Electronic Supplementary Information

Enantio- and Diastereodivergent Synthesis of Fused Indolizines Enabled by Synergistic Cu/Ir Catalysis

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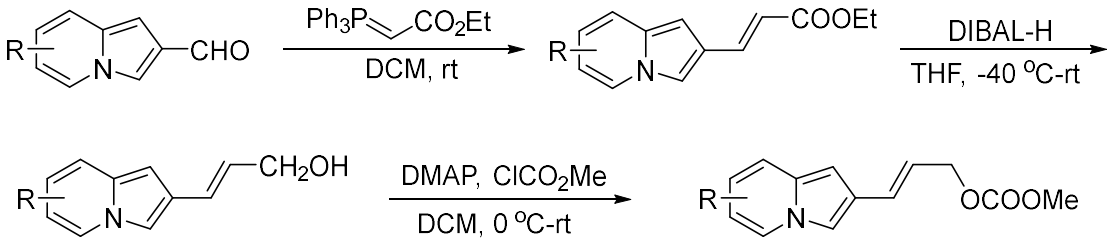
1. General Remarks

Unless otherwise stated, all reactions were set up under nitrogen atmosphere in oven-dried glassware using standard Schlenk techniques, monitored by TLC with silica-gel coated plates and purified by flash column chromatography. Commercially available reagents were used without further purification. Solvents were purified prior to use according to the standard methods. Aldimine esters[1], chiral ligands **L1**-**L4**,[2] **L6**[3], and 2-indolizine carbaldehyde[4] and 2-indolizine carbonates[5] were prepared according to the literature procedure. ^{1}H NMR spectra were recorded on a Bruker 400 MHz spectrometer in $CDCl_3$ (or DMSO). Chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard. The data are reported as (s = single, d = double, t = triple, q = quarte, m = multiple or unresolved, coupling constant(s) in Hz, integration). ^{13}C NMR spectra were recorded on a Bruker 100 MHz spectrometer in $CDCl_3$. Chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard. Enantiomeric excess values were determined by HPLC analysis employing AS-H, AD-H, IA, IC, ID, IE and OD-H chiral columns, using hexane and *i*-propanol as solvents. The racemic products were obtained by running reactions with racemic catalysts or blending equal amount of two enantiomers. The absolute configuration of compound **3k** was determined unequivocally according to the X-ray diffraction analysis.

2. Synthetic Procedures and Characterization for Substituted 2-Indolizine Carbonates



To a solution of indolizine-2-carbaldehyde (2.6 g, 18.1 mmol) in CH_2Cl_2 (60 mL) was added phosphorus ylide (7.3 g, 21.7 mmol) in one portion at 25 ºC. The reaction was then stirred at 25 ºC until complete consumption of starting material (detected by TLC). The mixture was concentrated under reduced pressure, and the residue was purified by a flash column chromatography (PE/EA = 5/1, with 1% Et_3N) to provide ethyl (*E*)-3-(indolizin-2-yl)acrylate (3.3 g, 90% yield) as a light yellow solid.

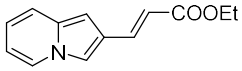
Under nitrogen atmosphere, to a solution of ethyl (*E*)-3-(indolizin-2-yl)acrylate (3.3 g, 16.3 mmol)

in anhydrous THF (50 mL) was added DIBAL-H (1.5 M, 16.3 mL, 24.5 mmol) dropwise at -40 ºC. After stirring at -40 ºC for 30 min, the reaction was then moved into 25 ºC and continuously stirred until complete consumption of starting material (detected by TLC). The reaction mixture was quenched with H_2O, extracted with EA (× 3) and filtered through celite to remove the colloid. The organic layer was combined, washed with brine, dried over anhydrous Na_2SO_4 before evaporation. Then the residue was purified by a flash column chromatography (PE/EA = 3/1, with 1% Et_3N) to afford (*E*)-3-(indolizin-2-yl)prop-2-en-1-ol (2.7 g, 95% yield) as a yellow solid.

(*E*)-3-(1-methyl-1*H*-indol-2-yl)prop-2-en-1-ol (2.7 g, 15.5 mmol) and DMAP (2.8 g, 23.3 mmol) were dissolved in CH_2Cl_2 (70 mL) before cooled to 0 ºC. Then methyl chlorocarbonate (1.4 mL, 18.6 mmol) was added dropwise *via* syringe at the same temperature. After stirring at 0 ºC for 30 min, the reaction was then moved into 25 ºC and continuously stirred until complete consumption of starting material (detected by TLC). Then the reaction mixture was quenched with a saturated solution of $NaHCO_3$ and extracted with CH_2Cl_2 (× 3). The organic layer was combined, washed with brine and dried over anhydrous Na_2SO_4. After filtration and evaporation, the residue was purified by a flash column chromatography (PE/EA = 5/1, with 1% Et_3N) to provide (*E*)-3-(indolizin-2-yl)allyl methyl carbonate **2a** (3.2 g, 90% yield) as a white solid.

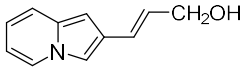
Characterization for Carbonates 2:

Ethyl (*E*)-3-(indolizin-2-yl)acrylate (2ac)



Yield (90%); Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 – 7.78 (m, 1H), 7.74 (d, *J* = 16.0 Hz, 1H), 7.43 (s, 1H), 7.29 (d, *J* = 9.2 Hz, 1H), 6.67 – 6.61 (m, 1H), 6.57 (s, 1H), 6.47 – 6.41 (m, 1H), 6.33 (d, *J* = 15.6 Hz, 1H), 4.25 (q, *J* = 7.2 Hz, 2H), 1.33 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.5, 138.5, 133.8, 125.1, 124.2, 119.4, 118.2, 116.8, 114.0, 111.3, 97.1, 60.2, 14.3.

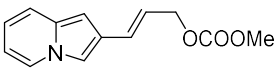
(*E*)-3-(indolizin-2-yl)prop-2-en-1-ol (2ad)



Yield (95%); Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 – 7.76 (m, 1H), 7.28 – 7.25 (m, 2H), 6.66 – 6.58 (m, 2H), 6.47 (s, 1H), 6.42 – 6.37 (m, 1H), 6.28 (dt, *J* = 16.0, 6.0 Hz, 1H), 4.29 (d, *J*

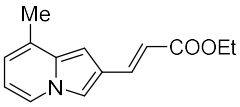
= 6.0 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 133.4, 127.5, 126.3, 124.93, 124.89, 118.9, 117.5, 111.2, 110.3, 96.1, 64.0.

(*E*)-3-(indolizin-2-yl)allyl methyl carbonate (2a)



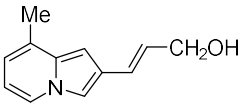
Yield (90%); White solid, m.p. = 103 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (d, *J* = 7.2 Hz, 1H), 7.29 – 7.24 (m, 2H), 6.72 (d, *J* = 16.0 Hz, 1H), 6.64 – 6.58 (m, 1H), 6.47 (s, 1H), 6.42 – 6.36 (m, 1H), 6.25 – 6.15 (m, 1H), 4.77 (d, *J* = 6.0 Hz, 2H), 3.79 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 155.7, 133.4, 128.7, 125.7, 124.9, 121.2, 118.9, 117.6, 111.6, 110.5, 96.3, 68.8, 54.7.

Ethyl (*E*)-3-(8-methylindolizin-2-yl)acrylate (2bc)



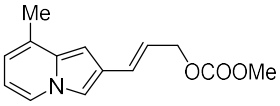
Yield (80%); Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 (d, *J* = 16.0 Hz, 1H), 7.71 (d, *J* = 6.8 Hz, 1H), 7.44 (s, 1H), 6.56 (s, 1H), 6.48 – 6.44 (m, 1H), 6.42 – 6.37 (m, 1H), 6.37 – 6.32 (m, 1H), 4.25 (q, *J* = 7.2 Hz, 2H), 2.36 (s, 3H), 1.33 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.6, 138.6, 135.0, 128.5, 123.8, 123.0, 117.2, 116.5, 114.6, 111.4, 95.7, 60.2, 18.0, 14.4.

(*E*)-3-(8-methylindolizin-2-yl)prop-2-en-1-ol (2bd)



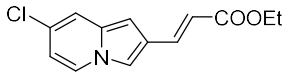
Yield (85%); Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 (d, *J* = 6.8 Hz, 1H), 7.27 – 7.25 (m, 1H), 6.64 (d, *J* = 16.0 Hz, 1H), 6.47 – 6.41 (m, 2H), 6.37 – 6.32 (m, 1H), 6.33 – 6.25 (m, 1H), 4.29 (d, *J* = 6.0 Hz, 2H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 134.5, 127.9, 127.2, 125.8, 125.0, 122.9, 116.6, 111.7, 110.4, 94.7, 64.0, 18.0.

(*E*)-methyl (3-(8-methylindolizin-2-yl)allyl) carbonate (2b)



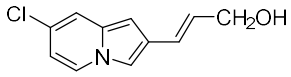
Yield (80%); White solid, m.p. = 87 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 (d, *J* = 6.8 Hz, 1H), 7.28 (s, 1H), 6.73 (d, *J* = 16.0 Hz, 1H), 6.46 (s, 1H), 6.45 – 6.40 (m, 1H), 6.39 – 6.32 (m, 1H), 6.22 (dt, *J* = 16.0, 6.8 Hz, 1H), 4.78 (d, *J* = 6.8 Hz, 2H), 3.80 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 155.7, 134.5, 128.9, 128.0, 125.2, 123.0, 120.9, 116.7, 112.2, 110.6, 94.9, 68.9, 54.7, 18.0.

Ethyl (*E*)-3-(7-chloroindolizin-2-yl)acrylate (2cc)



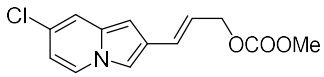
Yield (75%); Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 – 7.72 (m, 1H), 7.70 (d, *J* = 16.0 Hz, 1H), 7.41 (s, 1H), 7.28 (s, 1H), 6.52 (s, 1H), 6.44 – 6.40 (m, 1H), 6.32 (d, *J* = 16.0 Hz, 1H), 4.25 (q, *J* = 7.2 Hz, 2H), 1.33 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.3, 137.8, 133.4, 125.7, 125.3, 124.4, 117.7, 117.5, 114.3, 112.8, 97.3, 60.3, 14.3.

(*E*)-3-(7-chloroindolizin-2-yl)prop-2-en-1-ol (2cd)



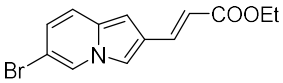
Yield (89%); Yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.18 (d, *J* = 7.2 Hz, 1H), 7.59 (s, 1H), 7.44 – 7.41 (m, 1H), 6.56 – 6.50 (m, 1H), 6.51 – 6.48 (m, 1H), 6.48 (s, 1H), 6.24 – 6.17 (m, 1H), 4.80 (t, *J* = 5.6 Hz, 1H), 4.12 – 4.06 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 133.5, 131.4, 128.7, 128.2, 123.6, 123.2, 117.9, 113.3, 112.0, 97.7, 62.8.

(*E*)-3-(7-chloroindolizin-2-yl)allyl methyl carbonate (2c)



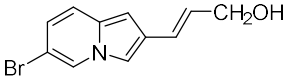
Yield (84%); White solid, m.p. = 120 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.20 (d, *J* = 7.2 Hz, 1H), 7.66 (s, 1H), 7.45 (s, 1H), 6.71 (d, *J* = 15.6 Hz, 1H), 6.53 (s, 1H), 6.53 – 6.49 (m, 1H), 6.24 – 6.15 (m, 1H), 4.73 (d, *J* = 6.0 Hz, 2H), 3.72 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 156.3, 133.6, 129.0, 128.3, 127.5, 124.0, 123.4, 118.1, 114.3, 112.4, 97.9, 69.4, 55.9.

Ethyl (*E*)-3-(6-bromoindolizin-2-yl)acrylate (2dc)



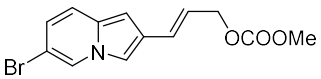
Yield (93%); Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 (s, 1H), 7.70 (d, *J* = 15.6 Hz, 1H), 7.40 (s, 1H), 7.22 – 7.17 (m, 1H), 6.73 – 6.68 (m, 1H), 6.61 (s, 1H), 6.33 (d, *J* = 15.6 Hz, 1H), 4.26 (q, *J* = 7.2 Hz, 2H), 1.33 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.3, 137.8, 132.0, 124.9, 124.8, 121.7, 120.0, 117.5, 114.1, 106.3, 98.6, 60.3, 14.4.

(*E*)-3-(6-bromoindolizin-2-yl)prop-2-en-1-ol (2dd)



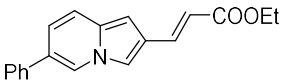
Yield (70%); Yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.50 (s, 1H), 7.57 (s, 1H), 7.31 (d, *J* = 9.6 Hz, 1H), 6.75 – 6.68 (m, 1H), 6.56 (s, 1H), 6.52 (d, *J* = 16.0 Hz, 1H), 6.21 (dt, *J* = 16.0, 5.2 Hz, 1H), 4.09 (d, *J* = 5.2 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 132.2, 131.4, 128.3, 126.5, 123.2, 121.4, 120.7, 113.4, 105.3, 98.7, 62.9.

(*E*)-3-(6-bromoindolizin-2-yl)allyl methyl carbonate (2d)



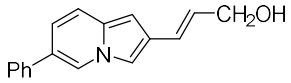
Yield (88%); White solid, m.p. = 120 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.51 (s, 1H), 7.63 (s, 1H), 7.32 (d, *J* = 9.6 Hz, 1H), 6.77 – 6.72 (m, 1H), 6.73 – 6.68 (m, 1H), 6.62 (s, 1H), 6.21 (dt, *J* = 16.0, 6.4 Hz, 1H), 4.73 (d, *J* = 6.4 Hz, 2H), 3.72 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 156.3, 132.3, 129.0, 127.1, 126.7, 123.4, 121.8, 120.9, 114.2, 105.7, 99.0, 69.4, 55.9.

Ethyl (*E*)-3-(6-phenylindolizin-2-yl)acrylate (2ec)



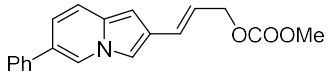
Yield (92%); Yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.03 (s, 1H), 7.76 (d, *J* = 15.6 Hz, 1H), 7.57 – 7.47 (m, 3H), 7.47 – 7.41 (m, 2H), 7.40 – 7.33 (m, 2H), 6.99 – 6.94 (m, 1H), 6.61 (s, 1H), 6.35 (d, *J* = 15.6 Hz, 1H), 4.26 (q, *J* = 7.2 Hz, 2H), 1.34 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.5, 138.4, 137.8, 133.0, 128.9, 127.5, 126.5, 125.5, 124.8, 122.3, 119.3, 119.2, 116.9, 114.5, 97.3, 60.2, 14.4.

(*E*)-3-(6-phenylindolizin-2-yl)prop-2-en-1-ol (2ed)



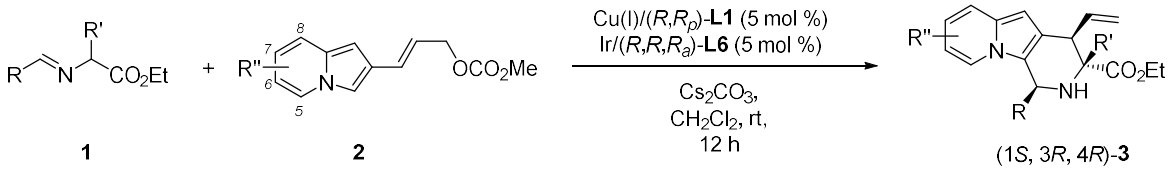
Yield (90%); Yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.53 (s, 1H), 7.67 – 7.60 (m, 3H), 7.48 – 7.39 (m, 3H), 7.36 – 7.31 (m, 1H), 7.04 – 6.99 (m, 1H), 6.57 (d, J = 16.0 Hz, 1H), 6.52 (s, 1H), 6.22 (dt, J = 16.0, 5.2 Hz, 1H), 4.81 (t, J = 5.6 Hz, 1H), 4.14 – 4.07 (m, 2H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 138.8, 133.0, 130.8, 130.2, 128.4, 128.2, 127.2, 124.1, 124.0, 123.7, 119.8, 118.8, 113.4, 97.4, 63.0.

(*E*)-methyl (3-(6-phenylindolizin-2-yl)allyl) carbonate (2e)



Yield (83%); Yellow solid, m.p. = 105 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.55 (s, 1H), 7.68 – 7.63 (m, 3H), 7.48 – 7.41 (m, 3H), 7.37 – 7.31 (m, 1H), 7.06 – 7.01 (m, 1H), 6.75 (d, J = 16.0 Hz, 1H), 6.58 (s, 1H), 6.21 (dt, J = 16.0, 6.4 Hz, 1H), 4.75 (d, J = 6.4 Hz, 2H), 3.72 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 156.4, 138.7, 133.1, 130.2, 129.5, 128.4, 127.3, 127.1, 124.4, 124.2, 122.8, 120.0, 119.2, 114.3, 97.6, 69.5, 55.9.

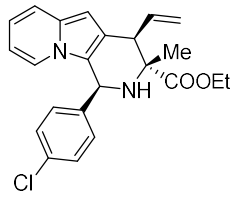
3. General Procedures and Characterization for Fused Indolizine



A flame dried Schlenk tube **A** was cooled to room temperature and filled with N_2. To this flask were added $[Ir(COD)Cl]_2$ (0.005 mmol), (*S,S,S*)-**L6** (0.010 mmol), degassed THF (0.5 mL) and degassed *n*-propylamine (0.5 mL). The reaction mixture was heated at 50 ºC for 30 min and then the volatile solvents were removed under vacuum to gain a pale-yellow solid. Meanwhile, $Cu(MeCN)_4BF_4$ (0.01 mmol) and (R,R_p)-^{i}Pr-Phosferrox-**L1** (0.011 mmol, 5.5 mol %) were dissolved in 1.0 mL of DCM in a Schlenk tube **B**, and stirred at room temperature for about 30 min. Aldimine esters (0.30 mmol), indolizine derived allylic carbonates (0.20 mmol), Ir complexs (0.01 mmol, 5 mol %), base (0.20 mmol)

and DCM (1.0 mL) were added into the Schlenk tube **A** and filled with N_2. The Cu/**L1** complex solution was then transferred from the Schlenk tube **B** to the Schlenk tube **A** *via* syringe. The reaction mixture was continuously stirred at room temperature under N_2 atmosphere. While the substrate was consumed (monitored by TLC), the reaction was purified by flash column chromatography to give the pure product. The dr value was determined by the crude ^{1}H NMR spectrum, and the enantiomeric excess was recorded by HPLC analysis in comparison with the racemic sample.

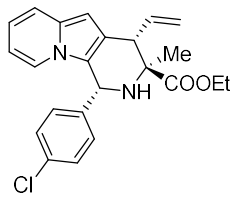
Ethyl (1*S*,3*R*,4*R*)-1-(4-chlorophenyl)-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3a



(1*S*,3*R*,4*R*)-**3a**

Yield (93%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -175.0 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.27 (m, 3H), 7.25 – 7.20 (m, 2H), 7.02 – 6.98 (m, 1H), 6.56 (m, 1H), 6.31 (s, 1H), 6.21 – 6.16 (m, 1H), 6.17 – 6.08 (m, 1H), 5.45 (s, 1H), 5.25 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.16 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.10 – 4.08 (m, 2H), 4.05 – 3.98 (m, 1H), 1.34 (s, 3H), 1.12 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.7, 140.3, 139.1, 133.8, 133.1, 129.8, 129.2, 126.4, 122.2, 118.8, 117.1, 116.4, 116.3, 109.4, 97.1, 62.1, 60.9, 54.9, 45.4, 25.0, 14.1. HRMS (ESI+) Calcd. For $C_{23}H_{23}ClN_2O_2$ ($[M+Na]^+$): 417.1340, found: 417.1340. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm); t_r = 6.41 and 10.82 min.

Ethyl (1*R*,3*S*,4*S*)-1-(4-chlorophenyl)-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*R*,3*S*,4*S*)-3a

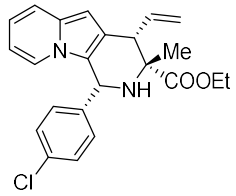


(1*R*,3*S*,4*S*)-**3a**

Yield (92%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = +171.5 (*c* 0.2, CH_2Cl_2). The product was analyzed by

HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm); t_r = 6.41 and 10.82 min.

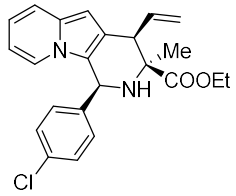
Ethyl (1*R*,3*R*,4*S*)-1-(4-chlorophenyl)-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*R*,3*R*,4*S*)-3a



(1*R*,3*R*,4*S*)-**3a**

Yield (90%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = +55.0 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.27 (m, 3H), 7.23 – 7.17 (m, 2H), 7.03 (m, 1H), 6.58 – 6.53 (m, 1H), 6.36 – 6.29 (m, 1H), 6.29 (s, 1H), 6.25 – 6.20 (m, 1H), 5.42 – 5.40 (m, 1H), 5.35 – 5.32 (m, 1H), 5.30 (s, 1H), 4.09 – 4.01 (m, 2H), 3.76 (d, *J* = 9.6 Hz, 1H), 1.43 (s, 3H), 1.12 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.4, 140.2, 137.5, 133.7, 132.7, 129.7, 129.2, 126.5, 121.9, 118.8, 118.7, 116.8, 115.9, 109.6, 96.4, 62.8, 60.5, 55.1, 51.1, 25.1, 14.1. HRMS (ESI+) Calcd. For $C_{23}H_{23}ClN_2O_2$ ($[M+H]^+$): 395.1520, found: 395.1515. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm); t_r = 7.20 and 13.66 min.

Ethyl (1*S*,3*S*,4*R*)-1-(4-chlorophenyl)-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*S*,4*R*)-3a

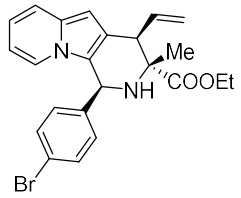


(1*S*,3*S*,4*R*)-**3a**

Yield (92%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -60.5 (*c* 0.2, CH_2Cl_2). The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm); t_r = 7.20 and 13.66 min.

Ethyl (1*S*,3*R*,4*R*)-1-(4-bromophenyl)-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]

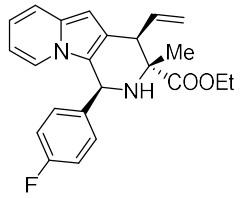
indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3b



(1*S*,3*R*,4*R*)-**3b**

Yield (85%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -89.5 (*c* 1.0, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 9.2 Hz, 1H), 7.17 (d, *J* = 8.4 Hz, 2H), 6.08 - 7.02 (m, 1H), 6.58 – 6.52(m, 1H), 6.31 (s, 1H), 6.22 – 6.16 (m, 1H), 6.17 – 6.08 (m, 1H), 5.44 (s, 1H), 5.25 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.15 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.12 – 4.04 (m, 2H), 4.05 – 3.99 (m, 1H), 1.33 (s, 3H), 1.12 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.7, 140.9, 139.1, 133.1, 132.2, 130.1, 126.4, 122.2, 121.9, 118.8, 117.0, 116.4, 116.3, 109.4, 97.1, 62.1, 60.9, 54.9, 45.4, 25.0, 14.1. HRMS (ESI+) Calcd. For $C_{23}H_{23}BrN_2O_2$ ($[M+H]^+$): 439.1016, found: 439.1005. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm); t_r = 5.82 and 9.52 min.

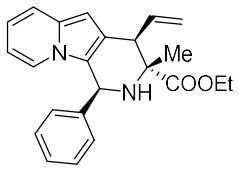
Ethyl (1*S*,3*R*,4*R*)-1-(4-fluorophenyl)-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-b]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3c



(1*S*,3*R*,4*R*)-**3c**

Yield (85%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -73.6 (*c* 0.5, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.24 (m, 3H), 7.04 – 6.97 (m, 3H), 6.57 – 6.51 (m, 1H), 6.31 (s, 1H), 6.21 – 6.09 (m, 2H), 5.47 (s, 1H), 5.29 – 5.22 (m, 1H), 5.18 – 5.13 (m, 1H), 4.11 – 4.05 (m, 2H), 4.05 – 3.99 (m, 1H), 1.34 (s, 3H), 1.12 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-d) δ 175.7, 162.4 (d, *J* = 244.9 Hz), 139.1, 137.5 (d, *J* = 3.0 Hz), 133.0, 130.0 (d, *J* = 8.1 Hz), 126.3, 122.2, 118.8, 117.4, 116.3 (d, *J* = 2.3 Hz), 116.0, 115.8, 109.3, 97.0, 62.1, 60.8, 54.8, 45.4, 24.9, 14.1. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -114.09. HRMS (ESI+) Calcd. For $C_{23}H_{23}FN_2O_2$ ($[M+H]^+$): 379.1816, found: 379.1810. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm); t_r = 4.93 and 7.49 min.

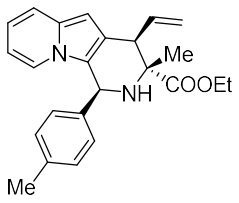
Ethyl (1*S*,3*R*,4*R*)-3-methyl-1-phenyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3d



(1*S*,3*R*,4*R*)-**3d**

Yield (88%); >20:1 dr; yellow solid; m.p. = 106 - 108 ºC. $[\alpha]^{20}_D$ = -264.0 (*c* 0.3, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.26 (m, 6H), 7.04 – 6.99 (m, 1H), 6.55 – 6.50 (m, 1H), 6.31 (s, 1H), 6.22 – 6.15 (m, 1H), 6.15 – 6.11 (m, 1H), 5.47 (s, 1H), 5.26 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.15 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.14 – 4.05 (m, 2H), 4.06 – 3.99 (m, 1H), 1.34 (s, 3H), 1.13 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.7, 141.6, 139.2, 132.9, 129.0, 128.4, 128.3, 128.1, 126.3, 122.40, 118.7, 117.6, 116.2, 109.2, 97.0, 62.1, 60.8, 55.6, 45.5, 25.0, 14.1. HRMS (ESI+) Calcd. For $C_{23}H_{24}N_2O_2$ ($[M+H]^+$): 361.1910, found: 361.1907. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 6.44 and 12.07 min.

Ethyl (1*S*,3*R*,4*R*)-3-methyl-1-(p-tolyl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3e

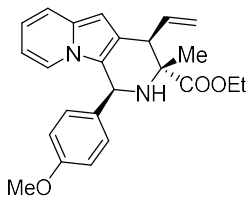


(1*S*,3*R*,4*R*)-**3e**

Yield (95%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -194.4 (*c* 0.5, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.28 – 7.25 (m, 1H), 7.18 – 7.10 (m, 4H), 7.06 – 7.02 (m, 1H), 6.55 – 6.49 (m, 1H), 6.31 (s, 1H), 6.21 – 6.14 (m, 1H), 6.15 – 6.11 (m, 1H), 5.42 (s, 1H), 5.25 (dd, *J* = 17.2, 1.0 Hz, 1H), 5.14 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.13 – 4.03 (m, 2H), 4.05 – 3.98 (m, 1H), 2.33 (s, 3H), 1.33 (s, 3H), 1.12 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.8, 139.4, 138.7, 137.8, 132.9, 129.7, 128.2, 126.3, 122.5, 118.7, 117.8, 116.10, 116.05, 109.1, 96.9, 62.1, 60.8, 55.2, 45.5, 25.0, 21.2, 14.1. HRMS (ESI+) Calcd. For $C_{24}H_{26}N_2O_2$ ($[M+H]^+$): 375.2067, found: 375.2063. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0

mL/min, λ = 254 nm); t_r = 7.84 and 11.78 min.

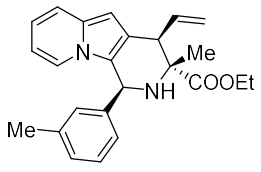
Ethyl (1*S*,3*R*,4*R*)-1-(4-methoxyphenyl)-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3f



(1*S*,3*R*,4*R*)-**3f**

Yield (92%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -127.2 (*c* 0.5, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.28 – 7.26 (m, 1H), 7.23 – 7.18 (m, 2H), 7.03 – 7.07 (m, 1H), 6.88 – 6.83 (m, 2H), 6.56 – 6.50 (m, 1H), 6.30 (s, 1H), 6.21 – 6.15 (m, 1H), 6.16 – 6.11 (m, 1H), 5.42 (s, 1H), 5.25 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.15 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.13 – 4.04 (m, 2H), 4.04 – 4.00 (m, 1H), 3.79 (s, 3H), 1.33 (s, 3H), 1.13 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.8, 159.4, 139.3, 133.8, 132.9, 129.4, 126.3, 122.6, 122.5, 118.7, 117.9, 116.1, 114.4, 109.1, 96.9, 62.1, 60.8, 55.3, 54.9, 45.5, 25.1, 14.2. HRMS (ESI+) Calcd. For $C_{24}H_{26}N_2O_3$ ($[M+H]^+$): 391.2016, found: 391.2010. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm); t_r = 6.35 and 8.56 min.

Ethyl (1*S*,3*R*,4*R*)-3-methyl-1-(m-tolyl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3g

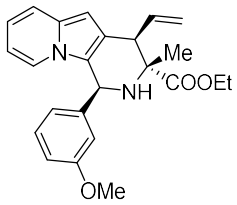


(1*S*,3*R*,4*R*)-**3g**

Yield (90%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -143.2 (*c* 0.3, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.25 (m, 1H), 7.23 – 7.18 (m, 1H), 7.13 – 7.01 (m, 4H), 6.57 – 6.49 (m, 1H), 6.31 (s, 1H), 6.22 – 6.15 (m, 1H), 6.16 – 6.11 (m, 1H), 5.41 (s, 1H), 5.26 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.15 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.14 – 4.04 (m, 2H), 4.05 – 4.00 (m, 1H), 2.31 (s, 3H), 1.34 (s, 3H), 1.13 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.7, 141.5, 139.3, 138.7, 132.92, 129.0, 128.90, 128.87, 126.3, 125.3, 122.5, 118.7, 117.7, 116.2, 116.1, 109.1, 96.9, 62.1, 60.8, 55.6, 45.5, 25.1, 21.4,

14.1. HRMS (ESI+) Calcd. For $C_{24}H_{26}N_2O_2$ ($[M+H]^+$): 375.2067, found: 375.2063. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 5.93 and 11.13 min.

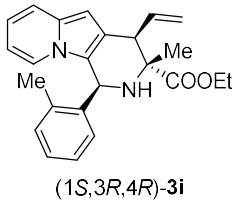
Ethyl (1*S*,3*R*,4*R*)-1-(3-methoxyphenyl)-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3h



(1*S*,3*R*,4*R*)-**3h**

Yield (91%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -146.5 (*c* 0.15, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.25 (m, 1H), 7.25 – 7.21 (m, 1H), 7.08 – 7.04 (m, 1H), 6.89 – 6.82 (m, 3H), 6.56 – 6.50 (m, 1H), 6.30 (s, 1H), 6.22 – 6.16 (m, 1H), 6.17 – 6.11 (m, 1H), 5.43 (s, 1H), 5.25 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.15 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.13 – 4.04 (m, 2H), 4.05 – 3.99 (m, 1H), 3.75 (s, 3H), 1.35 (s, 3H), 1.12 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.8, 160.1, 143.4, 139.2, 133.0, 130.0, 126.2, 122.5, 120.6, 118.7, 117.5, 116.22, 116.19, 113.9, 113.5, 109.2, 97.0, 62.1, 60.8, 55.6, 55.2, 45.5, 25.0, 14.1. HRMS (ESI+) Calcd. For $C_{24}H_{26}N_2O_3$ ($[M+H]^+$): 391.2016, found: 391.2008. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 80/20, flow rate 1.0 mL/min, λ = 254 nm); t_r = 4.48 and 6.22 min.

Ethyl (1*S*,3*R*,4*R*)-3-methyl-1-(o-tolyl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3i

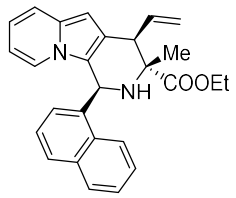


(1*S*,3*R*,4*R*)-**3i**

Yield (87%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -175.0 (*c* 0.1, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.24 (m, 2H), 7.21 – 7.16 (m, 1H), 7.08 – 7.00 (m, 1H), 6.87 – 6.78 (m, 2H), 6.56 – 6.48 (m, 1H), 6.33 (s, 1H), 6.19 – 6.13 (m, 1H), 6.14 – 6.08 (m, 1H), 5.74 (s, 1H), 5.24 (dd, *J* = 17.0 Hz,

2.0, 1H), 5.13 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.16 – 4.06 (m, 2H), 4.07 – 3.99 (m, 1H), 2.67 (s, 3H), 1.34 (s, 3H), 1.17 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.7, 139.2, 138.7, 136.1, 132.8, 130.8, 127.8, 127.7, 127.0, 126.7, 122.4, 118.7, 117.9, 116.1, 116.0, 109.2, 97.1, 62.0, 60.8, 50.9, 45.4, 25.1, 18.9, 14.2. HRMS (ESI+) Calcd. For $C_{24}H_{26}N_2O_2$ ([M+H]$^+$): 375.2067, found: 375.2063. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 4.06 and 4.63 min.

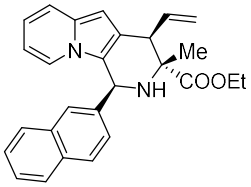
Ethyl (1*S*,3*R*,4*R*)-3-methyl-1-(naphthalen-1-yl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3j



(1S,3*R*,4*R*)-**3j**

Yield (86%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -346.0 (*c* 0.05, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.57 (d, *J* = 8.4 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.70 - 7.63 (m, 1H), 7.60 - 7.52 (m, 1H), 7.35 - 7.27(m, 2H), 6.95 (d, *J* = 7.2 Hz, 1H), 6.82 (d, *J* = 7.2 Hz, 1H), 6.58 - 6.51 (m, 1H), 6.39 (s, 1H), 6.39 - 6.34 (m, 1H), 6.16 - 6.08 (m, 1H), 6.09 - 6.03 (m, 1H), 5.25 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.14 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.21 - 4.11 (m, 2H), 4.12 - 4.04 (m, 1H), 1.34 (s, 3H), 1.20 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.8, 139.0, 135.9, 134.3, 133.1, 131.9, 129.1, 128.3, 127.2, 126.8, 126.1, 125.8, 124.8, 123.0, 118.7, 117.1, 116.4, 116.1, 115.8, 109.1, 97.2, 62.3, 60.9, 50.3, 45.6, 25.0, 14.2. HRMS (ESI+) Calcd. For $C_{27}H_{26}N_2O_2$ ([M+H]$^+$): 411.2067, found: 411.2066. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 4.64 and 6.20 min.

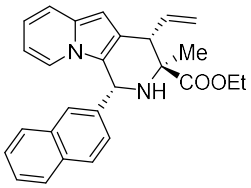
Ethyl (1*S*,3*R*,4*R*)-3-methyl-1-(naphthalen-2-yl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3k



(1*S*,3*R*,4*R*)-**3k**

Yield (95%); >20:1 dr; yellow solid; m.p. = 154- 156 ºC. $[\alpha]^{20}_{D}$ = -42.4 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (s, 1H), 7.85 – 7.79 (m, 2H), 7.77 – 7.73 (m, 1H), 7.50 – 7.44 (m, 2H), 7.31 – 7.25 (m, 2H), 7.09 – 7.04 (m, 1H), 6.53 – 6.46 (m, 1H), 6.35 (s, 1H), 6.29 – 6.18 (m, 1H), 6.09 – 6.04 (m, 1H), 5.64 (s, 1H), 5.31 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.18 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.16 – 4.08 (m, 2H), 4.09 – 4.03 (m, 1H), 1.35 (s, 3H), 1.15 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.8, 139.31, 139.29, 133.5, 133.3, 133.0, 129.1, 127.8, 127.7, 127.4, 126.5, 126.1, 126.0, 125.9, 122.4, 118.7, 117.4, 116.3, 116.1, 109.3, 97.0, 62.1, 60.8, 55.8, 45.6, 25.0, 14.2. HRMS (ESI+) Calcd. For $C_{27}H_{26}N_2O_2$ ($[M+H]^+$): 411.2067, found: 411.2062. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak IE, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 250 nm); t_r = 6.65 and 7.10 min.

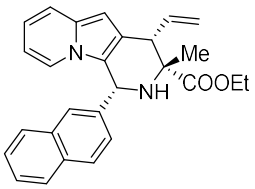
Ethyl (1*R*,3*S*,4*S*)-3-methyl-1-(naphthalen-2-yl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*R*,3*S*,4*S*)-3k



(1*R*,3*S*,4*S*)-**3k**

Yield (93%); >20:1 dr; yellow oil. $[\alpha]^{20}_{D}$ = +43.5 (*c* 0.2, CH_2Cl_2). The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak IE, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 250 nm); t_r = 6.65 and 7.10 min.

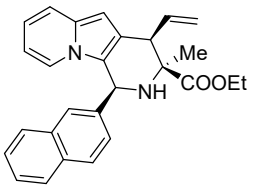
Ethyl (1*R*,3*R*,4*S*)-3-methyl-1-(naphthalen-2-yl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*R*,3*R*,4*S*)-3k



(1*R*,3*R*,4*S*)-**3k**

Yield (92%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = +143.0 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 – 7.78 (m, 3H), 7.78 – 7.74 (m, 1H), 7.50 – 7.44 (m, 2H), 7.33 - 7.26 (m, 2H), 7.12 – 7.07 (m, 1H), 6.55 – 6.48 (m, 1H), 6.40 – 6.31 (m, 1H), 6.33 (s, 1H), 6.14 – 6.09 (m, 1H), 5.60 (s, 1H), 5.39 – 5.34 (m, 1H), 5.34 – 5.31 (m, 1H), 4.13 – 4.04 (m, 2H), 3.84 (d, *J* = 10.0 Hz, 1H), 1.46 (s, 3H), 1.15 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.4, 139.2, 137.6, 133.5, 133.3, 132.7, 129.1, 127.9, 127.7, 127.3, 126.5, 126.1, 126.04, 126.02, 122.0, 118.73, 118.65, 117.2, 115.8, 109.5, 96.3, 62.8, 60.5, 56.0, 51.2, 25.2, 14.2. HRMS (ESI+) Calcd. For $C_{27}H_{26}N_2O_2$ ($[M+H]^+$): 411.2067, found: 411.2061. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak IE, *i*-propanol/hexane = 5/95, flow rate 0.5 mL/min, λ = 254 nm); t_r = 13.66 and 14.48 min.

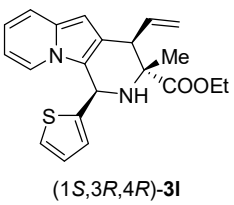
Ethyl (1*S*,3*S*,4*R*)-3-methyl-1-(naphthalen-2-yl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*S*,4*R*)-3k



(1*S*,3*S*,4*R*)-**3k**

Yield (93%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -149.0 (*c* 0.2, CH_2Cl_2). The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak IE, *i*-propanol/hexane = 5/95, flow rate 0.5 mL/min, λ = 254 nm); t_r = 13.66 and 14.48 min.

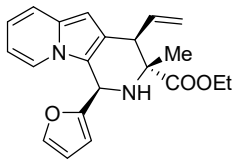
Ethyl (1*S*,3*R*,4*R*)-3-methyl-1-(thiophen-2-yl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3l



(1*S*,3*R*,4*R*)-**3l**

Yield (82%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -192.5 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.30 – 7.26 (m, 2H), 7.24 – 7.21 (m, 1H), 7.17 – 7.14 (m, 1H), 6.94 – 6.98 (m, 1H), 6.59 – 6.53 (m, 1H), 6.28 (s, 1H), 6.27 – 6.22 (m, 1H), 6.21 – 6.11 (m, 1H), 5.84 (s, 1H), 5.23 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.16 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.11 – 4.02 (m, 2H), 4.03 – 3.96 (m, 1H), 1.35 (s, 3H), 1.09 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.7, 146.7, 138.9, 133.1, 126.3, 126.1, 126.0, 125.7, 122.2, 118.7, 117.5, 116.5, 116.4, 109.4, 96.9, 62.2, 60.8, 50.3, 45.5, 24.8, 14.1. HRMS (ESI+) Calcd. For $C_{21}H_{22}N_2O_2S$ ($[M+H]^+$): 367.1474, found: 367.1470. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 8.02 and 12.30 min.

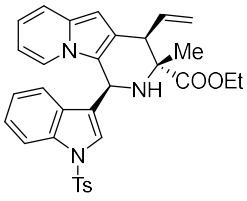
Ethyl (1*S*,3*R*,4*R*)-1-(furan-2-yl)-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3m



(1*S*,3*R*,4*R*)-**3m**

Yield (86%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -292.0 (*c* 0.1, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.34 (m, 1H), 7.31 – 7.26 (m, 2H), 6.60 – 6.54 (m, 1H), 6.34 – 6.31 (m, 1H), 6.31 – 6.27 (m, 1H), 6.28 (s, 1H), 6.28 – 6.24 (m, 1H), 6.19 – 6.07 (m, 1H), 5.67 (s, 1H), 5.21 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.15 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.10 – 4.02 (m, 2H), 4.03 – 3.97 (m, 1H), 1.36 (s, 3H), 1.09 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.6, 154.0, 142.6, 138.6, 133.1, 125.9, 122.2, 118.8, 116.7, 116.3, 115.4, 110.3, 109.5, 108.0, 97.0, 62.0, 60.9, 48.6, 45.4, 24.7, 14.1. HRMS (ESI+) Calcd. For $C_{21}H_{22}N_2O_3$ ($[M+H]^+$): 351.1703, found: 351.1700. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm); t_r = 6.22 and 7.89 min.

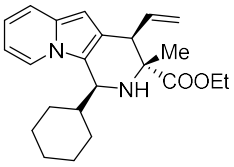
Ethyl (1*S*,3*R*,4*R*)-3-methyl-1-(1-tosyl-1H-indol-3-yl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3n



(1*S*,3*R*,4*R*)-**3n**

Yield (90%); >20:1 dr; yellow solid; m.p. = 80 - 82 ºC. $[\alpha]^{20}_D$ = -208.5 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.97 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.51 (s, 1H), 7.29 – 7.25 (m, 2H), 7.23 – 7.19 (m, 2H), 7.13 – 7.00 (m, 3H), 6.54 – 6.48 (m, 1H), 6.34 (s, 1H), 6.18 – 6.07 (m, 1H), 6.03 – 5.97 (m, 1H), 5.76 (s, 1H), 5.29 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.15 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.16 – 4.06 (m, 2H), 4.07 – 4.01 (m, 1H), 2.37 (s, 3H), 1.32 (s, 3H), 1.15 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.7, 145.0, 138.5, 135.8, 133.1, 129.9, 129.2, 127.0, 126.9, 126.0, 125.1, 125.0, 123.5, 122.5, 122.2, 120.0, 118.8, 116.3, 116.1, 116.0, 113.8, 109.2, 97.3, 61.9, 60.9, 46.9, 45.5, 25.0, 21.6, 14.2. HRMS (ESI+) Calcd. For $C_{32}H_{31}N_3O_4S$ ($[M+H]^+$): 554.2108, found: 554.2097. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm); t_r = 7.18 and 10.49 min.

Ethyl (1*S*,3*R*,4*R*)-1-cyclohexyl-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3o

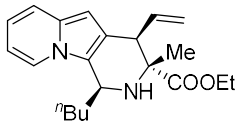


(1*S*,3*R*,4*R*)-**3o**

Yield (59%); 10:1 dr; yellow oil. $[\alpha]^{20}_D$ = -235.0 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 (d, *J* = 7.2 Hz, 1H), 7.27 (d, *J* = 7.6 Hz, 1H), 6.59 – 6.53 (m, 1H), 6.43 – 6.36 (m, 1H), 6.23 (s, 1H), 6.12 – 6.00 (m, 1H), 5.21 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.07 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.52 – 4.48 (m, 1H), 4.00 – 3.93 (m, 1H), 3.94 – 3.85 (m, 2H), 2.15 – 2.04 (m, 1H), 1.88 – 1.74 (m, 3H), 1.68 – 1.57 (m, 2H), 1.53 – 1.43 (m, 1H), 1.41 – 1.32 (m, 2H), 1.30 (s, 3H), 1.20 – 1.10 (m, 1H), 0.99 (t, *J* = 7.2 Hz, 3H), 0.85 – 0.78 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.5, 139.3, 132.9, 126.6, 122.6, 119.1, 118.5, 115.5, 115.3, 109.2, 97.1, 61.4, 60.4, 54.5, 46.1, 39.8, 29.9, 27.1, 26.5, 26.4, 26.2, 25.1, 14.1. HRMS (ESI+) Calcd. For $C_{23}H_{30}N_2O_2$ ($[M+H]^+$): 367.2380, found: 367.2376. The product was analyzed by HPLC to determine the enantiomeric excess: 96% ee (Chiralpak AD-H, *i*-

propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 4.71 and 8.48 min.

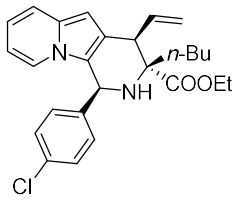
Ethyl (1*S*,3*R*,4*R*)-1-butyl-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3p



(1*S*,3*R*,4*R*)-**3p**

Yield (60%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -240.0 (*c* 0.3, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 – 7.60 (m, 1H), 7.30 – 7.26 (m, 1H), 6.61 – 6.54 (m, 1H), 6.44 - 6.38 (m, 1H), 6.23 (s, 1H), 6.12 – 6.01 (m, 1H), 5.20 – 5.13 (m, 1H), 5.13 – 5.09 (m, 1H), 4.57 – 4.52 (m, 1H), 4.03 – 3.97 (m, 1H), 3.97 – 3.89 (m, 2H), 2.00 – 1.93 (m, 1H), 1.79 – 1.67 (m, 1H), 1.53 – 1.36 (m, 2H), 1.35 (s, 3H), 1.34 – 1.25 (m, 2H), 1.01 (t, *J* = 7.2 Hz, 3H), 0.90 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.0, 138.9, 132.7, 125.4, 122.1, 119.5, 119.1, 116.2, 115.5, 109.3, 97.0, 61.7, 60.6, 49.7, 45.8, 34.0, 27.3, 24.8, 22.8, 14.06, 14.04. HRMS (ESI+) Calcd. For $C_{21}H_{28}N_2O_2$ ($[M+H]^+$): 341.2223, found: 341.2222. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak IA, *i*-propanol/hexane = 1/99, flow rate 0.3 mL/min, λ = 254 nm); t_r = 26.21 and 30.68 min.

Ethyl (1*S*,3*R*,4*R*)-3-butyl-1-(4-chlorophenyl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3q

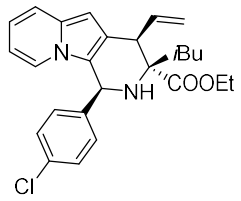


(1*S*,3*R*,4*R*)-**3q**

Yield (93%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -103.0 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.26 (m, 3H), 7.24 – 7.20 (m, 2H), 6.99 (m, 1H), 6.57 – 6.51 (m, 1H), 6.31 (s, 1H), 6.20 – 6.14 (m, 1H), 6.16 – 6.08 (m, 1H), 5.40 (s, 1H), 5.27 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.13 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.12 – 4.04 (m, 2H), 4.05 – 3.99 (m, 1H), 1.81 – 1.69 (m, 1H), 1.60 – 1.48 (m, 1H), 1.30 – 1.23 (m, 4H), 1.11 (t, *J* = 7.2 Hz, 3H), 0.87 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.6, 140.4, 139.2, 133.7, 133.1, 129.8, 129.2, 126.6, 122.2, 118.8, 117.3, 116.3, 115.8, 109.3, 97.0, 65.4, 60.6, 54.9, 44.5, 37.6, 25.5, 22.9, 14.3, 13.9. HRMS (ESI+) Calcd. For $C_{26}H_{29}ClN_2O_2$ ($[M+H]^+$):

437.1990, found: 437.1979. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 9.50 and 13.47 min.

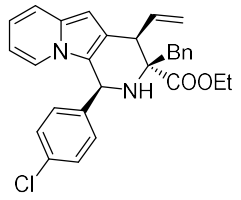
Ethyl (1*S*,3*R*,4*R*)-1-(4-chlorophenyl)-3-isobutyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3r



(1*S*,3*R*,4*R*)-**3r**

Yield (88%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -115.5 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.26 (m, 3H), 7.24 – 7.19 (m, 2H), 7.02 – 6.96 (m, 1H), 6.58 – 6.51 (m, 1H), 6.30 (s, 1H), 6.21 – 6.15 (m, 1H), 6.16 – 6.08 (m, 1H), 5.42 (s, 1H), 5.25 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.13 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.13 – 4.09 (m, 1H), 4.02 (q, *J* = 7.2 Hz, 2H), 1.82 – 1.71 (m, 2H), 1.49 – 1.41 (m, 1H), 1.10 (t, *J* = 7.2 Hz, 3H), 0.92 – 0.87 (m, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.7, 140.4, 139.4, 133.7, 133.0, 129.8, 129.2, 126.6, 122.2, 118.8, 117.2, 116.3, 115.9, 109.3, 96.9, 65.1, 60.6, 54.8, 46.9, 45.6, 24.4, 24.0, 23.7, 14.1. HRMS (ESI+) Calcd. For $C_{26}H_{29}ClN_2O_2$ ($[M+H]^+$): 437.1990, found: 437.1981. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 7.83 and 10.38 min.

Ethyl (1*S*,3*R*,4*R*)-3-benzyl-1-(4-chlorophenyl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3s

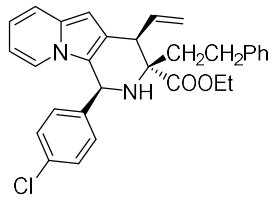


(1*S*,3*R*,4*R*)-**3s**

Yield (96%); >20:1 dr; yellow solid; m.p. = 62 - 64 ºC. $[\alpha]^{20}_D$ = -120.5 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.25 (m, 4H), 7.24 – 7.19 (m, 4H), 7.11 – 7.07 (m, 2H), 7.00 - 6.97 (m, 1H), 6.56 – 6.50 (m, 1H), 6.37 – 6.26 (m, 1H), 6.30 (s, 1H), 6.19 – 6.14 (m, 1H), 5.38 (dd, *J* = 17.2

Hz, 2.0 Hz, 1H), 5.36 (s, 1H), 5.23 (dd, *J* = 10.0 Hz, 2.0 Hz, 1H), 4.20 – 4.14 (m, 1H), 3.94 – 3.82 (m, 2H), 3.08 (d, *J* = 13.6 Hz, 1H), 2.88 (d, *J* = 13.6 Hz, 1H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 173.9, 140.7, 139.6, 136.0, 133.6, 133.1, 129.9, 129.8, 129.1, 128.4, 127.0, 126.2, 122.1, 118.8, 117.5, 116.4, 116.2, 109.4, 96.7, 66.4, 60.5, 54.9, 46.1, 44.2, 14.0. HRMS (ESI+) Calcd. For $C_{29}H_{27}ClN_2O_2$ ([M+H]$^+$): 471.1833, found: 471.1816. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 8.41 and 34.84 min.

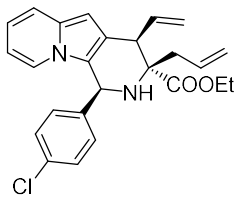
Ethyl (1*S*,3*R*,4*R*)-1-(4-chlorophenyl)-3-phenethyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3t



(1*S*,3*R*,4*R*)-**3t**

Yield (85%); >20:1 dr; yellow solid; m.p. = 61 - 62 ºC. $[\alpha]^{20}_D$ = -172.0 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.25 (m, 4H), 7.25 – 7.11 (m, 6H), 7.02 – 6.98 (m, 1H), 6.59 – 6.53 (m, 1H), 6.33 (s, 1H), 6.23 – 6.18 (m, 1H), 6.19 – 6.12 (m, 1H), 5.43 (s, 1H), 5.33 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.17 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.20 – 4.16 (m, 1H), 4.14 – 4.04 (m, 2H), 2.73 – 2.62 (m, 1H), 2.62 – 2.51 (m, 1H), 2.10 – 2.00 (m, 1H), 1.90 – 1.80 (m, 1H), 1.15 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.4, 141.3, 140.3, 139.0, 133.8, 133.1, 129.8, 129.2, 128.4, 128.3, 126.3, 126.0, 122.2, 118.8, 117.2, 116.4, 116.1, 109.4, 97.0, 65.3, 60.9, 54.9, 44.6, 39.7, 29.9, 14.4. HRMS (ESI+) Calcd. For $C_{30}H_{29}ClN_2O_2$ ([M+H]$^+$): 485.1990, found: 485.1980. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 12.45 and 27.72 min.

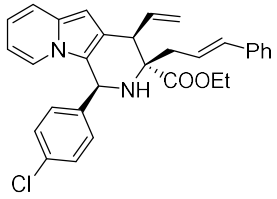
Ethyl (1*S*,3*R*,4*R*)-3-allyl-1-(4-chlorophenyl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3u



(1*S*,3*R*,4*R*)-**3u**

Yield (96%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -328.0 (*c* 0.05, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.26 (m, 3H), 7.24 – 7.20 (m, 2H), 7.03 – 6.98 (m, 1H), 6.58 – 6.52 (m, 1H), 6.30 (s, 1H), 6.22 – 6.16 (m, 1H), 6.18 – 6.11 (m, 1H), 5.78 – 5.66 (m, 1H), 5.46 (s, 1H), 5.29 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.15 (dd, *J* = 10.0, 2.0 Hz, 1H), 5.13 (s, 1H), 5.11 – 5.07 (m, 1H), 4.12 – 4.02 (m, 2H), 4.03 – 3.97 (m, 1H), 2.57 – 2.48 (m, 1H), 2.37 – 2.27 (m, 1H), 1.12 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.2, 140.5, 139.1, 133.7, 133.1, 131.9, 129.8, 129.2, 126.2, 122.2, 119.6, 118.8, 117.4, 116.4, 116.1, 109.4, 96.9, 65.0, 60.8, 54.9, 45.1, 42.4, 14.3. HRMS (ESI+) Calcd. For $C_{25}H_{25}ClN_2O_2$ ($[M+H]^+$): 421.1677, found: 421.1672. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak IA, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 8.59 and 9.54 min.

Ethyl (1*S*,3*R*,4*R*)-1-(4-chlorophenyl)-3-cinnamyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3v

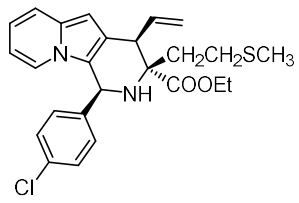


(1*S*,3*R*,4*R*)-**3v**

Yield (95%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -7.6 (*c* 0.25, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.25 (m, 8H), 7.24 – 7.19 (m, 2H), 7.02 – 6.98 (m, 1H), 6.57 – 6.52 (m, 1H), 6.44 (d, *J* = 15.6 Hz, 1H), 6.31 (s, 1H), 6.27 – 6.17 (m, 1H), 6.19 – 6.16 (m, 1H), 6.13 – 6.03 (m, 1H), 5.46 (s, 1H), 5.33 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.19 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.14 (d, *J* = 8.8 Hz, 1H), 4.10 – 3.98 (m, 2H), 2.71 – 2.64 (m, 1H), 2.51 – 2.44 (m, 1H), 1.09 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.3, 140.4, 139.2, 137.0, 134.3, 133.7, 133.1, 129.9, 129.2, 128.5, 127.4, 126.2, 126.2, 123.3, 122.2, 118.8, 117.4, 116.4, 116.2, 109.4, 96.9, 65.4, 60.8, 54.9, 45.2, 41.6, 14.3. HRMS (ESI+) Calcd. For $C_{31}H_{29}ClN_2O_2$ ($[M+H]^+$): 497.1990, found: 497.1982. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow

rate 1.0 mL/min, λ = 254 nm); t_r = 13.65 and 16.59 min.

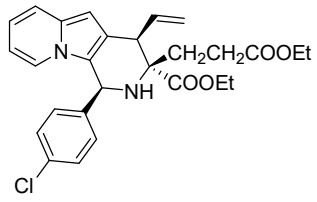
Ethyl (1*S*,3*R*,4*R*)-1-(4-chlorophenyl)-3-(2-(methylthio)ethyl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3w



(1*S*,3*R*,4*R*)-**3w**

Yield (97%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -104.0 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.26 (m, 3H), 7.24 – 7.20 (m, 2H), 7.01 – 6.97 (m, 1H), 6.60 – 6.52 (m, 1H), 6.30 (s, 1H), 6.21 – 6.17 (m , 1H), 6.18 – 6.09 (m, 1H), 5.40 (s, 1H), 5.31 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.16 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.12 – 4.04 (m, 2H), 4.06 – 4.01 (m, 1H), 2.59 – 2.40 (m, 2H), 2.06 (s, 3H), 2.07 – 2.02 (m, 1H), 1.88 – 1.79 (m, 1H), 1.12 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.0, 140.1, 138.7, 133.9, 133.1, 129.8, 129.2, 126.1, 122.2, 118.8, 117.0, 116.5, 116.3, 109.5, 96.9, 65.2, 61.0, 54.8, 44.6, 37.5, 28.0, 15.4, 14.3. HRMS (ESI+) Calcd. For $C_{25}H_{27}ClN_2O_2S$ ($[M+H]^+$): 455.1554, found: 455.1548. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 18.66 and 20.08 min.

Ethyl (1*S*,3*R*,4*R*)-1-(4-chlorophenyl)-3-(3-ethoxy-3-oxopropyl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3x

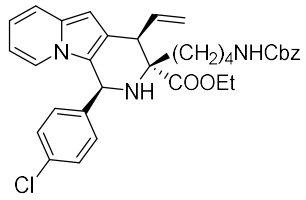


(1*S*,3*R*,4*R*)-**3x**

Yield (91%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -115.5 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.26 (m, 3H), 7.24 – 7.19 (m, 2H), 7.02 – 6.97 (m, 1H), 6.59 – 6.52 (m, 1H), 6.31 (s, 1H), 6.22 – 6.17 (m, 1H), 6.18 – 6.08 (m, 1H), 5.40 (s, 1H), 5.30 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.16 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.12 – 4.07 (m, 2H), 4.08 – 4.03 (m, 2H), 4.04 – 4.00 (m, 1H), 2.43 – 2.34 (m, 2H), 2.10 – 2.04 (m, 1H), 1.97 – 1.89 (m, 1H), 1.22 (t, *J* = 7.2 Hz, 3H), 1.11 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR

(100 MHz, Chloroform-*d*) δ 173.9, 172.8, 140.1, 138.6, 133.9, 133.1, 129.8, 129.2, 126.1, 122.2, 118.8, 117.1, 116.5, 116.4, 109.5, 97.0, 64.7, 61.0, 60.5, 54.8, 44.5, 32.3, 28.7, 14.2, 14.1. HRMS (ESI+) Calcd. For $C_{27}H_{29}ClN_2O_4$ ($[M+Na]^+$): 503.1708, found: 503.1707. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 18.72 and 31.11 min.

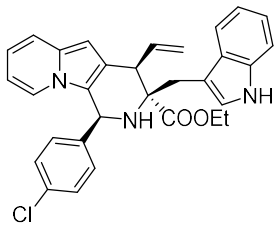
Ethyl (1*S*,3*R*,4*R*)-3-(4-(((benzyloxy)carbonyl)amino)butyl)-1-(4-chlorophenyl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3y



(1*S*,3*R*,4*R*)-**3y**

Yield (94%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -66.0 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.28 (m, 8H), 7.26 – 7.20 (m, 2H), 6.99 (d, *J* = 7.2 Hz, 1H), 6.58 – 6.51 (m, 1H), 6.30 (s, 1H), 6.20 – 6.16 (m, 1H), 6.16 – 6.06 (m, 1H), 5.39 (s, 1H), 5.27 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.12 (dd, *J* = 10.0, 2.0 Hz, 1H), 5.07 (s, 2H), 4.74 (br, 1H), 4.11 – 4.03 (m, 2H), 4.04 – 4.01 (m, 1H), 3.20 – 3.10 (m, 2H), 1.78 – 1.70 (m, 1H), 1.59 – 1.52 (m, 1H), 1.48 – 1.42 (m, 2H), 1.36 – 1.29 (m, 2H), 1.08 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.4, 156.3, 140.3, 139.1, 136.5, 133.8, 133.1, 129.8, 129.2, 128.8, 128.5, 128.1, 126.3, 122.1, 118.8, 117.1, 116.4, 115.9, 109.4, 96.9, 66.6, 65.2, 60.8, 54.9, 44.5, 40.7, 37.4, 30.0, 20.5, 14.2. HRMS (ESI+) Calcd. For $C_{34}H_{36}ClN_3O_4$ ($[M+H]^+$): 586.2467, found: 586.2455. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak ID, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 242 nm); t_r = 21.32 and 33.43 min.

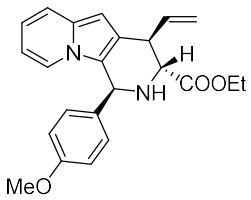
Ethyl (1*S*,3*R*,4*R*)-3-((1H-indol-3-yl)methyl)-1-(4-chlorophenyl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3z



(1*S*,3*R*,4*R*)-**3z**

Yield (55%); >20:1 dr; yellow solid; m.p. = 93 ºC. $[\alpha]^{20}_{D}$ = -2.0 (*c* 0.3, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (s, 1H), 7.50 – 7.46 (m, 1H), 7.30 – 7.25 (m, 4H), 7.18 – 7.10 (m, 3H), 7.05 – 6.96 (m, 3H), 6.56- 6.49 (m, 1H), 6.42 – 6.32 (m, 1H), 6.32 (s, 1H), 6.19 – 6.12 (m, 1H), 5.40 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.37 (s, 1H), 5.24 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.26 (d, *J* = 10.0 Hz, 1H), 3.74 (q, *J* = 7.2 Hz, 2H), 3.29 – 3.07 (m, 2H), 0.83 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.6, 140.9, 139.7, 136.0, 133.5, 133.1, 129.9, 129.0, 128.0, 126.3, 123.1, 122.2, 122.0, 119.4, 118.84, 118.75, 117.6, 116.3, 116.1, 111.1, 110.0, 109.3, 96.8, 65.8, 60.7, 54.9, 46.0, 33.7, 13.8. HRMS (ESI+) Calcd. For $C_{31}H_{28}ClN_3O_2$ ($[M+H]^+$): 510.1943, found: 510.1939. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm); t_r = 7.85 and 14.34 min.

Ethyl (1*S*,3*R*,4*R*)-1-(4-methoxyphenyl)-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-b]indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3A

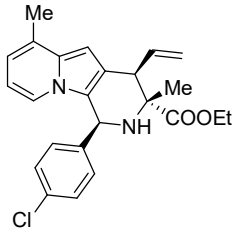


(1*S*, 3*R*, 4*R*)-**3A**

Yield (69%); 6:1 dr; yellow oil. $[\alpha]^{20}_{D}$ = -13.2 (*c* 0.5, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.31 (m, 1H), 7.18 – 7.14 (m, 2H), 7.02 – 6.98 (m, 1H), 6.90 – 6.85 (m, 2H), 6.61 – 6.55 (m, 1H), 6.33 (s, 1H), 6.24 – 6.19 (m, 1H), 5.85 – 5.73 (m, 1H), 5.33 – 5.27 (m, 1H), 5.27 – 5.21 (m, 2H), 4.18 (q, *J* = 7.2 Hz, 2H), 3.85 – 3.81 (m, 1H), 3.80 (s, 3H), 3.54 (d, *J* = 10.0 Hz, 1H), 1.26 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 172.1, 159.6, 137.3, 132.5, 131.7, 129.3, 126.3, 122.7, 118.7, 118.2, 117.7, 116.3, 114.6, 109.6, 96.9, 62.2, 60.8, 56.6, 55.3, 45.8, 14.2. HRMS (ESI+) Calcd. For $C_{23}H_{24}N_2O_3$ ($[M+H]^+$): 377.1860, found: 377.1857. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 20/80, flow rate

1.0 mL/min, λ = 254 nm); t_r = 7.30 and 9.25 min.

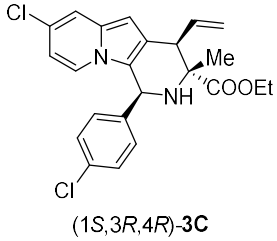
Ethyl (1*S*,3*R*,4*R*)-1-(4-chlorophenyl)-3,6-dimethyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3B



(1*S*,3*R*,4*R*)-**3B**

Yield (83%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -120.0 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.26 (m, 2H), 7.24 – 7.19 (m, 2H), 6.92 – 6.88 (m, 1H), 6.39 – 6.35 (m, 1H), 6.30 (s, 1H), 6.20 – 6.13 (m, 1H), 6.14 – 6.10 (m, 1H), 5.45 (s, 1H), 5.28 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.16 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.14 – 4.04 (m, 2H), 4.06 – 3.98 (m, 1H), 2.35 (s, 3H), 1.34 (s, 3H), 1.13 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.7, 140.5, 139.2, 134.0, 133.7, 129.8, 129.2, 127.8, 125.9, 120.3, 117.5, 116.2, 115.8, 109.5, 95.6, 62.1, 60.9, 54.9, 45.5, 25.0, 18.1, 14.1. HRMS (ESI+) Calcd. For $C_{24}H_{25}ClN_2O_2$ ($[M+H]^+$): 409.1677, found: 409.1670. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm); t_r = 4.91 and 18.32 min.

Ethyl (1*S*,3*R*,4*R*)-7-chloro-1-(4-chlorophenyl)-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3C

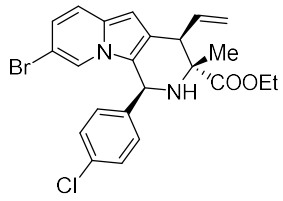


(1*S*,3*R*,4*R*)-**3C**

Yield (82%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -206.0 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.29 (m, 2H), 7.25 – 7.14 (m, 3H), 6.94 – 6.90 (m, 1H), 6.27 (s, 1H), 6.17 – 6.13 (m, 1H), 6.14 – 6.06 (m, 1H), 5.43 (s, 1H), 5.25 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.16 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.14 – 4.06 (m, 1H), 4.07 – 3.99 (m, 2H), 1.33 (s, 3H), 1.12 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.6, 139.9, 138.7, 134.0, 132.7, 129.7, 129.3, 127.5, 122.78, 122.76, 117.7, 117.2,

116.5, 110.8, 97.4, 62.0, 60.9, 54.7, 45.3, 24.8, 14.1. HRMS (ESI+) Calcd. For $C_{23}H_{22}Cl_2N_2O_2$ ($[M+H]^+$): 429.1131, found: 429.1126. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm); t_r = 5.46 and 12.81 min.

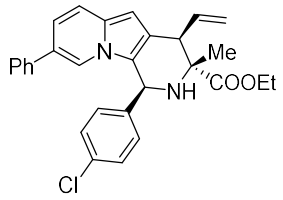
Ethyl (1*S*,3*R*,4*R*)-8-bromo-1-(4-chlorophenyl)-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3D



(1*S*,3*R*,4*R*)-**3D**

Yield (75%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -266.5 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.30 (m, 2H), 7.24 – 7.14 (m, 4H), 6.64 – 6.58 (m, 1H), 6.35 (s, 1H), 6.17 – 6.06 (m, 1H), 5.42 (s, 1H), 5.25 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.17 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.10 – 4.05 (m, 1H), 4.06 – 4.00 (m, 2H), 1.33 (s, 3H), 1.12 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 175.5, 139.7, 138.8, 134.1, 131.4, 129.7, 129.3, 127.1, 122.0, 119.8, 119.4, 118.0, 116.6, 104.5, 98.6, 62.0, 60.9, 54.8, 45.4, 24.9, 14.2. HRMS (ESI+) Calcd. For $C_{23}H_{22}BrClN_2O_2$ ($[M+H]^+$): 473.0626, found: 473.0613. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak IE, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 250 nm); t_r = 4.85 and 5.22 min.

Ethyl (1*S*,3*R*,4*R*)-1-(4-chlorophenyl)-3-methyl-8-phenyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*] indolizine-3-carboxylate (1*S*,3*R*,4*R*)-3E



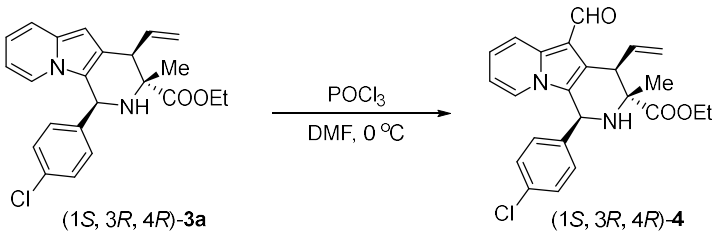
(1*S*,3*R*,4*R*)-**3E**

Yield (83%); >20:1 dr; yellow solid; m.p. = 74 ºC. $[\alpha]^{20}_D$ = -389.0 (*c* 0.5, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.30 (m, 5H), 7.27 – 7.16 (m, 6H), 6.88 – 6.81 (m, 1H), 6.34 (s, 1H), 6.21 – 6.10 (m, 1H), 5.50 (s, 1H), 5.27 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.17 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.13 – 4.05 (m, 2H), 4.06 – 3.99 (m, 1H), 1.35 (s, 3H), 1.13 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz,

Chloroform-*d*) δ 175.7, 140.3, 139.0, 138.4, 133.9, 132.2, 129.8, 129.2, 128.8, 127.0, 126.9, 126.3, 123.4, 119.7, 118.7, 117.8, 117.1, 116.4, 97.2, 62.1, 60.9, 54.9, 45.4, 25.0, 14.1. HRMS (ESI+) Calcd. For $C_{29}H_{27}ClN_2O_2$ ($[M+H]^+$): 471.1834, found: 471.1825. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 11.83 and 21.13 min.

4. Experimental Procedures and Characterization for Synthetic Applications

Ethyl (1*S*,3*R*,4*R*)-1-(4-chlorophenyl)-5-formyl-3-methyl-4-vinyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate[4] (1*S*,3*R*,4*R*)-4

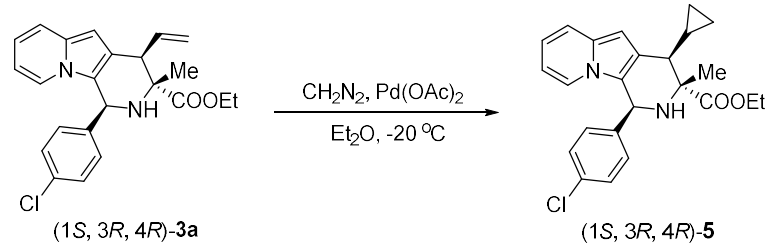


(1*S*,3*R*,4*R*)-**3a** (78.8 mg, 0.2 mmol) was dissolved in DMF (0.5 mL). A solution of distilled $POCl_3$ (36.8 mg, 0.24 mmol) in DMF (0.1 mL) was added to the solution at 0 °C. After stirring for 20 minutes in 0 °C, the reaction mixture was carefully quenched with cold water and extracted with EA. The organic phase was reextracted with water, washed with brine and dried over Na_2SO_4. The solvent was removed under reduced pressure to afford the product (1*S*,3*R*,4*R*)-**4**.

Yield (72%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -9.0 (*c* 0.3, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.13 (s, 1H), 8.24 (d, *J* = 8.8 Hz, 1H), 7.35 – 7.31 (m, 2H), 7.28 – 7.21 (m, 3H), 7.15 – 7.08 (m, 1H), 6.62 – 6.56 (m, 1H), 6.19 – 6.09 (m, 1H), 5.48 (s, 1H), 5.38 (dd, *J* = 17.2, 2.0 Hz, 1H), 5.27 (dd, *J* = 10.0, 2.0 Hz, 1H), 4.56 – 4.50 (m, 1H), 4.06 (q, *J* = 7.2 Hz, 2H), 1.38 (s, 3H), 1.10 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 182.7, 175.3, 139.1, 137.5, 137.0, 134.3, 129.6, 129.5, 129.1, 124.4, 123.6, 120.0, 119.2, 118.1, 113.5, 110.2, 61.9, 61.1, 54.4, 43.2, 24.6, 14.1. For $C_{24}H_{23}ClN_2O_3$ ($[M+H]^+$): 423.1469, found: 423.1462. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm); t_r = 8.70 and 11.94 min.

Ethyl (1*S*,3*R*,4*R*)-1-(4-chlorophenyl)-4-cyclopropyl-3-methyl-1,2,3,4-tetrahydropyrido[4,3-

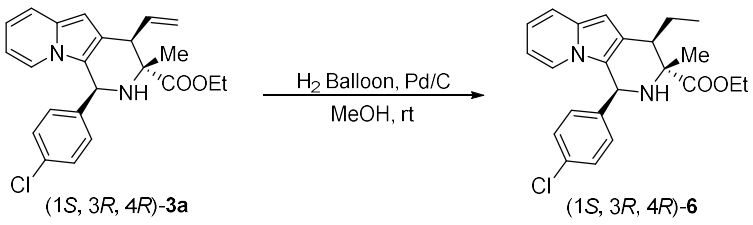
***b*]indolizine-3-carboxylate[5] (1*S*,3*R*,4*R*)-5**



Fresh prepared diazomethane solution (0.5 M in Et_2O, 2 mL) and (1*S*,3*R*,4*R*)-**3a** (78.8 mg, 0.2 mmol) were added into a Schlenk tube. Under a positive nitrogen pressure, the reaction was cooled to -20 °C, and $Pd(OAc)_2$ (1.5 mg, 1 mol %) was added in one portion with gas evolution. After stirring for 1 hour in -20 °C, the reaction was moved to room temperature and stirred overnight. While the reaction was partly completed, the solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (PE/EA = 8/1) to afford the product (1*S*,3*R*,4*R*)-**5**.

Yield (43%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -74.0 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.28 (m, 3H), 7.25 – 7.23 (m, 2H), 7.01 (d, *J* = 7.2 Hz, 1H), 6.58 – 6.53 (m, 1H), 6.33 (s, 1H), 6.20 – 6.16 (m, 1H), 5.45 (s, 1H), 4.06 – 3.96 (m, 2H), 2.64 (d, *J* = 10.0 Hz, 1H), 1.53 (s, 3H), 1.24 – 1.18 (m, 1H), 1.08 (t, *J* = 7.2 Hz, 3H), 0.89 – 0.84 (m, 1H), 0.73 – 0.68 (m, 1H), 0.56 – 0.52 (m, 1H), 0.51 – 0.50 (m, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.2, 140.7, 133.7, 132.8, 129.8, 129.2, 128.3, 122.1, 118.8, 116.9, 116.2, 109.3, 97.0, 63.5, 60.7, 55.0, 45.1, 24.8, 14.6, 14.1, 7.6, 2.2. HRMS (ESI+) Calcd. For $C_{24}H_{25}ClN_2O_2$ ($[M+H]^+$): 409.1677, found: 409.1678. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm); t_r = 7.12 and 12.05 min.

Ethyl (*1S*,*3R*,*4R*)-1-(4-chlorophenyl)-4-ethyl-3-methyl-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate[6] (1*S*,3*R*,4*R*)-6

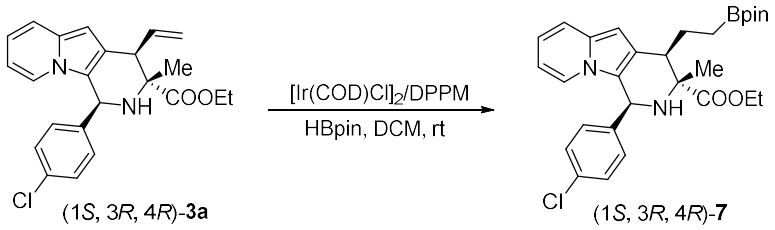


Pd/C (21.0 mg, palladium on activated carbon, 10% Pd basis, 1 mol %) was added to a solution of (1*S*,3*R*,4*R*)-**3a** (78.8 mg, 0.2 mmol) in anhydrous MeOH (4 mL). The reaction mixture was stirred under H_2 atmosphere (1 atm) at room temperature for 6 hours. After the reaction was completed

(monitored by TLC), the crude reaction mixture was filtrated with celite and washed with MeOH. The solvent was removed under reduced pressure, then the residue was purified by a flash column chromatography (PE/EA = 6/1) to afford the product (1*S*,3*R*,4*R*)-**6**.

Yield (93%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -52.1 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 - 7.25 (m, 3H), 7.23 - 7.18 (m, 2H), 7.04 - 7.00 (m, 1H), 6.58 – 6.52 (m, 1H), 6.33 (s, 1H), 6.22 – 6.16 (m, 1H), 5.45 (s, 1H), 4.00 (q, *J* = 7.2 Hz, 2H), 3.27 (dd, *J* = 10.8, 4.4 Hz, 1H), 1.96 – 1.89 (m, 1H), 1.65 – 1.53 (m, 1H), 1.38 (s, 3H), 1.11 (t, *J* = 7.2 Hz, 3H), 1.05 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.4, 140.8, 133.6, 132.3, 129.6, 129.2, 127.9, 121.9, 118.6, 117.0, 116.0, 109.2, 98.7, 63.0, 60.6, 55.0, 41.3, 24.4, 24.1, 14.1, 12.4. HRMS (ESI+) Calcd. For $C_{23}H_{25}ClN_2O_2$ ($[M+H]^+$): 397.1677, found: 397.1672. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm); t_r = 7.09 and 11.41 min.

Ethyl (1*S*,3*R*,4*R*)-1-(4-chlorophenyl)-3-methyl-4-(2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethyl)-1,2,3,4-tetrahydropyrido[4,3-*b*]indolizine-3-carboxylate[7] (1*S*,3*R*,4*R*)-7

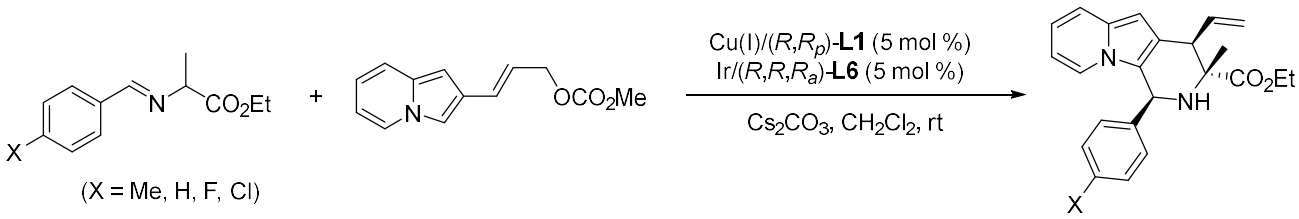


To a solution of $[Ir(COD)Cl]_2$ (6.7 mg, 5 mol %) and bis(diphenylphosphino)methane (DPPM, 7.7 mg, 10 mol %) in anhydrous DCM (2 mL) was added (1*S*,3*R*,4*R*)-**3a** (76.2 g, 0.2 mmol) in one portion under a positive argon pressure. Then 4,4,5,5-tetramethyl-1,3,2-dioxaborolane (HBpin, 58 μL, 0.4 mmol) was added at room temperature and the resulting solution was stirred overnight. The reaction mixture was quenched with MeOH (1 mL) and concentrated under reduced pressure. The residue was purified by silica-gel flash column chromatography (PE/EA = 8/1, with 1% MeOH) to afford the product (1*S*,3*R*,4*R*)-**7**.

Yield (83%); >20:1 dr; yellow oil. $[\alpha]^{20}_D$ = -38.0 (*c* 0.2, CH_2Cl_2); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.25 (m, 5H), 7.02 (d, *J* = 7.2 Hz, 1H), 6.57 – 6.50 (m, 1H), 6.35 (s, 1H), 6.21 – 6.15 (m, 1H), 5.45 (s, 1H), 4.04 - 3.92 (m, 2H), 3.30 – 3.24 (m, 1H), 2.05 – 1.99 (m, 1H), 1.70 – 1.63 (m, 1H), 1.40 (s, 3H), 1.22 (s, 6H), 1.15 (s, 6H), 1.12 – 1.07 (m, 1H), 1.05 (t, *J* = 7.2 Hz, 3H), 1.02 – 0.95 (m, 1H).

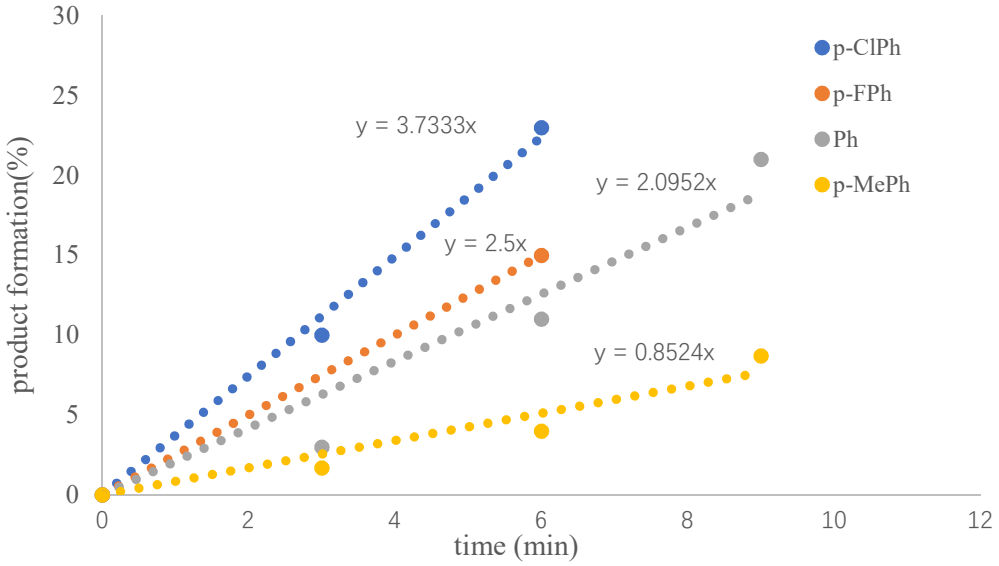
^{13}C NMR (100 MHz, Chloroform-*d*) δ 176.3, 140.7, 133.6, 132.2, 129.9, 129.1, 127.8, 121.9, 118.6, 116.9, 116.0, 109.2, 98.9, 82.9, 63.0, 60.6, 55.1, 41.7, 25.2, 24.9, 24.8, 24.4, 14.1. HRMS (ESI+) Calcd. For $C_{29}H_{36}BClN_2O_4$ ([M+H]$^+$): 523.2534, found: 523.2526. The product was analyzed by HPLC to determine the enantiomeric excess: 99% ee (Chiralpak AD-H, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm); t_r = 10.0 and 20.75 min.

5. Hammett Plot Studies



1 **2a** (1*S*, 3*R*, 4*R*)-**3**

To probe the electronic effects for this cascade allylation/Friedel-Crafts type reaction, the rate of synergistic Cu/Ir-catalyzed asymmetric cascade annulation of 2-indolizinyl allyl carbonate **2a** with *p*-X-C_6H_4CHO derived α-methyl substituted imino esters **1** containing electron-rich and electron-deficient substituted groups on the phenyl ring (X = CH_3, H, F, Cl) was measured by the ^{1}H NMR spectroscopic method. The hammett-plot study on imino esters **1** was performed using the initial rates and the corresponding substituent constants. All reactions were performed using the general procedure on 0.2 mmol scale, the product formation was determined by ^{1}H NMR every three minutes. The Hammett plot resulted in the linear fit with a positive slope, which indicated that the electron-deficient substituents should accelerate this cascade asymmetric transformation.



X	Me	H	F	Cl
K	0.8524	2.0952	2.5000	3.7333
K_X/K_H	0.41	1.00	1.19	1.78
$\log(K_X/K_H)$	-0.39	0.00	0.08	0.25
σ_p	-0.17	0.00	0.06	0.23

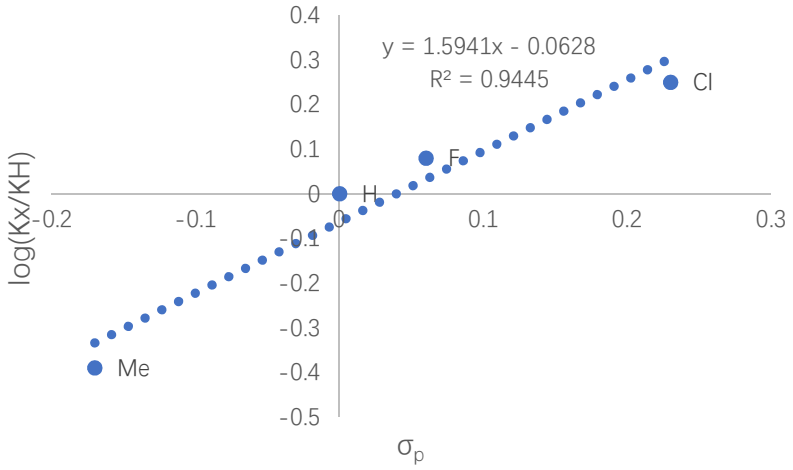


Figure S1. Hammett plot from synergistic Cu/Ir-catalyzed asymmetric [3 + 3] annulation of 2-indolizinyl formaldehyde derived allyl carbonate **2a** with *p*-X-C_6H_4CHO derived α-methyl substituted imino esters (X = Me, H, F, Cl).

6. Absolute configuration determination of (1*S*,3*R*,4*R*)-3k

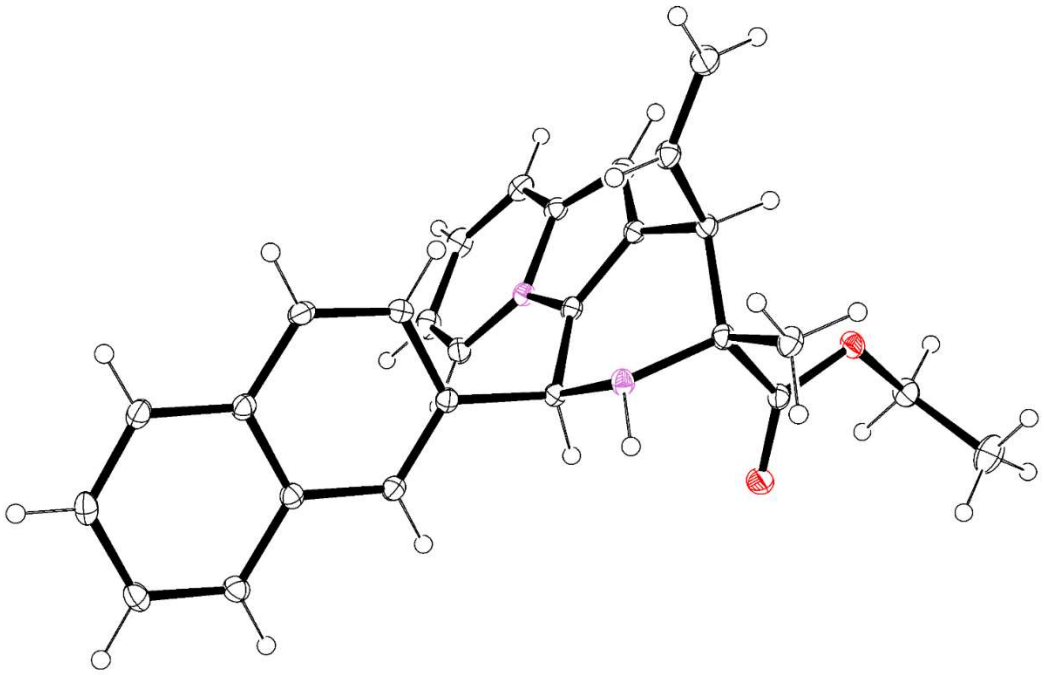


Figure S2. ORTEP representation of (1*S*,3*R*,4*R*)-**3k** (CCDC 2221435) at 30% probability for the drawing of thermal ellipsoids.

To a 30 mL oven-dried glass sample bottle was added 80 mg pure **3k** with 0.4 mL DCM to get clear solution, then 4 mL PE was slowly added. The mixture solution was sealed with filter paper to slowly grow crystals at room temperature. Crystal data for (1*S*,3*R*,4*R*)-**3k**: $C_{27}H_{26}N_2O_2$, M_r = 410.50, T = 100 K, orthorhombic, space group P 21 21 21, a= 6.94728(4), b= 13.79687(7), c= 22.55057(13) Å, V = 2161.49(2) Å^3, Z = 4, 4251 unique reflections, final R_1 = 0.0263 and wR_2 = 0.0673 for 4335 observed [I>2σ(I)] reflections, Flack χ = 0.08(6). CCDC 2221435 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK; fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

7. References

(1) Wang, C.-J.; Liang, G.; Xue, Z.-Y.; Gao, F. Highly Enantioselective 1,3-Dipolar Cycloaddition of Azomethine Ylides Catalyzed by Copper(I)/TF-BiphamPhos Complexes. *J. Am. Chem. Soc*. **2008**, *130*, 17250.

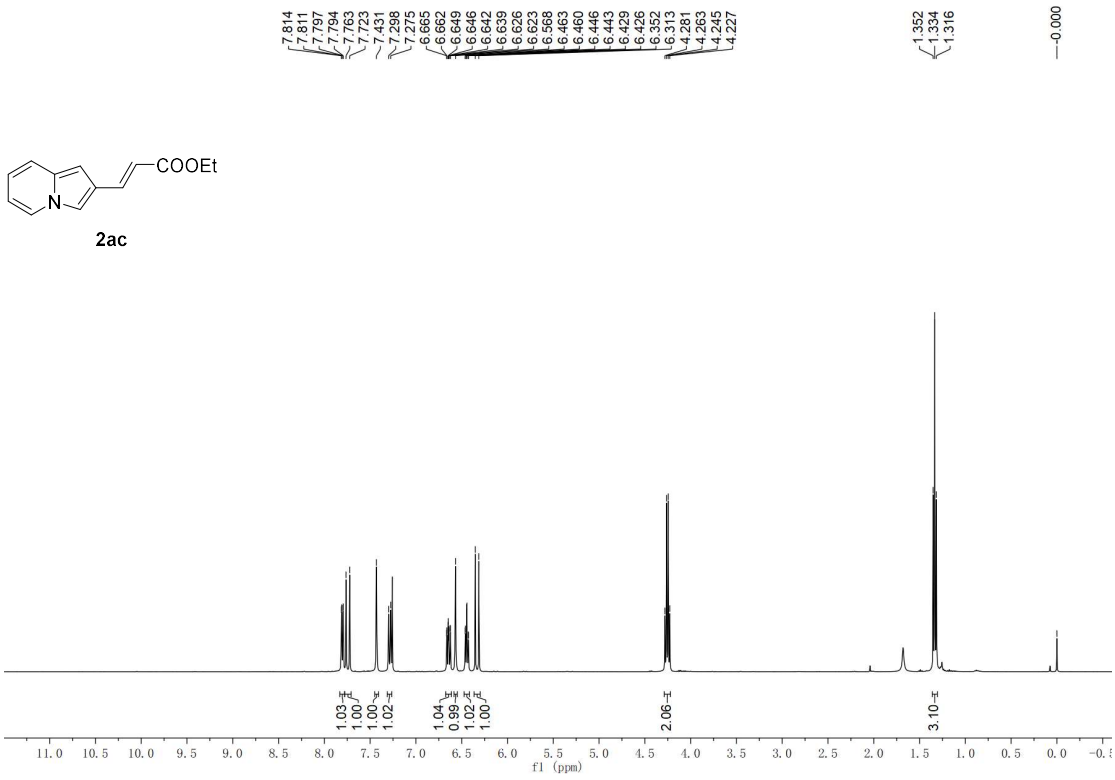
(2) Richards, C. J.; Mulvaney, A. W. Synthesis of phosphinoferrocenyloxazolines. New ligands for asymmetric catalysis. *Tetrahedron: Asymmetry* **1996**, *7*, 1419.

(3) Craig, R. S.; Daniel, J. M.; T. V. RajanBabu, (*R*)-2,2'-Binaphthoyl-(S,S)-Di(1-Phenylethyl) Aminophosphine. Scalable Protocols for the Syntheses of Phosphoramidite (Feringa) Ligands. *Org. Synth.* **2008**, 85.

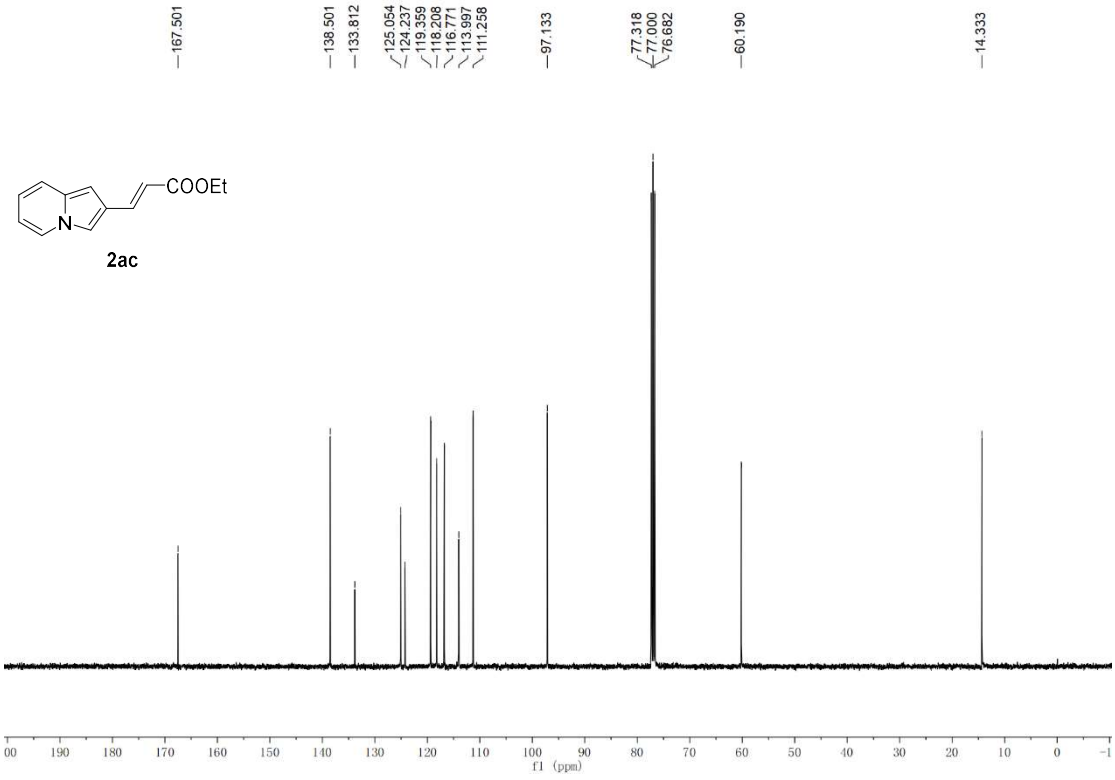
(4) Burnett, D. A.; Vacca, J. P. PCT Int. Appl., 2018119395, 28 Jun 2018.

(5) Stanley, L. M.; Hartwig, J. F. *Angew. Chem., Int. Ed.* **2009,** *48*, 7841.

