Supporting Information

A gold(I)-catalyzed chemoselective three-component reaction of phenols, α-diazocarbonyl compounds and allenamides

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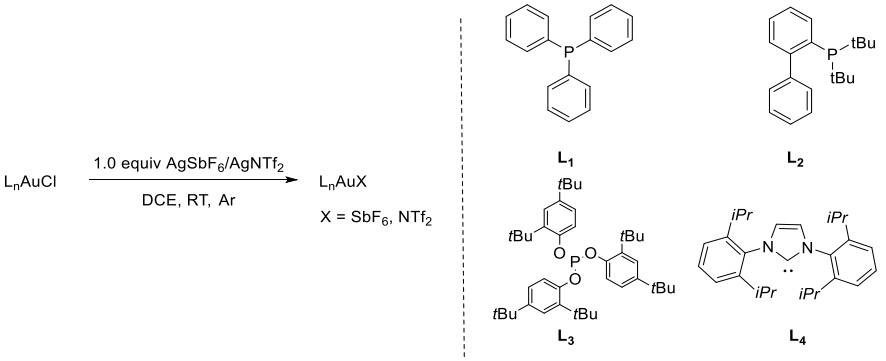
1. General Information

General. Unless noted all solvents were purified and dried using standard procedures. All reactions were carried out under an inert atmosphere in oven-dried Schlenk tubes with magnetic stirring using freshly distilled solvents. Analytical thin layer chromatography (TLC) plates were purchased from EM Science (silica gel 60 F254 plates). All NMR spectra were recorded on a Bruker spectrometer at 400 or 500 MHz (^{1}H NMR), 101 or 126 MHz (^{13}C NMR) and 376 or 471 MHz (^{19}F NMR). Chemical shifts (δ value) were reported in ppm with the solvent signals as reference (in $CDCl_3$ as solvent) and coupling constants (*J*) are given in Hertz (Hz). The peak information was described as: br = broad singlet, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, comp = composite of magnetically non-equivalent protons, down field from internal tetramethylsilane (TMS). Syringe pump was purchased from Longerpump. Needle filters were purchased from Anpel. Single-crystal X-ray diffraction data (**4i**) were collected in a Rikagu XtaLAB Synergy. HRMS (ESI) Mass Spectra were recorded on SHIMADZU LCMS-IT-TOF mass spectrometer. Liquid chromatography–mass spectrometry (LC-MS) was recorded on WATERS ACQUITY UPLC.

Materials. Phenols **1** and all dry solvents except toluene (99.9%, Extra Dry, with molecular sieves, Water ≤ 50 ppm (by K.F.), EnergySeal) were purchased from Energy Chemical. All catalysts including JohnphosAu(MeCN)SbF_6, $(PPh_3)AuCl$, IPr(NHC)AuCl, (2, 4-*t*BuPhO)$_3$PAuCl were purchased from Laajoo. $(C_6F_5)_3B$, CuI, $Cu(MeCN)_4PF_6$, $Cu(MeCN)_4BF_4$, CuOTf, $[PdCl(allyl)]_2$, $Pd(PhCN)_2Cl_2$, $NaBAr^F$, AgOTf were purchased from Energy Chemical. $Rh_2(OAc)_4$ was purchased from Sigma-Aldrich. Diazo compounds **2**[1], allenamide **3**[2], O-H insertion product **13a**[3], C-H insertion product **14a**[3], dimer product **15**[4], dimer product **16**[4] were prepared according to the literature procedures. Anhydrous toluene was distilled from Na under an atmosphere of argon. All other chemicals were obtained from commercial sources and used as received without further purification.

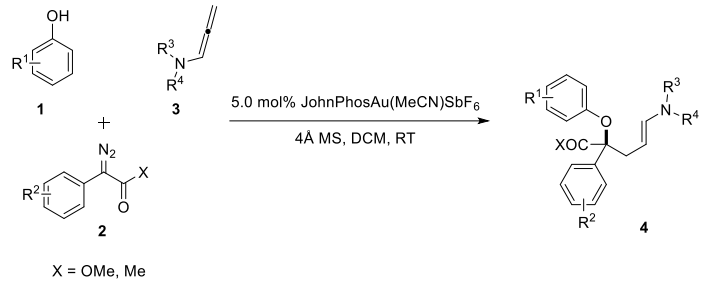
2. Experimental Procedures

2.1 General procedure for synthesis of L_nAuX[5]



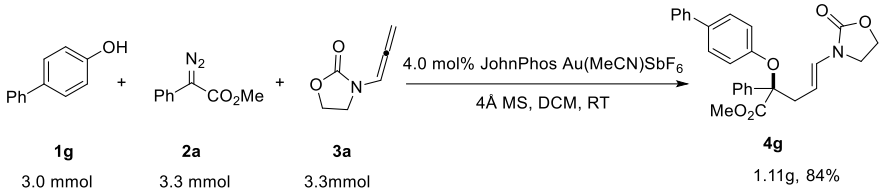
To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, L_nAuCl (0.02 mmol) was dissolved in dry DCE (1.0 mL) and AgX (X = SbF_6, NTf_2) (0.02 mmol) was added. The mixture was stirred under a dinitrogen atmosphere at room temperature for 20 mins, the precipitation of AgCl was removed by flirtation through needle filter. The filtrate was directly used without further purification.

2.2 General procedure for three-component reactions of 4



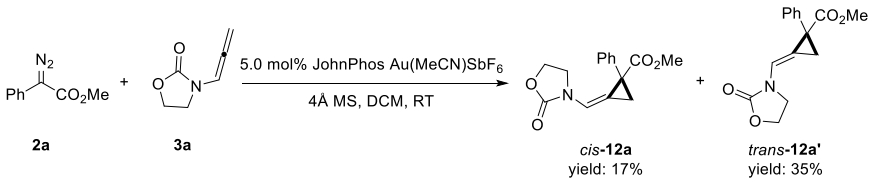
To a flame-dried 25-mL Schlenk flask charged with a magnetic stirring bar, 5.0 mol% JohnphosAu(MeCN)SbF_6, phenol **1** (0.40 mmol), and 100 mg 4 Å MS in 4.0 mL of DCM were sequentially added at room temperature. Diazocarbonyl compounds **2** (0.48 mmol) and allenamide **3** (0.48 mmol) dissolved in DCM (2.0 mL) were added by syringe pump over 1.0 hr under a dinitrogen atmosphere. The mixture was stirred for 1.0 hr under a dinitrogen atmosphere at room temperature. Few amount of pyridine was used for quenching reaction before the solvent was evaporated, and products were purified by column chromatography (10:1 to 2:1 gradient of hexanes: ethyl acetate as eluents) to afford the pure product.

2.3 Procedure for synthesis of 4g in gram scale



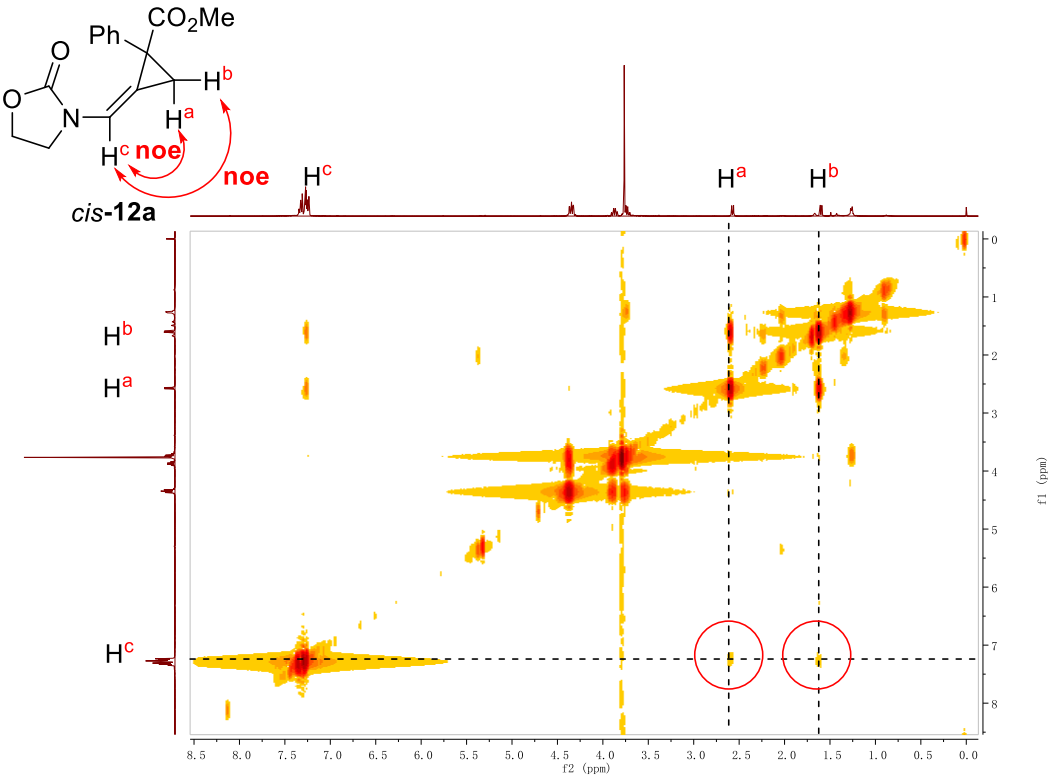
To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, JohnphosAu(MeCN)SbF_6 (96.0 mg, 4.0 mol%), phenol **1g** (510.6 mg, 3.0 mmol), 500 mg 4 Å MS in 10.0 mL of DCM were sequentially added at room temperature. Diazoacetate **2a** (581.4 mg, 3.3 mmol), allenamide **3a** (412.9 mg, 3.3 mmol) in DCM (5.0 mL) were introduced by syringe pump over 1.5 hr and the reaction solution was stirred for another 2.0 hrs under a dinitrogen atmosphere. After the completion of the reaction, few amount of pyridine was used for quenching reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (10:1 to 2:1 gradient of hexanes: ethyl acetate as eluents) to afford **4g** in 83% yield (1.1 g).

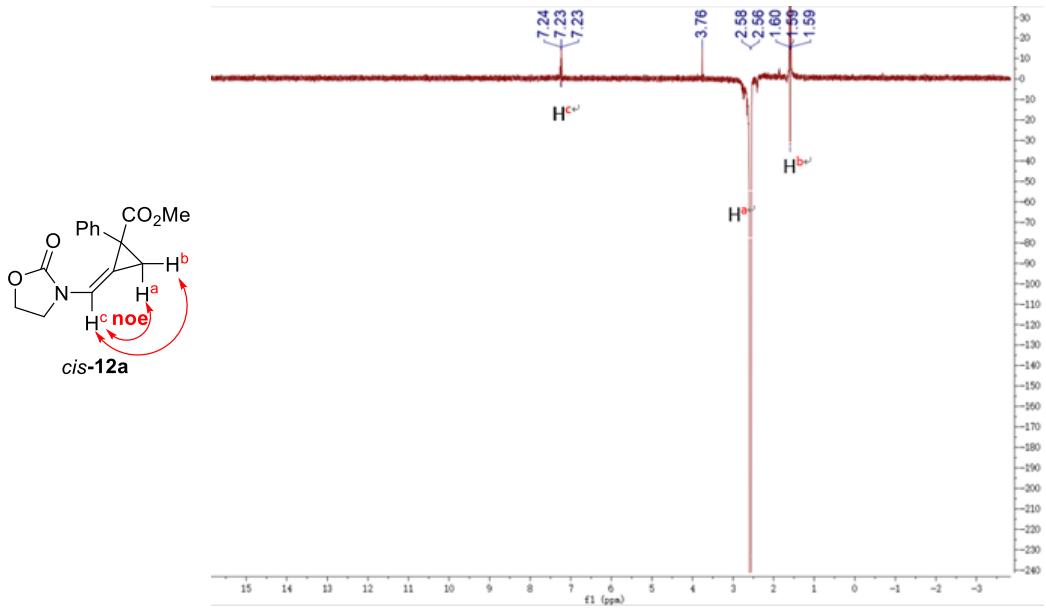
2.4 Procedure for synthesis of 12a and 12b.



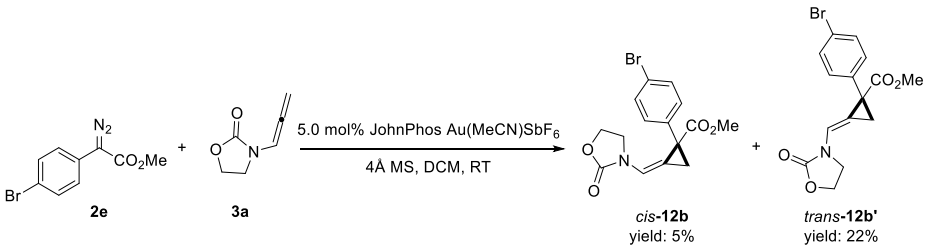
To a flame-dried 25-mL Schlenk flask charged with a magnetic stirring bar, 5.0 mol% JohnphosAu(MeCN)SbF_6, 50 mg 4 Å MS in 4.0 mL of DCM were sequentially added at room temperature. Aryldiazoacetate **2a** (0.40 mmol) and allenamide **3a** (0.60 mmol) dissolved in DCM (2.0 mL) were added by syringe pump over 1.0 hr under a dinitrogen atmosphere. The mixture was stirred for 4.0 hrs under a dinitrogen atmosphere at room temperature. Few amount of pyridine was used for quenching reaction before the solvent was evaporated, and products were purified by column chromatography (10:1 to 1:1 gradient of hexanes: ethyl acetate as eluents) to afford *cis*-**12a** (18.9 mg) and

tran-**12a'** (37.9 mg) in total yield of 52% (*cis*-**12a** : *tran*-**12a'** = 1:2). *cis*-**12a**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (ddd, *J* = 8.3, 4.3, 2.8 Hz, 2H), 7.29 – 7.26 (m, 2H), 7.25 (dd, *J* = 3.0, 1.6 Hz, 1H), 7.24 (t, *J* = 2.0 Hz, 1H), 4.40 – 4.29 (m, 2H), 3.87 (td, *J* = 9.0, 6.8 Hz, 1H), 3.77 (s, 3H), 3.76 – 3.70 (m, 1H), 2.57 (dd, *J* = 7.9, 2.1 Hz, 1H), 1.60 (dd, *J* = 7.9, 2.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.3, 155.7, 137.4, 129.2, 128.3, 127.7, 116.5, 108.2, 62.5, 52.8, 42.9, 31.3, 20.2. *tran*-**12a'**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (ddd, *J* = 8.3, 4.3, 2.8 Hz, 2H), 7.29 – 7.26 (m, 2H), 7.26 – 7.25 (m, 1H), 7.24 (t, *J* = 2.0 Hz, 1H), 4.40 – 4.29 (m, 2H), 3.87 (td, *J* = 9.0, 6.8 Hz, 1H), 3.77 (s, 3H), 3.76 – 3.70 (m, 1H), 2.57 (dd, *J* = 7.9, 2.1 Hz, 1H), 1.60 (dd, *J* = 7.9, 2.0 Hz, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 172.2, 155.6, 139.1, 128.6, 127.4, 127.3, 116.8, 107.2, 62.4, 52.8, 43.3, 33.4, 21.5. HRMS (ESI+) $[M+Na]^+$ calcd for $C_{15}H_{15}NO_4Na^+$: 296.0893, found 296.0891.

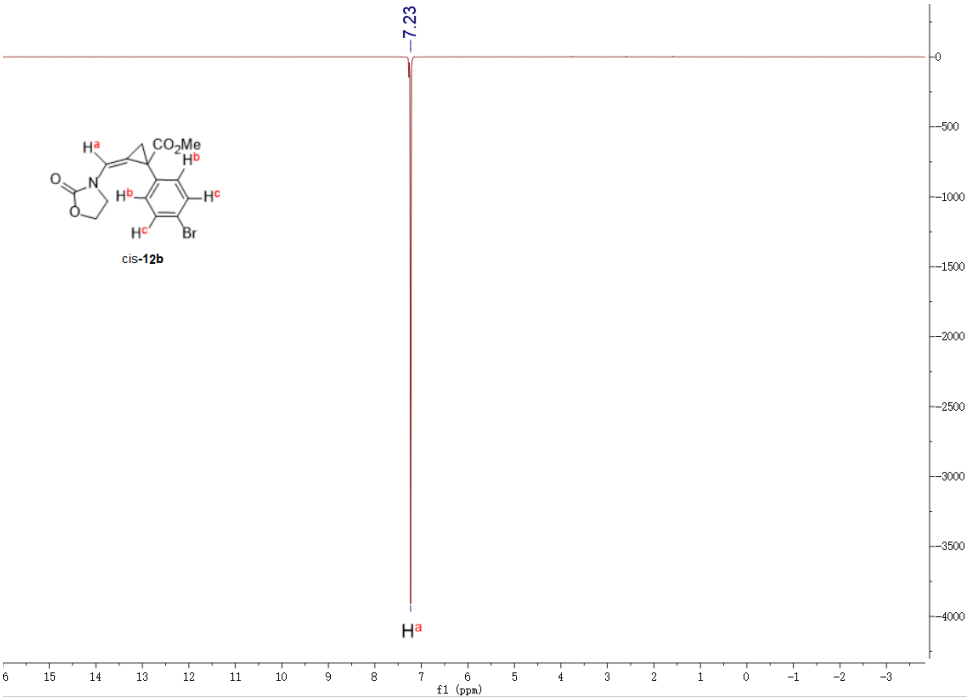




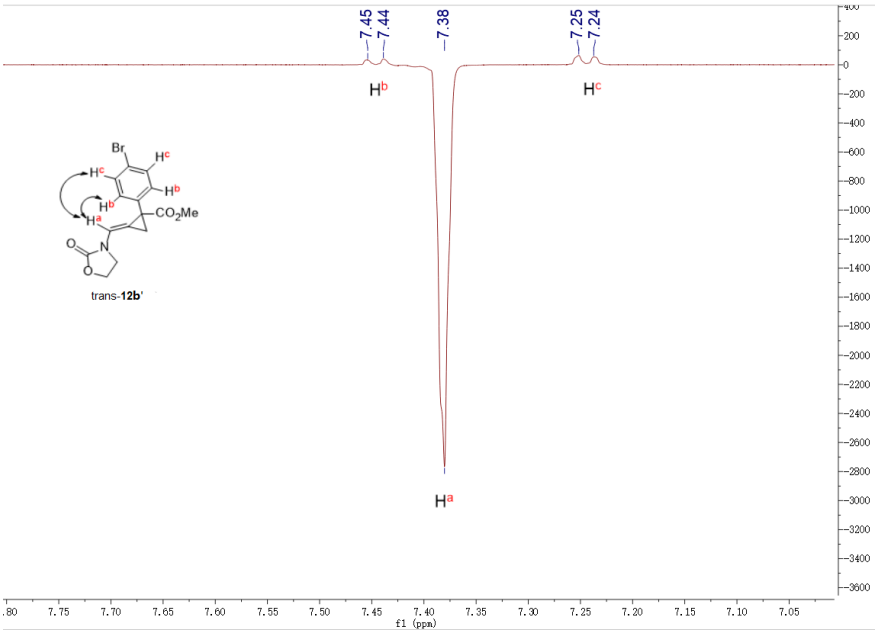
When H^c was motivated, H^a and H^b show response, which meant correlations among three hydrogen and in the same side.



The same procedure to obtain *cis*-**12b** (1.4 mg) and *trans*-**12b'** (30.9 mg) in total yield of 27% (*cis*-**12b**: *tran*-**12b'** = 5:22). *cis*-**12b**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (d, *J* = 7.9 Hz, 2H), 7.23 (s, 1H), 7.16 (d, *J* = 7.8 Hz, 2H), 4.43 – 4.27 (m, 2H), 3.81 (dd, *J* = 16.2, 8.5 Hz, 1H), 3.76 (s, 3H), 3.70 (dd, *J* = 17.5, 8.7 Hz, 1H), 2.59 (d, *J* = 8.0 Hz, 1H), 1.59 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 131.7, 129.2, 117.0, 106.9, 62.4, 52.9, 43.2, 32.7, 21.8. *tran*-**12b'**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, *J* = 7.5 Hz, 2H), 7.38 (s, 1H), 7.24 (d, *J* = 7.3 Hz, 2H), 4.46 (dd, *J* = 14.3, 7.5 Hz, 2H), 4.03 (q, *J* = 8.3 Hz, 1H), 3.91 (q, *J* = 8.4 Hz, 1H), 3.67 (s, 3H), 2.58 (d, *J* = 7.8 Hz, 1H), 1.83 (d, *J* = 7.8 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.8, 155.6, 136.4, 131.4, 130.9, 121.8, 116.9, 107.6, 62.4, 52.9, 42.9, 30.8, 20.3. HRMS (ESI+) $[M+Na]^+$ calcd for $C_{15}H_{14}NO_4BrNa^+$: 373.9998, found 373.9999.

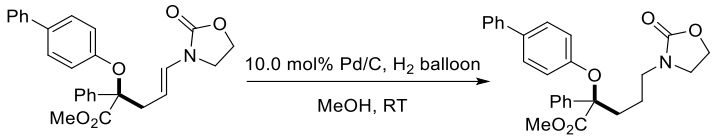


When H^a was motivated, H^b and H^c show no response, that meant no correlation among three hydrogen and not in the same side.



When H^a was motivated, H^b and H^c show response, which meant correlations among three hydrogen and in the same side.

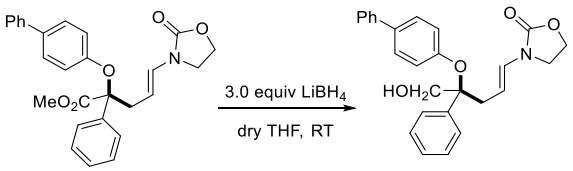
2.5 Procedure for synthesis of 5 from 4g



4g **5**
Yield: 78%

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **4g** （44.3 mg, 0.10mmol), Pd/C (1.1 mg, 10.0 mol%) in 4.0mL MeOH were sequentially added and stirred for overnight with a hydrogen-filled balloon. The reaction mixture the reaction mixture was filtered, and the filtrate were concentrated, the crude product was purified by flash chromatography on silica gel (5:1 to 2:1 gradient of hexanes: ethyl acetate as eluents) to afford the pure product **5** (34.7 mg, 78%, colorless oil). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.9 Hz, 2H), 7.51 (d, *J* = 7.8 Hz, 2H), 7.45 (d, *J* = 8.2 Hz, 2H), 7.39 (t, *J* = 7.3 Hz, 4H), 7.32 (dd, *J* = 15.6, 7.6 Hz, 2H), 6.89 (d, *J* = 8.2 Hz, 2H), 4.01 (t, *J* = 8.0 Hz, 2H), 3.71 (s, 3H), 3.19 – 3.10 (m, 2H), 3.09 – 2.98 (m, 2H), 2.71 – 2.57 (m, 1H), 2.47 – 2.31 (m, 1H), 1.39 (dtd, *J* = 25.8, 13.1, 6.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.5, 158.6, 154.4, 140.3, 139.0, 134.7, 128.9, 128.7, 128.3, 127.9, 127.0, 126.7, 125.7, 118.2, 84.3, 61.6, 53.0, 43.7, 43.5, 32.0, 20.7. HRMS (ESI) $[M+Na]^+$ calcd for $C_{27}H_{27}NO_5Na^+$, 468.1781, found 468.1779.

2.6 Procedure for synthesis of 6 from 4g

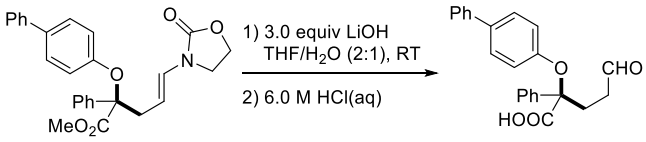


4g **6**
Yield: 85%

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **4g** (44.3 mg, 0.10 mmol), $LiBH_4$ (6.6 mg, 0.30 mmol) in 2.5 mL dry THF were sequentially added at room temperature and stirred for 4.0 hrs. The reaction solution was slowly added saturated NH_4Cl(aq) before extracted with EtOAc (5 x 3 mL). The organic layers were washed with brine. After drying over $MgSO_4$ and concentration in vacuo, the

crude product was purified by flash chromatography on silica gel (5:1 to 1:1 gradient of hexanes: ethyl acetate as eluents) to afford the pure product **6** (35.3 mg, 85%, white solid). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (s, 1H), 7.51 (dd, *J* = 11.1, 8.1 Hz, 3H), 7.42 (dd, *J* = 6.0, 2.7 Hz, 5H), 7.35 – 7.27 (m, 3H), 6.83 (d, *J* = 8.7 Hz, 2H), 6.71 (d, *J* = 14.3 Hz, 1H), 4.66 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.39 (t, *J* = 8.3 Hz, 2H), 4.04 (d, *J* = 10.9 Hz, 2H), 3.93 (d, *J* = 10.7 Hz, 2H), 3.62 (dt, *J* = 16.0, 8.5 Hz, 2H), 3.12 – 2.87 (m, 3H), 2.10 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 154.3, 144.2, 140.4, 135.1, 130.9, 130.2, 129.5, 128.8, 127.9, 127.1, 126.9, 126.7, 125.1, 123.0, 119.9, 104.1, 83.6, 66.4, 62.2, 42.5, 35.4. HRMS (ESI) [M+Na]+ calcd for $C_{24}H_{26}NO_4BrNa^+$, 438.1676, found 438.1676.

2.7 Procedure for synthesis of 7 from 4g

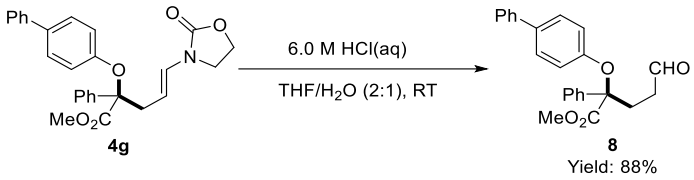


4g **7**
Yield: 80%

To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **4g** (44.3 mg, 0.10 mmol), LiOH (12.6 mg, 0.30 mmol) in 3.0 mL THF/H_2O(1: 0.5) were sequentially added at room temperature and stirred for overnight. The reaction solution was slowly added 6.0 M HCl(aq) to pH = 1～2 before extracted with EtOAc (5 x 3 mL). The organic layers were washed with brine. After drying over $MgSO_4$ and concentration in vacuo, the crude product was purified by flash chromatography on silica gel (10:1 to pure EtOAc gradient of hexanes: ethyl acetate as eluents) to afford the pure product **7** (28.8 mg, 80%, colorless oil). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.56 (s, 1H), 9.21 (s, 1H), 7.63 (d, *J* = 7.1 Hz, 2H), 7.46 (d, *J* = 7.3 Hz, 2H), 7.36 (d, *J* = 7.7 Hz, 6H), 7.28 (d, *J* = 7.1 Hz, 1H), 7.24 (d, *J* = 12.9 Hz, 1H), 6.84 (d, *J* = 8.1 Hz, 2H), 2.89 (d, *J* = 8.6 Hz, 1H), 2.77 – 2.67 (m, 1H), 2.43 (dt, *J* = 14.6, 11.1 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.8, 172.3, 154.4, 140.4, 138.4, 134.9, 128.8, 128.7, 128.4, 128.0, 126.9, 126.8,

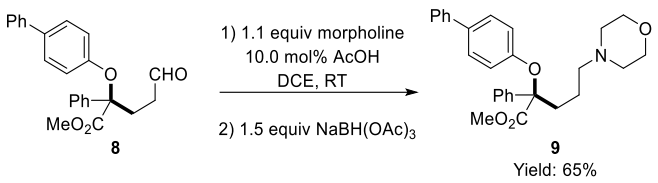
125.9, 117.9, 116.4, 115.7, 84.0, 53.0, 38.0, 29.0. HRMS (ESI) $[M+Na]^+$ calcd for $C_{23}H_{20}O_4Na^+$, 383.1254, found 383.1258.

2.8 Procedure for synthesis of 8 from 4g



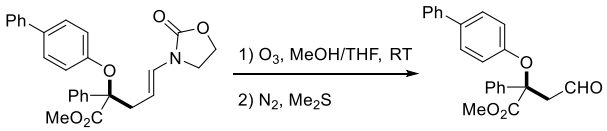
To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **4g** (44.3 mg, 0.10 mmol) in 3.0 mL THF/H_2O (2: 1) at room temperature, the reaction solution was slowly added 0.5 mL 6.0 M HCl(aq) and stirred for overnight. The reaction mixture was treated with saturated $NaHCO_3$(aq) before extracted with EtOAc (3 x 3 mL). The organic layers were washed with brine. After drying over $MgSO_4$ and concentration in vacuo, the crude product was purified by flash chromatography on silica gel (10:1 to 5:1 gradient of hexanes: ethyl acetate as eluents) to afford the pure product **8** (32.9 mg, 88%, colorless oil). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.62 (s, 1H), 7.68 (d, *J* = 7.7 Hz, 2H), 7.56 (d, *J* = 7.6 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.47 – 7.41 (m, 4H), 7.41 – 7.36 (m, 1H), 7.33 (t, *J* = 7.3 Hz, 1H), 6.92 (d, *J* = 8.1 Hz, 2H), 3.75 (s, 3H), 2.94 (ddd, *J* = 15.0, 9.8, 5.5 Hz, 1H), 2.76 (ddd, *J* = 14.9, 10.0, 5.1 Hz, 1H), 2.54 – 2.42 (m, 1H), 2.41 – 2.30 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.8, 172.3, 154.4, 140.4, 138.4, 134.9, 128.8, 128.7, 128.4, 128.0, 126.9, 126.8, 125.9, 117.9, 116.4, 115.7, 84.0, 53.0, 38.0, 29.0. HRMS (ESI) $[M+Na]^+$ calcd for $C_{24}H_{22}O_4Na^+$, 397.1410, found 397.1410.

2.9 Procedure for synthesis of 9 from 8



To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **8** (37.4 mg, 0.10 mmol), morpholine (9.6 mg, 0.11 mmol) and AcOH (0.6 mg, 10.0 mol%) in 3.0 mL DCE were sequentially added at room temperature and stirred for overnight. Sodium triacetoxyborohydride (31.8 mg, 0.15 mmol) was added to the reaction in one portion and then stirred for another 8.0 hrs. The mixture was concentrated in vacuo, the crude product was purified by flash chromatography on silica gel (10:1 to 5:1 gradient of hexanes: ethyl acetate as eluents) to afford the pure product **9** (32.9 mg, 65%, colorless oil). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.9 Hz, 2H), 7.52 (d, *J* = 7.8 Hz, 2H), 7.44 (d, *J* = 8.3 Hz, 2H), 7.40 (dd, *J* = 12.5, 7.1 Hz, 4H), 7.31 (dt, *J* = 14.5, 7.3 Hz, 2H), 6.89 (d, *J* = 8.2 Hz, 2H), 3.72 (s, 3H), 3.54 (t, *J* = 11.7 Hz, 4H), 2.69 – 2.59 (m, 1H), 2.45 – 2.35 (m, 1H), 2.18 (d, *J* = 8.2 Hz, 4H), 1.44 – 1.35 (m, 1H), 1.34 – 1.25 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.0, 154.6, 140.5, 139.3, 134.6, 128.8, 128.5, 128.0, 127.8, 126.9, 126.7, 125.8, 118.2, 84.7, 66.9, 58.0, 53.4, 52.8, 33.1, 19.6.HRMS (ESI) $[M+Na]^+$ calcd for $C_{28}H_{31}NO_4Na^+$, 446.2326, found 446.2322.

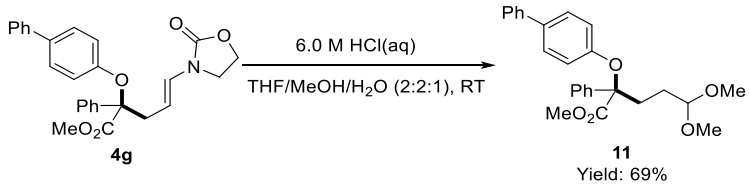
2.10 Procedure for synthesis of 10 from 4g



To a flame-dried 25-mL Schlenk flask charged with a magnetic stirring bar, **4g** (44.3 mg, 0.10 mmol) in 4.0 mL THF/MeOH (1:1) at room temperature, introducing ozone to reaction by ozonator (8 L/min) lasting 30 mins, and then introducing nitrogen instead for 0.5 hr. The reaction mixture was treated with Me_2S. The organic layers were washed with brine. After drying over $MgSO_4$ and concentration in vacuo, the crude product was purified by flash chromatography on silica gel (10:1 to 5:1 gradient of hexanes: ethyl acetate as eluents) to afford the pure product **10** (32.5 mg, 90%, colorless oil). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.63 (t, *J* = 2.1 Hz, 1H), 7.67 (d, *J* = 7.5 Hz, 2H), 7.58 – 7.53 (m, 2H), 7.50 – 7.41 (m, 7H), 7.34 (t, *J* = 7.3 Hz, 1H), 6.91 (d, *J* = 8.7 Hz, 2H), 3.81 (s, 3H), 3.57 – 3.39 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ

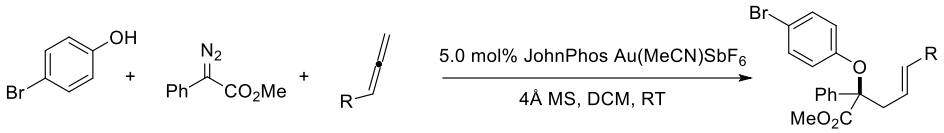
198.5, 171.5, 154.1, 140.3, 138.1, 135.9, 129.0, 128.8, 128.8, 128.7, 128.3, 128.1, 127.0, 126.8, 126.7, 125.9, 119.2, 115.7, 82.8, 53.2, 48.9. HRMS (ESI) $[M+Na]^+$ calcd for $C_{23}H_{20}O_4Na^+$, 383.1254, found 383.1254.

2.11 Procedure for synthesis of 11 from 4g



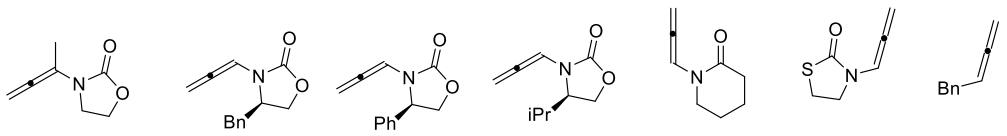
To a flame-dried 10-mL Schlenk flask charged with a magnetic stirring bar, **4g** (44.3 mg, 0.10 mmol) in 2.5 mL THF/MeOH/H_2O (2:2:1) at room temperature, the reaction solution was slowly added 0.5 mL 6.0 M HCl(aq) and stirred for overnight. The reaction mixture was treated with saturated $NaHCO_3$(aq) before extracted with EtOAc (3 x 3 mL). The organic layers were washed with brine. After drying over $MgSO_4$ and concentration in vacuo, the crude product was purified by flash chromatography on silica gel (510:1 to 1:1 gradient of hexanes: ethyl acetate as eluents) to afford the pure product **11** (29.0 mg, 69%, colorless oil). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.9 Hz, 2H), 7.52 (d, *J* = 7.8 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.39 (dd, *J* = 11.5, 7.2 Hz, 4H), 7.30 (dt, *J* = 14.6, 7.3 Hz, 2H), 6.89 (d, *J* = 8.0 Hz, 2H), 4.21 (t, *J* = 5.6 Hz, 1H), 3.71 (s, 3H), 3.11 (s, 6H), 2.68 – 2.57 (m, 1H), 2.45 – 2.33 (m, 1H), 1.53 (ddd, *J* = 17.6, 12.6, 5.0 Hz, 1H), 1.45 (dt, *J* = 18.6, 5.0 Hz, 1H). ^{13}C NMR (101 MHz, CDCl3) δ 173.0, 154.6, 140.5, 139.3, 134.6, 128.8, 128.5, 128.0, 127.8, 126.9, 126.7, 125.8, 118.2, 84.7, 66.9, 58.0, 53.4, 52.8, 33.1, 19.6. HRMS (ESI) $[M+Na]^+$ calcd for $C_{26}H_{28}O_5Na^+$, 443.1829, found 443.1831.

3. Table S1 for Detailed Investigation of Allenamides



1a	2a	3	4
0.40 mmol	0.48 mmol	0.48 mmol	yield<5%

Examples of failing to give desired products



3b 3c 3d 3e 3f 3g 3h

To a flame-dried 25-mL Schlenk flask charged with a magnetic stirring bar, 5.0 mol% JohnphosAu(MeCN)SbF_6, phenol **1a** (0.40 mmol), and 100 mg 4 Å MS in 4.0 mL of DCM were sequentially added at room temperature. Aryldiazoacetate **2** (0.48 mmol) and allene **3** (0.48 mmol) dissolved in DCM (2.0 mL) were added by syringe pump over 1.0 hr under a dinitrogen atmosphere. The mixture was stirred for 1.0 hr under a dinitrogen atmosphere at room temperature. Few amount of pyridine was used for quenching reaction before the solvent was evaporated, Few amount of pyridine was used for quenching reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. The crude product was detected by TLC and ^{1}H NMR using 1, 3, 5-trimethoxybenzene as an internal standard. Above examples failed to give desired products in detectable yields, the major side products of reactions contain **3b-3g** are insertion product **13a**, dimer of **3**. Reaction contains **3h** recover all **3h** and the major side products are **13a**.

4. Computational Details

We used the Gaussian 09 software[6] to carry out all the DFT calculations. The structures, were optimized at the M06/Lanl2dz+6-31G(d,p)[7] (Lanl2dz[8] for Au and 6-31G(d,p) for other atoms) level of theory. Frequency analysis calculations were carried out at the same level to characterize the structures (transition states show only one

negative frequency). The intrinsic reaction coordinate (IRC)[9] analysis has been calculated to prove the transition state was connecting the related reactant and product on the potential energy surface (PES). The single-point calculations were performed with solvent effects of dichloromethane by using the SMD model[10] at the M06/SDD+6-31+G(d,p) (SDD[11] for Au and 6-31+G(d,p) for other atoms) level of theory. All discussed Gibbs free energies were calculated at room temperature (298K) and corrected from the SMD solvation model.

To account for the crucial precursors preceding the O-H and C-H bond insertion,[12] we calculated the reaction pathways of α-diazoesters and catalyst AuL (L = Johnphos) in solution (Fig. S1). As shown in Fig. S1, the generation of the Au-carbene complex is drastically exothermic and easy with low energy barrier of 14.10 kcal/mol. Thus, we used the Au-carbene and phenol as the reactants for the O-H and C-H bond insertion reactions.

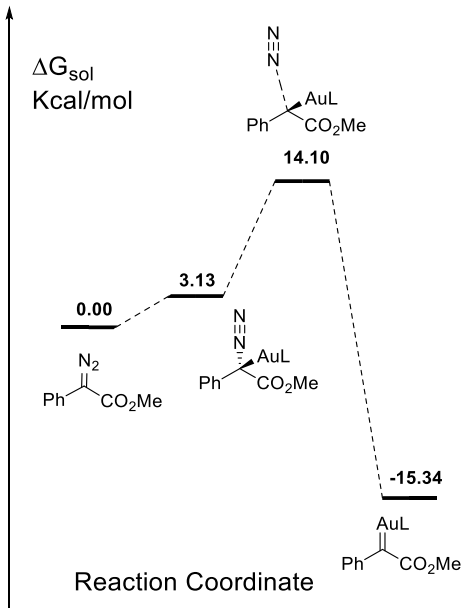
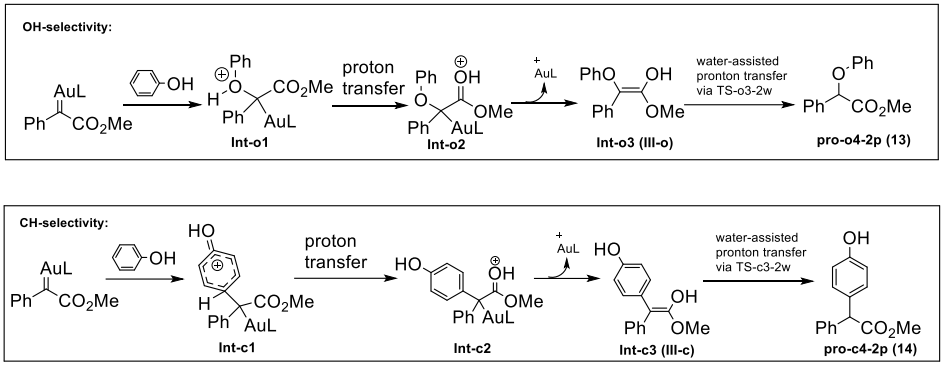


Fig S1. The calculated reaction pathway of α-Diazoesters and the catalyst AuL (L= Johnphos) in solution.

The reaction mechanisms and the Gibbs energy profiles for all the corresponding stationary structures from DFT calculations are listed below. In addition, the imaginary frequency and cartesian coordinates for all the transition states are also given below.



Scheme S1 Proposed Mechanism for the Au-catalyzed Two-Components O-H and C-H insertion Reactions. Int: intermediate, pro: product.

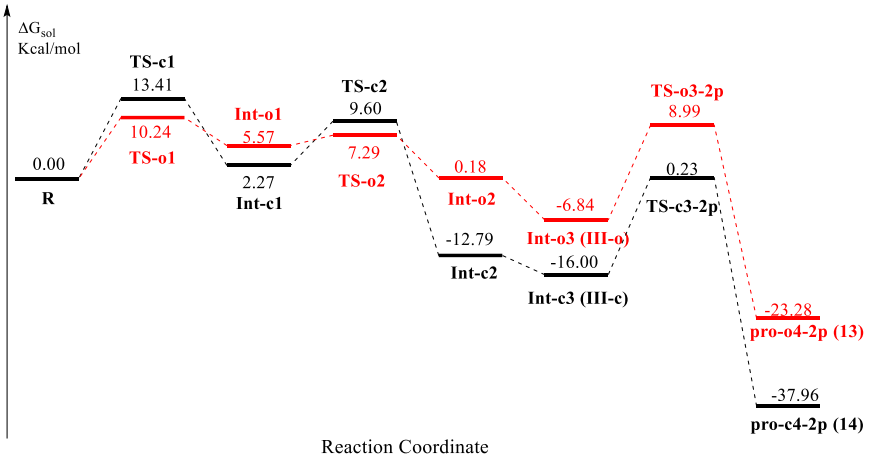
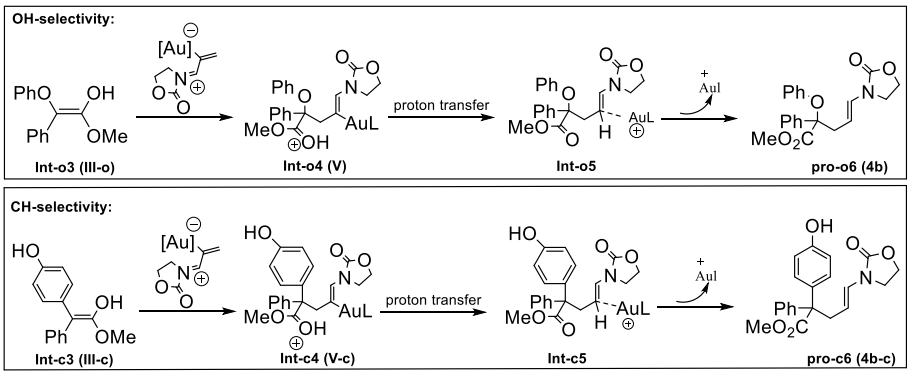


Fig S2. The calculated free energy profiles for the Au(I)-catalyzed Two-Components O-H (red) and C-H (black) insertion Reactions. R: reactant, Int: intermediate, TS: transition state, pro: product.



Scheme S2. Proposed Mechanism for the Au(I)-catalyzed Three-Components O-H and C-H insertion Reactions. Int: intermediate, TS: transition state, pro: product.

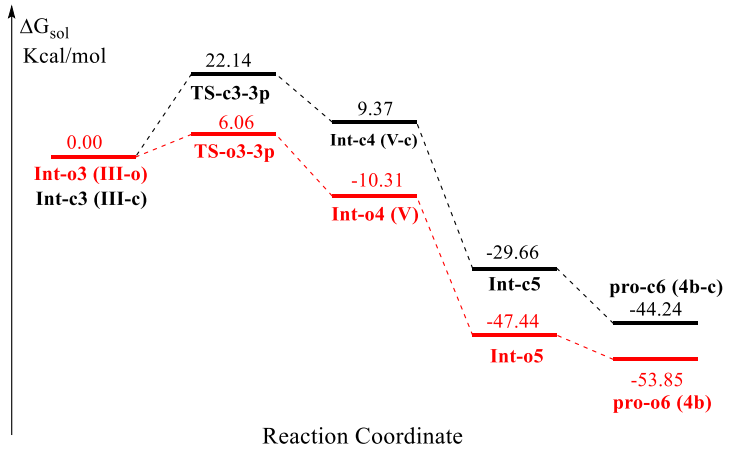


Fig S3. The calculated free energy profiles for the Au(I)-catalyzed Three-Components O-H (red) and C-H (black) insertion Reactions. Int: intermediate, TS: transition state, pro: product.

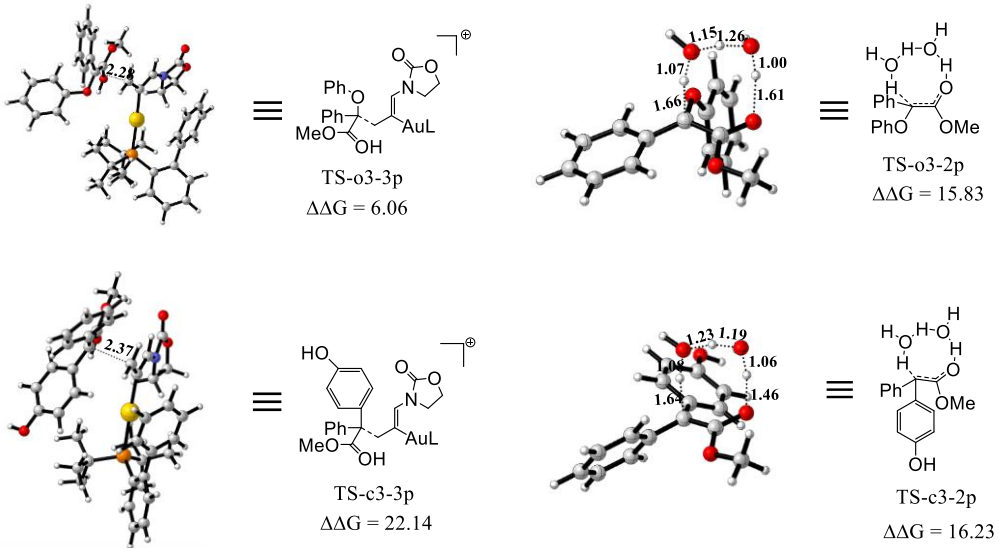
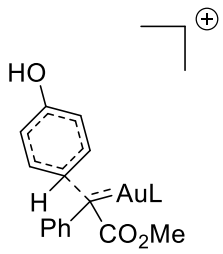


Fig S4. The Structures of transition states TS-o3-3p, TS-o3-2p, TS-c3-3p, TS-c3-2p in the O-H and C-H insertion Pathways of the three and two component reactions of phenol respectively. The values of ΔΔG are in the units of kcal/mol.

Cartesian coordinates for all the transition states in Scheme S1 and S2



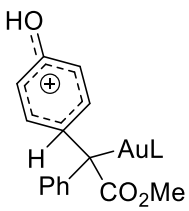
TS-c1

Gibbs free energies = -2059.374363 a.u.

C	-4.94778700	2.01637300	0.23036200
C	-4.08776800	1.07481900	0.77156100
C	-2.89912100	0.70383900	0.10504000

C	-2.63812800	1.29582500	-1.14780600
C	-3.51057600	2.21983300	-1.70271400
C	-4.66429200	2.58508600	-1.01131400
H	-5.84761100	2.30195300	0.76827400
H	-4.32335400	0.62419600	1.73355400
H	-1.72096100	1.02485400	-1.67121800
H	-3.28359600	2.67185700	-2.66550400
H	-5.34607500	3.31625700	-1.43915200
C	-1.97372500	-0.25701400	0.65733800
C	-1.99026100	-0.59614800	2.11139600
O	-1.93344700	-1.69609700	2.61598700
O	-1.90880500	0.54565100	2.81911100
C	-1.49021700	0.38191700	4.17613700
H	-1.50746900	1.37891100	4.61773100
H	-2.16010400	-0.29143400	4.71637800
H	-0.47378600	-0.03013700	4.20376800
C	-3.87967200	-2.22673500	0.44513300
C	-2.58848900	-2.19950200	-0.14237400
C	-2.49167400	-1.93847000	-1.53351600
C	-3.57377100	-1.47107700	-2.23184000
C	-4.81041600	-1.31808100	-1.56603100
C	-4.97338900	-1.75965000	-0.24217100
H	-3.97288500	-2.55513900	1.47634200
H	-1.52803300	-2.04062200	-2.03080500
H	-3.49527000	-1.20511700	-3.28509900
H	-5.96182400	-1.69975400	0.20453100
O	-5.87148300	-0.77654600	-2.15748800
H	-5.66308100	-0.49963600	-3.05940800
H	-1.77353200	-2.70694500	0.36842100
Au	0.09186700	-0.33372700	0.17833100
P	2.41329000	-0.79259200	-0.20173400
C	2.52284700	-1.59310200	-1.91572000
C	1.71922500	-2.89372400	-1.90769500
C	1.86301700	-0.59179100	-2.87016800
C	3.93532600	-1.87685500	-2.42312800
H	2.22029800	-3.68858000	-1.34278000
H	0.71173600	-2.75929200	-1.48926600
H	1.60925600	-3.25229700	-2.93982800
H	2.39085200	0.37045200	-2.87990900
H	1.89415400	-0.99632700	-3.89078100
H	0.81202700	-0.40033900	-2.61053400
H	3.85918000	-2.37197000	-3.40042400
H	4.51298200	-0.95885900	-2.57110100
H	4.50006200	-2.54444800	-1.76476700

C	2.97106900	-1.93252300	1.21512600
C	3.24009200	-1.02338100	2.41663400
C	1.81268200	-2.87212500	1.57530600
C	4.20335900	-2.78948300	0.92641800
H	4.09297700	-0.35502800	2.25585200
H	2.36168100	-0.41177300	2.66556200
H	3.46101400	-1.64818500	3.29194000
H	1.50530400	-3.50940400	0.73892700
H	2.14105800	-3.53421900	2.38753500
H	0.92871400	-2.32893600	1.93370900
H	4.43314700	-3.37752400	1.82488800
H	4.03373600	-3.50442600	0.11301400
H	5.09920400	-2.20410100	0.69852800
C	3.56393600	0.63883500	-0.26540500
C	3.12097700	1.97875800	-0.26126700
C	4.94076000	0.39079600	-0.39729300
C	4.06433900	3.00078600	-0.43225900
C	1.72046600	2.43561800	-0.05793300
C	5.86218200	1.41779400	-0.53801000
H	5.30806900	-0.63081300	-0.40158000
C	5.41810100	2.73407800	-0.56835300
H	3.71058200	4.02997900	-0.43277100
C	1.02485200	3.04847000	-1.10404000
C	1.13460800	2.39957400	1.21323500
H	6.92002900	1.18698200	-0.63095800
H	6.12450900	3.55134500	-0.68829900
C	-0.23382700	3.60152200	-0.88708800
H	1.48798300	3.10456900	-2.08859300
C	-0.11910200	2.96432500	1.43138500
H	1.68579600	1.95630100	2.04251400
C	-0.80879200	3.55970400	0.38004500
H	-0.76369400	4.07822300	-1.70940200
H	-0.55910900	2.93369000	2.42498700
H	-1.79190700	3.99519600	0.54878500



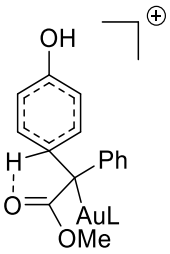
Int-c1

Gibbs free energies = -2059.391311 a.u.

C	-4.50986500	2.69295000	0.21214000
C	-3.78612800	1.66491800	0.80606000

C	-2.81790500	0.95109100	0.08774200
C	-2.60820200	1.30602400	-1.24904200
C	-3.34559900	2.31752900	-1.85513000
C	-4.30057100	3.01735200	-1.12527000
H	-5.24832500	3.23741200	0.79598900
H	-3.97031100	1.42299800	1.85182600
H	-1.82717800	0.79636900	-1.81681200
H	-3.15415800	2.57461800	-2.89493000
H	-4.87239900	3.81547500	-1.59215700
C	-2.09118300	-0.22231400	0.69021800
C	-1.89900600	-0.25546600	2.16846600
O	-1.95748200	-1.26474900	2.85188500
O	-1.56766600	0.94222400	2.68016600
C	-1.08838100	0.90917500	4.02289000
H	-0.84786800	1.94163600	4.28258100
H	-1.84348600	0.50904700	4.70496100
H	-0.19111600	0.28171000	4.08872900
C	-4.18577400	-1.60145900	0.78832700
C	-2.80185400	-1.59745900	0.29879900
C	-2.65694200	-1.90330300	-1.12325100
C	-3.72005800	-2.05759500	-1.95171300
C	-5.03038600	-1.92322000	-1.41762400
C	-5.25886400	-1.71261500	-0.03516700
H	-4.31917200	-1.46767000	1.86032700
H	-1.64082200	-1.96623300	-1.51415700
H	-3.59399000	-2.26350300	-3.01310900
H	-6.28611300	-1.65779500	0.31263600
O	-6.09732400	-2.00935300	-2.17500000
H	-5.87715900	-2.16021400	-3.10643700
H	-2.21811700	-2.31574800	0.90705600
Au	0.03553500	-0.34493700	0.17420700
P	2.34934100	-0.89366100	-0.15354000
C	2.47749200	-1.81186600	-1.80561100
C	1.62905800	-3.08128100	-1.73784300
C	1.87957400	-0.85521900	-2.84270000
C	3.89331500	-2.17420400	-2.25179800
H	2.07779500	-3.85006200	-1.09825100
H	0.61467100	-2.87947100	-1.36695800
H	1.54226500	-3.50867600	-2.74578700
H	2.45229200	0.07827100	-2.90992500
H	1.90921000	-1.33300400	-3.83128000
H	0.83497700	-0.59634600	-2.61764800
H	3.82892900	-2.71032800	-3.20821500
H	4.51101400	-1.28609700	-2.42012700

H	4.41094200	-2.83233200	-1.54601500
C	2.84372800	-1.95653800	1.34902700
C	3.14695700	-0.97634200	2.48465900
C	1.63993300	-2.81219600	1.76535000
C	4.03366800	-2.89441100	1.14285900
H	4.04809100	-0.38288400	2.29744200
H	2.30956500	-0.28586700	2.65722400
H	3.30065900	-1.54286900	3.41245300
H	1.29476800	-3.47851600	0.96646900
H	1.93851100	-3.44386300	2.61271200
H	0.78953900	-2.20311200	2.09704900
H	4.21870500	-3.42690600	2.08527000
H	3.83718500	-3.65666700	0.38025600
H	4.96303600	-2.37581900	0.89036900
C	3.56492100	0.48063400	-0.28386900
C	3.18560000	1.83470700	-0.40289400
C	4.93337000	0.16430700	-0.33711900
C	4.18554300	2.79872000	-0.59622300
C	1.80106700	2.37238300	-0.33493400
C	5.90821400	1.13532700	-0.50775200
H	5.25308500	-0.86982200	-0.25690600
C	5.52967000	2.46510600	-0.64665100
H	3.88044100	3.83922600	-0.68810700
C	1.23490300	2.95438800	-1.47355500
C	1.11410800	2.46076100	0.88117100
H	6.95643900	0.85016600	-0.53789700
H	6.27834200	3.24041600	-0.78771200
C	0.01038500	3.60841400	-1.39879500
H	1.77653600	2.90820900	-2.41770000
C	-0.10442800	3.13056700	0.95740800
H	1.56389900	2.03722100	1.77998000
C	-0.65783800	3.70408000	-0.18196700
H	-0.41923000	4.05631200	-2.29255800
H	-0.62667500	3.19688500	1.90843700
H	-1.61353300	4.22008100	-0.12202600

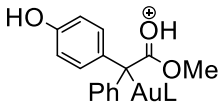


TS-c2

Gibbs free energies = -2059.380421 a.u.

