

Supporting Information

Nickel-catalyzed arylation cyclization of 1,6-enynes: arylation of unactivated alkene moieties

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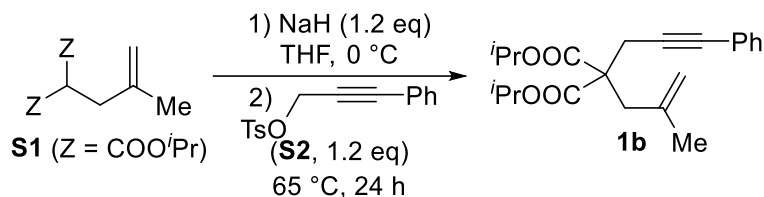
1. General Information

All anaerobic and moisture-sensitive manipulations were carried out with standard Schlenk techniques under argon. NMR spectra were recorded on Bruker AVANCE III 500MHz and Bruker AVANCE NEO 600MHz. Chemical shifts are reported in δ (ppm) referenced to the residual solvent peak of CDCl_3 (δ 7.26) for ^1H NMR and CDCl_3 (δ 77.0) for ^{13}C NMR. The following abbreviations are used to describe the multiplicities; s: singlet, d: doublet, t: triplet, q: quartet, quint: quintet, sext: sextet, hept: heptet, m: multipls. Coupling constants are reported in Hertz (Hz). HRESIMS spectras were acquired using the waters G2-Xs qtof mass spectrometer. GC-MS analyses were recorded on Shimadzu GCMS-QP2020 NX. For thin layer chromatography (TLC), NUO TAI precoated TLC plates (SHF254) were used, and compounds were visualized with a UV light at 254 nm. Further visualization was achieved by staining with KMnO_4 followed by heating. Flash column chromatography was performed with Silica gel (SANPONT). Enantiomeric excesses (ee) were determined by HPLC analysis on Shimazu (LC-16) HPLC with Daicel chiral columns. The products were further purified by GPC (Gel Permeation Chromatography) if necessary.

2. Materials

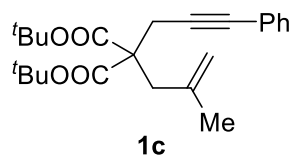
Tetrahydrofuran, dichloromethane, toluene and diethyl ether were taken from a solvent purification. Diisopropyl malonate, dimethyl malonate, cuprous iodide, potassium *tert*-butoxide, *N*-bromosuccinimide (NBS), *p*-toluene sulfonic acid, sodium borohydride, phenylacetone, tetrahydropyrrole, formaldehyde, propionic acid, hexanal, sodium hydride, arylboronics acid, $\text{Ni}(\text{cod})_2$, PCy_3 , $\text{Ni}(\text{cod})(\text{DQ})$, NiCl_2 , tris(4-methoxyphenyl)phosphine, $\text{PdCl}_2(\text{PPh}_3)_2$, and PPh_3 were purchased and used as received. **1a**¹ (CAS NO. 379228-69-0) and **1d**² (CAS NO. 1609650-63-9) were prepared according to the reported procedures.

3. Preparation of 1,6-Enynes



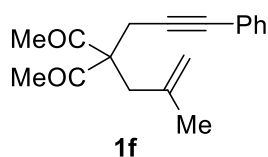
Under N_2 , a suspension of NaH (60% in mineral oil, 0.198 g, 4.95 mmol) in THF (10 mL) was added a solution of allylmalonate **S1**³ (CAS NO. 1912806-78-0, 1.00 g, 4.13 mmol) in THF (2.0 mL) dropwise at 0 °C. The mixture was stirred at room temperature for 30 min. A solution of alkyne **S2**⁴ (CAS NO. 21541-60-6, 1.42 g, 4.95 mmol) in THF (2.0 mL) was added at 0 °C. The mixture was stirred at 65 °C for 24 h, quenched with saturated aqueous NH_4Cl , and extracted with ethyl acetate. The combined organic layers were dried over MgSO_4 and filtered. The solvent was removed on a rotary evaporator. The residue was purified by flash column chromatography on silica gel (hexane/ ethyl acetate = 60:1) to give compound **1b** as a colorless oil (87% yield, 1.28 g, 3.59 mmol). $R_f = 0.4$ (hexane/ethyl acetate (30/1)). **¹H NMR** (600 MHz, CDCl_3): δ 7.38–7.34 (m, 2 H), 7.30–7.24 (m, 3H), 5.08 (hept, $J = 6.0$ Hz, 2H), 4.93 (s, 1H), 4.90 (s, 1H), 3.02 (s, 2H), 2.88 (s, 2H), 1.72 (s, 3H), 1.25 (d, $J = 6.3$ Hz, 12H); **¹³C NMR** (151 MHz, CDCl_3): δ 169.8, 140.3, 131.6, 128.2, 127.8, 123.4, 116.1, 85.0, 83.5, 69.1, 56.6, 39.4, 23.44, 23.41, 21.6, 21.5. **HRMS (ESI)** calcd for $\text{C}_{22}\text{H}_{28}\text{O}_4\text{Na}^+$ [$\text{M}+\text{Na}$]⁺ 379.1880, found 379.1880.

Similarly to the preparation of compound **1b**, 1,6-enynes **1c**, **1f** and **1y** were prepared with the corresponding allylmalonates.

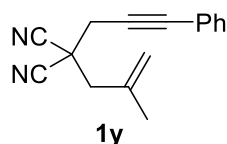


Compound 1c. (82% yield, 0.630 g, 1.36 mmol, a colorless oil, $R_f = 0.4$ (hexane/ethyl acetate (20/1))). **¹H NMR** (600 MHz, CDCl_3): δ 7.37–7.34 (m, 2H), 7.27–7.25 (m, 3H), 4.91 (s, 2H), 2.95 (s, 2H), 2.80 (s, 2H), 1.75 (s, 3H), 1.48 (s, 18H); **¹³C NMR** (151 MHz, CDCl_3): δ 169.4, 140.7, 131.5, 128.1, 127.7, 123.5, 115.8, 85.4, 83.4, 81.6, 57.5, 39.4, 27.8, 23.6, 23.5. **HRMS (ESI)** calcd for $\text{C}_{24}\text{H}_{32}\text{O}_4\text{Na}^+$ [$\text{M}+\text{Na}$]⁺ 407.2193, found

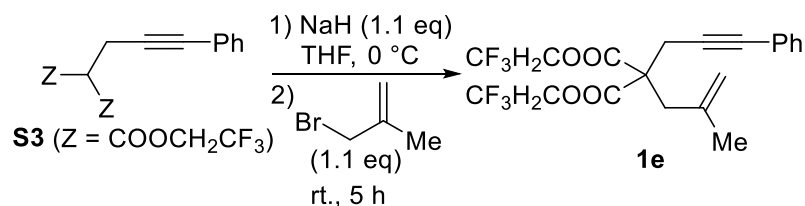
407.2198.



Compound 1f. (69% yield, 0.402 g, 1.50 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.36–7.32 (m, 2H), 7.30–7.27 (m, 3H), 4.91 (s, 1H), 4.79 (s, 1H), 3.06 (s, 2H), 2.91 (s, 2H), 2.21 (s, 6H), 1.68 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 205.1, 140.2, 131.6, 128.2, 128.1, 123.0, 115.5, 85.0, 84.2, 70.3, 38.6, 26.9, 23.8, 21.8. **HRMS (ESI)** calcd for $\text{C}_{18}\text{H}_{20}\text{O}_2\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 291.1356, found 291.1361.

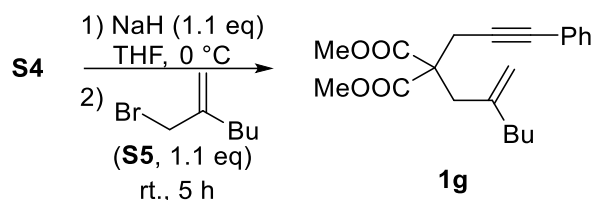


Compound 1y. (63% yield, 0.290 g, 1.24 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (20/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.47 (d, $J = 5.5$ Hz, 2H), 7.39–7.30 (m, 3H), 5.21 (s, 1H), 5.16 (s, 1H), 3.17 (s, 2H), 2.83 (s, 2H), 2.00 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 136.8, 131.9, 129.0, 128.4, 121.7, 119.2, 114.9, 87.2, 79.6, 43.8, 36.2, 29.6, 23.1. **HRMS (ESI)** calcd for $\text{C}_{16}\text{H}_{14}\text{N}_2^+$ $[\text{M}+\text{H}]^+$ 235.1230, found 235.1236.

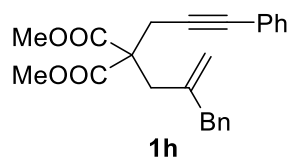


Under N_2 , a suspension of NaH (60% in mineral oil, 80.6 mg, 2.01 mmol) in THF (5.0 mL) was added a solution of **S3**⁵ (CAS NO. 2376294-99-2, 0.700 g, 1.83 mmol) in THF (1.0 mL) dropwise at 0 °C. The mixture was stirred at room temperature for 30 min. A solution of 3-bromo-2-methylpropene (0.271 g, 2.01 mmol) in THF (1.0 mL) was added at 0 °C. The mixture was stirred at room temperature for 5 h, quenched with saturated aqueous NH_4Cl , and extracted with ethyl acetate (20 mL \times 3). The combined organic layers were dried over MgSO_4 and filtered. The solvent was removed on a

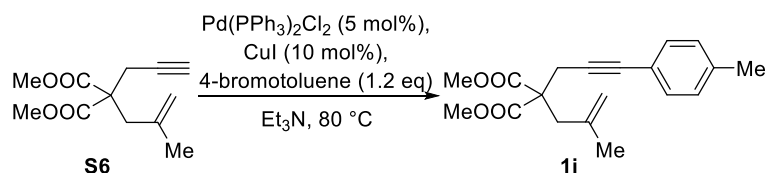
rotary evaporator. The residue was purified by flash column chromatography on silica gel (hexane/ ethyl acetate = 80:1) to give compound **1e** as a colorless oil (61% yield, 0.485 g, 1.11 mmol). $R_f = 0.4$ (hexane/ethyl acetate (40/1)). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.38–7.34 (m, 2H), 7.32–7.27 (m, 3H), 5.00 (quint, $J = 1.6$ Hz, 1H), 4.92 (s, 1H), 4.54 (q, $J = 8.2$ Hz, 4H), 3.13 (s, 2H), 2.97 (s, 2H), 1.73 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 168.0, 138.9, 131.6, 128.3, 122.8, 122.5 (q, $J = 277.5$ Hz), 117.2, 84.7, 82.9, 61.3 (q, $J = 37.5$ Hz), 57.1, 39.6, 29.7, 23.8, 23.2. $^{19}\text{F}\{^1\text{H}\}$ NMR (565 MHz, CDCl_3): δ -74.1 (s, 6F). **HRMS (ESI)** calcd for $\text{C}_{20}\text{H}_{18}\text{F}_6\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 459.1001, found 459.1008.



Under N_2 , a suspension of NaH (60% in mineral oil, 88.0 mg, 2.20 mmol) in THF (5.0 mL) was added a solution of phenylpropynemalonate **S4**⁶ (CAS NO. 346621-58-7, 0.493 g, 2.0 mmol) in THF (2.0 mL) dropwise at 0 °C. The mixture was stirred at room temperature for 30 min. A solution of **S5**⁷ (CAS NO. 123004-86-4, 390 mg, 2.20 mmol) was added to the mixture at 0 °C. The mixture was stirred at room temperature for 1.5 h before saturated aqueous NH_4Cl (10 mL) was added. The mixture was extracted with ethyl acetate. The combined organic layers were dried over MgSO_4 and filtered. The solvent was removed on a rotary evaporator. The residue was purified by flash column chromatography on silica gel (hexane/ ethyl acetate = 20:1) to give compound **1g** (76% yield, 0.521 g, 1.52 mmol) as a colorless oil. $R_f = 0.4$ (hexane/ethyl acetate (10/1)). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.39–7.34 (m, 2H), 7.29–7.26 (m, 3H), 4.93 (q, $J = 1.6$ Hz, 1H), 4.89 (s, 1H), 3.75 (s, 6H), 3.06 (s, 2H), 2.91 (s, 2H), 1.94 (t, $J = 8.0$ Hz, 2H), 1.42 (quint, $J = 7.4$ Hz, 2H), 1.29 (sext, $J = 7.3$ Hz, 2H), 0.88 (t, $J = 7.4$ Hz, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 170.7, 144.2, 131.6, 128.2, 127.9, 123.2, 114.8, 84.6, 83.9, 57.1, 52.7, 37.4, 36.3, 30.1, 23.5, 22.3, 13.9. **HRMS (ESI)** calcd for $\text{C}_{21}\text{H}_{26}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 365.1723, found 365.1727.

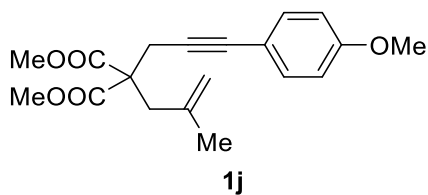


Similarly to the preparation of compound **1g**, 1,6-enyne **1h** was prepared from the compound **S4** and [2-(bromomethyl)-2-propen-1-yl]benzene² (CAS NO. 30457-89-7, 0.507 g, 2.4 mmol). Compound **1h** (92% yield, 0.693 g, 1.84 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (30/1), R_f = 0.4 (hexane/ethyl acetate (10/1))). **¹H NMR** (600 MHz, CDCl₃): δ 7.37–7.33 (m, 2H), 7.32–7.23 (m, 5H), 7.22–7.14 (m, 3H), 5.02 (s, 1H), 4.93 (q, J = 1.5 Hz, 1H), 3.77 (s, 6H), 3.29 (s, 2H), 3.13 (s, 2H), 2.89 (s, 2H); **¹³C NMR** (151 MHz, CDCl₃): δ 170.6, 143.4, 139.0, 131.6, 129.1, 128.3, 128.2, 128.0, 126.2, 123.1, 117.3, 84.5, 84.1, 57.2, 52.7, 43.5, 36.8, 23.8. **HRMS (ESI)** calcd for C₂₁H₂₆O₄Na⁺ [M+Na]⁺ 399.1567, found 399.1567.

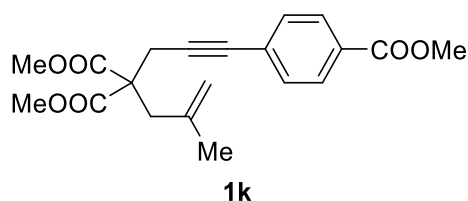


A dry Schlenk tube was charged with compound **S6**⁸ (CAS NO. 109468-75-9, 0.200 g, 0.891 mmol), Pd(PPh₃)₂Cl₂ (31.3 mg, 0.0446 mmol, 5 mol% of Pd), and CuI (17.0 mg, 0.0891 mmol, 10 mol%). Triethylamine (0.451 g, 4.46 mmol) and 4-bromotoluene (0.183 g, 1.07 mmol) were added. The mixture was stirred at 80 °C overnight. The reaction mixture was diluted with ethyl acetate, washed with water and brine, dried with anhydrous MgSO₄, and filtered. The solvent was removed on a rotary evaporator. The residue was purified by flash column chromatography on silica gel (hexane/ ethyl acetate = 20:1) to give compound **1i** (95% yield, 0.268 g, 0.851 mmol) as a colorless oil. R_f = 0.4 (hexane/ethyl acetate (10/1)). **¹H NMR** (600 MHz, CDCl₃): δ 7.28 (d, J = 8.2 Hz, 2H), 7.10 (d, J = 7.9 Hz, 2H), 4.96 (s, 1H), 4.91 (s, 1H), 3.77 (s, 6H), 3.07 (s, 2H), 2.94 (s, 2H), 2.34 (s, 3H), 1.72 (s, 3H); **¹³C NMR** (151 MHz, CDCl₃): δ 170.7, 139.9, 138.0, 131.5, 128.9, 120.2, 116.2, 83.9, 83.7, 56.9, 52.7, 39.7, 23.6, 23.2, 21.4. **HRMS (ESI)** calcd for C₁₉H₂₂O₄Na⁺ [M+Na]⁺ 337.1416, Found 337.1415.

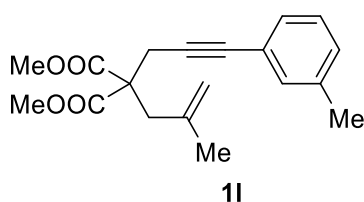
Similarly to the preparation of compound **1i**, 1,6-enynes **1j–1n** and **1t–1x** were prepared with the corresponding arylboromides.



Compound 1j. (95% yield, 0.281 g, 0.851 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.30 (d, $J = 8.8$ Hz, 2H), 6.80 (d, $J = 8.8$ Hz, 2H), 4.93 (s, 1H), 4.88 (s, 1H), 3.79 (s, 3H), 3.75 (s, 6H), 3.04 (s, 2H), 2.90 (s, 2H), 1.69 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 170.7, 159.3, 139.9, 133.0, 116.2, 115.4, 113.8, 83.6, 82.9, 56.9, 55.2, 52.7, 39.7, 23.6, 23.2. **HRMS (ESI)** calcd for $\text{C}_{19}\text{H}_{22}\text{O}_5\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 353.1359, Found 353.1364.

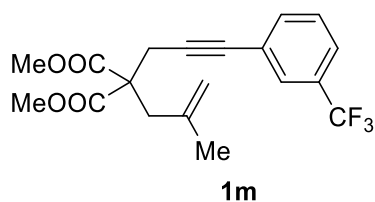


Compound 1k. (93% yield, 0.299 g, 0.833 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.95 (d, $J = 8.3$ Hz, 2H), 7.42 (d, $J = 8.4$ Hz, 2H), 4.94 (s, 1H), 4.88 (s, 1H), 3.91 (s, 3H), 3.77 (s, 6H), 3.08 (s, 2H), 2.91 (s, 2H), 1.69 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 170.6, 166.5, 139.8, 131.5, 129.41, 129.36, 127.9, 116.4, 88.0, 83.2, 56.7, 52.8, 52.2, 39.9, 23.7, 23.2. **HRMS (ESI)** calcd for $\text{C}_{20}\text{H}_{22}\text{O}_6\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 381.1309, Found 381.1306.

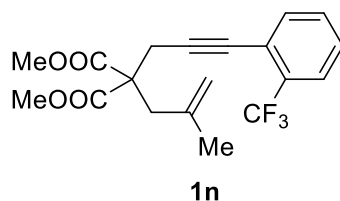


Compound 1l. (90% yield, 0.253 g, 0.806 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.19 (s, 1H), 7.16 (t, $J = 7.5$ Hz, 2H), 7.09 (d, $J = 6.8$ Hz, 1H), 4.94 (s, 1H), 4.89 (s, 1H), 3.76 (s, 6H), 3.06 (s, 2H), 2.92 (s, 2H), 2.31 (s, 3H), 1.70 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 170.7, 139.9, 137.8, 132.1, 128.8, 128.7, 128.1, 123.0, 116.3, 84.1, 84.0, 56.8, 52.7, 39.7, 23.6, 23.2, 21.1. **HRMS (ESI)** calcd

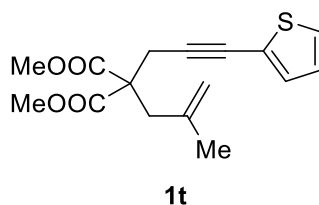
for $C_{19}H_{22}O_4Na^+$ $[M+Na]^+$ 337.1410, Found 337.1417.



Compound 1m. (83% yield, 0.274 g, 0.744 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). 1H NMR (600 MHz, $CDCl_3$): δ 7.62 (s, 1H), 7.54 (d, $J = 7.6$ Hz, 2H), 7.42 (t, $J = 7.8$ Hz, 1H), 4.97 (s, 1H), 4.89 (s, 1H), 3.78 (s, 6H), 3.09 (s, 2H), 2.92 (s, 2H), 1.71 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): 171.5, 140.8, 135.8, 131.9 (q, $J = 32.4$ Hz), 129.7, 129.3 (q, $J = 3.9$ Hz), 125.1, 125.6 (q, $J = 3.8$ Hz), 124.7 (q, $J = 273.2$ Hz), 117.4, 87.5, 83.4, 57.7, 53.7, 40.9, 24.6, 24.2. **HRMS (ESI)** calcd for $C_{19}H_{19}F_3O_4Na^+$ $[M+Na]^+$ 391.1128, Found 391.1136.

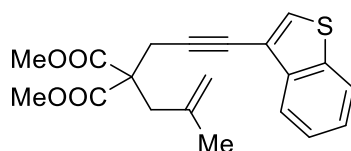


Compound 1n. (87% yield, 0.286 g, 0.776 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). 1H NMR (600 MHz, $CDCl_3$): δ 7.60 (d, $J = 7.9$ Hz, 1H), 7.51 (d, $J = 7.7$ Hz, 1H), 7.44 (t, $J = 7.6$ Hz, 1H), 7.35 (t, $J = 7.7$ Hz, 1H), 4.93 (s, 1H), 4.87 (s, 1H), 3.75 (s, 6H), 3.11 (s, 2H), 2.91 (s, 2H), 1.68 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 170.4, 139.9, 134.3, 131.33 (q, $J = 30.3$ Hz), 131.26, 127.7, 125.6 (q, $J = 5.1$ Hz), 123.5 (q, $J = 273.3$ Hz), 121.4, 116.3, 90.7, 79.6, 56.7, 52.7, 39.6, 23.7, 23.1. **HRMS (ESI)** calcd for $C_{19}H_{19}F_3O_4Na^+$ $[M+Na]^+$ 391.1128, Found 391.1136.



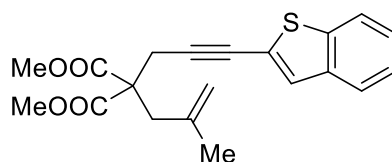
Compound 1t. (85% yield, 0.233 g, 0.762 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))).

$^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.18 (d, $J = 5.2$ Hz, 1H), 7.11 (d, $J = 3.6$ Hz, 1H), 6.92 (dd, $J = 5.2, 3.6$ Hz, 1H), 4.93 (s, 1H), 4.87 (s, 1H), 3.76 (s, 6H), 3.08 (s, 2H), 2.89 (s, 2H), 1.69 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 170.6, 139.8, 131.5, 126.8, 126.5, 123.2, 116.4, 88.6, 76.9, 56.7, 52.7, 39.8, 23.9, 23.2. **HRMS (ESI)** calcd for $\text{C}_{16}\text{H}_{18}\text{O}_4\text{SNa}^+$ $[\text{M}+\text{Na}]^+$ 329.0818, Found 329.0828.



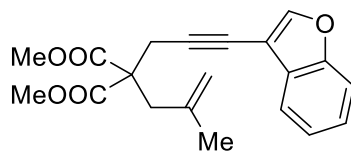
1u

Compound 1u. (83% yield, 0.265 g, 0.744 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.93 (d, $J = 8.0$ Hz, 1H), 7.85 (d, $J = 7.7$ Hz, 1H), 7.55 (s, 1H), 7.48 (t, $J = 7.6$ Hz, 1H), 7.40 (t, $J = 7.6$ Hz, 1H), 4.99 (s, 1H), 4.96 (s, 1H), 3.81 (s, 6H), 3.20 (s, 2H), 3.01 (s, 2H), 1.75 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 170.6, 139.9, 139.3, 138.7, 129.5, 124.9, 124.7, 122.9, 122.5, 118.2, 116.4, 87.1, 77.4, 56.8, 52.8, 39.9, 23.9, 23.2. **HRMS (ESI)** calcd for $\text{C}_{20}\text{H}_{20}\text{O}_4\text{SNa}^+$ $[\text{M}+\text{Na}]^+$ 379.0975, Found 379.0981.



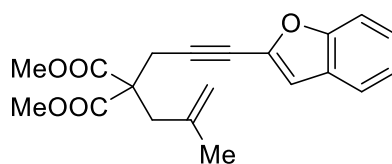
1v

Compound 1v. (85% yield, 0.271 g, 0.762 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.76–7.67 (m, 2H), 7.35 (s, 1H), 7.34–7.31 (m, 2H), 4.97 (s, 1H), 4.91 (s, 1H), 3.78 (s, 6H), 3.13 (s, 2H), 2.93 (s, 2H), 1.71 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 170.5, 139.9, 139.8, 139.0, 128.3, 125.3, 124.6, 123.6, 123.1, 121.9, 116.5, 90.9, 77.3, 56.7, 52.8, 39.9, 24.0, 23.2. **HRMS (ESI)** calcd for $\text{C}_{20}\text{H}_{20}\text{O}_4\text{SNa}^+$ $[\text{M}+\text{Na}]^+$ 3379.0975, Found 379.0971.



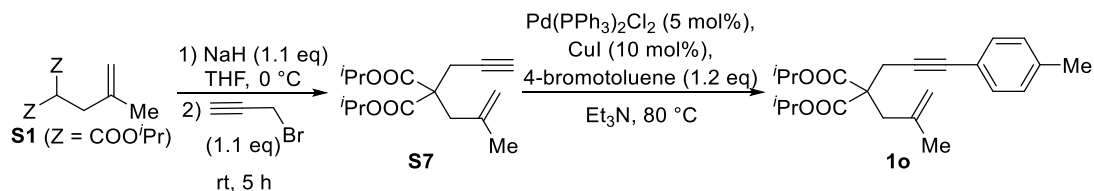
1w

Compound 1w. (89% yield, 0.271 g, 0.797 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.74 (s, 1H), 7.64 (d, $J = 7.1$ Hz, 1H), 7.47 (d, $J = 7.1$ Hz, 1H), 7.35–7.27 (m, 2H), 4.96 (s, 1H), 4.92 (s, 1H), 3.78 (s, 6H), 3.15 (s, 2H), 2.97 (s, 2H), 1.72 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 170.6, 154.5, 147.2, 139.9, 127.9, 125.1, 123.3, 120.3, 116.4, 111.5, 104.3, 89.3, 73.1, 56.8, 52.8, 39.8, 23.9, 23.2. **HRMS (ESI)** calcd for $\text{C}_{20}\text{H}_{20}\text{O}_5\text{Na}^+ [\text{M}+\text{Na}]^+$ 363.1203, Found 363.1207.



1x

Compound 1x. (89% yield, 0.271 g, 0.797 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.52 (d, $J = 7.8$ Hz, 1H), 7.42 (d, $J = 8.3$ Hz, 1H), 7.30 (t, $J = 7.8$ Hz, 1H), 7.21 (t, $J = 7.5$ Hz, 1H), 6.85 (s, 1H), 4.97 (s, 1H), 4.92 (s, 1H), 3.78 (s, 6H), 3.16 (s, 2H), 2.93 (s, 2H), 1.70 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 170.4, 154.6, 139.7, 138.5, 127.5, 125.4, 123.1, 121.0, 116.6, 111.12, 111.08, 91.2, 74.3, 56.5, 52.8, 39.9, 23.8, 23.1. **HRMS (ESI)** calcd for $\text{C}_{20}\text{H}_{20}\text{O}_5\text{Na}^+ [\text{M}+\text{Na}]^+$ 363.1203, Found 363.1205.

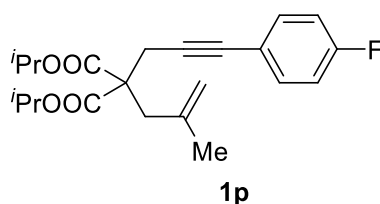


Under N_2 , a suspension of NaH (60% in mineral oil, 0.248 g, 6.81 mmol) in THF (7.0 mL) was added a solution of **S1** (1.50 g, 6.19 mmol) in THF (2.0 mL) dropwise at 0°C , and the mixture was stirred at room temperature for 10 min. A solution of 3-

bromopropyne (0.919 g, 6.81 mmol) was added at 0 °C. The mixture was stirred at room temperature for 5 h, quenched with saturated aqueous NH₄Cl, and extracted with ethyl acetate. The combined organic layers were dried over MgSO₄ and filtered. The solvent was removed on a rotary evaporator. The residue was purified by flash column chromatography on silica gel (hexane/ ethyl acetate = 40:1) to give compound **S7** as a white solid (95% yield, 1.65 g, 5.88 mmol). *R_f* = 0.4 (hexane/ethyl acetate (20/1)). ¹H NMR (600 MHz, CDCl₃): δ 5.06 (hept, *J* = 6.3 Hz, 2H), 4.90 (s, 1H), 4.87 (s, 1H), 2.82 (s, 2H), 2.81(d, *J* = 2.7 Hz, 2H), 2.01 (t, *J* = 2.7 Hz, 1H), 1.68 (s, 3H), 1.24 (d, *J* = 6.2 Hz, 12H); ¹³C NMR (151 MHz, CDCl₃): δ 169.6, 140.1, 116.1, 79.4, 71.4, 69.2, 56.2, 39.2, 23.3, 22.5, 21.5. HRMS (ESI) calcd for C₁₆H₂₄O₄Na⁺ [M+Na]⁺ 303.1567, found 303.1570.

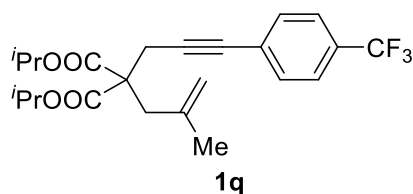
The synthesis method from **S7** to compound **1o** is similar to that of compound **1i**. ¹H NMR (600 MHz, CDCl₃): δ 7.29 (d, *J* = 8.7 Hz, 2H), 6.80 (d, *J* = 8.8 Hz, 2H), 5.07 (hept, *J* = 6.2 Hz, 2H), 4.92 (s, 1H), 4.90 (s, 1H), 3.79 (s, 3H), 3.00 (s, 2H), 2.87 (s, 2H), 1.71 (s, 3H), 1.25 (d, *J* = 6.3 Hz, 12H); ¹³C NMR (151 MHz, CDCl₃): δ 169.8, 140.4, 137.8, 131.5, 128.9, 120.4, 116.0, 84.2, 83.6, 69.1, 56.7, 39.5, 23.5, 23.4, 21.6, 21.5, 21.4. HRMS (ESI) calcd for C₂₃H₃₀O₄Na⁺ [M+Na]⁺ 393.2036, found 393.2041.

Similarly to the preparation of compound **1o**, 1,6-enynes **1p–1s** were prepared with the corresponding arylbromides.

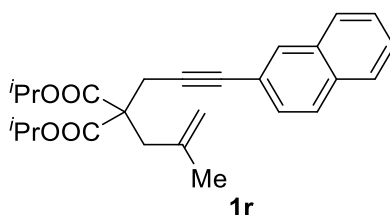


Compound 1p. (96% yield, 0.256 g, 0.684 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), *R_f* = 0.4 (hexane/ethyl acetate (20/1))). ¹H NMR (600 MHz, CDCl₃): δ 7.33 (dd, *J* = 8.6, 5.5 Hz, 2H), 6.96 (t, *J* = 8.7 Hz, 2H), 5.07 (hept, *J* = 6.2 Hz, 2H), 4.92 (s, 1H), 4.89 (s, 1H), 3.00 (s, 2H), 2.86 (s, 2H), 1.71 (s, 3H), 1.25 (d, *J* = 6.4 Hz, 6H), 1.24 (d, *J* = 6.4 Hz, 6H); ¹³C NMR (151 MHz, CDCl₃): δ 169.8, 162.3 (d, *J* = 248.9 Hz), 140.3, 133.4 (d, *J* = 8.2 Hz), 119.5 (d, *J* = 3.4 Hz), 116.1, 115.4 (d, *J* = 21.9 Hz), 84.7, 82.5, 69.1, 56.6, 39.5, 23.43, 23.39, 21.6, 21.5.

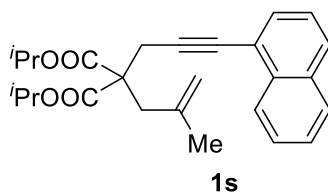
HRMS (ESI) calcd for $C_{22}H_{27}FO_4Na^+$ $[M+Na]^+$ 397.1786, found 397.1789.



Compound 1q. (90% yield, 0.272 g, 0.641 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). 1H NMR (600 MHz, $CDCl_3$): δ 7.53 (d, $J = 8.0$ Hz, 2H), 7.45 (d, $J = 8.0$ Hz, 2H), 5.08 (hept, $J = 6.3$ Hz, 2H), 4.93 (s, 1H), 4.88 (s, 1H), 3.07 (s, 2H), 2.87 (s, 2H), 1.71 (s, 3H), 1.254 (d, $J = 6.2$ Hz, 6H), 1.247 (d, $J = 6.3$ Hz, 6H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 169.7, 140.2, 131.8, 129.7 (q, $J = 32.6$ Hz), 127.2, 125.1 (q, $J = 3.8$ Hz), 123.9 (q, $J = 273.2$ Hz), 116.2, 88.0, 82.4, 69.3, 56.5, 39.4, 23.5, 23.4, 21.6, 21.5. **HRMS (ESI)** calcd for $C_{23}H_{27}F_3O_4Na^+$ $[M+Na]^+$ 447.1754, found 447.1753.



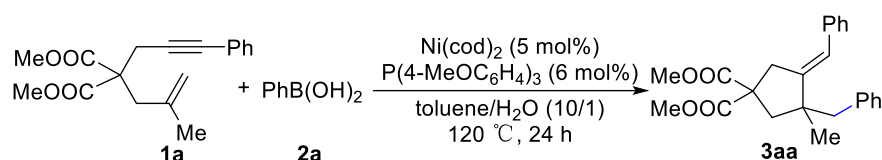
Compound 1r. (95% yield, 0.272 g, 0.669 mmol, a colorless solid, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). 1H NMR (600 MHz, $CDCl_3$): δ 7.87 (s, 1H), 7.80–7.75 (m, 2H), 7.74 (d, $J = 8.5$ Hz, 1H), 7.49–7.44 (m, 2H), 7.41 (d, $J = 6.8$ Hz, 1H), 5.10 (hept, $J = 6.2$ Hz, 2H), 4.95 (s, 2H), 3.08 (s, 2H), 2.92 (s, 2H), 1.74 (s, 3H), 1.27 (d, $J = 6.4$ Hz, 12H); ^{13}C NMR (151 MHz, $CDCl_3$): δ 169.8, 140.3, 133.0, 132.6, 131.2, 128.6, 127.8, 127.7, 127.6, 126.4, 120.7, 116.2, 85.4, 83.9, 69.2, 56.7, 39.5, 23.6, 23.4, 21.60, 21.56. **HRMS (ESI)** calcd for $C_{26}H_{30}O_4Na^+$ $[M+Na]^+$ 429.2036, found 429.2041.



Compound 1s. (95% yield, 0.272 g, 0.669 mmol, a colorless solid, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))).

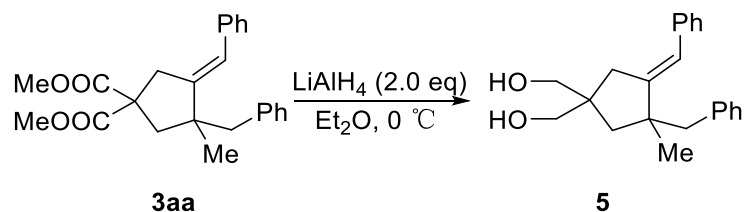
$^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.30 (d, $J = 8.3$ Hz, 1H), 7.82 (d, $J = 8.1$ Hz, 1H), 7.79 (d, $J = 8.3$ Hz, 1H), 7.60 (d, $J = 7.3$ Hz, 1H), 7.55 (t, $J = 6.8$ Hz, 1H), 7.50 (t, $J = 6.8$ Hz, 1H), 7.39 (t, $J = 8.1$ Hz, 1H), 5.11 (hept, $J = 6.3$ Hz, 2H), 4.95 (s, 2H), 3.20 (s, 2H), 2.97 (s, 2H), 1.75 (s, 3H), 1.26 (d, $J = 6.3$ Hz, 12H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 169.9, 140.3, 133.4, 133.1, 130.4, 128.3, 128.1, 126.6, 126.28, 126.26, 125.1, 121.1, 116.2, 89.9, 81.6, 69.2, 56.7, 39.6, 23.9, 23.5, 21.61, 21.57. **HRMS (ESI)** calcd for $\text{C}_{26}\text{H}_{30}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 429.2036, found 429.2044.

4. A Typical Procedure for Ni-Catalyzed Cascade Cyclization of 1,6-Enynes with $\text{ArB}(\text{OH})_2$ (Table 1, entry 1).



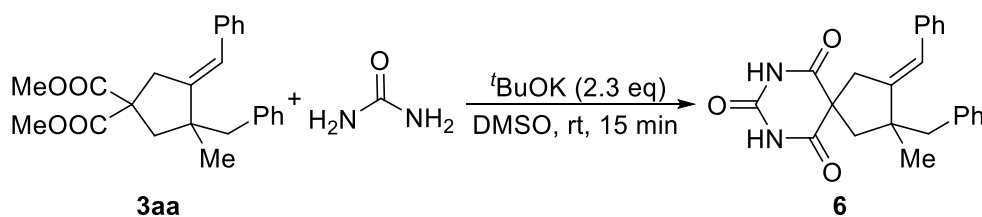
An oven-dried Schlenk tube equipped with a stir bar was charged with **1a** (30.0 mg, 0.100 mmol) and phenylboronic acid (36.6 mg, 0.300 mmol). $\text{Ni}(\text{cod})_2$ (1.38 mg, 5.00 μmol , 5.0 mol% of Ni), $\text{P}(4\text{-MeOC}_6\text{H}_4)_3$ (2.11 mg, 6.00 μmol , 6.0 mol%), toluene (1.0 mL), and H_2O (0.1 mL) were added to the mixture at room temperature in an argon-filled glovebox. Then the reaction was stirred at $120\text{ }^\circ\text{C}$ for 24 h. The mixture was passed through a short silica gel pad with ethyl acetate as eluent. The solvent was removed on a rotary evaporator. The crude product was subjected to chromatography on silica gel with hexane/ethyl acetate (40/1) as eluent to give compound **3aa** (91% yield, 34.4 mg, 0.0910 mmol) as a colorless oil.

5. Synthetic Manipulations.

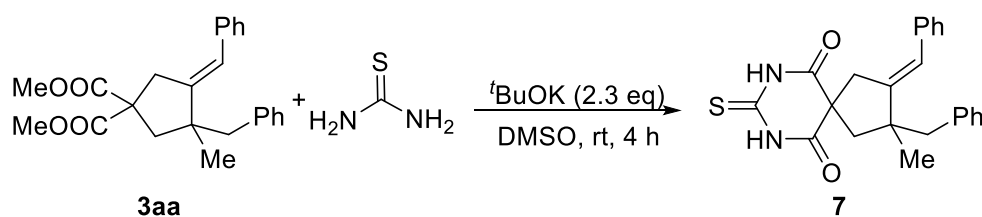


A solution of **3aa** (60.0 mg, 0.160 mmol) in ethyl ether (2.0 mL) was added LiAlH_4

(12.0 mg, 0.320 mmol) slowly at 0 °C. Then the resulting mixture was warmed to room temperature and stirred for 12 h. The reaction mixture was quenched by saturated potassium sodium tartrate and extracted with ethyl acetate. The combined organic layers were dried over MgSO₄ and filtered. The solvent was removed, and the residue was purified by flash column chromatography on silica gel (hexane/ethyl acetate = 8:1) to give compound **5** as a colorless oil (92% yield, 47.5 mg, 0.147 mmol). *R_f* = 0.3 (hexane/ethyl acetate (3/1)).

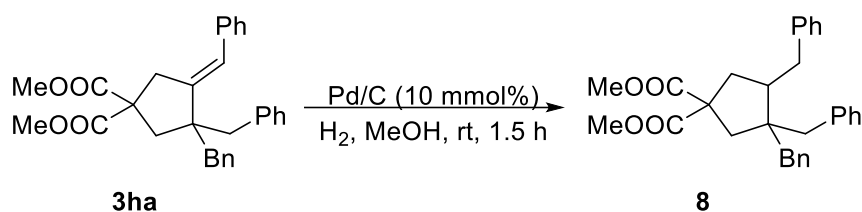


Urea (39.6 mg, 66.0 μmol) and ^tBuOK (11.2 mg, 0.284 mmol) was added to a solution of compound **3aa** (40.0 mg, 0.110 mmol) in dry DMSO (2.0 mL) was added. The mixture was stirred at room temperature for 15 min, diluted with ethyl acetate (10 mL), and washed with a HCl solution (0.1 N, 5.0 mL). The aqueous phase was extracted with ethyl acetate, washed with brine, and dried over MgSO₄. The solvent was removed and the residue was purified by flash column chromatography on silica gel (hexane/ethyl acetate = 20:1) to give compound **6** as a white solid (95% yield, 39.1 mg, 0.105 mmol). *R_f* = 0.3 (hexane/ethyl acetate (10/1)).



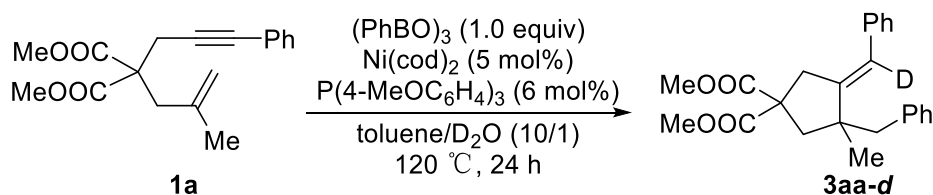
Thiourea (24.1 mg, 0.320 mmol) and ^tBuOK (13.7 mg, 0.122 mmol) was added to a solution of compound **3aa** (20.0 mg, 53.0 μmol) in dry DMSO (1.0 mL) was added. The mixture was stirred at room temperature for 15 min, diluted with ethyl acetate (5 mL), and washed with a HCl solution (0.1 N, 5 mL). The aqueous phase was extracted with ethyl acetate, washed with brine, and dried over MgSO₄. The solvent was removed and the residue was purified by flash column chromatography on silica gel (hexane/ethyl acetate = 20:1) to give compound **7** as a white solid (98% yield, 20.3 mg,

51.9 μmol). $R_f = 0.3$ (hexane/ethyl acetate (10/1)).

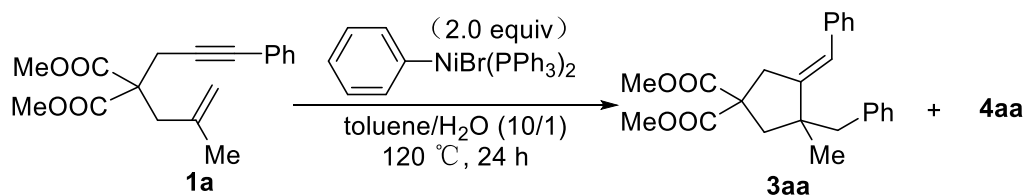


10% Pd/C (5.65 mg) was added to a solution of compound **3ha** (20.0 mg, 53.0 μmol) in dry MeOH (2.0 ml). The mixture was stirred under H_2 atmosphere (using H_2 balloon) at room temperature for 1.5 h. The solvent was removed, and the residue was purified by flash column chromatography on silica gel (hexane/ethyl acetate = 20:1) to give compound **8** as a white solid (94% yield, 22.7 mg, 49.7 μmol). $R_f = 0.3$ (hexane/ethyl acetate (10/1)).

6. Mechanism Studies

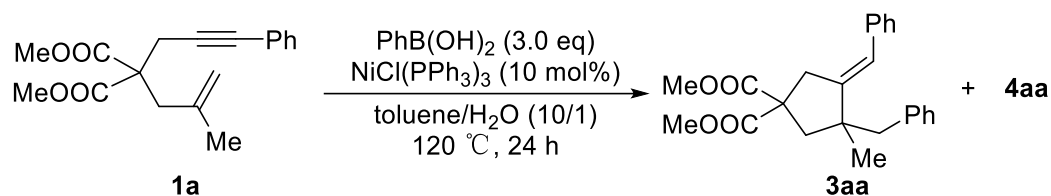


An oven-dried Schlenk flask equipped with a stir bar was charged with **1a** (30.0 mg, 0.100 mmol) and $(\text{PhBO})_3$ (31.2 mg, 0.100 mmol). $\text{Ni}(\text{cod})_2$ (1.38 mg, 5.00 μmol , 5.0 mol% of Ni), $\text{P}(4\text{-MeOC}_6\text{H}_4)_3$ (2.11 mg, 6.00 μmol , 6.0 mol%), toluene (1.0 mL) and D_2O (0.1 mL) were added to the mixture at room temperature in an argon-filled glovebox. Then the reaction was stirred at 120 $^\circ\text{C}$ for 24 h. The mixture was passed through a short silica gel pad with ethyl acetate as eluent. The solvent was removed on a rotary evaporator. The crude product was subjected to chromatography on silica gel with hexane/ethyl acetate (40/1) as eluent to give compound **3aa-d** (83% yield, 31.5 mg, 0.0830 mmol) as a colorless oil.



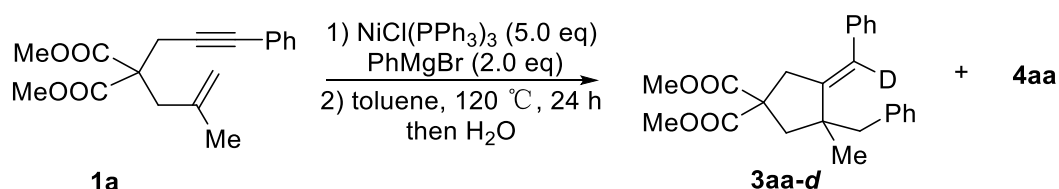
An oven-dried Schlenk tube equipped with a stir bar was charged with **1a** (30.0 mg,

0.100 mmol). Aryl-Ni(II) complex (3.70 mg, 5.00 μmol), toluene (1.0 mL) and H_2O (0.1 mL) were added to the mixture at room temperature in an argon-filled glovebox. Then the reaction was stirred at 120 $^\circ\text{C}$ for 24 h. The mixture was passed through a short silica gel pad with ethyl acetate as eluent. The solvent was removed on a rotary evaporator.



The Ni(I) precursor $(\text{PPh}_3)_3\text{NiCl}$ was synthesized by comproportionation of $\text{Ni}(\text{PPh}_3)_4$ and $(\text{PPh}_3)_2\text{NiCl}_2$ in ethyl ether according to Heimbach.⁹ Or to a scintillation vial was added $\text{Ni}(\text{cod})_2$ (0.100 g, 0.364 mmol) and $\text{NiCl}_2(\text{dme})$ (79.9 mg, 0.364 mmol.) as solids, followed by 5.0 mL of toluene. To this solution was added PPh_3 (573 mg, 2.18 mmol) dissolved in 3.0 mL toluene and the reaction mixture was stirred rt for 12 h before being filtered through Celite. The filtrate was concentrated in vacuo to a volume of 2.0 mL, layered with hexanes, and cooled to -30 $^\circ\text{C}$ to afford a yellow crystalline solid $\text{NiCl}(\text{PPh}_3)_3$ (74% yield, 77.9 mg, 0.269 mmol).¹⁰

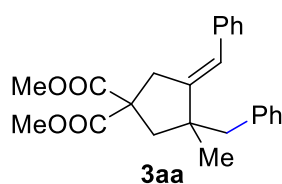
An oven-dried Schlenk tube equipped with a stir bar was charged with **1a** (30.0 mg, 0.100 mmol) and phenylboronic acid **2a** (36.6 mg, 0.300 mmol). $\text{NiCl}(\text{PPh}_3)_3$ (8.81 mg, 10.0 μmol , 10 mol% of Ni), toluene (1.0 mL) and H_2O (0.1 mL) were added to the mixture at room temperature in an argon-filled glovebox. Then the reaction was stirred at 120 $^\circ\text{C}$ for 24 h. The crude product was subjected to chromatography on silica gel with hexane/ethyl acetate (40/1) as eluent to give compound **3aa** (76% yield, 28.8 mg, 0.0500 mmol) as a colorless oil.



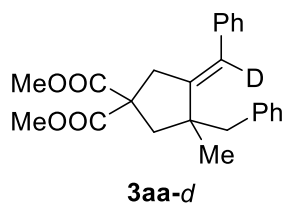
To a dry Schlenk tube was added $\text{NiCl}(\text{PPh}_3)_3$ (0.500 mmol, 145 mg), which was dissolved in 500 μL of toluene. The appropriate arylmagnesium bromide Grignard reagent (2.0 equiv, 0.200 mmol) was added to the mixture.

An oven-dried Schlenk tube equipped with a stir bar was charged with **1a** (30.0 mg, 0.100 mmol). Grignard-reagent-Ni(I) complex and toluene (1.0 mL) were added to the Schlenk tube at room temperature in an argon-filled glovebox. Then the reaction was stirred at 120 °C for 24 h. The reaction quenched with H₂O (0.1 mL). The crude product was subjected to chromatography on silica gel with hexane/ethyl acetate (40/1) as eluent to give compound **3aa-d** (21% yield, 7.97 mg, 0.0210 mmol) as a colorless oil.

7. Characterization of the Products

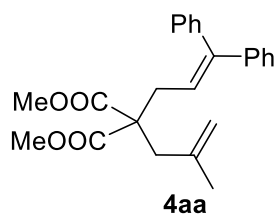


Compound 3aa. (Table 1, entry 1, 91% yield, 34.4 mg, 91.0 μmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), R_f = 0.4 (hexane/ethyl acetate (20/1)). The ee was measured by HPLC (Chiralpak IH column, 0.5 mL/min, hexane/2-propanol = 99/1, 230 nm, t_{minor} = 17.3 min, t_{major} = 20.1 min); $[\alpha]_D^{25} +1.02$ (c 0.850, CHCl₃) for 22% ee. **¹H NMR** (600 MHz, CDCl₃): δ 7.34 (t, J = 7.7 Hz, 2H), 7.28–7.24 (m, 4H), 7.24–7.19 (m, 2H), 7.17 (d, J = 6.7 Hz, 2H), 6.11 (t, J = 2.5 Hz, 1H), 3.74 (s, 3H), 3.67 (s, 3H), 3.38 (d, J = 17.9 Hz, 1H), 3.20 (dd, J = 17.1, 2.8 Hz, 1H), 2.73 (s, 2H), 2.58 (d, J = 13.8 Hz, 1H), 2.22 (d, J = 13.2 Hz, 1H), 1.15 (s, 3H); **¹³C NMR** (151 MHz, CDCl₃): δ 172.6, 172.4, 148.8, 138.4, 137.8, 130.7, 128.5, 128.2, 127.8, 126.3, 126.2, 122.3, 58.4, 52.9, 52.8, 47.9, 47.4, 44.7, 39.1, 27.0. **HRMS (ESI)** calcd for C₂₄H₂₆O₄Na⁺ [M+Na]⁺ 401.1723, found 401.1738.

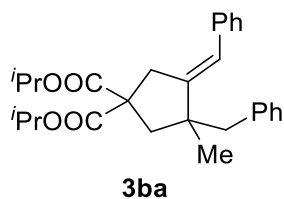


Compound 3aa-d. (Fig 3 (a), 83% yield, 31.5 mg, 83.0 μmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), R_f = 0.4 (hexane/ethyl acetate (20/1)). **¹H NMR** (600 MHz, CDCl₃): δ 7.34 (t, J = 7.7 Hz, 2H), 7.29–7.24 (m,

4H), 7.24–7.20 (m, 2H), 7.18 (d, $J = 6.7$ Hz, 2H), 3.74 (s, 3H), 3.68 (s, 3H), 3.39 (d, $J = 17.1$ Hz, 1H), 3.21 (d, $J = 17.1$ Hz, 1H), 2.73 (s, 2H), 2.58 (d, $J = 13.8$ Hz, 1H), 2.22 (d, $J = 13.8$ Hz, 1H), 1.16 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 172.6, 172.5, 148.8, 138.4, 137.8, 130.7, 128.5, 128.2, 127.8, 126.3, 126.3, 58.5, 52.9, 52.8, 47.9, 47.5, 44.8, 39.1, 27.3; $^2\text{H NMR}$ (92 MHz, CDCl_3): δ 6.12 (s, 1H). **HRMS (ESI)** calcd for $\text{C}_{24}\text{H}_{25}\text{DO}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 402.1786, found 402.1791.

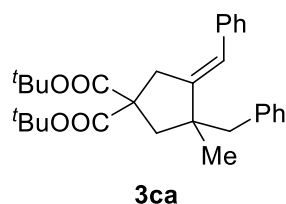


Compound 4aa. (Table 1, entry 2, 31% yield, 11.7 mg, 31.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.35 (t, $J = 7.5$ Hz, 2H), 7.30 (t, $J = 7.4$ Hz, 1H), 7.29–7.20 (m, 3H), 7.18 (d, $J = 6.5$ Hz, 2H), 7.13 (d, $J = 8.0$ Hz, 2H), 5.90 (t, $J = 7.2$ Hz, 1H), 4.77 (s, 1H), 4.64 (s, 1H), 3.67 (s, 6H), 2.82 (d, $J = 7.3$ Hz, 2H), 2.76 (s, 2H), 1.57 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 171.6, 145.0, 142.9, 140.3, 139.5, 129.9, 128.1, 127.6, 127.2, 123.1, 115.7, 57.5, 52.4, 40.5, 32.4, 23.2. **HRMS (ESI)** calcd for $\text{C}_{24}\text{H}_{26}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 401.1723, found 401.1728.

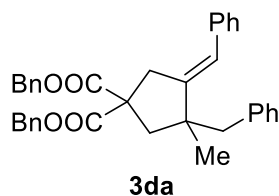


Compound 3ba. (Table 2, entry 2, 97% yield, 42.2 mg, 97.1 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). $^1\text{H NMR}$ (500 MHz, CDCl_3): δ 7.33 (t, $J = 7.6$ Hz, 2H), 7.29–7.24 (m, 4H), 7.24–7.17 (m, 4H), 6.08 (t, $J = 2.4$ Hz, 1H), 5.04 (hept, $J = 6.3$ Hz, 1H), 4.97 (hept, $J = 6.3$ Hz, 1H), 3.33 (d, $J = 16.9$ Hz, 1H), 3.11 (dd, $J = 16.9, 2.8$ Hz, 1H), 2.74 (s, 2H), 2.54 (d, $J = 13.9$ Hz, 1H), 2.19 (d, $J = 13.8$ Hz, 1H), 1.24 (d, $J = 6.3$ Hz, 3H), 1.21 (d, $J = 6.1$ Hz, 3H), 1.18 (d, $J = 6.3$ Hz, 3H), 1.17 (s, 3H), 1.13 (d, $J = 6.2$ Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3): δ 171.7, 171.5, 149.1, 138.5, 138.0, 130.7, 128.5, 128.1,

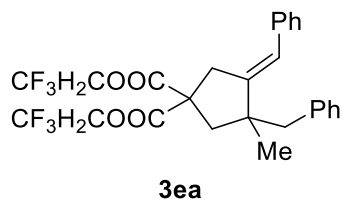
127.7, 126.19, 126.16, 122.2, 69.1, 68.9, 58.6, 48.1, 47.3, 44.5, 38.8, 27.0, 21.53, 21.51, 21.44, 21.40. **HRMS (ESI)** calcd for $C_{28}H_{34}O_4Na^+$ $[M+Na]^+$ 457.2349, found 457.2454.



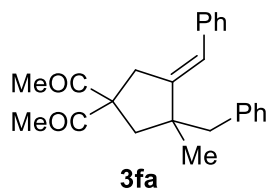
Compound 3ca. (Table 2, entry 3, entry 95% yield, 43.9 mg, 94.9 μ mol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), R_f = 0.4 (hexane/ethyl acetate (20/1))). **1H NMR** (600 MHz, $CDCl_3$): δ 7.33 (t, J = 7.5 Hz, 2H), 7.28–7.24 (m, 4H), 7.24–7.18 (m, 4H), 6.05 (t, J = 2.5 Hz, 1H), 3.27 (d, J = 16.2 Hz, 1H), 3.05 (d, J = 16.9 Hz, 1H), 2.76 (d, J = 13.1 Hz, 1H), 2.73 (d, J = 13.1 Hz, 1H), 2.50 (d, J = 13.8 Hz, 1H), 2.13 (d, J = 13.8 Hz, 1H), 1.45 (s, 9H), 1.37 (s, 9H), 1.17 (s, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 171.4, 171.2, 149.4, 138.7, 138.1, 130.7, 128.5, 128.1, 127.7, 126.1, 122.1, 81.4, 81.2, 59.9, 48.1, 47.3, 44.7, 38.8, 27.8, 27.7, 26.9. **HRMS (ESI)** calcd for $C_{30}H_{38}O_4Na^+$ $[M+Na]^+$ 485.2662, found 485.2667.



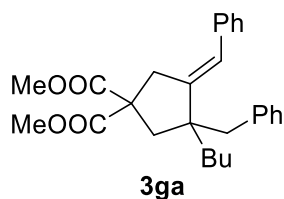
Compound 3da. (Table 2, entry 4, 86% yield, 45.6 mg, 85.9 μ mol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), R_f = 0.4 (hexane/ethyl acetate (20/1))). **1H NMR** (600 MHz, $CDCl_3$): δ 7.36–7.28 (m, 5H), 7.26–7.18 (m, 11H), 7.16–7.11 (m, 4H), 6.12 (t, J = 2.4 Hz, 1H), 5.17–4.97 (m, 4H), 3.39 (dd, J = 16.9, 2.0 Hz, 1H), 3.18 (dd, J = 16.9, 2.8 Hz, 1H), 2.71 (s, 2H), 2.58 (d, J = 13.9 Hz, 1H), 2.26 (d, J = 13.8 Hz, 1H), 1.15 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$): δ 171.8, 171.6, 148.8, 138.4, 137.8, 135.3, 130.7, 128.6, 128.5, 128.4, 128.3, 128.22, 128.20, 128.0, 127.9, 127.8, 126.3, 126.2, 122.5, 67.34, 67.25, 58.7, 48.1, 47.4, 44.5, 39.0, 27.1. **HRMS (ESI)** calcd for $C_{36}H_{34}O_4Na^+$ $[M+Na]^+$ 553.2349, found 553.2354.



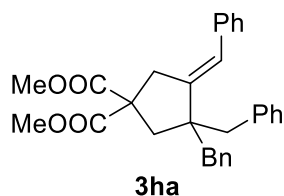
Compound 3ea. (Table 2, entry 5, 88% yield, 45.3 mg, 88.1 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (30/1), $R_f=0.4$ (hexane/ethyl acetate (15/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.35 (t, $J=7.7$ Hz, 2H), 7.30–7.21 (m, 6H), δ 7.16 (d, $J=6.9$ Hz, 2H), 6.18 (t, $J=2.5$ Hz, 1H), 4.57–4.37 (m, 4H), 3.38 (d, $J=16.5$ Hz, 1H), 3.09 (dd, $J=16.9, 2.9$ Hz, 1H), 2.76 (s, 2H), 2.63 (d, $J=14.1$ Hz, 1H), 2.30 (d, $J=14.0$ Hz, 1H), 1.22 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 169.9, 169.8, 147.2, 138.0, 137.5, 130.6, 128.5, 128.3, 127.9, 126.6, 126.5, 123.3, 122.53 (q, $J=277.4$ Hz), 122.49 (q, $J=277.7$ Hz), 61.3 (q, $J=37.4$ Hz), 61.3 (q, $J=37.0$ Hz), 58.1, 48.3, 47.4, 44.5, 39.0, 27.2. $^{19}\text{F}\{^1\text{H}\}$ NMR (565 MHz, CDCl_3): -74.2 (s, 3F), -74.3 (s, 3F). **HRMS (ESI)** calcd for $\text{C}_{26}\text{H}_{24}\text{F}_6\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 537.1471, found 537.1476.



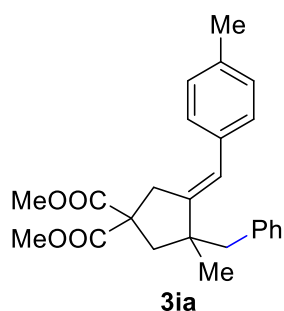
Compound 3fa. (Table 2, entry 6, 76% yield, 26.3 mg, 75.9 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f=0.4$ (hexane/ethyl acetate (20/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.36 (t, $J=7.6$ Hz, 2H), 7.27 (d, $J=7.6$ Hz, 3H), 7.25–7.20 (m, 3H), 7.16 (d, $J=7.4$ Hz, 2H), 6.12 (s, 1H), 3.29 (d, $J=17.0$ Hz, 1H), 3.00 (dd, $J=17.0, 2.8$ Hz, 1H), 2.68 (s, 2H), 2.44 (d, $J=13.8$ Hz, 1H), 2.15 (d, $J=14.1$ Hz, 1H), 2.07 (s, 3H), 2.02 (s, 3H), 1.15 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 205.4, 205.3, 148.5, 138.3, 137.7, 130.6, 128.6, 128.3, 127.8, 126.5, 126.3, 122.5, 73.4, 48.0, 47.5, 42.1, 35.8, 26.9, 26.6, 26.3. **HRMS (ESI)** calcd for $\text{C}_{24}\text{H}_{26}\text{O}_2\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 369.1825, found 369.1830.



Compound 3ga. (Table 2, entry 7, 91% yield, 38.3 mg, 91.1 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (500 MHz, CDCl_3): δ 7.34 (t, $J = 7.7$ Hz, 2H), 7.28–7.19 (m, 6H), 7.19–7.14 (m, 2H), 5.98 (t, $J = 2.5$ Hz, 1H), 3.72 (s, 3H), 3.70 (s, 3H), 3.30–3.16 (m, 2H), 2.76 (d, $J = 13.3$ Hz, 1H), 2.73 (d, $J = 13.3$ Hz, 1H), 2.55 (d, $J = 14.1$ Hz, 1H), 2.34 (d, $J = 14.1$ Hz, 1H), 1.51–1.28 (m, 6H), 0.91 (t, $J = 7.0$ Hz, 3H); $^{13}\text{C NMR}$ (126 MHz, CDCl_3): δ 172.7, 172.6, 147.4, 138.3, 137.9, 130.8, 128.6, 128.2, 127.7, 126.3, 126.2, 122.9, 58.3, 52.9, 52.8, 50.8, 45.1, 42.1, 39.5, 38.2, 26.6, 23.3, 14.1. **HRMS (ESI)** calcd for $\text{C}_{27}\text{H}_{32}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 443.2193, found 443.2196.

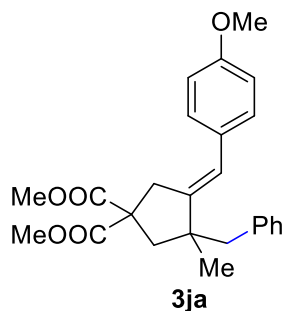


Compound 3ha. (Table 2, entry 8, 97% yield, 44.1 mg, 97.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.36 (t, $J = 7.6$ Hz, 2H), 7.31–7.22 (m, 13H), 6.36 (t, $J = 2.5$ Hz, 1H), 3.63 (s, 6H), 2.89 (d, $J = 13.2$ Hz, 2H), 2.85–2.79 (m, 4H), 2.52 (s, 2H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 172.2, 147.8, 138.1, 137.8, 131.1, 128.6, 128.3, 127.9, 126.42, 126.35, 123.7, 58.6, 52.7, 51.3, 46.5, 40.3, 39.0; **HRMS (ESI)** calcd for $\text{C}_{30}\text{H}_{30}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 477.2036, found 477.2041. The structure of **3ha** was confirmed by single crystal X-ray diffraction (Section 8).

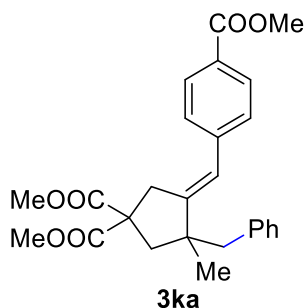


Compound 3ia. (Table 2, entry 9, 85% yield, 33.4 mg, 85.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.25 (t, $J = 7.5$ Hz, 2H), 7.22 (d, $J = 7.0$ Hz, 1H), 7.19–7.14 (m, 6H), 6.08 (t, $J = 2.6$ Hz, 1H), 3.74 (s, 3H), 3.67 (s, 3H), 3.37

(dd, $J = 17.1, 2.1$ Hz, 1H), 3.20 (dd, $J = 17.1, 2.9$ Hz, 1H), 2.72 (s, 2H), 2.57 (d, $J = 13.8$ Hz, 1H), 2.35 (s, 3H), 2.22 (d, $J = 13.8$ Hz, 1H), 1.15 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 172.7, 172.5, 147.9, 138.5, 136.0, 135.0, 130.7, 128.9, 128.5, 127.8, 126.2, 122.2, 58.4, 52.9, 52.8, 47.9, 47.4, 44.8, 39.1, 27.0, 21.1. **HRMS (ESI)** calcd for $\text{C}_{25}\text{H}_{28}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 415.1880, Found 415.1885.

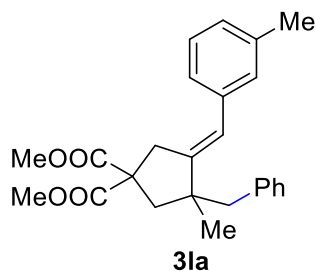


Compound 3ja. (Table 2, entry 10, 87% yield, 35.5 mg, 87.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.25 (t, $J = 9.7$ Hz, 2H), 7.21 (t, $J = 9.0$ Hz, 3H), 7.17 (d, $J = 7.1$ Hz, 2H), 6.88 (d, $J = 8.7$ Hz, 2H), 6.05 (t, $J = 2.5$ Hz, 1H), 3.82 (s, 3H), 3.74 (s, 3H), 3.67 (s, 3H), 3.35 (dd, $J = 17.0, 2.1$ Hz, 1H), 3.18 (dd, $J = 17.0, 2.7$ Hz, 1H), 2.71 (s, 2H), 2.57 (d, $J = 13.8$ Hz, 1H), 2.20 (d, $J = 13.8$ Hz, 1H), 1.14 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 172.7, 172.6, 158.1, 146.8, 138.5, 130.7, 130.6, 129.7, 127.8, 126.2, 121.7, 113.7, 58.5, 55.3, 52.9, 52.8, 48.0, 47.4, 44.8, 39.1, 27.0. **HRMS (ESI)** calcd for $\text{C}_{25}\text{H}_{28}\text{O}_5\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 431.1829, Found 431.1834.

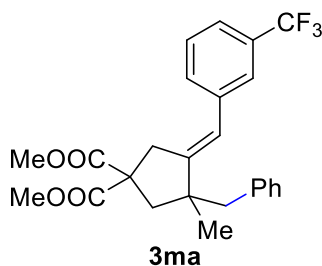


Compound 3ka. (Table 2, entry 11, 82% yield, 35.8 mg, 82.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.00 (d, $J = 8.4$ Hz, 2H), 7.31 (d, $J = 8.0$ Hz, 2H), 7.27 (t, $J = 7.8$ Hz, 2H), 7.23 (d, $J = 7.1$ Hz, 1H), 7.16 (d, $J = 8.1$ Hz, 2H), 6.13 (t, $J = 2.5$ Hz, 1H), 3.92 (s, 3H), 3.75 (s, 3H), 3.68 (s, 3H), 3.38 (d, $J = 16.5$ Hz,

1H), 3.20 (dd, $J = 17.2, 2.8$ Hz, 1H), 2.73 (s, 2H), 2.60 (d, $J = 13.8$ Hz, 1H), 2.23 (d, $J = 13.9$ Hz, 1H), 1.16 (s, 3H); ^{13}C NMR (151 MHz, CDCl_3): δ 172.4, 172.3, 167.0, 151.7, 142.5, 138.1, 130.7, 129.6, 128.4, 127.8, 126.4, 121.8, 58.4, 53.0, 52.9, 52.0, 47.9, 47.8, 44.7, 39.3, 27.0. **HRMS (ESI)** calcd for $\text{C}_{26}\text{H}_{28}\text{O}_6\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 459.1778, Found 459.1787.

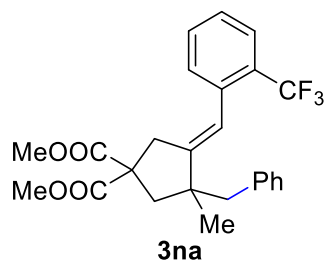


Compound 3la. (Table 2, entry 12, 86% yield, 33.8 mg, 86.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). ^1H NMR (600 MHz, CDCl_3): δ 7.28–7.25 (m, 2H), 7.24–7.20 (m, 2H), 7.18 (d, $J = 7.4$ Hz, 2H), 7.08 (d, $J = 5.8$ Hz, 2H), 7.03 (d, $J = 7.5$ Hz, 1H), 6.09 (s, 1H), 3.75 (d, $J = 1.4$ Hz, 3H), 3.68 (d, $J = 1.4$ Hz, 3H), 3.39 (d, $J = 17.1$ Hz, 1H), 3.21 (dd, $J = 17.2, 2.8$ Hz, 1H), 2.73 (s, 2H), 2.58 (d, $J = 13.8$ Hz, 1H), 2.37 (s, 3H), 2.21 (d, $J = 13.8$ Hz, 1H), 1.15 (s, 3H); ^{13}C NMR (151 MHz, CDCl_3): δ 172.7, 172.5, 148.6, 138.5, 137.8, 137.7, 130.7, 129.3, 128.1, 127.8, 127.1, 126.2, 125.6, 122.4, 58.4, 52.9, 52.8, 47.9, 47.5, 44.8, 39.1, 27.0, 21.5. **HRMS (ESI)** calcd for $\text{C}_{25}\text{H}_{28}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 415.1880, Found 415.1884.

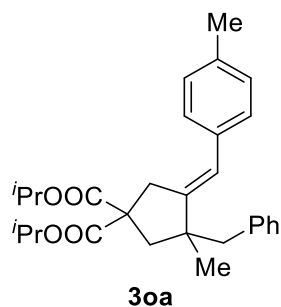


Compound 3ma. (Table 2, entry 13, 85% yield, 38.0 mg, 85.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). ^1H NMR (600 MHz, CDCl_3): δ 7.50–7.40 (m, 4H), 7.30–7.26 (m, 3H), 7.16 (d, $J = 8.1$ Hz, 2H), 6.11 (t, $J = 2.4$ Hz, 1H), 3.75 (s, 3H), 3.69 (s, 3H), 3.33 (d, $J = 17.1$ Hz, 1H), 3.16 (dd, $J = 17.0, 2.7$ Hz, 1H), 2.73 (s, 2H), 2.61 (d, $J = 13.9$ Hz, 1H),

2.23 (d, $J = 13.9$ Hz, 1H), 1.16 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 172.4, 172.3, 151.0, 138.6, 138.1, 131.5, 130.645, 130.636 (q, $J = 32.2$ Hz), 128.7, 127.8, 126.4, 124.2 (q, $J = 272.5$ Hz), 125.2 (q, $J = 3.8$ Hz), 123.0 (q, $J = 4.0$ Hz), 121.2, 58.4, 52.9, 52.8, 47.9, 47.5, 44.8, 38.9, 27.0. **HRMS (ESI)** calcd for $\text{C}_{25}\text{H}_{25}\text{F}_3\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 469.1597, Found 469.1601.

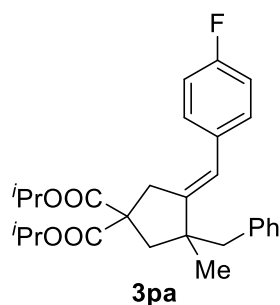


Compound 3na. (Table 2, entry 14, 83% yield, 37.1 mg, 83.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.64 (d, $J = 7.8$ Hz, 1H), 7.51 (t, $J = 7.6$ Hz, 1H), 7.36–7.31 (m, 2H), 7.31–7.27 (m, 2H), 7.25–7.21 (m, 3H), 6.42 (s, 1H), 3.71 (s, 3H), 3.63 (s, 3H), 3.06 (d, $J = 16.6$ Hz, 1H), 2.88 (d, $J = 16.7$ Hz, 1H), 2.77 (s, 2H), 2.61 (d, $J = 14.0$ Hz, 1H), 2.20 (d, $J = 13.9$ Hz, 1H), 1.19 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 172.3, 172.2, 151.8, 138.3, 137.0, 131.5, 130.7, 130.6, 128.2 (q, $J = 29.6$ Hz), 127.9, 126.6, 126.3, 125.7 (q, $J = 5.5$ Hz), 124.5 (q, $J = 273.4$ Hz), 119.1, 58.2, 52.8, 52.7, 48.0, 46.59, 44.6, 38.8, 27.2. **HRMS (ESI)** calcd for $\text{C}_{25}\text{H}_{25}\text{F}_3\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 469.1597, Found 469.1601.

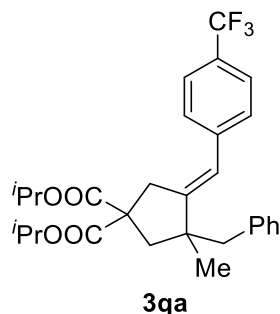


Compound 3oa. (Table 2, entry 15, 85% yield, 38.1 mg, 85.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.26 (t, $J = 7.3$ Hz, 2H), 7.22 (d, $J = 6.9$ Hz, 1H), 7.20–7.13 (m, 6H), 6.05 (s, 1H), 5.05 (hept, $J = 6.3$ Hz, 1H), 4.98 (hept, $J = 6.4$ Hz, 1H), 3.33 (d, $J = 16.9$ Hz, 1H), 3.12 (d, $J = 17.0$ Hz, 1H), 2.74 (s, 2H), 2.54

(d, $J = 13.8$ Hz, 1H), 2.35 (s, 3H), 2.19 (d, $J = 13.8$ Hz, 1H), 1.24 (d, $J = 6.3$ Hz, 3H), 1.22 (d, $J = 6.2$ Hz, 3H), 1.17 (s, 3H), 1.18 (d, $J = 6.3$ Hz, 3H), 1.15 (d, $J = 6.3$ Hz, 3H); ^{13}C NMR (151 MHz, CDCl_3): δ 171.8, 171.6, 148.2, 138.6, 135.8, 135.2, 130.7, 128.8, 128.4, 127.7, 126.1, 122.0, 69.0, 68.9, 58.6, 48.0, 47.3, 44.6, 38.8, 26.9, 21.5, 21.44, 21.41, 21.1. **HRMS (ESI)** calcd for $\text{C}_{29}\text{H}_{36}\text{O}_5\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 471.2506, found 471.2511.

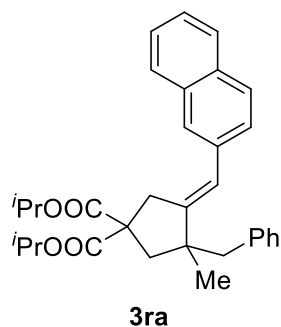


Compound 3pa. (Table 2, entry 16, 87% yield, 39.4 mg, 87.1 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). ^1H NMR (600 MHz, CDCl_3): δ 7.26 (t, $J = 6.9$ Hz, 2H), 7.24–7.19 (m, 3H), 7.17 (d, $J = 6.8$ Hz, 2H), 7.02 (t, $J = 8.8$ Hz, 2H), 6.03 (s, 1H), 5.04 (hept, $J = 6.2$ Hz, 1H), 4.97 (hept, $J = 6.3$ Hz, 1H), 3.27 (d, $J = 16.8$ Hz, 1H), 3.06 (dd, $J = 16.8, 2.8$ Hz, 1H), 2.73 (s, 2H), 2.54 (d, $J = 13.8$ Hz, 1H), 2.19 (d, $J = 13.9$ Hz, 1H), 1.24 (d, $J = 6.3$ Hz, 3H), 1.21 (d, $J = 6.3$ Hz, 3H), 1.174 (d, $J = 6.3$ Hz, 3H), 1.169 (s, 3H), 1.13 (d, $J = 6.2$ Hz, 3H); ^{13}C NMR (151 MHz, CDCl_3): δ 171.6, 171.5, 161.3 (d, $J = 245.7$ Hz), 148.9, 138.5, 134.1 (d, $J = 3.3$ Hz), 130.7, 130.0 (d, $J = 7.7$ Hz), 127.7, 126.2, 121.1, 115.0 (d, $J = 21.3$ Hz), 69.1, 69.0, 58.6, 48.1, 47.3, 44.6, 38.7, 26.9, 21.5, 21.43, 21.39. **HRMS (ESI)** calcd for $\text{C}_{28}\text{H}_{33}\text{FO}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 475.2255, found 475.2262.

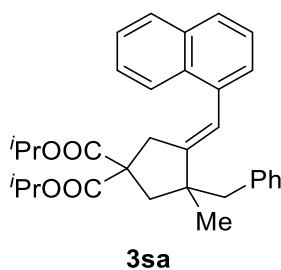


Compound 3qa. (Table 2, entry 17, 82% yield, 41.2 mg, 82.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). ^1H NMR (600 MHz, CDCl_3): δ 7.58 (d, $J = 7.8$ Hz, 2H), 7.35 (d, $J =$

8.0 Hz, 2H), 7.30–7.21 (m, 3H), 7.17 (d, $J = 7.3$ Hz, 2H), 6.09 (s, 1H), 5.05 (hept, $J = 6.3$ Hz, 1H), 4.98 (hept, $J = 6.3$ Hz, 1H), 3.30 (d, $J = 16.9$ Hz, 1H), 3.09 (d, $J = 14.2$ Hz, 1H), 2.75 (s, 2H), 2.58 (d, $J = 13.9$ Hz, 1H), 2.22 (d, $J = 13.8$ Hz, 1H), 1.24 (d, $J = 6.3$ Hz, 3H), 1.22 (d, $J = 6.2$ Hz, 3H), 1.19 (s, 3H), 1.18 (d, $J = 6.5$ Hz, 3H), 1.14 (d, $J = 6.3$ Hz, 3H); ^{13}C NMR (151 MHz, CDCl_3): δ 171.5, 171.4, 152.0, 141.5, 138.3, 130.7, 128.6, 128.1 (q, $J = 32.4$ Hz), 127.8, 126.3, 125.1 (q, $J = 3.8$ Hz), 124.3 (q, $J = 272.0$ Hz), 121.2, 69.2, 69.1, 58.6, 48.0, 47.5, 44.6, 38.9, 26.9, 21.5, 21.43, 21.39. **HRMS (ESI)** calcd for $\text{C}_{29}\text{H}_{33}\text{F}_3\text{O}_4\text{Na}^+ [\text{M}+\text{Na}]^+$ 525.2223, found 525.2225.

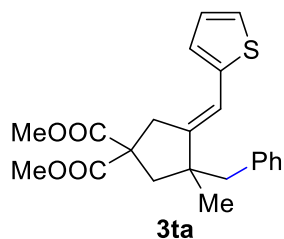


Compound 3ra. (Table 2, entry 18, 86% yield, 41.7 mg, 86.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). ^1H NMR (600 MHz, CDCl_3): δ 7.86–7.78 (m, 3H), 7.70 (s, 1H), 7.50–7.40 (m, 3H), 7.31–7.26 (m, 2H), 7.23 (d, $J = 7.7$ Hz, 3H), 6.24 (s, 1H), 5.07 (hept, $J = 6.2$ Hz, 1H), 4.98 (hept, $J = 6.3$ Hz, 1H), 3.43 (d, $J = 16.9$ Hz, 1H), 3.25 (d, $J = 16.9$ Hz, 1H), 2.80 (s, 2H), 2.59 (d, $J = 13.8$ Hz, 1H), 2.25 (d, $J = 13.8$ Hz, 1H), 1.25 (d, $J = 6.2$ Hz, 3H), 1.23 (s, 3H), 1.22 (d, $J = 6.2$ Hz, 3H), 1.18 (d, $J = 6.2$ Hz, 3H), 1.13 (d, $J = 6.3$ Hz, 3H); ^{13}C NMR (151 MHz, CDCl_3): δ 171.7, 171.5, 149.7, 138.5, 135.6, 133.4, 132.0, 130.8, 127.9, 127.7, 127.6, 127.5, 127.12, 127.05, 126.2, 126.0, 125.5, 122.3, 69.1, 69.0, 58.7, 48.1, 47.5, 44.6, 39.0, 27.0, 21.5, 21.43, 21.41. **HRMS (ESI)** calcd for $\text{C}_{32}\text{H}_{36}\text{O}_4\text{Na}^+ [\text{M}+\text{Na}]^+$ 507.2506, found 507.2511.

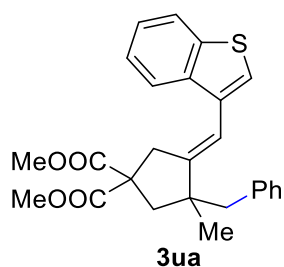


Compound 3sa. (Table 2, entry 19, 85% yield, 41.2 mg, 85.0 μmol , colorless oil,

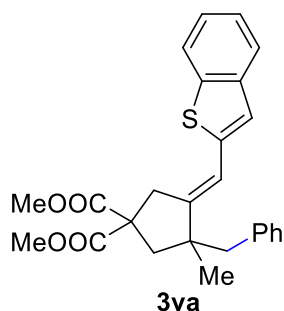
chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f = 0.4$ (hexane/ethyl acetate (20/1))). **$^1\text{H NMR}$** (600 MHz, CDCl_3): δ 7.87 (d, $J = 9.0$ Hz, 1H), 7.84 (d, $J = 8.8$ Hz, 1H), 7.75 (d, $J = 8.2$ Hz, 1H), 7.50–7.43 (m, 3H), 7.39 (d, $J = 7.0$ Hz, 1H), 7.34–7.28 (m, 5H), 6.59 (s, 1H), 5.01 (hept, $J = 6.2$ Hz, 1H), 4.91 (hept, $J = 6.3$ Hz, 1H), 3.13 (d, $J = 16.7$ Hz, 1H), 3.00 (d, $J = 16.5$ Hz, 1H), 2.89 (d, $J = 13.0$ Hz, 1H), 2.86 (d, $J = 13.2$ Hz, 1H), 2.60 (d, $J = 13.9$ Hz, 1H), 2.29 (d, $J = 13.8$ Hz, 1H), 1.34 (s, 3H), 1.21 (d, $J = 6.3$ Hz, 3H), 1.15 (d, $J = 6.2$ Hz, 3H), 1.12 (d, $J = 6.3$ Hz, 3H), 0.98 (d, $J = 6.3$ Hz, 3H); **$^{13}\text{C NMR}$** (151 MHz, CDCl_3): δ 171.7, 171.5, 150.9, 138.6, 135.3, 133.5, 131.9, 130.7, 128.3, 127.8, 127.0, 126.2, 126.1, 125.7, 125.6, 125.4, 124.8, 120.0, 69.0, 68.8, 58.2, 48.1, 46.7, 45.1, 38.6, 27.0, 21.5, 21.44, 21.37, 21.2. **HRMS (ESI)** calcd for $\text{C}_{32}\text{H}_{36}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 507.2506, found 507.2513.



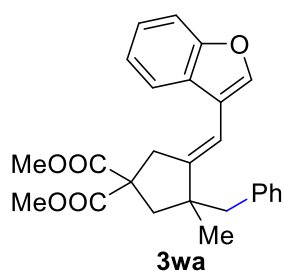
Compound 3ta. (Table 2, entry 20, 93% yield, 35.8 mg, 93.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). **$^1\text{H NMR}$** (600 MHz, CDCl_3): δ 7.28–7.24 (m, 3H), 7.22 (d, $J = 7.4$ Hz, 1H), 7.15 (d, $J = 6.6$ Hz, 2H), 7.05–7.01 (m, 1H), 6.93 (d, $J = 3.6$ Hz, 1H), 6.28 (t, $J = 2.6$ Hz, 1H), 3.77 (s, 3H), 3.71 (s, 3H), 3.46 (dd, $J = 17.7, 2.3$ Hz, 1H), 3.27 (dd, $J = 17.8, 2.7$ Hz, 1H), 2.72 (d, $J = 13.3$ Hz, 1H), 2.68 (d, $J = 13.3$ Hz, 1H), 2.61 (d, $J = 13.8$ Hz, 1H), 2.23 (d, $J = 13.8$ Hz, 1H), 1.11 (s, 3H); **$^{13}\text{C NMR}$** (151 MHz, CDCl_3): δ 172.6, 172.5, 147.6, 141.6, 138.3, 130.7, 127.8, 127.1, 126.3, 126.1, 124.7, 115.6, 58.5, 53.0, 52.9, 47.7, 47.6, 45.2, 39.5, 27.0. **HRMS (ESI)** calcd for $\text{C}_{26}\text{H}_{26}\text{O}_4\text{SNa}^+$ $[\text{M}+\text{Na}]^+$ 407.1288, Found 407.1293.



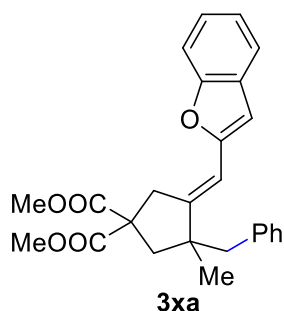
Compound 3ua. (Table 2, entry 21, 90% yield, 39.1 mg, 90.0 μ mol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f = 0.4 (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.87 (d, J = 7.1 Hz, 1H), 7.70 (d, J = 8.7 Hz, 1H), 7.42–7.34 (m, 2H), 7.29 (t, J = 7.6 Hz, 3H), 7.25 (d, J = 6.6 Hz, 1H), 7.21 (d, J = 8.0 Hz, 2H), 6.33 (t, J = 2.5 Hz, 1H), 3.75 (s, 3H), 3.68 (s, 3H), 3.41 (dd, J = 17.3, 2.8 Hz, 1H), 3.24 (dd, J = 17.3, 2.8 Hz, 1H), 2.80 (s, 2H), 2.64 (d, J = 13.9 Hz, 1H), 2.29 (d, J = 13.8 Hz, 1H), 1.24 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 172.6, 172.4, 150.8, 139.6, 138.9, 138.3, 133.0, 130.7, 127.9, 126.3, 124.4, 124.0, 122.7, 122.6, 121.9, 113.9, 58.2, 52.9, 52.9, 47.9, 47.4, 45.2, 39.7, 27.1. **HRMS (ESI)** calcd for $\text{C}_{26}\text{H}_{26}\text{O}_4\text{SNa}^+$ $[\text{M}+\text{Na}]^+$ 457.1444, Found 457.1445.



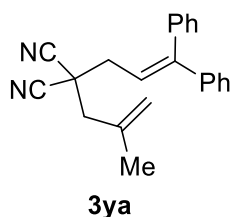
Compound 3va. (Table 2, entry 22, 90% yield, 39.1 mg, 90.0 μ mol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f = 0.4 (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.79 (d, J = 7.9 Hz, 1H), 7.73 (d, J = 7.8 Hz, 1H), 7.34 (t, J = 7.4 Hz, 1H), 7.29–7.23 (m, 4H), 7.17 (d, J = 7.8 Hz, 2H), 7.12 (s, 1H), 6.30 (t, J = 2.4 Hz, 1H), 3.78 (s, 3H), 3.72 (s, 3H), 3.58 (dd, J = 17.7, 2.4 Hz, 1H), 3.36 (dd, J = 17.8, 2.8 Hz, 1H), 2.75 (d, J = 13.3 Hz, 1H), 2.72 (d, J = 13.3 Hz, 1H), 2.63 (d, J = 13.7 Hz, 1H), 2.27 (d, J = 13.7 Hz, 1H), 1.15 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 172.5, 172.4, 150.5, 141.4, 139.79, 139.78, 138.1, 130.7, 127.9, 126.4, 124.4, 124.0, 123.2, 122.6, 122.0, 116.2, 58.4, 53.0, 53.0, 47.9, 47.7, 45.1, 39.5, 27.0. **HRMS (ESI)** calcd for $\text{C}_{26}\text{H}_{26}\text{O}_4\text{SNa}^+$ $[\text{M}+\text{Na}]^+$ 457.1444, Found 457.1449.



