[Electronic supplementary information]

Construction of Quaternary Stereogenic Center by Asymmetric Hydroformylation: A Straightforward Method to Prepare Chiral α-Quaternary Amino Acids

Dequan Zhang[†], Jialin Wen[†,‡]* and Xumu Zhang[†]*

[†] Department of Chemistry, Guangdong Provincial Key Laboratory of Catalysis, Southern University of Science and Technology, Shenzhen, 518055, China.

[‡] Academy for Advanced Interdisciplinary Studies, Southern University of Science and Technology, Shenzhen, 518055, China.

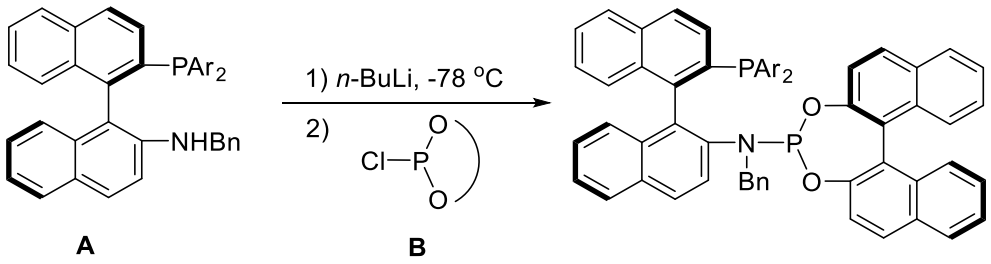
Contents

1. General remarks

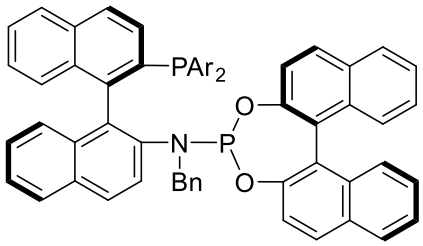
All the reactions dealing with air- or moisture- sensitive compounds were carried out in a dry reaction vessel under an argon atmosphere or in an argon-filled glove box. Unless otherwise noted, all reagents and solvents were purchased from commercial suppliers without further purification. Toluene was distilled over sodium chips and indicated by benzophenone under an argon atmosphere. Other anhydrous solvents were purchased from J&K Chemical and degassed by bubbling argon over a period of 30 min. Purification of products was carried out by flash chromatography using silica gel (200-300 mesh). Thin layer chromatography (TLC) was performed on EM reagents 0.25 mm silica 60-F plates. The metal precursor $Rh(acac)(CO)_2$ was purchased from Umicore.

^{1}H, ^{13}C, ^{19}F and ^{31}P NMR spectra were recorded on a Bruker Avance 400 MHz or on a Bruker Avance 600 MHz spectrometer with tetramethylsilane as the internal standard. Chemical shifts are reported in parts per million (ppm, δ scale) downfield from TMS at 0.00 ppm and referenced to the $CDCl_3$ at 7.27 ppm for ^{1}H NMR or 77.0 ppm for ^{13}C NMR. Data are reported as: multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant in hertz (Hz) and signal area integration in natural numbers. ^{13}C NMR and ^{31}P NMR analyses were recorded with ^{1}H decoupling. HPLC analysis was conducted on an Agilent 1260 Series instrument. GC analysis was carried out on Agilent 7890 Series instrument using chiral capillary columns. Optical rotations were measured using a 1 mL cell with a 1 dm path length on a Rudolph Autopol I polarimeter at 589 nm. All new products were further characterized by HRMS. A positive ion mass spectrum of sample was acquired on a Thermo LTQ-FT mass spectrometer with an electrospray ionization source. Crystal structure was measured with BRUKER APEX III diffractometer.

2. Procedures for the preparation of (*R*,*S*)-DTBM-Bn-YanPhos



(*R*,*S*)-DTBM-Bn-YanPhos was prepared according to the literature.[1,2] To a solution of A (3.3 mmol) in THF (30 mL) at -78 °C was added dropwise *n*-BuLi (5.0 mmol, 1.6 M in hexane). The reaction mixture was stirred for 1 h to give a deep red solution, and B (5.0 mmol) in THF (15 mL) was added dropwise. After addition, the cooling bath was removed and the mixture was stirred at room temperature overnight. The volatiles were evaporated under reduced pressure. To the residue was added CH_2Cl_2 (30 mL), and the mixture was filtered to remove the salt. The filtration was concentrated and subjected to chromatography on silica gel (eluted with hexane/EtOAc 100:1 to 10:1) to afford pure ligands.



(*R*,*S*)-DTBM-Bn-YanPhos
Ar = 3,5-*t*-Bu-4-OMe-C_6H_2

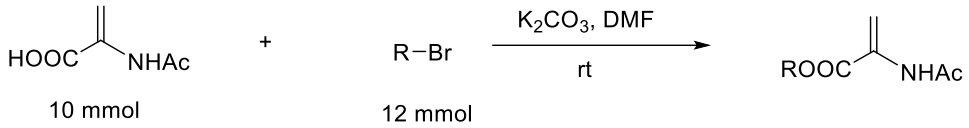
(*R*,*S*)-DTBM-Bn-YanPhos: white solid, 1.85 g, 49% yield. $[\alpha]^{22}_D$ = -123.7 (c = 1.0, $CHCl_3$). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.22 (dd, *J* = 15.72, 8.39 Hz, 2H), 7.95 (d, *J* = 8.80 Hz, 1H), 7.89 (d, *J* = 8.18 Hz, 1H), 7.77 (dd, *J* = 8.55, 2.80 Hz, 1H), 7.70 – 7.57 (m, 5H), 7.47 (d, *J* = 8.43 Hz, 1H), 7.41 (dt, *J* = 13.86, 7.36 Hz, 2H), 7.35 (d, *J* = 8.26 Hz, 1H), 7.31 – 7.20 (m, 6H), 7.16 (q, *J* = 7.64, 7.07 Hz, 2H), 7.12 – 7.00 (m, 9H), 6.67 (d, *J* = 8.47 Hz, 2H), 6.45 (t, *J* = 7.76 Hz, 1H), 6.29 (d, *J* = 8.54 Hz, 1H), 5.62 (d, *J* = 8.83 Hz, 1H), 3.87 (d, *J* = 14.43 Hz, 1H), 3.55 (s, 3H), 3.45 (s, 3H), 3.24 (d, *J* = 14.52 Hz, 1H), 1.14 (s, 18H), 0.86 (s, 18H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 160.2, 159.1, 149.9, 149.9, 149.7, 142.9, 142.8, 142.8, 141.5, 141.3, 139.8, 138.3, 138.0, 137.9, 137.7, 133.9, 133.8, 133.7, 133.7, 133.0, 132.4, 132.2, 132.2, 132.1, 131.6, 131.2, 131.1, 130.8,

130.6, 130.1, 130.0, 129.6, 129.2, 128.5, 128.4, 128.3, 128.1, 127.9, 127.7, 127.6, 127.3, 127.2, 127.0, 126.9, 126.8, 126.5, 125.9, 125.8, 125.5, 124.7, 124.5, 124.4, 122.7, 122.5, 122.2, 64.3, 64.0, 51.6, 35.6, 35.6, 32.0, 31.8. ^{31}P NMR (243 MHz, Chloroform-*d*) δ 133.85 (d, *J* = 92.29 Hz), -14.00 (d, *J* = 91.76 Hz). **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{77}H_{78}NO_4P_2$ = 1142.5406; Found 1142.5412.

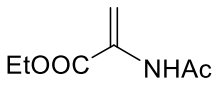
3. General procedure for the synthesis of substrates

The substrates of methyl 2-acetamidoacrylate (**1a**), methyl 2-((tert-butoxycarbonyl)amino)acrylate (**1g**), methyl 2-acetoxyacrylate (**1j**), 3-methylene-1-phenylazetidin-2-one (**1m**) and methyl 2-fluoroacrylate (**1u**) are commercially available.

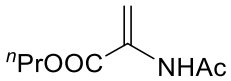
Preparation of compound 1b-1e:



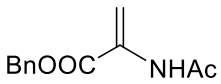
1b-1e were synthesized according to the literature procedure.[3] To a stirred mixture of 2-acetamidoacrylic acid (1.29 g, 10.0 mmol) and K_2CO_3 (1.66 g, 12 mmol) in DMF (15 mL) was added R-Br (12 mmol) at room temperature. After stirred at room temperature for 3 h, the reaction mixture was partitioned between 1:1 (v/v) of EtOAc and water (20mL), the aqueous layer was extracted with EtOAc (2 × 30 mL). The combined organic layers were washed with brine (2 × 25 mL), dried ($MgSO_4$), filtered, and concentrated in vacuo to provide **1b-1e**.



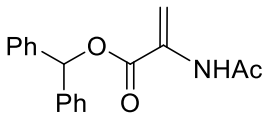
(4-methylpent-4-ene-2,2-diyldisulfonyl)dibenzene (1b)[3]: colourless oil, 1.49 g, 95% yield; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.78 (s, 1H), 6.58 (s, 1H), 5.88 (d, *J* = 1.5 Hz, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 2.13 (s, 3H), 1.35 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.9, 164.1, 131.1, 108.4, 62.2, 24.7, 14.1 ppm.



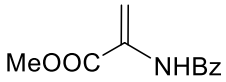
Propyl 2-acetamidoacrylate (1c)[4]: colourless oil, 1.57 g, 92% yield; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.79 (s, 1H), 6.58 (s, 1H), 5.88 (d, *J* = 1.5 Hz, 1H), 4.20 (t, *J* = 6.7 Hz, 2H), 2.13 (s, 3H), 1.74 (dtd, *J* = 14.0, 7.4, 6.6 Hz, 2H), 0.99 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.9, 164.2, 131.1, 108.3, 67.7, 24.6, 21.9, 10.3 ppm.



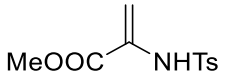
Penzyl 2-acetamidoacrylate (1d)[5]: white solid, 2.08 g, 95% yield; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 (s, 1H), 7.37 (d, *J* = 3.4 Hz, 5H), 6.61 (s, 1H), 5.94 (d, *J* = 1.5 Hz, 1H), 5.26 (s, 2H), 2.11 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.9, 164.1, 135.1, 131.0, 128.7, 128.6, 128.2, 109.0, 67.8, 24.7 ppm.



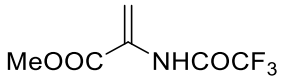
Penzhydryl 2-acetamidoacrylate (1e): white solid, 2.80 g, 95% yield; ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.71 (s, 1H), 7.36 (d, *J* = 4.7 Hz, 8H), 7.33 – 7.29 (m, 2H), 6.93 (s, 1H), 6.67 (s, 1H), 6.08 (d, *J* = 1.5 Hz, 1H), 2.09 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.8, 163.4, 139.4, 131.1, 128.7, 128.3, 127.0, 108.9, 24.7 ppm.



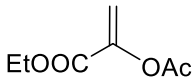
Methyl 2-benzamidoacrylate (1f)[6] was synthesized according to the literature procedure. Colourless oil, the ^{1}H NMR and ^{13}C NMR data obtained corresponded to the literature. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.54 (s, 1H), 7.88 – 7.81 (m, 2H), 7.58 – 7.51 (m, 1H), 7.51 – 7.44 (m, 2H), 6.80 (s, 1H), 6.00 (d, *J* = 1.4 Hz, 1H), 3.89 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.8, 164.8, 134.3, 132.1, 131.1, 128.8, 127.0, 108.9, 53.1 ppm.



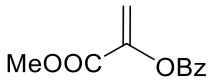
Methyl 2-((4-methylphenyl)sulfonamido)acrylate (1h)[7] was synthesized according to the literature procedure. Yellow oil, the ^{1}H NMR and ^{13}C NMR data obtained corresponded to the literature. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.77 – 7.73 (m, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.13 (s, 1H), 5.67 (d, *J* = 1.3 Hz, 1H), 5.64 (t, *J* = 1.5 Hz, 1H), 3.76 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 163.7, 144.4, 135.4, 130.8, 129.7, 127.6, 106.9, 53.2, 21.6 ppm.



Methyl 2-(2,2,2-trifluoroacetamido)acrylate (1i)[8] was synthesized according to the literature procedure. Yellow oil, the ^{1}H NMR and ^{13}C NMR data obtained corresponded to the literature. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.55 (s, 1H), 6.72 (d, *J* = 1.0 Hz, 1H), 6.15 (t, *J* = 1.2 Hz, 1H), 3.92 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.46, 154.95, 129.48, 116.65, 113.78, 112.38, 53.45 ppm.

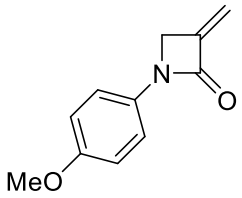


Ethyl 2-acetoxyacrylate (1k)[9] was synthesized according to the literature procedure. Colourless oil, the ^{1}H NMR and ^{13}C NMR data obtained corresponded to the literature. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.05 (d, *J* = 1.7 Hz, 1H), 5.47 (d, *J* = 1.7 Hz, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 2.24 (s, 3H), 1.32 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.0, 161.4, 144.8, 113.7, 61.8, 20.4, 14.0 ppm.



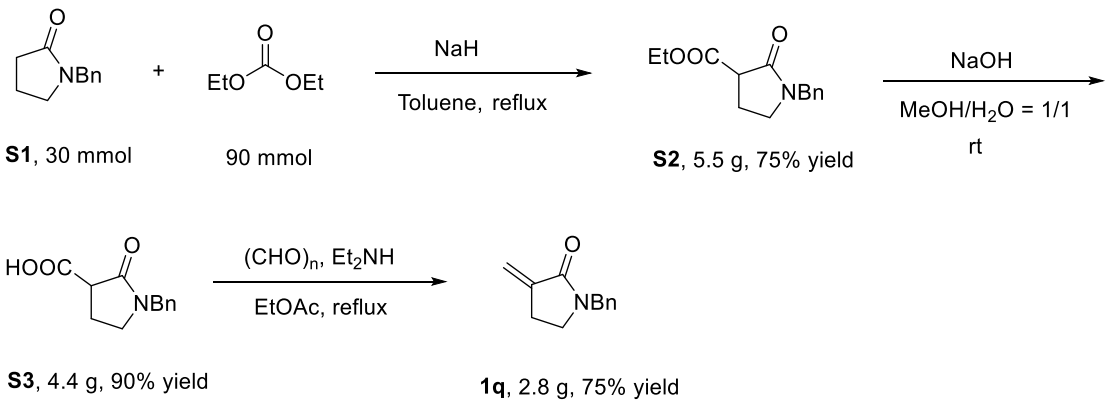
3-methoxy-3-oxoprop-1-en-2-yl benzoate (1l)[10] was synthesized according to the literature procedure. Colourless oil, the ^{1}H NMR and ^{13}C NMR data obtained corresponded to the literature. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.13 – 8.11 (m, 2H), 7.63 – 7.60 (m, 1H), 7.49 – 7.47 (m, 2H), 6.17 (d, *J* = 1.6 Hz, 1H), 5.62 (d, *J* = 1.6 Hz, 1H), 3.81

(d, J = 1.4 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.7, 162.1, 144.8, 133.9, 133.8, 130.3, 128.6, 114.4, 52.7 ppm.



1-(4-methoxyphenyl)-3-methyleneazetidin-2-one (1n)[11] was synthesized according to the literature procedure. Brown oil, the ^{1}H NMR and ^{13}C NMR data obtained corresponded to the literature. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 – 7.31 (m, 2H), 6.99 – 6.86 (m, 2H), 5.84 (q, J = 1.7 Hz, 1H), 5.32 (q, J = 1.4 Hz, 1H), 4.10 (t, J = 1.5 Hz, 2H), 3.81 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.8, 156.3, 143.5, 132.0, 117.7, 114.5, 110.6, 55.5, 47.9 ppm.

Preparation of compound 1o-1s: (**1q** as an example)[12]



S1, 30 mmol

90 mmol

S2, 5.5 g, 75% yield

S3, 4.4 g, 90% yield

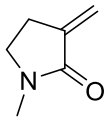
1q, 2.8 g, 75% yield

To a stirring solution of NaH (60%, 3.6 g, 90 mmol, 3.0 equiv) in toluene (150 mL) at 0 °C was slowly added a solution of **S1** (5.25 g, 30 mmol, 1.0 equiv, in 25 mL toluene) over 1 hour under the atmosphere of Argon. After addition, the resulting mixture was stirring at 0 °C for 1 hour. Diethyl carbonate (10.63 g, 90 mmol, 3.0 equiv, in 10 mL toluene) was injected into the mixture in five minutes. The mixture was then warm up to reflux and kept refluxing for 8 hours. Then the reaction was quenched with brine. Organic layer was collected and the aqueous layer was extracted with DCM. The combined organic layer was dried over anhydrous Na_2SO_4, filtrated, concentrated under vacuum. The residue was purified by flash chromatography on silica gel with EtOAc/PE (1/4) as eluents to give **S2** (5.5 g, 22.2 mmol, 75% yield) as colorless oil.

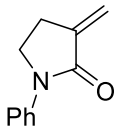
To a stirring solution of **S2** (5.5 g, 22.2 mmol, 1.0 equiv) in 35 mL MeOH was slowly added a solution of NaOH (890 mg, 22.2 mmol, 1.0 eq, in 35 mL H_2O). The mixture was then stirring overnight at the room tempretrue. The reaction was quenched with 2N HCl (25 mL) and extracted with DCM. The organic layer was dried over anhydrous Na_2SO_4, filtrated, concentrated under vacuum to give **S3** (4.4 g, 20 mmol, 90% yield) as white solid without any

purification.

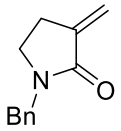
To a stirring solution of **S3** (4.4 g, 20 mmol, 1 equiv), paraformaldehyde (870 mg, 30 mmol, 1.5 equiv) in 50 ml EtOAc was added a solution of diethylamine (1.75 g, 24 mmol, 1.2 equiv, in 5 ml EtOAc) at 0 ºC. After the addition was finished, the mixture was heated to reflux for 4 hours and then cooled to room tempreture. 2N HCl (25 mL) was added to the mixture to quench the reaction. The organic layer was collected and dried with anhydrous Na_2SO_4, filtrated, concentrated under vacuum. The residue was purified by flash chromatography on silica gel with EtOAc/PE = 1/5 to give **1q** (2.8 g, 75% yield) as yellow oil.



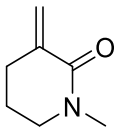
1-methyl-3-methylenepyrrolidin-2-one (1o)[12] : colourless oil, 58% yield (1.93 g, over three procedures); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.03 – 5.91 (m, 1H), 5.41 – 5.26 (m, 1H), 3.45 – 3.35 (m, 2H), 2.95 (s, 3H), 2.77 (tt, *J* = 6.4, 2.6 Hz, 2H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.1, 139.5, 115.0, 46.3, 30.2, 24.0 ppm.



3-methylene-1-phenylpyrrolidin-2-one (1p)[12] **:** colourless oil, 55% yield (2.86 g, over three procedures); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.81 – 7.69 (m, 2H), 7.48 – 7.38 (m, 2H), 7.24 – 7.11 (m, 1H), 6.16 (t, *J* = 2.9 Hz, 1H), 5.47 (t, *J* = 2.5 Hz, 1H), 3.89 (t, *J* = 6.9 Hz, 2H), 2.93 (tt, *J* = 6.7, 2.7 Hz, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.0, 140.2, 139.6, 128.9, 124.8, 119.7, 116.8, 45.2, 23.8 ppm.



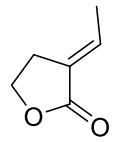
1-benzyl-3-methylenepyrrolidin-2-one (1q)[12] **:** colourless oil, 54% yield (3.03 g, over three procedures); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.24 (m, 5H), 6.06 (t, *J* = 2.8 Hz, 1H), 5.38 (t, *J* = 2.5 Hz, 1H), 4.57 (s, 2H), 3.32 – 3.21 (m, 2H), 2.75 (tt, *J* = 6.6, 2.7 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.9, 139.6, 136.3, 128.7, 128.3, 127.7, 115.8, 47.3, 43.5, 24.0 ppm.



1-methyl-3-methylenepiperidin-2-one (1r)[13] **:** colourless oil, 50% yield (1.88 g, over three procedures); ^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.09 (q, *J* = 1.7 Hz, 1H), 5.17 (q, *J* = 1.8 Hz, 1H), 3.31 (t, *J* = 6.0 Hz, 2H), 2.94 (s, 3H),

2.49 (ddd, *J* = 7.8, 3.8, 1.7 Hz, 2H), 1.82 (q, *J* = 6.2 Hz, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.3, 137.8, 120.9, 50.3, 35.1, 30.1, 23.1 ppm.

1-benzyl-3-methylenepiperidin-2-one (1s)[12] **：** colourless oil, 57% yield (3.44 g, over three procedures)；^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.14 (m, 5H), 6.21 (q, *J* = 1.7 Hz, 1H), 5.25 (q, *J* = 1.8 Hz, 1H), 4.60 (s, 2H), 3.30 – 3.15 (m, 2H), 2.55 – 2.45 (m, 2H), 1.79 – 1.75 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 164.4, 137.8, 137.2, 128.6, 128.1, 127.4, 122.0, 50.7, 47.8, 30.2, 23.1 ppm.



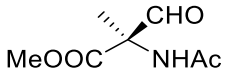
(*E*)-3-ethylidenedihydrofuran-2(3H)-one (1t)[14] was synthesized according to the literature procedure. Colourless oil, the ^{1}H NMR and ^{13}C NMR data obtained corresponded to the literature. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.70 (dtd, *J* = 10.1, 7.0, 3.0 Hz, 1H), 4.30 (t, *J* = 7.5 Hz, 2H), 2.81 (ddq, *J* = 7.4, 5.0, 2.4 Hz, 2H), 1.80 (dt, *J* = 7.2, 2.1 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 171.1, 135.5, 126.4, 65.4, 24.8, 15.6 ppm.

4. General Procedure for asymmetric hydroformylation

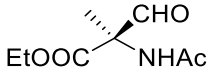
AHF procedure for substrate scope：

In an argon-filled glovebox, to a 5-mL vial equipped with a magnetic bar was added either the (*R,S*)-DTBM-Bn-YanPhos (0.006 mmol) ligand or the (*R,R*)-Ph-BPE (0.012 mmol) ligand and $Rh(acac)(CO)_2$ (0.004 mmol in 0.5 mL toluene). After stirring for 10 min, to the mixture was charged with terminal olefin (0.2 mmol). This vial was transferred into a Parr autoclave. The autoclave was pressurized with carbon monoxide (2.5 bar) and hydrogen (2.5 bar) sequentially. The reaction mixture was stirred at the desired temperature for 24 h. The autoclave was then cooled to room temperature and the synthetic gas was carefully released in a well-ventilated hood. The solution was concentrated in vacuo and the aldehyde was purified by flash chromatography (on silica, petroleum ether/ethyl acetate). The racemic products were prepared following the same procedure but with racemic Bn-YanPhos. The enantiomeric excesses of **2a-2t** were determined by HPLC or GC. The absolute configuration of **2a-2l** was compared to a previously reported literature[15]. The absolute configuration of **2p** was determined by XRD after condensation with 2,4-dinitrophenylhydrazine; configuration of **2m-2t** were assigned by analogy.

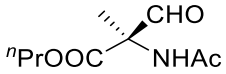
5. Characterization data of products



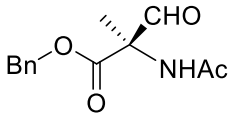
Methyl (*R*)-2-acetamido-2-methyl-3-oxopropanoate (2a)[15]**:** purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 2/1, v/v), colorless oil, 29.8 mg, 86% isolated yield; 96:4 *er*; $[\alpha]^{25}_{D}$ = +32.9 (c = 2.0, acetone), ref 15: $[\alpha]^{25}_{D}$ = +21.2 (c = 2.0, acetone, 60% ee); Enantiomeric excess was determined by GC with a Supelco's Beta Dex 120 column, Temperature program: 80 °C, stay 5 mins, 1 °C/min to 140 °C, stay 5 mins, Flow rate = 1 mL/min, t_{major} = 56.7 min, t_{minor} = 57.5 min. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.55 (s, 1H), 6.66 (s, 1H), 3.81 (s, 3H), 2.06 (s, 3H), 1.67 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 193.4, 169.7, 169.2, 66.6, 53.5, 22.6, 19.0 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_7H_{11}NO_4$ = 174.0766; Found 174.0759.



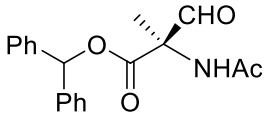
Ethyl (*R*)-2-acetamido-2-methyl-3-oxopropanoate (2b): purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 2/1, v/v), colorless oil, 34.0 mg, 91% isolated yield; 95:5 *er*; $[\alpha]^{25}_{D}$ = +15.7 (c = 0.9, acetone); Enantiomeric excess was determined by GC with a Supelco's Beta Dex 120 column, Temperature program: 70 °C, stay 5 mins, 0.4 °C/min to 130 °C, stay 5 mins, Flow rate = 1 mL/min, t_{major} = 139.0 min, t_{minor} = 140.4 min. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.55 (s, 1H), 6.69 (s, 1H), 4.26 (q, *J* = 7.13 Hz, 2H), 2.06 (s, 3H), 1.68 (s, 3H), 1.28 (t, *J* = 7.14 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 193.5, 169.7, 168.7, 66.6, 62.9, 22.6, 18.9, 14.0 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_8H_{13}NO_4$ = 188.0923; Found 188.0915.



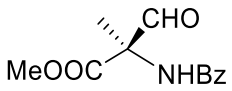
Propyl (*R*)-2-acetamido-2-methyl-3-oxopropanoate (2c): purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 2/1, v/v), colorless oil, 36.6 mg, 91% isolated yield; 95:5 *er*; $[\alpha]^{25}_{D}$ = +10.8 (c = 2.9, acetone); Enantiomeric excess was determined by GC with a Supelco's Beta Dex 120 column, Temperature program: 70 °C, stay 5 mins, 0.4 °C/min to 130 °C, stay 5 mins, Flow rate = 1 mL/min, t_{major} = 165.8 min, t_{minor} = 166.5 min. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.56 (s, 1H), 6.72 (s, 1H), 4.16 (t, *J* = 6.61 Hz, 2H), 2.06 (s, 3H), 1.69 - 1.66 (m, 5H), 0.93 (t, *J* = 7.43 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.5, 169.7, 168.8, 68.3, 66.7, 22.6, 21.8, 19.0, 10.2 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_9H_{15}NO_4$ = 202.1079; Found 202.1071.



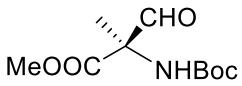
Benzyl (*R*)-2-acetamido-2-methyl-3-oxopropanoate (2d)[15]: purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 4/1, v/v), colorless oil, 45.3 mg, 91% isolated yield; 93:7 *er*; $[\alpha]^{25}_{D}$ = +10.9 (c = 0.8, acetone); The enantiomeric excess was determined by HPLC after condensation with 2,4-dinitrophenylhydrazine to the corresponding compound on Chiralpak OD-3 column, hexane: isopropanol = 85:15; flow rate = 0.45 mL/min; UV detection at 230 nm; t_{minor} = 14.9 min, t_{major} = 17.5 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.56 (s, 1H), 7.37 – 7.29 (m, 5H), 6.64 (s, 1H), 5.25 - 5.18 (m, 2H), 2.04 (s, 3H), 1.68 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.4, 169.7, 168.6, 134.7, 128.7, 128.7, 128.2, 68.3, 66.7, 22.6, 19.0 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{15}NO_4$ = 250.1079; Found 250.1069.



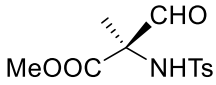
Benzhydryl (*R*)-2-acetamido-2-methyl-3-oxopropanoate (2e): purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 8/1, v/v), colorless oil, 52.0 mg, 80% isolated yield; 95:5 *er*; $[\alpha]^{25}_{D}$ = +17.1 (c = 1.0, acetone); The enantiomeric excess was determined by HPLC after $NaBH_4$ reduction to the corresponding alcohol on Chiralpak AD-3 column, hexane: isopropanol = 80:20; flow rate = 0.4 mL/min; UV detection at 210 nm; t_{major} = 3.2 min, t_{minor} = 3.7 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.57 (s, 1H), 7.40 – 7.24 (m, 10H), 6.90 (s, 1H), 6.73 (s, 1H), 2.05 (s, 3H), 1.72 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.3, 169.7, 167.8, 139.0, 138.9, 128.7, 128.7, 128.4, 128.3, 127.0, 126.9, 79.4, 66.9, 22.6, 18.9 ppm. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{19}H_{19}NO_4$ = 348.1212; Found 348.1212.



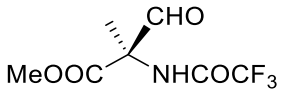
Methyl (*R*)-2-benzamido-2-methyl-3-oxopropanoate (2f)[16]: purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 4/1, v/v), colorless oil, 42.3 mg, 90% isolated yield; 95:5 *er*; $[\alpha]^{25}_{D}$ = +36.4 (c = 2.0, acetone); Enantiomeric excess was determined by GC with a Supelco's Beta Dex 225 column, Temperature program: 80 °C, stay 5 mins, 2 °C/min to 200 °C, stay 5 mins, Flow rate = 1 mL/min, t_{minor} = 63.7 min, t_{major} = 64.4 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.64 (s, 1H), 7.84 (d, *J* = 7.12 Hz, 2H), 7.55 (t, *J* = 7.38 Hz, 1H), 7.46 (t, *J* = 7.55 Hz, 2H), 7.37 (s, 1H), 3.83 (s, 3H), 1.80 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.3, 169.2, 166.6, 132.7, 132.3, 128.7, 127.3, 67.0, 53.7, 19.0 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{13}NO_4$ = 236.0923; Found 236.0913.



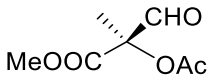
Methyl (*R*)-2-((tert-butoxycarbonyl)amino)-2-methyl-3-oxopropanoate (2g)[15]**:** purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 2/1, v/v), yellow oil, 35.1 mg, 76% isolated yield; 93:7 *er*; $[\alpha]^{25}_{D}$ = +54.1 (c = 0.7, acetone); Enantiomeric excess was determined by GC with a Supelco's Beta Dex 225 column, Temperature program: 80 °C, stay 5 mins, 2 °C/min to 200 °C, stay 5 mins, Flow rate = 1 mL/min, t_{minor} = 71.2 min, t_{major} = 72.8 min. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.57 (s, 1H), 5.64 (s, 1H), 3.80 (s, 3H), 1.64 (s, 3H), 1.44 (s, 9H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 193.9, 169.4, 154.6, 80.9, 66.7, 53.4, 28.2, 19.2 ppm. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{10}H_{17}NO_5$ = 254.1004; Found 254.0995.



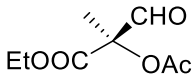
Methyl (*R*)-2-methyl-2-((4-methylphenyl)sulfonamido)-3-oxopropanoate (2h): purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 2/1, v/v), yellow oil, 39.4 mg, 75% isolated yield; 93:7 *er*; $[\alpha]^{25}_{D}$ = +17.2 (c = 1.3, acetone); The enantiomeric excess was determined by HPLC after reacting with (carbethoxymethylene)triphenylphosphorane to the corresponding compound on Chiralpak AD-3 column, hexane: isopropanol = 85:15; flow rate = 0.5 mL/min; UV detection at 210 nm; t_{major} = 8.4 min, t_{minor} = 9.5 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.42 (s, 1H), 7.68 (d, *J* = 8.36 Hz, 2H), 7.23 (d, *J* = 8.10 Hz, 2H), 5.90 (s, 1H), 3.66 (s, 3H), 2.35 (s, 3H), 1.49 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 192.6, 168.1, 143.8, 138.9, 129.7, 126.9, 69.1, 53.8, 21.5, 18.6 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{15}NO_5S$ = 286.0749; Found 286.0739.



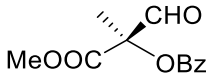
Methyl (*R*)-2-methyl-3-oxo-2-(2,2,2-trifluoroacetamido)propanoate (2i): purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 8/1, v/v), colorless oil, 36.3 mg, 80% isolated yield; 96:4 *er*; $[\alpha]^{21}_{D}$ = +25.3 (c = 1.0, acetone); Enantiomeric excess was determined by GC with a Supelco's Beta Dex 225 column, Temperature program: 80 °C, stay 5 mins, 2 °C/min to 210 °C, stay 5 mins, Flow rate = 1 mL/min, t_{major} = 17.6 min, t_{minor} = 17.9 min. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.42 (s, 1H), 7.43 (s, 1H), 3.78 (s, 3H), 1.76 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 191.0, 167.1, 156.6, 156.3, 116.3, 67.5, 54.1, 18.1 ppm. ^{19}F NMR (565 MHz, Chloroform-*d*) δ -75.7 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_7H_8F_3NO_4$ = 228.0484; Found 228.0476.



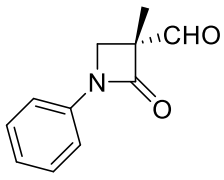
Methyl (*R*)-2-acetoxy-2-methyl-3-oxopropanoate (2j)[17]**:** purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 2/1, v/v), colorless oil, 33.4 mg, 96% isolated yield; 99:1 *er*; $[\alpha]^{25}_{D}$ = +9.8 (c = 1.0, acetone); Enantiomeric excess was determined by GC with a Supelco's Beta Dex 120 column, Temperature program: 80 °C, stay 5 mins, 1 °C/min to 140 °C, stay 5 mins, Flow rate = 0.5 mL/min, t_{minor} = 56.7 min, t_{major} = 57.5 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.88 (s, 1H), 3.84 (s, 3H), 2.18 (s, 3H), 1.60 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.7, 170.0, 169.0, 81.5, 53.1, 20.2, 19.4. ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_7H_{10}O_5$ = 175.0606; Found 175.0599.



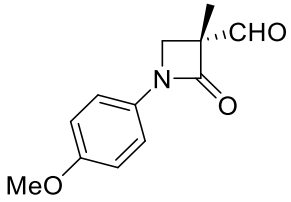
Ethyl (*R*)-2-acetoxy-2-methyl-3-oxopropanoate (2k): purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 4/1, v/v), colorless oil, 34.6 mg, 92% isolated yield; 96:4 *er*; $[\alpha]^{21}_{D}$ = +19.1 (c = 1.5, acetone); Enantiomeric excess was determined by GC with a Supelco's Beta Dex 225 column, Temperature program: 80 °C, stay 5 mins, 1 °C/min to 150 °C, stay 5 mins, Flow rate = 1 mL/min, t_{minor} = 26.0 min, t_{major} = 27.3 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.89 (s, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 2.17 (s, 3H), 1.59 (s, 3H), 1.31 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 193.9, 169.9, 168.5, 81.5, 62.3, 20.1, 19.4, 14.0 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_8H_{12}O_5$ = 189.0763; Found 189.0761.



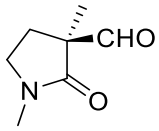
(*R*)-1-methoxy-2-methyl-1,3-dioxopropan-2-yl benzoate (2l)[17]**:** purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 4/1, v/v), colorless oil, 45.3 mg, 96% isolated yield; 93:7 *er*; $[\alpha]^{25}_{D}$ = +16.5 (c = 2.0, acetone); The enantiomeric excess was determined by HPLC after condensation with 2,4-dinitrophenylhydrazine to the corresponding compound on Chiralpak AS-3 column, hexane: isopropanol = 85:15; flow rate = 1.0 mL/min; UV detection at 220 nm; t_{major} = 21.4 min, t_{minor} = 29.5 min. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 10.00 (s, 1H), 8.09 – 8.07 (m, 2H), 7.50 – 7.45 (m, 3H), 3.85 (s, 3H), 1.75 (s, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 193.6, 169.0, 165.5, 133.9, 133.7, 130.2, 128.5, 81.9, 53.2, 19.5 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{12}O_5$ = 237.0763; Found 237.0752.



(*R*)-3-methyl-2-oxo-1-phenylazetidine-3-carbaldehyde (2m)[17]**:** purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 2/1, v/v), colorless oil, using (*R,S*)-DTBM-Bn-YanPhos got 27.2 mg, 72% isolated yield, 95:5 *er*, $[\alpha]^{25}_{D}$ = -36.6 (c = 2.4, acetone), absolute configuration: R; using (*R,R*)-Ph-BPE got 33.2 mg, 88% isolated yield, 97:3 *er*, $[\alpha]^{25}_{D}$ = +190.7 (c = 2.0, acetone) , absolute configuration: S; Enantiomeric excess was determined by GC with a Supelco's Beta Dex 225 column, Temperature program: 80 °C, stay 5 mins, 1 °C/min to 190 °C, stay 5 mins, Flow rate = 1 mL/min, t_{major} = 97.9 min, t_{minor} = 100.4 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.73 (s, 1H), 7.38 – 7.35 (m, 4H), 7.17 – 7.12 (m, 1H), 4.14 (d, *J* = 6.19 Hz, 1H), 3.49 (d, *J* = 6.16 Hz, 1H), 1.66 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 195.9, 162.3, 137.7, 129.3, 124.7, 116.6, 65.2, 46.2, 13.9 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{11}H_{11}NO_2$ = 190.0868; Found 190.0861.

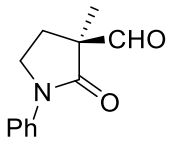


(*R*)-1-(4-methoxyphenyl)-3-methyl-2-oxoazetidine-3-carbaldehyde (2n): purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 2/1, v/v), colorless oil, using (*R,S*)-DTBM-Bn-YanPhos got 30.7 mg, 70% isolated yield; 95:5 *er*; $[\alpha]^{25}_{D}$ = -72.4 (c = 1.6, acetone) , absolute configuration: R; using (*R,R*)-Ph-BPE got 36.8 mg, 84% isolated yield, 97:3 *er*, $[\alpha]^{25}_{D}$ = +97.2 (c = 1.0, acetone) , absolute configuration: S; Enantiomeric excess was determined by GC with a Supelco's Beta Dex 225 column, Temperature program: 80 °C, stay 5 mins, 1 °C/min to 210 °C, stay 5 mins, Flow rate = 1 mL/min, t_{major} = 122.2 min, t_{minor} = 123.2 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.72 (s, 1H), 7.32 – 7.28 (m, 2H), 6.92 – 6.87 (m, 2H), 4.10 (d, *J* = 6.09 Hz, 1H), 3.80 (s, 3H), 3.46 (d, *J* = 6.13 Hz, 1H), 1.64 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 196.1, 161.7, 156.6, 131.3, 117.9, 114.5, 65.2, 55.6, 46.3, 13.8 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{13}NO_3$ = 220.0974; Found 220.0965.



(*S*)-1,3-dimethyl-2-oxopyrrolidine-3-carbaldehyde (2o): purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 1/1, v/v), colorless oil, 26.8 mg, 95% isolated yield; 99:1 *er*; $[\alpha]^{25}_{D}$ = +16.5 (c = 2.1, acetone); Enantiomeric excess was determined by GC with a Supelco's Beta Dex 225 column,

Temperature program: 80 °C, stay 5 mins, 1 °C/min to 210 °C, stay 5 mins, Flow rate = 1 mL/min, t_{minor} = 53.5 min, t_{major} = 58.3 min. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.60 (s, 1H), 3.38 – 3.32 (m, 2H), 2.87 (s, 3H), 2.64 (ddd, *J* = 13.17, 8.38, 4.76 Hz, 1H), 1.79 (dddd, *J* = 13.18, 8.72, 6.34, 0.65 Hz, 1H), 1.42 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 199.6, 172.2, 56.6, 46.2, 30.0, 26.0, 18.5 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_7H_{11}NO_2$ = 142.0868; Found 142.0861.



(*S*)-3-methyl-2-oxo-1-phenylpyrrolidine-3-carbaldehyde (2p): purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 2/1, v/v), colorless oil, 35.8 mg, 88% isolated yield; 98:2 *er*; $[\alpha]^{24}_{D}$ = -38.1 (c = 1.2, acetone); The enantiomeric excess was determined by HPLC after condensation with 2,4-dinitrophenylhydrazine to the corresponding compound on Chiralpak AS-3 column, hexane: isopropanol = 75:25; flow rate = 1.0 mL/min; UV detection at 210 nm; t_{minor} = 30.9 min, t_{major} = 35.3 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.69 (s, 1H), 7.64 – 7.60 (m, 2H), 7.42 – 7.37 (m, 2H), 7.21 – 7.17 (m, 1H), 3.89 – 3.80 (m, 2H), 2.77 (ddd, *J* = 13.0, 8.0, 4.9 Hz, 1H), 1.95 (dddd, *J* = 13.1, 8.5, 6.8, 0.8 Hz, 1H), 1.54 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 199.1, 171.5, 138.9, 129.0, 125.1, 119.9, 58.1, 45.5, 25.7, 18.7 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{12}H_{13}NO_2$ = 204.1025; Found 204.1021.

Product **2p** was condensed with 2,4-dinitrophenylhydrazine, and the resulting compound crystalized in dichloromethane and MeOH (by evaporation of solvent). CCDC No. 2121822.

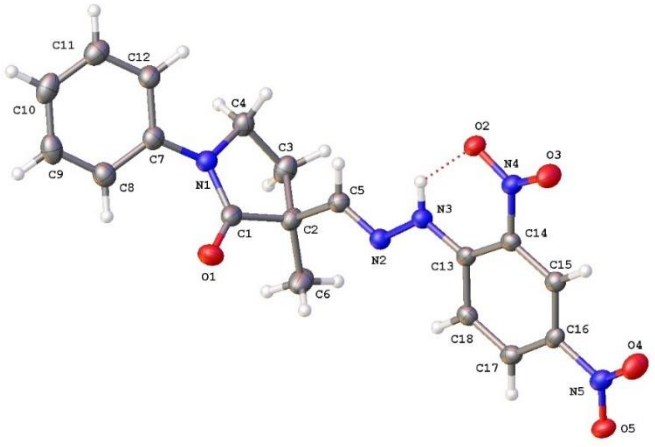
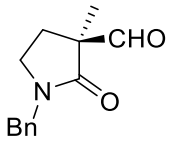


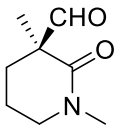
Table S1 Crystal data and structure refinement.

Identification code	1
Empirical formula	$C_{18}H_{17}N_5O_5$
Formula weight	383.36
Temperature/K	100.0

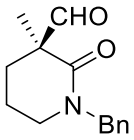
Crystal system	monoclinic
Space group	$P2_1$
a/Å	7.1241(5)
b/Å	34.022(2)
c/Å	7.3539(5)
α/°	90
β/°	90.288(4)
γ/°	90
Volume/Å^3	1782.4(2)
Z	4
ρ_{calc}g/cm^3	1.429
μ/mm^{-1}	0.901
F(000)	800.0
Crystal size/mm^3	0.12 × 0.11 × 0.1
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	5.194 to 144.19
Index ranges	$-8 \le h \le 8$, $-41 \le k \le 41$, $-8 \le l \le 9$
Reflections collected	34224
Independent reflections	6866 [R_{int} = 0.0455, R_{sigma} = 0.0343]
Data/restraints/parameters	6866/1/507
Goodness-of-fit on F^2	1.070
Final R indexes [I>=2σ (I)]	R_1 = 0.0348, wR_2 = 0.0815
Final R indexes [all data]	R_1 = 0.0391, wR_2 = 0.0843
Largest diff. peak/hole / e Å^{-3}	0.16/-0.24
Flack parameter	-0.12(7)



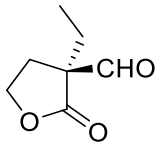
(*S*)-1-benzyl-3-methyl-2-oxopyrrolidine-3-carbaldehyde (2q): purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 2/1, v/v), colorless oil, 37.3 mg, 86% isolated yield; 95:5 *er*; $[\alpha]^{23}_D$ = +10.3 (c = 0.3, acetone); The enantiomeric excess was determined by HPLC after condensation with 2,4-dinitrophenylhydrazine to the corresponding compound on Chiralpak OD-3 column, hexane: isopropanol = 70:30; flow rate = 1.0 mL/min; UV detection at 210 nm; t_{major} = 19.6 min, t_{minor} = 25.1 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.67 (s, 1H), 7.37 – 7.30 (m, 3H), 7.23 – 7.20 (m, 2H), 4.47 (q, *J* = 14.7 Hz, 2H), 3.28 – 3.19 (m, 2H), 2.61 (ddd, *J* = 13.2, 8.3, 4.9 Hz, 1H), 1.79 – 1.74 (m, 1H), 1.47 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 199.6, 172.3, 135.9, 128.8, 128.0, 127.8, 56.8, 47.0, 43.5, 26.1, 18.5 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{15}NO_2$ = 218.1181; Found 218.1178.



(*S*)-1,3-dimethyl-2-oxopiperidine-3-carbaldehyde (2r): purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 1/1, v/v), colorless oil, 26.7 mg, 86% isolated yield; 98:2 *er*; $[\alpha]^{21}_{D}$ = -27.0 (c = 0.4, acetone); Enantiomeric excess was determined by GC with a Supelco's Beta Dex 225 column, Temperature program: 80 °C, stay 5 mins, 1 °C/min to 210 °C, stay 5 mins, Flow rate = 1 mL/min, t_{minor} = 61.6 min, t_{major} = 62.5 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.69 (s, 1H), 3.37 – 3.26 (m, 2H), 2.98 (s, 3H), 2.27 (dddd, *J* = 13.6, 7.2, 3.9, 0.9 Hz, 1H), 1.84 (dddd, *J* = 14.4, 7.6, 5.8, 3.8 Hz, 2H), 1.62 – 1.56 (m, 1H), 1.42 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 201.4, 169.6, 54.5, 50.2, 35.1, 28.6, 21.4, 19.8 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_8H_{13}NO_2$ = 156.1025; Found 156.1021.

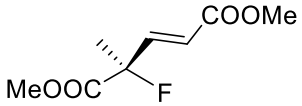


(*S*)-1-benzyl-3-methyl-2-oxopiperidine-3-carbaldehyde (2s): purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 2/1, v/v), colorless oil, 41.2 mg, 89% isolated yield; 98:2 *er*; $[\alpha]^{24}_{D}$ = -40.4 (c = 0.6, acetone); The enantiomeric excess was determined by HPLC after condensation with 2,4-dinitrophenylhydrazine to the corresponding compound on Chiralpak AS-3 column, hexane: isopropanol = 90:10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_{major}= 52.3 min, t_{minor} = 60.5 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.75 (s, 1H), 7.37 – 7.29 (m, 3H), 7.26 – 7.23 (m, 2H), 4.68 – 4.57 (m, 2H), 3.29 – 3.18 (m, 2H), 2.31 – 2.24 (m, 1H), 1.82 – 1.73 (m, 2H), 1.64 – 1.58 (m, 1H), 1.48 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 201.3, 169.6, 136.8, 128.7, 127.9, 127.6, 54.7, 50.5, 47.5, 28.6, 21.6, 19.8 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{14}H_{17}NO_2$ = 232.1338; Found 232.1338.



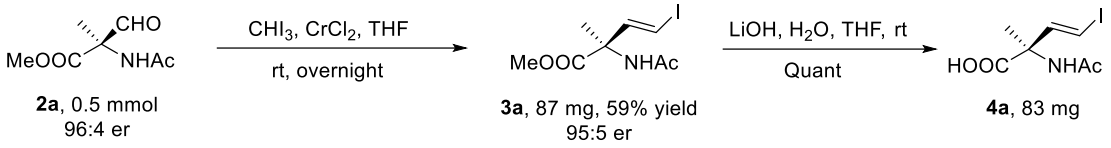
(*S*)-3-ethyl-2-oxotetrahydrofuran-3-carbaldehyde (2t): purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 2/1, v/v), colorless oil, 24.4 mg, 86% isolated yield; 98:2 *er*; $[\alpha]^{21}_{D}$ = -50.4 (c = 1.0, acetone); Enantiomeric excess was determined by GC with a Supelco's Beta Dex 225 column, Temperature program: 80 °C, stay 5 mins, 4 °C/min to 180 °C, stay 5 mins, Flow rate = 1 mL/min, t_{minor} = 26.4 min, t_{major} = 27.3 min. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.55 (d, *J* = 1.0 Hz, 1H), 4.33 (td, *J* = 8.9, 4.9 Hz,

1H), 4.26 (ddd, *J* = 9.1, 8.1, 7.5 Hz, 1H), 2.81 (ddd, *J* = 13.1, 8.1, 4.9 Hz, 1H), 2.13 – 2.04 (m, 2H), 1.96 (dq, *J* = 14.1, 7.5 Hz, 1H), 0.96 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 196.6, 174.5, 66.1, 60.2, 25.8, 25.7, 8.7 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_7H_{10}O_3$ = 143.0708; Found 143.0707.



Dimethyl (*R*,*E*)-4-fluoro-4-methylpent-2-enedioate (2u)[17]**:** Hydroformylation was conducted on a 0.2 mmol scale. After completion of the reaction, the crude material was treated with (carbethoxymethylene)triphenylphosphorane to facilitate **2t**. Purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 4/1, v/v), colorless oil, 27.4 mg, 72% isolated yield; 97:3 *er*; The absolute configuration was determined by comparison of the optical rotation of the corresponding carboxylic acid which was obtained by the oxidation of the crude aldehyde.[18] $[\alpha]_D^{20}$ = +17.5 (c = 1.3, MeOH), ref 17: $[\alpha]^{20}D$ = +19.4 (c = 1.0, MeOH); The enantiomeric excess was determined by HPLC on Chiralpak OD-3 column, hexane: isopropanol = 90:10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_{major}= 4.85 min, t_{minor} = 5.72 min. ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.03 (dd, *J* = 20.27, 15.74 Hz, 1H), 6.20 (d, *J* = 15.73 Hz, 1H), 3.82 (s, 3H), 3.77 (s, 3H), 1.71 (d, *J* = 21.32 Hz, 3H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.5 (d, *J* = 25.8 Hz), 166.0, 143.8 (d, *J* = 20.7 Hz), 121.3 (d, *J* = 10.1 Hz), 93.0 (d, *J* = 190.1 Hz), 53.2, 52.0, 24.1 (d, *J* = 24.0 Hz) ppm. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -158.3. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_8H_{11}FO_4$ = 213.0539; Found 213.0531.

6. Elaboration on chiral quaternary aldehydes for the synthesis of chiral *α*-quaternary amino acid derivatives.



2a, 0.5 mmol
96:4 er

3a, 87 mg, 59% yield
95:5 er

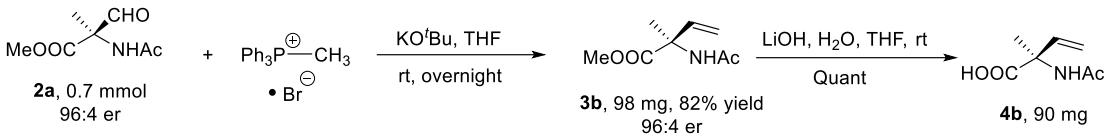
4a, 83 mg

3a was prepared according to the literature.[19] Chromium chloride (369 mg, 3 mmol) was suspended into 4.0 mL of THF under argon. Compound **2a** (87 mg, 0.5 mmol) and iodoform (393 mg, 1 mmol) were dissolved into 3.0 mL of THF and added to the stirring suspension. The mixture was stirred at room temperature overnight. Water was added, and the layers were separated. The aqueous layer was back extracted with ethyl acetate. Combined organic fractions were then washed with brine, dried (Na_2SO_4), filtered, and concentrated in vacuo. The residue was purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 4/1, v/v) to give the desired product **3a**.

To a solution of **3a** (0.295 mmol, 87 mg, 1.0 equiv) in THF (5.0 mL) was added LiOH (2.95 mmol, 71 mg, 10.0 equiv) and H_2O (5.0 mL), and the resulting solution was stirred at room temperature for 3 h. Then the mixture was acidified with 2 N HCl to pH~3 and extracted with ethyl acetate. Combined organic fractions were then washed with brine, dried (Na_2SO_4), filtered, and concentrated in vacuo to give the desired product **4a**.

Methyl (*R,E*)-2-acetamido-4-iodo-2-methylbut-3-enoate (3a): Yellow solid, 87.0 mg, 59% isolated yield; 95:5 *er*; $[\alpha]^{20}_D$ = +40.4 (c = 1.6, acetone); The enantiomeric excess was determined by HPLC on Chiralpak AS-3 column, hexane: isopropanol = 90:10; flow rate = 1.0 mL/min; UV detection at 210 nm; t_{minor} = 8.4 min, t_{major} = 10.1 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.62 (dd, *J* = 163.87, 14.77 Hz, 2H), 6.47 (s, 1H), 3.77 (s, 3H), 2.02 (s, 3H), 1.63 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.9, 169.3, 143.8, 78.6, 62.6, 53.2, 23.4, 22.8 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_8H_{12}INO_3$ = 297.9940; Found 297.9939.

(*R,E*)-2-acetamido-4-iodo-2-methylbut-3-enoic acid (4a): white solid, 83.0 mg; $[\alpha]^{20}_D$ = +59.2 (c = 1.0, acetone). ^{1}H NMR (400 MHz, Methanol-d_4) δ 6.73 (dd, *J* = 207.2, 14.8 Hz, 2H), 2.01 (s, 3H), 1.54 (s, 3H). ^{13}C NMR (101 MHz, Methanol-d_4) δ 173.6, 171.4, 145.1, 76.3, 62.0, 22.6, 21.2 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_7H_{10}INO_3$ = 283.9784; Found 283.9785.

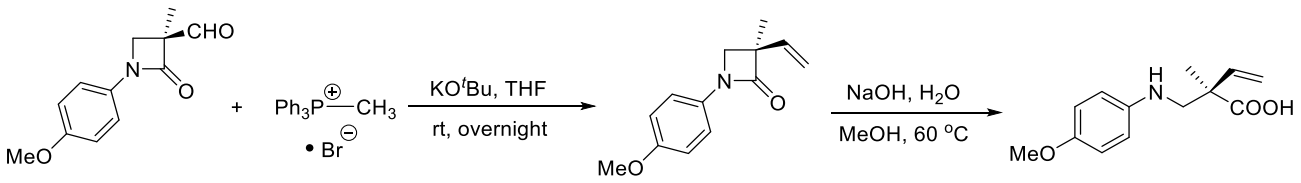


3b was prepared according to the literature.[20] To a mixture of the respective triphenylphosphonium bromide (330 mg, 1.3 eq.) and KO^{t}Bu (94.3 mg, 1.2 eq) was added THF (8 mL) at ambient temperature. The reaction mixture was stirred for approximately 1 hour. Compound **2a** (121 mg, 0.7 mmol) were dissolved into 1.0 mL THF and added to the stirring suspension. The mixture was stirred at room temperature overnight. Water was added, and the layers were separated. The aqueous layer was back extracted with ethyl acetate. Combined organic fractions were then washed with brine, dried (Na_2SO_4), filtered, and concentrated in vacuo. The residue was purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 4/1, v/v) to give the desired product **3b**.

To a solution of **3b** (0.57 mmol, 98 mg, 1.0 equiv) in THF (8.0 mL) was added LiOH (5.7 mmol, 136.8 mg, 10.0 equiv) and H_2O (8.0 mL), and the resulting solution was stirred at room temperature for 3 h. Then the mixture was acidified with 2 N HCl to pH~3 and extracted with ethyl acetate. Combined organic fractions were then washed with brine, dried (Na_2SO_4), filtered, and concentrated in vacuo to give the desired product **4b**.

Methyl (*R*)-2-acetamido-2-methylbut-3-enoate (3b)[21]**:** white solid, 98.0 mg, 82% isolated yield; 96:4 *er*; $[\alpha]_D^{20}$ = +28.2 (c = 1.0, acetone); Enantiomeric excess was determined by GC with a Supelco's Beta Dex 225 column, Temperature program: 80 °C, stay 5 mins, 0.5 °C/min to 115 °C, stay 5 mins, Flow rate = 1 mL/min, t_{major} = 61.8 min, t_{minor} = 63.3 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.23 (s, 1H), 6.08 (dd, *J* = 17.3, 10.5 Hz, 1H), 5.31 – 5.19 (m, 2H), 3.76 (s, 3H), 2.02 (s, 3H), 1.67 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.1, 169.2, 137.4, 115.6, 60.5, 53.0, 23.5, 22.6 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_8H_{13}NO_3$ = 172.0974; Found 172.0971.

(*R*,*E*)-2-acetamido-4-iodo-2-methylbut-3-enoic acid (4b)[22]**:** white solid, 90.0 mg; $[\alpha]_D^{20}$ = +18.8 (c = 1.0, acetone). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.92 – 6.65 (m, 4H), 5.96 (dd, *J* = 17.4, 11.0 Hz, 1H), 5.35 – 5.27 (m, 2H), 3.76 (s, 3H), 3.34 – 3.23 (m, 2H), 1.40 (s, 3H). ^{13}C NMR (101 MHz, Methanol-d_4) δ 174.8, 171.5, 137.9, 113.7, 60.0, 22.5, 21.3 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_7H_{11}NO_3$ = 158.0817; Found 158.0816.



2n, 0.3 mmol
97:3 er

3n, 58 mg, 89% yield

4n, 60 mg, 96 yield%
97:3 er

To a mixture of the respective triphenylphosphonium bromide (141 mg, 1.3 eq.) and KO^{t}Bu (40.5 mg, 1.2 eq) was added THF (3 mL) at ambient temperature. The reaction mixture was stirred for approximately 1 hour. Compound **2n** (66.0 mg, 0.3 mmol) were dissolved into 1.0 mL THF and added to the stirring suspension. The mixture was stirred at room temperature overnight. Water was added, and the layers were separated. The aqueous layer was back extracted with ethyl acetate. Combined organic fractions were then washed with brine, dried (Na_2SO_4), filtered, and concentrated in vacuo. The residue was purified by flash chromatography (on silica, petroleum ether/ ethyl acetate = 5/1, v/v) to give the desired product **3n**[20].

To a solution of **3o** (0.27 mmol, 58 mg, 1.0 equiv) in MeOH (2.0 mL) was added NaOH (1.4 mmol, 56 mg, 5.0 equiv) and H_2O (2.0 mL), and the resulting solution was stirred at 60 °C for 5 h. Then the mixture was acidified with 2 N HCl to pH~3 and extracted with ethyl acetate. Combined organic fractions were then washed with brine, dried (Na_2SO_4), filtered, and concentrated in vacuo to give the desired product **4n**.

(*R*)-2-(((4-methoxyphenyl)amino)methyl)-2-methylbut-3-enoic acid (4n): Brown oil, 60.0 mg, 96% isolated yield; 97:3 *er*; $[\alpha]^{21}_D$ = +21.0 (c = 1.0, acetone); The enantiomeric excess was determined by HPLC on Chiralpak OJ-3 column, hexane: isopropanol = 85:15; flow rate = 1.0 mL/min; UV detection at 254 nm; t_{minor} = 12.3 min, t_{major} = 14.9 min. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 (s, 1H), 6.79 (d, *J* = 9.0 Hz, 2H), 6.71 (d, *J* = 9.0 Hz, 2H), 6.00 (dd, *J* = 17.8, 10.5 Hz, 1H), 5.32 – 5.30 (m, 1H), 5.27 (d, *J* = 5.9 Hz, 1H), 3.75 (s, 3H), 3.36 – 3.24 (m, 2H), 1.40 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 179.0, 153.6, 140.9, 138.8, 116.5, 116.3, 114.9, 55.8, 53.1, 49.7, 20.6 ppm. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{17}NO_3$ = 236.1287; Found 236.1286.

7. Hammett study on the influence from electronic property on AHF of 1-arylstyrene

Derivation of kinetic equation:

According to Jörke and co-worders' research[23], the rate of hydroformylation shows a first-order kinetics in olefin substrate under a low syngas pressure. Under a certain reaction condition, we have:

$$rate = \frac{d(aldehyde)}{dt} = k[olefin]{P_{H2}}^{a}{P_{CO}}^{b} \quad (1)$$

$$\frac{d(linear)}{dt} = k_l[olefin]{P_{H2}}^{a}{P_{CO}}^{b} \quad (2)$$

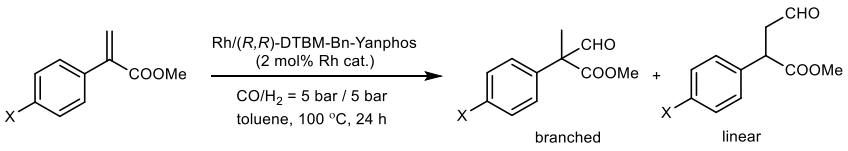
$$\frac{d(branched)}{dt} = k_b[olefin]{P_{H2}}^{a}{P_{CO}}^{b} \quad (3)$$

$$[linear\ alhyded] = \int \frac{d(linear)}{dt} = \int k_l[olefin]{P_{H2}}^{a}{P_{CO}}^{b} \quad (4)$$

$$[branched\ alhyded] = \int \frac{d(branched)}{dt} = \int k_b[olefin]{P_{H2}}^{a}{P_{CO}}^{b} \quad (5)$$

So, the $\frac{k_b}{k_l}$ roughly equals to the regiomeric ratio:

$$\frac{[linear]}{[branched]} = \frac{k_l}{k_b} \quad (6)$$



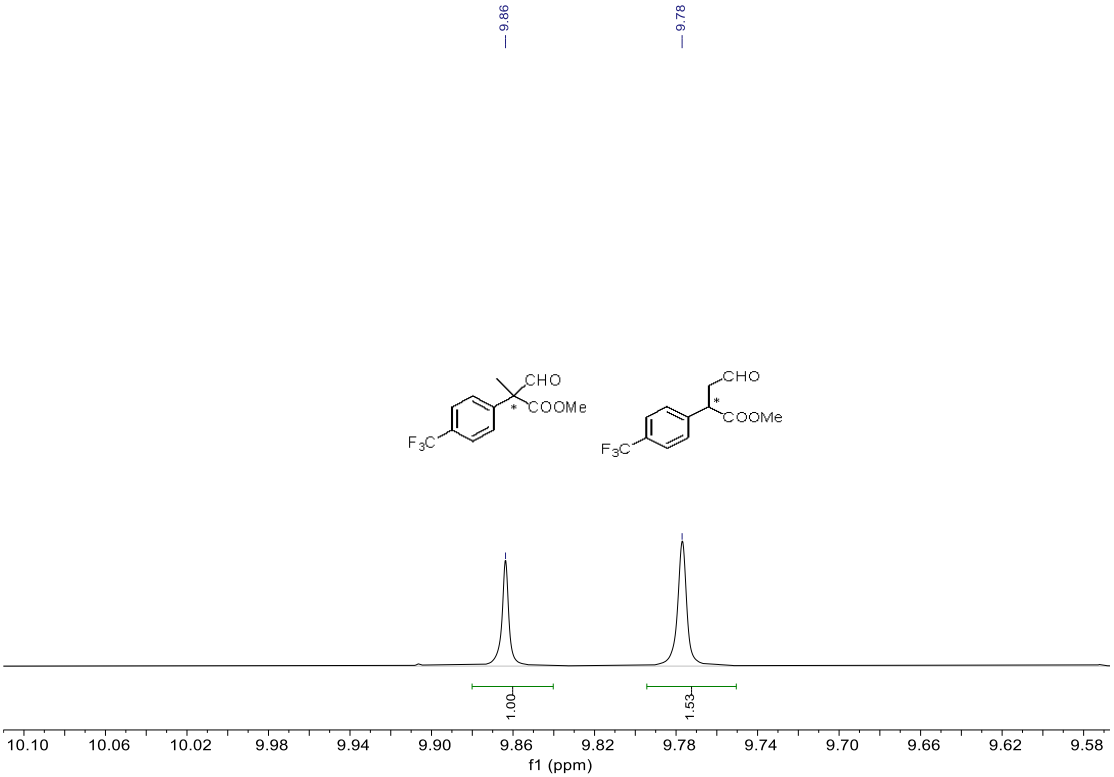
The hydroformylation of 1-arylstyrene was carried out using the standard procedure with modification on temperature. All the six parallel reactions were conducted in a 300-mL autoclave in a batch. 3 The results are showed in table S2.

Table S2. Results for AHF of 1-arylstyrene:

-X	σ_p	b	l	b/l	lg(b/l)
-CF_3	0.53	1	1.53	0.65	-0.18469
-F	0.15	1	2.65	0.38	-0.42325
-Cl	0.24	1	2.35	0.43	-0.37107
-Br	0.26	1	2.40	0.42	-0.38021
-Me	-0.14	1	5.59	0.18	-0.74741
-OMe	-0.12	1	7.28	0.14	-0.86213

Linear regression was performed with Origin 2017.

