 7.52 7.52 7.52 7.50 7.50 7.47 7.47 7.46 7.46 7.46 7.45 7.45 7.44 7.43 7.42 7.42 7.42 7.42 7.41 7.40 7.40 7.40 7.37 7.37 7.35 7.35 7.35 7.34 7.33 7.33 7.33 7.32 7.32 7.32 7.30 7.30 7.30 7.25 4.83 4.82 3.28 3.25 3.12 3.10
N
O
CF3
Cl
3qa
1.00 12.05 2.00 1.08 1.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)


158.19 147.23 140.69 139.24 132.32 131.90 129.61 129.49 129.41 128.99 128.56 128.53 126.08 124.46 123.95 123.31 122.16 86.80 77.46 77.14 76.82 50.79 43.96 43.69 43.42 43.14
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CF3
Cl
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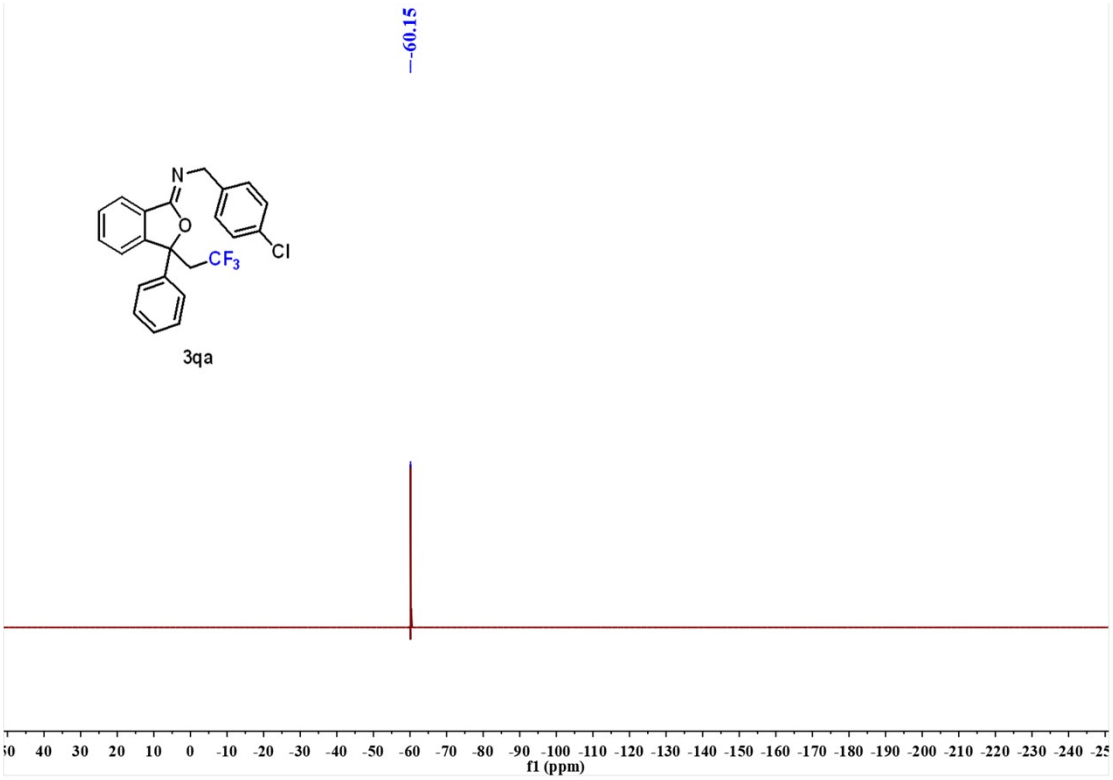
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)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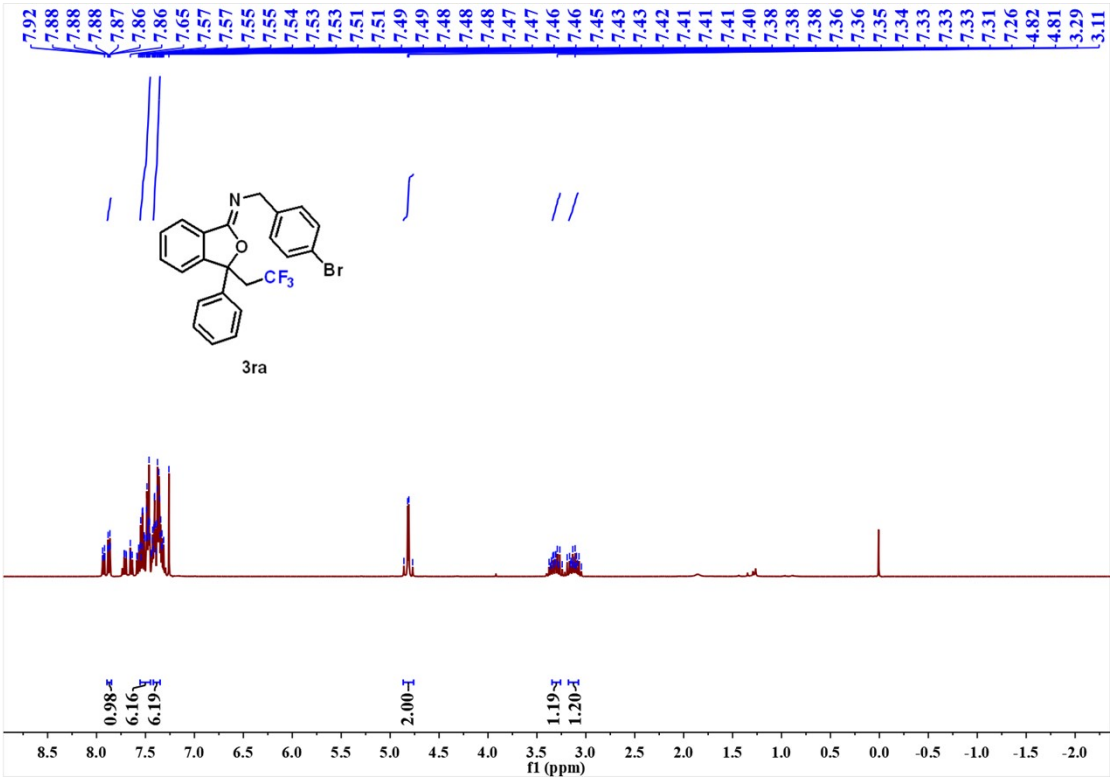
f1 (ppm)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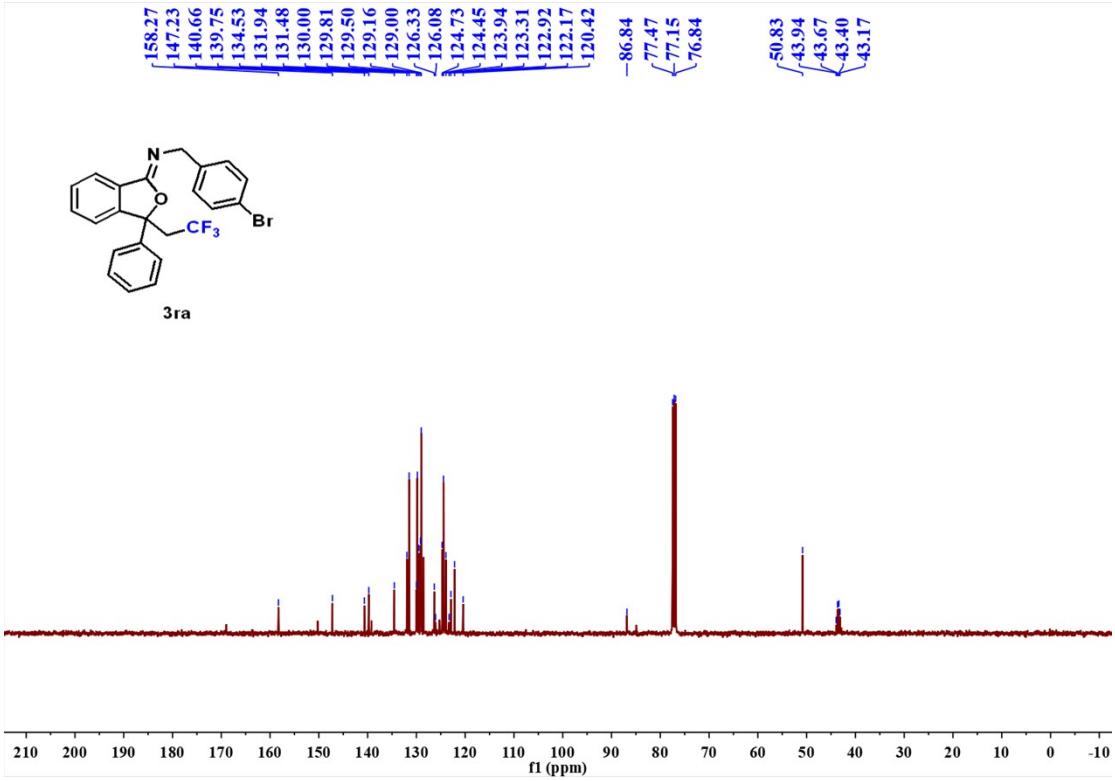
7.33
7.33
7.33
7.31
7.26
4.82
4.81
3.29
3.11
N
O
CF3
Br
3ra
0.98
6.16
6.19
2.00
1.19
1.20
f1 (ppm)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131.94
131.48
130.00
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129.50
129.16
129.00
126.33
126.08
124.73
124.45
123.94
123.31
122.92
122.17
120.42
86.84
77.47
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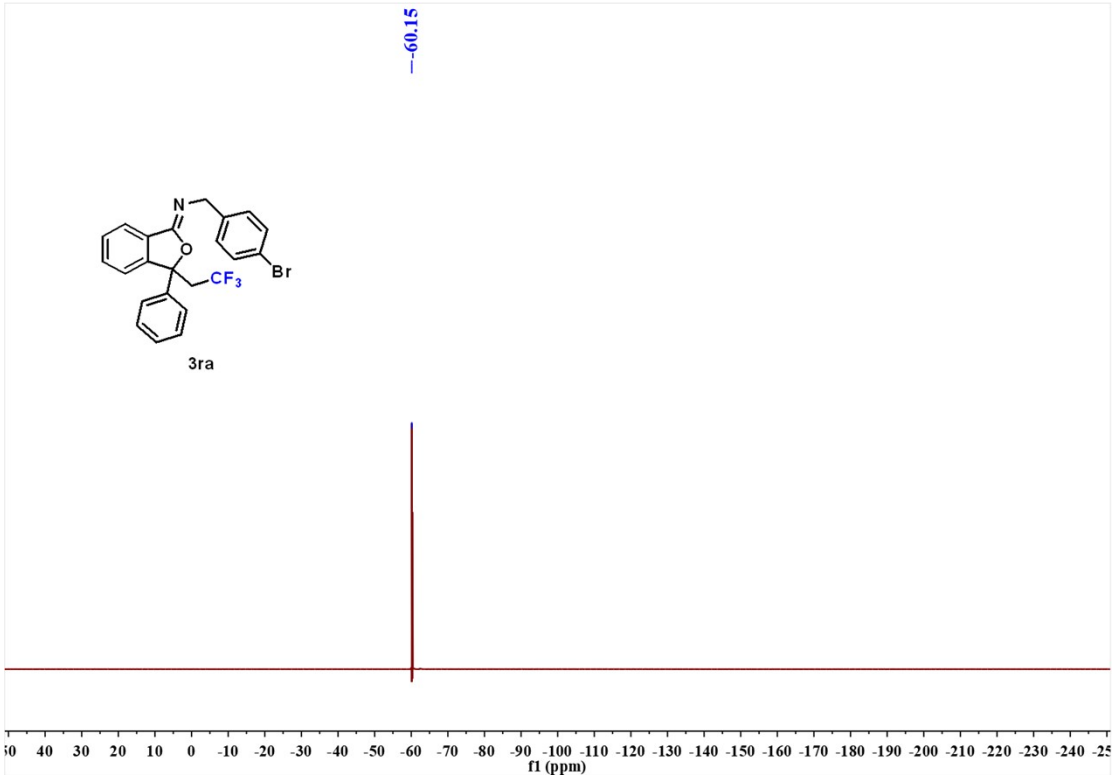
43.17
N
O
CF3
Br
3ra
f1 (ppm)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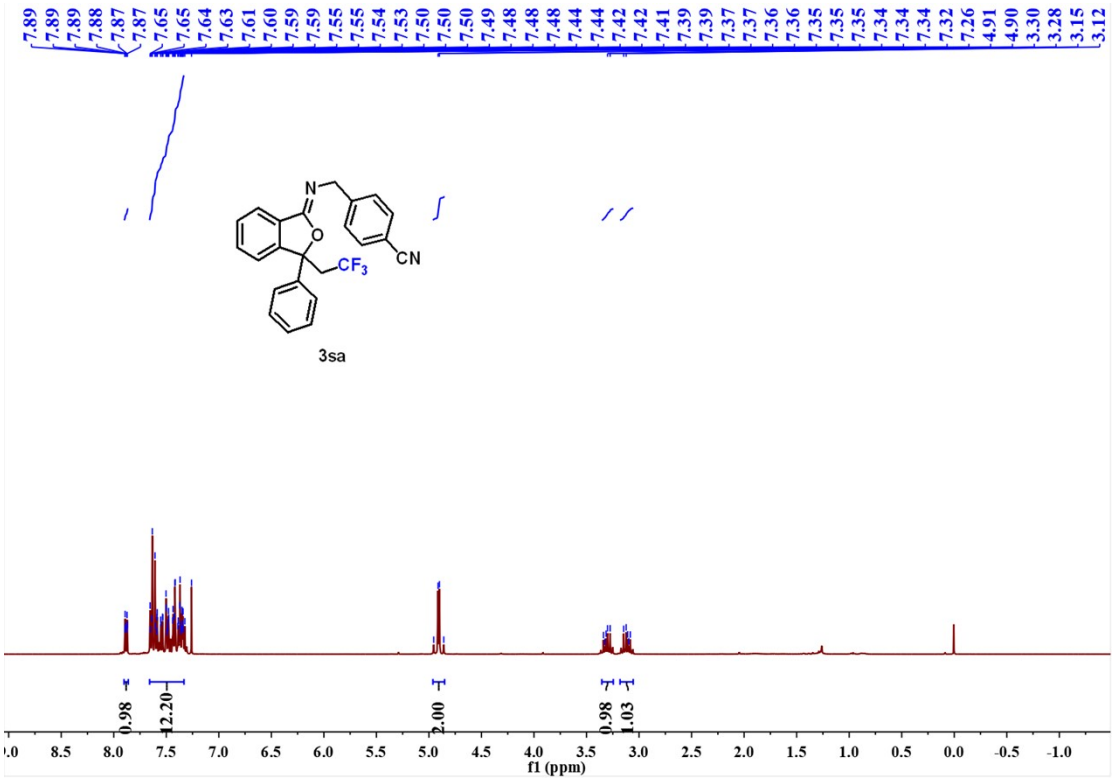
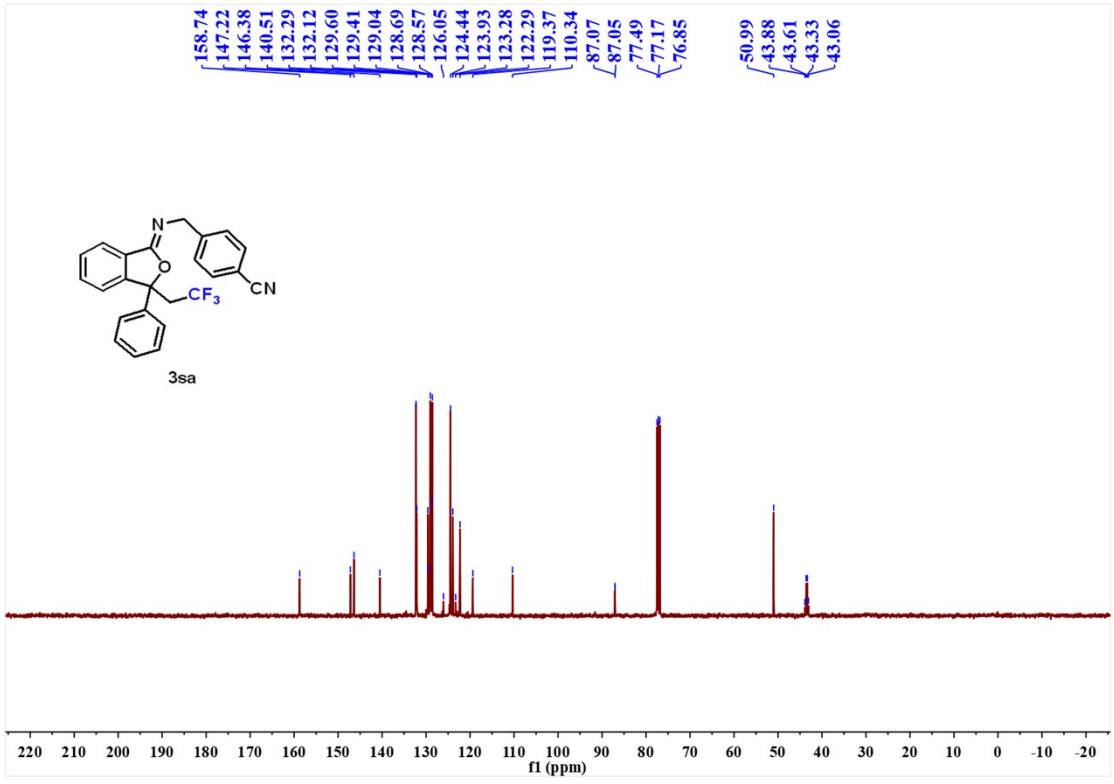
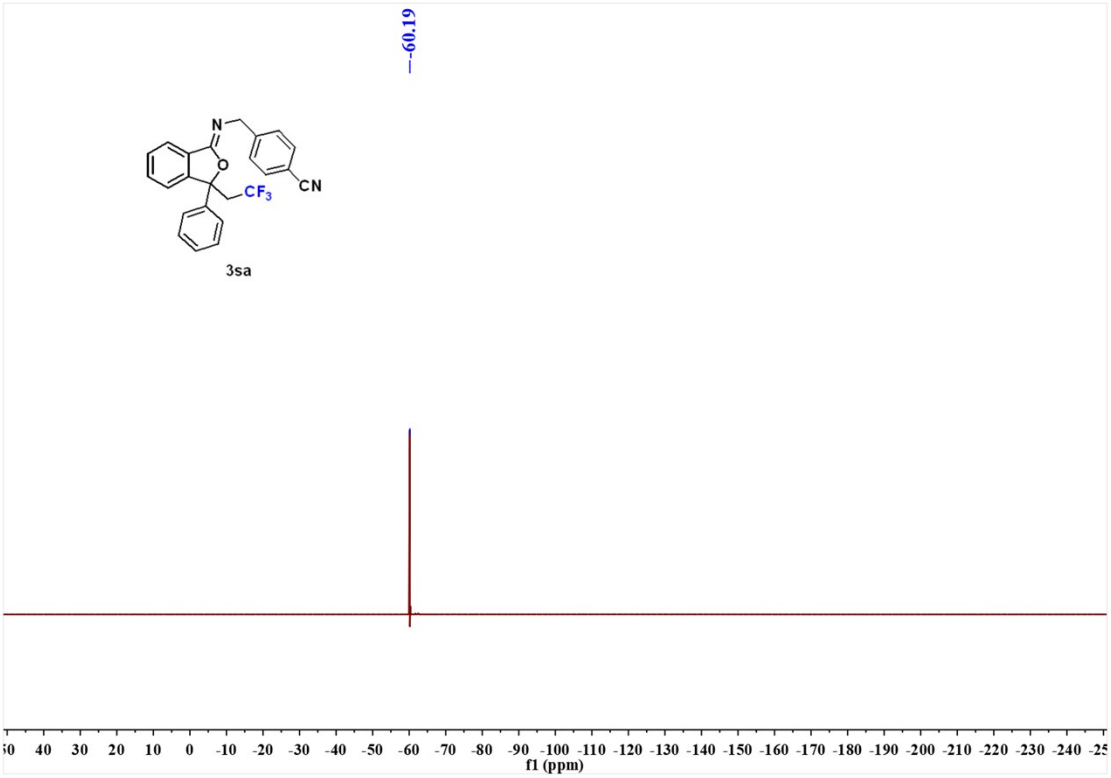
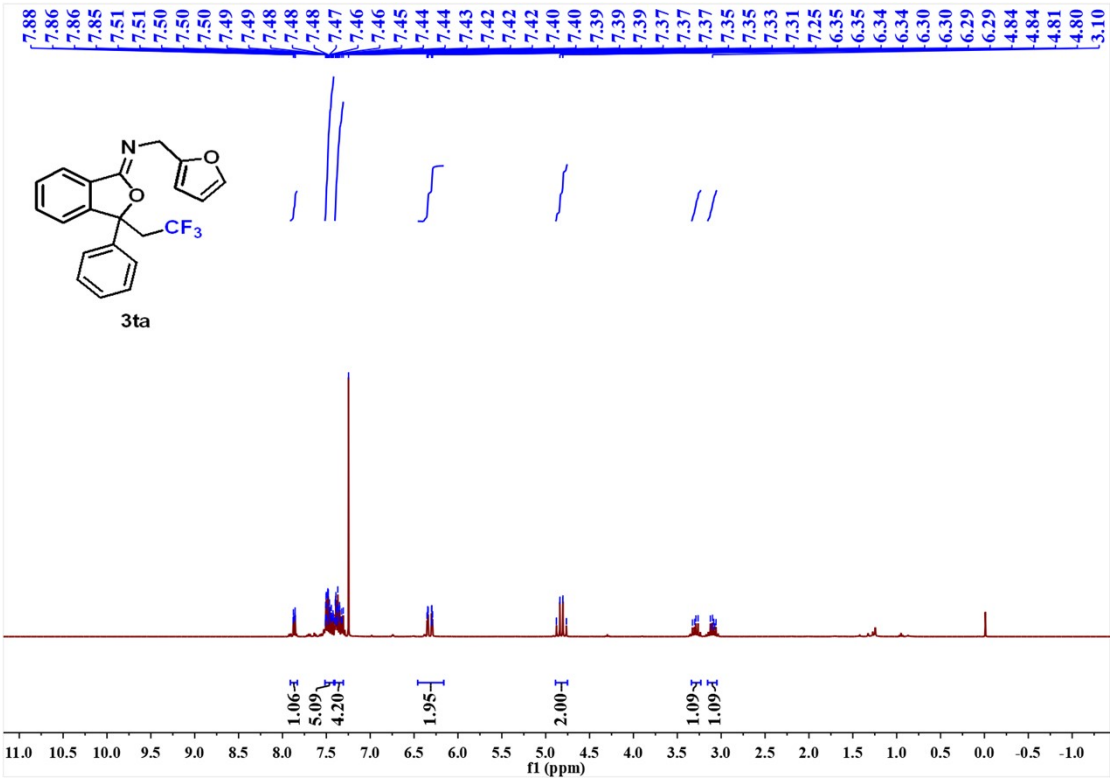
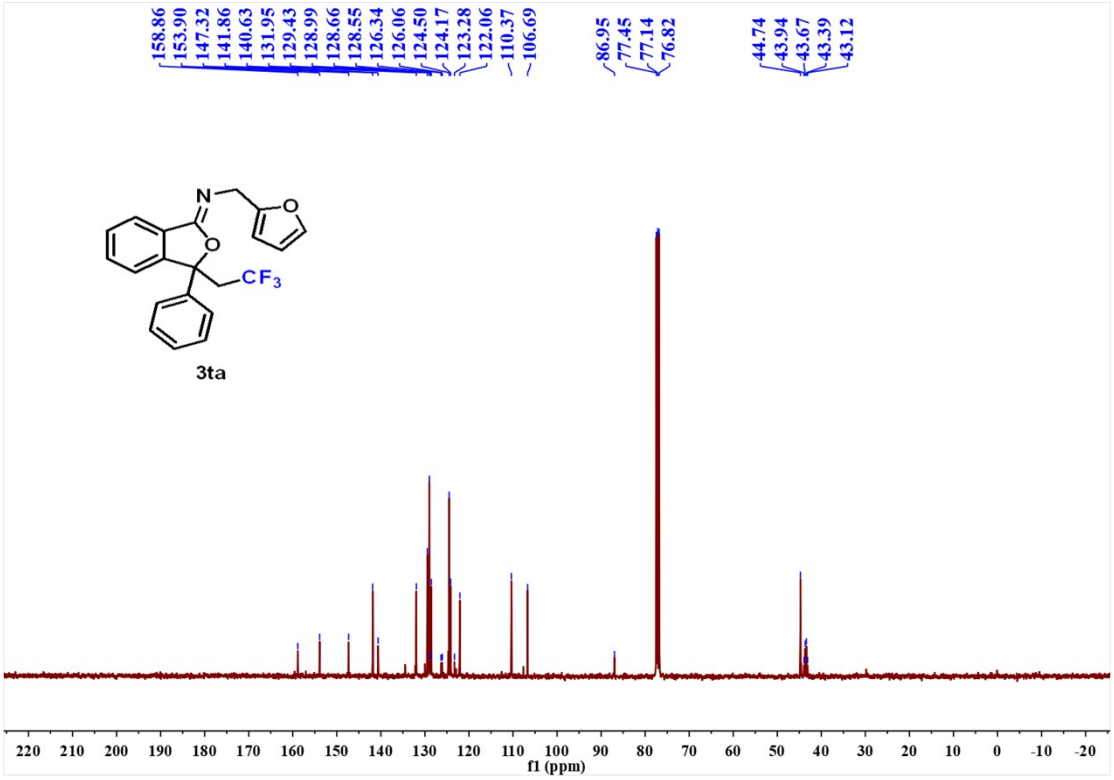
CF3
Br
3ra
f1 (ppm)