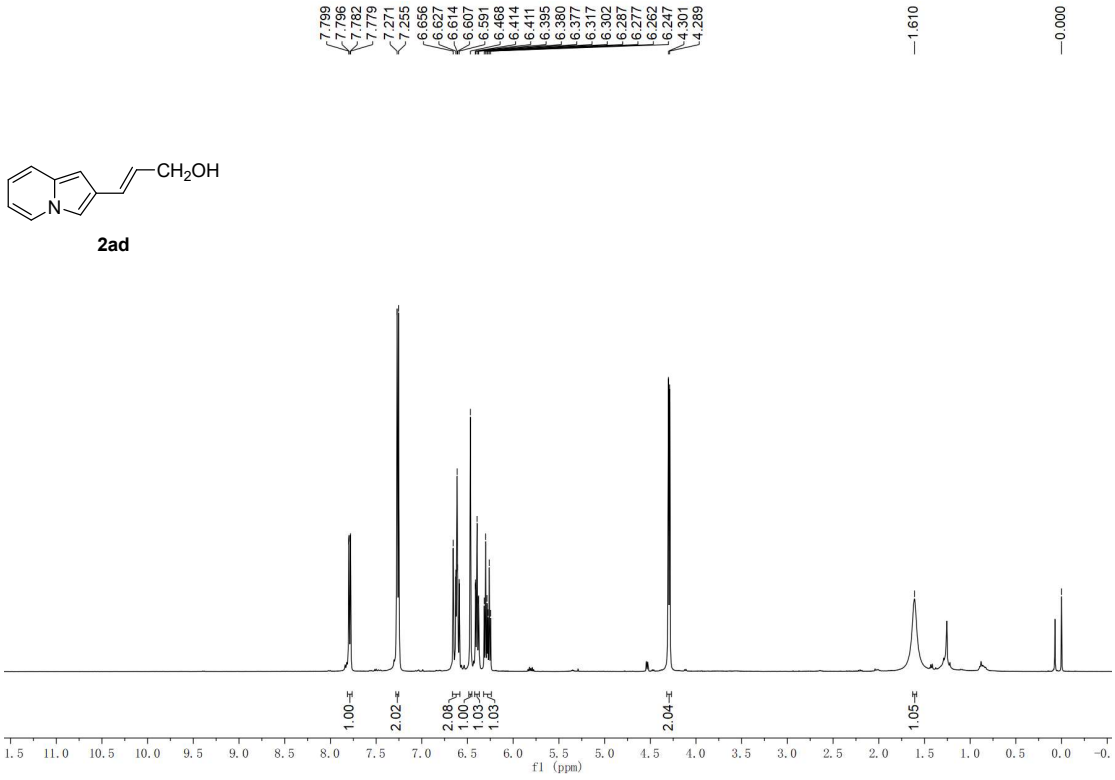
8. NMR and HPLC Spectra



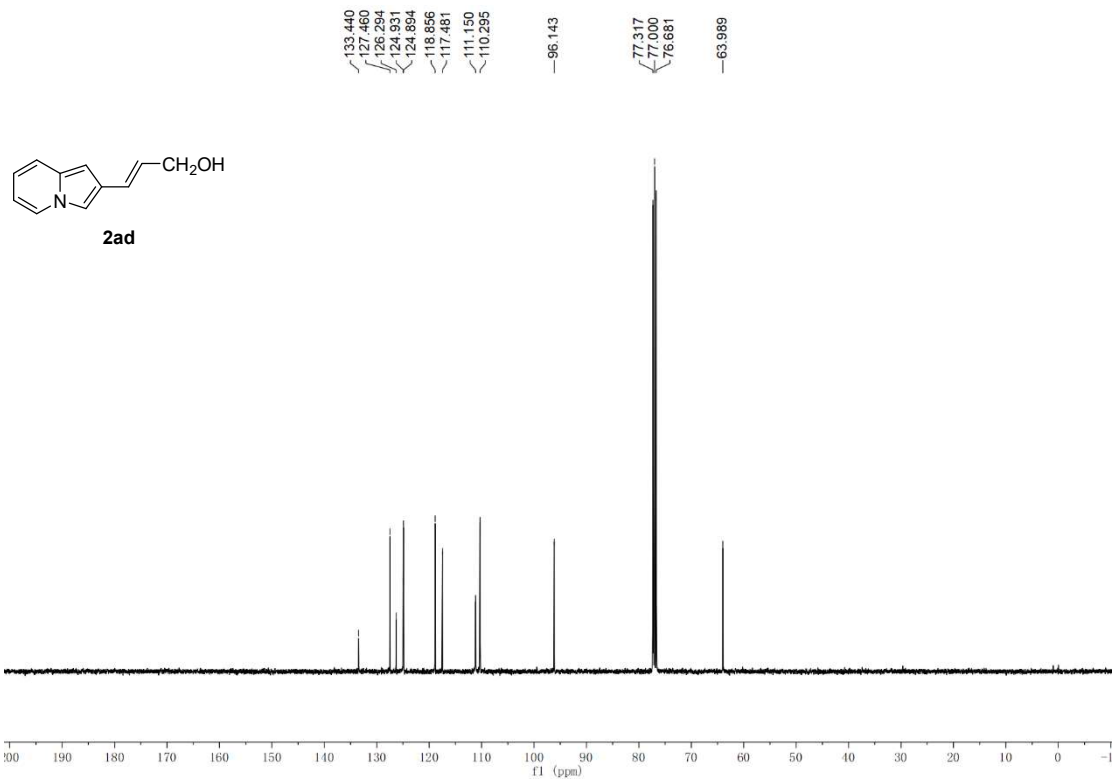
^{1}H NMR (400 MHz) of **2ac** in $CDCl_3$



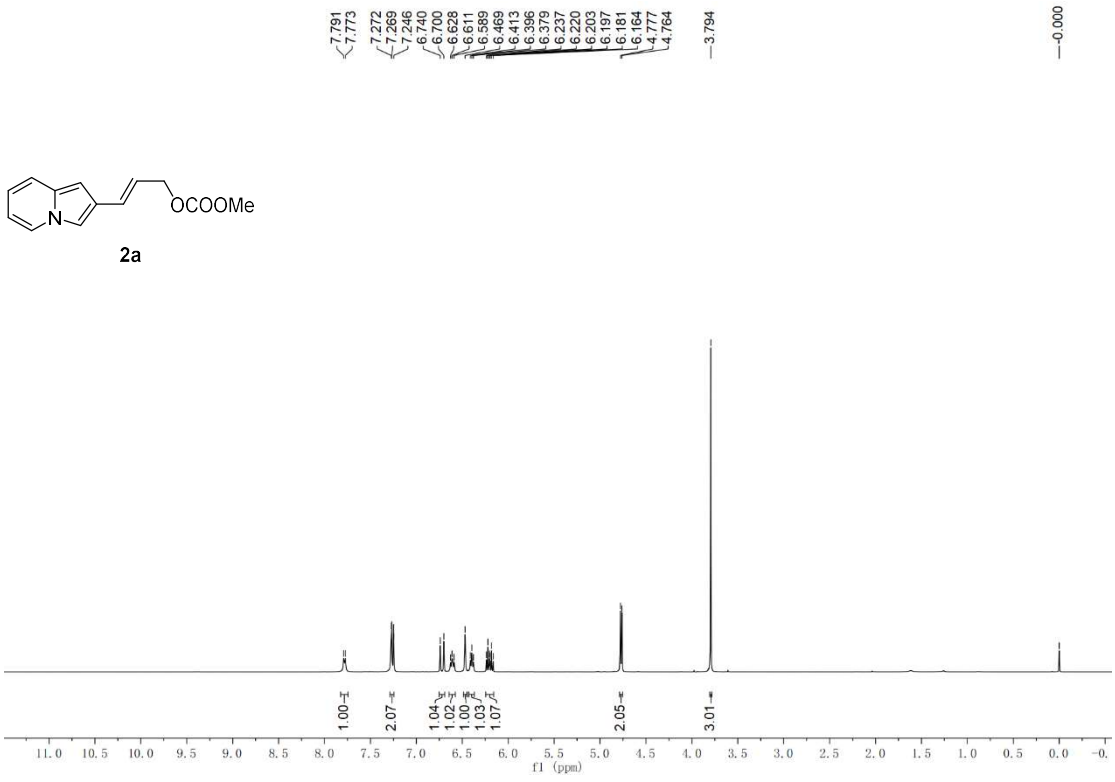
^{13}C NMR (100 MHz) of **2ac** in $CDCl_3$



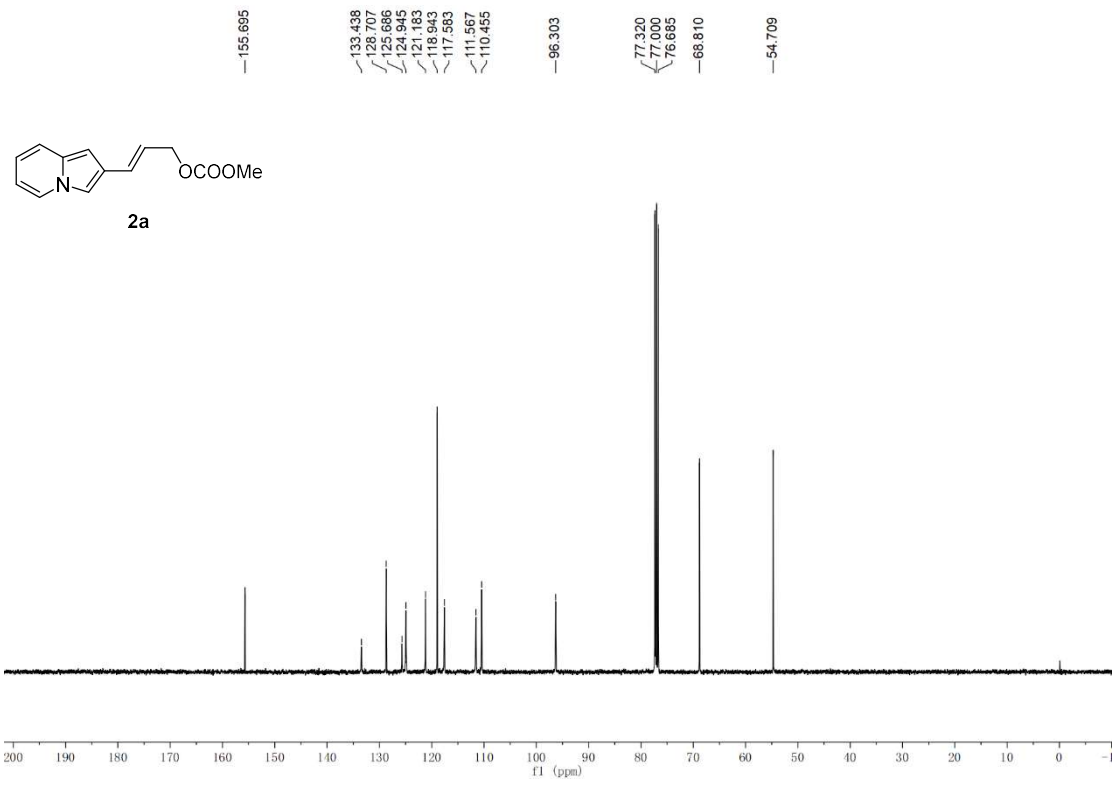
^{1}H NMR (400 MHz) of **2ad** in $CDCl_3$



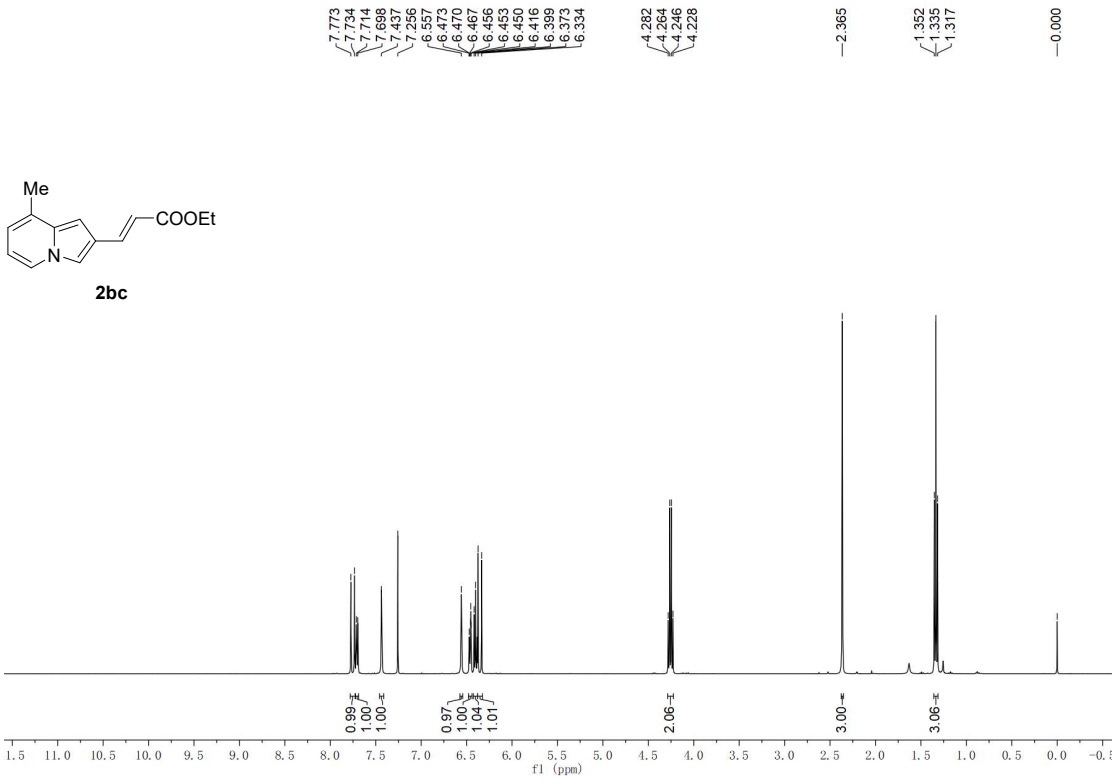
^{13}C NMR (100 MHz) of **2ad** in $CDCl_3$



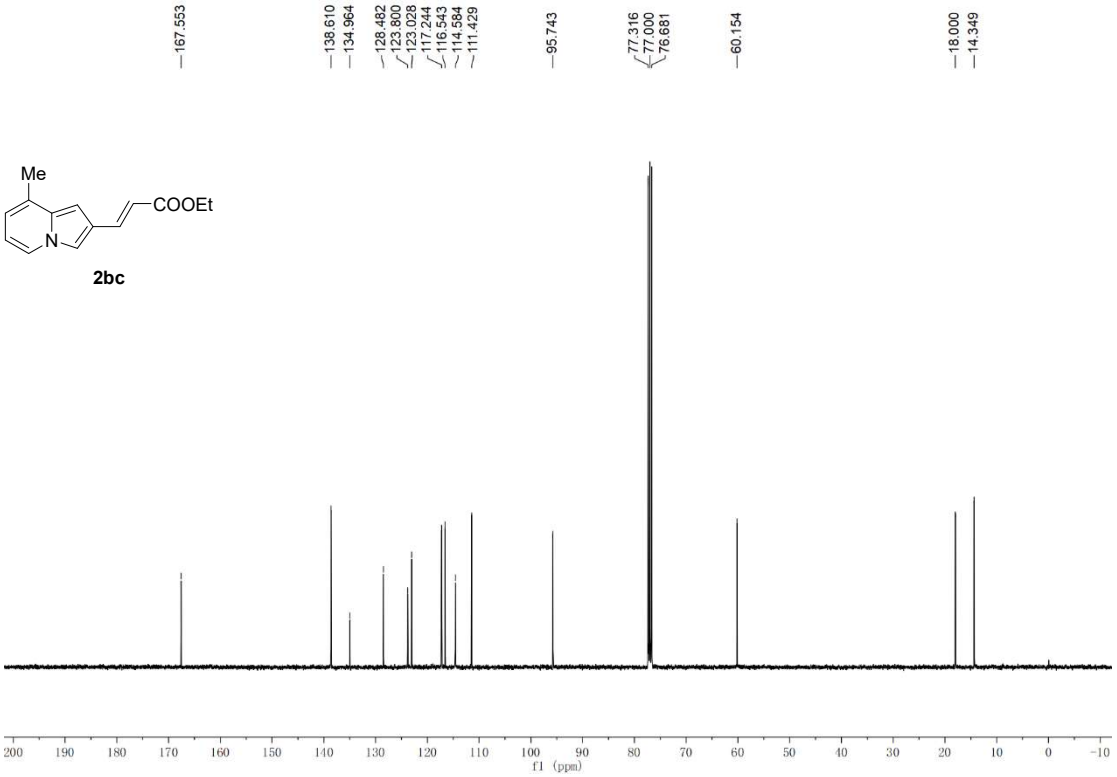
^{1}H NMR (400 MHz) of **2a** in $CDCl_3$



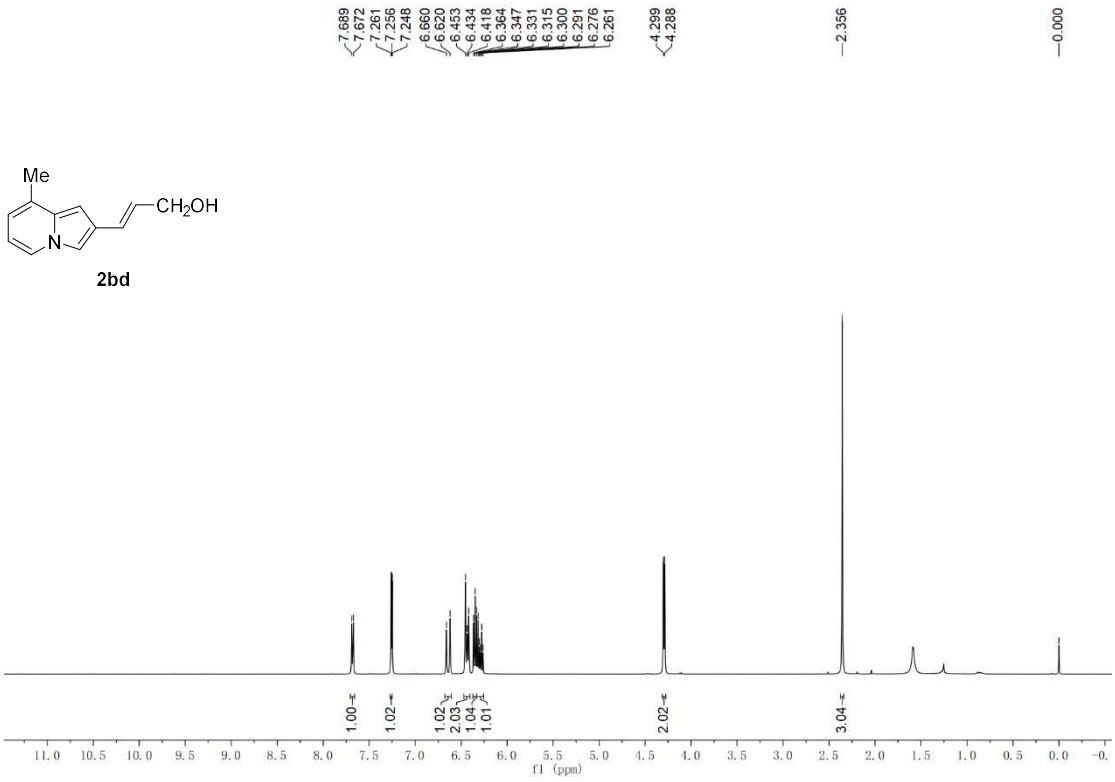
^{13}C NMR (100 MHz) of **2a** in $CDCl_3$



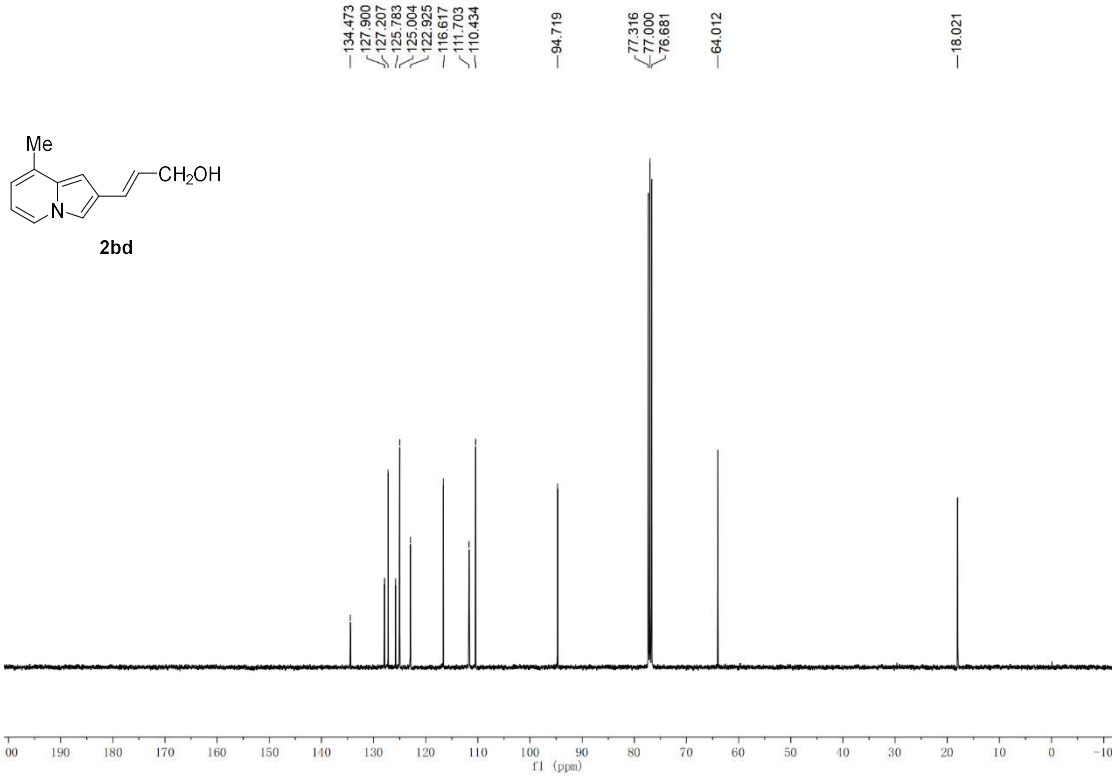
^{1}H NMR (400 MHz) of **2bc** in $CDCl_3$



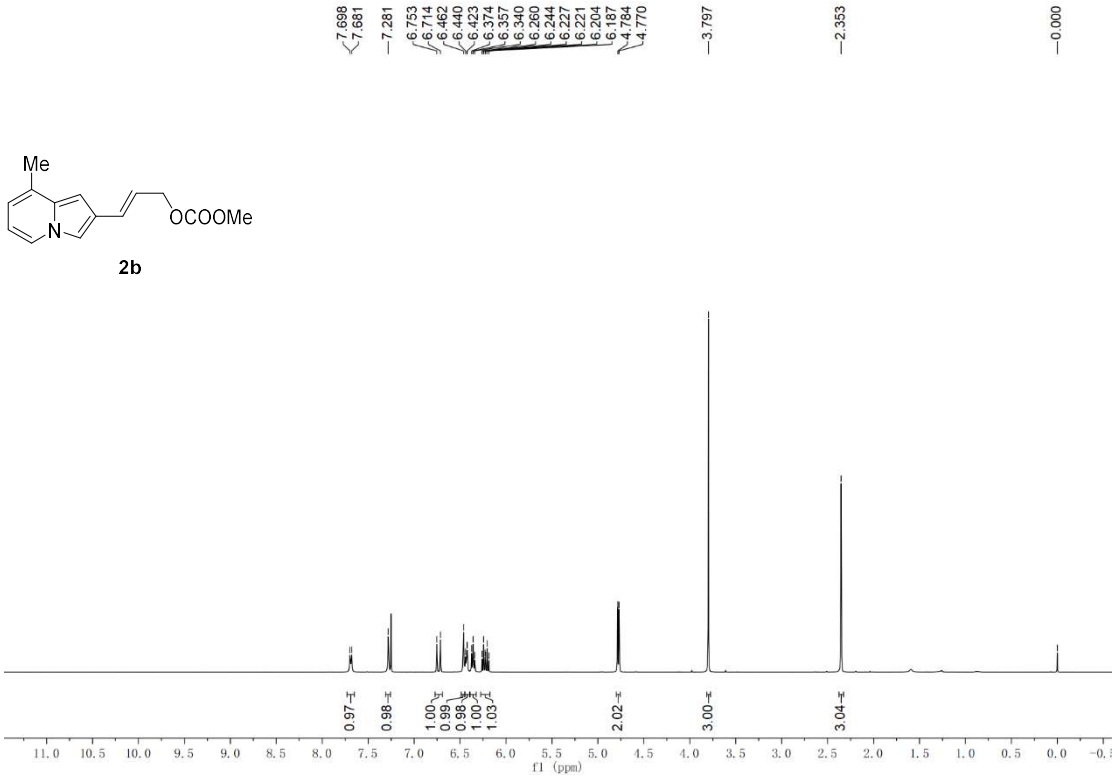
^{13}C NMR (100 MHz) of **2bc** in $CDCl_3$



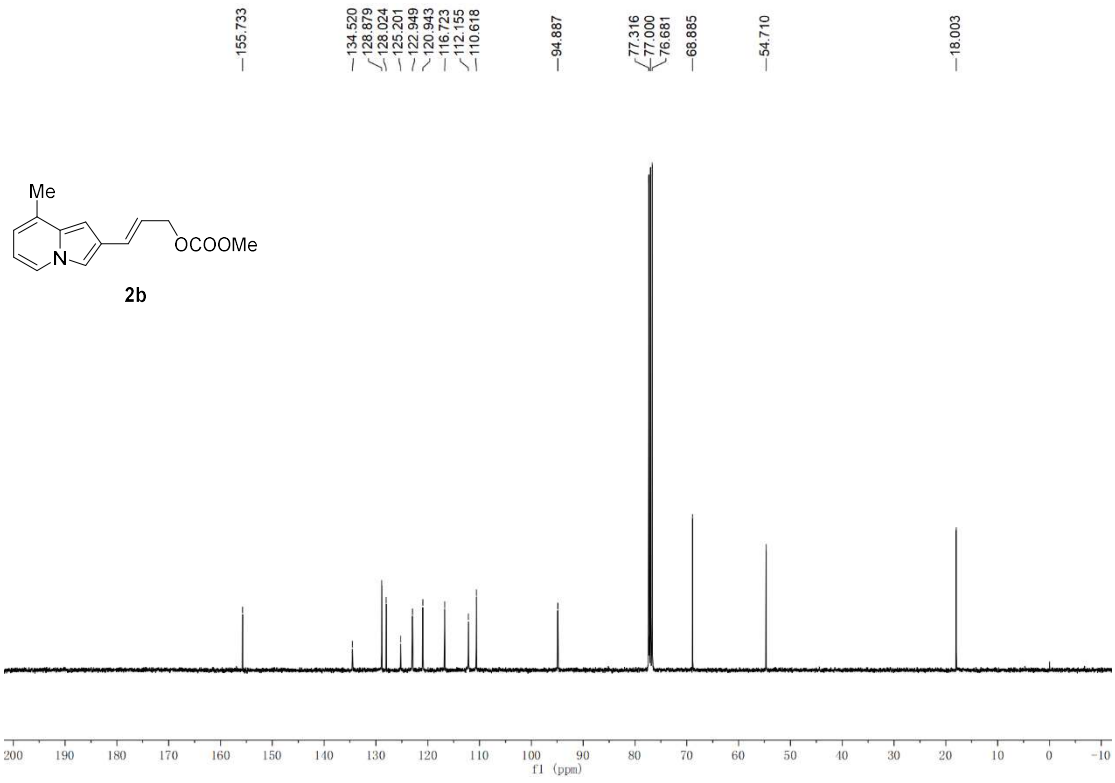
^{1}H NMR (400 MHz) of **2bd** in $CDCl_3$



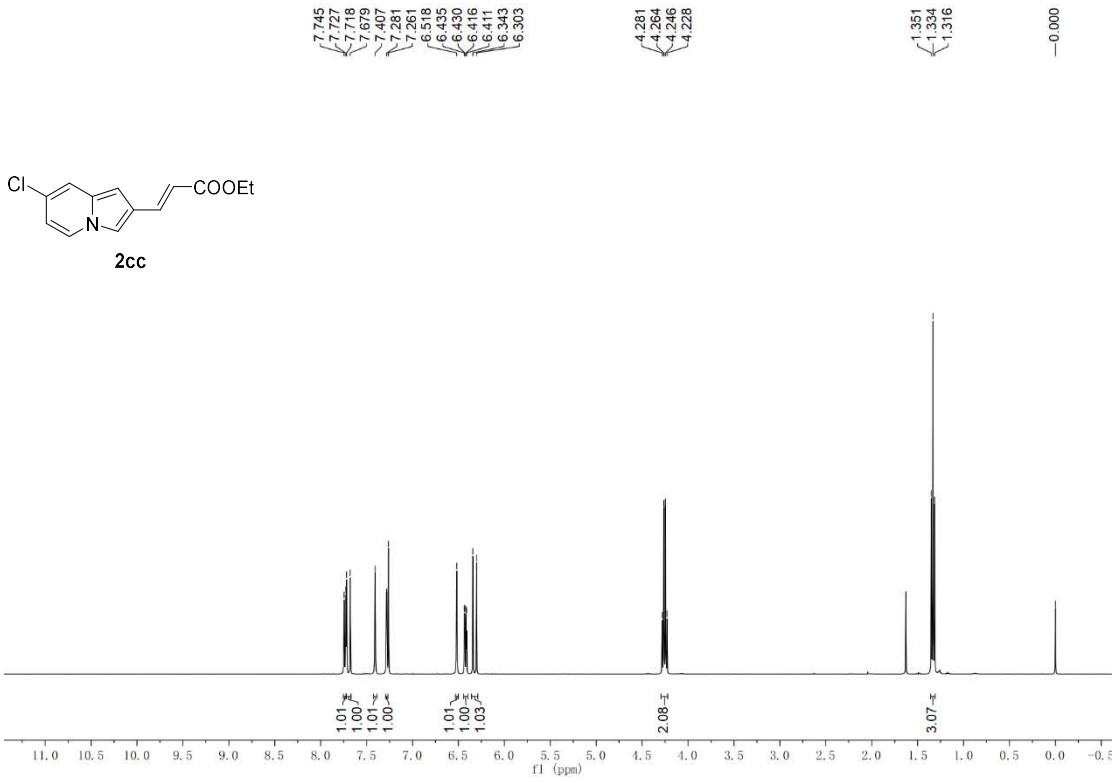
^{13}C NMR (100 MHz) of **2bd** in $CDCl_3$



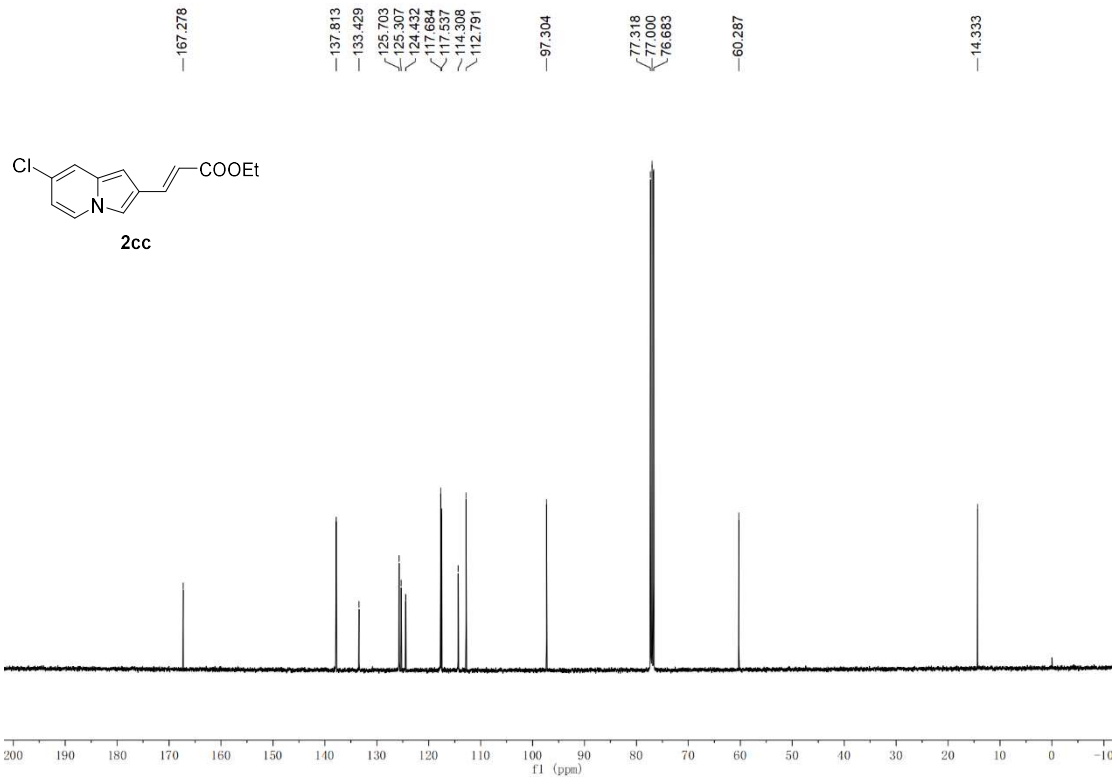
^{1}H NMR (400 MHz) of **2b** in $CDCl_3$



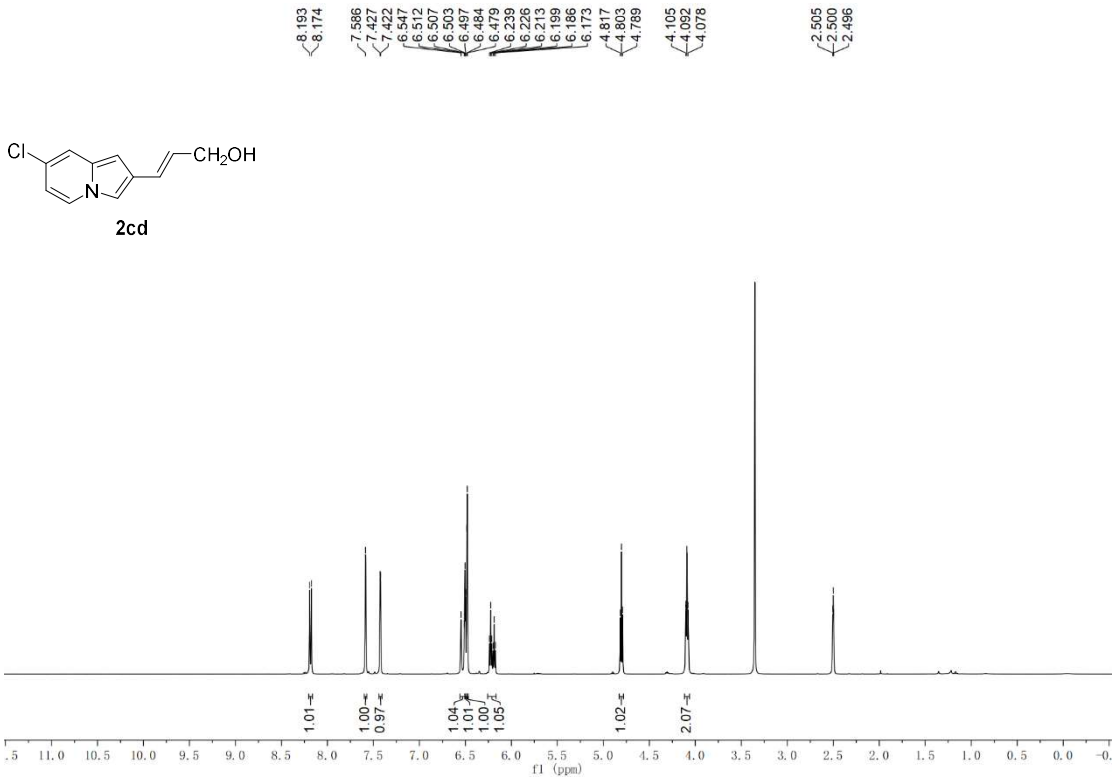
^{13}C NMR (100 MHz) of **2b** in $CDCl_3$



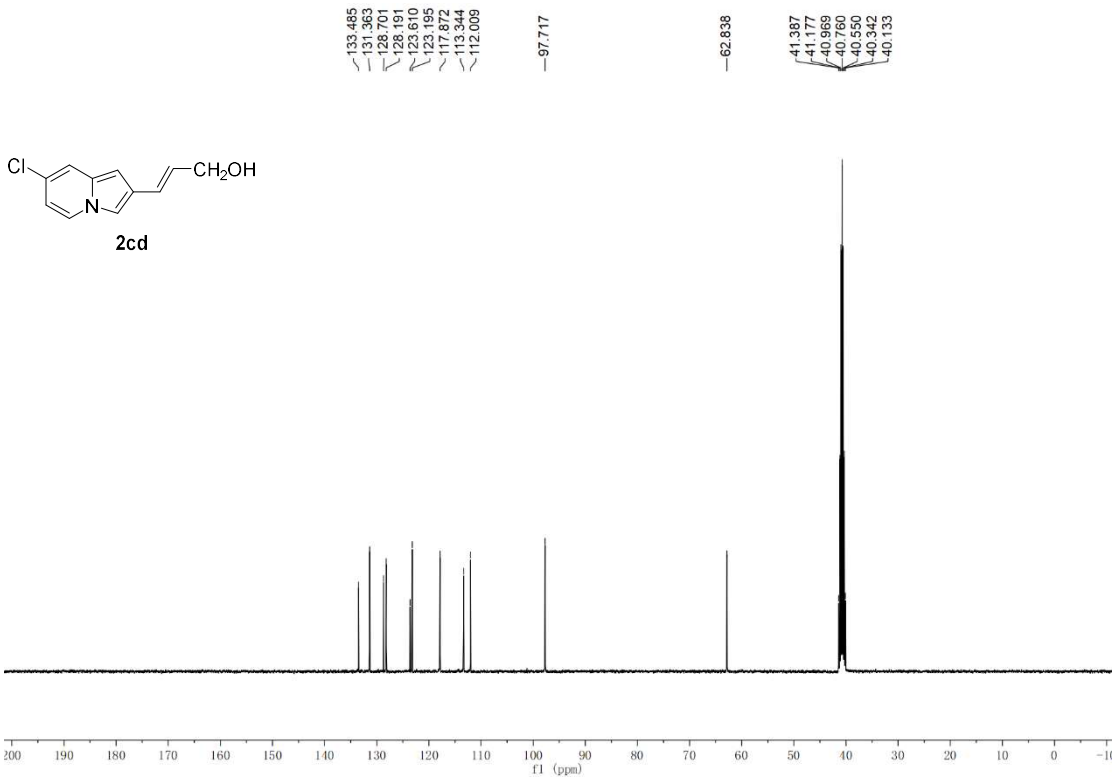
^{1}H NMR (400 MHz) of **2cc** in $CDCl_3$



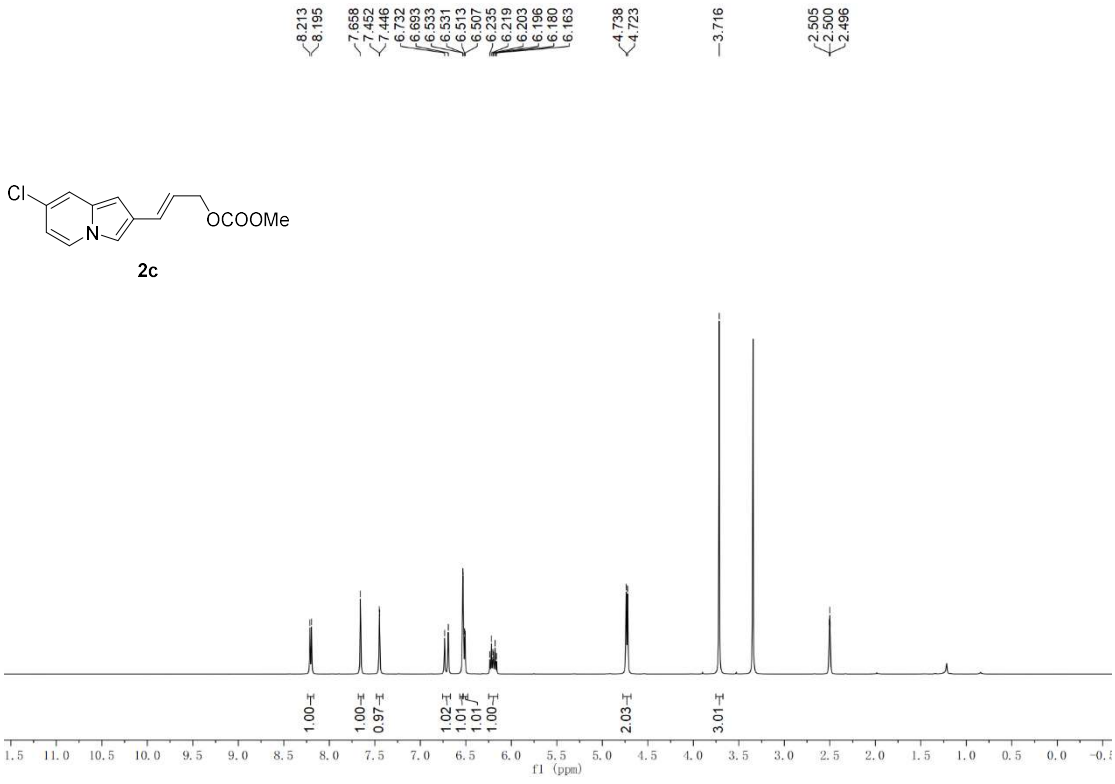
^{13}C NMR (100 MHz) of **2cc** in $CDCl_3$



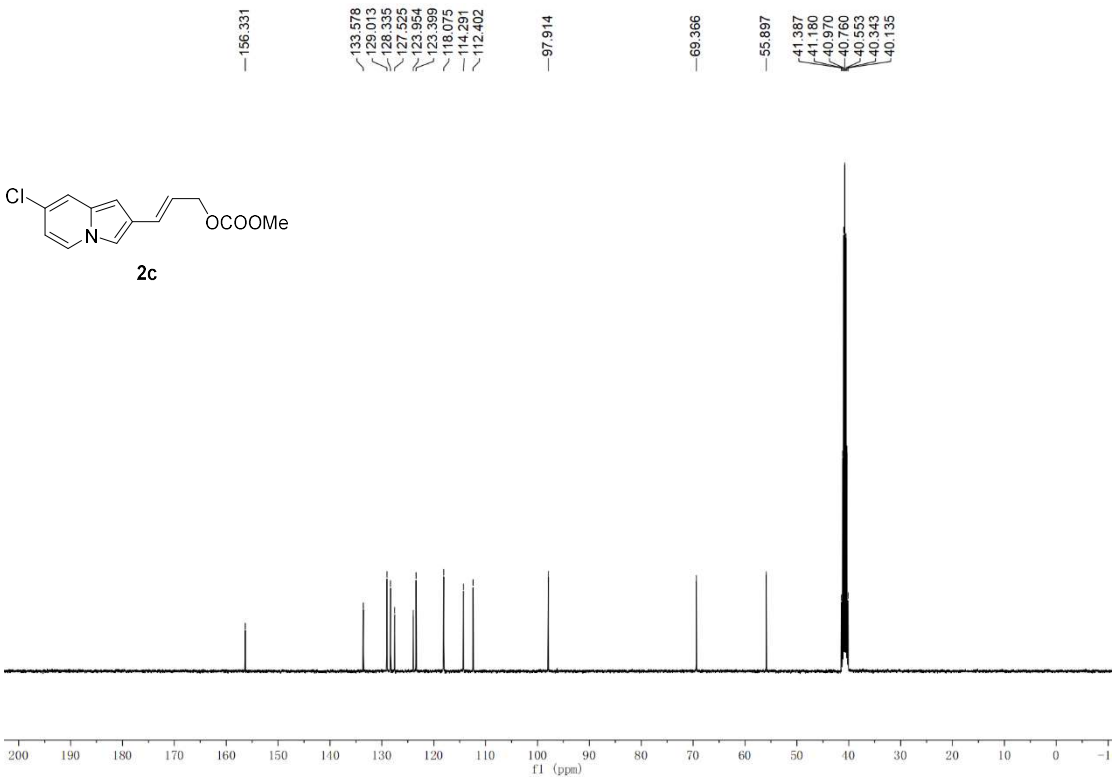
^{1}H NMR (400 MHz) of **2cd** in DMSO



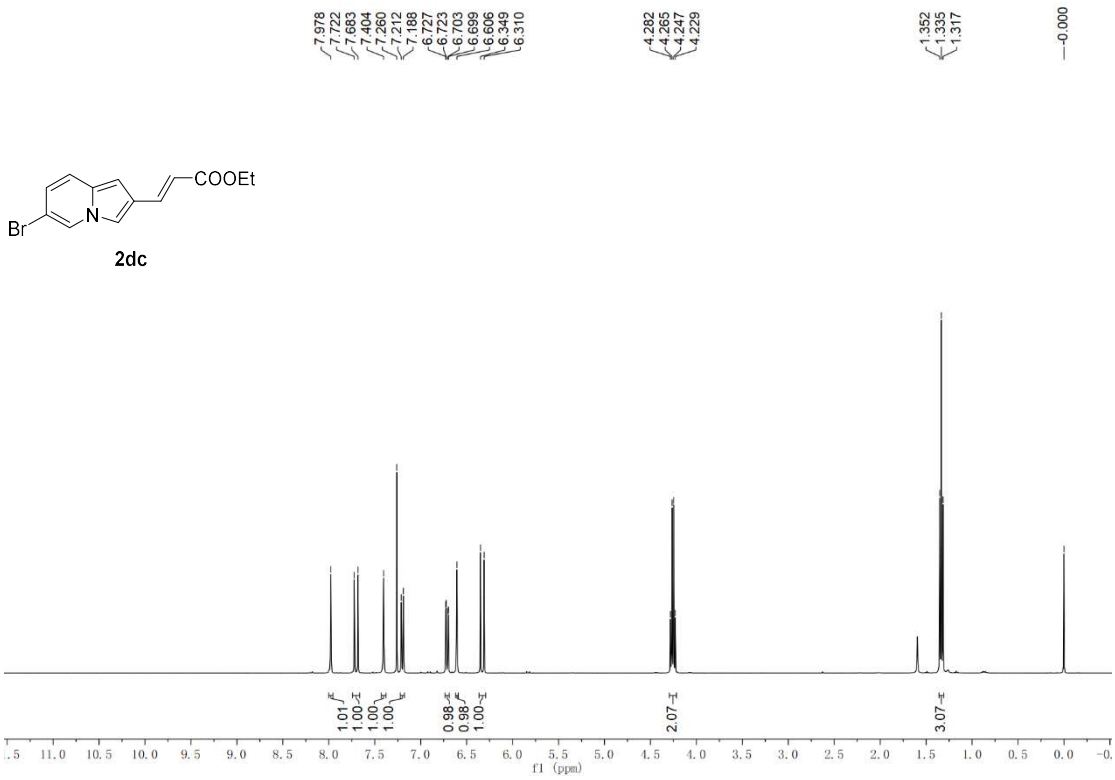
^{13}C NMR (100 MHz) of **2cd** in DMSO



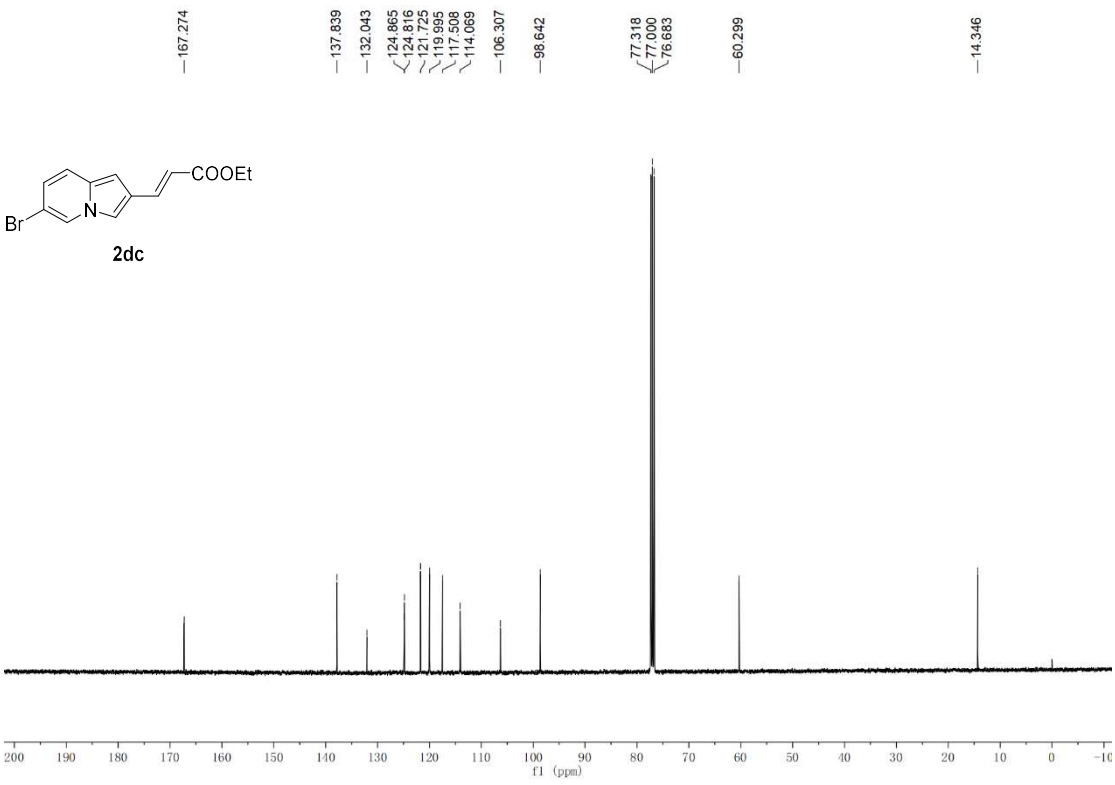
^{1}H NMR (400 MHz) of **2c** in DMSO



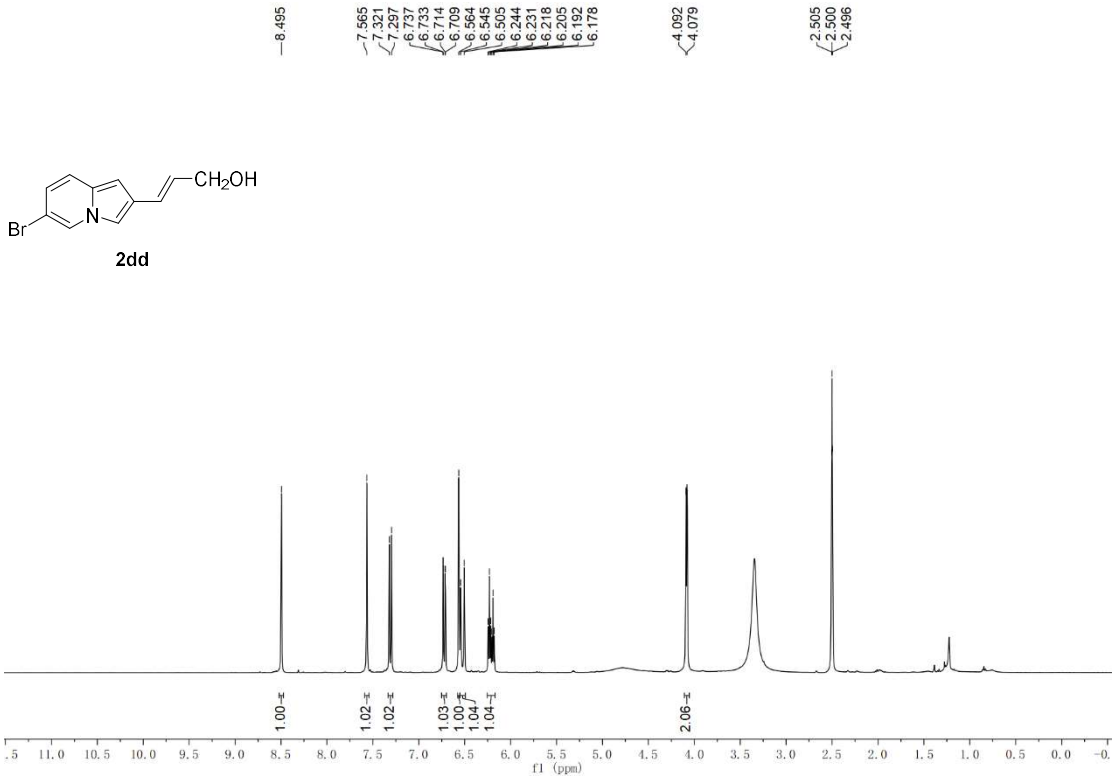
^{13}C NMR (100 MHz) of **2c** in DMSO



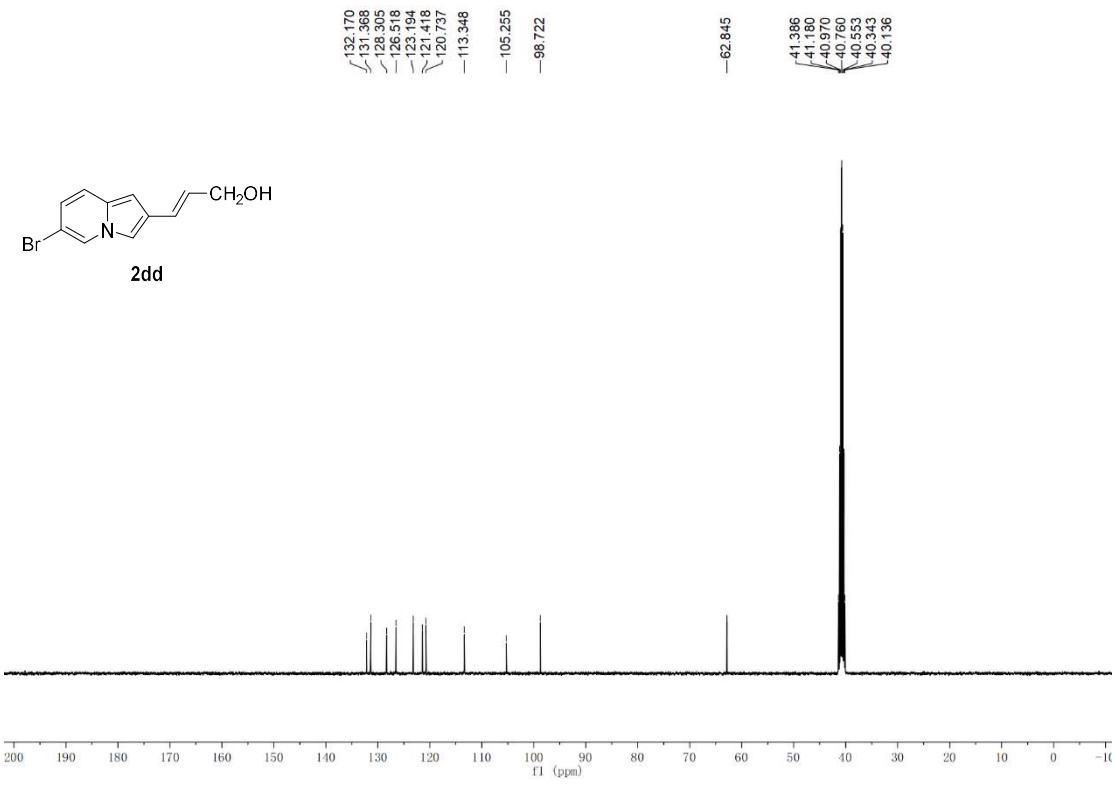
^{1}H NMR (400 MHz) of **2dc** in $CDCl_3$



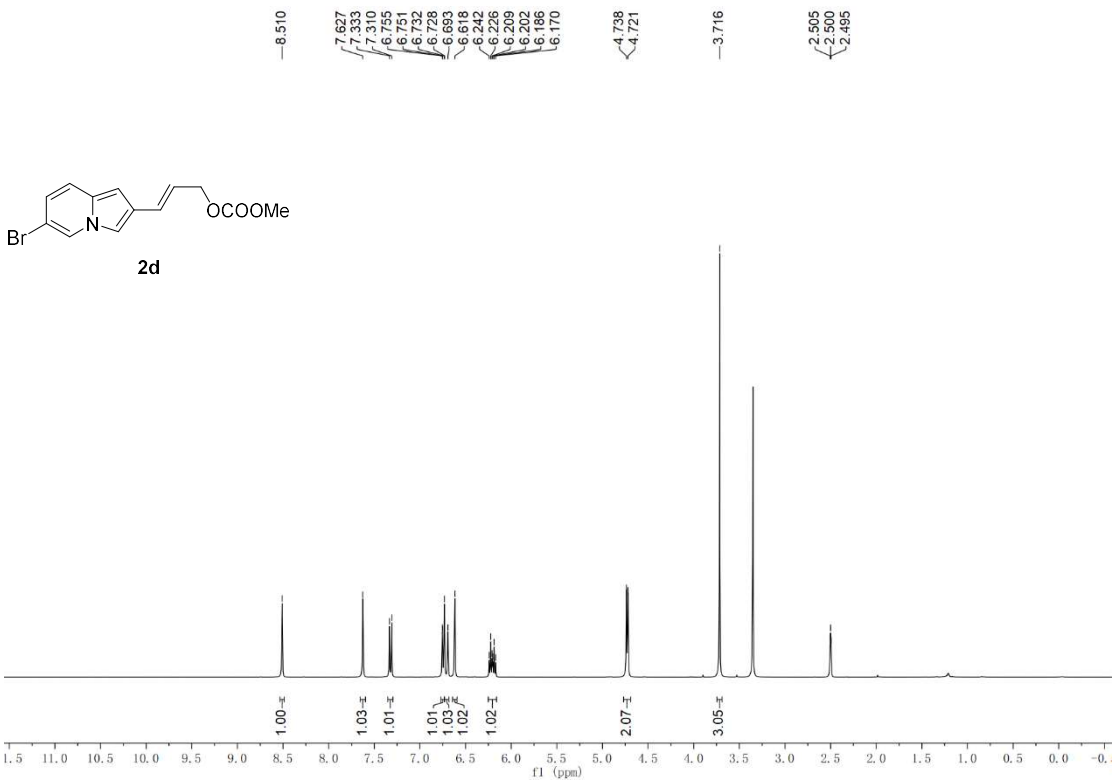
^{13}C NMR (100 MHz) of **2dc** in $CDCl_3$



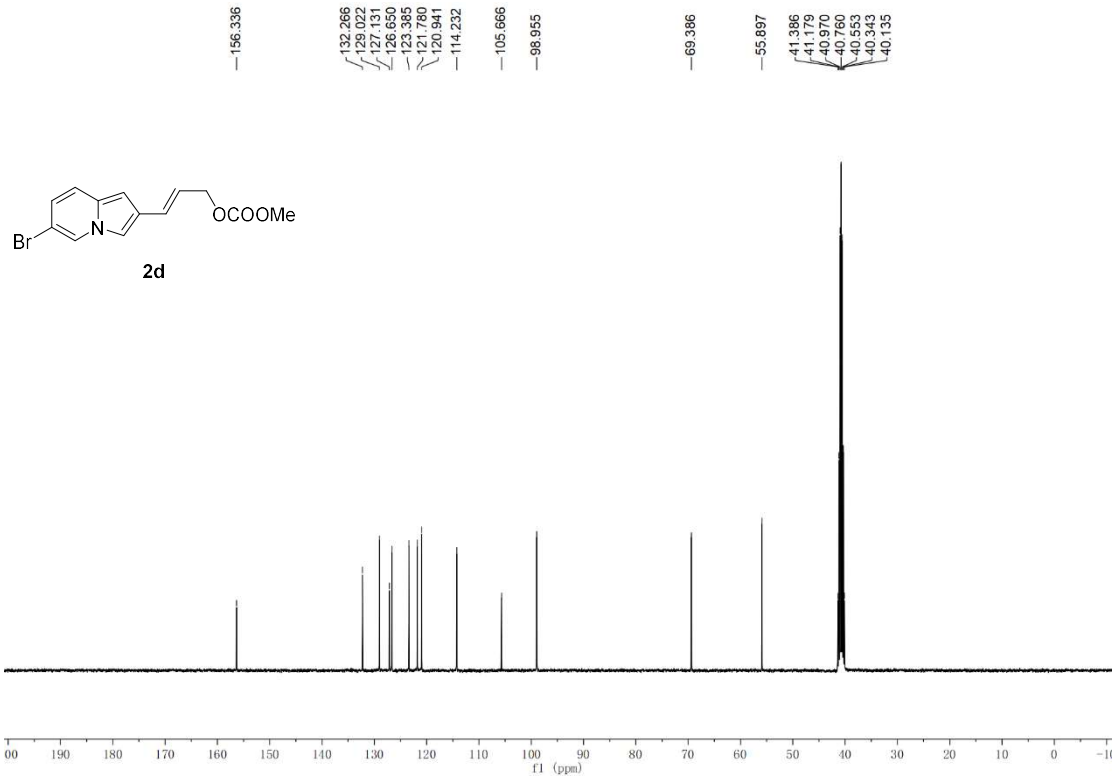
^{1}H NMR (400 MHz) of **2dd** in DMSO



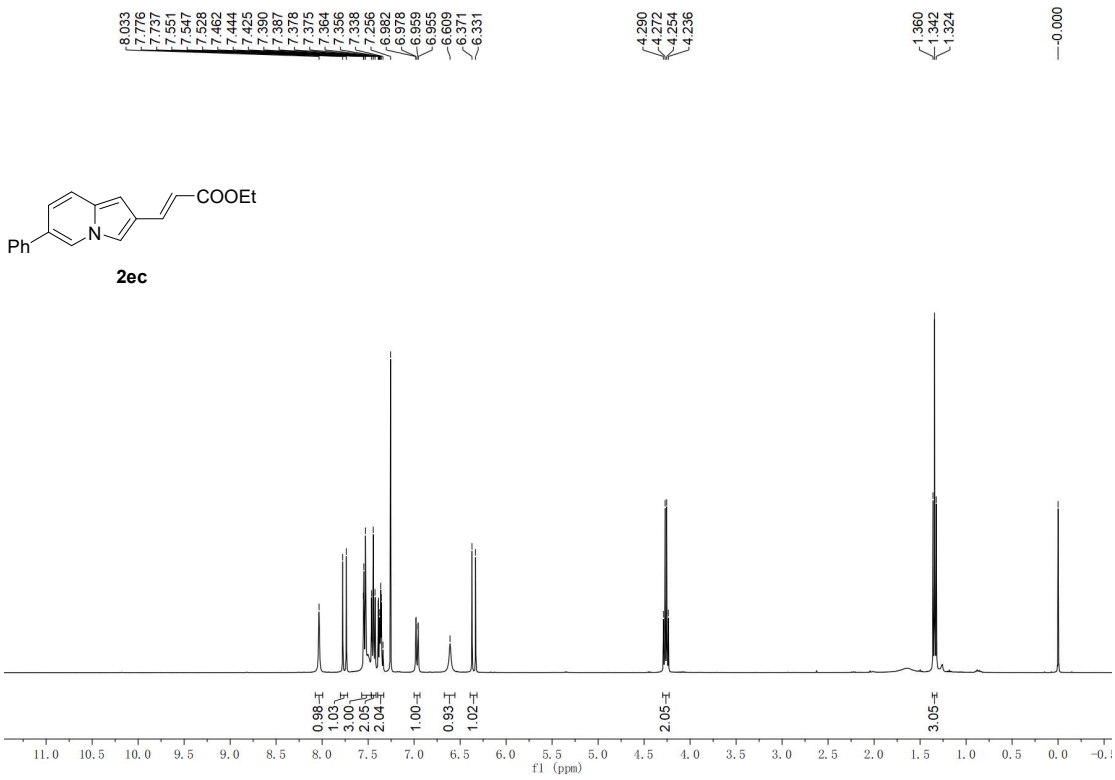
^{13}C NMR (100 MHz) of **2dd** in DMSO



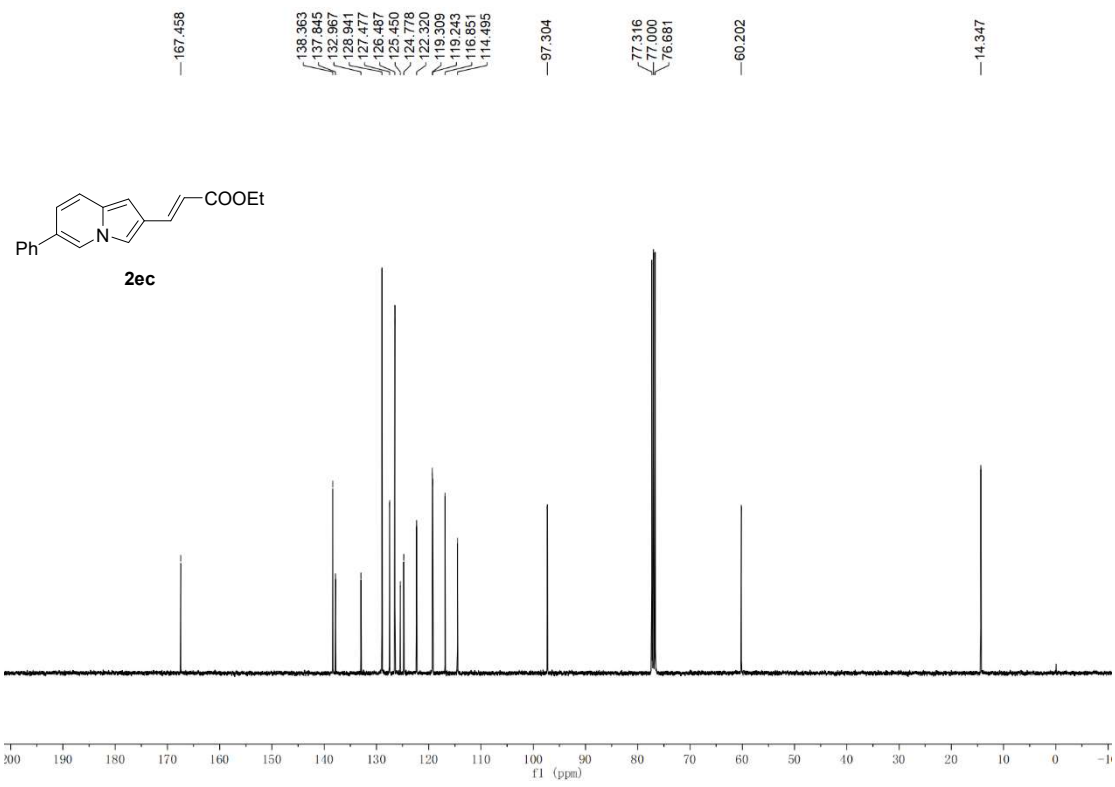
^{1}H NMR (400 MHz) of **2d** in DMSO



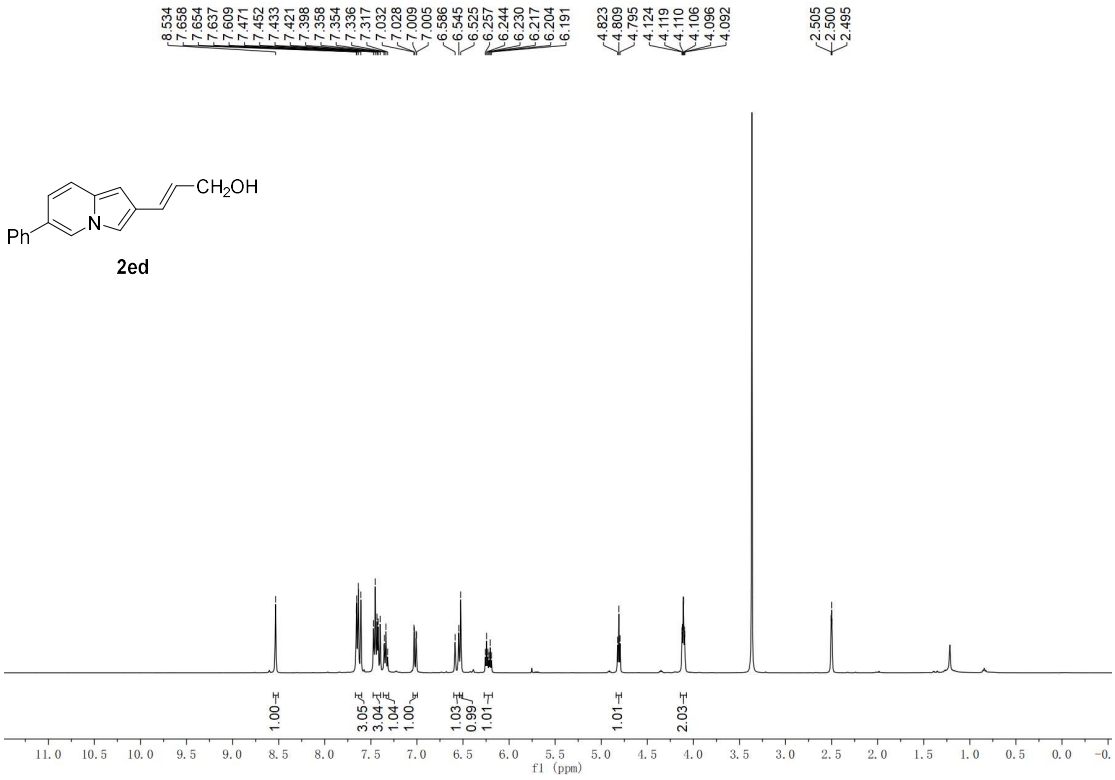
^{13}C NMR (100 MHz) of **2d** in DMSO



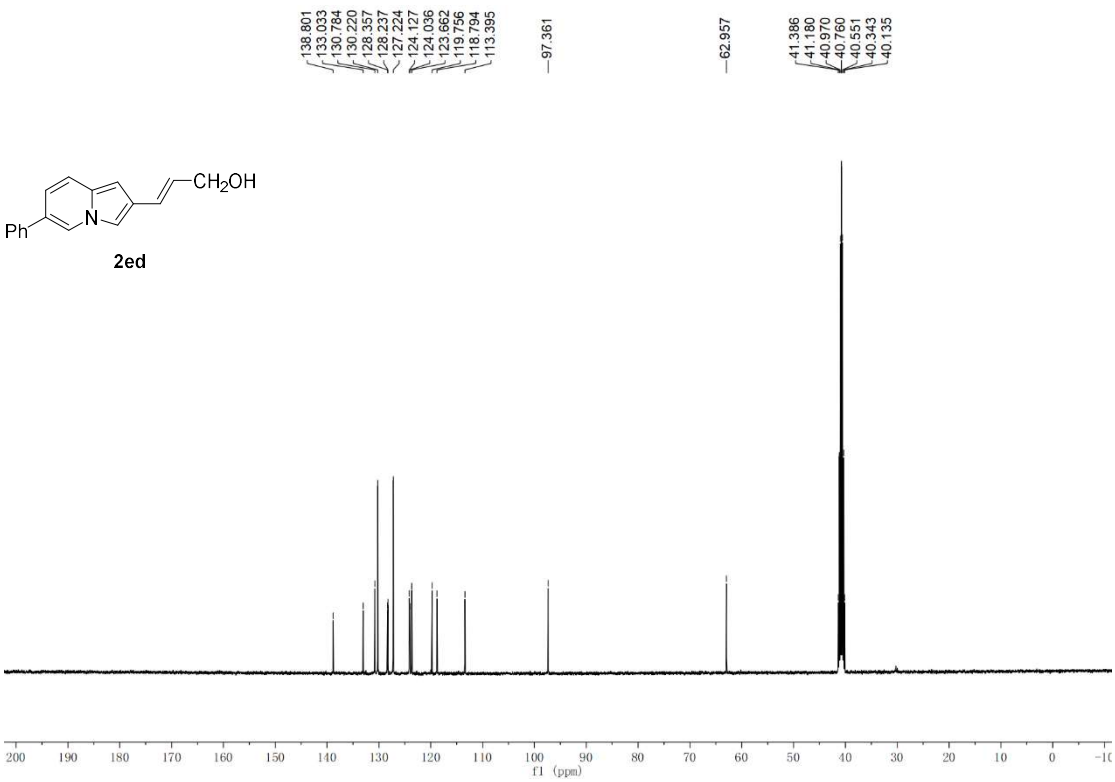
^{1}H NMR (400 MHz) of **2ec** in $CDCl_3$



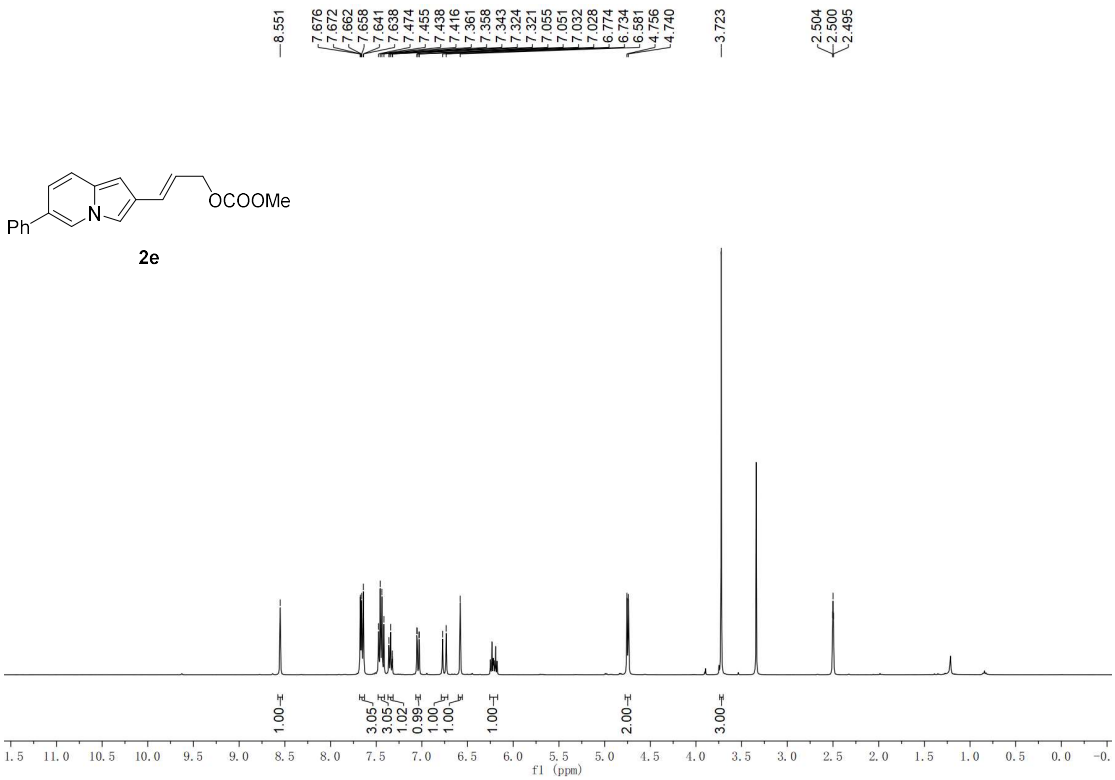
^{13}C NMR (100 MHz) of **2ec** in $CDCl_3$



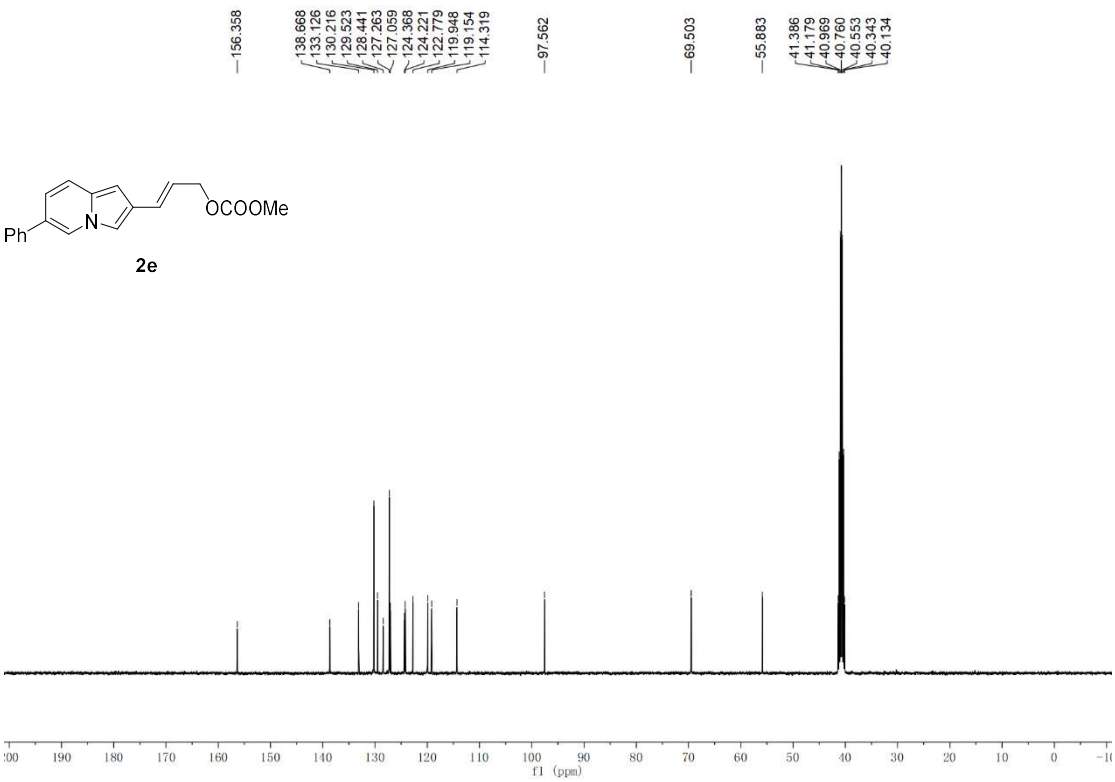
^{1}H NMR (400 MHz) of **2ed** in DMSO



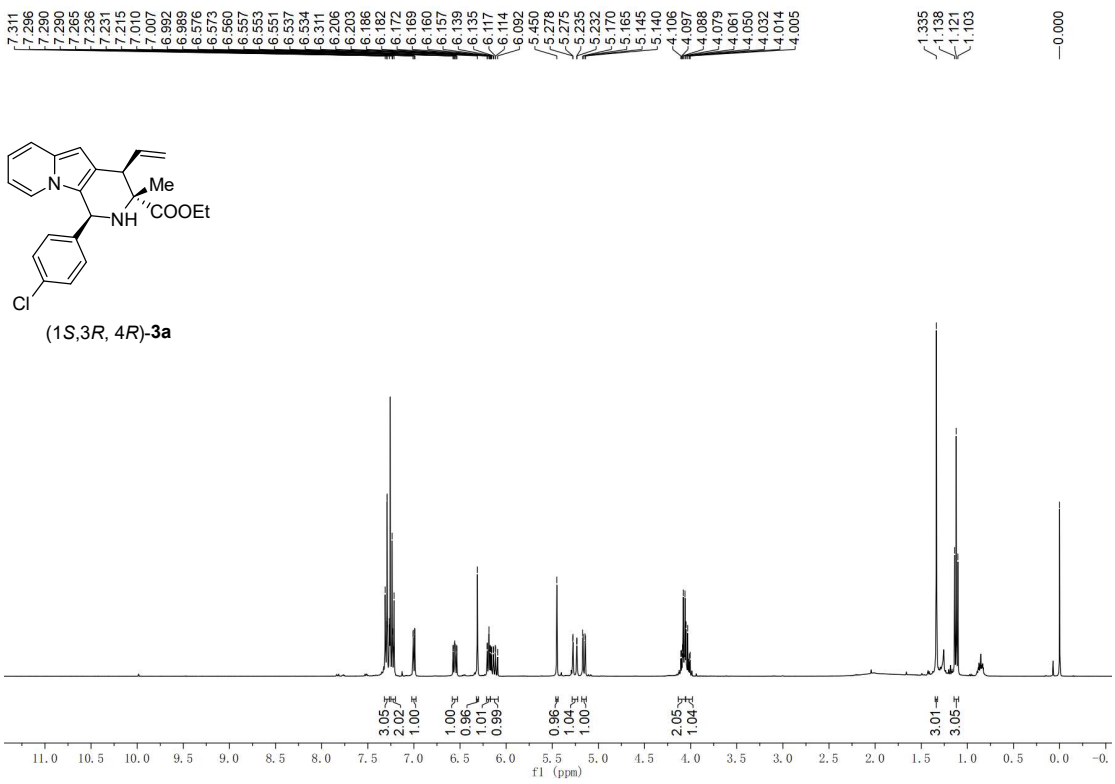
^{13}C NMR (100 MHz) of **2ed** in DMSO



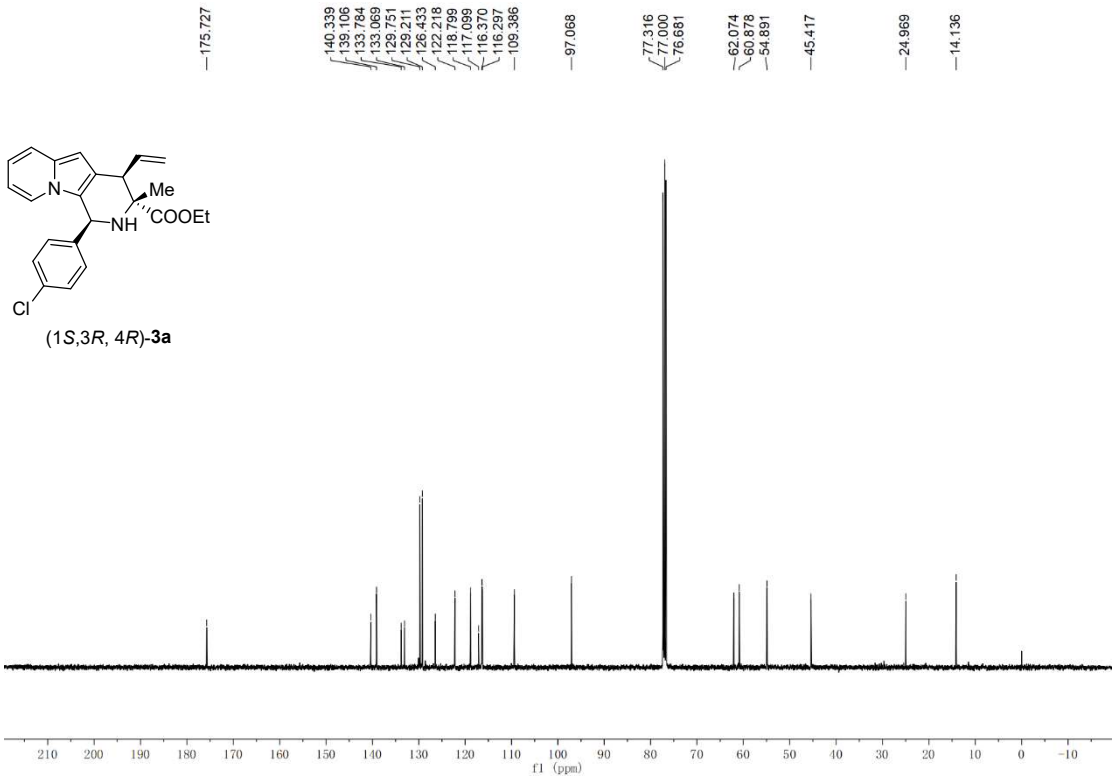
^{1}H NMR (400 MHz) of **2e** in DMSO



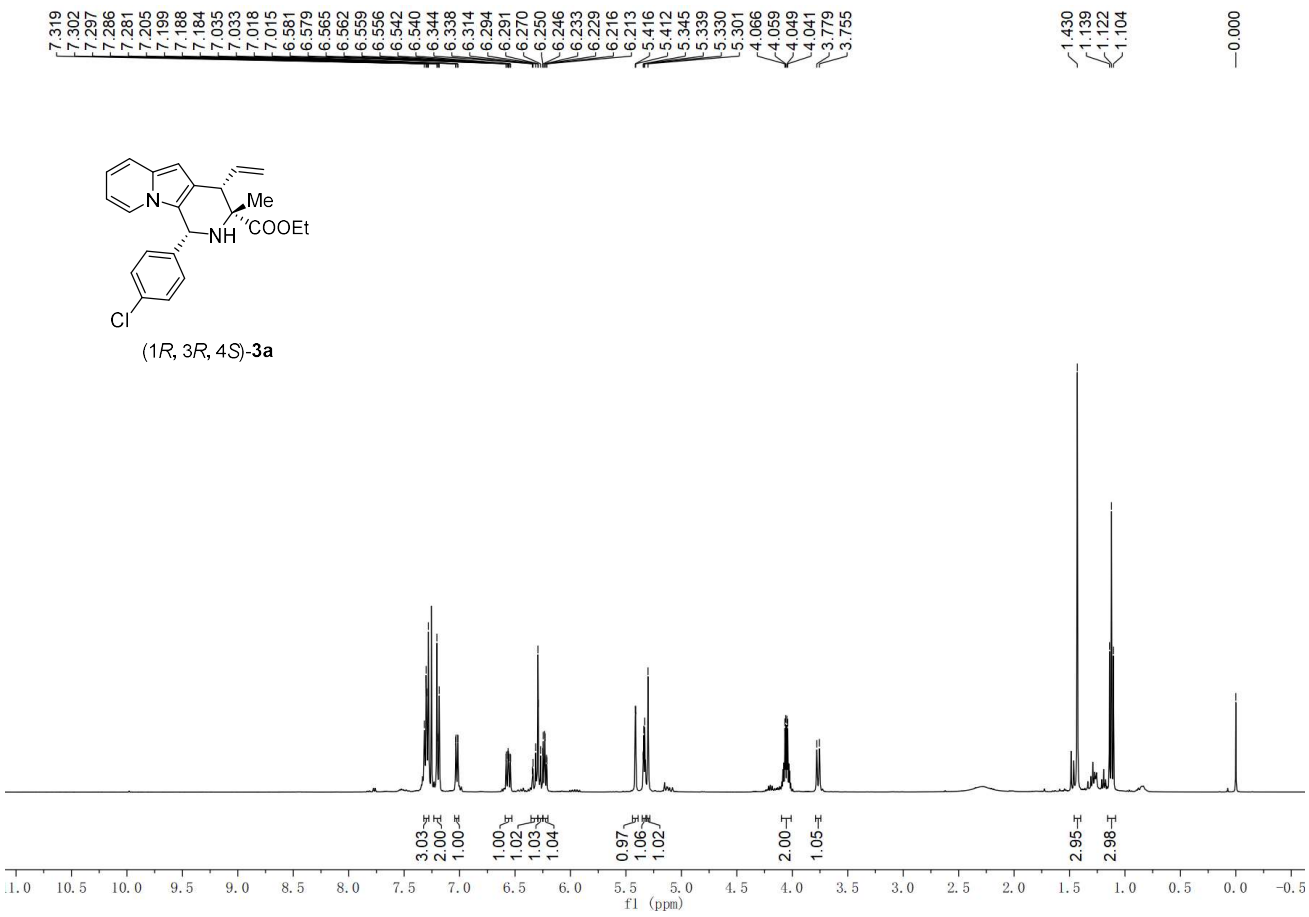
^{13}C NMR (100 MHz) of **2e** in DMSO



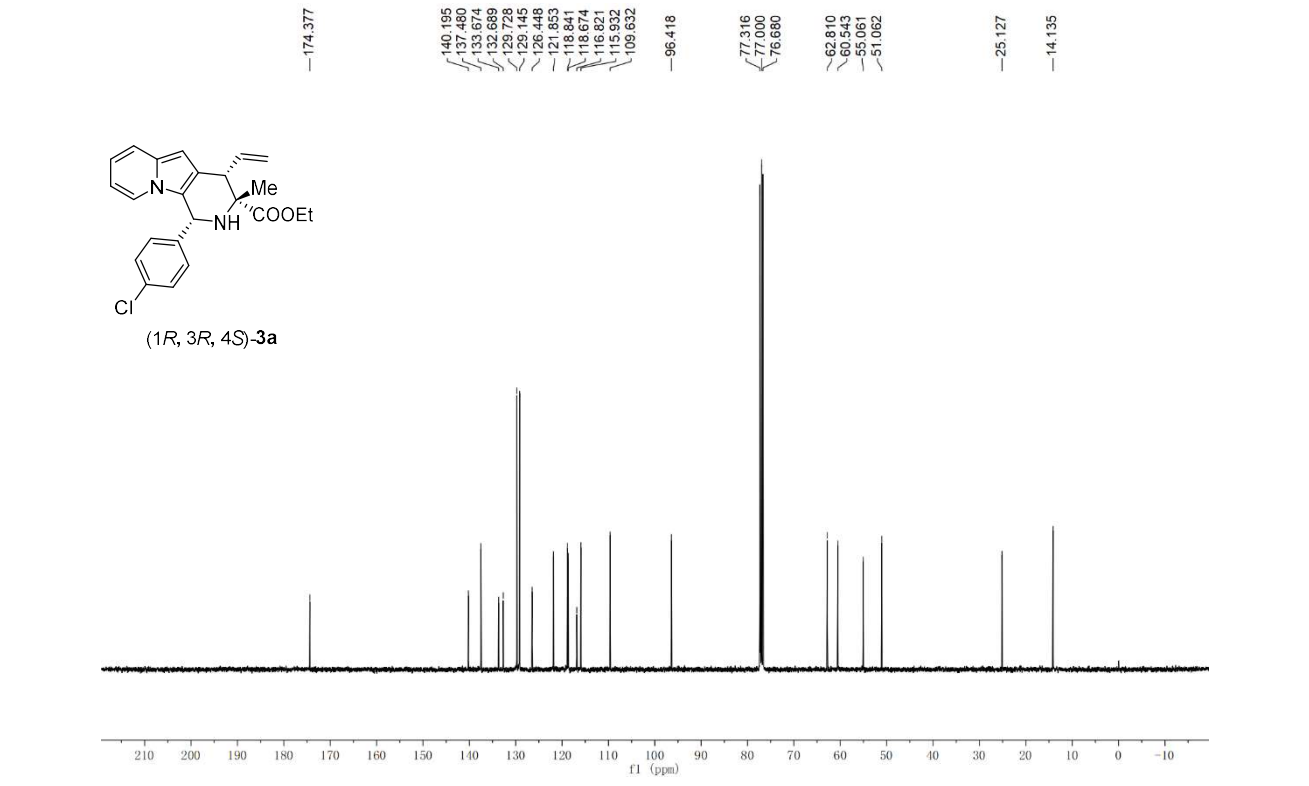
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3a** in $CDCl_3$



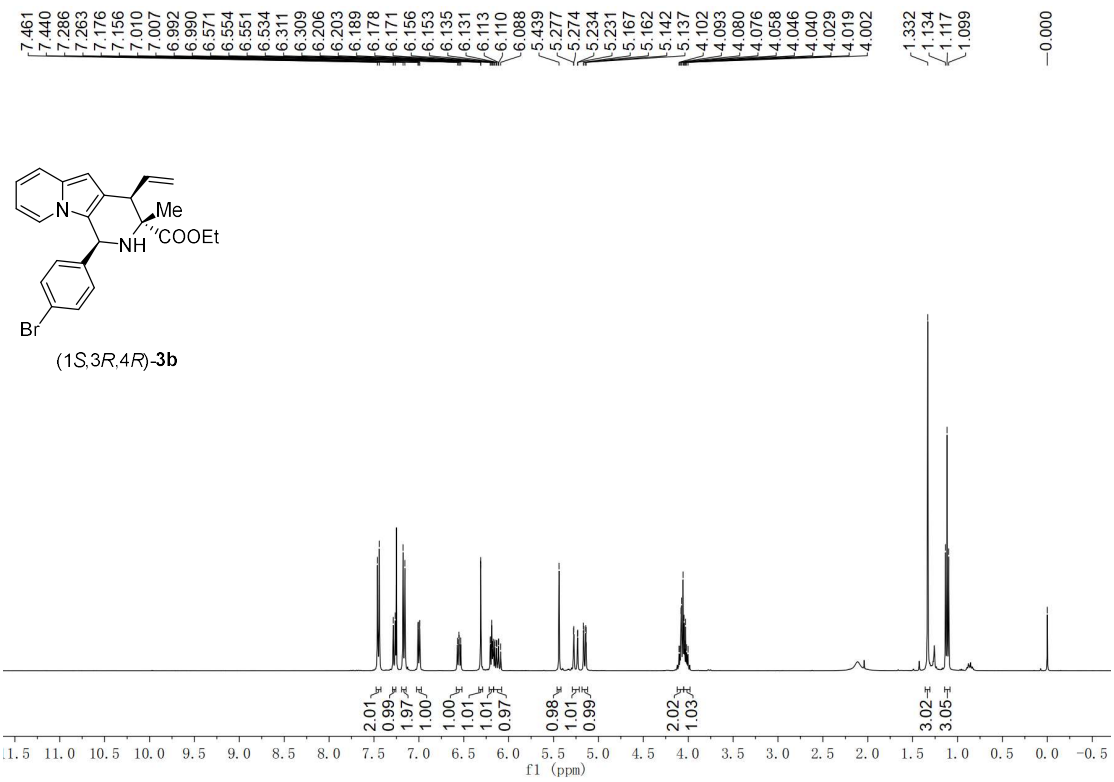
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3a** in $CDCl_3$



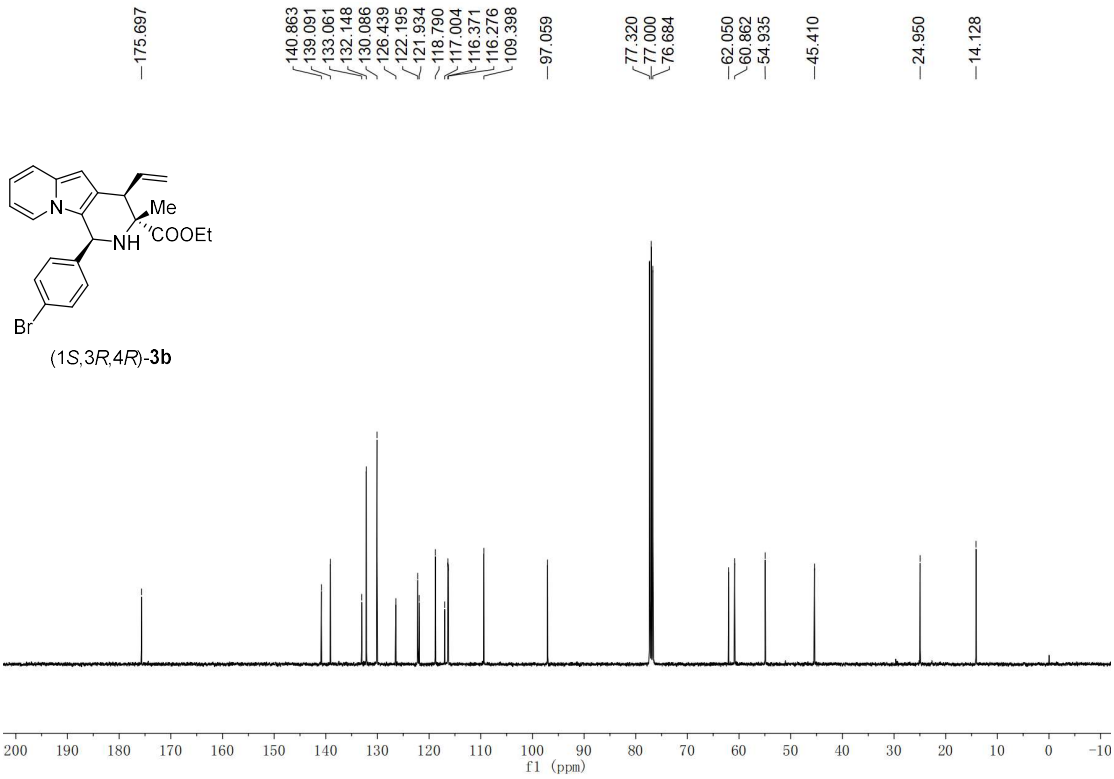
^{1}H NMR (400 MHz) of (1*R*, 3*R*, 4*S*)-**3a** in $CDCl_3$



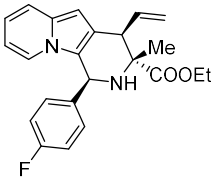
^{13}C NMR (100 MHz) of (1*R*, 3*R*, 4*S*)-**3a** in $CDCl_3$



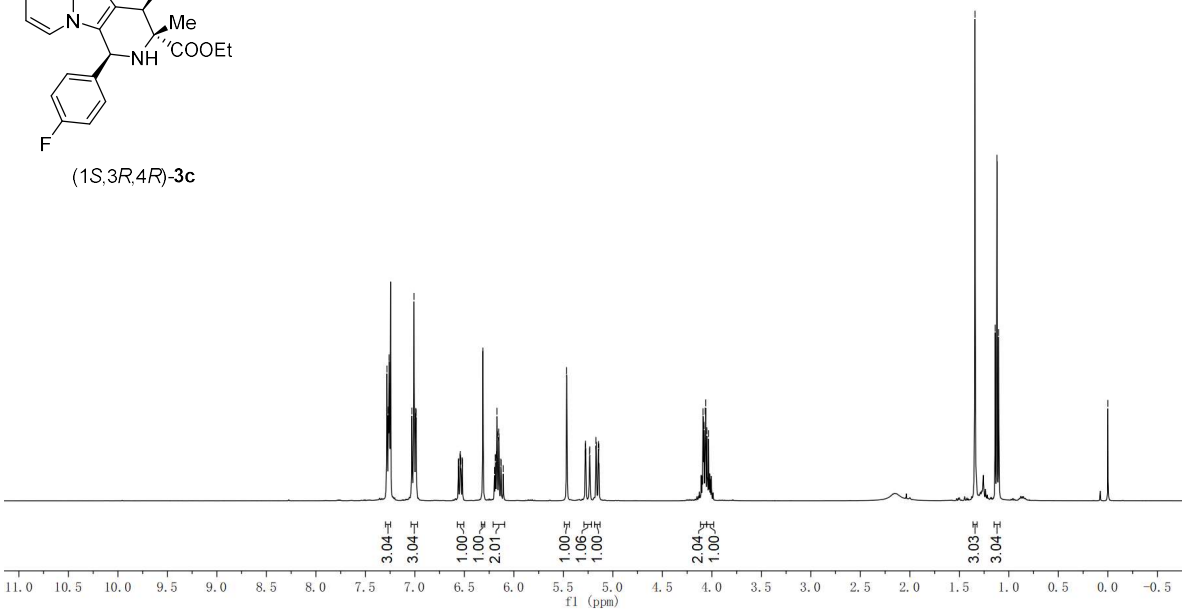
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3b** in $CDCl_3$



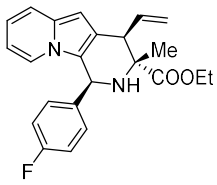
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3b** in $CDCl_3$



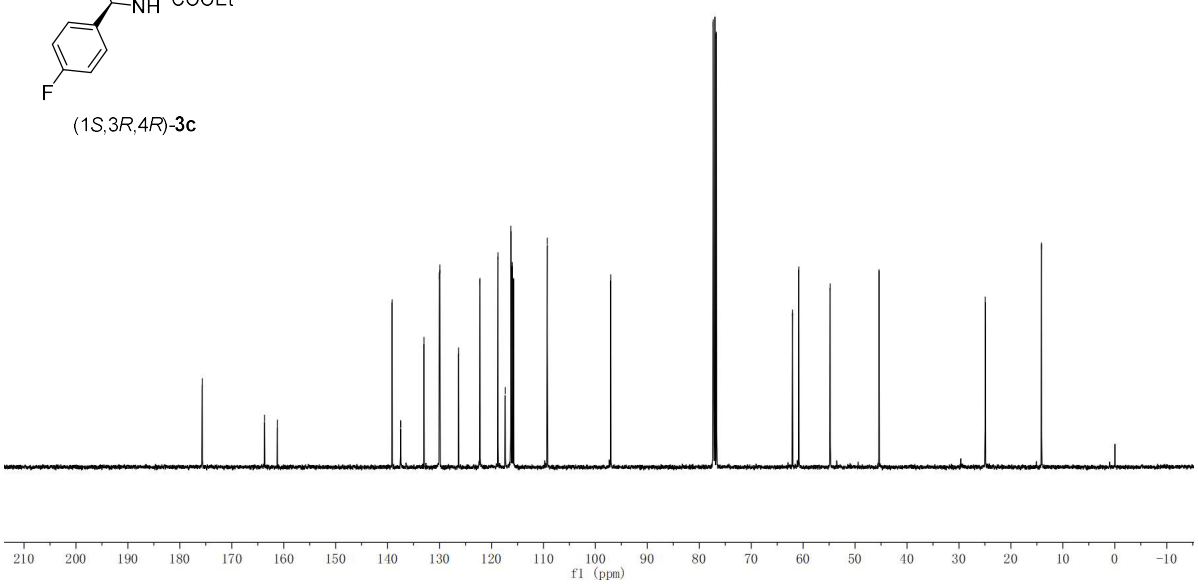
(1*S*,3*R*,4*R*)-**3c**



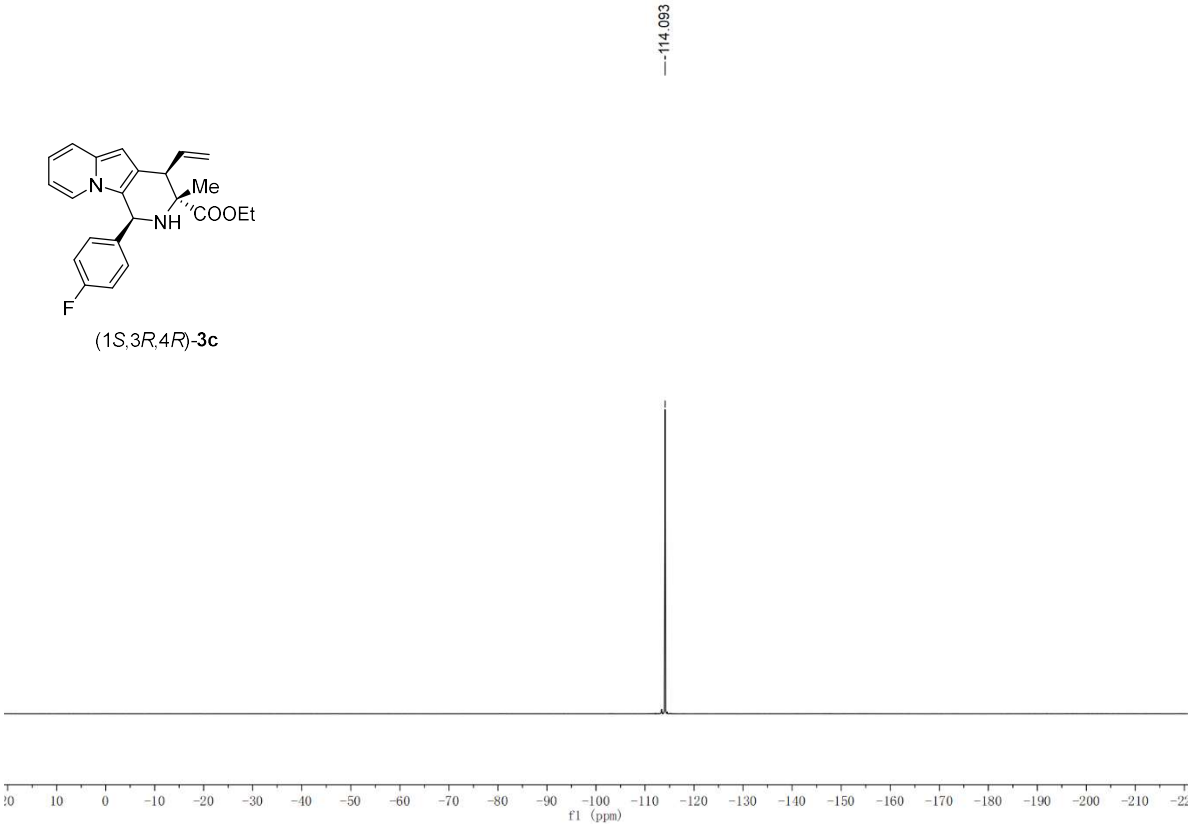
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3c** in $CDCl_3$