Raw NMR data: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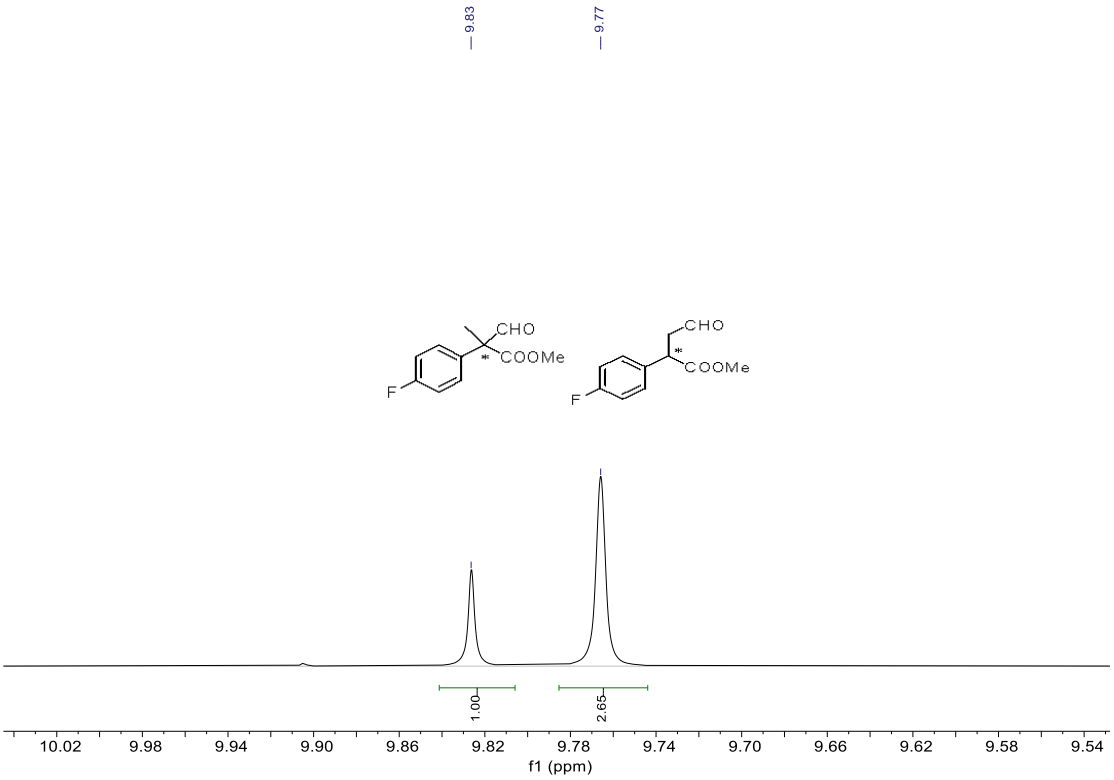
9.78
CHO
COOMe
F3C
1.00
1.53
10.10
10.06
10.02
9.98
9.94
9.90
9.86
9.82
9.78
9.74
9.70
9.66
9.62
9.58
f1 (ppm)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COOMe
F
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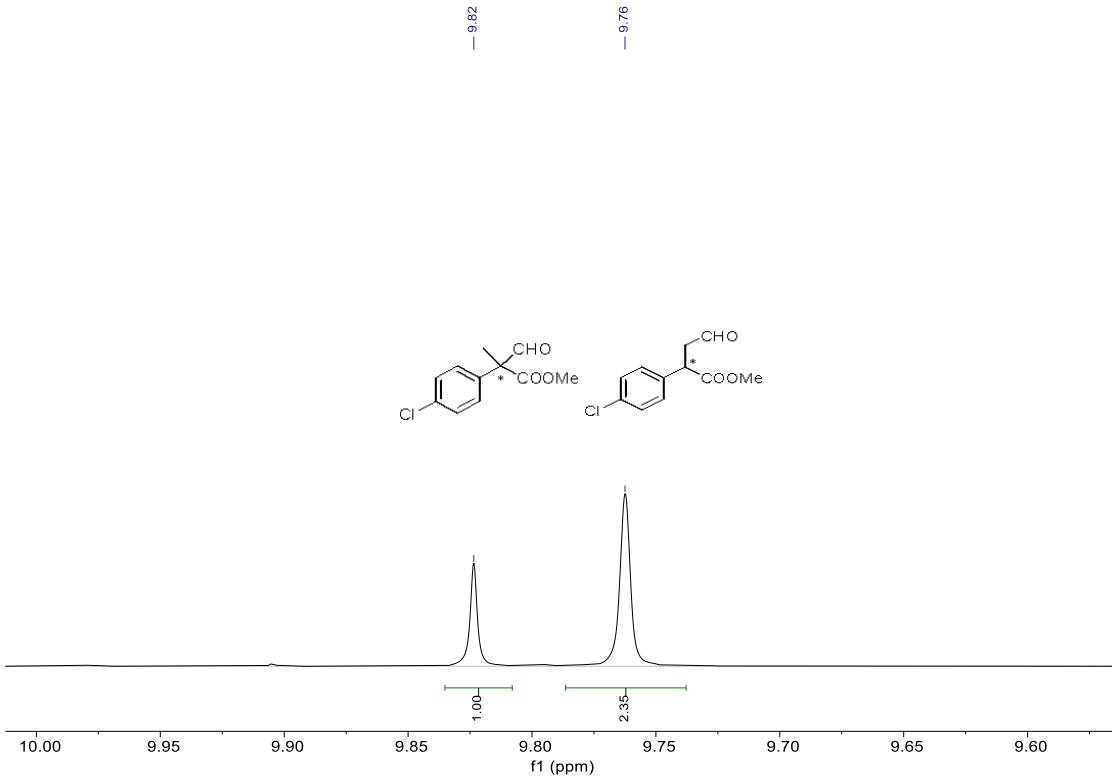
2.65
10.02
9.98
9.94
9.90
9.86
9.82
9.78
9.74
9.70
9.66
9.62
9.58
9.54
f1 (ppm)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COOMe
Cl
CHO
COOMe
Cl
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10.00
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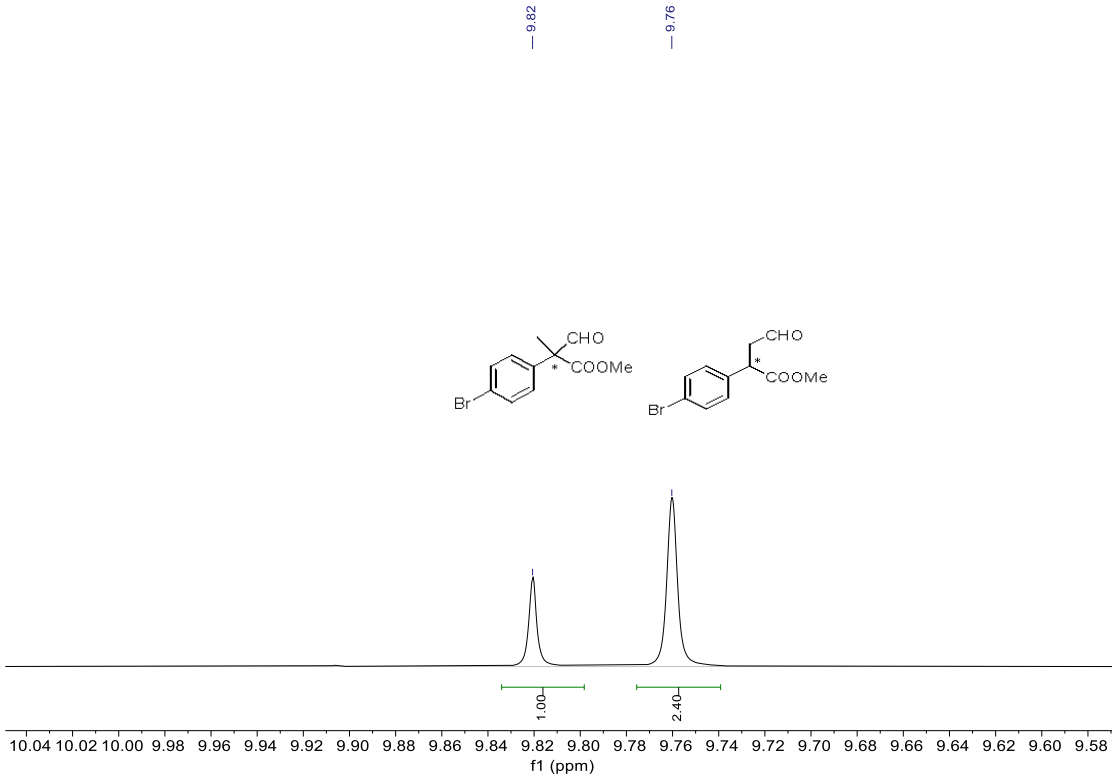
9.80
9.75
9.70
9.65
9.60
f1 (ppm)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9.76
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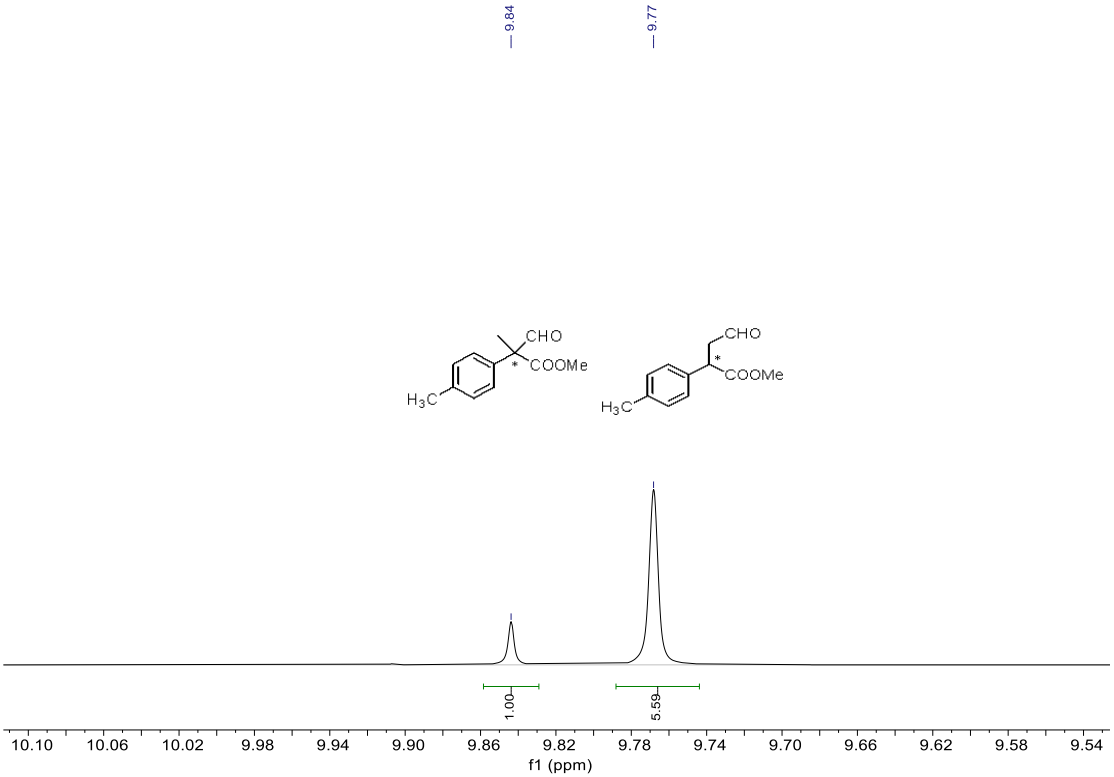
COOMe
Br
CHO
COOMe
Br
1.00
2.40
10.04 10.02 10.00 9.98 9.96 9.94 9.92 9.90 9.88 9.86 9.84 9.82 9.80 9.78 9.76 9.74 9.72 9.70 9.68 9.66 9.64 9.62 9.60 9.58
f1 (ppm)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9.77
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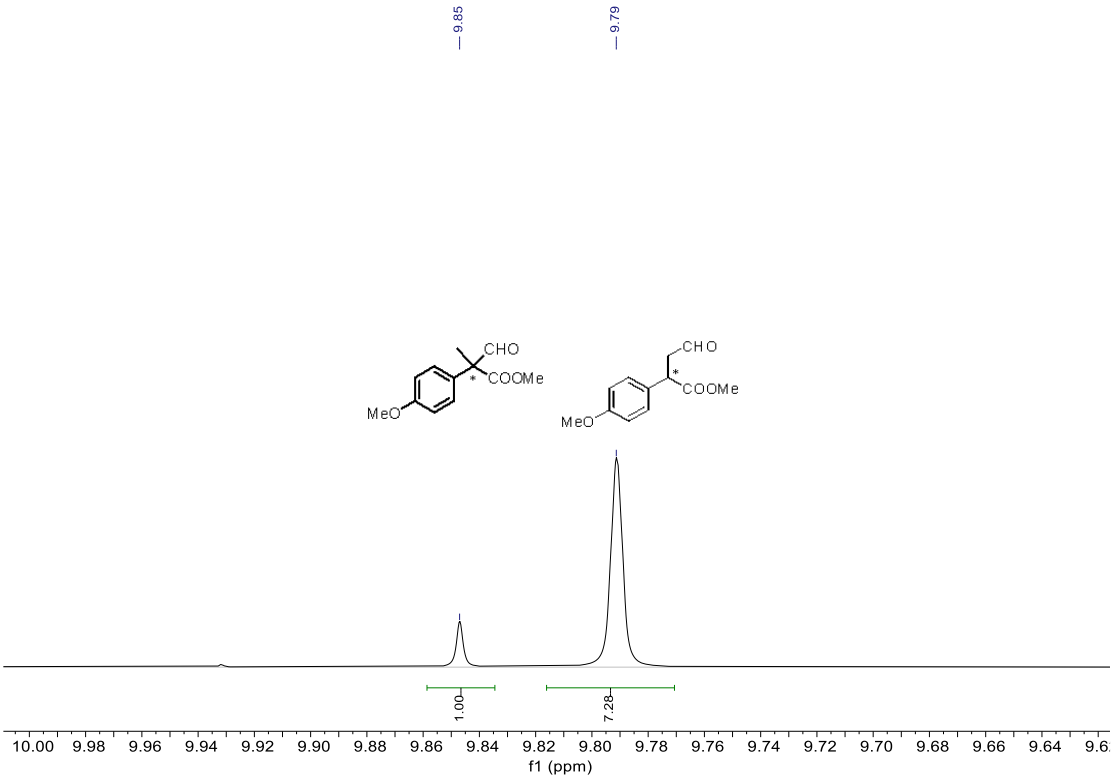
COOMe
H3C
CHO
COOMe
H3C
1.00
5.59
10.10 10.06 10.02 9.98 9.94 9.90 9.86 9.82 9.78 9.74 9.70 9.66 9.62 9.58 9.54
f1 (ppm)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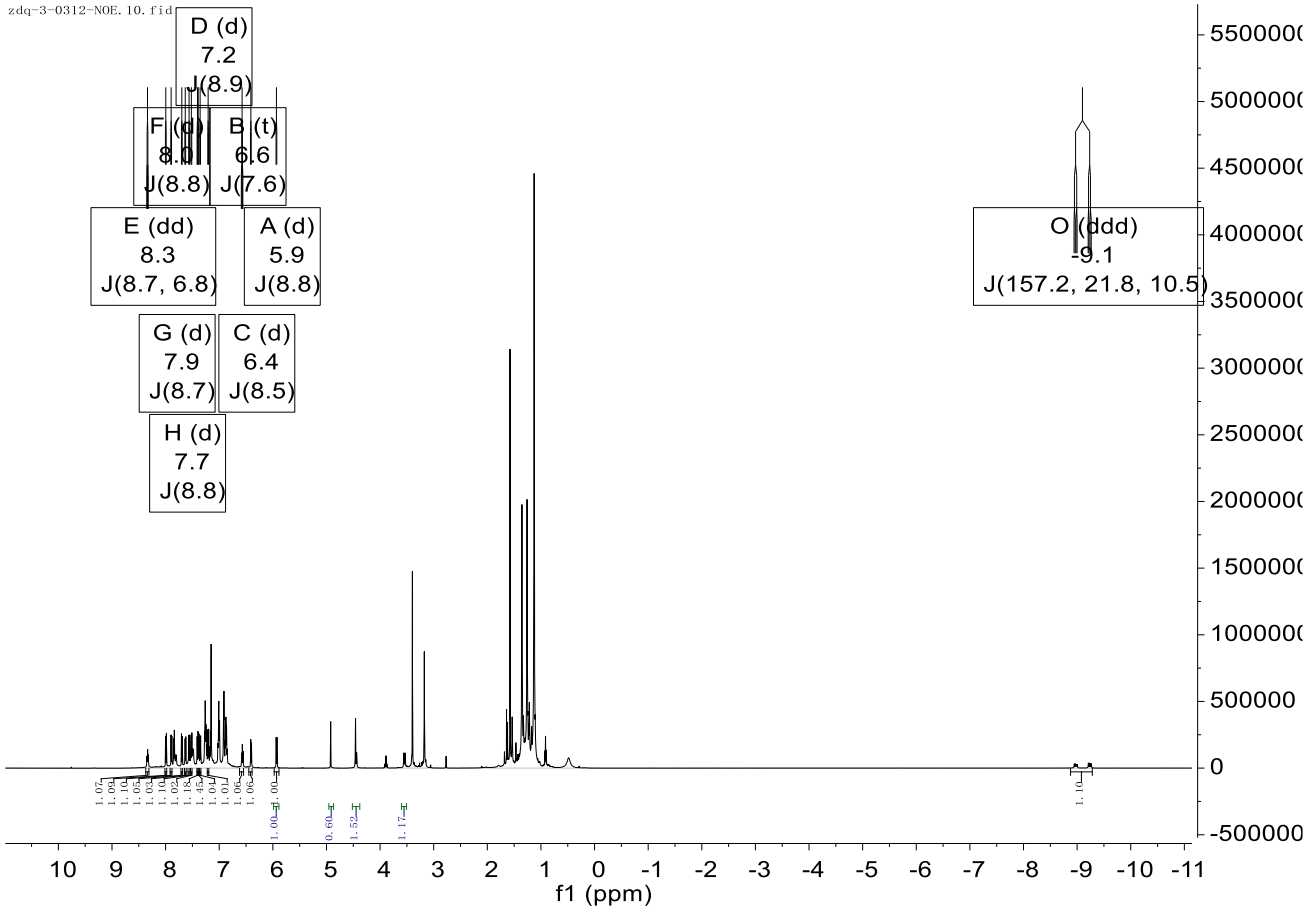
9.79
CHO
COOMe
MeO
CHO
COOMe
MeO
1.00
7.28
10.00 9.98 9.96 9.94 9.92 9.90 9.88 9.86 9.84 9.82 9.80 9.78 9.76 9.74 9.72 9.70 9.68 9.66 9.64
f1 (ppm)

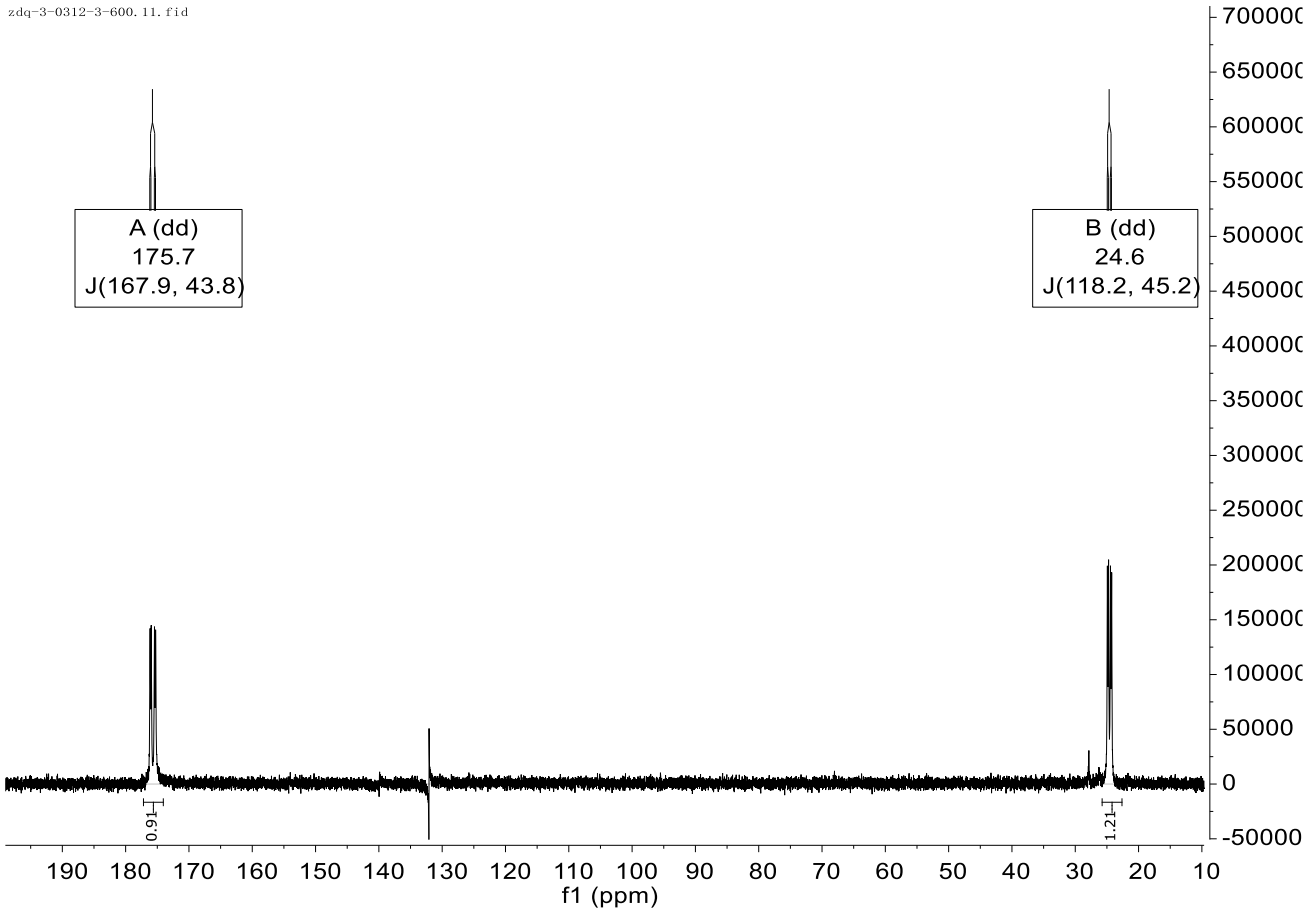
8. Preparation of Rh(DTBM-Bn-Yanphos)$(CO)_2H$ and its NMR data.

In an argon-filled glovebox, 11.4 mg (*R,S*)-DTBM-BN-Yanphos (0.010 mmol) and equimolar Rh(acac)$(CO)_2$ was dissolved in 0.5 mL benzene-*d6*. This mixture was stirred 0.5 hour before transferred into a Young Tube. This NMR tube was then attached to a Schlenk line and was freezed in liquid nitrogen. After being freezed for 15 minutes, this Tube was vacuumed by an oil pump for 15 minutes. The tube was then charged with syngas (CO/H_2 = 1:1) and was sealed afterwards. After being warmed to room temperature, this tube was shaken gently before heating in an oil bath at 60 ℃. After 1 hour heating, the color of the solution was changed from yellow to light yellow. This sample was analyzed by NMR spectroscopy.

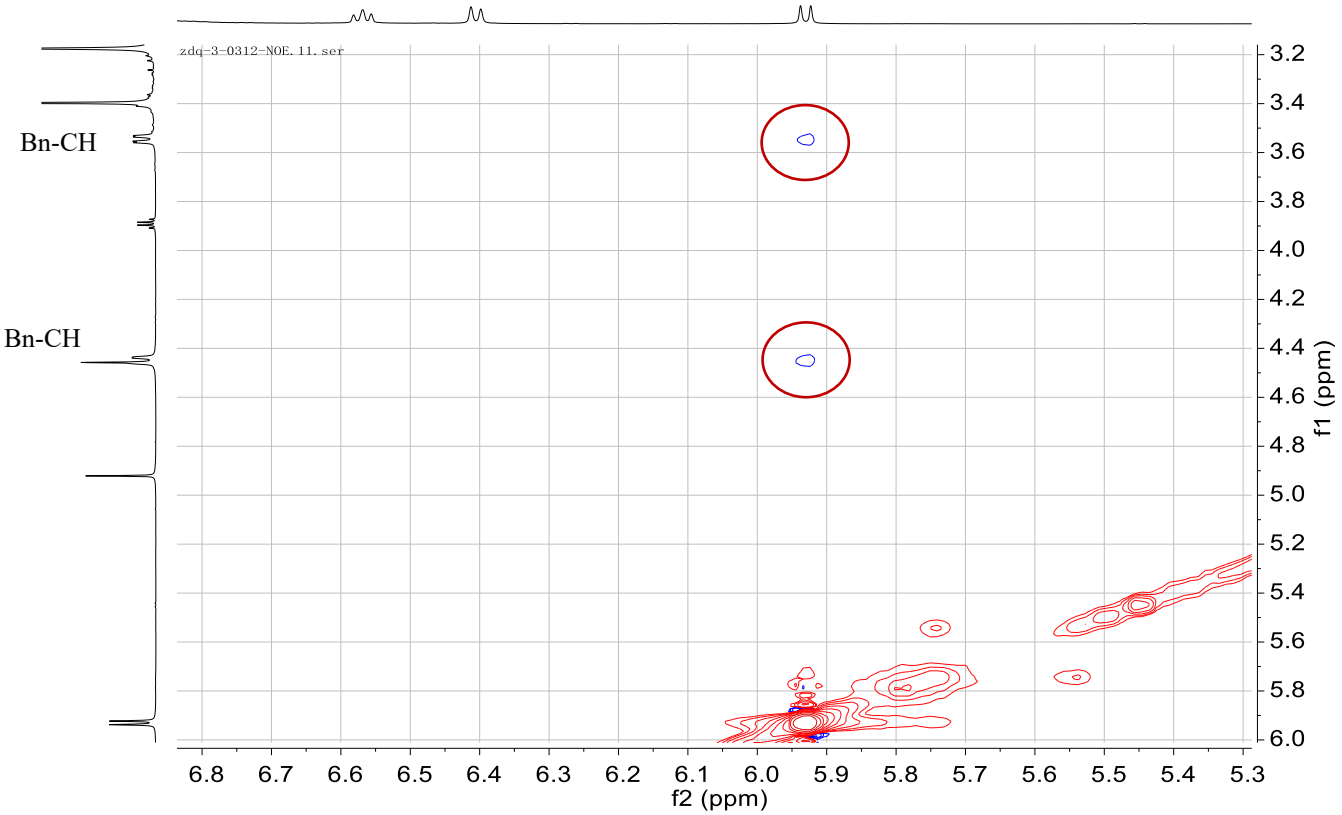
^{1}H NMR:



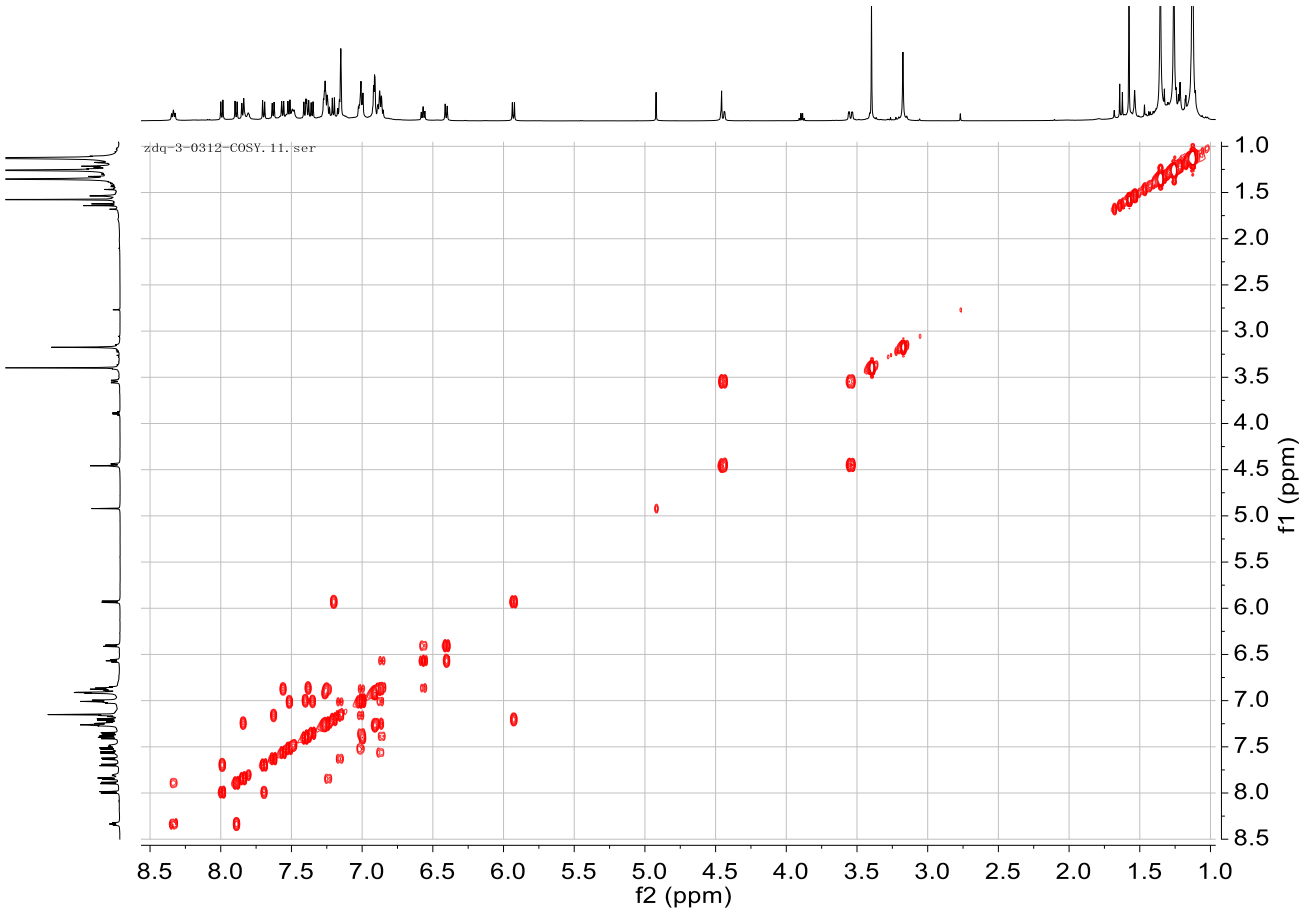
^{31}P NMR:


zdq-3-0312-3-600.11.fid
A (dd)
175.7
J(167.9, 43.8)
B (dd)
24.6
J(118.2, 45.2)
0.91
1.21
f1 (ppm)

NOESY:



COSY:



9. Details in DFT computational studies.

DFT calculations were performed using the Gaussian 16 package[24]. All the structures are optimized using the M06[25] functional with the basis set SDD for Rh[26,27] and 6-31G* for other main group atoms[28,29]. Geometric structures of all species were optimized at T = 298.15 K. Vibrational analyses were performed to ensure intermediates to have no imaginary frequencies. Single point calculations were performed using the M06 functional with the SDD basis set for Rh and the 6-311++G** basis set for all of the other main group atoms and solvent effects (benzene) were considered using the SMD mode.[30]

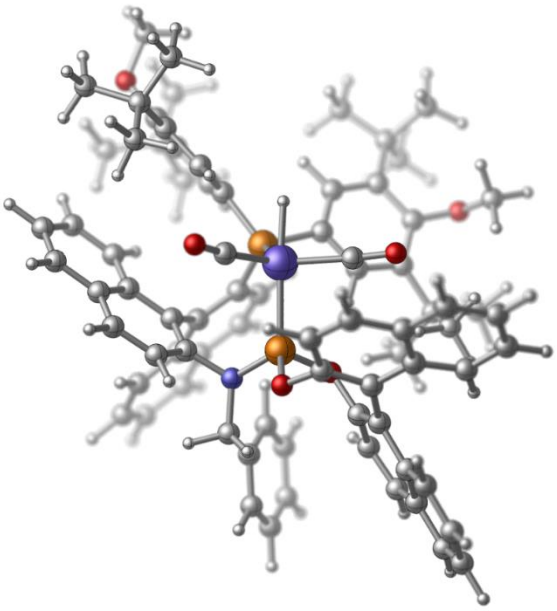
The outcome structure of Rh[(*R,S*)-DTBM-Bn-Yanphos](CO)H were analyzed by a web tool, SambVca 2.1[31] (https://www.molnac.unisa.it/OMtools/sambvca2.1/index.html). The rhodium atom was selected for the center of the sphere Rh-CO bond was selected as the z-axil and another Rh-H bond as the x-axil in the Cartesian coordinate system. Bondi atomic model (scaled by 1.17) was selected for atomic radii. Defined radius of the semi-sphere was set at 6.0 Å.

Different catalyst-substrate complexation structures were optimized using DFT calculation. The energies of such results were summarized in Table S3. Based on the analysis of topological of catalytically active species Rh[(*R,S*)-DTBM-Bn-Yanphos](CO)H and different diastereomers of catalyst-substrate complexes, we could tentatively draw the conclusion about the enantioinduction model in the manuscript.

Table S3. Energies of found diastereomers of Rh[(*R,S*)-DTBM-Bn-Yanphos](CO)(MAA)H (in Hartree)

	Electronic Energy	EE + Thermal Free Energy Correction	Single Point EE	Relative free energy in kcal/mol
cat-sub-1	-4755.119765	-4753.726368	-4756.270422	2.8
cat-sub-2	-4755.124397	-4753.73239	-4756.273571	0
cat-sub-3	-4755.105553	-4753.711521	-4756.261018	9.1
cat-sub-4	-4755.10567	-4753.712471	-4756.262414	7.7
cat-sub-5	-4755.11844	-4753.725842	-4756.27073	2.2
cat-sub-6	-4755.103918	-4753.711868	-4756.259016	9.2

Coordinates of optimized structures:
Rh[(*R,S*)-DTBM-Bn-Yanphos](CO)$_2$H



P	-1.74441600	-1.24319900	-0.70052300
C	1.26887200	-2.70288100	0.26281500
C	1.37573100	-1.87260100	1.49436900
C	1.38622600	-0.48619400	1.48714300
C	1.47402900	-2.58779100	2.73215800
C	1.49617800	0.21388300	2.72075600
H	1.49559400	1.30306500	2.71900100
C	0.03611100	-3.08971700	-0.22781100
C	2.34592300	-4.14692500	-1.42392100
C	1.65373200	-2.56527300	5.18028800
H	1.74369200	-1.99013900	6.10247600
C	1.59645000	-1.86420700	3.95317900
C	3.74986200	-2.83138100	0.08314700
H	3.84585600	-2.11761500	0.90200300
C	4.87340600	-3.31301400	-0.54151500
H	5.85900600	-2.97682300	-0.21840700
C	1.61304400	-0.45193900	3.91052900
H	1.70484100	0.10212400	4.84581900
C	2.45477400	-3.22047900	-0.34457000
C	3.52390200	-4.64403700	-2.03210800
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C	1.06201400	-4.55028300	-1.86093500
H	0.98485000	-5.25905400	-2.68534700
C	1.45425600	-4.65685700	4.00626800
H	1.39428700	-5.74351800	4.03410700
C	1.41091800	-4.00407800	2.79955900

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C	-0.06295900	-4.02457100	-1.28608900
H	-1.05765900	-4.29171900	-1.64576300
C	4.76204700	-4.23419100	-1.60567500
H	5.66128000	-4.61494500	-2.08811400
C	1.57757400	-3.93382100	5.21113900
H	1.61070300	-4.46484700	6.16083100
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C	4.08673500	0.63910100	0.49369800
C	3.55063300	0.14510300	-1.78381000
C	5.44848400	0.53170800	0.23503200
H	3.74895000	0.83241900	1.50801100
C	4.90256400	0.00772600	-2.12291500
H	2.78448500	-0.04319100	-2.53119500
C	5.83871700	0.28067300	-1.10528800
C	0.95093700	2.13349200	0.51214500
C	1.85962700	3.17800100	0.64124700
C	-0.34774100	2.31081000	0.96849000
C	1.46987500	4.42469200	1.13669400
H	2.89034600	3.00899400	0.34157600
C	-0.79183400	3.50548700	1.53256900
H	-1.04072400	1.47057100	0.90059100
C	0.11236600	4.58611000	1.50053600
C	-2.10307700	-3.37077400	1.01850300
H	-1.68910500	-4.39054600	0.97876000
H	0.78603300	0.93353400	-2.79228900
C	0.29061600	-1.31495800	-3.25681000
O	0.57660100	-2.00340000	-4.14221800
Rh	-0.21923000	0.00335600	-1.93897200
C	-1.40626500	1.51682000	-2.13988200
O	-2.08057400	2.43764700	-2.31268900
C	-2.18747000	3.46245300	2.18324700
C	-3.26382200	3.23247700	1.11365700
H	-4.25303900	3.14087900	1.58735900
H	-3.08484700	2.31358500	0.53783200
H	-3.30664100	4.06394500	0.39571200
C	-2.56985600	4.68630200	3.02134600
H	-3.49890500	4.45597700	3.56243600
H	-2.76373200	5.58277800	2.42403800
H	-1.79927500	4.93239800	3.76194600
C	-2.19755700	2.27130500	3.16383400
H	-1.43668000	2.40762900	3.94672400

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C	2.52183800	5.90257900	2.85780000
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H	2.77320300	5.03014500	3.47777100
H	1.54844900	6.28766200	3.17941200
C	3.92755500	5.03786500	1.02393200
H	4.03855800	4.80359700	-0.04431500
H	4.21209500	4.14703900	1.60336500
H	4.64894200	5.83044500	1.26454700
C	2.25723400	6.77797600	0.52558300
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H	3.11424000	7.46246700	0.60544700
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C	5.74557400	0.75180900	2.74459700
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H	5.20227800	1.70505200	2.82368800
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C	7.41817000	1.77935300	1.25788400
H	8.12978800	1.64059200	0.43943100
H	8.00159000	1.89379400	2.18287500
H	6.86952300	2.71782200	1.09020500
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H	7.78431400	-0.91787000	0.52859800
H	6.57375100	-1.56458100	1.66768900
H	7.98022200	-0.67282900	2.27986000
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H	6.11481500	1.46697600	-4.19942700
C	6.50913500	-1.29832700	-3.63942300
H	7.42524700	-0.75390100	-3.40150600
H	6.60966900	-1.69344900	-4.65989300
H	6.44681700	-2.15477600	-2.95249500
C	4.10580100	-1.34750200	-4.10120200
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C	-3.31908000	-3.69523200	3.16811400

C	-1.66453500	-1.95714900	3.10230800
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C	-1.94578300	-1.64477700	4.43082800
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H	-6.11097100	1.83455300	-1.20755400
C	-4.02756800	-0.44021700	0.56048000
C	-6.34407600	-0.59707500	-0.10575400
C	-4.74630900	0.68246800	-4.13148000
C	-4.55351500	-0.30041900	-1.87634600
C	-6.72374000	-0.63531100	1.26854300
C	-5.26418400	1.68123500	-4.99014400
H	-5.00400800	1.63895900	-6.04814400
C	-8.08710000	-0.78954300	1.61563200
H	-8.35107100	-0.80518800	2.67359600
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H	-6.01501400	-0.56147000	3.31387500
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H	-7.09595800	-0.78693800	-2.13036200
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C	-6.05403400	2.69068300	-4.50281200
H	-6.43766800	3.45938300	-5.17134100
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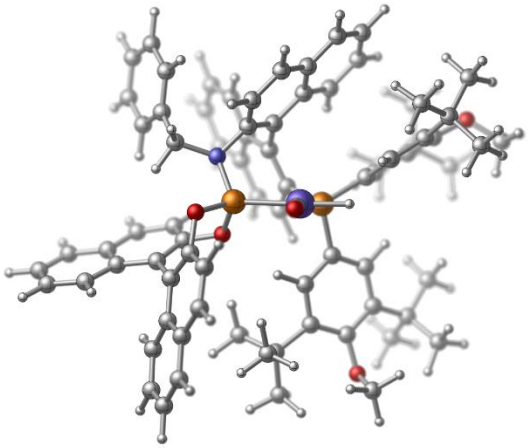
H	-3.62135000	-0.43174500	2.67528200
O	-2.95118900	-2.03361300	-1.54196500
O	-2.67174100	-0.32307000	0.31593600
O	-0.32148200	5.85089400	1.83346800

O	7.19298200	0.25597200	-1.35613300
C	-1.04626400	6.46508500	0.78623800
H	-1.94362500	5.88864500	0.51660200
H	-1.34806600	7.45535000	1.14456100
H	-0.42805200	6.57516600	-0.11755500
C	7.72924000	1.39178300	-2.00089700
H	8.75416800	1.52963400	-1.63571100
H	7.77047100	1.25662300	-3.09126700
H	7.14359000	2.29510100	-1.77452700

Rh[(*R*,*S*)-DTBM-Bn-Yanphos](CO)H



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C	0.77898100	-0.56692600	1.13322900
C	0.63237300	-2.82451600	2.04370400
C	0.48170500	-0.04831200	2.41941700
H	0.42994300	1.03151300	2.55733400
C	0.01003900	-2.79353100	-1.28566900
C	2.60222100	-3.56221900	-2.05458900
C	0.18106700	-3.15738000	4.43408200
H	-0.04701500	-2.72517700	5.40903300
C	0.35073100	-2.28352800	3.33337600
C	3.49639800	-2.76912700	0.07169500
H	3.34534500	-2.30151500	1.04450000
C	4.75648600	-3.15673200	-0.31283600
H	5.60243500	-2.98752800	0.35314400
C	0.26304300	-0.88050900	3.48483700
H	0.03480200	-0.47029900	4.46928300
C	2.38151400	-2.95020300	-0.78546800
C	3.90838200	-3.97097700	-2.41436500

H	4.05467500	-4.44149600	-3.38725700
C	1.50688700	-3.75308400	-2.92946400
H	1.68637800	-4.19448000	-3.90991500
C	0.63500500	-5.04959300	3.01542300
H	0.75200400	-6.12543600	2.89729400
C	0.76843100	-4.23105900	1.92257300
H	0.97894600	-4.66305700	0.94563700
C	0.24860000	-3.37449200	-2.55527500
H	-0.59238600	-3.49243100	-3.23899500
C	4.96715400	-3.77207200	-1.56480200
H	5.96964100	-4.08525200	-1.85352400
C	0.32639200	-4.51264100	4.28292300
H	0.21094600	-5.17536900	5.13923000
N	-1.33547500	-2.41229100	-0.95751000
P	1.20236000	0.59518800	-0.24722900
C	3.02784300	0.49902400	-0.20609600
C	3.69955500	0.43675400	1.01448600
C	3.75907100	0.42798300	-1.37837400
C	5.08607200	0.37361600	1.08941900
H	3.11188900	0.43225700	1.92894200
C	5.15626200	0.33249300	-1.38671000
H	3.20369900	0.42587800	-2.31277400
C	5.80296900	0.38397400	-0.13438800
C	0.82202900	2.25740500	0.41798000
C	1.78271700	3.11103500	0.95542200
C	-0.49965200	2.67996000	0.37495500
C	1.46623000	4.40525400	1.36437100
H	2.80574000	2.75849900	1.03652200
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H	-1.25170200	1.99027400	-0.00226400
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C	-2.36774700	-3.47153900	-1.01860700
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C	-0.56925300	0.49940900	-4.06122000
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C	-2.87325800	5.50522500	1.49416400
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C	2.02662500	5.64106900	3.46242000
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H	5.19440200	2.10974500	-3.49690300
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H	6.80052300	2.16070600	-2.75316800
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H	7.48042100	-0.87155000	-3.70630200
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H	5.47487800	-0.79106300	-4.65573800
H	-3.31593700	-3.01530600	-0.71142000
C	-2.08268500	-4.66764800	-0.15127100
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C	-2.57685000	-4.72374000	1.15298200
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H	-3.12865100	-3.86987600	1.54747000
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H	-1.57431500	-7.85095600	2.02610100
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H	-7.20016900	-0.40723100	-0.64510200
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C	-3.15325800	-1.24106700	1.95636200

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H	-0.50907700	7.92799700	0.48505300
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H	8.71020100	1.67523800	0.32946100
H	8.14157000	1.68719100	-1.35444300
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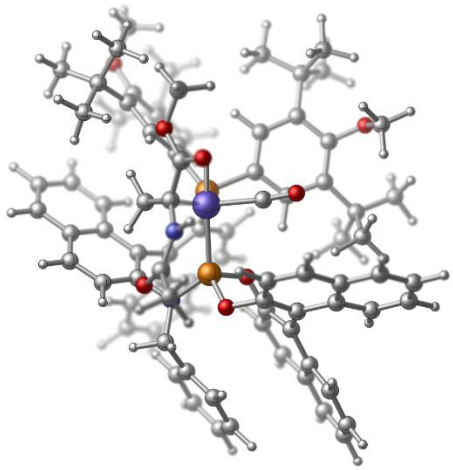
Rh[(*R,S*)-DTBM-Bn-Yanphos](CO)(MAA)H-1



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C	-2.17960600	-3.46082300	0.14819000
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C	-1.37953100	-4.62193100	2.14075300
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H	-3.08521300	0.07913300	-2.53110700
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C	-1.94551400	4.12579800	-1.45894200
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C	0.41390800	3.59930000	-1.95808300
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C	-3.16025500	5.05491000	-1.59856700
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C	-0.46542300	-0.18578200	4.01666900
C	-1.13793200	0.95291400	4.69475700
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O	-2.46033100	1.01758900	4.47476300
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O	1.35154500	-2.49882800	3.88370100
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H	3.59936900	-1.64130000	5.08918000
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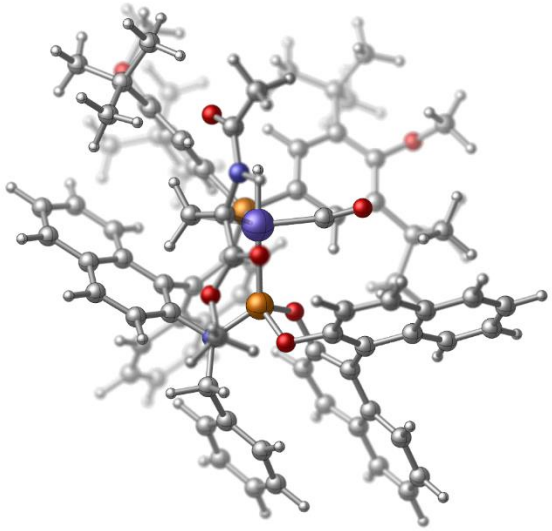
Rh[(*R,S*)-DTBM-Bn-Yanphos](CO)(MAA)H-2



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H	-3.13193000	-2.33768600	-1.69985100
C	-4.55440100	-3.56109700	-0.68566200
H	-5.38069800	-3.22996100	-1.31460300
C	-0.08718900	-0.75299900	-3.91445700
H	0.13085500	-0.23773300	-4.85057000
C	-2.20554400	-3.42507300	-0.06826500
C	-3.74833500	-4.91794700	1.12966900
H	-3.90573300	-5.65374900	1.91874200
C	-1.36088000	-4.83556800	1.73969700
H	-1.53933100	-5.58413500	2.51176700
C	-0.07501100	-4.95982500	-3.81939400
H	-0.10568700	-6.04807700	-3.80220600
C	-0.35873900	-4.25464500	-2.67545600
H	-0.60307900	-4.79456000	-1.76173300
C	-0.11855600	-4.29225100	1.57722000
H	0.69009800	-4.58631500	2.24327200

C	-4.78927800	-4.50059000	0.33948500
H	-5.79265800	-4.89313100	0.49713500
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H	0.48864000	-4.85840100	-5.91261000
N	1.45971800	-2.75427300	0.51995500
P	-1.24672900	0.35138500	-0.10640400
C	-3.06421400	0.15677500	-0.26373100
C	-3.63236200	0.17965100	-1.54026800
C	-3.88772500	-0.01185900	0.83642400
C	-5.00299700	0.11386200	-1.74269900
H	-2.97115400	0.26924200	-2.39719100
C	-5.27998900	-0.15768600	0.70489700
H	-3.43863400	-0.03313600	1.82748000
C	-5.81638200	0.00920300	-0.58611000
C	-1.01553100	2.07418600	-0.70892700
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C	-1.92824900	4.21982400	-1.41535200
H	-3.09662700	2.51742900	-0.84106500
C	0.51777600	3.85848800	-1.37721300
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C	-0.60663700	4.69875100	-1.55143900
C	2.59159600	-3.71185800	0.57352800
H	2.13890700	-4.70543200	0.68496100
H	-1.39339700	1.02305600	2.44013800
Rh	-0.16309300	0.11811100	1.99380300
C	0.84081600	1.77000500	2.14990000
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C	1.97891900	4.24422400	-1.67657600
C	2.65258500	4.79380500	-0.41192500
H	3.69254900	5.07834400	-0.63074400
H	2.67707800	4.03438900	0.38308800
H	2.13953500	5.67395600	-0.00774300
C	2.11136200	5.24082000	-2.83578200
H	3.17552800	5.36350200	-3.08139200
H	1.70318900	6.23050000	-2.62096900
H	1.60058300	4.86475300	-3.73351200
C	2.77702000	2.99987000	-2.10726200
H	2.27850300	2.45258000	-2.92168900
H	2.94834300	2.29681900	-1.28168800
H	3.76981500	3.30816000	-2.46528100
C	-3.16397500	5.04492100	-1.80774800
C	-3.05751300	5.44865900	-3.28454600
H	-3.94120100	6.03383200	-3.57933000

H	-3.01681500	4.55550300	-3.92504900
H	-2.16423700	6.05197700	-3.47555200
C	-4.45487100	4.22890800	-1.66091800
H	-4.65924700	3.94693100	-0.61742900
H	-4.43418900	3.30815800	-2.26318200
H	-5.30212500	4.83454300	-2.01186600
C	-3.33017800	6.29371500	-0.93454100
H	-2.56464400	7.04673000	-1.13957100
H	-3.29237400	6.03653700	0.13376100
H	-4.30664600	6.75915800	-1.13282100
C	-5.56764700	0.04754500	-3.17088800
C	-4.45472600	0.15963600	-4.21877900
H	-3.70448700	-0.63981900	-4.12464500
H	-3.93282800	1.12762900	-4.16853200
H	-4.89648300	0.07441100	-5.22073700
C	-6.57603700	1.16319000	-3.47480300
H	-7.51497200	1.02703700	-2.93124400
H	-6.81316000	1.16090200	-4.54845900
H	-6.16683700	2.15426700	-3.22914500
C	-6.24742500	-1.31351100	-3.37408100
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H	-5.51491000	-2.13010200	-3.28759600
H	-6.68833600	-1.36993700	-4.38044700
C	-6.07570500	-0.54489000	1.96615100
C	-6.31137200	0.68104200	2.85844300
H	-5.35787700	1.11362900	3.18972600
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H	-6.89010000	1.46618000	2.35385000
C	-7.40449800	-1.24910700	1.66437700
H	-8.16576600	-0.60276400	1.22075200
H	-7.81469800	-1.63999300	2.60599600
H	-7.25231900	-2.10034600	0.98470000
C	-5.24889300	-1.55194900	2.79045800
H	-4.40180700	-1.07580800	3.29665800
H	-4.87883700	-2.37979000	2.16593400
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H	3.19160600	-3.52856200	1.47437600
C	3.49273600	-3.75155700	-0.63092500
C	4.84564300	-3.43807500	-0.51536100
C	3.00753100	-4.21425900	-1.85507300
C	5.70170400	-3.58956100	-1.60243400
H	5.22986800	-3.06391900	0.43547300
C	3.85563600	-4.35976700	-2.94479800
H	1.95308300	-4.47359300	-1.94843600

C	5.20869900	-4.05168000	-2.81825800
H	6.75465300	-3.32711500	-1.50230400
H	3.45799500	-4.72268500	-3.89237100
H	5.87957600	-4.16379400	-3.66977100
C	3.73662100	-0.04504800	2.01575600
C	4.44056900	0.05257400	-0.36073700
C	5.55187800	2.74806400	0.32434900
H	5.58048200	2.41315600	-0.70970300
C	3.26551400	-0.35899200	-0.96301200
C	5.65767900	-0.09844400	-1.10262800
C	4.89537300	2.40685900	2.64552100
C	4.39811000	0.62740600	1.00218600
C	5.59930300	-0.49117300	-2.47191200
C	5.43838200	3.67864300	2.94972600
H	5.37429400	4.03278900	3.97888000
C	6.79885900	-0.62446400	-3.21075500
H	6.72831700	-0.91943300	-4.25876400
C	4.34852900	-0.81231000	-3.05252000
H	4.31929900	-1.13221400	-4.09436900
C	4.96215400	1.91239300	1.30790200
C	4.26657800	1.63082100	3.64628800
H	4.22468000	2.01684600	4.66442700
C	8.08504300	-0.08618900	-1.25131800
H	9.05415800	0.04366700	-0.77220900
C	3.67939600	0.43403200	3.33923400
H	3.14975300	-0.14274200	4.09620000
C	6.93648100	0.07506800	-0.51546400
H	7.00232000	0.32946500	0.54080400
C	8.02031300	-0.42377700	-2.61973000
H	8.93697900	-0.53973800	-3.19553100
C	6.07029100	3.97656600	0.65098300
H	6.51217000	4.59637700	-0.12812800
C	6.01981400	4.45073800	1.97787800
H	6.43137800	5.42805700	2.22356700
C	3.20631400	-0.78940000	-2.30309700
H	2.23885500	-1.08165000	-2.70867300
O	3.10901400	-1.25244500	1.74549500
O	2.06689000	-0.24327100	-0.30175100
O	-0.45930200	6.01932600	-1.91596600
O	-7.17790700	0.05061600	-0.78926900
C	-0.09168000	6.91691200	-0.88978400
H	0.99517500	7.08259200	-0.86918200
H	-0.57886600	7.87805000	-1.09517200
H	-0.41619700	6.55369900	0.09642400

C	-7.76754000	1.29143700	-0.45941600
H	-8.76374000	1.30566900	-0.91609600
H	-7.87620400	1.41830100	0.62704000
H	-7.17611200	2.13241300	-0.85408000
C	-1.28206200	-1.40952800	3.05766800
H	-2.35243500	-1.24143500	3.07701700
H	-0.96909000	-2.40540000	2.76282700
C	-0.47965700	-0.74357000	4.02079000
C	0.78918300	-1.31659600	4.51404500
O	1.42600400	-0.84474800	5.44314300
O	1.17698400	-2.43724700	3.87476500
C	2.37910500	-3.02771200	4.35083000
H	2.43585600	-4.01308300	3.87821700
H	3.24959900	-2.42970700	4.05606000
H	2.35857800	-3.12979900	5.44061100
N	-0.97998600	0.16236900	5.00231600
H	-0.27688600	0.41102400	5.69160100
C	-2.17074800	0.81431300	5.02708000
O	-3.06359100	0.66304900	4.20013700
C	-2.31636800	1.80164300	6.16059000
H	-2.17637200	2.81587500	5.76545000
H	-3.33595100	1.74106300	6.55365600
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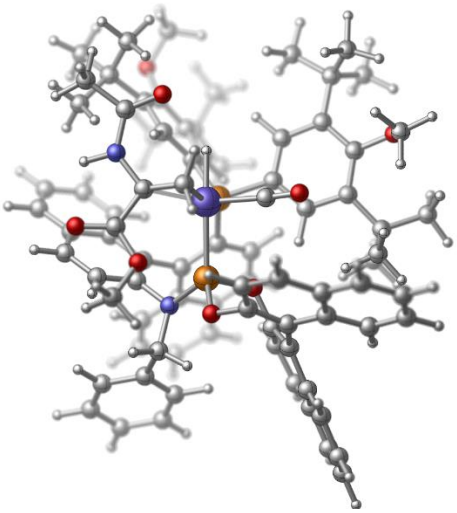
Rh[(*R*,*S*)-DTBM-Bn-Yanphos](CO)(MAA)H-3



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C	-0.40140100	-3.01728000	-2.49368900

C	-0.29734600	-0.25927500	-2.97181400
H	-0.29106700	0.81070800	-3.16940700
C	0.00124400	-2.91077700	0.87011200
C	-2.63652900	-3.79303900	1.34016600
C	0.09886500	-3.43660200	-4.86092900
H	0.34072100	-3.03830200	-5.84691300
C	-0.09727700	-2.52513700	-3.79596000
C	-3.34781200	-2.89362600	-0.81100200
H	-3.12542500	-2.35947200	-1.73463000
C	-4.62463200	-3.34031800	-0.57518500
H	-5.40773900	-3.15137300	-1.30901600
C	-0.04489000	-1.12741600	-4.00005100
H	0.17141400	-0.74735700	-4.99941700
C	-2.31144500	-3.10338700	0.13583400
C	-3.95698300	-4.25963100	1.54689700
H	-4.17858500	-4.79260600	2.47204100
C	-1.61777900	-4.02382500	2.29208400
H	-1.86243400	-4.52986300	3.22574600
C	-0.37424800	-5.27691500	-3.38297500
H	-0.48809500	-6.34833700	-3.22703700
C	-0.53093400	-4.41961500	-2.32348800
H	-0.75514500	-4.81954200	-1.33626700
C	-0.34117400	-3.59652800	2.05753900
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C	-4.93405600	-4.04223500	0.60914200
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C	-0.04538800	-4.78606800	-4.66378500
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N	1.35761100	-2.46273300	0.71132800
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C	-3.46387000	0.36145100	-1.76854600
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C	-4.83651300	0.36968200	-1.96685600
H	-2.79885500	0.33832600	-2.62703100
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H	-3.25901100	0.31755000	1.60054200
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C	-1.67517700	3.11833100	-0.98058300
C	0.54226500	2.40752200	-1.52905700
C	-1.36183200	4.44109300	-1.28581600
H	-2.67855200	2.86722500	-0.64914600
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H	1.28074100	1.60951300	-1.59344500
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H	2.43777000	-3.91181700	1.82978600
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Rh	-0.02144200	0.64482100	1.88145300
C	1.00399800	2.24405500	1.50651500
O	1.62921200	3.21230600	1.50075200
C	2.29582900	3.85326500	-2.55791500
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H	4.38656000	3.60777900	-2.03010900
H	3.29922700	2.53411300	-1.11937700
H	3.40258600	4.24835100	-0.69703200
C	2.57330900	5.21334900	-3.20724600
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C	-2.46541700	5.50910000	-1.29823600
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H	-3.33040500	6.89498900	-2.73041000
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C	-5.41196300	0.19911700	-3.38106400
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H	-5.60739200	-1.96566200	-3.23496900
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H	-4.92491100	1.77205600	2.85656300
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O	2.24769900	-0.10246000	-0.24541900
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C	-7.44041800	1.93288200	-0.81585700
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H	-7.40600900	2.22833900	0.24281800
H	-6.83054500	2.64369800	-1.39388000
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H	-0.27217800	1.84584100	4.27782700
H	1.24598200	0.80740700	4.26660300
C	-0.60369400	-0.25912800	3.91851000
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O	-0.55971700	-2.43749000	4.89927300
O	1.35093000	-1.58905600	4.07646800
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H	1.62085800	-3.63341600	4.41411000
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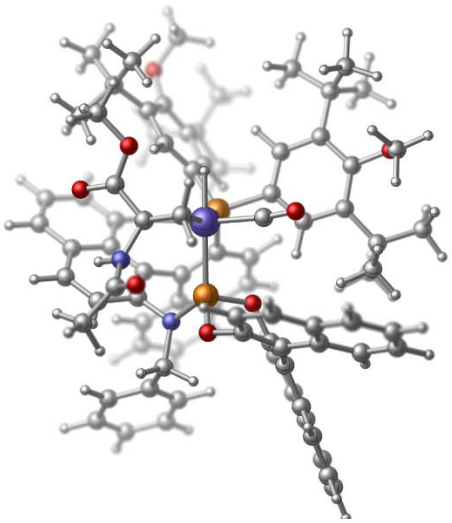
C	-3.97663100	0.44441100	5.48968900

H	-3.77757600	0.79097700	6.51205100
H	-4.84983100	0.99329300	5.12282300
H	-4.20951500	-0.62628900	5.52946200

Rh[(*R,S*)-DTBM-Bn-Yanphos](CO)(MAA)H-4



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H	-5.40798100	-3.18249200	-1.05631800
C	-0.26562000	-0.79675800	-4.05901000
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C	-3.63164300	-4.59798300	1.46224700
H	-3.73944400	-5.25599900	2.32445200
C	-1.21690100	-4.43653900	1.93599000
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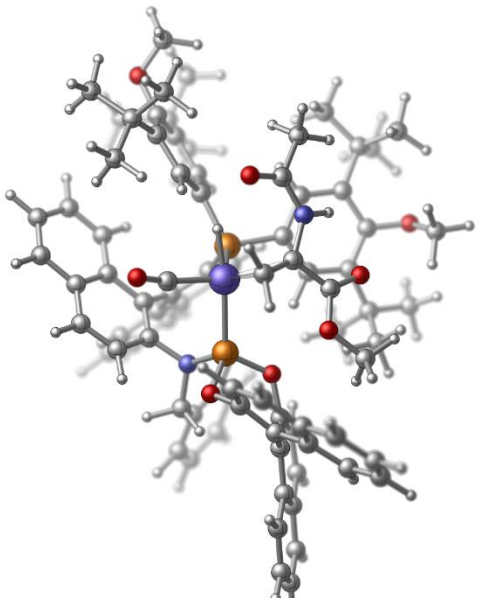
Rh[(*R*,*S*)-DTBM-Bn-Yanphos](CO)(MAA)H-5



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C	-2.74076500	4.09919400	-3.69750000
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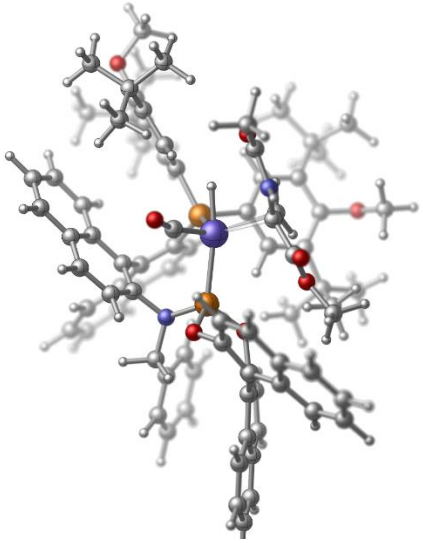
Rh[(*R*,*S*)-DTBM-Bn-Yanphos](CO)(MAA)H-6



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C	-8.02347900	-1.62667500	-0.74002500
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O	2.68766400	-4.52190500	-0.53508800
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N	0.06392600	-4.56435700	-0.76497800
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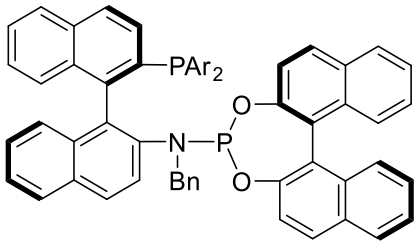
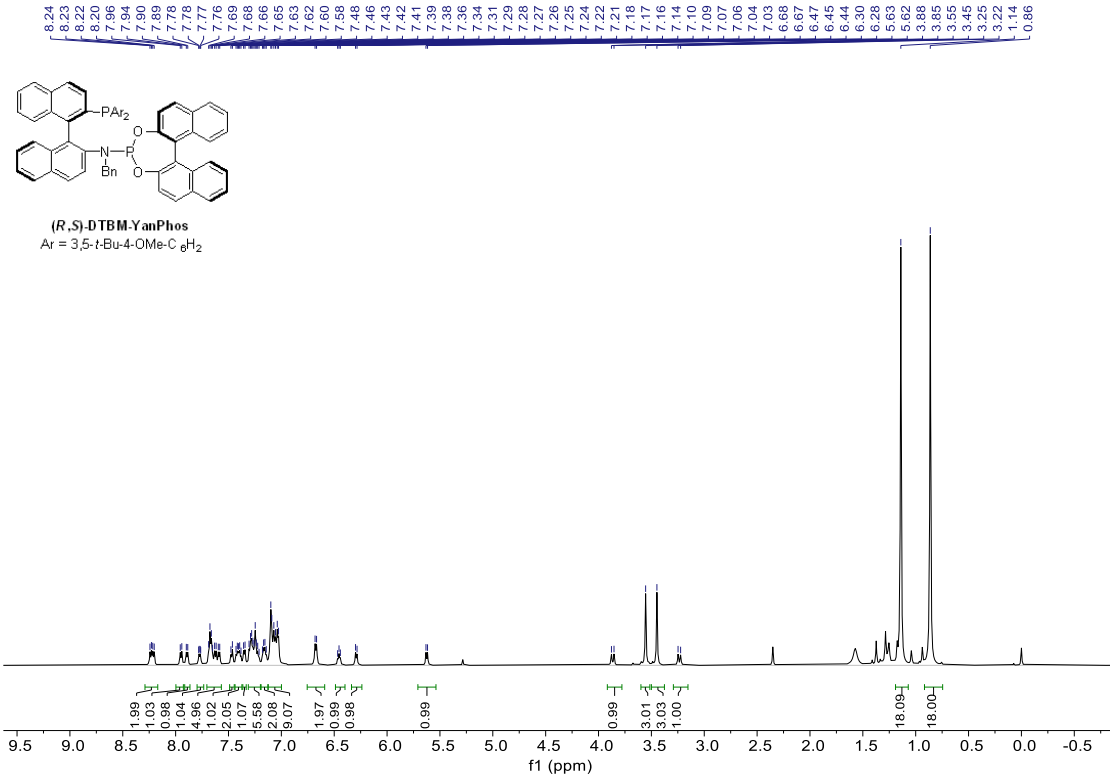
10. NMR spectra



