Supporting information

A practical strategy to access chiral *α*-aryloxy carboxylic acids through ion-pairing directed asymmetric hydrogenation

Lin Yao,[‡a] Haixia Ma,[‡a] Zhuang Nie,[b] Huifang Nie,[a] Dongxu Zhang,[a] Zhao Wei,[a] Zhanhong Shen,[a] Weiping Chen,[a] Ru Jiang,*[a] Shengyong Zhang*[a]

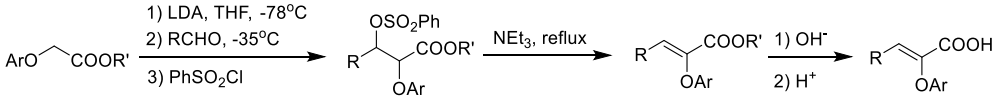
Contents

1. General information

Unless otherwise noted, all experiments dealing with air- or moisture-sensitive compounds were carried out in the argon-filled glove box or using standard Schlenk techniques and oil bath were utilized as the heat source. All commercially available chemicals including solvents were used without further purification. ^{1}H NMR, ^{13}C NMR were recorded on a Bruker ADVANCE III (400 MHz) spectrometer with $CDCl_3$, CD_3OD, DMSO-d as the solvent and tetramethylsilane (TMS) as the internal standard. Enantiomeric excesses were determined by Daicel chiral column on an Agilent 1260 Series HPLC instrument. Optical rotations were measured on a PERKIN ELMER polarimeter 343 instrument. High-Resolution Mass Spectroscopy (HRMS) was carried out on a VARIA FT-ICR MS.

The absolute configuration of the hydrogenation products was determined by comparison of analytical data with the literature.[1, 2]

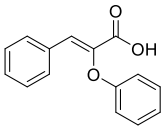
2. Preparation and characterization of *α*-aryloxy-substituted *α,β*-unsaturated acids



All the *α*-aryloxy substituted *α,β*-unsaturated acids were prepared following the above procedure according to literature.[1]

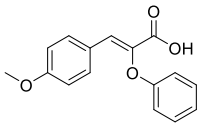
Characterization data of all the unsaturated acids was showed as followings:

(*Z*)-2-phenoxy-3-phenylacrylic acid (1a)



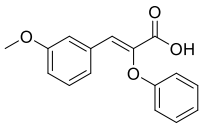
36% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.72 (m, 2H), 7.51 (s, 1H), 7.37-7.31 (m, 5H), 7.10-7.03 (m, 3H).

(*Z*)-3-(4-methoxyphenyl)-2-phenoxyacrylic acid (1b)



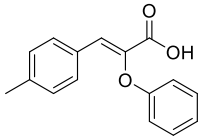
34% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 8.0 Hz, 2H), 7.49 (s, 1H), 7.34-7.30 (m, 2H), 7.08-7.03 (m, 3H), 6.88 (d, J = 8.0 Hz, 2H).

(*Z*)-3-(3-methoxyphenyl)-2-phenoxyacrylic acid (1c)



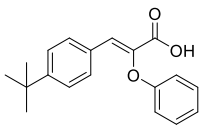
29% yield, yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (s, 1H), 7.34-7.27 (m, 5H), 7.09-7.02 (m, 3H), 6.94-6.91 (m, 1H), 3.73 (s, 3H).

(*Z*)-2-phenoxy-3-(p-tolyl)acrylic acid (1d)



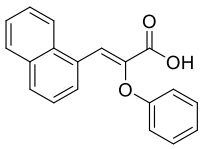
35% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 8.0 Hz, 1H), 7.49 (s, 1H), 7.34-7.28 (m, 2H), 7.17-7.16 (m, 2H), 7.08-7.02 (m, 3H), 2.36 (s, 3H).

(*Z*)-3-(4-(tert-butyl)phenyl)-2-phenoxyacrylic acid (1e)



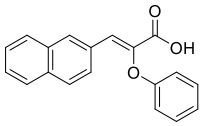
37% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70-7.68 (m, 2H), 7.53 (s, 1H), 7.40 (d, J = 8.0 Hz, 2H), 7.34 (t, J = 8.0 Hz, 2H), 7.10-7.05 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.21, 156.40, 153.74, 138.28, 130.66, 129.98, 129.79, 129.40, 125.85, 122.72, 115.35, 34.90, 31.10.

(*Z*)-3-(naphthalen-1-yl)-2-phenoxyacrylic acid (1f)



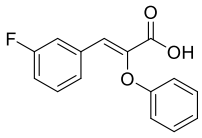
43% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 8.22 (d, J = 8.0 Hz, 1H), 8.11 (d, J = 4.0 Hz, 1H), 7.88 (t, J = 8.0 Hz, 2H), 7.65-7.62 (m, 1H), 7.58-7.55 (m, 1H), 7.48-7.42 (m, 1H), 7.32-7.29 (m, 2H), 7.06-7.04 (m, 3H).

(*Z*)-3-(naphthalen-2-yl)-2-phenoxyacrylic acid (1g)



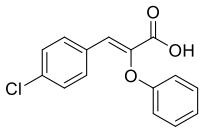
46% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.90-7.78 (m, 4H), 7.69 (s, 1H), 7.54-7.48 (m, 2H), 7.36-7.29 (m, 3H), 7.10 (d, J = 8.0 Hz, 2H).

(*Z*)-3-(3-fluorophenyl)-2-phenoxyacrylic acid (1h)



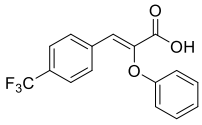
42% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52-7.35 (m, 3H), 7.36-7.32 (m, 3H), 7.11-7.07 (m, 2H), 7.04-7.02 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.30, 163.96, 161.52, 156.04, 139.89, 134.18, 134.09, 130.25, 130.17, 129.86, 128.25, 126.59, 123.10, 117.20, 117.06, 116.99, 116.84, 115.44. ^{19}F NMR (100 MHz, $CDCl_3$) δ -112.19.

(*Z*)-3-(4-chlorophenyl)-2-phenoxyacrylic acid (1i)



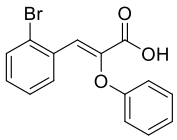
45% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, J = 8.0 Hz, 2H), 7.45 (s, 1H), 7.34-7.32 (m, 4H), 7.09 (t, J = 8.0 Hz, 1H), 7.03-7.01 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.18, 154.86, 138.65, 131.90, 130.71, 130.40, 130.16, 129.75, 128.90, 127.90, 116.77.

(*Z*)-2-phenoxy-3-(4-(trifluoromethyl)phenyl)acrylic acid (1j)



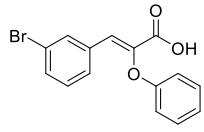
47% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, J = 8.0 Hz, 2H), 7.62 (d, J = 8.0 Hz, 2H), 7.52 (s, 1H), 7.35 (t, J = 8.0 Hz, 2H), 7.11 (t, J = 8.0 Hz, 1H), 7.03 (d, J = 8.0 Hz, 2H).

(*Z*)-3-(2-bromophenyl)-2-phenoxyacrylic acid (1k)



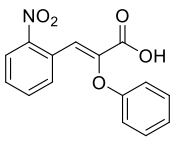
43% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94-7.93 (m, 1H), 7.85 (s, 1H), 7.62 (d, J = 8.0 Hz, 1H), 7.28-7.15 (m, 4H), 7.05-6.97 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.29, 156.34, 140.80, 133.01, 131.09, 130.77, 129.77, 127.59, 126.95, 122.86, 115.48.

(*Z*)-3-(3-bromophenyl)-2-phenoxyacrylic acid (1l)



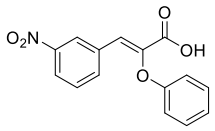
39% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.40 (s, 1H), 7.34 (t, J = 8.0 Hz, 2H), 7.25-7.21 (m, 1H), 7.11-7.08 (m, 1H), 7.02 (d, J = 8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.13, 156.05, 140.05, 133.38, 132.91, 130.29, 129.86, 128.94, 127.83, 123.11, 115.44, 114.65.

(*Z*)-3-(2-nitrophenyl)-2-phenoxyacrylic acid (1m)



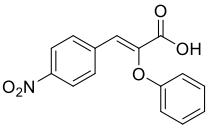
40% yield, light brown solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 8.0 Hz, 1H), 7.88-7.85 (m, 2H), 7.59 (t, J = 8.0 Hz, 1H), 7.49 (t, J = 8.0 Hz, 1H), 7.32-7.28 (m, 2H), 7.07-7.04 (m, 1H), 6.99-6.97 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.46, 156.47, 148.10, 141.06, 133.26, 131.46, 129.87, 129.81, 124.77, 124.71, 123.08, 115.45.

(*Z*)-3-(3-nitrophenyl)-2-phenoxyacrylic acid (1n)



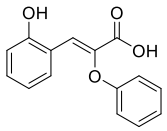
38% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (s, 1H), 8.21 (d, J = 8.0 Hz, 1H), 8.07 (d, J = 8.0 Hz, 1H), 7.57-7.52 (m, 2H), 7.36-7.33 (m, 2H), 7.11 (t, J = 8.0 Hz, 1H) 7.05-7.03 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.77, 155.82, 148.47, 141.30, 135.79, 133.76, 129.97, 129.82, 126.46, 125.14, 124.32, 123.41, 115.42.

(*Z*)-3-(4-nitrophenyl)-2-phenoxyacrylic acid (1o)



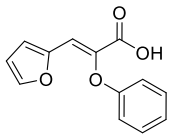
41% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, J = 8.0 Hz, 2H), 7.90 (d, J = 12.0 Hz, 2H), 7.49 (s, 1H), 7.36 (t, J = 8.0 Hz, 2H), 7.36 (t, J = 8.0 Hz, 2H), 7.03 (d, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.90, 155.81, 147.95, 141.83, 138.37, 131.05, 130.01, 126.21, 123.95, 123.55, 115.53.

(*Z*)-3-(2-hydroxyphenyl)-2-phenoxyacrylic acid (1p)



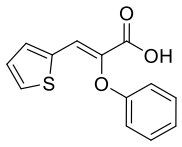
39% yield, light yellow solid. ^{1}H NMR (400 MHz, DMSO) δ ^{1}H NMR (400 MHz, DMSO) δ 10.18 (s, 1H), 7.76-7.72 (m, 2H), 7.34-7.30 (m, 2H), 7.19-7.15 (m, 1H), 7.04-7.01 (m, 1H), 6.96-6.90 (m, 3H), 6.72 (t, J=8.0 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.89, 156.89, 156.57, 139.50, 131.50, 130.25, 129.90, 122.60, 120.79, 119.76, 119.59, 116.09, 115.39.

(*Z*)-3-(furan-2-yl)-2-phenoxyacrylic acid (1q)



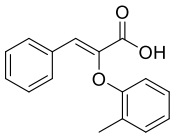
42% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (s, 2H), 7.32 (t, J = 8.0 Hz, 2H), 7.07 (t, J = 8.0 Hz, 1H), 7.01 (d, J = 8.0 Hz, 2H), 6.91 (d, J = 4.0 Hz, 1H), 6.47 (brs, 1H).

(*Z*)-2-phenoxy-3-(thiophen-2-yl)acrylic acid (1r)



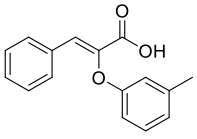
39% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.48-7.47 (m, 1H), 7.40 (brs, 1H), 7.35-7.31 (m, 2H), 7.10-7.03 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.27, 155.94, 136.40, 134.90, 132.50, 131.52, 129.70, 127.15, 124.06, 122.94, 115.23.

(*Z*)-3-phenyl-2-(o-tolyloxy)acrylic acid (1s)



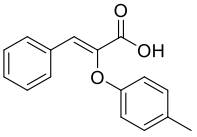
37% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.72 (m, 2H), 7.50 (s, 1H), 7.37-7.36 (m, 3H), 7.28-7.25 (m, 1H), 7.08 (t, J = 8.0 Hz, 1H), 7.00-6.97 (m, 1H), 6.77 (d, J = 8.0 Hz, 1H), 2.45 (s, 3H).

(*Z*)-3-phenyl-2-(m-tolyloxy)acrylic acid (1t)



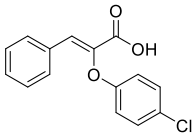
39% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.72 (m, 2H), 7.49 (s, 1H), 7.40-7.36 (m, 3H), 7.20 (t, J = 8.0 Hz, 1H), 6.90-6.83 (m, 2H), 2.35 (s, 3H).

(*Z*)-3-phenyl-2-(p-tolyloxy)acrylic acid (1u)



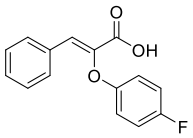
42% yield, yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (brs, 2H), 7.50 (s, 1H), 7.39-7.37 (m, 3H), 7.13 (d, J = 8.0 Hz, 2H), 6.95 (d, J = 8.0 Hz, 2H), 2.33 (s, 3H).

(*Z*)-2-(4-chlorophenoxy)-3-phenylacrylic acid (1v)



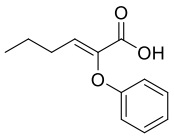
36% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (brs, 2H), 7.52 (s, 1H), 7.38-7.29 (m, 5H), 6.98-6.97 (m, 2H).

(*Z*)-2-(4-fluorophenoxy)-3-phenylacrylic acid (1w)



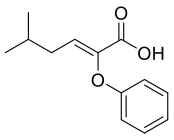
37% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (brs, 2H), 7.50 (s, 1H), 7.38 (brs, 3H), 7.00-6.99 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.52, 159.69, 157.30, 152.21, 139.09, 132.04, 130.70, 130.32, 129.92, 128.88, 116.65, 116.57, 116.38, 116.15. ^{19}F NMR (100 MHz, $CDCl_3$) δ -121.22.

(*Z*)-2-phenoxyhex-2-enoic acid (1x)



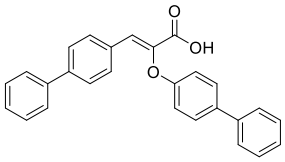
29% yield, white needle crystals. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.28 (m, 2H), 7.05-7.02 (m, 1H), 6.95-6.93 (m, 2H), 6.80 (t, J = 8.0 Hz, 1H), 2.23 (q, J = 8.0 Hz, 2H), 1.49 (q, J = 8.0 Hz, 2H), 0.94 (t, J = 8.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.86, 157.20, 140.25, 135.14, 129.69, 129.62, 122.24, 114.88, 28.03, 21.55, 13.88.

(*Z*)-5-methyl-2-phenoxyhex-2-enoic acid (1y)



31% yield, yellow viscous oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.28 (m, 2H), 7.04 (t, J = 8.0 Hz, 1H), 6.93 (d, J = 8.0 Hz, 2H), 6.81 (t, J = 8.0 Hz, 1H), 2.15 (t, J = 8.0 Hz, 2H), 1.82-1.71 (m, 1H), 0.94 (d, J = 8.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.17, 157.17, 140.62, 134.32, 129.61, 122.25, 114.92, 34.94, 28.01, 22.48.

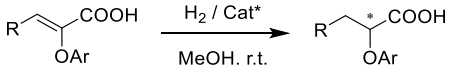
(*Z*)-3-([1,1'-biphenyl]-4-yl)-2-([1,1'-biphenyl]-4-yloxy)acrylic acid (1z)



53% yield, white solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, J = 8.0 Hz, 2H), 7.63-7.55 (m, 9H), 7.45 (q, J = 8.0 Hz, 4H), 7.40-7.34 (m, 2H), 7.16-7.13 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.60, 156.38, 141.57, 140.68, 140.05, 139.60, 135.04, 131.95, 131.16, 129.47, 129.38, 128.71, 128.39, 127.48, 127.13, 126.85, 126.45, 116.03.

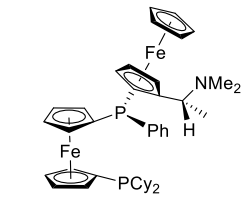
3. Asymmetric hydrogenation of *α*-aryloxy-substituted *α,β*-unsaturated acids

3.1 General procedure of asymmetric hydrogenation

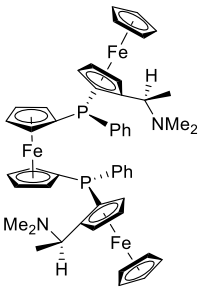


A solution of (R_C, S_{Fc}, S_P)-Chenphos (1.64mg, 0.0022 mmol) and $Rh(nbd)_2BF_4$ (0.46 mg, 0.002 mmol) in MeOH (1 mL) was stirred under nitrogen atmosphere. After 30 min, the clear yellow solution was transferred into a hydrogenation tube equipped with a stir bar, and the *α,β*-unsaturated carboxylic acids was added. The hydrogenation tube was then put into an autoclave. The air in the autoclave was replaced with hydrogen for three times. The autoclave was then charged with hydrogen to 20 atm, and the reaction mixture was stirred at room temperature for 20 h. After releasing the hydrogen, the reaction mixture was concentrated on a rotary evaporator. The conversion of substrate was determined by ^{1}H NMR analysis. The crude product was purified by flash chromatography on silica gel column to give the pure product. The product was reacted with aniline (1.1 eq) in the presence of DMAP and DCC in THF for 30 min to afford the corresponding amide. After a flash chromatography on neutral Al_2O_3 column, the desired amide was obtained and the *ee* values of the products were determined by chiral HPLC.

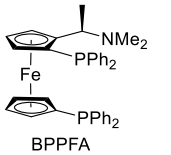
3.2 Ligands screened in the asymmetric hydrogenation



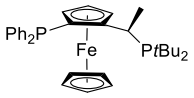
(R_C, S_{Fc}, S_P)-Chenphos



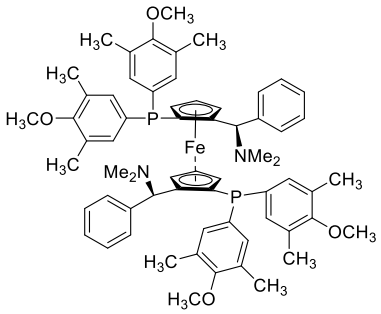
(R_C,R_C,S_{Fc},S_{Fc},S_P,S_P)-Trifer



BPPFA



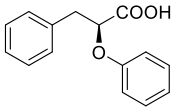
Josiphos



(S_P,S'_P)-Mandyphos

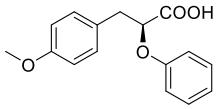
4. Analytical Data of the Hydrogenation Products

(*S*)-2-phenoxy-3-phenylpropionic acid (2a)



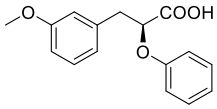
White solid, 97% yield, 98% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=95:5, flow rate=1.0 mL/min, 254 nm UV detector, t_R=16.35 min for major isomer, and t_R=20.85 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.26 (m, 7H), 6.98 (t, J = 16.0 Hz, 1H), 6.86 (d, J = 4.0 Hz, 2H), 4.84 (brs, 1H), 3.28 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.56, 136.32, 129.63, 129.55, 128.51, 127.04, 121.99, 115.41, 38.87.

(*S*)-3-(4-methoxyphenyl)-2-phenoxypropionic acid (2b)



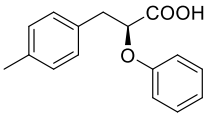
White solid, 98% yield, 98% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=19.11 min for major isomer, and t_R=21.80 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.25 (m, 5H), 7.01-6.97 (m, 1H), 6.87 (t, J = 16 Hz, 3H), 4.82 (brs, 1H), 3.25 (d, J = 4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.59, 157.60, 130.58, 129.64, 128.35, 121.94, 120.51, 115.41, 113.93, 55.25, 38.01.

(*S*)-3-(3-methoxyphenyl)-2-phenoxypropionic acid (2c)



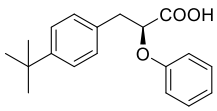
White solid, 97% yield, 95% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=17.26 min for major isomer, and t_R=21.54 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.23 (m, 2H), 7.02-6.99 (m, 1H), 6.95-6.88 (m, 4H), 6.84-6.82 (m, 2H), 4.88 (t, J = 6.0 Hz, 1H), 3.81 (s, 3H), 3.29 (d, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.31, 159.59, 157.72, 137.75, 129.65, 129.50, 122.04, 121.86, 115.38, 115.21, 112.60, 55.20, 38.91.

(*S*)-2-phenoxy-3-p-tolylpropionic acid (2d)



White solid, 97% yield, 98% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=12.75 min for major isomer, and t_R=14.18 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.22 (m, 4H), 7.15-7.13 (m, 2H), 7.01 (d, J = 6.0 Hz, 1H), 6.88 (d, J =8.0 Hz, 2H), 4.85 (t, J = 8.0 Hz, 1H), 3.28-3.27 (m, 2H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.33, 157.46, 136.65, 132.95, 129.64, 129.38, 129.21, 122.03, 115.35, 38.42, 21.22.

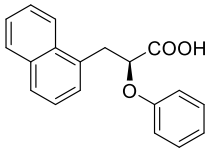
(*S*)-3-(4-(*tert*-butyl)phenyl)-2-phenoxypropanoic acid (2e)



White solid, 96% yield, 93% *ee*. HPLC condition: Chiralcel AS-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=7.47 min for major isomer, and t_R=9.74 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.29 (m, 6H), 7.01 (t, J = 6.0 Hz, 1H), 6.91-6.89 (m, 2H), 4.87 (brs,

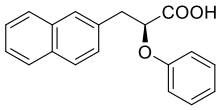
1H), 3.30-3.29 (m, 2H), 1.34 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.04, 157.57, 149.87, 133.20, 129.62, 129.17, 125.42, 121.95, 115.37, 38.38, 34.46, 31.37.

(*S*)-3-(naphthalen-1-yl)-2-phenoxypropionic acid (2f)



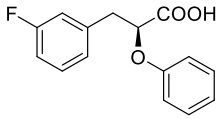
White solid, 97% yield, 95% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=85:15, flow rate=1.0 mL/min, 254 nm UV detector, t_R=9.58 min for major isomer, and t_R=13.60 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, J =8.0 Hz, 1H), 7.90 (d, J =8.0 Hz, 1H), 7.80 (d, J =8.0 Hz, 1H), 7.61-7.52 (m, 3H), 7.45-7.42 (m, 1H), 7.23-7.19 (m, 2H), 6.96-6.93 (m, 1H), 6.80-6.78 (m, 2H), 5.01-4.99 (m, 1H), 3.89-3.86 (m, 1H), 3.72-3.67 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.22, 157.60, 133.92, 132.32, 131.97, 129.54, 128.95, 128.12, 127.97, 126.30, 125.67, 125.43, 123.51, 121.93, 115.28, 36.27.

(*S*)-3-(naphthalen-2-yl)-2-phenoxypropionic acid (2g)



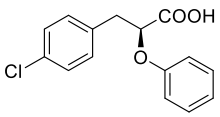
White solid, 98% yield, 98% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=85:15, flow rate=1.0 mL/min, 254 nm UV detector, t_R=11.69 min for major isomer, and t_R=14.75 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83-7.81 (m, 4H), 7.49 (brs, 3H), 7.27-7.25 (m, 2H), 6.99-6.97 (m, 1H), 6.91-6.89 (m, 2H), 4.97 (brs, 1H), 3.48 (brs, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.05, 157.52, 133.76, 133.47, 132.52, 129.64, 128.27, 128.12, 127.71, 127.66, 126.09, 125.74, 122.06, 115.42, 39.03.

(*S*)-3-(3-fluorophenyl)-2-phenoxypropanoic acid (2h)



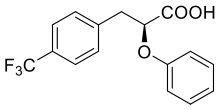
White solid, 98% yield, 97% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, t_R=9.83 min for major isomer, and t_R=12.84 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (brs, 4H), 7.12-7.06 (m, 2H), 7.02-6.95 (m, 2H), 6.87 (d, J = 8.0 Hz, 2H), 4.85 (brs, 1H), 3.30-3.29 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.99, 161.54, 157.43, 138.80, 129.98, 129.90, 129.68, 125.21, 122.10, 116.62, 116.40, 115.33, 114.10, 113.90, 38.43. ^{19}F NMR (100 MHz, $CDCl_3$) δ -113.24.

(*S*)-3-(4-chlorophenyl)-2-phenoxypropanoic acid (2i)



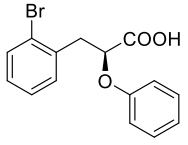
White solid, 97% yield, 95% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=15.99 min for major isomer (*S*), and t_R=20.45 min for minor isomer (*R*); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.29 (m, 6H), 7.02 (t, J = 6.0 Hz, 1H), 6.87 (d, J = 8.0 Hz, 2H), 4.84 (t, J = 6.0 Hz, 1H), 3.28-3.27 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.03, 157.37, 134.63, 133.00, 130.91, 129.71, 128.66, 122.17, 115.30, 38.13.

(*S*)-2-phenoxy-3-(4-(trifluoromethyl)phenyl)propanoic acid (2j)



White solid, 98% yield, 96% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=16.45 min for major isomer, and t_R=24.54 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60-7.58 (m, 2H), 7.48-7.46 (m, 2H), 7.31-7.27 (m, 2H), 7.02 (t, J = 16.0 Hz, 1H), 6.87 (d, J = 8.0 Hz, 2H), 4.89 (t, J=12.0 Hz, 1H), 3.37-3.36 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.96, 157.25, 140.21, 129.90, 129.73, 125.45, 125.42, 122.27, 115.23, 38.50.

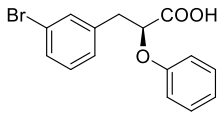
3-(2-bromophenyl)-2-phenoxypropanoic acid (2k)



White solid, 96% yield, 95% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=13.76 min for major isomer, and t_R=21.25 min for minor isomer; ^{1}H

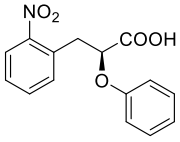
NMR (400 MHz, $CDCl_3$) δ 7.57-7.56 (m, 1H), 7.38-7.37 (m, 1H), 7.24-7.23 (m, 2H), 7.13-7.12 (m, 1H), 6.97-6.95 (m, 1H), 6.84 (brs, 2H), 4.95 (brs, 1H), 3.53-3.50 (m, 1H), 3.33 (brs, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.10, 157.64, 135.78, 132.85, 132.22, 129.56, 128.77, 127.41, 124.71, 121.92, 115.39, 39.28.

(*S*)-3-(3-bromophenyl)-2-phenoxypropanoic acid (2l)



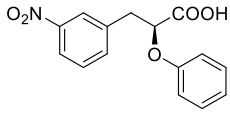
White solid, 97% yield, 96% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=15.65 min for major isomer, and t_R=19.96 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.40-7.39 (m, 1H), 7.19-7.18 (m, 4H), 6.99 (brs, 1H), 6.87 (s, 2H), 4.83 (s, 1H), 3.25 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.71, 157.41, 138.59, 132.62, 130.20, 130.02, 129.66, 122.41. 122.12, 115.37, 38.43.

(*S*)-3-(2-nitrophenyl)-2-phenoxypropanoic acid (2m)



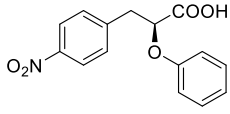
White solid, 98% yield, 92% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=85:15, flow rate=1.0 mL/min, 254 nm UV detector, t_R=9.26 min for major isomer, and t_R=11.41 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97-7.95 (m, 1H), 7.54 (brs, 2H), 7.44-7.42 (m, 1H), 7.26-7.22 (m, 2H), 6.98-6.95 (m, 1H), 6.84-6.82 (m, 2H), 5.02-5.01 (m, 1H), 3.74-3.71 (m, 1H), 3.60-3.54 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.14, 157.39, 149.85, 133.56, 132.99, 131.13, 129.60, 128.35, 124.90, 122.03, 115.16, 35.91.

(*S*)-3-(3-nitrophenyl)-2-phenoxypropanoic acid (2n)



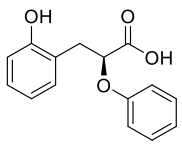
White solid, 98% yield, 97% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=85:15, flow rate=1.0 mL/min, 254 nm UV detector, t_R=18.44 min for major isomer, and t_R=24.93 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (brs, 1H), 8.13-8.11 (m, 1H), 7.70-7.68 (m, 1H), 7.51-7.47 (m, 1H), 7.28-7.25 (m, 2H), 7.01-6.98 (m, 1H), 6.87-6.85 (m, 2H), 4.89 (brs, 1H), 3.41 (brs, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.48, 157.18, 148.24, 138.21, 135.93, 129.74, 129.43, 124.57, 122.29, 115.22, 38.25.