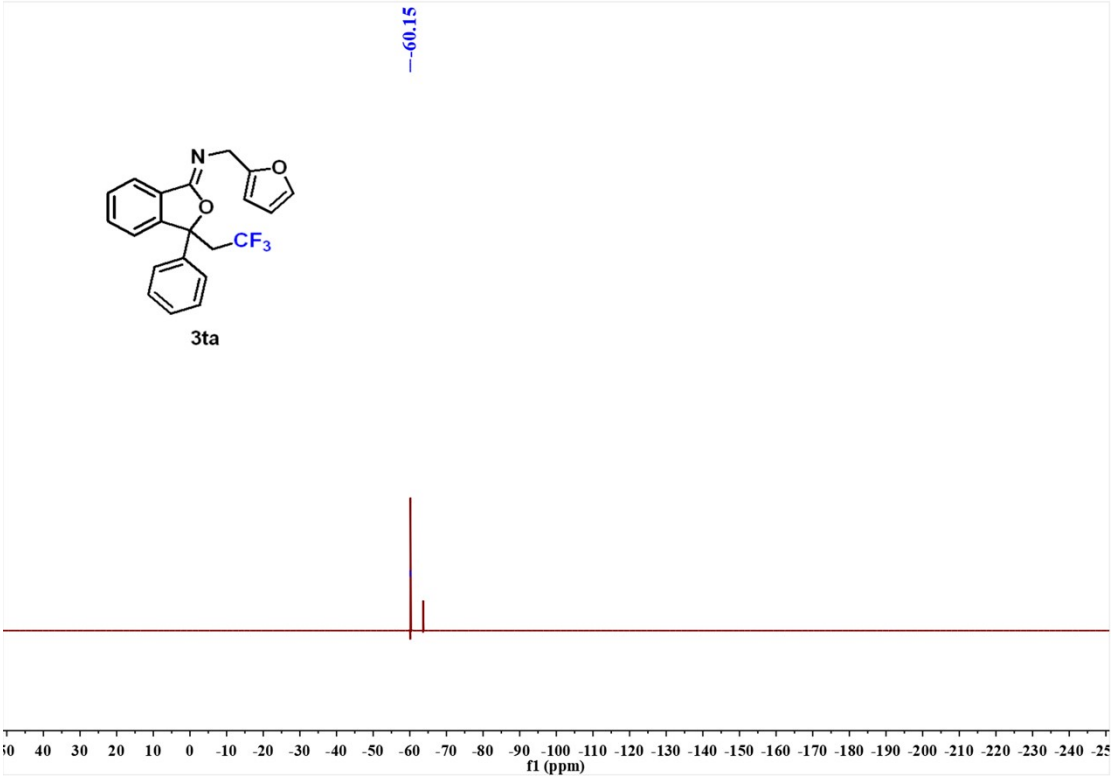

7.89 7.89 7.89 7.88 7.87 7.87 7.65 7.65 7.64 7.63 7.61 7.60 7.59 7.59 7.55 7.55 7.54 7.53 7.50 7.50 7.50 7.49 7.48 7.48 7.48 7.44 7.44 7.42 7.42 7.41 7.39 7.39 7.37 7.37 7.36 7.36 7.35 7.35 7.35 7.34 7.34 7.34 7.32 7.26 4.91 4.90 3.30 3.28 3.15 3.12
N
O
CF3
CN
3sa
0.98
12.20
2.00
0.98
1.03
f1 (ppm)