(1*S*,3*R*,4*R*)-**3c**

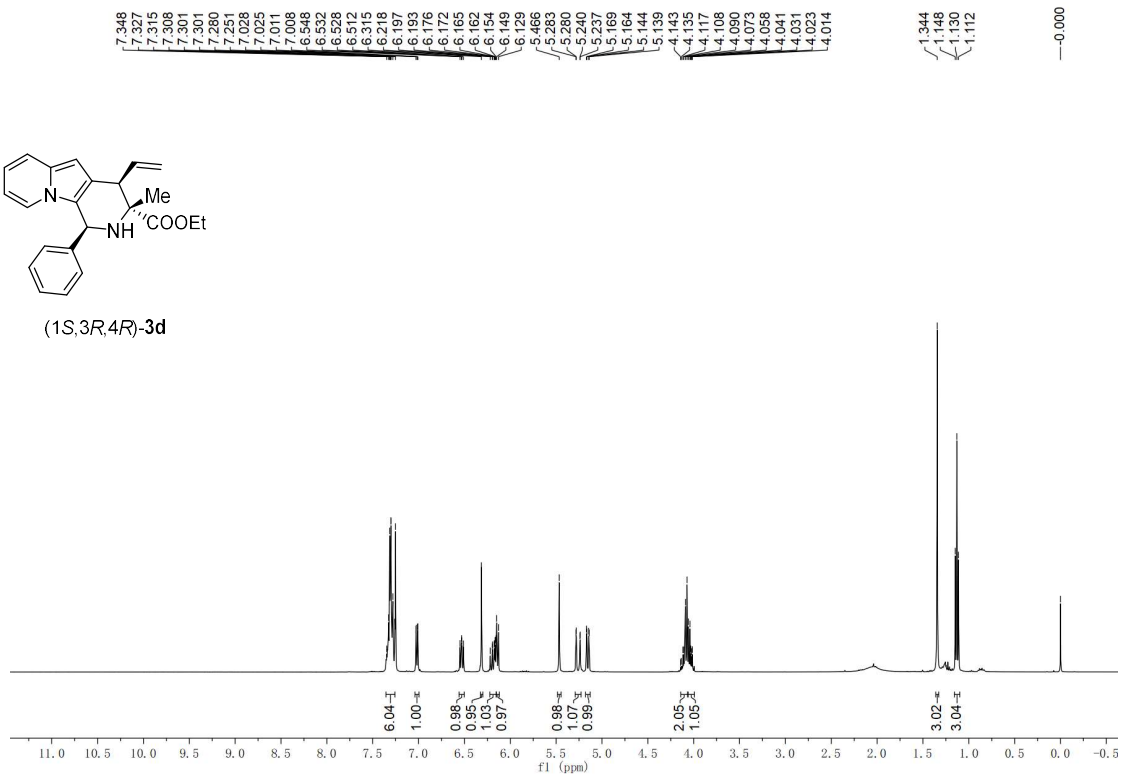


^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3c** in $CDCl_3$

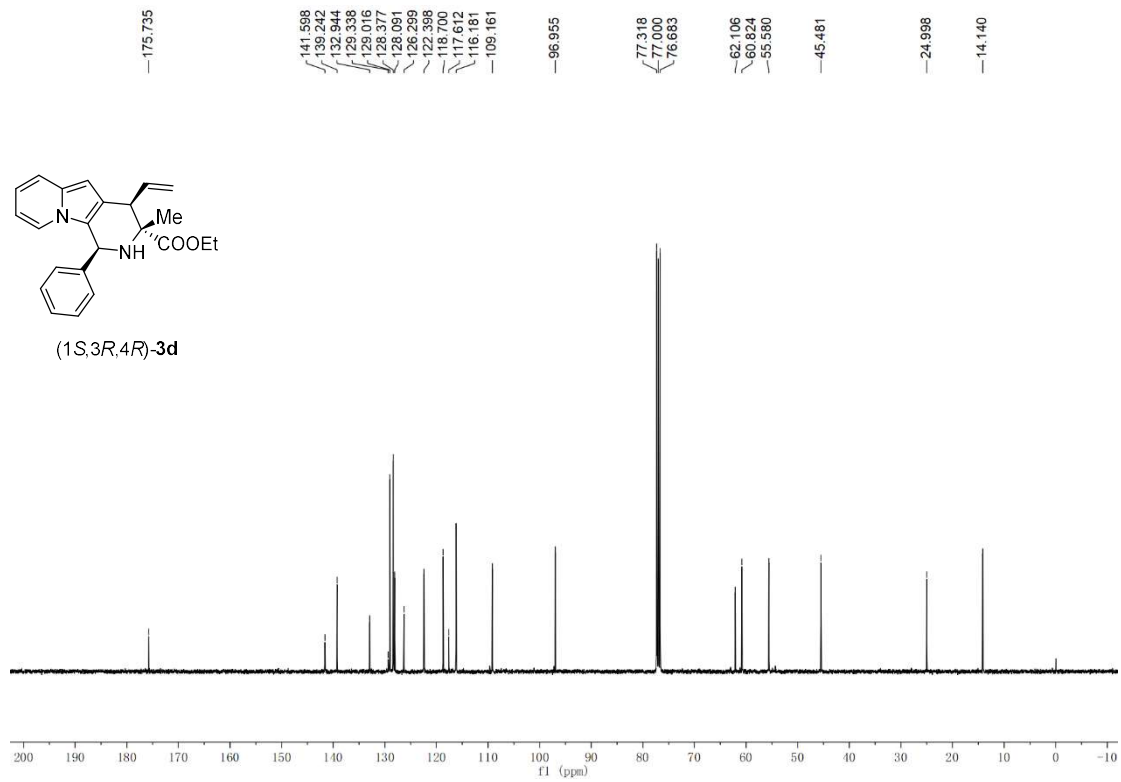


(1*S*,3*R*,4*R*)-**3c**

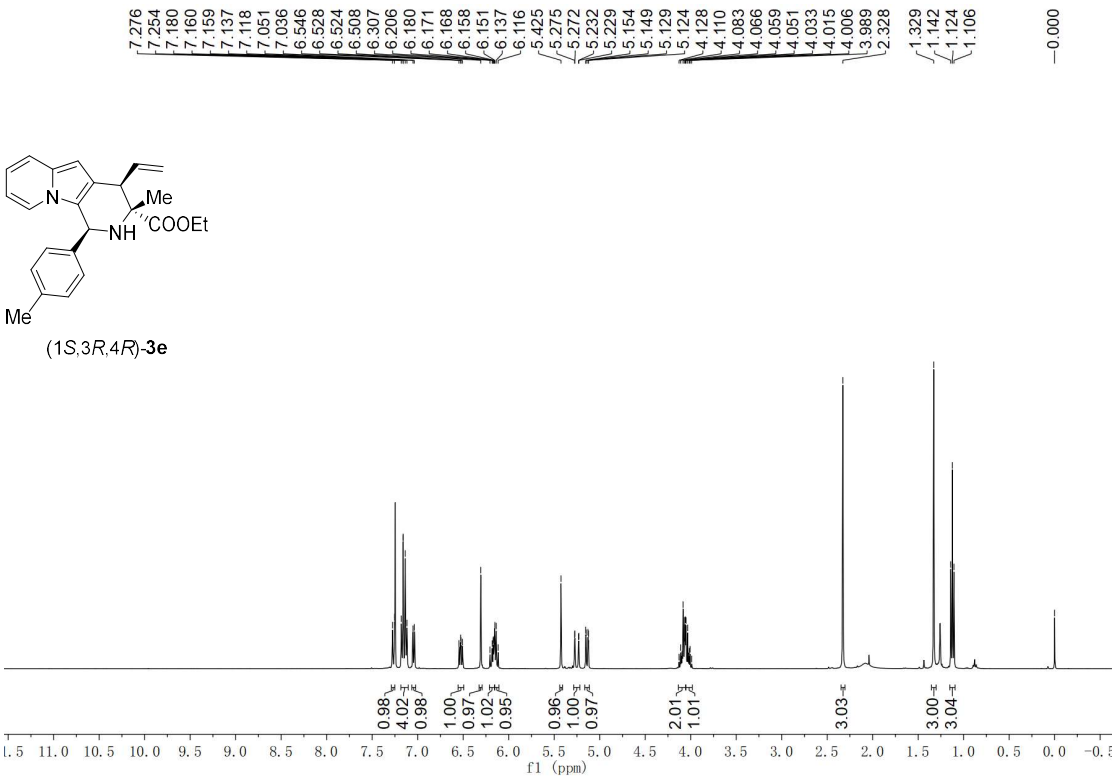
^{19}F NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3c** in $CDCl_3$



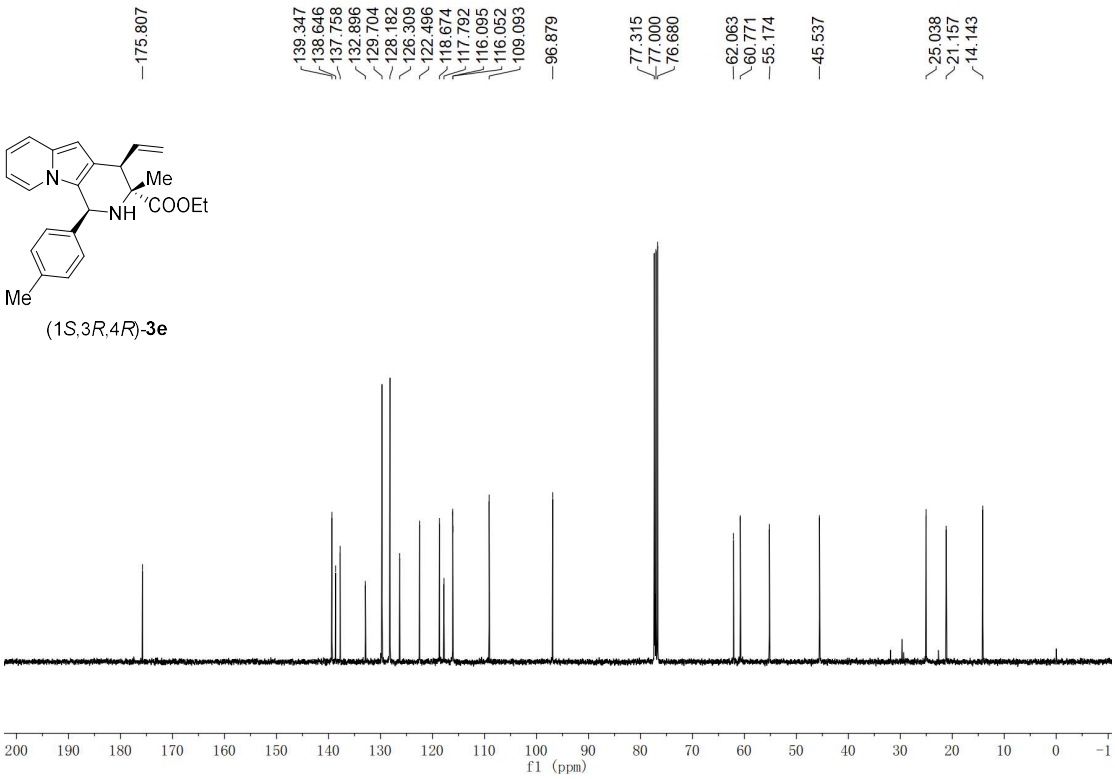
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3d** in $CDCl_3$



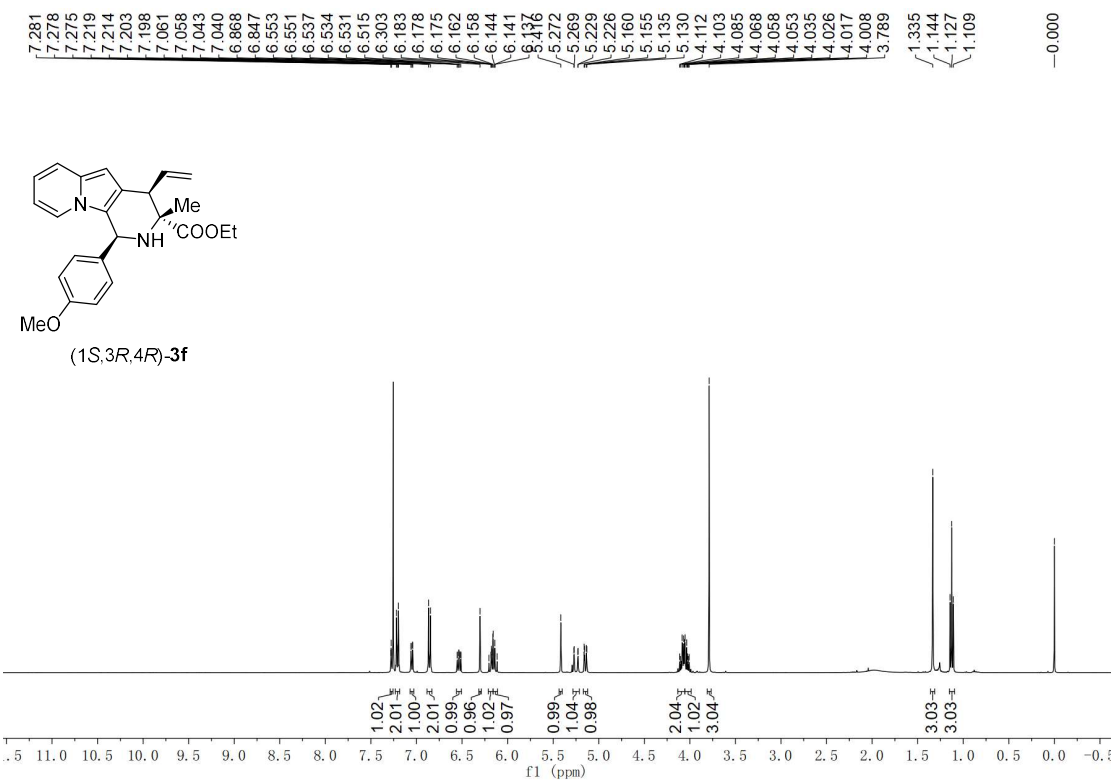
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3d** in $CDCl_3$



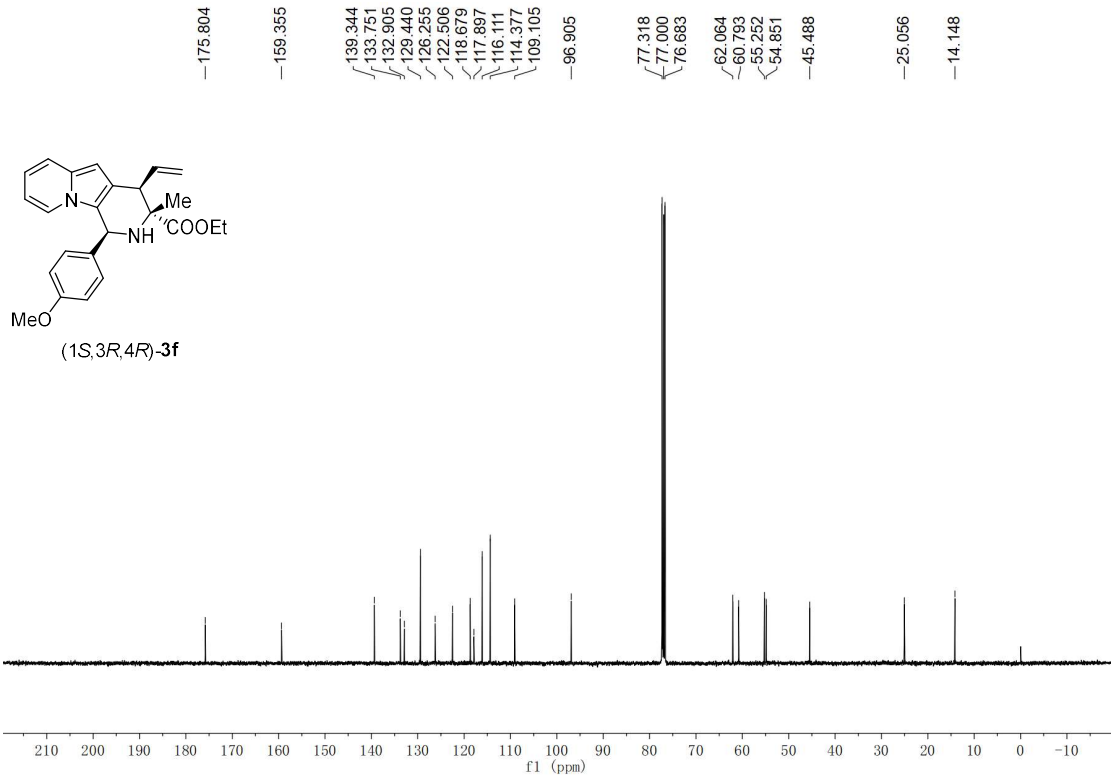
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3e** in $CDCl_3$



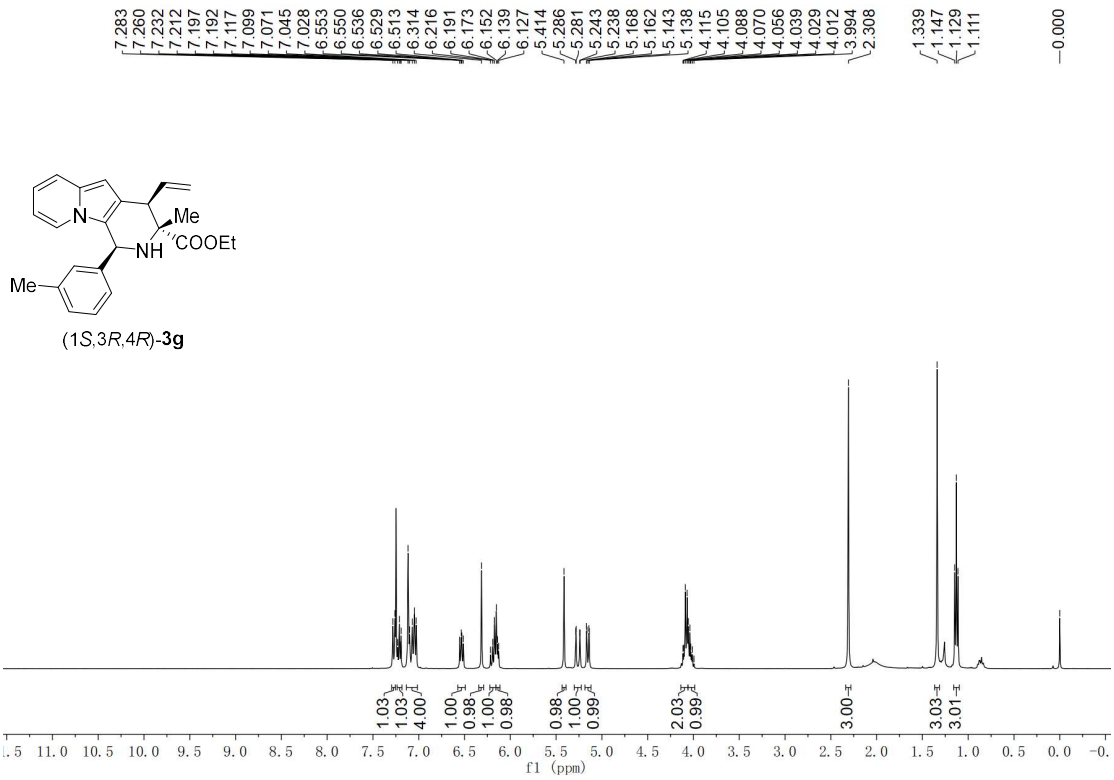
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3e** in $CDCl_3$



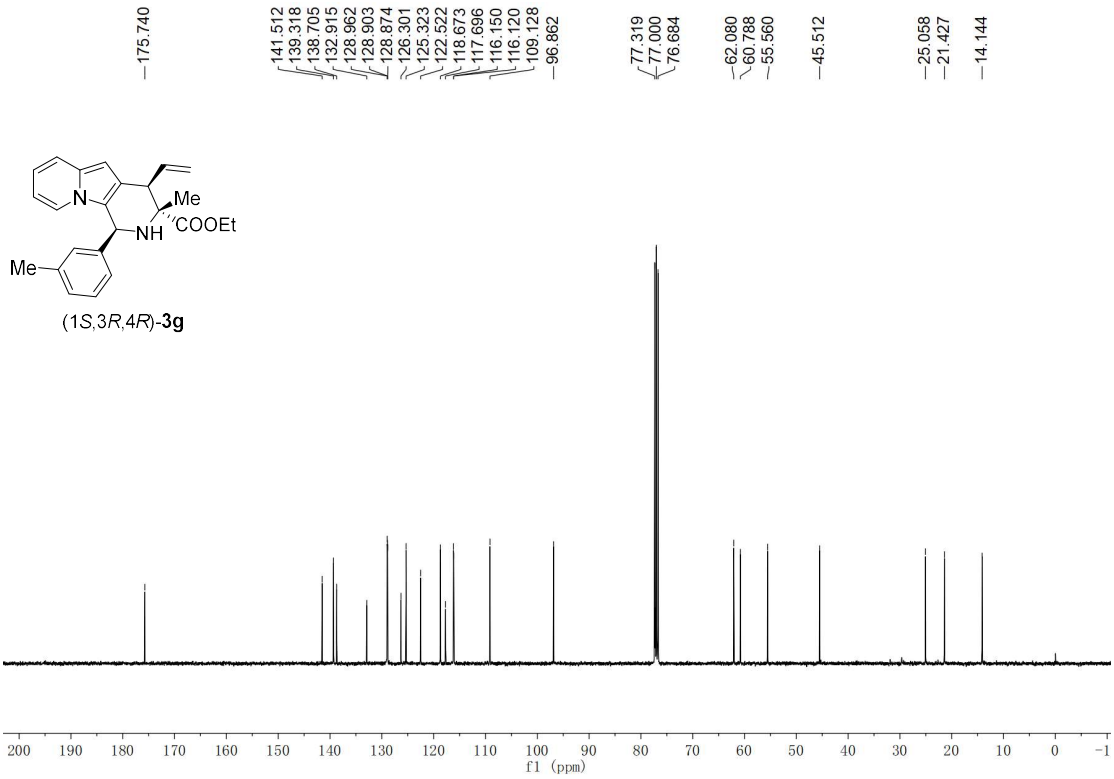
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3f** in $CDCl_3$



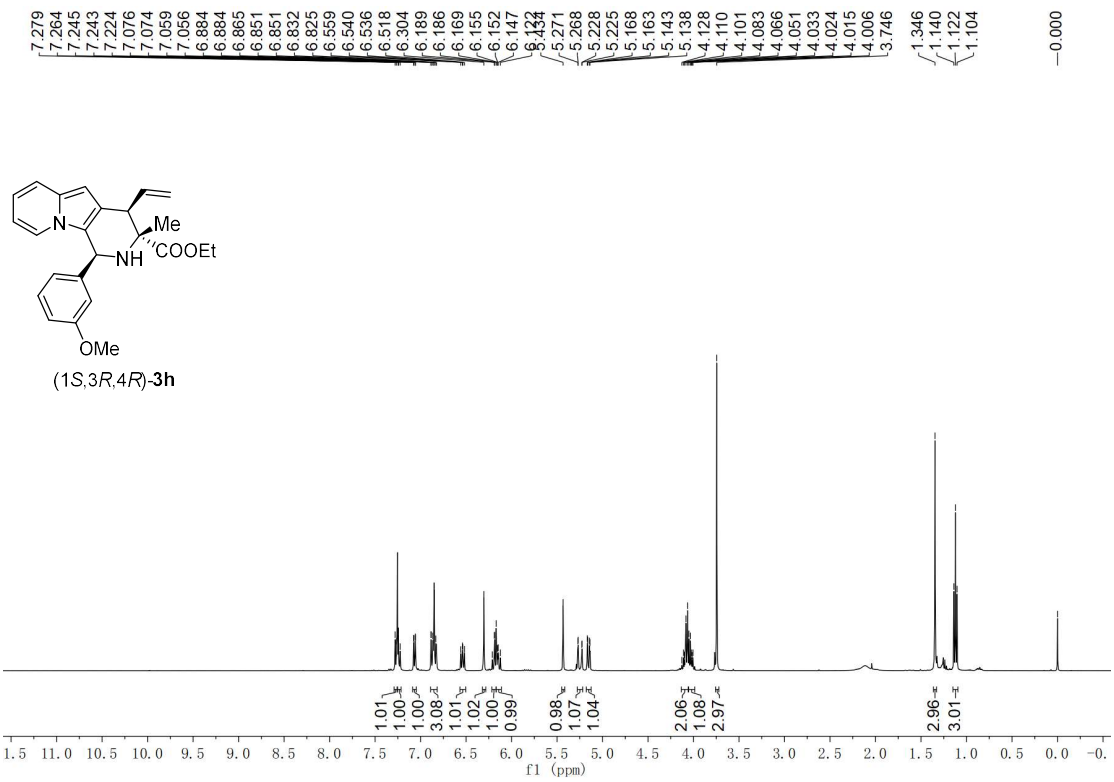
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3f** in $CDCl_3$



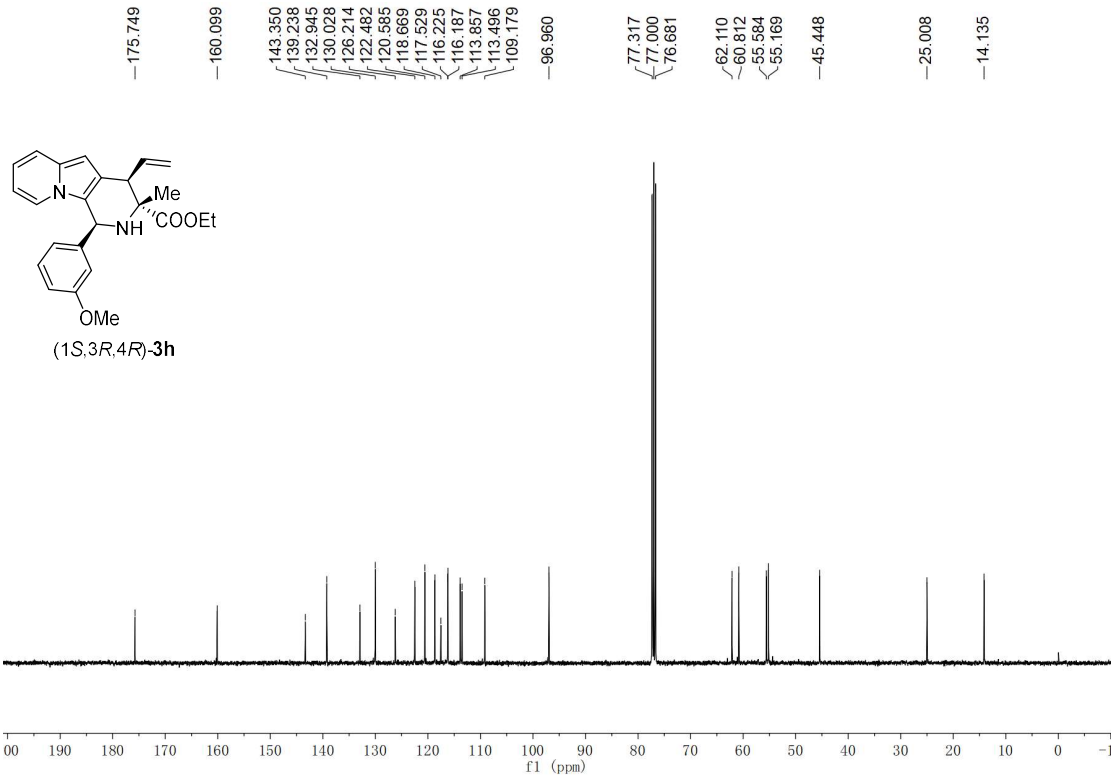
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3g** in $CDCl_3$



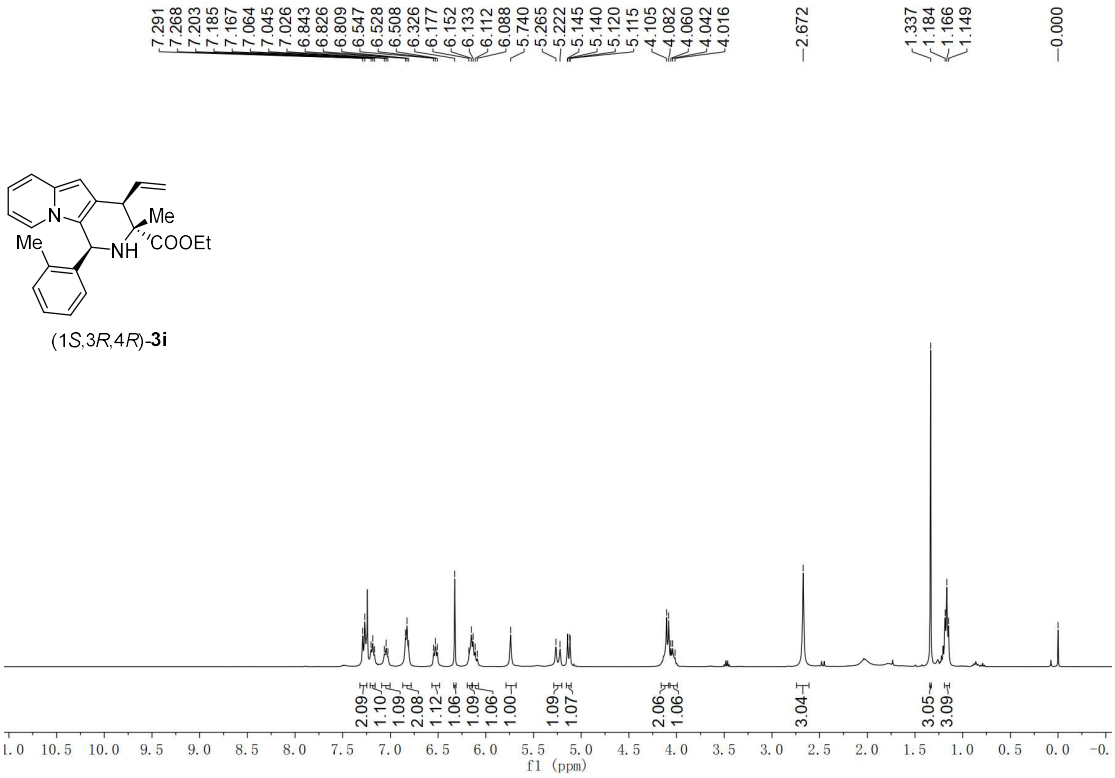
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3g** in $CDCl_3$



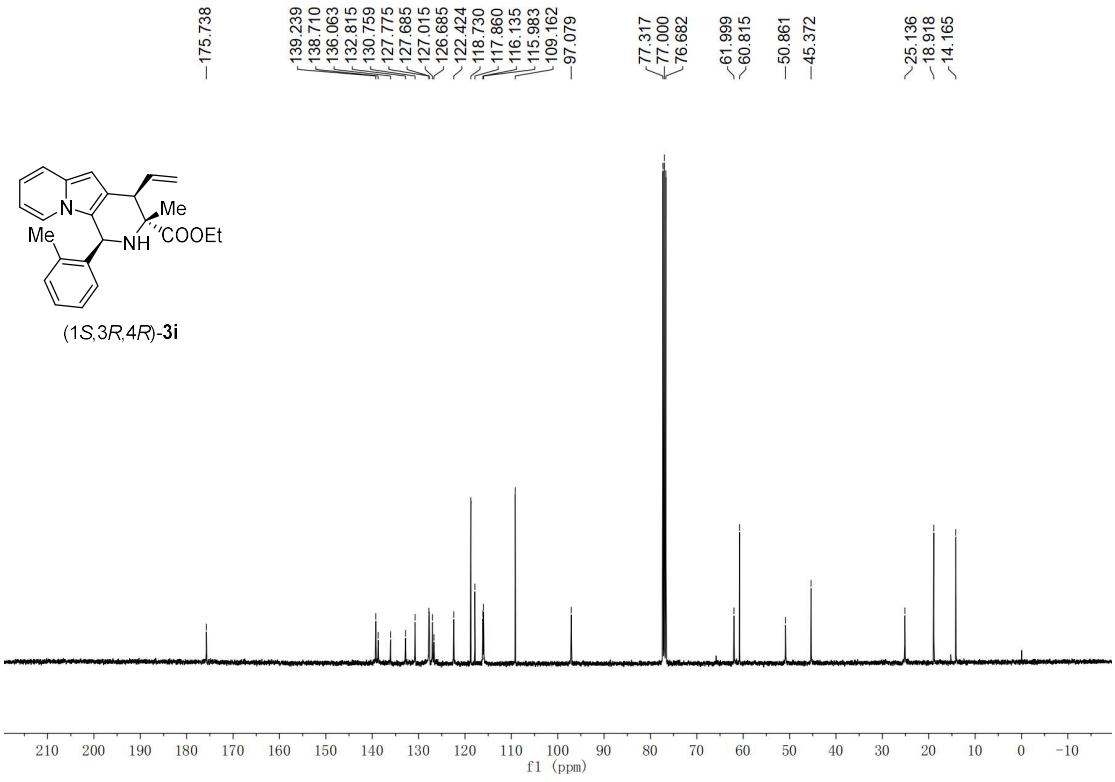
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3h** in $CDCl_3$



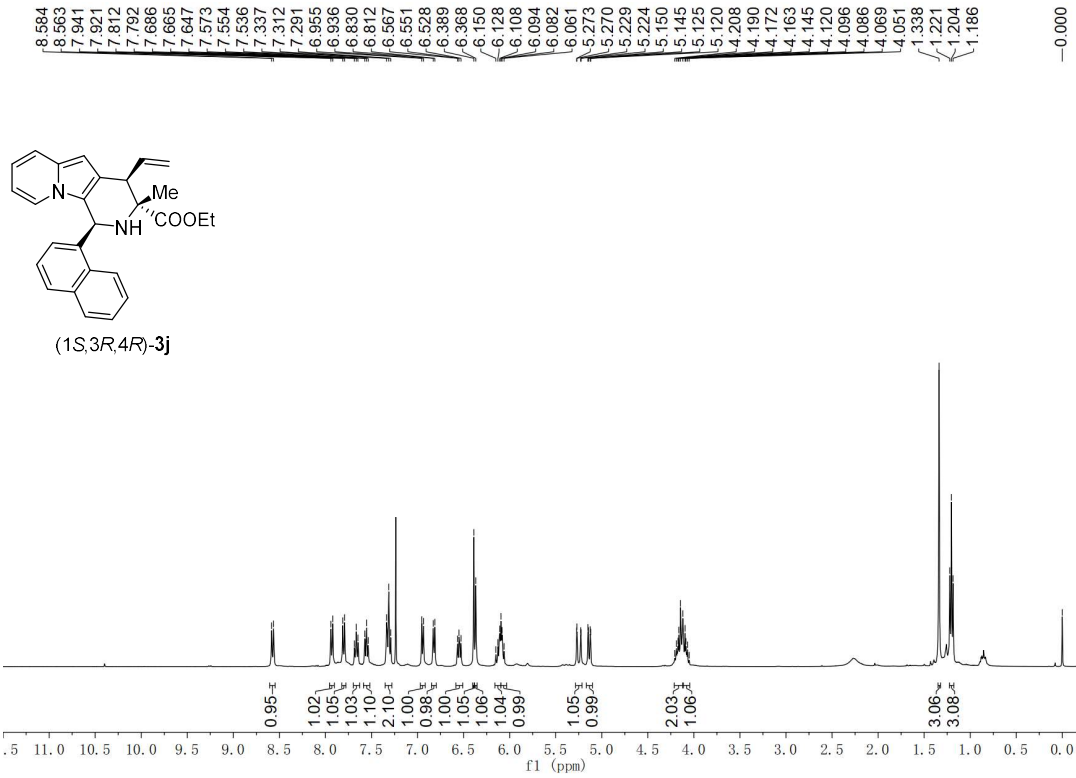
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3h** in $CDCl_3$



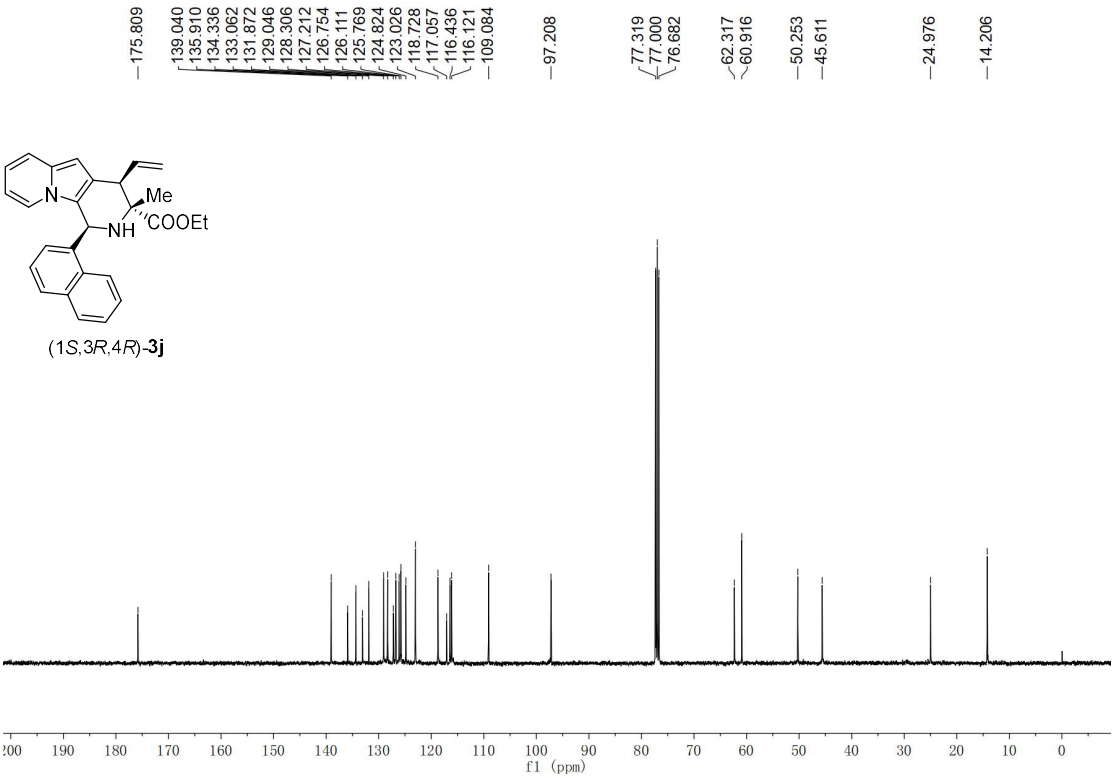
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3i** in $CDCl_3$



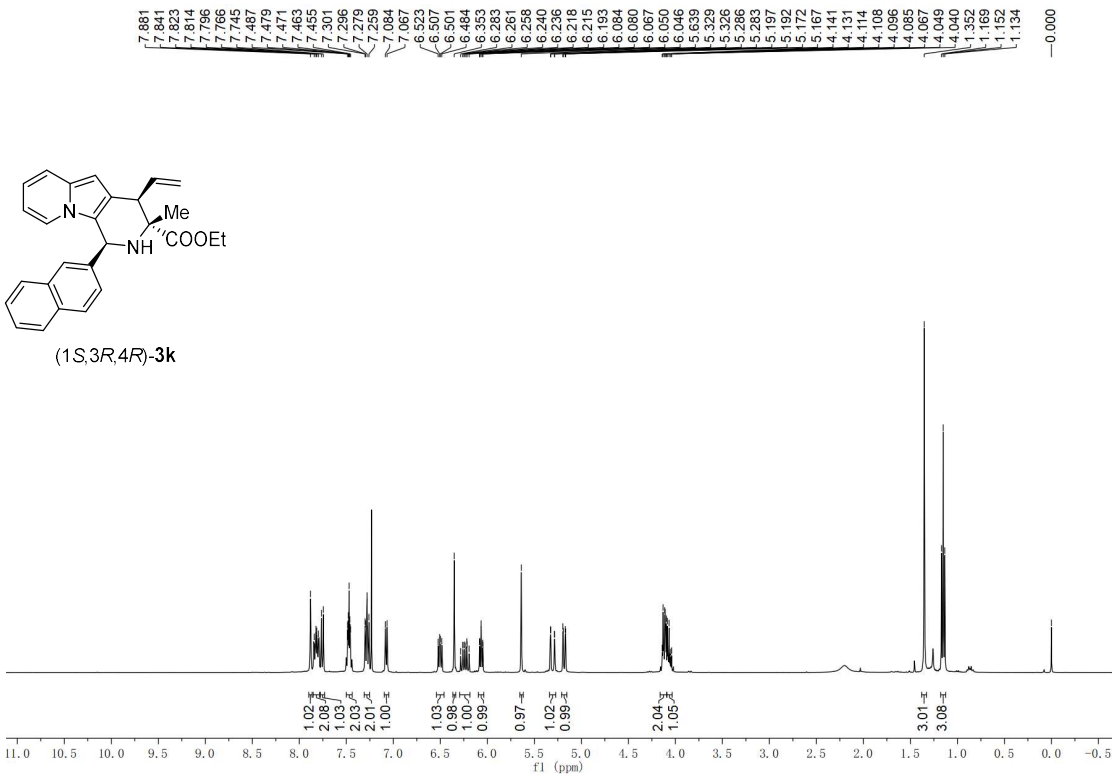
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3i** in $CDCl_3$



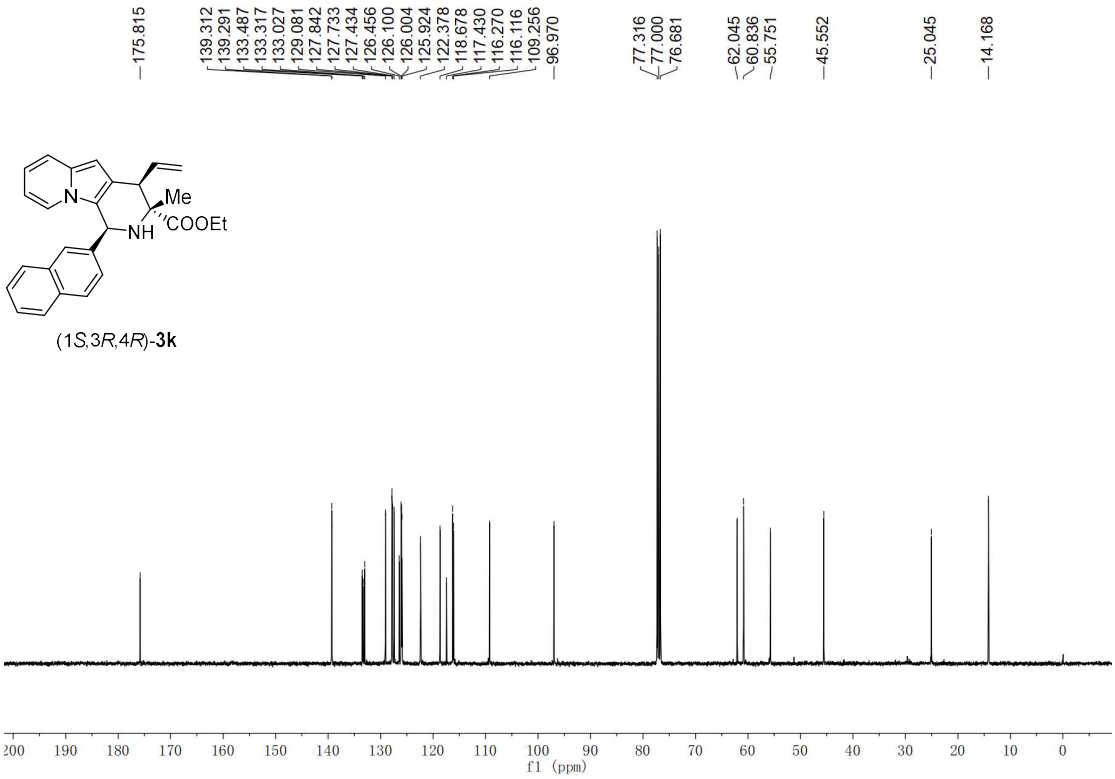
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3j** in $CDCl_3$



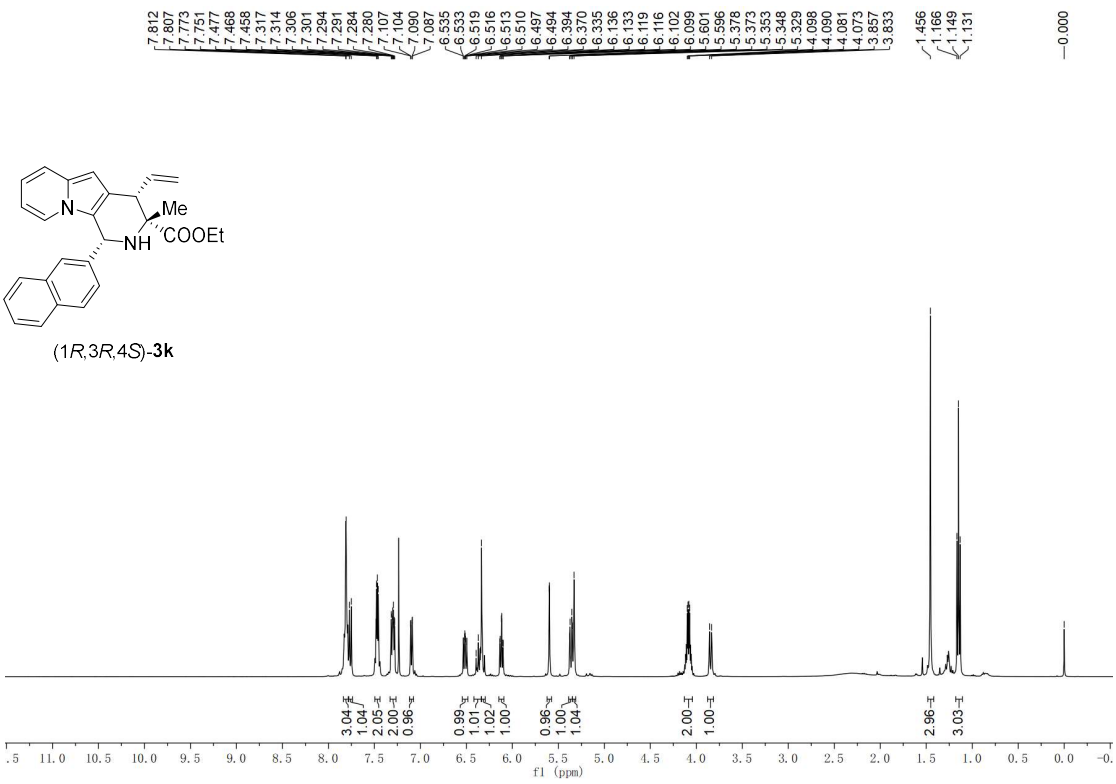
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3j** in $CDCl_3$



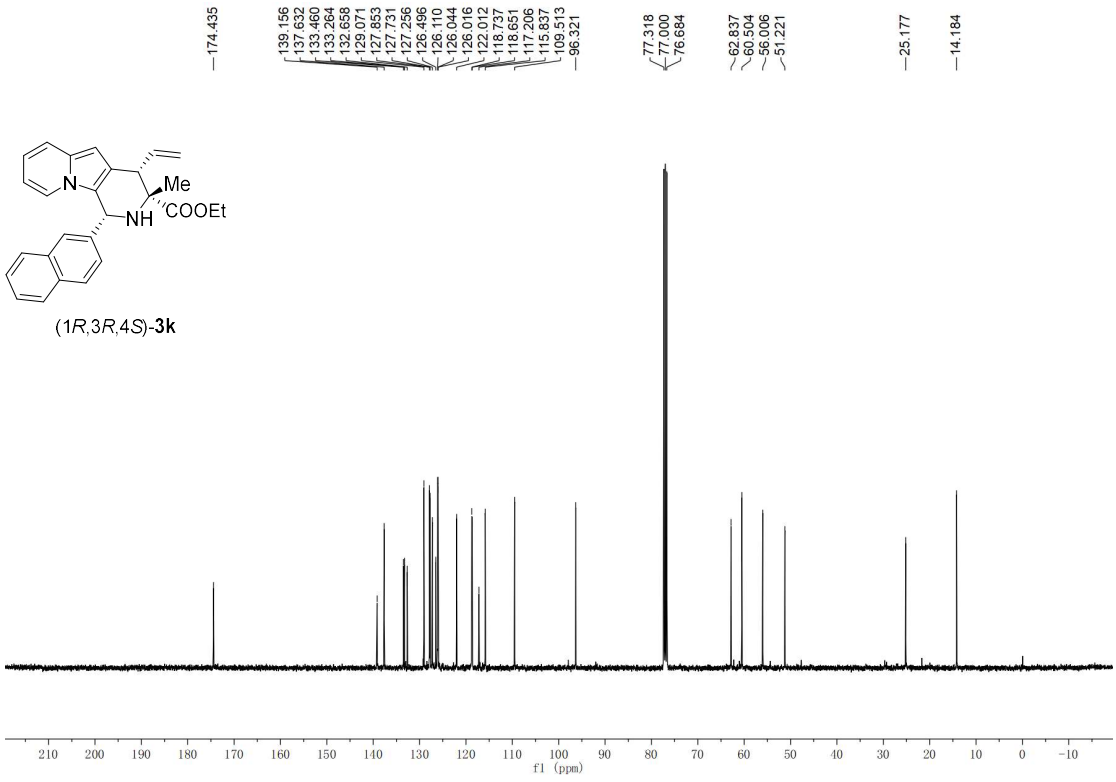
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3k** in $CDCl_3$



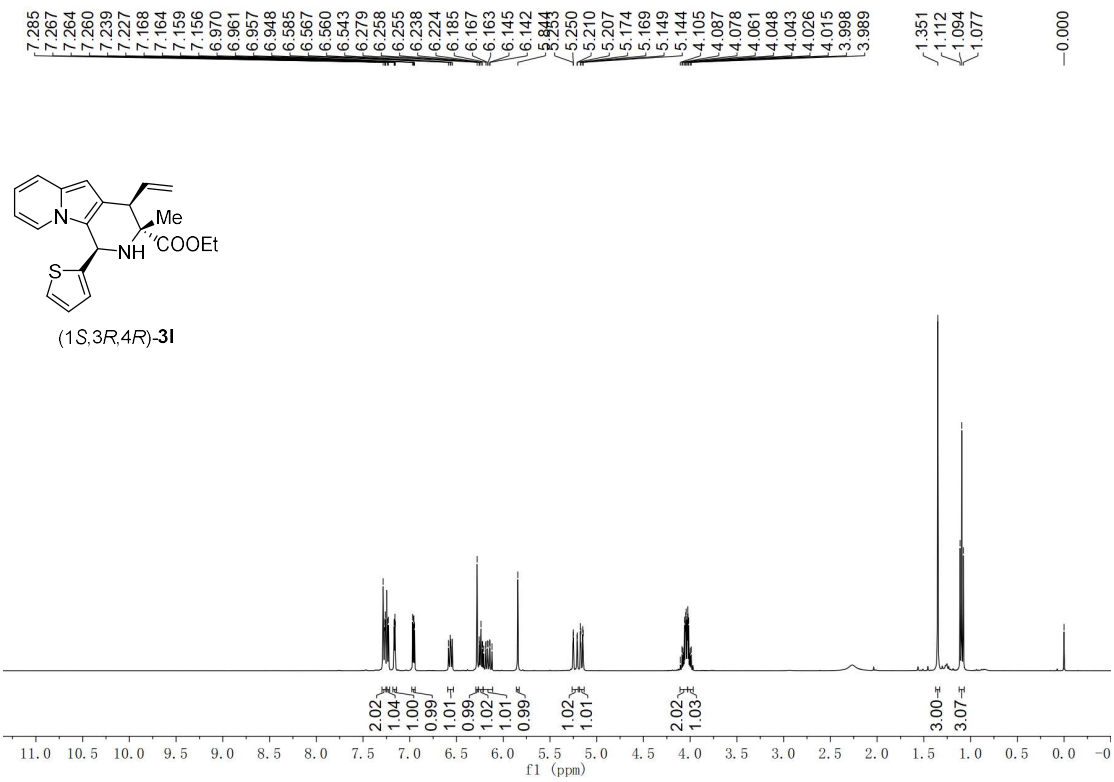
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3k** in $CDCl_3$



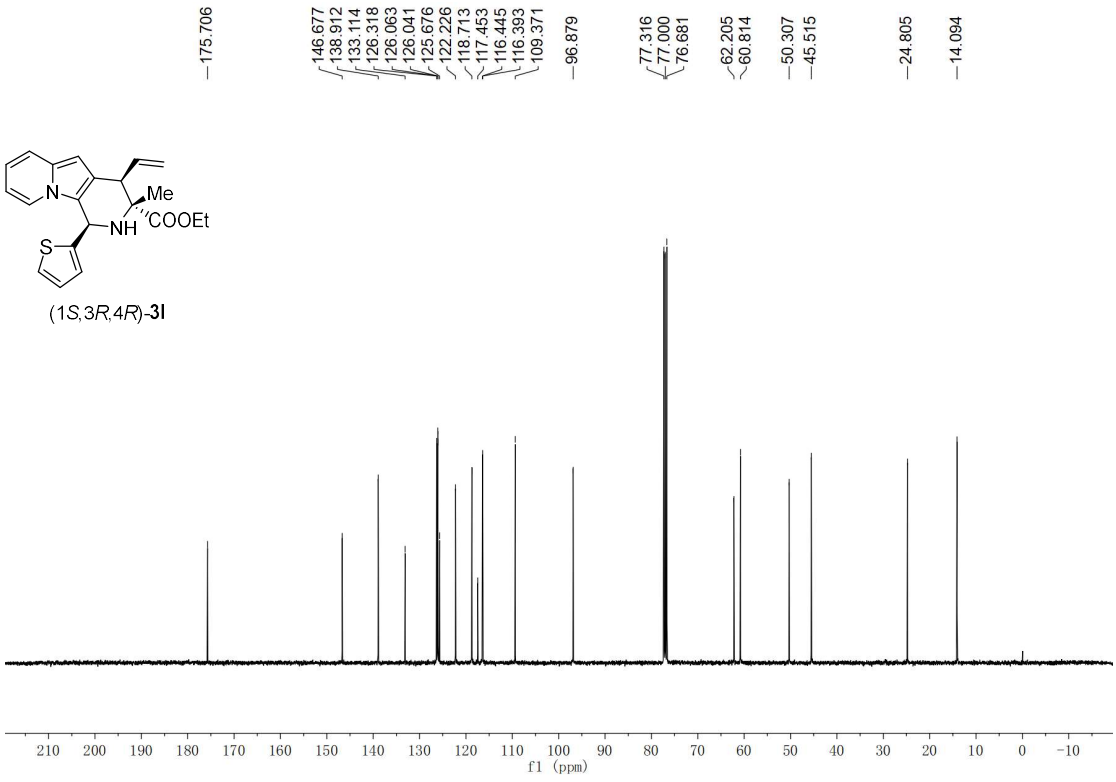
^{1}H NMR (400 MHz) of (1*R*, 3*R*, 4*S*)-**3k** in $CDCl_3$



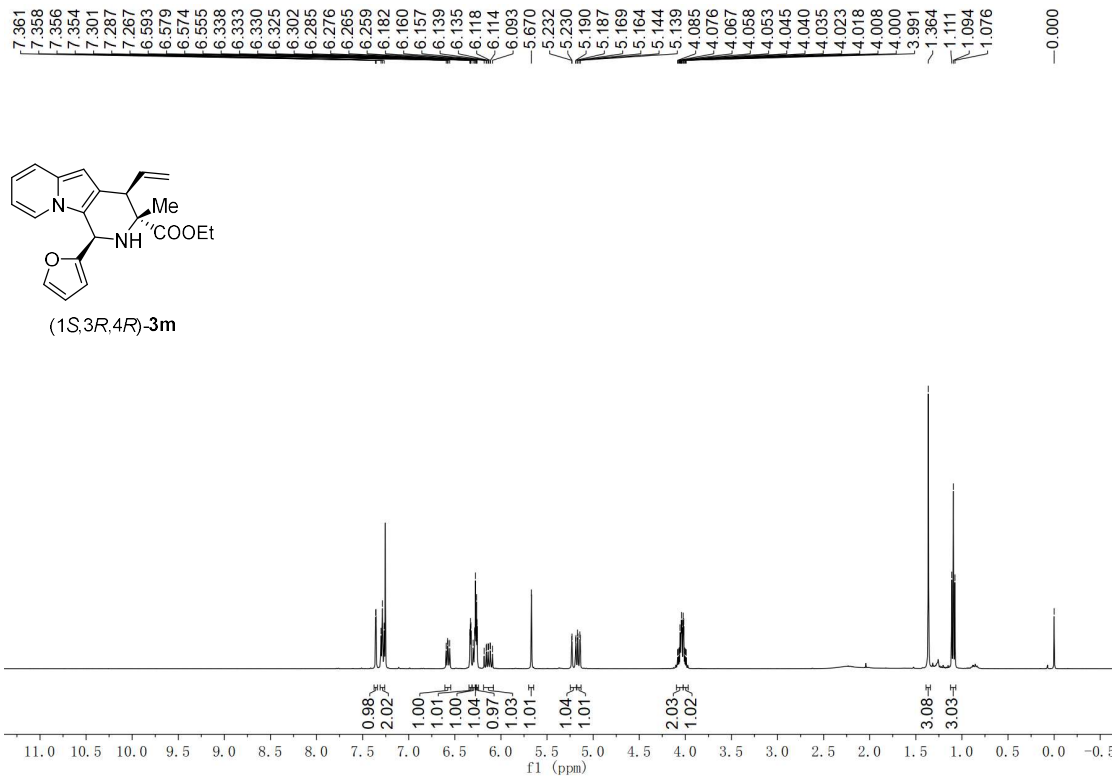
^{13}C NMR (100 MHz) of (1*R*, 3*R*, 4*S*)-**3k** in $CDCl_3$



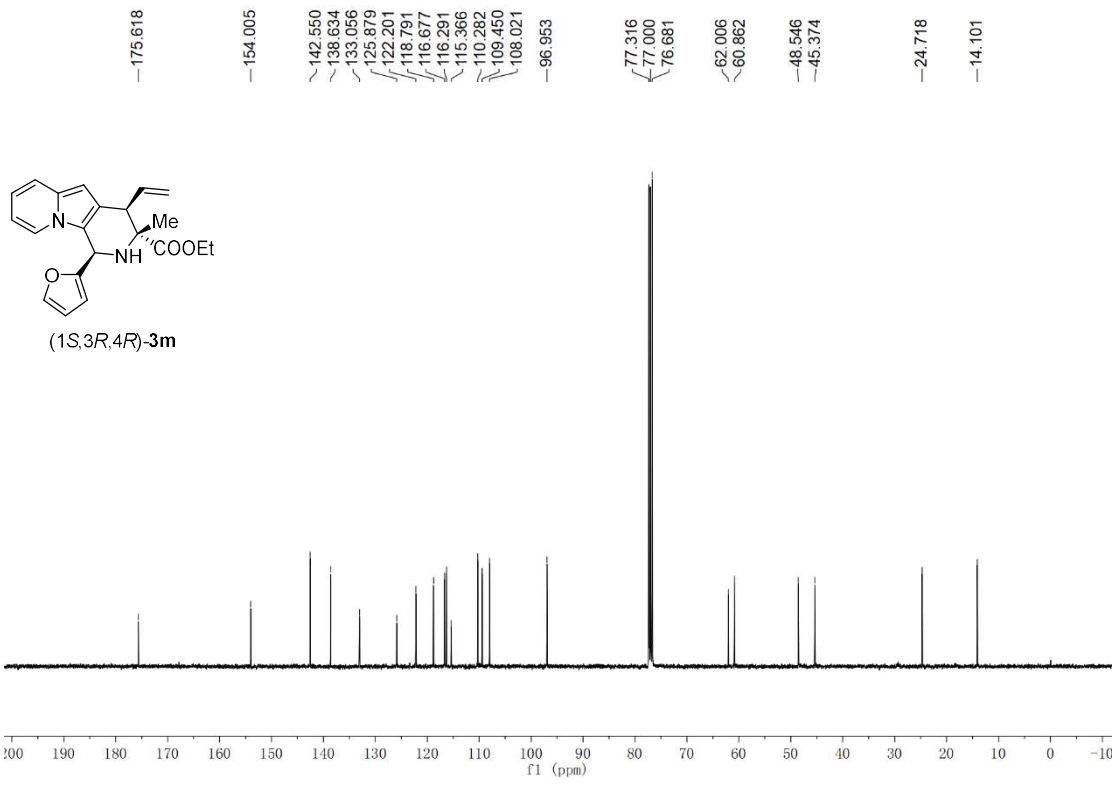
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3l** in $CDCl_3$



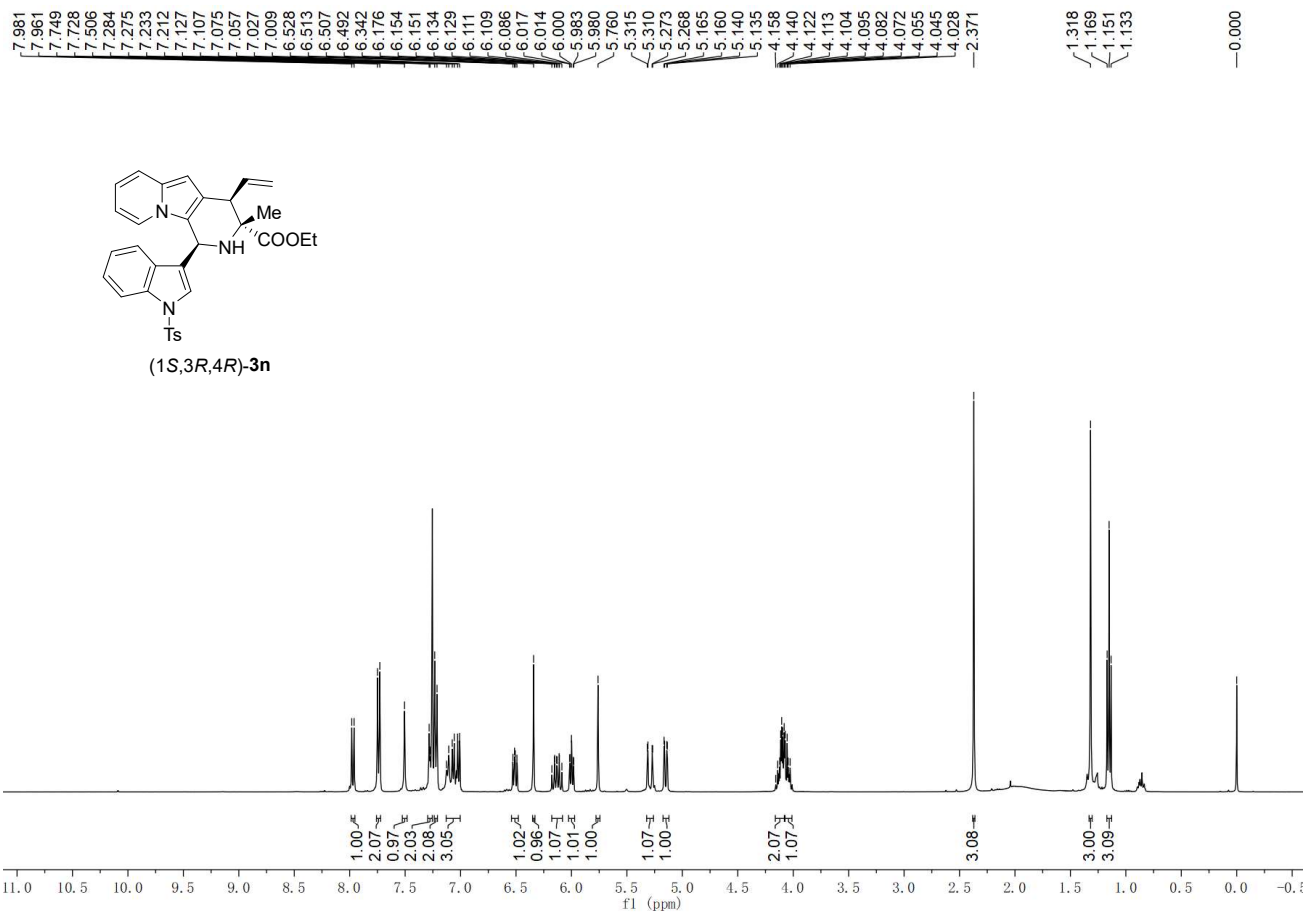
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3l** in $CDCl_3$



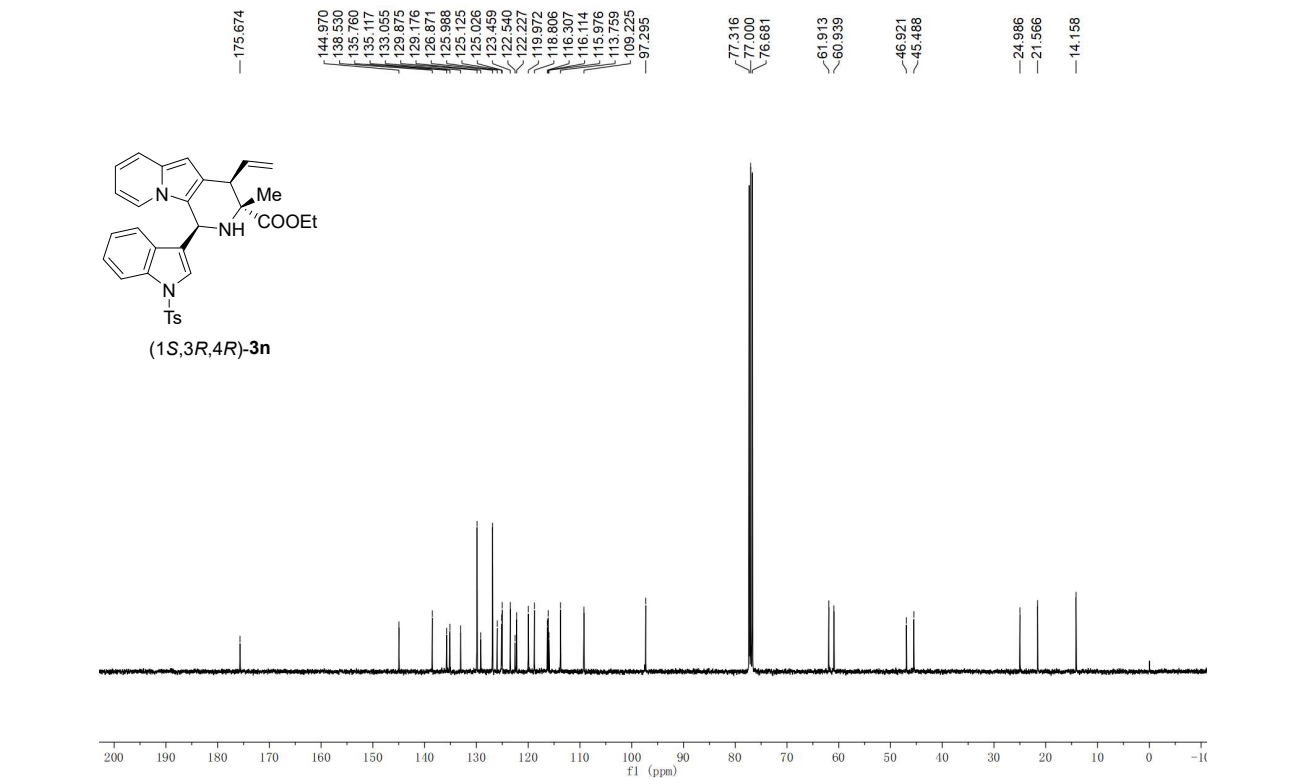
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3m** in $CDCl_3$



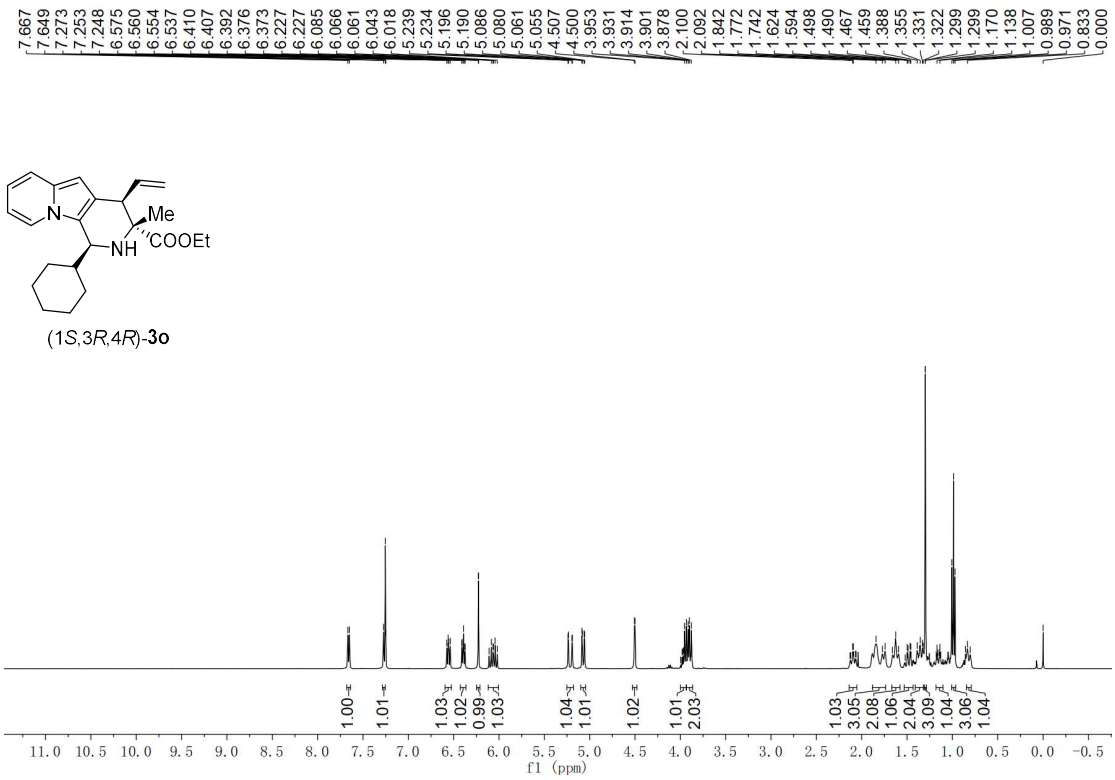
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3m** in $CDCl_3$



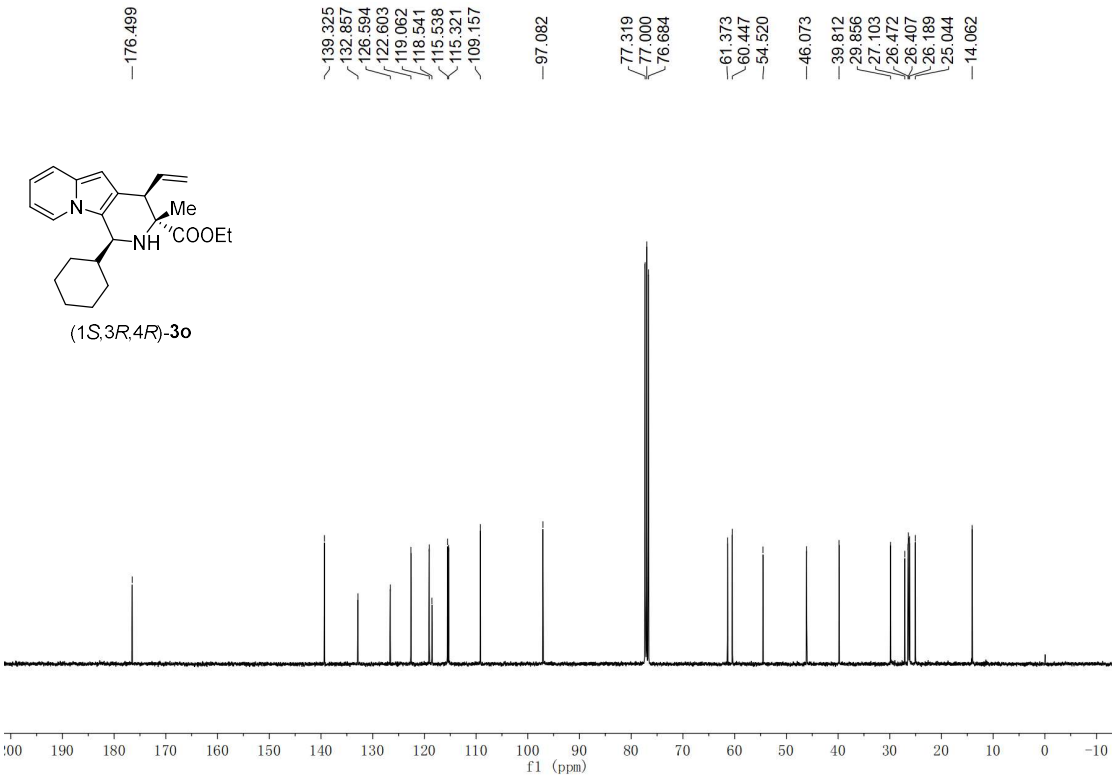
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3n** in $CDCl_3$



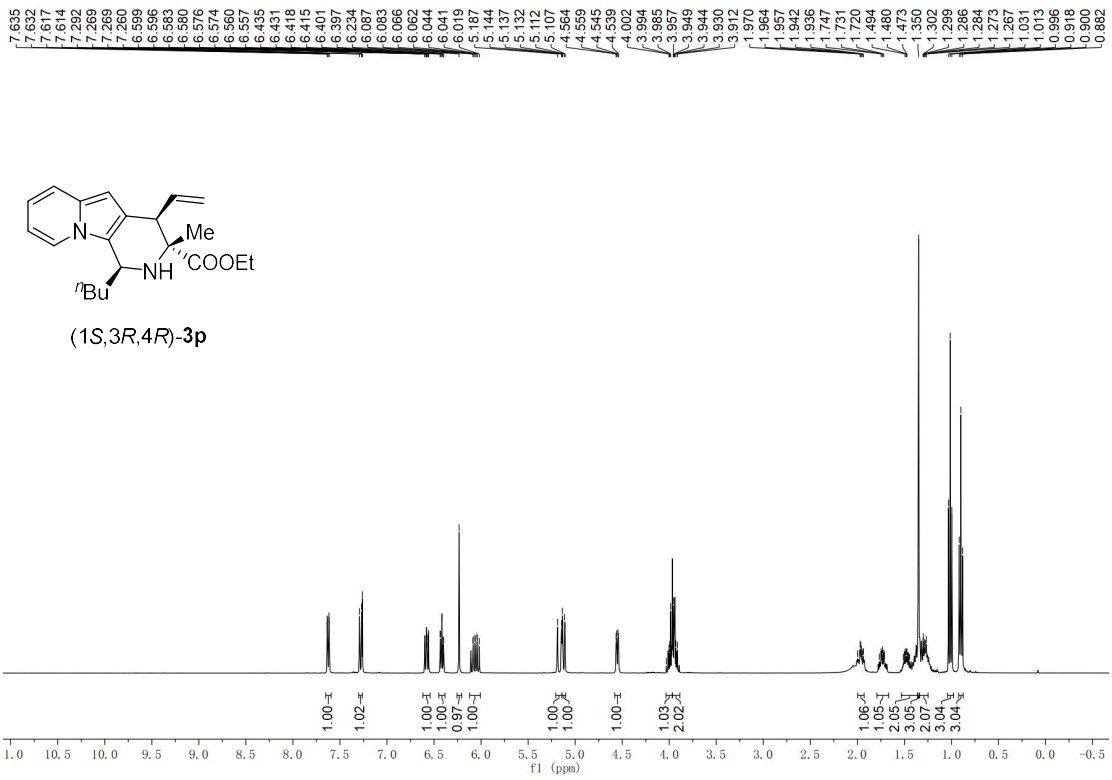
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3n** in $CDCl_3$



^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3o** in $CDCl_3$

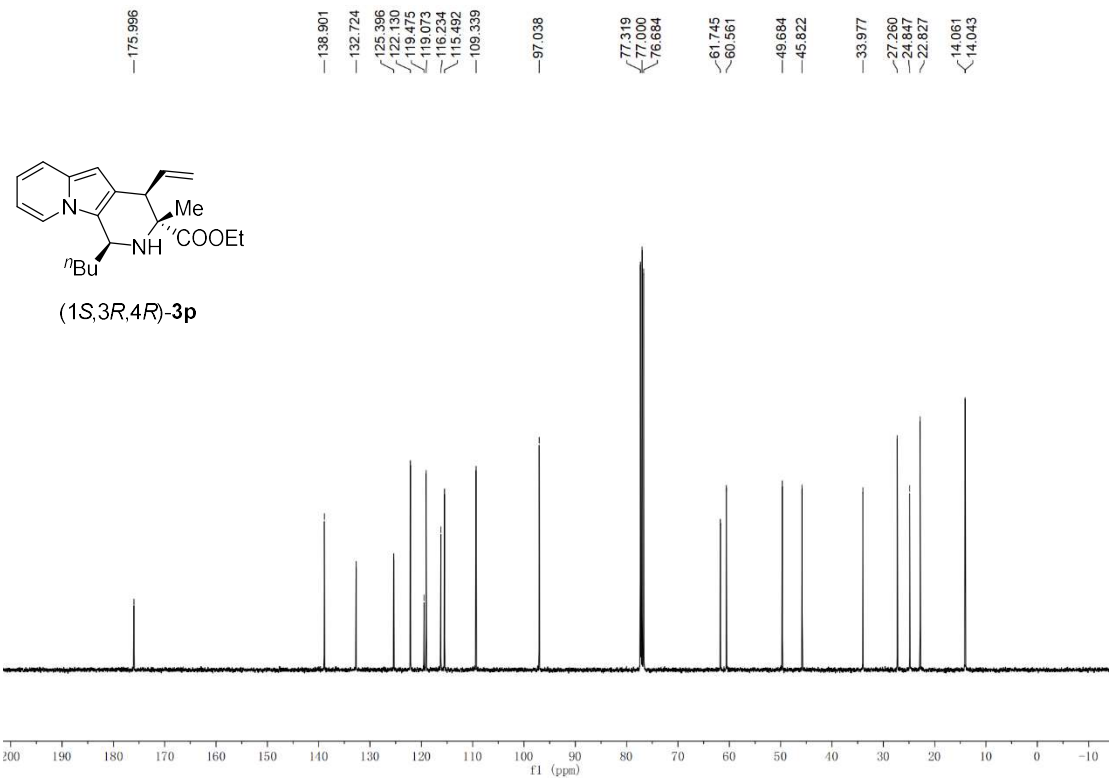


^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3o** in $CDCl_3$



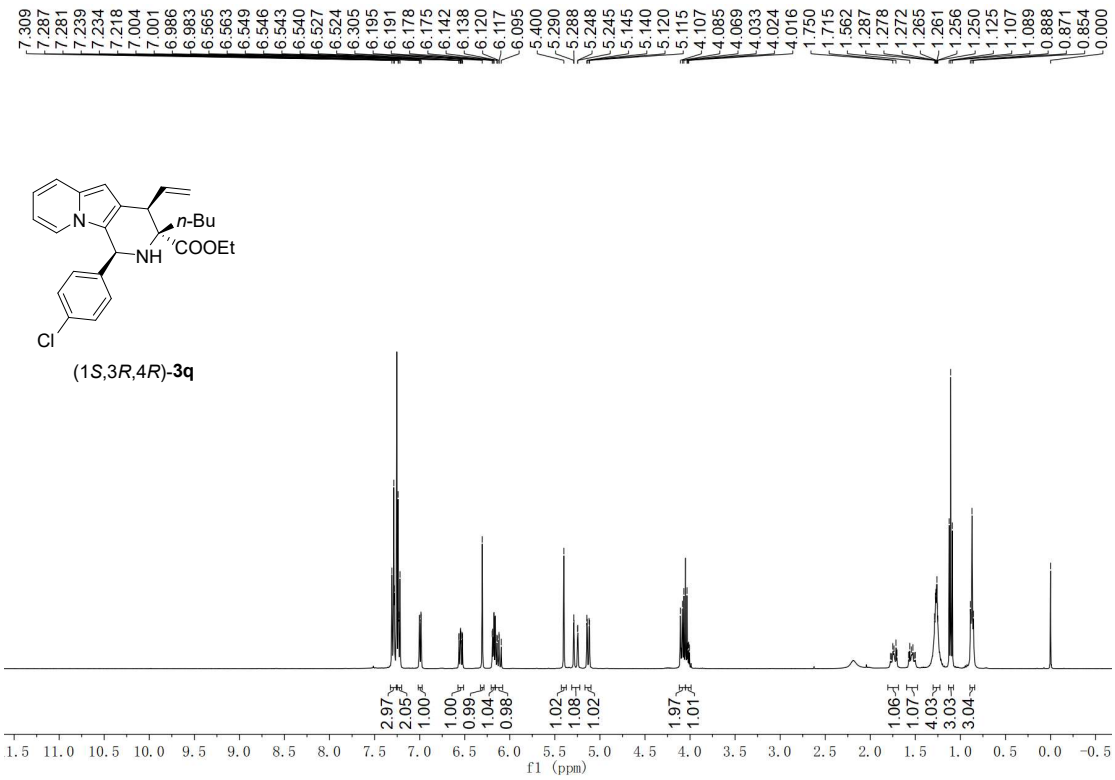
(1*S*,3*R*,4*R*)-**3p**

^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3p** in $CDCl_3$

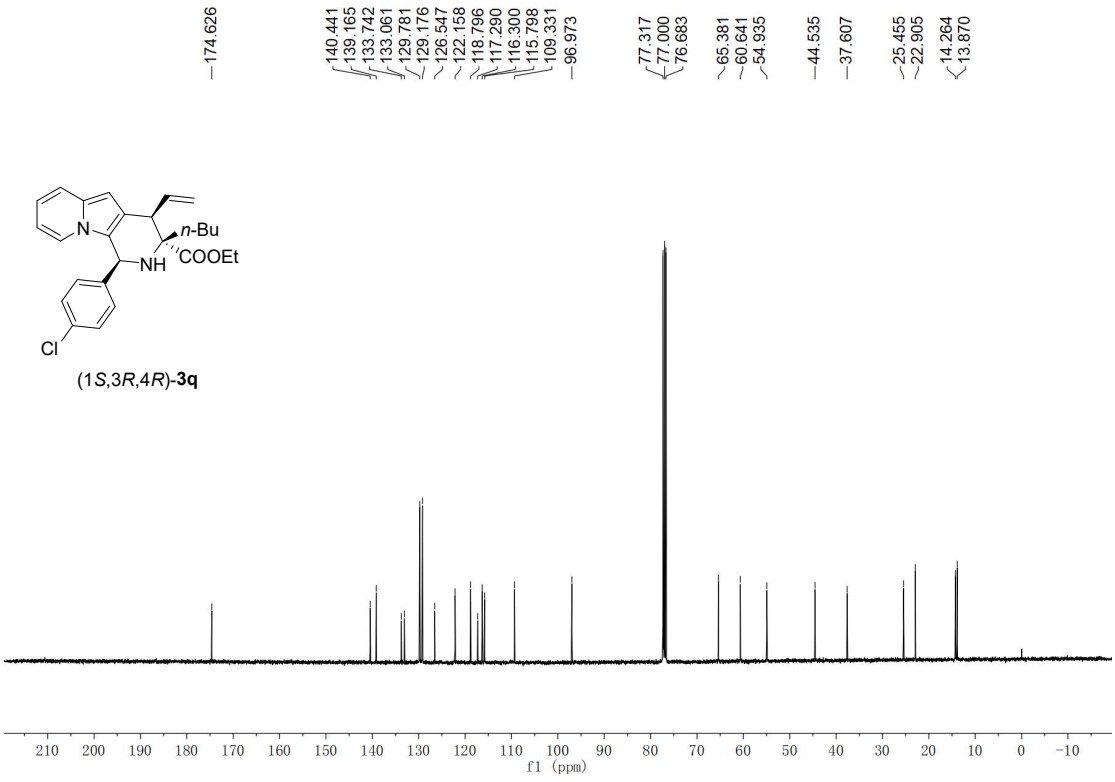


(1*S*,3*R*,4*R*)-**3p**

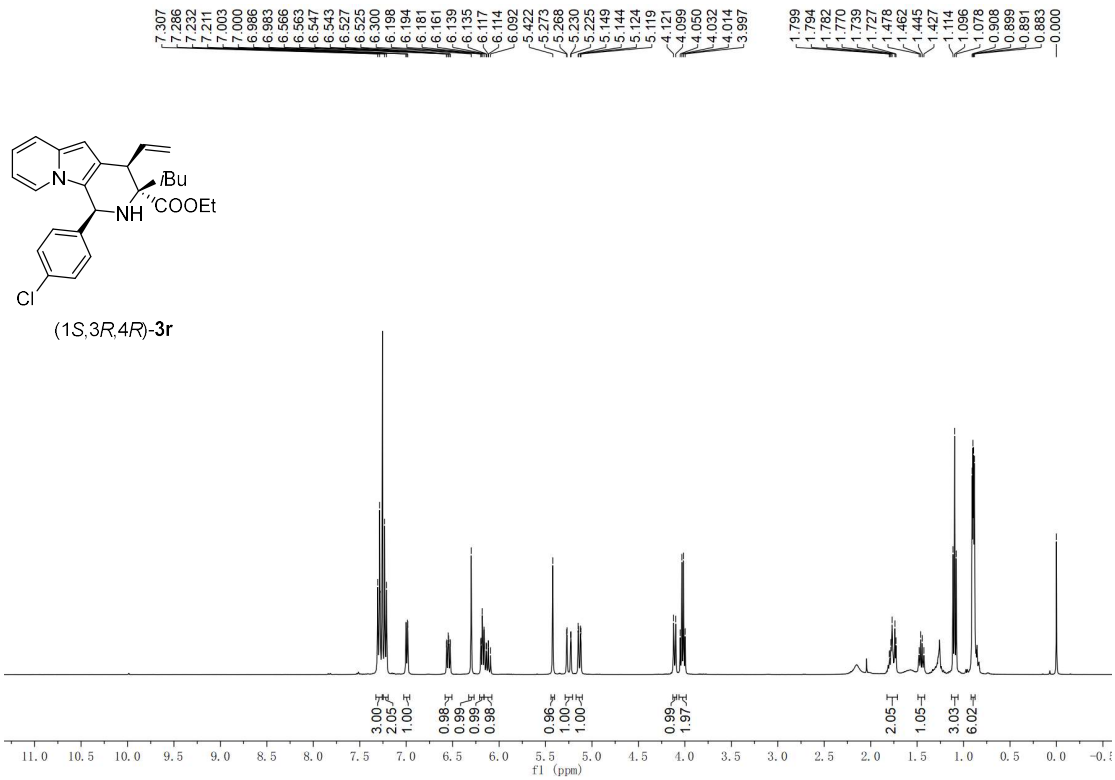
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3p** in $CDCl_3$



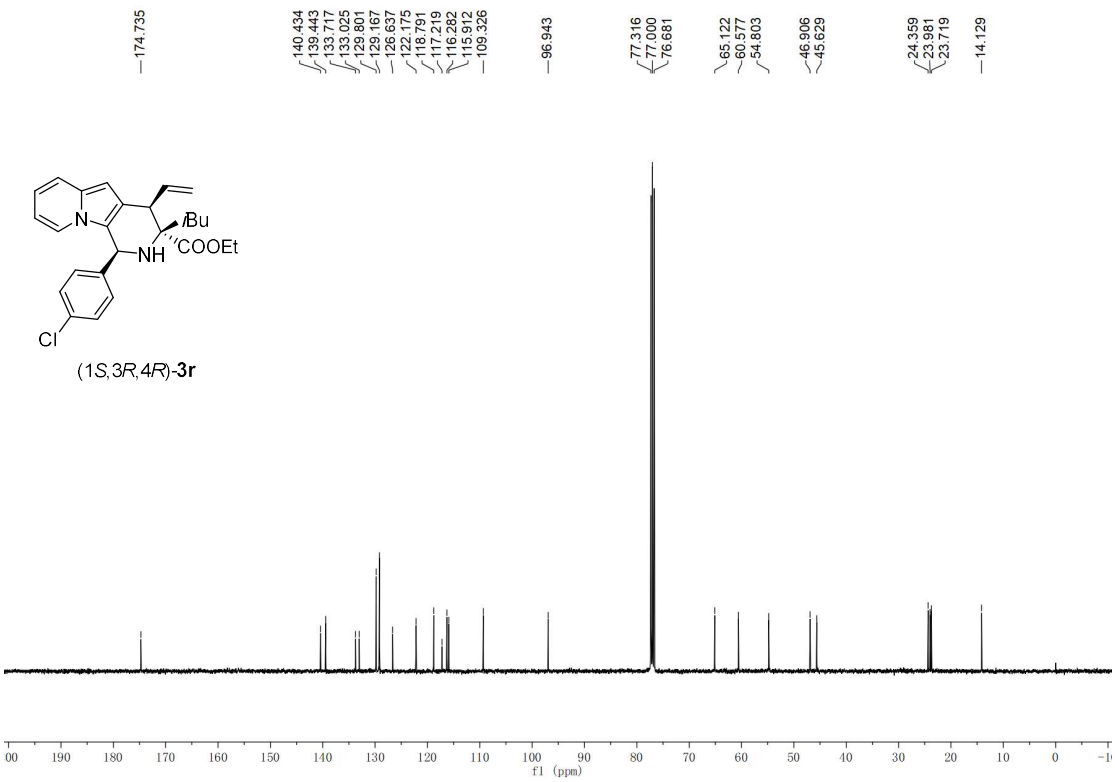
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3q** in $CDCl_3$



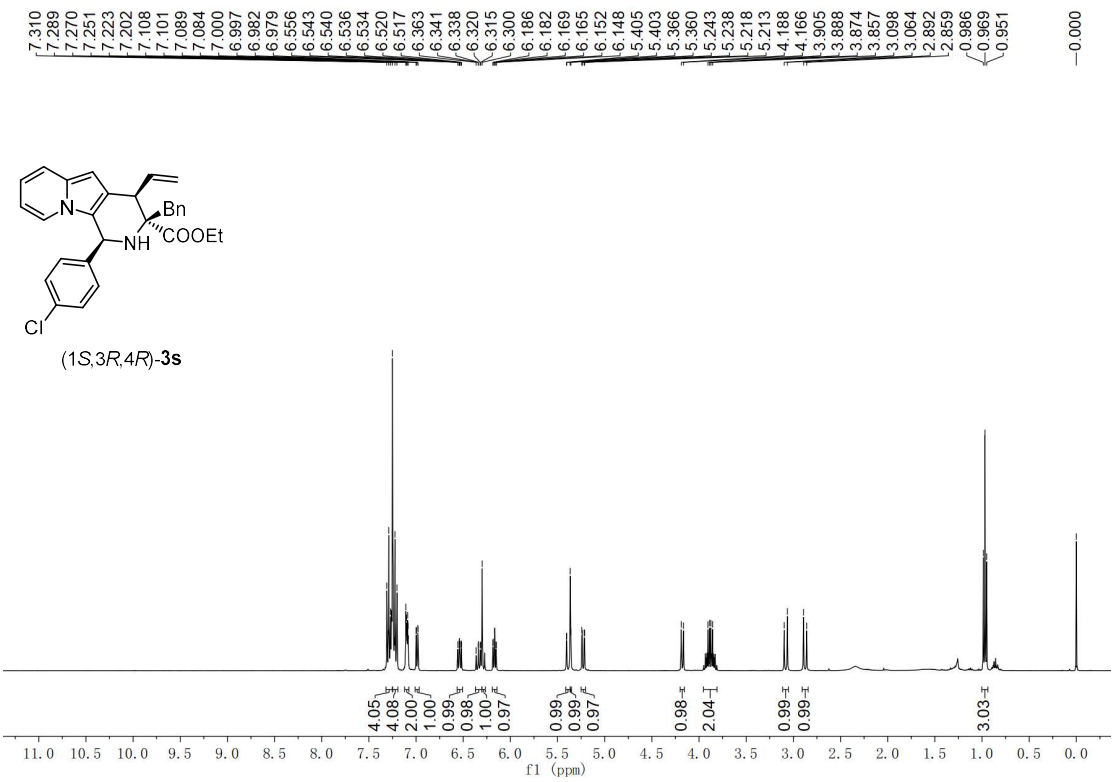
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3q** in $CDCl_3$



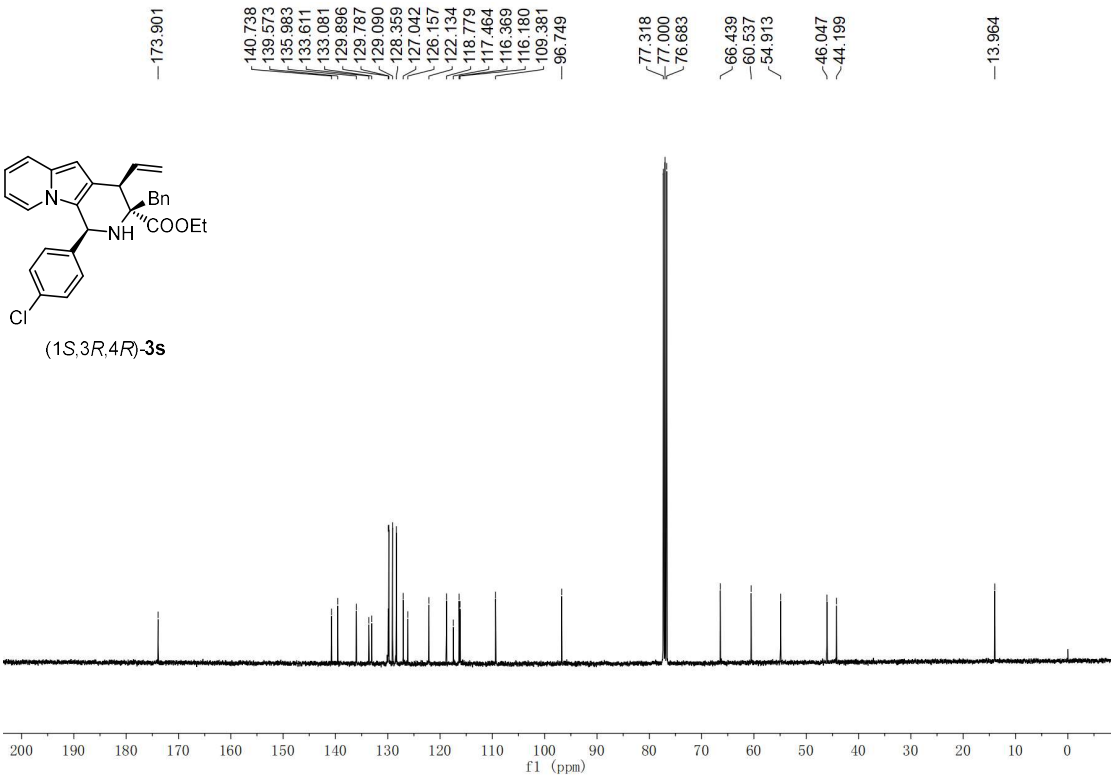
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3r** in $CDCl_3$



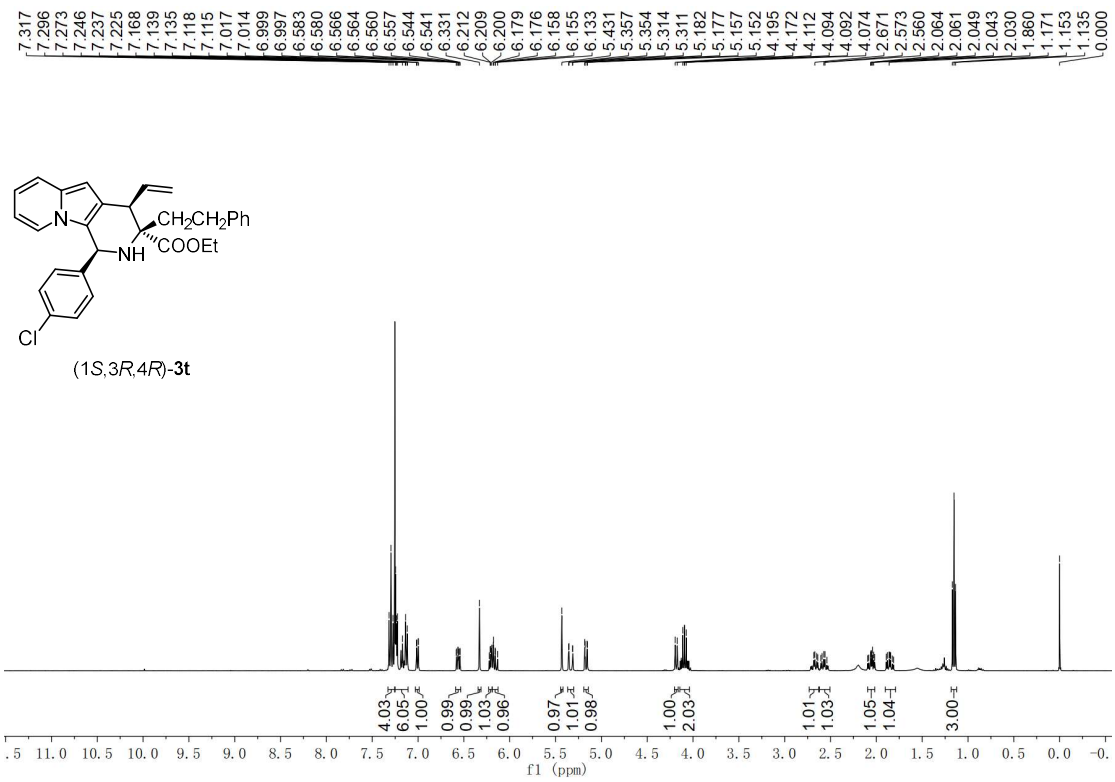
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3r** in $CDCl_3$