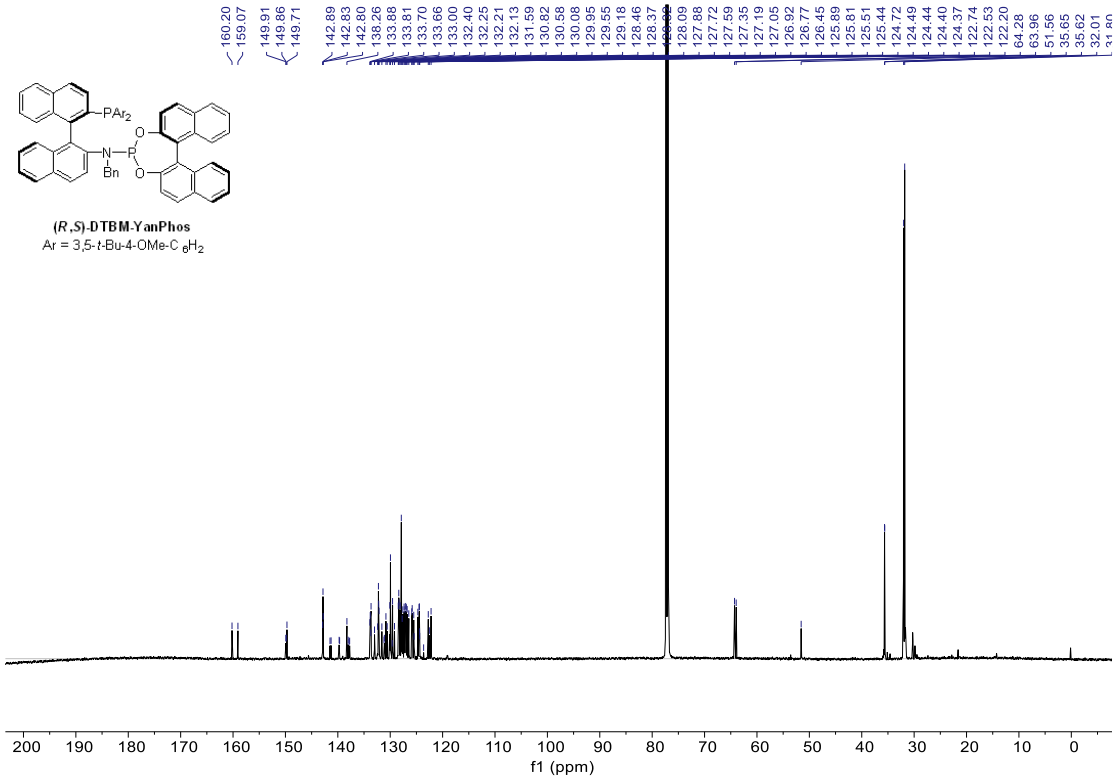
(*R*,*S*)-DTBM-YanPhos

Ar = 3,5-*t*-Bu-4-OMe-C_6H_2

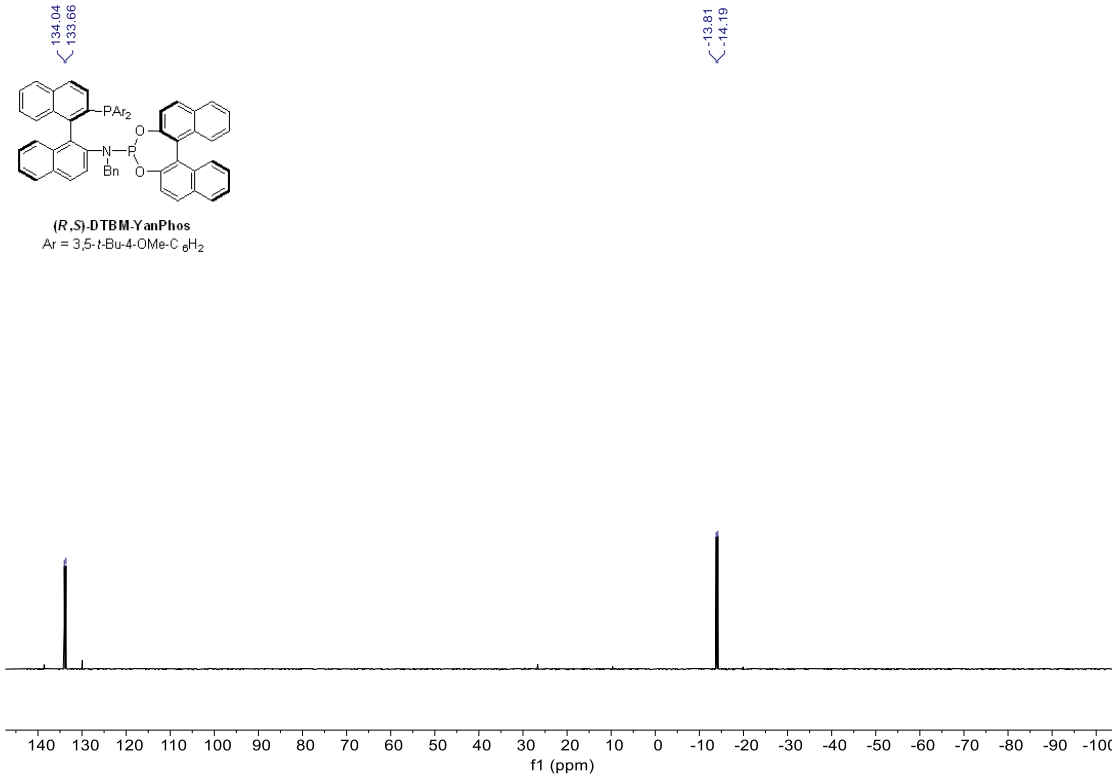
^{1}H NMR (600 MHz, Chloroform-*d*)

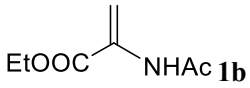


^{13}C NMR (151 MHz, Chloroform-*d*)



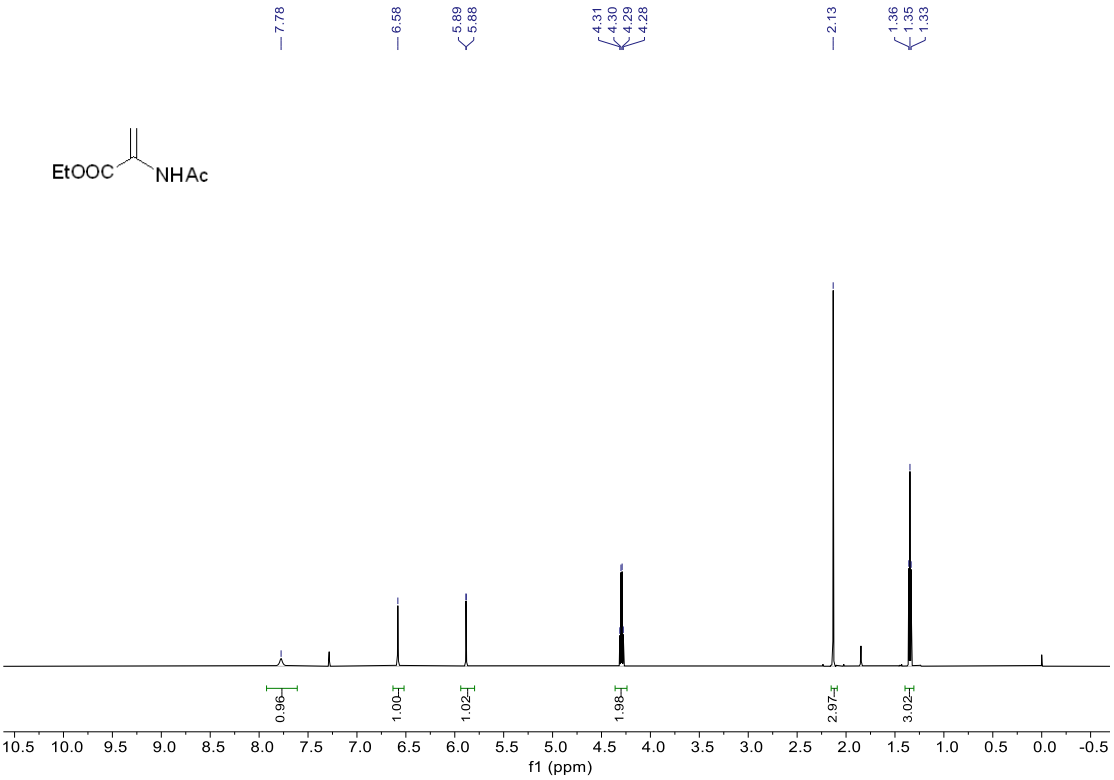
^{31}P NMR (243 MHz, Chloroform-*d*)



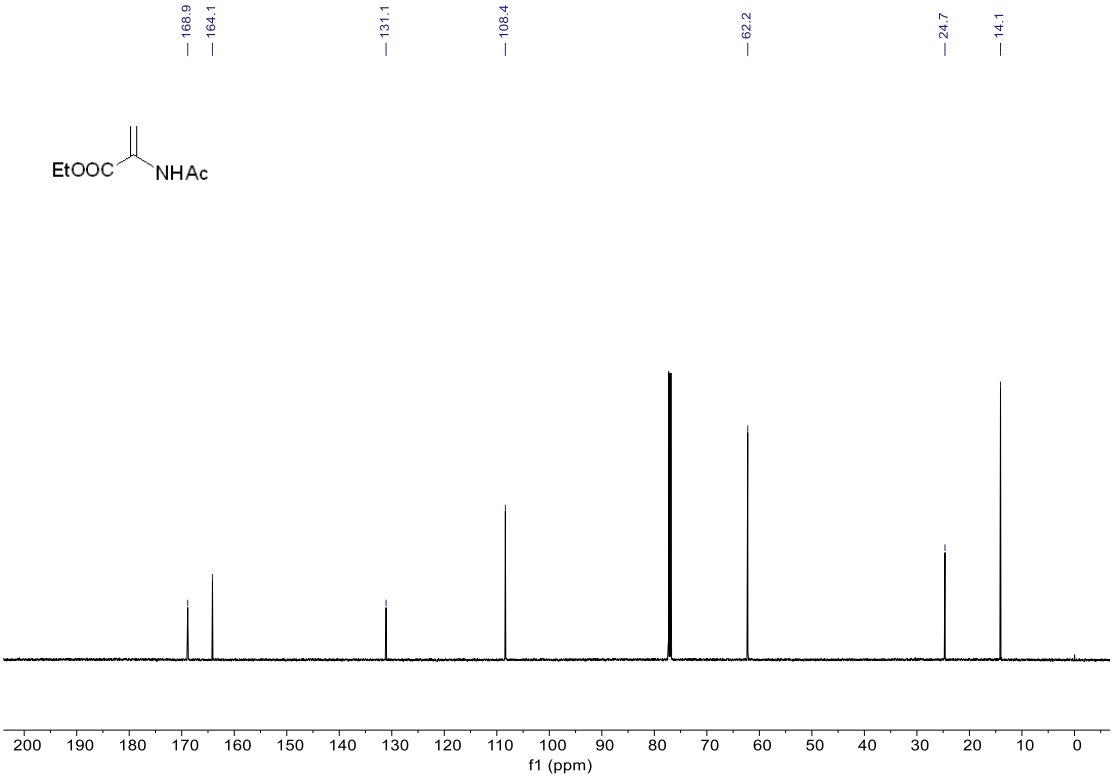


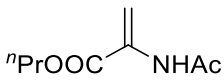
1b

^{1}H NMR (600 MHz, Chloroform-*d*)



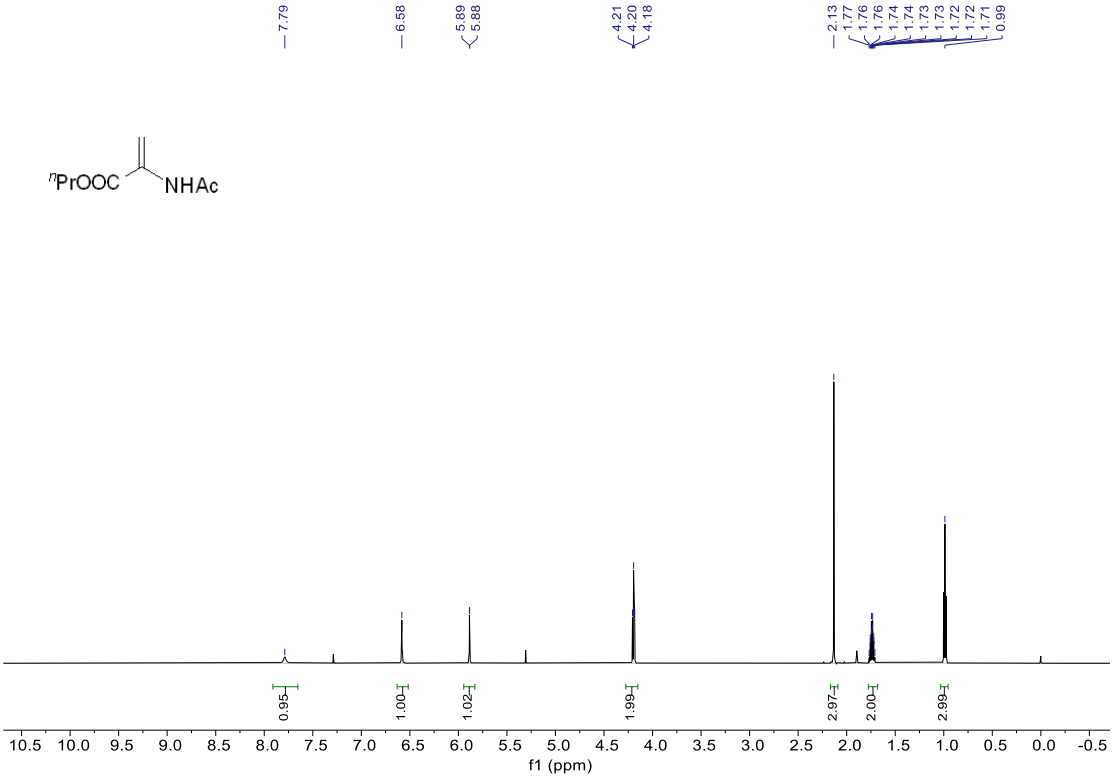
^{13}C NMR (151 MHz, Chloroform-*d*)



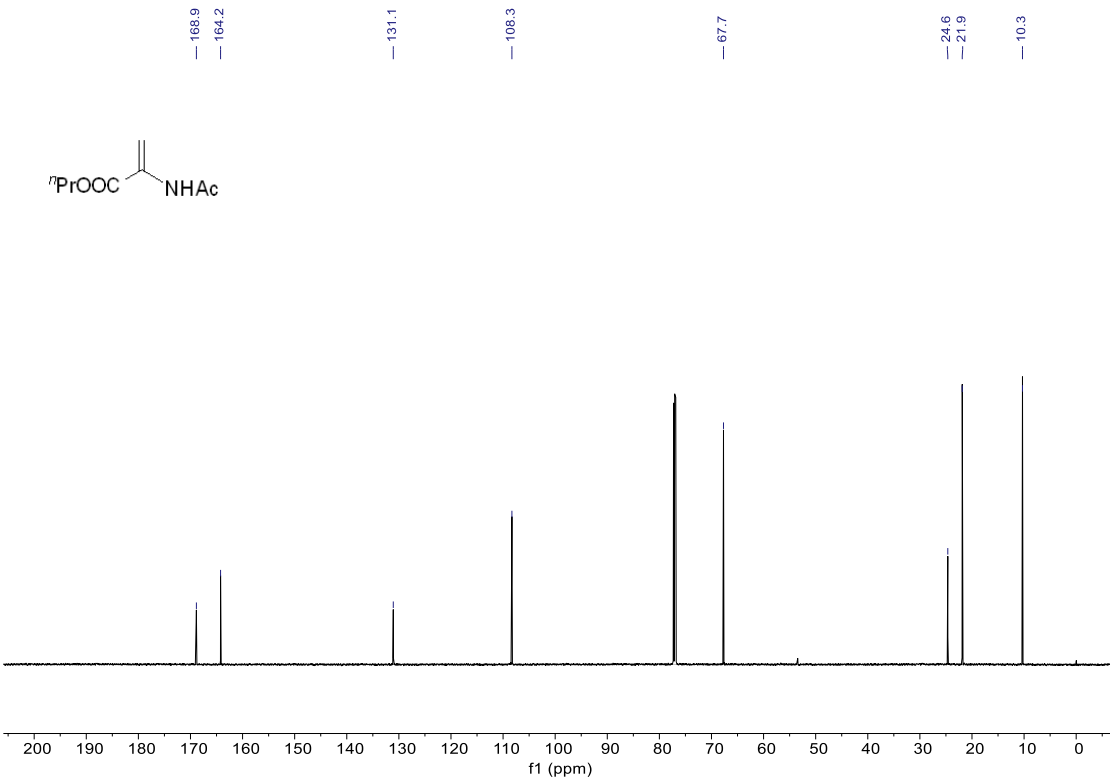


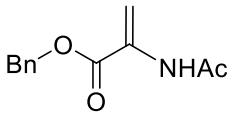
1c

^{1}H NMR (600 MHz, Chloroform-*d*)



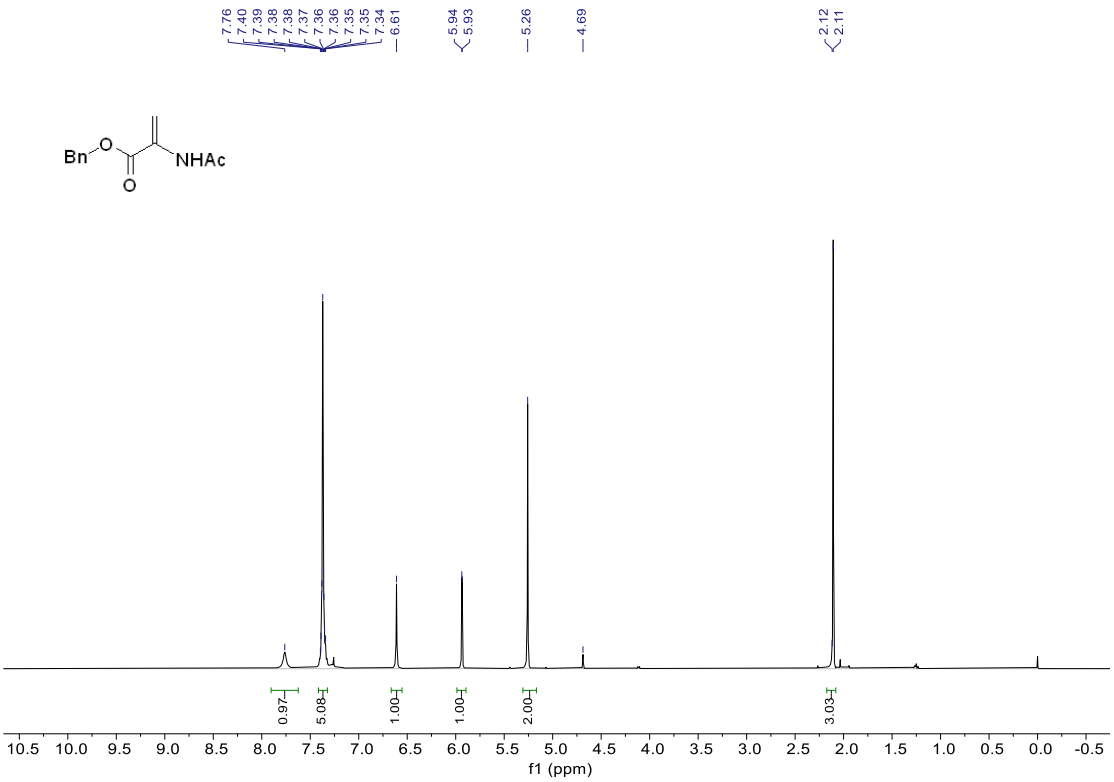
^{13}C NMR (151 MHz, Chloroform-*d*)



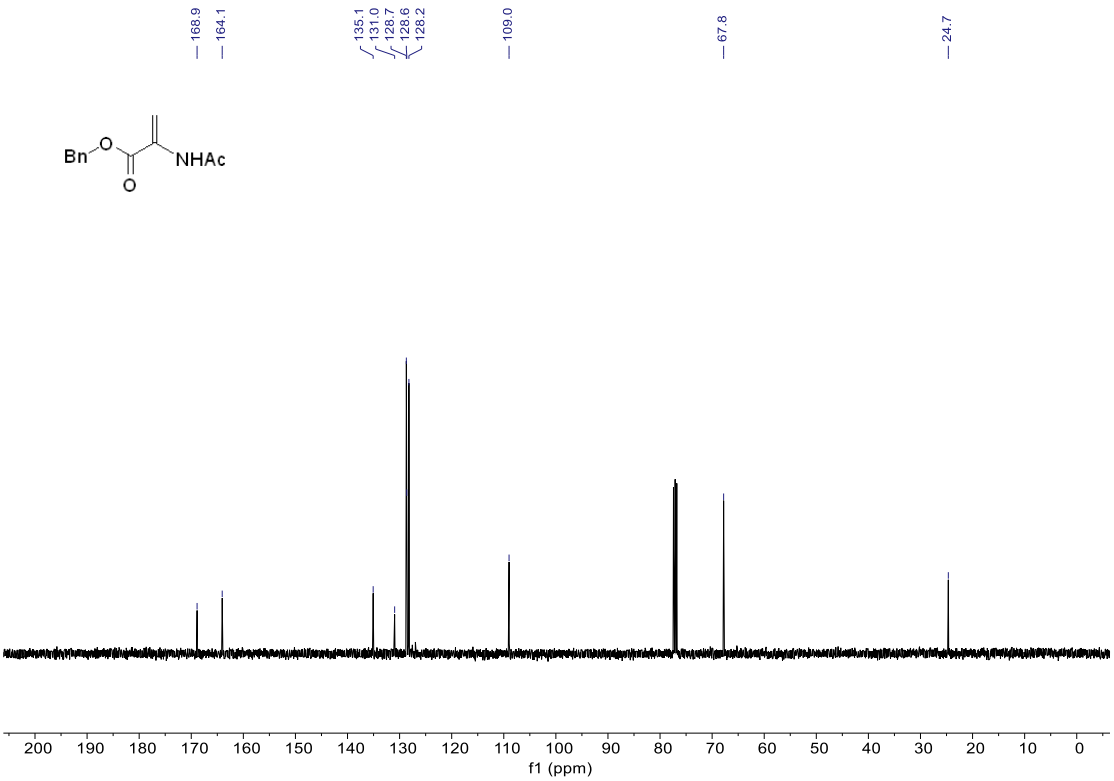


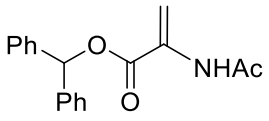
1d

^{1}H NMR (400 MHz, Chloroform-*d*)



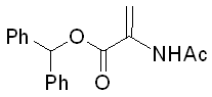
^{13}C NMR (101 MHz, Chloroform-*d*)

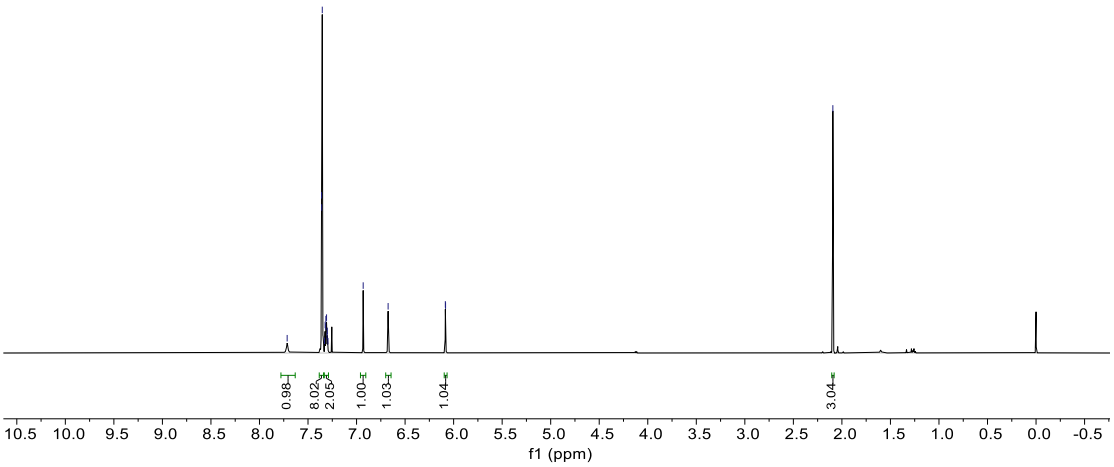




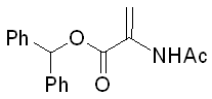
1e

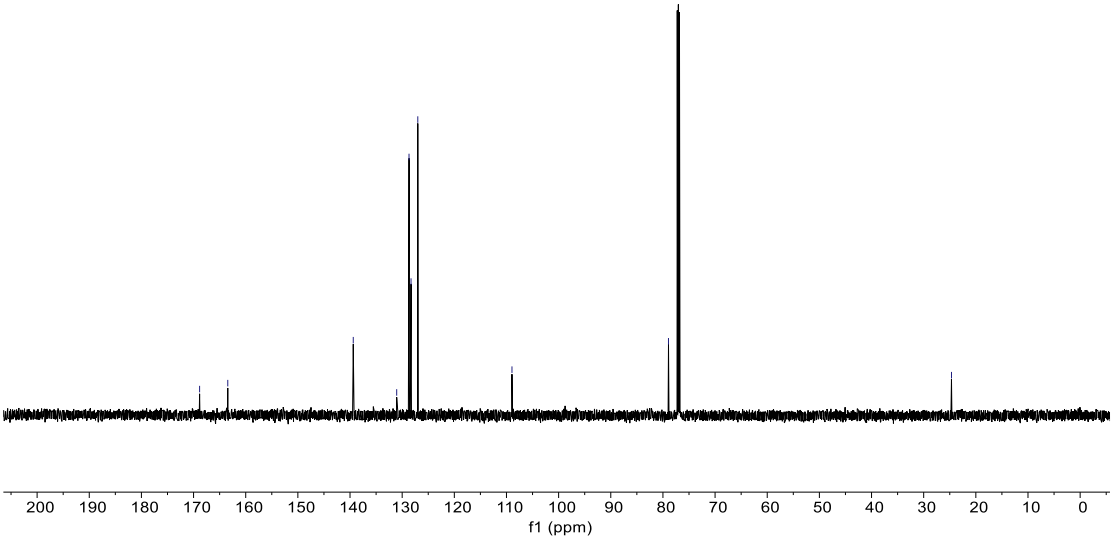
^{1}H NMR (600 MHz, Chloroform-*d*)

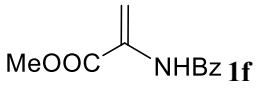




^{13}C NMR (151 MHz, Chloroform-*d*)

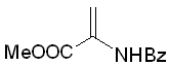


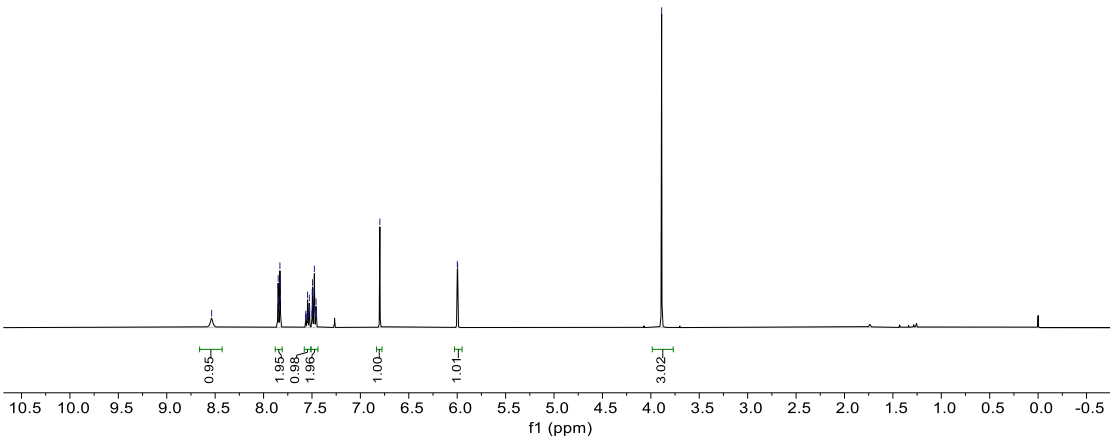




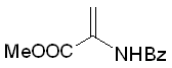
1f

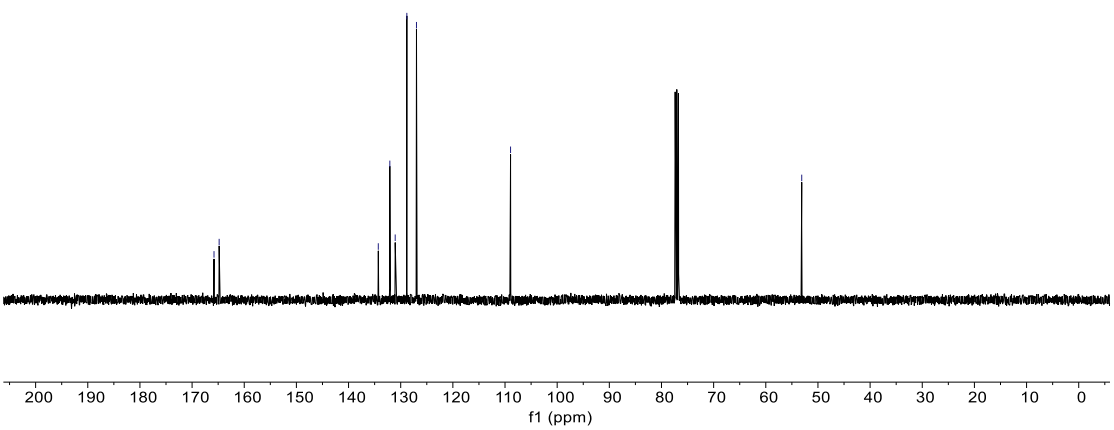
^{1}H NMR (400 MHz, Chloroform-*d*)

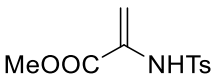




^{13}C NMR (101 MHz, Chloroform-*d*)

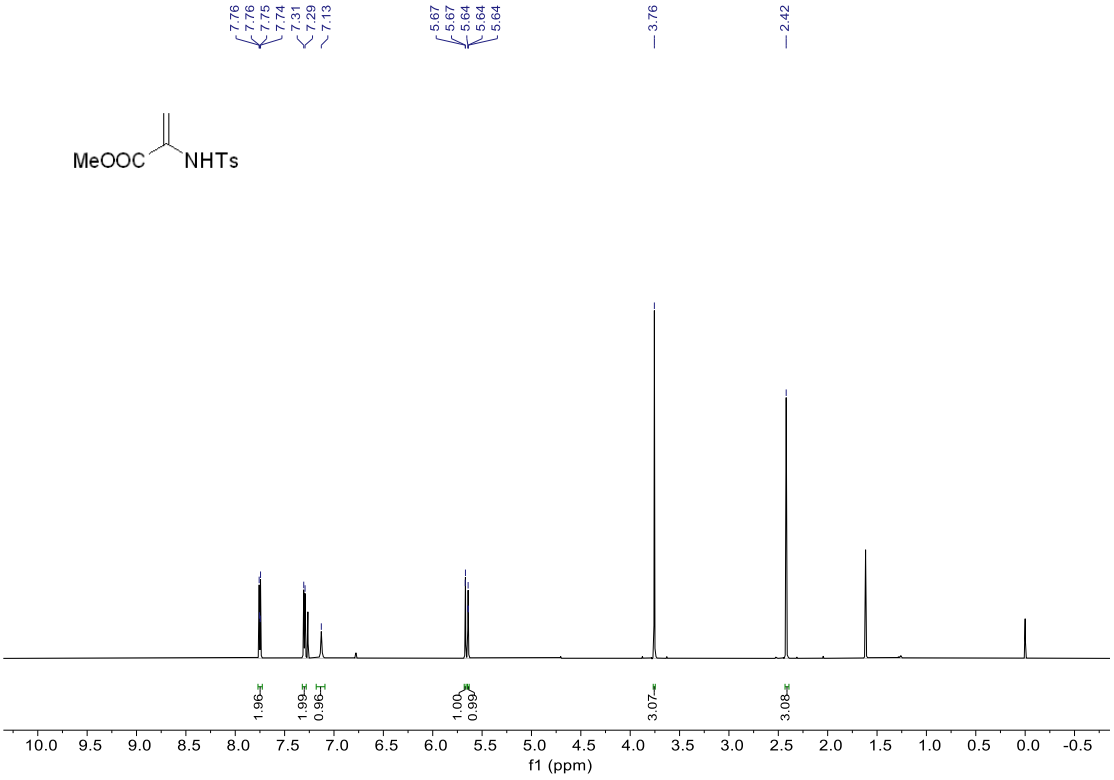




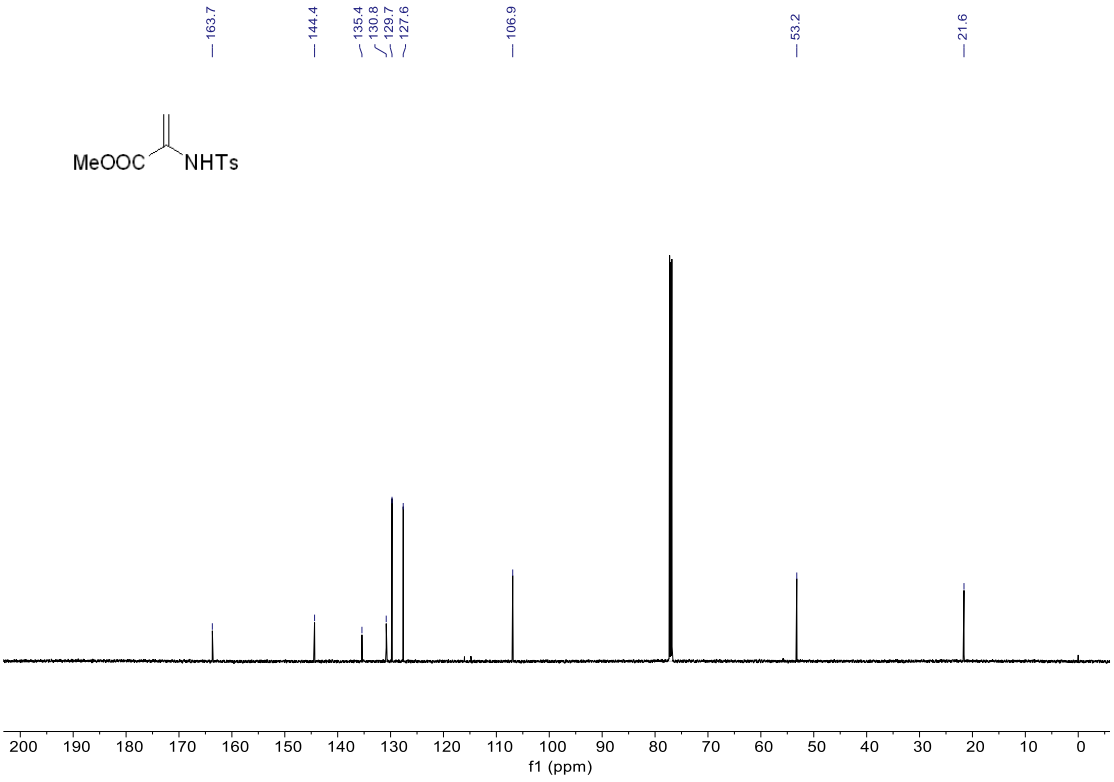


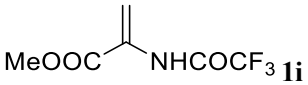
1h

^{1}H NMR (600 MHz, Chloroform-*d*)



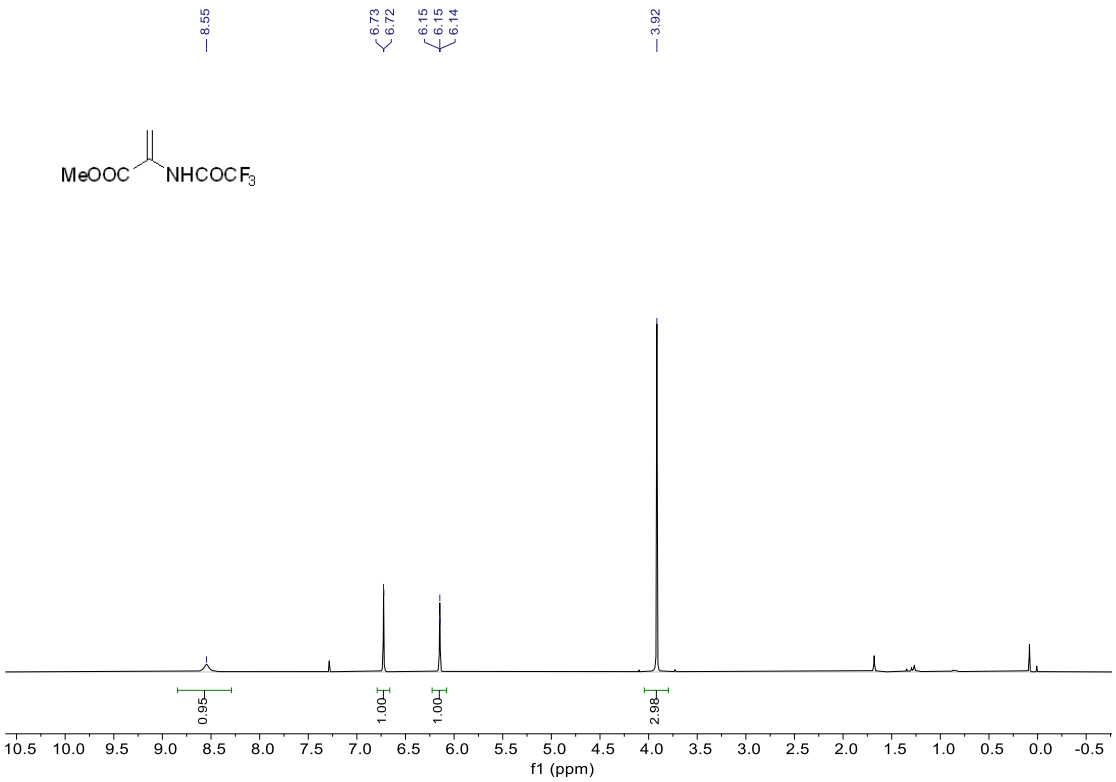
^{13}C NMR (151 MHz, Chloroform-*d*)



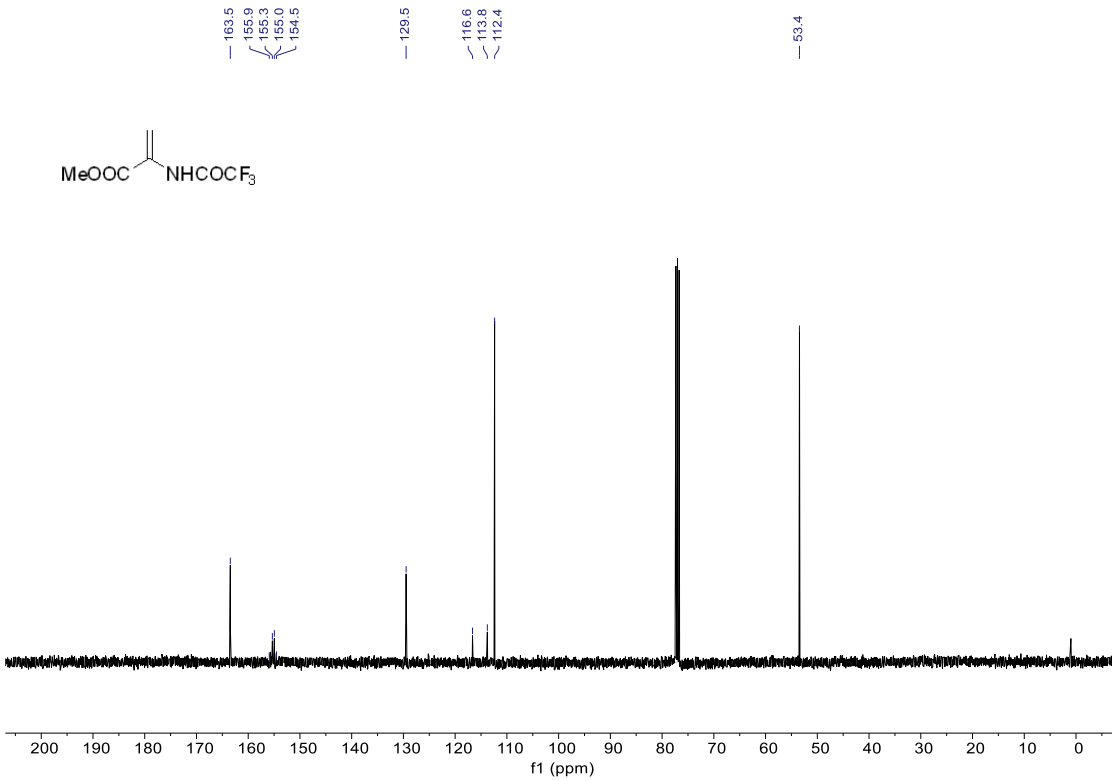


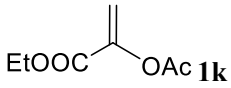
1i

^{1}H NMR (400 MHz, Chloroform-*d*)



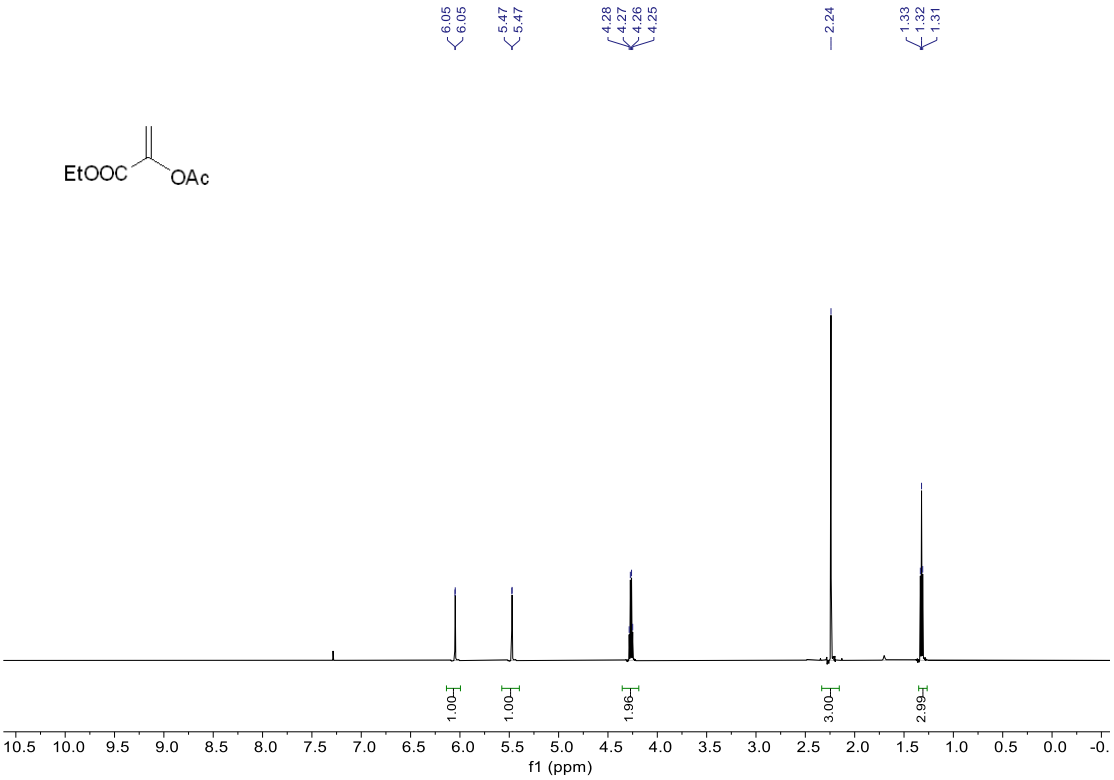
^{13}C NMR (101 MHz, Chloroform-*d*)



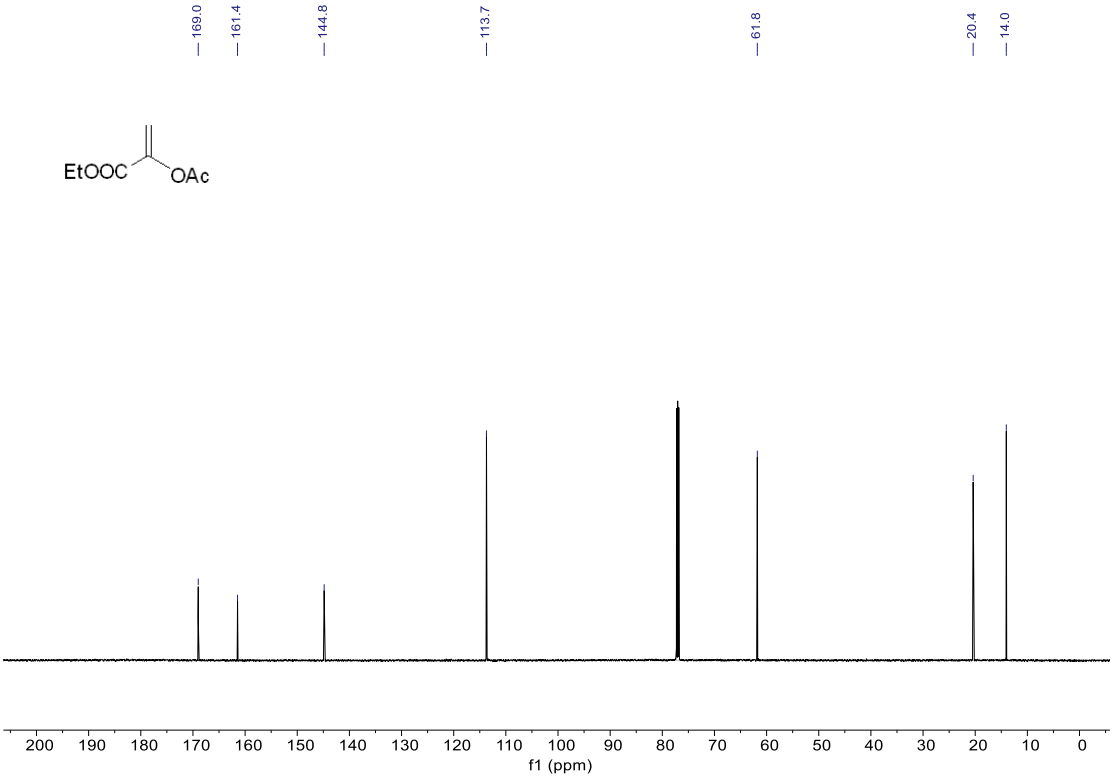


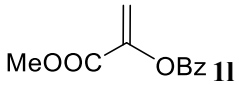
1k

^{1}H NMR (600 MHz, Chloroform-*d*)



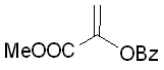
^{13}C NMR (151 MHz, Chloroform-*d*)

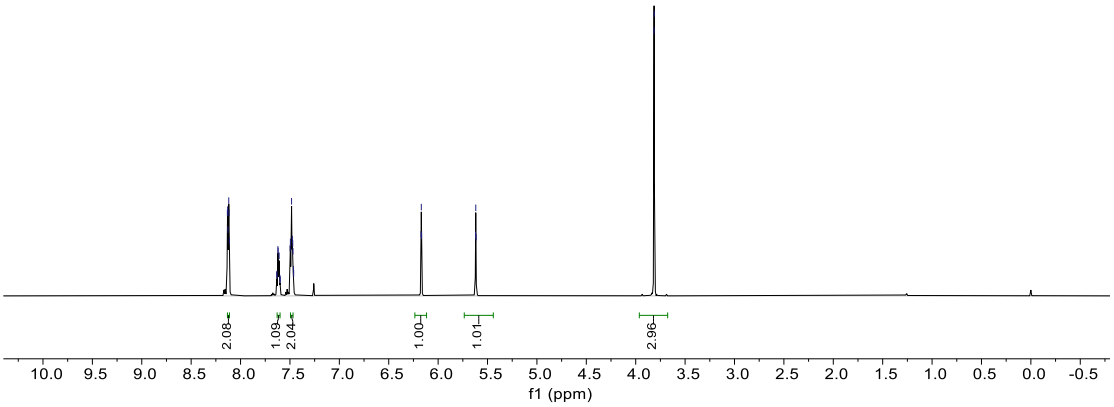




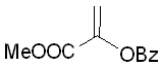
1l

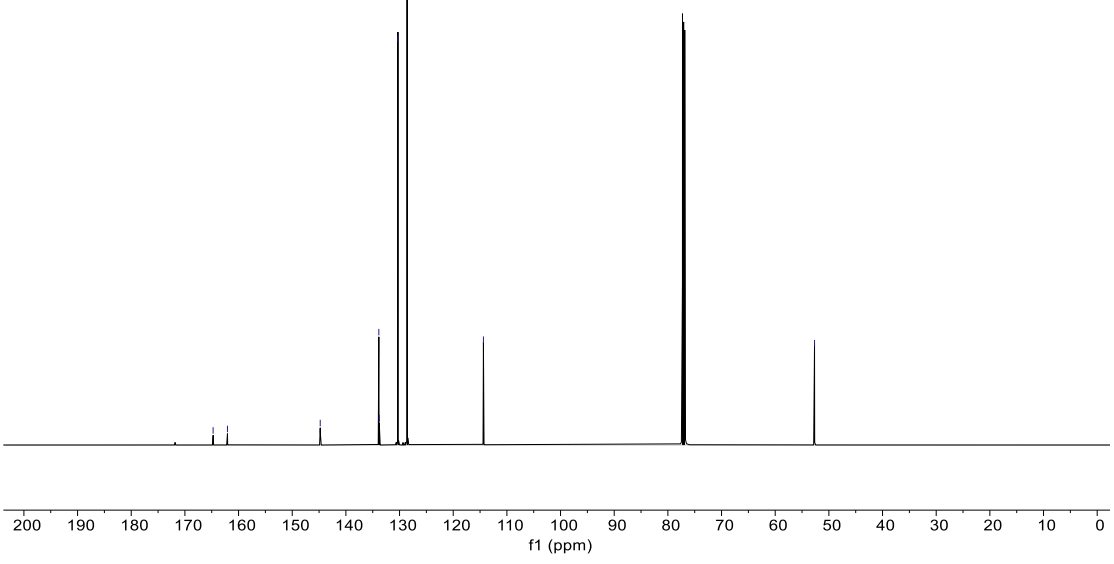
^{1}H NMR (600 MHz, Chloroform-*d*)

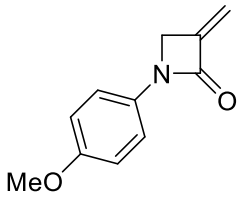




^{13}C NMR (151 MHz, Chloroform-*d*)

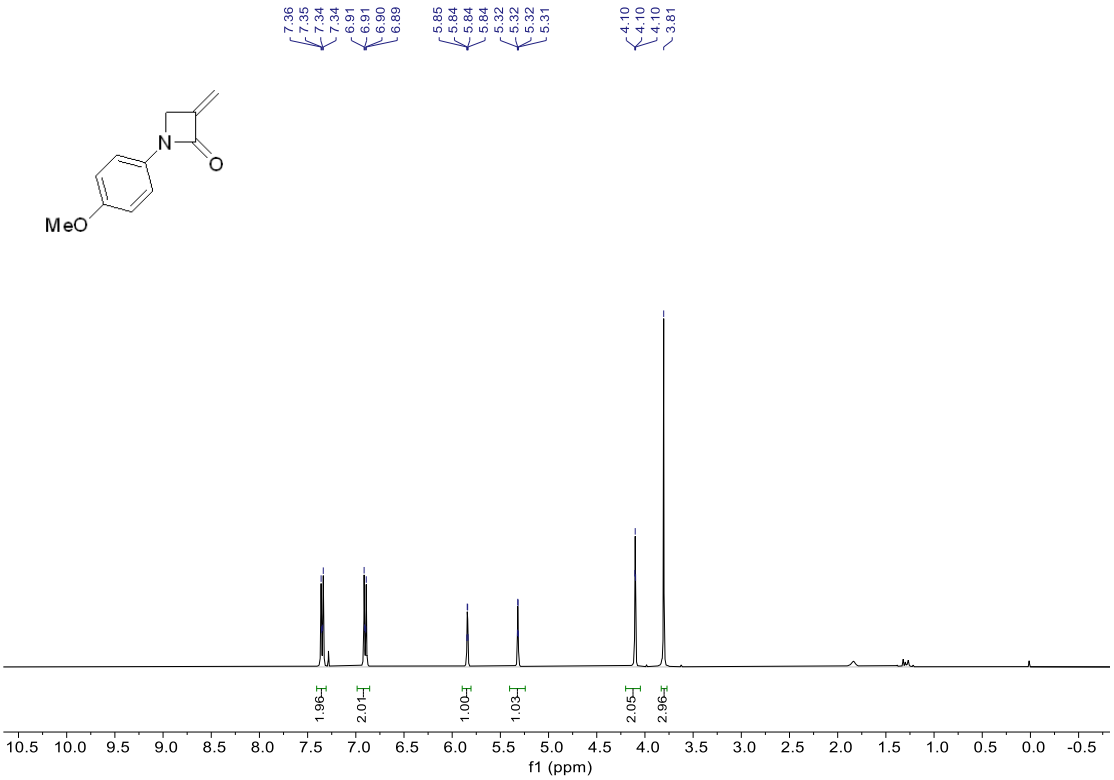




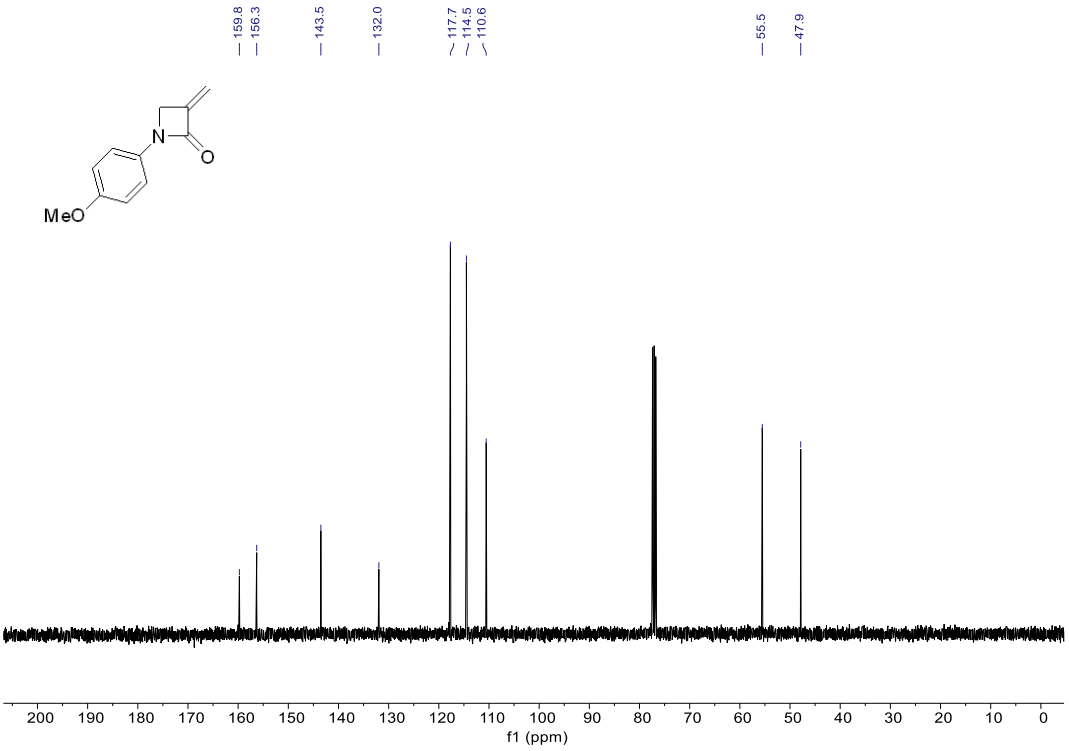


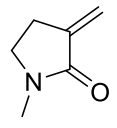
1n

^{1}H NMR (400 MHz, Chloroform-*d*)



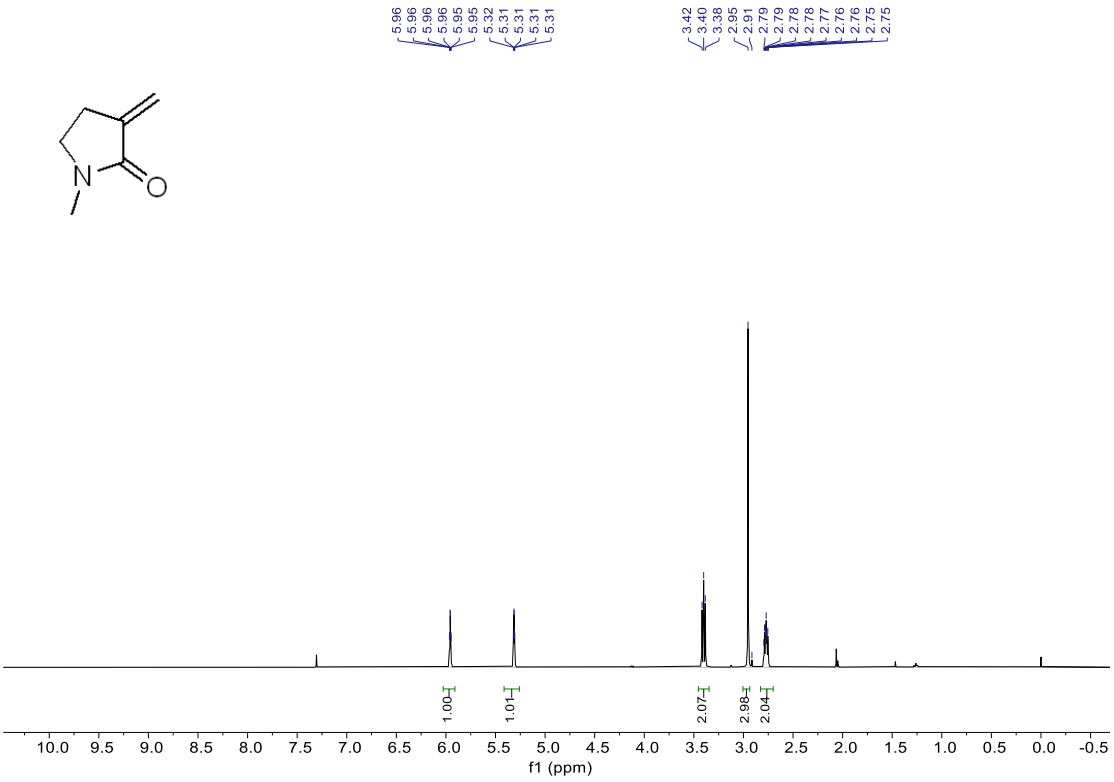
^{13}C NMR (101 MHz, Chloroform-*d*)



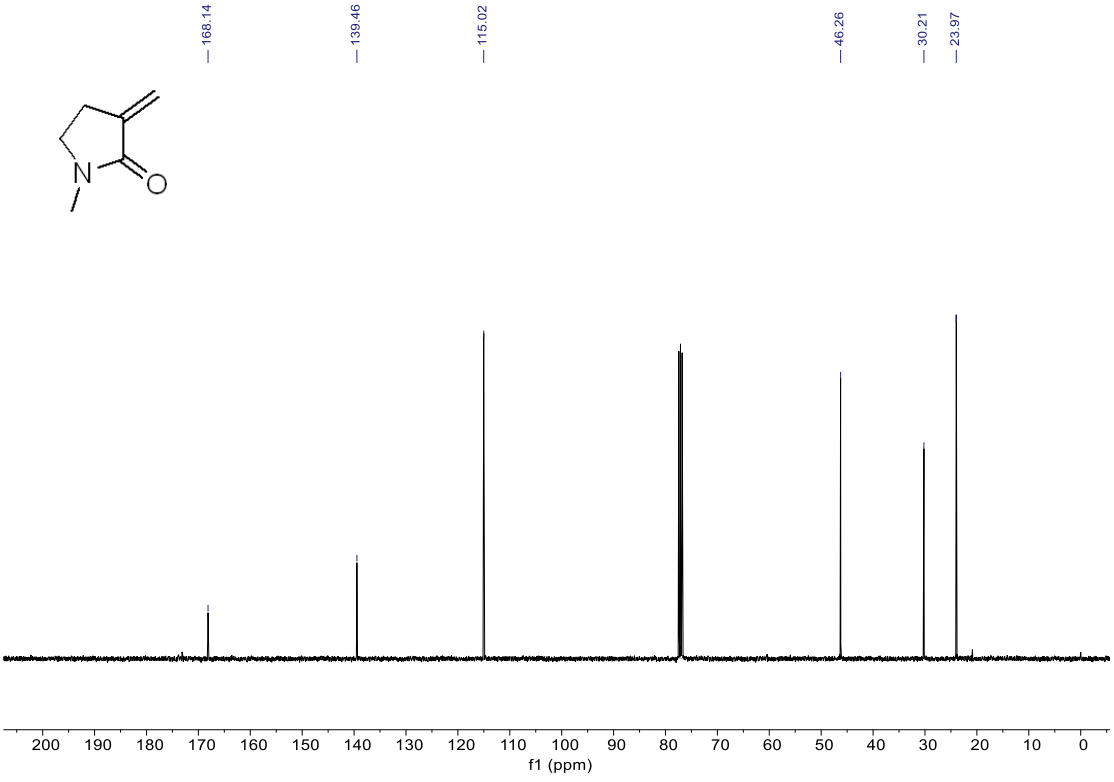


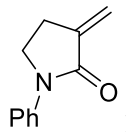
1o

^{1}H NMR (400 MHz, Chloroform-*d*)



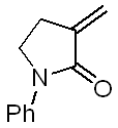
^{13}C NMR (101 MHz, Chloroform-*d*)

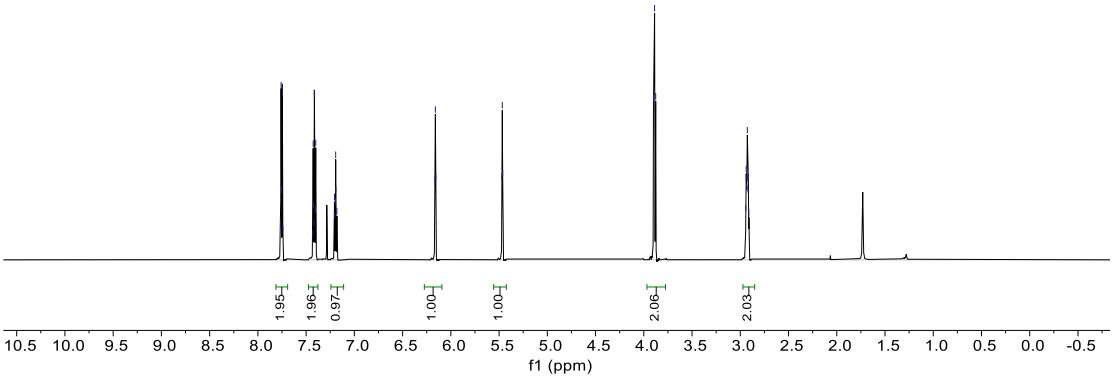




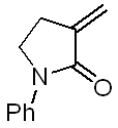
1p

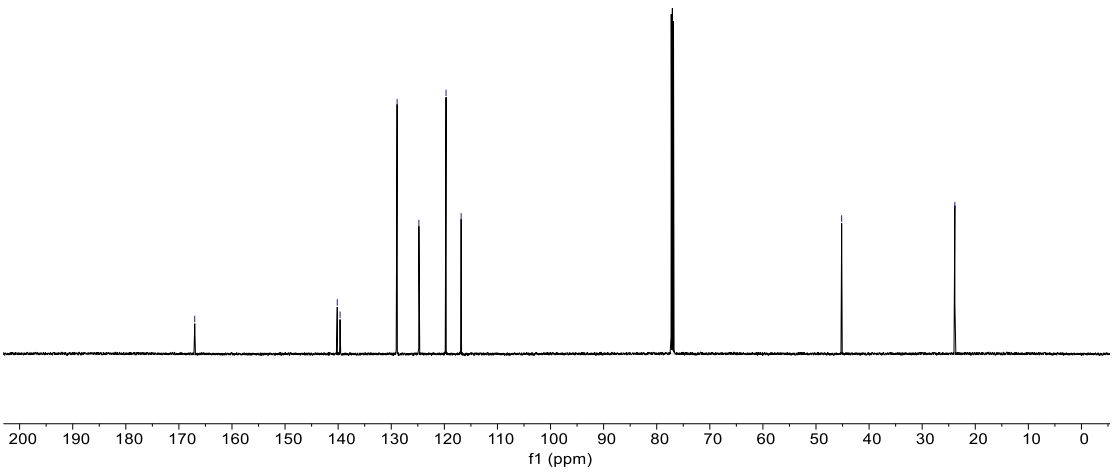
^{1}H NMR (600 MHz, Chloroform-*d*)

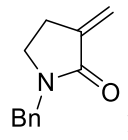




^{13}C NMR (151 MHz, Chloroform-*d*)