(*S*)-3-(4-nitrophenyl)-2-phenoxypropanoic acid (2o)



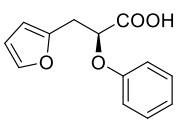
White solid, 98% yield, 96% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=85:15, flow rate=1.0 mL/min, 254 nm UV detector, t_R=25.36 min for major isomer, and t_R=33.68 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, J = 8.0 Hz, 2H), 7.49 (d, J = 8.0 Hz, 2H), 7.29-7.25 (m, 2H), 7.00 (t, J = 8.0 Hz, 1H), 6.84 (d, J = 8.0 Hz, 2H), 4.89 (brs, 1H), 3.38 (brs, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.17, 157.13, 147.16, 143.84, 130.48, 129.76, 123.66, 122.36, 115.19, 38.42.

(*S*)-3-(2-hydroxyphenyl)-2-phenoxypropanoic acid (2p)



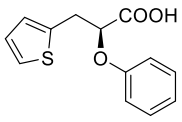
White solid, 97% yield, 95% *ee*. HPLC condition: Chiralcel AS-H column (25 cm × 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, t_R=22.27 min for major isomer, and t_R=25.75 min for minor isomer; ^{1}H NMR (400 MHz, DMSO) δ 7.25 (t, J=8.0 Hz, 2H), 7.15 (d, J=8.0 Hz, 1H), 7.06-7.03 (m, 1H), 6.93-6.90 (m, 1H), 6.81 (d, J=8.0 Hz), 6.72 (t, J=8.0 Hz), 4.89 (t, J=8.0 Hz, 1H), 3.21-3.17 (m, 1H), 3.08-3.02 (m, 1H). ^{13}C NMR (100 MHz, DMSO) δ 172.83, 158.21, 155.86, 131.64, 129.97, 128.24, 123.23, 121.47, 119.23, 115.32, 115.20, 75.75, 33.78.

(*S*)-3-(furan-2-yl)-2-phenoxypropanoic acid (2q)



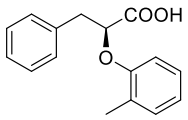
Brown solid, 99% yield, 97% *ee*. HPLC condition: Chiralcel AD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, t_R=20.44 min for minor isomer and t_R=22.86 min for major isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.30 (m, 3H), 7.04-7.01 (m, 1H), 6.91-6.85 (m, 2H), 6.32 (s, 1H), 6.23 (s, 1H), 4.98 (brs, 1H), 3.37-3.35 (d, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.70, 157.43, 149.81, 141.92, 129.66, 122.22, 115.59, 110.51, 108.04, 31.57.

(*S*)-2-phenoxy-3-(thiophen-2-yl)propanoic acid (2r)



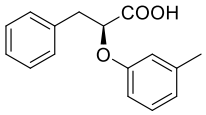
White solid, 99% yield, >99% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=15.25 min for major isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (brs, 1H), 7.31-7.29 (m, 2H), 7.21 (s, 1H), 7.03-6.95 (m, 5H), 4.86 (brs, 1H), 3.53 (brs, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.85, 157.39, 137.68, 129.66, 126.83, 126.78, 124.99, 122.18, 115.51, 33.11.

(*S*)-3-phenyl-2-(o-tolyloxy)propanoic acid (2s)



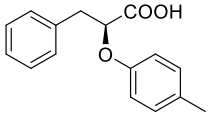
Colorless oil and solidified by standing. 95% yield, 98% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=11.34 min for major isomer, and t_R=12.89 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.29 (m, 5H), 7.16-7.10 (m, 2H), 6.90 (brs, 1H), 6.67-6.66 (m, 1H), 4.87 (brs, 1H), 3.34 (brs, 1H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.27, 163.51, 136.27, 131.10, 129.60, 128.43, 127.41, 127.03, 126.70, 121.49, 111.49, 39.07, 16.40.

(*S*)-3-phenyl-2-(m-tolyloxy)propanoic acid (2t)



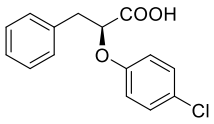
White solid, 96% yield, 97% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=10.27 min for major isomer, and t_R=11.93 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.28 (m, 5H), 7.16 (t, J = 8.0 Hz, 1H), 6.82 (d, J = 8.0 Hz, 1H), 6.72-6.67 (m, 2H), 4.88-4.85 (m, 1H), 3.30 (d, J = 4.0 Hz, 2H), 2.32 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.18, 157.53, 139.79, 136.28, 129.53, 129.33, 128.49, 127.03, 122.86, 116.32, 112.01, 38.91, 21.47.

(*S*)-3-phenyl-2-(p-tolyloxy)propanoic acid (2u)



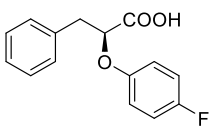
White solid, 97% yield, 97% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=11.00 min for major isomer, and t_R=12.26 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.29 (m, 5H), 7.08-7.07 (m, 1H), 6.78 (d, J = 8.0 Hz, 1H), 4.83 (brs, 1H), 3.30 (brs, 2H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.02, 155.51, 136.37, 131.38, 130.06, 129.52, 128.48, 127.00, 115.39, 38.89, 20.49.

(*S*)-2-(4-chlorophenoxy)-3-phenylpropanoic acid (2v)



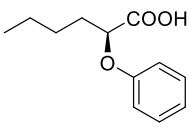
White solid, 93% yield, 95% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=16.09 min for major isomer, and t_R=18.15 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.21 (m, 7H), 6.79 (s, 2H), 4.80 (brs, 1H), 3.29 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.69, 156.18, 135.99, 129.49, 129.45, 128.54, 127.15, 127.00, 116.79, 38.80.

(*S*)-2-(4-fluorophenoxy)-3-phenylpropanoic acid (2w)



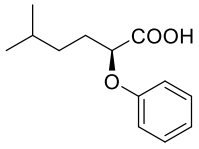
White solid, 95% yield, 93% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=0.8 mL/min, 254 nm UV detector, t_R=17.19 min for major isomer (*S*), and t_R=19.17 min for minor isomer (*R*); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.29 (m, 5H), 6.93-6.78 (m, 4H), 4.74 (brs, 1H), 3.26 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.09, 159.15, 156.77, 153.76, 136.16, 129.48, 128.54, 127.12, 116.96, 116.13, 115.90, 38.88.

(*S*)-2-phenoxyhexanoic acid (2x)



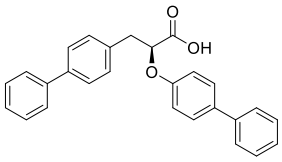
White solid, 97% yield, 88% *ee*. HPLC condition: Chiralcel OD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=92:8, flow rate=1.0 mL/min, 254 nm UV detector, t_R=8.69 min for major isomer, and t_R=9.83 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.29 (m, 2H), 7.03-6.94 (m, 3H), 4.67 (brs, 1H), 2.01 (brs, 2H), 1.46-1.24 (m, 4H), 0.96-0.93 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.71, 129.64, 121.80, 115.17, 36.74, 34.98, 32.44, 29.71, 27.36, 22.33, 13.87.

(*S*)-5-methyl-2-phenoxyhexanoic acid (2y)



White solid, 96% yield, 85% *ee*. HPLC condition: Chiralcel AD-H column (25 cm × 0.46 cm ID), hexane/2-propanol=90:10, flow rate=1.0 mL/min, 254 nm UV detector, t_R=7.94 min for major isomer, and t_R=9.41 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.29 (m, 3H), 7.03-7.00 (m, 1H), 6.93 (d, *J* = 8.0 Hz, 3H), 4.64 (brs, 1H), 2.02-2.00 (m, 2H), 1.64-1.61 (m, 1H), 1.50-1.41 (m, 2H), 0.94 (d, *J* = 8.0 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.03, 157.74, 129.64, 121.78, 115.16, 34.20, 30.74, 27.81, 22.52, 22.34.

(*S*)-5-methyl-2-phenoxyhexanoic acid (2y)



White solid, 97% yield, 90% *ee*, 95% *ee* after one recrystallization. HPLC condition: Chiralcel AS-H column (25 cm × 0.46 cm ID), hexane/2-propanol=90:10, flow rate=0.8 mL/min, 254 nm UV detector, t_R=18.44 min for major isomer, and t_R=28.75 min for minor isomer; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.51 (m, 8H), 7.47-7.41 (m, 6H), 7.38-7.32 (m, 2H), 6.98 (d, *J* = 8.0 Hz, 2H), 4.98 (t, *J*=4.0 Hz, 1H), 3.39 (t, *J*=4.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.21, 157.05, 140.80, 140.50, 139.98, 135.26, 135.17, 129.95, 128.76, 128.34, 127.24, 127.05, 126.80, 115.66, 38.50.

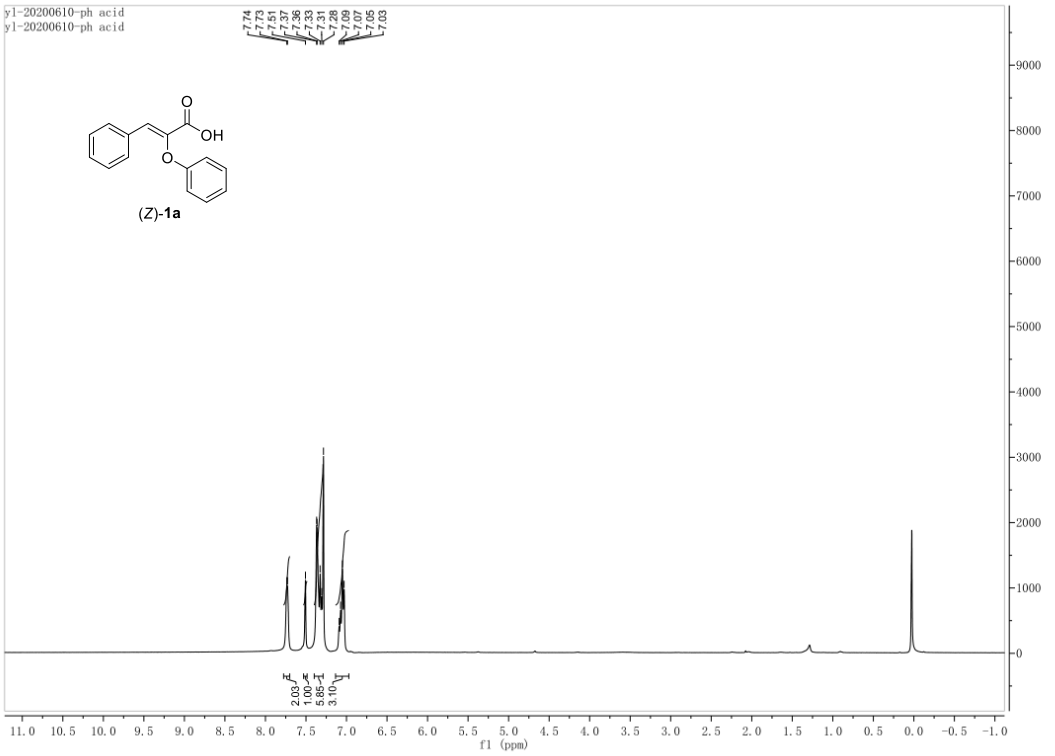
5. Reference

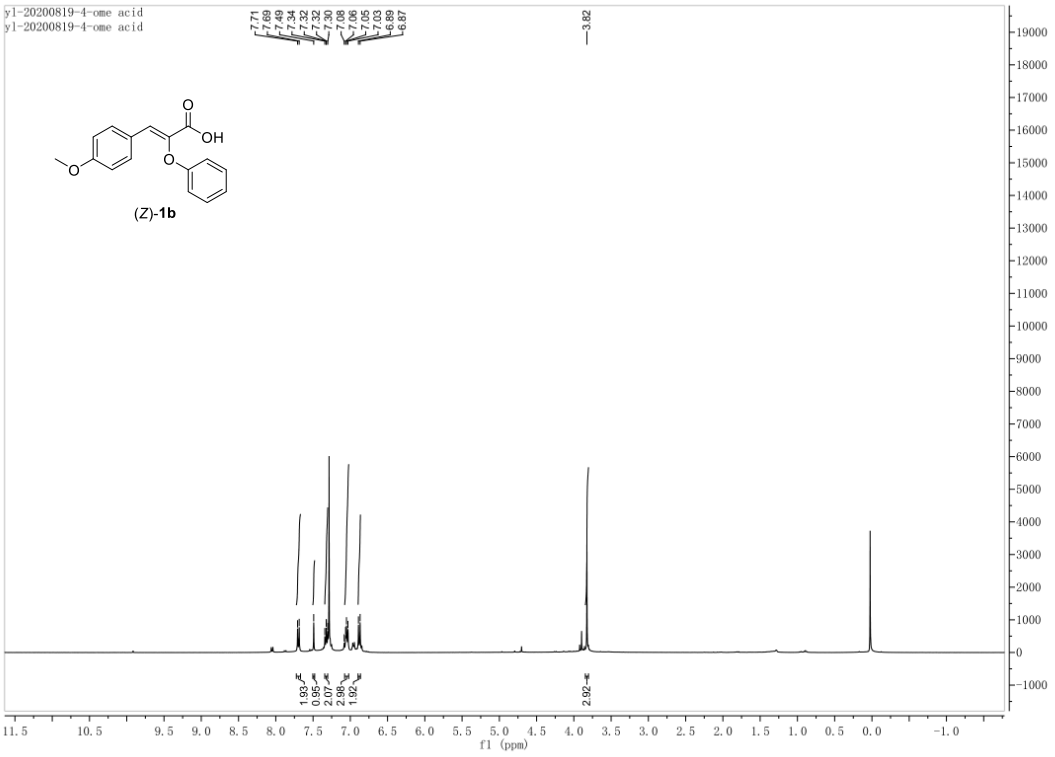
(1) S. Li, S.-F. Zhu, J.-H. Xie, S. Song, C.-M. Zhang and Q.-L. Zhou, *J. Am. Chem. Soc.*, **2010**, 132, 1172.

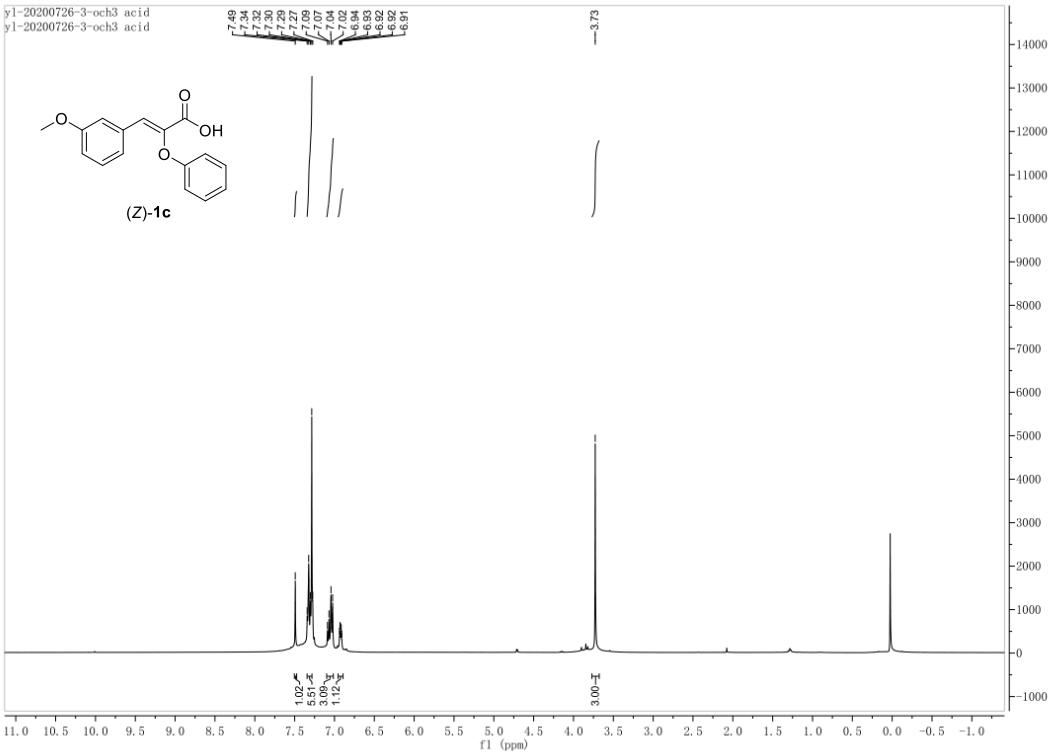
(2) W.-P. Chen, P.-J. McCormack, K. Mohammed, W. Mbafor, S.-M. Roberts, J. Whittall, *Angew. Chem. Int. Ed.*, **2007**, 46, 4141.

6. NMR Spectra

6.1 NMR Spectra of the substrates



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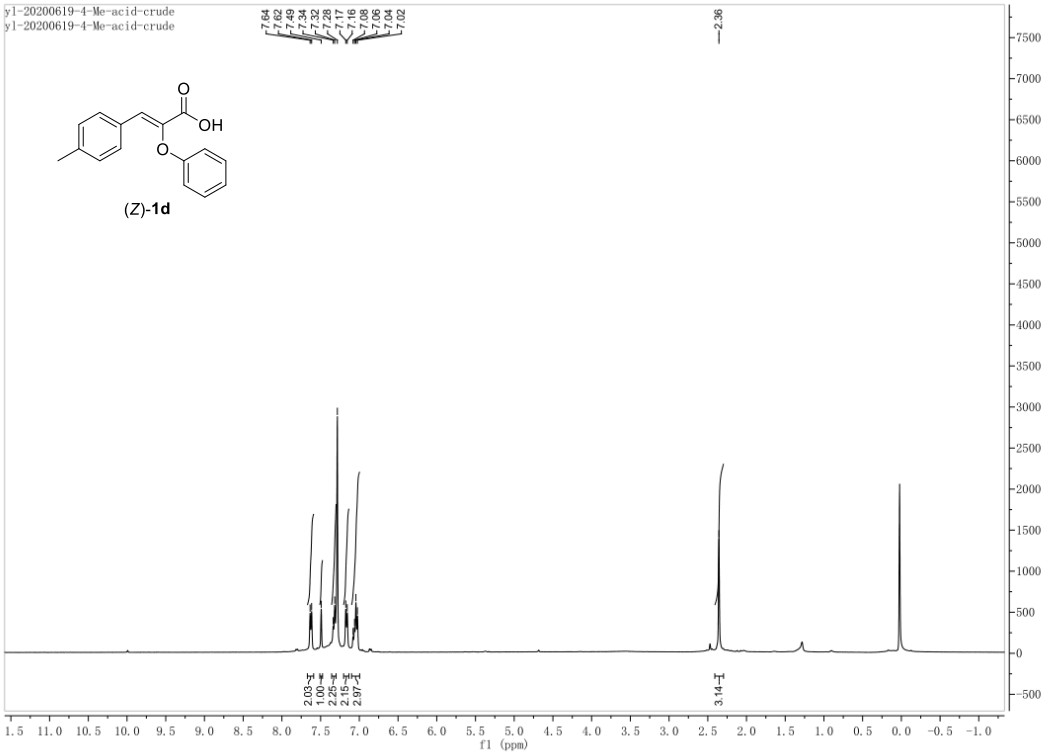
yl-20200726-3-och3 acid
7.49
7.34
7.32
7.30
7.29
7.27
7.09
7.07
7.04
7.02
6.94
6.93
6.92
6.92
6.91
3.73
O
OH
O
O
(Z)-1c
1.02
5.51
3.09
1.12
3.00
f1 (ppm)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yl-20200619-4-Me-acid-crude
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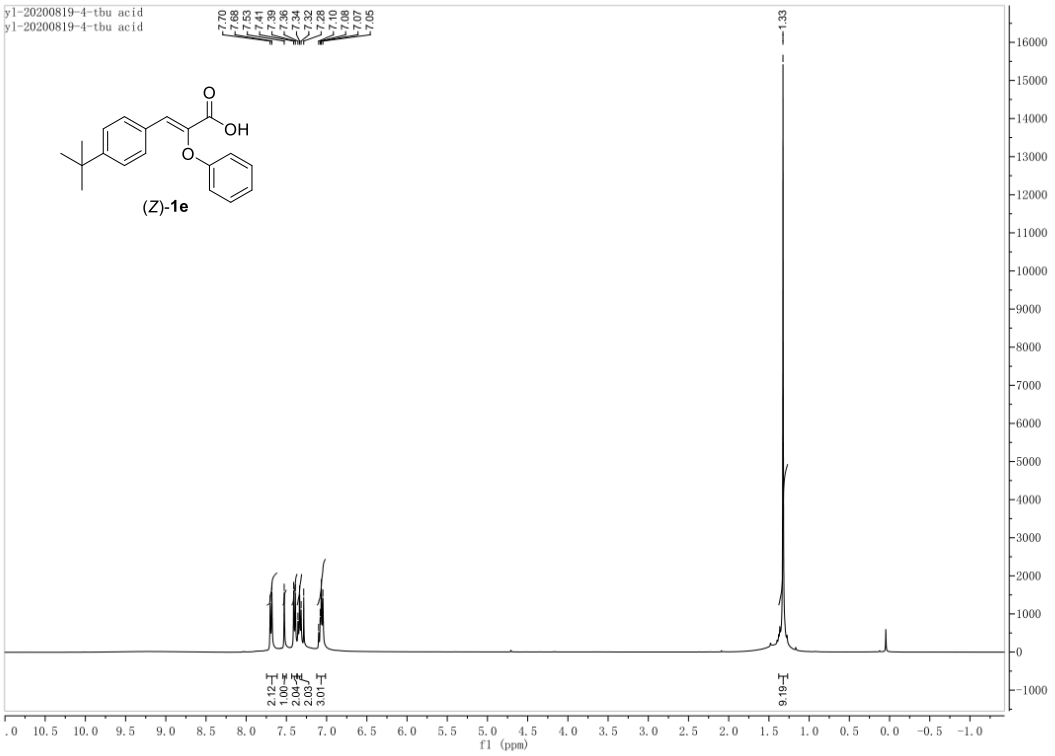
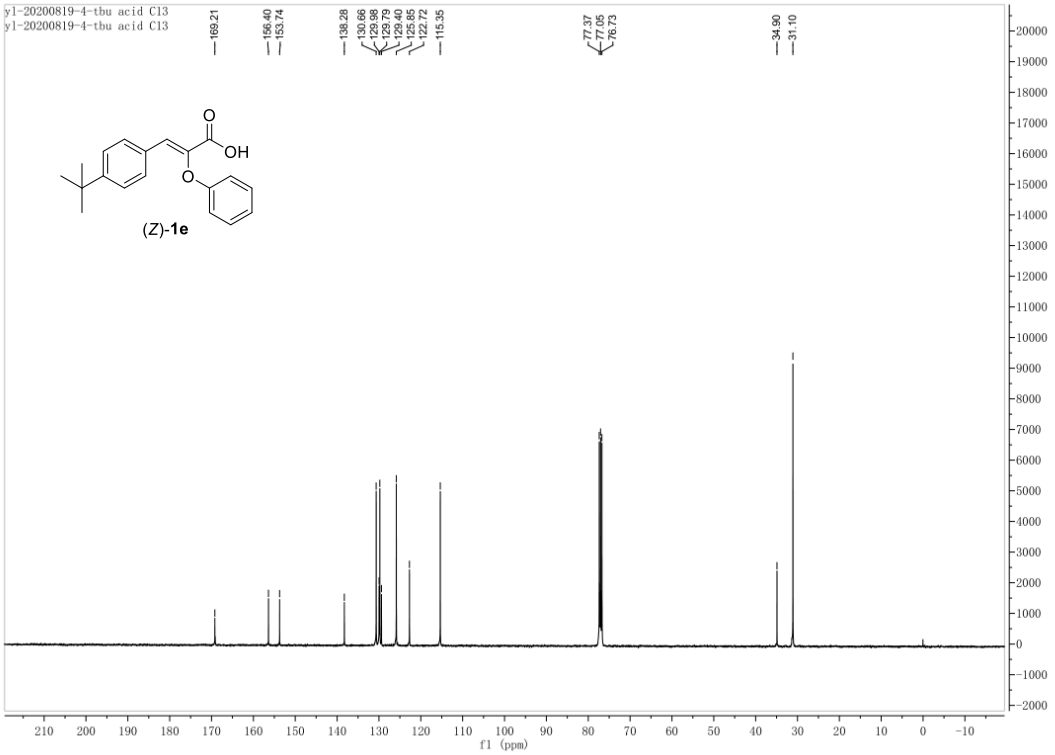
7.62
7.49
7.34
7.32
7.28
7.17
7.16
7.08
7.06
7.04
7.02
2.36
O
OH
O
(Z)-1d
2.03
2.00
2.05
2.15
2.97
3.14
f1 (ppm)


yl-20200819-4-tbu acid
yl-20200819-4-tbu acid
7.70
7.68
7.53
7.41
7.39
7.36
7.34
7.32
7.28
7.10
7.08
7.07
7.05
1.33
O
OH
O
(Z)-1e
2.12
1.00
2.04
2.03
3.01
9.19
fl (ppm)