C	-3.69860200	3.65874100	-0.20237300
C	-3.23906800	2.55648900	0.51384600
C	-2.62199800	1.48454500	-0.13946300
C	-2.49302300	1.54664300	-1.53269200
C	-2.96000600	2.64007700	-2.24982100
C	-3.56473900	3.70469500	-1.58577000
H	-4.17482800	4.48111500	0.32671300
H	-3.35584900	2.53855600	1.59564400
H	-2.00381600	0.72154900	-2.05460600
H	-2.84579000	2.66536700	-3.33101200
H	-3.93072800	4.56259300	-2.14410000
C	-2.19102400	0.23693900	0.57587500
C	-2.02347800	0.22357800	2.03750600
O	-2.31785900	-0.80922100	2.67722300
O	-1.50661000	1.28189700	2.63270600
C	-1.09821500	1.10482400	3.99395600
H	-0.67822600	2.06224500	4.30369900
H	-1.94837100	0.83485000	4.62522500
H	-0.34003300	0.31602500	4.05408400
C	-4.54664000	-0.72035000	0.40158000
C	-3.12655500	-0.97058500	0.30487900
C	-2.74813000	-2.06679100	-0.53863000
C	-3.67073700	-2.89726100	-1.12083000
C	-5.04284000	-2.63198900	-0.94796600
C	-5.47748200	-1.53624700	-0.17401500
H	-4.87044200	0.13766500	0.98999300
H	-1.68267300	-2.25628600	-0.66731000
H	-3.35654600	-3.74794200	-1.72298600
H	-6.54529600	-1.36615500	-0.07292400
O	-5.98827600	-3.38599800	-1.48646600
H	-5.61641800	-4.11525500	-2.00104200
H	-2.90486900	-1.39526700	1.46268800
Au	-0.06766400	-0.19579600	0.13155200
P	2.15142300	-1.07560000	-0.14703900
C	2.29783800	-1.81696000	-1.88401000
C	1.24022100	-2.90395200	-2.06206900
C	1.99692500	-0.66020000	-2.84204000
C	3.67471300	-2.38425800	-2.22464900
H	1.43105400	-3.78271600	-1.43480100
H	0.23221800	-2.52709400	-1.84363400
H	1.24727600	-3.24135700	-3.10701200
H	2.73296800	0.14770800	-2.74443700
H	2.04441800	-1.02985400	-3.87503300
H	0.99817000	-0.23159800	-2.67935000

H	3.65274500	-2.74829600	-3.26043800
H	4.46004500	-1.62368200	-2.16494000
H	3.95775600	-3.23013400	-1.58965300
C	2.33589000	-2.35885000	1.25322500
C	2.71408600	-1.57369500	2.51158400
C	0.96951400	-3.01599000	1.49583100
C	3.34489300	-3.48554100	1.01749300
H	3.72675000	-1.16086500	2.46300500
H	2.01637700	-0.74407100	2.69450000
H	2.66320500	-2.24487200	3.37897000
H	0.57465600	-3.51227200	0.60120800
H	1.08421400	-3.78338400	2.27310400
H	0.22017800	-2.29715000	1.85205500
H	3.36182100	-4.12297600	1.91163500
H	3.06514500	-4.12889500	0.17499200
H	4.37073500	-3.13984300	0.86317200
C	3.57509600	0.08416900	-0.04131300
C	3.43660900	1.48151200	-0.17369300
C	4.86929800	-0.44908900	0.07855700
C	4.59290100	2.27326900	-0.20536500
C	2.15581200	2.22723400	-0.28261400
C	6.00025800	0.35313100	0.07066600
H	5.00447000	-1.52235600	0.16445700
C	5.86080700	1.72754300	-0.08118800
H	4.47167600	3.34927800	-0.31383400
C	1.81778600	2.84585500	-1.48926900
C	1.35583900	2.45405600	0.84322000
H	6.98398400	-0.09750700	0.17246800
H	6.73556600	2.37239200	-0.09940300
C	0.69696700	3.66488000	-1.57375700
H	2.45192900	2.69132000	-2.36147600
C	0.24907200	3.29419500	0.76221700
H	1.62970800	1.99448700	1.79432300
C	-0.08277600	3.89898500	-0.44593200
H	0.43906700	4.13419300	-2.52055600
H	-0.36060700	3.47331400	1.64484300
H	-0.96083300	4.53803100	-0.51077700



Int-c2

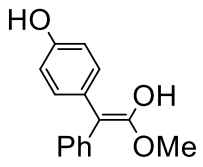
Gibbs free energies = -2059.416107 a.u.

C	-3.44887500	3.91459100	-0.28077400
C	-3.15215100	2.76558600	0.44741500

C	-2.54713900	1.66826700	-0.17184700
C	-2.26338800	1.74778900	-1.54094200
C	-2.55879800	2.89321500	-2.26751500
C	-3.15371500	3.98381800	-1.63836200
H	-3.93049000	4.75351000	0.21616800
H	-3.41025400	2.72289400	1.50282900
H	-1.82394100	0.88315000	-2.04113100
H	-2.33070100	2.93184500	-3.32992400
H	-3.39736300	4.87815700	-2.20633400
C	-2.33189000	0.35853700	0.52882100
C	-2.11516100	0.32362600	1.92824800
O	-2.35199500	-0.74252300	2.66859600
O	-1.66950200	1.36219200	2.59414000
C	-1.08091600	1.13910200	3.88349900
H	-0.69298500	2.10796700	4.19824700
H	-1.82450600	0.77795500	4.59741000
H	-0.26530200	0.41089900	3.79638200
C	-4.47371800	-0.50949900	-0.47069100
C	-3.17625800	-0.77835800	-0.00161200
C	-2.75676800	-2.11525800	-0.00564700
C	-3.58778800	-3.14314400	-0.44490100
C	-4.86734200	-2.84783800	-0.90918900
C	-5.30408900	-1.51878400	-0.91891200
H	-4.83285800	0.51759600	-0.48513300
H	-1.74354200	-2.36290200	0.31383200
H	-3.22976100	-4.17191000	-0.44315600
H	-6.30599000	-1.30631100	-1.28203000
O	-5.72582300	-3.77996200	-1.36255800
H	-5.32954800	-4.65726100	-1.31471200
H	-2.79685100	-1.41606500	2.11613900
Au	-0.10618800	-0.12448600	0.22554600
P	2.03022600	-1.13096300	-0.16315500
C	1.99339700	-1.81731100	-1.92518400
C	0.82822700	-2.79676400	-2.05653700
C	1.74340900	-0.60548100	-2.82794000
C	3.28993900	-2.49110600	-2.37145100
H	0.98333600	-3.71152700	-1.47101400
H	-0.12721400	-2.34403200	-1.75725000
H	0.73489300	-3.09822000	-3.10805100
H	2.55269400	0.13167400	-2.75373500
H	1.69704700	-0.94335100	-3.87151400
H	0.79724700	-0.09802200	-2.59645700
H	3.16310900	-2.82752200	-3.40881800
H	4.13938700	-1.80030800	-2.35669100

H	3.54456400	-3.37240200	-1.77418400
C	2.22210900	-2.46644200	1.18933500
C	2.76474000	-1.75504900	2.43168700
C	0.83556400	-3.02271400	1.53495000
C	3.10880100	-3.66080100	0.83206400
H	3.79996000	-1.42100900	2.31189000
H	2.15403400	-0.87972400	2.69546200
H	2.73017700	-2.44902800	3.28165000
H	0.34204400	-3.49308600	0.67573600
H	0.95229000	-3.79485700	2.30710900
H	0.17261200	-2.24752300	1.94127500
H	3.14776900	-4.33015700	1.70156800
H	2.69912900	-4.24244800	-0.00159800
H	4.14286900	-3.39679100	0.59523400
C	3.52920400	-0.06806300	-0.10718200
C	3.49103600	1.34091600	-0.16481900
C	4.78314600	-0.70245800	-0.09964900
C	4.70177500	2.04522000	-0.22346600
C	2.26407800	2.17915900	-0.18457600
C	5.96985800	0.01305200	-0.13890600
H	4.84235500	-1.78562700	-0.07394700
C	5.92874200	1.40036300	-0.20610100
H	4.65809900	3.13143100	-0.27003300
C	1.94225600	2.89139500	-1.34294300
C	1.49556400	2.37643300	0.96898400
H	6.91993500	-0.51430100	-0.12563700
H	6.84802800	1.97900000	-0.24318100
C	0.86801700	3.77416500	-1.35506500
H	2.55130200	2.75509700	-2.23589600
C	0.42665500	3.26894600	0.95696400
H	1.76933400	1.85241300	1.88577400
C	0.11386900	3.96882900	-0.20329600
H	0.62311800	4.31924800	-2.26387100
H	-0.16949000	3.42049800	1.85409900
H	-0.73490200	4.64861100	-0.21552300

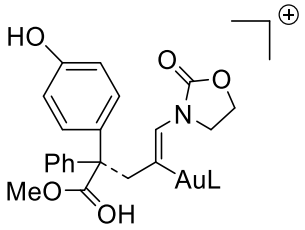
Int-c3



Gibbs free energies = -804.987753 a.u.

C	3.57406500	-1.66961600	0.47559900
C	2.70113600	-0.59150200	0.53441900

C	1.42729700	-0.65867100	-0.05033500
C	1.06749400	-1.86031100	-0.68094300
C	1.94068400	-2.93839600	-0.73566900
C	3.20310100	-2.85032900	-0.15917400
H	4.55451800	-1.58683900	0.94062500
H	3.00549100	0.31688400	1.04460600
H	0.08444300	-1.94252600	-1.14128900
H	1.63192900	-3.85272800	-1.23837200
H	3.88884700	-3.69328200	-0.20092800
C	0.45839100	0.45168000	-0.00245200
C	0.81352300	1.76287600	0.03831000
O	-0.05533300	2.78739900	0.14726700
O	2.08653200	2.17073000	-0.02314500
C	2.35452500	3.56341100	-0.02626000
H	1.87409900	4.06303500	-0.87403000
H	2.01830300	4.04022700	0.90044200
H	3.43846600	3.65223500	-0.11348500
C	-2.88020700	-1.01804800	1.03064800
C	-3.74499100	-0.47363700	0.07968000
C	-3.23913800	0.36171700	-0.91188100
C	-1.87926000	0.64369600	-0.94532900
C	-0.99218700	0.13069400	0.01390400
C	-1.52821500	-0.71313600	0.99591900
H	-3.27321700	-1.67688400	1.80543900
H	-3.92148200	0.76243800	-1.65687700
H	-1.48493500	1.26525400	-1.74895200
H	-0.86049000	-1.13851700	1.74289700
O	-5.07797800	-0.72671900	0.07121100
H	-0.94523200	2.41228400	0.23604900
H	-5.29382500	-1.31542000	0.80259600



TS-c3-3p

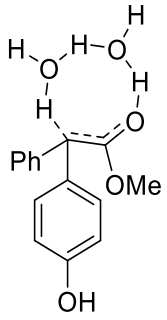
Gibbs free energies = -2497.058841 a.u.

C	5.90714700	-2.36924700	-2.02488800
C	5.14015500	-1.44620500	-1.32660300
C	4.39760300	-1.82788100	-0.19752800
C	4.46654600	-3.17201100	0.20194900
C	5.23882900	-4.09207900	-0.49492200
C	5.96013700	-3.69745200	-1.61587100

H	6.47038700	-2.04448300	-2.89645800
H	5.13935700	-0.41395300	-1.66261700
H	3.91680300	-3.49847200	1.08179400
H	5.27837100	-5.12383900	-0.15438900
H	6.56264700	-4.41706400	-2.16402400
C	3.54322600	-0.88395200	0.56907500
C	3.96221300	0.41921700	0.83632000
O	3.25681500	1.27995800	1.55630600
O	5.05661300	0.91897600	0.31392800
C	5.46867600	2.25526000	0.65790700
H	4.76939100	2.99887600	0.26340900
H	5.55539300	2.35710700	1.74254100
H	6.44548100	2.37583800	0.19120100
C	2.53769700	-1.28834400	2.85099000
C	2.49997900	-1.46443000	1.46156400
C	1.51615500	-2.32759600	0.94972900
C	0.61956300	-2.97630000	1.77716800
C	0.65377600	-2.75558800	3.15751900
C	1.61699700	-1.90651100	3.69267100
H	3.32626400	-0.68621300	3.30022400
H	1.48217300	-2.53208400	-0.11963700
H	-0.11512600	-3.67109100	1.37821800
H	1.67260700	-1.74983100	4.76925200
H	2.42016200	0.85556300	1.82268000
C	2.24345100	0.09587000	-1.14920400
C	1.34615500	1.08707700	-0.71564600
C	1.93318900	2.33661000	-0.76526500
H	2.95846400	2.45607200	-1.13405000
C	2.26633300	4.67511900	-0.36900500
C	0.12882700	3.84289500	0.16033200
C	0.16060400	5.37058500	0.15355600
H	0.04877300	3.41518600	1.17046800
H	-0.67858900	3.42799000	-0.45187500
H	-0.23558200	5.81802200	1.06714400
H	-0.36352900	5.79263400	-0.71066200
N	1.42529500	3.53974800	-0.41071300
O	1.54549000	5.71747200	0.04956200
O	3.43343900	4.69285100	-0.64170000
C	-3.91564500	-0.95841900	-0.68676100
C	-5.23235800	-1.27765600	-0.31405500
C	-5.99413000	-2.20016000	-1.01500600
C	-5.44279100	-2.84568200	-2.11519100
C	-4.14621000	-2.54410400	-2.50180600
C	-3.36766300	-1.60163400	-1.81553200

C	-2.01405500	-1.36732800	-2.38569500
C	-1.04914800	-2.37877700	-2.32635900
C	0.16260100	-2.24093600	-2.99749400
C	0.42276600	-1.09158800	-3.74033600
C	-0.52880600	-0.07752100	-3.80067600
C	-1.73987800	-0.21529100	-3.12959100
C	-2.94740800	-0.75077300	2.11325200
C	-2.74173700	-2.23701700	1.80761200
C	-4.20037900	-0.57927400	2.96926600
C	-1.74310300	-0.24239100	2.91453800
C	-3.84514400	1.80035600	0.45643600
C	-3.17858800	2.68805400	1.50885800
C	-3.64546700	2.40694400	-0.93600400
C	-5.34835500	1.75905900	0.73119400
H	-5.67435400	-0.80686600	0.55826200
H	-7.00944000	-2.41915800	-0.69511500
H	-6.02033200	-3.57876700	-2.67235700
H	-3.70960400	-3.03487900	-3.36965100
H	-1.27040100	-3.28935800	-1.76927600
H	0.89777700	-3.04297900	-2.95866400
H	1.36181900	-0.99244100	-4.28033800
H	-0.33610400	0.81605600	-4.38957800
H	-2.49996900	0.56107400	-3.20905700
H	-1.94288700	-2.38927100	1.06960000
H	-2.44347900	-2.75889200	2.72702300
H	-3.65177300	-2.70834200	1.42214400
H	-4.36018300	0.45798400	3.28580200
H	-4.07441200	-1.17560900	3.88331500
H	-5.11036200	-0.94384800	2.48205100
H	-1.79439500	0.83472100	3.11547900
H	-0.79417900	-0.45245000	2.40276400
H	-1.72032000	-0.76372800	3.88202200
H	-3.42184300	2.37030900	2.52952200
H	-3.54389800	3.71812700	1.39549900
H	-2.08626500	2.69956100	1.41130700
H	-4.14913400	1.81230300	-1.70877400
H	-4.08552300	3.41312200	-0.95811300
H	-2.58529900	2.48792200	-1.21113700
H	-5.59934300	1.30376300	1.69478900
H	-5.89636400	1.23883900	-0.06024900
H	-5.72129100	2.79197900	0.75581500
P	-2.93707000	0.13534400	0.42553800
Au	-0.62208000	0.58483000	-0.18965400
H	3.16200300	0.36756900	-1.67502900

H	1.92218000	-0.92904700	-1.30974000
O	-0.27287800	-3.38993900	3.91034300
H	-0.09918300	-3.23786800	4.84654400

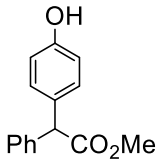


TS*-c3-2p

Gibbs free energies = -957.750343 a.u.

C	2.38393300	-2.98674400	-0.63496700
C	1.39897200	-2.00664400	-0.69968100
C	1.56134000	-0.75994100	-0.07488300
C	2.76293200	-0.54796500	0.62416600
C	3.75264400	-1.52038100	0.68086300
C	3.57078200	-2.75086900	0.05228500
H	2.22406900	-3.94085300	-1.13449000
H	0.48075000	-2.20904300	-1.24897400
H	2.91428700	0.40398800	1.13188700
H	4.66974000	-1.31988300	1.23229400
H	4.34175800	-3.51653100	0.10400100
C	0.49048400	0.26954100	-0.10627300
C	0.77569400	1.60285000	-0.52086900
O	-0.03542400	2.56114700	-0.53695300
O	2.05790000	1.84368200	-0.87429000
C	2.39114400	3.19794100	-1.14670200
H	3.46169200	3.20595100	-1.36274400
H	1.83947900	3.57778200	-2.01297800
H	2.18327800	3.84525900	-0.28812200
C	-3.15464400	-0.11801200	-1.20075100
C	-3.61827900	-1.06695500	-0.29146300
C	-2.73703600	-1.59019000	0.65487300
C	-1.42142600	-1.15152300	0.69039600
C	-0.92228500	-0.19262200	-0.20980900
C	-1.82699600	0.29675400	-1.16333300
H	-3.83378000	0.28595400	-1.95172100
H	-3.10175600	-2.33437000	1.35979100
H	-0.75021600	-1.57468000	1.43900500
H	-1.48867000	1.03672400	-1.88521900
O	-4.90075900	-1.51320700	-0.28029100
H	-1.15315000	2.55956200	0.54702200

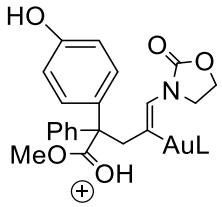
O	-1.67082200	2.45009800	1.42169600
O	0.08062900	1.17276700	2.43433300
H	-0.85687500	1.79512000	2.06501700
H	0.38177500	0.74339900	1.51376900
H	-2.44962400	1.90911700	1.21482000
H	-0.16933700	0.45640500	3.03891600
H	-5.38916700	-1.09124200	-1.00134000

pro-c4-2p 

Gibbs free energies = -805.022760 a.u.

C	3.90901100	-0.96478300	0.09379500
C	2.86392600	-0.12962700	0.46596300
C	1.53509700	-0.55727600	0.37865300
C	1.28018200	-1.85004000	-0.07555900
C	2.32705800	-2.69096300	-0.44756200
C	3.64319000	-2.25176200	-0.36836800
H	4.93489800	-0.61030000	0.16530800
H	3.08311000	0.87326800	0.83411600
H	0.25456200	-2.20707500	-0.14025100
H	2.10720100	-3.69605100	-0.80112600
H	4.45977400	-2.90721000	-0.66230100
C	0.43039500	0.36809900	0.85926600
C	0.66388100	1.81503800	0.45389500
O	0.60299900	2.75341200	1.21548300
O	0.90185200	1.94051900	-0.85678300
C	1.06026500	3.28125900	-1.32518700
H	1.25615800	3.20767300	-2.39554200
H	0.14972600	3.86192600	-1.14891900
H	1.89934900	3.77175800	-0.82259400
C	-1.94537600	-0.22883200	1.45705000
C	-0.98329300	-0.01492400	0.46817300
C	-1.37583600	-0.12744400	-0.86915800
C	-2.68257800	-0.45034000	-1.20816700
C	-3.63010600	-0.66057900	-0.20457900
C	-3.25679100	-0.54975100	1.13404000
H	-1.66208400	-0.14344300	2.50513000
H	-0.64584000	0.03883300	-1.65891700
H	-2.97543200	-0.53693100	-2.25400100
H	-4.00431600	-0.71623300	1.90598500
O	-4.91909600	-0.97365700	-0.47431800

H	-5.04566300	-1.02055200	-1.43292900
H	0.46835900	0.39368400	1.95743800



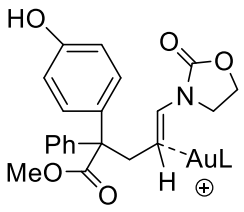
Int-c4

Gibbs free energies = -2497.079193 a.u.

C	-0.18156425	-0.89385474	0.00000000
C	0.98178275	-0.34801574	-0.52266600
C	1.94355975	-1.15518474	-1.14496800
C	1.70604575	-2.52905774	-1.21309500
C	0.54147575	-3.07798174	-0.68186400
C	-0.40677025	-2.26534174	-0.07700000
H	-0.91439225	-0.24370374	0.47108100
H	1.12954975	0.72841826	-0.45046900
H	2.43138475	-3.19164374	-1.67777800
H	0.38197375	-4.15141374	-0.74450300
H	-1.31630025	-2.69456474	0.33527100
C	3.24370375	-0.53933074	-1.68595700
C	2.96828075	0.50779426	-2.74099200
O	3.90850075	1.07126826	-3.40737900
O	1.77490975	0.87383526	-2.99312300
C	1.54683275	2.02290826	-3.86890900
H	2.04344175	2.89529926	-3.42990100
H	1.93675675	1.80078526	-4.86358500
H	0.46572675	2.13945826	-3.88653400
C	3.83018075	-2.02959974	-3.64572600
C	4.12422075	-1.60124074	-2.34789300
C	5.10123575	-2.30237874	-1.63511800
C	5.76214175	-3.38072374	-2.20135100
C	5.48778975	-3.76574974	-3.51408500
C	4.50717875	-3.08724774	-4.23760900
H	3.02950475	-1.55070874	-4.21178200
H	5.35276175	-2.02687474	-0.61307500
H	6.50639975	-3.94202574	-1.64184700
H	4.26560175	-3.39119174	-5.25514200
H	4.79042075	0.93428426	-2.95209800
C	3.97329875	0.22256626	-0.50180900
C	4.98017275	1.27461626	-0.90699400
C	4.45044375	2.51081226	-0.89970800
H	3.40459075	2.66646026	-0.60420500

C	4.20949775	4.63902326	-1.97318100
C	6.39504675	4.11912126	-1.37059000
C	6.23080175	5.61228826	-1.64661800
H	6.92936375	3.60116326	-2.18245100
H	6.91210275	3.90564026	-0.42664300
H	6.98011075	6.01956526	-2.32847500
H	6.22491775	6.20126726	-0.72158300
N	5.00600775	3.72355226	-1.31179500
O	4.94683075	5.72649326	-2.26766700
O	3.04770275	4.50049026	-2.27228500
C	10.31213175	-0.52706574	-1.16227500
C	11.59654775	-0.89024074	-1.60116800
C	12.51319475	-1.50834774	-0.76395300
C	12.15577575	-1.79370674	0.54831800
C	10.89036475	-1.45093474	0.99926400
C	9.95546875	-0.81377674	0.17170800
C	8.64930075	-0.50437774	0.81596500
C	7.77145275	-1.54664674	1.13395800
C	6.61496275	-1.29980174	1.86886800
C	6.32591975	-0.00905774	2.30460800
C	7.19580575	1.03348026	1.99957100
C	8.34883875	0.78837826	1.25908600
C	8.95819075	-1.16272274	-3.73766200
C	8.91738275	-2.50826374	-3.00963700
C	10.05865175	-1.19442174	-4.79505700
C	7.61637375	-0.94054374	-4.44260800
C	9.91633275	1.77450226	-3.02956300
C	9.01125375	2.33392626	-4.12935200
C	9.93548275	2.73168626	-1.83413000
C	11.34557175	1.68060326	-3.56624700
H	11.88836275	-0.70199774	-2.62994600
H	13.49786075	-1.77303174	-1.14018300
H	12.85839875	-2.28183074	1.21868900
H	10.60279075	-1.66806574	2.02631900
H	8.01760975	-2.56106974	0.81990700
H	5.94997075	-2.12335574	2.12319400
H	5.43136875	0.18202226	2.89285100
H	6.98214675	2.04099126	2.34923700
H	9.04465975	1.59882326	1.04437400
H	8.22332275	-2.48653974	-2.15994400
H	8.56213175	-3.28696574	-3.69968900
H	9.90334675	-2.80524174	-2.63668300
H	10.07935575	-0.28762274	-5.41014900
H	9.85964375	-2.03658974	-5.47183200

H	11.05570175	-1.35868174	-4.37400500
H	7.55982675	0.03544326	-4.93997700
H	6.77575775	-1.01873274	-3.74106400
H	7.48569575	-1.71459874	-5.21206500
H	9.06836175	1.74219726	-5.05080500
H	9.33650875	3.35262126	-4.38055000
H	7.95780375	2.38095626	-3.82276900
H	10.60243975	2.37096126	-1.04083900
H	10.31330475	3.70983826	-2.16179500
H	8.93842575	2.87944826	-1.40184700
H	11.45395275	0.97726726	-4.39785100
H	12.06251975	1.41579526	-2.78279100
H	11.63450075	2.67168126	-3.94136500
P	9.12793475	0.17178926	-2.38580900
Au	6.90343475	0.73546126	-1.54446700
H	3.18119575	0.68473726	0.09903700
H	4.40077575	-0.55778774	0.13686700
O	6.21325975	-4.78268374	-4.02390100
H	5.90145375	-5.00763774	-4.90816900



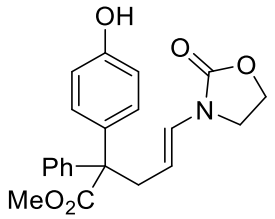
Int-c5

Gibbs free energies = -2497.141397 a.u.

C	-1.93638100	-0.39592500	0.18590000
C	-1.11061700	0.68897100	-0.45097300
C	-0.87948200	1.86191000	0.25538900
H	-1.53773300	-1.38718200	-0.05995400
H	-1.90239100	-0.30007500	1.28009600
H	-0.92729100	1.89402700	1.34601900
C	-0.14141100	4.14237800	0.45818200
C	-0.70913900	3.40722300	-1.71108800
C	-0.65704100	4.93077000	-1.61549400
H	-1.64018600	3.03653000	-2.15664900
H	0.14645400	2.97945600	-2.25681300
H	-1.66275400	5.36681400	-1.60915700
H	-0.05849800	5.40371300	-2.39536200
N	-0.64393800	3.07014900	-0.30324700
O	-0.04146800	5.20474400	-0.34933400
O	0.16597900	4.09059700	1.61437100
C	4.19932900	-1.45087200	-0.13837600

C	5.59248000	-1.53968100	0.01339400
C	6.30601900	-2.65893400	-0.38819000
C	5.62708900	-3.73693900	-0.94268300
C	4.25040300	-3.67184600	-1.09560200
C	3.51382900	-2.54142300	-0.71630400
C	2.04891600	-2.62992600	-0.97056000
C	1.45201100	-1.95727500	-2.04638100
C	0.10967100	-2.17016700	-2.36022900
C	-0.65021100	-3.05746600	-1.60167500
C	-0.06680800	-3.72858500	-0.52996300
C	1.27369500	-3.51991900	-0.22062300
C	4.24638900	1.58559300	-0.13540300
C	4.56677200	1.32114200	-1.60845400
C	5.52128800	1.98456100	0.60934900
C	3.26528300	2.76404600	-0.05992600
C	3.39730300	-0.14338300	2.39989400
C	2.80713900	1.11452900	3.03731600
C	2.49872300	-1.34341200	2.71563900
C	4.78545200	-0.41980700	2.97401800
H	6.13625300	-0.71790400	0.47029100
H	7.38454200	-2.68926200	-0.25964300
H	6.16722000	-4.62636400	-1.25641700
H	3.71377400	-4.50948400	-1.53693800
H	2.06007400	-1.29628200	-2.66389000
H	-0.34239100	-1.64690800	-3.20049700
H	-1.70119000	-3.22616000	-1.83680800
H	-0.65443900	-4.42974900	0.05838600
H	1.73754900	-4.06701400	0.59911800
H	3.67854600	0.99695700	-2.16812500
H	4.91983200	2.25487500	-2.06545900
H	5.34833300	0.56623200	-1.74368300
H	5.32825400	2.26847900	1.64987300
H	5.94658200	2.86665300	0.11254900
H	6.29802000	1.21376600	0.59589500
H	2.87841500	2.94740600	0.94905700
H	2.40806600	2.61311900	-0.73010700
H	3.78432400	3.67515900	-0.38609200
H	3.45233600	1.99174900	2.91348600
H	2.69574300	0.94592100	4.11626000
H	1.81413600	1.36100700	2.63701100
H	2.86859800	-2.26517300	2.24859900
H	2.48869700	-1.50165900	3.80197800
H	1.46130800	-1.18620700	2.38938700
H	5.49488900	0.39202000	2.78846800

H	5.21123800	-1.35314600	2.59001100
H	4.69380500	-0.52761900	4.06277200
P	3.35370600	0.03864800	0.51978300
Au	1.05524500	0.26573300	-0.07163700
C	-4.38021600	3.35712100	-0.94792200
C	-4.10605500	2.00779300	-1.17426400
C	-3.87846100	1.13832700	-0.10574400
C	-3.95497100	1.65639900	1.19433400
C	-4.21142900	3.00263400	1.41972000
C	-4.41903400	3.86453300	0.34501900
H	-4.57416700	4.01039200	-1.79686300
H	-4.05921000	1.64280900	-2.19624400
H	-3.81897300	0.98755200	2.04370400
H	-4.26033900	3.37832800	2.43884900
H	-4.63038700	4.91680000	0.51884900
C	-3.44282900	-0.32405000	-0.25393200
C	-3.44746000	-0.78196900	-1.72111800
O	-2.84582100	-0.21992800	-2.61604000
O	-4.12980800	-1.90738000	-1.91955400
C	-4.15022600	-2.38325900	-3.26760800
H	-4.58582600	-1.63320100	-3.93309400
H	-3.13505200	-2.60683600	-3.61326700
H	-4.75918000	-3.28673600	-3.25561100
H	-1.19954300	0.76454100	-1.53685600
C	-4.30497300	-1.23825600	0.61006900
C	-3.78394900	-2.32198600	1.31394600
C	-5.69024200	-1.03529900	0.65696800
C	-4.60559000	-3.16325400	2.05820400
H	-2.71759200	-2.53956000	1.29466000
C	-6.52044300	-1.86357200	1.38901700
H	-6.12674500	-0.20268100	0.10697500
C	-5.97866400	-2.93610000	2.10146500
H	-4.17481000	-3.99951300	2.60825300
H	-7.59408900	-1.70102700	1.42844600
O	-6.83405100	-3.70720200	2.80680300
H	-6.35215500	-4.41266900	3.25197400



pro-c6

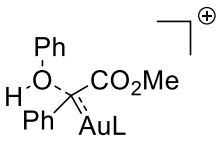
Gibbs free energies = -1242.731159 a.u.

C	-0.11169356	-0.26536312	-0.00292480

C	0.71407044	0.81953288	-0.63979780
C	0.94520544	1.99247188	0.06656420
H	0.28695444	-1.25662012	-0.24877880
H	-0.07770356	-0.16951312	1.09127120
H	0.89739644	2.02458888	1.15719420
C	1.68327644	4.27293988	0.26935720
C	1.11554844	3.53778488	-1.89991280
C	1.16764644	5.06133188	-1.80431880
H	0.18450144	3.16709188	-2.34547380
H	1.97114144	3.11001788	-2.44563780
H	0.16193344	5.49737588	-1.79798180
H	1.76618944	5.53427488	-2.58418680
N	1.18074944	3.20071088	-0.49207180
O	1.78321944	5.33530588	-0.53815880
O	1.99066644	4.22115888	1.42554620
C	6.02401644	-1.32031012	-0.32720080
C	7.41716744	-1.40911912	-0.17543080
C	8.13070644	-2.52837212	-0.57701480
C	7.45177644	-3.60637712	-1.13150780
C	6.07509044	-3.54128412	-1.28442680
C	5.33851644	-2.41086112	-0.90512880
C	3.87360344	-2.49936412	-1.15938480
C	3.27669844	-1.82671312	-2.23520580
C	1.93435844	-2.03960512	-2.54905380
C	1.17447644	-2.92690412	-1.79049980
C	1.75787944	-3.59802312	-0.71878780
C	3.09838244	-3.38935712	-0.40944780
C	6.07107644	1.71615488	-0.32422780
C	6.39145944	1.45170388	-1.79727880
C	7.34597544	2.11512288	0.42052420
C	5.08997044	2.89460788	-0.24875080
C	5.22199044	-0.01282112	2.21106920
C	4.63182644	1.24509088	2.84849120
C	4.32341044	-1.21285012	2.52681420
C	6.61013944	-0.28924512	2.78519320
H	7.96094044	-0.58734212	0.28146620
H	9.20922944	-2.55870012	-0.44846780
H	7.99190744	-4.49580212	-1.44524180
H	5.53846144	-4.37892212	-1.72576280
H	3.88476144	-1.16572012	-2.85271480
H	1.48229644	-1.51634612	-3.38932180
H	0.12349744	-3.09559812	-2.02563280
H	1.17024844	-4.29918712	-0.13043880
H	3.56223644	-3.93645212	0.41029320

H	5.50323344	1.12751888	-2.35694980
H	6.74451944	2.38543688	-2.25428380
H	7.17302044	0.69679388	-1.93250780
H	7.15294144	2.39904088	1.46104820
H	7.77126944	2.99721488	-0.07627580
H	8.12270744	1.34432788	0.40707020
H	4.70310244	3.07796788	0.76023220
H	4.23275344	2.74368088	-0.91893180
H	5.60901144	3.80572088	-0.57491680
H	5.27702344	2.12231088	2.72466120
H	4.52043044	1.07648288	3.92743520
H	3.63882344	1.49156888	2.44818620
H	4.69328544	-2.13461112	2.05977420
H	4.31338444	-1.37109712	3.61315320
H	3.28599544	-1.05564512	2.20056220
H	7.31957644	0.52258188	2.59964320
H	7.03592544	-1.22258412	2.40118620
H	6.51849244	-0.39705712	3.87394720
P	5.17839344	0.16920988	0.33095820
Au	2.87993244	0.39629488	-0.26046180
C	-2.55552856	3.48768288	-1.13674680
C	-2.28136756	2.13835488	-1.36308880
C	-2.05377356	1.26888888	-0.29456880
C	-2.13028356	1.78696088	1.00550920
C	-2.38674156	3.13319588	1.23089520
C	-2.59434656	3.99509488	0.15619420
H	-2.74947956	4.14095388	-1.98568780
H	-2.23452256	1.77337088	-2.38506880
H	-1.99428556	1.11811388	1.85487920
H	-2.43565156	3.50888988	2.25002420
H	-2.80569956	5.04736188	0.33002420
C	-1.61814156	-0.19348812	-0.44275680
C	-1.62277256	-0.65140712	-1.90994280
O	-1.02113356	-0.08936612	-2.80486480
O	-2.30512056	-1.77681812	-2.10837880
C	-2.32553856	-2.25269712	-3.45643280
H	-2.76113856	-1.50263912	-4.12191880
H	-1.31036456	-2.47627412	-3.80209180
H	-2.93449256	-3.15617412	-3.44443580
H	0.62514444	0.89510288	-1.72568080
C	-2.48028556	-1.10769412	0.42124420
C	-1.95926156	-2.19142412	1.12512120
C	-3.86555456	-0.90473712	0.46814320
C	-2.78090256	-3.03269212	1.86937920

H	-0.89290456	-2.40899812	1.10583520
C	-4.69575556	-1.73301012	1.20019220
H	-4.30205756	-0.07211912	-0.08184980
C	-4.15397656	-2.80553812	1.91264020
H	-2.35012256	-3.86895112	2.41942820
H	-5.76940156	-1.57046512	1.23962120
O	-5.00936356	-3.57664012	2.61797820
H	-4.52746756	-4.28210712	3.06314920



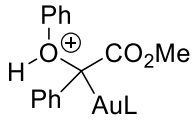
TS-o1

Gibbs free energies = -2059.377202 a.u.

Au	0.22402800	0.15178600	0.23135400
P	-2.12728500	0.61650200	0.02532900
C	-2.41246800	1.61508900	-1.56227100
C	-1.21860600	2.54536800	-1.77798500
C	-2.43091500	0.60008000	-2.70799700
C	-3.69350000	2.44122800	-1.57529000
H	-1.11602100	3.30249900	-0.99342900
H	-0.27405600	1.98688300	-1.83690700
H	-1.35366900	3.07599800	-2.73110000
H	-3.31407100	-0.04909900	-2.68390500
H	-2.44481700	1.14976400	-3.65913000
H	-1.53289400	-0.03505400	-2.70669900
H	-3.76499500	2.95801900	-2.54269200
H	-4.59644000	1.83001100	-1.47113300
H	-3.69286400	3.21036500	-0.79374800
C	-2.55213400	1.54030400	1.62760500
C	-2.04660100	0.64218900	2.76210600
C	-1.77149800	2.85461300	1.64064800
C	-4.02651200	1.84574500	1.88705000
H	-2.52041900	-0.34857700	2.74503000
H	-0.95616800	0.50571900	2.72606600
H	-2.29533700	1.11122100	3.72413300
H	-2.18068400	3.58543300	0.93219300
H	-1.84583200	3.29516900	2.64450800
H	-0.70589700	2.71043900	1.41786400
H	-4.08590900	2.46352300	2.79392200
H	-4.50104400	2.41105400	1.07756300
H	-4.61126200	0.94053200	2.07957300
C	-3.28343700	-0.81318300	-0.09866300
C	-2.85924100	-2.14356700	-0.29964800

C	-4.66456800	-0.55093000	-0.09199200
C	-3.82715400	-3.14618300	-0.45680900
C	-1.45361500	-2.61797600	-0.43356800
C	-5.60758300	-1.55712900	-0.24678200
H	-5.02204900	0.46672900	0.02255000
C	-5.18544100	-2.86899800	-0.42359500
H	-3.48759300	-4.16860900	-0.61356600
C	-0.97871600	-2.94861200	-1.70848200
C	-0.65914400	-2.90629300	0.68073900
H	-6.66635300	-1.31031200	-0.23540400
H	-5.90906600	-3.67123100	-0.54713000
C	0.26664100	-3.54807800	-1.86752100
H	-1.60659800	-2.74731500	-2.57611000
C	0.57799100	-3.52730500	0.52017200
H	-1.02280500	-2.66285900	1.68017400
C	1.04358400	-3.84814700	-0.75104600
H	0.62386100	-3.79701800	-2.86498700
H	1.17964400	-3.76338000	1.39430300
H	2.01248100	-4.32910700	-0.87370800
C	5.09900000	-2.22116400	-0.79823800
C	4.32780400	-1.50248700	0.10144400
C	3.12641100	-0.89988800	-0.31413400
C	2.73533000	-1.01764700	-1.65924700
C	3.51738400	-1.72419200	-2.56227000
C	4.69431200	-2.33069300	-2.12948100
H	6.02012100	-2.69427500	-0.46783600
H	4.65122900	-1.40934700	1.13704800
H	1.79861400	-0.55669300	-1.97554900
H	3.20432100	-1.81443900	-3.59948000
H	5.30297000	-2.89388000	-2.83319300
C	2.28763300	-0.15314700	0.60918500
C	2.43629100	-0.33683200	2.08113900
O	2.64525000	0.56983000	2.87758200
O	2.20410400	-1.58940000	2.42840300
C	2.06492500	-1.85013900	3.83397000
H	2.99291200	-1.61626800	4.36219600
H	1.24359800	-1.25875100	4.24979900
H	1.84269000	-2.91483400	3.91532700
C	2.85733400	2.64828200	-1.44833000
C	2.60518300	2.58270200	-0.08411700
C	1.84317000	3.54116800	0.57299100
C	1.32655700	4.60281900	-0.16354400
C	1.56114600	4.68688900	-1.53424200
C	2.32220000	3.70908600	-2.17237700

H	3.47673200	1.88870000	-1.91930500
H	1.66630900	3.45805700	1.64503600
H	0.73470600	5.36412700	0.33988800
H	2.51445400	3.77761300	-3.24022500
O	3.16156800	1.52857500	0.62224900
H	3.08185600	1.66340100	1.60400600
H	1.15346700	5.51730900	-2.10522500

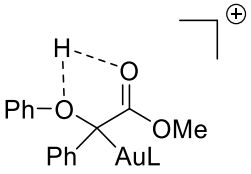
Int-o1 

Gibbs free energies = -2059.384638 a.u.

Au	0.23528300	0.19065200	0.23213700
P	-2.11693600	0.63539600	0.01711300
C	-2.38424400	1.61373400	-1.58822900
C	-1.21421000	2.57864200	-1.77991800
C	-2.33647500	0.58007700	-2.71691700
C	-3.68863600	2.39960300	-1.66325100
H	-1.17400100	3.35202600	-1.00597100
H	-0.25046400	2.05123300	-1.79167500
H	-1.33157100	3.08610700	-2.74771600
H	-3.19991800	-0.09559800	-2.70676300
H	-2.34037400	1.11316000	-3.67748500
H	-1.42002500	-0.02698700	-2.67876000
H	-3.74185400	2.88954400	-2.64573400
H	-4.57482300	1.76235400	-1.57593500
H	-3.74427700	3.18952000	-0.90486200
C	-2.53825300	1.57334200	1.61417800
C	-2.09461300	0.64861200	2.75343200
C	-1.70295700	2.85346800	1.65684200
C	-4.00407500	1.93903800	1.84277000
H	-2.61923400	-0.31573800	2.73003200
H	-1.01252700	0.45468000	2.73214600
H	-2.33076500	1.13019100	3.71246100
H	-2.06440600	3.61024200	0.94979800
H	-1.77823700	3.28589500	2.66415200
H	-0.64046400	2.66384100	1.45288700
H	-4.05958600	2.55878700	2.74860900
H	-4.43606900	2.52349900	1.02288800
H	-4.62997700	1.05877100	2.02077900
C	-3.29452200	-0.77855100	-0.09579100
C	-2.88999200	-2.11834900	-0.27478400
C	-4.67183100	-0.49612100	-0.09982800

C	-3.87235100	-3.10777700	-0.42639900
C	-1.49111800	-2.61723800	-0.38611200
C	-5.62923300	-1.48972300	-0.24852500
H	-5.01651300	0.52703800	0.00191200
C	-5.22647000	-2.80974700	-0.40722400
H	-3.54743500	-4.13733000	-0.56635000
C	-1.01551600	-2.99638500	-1.64726100
C	-0.70807500	-2.88382200	0.74127000
H	-6.68413000	-1.22658000	-0.24566700
H	-5.96128000	-3.60251700	-0.52600600
C	0.22172600	-3.61796700	-1.78057700
H	-1.63569200	-2.81284500	-2.52435000
C	0.51999900	-3.52811900	0.60720000
H	-1.07303300	-2.60425000	1.73068900
C	0.98873200	-3.89279100	-0.65103300
H	0.58000800	-3.90454100	-2.76744200
H	1.11171900	-3.75188800	1.49121000
H	1.95187000	-4.38962900	-0.75300900
C	5.02501300	-2.33192000	-0.77760900
C	4.29926400	-1.53168300	0.09594000
C	3.12298600	-0.90022800	-0.32832200
C	2.70098200	-1.07452400	-1.65088200
C	3.43644200	-1.86084600	-2.53151200
C	4.59522700	-2.49502600	-2.09343200
H	5.93140800	-2.82485300	-0.43419700
H	4.65035100	-1.39588900	1.11879500
H	1.77817100	-0.59170000	-1.97712700
H	3.09648500	-1.98853900	-3.55676500
H	5.16645500	-3.11864400	-2.77739800
C	2.35675300	-0.01339800	0.59100500
C	2.43548100	-0.28007400	2.05273300
O	2.72178400	0.61707600	2.84946800
O	2.12591400	-1.50730800	2.40251200
C	2.02456900	-1.76723000	3.81158700
H	2.99648700	-1.63874600	4.29549900
H	1.29280200	-1.09601000	4.26991700
H	1.69326800	-2.80281100	3.89639500
C	2.86628400	2.52803000	-1.49684400
C	2.59808500	2.47432600	-0.14068900
C	1.90802100	3.46124200	0.54223200
C	1.46025500	4.56286900	-0.18151400
C	1.70147300	4.64545400	-1.55093400
C	2.39782100	3.63140000	-2.20522900
H	3.43351300	1.73484600	-1.97664500

H	1.72718600	3.37225200	1.61226300
H	0.91958500	5.35506400	0.33064500
H	2.59420200	3.70281000	-3.27173100
O	3.10748600	1.37344700	0.58959500
H	3.13898700	1.54690000	1.59520200
H	1.35008000	5.50825000	-2.11104500



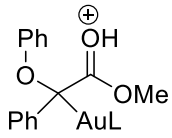
TS-o2

Gibbs free energies = -2059.381885 a.u.

Au	0.22986400	0.19279200	0.21537600
P	-2.13315100	0.58306700	0.01725800
C	-2.44349900	1.50476900	-1.61203500
C	-1.27813900	2.46127000	-1.87117000
C	-2.43170300	0.43347600	-2.70719000
C	-3.75254900	2.28734600	-1.66257100
H	-1.16935500	3.23358100	-1.10173800
H	-0.32167600	1.92580800	-1.94389800
H	-1.44623300	2.97168200	-2.82952300
H	-3.29773700	-0.23579100	-2.65079400
H	-2.45442600	0.93036400	-3.68603400
H	-1.51981300	-0.18025300	-2.66790400
H	-3.85067400	2.74460200	-2.65623600
H	-4.63207000	1.65147600	-1.51759200
H	-3.77742500	3.10210000	-0.92875500
C	-2.56930300	1.57629700	1.57610400
C	-2.05944500	0.73316200	2.75083100
C	-1.80527600	2.90174300	1.53659100
C	-4.04866400	1.87610200	1.82242000
H	-2.52907100	-0.25869300	2.77698100
H	-0.96899100	0.59920900	2.71858800
H	-2.30901900	1.24233500	3.69133200
H	-2.21872700	3.59581600	0.79416900
H	-1.89404200	3.38730700	2.51769800
H	-0.73636000	2.76558900	1.32558000
H	-4.11948300	2.53431500	2.69859900
H	-4.53053500	2.39771000	0.98842100
H	-4.62144700	0.97367600	2.05632700
C	-3.25721100	-0.87053600	-0.03187400
C	-2.80154200	-2.19564700	-0.19395400
C	-4.64396300	-0.63906000	-0.02494000

C	-3.74738700	-3.22342700	-0.31358000
C	-1.38613200	-2.63680600	-0.31757300
C	-5.56349200	-1.67089400	-0.14011500
H	-5.02419600	0.37308400	0.05631300
C	-5.11085300	-2.97677000	-0.27888800
H	-3.38242500	-4.24111800	-0.43721600
C	-0.93568000	-3.08404400	-1.56470400
C	-0.54571700	-2.77247400	0.79285600
H	-6.62748600	-1.45003700	-0.12862800
H	-5.81576100	-3.79892300	-0.37109500
C	0.32531900	-3.65298200	-1.70146000
H	-1.59815100	-3.00057700	-2.42572000
C	0.71080500	-3.35831600	0.65556400
H	-0.89440600	-2.44834100	1.77451000
C	1.14830200	-3.79729400	-0.58887800
H	0.66248500	-3.99693400	-2.67698500
H	1.35562400	-3.46295300	1.52455200
H	2.13546700	-4.24243400	-0.69472200
C	4.96941300	-2.38889400	-0.72621200
C	4.26060000	-1.54405400	0.11805800
C	3.10282700	-0.89662900	-0.32885700
C	2.67884600	-1.10612500	-1.64493900
C	3.39752600	-1.93544200	-2.49751600
C	4.54052800	-2.58159000	-2.03760600
H	5.86419200	-2.88954900	-0.36556400
H	4.61539000	-1.38457000	1.13591200
H	1.76638000	-0.61863800	-1.99224700
H	3.05514200	-2.08938200	-3.51802400
H	5.10079000	-3.23584100	-2.70083200
C	2.36865200	0.05494700	0.55081400
C	2.48575600	-0.11433900	2.02016000
O	2.85686900	0.85407100	2.70735000
O	2.14958700	-1.27330600	2.52016800
C	2.14906600	-1.38218600	3.95458800
H	3.14705700	-1.18276600	4.35181300
H	1.43675500	-0.67234800	4.38324400
H	1.84637000	-2.40712000	4.16760500
C	2.74636900	2.56159500	-1.60636100
C	2.52604900	2.49671200	-0.24141000
C	1.82248900	3.46389900	0.45843400
C	1.31168100	4.54655000	-0.25152600
C	1.50629600	4.63492900	-1.62762300
C	2.21857400	3.64549700	-2.30154500
H	3.33057000	1.78902800	-2.09904900

H	1.68286300	3.37300300	1.53494600
H	0.76352200	5.32314600	0.27636200
H	2.38121100	3.72490300	-3.37292400
O	3.09808400	1.42247800	0.46861500
H	3.15651900	1.56536400	1.54289400
H	1.10962300	5.48490400	-2.17634800



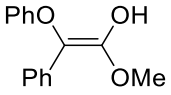
Int-o2

Gibbs free energies = -2059.393219 a.u.

Au	0.23630100	0.19040100	0.30732200
P	-2.10356900	0.61846300	-0.01020400
C	-2.32789300	1.56002500	-1.64128500
C	-1.14498300	2.50802500	-1.84185600
C	-2.28130500	0.50289100	-2.74876600
C	-3.63037300	2.35080800	-1.73427100
H	-1.06908400	3.28162600	-1.07094400
H	-0.18796900	1.96882300	-1.86794800
H	-1.26188200	3.01783500	-2.80786700
H	-3.14692900	-0.16893500	-2.72902400
H	-2.27475900	1.01432200	-3.72018800
H	-1.36828700	-0.10685700	-2.69093800
H	-3.68547400	2.81776600	-2.72664500
H	-4.51802800	1.71733300	-1.63209900
H	-3.68259700	3.15988400	-0.99567000
C	-2.59297800	1.60276300	1.53920800
C	-2.12916200	0.75310700	2.72863100
C	-1.82374500	2.92560400	1.53678100
C	-4.08012000	1.90525400	1.72980500
H	-2.55555400	-0.25898400	2.70529600
H	-1.03407500	0.67189100	2.76676900
H	-2.46129600	1.23054800	3.66013100
H	-2.21913700	3.63350700	0.79818100
H	-1.93174100	3.39515900	2.52373700
H	-0.75114600	2.78936000	1.34568200
H	-4.18127100	2.57017900	2.59773400
H	-4.52967500	2.42198500	0.87528000
H	-4.66232900	1.00508800	1.94864600
C	-3.23406800	-0.82568000	-0.12778900
C	-2.78399900	-2.15078300	-0.30618200
C	-4.61873600	-0.58275100	-0.15722700
C	-3.73416200	-3.16858700	-0.46763400
C	-1.37026600	-2.60015000	-0.42531200

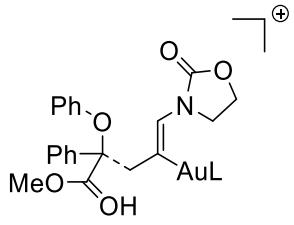
C	-5.54240400	-1.60482500	-0.31725400
H	-4.99372500	0.43088300	-0.07047800
C	-5.09630800	-2.91192100	-0.46427200
H	-3.37371300	-4.18627600	-0.60392900
C	-0.90609200	-2.98986700	-1.68672200
C	-0.55046200	-2.80815900	0.68915700
H	-6.60440600	-1.37502100	-0.33368500
H	-5.80473700	-3.72645500	-0.59044900
C	0.35049300	-3.56504000	-1.83526000
H	-1.55517500	-2.85681400	-2.55155400
C	0.69914000	-3.40596500	0.53875300
H	-0.91283400	-2.53297100	1.68121600
C	1.15409300	-3.77930100	-0.72019900
H	0.69680900	-3.86192100	-2.82282500
H	1.32460900	-3.58564600	1.40881100
H	2.13717800	-4.23122200	-0.83261700
C	4.99859600	-2.30332200	-0.69733100
C	4.29795300	-1.48069600	0.17584200
C	3.13161200	-0.82789600	-0.23754900
C	2.68975600	-1.00993500	-1.55098400
C	3.40161800	-1.81574800	-2.43287800
C	4.55443400	-2.46665000	-2.00694500
H	5.90138700	-2.80594800	-0.35983900
H	4.66826100	-1.33727200	1.19001900
H	1.77367600	-0.51998700	-1.88563500
H	3.04667500	-1.94293600	-3.45289700
H	5.11000600	-3.09903600	-2.69484200
C	2.44977500	0.12751600	0.69331500
C	2.27796500	-0.23271300	2.06608200
O	2.30264500	0.67989000	3.00157700
O	2.09460700	-1.46189600	2.43873700
C	1.62629900	-1.71468900	3.77594300
H	2.34673900	-1.35037900	4.51131500
H	0.65673000	-1.22869200	3.92680300
H	1.52356500	-2.79731200	3.84470500
C	2.90328400	2.41113600	-1.47992600
C	2.56658800	2.41890400	-0.13090400
C	1.83522100	3.46474600	0.42175600
C	1.41722400	4.51291500	-0.39173900
C	1.73117200	4.50935900	-1.74799200
C	2.47198600	3.46046500	-2.28687100
H	3.51331100	1.60396000	-1.87715400
H	1.60925600	3.45944100	1.48822100
H	0.85235300	5.33654700	0.03942000

H	2.73706300	3.46725200	-3.34104900
O	3.03599300	1.43429500	0.72274900
H	2.61454200	1.49671600	2.54970300
H	1.41255000	5.33260300	-2.38202600

Int-o3 

Gibbs free energies = -804.970944 a.u.

C	2.95302900	-2.17087900	0.70101200
C	2.36947000	-0.92076200	0.55064400
C	1.21913800	-0.75976600	-0.23911000
C	0.67264200	-1.89880000	-0.85081900
C	1.26010300	-3.14553200	-0.68913600
C	2.40571000	-3.29198000	0.08518800
H	3.84478000	-2.26920800	1.31654000
H	2.80343900	-0.06017300	1.04903300
H	-0.21822100	-1.79624900	-1.46497100
H	0.81605400	-4.01105000	-1.17623300
H	2.86469100	-4.26959000	0.21121200
C	0.56871900	0.52924900	-0.43500500
C	1.01300000	1.77902500	-0.15565300
O	0.29941400	2.87410400	-0.46368700
O	2.17748400	2.02488100	0.44784200
C	2.73311700	3.32541800	0.29440500
H	2.88692000	3.56797700	-0.76288600
H	2.09305900	4.08775300	0.74778000
H	3.69486200	3.29609000	0.80803400
C	-2.97622500	0.09012400	-1.07765800
C	-1.79241200	0.20045600	-0.35192800
C	-1.77812800	-0.00625500	1.02294600
C	-2.96978800	-0.32126300	1.66902200
C	-4.16017700	-0.42792900	0.95976900
C	-4.15653800	-0.22058600	-0.41717300
H	-2.94597600	0.25135500	-2.15255700
H	-0.84659400	0.07360500	1.57599300
H	-2.96031200	-0.48582900	2.74397900
H	-5.08073600	-0.30328200	-0.98438700
O	-0.67308800	0.53485100	-1.08626600
H	-0.46737600	2.55874200	-0.96851500
H	-5.08503000	-0.67395200	1.47484100



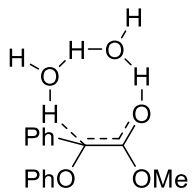
TS-o3-3p

Gibbs free energies = -2497.040626 a.u.