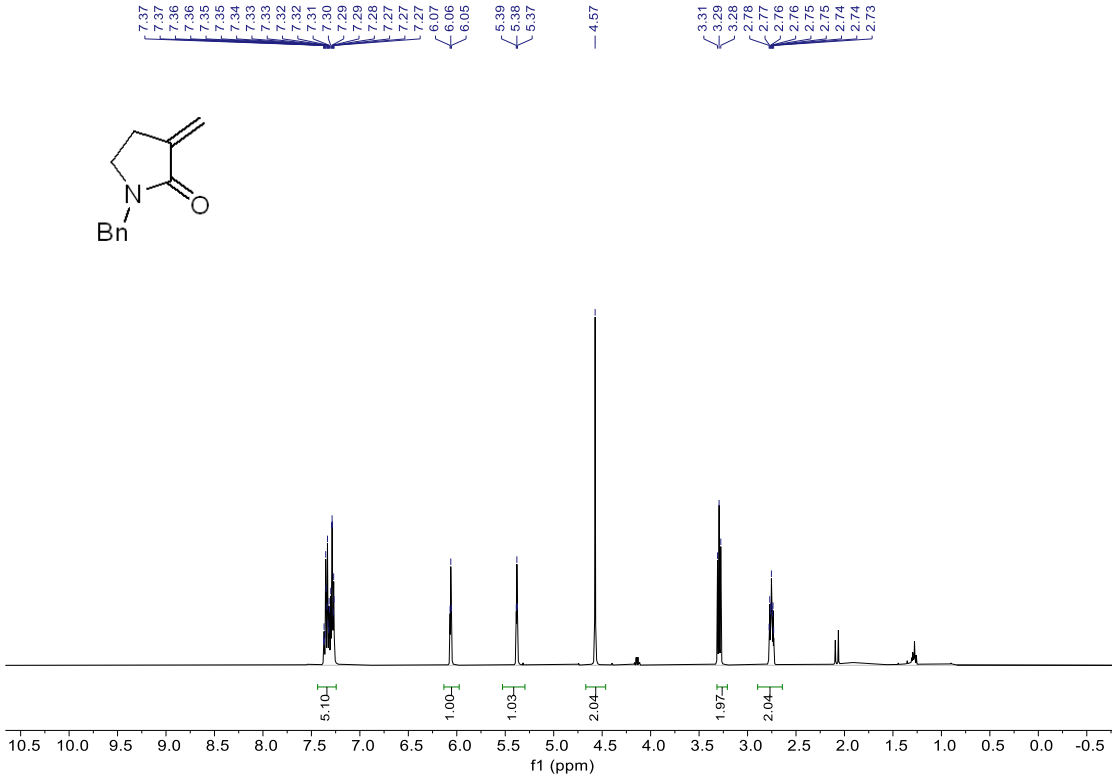




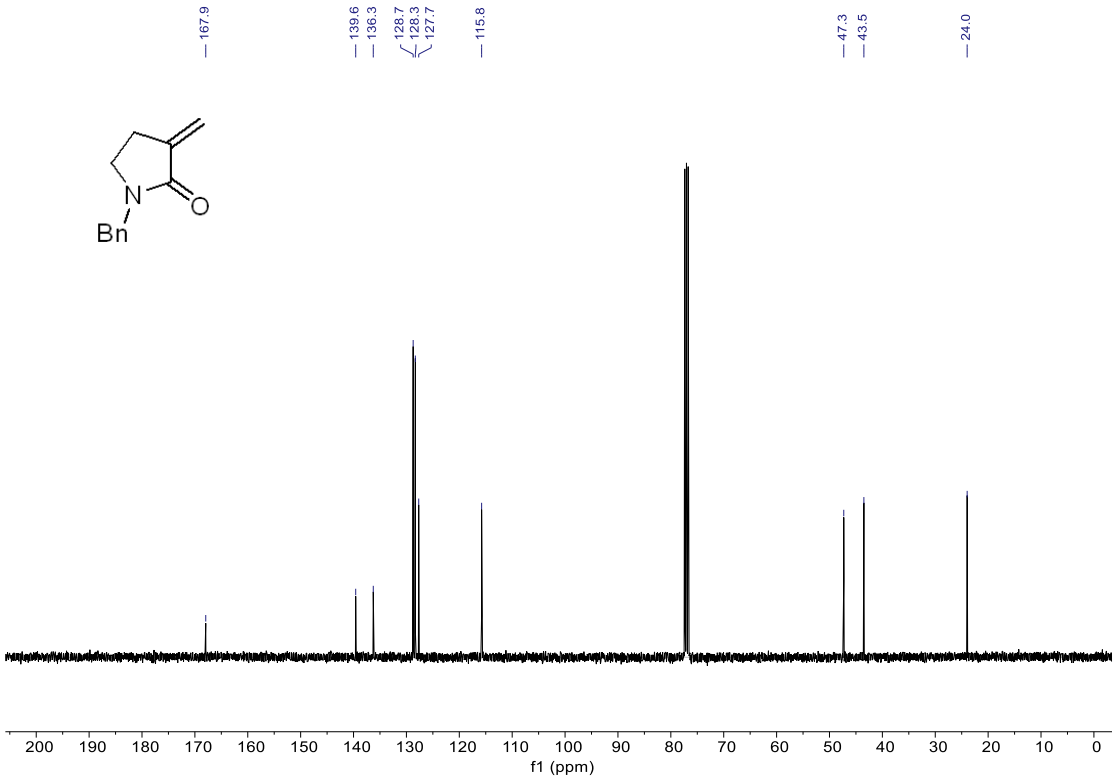


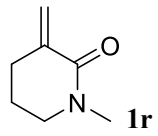
1q

^{1}H NMR (400 MHz, Chloroform-*d*)



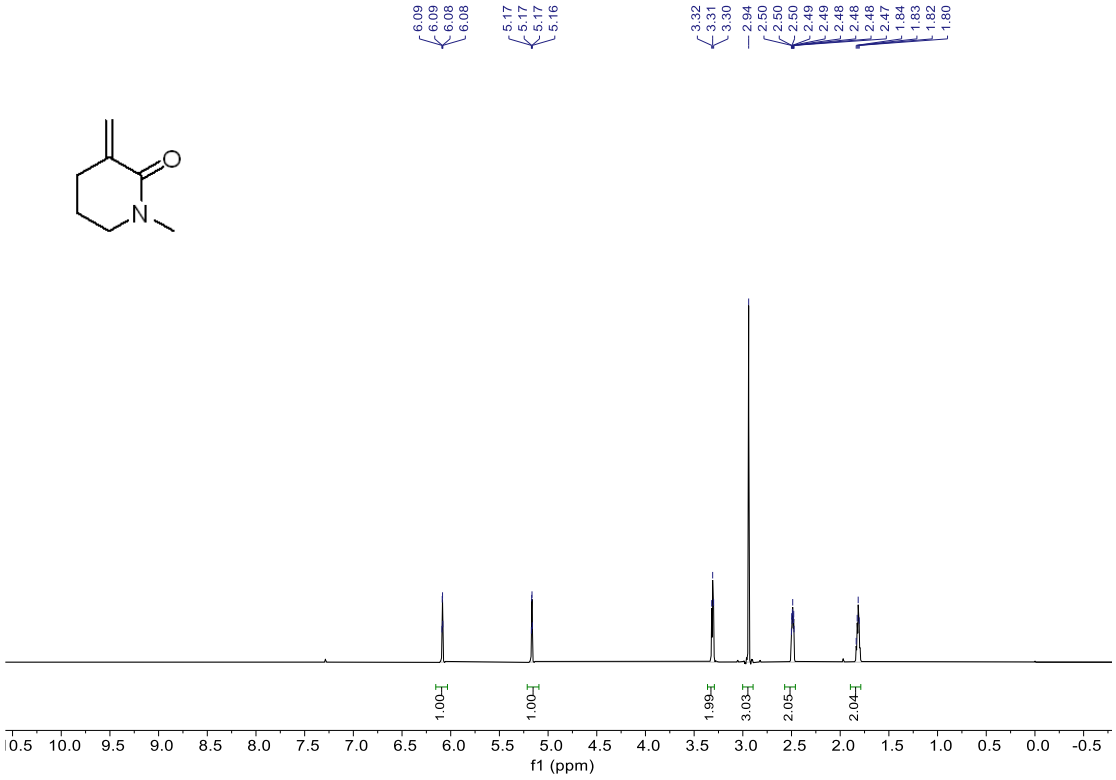
^{13}C NMR (101 MHz, Chloroform-*d*)



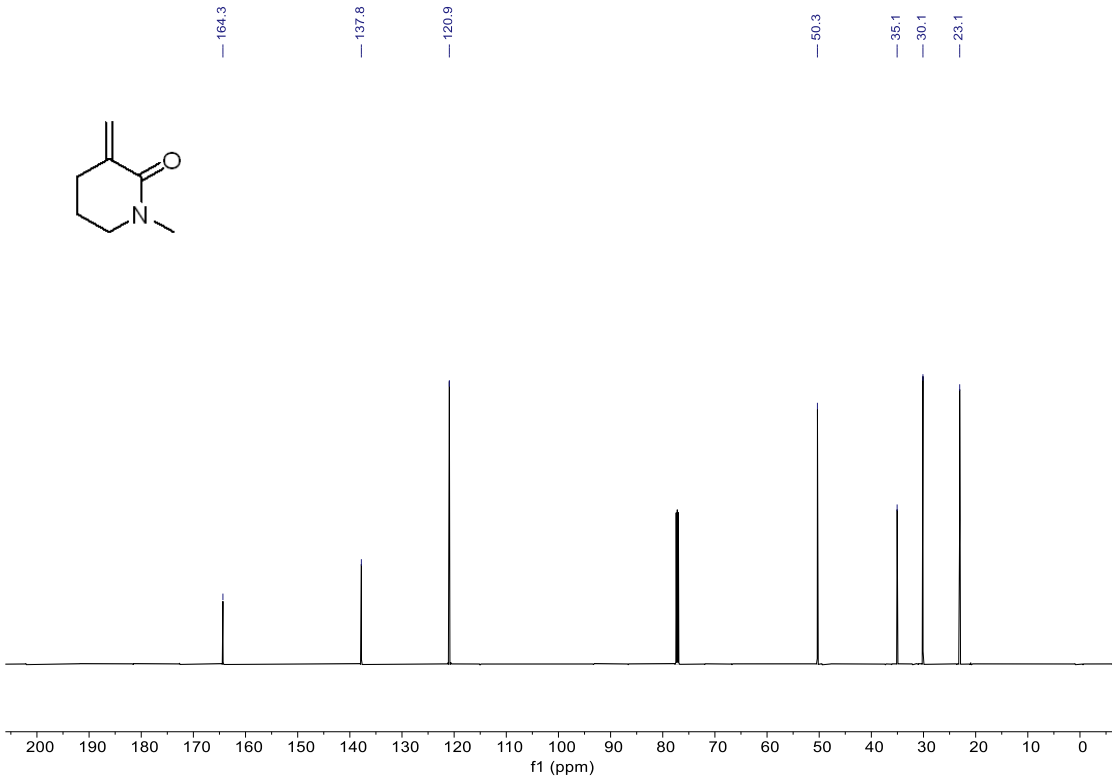


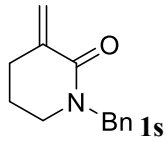
1r

^{1}H NMR (600 MHz, Chloroform-*d*)



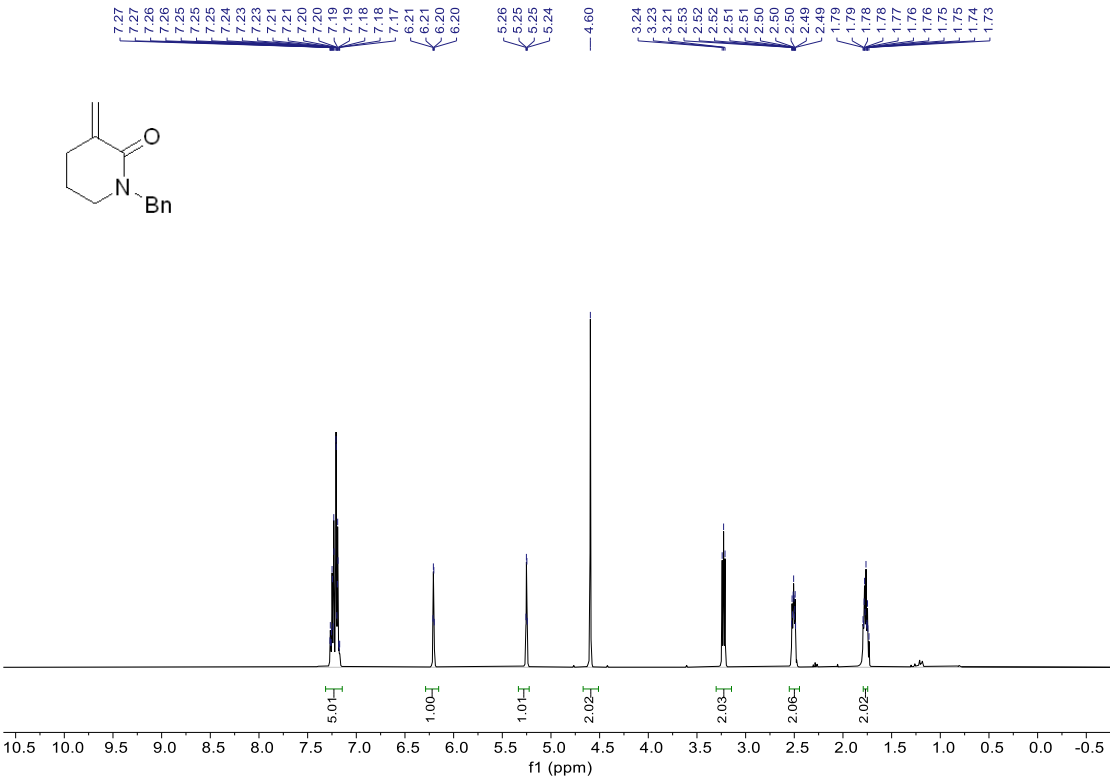
^{13}C NMR (151 MHz, Chloroform-*d*)



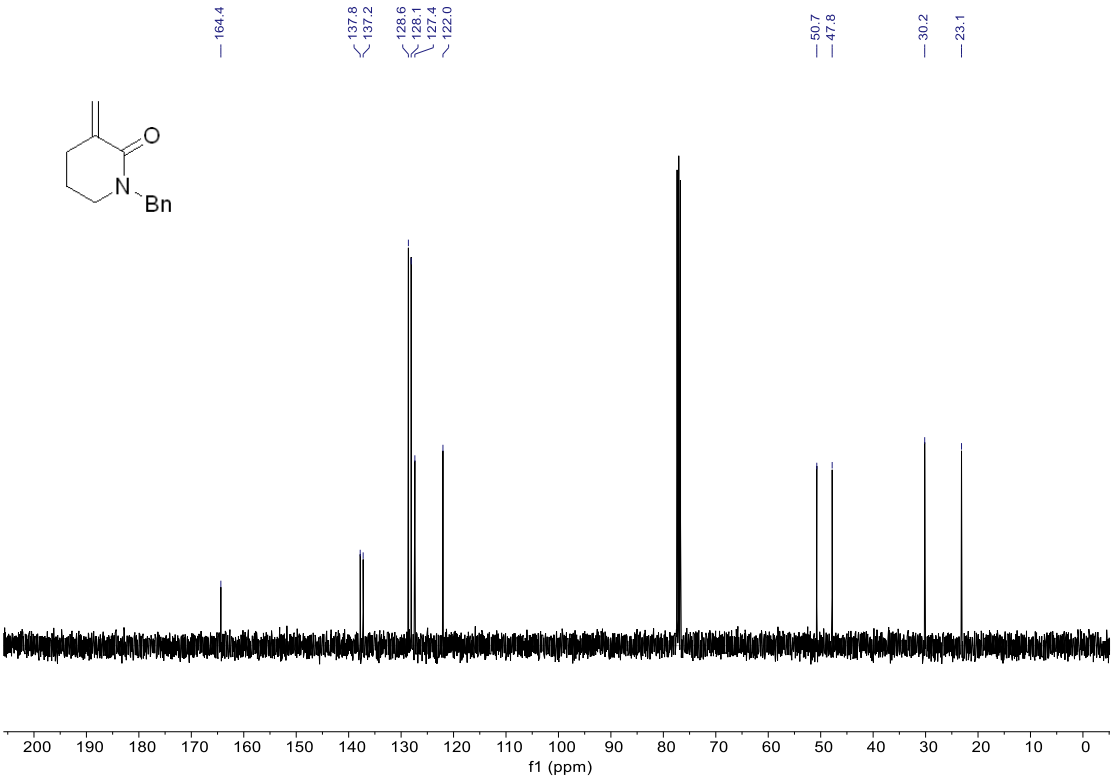


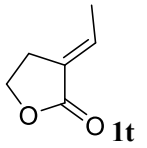
1s

^{1}H NMR (400 MHz, Chloroform-*d*)



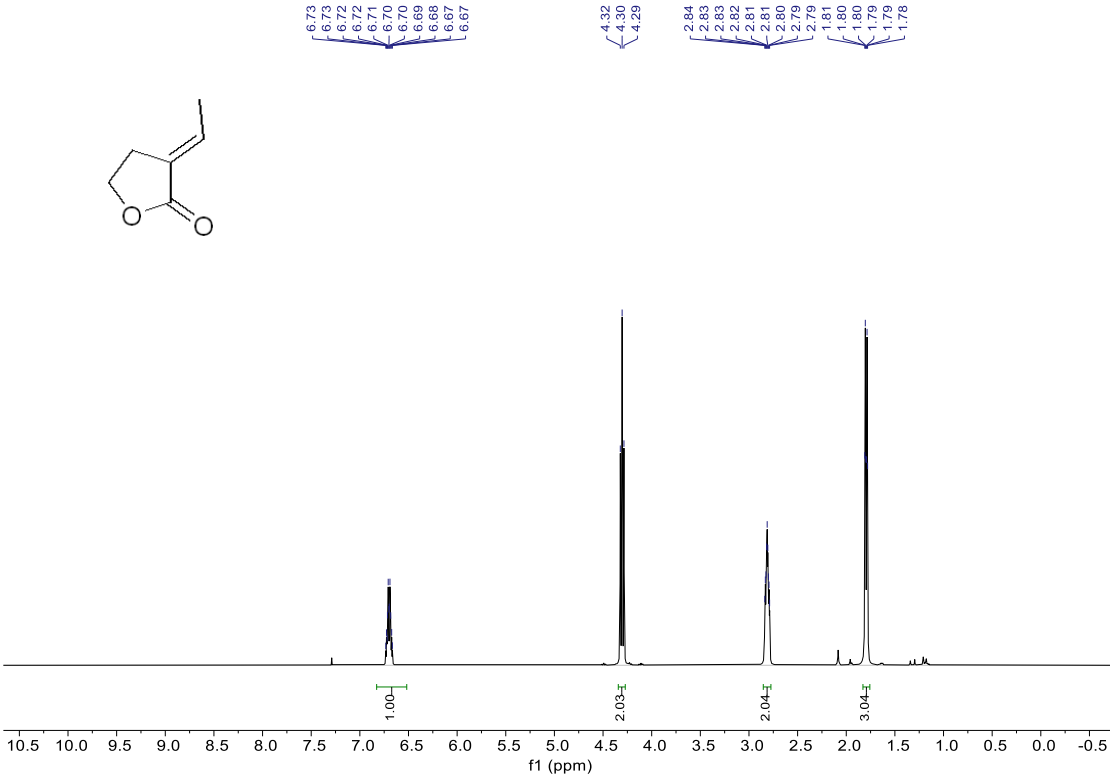
^{13}C NMR (101 MHz, Chloroform-*d*)



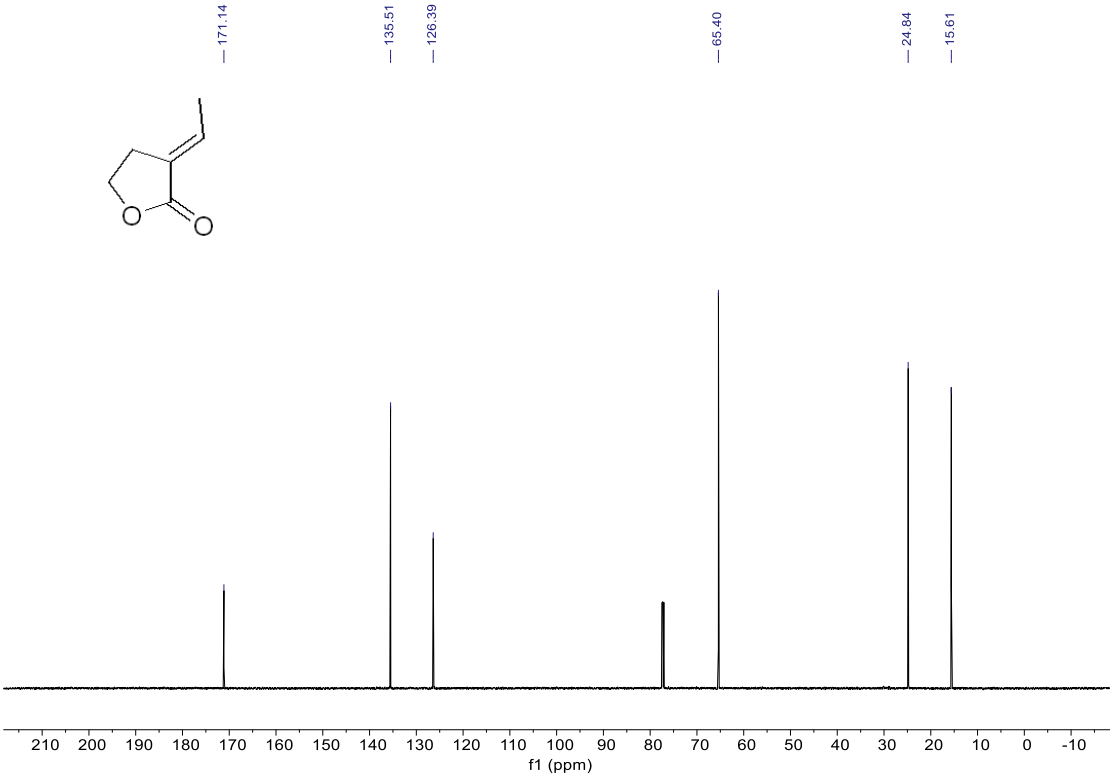


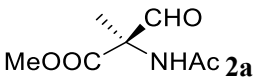
1t

^{1}H NMR (400 MHz, Chloroform-*d*)



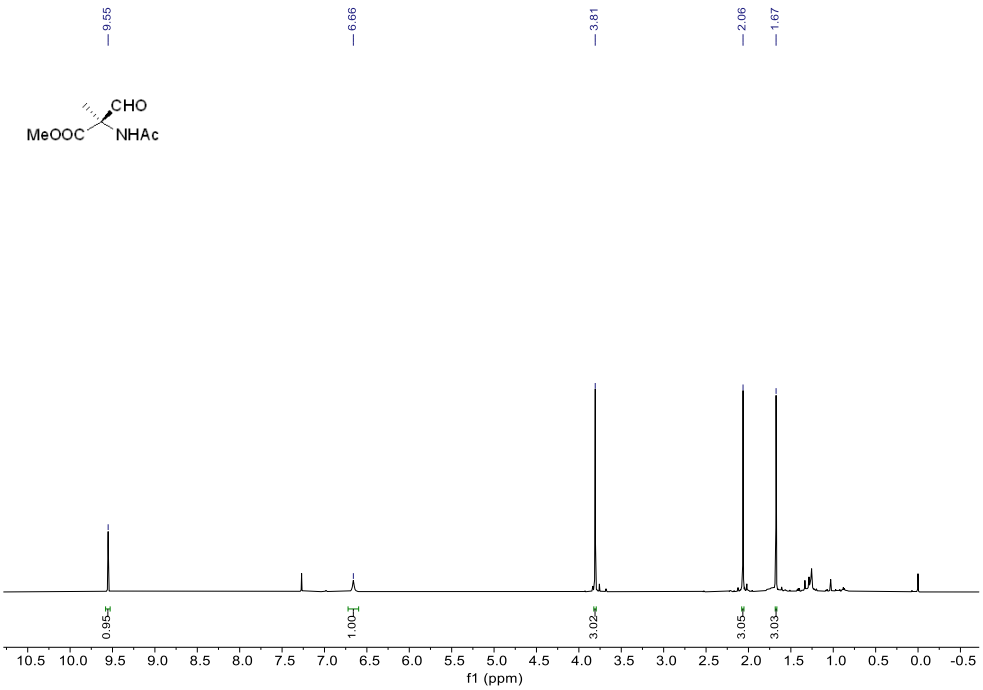
^{13}C NMR (151 MHz, Chloroform-*d*)



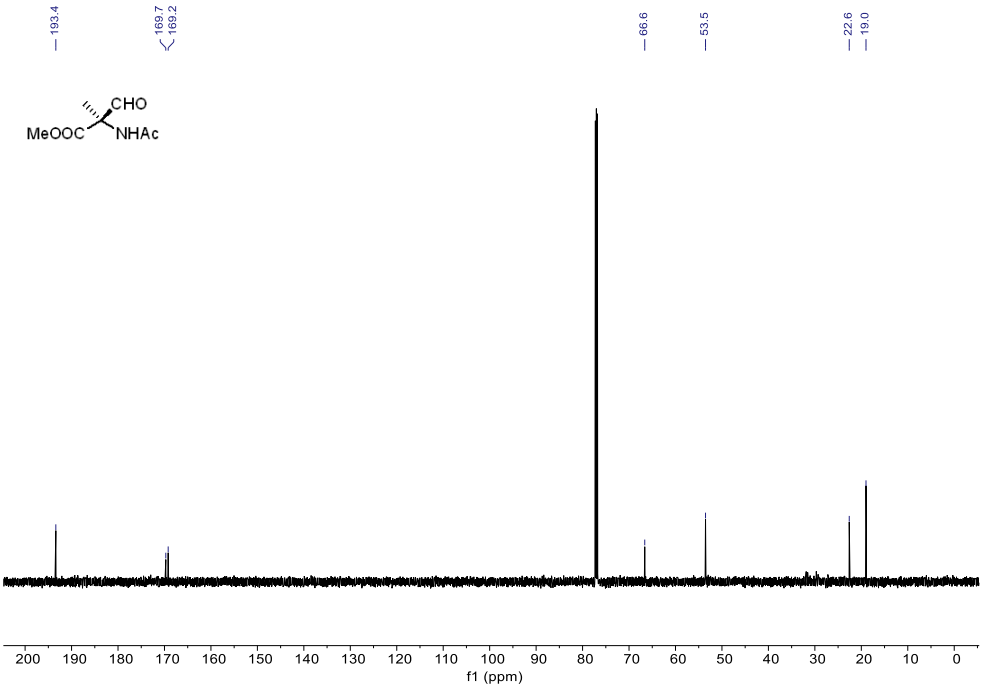


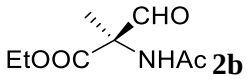
2a

^{1}H NMR (600 MHz, Chloroform-*d*)



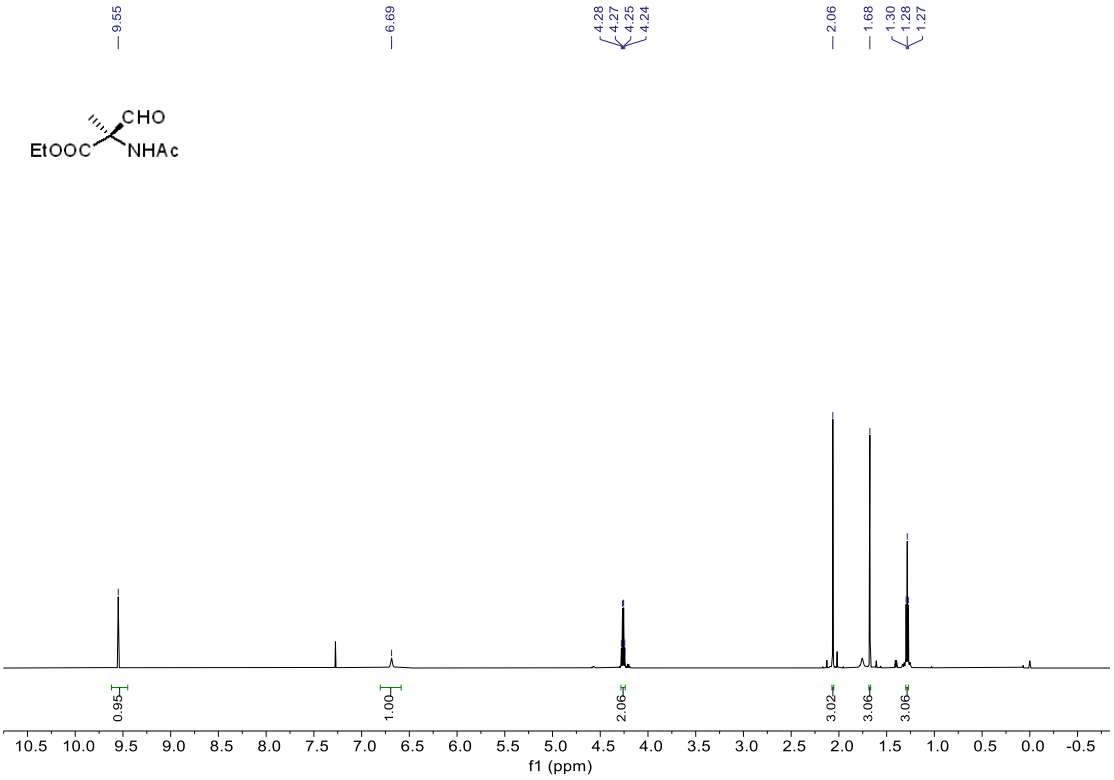
^{13}C NMR (151 MHz, Chloroform-*d*)



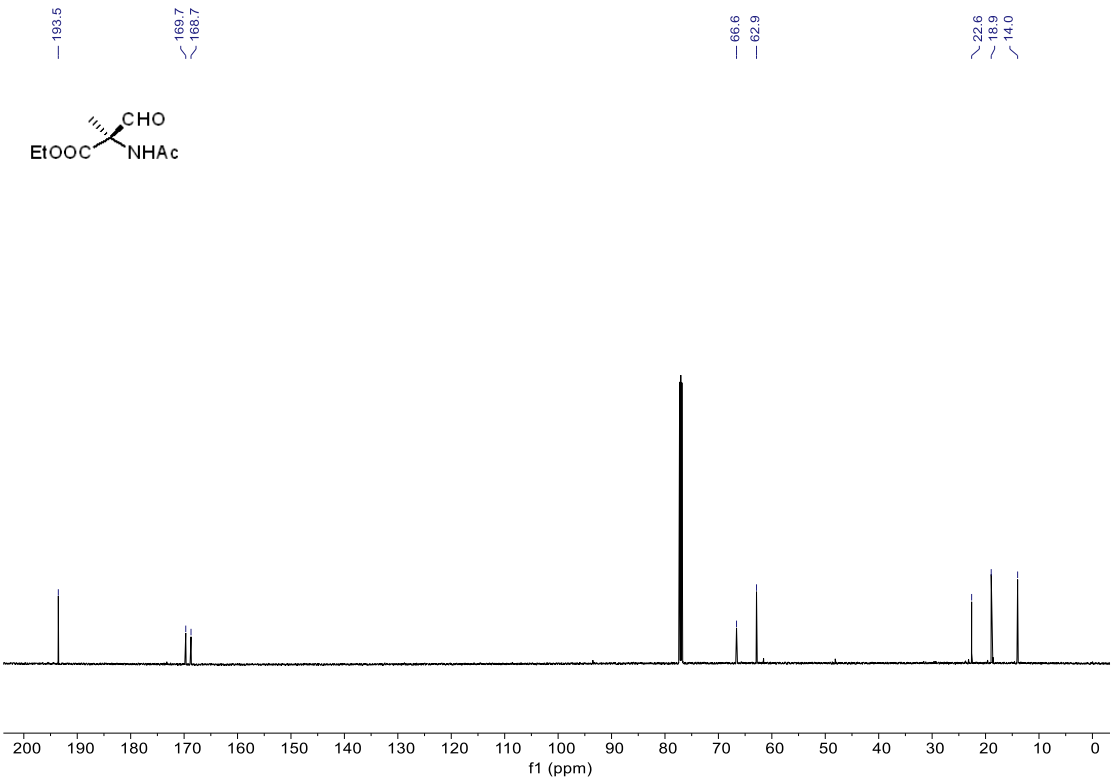


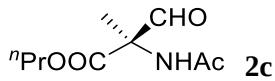
2b

^{1}H NMR (600 MHz, Chloroform-*d*)



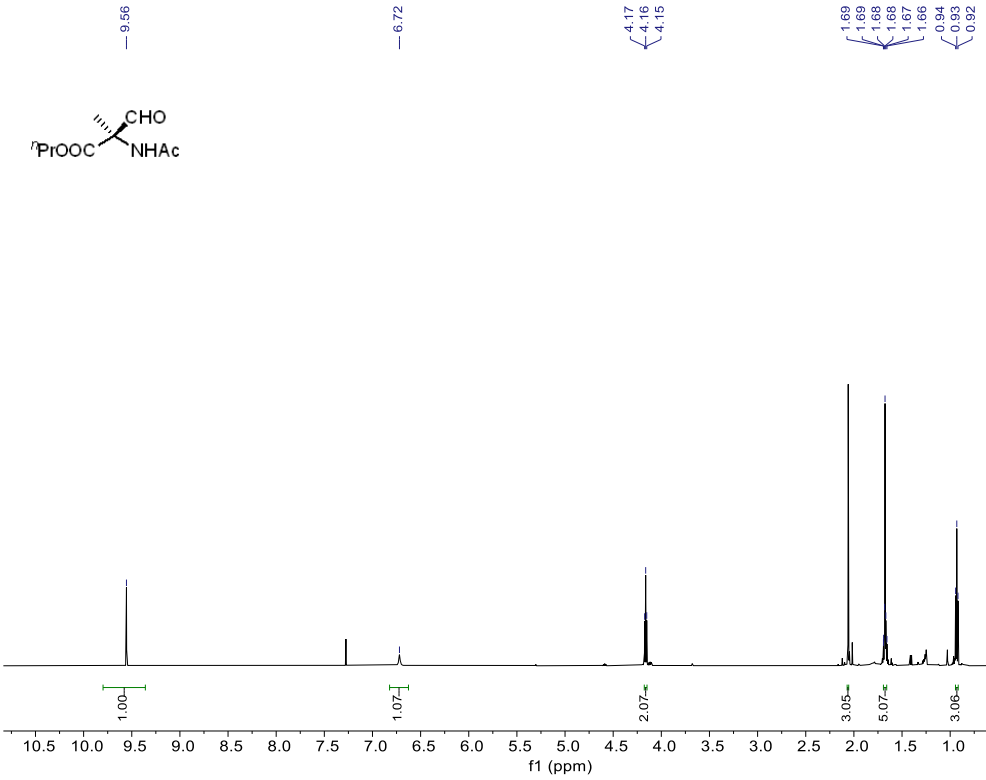
^{13}C NMR (151 MHz, Chloroform-*d*)



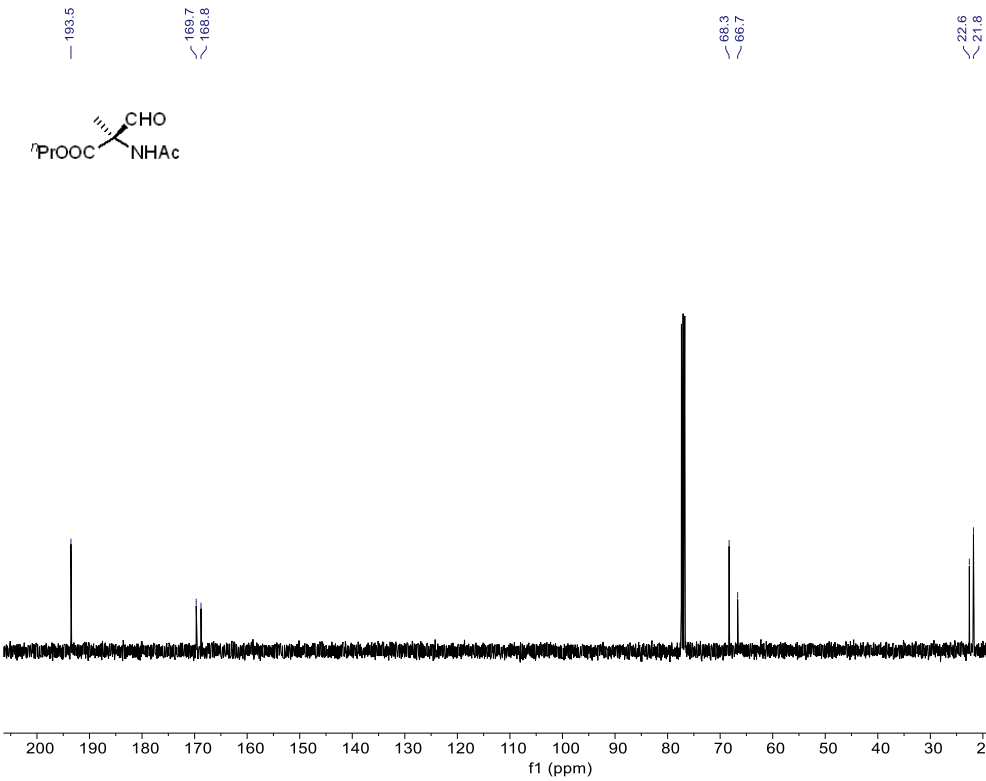


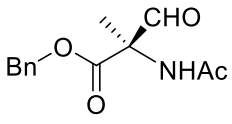
2c

^{1}H NMR (600 MHz, Chloroform-*d*)



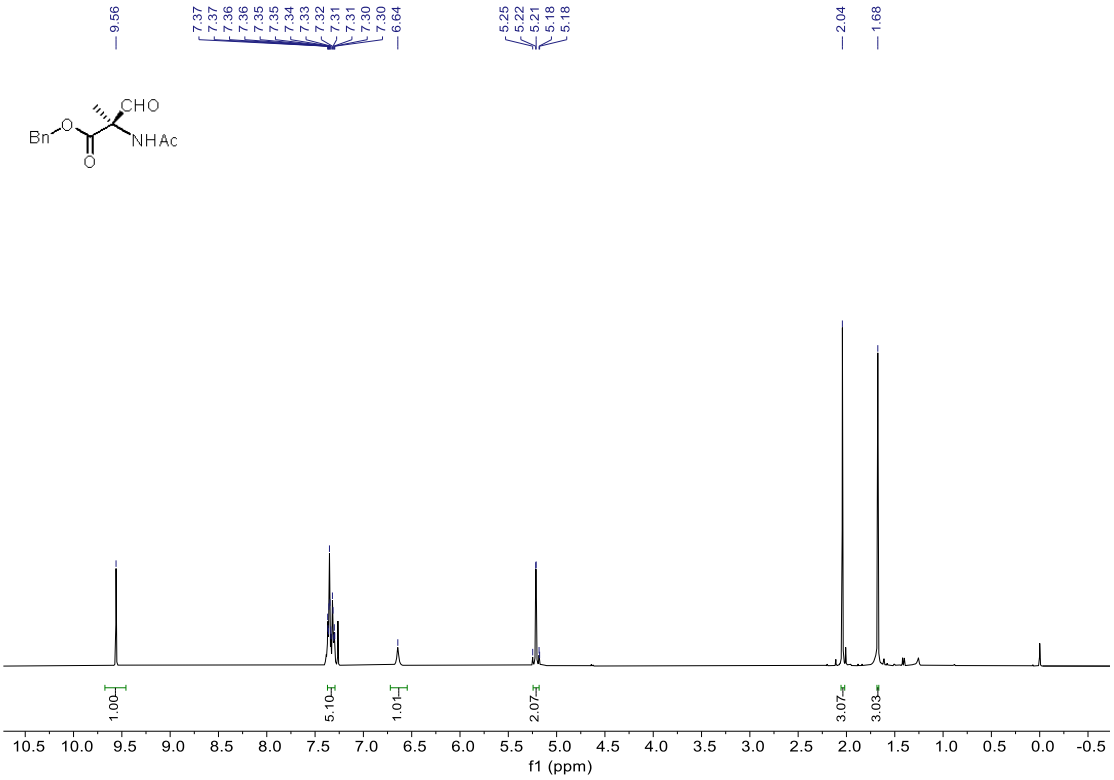
^{13}C NMR (101 MHz, Chloroform-*d*)



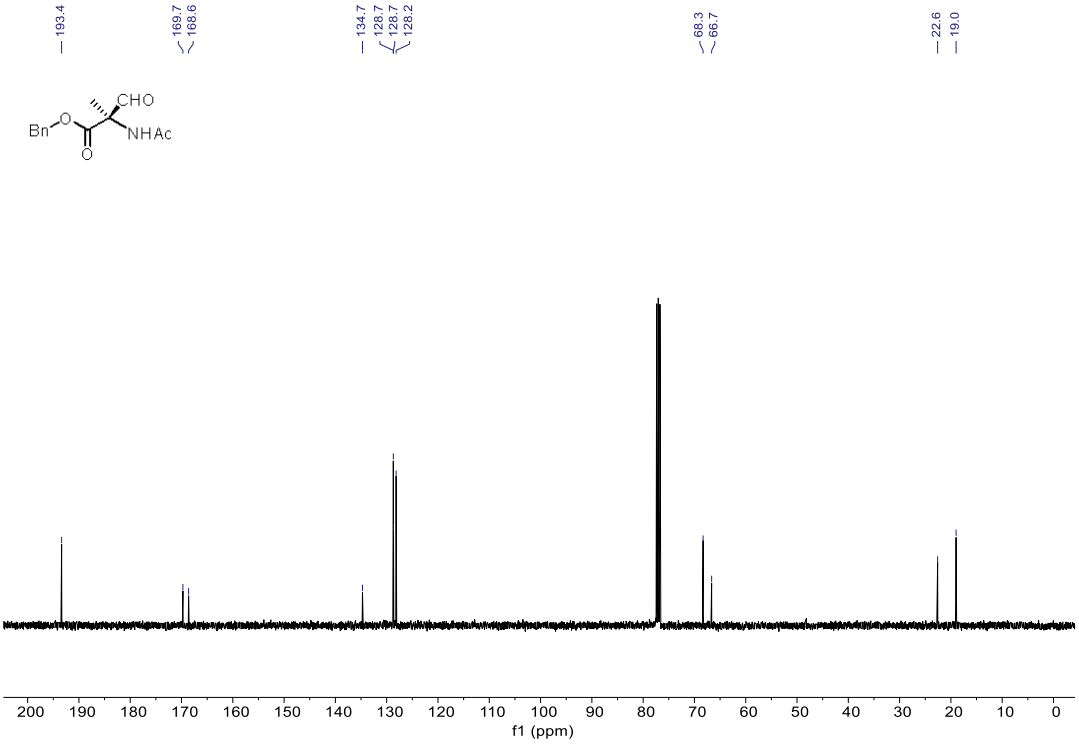


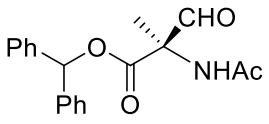
2d

^{1}H NMR (400 MHz, Chloroform-*d*)



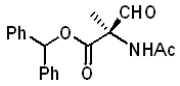
^{13}C NMR (101 MHz, Chloroform-*d*)

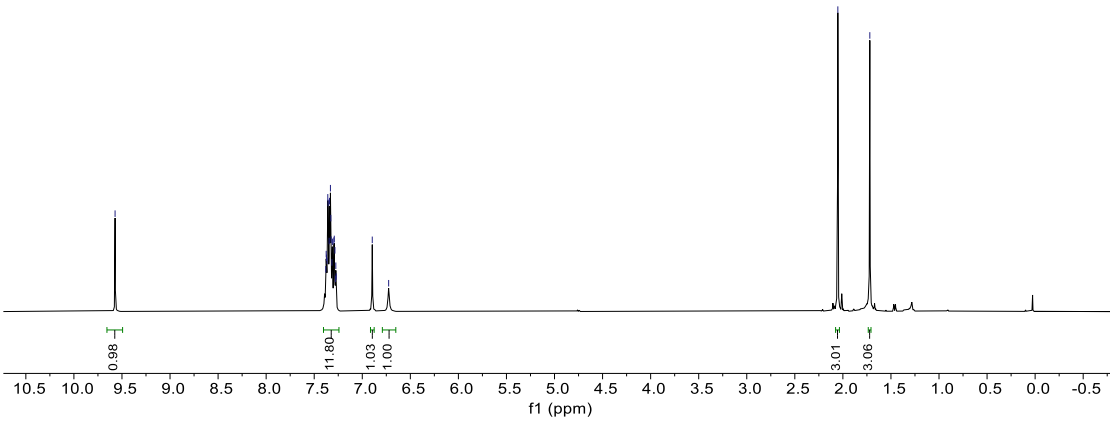




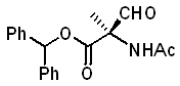
2e

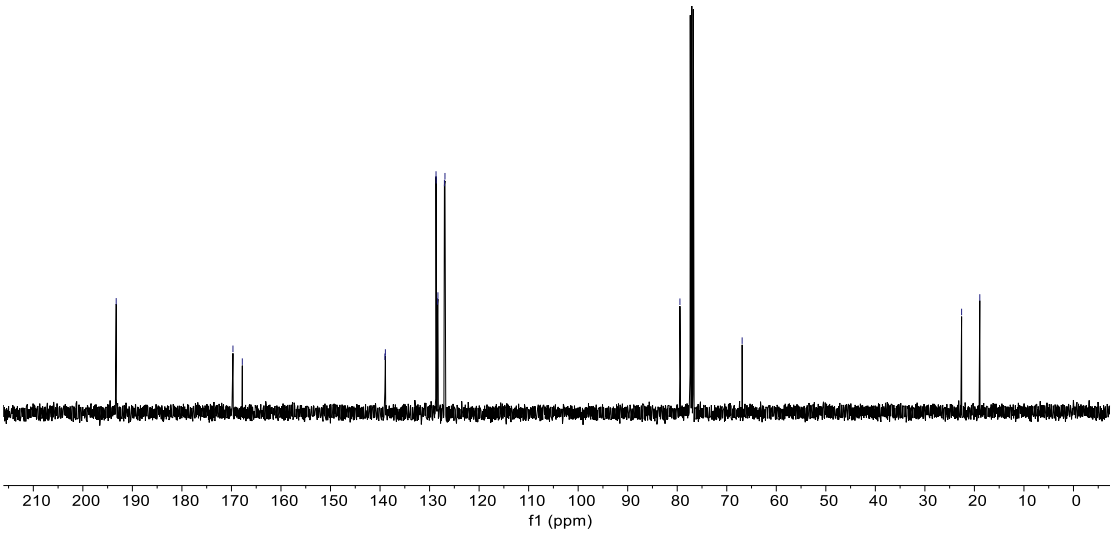
^{1}H NMR (400 MHz, Chloroform-*d*)

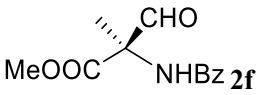




^{13}C NMR (101 MHz, Chloroform-*d*)

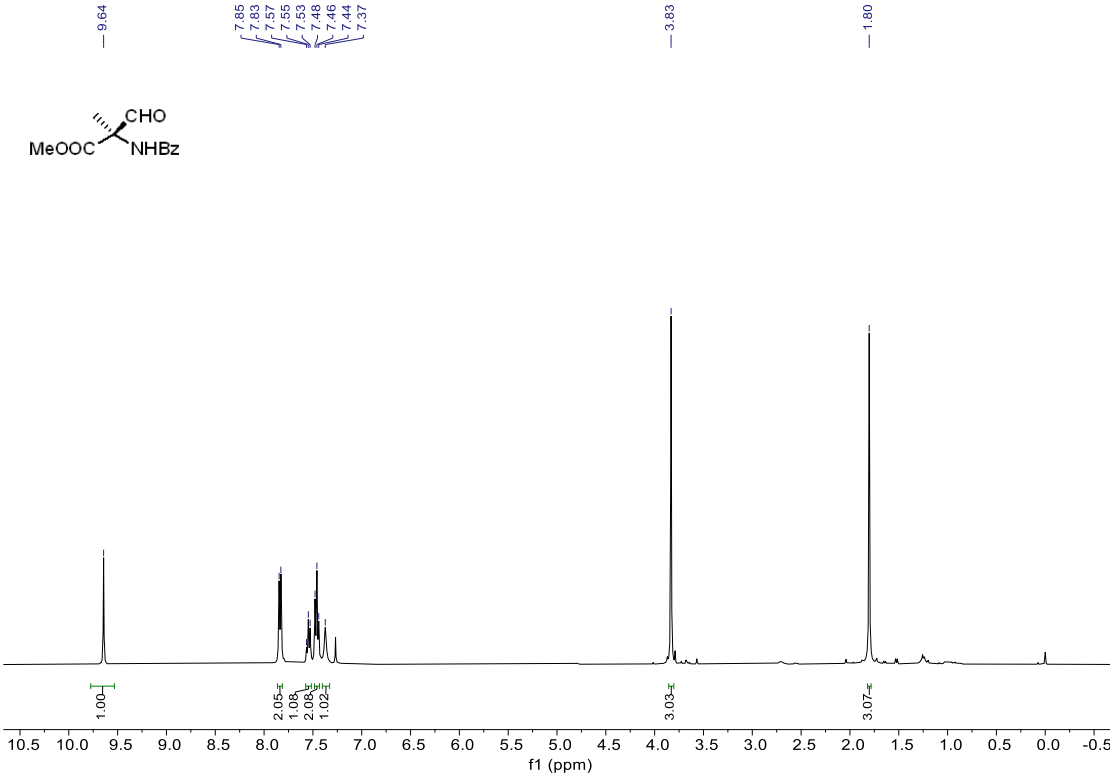




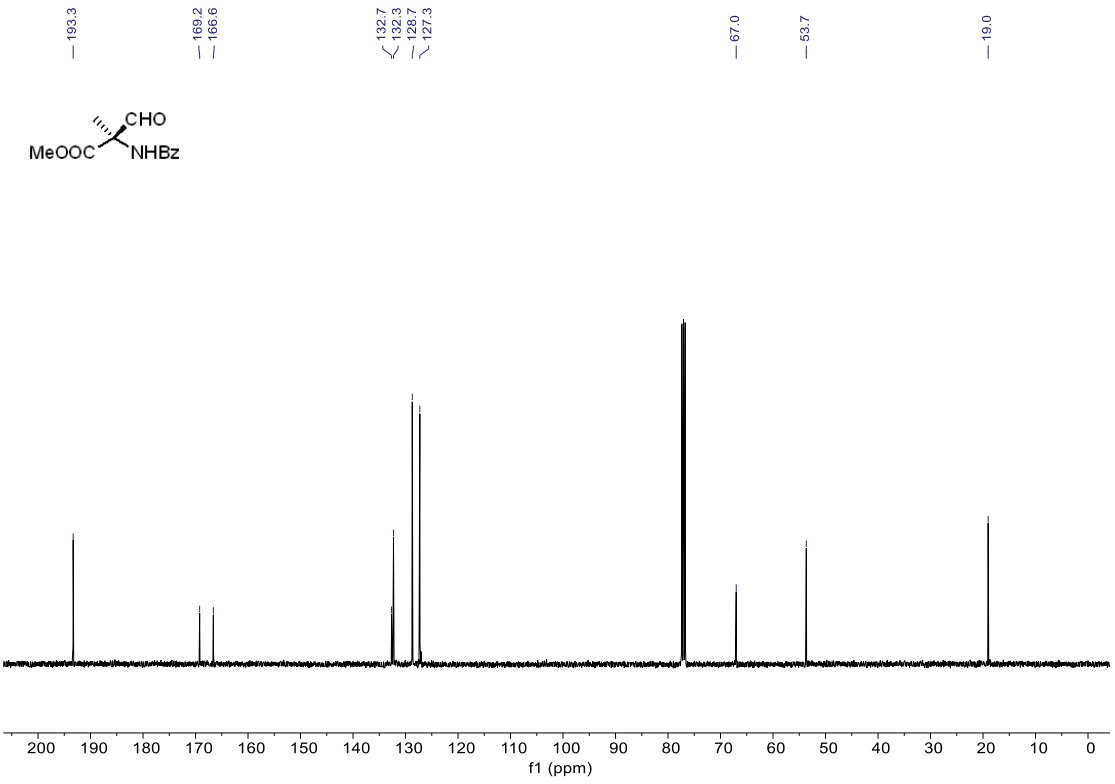


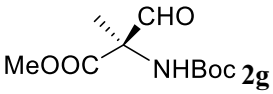
2f

^{1}H NMR (400 MHz, Chloroform-*d*)



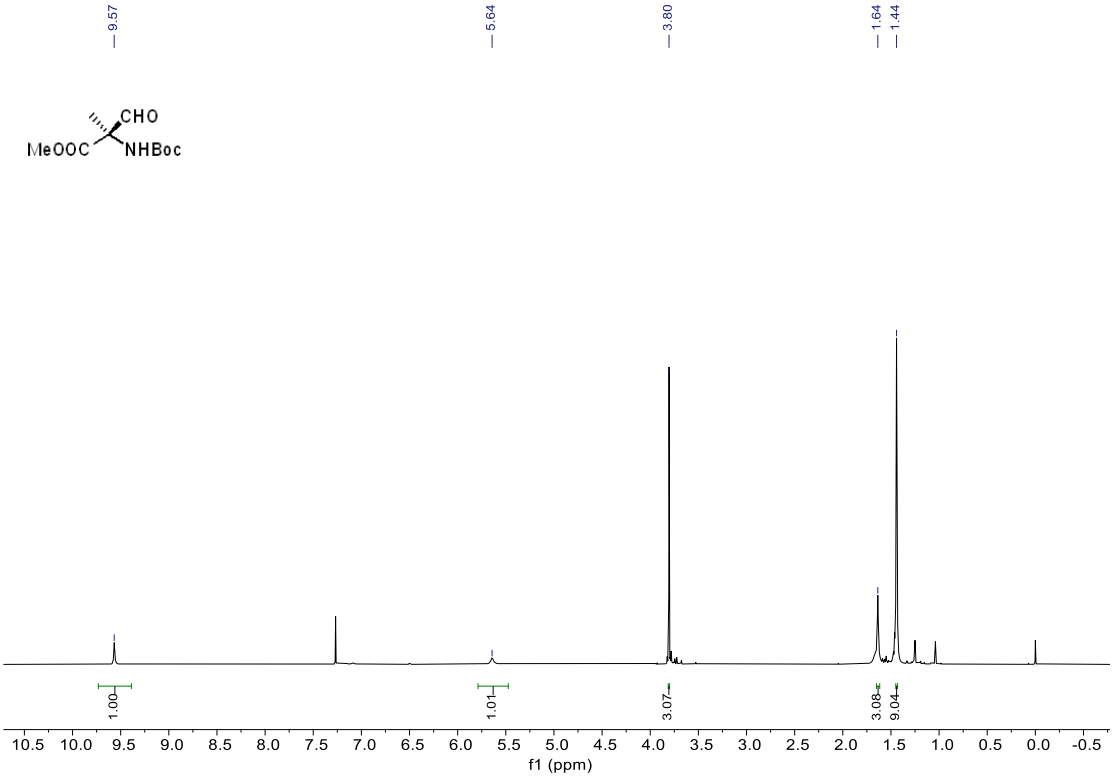
^{13}C NMR (101 MHz, Chloroform-*d*)



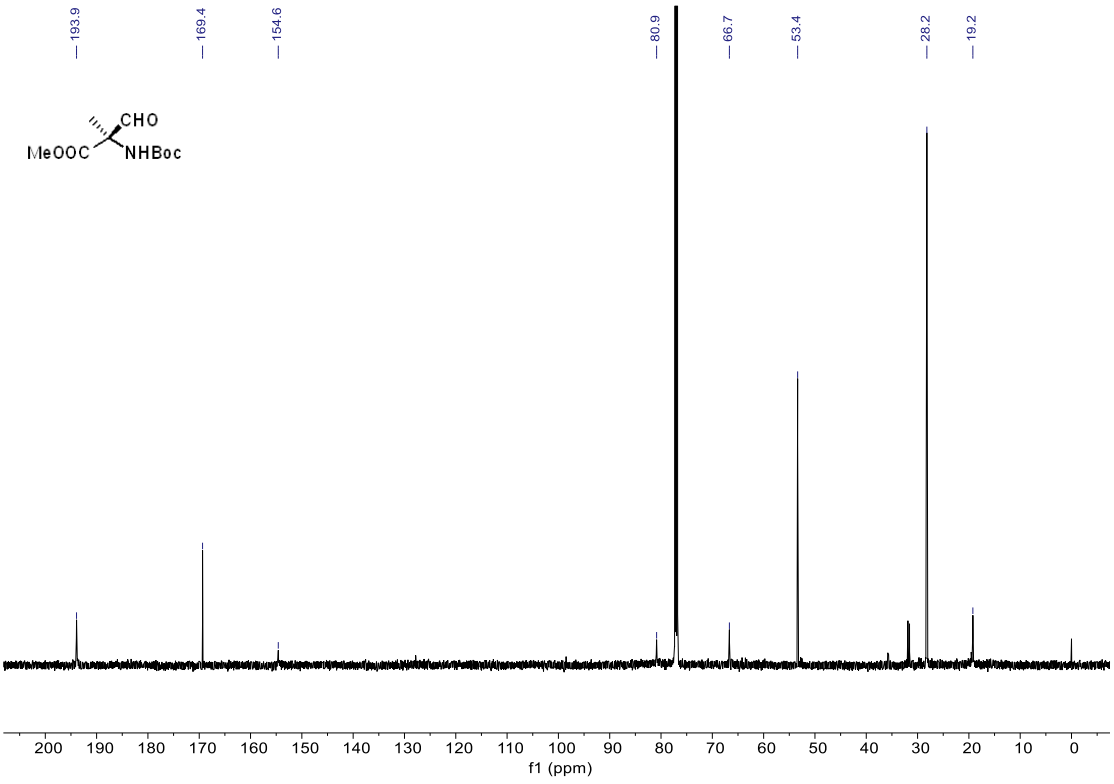


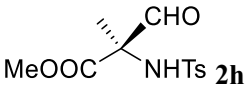
2g

^{1}H NMR (600 MHz, Chloroform-*d*)



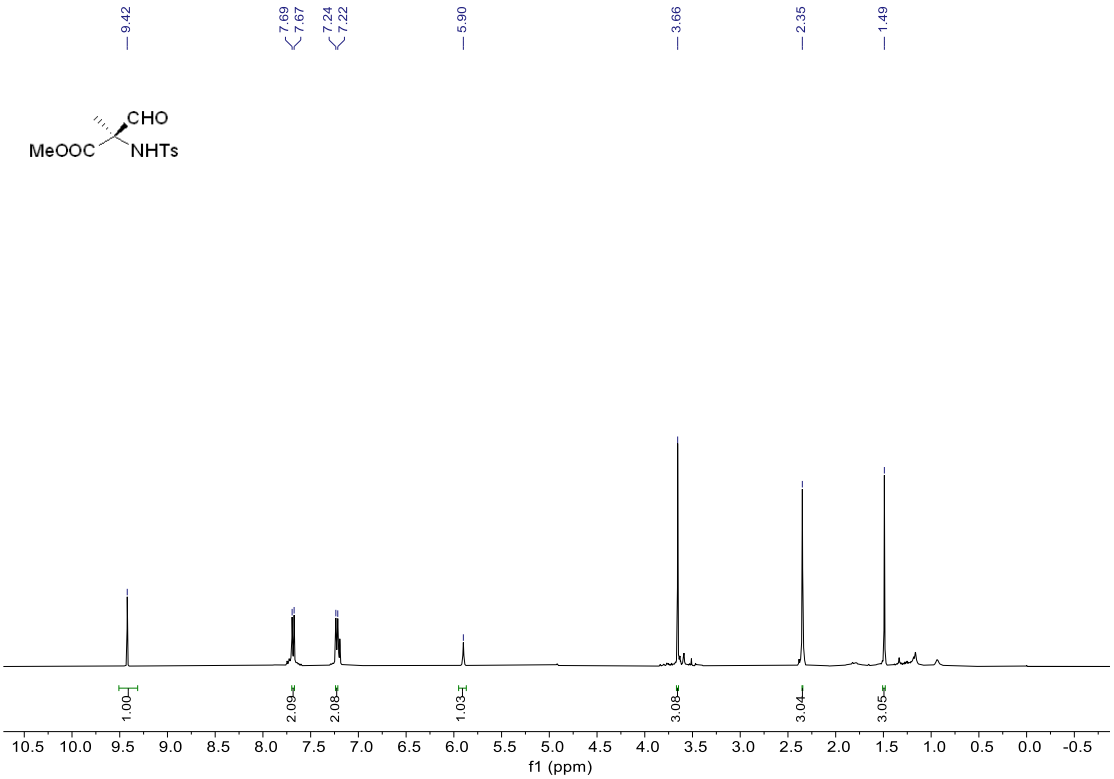
^{13}C NMR (151 MHz, Chloroform-*d*)



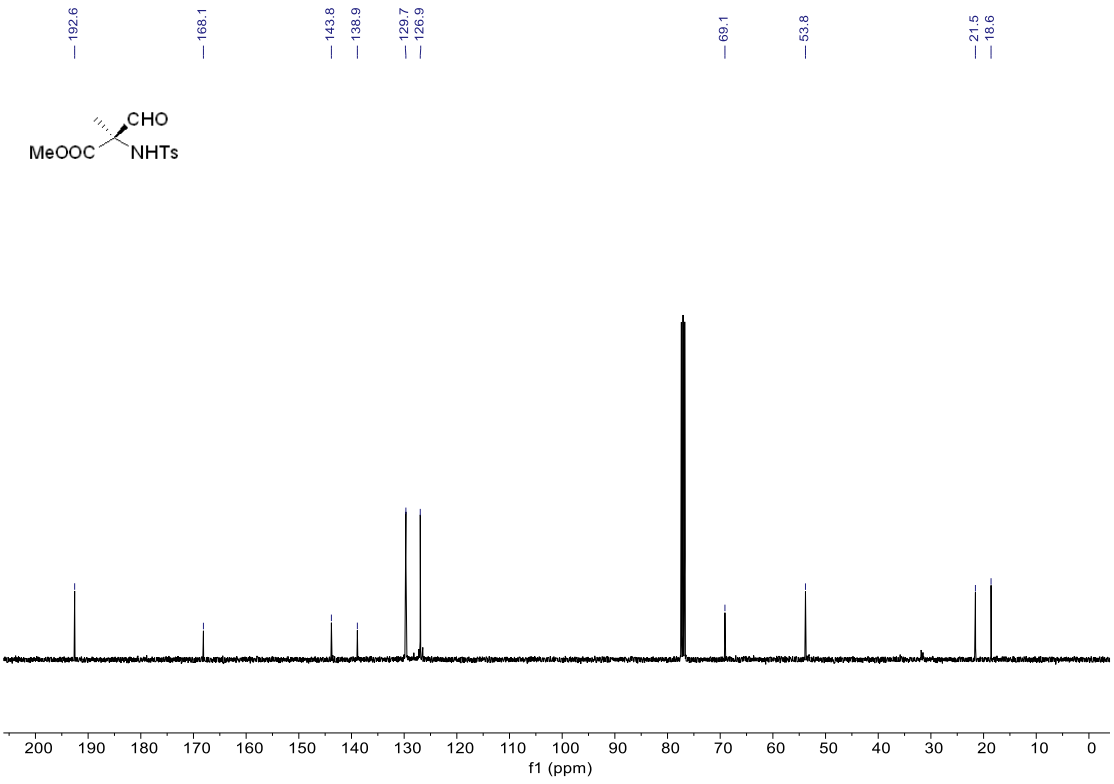


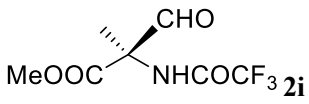
2h

^{1}H NMR (400 MHz, Chloroform-*d*)



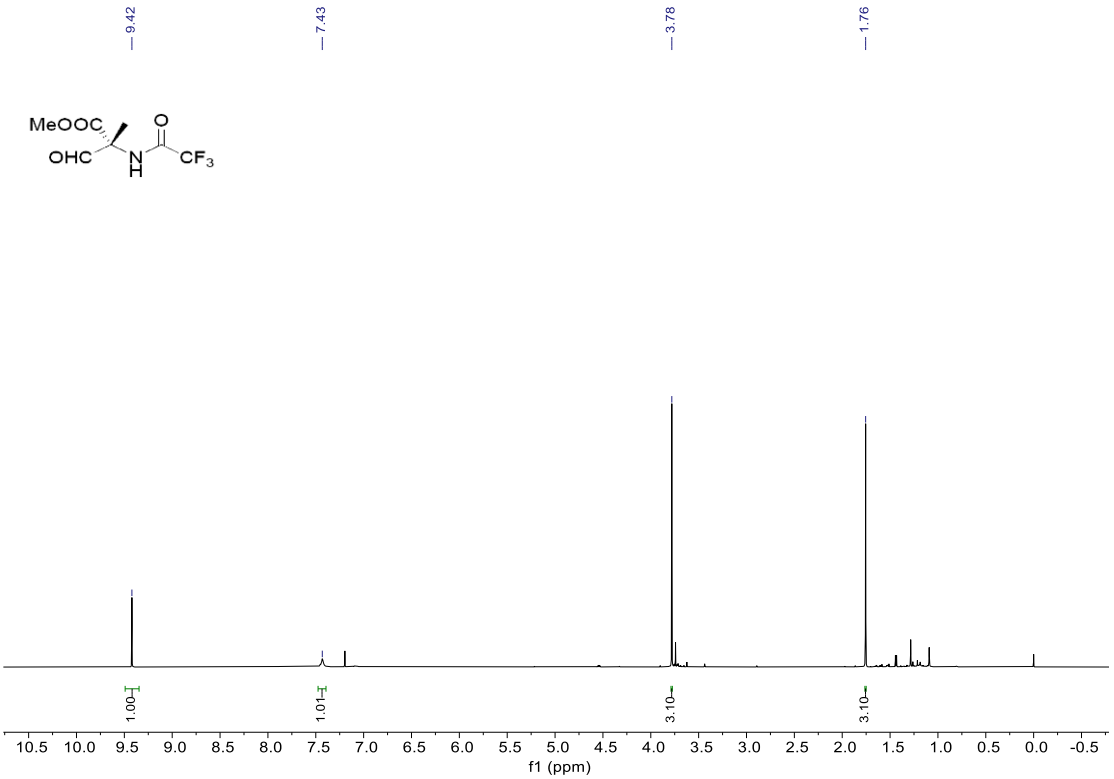
^{13}C NMR (101 MHz, Chloroform-*d*)