yl-20200819-4-tbu acid C13
yl-20200819-4-tbu acid C13
169.21
156.40
153.74
138.28
130.66
129.98
129.79
129.40
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77.37
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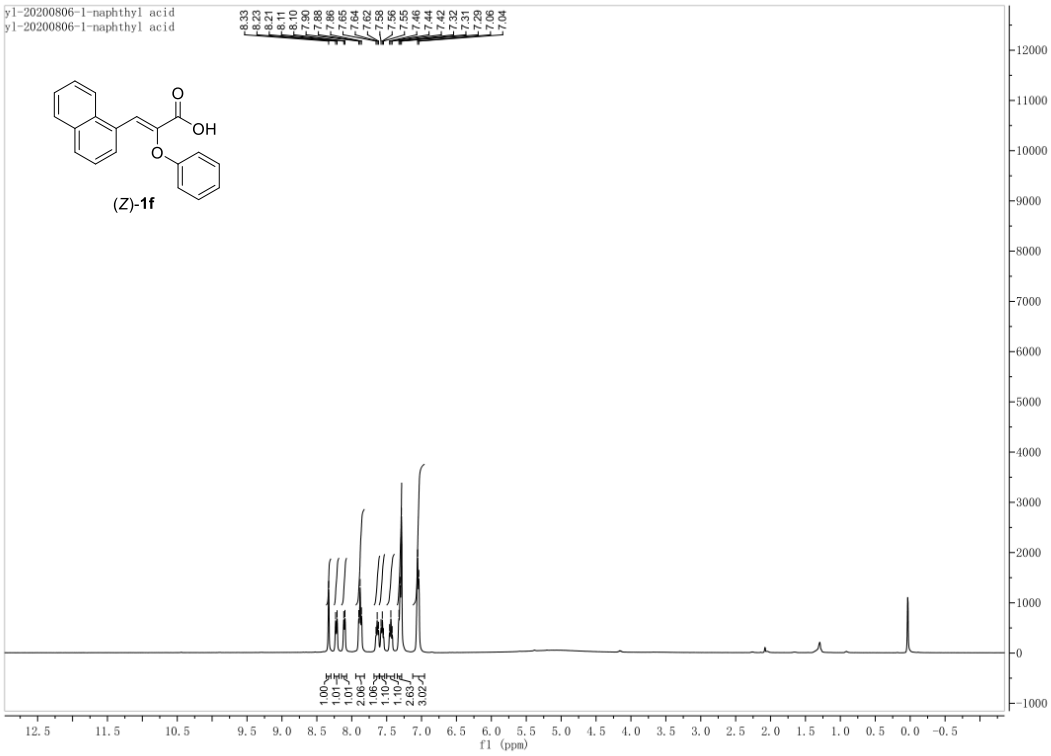
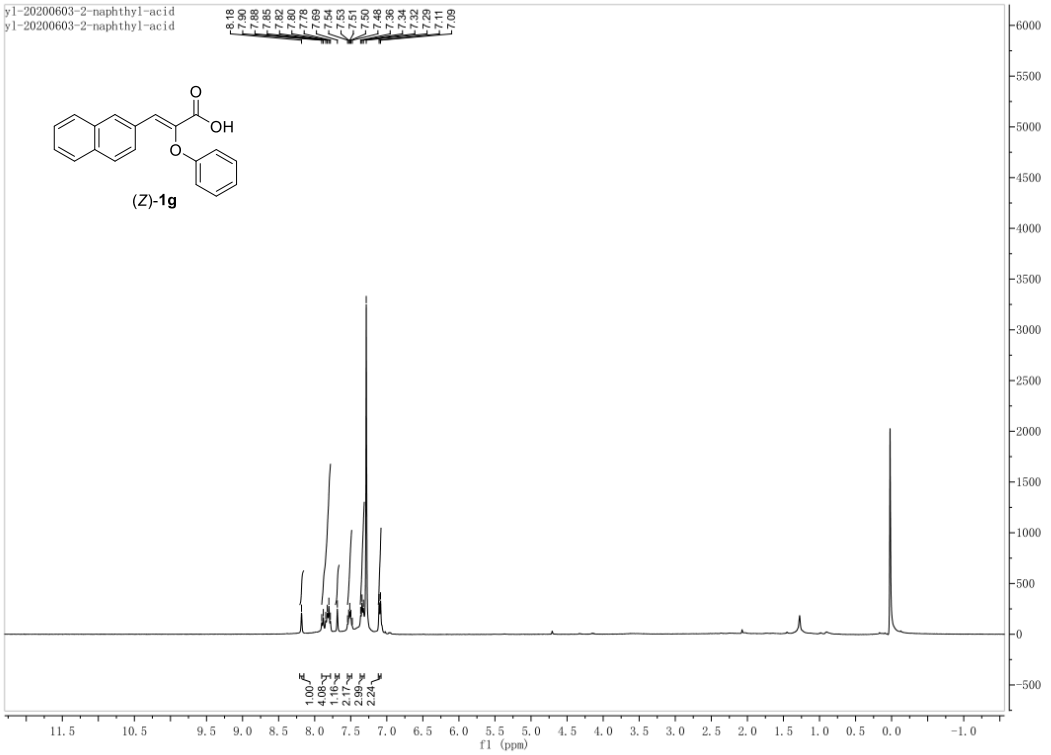
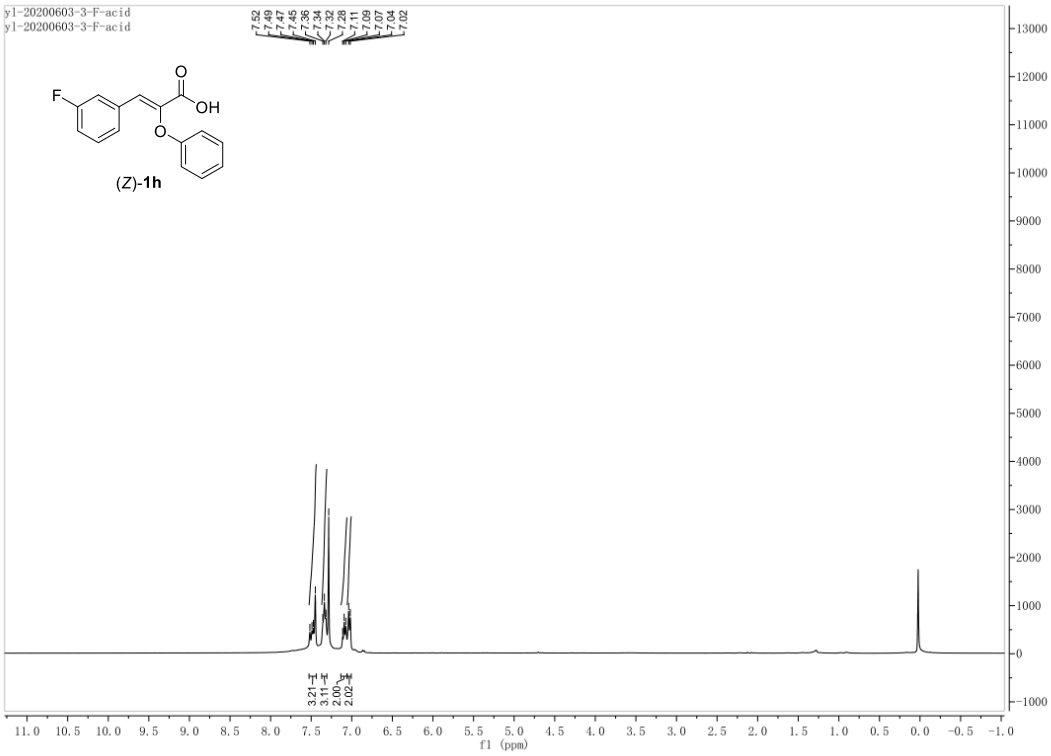
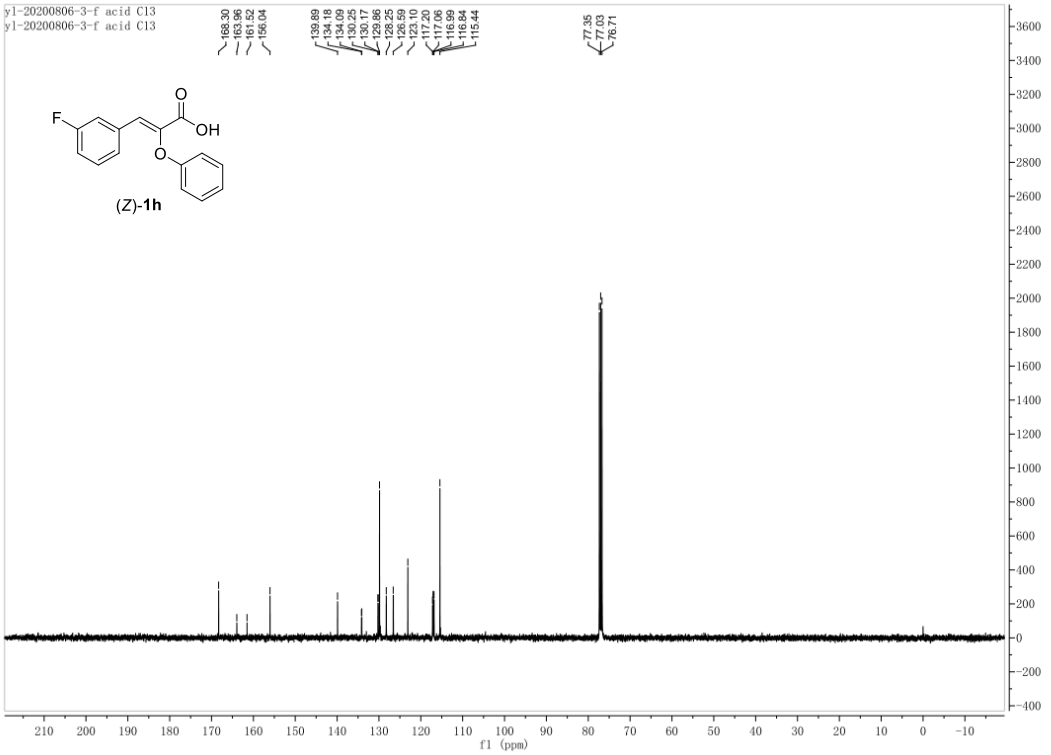
34.90
31.10
O
OH
O
(Z)-1e
fl (ppm)


yl-20200806-1-naphthyl acid
yl-20200806-1-naphthyl acid
(Z)-1f
f1 (ppm)


yl-20200603-2-naphthyl-acid
yl-20200603-2-naphthyl-acid
(Z)-1g
f1 (ppm)


yl-20200603-3-F-acid
yl-20200603-3-F-acid
7.52
7.49
7.47
7.45
7.36
7.34
7.32
7.28
7.11
7.09
7.07
7.04
7.02
F
O
OH
O
(Z)-1h
3.21
3.11
2.00
2.02
fl (ppm)


yl-20200806-3-f acid C13
yl-20200806-3-f acid C13
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163.96
161.52
160.04
139.89
134.18
134.09
130.25
130.17
129.86
128.35
126.59
123.10
117.20
117.06
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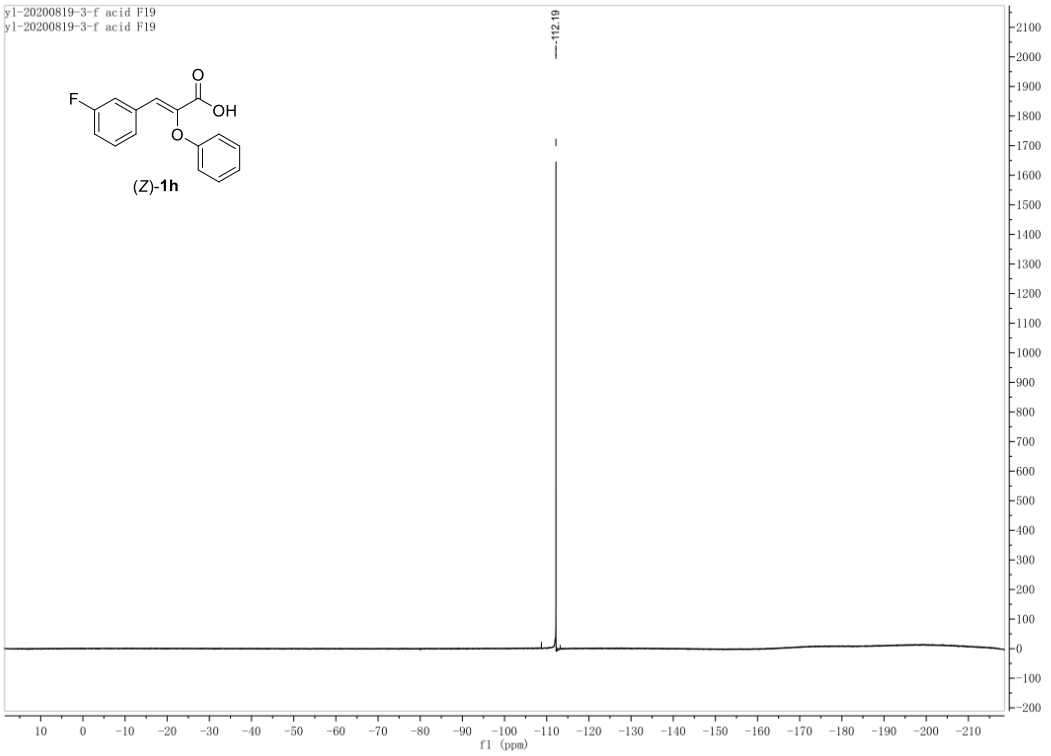
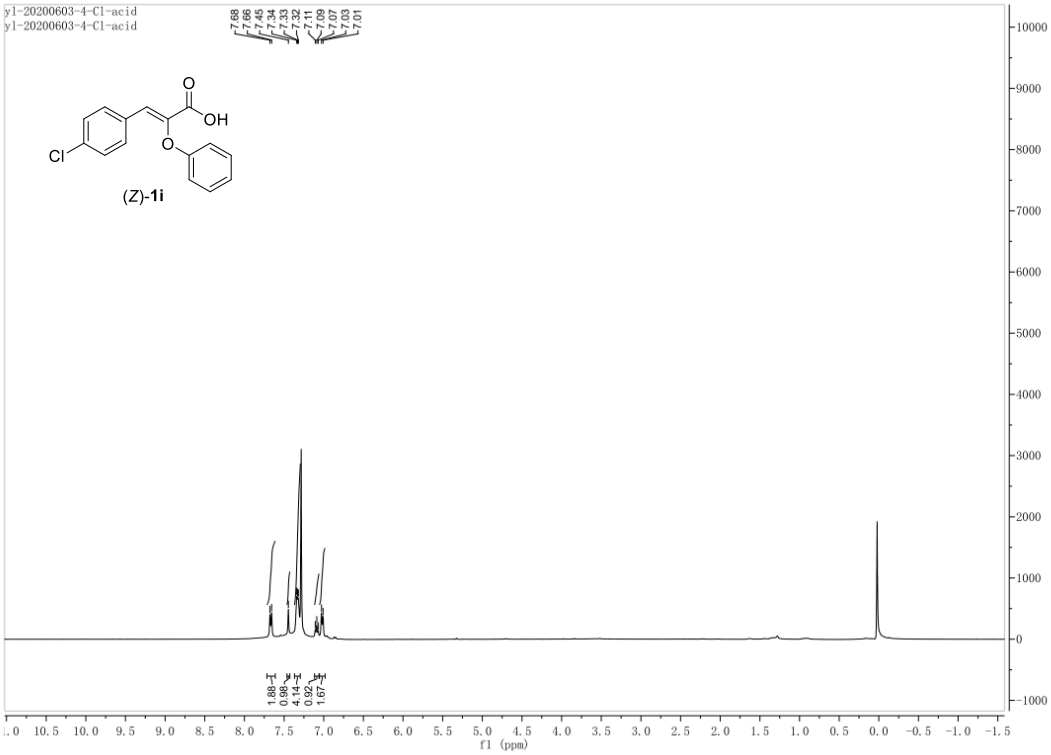
77.03
76.71
F
O
OH
O
(Z)-1h
fl (ppm)


yl-20200819-3-f acid F19
yl-20200819-3-f acid F19
-112.19
F
O
OH
O
(Z)-1h
f1 (ppm)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yl-20200603-4-Cl-acid
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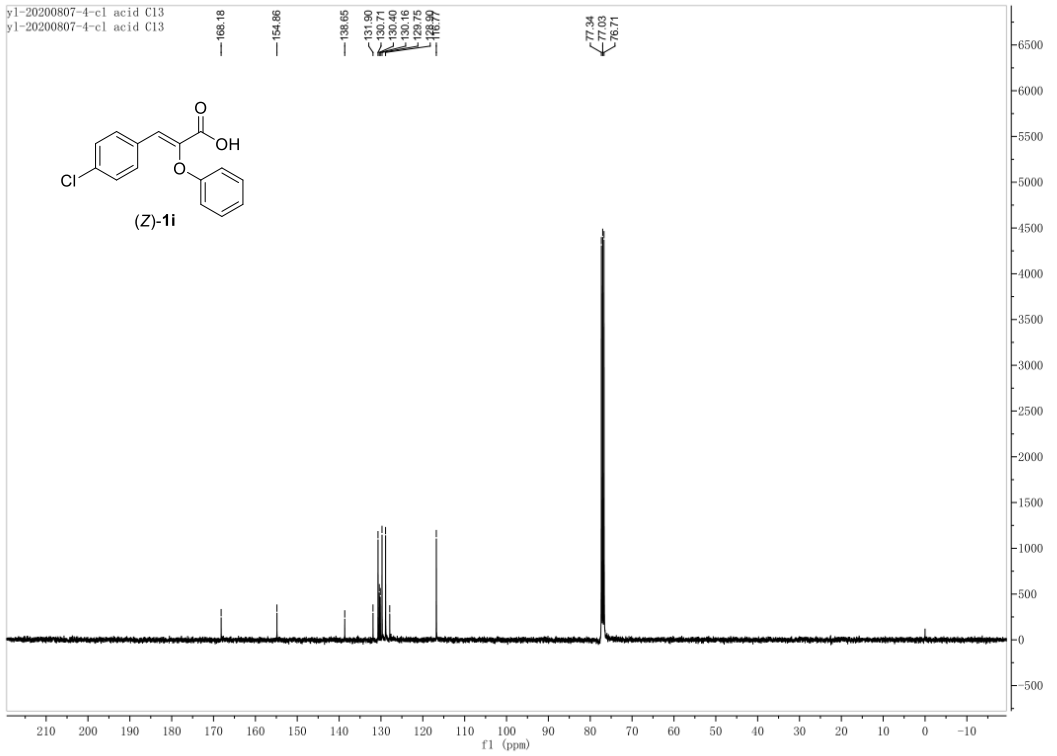
7.66
7.45
7.34
7.33
7.32
7.11
7.09
7.07
7.03
7.01
Cl
O
OH
O
(Z)-1i
1.88
0.98
4.14
0.92
1.67
f1 (ppm)


yl-20200807-4-cl acid C13
yl-20200807-4-cl acid C13
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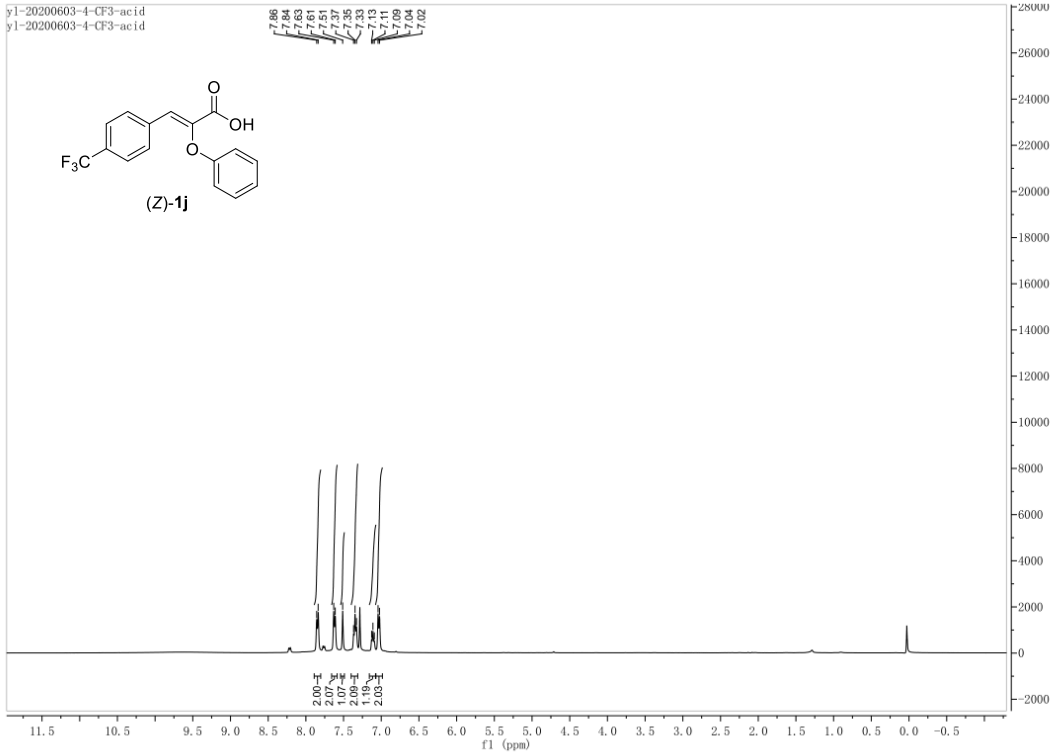
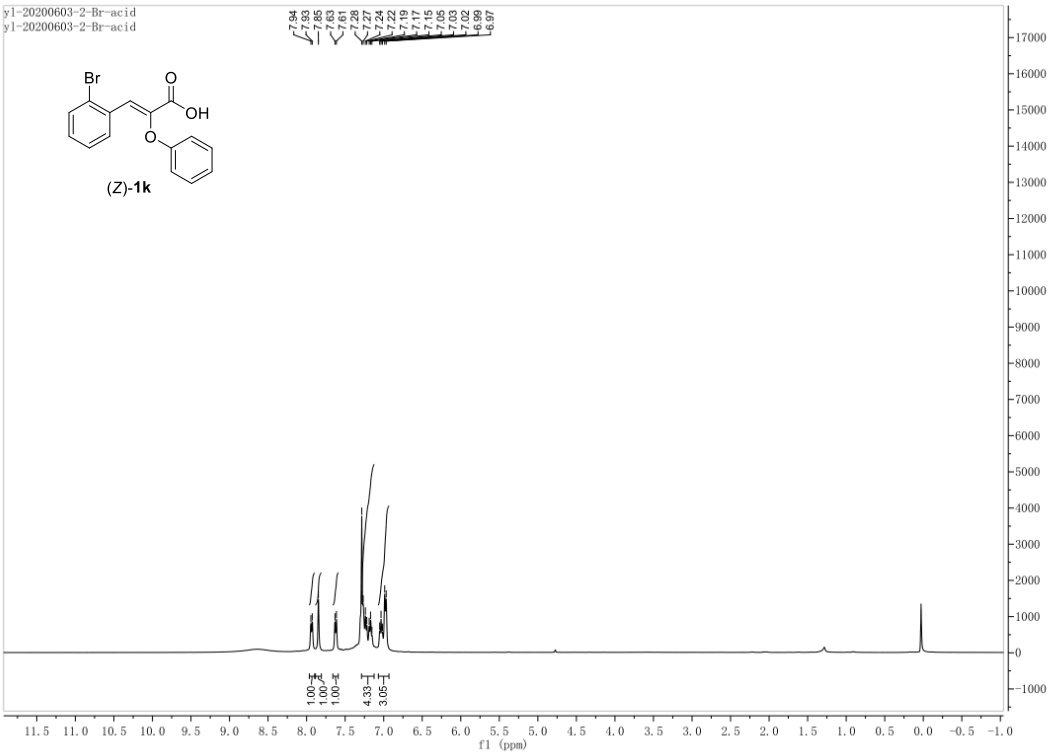
154.86
138.65
131.90
130.71
130.40
130.15
129.75
128.99
116.77
77.34
77.03
76.71
O
OH
Cl
O
(Z)-1i
fl (ppm)


yl-20200603-4-CF3-acid
yl-20200603-4-CF3-acid
7.86
7.84
7.63
7.61
7.51
7.37
7.35
7.33
7.13
7.11
7.09
7.04
7.02
O
OH
F3C
O
(Z)-1j
2.00
2.07
1.07
2.09
1.19
2.03
fl (ppm)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yl-20200603-2-Br-acid
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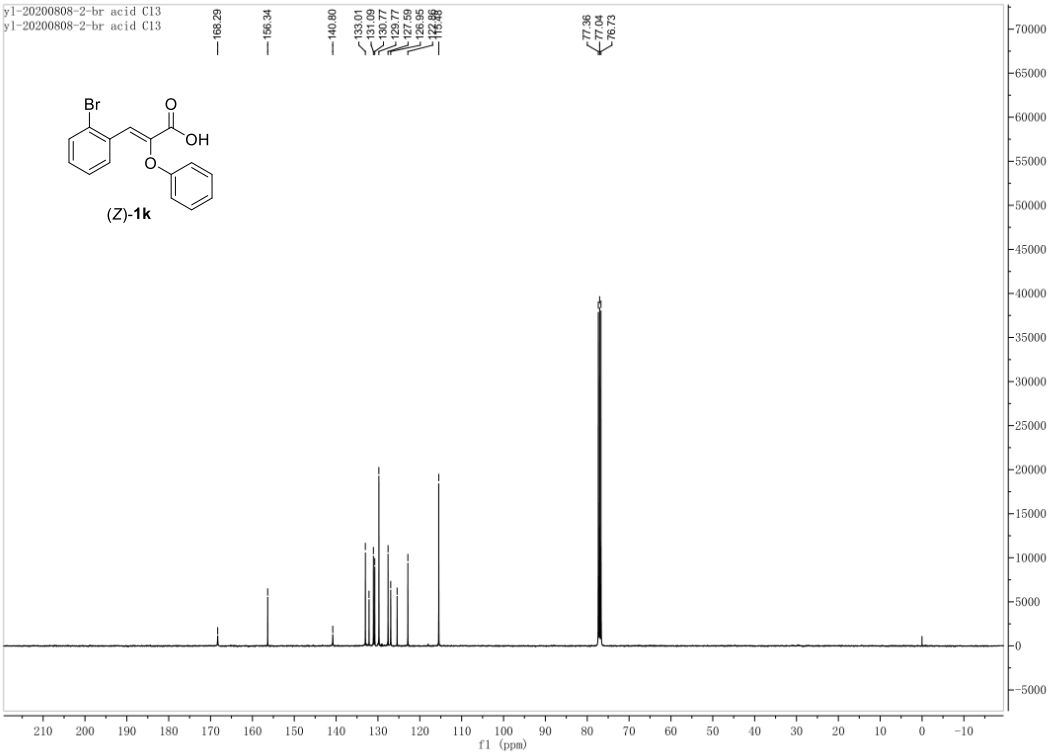
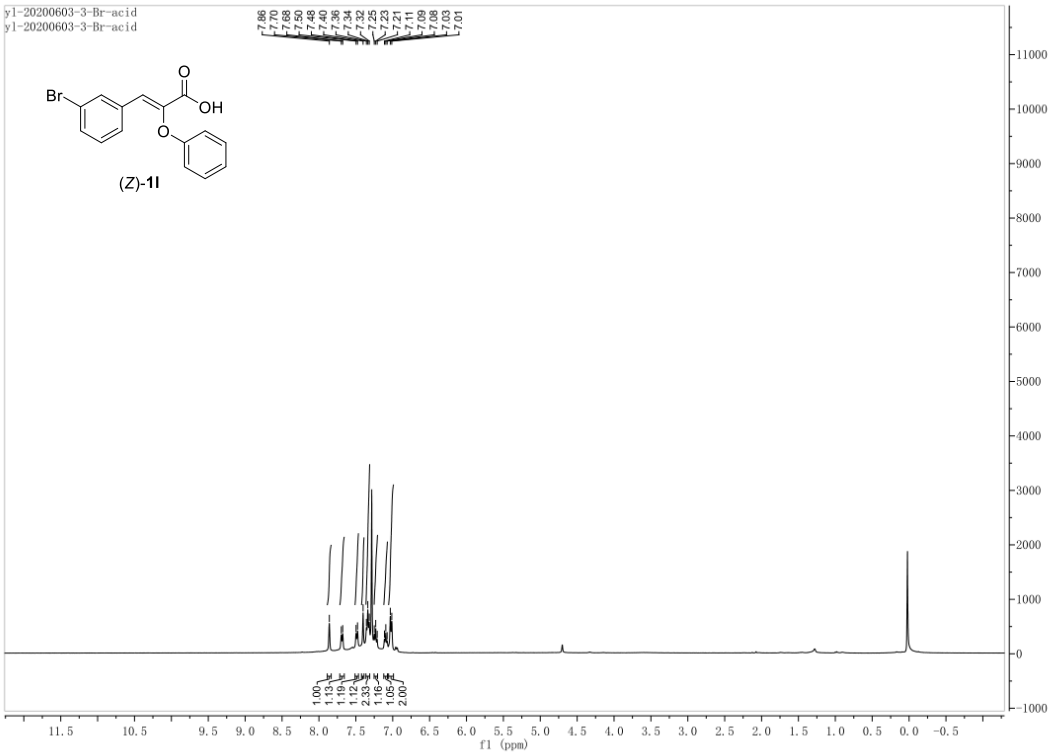
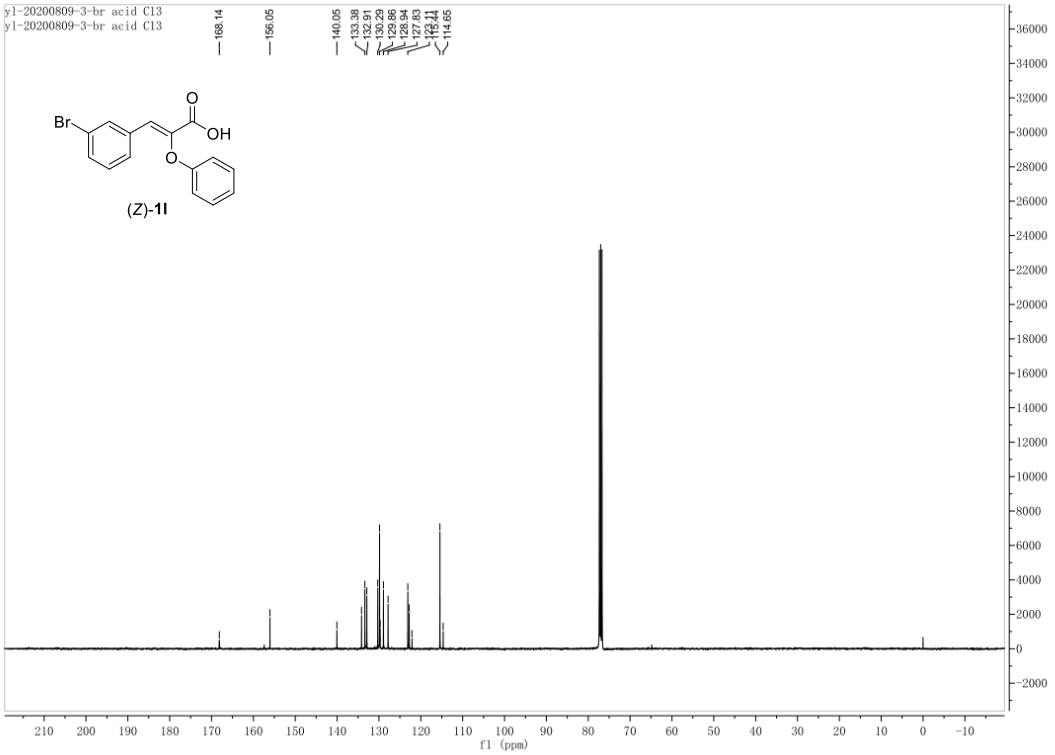
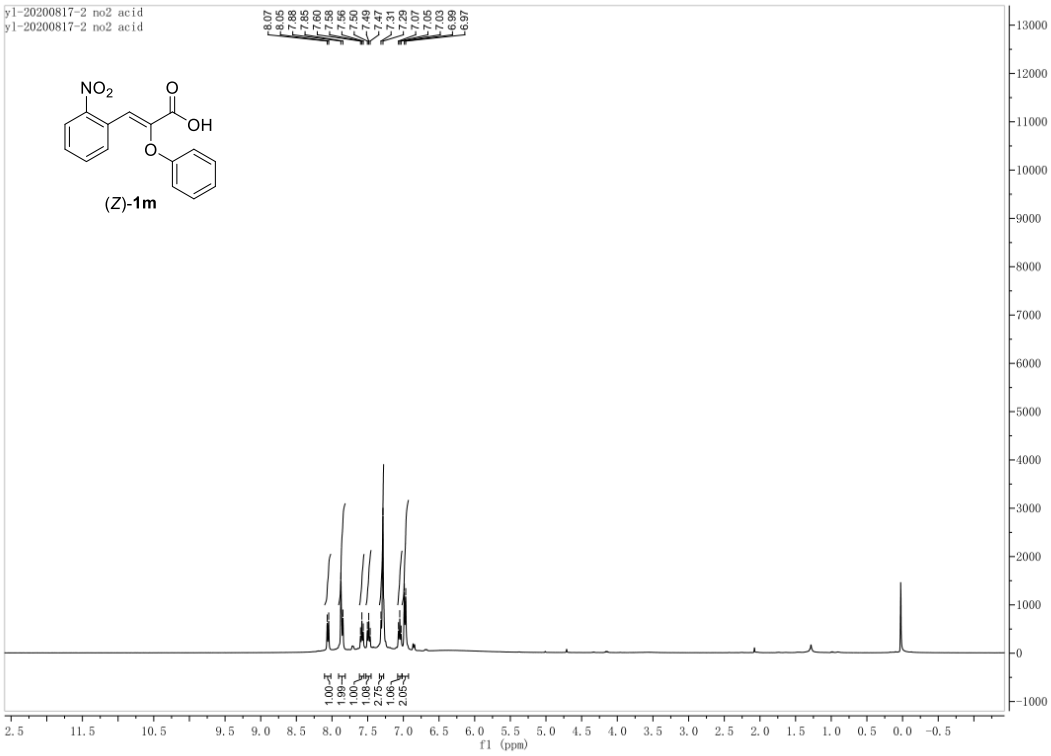
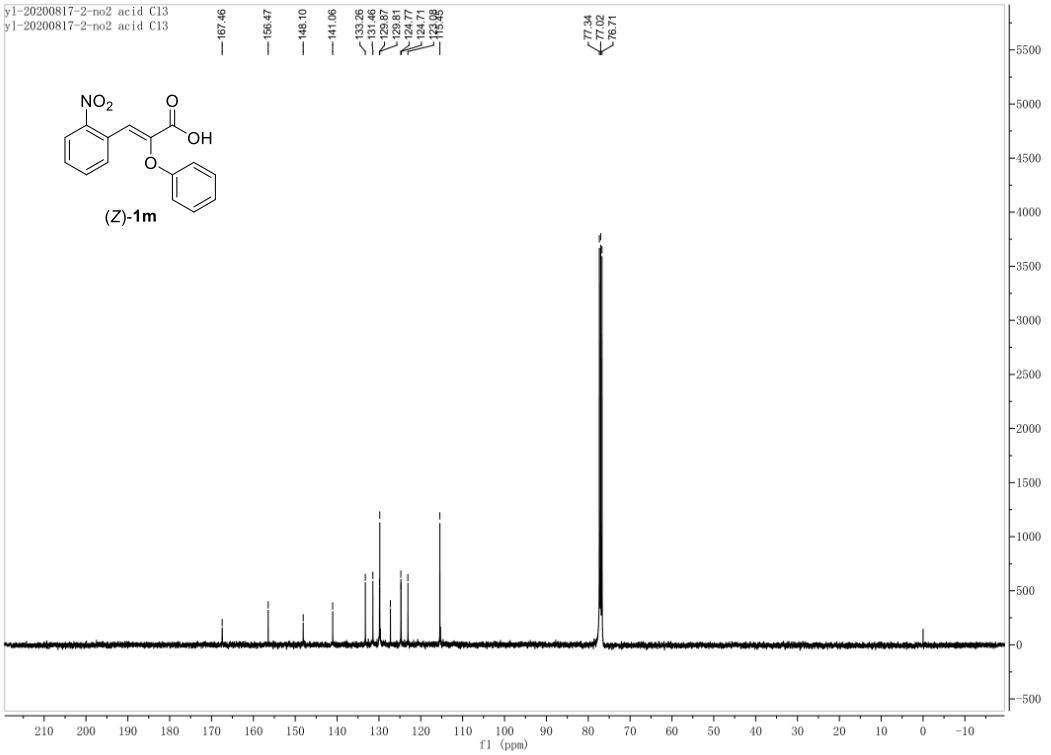
7.93
7.85
7.63
7.61
7.28
7.27
7.24
7.22
7.19
7.17
7.15
7.05
7.03
7.02
6.99
6.97
Br
O
OH
O
(Z)-1k
1.00
1.00
1.00
4.33
3.05
f1 (ppm)

