Supporting information

Electrochemical Synthesis of *Trans*-2,3-disubstituted Aziridines via Oxidative Dehydrogenative Intramolecular C(sp3)−H Amination

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Part I Experimental Section

1.1 General information

^1H NMR and ^{13}C NMR were recorded on a Bruker-400MHz Spectrometer (^1H NMR: 400MHz, ^{13}C NMR: 100MHz) using TMS as internal reference. The chemical shifts (δ) and coupling constants (*J*) were expressed in ppm and Hz respectively. The abbreviations used for explaining the multiplicities were as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. High resolution mass spectra (HRMS) were measured using electrospray ionization (ESI) and the time-of-flight (TOF) mass analyzer. Substrates **1a-1v** were prepared according to the literature procedures (*Chem. Commun.* **2003**, 2570; *J. Org. Chem.* **2004**, *69*, 8482). Flash chromatography was carried out using silica gel (100−200 mesh).

1.2 General procedure for the electrosynthesis

An undivided cell was equipped with a magnet stirrer, platinum plate (1.5 × 1.5 cm^2) electrode, as the working electrode and counter electrode. The substrate **1** (0.3 mmol) and electrolyte KI (100 mg, 0.6 mmol) was added to the mixed solvent THF/MeOH (6/4 mL). The resulting mixture was allowed to stir and electrolyze at constant current conditions (4 mA/cm^2) under room temperature for 3 h. After the reaction, the solvent was removed with a rotary evaporator and the residue was purified by flash column chromatography on silica gel (1% Et_3N is needed when packing the column in case of the product decomposition) to afford the desired product **2** as a colorless oil or white foam.

1.3 Scale-up synthesis

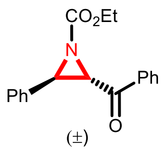
A beaker (500 mL) was equipped with a magnet stirrer, platinum plate (5 × 5 cm^2) electrode, as the working electrode and counter electrode. The substrate **1a** (2.97 g, 10 mmol) and electrolyte KI (3.4 g, 12 mmol) was added to the mixed solvent THF/MeOH (120/80 mL). The resulting mixture was allowed to stir and electrolyze at constant current conditions (4 mA/cm^2) under room temperature for 12 h. Then, the solvent was removed with a rotary evaporator and the residue was purified by flash column chromatography on silica gel (1% Et_3N was added when packing the column in case of the product decomposition) to afford the desired product **2a** (2.15 g) as a colorless oil.

1.4 Procedure for CV experiments

Cyclic voltammograms of **1a** and KI were performed in a three-electrode cell at room temperature with 0.1 M $LiClO_4$ in THF/MeOH (4 mL, 6/4 v/v) as the supporting electrolyte. The working electrode was a Pt wire electrode while the counter electrode was a Pt disk. The reference was an Ag/AgCl electrode. The scan rate was 100 mV/s, and the test window ranged from 0 V to 2.0 V.

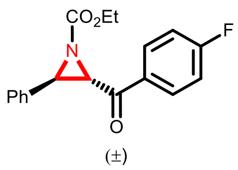
1.5 Characterization data

***Trans*-ethyl 2-benzoyl-3-phenylaziridine-1-carboxylate (2a)**:



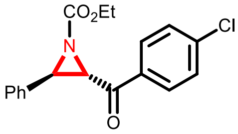
Colorless oil (83% yield, 74 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 – 7.96 (m, 2H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.40 – 7.33 (m, 5H), 4.29 – 4.22 (m, 2H), 4.05 (d, *J* = 2.5 Hz, 1H), 3.90 (d, *J* = 2.4 Hz, 1H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.2, 160.5, 136.5, 135.9, 134.1, 129.0, 128.8, 128.6, 126.5, 124.8, 62.9, 47.5, 47.3, 14.4. IR (NaCl): 2982, 1732, 1677, 1597, 1301 cm^{-1}. HRMS (ESI) m/z calcd for $C_{18}H_{17}NNaO_3$ $[M+Na]^+$ 318.1101, found 318.1112.

***Trans*-ethyl 2-(4-fluorobenzoyl)-3-phenylaziridine-1-carboxylate (2b):**



Colorless oil (66% yield, 62 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.46 – 7.35 (m, 5H), 7.19 (t, *J* = 8.5 Hz, 2H), 4.40 – 4.19 (m, 2H), 4.01 (d, *J* = 2.3 Hz, 1H), 3.92 (d, *J* = 2.1 Hz, 1H), 1.28 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.7, 166.4 (d, *J* = 256.8 Hz), 160.3, 135.8, 133.0, 131.3 (d, *J* = 9.5 Hz), 128.8, 128.7, 126.5, 116.2 (d, *J* = 22.1 Hz), 62.9, 47.5, 47.0, 14.4. IR (NaCl): 2984, 1732, 1678, 1598, 1297 cm^{-1}. HRMS (ESI) m/z calcd for $C_{18}H_{16}FNNaO_3$ $[M+Na]^+$ 336.1006, found 336.1009.

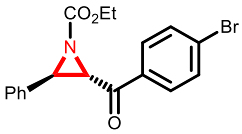
***Trans*-ethyl 2-(4-chlorobenzoyl)-3-phenylaziridine-1-carboxylate (2c):**



(±)

Colorless oil (64% yield, 63 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.91 (m, 2H), 7.49 – 7.45 (m, 2H), 7.38 – 7.35 (m, 5H), 4.29 – 4.17 (m, 2H), 3.99 (d, J = 2.4 Hz, 1H), 3.90 (d, J = 2.4 Hz, 1H), 1.25 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.1, 160.3, 140.8, 135.7, 134.8, 130.0, 129.4, 128.8, 128.7, 126.5, 63.0, 47.6, 47.1, 14.4. IR (NaCl): 2983, 1734, 1678, 1597, 1279 cm^{-1}. HRMS (ESI) m/z calcd for $C_{18}H_{16}ClNNaO_3$ $[M+Na]^+$ 352.0711, found 352.0714.

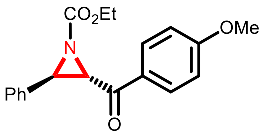
***Trans*-ethyl 2-(4-bromobenzoyl)-3-phenylaziridine-1-carboxylate (2d):**



(±)

Pale yellow oil (64% yield, 72 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 – 7.83 (m, 2H), 7.68 – 7.60 (m, 2H), 7.41 – 7.31 (m, 5H), 4.31 – 4.19 (m, 2H), 3.98 (d, J = 2.4 Hz, 1H), 3.90 (d, J = 2.4 Hz, 1H), 1.26 (t, J = 7.1 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.4, 160.3, 135.7, 135.2, 132.4, 130.0, 129.6, 128.8, 128.7, 126.5, 63.0, 47.7, 47.0, 14.4. IR (NaCl): 2981, 1732, 1677, 1598, 1302 cm^{-1}. HRMS (ESI) m/z calcd for $C_{18}H_{16}BrNNaO_3$ $[M+Na]^+$ 396.0206, found 396.0204.

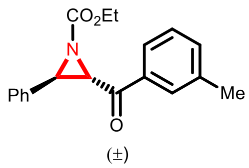
***Trans*-ethyl 2-(4-methoxybenzoyl)-3-phenylaziridine-1-carboxylate (2e):**



(±)

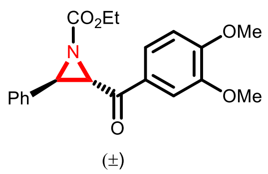
Colorless oil (65% yield, 63 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 7.93 (m, 2H), 7.43 – 7.28 (m, 5H), 7.01 – 6.93 (m, 2H), 4.24 (dt, J = 12.7, 6.4 Hz, 2H), 4.01 (d, J = 2.5 Hz, 1H), 3.88 (s, 3H), 1.26 (t, J = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.3, 164.4, 160.6, 136.1, 131.0, 129.6, 128.8, 128.5, 126.5, 114.2, 62.8, 55.7, 47.1, 47.0, 14.4. IR (NaCl): 2979, 1732, 1672, 1596, 1298 cm^{-1}. HRMS (ESI) m/z calcd for $C_{19}H_{19}NNaO_4$ $[M+Na]^+$ 348.1206, found 348.1210.

***Trans*-ethyl 2-(3-methylbenzoyl)-3-phenylaziridine-1-carboxylate (2f):**



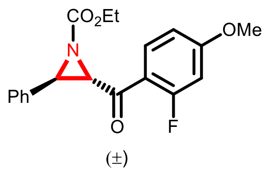
Colorless oil (77% yield, 72 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^1H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.8 Hz, 2H), 7.46 – 7.30 (m, 7H), 4.38 – 4.16 (m, 2H), 4.04 (d, *J* = 2.4 Hz, 1H), 3.89 (d, *J* = 2.4 Hz, 1H), 2.41 (s, 3H), 1.26 (t, *J* = 8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.4, 160.5, 138.9, 136.6, 136.0, 134.9, 129.1, 128.9, 128.8, 128.6, 126.6, 125.9, 62.9, 47.5, 47.3, 21.5, 14.5. IR (NaCl): 2981, 1732, 1674, 1597, 1300 cm^{-1}. HRMS (ESI) m/z calcd for $C_{19}H_{19}NNaO_3$ $[M+Na]^+$ 332.1257, found 332.1260.

***Trans*-ethyl 2-(3,4-dimethoxybenzoyl)-3-phenylaziridine-1-carboxylate (2g):**



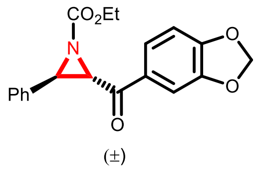
Colorless oil (58% yield, 62 mg), petroleum ether/ethyl acetate = 4 : 1 – 2:1 (v/v) as eluent for column chromatography; ^1H NMR (400 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.56 (d, *J* = 2.0 Hz, 1H), 7.42 – 7.33 (m, 5H), 6.90 (d, *J* = 8.4 Hz, 1H), 4.31-4.21 (m, 2H), 4.02 (d, *J* = 2.5 Hz, 1H), 3.95 (s, 3H), 3.93 (s, 3H), 3.89 (d, *J* = 2.5 Hz, 1H), 1.27 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.3, 160.6, 154.3, 149.4, 136.1, 129.8, 128.8, 128.5, 126.5, 123.7, 110.4, 110.2, 62.9, 56.3, 56.2, 47.2, 46.9, 14.5. IR (NaCl): 2977, 1732, 1668, 1597, 1296 cm^{-1}. HRMS (ESI) m/z calcd for $C_{20}H_{21}NNaO_5$ $[M+Na]^+$ 378.1312, found 378.1317.

***Trans*-ethyl 2-(2-fluoro-4-methoxybenzoyl)-3-phenylaziridine-1-carboxylate (2h):**



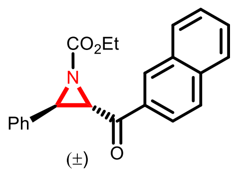
Colorless oil (73% yield, 75 mg), petroleum ether/ethyl acetate = 6 : 1 – 3:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (t, *J* = 8.7 Hz, 1H), 7.43 – 7.29 (m, 5H), 6.79 (dd, *J* = 8.8, 2.2 Hz, 1H), 6.61 (dd, *J* = 13.1, 2.2 Hz, 1H), 4.26 (dt, *J* = 7.2, 3.1 Hz, 2H), 4.04 (t, *J* = 2.4 Hz, 1H), 3.91 – 3.84 (m, 4H), 1.28 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.6 (d, *J* = 4.4 Hz), 165.8 (d, *J* = 11.9 Hz), 163.8 (d, *J* = 255.5 Hz), 160.6, 136.1, 132.5 (d, *J* = 4.3 Hz), 128.7, 128.5, 126.6, 118.1 (d, *J* = 12.9 Hz), 111.3 (d, *J* = 2.4 Hz), 101. 9 (d, *J* = 27 Hz), 62.8, 56.1, 50.0 (d, *J* = 13.1 Hz), 47.7, 14.5. IR (NaCl): 2983, 1732, 1677, 1598, 1297 cm^{-1}. HRMS (ESI) m/z calcd for $C_{19}H_{18}FNNaO_4$ $[M+Na]^+$ 366.1112, found 366.1115.

***Trans*-ethyl 2-(benzo[d][1,3]dioxole-5-carbonyl)-3-phenylaziridine-1-carboxylate (2i):**



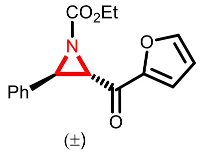
White foam (54% yield, 55 mg), petroleum ether/ethyl acetate = 6 : 1 – 3:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.46 (d, *J* = 1.7 Hz, 1H), 7.38-7.33 (m, 5H), 6.87 (d, *J* = 8.2 Hz, 1H), 6.07 (s, 2H), 4.30 – 4.19 (m, 2H), 3.95 (d, *J* = 2.5 Hz, 1H), 3.87 (d, *J* = 2.5 Hz, 1H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.9, 160.5, 152.8, 148.6, 136.0, 131.4, 128.8, 128.6, 126.5, 125.4, 108.22, 108.18, 102.2, 62.8, 47.2, 47.1, 14.4. IR (NaCl): 2978, 1732, 1670, 1596, 1297 cm^{-1}. HRMS (ESI) m/z calcd for $C_{19}H_{17}NNaO_5$ $[M+Na]^+$ 362.0999, found, 362.1003.

***Trans*-ethyl 2-(2-naphthoyl)-3-phenylaziridine-1-carboxylate (2j):**



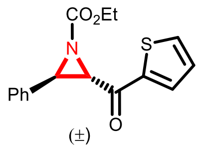
White foam (69% yield, 71 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (s, 1H), 8.04 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.98 – 7.87 (m, 3H), 7.67 – 7.54 (m, 2H), 7.47 – 7.32 (m, 5H), 4.27 (qd, *J* = 7.2, 4.0 Hz, 2H), 4.21 (d, *J* = 2.4 Hz, 1H), 3.98 (d, *J* = 2.4 Hz, 1H), 1.27 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.0, 160.6, 136.1, 133.9, 132.5, 130.8, 129.9, 129.3, 128.8, 128.6, 128.0, 127.3, 126.6, 123.9, 63.0, 47.6, 47.3, 14.5. IR (NaCl): 2982, 1732, 1675, 1598, 1300 cm^{-1}. HRMS (ESI) m/z calcd for $C_{22}H_{19}NNaO_3$ $[M+Na]^+$ 368.1257, found 368.1263.

***Trans*-ethyl 2-(furan-2-carbonyl)-3-phenylaziridine-1-carboxylate (2k):**



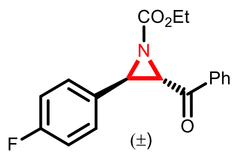
Colorless oil (59% yield, 51 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (s, 1H), 7.39 (dd, *J* = 4.5, 3.2 Hz, 6H), 6.62 (dd, *J* = 3.5, 1.6 Hz, 1H), 4.39 – 4.12 (m, 2H), 3.97 (d, *J* = 2.3 Hz, 1H), 3.94 (d, *J* = 2.3 Hz, 1H), 1.27 (t, *J* = 7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.4, 160.2, 143.4, 135.8, 135.6, 133.4, 128.8, 128.7, 128.6, 126.5, 62.9, 47.7, 47.1, 14.4. IR (NaCl): 2932, 1730, 1634 cm^{-1}. HRMS (ESI) m/z calcd for $C_{16}H_{16}NO_4$ $[M+H]^+$ 286.1074, found 286.1075.

***Trans*-ethyl 2-phenyl-3-(thiophene-2-carbonyl)aziridine-1-carboxylate (2l):**



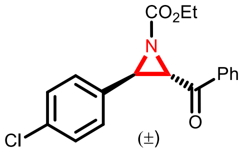
Colorless oil (57% yield, 51 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 3.8 Hz, 1H), 7.76 (d, *J* = 4.9 Hz, 1H), 7.45 – 7.32 (m, 5H), 7.21 – 7.15 (m, 1H), 4.24 (qd, *J* = 7.1, 3.9 Hz, 2H), 3.94 (d, *J* = 2.0 Hz, 1H), 3.89 (d, *J* = 2.1 Hz, 1H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.4, 160.2, 152.6, 147.8, 135.9, 128.8, 128.6, 126.6, 119.2, 113.0, 63.0, 47.1, 47.0, 14.4. IR (NaCl): 2955, 1731, 1632 cm^{-1}. HRMS (ESI) m/z calcd for $C_{16}H_{16}NO_3S$ $[M+H]^+$ 302.0845, found 302.0843.

***Trans*-ethyl 2-benzoyl-3-(4-fluorophenyl)aziridine-1-carboxylate (2m):**



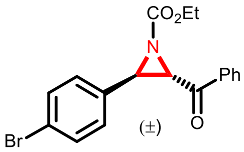
Colorless oil (70% yield, 66 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.94 (m, 2H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 2H), 7.40 – 7.33 (m, 2H), 7.09 – 7.03 (m, 2H), 4.26 (qd, *J* = 7.1, 4.7 Hz, 2H), 4.00 (d, J = 2.4 Hz, 1H), 3.88 (d, J = 2.4 Hz, 1H), 1.27 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.1, 163.0 (d, J = 247.3 Hz), 160.4, 136.5, 134.2, 131.8 (d, J = 3.1 Hz), 129.1, 128.6, 128.3 (d, J = 8.3 Hz), 115.8 (d, J = 21.8 Hz), 63.0, 47.3, 46.8, 14.5. IR (NaCl): 2984, 1732, 1678, 1598, 1297 cm^{-1}. HRMS (ESI) m/z calcd for $C_{18}H_{17}FNO_3$ $[M+H]^+$ 314.1187, found 314.1192.