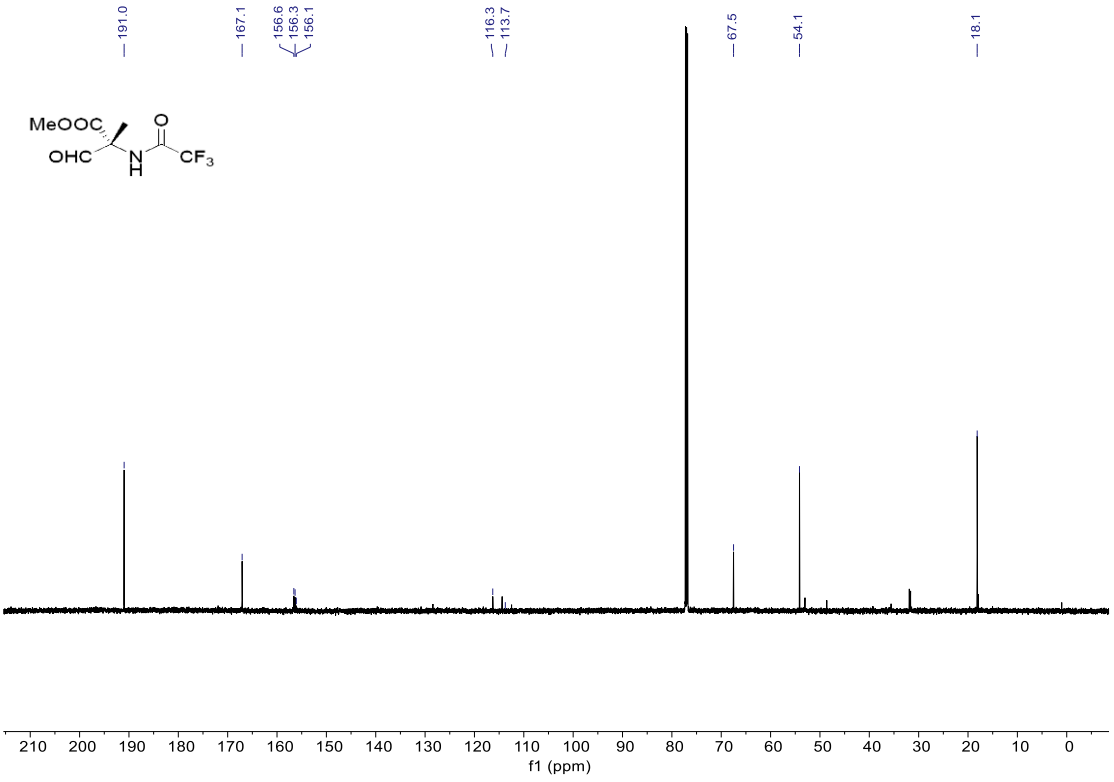


2i

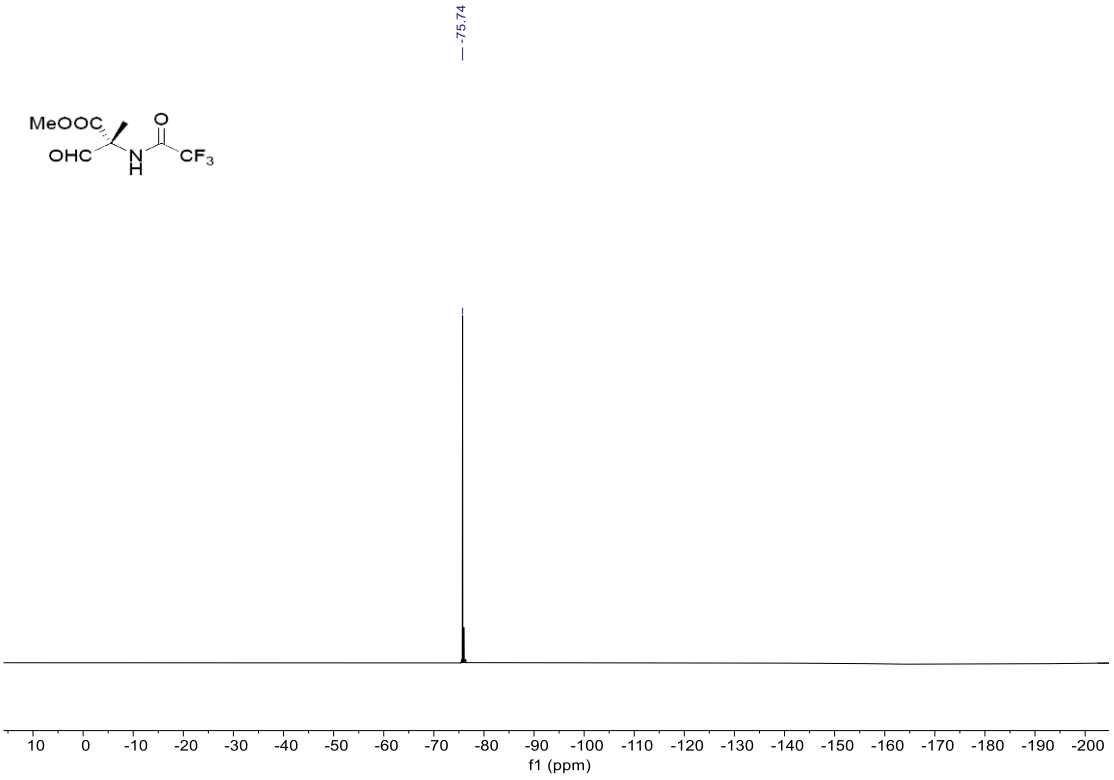
^{1}H NMR (600 MHz, Chloroform-*d*)

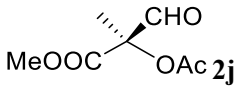


^{13}C NMR (151 MHz, Chloroform-*d*)



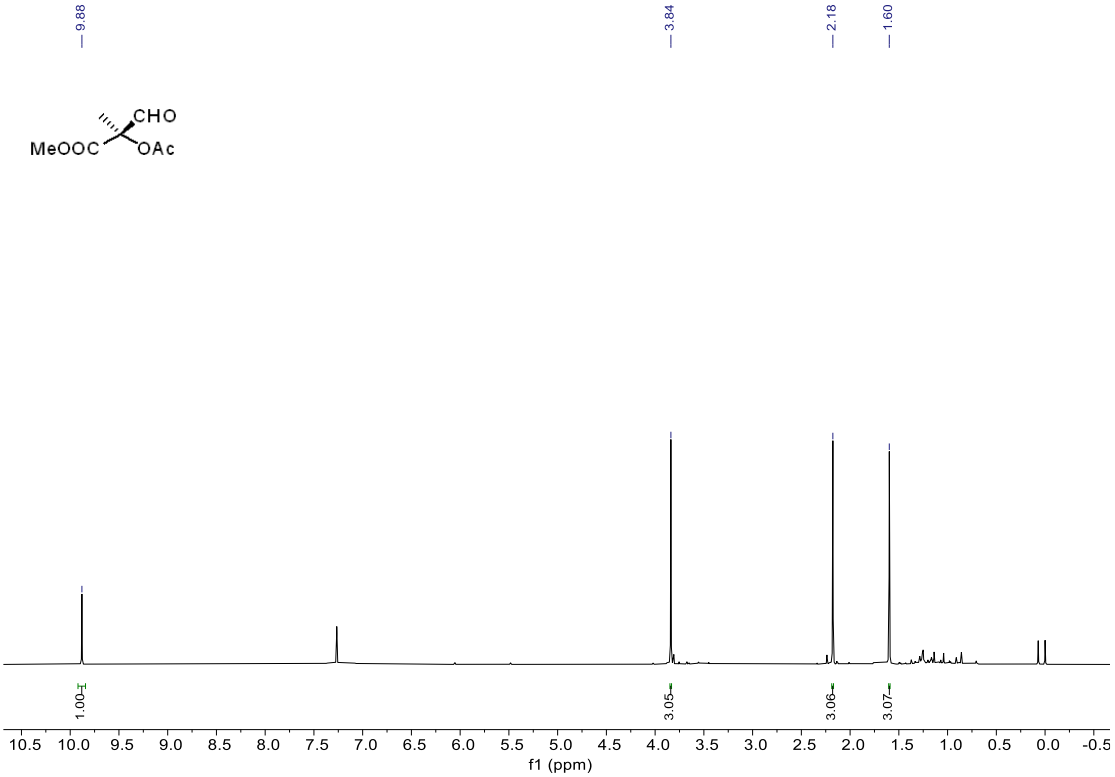
^{19}F NMR (565 MHz, Chloroform-*d*)



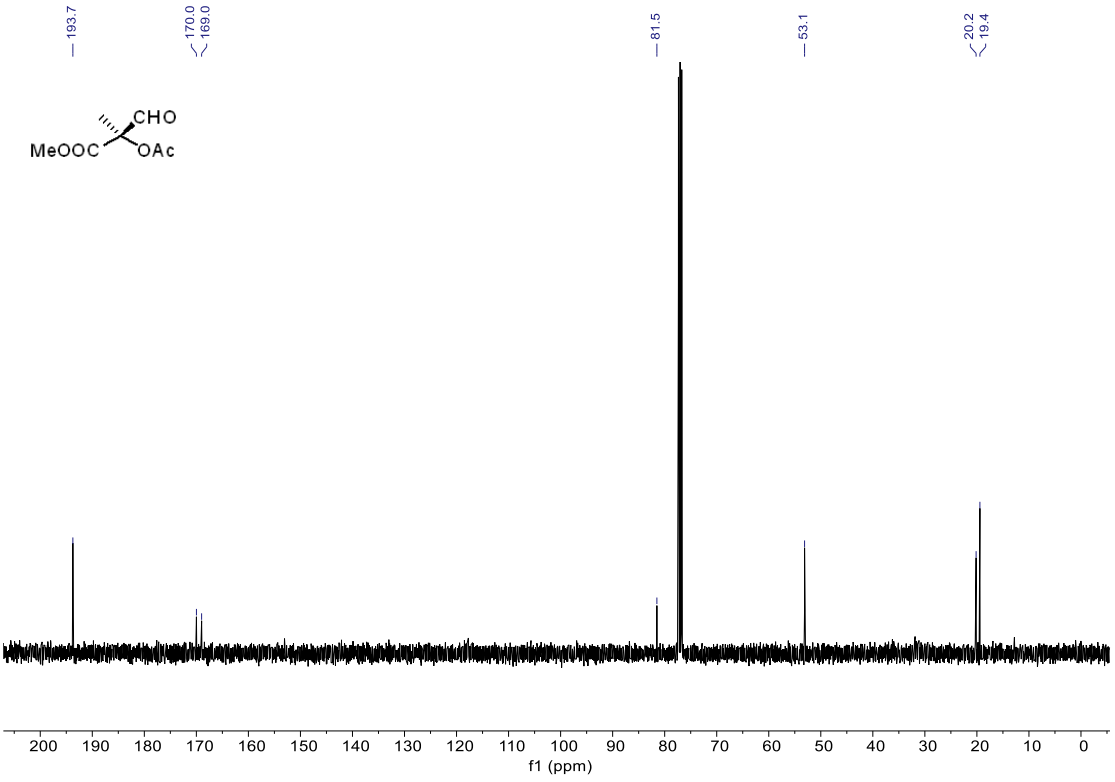


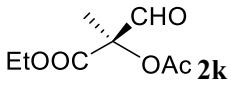
2j

^{1}H NMR (400 MHz, Chloroform-*d*)



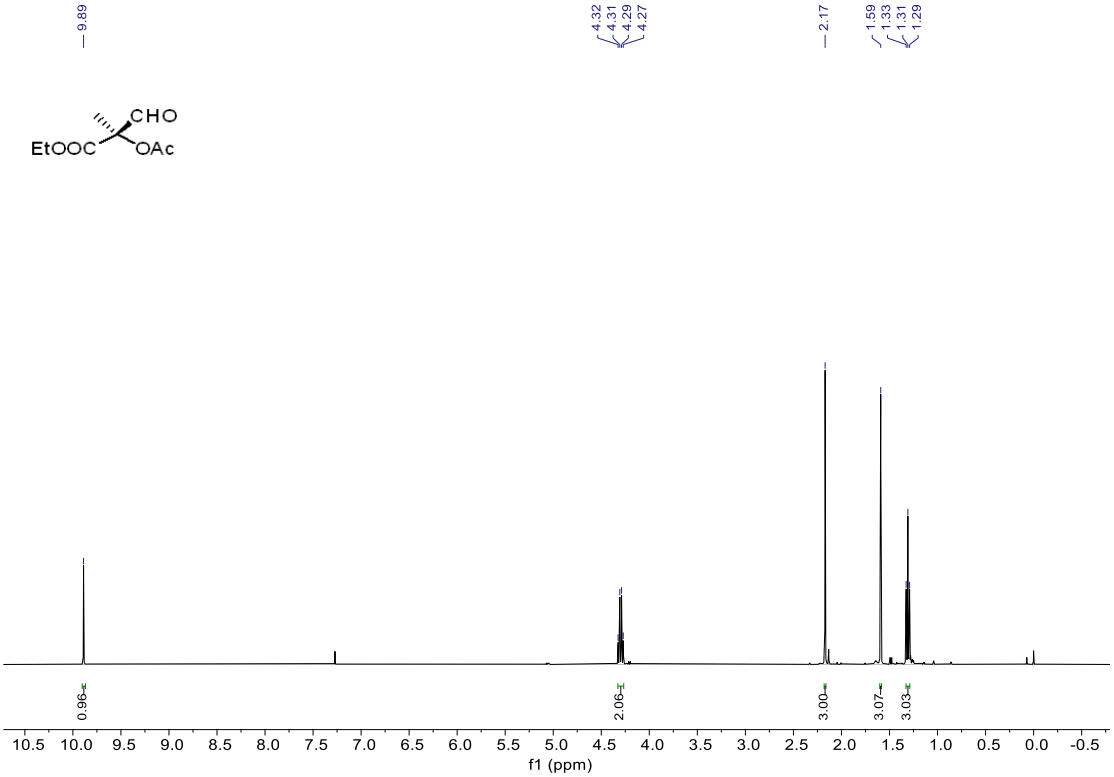
^{13}C NMR (101 MHz, Chloroform-*d*)



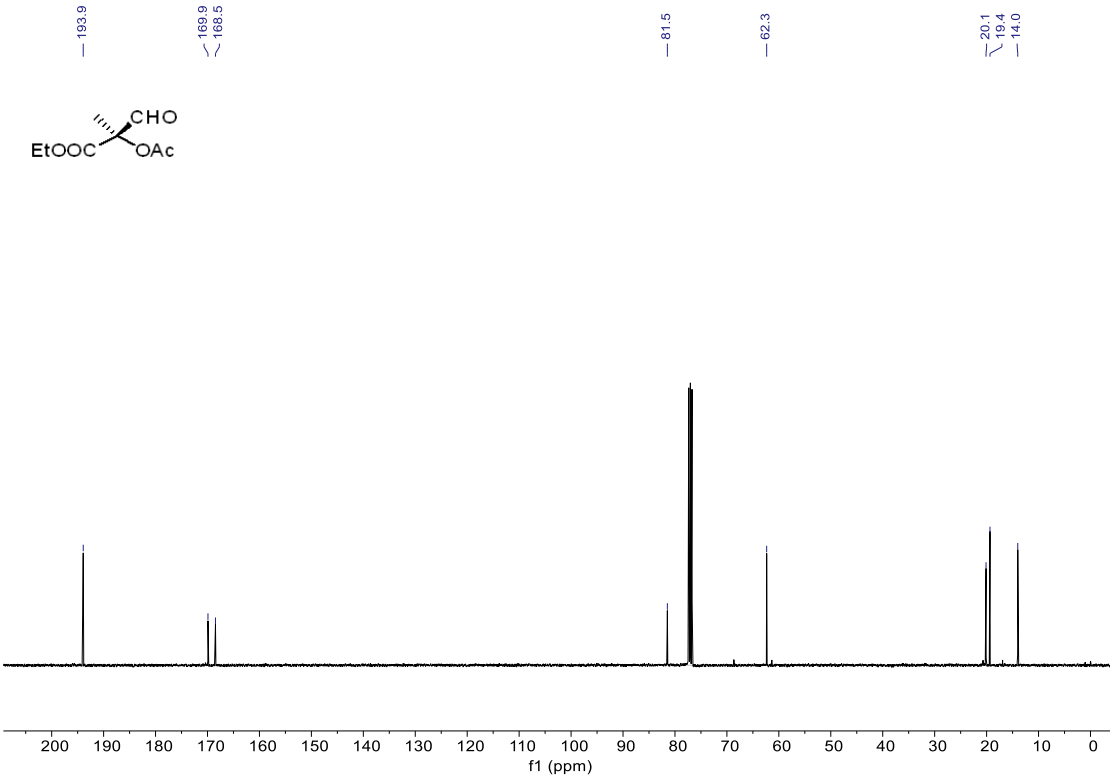


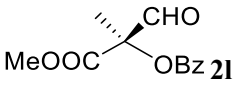
2k

^{1}H NMR (400 MHz, Chloroform-*d*)



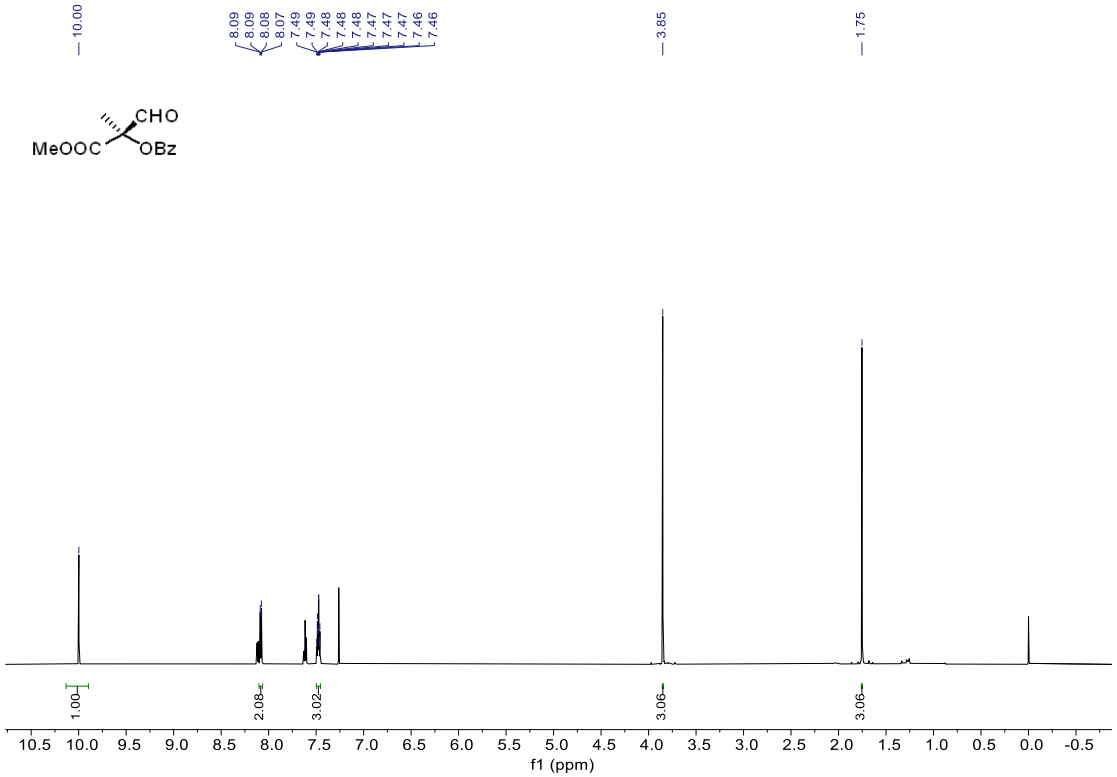
^{13}C NMR (101 MHz, Chloroform-*d*)



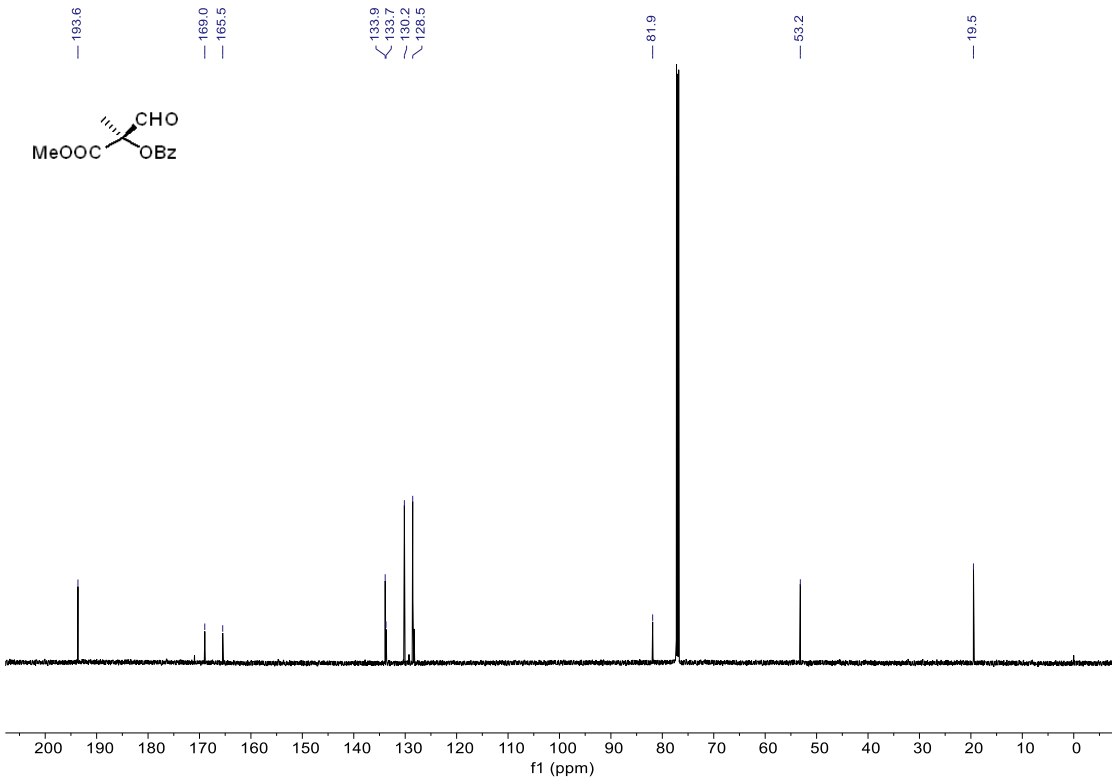


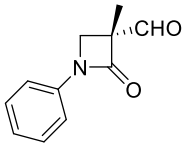
2l

^{1}H NMR (600 MHz, Chloroform-*d*)



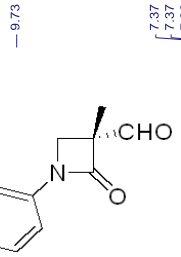
^{13}C NMR (151 MHz, Chloroform-*d*)



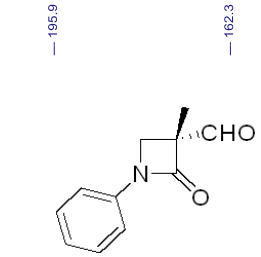


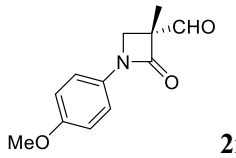
2m

^{1}H NMR (400 MHz, Chloroform-*d*)



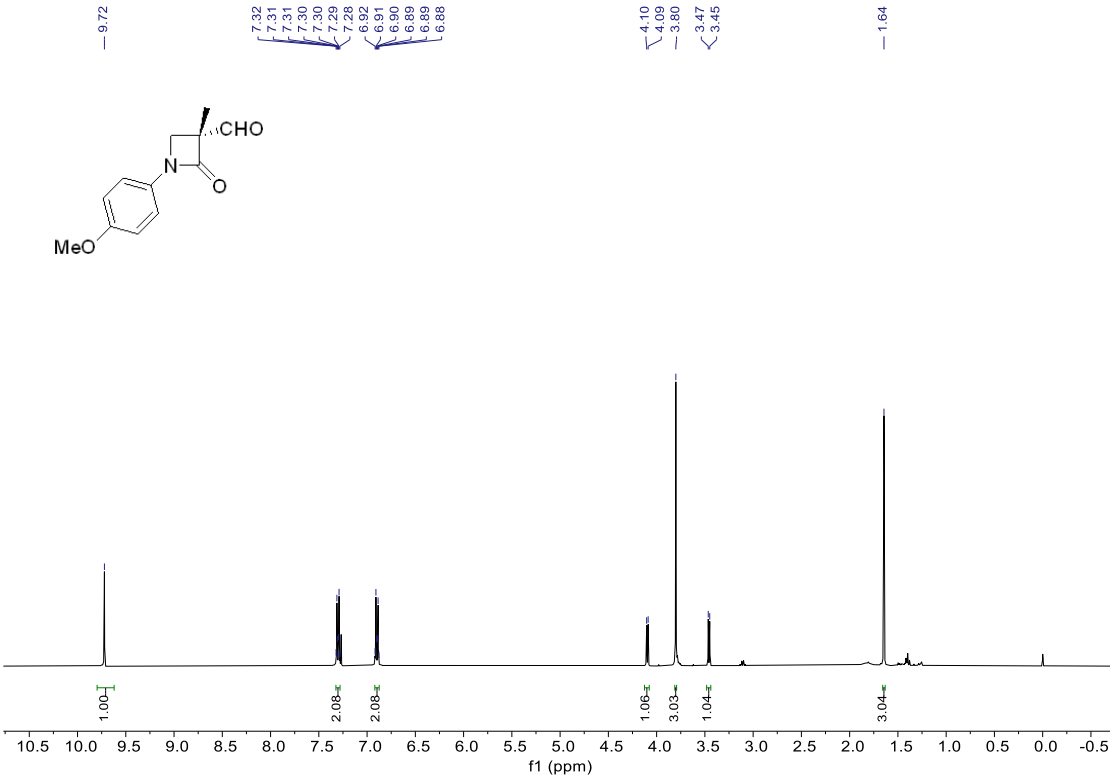
^{13}C NMR (101 MHz, Chloroform-*d*)



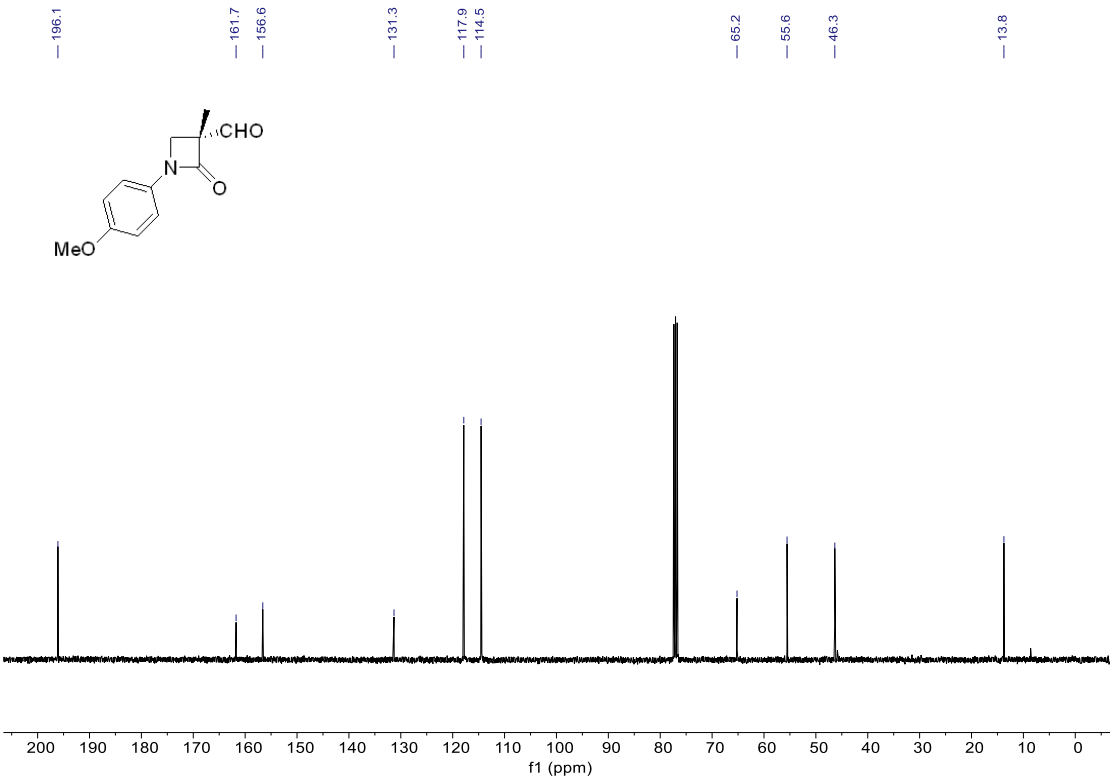


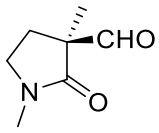
2n

^{1}H NMR (400 MHz, Chloroform-*d*)



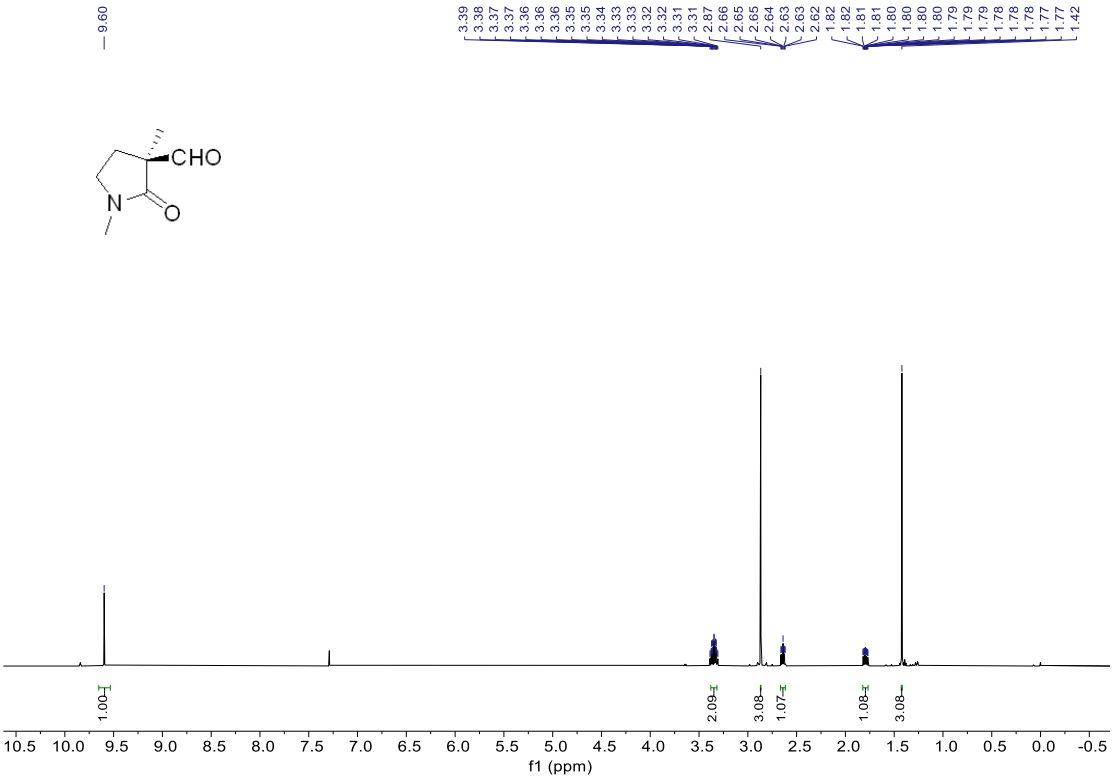
^{13}C NMR (101 MHz, Chloroform-*d*)



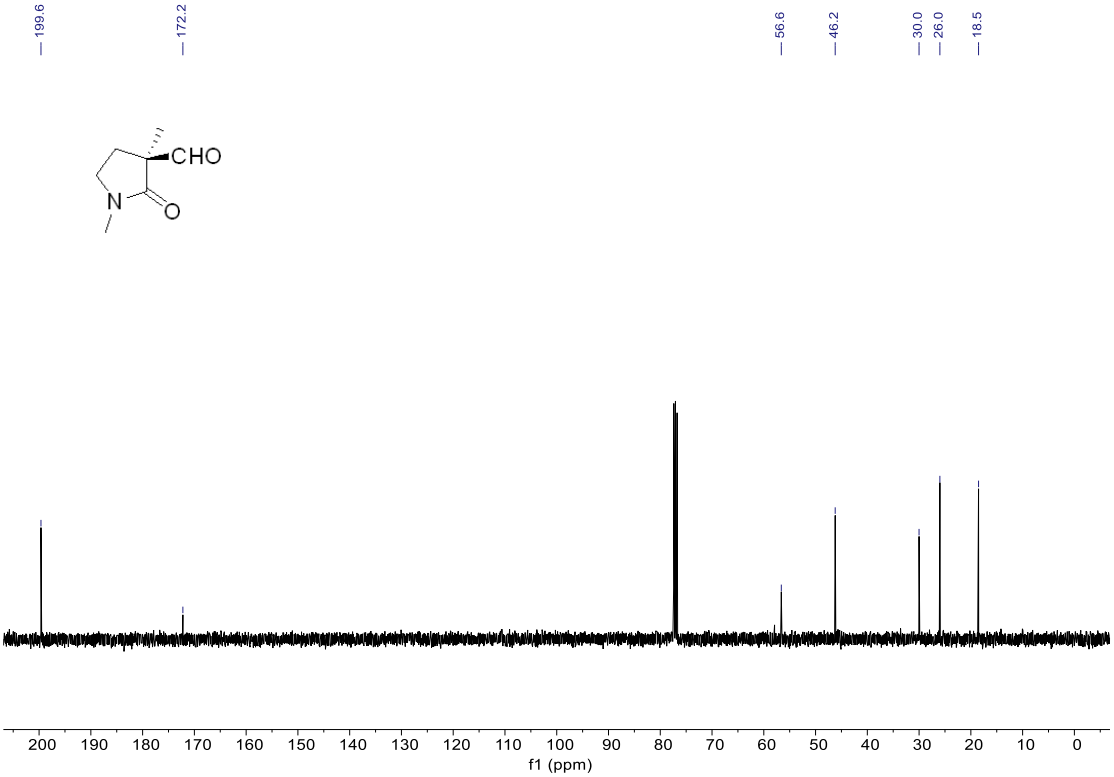


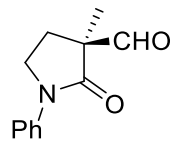
2o

^{1}H NMR (600 MHz, Chloroform-*d*)



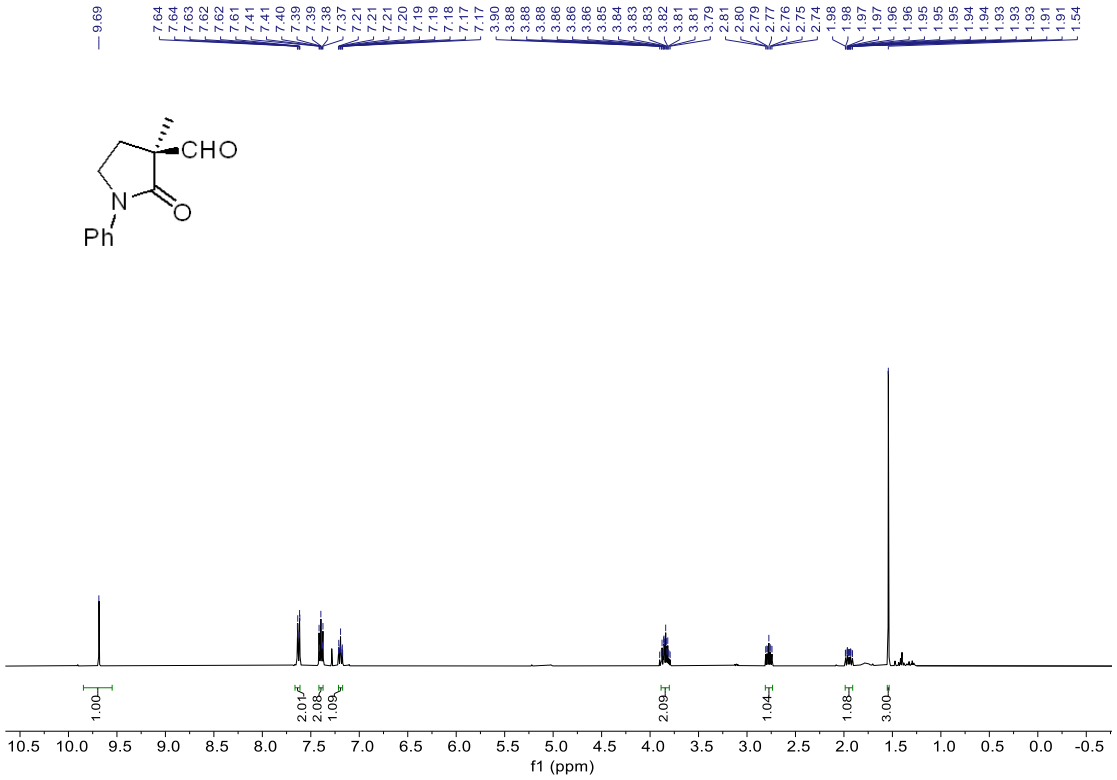
^{13}C NMR (101 MHz, Chloroform-*d*)



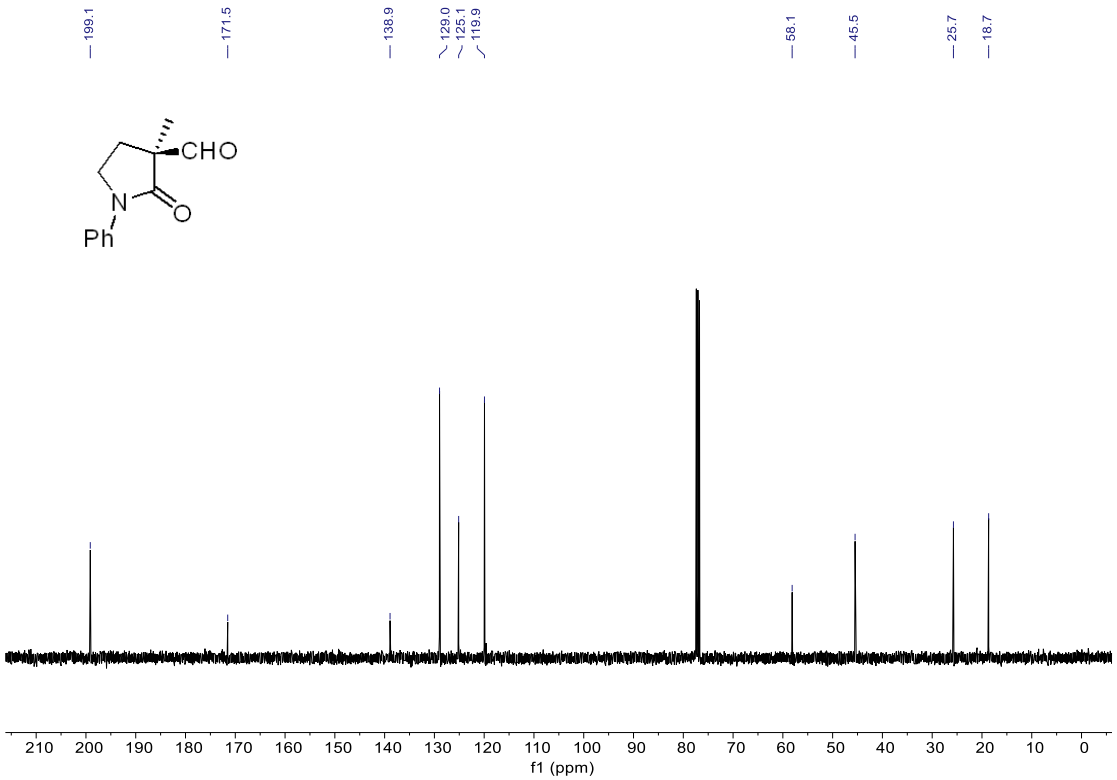


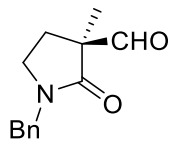
2p

^{1}H NMR (400 MHz, Chloroform-*d*)



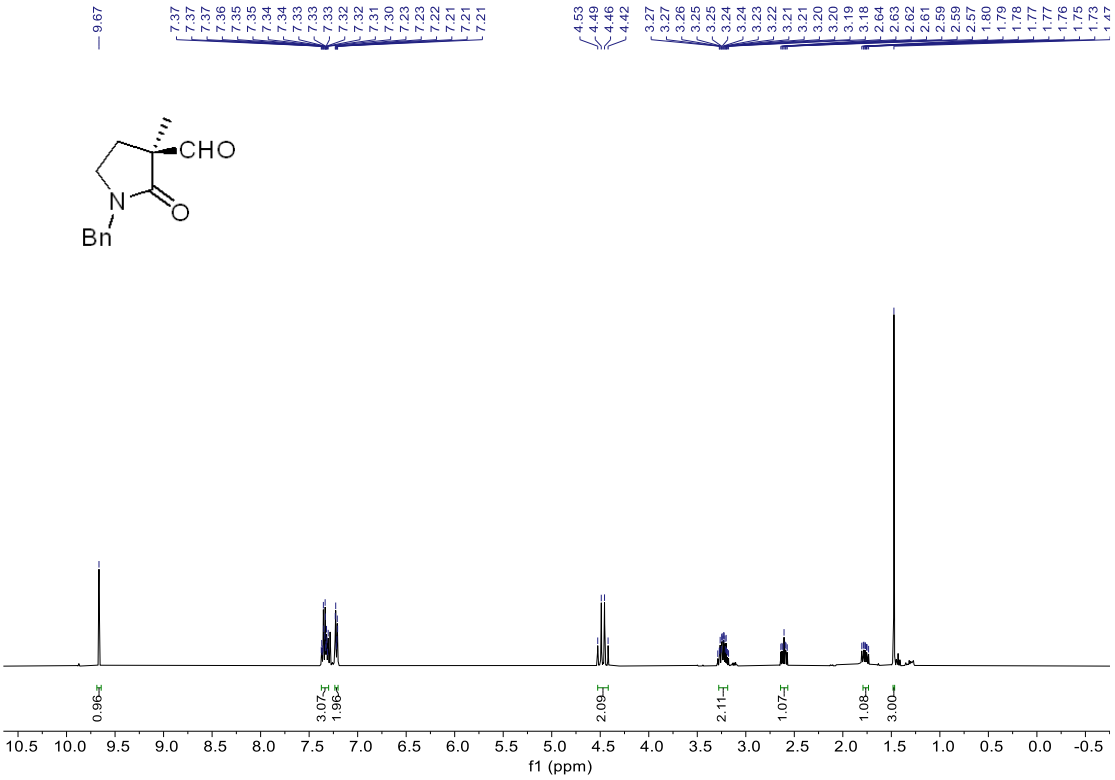
^{13}C NMR (101 MHz, Chloroform-*d*)



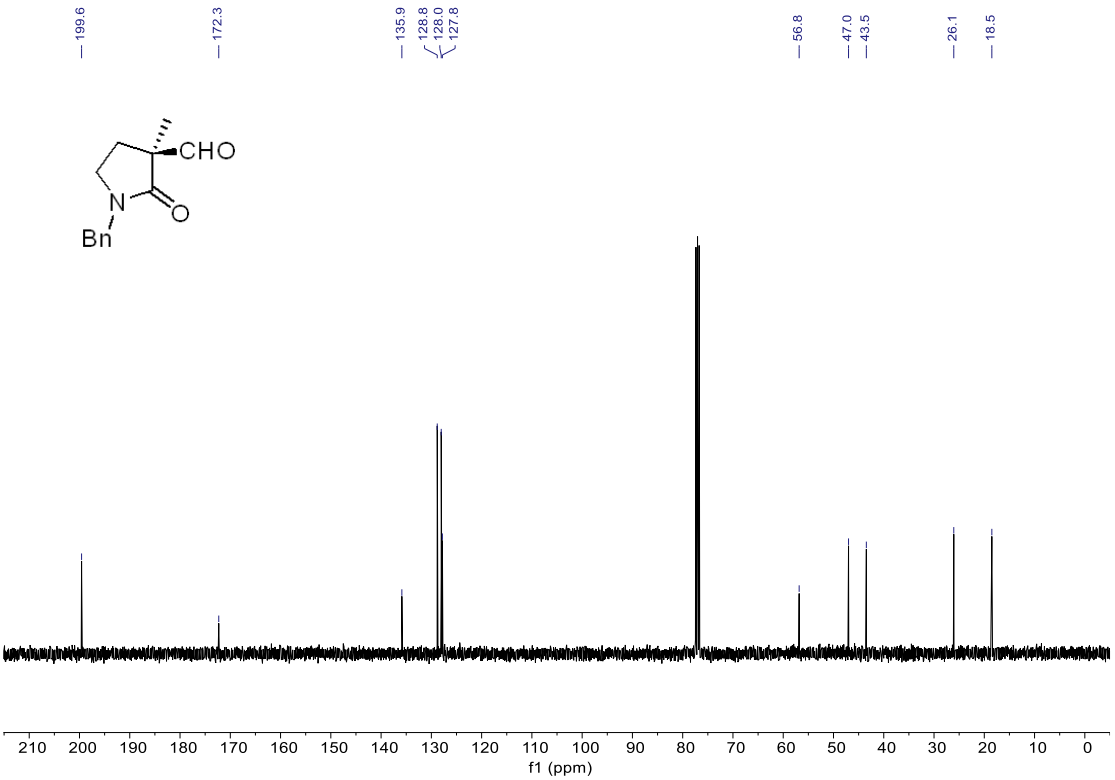


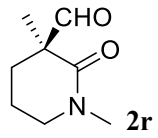
2q

^{1}H NMR (400 MHz, Chloroform-*d*)



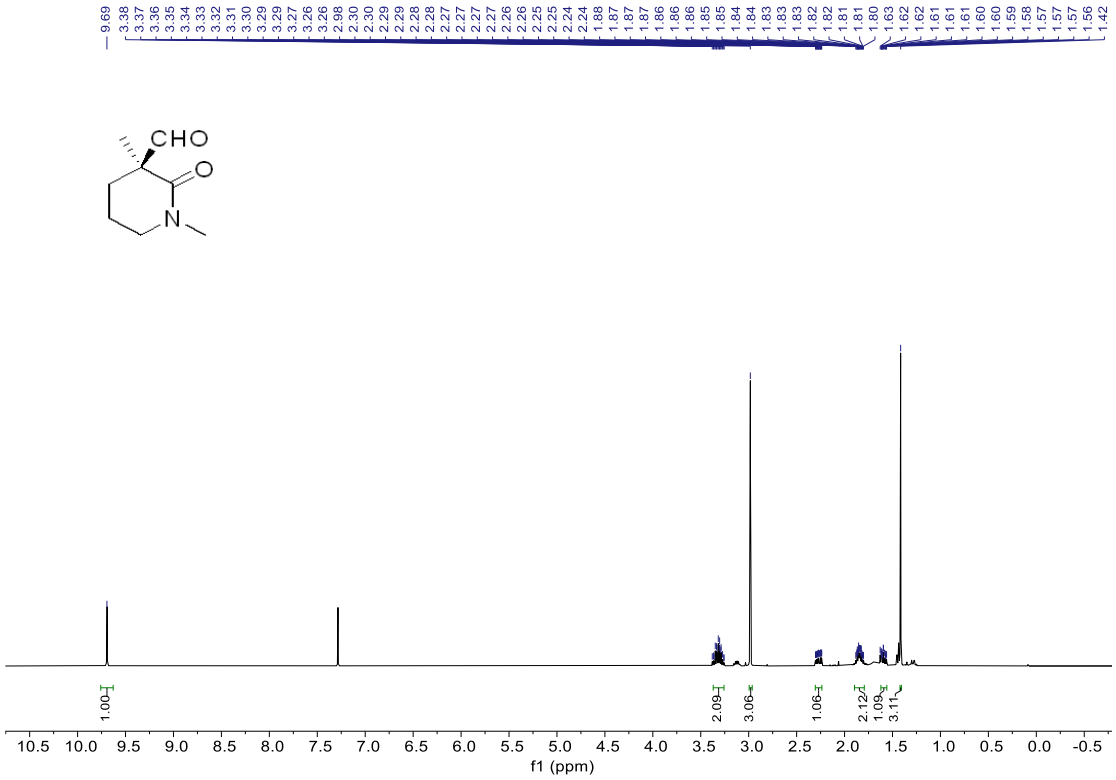
^{13}C NMR (101 MHz, Chloroform-*d*)



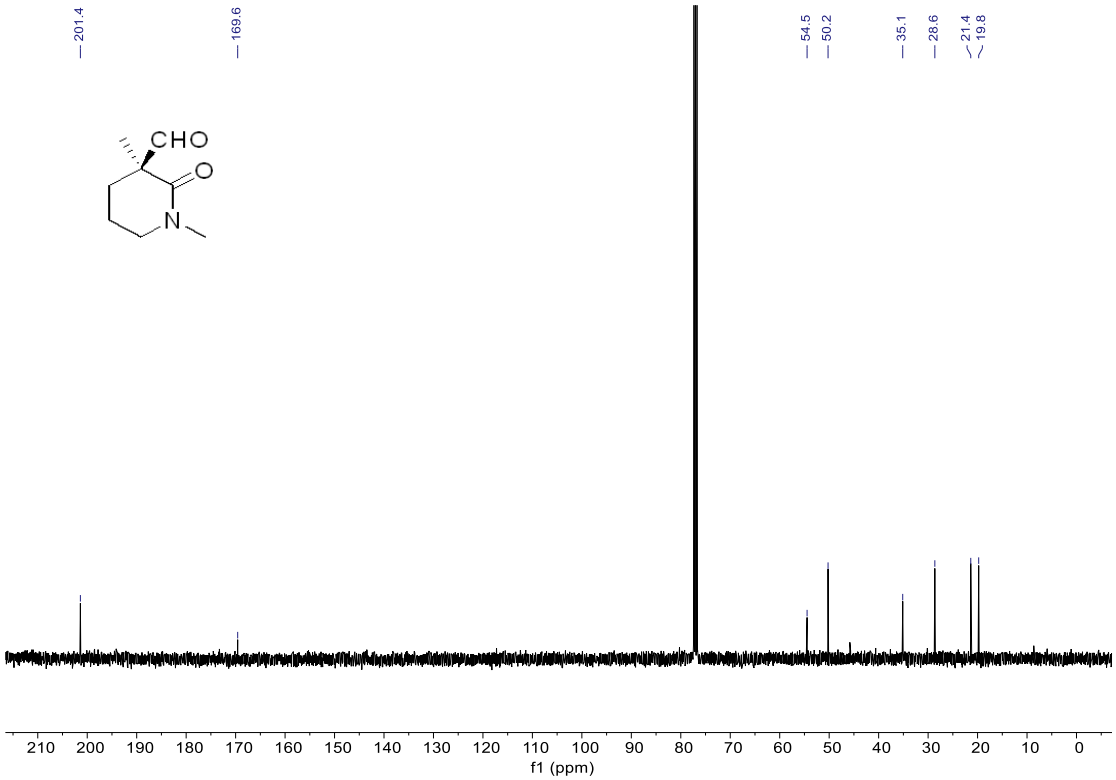


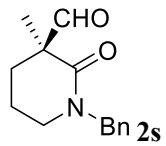
2r

^{1}H NMR (400 MHz, Chloroform-*d*)



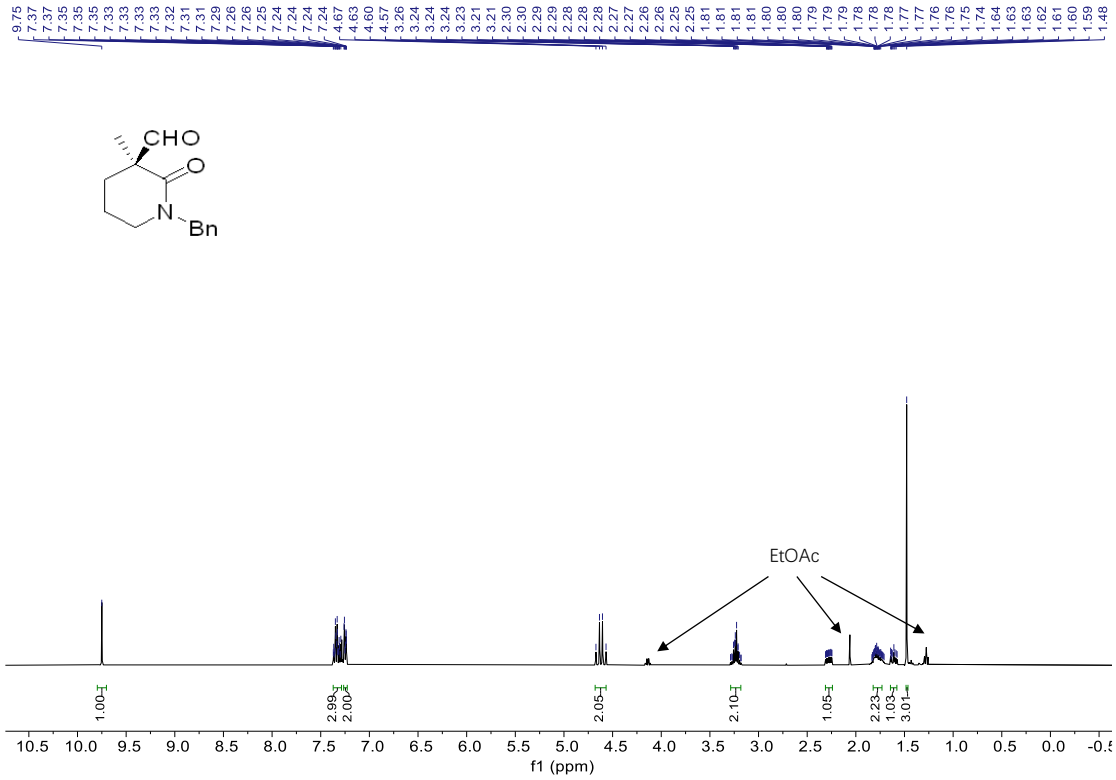
^{13}C NMR (101 MHz, Chloroform-*d*)



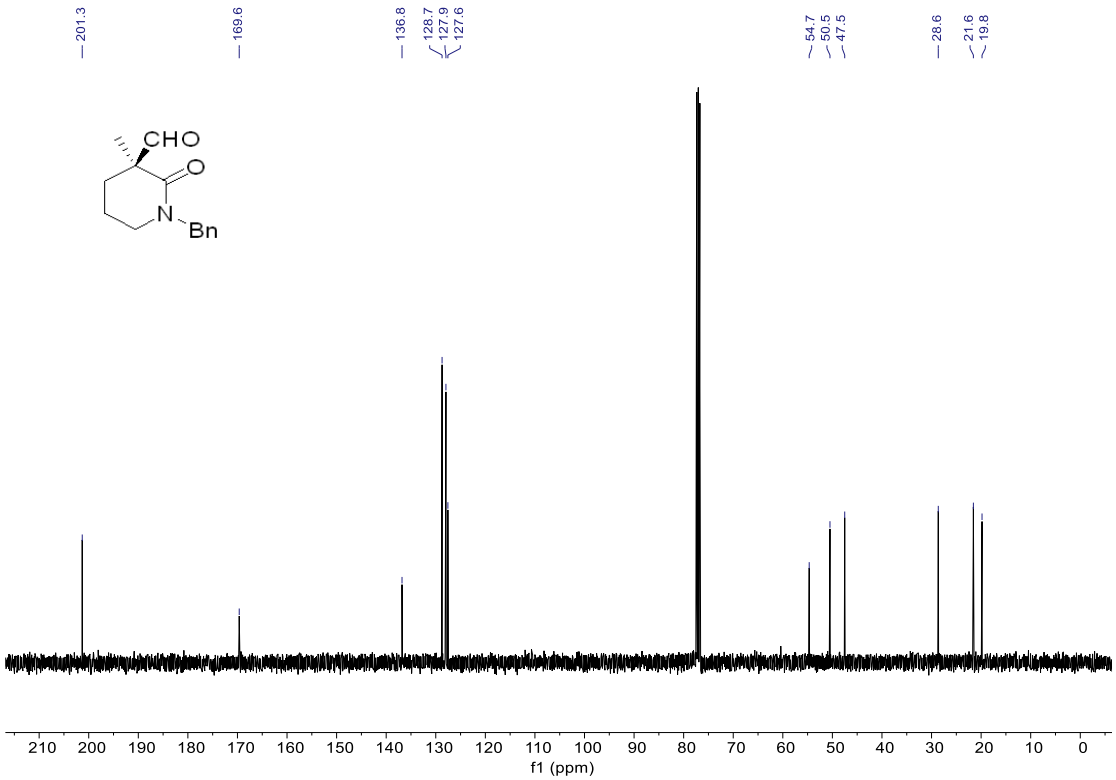


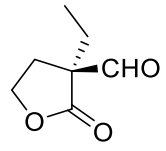
2s

^{1}H NMR (400 MHz, Chloroform-*d*)



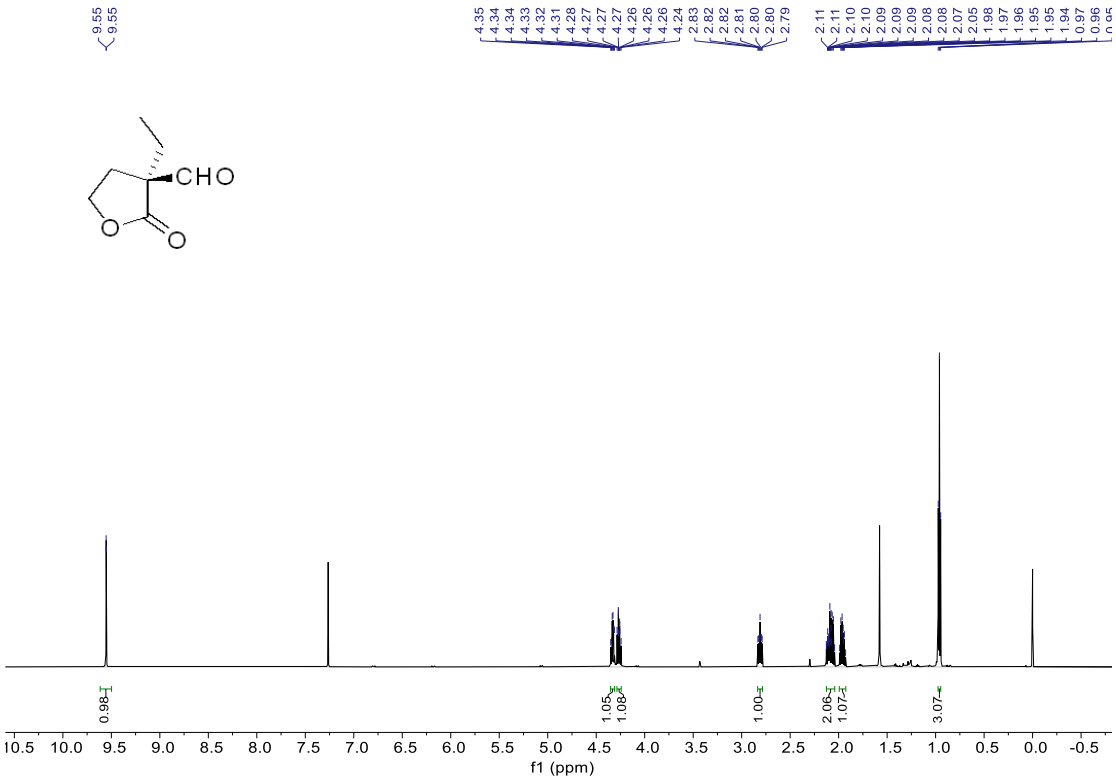
^{13}C NMR (101 MHz, Chloroform-*d*)



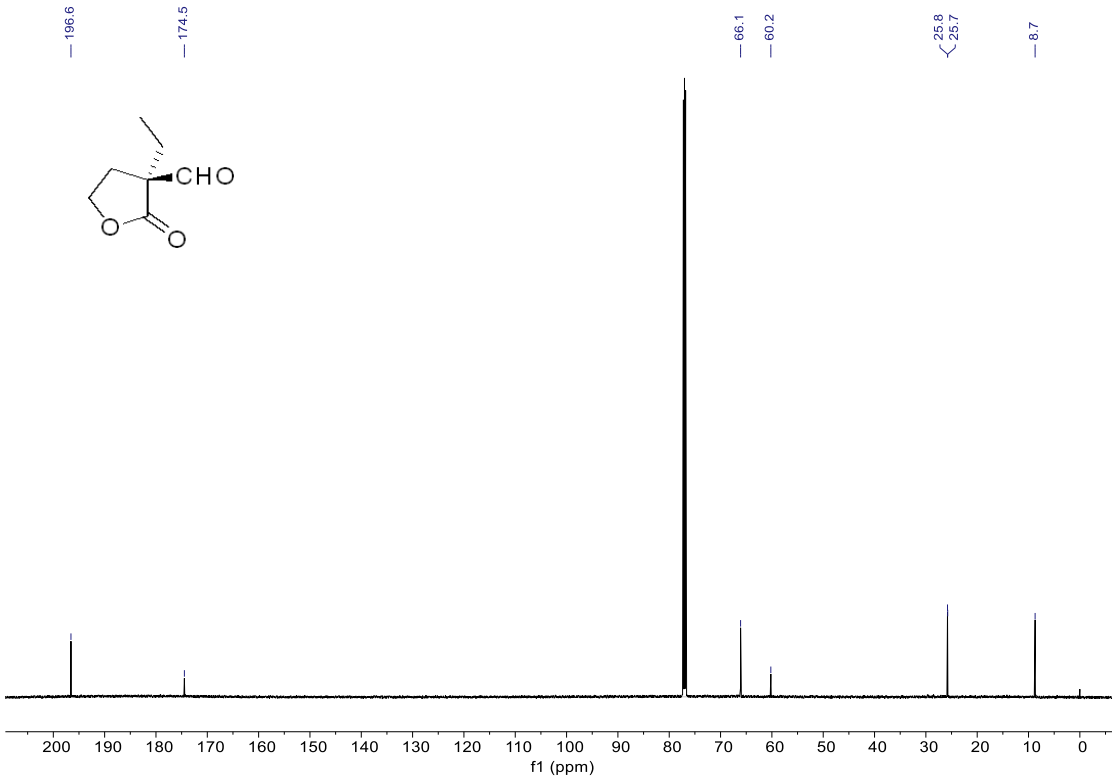


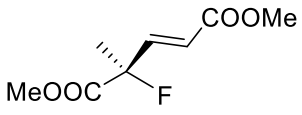
2t

^{1}H NMR (600 MHz, Chloroform-*d*)



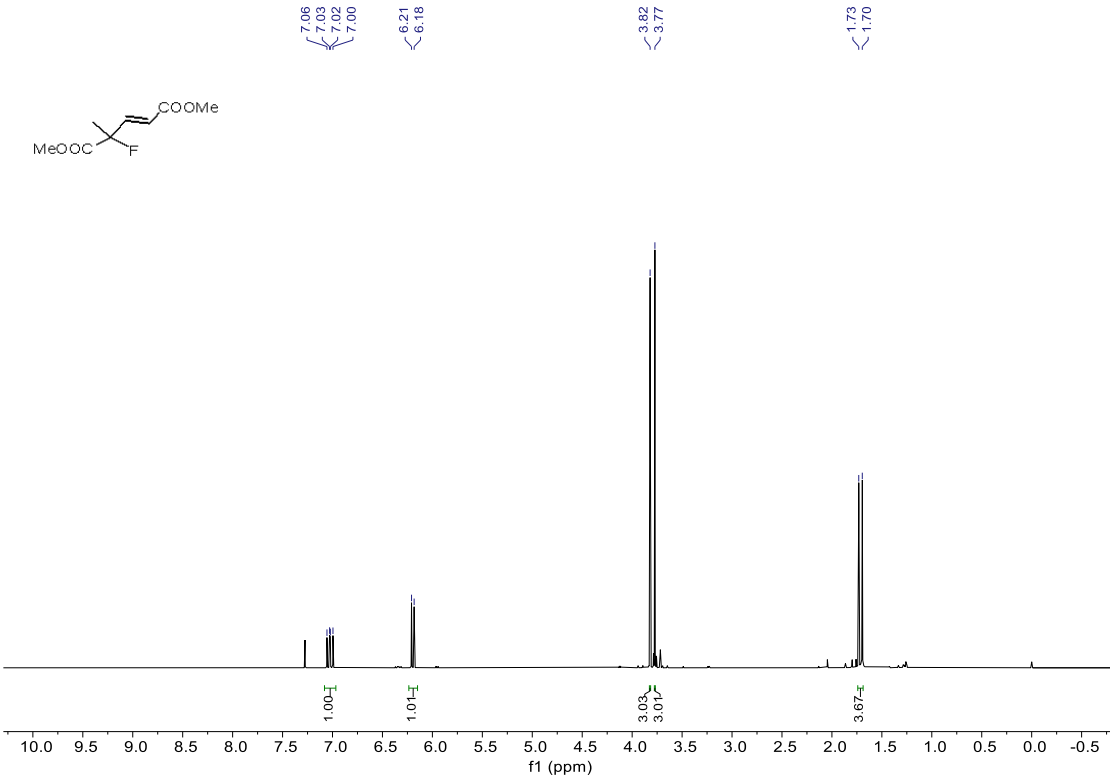
^{13}C NMR (151 MHz, Chloroform-*d*)