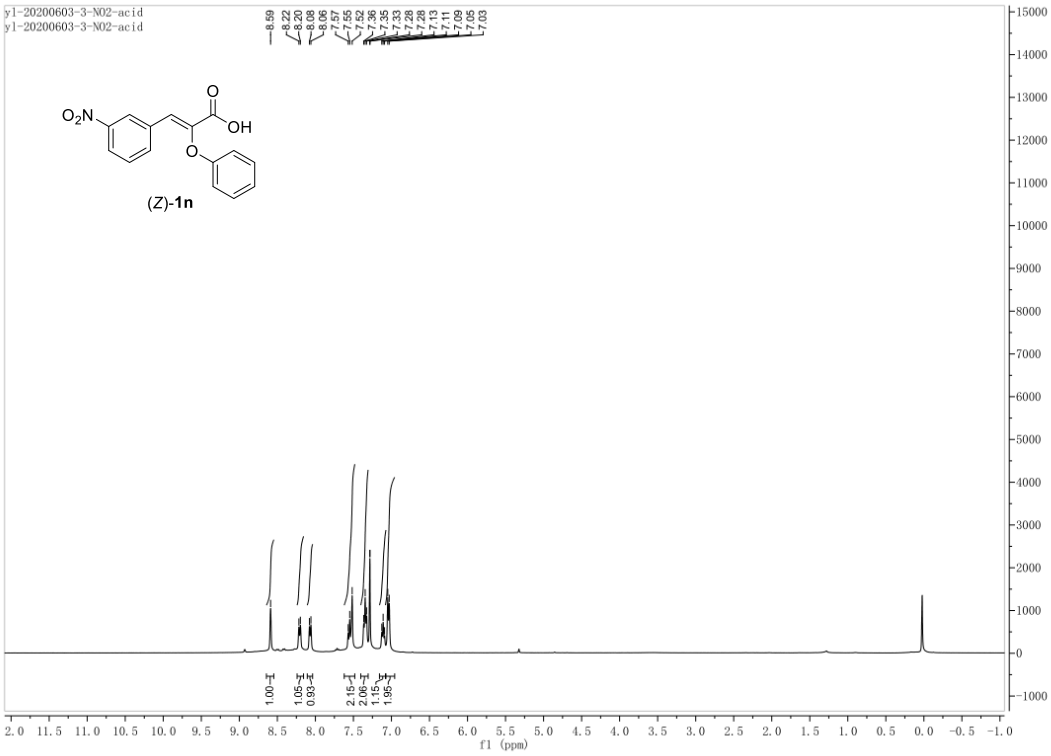

yl-20200808-2-br acid C13
yl-20200808-2-br acid C13
168.29
156.34
140.80
133.01
131.09
130.77
129.77
127.59
126.95
77.36
77.04
76.73
Br
O
OH
O
(Z)-1k
f1 (ppm)

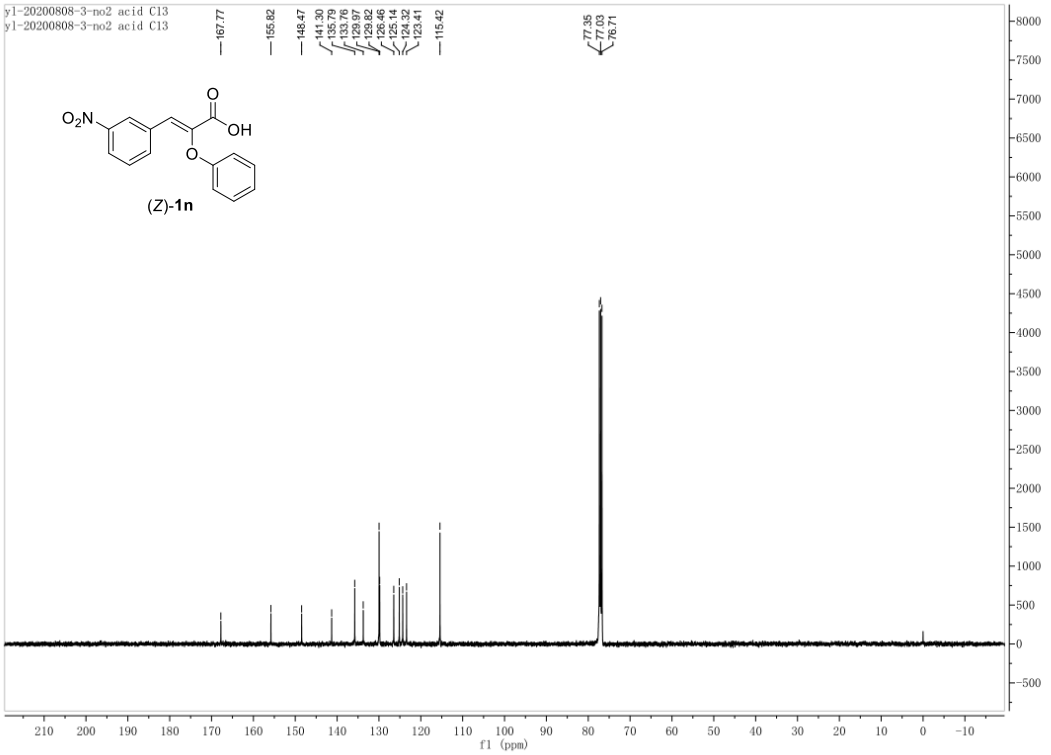

yl-20200603-3-Br-acid
yl-20200603-3-Br-acid
7.86
7.70
7.68
7.50
7.48
7.40
7.36
7.34
7.32
7.25
7.23
7.21
7.11
7.09
7.08
7.03
7.01
Br
O
OH
O
(Z)-1l
1.00
1.13
1.19
1.12
2.33
1.16
1.05
2.00
f1 (ppm)

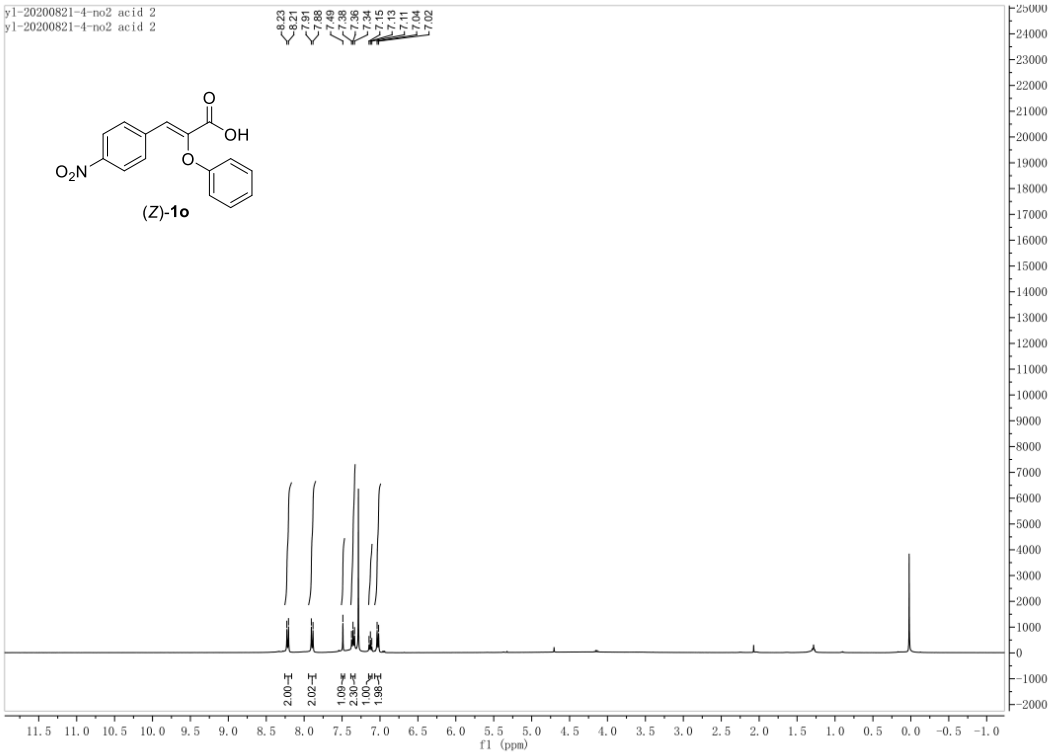

yl-20200809-3-br acid C13
yl-20200809-3-br acid C13
168.14
156.05
140.05
133.38
132.91
130.29
129.86
129.54
127.83
123.41
115.44
114.65
Br
O
OH
O
(Z)-1l
f1 (ppm)

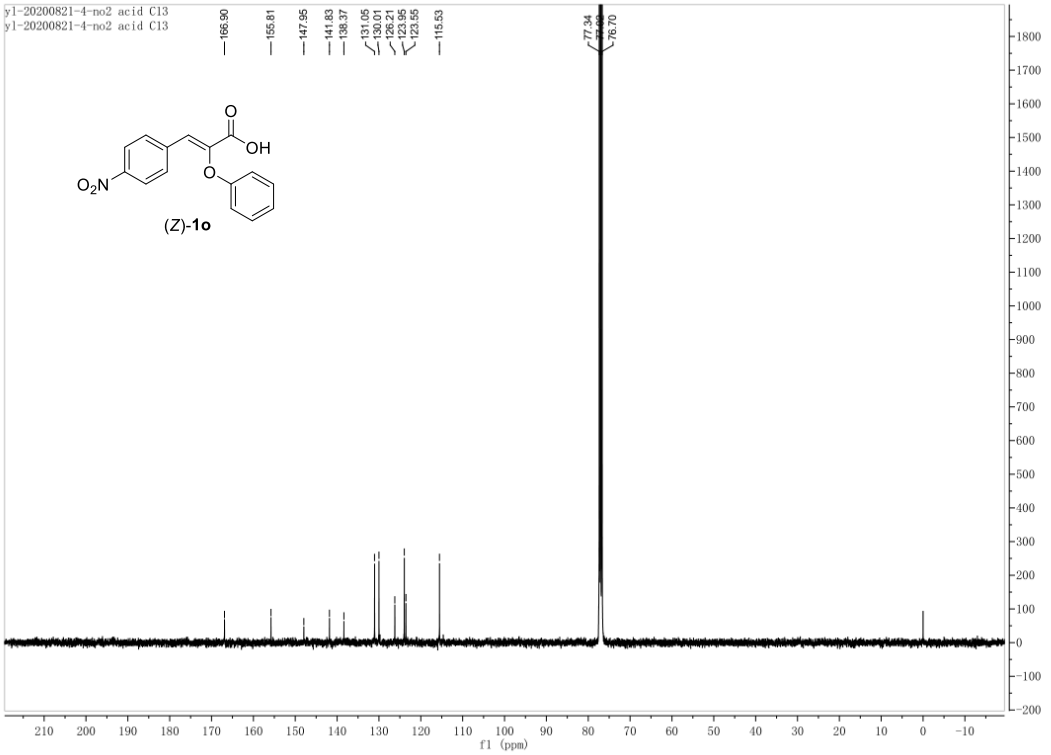

yl-20200817-2 no2 acid
yl-20200817-2 no2 acid
8.07
8.05
7.88
7.86
7.60
7.58
7.56
7.50
7.49
7.47
7.31
7.29
7.07
7.05
7.03
6.99
6.97
NO2
O
OH
O
(Z)-1m
1.00
1.99
1.00
1.08
2.75
1.06
2.05
f1 (ppm)

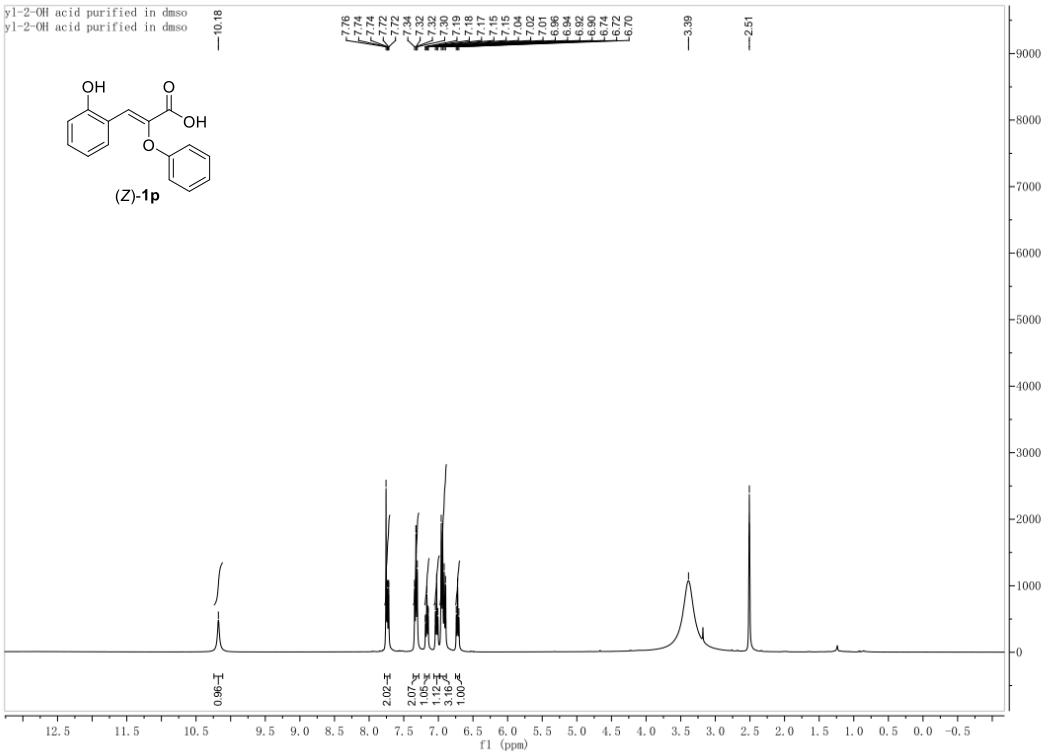

yl-20200817-2-no2 acid C13
yl-20200817-2-no2 acid C13
167.46
156.47
148.10
141.06
133.26
131.46
129.87
129.81
124.77
124.71
77.34
77.02
76.71
NO2
O
OH
O
(Z)-1m
f1 (ppm)

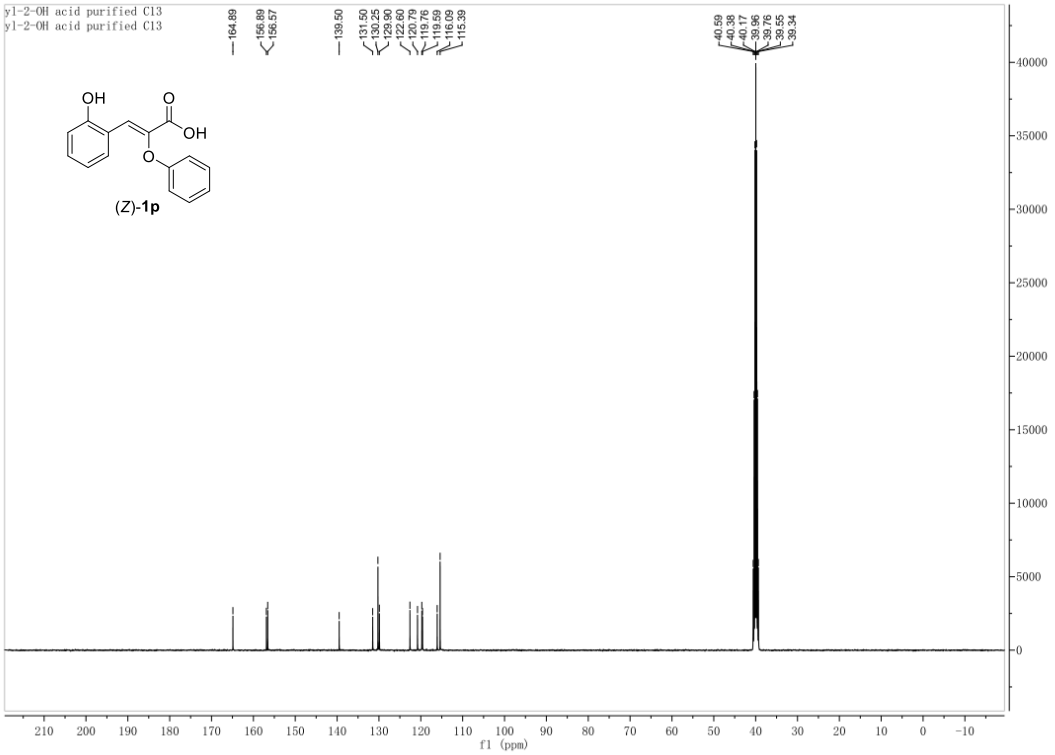

yl-20200603-3-N02-acid
yl-20200603-3-N02-acid
8.59
8.22
8.20
8.08
8.06
7.57
7.55
7.36
7.35
7.33
7.28
7.28
7.13
7.11
7.09
7.05
7.03
O2N
O
OH
O
(Z)-1n
1.00
1.05
0.93
2.15
2.06
2.05
1.95
f1 (ppm)

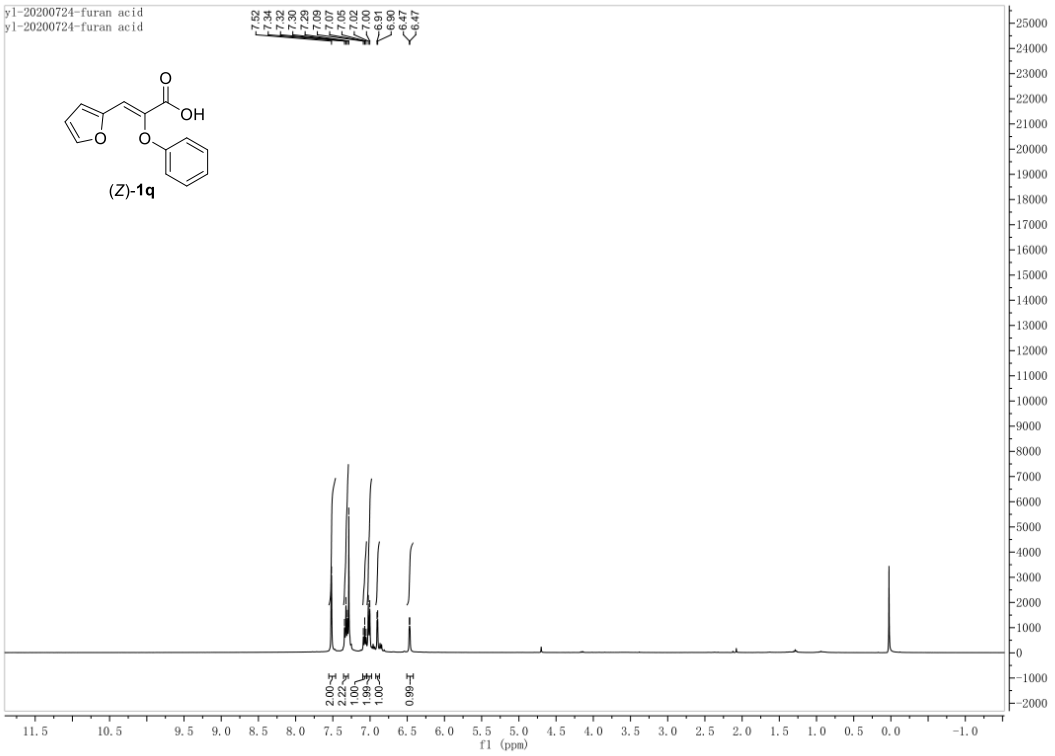

yl-20200808-3-no2 acid C13
yl-20200808-3-no2 acid C13
167.77
155.82
148.47
141.30
135.79
133.76
129.97
129.82
126.46
125.14
124.32
123.41
115.42
77.35
77.03
76.71
O2N
O
OH
O
(Z)-1n
f1 (ppm)

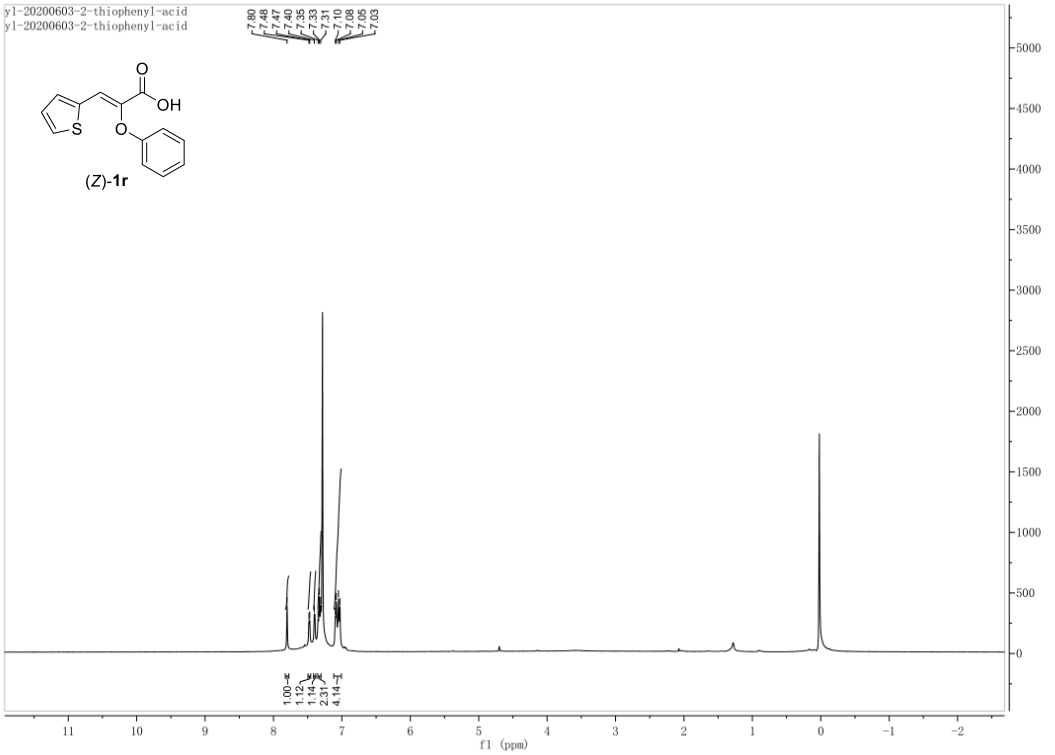

yl-20200821-4-no2 acid 2
yl-20200821-4-no2 acid 2
8.23
8.21
7.91
7.88
7.49
7.38
7.36
7.34
7.15
7.13
7.11
7.04
7.02
O
OH
O
O_2N
(Z)-1o
2.00
2.02
1.09
2.30
1.00
1.98
f1 (ppm)