C	6.70867600	1.52131700	-1.65388100
C	5.66505400	1.35197200	-0.75349800
C	4.72813800	0.32657500	-0.94353400
C	4.86682900	-0.51748000	-2.05495600
C	5.91397200	-0.34175600	-2.94874300
C	6.83899400	0.67871800	-2.75319500
H	7.43092000	2.31712700	-1.49007600
H	5.58353200	2.01516900	0.10196400
H	4.14921300	-1.32006500	-2.21216900
H	6.00706000	-1.00757600	-3.80290100
H	7.65858500	0.81547800	-3.45361900
C	3.58615400	0.11223700	-0.04771100
C	3.19983100	0.88066900	1.04471200
O	2.28116300	0.45355900	1.88835900
O	3.58903000	2.12452300	1.19761200
C	3.17349800	2.84669600	2.36656900
H	2.08294200	2.88775300	2.43477000
H	3.58297100	2.37761600	3.26556800
H	3.58213600	3.84912400	2.24326900
C	4.77135700	-2.07678500	1.36772700
C	3.76870400	-2.22106400	0.41790000
C	3.44888400	-3.46399100	-0.11369100
C	4.13941900	-4.58709700	0.32459900
C	5.14556900	-4.46422100	1.27916000
C	5.45910500	-3.21069600	1.79229000
H	5.02904200	-1.09611300	1.76168800
H	2.67206300	-3.52752600	-0.87248500
H	3.89717200	-5.56194900	-0.09091500
H	6.24927200	-3.10633300	2.53143400
O	2.99724700	-1.14852100	-0.03425400
H	5.68997500	-5.34236100	1.61508500
H	1.96055500	-0.40688800	1.55257500
C	1.94723600	1.15344400	-1.25164300
C	0.81525400	1.49065100	-0.49969300
C	0.78827900	2.82648000	-0.14905100
H	1.47896900	3.55108400	-0.59574300
C	-0.15602700	4.83811100	0.76390900

C	-1.02756800	2.80601600	1.59895900
C	-1.48000800	4.00910400	2.42866400
H	-0.55549300	2.01768100	2.19914000
H	-1.84856500	2.36513600	1.01722600
H	-1.00478700	4.04217500	3.41566100
H	-2.56424200	4.05756000	2.55344300
N	-0.05899500	3.42750900	0.71699900
O	-1.06374800	5.16214200	1.69237900
O	0.45972600	5.60352100	0.08196500
C	-4.01155000	-1.41510300	-0.51260200
C	-4.91211400	-2.49194900	-0.45045400
C	-6.23390900	-2.37809000	-0.85341000
C	-6.69963400	-1.15582600	-1.32083900
C	-5.82882200	-0.08049500	-1.39587700
C	-4.48180400	-0.18229400	-1.01720800
C	-3.68464300	1.05641200	-1.22334200
C	-2.70770600	1.13346600	-2.22211500
C	-2.07855600	2.34241200	-2.50711500
C	-2.41240600	3.49227800	-1.79679000
C	-3.39008900	3.42931200	-0.80616500
C	-4.02394300	2.22093700	-0.52554300
C	-1.60537100	-3.24580800	-0.60928200
C	-1.90673900	-3.14728900	-2.10632300
C	-2.10985100	-4.58235000	-0.06524800
C	-0.08254400	-3.21735900	-0.42663300
C	-2.61701800	-1.84391700	2.05143400
C	-1.28588600	-2.17327700	2.72840500
C	-3.08706100	-0.46158100	2.51403400
C	-3.66818700	-2.86727100	2.47734800
H	-4.57679700	-3.44874600	-0.06374800
H	-6.89441500	-3.23902000	-0.79437000
H	-7.73396500	-1.04120200	-1.63439100
H	-6.18069700	0.87420300	-1.78216200
H	-2.46730000	0.24299100	-2.80284500
H	-1.33002100	2.38654000	-3.29487700
H	-1.92609900	4.43849200	-2.02656500
H	-3.68072500	4.33029200	-0.26888700
H	-4.80758100	2.17537900	0.23066600
H	-1.56149700	-2.19296200	-2.52764500
H	-1.37358800	-3.95091800	-2.63133800
H	-2.97442400	-3.25238000	-2.32607900
H	-1.85217700	-4.72737900	0.99021900
H	-1.61977000	-5.38915600	-0.62660900
H	-3.18690700	-4.73067000	-0.18642000

H	0.22556600	-3.19773700	0.62615300
H	0.37831800	-2.35607600	-0.92822300
H	0.33505100	-4.13174800	-0.87155700
H	-0.94469300	-3.19047400	2.50292400
H	-1.41148500	-2.10775400	3.81736900
H	-0.49342800	-1.46764900	2.44123900
H	-4.02099800	-0.16199200	2.02145000
H	-3.27525200	-0.48979900	3.59559500
H	-2.33075800	0.30908700	2.31990800
H	-3.42904300	-3.88824700	2.16467000
H	-4.66606900	-2.61180900	2.10715500
H	-3.72158500	-2.86906700	3.57436200
P	-2.32274500	-1.67079800	0.18589800
Au	-0.68247000	0.07313000	-0.14841900
H	2.67037600	1.91880400	-1.55310200
H	1.98947300	0.22558700	-1.82061400

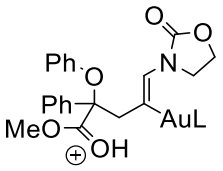


TS-o3-2p

Gibbs free energies = -957.734932 a.u.

C	2.44030100	-2.70515900	0.88241200
C	1.42668900	-1.75517400	0.86327300
C	1.58986300	-0.51614600	0.21329300
C	2.83472600	-0.27867300	-0.40359500
C	3.84154800	-1.23502300	-0.38154200
C	3.65844600	-2.45904700	0.25691800
H	2.27042800	-3.65177300	1.39283000
H	0.48815600	-1.97038000	1.36791000
H	3.01201000	0.66731100	-0.90391400
H	4.78746100	-1.01506200	-0.87408300
H	4.45095700	-3.20372000	0.26955700
C	0.50786600	0.47516800	0.27794600
C	0.23552100	1.54005800	-0.63799900
O	-0.81107500	2.21684700	-0.64224900
O	1.23612200	1.85299500	-1.48238800
C	1.04646900	3.02674000	-2.26817600
H	1.96691800	3.15380100	-2.84076800
H	0.19903200	2.91336600	-2.95090400
H	0.87773700	3.90449700	-1.63657900
C	-2.79304100	-0.97675400	0.86587300
C	-1.60814700	-0.67099600	0.19254700

C	-1.43232500	-1.07589400	-1.12987800
C	-2.45330700	-1.77261400	-1.77022200
C	-3.64067900	-2.07390500	-1.11036500
C	-3.80276800	-1.67235300	0.21374600
H	-2.90085900	-0.66308400	1.90330800
H	-0.50739200	-0.85033100	-1.65493700
H	-2.31137500	-2.08375600	-2.80315100
H	-4.72309900	-1.90251100	0.74652400
O	-0.67655900	0.01765300	0.91875400
H	-1.55537300	2.41904200	0.77477100
H	-4.43179500	-2.61656900	-1.62172800
O	-1.72581100	2.57395400	1.75773000
O	0.55909900	2.14381900	2.37897800
H	-0.56064900	2.36613900	2.20370500
H	0.78544600	1.49564600	1.55749300
H	-2.30458200	1.84769800	2.03690700
H	0.69579100	1.64616500	3.20105900



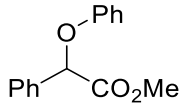
Int-o4

Gibbs free energies = -2497.066712 a.u.

C	6.83578100	-1.66622100	-0.34527700
C	5.63214600	-1.18418200	0.15331400
C	4.70261500	-0.58879200	-0.70438600
C	4.99436300	-0.46849300	-2.06196300
C	6.20056100	-0.95553400	-2.55769900
C	7.12124800	-1.55320200	-1.70349100
H	7.55102700	-2.13097400	0.32874700
H	5.40823800	-1.28381600	1.21525500
H	4.28384800	-0.01160700	-2.74576600
H	6.41787700	-0.86685000	-3.61932400
H	8.06226800	-1.93190100	-2.09529800
C	3.40847200	-0.05481200	-0.10285300
C	3.78247300	1.12673000	0.78374900
O	3.49378300	1.14353400	2.02841000
O	4.41819400	2.08896400	0.26137900
C	4.69741300	3.28847100	1.05003400
H	3.74757900	3.77701500	1.28767400
H	5.24880900	3.01032300	1.94967000
H	5.30142100	3.91452400	0.39673300
C	2.16154300	-2.95186000	1.79398100

C	2.57823400	-2.26804200	0.65218600
C	2.70102100	-2.92533000	-0.56838900
C	2.40995500	-4.28816200	-0.62629800
C	1.99575100	-4.98383500	0.50364200
C	1.86888000	-4.30678400	1.71560400
H	2.07980000	-2.40978600	2.73420000
H	3.03393600	-2.40677800	-1.46206500
H	2.51263800	-4.80436400	-1.57819000
H	1.54491700	-4.83547100	2.60940500
O	2.84811400	-0.93447200	0.86494700
H	1.77298100	-6.04604900	0.44226900
H	3.00639900	0.30412700	2.22927200
C	2.34866900	0.48109700	-1.08776800
C	1.18945400	1.13816300	-0.35691900
C	1.35332600	2.45821300	-0.14576100
H	2.18677800	3.01735500	-0.58445700
C	0.94113500	4.62632700	0.80643700
C	-0.44730200	2.93273400	1.58784700
C	-0.92514200	4.29710400	2.06648000
H	0.00800000	2.32404600	2.38478600
H	-1.25722400	2.35720400	1.12516300
H	-1.07802100	4.35453400	3.14616900
H	-1.84330400	4.60984100	1.55438100
N	0.55665700	3.32011900	0.61552900
O	0.12400500	5.20848600	1.70518700
O	1.87346800	5.20245700	0.28822300
C	-4.17820300	-0.57061900	-0.32999000
C	-5.35307700	-1.30189900	-0.08241500
C	-6.61651600	-0.79450600	-0.35184800
C	-6.74077300	0.48568600	-0.87698200
C	-5.59605100	1.21630600	-1.15573900
C	-4.30969900	0.70839800	-0.91618000
C	-3.20203200	1.59085600	-1.37039300
C	-2.42464000	1.25415000	-2.48366700
C	-1.48881700	2.15079700	-2.99081900
C	-1.31601200	3.39683500	-2.39394600
C	-2.08990300	3.74508500	-1.29025700
C	-3.02991900	2.85062800	-0.78616300
C	-2.40021900	-2.93017100	-0.80083300
C	-2.72975600	-2.59547500	-2.25614800
C	-3.27915100	-4.08640200	-0.33020600
C	-0.94017100	-3.38345300	-0.74704600
C	-2.72948200	-1.60311400	2.06224400
C	-1.52480000	-2.42721300	2.51949800

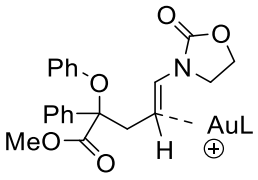
C	-2.64545700	-0.20882300	2.69123500
C	-4.00631800	-2.27245600	2.56718500
H	-5.28776400	-2.29756200	0.34240900
H	-7.49655300	-1.39777700	-0.14255400
H	-7.72111600	0.90910100	-1.08281100
H	-5.68336300	2.20642600	-1.59999700
H	-2.57778900	0.29137600	-2.96877800
H	-0.89988900	1.87845900	-3.86437000
H	-0.58423000	4.09801800	-2.79014000
H	-1.96414900	4.71996700	-0.82020600
H	-3.64790600	3.12788800	0.06881900
H	-2.06939800	-1.81086500	-2.64983600
H	-2.56674800	-3.49441600	-2.86670400
H	-3.77113000	-2.28149400	-2.39584000
H	-3.06099000	-4.37778500	0.70360100
H	-3.06919500	-4.95905300	-0.96466100
H	-4.35033500	-3.87875300	-0.42130600
H	-0.61427600	-3.66758600	0.25976600
H	-0.25796700	-2.60839000	-1.12109200
H	-0.82748200	-4.26934900	-1.38845400
H	-1.60870600	-3.48034400	2.22351600
H	-1.47477100	-2.39938800	3.61724300
H	-0.57607800	-2.03176600	2.13023300
H	-3.40220900	0.47888500	2.28719600
H	-2.81900100	-0.29321300	3.77318700
H	-1.65575700	0.24107600	2.54085500
H	-4.20152100	-3.24502800	2.10233500
H	-4.88783600	-1.63647800	2.43348600
H	-3.89330200	-2.44450600	3.64693900
P	-2.56457800	-1.31411400	0.18974500
Au	-0.54546500	0.01737600	-0.05607400
H	2.86115600	1.19771600	-1.74709900
H	2.02603800	-0.35929100	-1.71452500

pro-o4-2p 

Gibbs free energies = -804.997134 a.u.

C	2.72824000	0.07593000	1.46583300
C	1.45721600	-0.28075100	1.03267500
C	1.28716200	-0.90625100	-0.20431000
C	2.40885800	-1.16026500	-0.99409900
C	3.68050200	-0.80339300	-0.56238300
C	3.84067000	-0.18341000	0.67188100

H	2.84985500	0.56159000	2.43108000
H	0.59286100	-0.07108300	1.65592400
H	2.27778800	-1.63575600	-1.96582900
H	4.54516100	-1.01177500	-1.18785900
H	4.83333100	0.09742500	1.01627300
C	-0.06622800	-1.19476100	-0.79298800
C	-1.09540300	-1.74176600	0.19552400
O	-0.89852100	-2.01883000	1.35239100
O	-2.27164200	-1.92785600	-0.42143900
C	-3.31142100	-2.42203100	0.41812300
H	-4.19216200	-2.51959300	-0.21690900
H	-3.03833900	-3.39001400	0.84836000
H	-3.50657800	-1.72159900	1.23739500
C	-2.14331100	2.50006400	0.55610500
C	-1.15517100	3.47851000	0.53630600
C	0.02180700	3.25841800	-0.17358400
C	0.21754100	2.06254900	-0.85353000
C	-0.77261300	1.08414000	-0.82200300
C	-1.95820200	1.30077200	-0.12387100
H	-3.07041800	2.67286700	1.09780800
H	0.79575900	4.02190700	-0.19639900
H	1.13313700	1.86381500	-1.40596800
H	-2.72972500	0.53519400	-0.14232700
O	-0.58791700	-0.08453100	-1.52799800
H	0.04048800	-1.97509700	-1.56070300
H	-1.30439800	4.41531600	1.06744100



Int-o5

Gibbs free energies = -2497.125887 a.u.

C	1.88044200	-0.18231700	-0.26468900
C	1.02754000	0.43708300	0.80435500
C	0.65933500	1.76570700	0.97514100
H	1.56197300	-1.22029700	-0.41308300
H	1.78769300	0.31555400	-1.23540700
H	0.23433200	2.06357200	1.93619300
C	0.01555200	3.99701300	0.46356200
C	1.17106400	2.87205700	-1.25362900
C	1.07004200	4.37057300	-1.51828200
H	0.48616300	2.28066600	-1.88254000
H	2.19336500	2.49965700	-1.37745800

H	0.69434000	4.61818800	-2.51222200
H	2.03034600	4.87186900	-1.35213600
N	0.73966100	2.82396000	0.13299800
O	0.13063700	4.85633600	-0.55048600
O	-0.61313500	4.16405300	1.46877300
C	-4.32597300	-1.46881200	-0.26288000
C	-5.72548100	-1.52860600	-0.37477900
C	-6.39594700	-2.72569000	-0.57558800
C	-5.66929500	-3.90487100	-0.68483500
C	-4.28772900	-3.86780700	-0.57585500
C	-3.59262000	-2.67153400	-0.35166900
C	-2.11673100	-2.81374200	-0.22783800
C	-1.47832100	-2.73023000	1.01778300
C	-0.11839200	-3.01445800	1.13321600
C	0.61824700	-3.39078900	0.01268300
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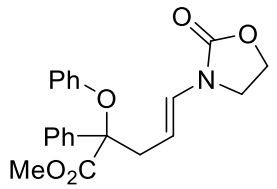

pro-o6

Gibbs free energies = -1242.702623 a.u.

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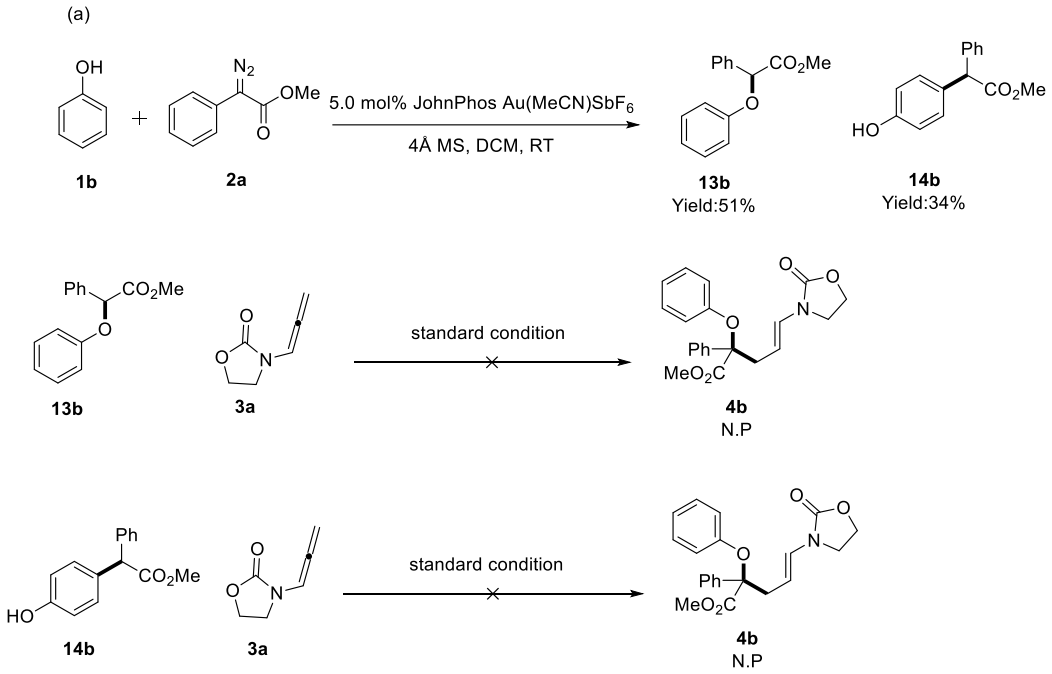
5. Control Experiments



To a flask charged with 5.0 mol% JohnphosAu(MeCN)SbF_6, phenol **1b** (0.30 mmol), and 50 mg 4 Å MS in 3.0 mL of DCM under a dinitrogen atmosphere was at room temperature. Aryldiazoacetate **2a** (0.36 mmol) in DCM (2.0 mL) were introduced by syringe pump over 1.0 hr and the reaction solution was stirred for another 0.5 hr. After the completion of the reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. And then the crude product was purified by flash chromatography on silica gel (EtOAc/light petroleum ether = 1:50) to give the pure product **13b** and **14b**.

To a flask charged with 5.0 mol% JohnphosAu(MeCN)SbF_6, **13b** or **14b** (0.1 mmol),

and 50 mg 4 Å MS in 1.0 mL of DCM under a dinitrogen atmosphere was at room temperature. **3a** (0.1 mmol) in DCM (1.0 mL) were introduced by syringe pump over 1.0 hr and the reaction solution was stirred for another 1.0 hr. Few amount of pyridine was used for quenching reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. The crude product was detected by TLC and ^{1}H NMR using 1, 3, 5-trimethoxybenzene as an internal standard.

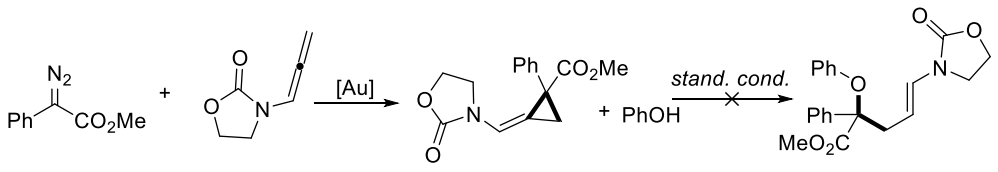
(b)

Entry	additive（mol%）	Yield of **4b**
1	none	N.R[b]
2	$TsOH{\cdot}H_2O$(10.0)	N.P[c]
3	TFA(10.0)	N.P[c]
4	*rac*-PA(10.0)[a]	N.P[c]
5	DBU(100.0)	N.R[b]
6	TEA(100.0)	N.R[b]
7	Cs_2CO_3(100.0)	N.R[b]

[a] *rac*-PA: *rac*-1,1'-Binaphthyl-2,2'-diyl hydrogenphosphate; [b] **13b** and **3a** were recovered. [c] **13b** was recovered.

To a flask charged with base or acid, **13b** (0.1 mmol), and 50 mg 4 Å MS in 1.0 mL of DCM under a dinitrogen atmosphere was at room temperature. **3a** (0.1 mmol) in DCM (1.0 mL) were introduced by syringe pump over 1.0 hr and the reaction solution was stirred for another 8.0 hr. The crude product was detected by TLC and ^{1}H NMR using 1, 3, 5-trimethoxybenzene as an internal standard.

c)



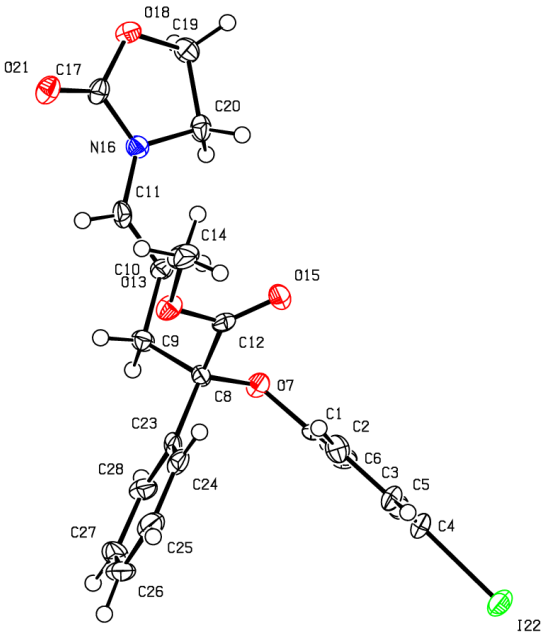
2a **3a** *cis*-**12a**; yield: 17%
trans-**12a'** yield: 35% **4b**

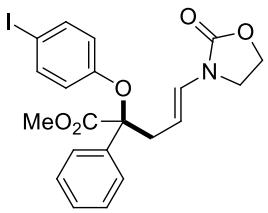
To a flame-dried 25-mL Schlenk flask charged with a magnetic stirring bar, 5.0 mol% JohnphosAu(MeCN)SbF_6, 50 mg 4 Å MS in 1.0 mL of DCM were sequentially added under a dinitrogen atmosphere at room temperature. Aryldiazoacetate **2a** (0.10 mmol) and allenamide **3a** (0.15 mmol) dissolved in DCM (1.0 mL) were added by syringe pump over 1.0 hr under a dinitrogen atmosphere. The mixture was stirred for 4.0 hrs at room temperature. Few amount of pyridine was used for quenching reaction before the solvent was evaporated, and products were purified by column chromatography (10:1 to 1:1 gradient of hexanes: ethyl acetate as eluents) to afford *cis*-**12a** and *tran*-**12a'** .

To a flask charged with 5.0 mol% JohnphosAu(MeCN)SbF_6, phenol **1b** (0.10 mmol), *cis*-**12a** or *tran*-**12a'** (0.10 mmol) and 50 mg 4 Å MS in 1.0 mL of DCM under a dinitrogen atmosphere was at room temperature. The reaction solution was stirred for 1.0 hr. After the completion of the reaction, few amount of pyridine was used for quenching reaction, the reaction mixture was filtrated and the filtrate was evaporated in vacuo to give the crude product. The crude product was detected by ^{1}H NMR using 1, 3, 5-trimethoxybenzene as an internal standard.

6. X-ray Diffraction Parameters and Data

4i (CCDC 1887654)





4i

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Bond precision:  C-C = 0.0150 A          Wavelength=1.54184

Cell:            a=15.6909(2)      b=8.2225(1)      c=30.5829(3)
                 alpha=90          beta=90          gamma=90
Temperature:     100 K
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	Calculated	Reported
Volume	3945.76(8)	3945.76(8)
Space group	P c a 21	P c a 21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C21 H20 I N O5	C21 H20 I N O5
Sum formula	C21 H20 I N O5	C21 H20 I N O5
Mr	493.28	493.28
Dx,g cm-3	1.661	1.661
Z	8	8
Mu (mm-1)	13.036	13.036
F000	1968.0	1968.0
F000'	1971.29	
h,k,lmax	18,9,36	18,9,36
Nref	7044[3596]	5398
Tmin,Tmax	0.083,0.272	0.290,1.000
Tmin'	0.011	

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Correction method= # Reported T Limits: Tmin=0.290 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.50/0.77      Theta(max)= 67.063

R(reflections)= 0.0419( 5146)     wR2(reflections)= 0.1139( 5398)

S = 1.089                  Npar= 507
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 Alert level B
PLAT926_ALERT_1_B Reported and Calculated   R1 Differ by .....      0.0074 Check
PLAT927_ALERT_1_B Reported and Calculated  wR2 Differ by .....      0.0179 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....       6 Check

 Alert level C
STRVA01_ALERT_4_C          Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack     0.390
          From the CIF: _refine_ls_abs_structure_Flack_su     0.006
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) .....       7.09 Note
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01503 Ang.
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage       52 %
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .       5 Check
PLAT928_ALERT_1_C Reported and Calculated    S value   Differ by .     0.171 Check
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.       0 Info
PLAT987_ALERT_1_C The Flack x is >> 0 -  Do a BASF/TWIN Refinement    Please Check

 Alert level G
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      20.22 Why ?
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............    0.00030 Ang.
PLAT792_ALERT_1_G Model has Chirality at C8        (Polar  SPGR)          S Verify
PLAT792_ALERT_1_G Model has Chirality at C36       (Polar  SPGR)          R Verify
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still       88% Note

 0 ALERT level A = Most likely a serious problem - resolve or explain
 3 ALERT level B = A potentially serious problem, consider carefully
 8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 5 ALERT level G = General information/check it is not something unexpected

 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 2 ALERT type 2 Indicator that the structure model may be wrong or deficient
 6 ALERT type 3 Indicator that the structure quality may be low
 2 ALERT type 4 Improvement, methodology, query or suggestion
 0 ALERT type 5 Informative message, check
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7. Notes and References

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Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09, Revision A.01*, Gaussian, Inc., Wallingford CT, 2009.

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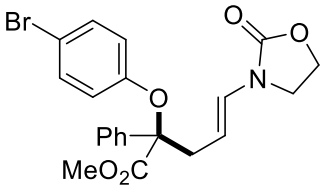
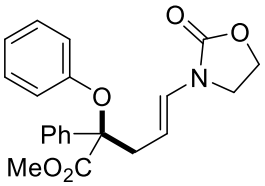
8. Analytical Data for the Products



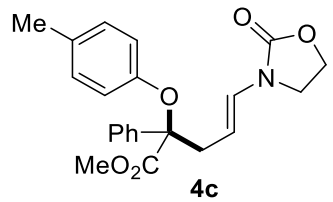
4a

Methyl(*E*)-2-(4-bromophenoxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate(4a): Colorless oil; 67% yield (119.3 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.50 (m, 2H), 7.34 (tdd, *J* = 6.9, 4.6, 2.1 Hz, 3H), 7.27 – 7.23 (m, 2H), 6.67 – 6.60 (m, 2H), 6.55 (d, *J* = 14.4 Hz, 1H), 4.57 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.36 (t, *J* = 8.1 Hz, 2H), 3.71 (s, 3H), 3.56 (td, *J* = 8.0, 5.5 Hz, 2H), 3.17 (ddd, *J* = 14.8, 8.0, 1.0 Hz, 1H), 3.08 (ddd, *J* = 14.8, 6.8, 1.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.6, 155.2, 154.4, 138.1, 132.0, 128.6, 128.4, 127.3, 126.2, 120.0, 114.2, 102.9, 85.4, 62.1, 52.8, 42.4, 38.4. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{20}NO_5BrNa^+$, 468.0417, found 468.0421.



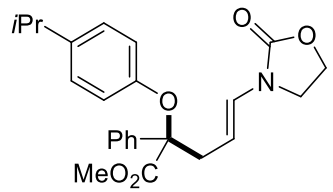
4b

Methyl (*E*)-5-(2-oxooxazolidin-3-yl)-2-phenoxy-2-phenylpent-4-enoate(4b): Colorless oil; 66% yield (96.9 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 5.3, 3.3 Hz, 2H), 7.39 – 7.33 (m, 2H), 7.33 – 7.28 (m, 1H), 7.21 – 7.15 (m, 2H), 6.93 (t, *J* = 7.4 Hz, 1H), 6.78 (dd, *J* = 8.7, 0.9 Hz, 2H), 6.48 (d, *J* = 14.4 Hz, 1H), 4.55 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.33 (t, *J* = 8.2 Hz, 2H), 3.70 (s, 3H), 3.59 – 3.47 (m, 2H), 3.23 (ddd, *J* = 14.8, 7.9, 0.8 Hz, 1H), 3.11 (ddd, *J* = 14.8, 6.9, 1.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.1, 155.2, 155.1, 138.7, 129.2, 128.5, 128.1, 127.1, 126.1, 121.9, 118.2, 103.1, 84.9, 62.1, 52.8, 42.4, 37.56. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{21}NO_5Na^+$, 390.1312, found 390.1312.



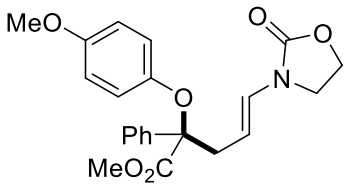
4c

Methyl (*E*)-5-(2-oxooxazolidin-3-yl)-2-phenyl-2-(p-tolyloxy)pent-4-enoate(4c): Colorless oil; 83% yield (130.1 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 5.3, 3.4 Hz, 2H), 7.39 – 7.32 (m, 2H), 7.30 (dd, *J* = 4.8, 3.5 Hz, 1H), 6.96 (d, *J* = 8.4 Hz, 2H), 6.69 – 6.64 (m, 2H), 6.48 (d, *J* = 14.4 Hz, 1H), 4.55 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.31 (t, *J* = 8.3 Hz, 2H), 3.69 (s, 3H), 3.59 – 3.44 (m, 2H), 3.21 (ddd, *J* = 14.8, 8.0, 1.0 Hz, 1H), 3.09 (ddd, *J* = 14.8, 6.9, 1.0 Hz, 1H), 2.23 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.3, 155.2, 152.8, 138.9, 131.3, 129.7, 128.5, 128.1, 127.0, 126.1, 118.3, 103.3, 84.8, 62.1, 52.7, 42.4, 37.2, 20.5. HRMS (ESI) $[M+Na]^+$ calcd for $C_{22}H_{23}NO_5Na^+$, 404.1468, found 404.1466.



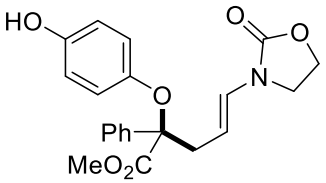
4d

Methyl(*E*)-2-(4-isopropylphenoxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate(4d): Colorless oil; 82% yield (134.7 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, *J* = 5.3, 3.4 Hz, 2H), 7.37 (dd, *J* = 8.4, 1.4 Hz, 2H), 7.32 – 7.29 (m, 1H), 7.03 (d, *J* = 8.6 Hz, 2H), 6.74 – 6.67 (m, 2H), 6.48 (d, *J* = 14.4 Hz, 1H), 4.55 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.34 (t, *J* = 8.2 Hz, 2H), 3.69 (s, 3H), 3.59 – 3.47 (m, 2H), 3.22 (ddd, *J* = 14.8, 7.8, 0.6 Hz, 1H), 3.10 (ddd, *J* = 14.9, 6.9, 1.0 Hz, 1H), 2.81 (dt, *J* = 13.8, 6.9 Hz, 1H), 1.19 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.3, 155.2, 152.9, 142.3, 139.0, 128.5, 128.1, 127.0, 126.9, 126.0, 118.1, 103.4, 84.8, 62.1, 52.7, 42.4, 37.0, 33.2, 24.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{24}H_{27}NO_5Na^+$, 432.1781, found 432.1782.



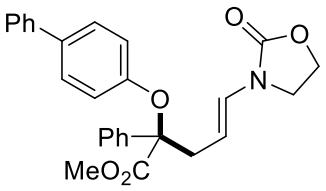
4e

Methyl(*E*)-2-(4-methoxyphenoxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate(4e): Colorless oil; 85% yield (137.8 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.2 Hz, 2H), 7.34 (dt, *J* = 13.8, 7.0 Hz, 3H), 6.71 (s, 4H), 6.52 (d, *J* = 14.4 Hz, 1H), 4.59 (dt, *J* = 14.5, 7.3 Hz, 2H), 4.36 (t, *J* = 8.2 Hz, 3H), 3.72 (s, 1H), 3.71 (s, 3H), 3.57 (dt, *J* = 17.3, 8.6 Hz, 2H), 3.16 (dd, *J* = 14.9, 7.9 Hz, 1H), 3.08 (dd, *J* = 14.9, 6.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.3, 155.2, 154.8, 148.6, 138.9, 128.5, 128.2, 127.0, 126.2, 120.1, 114.2, 103.4, 85.4, 62.1, 55.5, 52.7, 42.4, 36.9. HRMS (ESI) $[M+Na]^+$ calcd for $C_{22}H_{23}NO_6Na^+$, 420.1418, found 420.1419.



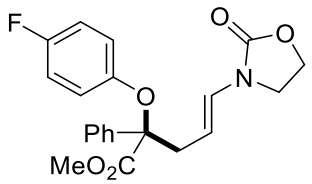
4f

Methyl(*E*)-2-(4-hydroxyphenoxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate(4f): Colorless oil; 35% yield (53.6 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.49 (m, 2H), 7.39 – 7.29 (m, 3H), 6.69 – 6.61 (m, 4H), 6.49 (d, *J* = 14.4 Hz, 1H), 5.97 (br, 1H), 4.59 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.36 (t, *J* = 8.2 Hz, 2H), 3.71 (s, 3H), 3.56 (dd, *J* = 17.1, 8.4 Hz, 2H), 3.15 (dd, *J* = 14.9, 8.0 Hz, 1H), 3.07 (dd, *J* = 15.0, 6.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.5, 155.5, 151.3, 148.2, 138.9, 128.5, 128.2, 126.9, 126.2, 120.4, 115.8, 103.7, 85.4, 62.3, 52.8, 42.4, 36.5. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{21}NO_6Na^+$, 406.1261, found 406.1263.



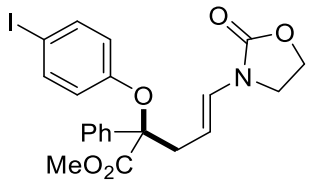
4g

Methyl(*E*)-2-([1,1'-biphenyl]-4-yloxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate(4g): White solid; 88% yield (158.0 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.8 Hz, 2H), 7.50 (d, *J* = 7.8 Hz, 2H), 7.41 (d, *J* = 8.7 Hz, 2H), 7.38 (t, *J* = 7.7 Hz, 4H), 7.32 (d, *J* = 7.3 Hz, 1H), 7.28 (dd, *J* = 13.8, 6.3 Hz, 1H), 6.84 (d, *J* = 8.7 Hz, 2H), 6.54 (d, *J* = 14.3 Hz, 1H), 4.59 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.33 (t, *J* = 8.1 Hz, 2H), 3.72 (s, 3H), 3.60 – 3.49 (m, 2H), 3.25 (dd, *J* = 14.8, 7.9 Hz, 1H), 3.14 (dd, *J* = 14.8, 6.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.0, 155.2, 154.7, 140.4, 138.7, 134.8, 128.8, 128.6, 128.3, 127.8, 127.2, 126.9, 126.7, 126.1, 118.5, 103.2, 85.1, 62.1, 52.8, 42.4, 37.8. HRMS (ESI) $[M+Na]^+$ calcd for $C_{27}H_{25}NO_5Na^+$, 466.1625, found 466.1628.



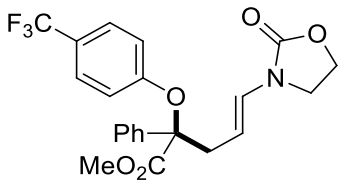
4h

Methyl(*E*)-2-(4-fluorophenoxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate(4h): Colorless oil; 90% yield (140.9 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.7 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.31 (t, *J* = 7.2 Hz, 1H), 6.85 (t, *J* = 8.6 Hz, 2H), 6.71 (dd, *J* = 9.1, 4.3 Hz, 2H), 6.54 (d, *J* = 14.3 Hz, 1H), 4.60 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.36 (t, *J* = 8.1 Hz, 2H), 3.71 (s, 3H), 3.62 – 3.52 (m, 2H), 3.16 (dd, *J* = 14.8, 8.0 Hz, 1H), 3.09 (dd, *J* = 14.8, 6.7 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.9, 158.8, 156.9, 155.2, 151.0, 151.0, 138.4, 128.5, 128.4, 127.2 (d, *J* = 11.5 Hz), 126.2, 120.0 (d, *J* = 2.3 Hz), 119.9 (d, *J* = 7.0 Hz), 115.7 (d, *J* = 6.4 Hz), 115.5 (d, *J* = 4.9 Hz), 103.1, 85.6, 62.1, 52.8, 52.7, 42.4, 37.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ -121.8. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{20}NO_5FNa^+$, 408.1218, found 408.1224.



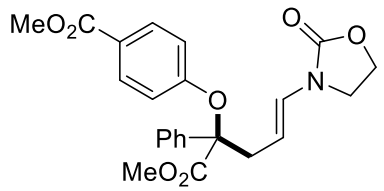
4i

Methyl (*E*)-2-(4-iodophenoxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate (**4i**): White solid; 63% yield (124.0 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.2 Hz, 2H), 7.46 (d, *J* = 8.8 Hz, 2H), 7.41 – 7.31 (m, 3H), 6.58 (d, *J* = 14.4 Hz, 1H), 6.55 (d, *J* = 8.8 Hz, 2H), 4.59 (dt, *J* = 14.6, 7.4 Hz, 1H), 4.40 (t, *J* = 8.1 Hz, 2H), 3.74 (s, 3H), 3.66 – 3.49 (m, 2H), 3.19 (dd, *J* = 14.7, 8.0 Hz, 1H), 3.10 (dd, *J* = 14.7, 6.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.5, 155.2, 138.0, 128.6, 128.3, 127.3, 126.1, 120.4, 102.8, 100.0, 85.3, 84.4, 62.1, 52.8, 42.4, 38.5. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{20}NO_5INa^+$, 516.0278, found 516.0276.



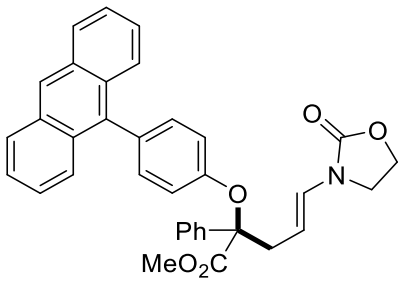
4j

Methyl(*E*)-5-(2-oxooxazolidin-3-yl)-2-phenyl-2-(4-(trifluoromethyl) phenoxy) pent-4-enoate (4j): Colorless oil; 68% yield (118.3 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (t, *J* = 1.8 Hz, 1H), 7.55 – 7.53 (m, 1H), 7.42 (d, *J* = 8.7 Hz, 2H), 7.39 – 7.30 (m, 3H), 6.81 (d, *J* = 8.6 Hz, 2H), 6.59 (d, *J* = 14.3 Hz, 1H), 4.59 (ddd, *J* = 14.6, 7.8, 7.0 Hz, 1H), 4.38 (t, *J* = 8.1 Hz, 2H), 3.73 (s, 3H), 3.64 – 3.53 (m, 2H), 3.18 (ddd, *J* = 14.6, 8.0, 0.8 Hz, 1H), 3.11 (ddd, *J* = 14.7, 6.8, 1.2 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ171.2, 160.0, 158.0, 155.2, 137.8, 128.7, 127.9 (d, *J* = 125.8 Hz), 127.4, 126.54, 126.52, 126.49, 126.46, 126.09, 126.50 (q, *J* = 3.7 Hz), 124.5 (d, *J* = 215.2 Hz), 123.3 (d, *J* = 23.3 Hz), 117.8, 102.7, 85.6, 62.1, 52.9, 42.4, 39.2. ^{19}F NMR (471 MHz, $CDCl_3$) δ -61.64. HRMS (ESI) $[M+Na]^+$ calcd for $C_{22}H_{20}NO_5F_3Na^+$, 458.1375, found 458.1375.



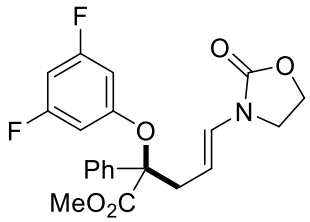
4k

Methyl (E)-4-((1-methoxy-1-oxo-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-en-2-yl)oxy)benzoate (4k). Colorless oil; 72% yield (122.4 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.3 Hz, 2H), 7.55 (d, *J* = 7.4 Hz, 2H), 7.36 (t, *J* = 7.2 Hz, 2H), 7.32 (d, *J* = 6.6 Hz, 1H), 6.77 (d, *J* = 8.3 Hz, 2H), 6.56 (d, *J* = 14.3 Hz, 1H), 4.57 (dt, *J* = 14.3, 7.2 Hz, 1H), 4.37 (t, *J* = 7.9 Hz, 2H), 3.85 (s, 3H), 3.72 (s, 3H), 3.57 (h, *J* = 8.5 Hz, 2H), 3.21 (dd, *J* = 14.4, 8.1 Hz, 1H), 3.12 (dd, *J* = 14.6, 6.5 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.4, 166.6, 159.3, 155.1, 137.9, 131.1, 128.6, 128.4, 127.5, 127.4, 126.1, 123.4, 117.4, 102.7, 85.5, 62.1, 52.9, 52.8, 52.0, 51.8, 42.4, 39.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{23}H_{23}NO_7Na^+$, 448.1367, found 448.1368.



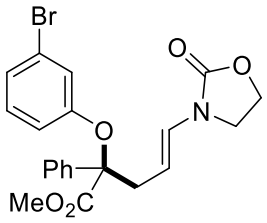
4l

Methyl(*E*)-2-(4-(anthracen-9-yl)phenoxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate(4l): White solid; 42% yield (90.1 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (s, 1H), 8.05 (d, *J* = 8.5 Hz, 2H), 7.71 (d, *J* = 7.8 Hz, 2H), 7.67 (d, *J* = 8.8 Hz, 2H), 7.47 (t, *J* = 7.5 Hz, 4H), 7.39 (dd, *J* = 14.4, 6.7 Hz, 3H), 7.27 (d, *J* = 8.9 Hz, 2H), 7.04 (t, *J* = 12.5 Hz, 2H), 6.64 (d, *J* = 14.3 Hz, 1H), 4.71 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.41 (t, *J* = 8.1 Hz, 2H), 3.84 (s, 3H), 3.65 (tt, *J* = 17.0, 8.6 Hz, 2H), 3.40 (dd, *J* = 14.9, 8.0 Hz, 1H), 3.28 (dd, *J* = 14.9, 6.7 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.2, 155.2, 154.6, 138.8, 136.4, 132.2, 132.0, 131.4, 130.4, 128.62, 128.3, 127.3, 126.8, 126.5, 126.2, 125.4, 125.1, 118.4, 103.2, 85.2, 62.1, 52.9, 42.5, 37.7. HRMS (ESI) $[M+Na]^+$ calcd for $C_{35}H_{29}NO_5Na^+$, 566.1938, found 566.1938.



4m

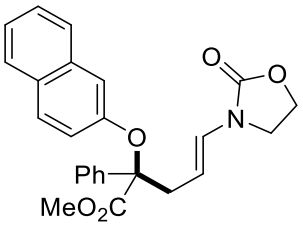
Methyl(*E*)-2-(3,5-difluorophenoxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate(4m): Colorless oil; 52% yield (83.6 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.1 Hz, 2H), 7.43 – 7.34 (m, 3H), 6.60 (d, *J* = 14.3 Hz, 1H), 6.48 – 6.38 (m, 1H), 6.33 – 6.25 (m, 2H), 4.60 (dt, *J* = 14.6, 7.4 Hz, 1H), 4.41 (t, *J* = 8.1 Hz, 2H), 3.77 (s, 3H), 3.66 – 3.55 (m, 2H), 3.19 (dd, *J* = 14.8, 8.1 Hz, 1H), 3.12 (dd, *J* = 14.7, 6.7 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.0, 164.0 (d, *J* = 15.7 Hz), 162.1 (d, *J* = 15.6 Hz), 157.1 (d, *J* = 13.4 Hz), 155.2, 137.6, 128.7, 128.6, 127.5, 126.1, 102.5, 102.0 (d, *J* = 7.0 Hz), 101.8 (d, *J* = 6.9 Hz), 97.5, 86.0, 62.1, 52.9, 42.4, 38.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -109.2. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{19}NO_5F_2Na^+$, 426.1124, found 426.1124.



4n

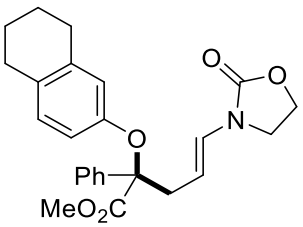
Methyl(*E*)-2-(3-bromophenoxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate(4n): Colorless oil; 80% yield (143.8 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.3 Hz, 2H), 7.36 (dt, *J* = 19.8, 7.0 Hz, 3H), 7.08 (d, *J* = 8.0 Hz, 1H), 7.05 – 6.98 (m, 2H), 6.63 (dd, *J* = 8.2, 2.0 Hz, 1H), 6.56 (d, *J* = 14.3 Hz, 1H), 4.59 (dt, *J* = 14.3, 7.3 Hz, 1H), 4.39 (t, *J* = 8.1 Hz, 2H), 3.74 (s, 3H), 3.65 – 3.52 (m, 2H), 3.20 (dd, *J* = 14.8, 8.0 Hz, 1H), 3.11 (dd, *J* = 14.8, 6.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.5, 156.0, 155.1, 138.1, 130.1, 128.6, 128.4, 127.3, 126.1, 125.0, 122.4, 122.0, 116.6, 102.8, 85.5, 62.1, 52.8, 42.4, 38.4. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{20}NO_5BrNa^+$,

468.0417, found 468.0417.



4o

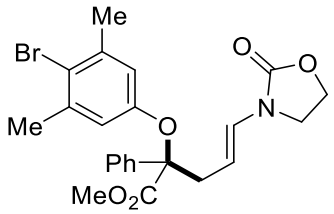
Methyl(*E*)-2-(naphthalen-2-yloxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate(4o): Colorless oil; 49% yield (81.7 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (t, *J* = 9.0 Hz, 2H), 7.62 (d, *J* = 7.4 Hz, 2H), 7.57 (d, *J* = 8.1 Hz, 1H), 7.41 – 7.31 (m, 5H), 7.15 (dd, *J* = 9.0, 2.6 Hz, 1H), 6.95 (d, *J* = 2.4 Hz, 1H), 6.52 (d, *J* = 14.3 Hz, 1H), 4.57 (dt, *J* = 14.6, 7.4 Hz, 1H), 4.34 (dd, *J* = 10.6, 5.7 Hz, 2H), 3.71 (s, 3H), 3.54 (dd, *J* = 16.3, 7.9 Hz, 2H), 3.33 (dd, *J* = 15.1, 7.8 Hz, 1H), 3.18 (dd, *J* = 15.2, 6.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.1, 155.1, 152.9, 138.6, 134.0, 129.4, 128.5, 128.2, 127.5, 127.2, 127.0, 126.3, 126.1, 124.3, 120.3, 112.5, 103.2, 85.2, 62.1, 52.8, 37.7. HRMS (ESI) $[M+Na]^+$ calcd for $C_{25}H_{23}NO_5Na^+$, 440.1468, found 440.1468.



4p

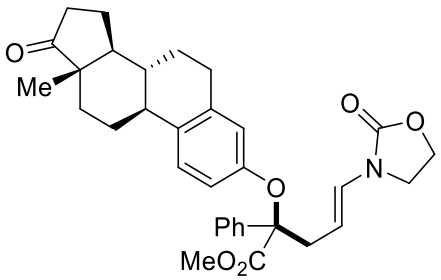
Methyl(*E*)-5-(2-oxooxazolidin-3-yl)-2-phenyl-2-((5,6,7,8-tetrahydronaphthalen-2-yl)oxy)pent-4-enoate(4p): Colorless oil; 69% yield (116.6 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.7 Hz, 2H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.1 Hz, 1H), 6.84 (d, *J* = 8.3 Hz, 1H), 6.53 (d, *J* = 2.2 Hz, 1H), 6.48 (dd, *J* = 8.2, 5.7 Hz, 2H), 4.53 (dt, *J* = 14.5, 7.3 Hz, 1H), 4.34 (t, *J* = 8.2 Hz, 2H), 3.70 (s, 3H), 3.59 – 3.46 (m, 2H), 3.22 (dd, *J* = 14.8, 7.8 Hz, 1H), 3.09 (dd, *J* = 14.8, 6.9 Hz, 1H), 2.65 (s, 4H), 1.76 – 1.69 (m, 4H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.4, 155.2, 152.5, 139.1, 138.1, 130.7, 129.5, 128.4, 128.1, 126.9, 126.0, 118.7, 115.5, 103.5, 84.6, 62.1, 52.7, 42.4, 36.9, 29.6,

28.6, 23.3, 23.0. HRMS (ESI) $[M+Na]^+$ calcd for $C_{25}H_{27}NO_5Na^+$, 444.1781, found 444.1780.



4q

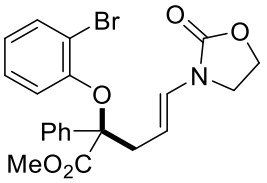
Methyl (*E*)-2-(4-bromo-3,5-dimethylphenoxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate(4q). Colorless oil; 73% yield (138.1 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.3 Hz, 2H), 7.34 (ddd, *J* = 11.0, 9.5, 5.7 Hz, 3H), 6.55 (d, *J* = 11.0 Hz, 3H), 4.56 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.36 (t, *J* = 8.1 Hz, 2H), 3.72 (s, 3H), 3.64 – 3.50 (m, 2H), 3.21 (dd, *J* = 14.8, 7.9 Hz, 1H), 3.11 (dd, *J* = 14.8, 6.8 Hz, 1H), 2.30 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 155.2, 153.6, 138.9, 138.5, 128.5, 128.3, 127.2, 126.0, 119.7, 118.0, 103.1, 85.0, 62.1, 52.8, 42.4, 37.8, 24.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{23}H_{24}NO_5BrNa^+$, 496.0730, found 496.0730.



4r

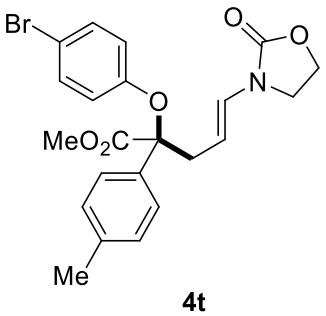
Methyl(*E*)-2-(((8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl)oxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate(4r): Colorless oil; 62% yield (134.4 mg); 1:1 d.r; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.1 Hz, 2H), 7.37 (t, *J* = 7.4 Hz, 2H), 7.32 (d, *J* = 7.2 Hz, 1H), 7.06 (d, *J* = 8.7 Hz, 1H), 6.57 (s, 1H), 6.53 – 6.49 (m, 1H), 6.46 (dd, *J* = 14.5, 2.5 Hz, 1H), 4.51 (dt, *J* = 14.5, 7.3 Hz, 1H), 4.35 (t, *J* = 8.1 Hz, 2H), 3.71 (s, 3H), 3.60 – 3.45 (m, 2H), 3.23 (dd, *J* = 16.0, 6.7 Hz, 1H), 3.10 (dd, *J* = 14.8, 6.8 Hz, 1H), 2.85 – 2.77 (m, 2H), 2.49 (dd, *J* = 18.8, 8.6 Hz, 1H), 2.33 (d, *J* = 10.8 Hz, 1H), 2.25 – 2.17 (m,

1H), 2.16 – 2.10 (m, 1H), 2.09 – 1.97 (m, 2H), 1.94 (t, *J* = 7.9 Hz, 1H), 1.68 – 1.41 (m, 6H), 0.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.4, 155.2, 152.8, 139.0, 137.7, 137.6, 133.3, 128.5, 128.1, 127.0, 126.0, 118.6, 118.5, 115.3, 115.2, 103.4, 103.3, 84.5, 84.5, 62.1, 52.8, 50.4, 48.0, 44.0, 42.4, 38.2, 38.1, 36.9, 36.9, 35.9, 31.6, 29.6, 29.5, 26.5, 25.7, 21.6, 13.9. HRMS (ESI) $[M+Na]^+$ calcd for $C_{33}H_{77}NO_6Na^+$, 566.2513, found 566.2513.



4s

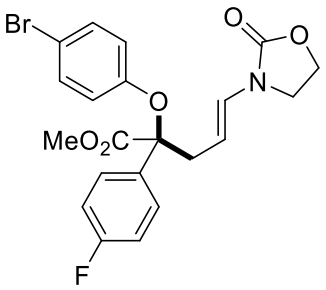
Methyl(*E*)-2-(2-bromophenoxy)-5-(2-oxooxazolidin-3-yl)-2-phenylpent-4-enoate(4s): Colorless oil; 39% yield (69.4 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.7 Hz, 2H), 7.55 (d, *J* = 7.0 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.2 Hz, 1H), 7.09 (t, *J* = 7.4 Hz, 1H), 6.85 (t, *J* = 7.6 Hz, 1H), 6.57 (d, *J* = 8.3 Hz, 1H), 6.31 (d, *J* = 14.3 Hz, 1H), 4.54 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.39 – 4.31 (m, 2H), 3.76 (s, 3H), 3.64 – 3.50 (m, 2H), 3.24 (dd, *J* = 15.0, 8.1 Hz, 1H), 3.08 (dd, *J* = 15.0, 6.7 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.0, 155.1, 151.5, 138.5, 133.8, 128.6, 128.3, 127.8, 127.1, 127.0, 125.8, 123.0, 117.4, 114.4, 102.7, 85.8, 62.1, 53.0, 52.9, 42.4, 37.6. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{20}NO_5BrNa^+$, 468.0417, found 468.0416.



4t

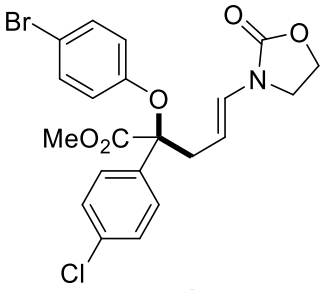
Methyl(*E*)-2-(4-bromophenoxy)-5-(2-oxooxazolidin-3-yl)-2-(p-tolyl)pent-4-enoate(4t): Colorless oil; 73% yield (133.7 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.2 Hz, 2H), 7.27 – 7.24 (m, 2H), 7.15 (d, *J* = 8.1 Hz, 2H), 6.62 (d, *J* = 8.9 Hz,

2H), 6.57 (d, *J* = 14.3 Hz, 1H), 4.60 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.38 (t, *J* = 8.1 Hz, 2H), 3.71 (s, 3H), 3.66 – 3.53 (m, 2H), 3.14 (dd, *J* = 14.7, 8.1 Hz, 1H), 3.07 (dd, *J* = 14.7, 6.7 Hz, 1H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 155.2, 154.4, 138.2, 135.1, 132.0, 129.3, 127.2, 126.1, 120.1, 114.2, 103.0, 85.4, 62.1, 52.7, 42.4, 38.3, 21.1. HRMS (ESI) $[M+Na]^+$ calcd for $C_{22}H_{22}NO_5BrNa^+$, 482.0574, found 482.0575.