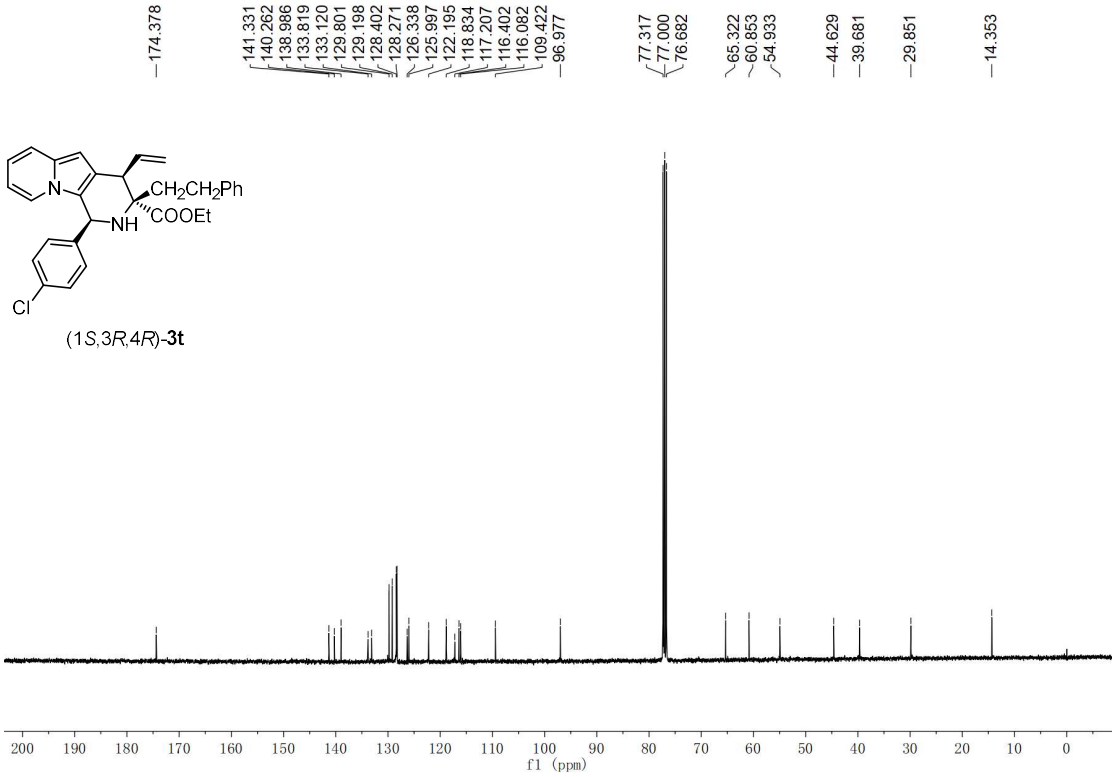
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3s** in $CDCl_3$



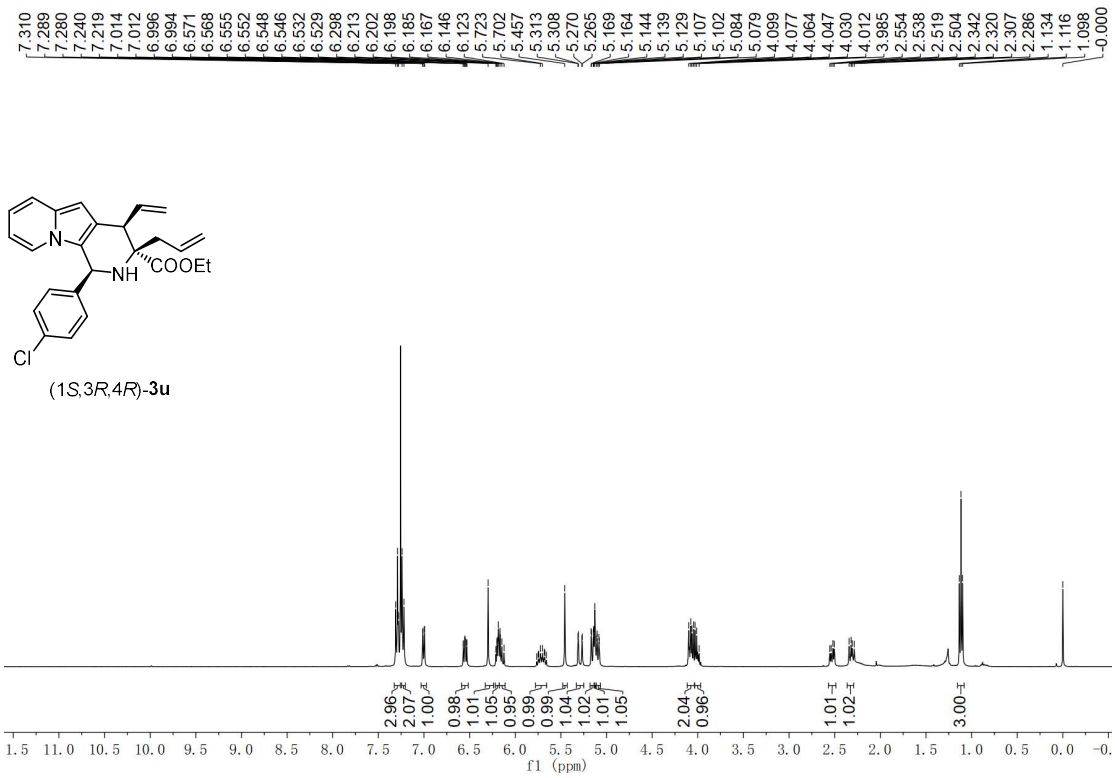
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3s** in $CDCl_3$



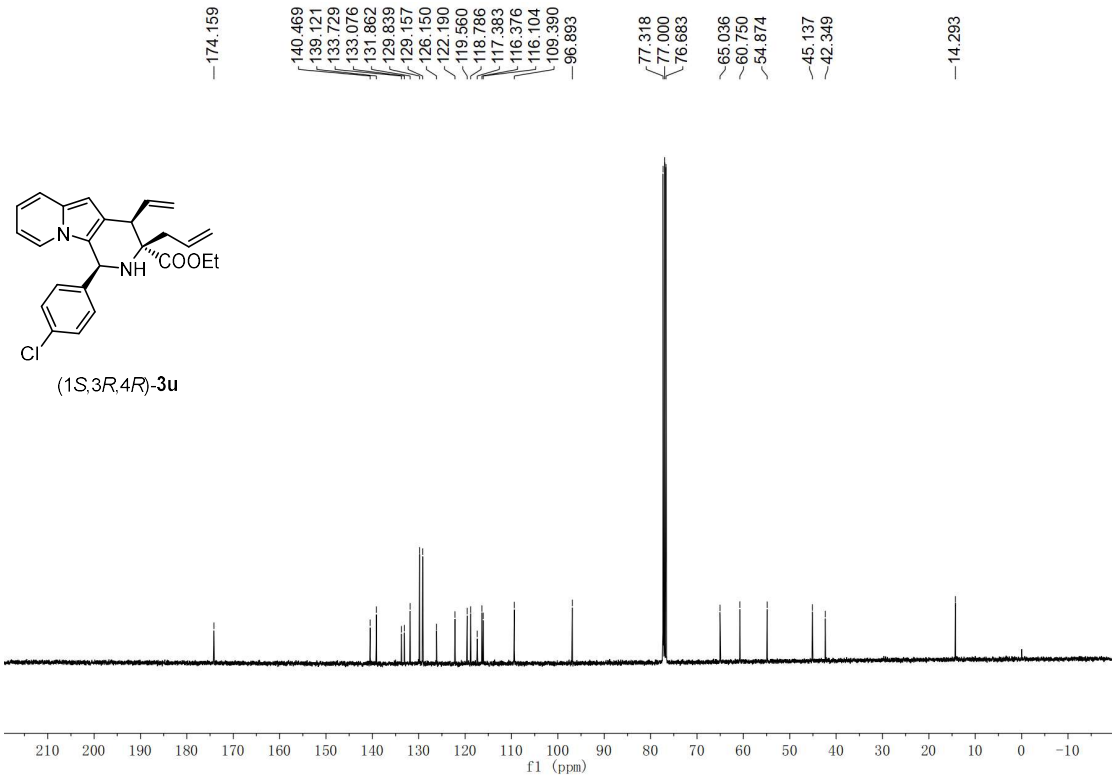
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3t** in $CDCl_3$



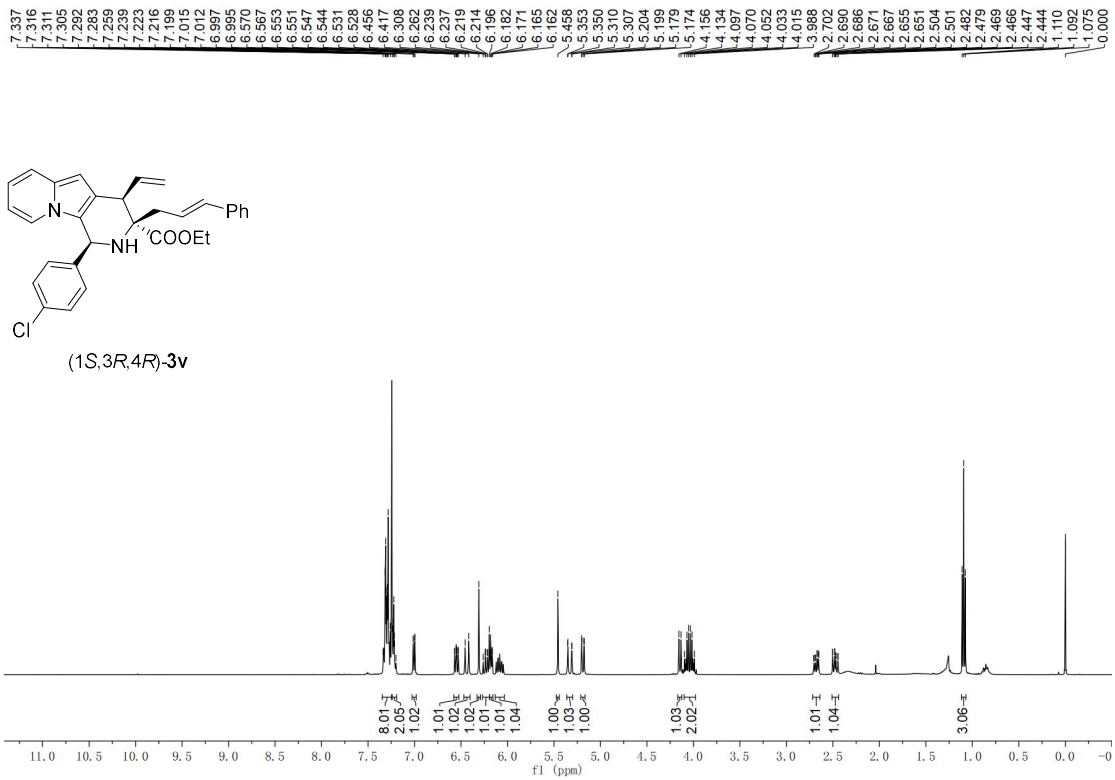
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3t** in $CDCl_3$



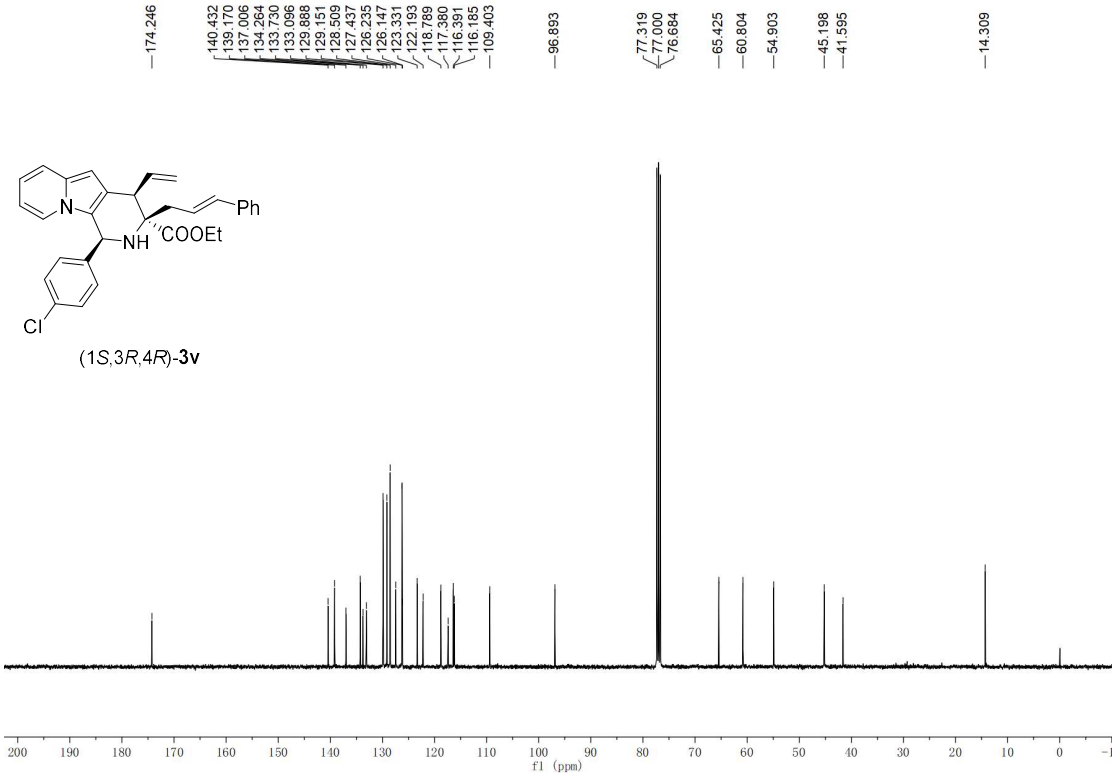
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3u** in $CDCl_3$



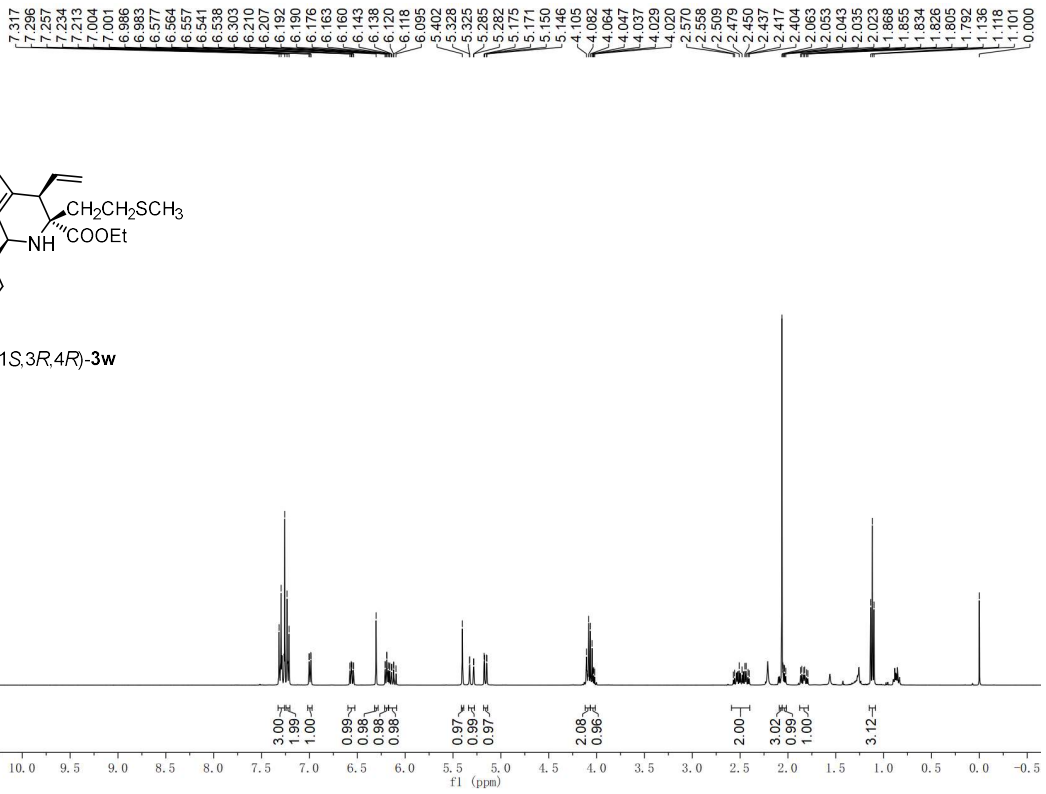
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3u** in $CDCl_3$



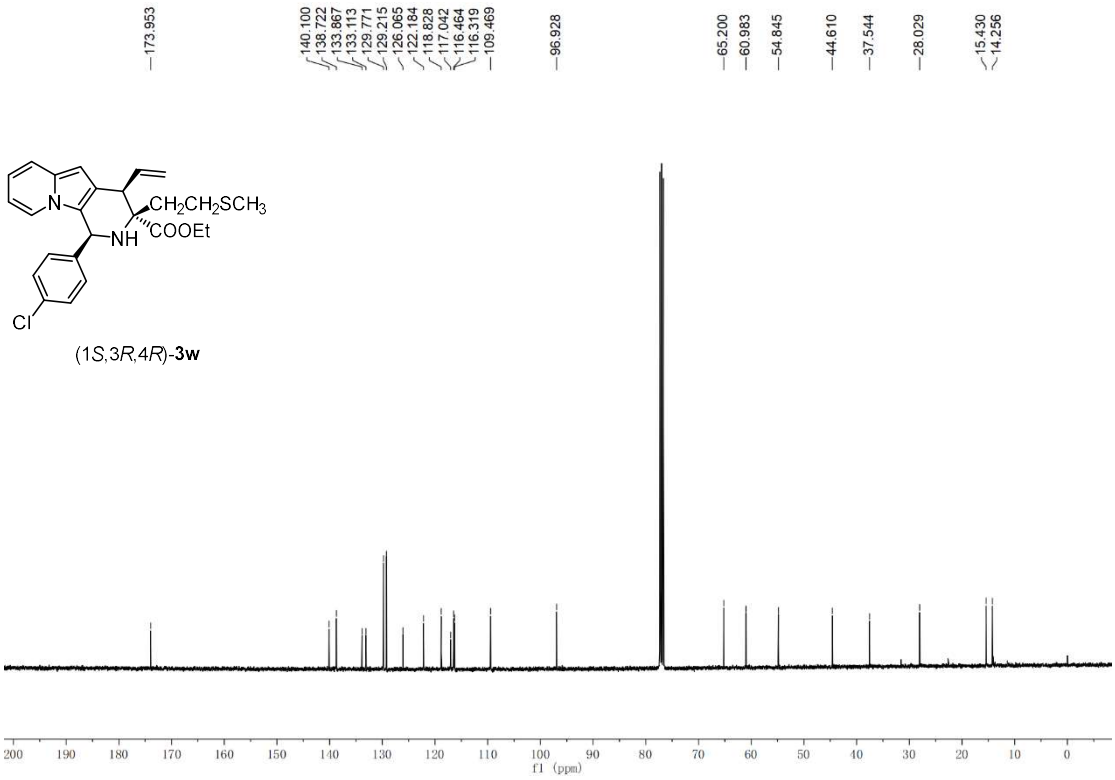
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3v** in $CDCl_3$



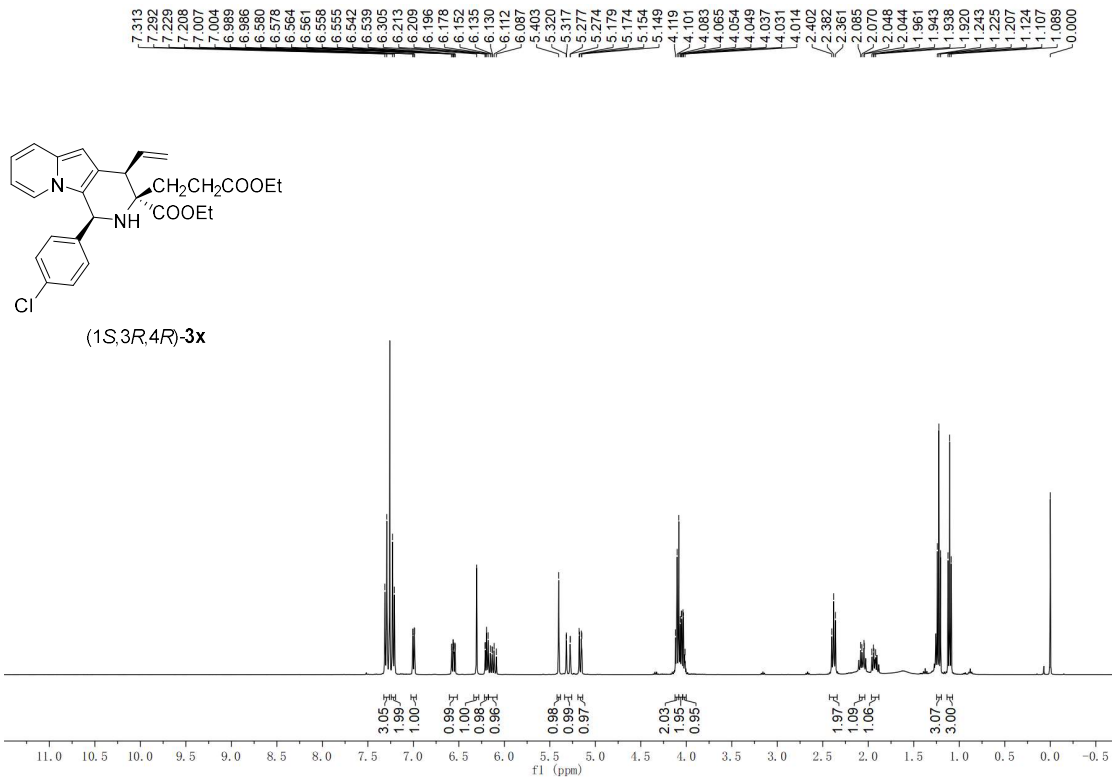
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3v** in $CDCl_3$



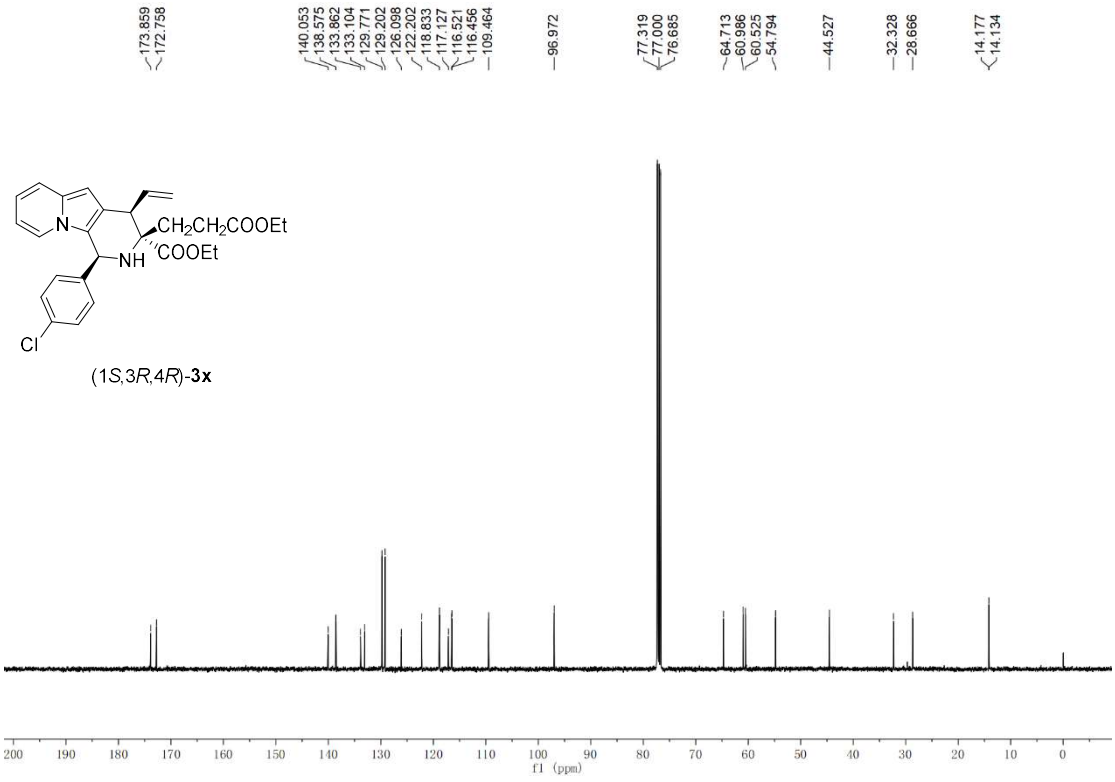
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3w** in $CDCl_3$



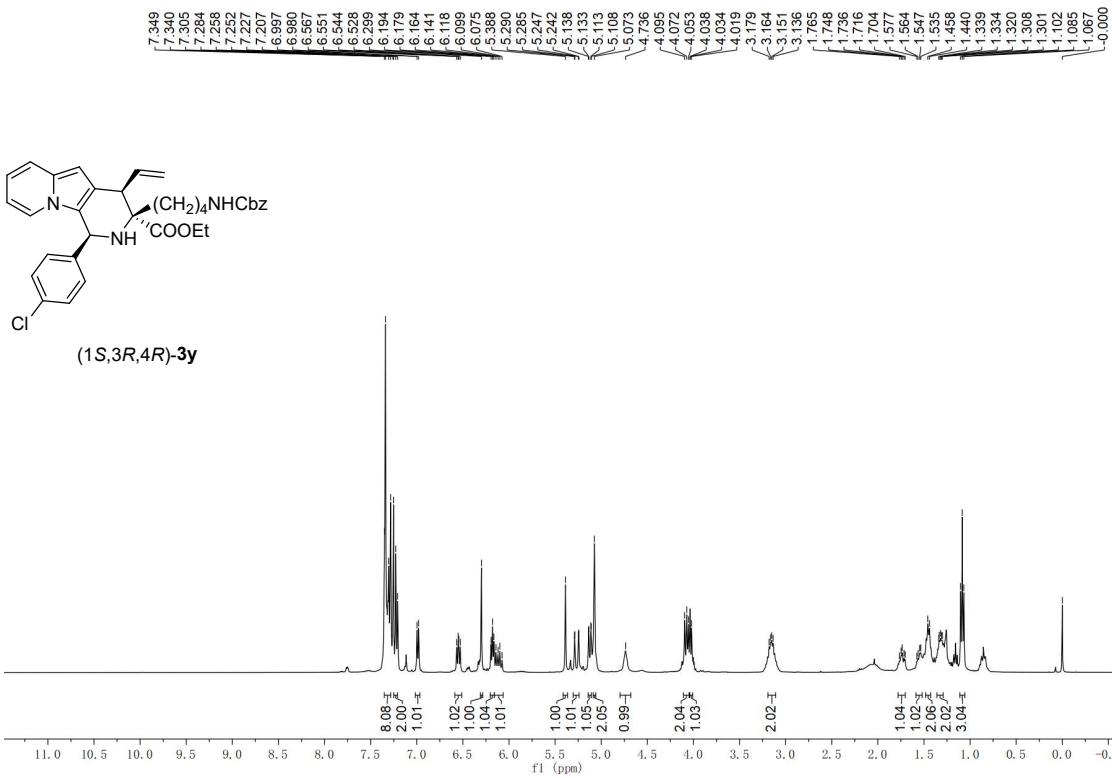
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3w** in $CDCl_3$



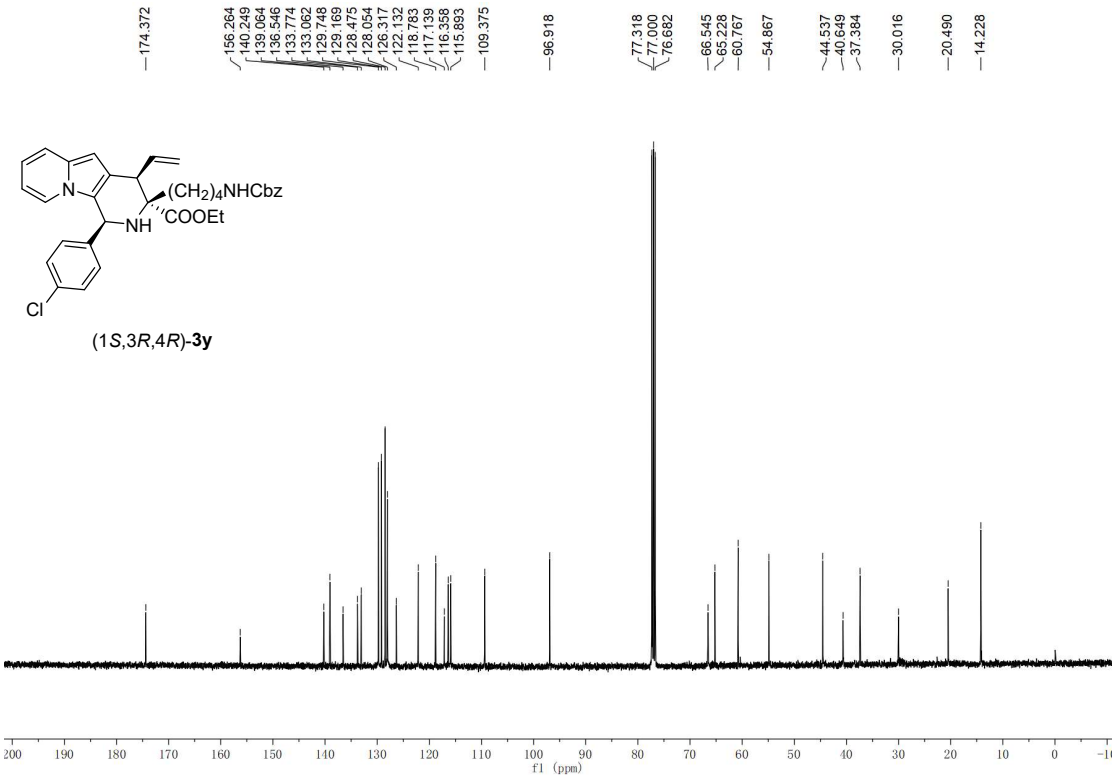
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3x** in $CDCl_3$



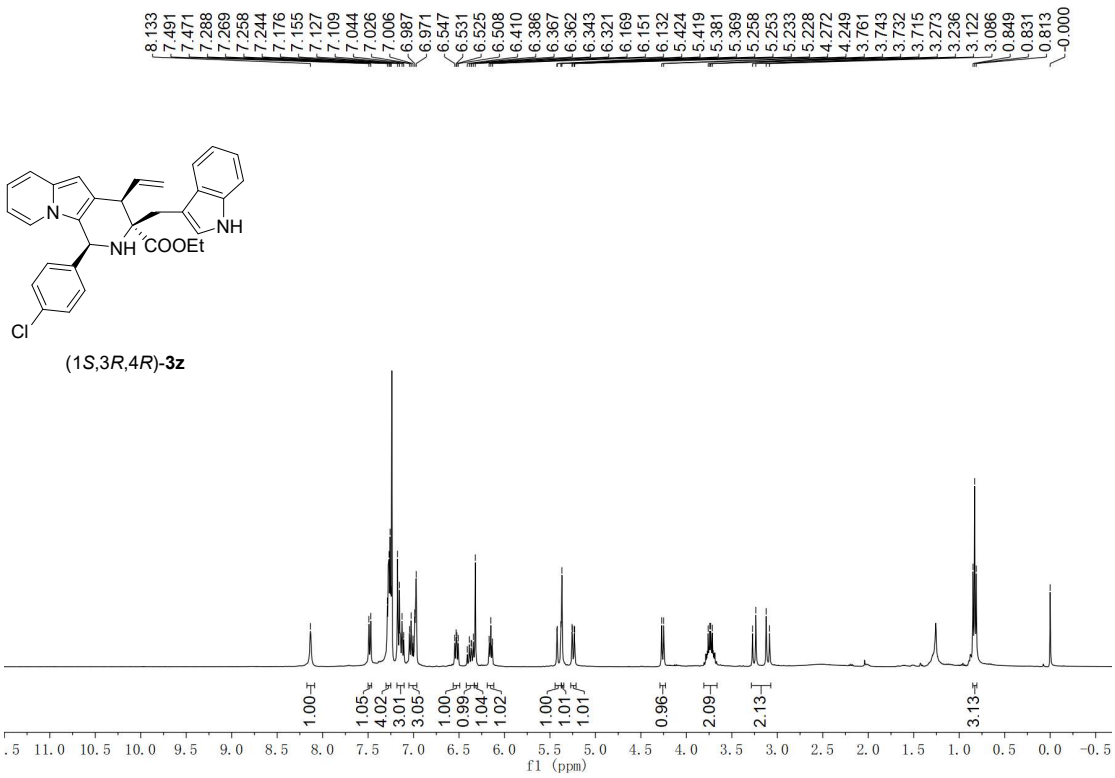
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3x** in $CDCl_3$



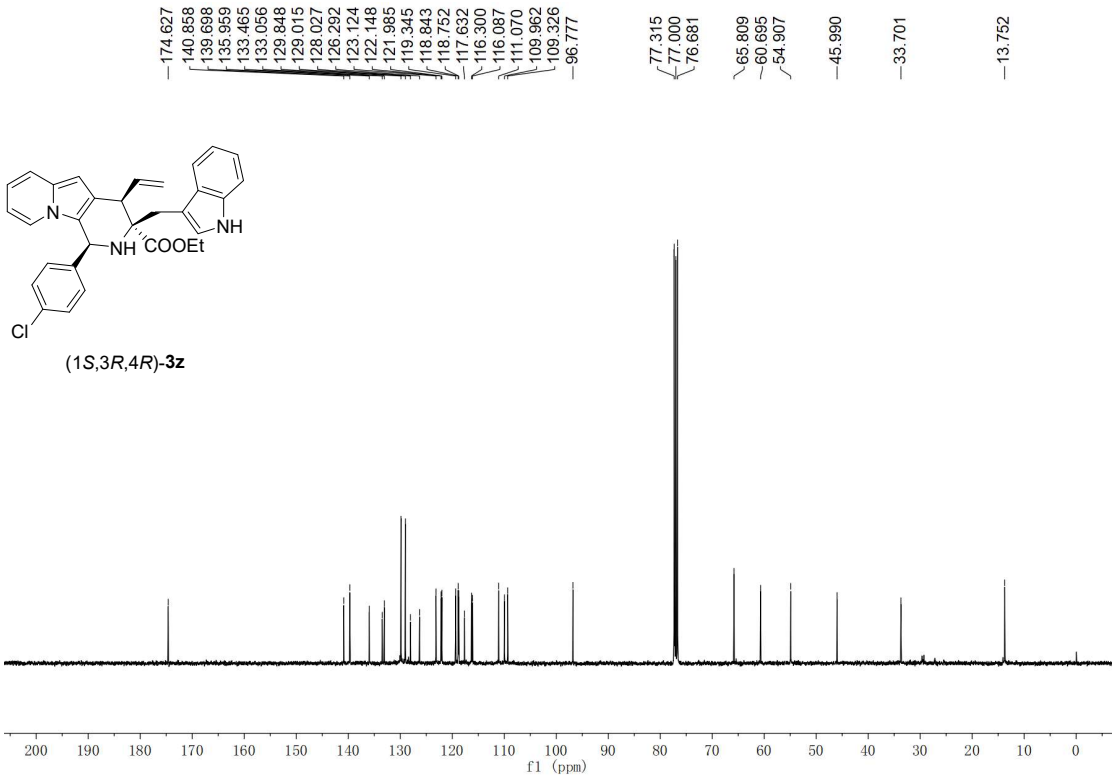
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3y** in $CDCl_3$



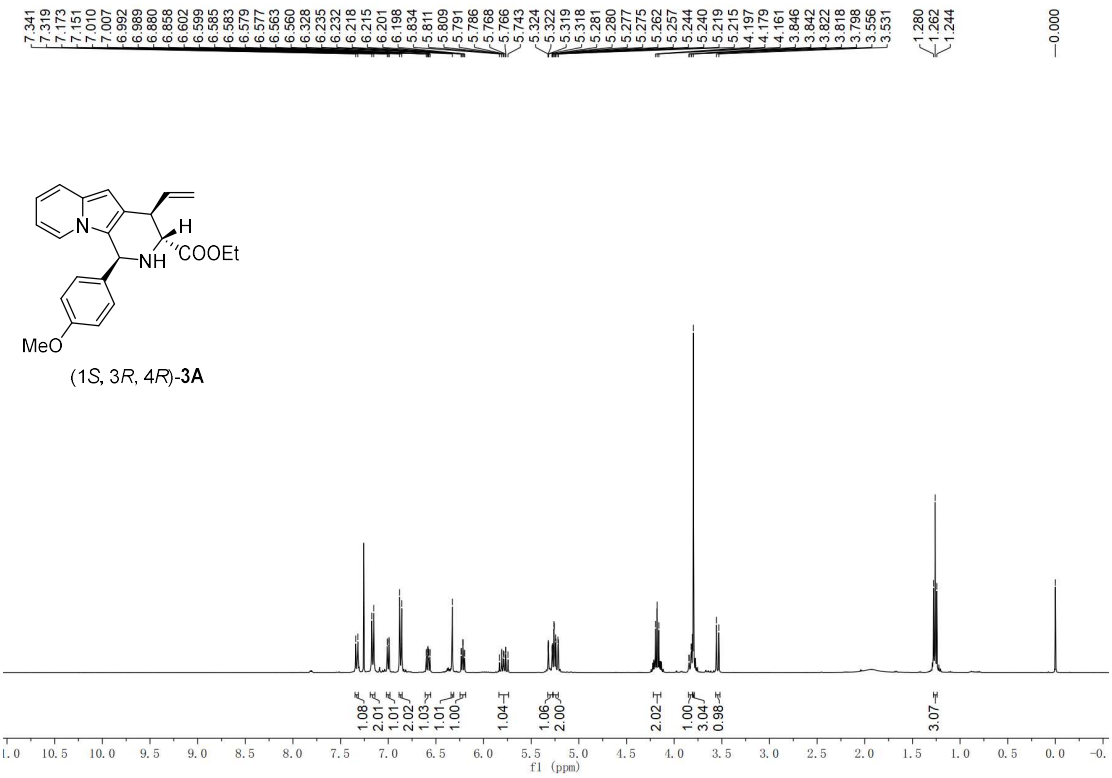
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3y** in $CDCl_3$



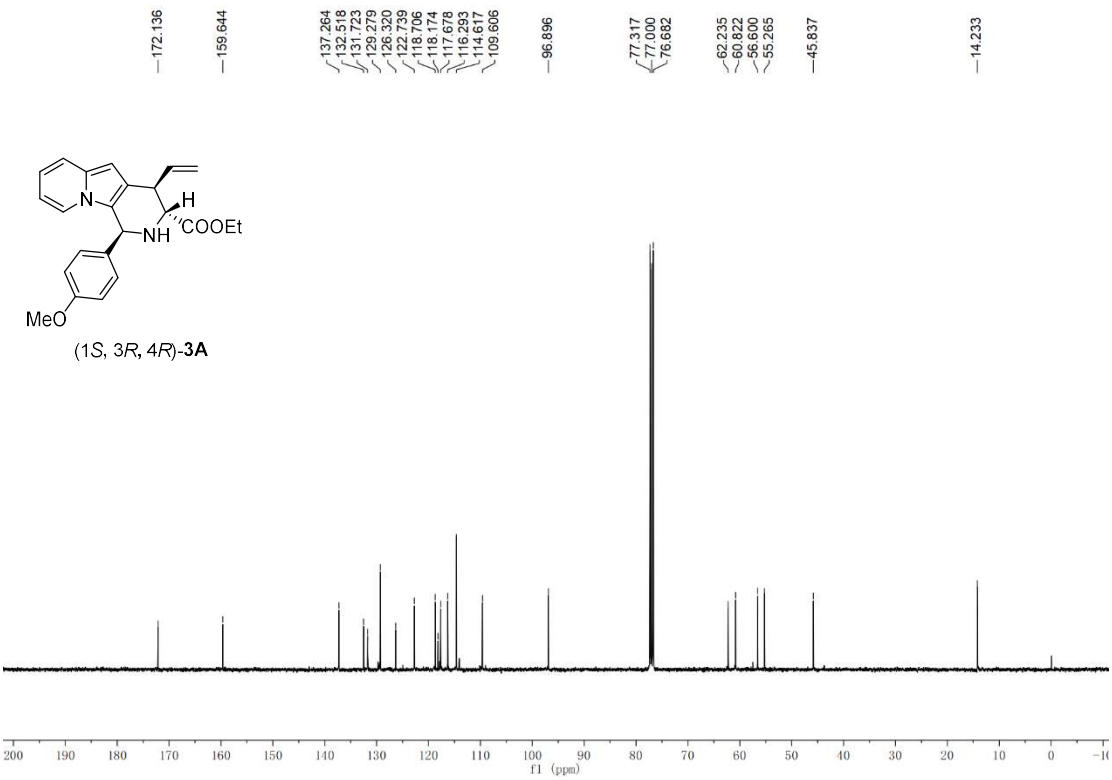
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3z** in $CDCl_3$



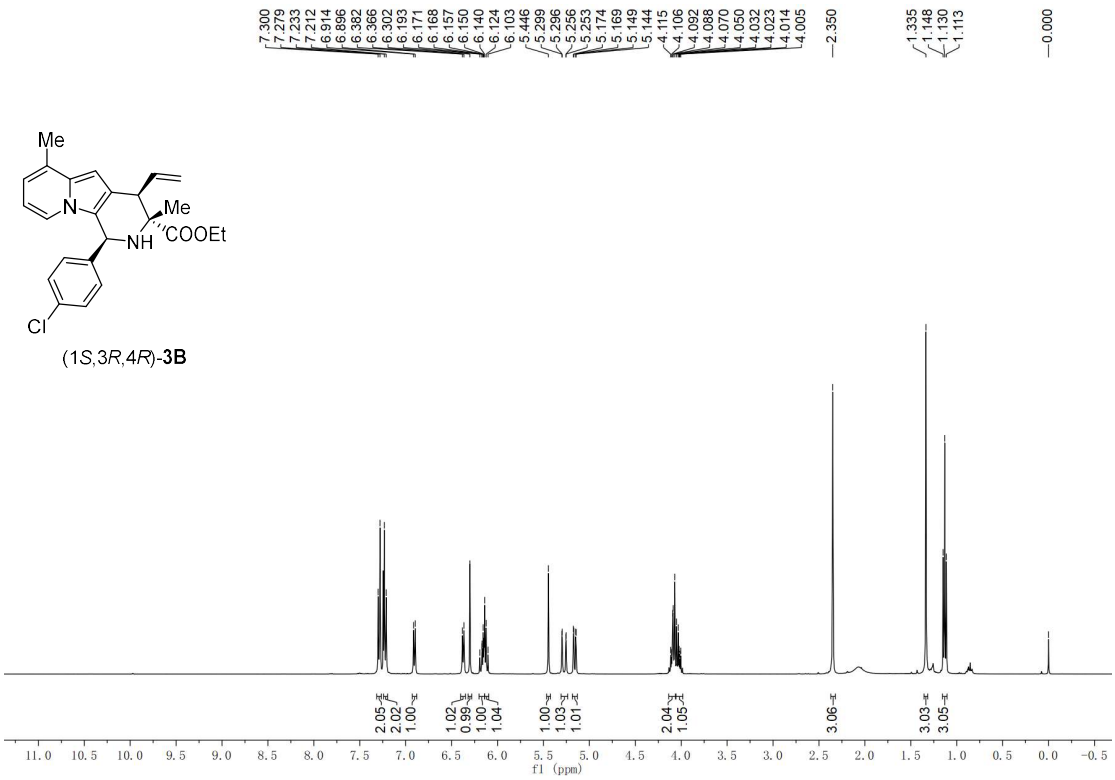
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3z** in $CDCl_3$



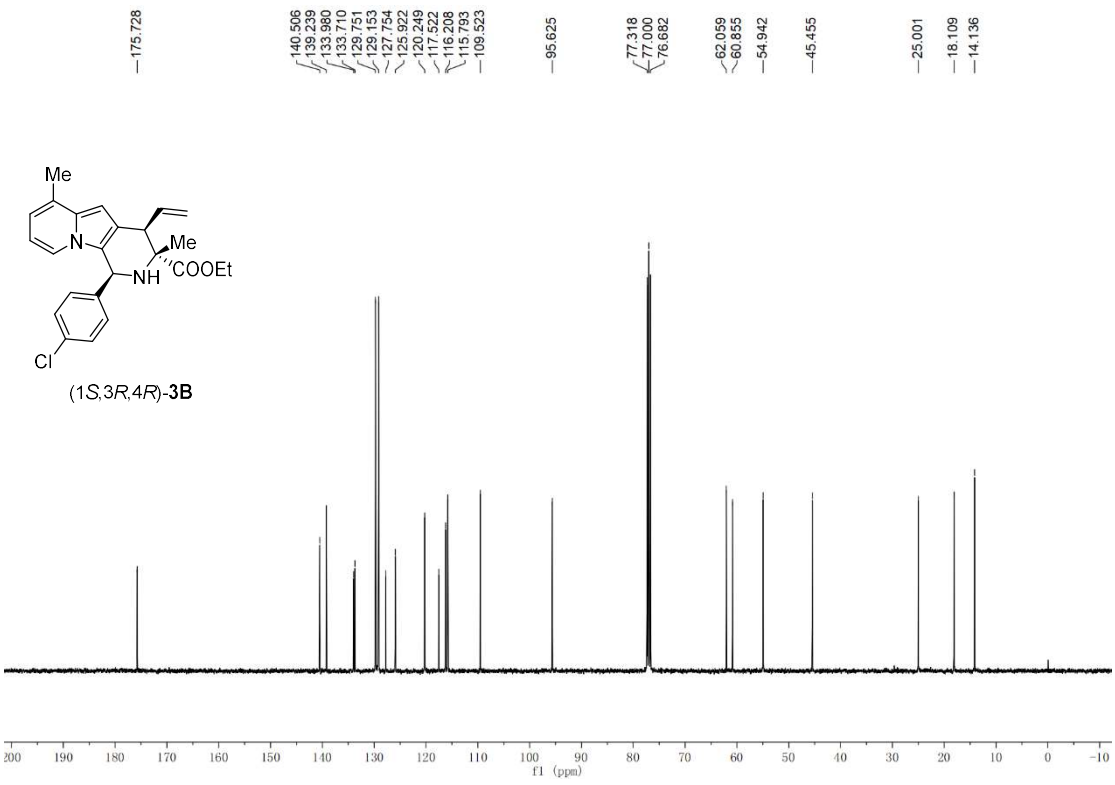
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3A** in $CDCl_3$



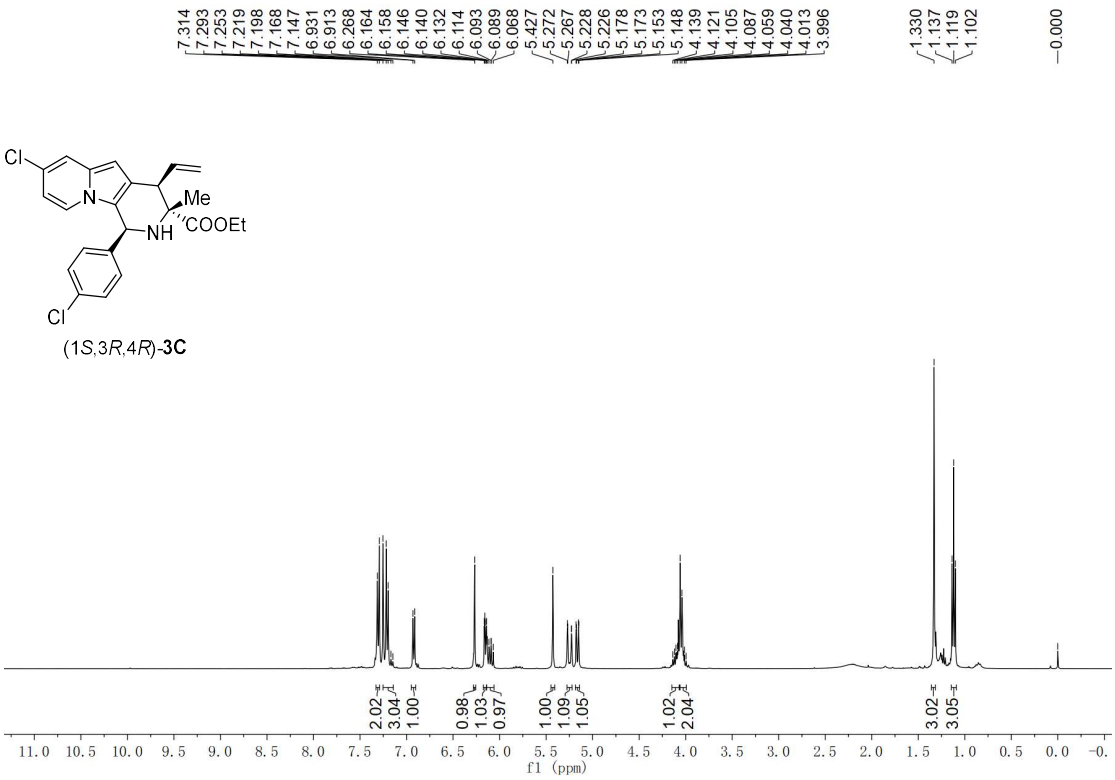
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3A** in $CDCl_3$



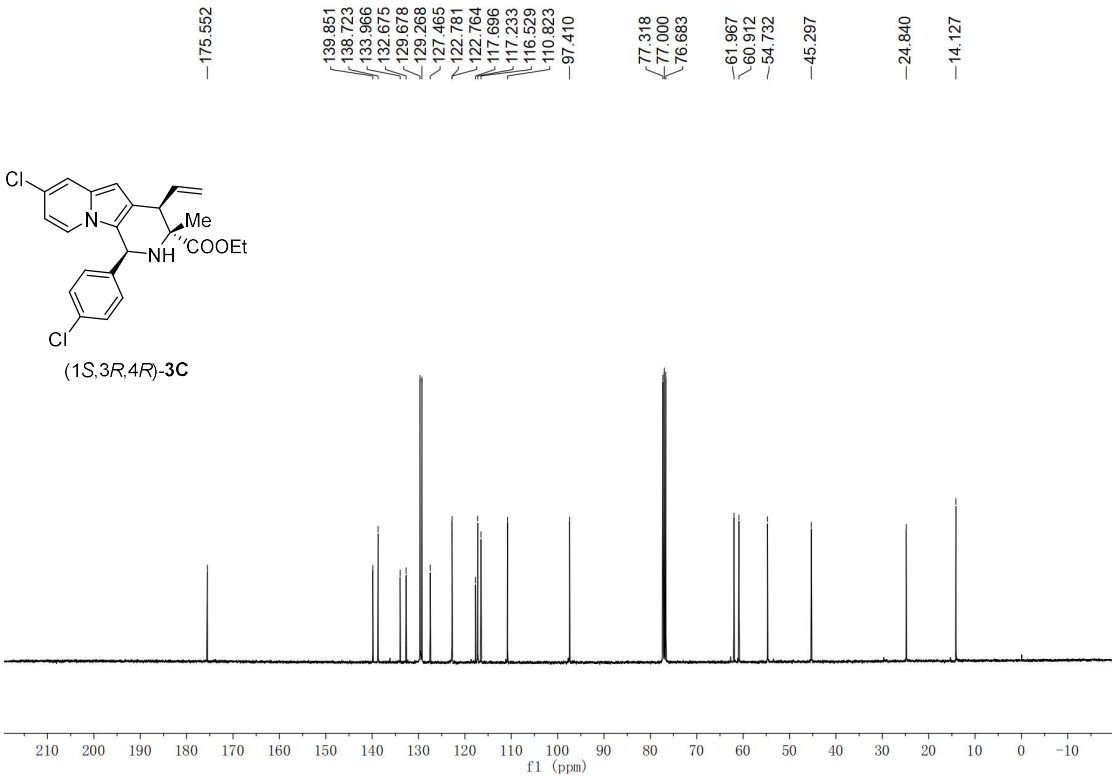
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3B** in $CDCl_3$



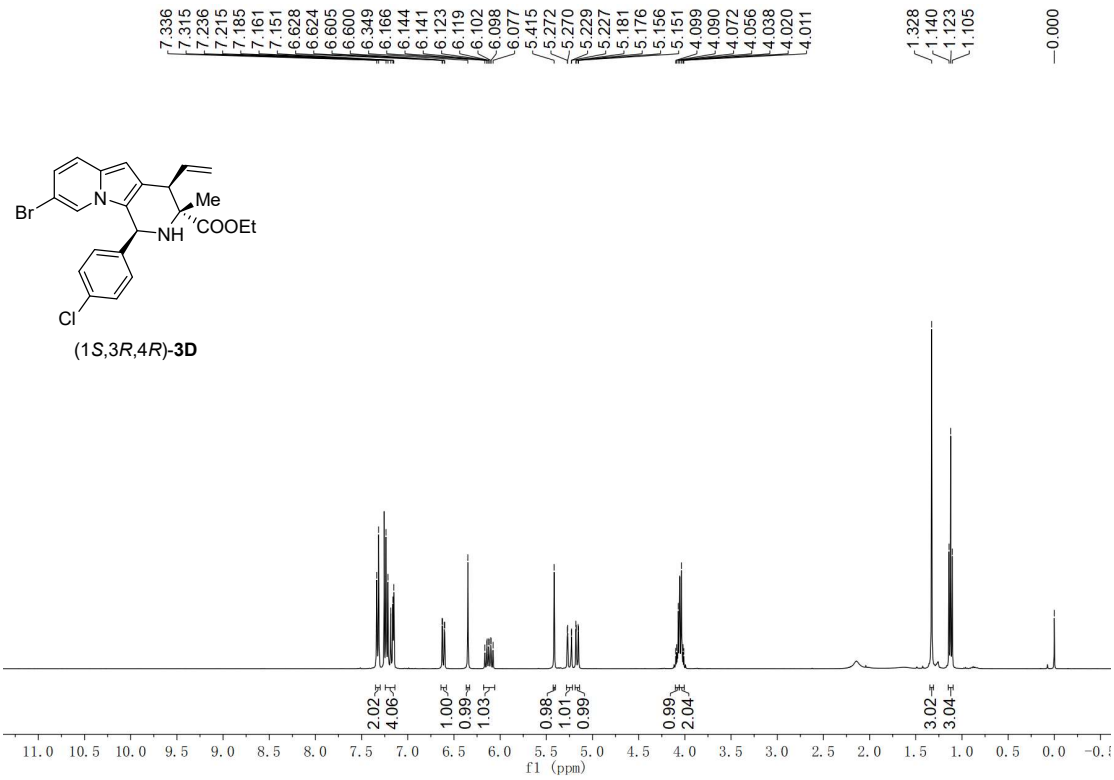
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3B** in $CDCl_3$



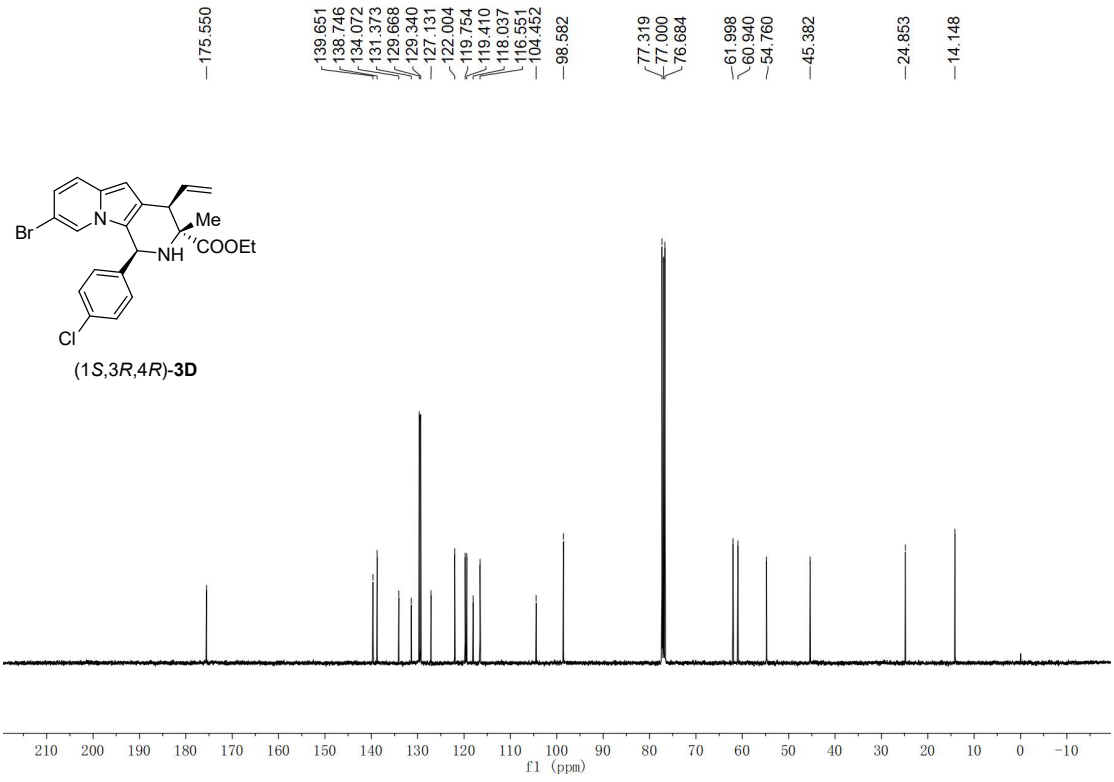
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3C** in $CDCl_3$



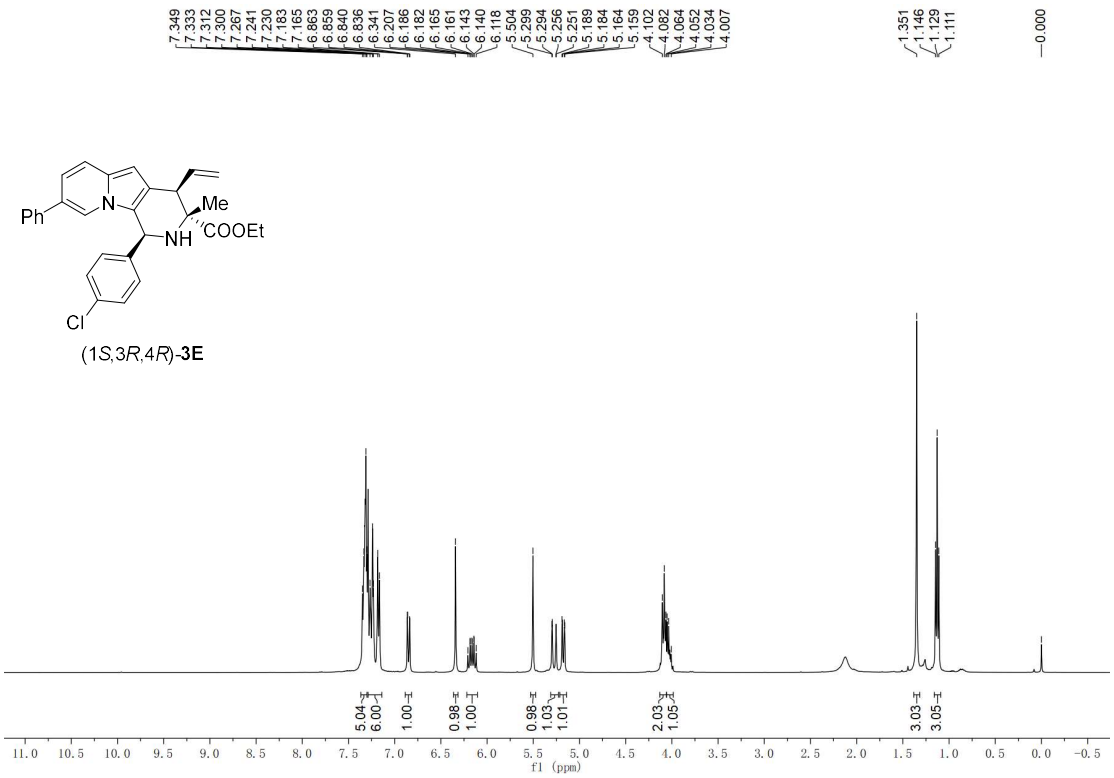
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3C** in $CDCl_3$



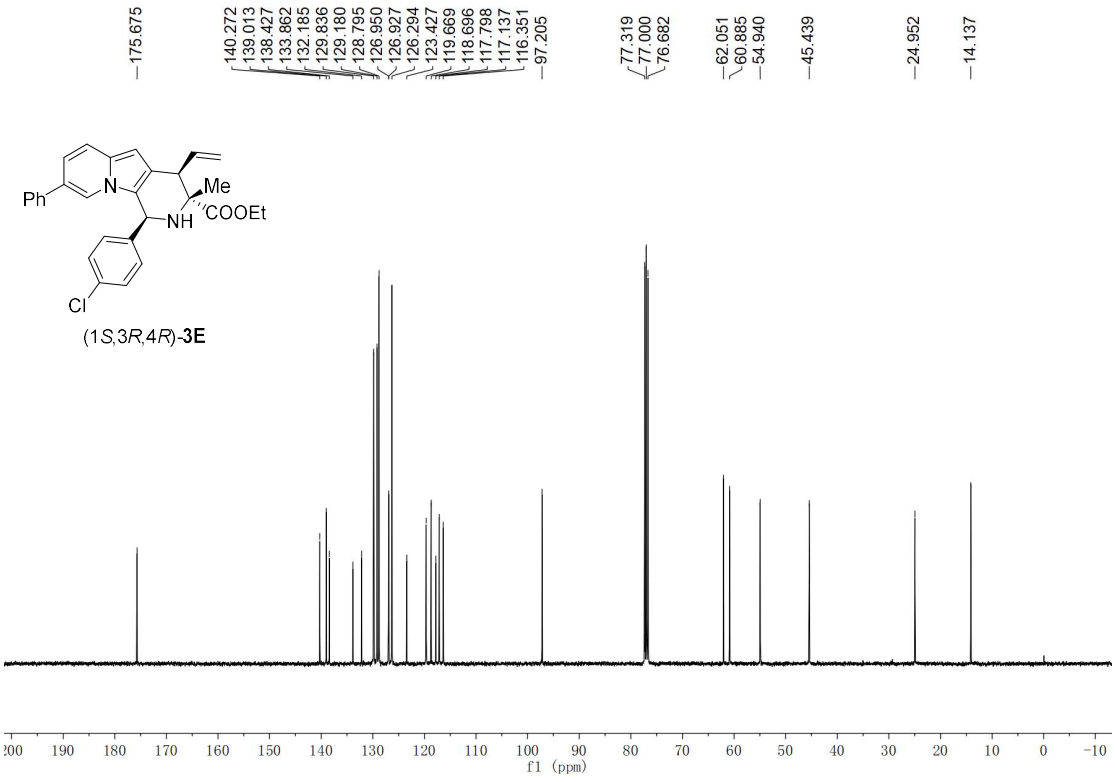
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3D** in $CDCl_3$



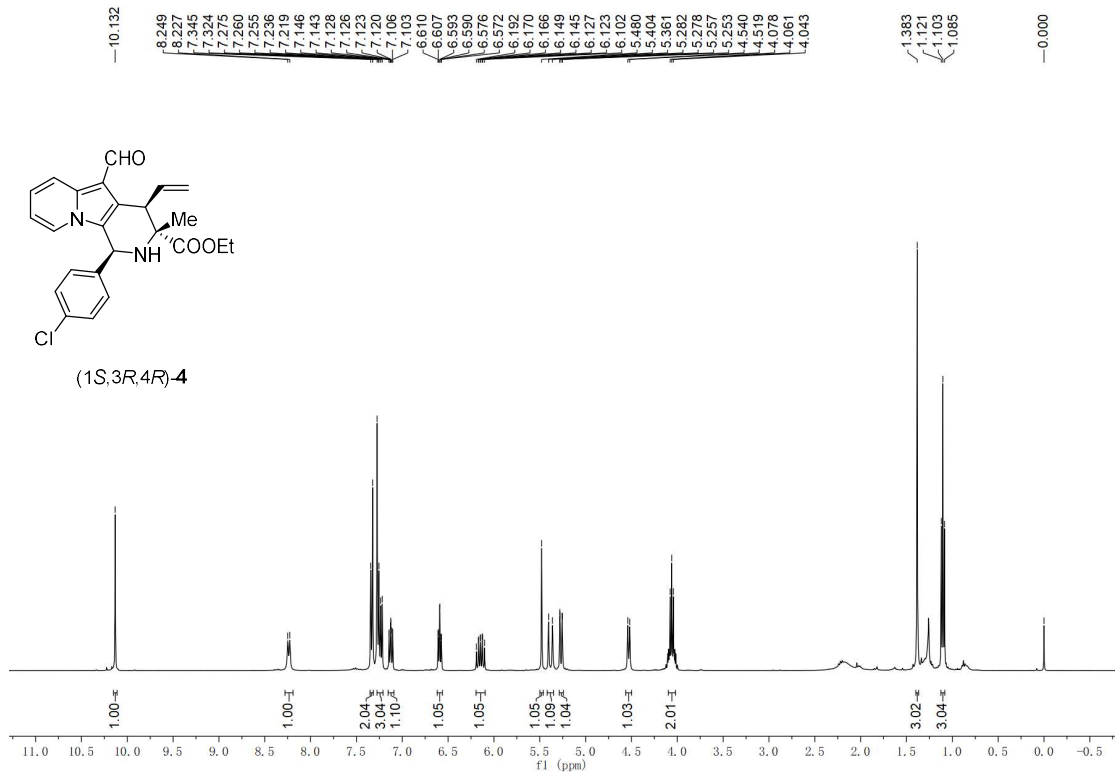
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3D** in $CDCl_3$



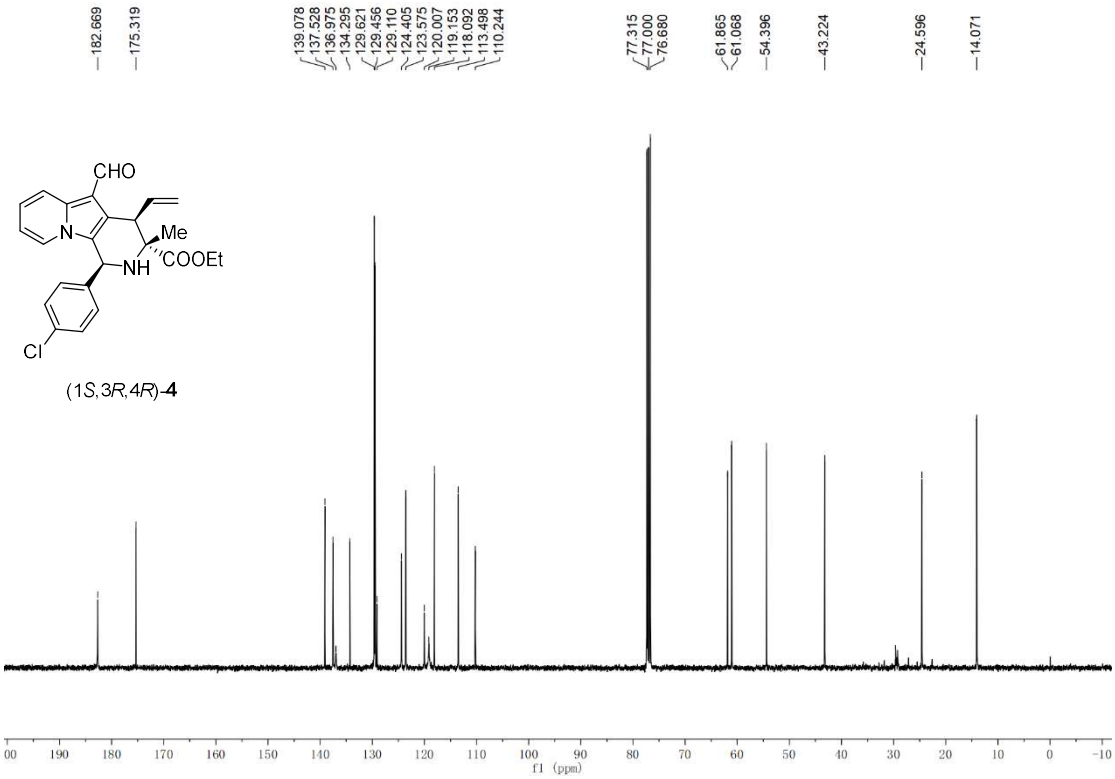
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**3E** in $CDCl_3$



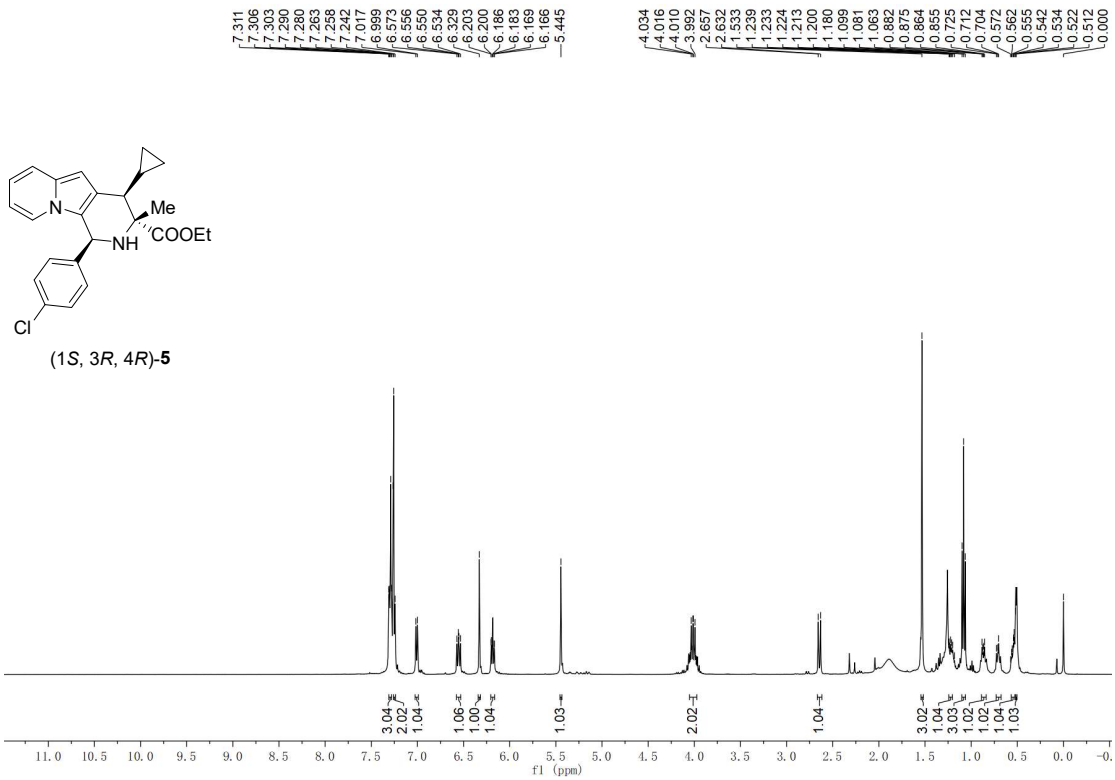
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**3E** in $CDCl_3$



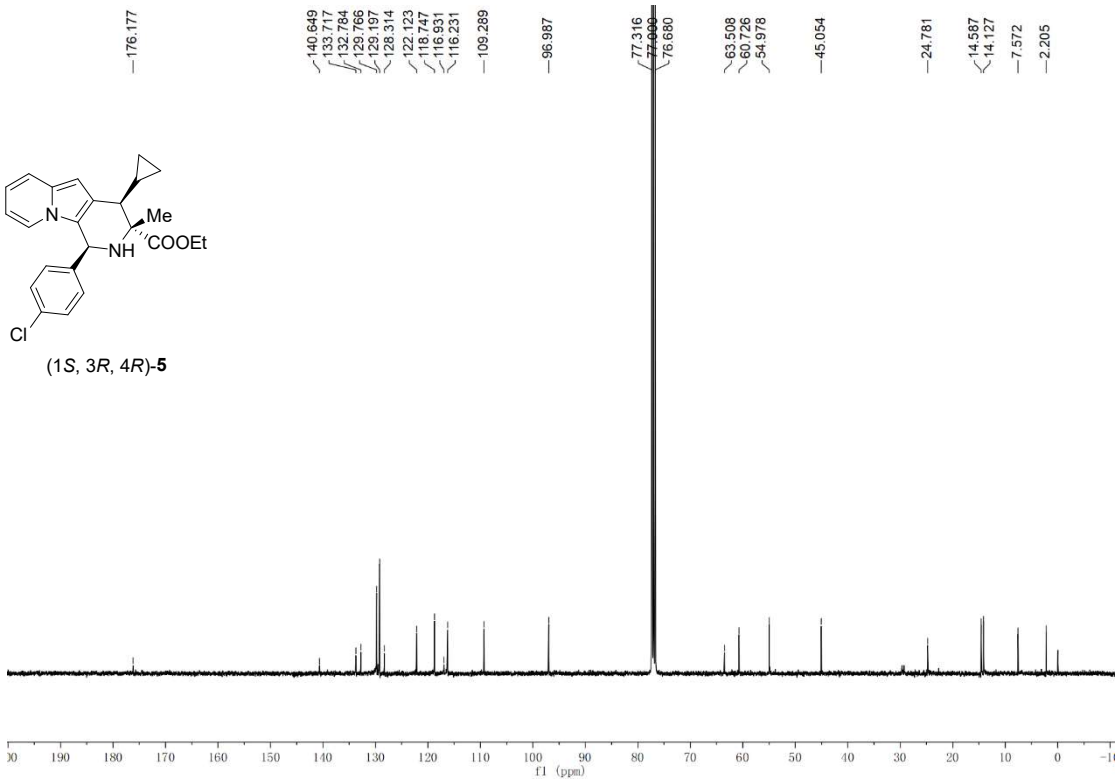
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**4** in $CDCl_3$



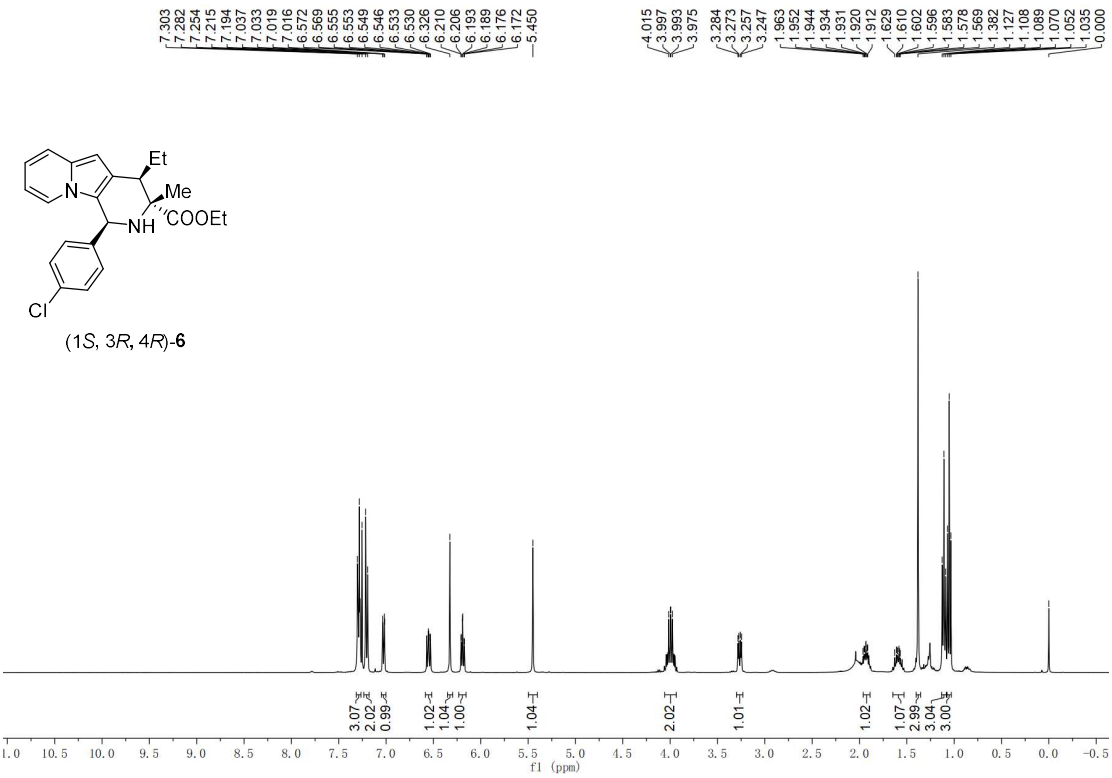
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**4** in $CDCl_3$



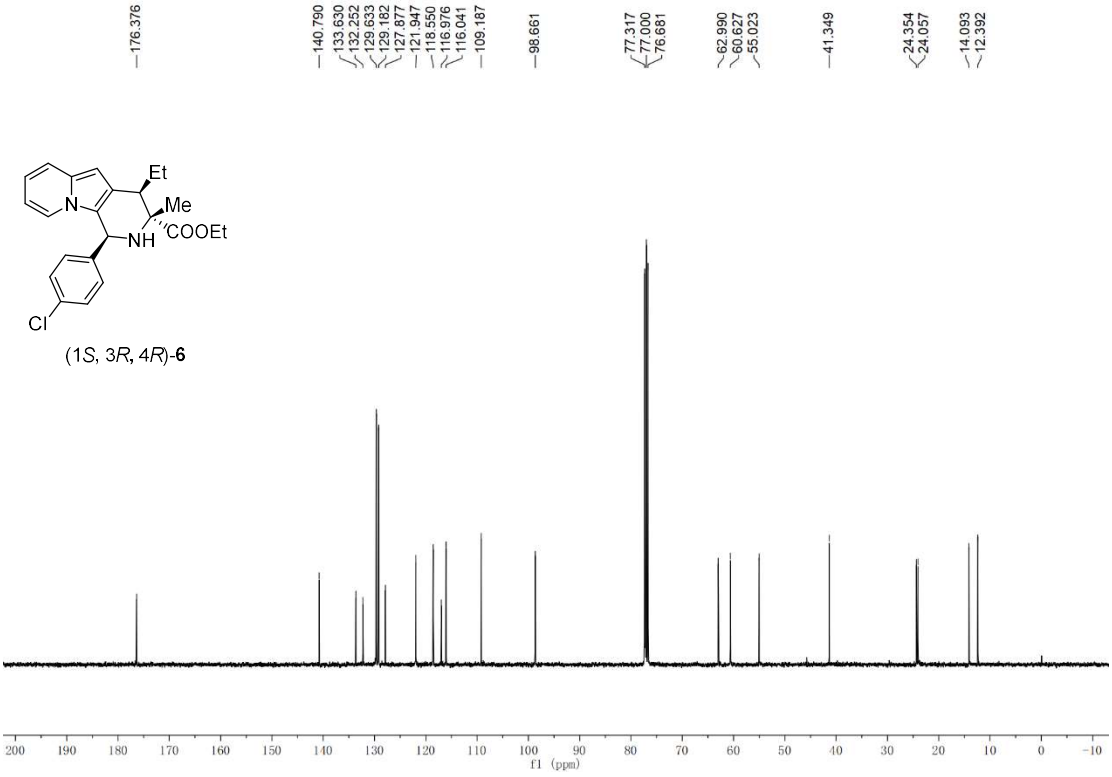
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**5** in $CDCl_3$



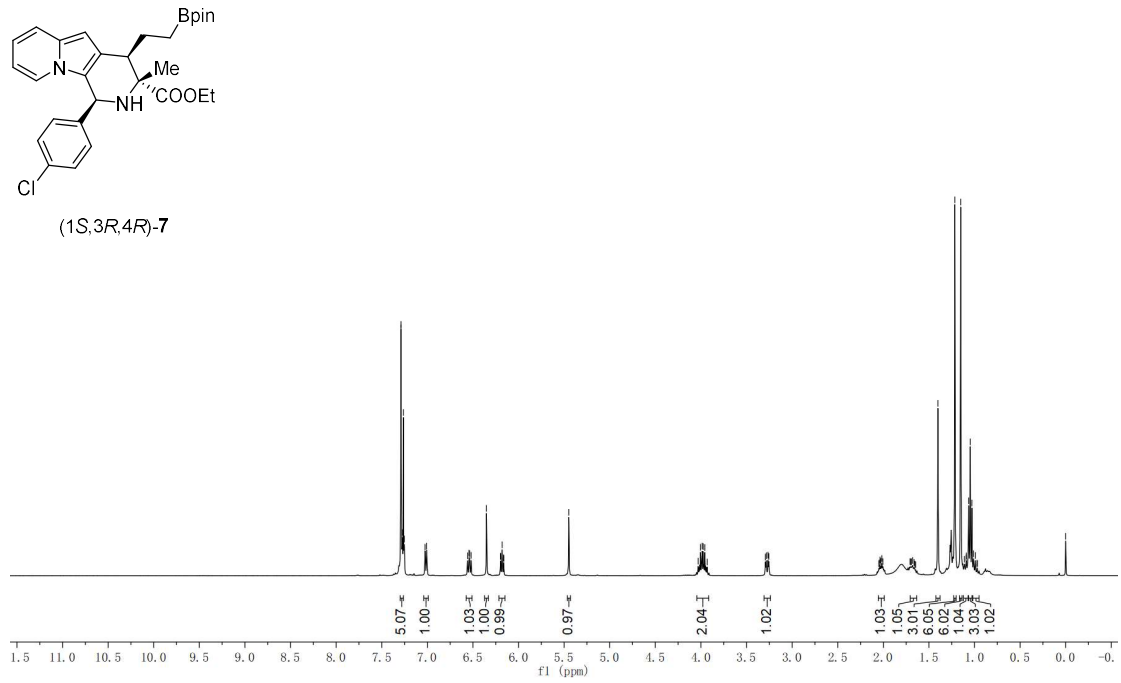
^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**5** in $CDCl_3$



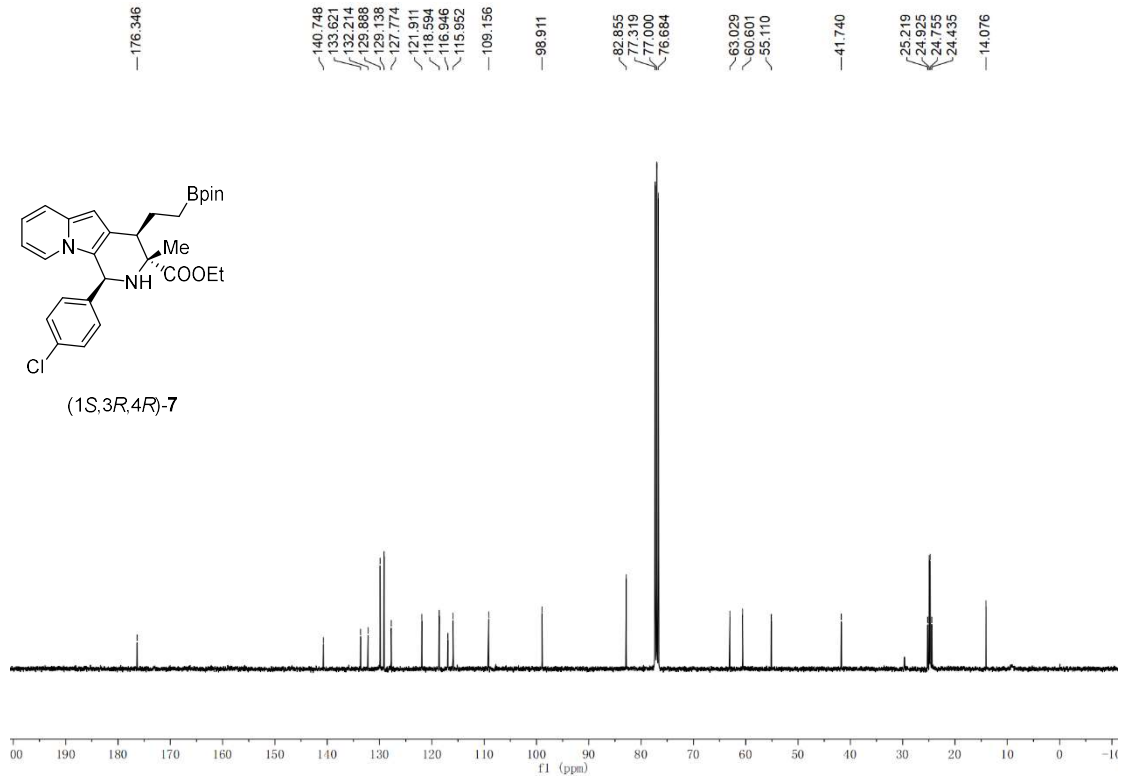
^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**6** in $CDCl_3$



^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**6** in $CDCl_3$

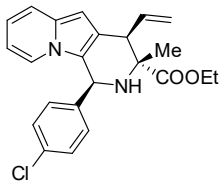


^{1}H NMR (400 MHz) of (1*S*, 3*R*, 4*R*)-**7** in $CDCl_3$



^{13}C NMR (100 MHz) of (1*S*, 3*R*, 4*R*)-**7** in $CDCl_3$

HPLC chromatogram of compound (*rac*)-3a



(1*S*,3*R*,4*R*)-**3a**

```
Data File D:\LC\DATA\ZBK\ZBK-3-58-1RAC 2021-05-12 09-22-42\ZBK-3-58-1RAC1.D
Sample Name: ZBK-3-58-1RAC

    ======================================================================
    Acq. Operator   : 系统                          Seq. Line :   2
    Sample Operator : 系统
    Acq. Instrument : 1200                          Location :   31
    Injection Date  : 5/12/2021 9:34:53 AM               Inj :   1
                                                    Inj Volume : 5.000 µl
    Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-58-1RAC 2021-05-12 09-22-42\P1-AD-H-90-10-254NM-1ML-
                      5UL-30MIN.M
    Last changed    : 5/12/2021 9:55:01 AM by 系统
                      (modified after loading)
    Analysis Method : D:\LC\DATA\ZBK\ZBK-3-58-1RAC 2021-05-12 09-22-42\P1-AD-H-90-10-254NM-1ML-
                      5UL-30MIN.M (Sequence Method)
    Last changed    : 7/28/2021 8:45:25 PM by 系统
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
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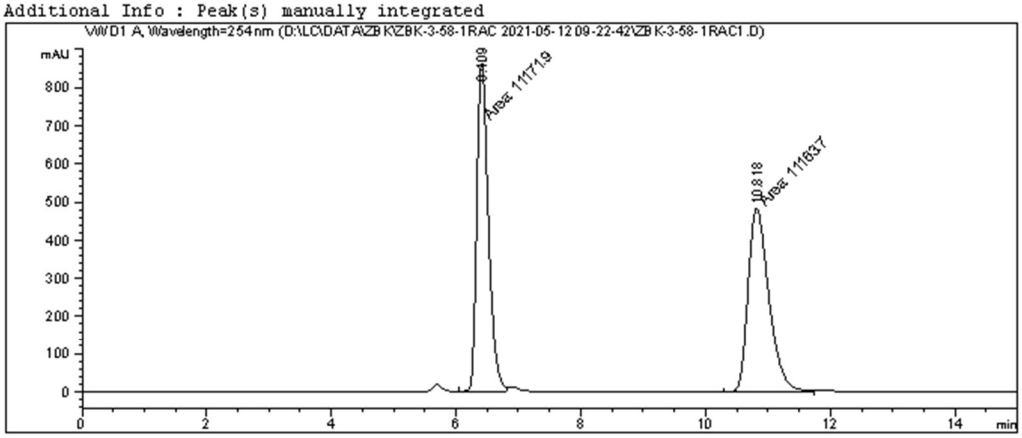


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    ======================================================================
                              Area Percent Report
    ======================================================================

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


    Signal 1: VWD1 A, Wavelength=254 nm

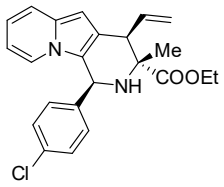
    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   6.409 MF    0.2160 1.11719e4   861.98682  50.0184
       2  10.818 MF    0.3860 1.11637e4   482.07657  49.9816

    Totals :                  2.23356e4  1344.06339

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

1200 7/28/2021 8:45:27 PM 系统                                  Page 1 of 1
```

HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3a



(1*S*,3*R*,4*R*)-**3a**

Data File D:\LC\DATA\ZBK\ZBK-3-58-1 2021-05-11 16-29-17\ZBK-3-58-11.D
Sample Name: ZBK-3-58R/R

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   73
Injection Date  : 5/11/2021 4:43:10 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-58-1 2021-05-11 16-29-17\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M
Last changed    : 5/7/2021 10:11:20 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-58-1 2021-05-11 16-29-17\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M (Sequence Method)
Last changed    : 7/28/2021 8:50:28 PM by 系统
                  (modified after loading)
Additional Info : Peak(s) manually integrated
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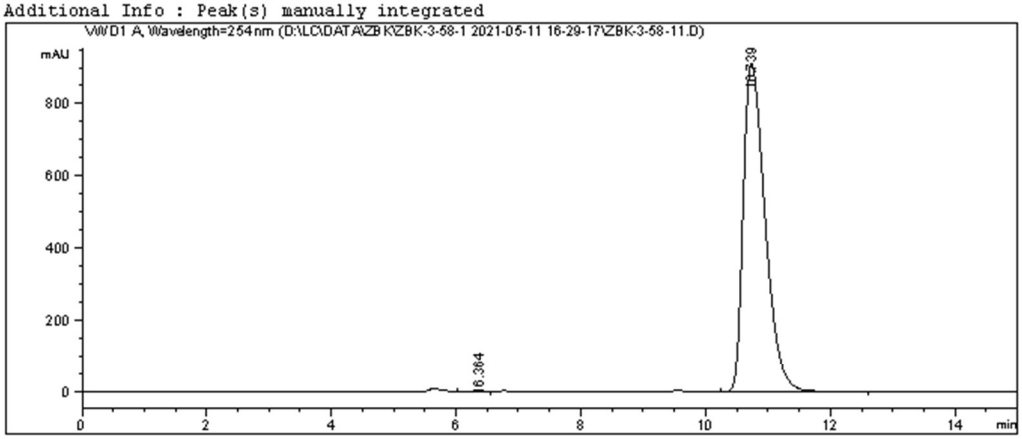


```
======================================================================
                        Area Percent Report
======================================================================

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


Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.364 VV    0.2592   39.57529    2.11342   0.1782
   2  10.739 BV R  0.3773 2.21704e4   910.35876  99.8218

Totals :                  2.22100e4   912.47218

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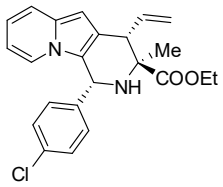
                        *** End of Report ***
```

HPLC chromatogram of compound (1*R*,3*S*,4*S*)-3a



(1*R*,3*S*,4*S*)-**3a**

Data File D:\LC\DATA\ZBK\ZBK-3-58-1 2021-05-11 16-29-17\ZBK-3-58-12.D
Sample Name: ZBK-3-58S/S

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :   3
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   74
Injection Date  : 5/11/2021 5:14:28 PM               Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-58-1 2021-05-11 16-29-17\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M
Last changed    : 5/11/2021 5:24:35 PM by 系统
                  (modified after loading)
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-58-1 2021-05-11 16-29-17\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M (Sequence Method)
Last changed    : 7/28/2021 8:48:36 PM by 系统
                  (modified after loading)
Additional Info : Peak(s) manually integrated
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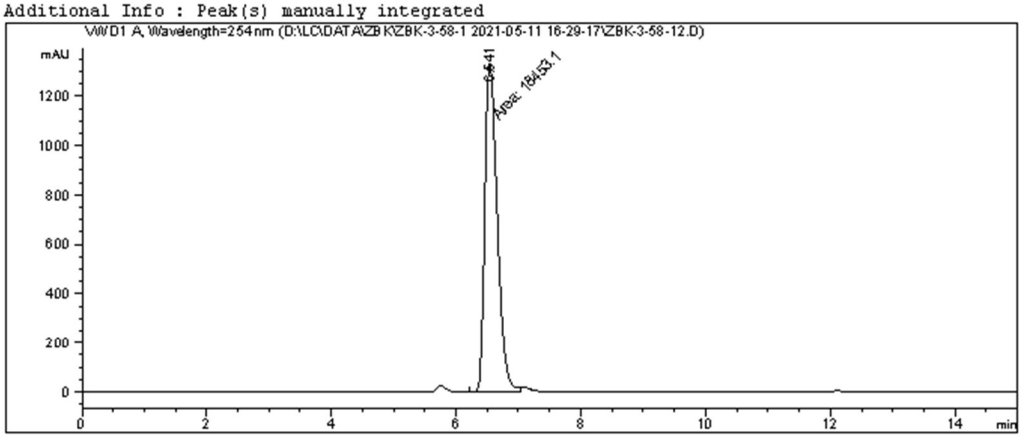



```
==================================================================
                        Area Percent Report
==================================================================

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


Signal 1: VWD1 A, Wavelength=254 nm

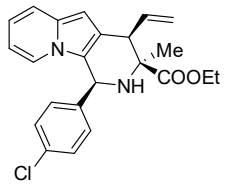
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.541 MF    0.2310 1.84531e4  1331.23181 100.0000

Totals :                  1.84531e4  1331.23181

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

1200 7/28/2021 8:48:39 PM 系统 Page 1 of 1

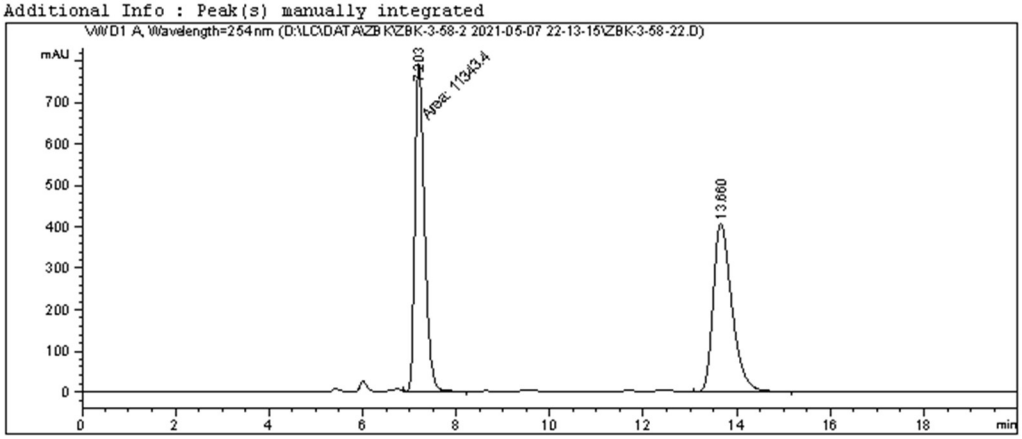
HPLC chromatogram of compound (*rac*)-3a



(1*S*,3*S*,4*R*)-**3a**

Data File D:\LC\DATA\ZBK\ZBK-3-58-2 2021-05-07 22-13-15\ZBK-3-58-22.D
Sample Name: ZBK-3-58-2RAC

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :   3
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   32
Injection Date  : 5/7/2021 10:56:44 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-58-2 2021-05-07 22-13-15\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M
Last changed    : 5/7/2021 10:11:20 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-58-2 2021-05-07 22-13-15\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M (Sequence Method)
Last changed    : 7/28/2021 8:52:06 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.203 FM    0.2387 1.13434e4   792.11041  50.1218
   2  13.660 BV R  0.4248 1.12883e4   406.05557  49.8782

Totals :                  2.26317e4  1198.16599

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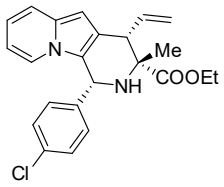
                        *** End of Report ***

1200 7/28/2021 8:52:10 PM 系统                          Page 1 of 1
```