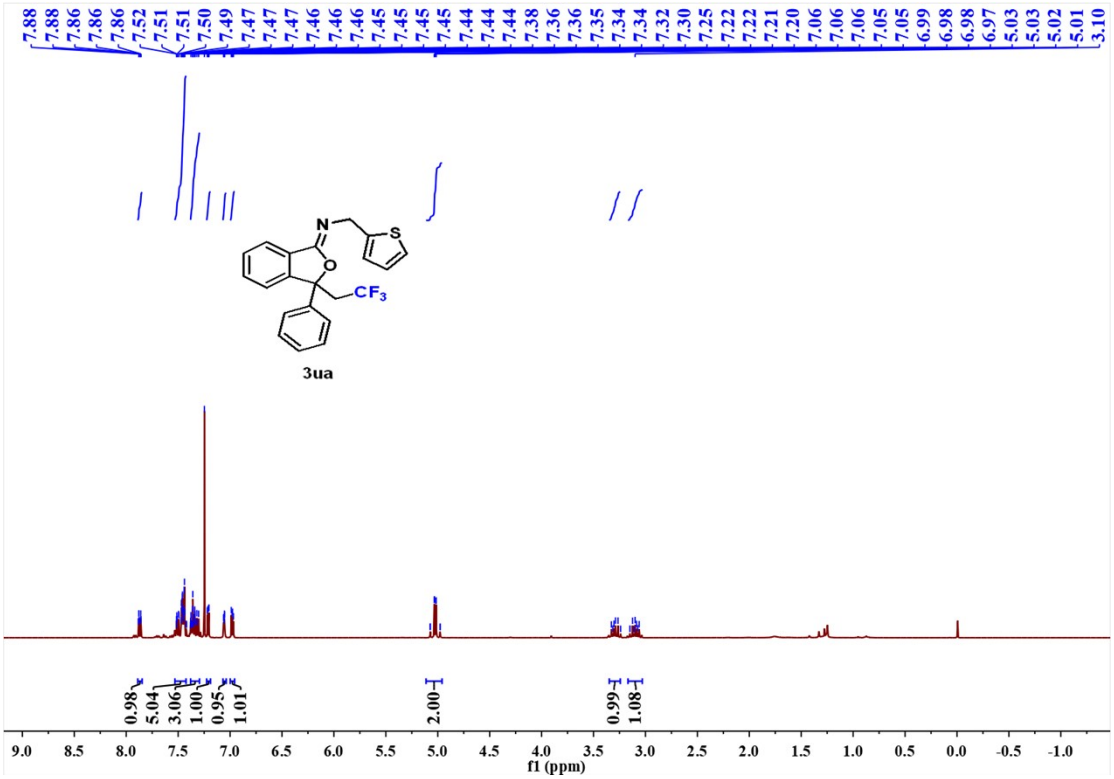

158.74 147.22 146.38 140.51 132.29 132.12 129.60 129.41 129.04 128.69 128.57 126.05 124.44 123.93 123.28 122.29 119.37 110.34 87.07 87.05 77.49 77.17 76.85 50.99 43.88 43.61 43.33 43.06
N
O
CF3
CN
3sa
f1 (ppm)


-60.19
N
O
CF3
CN
3sa
f1 (ppm)


7.88
7.86
7.86
7.85
7.51
7.51
7.50
7.50
7.50
7.49
7.49
7.48
7.48
7.48
7.47
7.46
7.46
7.45
7.44
7.44
7.43
7.42
7.42
7.42
7.40
7.40
7.39
7.39
7.39
7.37
7.37
7.37
7.35
7.35
7.33
7.31
7.25
6.35
6.35
6.34
6.34
6.30
6.30
6.29
6.29
4.84
4.84
4.81
4.80
3.10
N
O
O
CF3
3ta
1.06
5.09
4.20
1.95
2.00
1.09
1.09
f1 (ppm)


158.86
153.90
147.32
141.86
140.63
131.95
129.43
128.99
128.66
128.55
126.34
126.06
124.50
124.17
123.28
122.06
110.37
106.69
86.95
77.45
77.14
76.82
44.74
43.94
43.67
43.39
43.12
N
O
O
CF3
3ta
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


-60.15
N
O
O
CF3
3ta
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)


7.88
7.88
7.86
7.86
7.86
7.52
7.51
7.51
7.50
7.49
7.47
7.47
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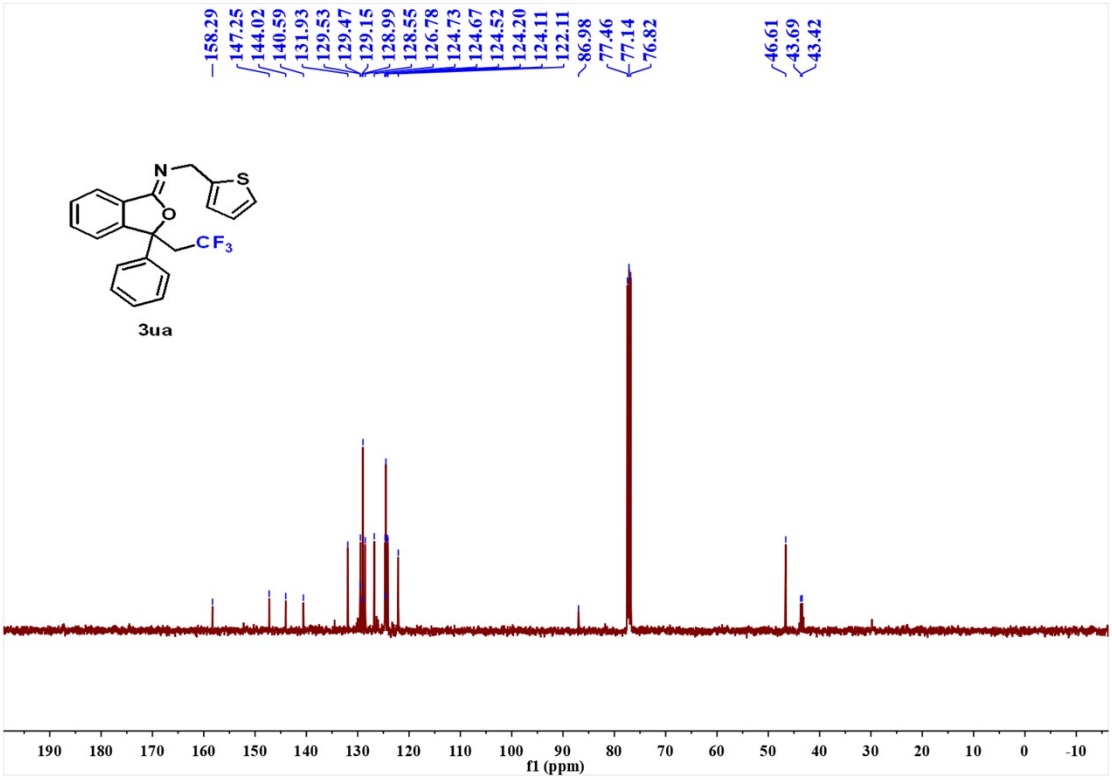
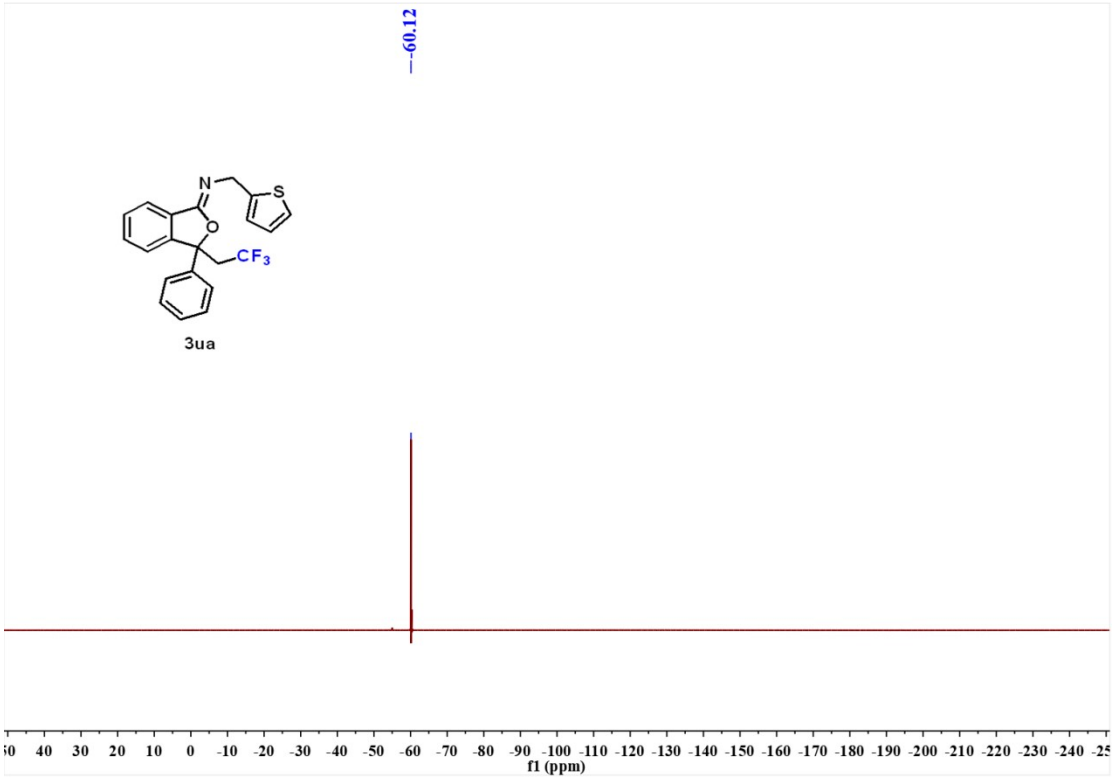
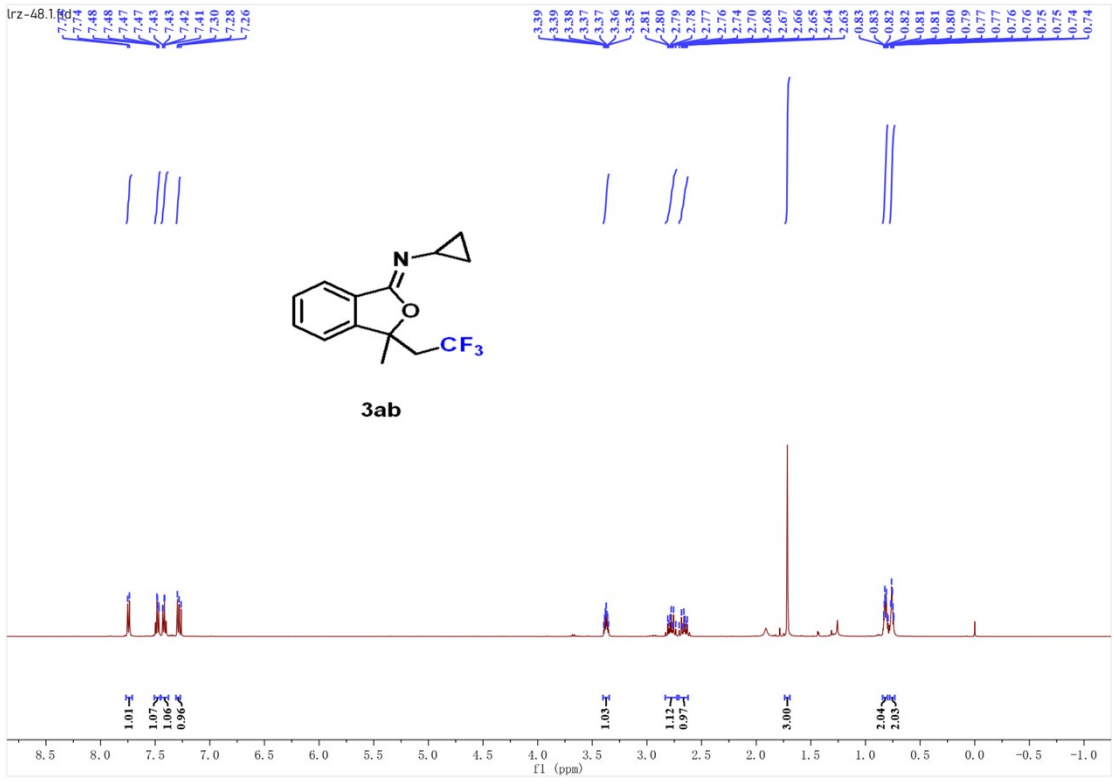
7.46
7.46
7.46
7.45
7.45
7.45
7.45
7.44
7.44
7.44
7.38
7.36
7.36
7.35
7.34
7.34
7.32
7.30
7.25
7.22
7.22
7.21
7.20
7.06
7.06
7.06
7.05
7.05
6.99
6.98
6.98
6.97
5.03
5.03
5.02
5.01
3.10
N
S
O
CF3
3ua
0.98
5.04
3.06
1.00
0.95
1.01
2.00
0.99
1.08
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


158.29
147.25
144.02
140.59
131.93
129.53
129.47
129.15
128.99
128.55
126.78
124.73
124.67
124.52
124.20
124.11
122.11
86.98
77.46
77.14
76.82
46.61
43.69
43.42
N
S
O
CF3
3ua
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

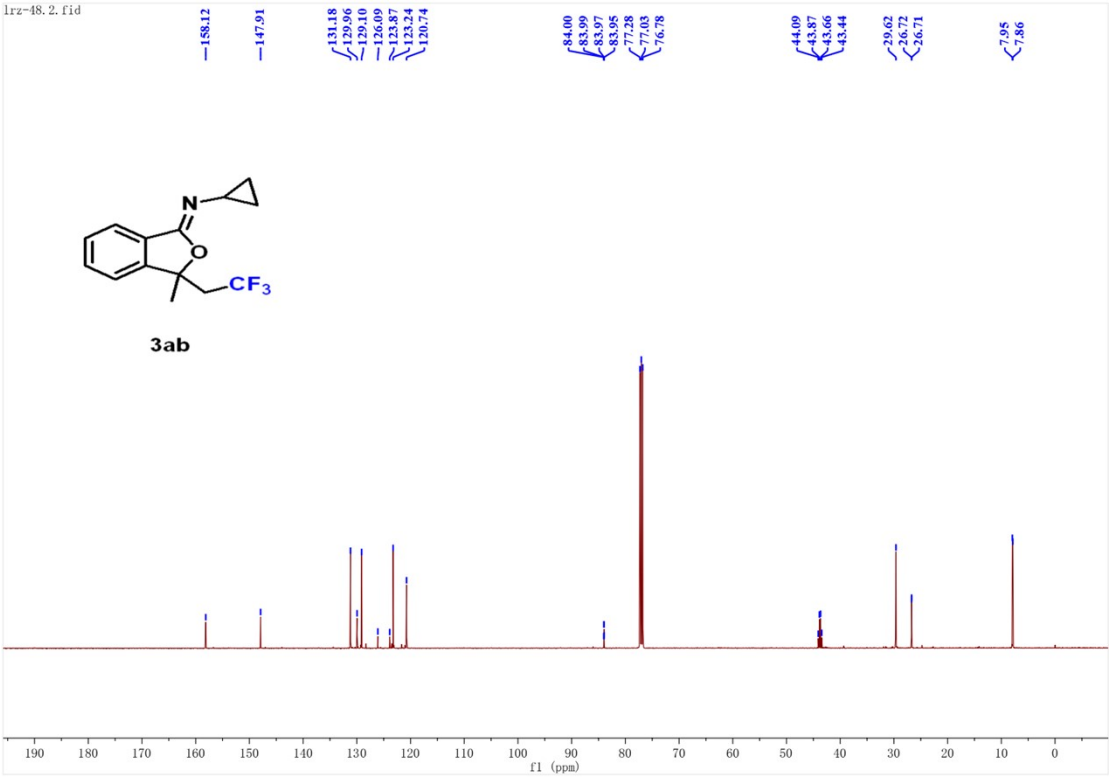

-60.12
N
S
O
CF3
f1 (ppm)