4u

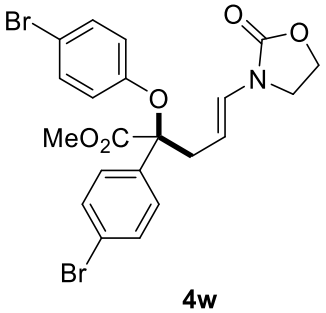
Methyl(*E*)-2-(4-bromophenoxy)-2-(4-fluorophenyl)-5-(2-oxooxazolidin-3-yl)pent-4-enoate(4u): Colorless oil; 64% yield (119.0 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.48 (m, 2H), 7.32 – 7.26 (m, 2H), 7.10 – 7.02 (m, 2H), 6.68 – 6.61 (m, 2H), 6.58 (d, *J* = 14.4 Hz, 1H), 4.56 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.40 (t, *J* = 8.1 Hz, 2H), 3.73 (s, 3H), 3.65 – 3.54 (m, 2H), 3.15 (ddd, *J* = 14.7, 7.9, 0.7 Hz, 1H), 3.07 (ddd, *J* = 14.8, 6.9, 1.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.5, 163.7, 161.2, 155.1, 154.2, 133.9 (d, *J* = 3.3 Hz), 128.2 (d, *J* = 8.1 Hz), 127.5, 119.9, 115.5 (d, *J* = 21.6 Hz), 114.4, 102.5, 85.0, 62.1, 52.9, 42.4, 38.8. ^{19}F NMR (471 MHz, $CDCl_3$) δ -113.5. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{19}NO_5FBrNa^+$, 486.0323, found 486.0322.



4v

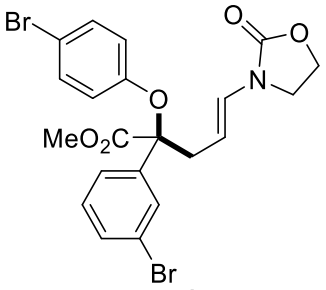
Methyl(*E*)-2-(4-bromophenoxy)-2-(4-chlorophenyl)-5-(2-oxooxazolidin-3-yl)pent-4-enoate(4v): White solid; 75% yield (143.6 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.28 (d, *J* = 9.0 Hz, 2H), 6.62 (d, *J* = 8.8

Hz, 2H), 6.57 (d, *J* = 14.3 Hz, 1H), 4.52 (dt, *J* = 14.5, 7.4 Hz, 1H), 4.38 (t, *J* = 8.0 Hz, 2H), 3.71 (s, 3H), 3.63 – 3.51 (m, 2H), 3.13 (dd, *J* = 14.7, 7.9 Hz, 1H), 3.04 (dd, *J* = 14.6, 6.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.3, 155.1, 154.2, 136.7, 133.9 (d, *J* = 3.3 Hz), 128.2 (d, *J* = 8.1 Hz), 127.8, 119.76, 115.5 (d, *J* = 21.6 Hz), 102.3, 100.0, 84.9, 62.1, 52.9, 42.4, 38.8. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{19}NO_5ClBr$, 502.0028, found 502.0027.



4w

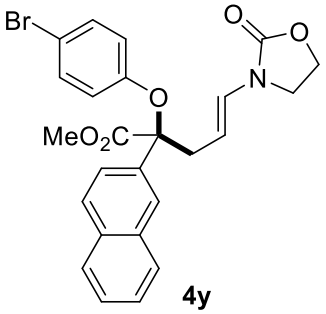
Methyl(*E*)-2-(4-bromophenoxy)-2-(4-bromophenyl)-5-(2-oxooxazolidin-3-yl)pent-4-enoate(4w): Colorless oil; 70% yield (146.4 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.8 Hz, 2H), 7.43 (d, *J* = 8.7 Hz, 2H), 7.27 (d, *J* = 9.0 Hz, 2H), 6.63 (t, *J* = 6.1 Hz, 2H), 6.56 (d, *J* = 14.3 Hz, 1H), 4.51 (dt, *J* = 14.6, 7.4 Hz, 1H), 4.38 (t, *J* = 8.1 Hz, 2H), 3.71 (s, 3H), 3.63 – 3.50 (m, 2H), 3.13 (dd, *J* = 14.8, 7.8 Hz, 1H), 3.03 (dd, *J* = 14.7, 6.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2, 155.1, 154.1, 137.2, 132.1, 131.7, 128.0, 127.6, 122.6, 119.7, 114.4, 102.3, 84.9, 62.1, 52.9, 42.4, 38.7. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{19}NO_5Br_2Na^+$, 545.9522, found 545.9525.



4x

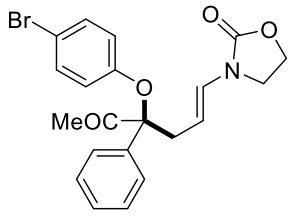
Methyl(*E*)-2-(4-bromophenoxy)-2-(3-bromophenyl)-5-(2-oxooxazolidin-3-yl)pent-4-enoate(4x): Colorless oil; 73% yield (152.7 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (t, *J* = 1.8 Hz, 1H), 7.48 – 7.42 (m, 2H), 7.31 – 7.26 (m, 2H), 7.23 (t, *J* = 7.9 Hz, 1H),

6.72 – 6.61 (m, 2H), 6.53 (d, J = 14.3 Hz, 1H), 4.49 (dt, J = 14.5, 7.4 Hz, 1H), 4.38 (t, J = 8.1 Hz, 2H), 3.71 (s, 3H), 3.63 – 3.51 (m, 2H), 3.14 (ddd, J = 14.7, 7.8, 0.7 Hz, 1H), 3.04 (ddd, J = 14.8, 7.0, 1.0 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2, 155.1, 154.1, 140.5, 132.2, 131.5, 130.2, 129.3, 127.6, 124.8, 122.8, 119.7, 114.5, 102.2, 84.6, 62.1, 53.0, 42.4, 38.5. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{19}NO_5Br_2Na^+$, 545.9522, found 545.9522.



4y

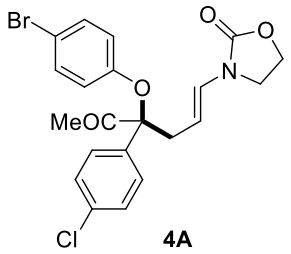
Methyl (*E*)-2-(4-bromophenoxy)-2-(naphthalen-2-yl)-5-(2-oxooxazolidin-3-yl)pent-4-enoate (4y): Colorless oil; 60% yield (119.0 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.89 – 7.83 (m, 3H), 7.62 (dd, J = 8.7, 1.8 Hz, 1H), 7.56 – 7.49 (m, 2H), 7.30 – 7.25 (m, 2H), 6.71 (d, J = 9.0 Hz, 2H), 6.63 (d, J = 14.3 Hz, 1H), 4.61 (dt, J = 14.5, 7.3 Hz, 1H), 4.37 (t, J = 8.3 Hz, 2H), 3.75 (s, 3H), 3.62 – 3.48 (m, 2H), 3.27 (qd, J = 14.8, 7.5 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.6, 155.2, 154.3, 135.6, 133.0, 132.9, 132.3, 132.1, 128.5, 128.5, 127.6, 127.4, 126.7, 126.5, 125.6, 123.6, 120.0, 116.6, 114.4, 102.8, 85.5, 62.1, 52.9, 42.4, 38.0. HRMS (ESI) $[M+Na]^+$ calcd for $C_{25}H_{22}NO_5BrNa^+$, 518.0574, found 518.0572.



4z

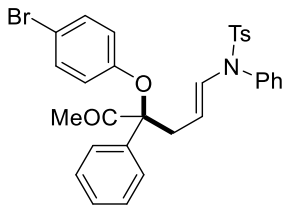
(*E*)-3-(4-(4-Bromophenoxy)-5-oxo-4-phenylhex-1-en-1-yl)oxazolidin-2-one (4z): Colorless oil; 55% yield (94.4 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 (d, J = 7.3 Hz, 2H), 7.39 (t, J = 7.1 Hz, 2H), 7.34 (d, J = 7.5 Hz, 3H), 6.72 (d, J = 8.0 Hz, 2H), 6.35 (d, J = 14.3 Hz, 1H), 4.33 (t, J = 7.7 Hz, 3H), 3.52 – 3.41 (m, 2H), 3.28 (dd, J = 15.1, 7.4 Hz, 1H), 3.07 (dd, J = 15.2, 6.8 Hz, 1H), 2.12 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ

207.9, 154.9, 153.9, 137.8, 132.5, 128.8, 128.3, 127.0, 125.7, 119.5, 114.5, 102.8, 100.0, 89.6, 62.0, 42.3, 33.5, 25.3. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{20}NO_4BrNa^+$, 452.0468, found 452.0470.



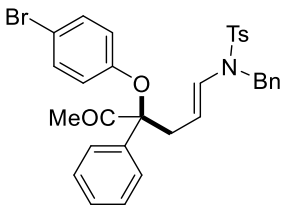
4A

(*E*)-3-(4-(4-bromophenoxy)-4-(4-chlorophenyl)-5-oxohex-1-en-1-yl)oxazolidin-2-one (4A): Colorless oil; 43% yield (79.6 mg); ^{1}H NMR (500 MHz, CDCl3) δ 7.45 (d, *J* = 8.2 Hz, 2H), 7.40 – 7.33 (m, 4H), 6.71 (d, *J* = 8.4 Hz, 2H), 6.37 (d, *J* = 14.2 Hz, 1H), 5.44 (d, *J* = 5.8 Hz, 1H), 4.27 (dt, *J* = 14.4, 7.3 Hz, 1H), 3.61 (t, *J* = 7.9 Hz, 1H), 3.47 (t, *J* = 7.4 Hz, 2H), 3.24 (dd, *J* = 14.9, 7.3 Hz, 1H), 3.02 (dd, *J* = 15.0, 6.9 Hz, 1H), 2.11 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 207.7, 153.7, 136.3, 134.4, 132.6, 129.9, 129.1, 127.2, 119.3, 114.7, 102.3, 97.1, 89.1, 87.9, 62.0, 42.3, 33.8, 25.3. HRMS (ESI) $[M+Na]^+$ calcd for $C_{21}H_{19}NO_4BrNa^+$, 486.0078, found 486.0078.



4B

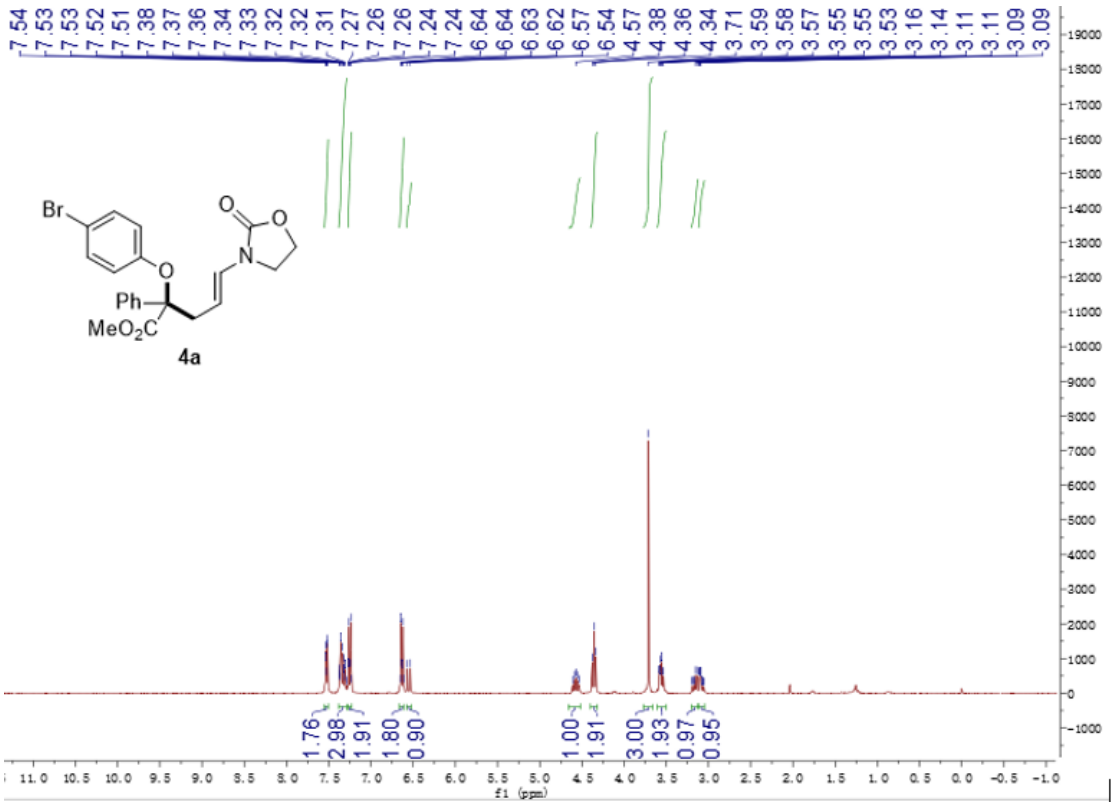
(*E*)-N-(4-(4-bromophenoxy)-5-oxo-4-phenylhex-1-en-1-yl)-4-methyl-N-phenylbenzenesulfonamide (4B): Colorless oil; 36% yield (84.8 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.34 (m, 8H), 7.33 – 7.29 (m, 2H), 7.25 (d, *J* = 8.8 Hz, 4H), 7.20 (d, *J* = 7.9 Hz, 2H), 7.16 (d, *J* = 7.7 Hz, 2H), 6.36 (s, 1H), 5.09 (s, 1H), 2.86 (d, *J* = 20.7 Hz, 1H), 2.72 (d, *J* = 20.6 Hz, 1H), 2.40 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.5, 144.0, 143.1, 138.6, 137.8, 137.0, 134.3, 131.4, 129.4, 129.3, 129.0, 128.6, 128.6, 128.5, 128.0, 127.9, 127.7, 124.8, 112.2, 64.0, 35.6, 21.6, 21.5. HRMS (ESI) $[M+H]^+$ calcd for $C_{31}H_{29}NO_4SBr^+$, 590.0995, found 590.0995.

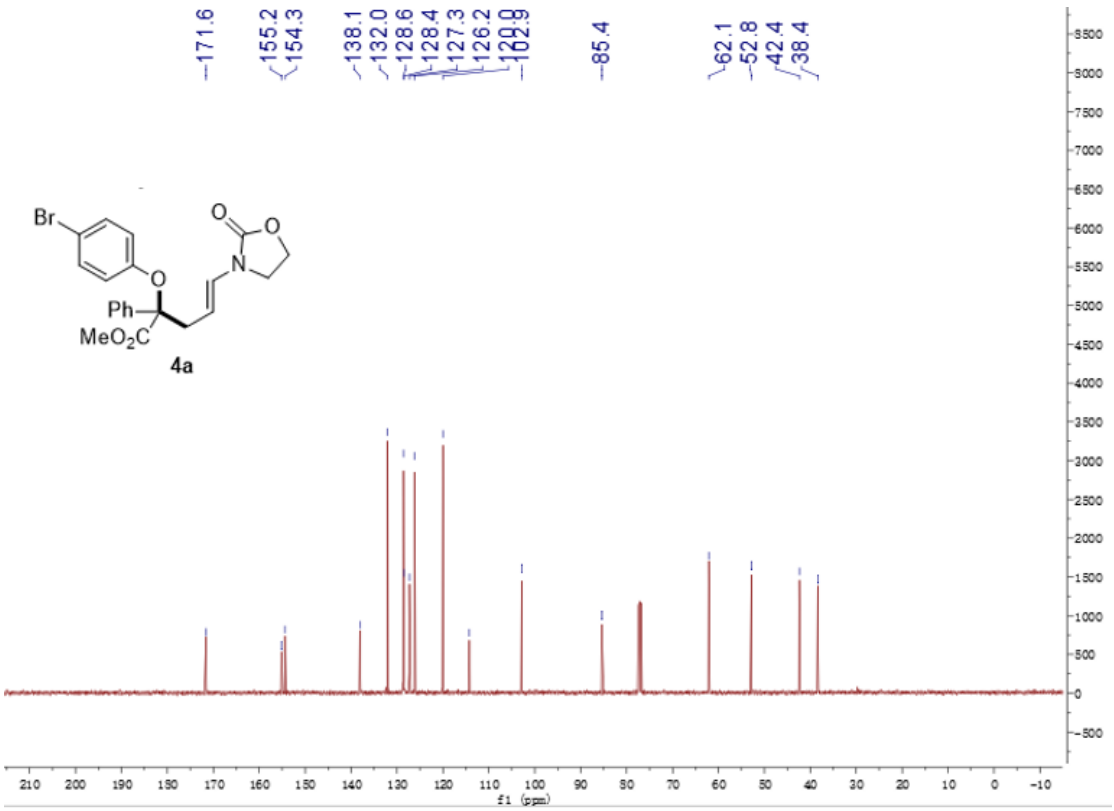


4C

(*E*)-N-benzyl-N-(4-(4-bromophenoxy)-5-oxo-4-phenylhex-1-en-1-yl)-4-methylbenzenesulfonamide (4C): Colorless oil; 43% yield (104.6 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.1 Hz, 2H), 7.52 (d, *J* = 8.1 Hz, 2H), 7.22 – 7.13 (m, 12H), 7.05 (s, 2H), 6.20 (s, 1H), 4.70 (d, *J* = 16.3 Hz, 1H), 4.45 (d, *J* = 15.7 Hz, 2H), 2.89 (s, 2H), 2.38 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.4, 143.7, 143.4, 137.9, 136.7, 136.5, 136.3, 129.6, 129.2, 128.3, 128.0, 127.7, 127.4, 127.4, 127.2, 123.5, 111.5, 62.5, 51.1, 49.1, 35.7, 21.6, 21.5. HRMS (ESI) $[M+H]^+$ calcd for $C_{32}H_{31}NO_4SBr^+$, 604.1152, found 604.1152.