***Trans*-ethyl 2-benzoyl-3-(4-chlorophenyl)aziridine-1-carboxylate (2n):**



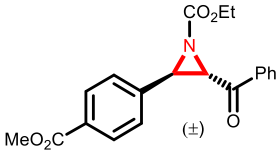
Colorless oil (74% yield, 73 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 7.5 Hz, 2H), 7.64 (t, J = 7.4 Hz, 1H), 7.51 (t, J = 7.7 Hz, 2H), 7.38 – 7.31 (m, 4H), 4.31 – 4.19 (m, 2H), 4.01 (d, J = 2.3 Hz, 1H), 3.87 (d, J = 2.2 Hz, 1H), 1.27 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.0, 160.3, 136.3, 134.5, 134.3, 129.0, 129.0, 128.6, 127.9, 124.8, 63.0, 47.3, 46.7, 14.4. IR (NaCl): 2983, 1734, 1678, 1597, 1343, 1279 cm^{-1}. HRMS (ESI) m/z calcd for $C_{18}H_{17}ClNO_3$ $[M+H]^+$ 330.0891, found 330.0892.

***Trans*-ethyl 2-benzoyl-3-(4-bromophenyl)aziridine-1-carboxylate (2o):**



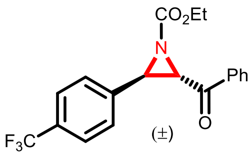
Pale yellow oil (74% yield, 83 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 – 7.96 (m, 2H), 7.66 – 7.61 (m, 1H), 7.53 – 7.48 (m, 4H), 7.28 – 7.27 (m, 1H), 7.26 – 7.25 (m, 1H), 4.32 – 4.19 (m, 2H), 4.00 (d, J = 2.4 Hz, 1H), 3.86 (d, J = 2.4 Hz, 1H), 1.26 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 160.3, 136.3, 135.0, 134.3, 131.9, 129.0, 128.6, 128.2, 122.6, 63.0, 47.2, 46.7, 14.4. IR (NaCl): 2981, 1732, 1677, 1598, 1302 cm^{-1}. HRMS (ESI) m/z calcd for $C_{18}H_{17}BrNO_3$ $[M+H]^+$ 374.0386, found 374.0388.

***Trans*-ethyl 2-benzoyl-3-(4-(methoxycarbonyl)phenyl)aziridine-1-carboxylate (2p):**



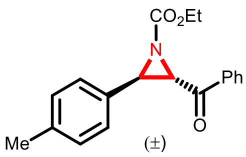
Colorless oil (65% yield, 69 mg), petroleum ether/ethyl acetate = 6 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.3 Hz, 2H), 8.02 – 7.98 (m, 2H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.54 – 7.44 (m, 4H), 4.26 (qd, *J* = 7.1, 4.3 Hz, 2H), 4.05 (d, *J* = 2.4 Hz, 1H), 3.95 (d, *J* = 2.3 Hz, 1H), 3.92 (s, 3H), 1.27 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 166.7, 160.2, 141.0, 136.4, 134.3, 130.4, 130.1, 129.1, 128.6, 126.6, 63.1, 52.3, 47.3, 46.8, 14.4. IR (NaCl): 2982, 1738, 1732, 1677, 1598, 1302 cm^{-1}. HRMS (ESI) m/z calcd for $C_{20}H_{20}NO_5$ $[M+H]^+$ 354.1336, found 354.1338.

***Trans*-ethyl 2-benzoyl-3-(4-(trifluoromethyl)phenyl)aziridine-1-carboxylate (2q):**



Colorless oil (76% yield, 83 mg), petroleum ether/ethyl acetate = 6 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01-7.98 (m, 2H), 7.65-7.62 (m, 3H), 7.53-7.48 (m, 4H), 4.31 – 4.21 (m, 2H), 4.09 – 4.00 (m, 1H), 4.00 – 3.91 (m, 1H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.8, 160.2, 140.0, 136.3, 134.3, 130.8 (d, *J* = 32.6 Hz), 129.1, 128.6, 126.9, 125.8 (q, *J* = 3.7 Hz), 123.9 (d, *J* = 228.5 Hz), 63.1, 47.2, 46.5, 14.4. IR (NaCl): 2982, 1732, 1677, 1599, 1303 cm^{-1}. HRMS (ESI) m/z calcd for $C_{19}H_{17}F_3NO_3$ $[M+H]^+$ 364.1155, found 364.1162.

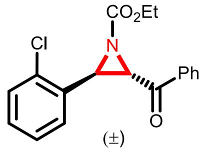
***Trans*-ethyl 2-benzoyl-3-(p-tolyl)aziridine-1-carboxylate (2r):**



Colorless oil (56% yield, 52 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.3 Hz, 2H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 7.8 Hz, 2H), 4.41 – 4.18 (m, 2H), 4.05 (d, *J* = 2.4 Hz, 1H), 3.88 (d, *J* = 2.2 Hz, 1H), 2.38 (s, 3H), 1.27 (t, *J* = 7.1 Hz, 3H). ^{13}C

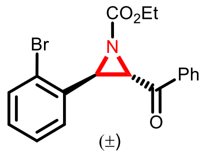
NMR (100 MHz, $CDCl_3$) δ 192.3, 160.6, 138.5, 136.6, 134.1, 133.0, 129.5, 129.0, 128.6, 126.5, 62.9, 47.6, 47.3, 21.3, 14.5. IR (NaCl): 2981, 1732, 1678, 1597, 1300 cm^{-1}. HRMS (ESI) m/z calcd for $C_{19}H_{20}NO_3$ $[M+H]^+$ 310.1438, found 310.1441.

***Trans*-ethyl 2-benzoyl-3-(2-chlorophenyl)aziridine-1-carboxylate (2s):**



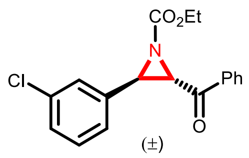
Colorless oil (81% yield, 80 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^1H NMR (400 MHz, $CDCl_3$) δ 8.08 – 7.97 (m, 2H), 7.64 (t, J = 7.4 Hz, 1H), 7.56 – 7.47 (m, 3H), 7.41 – 7.35 (m, 1H), 7.32 – 7.27 (m, 2H), 4.29 (qd, J = 7.1, 2.4 Hz, 2H), 4.12 (d, J = 2.5 Hz, 1H), 3.96 (d, J = 2.5 Hz, 1H), 1.29 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.1, 160.6, 136.4, 134.1, 134.1, 134.0, 129.6, 129.3, 129.0, 128.6, 127.9, 127.2, 63.0, 46.1, 45.7, 14.5. IR (NaCl): 2981, 1732, 1674, 1597, 1279 cm^{-1}. HRMS (ESI) m/z calcd for $C_{18}H_{17}ClNO_3$ $[M+H]^+$ 330.0891, found 330.0893.

***Trans*-ethyl 2-benzoyl-3-(2-bromophenyl)aziridine-1-carboxylate (2t):**



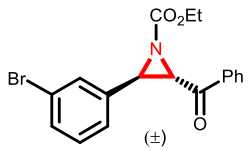
Colorless oil (87% yield, 98 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^1H NMR (400 MHz, $CDCl_3$) δ 8.01 – 7.98 (t, J = 7.4 Hz, 2H), 7.64 (t, J = 7.4 Hz, 1H), 7.55 – 7.47 (m, 4H), 7.41 – 7.35 (m, 1H), 7.28 – 7.21 (m, 1H), 4.26 (qd, J = 7.1, 2.4 Hz, 2H), 4.01 (d, J = 2.5 Hz, 1H), 3.96 (d, J = 2.5 Hz, 1H), 1.27 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 160.2, 138.3, 136.4, 134.3, 131.7, 130.4, 129.4, 129.1, 128.6, 125.4, 123.0, 63.1, 47.2, 46.5, 14.4. IR (NaCl): 2981, 1732, 1677, 1599, 1301 cm^{-1}. HRMS (ESI) m/z calcd for $C_{18}H_{17}BrNO_3$ $[M+H]^+$ 374.0386, found 374.0388.

***Trans*-ethyl 2-benzoyl-3-(3-chlorophenyl)aziridine-1-carboxylate (2u):**



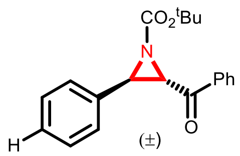
Colorless oil (70% yield, 69 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 7.94 (m, 2H), 7.67 – 7.61 (m, 1H), 7.51 (t, *J* = 7.8 Hz, 2H), 7.39 (d, *J* = 1.4 Hz, 1H), 7.32-7.29 (m, 3H), 4.26 (dt, *J* = 7.2, 2.7 Hz, 2H), 4.02 (d, *J* = 2.4 Hz, 1H), 3.87 (d, *J* = 2.4 Hz, 1H), 1.27 (t, *J* = 8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.9, 160.2, 138.0, 136.3, 134.9, 134.3, 130.1, 129.0, 128.8, 128.6, 126.5, 124.9, 63.1, 47.2, 46.5, 14.4. IR (NaCl): 2982, 1732, 1674, 1597, 1275 cm^{-1}. HRMS (ESI) m/z calcd for $C_{18}H_{17}ClNO_3$ $[M+H]^+$ 330.0891, found 330.0892.

***Trans*-ethyl 2-benzoyl-3-(3-bromophenyl)aziridine-1-carboxylate (2v):**



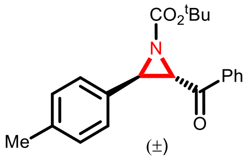
Colorless oil (71% yield, 80 mg), petroleum ether/ethyl acetate = 8 : 1 – 4:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 – 7.99 (m, 2H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.58 – 7.46 (m, 4H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.21 (td, *J* = 7.7, 1.5 Hz, 1H), 4.34 – 4.24 (m, 2H), 4.06 (d, *J* = 2.4 Hz, 1H), 3.95 (d, *J* = 2.5 Hz, 1H), 1.29 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.1, 160.6, 136.4, 135.7, 134.1, 132.4, 129.9, 128.9, 128.6, 128.3, 127.8, 123.7, 63.0, 48.1, 46.1, 14.5. IR (NaCl): 2981, 1732, 1677, 1599, 1302 cm^{-1}. HRMS (ESI) m/z calcd for $C_{18}H_{17}BrNO_3$ $[M+H]^+$ 374.0386, found 374.0388.

***Trans-tert*-butyl 2-benzoyl-3-phenylaziridine-1-carboxylate (2w)**



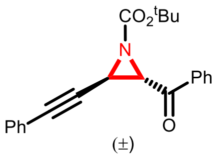
Colorless oil (85% yield, 83 mg), petroleum ether/ethyl acetate = 6 : 1 – 3:1 (v/v) as eluent for column chromatography; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 7.6 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.41 – 7.28 (m, 5H), 4.01 (s, 1H), 3.93 (d, *J* = 1.6 Hz, 1H), 1.44 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.5, 159.0, 136.8, 136.1, 133.9, 128.9, 128.8, 128.7, 128.6, 128.5, 126.6, 82.2, 47.2, 28.0. IR (NaCl): 2982, 1730, 1677, 1597, 1301 cm^{-1}. HRMS (ESI) m/z calcd for $C_{20}H_{22}NO_3$ $[M+H]^+$ 324.1594, found 324.1598.

***Trans-tert*-butyl 2-benzoyl-3-(p-tolyl)aziridine-1-carboxylate (2x)**



Colorless oil (74% yield, 75 mg), petroleum ether/ethyl acetate = 6 : 1 – 3:1 (v/v) as eluent for column chromatography; ^1H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 7.7 Hz, 2H), 7.61 (t, J = 7.3 Hz, 1H), 7.49 (t, J = 7.6 Hz, 2H), 7.26 (s, 2H), 7.17 (d, J = 7.7 Hz, 2H), 3.99 (d, J = 1.6 Hz, 1H), 3.89 (s, 1H), 2.35 (s, 3H), 1.44 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.6, 159.1, 138.4, 136.9, 133.9, 133.2, 129.4, 128.9, 128.5, 126.5, 82.1, 47.27, 47.23, 28.1, 21.3. IR (NaCl): 2982, 1730, 1677, 1595, 1300 cm^{-1}. HRMS (ESI) m/z calcd for $C_{21}H_{24}NO_3$ $[M+H]^+$ 338.1751, found 338.1756.

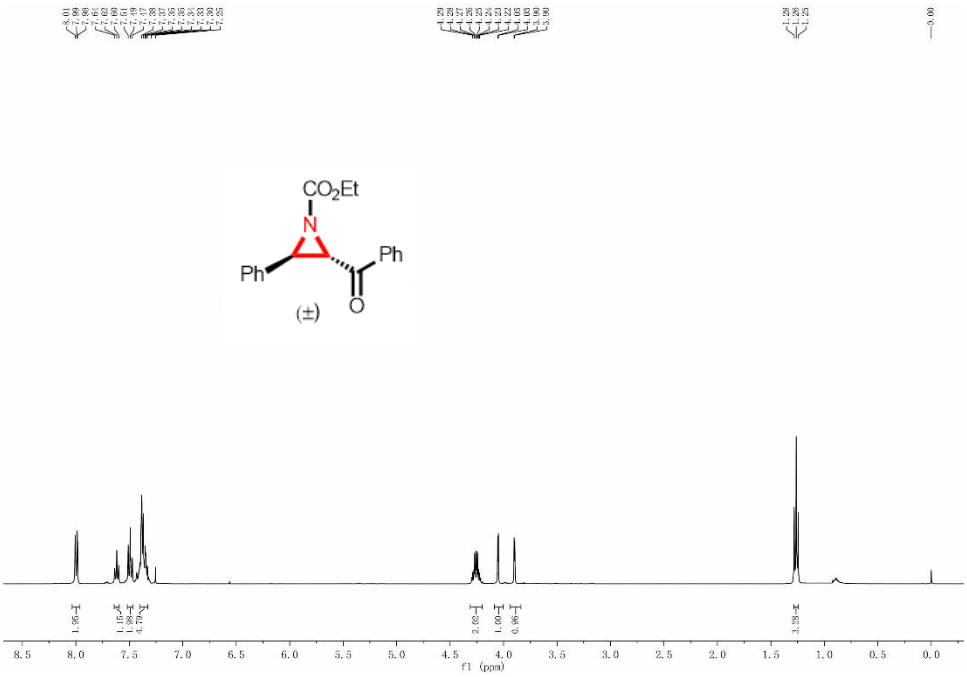
***Trans-tert*-butyl 2-benzoyl-3-(phenylethynyl)aziridine-1-carboxylate (2y)**



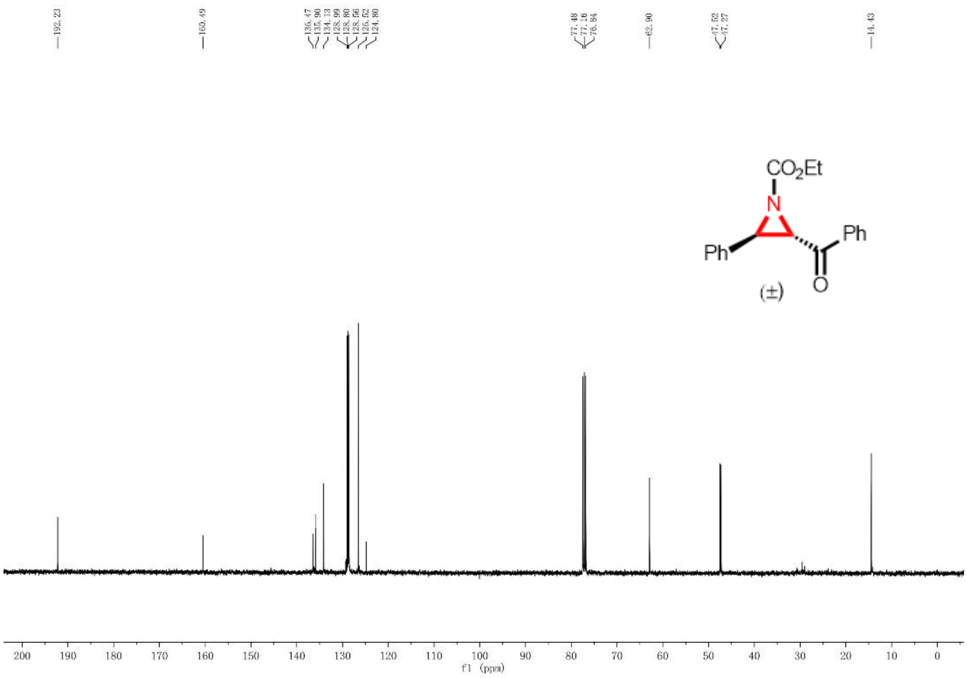
Colorless oil (51% yield, 53 mg), petroleum ether/ethyl acetate = 8 : 1 – 3:1 (v/v) as eluent for column chromatography; ^1H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 7.9 Hz, 2H), 7.65 (t, J = 7.2 Hz, 1H), 7.54 (t, J = 7.4 Hz, 2H), 7.45 (d, J = 7.5 Hz, 2H), 7.37 – 7.29 (m, 3H), 4.23 (s, 1H), 3.60 (s, 1H), 1.47 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.0, 158.5, 134.2, 132.1, 129.1, 129.0, 128.8, 128.5, 83.9, 83.5, 82.8, 45.0, 33.9, 28.1. IR (NaCl): 2982, 2156, 1730, 1676, 1297 cm^{-1}. HRMS (ESI) m/z calcd for $C_{22}H_{22}NO_3$ $[M+H]^+$ 348.1594, found 348.1597.