HPLC chromatogram of compound (1*R*,3*R*,4*S*)-3a



(1*R*,3*R*,4*S*)-**3a**

```
Data File D:\LC\DATA\ZBK\ZBK-3-58-2 2021-05-07 22-13-15\ZBK-3-58-21.D
Sample Name: ZBK-3-58R/S

    ======================================================================
    Acq. Operator   : 系统                          Seq. Line :   2
    Sample Operator : 系统
    Acq. Instrument : 1200                           Location :   31
    Injection Date  : 5/7/2021 10:25:30 PM              Inj :   1
                                                    Inj Volume : 5.000 µl
    Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-58-2 2021-05-07 22-13-15\P1-AD-H-90-10-254NM-1ML-5UL-
                      30MIN.M
    Last changed    : 5/7/2021 10:11:20 PM by 系统
    Analysis Method : D:\LC\DATA\ZBK\ZBK-3-58-2 2021-05-07 22-13-15\P1-AD-H-90-10-254NM-1ML-5UL-
                      30MIN.M (Sequence Method)
    Last changed    : 7/28/2021 8:53:49 PM by 系统
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
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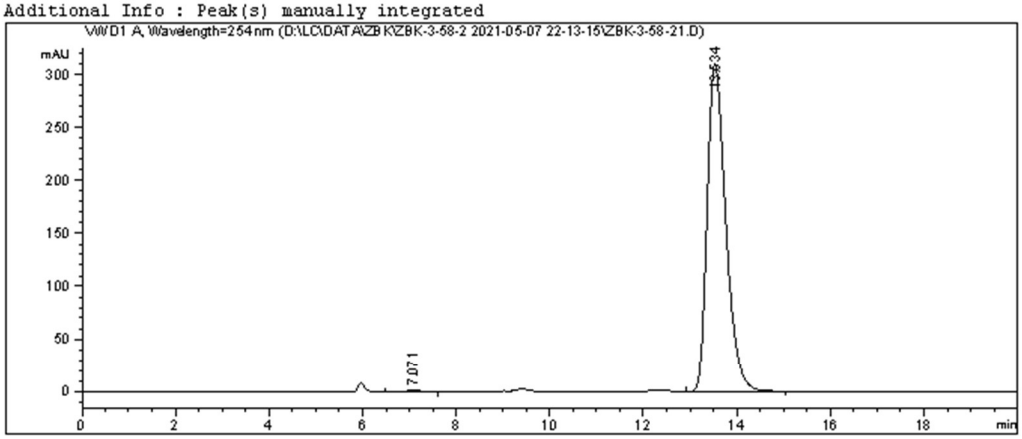


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    ======================================================================
                              Area Percent Report
    ======================================================================

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


    Signal 1: VWD1 A, Wavelength=254 nm

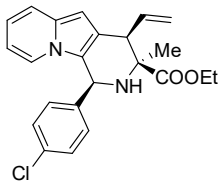
    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   7.071 VV R  0.2365   28.04296    1.71005   0.3259
       2  13.534 BB    0.4214 8575.84766  310.38681  99.6741

    Totals :                  8603.89062  312.09686


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

1200 7/28/2021 8:53:52 PM 系统                                  Page 1 of 1
```

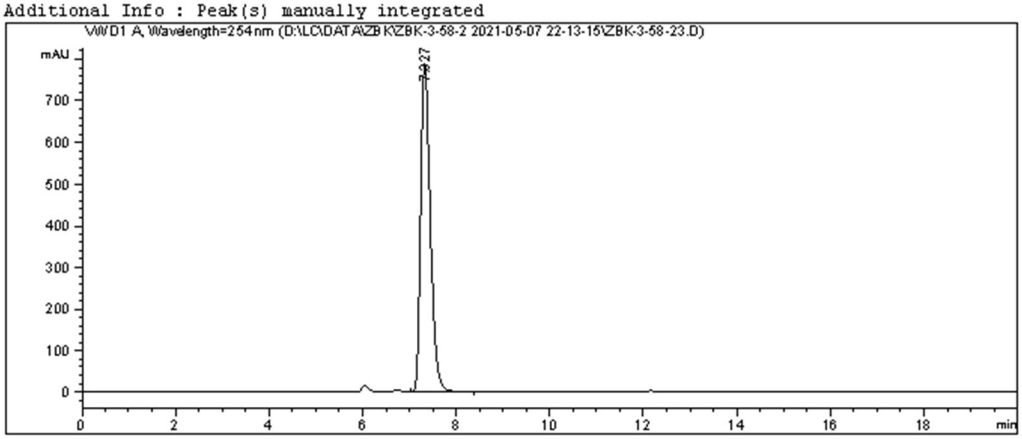
HPLC chromatogram of compound (1*S*,3*S*,4*R*)-3a



(1*S*,3*S*,4*R*)-**3a**

Data File D:\LC\DATA\ZBK\ZBK-3-58-2 2021-05-07 22-13-15\ZBK-3-58-23.D
Sample Name: ZBK-3-58S/R

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :   4
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   33
Injection Date  : 5/7/2021 11:27:59 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-58-2 2021-05-07 22-13-15\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M
Last changed    : 5/7/2021 10:11:20 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-58-2 2021-05-07 22-13-15\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M (Sequence Method)
Last changed    : 7/28/2021 8:55:04 PM by 系统
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```

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

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


Signal 1: VWD1 A, Wavelength=254 nm

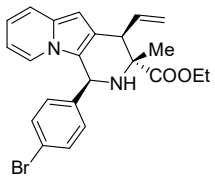
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.327 BB    0.2198 1.13153e4   788.81274 100.0000

Totals :                  1.13153e4   788.81274

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

1200 7/28/2021 8:55:08 PM 系统                          Page 1 of 1
```

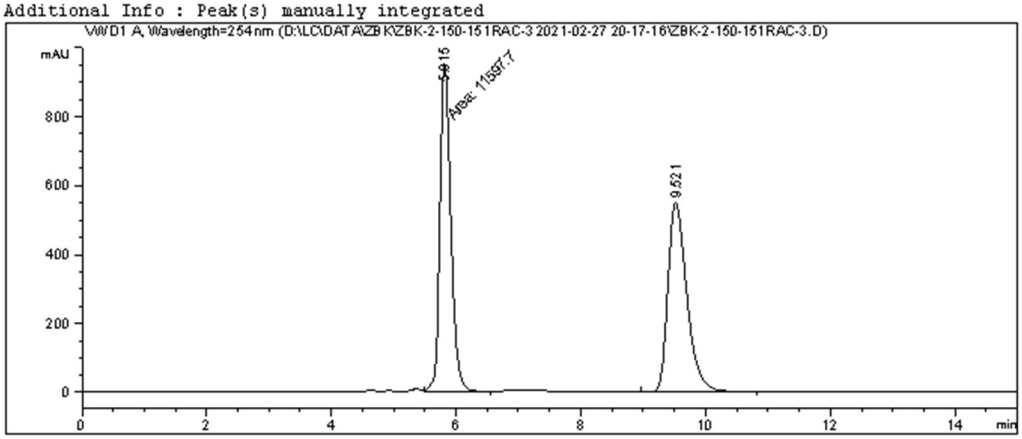
HPLC chromatogram of compound (*rac*)-3b



(1*S*,3*R*,4*R*)-**3b**

Data File D:\LC\DATA\ZBK\ZBK-2-150-151RAC-3 2021-02-27 20-17-16\ZBK-2-150-151RAC-3.D
Sample Name: ZBK-2-150-151RAC-2

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :   1
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   42
Injection Date  : 2/27/2021 8:18:45 PM               Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-150-151RAC-3 2021-02-27 20-17-16\P1-AD-H-80-20-254NM-
                  1ML-5UL-20MIN.M
Last changed    : 1/14/2021 2:49:11 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-2-150-151RAC-3 2021-02-27 20-17-16\P1-AD-H-80-20-254NM-
                  1ML-5UL-20MIN.M (Sequence Method)
Last changed    : 7/28/2021 8:00:37 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

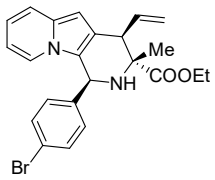
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.815 FM    0.2027 1.15977e4   953.43475  49.9684
   2   9.521 BV R  0.3227 1.16123e4   551.72522  50.0316

Totals :                  2.32100e4  1505.15997

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

1200 7/28/2021 8:00:39 PM 系统                          Page 1 of 1
```

HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3b



(1*S*,3*R*,4*R*)-**3b**

Data File D:\LC\DATA\ZBK\ZBK-2-150-151-2 2021-02-27 18-34-15\ZBK-2-150-151-21.D
Sample Name: ZBK-2-150-2

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                            Location :   42
Injection Date  : 2/27/2021 6:46:34 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-150-151-2 2021-02-27 18-34-15\P1-AD-H-80-20-254NM-1ML-
                  5UL-20MIN.M
Last changed    : 1/14/2021 2:49:11 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-2-150-151-2 2021-02-27 18-34-15\P1-AD-H-80-20-254NM-1ML-
                  5UL-20MIN.M (Sequence Method)
Last changed    : 7/28/2021 8:03:09 PM by 系统
                  (modified after loading)
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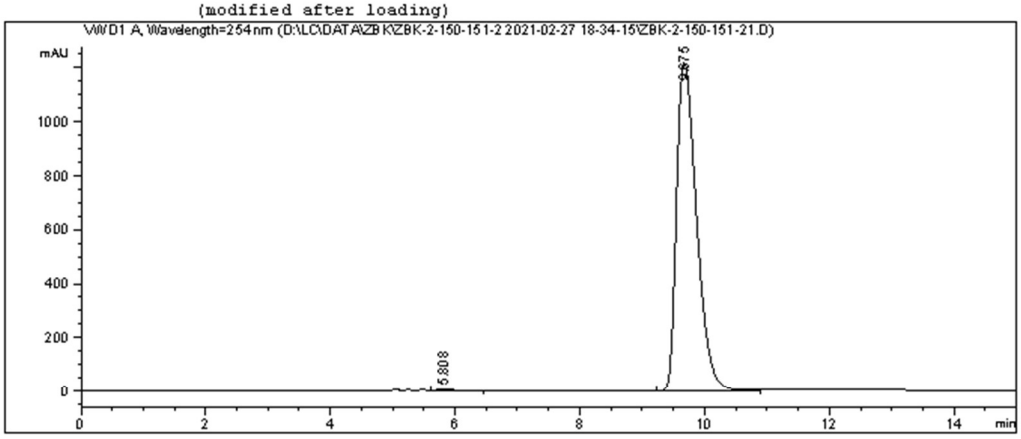


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==================================================================
                        Area Percent Report
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Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=254 nm

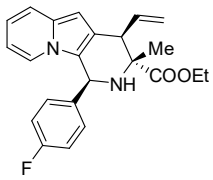
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.808 BV R  0.1678   50.66753    4.44867   0.1866
   2   9.675 BB    0.3471 2.71031e4  1217.16809  99.8134

Totals :                  2.71537e4  1221.61677


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


1200 7/28/2021 8:03:13 PM 系统                          Page 1 of 1
```

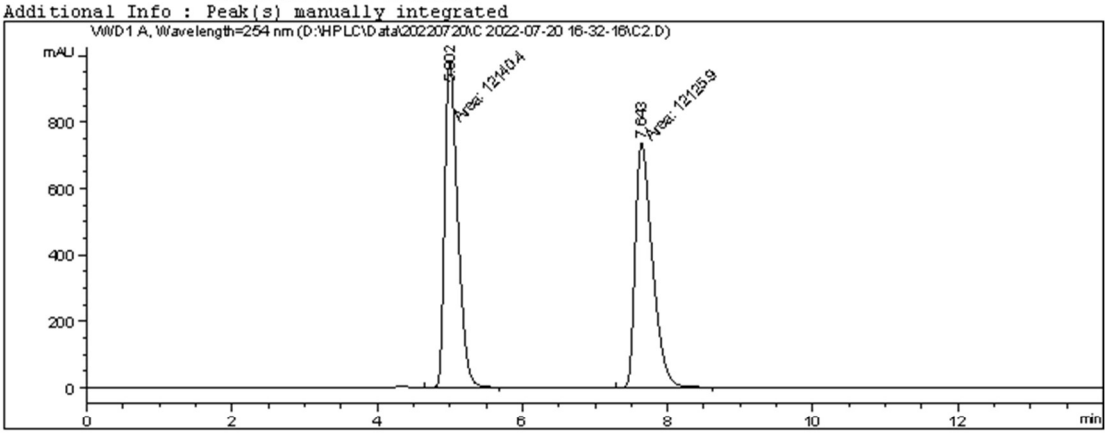
HPLC chromatogram of compound (*rac*)-3c



(1*S*,3*R*,4*R*)-**3c**

Data File D:\HPLC\Data\20220720\C 2022-07-20 16-32-16\C2.D
Sample Name: ZBK-4-117RAC

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Sample Operator : SYSTEM
Acq. Instrument : 1260                           Location :   1
Injection Date  : 7/20/2022 5:07:40 PM              Inj :   2
                                                Inj Volume : 10.000 µl
Acq. Method     : D:\HPLC\Data\20220720\C 2022-07-20 16-32-16\(1-6)-90-10-10uL-1ml-40min-254nm.M
Last changed    : 7/20/2022 5:06:52 PM by SYSTEM
Analysis Method : D:\HPLC\Data\20220720\C 2022-07-20 16-32-16\(1-6)-90-10-10uL-1ml-40min-254nm.M
                  (Sequence Method)
Last changed    : 11/24/2022 6:41:29 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




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

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

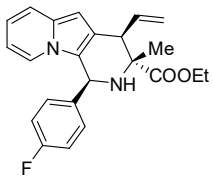

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.002 FM    0.2061 1.21404e4   981.62115  50.0299
   2   7.643 MF    0.2748 1.21259e4   735.54468  49.9701

Totals :                  2.42663e4  1717.16583

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

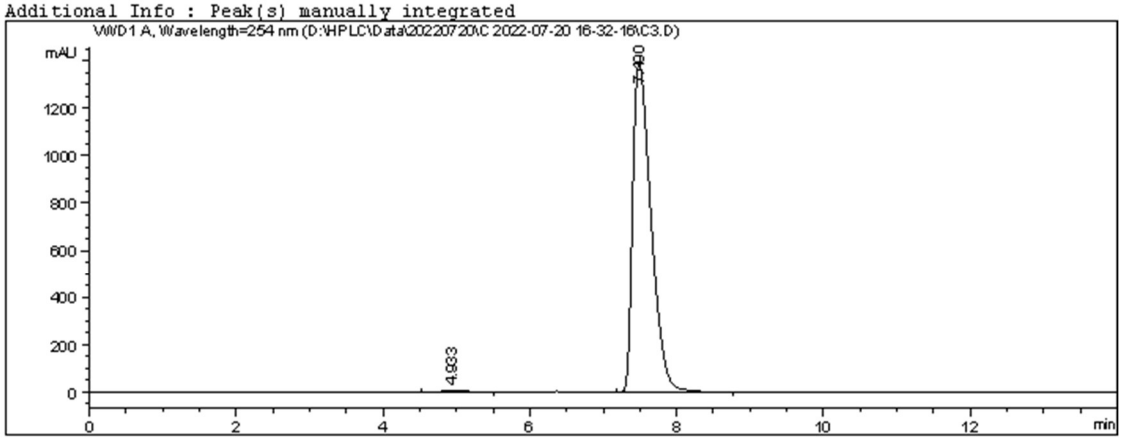
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3c



(1*S*,3*R*,4*R*)-**3c**

Data File D:\HPLC\Data\20220720\C 2022-07-20 16-32-16\C3.D
Sample Name: ZBK-4-117R/R

```
==================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   4
Sample Operator : SYSTEM
Acq. Instrument : 1260                          Location :   2
Injection Date  : 7/20/2022 5:28:29 PM              Inj :   1
                                               Inj Volume : 10.000 µl
Acq. Method     : D:\HPLC\Data\20220720\C 2022-07-20 16-32-16\(1-6)-90-10-10uL-1ml-40min-254nm.M
Last changed    : 7/20/2022 5:06:52 PM by SYSTEM
Analysis Method : D:\HPLC\Data\20220720\C 2022-07-20 16-32-16\(1-6)-90-10-10uL-1ml-40min-254nm.M
                  (Sequence Method)
Last changed    : 11/24/2022 6:45:51 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




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

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

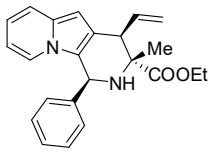

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.933 BB    0.2780  166.63431    9.12553   0.6844
   2   7.490 BB    0.2667 2.41814e4  1391.77112  99.3156

Totals :                  2.43481e4  1400.89665

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

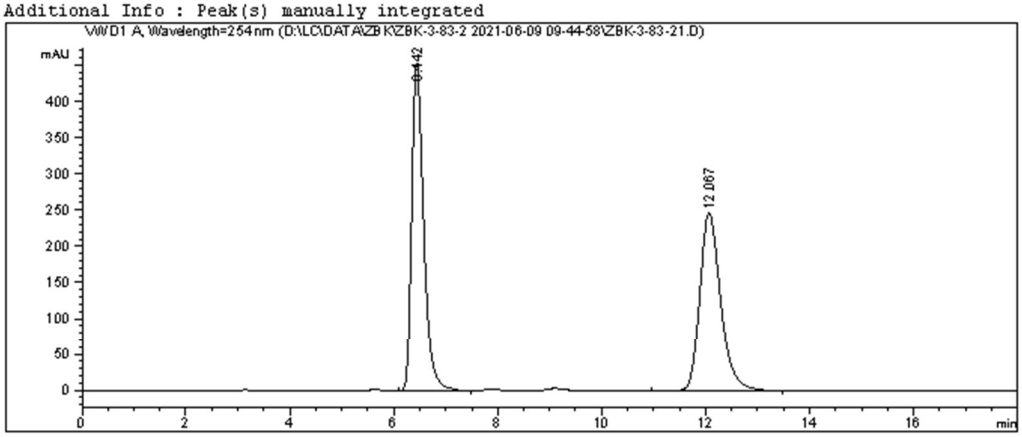
HPLC chromatogram of compound (*rac*)-3d



(1*S*,3*R*,4*R*)-**3d**

Data File D:\LC\DATA\ZBK\ZBK-3-83-2 2021-06-09 09-44-58\ZBK-3-83-21.D
Sample Name: ZBK-3-83RAC

```
==================================================================
Acq. Operator   : 采统                          Seq. Line :   2
Sample Operator : 采统
Acq. Instrument : 1200                            Location :   1
Injection Date  : 6/9/2021 9:56:56 AM                  Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-83-2 2021-06-09 09-44-58\P1-AD-H-95-5-254NM-1ML-5ul-
                  30min.M
Last changed    : 6/9/2021 10:21:37 AM by 采统
                  (modified after loading)
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-83-2 2021-06-09 09-44-58\P1-AD-H-95-5-254NM-1ML-5ul-
                  30min.M (Sequence Method)
Last changed    : 7/28/2021 9:06:05 PM by 采统
                  (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: VWD1 A, Wavelength=254 nm

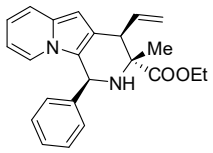
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.442 BB    0.2426 7207.07959  452.54630  51.2078
   2  12.067 BV R  0.4256 6867.10156  246.37842  48.7922

Totals :                  1.40742e4   698.92471


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

1200 7/28/2021 9:06:09 PM 采统                          Page 1 of 1
```

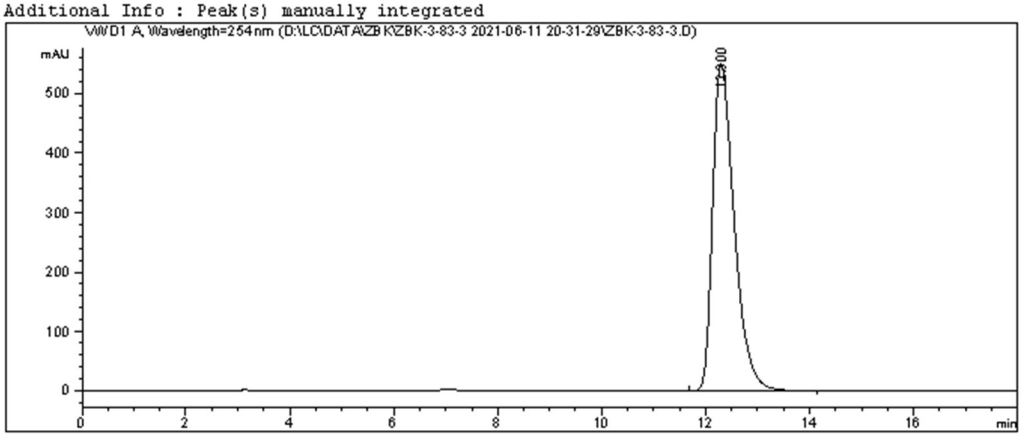
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3d



(1*S*,3*R*,4*R*)-**3d**

```
Data File D:\LC\DATA\ZBK\ZBK-3-83-3 2021-06-11 20-31-29\ZBK-3-83-3.D
Sample Name: ZBK-3-83R/R

    ======================================================================
    Acq. Operator   : 系统                          Seq. Line :   1
    Sample Operator : 系统
    Acq. Instrument : 1200                           Location :   3
    Injection Date  : 6/11/2021 8:32:54 PM              Inj :   1
                                                    Inj Volume : 5.000 µl
    Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-83-3 2021-06-11 20-31-29\P1-AD-H-95-5-254NM-1ML-5ul-
                      30min.M
    Last changed    : 6/11/2021 8:48:42 PM by 系统
                      (modified after loading)
    Analysis Method : D:\LC\DATA\ZBK\ZBK-3-83-3 2021-06-11 20-31-29\P1-AD-H-95-5-254NM-1ML-5ul-
                      30min.M (Sequence Method)
    Last changed    : 7/28/2021 9:04:38 PM by 系统
                      (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: VWD1 A, Wavelength=254 nm

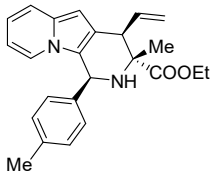
    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  12.300 BV R  0.4417 1.59170e4   551.32086 100.0000

    Totals :                  1.59170e4   551.32086


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

1200 7/28/2021 9:04:42 PM 系统                                  Page 1 of 1
```

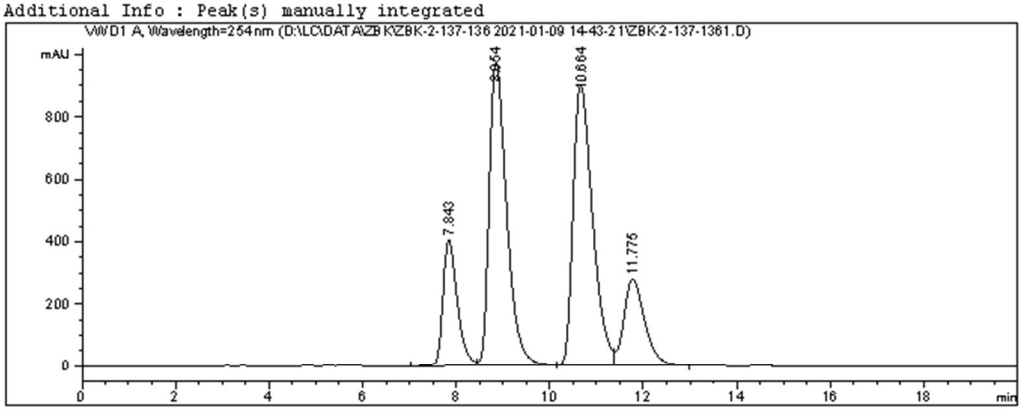
HPLC chromatogram of compound (*rac*)-3e



(1*S*,3*R*,4*R*)-**3e**

Data File D:\LC\DATA\ZBK\ZBK-2-137-136 2021-01-09 14-43-21\ZBK-2-137-1361.D
Sample Name: ZBK-2-137

```
======================================================================
Acq. Operator   : 采统                          Seq. Line :   2
Sample Operator : 采统
Acq. Instrument : 1200                           Location :   35
Injection Date  : 1/9/2021 2:55:41 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-137-136 2021-01-09 14-43-21\P1-AD-H-95-5-254NM-1ML-5ul
                  -30min.M
Last changed    : 12/29/2020 2:58:55 PM by 采统
Analysis Method : D:\LC\DATA\ZBK\ZBK-2-137-136 2021-01-09 14-43-21\P1-AD-H-95-5-254NM-1ML-5ul
                  -30min.M (Sequence Method)
Last changed    : 7/28/2021 5:42:13 PM by 采统
                  (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: VWD1 A, Wavelength=254 nm

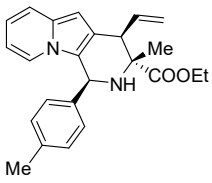
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.843 BV    0.3230 8635.95215  405.06708  12.6035
   2   8.854 VB    0.3968 2.51844e4   972.52118  36.7548
   3  10.664 BV    0.4480 2.60665e4   897.74261  38.0421
   4  11.775 VB    0.4668 8633.19727  279.40921  12.5995

Totals :                  6.85200e4  2554.74008


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

1200 7/28/2021 5:42:16 PM 采统 Page 1 of 1

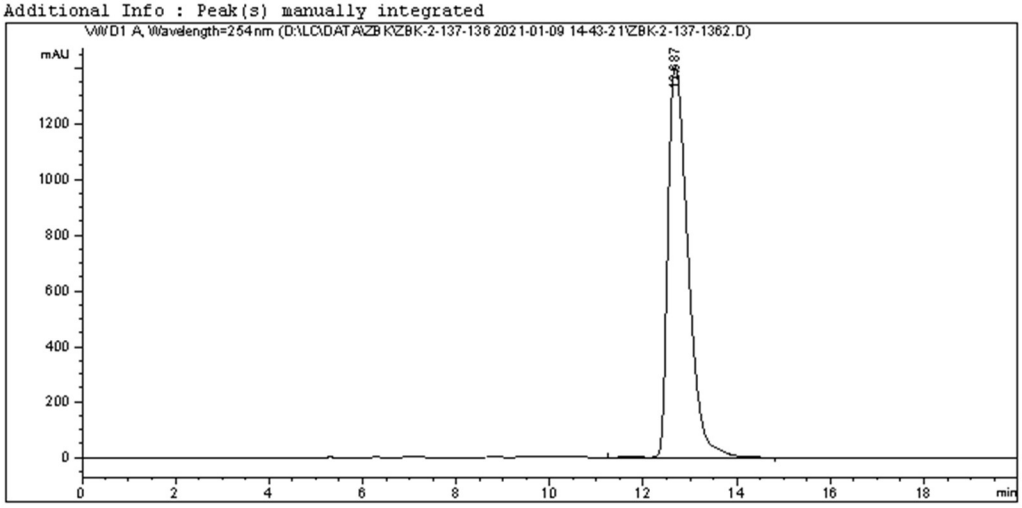
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3e



(1*S*,3*R*,4*R*)-**3e**

Data File D:\LC\DATA\ZBK\ZBK-2-137-136 2021-01-09 14-43-21\ZBK-2-137-1362.D
Sample Name: ZBK-2-136

```
    ======================================================================
    Acq. Operator   : 采统                          Seq. Line :   3
    Sample Operator : 采统
    Acq. Instrument : 1200                           Location :   36
    Injection Date  : 1/9/2021 3:26:59 PM                Inj :   1
                                                    Inj Volume : 5.000 µl
    Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-137-136 2021-01-09 14-43-21\P1-AD-H-95-5-254NM-1ML-5ul
                      -30min.M
    Last changed    : 12/29/2020 2:58:55 PM by 采统
    Analysis Method : D:\LC\DATA\ZBK\ZBK-2-137-136 2021-01-09 14-43-21\P1-AD-H-95-5-254NM-1ML-5ul
                      -30min.M (Sequence Method)
    Last changed    : 7/28/2021 7:37:11 PM by 采统
                      (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: VWD1 A, Wavelength=254 nm

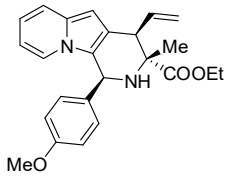
    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  12.687 VV R  0.4617 4.15618e4  1404.53491 100.0000

    Totals :                  4.15618e4  1404.53491

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

1200 7/28/2021 7:37:17 PM 采统                                Page 1 of 1
```

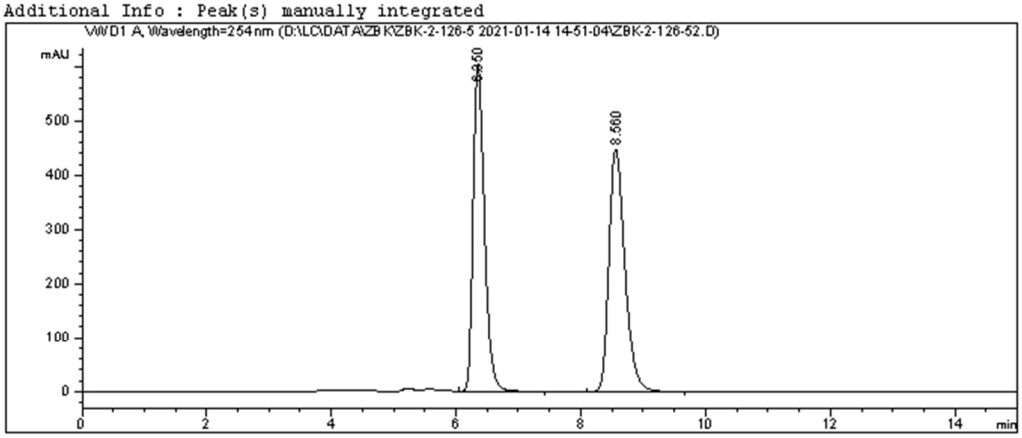
HPLC chromatogram of compound (*rac*)-3f



(1*S*,3*R*,4*R*)-**3f**

Data File D:\LC\DATA\ZBK\ZBK-2-126-5 2021-01-14 14-51-04\ZBK-2-126-52.D
Sample Name: ZBK-2-127S-2

```
=====================================================================
Acq. Operator   : 系统                          Seq. Line :   3
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   12
Injection Date  : 1/14/2021 3:24:38 PM               Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-126-5 2021-01-14 14-51-04\Pl-AD-H-80-20-254NM-1ML-5UL-
                  20MIN.M
Last changed    : 1/14/2021 3:42:14 PM by 系统
                  (modified after loading)
Analysis Method : D:\LC\DATA\ZBK\ZBK-2-126-5 2021-01-14 14-51-04\Pl-AD-H-80-20-254NM-1ML-5UL-
                  20MIN.M (Sequence Method)
Last changed    : 7/28/2021 5:19:41 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

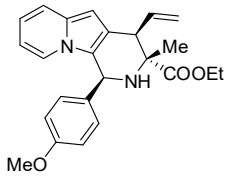
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.350 BB    0.1915 7589.51709  604.85889  48.8744
   2   8.560 BV R  0.2721 7939.08496  448.34076  51.1256

Totals :                  1.55286e4  1053.19965

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

1200 7/28/2021 5:19:49 PM 系统                              Page 1 of 1
```

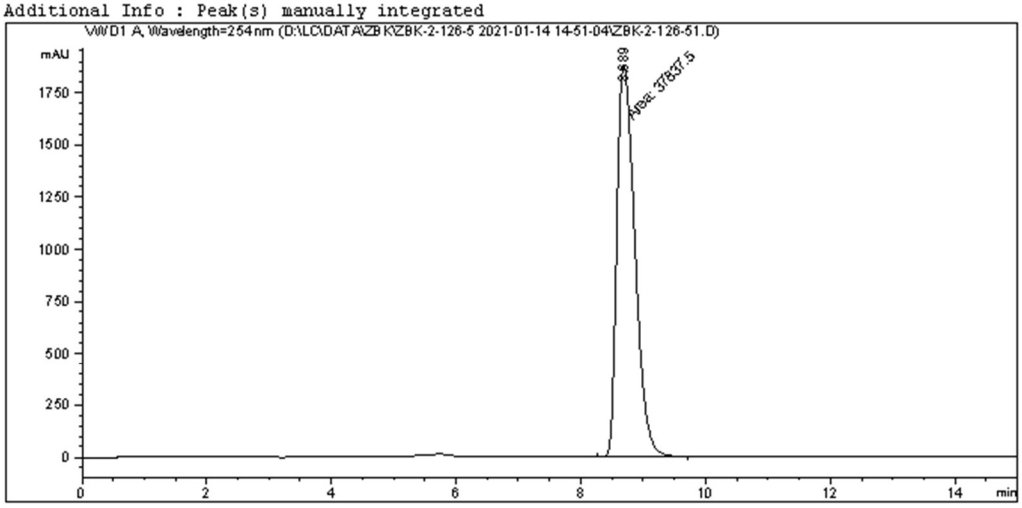
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3f



(1*S*,3*R*,4*R*)-**3f**

Data File D:\LC\DATA\ZBK\ZBK-2-126-5 2021-01-14 14-51-04\ZBK-2-126-51.D
Sample Name: ZBK-2-126-2

```
================================================================
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   11
Injection Date  : 1/14/2021 3:03:23 PM               Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-126-5 2021-01-14 14-51-04\P1-AD-H-80-20-254NM-1ML-5UL-
                  20MIN.M
Last changed    : 1/14/2021 2:49:11 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-2-126-5 2021-01-14 14-51-04\P1-AD-H-80-20-254NM-1ML-5UL-
                  20MIN.M (Sequence Method)
Last changed    : 7/28/2021 5:23:43 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

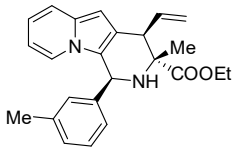
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.689 MM    0.3368 3.78375e4  1872.47302 100.0000

Totals :                  3.78375e4  1872.47302

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

1200 7/28/2021 5:23:46 PM 系统                          Page 1 of 1
```

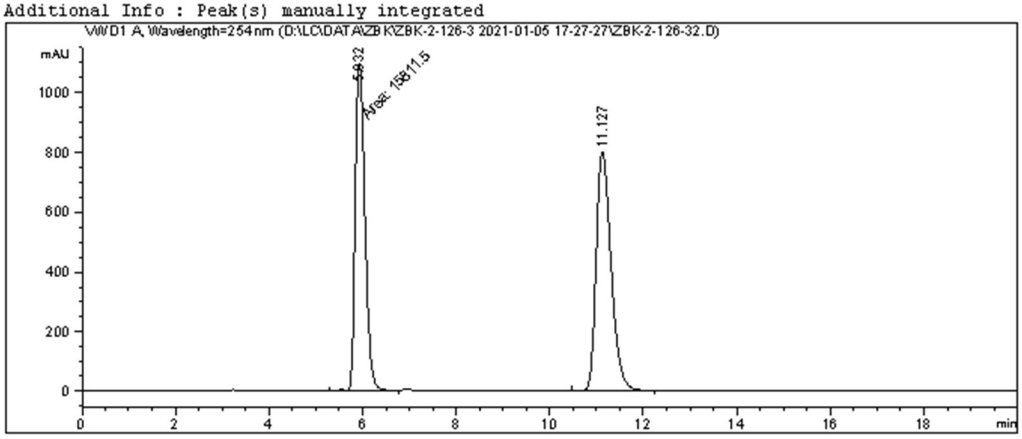
HPLC chromatogram of compound (*rac*)-3g



(1*S*,3*R*,4*R*)-**3g**

Data File D:\LC\DATA\ZBK\ZBK-2-126-3 2021-01-05 17-27-27\ZBK-2-126-32.D
Sample Name: ZBK-2-133S

```
==================================================================
Acq. Operator   : 采统                          Seq. Line :   3
Sample Operator : 采统
Acq. Instrument : 1200                           Location :   4
Injection Date  : 1/5/2021 6:26:05 PM                Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-126-3 2021-01-05 17-27-27\Pl-AD-H-95-5-254NM-1ML-5ul-
                  30min.M
Last changed    : 12/29/2020 2:58:55 PM by 采统
Analysis Method : D:\LC\DATA\ZBK\ZBK-2-126-3 2021-01-05 17-27-27\Pl-AD-H-95-5-254NM-1ML-5ul-
                  30min.M (Sequence Method)
Last changed    : 7/28/2021 5:29:35 PM by 采统
                  (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: VWD1 A, Wavelength=254 nm

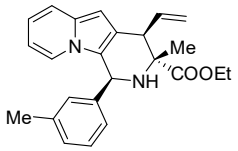
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.932 MF    0.2400 1.58115e4  1097.85315  47.1693
   2  11.127 BB    0.3420 1.77093e4   802.08563  52.8307

Totals :                  3.35208e4  1899.93878

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

1200 7/28/2021 5:29:39 PM 采统                          Page 1 of 1
```

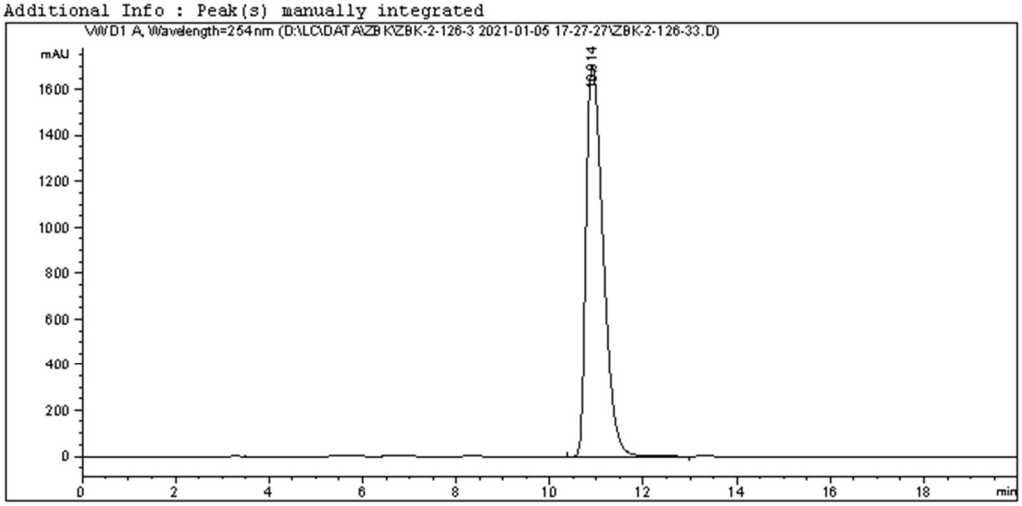
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3g



(1*S*,3*R*,4*R*)-**3g**

Data File D:\LC\DATA\ZBK\ZBK-2-126-3 2021-01-05 17-27-27\ZBK-2-126-33.D
Sample Name: ZBK-2-132

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :   4
Sample Operator : 系统
Acq. Instrument : 1200                            Location :   5
Injection Date  : 1/5/2021 6:57:21 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-126-3 2021-01-05 17-27-27\Pl-AD-H-95-5-254NM-1ML-5ul-
                  30min.M
Last changed    : 12/29/2020 2:58:55 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-2-126-3 2021-01-05 17-27-27\Pl-AD-H-95-5-254NM-1ML-5ul-
                  30min.M (Sequence Method)
Last changed    : 7/28/2021 5:32:07 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

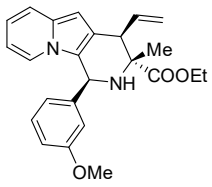
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.914 BV R  0.3990 4.30796e4  1700.21143 100.0000

Totals :                  4.30796e4  1700.21143


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

1200 7/28/2021 5:32:10 PM 系统                              Page 1 of 1
```

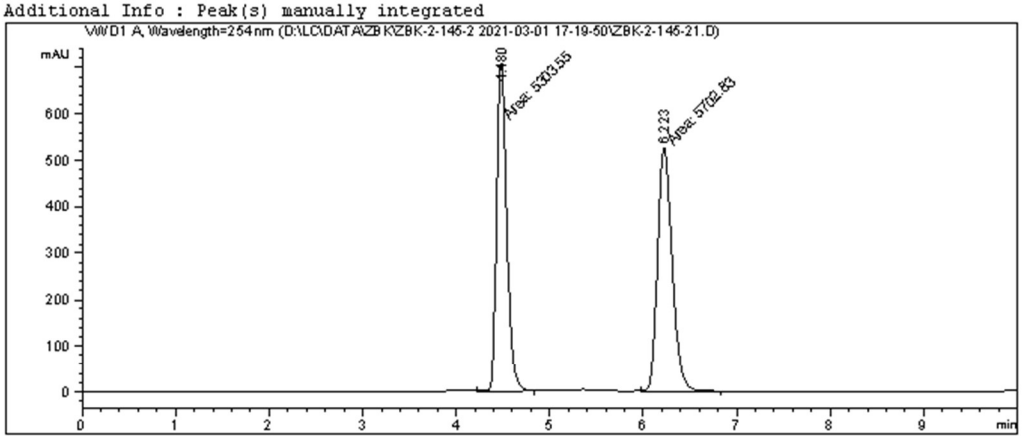
HPLC chromatogram of compound (*rac*)-3h



(1*S*,3*R*,4*R*)-**3h**

```
Data File D:\LC\DATA\ZBK\ZBK-2-145-2 2021-03-01 17-19-50\ZBK-2-145-21.D
Sample Name: ZBK-2-145-2

    ======================================================================
    Acq. Operator   : 系统                          Seq. Line :   2
    Sample Operator : 系统
    Acq. Instrument : 1200                           Location :   71
    Injection Date  : 3/1/2021 5:27:04 PM                Inj :   1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-145-2 2021-03-01 17-19-50\P1-AD-H-80-20-254NM-1ML-5UL-
                      20MIN.M
    Last changed    : 1/14/2021 2:49:11 PM by 系统
    Analysis Method : D:\LC\DATA\ZBK\ZBK-2-145-2 2021-03-01 17-19-50\P1-AD-H-80-20-254NM-1ML-5UL-
                      20MIN.M (Sequence Method)
    Last changed    : 7/28/2021 7:53:16 PM by 系统
                      (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: VWD1 A, Wavelength=254 nm

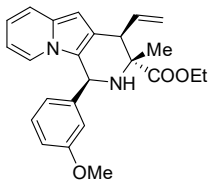
    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   4.480 FM    0.1250 5303.54932  706.87036  48.1862
       2   6.223 FM    0.1810 5702.82617  525.23358  51.8138

    Totals :                  1.10064e4  1232.10394

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

1200 7/28/2021 7:53:19 PM 系统                                  Page 1 of 1
```

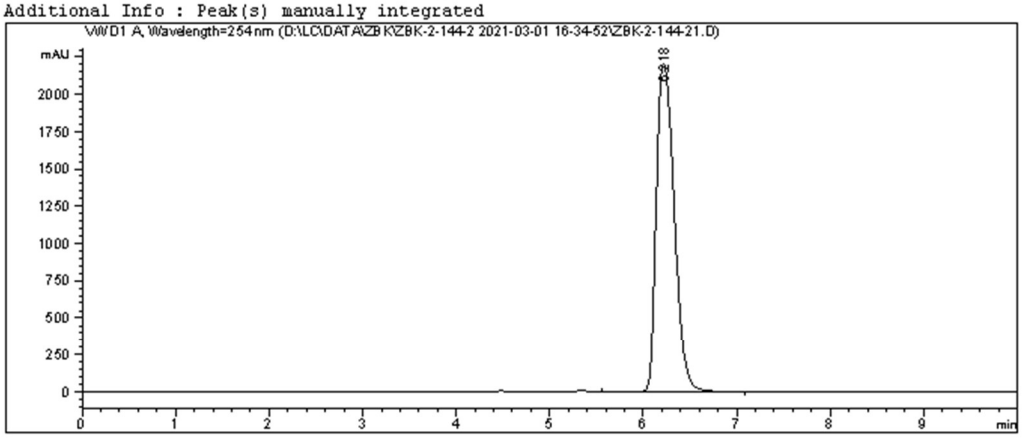
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3h



(1*S*,3*R*,4*R*)-**3h**

Data File D:\LC\DATA\ZBK\ZBK-2-144-2 2021-03-01 16-34-52\ZBK-2-144-21.D
Sample Name: ZBK-2-144-2

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   61
Injection Date  : 3/1/2021 4:47:14 PM                 Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-144-2 2021-03-01 16-34-52\Pl-AD-H-80-20-254NM-1ML-5UL-
                  20MIN.M
Last changed    : 3/1/2021 4:56:23 PM by 系统
                  (modified after loading)
Analysis Method : D:\LC\DATA\ZBK\ZBK-2-144-2 2021-03-01 16-34-52\Pl-AD-H-80-20-254NM-1ML-5UL-
                  20MIN.M (Sequence Method)
Last changed    : 7/28/2021 7:55:17 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

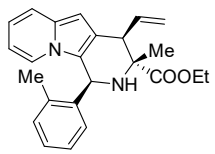
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.218 BB    0.2119 2.92913e4  2203.51538 100.0000

Totals :                  2.92913e4  2203.51538

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

1200 7/28/2021 7:55:20 PM 系统                          Page 1 of 1
```

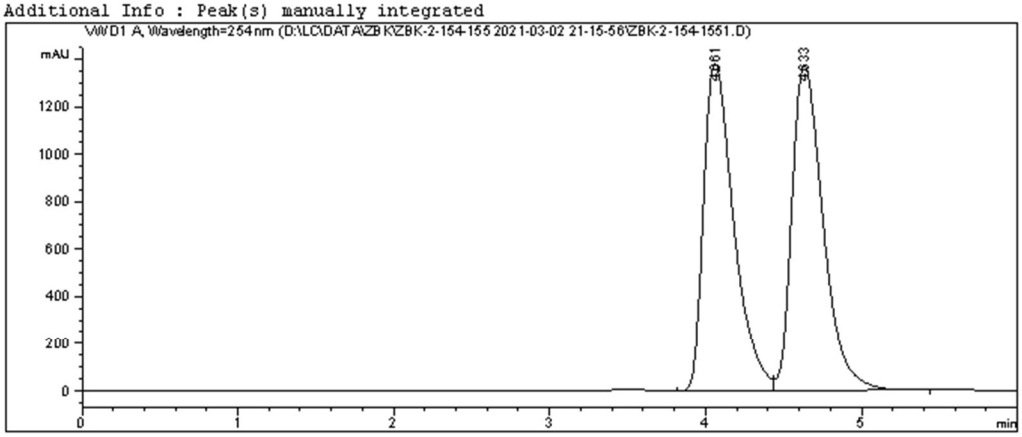
HPLC chromatogram of compound (*rac*)-3i



(1*S*,3*R*,4*R*)-**3i**

Data File D:\LC\DATA\ZBK\ZBK-2-154-155 2021-03-02 21-15-56\ZBK-2-154-1551.D
Sample Name: ZBK-2-155

```
======================================================================
Acq. Operator   : 采统                          Seq. Line :   2
Sample Operator : 采统
Acq. Instrument : 1200                            Location :   42
Injection Date  : 3/2/2021 9:23:15 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-154-155 2021-03-02 21-15-56\P1-AD-H-95-5-254NM-1ML-5ul
                  -30min.M
Last changed    : 3/2/2021 9:35:47 PM by 采统
                  (modified after loading)
Analysis Method : D:\LC\DATA\ZBK\ZBK-2-154-155 2021-03-02 21-15-56\P1-AD-H-95-5-254NM-1ML-5ul
                  -30min.M (Sequence Method)
Last changed    : 7/28/2021 8:04:57 PM by 采统
                  (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: VWD1 A, Wavelength=254 nm

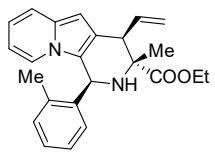
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.061 BV    0.2065 1.86251e4  1383.81360  49.3073
   2   4.633 VV R  0.2163 1.91485e4  1374.99561  50.6927

Totals :                  3.77736e4  2758.80920


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

1200 7/28/2021 8:05:02 PM 采统                                Page 1 of 1
```

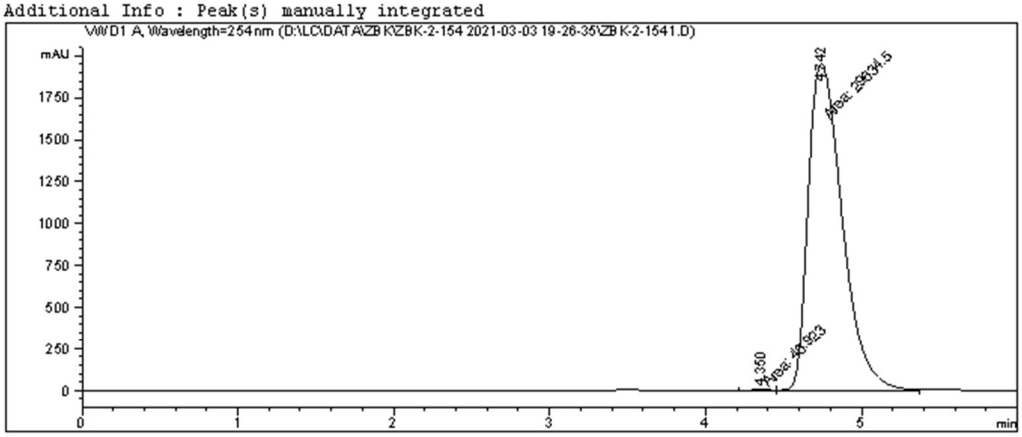
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3i



(1*S*,3*R*,4*R*)-**3i**

Data File D:\LC\DATA\ZBK\ZBK-2-154 2021-03-03 19-26-35\ZBK-2-1541.D
Sample Name: ZBK-2-154

```
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   61
Injection Date  : 3/3/2021 7:38:54 PM                 Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-154 2021-03-03 19-26-35\P1-AD-H-95-5-254NM-1ML-5ul-
                  30min.M
Last changed    : 3/3/2021 8:04:55 PM by 系统
                  (modified after loading)
Analysis Method : D:\LC\DATA\ZBK\ZBK-2-154 2021-03-03 19-26-35\P1-AD-H-95-5-254NM-1ML-5ul-
                  30min.M (Sequence Method)
Last changed    : 7/28/2021 8:09:07 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

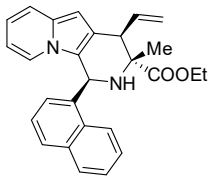
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.350 MM    0.1595   46.92297    4.90182   0.1581
   2   4.742 MM    0.2530 2.96345e4  1952.32861  99.8419

Totals :                  2.96814e4  1957.23044


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

1200 7/28/2021 8:09:10 PM 系统                          Page 1 of 1
```

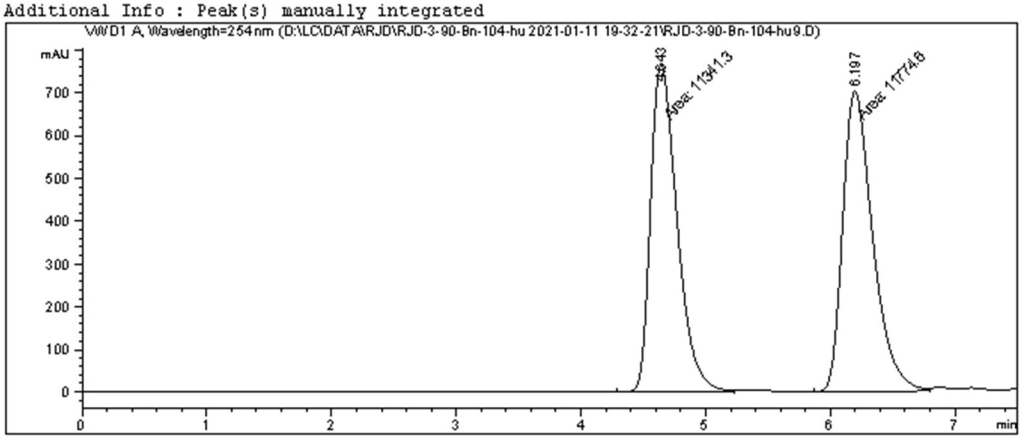
HPLC chromatogram of compound (*rac*)-3j



(1*S*,3*R*,4*R*)-**3j**

Data File D:\LC\DATA\RJD\RJD-3-90-Bn-104-hu 2021-01-11 19-32-21\RJD-3-90-Bn-104-hu9.D
Sample Name: ZBK-2-143S

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :  10
Sample Operator : 系统
Acq. Instrument : 1200                           Location :  41
Injection Date  : 1/11/2021 11:14:11 PM             Inj :  1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\RJD\RJD-3-90-Bn-104-hu 2021-01-11 19-32-21\P1-AD-H-95-5-254NM-
                  1ML-5UL-40MIN.M
Last changed    : 1/5/2021 5:23:59 PM by 系统
Analysis Method : D:\LC\DATA\RJD\RJD-3-90-Bn-104-hu 2021-01-11 19-32-21\P1-AD-H-95-5-254NM-
                  1ML-5UL-40MIN.M (Sequence Method)
Last changed    : 7/28/2021 7:48:56 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

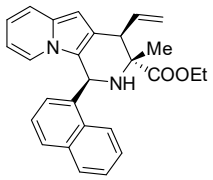
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.643 MF    0.2459 1.13413e4   768.53619  49.0627
   2   6.197 MF    0.2787 1.17746e4   704.12799  50.9373

Totals :                  2.31159e4  1472.66418

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

1200 7/28/2021 7:49:01 PM 系统 Page 1 of 1

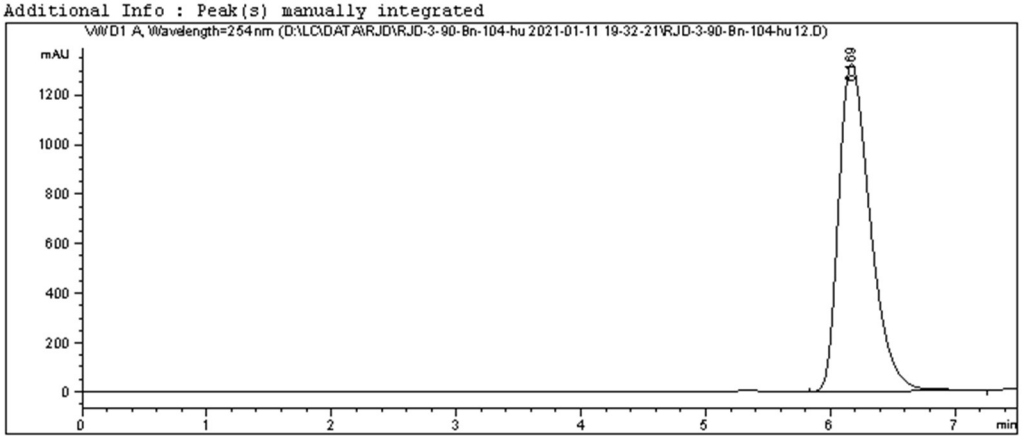
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3j



(1*S*,3*R*,4*R*)-**3j**

Data File D:\LC\DATA\RJD\RJD-3-90-Bn-104-hu 2021-01-11 19-32-21\RJD-3-90-Bn-104-hu12.D
Sample Name: ZBK-2-142

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :  13
Sample Operator : 系统
Acq. Instrument : 1200                            Location :   43
Injection Date  : 1/12/2021 12:47:40 AM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\RJD\RJD-3-90-Bn-104-hu 2021-01-11 19-32-21\P1-AD-H-95-5-254NM-
                  1ML-5UL-40MIN.M
Last changed    : 1/5/2021 5:23:59 PM by 系统
Analysis Method : D:\LC\DATA\RJD\RJD-3-90-Bn-104-hu 2021-01-11 19-32-21\P1-AD-H-95-5-254NM-
                  1ML-5UL-40MIN.M (Sequence Method)
Last changed    : 7/28/2021 7:47:07 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

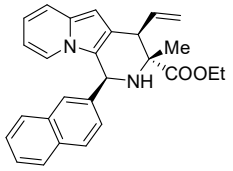
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.169 BV R  0.2724 2.34652e4  1326.30554 100.0000

Totals :                  2.34652e4  1326.30554


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

1200 7/28/2021 7:47:12 PM 系统 Page 1 of 1

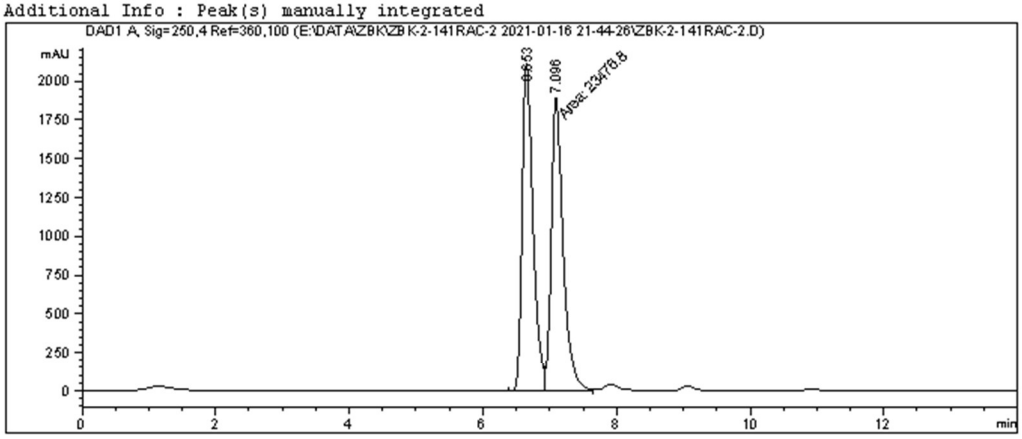
HPLC chromatogram of compound (*rac*)-3k



(1*S*,3*R*,4*R*)-**3k**

Data File E:\DATA\ZBK\ZBK-2-141RAC-2 2021-01-16 21-44-26\ZBK-2-141RAC-2.D
Sample Name: ZBK-2-141RAC

```
==================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   1
Acq. Instrument : 1260                          Location :   31
Injection Date  : 1/16/2021 9:45:56 PM              Inj :   1
                                               Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-141RAC-2 2021-01-16 21-44-26\4-IE--95-5-1ML-20MIN-5UL-
                  254NM-DAD.M
Last changed    : 1/16/2021 9:57:24 PM by SYSTEM
                  (modified after loading)
Analysis Method : E:\DATA\ZBK\ZBK-2-141RAC-2 2021-01-16 21-44-26\4-IE--95-5-1ML-20MIN-5UL-
                  254NM-DAD.M (Sequence Method)
Last changed    : 7/29/2021 3:15:33 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

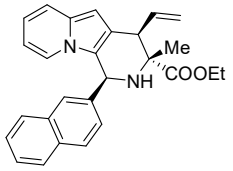

Signal 1: DAD1 A, Sig=250,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.653 BV    0.1727 2.40373e4  2113.82666  50.5897
   2   7.096 MF    0.2064 2.34768e4  1896.09497  49.4103

Totals :                  4.75141e4  4009.92163


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

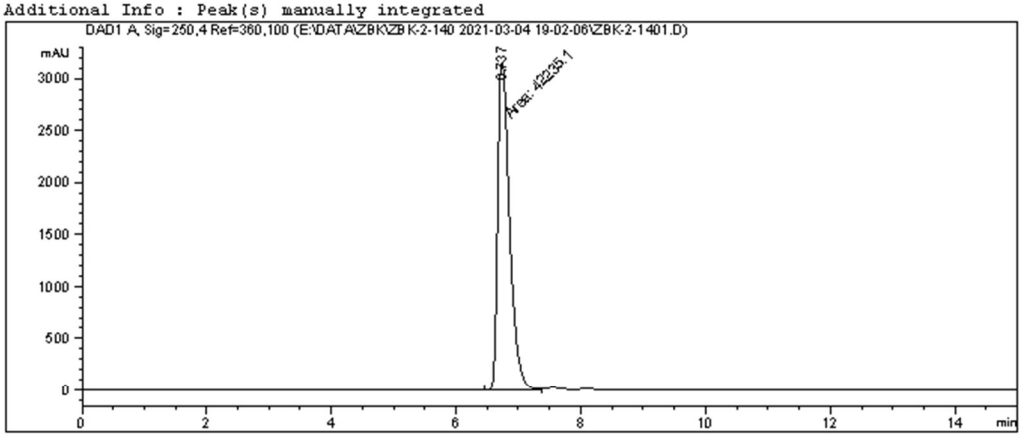
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3k



(1*S*,3*R*,4*R*)-**3k**

Data File E:\DATA\ZBK\ZBK-2-140 2021-03-04 19-02-06\ZBK-2-1401.D
Sample Name: ZBK-2-140

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : 1260                           Location :   63
Injection Date  : 3/4/2021 7:15:06 PM                Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-140 2021-03-04 19-02-06\4-IE--95-5-1ML-20MIN-5UL-254NM-
                  DAD.M
Last changed    : 3/4/2021 7:02:06 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-2-140 2021-03-04 19-02-06\4-IE--95-5-1ML-20MIN-5UL-254NM-
                  DAD.M (Sequence Method)
Last changed    : 7/29/2021 3:19:20 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




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

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


Signal 1: DAD1 A, Sig=250,4 Ref=360,100

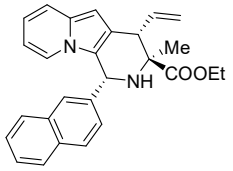
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.737 MF    0.2229 4.22351e4  3157.52173 100.0000

Totals :                  4.22351e4  3157.52173

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

1260 7/29/2021 3:19:23 PM SYSTEM

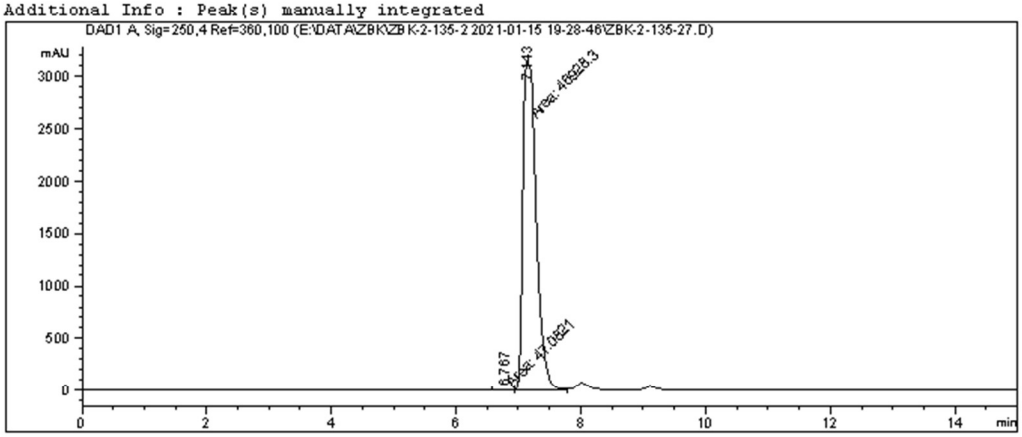
HPLC chromatogram of compound (1*R*,3*S*,4*S*)-3k



(1*R*,3*S*,4*S*)-**3k**

Data File E:\DATA\ZBK\ZBK-2-135-2 2021-01-15 19-28-46\ZBK-2-135-27.D
Sample Name: ZBK-2-140S,Sp

```
=====================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   8
Acq. Instrument : 1260                           Location :   44
Injection Date  : 1/15/2021 9:40:30 PM               Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-135-2 2021-01-15 19-28-46\4-IE--95-5-1ML-20MIN-5UL-254NM-
                  DAD.M
Last changed    : 1/15/2021 8:37:56 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-2-135-2 2021-01-15 19-28-46\4-IE--95-5-1ML-20MIN-5UL-254NM-
                  DAD.M (Sequence Method)
Last changed    : 7/29/2021 3:30:53 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




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

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

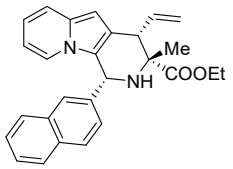

Signal 1: DAD1 A, Sig=250,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.767 MF    0.1821   47.08208    4.30997   0.1002
   2   7.143 FM    0.2495 4.69283e4  3134.67456  99.8998

Totals :                  4.69754e4  3138.98453

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

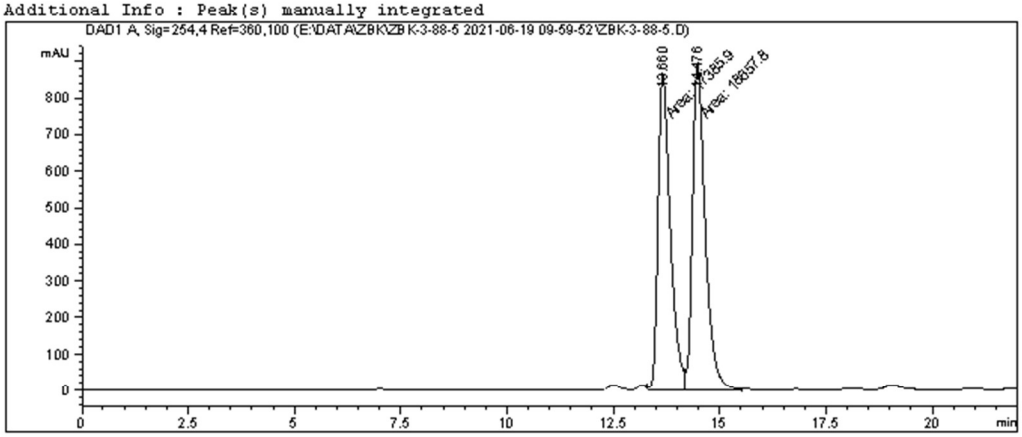
HPLC chromatogram of compound (*rac*)-3k



(1*R*,3*R*,4*S*)-**3k**

Data File E:\DATA\ZBK\ZBK-3-88-5 2021-06-19 09-59-52\ZBK-3-88-5.D
Sample Name: ZBK-3-88RAC

```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   1
Acq. Instrument : 1260                          Location :   72
Injection Date  : 6/19/2021 10:01:11 AM             Inj :   1
                                               Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-3-88-5 2021-06-19 09-59-52\IE-95-5-254NM-0.5ML-40MIN.M
Last changed    : 6/19/2021 10:01:21 AM by SYSTEM
                  (modified after loading)
Analysis Method : E:\DATA\ZBK\ZBK-3-88-5 2021-06-19 09-59-52\IE-95-5-254NM-0.5ML-40MIN.M (
                  Sequence Method)
Last changed    : 7/29/2021 3:46:19 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




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

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

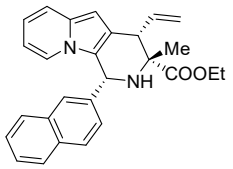

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.660 FM    0.3342 1.73859e4   866.98480  48.2357
   2  14.476 MF    0.3470 1.86578e4   896.11237  51.7643

Totals :                 3.60437e4  1763.09717

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

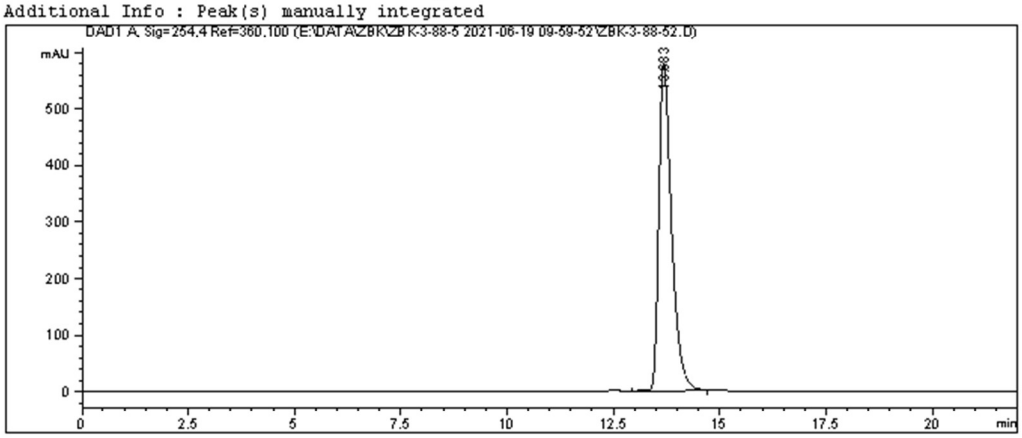
HPLC chromatogram of compound (1*R*,3*R*,4*S*)-3k



(1*R*,3*R*,4*S*)-**3k**

Data File E:\DATA\ZBK\ZBK-3-88-5 2021-06-19 09-59-52\ZBK-3-88-52.D
Sample Name: ZBK-3-88R/S

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Acq. Instrument : 1260                           Location :   51
Injection Date  : 6/19/2021 10:50:03 AM              Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-3-88-5 2021-06-19 09-59-52\IE-95-5-254NM-0.5ML-40MIN.M
Last changed    : 6/19/2021 10:01:21 AM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-3-88-5 2021-06-19 09-59-52\IE-95-5-254NM-0.5ML-40MIN.M (
                  Sequence Method)
Last changed    : 7/29/2021 3:48:07 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

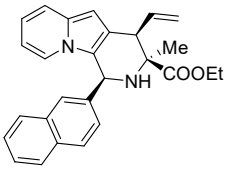

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|-------|
   1  13.683 VB R  0.3197 1.22386e4   579.28882 100.0000

Totals :                  1.22386e4   579.28882

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

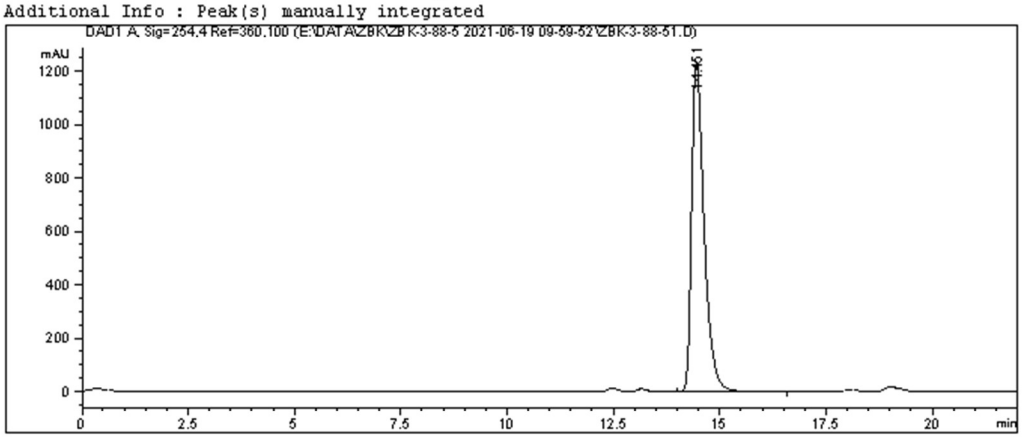
HPLC chromatogram of compound (1*S*,3*S*,4*R*)-3k



(1*S*,3*S*,4*R*)-**3k**

Data File E:\DATA\ZBK\ZBK-3-88-5 2021-06-19 09-59-52\ZBK-3-88-51.D
Sample Name: ZBK-3-88S/R

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : 1260                           Location :   52
Injection Date  : 6/19/2021 10:25:35 AM              Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-3-88-5 2021-06-19 09-59-52\IE-95-5-254NM-0.5ML-40MIN.M
Last changed    : 6/19/2021 10:01:21 AM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-3-88-5 2021-06-19 09-59-52\IE-95-5-254NM-0.5ML-40MIN.M (
                  Sequence Method)
Last changed    : 7/29/2021 3:48:07 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

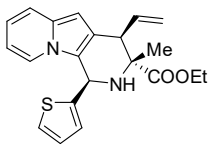

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|-------|
   1  14.451 BB    0.3092 2.52099e4  1229.79907 100.0000

Totals :                  2.52099e4  1229.79907

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

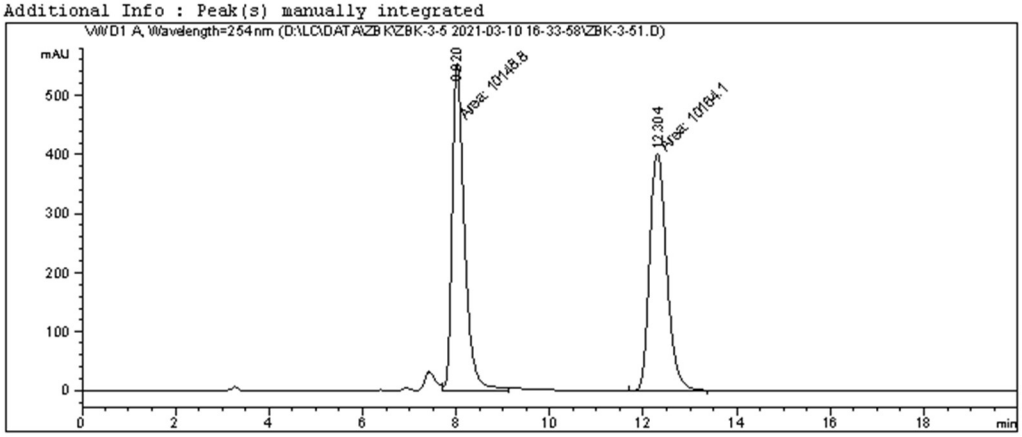
HPLC chromatogram of compound (*rac*)-3l



(1*S*,3*R*,4*R*)-**3l**

Data File D:\LC\DATA\ZBK\ZBK-3-5 2021-03-10 16-33-58\ZBK-3-51.D
Sample Name: ZBK-3-5S

```
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                          Location :   1
Injection Date  : 3/10/2021 4:46:15 PM              Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-5 2021-03-10 16-33-58\P1-AD-H-95-5-254NM-1ML-5ul-30min
                  .M
Last changed    : 3/10/2021 5:02:20 PM by 系统
                  (modified after loading)
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-5 2021-03-10 16-33-58\P1-AD-H-95-5-254NM-1ML-5ul-30min
                  .M (Sequence Method)
Last changed    : 7/28/2021 8:13:00 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

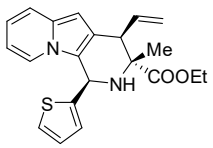
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.020 MM    0.3047 1.01488e4   555.21069  49.9624
   2  12.304 MF    0.4219 1.01641e4   401.52850  50.0376

Totals :                  2.03129e4   956.73920


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

1200 7/28/2021 8:13:04 PM 系统 Page 1 of 1

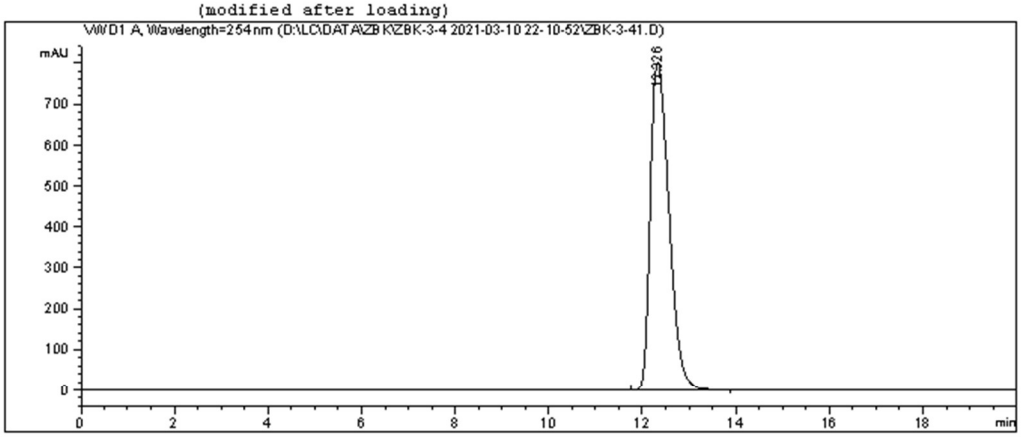
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3l



(1*S*,3*R*,4*R*)-**3l**

Data File D:\LC\DATA\ZBK\ZBK-3-4 2021-03-10 22-10-52\ZBK-3-41.D
Sample Name: ZBK-3-4

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                            Location :   4
Injection Date  : 3/10/2021 10:23:10 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-4 2021-03-10 22-10-52\P1-AD-H-95-5-254NM-1ML-5ul-30min
                  .M
Last changed    : 12/29/2020 2:58:55 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-4 2021-03-10 22-10-52\P1-AD-H-95-5-254NM-1ML-5ul-30min
                  .M (Sequence Method)
Last changed    : 7/28/2021 8:15:04 PM by 系统
                  (modified after loading)
```




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

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


Signal 1: VWD1 A, Wavelength=254 nm

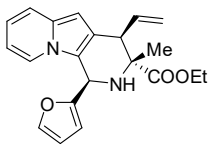
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.326 BB    0.4431 2.22550e4   802.03363 100.0000

Totals :                  2.22550e4   802.03363

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

1200 7/28/2021 8:15:08 PM 系统 Page 1 of 1

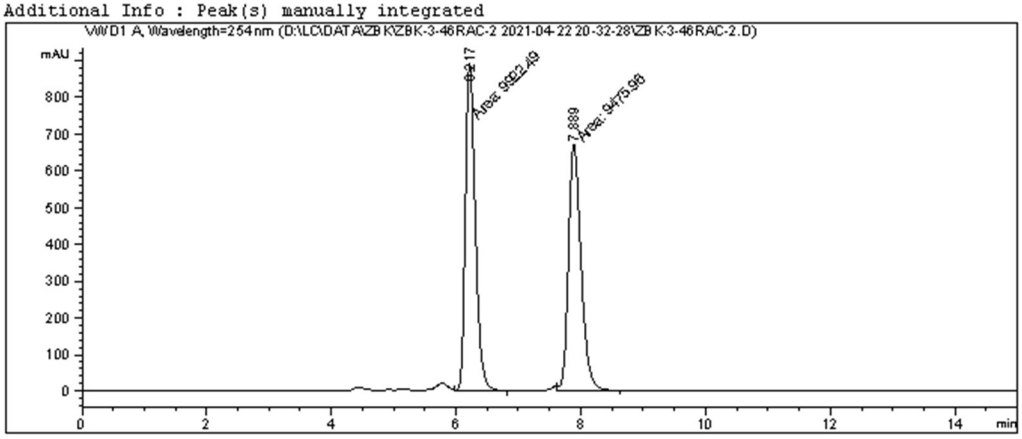
HPLC chromatogram of compound (*rac*)-3m



(1*S*,3*R*,4*R*)-**3m**

Data File D:\LC\DATA\ZBK\ZBK-3-46RAC-2 2021-04-22 20-32-28\ZBK-3-46RAC-2.D
Sample Name: ZBK-3-46RAC

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :   1
Sample Operator : 系统
Acq. Instrument : 1200                            Location :   73
Injection Date  : 4/22/2021 8:33:51 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-46RAC-2 2021-04-22 20-32-28\P1-AD-H-80-20-254NM-1ML-
                  5UL-20MIN.M
Last changed    : 1/14/2021 2:49:11 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-46RAC-2 2021-04-22 20-32-28\P1-AD-H-80-20-254NM-1ML-
                  5UL-20MIN.M (Sequence Method)
Last changed    : 7/28/2021 8:38:00 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

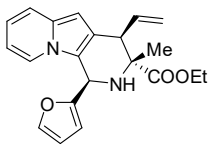
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.217 MM    0.1852 9922.48828  892.89410  51.1509
   2   7.889 MF    0.2354 9475.95898  670.79712  48.8491

Totals :                  1.93984e4  1563.69122

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

1200 7/28/2021 8:38:03 PM 系统                          Page 1 of 1
```

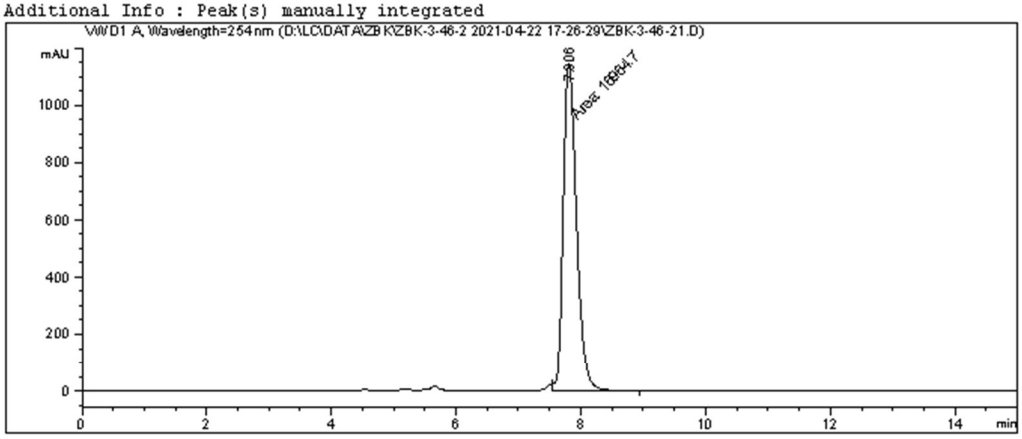
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3m



(1*S*,3*R*,4*R*)-**3m**

Data File D:\LC\DATA\ZBK\ZBK-3-46-2 2021-04-22 17-26-29\ZBK-3-46-21.D
Sample Name: ZBK-3-46R-2

```
==================================================================
Acq. Operator   : 采统                          Seq. Line :   2
Sample Operator : 采统
Acq. Instrument : 1200                            Location :   73
Injection Date  : 4/22/2021 5:38:36 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-46-2 2021-04-22 17-26-29\Pl-AD-H-80-20-254NM-1ML-5UL-
                  20MIN.M
Last changed    : 1/14/2021 2:49:11 PM by 采统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-46-2 2021-04-22 17-26-29\Pl-AD-H-80-20-254NM-1ML-5UL-
                  20MIN.M (Sequence Method)
Last changed    : 7/28/2021 8:41:07 PM by 采统
                  (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

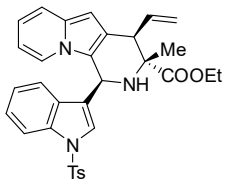

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.806 FM    0.2469 1.69647e4  1145.33398 100.0000

Totals :                  1.69647e4  1145.33398

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

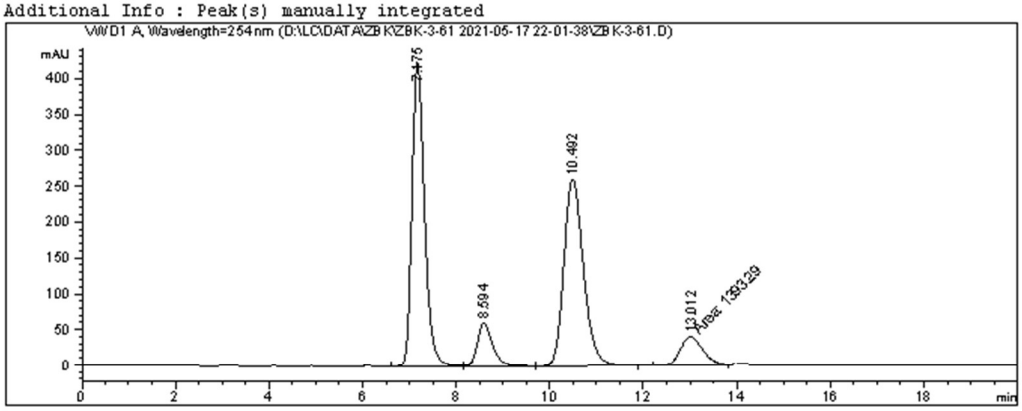
HPLC chromatogram of compound (*rac*)-3n



(1*S*,3*R*,4*R*)-**3n**

Data File D:\LC\DATA\ZBK\ZBK-3-61 2021-05-17 22-01-38\ZBK-3-61.D
Sample Name: ZBK-3-61RAC

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :   1
Sample Operator : 系统
Acq. Instrument : 1200                            Location :   23
Injection Date  : 5/17/2021 10:02:53 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-61 2021-05-17 22-01-38\P1-80-20-254NM-1ML-5ul-45min.M
Last changed    : 5/17/2021 10:24:39 PM by 系统
                  (modified after loading)
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-61 2021-05-17 22-01-38\P1-80-20-254NM-1ML-5ul-45min.M
                  (Sequence Method)
Last changed    : 7/28/2021 8:57:35 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

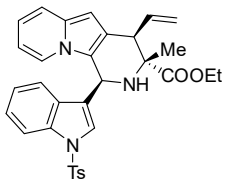
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.175 BV    0.2840 7830.61865  423.75073  43.1738
   2   8.594 VV R  0.3400 1339.46570   60.12615   7.3851
   3  10.492 VV R  0.4478 7574.04102  260.99268  41.7592
   4  13.012 MF    0.5674 1393.29395   40.92601   7.6819

Totals :                  1.81374e4   785.79556


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

1200 7/28/2021 8:57:37 PM 系统                          Page 1 of 1
```

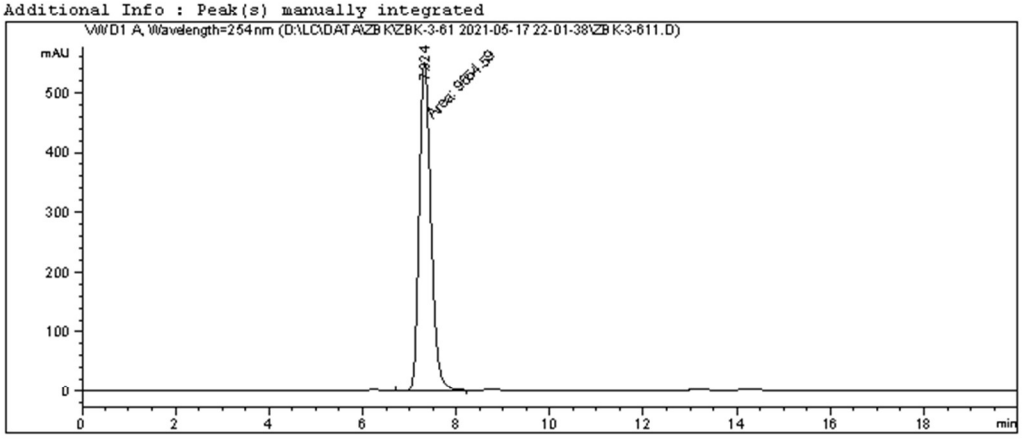
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3n



(1*S*,3*R*,4*R*)-**3n**

Data File D:\LC\DATA\ZBK\ZBK-3-61 2021-05-17 22-01-38\ZBK-3-611.D
Sample Name: ZBK-3-610PT

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                            Location :   11
Injection Date  : 5/17/2021 10:26:06 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-61 2021-05-17 22-01-38\P1-80-20-254NM-1ML-5ul-45min.M
Last changed    : 5/17/2021 10:24:39 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-61 2021-05-17 22-01-38\P1-80-20-254NM-1ML-5ul-45min.M
                  (Sequence Method)
Last changed    : 7/28/2021 9:00:10 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

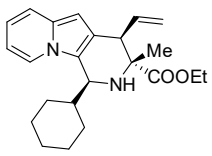
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.324 MF    0.2928 9654.58984  549.59149 100.0000

Totals :                  9654.58984  549.59149


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

1200 7/28/2021 9:00:13 PM 系统 Page 1 of 1

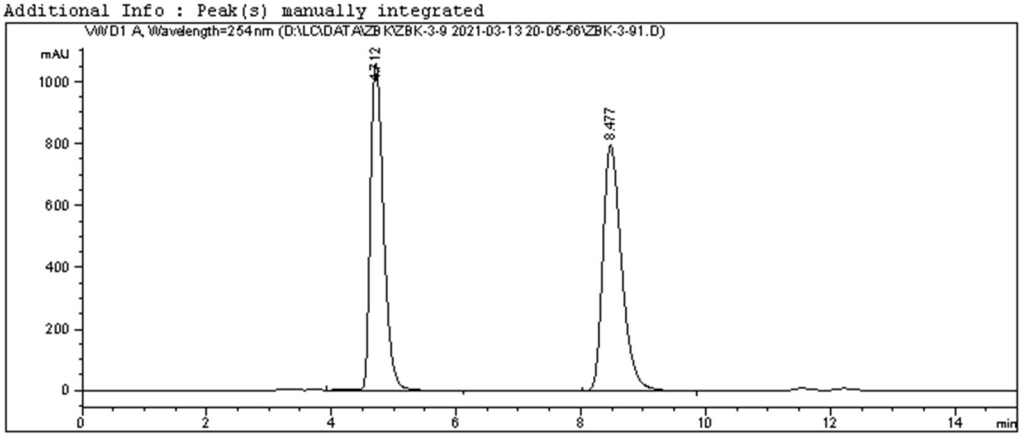
HPLC chromatogram of compound (*rac*)-3o



(1*S*,3*R*,4*R*)-**3o**

Data File D:\LC\DATA\ZBK\ZBK-3-9 2021-03-13 20-05-56\ZBK-3-91.D
Sample Name: ZBK-3-9

```
======================================================================
Acq. Operator   : 采统                          Seq. Line :   2
Sample Operator : 采统
Acq. Instrument : 1200                            Location :   3
Injection Date  : 3/13/2021 8:18:20 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-9 2021-03-13 20-05-56\P1-AD-H-95-5-254NM-1ML-5ul-30min
                  .M
Last changed    : 3/13/2021 8:31:18 PM by 采统
                  (modified after loading)
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-9 2021-03-13 20-05-56\P1-AD-H-95-5-254NM-1ML-5ul-30min
                  .M (Sequence Method)
Last changed    : 7/28/2021 8:17:20 PM by 采统
                  (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: VWD1 A, Wavelength=254 nm

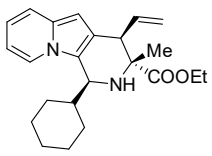
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.712 VV R  0.2261 1.53917e4  1058.06335  48.1640
   2   8.477 BB    0.3200 1.65652e4   795.85736  51.8360

Totals :                  3.19569e4  1853.92072


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

1200 7/28/2021 8:17:22 PM 采统                          Page 1 of 1
```

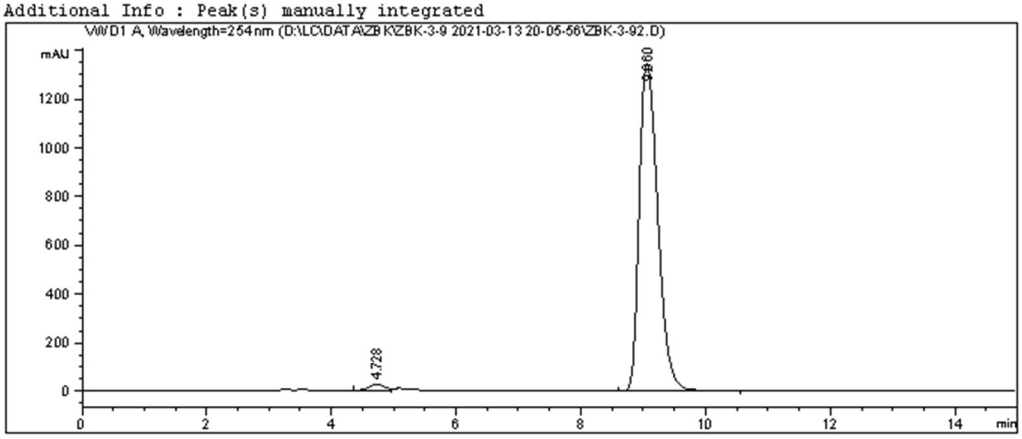
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3o



(1*S*,3*R*,4*R*)-**3o**

Data File D:\LC\DATA\ZBK\ZBK-3-9 2021-03-13 20-05-56\ZBK-3-92.D
Sample Name: ZBK-3-8

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :   3
Sample Operator : 系统
Acq. Instrument : 1200                            Location :   4
Injection Date  : 3/13/2021 8:34:35 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-9 2021-03-13 20-05-56\P1-AD-H-95-5-254NM-1ML-5ul-30min
                  .M
Last changed    : 3/13/2021 8:31:18 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-9 2021-03-13 20-05-56\P1-AD-H-95-5-254NM-1ML-5ul-30min
                  .M (Sequence Method)
Last changed    : 7/28/2021 8:21:32 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

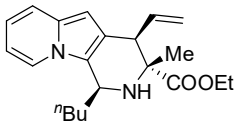
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.728 BV    0.2794  440.95612   24.54942   1.5645
   2   9.060 BV R  0.3251 2.77437e4  1344.77075  98.4355

Totals :                  2.81847e4  1369.32017


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

1200 7/28/2021 8:21:35 PM 系统                          Page 1 of 1
```

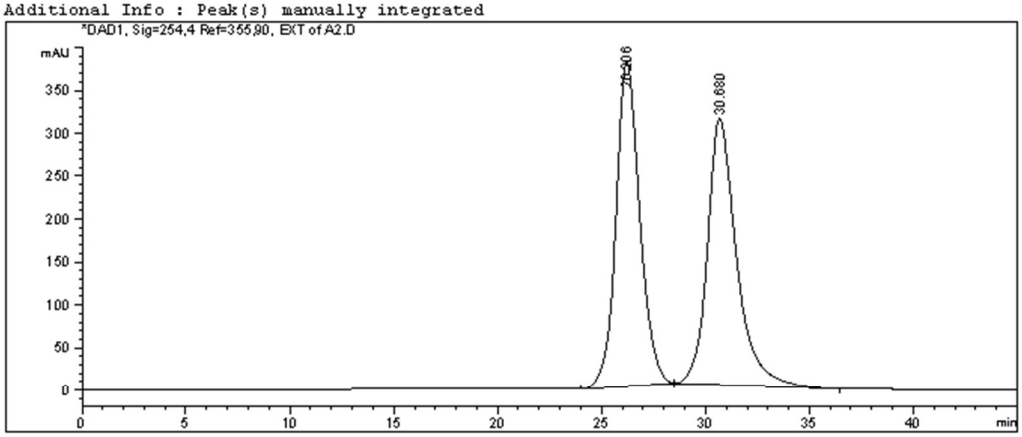
HPLC chromatogram of compound (*rac*)-3p



(1*S*,3*R*,4*R*)-**3p**

Data File D:\HPLC\DATA\20230215\A 2023-02-15 09-02-41\A2.D
Sample Name: ZBK-6-6RAC

```
==================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   3
Acq. Instrument : 1260                          Location :   21
Injection Date  : 2/15/2023 10:26:05 AM             Inj :   1
                                               Inj Volume : 5.000 µl
Acq. Method     : D:\HPLC\Data\20230215\A 2023-02-15 09-02-41\2-IA-99-1-0.3ML-5UL-70MIN-254NM
                  -DAD.M
Last changed    : 2/15/2023 9:02:42 AM by SYSTEM
Analysis Method : D:\HPLC\Data\20230215\A 2023-02-15 09-02-41\2-IA-99-1-0.3ML-5UL-70MIN-254NM
                  -DAD.M (Sequence Method)
Last changed    : 2/24/2023 6:53:46 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, Sig=254,4 Ref=355,90, EXT
 Signal has been modified after loading from rawdata file!

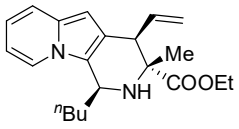
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  26.206 BB    1.1601 3.01921e4   377.88687  49.9061
   2  30.680 BB    1.3618 3.03058e4   310.74753  50.0939

Totals :                 6.04978e4   688.63440


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

1260 2/24/2023 6:53:49 PM SYSTEM                    Page 1 of 1
```

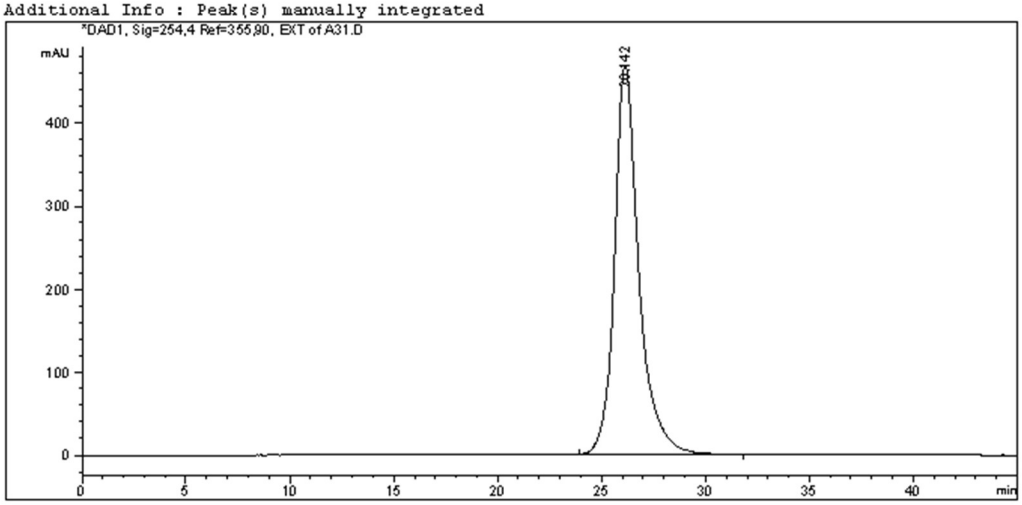
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3p



(1*S*,3*R*,4*R*)-**3p**

Data File D:\HPLC\DATA\20230223\A 2023-02-23 10-45-21\A31.D
Sample Name: ZBK-6-6R/R

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :  32
Acq. Instrument : 1260                           Location :  22
Injection Date  : 2/24/2023 4:10:23 AM               Inj :  2
                                                Inj Volume : 5.000 µl
Acq. Method     : D:\HPLC\Data\20230223\A 2023-02-23 10-45-21\2-IA-99-1-0.3ML-5UL-70MIN-254NM
                  -DAD.M
Last changed    : 2/23/2023 11:04:35 AM by SYSTEM
Analysis Method : D:\HPLC\Data\20230223\A 2023-02-23 10-45-21\2-IA-99-1-0.3ML-5UL-70MIN-254NM
                  -DAD.M (Sequence Method)
Last changed    : 2/24/2023 6:48:41 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, Sig=254,4 Ref=355,90, EXT
 Signal has been modified after loading from rawdata file!