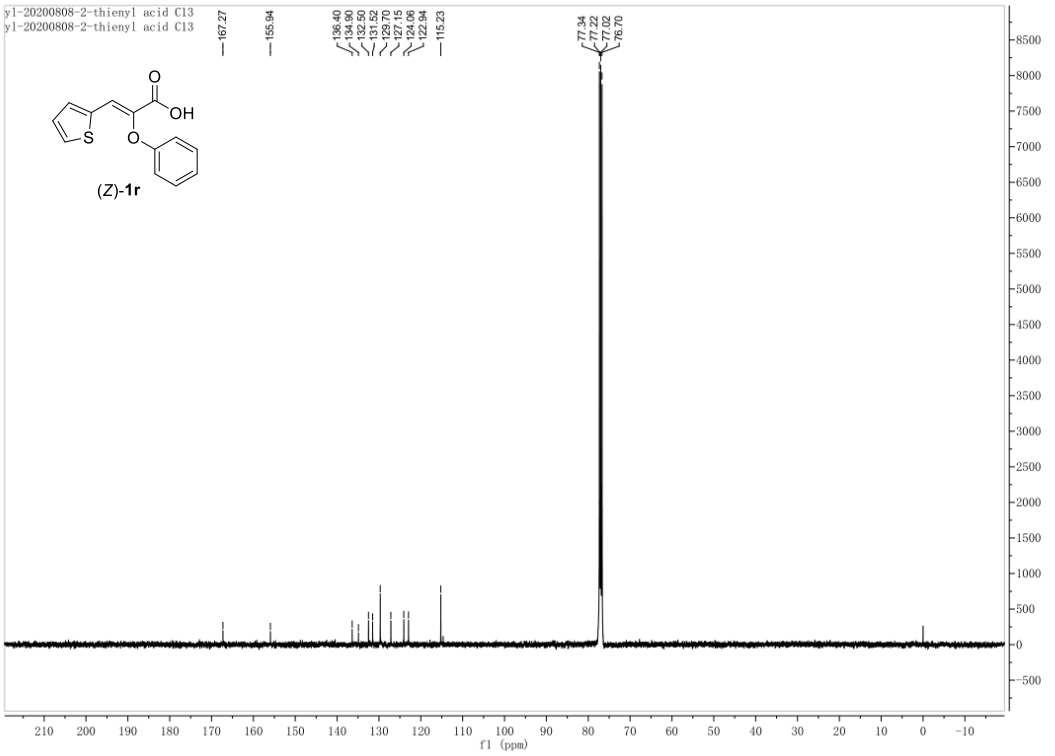

yl-20200821-4-no2 acid C13
yl-20200821-4-no2 acid C13
166.90
155.81
147.95
141.83
138.37
131.05
130.01
125.21
123.95
123.55
115.53
77.34
77.02
76.70
O
OH
O
O_2N
(Z)-1o
f1 (ppm)

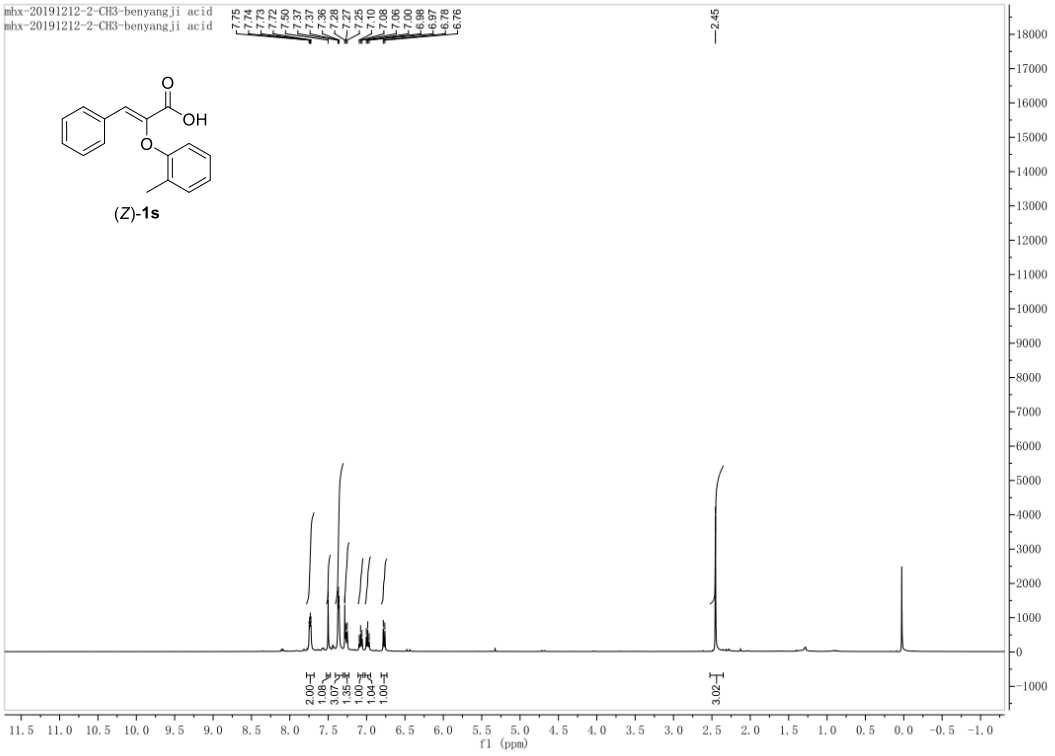

yl-2-OH acid purified in dmso
yl-2-OH acid purified in dmso
10.18
7.76
7.74
7.74
7.72
7.72
7.34
7.32
7.32
7.30
7.19
7.18
7.17
7.15
7.15
7.04
7.02
7.01
6.96
6.94
6.92
6.90
6.74
6.72
6.70
3.39
2.51
OH
O
OH
O
(Z)-1p
0.96
2.02
2.07
1.05
1.12
3.16
1.00
f1 (ppm)

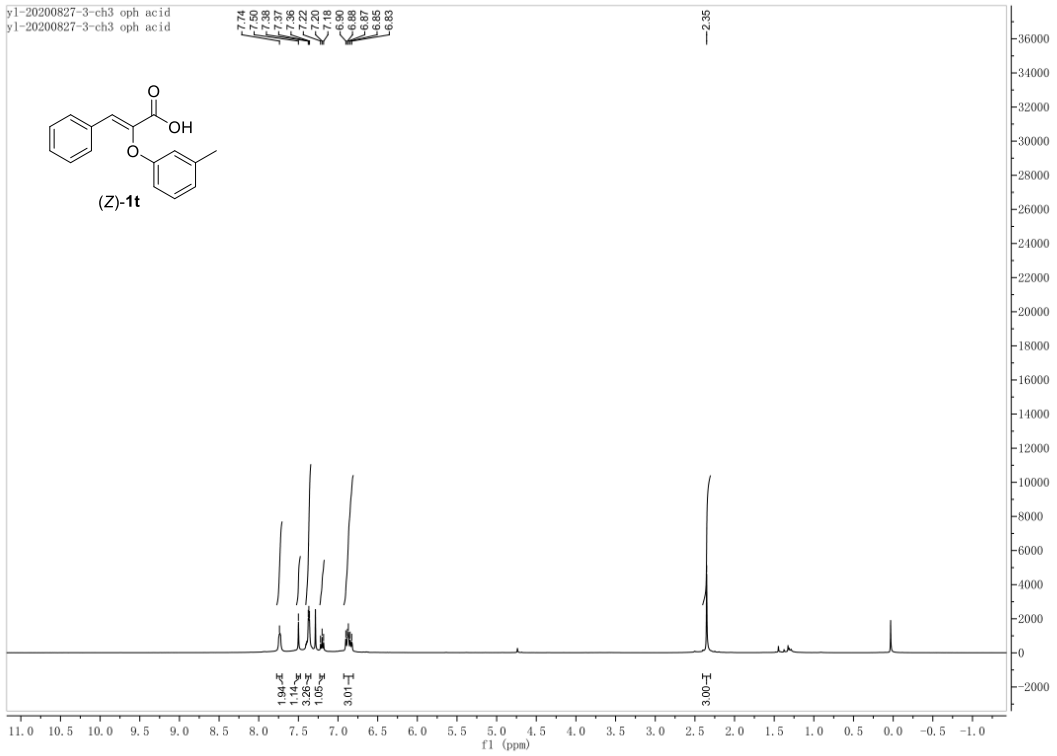

yl-2-OH acid purified C13
yl-2-OH acid purified C13
164.89
156.89
156.57
139.50
131.50
130.25
129.90
122.60
120.79
119.76
119.59
116.09
115.39
40.59
40.38
40.17
39.96
39.76
39.55
39.34
OH
O
OH
O
(Z)-1p
f1 (ppm)

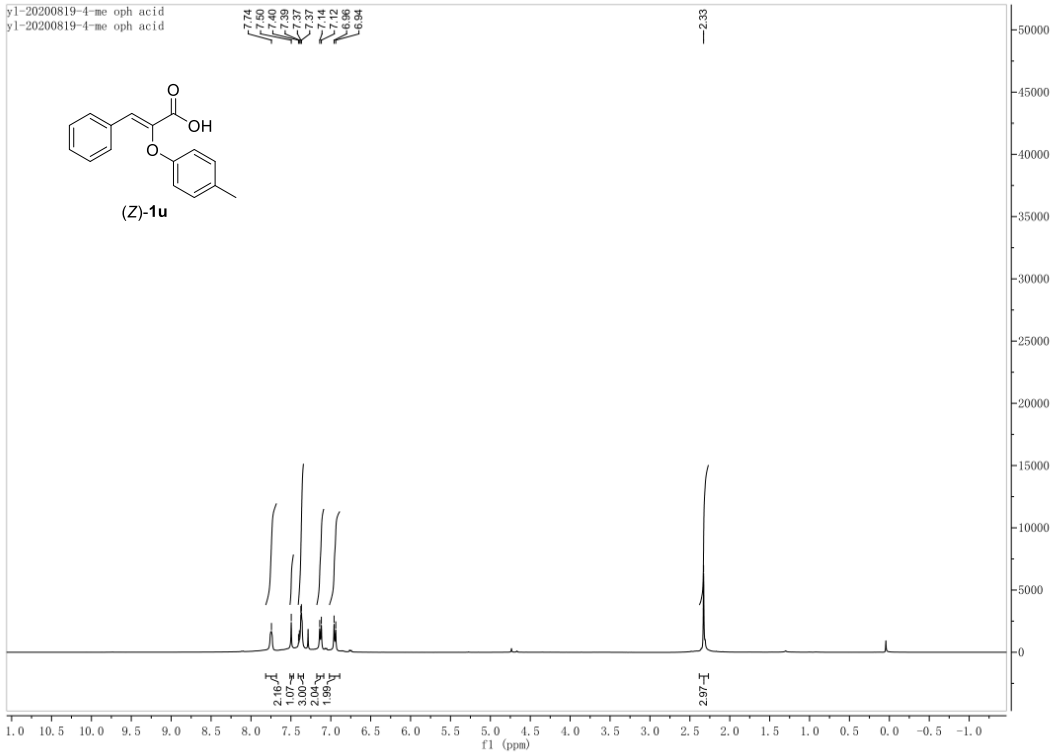

yl-20200724-furan acid
yl-20200724-furan acid
7.52
7.34
7.32
7.30
7.29
7.09
7.07
7.05
7.02
7.00
6.91
6.90
6.47
6.47
O
OH
O
O
(Z)-1q
2.00
2.22
1.00
1.99
1.00
0.99
fl (ppm)

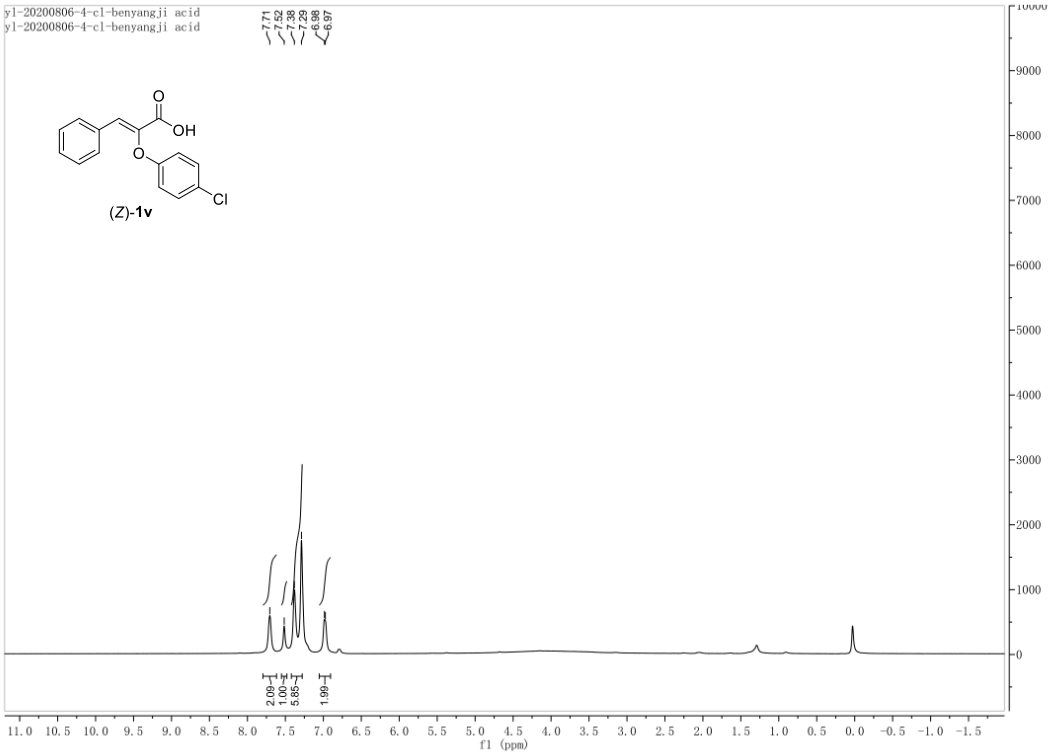

yl-20200603-2-thiophenyl-acid
yl-20200603-2-thiophenyl-acid
7.80
7.48
7.47
7.40
7.35
7.33
7.31
7.10
7.08
7.05
7.03
O
OH
S
O
(Z)-1r
1.00
1.12
1.14
2.31
4.14
fl (ppm)

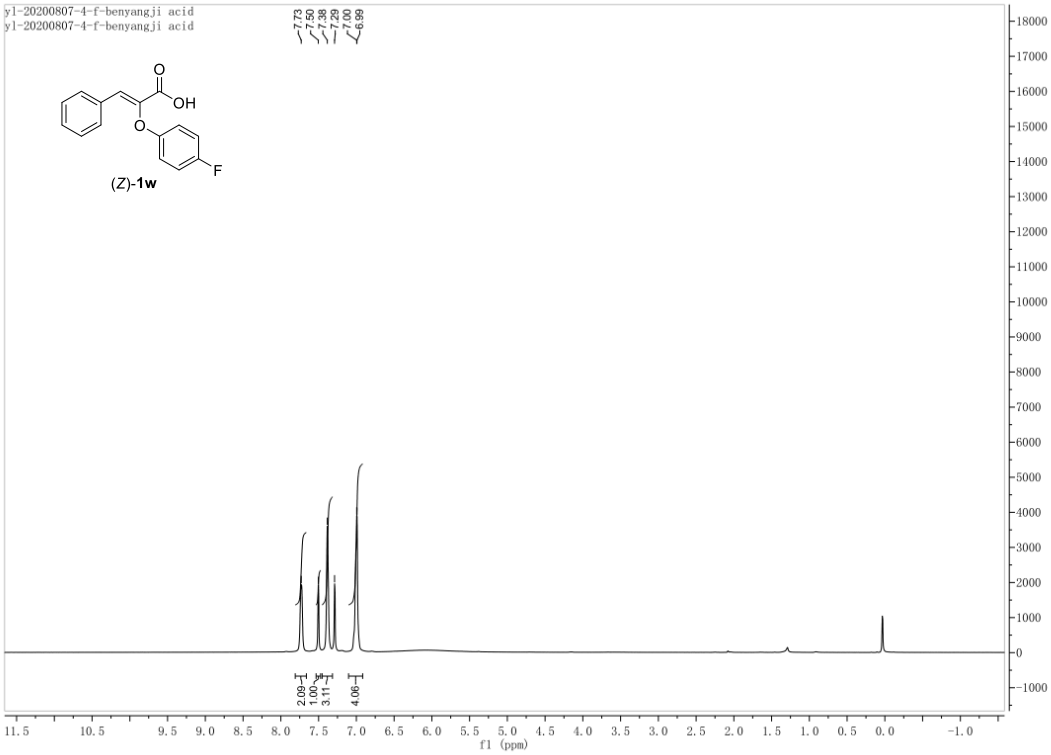

yl-20200808-2-thienyl acid C13
yl-20200808-2-thienyl acid C13
167.27
155.94
136.40
134.90
131.50
131.52
129.70
127.15
124.06
122.94
115.23
77.34
77.22
77.02
76.70
O
OH
S
O
(Z)-1r
f1 (ppm)

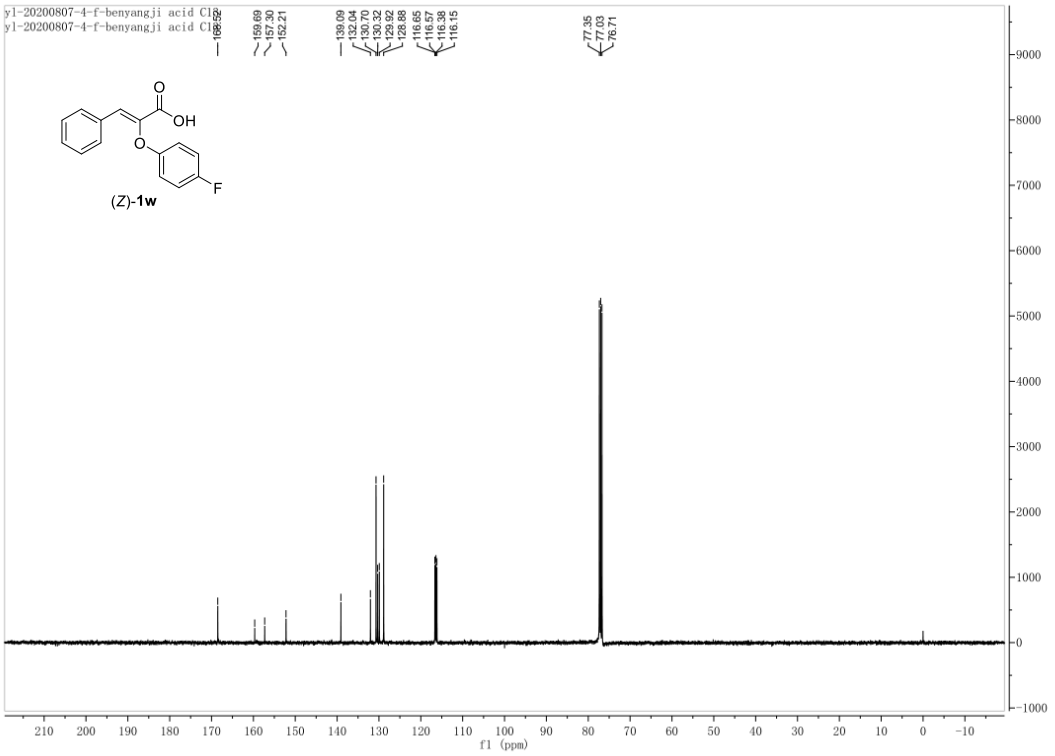

mhx-20191212-2-CH3-benyangji acid
mhx-20191212-2-CH3-benyangji acid
7.75
7.74
7.73
7.72
7.50
7.37
7.37
7.36
7.28
7.27
7.25
7.10
7.08
7.06
7.00
6.98
6.97
6.78
6.76
2.45
2.00
1.08
3.07
1.95
1.00
1.04
1.00
3.02
O
OH
O
(Z)-1s
f1 (ppm)

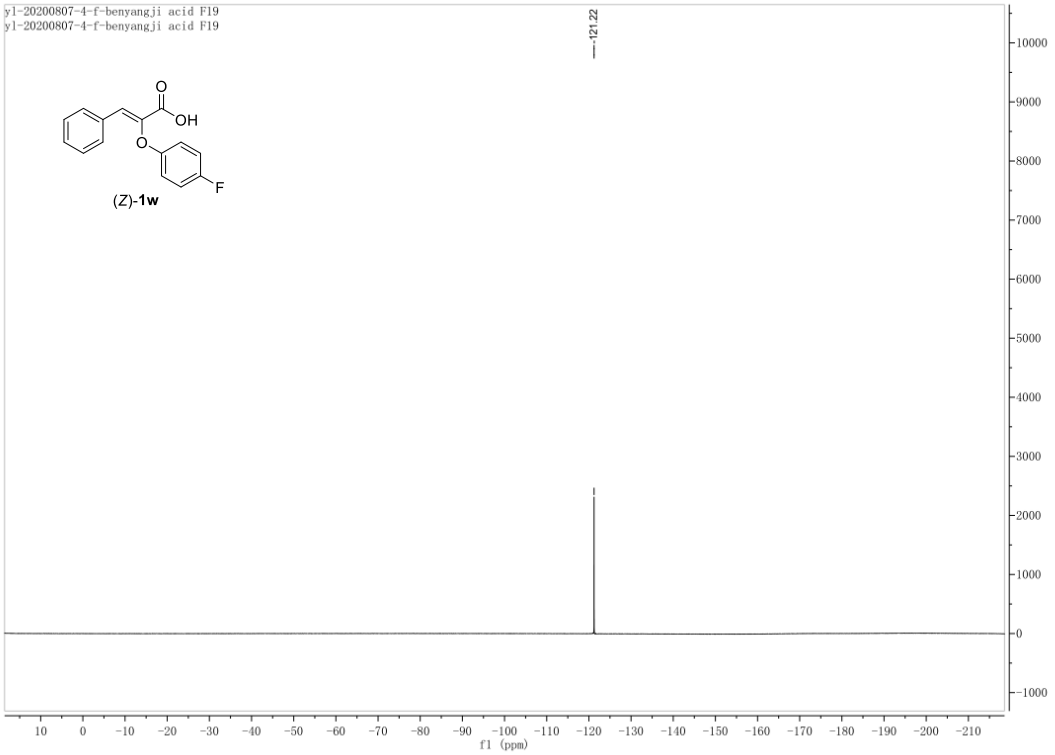

yl-20200827-3-ch3 oph acid
yl-20200827-3-ch3 oph acid
7.74
7.50
7.38
7.37
7.36
7.22
7.20
7.18
6.90
6.88
6.87
6.85
6.83
2.35
O
OH
O
(Z)-1t
1.94
1.44
3.26
1.05
3.01
3.00
f1 (ppm)

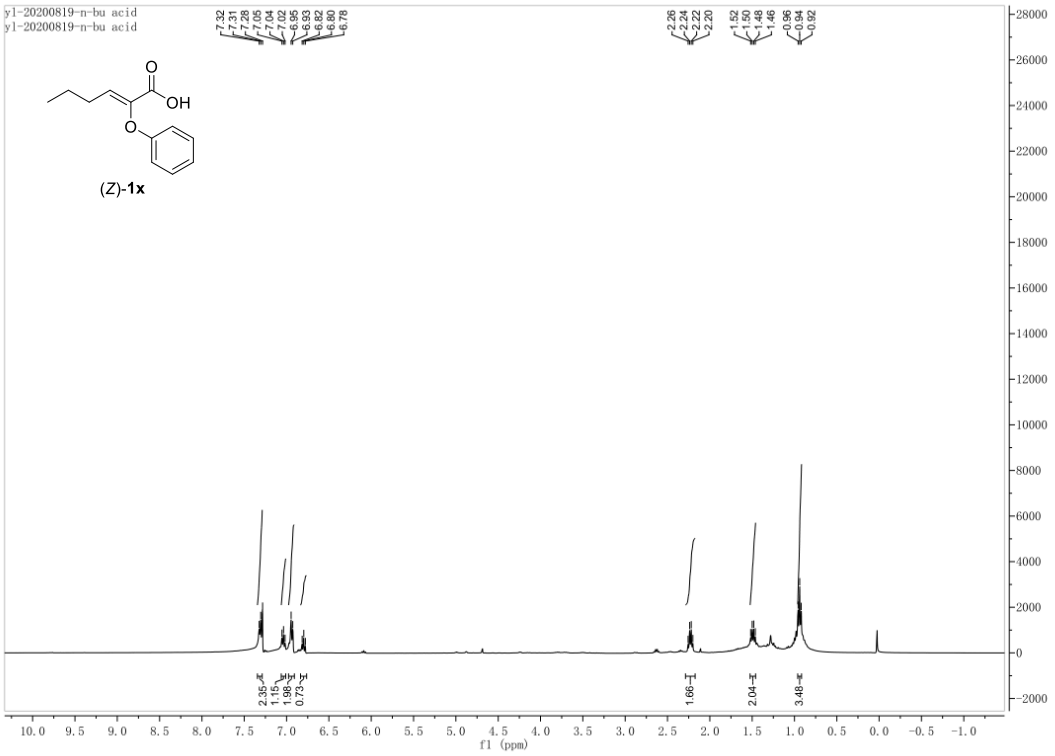

yl-20200819-4-me oph acid
yl-20200819-4-me oph acid
7.74
7.50
7.40
7.39
7.37
7.37
7.14
7.12
6.96
6.94
2.33
O
OH
O
(Z)-1u
2.16
1.07
3.00
2.04
1.99
2.97
f1 (ppm)

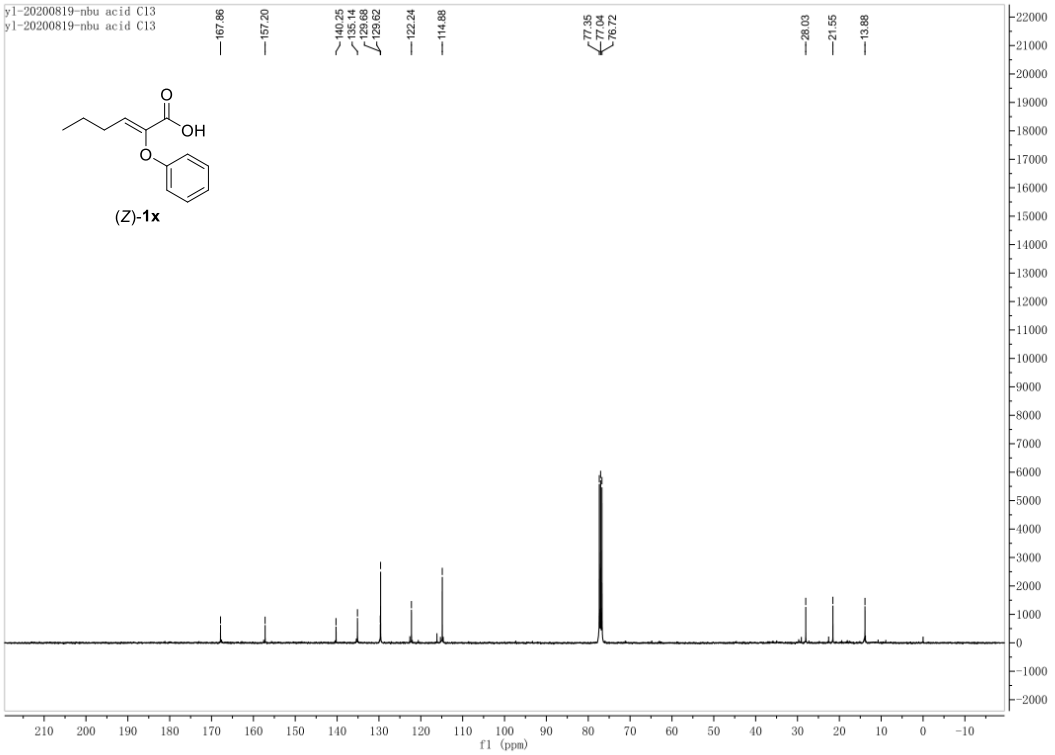

yl-20200806-4-cl-benyangji acid
yl-20200806-4-cl-benyangji acid
7.71
7.52
7.38
7.29
6.98
6.97
O
OH
O
Cl
(Z)-1v
2.09
1.00
5.85
1.99
f1 (ppm)

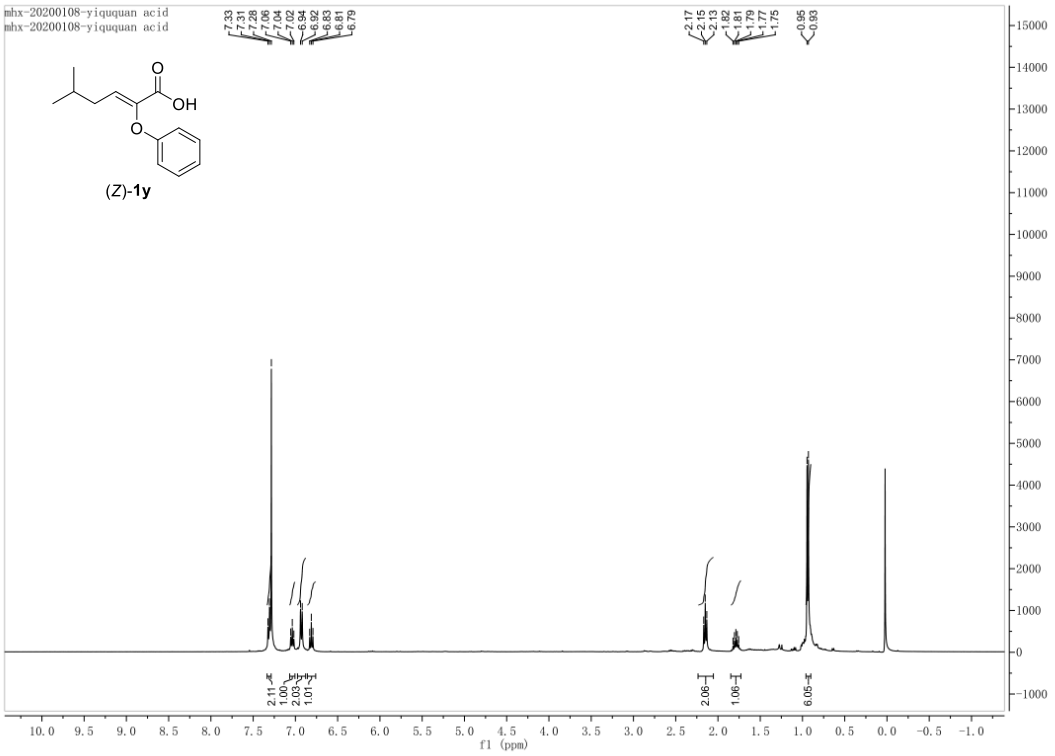

yl-20200807-4-f-benyangji acid
yl-20200807-4-f-benyangji acid
7.73
7.50
7.38
7.29
7.00
6.99
O
OH
O
F
(Z)-1w
2.09
1.00
3.11
4.06
f1 (ppm)