3ua

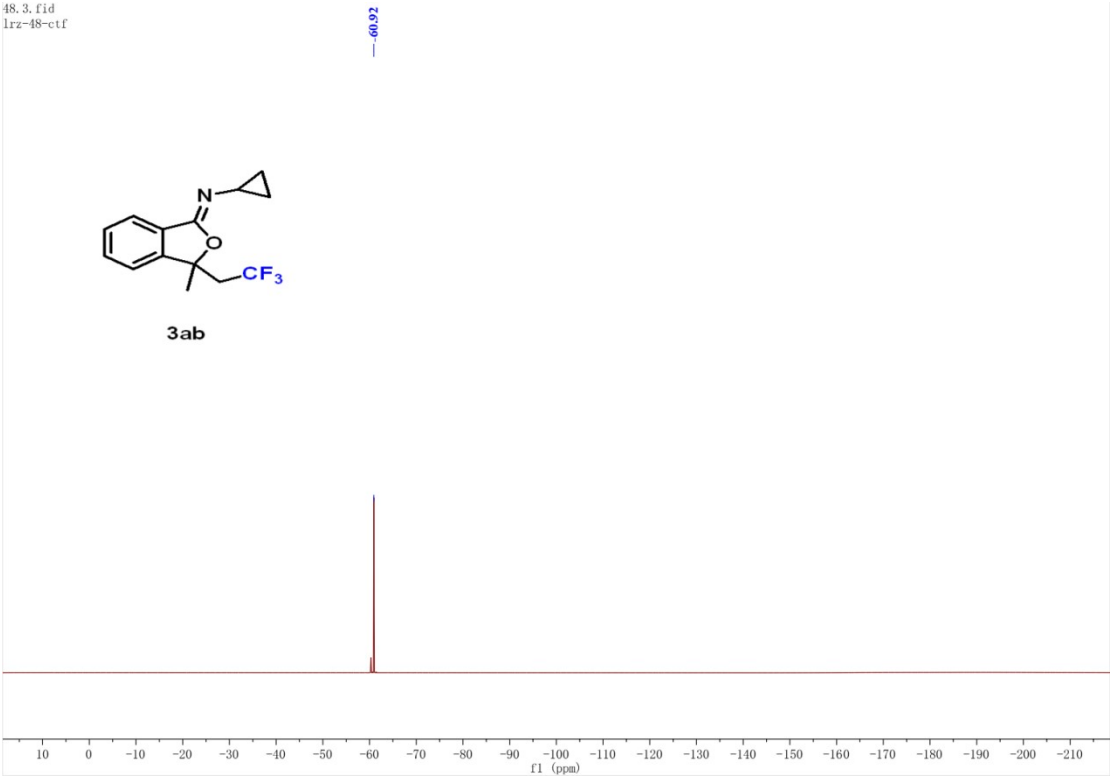

lrz-48.1.fid
N
O
CF3
1.01
1.07
1.06
0.96
1.03
1.12
0.97
3.00
2.04
2.03
f1 (ppm)

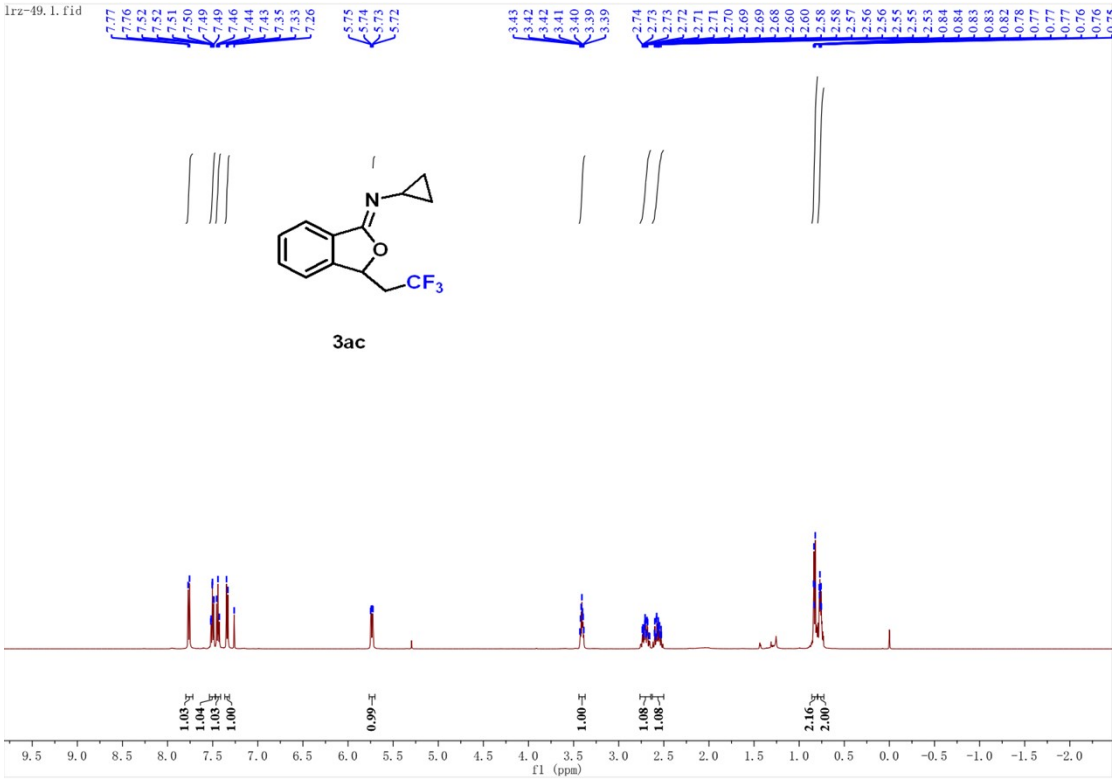
3ab

lrz-48.2.fid

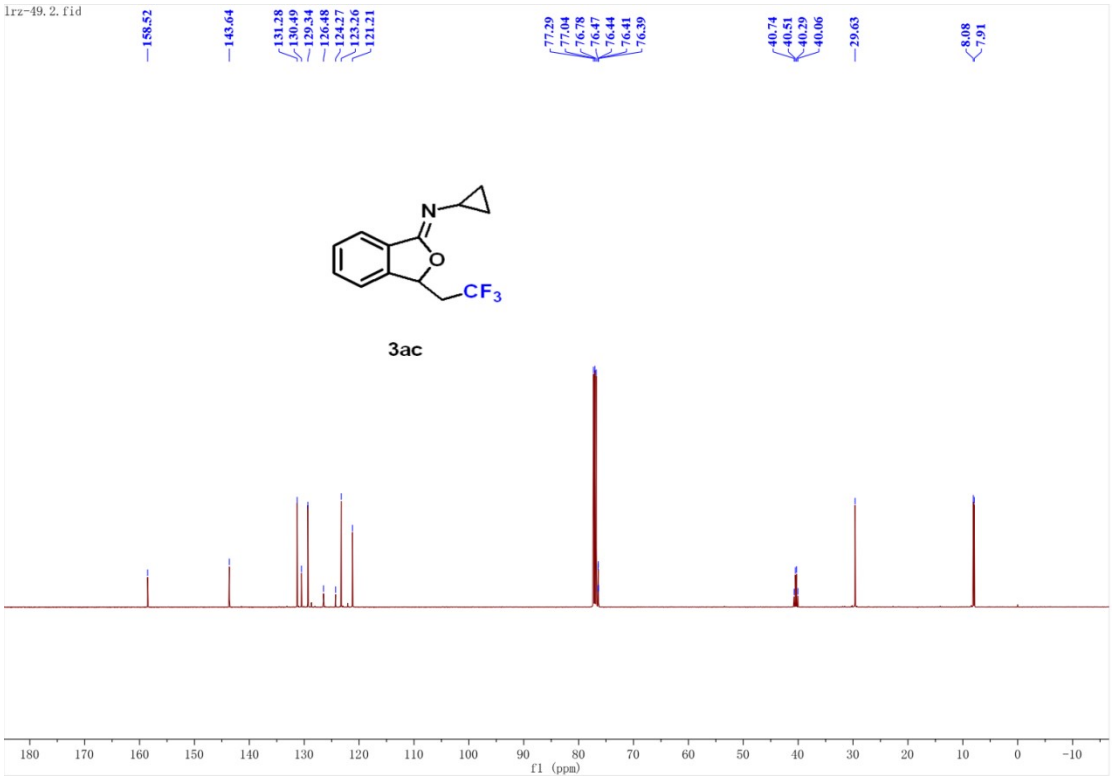


48.3.fid
lrz-48-ctf



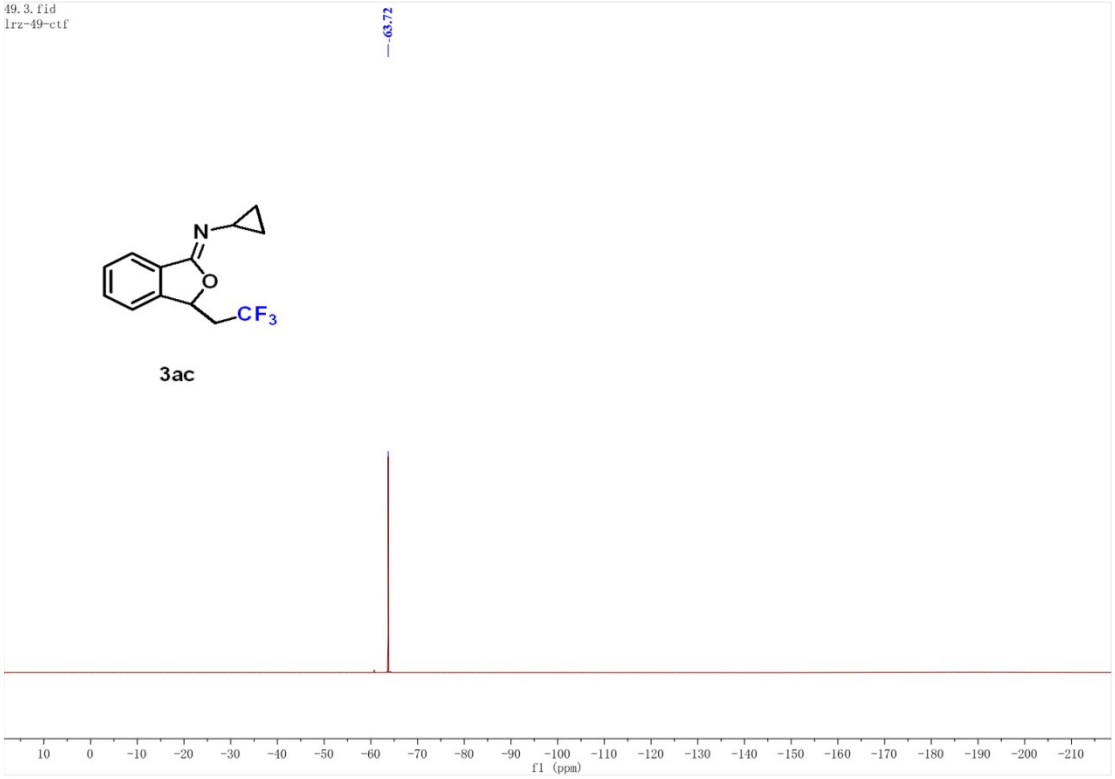

lrz-49.1.fid
7.77
7.76
7.52
7.52
7.51
7.50
7.49
7.49
7.46
7.44
7.43
7.35
7.33
7.26
5.75
5.74
5.73
5.72
3.43
3.42
3.42
3.41
3.40
3.39
3.39
2.74
2.73
2.73
2.72
2.71
2.71
2.70
2.69
2.69
2.68
2.60
2.60
2.58
2.58
2.57
2.56
2.56
2.55
2.55
2.53
0.84
0.84
0.83
0.83
0.82
0.78
0.77
0.77
0.77
0.76
0.76
N
O
CF3
1.03
1.04
1.03
1.00
0.99
1.00
1.08
1.08
2.16
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 -1.5 -2.0
f1 (ppm)

3ac

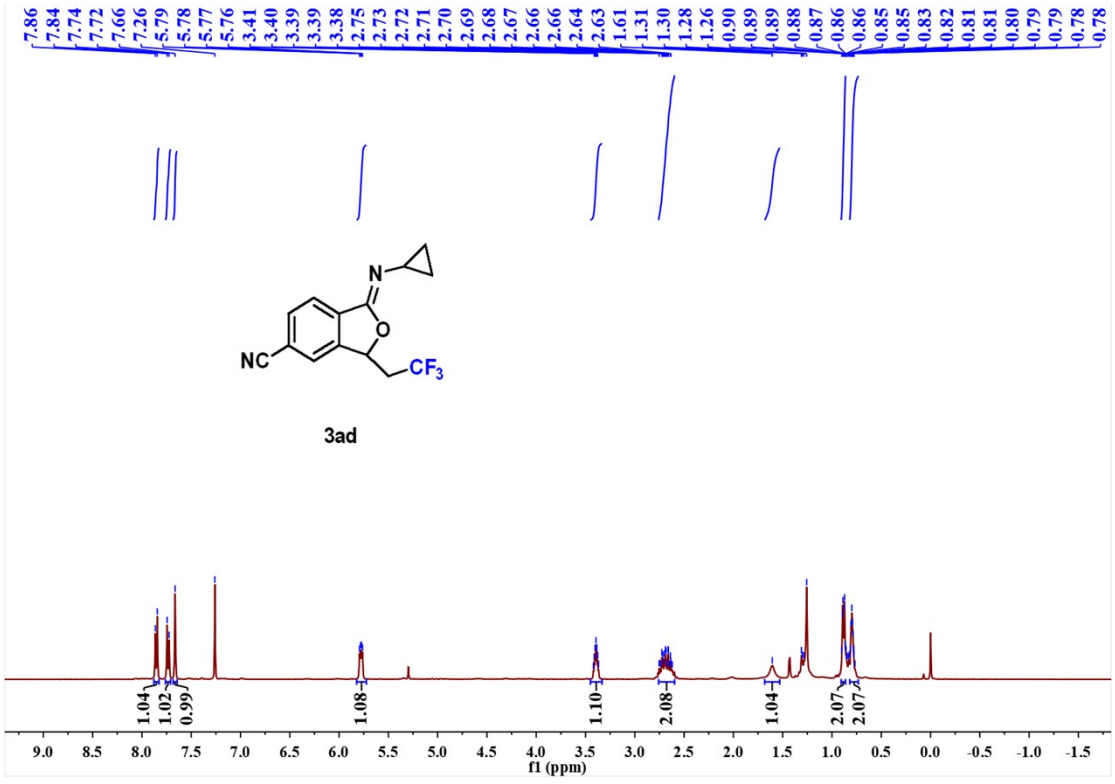

lrz-49.2.fid
158.52
143.64
131.28
130.49
129.34
126.48
124.27
123.26
121.21
77.29
77.04
76.78
76.47
76.44
76.41
76.39
40.74
40.51
40.29
40.06
29.63
8.08
7.91
N
O
CF3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ac