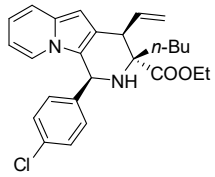
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  26.142 BB    1.1478 3.80922e4   467.91635 100.0000

Totals :                  3.80922e4   467.91635


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

1260 2/24/2023 6:48:44 PM SYSTEM                          Page 1 of 1
```

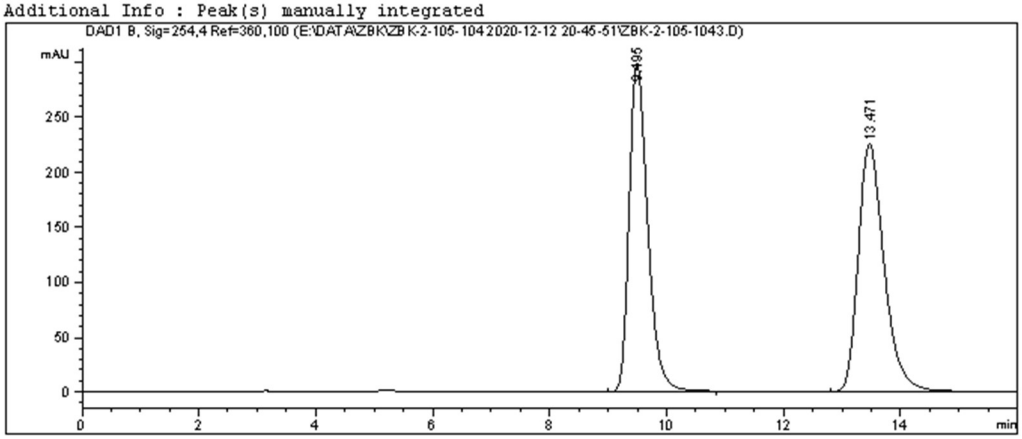
HPLC chromatogram of compound (*rac*)-3q



(1*S*,3*R*,4*R*)-**3q**

Data File E:\DATA\ZBK\ZBK-2-105-104 2020-12-12 20-45-51\ZBK-2-105-1043.D
Sample Name: ZBK-2-105X

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   4
Acq. Instrument : 1260                           Location :   43
Injection Date  : 12/12/2020 9:46:41 PM               Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-105-104 2020-12-12 20-45-51\2-AD-H-95-5-1ML--5UL-25MIN-
                  DAD.M
Last changed    : 12/12/2020 9:52:45 PM by SYSTEM
                  (modified after loading)
Analysis Method : E:\DATA\ZBK\ZBK-2-105-104 2020-12-12 20-45-51\2-AD-H-95-5-1ML--5UL-25MIN-
                  DAD.M (Sequence Method)
Last changed    : 7/29/2021 11:47:51 AM 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 B, Sig=254,4 Ref=360,100

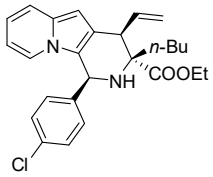
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.495 BB    0.3392 6575.32617  298.25720  48.5581
   2  13.471 BB    0.4723 6965.82080  225.58434  51.4419

Totals :                  1.354lle4   523.84154


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

1260 7/29/2021 11:48:07 AM SYSTEM                    Page 1 of 1
```

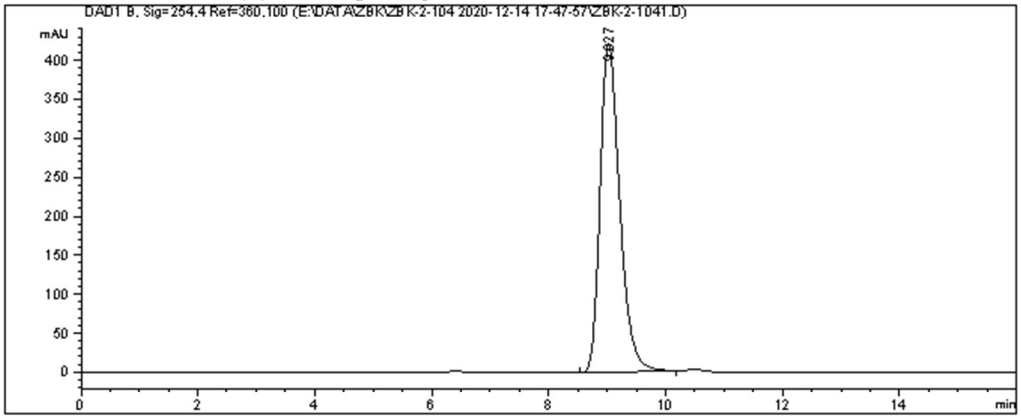
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3q



(1*S*,3*R*,4*R*)-**3q**

Data File E:\DATA\ZBK\ZBK-2-104 2020-12-14 17-47-57\ZBK-2-1041.D
Sample Name: ZBK-2-104-2

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : 1260                           Location :   11
Injection Date  : 12/14/2020 6:00:54 PM               Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-104 2020-12-14 17-47-57\2-AD-H-95-5-1ML--5UL-25MIN-DAD.M
Last changed    : 12/14/2020 5:47:58 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-2-104 2020-12-14 17-47-57\2-AD-H-95-5-1ML--5UL-25MIN-DAD.M
                  (Sequence Method)
Last changed    : 7/29/2021 11:51:04 AM 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

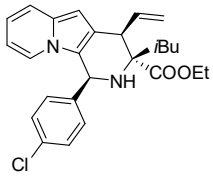

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.027 BB    0.3583 9831.44434  421.22473 100.0000

Totals :                  9831.44434  421.22473


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

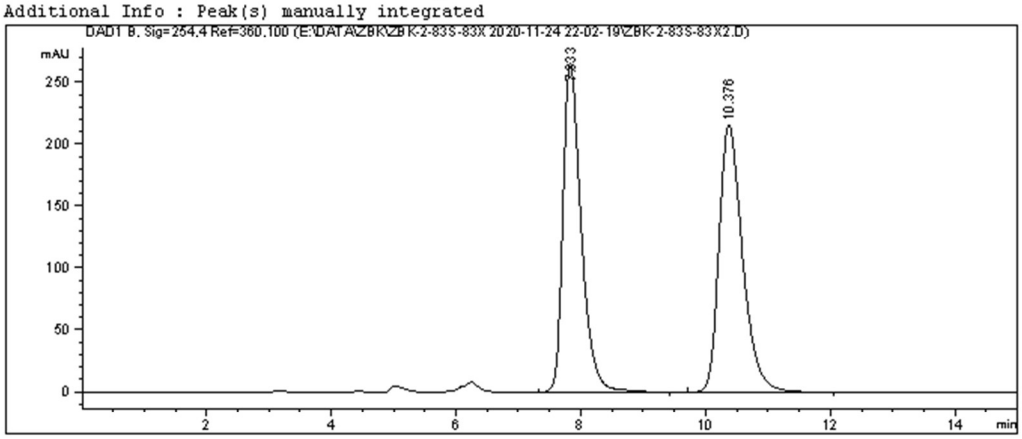
HPLC chromatogram of compound (*rac*)-3r



(1*S*,3*R*,4*R*)-**3r**

Data File E:\DATA\ZBK\ZBK-2-83S-83X 2020-11-24 22-02-19\ZBK-2-83S-83X2.D
Sample Name: ZBK-2-83X

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   3
Acq. Instrument : 1260                           Location :   52
Injection Date  : 11/24/2020 10:32:12 PM              Inj :   1
                                                Inj Volume : 10.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-83S-83X 2020-11-24 22-02-19\AD-H-5-95-1ML-25415MIN.M
Last changed    : 11/24/2020 10:02:19 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-2-83S-83X 2020-11-24 22-02-19\AD-H-5-95-1ML-25415MIN.M (
                  Sequence Method)
Last changed    : 7/28/2021 10:20:52 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




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

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

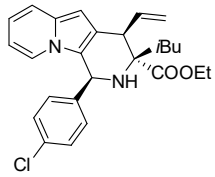

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.833 BB    0.3080 5418.37012  265.64490  48.8632
   2  10.376 BB    0.3998 5670.49414  216.32591  51.1368

Totals :                  1.10889e4   481.97081


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

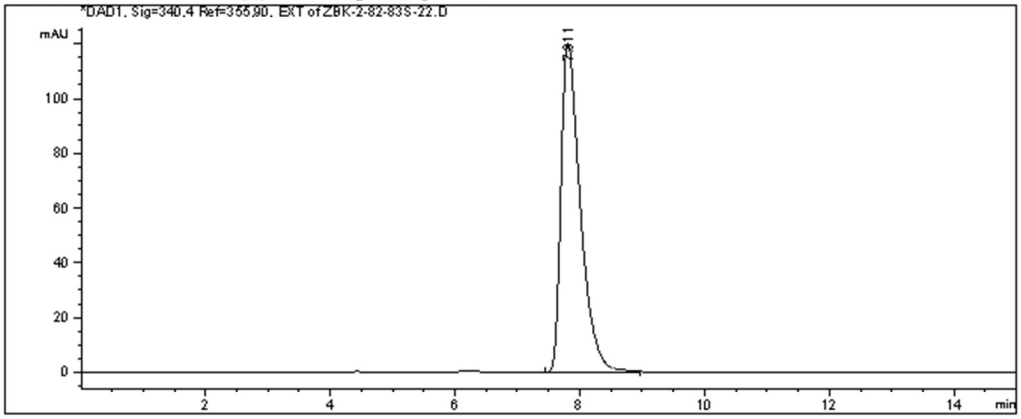
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3r



(1*S*,3*R*,4*R*)-**3r**

Data File E:\DATA\ZBK\ZBK-2-82-83S-2 2020-11-25 16-51-05\ZBK-2-82-83S-22.D
Sample Name: ZBK-2-82

```
    ======================================================================
    Acq. Operator   : SYSTEM                        Seq. Line :   3
    Acq. Instrument : 1260                           Location :   62
    Injection Date  : 11/25/2020 5:20:42 PM              Inj :   1
                                                  Inj Volume : 10.000 µl
    Acq. Method     : E:\DATA\ZBK\ZBK-2-82-83S-2 2020-11-25 16-51-05\AD-H-5-95-1ML-25415MIN.M
    Last changed    : 11/25/2020 4:51:05 PM by SYSTEM
    Analysis Method : E:\DATA\ZBK\ZBK-2-82-83S-2 2020-11-25 16-51-05\AD-H-5-95-1ML-25415MIN.M (
                      Sequence Method)
    Last changed    : 7/28/2021 10:25:56 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

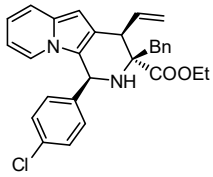

    Signal 1: DAD1, Sig=340,4 Ref=355,90, EXT
     Signal has been modified after loading from rawdata file!

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   7.811 BB    0.3289 2580.84229  119.99236 100.0000

    Totals :                   2580.84229  119.99236


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

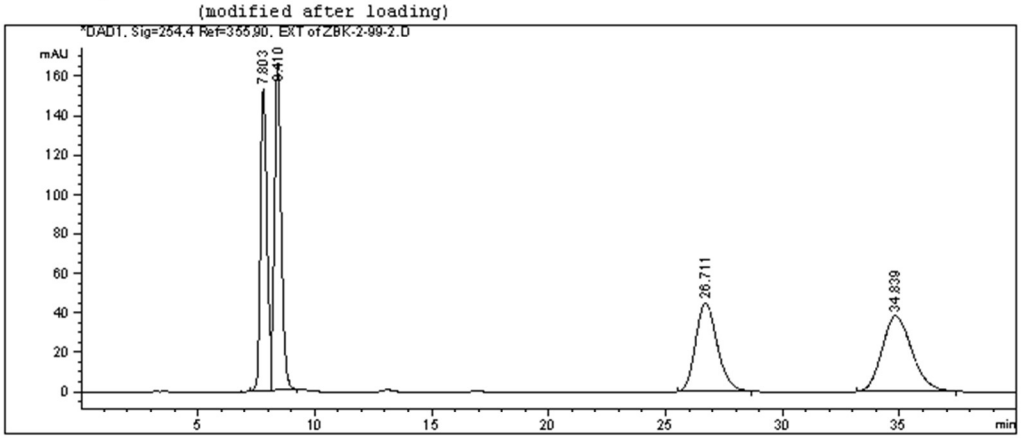
HPLC chromatogram of compound (*rac*)-3s



(1*S*,3*R*,4*R*)-**3s**

Data File E:\DATA\ZBK\ZBK-2-99-2 2020-12-09 20-17-09\ZBK-2-99-2.D
Sample Name: ZBK-2-99-2

```
=====================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   1
Acq. Instrument : 1260                           Location :   21
Injection Date  : 12/9/2020 8:18:42 PM               Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-99-2 2020-12-09 20-17-09\AD-H-95-5-254NM-1ML-5ul-40min-
                  DAD.M
Last changed    : 12/9/2020 8:17:09 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-2-99-2 2020-12-09 20-17-09\AD-H-95-5-254NM-1ML-5ul-40min-
                  DAD.M (Sequence Method)
Last changed    : 7/29/2021 11:33:58 AM by SYSTEM
                  (modified after loading)
```




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

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


Signal 1: DAD1, Sig=254,4 Ref=355,90, EXT
 Signal has been modified after loading from rawdata file!

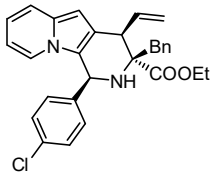
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.803 BV    0.2951 2954.52905  153.10089  23.3997
   2   8.410 VB    0.3126 3399.25610  165.48820  26.9219
   3  26.711 BB    0.7525 2878.74585   44.98803  22.7995
   4  34.839 BB    1.0347 3393.83472   38.45425  26.8790

Totals :                  1.26264e4   402.03138

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

1260 7/29/2021 11:34:00 AM SYSTEM                          Page 1 of 1
```

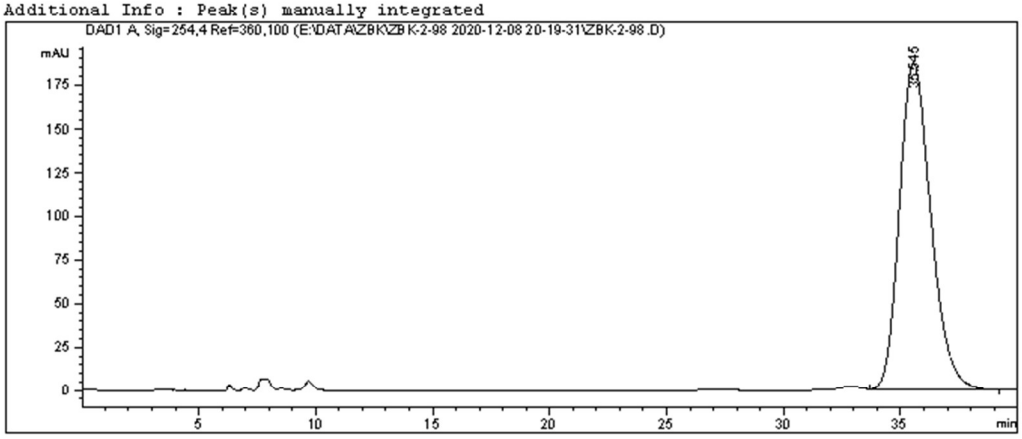
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3s



(1*S*,3*R*,4*R*)-**3s**

Data File E:\DATA\ZBK\ZBK-2-98 2020-12-08 20-19-31\ZBK-2-98.D
Sample Name: ZBK-2-98

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   1
Acq. Instrument : 1260                           Location :   11
Injection Date  : 12/8/2020 8:20:58 PM                Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-98 2020-12-08 20-19-31\AD-H-95-5-254NM-1ML-5ul-40min-DAD.
                  M
Last changed    : 12/8/2020 8:19:31 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-2-98 2020-12-08 20-19-31\AD-H-95-5-254NM-1ML-5ul-40min-DAD.
                  M (Sequence Method)
Last changed    : 8/19/2021 7:42:45 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=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  35.545 BB    1.1669 1.74810e4   186.95708 100.0000

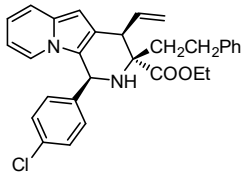
Totals :                  1.74810e4   186.95708


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

1260 8/19/2021 7:42:48 PM SYSTEM

Page 1 of 1

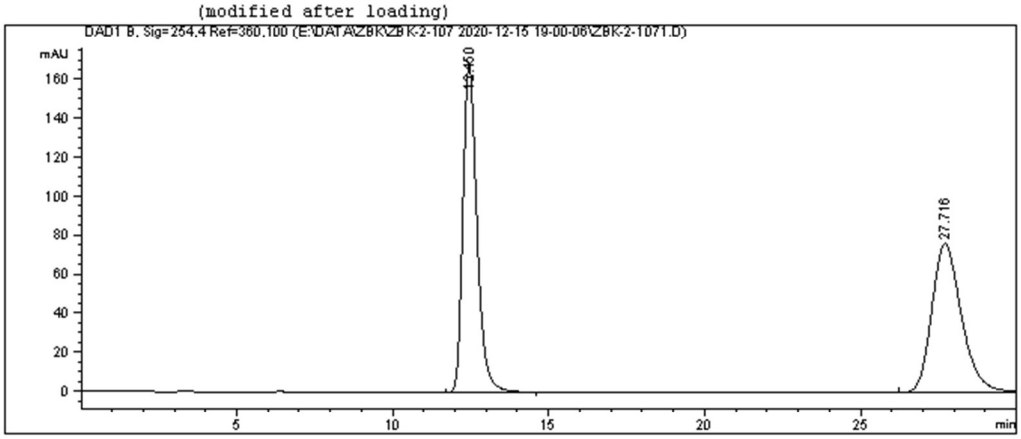
HPLC chromatogram of compound (*rac*)-3t



(1*S*,3*R*,4*R*)-**3t**

Data File E:\DATA\ZBK\ZBK-2-107 2020-12-15 19-00-06\ZBK-2-107l.D
Sample Name: ZBK-2-107S

```
==================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   2
Acq. Instrument : 1260                          Location :   41
Injection Date  : 12/15/2020 7:13:06 PM              Inj :   1
                                               Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-107 2020-12-15 19-00-06\2-AD-H-95-5-1ML--5UL-25MIN-DAD.M
Last changed    : 12/15/2020 7:27:47 PM by SYSTEM
                  (modified after loading)
Analysis Method : E:\DATA\ZBK\ZBK-2-107 2020-12-15 19-00-06\2-AD-H-95-5-1ML--5UL-25MIN-DAD.M
                  (Sequence Method)
Last changed    : 7/29/2021 11:53:14 AM by SYSTEM
                  (modified after loading)
```




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

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

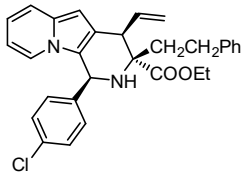

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.450 BB    0.4756 5252.69824  168.52895  51.3633
   2  27.716 BBA   0.9733 4973.86279   76.02758  48.6367

Totals :                  1.02266e4   244.55653


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

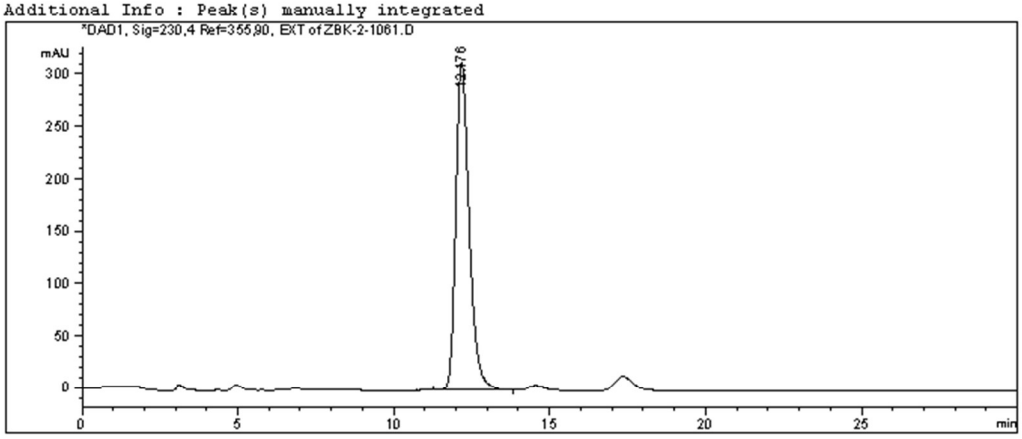
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3t



(1*S*,3*R*,4*R*)-**3t**

Data File E:\DATA\ZBK\ZBK-2-106 2020-12-17 20-51-38\ZBK-2-1061.D
Sample Name: ZBK-2-106

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : 1260                           Location :   61
Injection Date  : 12/17/2020 9:04:35 PM              Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-106 2020-12-17 20-51-38\AD-H-95-5-254NM-1ML-5ul-40min-DAD
                  .M
Last changed    : 12/17/2020 8:51:39 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-2-106 2020-12-17 20-51-38\AD-H-95-5-254NM-1ML-5ul-40min-DAD
                  .M (Sequence Method)
Last changed    : 7/29/2021 11:55:57 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




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

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

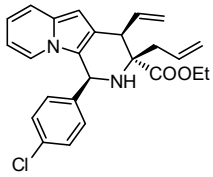

Signal 1: DAD1, Sig=230,4 Ref=355,90, EXT
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  12.176 BB    0.4614 9460.74805  313.21091 100.0000

Totals :                  9460.74805  313.21091


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

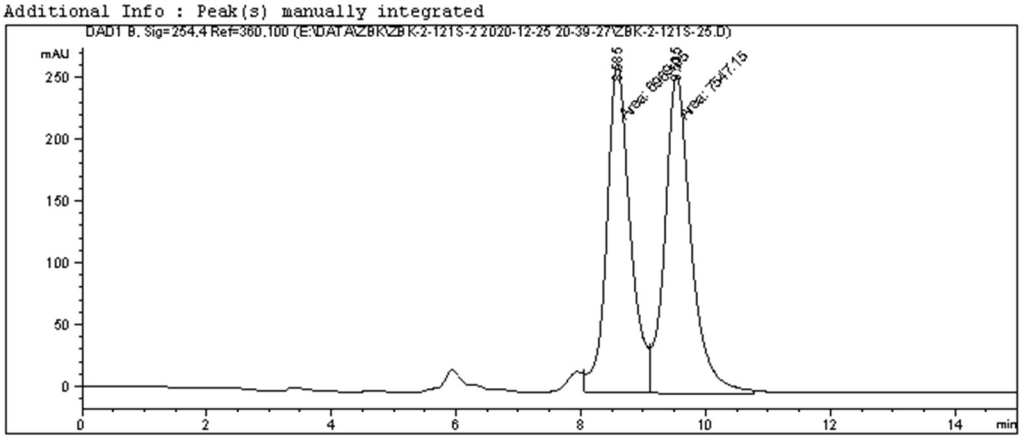
HPLC chromatogram of compound (*rac*)-3u



(1*S*,3*R*,4*R*)-**3u**

Data File E:\DATA\ZBK\ZBK-2-121S-2 2020-12-25 20-39-27\ZBK-2-121S-25.D
Sample Name: ZBK-2-121S

```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   6
Acq. Instrument : 1260                          Location :   43
Injection Date  : 12/25/2020 9:46:41 PM             Inj :   1
                                               Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-121S-2 2020-12-25 20-39-27\2-IA-95-5-1ML-5UL-20MIN-ALL.M
Last changed    : 12/25/2020 8:39:28 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-2-121S-2 2020-12-25 20-39-27\2-IA-95-5-1ML-5UL-20MIN-ALL.M
                  (Sequence Method)
Last changed    : 8/19/2021 8:47:25 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




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

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

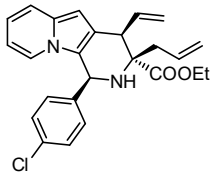

Signal 1: DAD1 B, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.585 FM    0.4364 6969.94824  266.21698  48.0120
   2   9.535 FM    0.4888 7547.15088  257.35364  51.9880

Totals :                  1.45171e4   523.57062


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

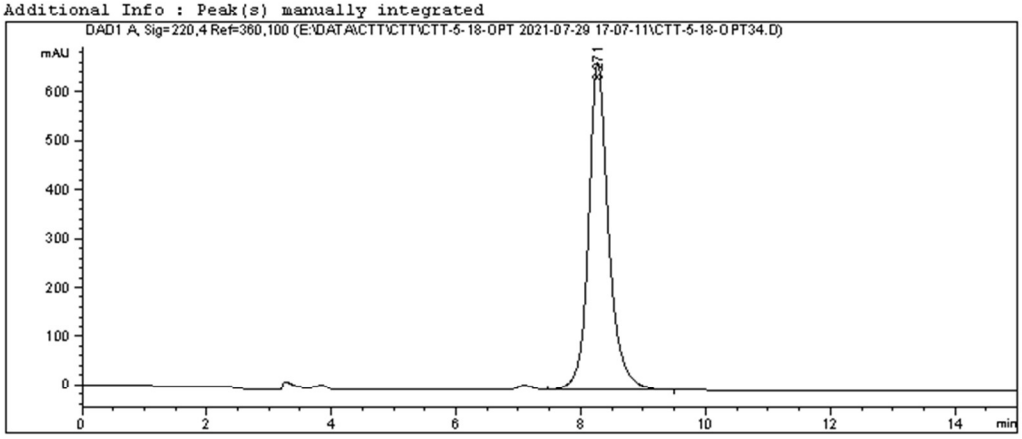
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3u



(1*S*,3*R*,4*R*)-**3u**

```
Data File E:\DATA\CTT\CTT\CTT-5-18-OPT 2021-07-29 17-07-11\CTT-5-18-OPT34.D
Sample Name: ZBK-2-120

    ======================================================================
    Acq. Operator   : SYSTEM                          Seq. Line :  35
    Acq. Instrument : 1260                            Location :   6
    Injection Date  : 7/30/2021 11:48:52 AM                Inj :   1
                                                    Inj Volume : 5.000 µl
    Acq. Method     : E:\DATA\CTT\CTT\CTT-5-18-OPT 2021-07-29 17-07-11\2-IA-95-5-1ML-5UL-20MIN-
                      ALL.M
    Last changed    : 7/29/2021 10:23:58 PM by SYSTEM
    Analysis Method : E:\DATA\CTT\CTT\CTT-5-18-OPT 2021-07-29 17-07-11\2-IA-95-5-1ML-5UL-20MIN-
                      ALL.M (Sequence Method)
    Last changed    : 8/19/2021 8:37:39 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=220,4 Ref=360,100

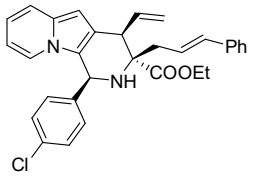
    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   8.271 BB    0.3326 1.49649e4   669.97913 100.0000

    Totals :                  1.49649e4   669.97913


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


1260 8/19/2021 8:37:42 PM SYSTEM                          Page 1 of 1
```

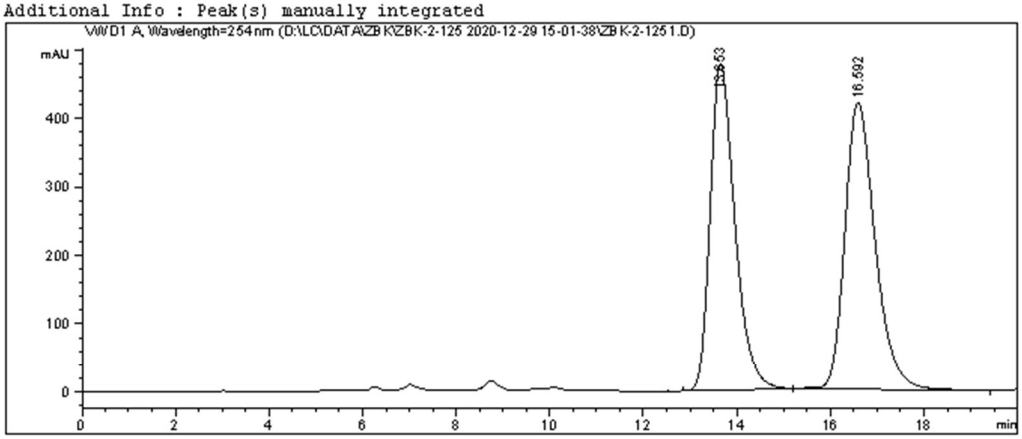
HPLC chromatogram of compound (*rac*)-3v



(1*S*,3*R*,4*R*)-**3v**

Data File D:\LC\DATA\ZBK\ZBK-2-125 2020-12-29 15-01-38\ZBK-2-125l.D
Sample Name: ZBK-2-125S

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   31
Injection Date  : 12/29/2020 3:19:35 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-125 2020-12-29 15-01-38\P1-AD-H-95-5-254NM-1ML-5ul-
                  30min.M
Last changed    : 12/29/2020 2:58:55 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-2-125 2020-12-29 15-01-38\P1-AD-H-95-5-254NM-1ML-5ul-
                  30min.M (Sequence Method)
Last changed    : 7/28/2021 4:59:59 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

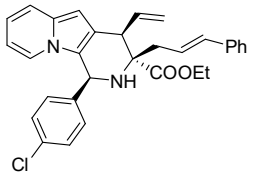
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  13.653 BB    0.5604 1.75939e4   478.04611  48.2078
   2  16.592 VV R  0.6912 1.89020e4   419.85510  51.7922

Totals :                  3.64959e4   897.90121

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

1200 7/28/2021 5:00:03 PM 系统                          Page 1 of 1
```

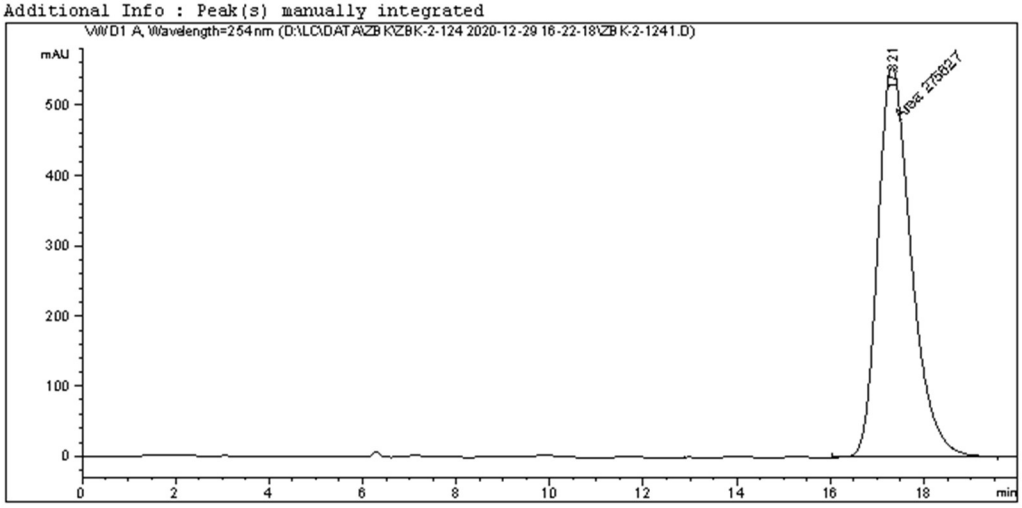
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3v



(1*S*,3*R*,4*R*)-**3v**

Data File D:\LC\DATA\ZBK\ZBK-2-124 2020-12-29 16-22-18\ZBK-2-1241.D
Sample Name: ZBK-2-124

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                            Location :   33
Injection Date  : 12/29/2020 4:31:14 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-2-124 2020-12-29 16-22-18\P1-AD-H-95-5-254NM-1ML-5ul-
                  30min.M
Last changed    : 12/29/2020 2:58:55 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-2-124 2020-12-29 16-22-18\P1-AD-H-95-5-254NM-1ML-5ul-
                  30min.M (Sequence Method)
Last changed    : 7/28/2021 5:15:24 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

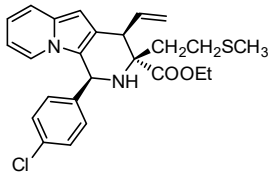
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.321 MM    0.8270 2.75627e4   555.45636 100.0000

Totals :                  2.75627e4   555.45636

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

1200 7/28/2021 5:15:27 PM 系统                          Page 1 of 1
```

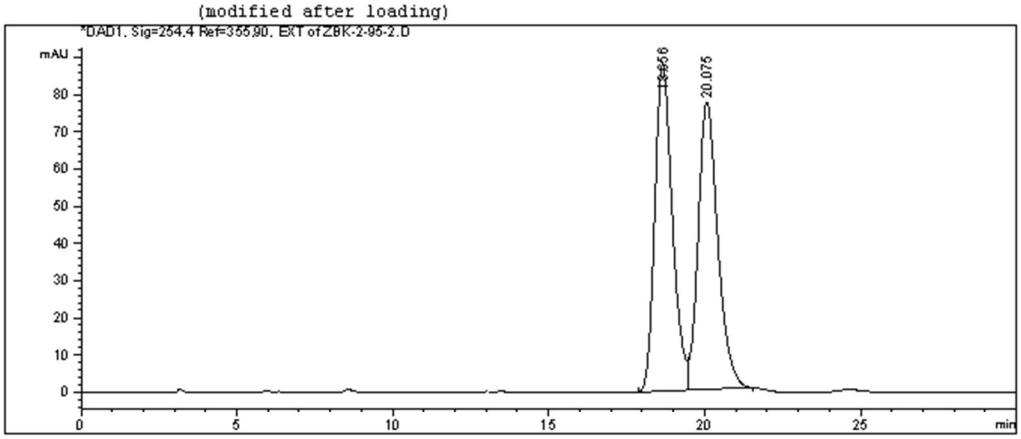
HPLC chromatogram of compound (*rac*)-3w



(1*S*,3*R*,4*R*)-**3w**

Data File E:\DATA\ZBK\ZBK-2-95-2 2020-12-04 16-07-01\ZBK-2-95-2.D
Sample Name: ZBK-2-95-2

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   1
Acq. Instrument : 1260                           Location :   12
Injection Date  : 12/4/2020 4:08:31 PM               Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-95-2 2020-12-04 16-07-01\AD-H-95-5-254NM-1ML-5ul-40min-
                  DAD.M
Last changed    : 12/4/2020 4:07:01 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-2-95-2 2020-12-04 16-07-01\AD-H-95-5-254NM-1ML-5ul-40min-
                  DAD.M (Sequence Method)
Last changed    : 7/29/2021 11:28:39 AM by SYSTEM
                  (modified after loading)
```




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

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

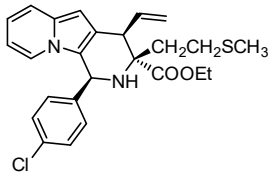

Signal 1: DAD1, Sig=254,4 Ref=355,90, EXT
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  18.656 BV    0.5824 3442.93726   88.01923  50.5357
   2  20.075 VB    0.6346 3369.94751   77.29643  49.4643

Totals :                  6812.88477  165.31567


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

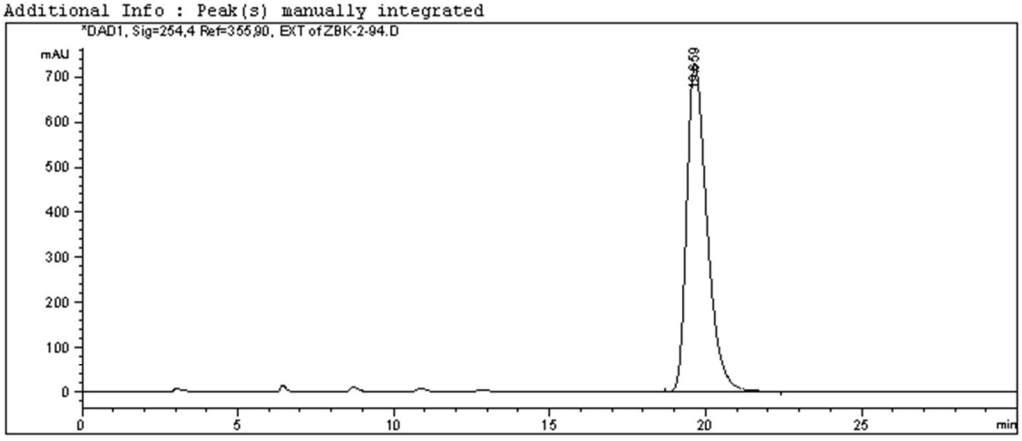
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3w



(1*S*,3*R*,4*R*)-**3w**

Data File E:\DATA\ZBK\ZBK-2-94 2020-12-03 22-23-50\ZBK-2-94.D
Sample Name: ZBK-2-94

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   1
Acq. Instrument : 1260                           Location :   61
Injection Date  : 12/3/2020 10:25:09 PM              Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-94 2020-12-03 22-23-50\AD-H-95-5-254NM-1ML-5ul-40min-DAD.
                  M
Last changed    : 12/3/2020 10:25:27 PM by SYSTEM
                  (modified after loading)
Analysis Method : E:\DATA\ZBK\ZBK-2-94 2020-12-03 22-23-50\AD-H-95-5-254NM-1ML-5ul-40min-DAD.
                  M (Sequence Method)
Last changed    : 7/29/2021 11:31:33 AM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




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

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

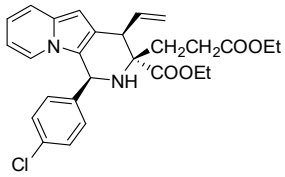

Signal 1: DAD1, Sig=254,4 Ref=355,90, EXT
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  19.659 BB    0.6849 3.29948e4   729.14325 100.0000

Totals :                  3.29948e4   729.14325

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

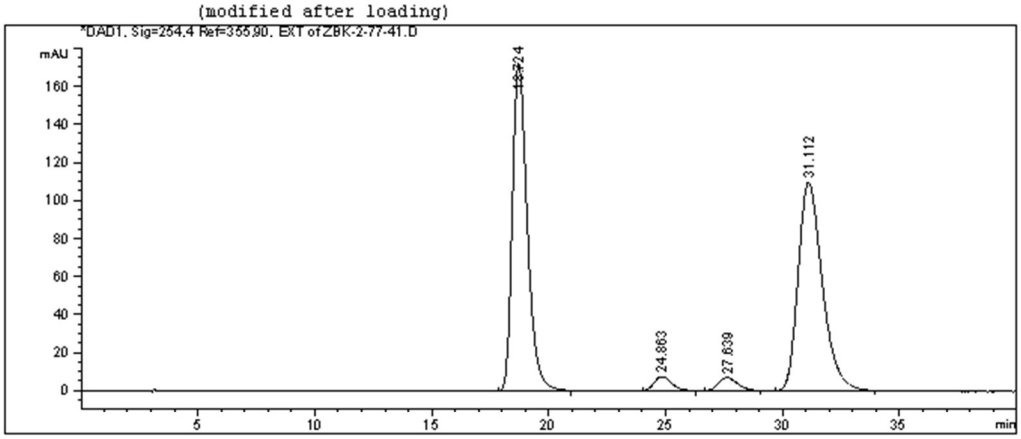
HPLC chromatogram of compound (*rac*)-3x



(1*S*,3*R*,4*R*)-**3x**

Data File E:\DATA\ZBK\ZBK-2-77-4 2020-12-09 18-44-49\ZBK-2-77-41.D
Sample Name: ZBK-2-77-4

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : 1260                           Location :   83
Injection Date  : 12/9/2020 6:57:43 PM               Inj :   1
                                               Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-77-4 2020-12-09 18-44-49\AD-H-95-5-254NM-1ML-5ul-40min-
                  DAD.M
Last changed    : 12/9/2020 6:44:50 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-2-77-4 2020-12-09 18-44-49\AD-H-95-5-254NM-1ML-5ul-40min-
                  DAD.M (Sequence Method)
Last changed    : 7/28/2021 10:13:14 PM by SYSTEM
                  (modified after loading)
```




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

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

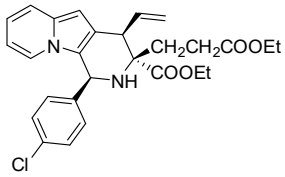

Signal 1: DAD1, Sig=254,4 Ref=355,90, EXT
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  18.724 BB    0.6499 7608.14551  172.04539  46.6162
   2  24.863 BB    0.6197  401.96313    7.62876   2.4629
   3  27.639 BB    0.6873  408.74911    6.97925   2.5045
   4  31.112 BB    0.8544 7901.95605  109.70082  48.4164

Totals :                  1.63208e4   296.35423

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

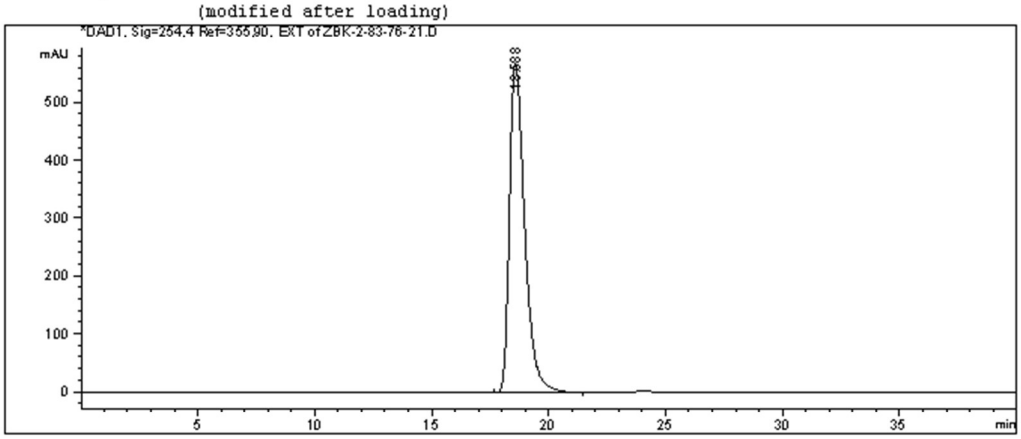
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3x



(1*S*,3*R*,4*R*)-**3x**

Data File E:\DATA\ZBK\ZBK-2-83-76-2 2020-11-23 17-32-48\ZBK-2-83-76-21.D
Sample Name: ZBK-2-76-2

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : 1260                           Location :   51
Injection Date  : 11/23/2020 5:46:11 PM              Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-83-76-2 2020-11-23 17-32-48\AD-H-95-5-254NM-1ML-5ul-40min
                  -DAD.M
Last changed    : 11/23/2020 5:32:48 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-2-83-76-2 2020-11-23 17-32-48\AD-H-95-5-254NM-1ML-5ul-40min
                  -DAD.M (Sequence Method)
Last changed    : 7/28/2021 10:16:53 PM by SYSTEM
                  (modified after loading)
```




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

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

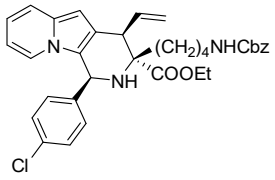

Signal 1: DAD1, Sig=254,4 Ref=355,90, EXT
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  18.588 BB    0.6901 2.57310e4   568.41187 100.0000

Totals :                  2.57310e4   568.41187


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

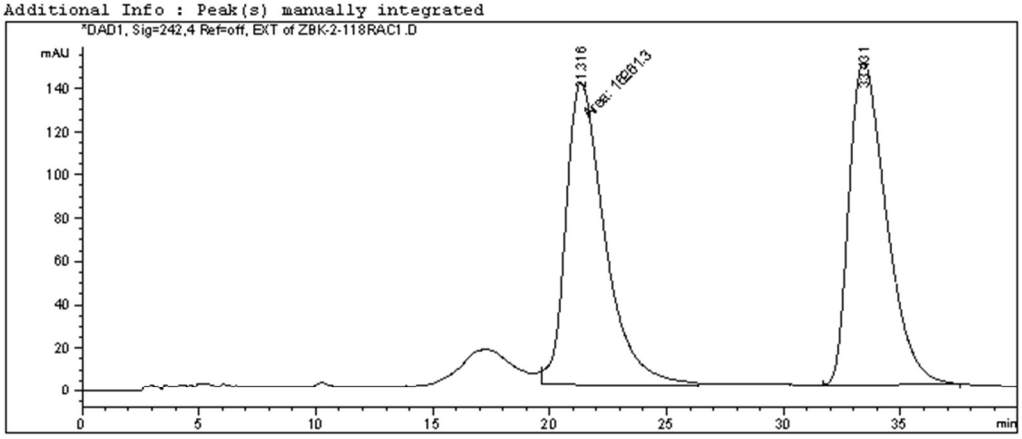
HPLC chromatogram of compound (*rac*)-3y



(1*S*,3*R*,4*R*)-**3y**

Data File E:\DATA\ZBK\ZBK-2-118RAC 2021-01-13 22-26-28\ZBK-2-118RAC1.D
Sample Name: ZBK-2-118RAC

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : 1260                          Location :   71
Injection Date  : 1/13/2021 10:38:47 PM              Inj :   1
                                               Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-118RAC 2021-01-13 22-26-28\3-ID-80-20-1ML-5ul-60MIN--DAD.
                  M
Last changed    : 1/13/2021 10:26:29 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-2-118RAC 2021-01-13 22-26-28\3-ID-80-20-1ML-5ul-60MIN--DAD.
                  M (Sequence Method)
Last changed    : 7/29/2021 2:51:55 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

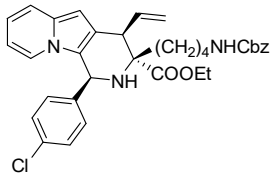

Signal 1: DAD1, Sig=242,4 Ref=off, EXT
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  21.316 FM    1.9358 1.62613e4   140.00591  49.5946
   2  33.431 BB    1.3016 1.65271e4   148.93541  50.4054

Totals :                  3.27884e4   288.94131

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

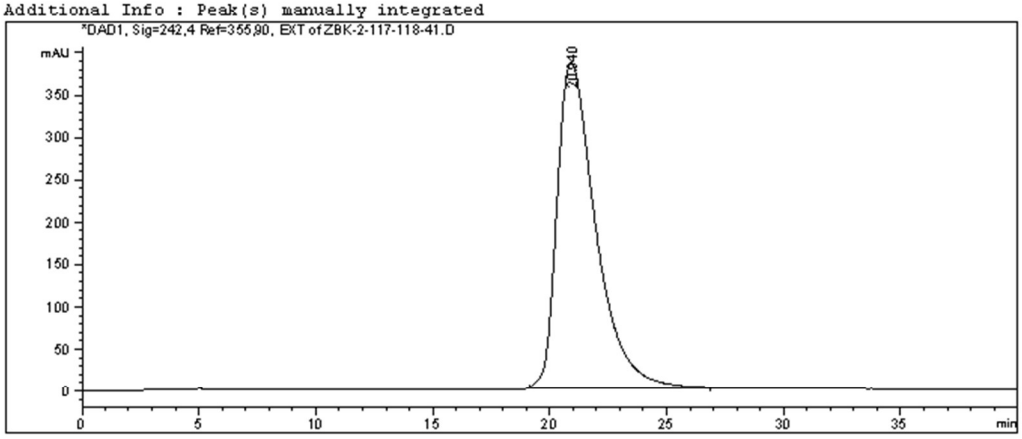
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3y



(1*S*,3*R*,4*R*)-**3y**

Data File E:\DATA\ZBK\ZBK-2-117-118-4 2021-01-13 20-39-06\ZBK-2-117-118-41.D
Sample Name: ZBK-2-117R,Rp

```
======================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : 1260                          Location :   71
Injection Date  : 1/13/2021 8:51:39 PM               Inj :   1
                                               Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-117-118-4 2021-01-13 20-39-06\3-ID-80-20-1ML-5UL-40MIN-
                  DAD.M
Last changed    : 1/13/2021 8:39:06 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-2-117-118-4 2021-01-13 20-39-06\3-ID-80-20-1ML-5UL-40MIN-
                  DAD.M (Sequence Method)
Last changed    : 7/29/2021 2:55:05 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

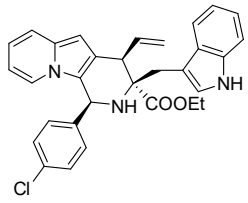

Signal 1: DAD1, Sig=242,4 Ref=355,90, EXT
 Signal has been modified after loading from rawdata file!

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  20.940 BB    1.3473 4.41605e4   384.40781 100.0000

Totals :                  4.41605e4   384.40781

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

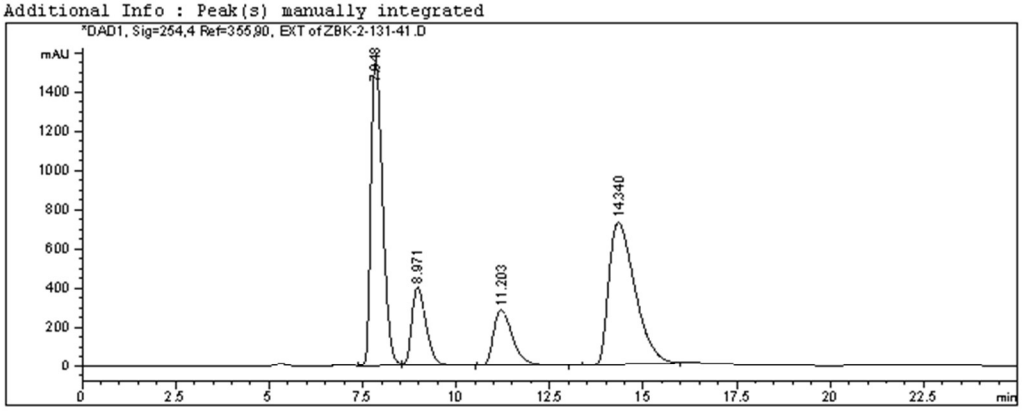
HPLC chromatogram of compound (*rac*)-3z



(1*S*,3*R*,4*R*)-**3z**

Data File E:\DATA\ZBK\ZBK-2-131-4 2021-01-04 18-40-32\ZBK-2-131-41.D
Sample Name: ZBK-2-131

```
======================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   2
Acq. Instrument : 1260                          Location :   11
Injection Date  : 1/4/2021 6:52:56 PM                Inj :   1
                                               Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-2-131-4 2021-01-04 18-40-32\ID-90-10-254NM-1ML-5ul-40min-
                  DAD.M
Last changed    : 1/4/2021 7:31:07 PM by SYSTEM
                  (modified after loading)
Analysis Method : E:\DATA\ZBK\ZBK-2-131-4 2021-01-04 18-40-32\ID-90-10-254NM-1ML-5ul-40min-
                  DAD.M (Sequence Method)
Last changed    : 7/29/2021 3:12:08 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, Sig=254,4 Ref=355,90, EXT
 Signal has been modified after loading from rawdata file!

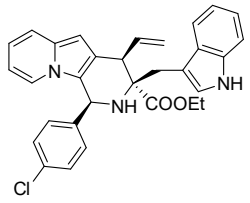
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.848 BV    0.3377 3.39642e4  1549.53247  37.5663
   2   8.971 VB    0.4091 1.07829e4   401.84921  11.9265
   3  11.203 BB    0.5549 1.02343e4   285.68988  11.3198
   4  14.340 BB    0.7305 3.54299e4   727.08154  39.1875

Totals :                  9.04113e4  2964.15311

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

1260 7/29/2021 3:12:10 PM SYSTEM                          Page 1 of 1
```

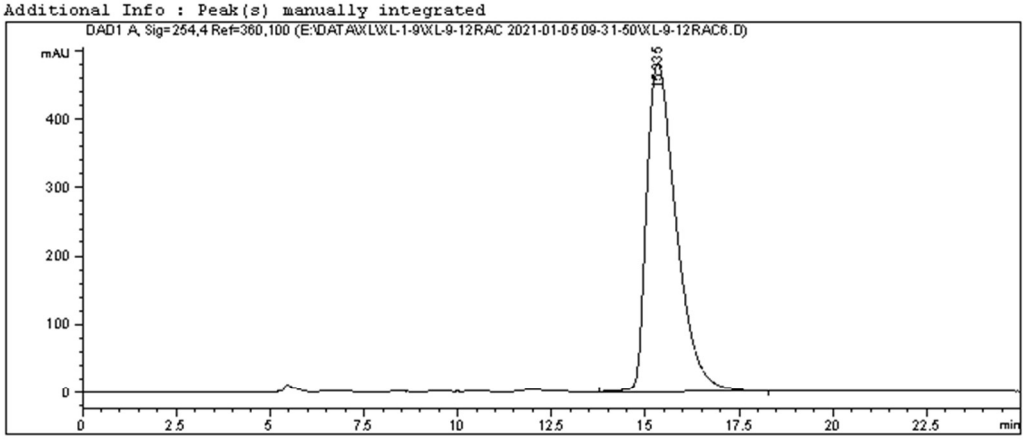
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3z



(1*S*,3*R*,4*R*)-**3z**

Data File E:\DATA\XL\XL-1-9\XL-9-12RAC 2021-01-05 09-31-50\XL-9-12RAC6.D
Sample Name: ZBK-2-130

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   7
Acq. Instrument : 1260                           Location :   61
Injection Date  : 1/5/2021 12:49:11 PM               Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\XL\XL-9-12RAC 2021-01-05 09-31-50\ID-90-10-254NM-1ML-5ul-30min-DAD.
                  M
Last changed    : 1/5/2021 11:57:14 AM by SYSTEM
Analysis Method : E:\DATA\XL\XL-1-9\XL-9-12RAC 2021-01-05 09-31-50\ID-90-10-254NM-1ML-5ul-
                  30min-DAD.M (Sequence Method)
Last changed    : 7/29/2021 3:08:05 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

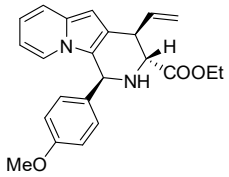

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  15.335 BB    0.8117 2.63744e4   481.00815 100.0000

Totals :                  2.63744e4   481.00815

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

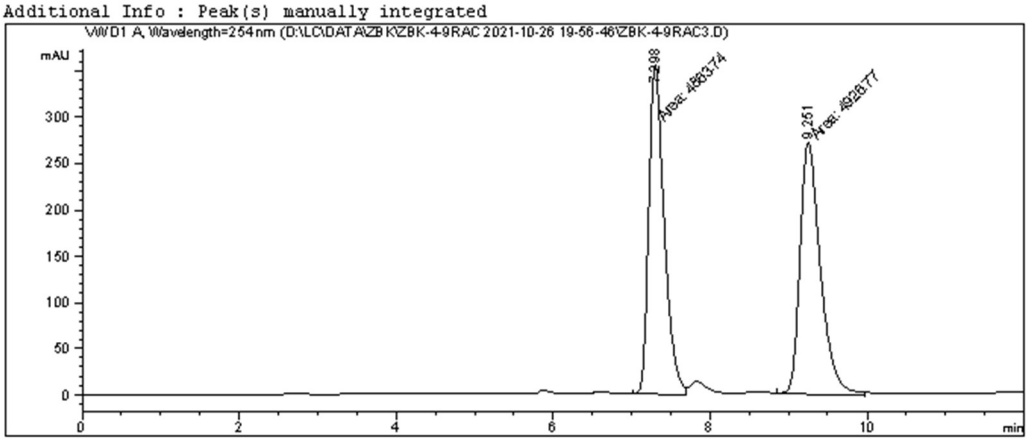
HPLC chromatogram of compound (*rac*)-3A



(1*S*,3*R*,4*R*)-**3A**

Data File D:\LC\DATA\ZBK\ZBK-4-9RAC 2021-10-26 19-56-46\ZBK-4-9RAC3.D
Sample Name: ZBK-4-9RAC

```
=====================================================================
Acq. Operator   : 系统                          Seq. Line :   4
Sample Operator : 系统
Acq. Instrument : 1200                            Location :   54
Injection Date  : 10/26/2021 8:46:13 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-4-9RAC 2021-10-26 19-56-46\P1-80-20-254NM-1ML-5ul-45min.
                  M
Last changed    : 10/26/2021 9:03:52 PM by 系统
                  (modified after loading)
Analysis Method : D:\LC\DATA\ZBK\ZBK-4-9RAC 2021-10-26 19-56-46\P1-80-20-254NM-1ML-5ul-45min.
                  M (Sequence Method)
Last changed    : 11/22/2022 4:52:37 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

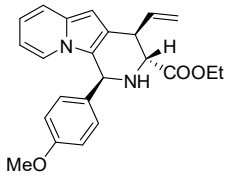
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.298 MM    0.2280 4863.73730  355.56787  49.6781
   2   9.251 MM    0.3023 4926.77295  271.59332  50.3219

Totals :                  9790.51025  627.16119

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

1200 11/22/2022 4:52:44 PM 系统                          Page 1 of 1
```

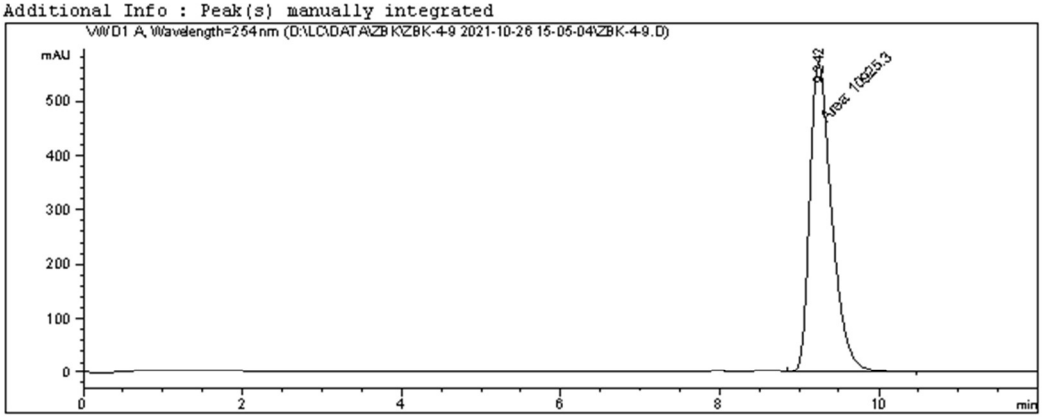
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3A



(1*S*,3*R*,4*R*)-**3A**

Data File D:\LC\DATA\ZBK\ZBK-4-9 2021-10-26 15-05-04\ZBK-4-9.D
Sample Name: ZBK-4-9SS

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :   1
Sample Operator : 系统
Acq. Instrument : 1200                            Location :   23
Injection Date  : 10/26/2021 3:06:16 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-4-9 2021-10-26 15-05-04\P1-80-20-254NM-1ML-5ul-45min.M
Last changed    : 10/26/2021 3:31:18 PM by 系统
                  (modified after loading)
Analysis Method : D:\LC\DATA\ZBK\ZBK-4-9 2021-10-26 15-05-04\P1-80-20-254NM-1ML-5ul-45min.M (
                  Sequence Method)
Last changed    : 11/22/2022 4:56:20 PM by 系统
                  (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

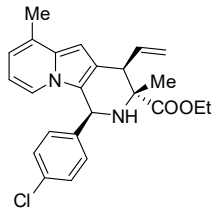

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.242 FM    0.3208 1.09253e4   567.68463 100.0000

Totals :                  1.09253e4   567.68463


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

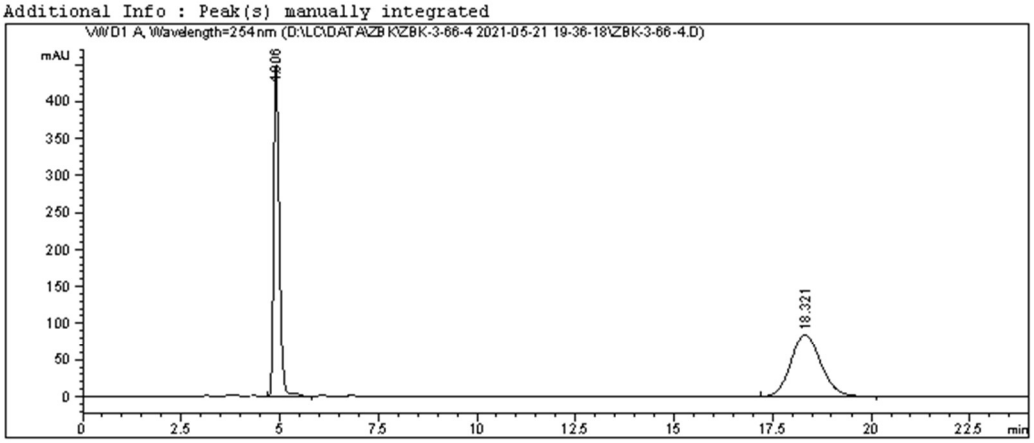
HPLC chromatogram of compound (*rac*)-3B



(1*S*,3*R*,4*R*)-**3B**

Data File D:\LC\DATA\ZBK\ZBK-3-66-4 2021-05-21 19-36-18\ZBK-3-66-4.D
Sample Name: ZBK-3-66RAC

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :   1
Sample Operator : 系统
Acq. Instrument : 1200                            Location :   12
Injection Date  : 5/21/2021 7:37:43 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-66-4 2021-05-21 19-36-18\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M
Last changed    : 5/21/2021 7:38:09 PM by 系统
                  (modified after loading)
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-66-4 2021-05-21 19-36-18\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M (Sequence Method)
Last changed    : 11/22/2022 4:59:20 PM by 系统
                  (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

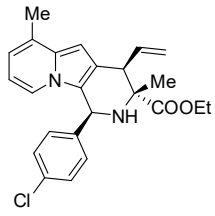

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.906 BV R  0.1519 4466.34814  449.39865  50.2664
   2  18.321 BV R  0.7936 4419.00537   84.90782  49.7336

Totals :                  8885.35352  534.30647

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

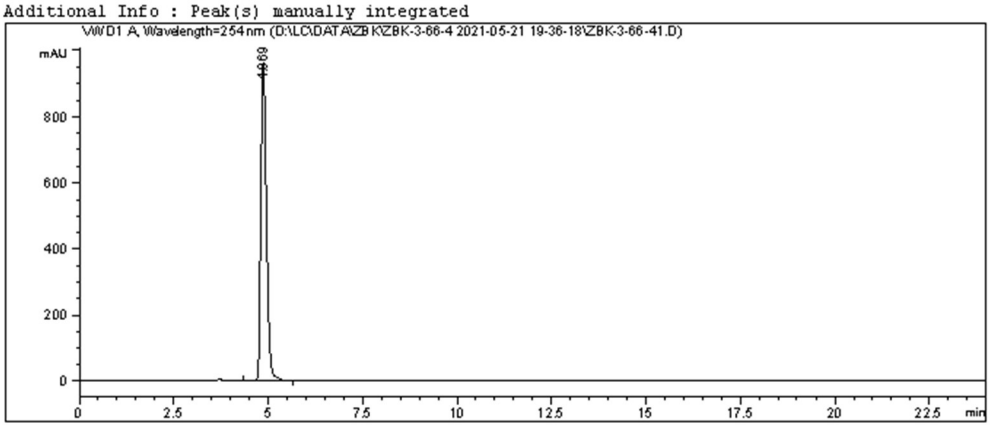
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3B



(1*S*,3*R*,4*R*)-**3B**

Data File D:\LC\DATA\ZBK\ZBK-3-66-4 2021-05-21 19-36-18\ZBK-3-66-41.D
Sample Name: ZBK-3-66R/R

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   11
Injection Date  : 5/21/2021 8:03:55 PM               Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-66-4 2021-05-21 19-36-18\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M
Last changed    : 5/21/2021 7:38:09 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-66-4 2021-05-21 19-36-18\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M (Sequence Method)
Last changed    : 11/22/2022 5:01:08 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

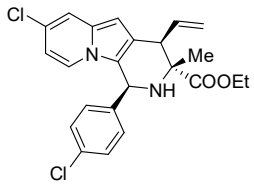
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.869 VB R  0.1577 9886.07324  962.55554 100.0000

Totals :                  9886.07324  962.55554

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

1200 11/22/2022 5:01:11 PM 系统 Page 1 of 1

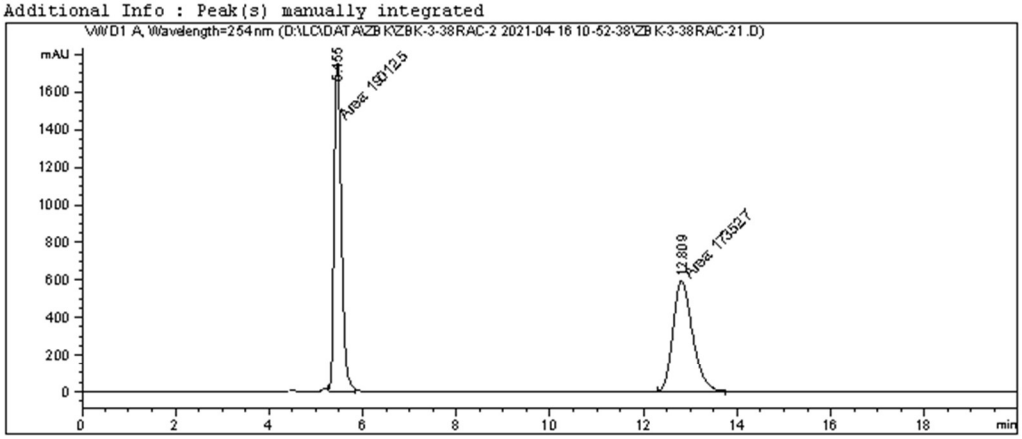
HPLC chromatogram of compound (*rac*)-3C



(1*S*,3*R*,4*R*)-**3C**

Data File D:\LC\DATA\ZBK\ZBK-3-38RAC-2 2021-04-16 10-52-38\ZBK-3-38RAC-21.D
Sample Name: ZBK-3-38RAC-2

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   3
Injection Date  : 4/16/2021 10:57:52 AM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-38RAC-2 2021-04-16 10-52-38\P1-AD-H-80-20-254NM-1ML-
                  5UL-20MIN.M
Last changed    : 1/14/2021 2:49:11 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-38RAC-2 2021-04-16 10-52-38\P1-AD-H-80-20-254NM-1ML-
                  5UL-20MIN.M (Sequence Method)
Last changed    : 7/28/2021 8:32:22 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

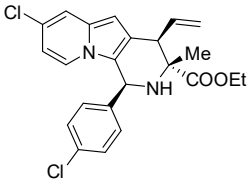
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.455 MF    0.1810 1.90125e4  1750.67407  52.2822
   2  12.809 FM    0.4866 1.73527e4   594.37946  47.7178

Totals :                  3.63652e4  2345.05353


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

1200 7/28/2021 8:32:25 PM 系统                          Page 1 of 1
```

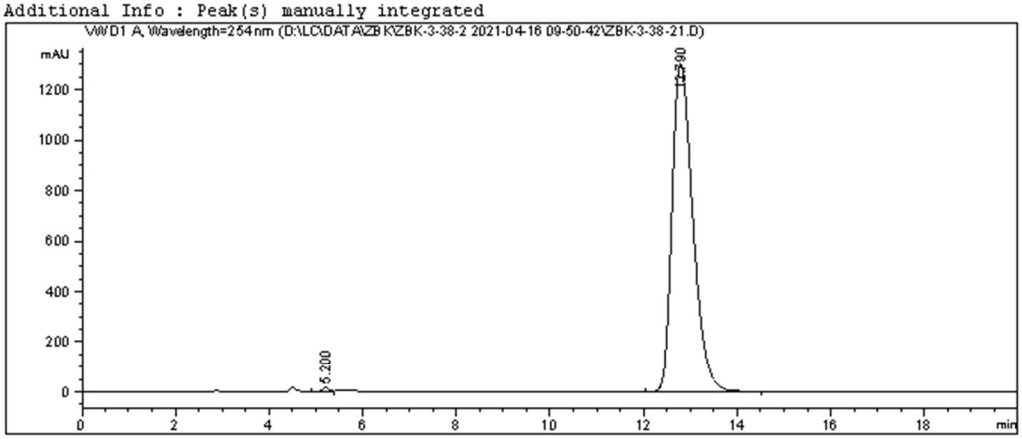
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3C



(1*S*,3*R*,4*R*)-**3C**

Data File D:\LC\DATA\ZBK\ZBK-3-38-2 2021-04-16 09-50-42\ZBK-3-38-21.D
Sample Name: ZBK-3-38R

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   3
Injection Date  : 4/16/2021 9:54:56 AM               Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-38-2 2021-04-16 09-50-42\P1-AD-H-80-20-254NM-1ML-5UL-
                  20MIN.M
Last changed    : 1/14/2021 2:49:11 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-38-2 2021-04-16 09-50-42\P1-AD-H-80-20-254NM-1ML-5UL-
                  20MIN.M (Sequence Method)
Last changed    : 7/28/2021 8:34:32 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

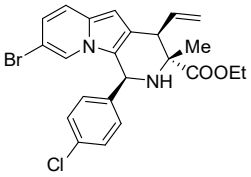
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.200 BV    0.1296  133.98087   15.54926   0.3321
   2  12.790 BB    0.4784 4.02095e4  1301.41541  99.6679

Totals :                  4.03435e4  1316.96467

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

1200 7/28/2021 8:34:35 PM 系统                          Page 1 of 1
```

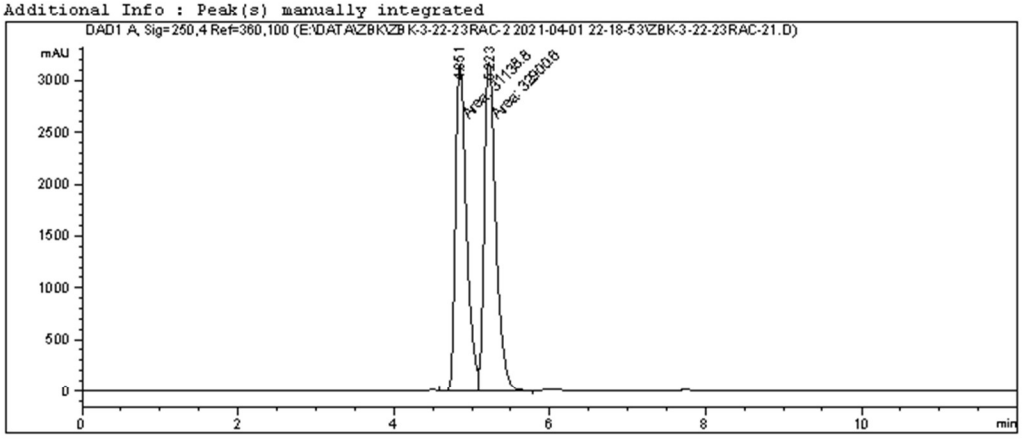
HPLC chromatogram of compound (*rac*)-3D



(1*S*,3*R*,4*R*)-**3D**

Data File E:\DATA\ZBK\ZBK-3-22-23RAC-2 2021-04-01 22-18-53\ZBK-3-22-23RAC-21.D
Sample Name: ZBK-3-22-23RAC

```
==================================================================
Acq. Operator   : SYSTEM                        Seq. Line :   2
Acq. Instrument : 1260                           Location :   23
Injection Date  : 4/1/2021 10:31:58 PM               Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-3-22-23RAC-2 2021-04-01 22-18-53\4-IE--95-5-1ML-20MIN-5UL-
                  254NM-DAD.M
Last changed    : 4/1/2021 10:18:54 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-3-22-23RAC-2 2021-04-01 22-18-53\4-IE--95-5-1ML-20MIN-5UL-
                  254NM-DAD.M (Sequence Method)
Last changed    : 7/29/2021 3:37:53 PM by SYSTEM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
```




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

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

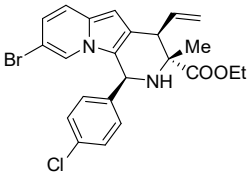

Signal 1: DAD1 A, Sig=250,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.851 MM    0.1650 3.11388e4  3144.90674  48.6244
   2   5.223 MF    0.1729 3.29006e4  3171.80933  51.3756

Totals :                  6.40394e4  6316.71606


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

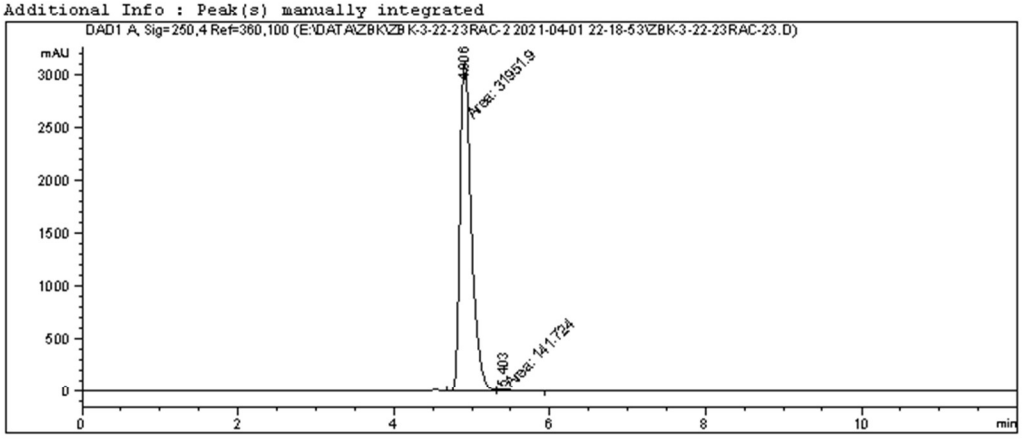
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3D



(1*S*,3*R*,4*R*)-**3D**

Data File E:\DATA\ZBK\ZBK-3-22-23RAC-2 2021-04-01 22-18-53\ZBK-3-22-23RAC-23.D
Sample Name: ZBK-3-22-2

```
==================================================================
Acq. Operator   : SYSTEM                       Seq. Line :   4
Acq. Instrument : 1260                          Location :   3
Injection Date  : 4/1/2021 11:05:12 PM              Inj :   1
                                               Inj Volume : 5.000 µl
Acq. Method     : E:\DATA\ZBK\ZBK-3-22-23RAC-2 2021-04-01 22-18-53\4-IE--95-5-1ML-20MIN-5UL-
                  254NM-DAD.M
Last changed    : 4/1/2021 10:18:54 PM by SYSTEM
Analysis Method : E:\DATA\ZBK\ZBK-3-22-23RAC-2 2021-04-01 22-18-53\4-IE--95-5-1ML-20MIN-5UL-
                  254NM-DAD.M (Sequence Method)
Last changed    : 7/29/2021 3:40:38 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

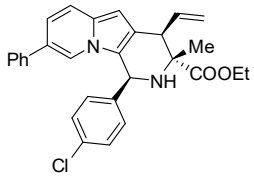

Signal 1: DAD1 A, Sig=250,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.906 FM    0.1708 3.19519e4  3117.61450  99.5584
   2   5.403 FM    0.2133  141.72401   11.07572   0.4416

Totals :                  3.20936e4  3128.69022

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

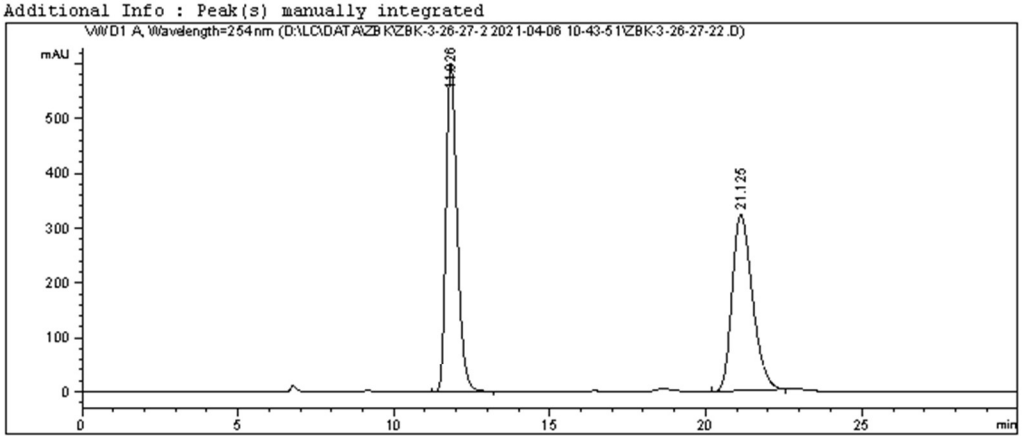
HPLC chromatogram of compound (*rac*)-3E



(1*S*,3*R*,4*R*)-**3E**

Data File D:\LC\DATA\ZBK\ZBK-3-26-27-2 2021-04-06 10-43-51\ZBK-3-26-27-22.D
Sample Name: ZBK-3-26-27RAC

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :   3
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   41
Injection Date  : 4/6/2021 11:27:23 AM               Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-26-27-2 2021-04-06 10-43-51\P1-AD-H-95-5-254NM-1ML-5ul
                  -30min.M
Last changed    : 12/29/2020 2:58:55 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-26-27-2 2021-04-06 10-43-51\P1-AD-H-95-5-254NM-1ML-5ul
                  -30min.M (Sequence Method)
Last changed    : 7/28/2021 8:27:28 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

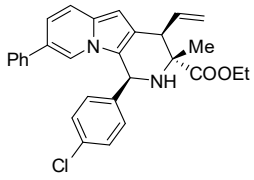
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.826 BV R  0.3764 1.47906e4   600.00867  50.2081
   2  21.125 BB    0.6980 1.46680e4   323.45261  49.7919

Totals :                  2.94585e4   923.46127


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

1200 7/28/2021 8:27:35 PM 系统                          Page 1 of 1
```

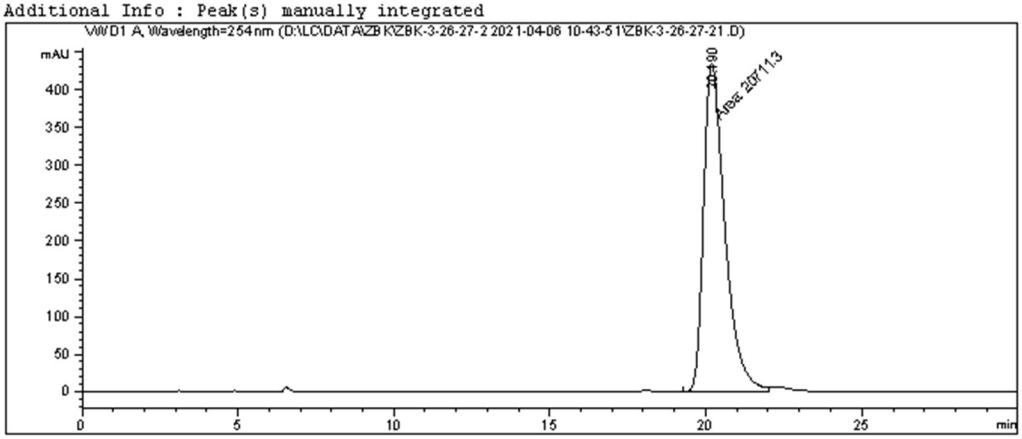
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-3E



(1*S*,3*R*,4*R*)-**3E**

Data File D:\LC\DATA\ZBK\ZBK-3-26-27-2 2021-04-06 10-43-51\ZBK-3-26-27-21.D
Sample Name: ZBK-3-26

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :   2
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   3
Injection Date  : 4/6/2021 10:56:08 AM               Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-26-27-2 2021-04-06 10-43-51\P1-AD-H-95-5-254NM-1ML-5ul
                  -30min.M
Last changed    : 12/29/2020 2:58:55 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-26-27-2 2021-04-06 10-43-51\P1-AD-H-95-5-254NM-1ML-5ul
                  -30min.M (Sequence Method)
Last changed    : 7/28/2021 8:29:46 PM by 系统
                  (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

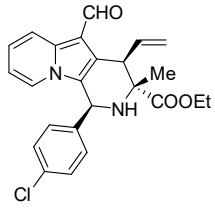

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  20.190 MF    0.7946 2.07113e4   434.41125 100.0000

Totals :                  2.07113e4   434.41125

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

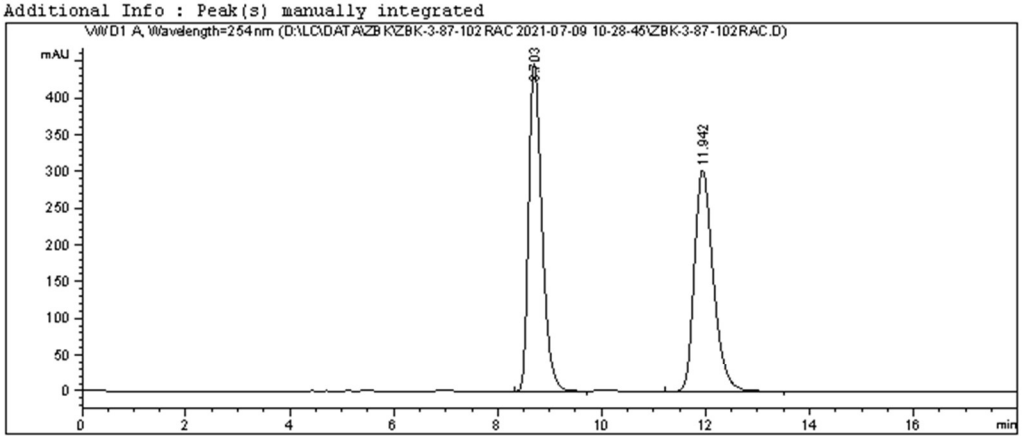
HPLC chromatogram of compound (*rac*)-4



(1*S*,3*R*,4*R*)-**4**

Data File D:\LC\DATA\ZBK\ZBK-3-87-102RAC 2021-07-09 10-28-45\ZBK-3-87-102RAC.D
Sample Name: ZBK-3-87-102RAC

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :   1
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   41
Injection Date  : 7/9/2021 10:30:10 AM               Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-87-102RAC 2021-07-09 10-28-45\P1-AD-H-80-20-254NM-1ML-
                  5UL-20MIN.M
Last changed    : 1/14/2021 2:49:11 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-87-102RAC 2021-07-09 10-28-45\P1-AD-H-80-20-254NM-1ML-
                  5UL-20MIN.M (Sequence Method)
Last changed    : 7/28/2021 9:16:20 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

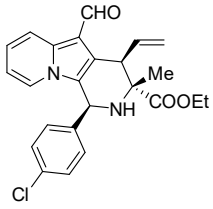
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.703 BB    0.2717 7960.23828  447.23532  50.9437
   2  11.942 VV R  0.3886 7665.32520  302.76563  49.0563

Totals :                  1.56256e4   750.00095

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

1200 7/28/2021 9:16:22 PM 系统                          Page 1 of 1
```

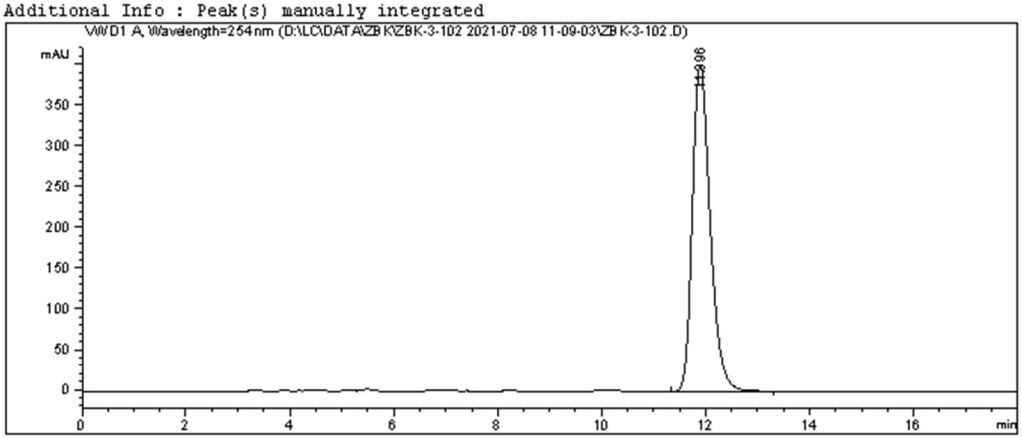
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-4



(1*S*,3*R*,4*R*)-**4**

Data File D:\LC\DATA\ZBK\ZBK-3-102 2021-07-08 11-09-03\ZBK-3-102.D
Sample Name: ZBK-3-102

```
==================================================================
Acq. Operator   : 系统                          Seq. Line :   1
Sample Operator : 系统
Acq. Instrument : 1200                            Location :   31
Injection Date  : 7/8/2021 11:10:28 AM                 Inj :   1
                                                  Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-102 2021-07-08 11-09-03\P1-AD-H-80-20-254NM-1ML-5UL-
                  20MIN.M
Last changed    : 1/14/2021 2:49:11 PM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-102 2021-07-08 11-09-03\P1-AD-H-80-20-254NM-1ML-5UL-
                  20MIN.M (Sequence Method)
Last changed    : 7/28/2021 9:17:59 PM by 系统
                  (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

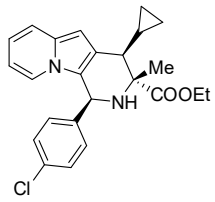

Signal 1: VWD1 A, Wavelength=254 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.896 BB    0.3630 9564.50098  402.67850 100.0000

Totals :                  9564.50098  402.67850

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

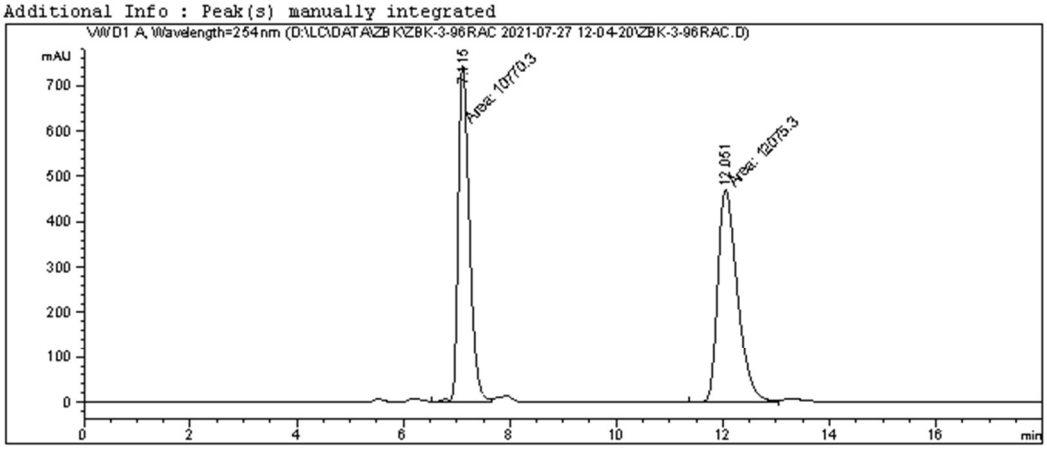
HPLC chromatogram of compound (*rac*)-5



(1*S*,3*R*,4*R*)-**5**

Data File D:\LC\DATA\ZBK\ZBK-3-96RAC 2021-07-27 12-04-20\ZBK-3-96RAC.D
Sample Name: ZBK-3-96RAC

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :   1
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   21
Injection Date  : 7/27/2021 12:05:45 PM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-96RAC 2021-07-27 12-04-20\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M
Last changed    : 7/27/2021 12:05:56 PM by 系统
                  (modified after loading)
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-96RAC 2021-07-27 12-04-20\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M (Sequence Method)
Last changed    : 7/28/2021 9:11:23 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

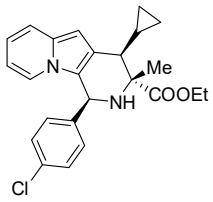
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.115 MF    0.2414 1.07703e4   743.47247  47.1437
   2  12.051 MF    0.4279 1.20753e4   470.28445  52.8563

Totals :                  2.28456e4  1213.75693


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

1200 7/28/2021 9:11:26 PM 系统                          Page 1 of 1
```

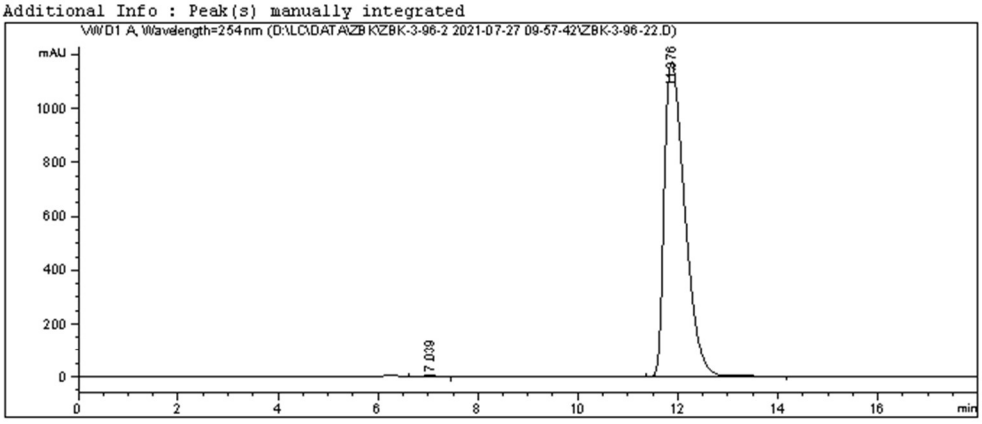
HPLC chromatogram of compound (1*S*,3*R*,4*R*)-5



(1*S*,3*R*,4*R*)-**5**

Data File D:\LC\DATA\ZBK\ZBK-3-96-2 2021-07-27 09-57-42\ZBK-3-96-22.D
Sample Name: ZBK-3-96-1

```
======================================================================
Acq. Operator   : 系统                          Seq. Line :   3
Sample Operator : 系统
Acq. Instrument : 1200                           Location :   14
Injection Date  : 7/27/2021 10:46:33 AM              Inj :   1
                                                 Inj Volume : 5.000 µl
Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-96-2 2021-07-27 09-57-42\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M
Last changed    : 7/27/2021 10:45:19 AM by 系统
Analysis Method : D:\LC\DATA\ZBK\ZBK-3-96-2 2021-07-27 09-57-42\P1-AD-H-90-10-254NM-1ML-5UL-
                  30MIN.M (Sequence Method)
Last changed    : 7/28/2021 9:13:07 PM by 系统
                  (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: VWD1 A, Wavelength=254 nm

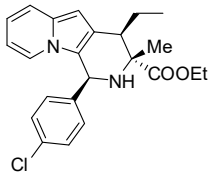
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.039 VB    0.2674   71.79204    4.00496   0.2133
   2  11.876 BV R  0.4443 3.35930e4  1174.70117  99.7867

Totals :                  3.36648e4  1178.70613


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

1200 7/28/2021 9:13:09 PM 系统                          Page 1 of 1
```

HPLC chromatogram of compound (*rac*)-6



(1*S*, 3*R*, 4*R*)-**6**

```
Data File D:\LC\DATA\ZBK\ZBK-3-115-2 2021-08-24 15-46-59\ZBK-3-115-25.D
Sample Name: ZBK-3-115RAC

    ======================================================================
    Acq. Operator   : 系统                          Seq. Line :   6
    Sample Operator : 系统
    Acq. Instrument : 1200                           Location :   43
    Injection Date  : 8/24/2021 5:37:06 PM              Inj :   1
                                                    Inj Volume : 5.000 µl
    Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-115-2 2021-08-24 15-46-59\P1-AD-H-90-10-254NM-1ML-5UL-
                      30MIN.M
    Last changed    : 8/24/2021 4:53:24 PM by 系统
    Analysis Method : D:\LC\DATA\ZBK\ZBK-3-115-2 2021-08-24 15-46-59\P1-AD-H-90-10-254NM-1ML-5UL-
                      30MIN.M (Sequence Method)
    Last changed    : 11/22/2022 4:46:37 PM by 系统
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
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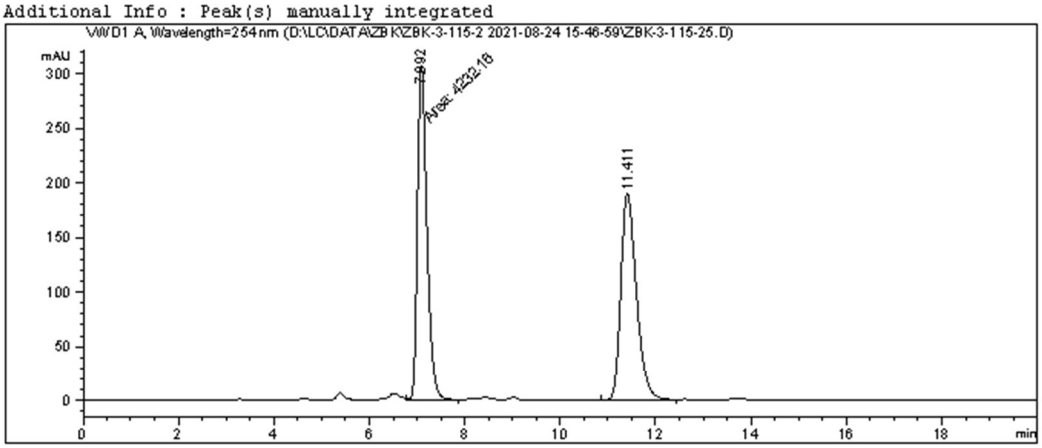


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    ======================================================================
                              Area Percent Report
    ======================================================================

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


    Signal 1: VWD1 A, Wavelength=254 nm

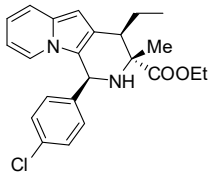
    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   7.092 FM    0.2297 4232.15576  307.08786  49.5648
       2  11.411 BV R  0.3483 4306.48291  189.38510  50.4352

    Totals :                  8538.63867  496.47296


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

1200 11/22/2022 4:46:41 PM 系统                                  Page 1 of 1
```

HPLC chromatogram of compound (1*S*,3*R*,4*R*)-6



(1*S*, 3*R*, 4*R*)-**6**

```
Data File D:\LC\DATA\ZBK\ZBK-3-115-3 2021-08-24 19-14-22\ZBK-3-115-32.D
Sample Name: ZBK-3-115-1

    ======================================================================
    Acq. Operator   : 采统                          Seq. Line :   3
    Sample Operator : 采统
    Acq. Instrument : 1200                           Location :   41
    Injection Date  : 8/24/2021 7:48:50 PM              Inj :   2
                                                    Inj Volume : 5.000 µl
    Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-115-3 2021-08-24 19-14-22\P1-AD-H-90-10-254NM-1ML-5UL-
                      30MIN.M
    Last changed    : 8/24/2021 7:22:48 PM by 采统
    Analysis Method : D:\LC\DATA\ZBK\ZBK-3-115-3 2021-08-24 19-14-22\P1-AD-H-90-10-254NM-1ML-5UL-
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    Last changed    : 11/22/2022 5:04:07 PM by 采统
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
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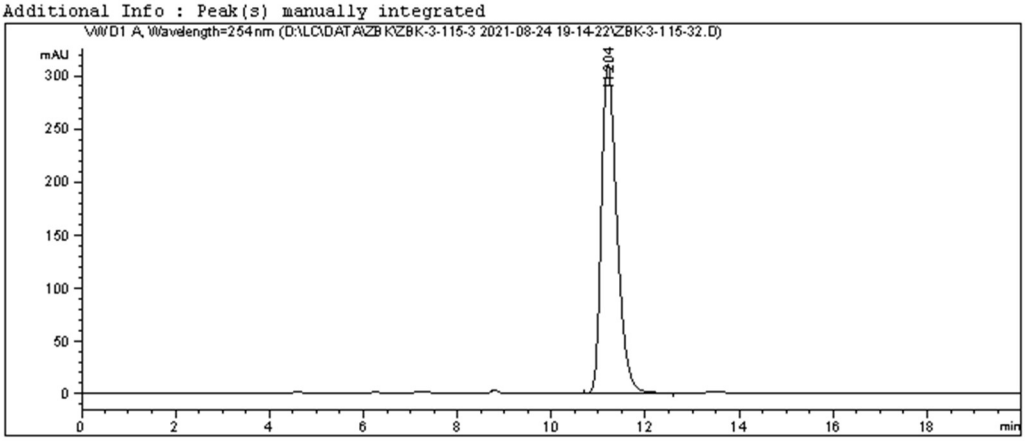


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    ======================================================================
                            Area Percent Report
    ======================================================================

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


    Signal 1: VWD1 A, Wavelength=254 nm

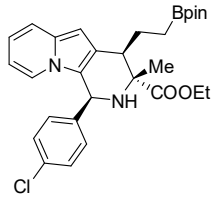
    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  11.204 BV R  0.3506 7129.33496  310.83817 100.0000

    Totals :                  7129.33496  310.83817


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


1200 11/22/2022 5:04:09 PM 采统                                  Page 1 of 1
```

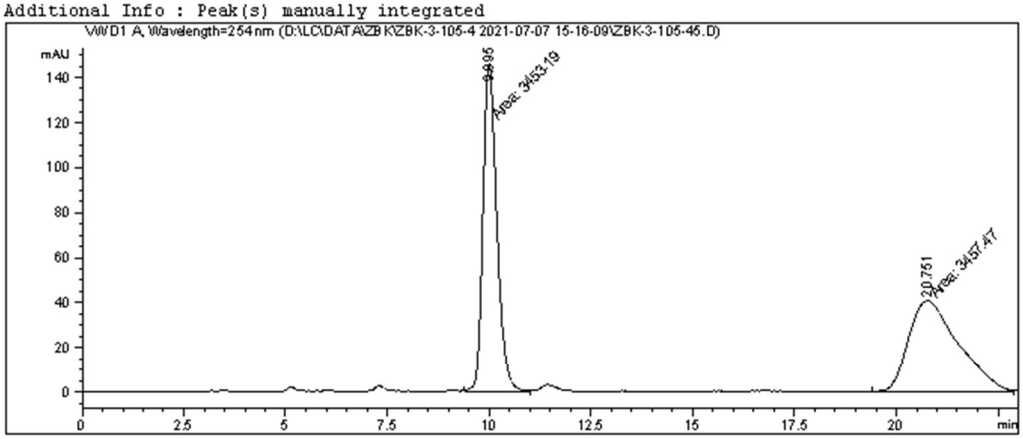
HPLC chromatogram of compound (*rac*)-7



(1*S*,3*R*,4*R*)-**7**

```
Data File D:\LC\DATA\ZBK\ZBK-3-105-4 2021-07-07 15-16-09\ZBK-3-105-45.D
Sample Name: ZBK-3-105RAC

    ======================================================================
    Acq. Operator   : 系统                          Seq. Line :   6
    Sample Operator : 系统
    Acq. Instrument : 1200                           Location :   41
    Injection Date  : 7/7/2021 5:30:58 PM                Inj :   1
                                                   Inj Volume : 5.000 µl
    Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-105-4 2021-07-07 15-16-09\P1-AD-H-95-5-254NM-1ML-5ul-
                      30min.M
    Last changed    : 7/7/2021 5:29:46 PM by 系统
    Analysis Method : D:\LC\DATA\ZBK\ZBK-3-105-4 2021-07-07 15-16-09\P1-AD-H-95-5-254NM-1ML-5ul-
                      30min.M (Sequence Method)
    Last changed    : 7/28/2021 9:26:07 PM by 系统
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
```

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

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


    Signal 1: VWD1 A, Wavelength=254 nm

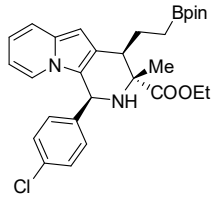
    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   9.995 FM    0.3950 3453.18652  145.71432  49.9690
       2  20.751 MF    1.4169 3457.47314   40.66933  50.0310

    Totals :                  6910.65967  186.38366


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

1200 7/28/2021 9:26:12 PM 系统                                Page 1 of 1
```

HPLC chromatogram of compound (1*S*,3*R*,4*R*)-7



(1*S*,3*R*,4*R*)-**7**

```
Data File D:\LC\DATA\ZBK\ZBK-3-105-3 2021-07-05 14-46-27\ZBK-3-105-33.D
Sample Name: ZBK-3-105-2