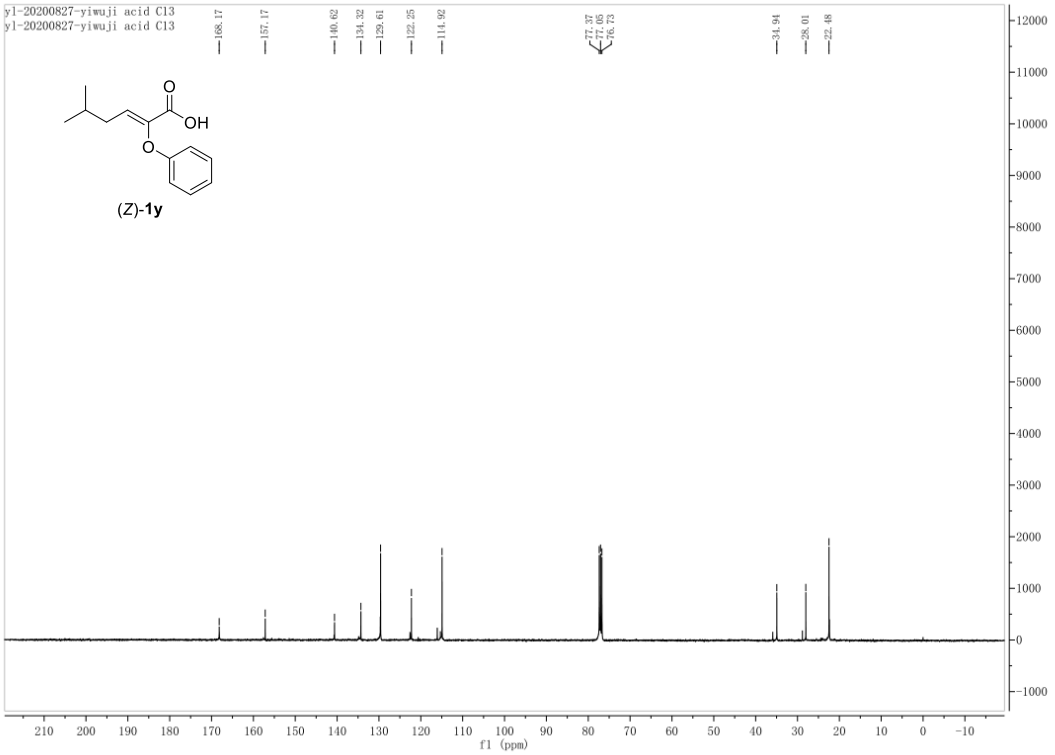

yl-20200807-4-f-benyangji acid C13
yl-20200807-4-f-benyangji acid C13
168.52
159.69
157.30
152.21
139.09
132.04
130.70
130.32
129.90
128.88
116.65
116.57
116.38
116.15
77.35
77.03
76.71
O
OH
O
F
(Z)-1w
f1 (ppm)

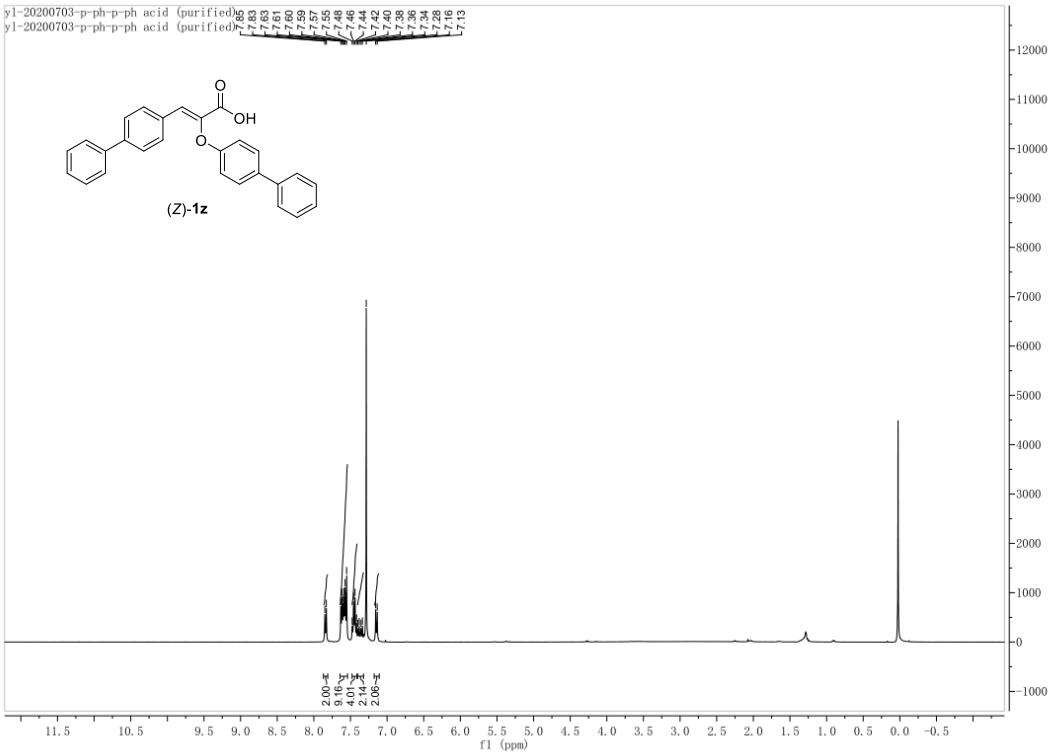

yl-20200807-4-f-benyangji acid F19
yl-20200807-4-f-benyangji acid F19
-121.22
O
OH
O
F
(Z)-1w
f1 (ppm)

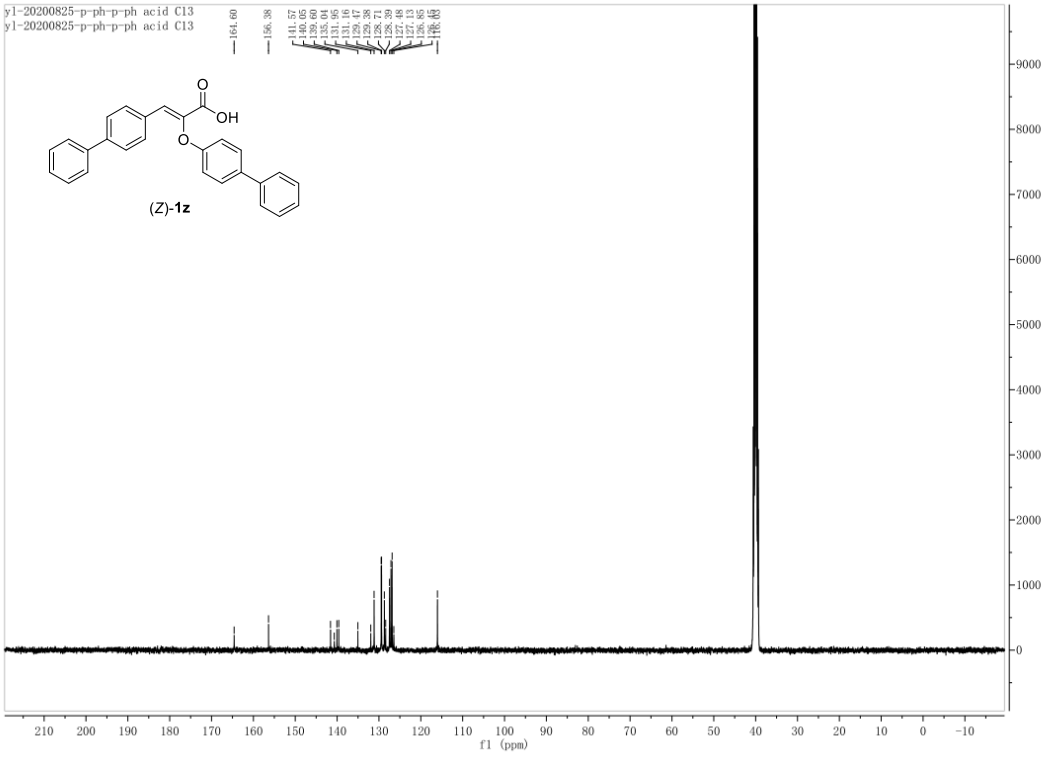

yl-20200819-n-bu acid
yl-20200819-n-bu acid
7.32
7.31
7.28
7.05
7.04
7.02
6.95
6.93
6.82
6.80
6.78
2.26
2.24
2.22
2.20
1.52
1.50
1.48
1.46
0.96
0.94
0.92
O
OH
O
(Z)-1x
2.35
1.15
1.98
0.73
1.66
2.04
3.48
f1 (ppm)


yl-20200819-nbu acid C13
yl-20200819-nbu acid C13
167.86
157.20
140.25
135.14
129.68
129.62
122.24
114.88
77.35
77.04
76.72
28.03
21.55
13.88
O
OH
O
(Z)-1x
f1 (ppm)

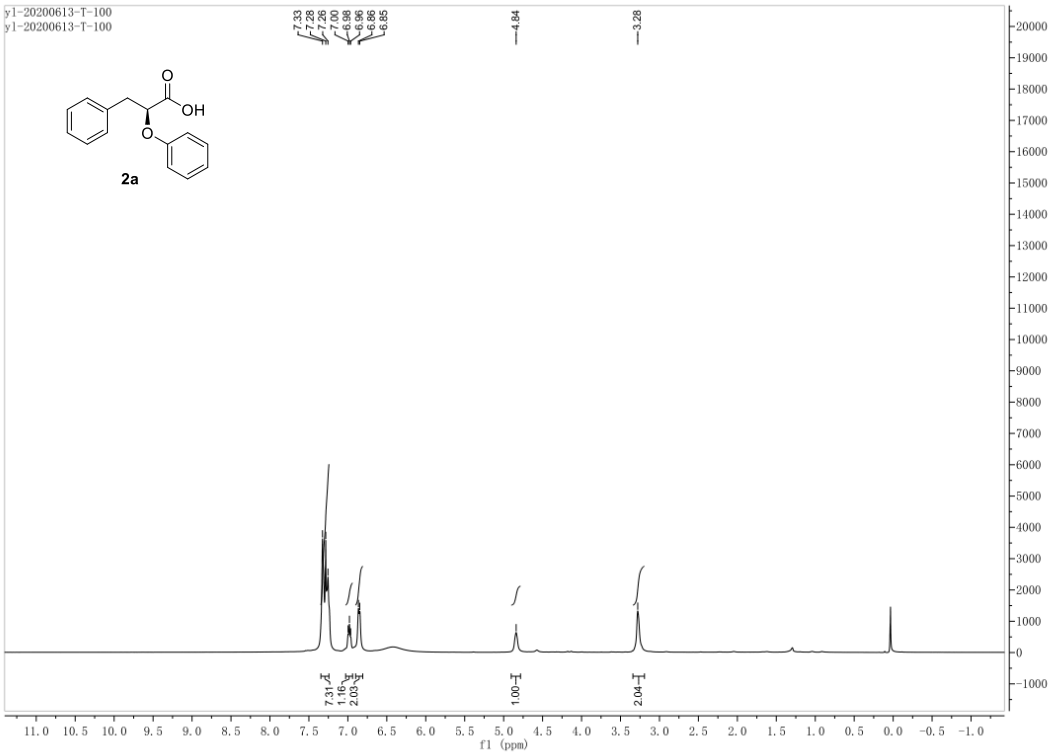

mhx-20200108-yiququan acid
mhx-20200108-yiququan acid
7.33
7.31
7.28
7.06
7.04
7.02
6.94
6.92
6.83
6.81
6.79
2.17
2.15
2.13
1.82
1.81
1.79
1.77
1.75
0.95
0.93
O
OH
O
(Z)-1y
2.11
1.00
2.03
1.01
2.06
1.06
6.05
f1 (ppm)

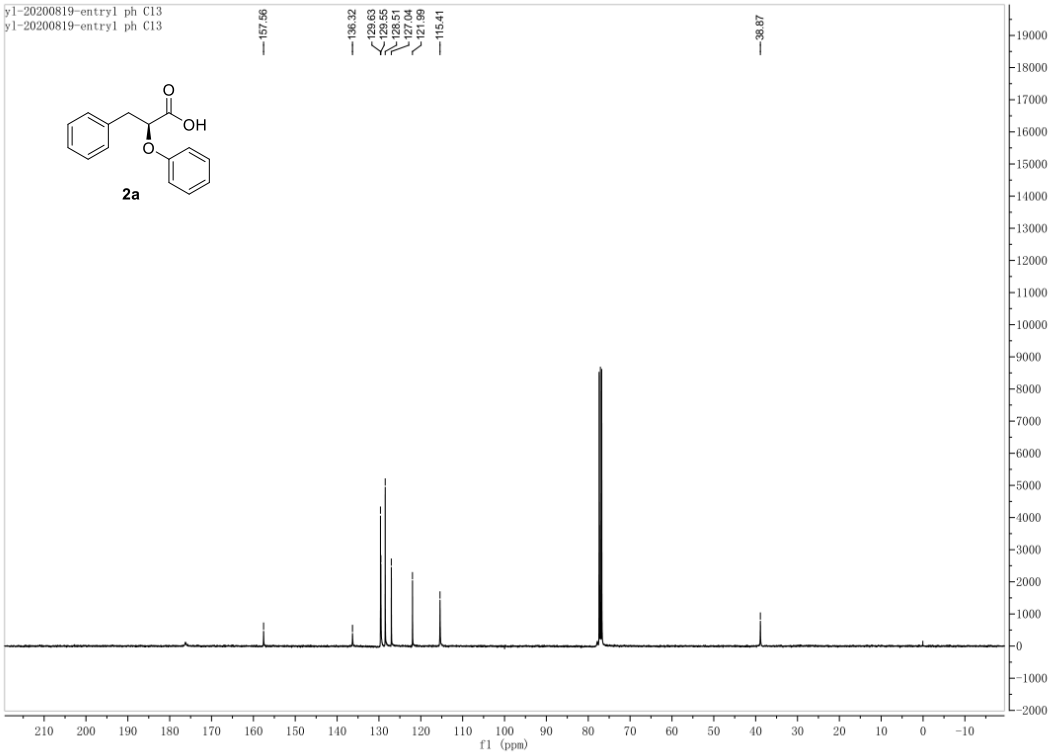

yl-20200827-yiwuji acid C13
yl-20200827-yiwuji acid C13
168.17
157.17
140.62
134.32
129.61
122.25
114.92
77.37
77.05
76.73
34.94
28.01
22.48
O
OH
O
(Z)-1y
f1 (ppm)

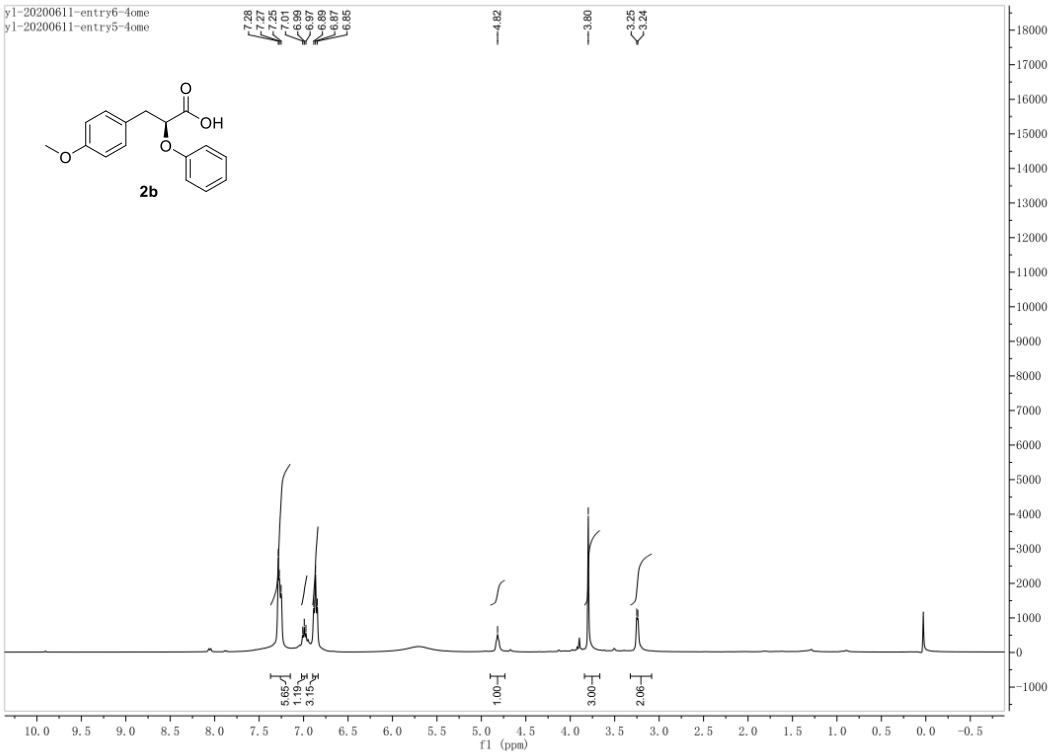


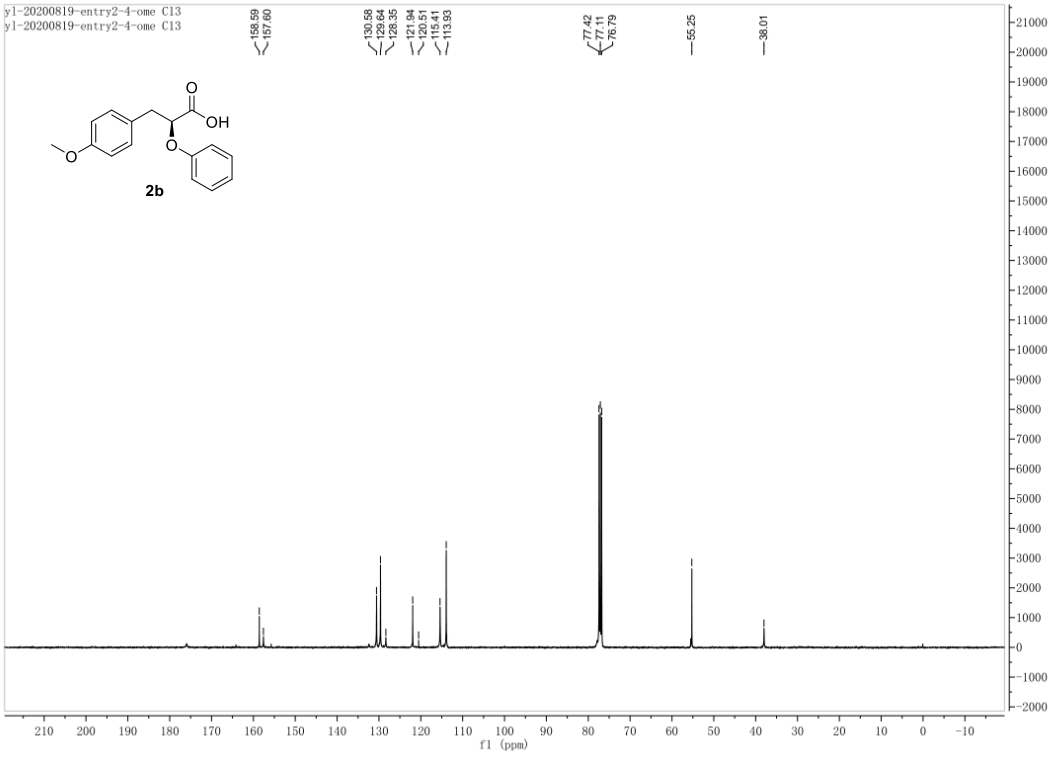


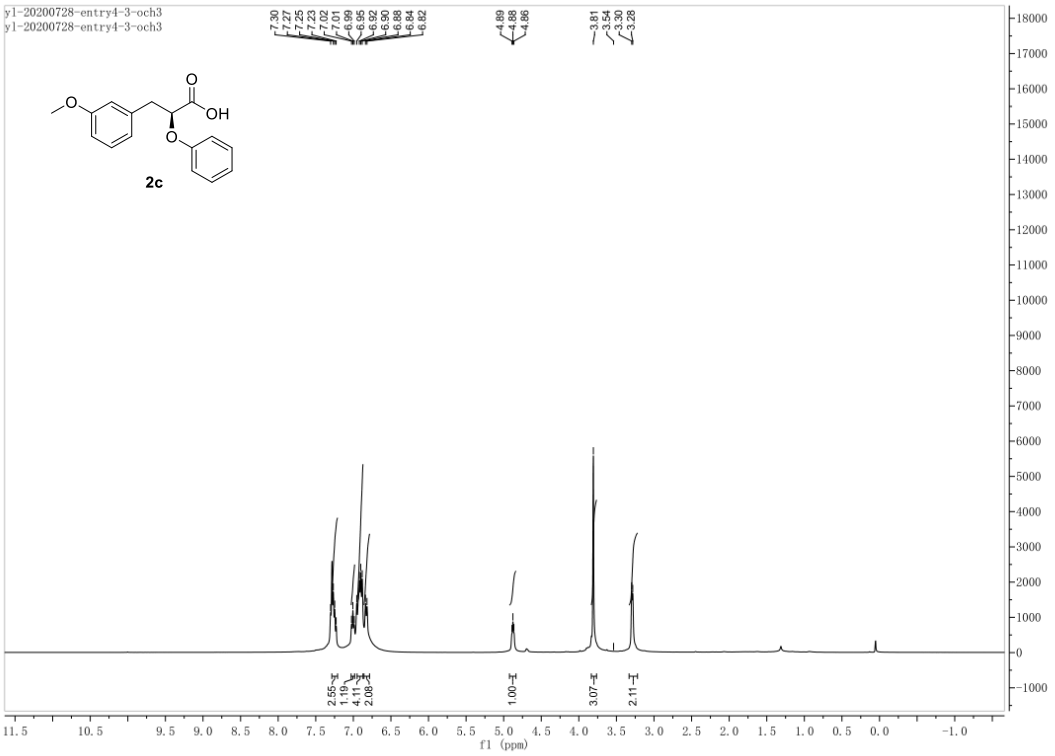
3.2 NMR spectra of chiral products

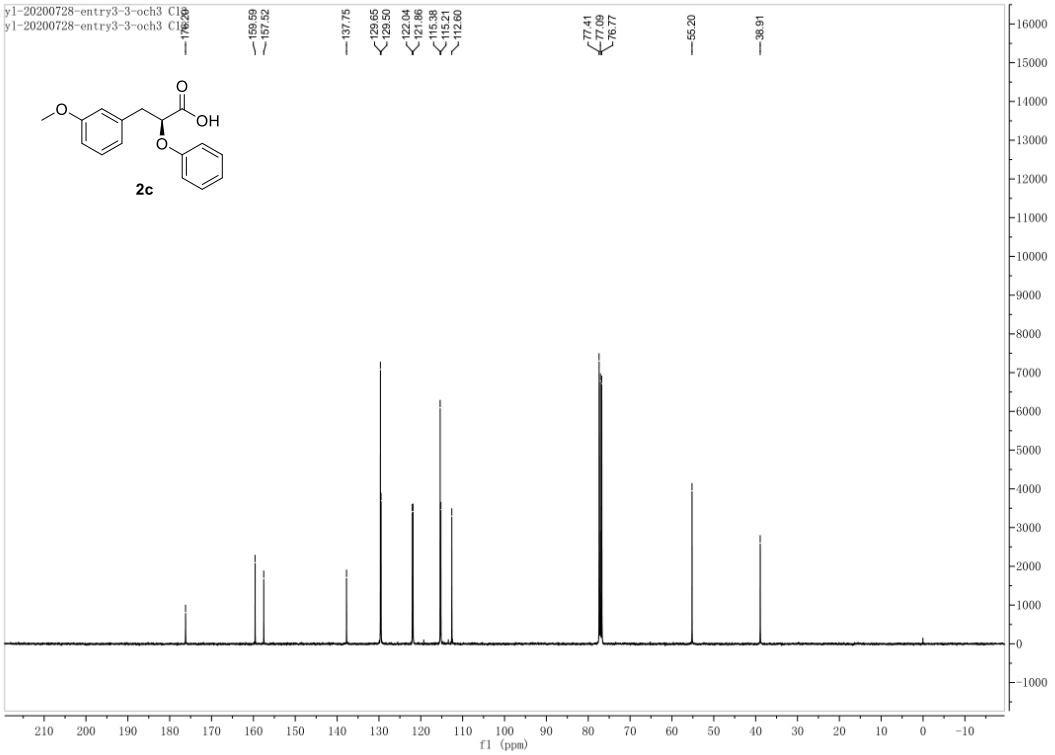

yl-20200613-T-100
yl-20200613-T-100
7.33
7.28
7.26
7.00
6.98
6.96
6.86
6.85
4.84
3.28
O
OH
O
2a
7.31
1.16
2.03
1.00
2.04
f1 (ppm)