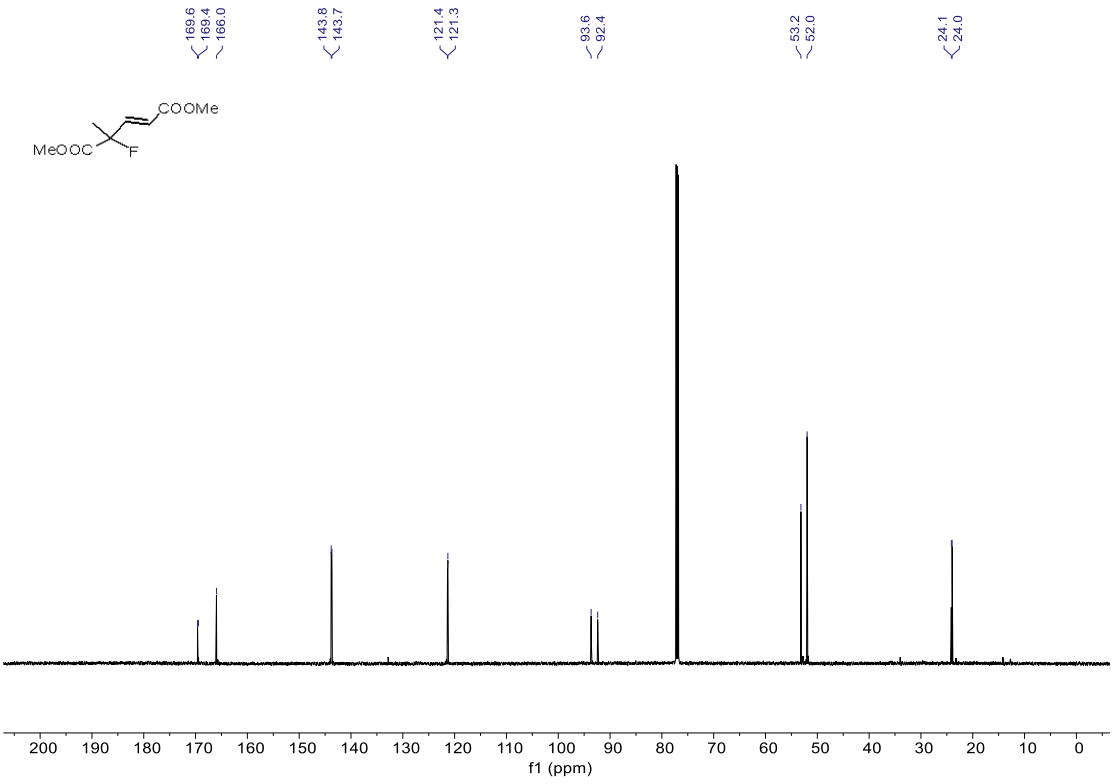


2u

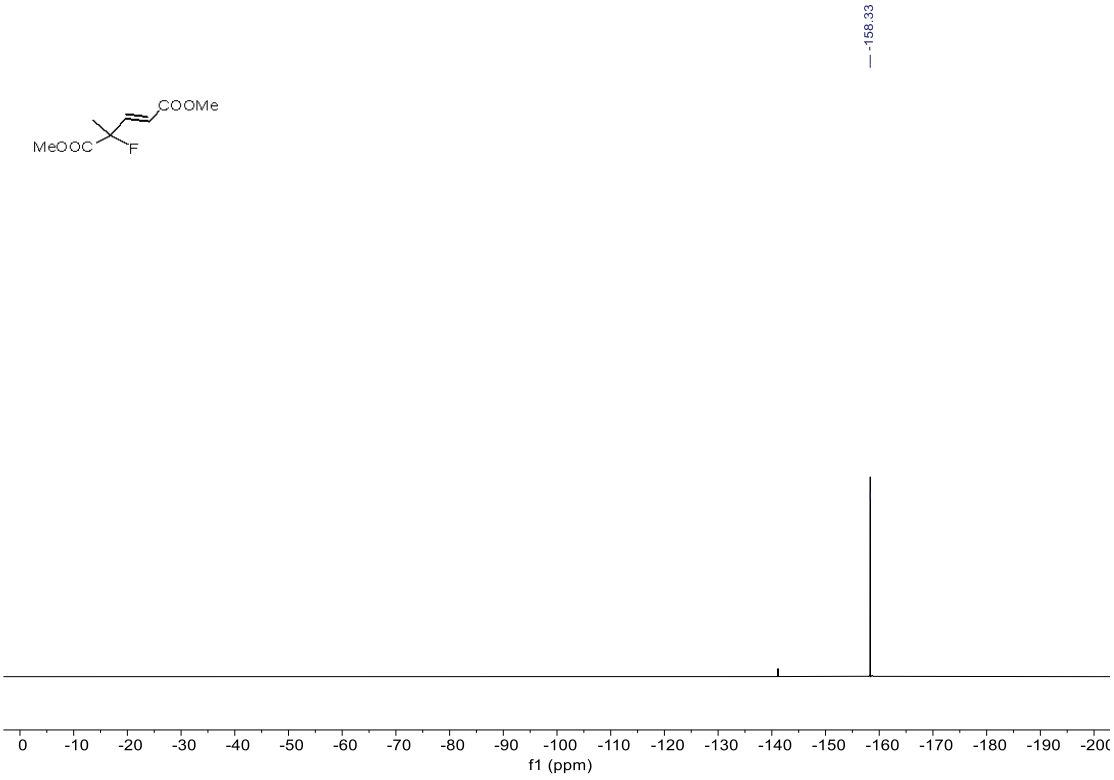
^{1}H NMR (600 MHz, Chloroform-*d*)

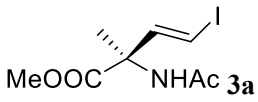


^{13}C NMR (151 MHz, Chloroform-*d*)



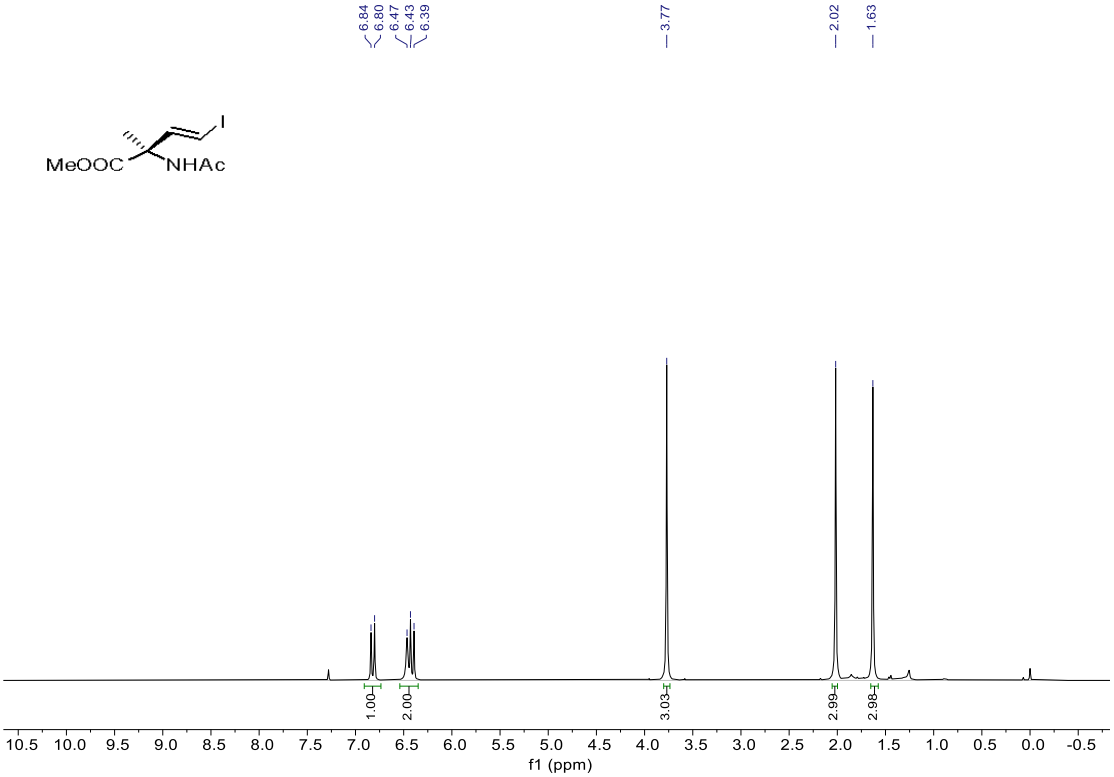
^{19}F NMR (376 MHz, Chloroform-*d*)



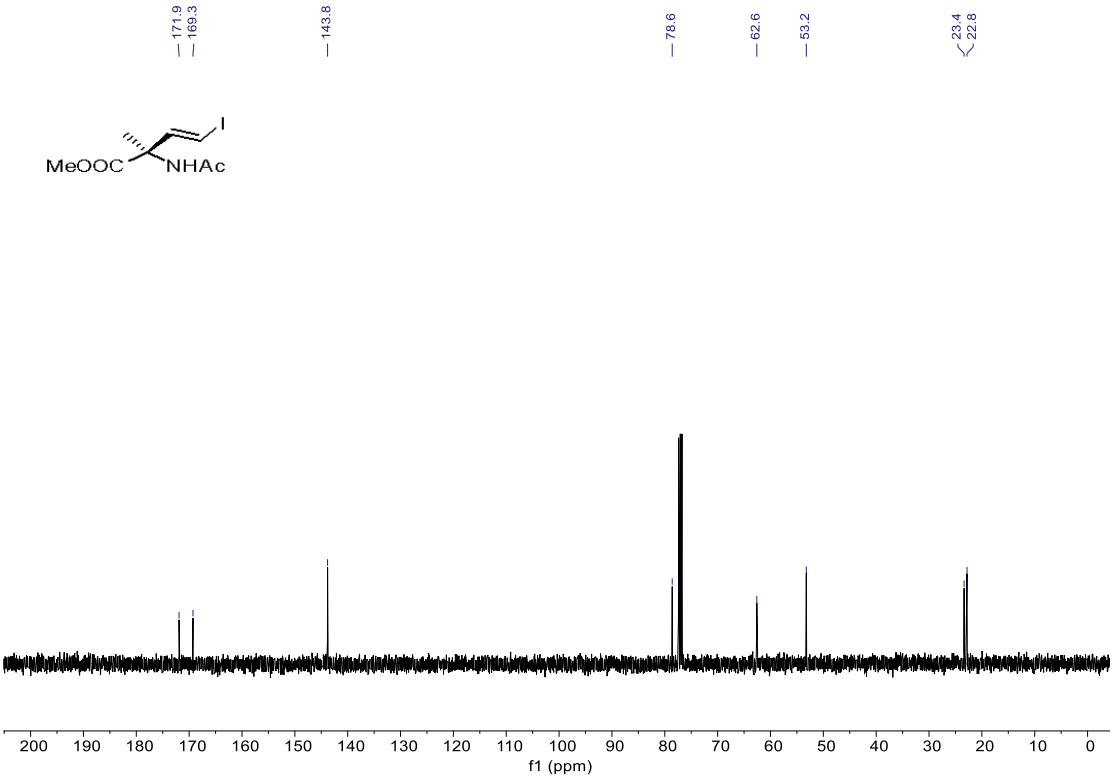


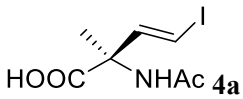
3a

^{1}H NMR (400 MHz, Chloroform-*d*)



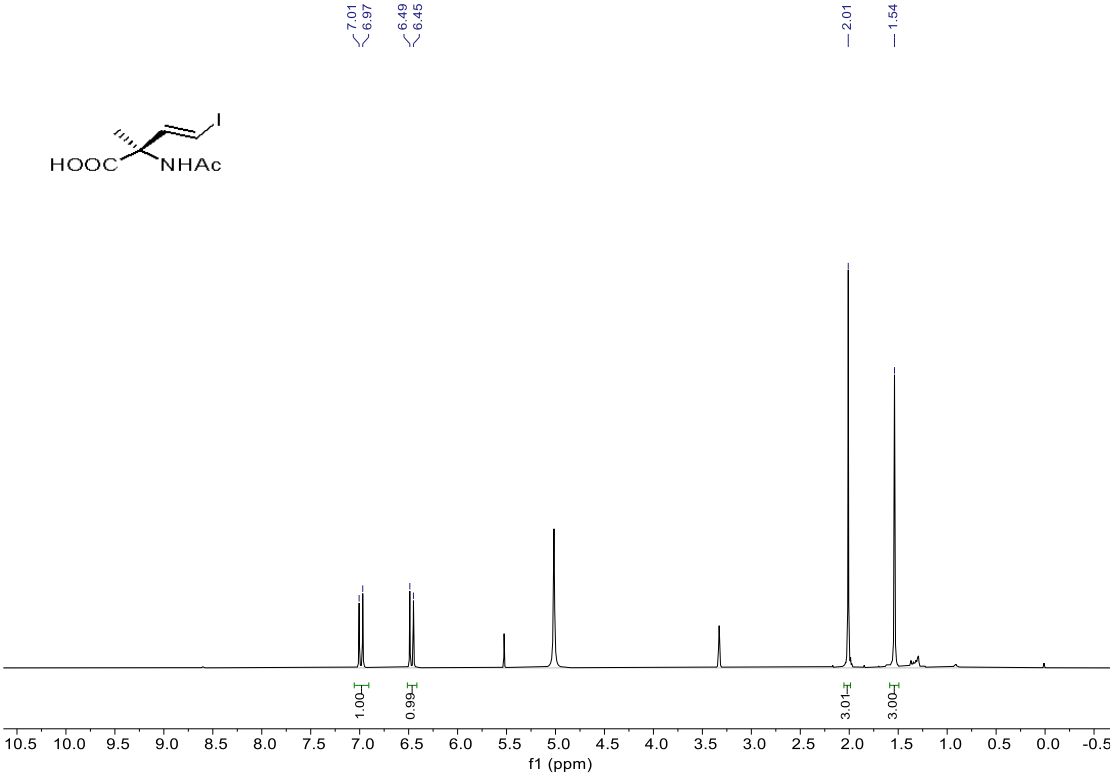
^{13}C NMR (101 MHz, Chloroform-*d*)



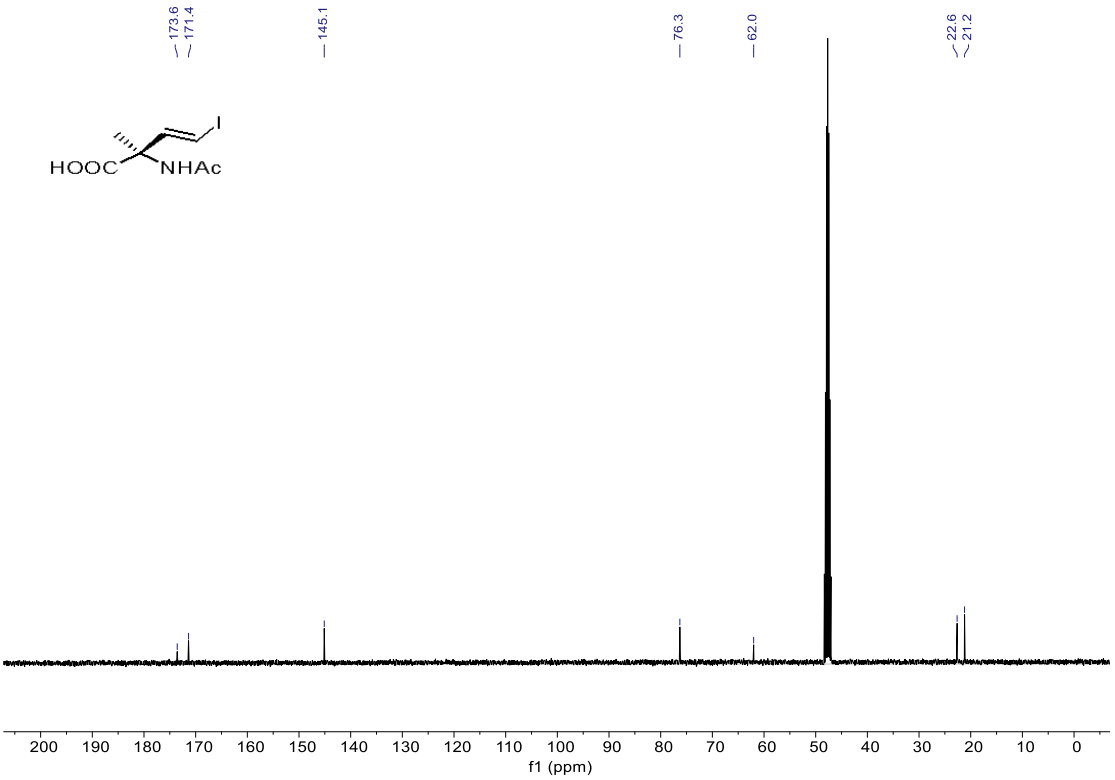


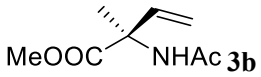
4a

^{1}H NMR (400 MHz, Methanol-d_4)



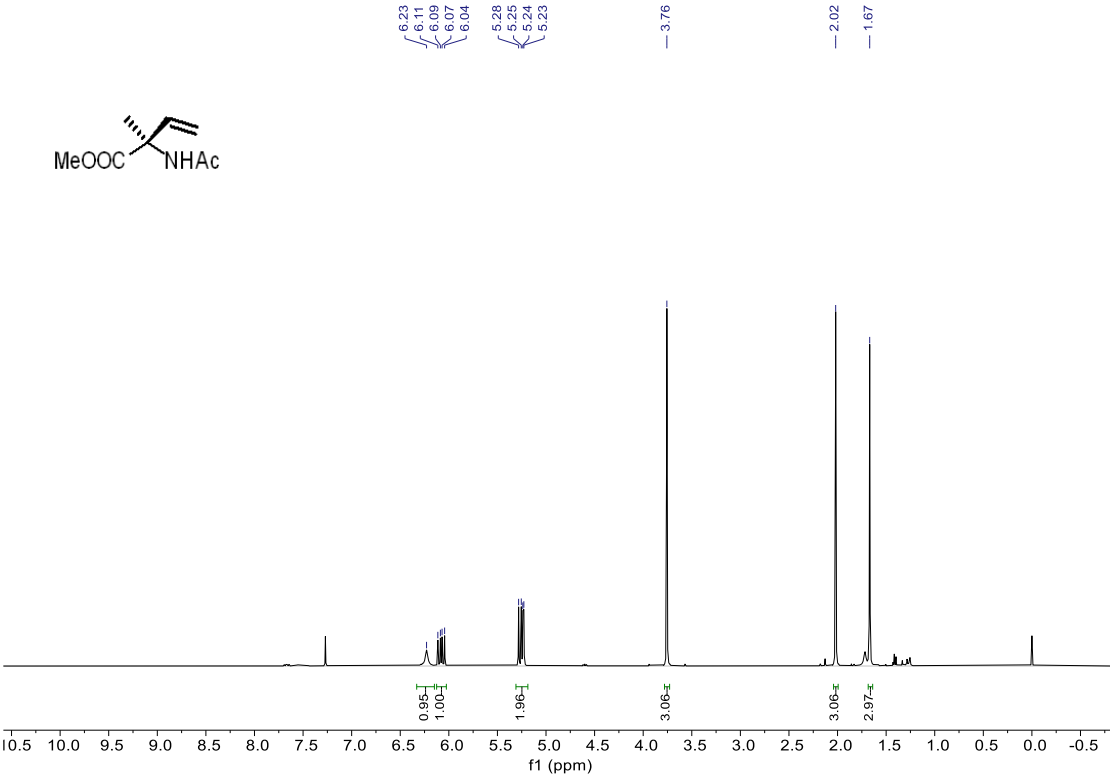
^{13}C NMR (101 MHz, Methanol-d_4)



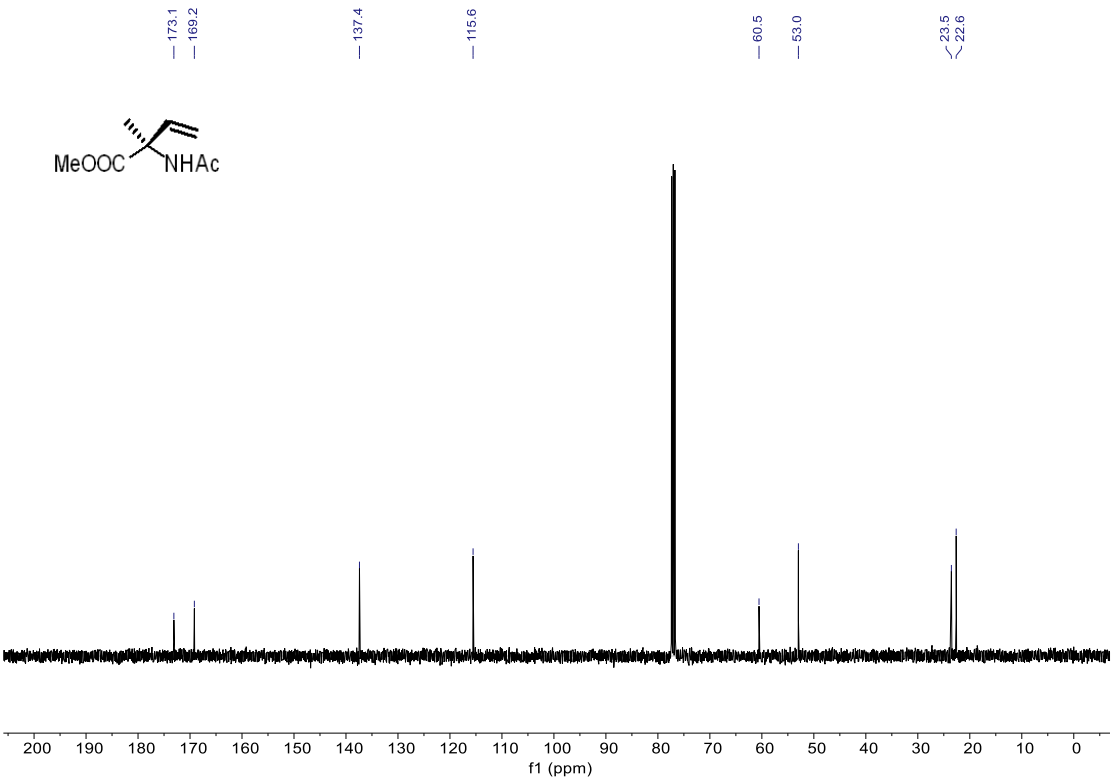


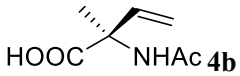
3b

^{1}H NMR (400 MHz, Chloroform-*d*)



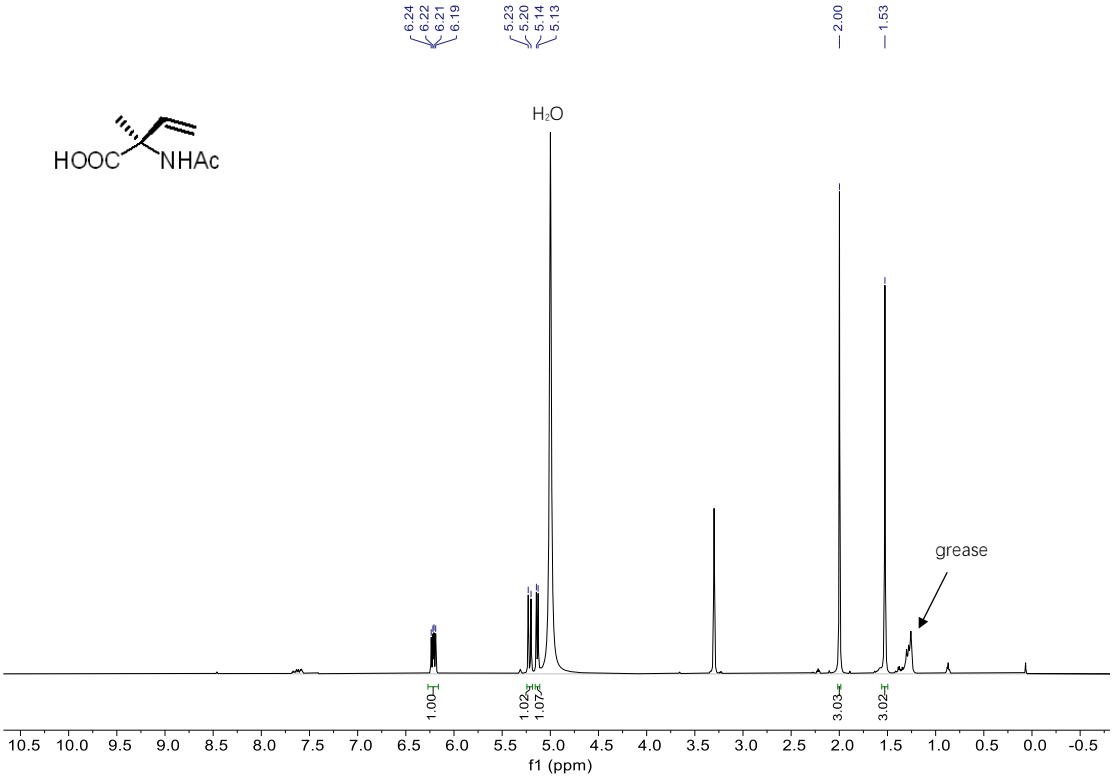
^{13}C NMR (101 MHz, Chloroform-*d*)



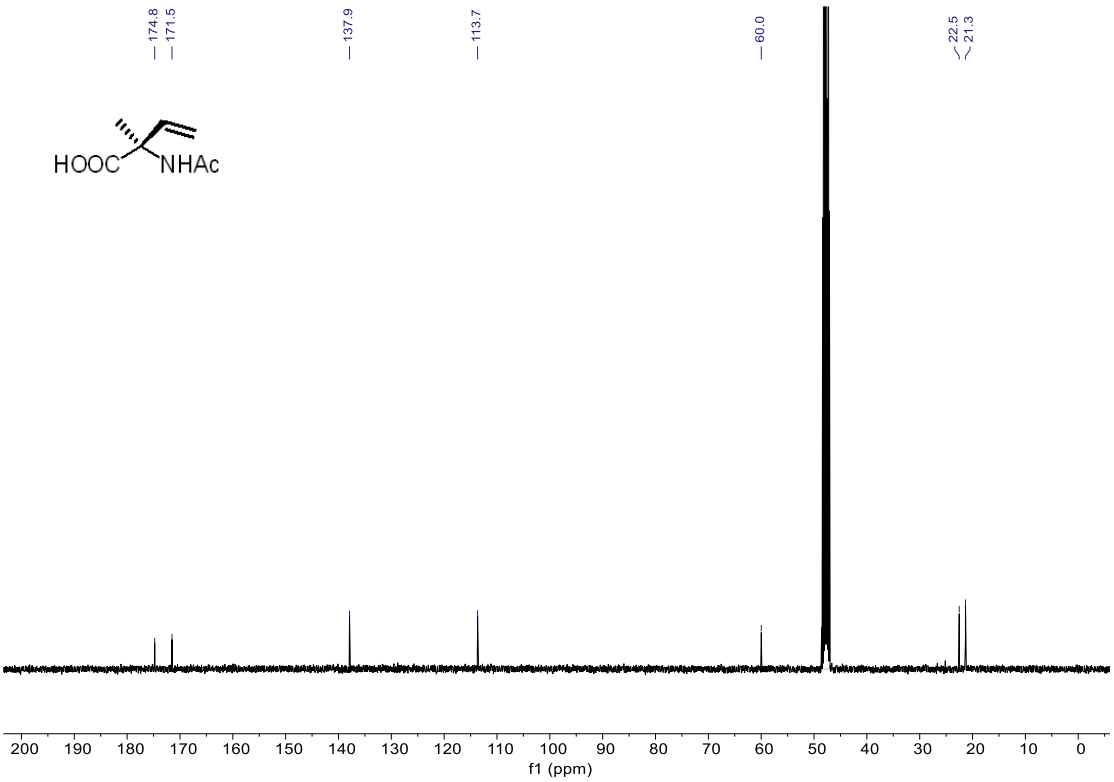


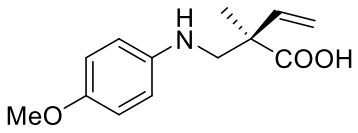
4b

^{1}H NMR (600 MHz, Methanol-d_4)



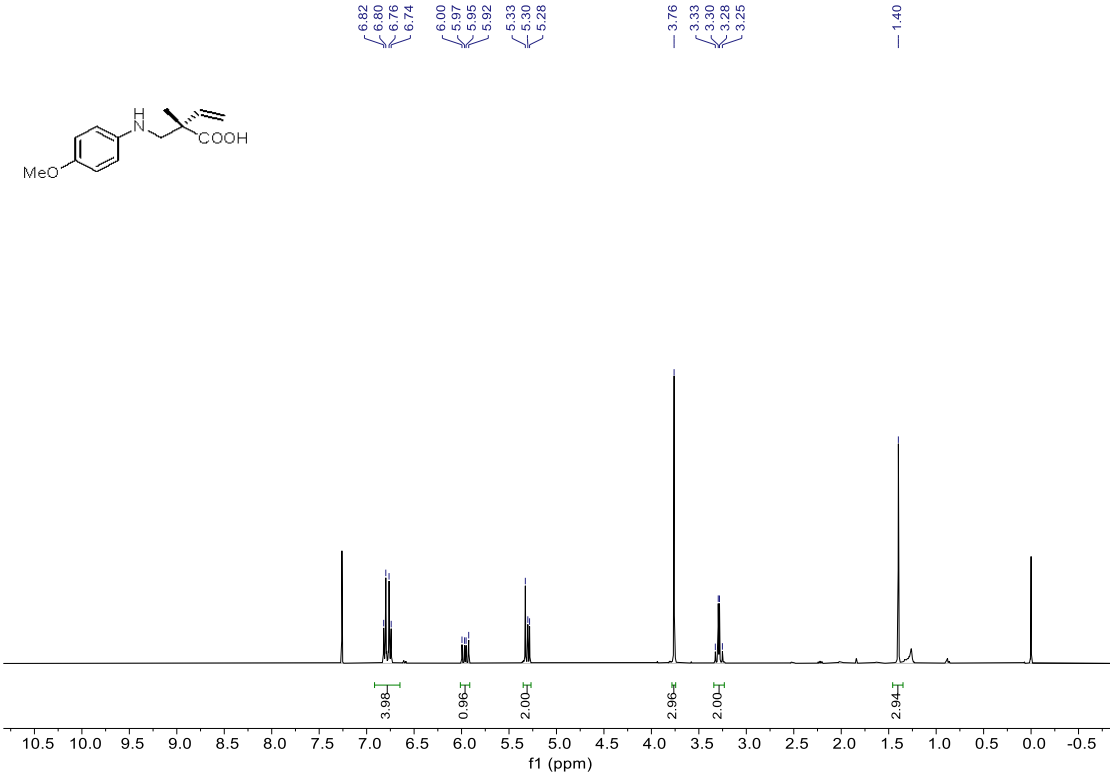
^{13}C NMR (101 MHz, Methanol-d_4)



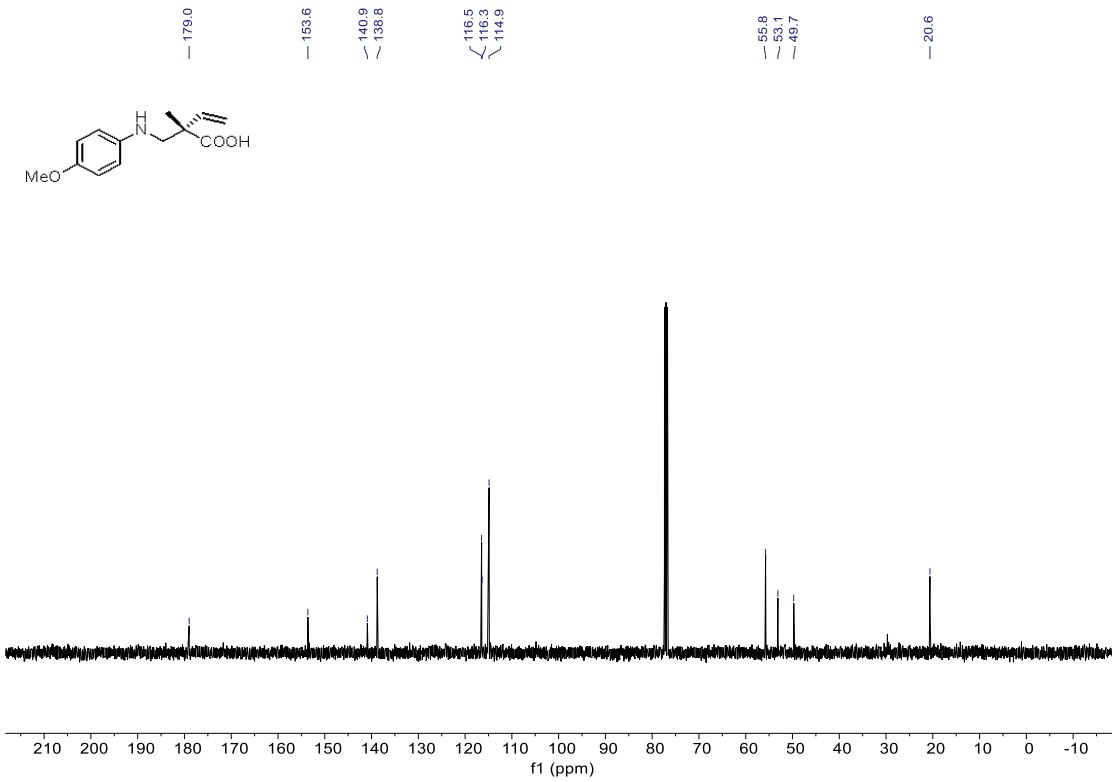


4n

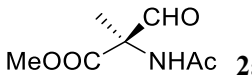
[1]H NMR (400 MHz, Chloroform-*d*)



[13]C NMR (101 MHz, Chloroform-*d*)


179.0
153.6
140.9
138.8
116.5
116.3
114.9
55.8
53.1
49.7
20.6
MeO
H
N
COOH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

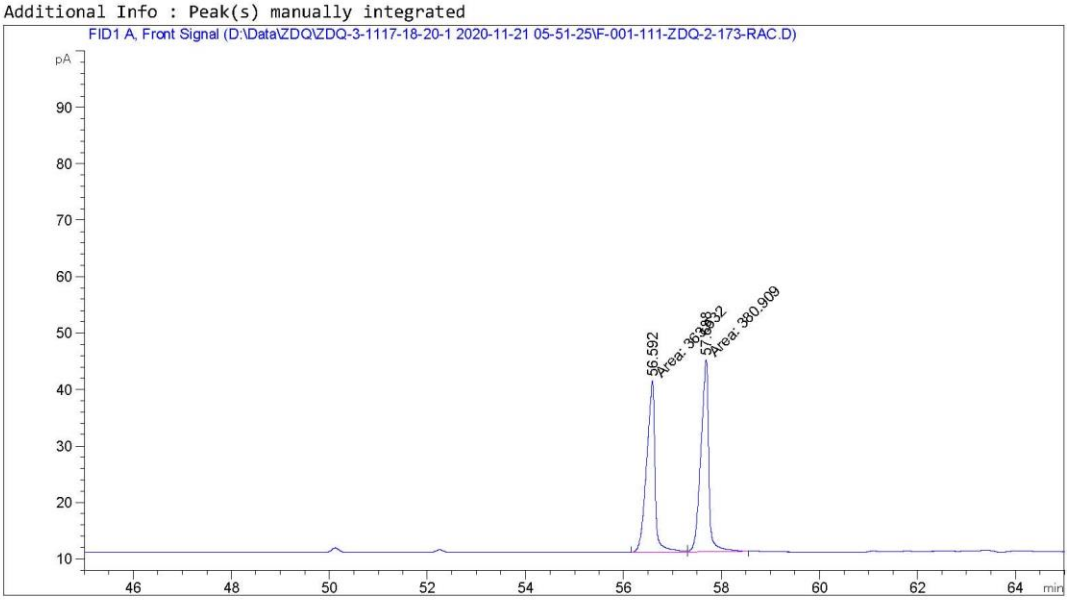
11. HPLC chromatograms



2a

Data File D:\Data\ZDQ\ZDQ-3-1117-18-20-1 2020-11-21 05-51-25\F-001-111-ZDQ-2-173-RAC.D
Sample Name: ZDQ-2-173-RAC

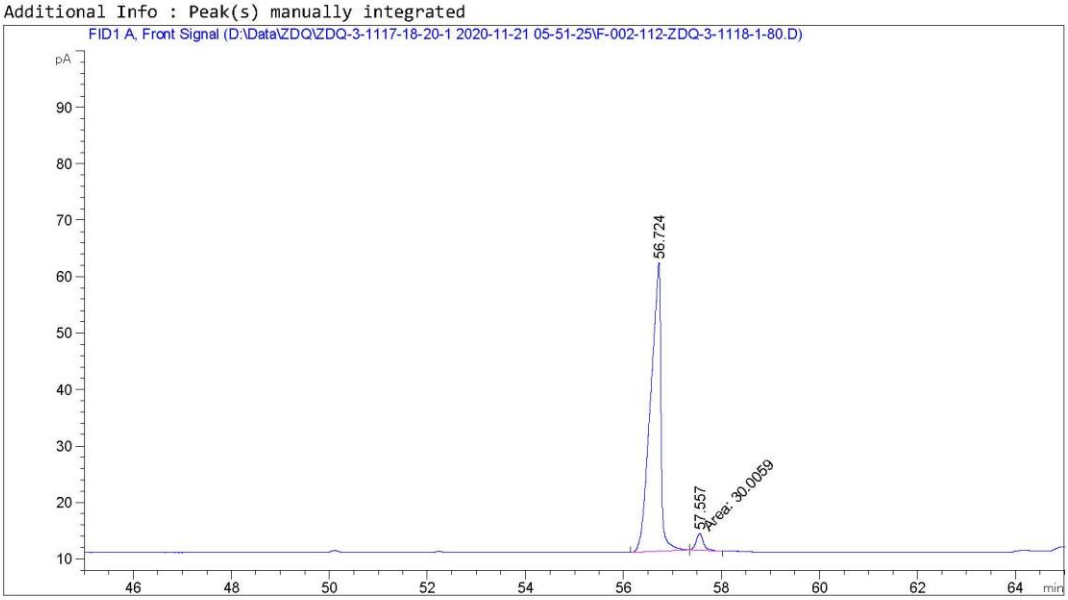
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   1
Acq. Instrument : GC7890B                       Location :   111  (F)
Injection Date  : 11/21/2020 5:53:26 AM              Inj :   1
                                               Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-3-1117-18-20-1 2020-11-21 05-51-25\ZDQ-B-120-80-1-140-70min
                  .M
Last changed    : 11/21/2020 5:42:30 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\ZDQ-3-1117-18-20-1 2020-11-21 05-51-25\ZDQ-B-120-80-1-140-70min
                  .M (Sequence Method)
Last changed    : 9/16/2021 4:31:53 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



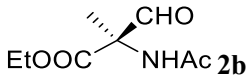

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  56.592 MF    0.1994  363.53186   30.39215 48.83285
   2  57.688 FM    0.1867  380.90942   34.00882 51.16715

Totals :                   744.44128   64.40097
```

Data File D:\Data\ZDQ\ZDQ-3-1117-18-20-1 2020-11-21 05-51-25\F-002-112-ZDQ-3-1118-1-80.D
Sample Name: ZDQ-3-1118-1-80

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : GC7890B                       Location :   112  (F)
Injection Date  : 11/21/2020 7:06:26 AM              Inj :   1
                                               Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-3-1117-18-20-1 2020-11-21 05-51-25\ZDQ-B-120-80-1-140-70min
                  .M
Last changed    : 11/21/2020 5:42:30 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\ZDQ-3-1117-18-20-1 2020-11-21 05-51-25\ZDQ-B-120-80-1-140-70min
                  .M (Sequence Method)
Last changed    : 9/16/2021 4:31:53 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



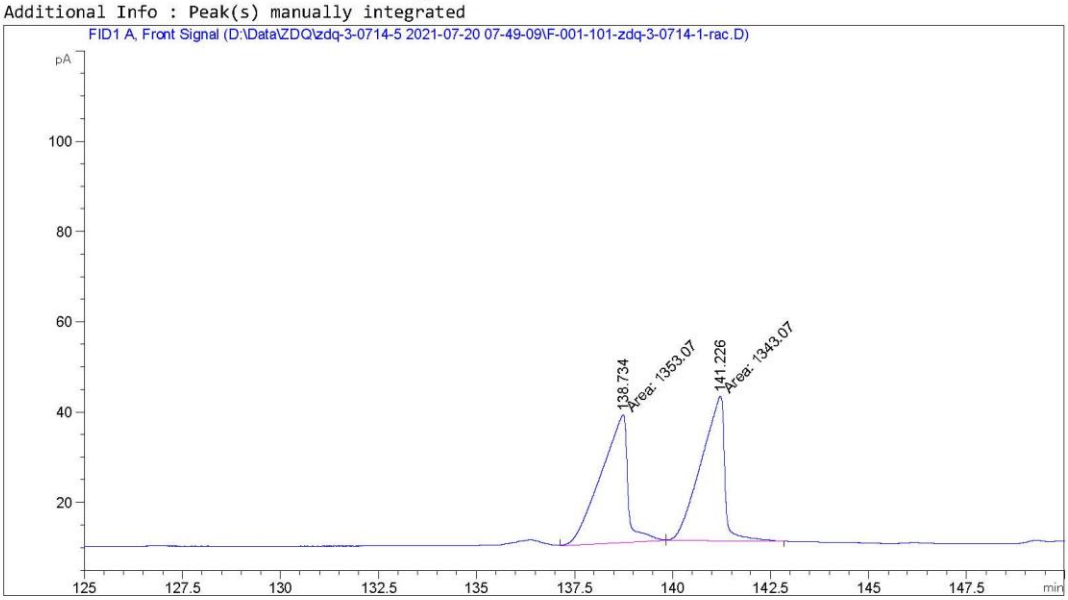

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  56.724 BB    0.1871  749.67950   51.11179 96.15154
   2  57.557 MM    0.1689   30.00588    2.96132  3.84846

Totals :                   779.68538   54.07311
```



2b

Data File D:\Data\ZDQ\zdq-3-0714-5 2021-07-20 07-49-09\F-001-101-zdq-3-0714-1-rac.D
Sample Name: zdq-3-0714-1-rac

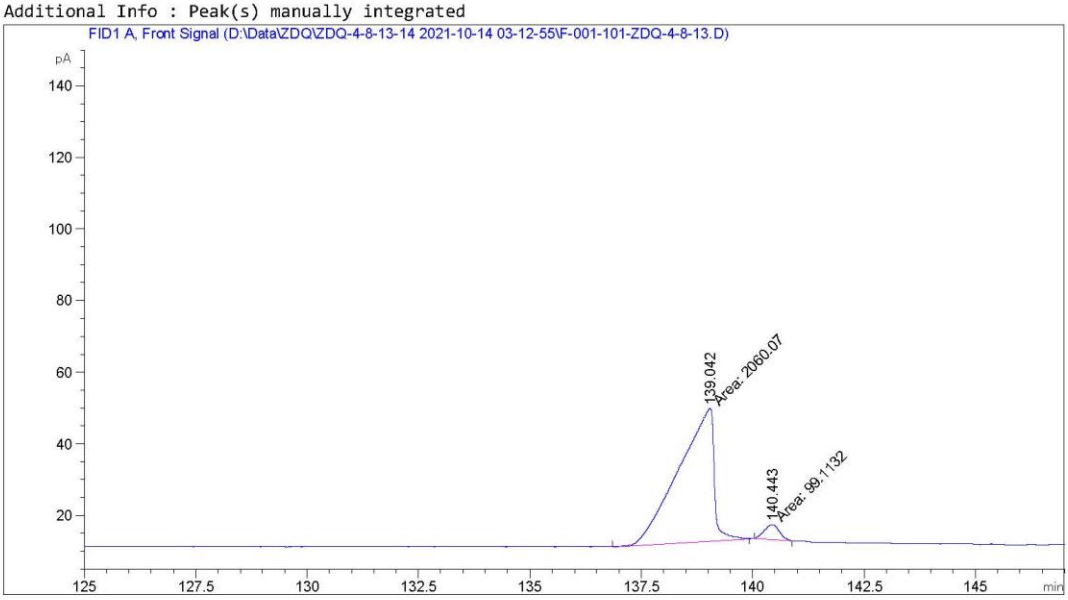
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   1
Acq. Instrument : GC7890B                      Location :   101  (F)
Injection Date  : 7/20/2021 7:51:26 AM              Inj :   1
                                              Inj Volume : 1 µl
Acq. Method     : D:\Data\ZDQ\zdq-3-0714-5 2021-07-20 07-49-09\ZDQ-B-120-70-0.4--5-130-185min
                  .M
Last changed    : 7/20/2021 7:39:26 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\zdq-3-0714-5 2021-07-20 07-49-09\ZDQ-B-120-70-0.4--5-130-185min
                  .M (Sequence Method)
Last changed    : 11/9/2021 6:32:39 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



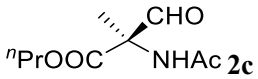

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1 138.734 MM    0.7989 1353.07239   28.22934 50.18547
   2 141.226 MM    0.6991 1343.07129   32.01870 49.81453

Totals :                  2696.14368   60.24804
```

Data File D:\Data\ZDQ\ZDQ-4-8-13-14 2021-10-14 03-12-55\F-001-101-ZDQ-4-8-13.D
Sample Name: ZDQ-4-8-13

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   1
Acq. Instrument : GC7890B                        Location :   101  (F)
Injection Date  : 10/14/2021 3:15:00 AM               Inj :   1
                                                Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 3 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-4-8-13-14 2021-10-14 03-12-55\ZDQ-B-120-70-0.4--5-130-
                  185min.M
Last changed    : 10/14/2021 6:26:02 AM by SYSTEM
                  (modified after loading)
Analysis Method : D:\Data\ZDQ\ZDQ-4-8-13-14 2021-10-14 03-12-55\ZDQ-B-120-70-0.4--5-130-
                  185min.M (Sequence Method)
Last changed    : 11/9/2021 6:39:16 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



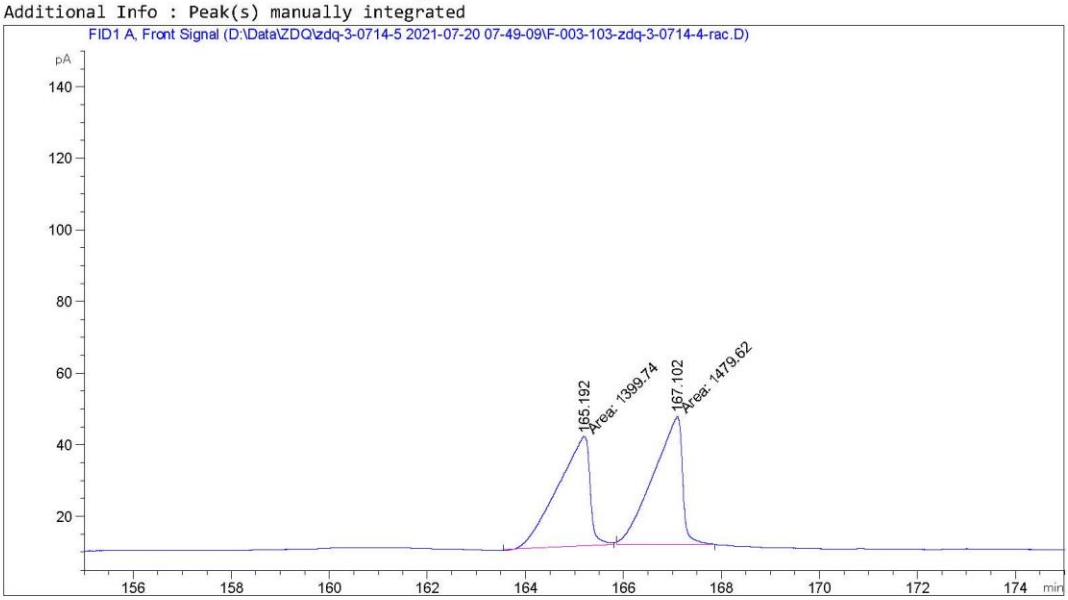

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1 139.042 MM    0.9255 2060.07178   37.09874 95.40970
   2 140.443 MM    0.3947   99.11315    4.18513  4.59030
```



2c

Data File D:\Data\ZDQ\zdq-3-0714-5 2021-07-20 07-49-09\F-003-103-zdq-3-0714-4-rac.D
Sample Name: zdq-3-0714-4-rac

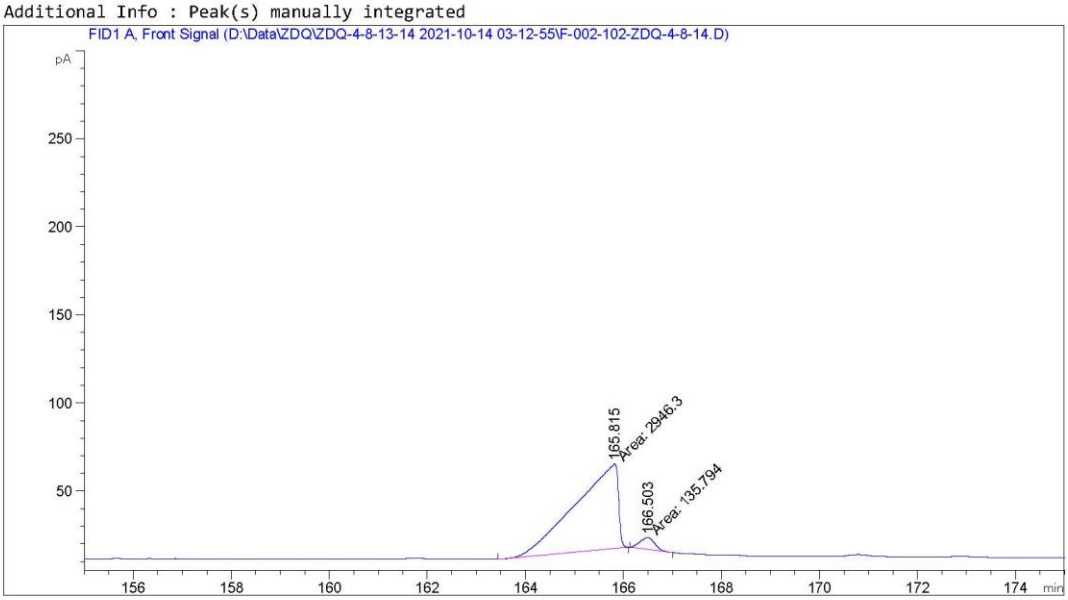
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   3
Acq. Instrument : GC7890B                      Location :   103  (F)
Injection Date  : 7/20/2021 2:07:50 PM              Inj :   1
                                              Inj Volume : 1 µl
Acq. Method     : D:\Data\ZDQ\zdq-3-0714-5 2021-07-20 07-49-09\ZDQ-B-120-70-0.4--5-130-185min
                  .M
Last changed    : 7/20/2021 7:39:26 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\zdq-3-0714-5 2021-07-20 07-49-09\ZDQ-B-120-70-0.4--5-130-185min
                  .M (Sequence Method)
Last changed    : 11/9/2021 6:35:13 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



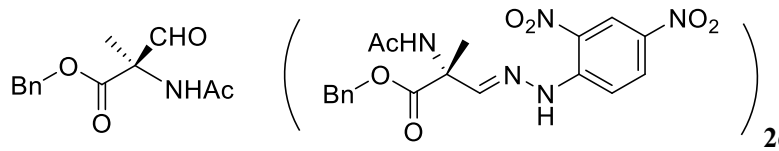

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1 165.192 MM    0.7641 1399.73914   30.53025 48.61282
   2 167.102 MM    0.6886 1479.62329   35.81320 51.38718

Totals :                  2879.36243   66.34345
```

Data File D:\Data\ZDQ\ZDQ-4-8-13-14 2021-10-14 03-12-55\F-002-102-ZDQ-4-8-14.D
Sample Name: ZDQ-4-8-14

```
=====================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : GC7890B                       Location :   102  (F)
Injection Date  : 10/14/2021 6:51:04 AM              Inj :   1
                                               Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 3 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-4-8-13-14 2021-10-14 03-12-55\ZDQ-B-120-70-0.4--5-130-
                  185min.M
Last changed    : 10/14/2021 6:26:02 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\ZDQ-4-8-13-14 2021-10-14 03-12-55\ZDQ-B-120-70-0.4--5-130-
                  185min.M (Sequence Method)
Last changed    : 11/9/2021 6:44:46 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



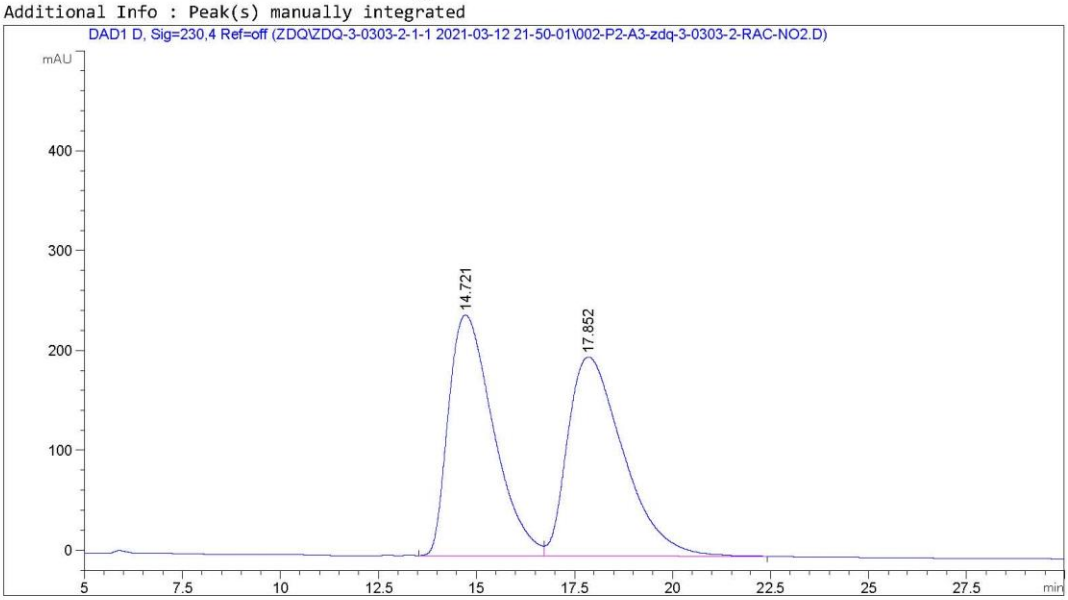

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1 165.815 MM    1.0222 2946.30420   48.03894 95.59409
   2 166.503 MM    0.3451  135.79446    6.55830  4.40591

Totals :                  3082.09866   54.59725
```



2d

Data File d:\Chem32\...Q-3-0303-2-1-1 2021-03-12 21-50-01\002-P2-A3-zdq-3-0303-2-RAC-NO2.D
Sample Name: zdq-3-0303-2-RAC-NO2

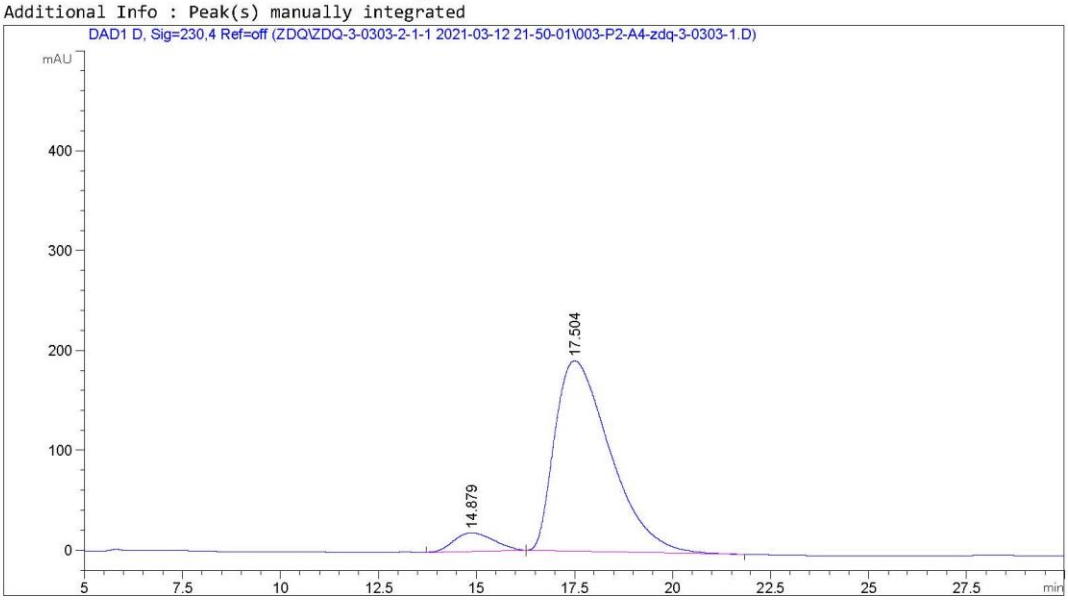
```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : 1290-DAD                       Location :   P2-A-03
Injection Date  : 3/12/2021 10:01:22 PM              Inj :   1
                                                Inj Volume : 1.000 µl
Acq. Method     : d:\Chem32\1\Data\ZDQ\ZDQ-3-0303-2-1-1 2021-03-12 21-50-01\OD-3-85-15-0.45-0
                  .5UL-30MIN-NO2.M
Last changed    : 3/12/2021 9:48:52 PM by SYSTEM
Analysis Method : d:\Chem32\1\Data\ZDQ\ZDQ-3-0303-2-1-1 2021-03-12 21-50-01\OD-3-85-15-0.45-0
                  .5UL-30MIN-NO2.M (Sequence Method)
Last changed    : 9/16/2021 6:35:25 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



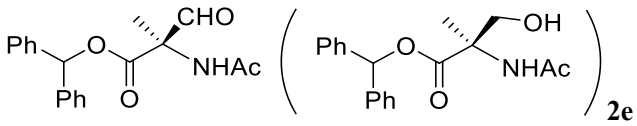

```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 D, Sig=230,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.721 BV    1.2304 1.90887e4   240.90775  49.3344
   2  17.852 VB    1.5025 1.96038e4   199.13431  50.6656

Totals :                  3.86925e4   440.04205
```

Data File d:\Chem32\...a\ZDQ\ZDQ-3-0303-2-1-1 2021-03-12 21-50-01\003-P2-A4-zdq-3-0303-1.D
Sample Name: zdq-3-0303-1

```
=====================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Acq. Instrument : 1290-DAD                      Location :   P2-A-04
Injection Date  : 3/12/2021 10:31:48 PM              Inj :   1
                                               Inj Volume : 1.000 µl
Acq. Method     : d:\Chem32\1\Data\ZDQ\ZDQ-3-0303-2-1-1 2021-03-12 21-50-01\OD-3-85-15-0.45-0
                  .5UL-30MIN-NO2.M
Last changed    : 3/12/2021 9:48:52 PM by SYSTEM
Analysis Method : d:\Chem32\1\Data\ZDQ\ZDQ-3-0303-2-1-1 2021-03-12 21-50-01\OD-3-85-15-0.45-0
                  .5UL-30MIN-NO2.M (Sequence Method)
Last changed    : 9/16/2021 6:35:25 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



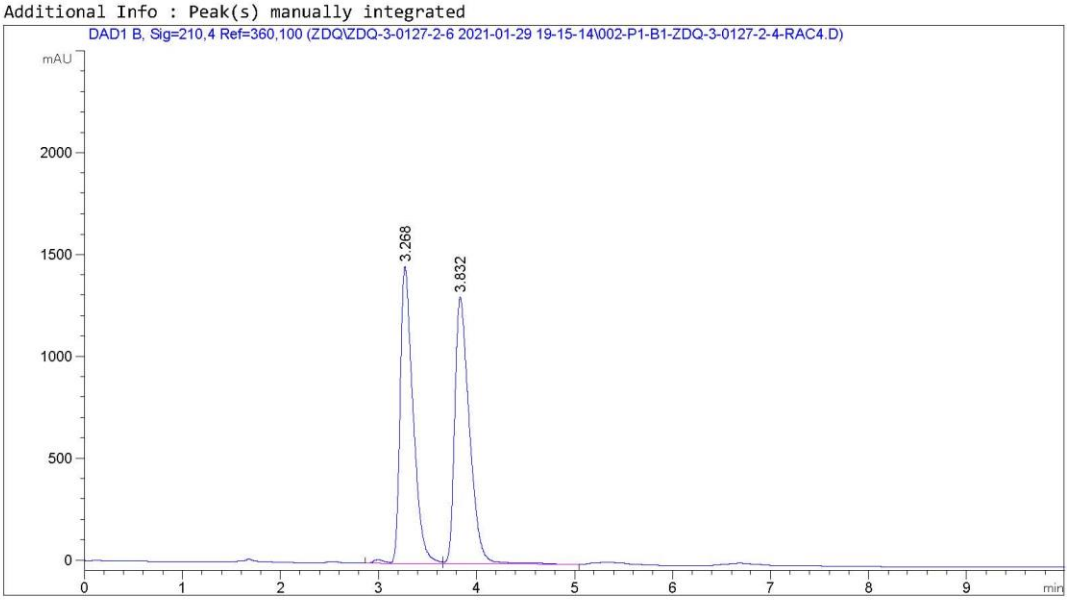

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 D, Sig=230,4 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.879 BB    1.1172 1306.08472   18.46432   6.5118
   2  17.504 BB    1.5370 1.87510e4   190.71869  93.4882

Totals :                  2.00571e4   209.18300
```



2e

Data File d:\Chem32\...\ZDQ-3-0127-2-6 2021-01-29 19-15-14\002-P1-B1-ZDQ-3-0127-2-4-RAC4.D
Sample Name: ZDQ-3-0127-2-4-RAC4

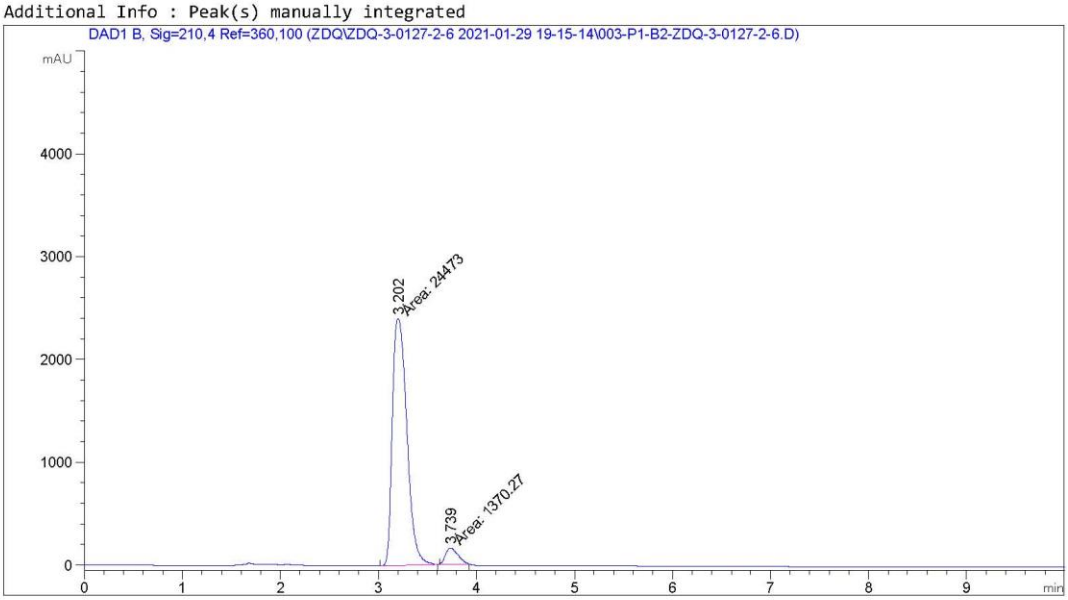
```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   2
    Acq. Instrument : 1290-DAD                       Location :   P1-B-01
    Injection Date  : 1/29/2021 7:21:37 PM               Inj :   1
                                                   Inj Volume : 1.000 µl
    Different Inj Volume from Sample Entry!  Actual Inj Volume : 0.500 µl
    Acq. Method     : d:\Chem32\1\Data\ZDQ\ZDQ-3-0127-2-6 2021-01-29 19-15-14\AD-3-80-20-0.4-1UL-
                      15MIN.M
    Last changed    : 1/29/2021 7:14:24 PM by SYSTEM
    Analysis Method : d:\Chem32\1\Data\ZDQ\ZDQ-3-0127-2-6 2021-01-29 19-15-14\AD-3-80-20-0.4-1UL-
                      15MIN.M (Sequence Method)
    Last changed    : 9/16/2021 6:23:12 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



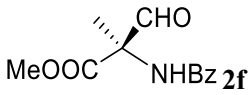

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 B, Sig=210,4 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   3.268 VV R  0.1337 1.33471e4  1459.26855  49.5824
       2   3.832 VV R  0.1542 1.35719e4  1309.95654  50.4176

    Totals :                  2.69190e4  2769.22510
```