    ======================================================================
    Acq. Operator   : 系统                          Seq. Line :   4
    Sample Operator : 系统
    Acq. Instrument : 1200                          Location :   63
    Injection Date  : 7/5/2021 3:57:25 PM              Inj :   1
                                                    Inj Volume : 5.000 µl
    Acq. Method     : D:\LC\DATA\ZBK\ZBK-3-105-3 2021-07-05 14-46-27\P1-AD-H-95-5-254NM-1ML-5ul-
                      30min.M
    Last changed    : 7/5/2021 3:56:09 PM by 系统
    Analysis Method : D:\LC\DATA\ZBK\ZBK-3-105-3 2021-07-05 14-46-27\P1-AD-H-95-5-254NM-1ML-5ul-
                      30min.M (Sequence Method)
    Last changed    : 7/28/2021 9:22:06 PM by 系统
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
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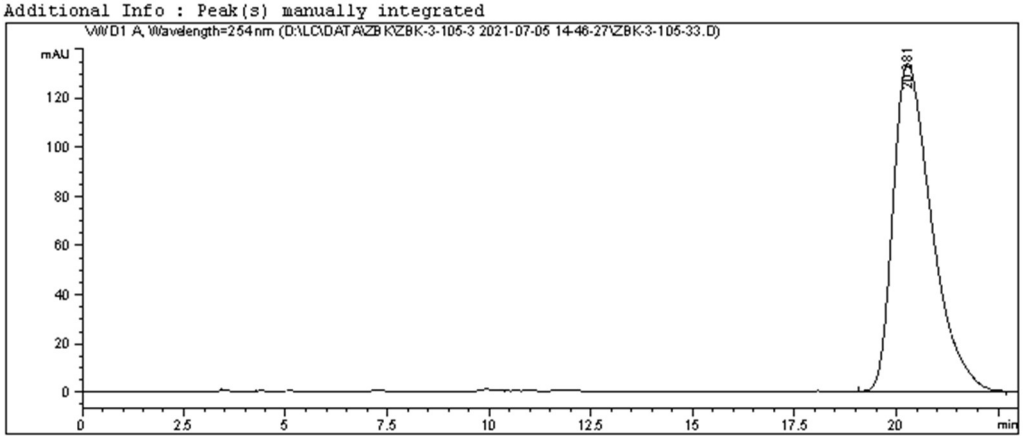


```
    ======================================================================
                            Area Percent Report
    ======================================================================

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


    Signal 1: VWD1 A, Wavelength=254 nm

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1  20.281 VV R  0.9891 8826.41992  133.86732 100.0000

    Totals :                  8826.41992  133.86732


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

Computational Details

All calculations were performed with Gaussian 09[1] at the M06-L[2] level of density functional theory. The M06-L functional and a mixed basis set of SDD[3] for Cu, Fe, and Ir and 6-31G(d) for other atoms were used for geometry optimizations and frequency calculations. Frequency outcomes were examined to confirm the stationary points as minima (no imaginary frequencies) or transition states (only one imaginary frequency). Single-point energies were then calculated with M06-L functional and the def2-TZVP[4] basis set for all atoms, in which the solvation effects were modeled by SMD[5] in CH_2Cl_2 ($\varepsilon = 8.93$) solvent. Free energies (kcal/mol) in solution were utilized in the discussions. The optimized geometries were represented by using CYLView.[6]

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö .; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*; Gaussian, Inc.: Wallingford, CT, 2009.
2. (a) Zhao, Y.; Truhlar, D. G. Density Functionals with Broad Applicability in Chemistry. *Acc. Chem. Res.* **2008**, *41*, 157–167. (b) Zhao, Y.; Truhlar, D. G. The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06-Class Functionals and 12 Other Functionals. *Theor. Chem. Acc.* **2008**, *120*, 215–241.
3. (a) Andrae, D.; Häussermann, U.; Dolg, M.; Stoll, H.; Preuss, H. Energy-Adjustedab initio pseudopotentials for the second and third row transition elements. *Theor. Chim. Acta* **1990**, *77*, 123–141. (b) Roy, L. E.; Hay, P. J.; Martin, R. L. Revised basis sets for the LANL effective core potentials. *J. Chem. Theory Comput.* **2008**, *4*, 1029–1031.
4. Weigend, F.; Ahlrichs, R. Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297–3305.
5. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *J. Phys. Chem. B* **2009**, *113*, 6378– 6396.
6. Legault, C. Y. *CYLview, 1.0b*; Universite′de Sherbrooke, 2009. http://www.cylview.org.

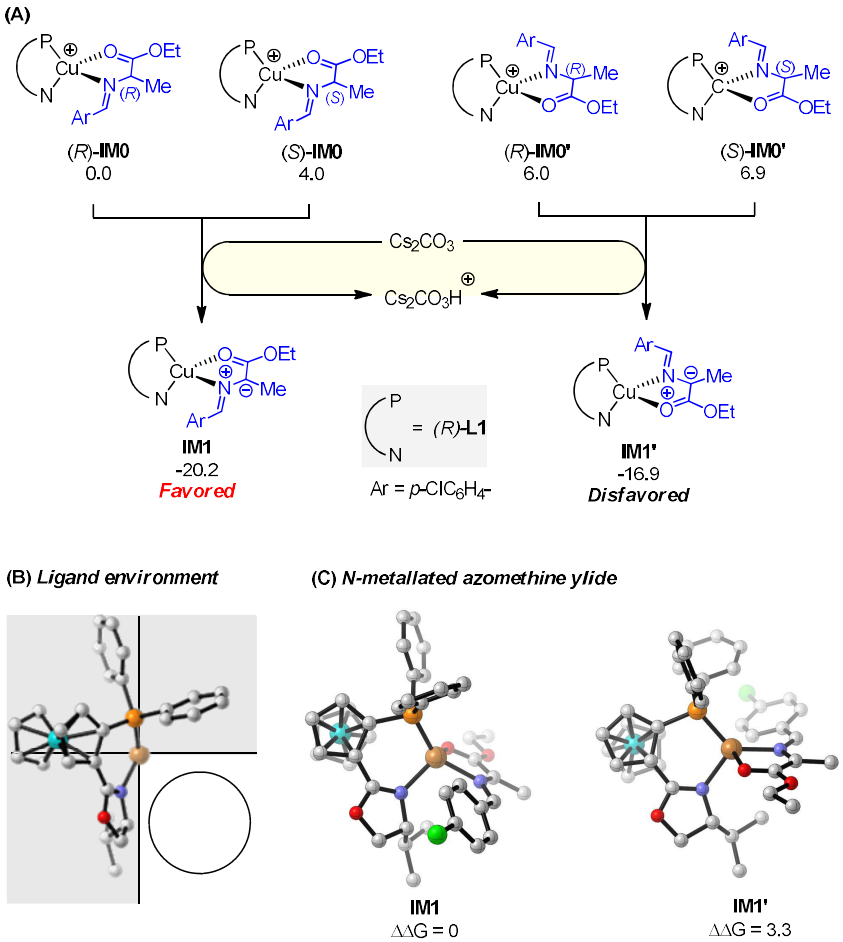

Fig. S3. (A) In situ generation of prochiral nucleophile **IM1**. Free energies are given in kcal/mol. (B) and (C) Structures of diastereomeric prochiral nucleophiles **IM1** and **IM1'**.

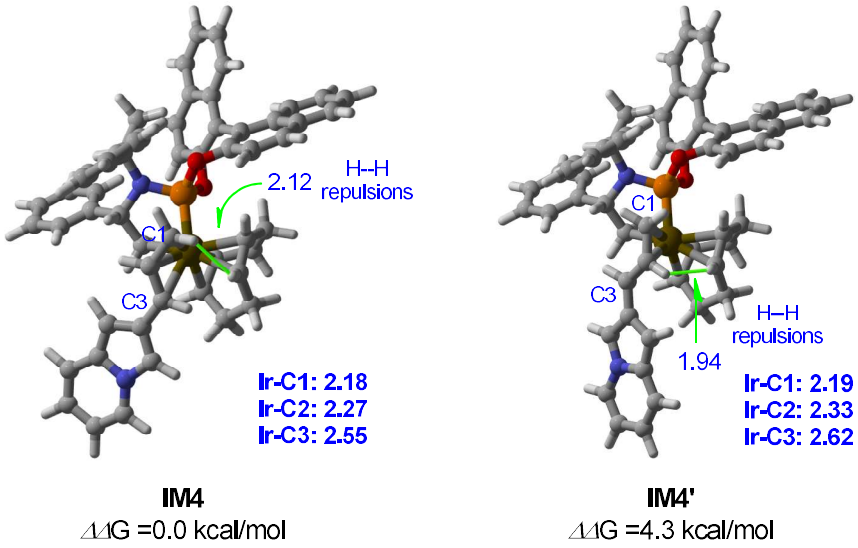

Fig. S4. Optimized structures of the π-allyliridium(III) species **IM4** and **IM4'**, with selected bond distances given in Å.

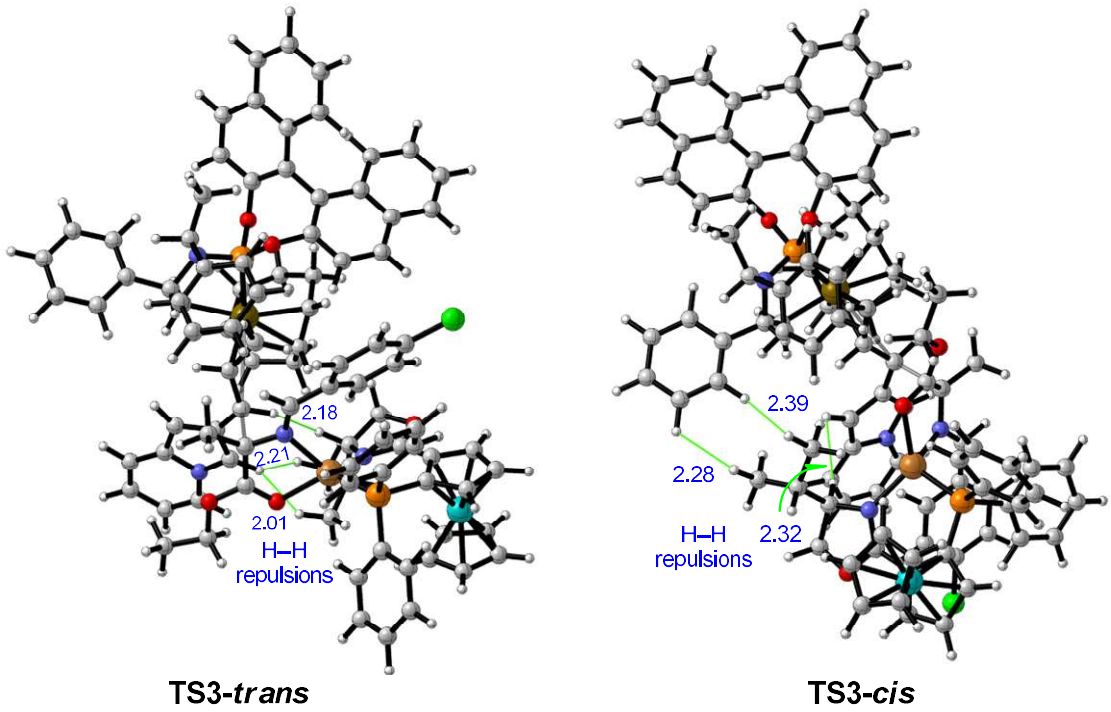

Fig. S5. Optimized structures of the *Re*-face−*Si*-face reaction pathways (**TS3**) enclosed strong steric hindrances between allyl moiety and oxazoline fragment, with selected bond distances given in Å.

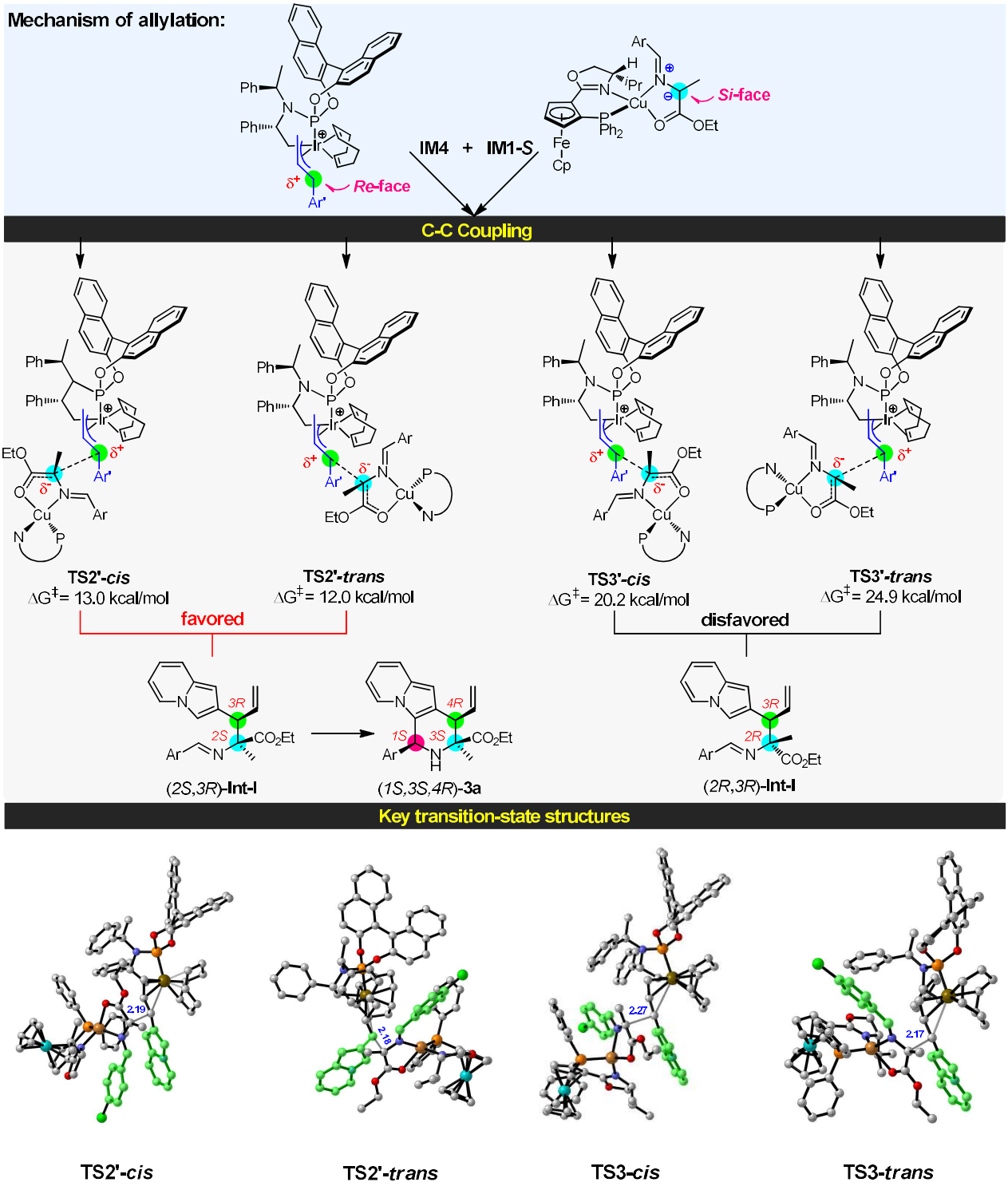

Fig. S6. Mechanism for the allylation of Cu^{I}-azomethine ylide **IM1-*S*** by allyl-Ir^{III} **IM4** [Cu(I)/(*S*,S_p)-**L1**+ Ir(I)/(*R*,*R*,R_a)-**L6**], and the optimized structures of bond-forming transition states. Free energies are given in kcal/mol (energy zero: **IM1-*S*** and **IM4**), and selected distances are shown in Å.

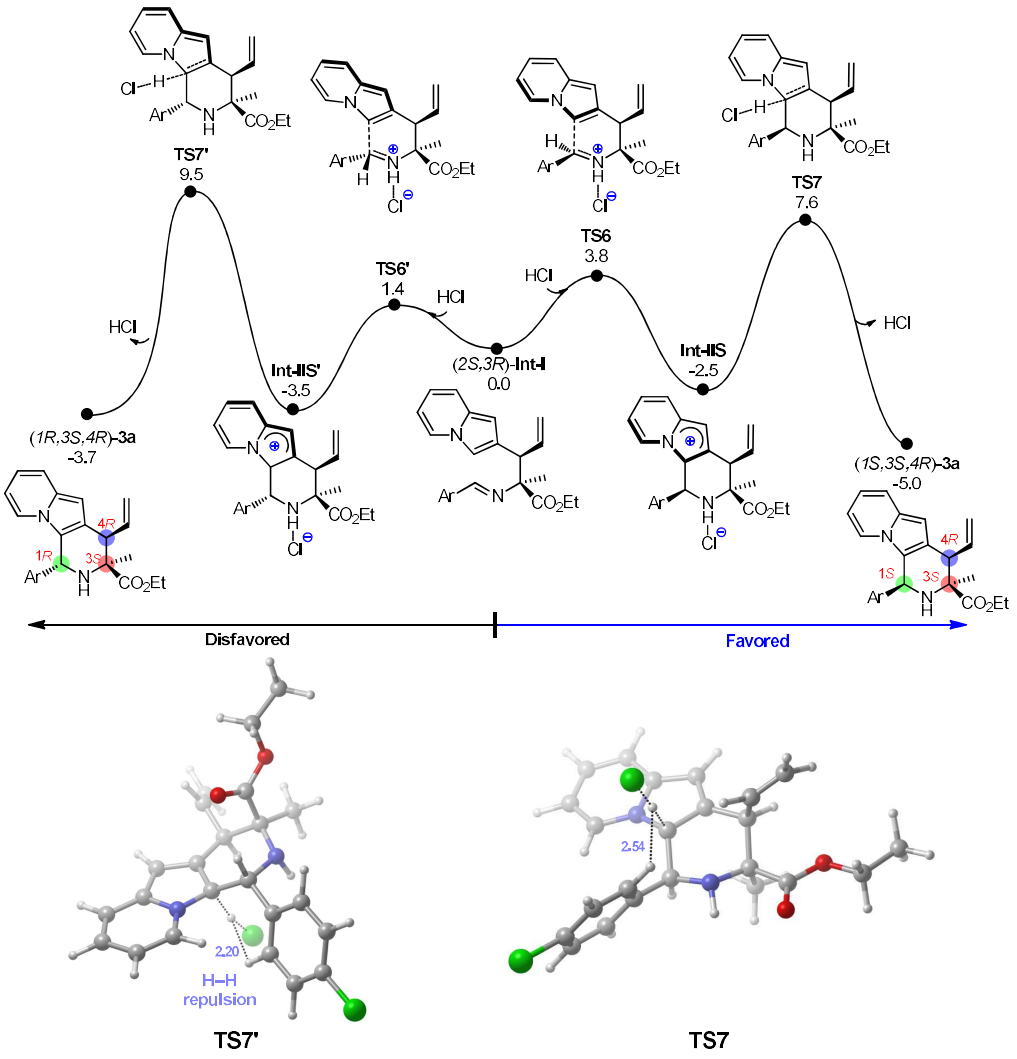

Fig. S7. Free energy profiles for Friedel-Crafts type reaction of (*2S,3R*)-**Int-I**.

Energies and Cartesian Coordinates (Å) for the Optimized Structures

(*R*)-**IM0**

M06-L SCF energy in solvent: -5590.968383 a.u

C	0.412413	-1.700265	1.879946
C	0.932121	-2.539371	2.922944
H	0.578122	-2.551478	3.947642
C	2.012377	-3.291730	2.388729
H	2.642188	-3.976909	2.945627
C	1.193127	-1.949484	0.678118
C	2.170174	-2.943197	1.018355
H	2.932592	-3.322203	0.345326
C	-2.012620	1.041056	2.064066
C	-2.516280	-0.000980	3.069167
H	-2.653991	0.386452	4.083230
N	-0.899454	0.344169	1.388192
C	-0.649780	-0.728034	2.074425
O	-1.455270	-0.981936	3.122260
H	-3.428407	-0.522532	2.756109
H	-2.781772	1.278814	1.314206
C	-1.574350	2.347101	2.744950
C	-0.740706	3.227634	1.829796
C	-2.806059	3.090085	3.246643
H	-0.952973	2.065179	3.613824
H	0.205639	2.750548	1.555120
H	-0.513593	4.185686	2.313136
H	-1.284925	3.448772	0.898179
H	-3.429293	2.477366	3.909745
H	-3.436364	3.404677	2.402881
H	-2.526518	3.990759	3.803367
P	0.926591	-1.147333	-0.918519
C	-0.089522	-2.351912	-1.842692
C	-0.274633	-2.160626	-3.220060
C	-0.802658	-3.366299	-1.193389
C	-1.150459	-2.971758	-3.931782
H	0.277548	-1.373720	-3.736665
C	-1.684335	-4.173668	-1.910514
H	-0.665493	-3.531782	-0.124624
C	-1.862837	-3.976091	-3.276567
H	-1.279260	-2.820686	-5.001760
H	-2.227339	-4.965725	-1.397931
H	-2.550760	-4.607976	-3.834289
C	2.553798	-1.194049	-1.734088
C	3.278088	-0.004040	-1.873839
C	3.103929	-2.393986	-2.204272
C	4.545650	-0.018701	-2.450817
H	2.840279	0.932962	-1.525473
C	4.369026	-2.404485	-2.781522
H	2.532747	-3.319762	-2.126922
C	5.092442	-1.218214	-2.900393
H	5.105555	0.908932	-2.554738
H	4.790367	-3.339349	-3.145354
H	6.081307	-1.228757	-3.354449
Cu	-0.158567	0.720849	-0.507001
O	1.244031	2.597983	-0.633326
C	0.667257	3.430367	-1.321597
O	1.024787	4.698112	-1.425380
C	-0.515760	3.098257	-2.206940
N	-1.281425	2.020583	-1.582526
C	-2.564436	2.068421	-1.726326
H	-3.020364	2.944067	-2.214164
C	-3.477803	1.050916	-1.243282
C	-4.803688	1.414741	-0.957689
C	-3.074805	-0.275612	-1.014366
C	-5.686980	0.505761	-0.394317
H	-5.137481	2.433034	-1.155781
C	-3.951342	-1.196680	-0.464405
H	-2.071125	-0.594592	-1.295623
C	-5.249017	-0.794047	-0.138990
H	-6.706818	0.791872	-0.153719
H	-3.639960	-2.224759	-0.294597
C	2.191484	5.107329	-0.650451
H	3.044531	4.507335	-0.986768
H	1.998464	4.855844	0.398602
C	3.021094	0.550165	1.619303
C	2.451476	0.598151	2.925977
H	1.585842	1.186191	3.216335
C	3.165931	-0.313002	3.757427
H	2.949249	-0.533267	4.797015
C	4.088706	-0.400518	1.640098
H	4.691578	-0.698809	0.787776
C	4.179172	-0.929161	2.963617
H	4.867152	-1.698627	3.296879
H	2.672585	1.115360	0.759274
Fe	2.347041	-1.285617	2.168141
Cl	-6.334534	-1.933091	0.582942

C	2.385443	6.578587	-0.875134
H	1.511335	7.148696	-0.545944
H	3.252161	6.926888	-0.305070
H	2.563550	6.799692	-1.931977
H	-1.133632	3.999343	-2.335801
C	0.011351	2.641588	-3.568541
H	0.602792	3.433141	-4.040083
H	0.639452	1.749854	-3.452772
H	-0.825549	2.391397	-4.228262

(*S*)-**IM0**

M06-L SCF energy in solvent: -5590.964102 a.u

C	-0.282588	-2.220428	-1.313007
C	-0.762086	-3.350950	-2.059115
H	-0.347146	-3.698915	-2.998225
C	-1.892430	-3.882748	-1.381967
H	-2.505848	-4.707895	-1.727220
C	-1.138688	-2.065598	-0.149499
C	-2.122185	-3.106048	-0.212363
H	-2.932253	-3.238351	0.497946
C	2.365103	0.200937	-2.102218
C	2.784709	-1.101694	-2.797449
H	2.928083	-1.000494	-3.878096
N	1.145508	-0.184727	-1.359470
C	0.843882	-1.395199	-1.719624
O	1.669658	-1.996444	-2.593907
H	3.670902	-1.577559	-2.361994
H	3.122012	0.520940	-1.372164
C	2.150145	1.354680	-3.090986
C	1.496656	2.559492	-2.436949
C	3.492276	1.741039	-3.702049
H	1.486185	0.983430	-3.891215
H	0.500815	2.324262	-2.047230
H	1.397209	3.384664	-3.152325
H	2.111650	2.920733	-1.598875
H	3.991844	0.902250	-4.202176
H	4.174610	2.112339	-2.923749
H	3.373996	2.537442	-4.444520
P	-0.930945	-0.816996	1.134866
C	0.032067	-1.684825	2.421854
C	0.157681	-1.097008	3.689483
C	0.772937	-2.836069	2.129402
C	1.002129	-1.653613	4.643382
H	-0.414972	-0.199526	3.929635
C	1.621380	-3.388295	3.087598
H	0.683210	-3.308859	1.151696
C	1.741461	-2.797285	4.341997
H	1.086039	-1.193228	5.625849
H	2.186334	-4.288312	2.851267
H	2.405926	-3.228740	5.087497
C	-2.598350	-0.631170	1.844955
C	-3.357921	0.489348	1.488675
C	-3.149952	-1.586567	2.708488
C	-4.655502	0.643227	1.968996
H	-2.920929	1.236775	0.824920
C	-4.444882	-1.427496	3.192021
H	-2.559154	-2.452848	3.007552
C	-5.199838	-0.315989	2.820184
H	-5.242192	1.515555	1.685216
H	-4.866263	-2.172385	3.864017
H	-6.211578	-0.194388	3.201665
Cu	0.227836	0.815505	0.211933
O	-1.210341	2.525584	-0.428160
C	-1.050667	3.469631	0.333141
O	-1.919457	4.459491	0.469382
C	0.136970	3.621666	1.274070
N	1.059274	2.508093	1.027937
C	2.320868	2.683533	1.227681
H	2.719046	3.672361	1.487513
C	3.295741	1.615944	1.070031
C	4.580711	1.930723	0.603464
C	2.976812	0.274713	1.334654
C	5.503586	0.929948	0.332737
H	4.848274	2.971068	0.418801
C	3.895665	-0.733987	1.085270
H	2.009792	0.021892	1.769522
C	5.147698	-0.399560	0.566096
H	6.491424	1.168582	-0.051406
H	3.649372	-1.771524	1.298604
C	-3.115310	4.380689	-0.360776
H	-3.621723	3.434182	-0.133771
H	-2.793927	4.341007	-1.407263
C	-2.847027	0.001200	-2.006094
C	-2.197259	-0.401211	-3.210484
H	-1.302903	0.053348	-3.627175
C	-2.881704	-1.540566	-3.726001
H	-2.606438	-2.104725	-4.610341
C	-3.933725	-0.896640	-1.771748

H	-4.594994	-0.887480	-0.910697
C	-3.955407	-1.846900	-2.836998
H	-4.639717	-2.683014	-2.931991
H	-2.536959	0.825619	-1.370973
Fe	-2.183709	-1.914565	-1.850392
Cl	6.288254	-1.657951	0.224559
C	-3.958202	5.582854	-0.048937
H	-3.423390	6.510850	-0.273467
H	-4.868742	5.562528	-0.655503
H	-4.251902	5.600080	1.005097
H	-0.284161	3.452167	2.280212
C	0.722037	5.027136	1.228236
H	1.228374	5.212002	0.273152
H	-0.076660	5.762935	1.340464
H	1.436668	5.196289	2.038709

(*R*)-**IM0'**

M06-L SCF energy in solvent: -5590.960353 a.u

C	-2.575070	0.055627	0.879575
C	-4.011673	0.066647	0.908486
H	-4.616695	0.026554	1.806898
C	-4.480365	0.091270	-0.431588
H	-5.519810	0.065622	-0.739505
C	-2.153398	0.061152	-0.513616
C	-3.353464	0.085225	-1.300429
H	-3.387629	0.102610	-2.385368
C	-0.164644	-0.604714	3.539157
C	-1.457067	-0.251968	4.271005
H	-1.772630	-0.982511	5.020320
N	-0.468248	-0.180983	2.157117
C	-1.762532	-0.115128	2.065617
O	-2.450606	-0.260568	3.217317
H	-1.454749	0.751237	4.715532
H	0.696038	-0.031193	3.913336
C	0.150437	-2.109694	3.619853
C	1.168129	-2.555122	2.582856
C	0.615230	-2.473203	5.024020
H	-0.799859	-2.635107	3.419021
H	0.850060	-2.301481	1.561819
H	1.322157	-3.639497	2.630447
H	2.142810	-2.081693	2.767439
H	-0.103660	-2.178024	5.798079
H	1.570412	-1.983518	5.256588
H	0.769053	-3.553220	5.119997
P	-0.449505	0.241298	-1.129395
C	-0.629025	1.579175	-2.361168
C	0.178652	1.600856	-3.505666
C	-1.522227	2.635697	-2.137440
C	0.080059	2.648345	-4.417058
H	0.876398	0.784843	-3.693727
C	-1.621071	3.677073	-3.055399
H	-2.143050	2.638320	-1.242372
C	-0.822672	3.685780	-4.197431
H	0.704827	2.647019	-5.307877
H	-2.335191	4.481435	-2.882876
H	-0.907983	4.496876	-4.917664
C	-0.090582	-1.229912	-2.143236
C	0.985553	-2.041533	-1.774174
C	-0.856136	-1.581220	-3.262794
C	1.292464	-3.190813	-2.498855
H	1.587448	-1.759826	-0.910675
C	-0.556234	-2.733054	-3.982148
H	-1.681989	-0.944311	-3.580191
C	0.516566	-3.539974	-3.600625
H	2.141704	-3.807328	-2.207857
H	-1.155462	-3.000173	-4.850565
H	0.751625	-4.436054	-4.171116
Cu	0.717502	0.656829	0.730664
C	-2.242230	-3.249587	-0.455765
C	-2.702106	-3.220543	0.891805
H	-2.074224	-3.225837	1.778215
C	-4.124500	-3.124136	0.876304
H	-4.768983	-3.045736	1.745109
C	-3.381329	-3.170203	-1.310980
H	-3.361958	-3.139332	-2.395063
C	-4.545349	-3.097502	-0.487677
H	-5.567234	-2.993809	-0.836475
H	-1.207006	-3.290598	-0.777114
Fe	-3.308033	-1.542242	-0.097325
O	-0.404130	2.855793	0.844464
C	0.520618	3.630114	1.029428
O	0.472076	4.937781	0.819214
C	1.857700	3.211803	1.611986
N	2.247371	1.902829	1.078877
C	3.497544	1.772974	0.767878
C	4.111202	0.536462	0.335406
C	5.366835	0.564878	-0.292873
C	3.494094	-0.705168	0.546996

C	5.966882	-0.602456	-0.739698
H	5.869596	1.519106	-0.447205
C	4.090176	-1.881852	0.125093
H	2.542553	-0.743004	1.080390
C	5.319511	-1.821885	-0.533055
H	6.929735	-0.578284	-1.242400
H	3.617517	-2.845412	0.304854
C	-0.797268	5.455598	0.325452
H	-1.562437	5.242877	1.080996
H	-1.052334	4.894224	-0.580966
Cl	6.052231	-3.285475	-1.093570
H	4.157223	2.651240	0.824423
C	-0.616540	6.924495	0.073384
H	-1.553623	7.354217	-0.294534
H	0.157759	7.103817	-0.678966
H	-0.337417	7.455465	0.988848
H	2.611511	3.971133	1.359030
C	1.707414	3.127096	3.130506
H	0.937436	2.390881	3.391969
H	1.416233	4.098506	3.543946
H	2.653716	2.823225	3.589388

(*S*)-**IM0'**

M06-L SCF energy in solvent: -5590.960336 a.u

C	-2.571764	0.047372	0.882948
C	-4.008445	0.047972	0.914994
H	-4.611199	0.013353	1.815153
C	-4.480151	0.053952	-0.424209
H	-5.520019	0.017351	-0.729687
C	-2.153350	0.039776	-0.511022
C	-3.355088	0.046682	-1.295405
H	-3.391700	0.051675	-2.380369
C	-0.150297	-0.566385	3.543543
C	-1.443956	-0.217044	4.274847
H	-1.751751	-0.942568	5.032216
N	-0.460608	-0.159456	2.157995
C	-1.755519	-0.105039	2.068902
O	-2.439820	-0.244213	3.223666
H	-1.448793	0.790504	4.709455
H	0.706431	0.018211	3.909752
C	0.177850	-2.067672	3.638523
C	1.195970	-2.514572	2.602619
C	0.650009	-2.413024	5.044796
H	-0.768535	-2.603231	3.445870
H	0.871911	-2.273866	1.580281
H	1.359800	-3.597004	2.660473
H	2.167059	-2.030543	2.778563
H	-0.068872	-2.115932	5.818146
H	1.601886	-1.913277	5.269528
H	0.812954	-3.490737	5.151262
P	-0.452345	0.224214	-1.134002
C	-0.645448	1.550197	-2.376877
C	0.160279	1.568995	-3.522842
C	-1.548662	2.599997	-2.161852
C	0.049444	2.606163	-4.444619
H	0.865896	0.758133	-3.703883
C	-1.660428	3.630448	-3.090634
H	-2.167158	2.606577	-1.265256
C	-0.864347	3.635842	-4.234301
H	0.672919	2.602426	-5.336339
H	-2.383003	4.428656	-2.925152
H	-0.959935	4.438191	-4.962951
C	-0.090590	-1.252935	-2.138494
C	0.990408	-2.058571	-1.770308
C	-0.859575	-1.612615	-3.252995
C	1.298395	-3.210061	-2.491142
H	1.595615	-1.770735	-0.911064
C	-0.558568	-2.766553	-3.968420
H	-1.688669	-0.979839	-3.570096
C	0.519044	-3.567420	-3.587896
H	2.151446	-3.821761	-2.201144
H	-1.160454	-3.039790	-4.833089
H	0.755329	-4.465168	-4.155283
Cu	0.715667	0.668377	0.717053
C	-2.217019	-3.270592	-0.414396
C	-2.675912	-3.229803	0.933286
H	-2.047450	-3.221860	1.819241
C	-4.099025	-3.144432	0.918319
H	-4.743217	-3.061332	1.786921
C	-3.357460	-3.208325	-1.269174
H	-3.338988	-3.188711	-2.353578
C	-4.521281	-3.135455	-0.445504
H	-5.544228	-3.043024	-0.794314
H	-1.181774	-3.308144	-0.736213
Fe	-3.295149	-1.567128	-0.073904
O	-0.417601	2.860280	0.805470
C	0.500301	3.643045	0.989067
O	0.439384	4.949381	0.774501

C	1.840301	3.238274	1.574718
N	2.238061	1.927646	1.052391
C	3.489293	1.802561	0.743454
C	4.110811	0.566317	0.321466
C	5.369914	0.596603	-0.299735
C	3.498049	-0.676876	0.536747
C	5.978640	-0.570785	-0.734624
H	5.869184	1.552160	-0.457121
C	4.102241	-1.853317	0.126098
H	2.543663	-0.716038	1.064940
C	5.335823	-1.791931	-0.524002
H	6.944880	-0.545239	-1.230740
H	3.632990	-2.817965	0.308950
C	-0.834125	5.450200	0.273557
H	-1.611789	5.170506	0.993512
H	-1.043926	4.928221	-0.667793
Cl	6.079621	-3.256300	-1.067538
H	4.143879	2.685010	0.793958
C	-0.697906	6.935524	0.103271
H	-1.637687	7.352552	-0.272079
H	0.092403	7.180889	-0.612924
H	-0.466014	7.425916	1.053906
H	2.588985	4.000371	1.315169
C	1.690907	3.164801	3.093902
H	0.926256	2.425051	3.361010
H	1.392965	4.137378	3.499606
H	2.639409	2.871120	3.554862

IM1

M06-L SCF energy in solvent: -5590.488844 a.u

C	0.256000	-1.710242	1.860881
C	0.731444	-2.599346	2.880964
H	0.400327	-2.596275	3.913559
C	1.746195	-3.419880	2.314403
H	2.335663	-4.158039	2.848422
C	0.987972	-1.996227	0.640133
C	1.899256	-3.060892	0.944949
H	2.618949	-3.478937	0.248267
C	-1.885123	1.243063	2.107699
C	-2.515495	0.226142	3.069163
H	-2.637262	0.592170	4.093868
N	-0.837882	0.456893	1.432874
C	-0.717627	-0.652270	2.082293
O	-1.564160	-0.864590	3.113376
H	-3.468937	-0.183416	2.714199
H	-2.609272	1.583865	1.354171
C	-1.307349	2.471962	2.827235
C	-0.450237	3.328229	1.908992
C	-2.443863	3.300103	3.415048
H	-0.678510	2.094428	3.654923
H	0.382716	2.767015	1.469508
H	-0.037674	4.186332	2.454206
H	-1.049993	3.719446	1.076378
H	-3.076395	2.730922	4.108276
H	-3.092289	3.678913	2.612266
H	-2.056392	4.167323	3.961862
P	0.713868	-1.167835	-0.949551
C	-0.385049	-2.346675	-1.818543
C	-0.714801	-2.071474	-3.154263
C	-1.005376	-3.425453	-1.177342
C	-1.634547	-2.860490	-3.832685
H	-0.252437	-1.220682	-3.657343
C	-1.933600	-4.211096	-1.859132
H	-0.764889	-3.653442	-0.139322
C	-2.251731	-3.930360	-3.184437
H	-1.881742	-2.632999	-4.868038
H	-2.412485	-5.044377	-1.347219
H	-2.983708	-4.539470	-3.711652
C	2.323184	-1.380779	-1.792671
C	3.171043	-0.271223	-1.892824
C	2.742186	-2.615038	-2.306821
C	4.431809	-0.405524	-2.470465
H	2.826842	0.697603	-1.526545
C	4.001268	-2.742936	-2.885809
H	2.073129	-3.475503	-2.258508
C	4.850599	-1.639901	-2.960945
H	5.086214	0.462035	-2.544590
H	4.320291	-3.705516	-3.282510
H	5.834903	-1.742297	-3.414957
Cu	-0.041867	0.835459	-0.473982
O	1.509959	2.275547	-0.722323
C	1.010011	3.289085	-1.286041
O	1.818304	4.333050	-1.622363
C	-0.354290	3.458127	-1.598703
N	-1.158491	2.401857	-1.288906
C	-2.471339	2.502410	-1.365962
H	-2.924937	3.466744	-1.620678
C	-3.391545	1.432607	-1.069578

C	-4.734233	1.745209	-0.771581
C	-3.027452	0.071167	-1.038175
C	-5.647953	0.768335	-0.403643
H	-5.053740	2.787342	-0.806853
C	-3.928514	-0.917393	-0.673767
H	-2.014340	-0.211126	-1.319752
C	-5.235965	-0.561489	-0.343634
H	-6.674419	1.029953	-0.158838
H	-3.624627	-1.962570	-0.664989
C	3.200959	4.172246	-1.303705
H	3.592262	3.279641	-1.813374
H	3.310964	3.995600	-0.224817
C	2.998739	0.362186	1.592440
C	2.448891	0.414179	2.907257
H	1.618419	1.042860	3.215593
C	3.115102	-0.557611	3.711215
H	2.893616	-0.789350	4.747728
C	4.008024	-0.650196	1.581964
H	4.583222	-0.962959	0.715725
C	4.082133	-1.215543	2.891929
H	4.724694	-2.034363	3.198754
H	2.668358	0.964475	0.748697
C	-0.907556	4.728698	-2.143999
H	-1.526974	4.549499	-3.036671
H	-0.107589	5.420358	-2.415911
H	-1.561559	5.243863	-1.418983
Fe	2.222752	-1.445211	2.120666
Cl	-6.372062	-1.799002	0.143295
C	3.911231	5.424145	-1.746316
H	3.510037	6.304439	-1.232635
H	4.981492	5.355605	-1.523092
H	3.795096	5.580179	-2.824164

IM1'

M06-L SCF energy in solvent: -5590.482432 a.u

C	-0.099175	-2.715460	-0.647394
C	-0.609536	-4.035536	-0.889788
H	-0.333434	-4.661602	-1.730081
C	-1.573993	-4.329603	0.108393
H	-2.170721	-5.233658	0.168735
C	-0.765520	-2.183707	0.533455
C	-1.662091	-3.211353	0.983226
H	-2.305577	-3.143004	1.854647
C	2.199809	-0.743839	-2.712636
C	2.207484	-2.151092	-3.323037
H	1.717278	-2.181040	-4.307740
N	1.163118	-0.831444	-1.666286
C	0.836838	-2.076255	-1.560697
O	1.418848	-2.948332	-2.421750
H	3.194802	-2.613972	-3.405168
H	3.148371	-0.521902	-2.195232
C	1.952790	0.341954	-3.761267
C	1.875884	1.730841	-3.152509
C	3.052118	0.280455	-4.817705
H	0.987700	0.109935	-4.246867
H	1.036882	1.829396	-2.457801
H	1.756576	2.491670	-3.933527
H	2.789977	1.965864	-2.588406
H	3.105706	-0.694066	-5.320675
H	4.034524	0.474257	-4.364996
H	2.893763	1.039083	-5.592303
P	-0.266613	-0.628883	1.346597
C	0.434939	-1.258832	2.919561
C	-0.354446	-1.563136	4.034185
C	1.820652	-1.451305	2.982901
C	0.232480	-2.062246	5.192789
H	-1.431406	-1.393030	3.998272
C	2.401792	-1.957823	4.142289
H	2.437894	-1.181994	2.122786
C	1.610340	-2.263963	5.246796
H	-0.386965	-2.291866	6.058375
H	3.480490	-2.101818	4.186429
H	2.067483	-2.651625	6.155916
C	-1.776537	0.250536	1.883734
C	-1.590081	1.578673	2.295301
C	-3.073746	-0.272171	1.873889
C	-2.672574	2.363140	2.675787
H	-0.586321	2.007702	2.277949
C	-4.160517	0.521745	2.235744
H	-3.248472	-1.292462	1.538743
C	-3.963480	1.839713	2.635820
H	-2.508588	3.397825	2.971620
H	-5.166585	0.105492	2.198358
H	-4.815165	2.462611	2.903149
Cu	1.155757	0.402737	0.070632
O	3.257739	0.026101	0.282027
C	3.820938	1.151233	0.353417
O	5.172706	1.215546	0.531354

C	3.173395	2.402898	0.258895
N	1.825715	2.349699	0.057695
C	1.099417	3.449316	0.019588
H	1.575057	4.412203	0.233673
C	-0.313883	3.508122	-0.253848
C	-1.005063	4.693473	0.078764
C	-1.068403	2.477375	-0.856717
C	-2.368687	4.835312	-0.122415
H	-0.446599	5.514723	0.529177
C	-2.430594	2.615594	-1.082483
H	-0.574299	1.550872	-1.157231
C	-3.080530	3.785212	-0.697947
H	-2.883099	5.750495	0.161581
H	-2.994647	1.828560	-1.577752
C	5.836937	-0.042169	0.652430
H	5.649545	-0.644789	-0.247087
H	5.411842	-0.599445	1.499177
C	-3.213975	-0.993978	-1.305793
C	-2.352045	-1.278101	-2.403948
H	-1.555834	-0.632393	-2.766522
C	-2.648816	-2.596054	-2.868732
H	-2.131503	-3.122393	-3.664555
C	-4.040894	-2.134310	-1.083203
H	-4.780161	-2.240862	-0.295494
C	-3.694339	-3.125397	-2.050862
H	-4.120234	-4.120461	-2.125777
H	-3.197715	-0.094256	-0.701040
C	3.897507	3.700855	0.355610
H	4.974676	3.542599	0.436030
H	3.581251	4.295583	1.228218
H	3.707560	4.332650	-0.527739
Cl	-4.803291	3.938194	-0.950642
Fe	-2.075657	-2.643657	-0.932609
C	7.303553	0.241486	0.843822
H	7.710082	0.795420	-0.009347
H	7.864368	-0.694389	0.943099
H	7.472900	0.839809	1.745466

Cs_2CO_3

M06-L SCF energy in solvent: -304.357982 a.u

O	-1.123135	1.806300	0.001059
C	0.000138	1.180650	-0.000025
O	1.122975	1.806938	-0.001051
O	0.000400	-0.155272	0.000075
Cs	-2.816330	-0.315872	-0.000066
Cs	2.816280	-0.315903	0.000057

$Cs_2CO_3 \cdot H^+$

M06-L SCF energy in solvent: -304.867520 a.u

H	0.849582	2.828372	0.000434
O	-1.134946	1.868732	-0.000494
C	-0.100968	1.181358	-0.000101
O	1.117094	1.896259	0.000478
O	0.048496	-0.067539	-0.000128
Cs	-3.007555	-0.353559	0.000040
Cs	2.998665	-0.364552	-0.000016

2a

M06-L SCF energy in solvent: -783.823347 a.u

C	2.474146	-0.566993	0.658540
H	2.839600	-0.505664	1.693118
H	2.570059	-1.614273	0.343354
C	1.087236	-0.071274	0.517525
H	0.922761	0.982074	0.751418
C	0.057771	-0.860762	0.174485
H	0.270573	-1.907098	-0.062917
O	3.342484	0.254006	-0.160188
C	4.643351	0.000681	0.024063
O	5.118727	-0.817635	0.779541
O	5.332436	0.821285	-0.784062
C	6.747540	0.664066	-0.681985
H	7.045646	-0.356838	-0.940620
H	7.090463	0.884381	0.333992
C	-1.332122	-0.466930	0.099993
C	-1.904797	0.795330	0.386162
C	-2.365559	-1.321327	-0.277957
C	-3.272854	0.701556	0.181336
H	-1.383542	1.687412	0.711651
H	-2.348370	-2.363045	-0.572596
C	-4.368084	1.584673	0.294089
C	-4.816897	-1.048813	-0.515652
C	-5.639484	1.159034	0.010829
H	-4.171103	2.606511	0.610262
C	-5.862321	-0.183034	-0.400580
H	-4.911308	-2.085624	-0.824739
H	-6.480093	1.842581	0.099092
H	-6.863447	-0.536916	-0.628747
N	-3.541179	-0.627027	-0.232851

H	7.170284	1.377189	-1.390734

IM2

M06-L SCF energy in solvent: -2352.941809 a.u

Ir	-1.605152	-1.769286	-0.549346
O	0.776678	0.121107	1.199450
O	0.806297	0.231254	-1.356686
C	1.931083	-0.643670	1.176102
C	2.016344	-1.718472	2.082163
H	1.189602	-1.880349	2.770230
C	3.130789	-2.518062	2.089141
H	3.207694	-3.349586	2.788832
C	4.185780	-2.292625	1.173059
C	5.308692	-3.152380	1.112929
H	5.352290	-3.996015	1.801785
C	6.313863	-2.942685	0.199547
H	7.168382	-3.615603	0.160046
C	6.229366	-1.858904	-0.698168
H	7.013955	-1.707390	-1.437255
C	5.160065	-0.994926	-0.654539
H	5.102269	-0.168472	-1.359533
C	4.112987	-1.172129	0.284097
C	2.980266	-0.296524	0.339966
C	2.902855	0.945500	-0.456198
C	3.896953	1.972177	-0.351590
C	4.967390	1.907009	0.575649
H	5.041531	1.047389	1.237180
C	5.897457	2.916299	0.662237
H	6.703557	2.842593	1.390037
C	5.812148	4.047174	-0.174605
H	6.556928	4.837134	-0.099178
C	4.776596	4.153354	-1.071211
H	4.685754	5.030107	-1.712519
C	3.793334	3.139931	-1.176433
C	2.696498	3.264823	-2.062614
H	2.630778	4.149043	-2.695858
C	1.714752	2.308233	-2.104424
H	0.851531	2.402823	-2.758984
C	1.813197	1.166423	-1.282807
P	-0.272830	-0.030704	-0.090673
N	-1.214093	1.327121	0.136631
C	-2.792744	-0.124710	-1.153488
H	-2.504209	0.067743	-2.202748
H	-3.868163	-0.359457	-1.181057
C	-2.618993	1.166971	-0.349742
H	-3.258987	1.113520	0.546683
C	-3.027847	2.381321	-1.152642
C	-2.286455	2.751181	-2.279997
H	-1.409335	2.158288	-2.545703
C	-2.655125	3.850070	-3.044866
H	-2.067060	4.126794	-3.918993
C	-3.780681	4.597455	-2.695599
H	-4.072532	5.458563	-3.294306
C	-4.526554	4.237514	-1.577522
H	-5.404605	4.817666	-1.297506
C	-4.147600	3.137965	-0.807736
H	-4.721749	2.863582	0.078722
C	-1.028498	2.550816	0.950295
H	-1.446122	3.359280	0.330139
C	-1.866195	2.486298	2.214185
C	-2.635580	3.589590	2.587084
H	-2.649914	4.468961	1.940524
C	-3.388724	3.571329	3.758259
H	-3.987076	4.438729	4.032518
C	-3.384677	2.439812	4.569015
H	-3.977409	2.418550	5.481961
C	-2.624391	1.330645	4.201304
H	-2.621760	0.440610	4.828903
C	-1.870346	1.352980	3.032222
H	-1.286627	0.480024	2.737708
C	0.401885	2.964060	1.267729
H	1.014991	3.021314	0.363338
H	0.888522	2.298198	1.983214
H	0.365740	3.966151	1.710916
C	-3.408259	-2.929980	-0.072353
H	-4.209087	-2.196646	0.040641
C	-3.008947	-3.254301	-1.378615
H	-3.510472	-2.716840	-2.187082
C	-2.313214	-4.539639	-1.773236
H	-2.656240	-4.838102	-2.771853
H	-2.623841	-5.351795	-1.103715
C	-0.781126	-4.406597	-1.790916
H	-0.315157	-5.403554	-1.711452
H	-0.471634	-4.009964	-2.767493
C	-0.244702	-3.475393	-0.732992
H	0.762493	-3.096632	-0.933723
C	-0.694868	-3.427632	0.601298
H	-0.011191	-2.990791	1.327671

C	-1.732854	-4.361272	1.190821
H	-1.472749	-4.576144	2.235227
H	-1.700832	-5.331994	0.679806
C	-3.150308	-3.772269	1.146289
H	-3.902573	-4.576206	1.219958
H	-3.304351	-3.135247	2.027595

IM3

M06-L SCF energy in solvent: -3136.790777 a.u

Ir	-0.976827	-0.805393	-1.486027
O	1.690972	-0.304158	0.830889
O	1.728913	1.038551	-1.336918
C	2.849373	-0.942403	0.424288
C	2.924139	-2.332473	0.643695
H	2.088051	-2.836213	1.129006
C	4.053846	-3.012983	0.267846
H	4.128851	-4.086393	0.437546
C	5.130359	-2.340755	-0.358273
C	6.274162	-3.044323	-0.806068
H	6.313649	-4.121629	-0.645369
C	7.305857	-2.392792	-1.437939
H	8.177487	-2.947337	-1.780216
C	7.225327	-1.002342	-1.654828
H	8.031199	-0.489544	-2.176621
C	6.134089	-0.286256	-1.220344
H	6.082400	0.784178	-1.405571
C	5.060658	-0.921230	-0.546282
C	3.906609	-0.204199	-0.088080
C	3.807438	1.270301	-0.178490
C	4.770243	2.146581	0.420610
C	5.825695	1.674088	1.240225
H	5.914653	0.605587	1.423034
C	6.723975	2.542849	1.815742
H	7.519323	2.152878	2.448529
C	6.619331	3.932168	1.601452
H	7.340067	4.608853	2.056360
C	5.595435	4.426747	0.830461
H	5.488564	5.499843	0.671867
C	4.643893	3.562900	0.237295
C	3.559708	4.073951	-0.516426
H	3.483556	5.150619	-0.666060
C	2.603292	3.231919	-1.024170
H	1.746175	3.599124	-1.585518
C	2.724988	1.842794	-0.825892
P	0.633095	0.316108	-0.293002
N	-0.082145	1.492671	0.664352
C	-1.739692	1.178137	-1.139391
H	-1.301842	1.857562	-1.890920
H	-2.823977	1.171753	-1.308491
C	-1.480391	1.746574	0.253151
H	-2.146619	1.218414	0.953962
C	-1.839429	3.213858	0.301731
C	-0.888943	4.228608	0.165378
H	0.165607	3.959402	0.088319
C	-1.278748	5.565338	0.147576
H	-0.525655	6.345798	0.045728
C	-2.623994	5.906018	0.263518
H	-2.927546	6.951355	0.249879
C	-3.578220	4.899866	0.405886
H	-4.633315	5.153500	0.502327
C	-3.187101	3.565682	0.429729
H	-3.930535	2.772803	0.537475
C	0.199889	1.837818	2.093925
H	-0.396673	2.751009	2.234481
C	-0.372723	0.805241	3.047957
C	-1.700454	0.937548	3.475889
H	-2.279363	1.804214	3.148914
C	-2.285319	-0.007969	4.315200
H	-3.322476	0.110607	4.625869
C	-1.541788	-1.096703	4.760373
H	-1.997361	-1.844349	5.407438
C	-0.210705	-1.223814	4.369392
H	0.386111	-2.066393	4.717645
C	0.367170	-0.285241	3.519047
H	1.405163	-0.405815	3.217486
C	1.638555	2.231915	2.373137
H	1.972808	2.993467	1.658850
H	2.337665	1.393885	2.324551
H	1.699104	2.659686	3.380597
C	-1.648754	-0.526635	-3.523693
H	-2.379318	0.286994	-3.571267
C	-0.273357	-0.133057	-3.407241
H	-0.097904	0.943970	-3.362227
C	0.899143	-0.924170	-3.976893
H	1.679936	-0.218675	-4.286395
H	0.588735	-1.438924	-4.897085
C	1.506344	-1.918757	-2.976824
H	1.991267	-2.757884	-3.504911

H	2.307844	-1.417520	-2.417782
C	0.506033	-2.457689	-1.983928
H	0.932442	-2.831781	-1.050449
C	-0.774366	-2.903658	-2.332115
H	-1.268695	-3.574107	-1.628396
C	-1.273274	-3.011127	-3.760885
H	-1.873433	-3.925406	-3.853564
H	-0.421245	-3.156429	-4.436551
C	-2.106468	-1.802159	-4.187287
H	-2.105198	-1.699054	-5.286856
H	-3.154791	-1.975475	-3.905320
C	-0.978099	-2.684420	0.986470
H	-0.011164	-2.348132	1.379463
H	-0.794512	-3.492847	0.269182
C	-1.745561	-1.539843	0.424180
H	-1.844734	-0.739348	1.164749
C	-2.815818	-1.656070	-0.521035
H	-2.982706	-2.634356	-0.976850
O	-1.723951	-3.257306	2.097450
C	-0.974817	-3.967709	2.937161
O	0.211141	-4.209895	2.836928
O	-1.768786	-4.379793	3.941668
C	-1.084736	-5.135547	4.936985
H	-0.328417	-4.522118	5.440449
H	-1.852682	-5.446221	5.646810
H	-0.591403	-6.008262	4.497889
C	-4.017241	-0.825008	-0.415840
C	-4.957660	-0.622126	-1.423037
C	-4.433652	-0.075261	0.707993
H	-4.994579	-0.992177	-2.440438
C	-5.619172	0.575542	0.382707
H	-3.949146	-0.052814	1.679156
C	-7.041169	0.717834	-1.582462
C	-6.499386	1.447926	1.052936
C	-7.882736	1.564708	-0.921793
H	-7.185863	0.391063	-2.608072
C	-7.613620	1.940146	0.419624
H	-6.265212	1.719690	2.080461
H	-8.757903	1.943137	-1.442065
H	-8.290238	2.613468	0.939904
N	-5.926736	0.224287	-0.953781

TS1

M06-L SCF energy in solvent: -3136.768141 a.u

Ir	-0.988914	-1.174094	-0.970012
O	1.799768	-0.023953	0.912383
O	1.616710	0.692506	-1.530027
C	2.900798	-0.813879	0.584932
C	2.965318	-2.092433	1.169584
H	2.194996	-2.376606	1.893476
C	4.030247	-2.901179	0.857602
H	4.111216	-3.890608	1.306712
C	5.032488	-2.479574	-0.049922
C	6.094892	-3.336220	-0.428299
H	6.133792	-4.334094	0.008402
C	7.049047	-2.929854	-1.329681
H	7.857585	-3.601150	-1.613139
C	6.971220	-1.642775	-1.898929
H	7.714120	-1.329107	-2.630169
C	5.961275	-0.779509	-1.543015
H	5.908404	0.207315	-1.997525
C	4.972041	-1.158074	-0.601155
C	3.897659	-0.288111	-0.221439
C	3.819327	1.113792	-0.687218
C	4.867136	2.063610	-0.452760
C	6.007369	1.762859	0.333818
H	6.094443	0.777255	0.784714
C	6.992657	2.699477	0.544980
H	7.853568	2.443523	1.159530
C	6.894548	3.987479	-0.019519
H	7.684090	4.717103	0.149222
C	5.791451	4.321310	-0.767466
H	5.690780	5.319112	-1.194193
C	4.751872	3.387498	-0.991735
C	3.595741	3.742715	-1.726675
H	3.526340	4.744959	-2.148223
C	2.567749	2.848946	-1.886836
H	1.664614	3.101192	-2.438738
C	2.684082	1.555763	-1.344917
P	0.658681	0.282111	-0.228335
N	-0.053649	1.641111	0.427800
C	-1.819007	0.807320	-1.077463
H	-1.484922	1.257126	-2.026005
H	-2.909434	0.710733	-1.135103
C	-1.478909	1.757590	0.060211
H	-2.076720	1.479937	0.943049
C	-1.880618	3.165828	-0.317967
C	-0.991915	4.071299	-0.900878

H	0.052003	3.778697	-1.023736
C	-1.422892	5.338270	-1.284675
H	-0.715827	6.038784	-1.726521
C	-2.750756	5.713924	-1.095891
H	-3.086555	6.705720	-1.393526
C	-3.644833	4.815602	-0.516797
H	-4.684034	5.101501	-0.360798
C	-3.209129	3.553646	-0.127170
H	-3.903724	2.846645	0.330724
C	0.307117	2.464973	1.631653
H	-0.069803	3.462412	1.362027
C	-0.500376	2.004017	2.827580
C	-1.619790	2.749947	3.209595
H	-1.850421	3.672711	2.672508
C	-2.447280	2.318109	4.242729
H	-3.317462	2.909317	4.524821
C	-2.161146	1.127805	4.905159
H	-2.809229	0.777035	5.706502
C	-1.042714	0.379872	4.539631
H	-0.825333	-0.555251	5.052285
C	-0.213660	0.815082	3.507264
H	0.649119	0.205105	3.235285
C	1.789677	2.636669	1.902075
H	2.330242	2.909084	0.988262
H	2.258488	1.750783	2.334341
H	1.904996	3.457883	2.618360
C	-1.810638	-1.349555	-2.976623
H	-2.588872	-0.591346	-3.099448
C	-0.459008	-0.895012	-3.053153
H	-0.330143	0.175140	-3.219746
C	0.704020	-1.736351	-3.555703
H	1.416091	-1.075622	-4.063902
H	0.345240	-2.429840	-4.328405
C	1.439816	-2.489432	-2.441878
H	1.923359	-3.398724	-2.836544
H	2.254909	-1.861757	-2.061282
C	0.556078	-2.860184	-1.280433
H	1.071431	-2.996513	-0.328761
C	-0.717341	-3.418322	-1.409971
H	-1.113684	-3.945176	-0.541322
C	-1.326580	-3.819060	-2.738165
H	-1.879624	-4.756896	-2.603139
H	-0.525147	-4.052797	-3.449928
C	-2.259709	-2.749779	-3.304853
H	-2.375713	-2.870464	-4.395603
H	-3.264716	-2.885809	-2.881918
C	-0.860789	-2.016668	1.343175
H	-0.092735	-1.511469	1.920284
H	-0.663355	-3.051553	1.100333
C	-2.068981	-1.387638	1.015332
H	-2.275824	-0.424632	1.484312
C	-2.987082	-1.891932	0.057386
H	-2.961299	-2.957286	-0.169715
O	-1.129055	-2.971953	3.404394
C	-0.070600	-2.694175	4.021798
O	1.015928	-2.243521	3.598747
O	-0.189713	-2.910928	5.397400
C	0.979784	-2.629594	6.138775
H	1.270682	-1.572912	6.057119
H	0.743594	-2.868223	7.180677
H	1.831467	-3.233768	5.801733
C	-4.253092	-1.220361	-0.192491
C	-5.216160	-1.630060	-1.112784
C	-4.738272	-0.046752	0.435651
H	-5.245211	-2.487180	-1.773974
C	-5.985937	0.245557	-0.100429
H	-4.260950	0.506990	1.237583
C	-7.434838	-0.753822	-1.780181
C	-6.956054	1.248623	0.103181
C	-8.361817	0.223887	-1.573138
H	-7.550661	-1.564130	-2.493612
C	-8.123952	1.245003	-0.615866
H	-6.752461	2.016608	0.846363
H	-9.280893	0.205090	-2.151151
H	-8.869941	2.018985	-0.455802
N	-6.263639	-0.751745	-1.064966

IM4

M06-L SCF energy in solvent: -2832.852159 a.u

Ir	-1.251828	-1.137950	0.061116
P	0.675576	0.096514	0.107036
N	0.289672	1.691762	0.383521
O	1.483899	-0.109198	-1.313566
O	1.865932	-0.103138	1.207814
C	2.912838	-1.006715	1.030975
C	2.999005	-2.043316	1.979083
H	2.265937	-2.072794	2.784202
C	4.009934	-2.965877	1.880386

H	4.098367	-3.764875	2.615020	H	2.800487	3.703458	1.633276
C	4.940857	-2.905183	0.815947	C	-1.143273	1.962827	0.145018
C	5.946322	-3.890092	0.663249	H	-1.644157	1.990813	1.127956
H	6.005466	-4.689760	1.400749	C	-1.737050	0.826507	-0.675828
C	6.821122	-3.848851	-0.395353	H	-1.392051	0.914388	-1.718208
H	7.586765	-4.613678	-0.504054	H	-2.831676	0.908740	-0.700431
C	6.711434	-2.821604	-1.353926	C	-1.373502	3.298007	-0.523563
H	7.384259	-2.807774	-2.208812	C	-0.498449	3.792016	-1.494186
C	5.757352	-1.839215	-1.225133	H	0.410468	3.233244	-1.720045
H	5.682471	-1.063236	-1.982323	C	-0.767521	4.994100	-2.139659
C	4.856799	-1.832819	-0.130882	H	-0.074505	5.373551	-2.888388
C	3.851161	-0.820540	0.027295	C	-1.915733	5.717405	-1.822888
C	3.794828	0.357530	-0.866749	H	-2.123519	6.659716	-2.325571
C	4.913655	1.236851	-1.057907	C	-2.789244	5.236522	-0.850907
C	6.104303	1.135788	-0.296673	H	-3.679737	5.804113	-0.588255
H	6.182956	0.366269	0.467721	C	-2.515382	4.035576	-0.202761
C	7.153301	2.002192	-0.502553	H	-3.192715	3.664138	0.569645
H	8.053098	1.909266	0.102060	C	-1.375565	-0.857003	2.223861
C	7.072627	3.011297	-1.483178	H	-1.228386	-1.828977	2.699336
H	7.913860	3.682372	-1.641904	H	-0.790188	-0.056197	2.680879
C	5.923706	3.154324	-2.221645	C	-2.662026	-0.502708	1.720883
H	5.838076	3.942704	-2.968442	H	-2.905225	0.558046	1.657149
C	4.817363	2.293827	-2.022096	C	-3.561692	-1.393473	1.120217
C	3.615890	2.473079	-2.749041	H	-3.477186	-2.457269	1.335804
H	3.564249	3.263251	-3.496671	C	-0.845453	-1.710704	-2.042193
C	2.523979	1.681119	-2.499152	H	-0.577582	-0.787840	-2.555998
H	1.583295	1.806622	-3.031525	C	-2.218365	-1.909229	-1.789127
C	2.627594	0.657149	-1.543282	H	-2.912429	-1.133114	-2.123179
C	0.960998	2.662755	1.322025	C	-2.843418	-3.261003	-1.562631
H	0.477137	3.611049	1.047696	H	-2.980961	-3.763815	-2.533719
C	0.585161	2.371370	2.761858	H	-3.855754	-3.100331	-1.172053
C	-0.617302	2.883987	3.267474	C	-2.057724	-4.162978	-0.603606
H	-1.213841	3.552165	2.643348	H	-2.752087	-4.857664	-0.115703
C	-1.044577	2.579001	4.557299	H	-1.354885	-4.799622	-1.156063
H	-1.980873	2.989873	4.930138	C	-1.294156	-3.411243	0.469281
C	-0.260811	1.768472	5.374277	H	-1.668478	-3.515553	1.489074
H	-0.586300	1.532173	6.385391	C	0.039349	-3.032823	0.337405
C	0.957997	1.287154	4.899913	H	0.604458	-2.868819	1.256621
H	1.591784	0.681126	5.544923	C	0.864512	-3.245747	-0.903526
C	1.378396	1.587137	3.607456	H	1.175206	-4.302235	-0.945438
H	2.335111	1.207492	3.255820	H	1.793224	-2.671170	-0.805878
C	2.442315	2.841971	1.059287	C	0.154980	-2.842193	-2.203042
H	2.623795	3.041542	-0.003138	H	0.911451	-2.531143	-2.931549
H	3.044513	1.977762	1.351528	H	-0.353140	-3.704665	-2.653939

C	-4.779381	-0.963197	0.479182
C	-5.777974	-1.833119	0.033802
C	-5.205325	0.359402	0.192139
H	-5.856676	-2.911169	0.099702
C	-6.450032	0.281847	-0.416764
H	-4.691760	1.283875	0.428200
C	-7.976966	-1.503481	-1.056902
C	-7.373257	1.223140	-0.921591
C	-8.856331	-0.582340	-1.537657
H	-8.141933	-2.576126	-1.072701
C	-8.554684	0.804926	-1.472681
H	-7.118487	2.278113	-0.860011
H	-9.790569	-0.927813	-1.969173
H	-9.265696	1.528447	-1.861454
N	-6.787203	-1.088410	-0.504162

IM3'

M06-L SCF energy in solvent: -3136.773999 a.u

Ir	-0.993321	-0.616235	-1.523400
O	1.709111	-0.262652	0.825038
O	1.704623	1.089004	-1.317617
C	2.810556	-0.954043	0.360535
C	2.823054	-2.350585	0.546858
H	1.990656	-2.824209	1.065654
C	3.904386	-3.076007	0.115419
H	3.933547	-4.154904	0.265383
C	4.989348	-2.444516	-0.537862
C	6.082361	-3.191880	-1.038562
H	6.075650	-4.272942	-0.898626
C	7.122209	-2.577381	-1.693821
H	7.954613	-3.165356	-2.076207
C	7.101091	-1.180461	-1.882333
H	7.913486	-0.695667	-2.420800
C	6.060480	-0.422820	-1.397599
H	6.053118	0.653025	-1.558369
C	4.981181	-1.019907	-0.698164
C	3.881010	-0.259241	-0.183983
C	3.836679	1.218054	-0.239455
C	4.854595	2.045538	0.337423
C	5.930384	1.516332	1.094482
H	5.991344	0.440723	1.244020
C	6.883232	2.338521	1.650177
H	7.693626	1.904490	2.233348
C	6.815992	3.735970	1.478279
H	7.578898	4.375990	1.917613
C	5.774843	4.284886	0.769110
H	5.697152	5.364977	0.644059
C	4.768561	3.469707	0.198095
C	3.667866	4.035975	-0.489594
H	3.621086	5.118452	-0.606946
C	2.662402	3.239446	-0.974535
H	1.793828	3.650351	-1.485831
C	2.743147	1.840553	-0.821485
P	0.600342	0.362246	-0.268133
N	-0.038279	1.568795	0.734464
C	-1.772337	1.330378	-1.013468
H	-1.410951	2.046816	-1.766813
H	-2.867746	1.293263	-1.111632
C	-1.431805	1.884239	0.371463
H	-2.095897	1.393644	1.100332
C	-1.730605	3.366526	0.429451
C	-0.742377	4.348072	0.323480
H	0.302053	4.039563	0.262184
C	-1.083776	5.698720	0.308447
H	-0.300959	6.451890	0.227480
C	-2.417318	6.088099	0.398124
H	-2.682865	7.143679	0.384993
C	-3.410330	5.116350	0.510533
H	-4.456811	5.410027	0.582030
C	-3.066244	3.769505	0.530126
H	-3.841074	3.002876	0.604710
C	0.286427	1.866819	2.163621
H	-0.264642	2.802585	2.343170
C	-0.318856	0.833606	3.098490
C	-1.618554	1.029051	3.584838
H	-2.139113	1.957822	3.338338
C	-2.249894	0.066815	4.371321
H	-3.266914	0.235530	4.723610
C	-1.577423	-1.104255	4.710297
H	-2.066742	-1.866258	5.314850
C	-0.266222	-1.287490	4.277627
H	0.286066	-2.182499	4.560219
C	0.355874	-0.333030	3.478116
H	1.374259	-0.504606	3.138968
C	1.746806	2.186257	2.430147
H	2.103455	2.947272	1.726214
H	2.405163	1.318299	2.347929
H	1.841842	2.589407	3.445301

C	-2.407172	-0.712503	-3.136133
H	-3.307828	-0.134550	-2.902258
C	-1.245976	0.051954	-3.524705
H	-1.376934	1.136518	-3.522013
C	-0.203936	-0.429156	-4.522849
H	0.156144	0.426328	-5.107788
H	-0.664919	-1.106569	-5.254826
C	0.983932	-1.094605	-3.825311
H	1.503349	-1.792683	-4.504185
H	1.720736	-0.328553	-3.554248
C	0.596897	-1.816730	-2.560124
H	1.425765	-1.987428	-1.868263
C	-0.519410	-2.658498	-2.431133
H	-0.468552	-3.402016	-1.636596
C	-1.452332	-3.013650	-3.574607
H	-1.771488	-4.057299	-3.455115
H	-0.895499	-2.990978	-4.520724
C	-2.683522	-2.105388	-3.649363
H	-3.086313	-2.088012	-4.677817
H	-3.482537	-2.544881	-3.032573
C	-0.808614	-2.804680	0.920058
H	-0.218577	-1.997150	1.373444
H	-0.136592	-3.412751	0.302504
C	-1.986941	-2.264840	0.190994
H	-2.521171	-2.937812	-0.482035
C	-2.603270	-1.145949	0.676456
H	-2.088316	-0.624127	1.488817
O	-1.320832	-3.648009	1.994332
C	-0.375212	-4.169279	2.772250
O	0.826605	-4.080419	2.620222
O	-0.986016	-4.816996	3.777262
C	-0.084884	-5.454363	4.681015
H	0.589573	-4.724789	5.141124
H	-0.715618	-5.921023	5.438313
H	0.515503	-6.209578	4.164192
C	-3.920542	-0.650298	0.359765
C	-4.537175	0.367635	1.088346
C	-4.812783	-1.043843	-0.664336
H	-4.198323	0.906451	1.965885
C	-5.956947	-0.266966	-0.555944
H	-4.636246	-1.796944	-1.422748
C	-6.730298	1.509130	0.921971
C	-7.175676	-0.174041	-1.261772
C	-7.901213	1.584405	0.229339
H	-6.483043	2.129098	1.778924
C	-8.133119	0.730003	-0.882381
H	-7.328513	-0.838838	-2.108741
H	-8.649139	2.306967	0.542105
H	-9.070679	0.798283	-1.428118
N	-5.768230	0.604092	0.546200

TS1'

M06-L SCF energy in solvent: -3136.761719 a.u

Ir	-1.470382	-0.305664	-0.600429
O	1.766722	-0.076667	0.913931
O	1.637104	-0.451553	-1.599002
C	2.181798	-1.391095	1.103233
C	1.624617	-2.077909	2.198545
H	0.952015	-1.535758	2.866889
C	1.989799	-3.383525	2.409899
H	1.580773	-3.933926	3.256637
C	2.883636	-4.044704	1.532439
C	3.202361	-5.413703	1.700855
H	2.750611	-5.949268	2.535694
C	4.047903	-6.058651	0.830674
H	4.279600	-7.112936	0.970481
C	4.605605	-5.353371	-0.254852
H	5.257596	-5.869924	-0.957103
C	4.328871	-4.018426	-0.439516
H	4.759516	-3.488301	-1.286350
C	3.476471	-3.316985	0.449488
C	3.151294	-1.930864	0.272998
C	3.793623	-1.095481	-0.765115
C	5.216651	-0.930958	-0.839851
C	6.098067	-1.473161	0.129079
H	5.685778	-2.033279	0.964812
C	7.457761	-1.286615	0.038313
H	8.109673	-1.706370	0.802177
C	8.014183	-0.550213	-1.027034
H	9.092068	-0.414643	-1.090291
C	7.188555	0.008435	-1.972114
H	7.600612	0.597718	-2.791288
C	5.783823	-0.150863	-1.900640
C	4.928410	0.463473	-2.846154
H	5.369036	1.040885	-3.658195
C	3.566604	0.361702	-2.725027
H	2.889281	0.848802	-3.423247
C	3.015911	-0.393989	-1.671959

P	0.782386	0.275897	-0.359919
N	0.936808	1.929156	-0.399411
C	-1.336332	1.688640	-1.373765
H	-1.110840	1.574871	-2.444915
H	-2.318211	2.176678	-1.326370
C	-0.304801	2.646100	-0.779659
H	-0.706480	3.114966	0.134377
C	-0.027576	3.753675	-1.772567
C	0.721060	3.500677	-2.926317
H	1.145028	2.504816	-3.070464
C	0.938828	4.501881	-3.865007
H	1.531157	4.292803	-4.754544
C	0.398359	5.772408	-3.667619
H	0.566155	6.557551	-4.402646
C	-0.352039	6.032496	-2.524802
H	-0.772678	7.023306	-2.361648
C	-0.559270	5.028561	-1.580298
H	-1.128374	5.236542	-0.673242
C	2.003655	2.848614	0.116573
H	2.157853	3.558119	-0.711264
C	1.492433	3.643289	1.301149
C	1.450185	5.037199	1.222492
H	1.764538	5.528075	0.299579
C	1.006288	5.795494	2.302450
H	0.978760	6.881806	2.227546
C	0.588849	5.160635	3.468827
H	0.229329	5.748456	4.311871
C	0.623783	3.770121	3.558021
H	0.274824	3.270209	4.459450
C	1.079104	3.014239	2.480106
H	1.108618	1.925407	2.563014
C	3.361769	2.239096	0.420187
H	3.772728	1.687595	-0.430294
H	3.349687	1.588112	1.296788
H	4.042520	3.071127	0.633569
C	-2.453479	-0.743537	-2.503080
H	-2.813896	0.194438	-2.935925
C	-1.052120	-0.991897	-2.611215
H	-0.474577	-0.214378	-3.114898
C	-0.434306	-2.379052	-2.719099
H	0.471475	-2.304952	-3.331626
H	-1.119666	-3.031004	-3.278872
C	-0.060888	-3.017546	-1.370860
H	-0.134904	-4.115815	-1.434245
H	0.988681	-2.802430	-1.146041
C	-0.907382	-2.539830	-0.219371
H	-0.445560	-2.569921	0.768913
C	-2.293324	-2.473779	-0.286970
H	-2.834594	-2.426294	0.654144
C	-3.110160	-2.953907	-1.466362
H	-4.022774	-3.425026	-1.080774
H	-2.559420	-3.748167	-1.987099
C	-3.493314	-1.829771	-2.428541
H	-3.686905	-2.231419	-3.437809
H	-4.437896	-1.382934	-2.096519
C	-1.277732	0.685850	1.702434
H	-1.169984	1.730485	1.429720
H	-0.471087	0.204833	2.247197
C	-2.449624	-0.020837	1.414753
H	-2.592252	-0.970454	1.931996
C	-3.413033	0.419952	0.470873
H	-3.383725	1.477060	0.205807
O	-1.548828	1.409169	3.826881
C	-0.643964	0.829443	4.482367
O	0.132909	-0.088379	4.144470
O	-0.510957	1.354625	5.767838
C	0.536192	0.784515	6.526928
H	1.513236	0.946790	6.051519
H	0.510316	1.282152	7.501512
H	0.402973	-0.296664	6.656232
C	-4.707795	-0.214243	0.286783
C	-5.689450	0.265924	-0.579339
C	-5.216985	-1.383224	0.899133
H	-5.688520	1.129003	-1.233957
C	-6.493604	-1.610433	0.400476
H	-4.740733	-1.978532	1.669298
C	-7.959191	-0.514840	-1.202392
C	-7.491650	-2.583694	0.610989
C	-8.911846	-1.467525	-0.992427
H	-8.069313	0.318664	-1.889543
C	-8.680577	-2.521318	-0.069917
H	-7.289956	-3.379153	1.324727
H	-9.846617	-1.402726	-1.541427
H	-9.447116	-3.274311	0.093138
N	-6.767721	-0.573644	-0.522985

IM4'

M06-L SCF energy in solvent: -2832.846291 a.u

Ir	-1.413144	-0.590334	-0.074494
O	1.791703	-0.201018	1.201890
O	1.538553	-0.211173	-1.335406
C	2.604975	-1.328905	1.108741
C	2.397449	-2.317216	2.087776
H	1.636778	-2.144709	2.847509
C	3.168566	-3.451521	2.073912
H	3.029542	-4.220876	2.831839
C	4.144362	-3.646902	1.067793
C	4.903179	-4.840414	1.008034
H	4.732710	-5.601888	1.768067
C	5.827026	-5.041386	0.011313
H	6.403447	-5.963139	-0.024617
C	6.016001	-4.054237	-0.976409
H	6.729114	-4.225387	-1.780169
C	5.306383	-2.876202	-0.938609
H	5.461394	-2.131005	-1.714629
C	4.364109	-2.622886	0.089368
C	3.610558	-1.401987	0.157876
C	3.869755	-0.270452	-0.760802
C	5.165531	0.333343	-0.892239
C	6.256911	-0.011337	-0.057326
H	6.118418	-0.762172	0.716723
C	7.480946	0.600873	-0.200465
H	8.300225	0.324106	0.459929
C	7.683176	1.585416	-1.188226
H	8.659038	2.053401	-1.296344
C	6.640609	1.961196	-1.999755
H	6.775973	2.735315	-2.754017
C	5.362895	1.366981	-1.866683
C	4.275155	1.792534	-2.666599
H	4.443435	2.559192	-3.421444
C	3.021315	1.269327	-2.476152
H	2.164132	1.591551	-3.063741
C	2.838119	0.268650	-1.506856
P	0.726894	0.210105	0.035877
N	0.684623	1.859469	0.258120
C	-1.395504	1.411237	-0.907506
H	-0.935249	1.360786	-1.907680
H	-2.423745	1.754691	-1.069779
C	-0.633635	2.430872	-0.076858
H	-1.185230	2.607908	0.864582
C	-0.529675	3.754861	-0.798325
C	0.518180	4.033343	-1.679359
H	1.321587	3.304786	-1.794410
C	0.552848	5.237240	-2.375322
H	1.379561	5.447314	-3.051674
C	-0.461414	6.176418	-2.201911
H	-0.432256	7.118946	-2.744603
C	-1.505994	5.909785	-1.320189
H	-2.293745	6.645073	-1.168726
C	-1.535466	4.707583	-0.619663
H	-2.347998	4.502581	0.081146
C	1.521448	2.701760	1.188840
H	1.279679	3.718125	0.846868
C	1.025818	2.588267	2.616010
C	-0.023535	3.416747	3.034482
H	-0.406425	4.175488	2.348963
C	-0.565442	3.301002	4.312272
H	-1.379678	3.955446	4.617835
C	-0.051666	2.360625	5.200894
H	-0.467927	2.268857	6.202134
C	1.018985	1.558035	4.811039
H	1.447774	0.845076	5.513243
C	1.555198	1.672444	3.531968
H	2.398528	1.047198	3.247281
C	3.016294	2.534457	1.004744
H	3.291783	2.644201	-0.050664
H	3.398894	1.573949	1.358991
H	3.527093	3.320979	1.570876
C	-2.471489	-1.191947	-1.923930
H	-2.964731	-0.299172	-2.318545
C	-1.078545	-1.297099	-2.138445
H	-0.614374	-0.468648	-2.672882
C	-0.332332	-2.614580	-2.249937
H	0.487148	-2.487808	-2.965608
H	-1.001464	-3.363671	-2.692332
C	0.247852	-3.120304	-0.924163
H	0.344281	-4.217988	-0.939857
H	1.268548	-2.739017	-0.803636
C	-0.559888	-2.728855	0.283937
H	-0.005552	-2.674576	1.222507
C	-1.943538	-2.831526	0.367024
H	-2.359958	-2.858757	1.372940
C	-2.821874	-3.410187	-0.722488
H	-3.654747	-3.943590	-0.249196
H	-2.256244	-4.177091	-1.266405
C	-3.389517	-2.362638	-1.685035

H	-3.647421	-2.827824	-2.650487
H	-4.335050	-1.980305	-1.280795
C	-1.458681	0.031956	2.021789
H	-1.204392	1.088792	2.122911
H	-0.909478	-0.596156	2.726394
C	-2.817127	-0.338095	1.764768
H	-3.180559	-1.284419	2.161039
C	-3.659772	0.353493	0.900311
H	-3.381387	1.368153	0.620047
C	-4.966913	-0.090377	0.504859
C	-5.782939	0.598848	-0.395165
C	-5.648382	-1.274005	0.887738
H	-5.631682	1.541062	-0.907499
C	-6.869479	-1.289226	0.229858
H	-5.309024	-2.031635	1.584470
C	-8.025935	0.166984	-1.346361
C	-7.976198	-2.166716	0.194381
C	-9.080552	-0.692232	-1.371121
H	-7.974267	1.091712	-1.912179
C	-9.060863	-1.879647	-0.589736
H	-7.940793	-3.065548	0.804539
H	-9.936734	-0.451359	-1.993361
H	-9.912446	-2.553841	-0.615878
N	-6.930857	-0.118445	-0.563578

CO_2

M06-L SCF energy in solvent: -188.652161 a.u

O	0.000000	0.000000	1.168437
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	-1.168437

MeOH

M06-L SCF energy in solvent: -115.753470 a.u

C	0.655674	-0.019227	0.000000
H	1.073332	0.991531	-0.000001
H	1.037125	-0.541756	-0.893053
H	1.037125	-0.541754	0.893054
O	-0.744895	0.121784	0.000000
H	-1.122472	-0.766936	0.000000

TS2-*cis*

M06-L SCF energy in solvent: -8423.353163 a.u

C	-6.834606	-2.001876	0.177952
C	-7.928311	-2.924226	0.067317
H	-8.800318	-2.933598	0.711378
C	-7.632416	-3.838967	-0.978431
H	-8.241791	-4.687375	-1.269981
C	-5.844783	-2.356785	-0.828483
C	-6.368723	-3.492882	-1.532817
H	-5.854307	-4.030143	-2.322307
C	-6.087523	0.403301	2.832062
C	-7.610497	0.473578	2.661046
H	-8.173580	0.281931	3.579690
N	-5.666577	-0.474195	1.724205
C	-6.738658	-0.996132	1.222528
O	-7.918134	-0.598296	1.737436
H	-7.964541	1.406550	2.207777
H	-5.621013	1.390619	2.691366
C	-5.666144	-0.144537	4.204083
C	-4.189190	-0.498146	4.248221
C	-6.011744	0.866823	5.289885
H	-6.253692	-1.064433	4.377481
H	-3.928830	-1.259318	3.505192
H	-3.905384	-0.870506	5.240004
H	-3.575320	0.391557	4.041641
H	-7.074246	1.139592	5.297333
H	-5.435245	1.792146	5.151183
H	-5.770052	0.475228	6.283949
P	-4.277051	-1.494460	-1.135355
C	-4.637819	-0.566150	-2.674046
C	-3.623327	-0.277282	-3.598395
C	-5.912059	-0.022079	-2.879761
C	-3.879861	0.529654	-4.702484
H	-2.625243	-0.694615	-3.457082
C	-6.167630	0.785411	-3.985373
H	-6.714538	-0.244807	-2.174174
C	-5.153167	1.062296	-4.900149
H	-3.080815	0.739776	-5.411669
H	-7.166053	1.192769	-4.136748
H	-5.354876	1.689668	-5.765998
C	-3.138788	-2.812949	-1.688747
C	-2.086333	-3.204842	-0.851710
C	-3.295715	-3.445816	-2.930073
C	-1.225391	-4.229690	-1.239006
H	-1.934975	-2.692913	0.099568
C	-2.433817	-4.467181	-3.313985
H	-4.086715	-3.121793	-3.606820
C	-1.400329	-4.864725	-2.465865

H	-0.405125	-4.521037	-0.583959	N	4.801785	1.824221	0.656313
H	-2.564385	-4.951078	-4.279993	C	5.394080	-1.952571	0.610329
H	-0.725067	-5.662713	-2.769052	C	4.575458	-2.997964	1.077473
Cu	-3.835557	-0.390784	0.705728	H	3.717334	-2.742105	1.698474
O	-2.151661	-1.209646	1.778551	C	4.884997	-4.294436	0.753881
C	-1.496330	-0.279133	2.277639	H	4.268715	-5.116751	1.115686
O	-0.489055	-0.515487	3.121456	C	6.000698	-4.585921	-0.067291
C	-1.695363	1.129348	1.944515	C	6.297960	-5.914941	-0.453733
N	-2.982165	1.365279	1.444210	H	5.655413	-6.716144	-0.089113
C	-3.435952	2.587783	1.427457	C	7.363951	-6.191903	-1.274878
H	-2.864249	3.382012	1.920356	H	7.581262	-7.217631	-1.565165
C	-4.640972	3.050670	0.770911	C	8.170448	-5.139378	-1.752392
C	-4.991575	4.402861	0.936208	H	9.000214	-5.357084	-2.421906
C	-5.447908	2.261111	-0.068517	C	7.916922	-3.838064	-1.385956
C	-6.105317	4.947513	0.315805	H	8.543876	-3.038225	-1.772355
H	-4.361211	5.040019	1.556608	C	6.841310	-3.516984	-0.520150
C	-6.568742	2.788578	-0.689393	C	6.552818	-2.170304	-0.117918
H	-5.170607	1.222888	-0.259447	C	7.428316	-1.032676	-0.480221
C	-6.893640	4.131832	-0.492911	C	8.823868	-1.002821	-0.152072
H	-6.361811	5.995447	0.446561	C	9.438816	-1.993336	0.653959
H	-7.183269	2.173146	-1.343140	H	8.835166	-2.809120	1.044955
C	-0.156898	-1.907458	3.326163	C	10.778277	-1.929324	0.960742
H	0.022957	-2.366556	2.342536	H	11.222798	-2.697984	1.590028
H	-1.027006	-2.410788	3.765886	C	11.578426	-0.875645	0.475161
C	-4.450836	-4.089047	1.514885	H	12.638070	-0.841460	0.718921
C	-5.574720	-3.995807	2.387571	C	11.010685	0.114044	-0.290002
H	-5.737600	-3.215261	3.125229	H	11.611676	0.946559	-0.654787
C	-6.476631	-5.052095	2.067710	C	9.631422	0.090227	-0.608137
H	-7.442779	-5.227204	2.528463	C	9.032136	1.137469	-1.348990
C	-4.660911	-5.205327	0.646082	H	9.658119	1.953673	-1.707707
H	-4.006633	-5.513753	-0.163771	C	7.680687	1.143720	-1.583647
C	-5.911852	-5.801209	0.992221	H	7.190656	1.949266	-2.126778
H	-6.374338	-6.647253	0.495302	C	6.894639	0.070914	-1.124284
H	-3.613055	-3.395810	1.493345	C	3.760654	2.843437	0.398926
C	-1.000589	2.165937	2.776618	H	3.034427	2.809322	1.232617
H	-0.816679	3.080023	2.195963	C	4.328280	4.240854	0.338088
H	-0.036751	1.790556	3.128204	C	5.558403	4.506439	-0.270062
H	-1.596388	2.447524	3.657828	H	6.151419	3.670788	-0.645404
Fe	-6.164678	-3.862210	0.446054	C	6.027650	5.811697	-0.371990
Cl	-8.280045	4.802788	-1.294302	H	6.990549	6.005349	-0.841623
Ir	2.307205	0.471508	-0.951963	C	5.271852	6.870228	0.129419
P	4.459216	0.390973	-0.145877	H	5.642087	7.890541	0.051910
O	5.038841	-0.665502	0.984986	C	4.045963	6.615182	0.738164
O	5.534190	0.127435	-1.385433	H	3.454726	7.436084	1.140346

C	3.581505	5.307090	0.843758
H	2.623039	5.101737	1.327524
C	3.025699	2.499752	-0.886776
H	3.686545	2.695104	-1.747180
H	2.159803	3.165632	-0.996752
C	5.545507	2.015461	1.946435
H	5.658422	3.108251	1.988355
C	4.701909	1.626916	3.146316
C	3.796132	2.559302	3.669334
H	3.758997	3.561105	3.236394
C	2.972491	2.239633	4.745995
H	2.278146	2.981742	5.136959
C	3.058896	0.982167	5.335510
H	2.427978	0.730868	6.186512
C	3.980822	0.056953	4.848753
H	4.074512	-0.919021	5.323916
C	4.790958	0.373739	3.762788
H	5.505102	-0.359685	3.396193
C	6.951227	1.446890	1.945444
H	7.508498	1.802782	1.072116
H	6.983161	0.354368	1.944012
H	7.472173	1.793461	2.845133
C	1.688597	0.277009	1.111511
H	1.300927	-0.727368	1.299890
H	2.407117	0.604038	1.869792
C	0.825365	1.267171	0.542322
H	1.111606	2.302595	0.739139
C	-0.555463	1.129302	0.143130
H	-0.902457	0.138799	-0.167869
C	2.874010	0.404909	-3.046666
H	3.698584	1.102842	-3.205327
C	1.573912	0.986132	-2.941945
H	1.509890	2.072988	-3.045904
C	0.304088	0.255441	-3.302745
H	0.184818	0.209533	-4.400227
H	-0.541294	0.854545	-2.936566
C	0.223581	-1.149086	-2.697630
H	0.581480	-1.908116	-3.406658
H	-0.827505	-1.411137	-2.509048
C	0.982331	-1.292367	-1.388598
H	0.360369	-1.476107	-0.506765
C	2.307813	-1.752015	-1.301818
H	2.592288	-2.251715	-0.373166
C	3.188454	-2.062511	-2.485795
H	4.223410	-2.142187	-2.126052
H	2.933043	-3.057797	-2.888084
C	3.122808	-0.996430	-3.586397
H	2.350813	-1.248553	-4.326447
H	4.069010	-1.000552	-4.140560
C	-1.175628	2.230558	-0.568062
C	-2.289472	2.094553	-1.394821
C	-0.874670	3.614590	-0.483927
H	-2.852194	1.211623	-1.674103
C	-1.803208	4.300785	-1.261700
H	-0.058646	4.079369	0.058658
C	-3.736003	3.685762	-2.612522
C	-2.047960	5.656144	-1.569096
C	-3.965980	4.999855	-2.887571
H	-4.348791	2.862234	-2.970458
C	-3.108533	6.005026	-2.364813
H	-1.378435	6.407076	-1.156469
H	-4.818506	5.262987	-3.507198
H	-3.298600	7.049219	-2.598593
N	-2.669391	3.333026	-1.820080
C	1.058358	-1.950351	4.207593
H	1.368279	-2.988191	4.370505
H	1.892374	-1.403254	3.753225
H	0.855220	-1.498205	5.184118

TS2-*trans*

M06-L SCF energy in solvent: -8423.347943 a.u

C	-6.818833	1.803271	0.389564
C	-8.190392	2.223671	0.412921
H	-8.610899	2.937138	1.112734
C	-8.892771	1.492258	-0.582730
H	-9.958699	1.547970	-0.776222
C	-6.675560	0.792910	-0.643135
C	-7.971846	0.625431	-1.236262
H	-8.208918	-0.085439	-2.021260
C	-4.231606	2.322598	2.900547
C	-4.888125	3.690992	2.742005
H	-5.219268	4.155203	3.675100
N	-4.772228	1.577430	1.748561
C	-5.824223	2.224871	1.358731
O	-6.071773	3.409448	1.955558
H	-4.277774	4.402992	2.171359
H	-3.137712	2.383042	2.814265
C	-4.590197	1.648042	4.236549

C	-4.279152	0.159894	4.243860
C	-3.864451	2.352160	5.375980
H	-5.678753	1.778544	4.376208
H	-4.778258	-0.372879	3.426901
H	-4.587036	-0.296825	5.192345
H	-3.199061	-0.008081	4.134744
H	-4.076350	3.427823	5.415754
H	-2.776215	2.234555	5.266073
H	-4.143817	1.928639	6.346847
P	-5.110663	0.026521	-1.147951
C	-4.684722	1.026538	-2.624551
C	-3.529801	0.698244	-3.348542
C	-5.424200	2.150240	-3.012703
C	-3.134388	1.458515	-4.444031
H	-2.934129	-0.159161	-3.032942
C	-5.022075	2.918642	-4.103794
H	-6.318929	2.433002	-2.461378
C	-3.881321	2.574660	-4.823593
H	-2.236441	1.187829	-4.996851
H	-5.605726	3.791268	-4.390424
H	-3.569280	3.176317	-5.674670
C	-5.673460	-1.568334	-1.837601
C	-5.519651	-2.723035	-1.059961
C	-6.329013	-1.652571	-3.072149
C	-6.068267	-3.929003	-1.487170
H	-4.967330	-2.670530	-0.119798
C	-6.860191	-2.864695	-3.503011
H	-6.425593	-0.762918	-3.695853
C	-6.743399	-4.000501	-2.704092
H	-5.951321	-4.822394	-0.875067
H	-7.371209	-2.921891	-4.462690
H	-7.164864	-4.946968	-3.039134
Cu	-3.816541	0.067171	0.632061
O	-3.635941	-1.863728	1.609713
C	-2.576676	-1.935504	2.252575
O	-2.285296	-3.018647	2.994021
C	-1.535550	-0.923884	2.234479
N	-1.894310	0.180598	1.482161
C	-1.192934	1.282103	1.539360
H	-0.375446	1.397538	2.262729
C	-1.490823	2.422889	0.689940
C	-1.181265	3.725632	1.116430
C	-2.109024	2.267862	-0.562991
C	-1.525216	4.836515	0.354925
H	-0.688753	3.871190	2.078234
C	-2.457369	3.364578	-1.337088
H	-2.295405	1.262037	-0.941923
C	-2.179331	4.645932	-0.861365
H	-1.291543	5.842041	0.695344
H	-2.921886	3.229609	-2.310819
C	-3.314123	-4.030163	3.036637
H	-3.554098	-4.328643	2.006858
H	-4.221983	-3.583804	3.463753
C	-7.157416	-1.314509	1.771363
C	-7.685779	-0.340313	2.669864
H	-7.108891	0.241302	3.383563
C	-9.081374	-0.204208	2.412006
H	-9.756144	0.488834	2.902876
C	-8.233010	-1.779611	0.950863
H	-8.150062	-2.490918	0.134995
C	-9.420043	-1.094705	1.350120
H	-10.399002	-1.198507	0.894671
H	-6.112055	-1.610625	1.697019
C	-0.608332	-0.786993	3.401611
H	0.382306	-0.423328	3.105748
H	-0.484300	-1.742102	3.917739
H	-0.998536	-0.056365	4.130764
Fe	-7.997823	0.222617	0.742998
Cl	-2.628231	6.025119	-1.823729
Ir	2.687866	-1.335471	-0.614790
P	4.433920	0.084401	-0.194624
O	5.332688	0.122031	1.186693
O	5.624736	-0.092066	-1.339380
N	3.848518	1.650209	-0.155706
C	6.377087	-0.773187	1.378952
C	6.210178	-1.729099	2.398498
H	5.290687	-1.709193	2.981864
C	7.202805	-2.645928	2.633628
H	7.090534	-3.388997	3.421976
C	8.376413	-2.657019	1.842233
C	9.374723	-3.643863	2.023075
H	9.229156	-4.392283	2.801406
C	10.496761	-3.669093	1.229954
H	11.254248	-4.436097	1.376068
C	10.658901	-2.704511	0.215159
H	11.537227	-2.738292	-0.426166
C	9.714617	-1.722523	0.023071
H	9.851011	-0.990762	-0.769653

C	8.553806	-1.655794	0.832821
C	7.545894	-0.652340	0.645381
C	7.716843	0.467232	-0.306226
C	8.829388	1.368636	-0.228671
C	9.776063	1.317580	0.824891
H	9.663553	0.568916	1.605295
C	10.824064	2.206550	0.882031
H	11.532404	2.150141	1.706317
C	10.985431	3.193109	-0.111422
H	11.822868	3.885630	-0.058594
C	10.074681	3.284304	-1.136249
H	10.177576	4.052061	-1.902439
C	8.976120	2.394860	-1.217231
C	8.012786	2.508618	-2.248253
H	8.146552	3.272747	-3.012853
C	6.913235	1.687383	-2.274000
H	6.153565	1.765749	-3.048767
C	6.763941	0.699535	-1.283072
C	2.519101	1.766146	-0.792533
H	1.752769	1.826982	0.006316
C	2.412556	3.014694	-1.639219
C	3.510151	3.514174	-2.345851
H	4.480629	3.032296	-2.222801
C	3.373301	4.624723	-3.172250
H	4.238681	5.007578	-3.711174
C	2.135202	5.250190	-3.306765
H	2.029304	6.120287	-3.951848
C	1.037124	4.762258	-2.602753
H	0.066609	5.249149	-2.694257
C	1.179084	3.655286	-1.770575
H	0.321162	3.276624	-1.213174
C	2.245353	0.514768	-1.625036
H	2.826277	0.572013	-2.560716
H	1.187418	0.513792	-1.922319
C	4.190010	2.758636	0.795181
H	3.693463	3.623231	0.330811
C	3.531585	2.552821	2.148172
C	2.220745	3.006206	2.344253
H	1.721320	3.552461	1.540251
C	1.558467	2.783744	3.550785
H	0.542248	3.153308	3.695636
C	2.196829	2.107363	4.586325
H	1.681441	1.935142	5.529824
C	3.511552	1.680434	4.415001
H	4.031153	1.176816	5.228336
C	4.173489	1.908559	3.212676
H	5.201763	1.574758	3.099224
C	5.667890	3.095528	0.851279
H	6.060225	3.270858	-0.156759
H	6.275768	2.316634	1.318688
H	5.800673	4.015139	1.432272
C	1.930305	-0.654411	1.276867
H	2.141669	-1.353444	2.094868
H	2.180452	0.375596	1.539209
C	0.752883	-0.908791	0.485019
H	0.334283	-0.083382	-0.095854
C	-0.144359	-1.982594	0.756521
H	0.163454	-2.681885	1.538389
C	3.543497	-2.105056	-2.472414
H	3.886892	-1.251576	-3.060038
C	2.143560	-2.355798	-2.473425
H	1.521506	-1.691327	-3.079887
C	1.554727	-3.728211	-2.242548
H	1.712861	-4.356751	-3.135542
H	0.468082	-3.622561	-2.143457
C	2.107066	-4.434096	-0.996510
H	2.919276	-5.122706	-1.267318
H	1.321687	-5.068932	-0.566316
C	2.608389	-3.492640	0.085219
H	2.047125	-3.500812	1.020323
C	3.933933	-3.055094	0.179998
H	4.287435	-2.773809	1.172618
C	5.018852	-3.366055	-0.819147
H	5.861603	-2.689844	-0.624946
H	5.403731	-4.383806	-0.638266
C	4.575851	-3.203267	-2.277474
H	4.176982	-4.149231	-2.668821
H	5.456055	-2.979585	-2.891459
C	-2.789278	-5.170168	3.863721
H	-2.548544	-4.843086	4.880349
H	-3.540237	-5.963699	3.931623
H	-1.881485	-5.596787	3.422261
C	-1.045764	-2.534397	-0.222052
C	-1.505380	-1.960969	-1.432624
C	-1.530739	-3.840583	-0.160165
C	-2.235995	-2.930789	-2.111634
H	-1.271176	-0.968322	-1.802633
H	-1.366067	-4.615193	0.579830

C	-2.892123	-3.010843	-3.360883
C	-2.816614	-5.267509	-1.718342
C	-3.472660	-4.181576	-3.769716
H	-2.917231	-2.126578	-3.993535
C	-3.424637	-5.329314	-2.934656
H	-2.742024	-6.100653	-1.025524
H	-3.973195	-4.236539	-4.732865
H	-3.878877	-6.264758	-3.248417
N	-2.231791	-4.094505	-1.303893

TS3-*cis*

M06-L SCF energy in solvent: -8423.343394 a.u

C	-6.659545	-1.129226	1.041922
C	-7.931815	-1.551976	1.560910
H	-8.209663	-1.548667	2.608412
C	-8.717655	-2.024592	0.476284
H	-9.710540	-2.454071	0.554783
C	-6.668438	-1.352174	-0.394285
C	-7.951865	-1.906594	-0.717013
H	-8.265954	-2.211641	-1.710304
C	-3.556735	-0.345367	2.820435
C	-4.671773	-0.093654	3.841490
H	-4.567899	-0.657752	4.773925
N	-4.293790	-0.603681	1.572832
C	-5.543196	-0.751811	1.887205
O	-5.868431	-0.562819	3.185259
H	-4.817546	0.968565	4.078912
H	-2.940294	0.552920	2.671696
C	-2.637167	-1.513830	3.199978
C	-1.723790	-1.922180	2.054126
C	-1.831091	-1.149018	4.439974
H	-3.291371	-2.369155	3.447071
H	-2.284116	-2.232882	1.164523
H	-1.072147	-2.753799	2.352609
H	-1.075150	-1.088618	1.741804
H	-2.460003	-0.820892	5.277528
H	-1.119527	-0.338732	4.222854
H	-1.247751	-2.007074	4.791694
P	-5.327154	-0.920861	-1.527030
C	-6.035178	0.408178	-2.557725
C	-5.285262	0.811452	-3.672513
C	-7.217418	1.088987	-2.251671
C	-5.718358	1.858611	-4.476325
H	-4.356317	0.288405	-3.910937
C	-7.650297	2.138349	-3.060377
H	-7.803050	0.800895	-1.378658
C	-6.906373	2.523553	-4.172531
H	-5.131245	2.154071	-5.344631
H	-8.574708	2.658694	-2.814424
H	-7.250347	3.341442	-4.803126
C	-5.226788	-2.322888	-2.694921
C	-4.122397	-3.180397	-2.622020
C	-6.217093	-2.563808	-3.655981
C	-4.030118	-4.282198	-3.469729
H	-3.331872	-2.970683	-1.897984
C	-6.122220	-3.662823	-4.503044
H	-7.057311	-1.875101	-3.751335
C	-5.032254	-4.527453	-4.405855
H	-3.169790	-4.946544	-3.404460
H	-6.896502	-3.842637	-5.246429
H	-4.958823	-5.386207	-5.070304
Cu	-3.575573	-0.279492	-0.327153
O	-1.689434	-0.994531	-1.084138
C	-1.273496	-0.186997	-1.927398
O	-0.437662	-0.546752	-2.902506
C	-1.603496	1.242679	-1.924458
N	-2.804566	1.468210	-1.243196
C	-3.478820	2.562324	-1.460717
H	-3.203935	3.232752	-2.285175
C	-4.630922	2.966778	-0.684213
C	-5.488428	3.967180	-1.168650
C	-4.900933	2.412722	0.577931
C	-6.609818	4.360084	-0.450465
H	-5.285933	4.422926	-2.138169
C	-6.023344	2.783660	1.300884
H	-4.188757	1.709446	1.003446
C	-6.879920	3.750821	0.773653
H	-7.281198	5.122947	-0.836732
H	-6.230090	2.349789	2.277570
C	-0.012371	-1.929775	-2.900445
H	-0.898938	-2.558421	-3.058084
H	0.394034	-2.168712	-1.911389
C	-5.286580	-4.192890	0.447410
C	-5.711190	-4.133804	1.808215
H	-5.148544	-3.706303	2.633105
C	-7.035810	-4.654243	1.881841
H	-7.653343	-4.700305	2.772154
C	-6.352130	-4.752905	-0.323250

H	-6.353515	-4.892383	-1.399734
C	-7.431033	-5.038376	0.565873
H	-8.401087	-5.433031	0.283153
H	-4.338790	-3.831506	0.061235
C	-1.289502	2.041105	-3.161569
H	-0.336491	1.723469	-3.591683
H	-1.210929	3.113719	-2.940541
H	-2.062582	1.926436	-3.935842
Fe	-6.961824	-3.061732	0.618916
Cl	-8.289685	4.222272	1.675314
Ir	2.966219	1.658848	0.090791
P	4.576572	0.043020	0.328062
O	5.177703	-0.945595	-0.852466
O	5.981335	0.725788	0.899875
N	4.010201	-1.139771	1.368920
C	6.148475	-0.472626	-1.725074
C	5.755180	-0.293458	-3.064418
H	4.727796	-0.534376	-3.334756
C	6.666784	0.160722	-3.982610
H	6.380355	0.296224	-5.024839
C	7.989111	0.477710	-3.588422
C	8.922325	1.002726	-4.513919
H	8.604474	1.142151	-5.546875
C	10.195143	1.339816	-4.121949
H	10.902064	1.745567	-4.842354
C	10.578503	1.174430	-2.776018
H	11.577935	1.467056	-2.460167
C	9.700121	0.654723	-1.853681
H	10.011141	0.547044	-0.817602
C	8.387350	0.270878	-2.226857
C	7.448818	-0.274437	-1.288099