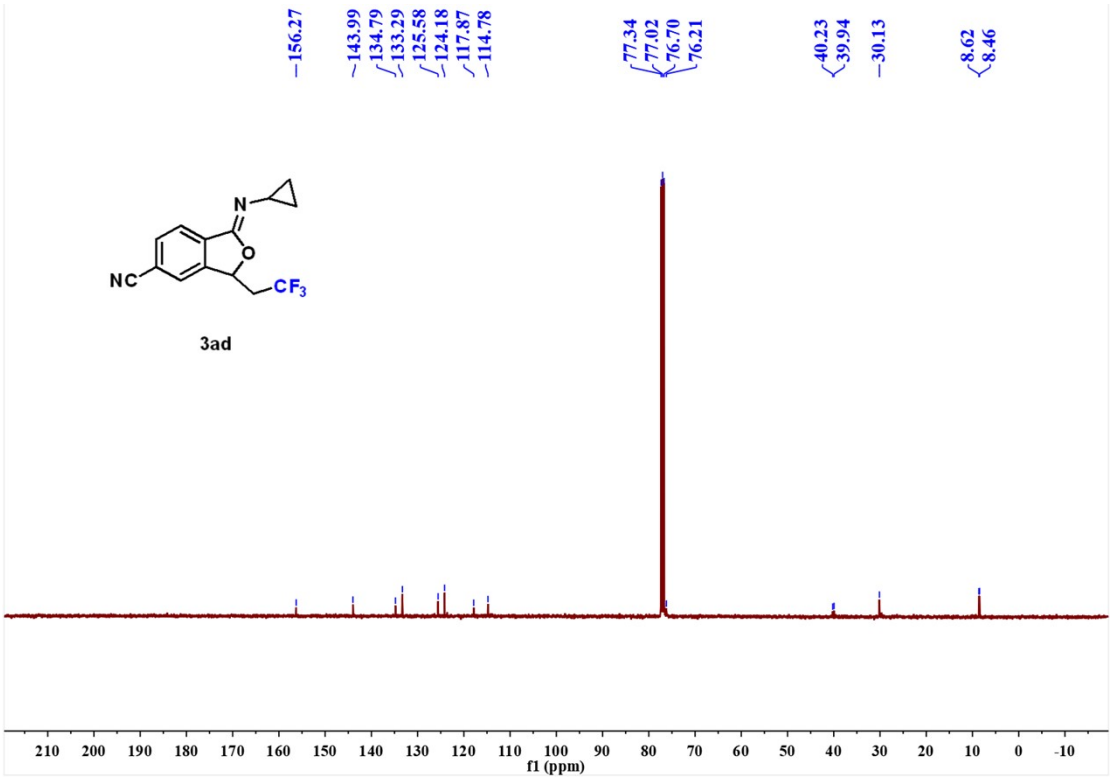
49.3.fid
lrz-49-ctf

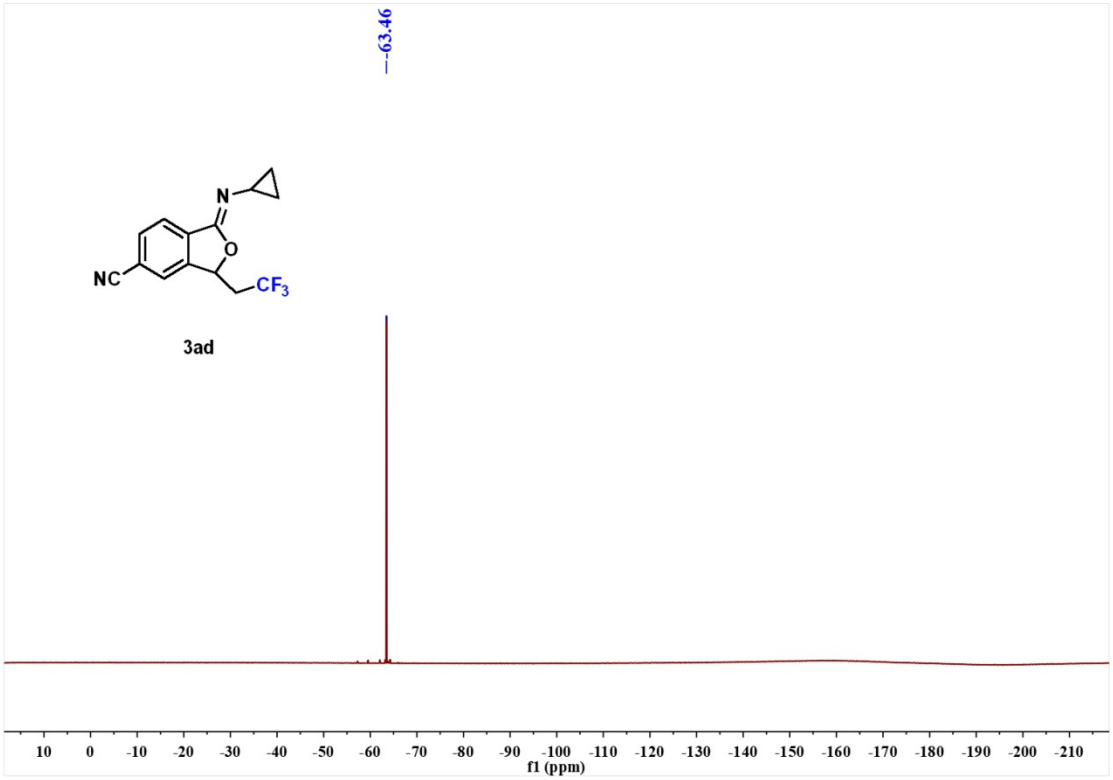


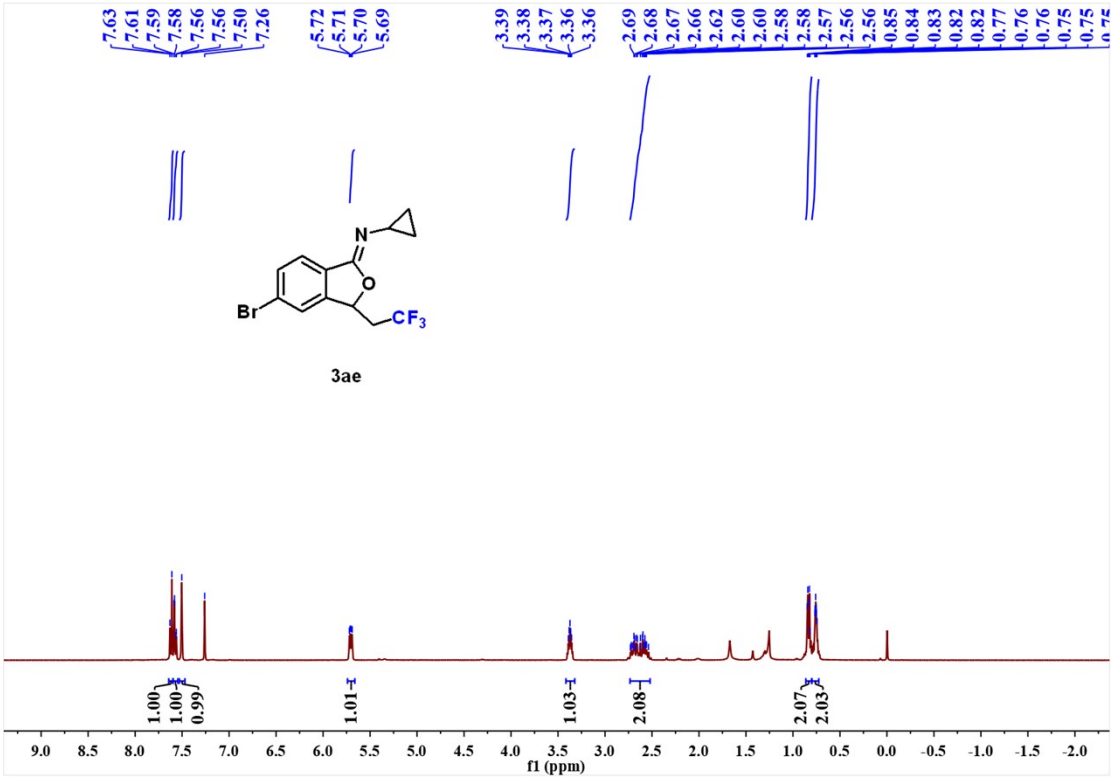
3ac

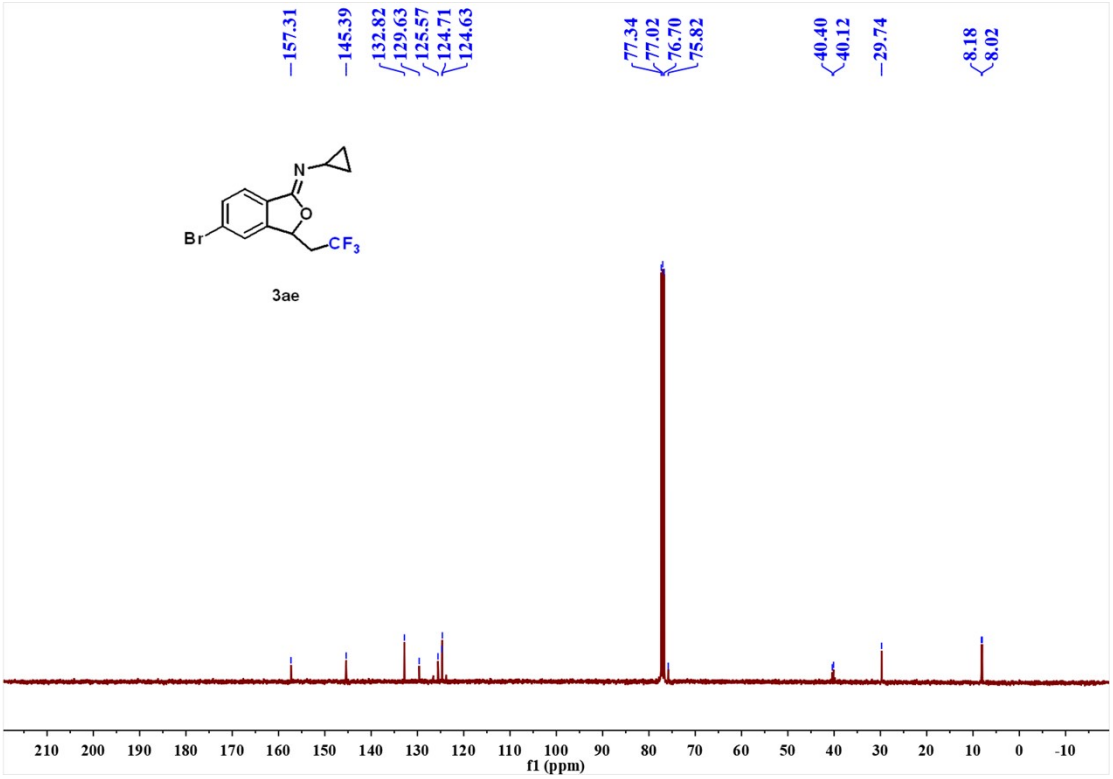


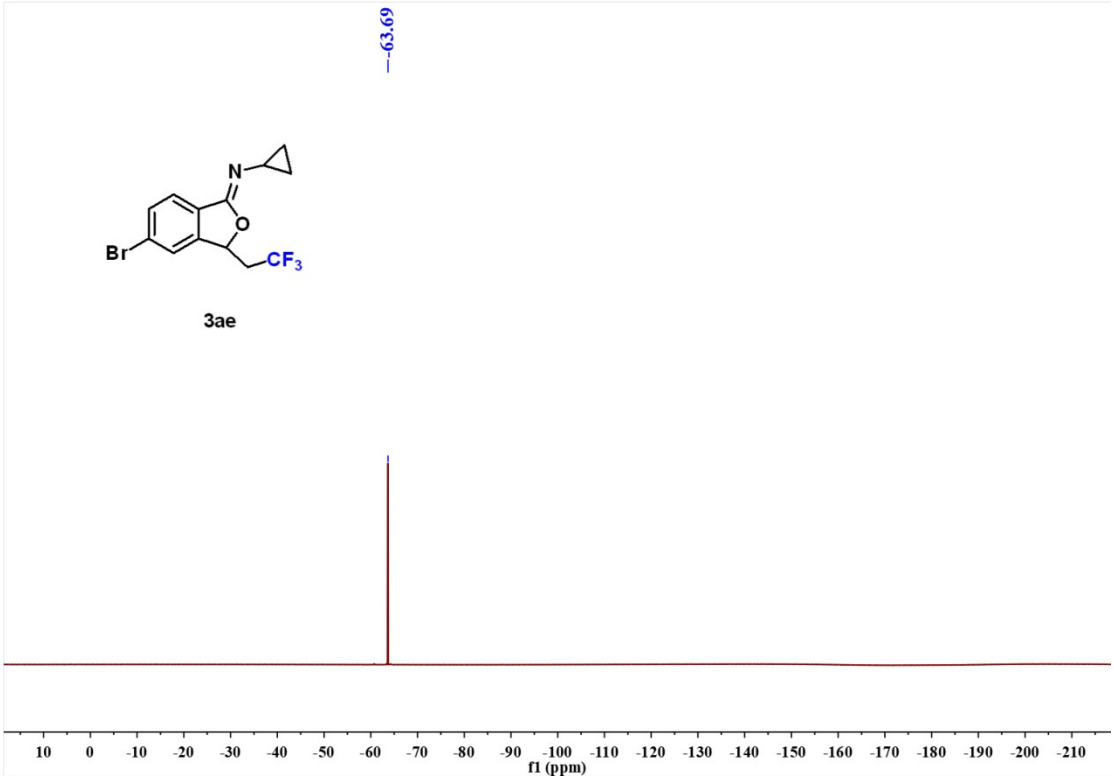
3ad

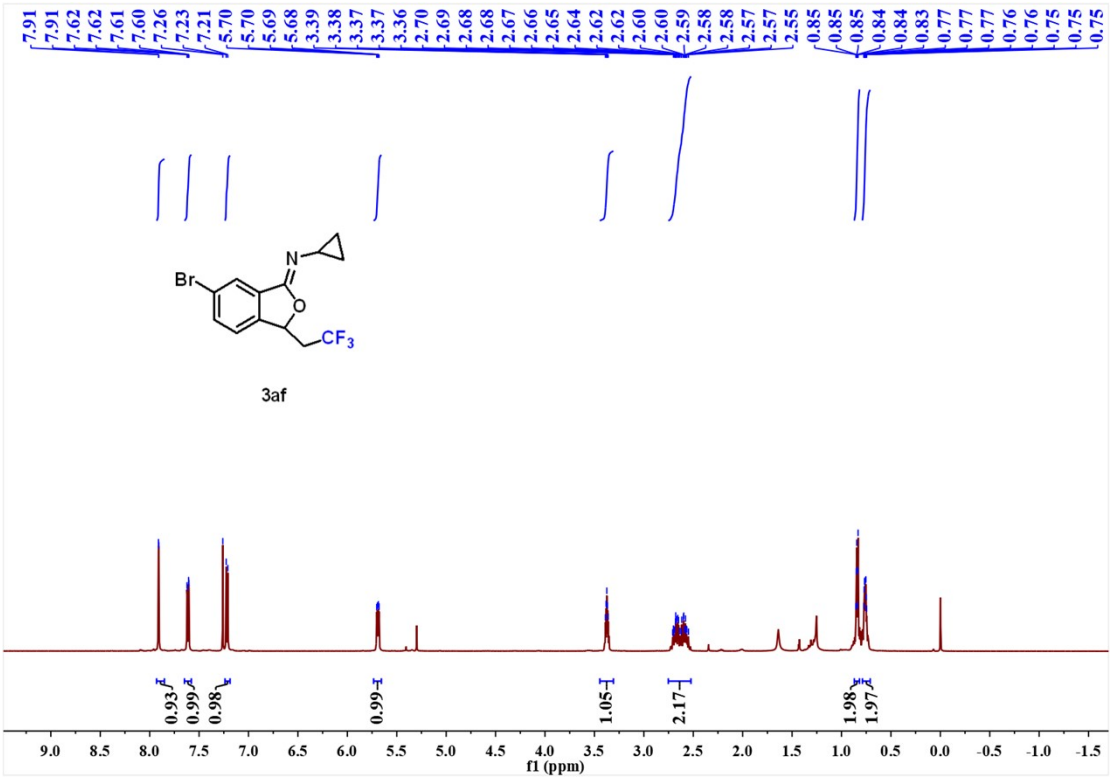

156.27
143.99
134.79
133.29
125.58
124.18
117.87
114.78
77.34
77.02
76.70
76.21
40.23
39.94
30.13
8.62
8.46
N
O
NC
CF3
3ad
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