Data File d:\Chem32\...a\ZDQ\ZDQ-3-0127-2-6 2021-01-29 19-15-14\003-P1-B2-ZDQ-3-0127-2-6.D
Sample Name: ZDQ-3-0127-2-6

```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   3
    Acq. Instrument : 1290-DAD                      Location :   P1-B-02
    Injection Date  : 1/29/2021 7:37:04 PM               Inj :   1
                                                   Inj Volume : 1.000 µl
    Different Inj Volume from Sample Entry!  Actual Inj Volume : 0.500 µl
    Acq. Method     : d:\Chem32\1\Data\ZDQ\ZDQ-3-0127-2-6 2021-01-29 19-15-14\AD-3-80-20-0.4-1UL-
                      15MIN.M
    Last changed    : 1/29/2021 7:14:24 PM by SYSTEM
    Analysis Method : d:\Chem32\1\Data\ZDQ\ZDQ-3-0127-2-6 2021-01-29 19-15-14\AD-3-80-20-0.4-1UL-
                      15MIN.M (Sequence Method)
    Last changed    : 9/16/2021 6:24:34 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



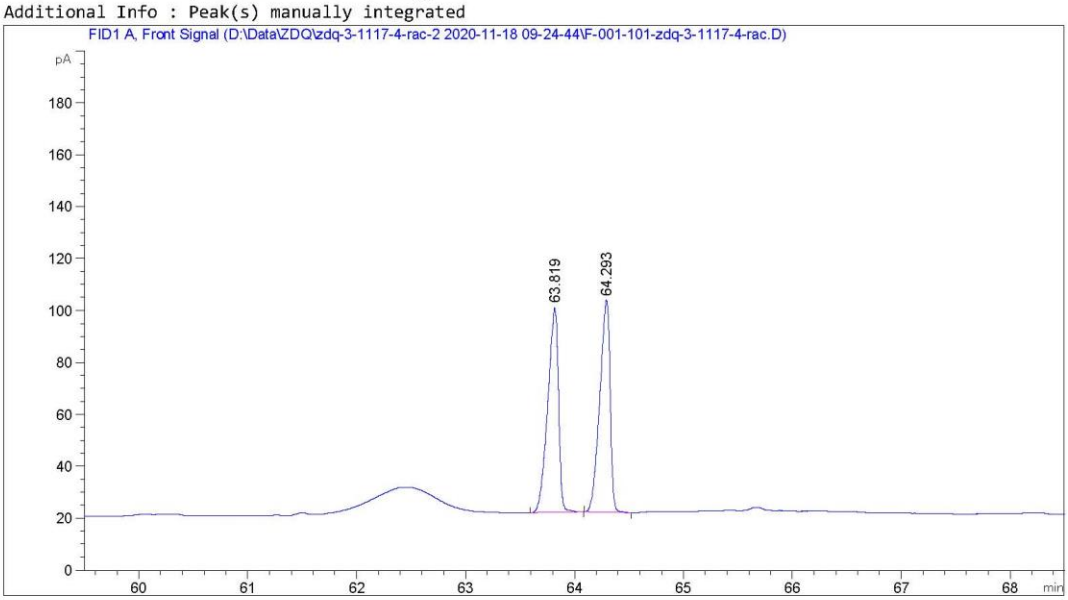

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 B, Sig=210,4 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   3.202 MM    0.1699 2.44730e4  2400.94482  94.6978
       2   3.739 MM    0.1443 1370.27063  158.24394   5.3022

    Totals :                  2.58432e4  2559.18877
```



2f

Data File D:\Data\ZDQ\zdq-3-1117-4-rac-2 2020-11-18 09-24-44\F-001-101-zdq-3-1117-4-rac.D
Sample Name: zdq-3-1117-4-rac

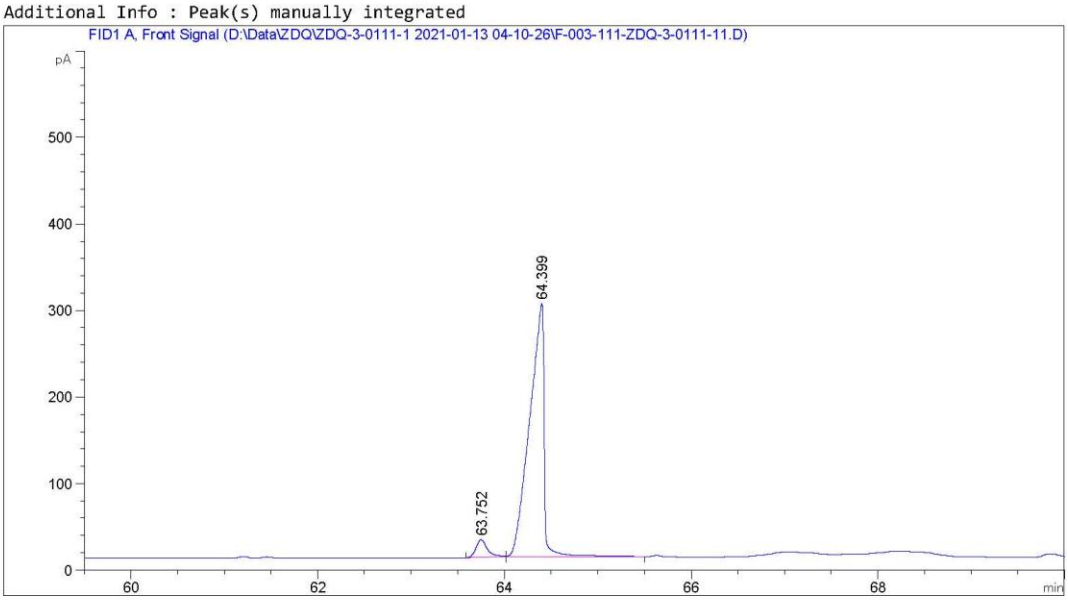
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   1
Acq. Instrument : GC7890B                       Location :   101  (F)
Injection Date  : 11/18/2020 9:26:42 AM              Inj :   1
                                               Inj Volume : 1 µl
Acq. Method     : D:\Data\ZDQ\zdq-3-1117-4-rac-2 2020-11-18 09-24-44\ZDQ-B-225-80-2-200-80min
                  .M
Last changed    : 11/18/2020 9:12:11 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\zdq-3-1117-4-rac-2 2020-11-18 09-24-44\ZDQ-B-225-80-2-200-80min
                  .M (Sequence Method)
Last changed    : 9/16/2021 4:38:30 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



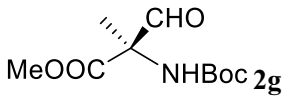

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  63.819 BB    0.0938  540.03967   79.00208 50.00649
   2  64.293 BB    0.0930  539.89960   81.76865 49.99351

Totals :                  1079.93927  160.77072
```

Data File D:\Data\ZDQ\ZDQ-3-0111-1 2021-01-13 04-10-26\F-003-111-ZDQ-3-0111-11.D
Sample Name: ZDQ-3-0111-11

```
==========================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Acq. Instrument : GC7890B                       Location :   111  (F)
Injection Date  : 1/13/2021 6:59:31 AM               Inj :   1
                                               Inj Volume : 1 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-3-0111-1 2021-01-13 04-10-26\ZDQ-B-225-80-2-200-80-1min.M
Last changed    : 1/13/2021 4:09:21 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\ZDQ-3-0111-1 2021-01-13 04-10-26\ZDQ-B-225-80-2-200-80-1min.M (
                  Sequence Method)
Last changed    : 9/16/2021 4:42:34 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



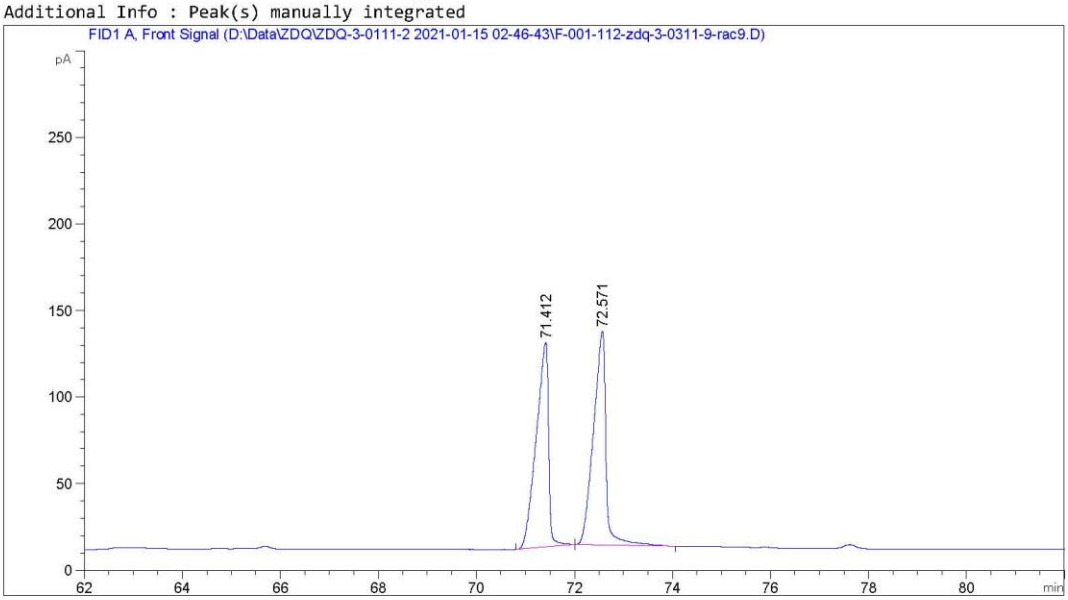

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  63.752 BB    0.1228  164.31439   20.21761  4.96064
   2  64.399 BB    0.1427 3148.04883  292.08099 95.03936

Totals :                  3312.36322  312.29861
```



2g

Data File D:\Data\ZDQ\ZDQ-3-0111-2 2021-01-15 02-46-43\F-001-112-zdq-3-0311-9-rac9.D
Sample Name: zdq-3-0311-9-rac9

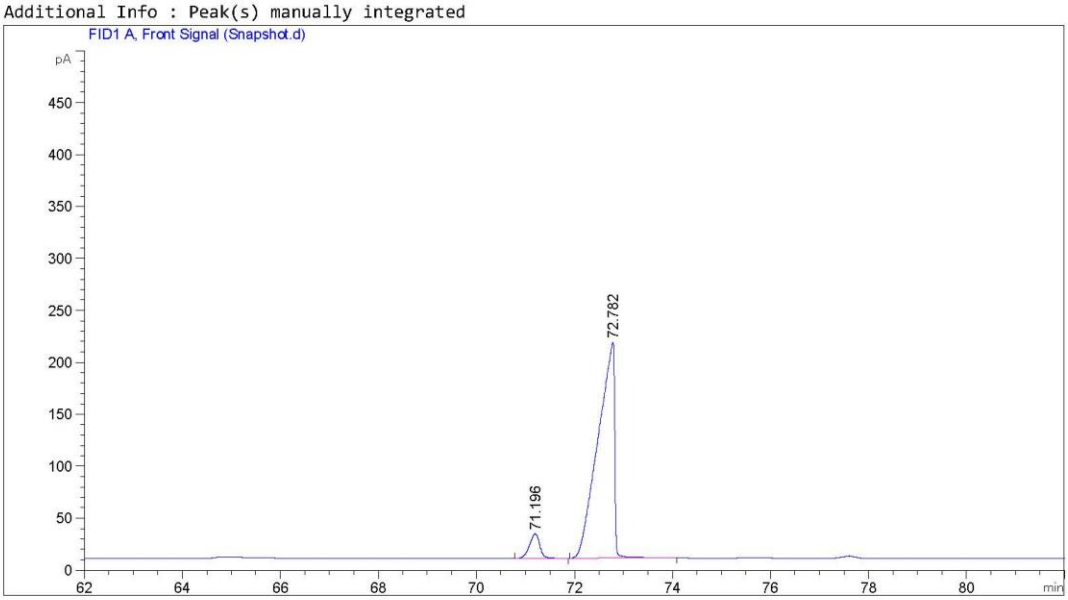
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   1
Acq. Instrument : GC7890B                       Location :   112  (F)
Injection Date  : 1/15/2021 2:48:48 AM               Inj :   1
                                               Inj Volume : 1 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-3-0111-2 2021-01-15 02-46-43\ZDQ-B-225-80-1-1-150-110min.M
Last changed    : 1/15/2021 2:47:50 AM by SYSTEM
                  (modified after loading)
Analysis Method : D:\Data\ZDQ\ZDQ-3-0111-2 2021-01-15 02-46-43\ZDQ-B-225-80-1-1-150-110min.M
                  (Sequence Method)
Last changed    : 9/16/2021 5:23:41 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



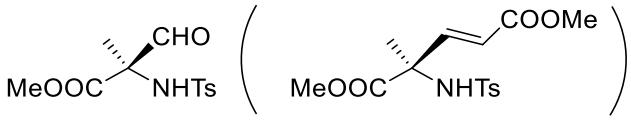

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  71.412 BB    0.2261 2078.12183  118.20456 48.60412
   2  72.571 BB    0.2297 2197.48682  123.42546 51.39588

Totals :                  4275.60864  241.63002
```

Data File C:\Chem32\1\Data\Snapshot.d
Sample Name:

```
=====================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   1
                                                 Location :   103
Injection Date  : 9/16/2021 4:05:50 AM               Inj :   1
Acq. Method     : ZDQ-B-225-80-1-1-130-210min.M
Analysis Method : D:\Data\ZDQ\ZDQ-3-0318-rac-1 2021-03-19 06-05-04\ZDQ-B-225-80-2-200-70min.M
                  (Sequence Method)
Last changed    : 9/16/2021 5:45:28 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



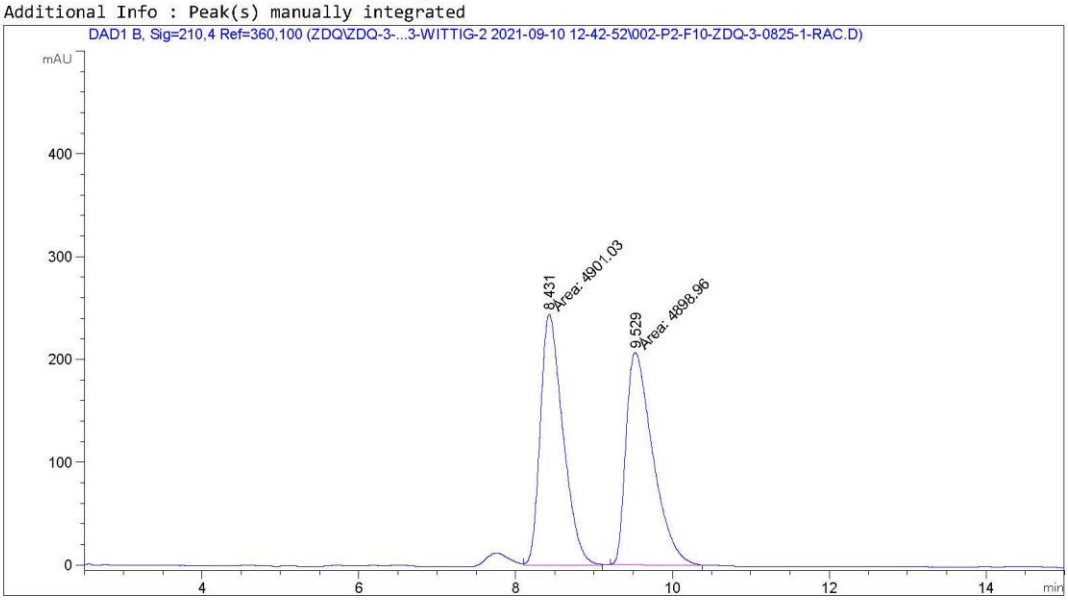

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  71.196 BB    0.1854  339.37476   23.65181  6.48488
   2  72.782 BB    0.2939 4893.94629  207.67484 93.51512

Totals :                  5233.32104  231.32665


=====================================================================
                        *** End of Report ***
```



2h

Data File d:\Chem32\...3-0905-3-WITTIG-2 2021-09-10 12-42-52\002-P2-F10-ZDQ-3-0825-1-RAC.D
Sample Name: ZDQ-3-0825-1-RAC

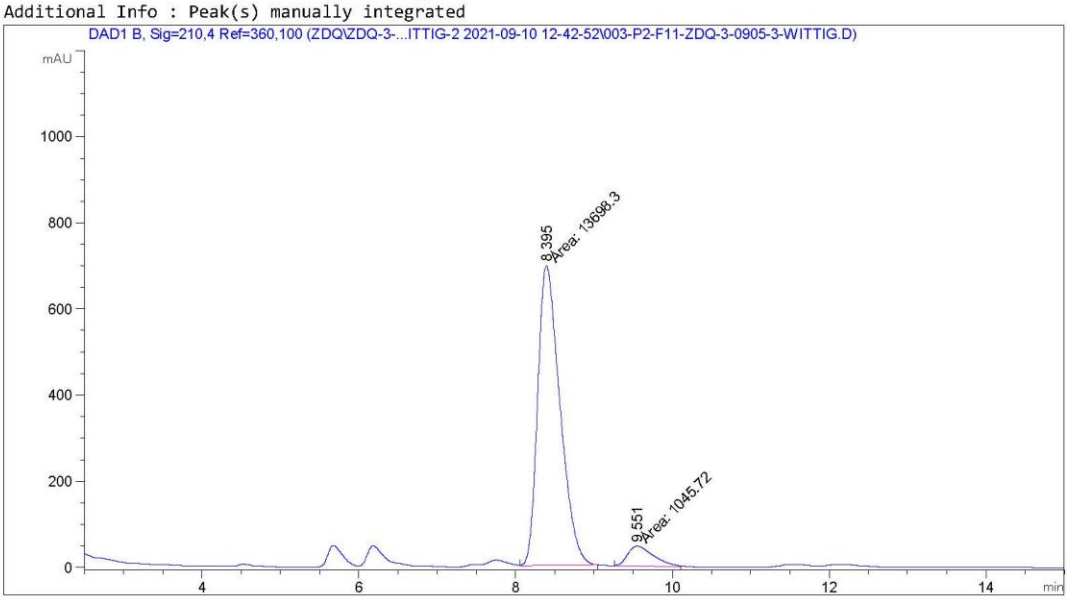
```
==================================================================
Acq. Operator   : SYSTEM                      Seq. Line :   2
Acq. Instrument : 1290-DAD                     Location :   P2-F-10
Injection Date  : 9/10/2021 12:49:14 PM             Inj :   1
                                             Inj Volume : 1.000 µl
Acq. Method     : d:\Chem32\1\Data\ZDQ\ZDQ-3-0905-3-WITTIG-2 2021-09-10 12-42-52\AD-3-85-15-0
                  .5-1UL-15MIN.M
Last changed    : 9/10/2021 11:28:24 AM by SYSTEM
Analysis Method : d:\Chem32\1\Data\ZDQ\ZDQ-3-0905-3-WITTIG-2 2021-09-10 12-42-52\AD-3-85-15-0
                  .5-1UL-15MIN.M (Sequence Method)
Last changed    : 11/9/2021 7:46:24 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



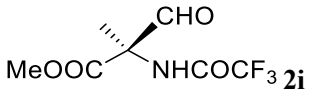

```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.431 MM    0.3345 4901.03467  244.17332  50.0106
   2   9.529 MM    0.3954 4898.95654  206.48215  49.9894

Totals :                  9799.99121  450.65547
```

Data File d:\Chem32\...905-3-WITTIG-2 2021-09-10 12-42-52\003-P2-F11-ZDQ-3-0905-3-WITTIG.D
Sample Name: ZDQ-3-0905-3-WITTIG

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Acq. Instrument : 1290-DAD                      Location :   P2-F-11
Injection Date  : 9/10/2021 1:04:40 PM               Inj :   1
                                               Inj Volume : 1.000 µl
Acq. Method     : d:\Chem32\1\Data\ZDQ\ZDQ-3-0905-3-WITTIG-2 2021-09-10 12-42-52\AD-3-85-15-0
                  .5-1UL-15MIN.M
Last changed    : 9/10/2021 11:28:24 AM by SYSTEM
Analysis Method : d:\Chem32\1\Data\ZDQ\ZDQ-3-0905-3-WITTIG-2 2021-09-10 12-42-52\AD-3-85-15-0
                  .5-1UL-15MIN.M (Sequence Method)
Last changed    : 11/9/2021 7:48:52 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



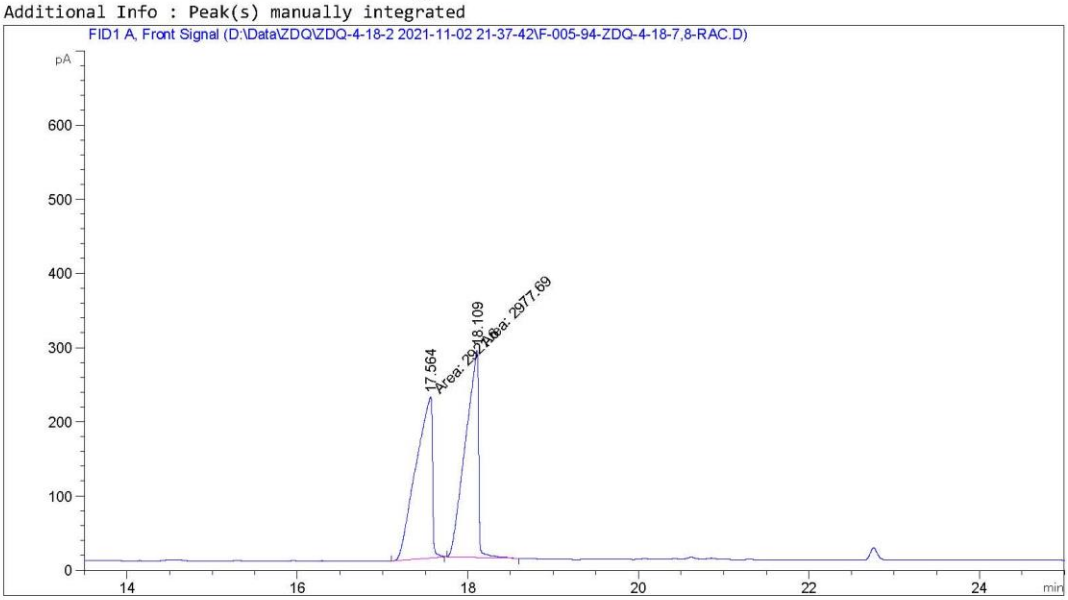

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.395 MM    0.3280 1.36983e4   696.11493  92.9075
   2   9.551 MM    0.3804 1045.71692   45.82208   7.0925

Totals :                  1.47440e4   741.93701
```



2i

Data File D:\Data\ZDQ\ZDQ-4-18-2 2021-11-02 21-37-42\F-005-94-ZDQ-4-18-7,8-RAC.D
Sample Name: ZDQ-4-18-7,8-RAC

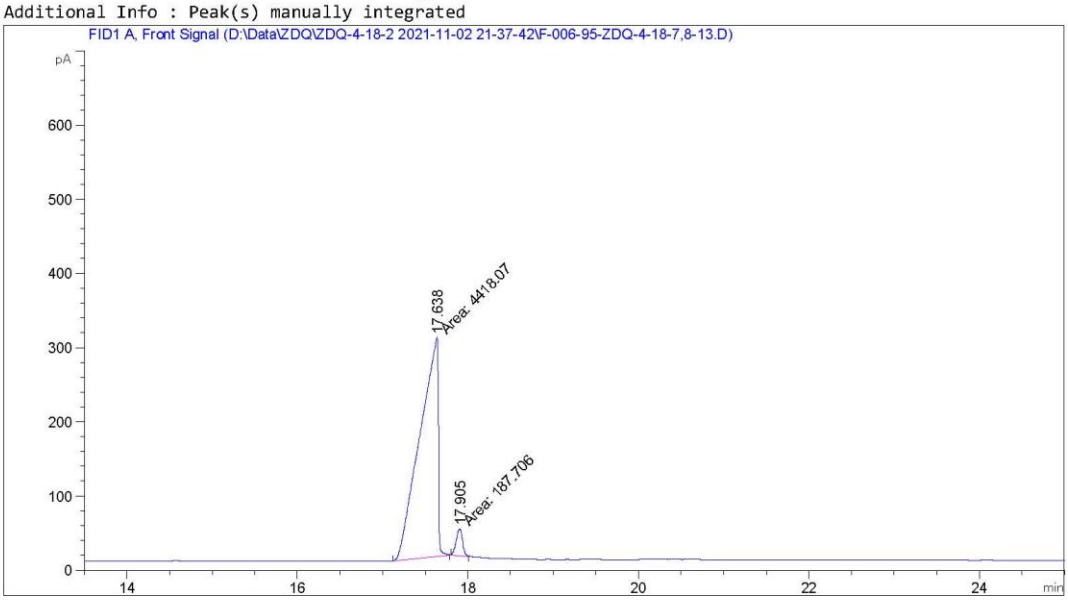
```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   5
Acq. Instrument : GC7890B                        Location :   94  (F)
Injection Date  : 11/3/2021 1:13:58 AM               Inj :   1
                                                Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-4-18-2 2021-11-02 21-37-42\ZDQ-B-225-80-2-210-90min.M
Last changed    : 10/22/2021 9:14:14 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\ZDQ-4-18-2 2021-11-02 21-37-42\ZDQ-B-225-80-2-210-90min.M (
                  Sequence Method)
Last changed    : 11/9/2021 7:00:33 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



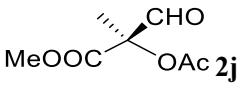

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]         %
----|-------|----|-------|----------|----------|--------|
   1  17.564 MM    0.2242 2921.60132  217.16211 49.52460
   2  18.109 MM    0.1774 2977.69238  279.69171 50.47540

Totals :                  5899.29370  496.85382
```

Data File D:\Data\ZDQ\ZDQ-4-18-2 2021-11-02 21-37-42\F-006-95-ZDQ-4-18-7,8-13.D
Sample Name: ZDQ-4-18-7,8-13

```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   6
    Acq. Instrument : GC7890B                        Location :   95  (F)
    Injection Date  : 11/3/2021 2:47:36 AM               Inj :   1
                                                   Inj Volume : 1 µl
    Different Inj Volume from Sample Entry!  Actual Inj Volume : 3 µl
    Acq. Method     : D:\Data\ZDQ\ZDQ-4-18-2 2021-11-02 21-37-42\ZDQ-B-225-80-2-210-90min.M
    Last changed    : 10/22/2021 9:14:14 AM by SYSTEM
    Analysis Method : D:\Data\ZDQ\ZDQ-4-18-2 2021-11-02 21-37-42\ZDQ-B-225-80-2-210-90min.M (
                      Sequence Method)
    Last changed    : 11/9/2021 6:57:57 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



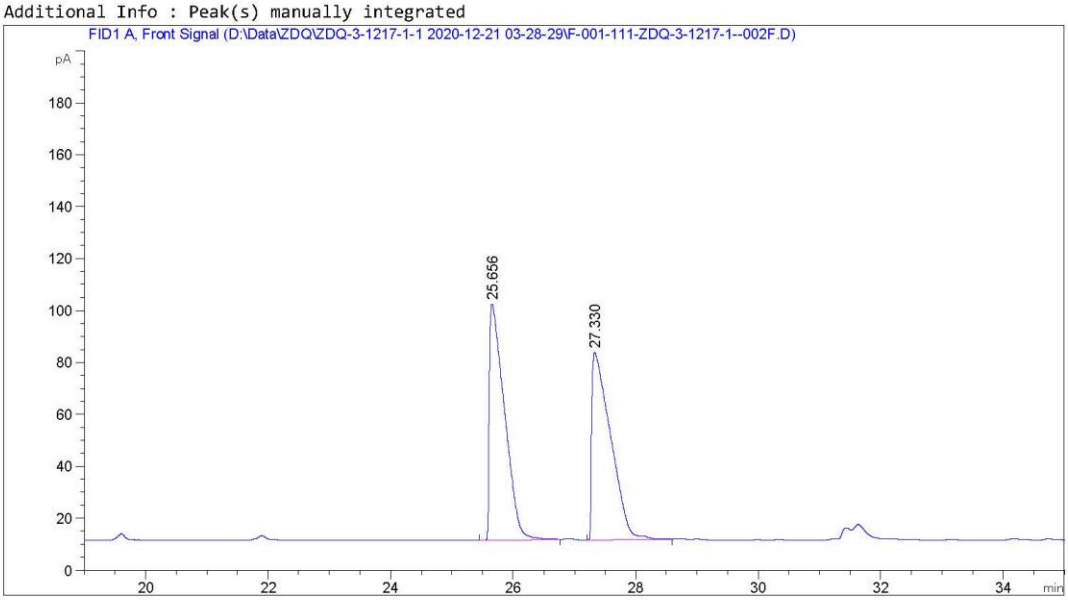

```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: FID1 A, Front Signal

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [pA*s]      [pA]        %
    ----|-------|----|-------|----------|----------|--------|
       1  17.638 MM    0.2495 4418.07178  295.07874 95.92455
       2  17.905 MM    0.0852  187.70630   36.72895  4.07545

    Totals :                  4605.77808  331.80768
```



2j

Data File D:\Data\ZDQ\ZDQ-3-1217-1-1 2020-12-21 03-28-29\F-001-111-ZDQ-3-1217-1--002F.D
Sample Name: RAC

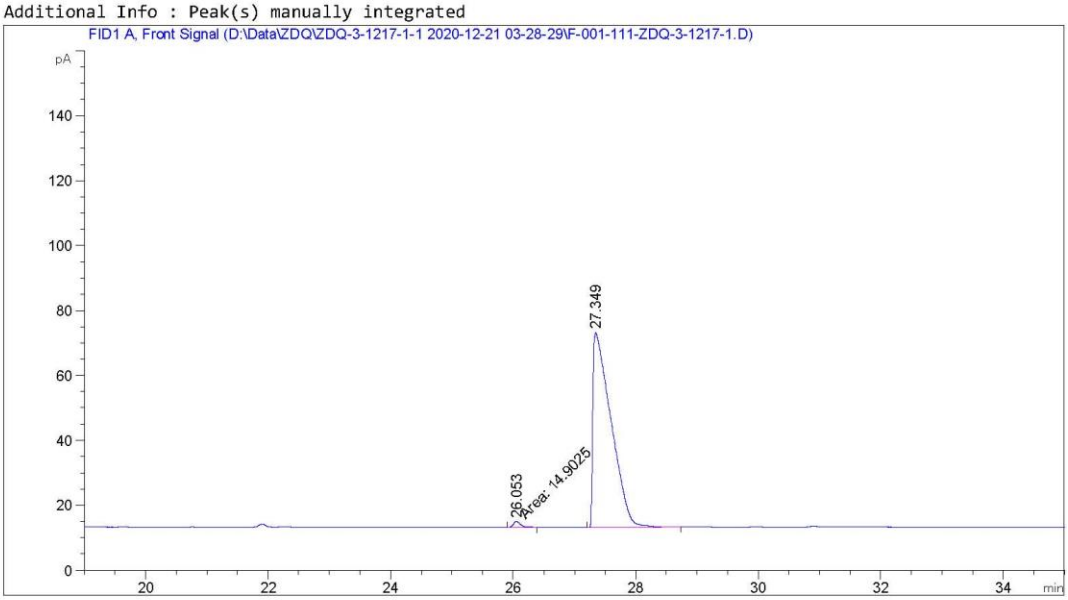
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   2
Acq. Instrument : GC7890B                      Location :   112  (F)
Injection Date  : 12/21/2020 5:03:33 AM             Inj :   1
                                              Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-3-1217-1-1 2020-12-21 03-28-29\ZDQ-B-225-80-1-150-80min.M
Last changed    : 12/21/2020 5:06:30 AM by SYSTEM
                  (modified after loading)
Analysis Method : D:\Data\ZDQ\ZDQ-3-1217-1-1 2020-12-21 03-28-29\ZDQ-B-225-80-1-150-80min.M (
                  Sequence Method)
Last changed    : 9/16/2021 5:34:30 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



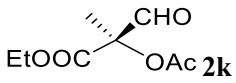

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  25.656 BB    0.2237 1556.80664   90.94520 50.28106
   2  27.330 BB    0.2695 1539.40234   72.26604 49.71894

Totals :                  3096.20898  163.21124
```

Data File D:\Data\ZDQ\ZDQ-3-1217-1-1 2020-12-21 03-28-29\F-001-111-ZDQ-3-1217-1.D
Sample Name: ZDQ-3-1217-1

```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   1
    Acq. Instrument : GC7890B                        Location :   111  (F)
    Injection Date  : 12/21/2020 3:30:28 AM               Inj :   1
                                                   Inj Volume : 1 µl
    Different Inj Volume from Sample Entry!  Actual Inj Volume : 3 µl
    Acq. Method     : D:\Data\ZDQ\ZDQ-3-1217-1-1 2020-12-21 03-28-29\ZDQ-B-225-80-1-150-80min.M
    Last changed    : 12/21/2020 5:00:13 AM by SYSTEM
                      (modified after loading)
    Analysis Method : D:\Data\ZDQ\ZDQ-3-1217-1-1 2020-12-21 03-28-29\ZDQ-B-225-80-1-150-80min.M (
                      Sequence Method)
    Last changed    : 9/16/2021 5:36:23 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



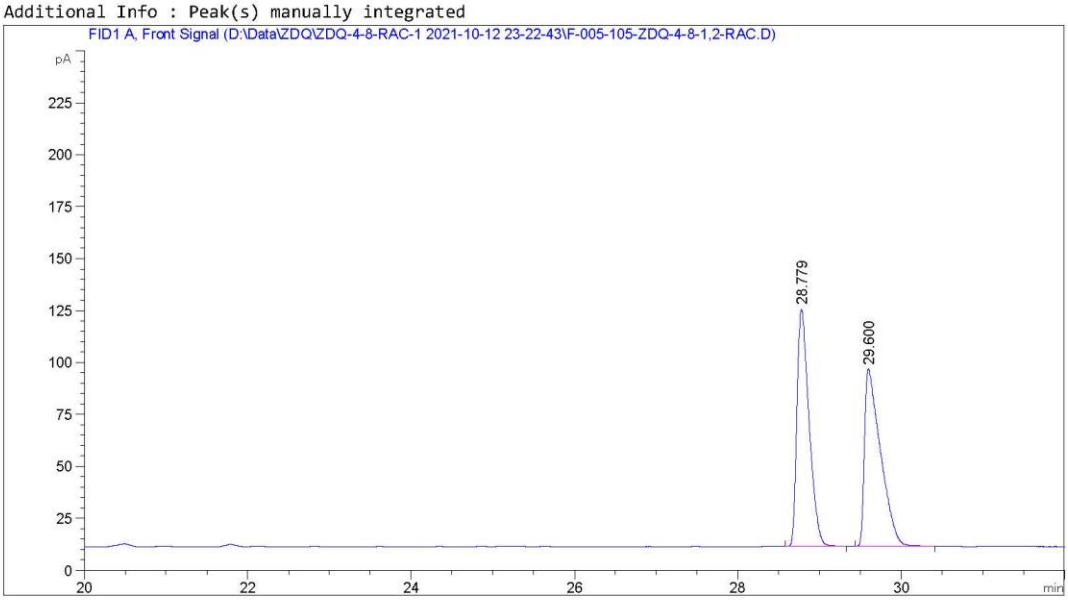

```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: FID1 A, Front Signal

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [pA*s]      [pA]        %
    ----|-------|----|-------|----------|----------|--------|
       1  26.053 MM    0.1377   14.90253    1.80415  1.19459
       2  27.349 BB    0.2634 1232.59705   60.05963 98.80541

    Totals :                  1247.49957   61.86378
```



2k

Data File D:\Data\ZDQ\ZDQ-4-8-RAC-1 2021-10-12 23-22-43\F-005-105-ZDQ-4-8-1,2-RAC.D
Sample Name: ZDQ-4-8-1,2-RAC

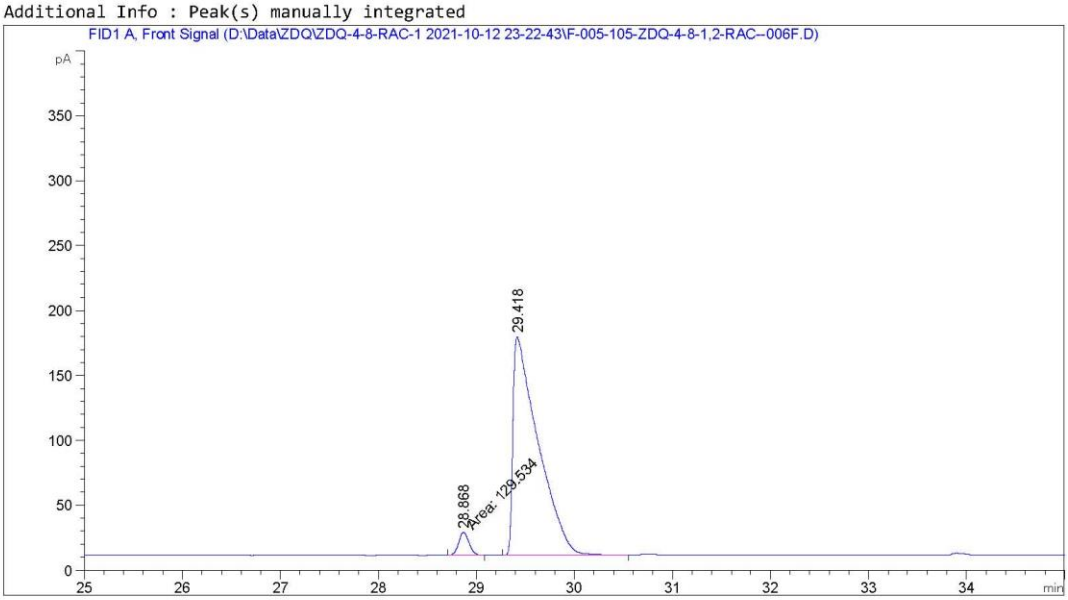
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   5
Acq. Instrument : GC7890B                       Location :   105  (F)
Injection Date  : 10/13/2021 8:46:58 AM              Inj :   1
                                               Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 3 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-4-8-RAC-1 2021-10-12 23-22-43\ZDQ-B-225-80-1-210-155min.M
Last changed    : 10/13/2021 9:27:22 AM by SYSTEM
                  (modified after loading)
Analysis Method : D:\Data\ZDQ\ZDQ-4-8-RAC-1 2021-10-12 23-22-43\ZDQ-B-225-80-1-210-155min.M (
                  Sequence Method)
Last changed    : 11/9/2021 6:48:12 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



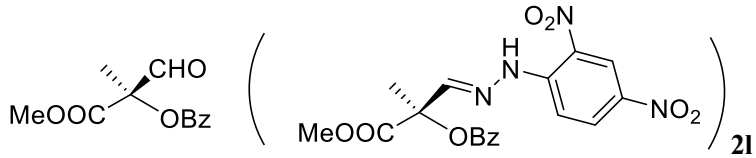

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  28.779 BB    0.1454 1169.79016  114.31574 50.21287
   2  29.600 BB    0.1805 1159.87207   85.36095 49.78713

Totals :                  2329.66223  199.67670
```

Data File D:\Data\ZDQ\ZDQ-4-8-RAC-1 2021-10-12 23-22-43\F-005-105-ZDQ-4-8-1,2-RAC--006F.D
Sample Name: ZDQ-4-8-3

```
=====================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   6
Acq. Instrument : GC7890B                        Location :   106  (F)
Injection Date  : 10/13/2021 9:53:58 AM               Inj :   1
                                                Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 3 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-4-8-RAC-1 2021-10-12 23-22-43\ZDQ-B-225-80-1-210-155min.M
Last changed    : 10/13/2021 10:00:54 AM by SYSTEM
                  (modified after loading)
Analysis Method : D:\Data\ZDQ\ZDQ-4-8-RAC-1 2021-10-12 23-22-43\ZDQ-B-225-80-1-210-155min.M (
                  Sequence Method)
Last changed    : 11/9/2021 6:49:49 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



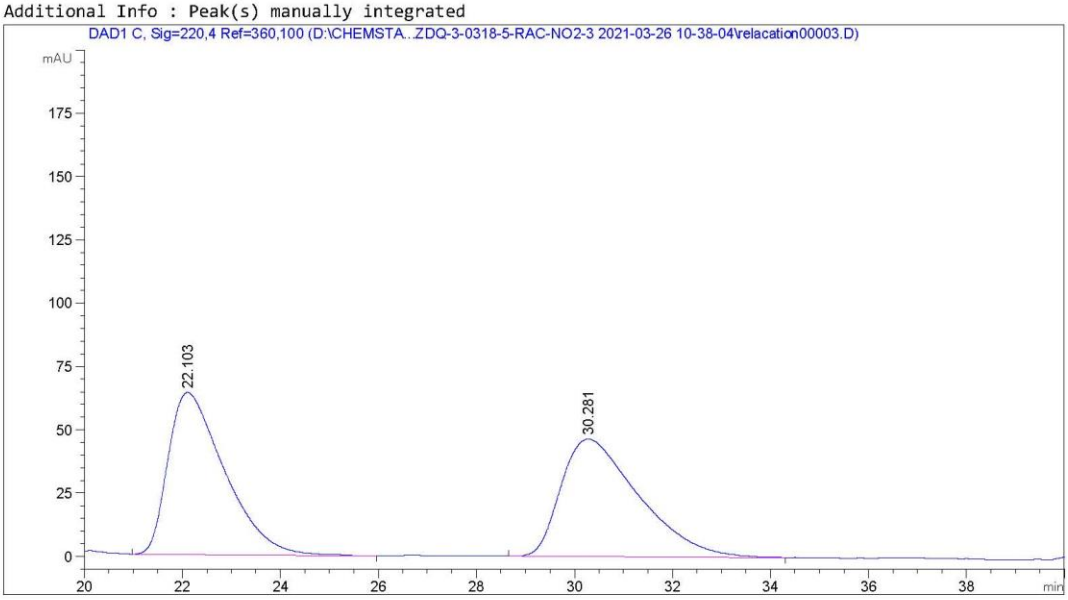

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  28.868 MM    0.1219  129.53400   17.70324  4.16593
   2  29.418 BB    0.2260 2979.83472  167.96803 95.83407

Totals :                  3109.36871  185.67127
```



2l

Data File D:\CHEMSTA...AC-NO2\ZDQ-3-0318-5-RAC-NO2-3 2021-03-26 10-38-04\relacation00003.D
Sample Name: ZDQ-3-0318-5-RAC

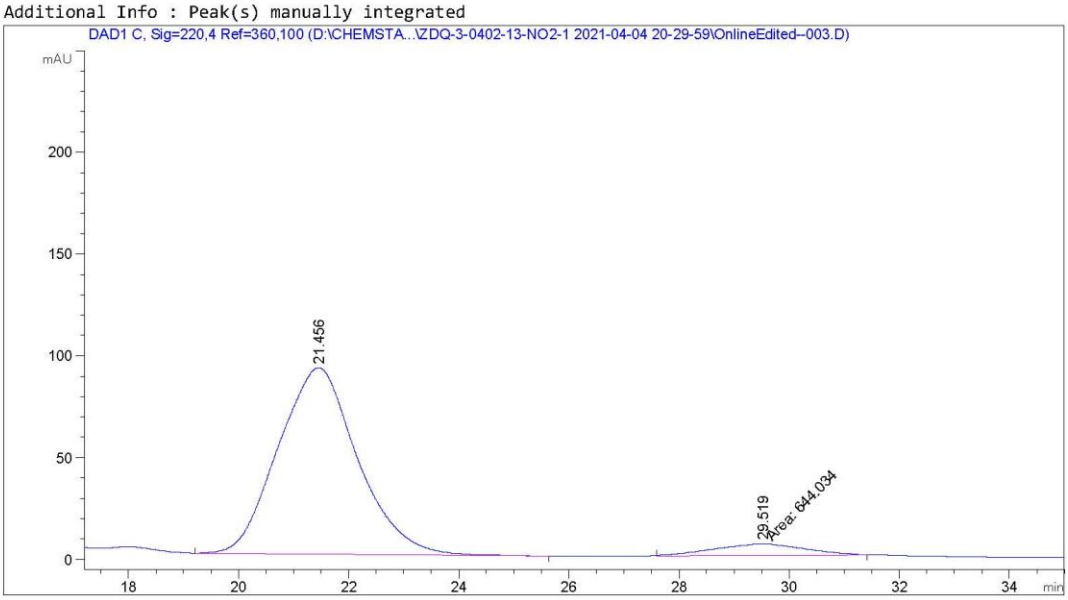
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   3
Sample Operator : SYSTEM
Acq. Instrument : LC                           Location :   P2-F-01
Injection Date  : 3/26/2021 11:30:19 AM             Inj :   1
                                              Inj Volume : 0.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 6.000 µl
Acq. Method     : D:\ChemStation\1\Data\YC\ZDQ-3-0318-5-RAC-NO2\ZDQ-3-0318-5-RAC-NO2-3 2021-
                  03-26 10-38-04\4-AS3-85-15-1ml-40min.M
Last changed    : 9/19/2019 7:49:52 PM by SYSTEM
Analysis Method : D:\ChemStation\1\Data\YC\ZDQ-3-0318-5-RAC-NO2\ZDQ-3-0318-5-RAC-NO2-3 2021-
                  03-26 10-38-04\4-AS3-85-15-1ml-40min.M (Sequence Method)
Last changed    : 9/16/2021 7:08:25 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



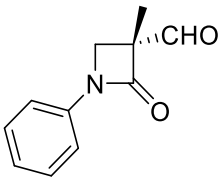

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 C, Sig=220,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  22.103 BB    1.1712 5124.48682   63.92703  50.1571
   2  30.281 BB    1.5572 5092.38965   46.37289  49.8429
```

Data File D:\CHEMSTA...-13-NO2\ZDQ-3-0402-13-NO2-1 2021-04-04 20-29-59\OnlineEdited--003.D
Sample Name: ZDQ-3-0402-13-NO2

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Sample Operator : SYSTEM
Acq. Instrument : LC                           Location :   P2-F-02
Injection Date  : 4/4/2021 9:19:37 PM               Inj :   1
                                              Inj Volume : 0.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 20.000 µl
Acq. Method     : D:\ChemStation\1\Data\YC\ZDQ-3-0402-13-NO2\ZDQ-3-0402-13-NO2-1 2021-04-04
                  20-29-59\4-AS3-85-15-1ml-40min.M
Last changed    : 4/4/2021 9:18:37 PM by SYSTEM
Analysis Method : D:\ChemStation\1\Data\YC\ZDQ-3-0402-13-NO2\ZDQ-3-0402-13-NO2-1 2021-04-04
                  20-29-59\4-AS3-85-15-1ml-40min.M (Sequence Method)
Last changed    : 9/16/2021 7:01:19 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



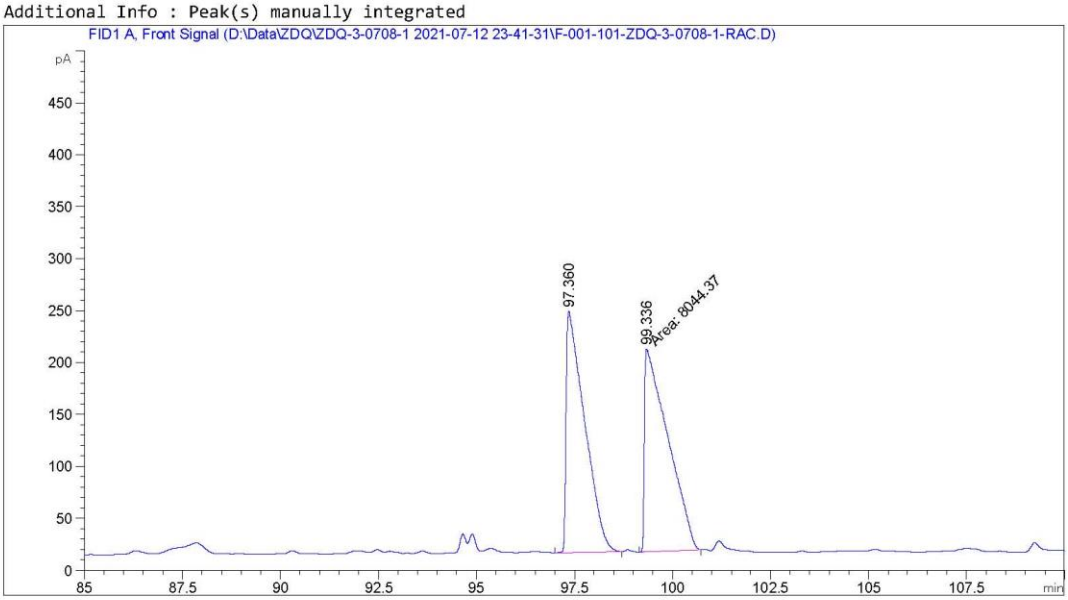

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 C, Sig=220,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  21.456 BB    1.4230 9159.53418   91.56680  93.4306
   2  29.519 MM    1.8729  644.03430    5.73108   6.5694
```



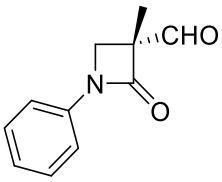
2m

Data File D:\Data\ZDQ\ZDQ-3-0708-1 2021-07-12 23-41-31\F-001-101-ZDQ-3-0708-1-RAC.D
Sample Name: ZDQ-3-0708-1-RAC

```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   1
Acq. Instrument : GC7890B                       Location :   101  (F)
Injection Date  : 7/12/2021 11:43:35 PM              Inj :   1
                                               Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-3-0708-1 2021-07-12 23-41-31\ZDQ-B-225-80-1-190--25-140min.
                  M
Last changed    : 7/12/2021 11:38:00 PM by SYSTEM
Analysis Method : D:\Data\ZDQ\ZDQ-3-0708-1 2021-07-12 23-41-31\ZDQ-B-225-80-1-190--25-140min.
                  M (Sequence Method)
Last changed    : 9/16/2021 4:56:54 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



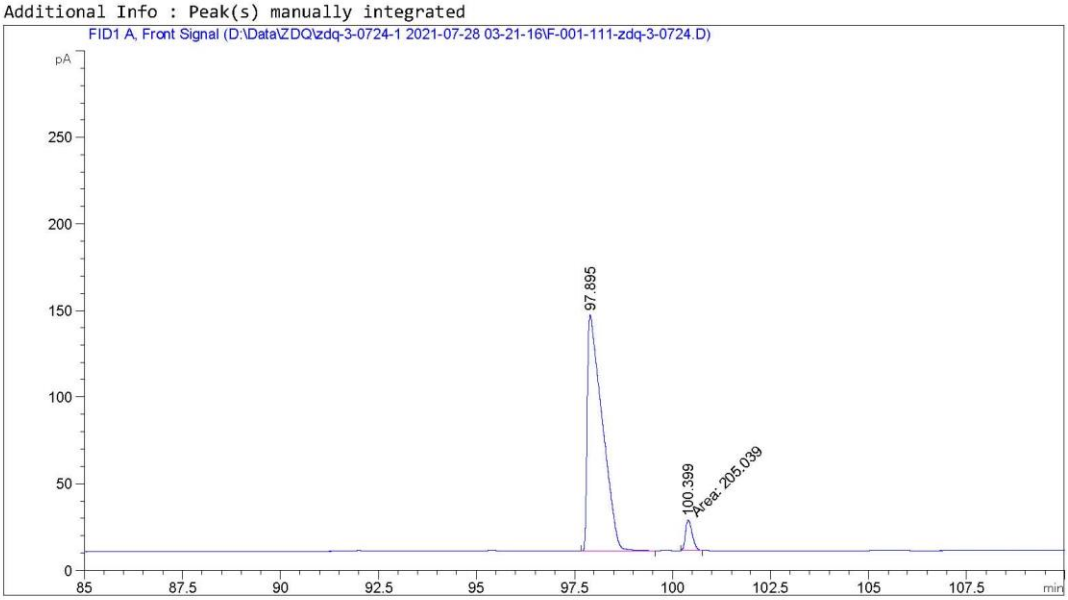

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  97.360 BB    0.3920 7589.47900  232.39511 48.54518
   2  99.336 MM    0.6873 8044.36621  195.07829 51.45482

Totals :                  1.56338e4   427.47340
```



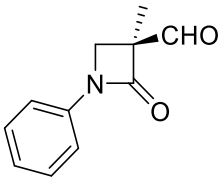
2m with (*R,S*)-DTBM-Bn-YanPhos

Data File D:\Data\ZDQ\zdq-3-0724-1 2021-07-28 03-21-16\F-001-111-zdq-3-0724.D
Sample Name: zdq-3-0724

```
=====================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   1
Acq. Instrument : GC7890B                       Location :   111  (F)
Injection Date  : 7/28/2021 3:23:20 AM               Inj :   1
                                                Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 2 µl
Acq. Method     : D:\Data\ZDQ\zdq-3-0724-1 2021-07-28 03-21-16\ZDQ-B-225-80-1-190--25-140min.
                  M
Last changed    : 7/28/2021 3:14:18 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\zdq-3-0724-1 2021-07-28 03-21-16\ZDQ-B-225-80-1-190--25-140min.
                  M (Sequence Method)
Last changed    : 9/16/2021 5:06:14 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



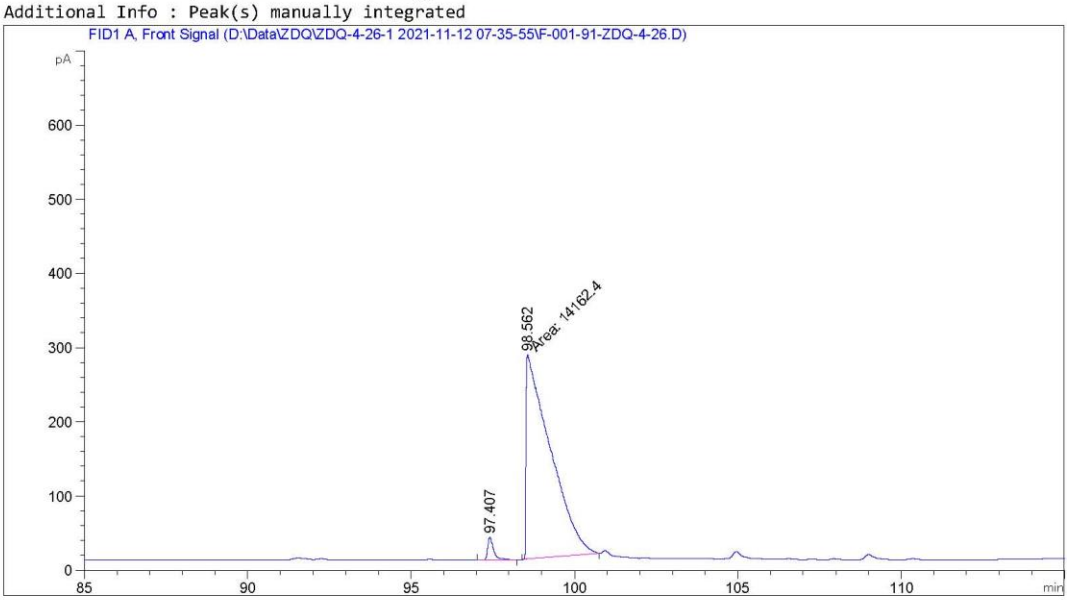

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  97.895 BB    0.3129 3609.92212  136.35985 94.62541
   2 100.399 MM    0.1954  205.03851   17.48654  5.37459

Totals :                  3814.96063  153.84639
```



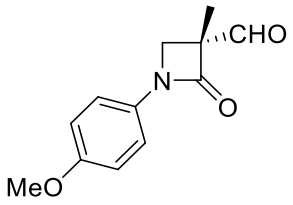
2m with (*R,R*)-Ph-BPE

Data File D:\Data\ZDQ\ZDQ-4-26-1 2021-11-12 07-35-55\F-001-91-ZDQ-4-26.D
Sample Name: ZDQ-4-26

```
=====================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   1
Acq. Instrument : GC7890B                         Location :   91  (F)
Injection Date  : 11/12/2021 7:43:05 AM               Inj :   1
                                                 Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-4-26-1 2021-11-12 07-35-55\ZDQ-B-225-80-1-210-155min.M
Last changed    : 8/18/2021 8:34:44 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\ZDQ-4-26-1 2021-11-12 07-35-55\ZDQ-B-225-80-1-210-155min.M (
                  Sequence Method)
Last changed    : 11/12/2021 8:12:20 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



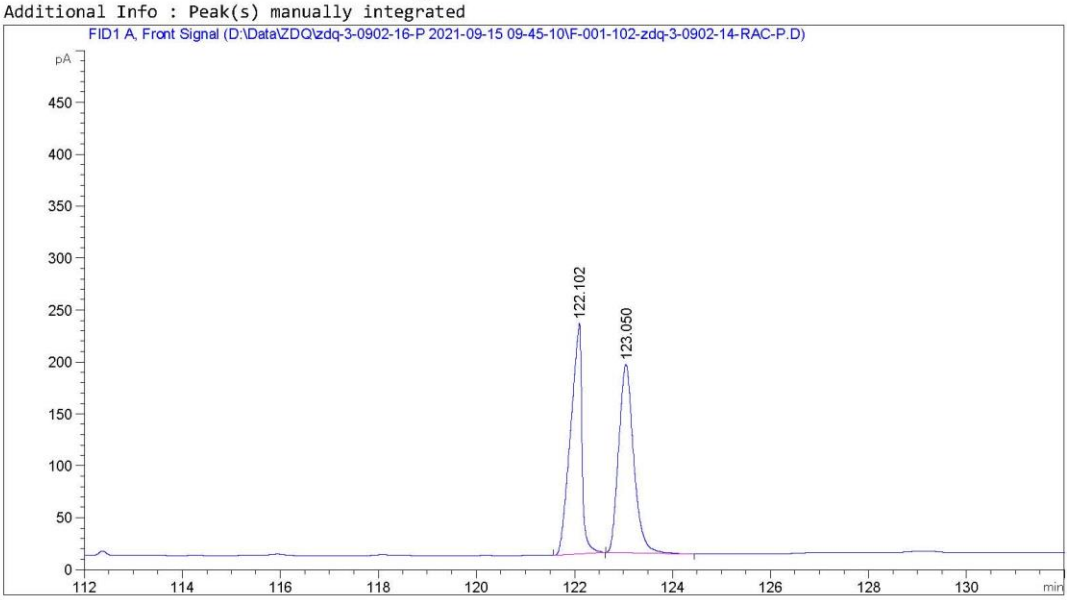

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  97.407 BB    0.1738  377.32901   30.61825  2.59516
   2  98.562 MM    0.8578 1.41624e4   275.17197 97.40484

Totals :                  1.45397e4   305.79022
```



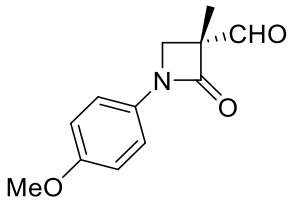
2n

Data File D:\Data\ZDQ\zdq-3-0902-16-P 2021-09-15 09-45-10\F-001-102-zdq-3-0902-14-RAC-P.D
Sample Name: zdq-3-0902-14-RAC-P

```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   1
    Acq. Instrument : GC7890B                        Location :   102  (F)
    Injection Date  : 9/15/2021 9:47:09 AM                Inj :   1
                                                   Inj Volume : 1 µl
    Different Inj Volume from Sample Entry!  Actual Inj Volume : 3 µl
    Acq. Method     : D:\Data\ZDQ\zdq-3-0902-16-P 2021-09-15 09-45-10\ZDQ-B-225-80-1-210-155min.M
    Last changed    : 8/18/2021 8:34:44 AM by SYSTEM
    Analysis Method : D:\Data\ZDQ\zdq-3-0902-16-P 2021-09-15 09-45-10\ZDQ-B-225-80-1-210-155min.M
                      (Sequence Method)
    Last changed    : 9/16/2021 5:17:23 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



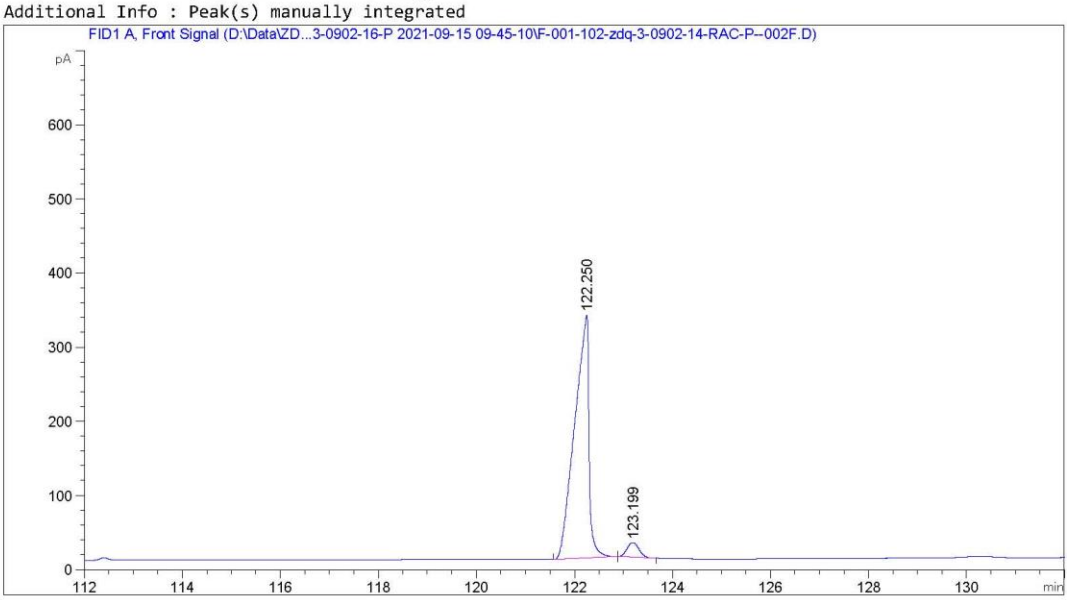

```
    ======================================================================
                           Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: FID1 A, Front Signal

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [pA*s]      [pA]        %
    ----|-------|----|-------|----------|----------|--------|
       1 122.102 BB    0.2073 3570.20654  222.35925 48.04352
       2 123.050 BB    0.2559 3860.98560  181.69611 51.95648

    Totals :                  7431.19214  404.05536
```



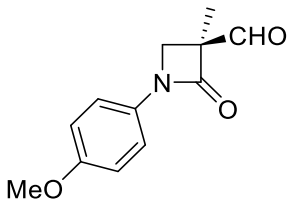
2n with (*R,S*)-DTBM-Bn-YanPhos

Data File D:\Data\ZD...0902-16-P 2021-09-15 09-45-10\F-001-102-zdq-3-0902-14-RAC-P--002F.D
Sample Name: zdq-3-0902-16-P16

```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   2
Acq. Instrument : GC7890B                      Location :   103  (F)
Injection Date  : 9/15/2021 12:25:58 PM             Inj :   1
                                               Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5 µl
Acq. Method     : D:\Data\ZDQ\zdq-3-0902-16-P 2021-09-15 09-45-10\ZDQ-B-225-80-1-210-155min.M
Last changed    : 8/18/2021 8:34:44 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\zdq-3-0902-16-P 2021-09-15 09-45-10\ZDQ-B-225-80-1-210-155min.M
                  (Sequence Method)
Last changed    : 9/16/2021 5:18:42 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

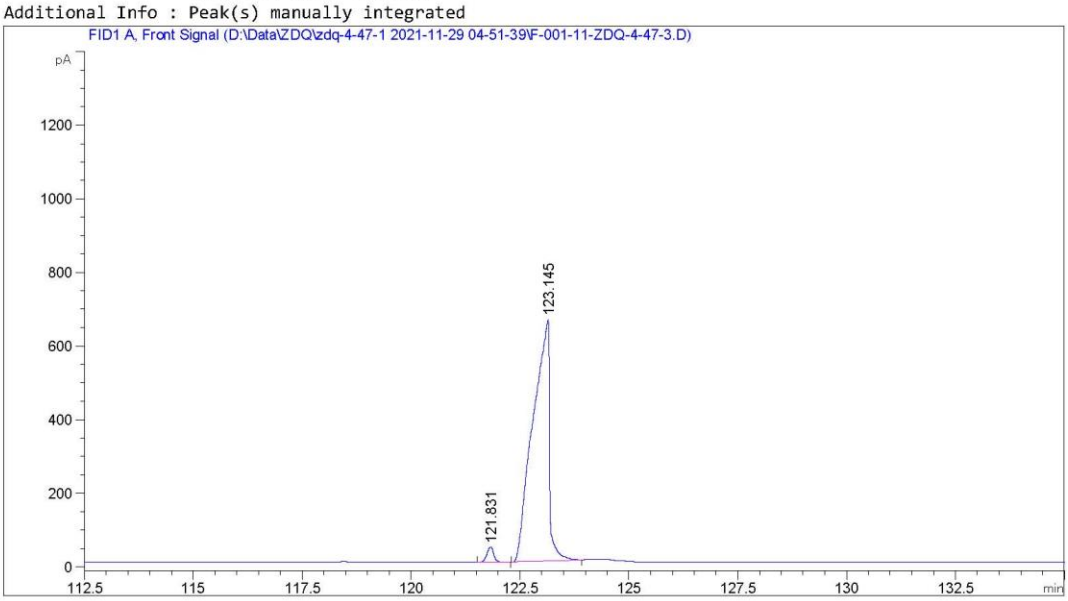



```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1 122.250 BB    0.2589 6672.19580  327.15692 95.26250
   2 123.199 BB    0.2045  331.81476   19.50583  4.73750

Totals :                  7004.01056  346.66275
```