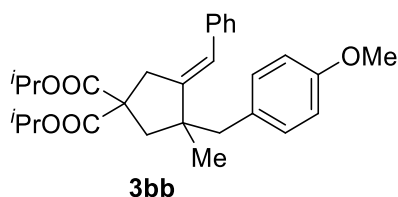
Compound 3wa. (Table 2, entry 23, 97% yield, 40.6 mg, 0.097.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f = 0.4 (hexane/ethyl acetate (25/1))). **$^1\text{H NMR}$** (600 MHz, CDCl_3): δ 7.60 (s, 1H), 7.54 (d, J = 7.2 Hz, 1H), 7.49 (d, J = 8.2 Hz, 1H), 7.32 (d, J = 7.3 Hz, 1H), 7.27 (t, J = 8.8 Hz, 2H), 7.26–7.21 (m, 2H), 7.18 (d, J = 6.8 Hz, 2H), 6.10 (t, J = 2.7 Hz, 1H), 3.76 (s, 3H), 3.70 (s, 3H), 3.31 (dd, J = 17.5, 2.2 Hz, 1H), 3.18 (dd, J = 17.4, 2.7 Hz, 1H), 2.76 (s, 2H), 2.64 (d, J = 13.8 Hz, 1H), 2.28 (d, J = 13.8 Hz, 1H), 1.19 (s, 3H); **$^{13}\text{C NMR}$** (151 MHz, CDCl_3): δ 172.6, 172.5, 154.7, 150.3, 141.7, 138.3, 130.7, 127.8, 127.5, 126.3, 124.5, 122.5, 119.6, 118.2, 111.4, 109.8, 58.2, 53.0, 52.9, 47.8, 47.3, 45.4, 40.1, 27.0. **HRMS (ESI)** calcd for $\text{C}_{26}\text{H}_{26}\text{O}_5\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 441.1672, Found 441.1683.



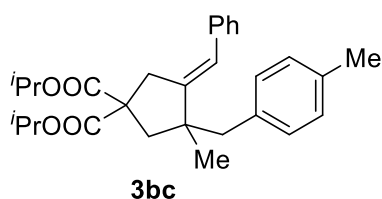
Compound 3xa. (Table 2, entry 24, 95% yield, 39.8 mg, 95.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f = 0.4 (hexane/ethyl acetate (25/1))). **$^1\text{H NMR}$** (600 MHz, CDCl_3): δ 7.53 (d, J = 7.5 Hz, 1H), 7.46 (d, J = 8.0 Hz, 1H), 7.29–7.19 (m, 5H), 7.16 (d, J = 7.0 Hz, 2H), 6.54 (s, 1H), 6.07 (t, J = 2.4 Hz, 1H), 3.79 (s, 3H), 3.72 (s, 3H), 3.68 (dd, J = 18.4, 2.3 Hz, 1H), 3.47 (dd, J = 18.4, 2.7 Hz, 1H), 2.75 (d, J = 13.2 Hz, 1H), 2.71 (d, J = 13.3 Hz, 1H), 2.64 (d, J = 13.8 Hz, 1H), 2.25 (d, J = 13.7 Hz, 1H), 1.14 (s, 3H); **$^{13}\text{C NMR}$** (151 MHz, CDCl_3): δ 172.6, 172.5, 155.2, 154.5, 152.2, 138.0, 130.6, 129.0, 127.9, 126.4, 124.0, 122.7, 120.6, 111.3, 111.0, 104.6, 58.4, 53.0, 52.9, 48.0, 47.6, 45.0, 40.0, 26.9. **HRMS (ESI)** calcd for $\text{C}_{26}\text{H}_{26}\text{O}_5\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 441.1672, Found 441.1672.



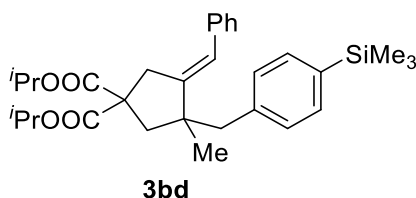
Compound 3ya. (Table 2, entry 25, 36% yield, 11.3 mg, 36.2 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (30/1), $R_f=0.4$ (hexane/ethyl acetate (15/1))). $^1\text{H NMR}$ (500 MHz, CDCl_3): δ 7.46–7.35 (m, 3H), 7.35–7.25 (m, 5H), 7.23–7.18 (m, 2H), 6.20 (t, $J=7.4$ Hz, 1H), 5.11 (quint, $J=1.4$ Hz, 1H), 5.03 (quint, $J=1.0$ Hz, 1H), 2.81 (d, $J=7.4$ Hz, 2H), 2.55 (s, 2H), 1.91 (dd, $J=1.6, 0.9$ Hz, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 148.9, 141.0, 138.5, 137.2, 129.6, 128.6, 128.3, 128.2, 127.9, 127.5, 118.6, 118.3, 115.5, 44.6, 38.1, 36.8, 23.0. **HRMS (ESI)** calcd for $\text{C}_{22}\text{H}_{20}\text{N}_2\text{H}^+$ $[\text{M}+\text{H}]^+$ 313.1699, found 313.1708.



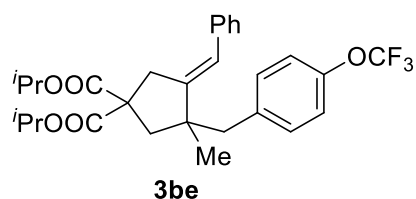
Compound 3bb. (Table 3, entry 1, 93% yield, 43.2 mg, 93.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (40/1), $R_f=0.4$ (hexane/ethyl acetate (20/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.33 (t, $J=7.7$ Hz, 2H), 7.28–7.24 (m, 2H), 7.20 (t, $J=7.4$ Hz, 1H), 7.10 (d, $J=8.6$ Hz, 2H), 6.80 (d, $J=8.6$ Hz, 2H), 6.08 (t, $J=2.4$ Hz, 1H), 5.04 (hept, $J=6.3$ Hz, 1H), 4.97 (hept, $J=6.2$ Hz, 1H), 3.79 (s, 3H), 3.33 (d, $J=17.2$ Hz, 1H), 3.10 (dd, $J=16.9, 2.8$ Hz, 1H), 2.68 (s, 2H), 2.52 (d, $J=13.8$ Hz, 1H), 2.18 (d, $J=14.8$ Hz, 1H), 1.24 (d, $J=6.3$ Hz, 3H), 1.21 (d, $J=6.3$ Hz, 3H), 1.17 (d, $J=6.2$ Hz, 3H), 1.16 (s, 3H), 1.13 (d, $J=6.3$ Hz, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 171.7, 171.5, 158.1, 149.2, 138.0, 131.6, 130.7, 128.5, 128.1, 126.1, 122.1, 113.1, 69.1, 69.0, 58.6, 55.2, 47.4, 47.2, 44.5, 38.9, 26.9, 21.52, 21.51, 21.44, 21.39. **HRMS (ESI)** calcd for $\text{C}_{29}\text{H}_{36}\text{O}_5\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 487.2455, found 487.2456.



Compound 3bc. (Table 3, entry 2, 81% yield, 36.3 mg, 80.9 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f = 0.4 (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.34 (t, J = 7.7 Hz, 2H), 7.29–7.25 (m, 2H), 7.20 (t, J = 7.4 Hz, 1H), 7.07 (t, J = 8.7 Hz, 4H), 6.10 (t, J = 2.4 Hz, 1H), 5.04 (hept, J = 6.2 Hz, 1H), 4.97 (hept, J = 6.3 Hz, 1H), 3.33 (dd, J = 16.9, 2.7 Hz, 1H), 3.12 (dd, J = 16.9, 2.8 Hz, 1H), 2.70 (s, 2H), 2.54 (d, J = 13.8 Hz, 1H), 2.32 (s, 3H), 2.18 (d, J = 13.8 Hz, 1H), 1.24 (d, J = 6.3 Hz, 3H), 1.21 (d, J = 6.2 Hz, 3H), 1.18 (d, J = 6.7 Hz, 3H), 1.17 (s, 3H), 1.13 (d, J = 6.2 Hz, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 171.7, 171.5, 149.3, 138.1, 135.6, 135.4, 130.6, 128.5, 128.4, 128.1, 126.1, 122.1, 69.1, 68.9, 58.6, 47.6, 47.3, 44.5, 38.8, 26.6, 21.51, 21.50, 21.44, 21.39, 21.0. **HRMS (ESI)** calcd for $\text{C}_{29}\text{H}_{36}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 471.2506, found 471.2614.

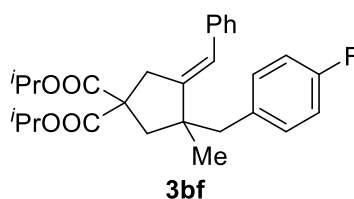


Compound 3bd. (Table 3, entry 3, 83% yield, 42.1 mg, 83.1 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f = 0.4 (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.41 (d, J = 7.8 Hz, 2H), 7.34 (t, J = 7.7 Hz, 2H), 7.28–7.25 (m, 2H), 7.22–7.16 (m, 3H), 6.10 (t, J = 2.5 Hz, 1H), 5.04 (hept, J = 6.3 Hz, 1H), 4.97 (hept, J = 6.3 Hz, 1H), 3.34 (dd, J = 16.5, 1.7 Hz, 1H), 3.17 (dd, J = 16.9, 2.7 Hz, 1H), 2.73 (s, 2H), 2.55 (d, J = 13.8 Hz, 1H), 2.18 (d, J = 13.8 Hz, 1H), 1.23 (d, J = 6.2 Hz, 3H), 1.21 (d, J = 6.3 Hz, 3H), 1.18 (d, J = 6.1 Hz, 3H), 1.17 (s, 3H), 1.14 (d, J = 6.2 Hz, 3H), 0.26 (s, 9H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 171.7, 171.5, 149.3, 139.1, 138.0, 137.7, 132.8, 130.2, 128.5, 128.1, 126.2, 122.1, 69.1, 69.0, 58.7, 48.0, 47.4, 44.5, 38.8, 27.0, 21.54, 21.52, 21.45, 21.41, -1.06. **HRMS (ESI)** calcd for $\text{C}_{31}\text{H}_{42}\text{O}_4\text{SiNa}^+$ $[\text{M}+\text{Na}]^+$ 529.2745, found 529.2753.

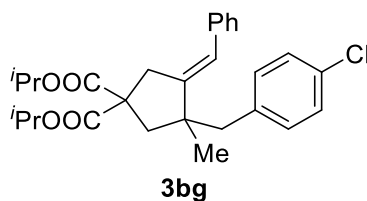


Compound 3be. (Table 3, entry 4, 86% yield, 44.6 mg, 86.0 μmol , a colorless oil,

chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.34 (t, $J = 7.7$ Hz, 2H), 7.26–7.18 (m, 5H), 7.11 (d, $J = 8.1$ Hz, 2H), 6.05 (t, $J = 2.5$ Hz, 1H), 5.04 (hept, $J = 6.3$ Hz, 1H), 4.97 (hept, $J = 6.3$ Hz, 1H), 3.35 (dd, $J = 17.0, 2.0$ Hz, 1H), 3.11 (dd, $J = 17.0, 2.7$ Hz, 1H), 2.74 (s, 2H), 2.51 (d, $J = 13.8$ Hz, 1H), 2.19 (d, $J = 13.8$ Hz, 1H), 1.23 (d, $J = 6.3$ Hz, 3H), 1.21 (d, $J = 6.3$ Hz, 3H), 1.18 (d, $J = 6.2$ Hz, 3H), 1.17 (s, 3H), 1.14 (d, $J = 6.3$ Hz, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 171.7, 171.4, 148.6, 147.8, 137.8, 137.3, 131.9, 128.5, 128.2, 126.4, 122.5, 120.5 (q, $J = 263.9$ Hz), 120.2, 69.2, 69.1, 59.6, 47.3, 47.1, 44.6, 38.8, 26.9, 21.5, 21.44, 21.40. **HRMS (ESI)** calcd for $\text{C}_{29}\text{H}_{33}\text{F}_3\text{O}_5\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 541.2172, found 541.2173.

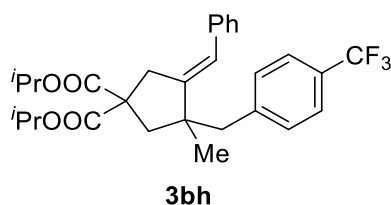


Compound 3bf. (Table 3, entry 5, 86% yield, 38.9 mg, 86.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.34 (t, $J = 7.6$ Hz, 2H), 7.26 (d, $J = 9.5$ Hz, 2H), 7.21 (t, $J = 8.3$ Hz, 1H), 7.14 (dd, $J = 8.4, 5.6$ Hz, 2H), 6.95 (t, $J = 8.7$ Hz, 2H), 6.06 (t, $J = 2.4$ Hz, 1H), 5.04 (hept, $J = 6.3$ Hz, 1H), 4.98 (hept, $J = 6.3$ Hz, 1H), 3.34 (dd, $J = 16.9, 2.0$ Hz, 1H), 3.09 (dd, $J = 17.0, 2.8$ Hz, 1H), 2.72 (s, 2H), 2.51 (d, $J = 13.8$ Hz, 1H), 2.20 (d, $J = 13.8$ Hz, 1H), 1.24 (d, $J = 6.3$ Hz, 3H), 1.22 (d, $J = 6.3$ Hz, 3H), 1.18 (d, $J = 6.3$ Hz, 3H), 1.17 (s, 3H), 1.14 (d, $J = 6.3$ Hz, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 171.7, 171.4, 161.6 (d, $J = 244.3$ Hz), 148.7, 137.8, 134.2 (d, $J = 3.2$ Hz), 132.0 (d, $J = 7.7$ Hz), 128.5, 128.2, 126.3, 122.4, 114.5 (d, $J = 20.8$ Hz), 69.1, 69.0, 58.6, 47.3, 47.1, 44.5, 38.8, 26.8, 21.5, 21.39, 21.42, 21.38. **HRMS (ESI)** calcd for $\text{C}_{28}\text{H}_{33}\text{FO}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 475.2155, found 475.2262.

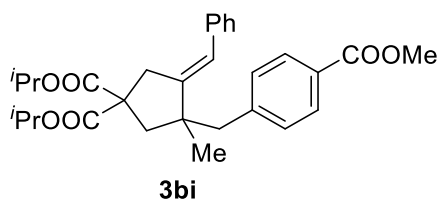


Compound 3bg. (Table 3, entry 6, 84% yield, 39.4 mg, 84.0 μmol , a colorless oil,

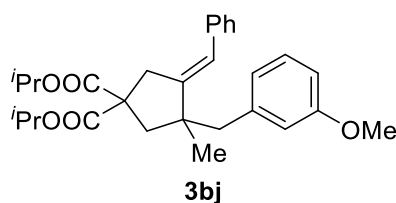
chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). **$^1\text{H NMR}$** (600 MHz, CDCl_3): δ 7.33 (t, $J = 7.7$ Hz, 2H), 7.26–7.19 (m, 5H), 7.11 (d, $J = 8.3$ Hz, 2H), 6.05 (t, $J = 2.4$ Hz, 1H), 5.04 (hept, $J = 6.2$ Hz, 1H), 4.97 (hept, $J = 6.3$ Hz, 1H), 3.34 (dd, $J = 16.6, 2.0$ Hz, 1H), 3.09 (dd, $J = 17.0, 2.8$ Hz, 1H), 2.70 (s, 2H), 2.49 (d, $J = 13.9$ Hz, 1H), 2.18 (d, $J = 14.4$ Hz, 1H), 1.23 (d, $J = 6.3$ Hz, 3H), 1.21 (d, $J = 6.3$ Hz, 3H), 1.18 (d, $J = 6.3$ Hz, 3H), 1.17 (s, 3H), 1.14 (d, $J = 6.3$ Hz, 3H); **$^{13}\text{C NMR}$** (151 MHz, CDCl_3): δ 171.7, 171.4, 148.7, 137.8, 137.0, 132.2, 132.0, 128.5, 128.2, 127.9, 126.3, 122.5, 69.2, 69.0, 58.6, 47.3, 47.2, 44.6, 38.8, 26.8, 21.51, 21.45, 21.4. **HRMS (ESI)** calcd for $\text{C}_{28}\text{H}_{33}\text{ClO}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 491.1960, found 491.1967.



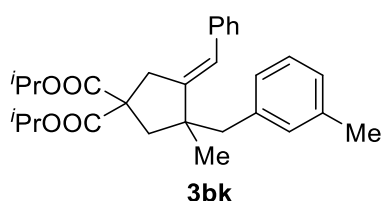
Compound 3bh. (Table 3, entry 7, 71% yield, 35.7 mg, 71.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). **$^1\text{H NMR}$** (600 MHz, CDCl_3): δ 7.33 (t, $J = 7.6$ Hz, 2H), 7.25 (d, $J = 8.5$ Hz, 2H), 7.23–7.15 (m, 4H), 7.06 (d, $J = 6.3$ Hz, 1H), 6.08 (t, $J = 2.4$ Hz, 1H), 5.04 (hept, $J = 6.3$ Hz, 1H), 4.97 (hept, $J = 6.2$ Hz, 1H), 3.32 (d, $J = 17.0, 2.2$ Hz, 1H), 3.12 (dd, $J = 17.0, 2.8$ Hz, 1H), 2.71 (s, 2H), 2.49 (d, $J = 13.9$ Hz, 1H), 2.20 (d, $J = 13.9$ Hz, 1H), 1.24 (d, $J = 6.3$ Hz, 3H), 1.21 (d, $J = 6.2$ Hz, 3H), 1.18 (d, $J = 6.7$ Hz, 3H), 1.17 (s, 3H), 1.13 (d, $J = 6.3$ Hz, 3H); **$^{13}\text{C NMR}$** (151 MHz, CDCl_3): δ 171.7, 171.3, 148.5, 142.7, 137.7, 131.0, 128.6 (q, $J = 32.5$ Hz), 128.5, 128.3, 126.4, 124.6 (q, $J = 3.8$ Hz), 124.4 (q, $J = 272.4$ Hz), 122.6, 69.2, 69.1, 68.7, 58.6, 47.6, 47.3, 44.6, 38.8, 26.9, 21.5, 21.43, 21.38. **HRMS (ESI)** calcd for $\text{C}_{29}\text{H}_{33}\text{F}_3\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 525.2223, found 525.2229.



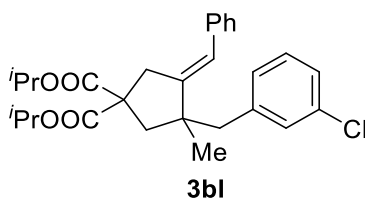
Compound 3bi. (Table 2, entry 8, 87% yield, 42.9 mg, 87.1 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f=0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.93 (d, $J = 8.3$ Hz, 2H), 7.33 (t, $J = 7.6$ Hz, 2H), 7.25 (d, $J = 7.3$ Hz, 2H), 7.24 (d, $J = 7.3$ Hz, 2H), 7.21 (t, $J = 7.2$ Hz, 1H), 6.06 (t, $J = 2.4$ Hz, 1H), 5.04 (hept, $J = 6.3$ Hz, 1H), 4.97 (hept, $J = 6.3$ Hz, 1H), 3.90 (s, 3H), 3.33 (d, $J = 17.1$ Hz, 1H), 3.11 (dd, $J = 17.0, 2.8$ Hz, 1H), 2.79 (t, $J = 13.0$ Hz, 2H), 2.51 (d, $J = 13.8$ Hz, 1H), 2.20 (d, $J = 13.8$ Hz, 1H), 1.23 (d, $J = 6.3$ Hz, 3H), 1.21 (d, $J = 6.3$ Hz, 3H), 1.168 (d, $J = 6.3$ Hz, 3H), 1.167 (s, 3H), 1.13 (d, $J = 6.3$ Hz, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 171.7, 171.4, 167.2, 148.5, 144.1, 137.7, 130.7, 129.0, 128.5, 128.20, 128.17, 126.4, 122.5, 69.2, 69.0, 58.6, 52.0, 47.9, 47.3, 44.7, 38.8, 26.8, 21.53, 21.51, 21.43, 21.38. **HRMS (ESI)** calcd for $\text{C}_{30}\text{H}_{36}\text{O}_6\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 515.2404, found 515.2404.



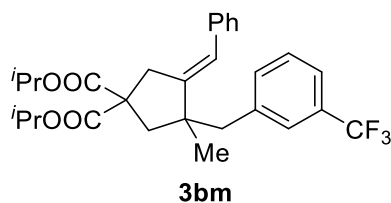
Compound 3bj. (Table 3, entry 9, 93% yield, 43.2 mg, 93.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f=0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.33 (t, $J = 7.6$ Hz, 2H), 7.27 (d, $J = 7.5$ Hz, 2H), 7.23–7.15 (m, 2H), 6.77 (m, 3H), 6.11 (t, $J = 2.4$ Hz, 1H), 5.04 (hept, $J = 6.2$ Hz, 1H), 4.98 (hept, $J = 6.3$ Hz, 1H), 3.74 (s, 3H), 3.34 (dd, $J = 16.9, 2.0$ Hz, 1H), 3.13 (dd, $J = 16.9, 2.8$ Hz, 1H), 2.73 (s, 2H), 2.55 (d, $J = 13.8$ Hz, 1H), 2.21 (d, $J = 13.8$ Hz, 1H), 1.24 (d, $J = 6.3$ Hz, 3H), 1.22 (d, $J = 6.2$ Hz, 3H), 1.19 (s, 3H), 1.18 (d, $J = 6.3$ Hz, 3H), 1.14 (d, $J = 6.2$ Hz, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 171.7, 171.5, 159.1, 149.1, 140.1, 138.0, 128.6, 128.5, 128.1, 126.2, 123.2, 122.2, 116.3, 111.7, 69.1, 68.9, 58.6, 55.1, 48.1, 47.3, 44.6, 38.8, 27.0, 21.50, 21.49, 21.42, 21.38. **HRMS (ESI)** calcd for $\text{C}_{29}\text{H}_{36}\text{O}_5\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 487.2455, found 487.2463.



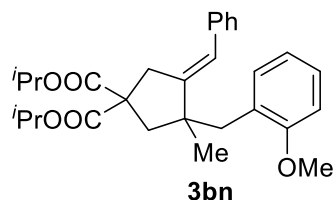
Compound 3bk. (Table 3, entry 10, 92% yield, 41.3 mg, 92.1 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.33 (t, $J = 7.7$ Hz, 2H), 7.28–7.24 (m, 2H), 7.20 (t, $J = 7.3$ Hz, 1H), 7.15 (t, $J = 7.7$ Hz, 1H), 7.03 (d, $J = 7.6$ Hz, 1H), 7.00 (s, 1H), 6.99 (d, $J = 7.8$ Hz, 1H), 6.09 (t, $J = 2.4$ Hz, 1H), 5.04 (hept, $J = 6.2$ Hz, 1H), 4.97 (hept, $J = 6.3$ Hz, 1H), 3.32 (d, $J = 16.9$ Hz, 1H), 3.12 (dd, $J = 16.9, 2.8$ Hz, 1H), 2.70 (s, 2H), 2.54 (d, $J = 13.8$ Hz, 1H), 2.31 (s, 3H), 2.20 (d, $J = 13.8$ Hz, 1H), 1.24 (d, $J = 6.3$ Hz, 3H), 1.22 (d, $J = 6.2$ Hz, 3H), 1.18 (s, 3H), 1.1747 (d, $J = 6.23$ Hz, 3H), 1.13 (d, $J = 6.3$ Hz, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 171.7, 171.6, 149.3, 138.5, 138.0, 137.1, 131.6, 128.5, 128.1, 127.7, 127.6, 126.9, 126.2, 122.2, 69.1, 68.9, 58.6, 48.0, 47.3, 44.5, 38.8, 26.9, 21.54, 21.51, 21.44, 21.40. **HRMS (ESI)** calcd for $\text{C}_{29}\text{H}_{36}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 471.2506, found 471.2507.



Compound 3bl. (Table 3, entry 11, 87% yield, 40.8 mg, 87.1 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.33 (t, $J = 7.6$ Hz, 2H), 7.25 (d, $J = 7.6$ Hz, 2H), 7.23–7.14 (m, 4H), 7.06 (d, $J = 6.4$ Hz, 1H), 6.07 (t, $J = 2.5$ Hz, 1H), 5.04 (hept, $J = 6.3$ Hz, 1H), 4.97 (hept, $J = 6.2$ Hz, 1H), 3.32 (d, $J = 16.6$ Hz, 1H), 3.12 (dd, $J = 17.0, 2.8$ Hz, 1H), 2.71 (s, 2H), 2.49 (d, $J = 13.9$ Hz, 1H), 2.20 (d, $J = 13.9$ Hz, 1H), 1.24 (d, $J = 6.3$ Hz, 3H), 1.22 (d, $J = 6.2$ Hz, 3H), 1.18 (d, $J = 6.4$ Hz, 3H), 1.17 (s, 3H), 1.14 (d, $J = 6.3$ Hz, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 171.7, 171.4, 148.7, 140.6, 137.8, 133.6, 130.7, 129.0, 128.9, 128.5, 128.2, 126.4, 126.3, 122.5, 69.2, 69.0, 58.6, 47.6, 47.3, 44.5, 38.8, 26.9, 21.6, 21.51, 21.45, 21.4. **HRMS (ESI)** calcd for $\text{C}_{28}\text{H}_{33}\text{ClO}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 491.1960, found 491.1960.

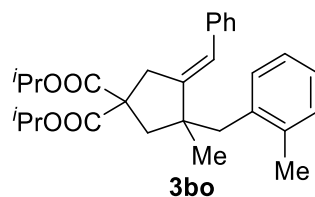


Compound 3bm. (Table 3, entry 12, 89% yield, 44.7 mg, 88.9 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f = 0.4 (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.50–7.46 (m, 1H), 7.43 (s, 1H), 7.37 (d, J = 5.3 Hz, 2H), 7.33 (t, J = 7.6 Hz, 2H), 7.26–7.18 (m, 3H), 6.04 (t, J = 2.4 Hz, 1H), 5.04 (hept, J = 6.3 Hz, 1H), 4.97 (hept, J = 6.3 Hz, 1H), 3.33 (dd, J = 16.9, 2.0 Hz, 1H), 3.12 (dd, J = 17.0, 2.8 Hz, 1H), 2.80 (s, 2H), 2.48 (d, J = 13.9 Hz, 1H), 2.23 (d, J = 13.9 Hz, 1H), 1.23 (d, J = 6.6 Hz, 3H), 1.21 (d, J = 6.6 Hz, 3H), 1.178 (s, 3H), 1.176 (d, J = 6.1 Hz, 3H), 1.13 (d, J = 6.3 Hz, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 171.6, 171.4, 148.3, 139.5, 137.7, 134.0, 130.1 (q, J = 31.9 Hz), 128.5, 128.2, 128.1, 127.3 (q, J = 3.8 Hz), 126.4, 124.2 (q, J = 272.6 Hz), 123.1 (q, J = 3.9 Hz), 122.8, 69.2, 69.1, 58.6, 47.7, 47.3, 44.6, 38.8, 26.8, 21.5, 21.43, 21.39. **HRMS (ESI)** calcd for $\text{C}_{29}\text{H}_{33}\text{F}_3\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 525.2223, found 525.2231.

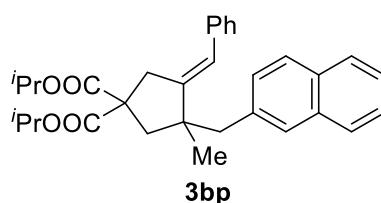


Compound 3bn. (Table 3, entry 13, 63% yield, 29.3 mg, 63.1 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f = 0.4 (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.30 (t, J = 7.6 Hz, 2H), 7.23 (d, J = 7.7 Hz, 2H), 7.17 (t, J = 7.6 Hz, 2H), 7.12 (d, J = 7.4 Hz, 1H), 6.84 (t, J = 7.4 Hz, 1H), 6.80 (d, J = 8.2 Hz, 1H), 5.96 (s, 1H), 5.07 (hept, J = 6.3 Hz, 1H), 4.98 (hept, J = 6.2 Hz, 1H), 3.75 (s, 3H), 3.32 (d, J = 16.8 Hz, 1H), 3.19 (d, J = 16.7 Hz, 1H), 2.98 (d, J = 13.0 Hz, 1H), 2.63 (d, J = 13.0 Hz, 1H), 2.56 (d, J = 13.8 Hz, 1H), 2.25 (d, J = 13.8 Hz, 1H), 1.23 (d, J = 6.7 Hz, 3H), 1.21 (d, J = 6.7 Hz, 3H), 1.17 (s, 3H), 1.16 (d, J = 4.7 Hz, 3H), 1.11 (d, J = 6.1 Hz, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 171.81, 171.75, 158.1, 149.3, 138.2, 132.2, 128.5, 128.0, 127.4, 127.2, 126.0, 121.6, 119.5, 110.2, 68.9, 68.8,

58.7, 55.1, 48.0, 45.3, 40.9, 38.8, 26.4, 21.6, 21.53, 21.45, 21.4. **HRMS (ESI)** calcd for $C_{29}H_{36}O_5Na^+$ $[M+Na]^+$ 487.2455, found 487.2467.

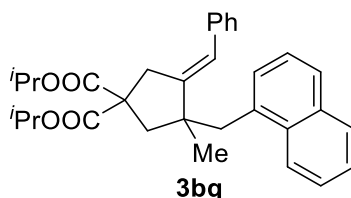


Compound 3bo. (Table 3, entry 14, 52% yield, 23.3 mg, 51.9 μ mol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f =0.4 (hexane/ethyl acetate (25/1))). **1H NMR** (600 MHz, $CDCl_3$): δ 7.32 (t, J = 7.6 Hz, 2H), 7.24–7.17 (m, 3H), 7.15 (d, J = 6.4 Hz, 1H), 7.12–7.06 (m, 3H), 5.90 (t, J = 2.4 Hz, 1H), 5.04 (hept, J = 6.2 Hz, 1H), 4.97 (hept, J = 6.2 Hz, 1H), 3.34 (dd, J = 16.9, 2.2 Hz, 1H), 3.21 (dd, J = 17.0, 2.8 Hz, 1H), 2.89 (d, J = 13.6 Hz, 1H), 2.69 (d, J = 13.6 Hz, 1H), 2.50 (d, J = 13.7 Hz, 1H), 2.35 (d, J = 13.7 Hz, 1H), 2.28 (s, 3H), 1.23 (d, J = 6.6 Hz, 3H), 1.22 (d, J = 6.6 Hz, 3H), 1.20 (s, 3H), 1.18 (d, J = 6.3 Hz, 3H), 1.12 (d, J = 6.3 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$): δ 171.8, 171.5, 148.5, 138.0, 137.4, 136.9, 131.4, 130.3, 128.5, 128.1, 126.3, 126.2, 125.1, 122.5, 69.1, 69.0, 58.7, 48.2, 46.0, 43.8, 38.9, 26.8, 21.54, 21.51, 21.45, 21.4, 20.4. **HRMS (ESI)** calcd for $C_{29}H_{36}O_4Na^+$ $[M+Na]^+$ 471.2506, found 471.2514.

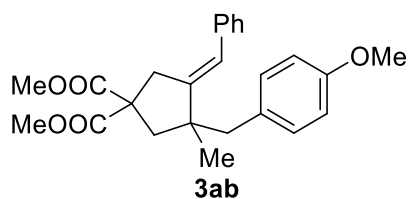


Compound 3bp. (Table 3, entry 15, 92% yield, 44.6 mg, 92.0 μ mol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f =0.4 (hexane/ethyl acetate (25/1))). **1H NMR** (600 MHz, $CDCl_3$): δ 7.81 (d, J = 7.2 Hz, 1H), 7.78 (d, J = 7.1 Hz, 1H), 7.74 (d, J = 8.3 Hz, 1H), 7.65 (s, 1H), 7.48–7.40 (m, 2H), 7.34 (t, J = 7.7 Hz, 3H), 7.27 (s, 2H), 7.21 (t, J = 7.3 Hz, 1H), 6.13 (t, J = 2.4 Hz, 1H), 5.04 (hept, J = 6.2 Hz, 1H), 4.98 (hept, J = 6.2 Hz, 1H), 3.37 (dd, J = 16.8, 2.0 Hz, 1H), 3.15 (dd, J = 16.9, 2.8 Hz, 1H), 2.92 (s, 2H), 2.63 (d, J = 13.8 Hz, 1H), 2.23 (d, J = 13.8 Hz, 1H), 1.23 (s, 3H), 1.22 (d, J = 6.0 Hz, 3H), 1.20 (d, J = 6.2 Hz, 3H), 1.17 (d, J = 6.2 Hz, 3H), 1.14 (d, J = 6.3 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$): δ 171.7, 171.5, 149.1, 138.0,

136.2, 133.2, 132.1, 129.4, 129.1, 128.5, 128.1, 127.6, 127.5, 127.0, 126.2, 125.7, 125.3, 122.4, 69.1, 69.0, 58.7, 48.2, 47.6, 44.7, 38.9, 27.0, 21.51, 21.48, 21.44, 21.39. **HRMS (ESI)** calcd for $C_{32}H_{36}O_4Na^+$ $[M+Na]^+$ 507.2506, found 507.2516.

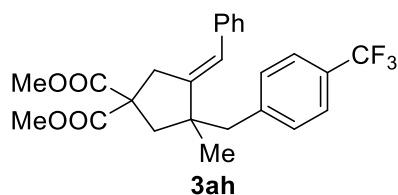


Compound 3bq. (Table 3, entry 16, 87% yield, 42.2 mg, 87.1 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f=0.4$ (hexane/ethyl acetate (25/1))). **1H NMR** (600 MHz, $CDCl_3$): δ 8.13 (d, $J = 8.4$ Hz, 1H), 7.83 (d, $J = 8.0$ Hz, 1H), 7.74 (d, $J = 7.8$ Hz, 1H), 7.48–7.35 (m, 4H), 7.30 (t, $J = 7.6$ Hz, 2H), 7.18 (t, $J = 7.4$ Hz, 1H), 7.13 (d, $J = 7.6$ Hz, 2H), 5.95 (s, 1H), 5.04 (hept, $J = 6.3$ Hz, 1H), 4.97 (hept, $J = 6.2$ Hz, 1H), 3.38 (d, $J = 13.8$ Hz, 1H), 3.32 (d, $J = 16.9$ Hz, 1H), 3.24 (dd, $J = 16.9, 2.8$ Hz, 1H), 3.18 (d, $J = 13.8$ Hz, 1H), 2.64 (d, $J = 13.8$ Hz, 1H), 2.36 (d, $J = 13.8$ Hz, 1H), 1.24 (s, 3H), 1.21 (d, $J = 5.4$ Hz, 3H), 1.20 (d, $J = 5.4$ Hz, 3H), 1.17 (d, $J = 6.3$ Hz, 3H), 1.12 (d, $J = 6.3$ Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$): δ 171.8, 171.5, 148.6, 137.9, 135.0, 133.8, 133.4, 129.0, 128.6, 128.5, 128.0, 127.0, 126.1, 125.4, 125.1, 124.9, 122.9, 69.1, 68.9, 58.6, 48.3, 45.7, 43.1, 38.9, 27.3, 21.5, 21.44, 21.42, 21.37. **HRMS (ESI)** calcd for $C_{32}H_{36}O_4Na^+$ $[M+Na]^+$ 507.2506, found 507.2519.

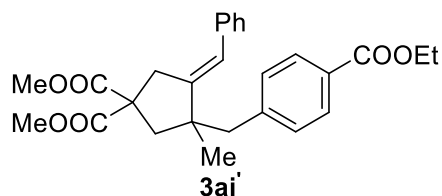


Compound 3ab. (Table 3, entry 17, 91% yield, 37.2 mg, 91.0 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f=0.4$ (hexane/ethyl acetate (25/1))). **1H NMR** (600 MHz, $CDCl_3$): δ 7.34 (t, $J = 8.1$ Hz, 2H), 7.27 (d, $J = 7.4$ Hz, 2H), 7.21 (t, $J = 7.3$ Hz, 1H), 7.09 (d, $J = 8.6$ Hz, 2H), 6.81 (d, $J = 8.6$ Hz, 2H), 6.11 (t, $J = 2.5$ Hz, 1H), 3.79 (s, 3H), 3.74 (s, 3H), 3.68 (s, 3H), 3.38 (dd, $J = 17.2, 2.7$ Hz, 1H), 3.19 (dd, $J = 17.1, 2.8$ Hz, 1H), 2.67 (s, 2H), 2.56 (d, $J = 13.8$ Hz, 1H), 2.21 (d, $J = 13.8$ Hz, 1H), 1.14 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$): δ 172.6, 172.5, 158.1, 148.9, 137.9, 131.6, 130.5, 128.5, 128.2, 126.3, 122.3, 113.2, 58.4, 55.2, 52.9, 52.8,

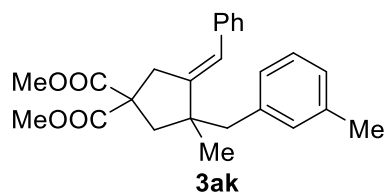
47.5, 47.0, 44.7, 39.1, 27.0. **HRMS (ESI)** calcd for $C_{25}H_{28}O_5Na^+$ $[M+Na]^+$ 431.1829, Found 431.1830.



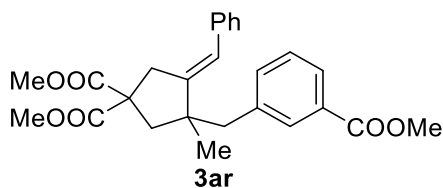
Compound 3ah. (Table 3, entry 18, 82% yield, 36.6 mg, 82.0 μ mol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f = 0.4 (hexane/ethyl acetate (25/1))). **1H NMR** (600 MHz, $CDCl_3$): δ 7.52 (d, J = 8.0 Hz, 2H), 7.35 (t, J = 7.7 Hz, 2H), 7.29 (d, J = 7.9 Hz, 2H), 7.26 (d, J = 8.1 Hz, 2H), 7.23 (t, J = 7.4 Hz, 1H), 6.09 (t, J = 2.5 Hz, 1H), 3.75 (s, 3H), 3.68 (s, 3H), 3.41 (dd, J = 17.1, 2.2 Hz, 1H), 3.22 (dd, J = 17.2, 2.8 Hz, 1H), 2.79 (s, 2H), 2.56 (d, J = 13.8 Hz, 1H), 2.21 (d, J = 13.9 Hz, 1H), 1.15 (s, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$): δ 172.6, 172.3, 148.2, 142.5, 137.5, 130.9, 128.6 (q, J = 48.7 Hz), 128.4, 128.3, 126.5, 124.7 (q, J = 5.7 Hz), 124.3 (q, J = 407.8 Hz), 122.70, 58.3, 53.0, 52.9, 47.5, 47.4, 44.8, 39.0, 26.9. **HRMS (ESI)** calcd for $C_{25}H_{25}F_3O_4Na^+$ $[M+Na]^+$ 469.1597, Found 469.1605.



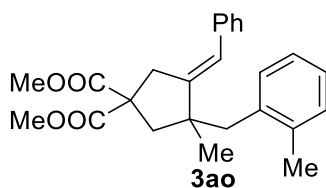
Compound 3ai'. (Table 3, entry 19, 83% yield, 37.4 mg, 83.0 μ mol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f = 0.4 (hexane/ethyl acetate (25/1))). **1H NMR** (600 MHz, $CDCl_3$): δ 7.94 (d, J = 8.2 Hz, 2H), 7.34 (t, J = 7.7 Hz, 2H), 7.27–7.20 (m, 5H), 6.10 (t, J = 2.5 Hz, 1H), 4.36 (q, J = 7.1 Hz, 2H), 3.74 (s, 3H), 3.67 (s, 3H), 3.39 (dd, J = 17.1, 2.2 Hz, 1H), 3.20 (dd, J = 17.2, 2.8 Hz, 1H), 2.79 (s, 2H), 2.55 (d, J = 13.9 Hz, 1H), 2.22 (d, J = 13.8 Hz, 1H), 1.39 (t, J = 7.1 Hz, 3H), 1.15 (s, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$): δ 172.5, 172.3, 166.7, 148.3, 143.8, 137.6, 130.6, 129.0, 128.6, 128.5, 128.3, 126.5, 122.6, 60.8, 58.3, 52.9, 52.8, 47.8, 47.5, 44.8, 39.0, 26.9, 14.3. **HRMS (ESI)** calcd for $C_{27}H_{30}O_6Na^+$ $[M+Na]^+$ 473.1935, Found 473.1934.



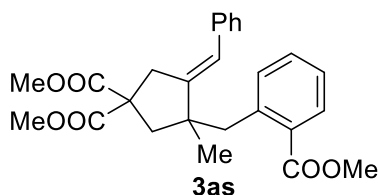
Compound 3ak. (Table 3, entry 20, 86% yield, 33.8 mg, 86.0 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f = 0.4 (hexane/ethyl acetate (25/1))). **¹H NMR** (600 MHz, CDCl₃): δ 7.34 (t, J = 7.7 Hz, 2H), 7.27 (d, J = 6.4 Hz, 2H), 7.21 (t, J = 7.4 Hz, 1H), 7.15 (t, J = 7.8 Hz, 1H), 7.03 (d, J = 7.5 Hz, 1H), 6.98 (d, J = 7.3 Hz, 2H), 6.12 (t, J = 2.6 Hz, 1H), 3.75 (s, 3H), 3.68 (s, 3H), 3.37 (dd, J = 17.1, 2.5 Hz, 1H), 3.21 (dd, J = 17.1, 2.8 Hz, 1H), 2.69 (s, 2H), 2.58 (d, J = 13.8 Hz, 1H), 2.31 (s, 3H), 2.22 (d, J = 13.8 Hz, 1H), 1.15 (s, 3H); **¹³C NMR** (151 MHz, CDCl₃): δ 172.6, 172.5, 149.0, 138.3, 137.9, 137.2, 131.5, 128.5, 128.2, 127.7, 127.6, 126.9, 126.3, 122.3, 58.4, 52.9, 52.8, 47.9, 47.4, 44.7, 39.1, 27.0, 21.4. **HRMS (ESI)** calcd for C₂₅H₂₈O₄Na⁺ [M+Na]⁺ 415.1880, Found 415.1887.



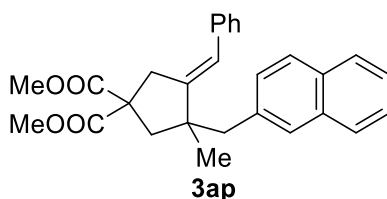
Compound 3ar. (Table 3, entry 21, 86% yield, 37.5 mg, 86.0 mmol, a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), R_f = 0.4 (hexane/ethyl acetate (25/1))). **¹H NMR** (600 MHz, CDCl₃): δ 7.90 (d, J = 7.6 Hz, 1H), 7.85 (s, 1H), 7.38–7.32 (m, 4H), 7.26–7.24 (m, 2H), 7.21 (t, J = 7.3 Hz, 1H), 6.08 (t, J = 2.5 Hz, 1H), 3.87 (s, 3H), 3.76 (s, 3H), 3.68 (s, 3H), 3.36 (dd, J = 17.1, 2.1 Hz, 1H), 3.25 (dd, J = 17.2, 2.8 Hz, 1H), 2.77 (s, 2H), 2.54 (d, J = 13.8 Hz, 1H), 2.24 (d, J = 13.9 Hz, 1H), 1.16 (s, 3H); **¹³C NMR** (151 MHz, CDCl₃): δ 172.6, 172.4, 167.2, 148.3, 138.7, 137.7, 135.2, 131.6, 129.7, 128.6, 128.2, 127.8, 127.6, 126.4, 122.7, 58.3, 53.0, 52.9, 52.0, 47.5, 44.7, 39.02, 26.7. **HRMS (ESI)** calcd for C₂₆H₂₈O₆Na⁺ [M+Na]⁺ 459.1778, Found 459.1788.



Compound 3ao. (Table 3, entry 22, 74% yield, 29.0 mg, 74.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f=0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.34 (t, $J=7.7$ Hz, 2H), 7.24–7.19 (m, 3H), 7.16–7.07 (m, 4H), 6.12 (t, $J=2.6$ Hz, 1H), 3.75 (s, 3H), 3.68 (s, 3H), 3.37 (dd, $J=17.1, 2.5$ Hz, 1H), 3.21 (dd, $J=17.1, 2.8$ Hz, 1H), 2.69 (s, 2H), 2.58 (d, $J=13.8$ Hz, 1H), 2.31 (s, 3H), 2.22 (d, $J=13.8$ Hz, 1H), 1.15 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 172.6, 172.5, 148.1, 137.9, 137.3, 136.7, 131.3, 130.3, 128.5, 128.2, 126.3, 126.7, 125.2, 122.6, 58.4, 52.9, 52.8, 47.9, 47.4, 44.7, 39.1, 27.0, 21.4. **HRMS (ESI)** calcd for $\text{C}_{25}\text{H}_{28}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 415.1880, Found 415.1887.

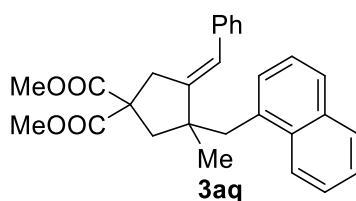


Compound 3as. (Table 3, entry 23, 88% yield, 38.4 mg, 88.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f=0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.80 (d, $J=7.8$ Hz, 1H), 7.37 (t, $J=7.6$ Hz, 1H), 7.32 (t, $J=7.7$ Hz, 2H), 7.29–7.18 (m, 5H), 5.87 (t, $J=2.3$ Hz, 1H), 3.76 (s, 3H), 3.75 (s, 3H), 3.66 (s, 3H), 3.54 (d, $J=13.1$ Hz, 1H), 3.40 (d, $J=17.1$ Hz, 1H), 3.20 (dd, $J=17.1, 2.8$ Hz, 1H), 3.09 (d, $J=13.1$ Hz, 1H), 2.55 (d, $J=13.8$ Hz, 1H), 2.28 (d, $J=13.4$ Hz, 1H), 1.08 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 172.5, 172.5, 168.6, 148.1, 139.6, 137.8, 133.0, 131.5, 130.9, 130.2, 128.6, 128.1, 126.3, 126.2, 122.8, 58.4, 52.9, 52.8, 51.8, 48.1, 46.0, 43.4, 39.0, 26.4. **HRMS (ESI)** calcd for $\text{C}_{26}\text{H}_{28}\text{O}_6\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 459.1778, Found 459.1787.

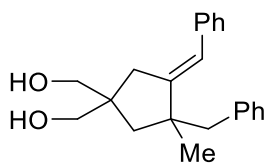


Compound 3ap. (Table 3, entry 24, 97% yield, 41.6 mg, 97.0 μmol , a colorless oil,

chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.82 (d, $J = 7.1$ Hz, 1H), 7.79 (d, $J = 7.1$ Hz, 1H), 7.75 (d, $J = 8.4$ Hz, 1H), 7.65 (s, 1H), 7.49–7.42 (m, 2H), 7.37–7.33 (m, 3H), 7.28 (d, $J = 7.3$ Hz, 2H), 7.23 (t, $J = 7.3$ Hz, 1H), 6.17 (t, $J = 2.4$ Hz, 1H), 3.74 (s, 3H), 3.68 (s, 3H), 3.42 (dd, $J = 17.1, 2.1$ Hz, 1H), 3.25 (dd, $J = 17.1, 2.7$ Hz, 1H), 2.92 (s, 2H), 2.68 (d, $J = 13.8$ Hz, 1H), 2.26 (d, $J = 13.8$ Hz, 1H), 1.22 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 172.6, 172.5, 148.9, 137.8, 136.0, 133.2, 132.1, 129.3, 129.1, 128.5, 128.2, 127.6, 127.5, 127.1, 126.3, 125.8, 125.3, 122.4, 58.4, 52.9, 52.8, 48.0, 47.7, 44.8, 39.1, 27.1. **HRMS (ESI)** calcd for $\text{C}_{28}\text{H}_{28}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 451.1880, Found 451.1890.



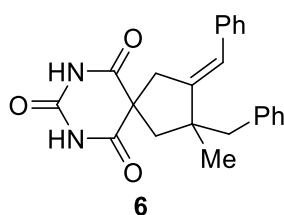
Compound 3aq. (Table 3, entry 25, 82% yield, 35.1 mg, 82.0 μmol , a colorless oil, chromatography on silica gel, eluent: hexane/ethyl acetate (50/1), $R_f = 0.4$ (hexane/ethyl acetate (25/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.11 (d, $J = 8.3$ Hz, 1H), 7.83 (d, $J = 8.8$ Hz, 1H), 7.74 (d, $J = 8.0$ Hz, 1H), 7.48–7.36 (m, 3H), 7.35 (d, $J = 7.1$ Hz, 1H), 7.31 (t, $J = 7.7$ Hz, 2H), 7.19 (t, $J = 7.4$ Hz, 1H), 7.15 (d, $J = 7.2$ Hz, 2H), 5.99 (t, $J = 2.5$ Hz, 1H), 3.72 (s, 3H), 3.67 (s, 3H), 3.37 (dd, $J = 17.1, 2.0$ Hz, 1H), 3.36 (d, $J = 13.8$ Hz, 1H), 3.31 (dd, $J = 17.1, 2.8$ Hz, 1H), 3.17 (d, $J = 13.8$ Hz, 1H), 2.70 (d, $J = 13.8$ Hz, 1H), 2.36 (d, $J = 13.8$ Hz, 1H), 1.20 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 172.7, 172.5, 148.3, 137.8, 134.9, 133.8, 133.3, 129.0, 128.6, 128.5, 128.1, 127.1, 126.3, 125.5, 125.2, 124.9, 124.8, 122.9, 58.4, 52.9, 52.8, 48.4, 46.0, 42.9, 39.0, 27.3. **HRMS (ESI)** calcd for $\text{C}_{28}\text{H}_{28}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 451.1880, Found 451.1879.



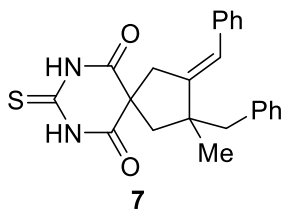
5

Compound 5. (92% yield, 47.5 mg, 147 μmol , a colorless oil, chromatography on silica

gel, eluent: hexane/ethyl acetate (6/1), $R_f = 0.4$ (hexane/ethyl acetate (3/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 7.33 (t, $J = 7.7$ Hz, 2H), 7.27–7.23 (m, 4H), 7.23–7.19 (m, 2H), 7.17 (d, $J = 7.8$ Hz, 2H), 6.22 (t, $J = 2.2$ Hz, 1H), 3.57–3.45 (m, 4H), 2.77 (s, 2H), 2.60 (d, $J = 16.2$ Hz, 1H), 2.32 (s, 2H), 2.14 (dd, $J = 16.3, 2.8$ Hz, 1H), 1.85 (d, $J = 14.0$ Hz, 1H), 1.45 (d, $J = 14.0$ Hz, 1H), 1.27 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 151.2, 139.0, 138.9, 130.7, 128.6, 128.2, 127.7, 126.22, 126.16, 122.3, 71.0, 69.8, 49.8, 47.1, 46.9, 42.2, 37.6, 29.0. **HRMS (ESI)** calcd for $\text{C}_{22}\text{H}_{26}\text{O}_2\text{Na}^+ [\text{M}+\text{Na}]^+$ 345.1825, found 345.1830.

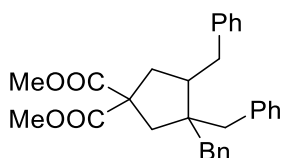


Compound 6. (95% yield, 39.1 mg, 105 μmol , a white solid, chromatography on silica gel, eluent: hexane/ethyl acetate (20/1), $R_f = 0.4$ (hexane/ethyl acetate (10/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.70 (s, 1H), 8.53 (s, 1H), 7.31 (t, $J = 7.6$ Hz, 2H), 7.26 (t, $J = 7.4$ Hz, 2H), 7.21 (t, $J = 6.9$ Hz, 2H), 7.20–7.16 (m, 4H), 6.16 (t, $J = 2.4$ Hz, 1H), 3.39 (d, $J = 16.2$ Hz, 1H), 3.24 (dd, $J = 16.2, 2.7$ Hz, 1H), 2.90 (s, 2H), 2.59 (d, $J = 13.9$ Hz, 1H), 2.06 (d, $J = 13.8$ Hz, 1H), 1.33 (s, 3H); $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ 172.7, 172.4, 148.9, 148.1, 138.2, 137.6, 130.8, 128.7, 128.2, 127.8, 126.6, 126.4, 122.7, 55.5, 48.8, 48.0, 46.9, 41.1, 26.3. **HRMS (ESI)** calcd for $\text{C}_{23}\text{H}_{22}\text{O}_3\text{Na}^+ [\text{M}+\text{Na}]^+$ 397.1523, found 397.1528.



Compound 7. (98% yield, 20.3 mg, 51.9 μmol , a white solid, chromatography on silica gel, eluent: hexane/ethyl acetate (20/1), $R_f = 0.4$ (hexane/ethyl acetate (10/1))). $^1\text{H NMR}$ (600 MHz, CDCl_3): δ 8.89 (s, 1H), 8.75 (s, 1H), 7.33 (t, $J = 7.7$ Hz, 2H), 7.28 (m, $J = 7.3$ Hz, 2H), 7.23 (t, $J = 7.3$ Hz, 2H), 7.18 (d, $J = 4.8$ Hz, 4H), 6.19 (s, 1H), 3.29 (d, $J = 16.2$ Hz, 1H), 3.23 (d, $J = 16.2$ Hz, 1H), 2.91 (s, 2H), 2.62 (d, $J = 13.9$ Hz, 1H),

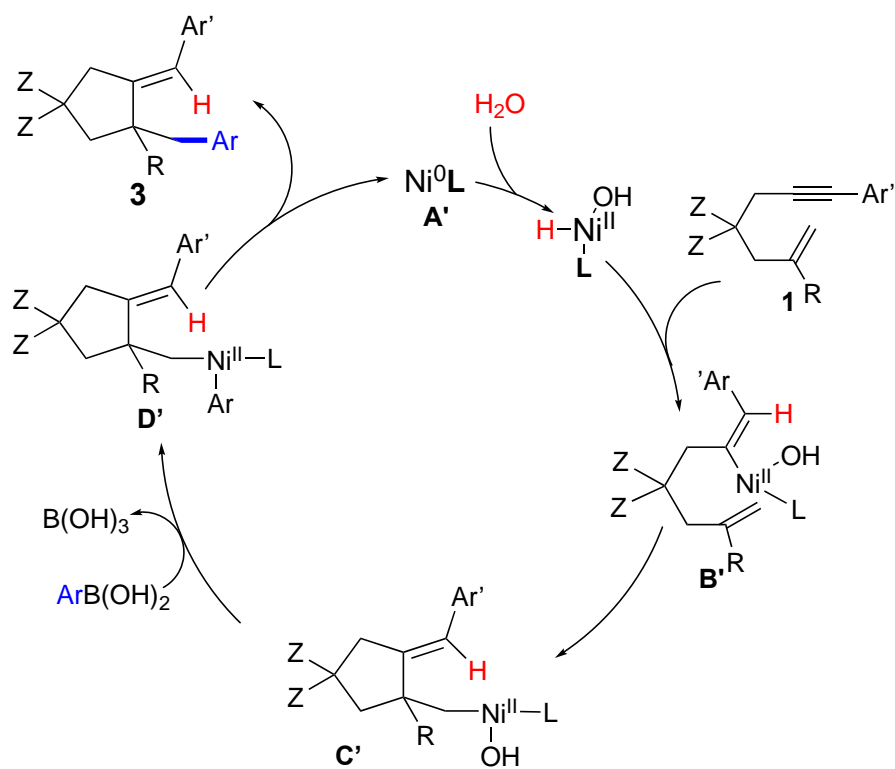
2.09 (d, $J = 13.8$ Hz, 1H), 1.35 (s, 3H); ^{13}C NMR (151 MHz, CDCl_3): δ 175.8, 170.4, 170.1, 147.8, 138.1, 137.5, 130.8, 128.7, 128.3, 127.9, 126.7, 126.4, 123.0, 55.8, 48.8, 48.1, 46.9, 41.2, 26.4. **HRMS (ESI)** calcd for $\text{C}_{23}\text{H}_{22}\text{O}_2\text{SNa}^+$ $[\text{M}+\text{Na}]^+$ 413.1294, found 413.1299.



8

Compound 8. (94% yield, 22.7 mg, 49.7 μmol , a white solid, chromatography on silica gel, eluent: hexane/ethyl acetate (20/1), $R_f = 0.4$ (hexane/ethyl acetate (10/1))). ^1H NMR (600 MHz, CDCl_3): δ 7.34 (t, $J = 7.5$ Hz, 2H), 7.32–7.27 (m, 7H), 7.25–7.17 (m, 4H), 7.12 (d, $J = 7.4$ Hz, 2H), 3.77 (s, 3H), 3.41 (s, 3H), 3.11 (d, $J = 13.4$ Hz, 1H), 2.83 (d, $J = 13.7$ Hz, 1H), 2.75 (d, $J = 13.1$ Hz, 1H), 2.68 (dd, $J = 13.4, 7.0$ Hz, 2H), 2.55–2.46 (m, 2H), 2.26–2.17 (m, 2H), 2.15–2.03 (m, 2H); ^{13}C NMR (151 MHz, CDCl_3): δ 173.5, 172.7, 140.8, 138.3, 137.6, 131.3, 131.1, 128.6, 128.5, 128.0, 127.9, 126.4, 126.2, 126.0, 56.8, 52.7, 52.5, 48.6, 45.4, 40.7, 40.0, 38.1, 37.8, 34.8. **HRMS (ESI)** calcd for $\text{C}_{30}\text{H}_{32}\text{O}_4\text{Na}^+$ $[\text{M}+\text{Na}]^+$ 479.2193, found 479.2198.

8. Another Possible Catalytic cycle



9. Single Crystal X-ray Diffraction Data for Compound 3ha (CCDC 2307259)

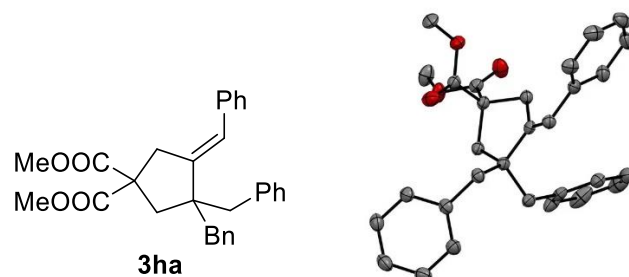


Figure S1. ORTEP illustration of compound **3ha** with thermal ellipsoids drawn at 50% probability level

Table S1 Crystal data and structure refinement for 3ha.

Identification code	3ha
Empirical formula	C ₃₀ H ₃₀ O ₄
Formula weight	454.54
Temperature/K	149.99(10)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	10.29250(10)
b/Å	15.4717(2)
c/Å	15.4935(2)
α/°	90
β/°	94.9010(10)
γ/°	90
Volume/Å ³	2458.20(5)
Z	4
ρ _{calc} /cm ³	1.228
μ/mm ⁻¹	0.640
F(000)	968.0
Crystal size/mm ³	0.15 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	8.09 to 142.848
Index ranges	-12 ≤ h ≤ 12, -18 ≤ k ≤ 17, -12 ≤ l ≤ 18
Reflections collected	13337
Independent reflections	4702 [R _{int} = 0.0248, R _{sigma} = 0.0256]
Data/restraints/parameters	4702/0/310
Goodness-of-fit on F ²	1.023
Final R indexes [I >= 2σ (I)]	R ₁ = 0.0377, wR ₂ = 0.0985

Final R indexes [all data] $R_1 = 0.0401$, $wR_2 = 0.1005$

Largest diff. peak/hole / $e \text{ \AA}^{-3}$ 0.27/-0.17

10. Details for the DFT Calculations

Computational details

All calculations were performed using Gaussian 09 program package,¹¹ employing the B3LYP-D3(BJ)^{12,13} functional and mixed basis set (the lanL2DZ ECP¹⁴ for Ni atom, and the 6-31G**¹⁵ basis set for the other atoms). Geometries were optimized in the mixed solvent (toluene/H₂O=10/1), and characterized by frequency analysis at 373 K. The self-consistent reaction field (SCRF) method based on the universal solvation model SMD¹⁶ was adopted to evaluate the effect of solvent. The intrinsic reaction coordinate (IRC) path¹⁷ was traced to check the energy profiles connecting each transition state to two associated minima of the proposed mechanism.

Table S2 The corrected electronic energies (E_{ZPE}), enthalpies (H), and Gibbs free energies (G) for all stationary points (in Hartree) in the reaction, obtained at the B3LYP/[6-31G**, Lan12DZ] (SMD, toluene/H₂O=10/1) theoretical level at 373K.

Structure	^a ZPE	^b H _c	^c G _c	E _{ZEP}	H	G
cod	0.18046	0.19308	0.13848	-311.91634	-311.90372	-311.95832
H ₂ O	0.02118	0.02591	-0.00198	-76.40611	-76.40137	-76.42927
PhB(OH) ₂	0.12513	0.13824	0.07951	-408.20138	-408.18826	-408.24700
B(OH) ₃	0.04818	0.05594	0.01330	-252.45493	-252.44717	-252.48981
I-IM0	0.70968	0.78186	0.58770	-2435.68690	-2435.61473	-2435.80888
I-TS1	0.70951	0.77998	0.58749	-2435.65453	-2435.58407	-2435.77656
I-IM1	0.71278	0.78279	0.59237	-2435.68710	-2435.61710	-2435.80751
I-IM2	0.89597	0.97949	0.76286	-2747.61426	-2747.53074	-2747.74737
I-TS2	0.89575	0.97857	0.76348	-2747.60687	-2747.52404	-2747.73913
I-IM3	0.89694	0.97854	0.76815	-2747.66854	-2747.58695	-2747.79734
I-IM4	0.92157	1.00952	0.78122	-2824.08739	-2823.99944	-2824.22774
I-TS3	0.91735	1.00382	0.77833	-2824.07910	-2823.99264	-2824.21813
I-IM5	0.92330	1.00893	0.78662	-2824.11536	-2824.02972	-2824.25204
3	0.45058	0.49163	0.36810	-1230.86832	-1230.82727	-1230.95080
Ni-OH	0.47040	0.51400	0.38476	-1593.25299	-1593.20938	-1593.33863
I-TS4	0.59680	0.65481	0.49297	-2001.46680	-2001.40879	-2001.57062
I-IM6	0.59722	0.65556	0.49368	-2001.48091	-2001.42257	-2001.58445
I-TS5	0.59570	0.65395	0.49095	-2001.45967	-2001.40142	-2001.56442
[Ni]-Ar	0.54700	0.59754	0.45034	-1749.00052	-1748.94998	-1749.09718
I-TS2'	0.89340	0.97685	0.75646	-2747.59434	-2747.51089	-2747.73128

II-IM0	0.62215	0.68343	0.51613	-2204.11871	-2204.05744	-2204.22473
II-TS1	0.62084	0.68065	0.51776	-2204.07798	-2204.01817	-2204.18106
II-IM1	0.62158	0.68201	0.51794	-2204.11540	-2204.05497	-2204.21904
II-IM2	0.80404	0.87973	0.67798	-2516.03979	-2515.96411	-2516.16585
II-IM3	0.82967	0.90649	0.70520	-2592.47361	-2592.39679	-2592.59808
II-TS2	0.82755	0.90512	0.70182	-2592.44389	-2592.36632	-2592.56962
II-IM4	0.82992	0.90886	0.69926	-2592.48125	-2592.40230	-2592.61190
II-TS3	0.95680	1.04732	0.81822	-3000.67797	-3000.58745	-3000.81655
II-IM5	0.95802	1.05041	0.81356	-3000.70774	-3000.61534	-3000.85219
II-IM6	0.90794	0.99179	0.77515	-2748.23425	-2748.15040	-2748.36704
II-TS4	0.90617	0.98957	0.77267	-2748.21795	-2748.13455	-2748.35146
II-IM7	0.90985	0.99379	0.77079	-2748.26870	-2748.18476	-2748.40776
Ni⁰(cod)₂PPh₃	0.64076	0.69505	0.54280	-1829.34870	-1829.29441	-1829.44666

^a Zero-point energy.

^b Thermal correction to enthalpy.

^c Thermal correction to Gibbs free energy.

11. Cartesian coordinates of all stationary points

cod

C	3.15588600	4.74138800	-1.79630000
C	3.53116500	5.13769500	-3.23949700
H	2.10939200	4.39989800	-1.78412100
H	3.37694500	4.29191600	-3.91165000
H	2.82127600	5.90823900	-3.56163900
C	5.25314700	2.59349300	-3.05829100
H	4.37826000	2.64888900	-3.70822300
H	5.63463100	1.57074300	-3.15777200
C	6.35333300	3.54650700	-3.57011900
H	7.27151400	3.35466700	-2.99827800
H	6.60266800	3.27441700	-4.60730600
C	4.87888700	2.82499000	-1.61253000
H	5.40847700	2.19707200	-0.89603900
C	4.01444400	3.71245500	-1.10485400
H	3.89637200	3.70885600	-0.02048200
C	6.08467000	5.02885400	-3.50434900
H	6.98790800	5.63564500	-3.58076600
C	4.93046600	5.69370300	-3.36886900
H	4.99810200	6.78045700	-3.31892500
H	3.16580500	5.64697400	-1.17449500

H₂O

O	0.59463300	-0.78047500	0.00000000
H	1.56063100	-0.72724300	0.00000000

H	0.32235600	0.14788400	0.00000000
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PhB(OH)₂

B	-0.03950800	-0.42533900	-0.15221500
O	0.73019300	-0.66803700	-1.25802200
H	1.18770200	-1.51842600	-1.18893500
O	-0.04681100	-1.37511400	0.83755900
H	-0.60689300	-1.14856300	1.59099100
C	-0.85330300	0.91549300	-0.09821700
C	-1.67244900	1.25709300	0.99241100
C	-0.77819700	1.82717400	-1.16760200
C	-2.38710100	2.45474400	1.01916400
H	-1.76529700	0.58684500	1.84477600
C	-1.48862300	3.02676800	-1.15026200
H	-0.15258300	1.58719300	-2.02208200
C	-2.29573500	3.34288000	-0.05458400
H	-3.01299900	2.69515900	1.87366400
H	-1.41466800	3.71479500	-1.98767800
H	-2.85081900	4.27656500	-0.03733800

B(OH)₃

B	0.11439700	-0.43413200	0.02806400
O	-0.49230100	0.76237300	0.31884500
H	-1.45626600	0.73308000	0.27995200
O	1.48340600	-0.44054000	0.07210500
H	1.83067400	-1.31559100	-0.14457700
O	-0.53881300	-1.60242100	-0.29767300
H	-1.50193800	-1.53554400	-0.31365300

I-IM0

C	-1.99258100	-2.38059700	0.60279400
C	-2.99343200	-3.34356800	0.39770000
C	-0.96577000	-2.65203600	1.52060700
C	-2.97120600	-4.54615200	1.10532400
H	-3.78631200	-3.15569700	-0.31860200
C	-0.94837700	-3.85259500	2.23261200
H	-0.17982900	-1.91910600	1.67018800
C	-1.95178300	-4.80145500	2.02677700
H	-3.75092300	-5.28365400	0.93876900
H	-0.14851500	-4.04724000	2.94124900
H	-1.93662200	-5.73854200	2.57545300
C	-3.18041700	0.27060200	0.63065000
C	-3.03878800	1.66452100	0.55905900
C	-4.24632000	-0.27503800	1.35956400

C	-3.96121000	2.49876500	1.19067900
H	-2.20037900	2.08574700	0.01614600
C	-5.15989000	0.56215200	2.00088900
H	-4.36092900	-1.35079500	1.43455100
C	-5.02180300	1.94955000	1.91420600
H	-3.83949100	3.57604600	1.13186500
H	-5.97936800	0.13002900	2.56826900
H	-5.73369000	2.59914400	2.41539600
C	0.62175700	0.67535000	1.60201300
C	1.65249100	0.09379300	1.19121100
Ni	0.25985800	0.11129800	-0.31512100
P	-1.95078600	-0.75963200	-0.26598800
C	2.09105600	-0.80540300	-1.75976700
C	3.15433400	-1.50591200	-0.94219700
H	2.73341500	-2.40815100	-0.49057800
H	3.92937700	-1.83684500	-1.64136600
C	2.97071200	-0.52483800	1.42994000
H	2.79979300	-1.51251400	1.87658100
H	3.51661100	0.07219200	2.16546700
C	3.87176300	-0.72855300	0.19181900
C	0.86412200	-1.37757400	-1.91778600
H	0.18615300	-1.03635100	-2.69177300
H	0.61655900	-2.30985400	-1.41646400
C	2.51767300	0.34535000	-2.63736400
H	2.76618300	1.23708000	-2.05851100
H	3.40500800	0.06063700	-3.21502300
H	1.71943500	0.62432900	-3.32600900
C	-0.28337700	1.38728700	2.46714300
C	-0.27986300	2.79352400	2.49922200
C	-1.18106900	0.68458700	3.29174000
C	-1.14518800	3.47644200	3.35106200
H	0.39555600	3.33634000	1.84785500
C	-2.04458200	1.37563600	4.13758700
H	-1.20032200	-0.39905500	3.25479700
C	-2.02892400	2.77235300	4.17320800
H	-1.13255200	4.56242100	3.36894800
H	-2.73758300	0.82230100	4.76422500
H	-2.70736000	3.30828300	4.83026300
C	-2.80801000	-1.12468900	-1.85227700
C	-2.37708600	-2.20698000	-2.63891300
C	-3.82245800	-0.29174700	-2.34615700
C	-2.95067800	-2.44922500	-3.88674500
H	-1.60332900	-2.87170500	-2.26932200
C	-4.39025800	-0.53281300	-3.59858100

H	-4.16835500	0.54905400	-1.75518900
C	-3.95732700	-1.61043000	-4.37285300
H	-2.61180800	-3.29435100	-4.47911900
H	-5.17547500	0.12234000	-3.96479400
H	-4.40268200	-1.79797500	-5.34544000
C	4.43182500	0.61740600	-0.27660700
O	4.12630200	1.70293900	0.16785800
O	5.33641500	0.43050200	-1.25201900
C	5.07337800	-1.57171000	0.65631400
O	5.30199800	-2.71482900	0.32564100
O	5.82775500	-0.87354300	1.52015900
C	5.93170800	1.62482000	-1.79724600
H	6.45315600	2.18194000	-1.01557200
H	6.63643100	1.28156400	-2.55406900
H	5.16647500	2.25917700	-2.25064600
C	6.98279200	-1.55784600	2.04972700
H	7.66628200	-1.82961900	1.24190200
H	7.45730400	-0.84867600	2.72726600
H	6.67914200	-2.45700800	2.59090800
C	-0.02753400	1.80431300	-1.34530500
C	-0.91180400	1.96494500	-2.43152800
C	0.74414800	2.93999400	-1.01879100
C	-1.03293500	3.16785000	-3.13840300
H	-1.53594300	1.12909400	-2.74125500
C	0.63644500	4.15274700	-1.71002900
H	1.46734700	2.87578500	-0.20693400
C	-0.25915400	4.27419000	-2.77669400
H	-1.73200000	3.24315500	-3.96985700
H	1.25173800	5.00292500	-1.41962900
H	-0.35077900	5.21301600	-3.31746000

I-TS1

C	0.79240200	0.93879800	-2.38334000
C	1.43425900	1.24678300	-3.59370000
C	-0.57837500	1.20425100	-2.24650000
C	0.71630200	1.82387800	-4.64107500
H	2.49073800	1.03194800	-3.71682200
C	-1.29624400	1.77703000	-3.29800200
H	-1.08118000	0.95103600	-1.31971800
C	-0.64830600	2.08949700	-4.49454300
H	1.22127400	2.06075200	-5.57305400
H	-2.36072400	1.95114400	-3.18459800
H	-1.20585900	2.53088700	-5.31550400
C	2.56919300	1.58511500	-0.16910100

C	2.99540600	1.41338900	1.15750900
C	2.78991000	2.81263800	-0.80785600
C	3.63890000	2.45120100	1.82930700
H	2.80171400	0.47444100	1.66371100
C	3.42723100	3.85236000	-0.12895300
H	2.45474500	2.96524100	-1.82783300
C	3.85204600	3.67450500	1.18921500
H	3.95319200	2.31118700	2.85921100
H	3.58676400	4.80274000	-0.63019800
H	4.33984000	4.48812700	1.71799500
C	-0.48086800	0.41239000	1.54535700
C	-1.56860000	-0.12572900	1.04393500
Ni	0.37253700	-1.00037900	0.55226600
P	1.67803400	0.19595200	-0.96352000
C	-1.75704800	-1.86083700	0.29286500
C	-2.87084300	-1.46882800	-0.67410200
H	-2.43658100	-1.00453900	-1.56149400
H	-3.41333100	-2.35915800	-1.00199600
C	-2.96600400	0.43020200	0.91988800
H	-2.90027200	1.45937100	0.55446100
H	-3.44085300	0.47304800	1.90382700
C	-3.82569500	-0.44651800	-0.02205100
C	-0.57910900	-2.45279200	-0.37408200
H	-0.26701800	-3.43467300	-0.03101100
H	-0.51531700	-2.31430200	-1.45272800
C	-2.20304900	-2.66569500	1.51576400
H	-2.92749100	-2.13243400	2.13372800
H	-2.66058300	-3.60817200	1.19075700
H	-1.33769200	-2.90345200	2.14079200
C	-0.17917700	1.67732400	2.18878700
C	0.08544500	1.74357600	3.56952000
C	-0.08609100	2.86105300	1.43004700
C	0.42462100	2.95543900	4.17068200
H	0.02580000	0.83640400	4.16378300
C	0.26238000	4.06622400	2.03466200
H	-0.26460200	2.82006700	0.36057100
C	0.51832800	4.12240900	3.40799300
H	0.62265500	2.98583900	5.23873900
H	0.33960000	4.96529400	1.42960700
H	0.79297500	5.06293400	3.87636900
C	2.97905200	-0.82508000	-1.74597400
C	2.58765000	-1.81226700	-2.66594800
C	4.32517200	-0.73119700	-1.37305300
C	3.53077100	-2.68434900	-3.20585400

H	1.54531300	-1.89797100	-2.95861100
C	5.26652200	-1.61276500	-1.90969900
H	4.63992800	0.02325800	-0.66020300
C	4.87325400	-2.58982600	-2.82491100
H	3.21784800	-3.44119500	-3.91930100
H	6.30790600	-1.53214500	-1.61170600
H	5.60651200	-3.27449200	-3.24077400
C	-4.96265200	-1.13592900	0.74639600
O	-5.18855500	-1.03324300	1.93375000
O	-5.69778400	-1.88366000	-0.09103000
C	-4.48169800	0.43633100	-1.08754300
O	-4.15780000	0.49619500	-2.25540300
O	-5.45500700	1.18143500	-0.54176500
C	-6.81704100	-2.57753900	0.49739100
H	-7.51870600	-1.86457900	0.93652600
H	-7.28855900	-3.11978700	-0.32172300
H	-6.47319400	-3.27326900	1.26625800
C	-6.13528000	2.09038000	-1.43254200
H	-6.60795200	1.54126000	-2.25014400
H	-6.88906700	2.58714500	-0.82241400
H	-5.43316900	2.82172700	-1.84025100
C	1.72878600	-2.06072700	1.42888300
C	2.49963500	-3.03942700	0.77930100
C	2.02245100	-1.79786300	2.78023200
C	3.53501000	-3.71049900	1.43765500
H	2.30717800	-3.27359600	-0.26312500
C	3.05049100	-2.47430700	3.44937800
H	1.45885000	-1.04148400	3.31995100
C	3.81472300	-3.43118400	2.77812500
H	4.12381700	-4.45188200	0.90185700
H	3.25688200	-2.24637100	4.49292500
H	4.61709300	-3.95331300	3.29266700

I-IM1

C	1.00708500	-2.46222600	0.05453900
C	1.71150700	-3.30105700	-0.81996700
C	0.95384400	-2.80419900	1.41347600
C	2.37745200	-4.43527600	-0.34004300
H	1.77152500	-3.06567700	-1.87888000
C	1.60857200	-3.94293200	1.89414300
H	0.40822800	-2.17294400	2.11033000
C	2.32863400	-4.75969300	1.01861700
H	2.93352200	-5.06557000	-1.03015300
H	1.56166000	-4.18623500	2.95285500

H	2.84214700	-5.64232300	1.38999600
C	-0.81930100	1.57766700	1.30100300
C	-1.50014900	2.77295100	0.98889500
C	0.21279400	1.63866900	2.25628100
C	-1.16261800	3.97341100	1.61324700
H	-2.29251100	2.75082600	0.24702300
C	0.54558200	2.83940600	2.88313000
H	0.76056800	0.73364600	2.49895800
C	-0.13693900	4.01569900	2.56202900
H	-1.70018600	4.88211200	1.35442100
H	1.34388600	2.85648100	3.62011200
H	0.12765400	4.95299400	3.04294900
C	-1.34731700	-1.68878500	-1.17031500
C	-1.12376100	0.31557600	0.60812900
C	-2.34574300	-0.24732100	0.54707300
C	-2.54397700	-1.52477400	-0.23713600
C	-3.69288500	0.21357100	1.04535400
C	-4.65154200	-0.16210800	-0.13135300
C	-3.90048900	-1.27010400	-0.96063600
H	-1.42935000	-1.04297100	-2.05840400
H	-1.14826300	-2.71681700	-1.47615700
H	-3.97822000	-0.35531600	1.93897400
H	-3.75612900	1.27268900	1.28560300
H	-3.71989100	-0.89899100	-1.97221500
H	-4.50551600	-2.17338600	-1.04954700
C	-5.99857200	-0.56313500	0.45365400
O	-6.88276200	0.23066600	0.71071400
O	-6.06881600	-1.87328200	0.73461800
C	-4.88912900	1.04889900	-1.03369200
O	-4.37986800	2.14406600	-0.90870200
O	-5.71728600	0.72824300	-2.04067400
C	-7.27321500	-2.31040800	1.39583600
H	-8.14652500	-2.11580600	0.76890900
H	-7.14866200	-3.38167300	1.55218700
H	-7.39135400	-1.79718100	2.35317400
C	-6.00219500	1.78054200	-2.98247300
H	-6.68644300	1.34535500	-3.71085500
H	-6.47388100	2.62783500	-2.47891200
H	-5.08522000	2.11369100	-3.47546500
C	-2.67007500	-2.74112000	0.70233200
H	-3.51059500	-2.62952900	1.39328600
H	-2.84185500	-3.65220400	0.11681700
H	-1.75563000	-2.87836000	1.28405400
Ni	0.22332600	-0.75495200	-0.44211800

P	2.38339600	0.35463000	-0.29710400
C	3.40866400	0.05817900	1.18494700
C	3.62982000	1.07185900	2.12985800
C	3.88081700	-1.23863100	1.44999000
C	4.32080900	0.79673800	3.31080000
H	3.26055200	2.07380500	1.94712800
C	4.57650600	-1.50591700	2.62853600
H	3.70770200	-2.03789600	0.73921700
C	4.79652100	-0.49145000	3.56328100
H	4.48564600	1.59182400	4.03220900
H	4.93655800	-2.51286300	2.81771700
C	2.50829000	2.15032200	-0.63953100
C	1.34125200	2.84846400	-0.97070900
C	3.74159600	2.82153400	-0.64331600
C	1.39950900	4.20864100	-1.28202000
H	0.39021000	2.32940100	-0.97038900
C	3.79715100	4.17877300	-0.95393700
H	4.65272500	2.28280500	-0.40235100
C	2.62530700	4.87482200	-1.26958000
H	0.48707100	4.74501400	-1.52441800
H	4.75329900	4.69400100	-0.95186600
C	3.32026300	-0.37037500	-1.70092700
C	2.59568000	-0.61167800	-2.87928300
C	4.68648100	-0.67448200	-1.66302400
C	3.22455100	-1.15315800	-3.99975500
H	1.53371900	-0.37727700	-2.91436200
C	5.31265800	-1.22570800	-2.78286500
H	5.26025000	-0.49355300	-0.76072100
C	4.58527200	-1.46788500	-3.95009500
H	2.65310000	-1.33794200	-4.90466100
H	6.37134500	-1.46533500	-2.74214300
H	2.67149700	5.93347300	-1.50806800
H	5.07563900	-1.90035800	-4.81722600
H	5.33525300	-0.70389400	4.48214000

I-IM2

C	-1.96415400	2.54812500	0.01546200
C	-2.72216500	3.16269400	-1.17535800
H	-2.30329000	1.51733300	0.17167600
H	-2.50442100	2.60068800	-2.08461100
H	-3.79231500	3.02463300	-0.99220500
C	0.05377800	3.14849700	-2.49699700
H	-0.76736200	2.55058800	-2.89562000
H	0.92614400	2.90994300	-3.11496200

C	-0.23952400	4.64930900	-2.68909500
H	0.64904500	5.21736300	-2.37980600
H	-0.34421400	4.85163300	-3.76603800
C	0.37317300	2.77457200	-1.06863600
H	1.43433400	2.74748700	-0.83267600
C	-0.46281800	2.53294900	-0.04515100
H	0.00597800	2.29349200	0.90688700
C	-1.42703800	5.23762900	-1.97153700
H	-1.42876700	6.32871700	-1.96982800
C	-2.45422400	4.63872300	-1.35558200
H	-3.18738100	5.29454200	-0.88513100
H	-2.25373800	3.08101700	0.93109100
C	1.02047100	-1.98819300	-1.64115900
C	1.59154600	-2.00604800	-2.92018900
C	0.99886800	-3.18118200	-0.90335900
C	2.16418000	-3.17624000	-3.43275000
H	1.61000200	-1.10608800	-3.52743700
C	1.55495200	-4.35645200	-1.41868300
H	0.54844800	-3.19337100	0.08469400
C	2.14848500	-4.35605800	-2.68337600
H	2.61880200	-3.16559500	-4.42071000
H	1.53213600	-5.26806900	-0.82643400
H	2.58670800	-5.26578400	-3.08461600
C	-0.61081200	-0.66155200	2.23203600
C	-1.25019500	0.32476700	3.01272200
C	0.38158600	-1.44926200	2.84935800
C	-0.90483900	0.51455700	4.35107800
H	-2.02675200	0.93238900	2.55986300
C	0.71712900	-1.26558100	4.19028300
H	0.89902300	-2.19895200	2.25935400
C	0.08157200	-0.27691100	4.94795900
H	-1.40934000	1.28298000	4.93119300
H	1.48814900	-1.88509600	4.63957400
H	0.35182000	-0.12480000	5.98890800
C	-1.23640900	-0.52018700	-1.85720800
C	-0.92030500	-0.82898800	0.80733700
C	-2.11557800	-1.21978000	0.33445500
C	-2.35993600	-1.28409700	-1.15874100
C	-3.42250900	-1.49334600	1.04002600
C	-4.48038100	-0.81754100	0.10533700
C	-3.76123400	-0.60929200	-1.27710700
H	-1.40992700	0.56175300	-1.85280300
H	-1.02180100	-0.85920900	-2.87193700
H	-3.61573200	-2.57163800	1.09239300

H	-3.48133300	-1.09126300	2.04986800
H	-3.64154900	0.46034800	-1.45447100
H	-4.35539300	-1.01231300	-2.09841100
C	-5.73510500	-1.68240400	0.07413400
O	-6.62919100	-1.59594500	0.89414100
O	-5.71744100	-2.59270400	-0.91092200
C	-4.91929800	0.53043900	0.68680300
O	-4.57653900	0.99550700	1.75374600
O	-5.75312500	1.15801800	-0.16125500
C	-6.83640700	-3.50075800	-0.94823200
H	-7.76924600	-2.95152500	-1.09631200
H	-6.64623500	-4.16254300	-1.79290800
H	-6.89684500	-4.07451400	-0.02042300
C	-6.30153300	2.40576800	0.30532600
H	-6.87687600	2.80541700	-0.52965500
H	-6.95317900	2.23170300	1.16552800
H	-5.50738400	3.10006300	0.58730700
C	-2.43740300	-2.73890600	-1.66160000
H	-3.22256100	-3.30014900	-1.14836900
H	-2.67015100	-2.75437600	-2.73318500
H	-1.48627800	-3.25322900	-1.51216500
Ni	0.36263200	-0.41901900	-0.71254100
P	2.60390000	0.10389500	0.20366000
C	3.51714600	-1.22232700	1.08428600
C	3.83528900	-1.14720200	2.44666000
C	3.85718800	-2.38018100	0.36421200
C	4.47345700	-2.21535100	3.08068000
H	3.58723400	-0.25939800	3.01616700
C	4.49397500	-3.44399300	1.00143400
H	3.63178400	-2.44664000	-0.69292700
C	4.79981300	-3.36726100	2.36263100
H	4.71685100	-2.14279200	4.13681500
H	4.74747400	-4.33326300	0.43166000
C	2.81284600	1.59920200	1.25527300
C	2.03577600	1.71529400	2.41980800
C	3.67435600	2.65000300	0.90581400
C	2.13394500	2.84824400	3.22734000
H	1.35276500	0.92282200	2.69302800
C	3.75770500	3.78932600	1.70863200
H	4.27602100	2.58668300	0.00674700
C	2.99132300	3.89127400	2.87110300
H	1.52849300	2.91589500	4.12604000
H	4.42432200	4.59785600	1.42290500
C	3.68722700	0.44754800	-1.23680200

C	3.09560700	0.91012700	-2.42014800
C	5.08105100	0.29800900	-1.18324500
C	3.88036700	1.23203200	-3.52805900
H	2.01721800	1.00969400	-2.47480400
C	5.86510200	0.61180600	-2.29393800
H	5.55176000	-0.06272600	-0.27477600
C	5.26728100	1.08255800	-3.46618600
H	3.40920500	1.58815800	-4.43949500
H	6.94332200	0.49177400	-2.24288900
H	3.05935000	4.77893800	3.49307400
H	5.87998600	1.32613000	-4.32922900
H	5.29387800	-4.19777100	2.85831800

I-TS2

C	-1.97346700	2.51926800	0.63236200
C	-2.65271100	3.35187400	-0.47118400
H	-2.31826700	1.47959900	0.57234200
H	-2.40330200	2.94284600	-1.45104500
H	-3.73409800	3.22234100	-0.36385900
C	0.19330900	3.46020100	-1.63433300
H	-0.61503800	2.94592700	-2.15582400
H	1.09212900	3.28672000	-2.23698800
C	-0.06587200	4.97997300	-1.62275900
H	0.82057200	5.47923900	-1.20725000
H	-0.13051600	5.33405700	-2.66287300
C	0.42553800	2.88013000	-0.25876900
H	1.46879400	2.81281700	0.04265500
C	-0.47148500	2.50237700	0.66609800
H	-0.06390100	2.12220200	1.60032400
C	-1.26716200	5.48299100	-0.86331300
H	-1.24061500	6.55844200	-0.68194200
C	-2.33468900	4.82676500	-0.39108000
H	-3.06805200	5.42188500	0.15357500
H	-2.32159600	2.87651500	1.61071000
C	0.72409200	-0.84784600	-2.42758000
C	1.32192900	0.01567800	-3.36242000
C	0.92195100	-2.22954700	-2.56551700
C	2.14424600	-0.48782400	-4.37165500
H	1.15343200	1.08665900	-3.29704400
C	1.73853100	-2.73197300	-3.58381700
H	0.46867800	-2.91333400	-1.85682800
C	2.35682400	-1.86488000	-4.48828500
H	2.61970600	0.19788100	-5.06790800
H	1.89520500	-3.80493300	-3.66281100