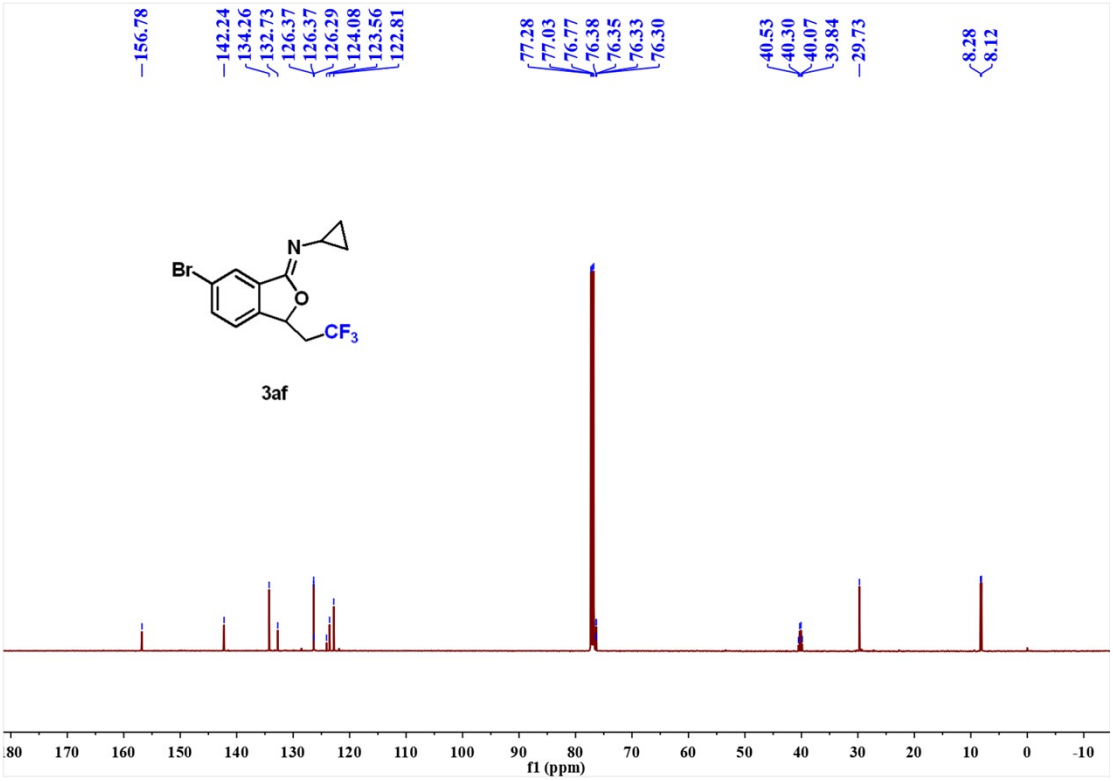

63.46
N
O
NC
CF3
3ad
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

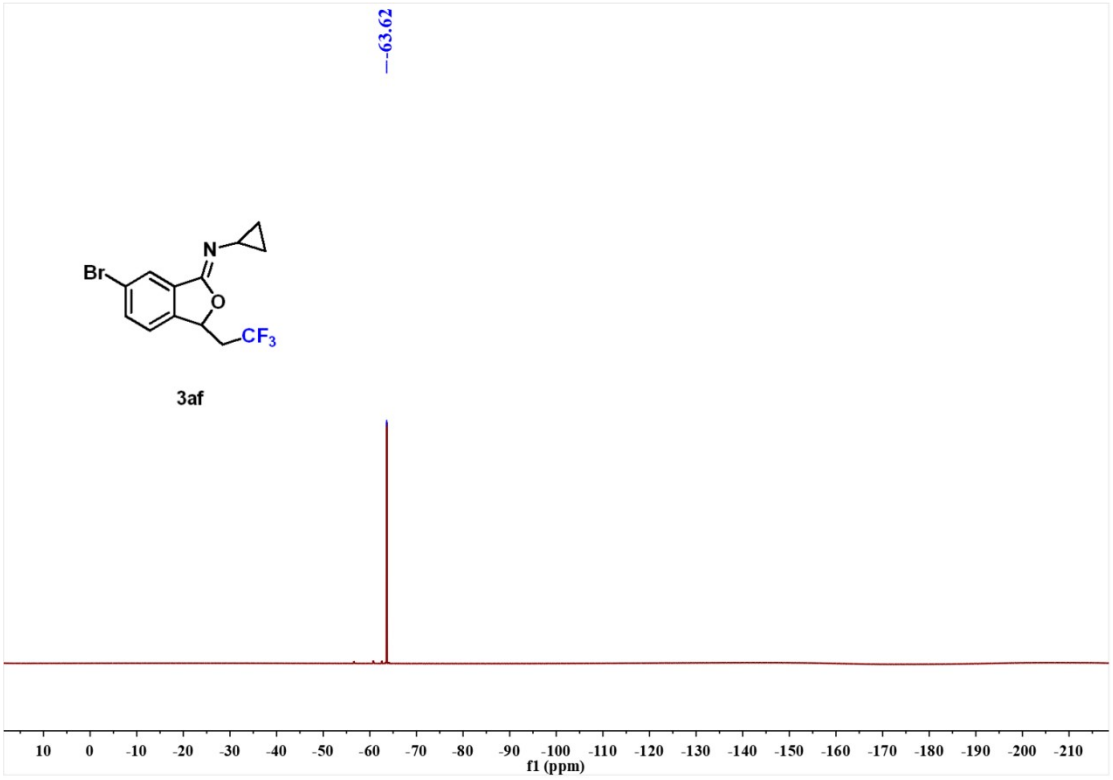

7.63
7.61
7.59
7.58
7.56
7.56
7.50
7.26
5.72
5.71
5.70
5.69
3.39
3.38
3.37
3.36
3.36
2.69
2.68
2.67
2.66
2.62
2.60
2.60
2.58
2.58
2.57
2.56
2.56
0.85
0.84
0.83
0.82
0.82
0.77
0.76
0.76
0.75
0.75
N
O
Br
CF3
3ae
1.00
1.00
0.99
1.01
1.03
2.08
2.07
2.03
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

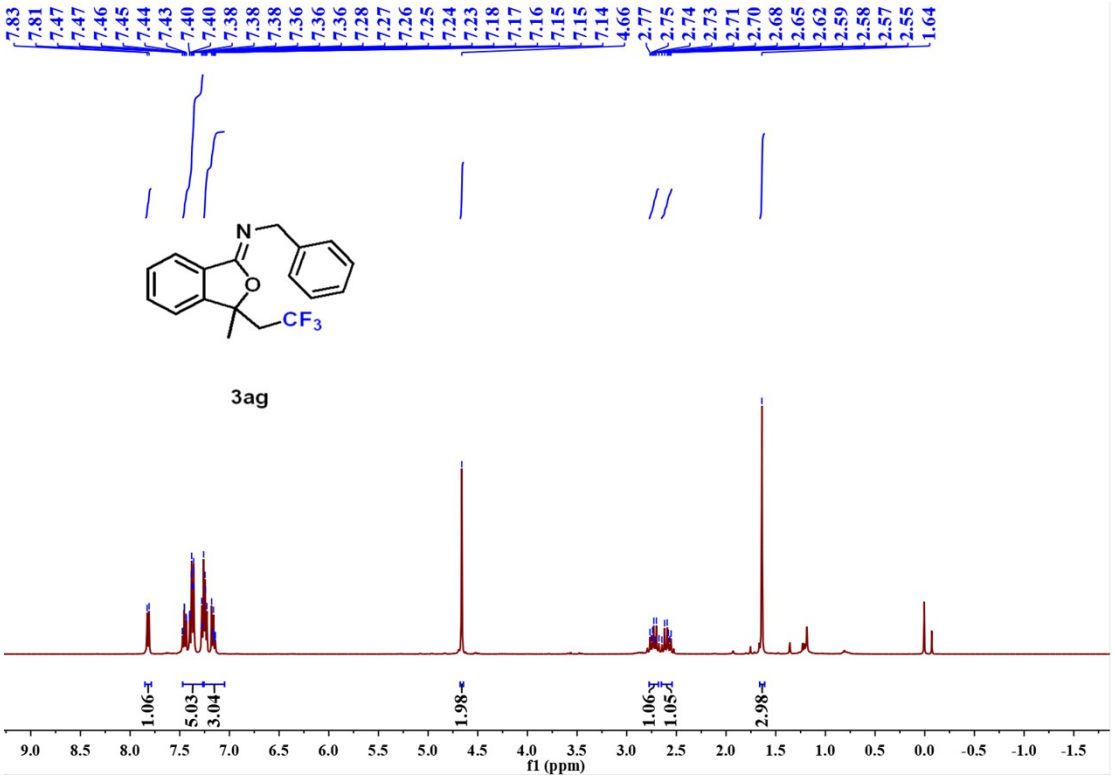

157.31
145.39
132.82
129.63
125.57
124.71
124.63
77.34
77.02
76.70
75.82
40.40
40.12
29.74
8.18
8.02
N
O
Br
CF3
3ae
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

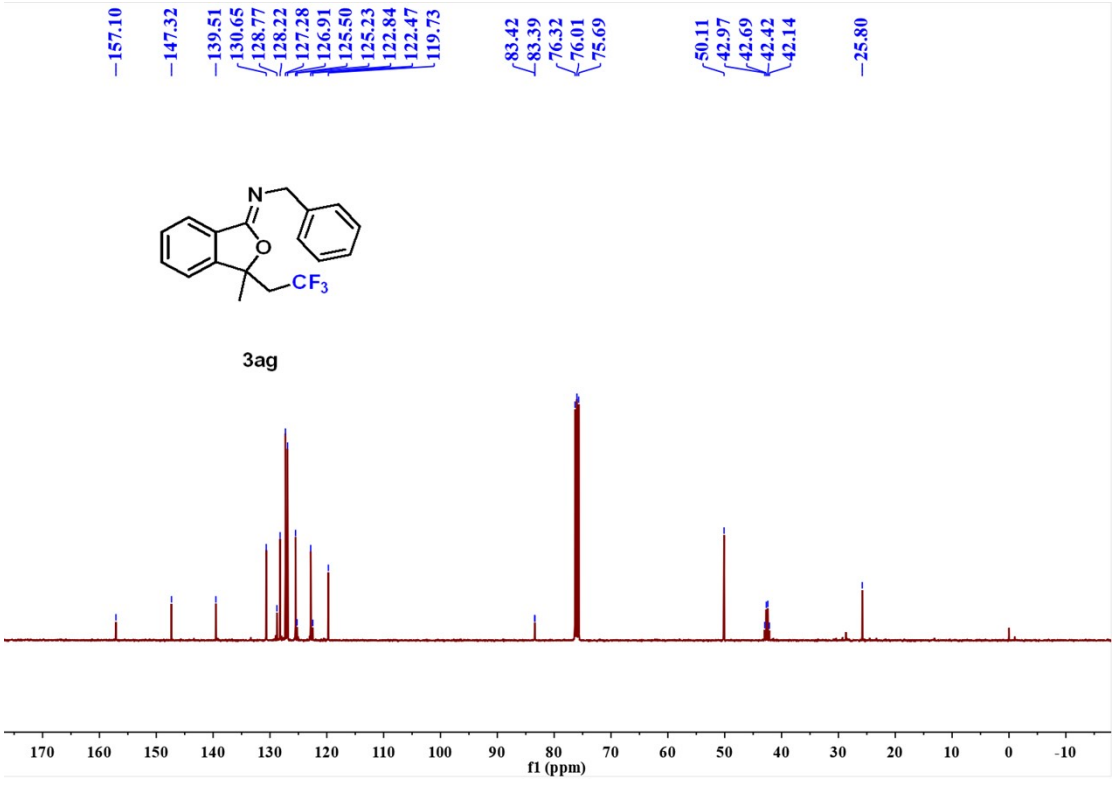

-63.69
N
O
Br
CF3
3ae
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

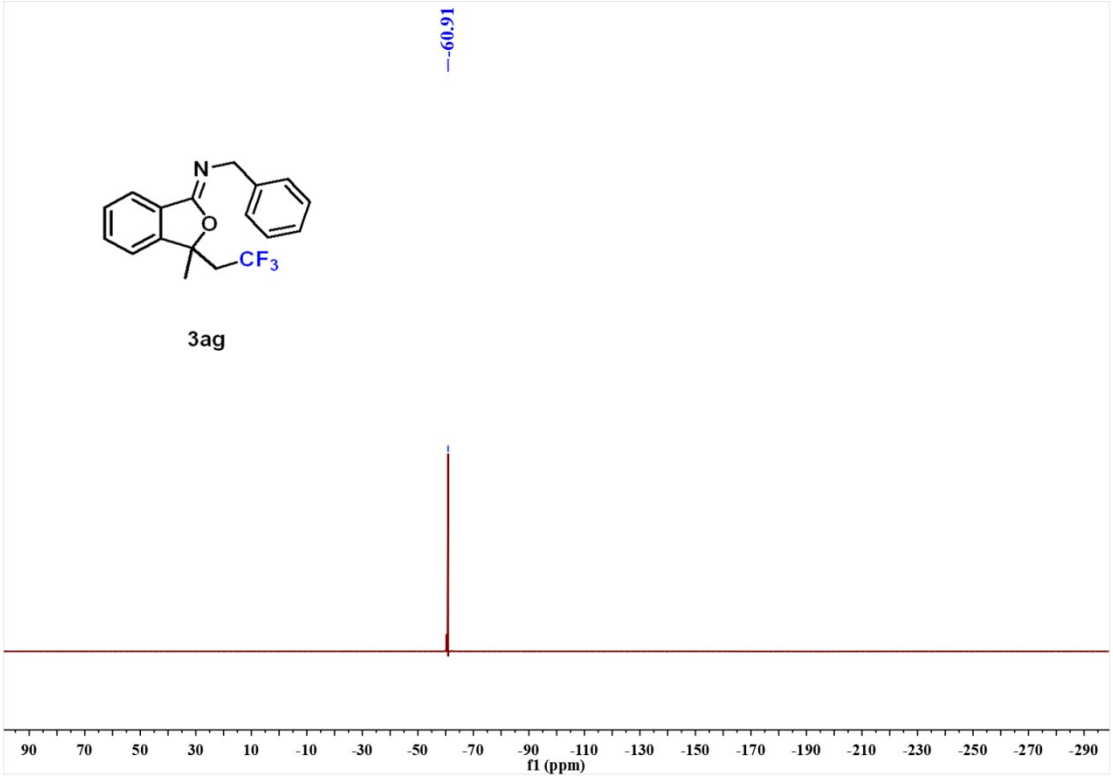

7.91 7.91 7.62 7.62 7.61 7.60 7.26 7.23 7.21 5.70 5.70 5.69 5.68 3.39 3.38 3.37 3.37 3.36 2.70 2.69 2.68 2.68 2.67 2.66 2.65 2.64 2.62 2.62 2.60 2.60 2.59 2.58 2.58 2.57 2.57 2.55 0.85 0.85 0.84 0.84 0.83 0.77 0.77 0.76 0.76 0.75 0.75 0.75
N
Br
O
CF3
3af
0.93 0.99 0.98 0.99 1.05 2.17 1.98 1.97
9.0 8.5 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
f1 (ppm)