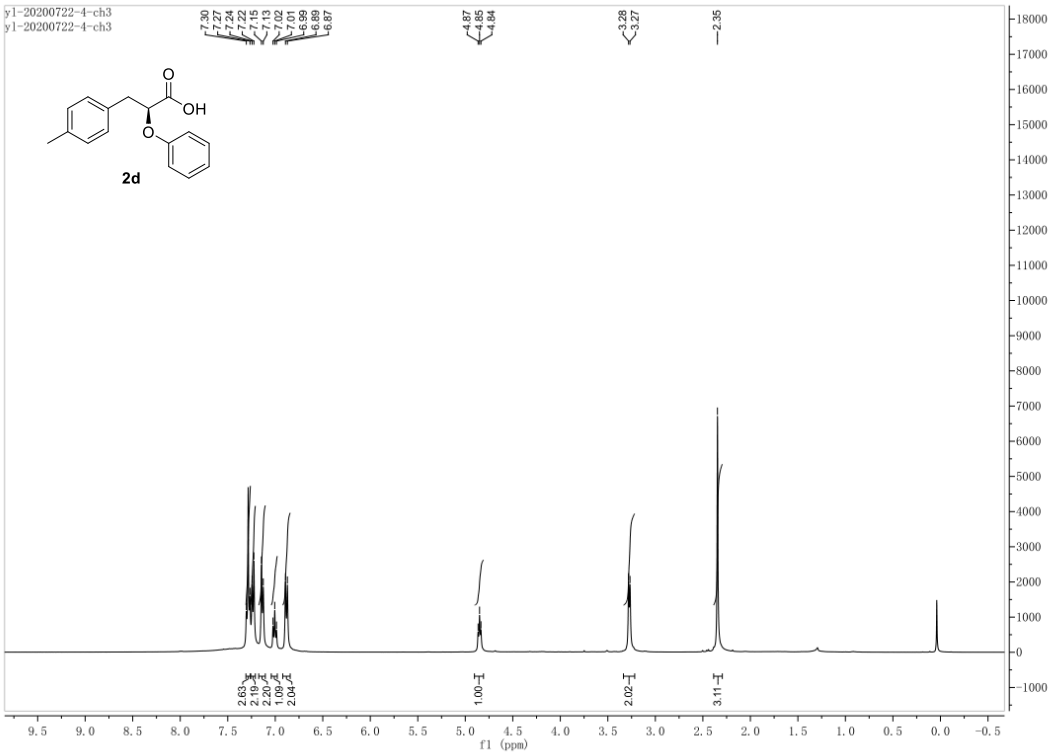

yl-20200819-entryl ph C13
yl-20200819-entryl ph C13
157.56
136.32
129.63
129.55
128.51
127.04
121.99
115.41
38.87
O
OH
O
2a
f1 (ppm)


yl-20200611-entry6-4ome
yl-20200611-entry5-4ome
7.28
7.27
7.25
7.01
6.99
6.97
6.89
6.87
6.85
4.82
3.80
3.25
3.24
O
OH
O
O
2b
5.65
1.19
3.15
1.00
3.00
2.06
f1 (ppm)


yl-20200819-entry2-4-ome C13
yl-20200819-entry2-4-ome C13
158.59
157.60
130.58
129.64
128.35
121.94
120.51
115.41
113.93
77.42
77.11
76.79
55.25
38.01
O
OH
O
O
2b
f1 (ppm)


yl-20200728-entry4-3-och3
yl-20200728-entry4-3-och3
7.30
7.27
7.25
7.23
7.02
7.01
6.99
6.95
6.92
6.90
6.88
6.84
6.82
4.89
4.88
4.86
3.81
3.54
3.30
3.28
O
OH
O
O
2c
2.55
1.19
4.11
2.08
1.00
3.07
2.11
f1 (ppm)


yl-20200728-entry3-3-och3 Cl
yl-20200728-entry3-3-och3 Cl
176.20
159.59
157.52
137.75
129.65
129.50
122.04
121.86
115.38
115.21
112.60
77.41
77.09
76.77
55.20
38.91
O
OH
O
O
2c
f1 (ppm)


y1-20200722-4-ch3
y1-20200722-4-ch3
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7.27
7.24
7.22
7.15
7.13
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7.01
6.99
6.89
6.87
4.87
4.85
4.84
3.28
3.27
2.35
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O
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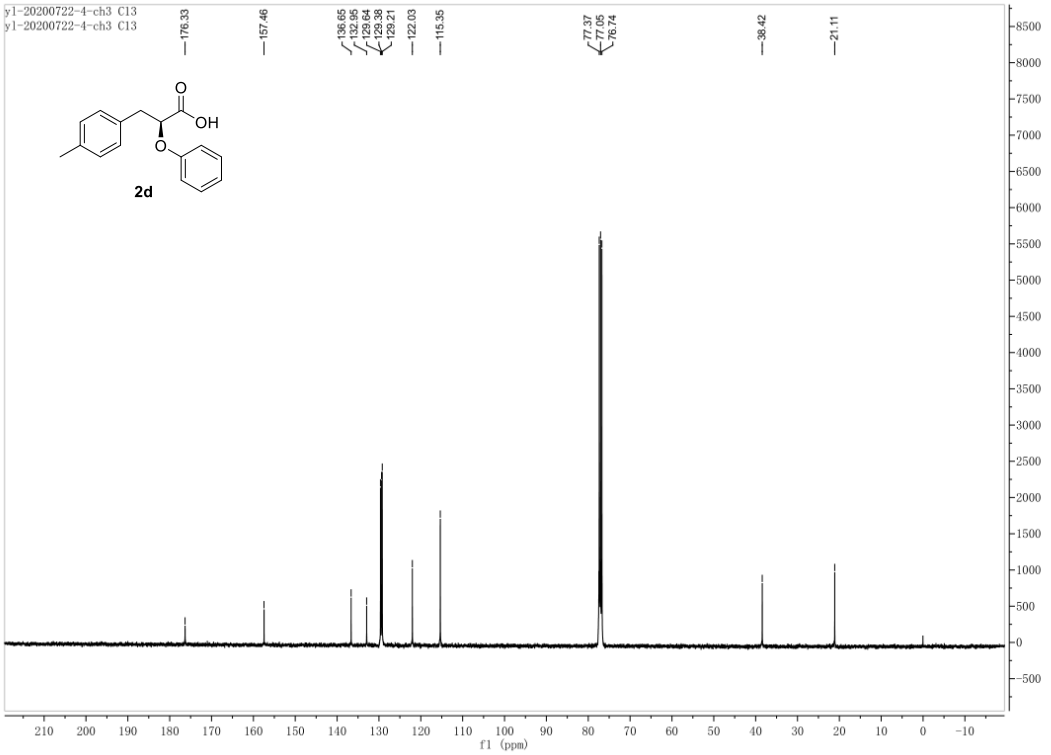
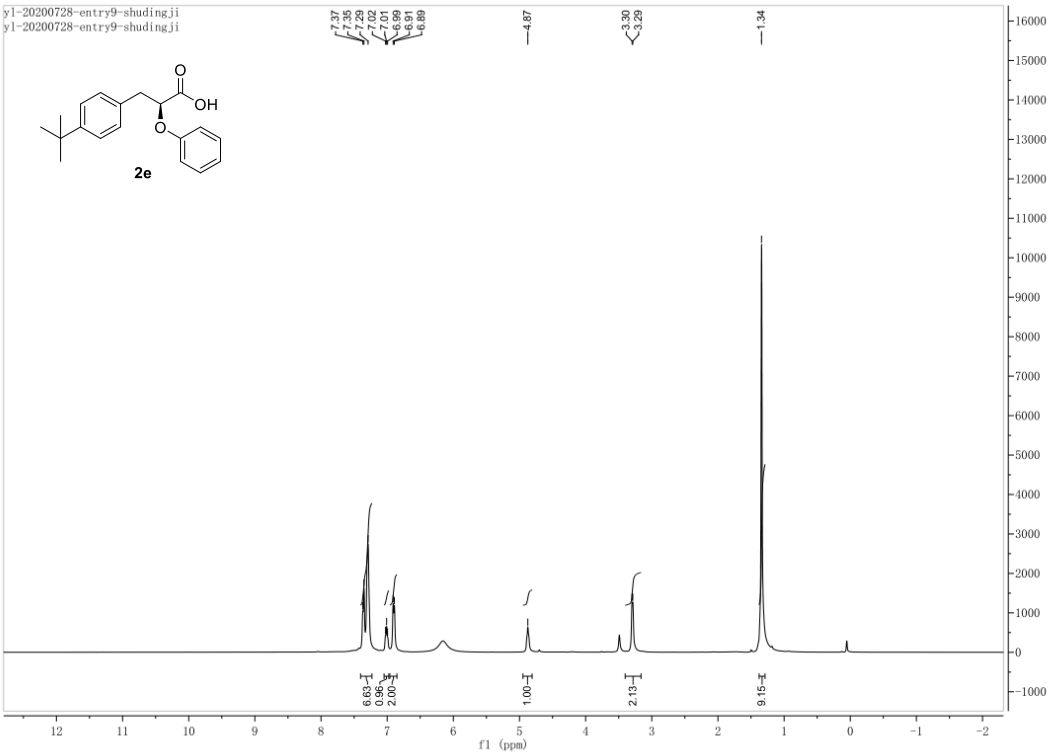
2.63
2.19
2.20
1.09
2.04
1.00
2.02
3.11
f1 (ppm)


y1-20200722-4-ch3 C13
y1-20200722-4-ch3 C13
176.33
157.46
136.65
132.95
129.64
129.38
129.21
122.03
115.35
77.37
77.05
76.74
38.42
21.11
OH
O
O
2d
f1 (ppm)


yl-20200728-entry9-shudingji
yl-20200728-entry9-shudingji
7.37
7.35
7.29
7.02
7.01
6.99
6.91
6.89
4.87
3.30
3.29
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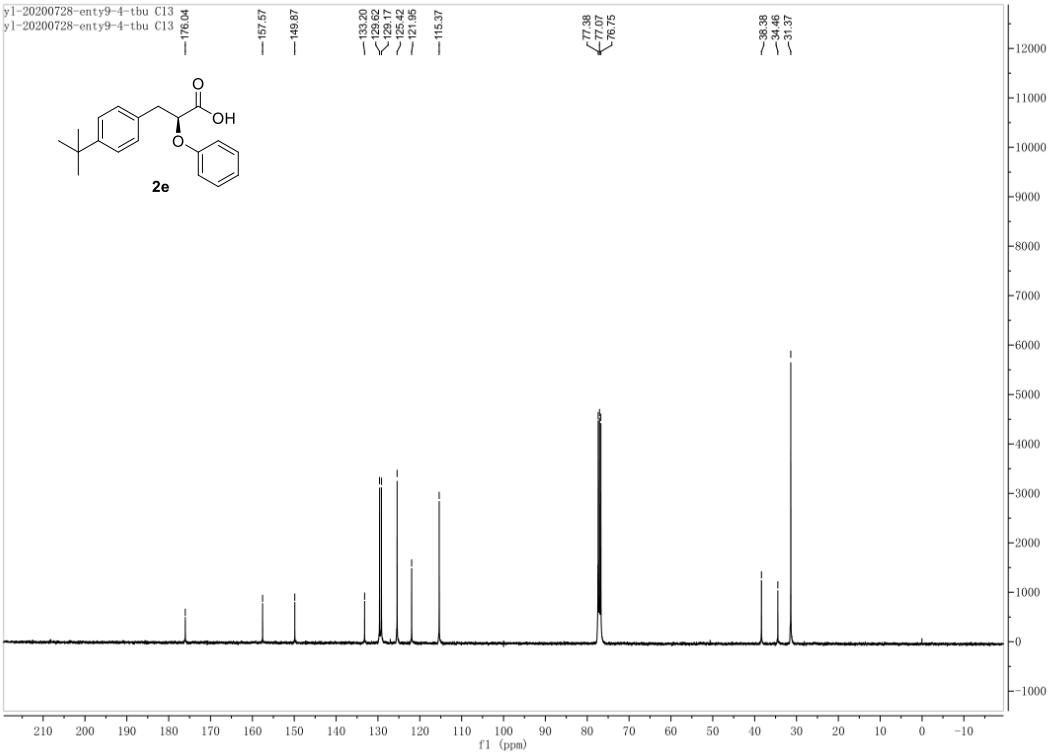
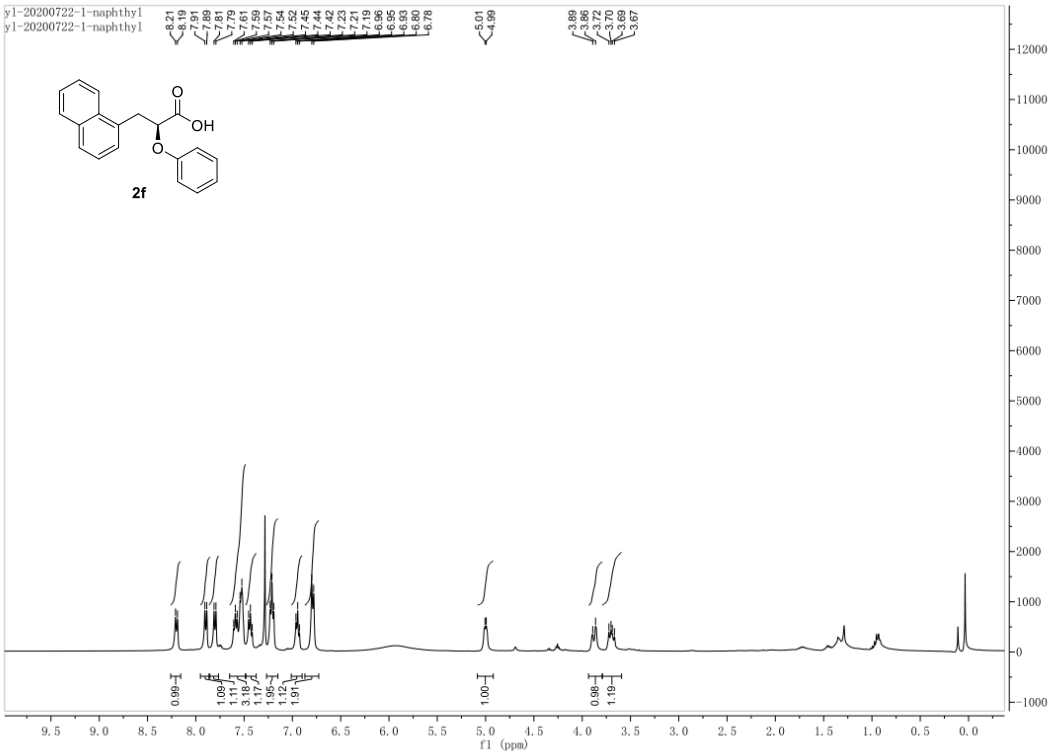
OH
O
O
2e
6.63
0.96
2.00
1.00
2.13
9.15
f1 (ppm)


yl-20200728-enty9-4-tbu C13
yl-20200728-enty9-4-tbu C13
176.04
157.57
149.87
133.20
129.62
129.17
125.42
121.95
115.37
77.38
77.07
76.75
38.38
34.46
31.37
OH
O
O
2e
f1 (ppm)


yl-20200722-1-naphthyl
yl-20200722-1-naphthyl
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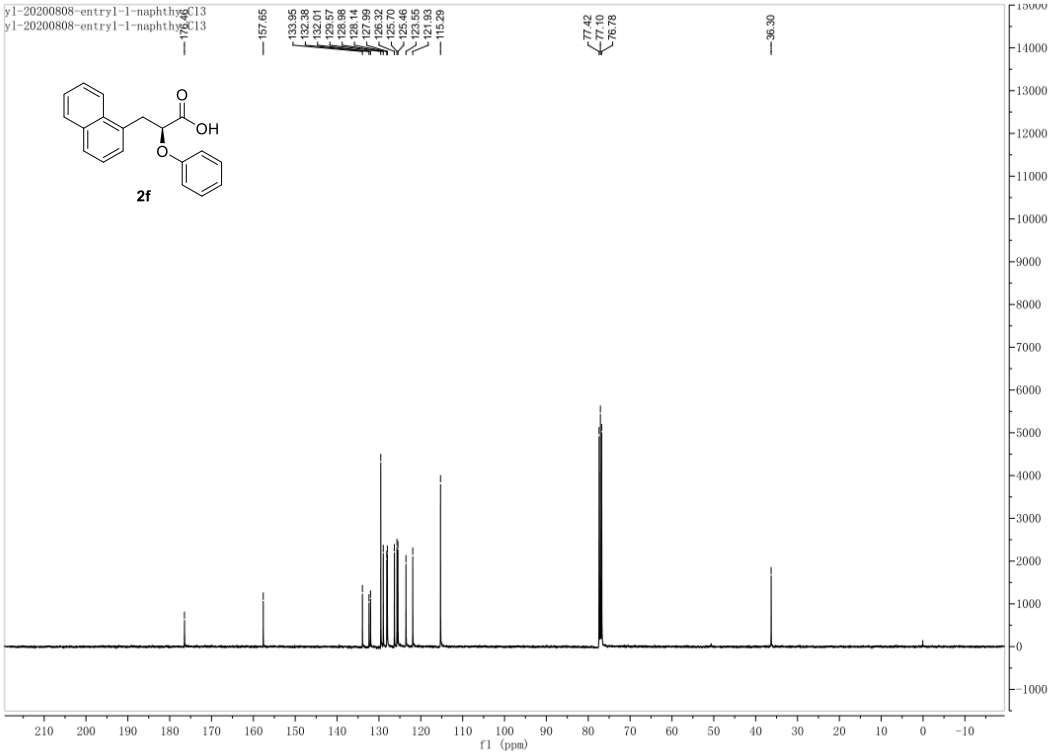
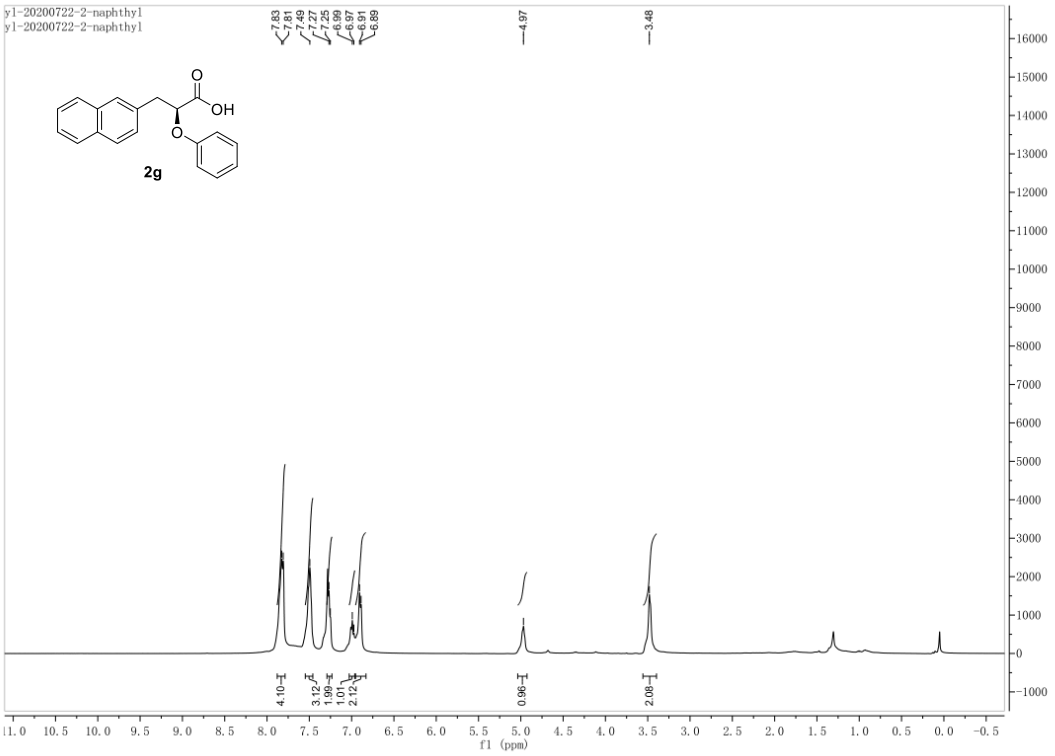
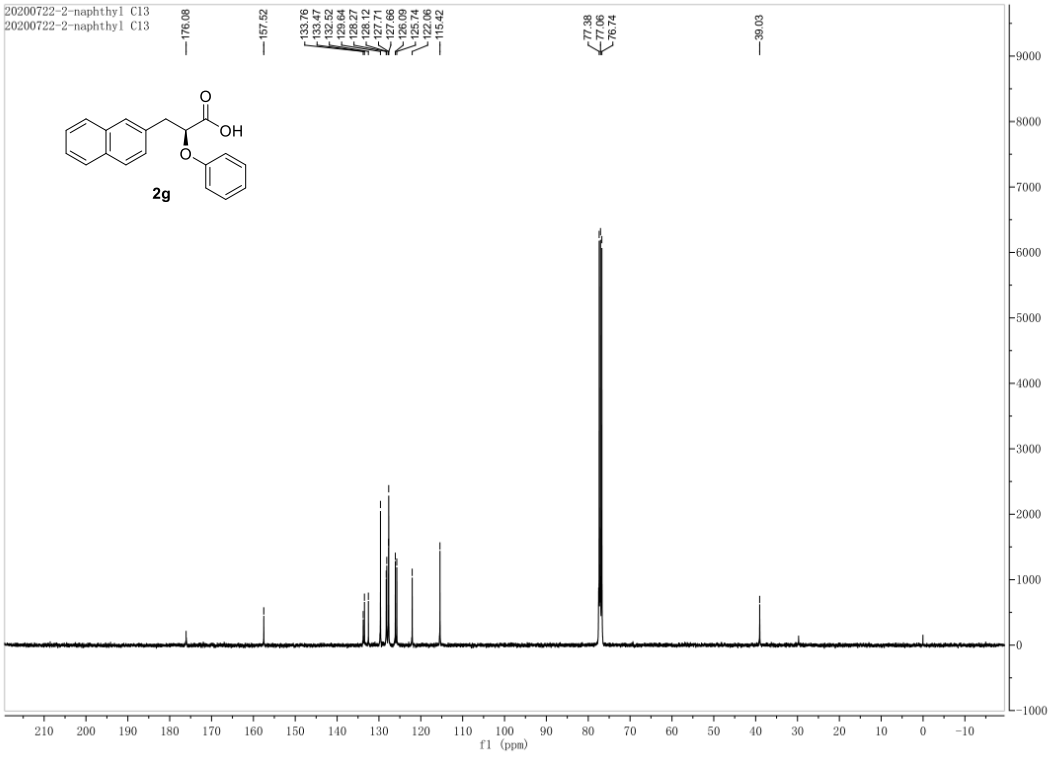
8.19
7.91
7.89
7.81
7.79
7.61
7.59
7.57
7.54
7.52
7.45
7.44
7.42
7.23
7.21
7.19
6.96
6.95
6.93
6.80
6.78
5.01
4.99
3.89
3.86
3.72
3.70
3.69
3.67
O
OH
O
2f
0.99
1.09
1.11
3.18
1.17
1.95
1.12
1.91
1.00
0.98
1.19
f1 (ppm)


yl-20200808-entryl-1-naphthyl-C13
yl-20200808-entryl-1-naphthyl-C13
178.49
157.65
133.95
132.38
132.01
129.57
128.98
128.14
127.99
126.32
125.70
125.46
123.55
121.93
115.29
77.42
77.10
76.78
36.30
O
OH
O
2f
f1 (ppm)


y1-20200722-2-naphthyl
y1-20200722-2-naphthyl
7.83
7.81
7.49
7.27
7.25
6.99
6.97
6.91
6.89
4.97
3.48
O
OH
O
2g
4.10
3.12
1.99
1.01
2.12
0.96
2.08
f1 (ppm)


20200722-2-naphthyl C13
20200722-2-naphthyl C13
176.08
157.52
133.76
133.47
132.52
129.64
128.27
128.12
127.71
127.66
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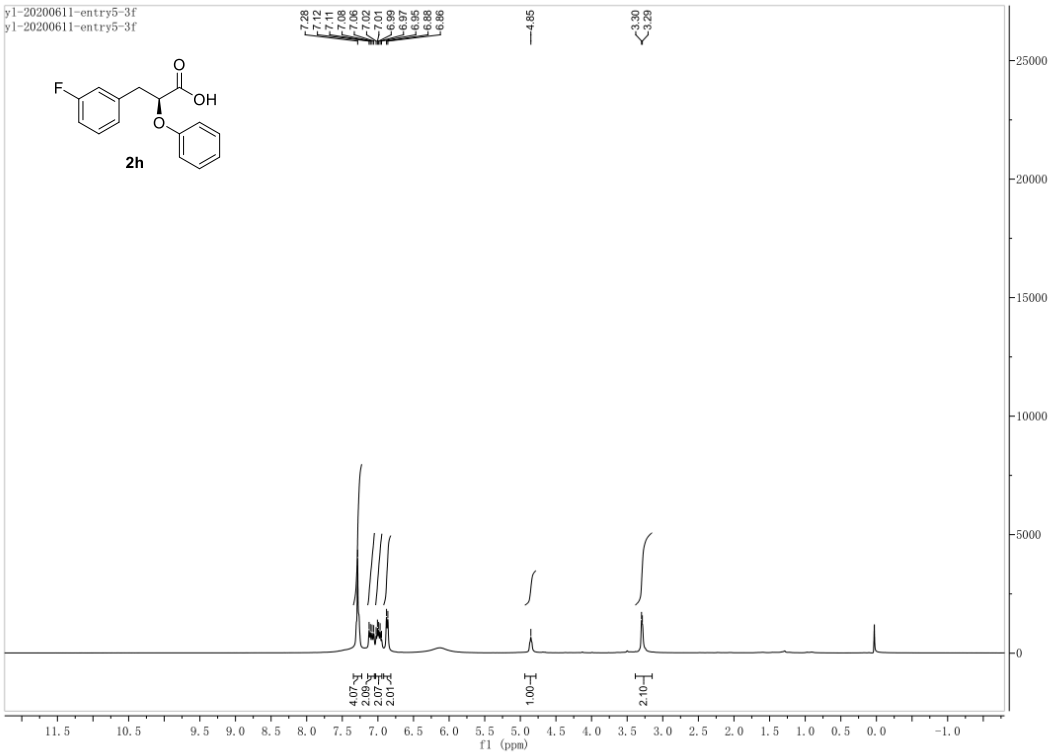
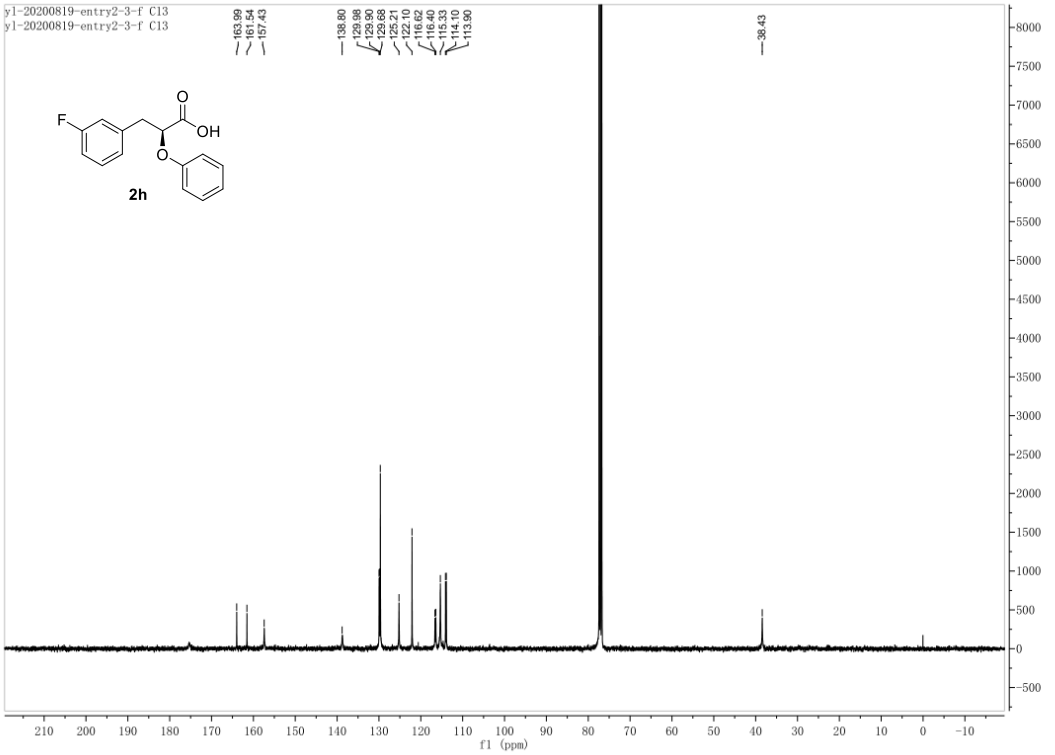
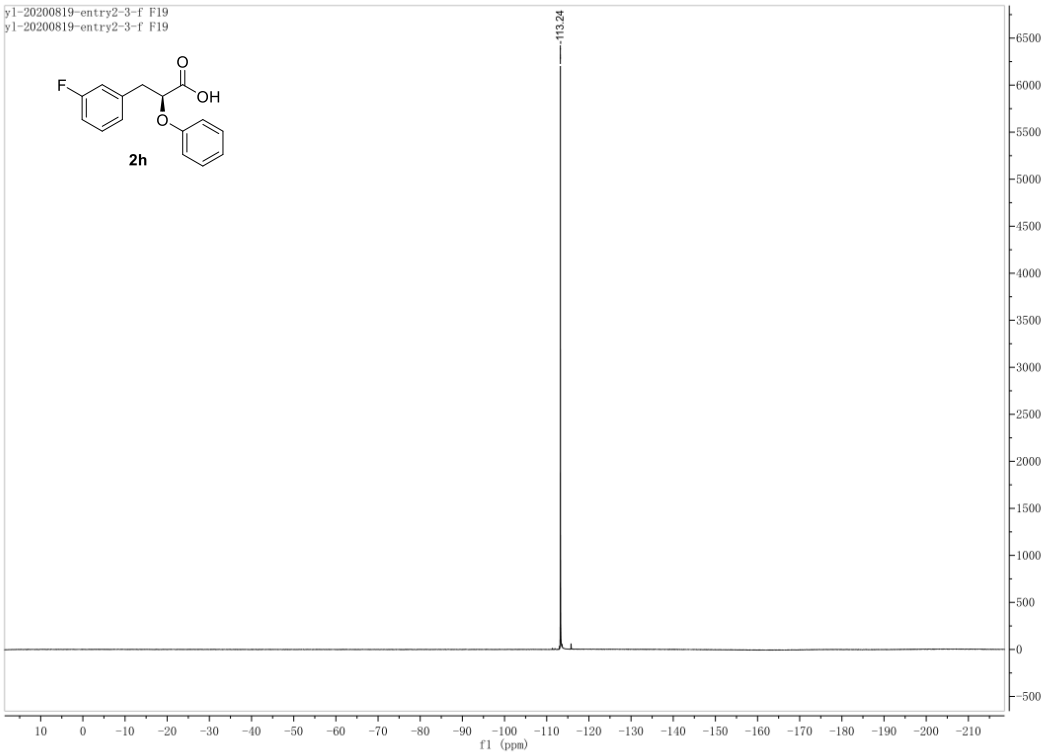
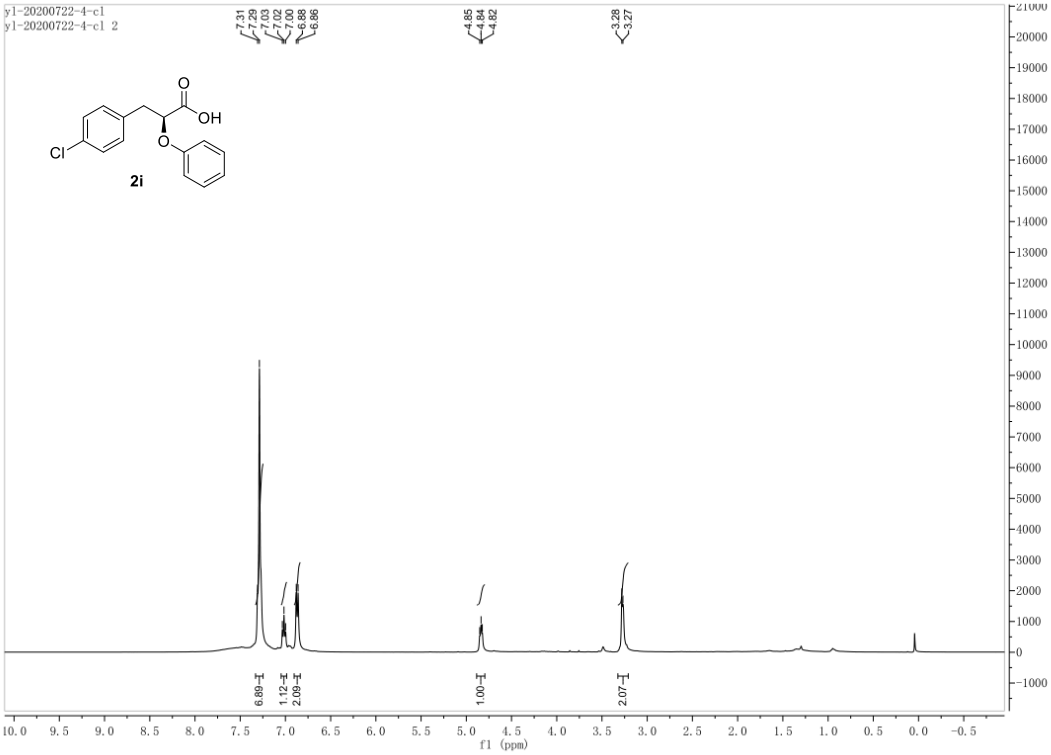
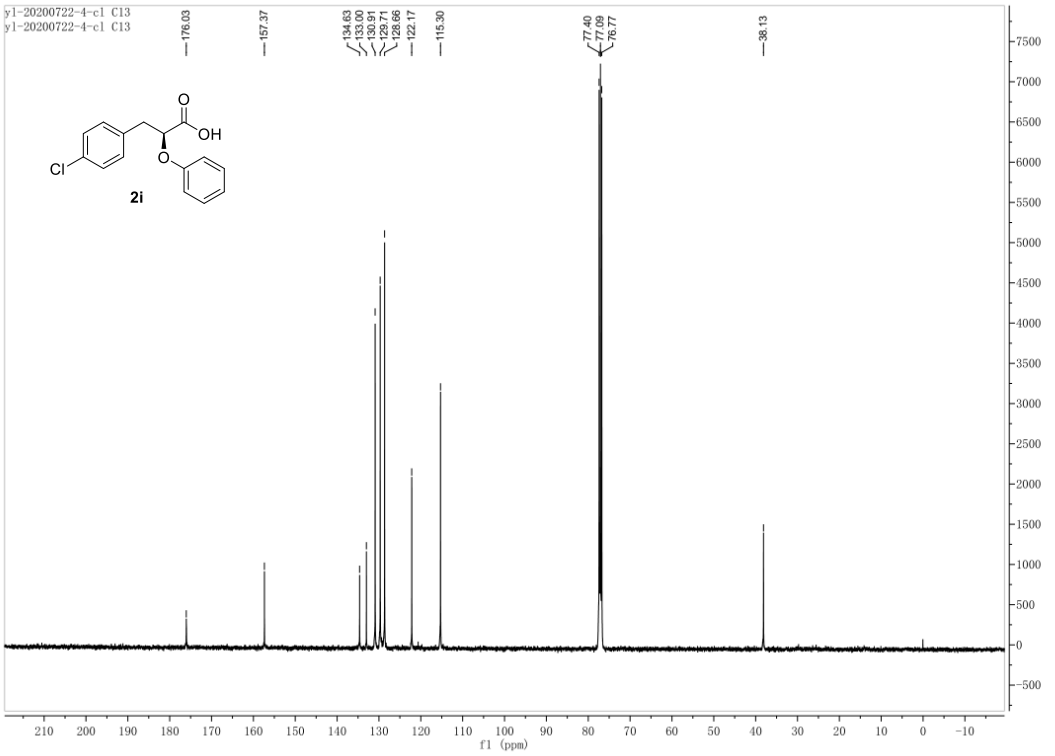
122.06
115.42
77.38
77.06
76.74
39.03
O
OH
O
2g
f1 (ppm)