H	2.99055100	-2.25639600	-5.27867300
C	-0.65925300	-1.24938700	2.05656500
C	-1.29321600	-0.40426100	2.99374000
C	0.26380800	-2.19187700	2.55179500
C	-1.00540200	-0.49145200	4.35636500
H	-2.02208500	0.31683600	2.63982400
C	0.54635000	-2.28255100	3.91475400
H	0.77168300	-2.84706100	1.85273200
C	-0.07850900	-1.42694200	4.82657100
H	-1.50831700	0.17370100	5.05421700
H	1.26725100	-3.01728700	4.26286600
H	0.15179000	-1.48908200	5.88631700
C	-1.24797800	-0.06520400	-1.97159100
C	-0.89162700	-1.08637400	0.61216300
C	-2.08673900	-1.30809300	0.03798000
C	-2.32873800	-0.99447000	-1.42767700
C	-3.41308900	-1.71147300	0.64602500
C	-4.45028600	-0.80225500	-0.09087700
C	-3.71951900	-0.28454900	-1.38243600
H	-1.33275000	0.94740000	-1.56477500
H	-1.27119000	0.00831400	-3.05535100
H	-3.63566100	-2.76383600	0.43146200
H	-3.46860300	-1.56930000	1.72419400
H	-3.58611000	0.79452300	-1.30275500
H	-4.31122400	-0.47240900	-2.27988800
C	-5.72561000	-1.59966400	-0.33882600
O	-6.67629000	-1.60821900	0.41950000
O	-5.65874900	-2.34854400	-1.45066700
C	-4.87059600	0.37288400	0.79895700
O	-4.57918700	0.52801200	1.96616500
O	-5.62968200	1.23864700	0.10396300
C	-6.78652900	-3.21233800	-1.69720100
H	-7.69595500	-2.62321400	-1.83707600
H	-6.54291900	-3.75743200	-2.60900000
H	-6.92677300	-3.90586600	-0.86464300
C	-6.16854600	2.34409200	0.85345600
H	-6.67813700	2.97374500	0.12419200
H	-6.87857300	1.98118900	1.60131500
H	-5.37369100	2.90416200	1.35019200
C	-2.45325700	-2.27698500	-2.27532400
H	-3.30592600	-2.87804700	-1.95227900
H	-2.61171000	-2.02179100	-3.33018600
H	-1.55554000	-2.89062600	-2.20548700
Ni	0.37904600	-0.16458700	-0.65315900

P	2.59955200	-0.11176500	0.29831700
C	3.21900100	-1.70224800	0.97000100
C	3.89268900	-1.79201800	2.19483600
C	2.97881100	-2.87250700	0.23260000
C	4.30974300	-3.03357200	2.67871900
H	4.08502400	-0.89836000	2.77730100
C	3.40269300	-4.11028500	0.71493300
H	2.46412300	-2.80971800	-0.71848700
C	4.06188400	-4.19493200	1.94452400
H	4.82594600	-3.09121500	3.63265300
H	3.21030000	-5.00848500	0.13526500
C	2.92490600	1.07793900	1.65831000
C	2.02497400	1.08764000	2.73681400
C	4.01373500	1.96042100	1.66724500
C	2.21144800	1.96685400	3.80265500
H	1.18279300	0.40585500	2.74147200
C	4.18843100	2.84977100	2.72990200
H	4.72339300	1.95783800	0.84753200
C	3.29104600	2.85406700	3.79956300
H	1.50867200	1.96092900	4.63042000
H	5.03222600	3.53388500	2.72295200
C	3.83399400	0.32857500	-0.99081600
C	3.68799500	1.55912900	-1.65238900
C	4.86119700	-0.53555800	-1.39025900
C	4.55919300	1.92598400	-2.67552700
H	2.89135000	2.23388600	-1.36329700
C	5.72219000	-0.17527400	-2.43000100
H	4.99167500	-1.49166200	-0.89659600
C	5.57689500	1.05463300	-3.07293500
H	4.43430100	2.88473300	-3.17061300
H	6.51166500	-0.85745200	-2.73209300
H	3.43132700	3.54614300	4.62475400
H	6.24958600	1.33326500	-3.87873600
H	4.38435800	-5.15973800	2.32486600

I-IM3

C	-1.77059200	2.51552000	0.76550500
C	-2.14910500	3.79086700	-0.00741200
H	-2.18247300	1.63864300	0.25154700
H	-1.67819700	3.78048600	-0.99225700
H	-3.22852300	3.75690200	-0.19186800
C	0.90770500	4.06600800	-0.36385600
H	0.23126900	3.99219700	-1.21542100
H	1.91893600	4.07125900	-0.78539600

C	0.69402200	5.41422500	0.34839100
H	1.41645100	5.49609400	1.17325200
H	0.96293000	6.22606700	-0.34462700
C	0.78702100	2.87357900	0.55535900
H	1.73455200	2.49278300	0.93190900
C	-0.31121900	2.25357400	1.01421800
H	-0.13819900	1.42448600	1.69559900
C	-0.67490300	5.70396000	0.90681800
H	-0.69729900	6.59791800	1.53209300
C	-1.84006800	5.06057300	0.75450500
H	-2.69202100	5.48146100	1.28935000
H	-2.27712100	2.52822800	1.74031400
C	-0.38080000	0.28067400	-2.76825400
C	0.34258600	1.49137200	-2.92628400
C	0.30638000	-0.91529300	-3.08817000
C	1.64168300	1.51247800	-3.42865500
H	-0.15519200	2.42550400	-2.68692200
C	1.61048700	-0.88552100	-3.60975000
H	-0.18939100	-1.86952700	-2.98053200
C	2.27639100	0.32157600	-3.80026200
H	2.15942200	2.46044700	-3.53523400
H	2.09961300	-1.82259600	-3.85865200
H	3.28822100	0.33793900	-4.19057200
C	-0.80391900	-1.46294500	1.49679500
C	-1.32918900	-0.76797700	2.60707200
C	0.00857800	-2.58377500	1.76418400
C	-1.03833000	-1.16361700	3.91449400
H	-1.99014900	0.07349800	2.43415900
C	0.29452100	-2.98300000	3.06944700
H	0.42732600	-3.13751900	0.93127600
C	-0.21905600	-2.26959800	4.15688200
H	-1.45844400	-0.60533900	4.74779400
H	0.93007600	-3.84912000	3.23600400
H	0.01308400	-2.57180100	5.17410800
C	-1.87095900	0.41179500	-2.50027200
C	-1.02844100	-1.00580300	0.10611500
C	-2.25325500	-1.13061600	-0.44068000
C	-2.70028800	-0.70618100	-1.84106700
C	-3.50340700	-1.66726700	0.24034200
C	-4.61876100	-0.68143400	-0.21047700
C	-4.13314400	-0.13421200	-1.59348600
H	-2.00108900	1.31601500	-1.89881300
H	-2.34870700	0.63345200	-3.46669500
H	-3.75033400	-2.67132300	-0.12253300

H	-3.43146600	-1.70802700	1.32515000
H	-4.11119600	0.95517100	-1.55952000
H	-4.82214600	-0.41503400	-2.39203300
C	-5.96612500	-1.38921400	-0.26355200
O	-6.86229900	-1.23656700	0.54412900
O	-6.03355400	-2.25742500	-1.28804200
C	-4.77935800	0.44076300	0.82588400
O	-4.40813900	0.39314700	1.97989200
O	-5.41771300	1.50146200	0.30266500
C	-7.23473900	-3.04995000	-1.36160800
H	-8.10807400	-2.41042000	-1.51124700
H	-7.09719400	-3.70971800	-2.21796600
H	-7.36497000	-3.63345200	-0.44712700
C	-5.69490900	2.57797600	1.21693100
H	-6.15541000	3.36310900	0.61717100
H	-6.38435300	2.24432600	1.99707000
H	-4.77514700	2.94136600	1.67959000
C	-2.84255300	-1.94824100	-2.75699100
H	-3.67030100	-2.57980900	-2.42394700
H	-3.05880100	-1.64422000	-3.78832700
H	-1.94478500	-2.56931100	-2.76401800
Ni	0.54657500	-0.11551200	-0.73129200
P	2.69566100	-0.44569900	0.09038500
C	3.08737300	-2.23610400	0.21627200
C	3.90853600	-2.76419500	1.22065000
C	2.52294700	-3.10268000	-0.73258000
C	4.15549200	-4.13723200	1.27791200
H	4.34899400	-2.10722200	1.96283800
C	2.78145500	-4.47228600	-0.68242200
H	1.86890300	-2.69953100	-1.49803400
C	3.59443500	-4.99337700	0.32773200
H	4.78679300	-4.53708000	2.06620400
H	2.33723900	-5.13276100	-1.42157800
C	3.13737600	0.20544000	1.75333900
C	2.16002600	0.15663000	2.75869600
C	4.40561300	0.72200200	2.05866500
C	2.44517600	0.61428100	4.04456200
H	1.17825000	-0.24025700	2.53597200
C	4.68585700	1.18620800	3.34524400
H	5.17515900	0.76157500	1.29583300
C	3.70804200	1.13182400	4.34125400
H	1.67691900	0.56674400	4.81038100
H	5.67114200	1.58496500	3.56980900
C	4.05192900	0.21169100	-0.96427000

C	4.11473800	1.59944400	-1.17302000
C	4.97564600	-0.61498800	-1.61429100
C	5.08649800	2.14724900	-2.00697800
H	3.40049700	2.25233700	-0.68159800
C	5.94119200	-0.06535300	-2.46282700
H	4.94477500	-1.68833300	-1.46240000
C	6.00001400	1.31438000	-2.66162100
H	5.12544200	3.22276000	-2.15457400
H	6.64987500	-0.71924200	-2.96314200
H	3.92920300	1.49264000	5.34164400
H	6.75205700	1.73992600	-3.31951900
H	3.78686600	-6.06118200	0.37584800

I-IM4

O	0.88624600	1.80381300	-2.12438400
C	-0.71098700	1.22557800	2.54400700
C	-1.48751600	2.55690000	2.62026000
H	-1.33048400	0.48916800	2.02244100
H	-1.73179800	2.91060800	1.61832800
H	-2.44797100	2.33897600	3.10004800
C	0.66338800	3.51582500	0.66018700
H	-0.36942700	3.35182900	0.35166200
H	1.20548600	3.81344600	-0.24512200
C	0.74796900	4.69702300	1.64898600
H	1.80761300	4.94796000	1.79410600
H	0.30578300	5.58631700	1.17404700
C	1.28556300	2.24739000	1.19522400
H	2.37265800	2.23150900	1.15876200
C	0.68388100	1.25911000	1.94244200
H	1.35608800	0.51531500	2.36583600
C	0.13585600	4.50608700	3.01440300
H	0.51638200	5.20015700	3.76495100
C	-0.78513000	3.62440300	3.42390400
H	-1.05696300	3.65650900	4.47948000
H	-0.59831700	0.84117200	3.56676000
C	-3.19752500	2.47322400	-1.19362200
C	-4.36220000	2.82799500	-0.49465200
C	-2.83425300	3.25290400	-2.30289100
C	-5.14327400	3.91362400	-0.89362500
H	-4.65207600	2.24123500	0.37143200
C	-3.61048300	4.34106900	-2.70639600
H	-1.93671500	3.00521000	-2.86347900
C	-4.77074800	4.67482000	-2.00351000
H	-6.03981800	4.16665700	-0.33424600

H	-3.30769300	4.93018500	-3.56765400
H	-5.37457000	5.52249900	-2.31437200
C	0.03068700	-2.26621800	0.39896100
C	-0.15174900	-2.42764900	1.78894400
C	0.73267800	-3.28121800	-0.27930000
C	0.34166200	-3.54345800	2.46349700
H	-0.70607000	-1.67112300	2.33400900
C	1.23638200	-4.39472100	0.39592300
H	0.88546000	-3.18935400	-1.34890300
C	1.04782000	-4.53495300	1.77368600
H	0.17410800	-3.64005100	3.53350700
H	1.77846600	-5.15511400	-0.16021600
H	1.44063100	-5.40051800	2.29945200
C	-2.37032300	1.29852600	-0.73340300
C	-0.50478600	-1.07224600	-0.30045800
C	-1.76160500	-1.16710000	-0.78265000
C	-2.59270400	-0.05379500	-1.46122300
C	-2.67309000	-2.38055500	-0.66297500
C	-4.04444500	-1.75574100	-0.35788100
C	-4.07118600	-0.53964400	-1.32014500
H	-1.30783200	1.54285000	-0.82675400
H	-2.55927500	1.13236700	0.32633900
H	-2.75861400	-2.92190400	-1.61336200
H	-2.36349500	-3.09066000	0.10293200
H	-4.75311700	0.23907300	-0.98219200
H	-4.43638700	-0.89173300	-2.28980500
C	-5.20838100	-2.68829900	-0.67381000
O	-5.17300400	-3.60134200	-1.47214000
O	-6.31411800	-2.33486700	0.00693200
C	-4.09833700	-1.41089200	1.13327600
O	-3.83667800	-2.21357300	2.00651000
O	-4.46896600	-0.14413000	1.38880000
C	-7.49214200	-3.12525200	-0.24767900
H	-7.32087400	-4.16781800	0.03112100
H	-8.27666900	-2.69150100	0.37223800
H	-7.76902700	-3.07328400	-1.30331100
C	-4.56708500	0.20384000	2.78333500
H	-4.86038900	1.25293300	2.80551400
H	-5.32559000	-0.41064400	3.27447200
H	-3.60773700	0.06171900	3.28485000
C	-2.23609400	0.05272400	-2.95292700
H	-2.33567500	-0.92224800	-3.44112200
H	-2.88675100	0.76018500	-3.47793700
H	-1.20061500	0.38013600	-3.08362200

Ni	0.76183800	0.50718300	-0.13235000
P	3.04751400	-0.12640300	-0.41498700
C	3.40232600	-1.62307000	-1.41873500
C	4.27650800	-2.64308100	-1.02212200
C	2.75127800	-1.72648900	-2.65767900
C	4.48622200	-3.75133300	-1.84534400
H	4.78490200	-2.58272500	-0.06635200
C	2.97036600	-2.82710800	-3.48491600
H	2.05441700	-0.95327500	-2.96751600
C	3.83406900	-3.84718200	-3.07613900
H	5.15906500	-4.54043200	-1.52205000
H	2.45686400	-2.89593000	-4.43949100
C	3.73064100	-0.49228400	1.24873600
C	3.26736400	-1.62434400	1.93954300
C	4.58492100	0.40463500	1.90631800
C	3.66309000	-1.85859700	3.25533600
H	2.59961300	-2.32132400	1.44938900
C	4.97038200	0.17184900	3.22869000
H	4.95193100	1.28464500	1.38968800
C	4.51276600	-0.95937600	3.90614200
H	3.29922200	-2.74170700	3.77185400
H	5.63190600	0.87557000	3.72587700
C	4.27096300	1.07354000	-1.09085200
C	3.89029900	2.40583400	-1.29535500
C	5.59332400	0.68971800	-1.36682100
C	4.81789300	3.34378000	-1.75573400
H	2.86550200	2.69673200	-1.10882900
C	6.51754300	1.62599600	-1.82731500
H	5.90087900	-0.34074900	-1.22001200
C	6.13203000	2.95647100	-2.01984100
H	4.51124800	4.37458100	-1.90983500
H	7.53834100	1.31902700	-2.03647200
H	4.81448600	-1.13954800	4.93384900
H	6.85367500	3.68472400	-2.37859200
H	3.99638900	-4.71202500	-3.71271100
H	0.65849200	1.16126400	-2.81190700
H	0.17935600	2.46526800	-2.15497800

I-TS3

C	1.15335200	-0.30721800	2.96357000
C	2.35144900	-0.79677400	3.81457400
H	1.47563200	0.58204800	2.40881500
H	3.24964300	-0.82568500	3.19918100
H	2.54119700	-0.03257900	4.57675900

C	2.58635400	-2.74021200	1.45258900
H	3.22624000	-1.86926100	1.57123700
H	2.88993900	-3.22204400	0.51792600
C	2.82036300	-3.74505400	2.60514400
H	2.32271500	-4.68785600	2.34311300
H	3.89303500	-3.98721400	2.64664400
C	1.13895900	-2.33772900	1.36008500
H	0.48866500	-3.05101600	0.85869600
C	0.53330700	-1.31502100	2.02075300
H	-0.55083300	-1.27844900	1.95736100
C	2.33785200	-3.34658500	3.98114600
H	2.13154900	-4.19394000	4.63563500
C	2.12918700	-2.12597900	4.49265200
H	1.74585700	-2.07693700	5.51192300
H	0.35923700	0.03434600	3.63762100
C	-1.18803700	3.02517600	1.02952100
C	-2.03949200	4.07358300	0.65457000
C	0.05199800	3.36326300	1.59802900
C	-1.65827400	5.40780700	0.82788000
H	-3.00682600	3.86125000	0.21716100
C	0.43463400	4.69110300	1.77898800
H	0.72994400	2.56797300	1.89322100
C	-0.42016700	5.72461500	1.38708200
H	-2.33525800	6.20015200	0.52037800
H	1.40172700	4.91771600	2.21906800
H	-0.12472500	6.76174400	1.51655000
C	-1.51115500	1.55042700	0.87372900
C	-2.54309300	1.08613300	-0.18393800
C	-3.91498400	-0.89428600	0.40647200
C	-4.87314900	0.24070000	-0.01571000
C	-3.99843600	1.49862000	0.20082300
H	-1.82577300	1.15514100	1.84975000
H	-0.56902100	1.03127000	0.64509400
H	-4.23813200	-1.87671700	0.06403300
H	-3.88868700	-0.91495300	1.50271000
H	-4.05166000	1.77531800	1.25592700
H	-4.37650400	2.33157100	-0.39284900
C	-5.29362700	0.12902800	-1.48812800
O	-5.43743500	1.07428200	-2.23664100
O	-5.49529600	-1.14363800	-1.85437100
C	-6.16386600	0.27079400	0.79243400
O	-7.28090900	0.24417600	0.31297000
O	-5.92516600	0.33364700	2.11322800
C	-5.92177600	-1.34312000	-3.21504700

H	-5.18763000	-0.93028200	-3.91113800
H	-5.99953300	-2.42254500	-3.34368700
H	-6.89150000	-0.86863400	-3.38517000
C	-7.09298600	0.36446000	2.95782000
H	-6.71550300	0.42506000	3.97842900
H	-7.70992000	1.23652300	2.72817900
H	-7.68503400	-0.54422800	2.82464000
C	-2.17081500	1.61003500	-1.58132900
H	-2.85145300	1.21768900	-2.33996000
H	-2.21454400	2.70104900	-1.62297700
H	-1.15813300	1.30823200	-1.84403500
C	-1.57707000	-1.25955600	-0.60098000
C	-2.57266000	-0.46204400	-0.15558600
C	-1.66486900	-2.73316300	-0.50923800
C	-1.17570500	-3.52524000	-1.57141400
C	-2.12341800	-3.41233500	0.63976700
C	-1.17134700	-4.91705600	-1.49982700
H	-0.78595300	-3.02528400	-2.45283300
C	-2.10531500	-4.80545100	0.71913900
H	-2.46653000	-2.83750600	1.49335800
C	-1.63478500	-5.56867700	-0.35192200
H	-0.79766300	-5.49753500	-2.33972300
H	-2.45780600	-5.29568700	1.62313100
H	-1.62291300	-6.65324000	-0.29174900
Ni	0.67415600	-0.74265800	-0.30402900
H	-0.69362100	-0.85549300	-1.69313000
O	0.24840500	-0.74498600	-2.39117100
H	0.28515500	0.15236200	-2.75161300
P	2.73140000	0.30668700	-0.66387000
C	3.87363000	-0.83294600	-1.53703000
C	3.32063400	-2.00179300	-2.08349900
C	5.24628200	-0.58526700	-1.69428700
C	4.12884900	-2.91081900	-2.76770800
H	2.25522100	-2.17966600	-1.98042800
C	6.05229000	-1.49820600	-2.37584100
H	5.68774800	0.31460300	-1.27925300
C	5.49581200	-2.66274100	-2.91118200
H	3.69065100	-3.81256200	-3.18574700
H	7.11394000	-1.29865700	-2.48889800
C	3.77626200	1.09712600	0.63497900
C	4.74531500	0.36101900	1.33584200
C	3.53734400	2.42740200	1.01547000
C	5.45226200	0.93964400	2.39135100
H	4.96175200	-0.66260900	1.05194900

C	4.24046000	3.00103700	2.07515200
H	2.80358900	3.02185700	0.48401000
C	5.19866100	2.25913900	2.76942000
H	6.20084300	0.35481200	2.91784400
H	4.04411600	4.03306200	2.35133200
C	2.46159500	1.68793800	-1.85079700
C	1.34726900	2.51189700	-1.62982300
C	3.29807400	1.95471600	-2.94326900
C	1.08772600	3.60114000	-2.46159600
H	0.68328500	2.30435300	-0.80050400
C	3.02714200	3.03403600	-3.78691200
H	4.15574500	1.32181800	-3.14298000
C	1.92799600	3.86249700	-3.54556000
H	0.22796300	4.23399200	-2.26344200
H	3.67793100	3.22877700	-4.63455300
H	5.74672600	2.70776100	3.59256100
H	1.72487600	4.70319100	-4.20245600
H	6.12588300	-3.37318300	-3.43852200

3

H	2.19836700	0.41829500	1.54780600
C	0.28391400	-2.31097900	0.22121400
C	1.51861000	0.85155400	0.81803900
C	0.37281200	0.19225200	0.57907500
C	-0.00216100	-1.13540200	1.22238600
C	-0.76855000	0.64140700	-0.30153900
C	-2.03326200	-0.10129200	0.22769300
C	-1.53107200	-0.99144400	1.39682300
H	-0.30037800	-2.14643300	-0.68812700
H	-0.09770300	-3.22717000	0.68612300
H	-0.89526200	1.72645900	-0.28298700
H	-0.61946700	0.35975300	-1.34908500
H	-2.04304800	-1.95598300	1.43433500
H	-1.74865000	-0.46537500	2.32930400
C	-3.06367600	0.92501600	0.70504600
O	-3.33140900	1.18456500	1.85814800
O	-3.61197900	1.55089800	-0.35117100
C	-2.69402700	-0.94104200	-0.86882800
O	-2.25962000	-1.13114100	-1.98615400
O	-3.83953900	-1.47372700	-0.41374800
C	-4.57826400	2.57792200	-0.04885600
H	-4.11460900	3.38055100	0.52934300
H	-4.91710200	2.95373400	-1.01389300
H	-5.41728900	2.16022600	0.51226200

C	-4.57566200	-2.28785600	-1.34926200
H	-4.85201000	-1.70277200	-2.22935800
H	-3.98070000	-3.15115200	-1.65592900
H	-5.46759200	-2.61332600	-0.81500000
C	1.98648400	2.12177600	0.24809700
C	2.92369600	2.87701900	0.98077200
C	1.57766800	2.61946700	-1.00436400
C	3.40473700	4.09341600	0.50380600
H	3.26777200	2.49900500	1.93999600
C	2.06168000	3.83688200	-1.48283700
H	0.90391600	2.04148700	-1.62435300
C	2.97053700	4.58340600	-0.73090500
H	4.12178600	4.65824700	1.09268400
H	1.73383700	4.19700000	-2.45394400
H	3.34573800	5.53039300	-1.10735500
C	0.67485300	-1.40731600	2.56610300
H	0.48814600	-0.58726000	3.26615800
H	0.28108700	-2.32881000	3.00851200
H	1.75601900	-1.52827800	2.46247000
C	1.73342600	-2.49140100	-0.15143300
C	2.56353600	-3.36429000	0.56529100
C	2.29211100	-1.76594100	-1.21368400
C	3.91445800	-3.50075700	0.23998700
H	2.14499400	-3.94278800	1.38436000
C	3.64109400	-1.89821500	-1.54325900
H	1.66037400	-1.09507900	-1.78785600
C	4.45875300	-2.76498300	-0.81430100
H	4.53972800	-4.18428700	0.80739900
H	4.05318600	-1.32610100	-2.36971000
H	5.50907700	-2.87029200	-1.07012700

I-IM5

C	0.98075300	-0.90098900	2.58364300
C	2.15544400	-1.48570700	3.39677900
H	1.24385000	0.11726500	2.27506800
H	3.07320600	-1.43845700	2.81206400
H	2.31619600	-0.82344600	4.25448100
C	2.57346500	-3.17023300	0.86405500
H	3.24525400	-2.35881900	1.14011300
H	2.93918900	-3.55684200	-0.09358200
C	2.65374400	-4.31671100	1.89394800
H	2.10790200	-5.18006700	1.49043500
H	3.70073500	-4.64764000	1.96911100
C	1.16267600	-2.67050500	0.67060200

H	0.53830400	-3.29620500	0.03180500
C	0.50604900	-1.70174400	1.39150700
H	-0.56372400	-1.62793300	1.20542900
C	2.11559200	-4.04766200	3.27801400
H	1.87009800	-4.95409800	3.83293300
C	1.90161700	-2.88393000	3.90609700
H	1.47418500	-2.94039000	4.90753400
H	0.11766800	-0.79036100	3.25302200
C	-1.16134800	2.87033600	0.66093800
C	-1.88345300	3.97275400	0.18883300
C	-0.00293800	3.12366400	1.41587700
C	-1.45753700	5.27936400	0.45243400
H	-2.78425700	3.82951200	-0.39373700
C	0.42647200	4.42105800	1.68044900
H	0.56924600	2.28149300	1.79526800
C	-0.30192700	5.51174400	1.19536700
H	-2.03676300	6.11518100	0.06936500
H	1.33234000	4.58320000	2.25787000
H	0.02985000	6.52671800	1.39412500
C	-1.52728000	1.41501000	0.42511600
C	-2.70572900	1.04954000	-0.51548000
C	-4.13082000	-0.73818500	0.44778000
C	-5.04952600	0.45645200	0.09834300
C	-4.05612600	1.64148200	0.00476400
H	-1.72668600	0.95852000	1.40401900
H	-0.63253400	0.90423000	0.04424800
H	-4.60449100	-1.69855500	0.24737500
H	-3.89398600	-0.69435600	1.51713500
H	-3.92726500	2.06556500	1.00294300
H	-4.45586400	2.41801600	-0.64773600
C	-5.74448600	0.22905200	-1.25171200
O	-5.76563400	1.02097500	-2.17096400
O	-6.33562500	-0.97367500	-1.29439100
C	-6.14655000	0.73996400	1.11651300
O	-7.28311100	1.06031200	0.82847100
O	-5.69671000	0.64039100	2.37722300
C	-7.03775200	-1.28250600	-2.51378700
H	-6.34918800	-1.27558700	-3.36216000
H	-7.45156500	-2.28055500	-2.37021800
H	-7.83839900	-0.55959500	-2.68794300
C	-6.65320000	0.94519000	3.41247600
H	-6.11142800	0.83720800	4.35201700
H	-7.02555300	1.96641000	3.30308300
H	-7.49121800	0.24495000	3.37445000

C	-2.39820700	1.45924400	-1.96703400
H	-3.22532300	1.18088200	-2.62482800
H	-2.24960700	2.53836900	-2.05205700
H	-1.48770800	0.96622100	-2.31906500
C	-2.09813600	-1.36214100	-0.98679400
C	-2.90862300	-0.47167800	-0.39080000
C	-2.08045300	-2.82729600	-0.89044300
C	-1.39789500	-3.53594600	-1.90113500
C	-2.61739100	-3.56372600	0.18297600
C	-1.28851200	-4.92396500	-1.86189300
H	-0.93315400	-2.97011300	-2.70331700
C	-2.50421000	-4.95366300	0.22303200
H	-3.09426500	-3.05052800	1.00931900
C	-1.84630300	-5.64184400	-0.79946300
H	-0.76118100	-5.44599900	-2.65564100
H	-2.92137300	-5.49999100	1.06446900
H	-1.75839000	-6.72377800	-0.76264700
Ni	1.07080600	-0.96797900	-0.61211100
H	-1.31903100	-0.96841500	-1.63576100
O	0.56589500	-0.58429200	-2.39448400
H	1.32078400	-0.41499300	-2.97167400
P	2.94857300	0.40797500	-0.47365200
C	4.13233000	-0.12950200	-1.77755700
C	4.00591200	-1.42184200	-2.30653700
C	5.15794300	0.70529900	-2.24603700
C	4.89519100	-1.87687300	-3.28320000
H	3.20710700	-2.06631200	-1.95217700
C	6.04286200	0.25163100	-3.22310300
H	5.26078800	1.71089900	-1.85136700
C	5.91380700	-1.04056800	-3.74225700
H	4.78838200	-2.88014500	-3.68550100
H	6.83253500	0.90586000	-3.58132700
C	4.01597500	0.52704300	1.01635200
C	5.13862300	-0.30163300	1.16260200
C	3.64456200	1.35917700	2.08546600
C	5.87229200	-0.29763500	2.35084300
H	5.44223600	-0.95071700	0.34806100
C	4.38459900	1.36894000	3.26722300
H	2.78006800	2.00703600	1.99056800
C	5.49894600	0.53717100	3.40546900
H	6.73865000	-0.94544900	2.44800100
H	4.08774400	2.02339300	4.08160700
C	2.58980800	2.15659400	-0.91411300
C	1.44705500	2.39856600	-1.69285600

C	3.39833600	3.23585900	-0.52520200
C	1.11365400	3.70198400	-2.06252100
H	0.83619100	1.55299900	-2.00352000
C	3.05808900	4.53710500	-0.89590500
H	4.28535800	3.06628600	0.07534000
C	1.91163200	4.77349600	-1.65873100
H	0.21974200	3.88053700	-2.65247800
H	3.68602600	5.36667000	-0.58340700
H	6.07140000	0.54059700	4.32818400
H	1.64072600	5.78879500	-1.93302500
H	6.60335800	-1.39077800	-4.50485200

Ni-OH

C	-3.72723500	-2.06572300	0.33764600
C	-4.64296100	-1.44688900	-0.73496800
H	-3.26855500	-2.97499900	-0.06907300
H	-4.04889600	-1.12609100	-1.59273500
H	-5.29335500	-2.24751700	-1.10435300
C	-2.68965600	0.94099200	-0.57585900
H	-2.80351700	0.35000800	-1.48586000
H	-1.89691600	1.66366100	-0.78394400
C	-3.97590300	1.73543600	-0.28646400
H	-3.79038000	2.39248600	0.57512500
H	-4.15978900	2.41933000	-1.12890200
C	-2.23758400	0.08419300	0.58588100
H	-1.64728600	0.61388200	1.33109100
C	-2.64641100	-1.18266700	0.93193600
H	-2.28144600	-1.54270300	1.89474700
C	-5.23638800	0.95832300	-0.01110800
H	-6.03740200	1.57220000	0.40366400
C	-5.52010500	-0.33687000	-0.20142400
H	-6.51690100	-0.65940400	0.10104000
H	-4.35545900	-2.39738400	1.17637100
Ni	-0.87537600	-1.41629500	-0.28555200
P	0.95531500	-0.05204700	-0.03096100
C	2.34244000	-0.47320300	-1.15995000
C	3.46468900	0.35494900	-1.32501700
C	2.27302100	-1.69220200	-1.85199800
C	4.51041600	-0.03911800	-2.15817500
H	3.51640000	1.31071000	-0.81380700
C	3.32714100	-2.08255300	-2.68283600
H	1.38319400	-2.31409700	-1.74798400
C	4.44540700	-1.26167500	-2.83435900
H	5.37491900	0.60687300	-2.28195400

H	3.26912200	-3.02669000	-3.21732400
C	1.67211600	-0.19718000	1.65560700
C	2.72815600	0.60951200	2.10812400
C	1.14248100	-1.17301900	2.51198100
C	3.24281000	0.43915300	3.39221500
H	3.14218600	1.37607000	1.46199300
C	1.66049900	-1.34482100	3.79789500
H	0.32319500	-1.79679200	2.16417500
C	2.71102300	-0.53882300	4.23873000
H	4.05880500	1.06950900	3.73353400
H	1.24239400	-2.10388200	4.45259300
C	0.72225800	1.75063100	-0.26259500
C	0.72345000	2.28885200	-1.55987900
C	0.35363800	2.57252500	0.81343700
C	0.37108500	3.62135300	-1.77288400
H	0.99765600	1.66462300	-2.40464000
C	-0.00504300	3.90410900	0.59617100
H	0.34573800	2.17495600	1.82276000
C	0.00185300	4.43232700	-0.69612900
H	0.38130600	4.02537100	-2.78098800
H	-0.28714300	4.52798500	1.43933200
H	3.11454500	-0.66841600	5.23872100
H	-0.27741400	5.46827300	-0.86379400
H	5.26220900	-1.56668800	-3.48237700
O	-0.66256200	-2.97989400	-1.25481800
H	-0.33308900	-3.68081800	-0.67486000

I-TS4

C	3.02759700	1.18824400	-2.03553000
C	4.07336800	1.72066900	-1.02939900
H	3.13692600	0.09915500	-2.09554000
H	3.96902300	1.19499700	-0.08090300
H	5.06094400	1.44523100	-1.41748200
C	1.61155300	2.01679100	0.75610400
H	2.32416300	1.20408800	0.88411900
H	0.83279000	1.85640300	1.50596900
C	2.26828500	3.38313700	1.04980800
H	1.47099200	4.13371400	1.13152800
H	2.72658500	3.34211500	2.04949800
C	0.98059500	1.96440500	-0.61186300
H	0.02198900	2.47271400	-0.69694000
C	1.57939700	1.58003100	-1.78745300
H	1.00663400	1.77127600	-2.69520700
C	3.27785400	3.89687400	0.05127100

H	3.39468300	4.98125000	0.05826000
C	4.02838700	3.21442400	-0.82365200
H	4.67720000	3.79696200	-1.47842800
H	3.28223700	1.56848700	-3.03331500
C	2.81615600	-2.10250000	0.40829600
C	3.80509900	-1.29572400	0.99671700
C	3.64766800	-0.75916800	2.27809000
C	2.48581800	-1.02371300	3.00615900
C	1.49341400	-1.83463700	2.44774800
C	1.66258900	-2.36554200	1.16876900
H	4.71385600	-1.08893300	0.43981600
H	4.42817000	-0.13535300	2.70594600
H	2.35547700	-0.60616400	4.00086300
H	0.59119900	-2.05754000	3.01039200
H	0.87607600	-2.98652100	0.75258700
Ni	0.51272900	-0.15400300	-1.08669900
P	-1.55814500	0.01292700	-0.09691300
C	-2.28550800	-1.59511800	0.41010200
C	-3.34903200	-1.70199300	1.31933300
C	-1.75679000	-2.75576200	-0.17652100
C	-3.87701400	-2.95336400	1.63638900
H	-3.75616700	-0.81134000	1.78644900
C	-2.29186200	-4.00596300	0.14331900
H	-0.91399900	-2.66659700	-0.86094500
C	-3.34940700	-4.10726900	1.04920700
H	-4.69773400	-3.02854900	2.34400000
H	-1.87510900	-4.90159500	-0.30918000
C	-2.79270700	0.70338800	-1.27035200
C	-4.12594400	0.94949800	-0.90640600
C	-2.38025600	0.97205100	-2.58253300
C	-5.02795700	1.45279300	-1.84209200
H	-4.45689200	0.75376100	0.10841300
C	-3.28565100	1.47437600	-3.52060800
H	-1.34760800	0.78241700	-2.86316900
C	-4.60943700	1.71514600	-3.15074100
H	-6.05770800	1.64101500	-1.55217800
H	-2.95640600	1.67841100	-4.53539400
C	-1.72431200	1.07724500	1.38524900
C	-1.33861500	0.58377600	2.64220000
C	-2.05741800	2.43449100	1.26190400
C	-1.29313600	1.42843800	3.75066000
H	-1.06650900	-0.45990300	2.75243900
C	-2.00688300	3.27911500	2.37271100
H	-2.35855700	2.83431000	0.29952200

C	-1.62327600	2.78015100	3.61884600
H	-0.99453300	1.03162600	4.71666000
H	-2.26942500	4.32723700	2.26211500
H	-5.31504800	2.10662700	-3.87768700
H	-1.58261400	3.43857700	4.48141800
H	-3.75986300	-5.08081700	1.30151500
O	0.92617700	-1.86014900	-1.76661100
H	0.76631400	-1.92470400	-2.71815500
B	3.04344000	-2.73212500	-1.02487300
O	4.09139300	-2.21359600	-1.75743600
O	2.52279300	-3.95073200	-1.42867500
H	4.18235300	-2.70934100	-2.58303900
H	1.57077000	-3.91415000	-1.26092500

I-IM6

C	2.93381700	0.70458100	-2.16143500
C	4.32314500	0.84763600	-1.50923500
H	2.76066200	-0.35895600	-2.37338600
H	4.36102000	0.27040000	-0.58505200
H	5.04562400	0.37703200	-2.18547300
C	2.70104100	1.60025300	0.98429900
H	3.27933100	0.68090800	0.93049100
H	2.19943600	1.57588000	1.95734600
C	3.63261200	2.82909400	0.97979700
H	3.02954200	3.72522200	1.18196800
H	4.31829400	2.74754300	1.83701700
C	1.64639500	1.66096200	-0.09371000
H	0.77570900	2.26452000	0.15868800
C	1.74767700	1.29155700	-1.41553600
H	0.93868300	1.62807300	-2.06240100
C	4.43830400	3.09414400	-0.26672600
H	4.83814700	4.10778900	-0.31664200
C	4.73261300	2.28494700	-1.29259600
H	5.32364600	2.71820400	-2.09990200
H	2.95738300	1.19280000	-3.14432300
C	1.94953300	-2.47257500	0.31696600
C	3.34333600	-2.30002900	0.42465500
C	3.93900300	-1.80615500	1.58804900
C	3.14833200	-1.45240300	2.68697800
C	1.76209900	-1.58971300	2.60734700
C	1.17646200	-2.09308000	1.43776500
H	3.96489300	-2.59029400	-0.41786800
H	5.01998700	-1.70106800	1.64337400
H	3.60996300	-1.06985500	3.59325100

H	1.13580700	-1.31766800	3.45220900
H	0.10076500	-2.25319900	1.41277400
Ni	0.69409000	-0.33037500	-0.50594400
P	-1.50253300	0.23316600	-0.01811500
C	-2.83134700	-0.84412300	-0.66715200
C	-4.10112200	-0.34608700	-1.00050300
C	-2.56524400	-2.21580600	-0.79862400
C	-5.09731200	-1.21226100	-1.45198900
H	-4.31018300	0.71494600	-0.90834500
C	-3.56991700	-3.07615900	-1.24689500
H	-1.57946600	-2.61789200	-0.58210900
C	-4.83352000	-2.57956300	-1.57310600
H	-6.07727100	-0.82055900	-1.70940000
H	-3.35529400	-4.13604000	-1.35068800
C	-1.90037100	1.88692600	-0.70555900
C	-2.23120800	2.99034600	0.09060100
C	-1.79046400	2.05245600	-2.09719100
C	-2.45292100	4.23954700	-0.49636400
H	-2.31763300	2.87755700	1.16605300
C	-2.02018100	3.29712100	-2.67979800
H	-1.53065200	1.20234000	-2.72239700
C	-2.34921600	4.39566600	-1.87913100
H	-2.70949600	5.08900600	0.13002900
H	-1.93846400	3.41177700	-3.75673900
C	-1.86744000	0.38304000	1.77268800
C	-3.12618400	0.10099200	2.32199100
C	-0.82881000	0.80121300	2.61886700
C	-3.34086800	0.24186100	3.69403500
H	-3.93609200	-0.23174800	1.68191900
C	-1.04818700	0.95080400	3.98828200
H	0.15120900	0.99935500	2.20108300
C	-2.30529100	0.66904300	4.52853600
H	-4.31809600	0.01653200	4.11103400
H	-0.23624400	1.27698700	4.63178800
H	-2.52236400	5.36676700	-2.33329800
H	-2.47611700	0.77613900	5.59566100
H	-5.60933100	-3.25244900	-1.92734100
O	0.52758300	-1.92827800	-1.74196300
H	0.98689200	-1.80034400	-2.58116200
B	1.23813900	-3.09491100	-1.02460700
O	2.24710900	-3.63331500	-1.92630000
O	0.15987000	-4.02618000	-0.69837600
H	1.83218500	-4.36186100	-2.40458300
H	0.43519100	-4.58351500	0.03887700

I-TS5

C	2.98838100	1.11800600	-1.99475100
C	4.36292600	1.41298700	-1.35372700
H	2.95419000	0.05673600	-2.27369500
H	4.53398900	0.73602400	-0.51695600
H	5.12757200	1.16803100	-2.10000000
C	2.69500000	1.51940500	1.22221500
H	3.35290600	0.67896300	1.01076600
H	2.20249500	1.28338800	2.17217600
C	3.50466000	2.81782800	1.43318400
H	2.83032700	3.58184500	1.84260000
H	4.24995200	2.64136700	2.22343200
C	1.63755900	1.66590000	0.15730000
H	0.70076000	2.10223400	0.49878600
C	1.76290600	1.48424200	-1.18421000
H	0.89643000	1.77013300	-1.78176400
C	4.18722500	3.41999000	0.22883800
H	4.41515500	4.48059100	0.34130400
C	4.54210900	2.85073600	-0.93038500
H	5.00354000	3.50000400	-1.67478700
H	2.92152400	1.67407200	-2.93913900
C	1.90482800	-1.91741800	0.08343200
C	3.31121800	-1.83621400	0.15217100
C	4.04506500	-2.31960500	1.24025100
C	3.38470900	-2.91545500	2.31852600
C	1.99299400	-3.04082200	2.28154700
C	1.27901000	-2.56627500	1.17576300
H	3.85181800	-1.38700000	-0.67659100
H	5.12968700	-2.23266500	1.24969300
H	3.94791300	-3.29068000	3.16914900
H	1.46810500	-3.51636700	3.10740900
H	0.19797500	-2.69844400	1.16561400
Ni	0.58893500	-0.46577700	-0.52600400
P	-1.54452600	0.20560900	0.01809700
C	-2.89938800	-0.79993900	-0.69426100
C	-4.19231800	-0.30156800	-0.91381100
C	-2.61022500	-2.13770300	-1.00500400
C	-5.18819600	-1.13697300	-1.42208000
H	-4.41810000	0.73667700	-0.69209600
C	-3.61167400	-2.97029200	-1.50681800
H	-1.60082400	-2.51882000	-0.88084300
C	-4.90020200	-2.47283700	-1.71500800
H	-6.18738400	-0.74532700	-1.59014100

H	-3.37950000	-4.00357600	-1.74864300
C	-1.98717200	1.93229600	-0.41589200
C	-2.19541200	2.93076000	0.54430500
C	-1.99490700	2.28096500	-1.77820500
C	-2.40985500	4.25435100	0.14961100
H	-2.18972800	2.67915600	1.59937500
C	-2.22077300	3.59933400	-2.16884800
H	-1.82837700	1.51568700	-2.53190600
C	-2.42376200	4.59169000	-1.20401400
H	-2.56752600	5.01993400	0.90394500
H	-2.23138000	3.85459400	-3.22458600
C	-1.81194000	0.10632500	1.83139100
C	-3.08746100	0.07140900	2.41479900
C	-0.67879900	0.06028600	2.65678100
C	-3.22296400	-0.00192200	3.80122800
H	-3.97241900	0.09425800	1.78694100
C	-0.81591800	-0.01122900	4.04389800
H	0.30822400	0.06757900	2.20685500
C	-2.08843000	-0.04071000	4.61775400
H	-4.21376800	-0.03066100	4.24522800
H	0.06955900	-0.05036500	4.67156900
H	-2.59083000	5.62085100	-1.50803200
H	-2.19801900	-0.10072800	5.69664800
H	-5.67620900	-3.12075300	-2.11256500
O	0.29236700	-1.40140600	-2.44362600
H	0.76813200	-0.83877300	-3.06976700
B	1.17621100	-2.42241300	-1.95895000
O	2.40325200	-2.43013200	-2.64360500
O	0.47716800	-3.58443200	-1.59437800
H	3.00083500	-3.10210800	-2.29516100
H	0.98216700	-4.11369900	-0.96641100

[Ni]-Ar

C	-0.91097500	2.55350400	-0.56046600
C	-2.18995600	2.47507500	-1.15709400
C	-3.13836900	3.49869900	-1.05115300
C	-2.84408500	4.65541500	-0.32372500
C	-1.59064900	4.77515300	0.28333600
C	-0.65075800	3.74583400	0.15307000
H	-4.11096700	3.39201300	-1.52839800
H	-2.46825800	1.58064900	-1.71100800
H	-3.58031900	5.44999900	-0.23023300
H	-1.34786400	5.67008700	0.85360900
H	0.31888000	3.87615900	0.63638100

C	3.07687600	1.53598900	-2.04548200
C	4.15471900	0.44714100	-1.85858900
H	2.30242100	1.15532000	-2.72914200
H	3.70383800	-0.46785900	-1.47204900
H	4.53980600	0.19572200	-2.85329500
C	2.95005900	0.23653300	0.96412700
H	2.85275100	-0.56814100	0.23740800
H	2.38414900	-0.08389100	1.84398100
C	4.42428600	0.40185600	1.38746100
H	4.46546900	1.11331600	2.22360400
H	4.77607300	-0.55256200	1.80760000
C	2.34397000	1.52757200	0.45809600
H	1.95502300	2.17796600	1.24167400
C	2.42361500	2.08481800	-0.79271100
H	2.07295300	3.11072800	-0.88357800
C	5.40685800	0.87129400	0.34387700
H	6.33907000	1.24772600	0.76707000
C	5.30860500	0.89332100	-0.99188800
H	6.15649700	1.30944500	-1.53621500
H	3.52897600	2.38652900	-2.57124800
Ni	0.43553200	1.11184500	-0.60707800
P	-0.62692200	-0.82514300	-0.03481100
C	-2.42417900	-0.95630700	-0.39084700
C	-2.81064500	-1.16317500	-1.72578800
C	-3.41025800	-0.78121500	0.58637000
C	-4.15957900	-1.19761200	-2.07280800
H	-2.05359300	-1.29589100	-2.49416100
C	-4.76240800	-0.80967100	0.23428100
H	-3.12929300	-0.62017100	1.62124800
C	-5.14064300	-1.01654200	-1.09233400
H	-4.44598700	-1.36048500	-3.10786700
H	-5.51869400	-0.67204700	1.00177100
H	-6.19216800	-1.03681900	-1.36320200
C	-0.50421300	-0.91448100	1.79523700
C	-0.09785000	-2.06183600	2.48920500
C	-0.76301200	0.26580800	2.51572000
C	0.04062200	-2.03212600	3.87909100
H	0.11950900	-2.97686400	1.94993000
C	-0.63566800	0.28745100	3.90382300
H	-1.05560100	1.16594000	1.98367400
C	-0.23111000	-0.86165500	4.58938600
H	0.36077900	-2.92690400	4.40528000
H	-0.84408100	1.20377200	4.44859100
H	-0.12317700	-0.84214400	5.66989100

C	0.00771600	-2.43176900	-0.64764600
C	1.22206000	-2.43708900	-1.34661500
C	-0.67993300	-3.64160800	-0.45969700
C	1.75658300	-3.63170100	-1.83313300
H	1.74082000	-1.49929100	-1.51946100
C	-0.14681400	-4.83453500	-0.94676900
H	-1.63229300	-3.64779600	0.06126000
C	1.07414200	-4.83206300	-1.62890400
H	2.69891000	-3.62221100	-2.37288800
H	-0.68389400	-5.76642200	-0.79579300
H	1.48516600	-5.76284400	-2.00866600

I-TS2'

C	-1.17304900	3.48831200	-2.37708400
C	0.20806700	3.61922700	-1.71131000
H	-1.20181700	2.55021400	-2.94844400
H	0.36260100	2.78094900	-1.03101400
H	0.96434000	3.50507300	-2.49568500
C	-1.40249400	3.30595000	0.88857000
H	-0.65662600	2.56736400	0.58702900
H	-1.85402700	2.90919200	1.80427500
C	-0.71776900	4.63302800	1.26290000
H	-1.48256500	5.32067300	1.65107000
H	-0.03725900	4.45159500	2.10636200
C	-2.48907100	3.45899200	-0.15186000
H	-3.49739800	3.54510400	0.25307200
C	-2.38496100	3.53450700	-1.48551900
H	-3.31986400	3.63941800	-2.03636000
C	0.04274300	5.35807700	0.18469600
H	0.31383100	6.37802400	0.46234600
C	0.43243900	4.95028900	-1.03075000
H	0.96399300	5.68357700	-1.63758800
H	-1.28234500	4.28257300	-3.12922500
C	0.13811500	-0.81321100	1.61906200
C	-0.62357800	-0.27517500	2.67189800
C	0.72566800	-2.07791300	1.77767600
C	-0.87426000	-1.02930800	3.81957800
H	-1.03725200	0.72468600	2.58789900
C	0.49658300	-2.81516200	2.94272500
H	1.36797200	-2.47553400	1.00168600
C	-0.31463000	-2.30248200	3.96093900
H	-1.50494600	-0.61665300	4.60254500
H	0.95741700	-3.79338400	3.05446100

H	-0.49532100	-2.88235200	4.86131000
H	-0.00168900	-1.29437700	-2.48928800
C	1.45192000	0.44520700	0.66043400
C	0.49254600	-1.23383900	-1.51190600
C	1.89615100	-0.64422000	-1.61613300
C	2.27987500	0.11981800	-0.35604700
C	3.07367600	-1.64734100	-1.73969400
C	4.31887000	-0.95741900	-1.07993500
C	3.77510400	0.34489500	-0.39051500
H	2.82507600	-2.56019900	-1.19199100
H	3.29937600	-1.92356700	-2.77121000
H	4.04005700	1.21340900	-1.00126200
H	4.20751000	0.50141100	0.59696100
C	4.91005300	-1.94366000	-0.08174700
O	5.85176500	-2.67751300	-0.30959800
O	4.20739100	-1.96208400	1.06277400
C	5.40870700	-0.62900900	-2.09643200
O	5.40891200	-0.94271600	-3.26845100
O	6.38510700	0.09209300	-1.51952200
C	4.60069800	-2.94378500	2.03873000
H	5.64665100	-2.80639100	2.32285700
H	3.94940200	-2.77936100	2.89650400
H	4.46107300	-3.95371100	1.64409300
C	7.49105100	0.44512400	-2.37136000
H	8.17340200	1.02026900	-1.74537700
H	7.98675800	-0.45398900	-2.74594000
H	7.15063500	1.05023900	-3.21552900
Ni	-0.42005800	-0.08341100	-0.08382200
C	1.92103900	1.34225200	1.74585800
C	2.16314400	2.69433600	1.44575500
C	2.20750500	0.89730700	3.05076200
C	2.65128500	3.57609100	2.41120900
H	1.95738600	3.05799500	0.44628800
C	2.69914000	1.77653000	4.01495900
H	2.06143100	-0.14622000	3.30185700
C	2.91667100	3.12208300	3.70390600
H	2.82007400	4.61652100	2.14776000
H	2.91975500	1.40747400	5.01300900
H	3.29439000	3.80494700	4.45952900
P	-2.66033900	-0.74159100	-0.39003900
C	-2.72875900	-2.51086300	-0.86935400
C	-3.50973600	-2.97489100	-1.93541200
C	-1.95754900	-3.42549700	-0.13357700
C	-3.51409200	-4.33207100	-2.26532700

H	-4.11313900	-2.28071700	-2.50999800
C	-1.97270600	-4.78111700	-0.45878300
H	-1.34746500	-3.07433000	0.69107600
C	-2.74743800	-5.23708000	-1.52927800
H	-4.12070700	-4.68016100	-3.09640100
H	-1.37444000	-5.47966100	0.11926300
C	-3.58438400	0.10631700	-1.72544400
C	-2.90851900	0.33159900	-2.93597100
C	-4.91106300	0.53541600	-1.59108100
C	-3.55173100	0.97255300	-3.99391900
H	-1.87893900	0.00518200	-3.04575200
C	-5.54768500	1.19008200	-2.64766400
H	-5.44702900	0.36272400	-0.66406700
C	-4.87114500	1.41038200	-3.84944200
H	-3.01886500	1.14144900	-4.92515500
H	-6.57515000	1.52302300	-2.53201700
C	-3.75259000	-0.64491900	1.08147400
C	-3.89453100	0.60337500	1.70883000
C	-4.36170200	-1.76765100	1.65668400
C	-4.63281800	0.72878000	2.88357000
H	-3.42855500	1.47721500	1.26965000
C	-5.09047400	-1.64298800	2.84197400
H	-4.26352000	-2.74001900	1.18771800
C	-5.22673900	-0.39858000	3.45905900
H	-4.73575700	1.70201500	3.35488700
H	-5.55335600	-2.52215100	3.28094900
H	-5.36915800	1.91854700	-4.66989200
H	-5.79132900	-0.30600400	4.38215000
H	-2.75300900	-6.29198200	-1.78767800
H	0.49824100	-2.24061000	-1.08095600
C	1.93562400	0.33843100	-2.81198600
H	2.88731600	0.87062600	-2.90357800
H	1.13861200	1.08091400	-2.71415900
H	1.77634800	-0.21458700	-3.74438700

II-IM0

C	0.54811600	1.65024900	0.20871100
C	1.62814100	0.99305600	0.41834600
Ni	0.22451700	-0.23606300	0.13240300
C	1.89619900	-1.94911400	-0.08356700
C	3.12692300	-1.55356400	0.70785900
H	2.87703700	-1.51806400	1.77084000
H	3.85823000	-2.35993400	0.58289300
C	3.05054100	1.01669000	0.82462100

H	3.09182100	1.05306700	1.92119800
H	3.54790400	1.91598000	0.45086900
C	3.85789200	-0.22501200	0.37428500
C	0.77326700	-2.39880000	0.56453600
H	0.02438200	-2.97738400	0.03434500
H	0.71152200	-2.38976500	1.64974600
C	2.05974800	-2.19976500	-1.56706400
H	2.18651700	-1.27434000	-2.13400800
H	2.94584000	-2.81959700	-1.74744100
H	1.19128200	-2.72226500	-1.97174300
C	-0.13941900	2.91447000	0.04226000
C	0.14880900	3.73909800	-1.06208200
C	-1.12891900	3.33331000	0.95109600
C	-0.53199800	4.94155800	-1.24844700
H	0.90379600	3.41966100	-1.77445900
C	-1.79974800	4.54004900	0.76676100
H	-1.36909100	2.69919500	1.79806100
C	-1.50901300	5.34843600	-0.33618300
H	-0.29870500	5.56151600	-2.10990900
H	-2.56346600	4.84405700	1.47702500
H	-2.04210300	6.28279800	-0.48602100
C	4.21140000	-0.10522700	-1.11068800
O	3.83202400	0.76757200	-1.86170900
O	5.02711000	-1.10940800	-1.48049100
C	5.18341400	-0.20740600	1.15109600
O	5.49736300	-0.98092500	2.03009200
O	5.94550600	0.82561100	0.75391900
C	5.43711600	-1.11107100	-2.86176200
H	5.97888100	-0.19277000	-3.10018900
H	6.08921500	-1.97696300	-2.97358100
H	4.56952200	-1.20288800	-3.51955800
C	7.20437700	0.98332200	1.43998000
H	7.82563900	0.09459100	1.30676700
H	7.68020800	1.85107300	0.98380000
H	7.03817600	1.15722800	2.50585700
C	-2.62780800	-1.86615800	-1.15320200
C	-3.97045500	-2.27529800	-1.10905000
C	-1.80195900	-2.34443800	-2.17733200
C	-4.46535600	-3.16735300	-2.05881300
H	-4.62728700	-1.89477300	-0.33281400
C	-2.29951100	-3.23253200	-3.13449400
H	-0.77265300	-2.00673200	-2.22573700
C	-3.62965100	-3.64882100	-3.07248900
H	-5.50392900	-3.48231600	-2.01417100

H	-1.64914200	-3.59503100	-3.92540200
H	-4.01890600	-4.34069200	-3.81378100
C	-2.41880200	-1.26742800	1.69040200
C	-2.29089700	-0.39791900	2.78819500
C	-2.75490500	-2.60769400	1.92528800
C	-2.52309200	-0.85291200	4.08486400
H	-2.01147100	0.63836500	2.62509800
C	-2.97503500	-3.06465500	3.22752900
H	-2.84651600	-3.29923000	1.09514600
C	-2.86574600	-2.18988900	4.30893900
H	-2.43153900	-0.16502200	4.92055400
H	-3.23556500	-4.10627400	3.39251300
H	-3.04150100	-2.54562800	5.31989800
P	-1.93407600	-0.64170500	0.03309600
C	-3.05586900	0.78162700	-0.28780000
C	-2.76201800	1.56620600	-1.41401100
C	-4.17379000	1.09970400	0.49245300
C	-3.57440900	2.64325500	-1.75895600
H	-1.88226900	1.33938700	-2.00908000
C	-4.98001900	2.19026400	0.15389900
H	-4.41632100	0.50599000	1.36723300
C	-4.68412200	2.96187600	-0.97078700
H	-3.32987100	3.24624700	-2.62812500
H	-5.84153600	2.43338800	0.76959100
H	-5.30985300	3.81099200	-1.22998700

II-TS1

C	-2.87722900	0.20166900	1.68059500
C	-4.22304000	0.53268400	1.90267900
C	-1.95133000	0.33095700	2.72359500
C	-4.62716700	1.01548200	3.14651300
H	-4.94978700	0.40999000	1.10568800
C	-2.35982000	0.81051700	3.96945000
H	-0.91660600	0.04861800	2.55467300
C	-3.69531600	1.15851200	4.17933500
H	-5.66843400	1.27603400	3.31147100
H	-1.63593100	0.90881900	4.77288300
H	-4.01380000	1.53152100	5.14829100
C	-2.74913200	0.76443900	-1.20604800
C	-2.49079700	0.42033900	-2.54356500
C	-3.24889800	2.03612900	-0.90696800
C	-2.75195700	1.33030400	-3.56564700
H	-2.08635000	-0.55947400	-2.78196900
C	-3.49971800	2.94874400	-1.93404000

H	-3.43092100	2.32376000	0.12133400
C	-3.25859400	2.59766400	-3.26231900
H	-2.55456700	1.05305900	-4.59692800
H	-3.87753600	3.93704700	-1.68995900
H	-3.45417900	3.30990300	-4.05845700
C	0.54454600	0.45548100	-0.24429100
C	1.73585000	-0.13978800	-0.33216800
Ni	-0.30024400	-1.14646300	0.11346900
P	-2.31913500	-0.46559000	0.07250500
C	2.01024500	-1.71443900	-0.28182600
C	3.32589100	-1.70299400	0.52832500
H	3.09548500	-1.62203300	1.59286000
H	3.89616600	-2.62281000	0.37728200
C	3.07430700	0.55924200	-0.44715100
H	3.06536500	1.51188900	0.08724700
H	3.32706500	0.77735800	-1.48900300
C	4.12763300	-0.43512000	0.12746400
C	0.94821700	-2.66640200	0.35177800
H	0.90141700	-3.60535600	-0.20447600
H	1.20326900	-2.88584400	1.39485300
C	2.25276900	-2.14919900	-1.74437400
H	2.90601400	-1.46427300	-2.29150000
H	2.71323400	-3.14344600	-1.76372600
H	1.29830100	-2.20369200	-2.27753300
C	0.20725300	1.87263900	-0.35284200
C	0.23112200	2.51491400	-1.60438900
C	-0.15404000	2.62386300	0.78001800
C	-0.09866900	3.86441500	-1.71784800
H	0.49769600	1.94149900	-2.48625600
C	-0.47633600	3.97519400	0.66500500
H	-0.17663500	2.14132300	1.75025800
C	-0.45293400	4.60072700	-0.58427300
H	-0.08329100	4.34094000	-2.69386400
H	-0.74677200	4.54044800	1.55255200
H	-0.71203400	5.65167100	-0.67435100
C	-3.47425900	-1.86111100	-0.22217100
C	-3.23292600	-3.06081900	0.46599000
C	-4.59473500	-1.75784300	-1.05762300
C	-4.10627300	-4.13817500	0.32602100
H	-2.35917700	-3.14544400	1.10577800
C	-5.46241900	-2.84286200	-1.20074400
H	-4.79355300	-0.83717400	-1.59483800
C	-5.22040800	-4.03252300	-0.51136500
H	-3.91279500	-5.06166700	0.86392400

H	-6.32743100	-2.75580600	-1.85177300
H	-5.89717100	-4.87429000	-0.62532300
C	5.21458100	-0.75948500	-0.89883800
O	5.25225400	-0.37651300	-2.04995700
O	6.14409400	-1.56017800	-0.35083700
C	4.80111500	0.20659600	1.34172200
O	4.53891400	-0.02275900	2.50321300
O	5.70076500	1.12388100	0.94586700
C	7.24605600	-1.92463400	-1.20533800
H	7.79288400	-1.03327700	-1.52319500
H	7.88657500	-2.56612000	-0.60029300
H	6.88753500	-2.46531600	-2.08446800
C	6.38059800	1.83898000	1.99667700
H	6.93969200	1.14678100	2.63109000
H	7.06155100	2.52414200	1.49200400
H	5.66526800	2.39601200	2.60671800

II-IMI

C	-3.84046300	-0.55851000	-1.09797000
C	-5.13880300	-0.71068500	-0.58549600
C	-3.54213900	-1.05767200	-2.37251700
C	-6.11394100	-1.37201600	-1.32984000
H	-5.38326000	-0.31309000	0.39450900
C	-4.52146300	-1.71716800	-3.11888400
H	-2.54511600	-0.92471400	-2.78009100
C	-5.80548300	-1.87847000	-2.59666500
H	-7.11490300	-1.48896900	-0.92508800
H	-4.27984500	-2.10154100	-4.10538000
H	-6.56741200	-2.39246800	-3.17532300
C	-2.44756900	-0.46296300	1.46953800
C	-1.69156000	0.17865400	2.46545300
C	-3.01018400	-1.71575700	1.73762500
C	-1.52258600	-0.41630600	3.71378100
H	-1.23568100	1.14241700	2.25948600
C	-2.83283500	-2.31213800	2.98832400
H	-3.57471500	-2.23424800	0.97196000
C	-2.09484100	-1.66419300	3.97879700
H	-0.94020600	0.09069900	4.47754500
H	-3.27037200	-3.28687800	3.18301900
H	-1.95862900	-2.13112100	4.94982400
C	0.71331300	-0.34370300	-0.30572800
C	1.95477200	0.13648600	-0.09512200
Ni	-0.47193600	0.91690600	-1.03891200
P	-2.53394200	0.33432000	-0.17241900

C	2.24594700	1.52319700	-0.61025800
C	3.66903000	1.34426300	-1.19552200
H	3.60273800	0.92988900	-2.20423100
H	4.24570000	2.27112400	-1.25168400
C	3.21672600	-0.52841900	0.39404100
H	3.24815900	-1.59544200	0.15614900
H	3.34768000	-0.43850400	1.47688400
C	4.37194600	0.27304900	-0.30441800
C	1.11787800	1.82430700	-1.61789700
H	0.87640900	2.89715400	-1.70294600
H	1.37390200	1.44653800	-2.61762800
C	2.24373000	2.56043400	0.52938000
H	2.93279100	2.28892900	1.33522000
H	2.53555300	3.54898000	0.15445700
H	1.23912000	2.64220600	0.95851200
C	0.25777300	-1.70617600	0.00375800
C	0.57205900	-2.33185600	1.22571200
C	-0.52712000	-2.42085500	-0.92013000
C	0.12732500	-3.62409800	1.50317200
H	1.14615900	-1.78656500	1.96736700
C	-0.97674400	-3.71010400	-0.64142100
H	-0.77670000	-1.94677200	-1.86302000
C	-0.65098600	-4.31922500	0.57359700
H	0.37477300	-4.08375600	2.45602900
H	-1.58408400	-4.23788800	-1.37176900
H	-1.00522300	-5.32132600	0.79721000
C	-3.31155300	1.96774400	0.15386500
C	-3.12524500	2.96121800	-0.82166300
C	-4.06407500	2.26350400	1.29832100
C	-3.68906400	4.22696800	-0.65995700
H	-2.54153900	2.73819200	-1.71345000
C	-4.62356500	3.53213000	1.46041600
H	-4.20638500	1.50851800	2.06418800
C	-4.43803100	4.51420700	0.48401600
H	-3.53974800	4.98723100	-1.42096600
H	-5.20499800	3.75376700	2.35072700
H	-4.87392700	5.50021700	0.61481300
C	5.29105600	0.93620900	0.72286500
O	5.12928600	0.95792100	1.92596600
O	6.32185700	1.53710400	0.10311800
C	5.21405500	-0.68971500	-1.14015800
O	5.17131400	-0.81259900	-2.34593100
O	5.98838800	-1.44635400	-0.34054000
C	7.26253000	2.21712200	0.95634800

H	7.71630300	1.51666900	1.66162200
H	8.02008700	2.62833900	0.28917800
H	6.76808900	3.02014300	1.50861800
C	6.79568000	-2.44160300	-0.99895500
H	7.49221900	-1.97069000	-1.69708300
H	7.34160700	-2.94893900	-0.20359700
H	6.16463000	-3.15200600	-1.53861000

II-IM2

C	0.45526900	1.01377900	-1.10997300
C	1.23338100	0.02766000	1.15623900
C	2.19598900	0.78528500	0.59956900
C	1.84206000	1.51649000	-0.66898500
C	3.67658400	0.93513100	0.83993400
C	4.26571300	0.94120300	-0.61969500
C	3.03611100	1.12931200	-1.58212900
H	0.52279100	0.23758200	-1.88701000
H	-0.18385100	1.82192000	-1.47753900
H	3.90411100	1.89707000	1.31406600
H	4.12330200	0.15926500	1.45849000
H	2.81597700	0.17992900	-2.07908300
H	3.27048200	1.87009500	-2.34912700
C	5.29679900	2.05676400	-0.77583800
O	5.23848200	2.98206800	-1.55855600
O	6.29054300	1.89800000	0.11544800
C	4.95538300	-0.35848000	-1.00933100
O	5.86198200	-0.43223200	-1.81546000
O	4.39595100	-1.43292000	-0.42412100
C	7.33356700	2.88981900	0.07709000
H	6.92717600	3.88395000	0.27978400
H	8.04010800	2.60499900	0.85672200
H	7.82597700	2.89081300	-0.89855300
C	4.91558300	-2.71294600	-0.83380100
H	4.34648000	-3.45448800	-0.27496300
H	4.77908600	-2.85626300	-1.90818500
H	5.97816400	-2.78929300	-0.59121800
C	1.34698200	-0.80509200	2.36417000
C	0.30609300	-0.76643200	3.31507500
C	2.38713000	-1.73474400	2.56812100
C	0.30188300	-1.61607200	4.42117300
H	-0.50948800	-0.06309200	3.16593900
C	2.38137500	-2.58701800	3.67209500
H	3.18392800	-1.80072000	1.83571000
C	1.33874900	-2.53546800	4.60301000

H	-0.51350700	-1.56435900	5.13802900
H	3.18973200	-3.30179300	3.80416100
H	1.33416400	-3.20464800	5.45866400
C	1.81437300	3.04373300	-0.46178300
H	2.76921900	3.42970200	-0.09138100
H	1.60063900	3.55184600	-1.40969900
H	1.03242400	3.31835300	0.25218900
C	1.23424300	-2.96602200	-0.45506700
C	1.18402100	-3.22422200	-1.97137400
H	1.88615800	-2.10722800	-0.25996100
H	0.73612900	-2.36809400	-2.47896100
H	2.21874900	-3.27502300	-2.32827100
C	-1.79321700	-2.49288900	-1.64277500
H	-1.12826300	-1.89899000	-2.27022300
H	-2.75524100	-1.97619900	-1.66675500
C	-2.01183400	-3.88509000	-2.26292200
H	-2.75182200	-4.42566200	-1.65515600
H	-2.49309000	-3.75635600	-3.24460000
C	-1.31546200	-2.53453400	-0.21021800
H	-2.10519600	-2.48579500	0.53661600
C	-0.07047100	-2.74415500	0.26363500
H	0.02032900	-2.80433400	1.34469400
C	-0.81534300	-4.78361600	-2.43163300
H	-1.08335300	-5.81043900	-2.68577000
C	0.49358800	-4.52016300	-2.32915900
H	1.16727600	-5.36307900	-2.48528800
H	1.72861200	-3.82013000	0.02853500
Ni	-0.43578100	-0.03791000	0.23880500
P	-2.56277700	0.71249700	-0.11798700
C	-3.65257300	-0.03014800	1.16567300
C	-4.32852900	-1.23742600	0.91984200
C	-3.69237200	0.51595600	2.45771300
C	-5.02898500	-1.87818200	1.94188100
H	-4.31447500	-1.67596800	-0.07206800
C	-4.38742100	-0.13197800	3.48043700
H	-3.18108800	1.44903500	2.66804200
C	-5.05723200	-1.33021600	3.22689500
H	-5.55290000	-2.80640400	1.73267400
H	-4.40863000	0.30579400	4.47426900
C	-3.51657600	0.61385000	-1.68159700
C	-4.91817400	0.57233700	-1.72948500
C	-2.79077700	0.61619500	-2.88276200
C	-5.57927800	0.52668600	-2.95803600
H	-5.49368700	0.57228100	-0.81022400

C	-3.45388500	0.57854600	-4.10917800
H	-1.70654000	0.63921700	-2.85413800
C	-4.84938700	0.52925200	-4.14888600
H	-6.66458700	0.49109500	-2.98361600
H	-2.88123400	0.57879500	-5.03200300
C	-2.60488800	2.50820500	0.28928300
C	-1.61678600	3.00835300	1.15144300
C	-3.58948300	3.37856600	-0.19845300
C	-1.62188100	4.35118000	1.53137500
H	-0.83985200	2.33929200	1.50887300
C	-3.58644600	4.72377400	0.17378900
H	-4.35647100	3.01180100	-0.87176200
C	-2.60627700	5.21215400	1.04120400
H	-0.85174700	4.72457700	2.20009100
H	-4.35137600	5.39031200	-0.21421800
H	-5.36572900	0.49183700	-5.10362900
H	-2.60697900	6.25955200	1.32864300
H	-5.59963000	-1.83210700	4.02258100

II-IM3

H	-0.63212100	-1.12933300	2.92277700
C	0.45678000	1.15559600	-0.63567600
C	1.32583000	0.09269600	1.58293400
C	2.25107000	0.85460900	0.97330400
C	1.80305800	1.73072800	-0.16653700
C	3.75178100	0.92641200	1.08361200
C	4.19022100	0.97789800	-0.41702000
C	2.98051700	1.62846100	-1.18638800
H	0.63757200	0.31537900	-1.31806100
H	-0.14611100	1.90147100	-1.16636400
H	4.06569600	1.85600800	1.57276900
H	4.21482600	0.08893200	1.60382300
H	2.70822500	0.99816100	-2.03334100
H	3.26685300	2.60304700	-1.58546100
C	5.49671900	1.75017800	-0.54984100
O	6.58575200	1.24325600	-0.73889200
O	5.31467800	3.06985300	-0.37340100
C	4.48309100	-0.44008300	-0.92297900
O	4.63443300	-1.42264900	-0.22545400
O	4.57120600	-0.46731000	-2.26239500
C	6.50859000	3.87571000	-0.39911600
H	7.00868700	3.79016300	-1.36697100
H	6.17503800	4.90026400	-0.23478100
H	7.19628300	3.56827900	0.39265000

C	4.93958000	-1.73126300	-2.84450100
H	4.92465900	-1.57375200	-3.92303500
H	5.94237100	-2.02074900	-2.51905500
H	4.22920000	-2.51114700	-2.56351800
C	1.65265900	-0.83331100	2.68600000
C	1.09789200	-0.65235800	3.97265500
C	2.47266500	-1.96324200	2.48534400
C	1.33550400	-1.56770900	5.00362100
H	0.50228200	0.23756000	4.16853100
C	2.70846900	-2.87349000	3.51384200
H	2.93265900	-2.10925300	1.51482000
C	2.13267100	-2.68968300	4.77564700
H	0.89786700	-1.39881900	5.98391400
H	3.34396700	-3.73587600	3.32909700
H	2.31213200	-3.40725600	5.57095600
C	1.64640000	3.19203800	0.29648900
H	2.59311200	3.59577000	0.67153500
H	1.32045700	3.82995100	-0.53414900
H	0.90136100	3.26341400	1.09420600
C	1.58047500	-2.96196000	-1.06401200
C	0.72957000	-2.38849500	-2.21311700
H	2.05033300	-2.12347800	-0.53485400
H	-0.00011500	-1.69085700	-1.80787000
H	1.39442100	-1.79292200	-2.85037200
C	-1.58239700	-3.22586100	-0.39266700
H	-1.34304500	-2.17084500	-0.52838000
H	-2.41274200	-3.24912700	0.32068000
C	-2.10600700	-3.84128700	-1.70894800
H	-2.53513400	-4.82714400	-1.48198900
H	-2.95020200	-3.23353900	-2.06528100
C	-0.41931400	-3.96883300	0.21844500
H	-0.68887700	-4.70615800	0.97540000
C	0.88449400	-3.84894900	-0.06349900
H	1.56586500	-4.47891200	0.50888500
C	-1.12663300	-4.02948200	-2.84053000
H	-1.44998700	-4.76349800	-3.58008000
C	0.05322000	-3.43562300	-3.06058300
H	0.60770100	-3.75193000	-3.94458500
H	2.41452000	-3.53580500	-1.48977000
Ni	-0.46315200	0.25110600	0.81661700
P	-2.53298600	0.77093600	-0.05063700
C	-3.92496900	0.44686000	1.11198300
C	-4.17501900	-0.87889000	1.51214800
C	-4.70910400	1.47538200	1.65364700

C	-5.18452900	-1.16506800	2.43138600
H	-3.57524200	-1.68558200	1.10664200
C	-5.71658500	1.18540700	2.57625500
H	-4.53887000	2.50314200	1.35441500
C	-5.95797000	-0.13259600	2.96737100
H	-5.36500900	-2.19448900	2.72678300
H	-6.31639100	1.99345000	2.98485500
C	-3.07968000	-0.03193600	-1.61131600
C	-4.39213400	-0.47988600	-1.81854300
C	-2.13628500	-0.18132300	-2.63978700
C	-4.74868300	-1.07615400	-3.03030800
H	-5.13675300	-0.36611200	-1.03873900
C	-2.49504400	-0.77612300	-3.84833000
H	-1.12139200	0.16681600	-2.49316300
C	-3.80199800	-1.22828600	-4.04561700
H	-5.76799200	-1.42067500	-3.17874800
H	-1.75088800	-0.89514600	-4.62950600
C	-2.69984300	2.56275100	-0.39861000
C	-2.03889100	3.45741800	0.45643900
C	-3.47661100	3.06350300	-1.45090700
C	-2.15992300	4.83344500	0.26688400
H	-1.42238900	3.06774500	1.26065100
C	-3.58954000	4.44173400	-1.64453100
H	-3.99085200	2.38067500	-2.11873100
C	-2.93446300	5.32754800	-0.78627000
H	-1.64216800	5.51775800	0.93261600
H	-4.19027600	4.82194700	-2.46568200
H	-4.08035700	-1.69863700	-4.98402000
H	-3.02298100	6.39903200	-0.94001700
H	-6.74233700	-0.35451400	3.68479700
O	-1.29146600	-0.97261400	2.22126800
H	-2.09144300	-0.63159600	2.65073700

II-TS2

H	0.34820600	0.31513200	-2.50859000
C	0.23022100	2.76235900	2.10094700
C	-0.73185300	3.62632700	2.94124500
H	0.36911200	1.79698200	2.60949100
H	-1.67659100	3.09933600	3.07742700
H	-0.29576900	3.72457900	3.94233500
C	-2.64395100	3.06708200	0.60120700
H	-2.81501700	2.65156000	1.59451100
H	-3.44280100	2.66323600	-0.03022700
C	-2.80440100	4.60058000	0.62352700

H	-2.76282900	4.96691200	-0.41166900
H	-3.81927500	4.84719800	0.97189200
C	-1.31820300	2.61495700	0.03822700
H	-1.31957000	2.36708800	-1.02185100
C	-0.14005000	2.49729500	0.66650700
H	0.69166200	2.14555600	0.06168000
C	-1.80584400	5.39967200	1.42284200
H	-1.79408800	6.45942400	1.16338100
C	-0.94951800	5.01062800	2.37648800
H	-0.29921100	5.78168400	2.79055700
H	1.22339600	3.22998900	2.10579300
O	-0.87147500	0.54776100	-2.70099400
H	-1.26571900	-0.15944900	-3.23284900
C	3.11284100	-2.21126900	0.32705500
C	4.07746300	-0.99971300	0.40925200
C	3.91788100	-0.36130500	-0.99415400
H	2.81299800	-2.56875300	1.31312700
H	3.63794700	-3.02301400	-0.18131600
H	4.48239900	-0.97512700	-1.70739600
H	4.30110200	0.65540200	-1.04142100
C	3.66732500	-0.00435200	1.50137400
O	3.55888800	1.19630100	1.35363300
O	3.45723500	-0.62686400	2.67030400
C	5.53082700	-1.36523700	0.68994600
O	6.25207700	-0.76967200	1.46659300
O	5.94081400	-2.39844300	-0.06208300
C	3.13855100	0.22440700	3.78672600
H	2.20620100	0.76480900	3.60629500
H	3.02927300	-0.44171500	4.64238300
H	3.94469100	0.94071500	3.96283000
C	7.32459500	-2.77334600	0.08731300
H	7.47754900	-3.60841400	-0.59609400
H	7.97848100	-1.93926300	-0.17833200
H	7.52897200	-3.08152000	1.11556100
C	0.72326200	-1.24885400	0.33298500
C	1.61443600	0.37351100	-1.90117100
C	2.43322400	-0.49349100	-1.27142600
C	1.90652400	-1.72661200	-0.52839000
H	1.05338900	-0.50585300	1.06731500
H	0.25503200	-2.08521000	0.86205500
C	2.07850300	1.68629500	-2.42207400
C	1.81998700	2.05490400	-3.75562200
C	2.72295900	2.62627000	-1.59317500
C	2.20855700	3.30076900	-4.24902500

H	1.30862100	1.35354500	-4.40849500
C	3.10551900	3.87414200	-2.08506300
H	2.92268000	2.36636600	-0.55905600
C	2.85285900	4.21847700	-3.41559000
H	2.00358000	3.55723300	-5.28513600
H	3.60048700	4.58136600	-1.42443900
H	3.15016400	5.19149500	-3.79655800
C	1.46687900	-2.83700200	-1.49778000
H	2.29676900	-3.14501600	-2.14346200
H	1.11696600	-3.71644600	-0.94664900
H	0.64594700	-2.49285200	-2.13380600
Ni	-0.34508400	-0.30098900	-0.95632300
P	-2.22168700	-1.10500600	-0.15650700
C	-3.68990200	-0.83420200	-1.21936800
C	-3.80892900	0.39024400	-1.89535700
C	-4.71748800	-1.78378800	-1.32782900
C	-4.94733600	0.66521700	-2.65410300
H	-3.00241400	1.11022800	-1.84056600
C	-5.85062500	-1.50629200	-2.09389400
H	-4.63869500	-2.73306100	-0.80944900
C	-5.96893300	-0.28168400	-2.75586700
H	-5.03060900	1.61640300	-3.17176300
H	-6.64169500	-2.24664700	-2.17021500
C	-2.73360900	-0.43370500	1.47227300
C	-4.07643300	-0.15800700	1.76723200
C	-1.75348700	-0.18867000	2.44553900
C	-4.43086000	0.35301700	3.01689100
H	-4.84451000	-0.33229000	1.02241000
C	-2.11260700	0.30935600	3.69728500
H	-0.71298400	-0.38298600	2.22169300
C	-3.45187100	0.58525100	3.98486400
H	-5.47299400	0.56957700	3.23235200
H	-1.34487500	0.49111200	4.44327200
C	-2.18792900	-2.92205800	0.06923200
C	-1.90602900	-3.71139000	-1.05670200
C	-2.39053200	-3.53836100	1.30903000
C	-1.83193700	-5.09762100	-0.94342800
H	-1.74391200	-3.23695600	-2.01996300
C	-2.30786300	-4.92918300	1.42146800
H	-2.60957900	-2.93855900	2.18561700
C	-2.02878300	-5.70939300	0.29888600
H	-1.61478200	-5.69961900	-1.82082100
H	-2.46337700	-5.40034700	2.38757200
H	-3.73004000	0.98239100	4.95658900

H	-1.96482400	-6.78979600	0.38877600
H	-6.85274500	-0.06765400	-3.34973300

II-IM4

H	1.05449400	0.21515700	-3.23549700
C	0.81135800	1.36424100	3.27125500
C	1.36864900	2.61741300	3.98239400
H	-0.07661900	1.01773800	3.82321500
H	0.58772200	3.37345200	4.07856900
H	1.63295200	2.32528000	5.00566900
C	0.15049500	4.02287500	1.54490800
H	-0.31016100	4.10056900	2.53141100
H	-0.50271600	4.58163300	0.86521000
C	1.52618500	4.72488600	1.53685200
H	1.85482400	4.81424600	0.49455400
H	1.39887600	5.75986700	1.89019200
C	0.20381300	2.58745300	1.07950400
H	0.00114500	2.43577700	0.02111800
C	0.47114300	1.49535000	1.80779700
H	0.44449600	0.54467900	1.27515900
C	2.64823000	4.07131400	2.30554300
H	3.64257600	4.37014300	1.97037900
C	2.59504100	3.19224600	3.31488200
H	3.54708900	2.82420000	3.69846400
H	1.54056900	0.55175300	3.35851200
O	-0.99508400	1.67961500	-2.00054500
H	-1.85812400	1.61739700	-2.43167700
C	2.27743900	-2.91205400	-1.04179100
C	3.00913900	-2.11611200	0.07502200
C	2.85763400	-0.61572400	-0.33402500
H	1.85255700	-3.84430000	-0.66873500
H	2.99640100	-3.15102000	-1.83042400
H	3.81853000	-0.17533200	-0.61246800
H	2.48522200	-0.05225200	0.52344400
C	2.41497800	-2.36780300	1.46736700
O	2.20542500	-1.50965400	2.30066600
O	2.18052500	-3.66968900	1.67193200
C	4.48752600	-2.48631000	0.18806500
O	5.04684800	-2.79982100	1.22032800
O	5.11090900	-2.38876000	-0.99647500
C	1.69181900	-4.01964800	2.98092800
H	0.73107000	-3.53646700	3.16949600
H	1.57533900	-5.10332600	2.96973300
H	2.41062200	-3.72105600	3.74779100

C	6.52471000	-2.67148100	-0.98835400
H	6.85341800	-2.54426300	-2.01957600
H	7.05054700	-1.97370500	-0.33218500
H	6.70850500	-3.69510500	-0.65323600
C	-0.01634200	-1.76196900	-0.69518000
C	1.68406500	0.42557900	-2.37530900
C	1.90727100	-0.59140300	-1.51036000
C	1.21061600	-1.94998700	-1.60103600
H	0.23726500	-1.77068400	0.36896000
H	-0.76861700	-2.54029700	-0.86807900
C	2.29862000	1.75961600	-2.40115400
C	2.31403600	2.44891500	-3.62907100
C	2.89178900	2.38200800	-1.28721300
C	2.92438600	3.69466700	-3.75251200
H	1.84559900	1.98849100	-4.49507700
C	3.50978000	3.62614800	-1.41373800
H	2.84320700	1.91896800	-0.31131700
C	3.53472700	4.28712900	-2.64371000
H	2.92491300	4.20274400	-4.71276100
H	3.96609100	4.08323200	-0.54087700
H	4.01559300	5.25672000	-2.73517900
C	0.77655100	-2.36318000	-3.00870600
H	1.62090400	-2.36403000	-3.70628000
H	0.34951500	-3.37163300	-2.98321600
H	0.00550500	-1.69210000	-3.40112100
Ni	-0.59877600	0.03204700	-1.19871100
P	-2.50762700	-0.24064600	-0.23219200
C	-3.23676000	1.19081500	0.65752600
C	-2.94893300	2.49059400	0.21540000
C	-4.10442500	1.00626100	1.74576900
C	-3.53051700	3.58821400	0.85066600
H	-2.25233600	2.61241200	-0.61055100
C	-4.67728100	2.10968500	2.38031100
H	-4.33146700	0.00797600	2.10252700
C	-4.39166300	3.40193300	1.93461900
H	-3.30015300	4.59182800	0.50492500
H	-5.34508300	1.95732900	3.22325000
C	-2.58830500	-1.58385600	1.00925800
C	-1.89963500	-1.40939700	2.22049400
C	-3.24949000	-2.79269500	0.76302100
C	-1.89174800	-2.42253400	3.17697500
H	-1.37827500	-0.47869700	2.41606300
C	-3.22923400	-3.81147400	1.71954500
H	-3.78092600	-2.94285400	-0.17053600

C	-2.55482800	-3.62852600	2.92716500
H	-1.36717300	-2.27028300	4.11561800
H	-3.74581700	-4.74563600	1.51921500
C	-3.76514700	-0.68986800	-1.48834500
C	-3.33293400	-1.26130800	-2.69429800
C	-5.13771900	-0.50115600	-1.26872500
C	-4.25991400	-1.64806600	-3.66314800
H	-2.27012900	-1.39975900	-2.86692400
C	-6.06149200	-0.88471200	-2.24067900
H	-5.48392700	-0.05210500	-0.34386600
C	-5.62490100	-1.45955900	-3.43745800
H	-3.91541800	-2.09065600	-4.59317300
H	-7.12230200	-0.73262900	-2.06441300
H	-2.54449600	-4.41955300	3.67125300
H	-6.34688800	-1.75530900	-4.19292800
H	-4.83613900	4.25917900	2.43217400

II-TS3

C	-0.06435500	-4.23578100	2.47042200
C	-1.54526300	-3.80293600	2.44251900
H	0.20223800	-4.67280200	1.49711800
H	-1.72494700	-3.12792000	1.60722600
H	-2.14417000	-4.69587200	2.23101300
C	-0.30609800	-0.99864200	2.33043600
H	-0.82313600	-1.43215300	1.47476600
H	0.07327300	-0.03315100	1.98146500
C	-1.29775500	-0.72501400	3.47849200
H	-0.77424600	-0.15499500	4.25847700
H	-2.08423400	-0.04866000	3.11270800
C	0.87028400	-1.84453200	2.75286800
H	1.74405100	-1.28468800	3.07966400
C	0.96003900	-3.18271400	2.80661500
H	1.91444800	-3.58707700	3.14567200
C	-1.93979000	-1.91749700	4.14282500
H	-2.37980900	-1.68536900	5.11348500
C	-2.03918300	-3.18939200	3.73191900
H	-2.52990100	-3.88345400	4.41458000
H	0.04988700	-5.04804100	3.20056500
H	-2.85413000	-1.07940400	-2.37639800
C	0.11095600	0.90253000	-1.18419600
C	-3.04637700	-0.70845100	-1.37505400
C	-2.35064800	0.35980100	-0.96150300
C	-1.30712100	1.10270300	-1.78390000
C	-2.61497500	1.17826100	0.27275400