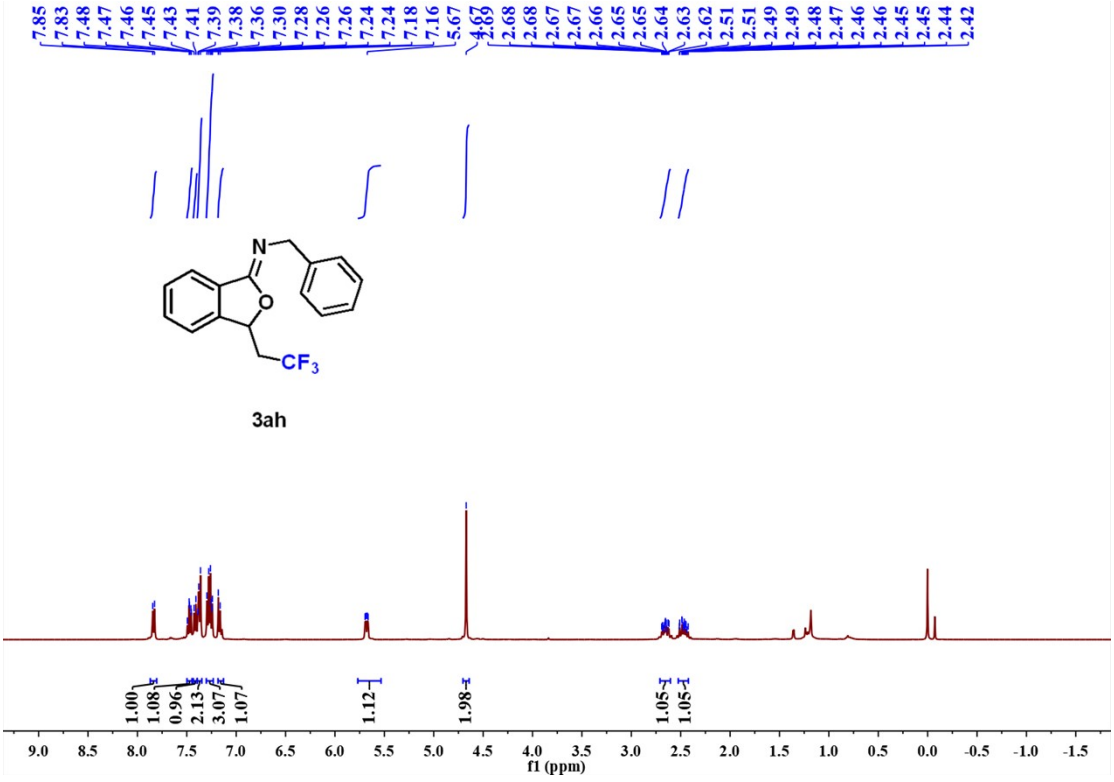

156.78
142.24
134.26
132.73
126.37
126.37
126.29
124.08
123.56
122.81
77.28
77.03
76.77
76.38
76.35
76.33
76.30
40.53
40.30
40.07
39.84
29.73
8.28
8.12
N
Br
O
CF3
3af
f1 (ppm)

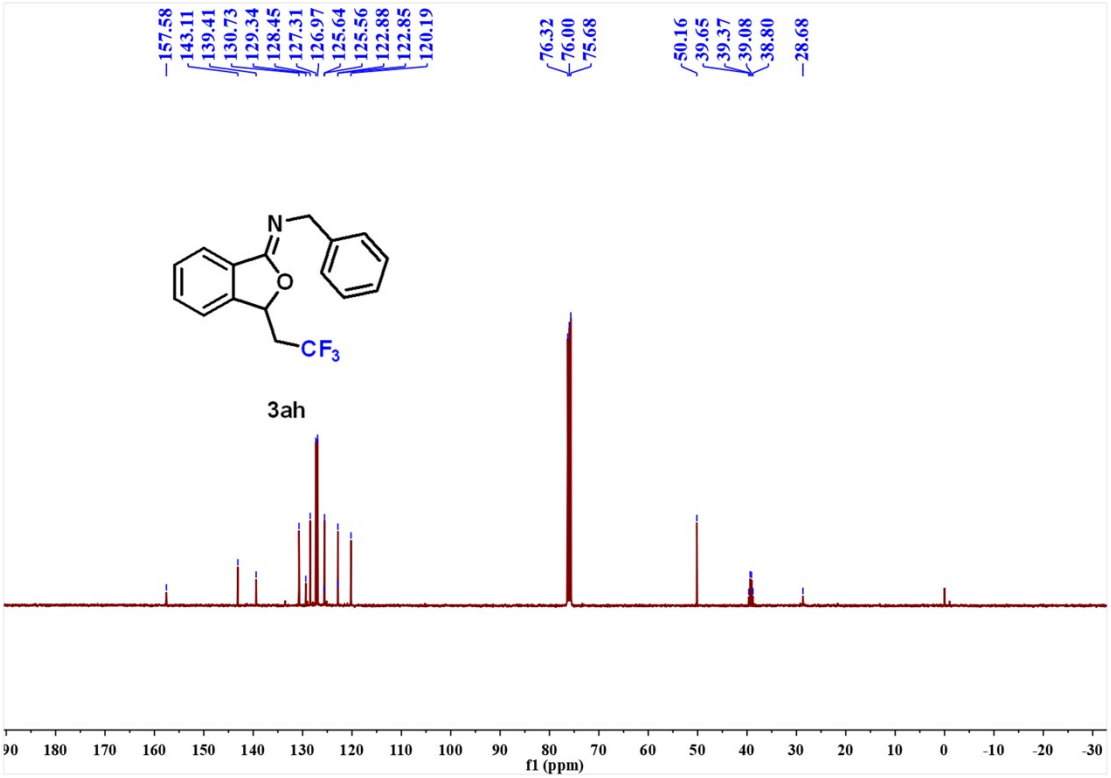

63.62
N
Br
O
CF3
3af
f1 (ppm)

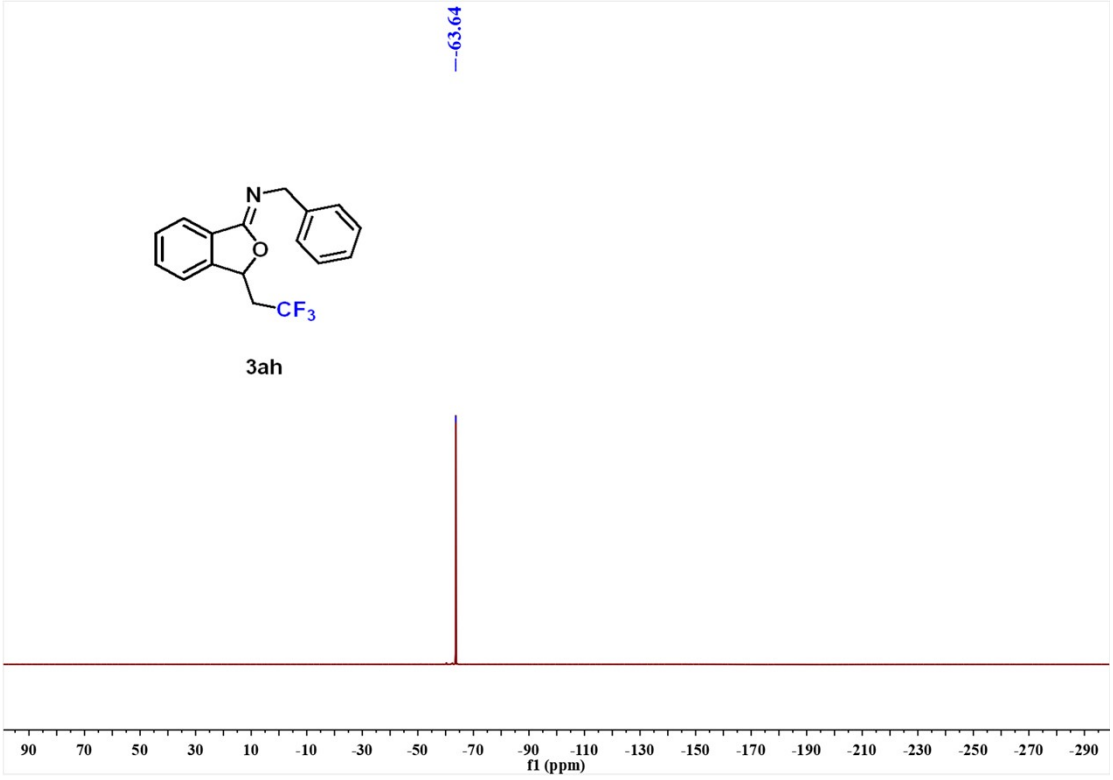

7.83
7.81
7.47
7.47
7.46
7.45
7.44
7.43
7.40
7.40
7.38
7.38
7.36
7.36
7.36
7.28
7.27
7.26
7.25
7.24
7.23
7.18
7.17
7.16
7.15
7.15
7.14
4.66
2.77
2.75
2.74
2.73
2.71
2.70
2.68
2.65
2.62
2.59
2.58
2.57
2.55
1.64
N
O
CF3
3ag
1.06
5.03
3.04
1.98
1.06
1.05
2.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

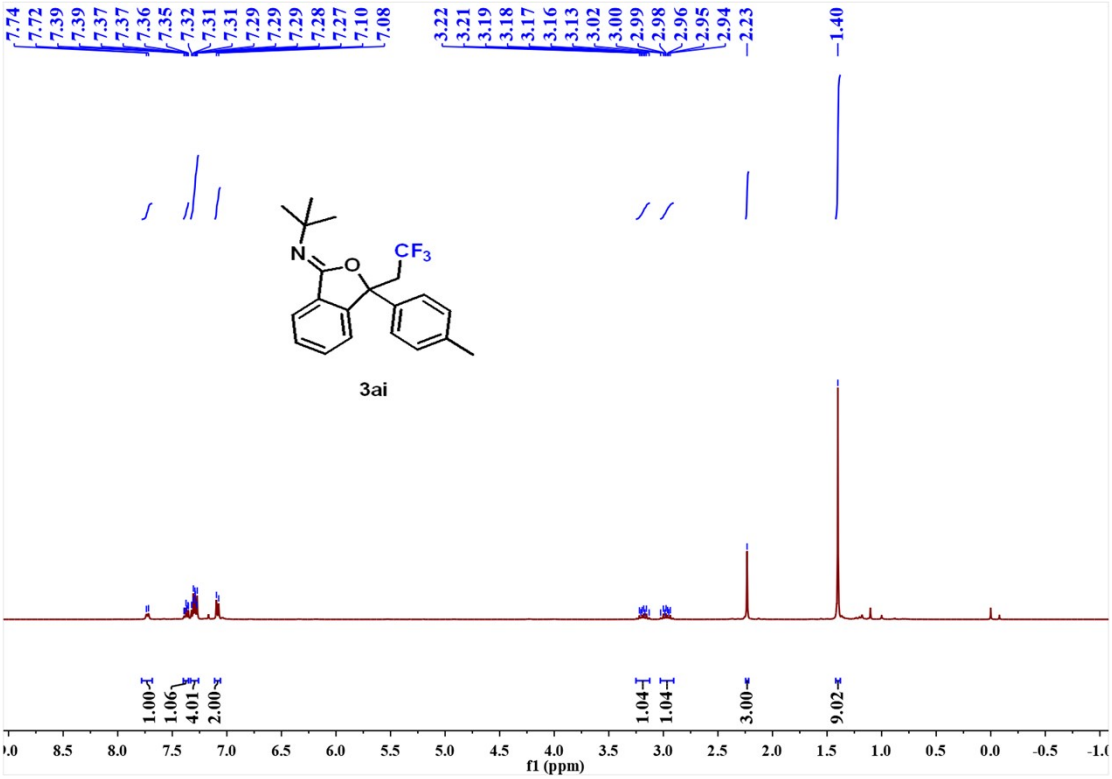

157.10
147.32
139.51
130.65
128.77
128.22
127.28
126.91
125.50
125.23
122.84
122.47
119.73
83.42
83.39
76.32
76.01
75.69
50.11
42.97
42.69
42.42
42.14
25.80
N
O
CF3
3ag
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


-60.91
N
O
CF3
3ag
90 70 50 30 10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)