9. NMR Spectra for the Products

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154.3
138.1
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128.6
128.4
127.3
126.2
120.9
102.9
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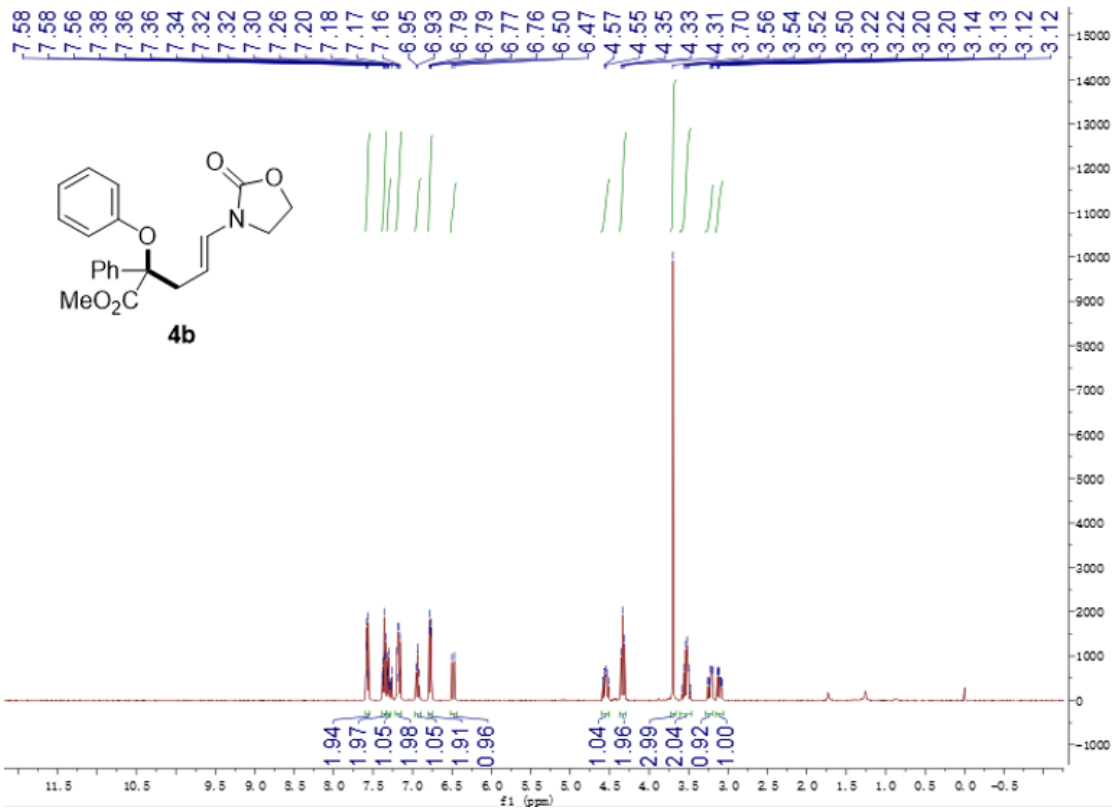
62.1
52.8
42.4
38.4
Br
O
O
N
O
Ph
MeO2C
4a
f1 (ppm)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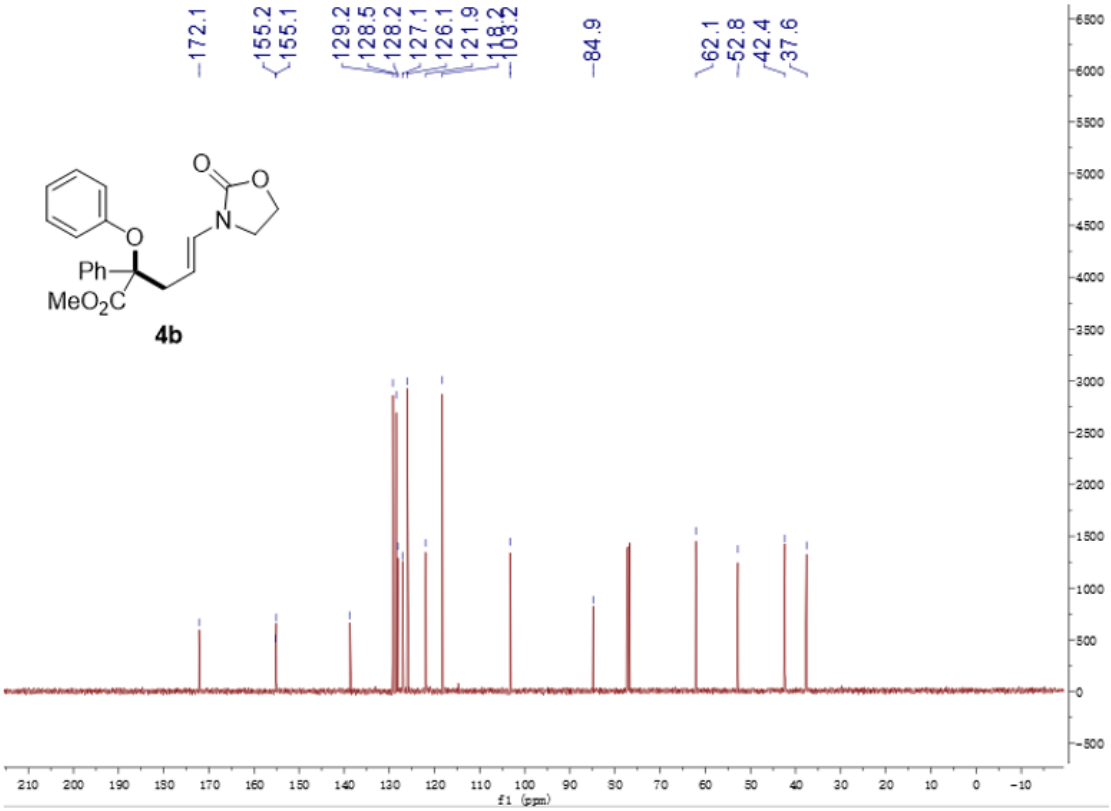
7.20
7.18
7.17
7.16
6.95
6.93
6.79
6.79
6.77
6.76
6.50
6.47
4.57
4.55
4.35
4.33
4.31
3.70
3.56
3.54
3.52
3.50
3.22
3.22
3.20
3.20
3.14
3.13
3.12
3.12
O
O
N
O
Ph
MeO2C
4b
1.94
1.97
1.05
1.98
1.05
1.91
0.96
1.04
1.96
2.99
2.04
0.92
1.00
f1 (ppm)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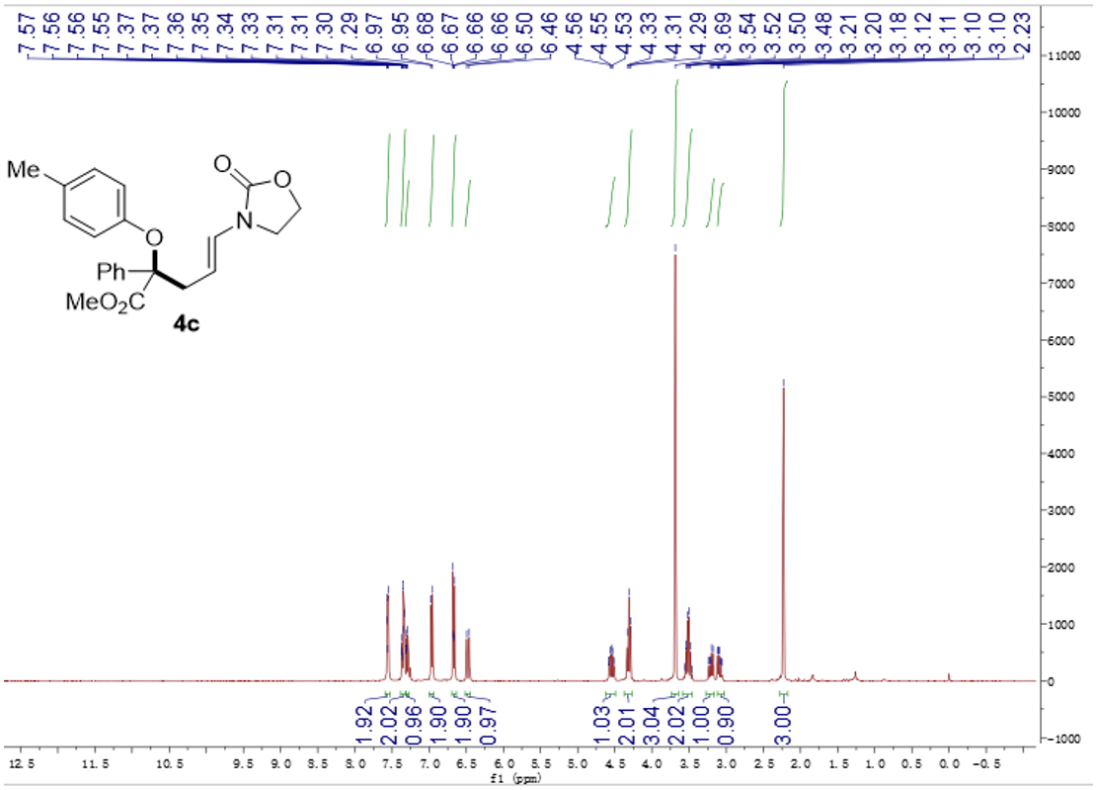
42.4
37.6
Ph
MeO2C
4b
f1 (ppm)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6.95
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6.66
6.66
6.50
6.46
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4.55
4.53
4.33
4.31
4.29
3.69
3.54
3.52
3.50
3.48
3.21
3.20
3.18
3.12
3.11
3.10
3.10
2.23
Me
Ph
MeO2C
4c
1.92
2.02
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0.97
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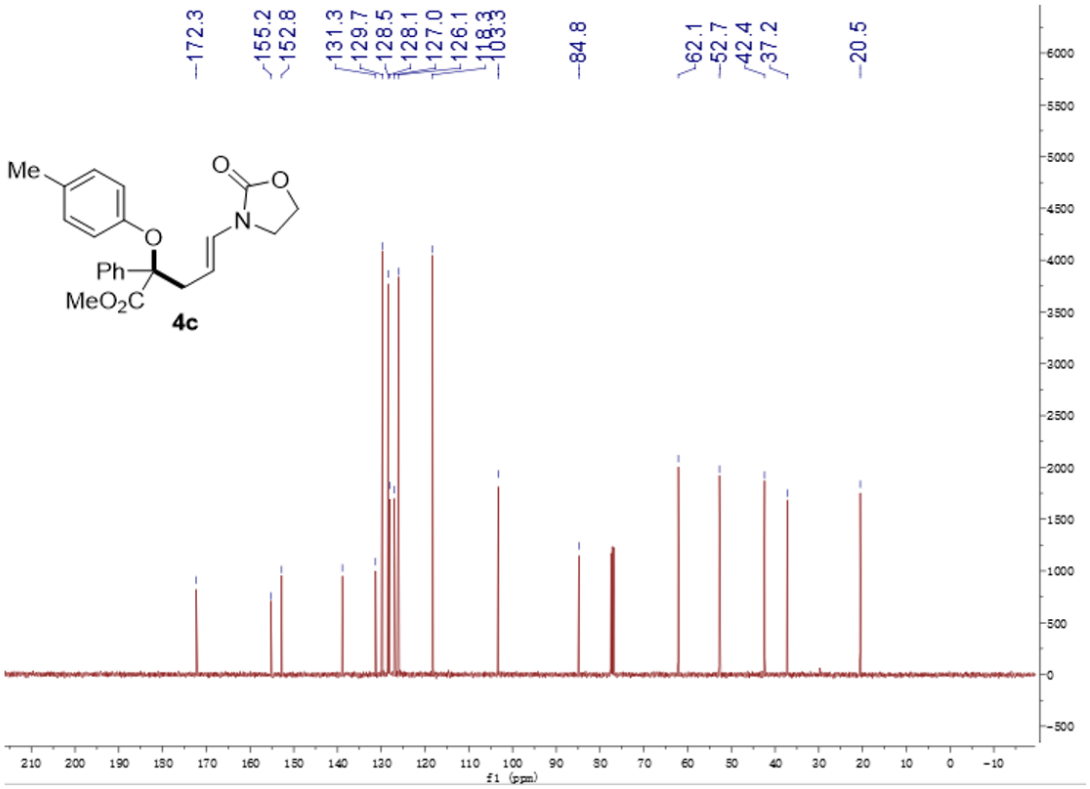
f1 (ppm)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118.3
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84.8
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N
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Ph
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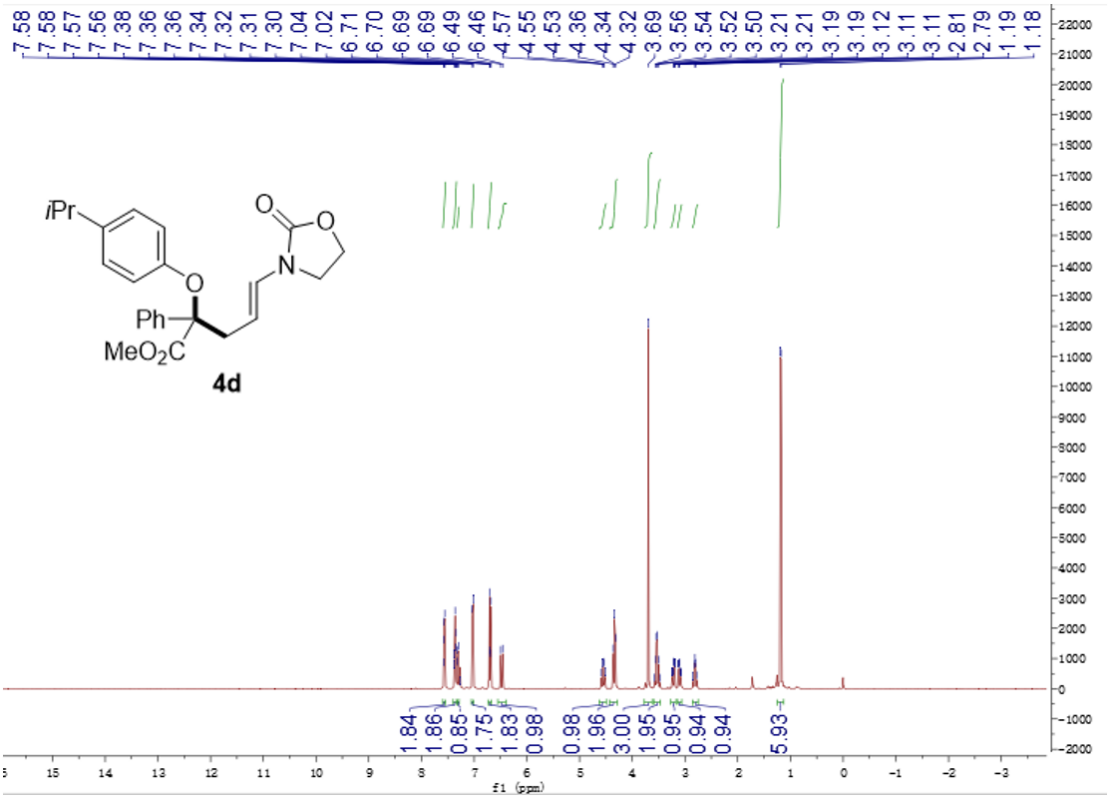
4c
f1 (ppm)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3.50
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3.21
3.19
3.19
3.12
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2.81
2.79
1.19
1.18
iPr
O
O
N
O
Ph
MeO2C
4d
1.84
1.86
0.85
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0.98
1.96
3.00
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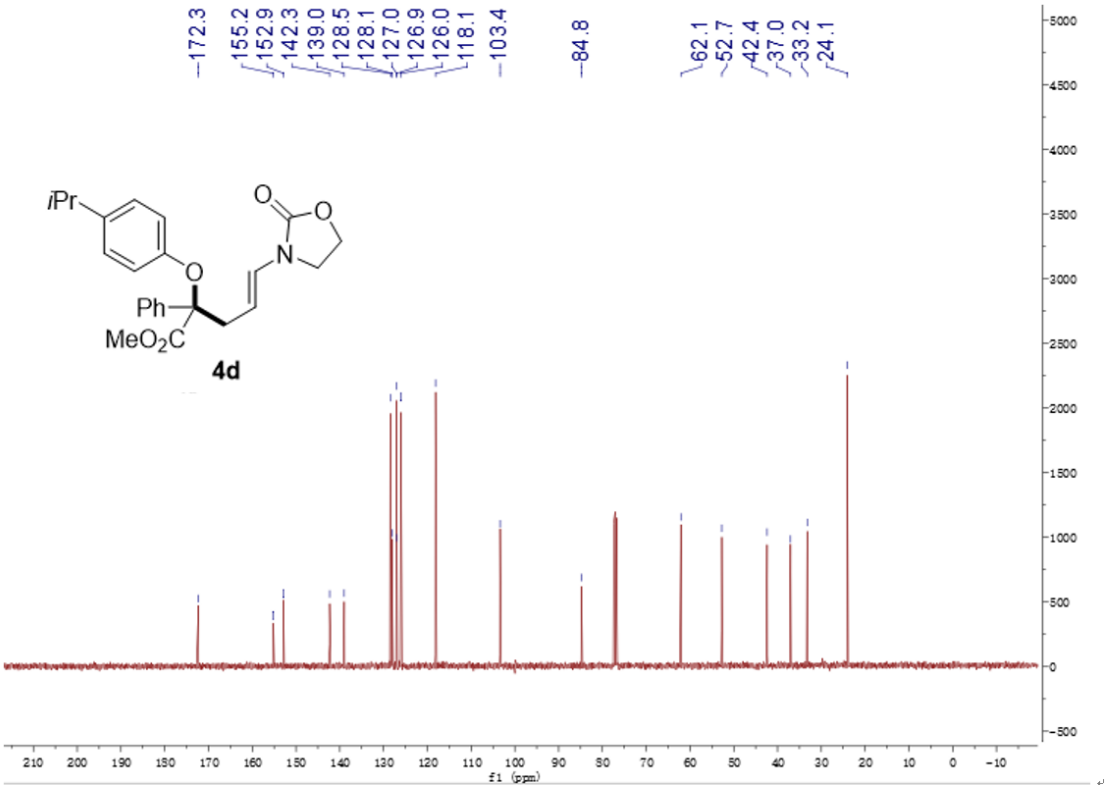
0.94
0.94
5.93
f1 (ppm)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84.8
62.1
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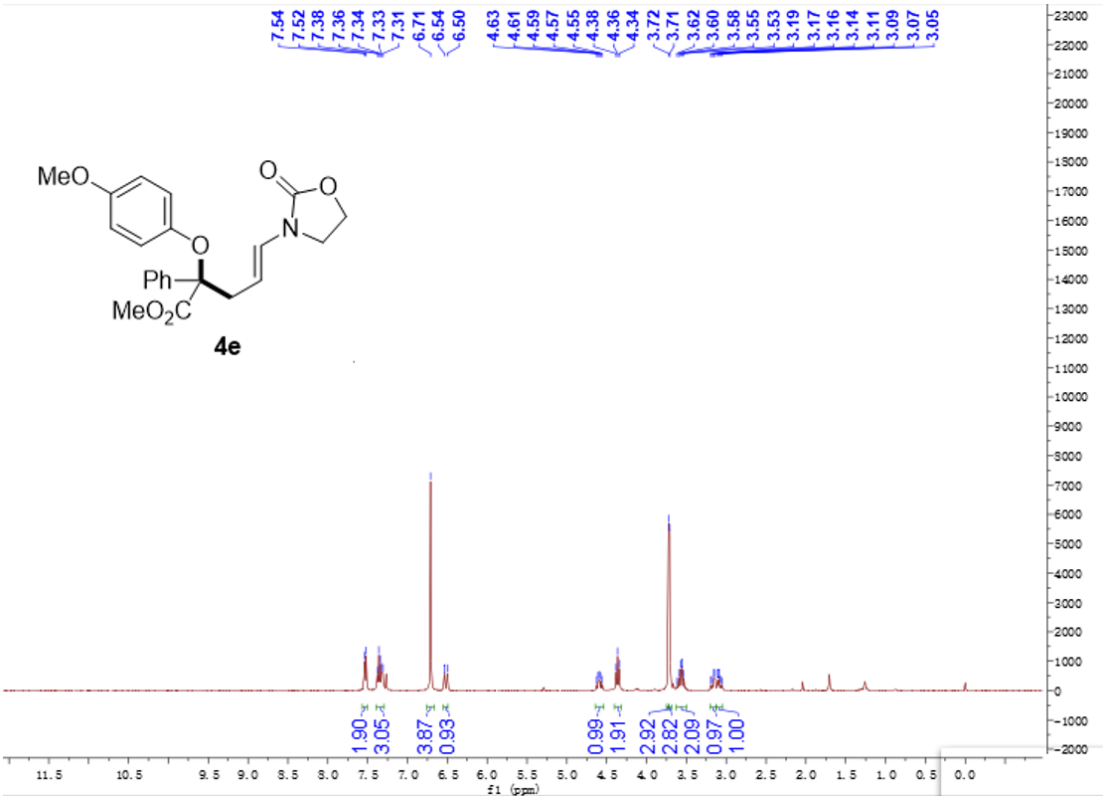
33.2
24.1
iPr
O
O
N
O
Ph
MeO2C
4d
f1 (ppm)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4.57
4.55
4.38
4.36
4.34
3.72
3.71
3.62
3.60
3.58
3.55
3.53
3.19
3.17
3.16
3.14
3.11
3.09
3.07
3.05
MeO
O
O
N
O
Ph
MeO2C
4e
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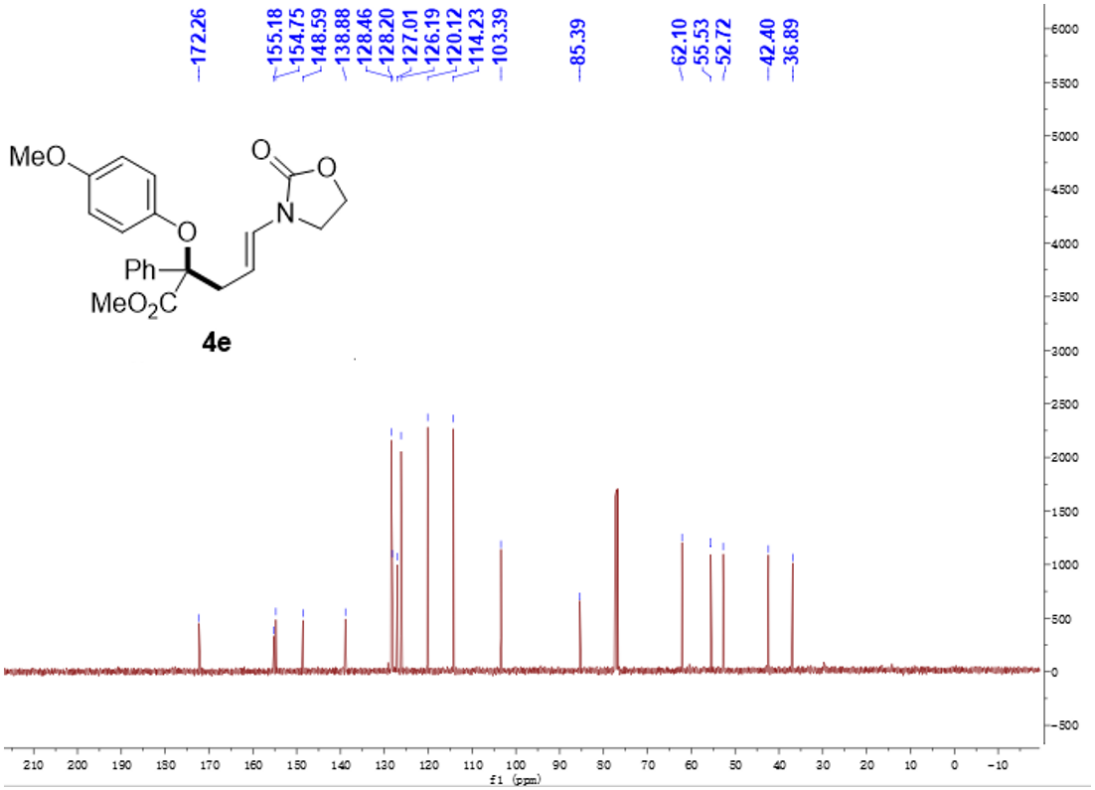
1.00
f1 (ppm)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114.23
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85.39
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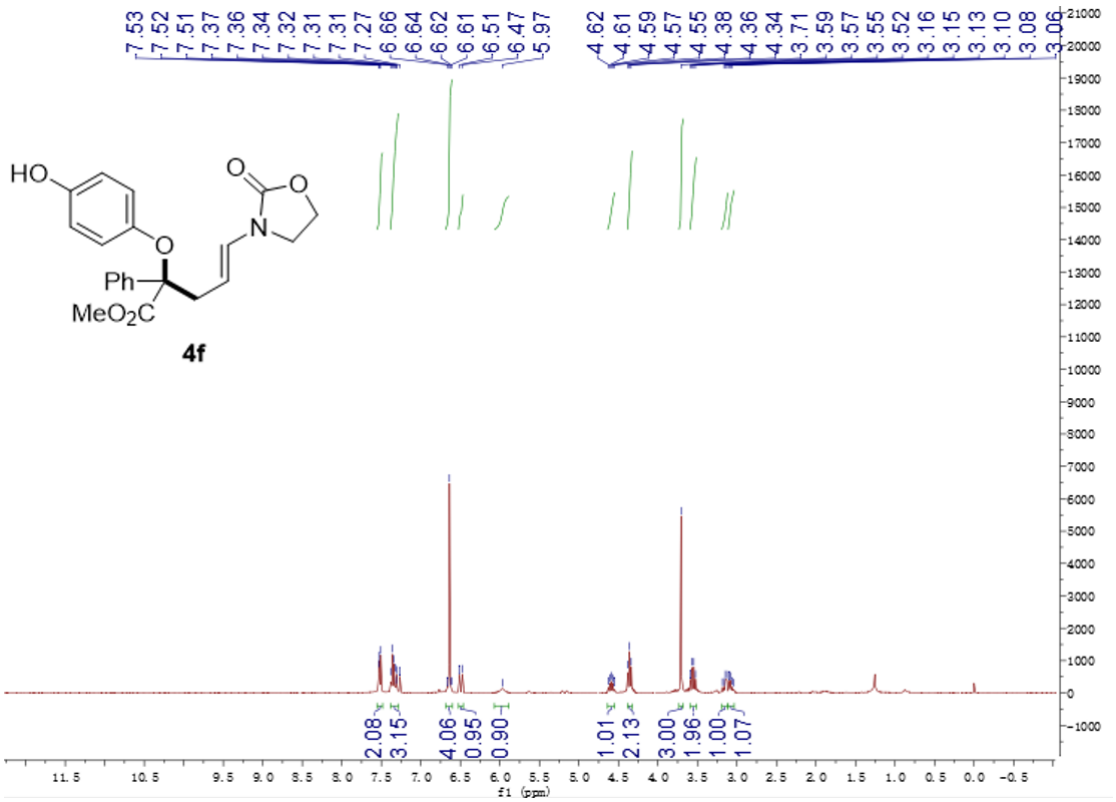
42.40
36.89
MeO
O
O
N
O
Ph
MeO2C
4e
f1 (ppm)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4.61
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4.57
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4.36
4.34
3.71
3.59
3.57
3.55
3.52
3.16
3.15
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3.10
3.08
3.06
HO
O
O
N
O
Ph
MeO2C
4f
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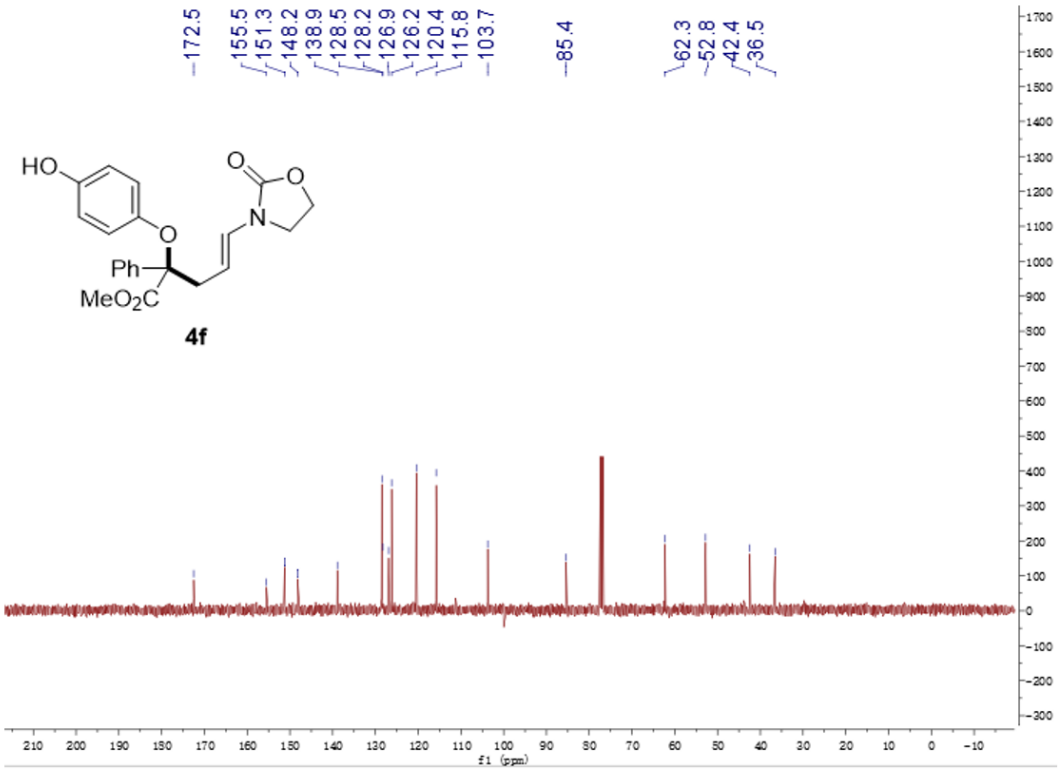
1.07
f1 (ppm)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126.9
126.2
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115.8
103.7
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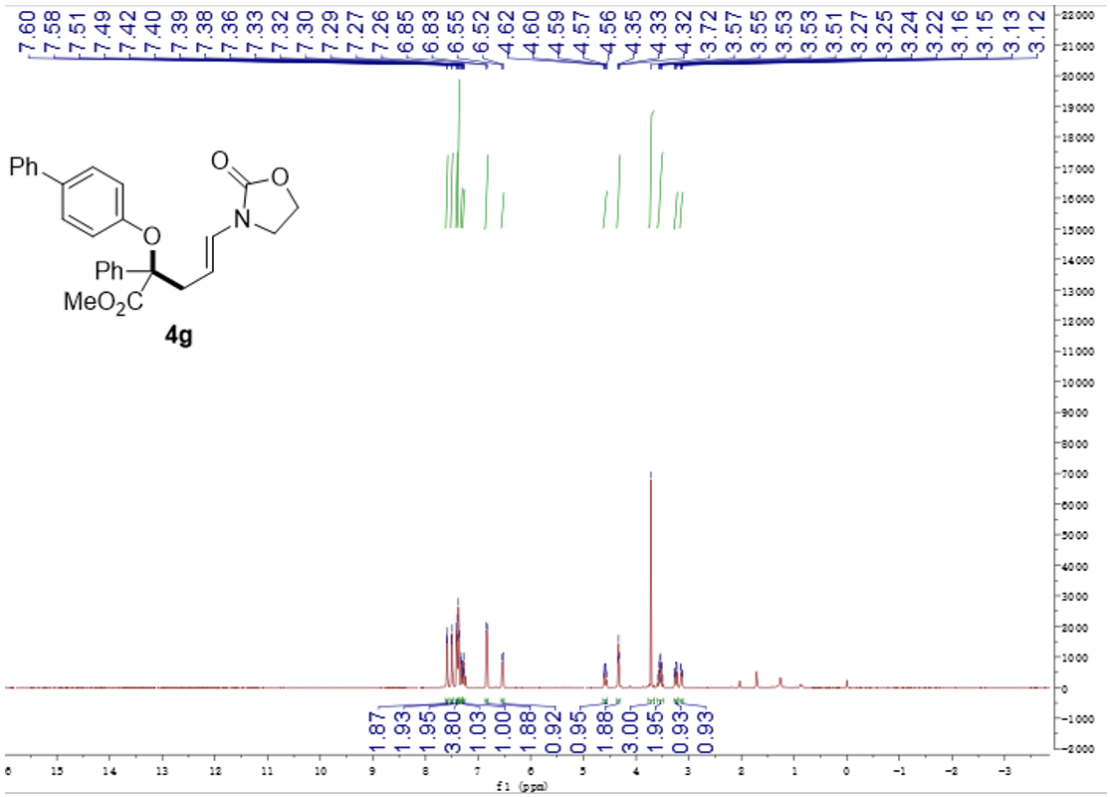
42.4
36.5
HO
O
O
N
O
Ph
MeO2C
4f
f1 (ppm)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7.27
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6.83
6.55
6.52
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4.56
4.35
4.33
4.32
3.72
3.57
3.55
3.53
3.53
3.51
3.27
3.25
3.24
3.22
3.16
3.15
3.13
3.12
Ph
O
O
N
O
Ph
MeO2C
4g
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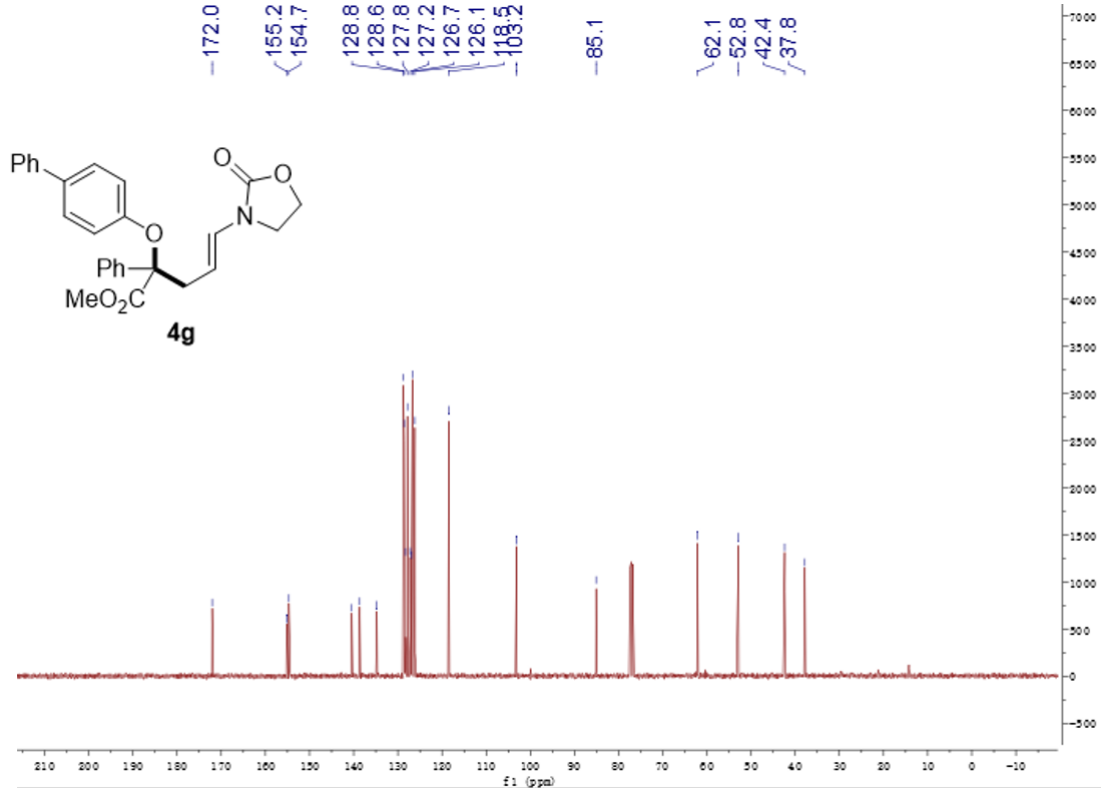
0.93
f1 (ppm)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127.8
127.2
126.7
126.1
118.5
103.2
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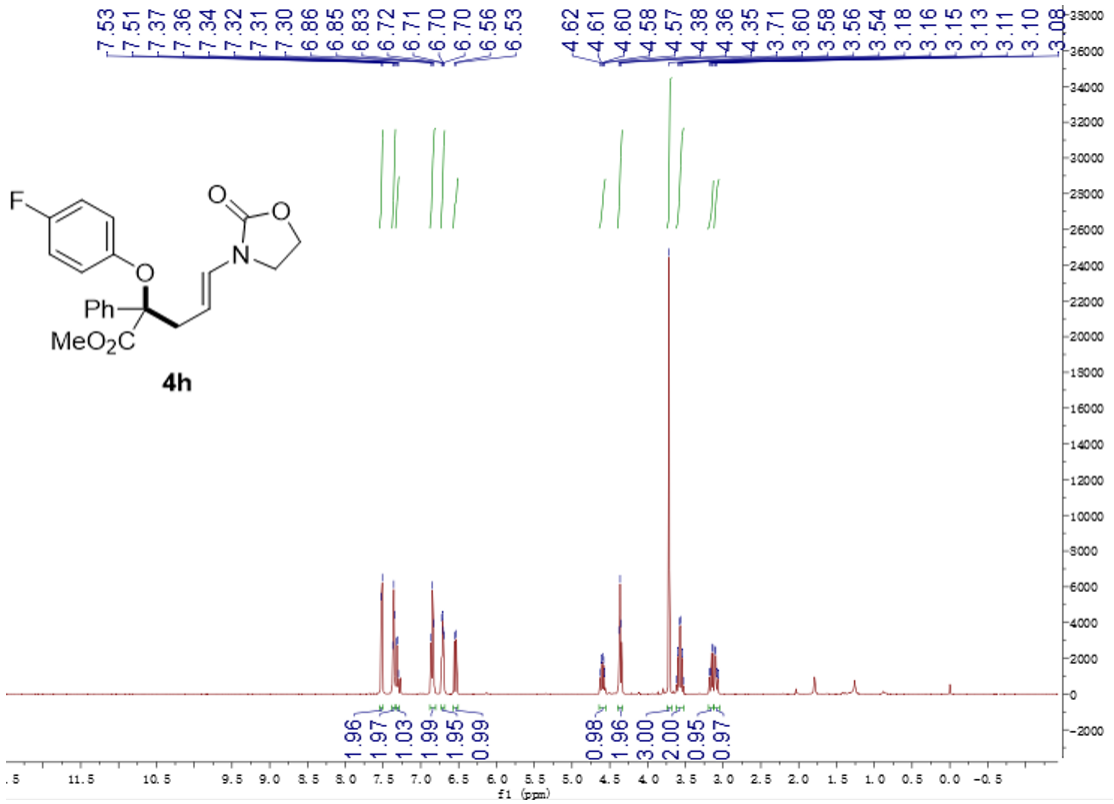
52.8
42.4
37.8
Ph
O
O
N
O
Ph
MeO2C
4g
f1 (ppm)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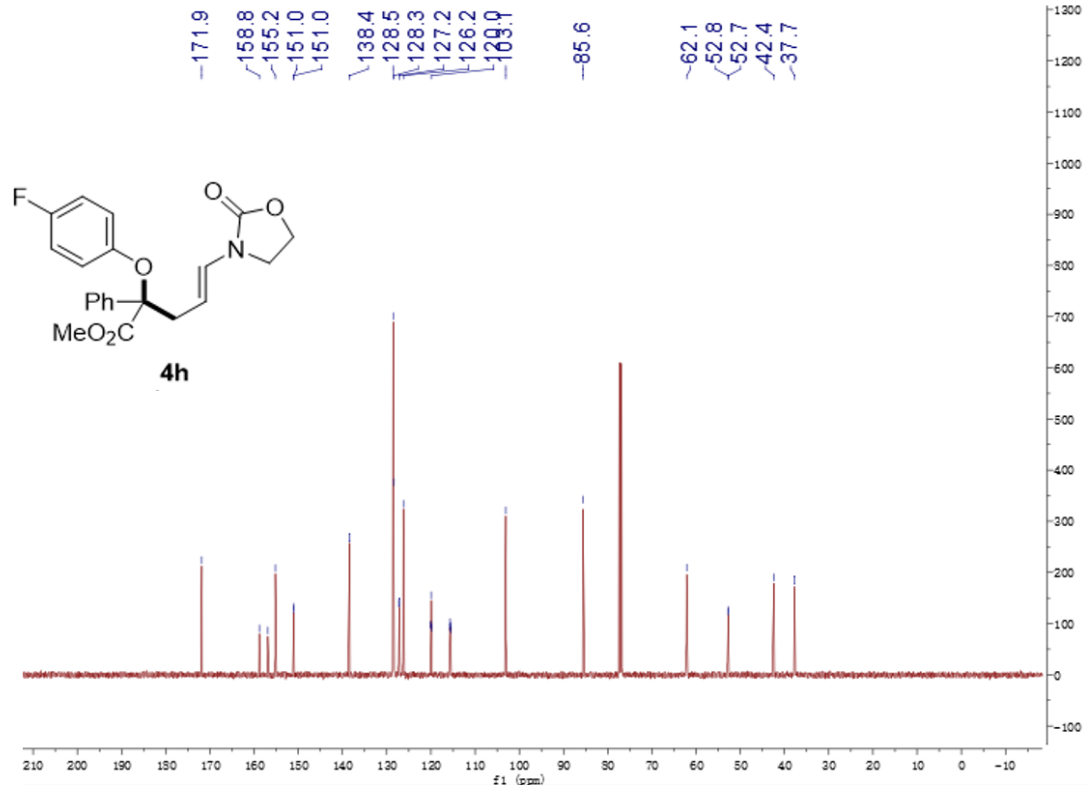
6.72
6.71
6.70
6.70
6.56
6.53
4.62
4.61
4.60
4.58
4.57
4.38
4.36
4.35
3.71
3.60
3.58
3.56
3.54
3.18
3.16
3.15
3.13
3.11
3.10
3.08
1.96
1.97
1.03
1.99
1.95
0.99
0.98
1.96
3.00
2.00
0.95
0.97
F
O
O
N
O
Ph
MeO2C
4h
f1 (ppm)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127.2
126.2
85.6
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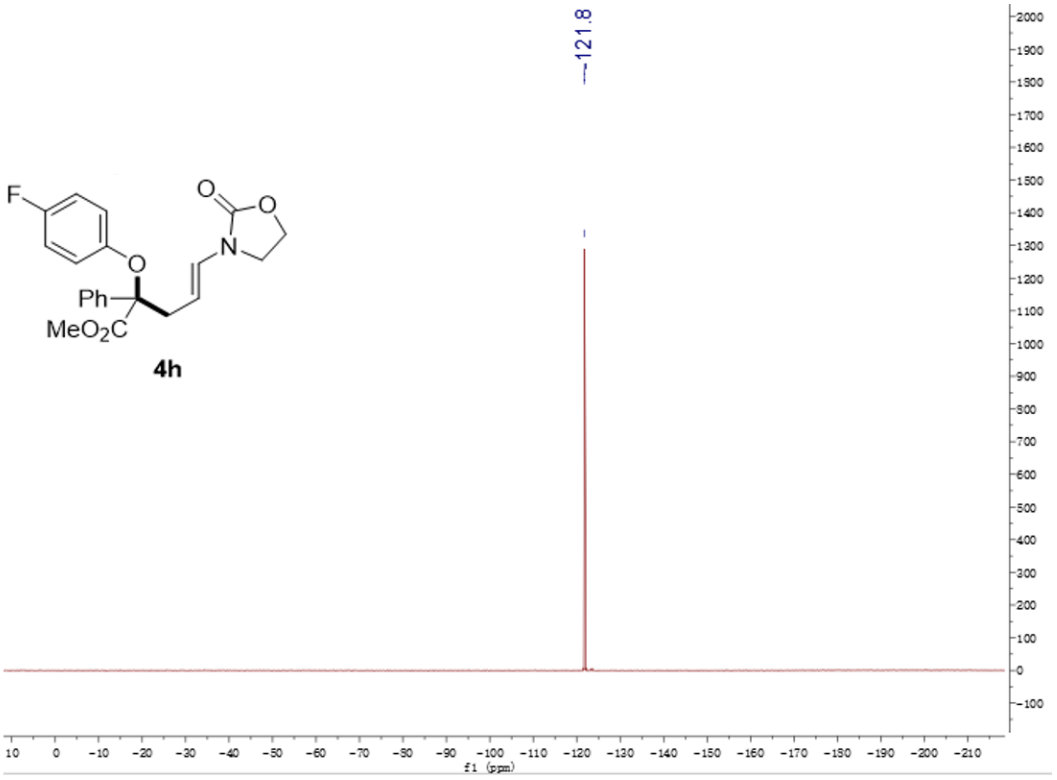
52.7
42.4
37.7
F
O
O
N
O
Ph
MeO2C
4h
f1 (ppm)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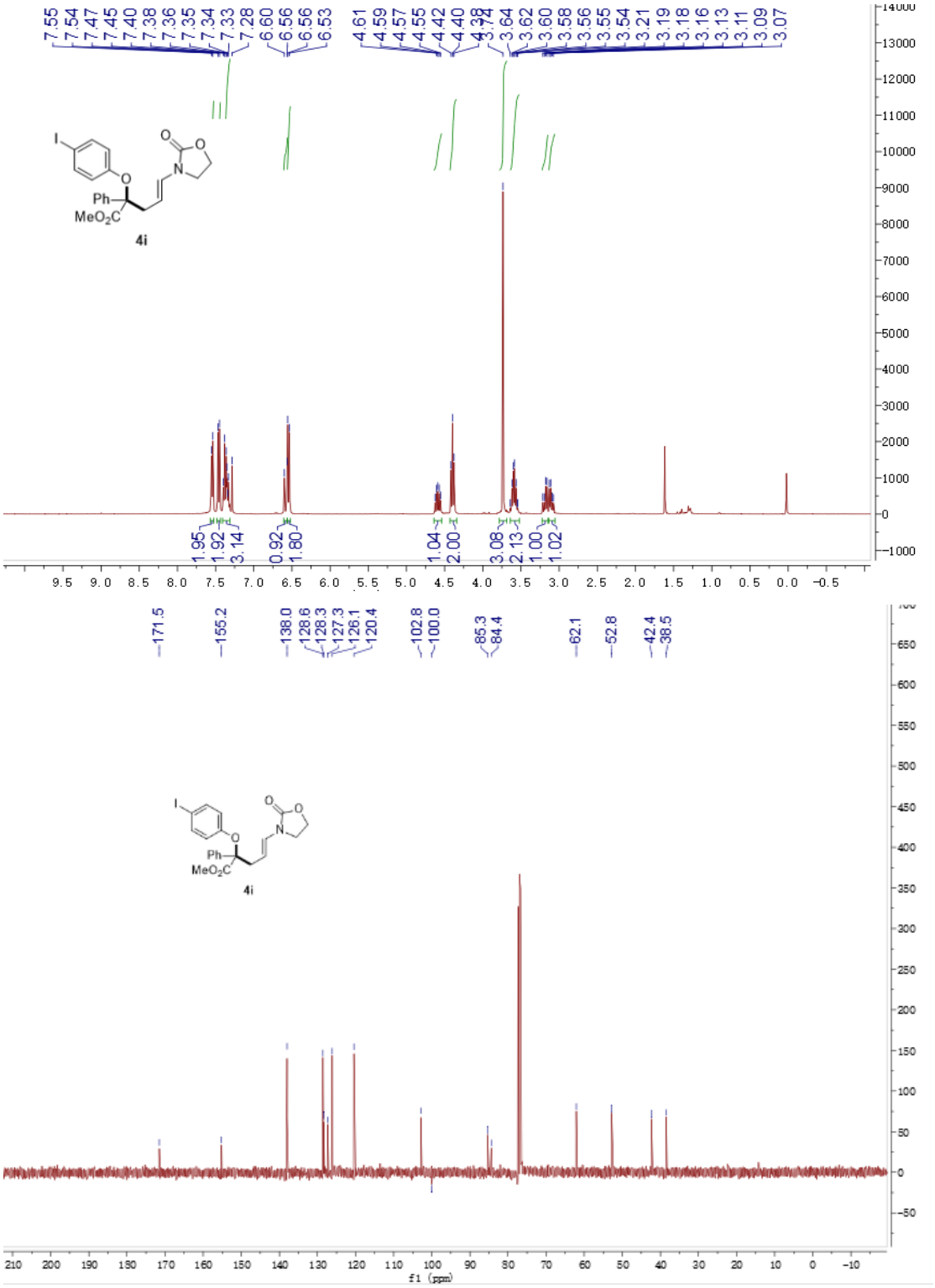
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3.09
3.07
I
O
O
N
O
Ph
MeO2C
4i
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1.04
2.00
3.08
2.13
1.00
1.02
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128.3
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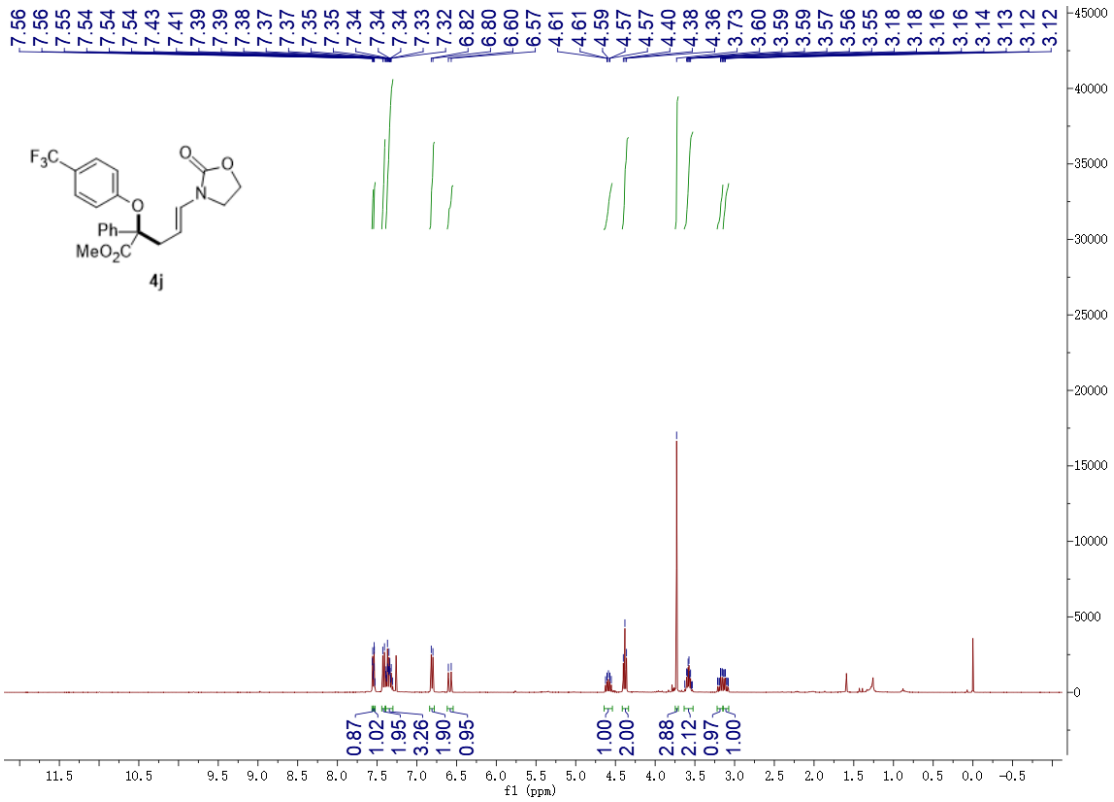
52.8
42.4
38.5
f1 (ppm)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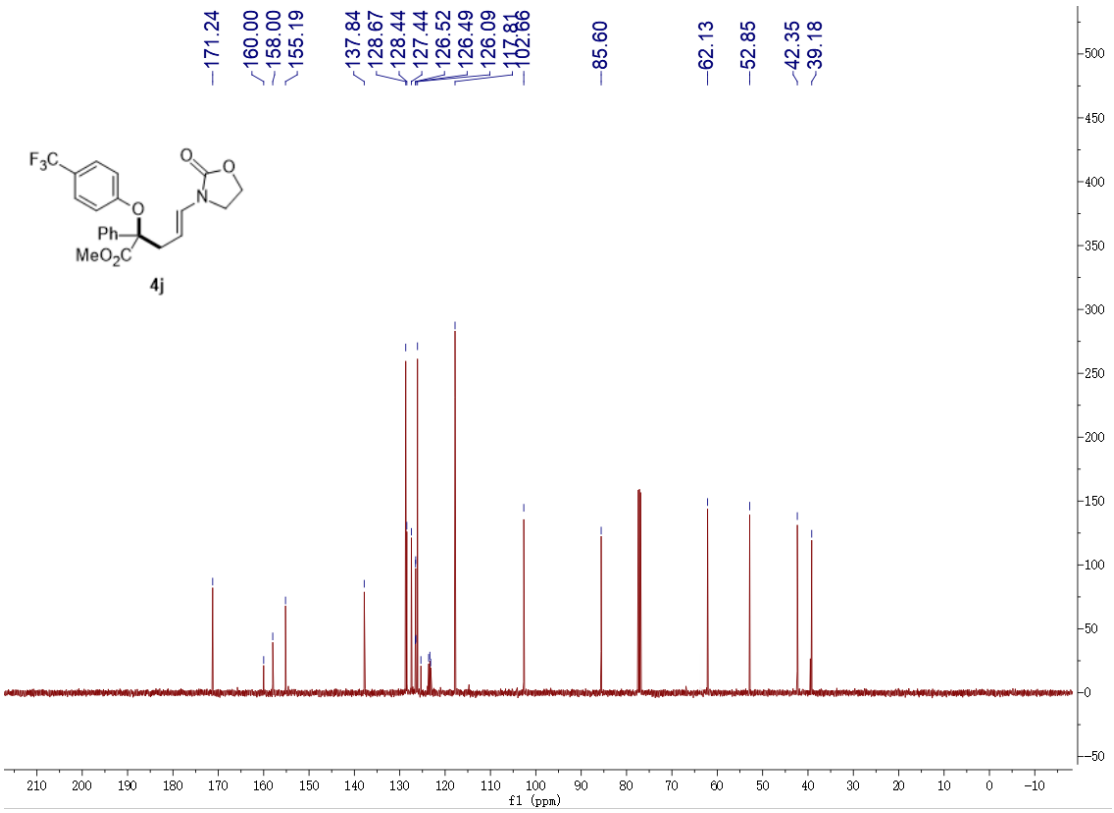
F3C
O
O
N
O
Ph
MeO2C
4j
0.87 1.02 1.95 3.26 1.90 0.95 1.00 2.00 2.88 2.12 0.97 1.00
f1 (ppm)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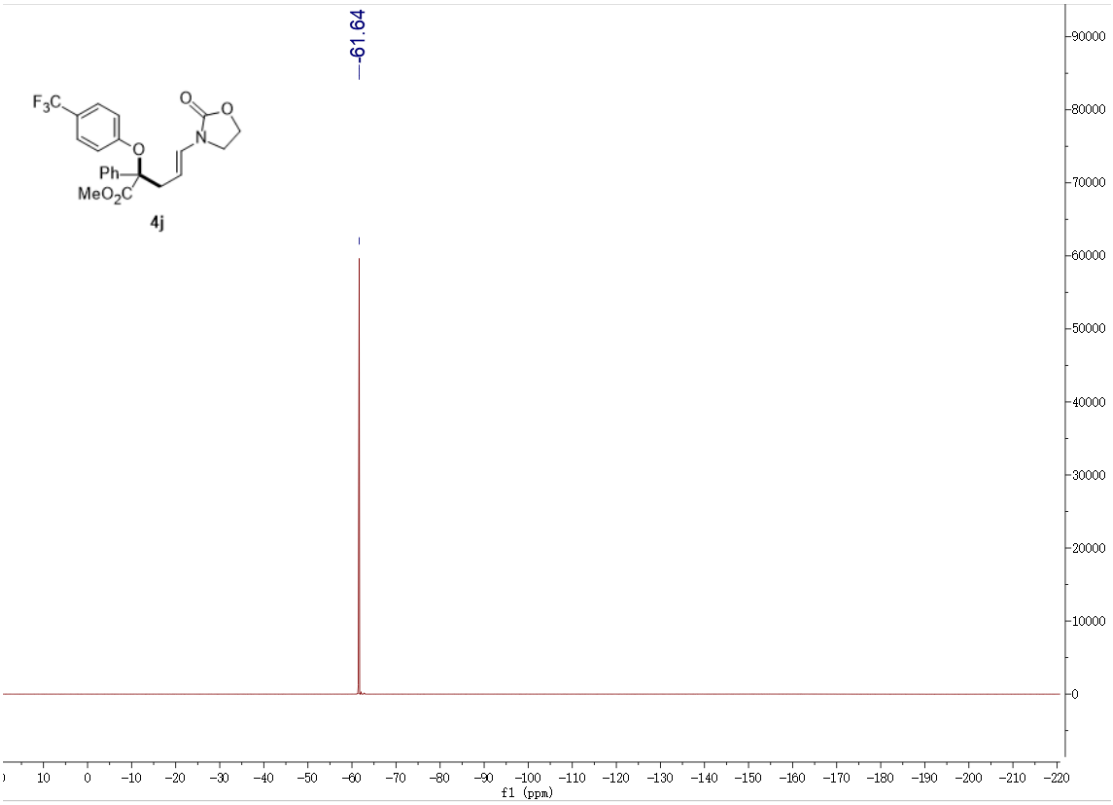
O
N
O
Ph
MeO2C
4j
f1 (ppm)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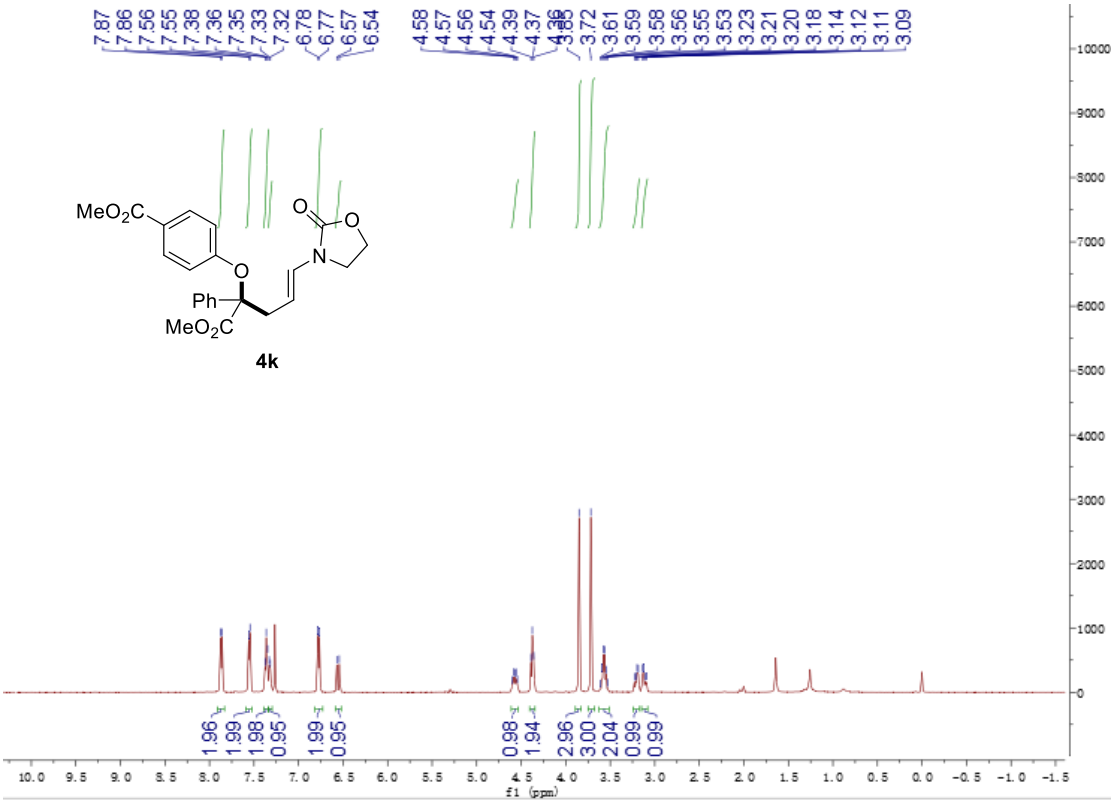
4j
f1 (ppm)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3.61
3.59
3.58
3.56
3.55
3.53
3.23
3.21
3.20
3.18
3.14
3.12
3.11
3.09
MeO2C
O
O
N
O
Ph
MeO2C
4k
1.96
1.99
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1.94
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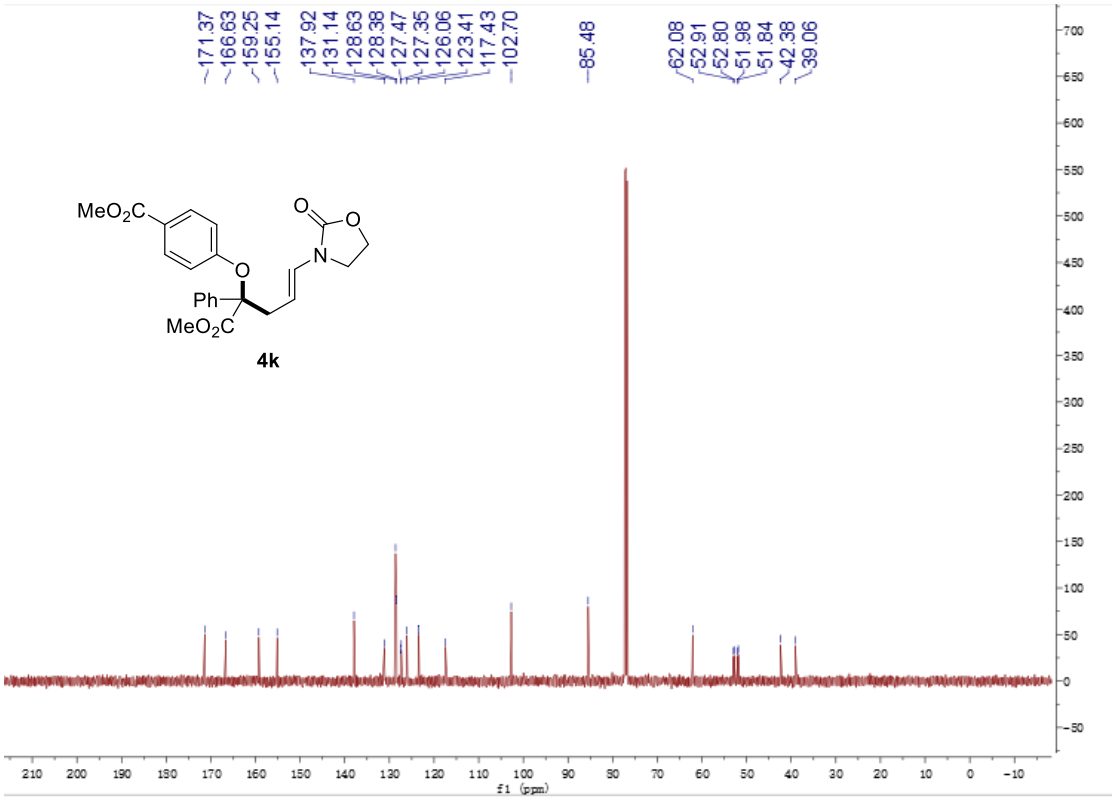
f1 (ppm)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102.70
85.48
62.08
52.91
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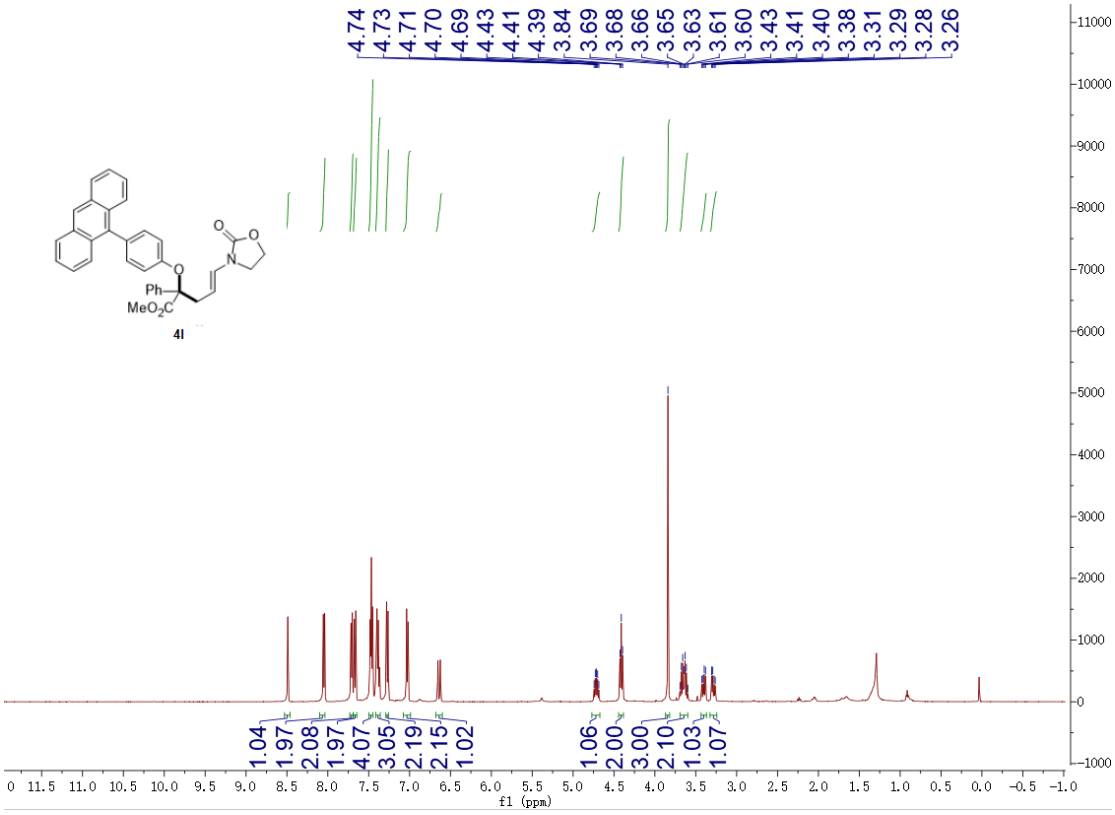
39.06
MeO2C
O
O
N
O
Ph
MeO2C
4k
f1 (ppm)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3.63
3.61
3.60
3.43
3.41
3.40
3.38
3.31
3.29
3.28
3.26
Ph
MeO2C
4l
1.04
1.97
2.08
1.97
4.07
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2.15
1.02
1.06
2.00
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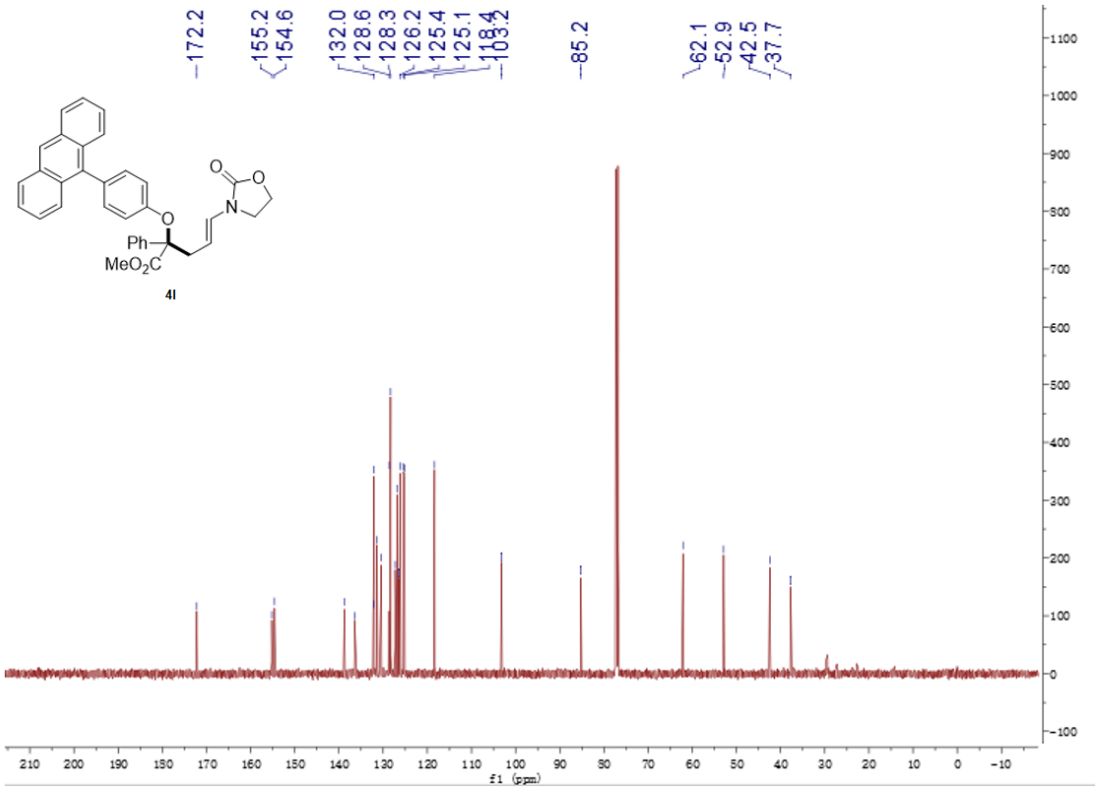
2.10
1.03
1.07
f1 (ppm)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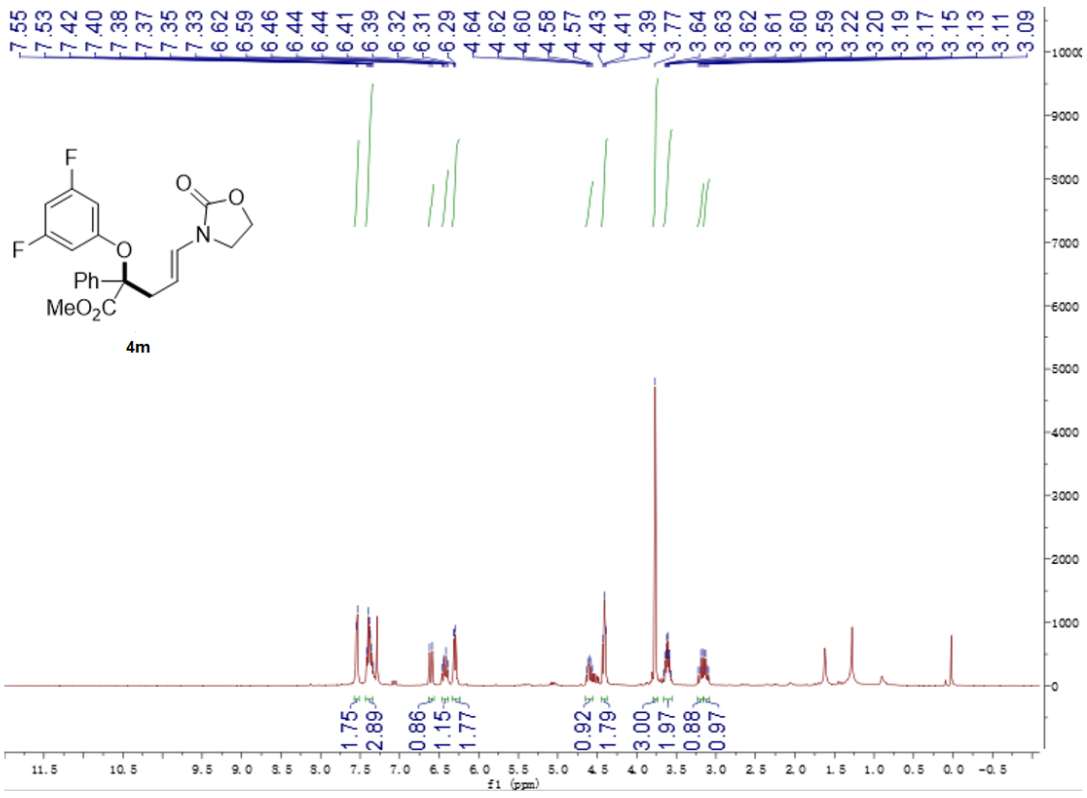
128.3
126.2
125.4
125.1
118.4
103.2
85.2
62.1
52.9
42.5
37.7
Ph
MeO2C
4l
f1 (ppm)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6.44
6.44
6.41
6.39
6.32
6.31
6.29
4.64
4.62
4.60
4.58
4.57
4.43
4.41
4.39
3.77
3.64
3.63
3.62
3.61
3.60
3.59
3.22
3.20
3.19
3.17
3.15
3.13
3.11
3.09
F
F
Ph
MeO2C
4m
1.75
2.89
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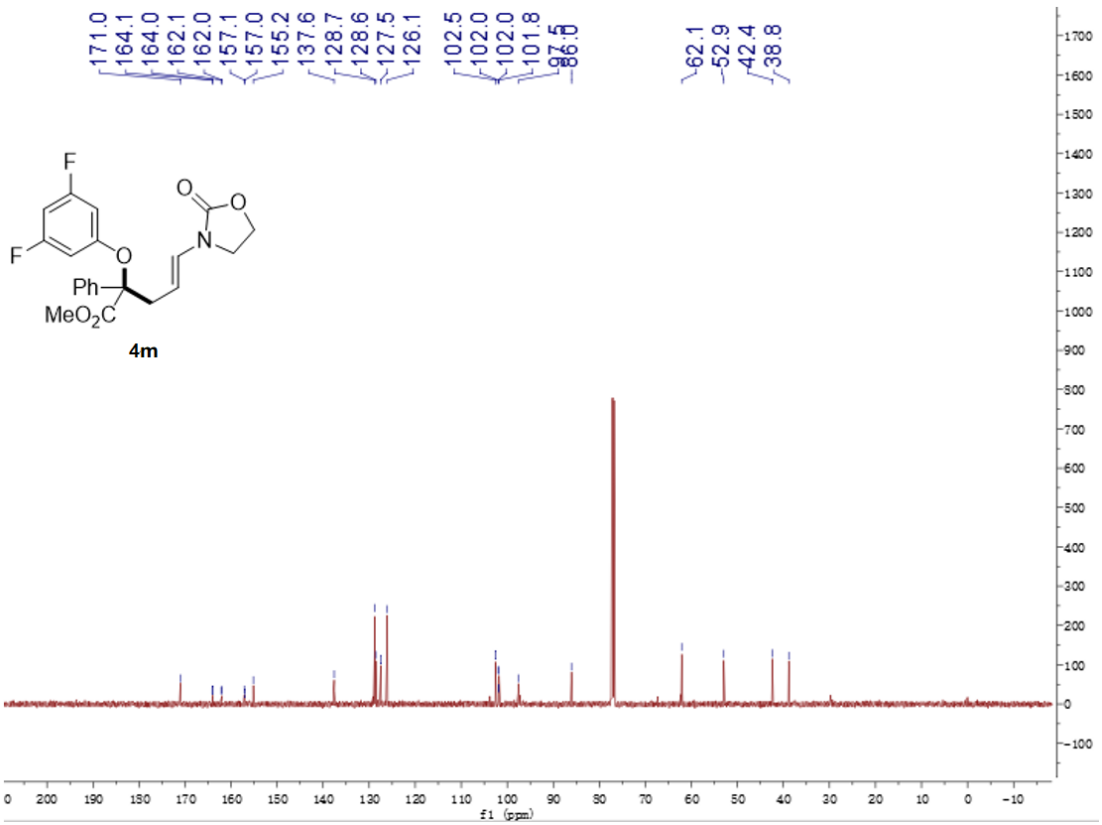
1.15
1.77
0.92
1.79
3.00
1.97
0.88
0.97
f1 (ppm)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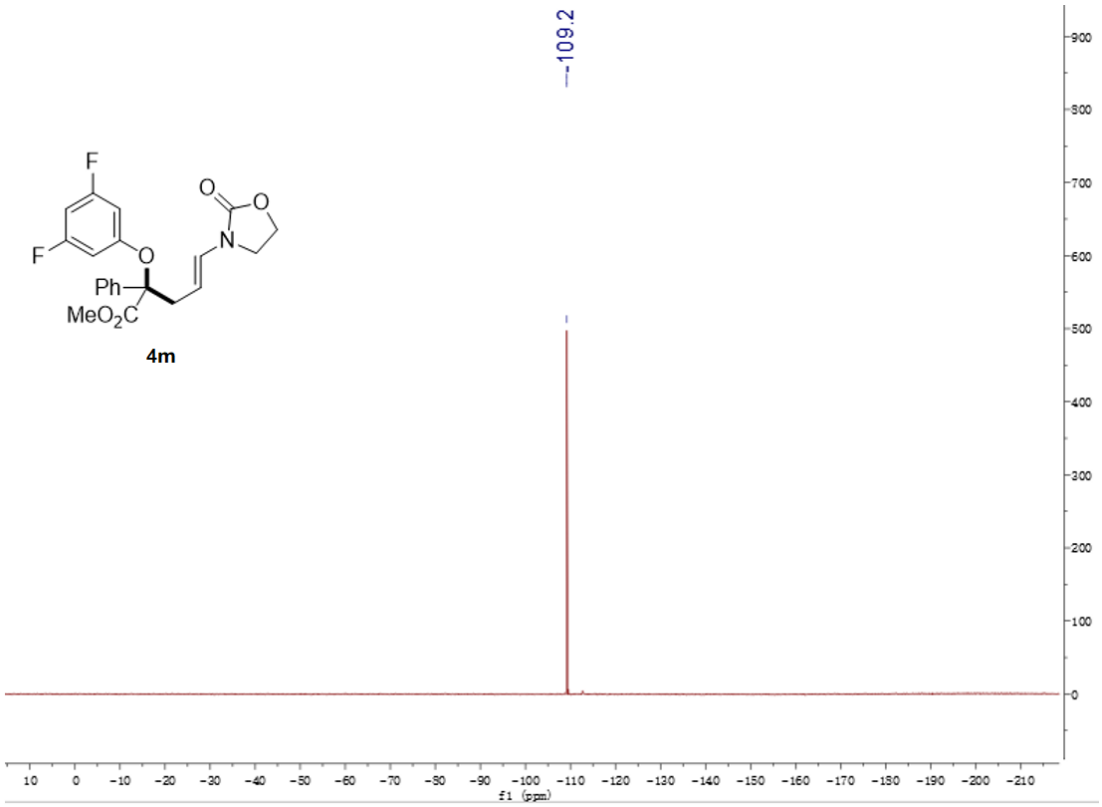
164.1
164.0
162.1
162.0
157.1
157.0
155.2
137.6
128.7
128.6
127.5
126.1
102.5
102.0
102.0
101.8
97.5
96.0
62.1
52.9
42.4
38.8
F
F
O
O
O
N
Ph
MeO2C
f1 (ppm)

4m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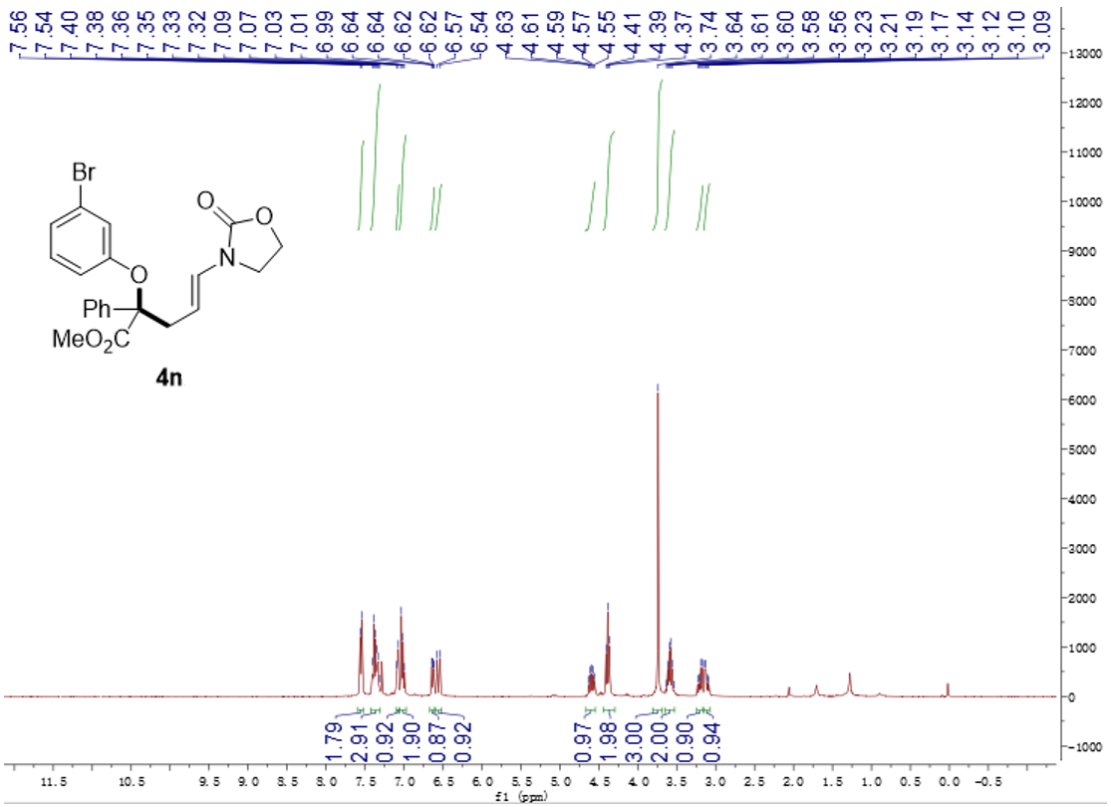
F
F
O
O
O
N
Ph
MeO2C
f1 (ppm)

4m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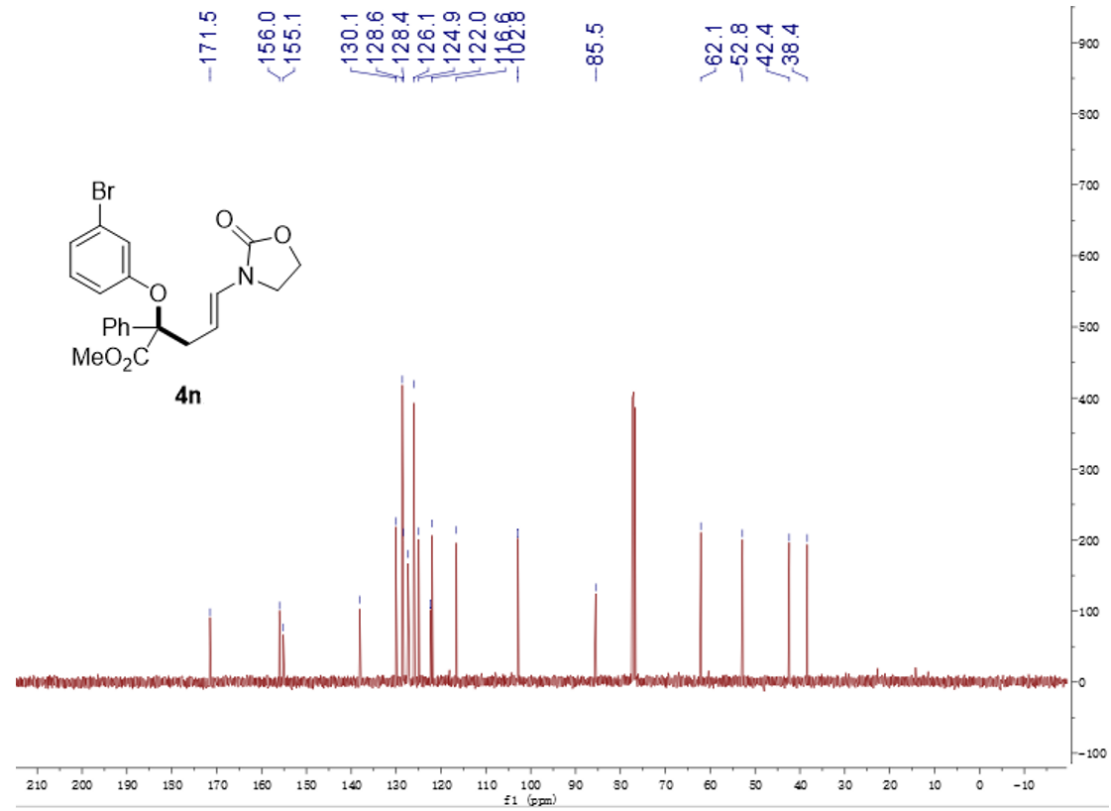
7.35
7.33
7.32
7.09
7.07
7.03
7.01
6.99
6.64
6.64
6.62
6.62
6.57
6.54
4.63
4.61
4.59
4.57
4.55
4.41
4.39
4.37
3.74
3.64
3.61
3.60
3.58
3.56
3.23
3.21
3.19
3.17
3.14
3.12
3.10
3.09
Br
O
O
N
O
Ph
MeO2C
4n
1.79
2.91
0.92
1.90
0.87
0.92
0.97
1.98
3.00
2.00
0.90
0.94
f1 (ppm)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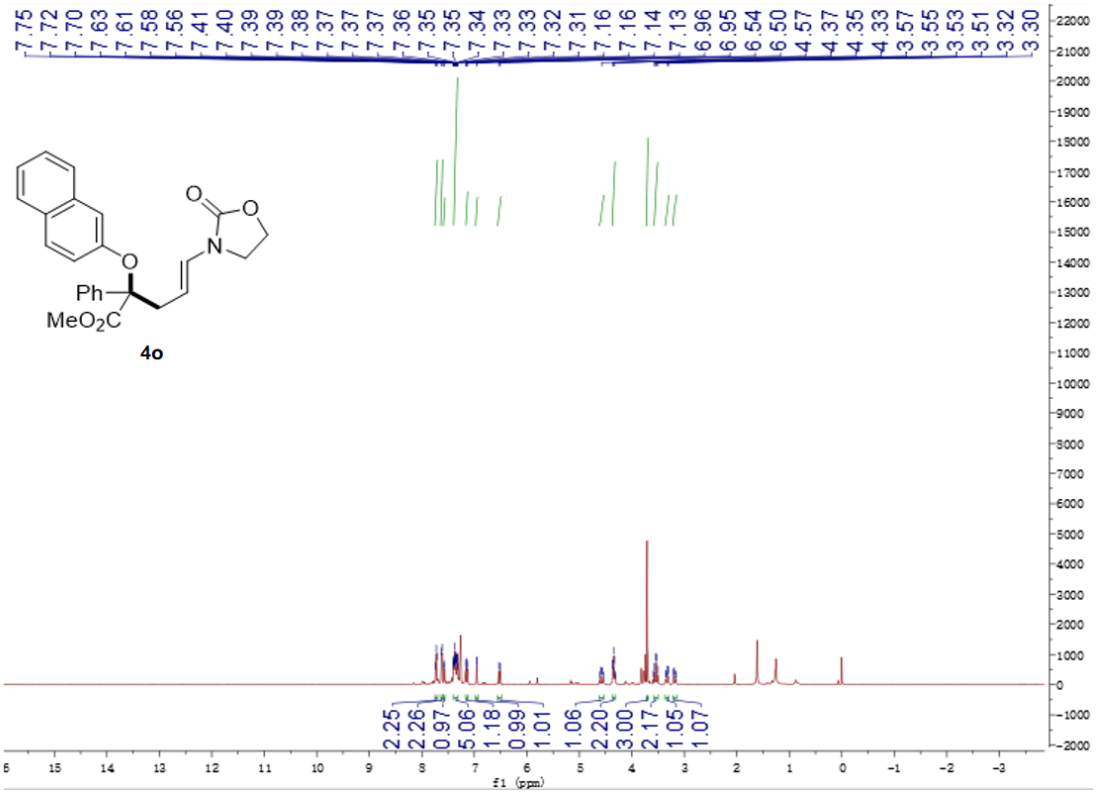
155.1
130.1
128.6
128.4
126.1
124.9
122.0
116.6
102.8
85.5
62.1
52.8
42.4
38.4
Br
O
O
N
O
Ph
MeO2C
4n
f1 (ppm)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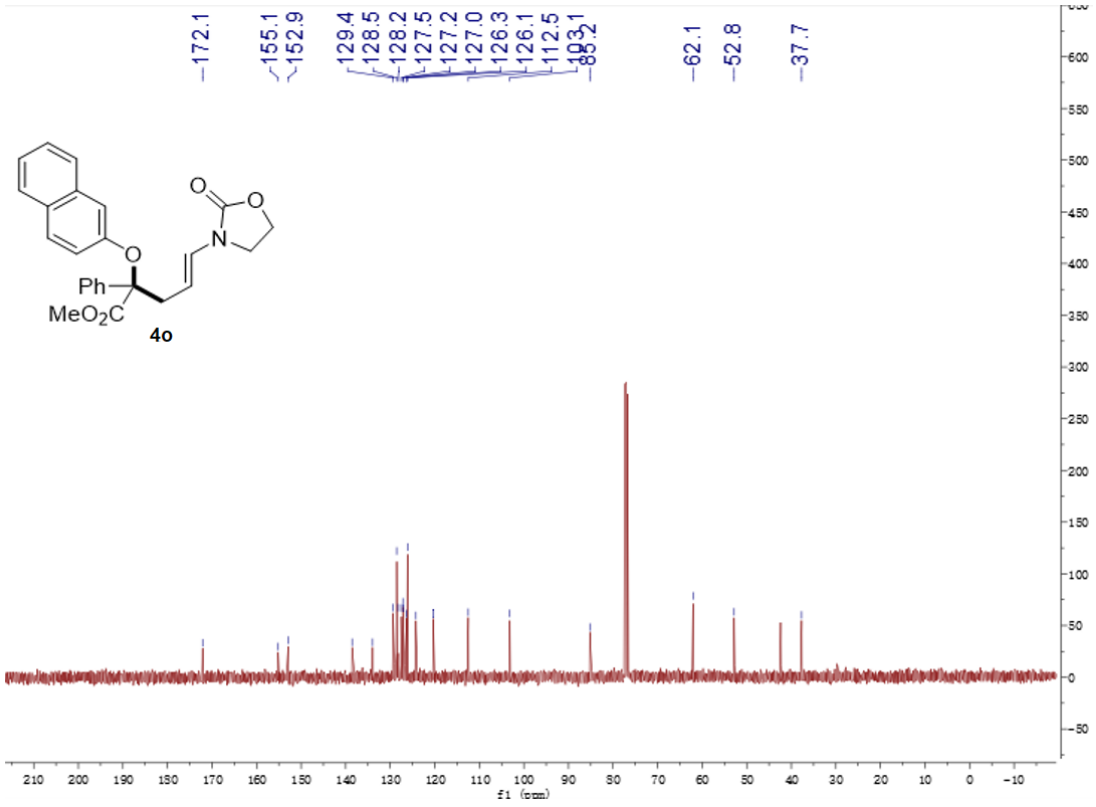
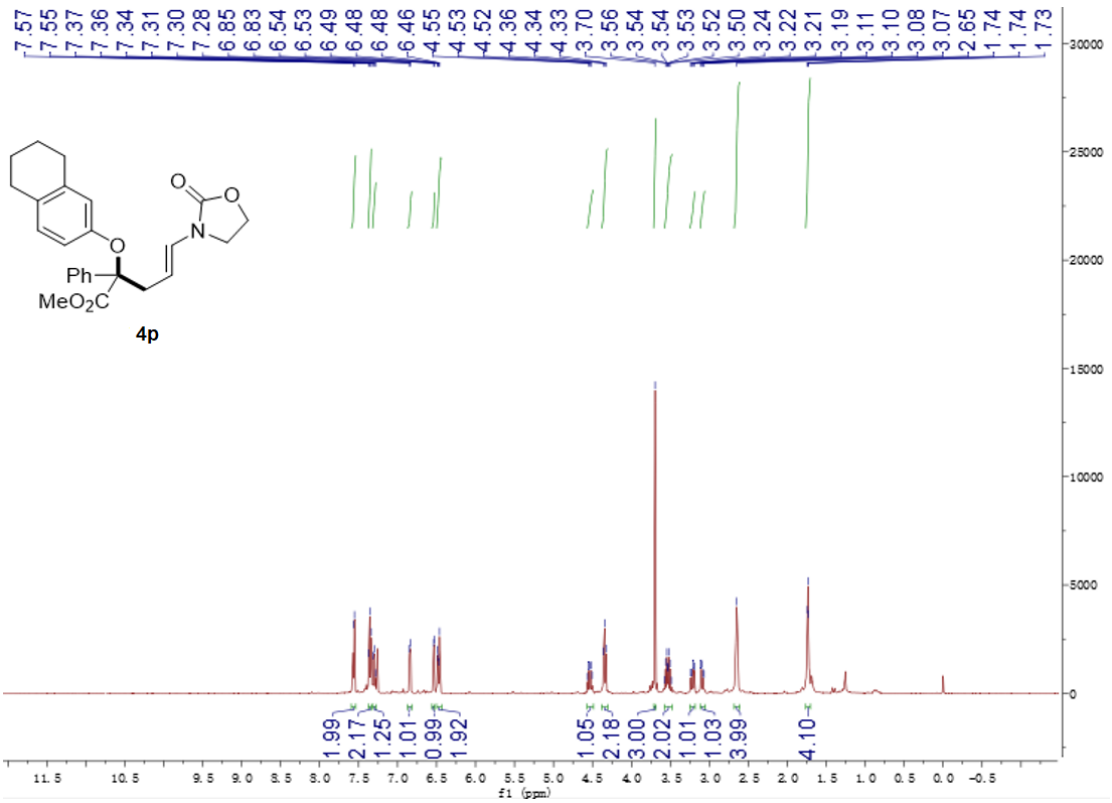
2.25 2.26 0.97 5.06 1.18 0.99 1.01 1.06 2.20 3.00 2.17 1.05 1.07
f1 (ppm)
Ph
MeO2C