C	-2.66920000	2.61755700	-0.30533600
C	-1.69735400	2.60511100	-1.52114700
H	0.08839400	1.36591500	-0.19379700
H	0.78946200	1.53266000	-1.77785700
H	-3.53027300	0.91338500	0.80023600
H	-1.79314000	1.12693600	0.99214100
H	-0.80946400	3.20797100	-1.31932700
H	-2.20597200	3.03465300	-2.38590800
C	-4.10729300	2.87672200	-0.77205900
O	-4.49241000	2.89254900	-1.92133300
O	-4.91949200	3.04177300	0.28778800
C	-2.31637900	3.66760900	0.73852300
O	-1.99048200	3.44566100	1.88675800
O	-2.42096500	4.90051800	0.21259800
C	-6.31848500	3.21713300	-0.01005700
H	-6.70573100	2.34679600	-0.54521600
H	-6.81373900	3.31884300	0.95559400
H	-6.47302900	4.11521800	-0.61303400
C	-2.17755700	6.00025100	1.11099600
H	-2.85623800	5.95144500	1.96616200
H	-1.14411100	5.98938400	1.46240400
H	-2.36684900	6.90155100	0.52800800
C	-4.06669500	-1.45760800	-0.62737800
C	-5.12004200	-2.07096700	-1.33181200
C	-4.00834300	-1.64664300	0.76587400
C	-6.09559600	-2.81237200	-0.66780300
H	-5.16553500	-1.95852800	-2.41185500
C	-4.98317200	-2.38995600	1.43169100
H	-3.17406700	-1.24306300	1.32625200
C	-6.03487900	-2.97166700	0.72027200
H	-6.90183000	-3.27150000	-1.23334700
H	-4.90280600	-2.52978100	2.50578600
H	-6.79062300	-3.55518900	1.23806300
C	-1.33747600	0.80495000	-3.28125100
H	-2.33031600	0.99391500	-3.70317300
H	-0.61997300	1.44928300	-3.80251300
H	-1.06599500	-0.22938300	-3.49035800
Ni	1.13529900	-0.69173600	-0.71571500
P	2.79265200	0.68139400	0.05691500
C	3.70489400	0.10871200	1.54511400
C	3.60435100	0.75701900	2.78406000
C	4.47403700	-1.06482500	1.45069700
C	4.23411500	0.22756800	3.91253600
H	3.04007900	1.67640900	2.87923400

C	5.10121600	-1.58841500	2.57989300
H	4.56896900	-1.57233500	0.49995000
C	4.97615400	-0.95017700	3.81663900
H	4.14407700	0.74190300	4.86485400
H	5.68763800	-2.49830100	2.49151100
C	2.43396800	2.45139200	0.37305500
C	3.05199100	3.47831600	-0.35344400
C	1.45907700	2.78590400	1.32856300
C	2.71642800	4.81254200	-0.11371300
H	3.79418700	3.24320000	-1.10717100
C	1.13835600	4.11912500	1.57817500
H	0.94408800	2.00466600	1.87760300
C	1.76563200	5.13645800	0.85503000
H	3.20290100	5.59751800	-0.68520800
H	0.37873500	4.35284800	2.31493200
C	4.06396500	0.70002700	-1.25814300
C	5.39133300	1.07410600	-0.99536900
C	3.68478500	0.37207200	-2.56652400
C	6.32012300	1.13133900	-2.03362100
H	5.69413900	1.32436900	0.01623300
C	4.61617700	0.43403900	-3.60412700
H	2.66590400	0.05662600	-2.76350300
C	5.93289500	0.81419700	-3.33924100
H	7.34515400	1.42298900	-1.82442800
H	4.31477500	0.17485500	-4.61483100
H	1.50896700	6.17522400	1.04108900
H	6.65935800	0.85806900	-4.14560400
H	5.46074800	-1.36392900	4.69609700
C	0.27031100	-2.40887700	-1.84028900
C	-0.85242200	-3.02057100	-1.23820100
C	-1.88558600	-3.58679800	-1.98309300
C	-1.85661500	-3.50214100	-3.37820900
C	-0.79234400	-2.85381500	-4.01317900
C	0.24979800	-2.32371800	-3.24936200
H	-0.88019500	-3.11615200	-0.15863900
H	-2.71669900	-4.07518500	-1.48371600
H	-2.65639400	-3.94262200	-3.96779100
H	-0.76868600	-2.78258500	-5.09775100
H	1.10585900	-1.88385100	-3.75433700
O	2.25559900	-2.16535200	-0.03901300
H	1.85144400	-2.47006800	0.79447800
B	1.91873100	-3.03526100	-1.16308900
O	1.64705100	-4.36604500	-0.70278000
O	2.90262900	-2.85435600	-2.17771700

H	0.99080000	-4.80136300	-1.25711700
H	2.84014400	-3.57480500	-2.81491800

II-IM5

C	-0.86757600	-3.73634000	2.95206100
C	-2.30271900	-3.23917600	2.69215400
H	-0.55528400	-4.38720900	2.12452400
H	-2.34847100	-2.69775300	1.74833100
H	-2.93338200	-4.12411200	2.55078800
C	-0.88196800	-0.52440100	2.33413700
H	-1.38539900	-1.02320700	1.50686000
H	-0.42619000	0.37342700	1.90953400
C	-1.91131500	-0.05930000	3.38056400
H	-1.38600600	0.52904900	4.14593400
H	-2.59735000	0.65488600	2.90325800
C	0.21225700	-1.38325400	2.91556200
H	1.10887900	-0.84152200	3.20629000
C	0.20836500	-2.70368300	3.16342200
H	1.12127600	-3.11197100	3.59936000
C	-2.71897300	-1.11506800	4.09002900
H	-3.24503200	-0.73459000	4.96699600
C	-2.88502700	-2.41737000	3.81964600
H	-3.51070100	-2.97698100	4.51543500
H	-0.87548100	-4.38120000	3.84197100
H	-2.80803300	-1.02407400	-2.81987600
C	0.03319600	0.90568700	-1.42054400
C	-3.11487800	-0.60610300	-1.86483400
C	-2.47347900	0.48753500	-1.42423900
C	-1.31949100	1.17999800	-2.13258300
C	-2.81447800	1.28961600	-0.19618300
C	-2.44358400	2.76100500	-0.54693900
C	-1.67422200	2.68126400	-1.89779500
H	-0.02023400	1.36238800	-0.42361200
H	0.79628700	1.46967200	-1.97408900
H	-3.85953000	1.19253300	0.10199500
H	-2.20780100	0.98542400	0.65835200
H	-0.78671300	3.31838300	-1.90896000
H	-2.35062700	3.03732500	-2.67920700
C	-3.72932000	3.58235500	-0.68412400
O	-4.20653600	4.00372400	-1.71555600
O	-4.30054500	3.74741700	0.52383500
C	-1.61769800	3.40492600	0.56628100
O	-1.12335400	2.83003400	1.51679100
O	-1.50114100	4.72883000	0.36707000

C	-5.52654700	4.50336300	0.54587500
H	-6.29310700	4.00986400	-0.05635500
H	-5.83155800	4.53735700	1.59173700
H	-5.35955100	5.51415000	0.16536000
C	-0.89751800	5.47853100	1.44112400
H	-1.53019400	5.42690900	2.33110500
H	0.09517900	5.09542200	1.68168500
H	-0.83447100	6.50577500	1.08296400
C	-4.18854300	-1.35383500	-1.19739800
C	-5.07978000	-2.11238200	-1.98141600
C	-4.33936000	-1.40847900	0.20207800
C	-6.09885300	-2.86191400	-1.39778800
H	-4.96153700	-2.10790300	-3.06194200
C	-5.35705800	-2.16127900	0.78795900
H	-3.63163000	-0.89531500	0.84020900
C	-6.24697200	-2.88636600	-0.00737700
H	-6.77620500	-3.43288700	-2.02711400
H	-5.43774900	-2.19261100	1.87097600
H	-7.03691900	-3.47545500	0.44963200
C	-1.23440900	0.90510300	-3.63447800
H	-2.17215900	1.16732800	-4.13696700
H	-0.43248100	1.50644000	-4.07883000
H	-1.01636400	-0.14276600	-3.84022600
Ni	0.94173900	-0.68799900	-0.81419600
P	2.82498500	0.53315800	-0.02088400
C	3.17943200	0.44473500	1.78452100
C	2.82245300	1.48080600	2.65934800
C	3.69948500	-0.74545700	2.32291900
C	2.98044200	1.33072500	4.03853000
H	2.42442100	2.41130000	2.27193000
C	3.86640200	-0.88794400	3.70019400
H	3.97389800	-1.56094300	1.66469800
C	3.50260700	0.14773700	4.56436600
H	2.69771400	2.14418600	4.70040000
H	4.27611900	-1.81215900	4.09740700
C	3.01752200	2.30893500	-0.47020700
C	4.08605600	2.75619100	-1.26249800
C	2.01561600	3.22771100	-0.10937200
C	4.15774800	4.08792400	-1.67547800
H	4.86554300	2.06665000	-1.56335000
C	2.09137600	4.55799900	-0.52318700
H	1.17122000	2.90417300	0.48747100
C	3.16081300	4.99219100	-1.30882100
H	4.99384400	4.41452000	-2.28719000

H	1.30576600	5.25271300	-0.24759000
C	4.29520700	-0.24206600	-0.79360200
C	5.58316400	-0.15549800	-0.24230400
C	4.11662200	-0.89658900	-2.01997500
C	6.67036300	-0.72629300	-0.90334200
H	5.73490900	0.35823600	0.70125400
C	5.20725000	-1.45931600	-2.68489600
H	3.11938600	-0.97323200	-2.44204100
C	6.48361000	-1.37880700	-2.12591800
H	7.66302500	-0.65863400	-0.46761100
H	5.05637500	-1.96949300	-3.63181100
H	3.21207000	6.02643700	-1.63618900
H	7.33183000	-1.82320500	-2.63877000
H	3.62577900	0.03375700	5.63724700
C	-0.14054000	-1.95268400	-1.70890700
C	-0.98239400	-2.81639500	-0.98529700
C	-1.64879600	-3.88664400	-1.58924000
C	-1.48570600	-4.13089700	-2.95531600
C	-0.63532800	-3.30412700	-3.69605100
C	0.02412500	-2.23512500	-3.07736400
H	-1.12698300	-2.65623900	0.07795800
H	-2.30563800	-4.51862200	-0.99528700
H	-2.00859600	-4.95428100	-3.43516100
H	-0.48861400	-3.48965400	-4.75840900
H	0.68014200	-1.61275300	-3.68183500
O	1.80519400	-2.27482300	0.33254300
H	1.32560400	-2.24931700	1.18679000
B	1.96013300	-3.56708800	-0.14628300
O	1.47042600	-4.58426400	0.63105700
O	2.64810700	-3.70719900	-1.31426500
H	1.59346000	-5.46800700	0.26138400
H	2.70046900	-4.61519800	-1.63682500

II-IM6

C	0.02809900	-1.95042400	-1.82052700
C	-0.92685600	-2.97809800	-1.73484800
C	-1.06491700	-3.94368600	-2.73799600
C	-0.24569100	-3.90855700	-3.86979200
C	0.70035500	-2.88769800	-3.99004700
C	0.82225700	-1.92021100	-2.98548600
H	-1.59077500	-3.02973200	-0.88132700
H	-1.81555700	-4.72436900	-2.63361100
H	-0.35180000	-4.65731200	-4.65033400
H	1.33468400	-2.83462400	-4.87244100

H	1.54413200	-1.11856900	-3.12454100
C	1.67366500	-3.91603900	0.52181200
C	1.98396900	-4.96973500	1.60500700
H	0.83161200	-4.22587900	-0.09442100
H	2.18247500	-5.93222700	1.10973000
H	2.93145300	-4.69886800	2.09075500
C	-1.07165400	-2.62826300	1.71892000
H	-1.74805400	-2.19684500	0.97485600
H	-1.46191100	-2.28445900	2.68581100
C	-1.17077500	-4.16599900	1.67711900
H	-2.22375700	-4.42343200	1.83829600
H	-0.92132100	-4.53144800	0.68099900
C	0.29269900	-2.00871000	1.56657100
H	0.36514900	-1.01871400	2.01652400
C	1.44789100	-2.54449600	1.10164500
H	2.35408400	-1.96884600	1.26611500
C	-0.33785900	-4.84981200	2.73580800
H	-0.86958100	-5.08308500	3.65867500
C	0.96074000	-5.17605700	2.69453900
H	1.36501200	-5.67126800	3.57850000
H	2.53760700	-3.86417100	-0.14981100
H	-3.29313700	-1.49920200	-1.84897800
C	-0.31408200	0.70610700	-1.36924800
C	-3.40633900	-0.97926600	-0.90252900
C	-2.71034800	0.16067700	-0.74943200
C	-1.79956900	0.77069200	-1.80820700
C	-2.80270800	1.13744500	0.39445800
C	-2.63935600	2.54328500	-0.26561900
C	-2.24116900	2.26240000	-1.74370100
H	-0.16902000	1.42039600	-0.55046900
H	0.31289300	1.04507200	-2.20143700
H	-3.73961800	1.05784600	0.94743400
H	-1.99110100	0.99894800	1.11644600
H	-1.46067800	2.93944400	-2.09739700
H	-3.12935600	2.41906700	-2.36120000
C	-3.98129900	3.27711200	-0.18345200
O	-4.77908800	3.40775600	-1.08663600
O	-4.19452700	3.71850600	1.06950900
C	-1.60365100	3.39591300	0.46636500
O	-0.90407500	3.03761600	1.39314900
O	-1.56187500	4.63125000	-0.06051300
C	-5.45598000	4.37546000	1.30249600
H	-6.28576400	3.69649100	1.09181100
H	-5.45169000	4.65275300	2.35651400

H	-5.54639400	5.26603600	0.67567400
C	-0.71731200	5.58506200	0.61462200
H	-1.06930300	5.73960000	1.63780400
H	0.32037700	5.24882400	0.63571000
H	-0.80416900	6.50824300	0.04217900
C	-4.33528900	-1.63974900	0.02444900
C	-5.27536900	-2.54232200	-0.51331500
C	-4.32627500	-1.46377700	1.42305300
C	-6.18500900	-3.21431000	0.29959400
H	-5.28621700	-2.70786800	-1.58750300
C	-5.23542600	-2.13898600	2.23765000
H	-3.58051600	-0.82937600	1.88429200
C	-6.17337800	-3.01234900	1.68267200
H	-6.90118100	-3.89973000	-0.14513900
H	-5.20138800	-1.98910500	3.31329800
H	-6.87792800	-3.53841500	2.32022000
C	-2.00751500	0.22766600	-3.22232800
H	-3.05149100	0.33887000	-3.53518900
H	-1.38141600	0.78393600	-3.92899700
H	-1.73192200	-0.82435700	-3.29788900
Ni	0.56953200	-0.75466900	-0.47615300
P	2.45481600	0.63084800	0.21424500
C	2.79064000	1.40716800	1.85330600
C	3.38143100	2.67117900	2.00031900
C	2.47162300	0.67208300	3.00640800
C	3.63553000	3.19107100	3.27076000
H	3.64623800	3.25180100	1.12437000
C	2.73296300	1.18941600	4.27501100
H	2.02777400	-0.31295400	2.91668900
C	3.31212700	2.45313900	4.41093000
H	4.09241400	4.17188400	3.36695100
H	2.48144500	0.60611100	5.15596700
C	2.66770100	2.02104400	-0.96791300
C	3.53330400	1.93638000	-2.06686800
C	1.85402100	3.15878000	-0.83107400
C	3.58793700	2.97035900	-3.00468700
H	4.16954300	1.06746900	-2.19493100
C	1.91410400	4.19154400	-1.76538300
H	1.18107800	3.23786000	0.01542200
C	2.77986700	4.09903400	-2.85844000
H	4.26765800	2.89209100	-3.84842800
H	1.28090100	5.06528900	-1.64221200
C	3.97697500	-0.36841200	-0.06217100
C	5.19018100	-0.09362600	0.58454400

C	3.91562800	-1.43265100	-0.97539700
C	6.32162400	-0.86586000	0.31628500
H	5.25310100	0.72319500	1.29565500
C	5.04986700	-2.19807900	-1.24895400
H	2.97626100	-1.66387300	-1.46634400
C	6.25463200	-1.91845600	-0.59981800
H	7.25572300	-0.64546600	0.82505400
H	4.98745200	-3.01664400	-1.96025800
H	2.82400900	4.90075600	-3.58977100
H	7.13685800	-2.51759000	-0.80579200
H	3.51046100	2.85911200	5.39852500

II-TS4

C	1.25162900	-5.29777000	0.06011500
C	2.48113800	-4.72804300	-0.67829400
H	1.48754200	-5.36395300	1.13353600
H	2.74461800	-3.75284700	-0.27094000
H	3.33103300	-5.38158400	-0.45228300
C	0.66839700	-2.29321700	-1.02159100
H	1.56834600	-2.28841000	-0.41106700
H	0.21086200	-1.30716600	-0.88260000
C	1.03986000	-2.44328600	-2.50727500
H	0.12705800	-2.34237200	-3.10667800
H	1.67042200	-1.59288800	-2.80559900
C	-0.31139200	-3.34018900	-0.55850500
H	-1.35679600	-3.04812100	-0.63153000
C	-0.06280300	-4.57807000	-0.11283000
H	-0.93027700	-5.17618100	0.17087000
C	1.72077900	-3.72247100	-2.92102600
H	1.71677700	-3.88546800	-4.00008700
C	2.31518200	-4.66667900	-2.17931800
H	2.71958500	-5.52375300	-2.71884700
H	1.10270700	-6.33819000	-0.26131600
H	3.20264400	-0.79920500	2.37535300
C	0.37372800	1.52101600	2.17387100
C	3.24233600	-0.40373900	1.36425200
C	2.61055700	0.76298300	1.14347000
C	1.91757100	1.57193800	2.24049600
C	2.64443900	1.57631200	-0.13100800
C	2.35710100	3.04795100	0.29920900
C	2.35359800	3.00875900	1.84841000
H	0.00109900	2.16287800	1.33285600
H	-0.03524400	1.99116800	3.06850300
H	3.61548800	1.48817600	-0.62579600

H	1.88743300	1.26307600	-0.85587400
H	1.71821700	3.78073100	2.28686400
H	3.37959200	3.18484000	2.18239200
C	3.46991000	3.96000300	-0.22543800
O	4.42998600	4.33658700	0.41198600
O	3.27019600	4.25399300	-1.52093300
C	1.03663000	3.54401600	-0.30602400
O	0.37727600	2.96401600	-1.14629200
O	0.69837600	4.73567000	0.20484100
C	4.28259600	5.06680000	-2.14931200
H	5.24388700	4.54760900	-2.14501400
H	3.94005700	5.22185500	-3.17213700
H	4.38090600	6.02327700	-1.63090100
C	-0.52935700	5.31090100	-0.29080000
H	-0.46689800	5.47438800	-1.36921200
H	-1.37447700	4.65524000	-0.06837200
H	-0.63645900	6.26075100	0.23263700
C	4.03574000	-1.23206800	0.44908300
C	4.89693600	-2.19307600	1.01807500
C	3.98259800	-1.15259900	-0.95704600
C	5.69055500	-3.01729500	0.22452300
H	4.94006500	-2.28210000	2.10052700
C	4.77402100	-1.98158600	-1.75094600
H	3.29432000	-0.47118500	-1.43800800
C	5.63571300	-2.91292200	-1.16803100
H	6.34771700	-3.74527900	0.69191400
H	4.70485900	-1.90891700	-2.83224000
H	6.24603800	-3.55994100	-1.79103900
C	2.38011400	1.22907700	3.65950200
H	3.47066200	1.27025300	3.73953900
H	1.95814200	1.94566800	4.37220900
H	2.04640900	0.23238900	3.95894800
Ni	-0.75617300	0.52813800	0.93213900
P	-2.45537300	0.09392600	-0.34687200
C	-2.18242600	-0.36763500	-2.10635200
C	-1.25532900	0.40841200	-2.82436200
C	-2.82962800	-1.42920600	-2.74944200
C	-1.00749700	0.14249400	-4.16969300
H	-0.73323900	1.22100300	-2.32608200
C	-2.56674000	-1.70273900	-4.09518900
H	-3.54082000	-2.04192000	-2.20635900
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H	-3.60607200	-3.87429700	2.36676500
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H	-5.99603100	-3.93296900	1.67173900
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C	0.02879000	-2.48741100	3.47222800
C	-0.92768400	-2.33279700	4.47895200
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H	-1.11310300	-3.13240400	5.19039800
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II-IM7

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H	3.75828000	-5.42501900	2.44717400
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C	-4.18531600	-1.28788400	-2.09792500
C	-3.90154200	-2.37926800	0.03748100
C	-4.54792000	-2.51026300	-2.67005200
H	-4.14891100	-0.39693400	-2.71549300
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H	-3.61878100	-2.32521800	1.08539000
C	-4.59549200	-3.66658200	-1.88802400
H	-4.79114800	-2.55850700	-3.72783100
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H	-8.23603600	2.77297900	1.84915900

H	-4.87349100	-4.61650500	-2.33549700
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C	0.18010700	0.56961100	2.22305700
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C	-0.61178000	-1.75821200	2.39916300
C	-1.41687600	-1.41314000	3.50202500
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C	-0.64787500	0.89994900	3.32792200
H	0.77063800	-1.04053400	0.89859700
H	-0.60051700	-2.77723100	2.02788400
H	-2.03073000	-2.16594600	3.98594400
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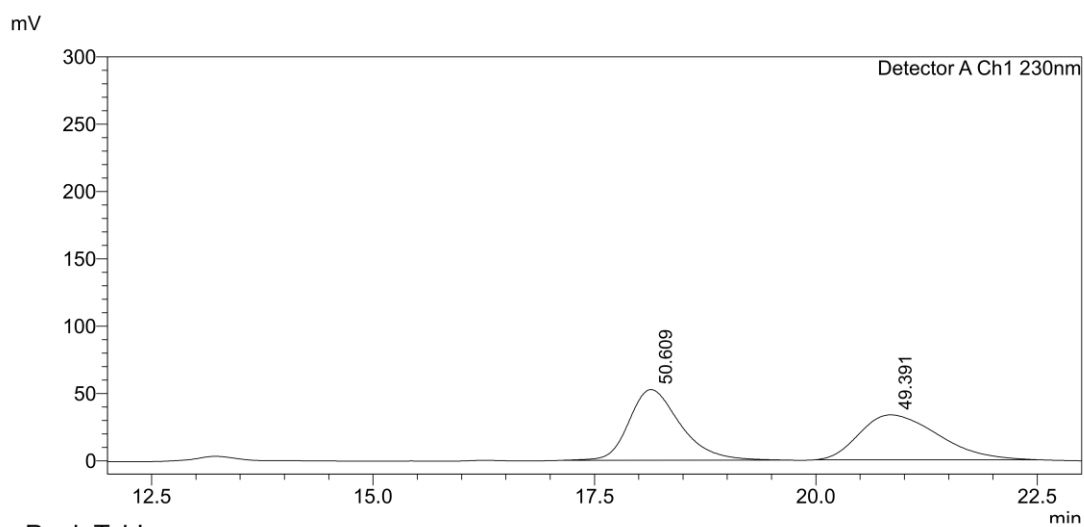
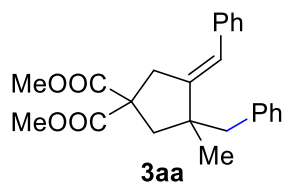
Ni⁰(cod)₂PPh₃

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H	-1.74066700	-3.50591100	1.78182400
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H	1.40259300	-2.65931600	0.28811700
C	0.41489500	-4.54187800	0.03299900
H	1.04566400	-4.73016000	-0.84636900
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C	-1.77907500	-2.09581200	-0.89871600
H	-2.21022300	-2.05832300	-1.89852700
C	-0.89529800	-5.26158000	-0.19086100
H	-0.80372600	-6.18377600	-0.76648800
C	-2.12436500	-4.92637800	0.22298700
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H	-3.76505200	-2.55691700	-0.28188100
Ni	-0.78253000	-0.33119500	-0.64042500
C	-2.19736500	2.04303000	0.94395000
C	-3.67142700	1.88225300	1.36958000
H	-1.57427700	1.45065400	1.62548500
H	-3.96156300	0.83142200	1.31582200
H	-3.73737600	2.15883900	2.42808600
C	-3.92680500	0.35204600	-1.28428300
H	-4.08066900	-0.11957500	-0.31702800
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C	-5.04591700	1.37746500	-1.55424000
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C	-2.54627700	0.95482400	-1.40660800
H	-2.17778200	1.00671900	-2.43284300
C	-1.84921400	1.71192400	-0.49567200
H	-1.02847400	2.29915500	-0.89566300
C	-5.16105700	2.55388400	-0.61921700
H	-5.80684500	3.34615900	-1.00115800
C	-4.61410500	2.76471700	0.58530600
H	-4.84292800	3.71897400	1.06046500
H	-1.90360600	3.08664600	1.11563500
P	1.18982300	0.46478700	-0.07426200
C	1.65997300	2.19361300	-0.53909100
C	1.15311100	3.26752700	0.21319000
C	2.40824800	2.47661900	-1.69061800
C	1.39699100	4.58574400	-0.17097700
H	0.57082600	3.07399000	1.10801300
C	2.64675200	3.79741600	-2.07786200
H	2.81717800	1.66762300	-2.28626500
C	2.14437200	4.85653600	-1.32009700
H	1.00231900	5.40116300	0.42875500
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H	2.33339600	5.88299300	-1.62047900
C	2.60933100	-0.50412000	-0.74463500
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H	-0.30941900	-0.69893100	2.07185200
C	2.65114800	1.14997000	3.75340800
H	3.22688300	1.71895700	1.76100600
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12. Chiral HPLC charts and NMR Spectra

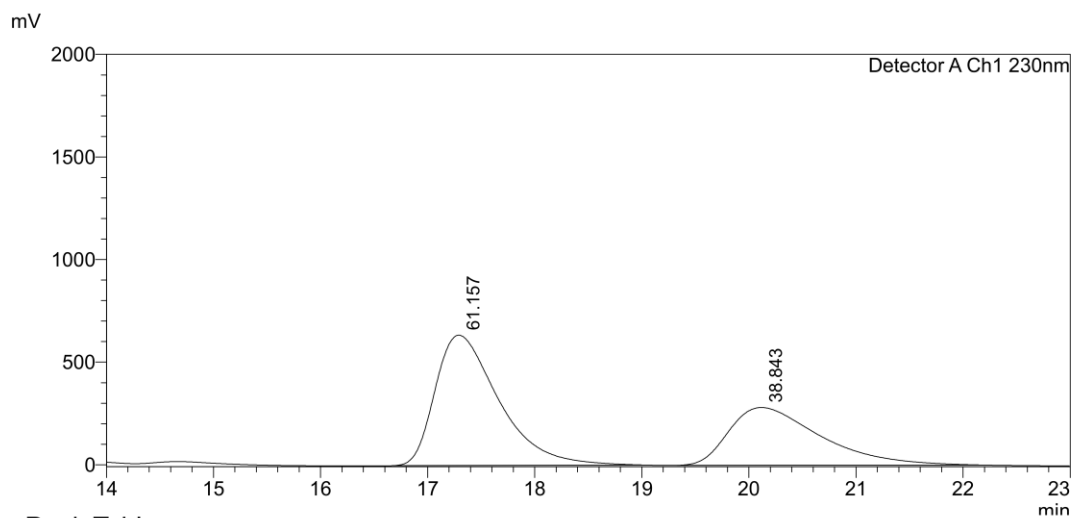


<Peak Table>

Detector A Ch1 230nm

Peak#	Ret. Time	Area	Height	Area%
1	18.138	2116795	52477	50.609
2	20.844	2065859	33385	49.391
总计		4182654	85862	100.000

Supplementary Figure 1. HPLC spectrum of 3aa-rac

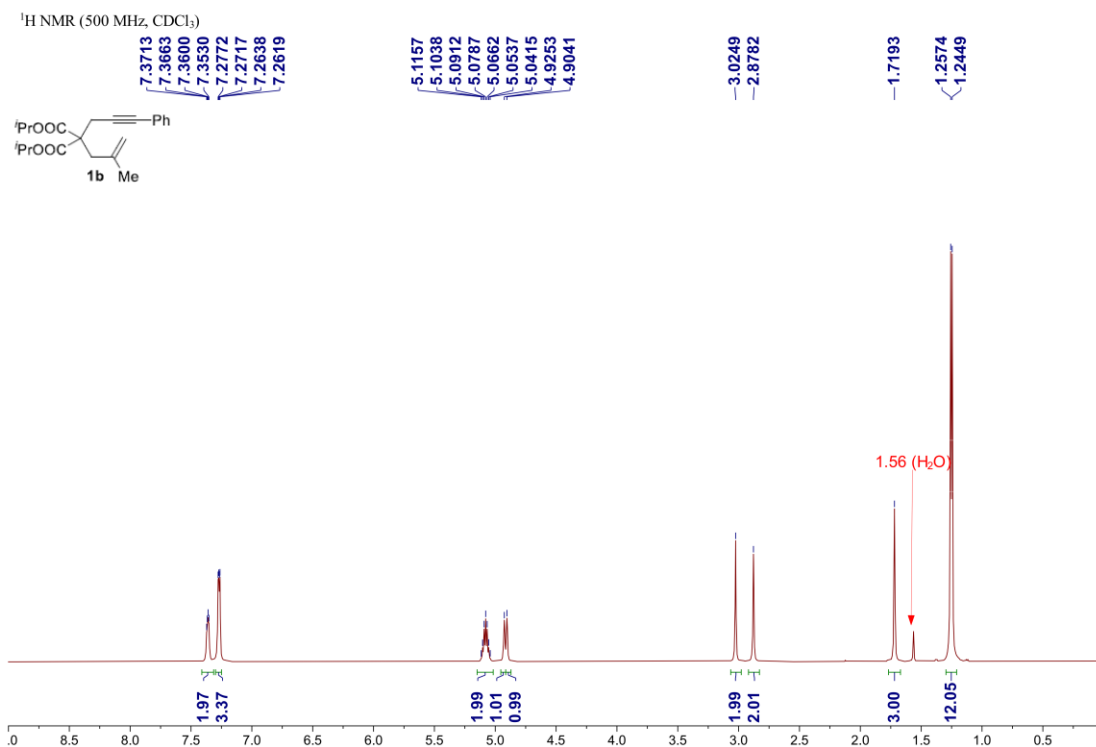


<Peak Table>

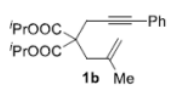
Detector A Ch1 230nm

Peak#	Ret. Time	Area	Height	Area%
1	17.291	26204556	634948	61.157
2	20.117	16643598	281129	38.843
总计		42848154	916077	100.000

Supplementary Figure 2. HPLC spectrum of 3aa



¹³C NMR (126 MHz, CDCl₃)



— 169.7978

— 140.2885

— 131.5721

— 128.1645

— 127.8342

— 123.4116

— 116.1146

— 84.9751

— 83.5457

— 77.2533

— 77.0000

— 76.7459

— 69.1063

— 56.5849

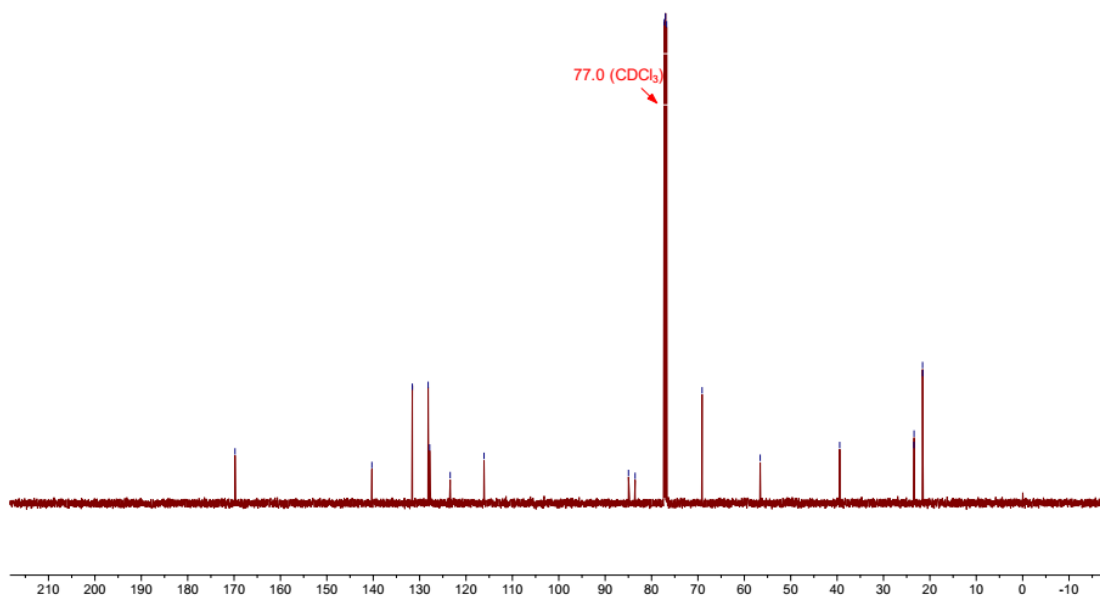
— 39.4433

— 23.4388

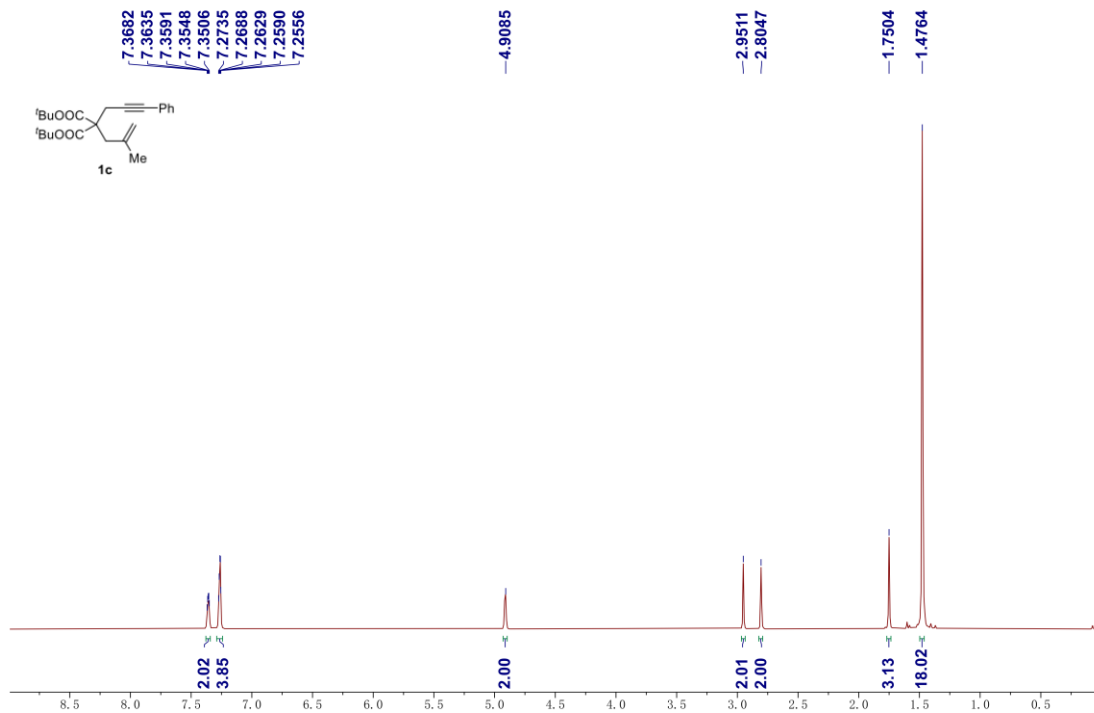
— 23.4121

— 21.5750

— 21.5413

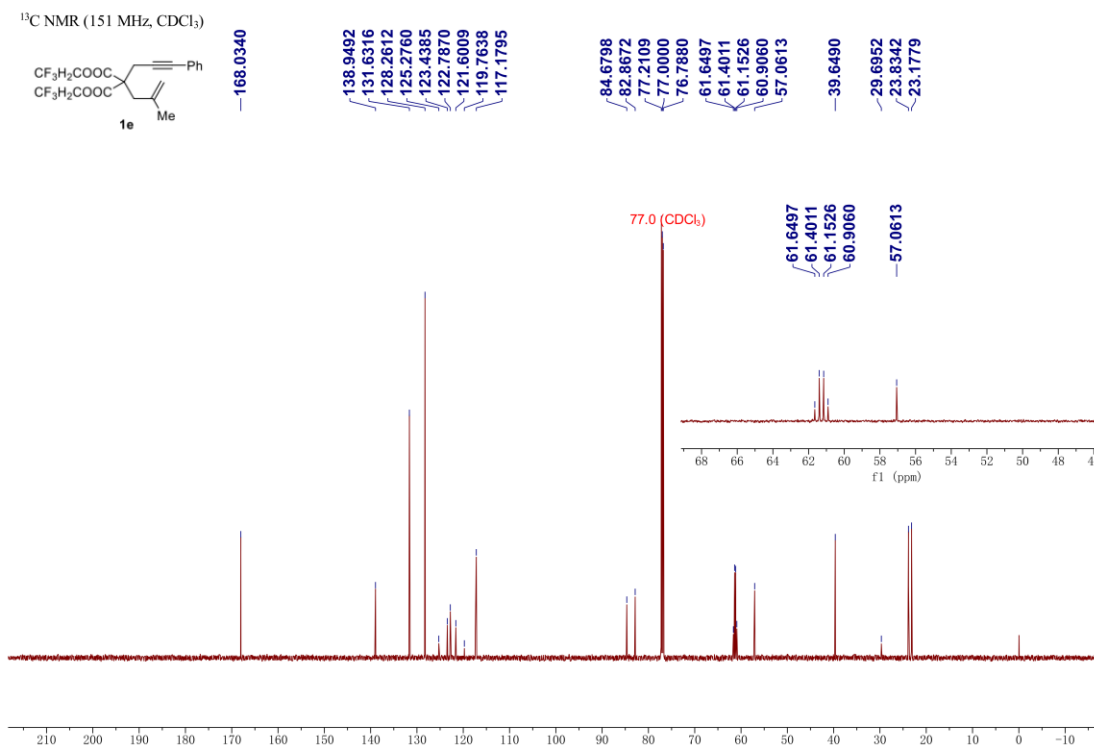
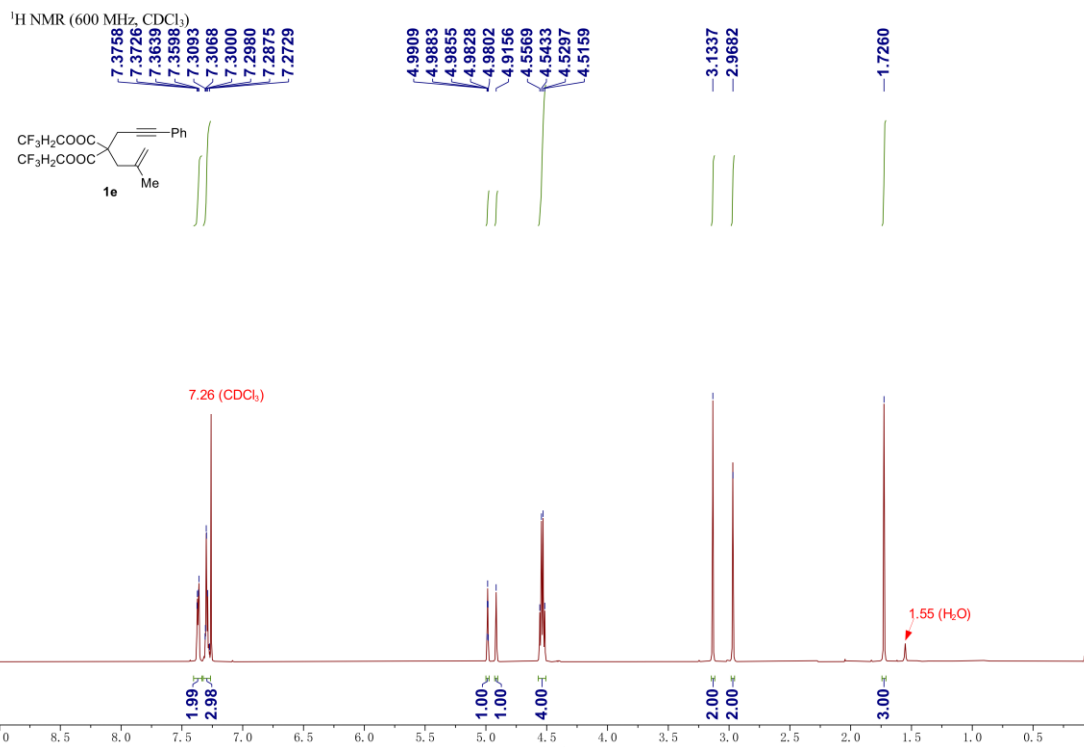


¹H NMR (600 MHz, CDCl₃)

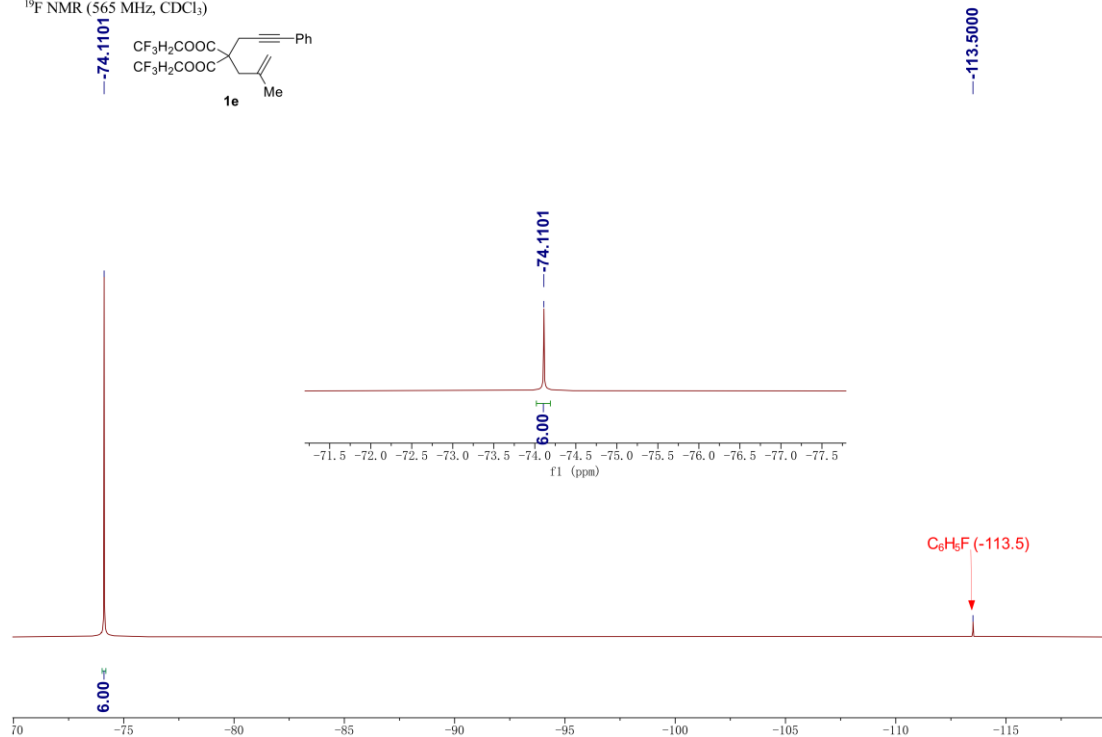
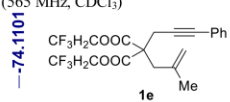


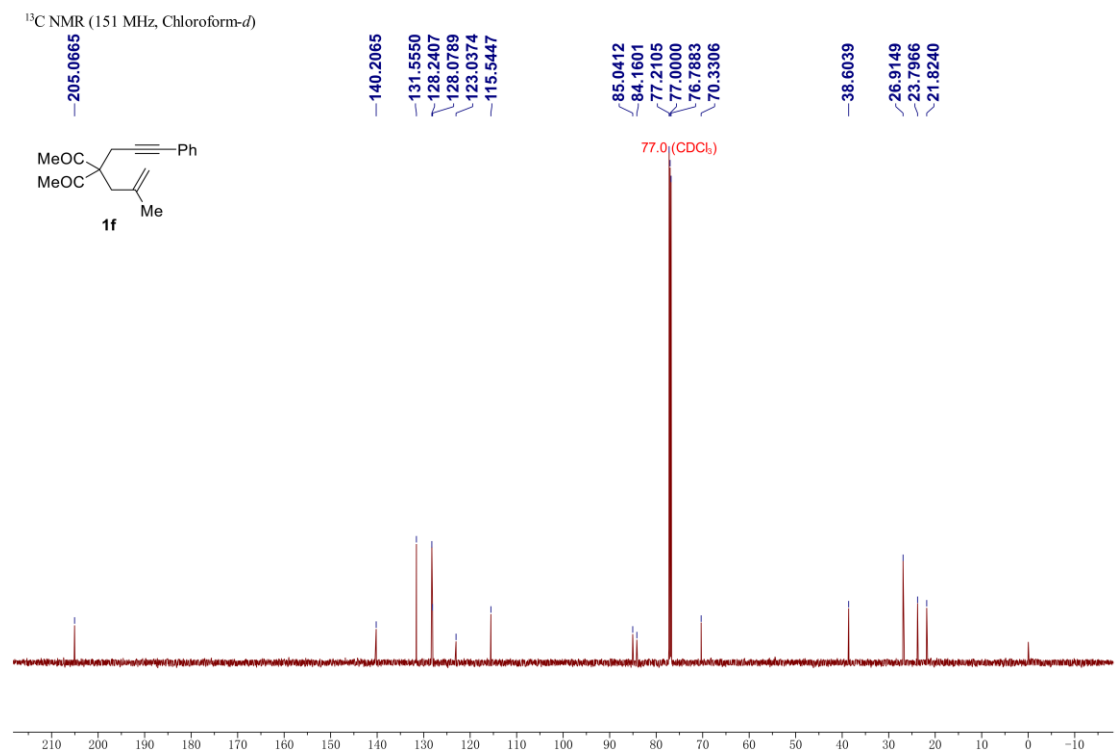
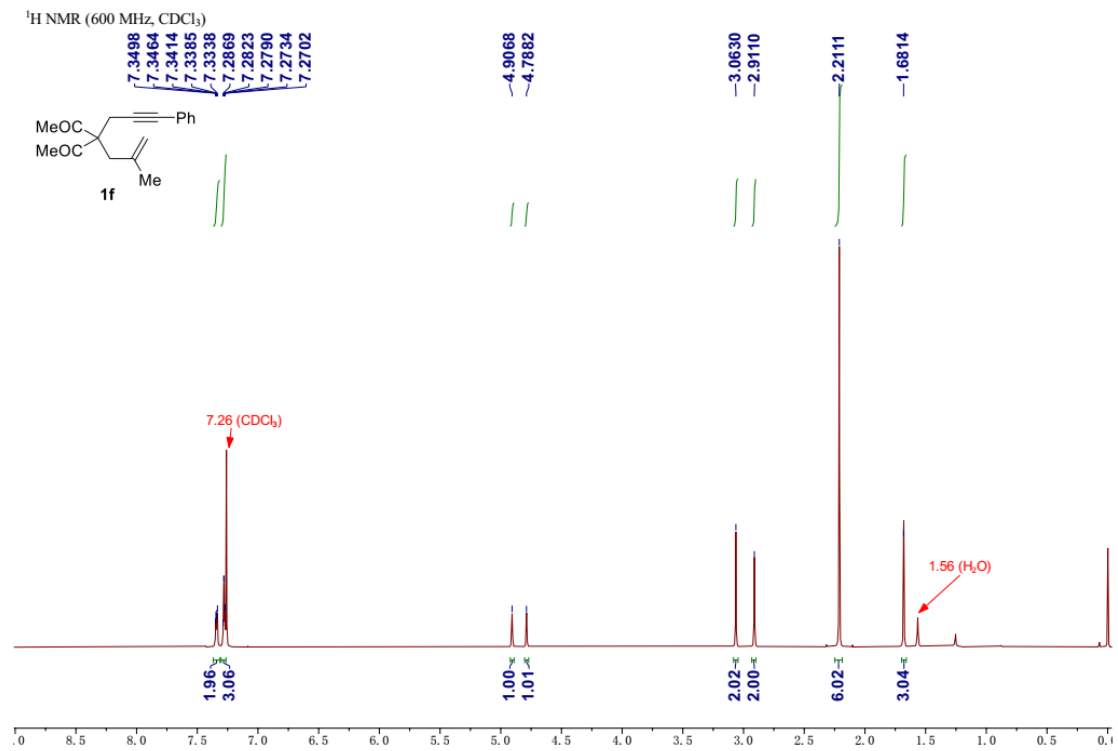
¹³C NMR (151 MHz, CDCl₃)

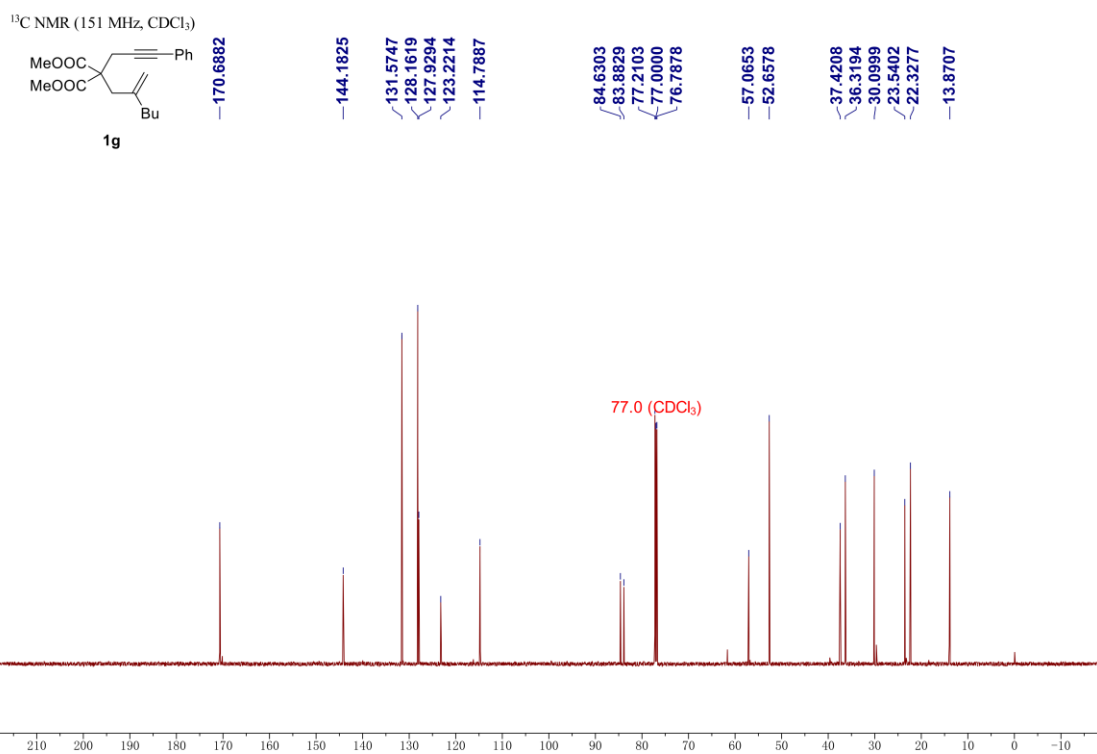
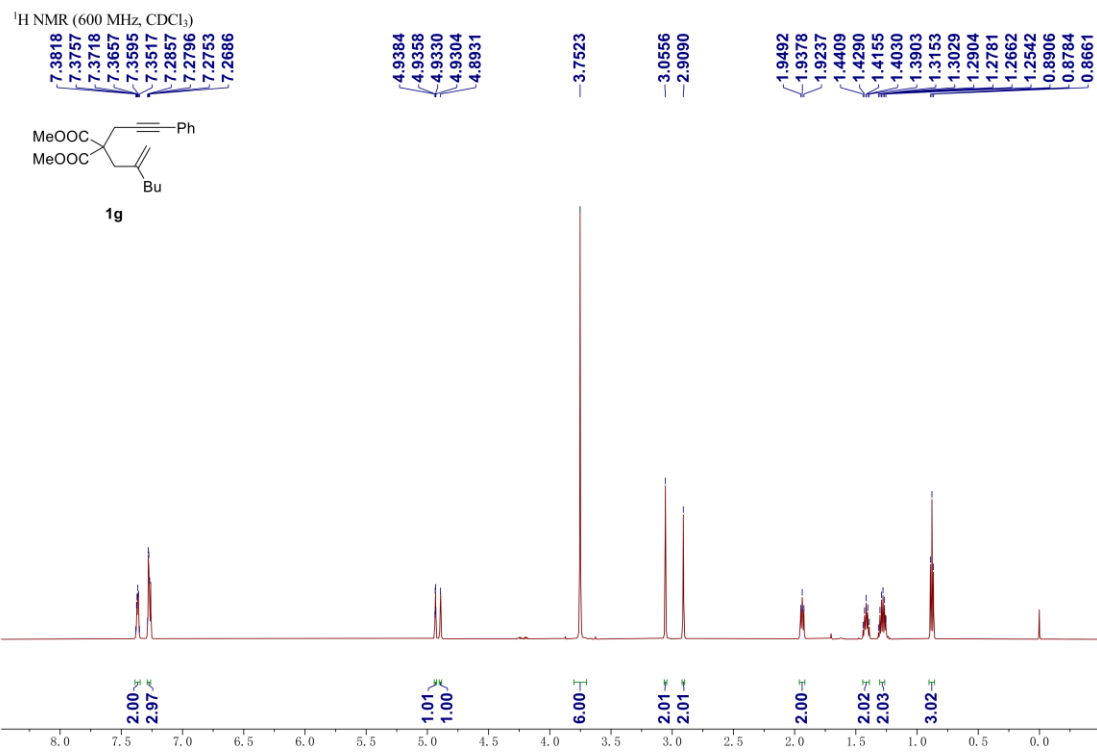




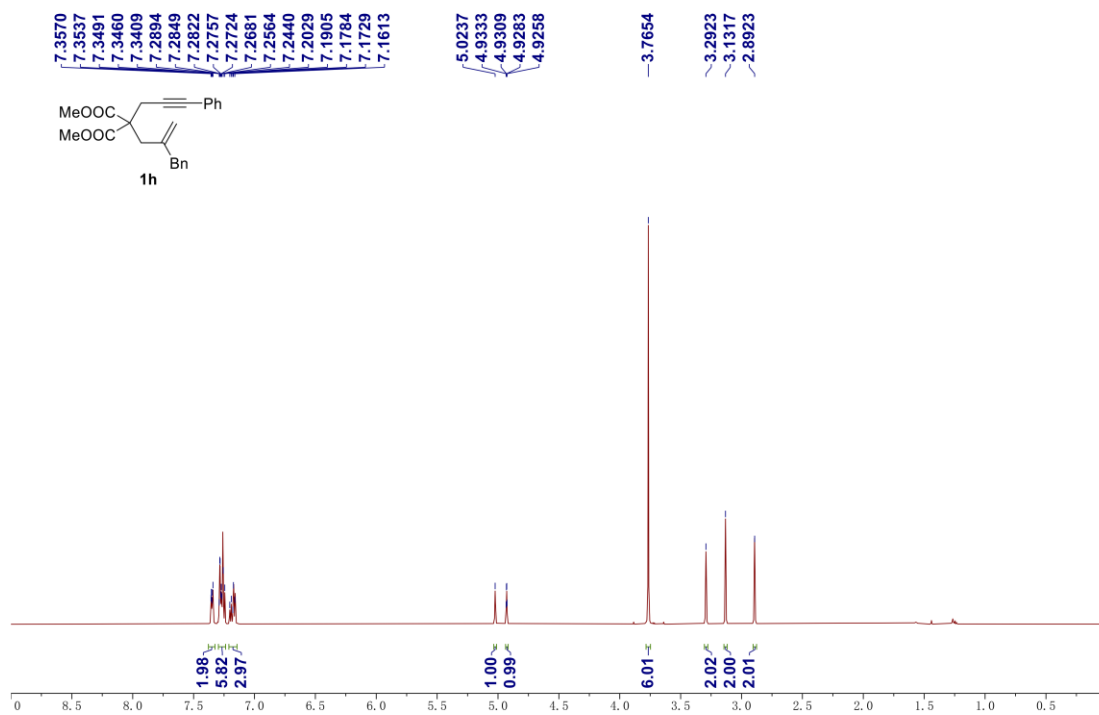
¹⁹F NMR (565 MHz, CDCl₃)



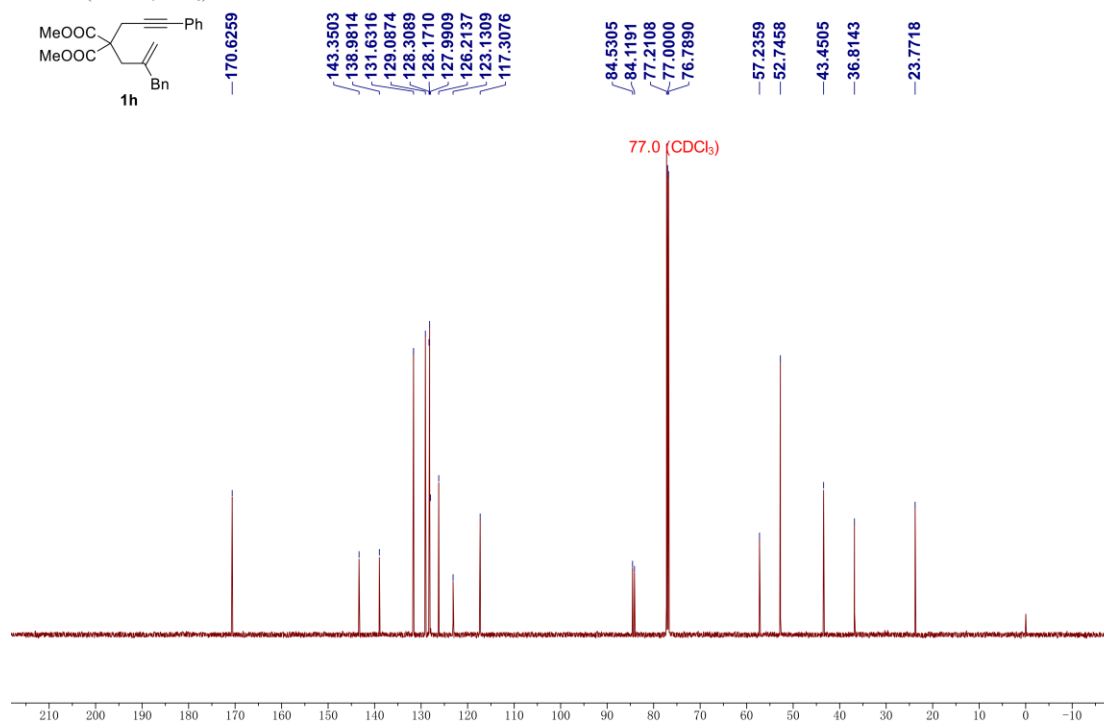


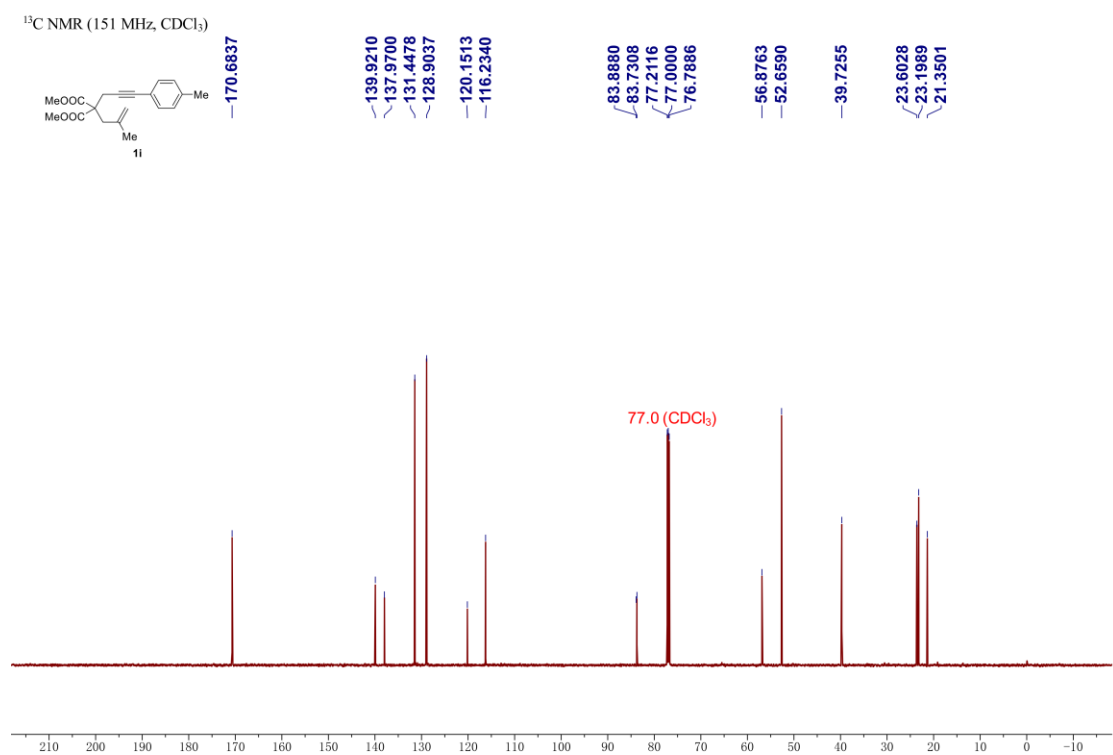
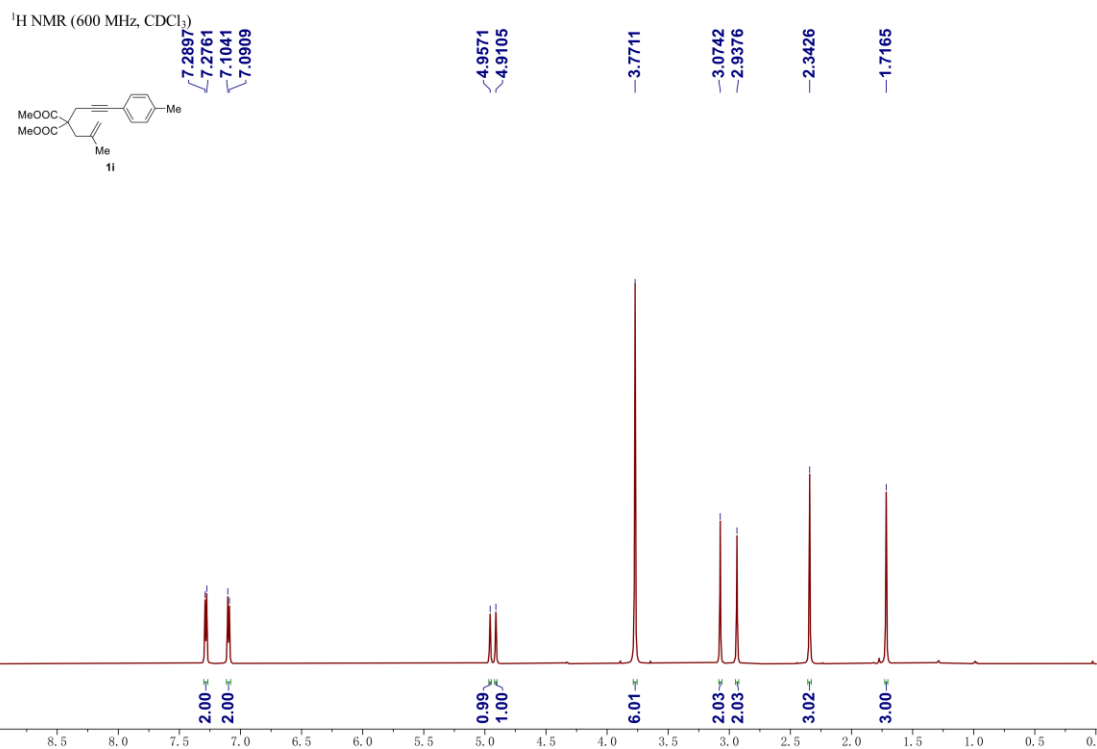


¹H NMR (600 MHz, CDCl₃)

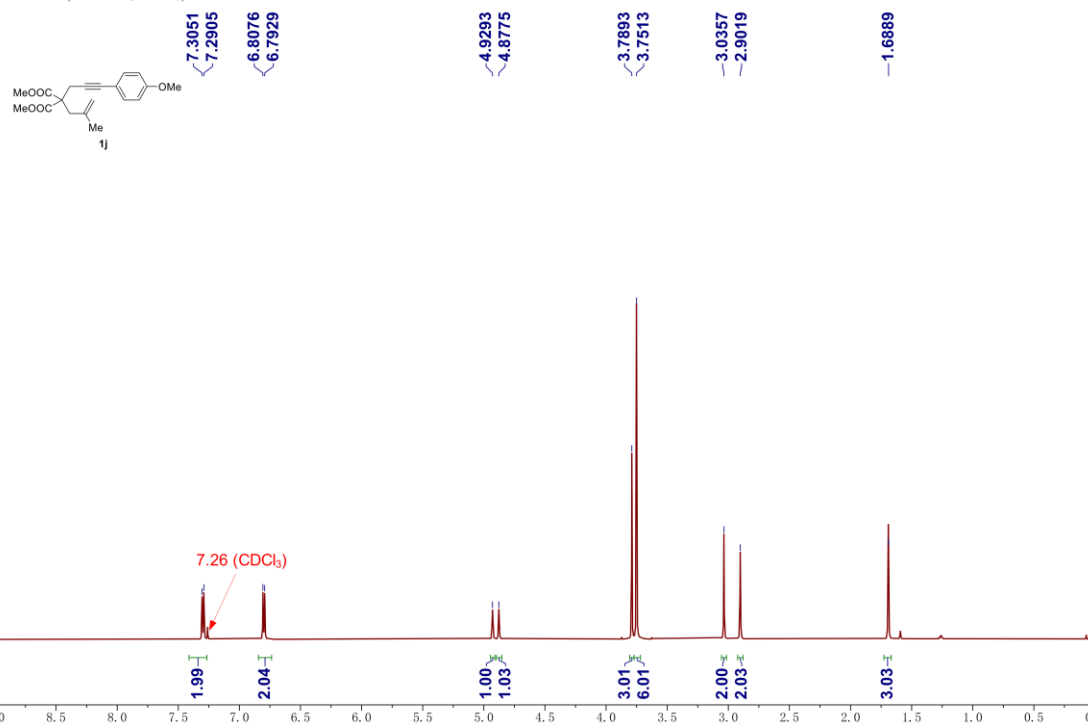


¹³C NMR (151 MHz, CDCl₃)

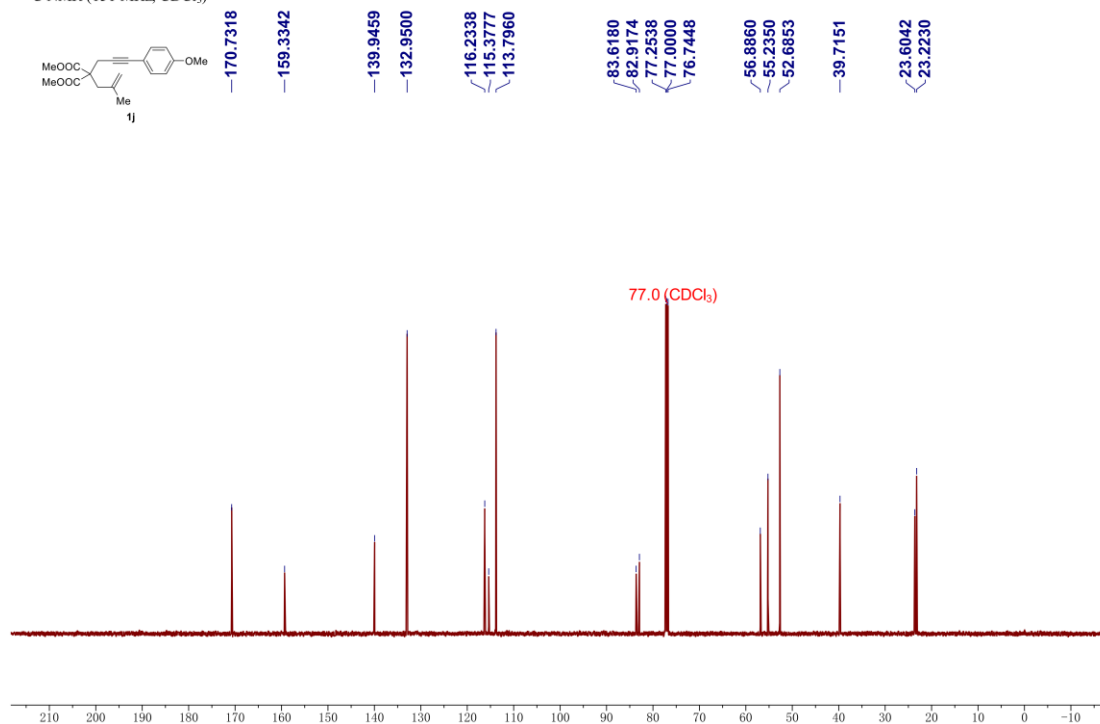




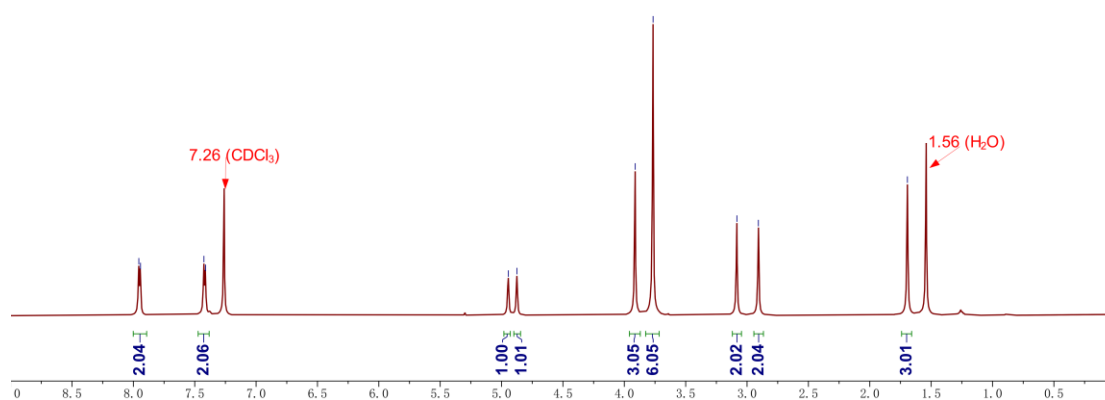
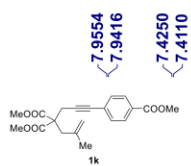
¹H NMR (600 MHz, CDCl₃)



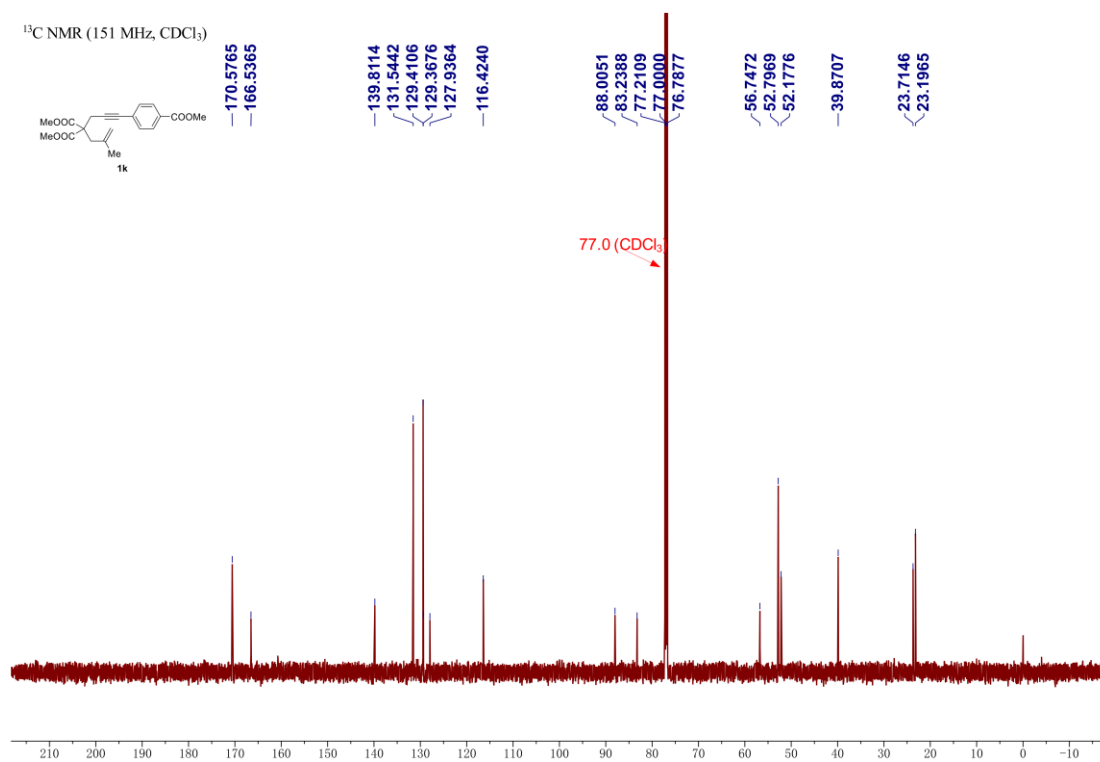
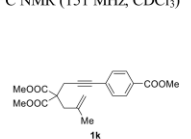
¹³C NMR (151 MHz, CDCl₃)



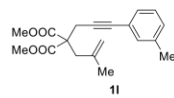
¹H NMR (600 MHz, CDCl₃)



¹³C NMR (151 MHz, CDCl₃)



¹H NMR (600 MHz, CDCl₃)



7.1902
7.1709
7.1585
7.1460
7.0943
7.0829

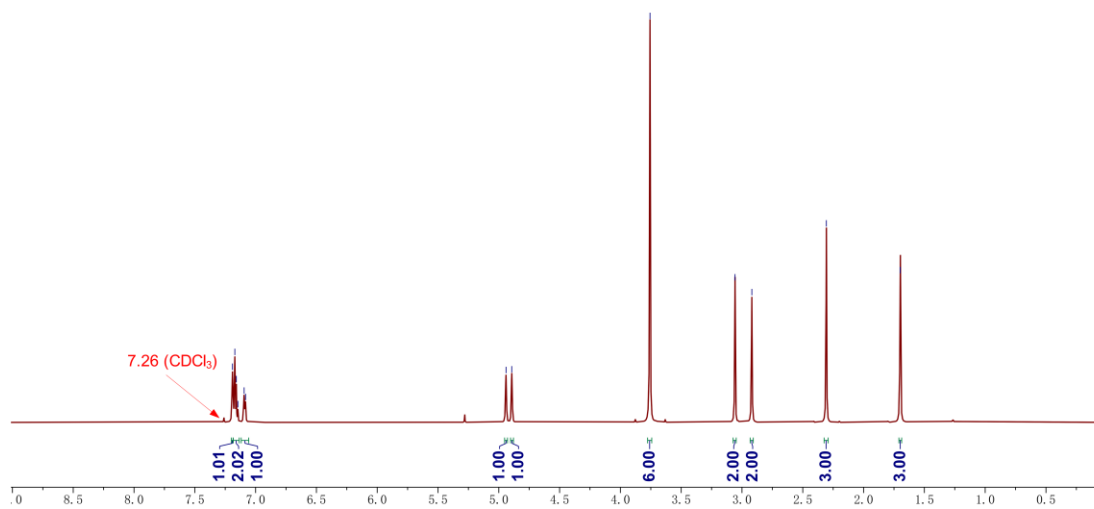
4.9404
4.8934

3.7564

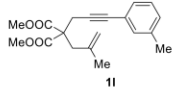
3.0573
2.9190

2.3059

1.6991



¹³C NMR (151 MHz, CDCl₃)



170.6530

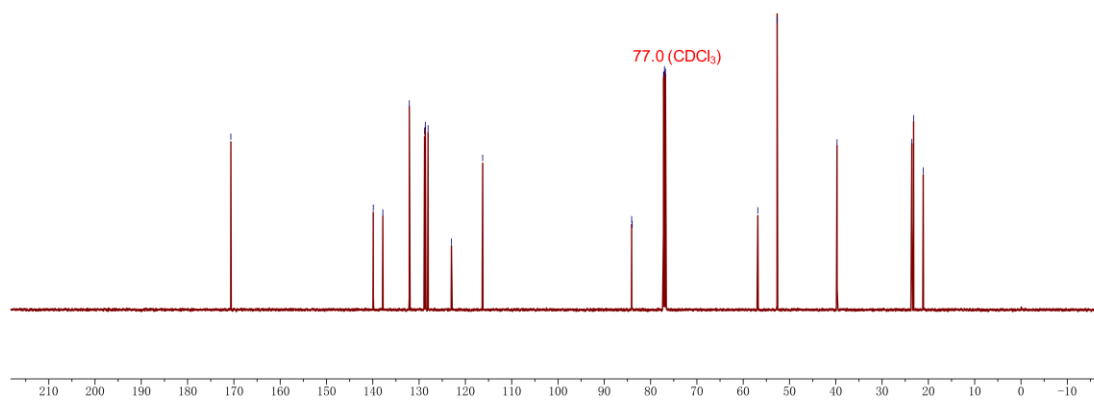
139.8957
137.8307
132.1116
128.8187
128.6576
128.0596
123.0152
116.2640

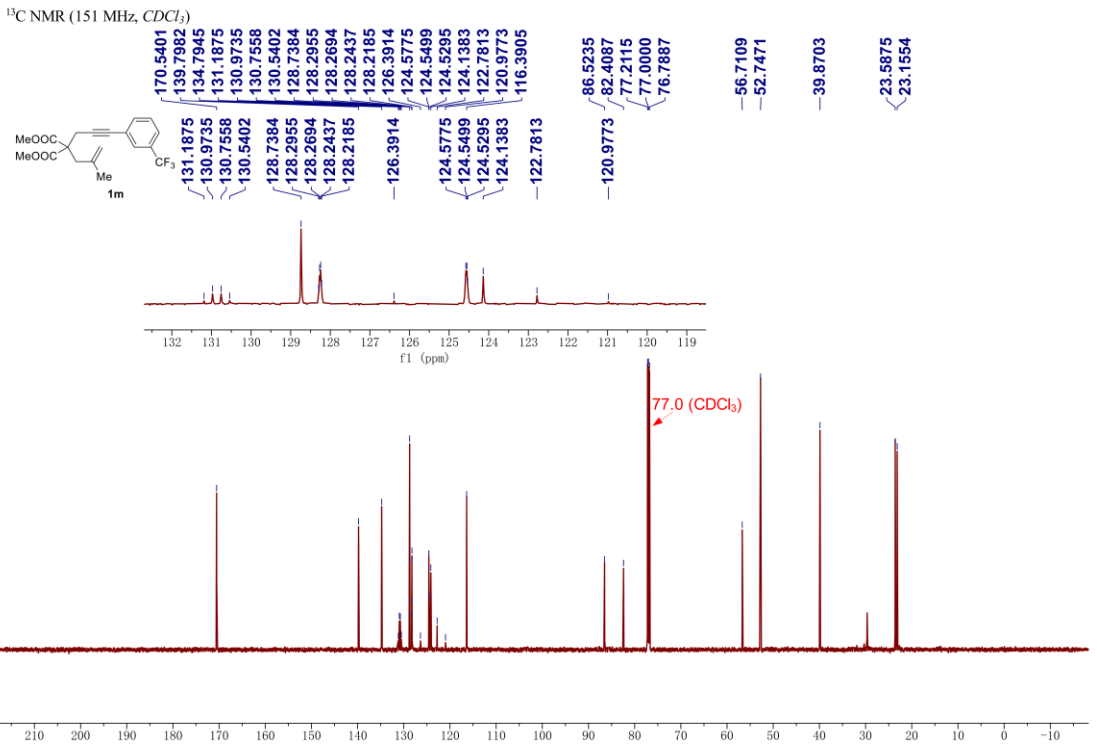
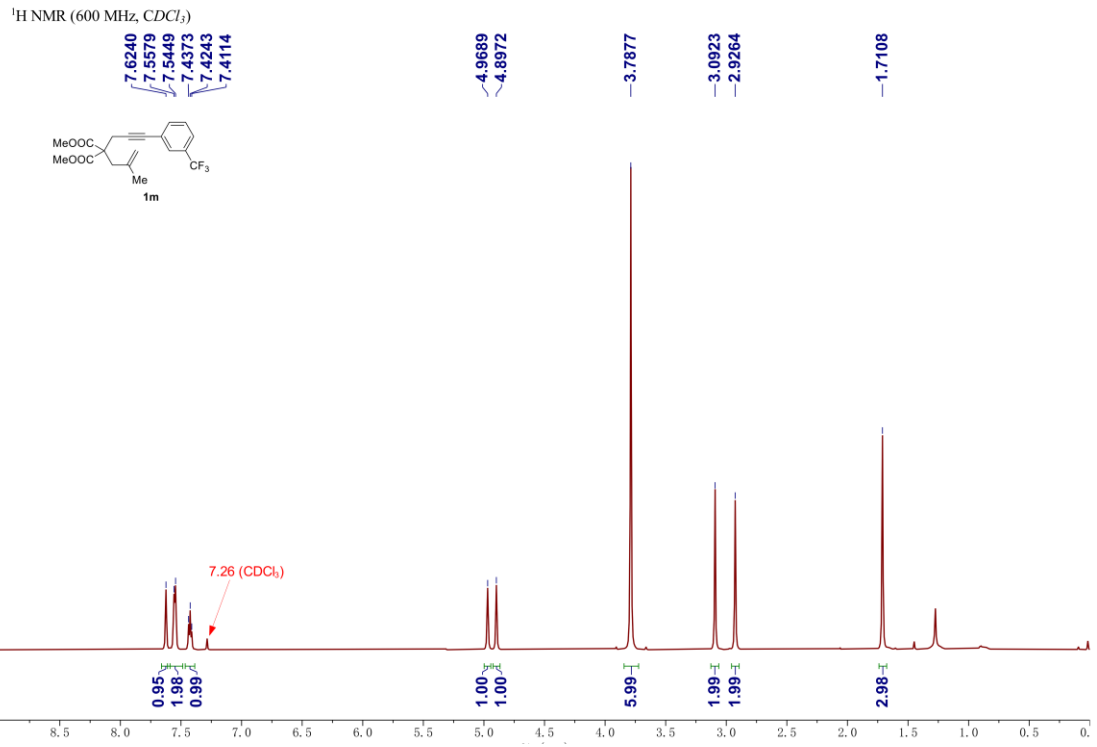
84.0921
83.9693
77.2119
77.0000
76.7880

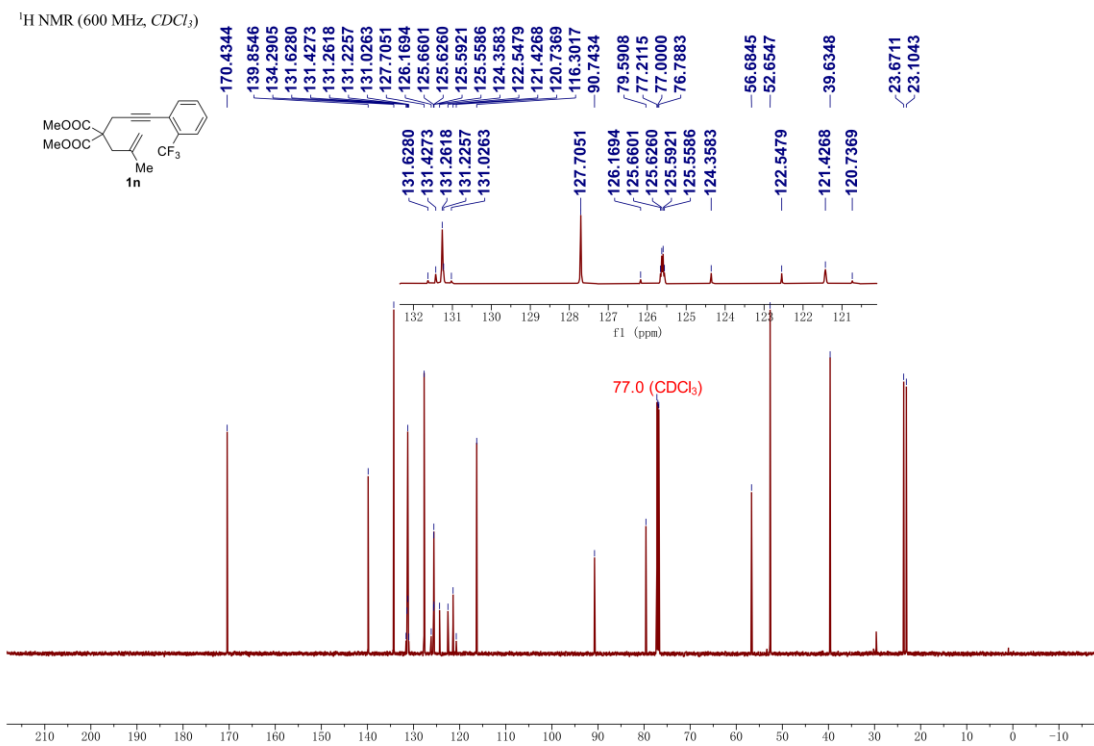
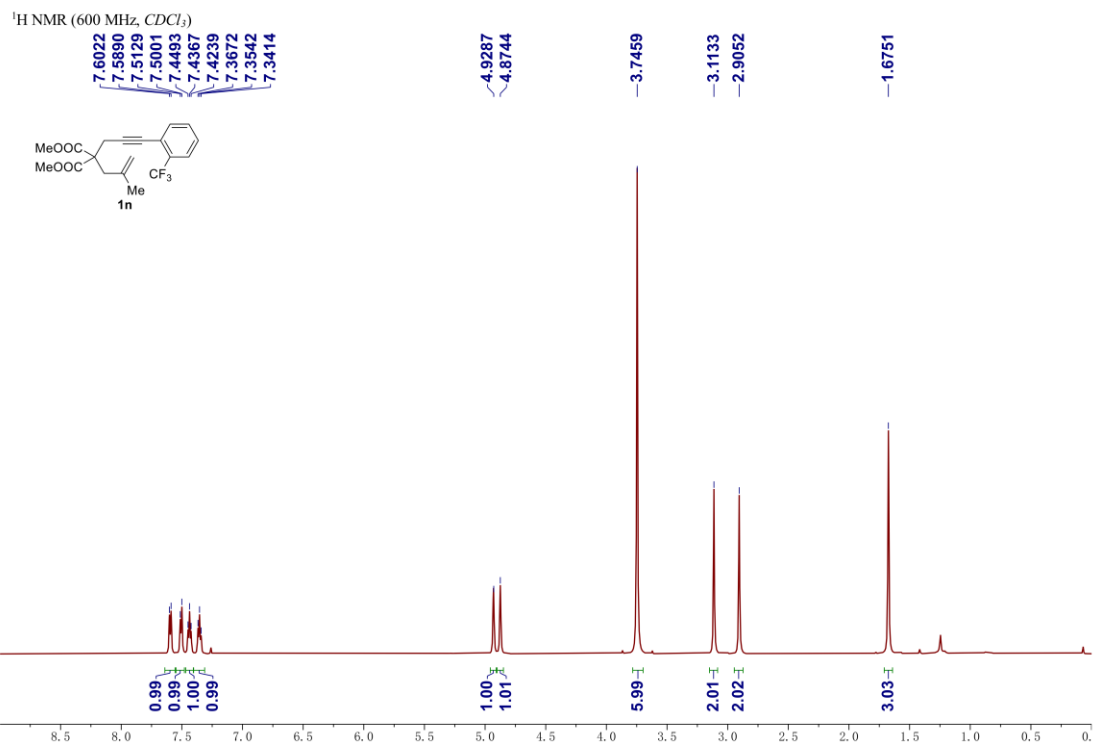
56.8367
52.6690