Part II NMR Spectra

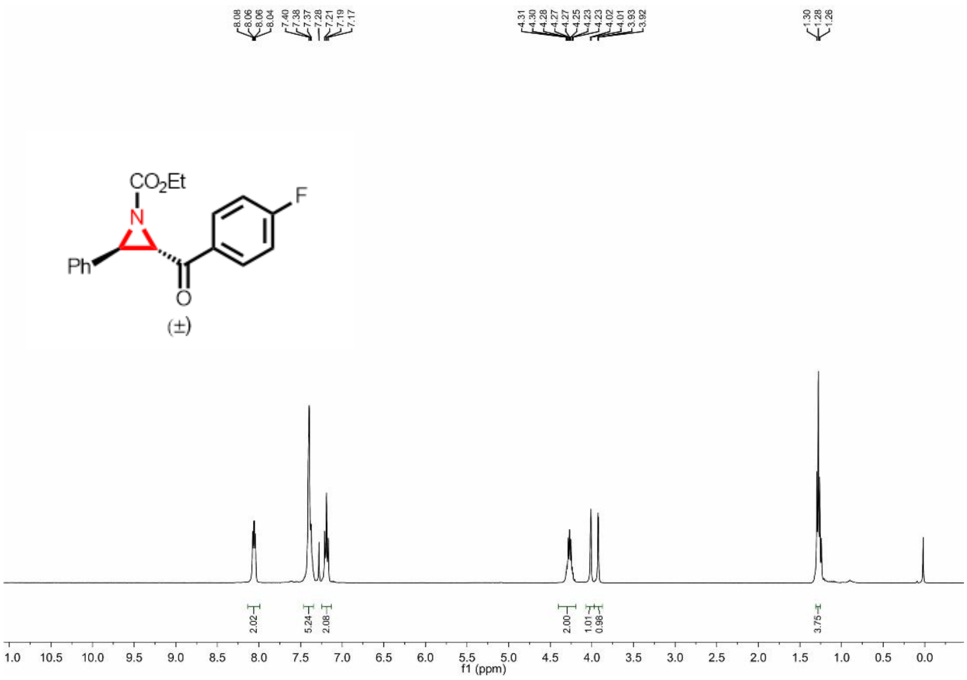
^{1}HNMR of **2a** (400 MHz, $CDCl_3$)



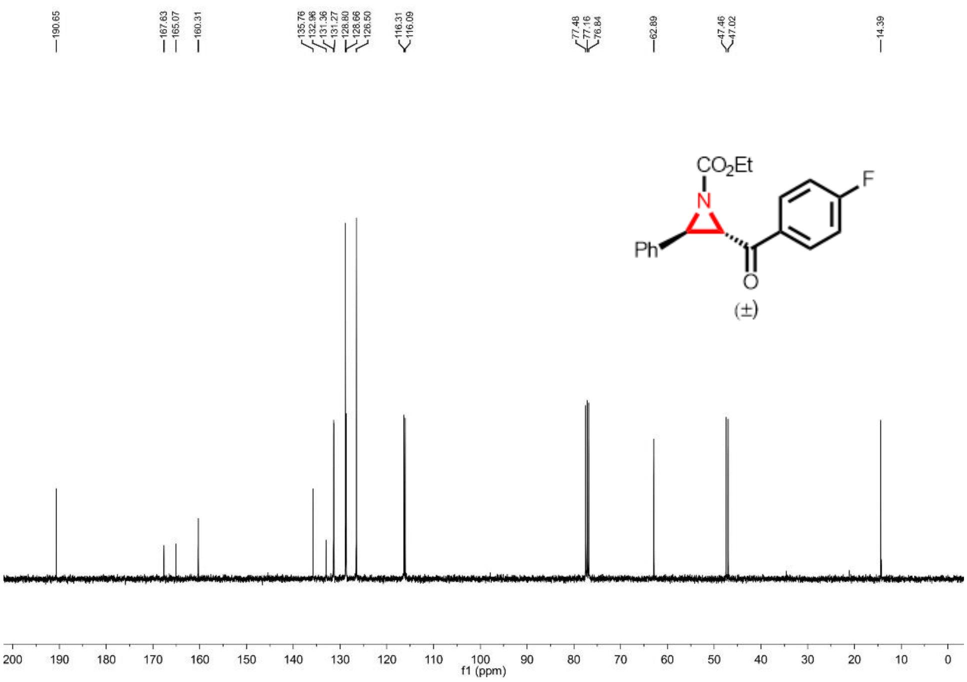
^{13}CNMR of **2a** (100 MHz, $CDCl_3$)



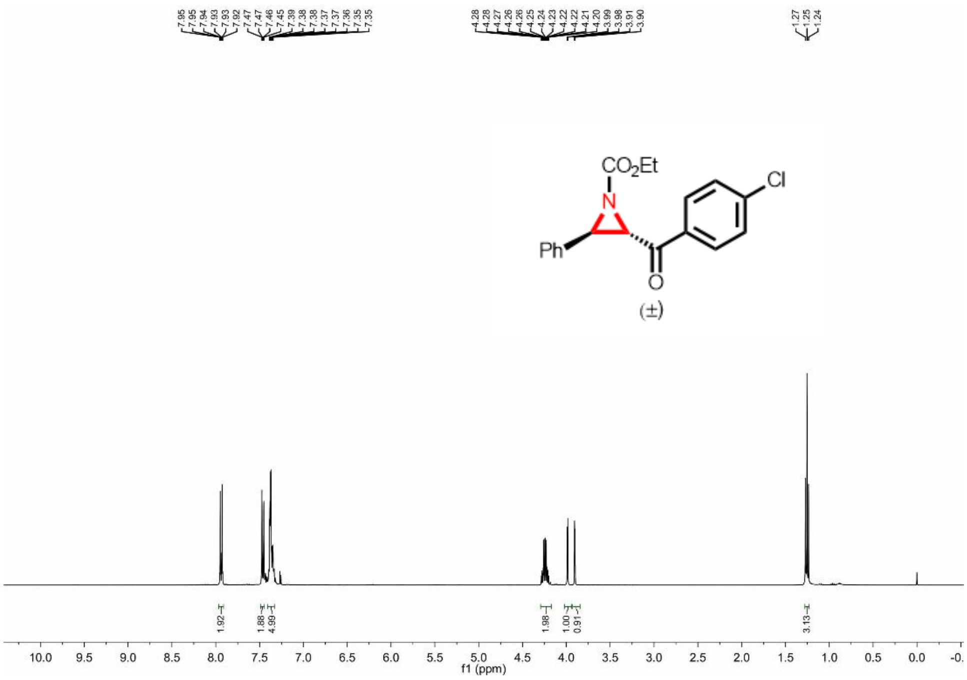
^{1}HNMR of **2b** (400 MHz, $CDCl_3$)



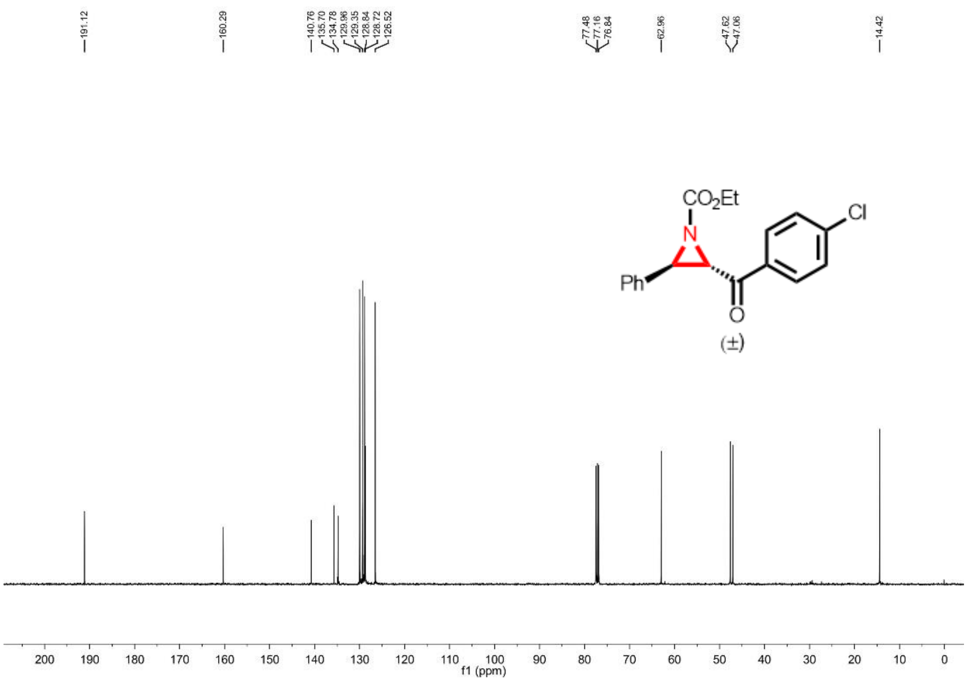
^{13}CNMR of **2b** (100 MHz, $CDCl_3$)



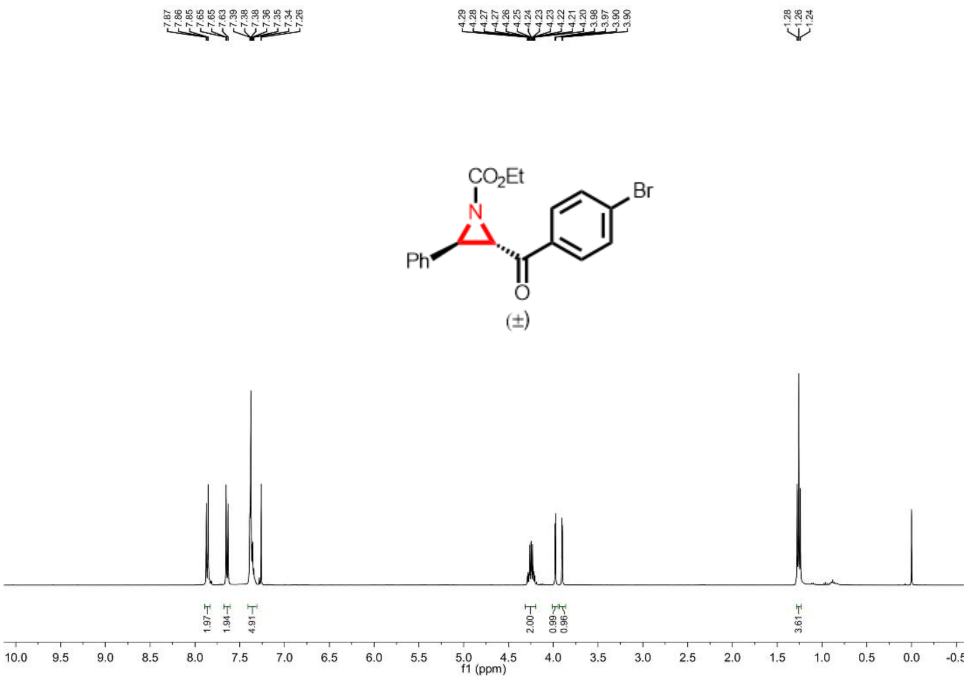
^{1}HNMR of **2c** (400 MHz, $CDCl_3$)



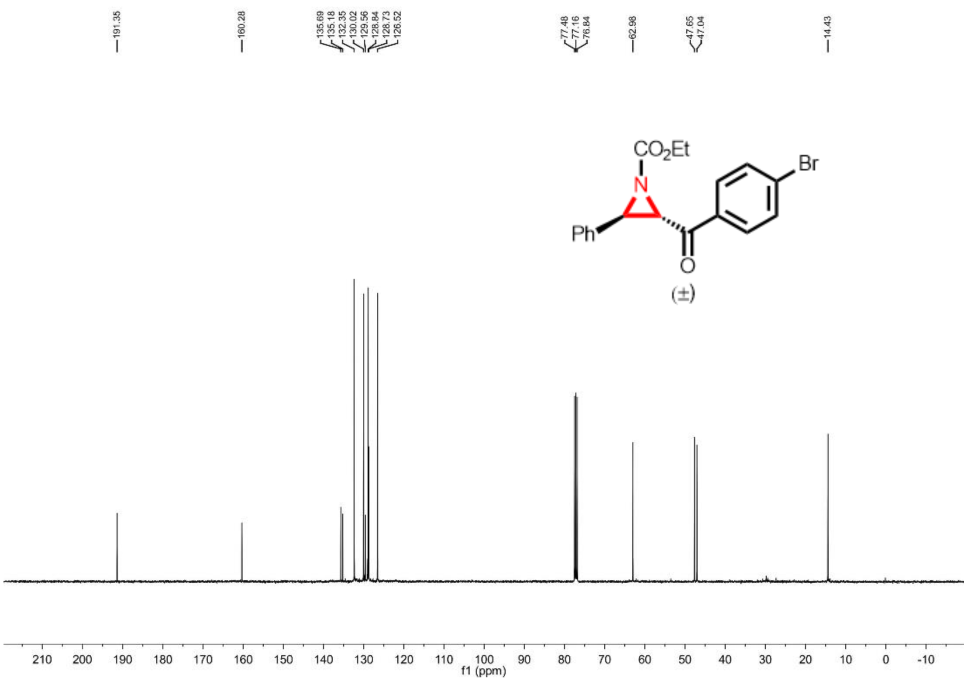
^{13}CNMR of **2c** (100 MHz, $CDCl_3$)



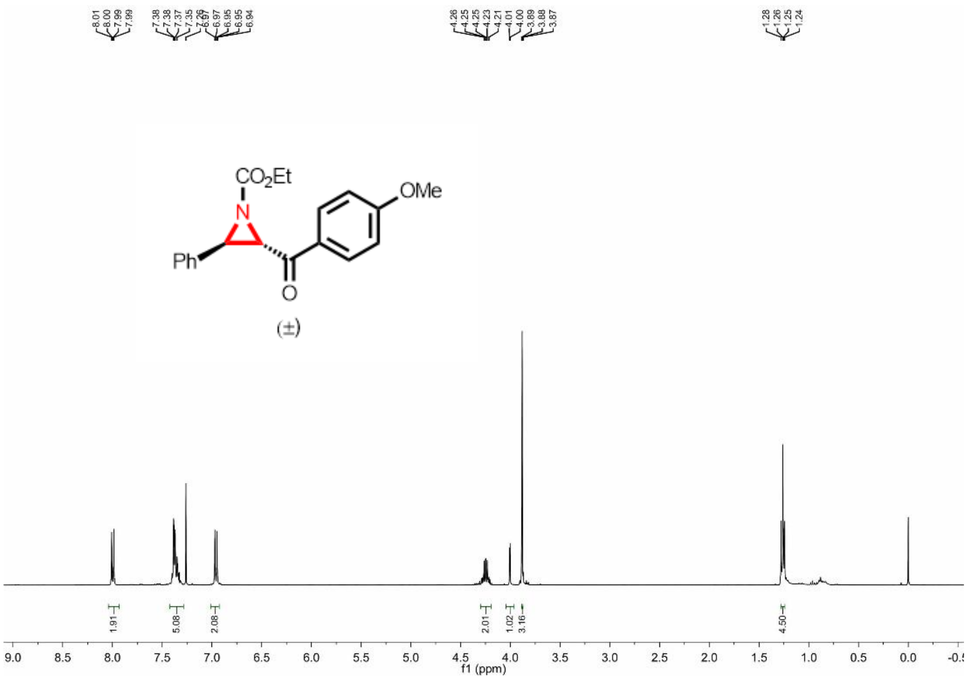
^{1}HNMR of **2d** (400 MHz, $CDCl_3$)



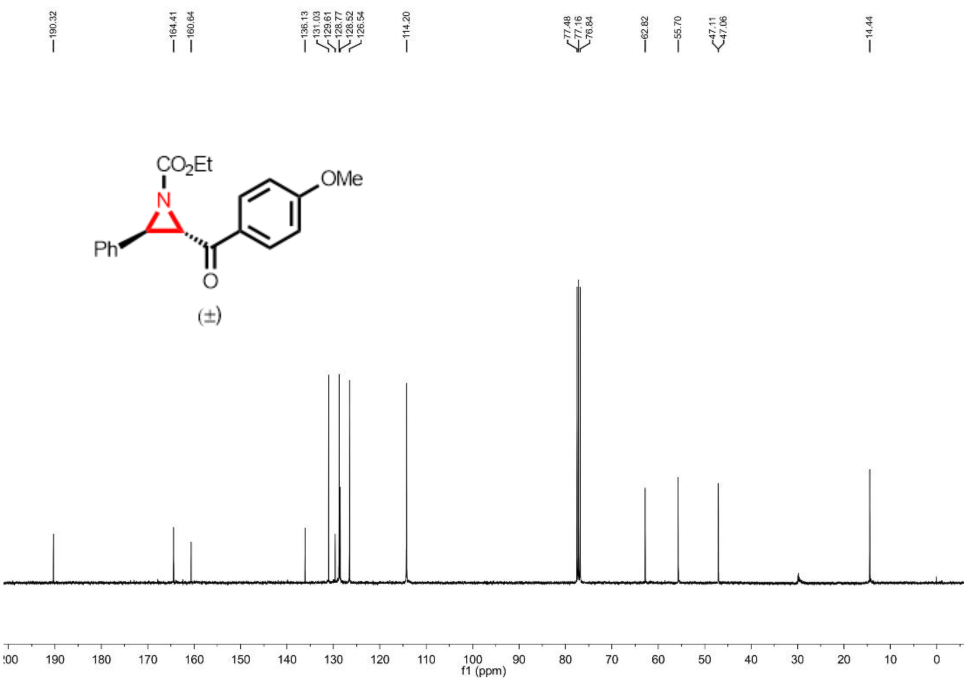
^{13}CNMR of **2d** (100 MHz, $CDCl_3$)