C	7.825913	-0.588278	0.108909
C	8.913872	-1.466021	0.432878
C	9.623393	-2.198959	-0.551205
H	9.337906	-2.099282	-1.595863
C	10.653340	-3.042532	-0.204717
H	11.175714	-3.598658	-0.980631
C	11.035782	-3.196919	1.142964
H	11.859105	-3.859215	1.402120
C	10.356107	-2.518657	2.125502
H	10.627482	-2.640927	3.173780
C	9.279044	-1.657531	1.806418
C	8.546621	-0.996480	2.821586
H	8.847749	-1.129130	3.860054
C	7.457203	-0.224902	2.506734
H	6.864357	0.278039	3.268252
C	7.095415	-0.055754	1.157474
C	2.800679	-0.705701	2.099053
H	1.914014	-1.137807	1.595079
C	2.817574	-1.190422	3.529832
C	3.983864	-1.128642	4.298839
H	4.907703	-0.792301	3.825909
C	3.971913	-1.512583	5.634793
H	4.888037	-1.464603	6.220857
C	2.791247	-1.963478	6.223940
H	2.782130	-2.266007	7.268954
C	1.627145	-2.033521	5.464726
H	0.704843	-2.395705	5.917603
C	1.644401	-1.654526	4.124350
H	0.735419	-1.712667	3.521986
C	2.691135	0.812509	2.048654
H	3.430641	1.246666	2.741599
H	1.702765	1.110750	2.423709
C	4.206856	-2.622608	1.314438
H	3.877144	-2.943100	2.313336
C	3.263294	-3.285479	0.327285
C	1.970047	-3.624338	0.746171
H	1.676705	-3.413854	1.776925
C	1.076292	-4.261306	-0.110921
H	0.077791	-4.519758	0.239833
C	1.473838	-4.592291	-1.403966
H	0.786864	-5.109588	-2.073530
C	2.758701	-4.266278	-1.832873
H	3.082721	-4.535084	-2.837577
C	3.642326	-3.612527	-0.979265
H	4.644579	-3.373409	-1.328142
C	5.653045	-3.065140	1.193132
H	6.258665	-2.612603	1.985671
H	6.109081	-2.815424	0.231719
H	5.698333	-4.153449	1.313127
C	1.815612	0.222265	-1.041504
H	1.860170	0.434683	-2.113367
H	2.011528	-0.829596	-0.808732
C	0.854703	0.912797	-0.231387
H	0.544093	0.385214	0.674343
C	-0.058620	1.959550	-0.646783
H	0.293045	2.600766	-1.452659
C	4.172991	3.221896	1.005164

H	4.613764	2.828236	1.922864
C	2.799589	3.599526	1.080846
H	2.307528	3.484821	2.050874
C	2.184233	4.656549	0.195095
H	2.490811	5.661918	0.531656
H	1.096915	4.615036	0.336772
C	2.504338	4.471365	-1.292932
H	3.359218	5.092833	-1.592096
H	1.660485	4.839563	-1.893606
C	2.779649	3.029031	-1.684396
H	2.058898	2.580746	-2.372278
C	4.062130	2.460260	-1.715527
H	4.215520	1.637627	-2.415958
C	5.320423	3.161535	-1.271220
H	6.116426	2.410643	-1.180162
H	5.652550	3.854863	-2.062220
C	5.164478	3.892606	0.066572
H	4.863985	4.937343	-0.095069
H	6.142487	3.943484	0.559485
C	1.002751	-2.085749	-3.997701
H	1.906420	-1.502404	-3.785541
H	1.296601	-3.136550	-4.084638
H	0.598227	-1.761311	-4.962242
C	-0.817806	2.649585	0.379527
C	-1.147324	2.171217	1.669078
C	-1.464569	3.874940	0.211383
C	-1.990605	3.098253	2.270965
H	-0.795683	1.255486	2.131486
H	-1.454127	4.571310	-0.619256
C	-2.660170	3.188090	3.510808
C	-3.026435	5.197846	1.607810
C	-3.496763	4.242439	3.774079
H	-2.487631	2.403586	4.246563
C	-3.684671	5.258252	2.799248
H	-3.126810	5.934699	0.816398
H	-4.013251	4.309847	4.728326
H	-4.356456	6.090611	2.985854
N	-2.180674	4.148190	1.343512

TS3-*trans*

M06-L SCF energy in solvent: -8423.346636 a.u

C	-4.545172	-2.396240	-1.253560
C	-4.946142	-3.611821	-1.907404
H	-4.643919	-3.911763	-2.904496
C	-5.849002	-4.297377	-1.051088
H	-6.362981	-5.223866	-1.283873
C	-5.218823	-2.336099	0.034598
C	-6.024036	-3.519964	0.128665
H	-6.669559	-3.770121	0.965114
C	-2.946423	0.573802	-2.623498
C	-2.430527	-0.565579	-3.500447
H	-2.554829	-0.411796	-4.576202
N	-3.533737	-0.153159	-1.485924
C	-3.770758	-1.358015	-1.903641
O	-3.274209	-1.681954	-3.120902
H	-1.388876	-0.845825	-3.287234
H	-2.132380	1.217154	-2.256161
C	-3.994767	1.436813	-3.354144
C	-4.884983	2.231706	-2.411003
C	-3.310006	2.338491	-4.373897
H	-4.638708	0.728616	-3.905217
H	-5.353959	1.583458	-1.661989
H	-5.676662	2.743227	-2.971653
H	-4.325078	2.992241	-1.851538
H	-2.706399	1.774405	-5.096541
H	-2.635156	3.052886	-3.879133
H	-4.043947	2.918105	-4.945066
P	-4.951828	-1.091899	1.330463
C	-4.377974	-2.084631	2.757818
C	-4.242888	-1.419824	3.986829
C	-4.047656	-3.441623	2.684486
C	-3.823113	-2.105793	5.119981
H	-4.483498	-0.357483	4.054116
C	-3.629172	-4.126788	3.823702
H	-4.107031	-3.971714	1.735059
C	-3.520927	-3.465647	5.042582
H	-3.738156	-1.580138	6.069582
H	-3.381247	-5.185177	3.750046
H	-3.201411	-4.005769	5.931876
C	-6.629019	-0.588950	1.861787
C	-7.079437	0.689312	1.513761
C	-7.469495	-1.433019	2.599017
C	-8.362428	1.104007	1.862404
H	-6.410492	1.359853	0.968751
C	-8.748992	-1.015454	2.951911
H	-7.109525	-2.412337	2.916772
C	-9.198985	0.250190	2.577441
H	-8.705589	2.099119	1.585199

H	-9.394623	-1.675279	3.528512
H	-10.198895	0.576042	2.857449
Cu	-3.589365	0.413611	0.512933
O	-3.675049	2.530573	0.604366
C	-2.769919	2.989045	1.326401
O	-2.735450	4.275550	1.680152
C	-1.629618	2.211937	1.790895
N	-1.830353	0.843203	1.615374
C	-1.132358	-0.027092	2.287356
H	-0.497157	0.280005	3.129208
C	-1.095113	-1.432558	1.930656
C	-0.685584	-2.391057	2.868961
C	-1.379896	-1.863145	0.621033
C	-0.608460	-3.735850	2.535648
H	-0.447947	-2.075097	3.883906
C	-1.315848	-3.204888	0.273531
H	-1.625485	-1.120150	-0.137703
C	-0.943699	-4.136177	1.243641
H	-0.314000	-4.477046	3.274750
H	-1.535277	-3.530260	-0.742359
C	-3.772543	5.121980	1.134481
H	-4.725028	4.839639	1.600055
H	-3.856140	4.918273	0.060078
C	-7.558047	-0.667657	-1.607466
C	-7.052427	-1.037242	-2.887662
H	-6.342793	-0.468128	-3.481476
C	-7.592351	-2.311579	-3.227180
H	-7.364994	-2.883234	-4.120378
C	-8.411086	-1.717099	-1.149114
H	-8.914726	-1.750020	-0.187995
C	-8.434061	-2.731372	-2.153361
H	-8.959033	-3.678580	-2.091153
H	-7.311615	0.234369	-1.058050
C	-0.798699	2.732555	2.921674
H	-0.689231	3.817886	2.849511
H	0.204307	2.285715	2.922937
H	-1.253903	2.505845	3.897955
Fe	-6.541629	-2.430581	-1.489492
Cl	-0.904996	-5.828623	0.836334
Ir	2.428641	1.404837	-1.069127
P	4.136289	0.211761	-0.101678
O	3.982505	-1.245968	0.650664
O	5.298745	-0.152970	-1.224597
N	4.746064	1.082660	1.198021
C	3.763279	-2.383614	-0.110865
C	2.486504	-2.967745	-0.015796
H	1.748309	-2.504495	0.639687
C	2.214119	-4.101156	-0.737826
H	1.237643	-4.579946	-0.666664
C	3.188799	-4.655027	-1.603102
C	2.891728	-5.781237	-2.406997
H	1.900738	-6.227295	-2.324549
C	3.822793	-6.295400	-3.276889
H	3.580596	-7.159208	-3.892348
C	5.092115	-5.691453	-3.379806
H	5.820270	-6.083962	-4.086698
C	5.420593	-4.607841	-2.597611
H	6.402957	-4.151347	-2.693898
C	4.493648	-4.064153	-1.673990
C	4.801925	-2.932815	-0.845529
C	6.161749	-2.351491	-0.749485
C	7.303758	-3.150270	-0.400191
C	7.198945	-4.513239	-0.023594
H	6.218230	-4.980366	0.018365
C	8.313564	-5.249832	0.305445
H	8.200487	-6.292297	0.597023
C	9.596505	-4.667843	0.277347
H	10.470129	-5.263576	0.532505
C	9.732968	-3.341502	-0.052480
H	10.714707	-2.868658	-0.056420
C	8.606235	-2.550695	-0.380815
C	8.743753	-1.172396	-0.669924
H	9.739245	-0.730047	-0.667350
C	7.640858	-0.398548	-0.921068
H	7.717841	0.667519	-1.123071
C	6.365402	-0.992824	-0.937228
C	4.167038	2.443068	1.261271
H	3.288526	2.410650	1.932300
C	5.133083	3.456556	1.824041
C	6.484964	3.459938	1.468235
H	6.861158	2.670750	0.815432
C	7.338755	4.444484	1.954491
H	8.390751	4.434671	1.675317
C	6.852002	5.440812	2.799209
H	7.522674	6.207589	3.181732
C	5.506621	5.446601	3.157359
H	5.121179	6.217499	3.822273
C	4.655594	4.456403	2.673781

H	3.599547	4.453229	2.955764
C	3.689061	2.854158	-0.120066
H	4.561305	3.067593	-0.758799
H	3.120706	3.789769	-0.040638
C	5.194860	0.539667	2.525257
H	5.651564	1.421412	2.997784
C	4.012925	0.150020	3.396617
C	3.346412	1.148818	4.119094
H	3.740365	2.166745	4.102229
C	2.213714	0.859157	4.876885
H	1.714759	1.652605	5.431619
C	1.739894	-0.448465	4.942581
H	0.864639	-0.683284	5.548264
C	2.417976	-1.459836	4.263382
H	2.074593	-2.491545	4.333080
C	3.543813	-1.164222	3.501610
H	4.061577	-1.966080	2.981196
C	6.293801	-0.499371	2.416474
H	7.124738	-0.110194	1.818156
H	5.968352	-1.440058	1.964325
H	6.673972	-0.723744	3.419401
C	1.357059	0.753071	0.703369
H	0.680884	-0.061992	0.434175
H	1.970498	0.522207	1.580412
C	0.924106	2.104401	0.497309
H	1.454183	2.882902	1.050097
C	-0.366628	2.497571	0.018793
H	-0.956202	1.733859	-0.492304
C	3.467707	1.821094	-2.917488
H	4.482830	2.142965	-2.675501
C	2.446243	2.806303	-2.735207
H	2.776891	3.792525	-2.397305
C	1.149383	2.823036	-3.504969
H	1.303877	3.228071	-4.519920
H	0.465599	3.521347	-3.001884
C	0.492195	1.443313	-3.573478
H	0.809546	0.899544	-4.473622
H	-0.593486	1.570344	-3.685075
C	0.769034	0.583287	-2.349347
H	-0.086847	0.399685	-1.693040
C	1.787675	-0.381728	-2.297999
H	1.632897	-1.227546	-1.625269
C	2.802475	-0.600992	-3.392174
H	3.610391	-1.221578	-2.983307
H	2.350182	-1.196737	-4.203247
C	3.399856	0.701171	-3.945074
H	2.840242	1.043856	-4.826115
H	4.414105	0.495267	-4.306859
C	-3.384173	6.545845	1.420328
H	-4.129508	7.229474	1.000476
H	-3.317481	6.731932	2.497228
H	-2.413857	6.782675	0.969679
C	-0.592544	3.850832	-0.444441
C	-1.628807	4.205555	-1.305661
C	0.144612	5.021765	-0.150624
H	-2.408494	3.599716	-1.749501
C	-0.445653	6.077487	-0.835197
H	1.015562	5.102330	0.490379
C	-2.367139	6.343649	-2.312717
C	-0.202462	7.463997	-0.944331
C	-2.122039	7.680910	-2.399515
H	-3.184594	5.832859	-2.815343
C	-1.022470	8.255247	-1.706407
H	0.644499	7.881754	-0.405481
H	-2.776770	8.295859	-3.009216
H	-0.834922	9.322586	-1.786152
N	-1.550248	5.547718	-1.545905

(*2R,3R*)-**Int-I**

M06-L SCF energy in solvent: -1610.714056 a.u

O	0.923842	-1.206371	-2.134153
C	1.320869	-1.697289	-1.105479
O	2.552935	-2.238448	-0.954143
C	0.522085	-1.830322	0.196863
N	-0.684527	-1.047344	0.015121
C	-1.838440	-1.571752	0.136576
H	-2.005220	-2.637968	0.375409
C	-3.057077	-0.780169	-0.038774
C	-4.306830	-1.365254	0.188362
C	-2.997756	0.560539	-0.445273
C	-5.478957	-0.638249	0.021442
H	-4.360479	-2.408396	0.501205
C	-4.157219	1.298996	-0.618675
H	-2.020136	0.999430	-0.636565
C	-5.390949	0.690212	-0.382786
H	-6.451565	-1.090254	0.196210
H	-4.119424	2.336792	-0.940130
C	3.402733	-2.111184	-2.110531

H	3.502779	-1.044335	-2.347531
H	2.906265	-2.585378	-2.965770
C	0.337054	-3.315175	0.511099
H	-0.185757	-3.448228	1.465535
H	1.312705	-3.804255	0.587521
H	-0.233904	-3.825194	-0.273996
Cl	-6.855621	1.606582	-0.609374
C	0.743322	-1.827978	3.687932
H	1.557182	-2.553298	3.726016
H	0.126121	-1.743944	4.579833
C	0.531262	-1.077896	2.608164
H	-0.289634	-0.357117	2.599292
C	1.348206	-1.144430	1.351574
H	2.210898	-1.802250	1.526841
C	4.720228	-2.756910	-1.778698
H	4.589653	-3.815723	-1.530553
H	5.401271	-2.689663	-2.633782
H	5.199224	-2.266282	-0.924011
C	1.860150	0.209590	0.953220
C	1.123543	1.400984	0.798505
C	3.190139	0.490205	0.673507
C	2.008906	2.405276	0.425502
H	0.054276	1.519890	0.921882
H	4.064353	-0.149059	0.686778
C	1.900650	3.778865	0.126946
C	4.402480	2.552246	0.013324
C	3.009656	4.510099	-0.213976
H	0.915617	4.237657	0.177561
C	4.281475	3.879991	-0.269449
H	5.340792	2.005274	-0.008442
H	2.921453	5.569375	-0.442016
H	5.171101	4.442634	-0.536838
N	3.294612	1.817998	0.354168

TS4

M06-L SCF energy in solvent: -2071.549206 a.u

C	4.097280	1.888309	2.420659
H	4.905812	2.105857	1.720383
H	4.267078	2.161770	3.459674
C	2.959650	1.317740	2.029424
H	2.166253	1.095748	2.750231
C	2.700021	0.937439	0.598019
H	3.586554	1.171288	-0.004442
O	3.480046	-0.266573	-1.794661
C	2.824229	-0.969129	-1.054931
O	2.351376	-2.177739	-1.397057
C	2.479680	-0.632167	0.407796
N	1.114009	-1.045957	0.696820
C	0.128448	-0.500549	-0.047649
H	0.413152	-0.285715	-1.083055
C	-1.288552	-0.836813	0.101180
C	-1.844291	-1.372819	1.273628
C	-2.130861	-0.561500	-0.988035
C	-3.207439	-1.622116	1.346344
H	-1.216073	-1.549279	2.147685
C	-3.494179	-0.815257	-0.926305
H	-1.707356	-0.141203	-1.901845
C	-4.021458	-1.342481	0.249271
H	-3.641633	-2.031063	2.254584
H	-4.142310	-0.605042	-1.772950
C	2.688447	-2.610247	-2.734598
H	3.779781	-2.593285	-2.839120
H	2.285309	-1.878561	-3.445852
C	3.418937	-1.417787	1.318408
H	3.142598	-1.247648	2.365413
H	4.452984	-1.085093	1.180742
H	3.350716	-2.488274	1.102109
C	1.529503	1.662179	0.040655
C	0.218071	1.464505	0.572704
C	0.068977	2.758105	-1.296076
C	-0.653992	3.467447	-2.267985
C	-1.988970	2.386246	-0.067568
C	-2.014485	3.633782	-2.126033
H	-0.118468	3.882614	-3.117867
C	-2.688487	3.092010	-1.008775
H	-2.425992	1.933020	0.817990
H	-2.574150	4.188756	-2.874934
H	-3.758658	3.222056	-0.881960
Cl	-5.730955	-1.656352	0.348923
H	-0.041739	1.241052	1.613815
H	0.904311	-1.113996	1.721061
Cl	0.348096	-0.364505	3.588453
C	1.421032	2.400206	-1.127568
H	2.222260	2.640144	-1.816439
C	2.105286	-3.983346	-2.920648
H	2.331136	-4.354728	-3.925674
H	2.520530	-4.689341	-2.194450
H	1.017486	-3.970450	-2.797046

N	-0.643070	2.222802	-0.215565

Int-II

M06-L SCF energy in solvent: -2071.559056 a.u

C	3.885562	2.366814	2.133588
H	4.668474	2.543439	1.393873
H	4.049527	2.784062	3.124459
C	2.787704	1.669288	1.848340
H	2.010668	1.499196	2.600688
C	2.532536	1.087390	0.480918
H	3.396976	1.317092	-0.159178
O	2.444036	-0.404459	-1.920629
C	2.751330	-0.985190	-0.895188
O	3.446389	-2.128354	-0.872227
C	2.350503	-0.499810	0.502695
N	0.968902	-0.953883	0.693760
C	-0.035105	-0.302458	-0.100105
H	0.269889	-0.326727	-1.153873
C	-1.410051	-0.900823	0.003918
C	-1.991790	-1.255506	1.226451
C	-2.155935	-1.056211	-1.169353
C	-3.289669	-1.752974	1.269563
H	-1.441607	-1.105756	2.157966
C	-3.455145	-1.551567	-1.140935
H	-1.710615	-0.784977	-2.127838
C	-4.010675	-1.896199	0.086818
H	-3.742652	-2.026661	2.219152
H	-4.029541	-1.674508	-2.055639
C	3.793932	-2.660902	-2.170435
H	4.338089	-1.888262	-2.726709
H	2.865648	-2.861393	-2.718844
C	3.186258	-1.119627	1.610124
H	2.813348	-0.782128	2.583763
H	4.237176	-0.824292	1.525532
H	3.122261	-2.209078	1.567536
C	1.325435	1.727329	-0.093307
C	-0.006885	1.244259	0.314979
C	-0.188270	2.917128	-1.281562
C	-0.897543	3.779314	-2.125467
C	-2.257485	2.107820	-0.363183
C	-2.278037	3.790859	-2.074972
H	-0.348030	4.431979	-2.797902
C	-2.968668	2.954448	-1.180100
H	-2.701319	1.438345	0.368087
H	-2.836783	4.461671	-2.723507
H	-4.051485	2.969435	-1.114497
Cl	-5.640908	-2.516375	0.143370
H	-0.224626	1.258007	1.411776
H	0.726007	-0.880422	1.694315
Cl	-0.024041	0.386903	3.473357
C	1.196136	2.682148	-1.058964
H	1.995786	3.175747	-1.599075
C	4.612878	-3.900742	-1.942015
H	4.905747	-4.340517	-2.901212
H	5.523832	-3.672174	-1.379163
H	4.045525	-4.650643	-1.381449
N	-0.906568	2.088648	-0.442420

TS5

M06-L SCF energy in solvent: -2071.539766 a.u

C	3.570463	1.021661	3.269109
H	4.597562	0.965629	2.906104
H	3.430756	1.405660	4.277040
C	2.540283	0.649787	2.512758
H	1.518783	0.730102	2.892194
C	2.678388	0.143059	1.103179
H	3.741275	0.117358	0.831098
O	3.538256	-1.442152	-1.062460
C	2.593210	-1.845013	-0.420777
O	1.822216	-2.889698	-0.797733
C	2.109410	-1.287195	0.929807
N	0.645835	-1.227514	1.027761
C	-0.027916	-0.524438	-0.070736
H	0.208054	-0.980076	-1.058880
C	-1.522989	-0.651167	0.111615
C	-2.133173	-0.359367	1.334998
C	-2.317959	-1.095696	-0.947069
C	-3.509129	-0.479232	1.488122
H	-1.523108	-0.027160	2.171556
C	-3.697819	-1.219926	-0.813622
H	-1.847894	-1.342390	-1.901010
C	-4.280610	-0.903174	0.409217
H	-3.984842	-0.240081	2.435653
H	-4.314283	-1.561799	-1.641126
C	2.172189	-3.487379	-2.063815
H	3.152794	-3.968663	-1.961567
H	2.281128	-2.687313	-2.805791
C	2.618713	-2.226035	2.019083

H	2.254716	-1.891512	2.995506
H	3.714428	-2.231211	2.045143
H	2.273379	-3.251457	1.842979
C	1.952350	1.049303	0.157548
C	0.557749	0.879589	-0.084228
C	1.346862	2.641207	-1.313889
C	1.201466	3.732928	-2.185613
C	-0.971555	2.075835	-1.662065
C	-0.007081	3.967722	-2.797911
H	2.060056	4.377001	-2.356916
C	-1.108062	3.126013	-2.527745
H	-1.783065	1.412656	-1.381367
H	-0.122236	4.809061	-3.476883
H	-2.076589	3.305378	-2.983947
Cl	-6.008600	-1.047077	0.597713
H	-0.016453	1.667973	1.102342
H	0.281076	-2.177095	1.055075
Cl	-0.596738	2.592673	2.074557
C	2.412440	2.147532	-0.540816
H	3.407583	2.575365	-0.507883
N	0.238898	1.819576	-1.087959
C	1.082536	-4.461451	-2.417919
H	1.299348	-4.940568	-3.378483
H	0.987585	-5.245945	-1.659873
H	0.115203	-3.953043	-2.502016

3a

M06-L SCF energy in solvent: -1610.726950 a.u

C	2.532747	0.681939	4.072150
H	3.553617	1.042318	3.940389
H	2.142958	0.689181	5.087936
C	1.803622	0.265636	3.038803
H	0.780718	-0.089819	3.191614
C	2.272631	0.267046	1.612606
H	3.339301	0.528351	1.583348
O	3.945930	-0.480403	-0.556957
C	2.936962	-1.120211	-0.358060
O	2.420482	-1.997417	-1.250214
C	2.114812	-1.118382	0.941000
N	0.684389	-1.382818	0.748943
C	-0.006425	-0.549011	-0.249899
H	0.226754	-0.876395	-1.287093
C	-1.499396	-0.725560	-0.049987
C	-2.265630	-1.430063	-0.976307
C	-2.124618	-0.207197	1.086786
C	-3.632127	-1.623521	-0.783965
H	-1.786089	-1.837476	-1.868473
C	-3.484533	-0.386326	1.297809
H	-1.528048	0.348912	1.810113
C	-4.227042	-1.098336	0.356848
H	-4.229060	-2.174461	-1.506313
H	-3.973420	0.019304	2.180011
C	3.152929	-2.105687	-2.488221
H	4.160898	-2.477283	-2.265519
H	3.267131	-1.101063	-2.912295
C	2.681575	-2.232101	1.817992
H	2.103165	-2.306730	2.744552
H	3.725341	-2.023453	2.077498
H	2.641737	-3.198296	1.299830
C	1.494249	1.255745	0.796190
C	0.471615	0.847287	-0.047026
C	0.685159	3.097996	-0.219164
C	0.329796	4.351819	-0.753281
C	-1.021308	2.069066	-1.621710
C	-0.667406	4.456930	-1.689804
H	0.871246	5.228148	-0.403695
C	-1.349656	3.292061	-2.127215
H	-1.508292	1.142029	-1.909155
H	-0.937189	5.427318	-2.099234
H	-2.140869	3.355402	-2.868606
Cl	-5.936845	-1.333435	0.618720
H	0.554940	-2.356968	0.487546
C	1.625732	2.650415	0.702683
H	2.332249	3.275725	1.235840
N	-0.026207	1.960182	-0.680235
C	2.382361	-3.031853	-3.388867
H	1.380586	-2.637829	-3.594223
H	2.902284	-3.150457	-4.345386
H	2.271548	-4.023188	-2.936649

TS4'

M06-L SCF energy in solvent: -2071.548760 a.u

C	-4.327891	1.520813	1.490815
H	-4.212086	0.853946	2.345208
H	-5.232957	2.123285	1.456195
C	-3.398548	1.592568	0.540267
H	-3.540619	2.271757	-0.305522
C	-2.132343	0.797167	0.564342

H	-2.071777	0.188514	1.481950
O	-2.974686	-2.374386	0.207480
C	-3.151671	-1.332783	-0.377483
O	-4.335851	-0.917271	-0.855022
C	-2.054843	-0.295682	-0.630182
N	-0.793286	-1.010193	-0.507579
C	0.349624	-0.338263	-0.749207
H	0.279240	0.416975	-1.534382
C	1.676419	-0.936578	-0.621617
C	1.956378	-2.030684	0.213275
C	2.724481	-0.338692	-1.339557
C	3.255462	-2.506257	0.322021
H	1.167591	-2.471813	0.823663
C	4.025374	-0.812988	-1.241421
H	2.512738	0.513284	-1.987216
C	4.278075	-1.896170	-0.404087
H	3.479835	-3.346488	0.973390
H	4.834897	-0.350905	-1.799917
C	-5.452168	-1.770509	-0.516786
H	-5.256207	-2.773040	-0.914400
H	-5.495646	-1.857208	0.575625
C	-2.204938	0.369781	-1.991799
H	-1.528724	1.224813	-2.104501
H	-1.998857	-0.346931	-2.794137
H	-3.225542	0.735966	-2.118040
C	-0.906335	1.630256	0.478808
C	0.357776	1.065734	0.809537
C	0.685792	3.151635	-0.046566
C	1.502957	4.215035	-0.463822
C	2.655828	1.981643	0.752903
C	2.864764	4.151101	-0.269887
H	1.038403	5.079908	-0.930639
C	3.447496	3.022652	0.351658
H	3.015000	1.081479	1.243408
H	3.497232	4.976598	-0.587158
H	4.518010	2.967555	0.523197
Cl	5.905829	-2.497601	-0.260714
H	0.514696	0.299944	1.583234
H	-0.781318	-1.631296	0.328677
Cl	-0.421591	-1.582642	2.540985
C	-6.688302	-1.143040	-1.098724
H	-6.848655	-0.139317	-0.690750
H	-7.566743	-1.751931	-0.861250
H	-6.615496	-1.061098	-2.188415
C	-0.695676	2.885238	-0.085199
H	-1.441037	3.562899	-0.485450
N	1.308143	2.044282	0.544610

Int-II'

M06-L SCF energy in solvent: -2071.562234 a.u

C	-4.469585	1.444531	1.184601
H	-4.339482	0.871718	2.103135
H	-5.421506	1.954814	1.053783
C	-3.502676	1.510499	0.270509
H	-3.660647	2.090963	-0.643693
C	-2.192543	0.810227	0.409424
H	-2.103891	0.332483	1.404295
O	-2.851978	-2.300300	0.638696
C	-3.038397	-1.463601	-0.213262
O	-4.199174	-1.292776	-0.868833
C	-1.994945	-0.422438	-0.618682
N	-0.699898	-1.047695	-0.416653
C	0.431555	-0.181841	-0.599881
H	0.366132	0.268711	-1.601417
C	1.757360	-0.884971	-0.495412
C	2.115962	-1.611056	0.646406
C	2.679208	-0.760891	-1.537911
C	3.374920	-2.194071	0.741239
H	1.416973	-1.690977	1.484429
C	3.942584	-1.338308	-1.455967
H	2.407856	-0.198162	-2.432227
C	4.278737	-2.049232	-0.308443
H	3.656279	-2.755119	1.628507
H	4.658836	-1.239815	-2.267584
C	-5.275363	-2.141603	-0.414032
H	-5.006874	-3.183726	-0.624199
H	-5.355630	-2.042333	0.675068
C	-2.165572	0.051708	-2.056544
H	-1.518849	0.909696	-2.277085
H	-1.914458	-0.756339	-2.751739
H	-3.197293	0.356530	-2.244206
C	-1.005470	1.667947	0.249526
C	0.310461	1.033152	0.424974
C	0.541780	3.266519	-0.161363
C	1.273850	4.424798	-0.447168
C	2.584196	2.086849	0.302515
C	2.651824	4.394913	-0.360167
H	0.741441	5.330655	-0.723706

C	3.316031	3.216235	0.026716
H	3.011993	1.144283	0.630347
H	3.227471	5.291321	-0.578240
H	4.396061	3.184159	0.125110
Cl	5.867343	-2.760087	-0.179147
H	0.409833	0.577783	1.452877
H	-0.682432	-1.491602	0.510842
Cl	-0.320677	-0.734283	2.933261
C	-6.522354	-1.705256	-1.131878
H	-6.757453	-0.659381	-0.906012
H	-7.372859	-2.321100	-0.821320
H	-6.409546	-1.802531	-2.216894
C	-0.849942	2.974512	-0.121799
H	-1.630605	3.699451	-0.323831
N	1.234871	2.119934	0.183010

TS5'

M06-L SCF energy in solvent: -2071.539063 a.u

C	-4.454628	1.073034	1.321101
H	-4.231473	0.512734	2.229801
H	-5.456090	1.489345	1.235790
C	-3.536907	1.240884	0.369674
H	-3.786647	1.812522	-0.528917
C	-2.161252	0.658522	0.427360
H	-1.983503	0.267544	1.444339
O	-2.621086	-2.310440	1.009788
C	-2.881864	-1.663195	0.017755
O	-4.040175	-1.737937	-0.651990
C	-1.952613	-0.587052	-0.531988
N	-0.598112	-1.121602	-0.397113
C	0.492969	-0.205055	-0.725706
H	0.443462	-0.039720	-1.819057
C	1.803492	-0.917100	-0.452849
C	2.708680	-0.525857	0.534059
C	2.107257	-2.043745	-1.226352
C	3.894929	-1.225676	0.739960
H	2.493859	0.325956	1.175305
C	3.283609	-2.755355	-1.034690
H	1.395550	-2.371232	-1.983487
C	4.173984	-2.333510	-0.049307
H	4.591367	-0.915844	1.514342
H	3.515549	-3.627716	-1.640113
C	-5.040865	-2.585605	-0.045063
H	-4.699838	-3.625812	-0.109292
H	-5.106777	-2.329095	1.019060
C	-2.231041	-0.218460	-1.980690
H	-1.619516	0.639167	-2.288714
H	-1.998235	-1.062376	-2.638498
H	-3.280227	0.050469	-2.125673
C	-1.075431	1.624947	0.114983
C	0.264017	1.154794	-0.069709
C	0.195602	3.440036	-0.273695
C	0.773069	4.705354	-0.462472
C	2.304124	2.410735	-0.821369
C	2.092011	4.810531	-0.838832
H	0.151880	5.585361	-0.316435
C	2.860140	3.643151	-1.036112
H	2.839558	1.475461	-0.947603
H	2.541659	5.788225	-0.992486
H	3.895684	3.700013	-1.356893
Cl	5.662790	-3.208968	0.194266
H	0.469675	0.954889	1.404037
H	-0.481806	-1.481959	0.550826
Cl	0.547427	0.737681	2.874694
C	-6.331086	-2.346787	-0.779362
H	-6.236358	-2.596272	-1.841487
H	-7.128818	-2.964573	-0.353722
H	-6.632706	-1.296413	-0.701277
C	-1.100465	3.003324	0.053593
H	-1.943828	3.652279	0.258532
N	1.003482	2.308525	-0.420718

3a'

M06-L SCF energy in solvent: -1610.725967 a.u

C	4.250556	1.200466	-1.724663
H	4.114412	0.430948	-2.485980
H	5.202305	1.727569	-1.728912
C	3.291712	1.479826	-0.841477
H	3.455465	2.262520	-0.095616
C	1.983394	0.755314	-0.758902
H	1.842700	0.199155	-1.700455
O	2.675001	-2.152050	-1.067259
C	2.932587	-1.432414	-0.123134
O	4.093479	-1.453191	0.544172
C	1.974246	-0.352211	0.368906
N	0.667788	-1.018533	0.446410
C	-0.475588	-0.145646	0.774510
H	-0.480706	-0.029554	1.877147

C	-1.737537	-0.897424	0.404167
C	-2.490803	-0.576549	-0.726005
C	-2.130343	-1.986089	1.187522
C	-3.621664	-1.314512	-1.065500
H	-2.192933	0.265986	-1.350588
C	-3.252793	-2.737382	0.862751
H	-1.535499	-2.252858	2.060533
C	-3.992004	-2.389610	-0.265483
H	-4.211722	-1.059189	-1.941683
H	-3.556586	-3.584285	1.472585
C	5.087352	-2.361639	0.023057
H	4.750301	-3.388314	0.211436
H	5.139632	-2.231076	-1.064124
C	2.345900	0.216639	1.728464
H	1.672380	1.038289	1.999003
H	2.271758	-0.560173	2.496149
H	3.368591	0.602578	1.729127
C	0.812589	1.654276	-0.518462
C	-0.315271	1.201179	0.152854
C	-0.595560	3.405786	-0.315970
C	-1.332422	4.605268	-0.290332
C	-2.394737	2.327390	0.924694
C	-2.556101	4.661873	0.328838
H	-0.900380	5.481900	-0.768380
C	-3.087863	3.501915	0.948240
H	-2.748439	1.402310	1.369852
H	-3.119893	5.591183	0.347434
H	-4.052051	3.529122	1.447682
Cl	-5.411325	-3.317818	-0.679085
H	0.499080	-1.467746	-0.453306
C	6.386182	-2.039042	0.708893
H	6.301403	-2.156960	1.794226
H	7.178984	-2.705610	0.353308
H	6.686458	-1.006331	0.500597
C	0.643460	3.016568	-0.818867
H	1.337673	3.659488	-1.347579
N	-1.172074	2.265961	0.299601

TS2'-*trans*

M06-L SCF energy in solvent: -8423.353065 a.u

Ir	1.942639	1.427205	-1.075457
P	3.852144	0.516782	-0.199189
O	3.938763	-0.856767	0.709476
O	4.917796	0.141588	-1.414998
C	3.778633	-2.090984	0.101847
C	2.604138	-2.800444	0.415233
H	1.897381	-2.348377	1.111816
C	2.394060	-4.031946	-0.150512
H	1.498419	-4.605897	0.087951
C	3.322648	-4.566187	-1.076740
C	3.082834	-5.800631	-1.727288
H	2.175914	-6.350999	-1.473322
C	3.965206	-6.295513	-2.657849
H	3.766843	-7.244080	-3.152814
C	5.127974	-5.565252	-2.977468
H	5.813886	-5.946278	-3.731354
C	5.405116	-4.376081	-2.343978
H	6.304740	-3.821620	-2.601979
C	4.527366	-3.845407	-1.366705
C	4.788186	-2.604612	-0.695016
C	6.074364	-1.881006	-0.818674
C	7.329169	-2.512110	-0.516905
C	7.418157	-3.822528	0.015409
H	6.505321	-4.378722	0.214173
C	8.636435	-4.393697	0.302477
H	8.673433	-5.398529	0.718798
C	9.834822	-3.689860	0.069895
H	10.792005	-4.156678	0.292587
C	9.786003	-2.408372	-0.421680
H	10.702296	-1.842350	-0.587314
C	8.549160	-1.782782	-0.709122
C	8.497078	-0.442575	-1.160366
H	9.430603	0.095489	-1.320600
C	7.292516	0.179086	-1.365145
H	7.224371	1.214555	-1.691618
C	6.099221	-0.540534	-1.169312
C	1.108865	0.888203	0.849928
H	0.500317	-0.012941	0.744813
H	1.812900	0.833336	1.686943
C	0.526117	2.162949	0.543464
H	1.005531	3.036929	0.990457
C	-0.805756	2.392526	0.071622
H	-1.318749	1.563067	-0.418582
C	2.731485	1.720871	-3.073060
H	3.727971	2.158481	-2.985150
C	1.632505	2.611414	-2.878906
H	1.875705	3.659090	-2.683510
C	0.276092	2.400126	-3.503272

H	0.309195	2.640286	-4.579985
H	-0.414970	3.126850	-3.057893
C	-0.276790	0.985335	-3.292335
H	-0.072355	0.355234	-4.171091
H	-1.374950	1.032208	-3.218245
C	0.261083	0.285316	-2.052060
H	-0.481829	0.054766	-1.281519
C	1.387998	-0.548823	-2.040403
H	1.393322	-1.337945	-1.284915
C	2.300479	-0.785225	-3.215284
H	3.219341	-1.256253	-2.843754
H	1.842212	-1.524305	-3.894705
C	2.658841	0.497495	-3.973188
H	1.940399	0.681745	-4.784286
H	3.627799	0.360321	-4.467396
C	-5.441774	-2.965967	0.343269
C	-6.568097	-3.830716	0.132894
H	-7.131855	-4.318611	0.920048
C	-6.835898	-3.877045	-1.261085
H	-7.657142	-4.405644	-1.732682
C	-5.007668	-2.471477	-0.952921
C	-5.882645	-3.057548	-1.927637
H	-5.849993	-2.863199	-2.994354
C	-4.251660	-1.493593	3.464811
C	-4.576716	-2.944302	3.820138
H	-5.247898	-3.067737	4.674407
N	-4.328276	-1.499509	1.989944
C	-4.964264	-2.578157	1.658850
O	-5.273697	-3.437457	2.650597
H	-3.687214	-3.571862	3.960893
H	-3.232624	-1.222669	3.771211
C	-5.235315	-0.493274	4.094646
C	-5.117376	0.892559	3.482781
C	-5.009958	-0.431482	5.600378
H	-6.253546	-0.878420	3.903836
H	-5.315743	0.887191	2.405749
H	-5.816828	1.590547	3.958720
H	-4.102959	1.291517	3.631921
H	-5.096584	-1.410115	6.088128
H	-4.006169	-0.040754	5.820826
H	-5.733889	0.236144	6.079919
P	-3.578914	-1.390930	-1.259178
C	-2.354793	-2.596255	-1.901503
C	-1.488522	-2.275208	-2.952733
C	-2.224217	-3.846234	-1.280557
C	-0.520912	-3.180929	-3.376537
H	-1.581383	-1.315470	-3.457529
C	-1.244974	-4.745037	-1.696919
H	-2.900741	-4.121892	-0.469515
C	-0.388711	-4.414362	-2.745693
H	0.127493	-2.922595	-4.212241
H	-1.160223	-5.714949	-1.206364
H	0.373104	-5.117447	-3.077128
C	-4.071367	-0.431397	-2.735061
C	-4.343450	0.933681	-2.582751
C	-4.209060	-1.014425	-4.002628
C	-4.756004	1.695962	-3.673690
H	-4.231606	1.392491	-1.599729
C	-4.615202	-0.248980	-5.090948
H	-3.976908	-2.070110	-4.143102
C	-4.891899	1.107650	-4.928731
H	-4.974566	2.755450	-3.539962
H	-4.714179	-0.712269	-6.070663
H	-5.207735	1.704361	-5.782052
Cu	-3.251947	-0.311798	0.631379
O	-3.971224	1.754957	0.530566
C	-3.272137	2.479699	1.261047
O	-3.602631	3.748537	1.515193
C	-2.013229	2.053721	1.851568
N	-1.907654	0.662001	1.905919
C	-1.122188	0.096523	2.778672
H	-0.626014	0.694462	3.553195
C	-0.845057	-1.327478	2.817499
C	-0.399547	-1.892992	4.024907
C	-0.985266	-2.175070	1.703785
C	-0.136299	-3.250051	4.140501
H	-0.270720	-1.247197	4.893330
C	-0.724332	-3.534273	1.804939
H	-1.277019	-1.758322	0.736642
C	-0.303877	-4.066843	3.023106
H	0.202207	-3.676121	5.081390
H	-0.818155	-4.177481	0.933824
C	-4.784958	4.243062	0.846724
H	-4.688489	4.032966	-0.227174
H	-5.650922	3.678827	1.216977
C	-6.908039	0.065060	-0.332270
C	-7.577294	-0.572214	0.754431
H	-7.269480	-0.535444	1.795679

C	-8.663245	-1.331164	0.228321
H	-9.336604	-1.961094	0.799448
C	-7.582578	-0.304930	-1.537859
H	-7.290554	-0.019687	-2.544009
C	-8.666962	-1.166274	-1.189109
H	-9.349003	-1.644969	-1.883646
H	-6.016656	0.683248	-0.250653
C	-1.363176	2.912549	2.889578
H	-0.286918	2.703142	2.960460
H	-1.490170	3.969304	2.639533
H	-1.794205	2.752419	3.890180
Fe	-6.899538	-1.951364	-0.573938
C	3.847780	2.901462	0.883202
C	5.159368	1.252033	2.231452
C	3.143785	3.091400	-0.450130
N	4.510139	1.579023	0.917376
Cl	0.036747	-5.766011	3.139297
H	5.609791	2.213356	2.517495
H	3.084593	2.922599	1.682748
H	3.894223	3.308339	-1.227463
H	2.497114	3.976278	-0.386731
C	4.116581	0.935288	3.288615
C	3.501775	1.994498	3.969609
C	3.722406	-0.369867	3.602694
C	2.487433	1.766215	4.896160
H	3.845565	3.013540	3.782451
C	2.719321	-0.603681	4.538006
H	4.204521	-1.212659	3.113640
C	2.088375	0.462465	5.177421
H	2.026813	2.605475	5.415140
H	2.436480	-1.628542	4.773849
H	1.313381	0.278185	5.921352
C	4.823166	4.026380	1.137316
C	4.420431	5.142500	1.873384
C	6.112241	4.003441	0.596673
C	5.283407	6.219011	2.063203
H	3.414602	5.162848	2.300297
C	6.978124	5.073922	0.790004
H	6.432829	3.125604	0.033800
C	6.565966	6.185693	1.523079
H	4.957151	7.081042	2.642191
H	7.981995	5.041020	0.369952
H	7.246056	7.021109	1.676878
C	6.303861	0.262198	2.130021
H	5.987929	-0.752491	1.873828
H	7.027527	0.591833	1.376190
H	6.819479	0.217662	3.095932
C	-1.198600	3.710025	-0.387987
C	-2.226216	3.936234	-1.302755
C	-0.688000	4.968115	0.008908
H	-2.833928	3.233362	-1.862284
C	-1.408945	5.949406	-0.660544
H	0.105854	5.156109	0.723042
C	-3.229303	5.979924	-2.279313
C	-1.402964	7.360661	-0.679324
C	-3.209723	7.341852	-2.284835
H	-3.904178	5.373872	-2.876974
C	-2.285707	8.049512	-1.470038
H	-0.682157	7.879586	-0.052100
H	-3.908738	7.873846	-2.923076
H	-2.279445	9.135961	-1.482031
N	-2.355778	5.284848	-1.477242
C	-4.876220	5.715437	1.134427
H	-5.744519	6.144871	0.623748
H	-4.982539	5.905067	2.207445
H	-3.980624	6.238529	0.780675

TS2'-*cis*

M06-L SCF energy in solvent: -8423.351719 a.u

C	-6.342171	1.044502	-0.059035
C	-7.605802	1.482556	-0.583718
H	-8.574973	1.199919	-0.188266
C	-7.353873	2.395479	-1.641605
H	-8.107582	2.937185	-2.202840
C	-5.289358	1.698006	-0.819862
C	-5.946013	2.532624	-1.787949
H	-5.443814	3.172541	-2.506345
C	-5.585710	-0.717766	3.055638
C	-7.082141	-0.974378	2.812726
H	-7.728470	-0.551718	3.591848
N	-5.165971	0.052881	1.875069
C	-6.221185	0.256937	1.153947
O	-7.380598	-0.279593	1.583297
H	-7.341432	-2.027921	2.666223
H	-5.020581	-1.663966	3.069830
C	-5.295193	0.020954	4.368099
C	-3.827642	0.399127	4.481069
C	-5.719818	-0.838877	5.552055

H	-3.501463	1.045871	3.658786
H	-3.627156	0.916713	5.427001
H	-3.195644	-0.502112	4.460865
H	-6.779850	-1.119242	5.517237
H	-5.133072	-1.767882	5.583115
H	-5.553374	-0.315486	6.499858
P	-3.503676	1.400898	-0.669049
C	-3.041728	0.894487	-2.366327
C	-1.690853	0.983754	-2.728067
C	-3.953451	0.372140	-3.289608
C	-1.261196	0.588378	-3.989578
H	-0.969488	1.387986	-2.016211
C	-3.521299	-0.034761	-4.551472
H	-5.010749	0.307243	-3.034192
C	-2.178434	0.073866	-4.905673
H	-0.208960	0.693809	-4.254797
H	-4.243776	-0.428199	-5.265046
H	-1.848136	-0.234978	-5.895387
C	-2.771355	3.073397	-0.562110
C	-2.178834	3.476419	0.639952
C	-2.835040	3.977336	-1.631172
C	-1.688205	4.774798	0.779596
H	-2.099613	2.761404	1.462335
C	-2.356927	5.275156	-1.484058
H	-3.245811	3.657413	-2.588828
C	-1.783288	5.676439	-0.277375
H	-1.226570	5.086378	1.715205
H	-2.426316	5.975802	-2.314830
H	-1.402923	6.689737	-0.164853
Cu	-3.231050	0.030715	1.007685
O	-1.479265	0.254470	2.261595
C	-1.152562	-0.850850	2.716953
O	-0.230318	-0.982751	3.675365
C	-1.682877	-2.126800	2.242148
N	-2.848092	-1.965167	1.498788
C	-3.642306	-2.984350	1.318376
H	-3.473776	-3.914386	1.874220
C	-4.805034	-2.989638	0.454975
C	-5.785377	-3.979137	0.646936
C	-4.994371	-2.067624	-0.589669
C	-6.937840	-4.017255	-0.125608
H	-5.641808	-4.725413	1.429393
C	-6.139306	-2.092730	-1.368425
H	-4.205880	-1.347481	-0.811292
C	-7.114062	-3.059004	-1.122628
H	-7.695886	-4.778848	0.036695
H	-6.279521	-1.376914	-2.175795
C	-5.539379	3.745805	1.740678
C	-6.899668	3.437480	2.043908
H	-7.244043	2.691336	2.754004
C	-7.730759	4.217205	1.188398
H	-8.813370	4.172699	1.139711
C	-5.531965	4.724681	0.699730
H	-4.649745	5.145183	0.225789
C	-6.886047	5.011984	0.358951
H	-7.217198	5.683466	-0.425992
H	-4.666697	3.275537	2.185362
C	-1.510456	-3.337836	3.111490
H	-1.517074	-4.262766	2.520696
H	-0.567169	-3.291267	3.659106
H	-2.323211	-3.423796	3.850615
Fe	-6.484428	3.029821	0.100594
C	0.383021	0.240378	4.144022
H	-0.407504	0.892521	4.539201
H	0.835517	0.754085	3.289181
H	-5.898524	0.946010	4.362024
Cl	-8.555754	-3.079755	-2.091136
Ir	2.523656	-1.513992	-0.627454
P	4.040923	0.191897	-0.410343
O	4.830092	0.648003	0.967465
O	5.332180	-0.049943	-1.432026
C	5.839473	-0.158466	1.470650
C	5.570094	-0.829097	2.678470
H	4.602046	-0.667108	3.150999
C	6.523320	-1.654469	3.217596
H	6.336571	-2.176468	4.155339
C	7.751663	-1.868872	2.546285
C	8.706809	-2.787793	3.042456
H	8.484650	-3.315907	3.969443
C	9.879335	-3.024340	2.366637
H	10.601938	-3.738560	2.755427
C	10.138504	-2.348869	1.157056
H	11.056110	-2.555548	0.609727
C	9.240053	-1.434263	0.657087
H	9.451101	-0.925795	-0.281052
C	8.028930	-1.152660	1.336076
C	7.065591	-0.217028	0.830327
C	7.344184	0.670496	-0.321105

C	8.481539	1.548015	-0.327914
C	9.338898	1.697359	0.791256
H	9.131019	1.136899	1.698911
C	10.418070	2.549555	0.754164
H	11.054079	2.647844	1.631718
C	10.704360	3.299538	-0.403754
H	11.566826	3.962283	-0.423453
C	9.879152	3.201648	-1.497263
H	10.073594	3.790723	-2.393117
C	8.749994	2.347545	-1.486689
C	7.871200	2.283433	-2.593340
H	8.092552	2.880959	-3.476736
C	6.742934	1.505668	-2.546362
H	6.041240	1.461616	-3.376210
C	6.478878	0.727464	-1.403259
C	1.607257	-0.758359	1.166405
H	1.925422	-1.304102	2.060872
H	1.673350	0.327599	1.281448
C	0.521690	-1.294036	0.390740
H	-0.063281	-0.583204	-0.201284
C	-0.175956	-2.519273	0.705725
H	0.332973	-3.194984	1.393789
C	3.504264	-2.382121	-2.379887
H	3.732440	-1.572962	-3.076495
C	2.153513	-2.828533	-2.333038
H	1.441503	-2.346959	-3.010145
C	1.779901	-4.234654	-1.930762
H	2.066425	-4.940659	-2.728866
H	0.687600	-4.288052	-1.865536
C	2.388092	-4.679568	-0.590560
H	3.271845	-5.312054	-0.756457
H	1.667670	-5.323678	-0.068407
C	2.771967	-3.542626	0.343012
H	2.245570	-3.514524	1.297613
C	4.024678	-2.918298	0.350194
H	4.340815	-2.477853	1.296244
C	5.140606	-3.218148	-0.616247
H	5.897944	-2.429848	-0.523766
H	5.643294	-4.150850	-0.308971
C	4.673366	-3.303307	-2.071565
H	4.398058	-4.336132	-2.328402
H	5.512487	-3.050838	-2.730647
C	1.928722	1.472494	-1.329908
C	3.512334	2.970186	-0.071986
C	1.793041	0.057973	-1.885774
N	3.263678	1.639829	-0.708248
H	2.896901	3.646828	-0.682768
H	2.321979	0.002194	-2.850578
H	0.736586	-0.138991	-2.106192
H	1.159318	1.624410	-0.545251
C	4.943524	3.449614	-0.221903
H	5.668503	2.826034	0.309657
H	5.225419	3.463916	-1.280085
H	5.028123	4.470151	0.168452
C	2.955159	3.053391	1.339479
C	1.594320	3.334691	1.518442
C	3.751246	2.897101	2.479424
C	1.042304	3.437052	2.792907
H	0.964163	3.508441	0.643737
C	3.204639	3.006899	3.754681
H	4.815139	2.698551	2.369024
C	1.847737	3.278163	3.916899
H	-0.020788	3.646137	2.910651
H	3.847303	2.895954	4.627092
H	1.420999	3.374150	4.914881
C	1.721724	2.515722	-2.406871
C	2.588654	2.568732	-3.505102
C	0.676889	3.437874	-2.332818
C	2.396103	3.500230	-4.517638
H	3.425019	1.869185	-3.550605
C	0.476962	4.369319	-3.350484
H	0.008546	3.425310	-1.467744
C	1.332562	4.400487	-4.445965
H	3.076235	3.527661	-5.367307
H	-0.345798	5.078172	-3.277443
H	1.180610	5.130214	-5.238881
C	1.397929	-0.138307	5.185598
H	1.893390	0.761996	5.563784
H	0.933620	-0.657459	6.030650
H	2.168268	-0.793834	4.763574
C	-1.021203	-3.154767	-0.275129
C	-1.610943	-2.553029	-1.412041
C	-1.487626	-4.471279	-0.204369
C	-2.411856	-3.504038	-2.030638
H	-1.470782	-1.533877	-1.758862
H	-1.233231	-5.278574	0.472568
C	-3.258477	-3.510993	-3.160338
C	-3.028611	-5.819560	-1.603434

C	-3.970430	-4.635152	-3.485513
H	-3.333746	-2.595959	-3.744763
C	-3.849201	-5.806773	-2.690927
H	-2.884849	-6.677818	-0.953881
H	-4.627269	-4.638967	-4.351440
H	-4.404054	-6.706342	-2.939142
N	-2.319537	-4.691138	-1.268839

TS3'-*trans*

M06-L SCF energy in solvent: -8423.334517 a.u

Ir	2.662887	1.857099	-0.473717
P	3.762864	0.180066	0.653803
O	3.890001	-1.400755	0.171534
O	5.372032	0.572217	0.770003
C	4.593109	-1.670633	-0.993665
C	3.836847	-2.058552	-2.116472
H	2.756200	-2.147416	-2.008757
C	4.478136	-2.314967	-3.301327
H	3.913327	-2.627350	-4.178811
C	5.879361	-2.140985	-3.413850
C	6.541148	-2.309778	-4.653789
H	5.949670	-2.601134	-5.521220
C	7.893603	-2.097047	-4.769389
H	8.388451	-2.224377	-5.729928
C	8.638030	-1.697182	-3.641419
H	9.704410	-1.503823	-3.739633
C	8.029097	-1.542854	-2.417147
H	8.615624	-1.226310	-1.557862
C	6.640676	-1.774584	-2.256209
C	5.976207	-1.608584	-0.994274
C	6.715019	-1.369339	0.266573
C	7.758235	-2.255742	0.705350
C	8.054418	-3.473800	0.043002
H	7.465532	-3.767736	-0.822114
C	9.061135	-4.300097	0.486704
H	9.259522	-5.232902	-0.037776
C	9.830673	-3.956414	1.615651
H	10.629592	-4.614456	1.950961
C	9.553166	-2.797436	2.298991
H	10.123605	-2.526477	3.186880
C	8.514218	-1.933239	1.878715
C	8.200133	-0.762136	2.608380
H	8.794017	-0.512178	3.486523
C	7.147923	0.031487	2.233694
H	6.869736	0.921903	2.793416
C	6.398546	-0.297549	1.087575
C	4.264106	3.306320	-0.155193
H	4.568791	3.257436	0.892032
C	3.055866	4.012250	-0.429662
H	2.535000	4.461378	0.420903
C	2.791648	4.698354	-1.747970
H	3.389965	5.622925	-1.818685
H	1.744177	5.021555	-1.749315
C	3.046453	3.801535	-2.962833
H	4.050307	3.974095	-3.374978
H	2.353670	4.075229	-3.771173
C	2.884682	2.319726	-2.668406
H	2.061841	1.823311	-3.189101
C	3.956840	1.491118	-2.304339
H	3.879881	0.438021	-2.577103
C	5.356230	1.994150	-2.059673
H	5.938844	1.184333	-1.606906
H	5.839489	2.201527	-3.029370
C	5.411353	3.227338	-1.151140
H	5.430662	4.149077	-1.749648
H	6.358446	3.218481	-0.598677
C	-3.995389	-2.421608	1.449511
C	-4.250827	-3.602937	2.230003
H	-3.805285	-3.820613	3.194838
C	-5.226827	-4.380260	1.552382
H	-5.659471	-5.307187	1.912908
C	-4.839701	-2.478533	0.263714
C	-5.597920	-3.693477	0.361818
H	-6.351002	-4.015787	-0.350526
C	-2.408908	0.710910	2.436406
C	-1.945577	-0.299537	3.480687
H	-2.100726	0.000192	4.521940
N	-2.966124	-0.165733	1.388128
C	-3.230472	-1.300711	1.961507
O	-2.789967	-1.447065	3.232227
H	-0.904289	-0.621049	3.343835
H	-1.563066	1.278106	2.015944
C	-3.463741	1.690446	2.983812
C	-4.187015	2.455795	1.887711
C	-2.813684	2.650286	3.972923
H	-4.205977	1.077359	3.527058
H	-4.684479	1.783679	1.177469
H	-4.946020	3.119984	2.319347

H	-3.494687	3.070898	1.299105
H	-2.359557	2.135557	4.828794
H	-2.018613	3.234080	3.485339
H	-3.547036	3.359941	4.372573
P	-4.814082	-1.271708	-1.094388
C	-4.530488	-2.239385	-2.616799
C	-4.455066	-1.492387	-3.803497
C	-4.351145	-3.624401	-2.678074
C	-4.239496	-2.119699	-5.023911
H	-4.574564	-0.407208	-3.763107
C	-4.134853	-4.250976	-3.904285
H	-4.368175	-4.221890	-1.768036
C	-4.082962	-3.504892	-5.077465
H	-4.195531	-1.527533	-5.936473
H	-3.997699	-5.331316	-3.934872
H	-3.917021	-3.998930	-6.033025
C	-6.552026	-0.739867	-1.290806
C	-6.903649	0.543366	-0.856436
C	-7.539934	-1.577823	-1.822803
C	-8.228845	0.968585	-0.915428
H	-6.126805	1.209175	-0.472537
C	-8.862769	-1.150715	-1.883743
H	-7.269279	-2.564935	-2.200016
C	-9.209871	0.119409	-1.422219
H	-8.495064	1.966170	-0.570651
H	-9.625712	-1.808438	-2.296109
H	-10.245418	0.450368	-1.469904
Cu	-3.284900	0.236489	-0.600531
O	-3.563427	2.270286	-1.119050
C	-2.894985	2.567165	-2.121435
O	-3.107630	3.708468	-2.785856
C	-1.793726	1.762704	-2.638915
N	-1.850196	0.453683	-2.142827
C	-1.274301	-0.510835	-2.798645
H	-0.835806	-0.323399	-3.787299
C	-1.205341	-1.882361	-2.346365
C	-0.907599	-2.884394	-3.284921
C	-1.448676	-2.265237	-1.015447
C	-0.922287	-4.226883	-2.936144
H	-0.703349	-2.602777	-4.318168
C	-1.488853	-3.603689	-0.659348
H	-1.593342	-1.498568	-0.253473
C	-1.242694	-4.576641	-1.626473
H	-0.722738	-4.999377	-3.674283
H	-1.693380	-3.897790	0.366328
C	-4.053700	4.617290	-2.177722
H	-5.025448	4.114090	-2.107099
H	-3.718170	4.829902	-1.153276
C	-6.672502	-0.667442	2.389491
C	-6.222077	-1.315566	3.581008
H	-5.411460	-0.986307	4.224141
C	-6.955304	-2.529214	3.725140
H	-6.809609	-3.272102	4.501813
C	-7.688289	-1.482314	1.803239
H	-8.203342	-1.284668	0.868213
C	-7.859245	-2.631227	2.627139
H	-8.526708	-3.462770	2.428272
H	-6.276850	0.255164	1.972746
C	-1.340382	2.012324	-4.050115
H	-1.365932	3.080763	-4.278407
H	-0.313449	1.660566	-4.218955
H	-1.981533	1.500259	-4.784204
Fe	-5.928842	-2.505420	1.968098
C	1.971770	0.895501	2.443675
C	3.075580	-1.274598	3.030571
C	2.141735	2.145057	1.584485
N	3.053580	-0.067997	2.152135
C	-0.130164	2.627324	-1.551074
C	0.424644	1.598518	-0.708093
H	0.363994	2.791029	-2.506851
H	-0.007764	1.564366	0.295521
C	1.156827	0.429379	-1.092133
H	1.278123	0.187490	-2.151996
H	1.040497	-0.462555	-0.471393
Cl	-1.358441	-6.255305	-1.183232
H	1.000424	0.408428	2.212346
H	2.930855	2.761226	2.042942
H	1.220877	2.741729	1.635674
H	2.924959	-0.858066	4.035852
C	1.947689	1.332202	3.891907
C	0.731228	1.679019	4.480615
C	3.124513	1.523872	4.622742
C	0.680937	2.198430	5.770681
H	-0.186309	1.565518	3.900104
C	3.078890	2.034325	5.915617
H	4.080014	1.262880	4.163153
C	1.857149	2.372180	6.495233
H	-0.277308	2.471035	6.211709

H	4.002606	2.171616	6.475065
H	1.823205	2.771364	7.506815
C	1.918099	-2.230813	2.799591
C	0.914881	-2.332742	3.768639
C	1.868284	-3.095778	1.699489
C	-0.108166	-3.274106	3.651299
H	0.950540	-1.674193	4.639743
C	0.852518	-4.036326	1.581152
H	2.645051	-3.046290	0.942503
C	-0.140169	-4.130563	2.555802
H	-0.875406	-3.339035	4.421426
H	0.840079	-4.711168	0.726210
H	-0.922197	-4.884792	2.466500
C	4.412321	-1.995158	3.076941
H	4.673520	-2.486535	2.135747
H	5.221177	-1.307171	3.345251
H	4.360294	-2.768400	3.850870
C	-4.102258	5.847518	-3.039638
H	-4.463180	5.614774	-4.046856
H	-4.772603	6.591841	-2.597889
H	-3.108072	6.299363	-3.131653
C	-0.631794	3.840833	-0.922673
C	-1.105996	4.002989	0.400844
C	-0.758000	5.073540	-1.563853
C	-1.521762	5.319599	0.553439
H	-1.161742	3.244127	1.172987
H	-0.526993	5.363282	-2.582248
C	-2.106526	6.071721	1.594182
C	-1.597589	7.299026	-0.863643
C	-2.428551	7.389894	1.402887
H	-2.294891	5.576213	2.544135
C	-2.163252	8.009258	0.151844
H	-1.360596	7.709885	-1.840581
H	-2.881595	7.966846	2.204440
H	-2.400537	9.056083	-0.011774
N	-1.289993	5.970860	-0.682742

TS3'-*cis*

M06-L SCF energy in solvent: -8423.340936 a.u

Ir	-3.080819	1.421776	-0.725354
P	-4.613940	-0.197999	-0.212060
O	-5.358987	-0.379922	1.248155
O	-5.917428	-0.115744	-1.236158
C	-6.456802	0.413549	1.561659
C	-6.281326	1.368455	2.580055
H	-5.311958	1.428452	3.072940
C	-7.326329	2.187553	2.924270
H	-7.207556	2.929998	3.712269
C	-8.566014	2.099376	2.246130
C	-9.628754	2.987601	2.539182
H	-9.478827	3.737079	3.315658
C	-10.817766	2.918625	1.854334
H	-11.624442	3.611385	2.084816
C	-10.987263	1.954338	0.840261
H	-11.921602	1.915518	0.283700
C	-9.980896	1.066247	0.541062
H	-10.124546	0.332857	-0.248811
C	-8.746415	1.098377	1.236483
C	-7.672478	0.197126	0.934105
C	-7.823186	-0.917733	-0.027176
C	-8.828222	-1.926827	0.129922
C	-9.676215	-1.984397	1.263741
H	-9.563545	-1.241602	2.049565
C	-10.627906	-2.969367	1.389751
H	-11.262577	-2.993849	2.273243
C	-10.783911	-3.950222	0.389749
H	-11.545136	-4.719798	0.497955
C	-9.961803	-3.939120	-0.711425
H	-10.059778	-4.701600	-1.483576
C	-8.962850	-2.947898	-0.866307
C	-8.085092	-2.954141	-1.977398
H	-8.207839	-3.721234	-2.740991
C	-7.079840	-2.025066	-2.083764
H	-6.383229	-2.020390	-2.919674
C	-6.949851	-1.032965	-1.094610
C	-4.180927	2.190762	-2.444301
H	-4.534095	1.332288	-3.017203
C	-2.804745	2.524921	-2.593475
H	-2.220798	1.915528	-3.288926
C	-2.240215	3.903831	-2.353670
H	-2.453957	4.561164	-3.213831
H	-1.147614	3.809732	-2.310199
C	-2.736366	4.546849	-1.053731
H	-3.621047	5.170210	-1.238852
H	-1.969729	5.237570	-0.677217
C	-3.059165	3.541146	0.038297
H	-2.405674	3.563869	0.912060
C	-4.339111	3.010961	0.260114

H	-4.561909	2.682612	1.276197
C	-5.548277	3.287387	-0.597639
H	-6.323852	2.552429	-0.342773
H	-5.971568	4.270687	-0.331971
C	-5.256829	3.207946	-2.100368
H	-4.967971	4.192393	-2.492208
H	-6.179649	2.941505	-2.628984
C	6.054940	-1.410769	-0.951861
C	6.672136	-2.559390	-1.554124
H	6.881438	-2.671564	-2.612372
C	6.993349	-3.481016	-0.522238
H	7.500205	-4.430434	-0.656935
C	6.001431	-1.630689	0.486739
C	6.595396	-2.916869	0.722949
H	6.710487	-3.380981	1.697975
C	5.282335	1.895665	-2.299332
C	5.711994	1.078908	-3.515629
H	6.516357	1.521976	-4.109486
N	5.104202	0.851642	-1.272238
C	5.746244	-0.196573	-1.683285
O	6.224645	-0.151463	-2.948528
H	4.871995	0.820817	-4.174448
H	4.322035	2.399284	-2.473733
C	6.317320	2.937774	-1.843862
C	5.949710	3.515563	-0.485377
C	6.465068	4.046275	-2.876761
H	7.283759	2.410213	-1.751405
H	5.953874	2.746570	0.297277
H	6.651682	4.305280	-0.191415
H	4.938572	3.948290	-0.504855
H	6.674712	3.667438	-3.885514
H	5.544259	4.640254	-2.934806
H	7.282685	4.723253	-2.605734
P	5.155868	-0.548231	1.677693
C	4.190690	-1.691449	2.724777
C	3.734777	-1.222058	3.966458
C	3.757280	-2.944282	2.279676
C	2.883220	-1.994546	4.747998
H	4.054091	-0.241193	4.323300
C	2.906985	-3.718913	3.066849
H	4.078834	-3.318676	1.308610
C	2.467638	-3.249079	4.301352
H	2.546118	-1.618021	5.712574
H	2.586933	-4.696757	2.707435
H	1.803922	-3.857116	4.914181
C	6.415616	0.089121	2.836038
C	6.516161	1.474182	3.008345
C	7.283267	-0.752899	3.542276
C	7.488260	2.010767	3.851722
H	5.825099	2.129389	2.473355
C	8.254645	-0.216749	4.380113
H	7.200785	-1.834243	3.428300
C	8.362139	1.166375	4.530395
H	7.562937	3.089300	3.976986
H	8.929477	-0.877360	4.922121
H	9.123886	1.583208	5.186282
Cu	3.996245	0.867856	0.435285
O	3.279753	2.711907	1.207779
C	2.211884	2.511340	1.813205
O	1.672342	3.465169	2.595541
C	1.406221	1.308431	1.704448
N	1.967599	0.370229	0.851366
C	1.459157	-0.828024	0.749426
H	0.678905	-1.178371	1.438962
C	1.900456	-1.770231	-0.261658
C	1.602718	-3.137013	-0.124346
C	2.627746	-1.362838	-1.394940
C	2.070610	-4.074864	-1.033851
H	1.020324	-3.467211	0.736438
C	3.096223	-2.287028	-2.317025
H	2.803583	-0.299067	-1.553683
C	2.833590	-3.642697	-2.118312
H	1.848888	-5.132421	-0.912294
H	3.667255	-1.967709	-3.187799
C	2.451682	4.669873	2.741424
H	3.445857	4.398686	3.118018
H	2.597137	5.118321	1.749873
C	8.948992	-0.121947	0.586316
C	9.014626	-0.094378	-0.837081
H	8.639126	0.695585	-1.480499
C	9.587605	-1.321276	-1.282528
H	9.729483	-1.620343	-2.315522
C	9.483929	-1.371371	1.024411
H	9.550335	-1.710662	2.052514
C	9.878869	-2.111391	-0.130348
H	10.291229	-3.114765	-0.134491
H	8.524730	0.649765	1.221547
C	0.565904	0.890758	2.871083

H	0.193852	1.760208	3.419335
H	-0.294143	0.283866	2.572064
H	1.158737	0.274113	3.566110
Fe	7.900737	-1.681836	-0.212854
C	-2.627865	-1.630400	-1.093484
C	-3.990185	-2.877696	0.603095
C	-2.601421	-0.328576	-1.885306
N	-3.887538	-1.705735	-0.326611
C	-0.129632	2.153888	0.266851
C	-1.033106	1.052363	0.190402
H	-0.373313	2.969232	0.950955
H	-0.654516	0.204882	-0.387041
C	-2.115511	0.791420	1.097750
H	-2.278019	1.494017	1.922725
H	-2.305329	-0.245680	1.384989
Cl	3.453467	-4.807639	-3.253151
H	-3.515653	-3.680963	0.020863
C	-5.409474	-3.338072	0.878204
H	-5.991610	-2.634452	1.478300
H	-5.948180	-3.507497	-0.061080
H	-5.371298	-4.288757	1.422066
C	-3.131203	-2.679070	1.838169
C	-1.775368	-3.027754	1.783253
C	-3.625548	-2.129994	3.026931
C	-0.929256	-2.801164	2.866788
H	-1.385803	-3.491522	0.873446
C	-2.782691	-1.903357	4.111849
H	-4.679131	-1.870502	3.102511
C	-1.429778	-2.228046	4.032625
H	0.124541	-3.079369	2.811354
H	-3.188014	-1.478874	5.028899
H	-0.767495	-2.048828	4.879146
H	-1.784984	-1.612934	-0.375127
H	-3.288136	-0.412579	-2.743588
H	-1.597398	-0.189817	-2.307163
C	-2.428698	-2.812074	-2.014665
C	-1.127705	-3.148919	-2.397641
C	-3.497871	-3.533531	-2.551799
C	-0.894557	-4.185794	-3.295422
H	-0.289693	-2.582683	-1.984907
C	-3.266976	-4.572895	-3.449116
H	-4.515829	-3.280495	-2.250269
C	-1.966389	-4.902989	-3.823008
H	0.126968	-4.437599	-3.578250
H	-4.108393	-5.131815	-3.855548
H	-1.788514	-5.718204	-4.521660
C	1.705904	5.577096	3.679927
H	2.259187	6.511311	3.819750
H	0.714456	5.825066	3.286185
H	1.575065	5.108705	4.660655
C	0.684632	2.490680	-0.879016
C	0.922333	1.672806	-2.009625
C	1.332361	3.706876	-1.093389
C	1.689775	2.396331	-2.908998
H	0.554050	0.665588	-2.171268
H	1.378344	4.600575	-0.482777
C	2.217363	2.156013	-4.196250
C	2.644638	4.636342	-2.979869
C	2.928072	3.130435	-4.850455
H	2.031834	1.184593	-4.651203
C	3.136861	4.390993	-4.227482
H	2.770207	5.574744	-2.447267
H	3.322341	2.949973	-5.847454
H	3.690841	5.175854	-4.733871
N	1.932801	3.664679	-2.319792

(*2S,3R*)-**Int-I**

M06-L SCF energy in solvent: -1610.714158 a.u

C	0.858090	-1.289539	-0.430567
N	-0.420770	-0.684332	-0.086456
C	-1.468659	-1.066863	-0.706454
H	-1.456054	-1.831951	-1.501869
C	-2.785321	-0.501395	-0.415637
C	-3.890885	-0.892858	-1.178360
C	-2.969198	0.440475	0.606756
C	-5.151341	-0.356884	-0.944640
H	-3.758602	-1.630420	-1.970113
C	-4.218534	0.985191	0.853741
H	-2.109170	0.730980	1.206879
C	-5.301270	0.582855	0.070410
H	-6.010032	-0.658284	-1.538455
H	-4.365576	1.717468	1.643373
Cl	-6.873131	1.273117	0.371397
C	2.212356	-1.874044	2.747568
H	3.104761	-2.397082	2.399784
H	1.892763	-2.083058	3.766223
C	1.557872	-1.019416	1.963358
H	0.662678	-0.511811	2.328319

C	1.938208	-0.709508	0.543146
H	2.875059	-1.235603	0.315270
C	2.169516	0.757771	0.327778
C	1.256485	1.822675	0.475629
C	3.385917	1.293007	-0.072395
C	1.921812	3.002578	0.161563
H	0.215423	1.743768	0.759629
H	4.335301	0.813834	-0.279271
C	1.570360	4.366679	0.104837
C	4.174546	3.601028	-0.535383
C	2.493999	5.312071	-0.261028
H	0.549109	4.642727	0.357954
C	3.819056	4.916007	-0.584188
H	5.167087	3.227111	-0.769840
H	2.218584	6.362785	-0.303208
H	4.565583	5.650194	-0.873372
N	3.251202	2.652293	-0.174696
C	1.241234	-0.994894	-1.884478
H	2.247846	-1.367280	-2.103379
H	1.222031	0.086931	-2.052194
H	0.540533	-1.466648	-2.583377
C	0.802735	-2.815805	-0.234456
O	-0.189703	-3.472997	-0.017474
O	2.035541	-3.350364	-0.360638
C	2.100598	-4.775130	-0.143674
C	3.533768	-5.193333	-0.324523
H	1.723900	-4.985375	0.865086
H	1.422995	-5.267918	-0.851235
H	3.634827	-6.272948	-0.171354
H	4.186792	-4.685427	0.393567
H	3.889593	-4.957836	-1.333218

TS6

M06-L SCF energy in solvent: -2071.549248 a.u

C	3.955205	0.957622	1.969469
H	4.638491	1.589852	1.398741
H	4.291651	0.637021	2.952916
C	2.764333	0.599630	1.492772
H	2.093500	-0.044834	2.073379
C	2.277072	1.018369	0.132660
H	3.037681	1.651575	-0.346247
C	2.101065	-0.247404	-0.850700
N	0.861621	-0.959846	-0.593142
C	-0.294758	-0.292378	-0.797547
H	-0.251141	0.445199	-1.600856
C	-1.618602	-0.891799	-0.644257
C	-1.865004	-2.086154	0.050807
C	-2.697710	-0.209654	-1.230662
C	-3.160255	-2.572950	0.160632
H	-1.050686	-2.613625	0.541986
C	-3.995269	-0.689722	-1.127716
H	-2.512571	0.714764	-1.780575
C	-4.213215	-1.872029	-0.425065
H	-3.355746	-3.493695	0.703429
H	-4.827486	-0.161582	-1.585099
C	0.983221	1.746204	0.197059
C	-0.189094	1.118747	0.717015
C	-0.757715	3.155516	-0.138408
C	-1.688451	4.155703	-0.459977
C	-2.514442	1.907790	0.978171
C	-3.000658	4.024765	-0.059596
H	-1.352167	5.026204	-1.017302
C	-3.416275	2.890998	0.674262
H	-2.741514	1.004146	1.537519
H	-3.721650	4.801825	-0.301445
H	-4.444536	2.784032	1.005577
Cl	-5.836221	-2.486759	-0.283860
H	-0.236606	0.353952	1.510362
H	0.882909	-1.570511	0.247576
Cl	0.262306	-1.655595	2.453728
C	0.618640	2.959927	-0.370379
H	1.263347	3.651917	-0.900740
N	-1.219182	2.039835	0.569675
C	2.166293	0.252079	-2.292978
H	3.182701	0.580106	-2.523357
H	1.886983	-0.542747	-2.993115
H	1.499393	1.108290	-2.451550
C	3.241398	-1.219770	-0.554296
O	3.101730	-2.319849	-0.077463
O	4.422165	-0.657328	-0.863552
C	5.575444	-1.434795	-0.467735
C	6.796574	-0.604473	-0.749354
H	5.565130	-2.376884	-1.028574
H	5.467416	-1.684498	0.594317
H	7.699288	-1.158439	-0.471633
H	6.867801	-0.349091	-1.812092
H	6.779340	0.327223	-0.173642

Int-IIS

M06-L SCF energy in solvent: -2071.559605 a.u

C	4.007192	1.036271	1.809873
H	4.727699	1.547186	1.167860
H	4.324720	0.819720	2.827389
C	2.797308	0.689089	1.374174
H	2.086914	0.175580	2.032782
C	2.337771	0.954093	-0.036421
H	3.122065	1.510854	-0.569569
C	2.078983	-0.406277	-0.842664
N	0.807765	-1.033223	-0.519493
C	-0.338597	-0.190656	-0.686350
H	-0.295685	0.258754	-1.689002
C	-1.666916	-0.882554	-0.565220
C	-1.921603	-1.877204	0.384464
C	-2.702963	-0.481327	-1.415700
C	-3.188925	-2.439900	0.492464
H	-1.143855	-2.186131	1.080148
C	-3.975403	-1.034510	-1.320452
H	-2.511804	0.284159	-2.169880
C	-4.205415	-2.010286	-0.355452
H	-3.387312	-3.204803	1.238352
H	-4.776486	-0.721044	-1.984988
C	1.070138	1.723817	-0.037219
C	-0.175865	1.038338	0.333839
C	-0.600114	3.234341	-0.280224
C	-1.427079	4.343095	-0.486012
C	-2.474642	1.982262	0.558780
C	-2.770557	4.250949	-0.172563
H	-0.997186	5.261969	-0.874813
C	-3.299423	3.064957	0.366457
H	-2.782480	1.038653	0.999503
H	-3.420494	5.109538	-0.324286
H	-4.344219	2.992224	0.650069
Cl	-5.799833	-2.705487	-0.210194
H	-0.202036	0.557091	1.358707
H	0.836705	-1.457811	0.413972
Cl	-0.041581	-0.789287	2.884461
C	0.796139	3.000620	-0.440168
H	1.501266	3.738279	-0.807124
N	-1.170473	2.074023	0.205824
C	2.168232	-0.103571	-2.338332
H	1.870477	-0.980887	-2.921857
H	3.189971	0.172762	-2.610184
H	1.514857	0.732436	-2.617034
C	3.172441	-1.380119	-0.407573
O	2.989183	-2.356314	0.280157
O	4.377162	-0.964449	-0.840039
C	5.491293	-1.736398	-0.338722
C	6.752216	-1.064296	-0.806502
H	5.412400	-1.777445	0.754017
H	5.396879	-2.763334	-0.711591
H	7.627618	-1.620834	-0.455776
H	6.821391	-0.042552	-0.417485
H	6.795545	-1.017109	-1.899891

TS7

M06-L SCF energy in solvent: -2071.539457 a.u

C	3.570818	0.370559	2.313474
H	4.482531	0.783770	1.879587
H	3.624994	0.046073	3.350086
C	2.444538	0.273371	1.610342
H	1.540523	-0.136799	2.064495
C	2.316735	0.706046	0.173558
H	3.242495	1.214242	-0.130050
C	2.080042	-0.503048	-0.779778
N	0.758481	-1.044178	-0.471510
C	-0.379309	-0.225313	-0.865588
H	-0.394802	0.001215	-1.956085
C	-1.654118	-0.980666	-0.563501
C	-1.839466	-1.610969	0.670131
C	-2.653876	-1.091196	-1.532446
C	-3.007908	-2.311287	0.942280
H	-1.058509	-1.545909	1.423450
C	-3.831173	-1.788577	-1.278639
H	-2.509170	-0.623567	-2.508073
C	-3.996514	-2.389938	-0.035025
H	-3.156029	-2.789354	1.906961
H	-4.606666	-1.876720	-2.035114
C	1.151303	1.626324	-0.010693
C	-0.176564	1.109263	-0.146119
C	-0.213187	3.397443	-0.283756
C	-0.854062	4.642329	-0.377725
C	-2.329059	2.294233	-0.616758
C	-2.208423	4.699472	-0.611030
H	-0.259160	5.543914	-0.256747
C	-2.953600	3.507072	-0.730316
H	-2.842645	1.338693	-0.657006

H	-2.709943	5.661141	-0.687107
H	-4.026557	3.530772	-0.893215
Cl	-5.468076	-3.264996	0.300792
H	-0.558264	0.937259	1.266837
H	0.674155	-1.994993	-0.819801
Cl	-1.061221	0.962730	2.678627
C	1.116804	3.004618	-0.040053
H	1.944963	3.686386	0.115671
N	-0.980045	2.240926	-0.427512
C	2.261068	-0.060972	-2.240501
H	3.292512	0.255036	-2.428846
H	2.019589	-0.880744	-2.928393
H	1.604010	0.785708	-2.473641
C	3.080753	-1.615872	-0.495868
O	2.791417	-2.782221	-0.342734
O	4.336756	-1.137160	-0.483893
C	5.353458	-2.108549	-0.156696
C	6.677740	-1.396642	-0.175886
H	5.301399	-2.927744	-0.883784
H	5.116150	-2.530038	0.827987
H	7.485308	-2.094793	0.067871
H	6.882885	-0.969766	-1.163406
H	6.697849	-0.583654	0.557933

(*1S,3S,4R*)-**3a**

M06-L SCF energy in solvent: -1610.725798 a.u

C	3.331832	0.451980	2.571096
H	4.153903	1.104930	2.274487
H	3.389498	0.018463	3.567295
C	2.309230	0.209259	1.753518
H	1.496014	-0.451987	2.061558
C	2.166971	0.784215	0.371576
H	3.058850	1.388813	0.151152
C	2.054163	-0.337279	-0.703045
N	0.749774	-0.975912	-0.521299
C	-0.406253	-0.186952	-0.947969
H	-0.469153	-0.081023	-2.057074
C	-1.662094	-0.910958	-0.504471
C	-1.951755	-1.049086	0.855062
C	-2.537384	-1.462010	-1.438451
C	-3.093147	-1.717108	1.276918
H	-1.266811	-0.620522	1.586007
C	-3.688093	-2.137108	-1.037265
H	-2.318815	-1.360095	-2.502779
C	-3.953246	-2.256778	0.321656
H	-3.322934	-1.822193	2.334242
H	-4.371474	-2.565354	-1.765985
C	0.933609	1.633308	0.264585
C	-0.227741	1.163006	-0.333046
C	-0.581062	3.301996	0.331891
C	-1.374446	4.458030	0.465482
C	-2.437265	2.214570	-0.809347
C	-2.655588	4.488344	-0.023512
H	-0.938084	5.321535	0.963013
C	-3.187670	3.344536	-0.672604
H	-2.789564	1.307841	-1.291009
H	-3.263256	5.383830	0.079785
H	-4.198185	3.349336	-1.070938
Cl	-5.390744	-3.099451	0.841513
H	0.748466	-1.897414	-0.950258
C	0.717960	2.955558	0.687808
H	1.422126	3.600579	1.200597
N	-1.155614	2.175509	-0.311815
C	2.291276	0.235105	-2.109797
H	3.304280	0.640570	-2.202011
H	2.161832	-0.543614	-2.872003
H	1.581418	1.042967	-2.319843
C	3.100948	-1.415929	-0.458935
O	2.873713	-2.605204	-0.400616
O	4.327414	-0.874579	-0.355106
C	5.379631	-1.809058	-0.040962
C	6.643201	-1.015498	0.145091
H	5.454767	-2.540416	-0.855078
H	5.090332	-2.357675	0.863894
H	7.476201	-1.682015	0.392009
H	6.904358	-0.466559	-0.765995
H	6.532288	-0.291109	0.959149

TS6'

M06-L SCF energy in solvent: -2071.551480 a.u

C	-4.463189	0.748816	2.200221
H	-4.235767	0.167568	3.093568
H	-5.449397	1.204832	2.149682
C	-3.569258	0.896590	1.224835
H	-3.828250	1.489429	0.341440
C	-2.201161	0.290635	1.238920
H	-1.993045	-0.182399	2.212045
C	-2.122584	-0.975598	0.227206

N	-0.737545	-1.397574	0.048229
C	0.196842	-0.538494	-0.410780
H	-0.160398	0.170381	-1.155854
C	1.609961	-0.897546	-0.511470
C	2.224675	-1.879985	0.282303
C	2.392914	-0.165109	-1.417656
C	3.584878	-2.124391	0.158352
H	1.648430	-2.416803	1.038093
C	3.752812	-0.409566	-1.554602
H	1.922983	0.609104	-2.025527
C	4.336886	-1.392257	-0.761387
H	4.066901	-2.877631	0.775824
H	4.355719	0.154714	-2.261165
C	-1.118323	1.259689	0.950100
C	0.240056	0.880863	1.139811
C	0.181277	2.942252	0.180722
C	0.793719	4.073760	-0.384200
C	2.374899	2.072692	0.752275
C	2.164995	4.192459	-0.369452
H	0.163861	4.843383	-0.822938
C	2.965285	3.181664	0.212262
H	2.910164	1.249886	1.217680
H	2.638621	5.069888	-0.803209
H	4.046992	3.268511	0.238653
Cl	6.042472	-1.707983	-0.913649
H	0.603903	0.168377	1.887471
H	-0.430557	-1.957384	0.874091
Cl	0.017439	-1.970554	2.947353
C	-1.144907	2.503789	0.329782
H	-2.014443	3.047509	-0.019255
N	1.014913	1.956177	0.727556
C	-2.885084	-2.134320	0.849403
H	-3.903183	-1.828537	1.101802
H	-2.942301	-2.980213	0.157939
H	-2.366202	-2.449767	1.762906
C	-2.706532	-0.506103	-1.103924
O	-2.175006	0.291462	-1.853247
O	-3.924532	-1.019734	-1.320058
C	-4.593629	-0.533873	-2.505721
C	-5.956731	-1.166748	-2.541465
H	-3.982141	-0.792168	-3.378297
H	-4.634687	0.561263	-2.452600
H	-6.506243	-0.827227	-3.425634
H	-5.883453	-2.258185	-2.583728
H	-6.538088	-0.898764	-1.653220

Int-IIS'

M06-L SCF energy in solvent: -2071.563473 a.u

C	-4.605649	1.352781	1.780589
H	-4.365433	1.130586	2.820237
H	-5.619028	1.689789	1.573335
C	-3.697481	1.218175	0.815402
H	-3.967311	1.448405	-0.219818
C	-2.300990	0.733920	1.038083
H	-2.059840	0.681602	2.117026
C	-2.095806	-0.790148	0.579537
N	-0.689802	-1.183270	0.535003
C	0.229840	-0.309365	-0.147065
H	-0.103177	-0.177313	-1.183800
C	1.637090	-0.841146	-0.143226
C	2.313212	-1.112671	1.052898
C	2.303833	-1.026299	-1.356419
C	3.628246	-1.564083	1.031023
H	1.808885	-0.956902	2.012582
C	3.619430	-1.477287	-1.393336
H	1.785258	-0.815972	-2.292396
C	4.269846	-1.742727	-0.192790
H	4.154775	-1.778220	1.957875
H	4.135680	-1.624557	-2.338595
C	-1.265732	1.579355	0.424976
C	0.133762	1.127177	0.525711
C	-0.017695	3.105501	-0.680237
C	0.503763	4.177868	-1.415764
C	2.206964	2.272452	-0.318052
C	1.868668	4.277396	-1.594430
H	-0.178946	4.915328	-1.828120
C	2.734054	3.319508	-1.034003
H	2.799836	1.499686	0.161998
H	2.280737	5.108646	-2.161972
H	3.810291	3.396495	-1.146686
Cl	5.919273	-2.311616	-0.224124
H	0.459137	0.999274	1.585531
H	-0.376707	-1.317747	1.506933
Cl	-0.021983	-0.129964	3.506221
C	-1.334263	2.734711	-0.300223
H	-2.225925	3.290791	-0.565654
N	0.865125	2.171278	-0.171112
C	-2.792009	-1.696068	1.580931

H	-3.858057	-1.459930	1.646536
H	-2.687170	-2.744195	1.289087
H	-2.332535	-1.551117	2.566957
C	-2.637609	-0.914075	-0.845315
O	-2.318939	-0.167320	-1.753517
O	-3.493339	-1.932596	-0.992241
C	-4.011408	-2.112213	-2.328828
C	-4.909188	-3.318193	-2.303165
H	-3.164954	-2.228805	-3.015596
H	-4.539965	-1.195837	-2.619413
H	-5.333813	-3.493538	-3.297172
H	-4.354790	-4.214051	-2.005388
H	-5.735162	-3.179693	-1.598083

TS7'

M06-L SCF energy in solvent: -2071.535337 a.u

C	-4.500457	0.929038	2.071096
H	-4.151358	0.825314	3.098832
H	-5.555600	1.156660	1.935610
C	-3.671069	0.788651	1.038195
H	-4.048694	0.914764	0.018802
C	-2.213406	0.459491	1.155523
H	-1.929903	0.499841	2.221405
C	-1.883870	-1.013641	0.706217
N	-0.443834	-1.261488	0.531554
C	0.339081	-0.328860	-0.292232
H	0.014308	-0.480632	-1.334208
C	1.785867	-0.770385	-0.201603
C	2.778284	-0.079177	0.494615
C	2.126478	-1.976627	-0.823503
C	4.081859	-0.567250	0.561493
H	2.542048	0.852785	1.005166
C	3.417982	-2.481067	-0.767096
H	1.352615	-2.531775	-1.352315
C	4.389579	-1.764636	-0.071829
H	4.848997	-0.025613	1.108369
H	3.676652	-3.417112	-1.255486
C	-1.349778	1.428068	0.421699
C	-0.012324	1.102933	0.064820
C	-0.496793	3.243222	-0.596073
C	-0.183847	4.483157	-1.178722
C	1.632955	2.381680	-1.331136
C	1.011114	4.654690	-1.835810
H	-0.915043	5.284669	-1.109958
C	1.923323	3.579702	-1.923451
H	2.289596	1.519351	-1.362192
H	1.251109	5.609377	-2.297553
H	2.861526	3.682889	-2.460210
Cl	6.020086	-2.382465	0.001110
H	0.453998	1.183694	1.626056
H	-0.017920	-1.301609	1.458118
Cl	0.738121	1.036096	3.020286
C	-1.619945	2.741667	0.076389
H	-2.522265	3.300872	0.293879
N	0.459105	2.219613	-0.650250
C	-2.371325	-1.985893	1.768333
H	-1.855175	-1.780506	2.715467
H	-3.446568	-1.880899	1.938152
H	-2.164526	-3.018854	1.476704
C	-2.536617	-1.239499	-0.657322
O	-2.302282	-0.557205	-1.636012
O	-3.415101	-2.253954	-0.657226
C	-4.072145	-2.491269	-1.921640
C	-4.973951	-3.681150	-1.744035
H	-3.303886	-2.651503	-2.687328
H	-4.619555	-1.582204	-2.200899
H	-5.498641	-3.899372	-2.680202
H	-4.401283	-4.569800	-1.459015
H	-5.723760	-3.496747	-0.967714

(*1R,3S,4R*)-**3a**

M06-L SCF energy in solvent: -1610.724744 a.u

C	4.202052	0.685093	-3.059164
H	3.649562	0.403366	-3.957070
H	5.236889	0.989236	-3.202908
C	3.635162	0.658913	-1.853515
H	4.204308	0.948176	-0.971119
C	2.209231	0.254397	-1.618006
H	1.729569	0.140110	-2.605043
C	2.013326	-1.133642	-0.950005
N	0.559858	-1.350052	-0.845241
C	-0.140655	-0.519987	0.151026
H	0.058959	-0.867569	1.191169
C	-1.629866	-0.669487	-0.088481
C	-2.201282	-0.183415	-1.267156
C	-2.445452	-1.314131	0.839146
C	-3.558179	-0.333385	-1.516236
H	-1.561455	0.314300	-1.995714

C	-3.810268	-1.475927	0.609500
H	-2.007104	-1.698404	1.762143
C	-4.351997	-0.982130	-0.571182
H	-4.005296	0.044923	-2.432007
H	-4.446627	-1.978668	1.333346
C	1.436888	1.258220	-0.817431
C	0.371991	0.869904	-0.017092
C	0.665674	3.105104	0.218311
C	0.340593	4.358940	0.768675
C	-1.122745	2.112003	1.540376
C	-0.681883	4.482526	1.675971
H	0.926506	5.220819	0.457231
C	-1.420060	3.335583	2.064437
H	-1.654029	1.198964	1.791251
H	-0.927137	5.453328	2.099519
H	-2.230953	3.411715	2.783092
Cl	-6.058886	-1.178072	-0.879942
C	1.622245	2.641945	-0.680782
H	2.375757	3.248948	-1.168568
N	-0.104028	1.985112	0.626881
C	2.580462	-2.242390	-1.828877
H	2.065151	-2.238250	-2.796458
H	3.650275	-2.090075	-2.005813
H	2.441360	-3.225235	-1.364462
C	2.697215	-1.202028	0.423142
O	3.530725	-0.444785	0.868195
O	2.232592	-2.275240	1.110447
C	2.784541	-2.432391	2.432804
C	2.073183	-3.585551	3.085994
H	2.649420	-1.490032	2.977679
H	3.865012	-2.598798	2.342679
H	2.460859	-3.745624	4.097552
H	0.997116	-3.392183	3.161265
H	2.212765	-4.511412	2.517827
H	0.391755	-2.324613	-0.605936