39.7257

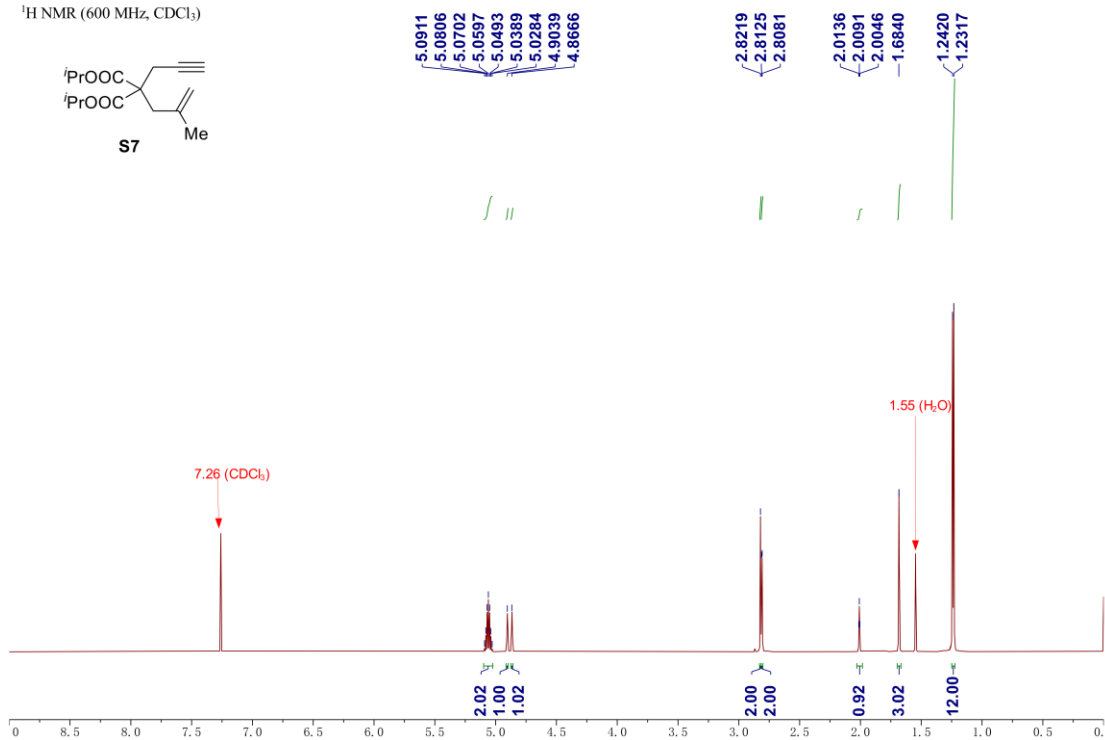
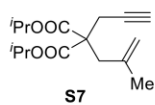
23.5789
23.1954
21.1133



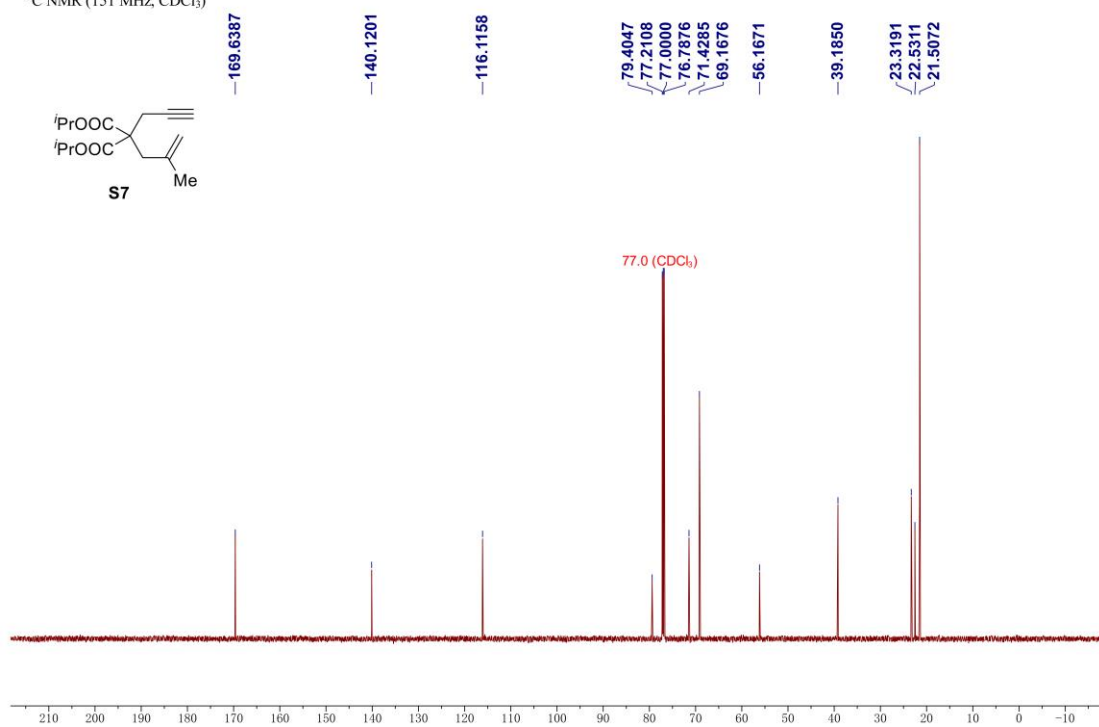
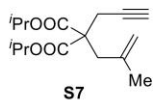




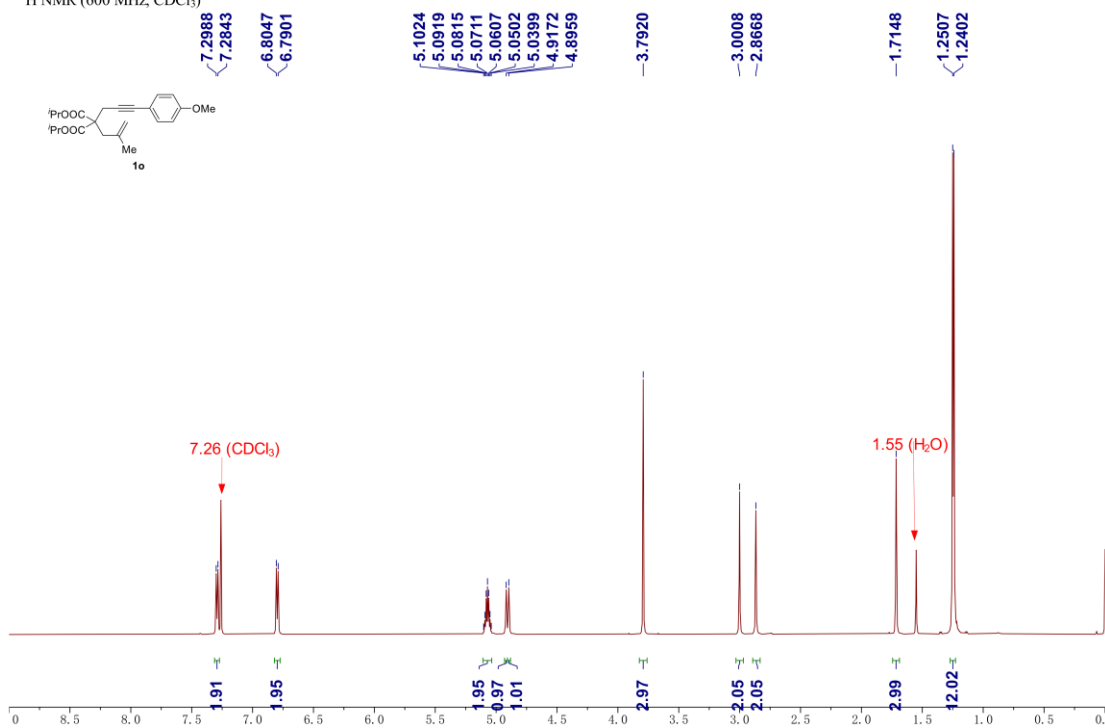
¹H NMR (600 MHz, CDCl₃)



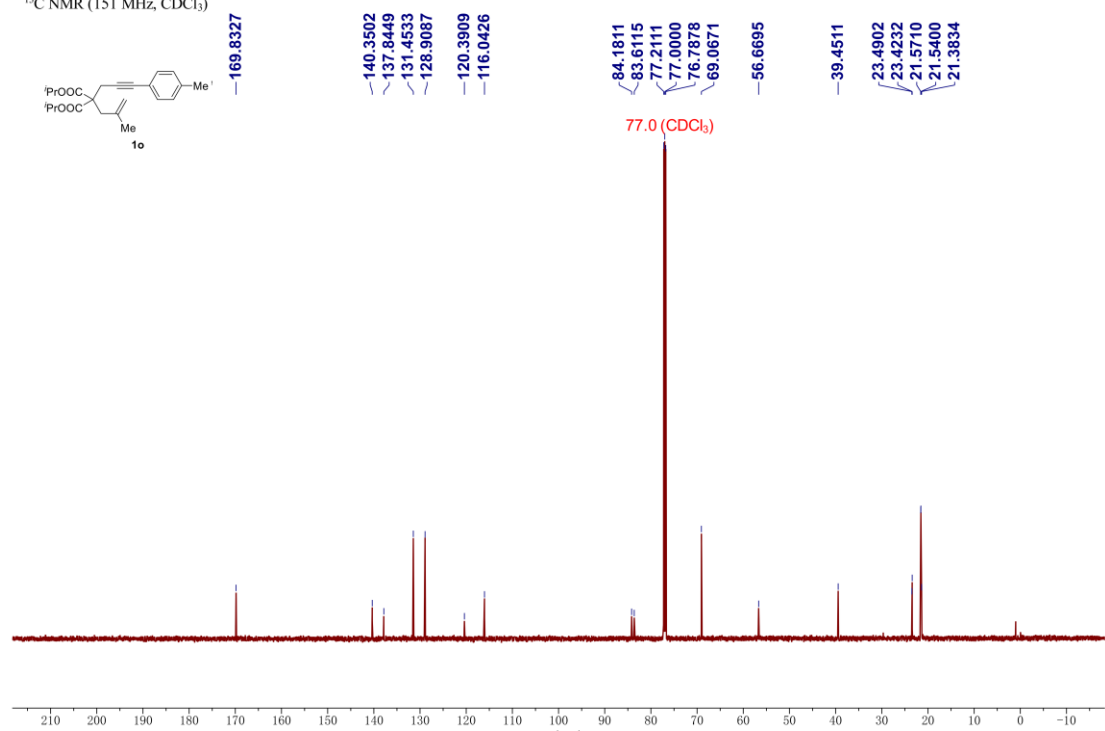
¹³C NMR (151 MHz, CDCl₃)



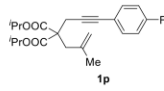
¹H NMR (600 MHz, CDCl₃)



¹³C NMR (151 MHz, CDCl₃)



¹H NMR (600 MHz, CDCl₃)

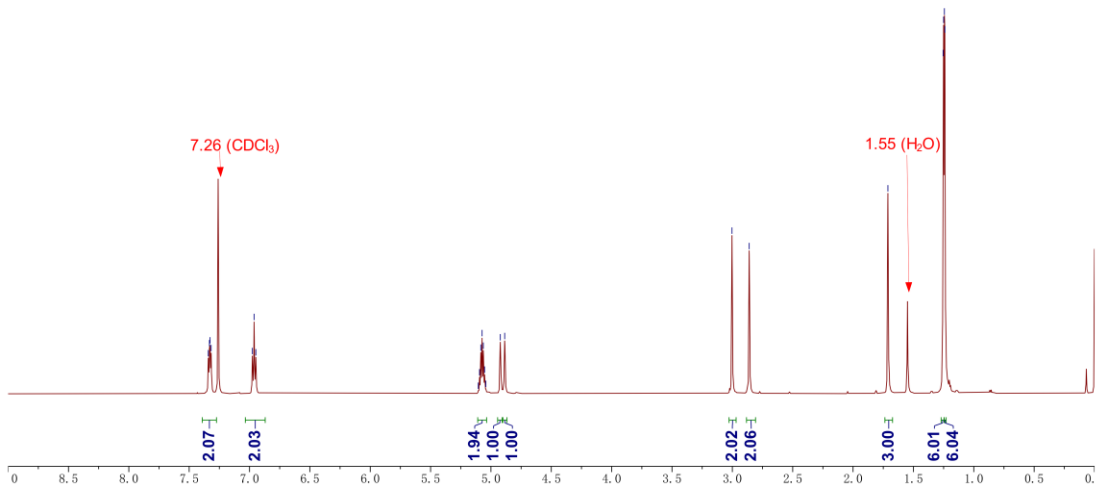


7.3414
7.3322
7.3271
7.3179
6.9766
6.9621
6.9477

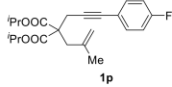
5.1048
5.0944
5.0839
5.0735
5.0631
5.0527
5.0424
4.9226
4.8862

3.0029
2.8604

1.7115
1.2540
1.2500
1.2434
1.2393



¹³C NMR (151 MHz, CDCl₃)



169.7677
163.0838
161.4352

140.2830
133.4042
133.3497

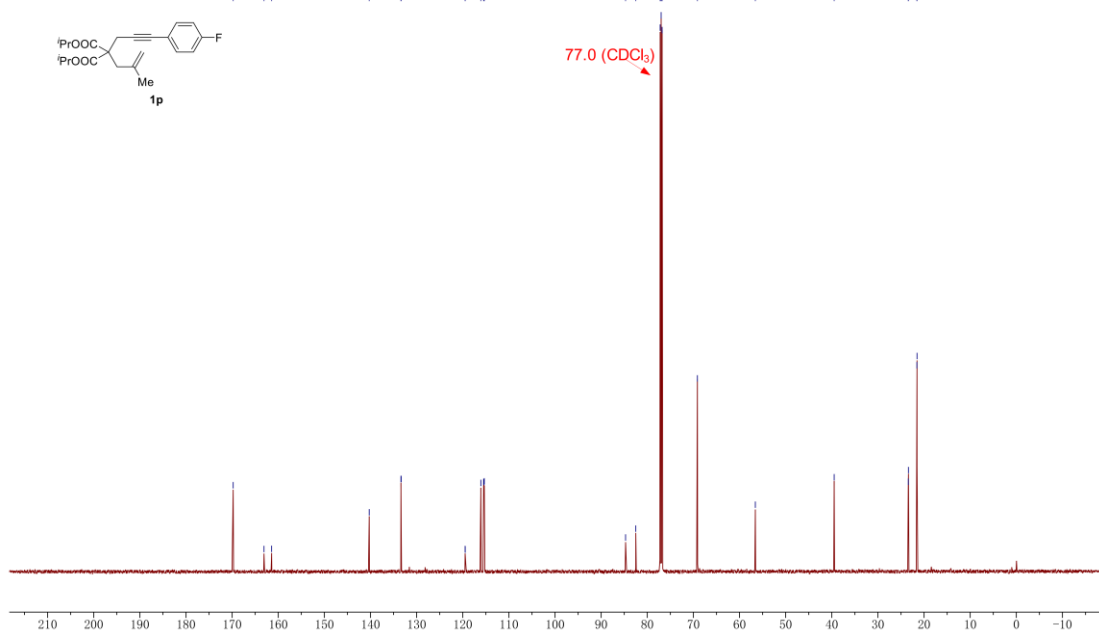
119.4623
119.4696
116.0867
115.4808
115.3356

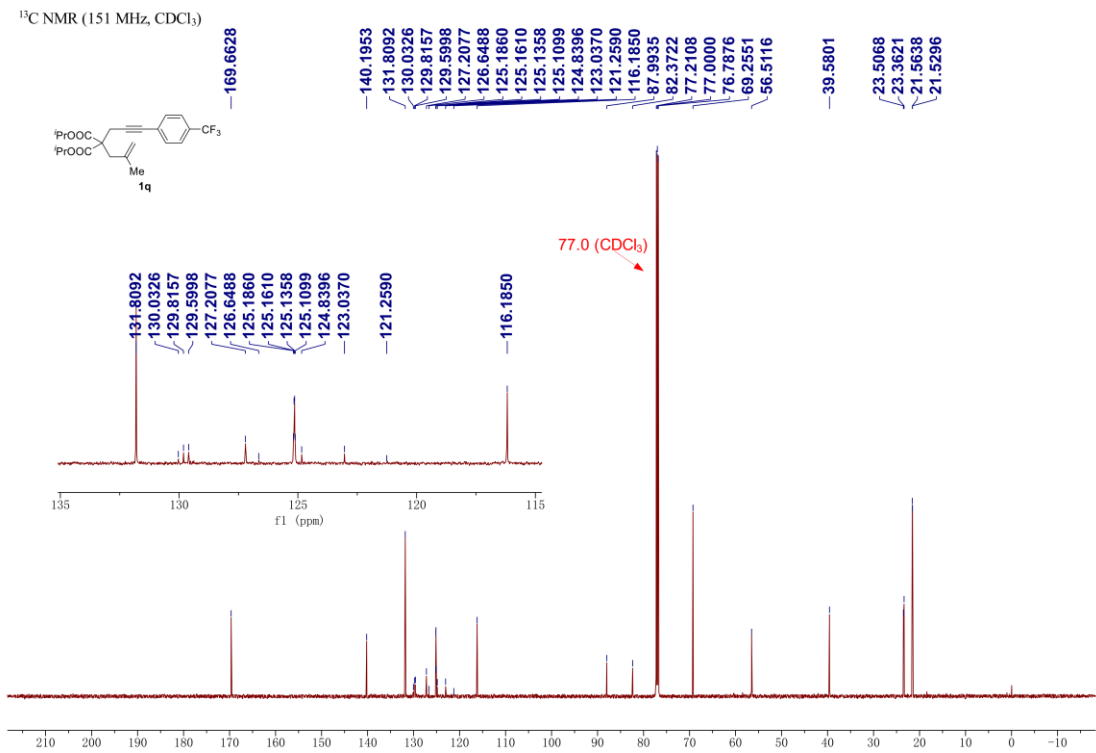
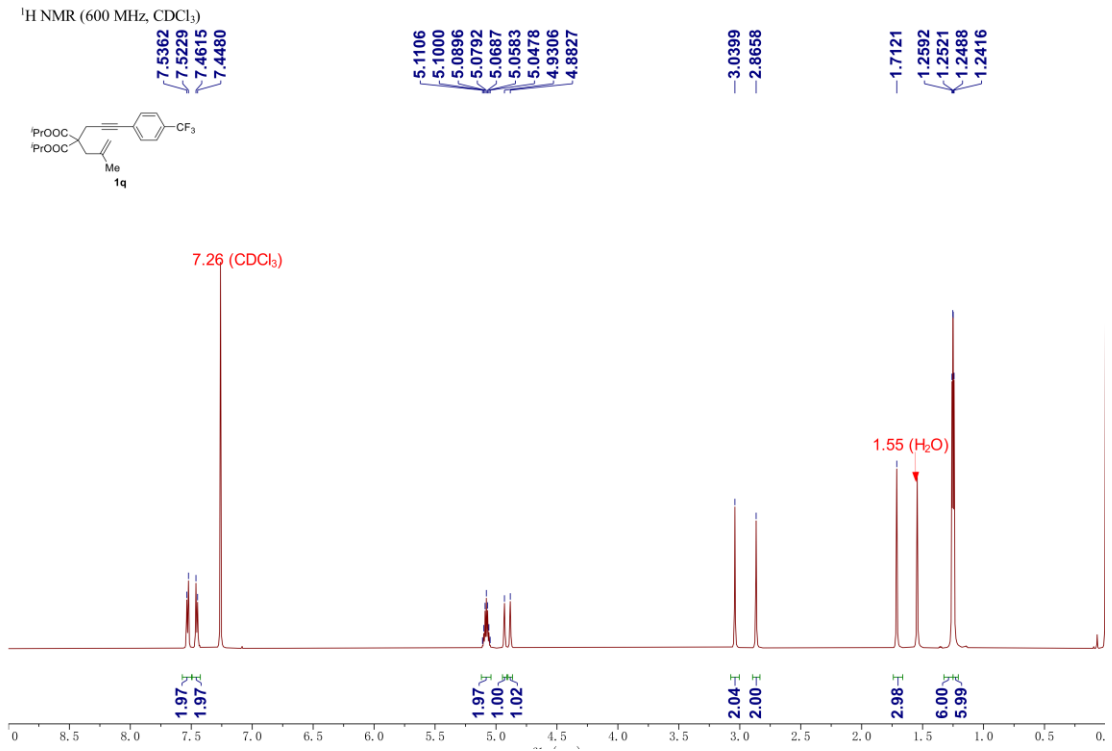
84.7084
82.4930
77.2119
77.0000
76.7880
69.1366

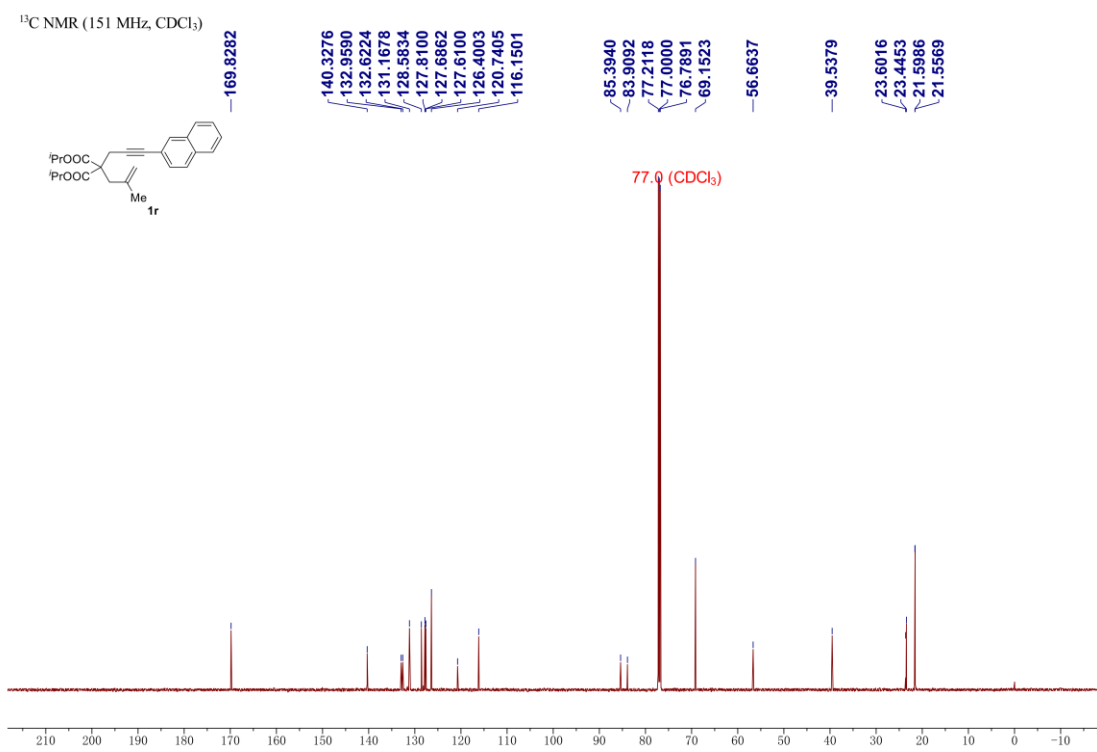
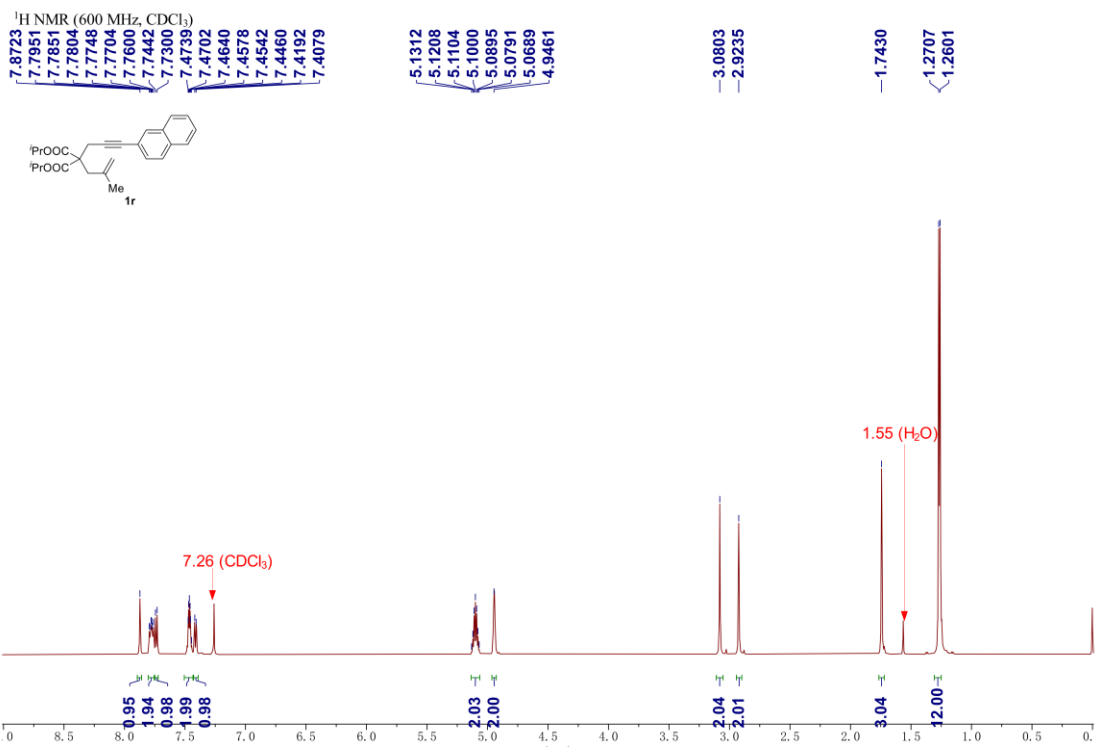
56.5813

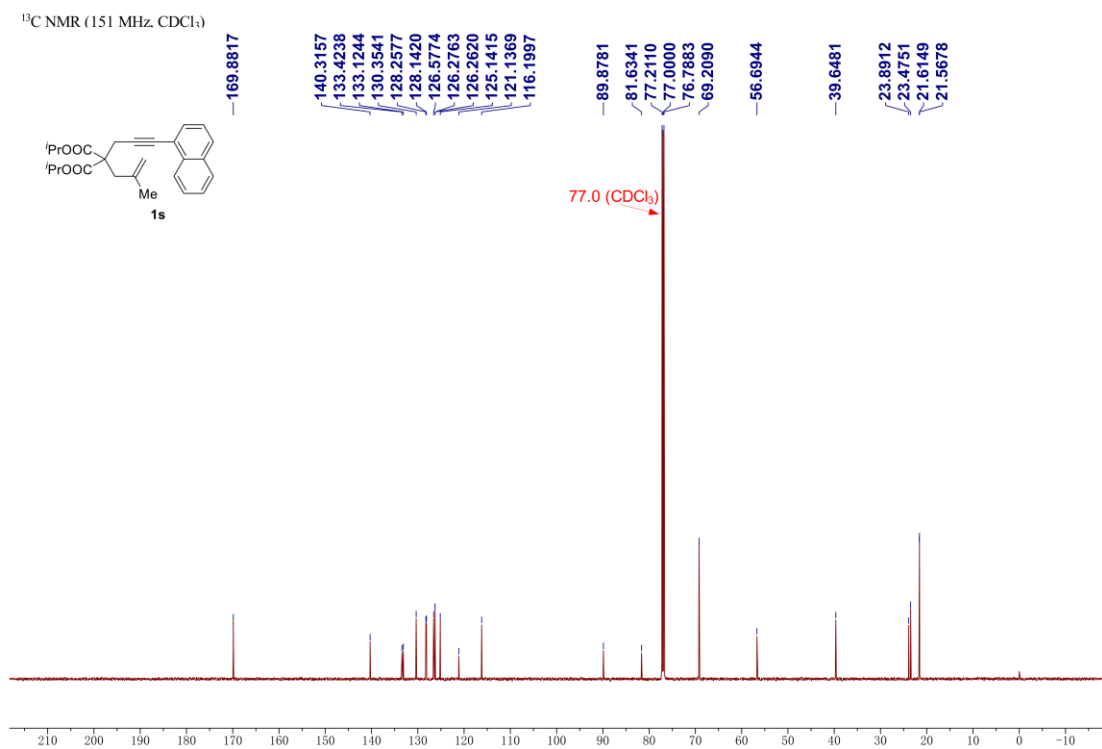
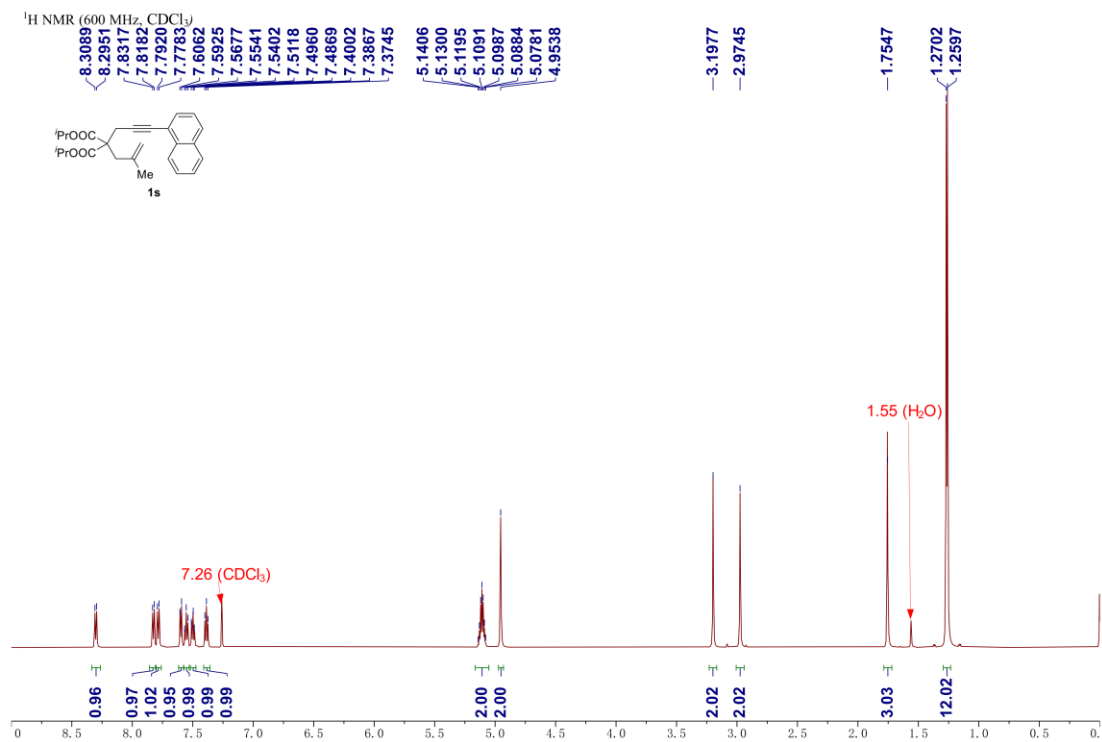
39.4913

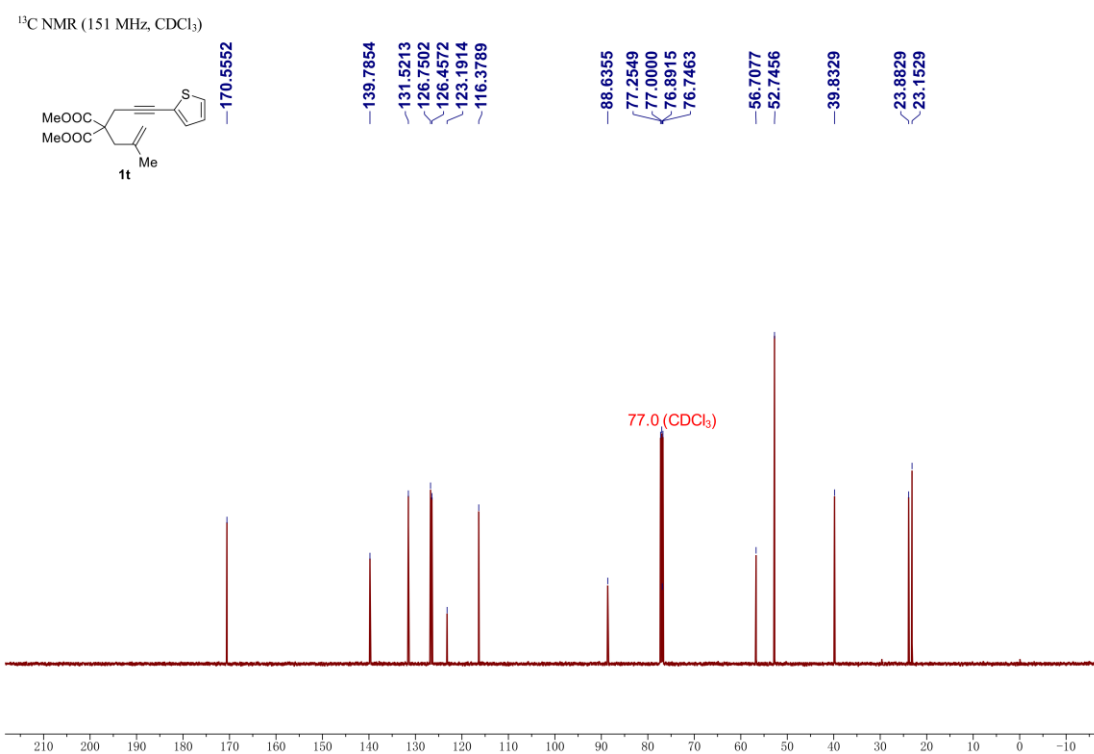
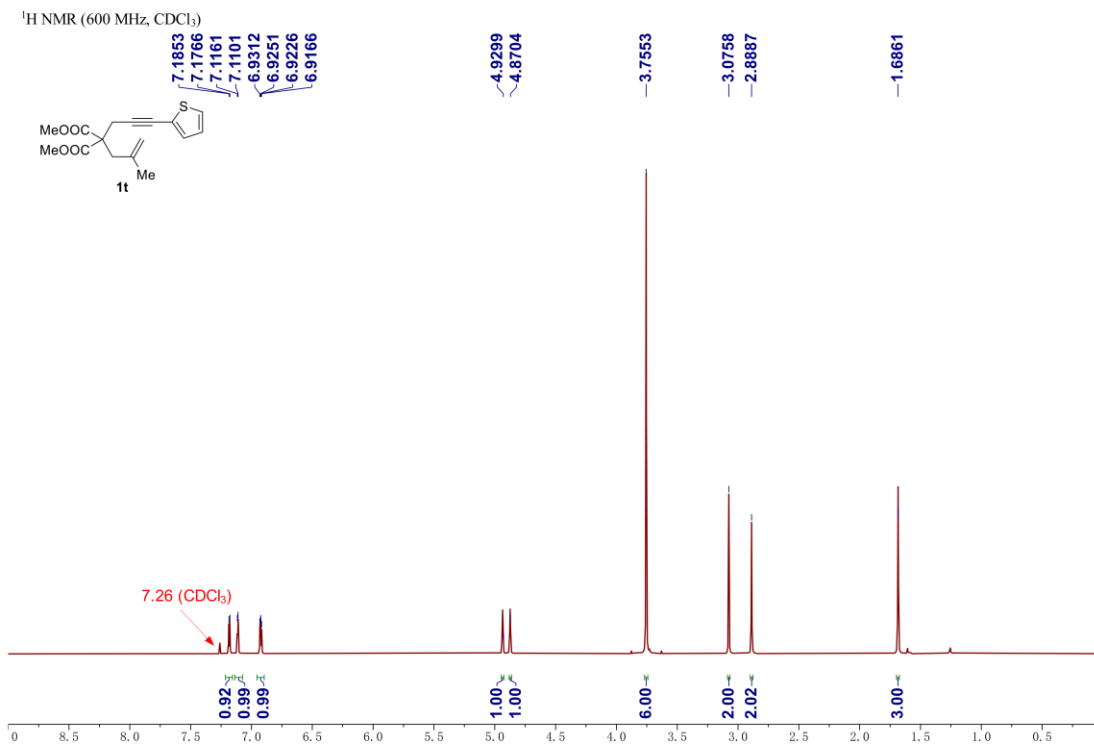
23.4276
23.3939
21.5656
21.5316

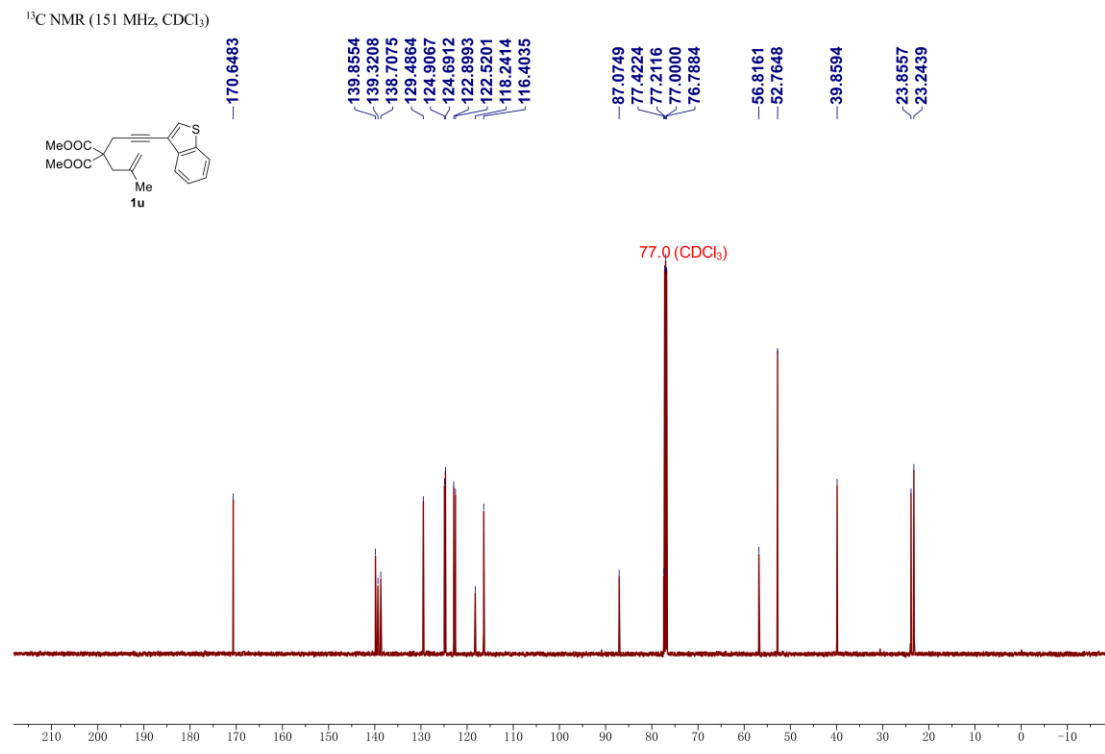
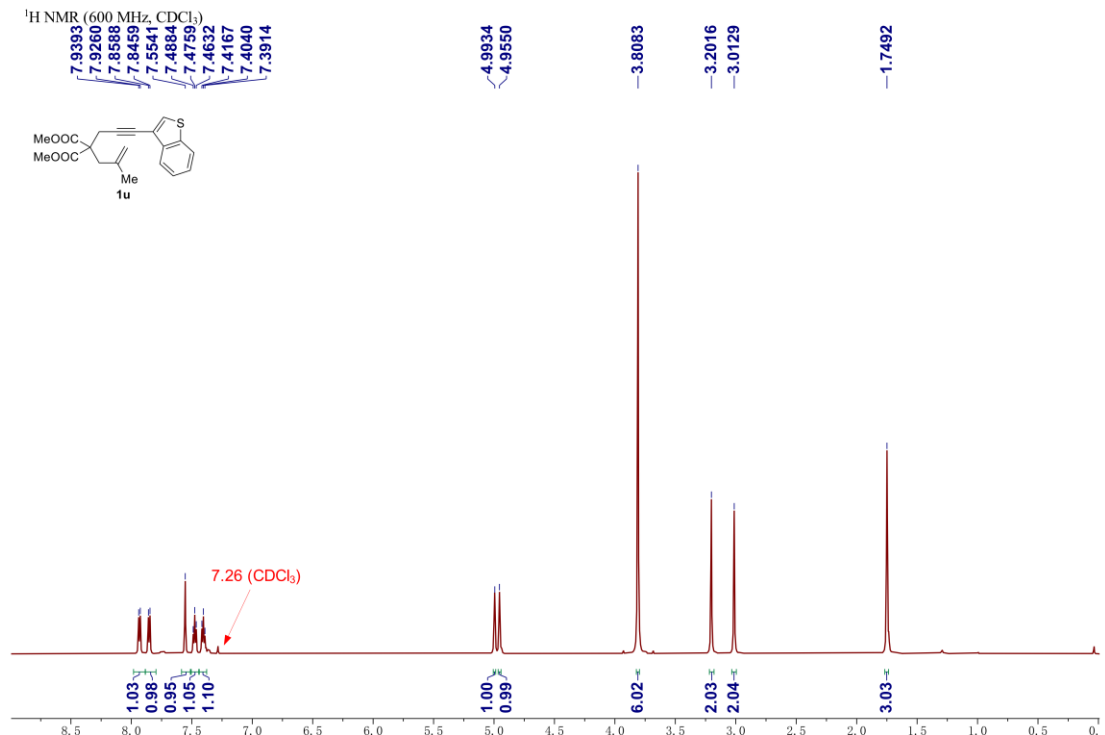


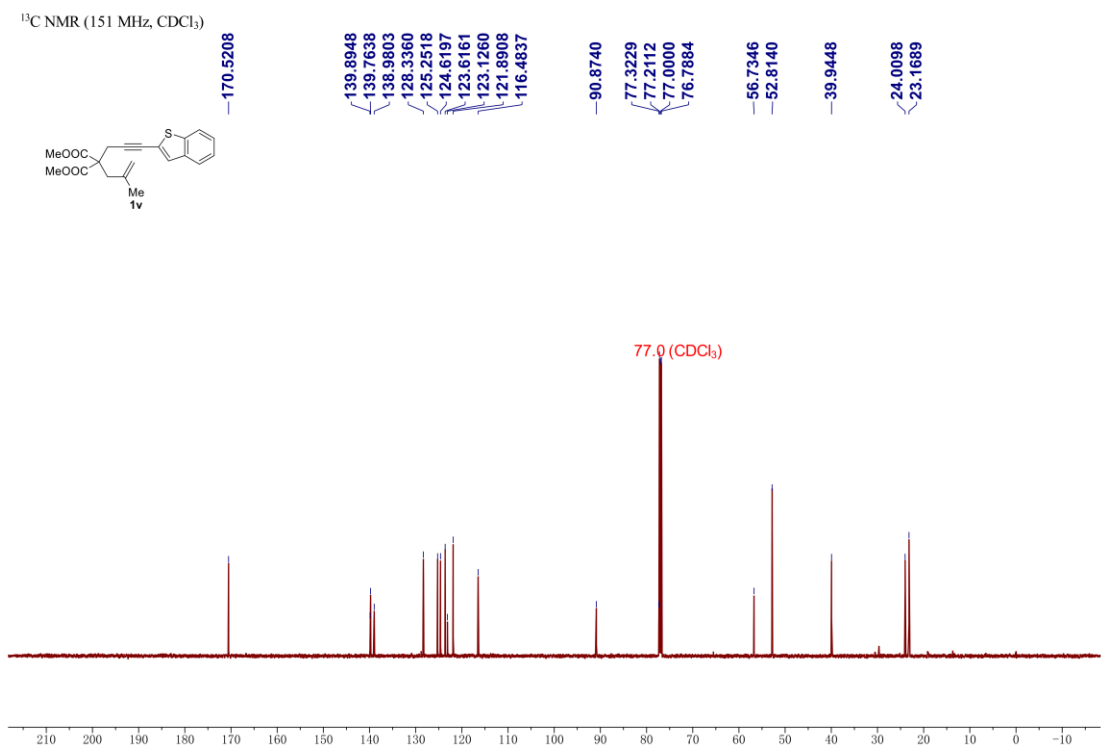
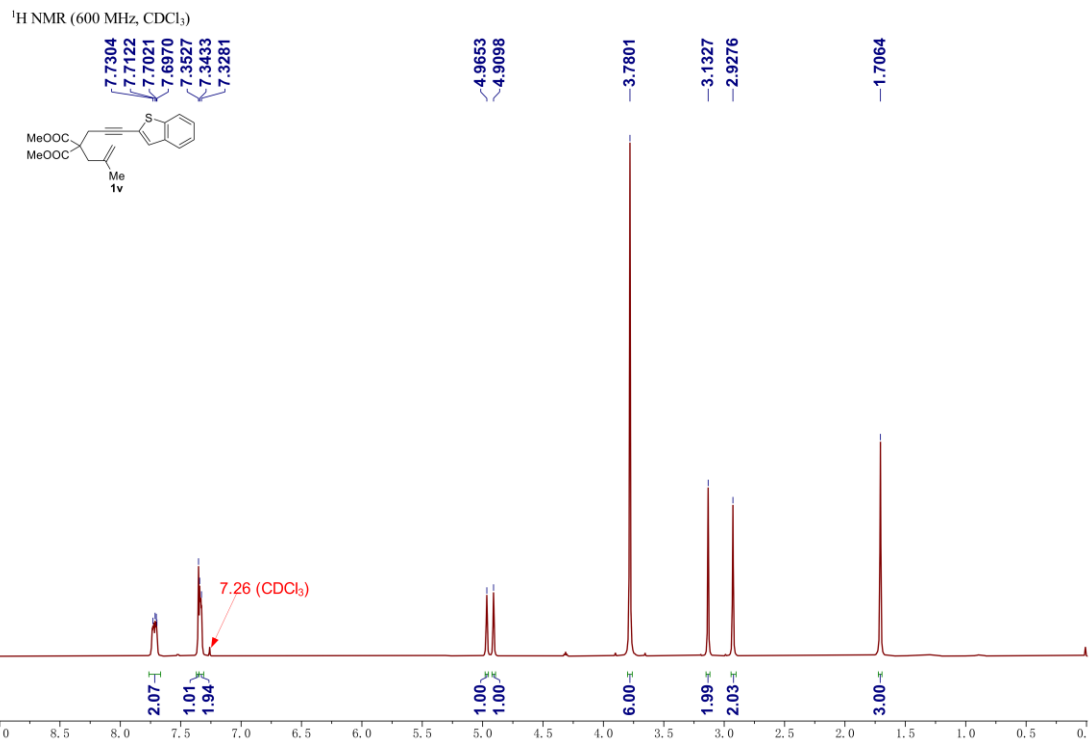


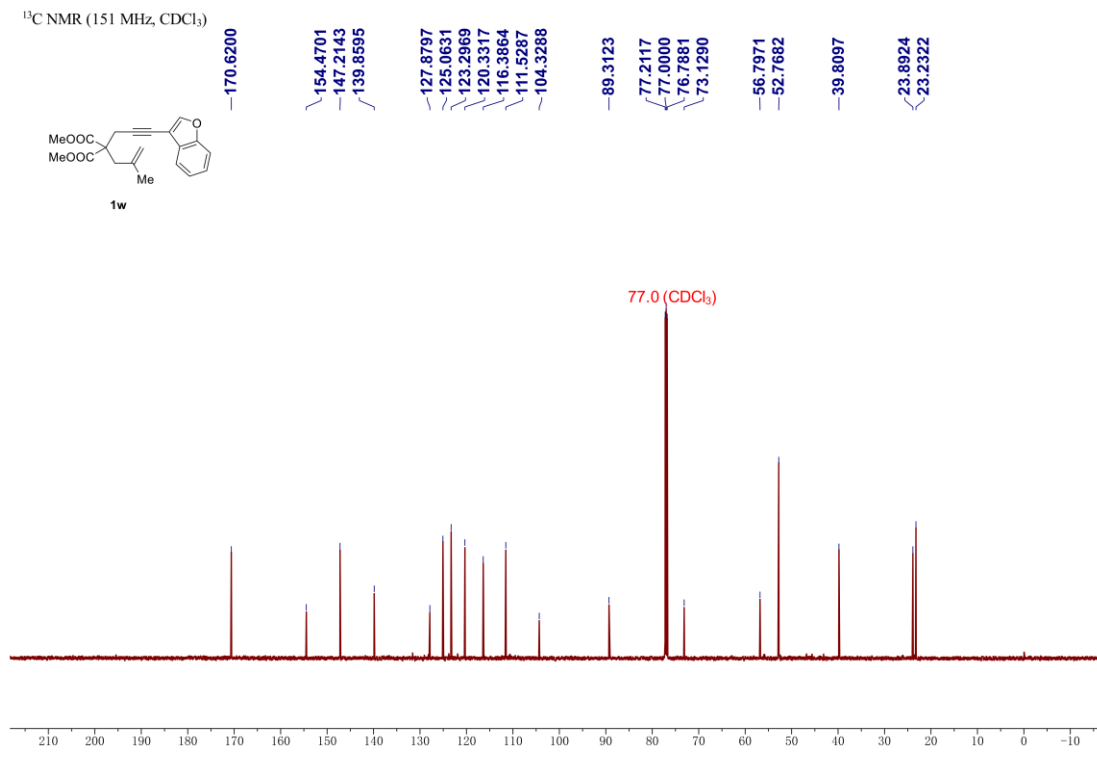
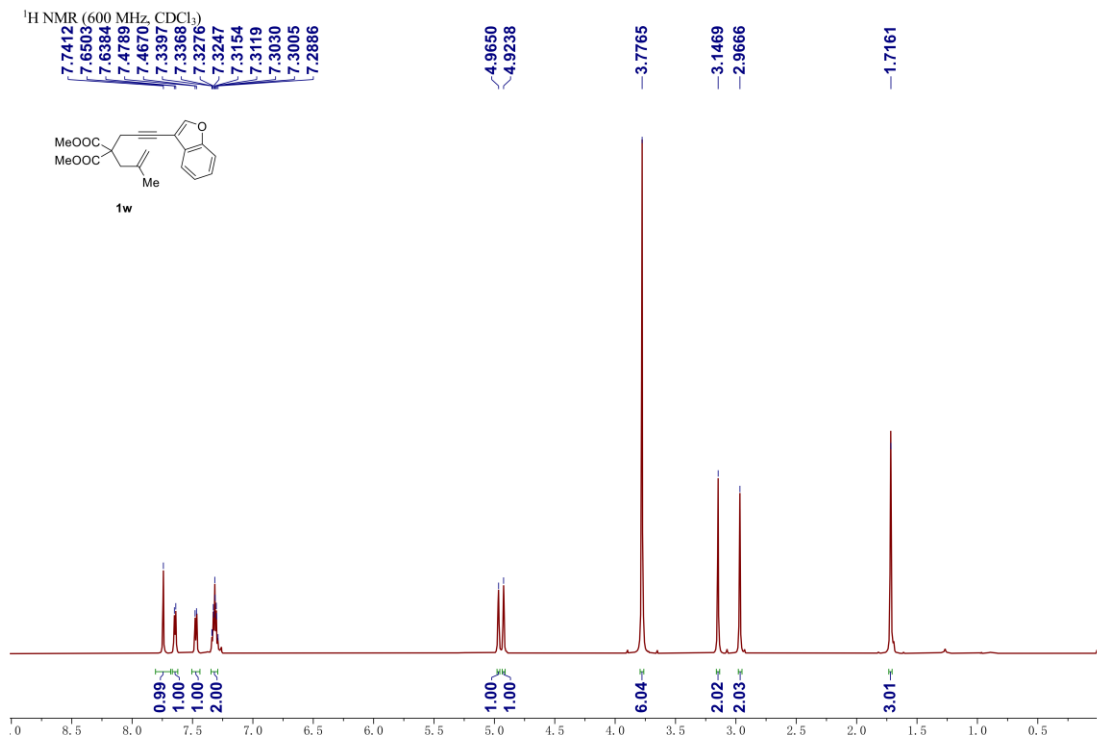






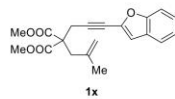






¹H NMR (600 MHz, CDCl₃)

7.5219
7.5090
7.4269
7.4131
7.3163
7.3039
7.2904
7.2268
7.2143
7.2018
6.8533

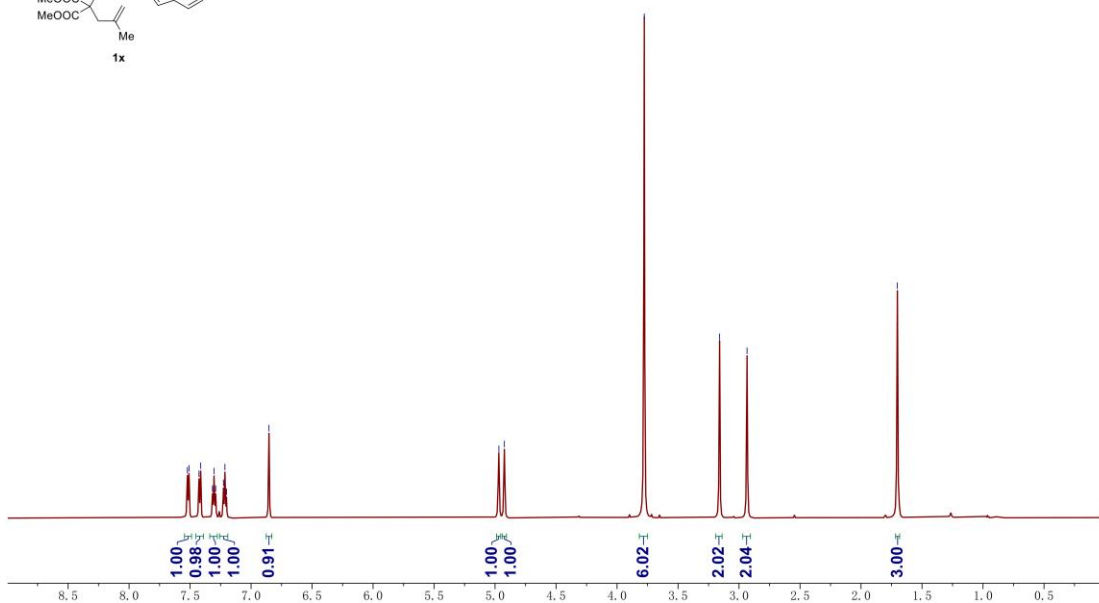


4.9685
4.9237

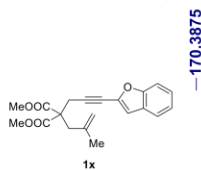
3.7771

3.1597
2.9344

1.7022



¹³C NMR (151 MHz, CDCl₃)



170.3875

154.5703

139.6531

138.4509

127.5277

125.3601

123.1410

121.0035

116.6017

111.1280

111.0811

91.1928

77.2116

77.0000

76.7897

74.3448

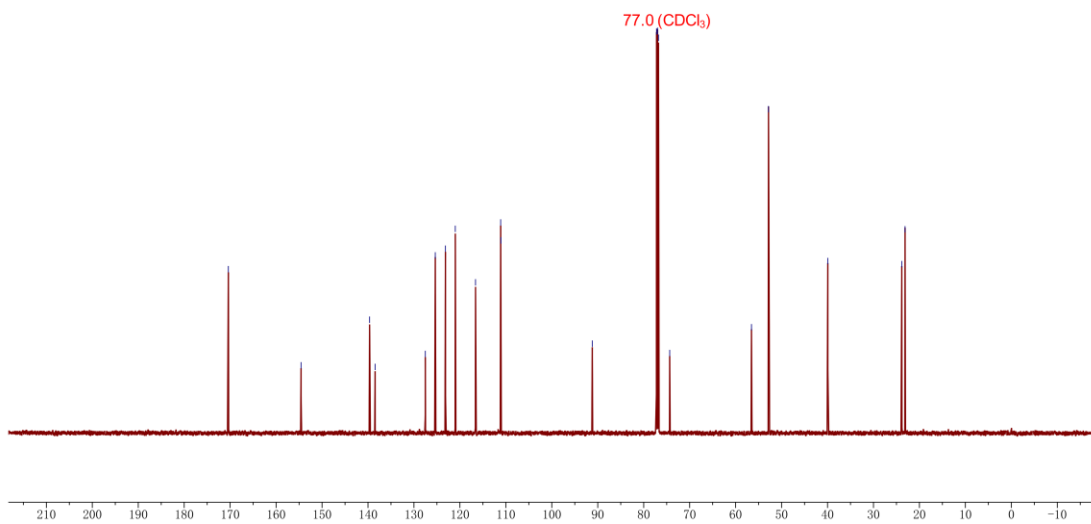
56.5469

52.8471

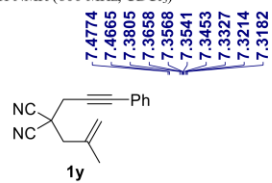
39.9389

23.8387

23.1296



¹H NMR (600 MHz, CDCl₃)



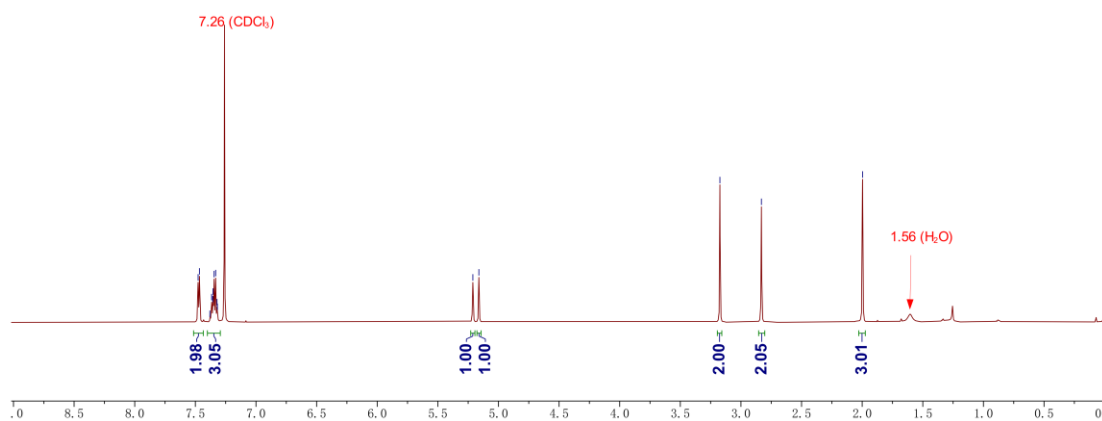
7.4774
7.4665
7.3805
7.3658
7.3541
7.3453
7.3327
7.3214
7.3182

5.2111
5.1616

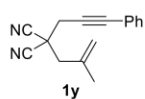
3.1735

2.8312

1.9969



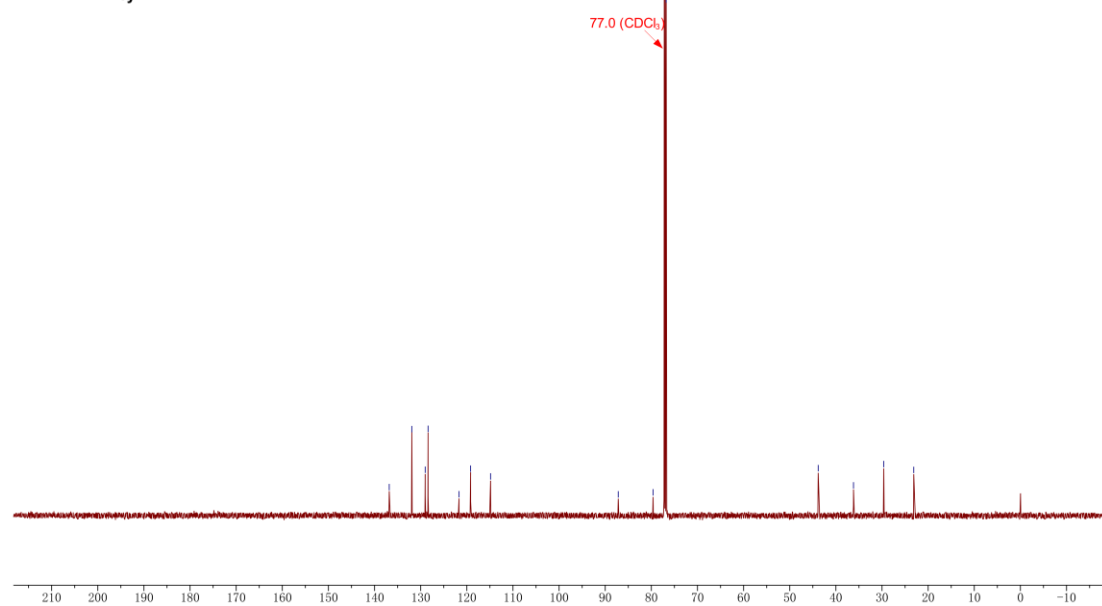
¹³C NMR (151 MHz, Chloroform-*d*)

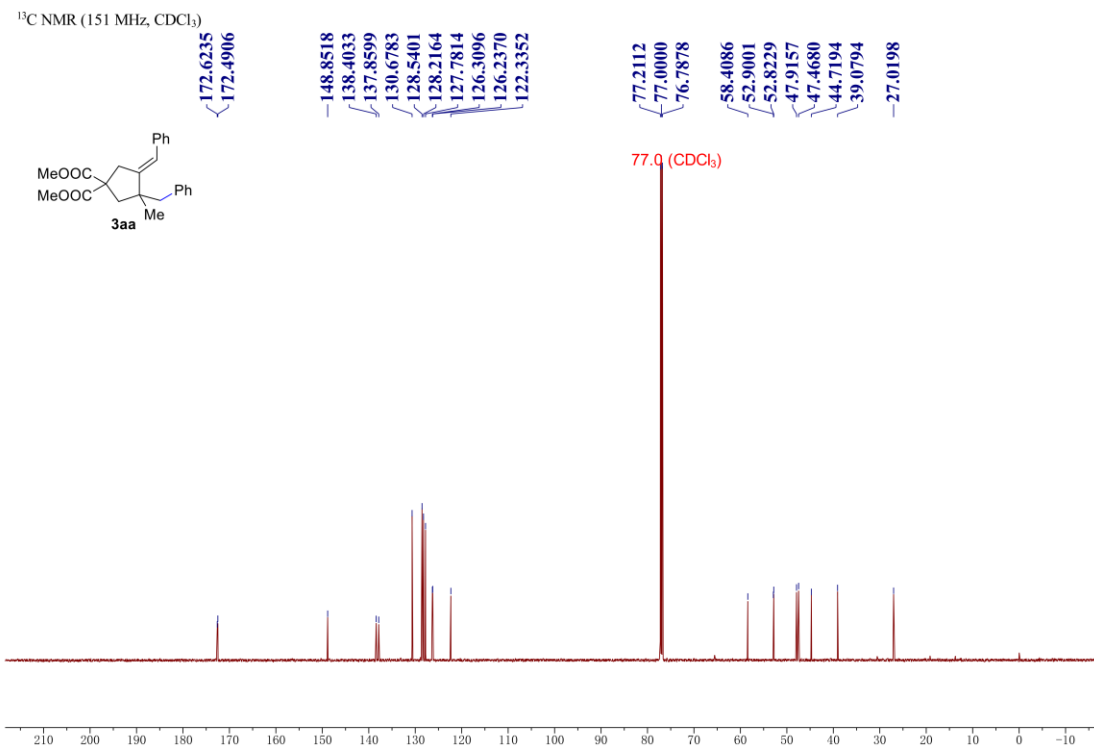
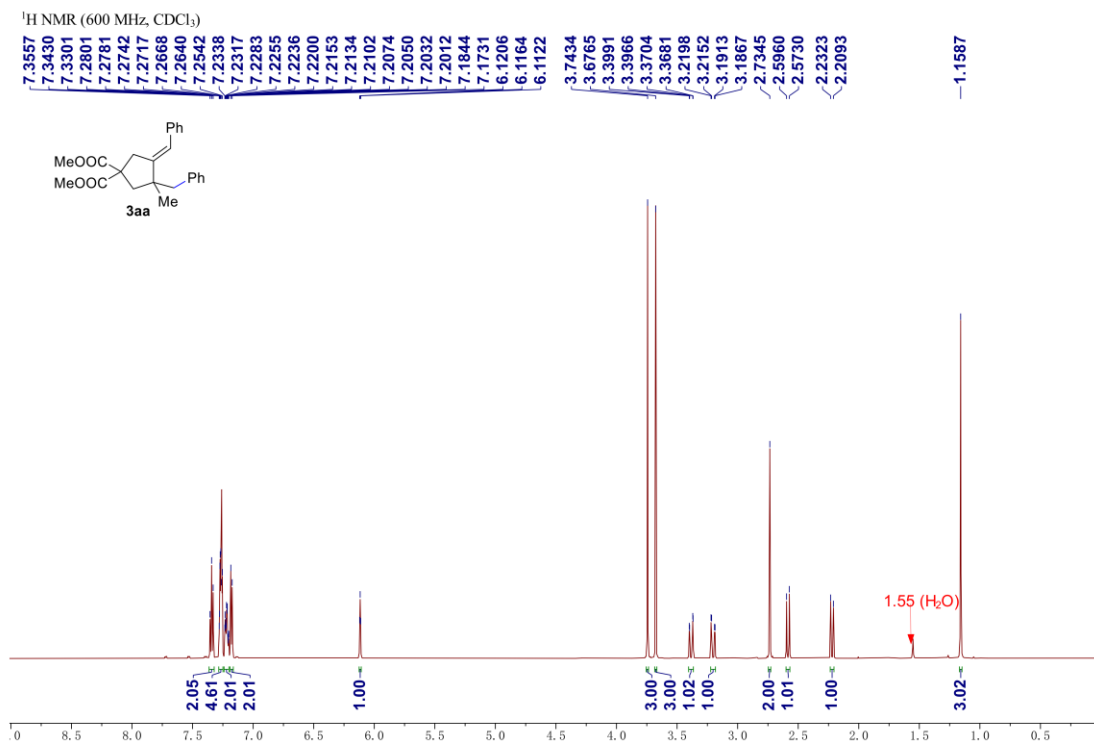


136.8230
131.9250
129.0307
128.4060
121.7030
119.1820
114.8589

87.1795
79.6283
77.2104
77.0000
76.7884

43.8355
36.1846
29.6282
23.1202



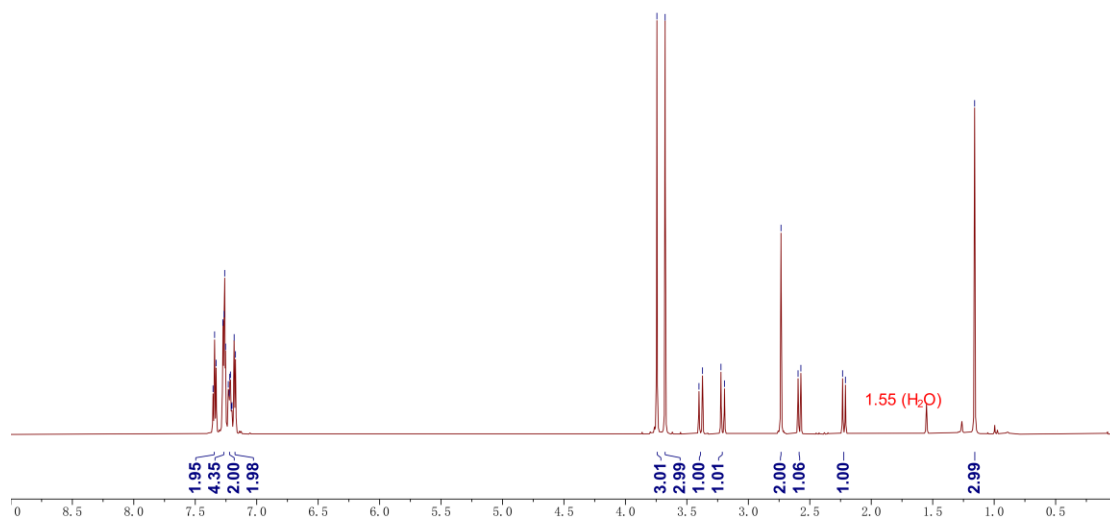
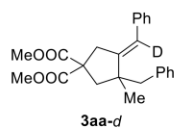


¹H NMR (600 MHz, CDCl₃)

7.3554
7.3426
7.3298
7.2751
7.2656
7.2601
7.2534
7.2314
7.2232
7.2194
7.2134
7.2011
7.1836
7.1724

3.7441
3.6772
3.4017
3.3732
3.2228
3.1943
2.7343
2.5956
2.5726
2.2331
2.2101

— 1.1590



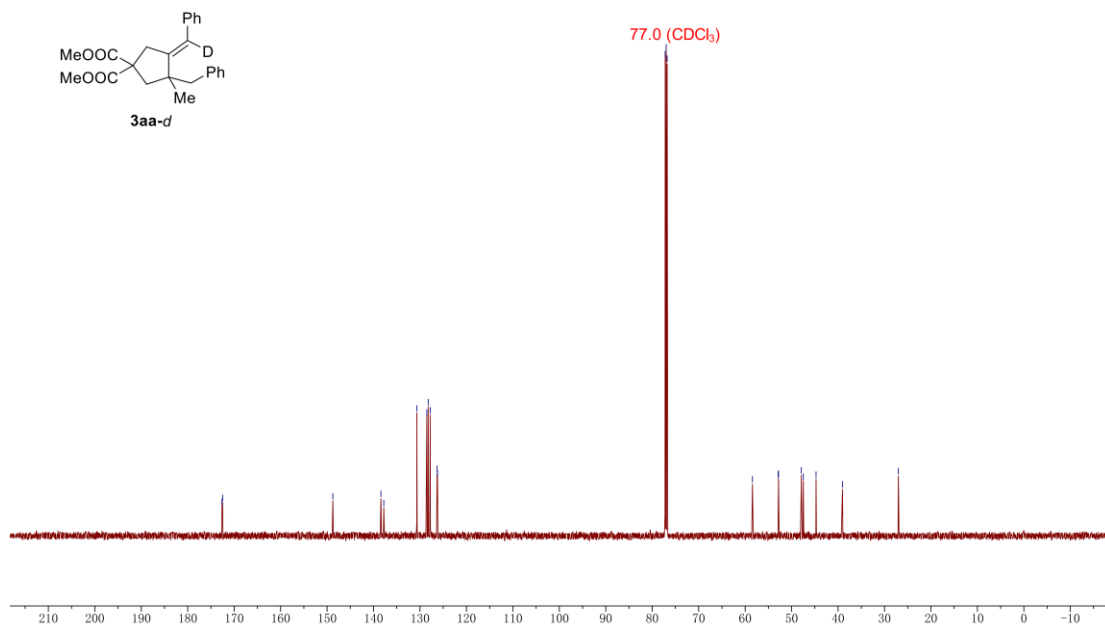
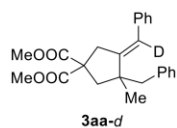
¹³C NMR (151 MHz, CDCl₃)

172.6244
172.4931

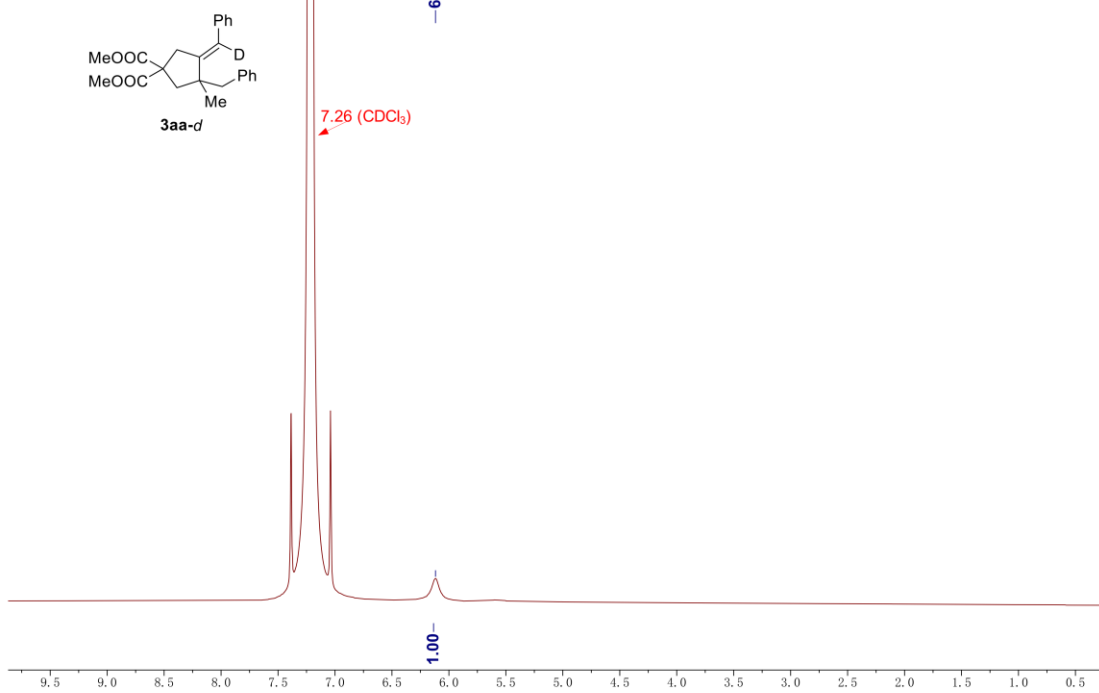
148.7565
138.4077
137.7979
130.6800
128.5259
128.2211
127.7805
126.3116
126.2369

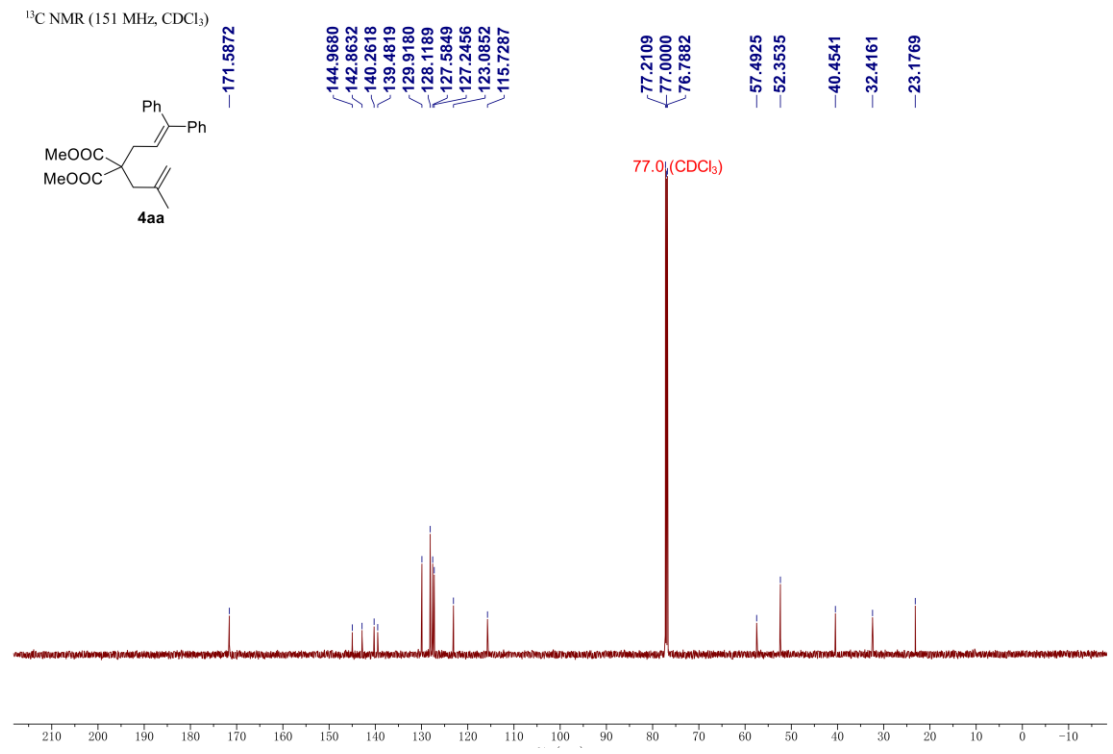
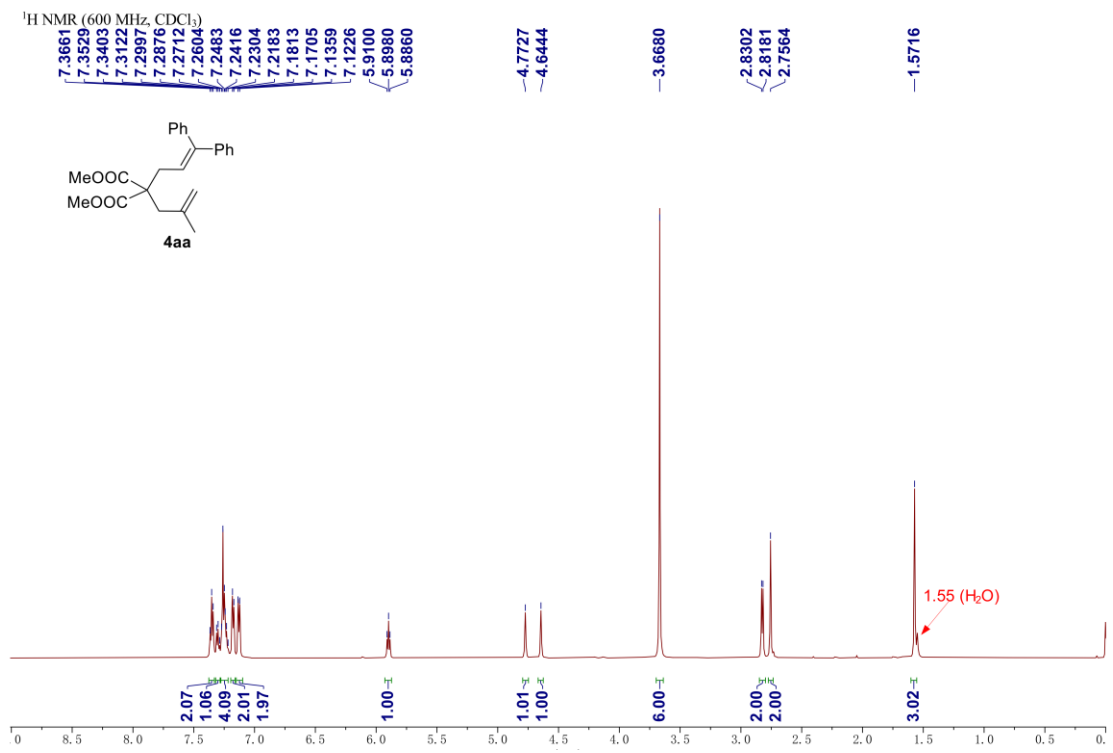
77.2118
77.0000
76.7901

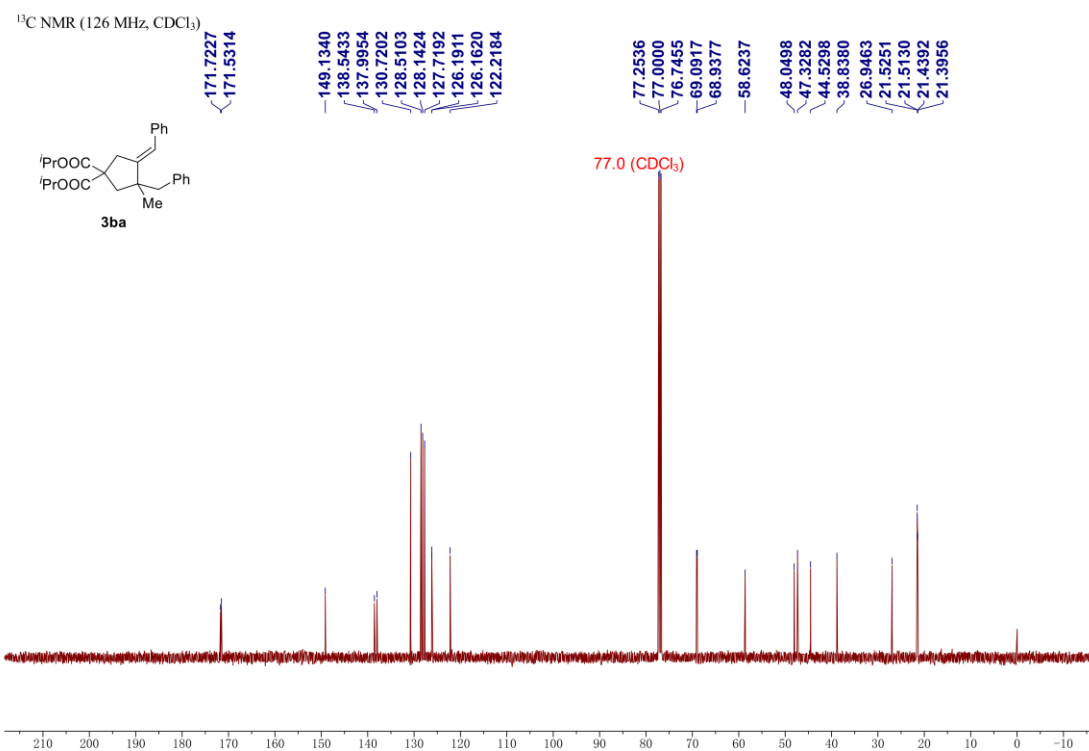
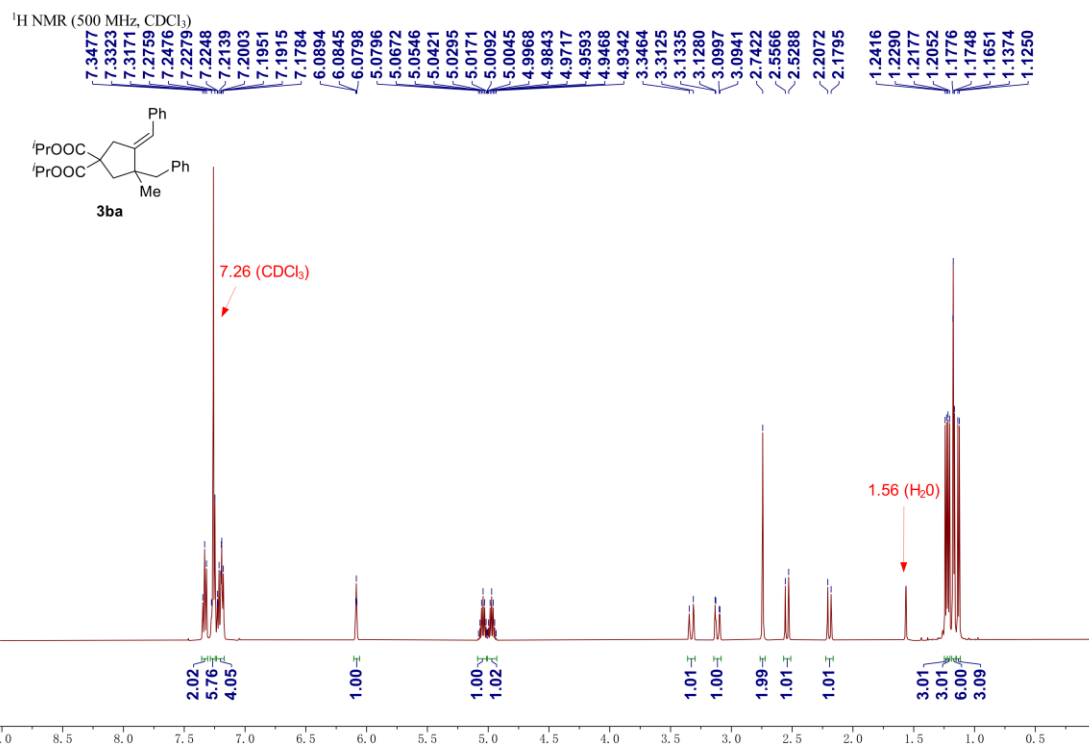
77.0 (CDCl₃)



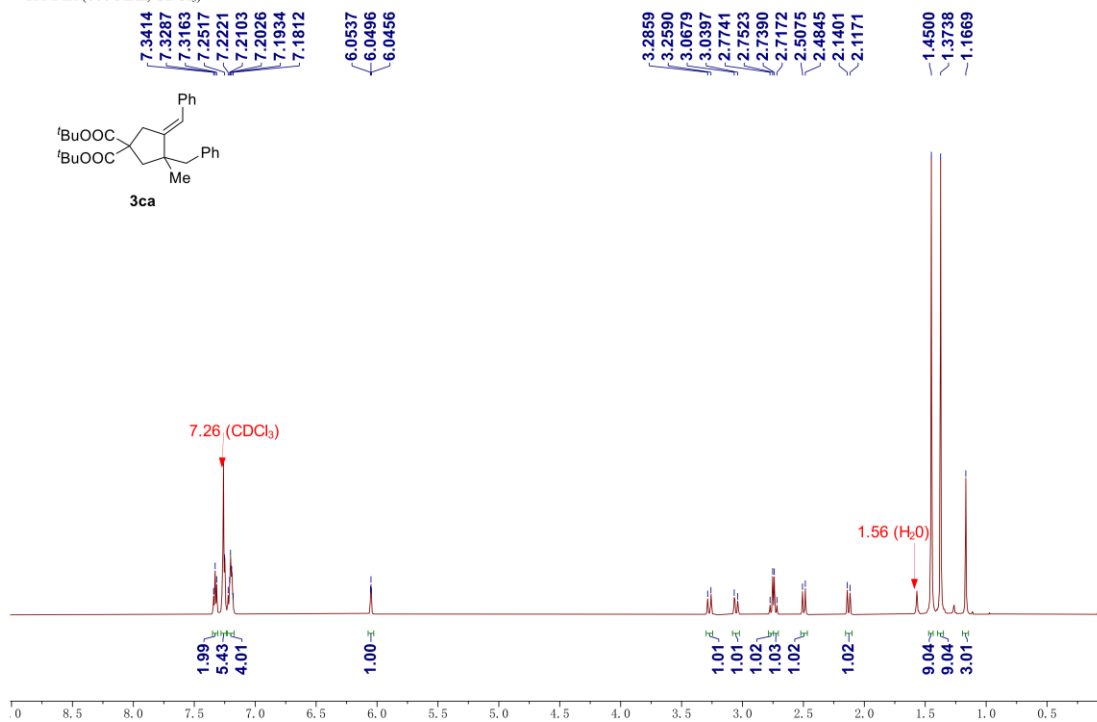
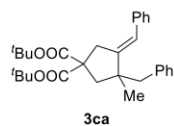
^2H NMR (92 MHz, CDCl_3)