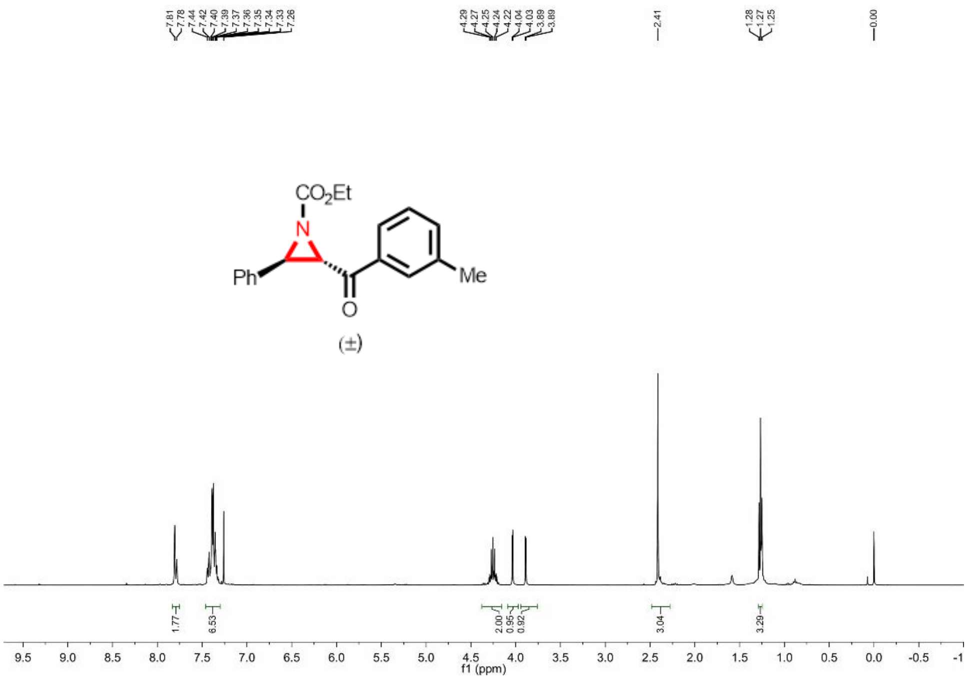
[1]HNMR of **2e** (400 MHz, $CDCl_3$)



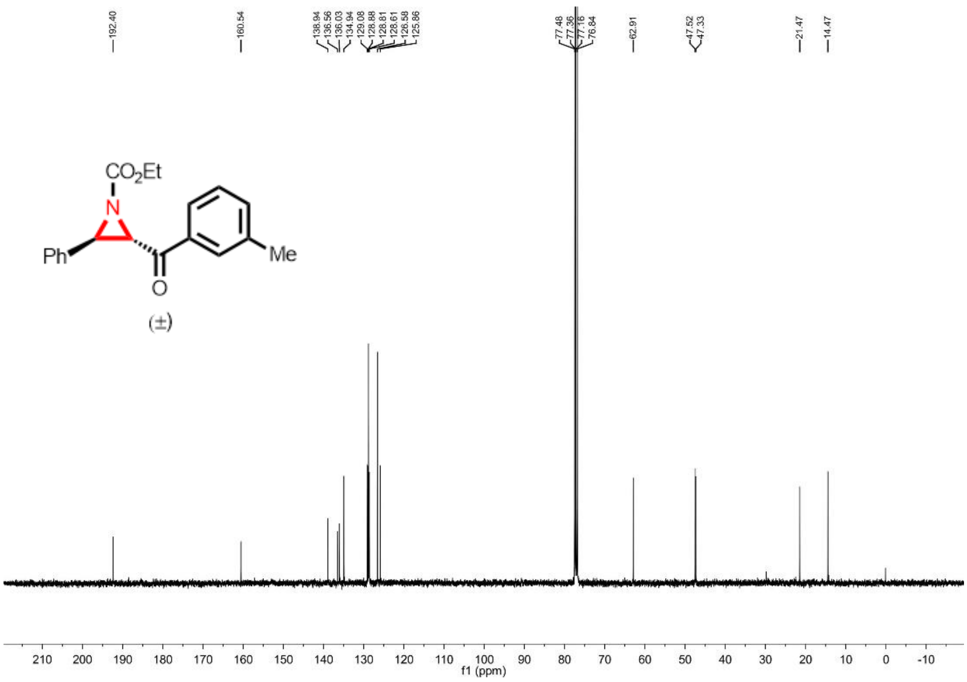
[13]CNMR of **2e** (100 MHz, $CDCl_3$)



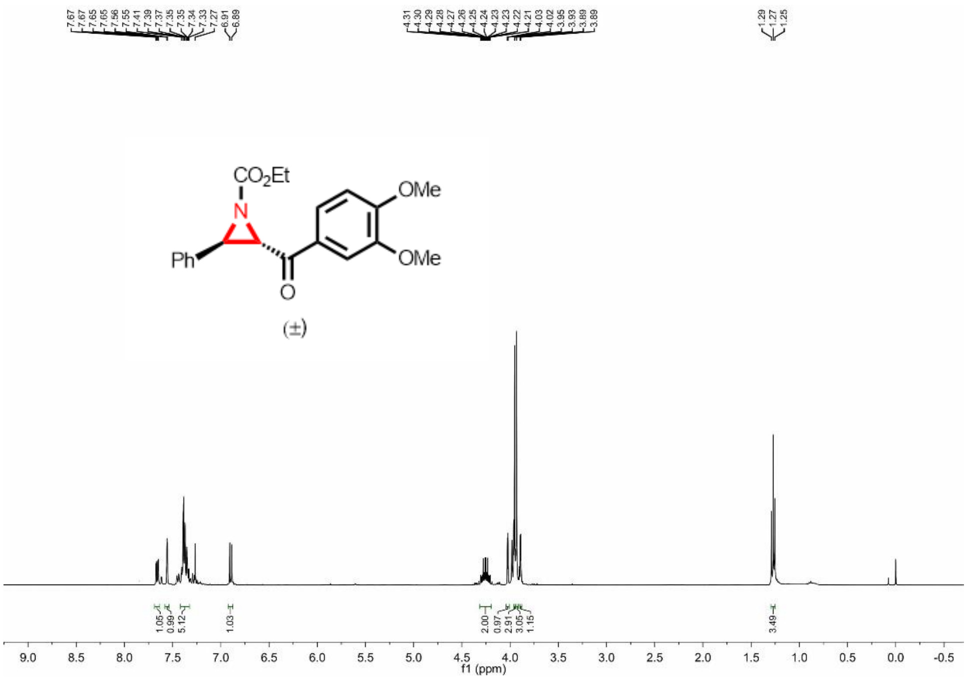
[1]HNMR of **2f** (400 MHz, $CDCl_3$)



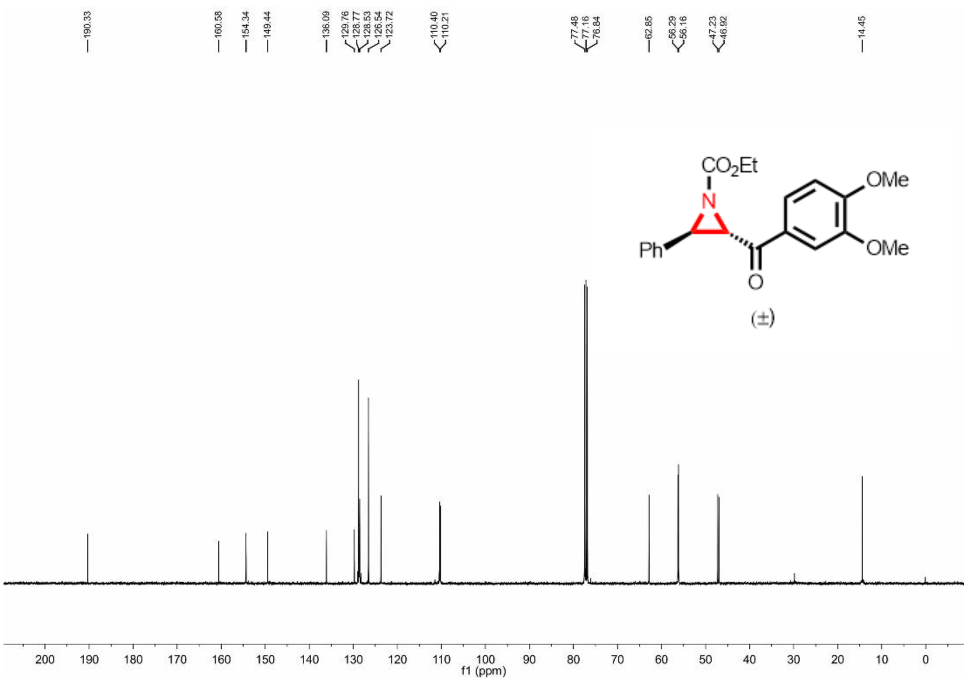
[13]CNMR of **2f** (100 MHz, $CDCl_3$)



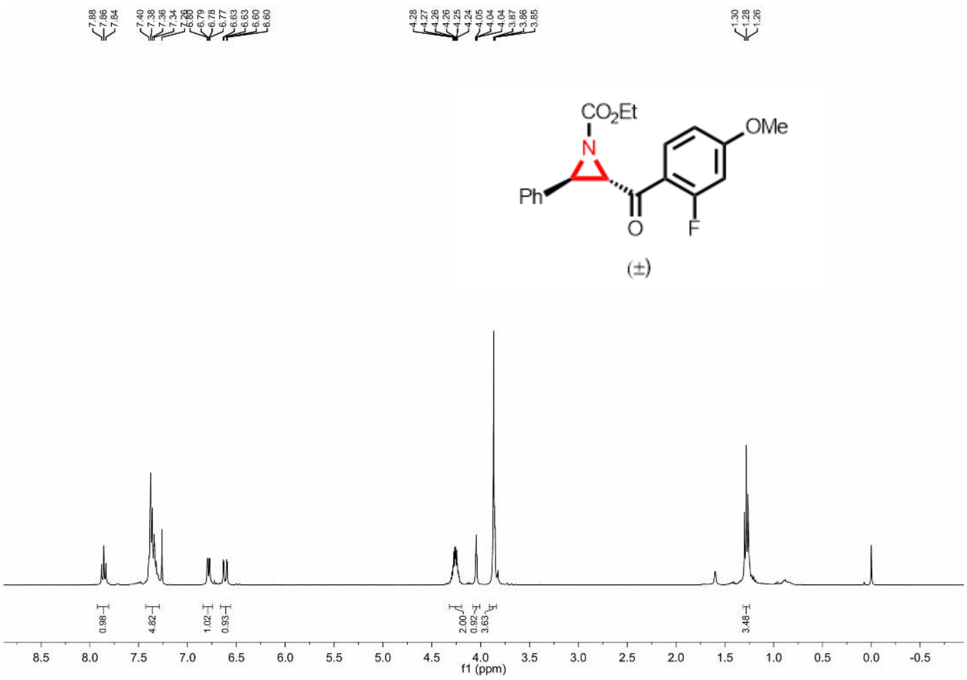
^{1}HNMR of **2g** (400 MHz, $CDCl_3$)



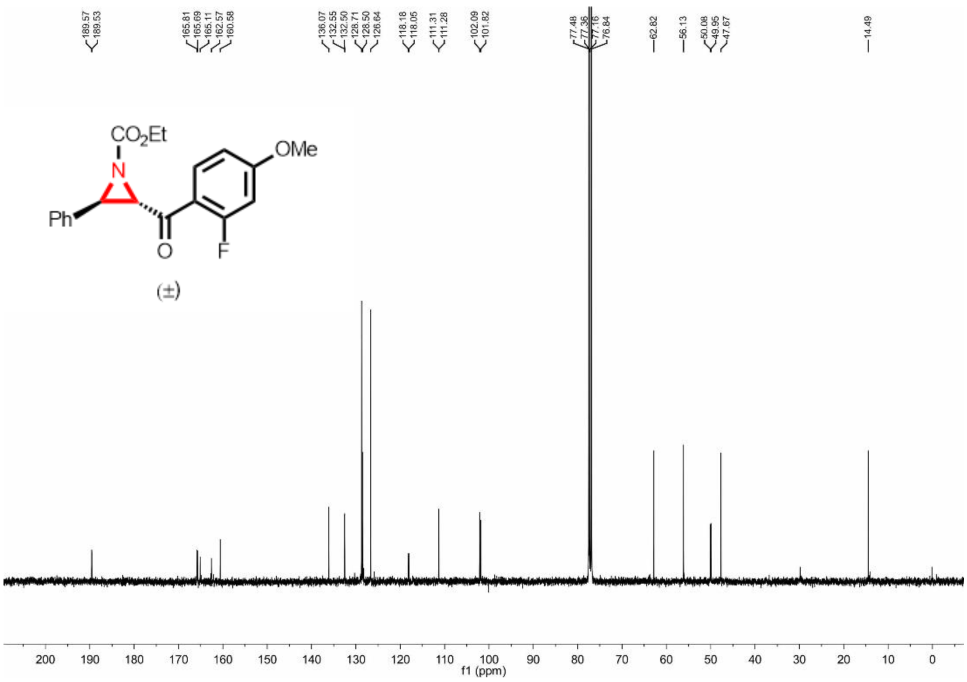
^{13}CNMR of **2g** (100 MHz, $CDCl_3$)



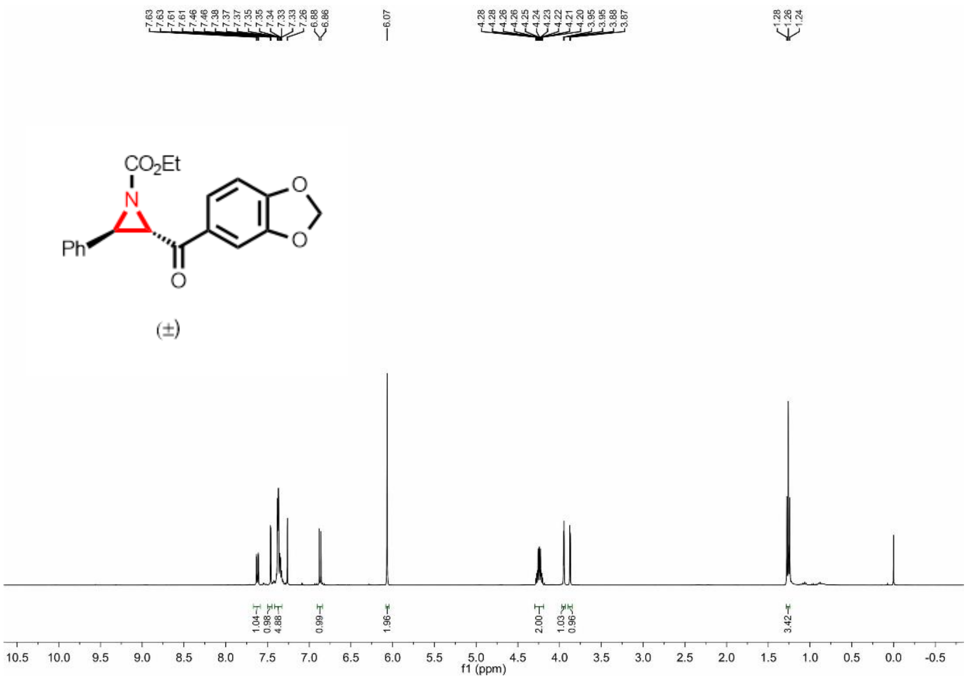
^{1}HNMR of **2h** (400 MHz, $CDCl_3$)



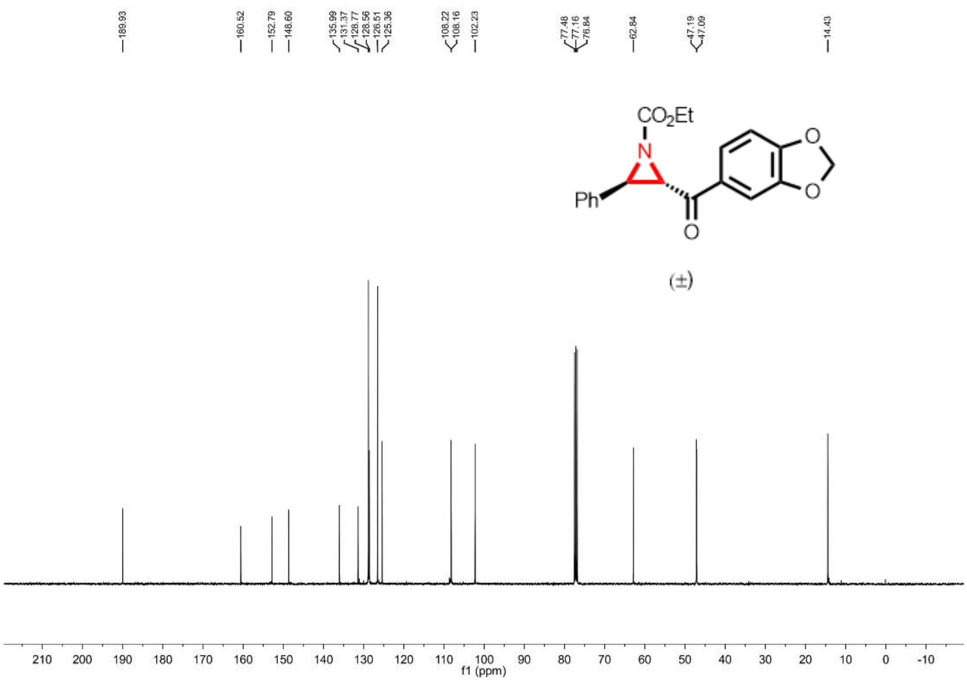
^{13}CNMR of **2h** (100 MHz, $CDCl_3$)