4o


172.1 155.1 152.9 129.4 128.5 128.2 127.5 127.2 127.0 126.3 126.1 112.5 103.1 85.2 62.1 52.8 37.7
f1 (ppm)
Ph
MeO2C

4o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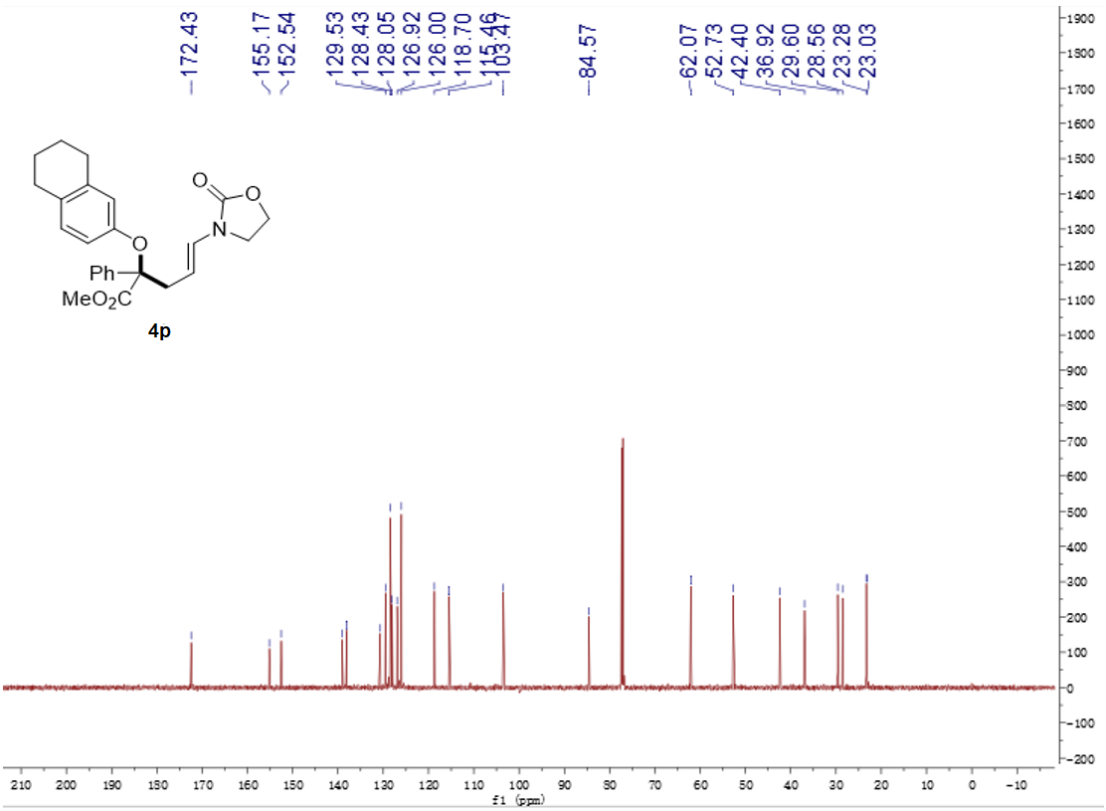
6.85
6.83
6.54
6.53
6.49
6.48
6.48
6.46
4.55
4.53
4.52
4.36
4.34
4.33
3.70
3.56
3.54
3.54
3.53
3.52
3.50
3.24
3.22
3.21
3.19
3.11
3.10
3.08
3.07
2.65
1.74
1.74
1.73
Ph
MeO2C
4p
1.99
2.17
1.25
1.01
0.99
1.92
1.05
2.18
3.00
2.02
1.01
1.03
3.99
4.10
f1 (ppm)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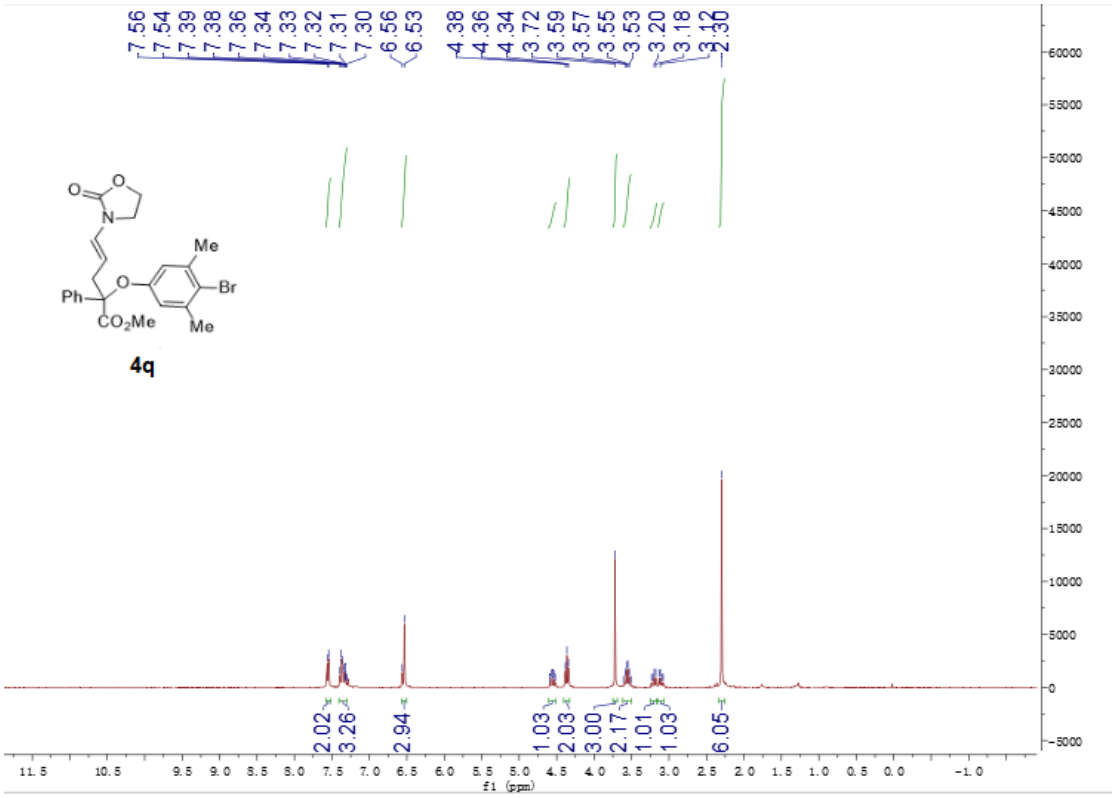
128.05
126.92
126.00
118.70
115.46
103.47
84.57
62.07
52.73
42.40
36.92
29.60
28.56
23.28
23.03
Ph
MeO2C
4p
f1 (ppm)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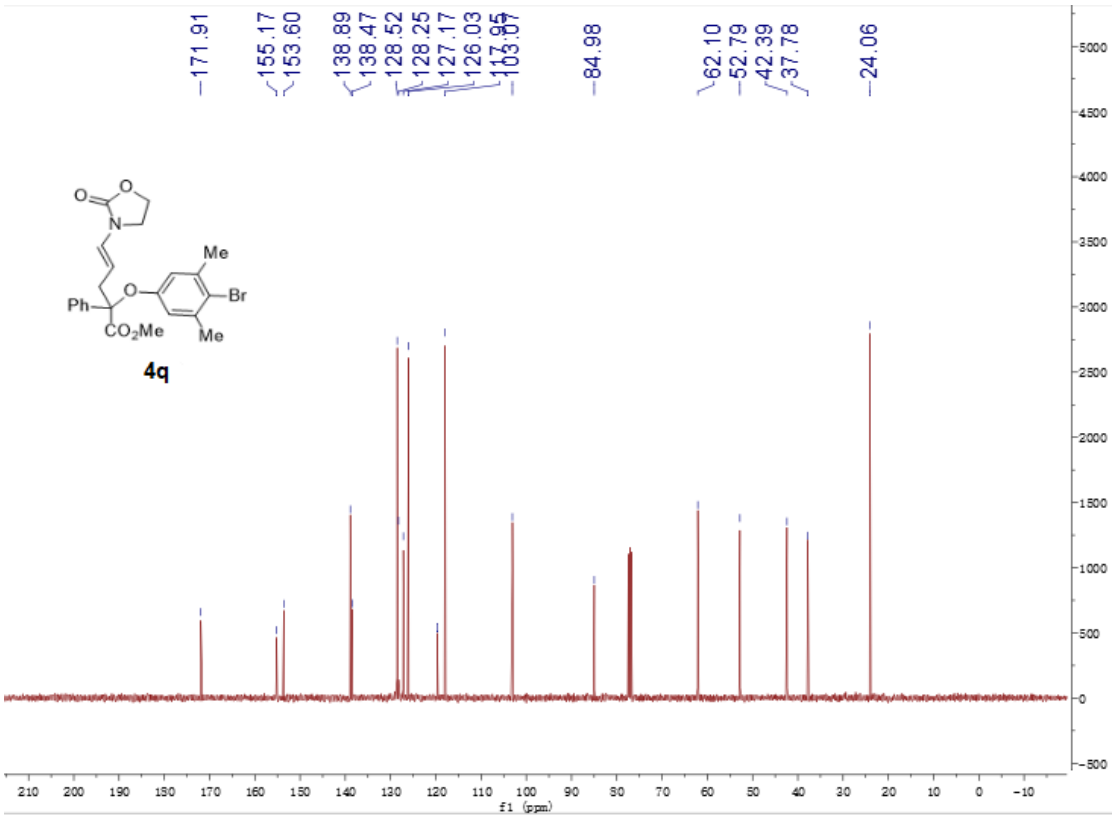
7.54
7.39
7.38
7.36
7.34
7.33
7.32
7.31
7.30
6.56
6.53
4.38
4.36
4.34
3.72
3.59
3.57
3.55
3.53
3.20
3.18
3.12
2.30
Me
Br
Ph
O
CO2Me
Me
4q
2.02
3.26
2.94
1.03
2.03
3.00
2.17
1.01
1.03
6.05
f1 (ppm)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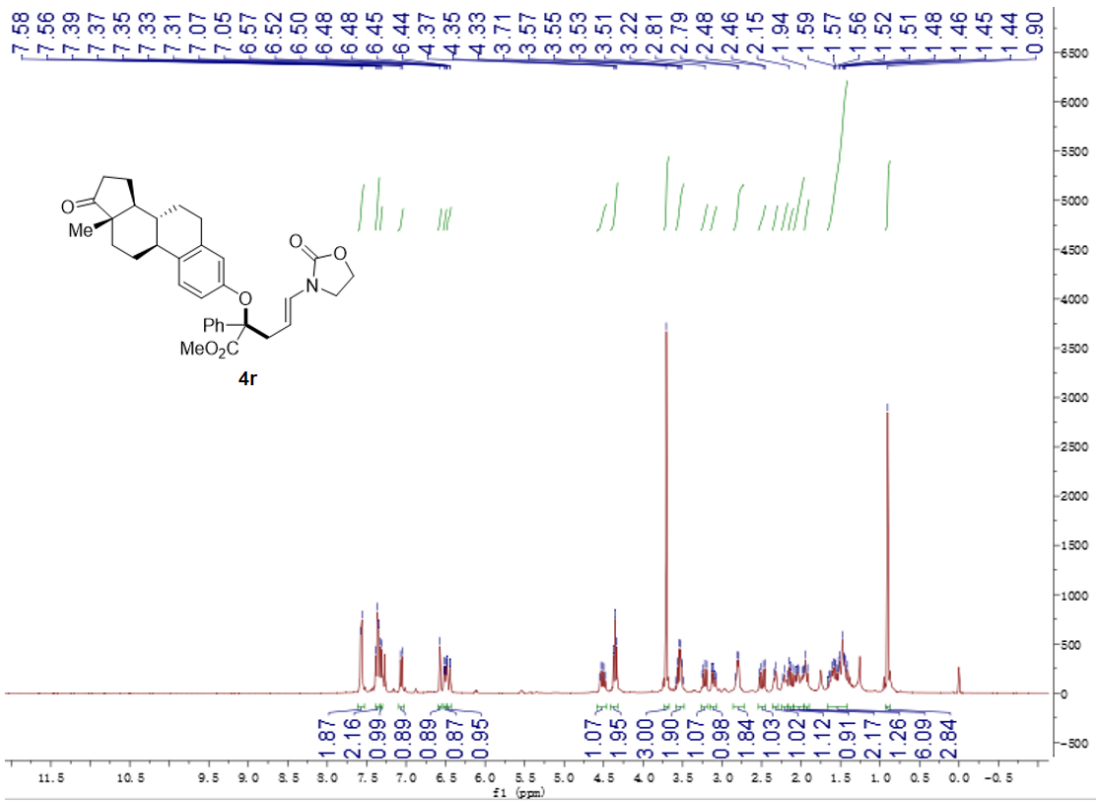
155.17
153.60
138.89
138.47
128.52
128.25
127.17
126.03
84.98
62.10
52.79
42.39
37.78
24.06
Me
Br
Ph
O
CO2Me
Me
4q
f1 (ppm)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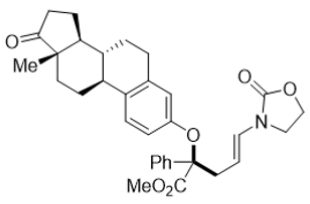
7.33
7.31
7.07
7.05
6.57
6.52
6.50
6.48
6.48
6.45
6.44
4.37
4.35
4.33
3.71
3.57
3.55
3.53
3.51
3.22
2.81
2.79
2.48
2.46
2.15
1.94
1.59
1.57
1.56
1.52
1.51
1.48
1.46
1.45
1.44
0.90
1.87
2.16
0.99
0.89
0.89
0.87
0.95
1.07
1.95
3.00
1.90
1.07
0.98
1.84
1.03
1.02
1.12
0.91
2.17
1.26
6.09
2.84
f1 (ppm)

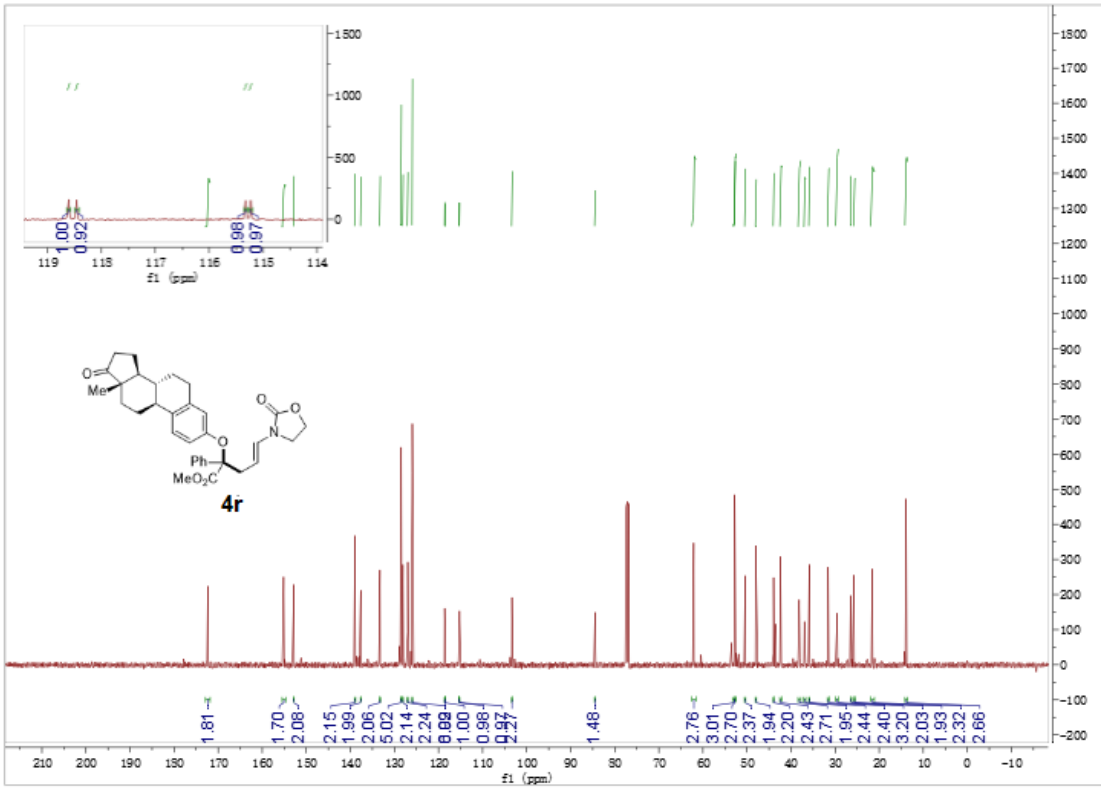

O
Me
O
O
N
O
Ph
MeO2C

4r

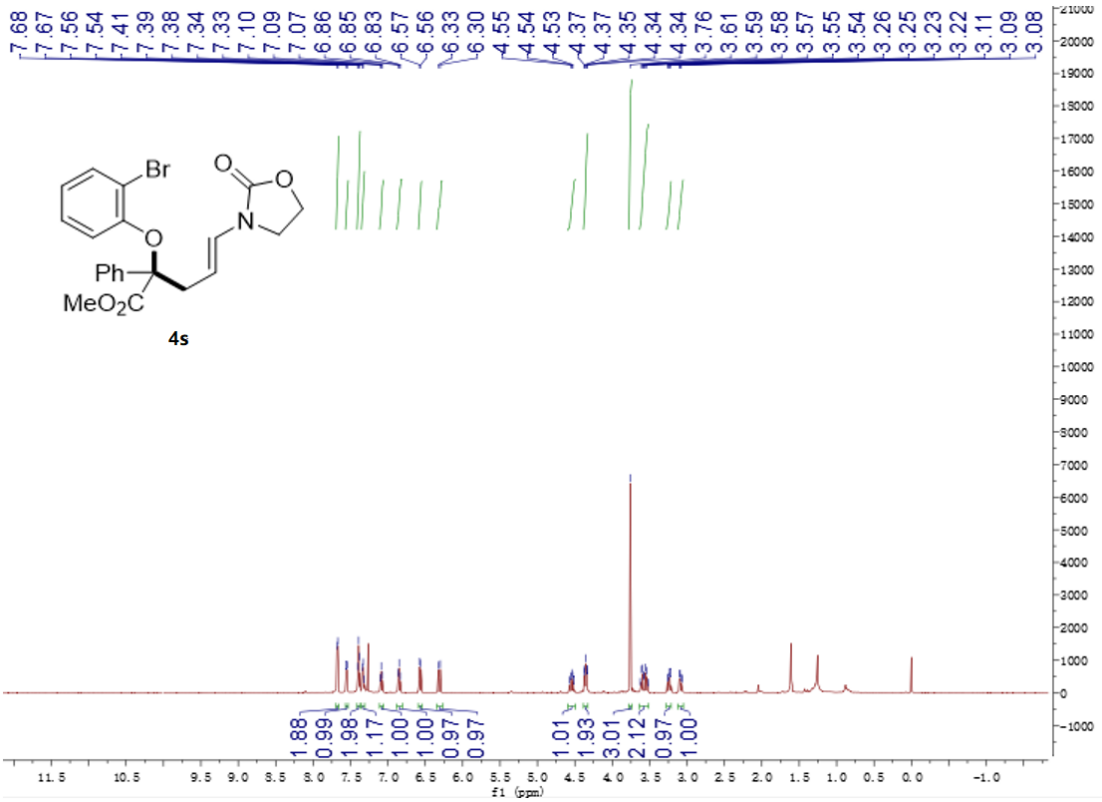
172.4
155.2
152.8
139.0
133.3
128.5
128.1
127.0
126.9
103.4
103.3
84.5
84.5
62.1
52.8
50.4
48.0
44.0
42.4
38.2
38.1
36.9
35.9
31.6
29.6
29.5
26.5
25.7
21.6
13.9
f1 (ppm)

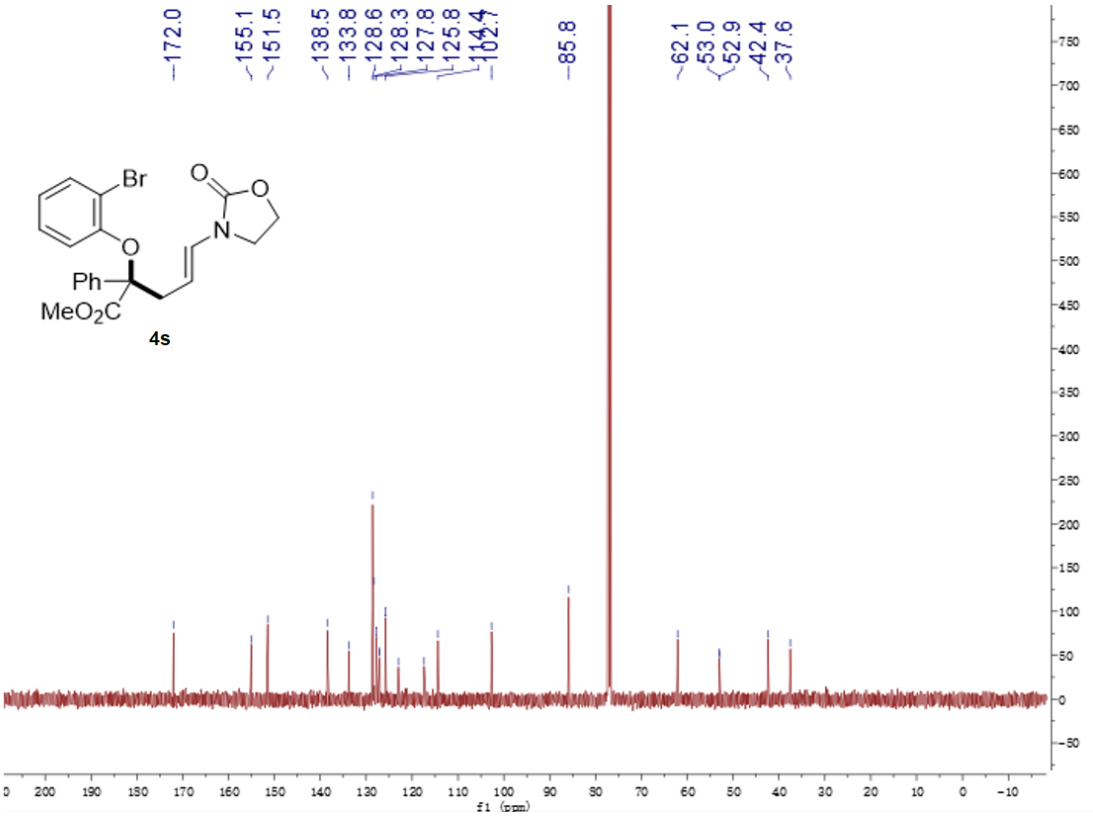
O
Me
O
O
N
O
Ph
MeO2C

4r



Quantitative ^{13}C NMR of **4r**

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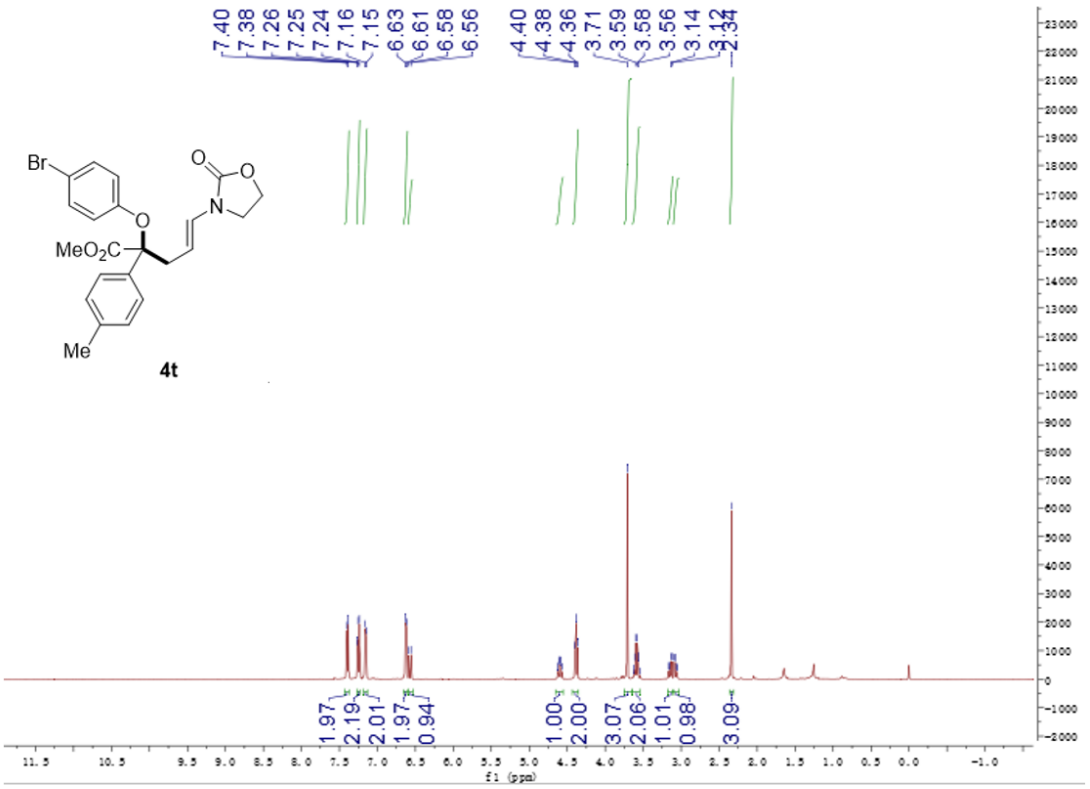
151.5
138.5
133.8
128.6
128.3
127.8
125.8
114.4
102.7
85.8
62.1
53.0
52.9
42.4
37.6
Br
O
O
N
O
Ph
MeO2C
4s
f1 (ppm)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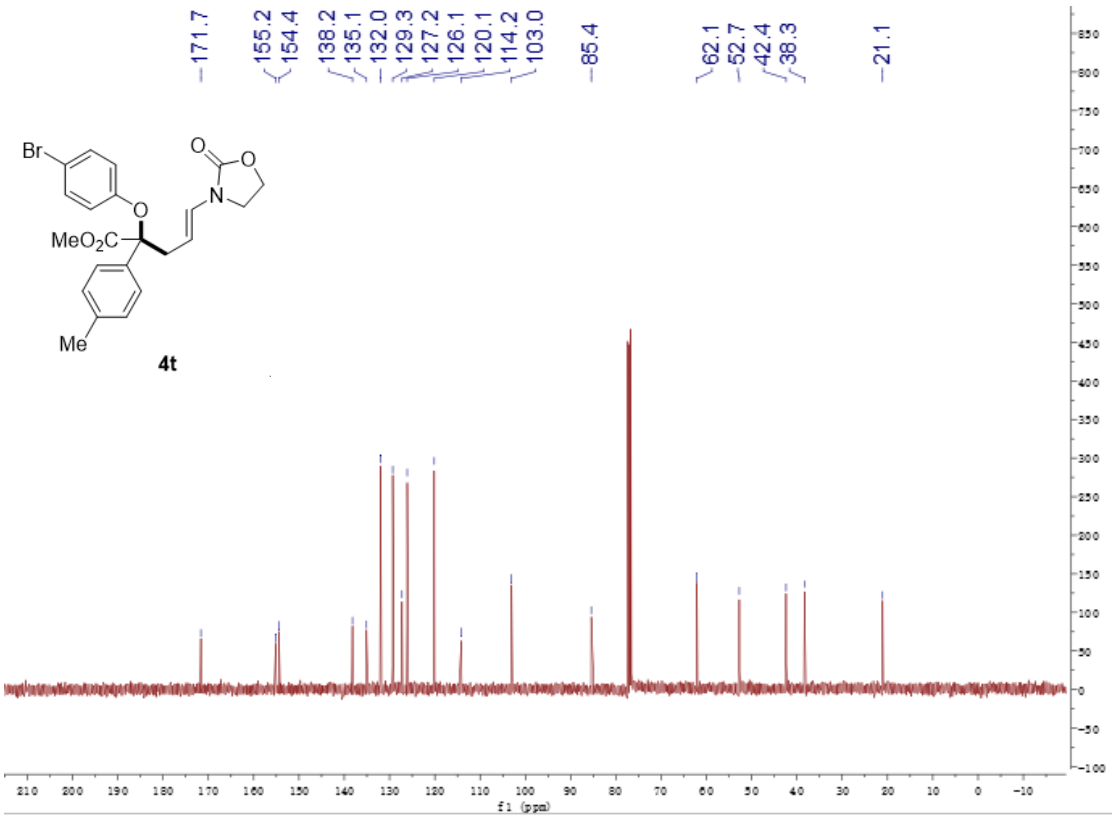
6.63
6.61
6.58
6.56
4.40
4.38
4.36
3.71
3.59
3.58
3.56
3.14
3.12
2.34
Br
O
O
N
O
MeO2C
Me
4t
1.97
2.19
2.01
1.97
0.94
1.00
2.00
3.07
2.06
1.01
0.98
3.09
f1 (ppm)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138.2
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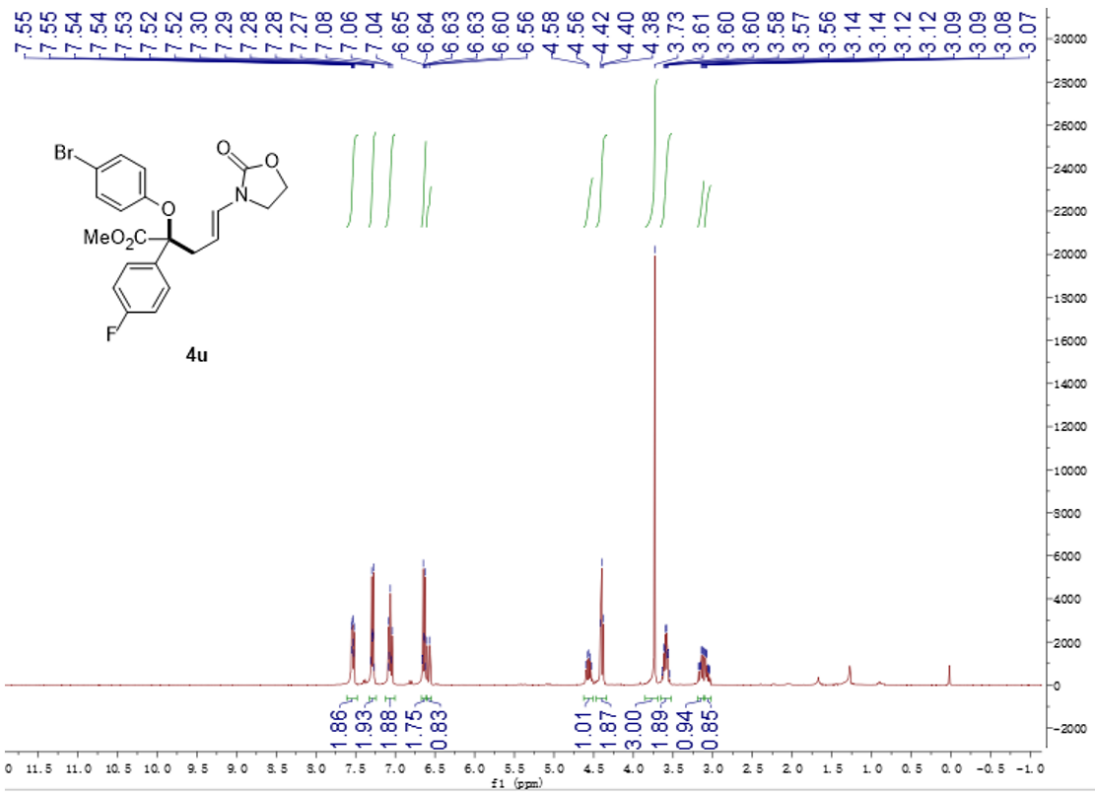
132.0
129.3
127.2
126.1
120.1
114.2
103.0
85.4
62.1
52.7
42.4
38.3
21.1
Br
O
O
N
MeO2C
Me
4t
f1 (ppm)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7.54
7.53
7.52
7.52
7.30
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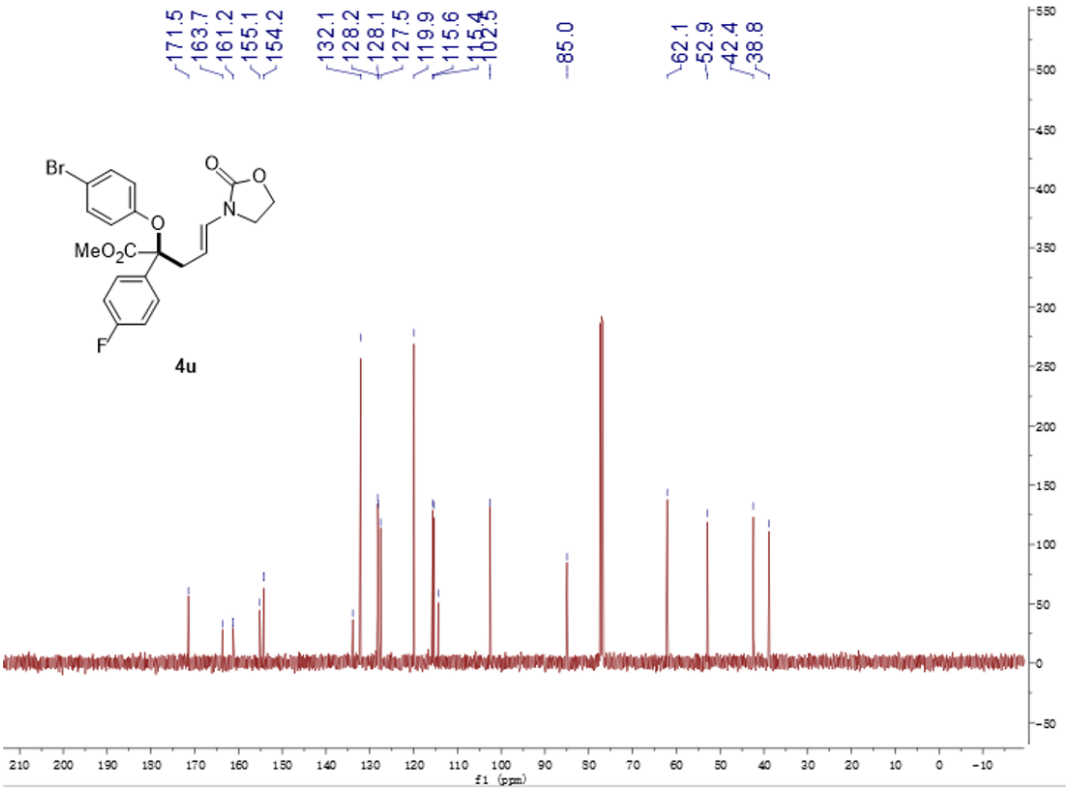
7.28
7.28
7.27
7.08
7.06
7.04
6.65
6.64
6.63
6.63
6.60
6.56
4.58
4.56
4.42
4.40
4.38
3.73
3.61
3.60
3.60
3.58
3.57
3.56
3.14
3.14
3.12
3.12
3.09
3.09
3.08
3.07
Br
O
O
N
MeO2C
F
4u
1.86
1.93
1.88
1.75
0.83
1.01
1.87
3.00
1.89
0.94
0.85
f1 (ppm)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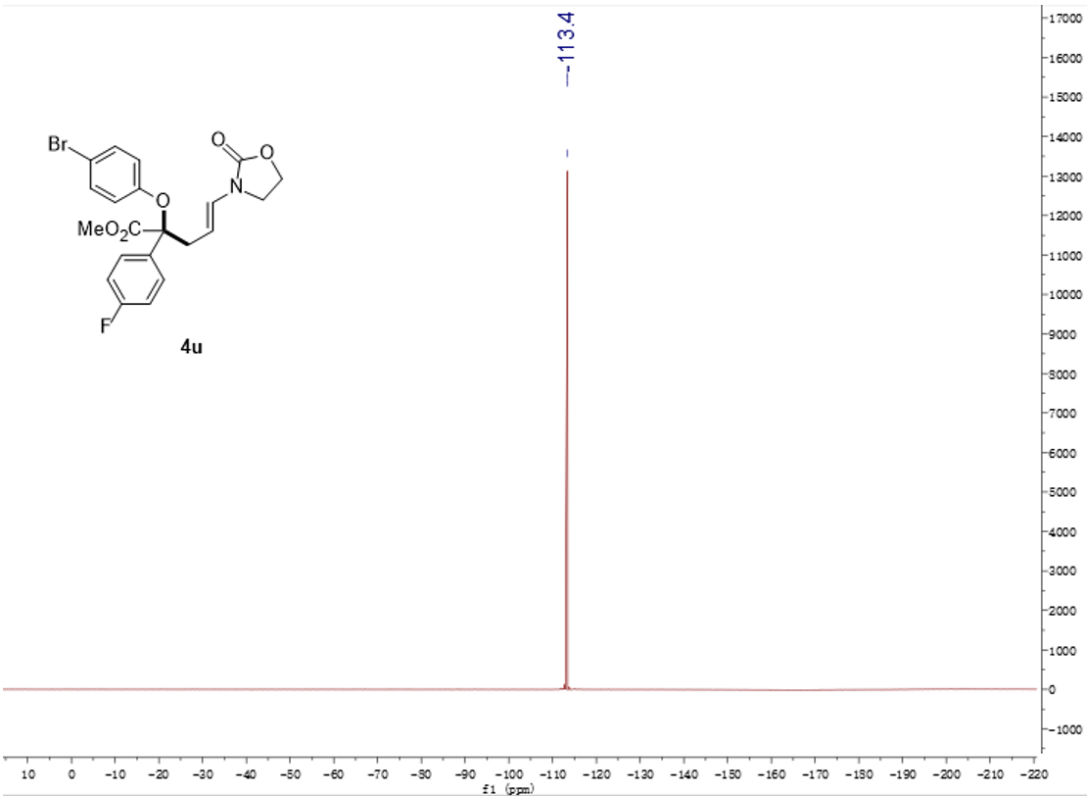
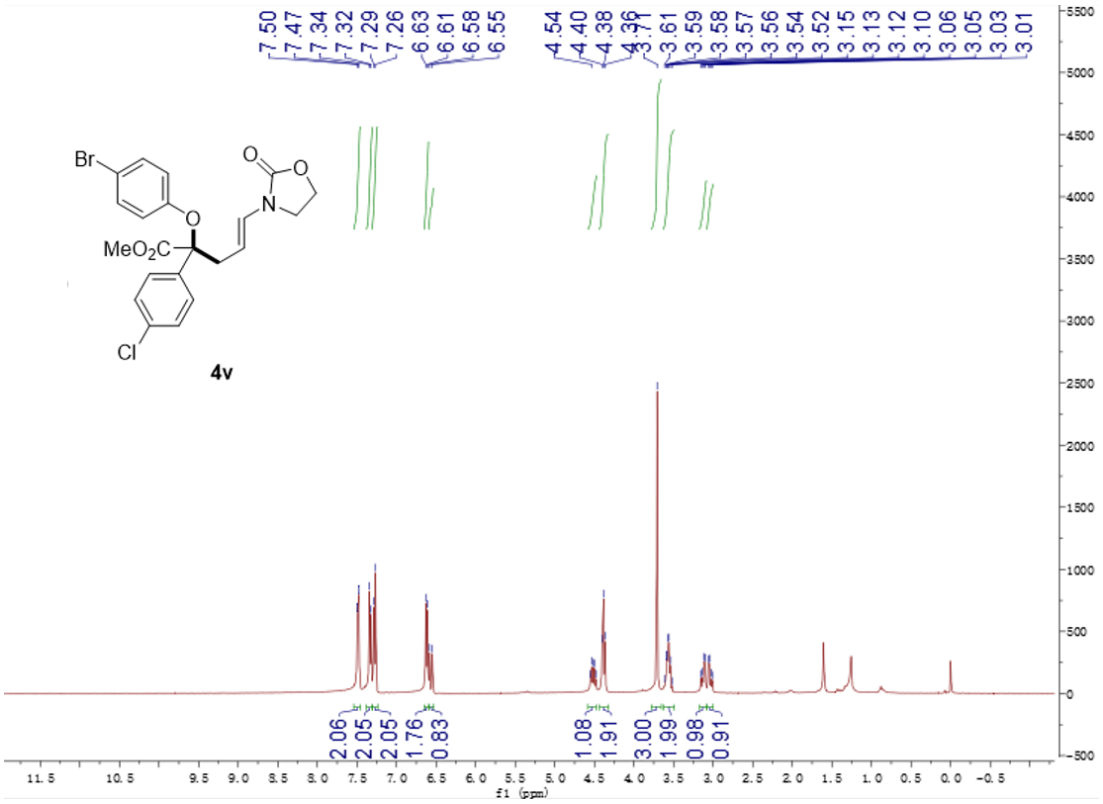
163.7
161.2
155.1
154.2
132.1
128.2
128.1
127.5
119.9
115.6
115.4
102.5
85.0
62.1
52.9
42.4
38.8
Br
O
O
N
O
MeO2C
F
4u
f1 (ppm)


113.4
Br
O
O
N
O
MeO2C
F
4u
f1 (ppm)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7.26
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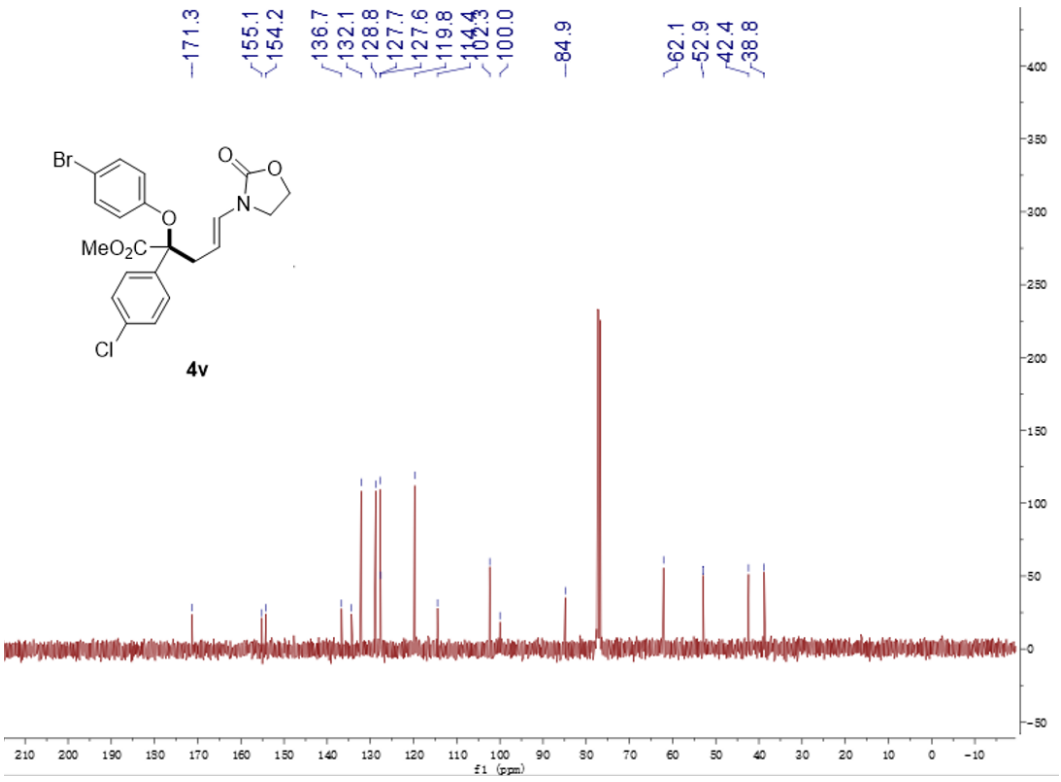
6.61
6.58
6.55
4.54
4.40
4.38
4.36
3.71
3.61
3.59
3.58
3.57
3.56
3.54
3.52
3.15
3.13
3.12
3.10
3.06
3.05
3.03
3.01
Br
O
O
N
O
MeO2C
Cl
4v
2.06
2.05
2.05
1.76
0.83
1.08
1.91
3.00
1.99
0.98
0.91
f1 (ppm)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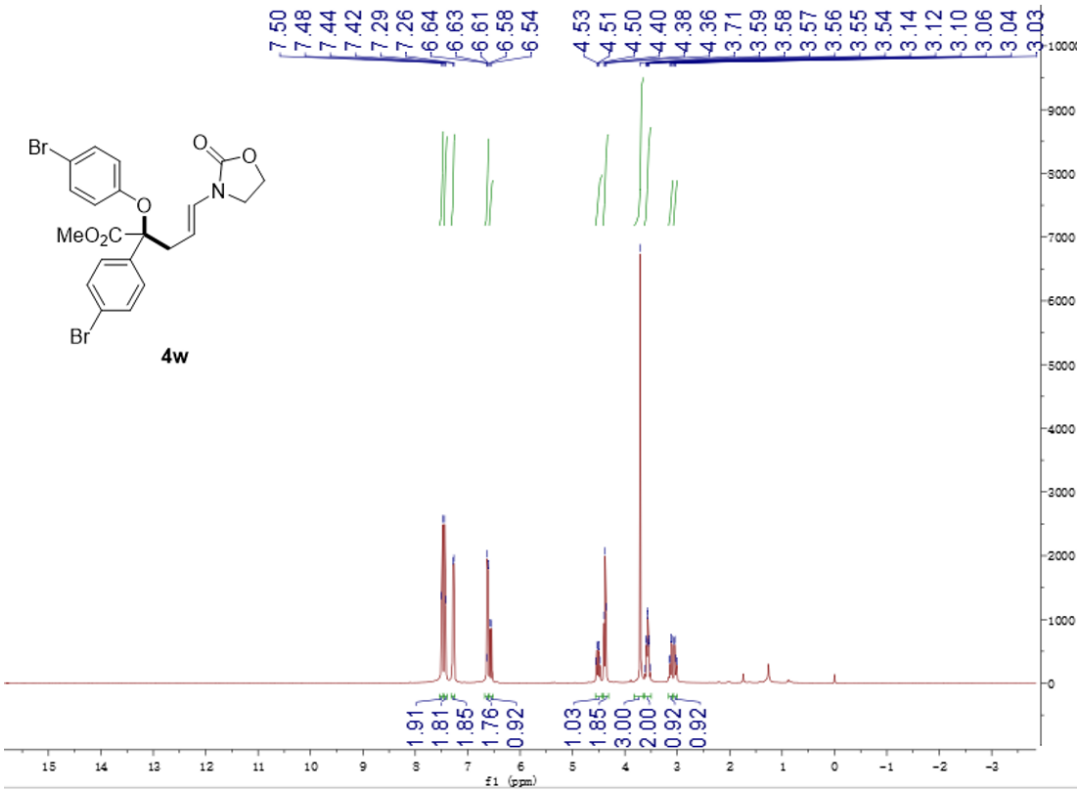
154.2
136.7
132.1
128.8
127.7
127.6
119.8
114.4
102.3
100.0
84.9
62.1
52.9
42.4
38.8
Br
O
O
N
O
MeO2C
Cl
4v
f1 (ppm)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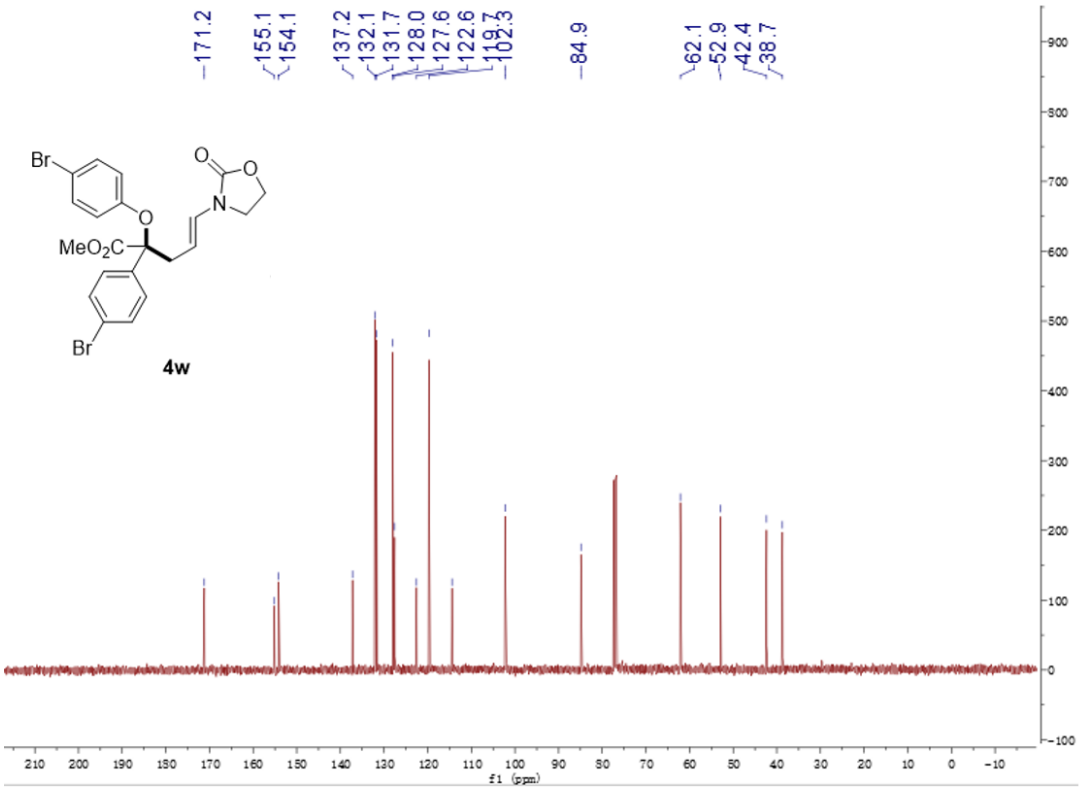
7.26
6.64
6.63
6.61
6.58
6.54
4.53
4.51
4.50
4.40
4.38
4.36
3.71
3.59
3.58
3.57
3.56
3.55
3.54
3.14
3.12
3.10
3.06
3.04
3.03
1.91
1.81
1.85
1.76
0.92
1.03
1.85
3.00
2.00
0.92
0.92
f1 (ppm)
Br
O
O
N
MeO2C
Br
4w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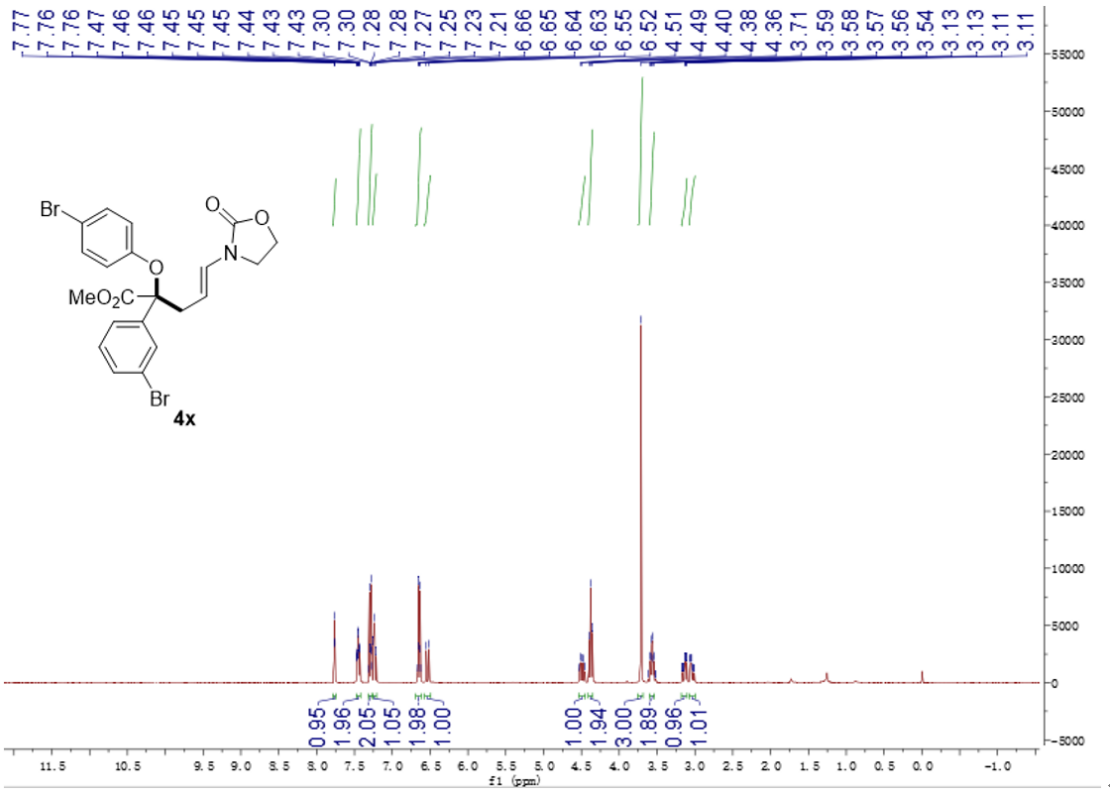
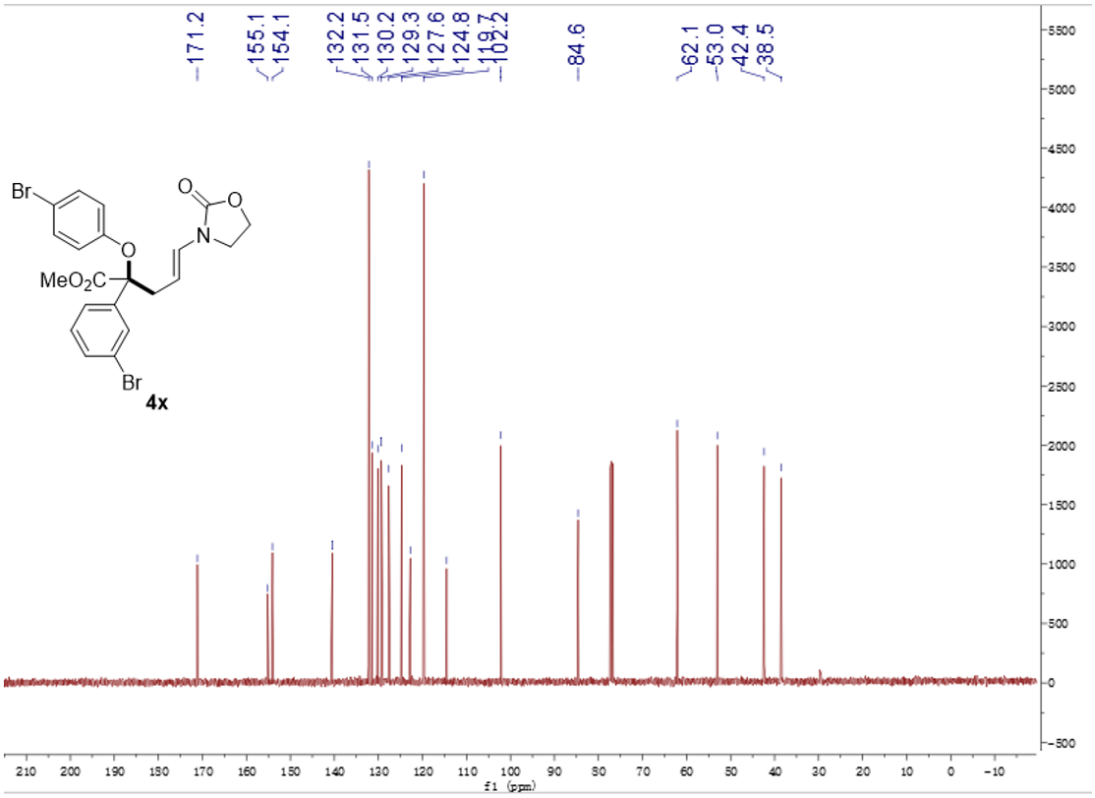
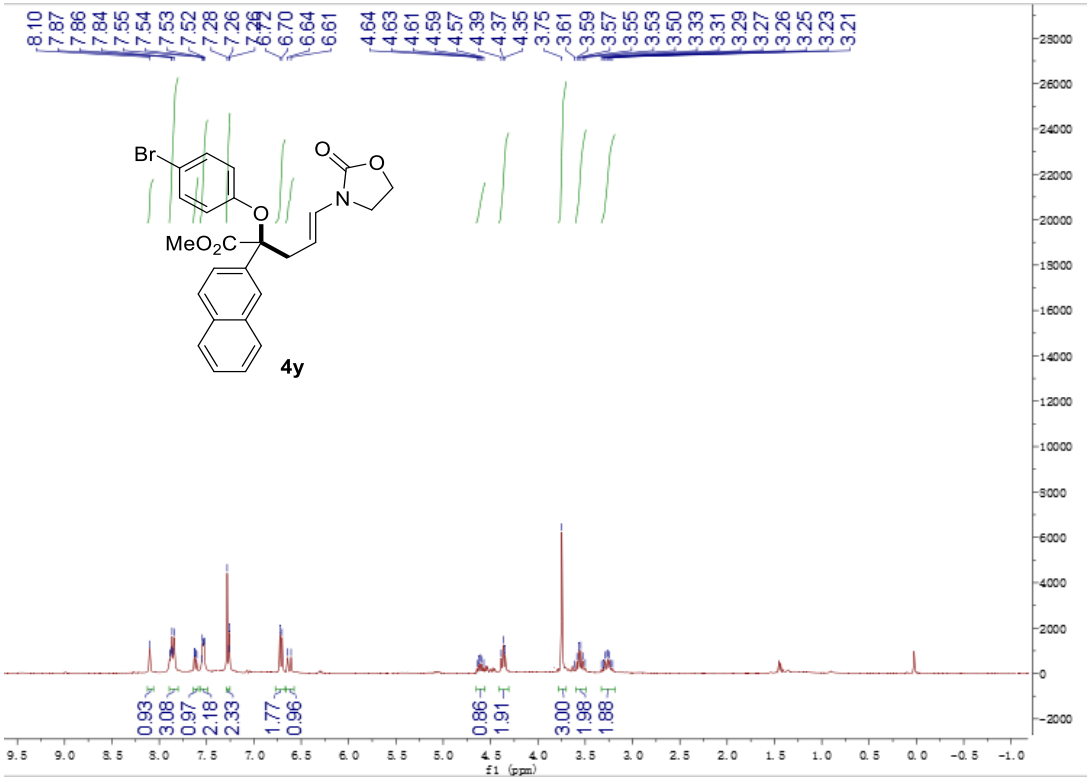
154.1
137.2
132.1
131.7
128.0
127.6
122.6
119.7
102.3
84.9
62.1
52.9
42.4
38.7
f1 (ppm)
Br
O
O
N
MeO2C
Br
4w