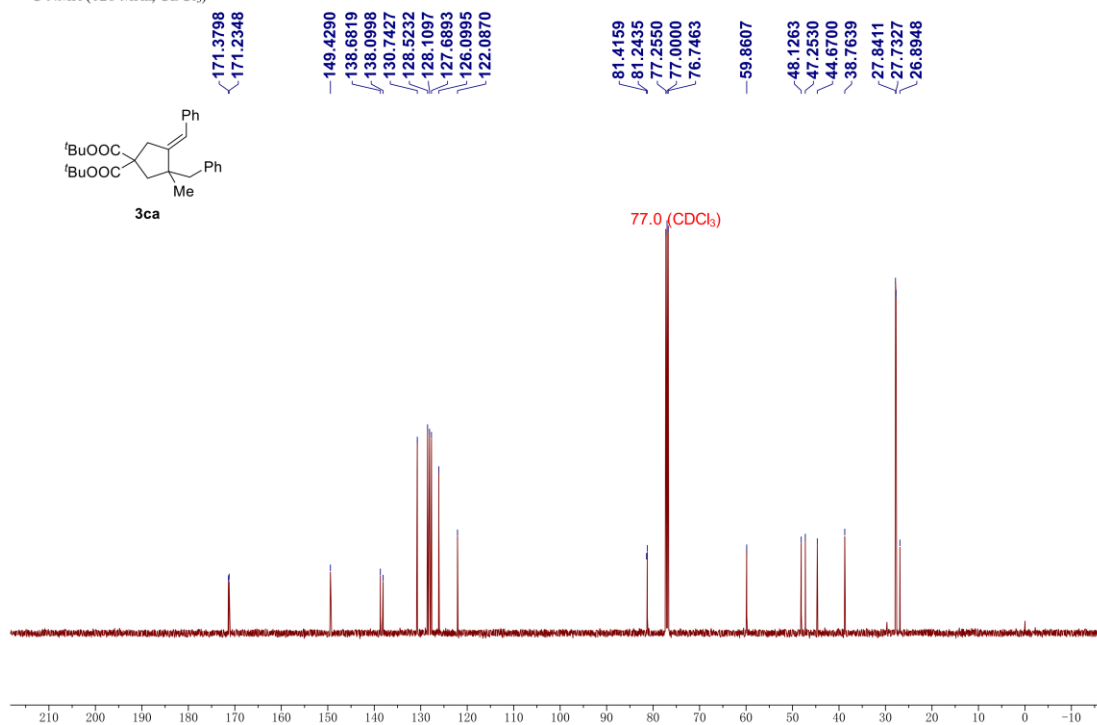
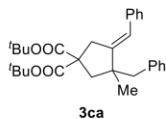


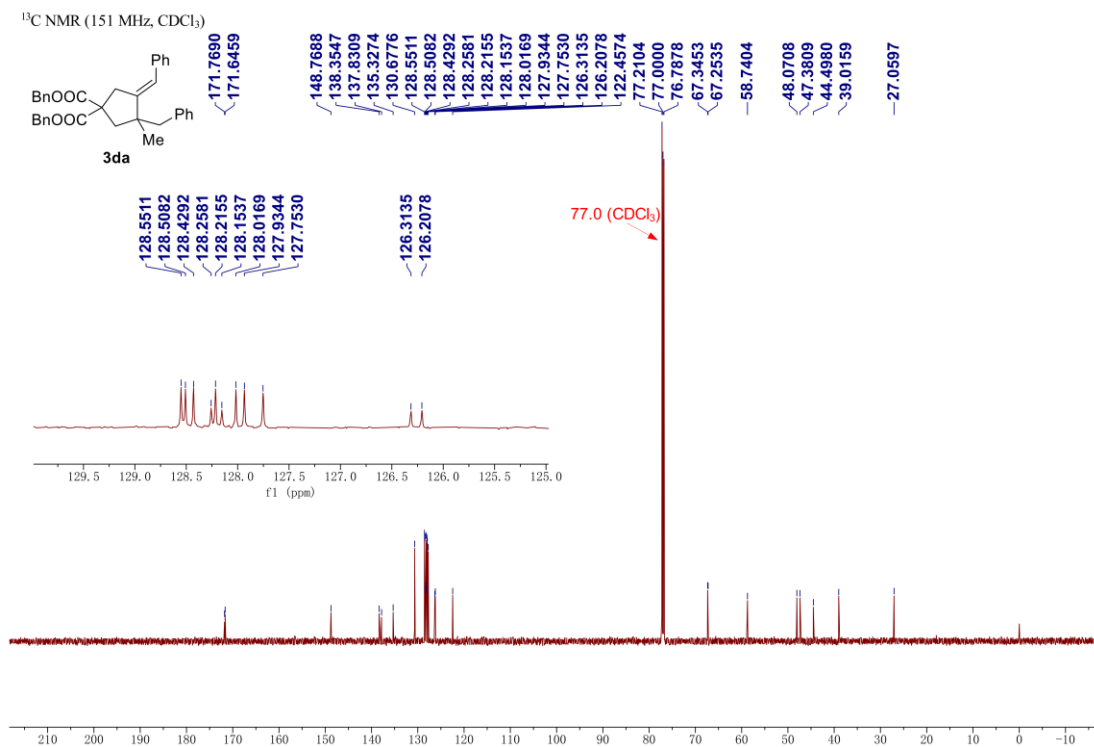
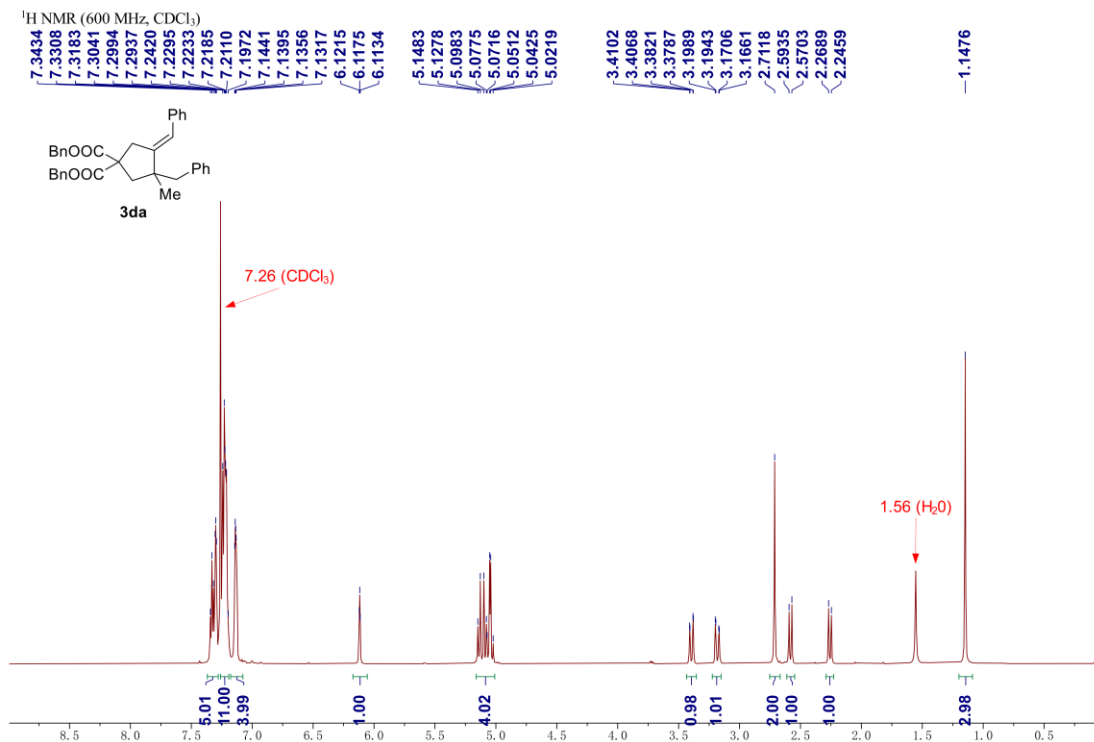


¹H NMR (600 MHz, CDCl₃)



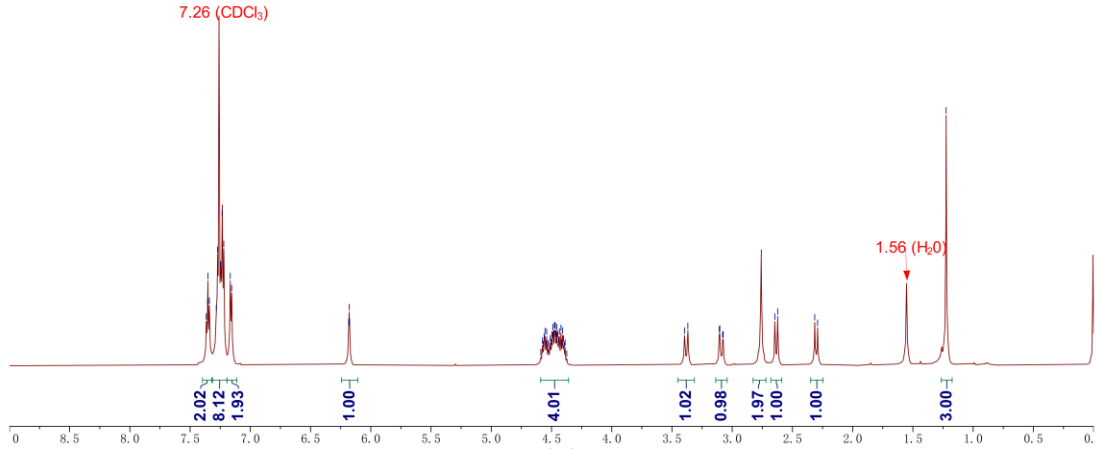
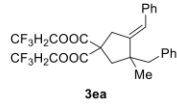
¹³C NMR (126 MHz, CDCl₃)



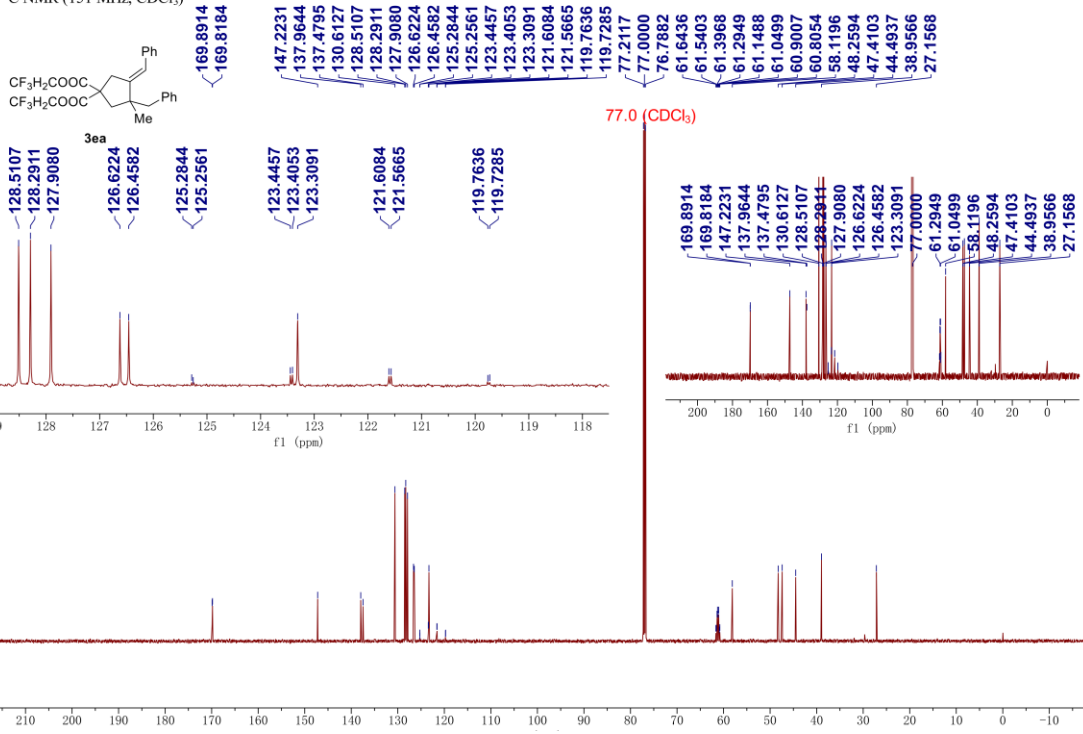


¹H NMR (600 MHz, CDCl₃)

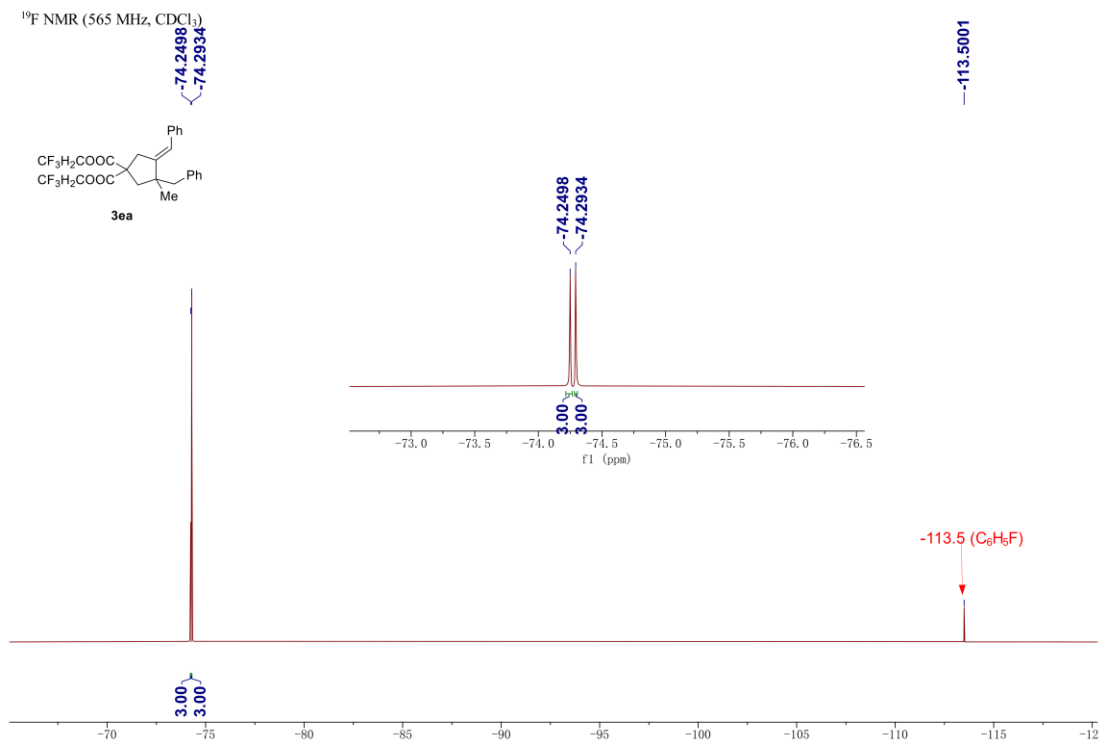
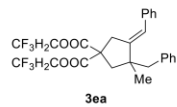
7.3656
7.3553
7.3519
7.3398
7.2829
7.2719
7.2470
7.2347
7.2203
7.1663
7.1548
6.1837
6.1797
6.1756
4.5749
4.5676
4.5612
4.5539
4.5474
4.5401
4.5264
4.5240
4.5102
4.5028
4.4965
4.4891
4.4827
4.4754
4.4690
4.4617
4.4554
4.4480
4.4416
4.4346
4.4216
4.4145
4.4081
4.4007
4.3944
4.3870
3.3960
3.3685
3.1076
3.1028
3.0794
3.0746
2.7584
2.6459
2.6224
2.3147
2.2914
1.9244

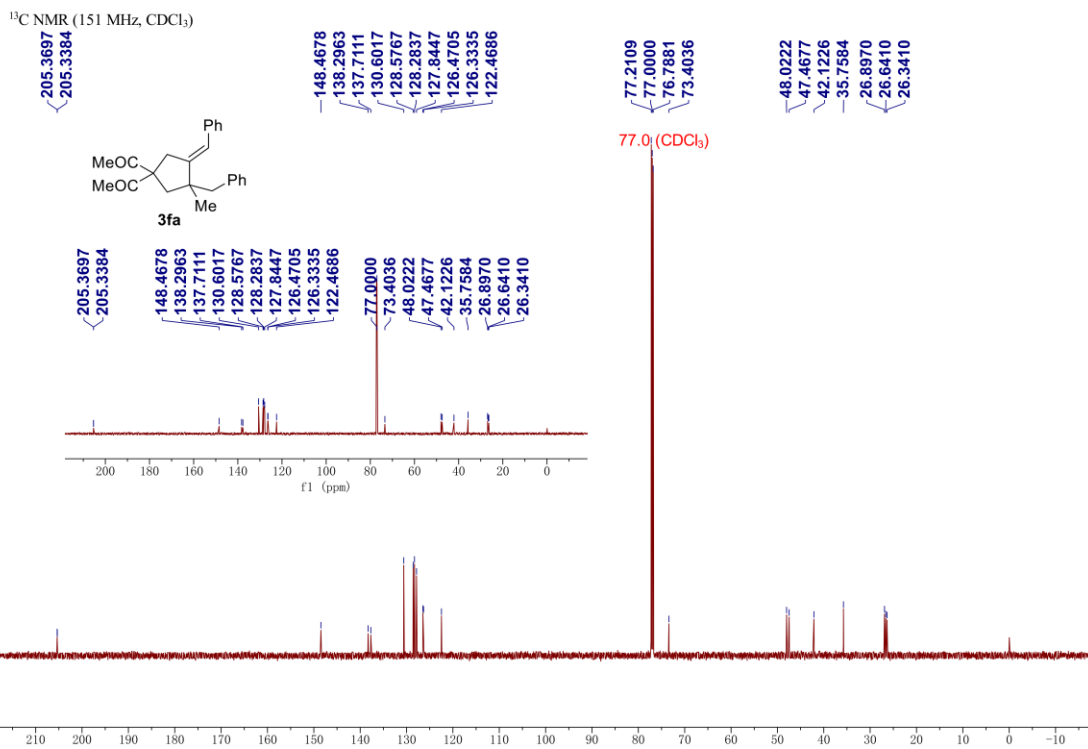
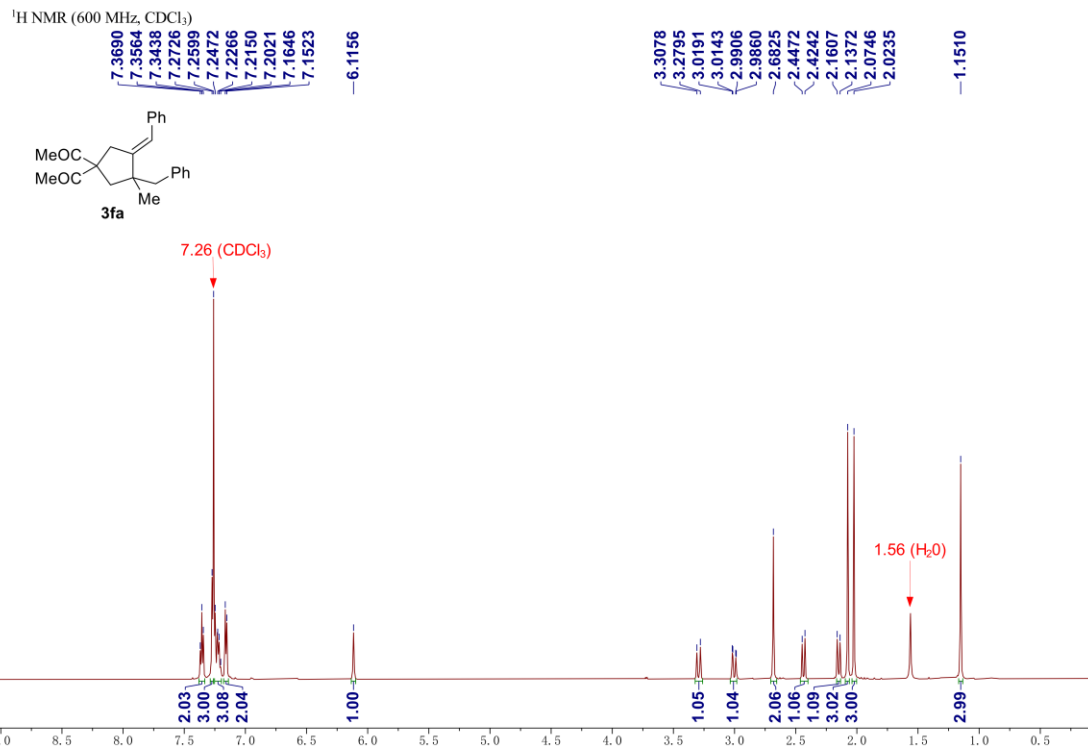


¹³C NMR (151 MHz, CDCl₃)

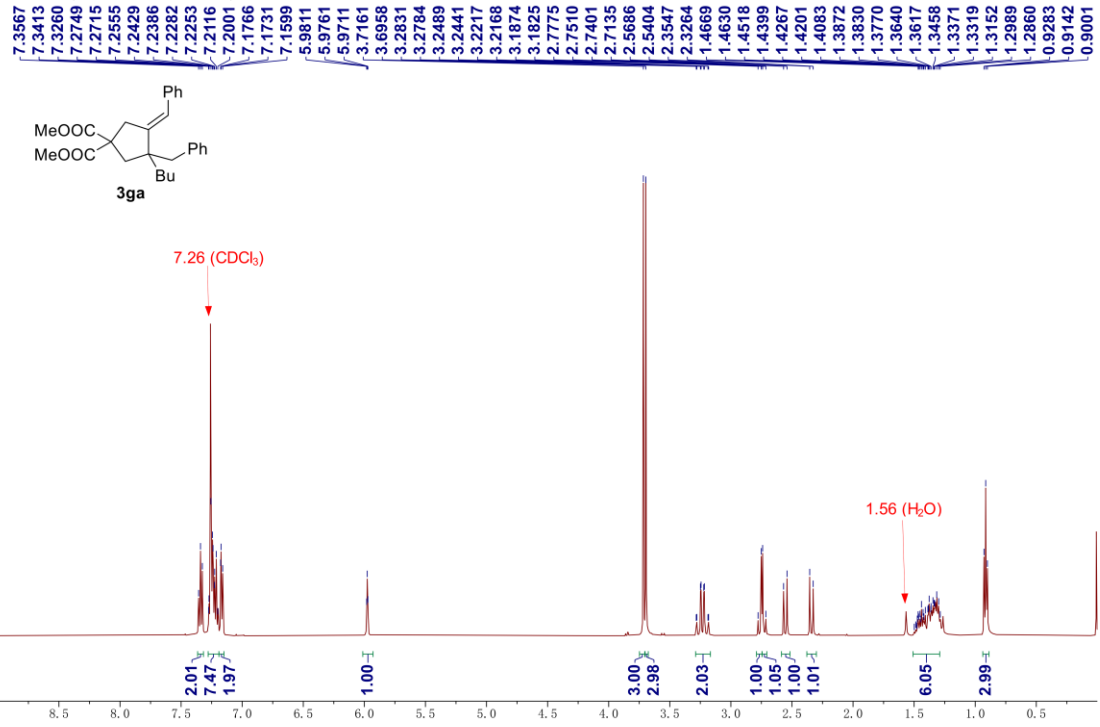


¹⁹F NMR (565 MHz, CDCl₃)

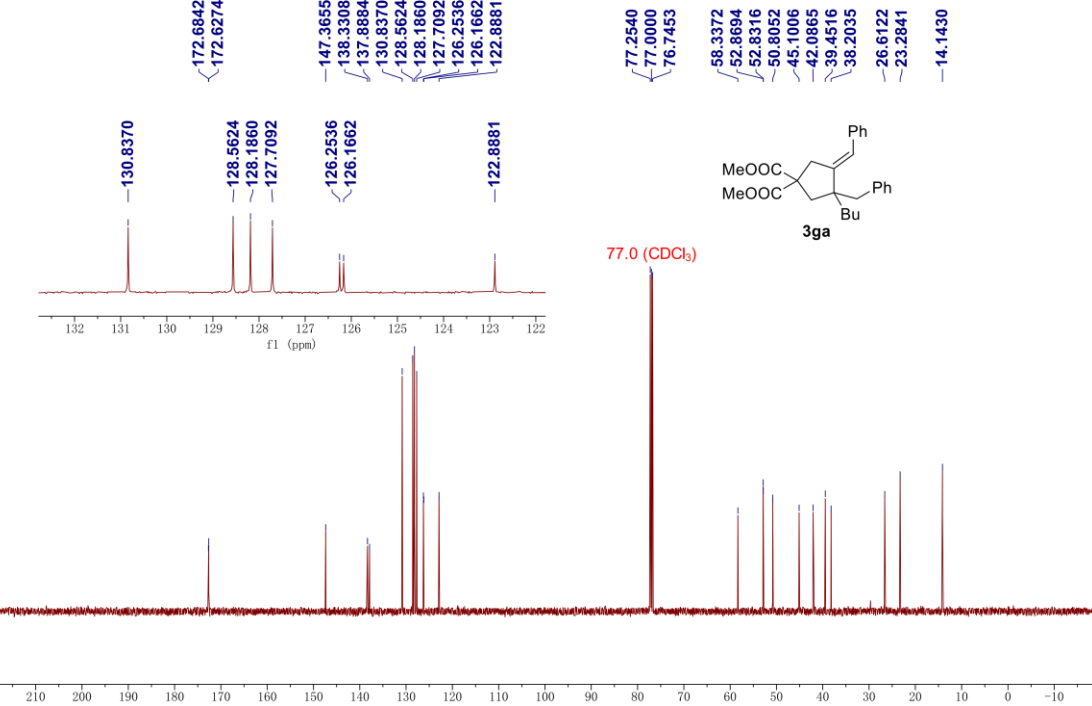




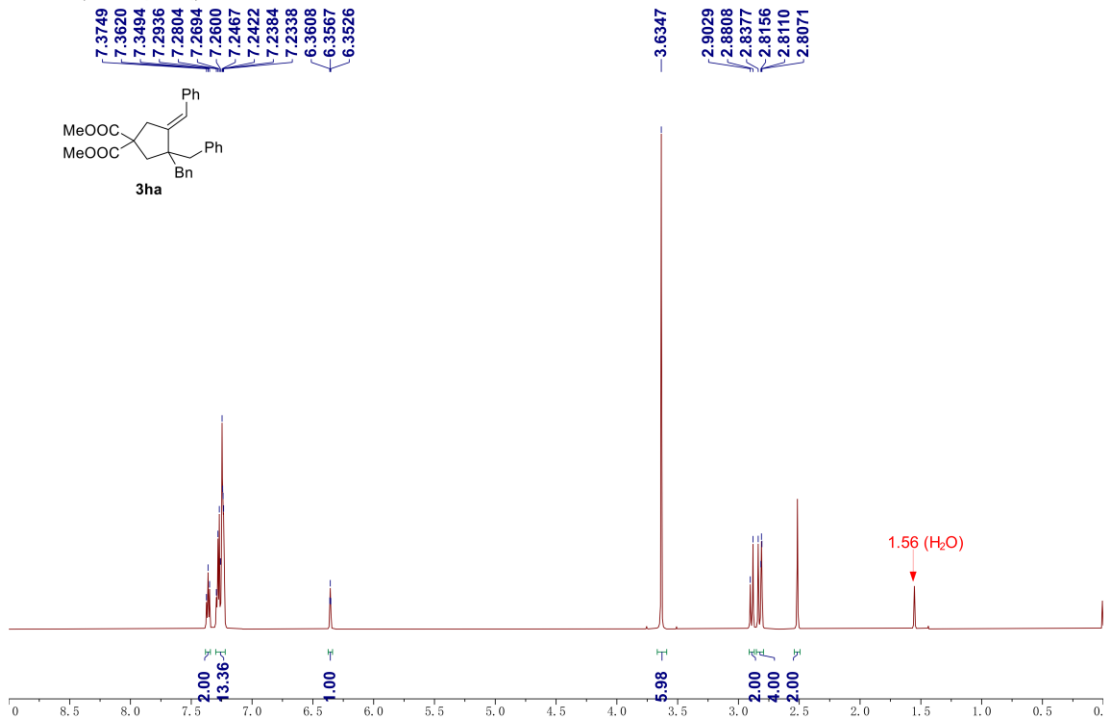
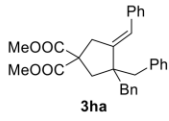
¹H NMR (500 MHz, Chloroform-*d*)



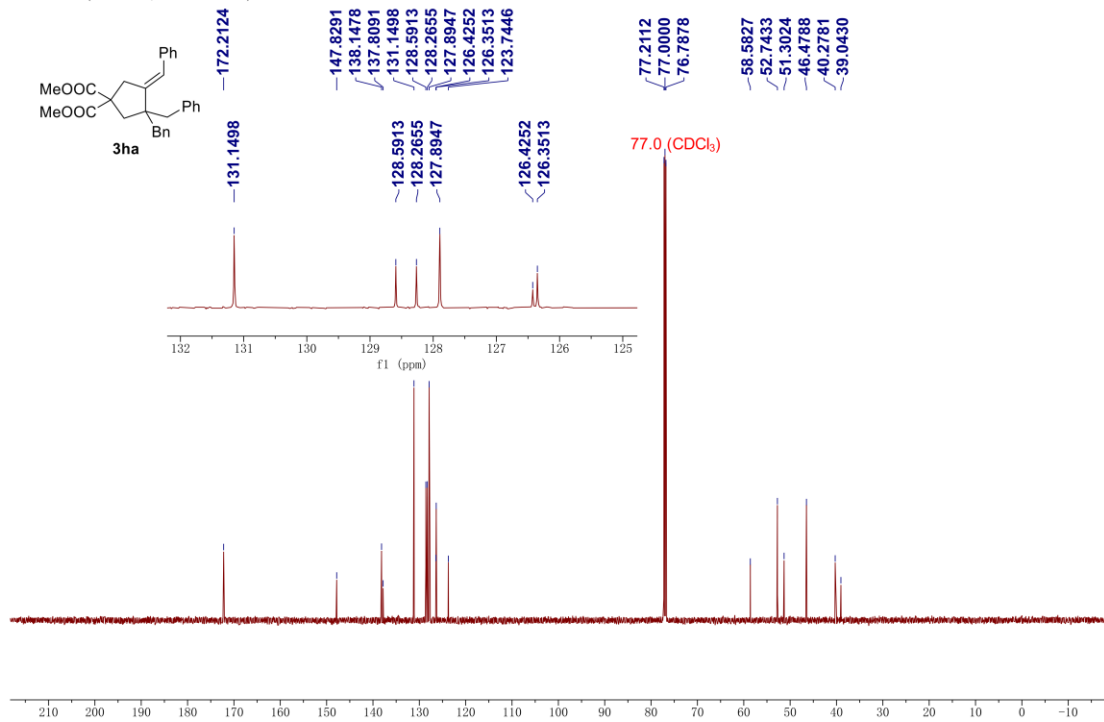
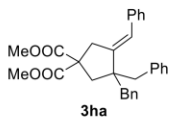
¹³C NMR (126 MHz, CDCl₃)



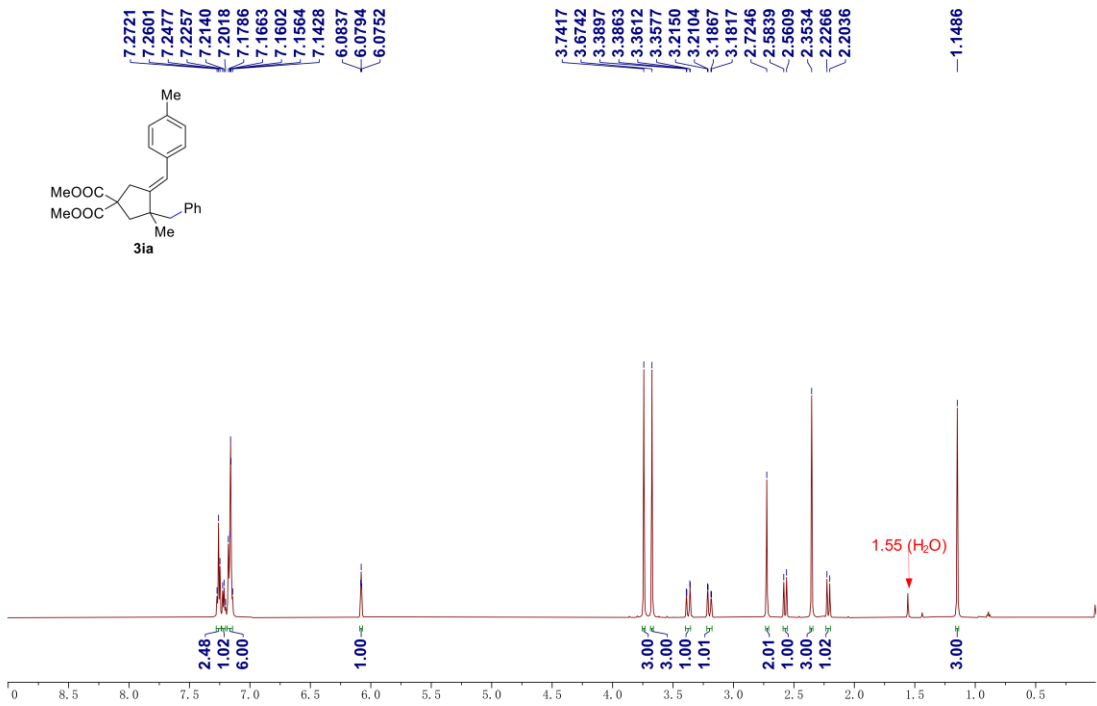
¹H NMR (600 MHz, CDCl₃)



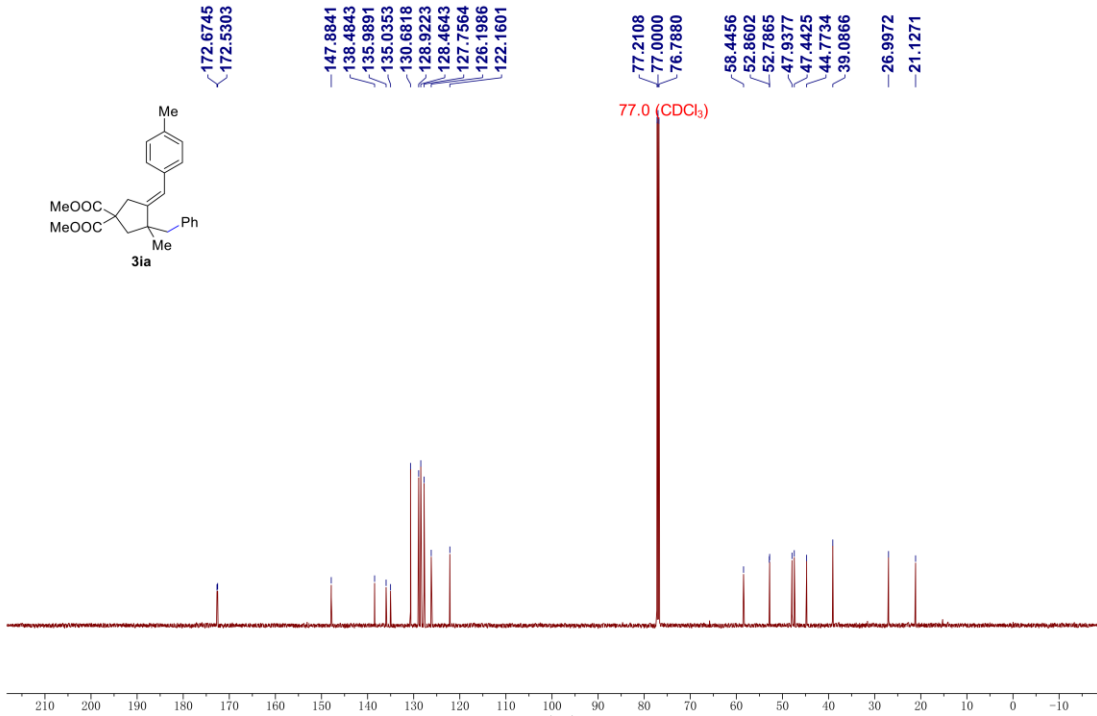
¹³C NMR (151 MHz, Chloroform-*d*)

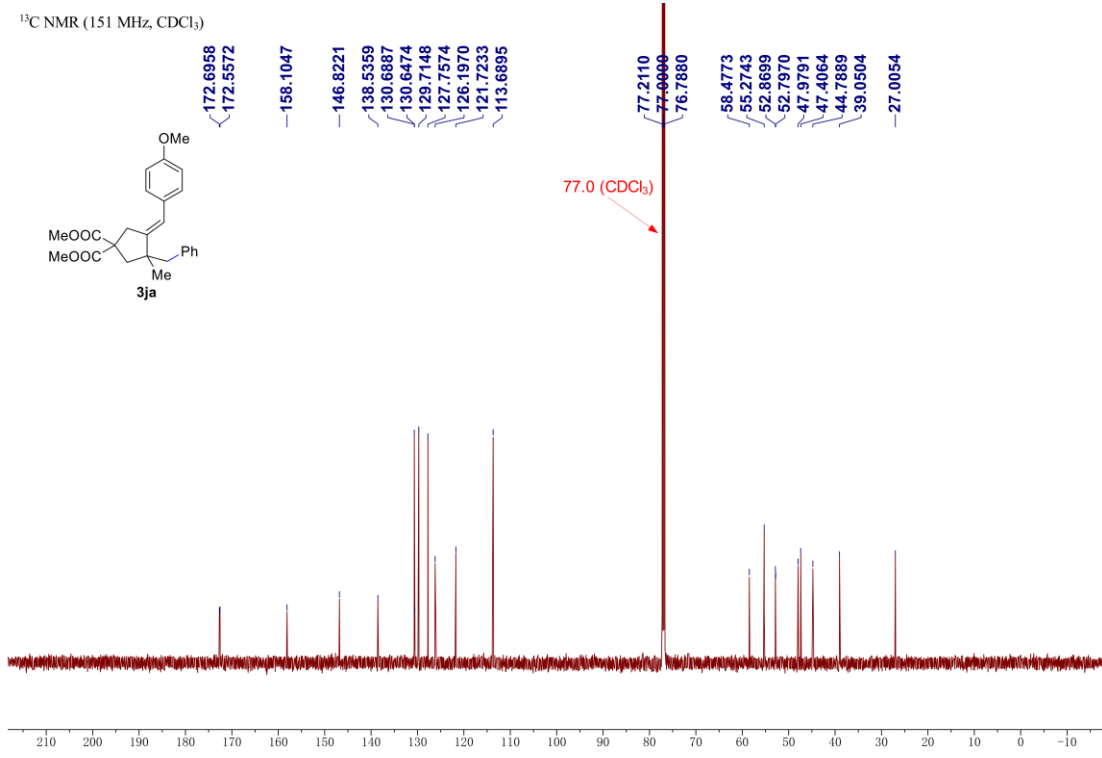
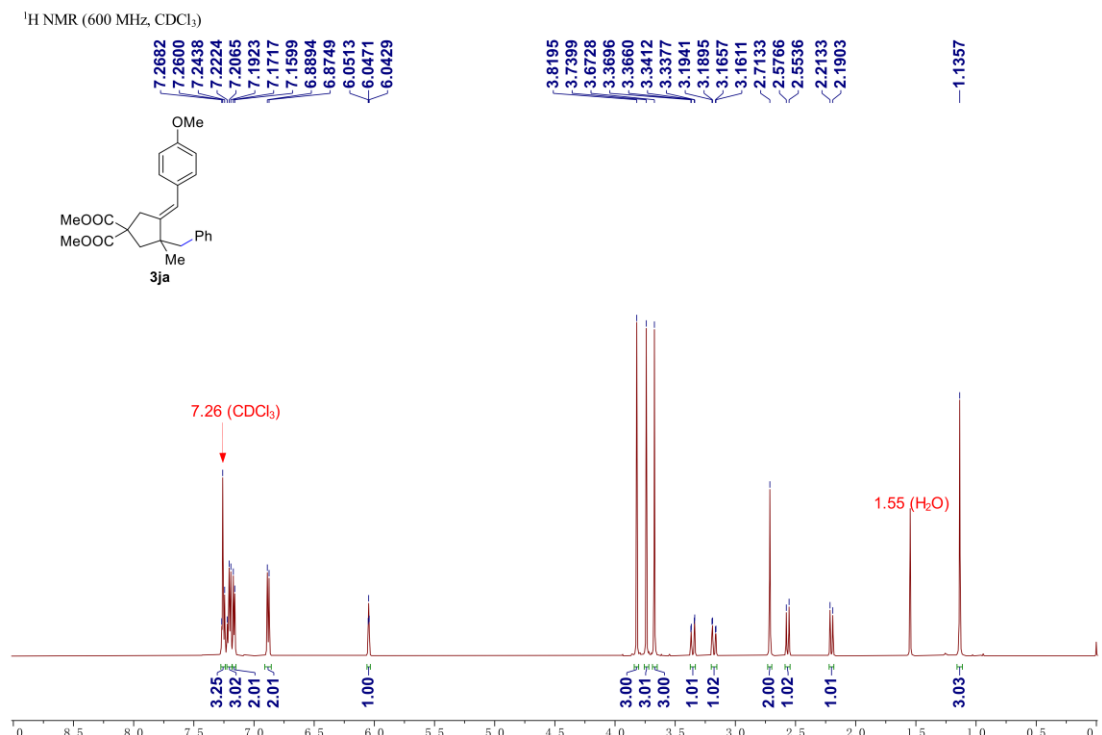


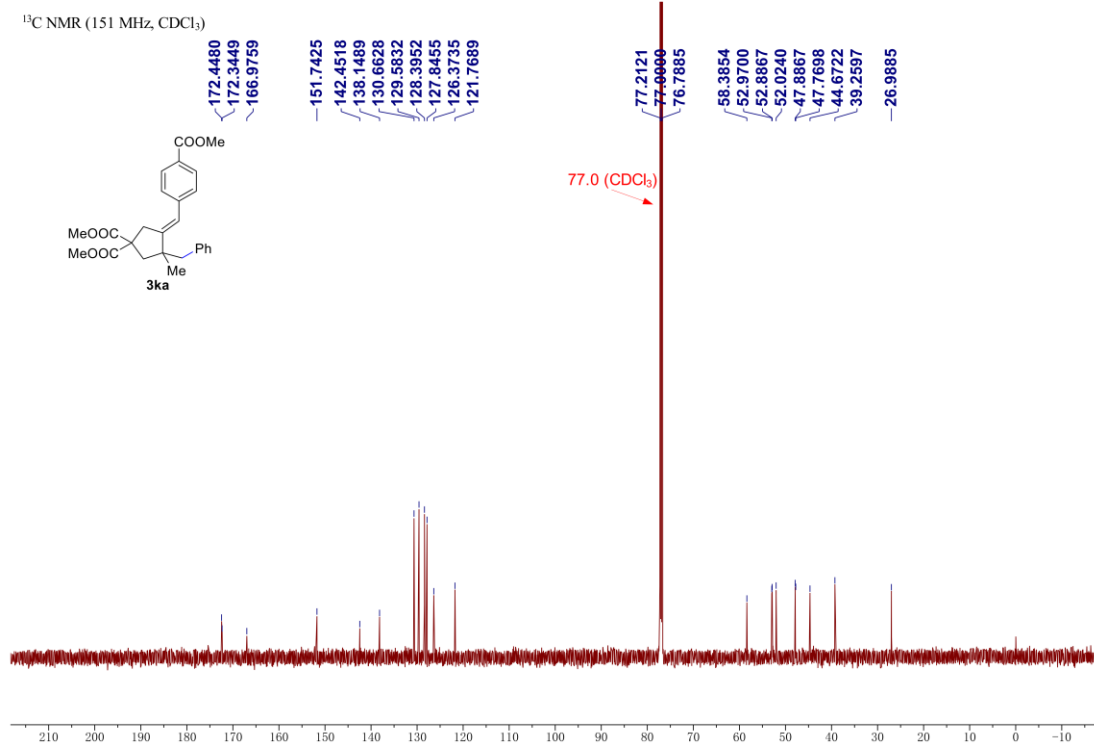
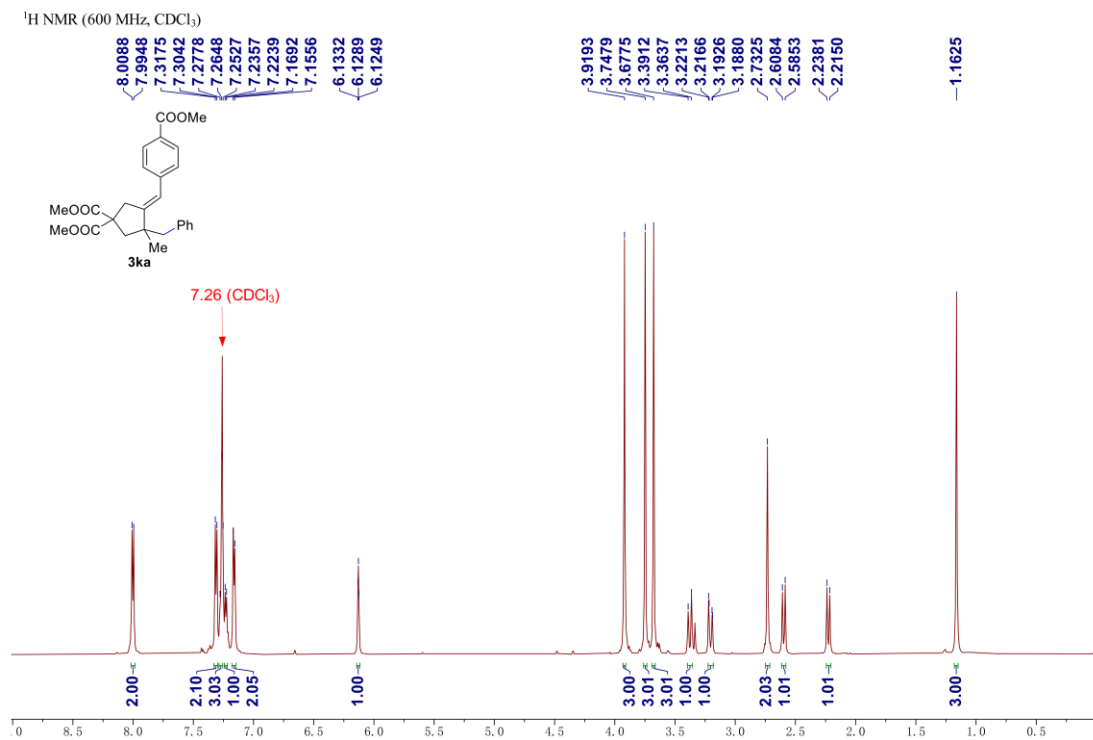
¹H NMR (600 MHz, CDCl₃)

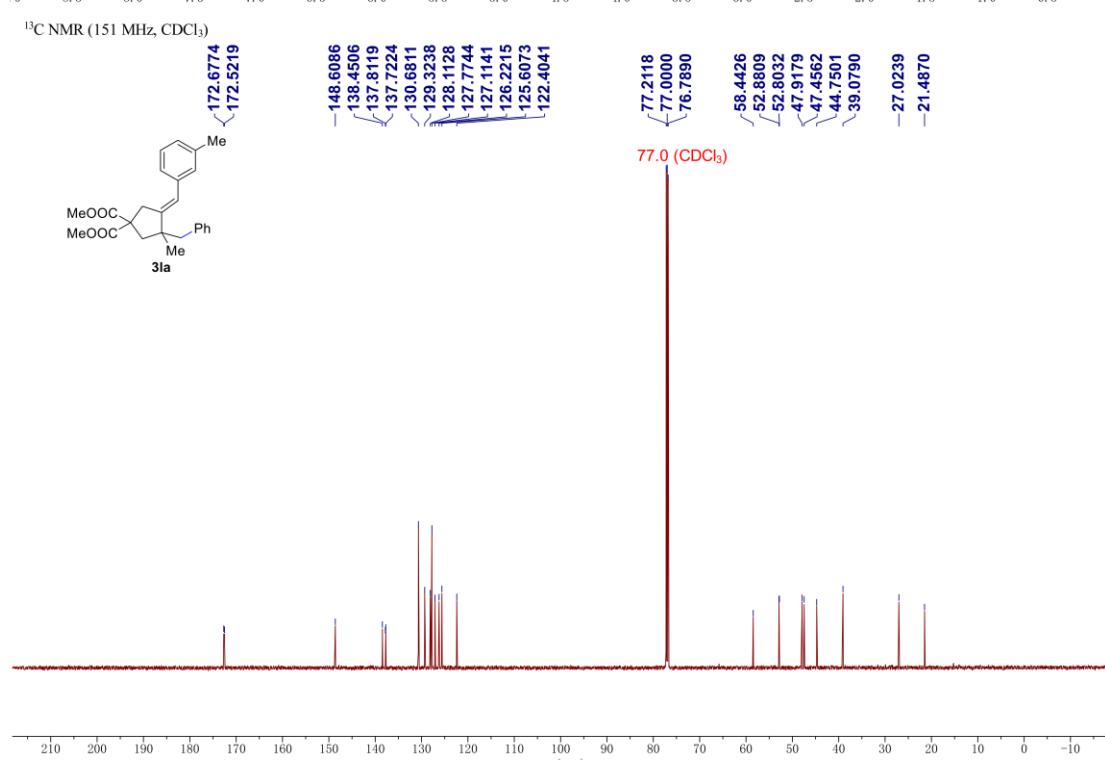
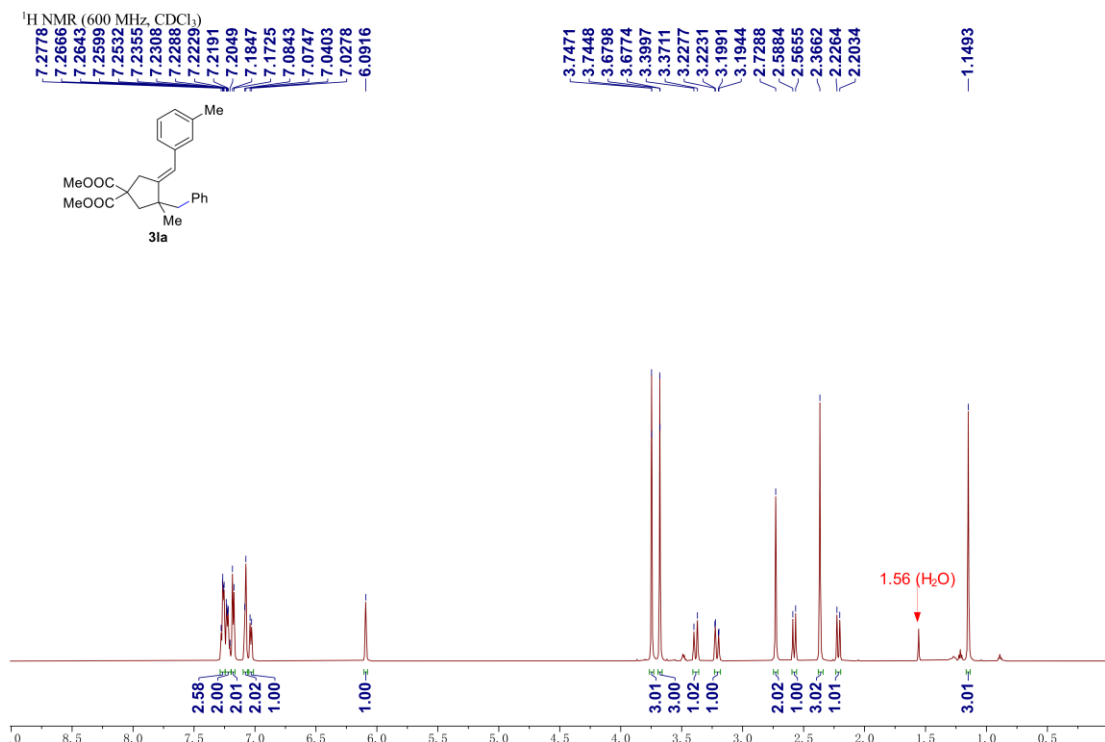


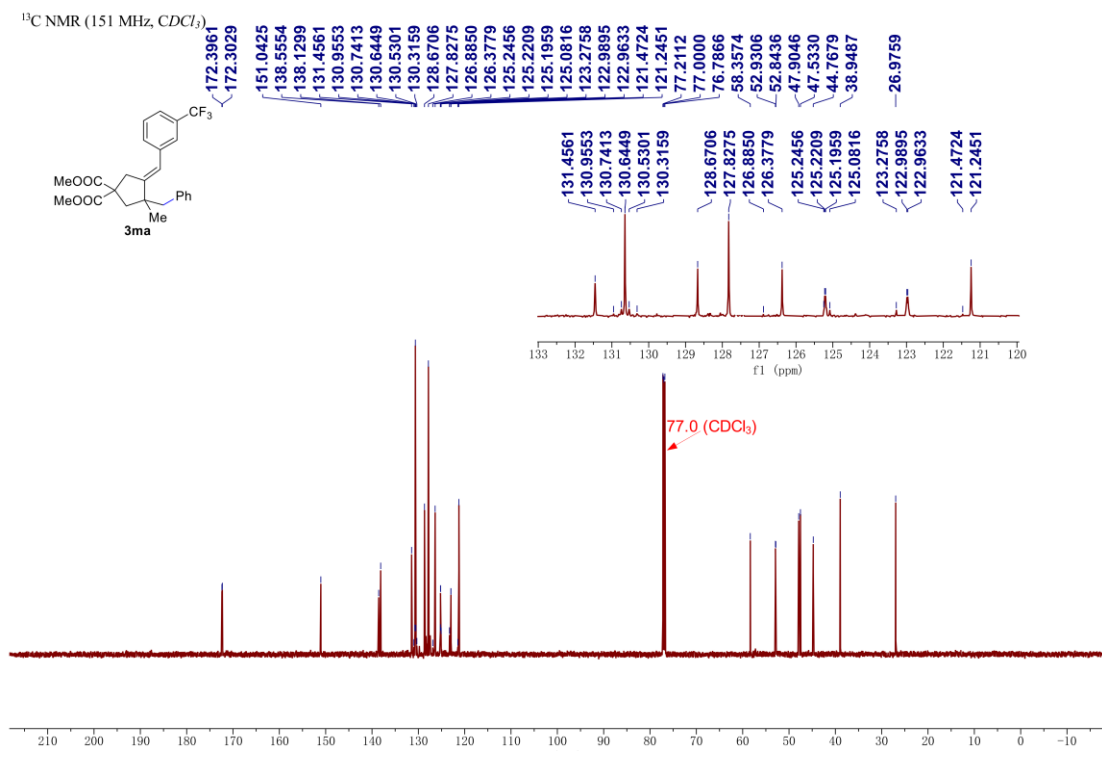
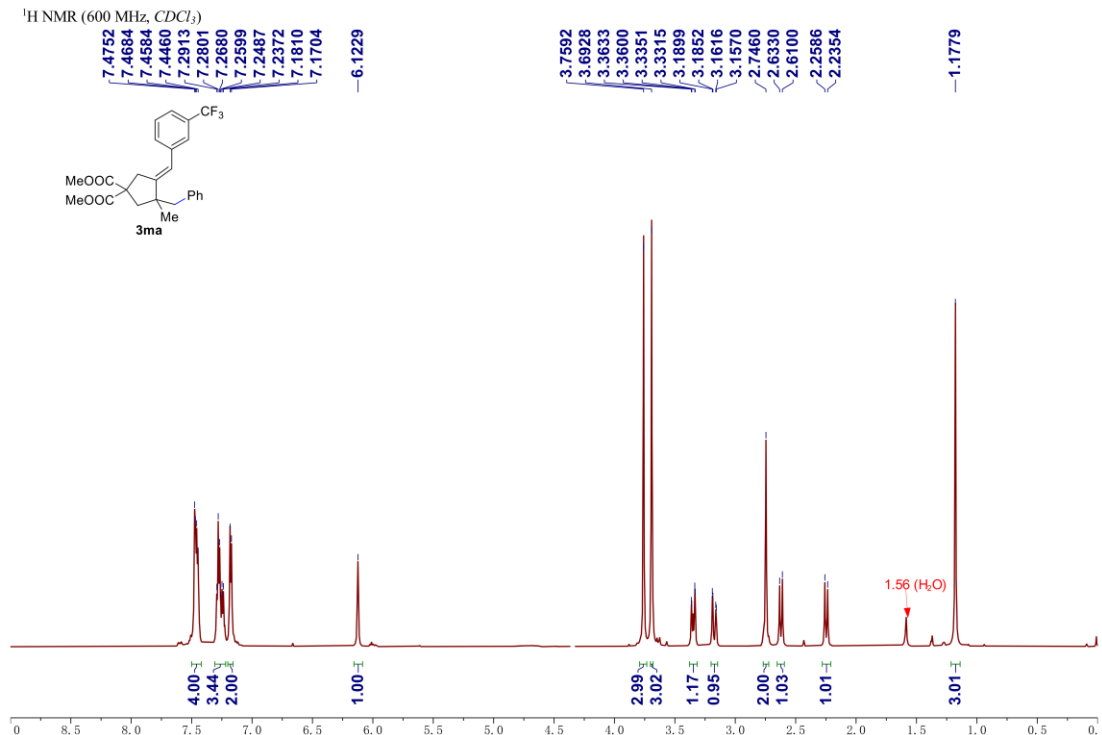
¹³C NMR (151 MHz, CDCl₃)

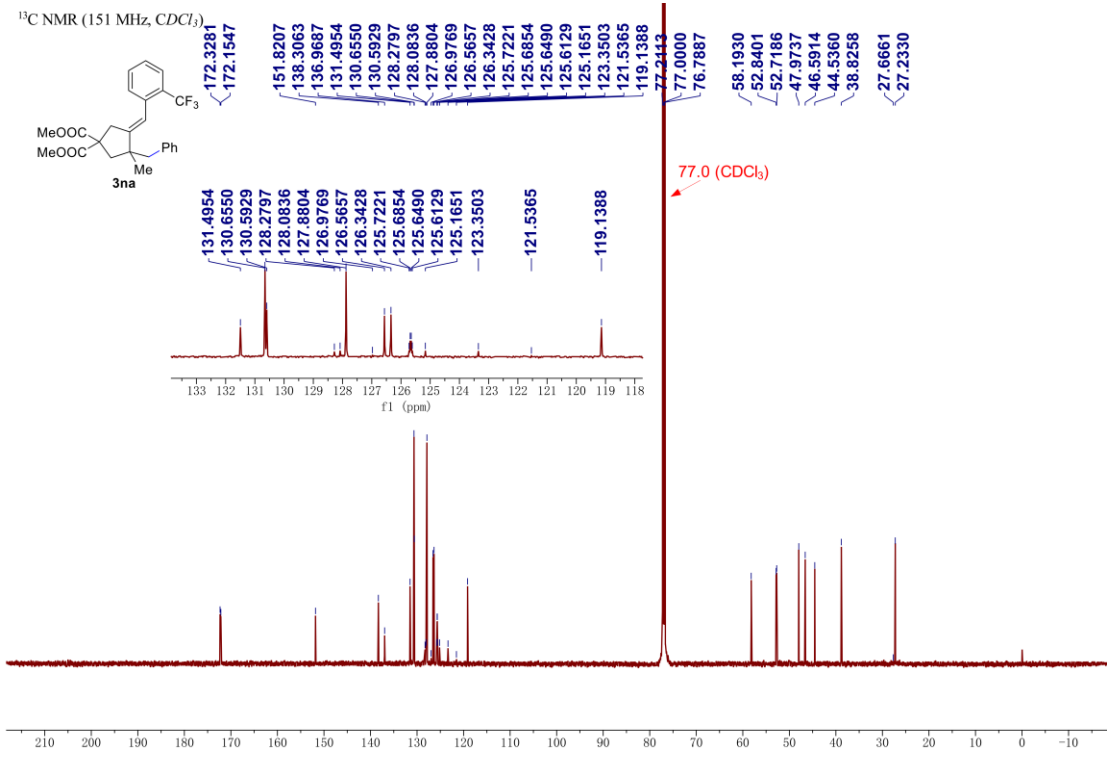
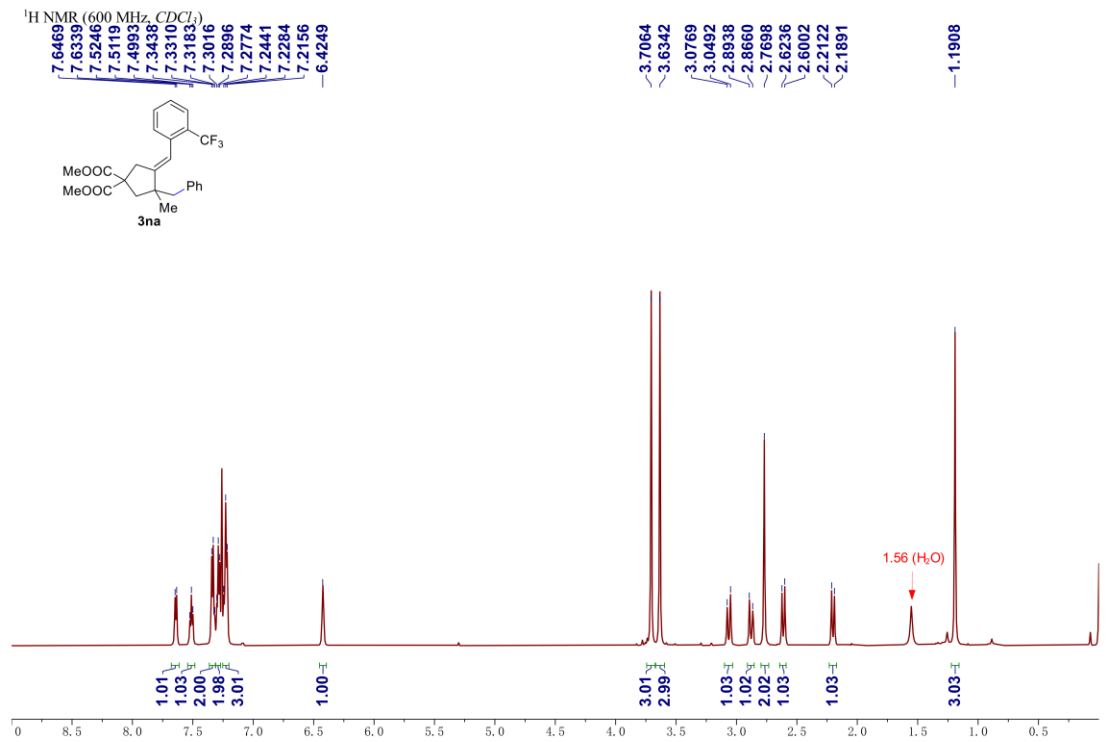




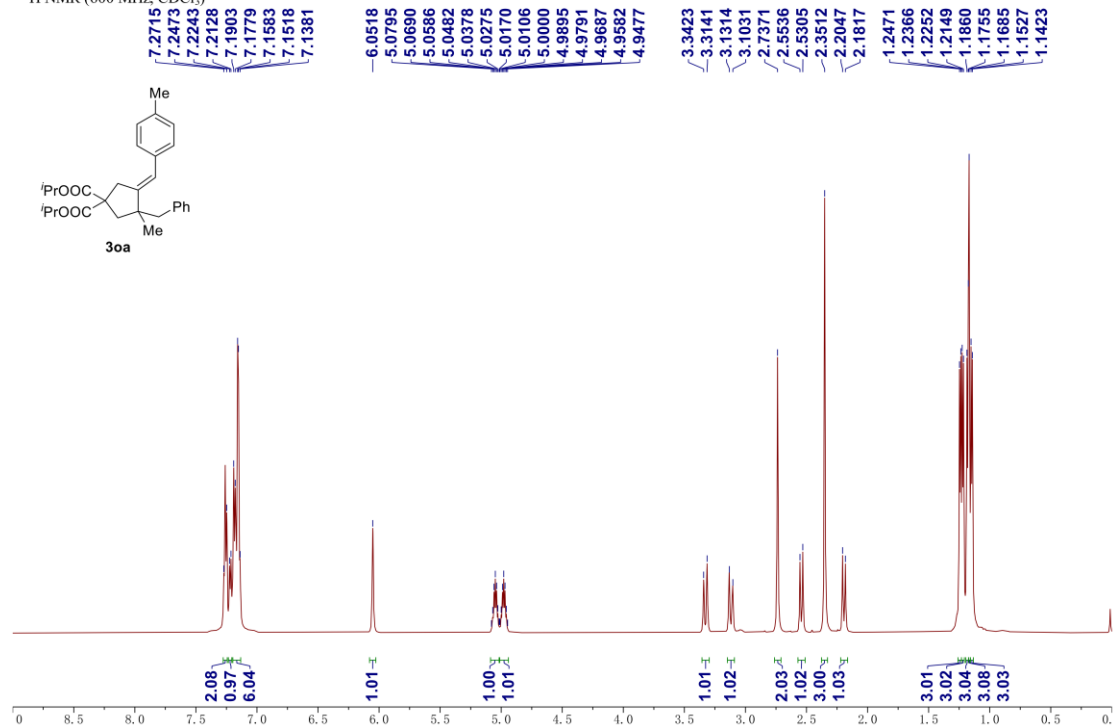




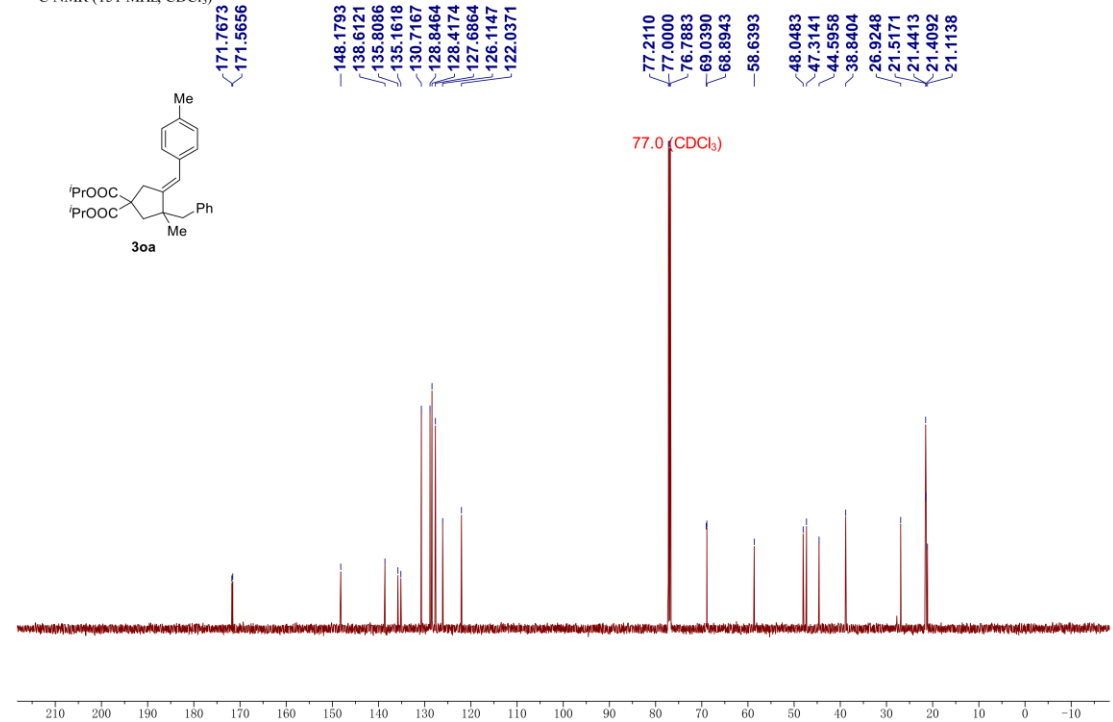




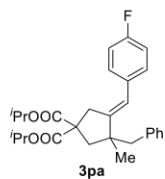
¹H NMR (600 MHz, CDCl₃)



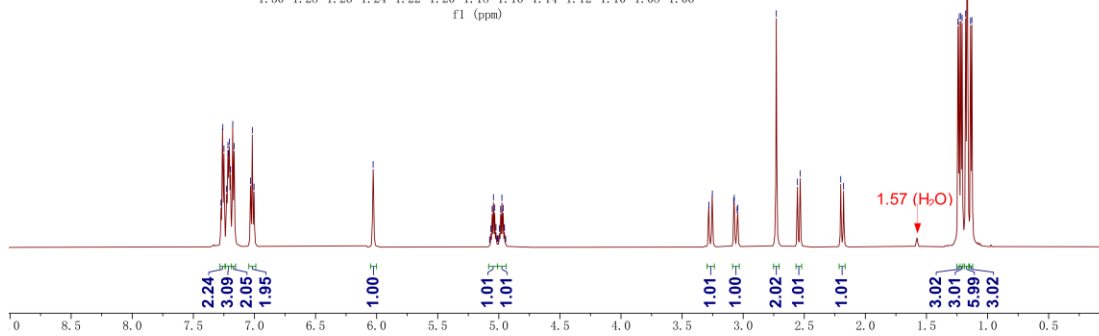
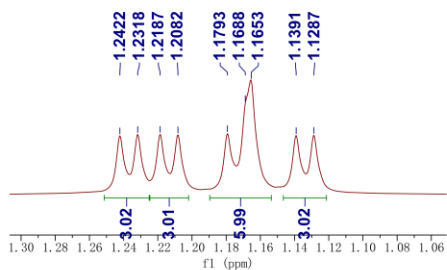
¹³C NMR (151 MHz, CDCl₃)



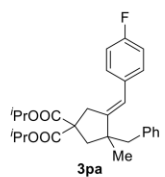
¹H NMR (600 MHz, CDCl₃)



7.2736, 7.2591, 7.2493, 7.2280, 7.2166, 7.2102, 7.2051, 7.1960, 7.1774, 7.1660, 7.0320, 7.0174, 7.0032, 6.0285, 5.0753, 5.0649, 5.0544, 5.0440, 5.0336, 5.0232, 5.0128, 5.0059, 4.9954, 4.9850, 4.9746, 4.9641, 4.9538, 4.9433, 3.2803, 3.2523, 3.0775, 3.0728, 3.0494, 3.0448, 2.7290, 2.5563, 2.5333, 2.2015, 2.1784, 1.2422, 1.2318, 1.2187, 1.2082, 1.1793, 1.1688, 1.1653, 1.1391, 1.1287



¹³C NMR (151 MHz, CDCl₃)



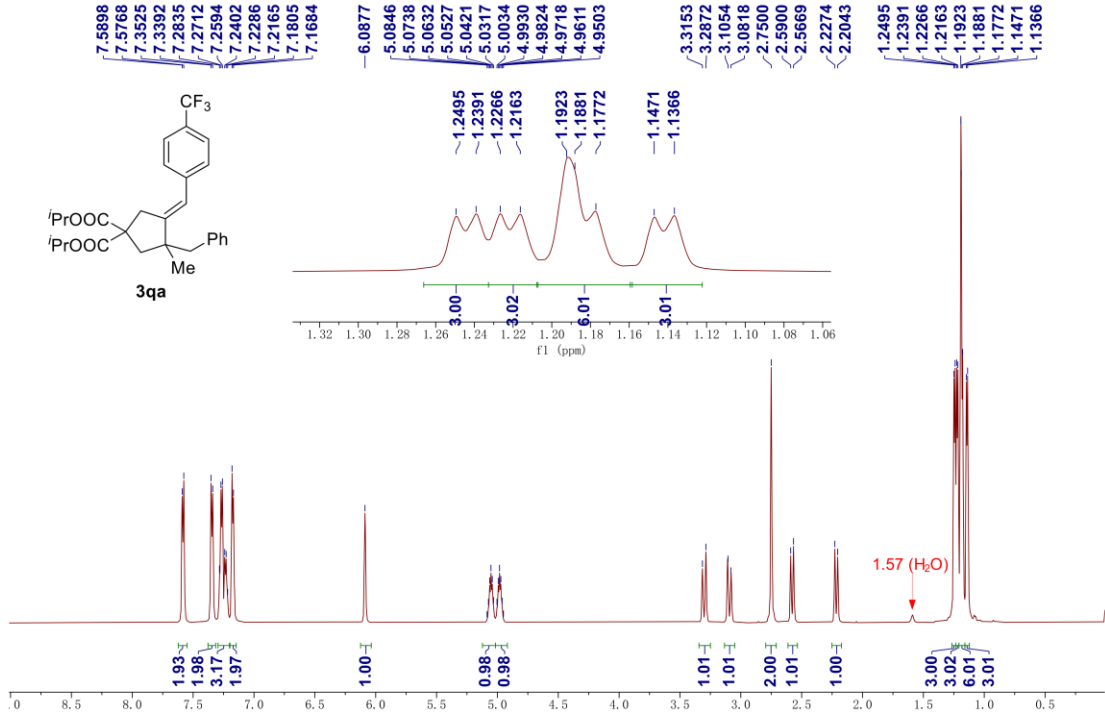
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77.0 (CDCl₃)

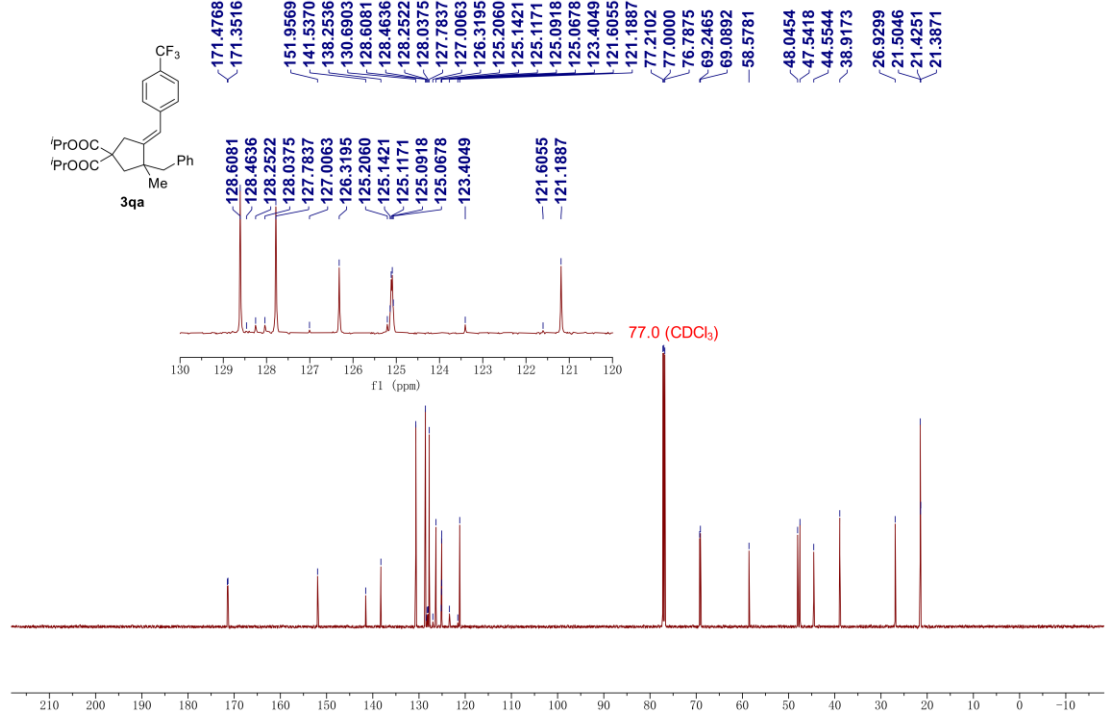
77.2113, 77.0000, 76.7880, 69.1340, 68.9717, 58.5974, 48.0642, 47.2654, 44.5567, 38.7281, 26.9010, 21.5111, 21.4310, 21.3940

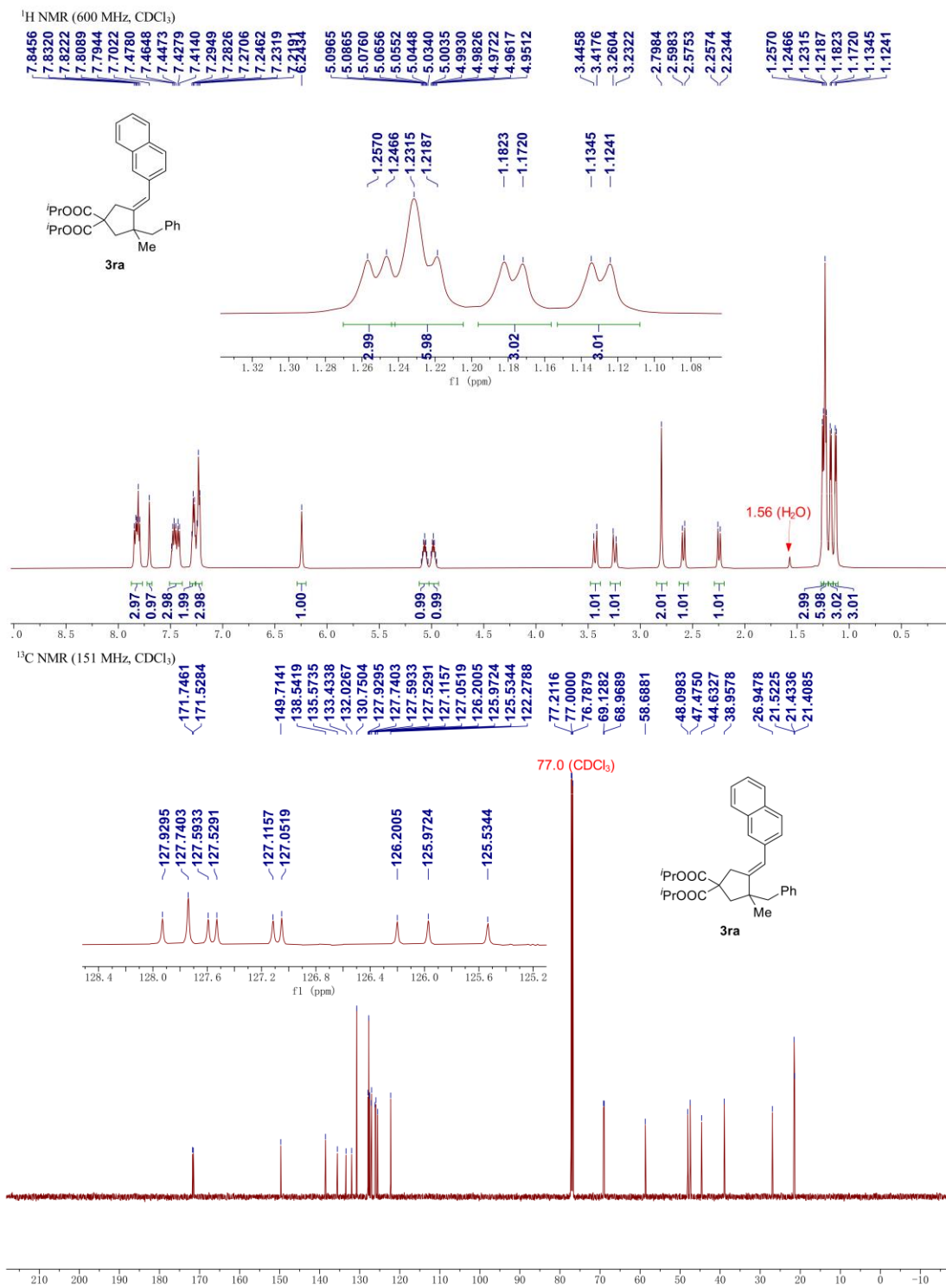
210, 200, 190, 180, 170, 160, 150, 140, 130, 120, 110, 100, 90, 80, 70, 60, 50, 40, 30, 20, 10, 0, -10

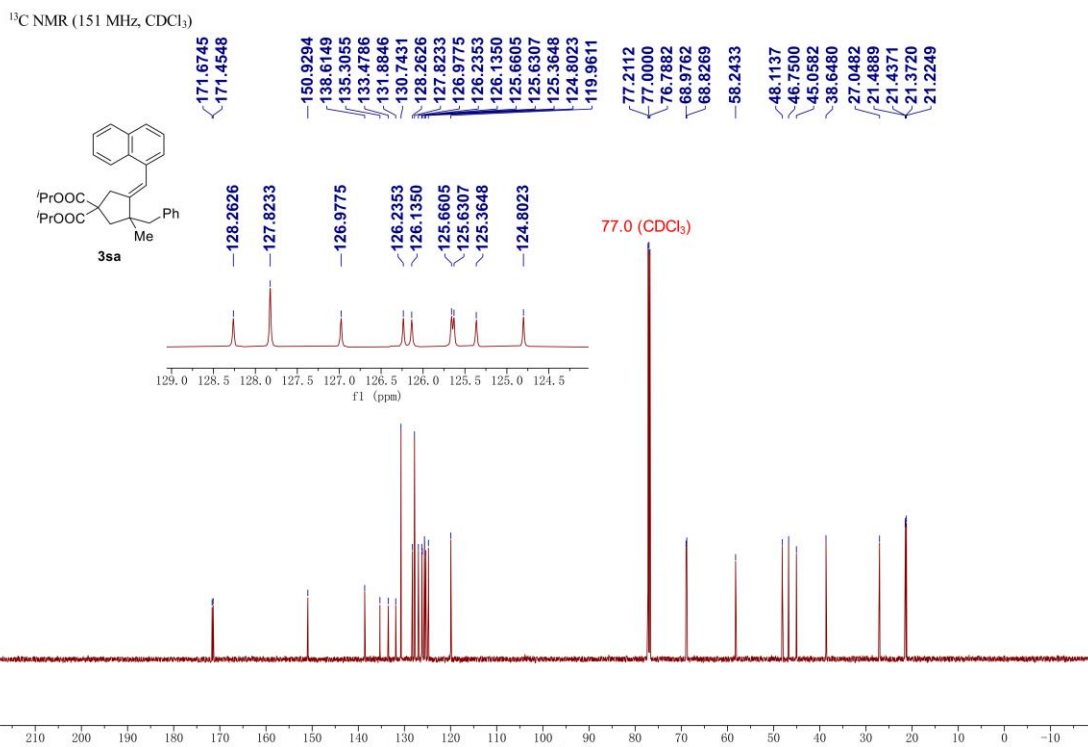
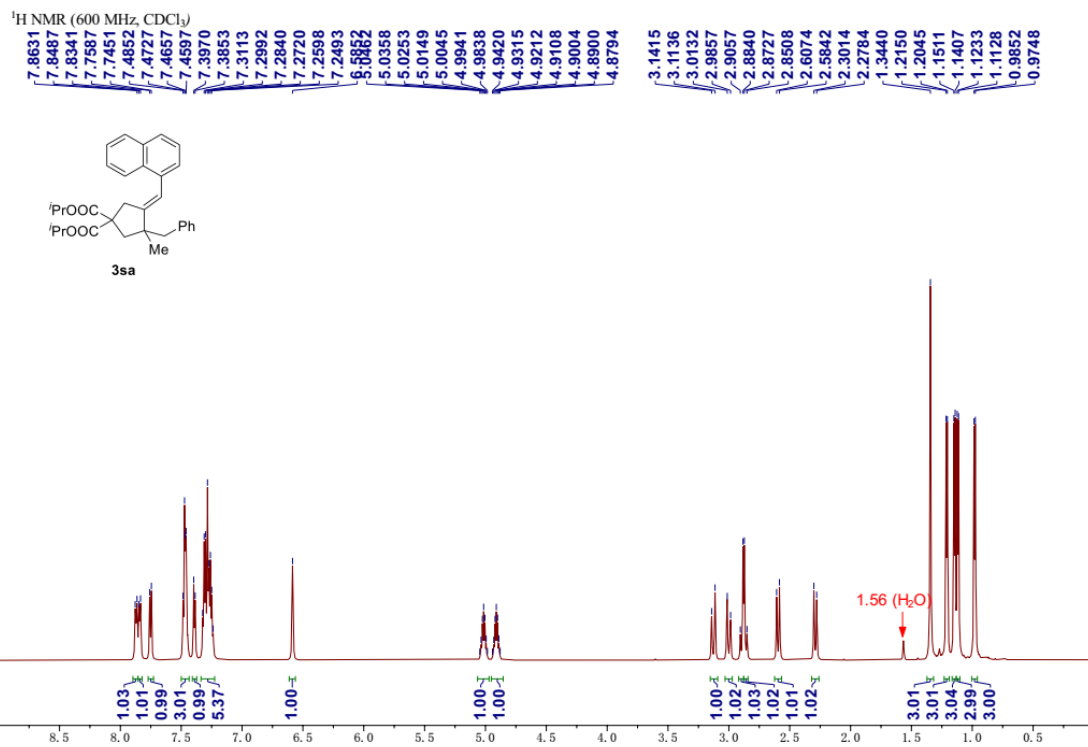
¹H NMR (600 MHz, CDCl₃)

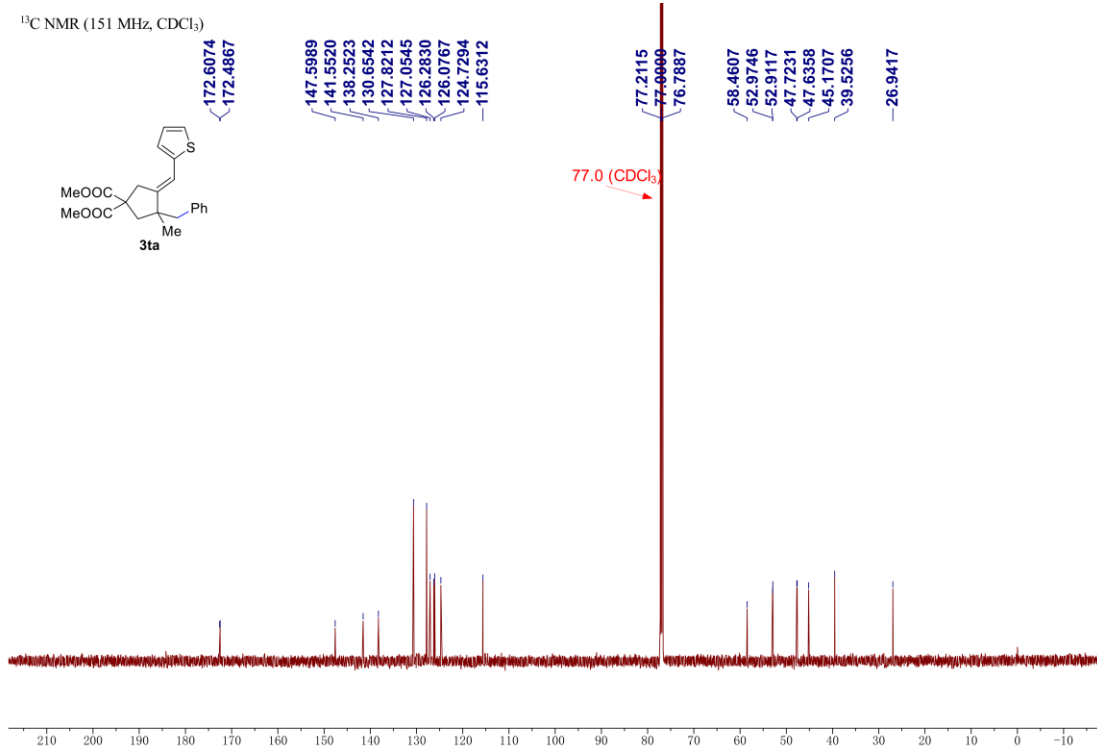
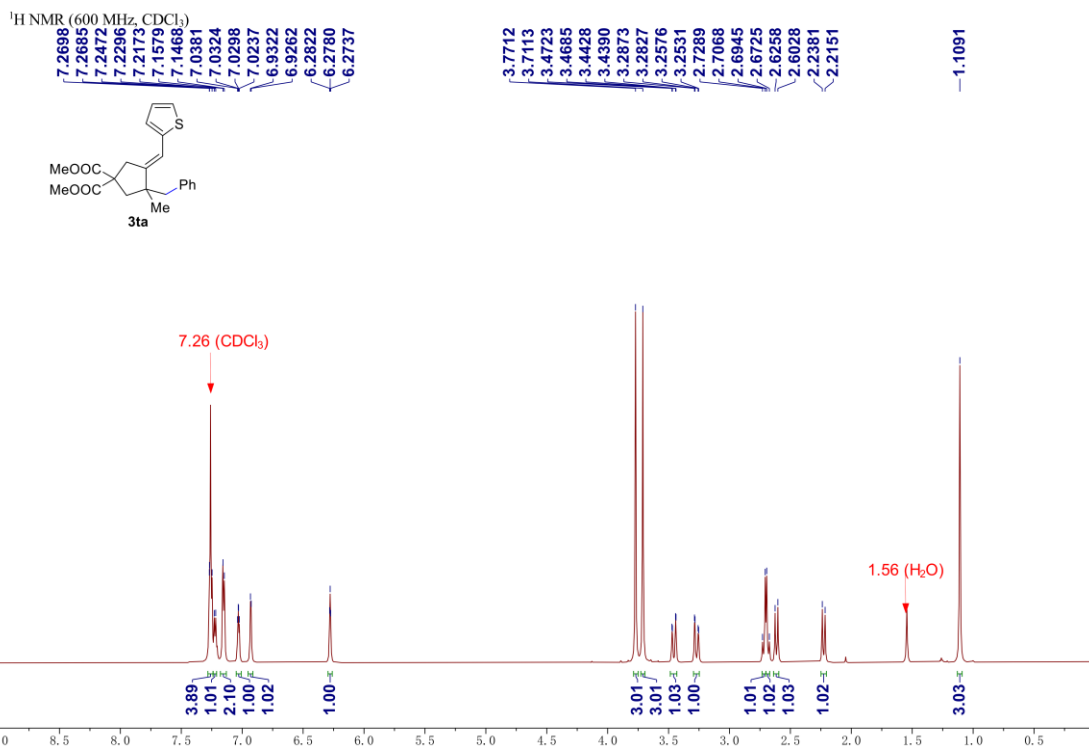