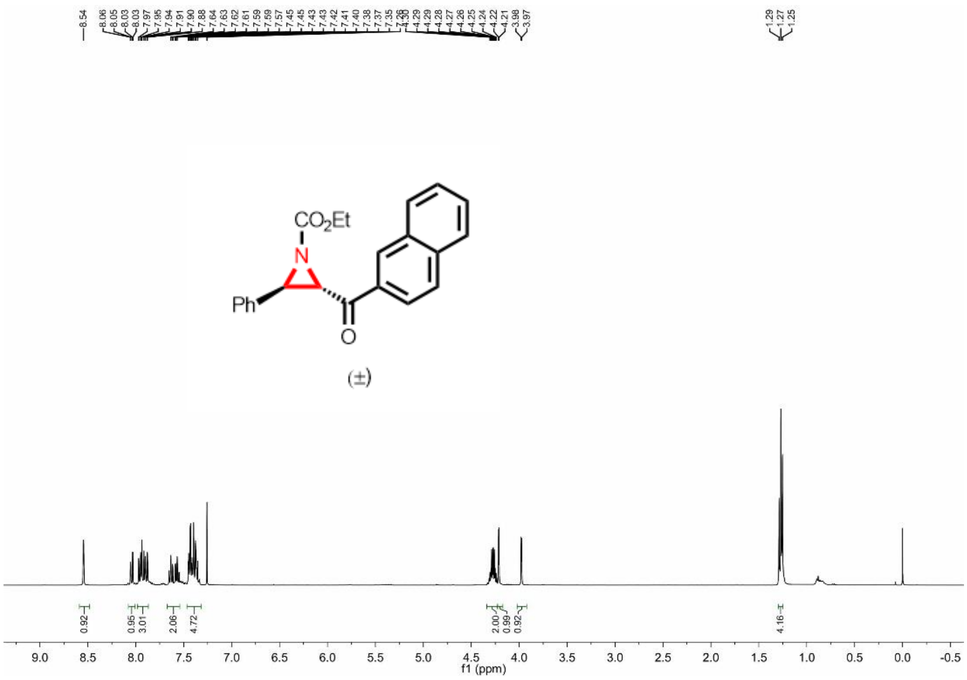
^{1}HNMR of **2i** (400 MHz, $CDCl_3$)



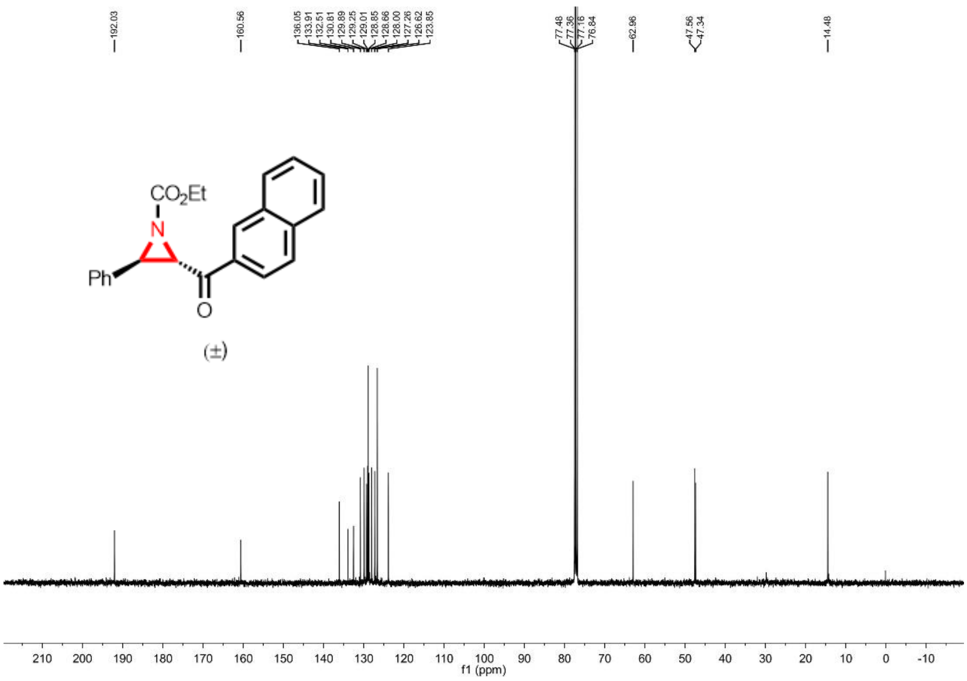
^{13}CNMR of **2i** (100 MHz, $CDCl_3$)



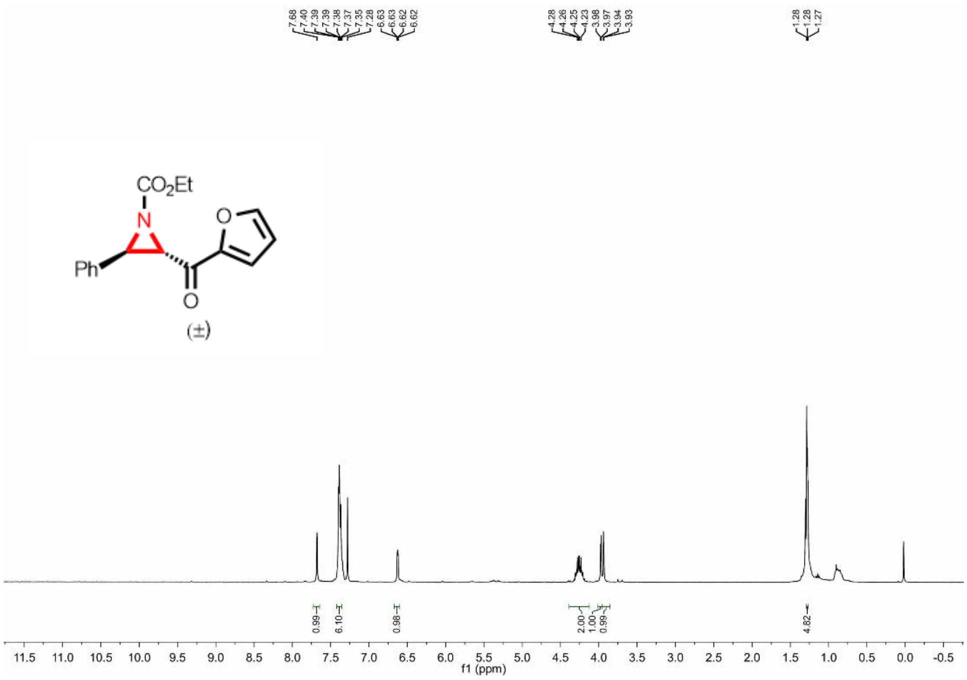
^{1}HNMR of **2j** (400 MHz, $CDCl_3$)



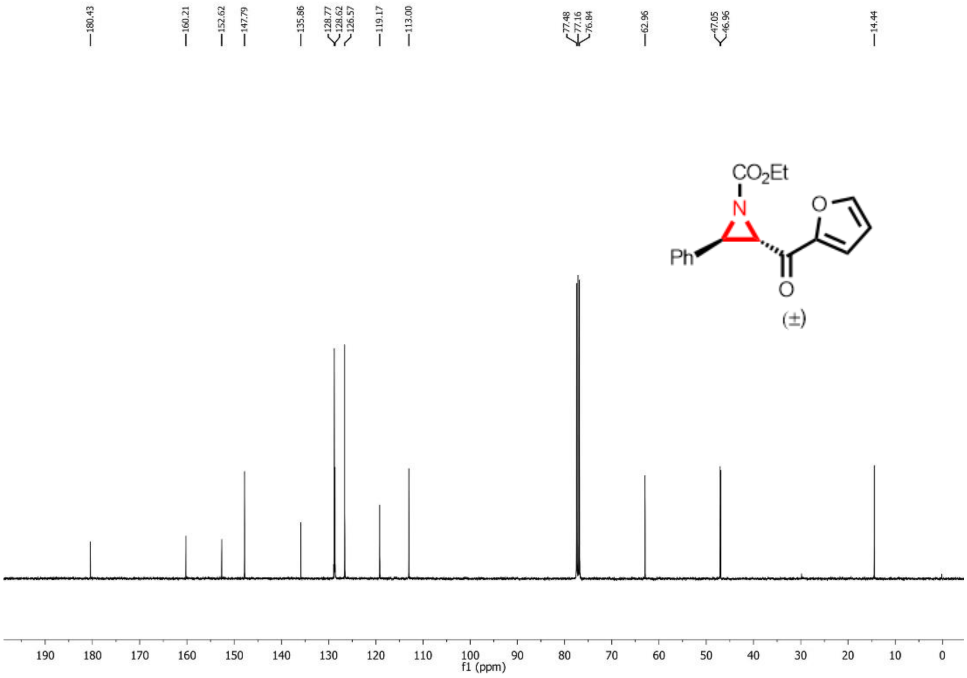
^{13}CNMR of **2j** (100 MHz, $CDCl_3$)



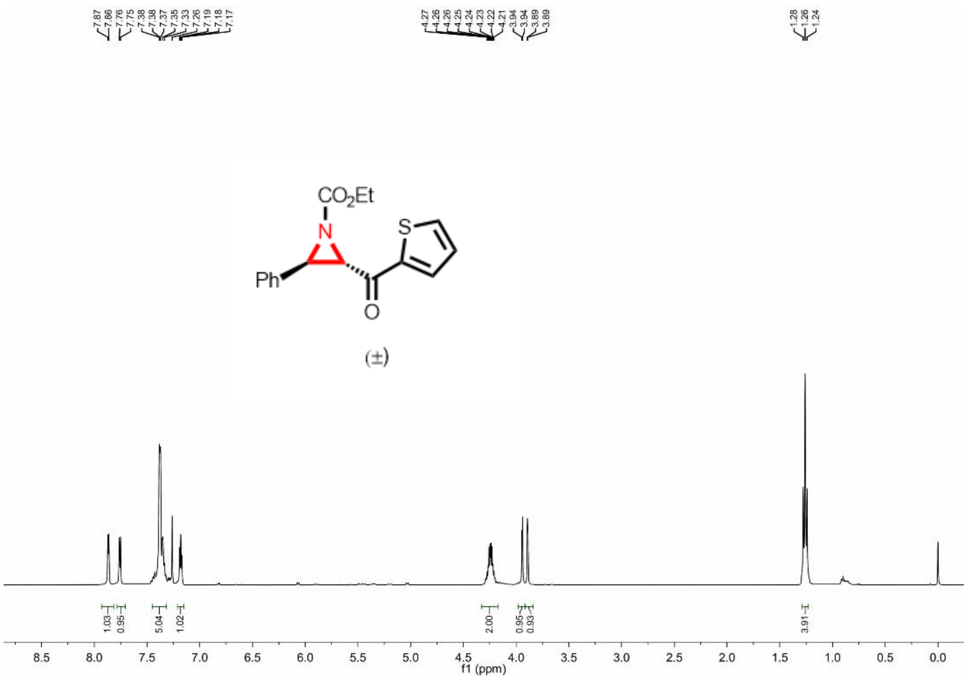
^{1}HNMR of **2k** (400 MHz, $CDCl_3$)



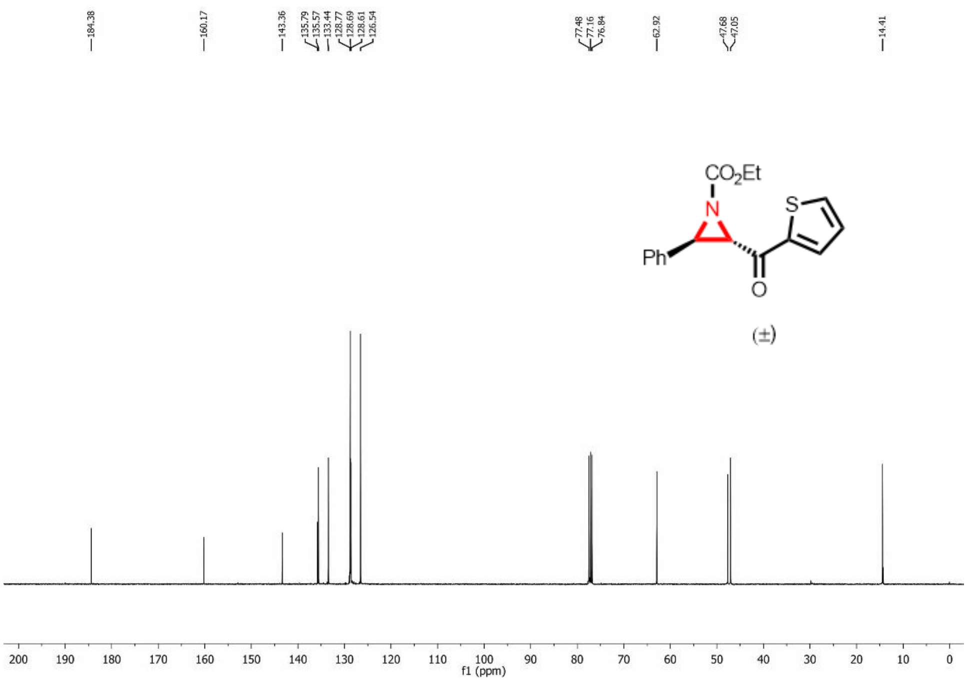
^{13}CNMR of **2k** (100 MHz, $CDCl_3$)



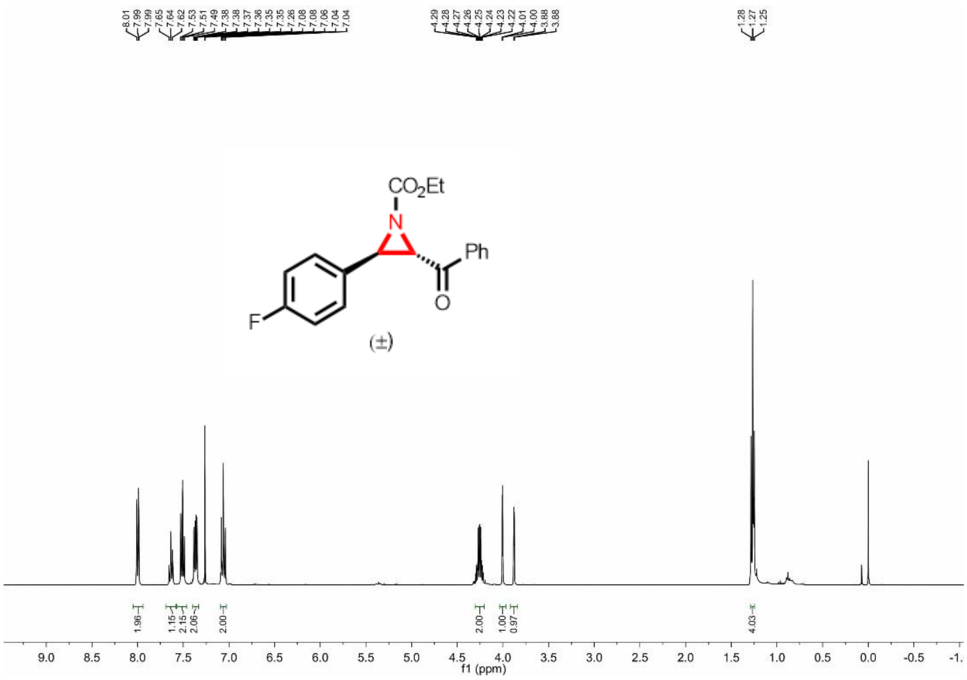
[1]HNMR of **2l** (400 MHz, $CDCl_3$)



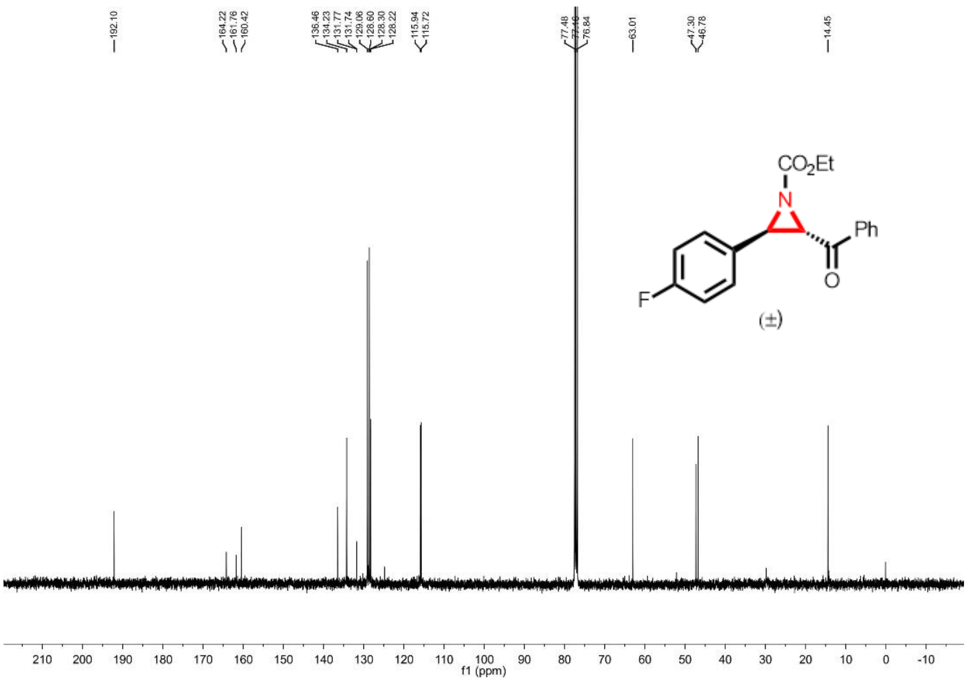
[13]CNMR of **2l** (100 MHz, $CDCl_3$)