7.77 7.76 7.76 7.47 7.46 7.46 7.45 7.45 7.45 7.44 7.43 7.43 7.30 7.30 7.28 7.28 7.27 7.25 7.23 7.21 6.66 6.65 6.64 6.63 6.55 6.52 4.51 4.49 4.40 4.38 4.36 3.71 3.59 3.58 3.57 3.56 3.54 3.13 3.13 3.11 3.11
Br
O
O
N
O
MeO2C
Br
4x
0.95 1.96 2.05 1.05 1.98 1.00 1.00 1.94 3.00 1.89 0.96 1.01
f1 (ppm)


171.2
155.1
154.1
132.2
131.5
130.2
129.3
127.6
124.8
119.7
102.2
84.6
62.1
53.0
42.4
38.5
Br
O
O
N
O
MeO2C
Br
4x
f1 (ppm)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4.64
4.63
4.61
4.59
4.57
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3.57
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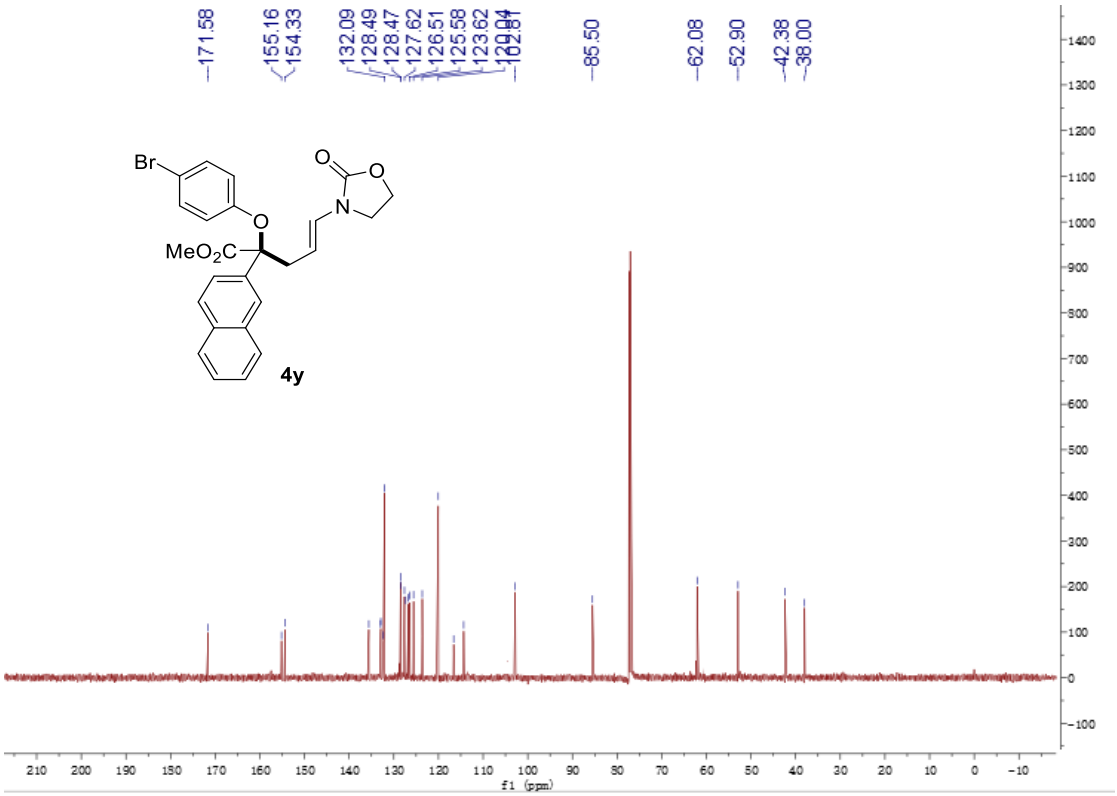
3.53
3.50
3.33
3.31
3.29
3.27
3.26
3.25
3.23
3.21
Br
O
O
N
O
MeO2C
4y
0.93
3.08
0.97
2.18
2.33
1.77
0.96
0.86
1.91
3.00
1.98
1.88
f1 (ppm)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128.49
128.47
127.62
126.51
125.58
123.62
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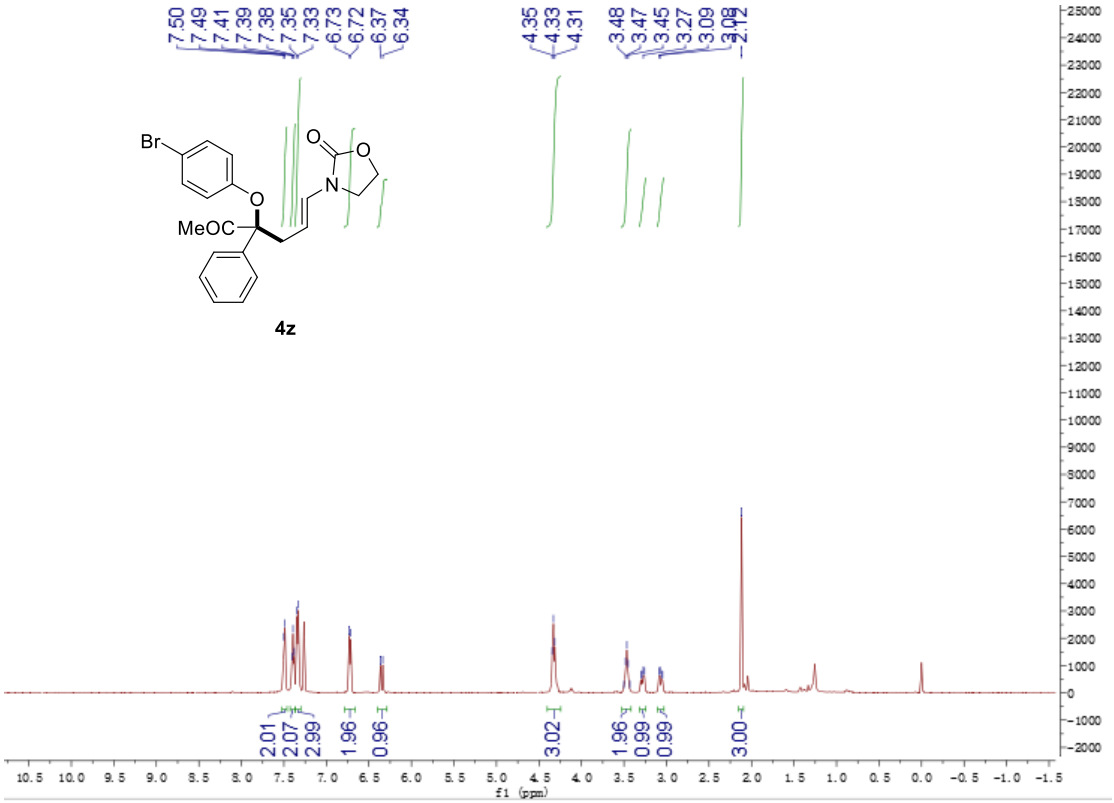
52.90
42.38
38.00
Br
O
O
N
O
MeO2C
4y
f1 (ppm)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7.33
6.73
6.72
6.37
6.34
4.35
4.33
4.31
3.48
3.47
3.45
3.27
3.09
3.08
2.12
Br
O
O
N
O
MeOC
O
4z
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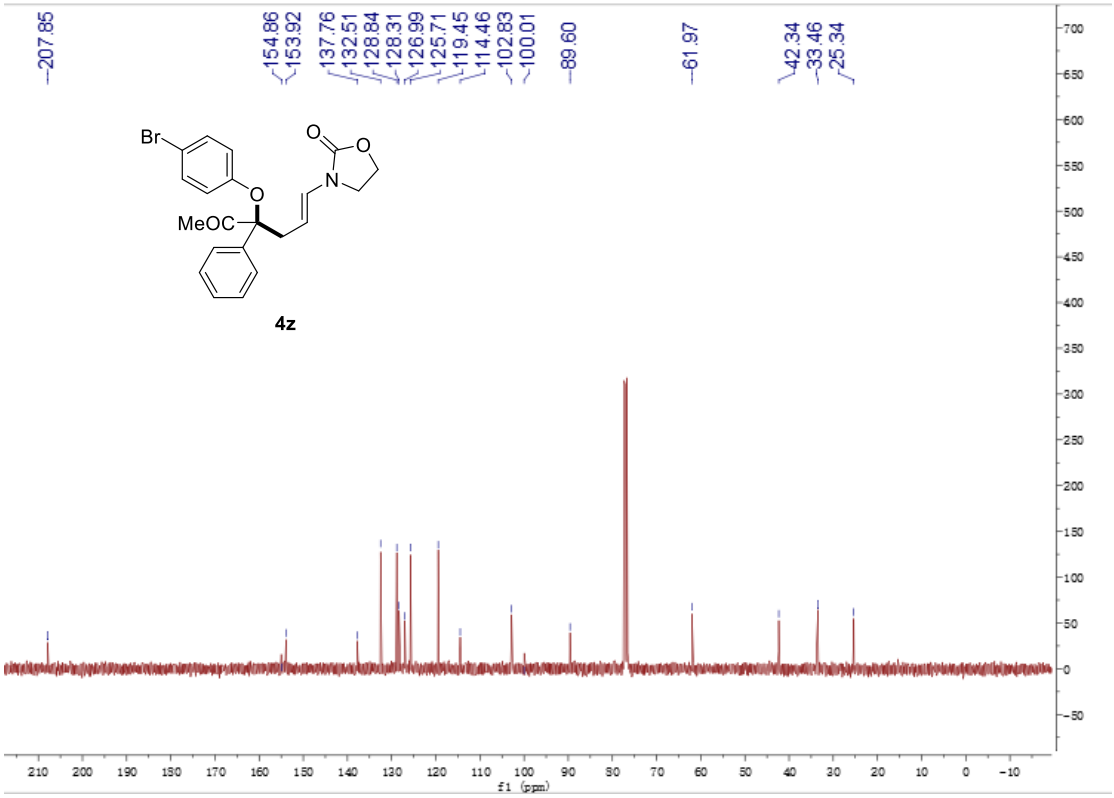
2.07
2.99
1.96
0.96
3.02
1.96
0.99
0.99
3.00
f1 (ppm)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153.92
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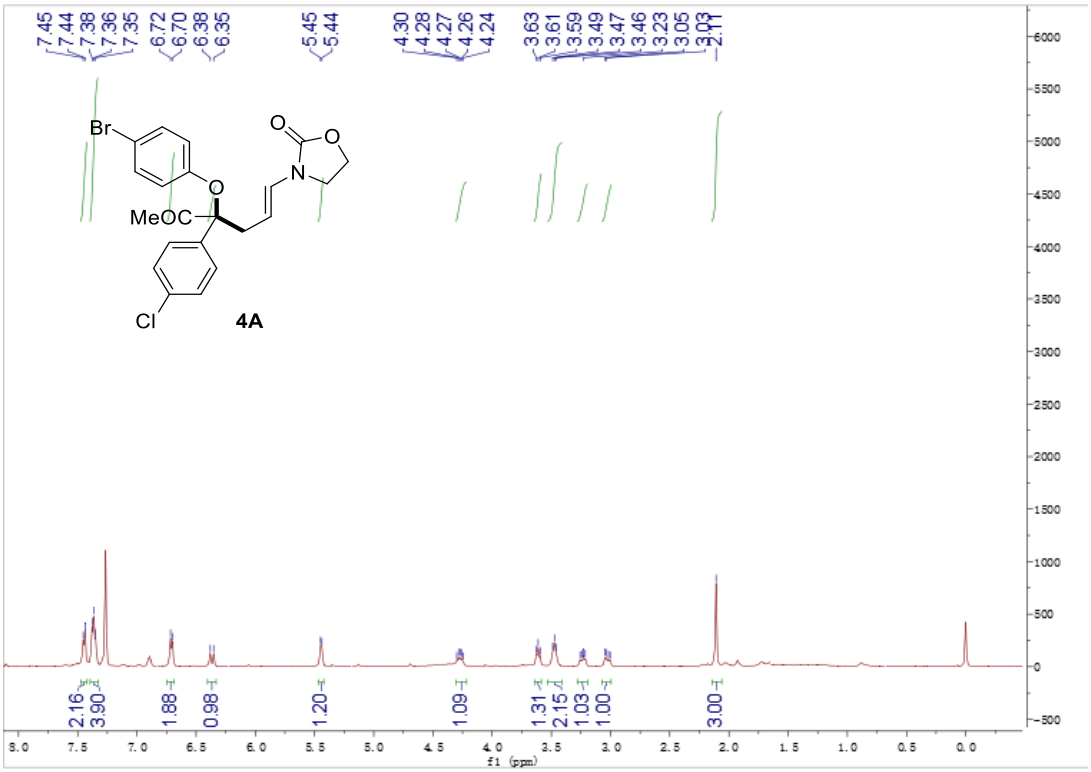
132.51
128.84
128.31
126.99
125.71
119.45
114.46
102.83
100.01
89.60
61.97
42.34
33.46
25.34
Br
O
O
N
O
MeOC
O
4z
f1 (ppm)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6.70
6.38
6.35
5.45
5.44
4.30
4.28
4.27
4.26
4.24
3.63
3.61
3.59
3.49
3.47
3.46
3.23
3.05
3.03
2.11
Br
O
O
N
O
MeOC
Cl
4A
2.16
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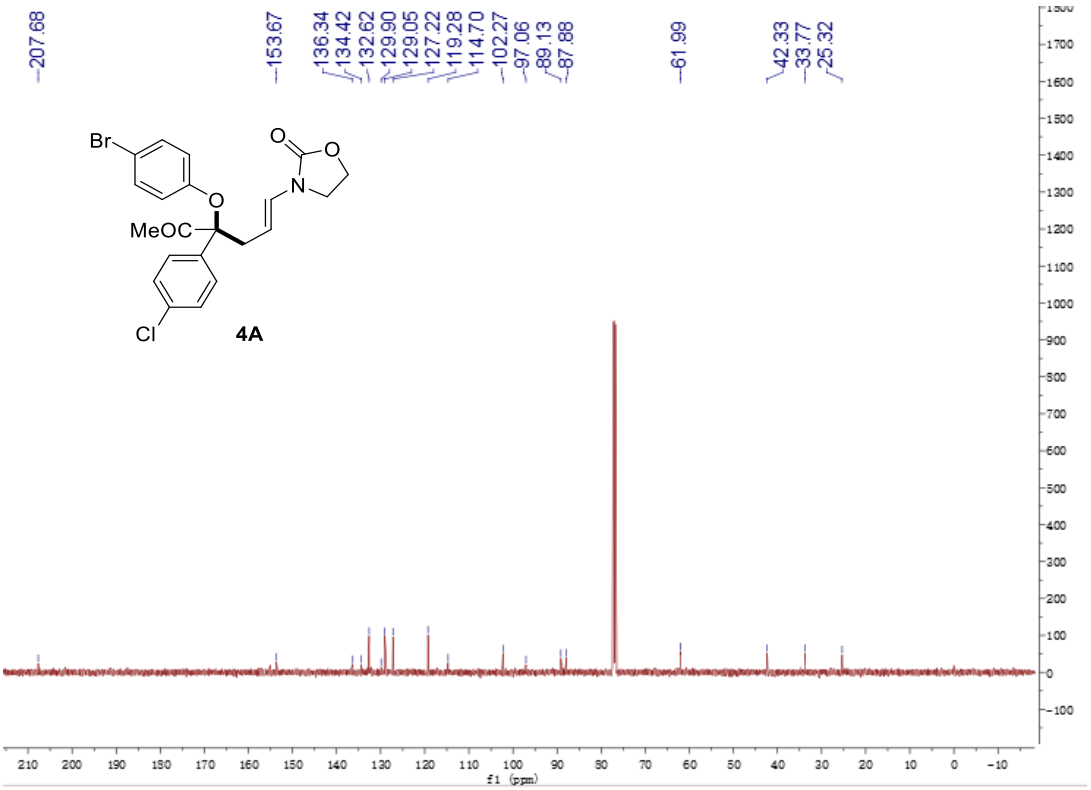
0.98
1.20
1.09
1.31
2.15
1.03
1.00
3.00
f1 (ppm)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129.90
129.05
127.22
119.28
114.70
102.27
97.06
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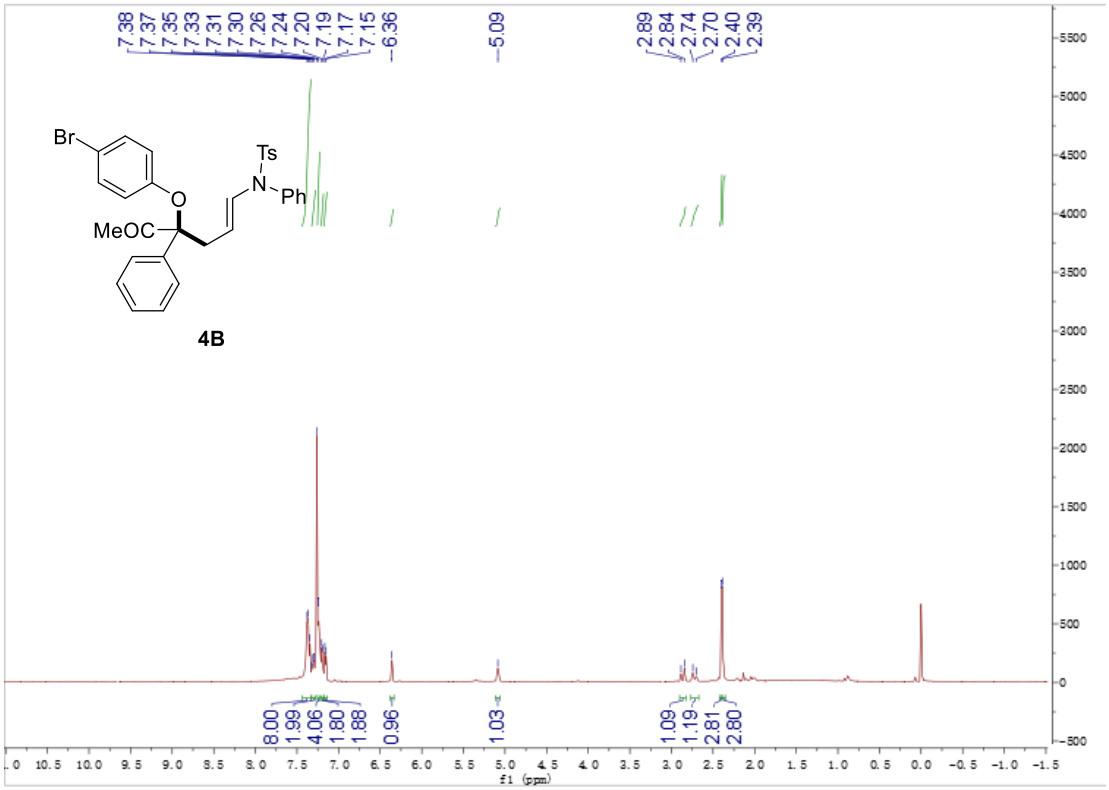
87.88
61.99
42.33
33.77
25.32
Br
O
O
N
O
MeOC
Cl
4A
f1 (ppm)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7.37
7.35
7.33
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7.30
7.26
7.24
7.20
7.19
7.17
7.15
6.36
5.09
2.89
2.84
2.74
2.70
2.40
2.39
Br
Ts
N
Ph
O
MeOC
4B
8.00
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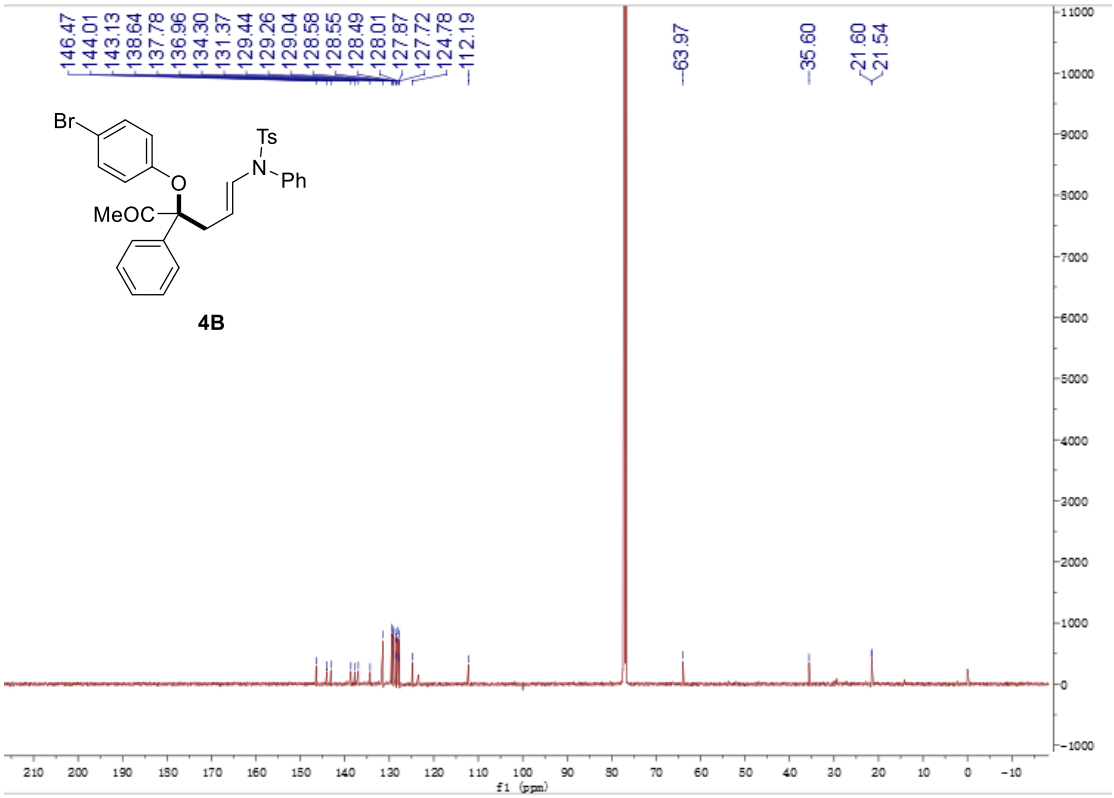
1.80
1.88
0.96
1.03
1.09
1.19
2.81
2.80
f1 (ppm)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129.26
129.04
128.58
128.55
128.49
128.01
127.87
127.72
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35.60
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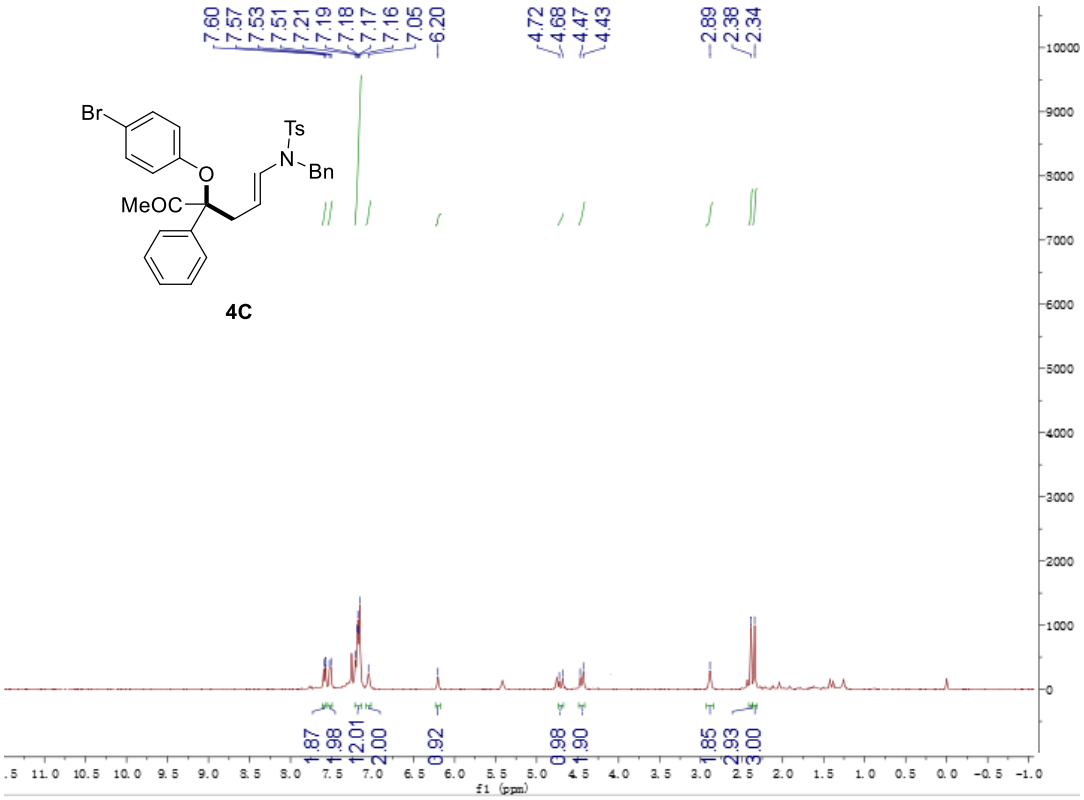
21.54
Br
Ts
N
Ph
O
MeOC
4B
f1 (ppm)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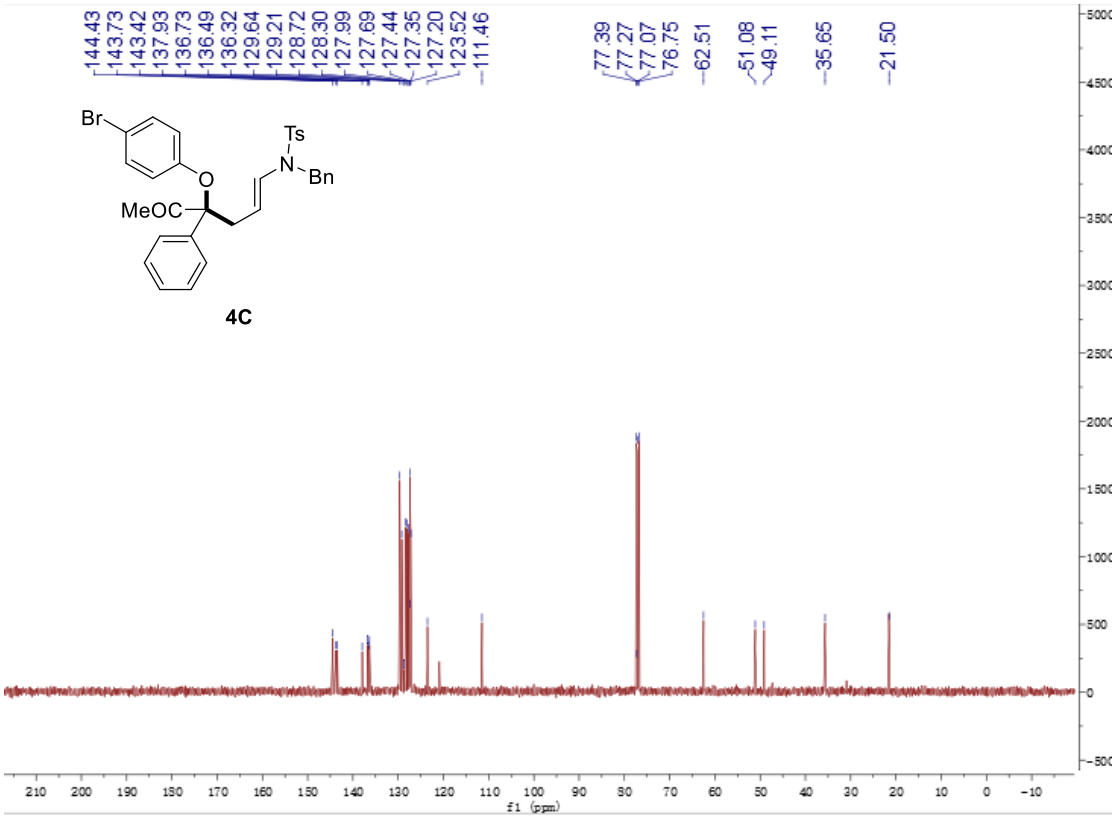
7.57
7.53
7.51
7.21
7.19
7.18
7.17
7.16
7.05
6.20
4.72
4.68
4.47
4.43
2.89
2.38
2.34
Br
O
MeOC
Ts
N
Bn
4C
1.87
1.98
2.01
2.00
0.92
0.98
1.90
1.85
2.93
3.00
f1 (ppm)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143.42
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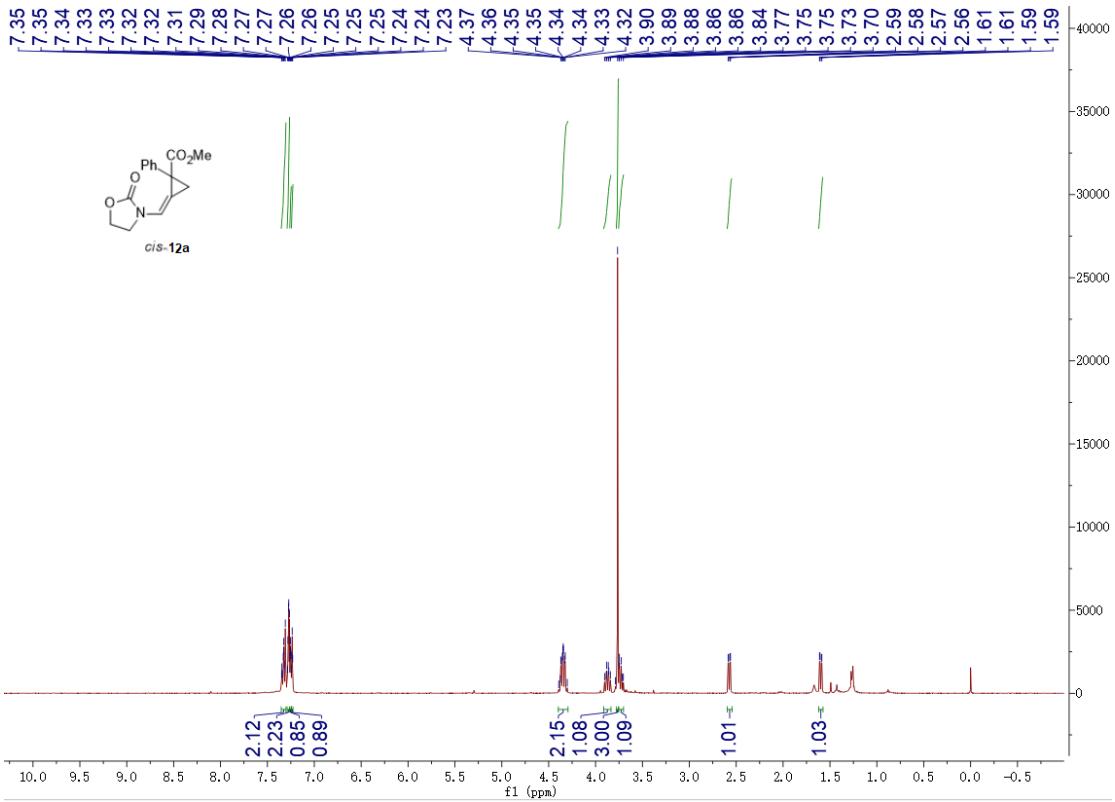
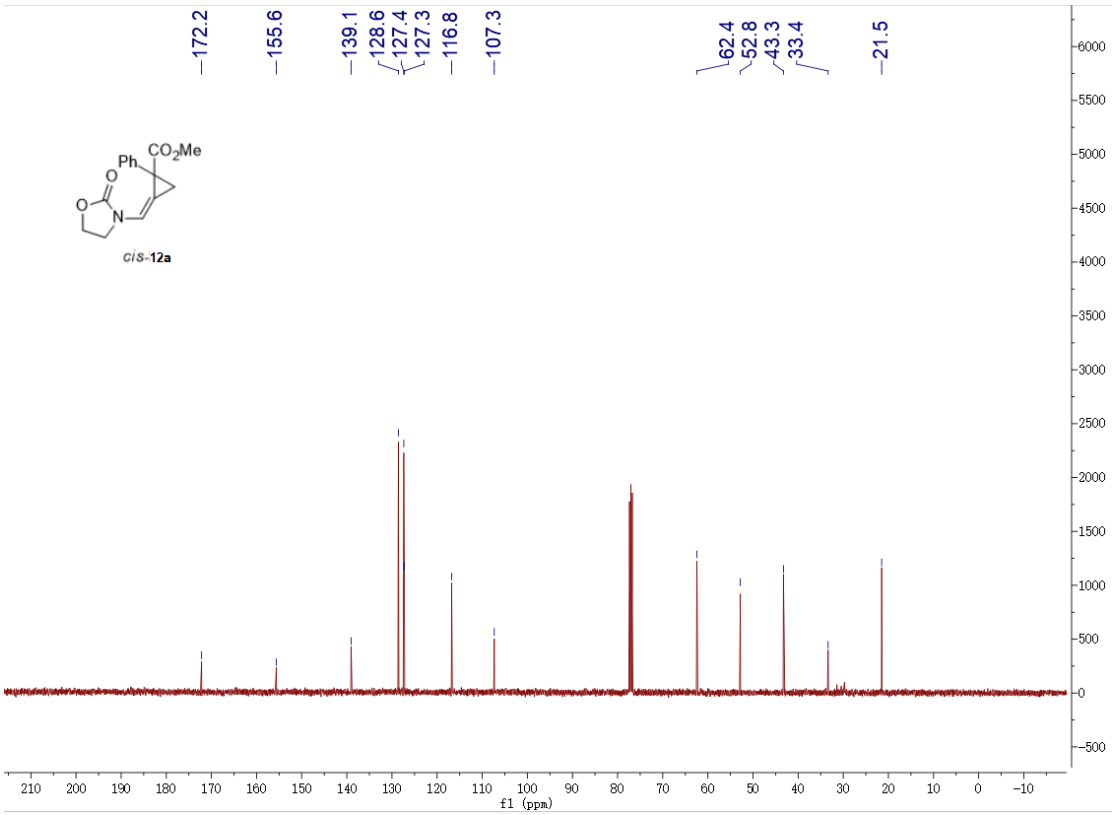
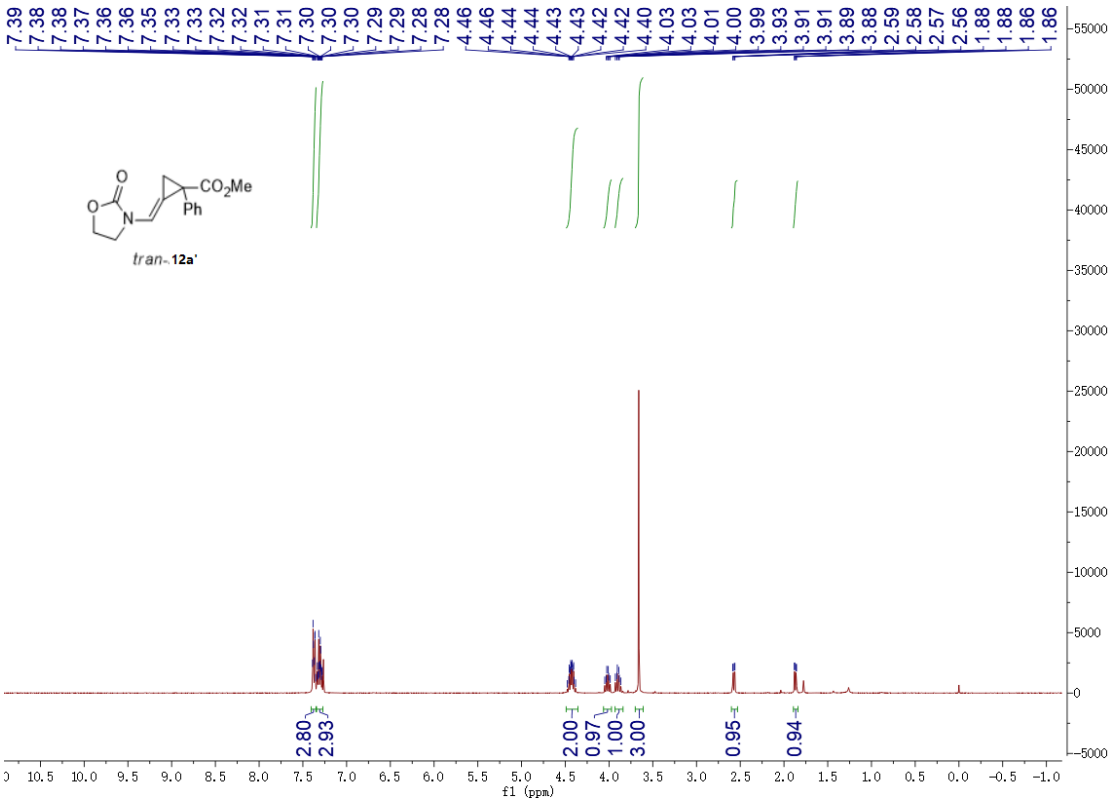
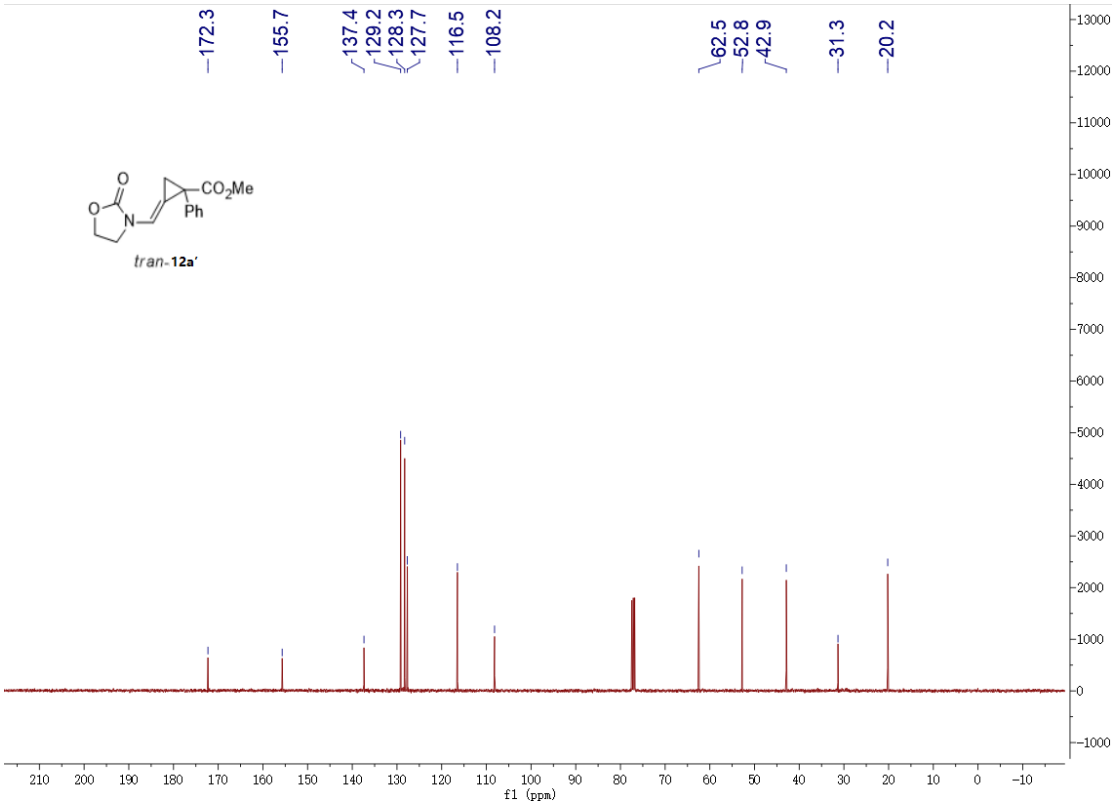
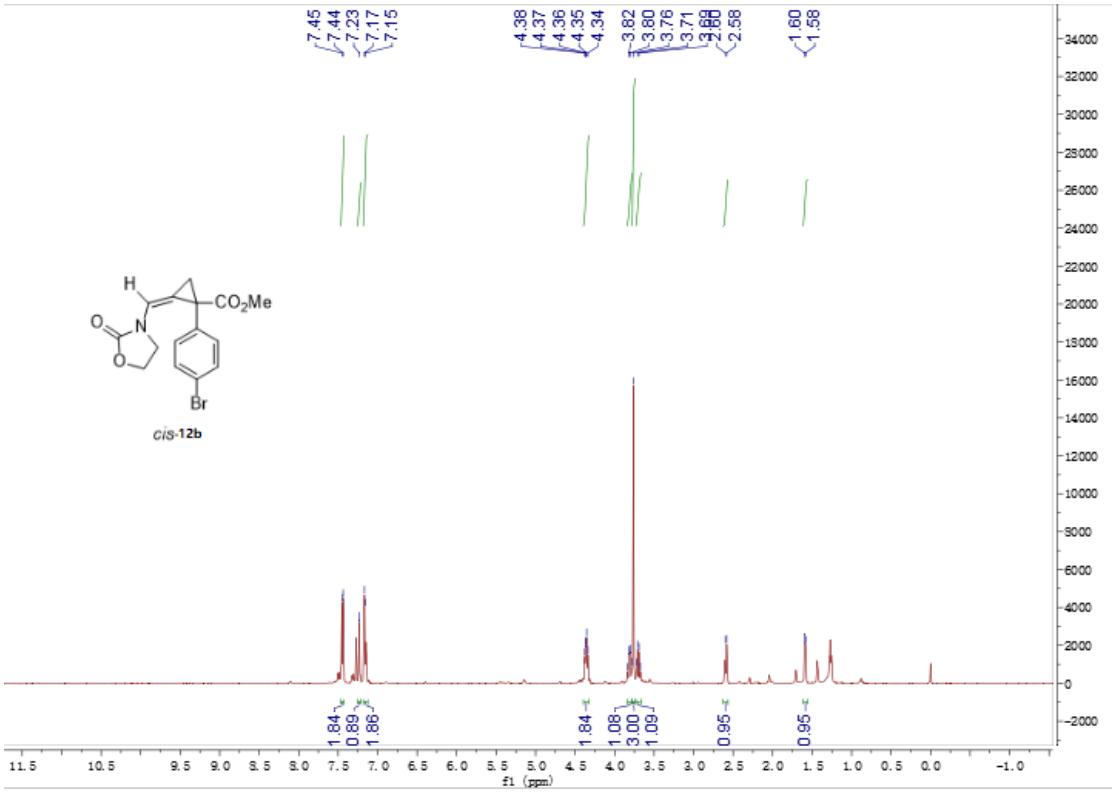
136.49
136.32
129.64
129.21
128.72
128.30
127.99
127.69
127.44
127.35
127.20
123.52
111.46
77.39
77.27
77.07
76.75
62.51
51.08
49.11
35.65
21.50
Br
O
MeOC
Ts
N
Bn
4C
f1 (ppm)


7.35 7.35 7.34 7.33 7.33 7.32 7.32 7.31 7.29 7.28 7.27 7.27 7.26 7.26 7.25 7.25 7.24 7.24 7.23
4.37 4.36 4.35 4.35 4.34 4.34 4.33 4.32 3.90 3.89 3.88 3.86 3.86 3.84 3.77 3.75 3.73 3.70 2.59 2.58 2.57 2.56 1.61 1.61 1.59 1.59
Ph
CO2Me
O
O
N
cis-12a
2.12 2.23 0.85 0.89 2.15 1.08 3.00 1.09 1.01 1.03
f1 (ppm)


172.2 155.6 139.1 128.6 127.4 127.3 116.8 107.3
62.4 52.8 43.3 33.4 21.5
Ph
CO2Me
O
O
N
cis-12a
f1 (ppm)


7.39 7.38 7.38 7.37 7.36 7.36 7.35 7.33 7.33 7.32 7.32 7.31 7.31 7.30 7.30 7.30 7.29 7.29 7.28 7.28
4.46 4.46 4.44 4.44 4.43 4.43 4.42 4.42 4.40 4.03 4.01 4.00 3.99 3.93 3.91 3.91 3.89 3.88 2.59 2.58 2.57 2.56 1.88 1.88 1.86 1.86
CO2Me
Ph
tran-12a'
2.80 2.93 2.00 0.97 1.00 3.00 0.95 0.94
f1 (ppm)


172.3 155.7 137.4 129.2 128.3 127.7 116.5 108.2
62.5 52.8 42.9 31.3 20.2
CO2Me
Ph
tran-12a'
f1 (ppm)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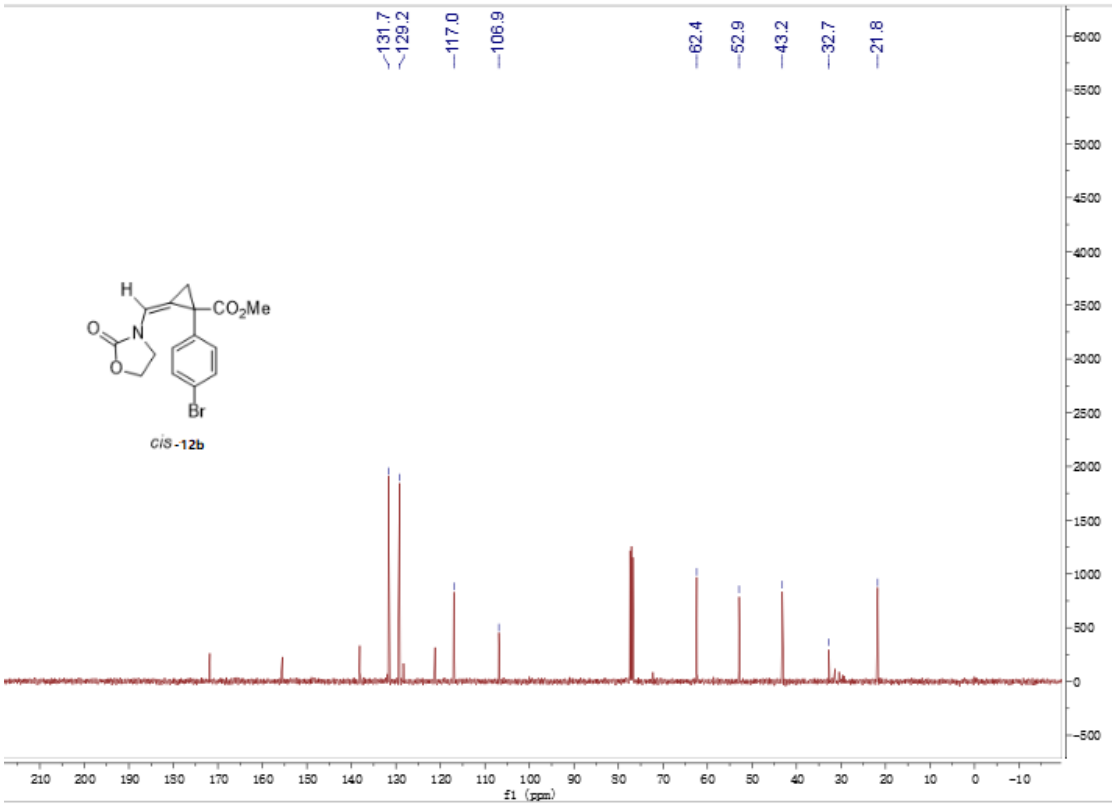
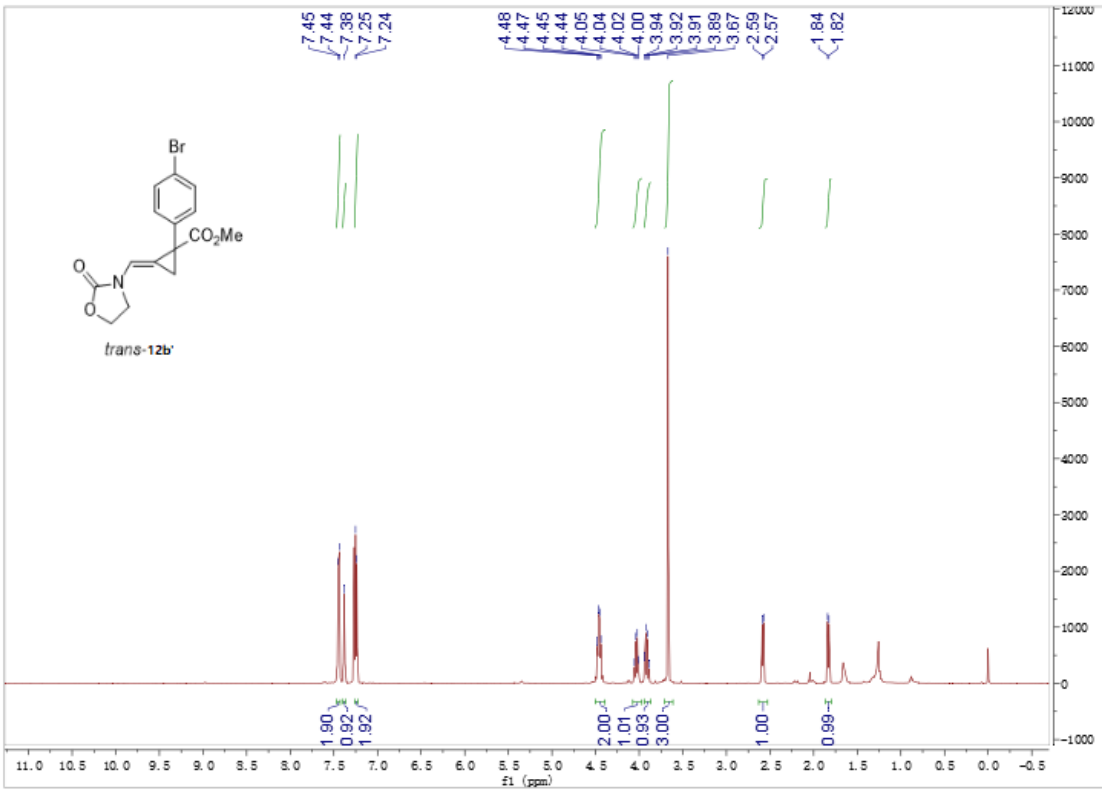
7.44
7.23
7.17
7.15
4.38
4.37
4.36
4.35
4.34
3.82
3.80
3.76
3.71
2.58
1.60
1.58
H
CO2Me
O
N
O
Br
cis-12b
1.84
0.89
1.86
1.84
1.08
3.00
1.09
0.95
0.95
f1 (ppm)