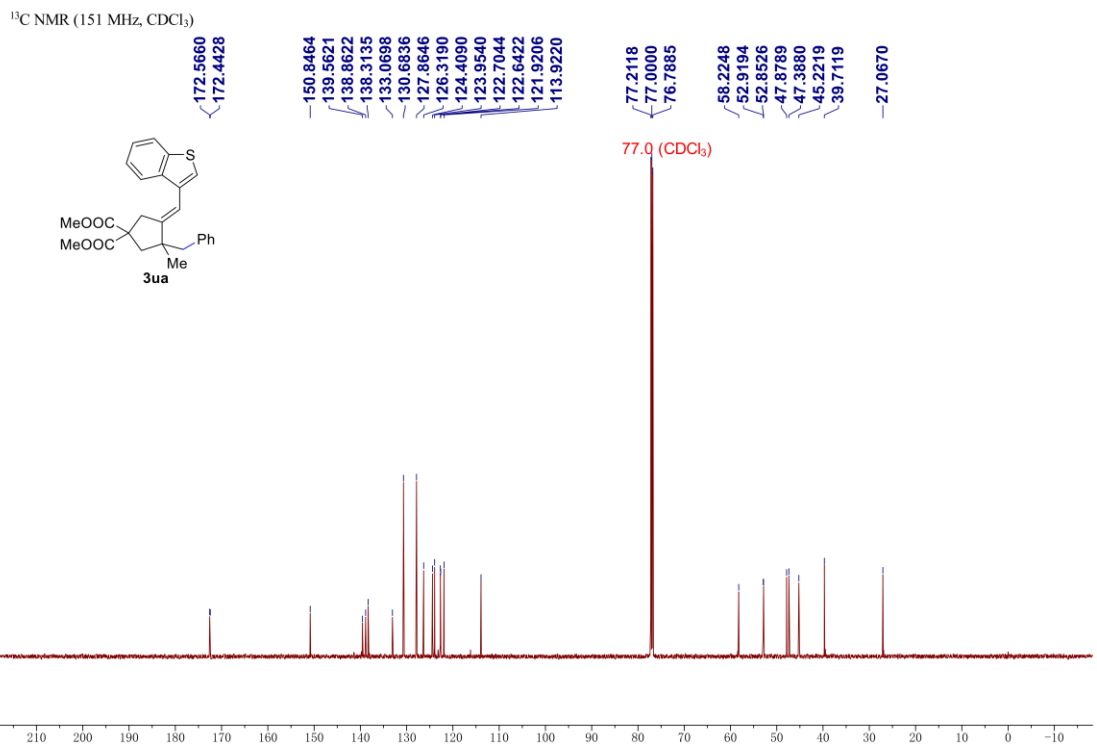
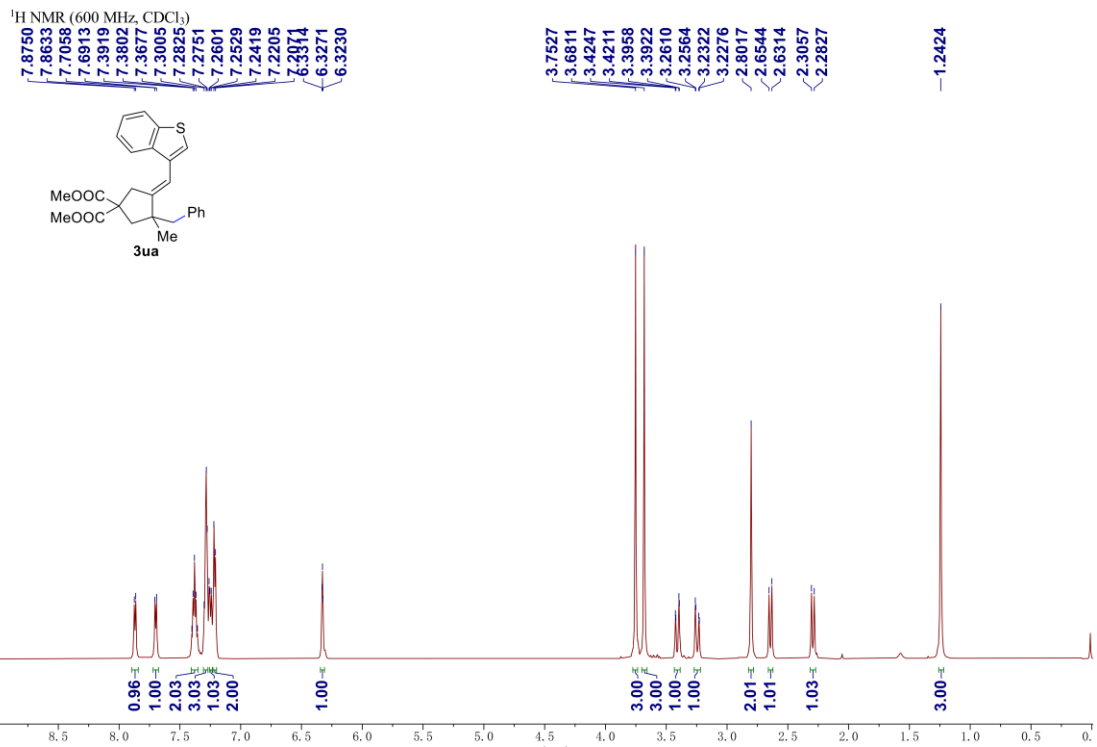
¹³C NMR (151 MHz, CDCl₃)

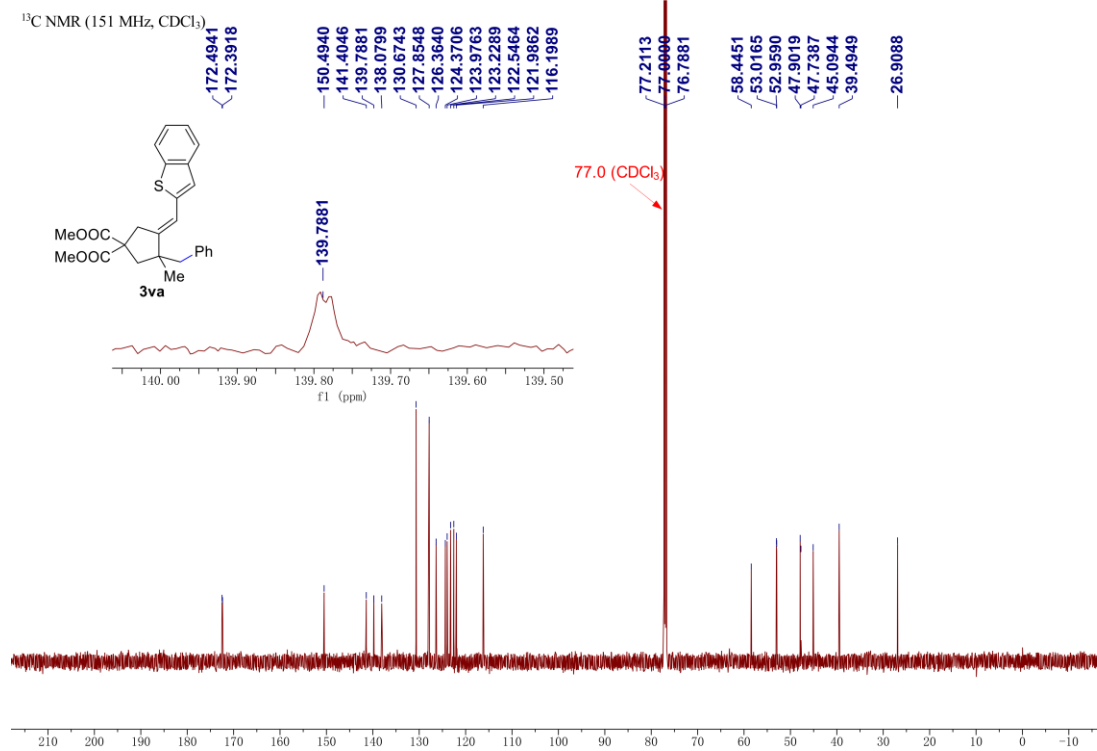
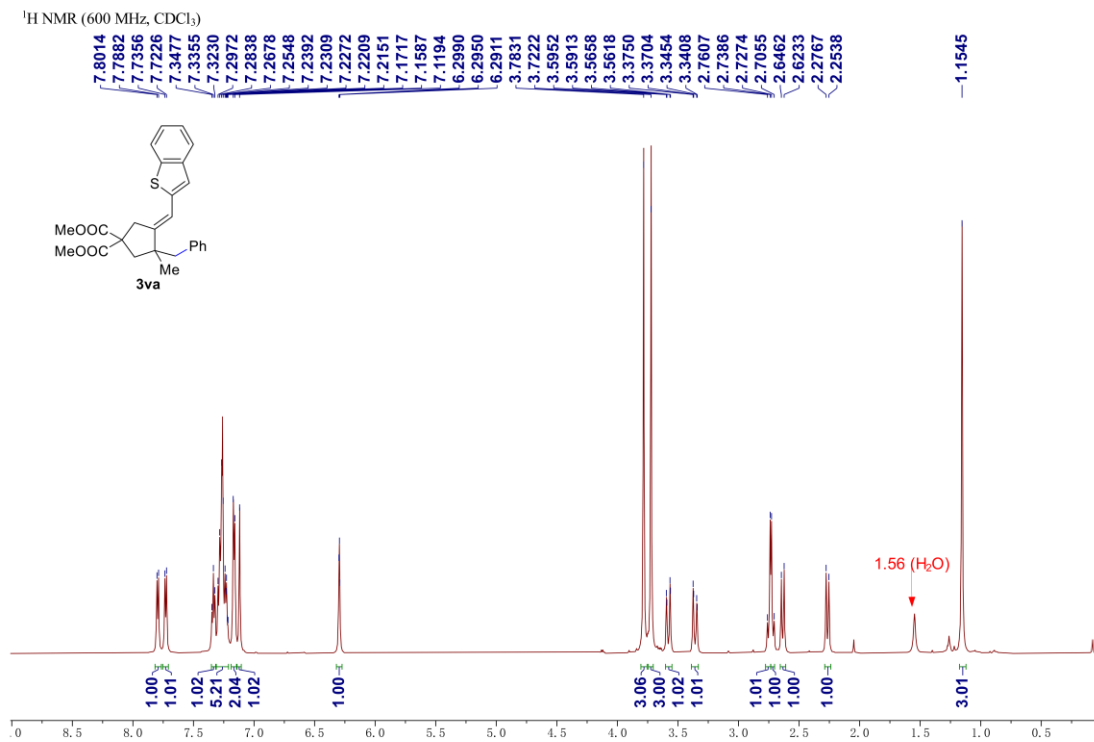


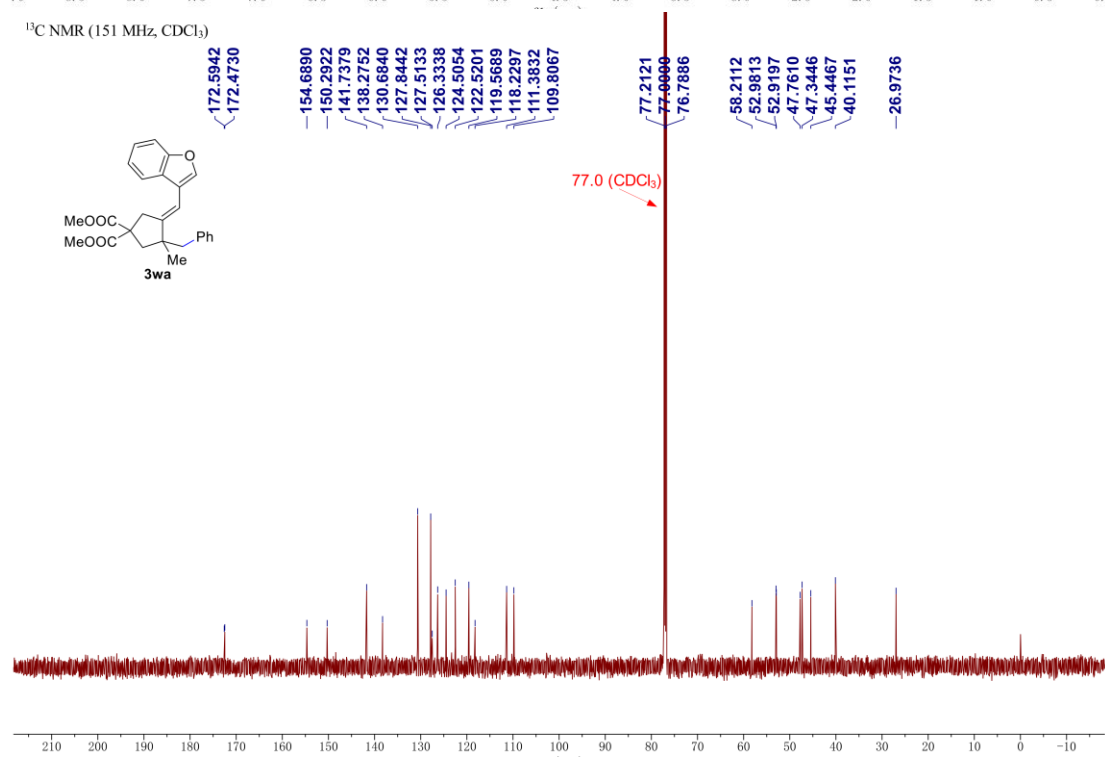
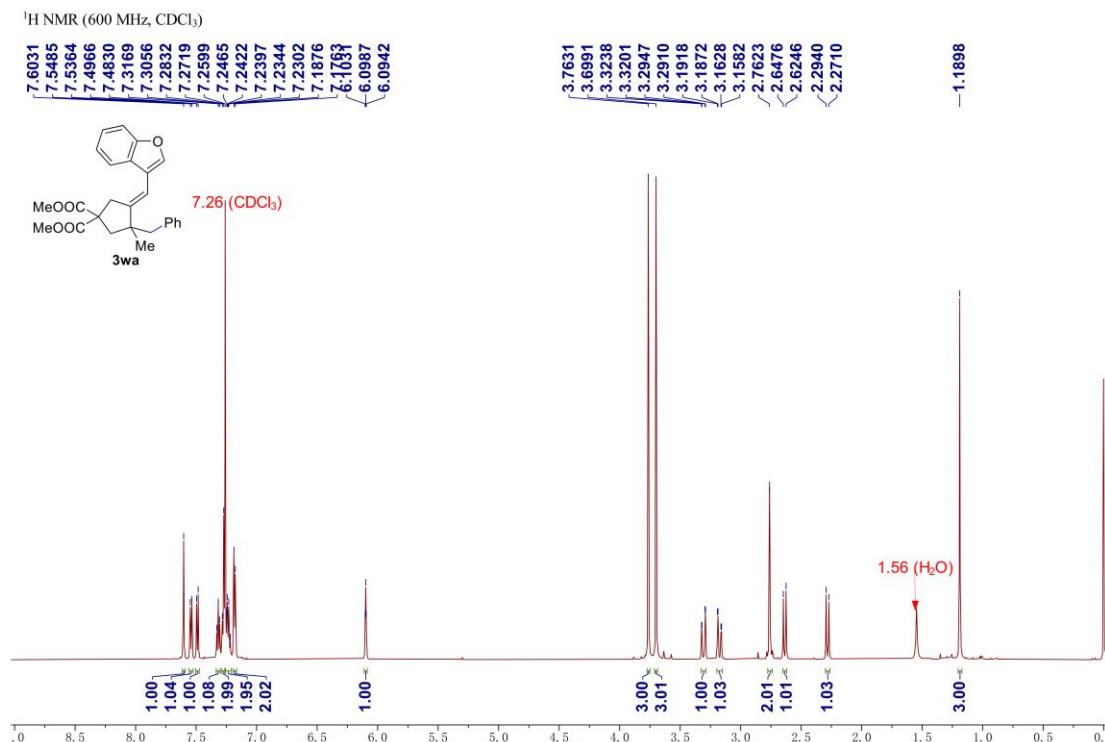


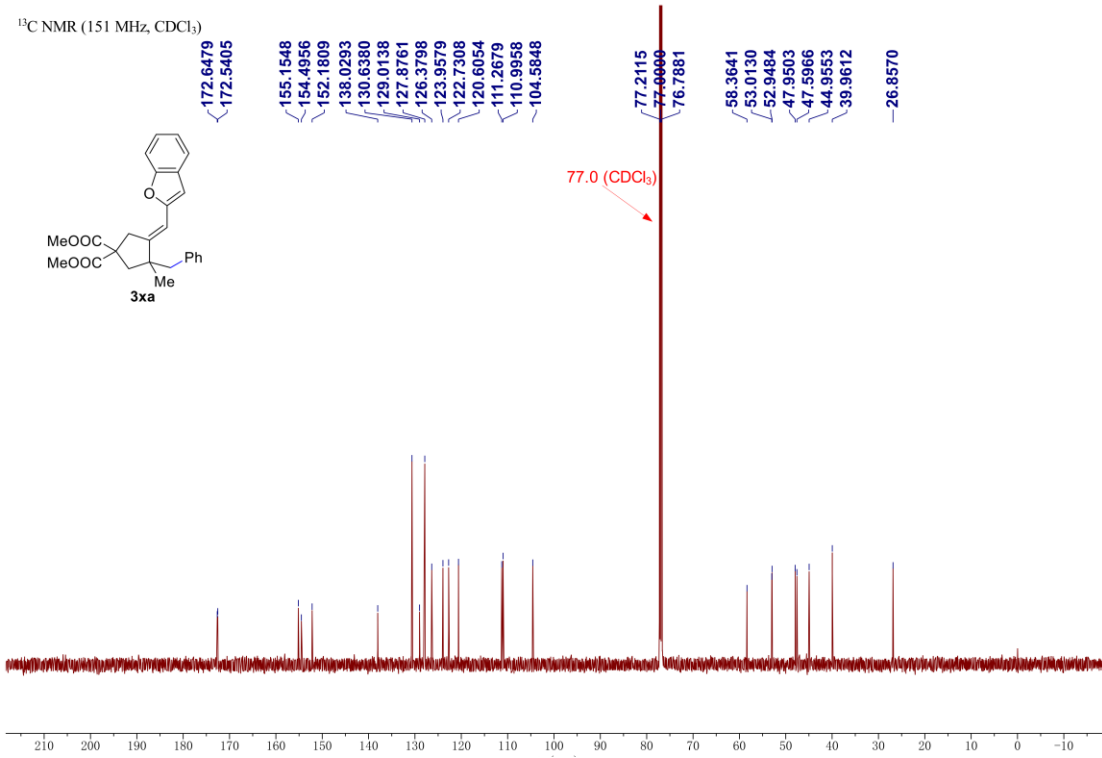
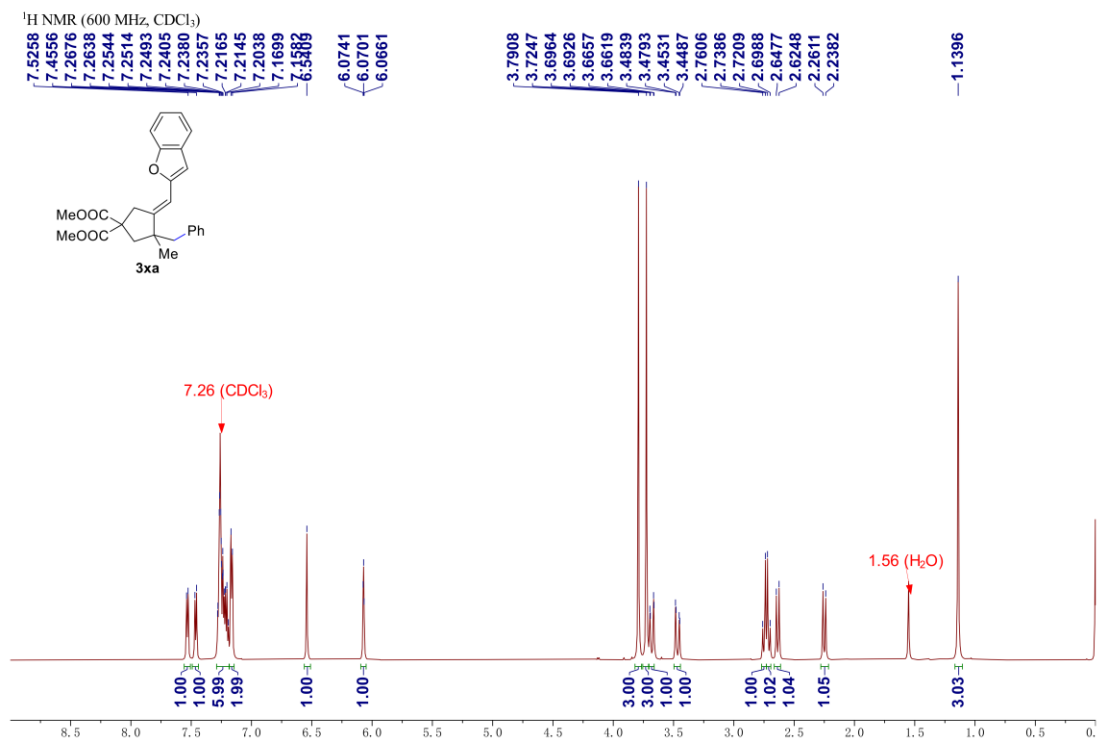


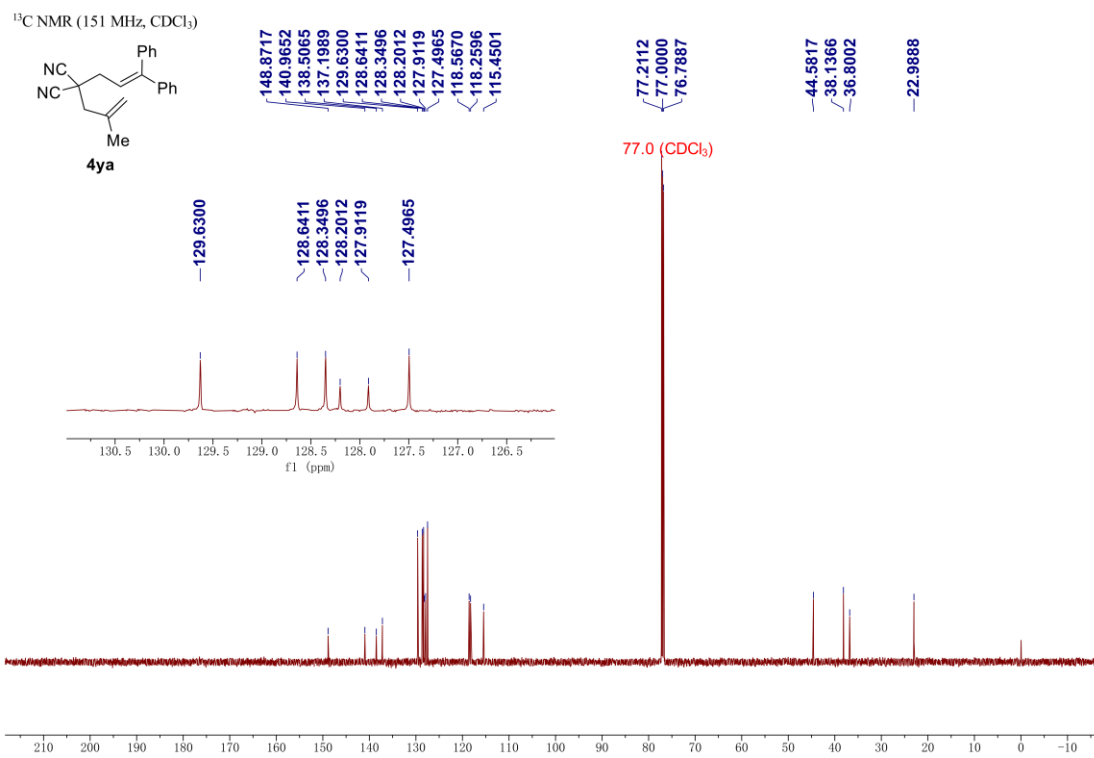


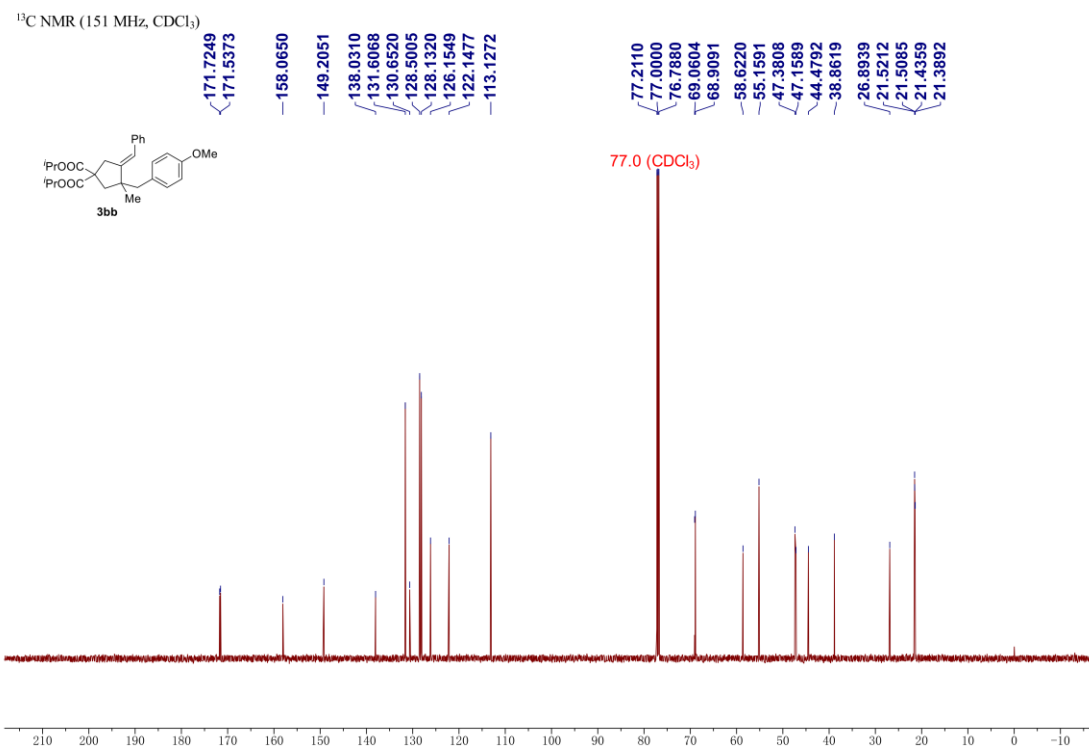
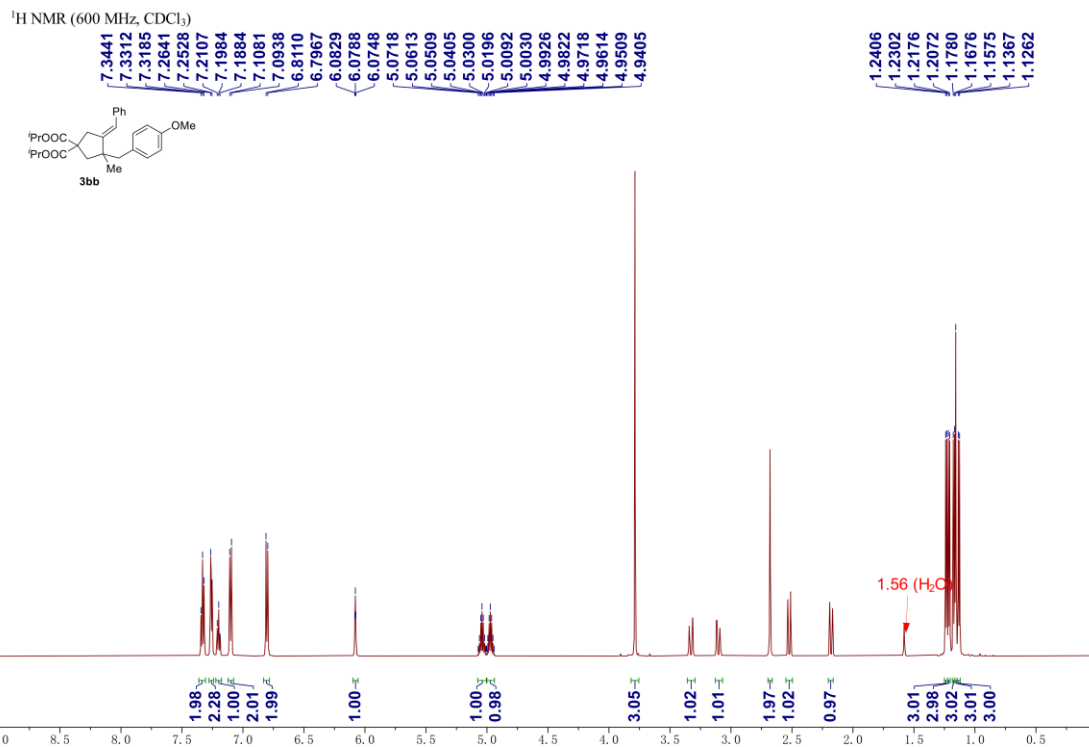


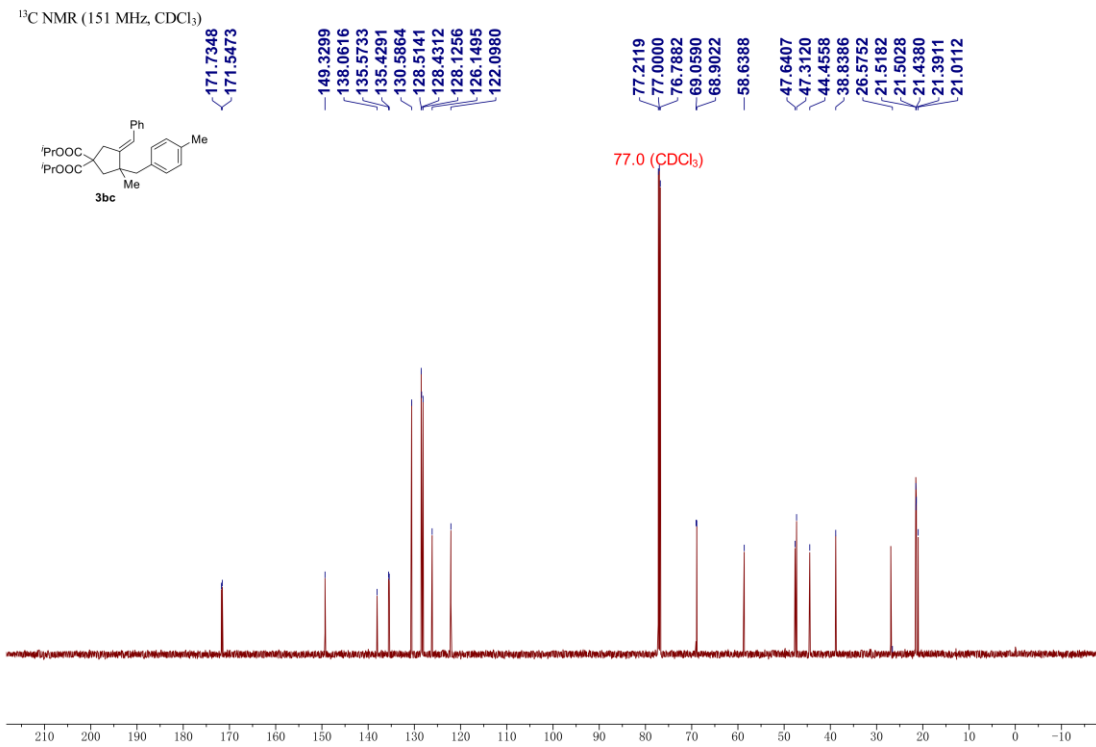
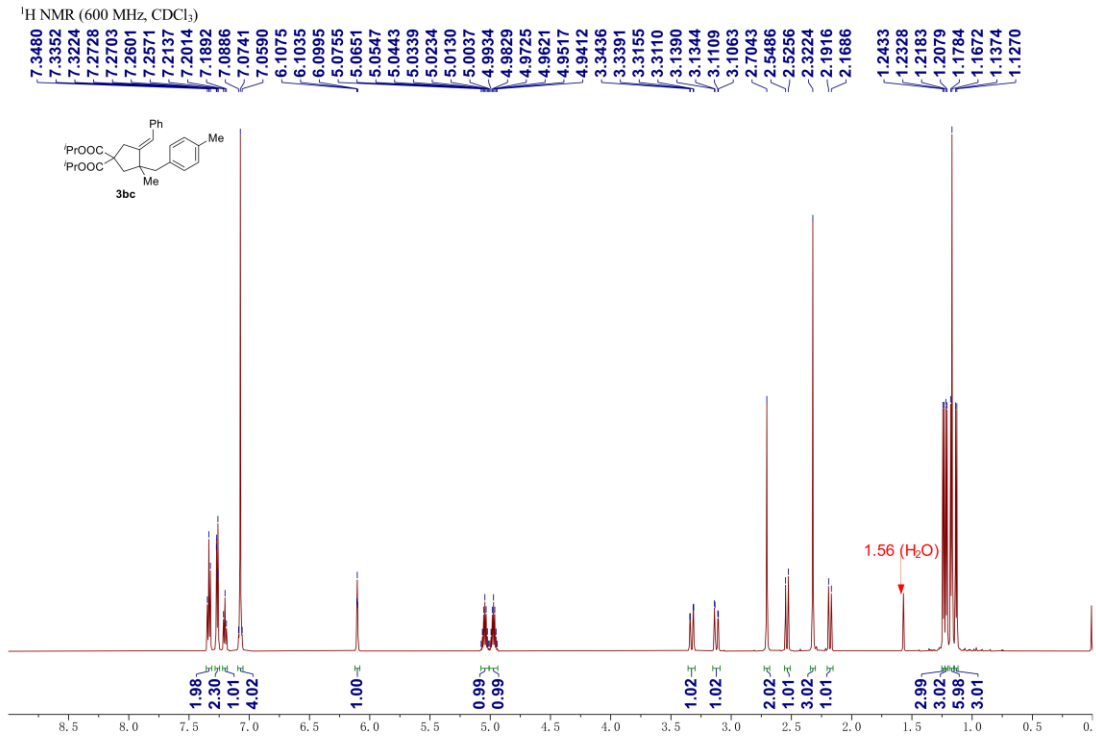


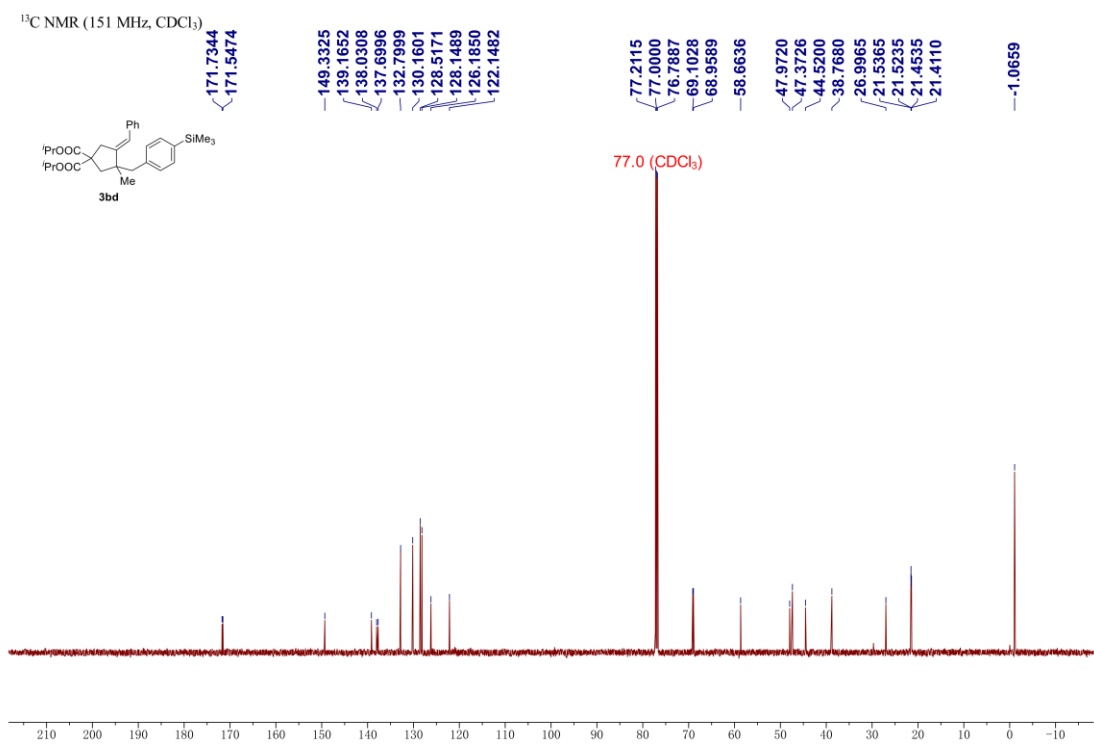
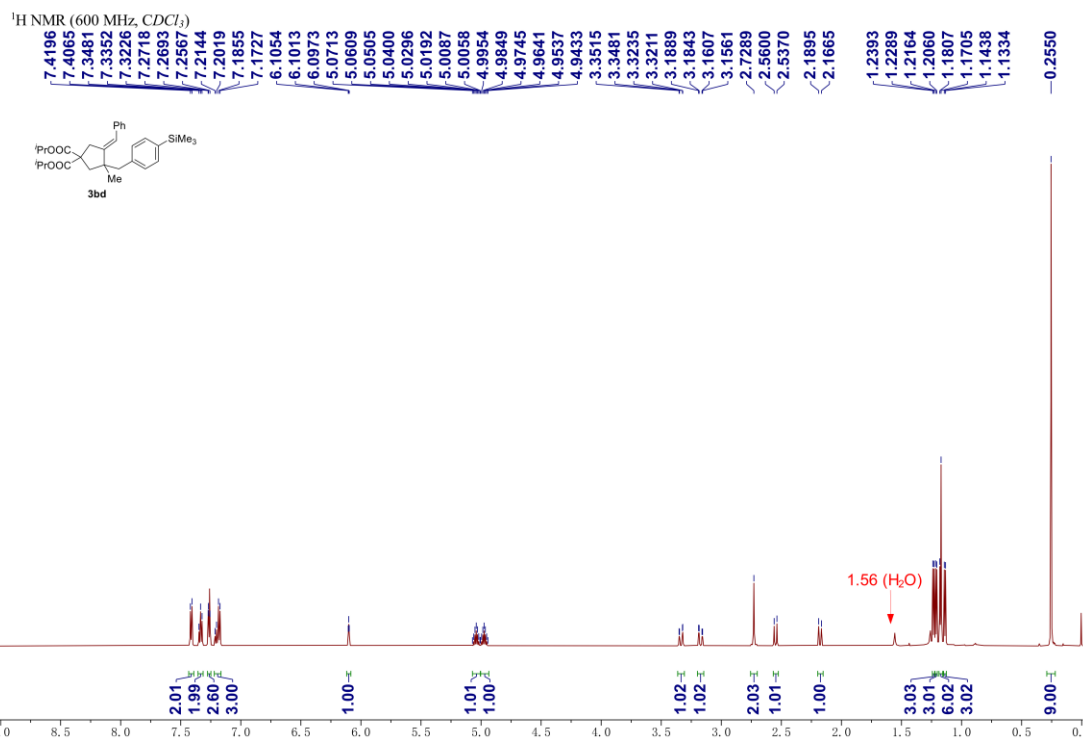


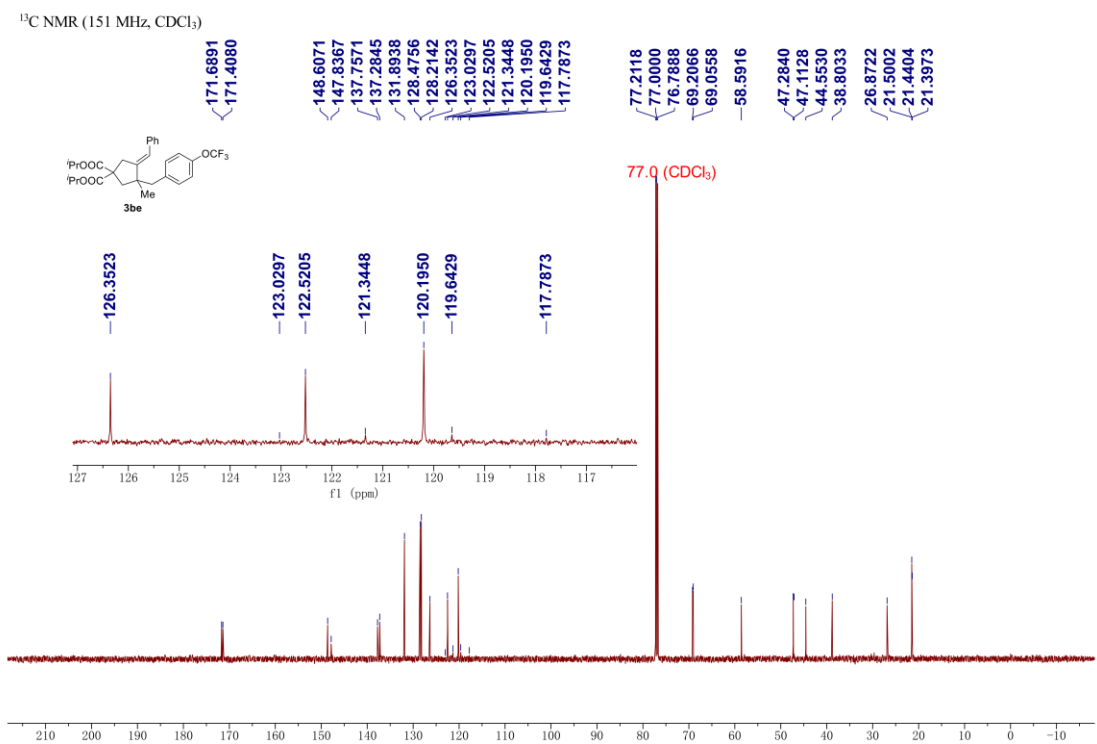
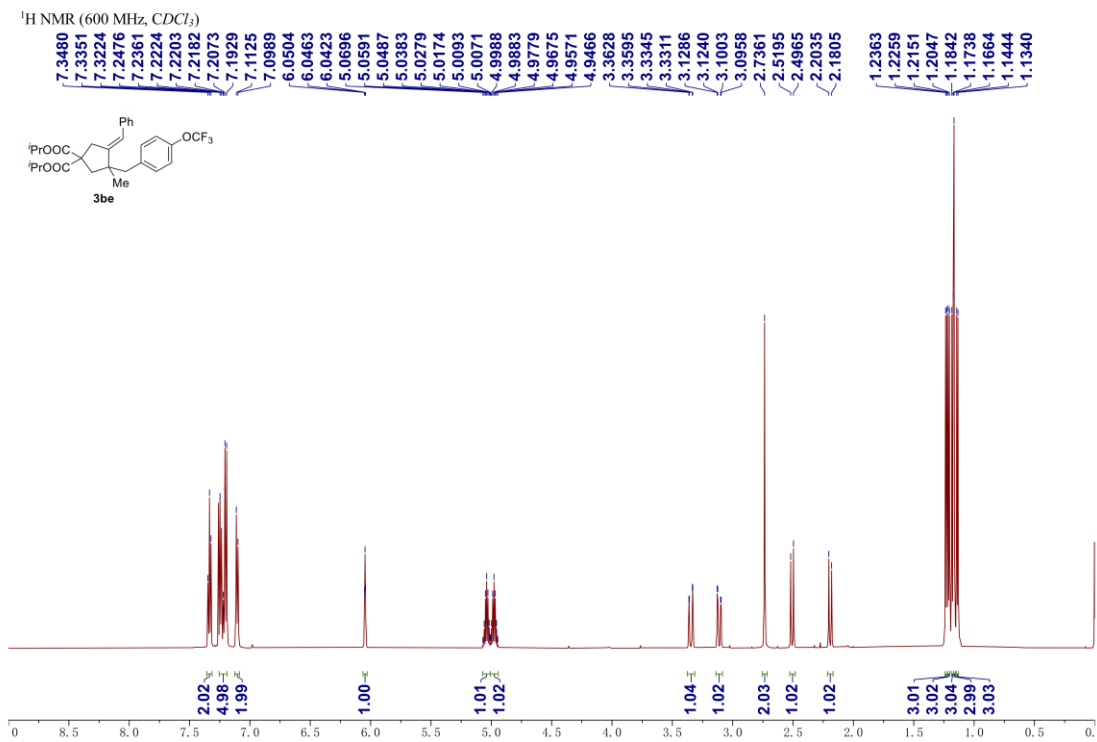


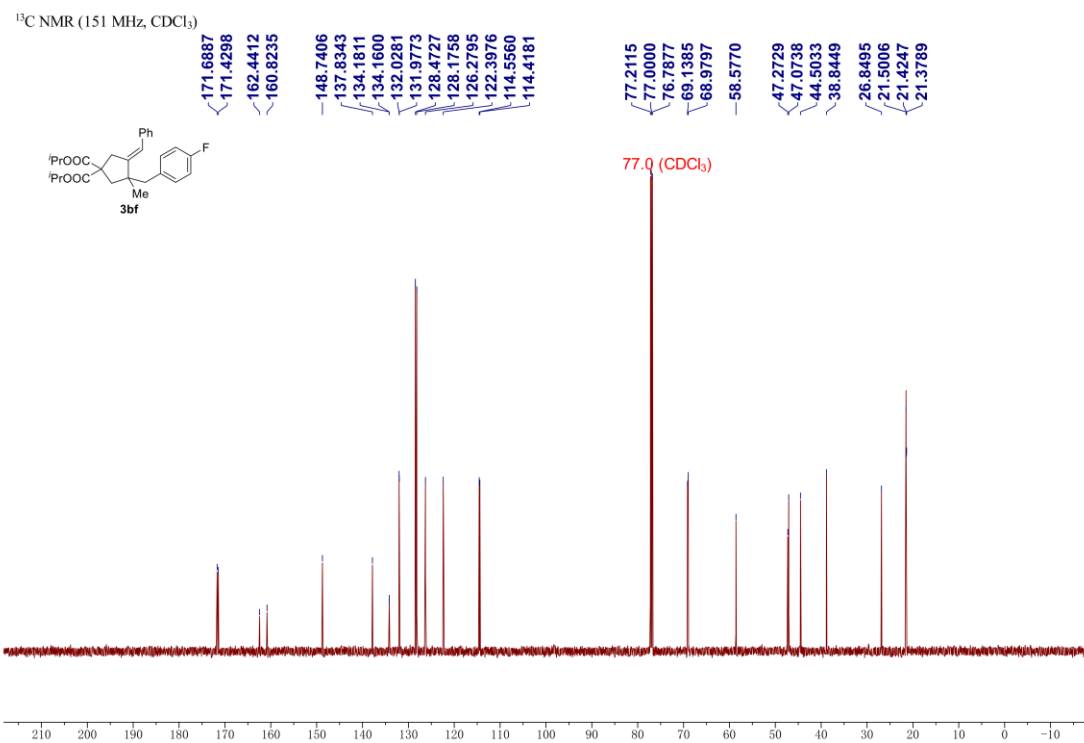
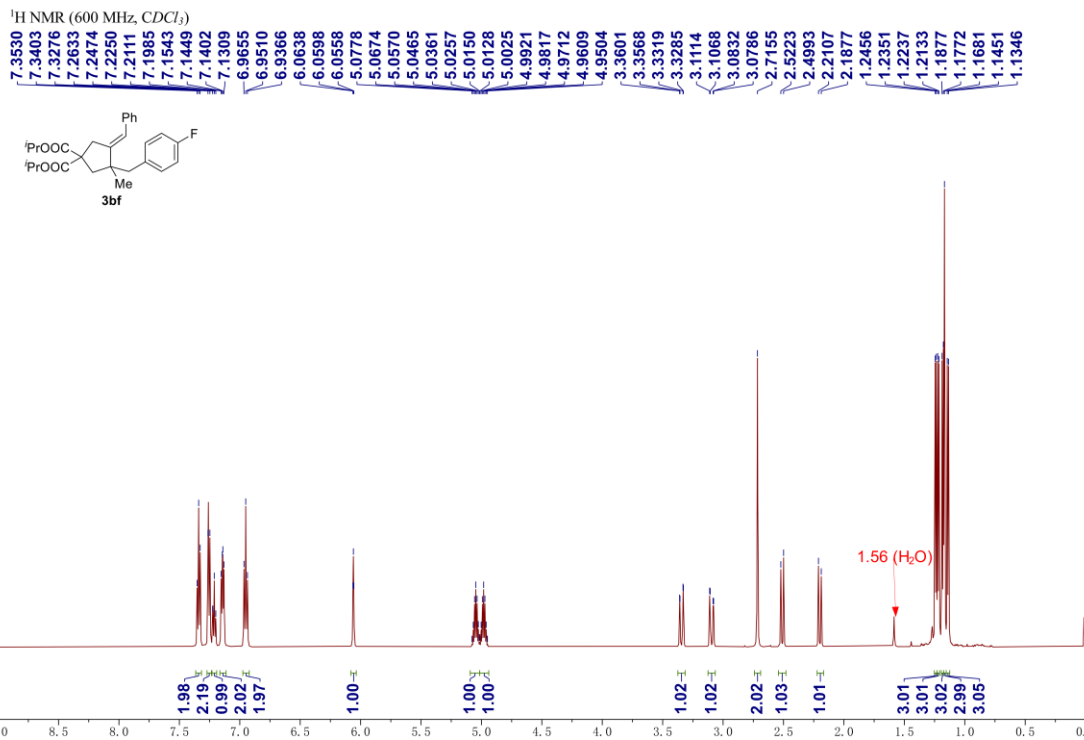


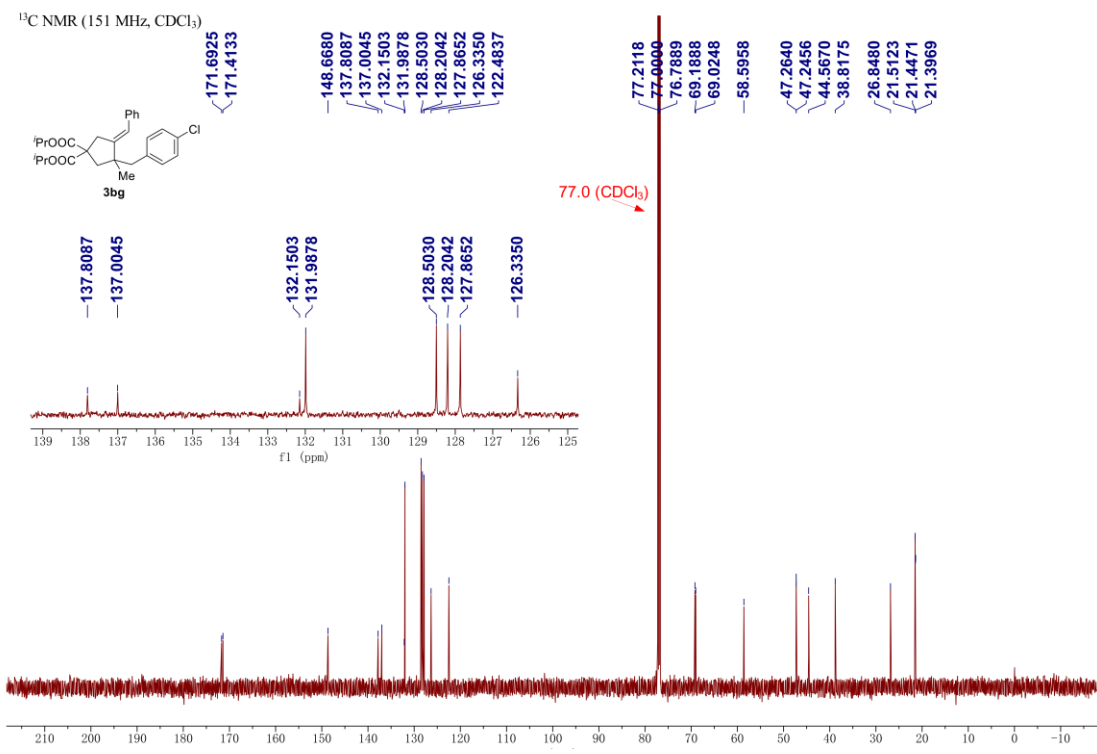
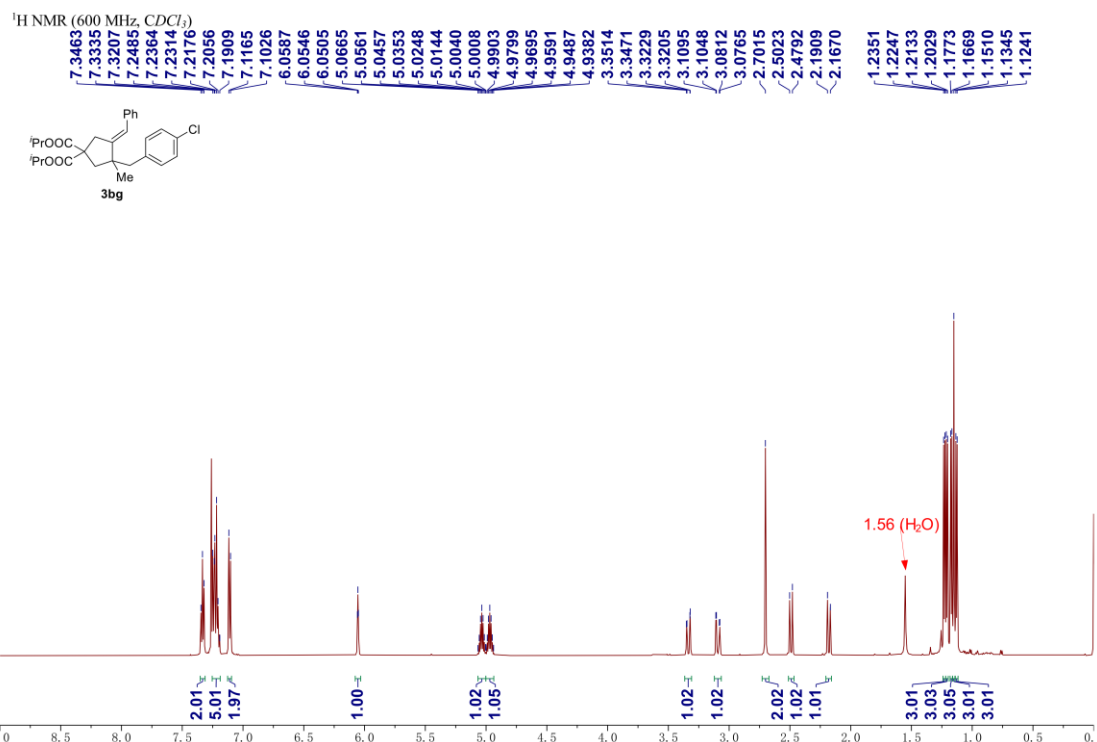


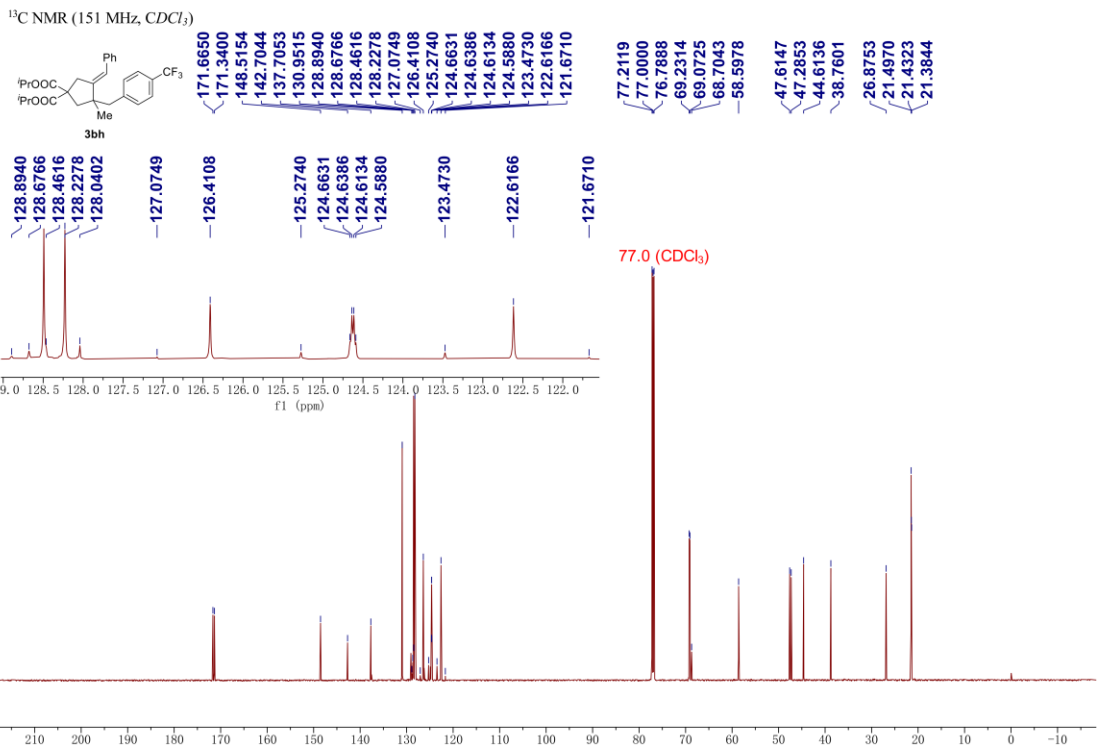
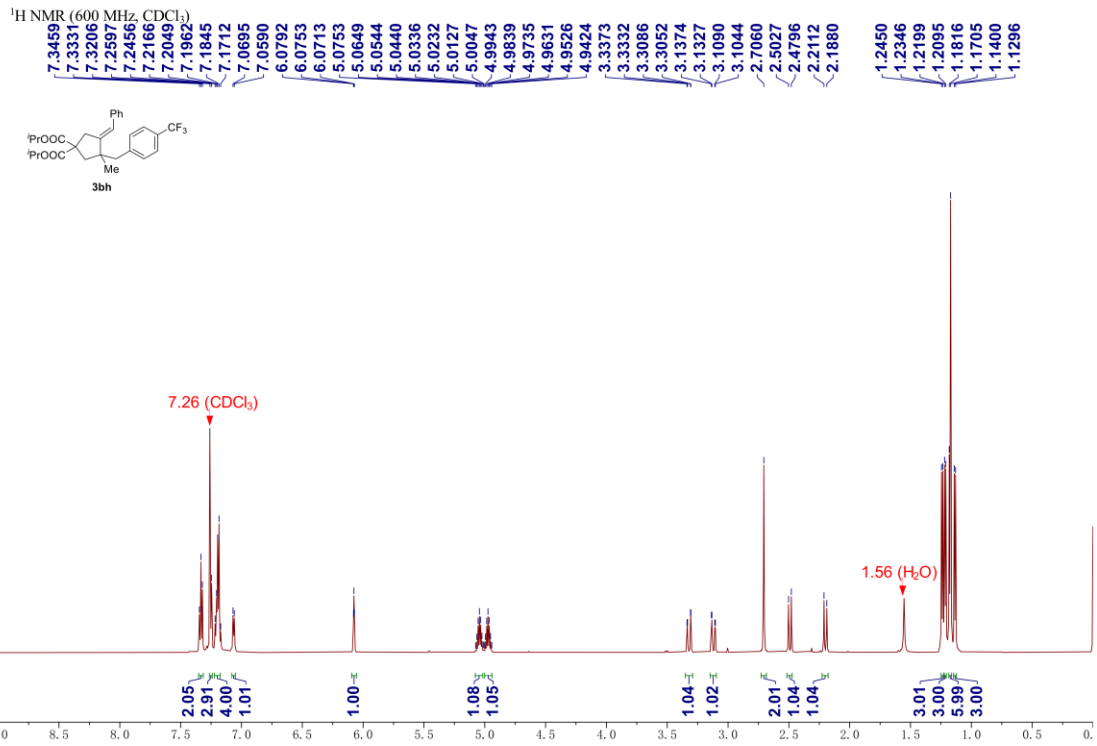




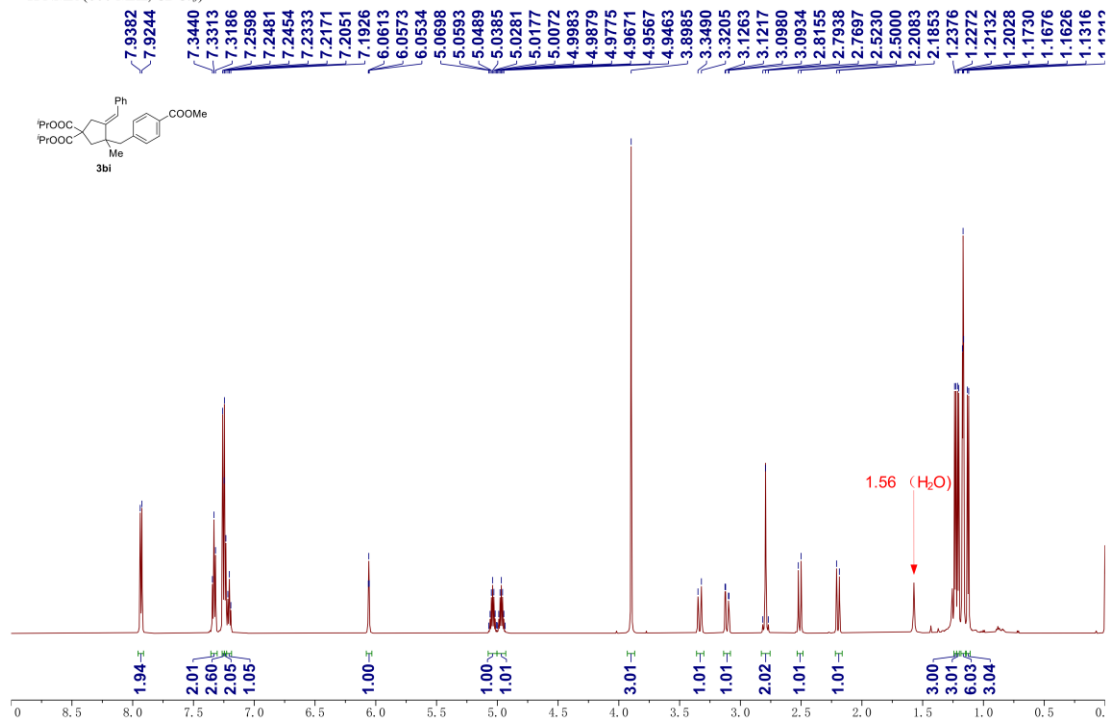




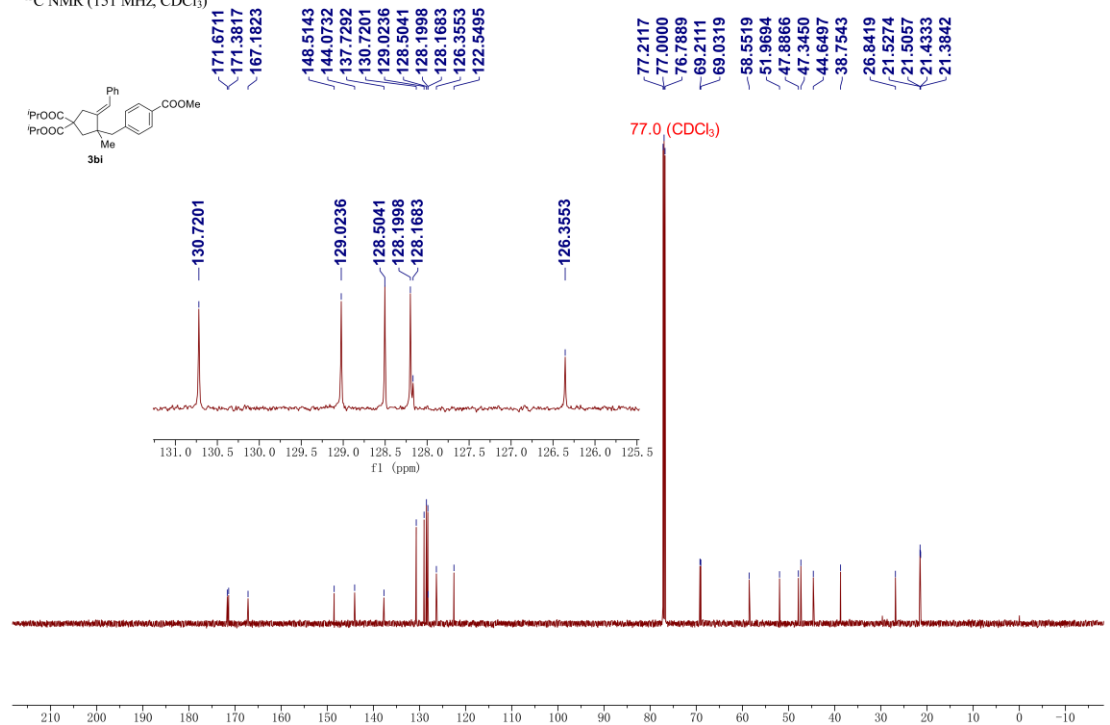




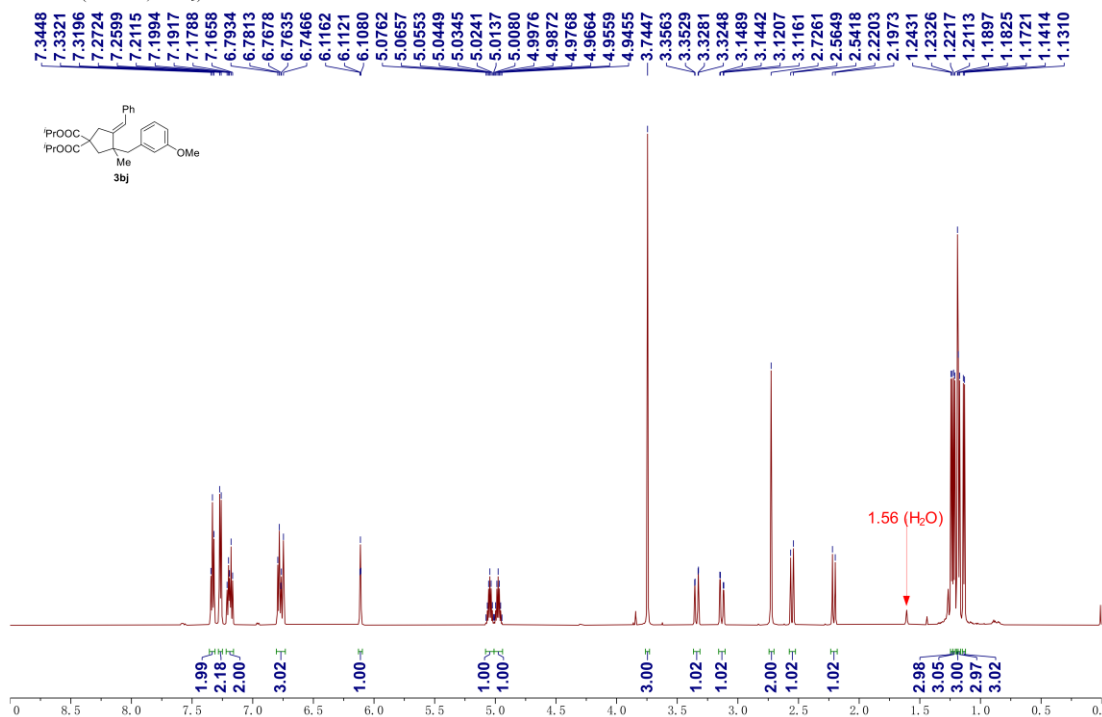
¹H NMR (600 MHz, CDCl₃)



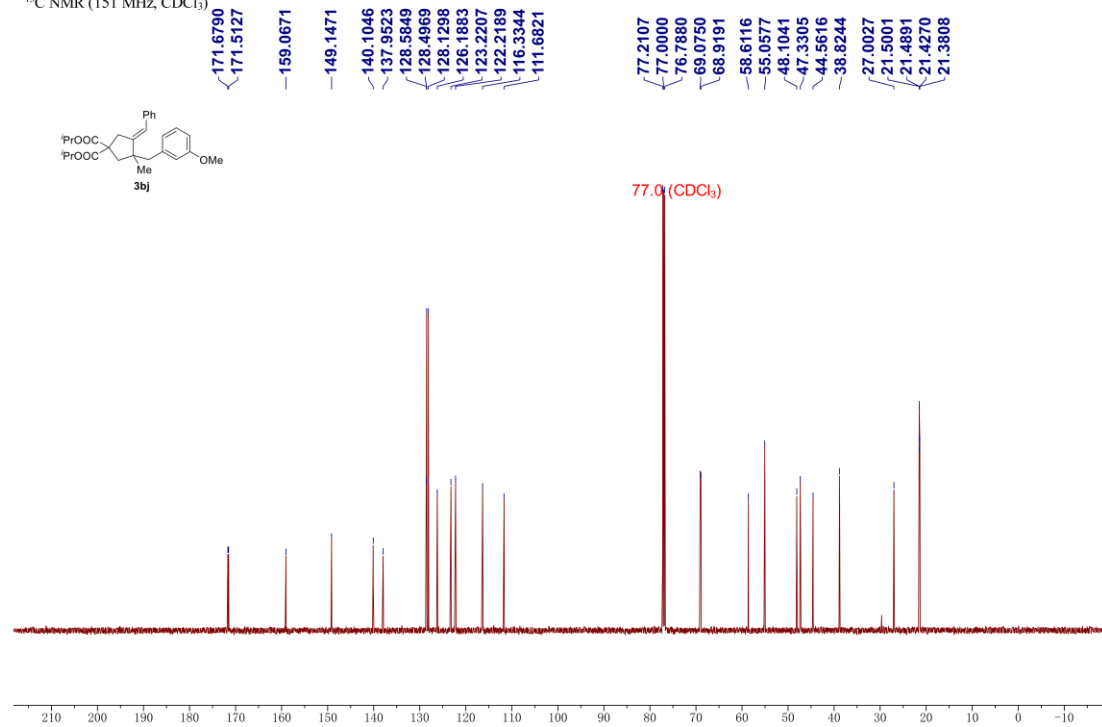
¹³C NMR (151 MHz, CDCl₃)

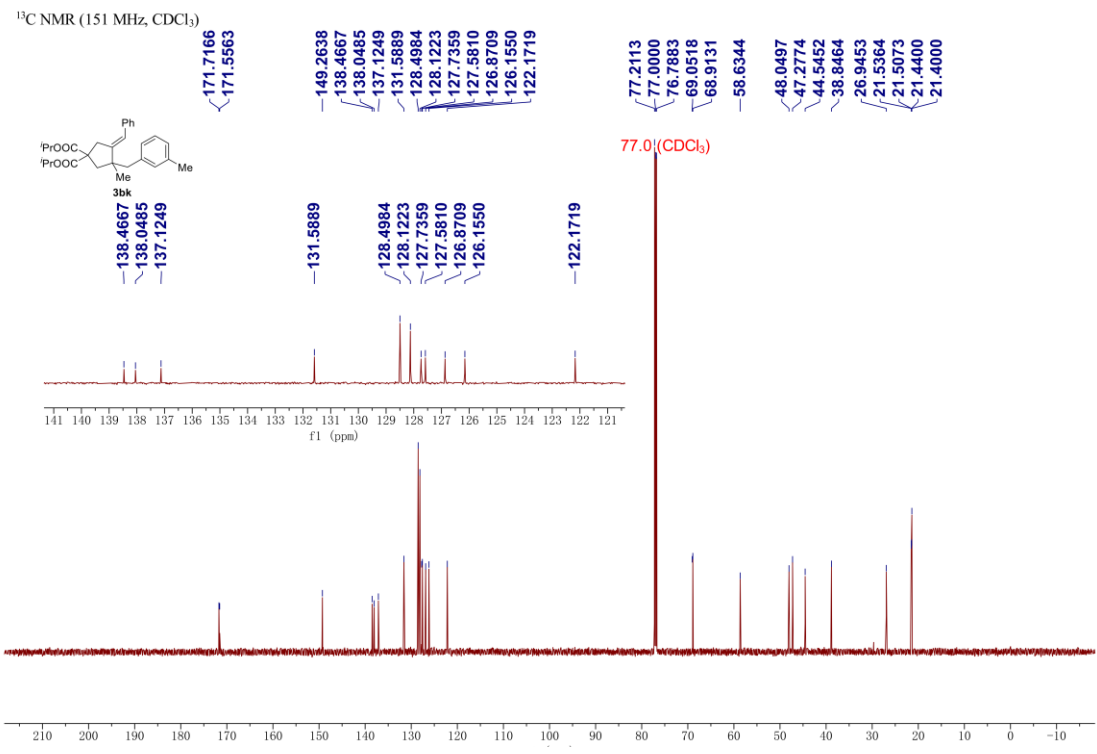
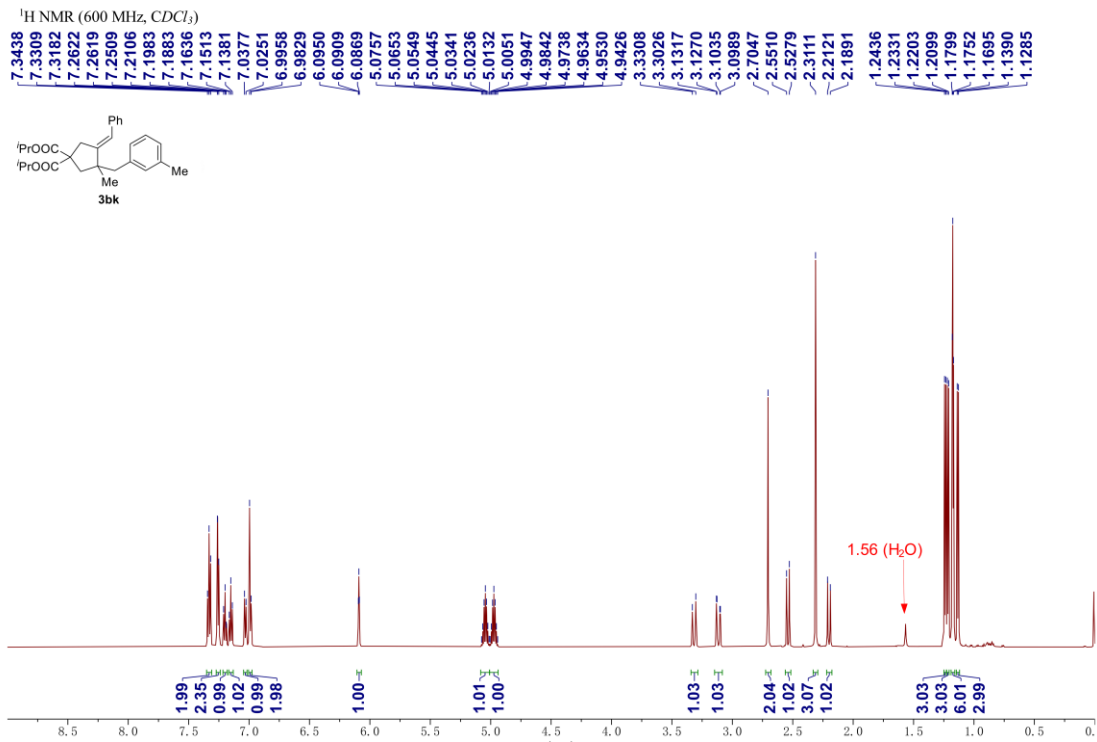


¹H NMR (600 MHz, CDCl₃)

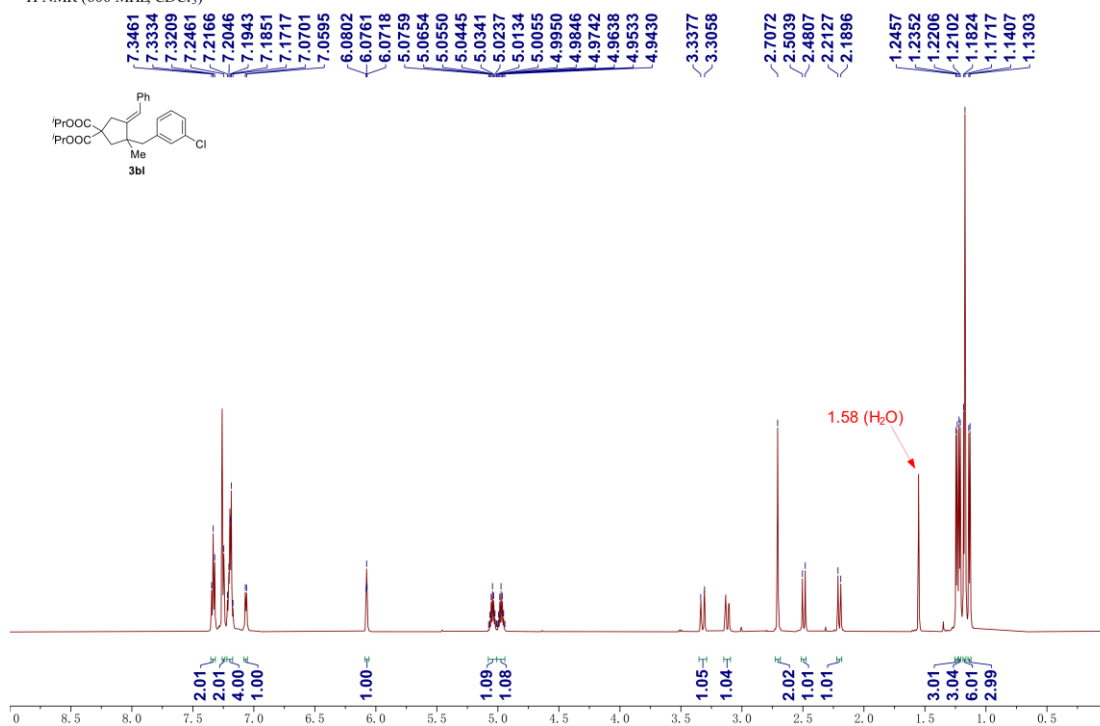
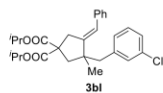


¹³C NMR (151 MHz, CDCl₃)

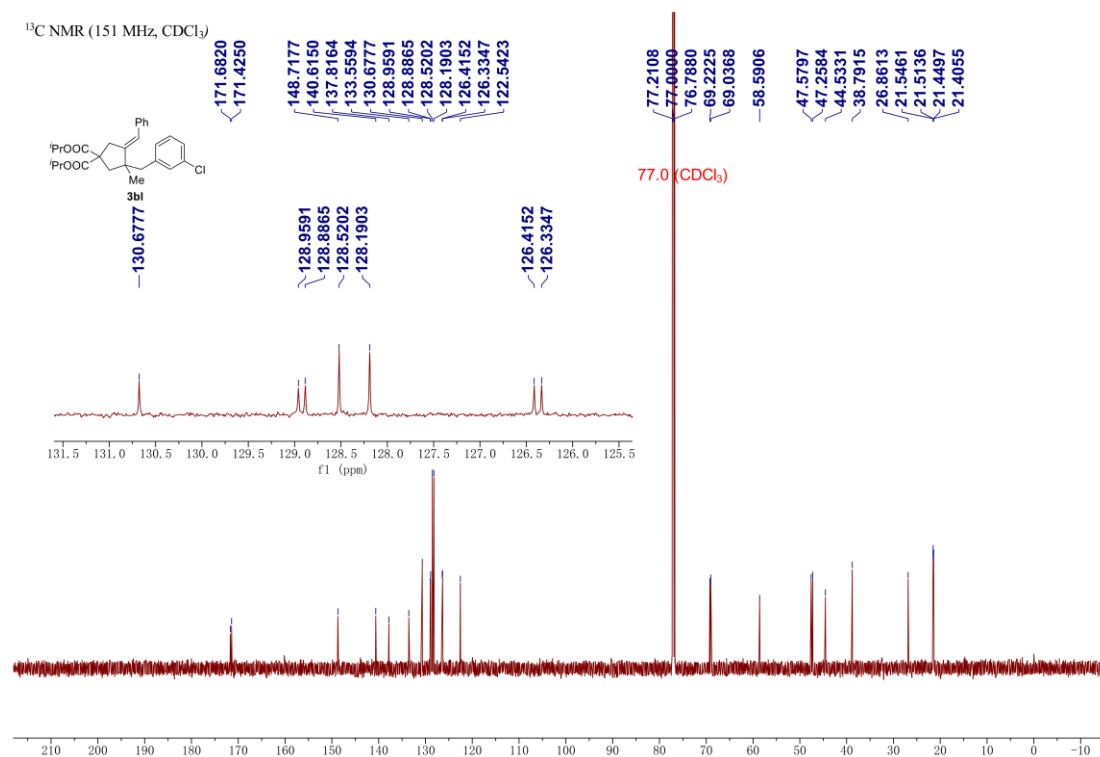
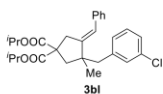




¹H NMR (600 MHz, CDCl₃)

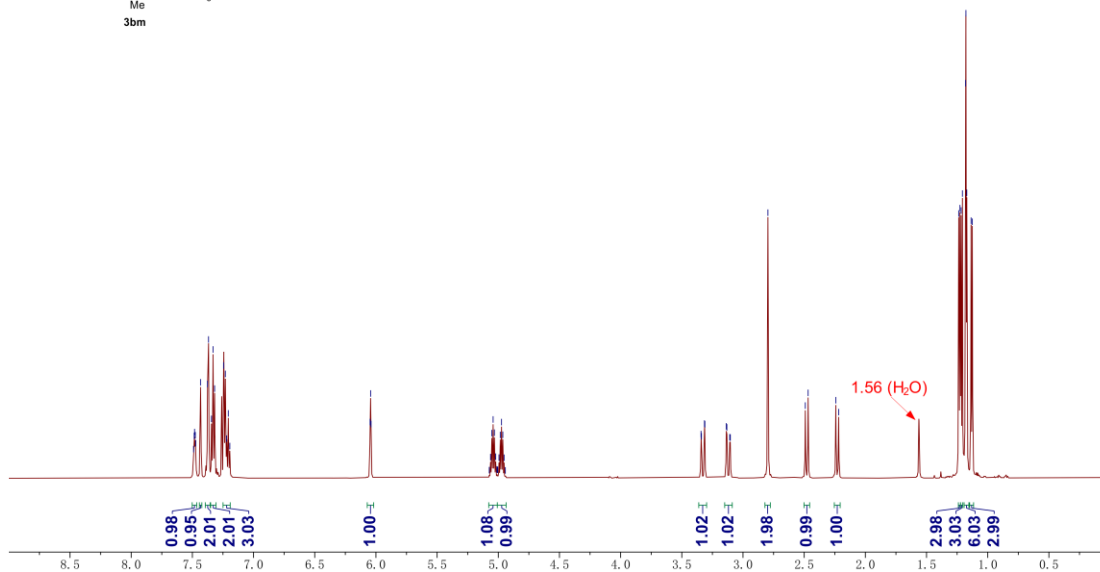
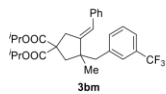


¹³C NMR (151 MHz, CDCl₃)



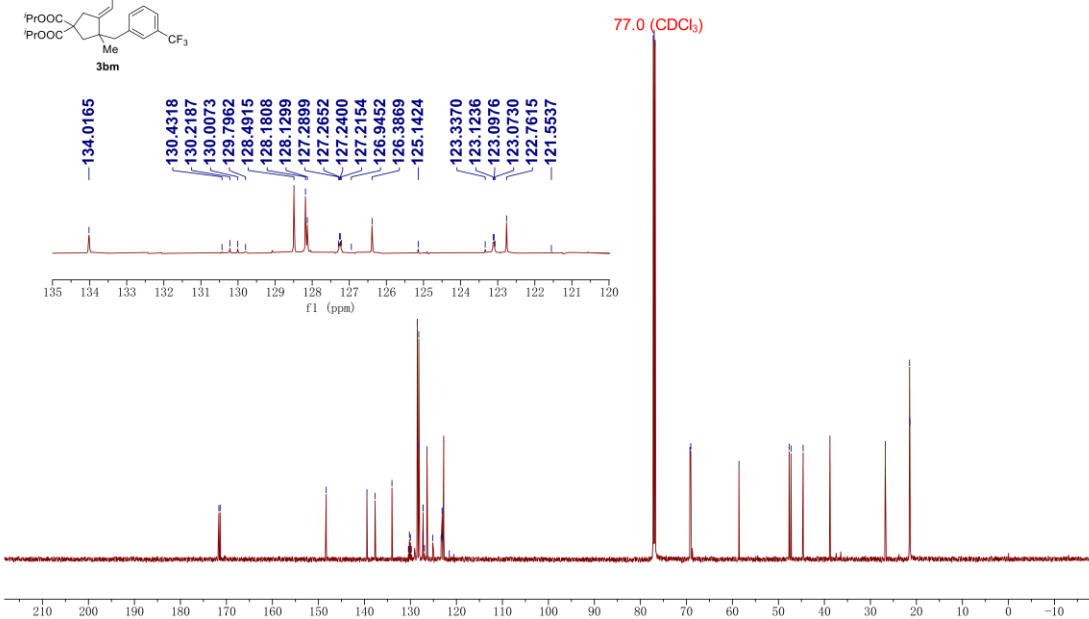
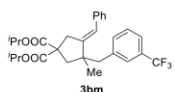
¹H NMR (600 MHz, CDCl₃)

7.4903, 7.4851, 7.4822, 7.4761, 7.4727, 7.4330, 7.3767, 7.3679, 7.3437, 7.3310, 7.3184, 7.2449, 7.2307, 7.2205, 7.2067, 7.1941, 6.0476, 6.0435, 6.0397, 5.0630, 5.0526, 5.0422, 5.0317, 5.0213, 5.0109, 5.0046, 4.9942, 4.9838, 4.9734, 4.9629, 4.9525, 4.9421, 3.3430, 3.3397, 3.3149, 3.3115, 3.1366, 3.1320, 3.1083, 3.1036, 2.7963, 2.4907, 2.4676, 2.2414, 2.2183, 1.2371, 1.2267, 1.2172, 1.2068, 1.1812, 1.1780, 1.1710, 1.1361, 1.1257