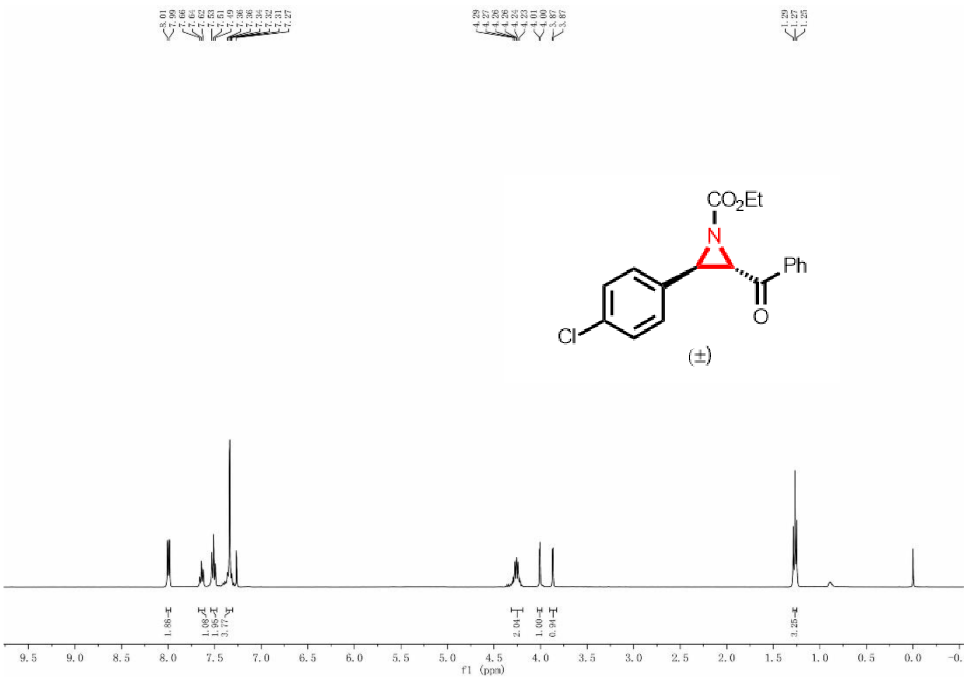
^{1}HNMR of **2m** (400 MHz, $CDCl_3$)



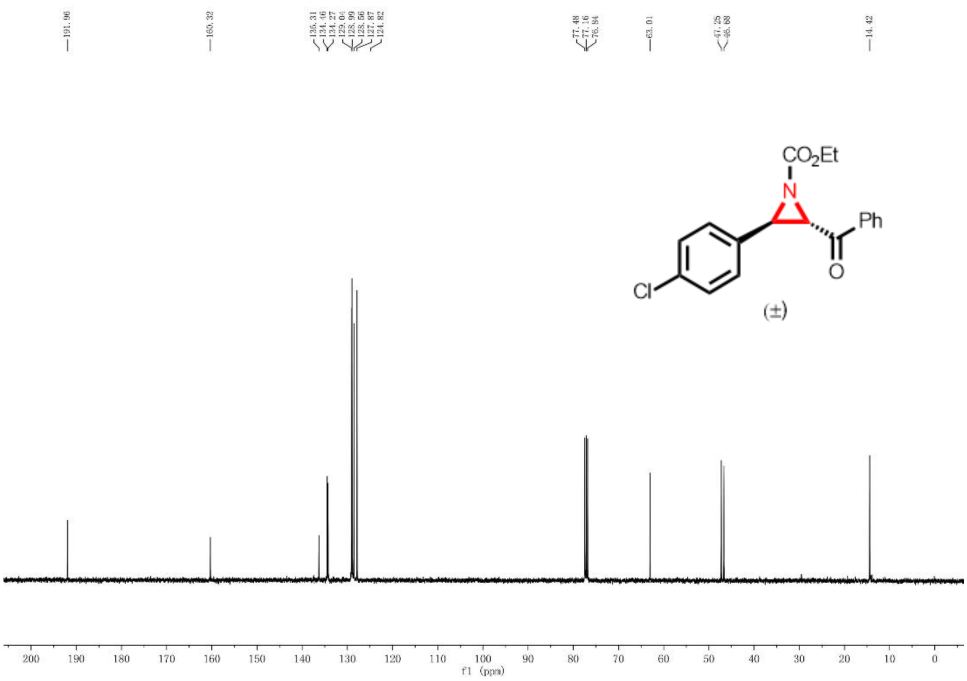
^{13}CNMR of **2m** (100 MHz, $CDCl_3$)



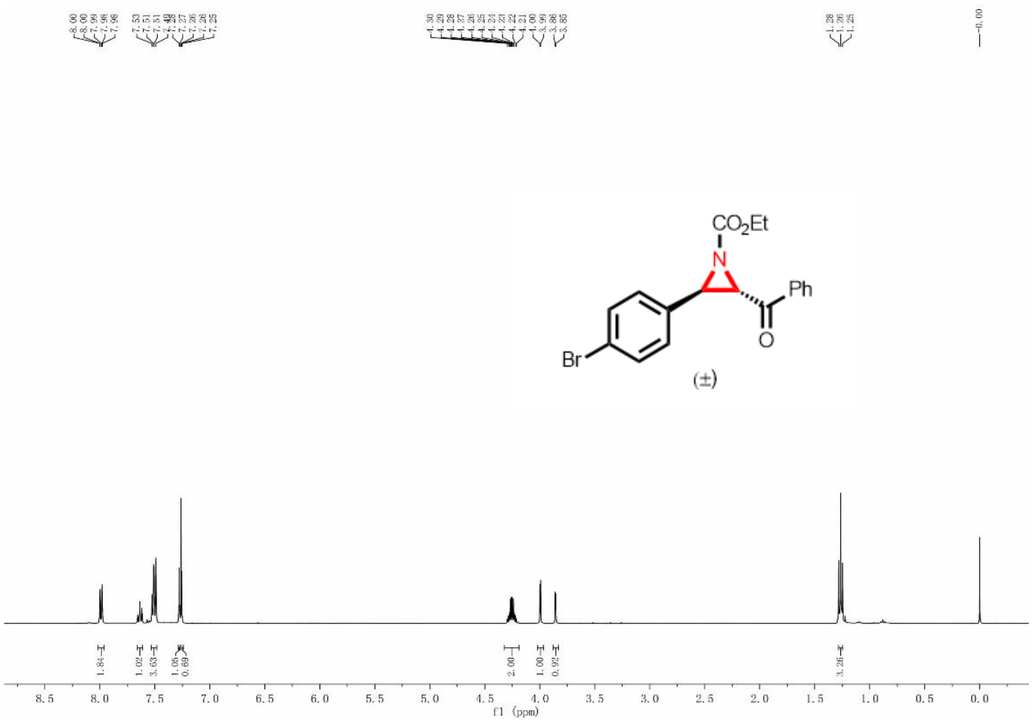
^{1}HNMR of **2n** (400 MHz, $CDCl_3$)



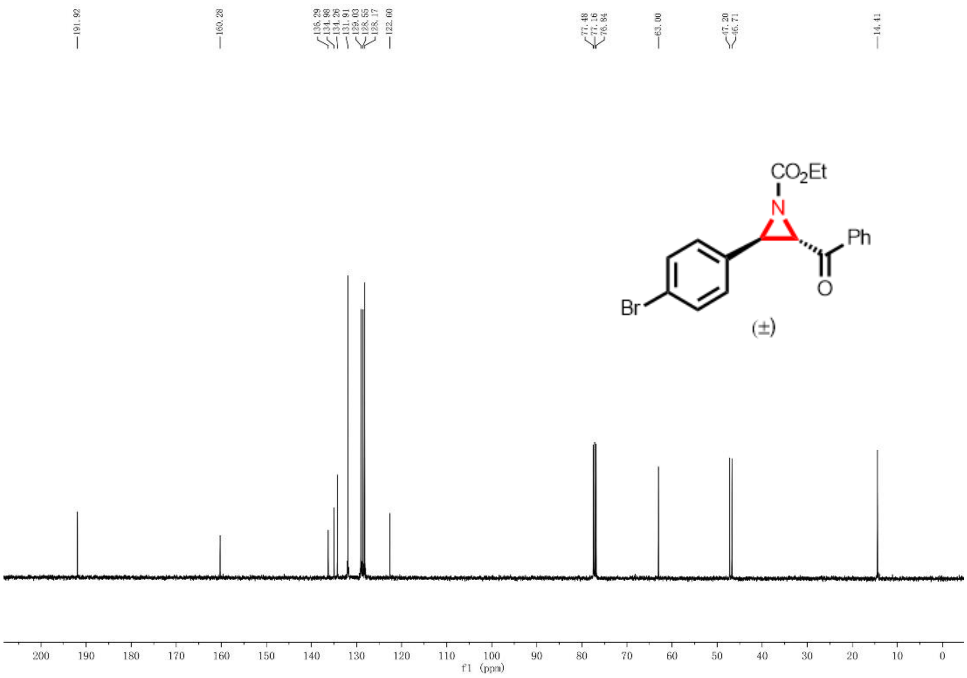
^{13}CNMR of **2n** (100 MHz, $CDCl_3$)



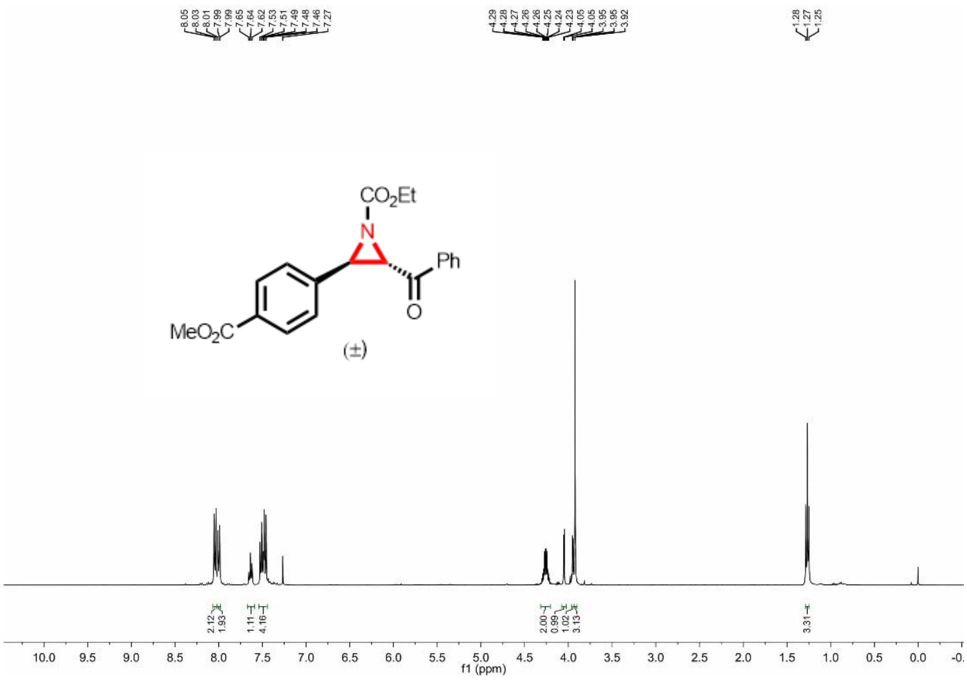
^{1}HNMR of **2o** (400 MHz, $CDCl_3$)



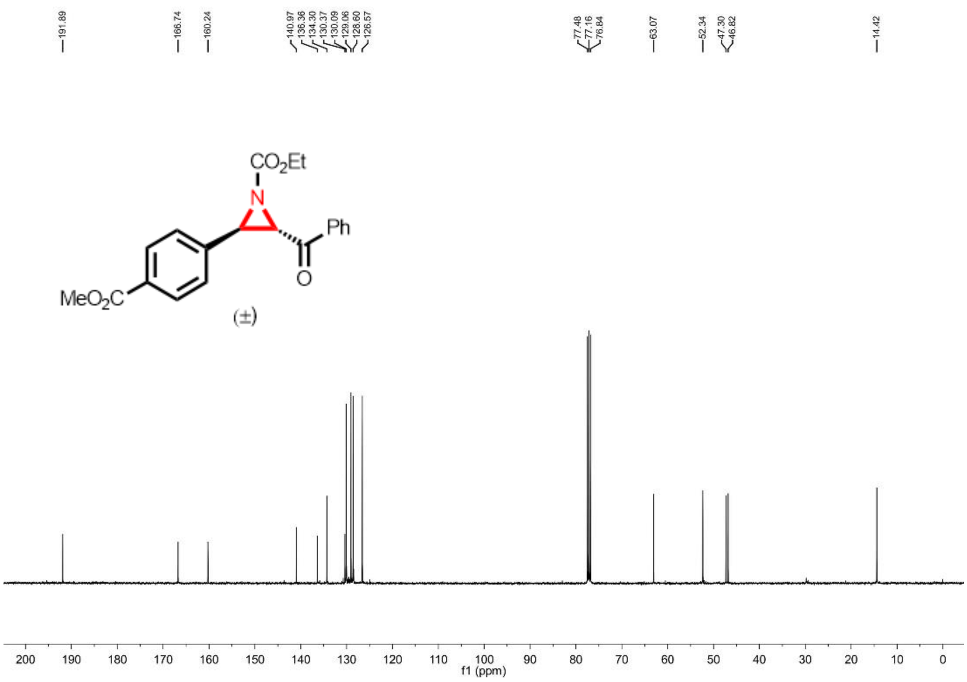
^{13}CNMR of **2o** (100 MHz, $CDCl_3$)



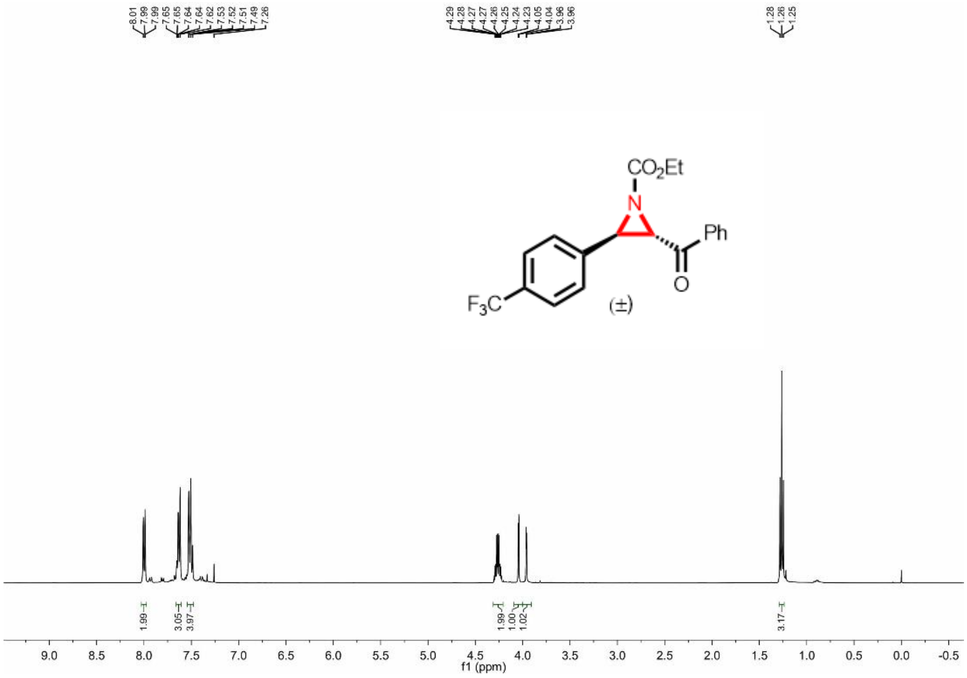
^{1}HNMR of **2p** (400 MHz, $CDCl_3$)



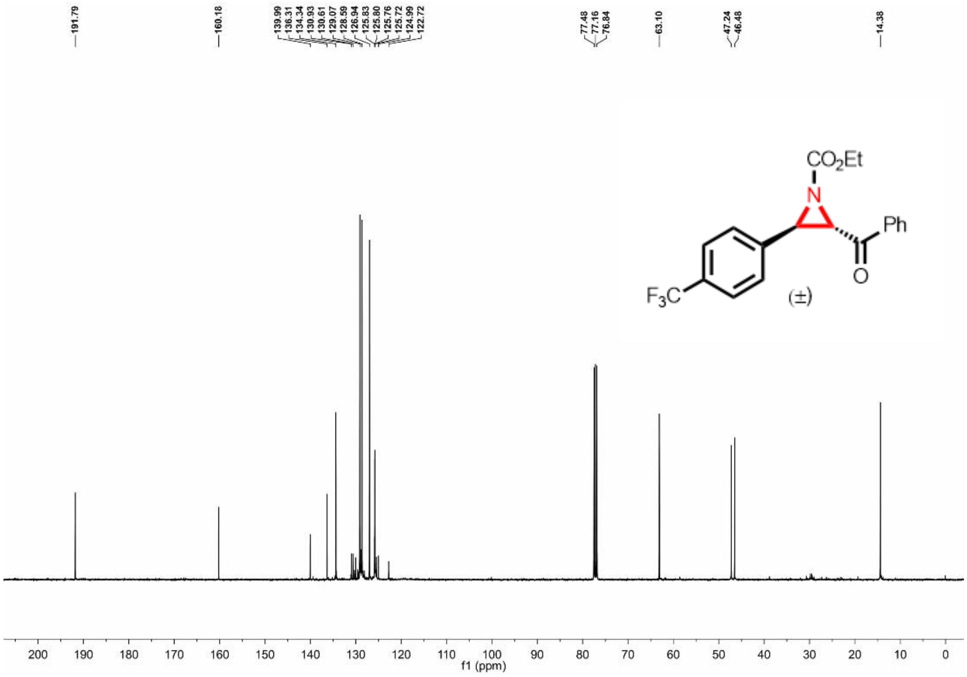
^{13}CNMR of **2p** (100 MHz, $CDCl_3$)