131.7
129.2
117.0
106.9
62.4
52.9
43.2
32.7
21.8
H
CO2Me
O
N
O
Br
cis-12b
f1 (ppm)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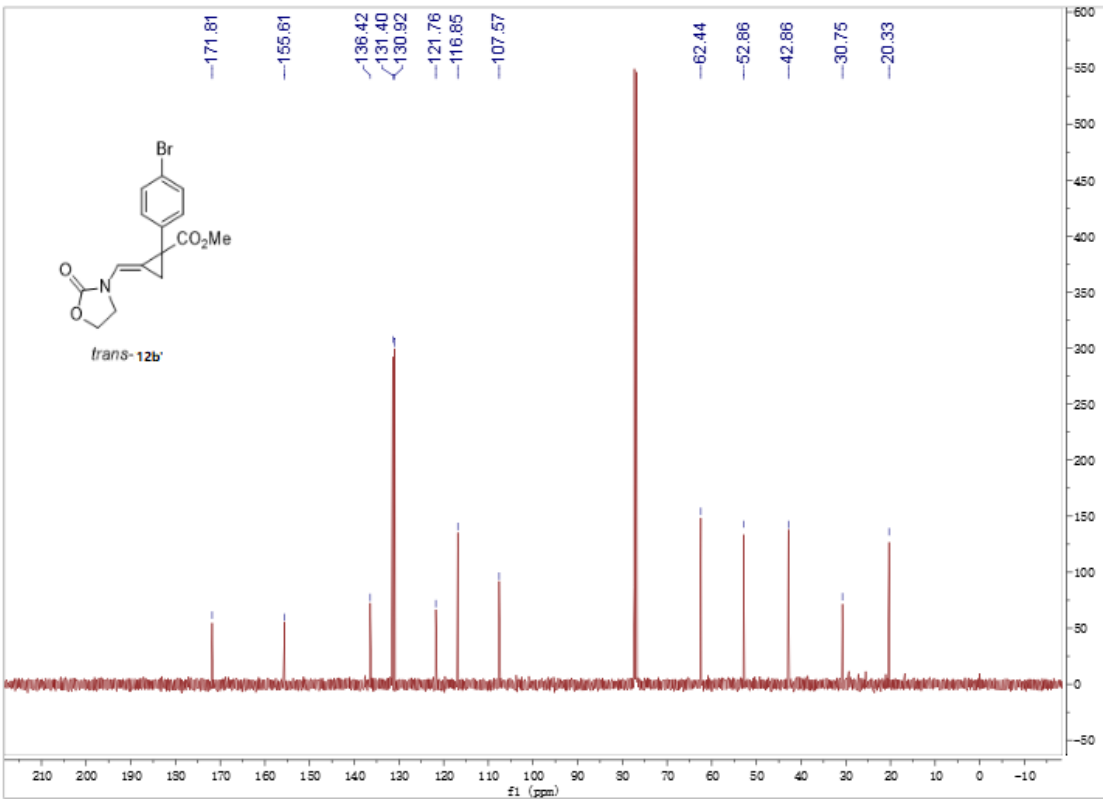
7.44
7.38
7.25
7.24
4.48
4.47
4.45
4.44
4.05
4.04
4.02
4.00
3.94
3.92
3.91
3.89
3.67
2.59
2.57
1.84
1.82
Br
CO2Me
O
N
O
trans-12b'
1.90
0.92
1.92
2.00
1.01
0.93
3.00
1.00
0.99
f1 (ppm)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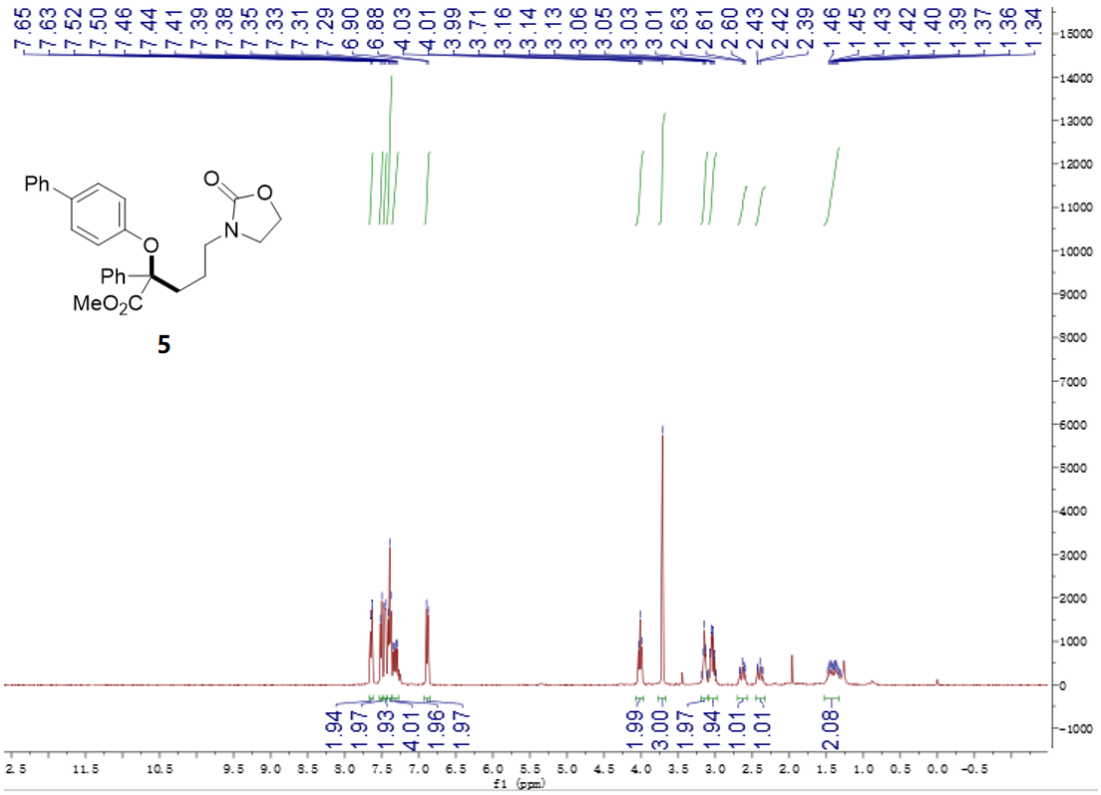
131.40
130.92
121.76
116.85
107.57
62.44
52.86
42.86
30.75
20.33
Br
CO2Me
O
N
O
trans-12b'
f1 (ppm)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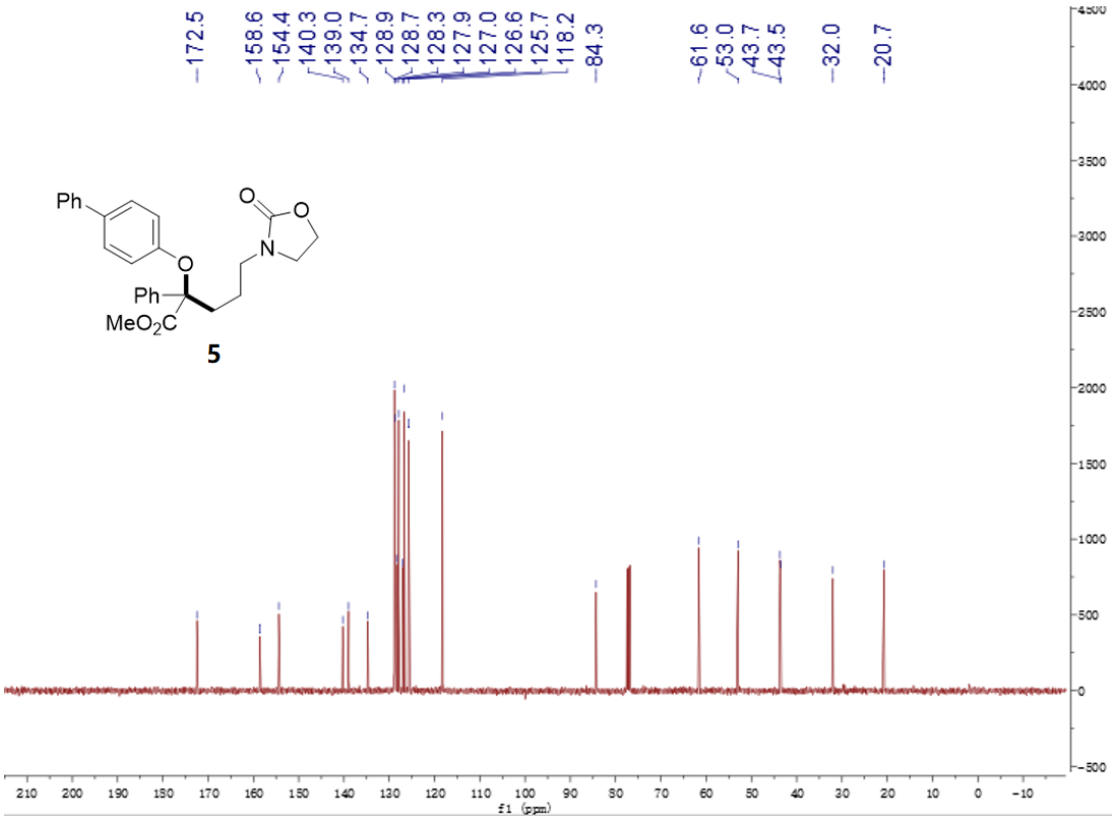
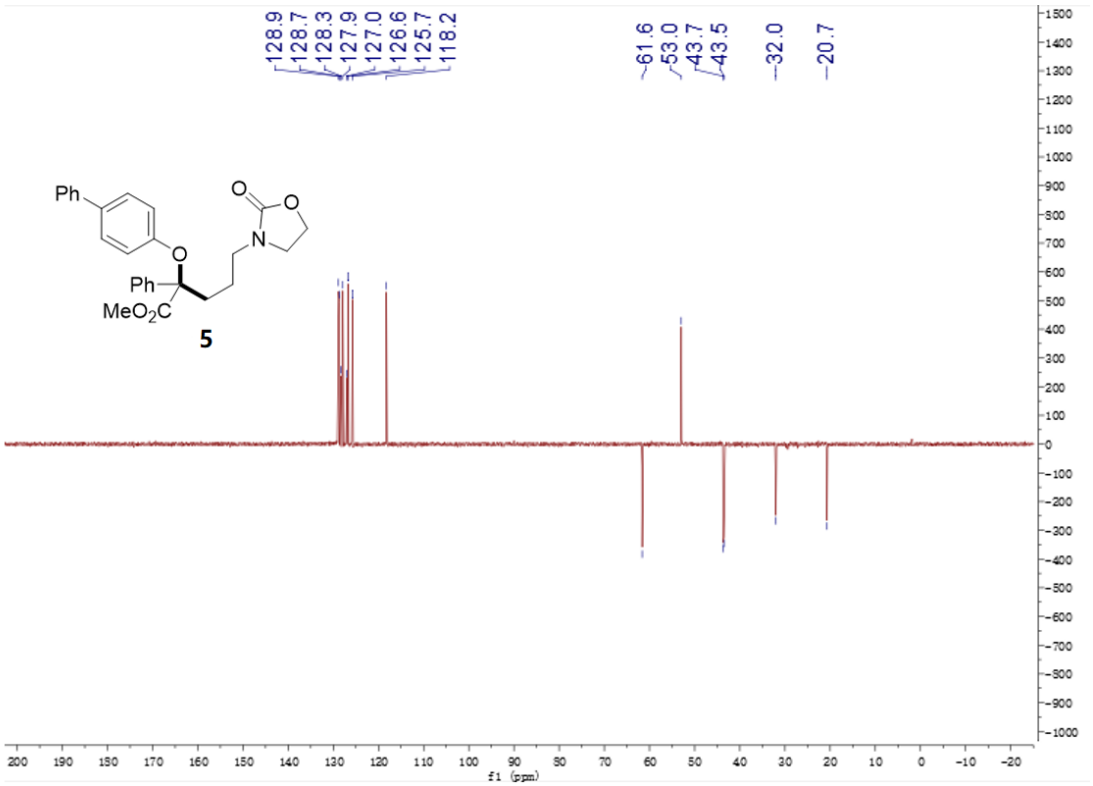
Ph
O
O
N
Ph
MeO2C
1.94 1.97 1.93 4.01 1.96 1.97 1.99 3.00 1.97 1.94 1.01 1.01 2.08
f1 (ppm)

5


172.5 158.6 154.4 140.3 139.0 134.7 128.9 128.7 128.3 127.9 127.0 126.6 125.7 118.2 84.3 61.6 53.0 43.7 43.5 32.0 20.7
Ph
O
O
N
Ph
MeO2C
f1 (ppm)

5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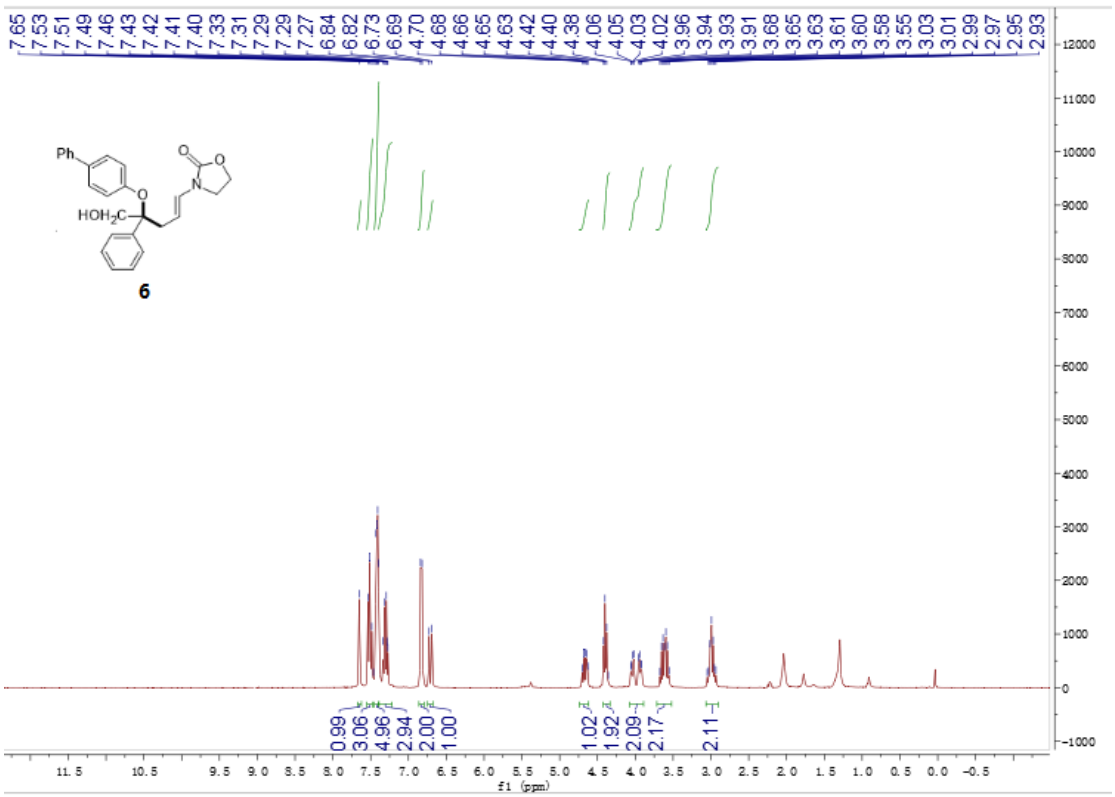
128.3
127.9
127.0
126.6
125.7
118.2
61.6
53.0
43.7
43.5
32.0
20.7
Ph
O
O
N
Ph
MeO2C
5
f1 (ppm)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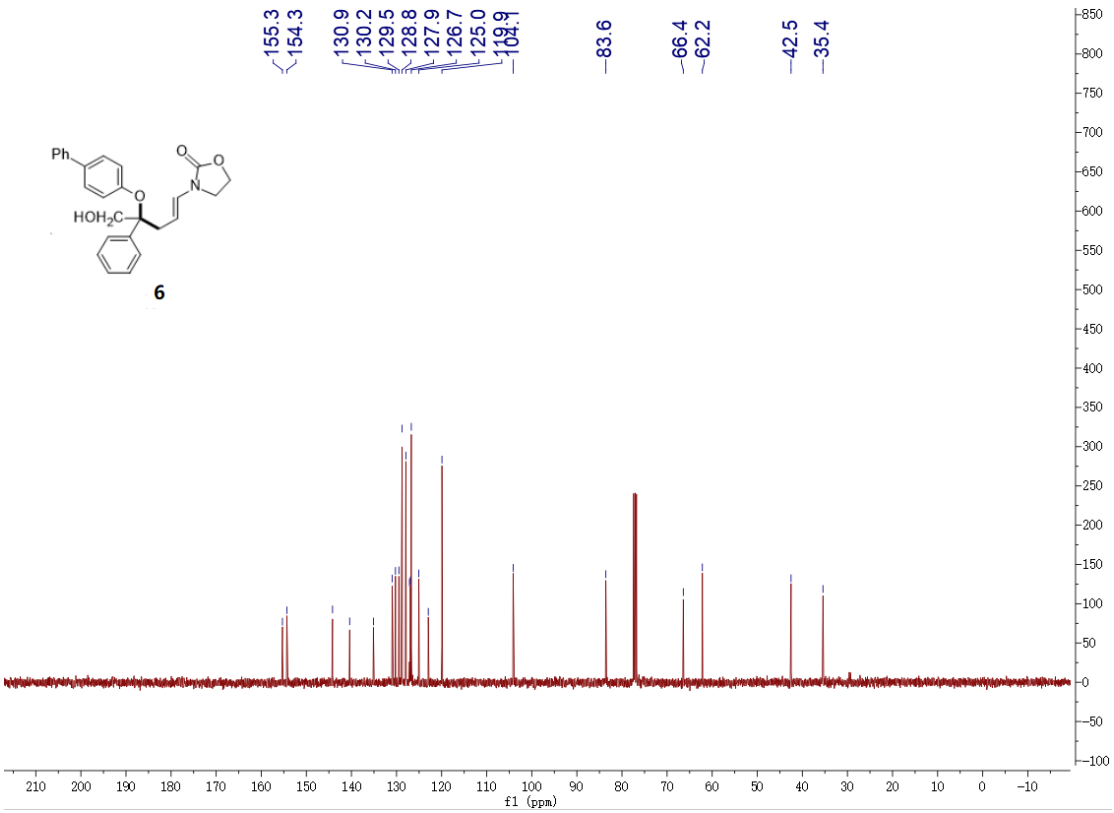
7.31
7.29
7.29
7.27
6.84
6.82
6.73
6.69
4.70
4.68
4.66
4.65
4.63
4.42
4.40
4.38
4.06
4.05
4.03
4.02
3.96
3.94
3.93
3.91
3.68
3.65
3.63
3.61
3.60
3.58
3.55
3.03
3.01
2.99
2.97
2.95
2.93
Ph
O
O
N
HOH2C
6
0.99
3.06
4.96
2.94
2.00
1.00
1.02
1.92
2.09
2.17
2.11
f1 (ppm)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154.3
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130.2
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128.8
127.9
126.7
125.0
119.9
104.1
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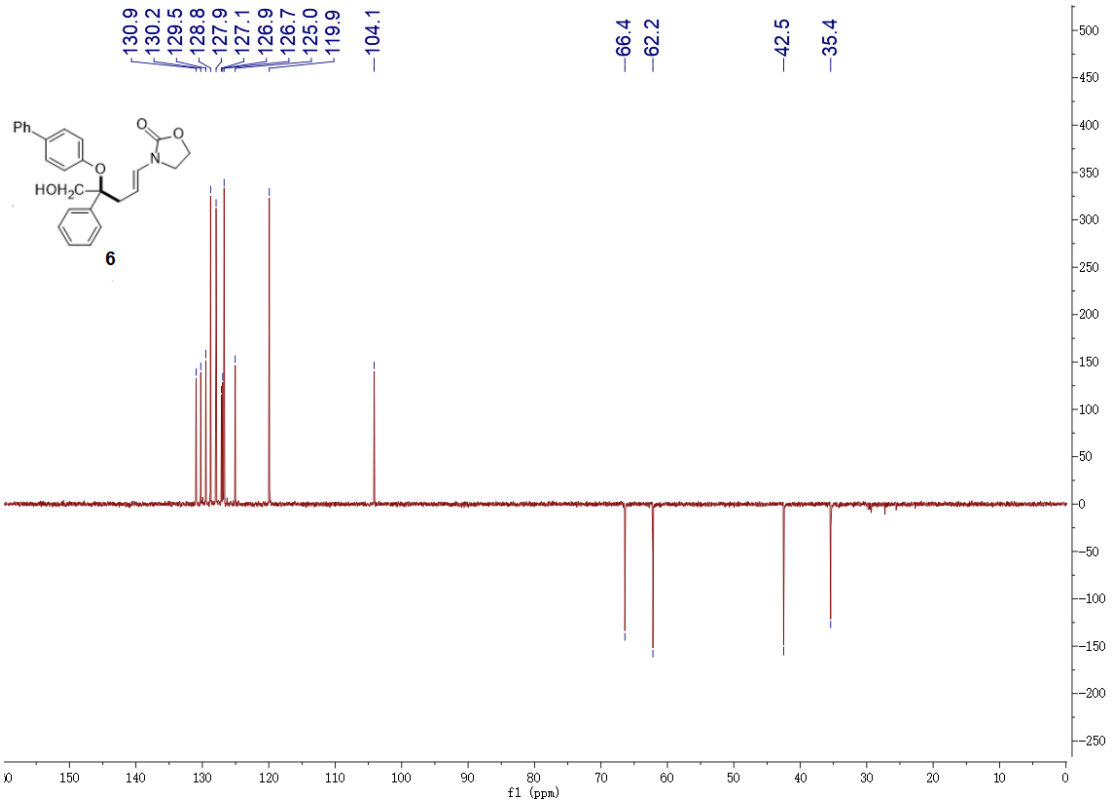
66.4
62.2
42.5
35.4
Ph
O
O
N
O
HOH2C
6
f1 (ppm)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127.9
127.1
126.9
126.7
125.0
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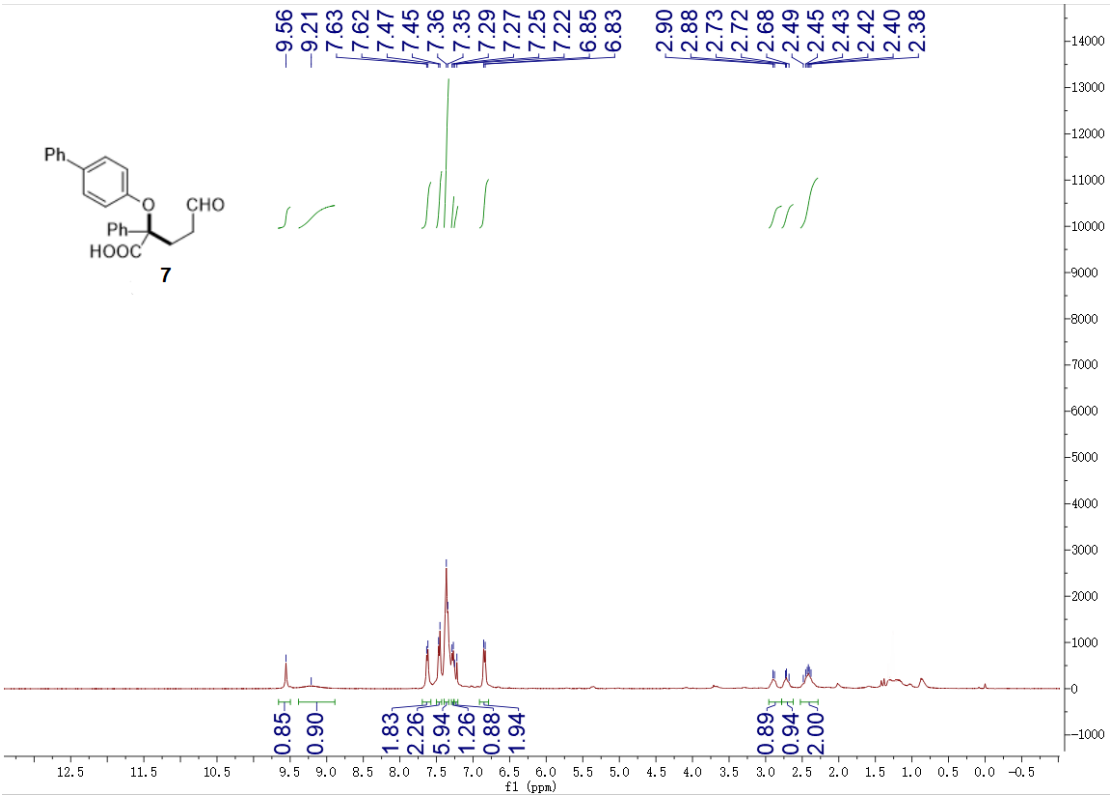
62.2
42.5
35.4
Ph
O
O
N
O
HOH2C
6
f1 (ppm)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7.25
7.22
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6.83
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2.88
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2.72
2.68
2.49
2.45
2.43
2.42
2.40
2.38
Ph
O
CHO
Ph
HOOC
7
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0.90
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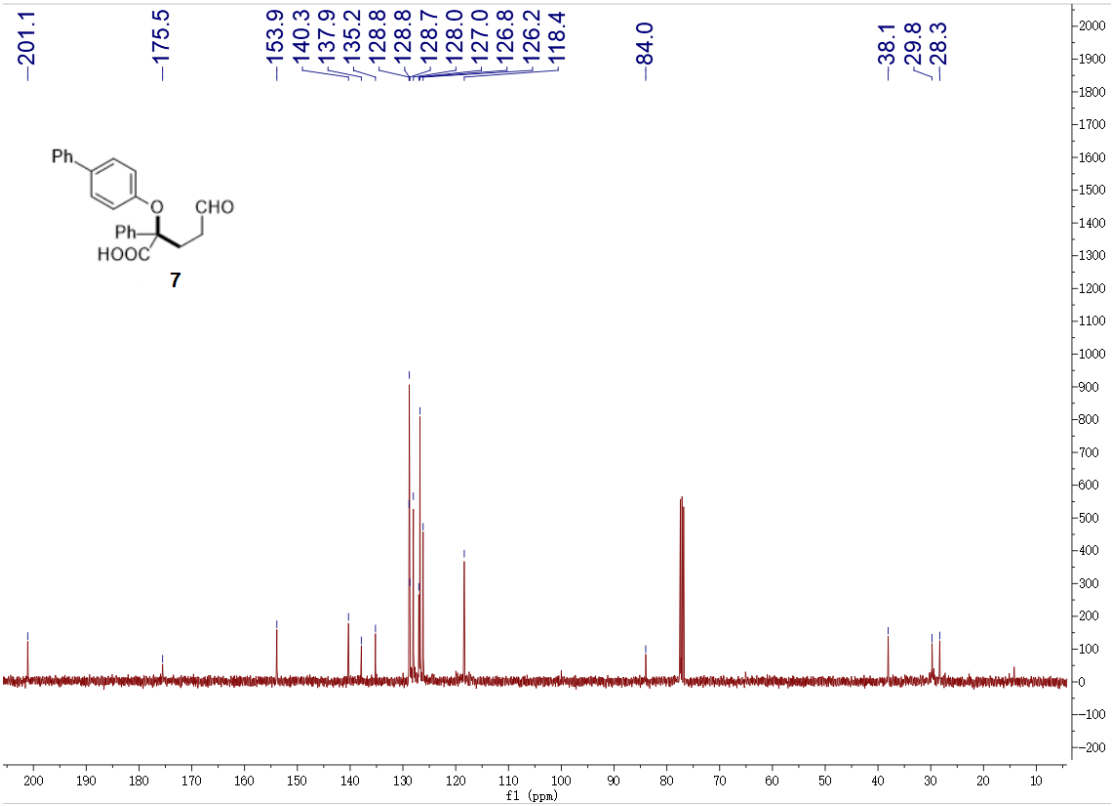
2.26
5.94
1.26
0.88
1.94
0.89
0.94
2.00
f1 (ppm)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135.2
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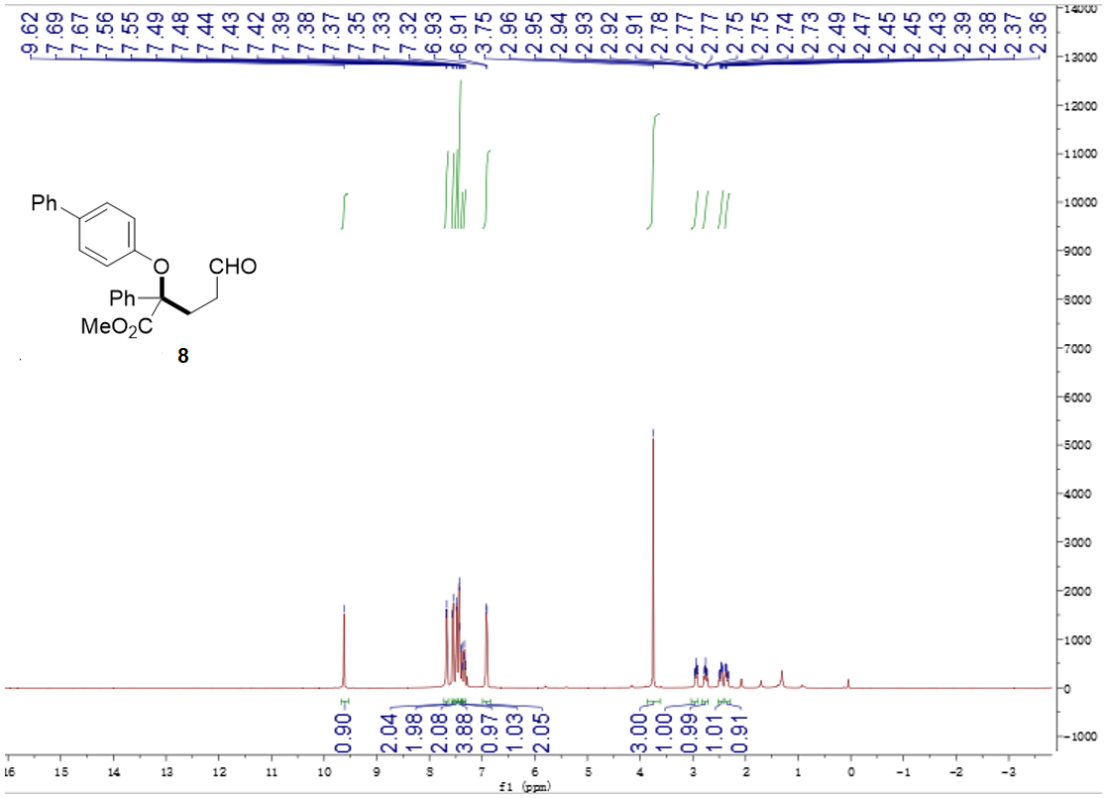
128.8
128.7
128.0
127.0
126.8
126.2
118.4
84.0
38.1
29.8
28.3
Ph
O
CHO
Ph
HOOC
7
f1 (ppm)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7.35
7.33
7.32
6.93
6.91
3.75
2.96
2.95
2.94
2.93
2.92
2.91
2.78
2.77
2.77
2.75
2.75
2.74
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2.47
2.45
2.45
2.43
2.39
2.38
2.37
2.36
Ph
O
CHO
Ph
MeO2C
8
0.90
2.04
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2.08
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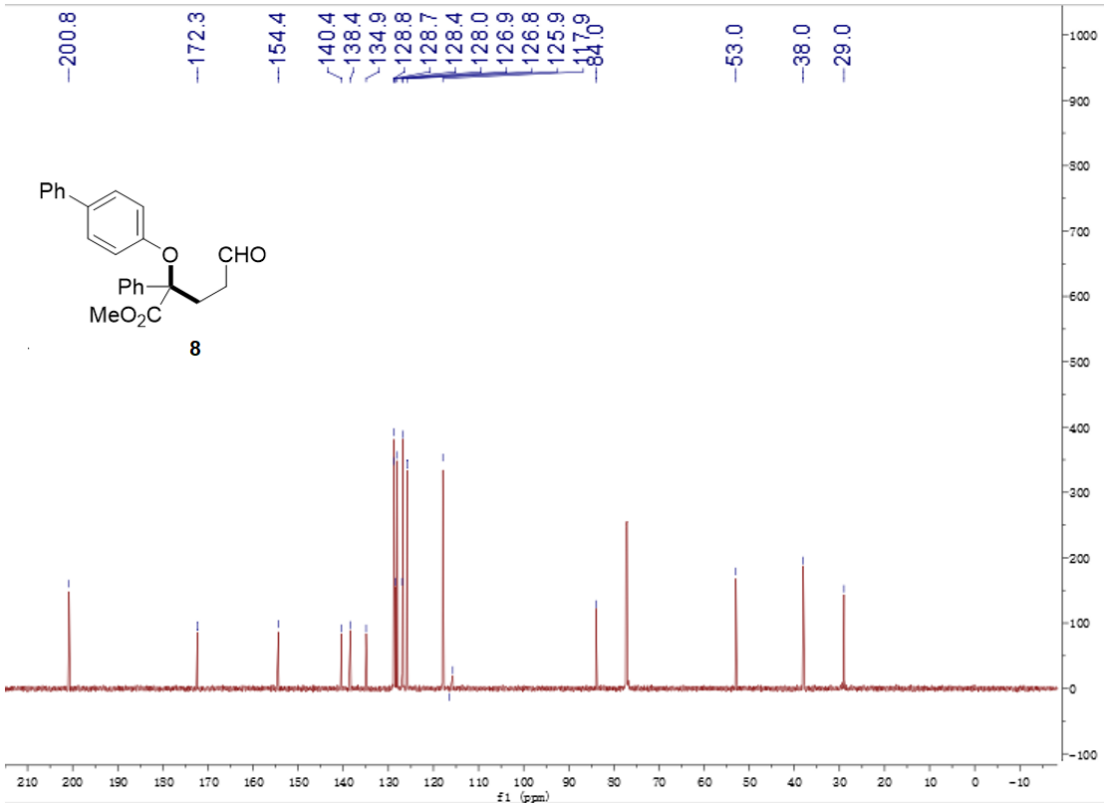
0.97
1.03
2.05
3.00
1.00
0.99
1.01
0.91
f1 (ppm)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128.7
128.4
128.0
126.9
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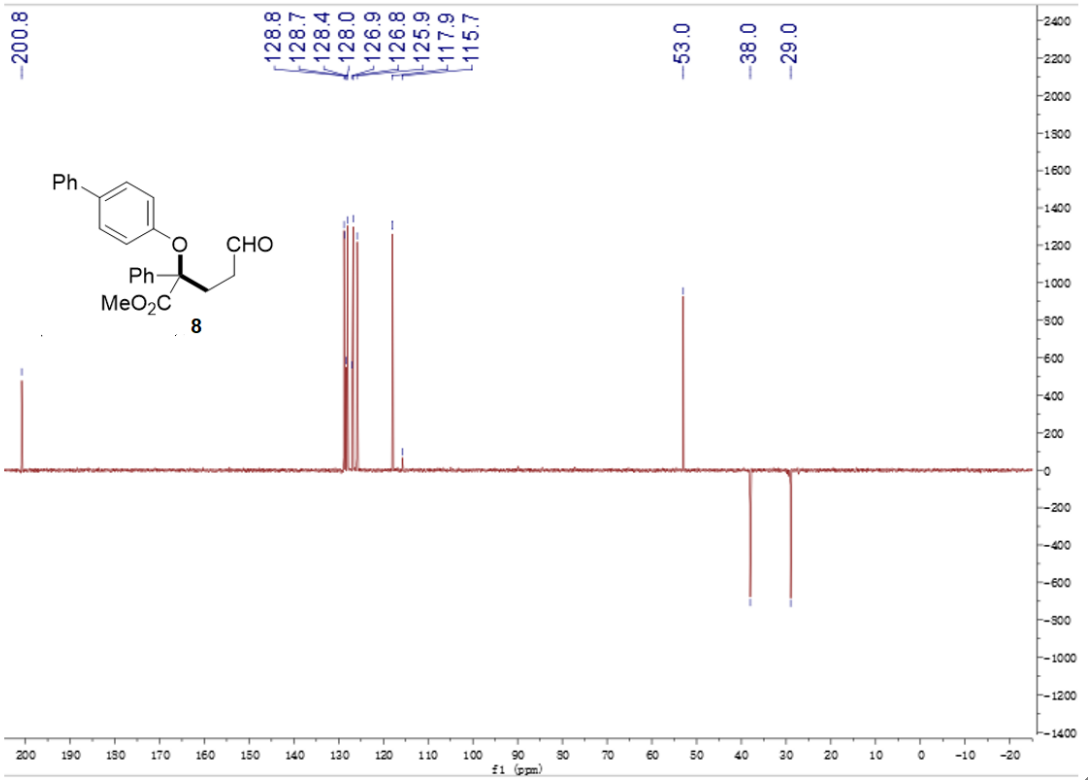
125.9
117.9
84.0
53.0
38.0
29.0
Ph
O
CHO
Ph
MeO2C
8
f1 (ppm)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126.9
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117.9
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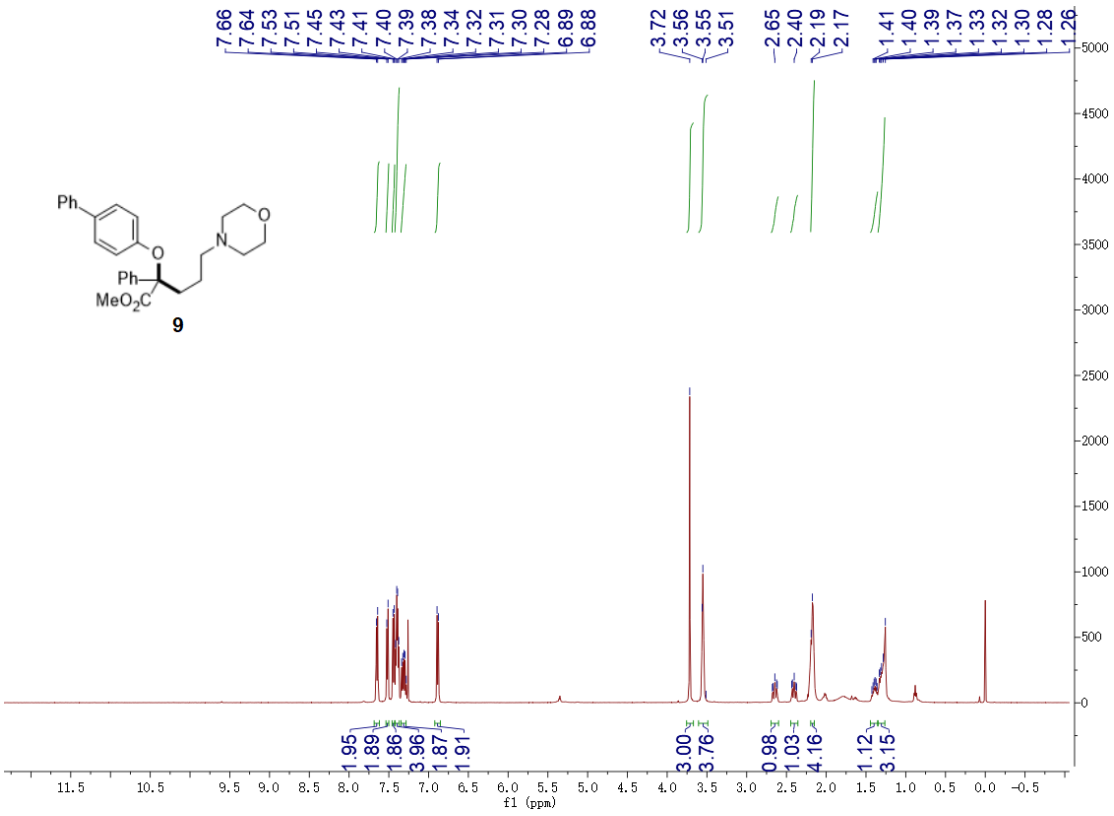
53.0
38.0
29.0
Ph
O
CHO
Ph
MeO2C
8
f1 (ppm)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6.89
6.88
3.72
3.56
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3.51
2.65
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1.41
1.40
1.39
1.37
1.33
1.32
1.30
1.28
1.26
Ph
O
N
O
Ph
MeO2C
9
1.95
1.89
1.86
3.96
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3.76
0.98
1.03
4.16
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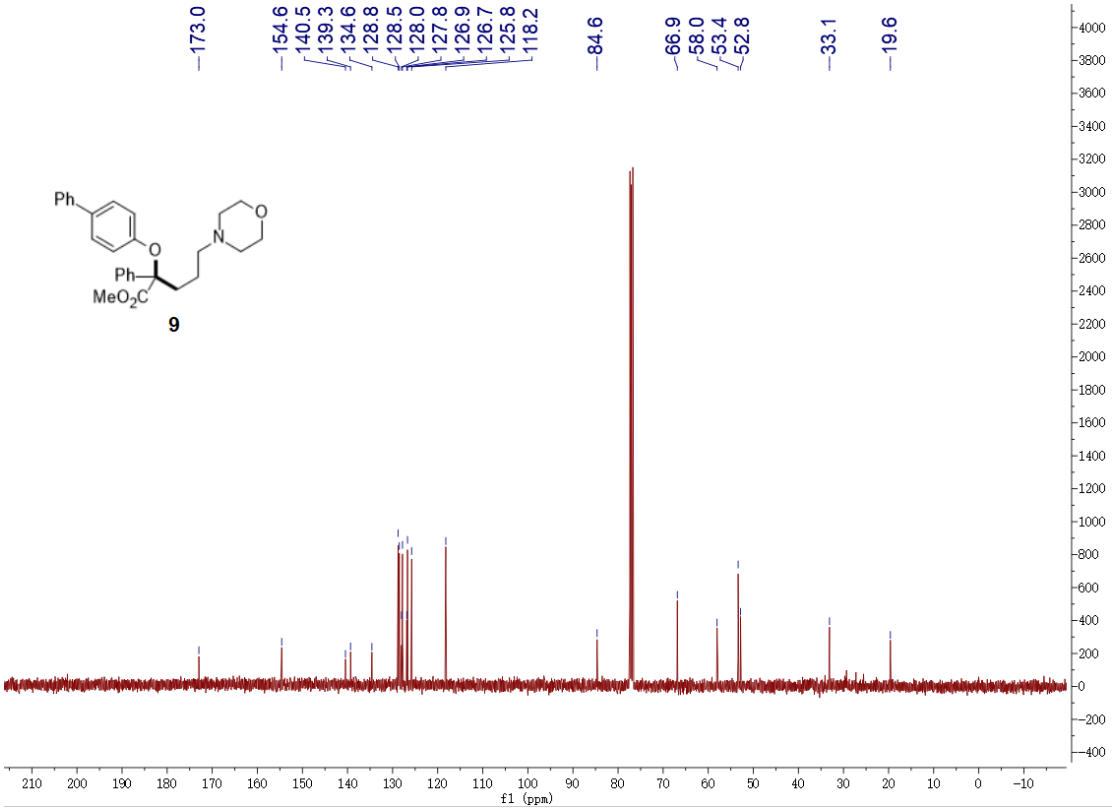
3.15
f1 (ppm)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139.3
134.6
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126.7
125.8
118.2
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33.1
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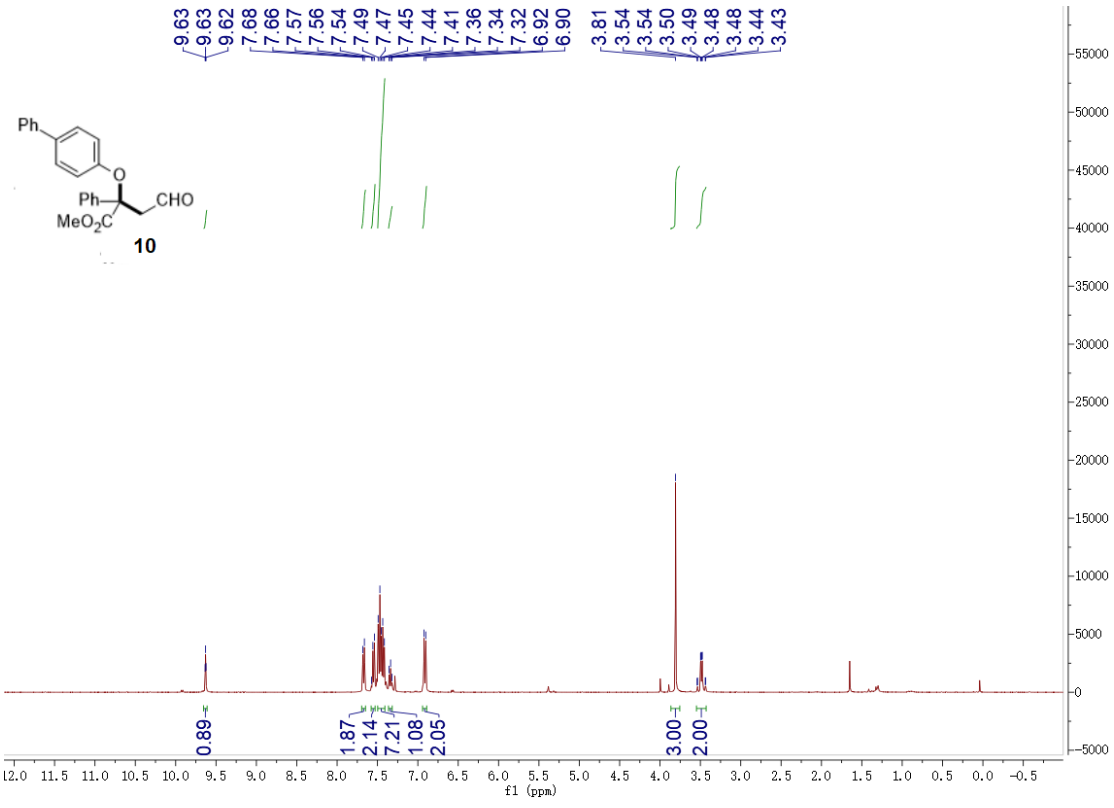
O
N
Ph
MeO2C
9
f1 (ppm)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7.36
7.34
7.32
6.92
6.90
3.81
3.54
3.54
3.50
3.49
3.48
3.48
3.44
3.43
Ph
O
Ph
CHO
MeO2C
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0.89
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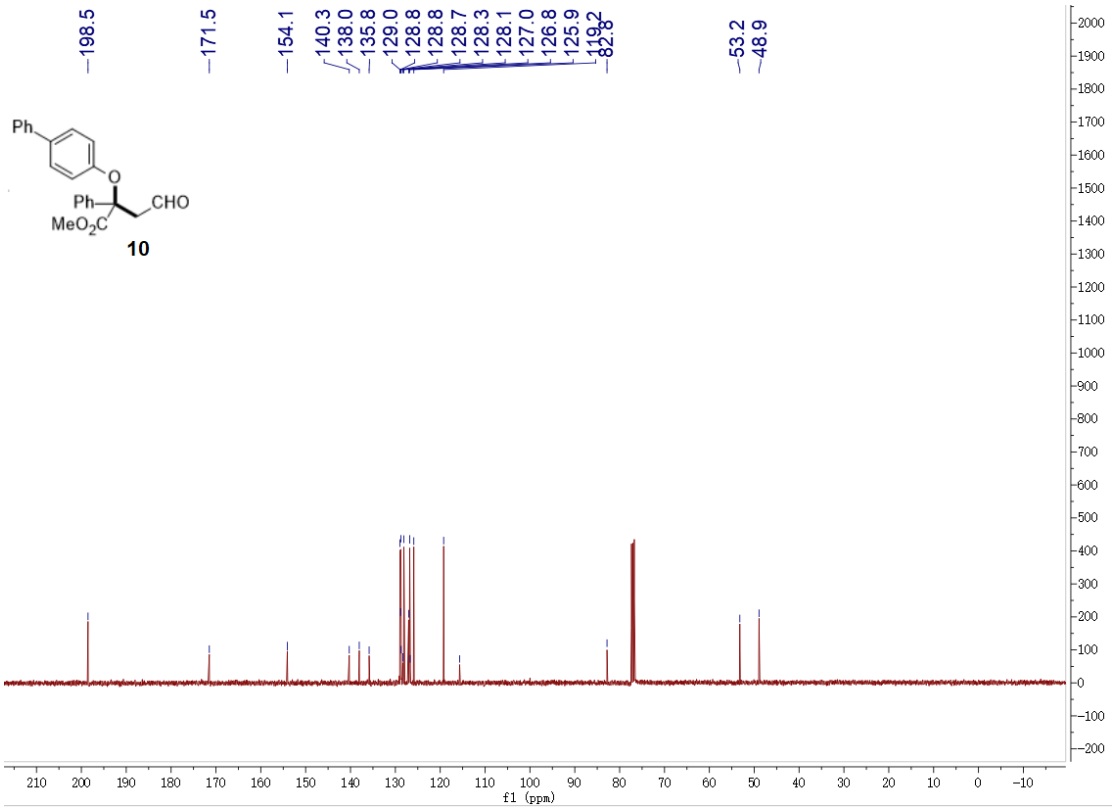
2.14
7.21
1.08
2.05
3.00
2.00
f1 (ppm)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129.0
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128.3
128.1
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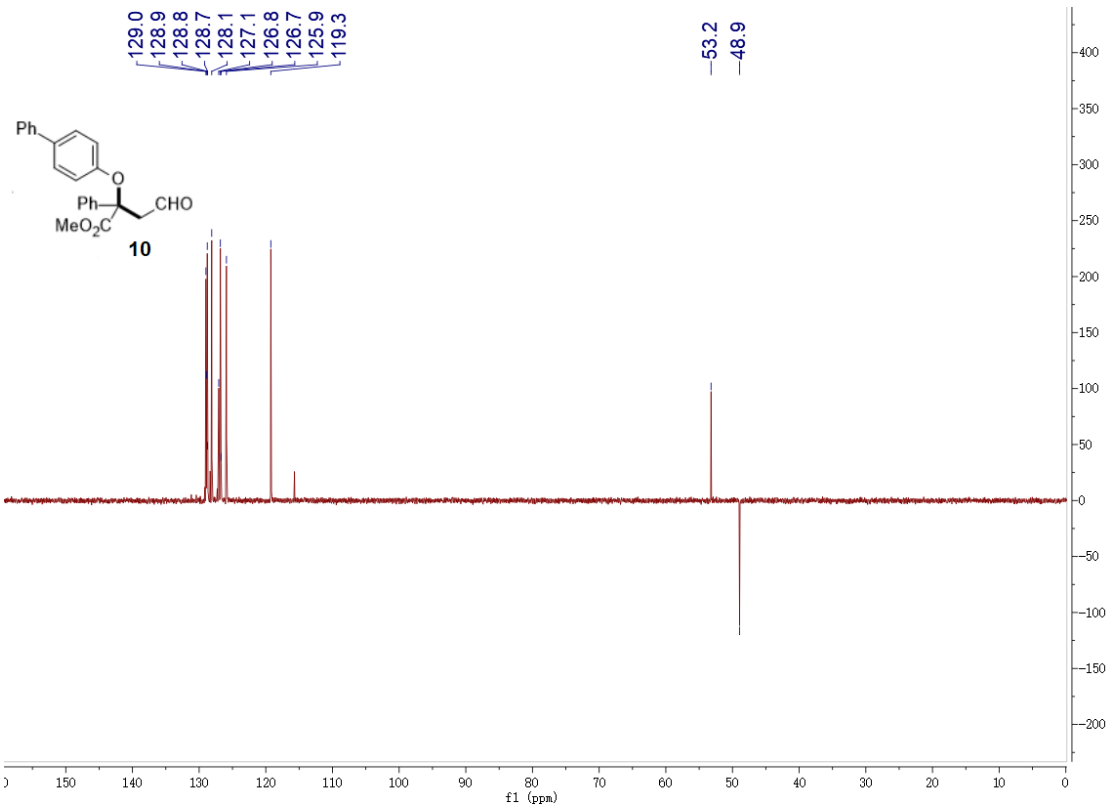
125.9
119.2
82.8
53.2
48.9
Ph
O
Ph
CHO
MeO2C
10
f1 (ppm)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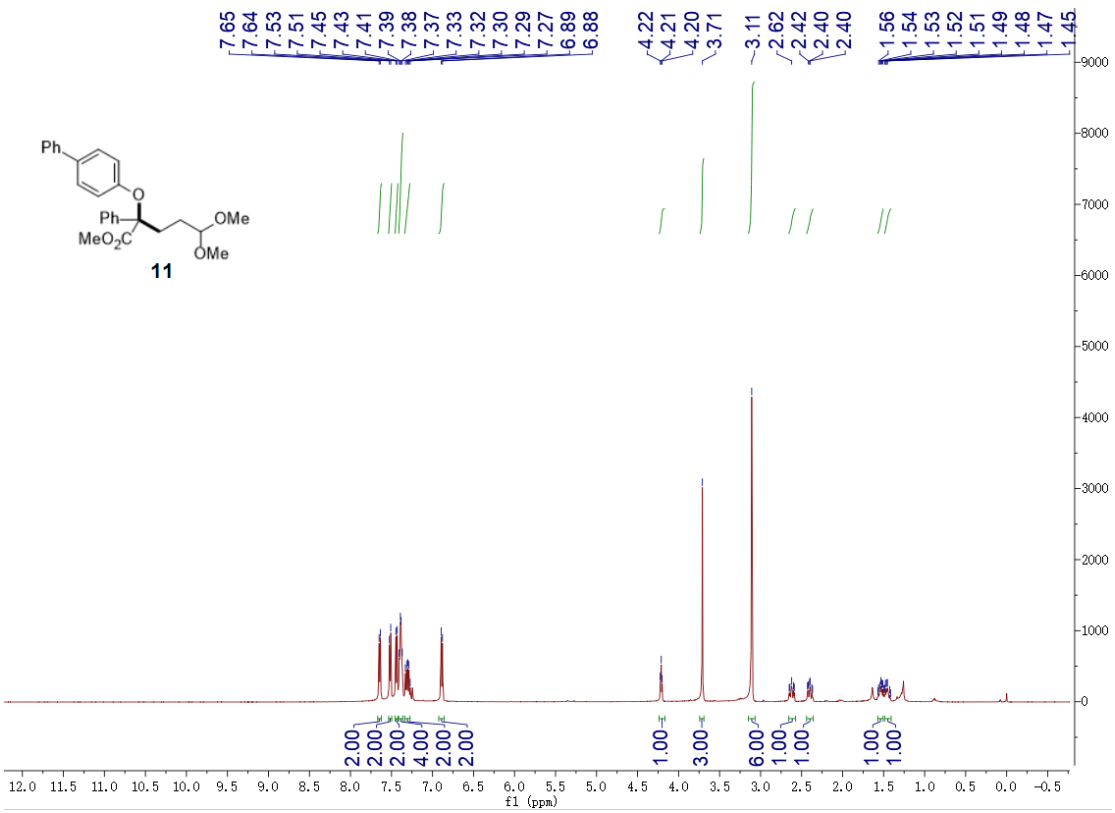
53.2
48.9
Ph
O
Ph
CHO
MeO2C
10
f1 (ppm)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7.29
7.27
6.89
6.88
4.22
4.21
4.20
3.71
3.11
2.62
2.42
2.40
2.40
1.56
1.54
1.53
1.52
1.51
1.49
1.48
1.47
1.45
Ph
O
Ph
MeO2C
OMe
OMe
11
2.00
2.00
2.00
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2.00
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3.00
6.00
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1.00
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1.00
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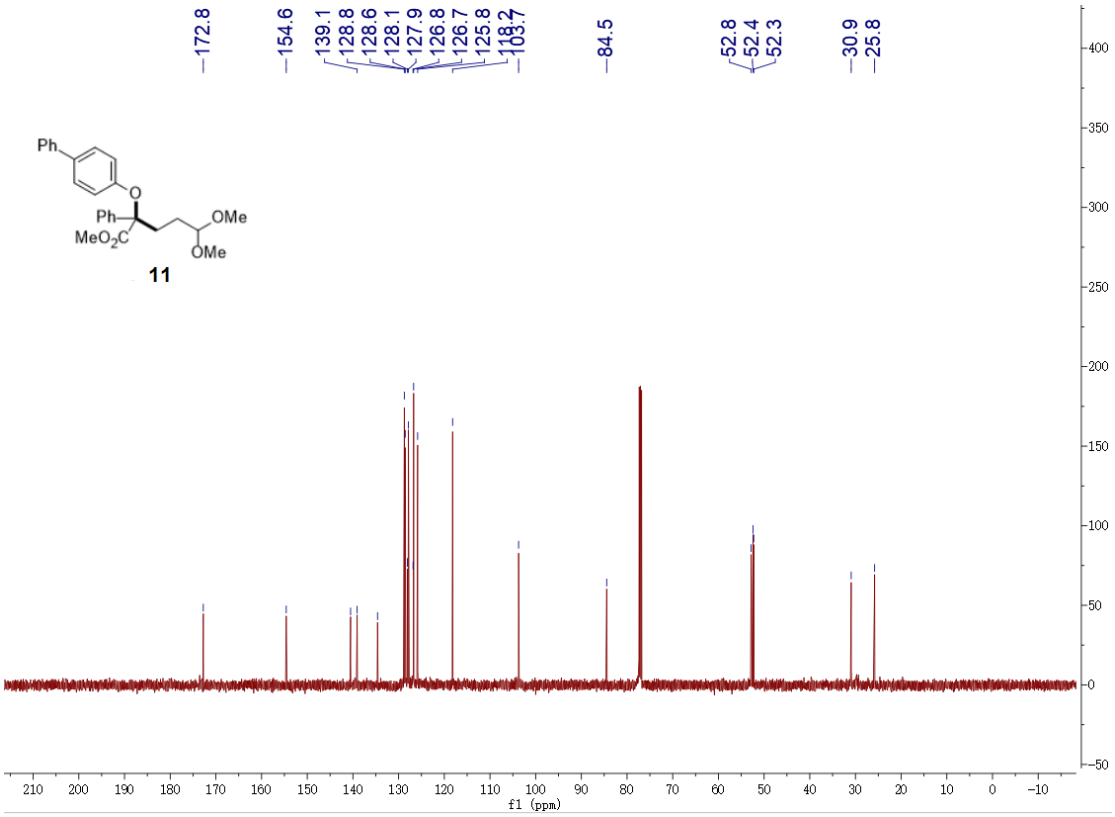
172.8
154.6
139.1
128.8
128.6
128.1
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118.2
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52.8
52.4
52.3
30.9
25.8
Ph
O
Ph
MeO2C
OMe
OMe
11
f1 (ppm)