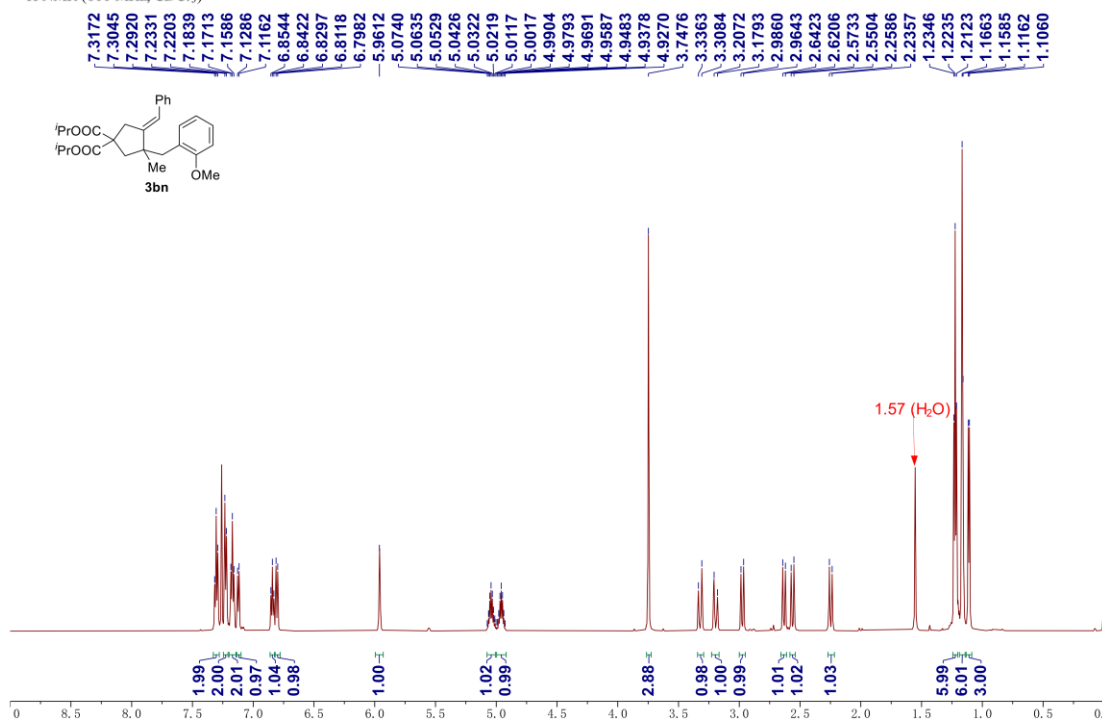


¹³C NMR (151 MHz, CDCl₃)

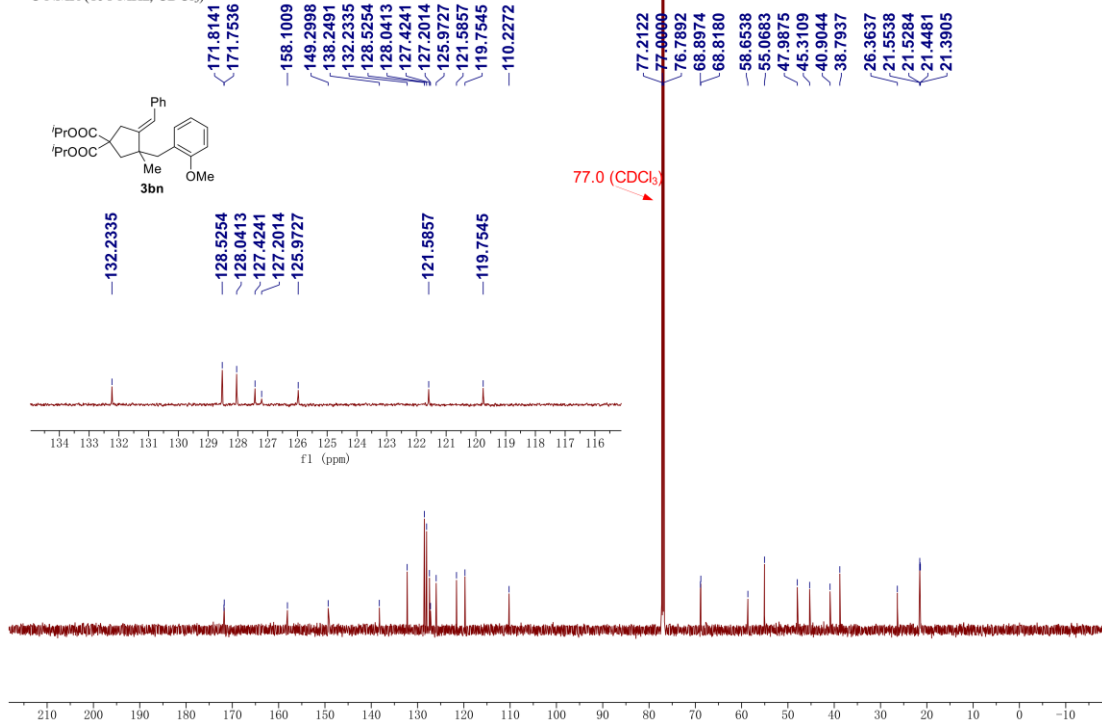
171.6488, 171.3619, 148.3198, 139.4581, 137.6787, 134.0165, 130.4318, 130.2187, 130.0073, 129.7962, 128.4915, 128.1808, 128.1299, 127.2899, 127.2652, 127.2400, 127.2154, 127.2154, 126.9452, 126.3869, 125.1424, 123.3370, 123.1236, 123.0976, 123.0730, 122.7615, 121.5537, 77.2114, 77.0000, 76.7884, 69.2295, 69.0560, 58.5801, 47.6586, 47.2614, 44.6208, 38.7934, 26.7663, 21.4839, 21.4295, 21.3859

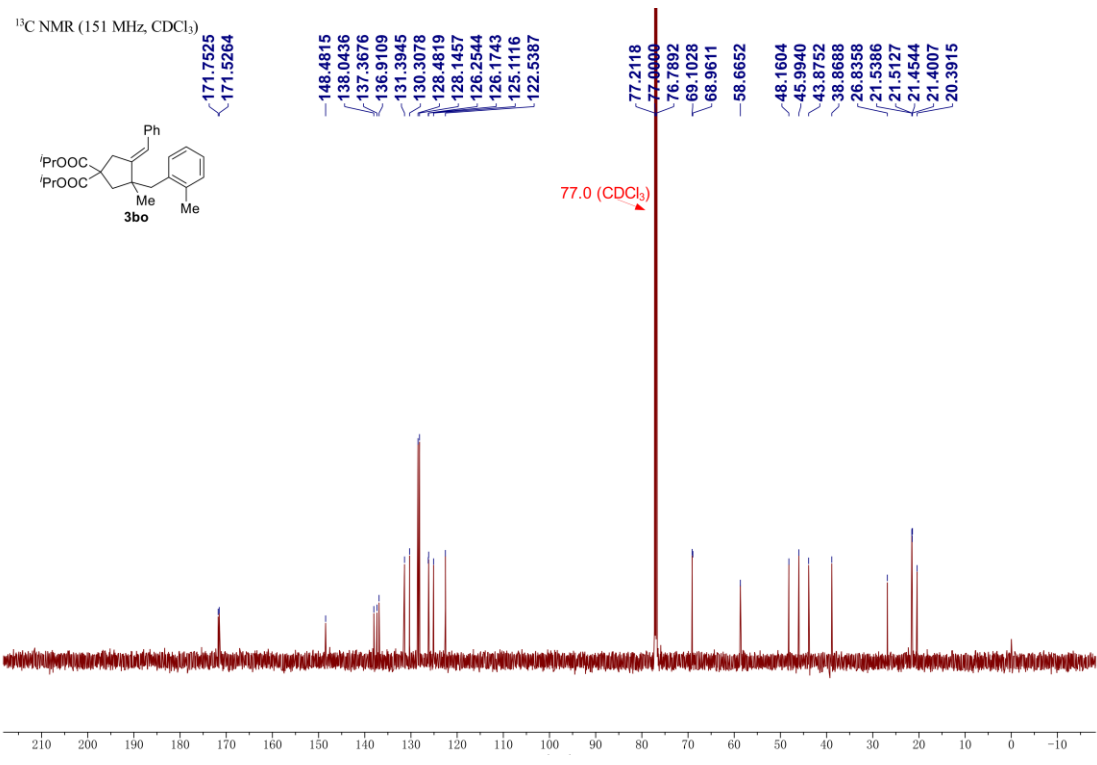
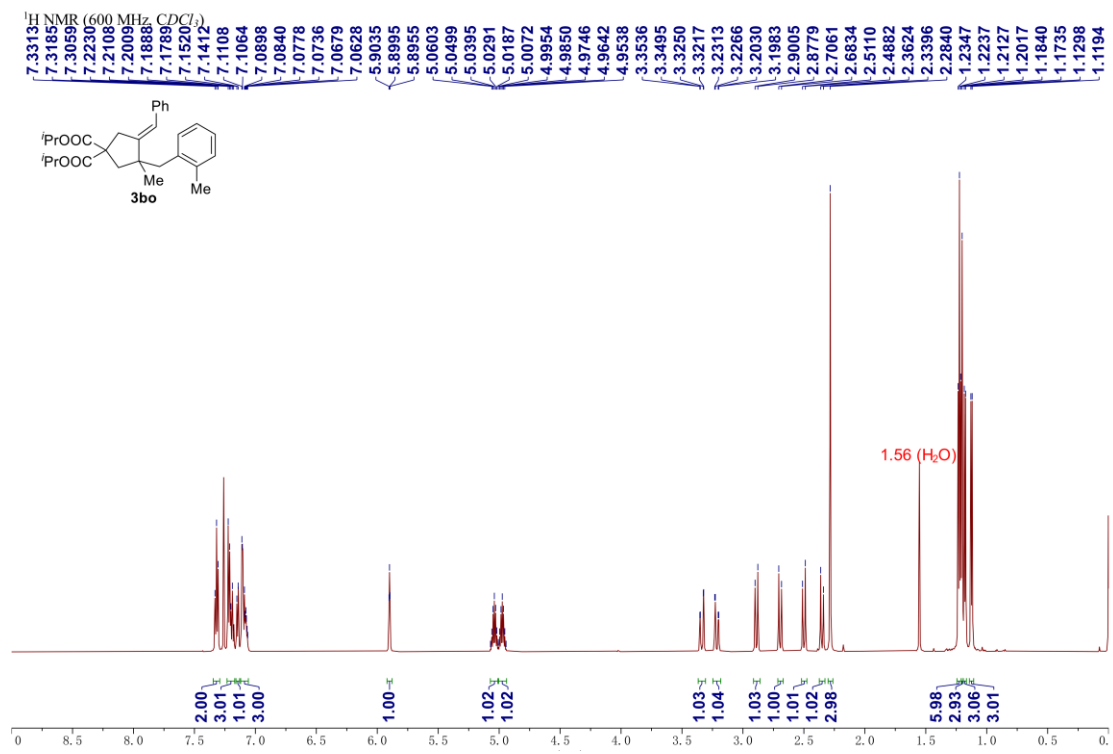


¹H NMR (600 MHz, CDCl₃)



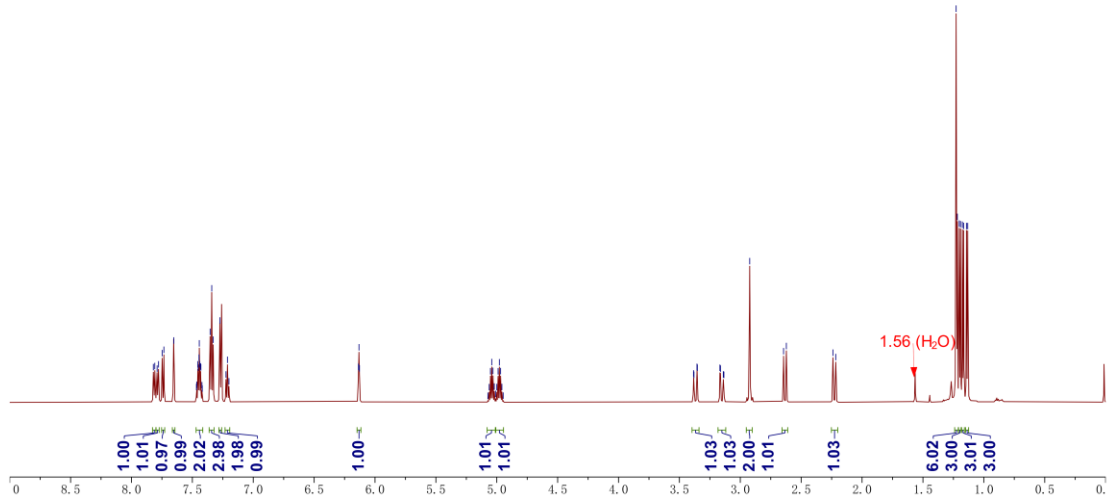
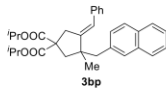
¹³C NMR (151 MHz, CDCl₃)



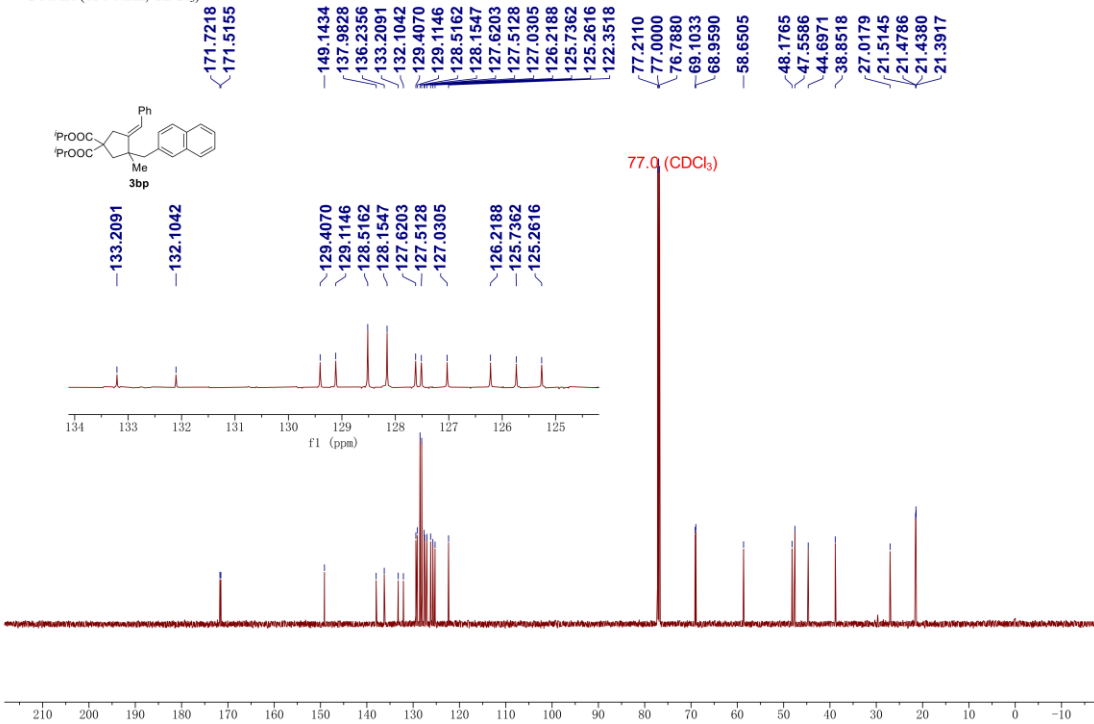


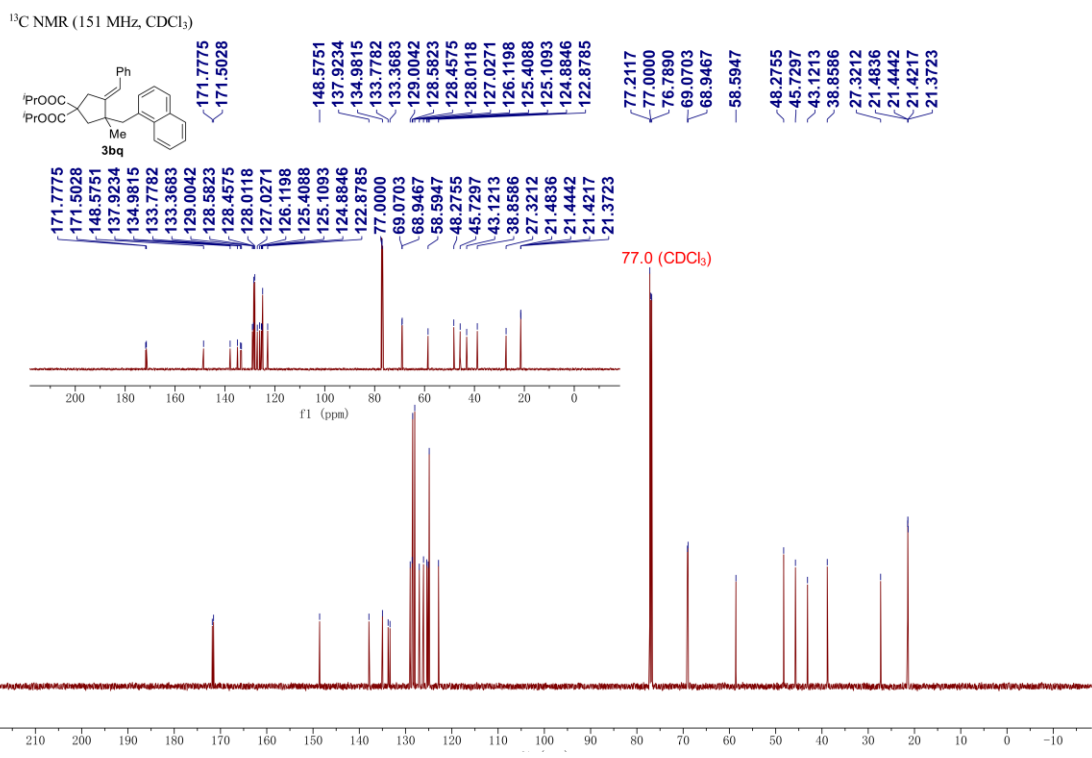
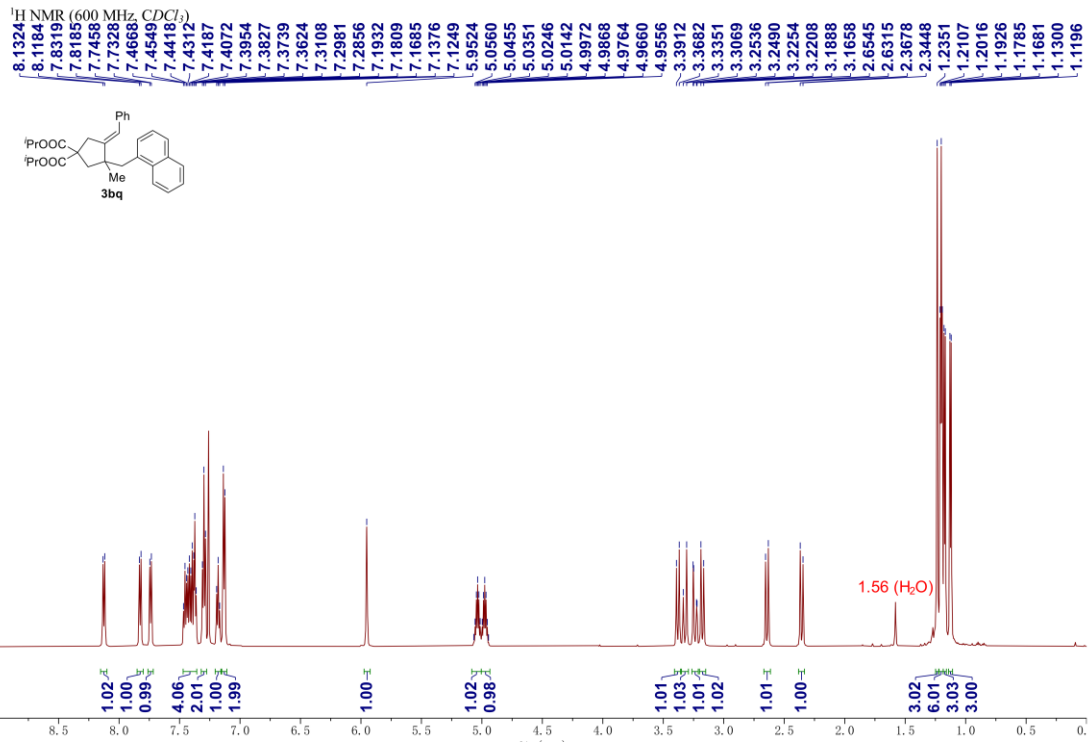
¹H NMR (600 MHz, CDCl₃)

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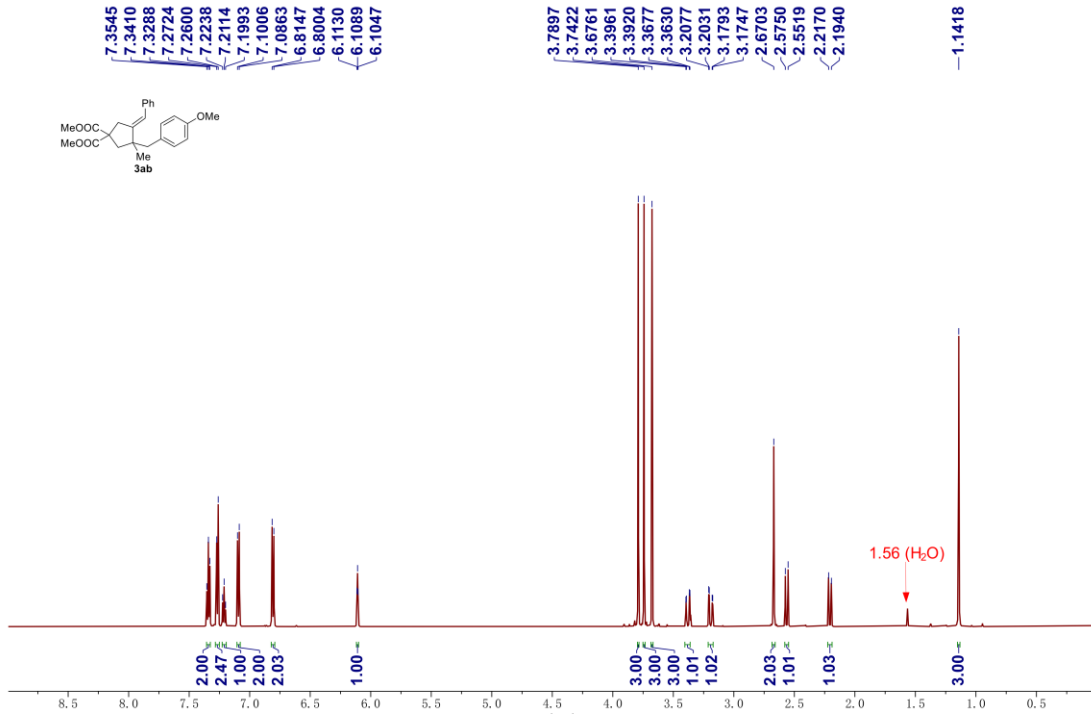
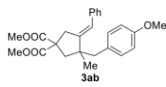


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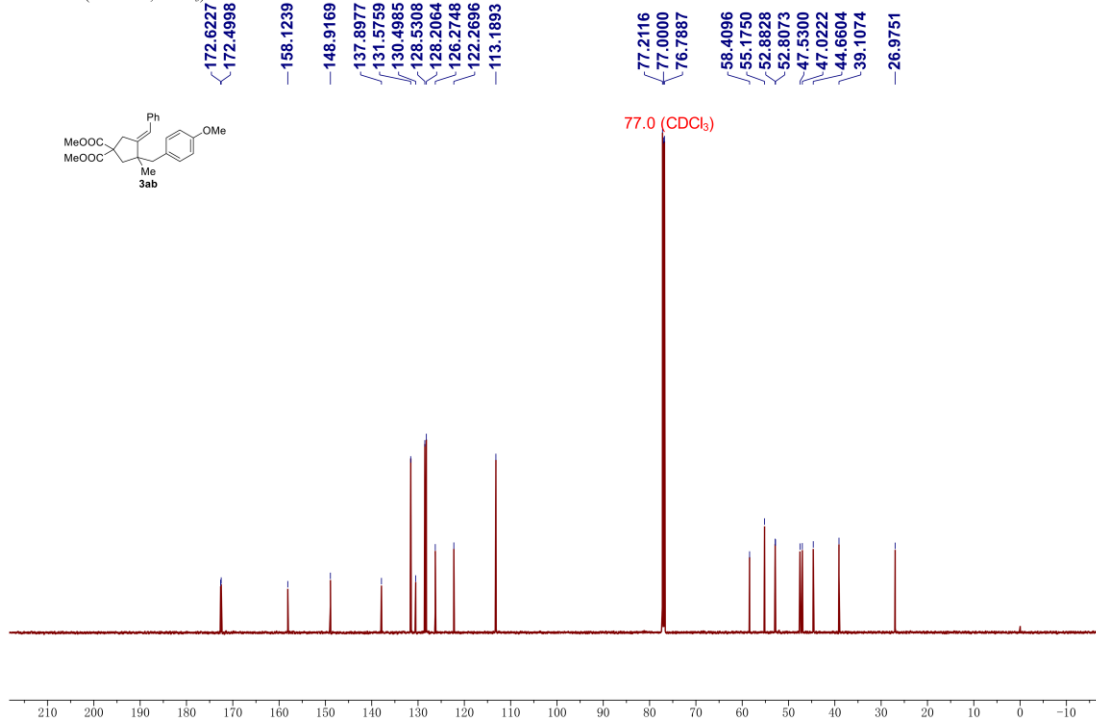
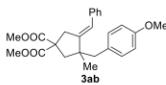


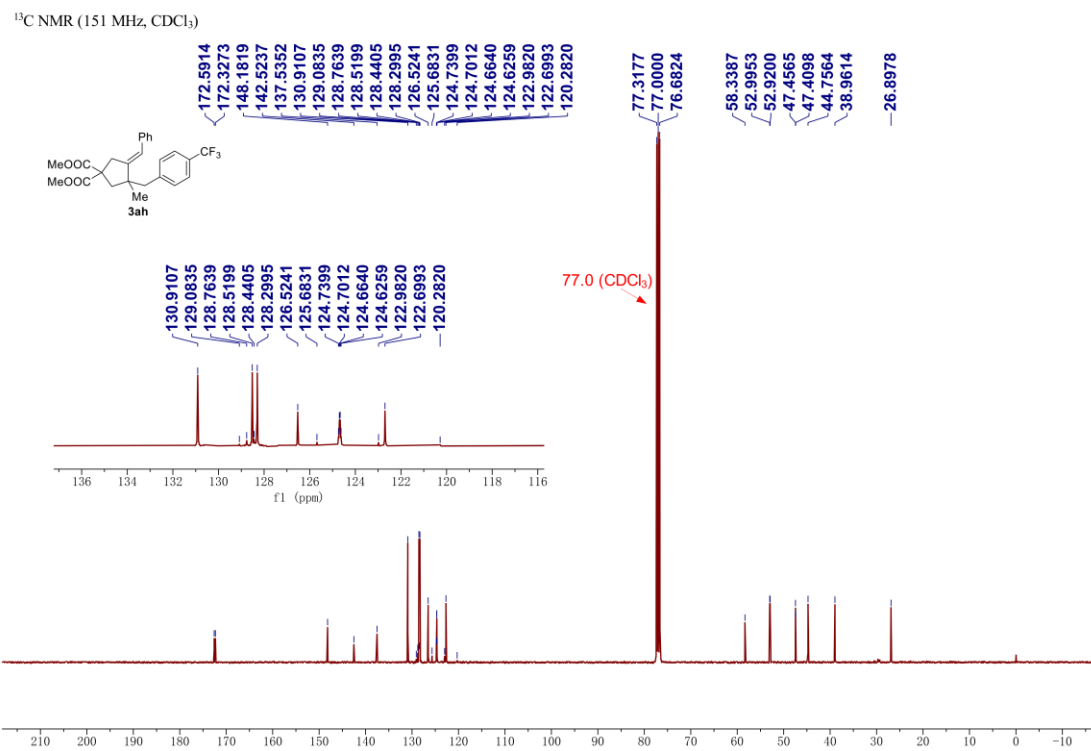
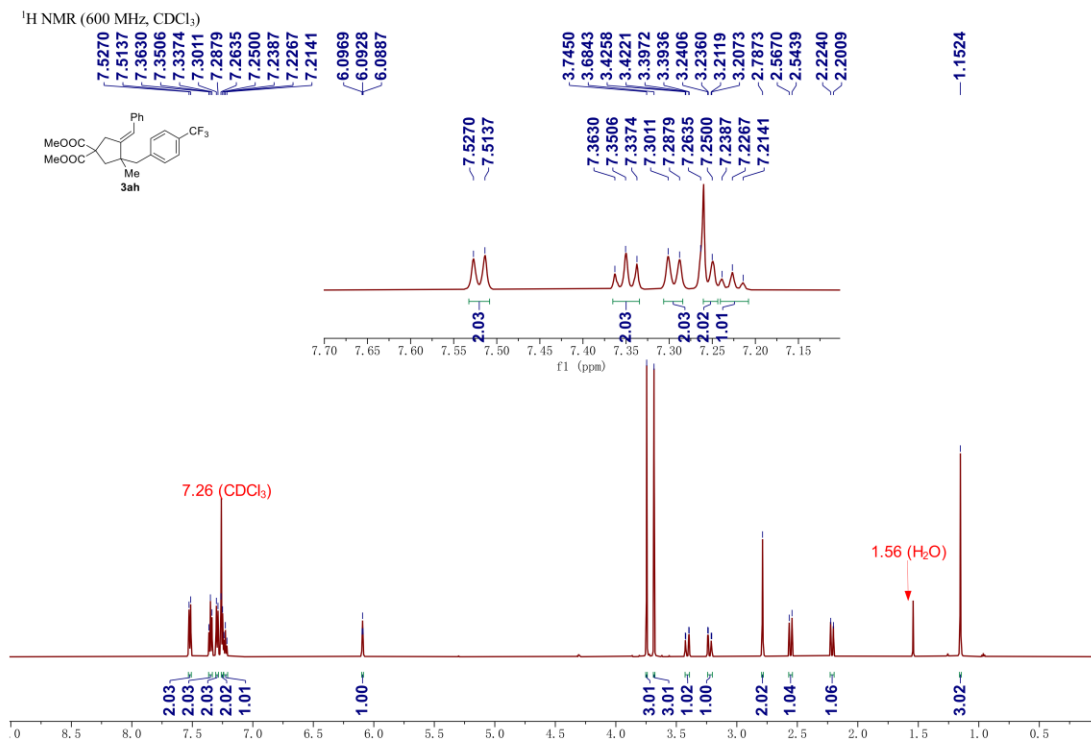


¹H NMR (600 MHz, CDCl₃)

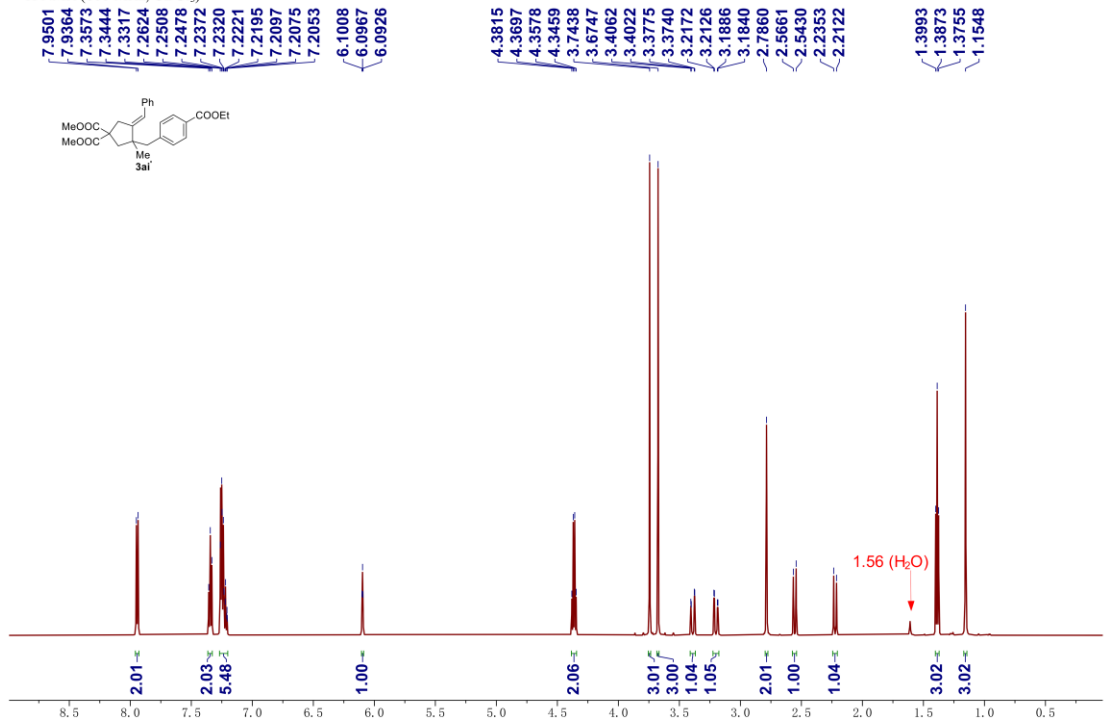


¹³C NMR (151 MHz, CDCl₃)

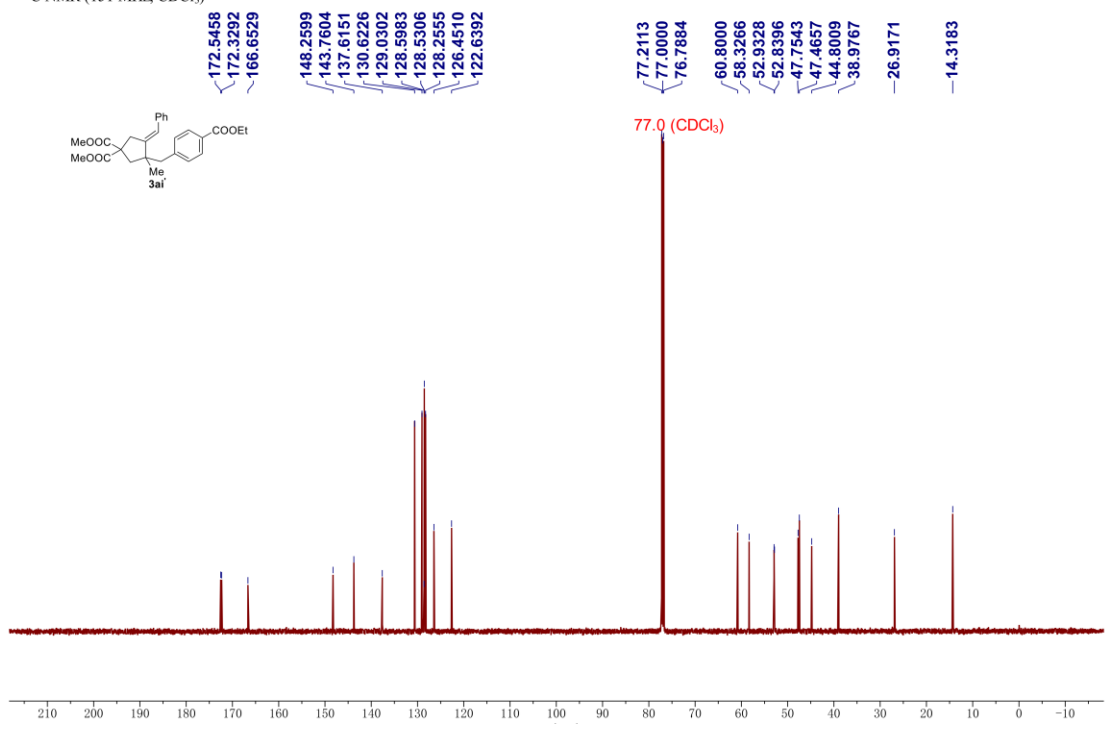


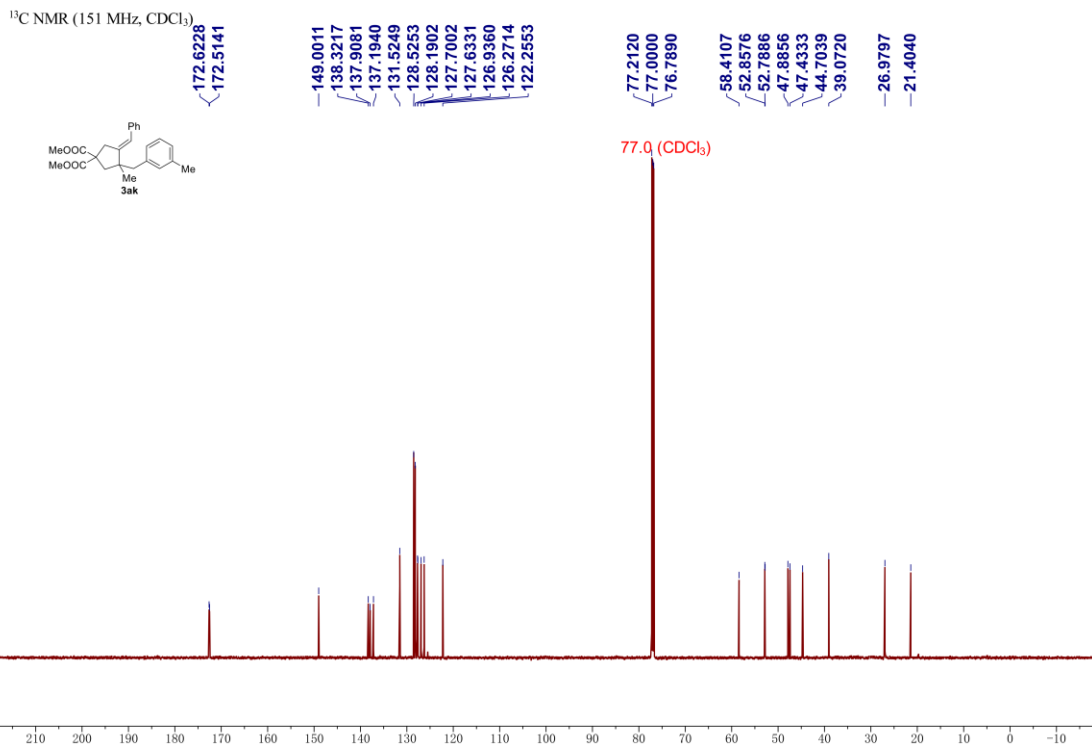
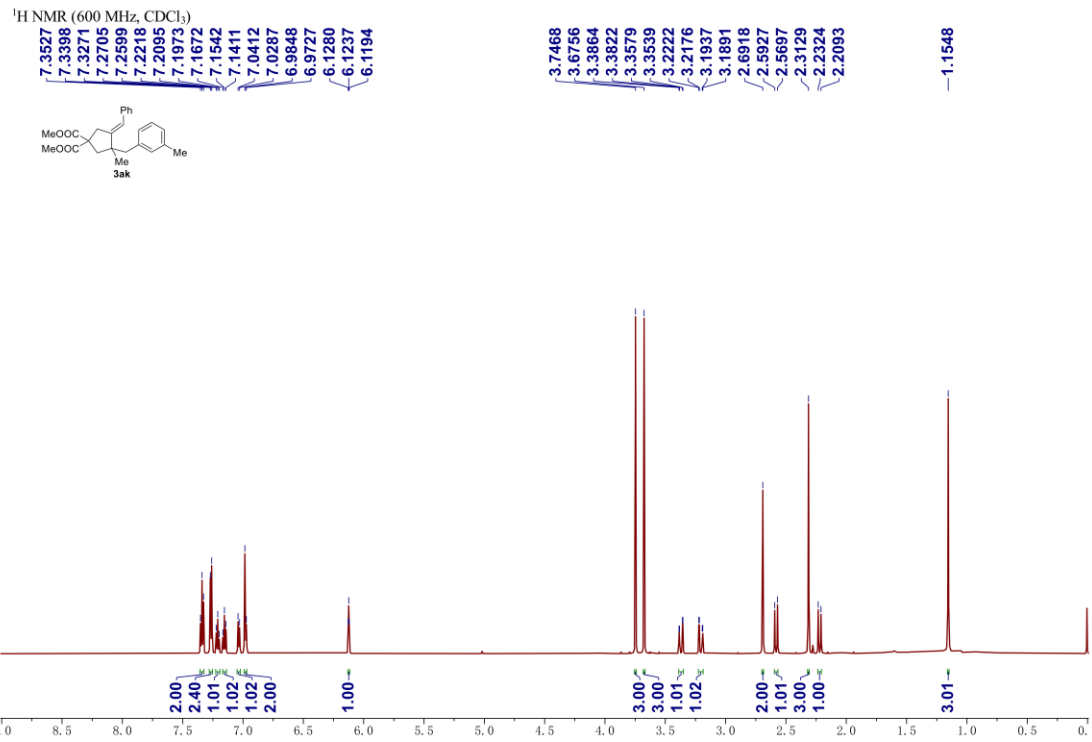


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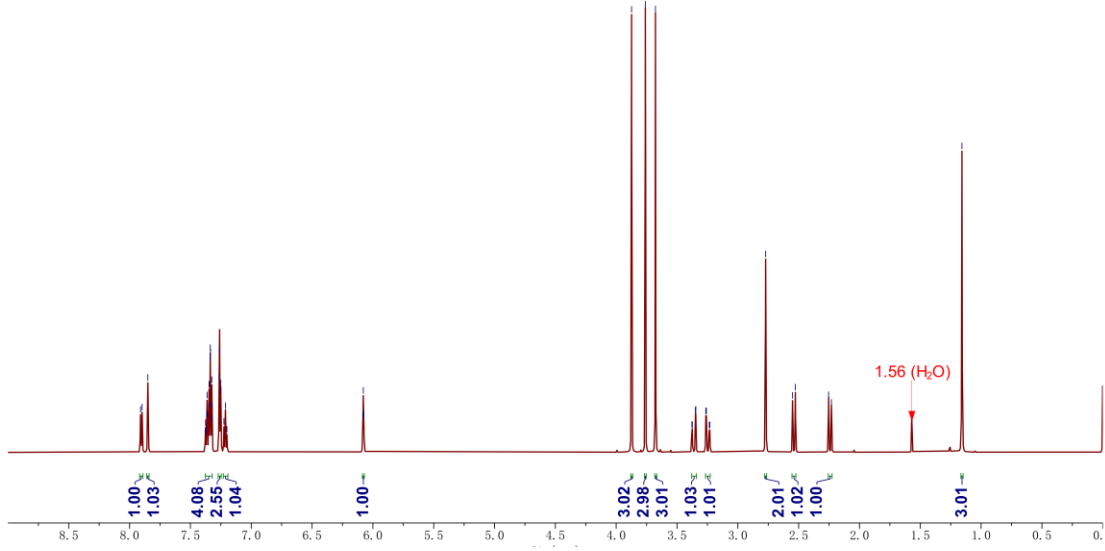
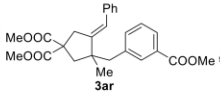
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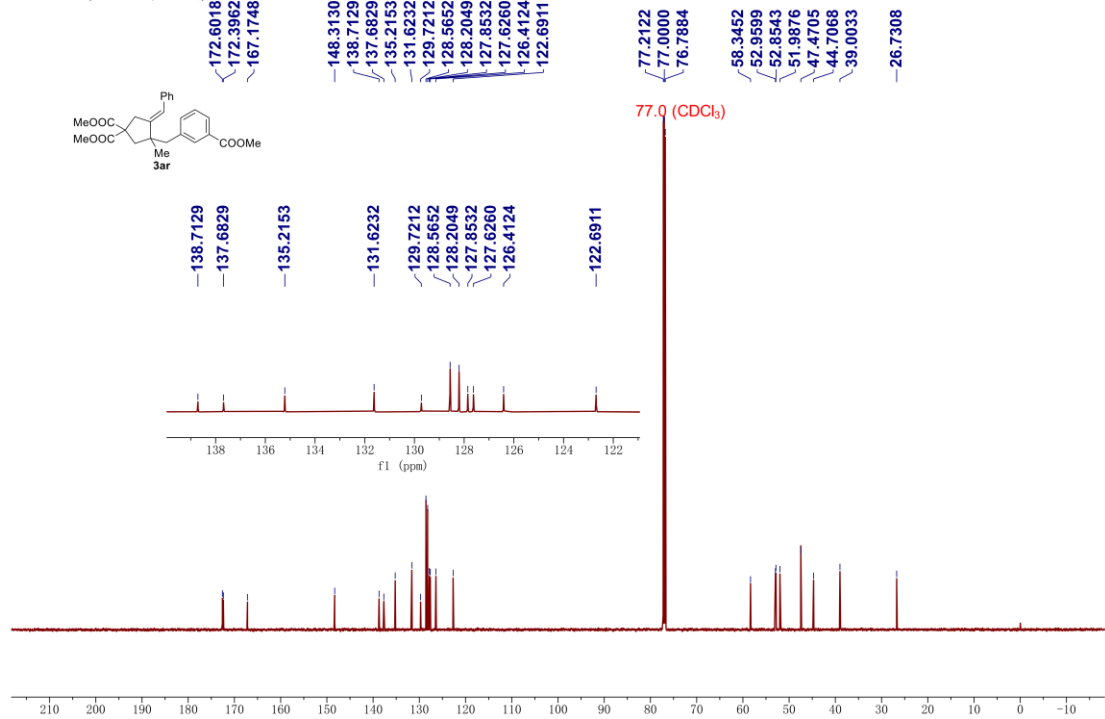
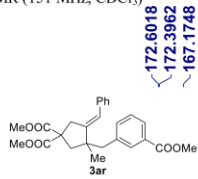


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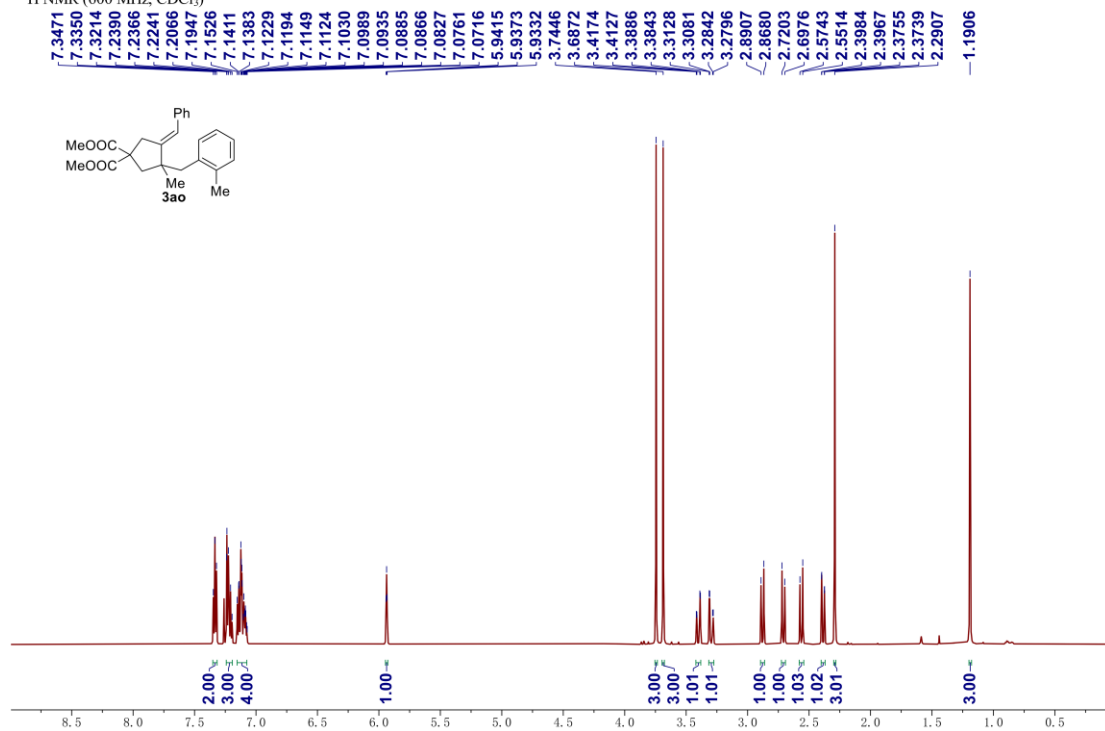
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2.2537
2.2306



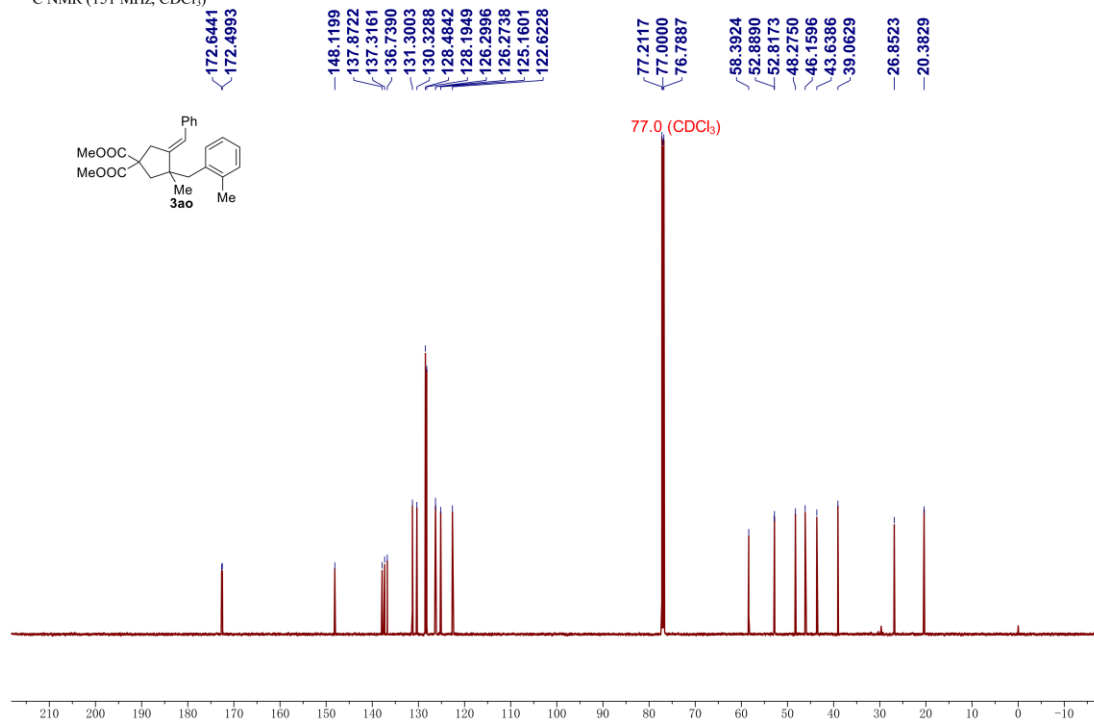
¹³C NMR (151 MHz, CDCl₃)

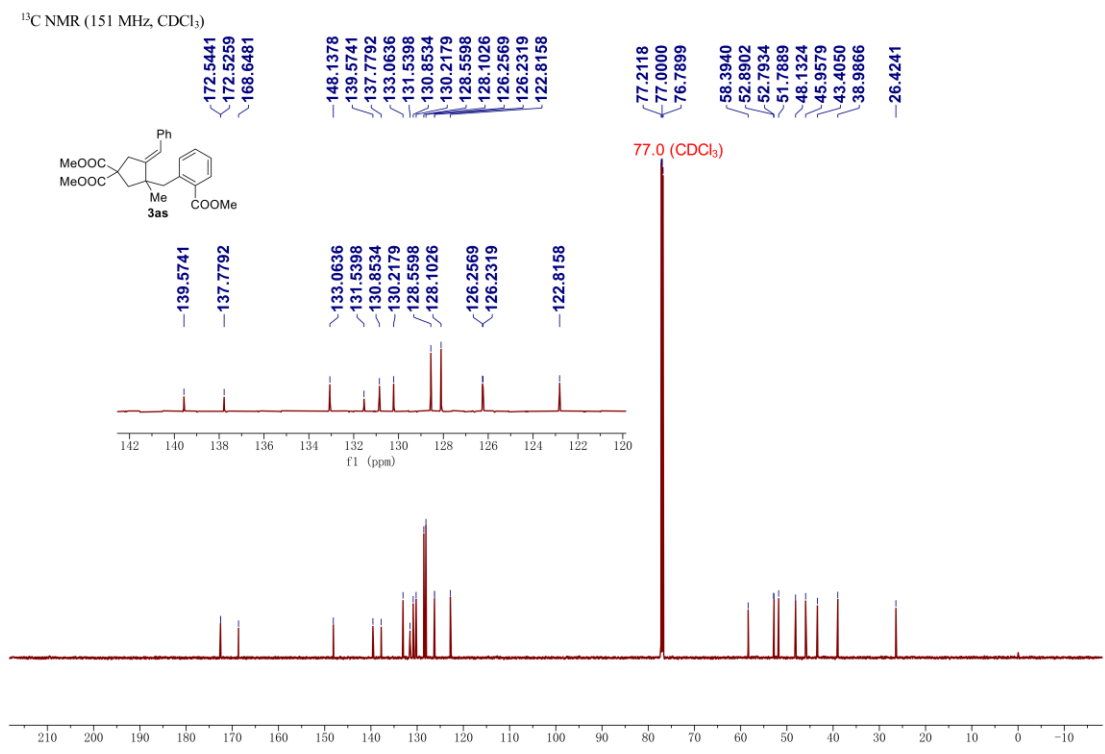
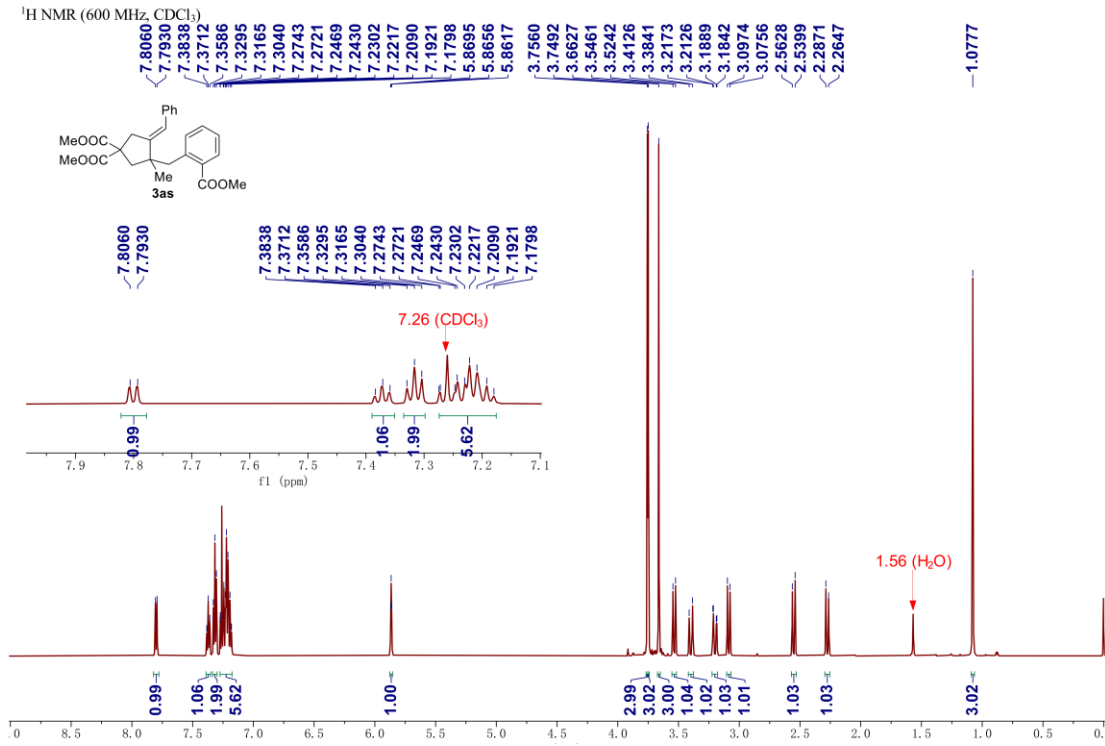


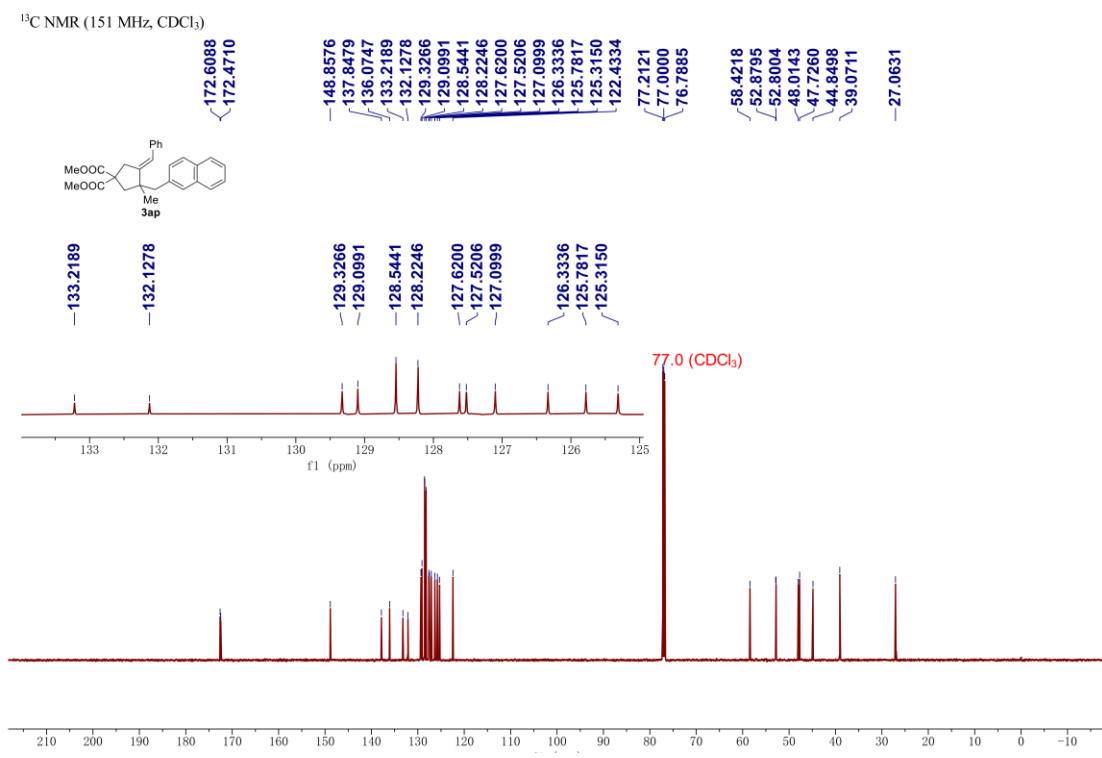
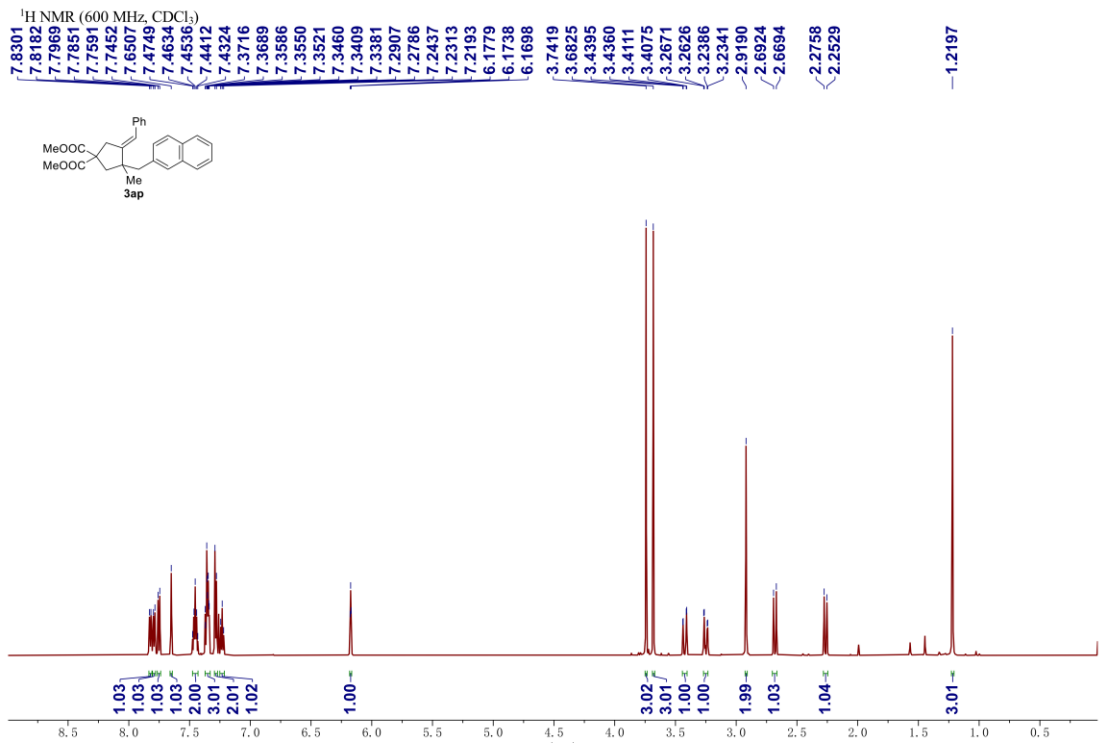
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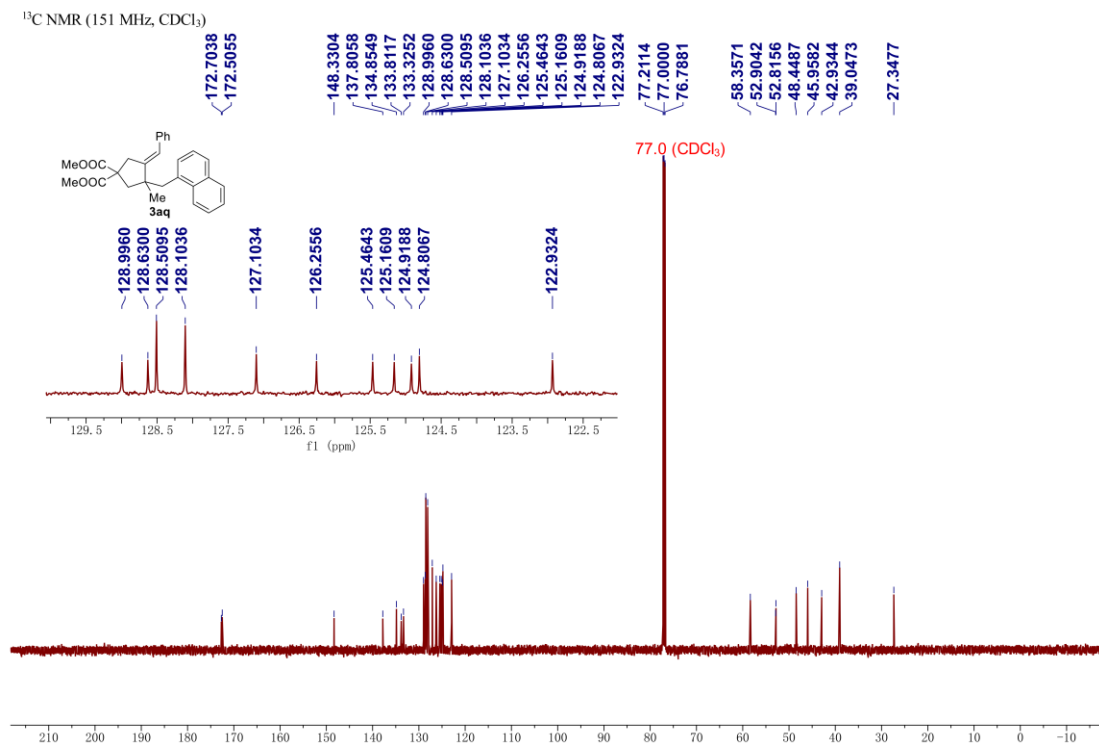
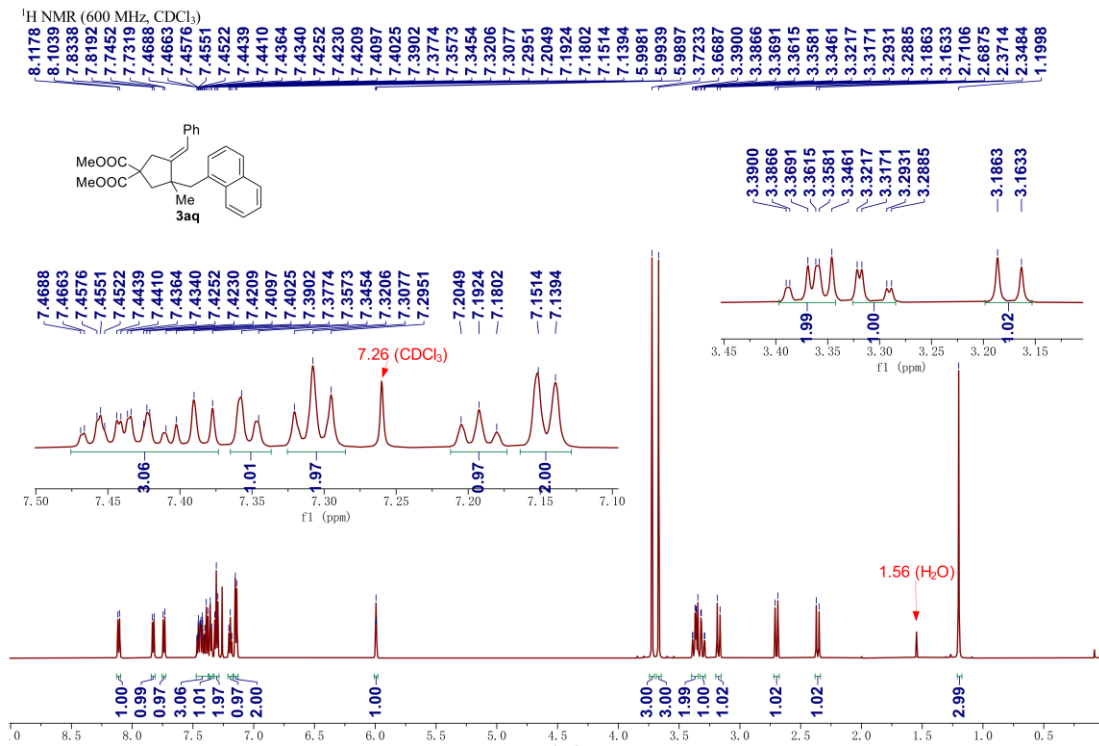


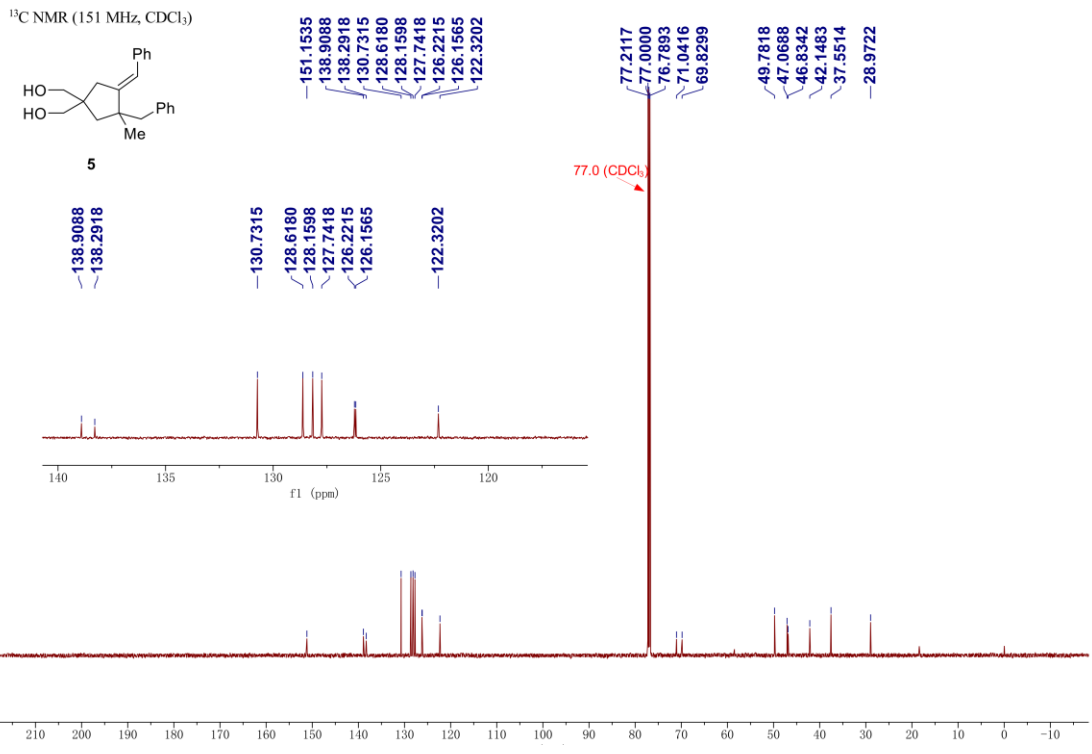
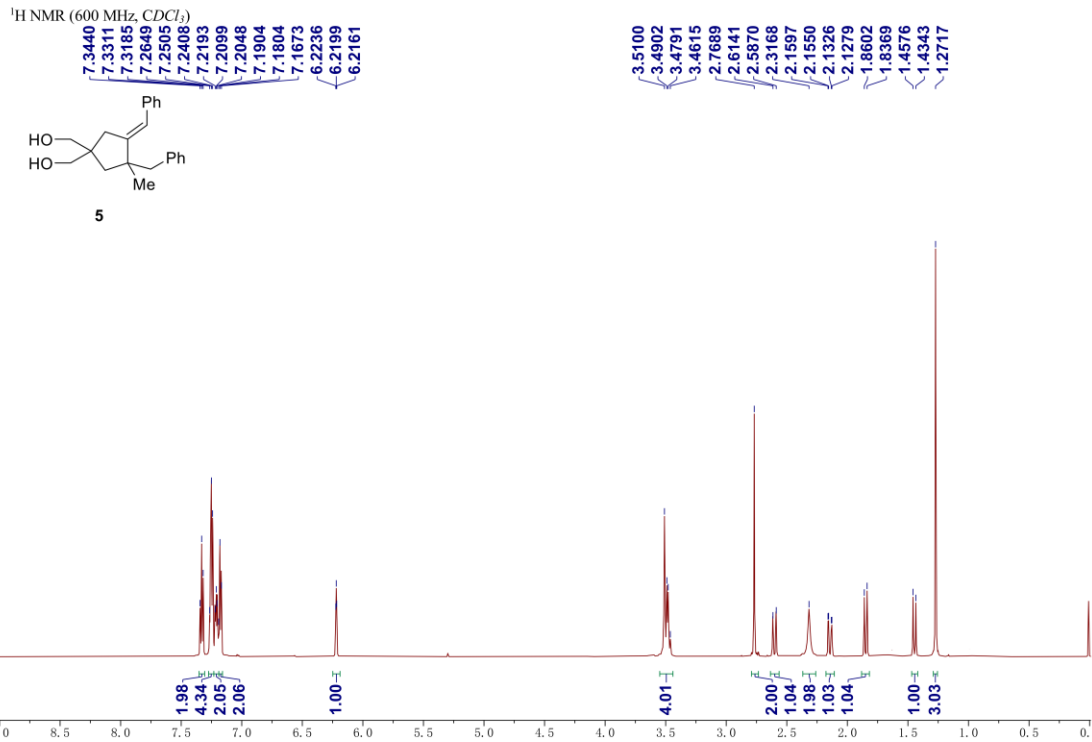
¹³C NMR (151 MHz, CDCl₃)



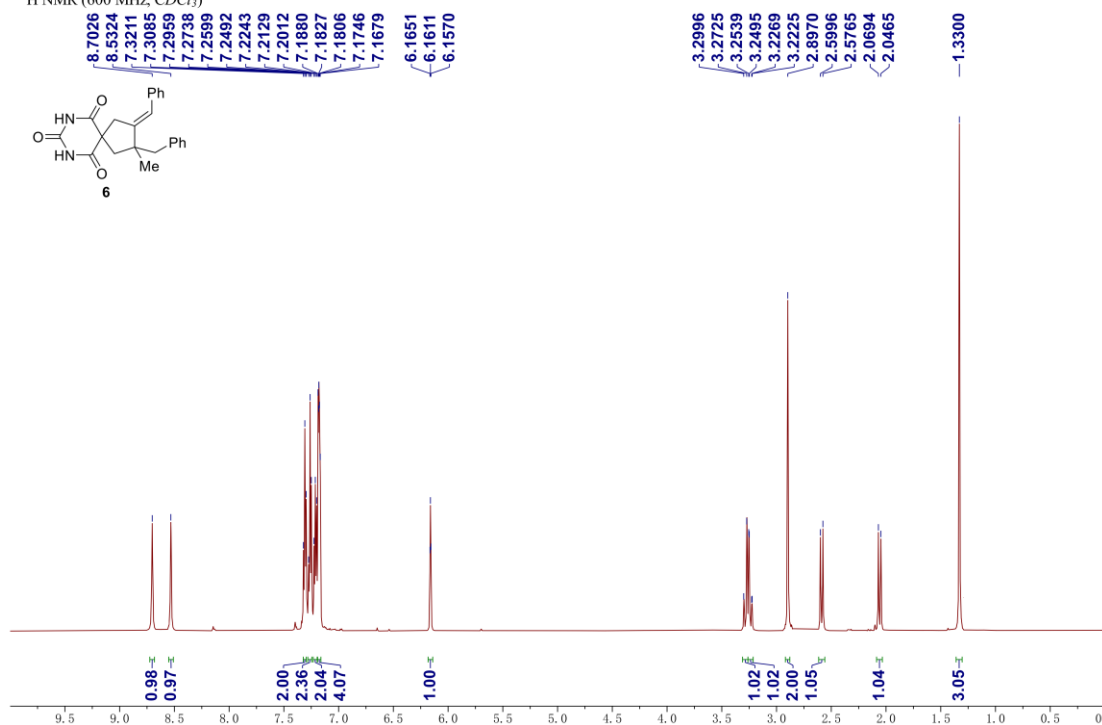
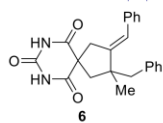




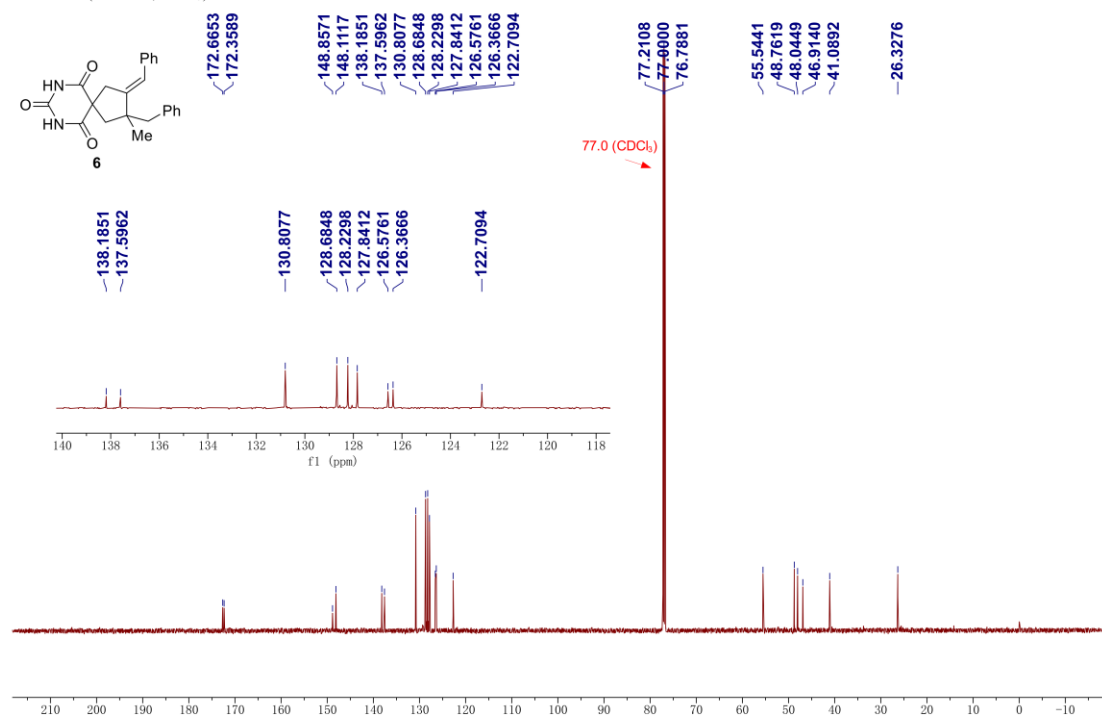
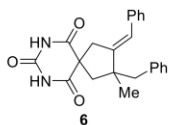




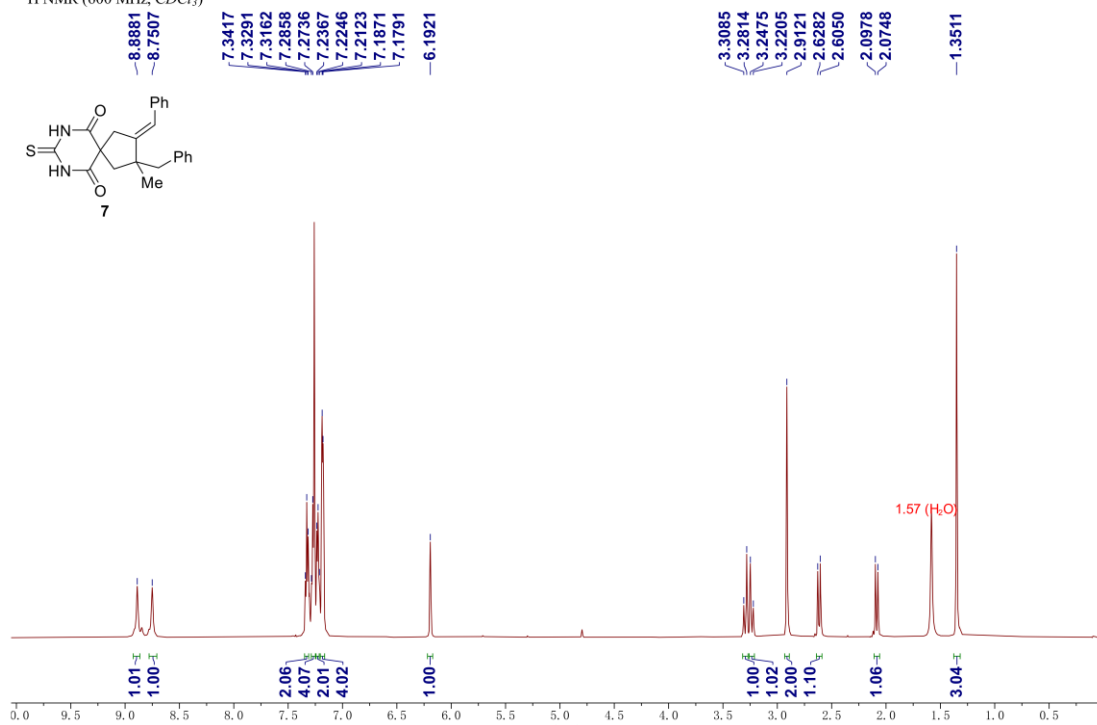
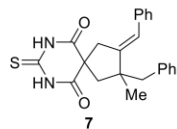
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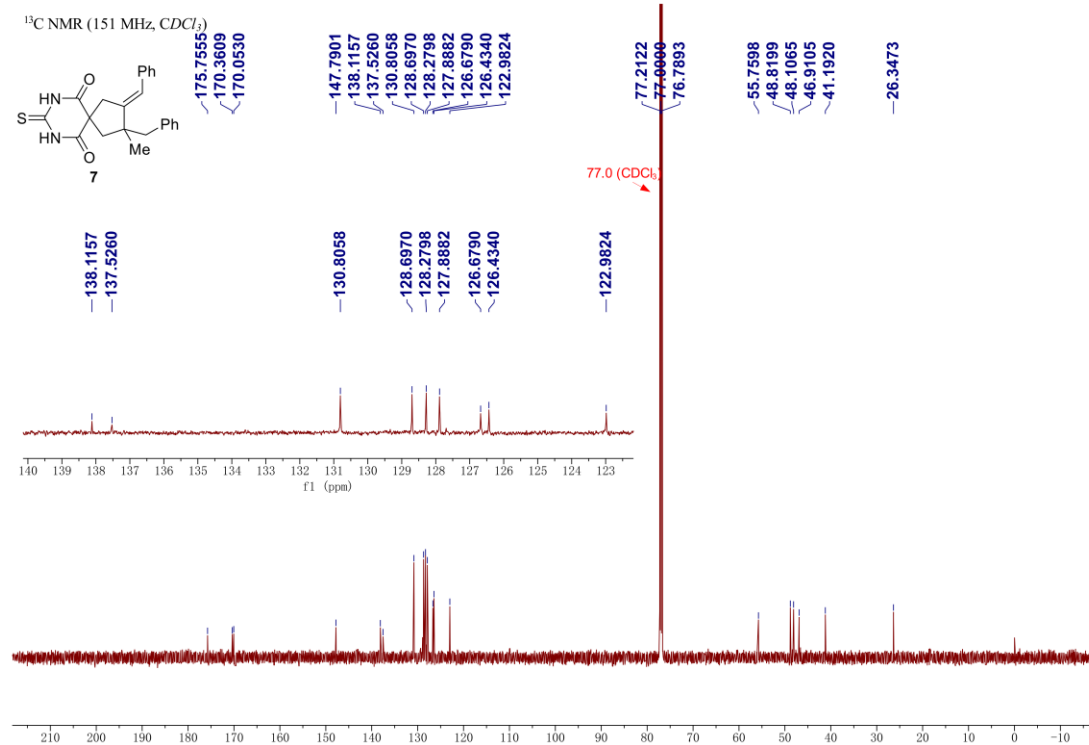
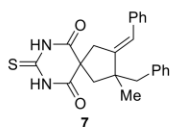
¹³C NMR (151 MHz, CDCl₃)



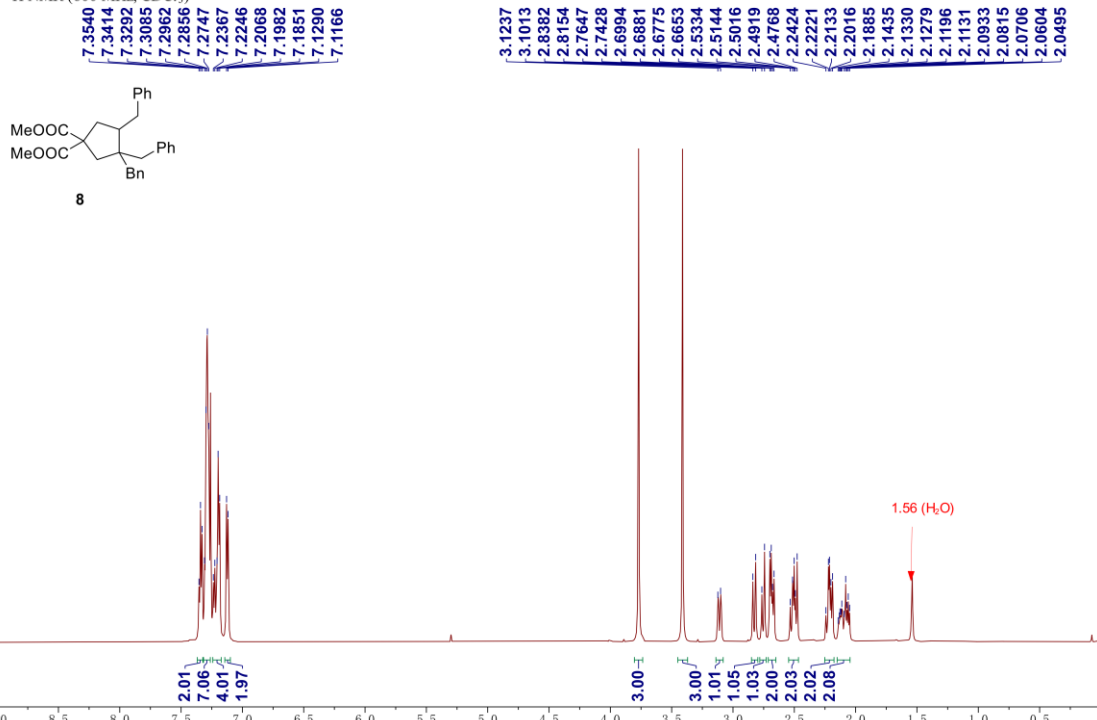
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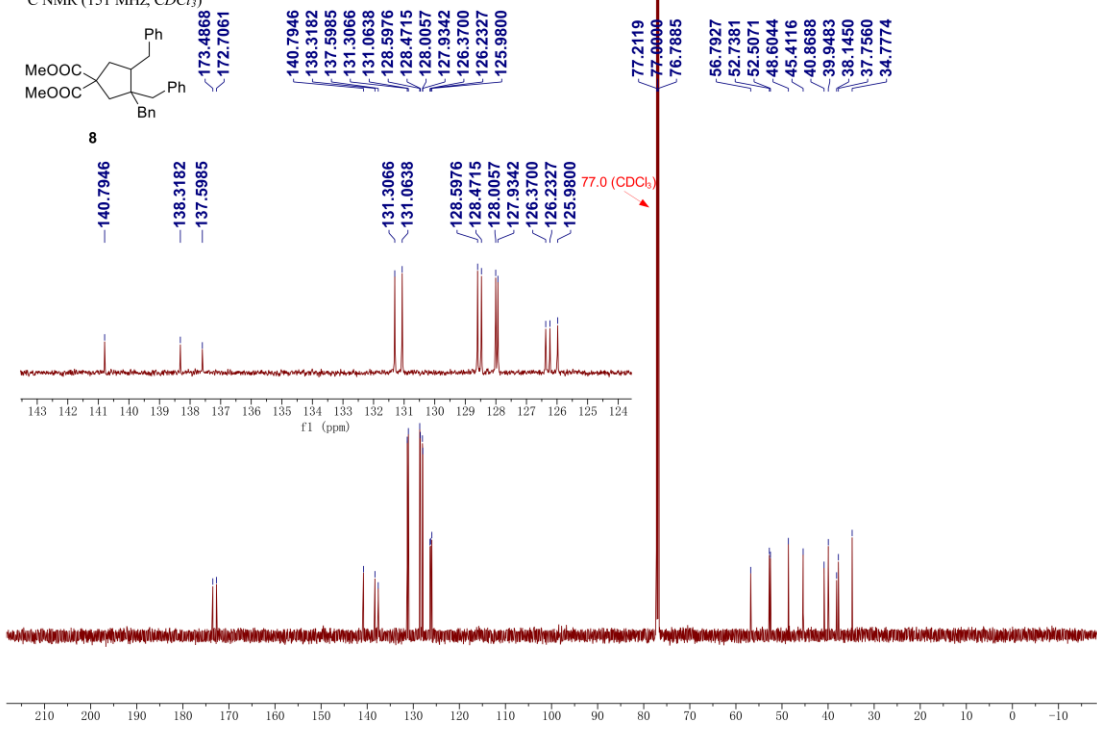
¹³C NMR (151 MHz, CDCl₃)



¹H NMR (600 MHz, CDCl₃)



¹³C NMR (151 MHz, CDCl₃)



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