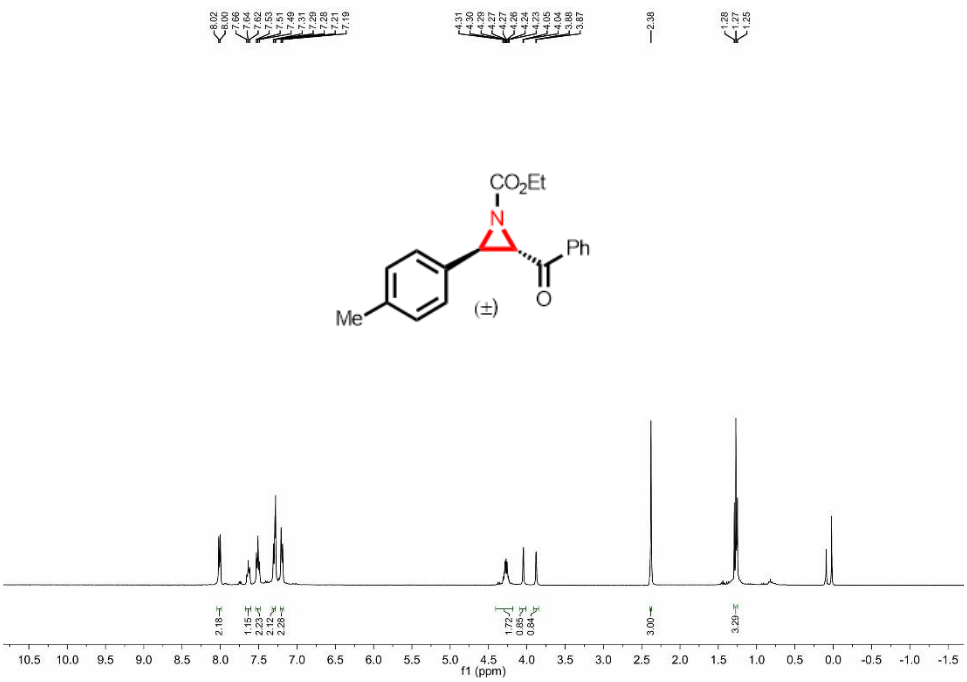
^{1}HNMR of **2q** (400 MHz, CDCl$_3$)



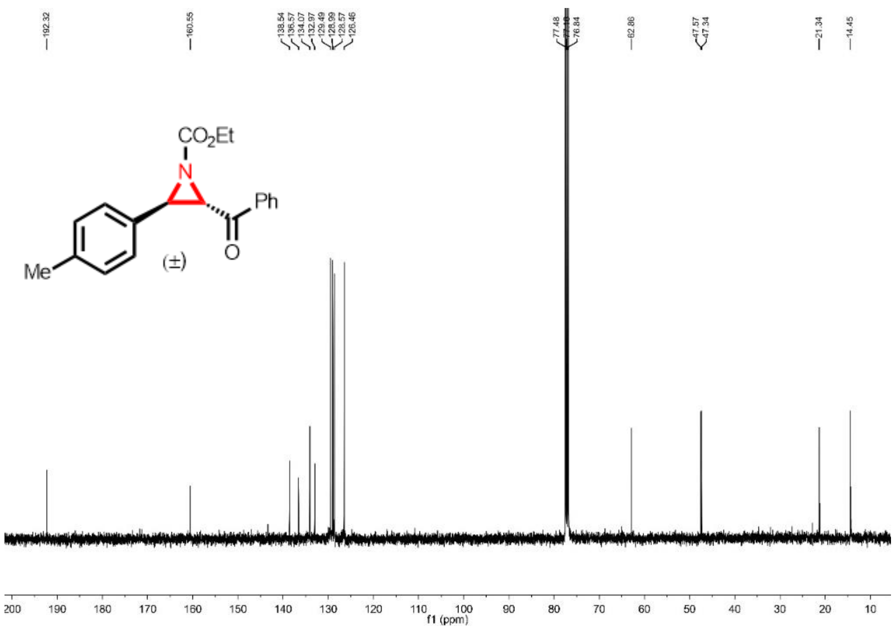
^{13}CNMR of **2q** (100 MHz, CDCl$_3$)



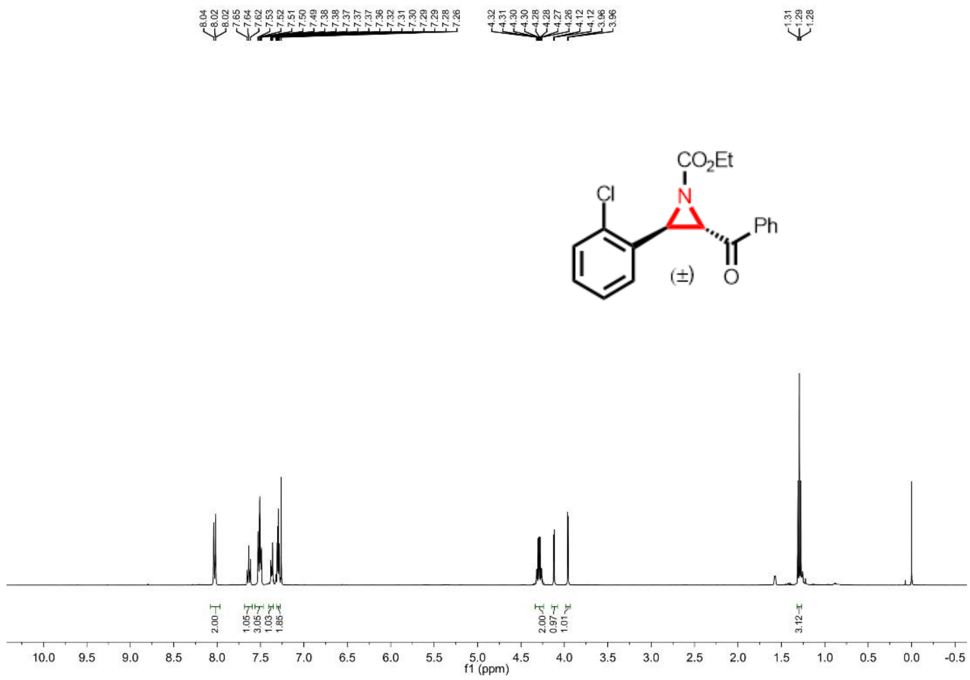
^{1}HNMR of **2r** (400 MHz, $CDCl_3$)



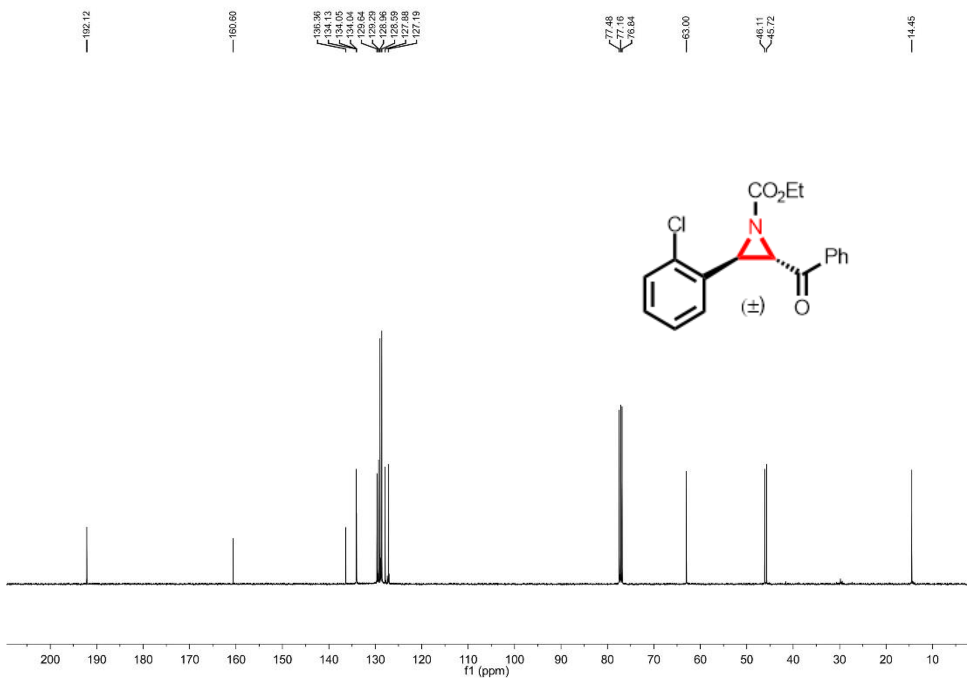
^{13}CNMR of **2r** (100 MHz, $CDCl_3$)



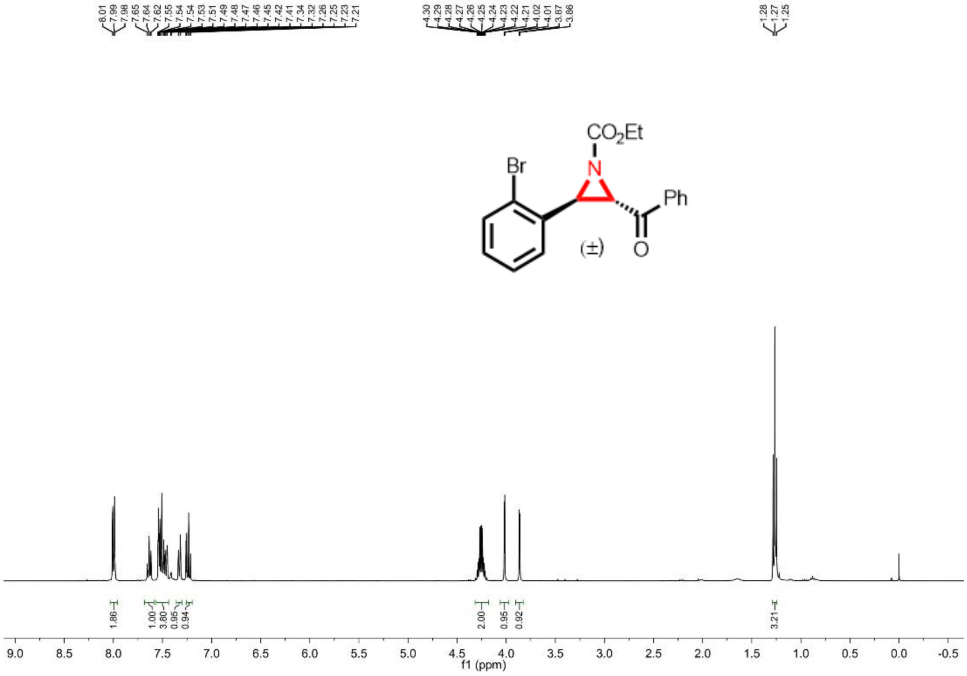
^{1}HNMR of **2s** (400 MHz, $CDCl_3$)



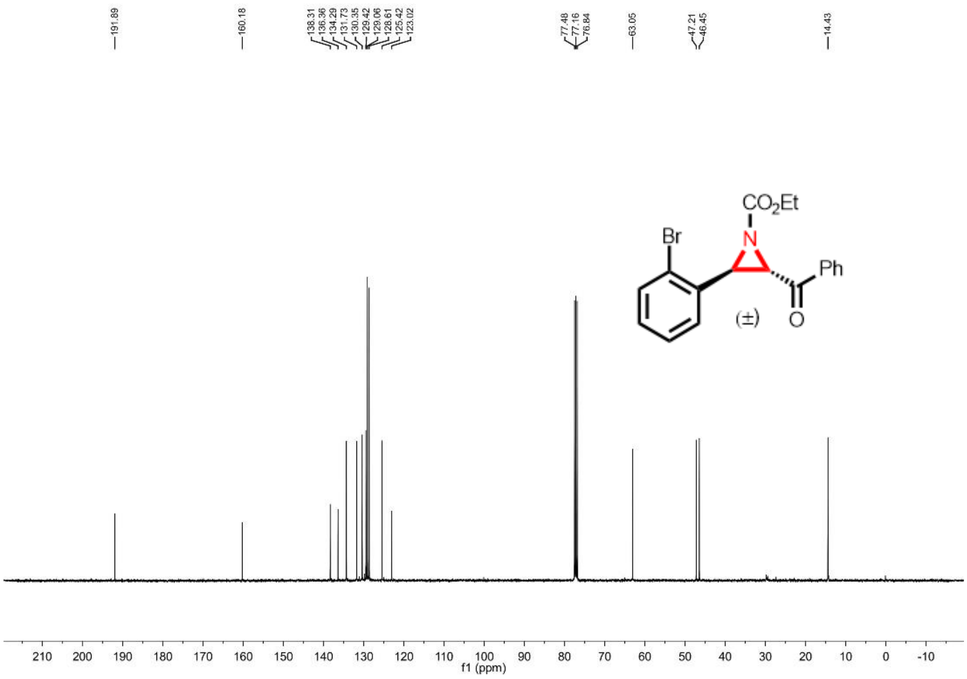
^{13}CNMR of **2s** (100 MHz, $CDCl_3$)



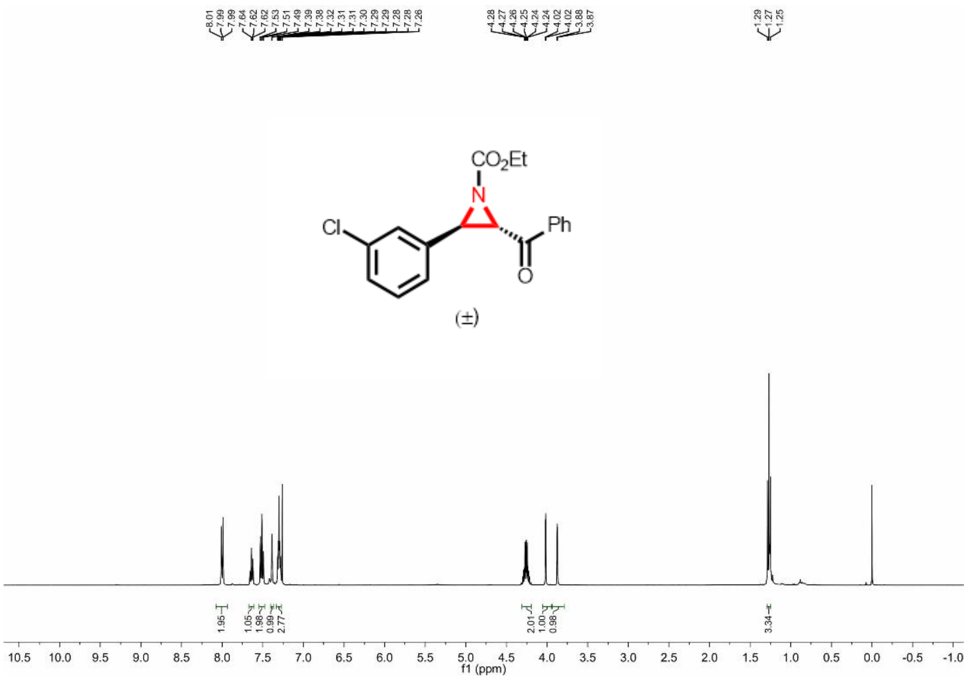
^{1}HNMR of **2t** (400 MHz, $CDCl_3$)



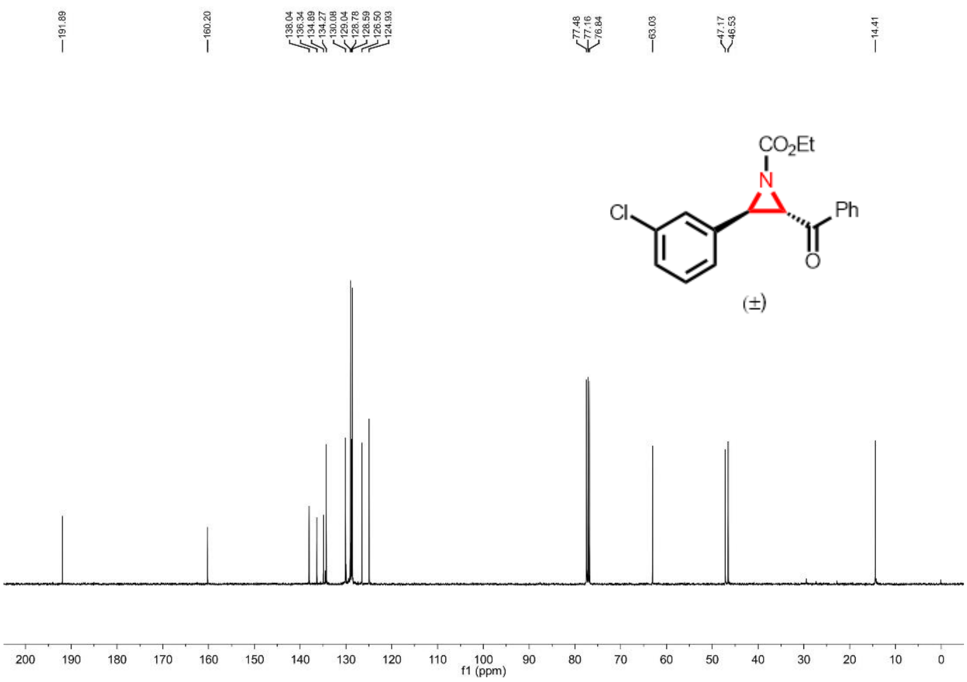
^{13}CNMR of **2t** (100 MHz, $CDCl_3$)



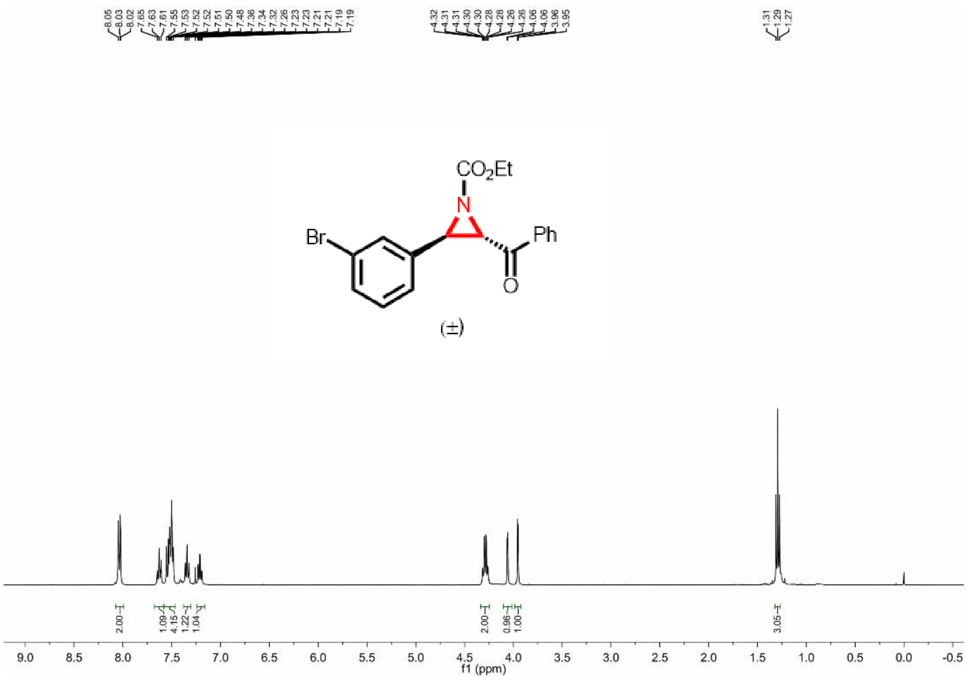
^{1}HNMR of **2u** (400 MHz, $CDCl_3$)