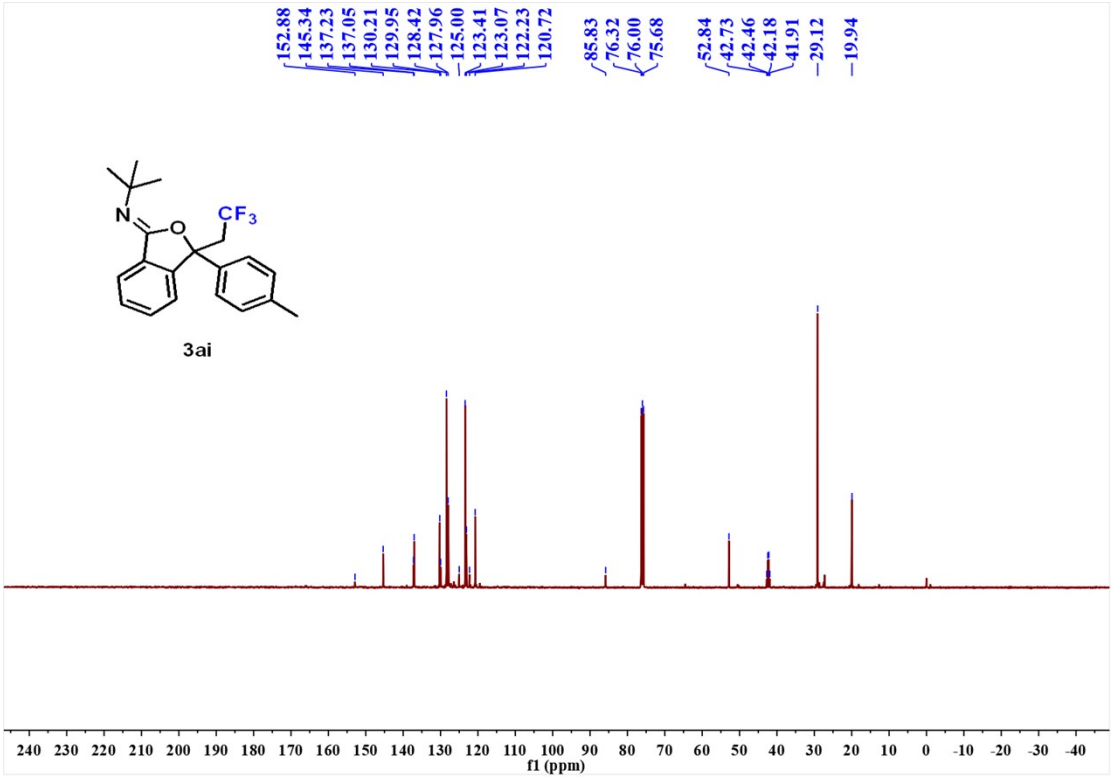

7.85 7.83 7.48 7.47 7.46 7.45 7.43 7.41 7.39 7.38 7.36 7.30 7.28 7.26 7.26 7.24 7.24 7.18 7.16 5.67 4.67 4.65 2.68 2.68 2.67 2.67 2.66 2.65 2.65 2.64 2.63 2.62 2.51 2.49 2.49 2.48 2.47 2.46 2.46 2.45 2.45 2.44 2.42
N
O
CF3
3ah
1.00 1.08 0.96 2.13 3.07 1.07 1.12 1.98 1.05 1.05
9.0 8.5 8.0 7.5 7.0 6.5 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
f1 (ppm)


157.58
143.11
139.41
130.73
129.34
128.45
127.31
126.97
125.64
125.56
122.88
122.85
120.19
76.32
76.00
75.68
50.16
39.65
39.37
39.08
38.80
28.68
N
O
CF3
3ah
f1 (ppm)

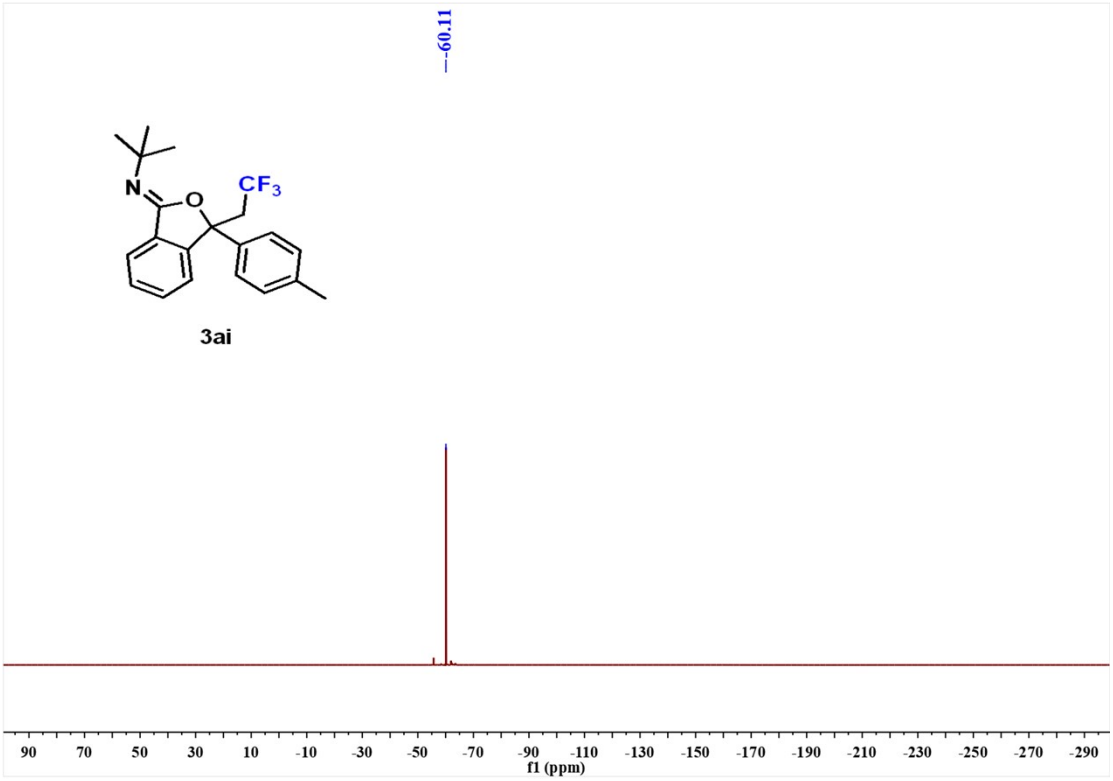

63.64
N
O
CF3
3ah
f1 (ppm)

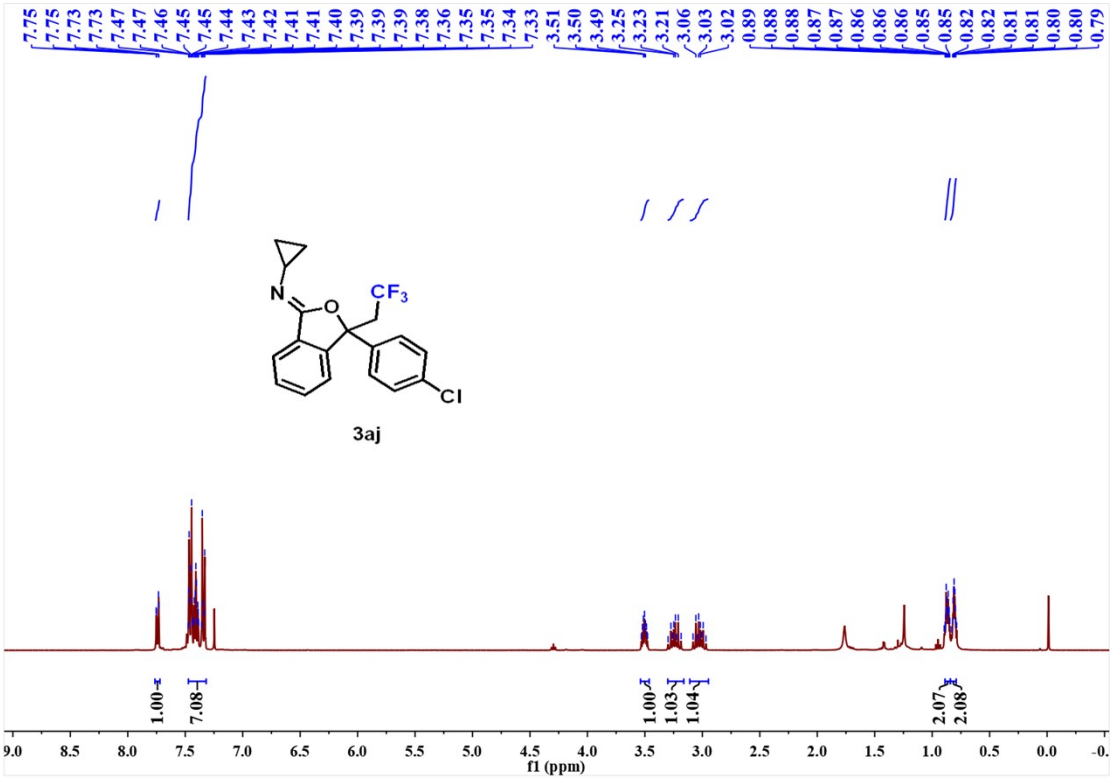

7.74
7.72
7.39
7.39
7.37
7.37
7.36
7.35
7.32
7.31
7.31
7.29
7.29
7.29
7.28
7.27
7.10
7.08
3.22
3.21
3.19
3.18
3.17
3.16
3.13
3.02
3.00
2.99
2.98
2.96
2.95
2.94
2.23
1.40
N
O
CF3
1.00
1.06
4.01
2.00
1.04
1.04
3.00
9.02
f1 (ppm)

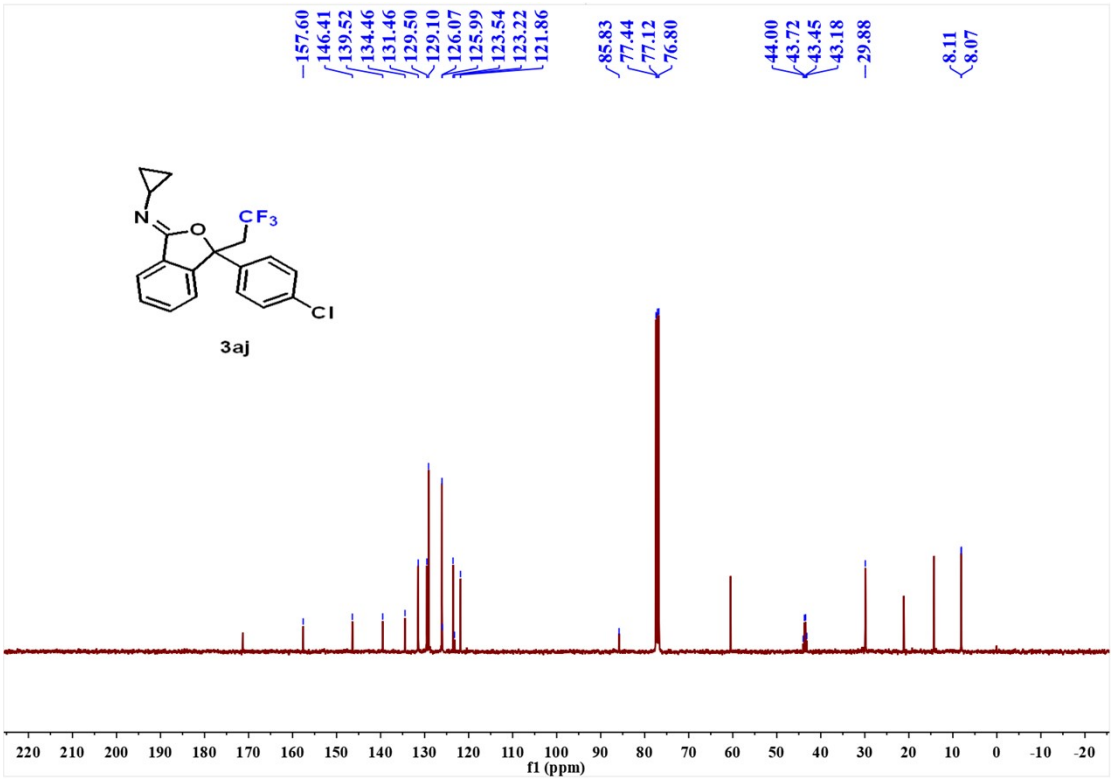
3ai

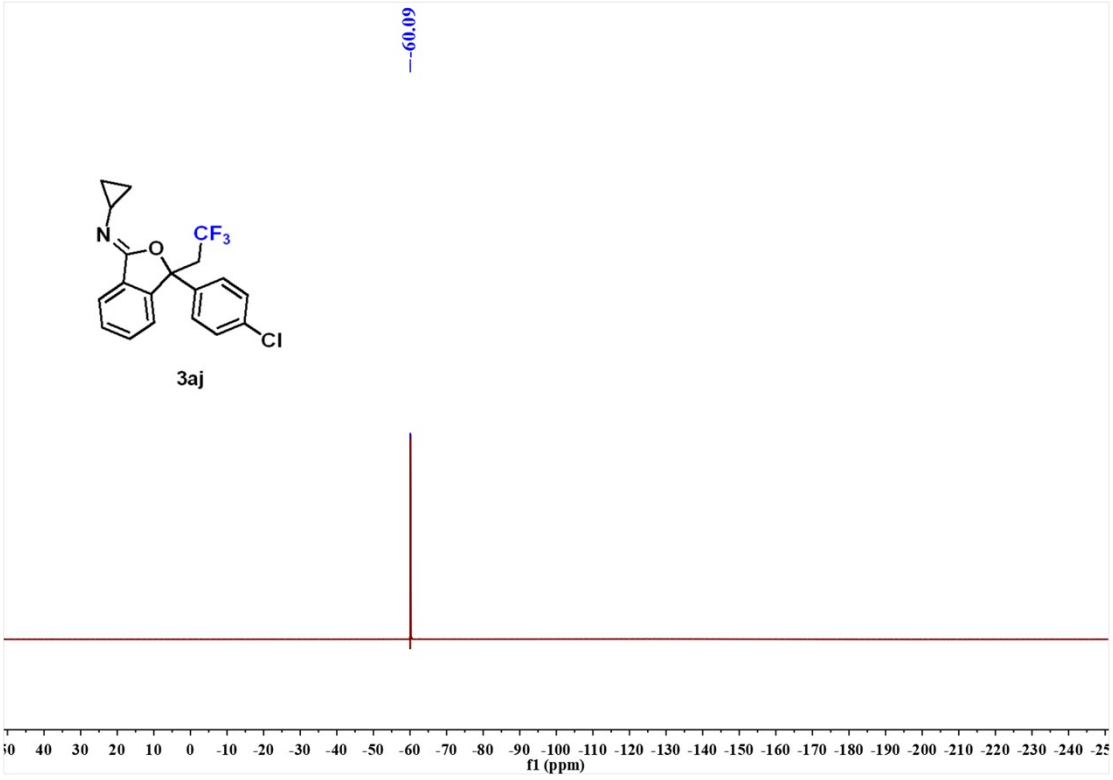

152.88
145.34
137.23
137.05
130.21
129.95
128.42
127.96
125.00
123.41
123.07
122.23
120.72
85.83
76.32
76.00
75.68
52.84
42.73
42.46
42.18
41.91
29.12
19.94
N
O
CF3
f1 (ppm)

3ai


-60.11
N
O
CF3
3ai
90 70 50 30 10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210 -230 -250 -270 -290
f1 (ppm)


7.75 7.75 7.73 7.73 7.47 7.47 7.46 7.45 7.45 7.44 7.43 7.42 7.41 7.41 7.40 7.39 7.39 7.38 7.36 7.35 7.35 7.34 7.33
3.51 3.50 3.49 3.25 3.23 3.21 3.06 3.03 3.02
0.89 0.88 0.88 0.87 0.87 0.86 0.86 0.86 0.85 0.85 0.82 0.82 0.81 0.81 0.80 0.80 0.79
N
O
CF3
Cl
3aj
1.00 7.08 1.00 1.03 1.04 2.07 2.08
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


157.60
146.41
139.52
134.46
131.46
129.50
129.10
126.07
125.99
123.54
123.22
121.86
85.83
77.44
77.12
76.80
44.00
43.72
43.45
43.18
29.88
8.11
8.07
N
O
CF3
Cl
3aj
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


-60.09
N
O
CF3
Cl
3aj
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)