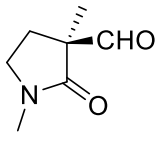


2n with (*R,R*)-Ph-BPE

```
Data File D:\Data\ZDQ\zdq-4-47-1 2021-11-29 04-51-39\F-001-11-ZDQ-4-47-3.D
Sample Name: ZDQ-4-47-3

    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   1
    Acq. Instrument : GC7890B                       Location :   11  (F)
    Injection Date  : 11/29/2021 4:53:42 AM              Inj :   1
                                                   Inj Volume : 1 µl
    Different Inj Volume from Sample Entry!  Actual Inj Volume : 2 µl
    Acq. Method     : D:\Data\ZDQ\zdq-4-47-1 2021-11-29 04-51-39\ZDQ-B-225-80-1-210-155min.M
    Last changed    : 11/29/2021 5:35:47 AM by SYSTEM
                      (modified after loading)
    Analysis Method : D:\Data\ZDQ\zdq-4-47-1 2021-11-29 04-51-39\ZDQ-B-225-80-1-210-155min.M (
                      Sequence Method)
    Last changed    : 12/14/2021 9:37:51 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



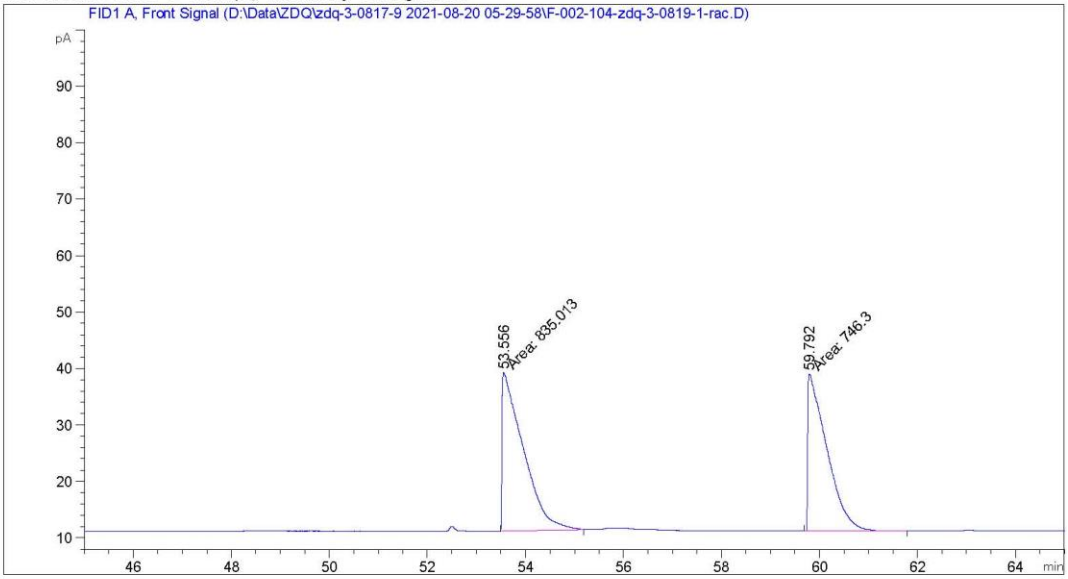

```
    ======================================================================
                              Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: FID1 A, Front Signal

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [pA*s]      [pA]        %
    ----|-------|----|-------|----------|----------|--------|
       1 121.831 BB    0.1605  444.79199   41.34258  2.48704
       2 123.145 BB    0.3220 1.74396e4   656.34039 97.51296

    Totals :                  1.78844e4   697.68297

GC7890B 12/14/2021 9:38:15 PM SYSTEM                          Page   1 of 2
```



2o

Data File D:\Data\ZDQ\zdq-3-0817-9 2021-08-20 05-29-58\F-002-104-zdq-3-0819-1-rac.D
Sample Name: zdq-3-0819-1-rac

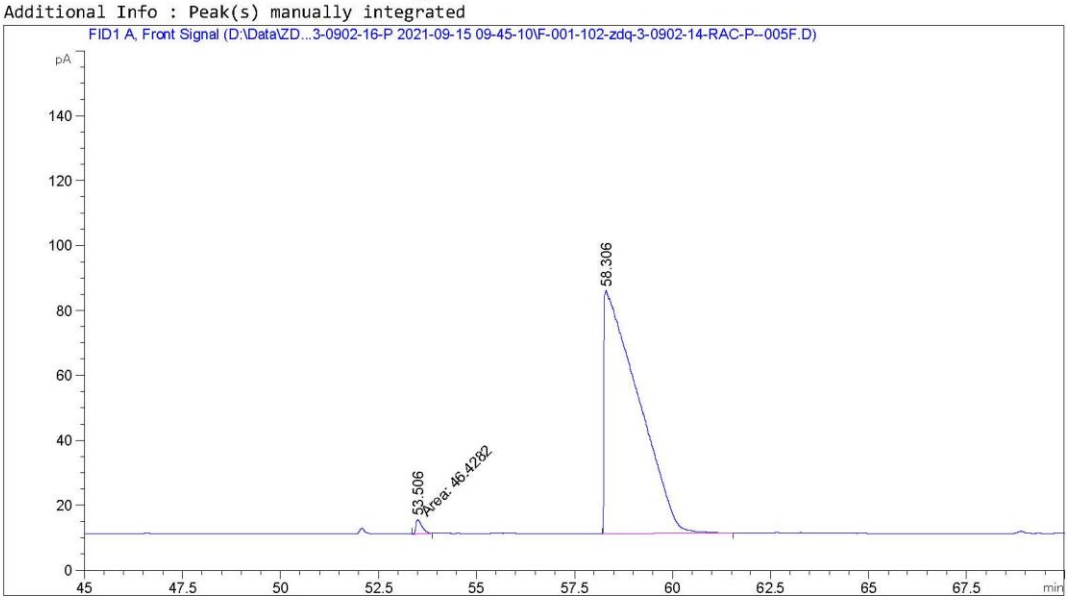
```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : GC7890B                       Location :   104  (F)
Injection Date  : 8/20/2021 8:11:36 AM               Inj :   1
                                               Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 2 µl
Acq. Method     : D:\Data\ZDQ\zdq-3-0817-9 2021-08-20 05-29-58\ZDQ-B-225-80-1-210-155min.M
Last changed    : 8/18/2021 8:34:44 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\zdq-3-0817-9 2021-08-20 05-29-58\ZDQ-B-225-80-1-210-155min.M (
                  Sequence Method)
Last changed    : 9/16/2021 5:12:49 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



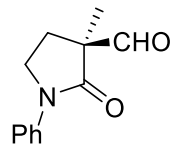

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  53.556 MM    0.4972  835.01349   27.99298 52.80507
   2  59.792 MM    0.4483  746.29968   27.74577 47.19493

Totals :                  1581.31317   55.73874
```

Data File D:\Data\ZD...0902-16-P 2021-09-15 09-45-10\F-001-102-zdq-3-0902-14-RAC-P--005F.D
Sample Name: zdq-3-0910-P

```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   5
    Acq. Instrument : GC7890B                        Location :   106  (F)
    Injection Date  : 9/15/2021 8:21:58 PM               Inj :   1
                                                   Inj Volume : 1 µl
    Different Inj Volume from Sample Entry!  Actual Inj Volume : 5 µl
    Acq. Method     : D:\Data\ZDQ\zdq-3-0902-16-P 2021-09-15 09-45-10\ZDQ-B-225-80-1-210-155min.M
    Last changed    : 8/18/2021 8:34:44 AM by SYSTEM
    Analysis Method : D:\Data\ZDQ\zdq-3-0902-16-P 2021-09-15 09-45-10\ZDQ-B-225-80-1-210-155min.M
                      (Sequence Method)
    Last changed    : 9/16/2021 5:14:12 AM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



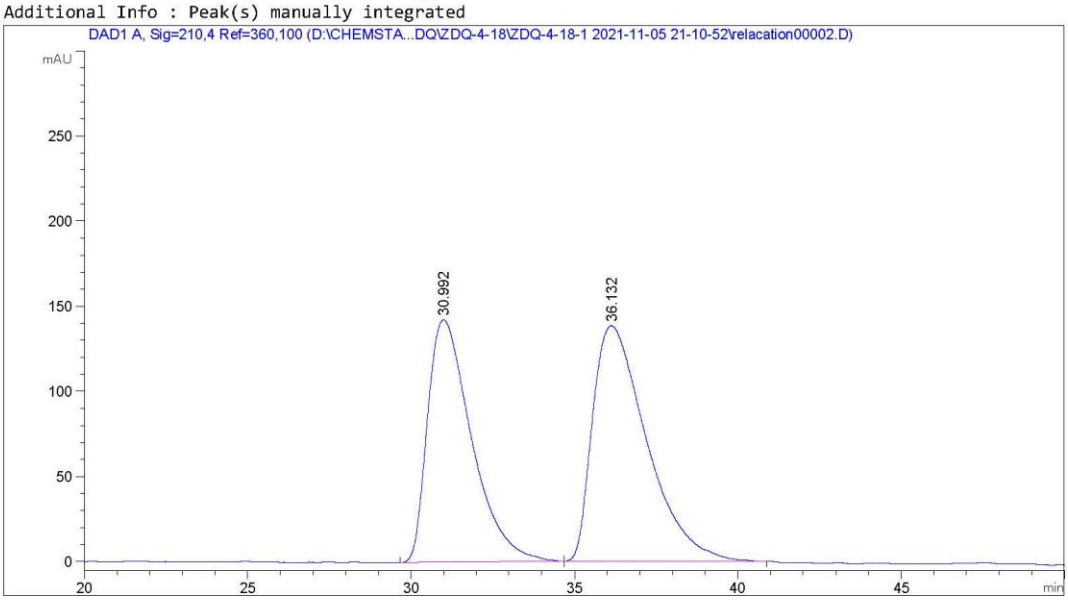

```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: FID1 A, Front Signal

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [pA*s]      [pA]        %
    ----|-------|----|-------|----------|----------|--------|
       1  53.506 MM    0.1763   46.42824    4.38864  1.02054
       2  58.306 BB    0.7092 4502.95605   74.91952 98.97946

    Totals :                  4549.38430   79.30816
```



2p

Data File D:\CHEMSTA...\DATA\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\relacation00002.D
Sample Name: ZDQ-4-18-9,10-RAC

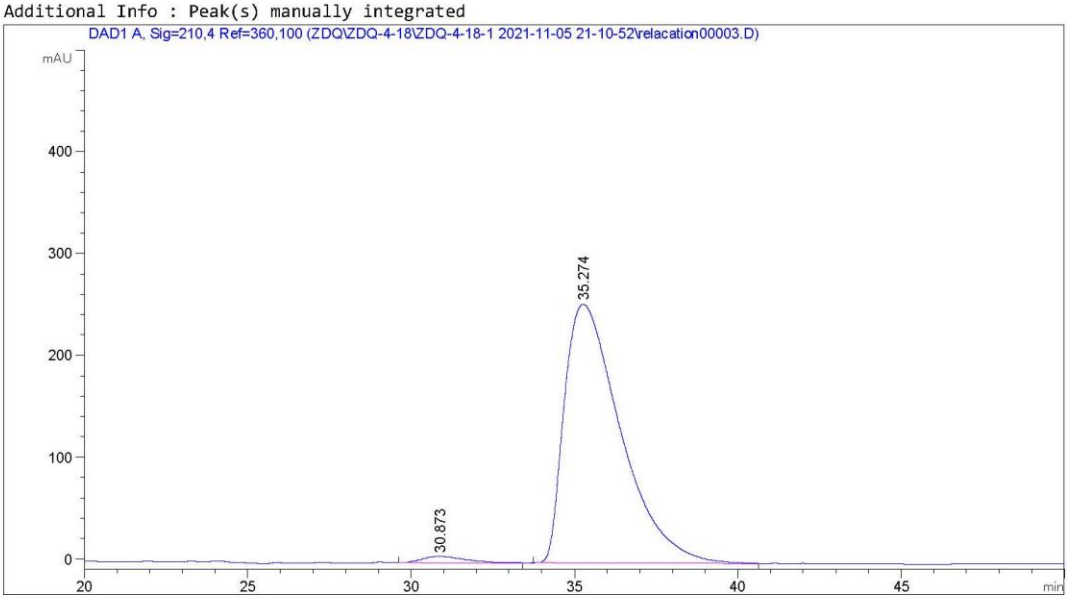
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   2
Sample Operator : SYSTEM
Acq. Instrument : LC                           Location :   P1-D-01
Injection Date  : 11/5/2021 9:22:09 PM              Inj :   1
                                              Inj Volume : 0.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5.000 µl
Acq. Method     : D:\ChemStation\1\Data\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\4-AS3-75-
                  25-1ml-60min.M
Last changed    : 11/5/2021 10:17:03 PM by SYSTEM
                  (modified after loading)
Analysis Method : D:\ChemStation\1\Data\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\4-AS3-75-
                  25-1ml-60min.M (Sequence Method)
Last changed    : 11/9/2021 8:11:02 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



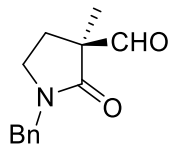

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  30.992 BB    1.3421 1.32992e4   142.32658  45.5660
   2  36.132 BB    1.5442 1.58874e4   138.30188  54.4340
```

Data File D:\ChemSta...\Data\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\relacation00003.D
Sample Name: ZDQ-4-18-11

```
==========================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Sample Operator : SYSTEM
Acq. Instrument : LC                            Location :   P1-D-02
Injection Date  : 11/5/2021 10:17:57 PM              Inj :   1
                                               Inj Volume : 0.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5.000 µl
Acq. Method     : D:\ChemStation\1\Data\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\4-AS3-75-
                  25-1ml-60min.M
Last changed    : 11/5/2021 10:17:03 PM by SYSTEM
Analysis Method : D:\ChemStation\1\Data\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\4-AS3-75-
                  25-1ml-60min.M (Sequence Method)
Last changed    : 11/9/2021 8:12:48 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



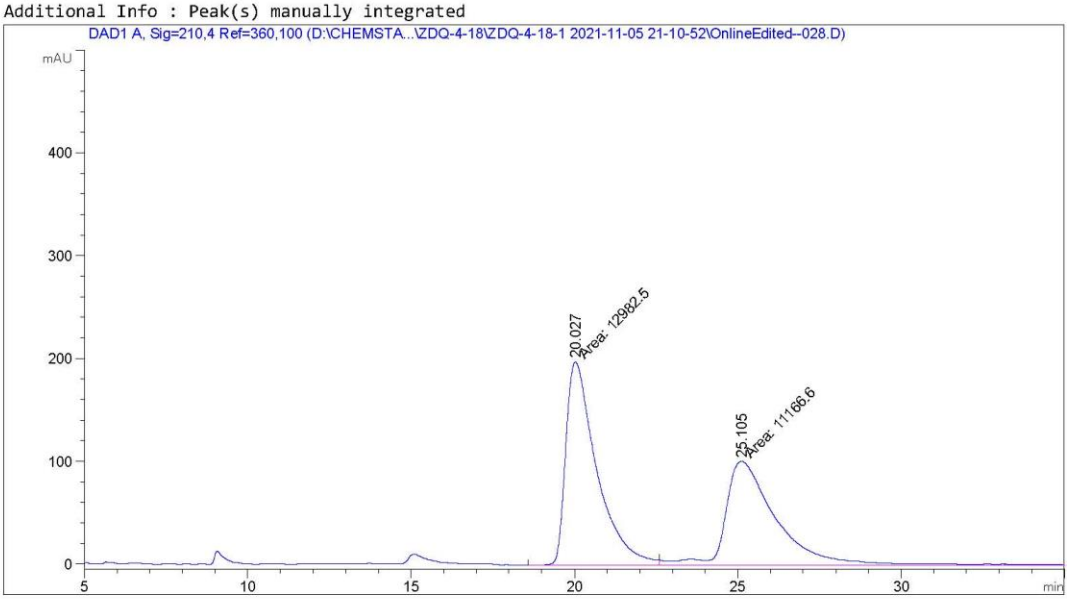

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  30.873 BB    1.0553  557.63074    6.23585   1.7968
   2  35.274 BB    1.4611 3.04772e4   254.14279  98.2032
```



2q

Data File D:\CHEMSTA...ATA\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\OnlineEdited--028.D
Sample Name: ZDQ-4-18-1,2-rac

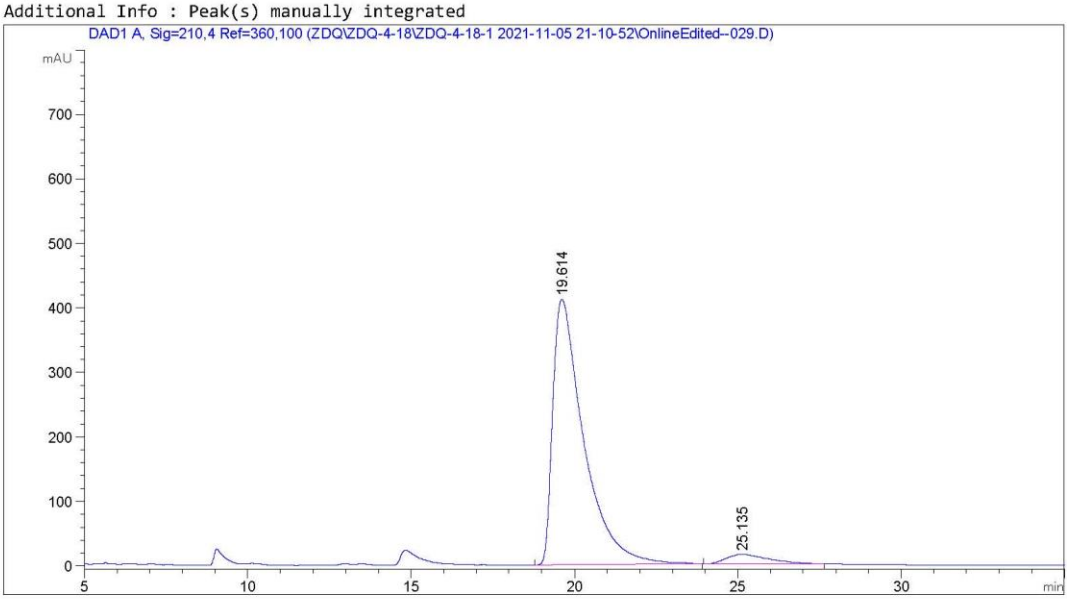
```
==========================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  28
Sample Operator : SYSTEM
Acq. Instrument : LC                            Location :   P1-D-05
Injection Date  : 11/6/2021 12:04:08 PM              Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5.000 µl
Acq. Method     : D:\ChemStation\1\Data\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\2-OD3-70-
                  30-2ul-1.0ml-40min.M
Last changed    : 12/24/2020 7:38:44 PM by SYSTEM
Analysis Method : D:\ChemStation\1\Data\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\2-OD3-70-
                  30-2ul-1.0ml-40min.M (Sequence Method)
Last changed    : 11/9/2021 8:19:50 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



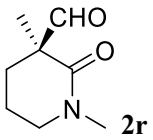

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  20.027 MF    1.0942 1.29825e4   197.75032  53.7599
   2  25.105 FM    1.8398 1.11666e4   101.15859  46.2401
```

Data File D:\ChemSta...ata\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\OnlineEdited--029.D
Sample Name: ZDQ-4-18-3

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  29
Sample Operator : SYSTEM
Acq. Instrument : LC                            Location :   P1-D-06
Injection Date  : 11/6/2021 12:45:03 PM              Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5.000 µl
Acq. Method     : D:\ChemStation\1\Data\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\2-OD3-70-
                  30-2ul-1.0ml-40min.M
Last changed    : 12/24/2020 7:38:44 PM by SYSTEM
Analysis Method : D:\ChemStation\1\Data\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\2-OD3-70-
                  30-2ul-1.0ml-40min.M (Sequence Method)
Last changed    : 11/9/2021 8:24:36 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



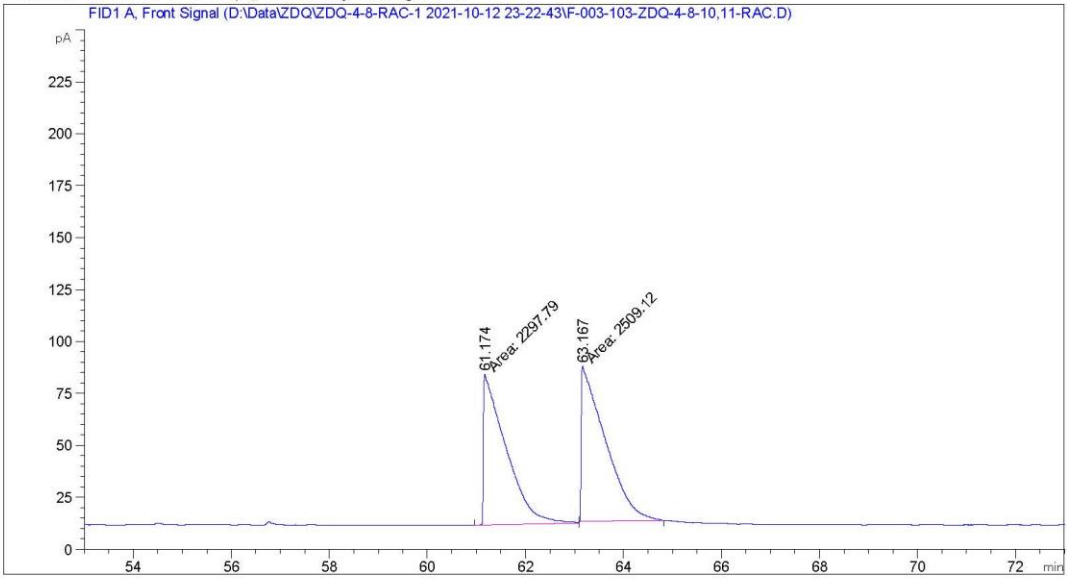

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  19.614 BB    0.9351 2.69698e4   411.22623  95.3686
   2  25.135 BB    1.0975 1309.74841   14.42230   4.6314
```



2r

Data File D:\Data\ZDQ\ZDQ-4-8-RAC-1 2021-10-12 23-22-43\F-003-103-ZDQ-4-8-10,11-RAC.D
Sample Name: ZDQ-4-8-10,11-RAC

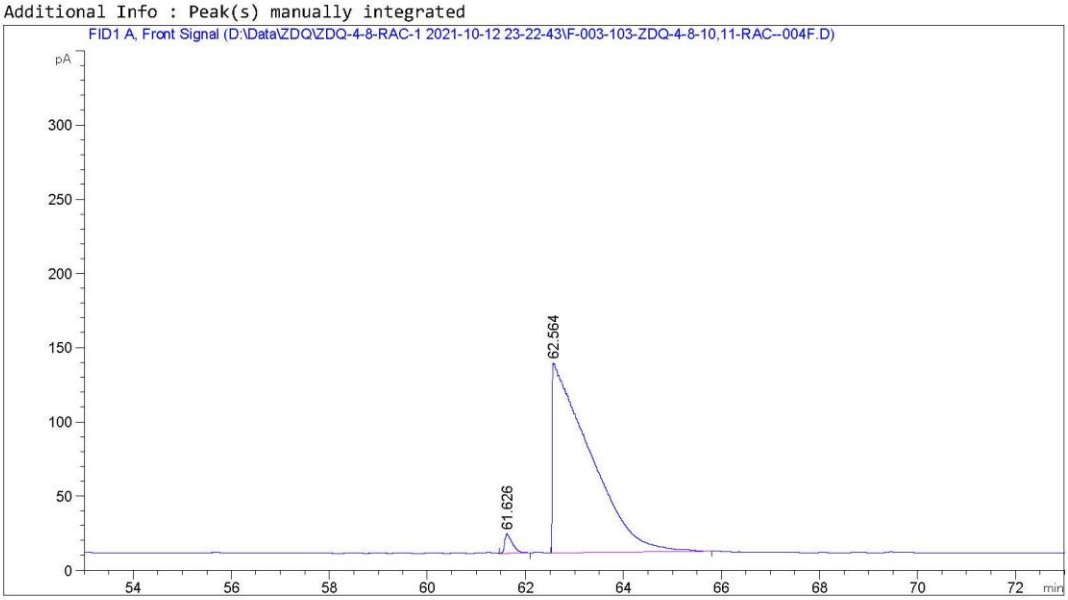
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   3
Acq. Instrument : GC7890B                       Location :   103  (F)
Injection Date  : 10/13/2021 4:47:15 AM              Inj :   1
                                               Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 3 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-4-8-RAC-1 2021-10-12 23-22-43\ZDQ-B-225-80-1-210-155min.M
Last changed    : 10/13/2021 6:36:03 AM by SYSTEM
                  (modified after loading)
Analysis Method : D:\Data\ZDQ\ZDQ-4-8-RAC-1 2021-10-12 23-22-43\ZDQ-B-225-80-1-210-155min.M (
                  Sequence Method)
Last changed    : 11/9/2021 6:53:24 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



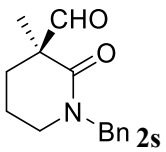

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  61.174 MM    0.5281 2297.79150   72.51940 47.80182
   2  63.167 MM    0.5616 2509.12085   74.46576 52.19818

Totals :                  4806.91235  146.98516
```

Data File D:\Data\ZD...Q-4-8-RAC-1 2021-10-12 23-22-43\F-003-103-ZDQ-4-8-10,11-RAC--004F.D
Sample Name: ZDQ-4-8-12

```
=====================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   4
Acq. Instrument : GC7890B                        Location :   104  (F)
Injection Date  : 10/13/2021 7:00:17 AM               Inj :   1
                                                Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 3 µl
Acq. Method     : D:\Data\ZDQ\ZDQ-4-8-RAC-1 2021-10-12 23-22-43\ZDQ-B-225-80-1-210-155min.M
Last changed    : 10/13/2021 7:42:37 AM by SYSTEM
                  (modified after loading)
Analysis Method : D:\Data\ZDQ\ZDQ-4-8-RAC-1 2021-10-12 23-22-43\ZDQ-B-225-80-1-210-155min.M (
                  Sequence Method)
Last changed    : 11/9/2021 6:54:15 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



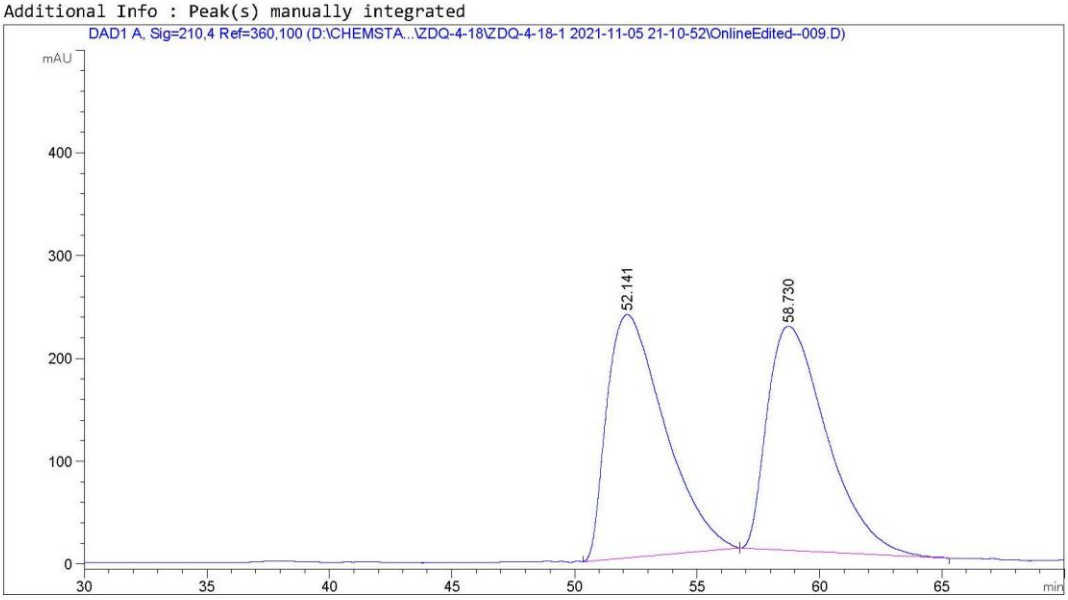

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  61.626 BB    0.1459  138.76862   12.96538  1.99618
   2  62.564 BB    0.6294 6812.92529  127.90112 98.00382

Totals :                  6951.69391  140.86650
```



2s

Data File D:\CHEMSTA...ATA\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\OnlineEdited--009.D
Sample Name: ZDQ-4-18-4,5-rac

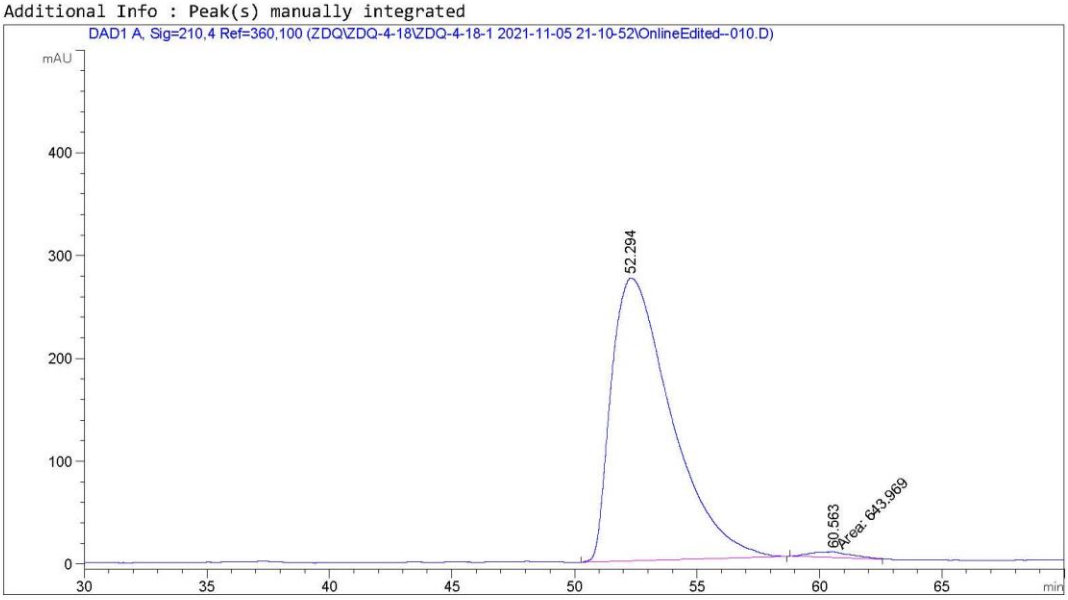
```
==========================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   9
Sample Operator : SYSTEM
Acq. Instrument : LC                            Location :   P1-D-03
Injection Date  : 11/6/2021 2:15:44 AM               Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5.000 µl
Acq. Method     : D:\ChemStation\1\Data\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\4-AS3-90-
                  10-1ml-70min.M
Last changed    : 6/20/2019 10:00:36 PM by SYSTEM
Analysis Method : D:\ChemStation\1\Data\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\4-AS3-90-
                  10-1ml-70min.M (Sequence Method)
Last changed    : 11/9/2021 8:14:29 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



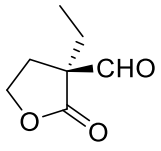

```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  52.141 BB    1.9549 3.87374e4   236.50540  51.2308
   2  58.730 BB    1.9869 3.68760e4   217.40118  48.7692
```

Data File D:\ChemSta...ata\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\OnlineEdited--010.D
Sample Name: ZDQ-4-18-6

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  10
Sample Operator : SYSTEM
Acq. Instrument : LC                            Location :   P1-D-04
Injection Date  : 11/6/2021 3:26:39 AM               Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5.000 µl
Acq. Method     : D:\ChemStation\1\Data\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\4-AS3-90-
                  10-1ml-70min.M
Last changed    : 6/20/2019 10:00:36 PM by SYSTEM
Analysis Method : D:\ChemStation\1\Data\ZDQ\ZDQ-4-18\ZDQ-4-18-1 2021-11-05 21-10-52\4-AS3-90-
                  10-1ml-70min.M (Sequence Method)
Last changed    : 11/9/2021 8:14:29 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



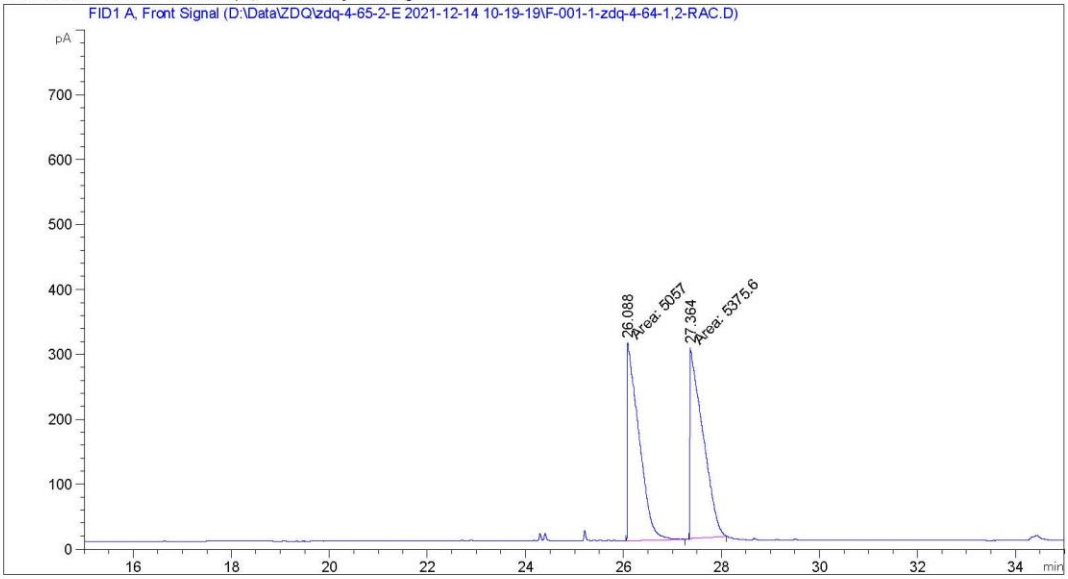

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  52.294 BB    2.0486 4.67723e4   274.95660  98.6419
   2  60.563 MM    1.9898  643.96948    5.39389   1.3581
```



2t

Data File D:\Data\ZDQ\zdq-4-65-2-E 2021-12-14 10-19-19\F-001-1-zdq-4-64-1,2-RAC.D
Sample Name: zdq-4-64-1,2-RAC

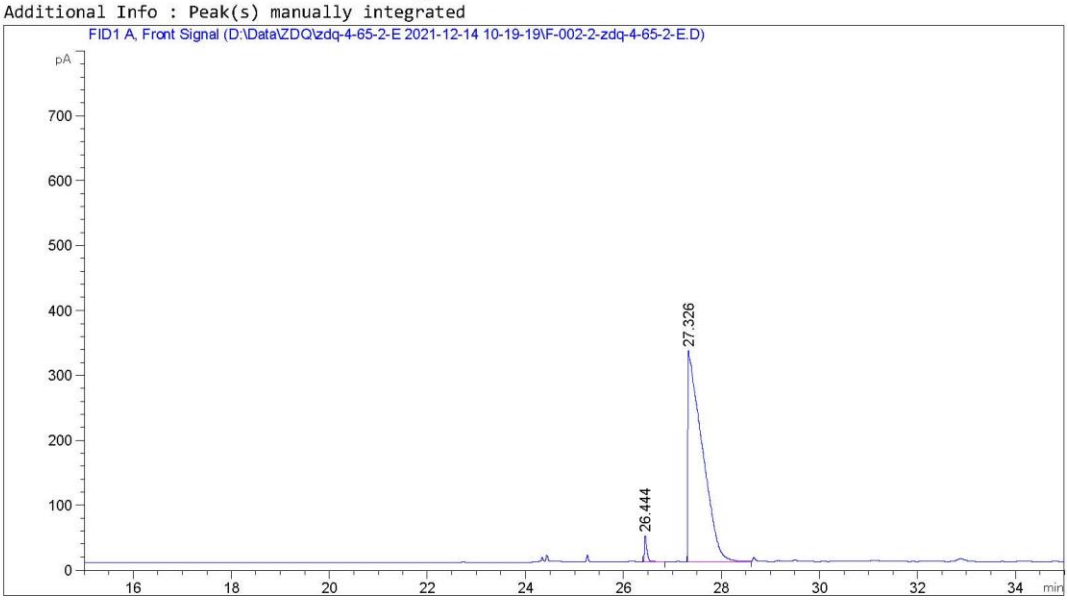
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   1
Acq. Instrument : GC7890B                       Location :   1  (F)
Injection Date  : 12/14/2021 10:21:24 AM             Inj :   1
                                               Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5 µl
Acq. Method     : D:\Data\ZDQ\zdq-4-65-2-E 2021-12-14 10-19-19\ZDQ-B-225-80-4-180-35min.M
Last changed    : 12/14/2021 10:06:22 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\zdq-4-65-2-E 2021-12-14 10-19-19\ZDQ-B-225-80-4-180-35min.M (
                  Sequence Method)
Last changed    : 12/14/2021 9:40:22 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



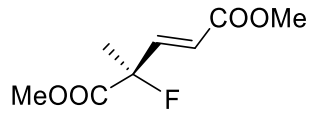

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  26.088 MM    0.2756 5057.00049  305.83853 48.47306
   2  27.364 MM    0.3049 5375.59912  293.79919 51.52694

Totals :                  1.04326e4   599.63773
```

Data File D:\Data\ZDQ\zdq-4-65-2-E 2021-12-14 10-19-19\F-002-2-zdq-4-65-2-E.D
Sample Name: zdq-4-65-2-E

```
=====================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : GC7890B                        Location :   2  (F)
Injection Date  : 12/14/2021 10:59:36 AM              Inj :   1
                                                Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 5 µl
Acq. Method     : D:\Data\ZDQ\zdq-4-65-2-E 2021-12-14 10-19-19\ZDQ-B-225-80-4-180-35min.M
Last changed    : 12/14/2021 10:06:22 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\zdq-4-65-2-E 2021-12-14 10-19-19\ZDQ-B-225-80-4-180-35min.M (
                  Sequence Method)
Last changed    : 12/14/2021 9:40:22 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



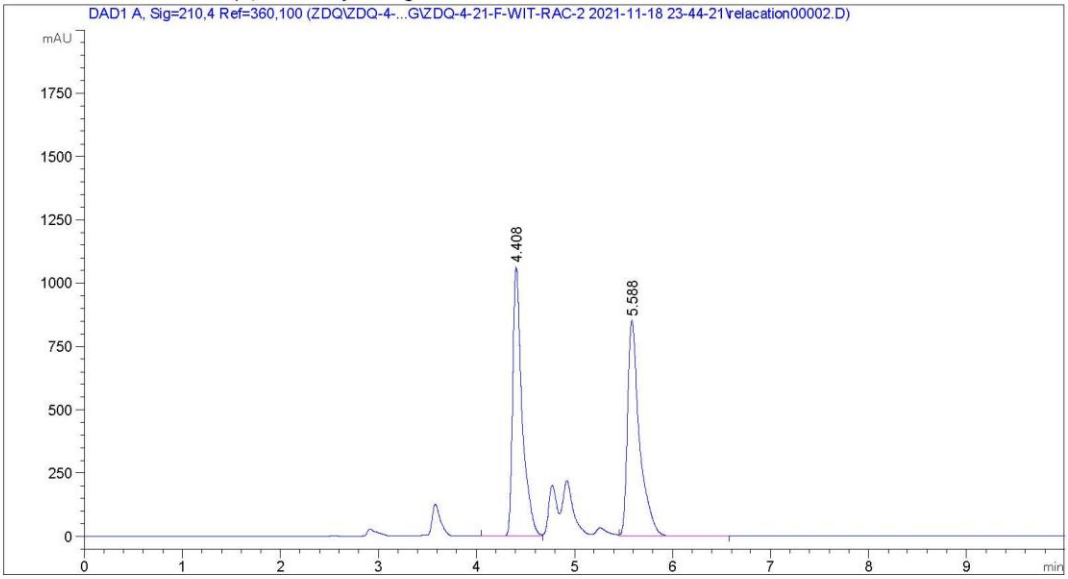

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  26.444 BB    0.0513  136.72021   39.58947  2.04083
   2  27.326 BV    0.2438 6562.50977  324.64966 97.95917

Totals :                  6699.22998  364.23912
```



2u

Data File D:\ChemSta...F-WITTIG\ZDQ-4-21-F-WIT-RAC-2 2021-11-18 23-44-21\relacation00002.D
Sample Name: F-WIT-RAC

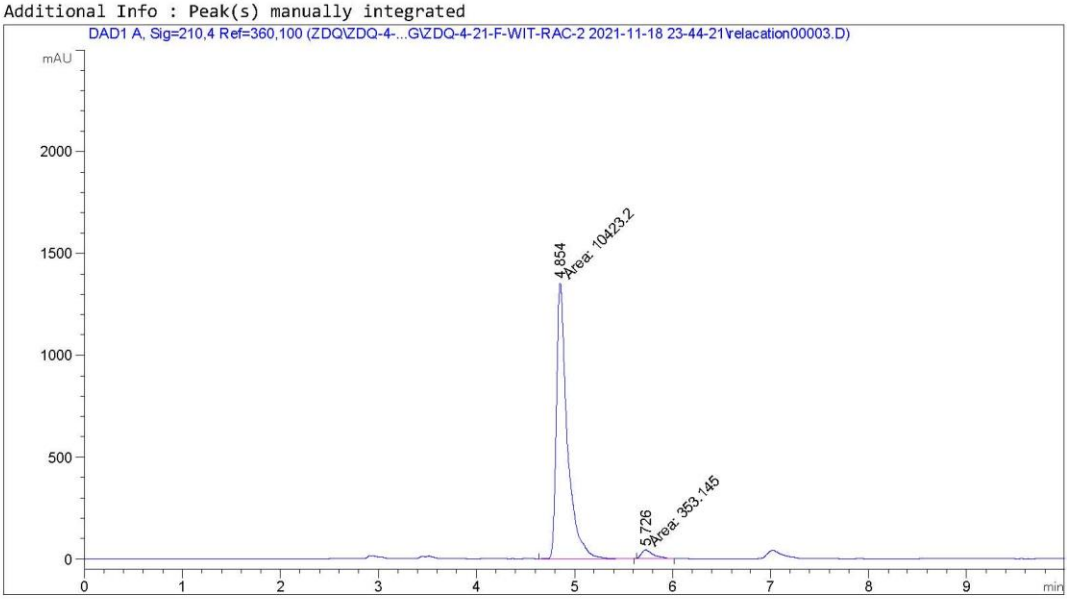
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   2
Sample Operator : SYSTEM
Acq. Instrument : LC                           Location :   P2-E-10
Injection Date  : 11/19/2021 12:00:35 AM            Inj :   1
                                              Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 1.000 µl
Acq. Method     : D:\ChemStation\1\Data\ZDQ\ZDQ-4-F-WITTIG\ZDQ-4-21-F-WIT-RAC-2 2021-11-18 23
                  -44-21\2-OD3-90-10-1.0ml-30min.M
Last changed    : 1/2/2020 5:16:24 PM by SYSTEM
Analysis Method : D:\ChemStation\1\Data\ZDQ\ZDQ-4-F-WITTIG\ZDQ-4-21-F-WIT-RAC-2 2021-11-18 23
                  -44-21\2-OD3-90-10-1.0ml-30min.M (Sequence Method)
Last changed    : 12/13/2021 8:06:31 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



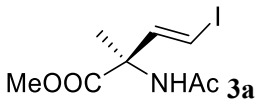

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.408 BV    0.0971 7029.13525 1063.02185  49.4544
   2   5.588 VB    0.1224 7184.24512  851.68402  50.5456
```

Data File D:\ChemSta...F-WITTIG\ZDQ-4-21-F-WIT-RAC-2 2021-11-18 23-44-21\relacation00003.D
Sample Name: F-WIT-RAC

```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   3
Sample Operator : SYSTEM
Acq. Instrument : LC                           Location :   P2-E-11
Injection Date  : 11/19/2021 12:31:26 AM            Inj :   1
                                              Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 1.000 µl
Acq. Method     : D:\ChemStation\1\Data\ZDQ\ZDQ-4-F-WITTIG\ZDQ-4-21-F-WIT-RAC-2 2021-11-18 23
                  -44-21\2-OD3-90-10-1.0ml-30min.M
Last changed    : 1/2/2020 5:16:24 PM by SYSTEM
Analysis Method : D:\ChemStation\1\Data\ZDQ\ZDQ-4-F-WITTIG\ZDQ-4-21-F-WIT-RAC-2 2021-11-18 23
                  -44-21\2-OD3-90-10-1.0ml-30min.M (Sequence Method)
Last changed    : 12/13/2021 8:08:03 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



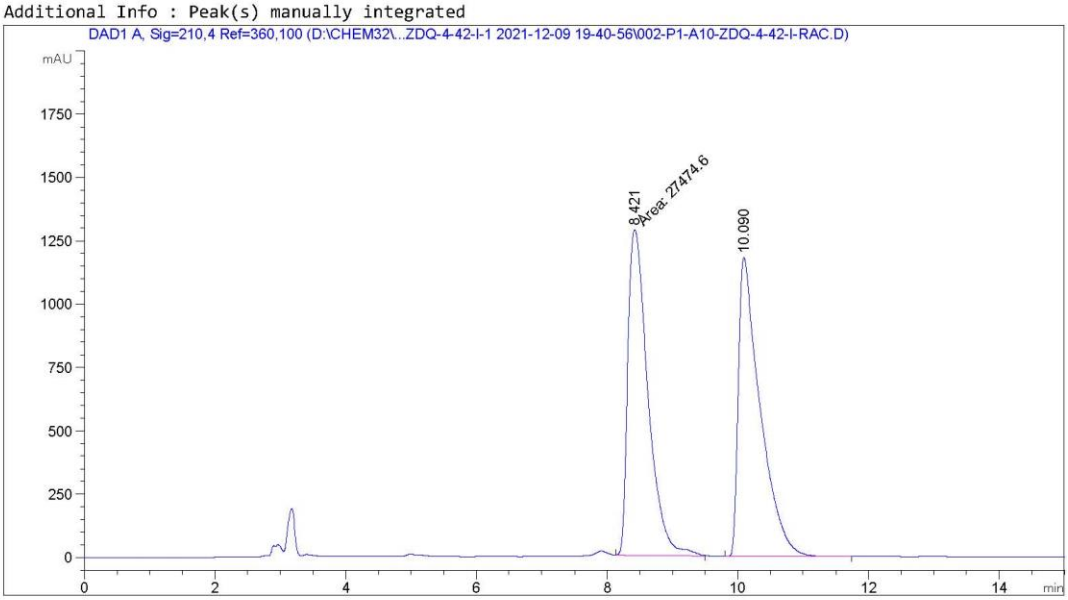

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.854 MM    0.1281 1.04232e4  1356.30066  96.7230
   2   5.726 MM    0.1387  353.14508   42.42539   3.2770
```



3a

Data File D:\CHEM32\...4-42-I\ZDQ-4-42-I-1 2021-12-09 19-40-56\002-P1-A10-ZDQ-4-42-I-RAC.D
Sample Name: ZDQ-4-42-I-RAC

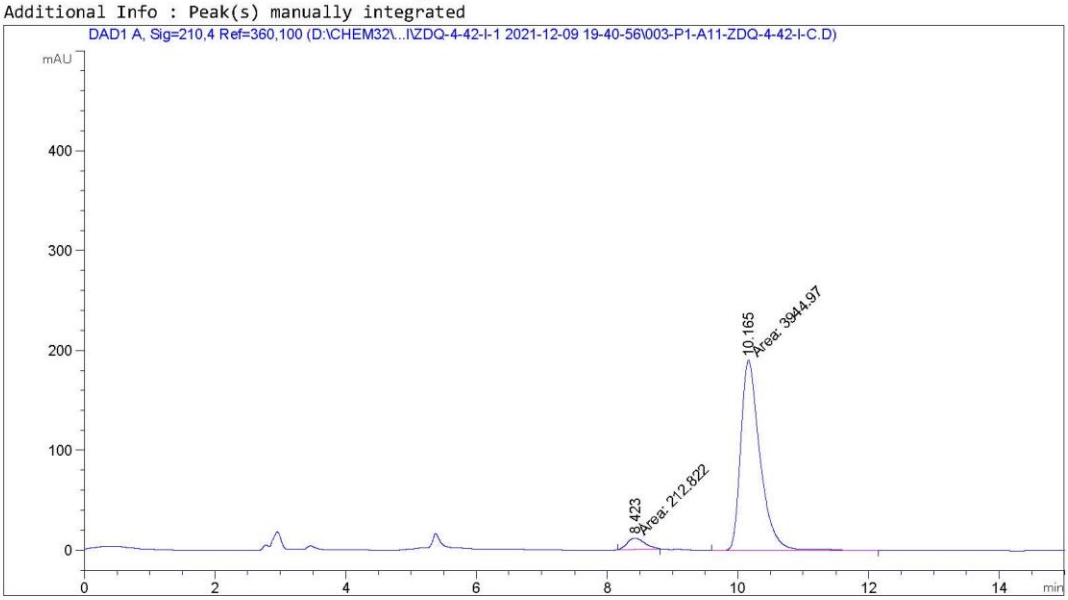
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   2
Acq. Instrument : 1260-DAD                      Location :   P1-A-10
Injection Date  : 12/9/2021 19:52:13                Inj :   1
                                               Inj Volume : 2.000 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 3.000 µl
Acq. Method     : D:\Chem32\1\Data\ZDQ\zdq-4-42-I\ZDQ-4-42-I-1 2021-12-09 19-40-56\ZDQ-AS3-90
                  -10-1ML-20MIN.M
Last changed    : 10/24/2019 20:52:44 by SYSTEM
Analysis Method : d:\Chem32\1\Data\ZDQ\zdq-4-42-I\ZDQ-4-42-I-1 2021-12-09 19-40-56\ZDQ-AS3-90
                  -10-1ML-20MIN.M (Sequence Method)
Last changed    : 12/13/2021 20:02:07 by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



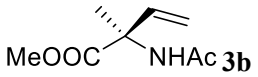

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.421 MM    0.3560 2.74746e4  1286.20959  50.1929
   2  10.090 BB    0.3212 2.72634e4  1181.37341  49.8071

Totals :                  5.47381e4  2467.58301
```

Data File D:\CHEM32\...Q-4-42-I\ZDQ-4-42-I-1 2021-12-09 19-40-56\003-P1-A11-ZDQ-4-42-I-C.D
Sample Name: ZDQ-4-42-I-C

```
=====================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Acq. Instrument : 1260-DAD                      Location :   P1-A-11
Injection Date  : 12/9/2021 20:13:08                 Inj :   1
                                               Inj Volume : 2.000 µl
Acq. Method     : D:\Chem32\1\Data\ZDQ\zdq-4-42-I\ZDQ-4-42-I-1 2021-12-09 19-40-56\ZDQ-AS3-90
                  -10-1ML-20MIN.M
Last changed    : 10/24/2019 20:52:44 by SYSTEM
Analysis Method : d:\Chem32\1\Data\ZDQ\zdq-4-42-I\ZDQ-4-42-I-1 2021-12-09 19-40-56\ZDQ-AS3-90
                  -10-1ML-20MIN.M (Sequence Method)
Last changed    : 12/13/2021 20:04:56 by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



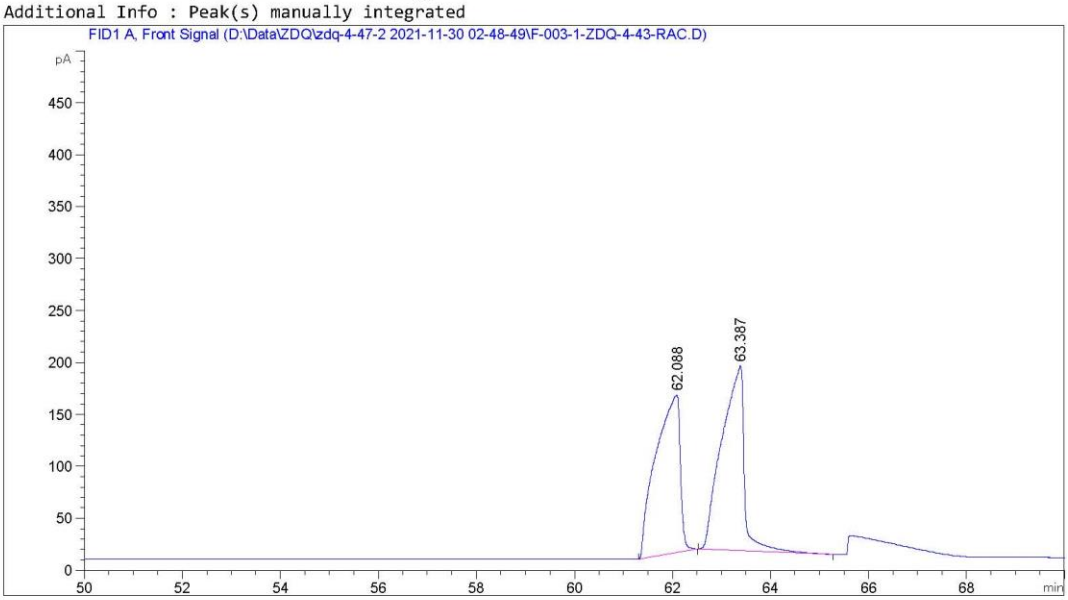

```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.423 MM    0.3133  212.82222   11.32204   5.1186
   2  10.165 MM    0.3450 3944.96777  190.56757  94.8814

Totals :                  4157.78999  201.88961
```



3b

Data File D:\Data\ZDQ\zdq-4-47-2 2021-11-30 02-48-49\F-003-1-ZDQ-4-43-RAC.D
Sample Name: ZDQ-4-43-RAC

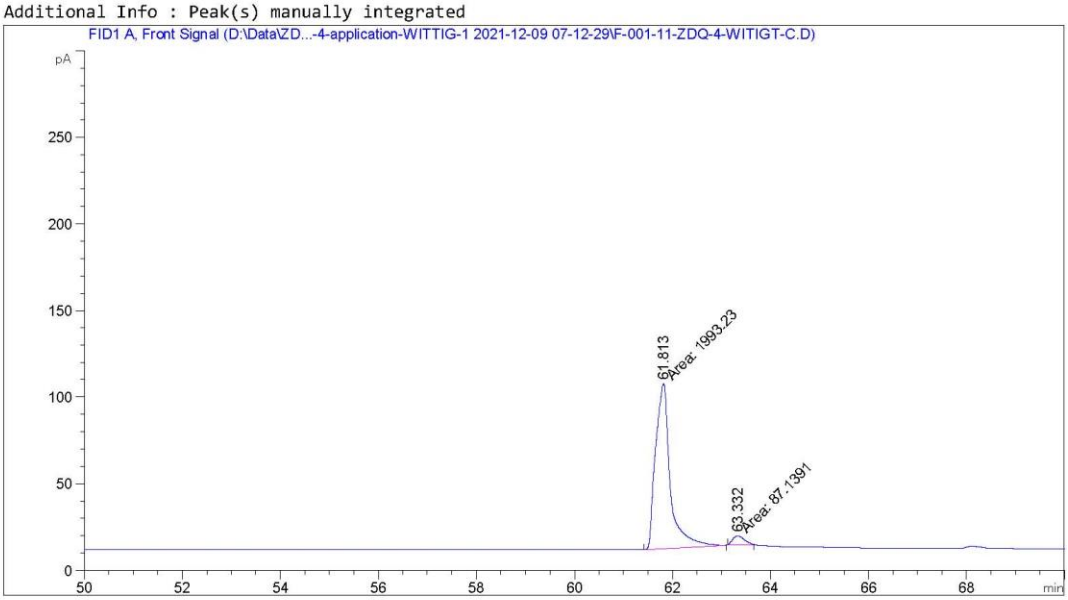
```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Acq. Instrument : GC7890B                        Location :   1  (F)
Injection Date  : 11/30/2021 8:39:02 AM               Inj :   1
                                                 Inj Volume : 1 µl
Different Inj Volume from Sample Entry!  Actual Inj Volume : 4 µl
Acq. Method     : D:\Data\ZDQ\zdq-4-47-2 2021-11-30 02-48-49\ZDQ-B-225-80-0.5-115-80min.M
Last changed    : 11/30/2021 2:44:19 AM by SYSTEM
Analysis Method : D:\Data\ZDQ\zdq-4-47-2 2021-11-30 02-48-49\ZDQ-B-225-80-0.5-115-80min.M (
                  Sequence Method)
Last changed    : 11/30/2021 11:17:50 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```



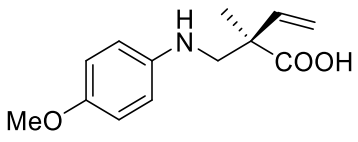

```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: FID1 A, Front Signal

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [pA*s]      [pA]        %
----|-------|----|-------|----------|----------|--------|
   1  62.088 BB    0.4254 5241.80762  151.97835 48.04500
   2  63.387 BB    0.3918 5668.39648  177.89108 51.95500

Totals :                  1.09102e4   329.86943
```

Data File D:\Data\ZD...-application-WITTIG-1 2021-12-09 07-12-29\F-001-11-ZDQ-4-WITIGT-C.D
Sample Name: ZDQ-4-WITIGT-C

```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   1
    Acq. Instrument : GC7890B                        Location :   11  (F)
    Injection Date  : 12/9/2021 7:21:29 AM               Inj :   1
                                                   Inj Volume : 1 µl
    Different Inj Volume from Sample Entry!  Actual Inj Volume : 5 µl
    Acq. Method     : D:\Data\ZDQ\zdq-4-application-WITTIG-1 2021-12-09 07-12-29\ZDQ-B-225-80-0.5
                      -115-80min.M
    Last changed    : 11/30/2021 2:44:19 AM by SYSTEM
    Analysis Method : D:\Data\ZDQ\zdq-4-application-WITTIG-1 2021-12-09 07-12-29\ZDQ-B-225-80-0.5
                      -115-80min.M (Sequence Method)
    Last changed    : 12/12/2021 10:38:53 PM by SYSTEM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```



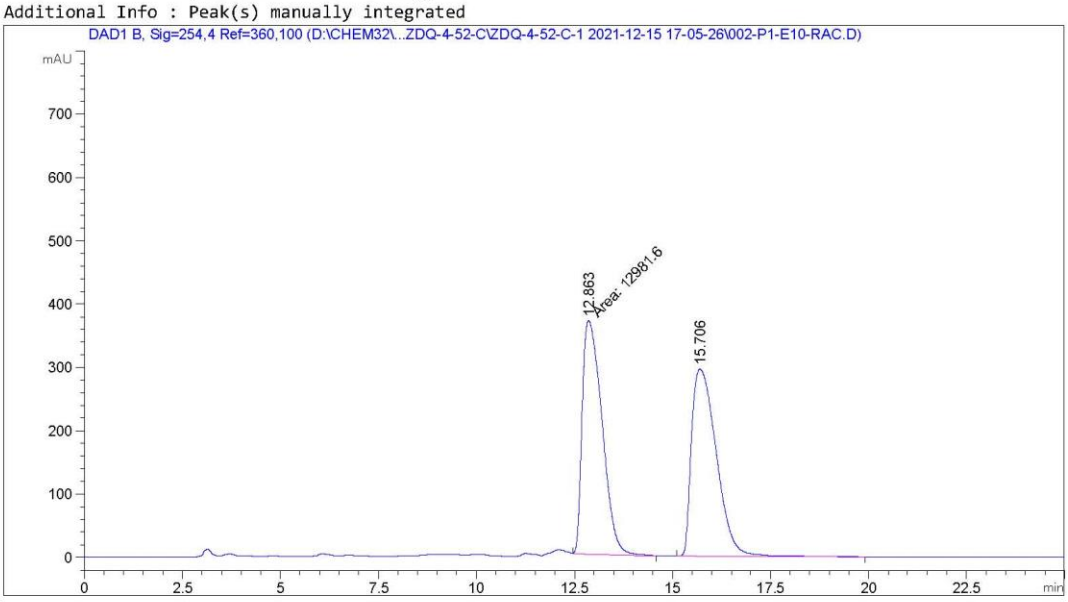

```
    ======================================================================
                            Area Percent Report
    ======================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: FID1 A, Front Signal

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [pA*s]      [pA]        %
    ----|-------|----|-------|----------|----------|--------|
       1  61.813 MM    0.3479 1993.23157   95.50225 95.81137
       2  63.332 MM    0.2787   87.13911    5.21163  4.18863

    Totals :                  2080.37068  100.71388
```



4n

Data File D:\CHEM32\...TA\ZDQ\ZDQ-4-52-C\ZDQ-4-52-C-1 2021-12-15 17-05-26\002-P1-E10-RAC.D
Sample Name: RAC

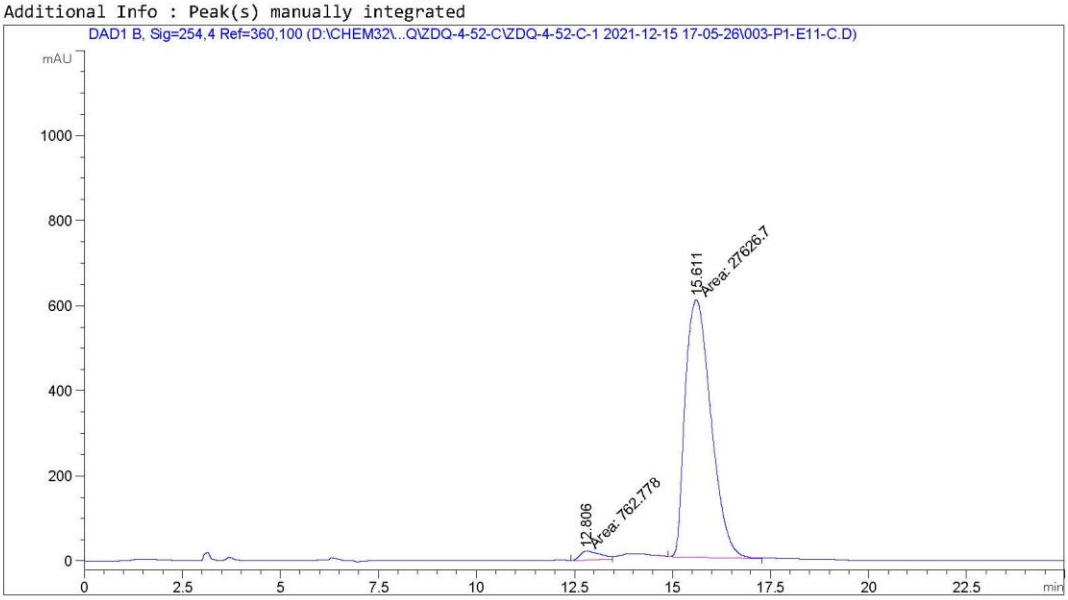
```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   2
Acq. Instrument : 1260-DAD                     Location :   P1-E-10
Injection Date  : 12/15/2021 17:16:45               Inj :   1
                                              Inj Volume : 2.000 µl
Acq. Method     : D:\Chem32\1\Data\ZDQ\ZDQ-4-52-C\ZDQ-4-52-C-1 2021-12-15 17-05-26\OJ-3-85-15
                  -1ML-25MIN.M
Last changed    : 12/15/2021 17:02:00 by SYSTEM
Analysis Method : D:\Chem32\1\Data\ZDQ\ZDQ-4-52-C\ZDQ-4-52-C-1 2021-12-15 17-05-26\OJ-3-85-15
                  -1ML-25MIN.M (Sequence Method)
Last changed    : 12/15/2021 19:51:07 by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.863 MM    0.5864 1.29816e4   368.98154  50.0817
   2  15.706 BB    0.7051 1.29393e4   295.35507  49.9183

Totals :                  2.59209e4   664.33661
```

Data File D:\CHEM32\1\DATA\ZDQ\ZDQ-4-52-C\ZDQ-4-52-C-1 2021-12-15 17-05-26\003-P1-E11-C.D
Sample Name: C

```
=====================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Acq. Instrument : 1260-DAD                      Location :   P1-E-11
Injection Date  : 12/15/2021 17:42:35               Inj :   1
                                               Inj Volume : 2.000 µl
Acq. Method     : D:\Chem32\1\Data\ZDQ\ZDQ-4-52-C\ZDQ-4-52-C-1 2021-12-15 17-05-26\OJ-3-85-15
                  -1ML-25MIN.M
Last changed    : 12/15/2021 17:02:00 by SYSTEM
Analysis Method : D:\Chem32\1\Data\ZDQ\ZDQ-4-52-C\ZDQ-4-52-C-1 2021-12-15 17-05-26\OJ-3-85-15
                  -1ML-25MIN.M (Sequence Method)
Last changed    : 12/15/2021 19:52:49 by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.806 MM    0.6074  762.77753   20.93088   2.6868
   2  15.611 MM    0.7610 2.76267e4   605.07977  97.3132

Totals :                  2.83894e4   626.01065
```

References

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