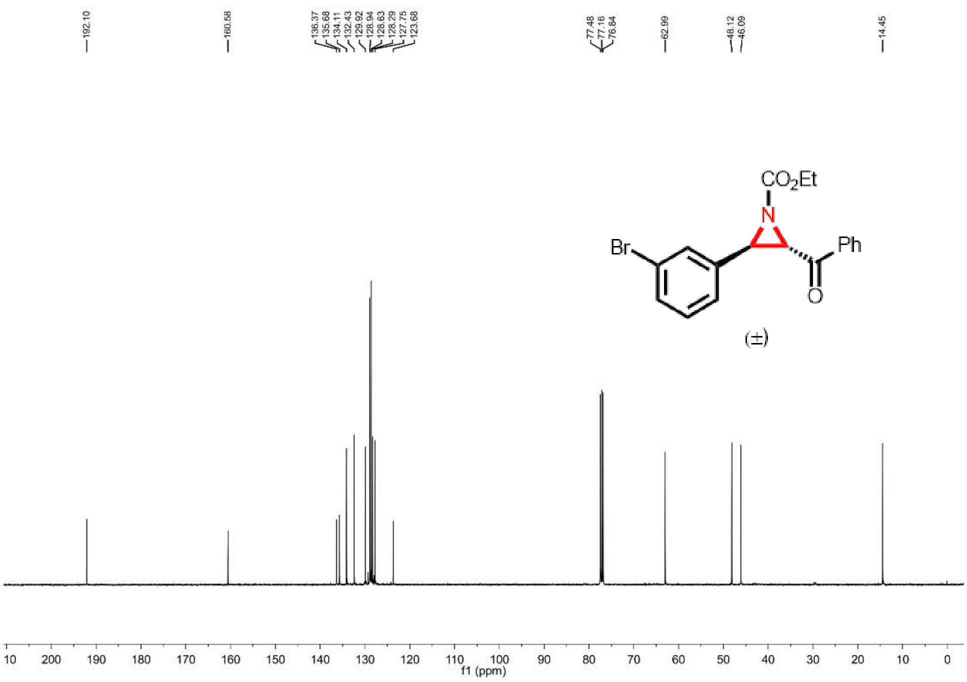
^{13}CNMR of **2u** (100 MHz, $CDCl_3$)



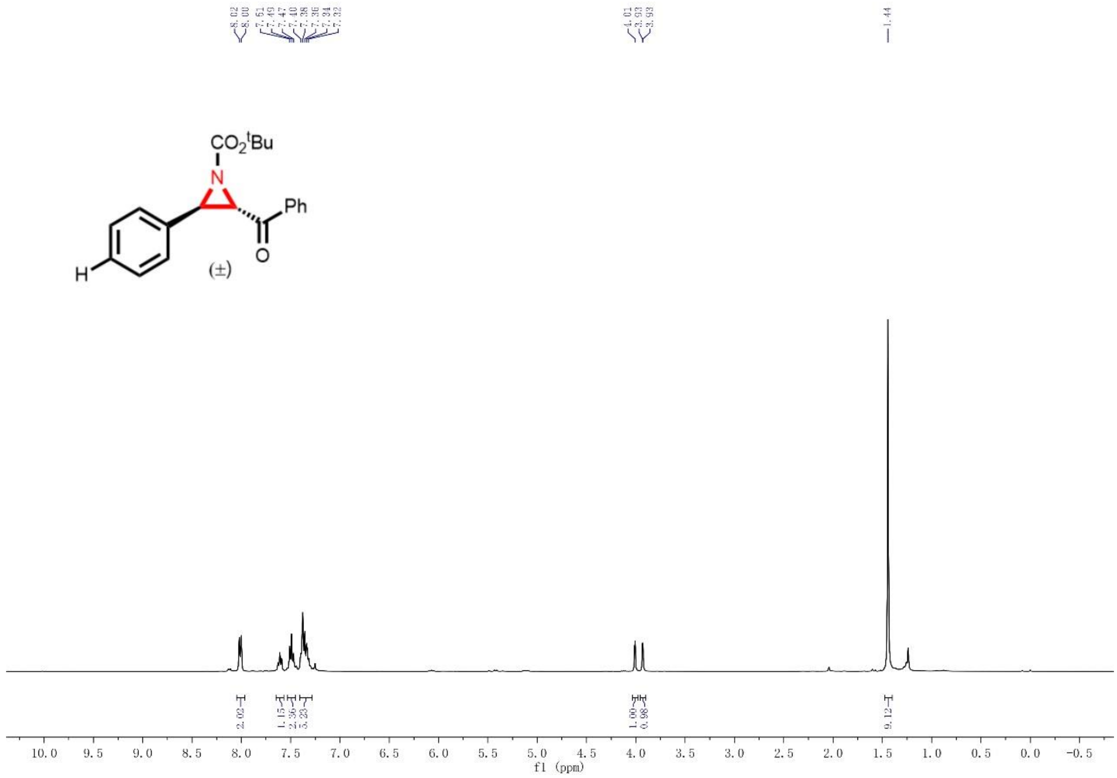
^{1}HNMR of **2v** (400 MHz, $CDCl_3$)



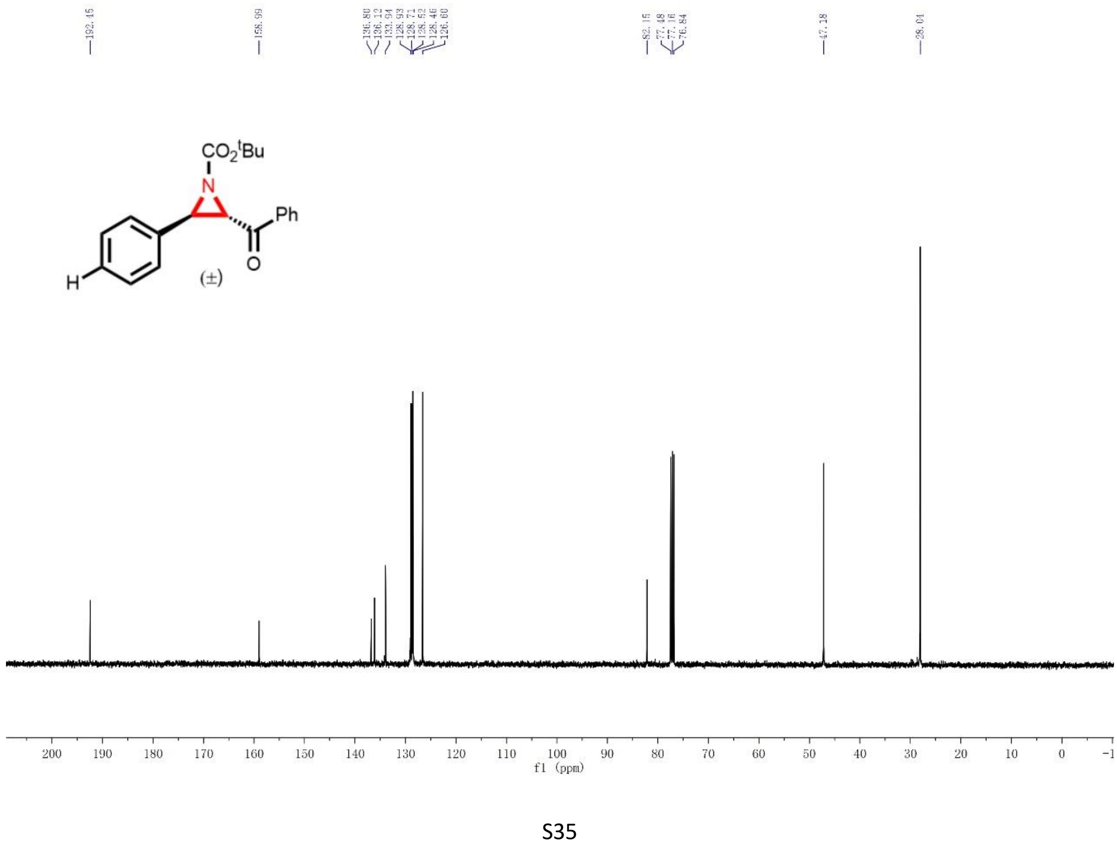
^{13}CNMR of **2v** (100 MHz, $CDCl_3$)



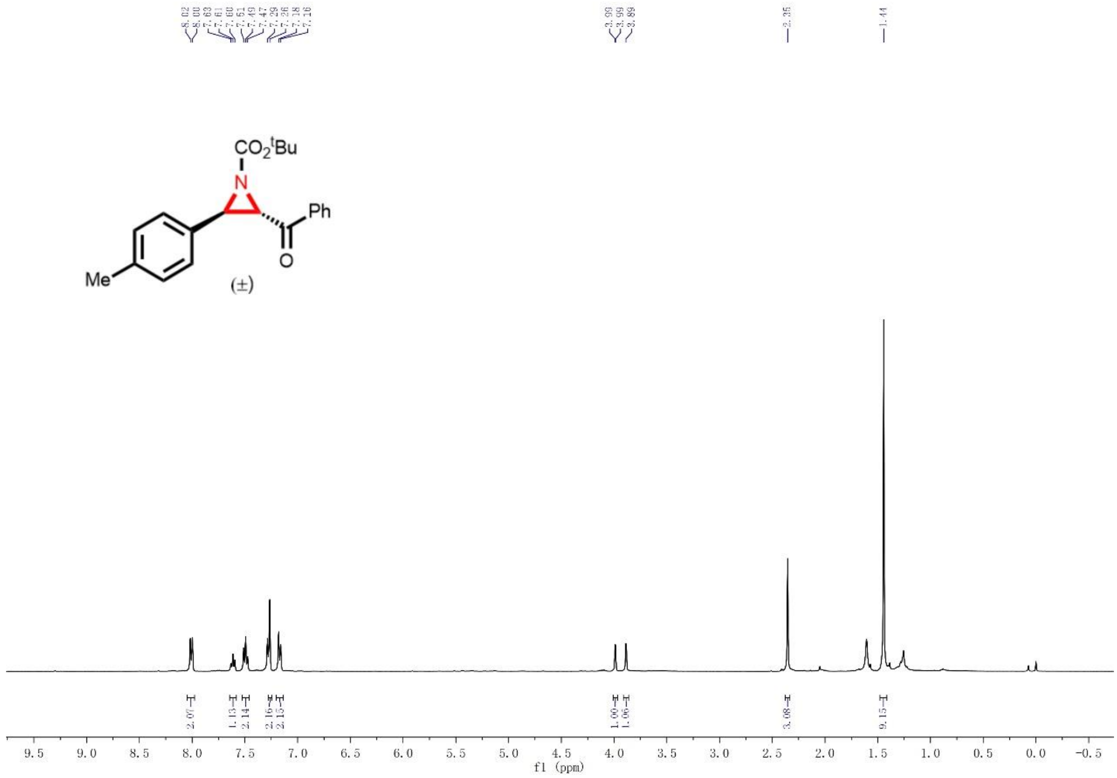
^{1}HNMR of **2w** (400 MHz, $CDCl_3$)



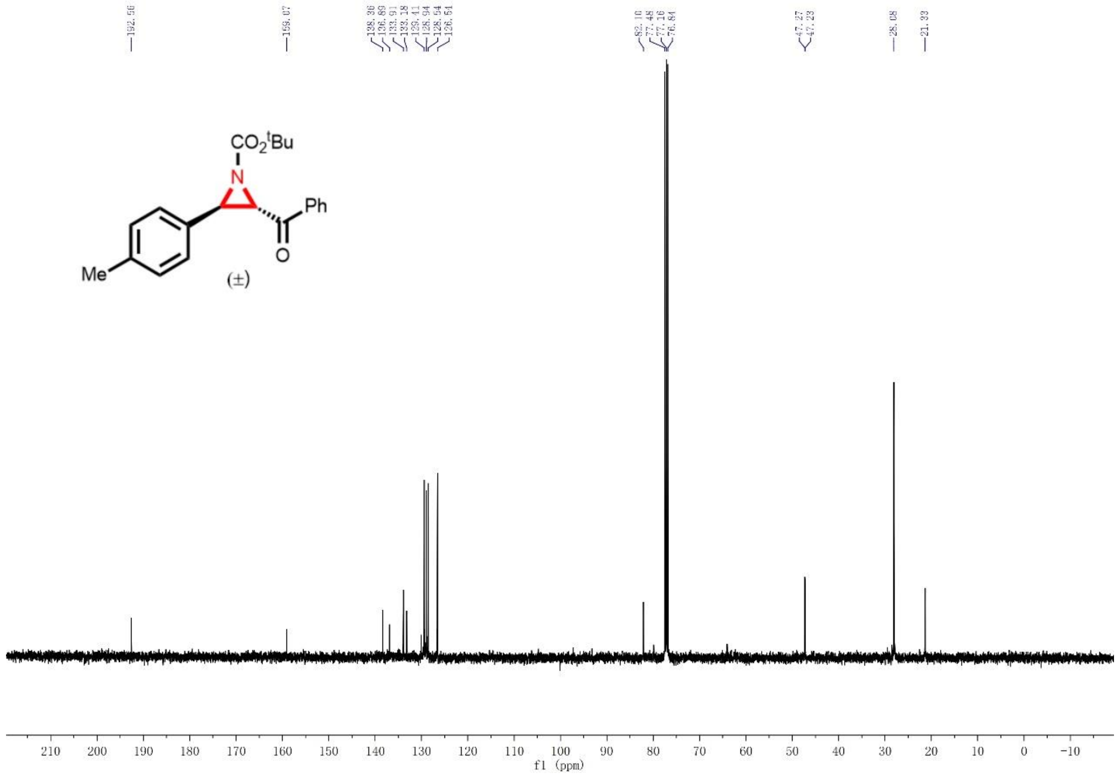
^{13}CNMR of **2w** (100 MHz, $CDCl_3$)



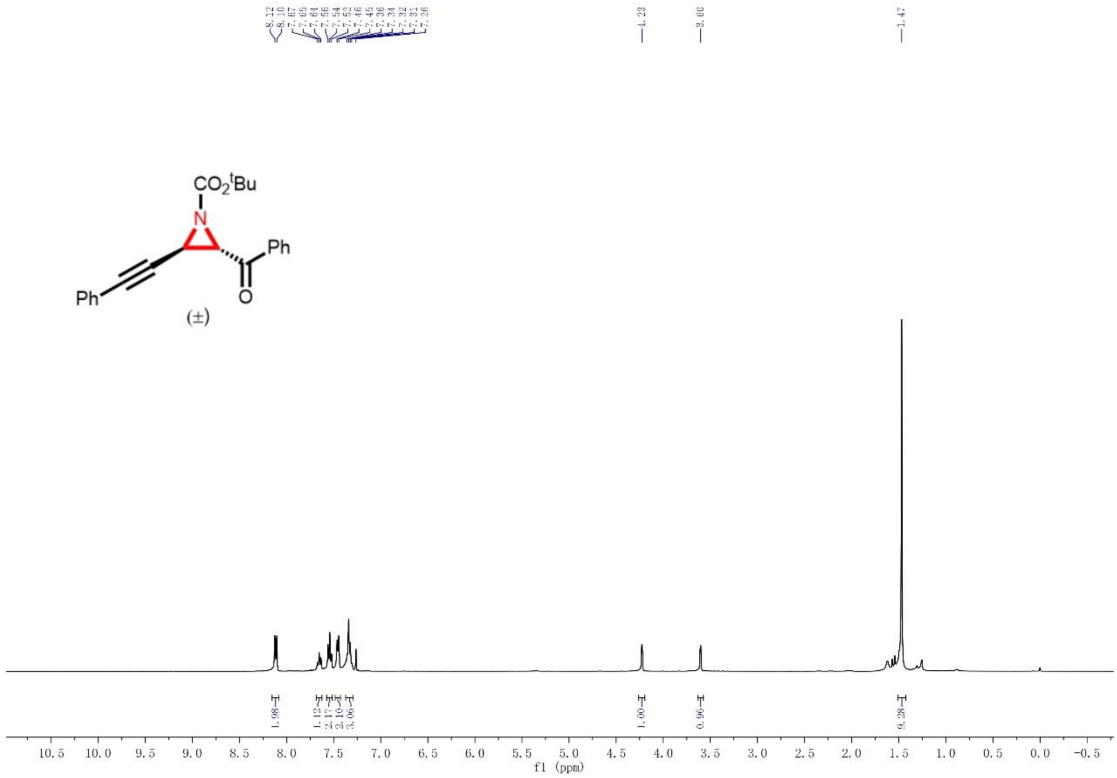
^{1}HNMR of **2x** (400 MHz, $CDCl_3$)



^{13}CNMR of **2x** (100 MHz, $CDCl_3$)



^{1}HNMR of **2y** (400 MHz, $CDCl_3$)



^{13}CNMR of **2y** (100 MHz, $CDCl_3$)