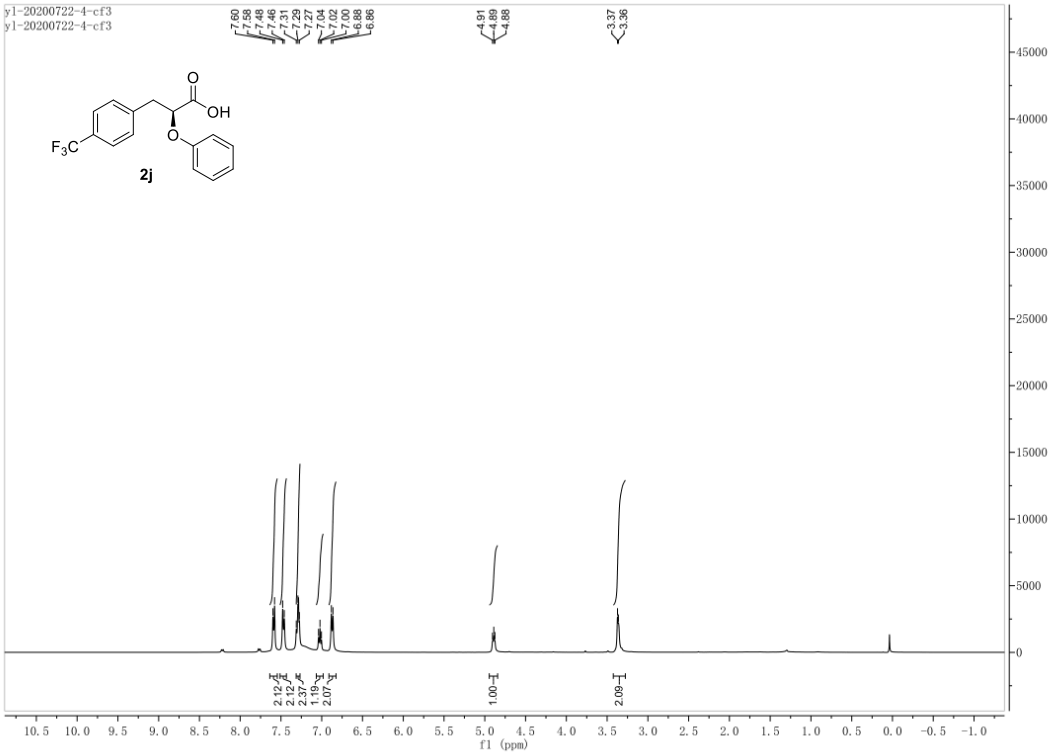

yl-20200611-entry5-3f
yl-20200611-entry5-3f
7.28
7.12
7.11
7.08
7.06
7.02
7.01
6.99
6.97
6.95
6.88
6.86
4.85
3.30
3.29
F
O
OH
O
2h
4.07
2.09
2.07
2.01
1.00
2.10
fl (ppm)

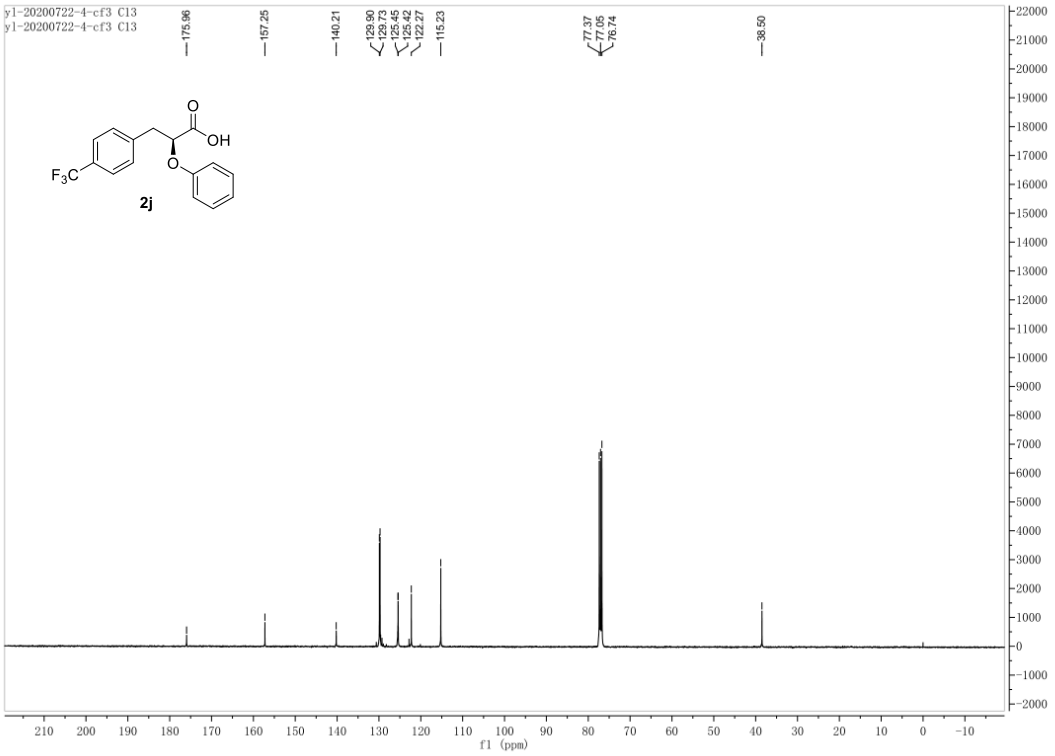

yl-20200819-entry2-3-f C13
yl-20200819-entry2-3-f C13
163.99
161.54
157.43
138.80
129.98
129.90
129.68
125.21
122.10
116.62
116.40
115.33
114.10
113.90
38.43
F
O
OH
O
2h
fl (ppm)


yl-20200819-entry2-3-f F19
yl-20200819-entry2-3-f F19
-113.24
F
O
OH
O
2h
f1 (ppm)


yl-20200722-4-cl
yl-20200722-4-cl 2
7.31
7.29
7.03
7.02
7.00
6.88
6.86
4.85
4.84
4.82
3.28
3.27
Cl
O
OH
O
2i
6.89
1.12
2.09
1.00
2.07
f1 (ppm)


yl-20200722-4-cl C13
yl-20200722-4-cl C13
176.03
157.37
134.63
133.00
130.91
129.71
128.66
122.17
115.30
77.40
77.09
76.77
38.13
O
OH
Cl
O
2i
f1 (ppm)


yl-20200722-4-cf3
yl-20200722-4-cf3
7.60
7.59
7.48
7.46
7.31
7.29
7.27
7.04
7.02
7.00
6.88
6.86
4.91
4.89
4.88
3.37
3.36
O
OH
F3C
O
2j
2.12
2.12
2.37
1.19
2.07
1.00
2.09
f1 (ppm)


yl-20200722-4-cf3 C13
yl-20200722-4-cf3 C13
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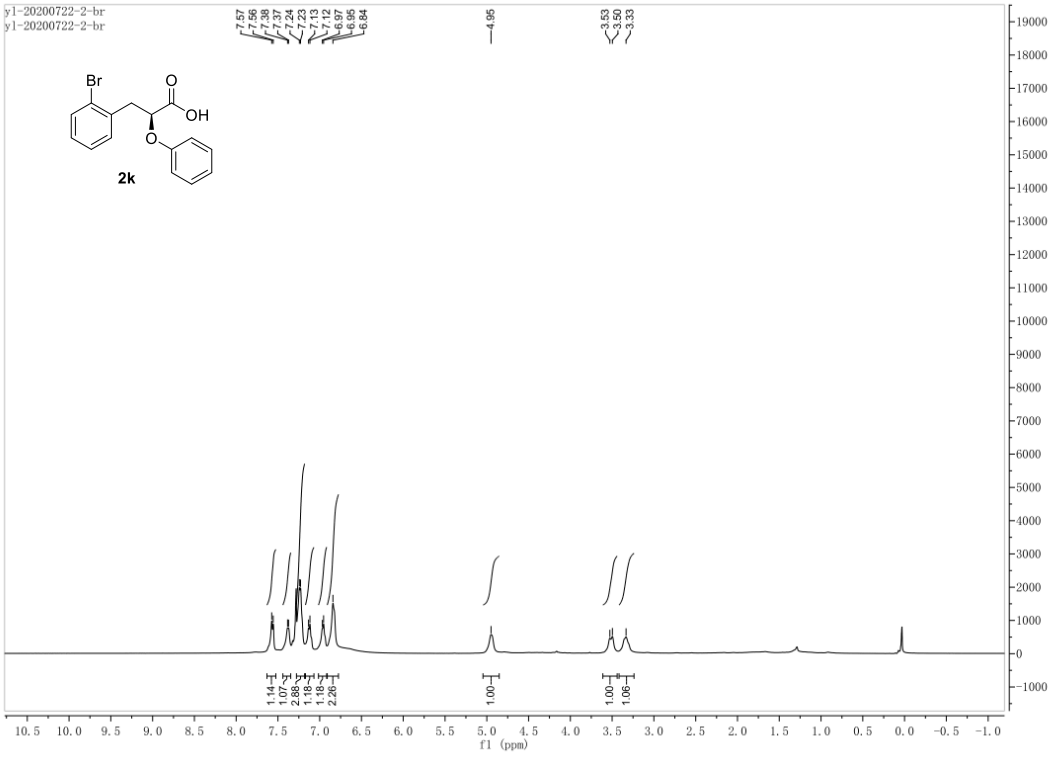
157.25
140.21
129.90
129.73
125.45
125.42
122.27
115.23
77.37
77.05
76.74
38.50
O
OH
F3C
O
2j
f1 (ppm)


yl-20200722-2-br
yl-20200722-2-br
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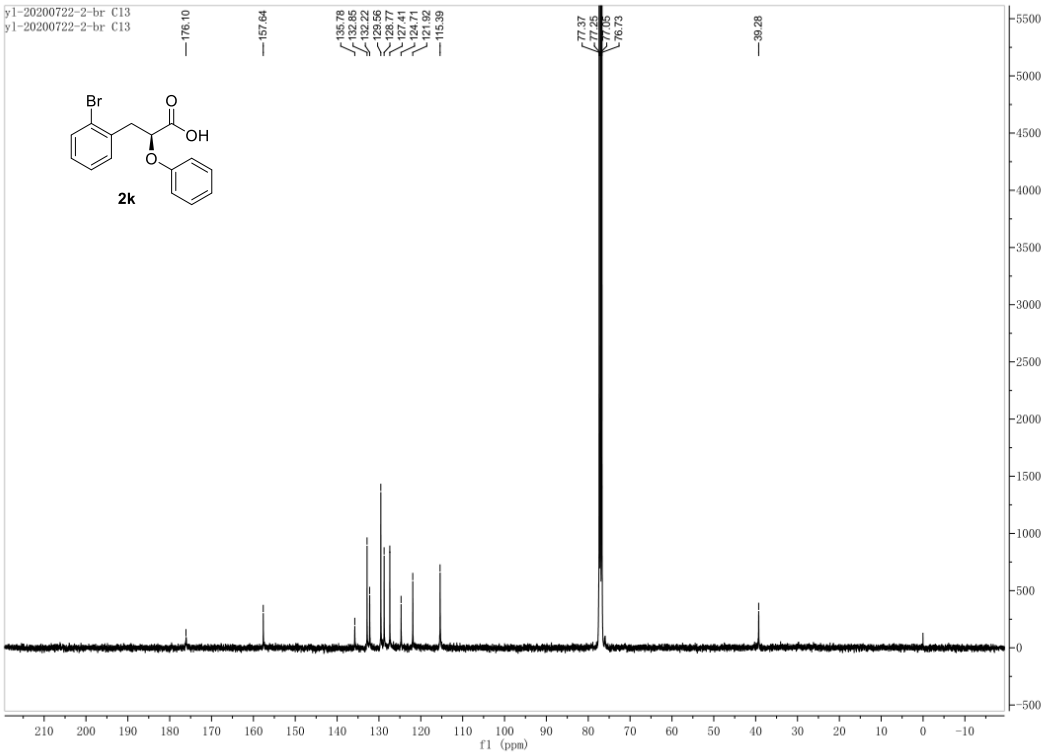
7.56
7.38
7.37
7.24
7.23
7.13
7.12
6.97
6.95
6.84
4.95
3.53
3.50
3.33
Br
O
OH
O
2k
1.14
1.07
2.88
1.18
1.18
2.28
1.00
1.00
1.06
f1 (ppm)


yl-20200722-2-br C13
yl-20200722-2-br C13
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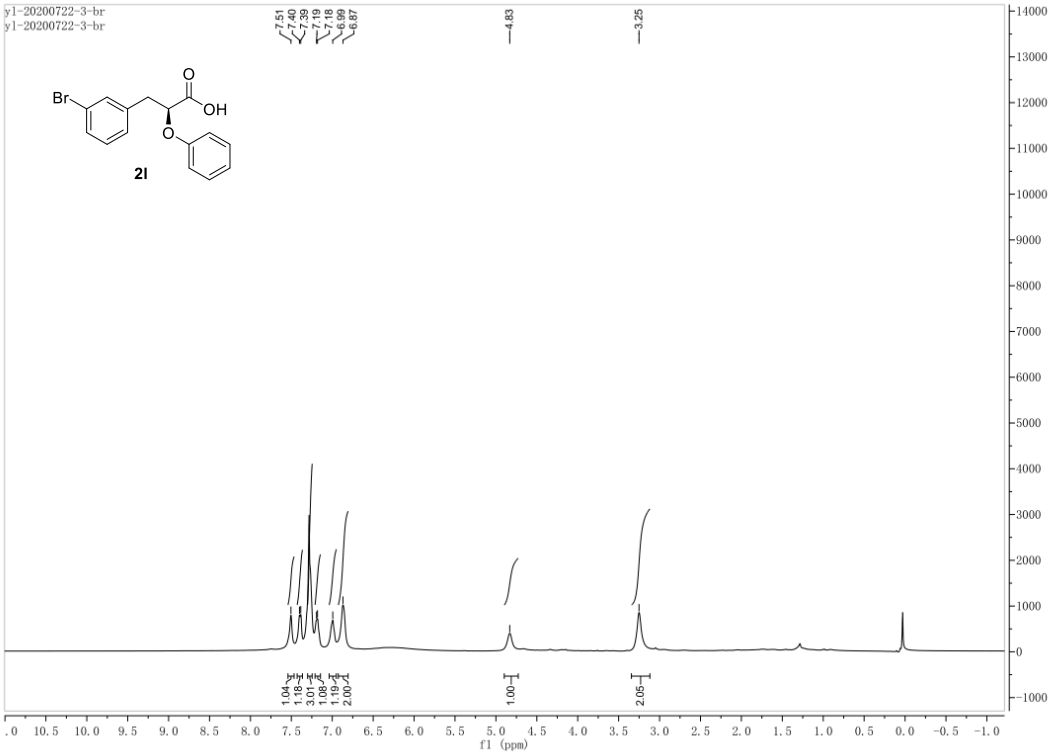
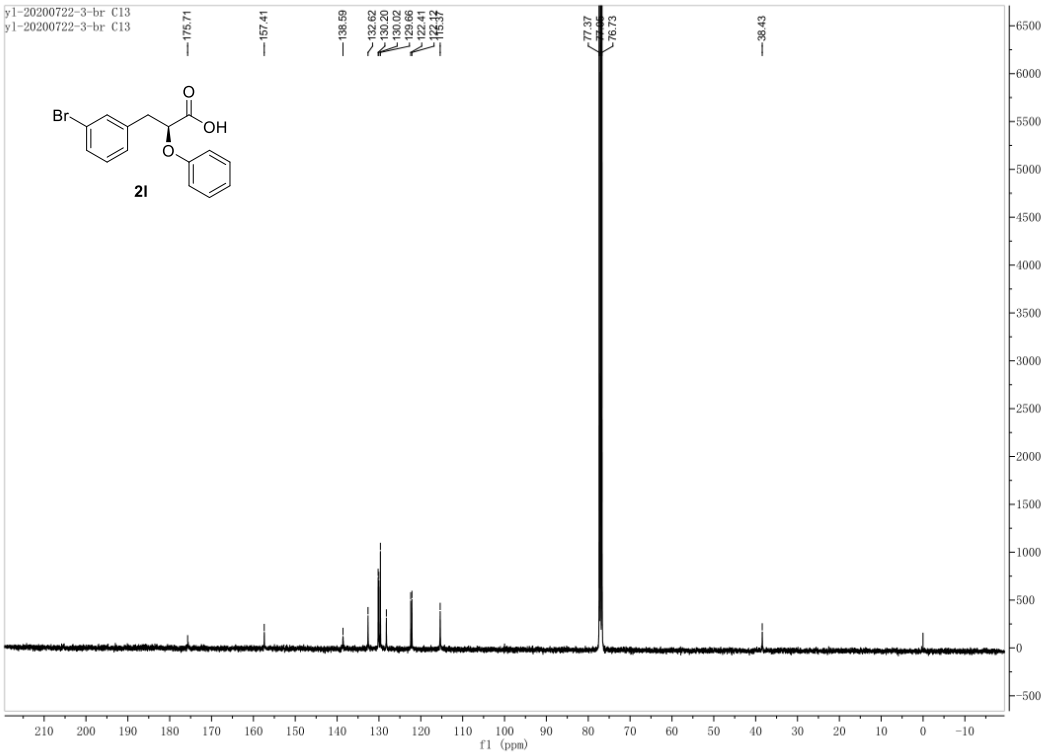
157.64
135.78
132.85
132.22
129.56
129.27
127.41
124.71
121.92
115.39
77.37
77.25
77.05
76.73
39.28
Br
O
OH
O
2k
f1 (ppm)


yl-20200722-3-br
yl-20200722-3-br
7.51
7.40
7.39
7.19
7.18
6.99
6.87
4.83
3.25
Br
O
OH
O
2l
1.04
1.18
3.01
1.08
1.19
2.00
1.00
2.05
f1 (ppm)


yl-20200722-3-br C13
yl-20200722-3-br C13
175.71
157.41
138.59
132.62
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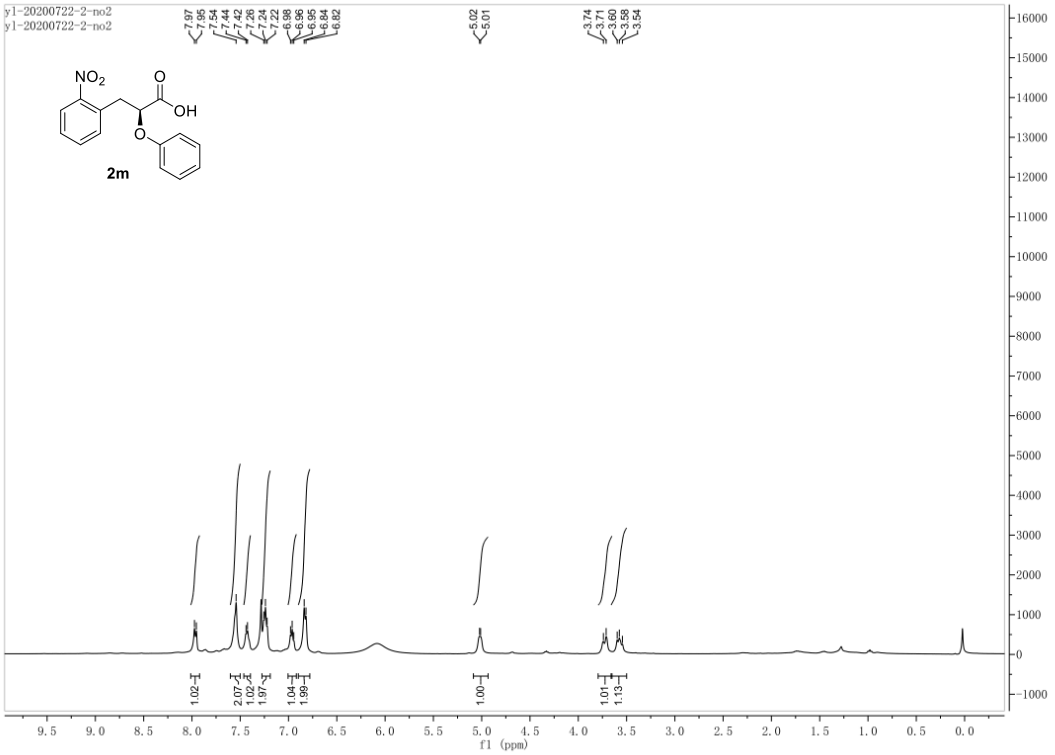
129.66
122.41
77.37
76.73
38.43
Br
O
OH
O
2l
f1 (ppm)


yl-20200722-2-no2
yl-20200722-2-no2
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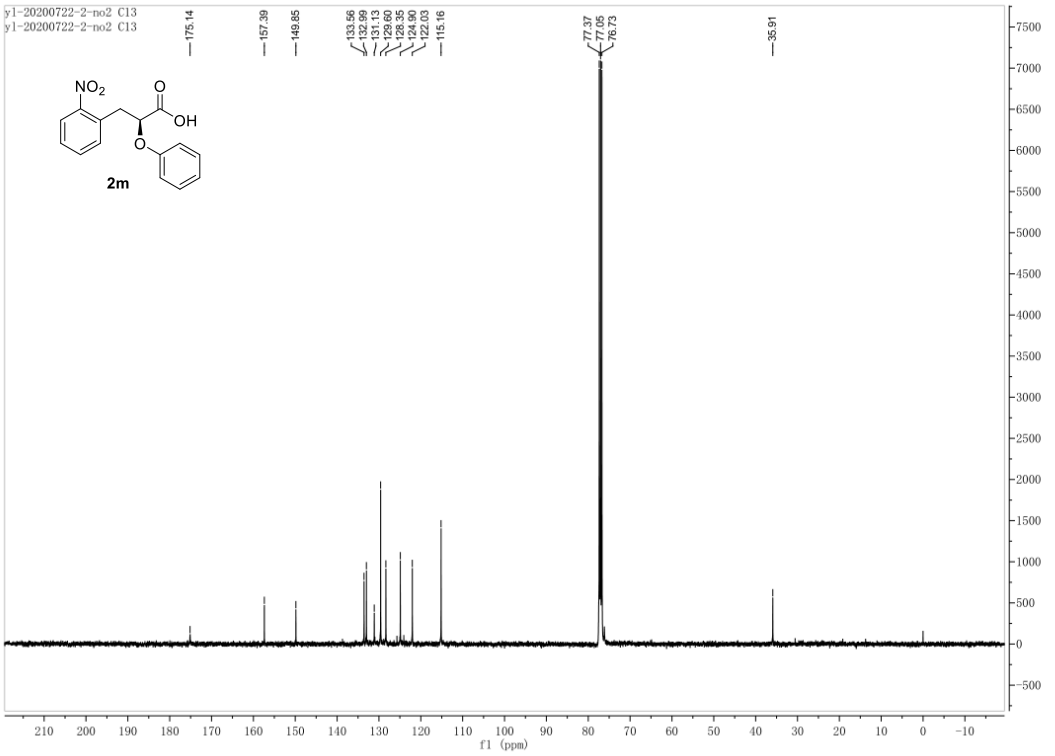
7.54
7.44
7.42
7.26
7.24
7.22
6.98
6.96
6.95
6.84
6.82
5.02
5.01
3.74
3.71
3.60
3.58
3.54
NO2
O
OH
O
2m
1.02
2.07
1.02
1.07
1.04
1.99
1.00
1.01
1.13
f1 (ppm)


yl-20200722-2-no2 C13
yl-20200722-2-no2 C13
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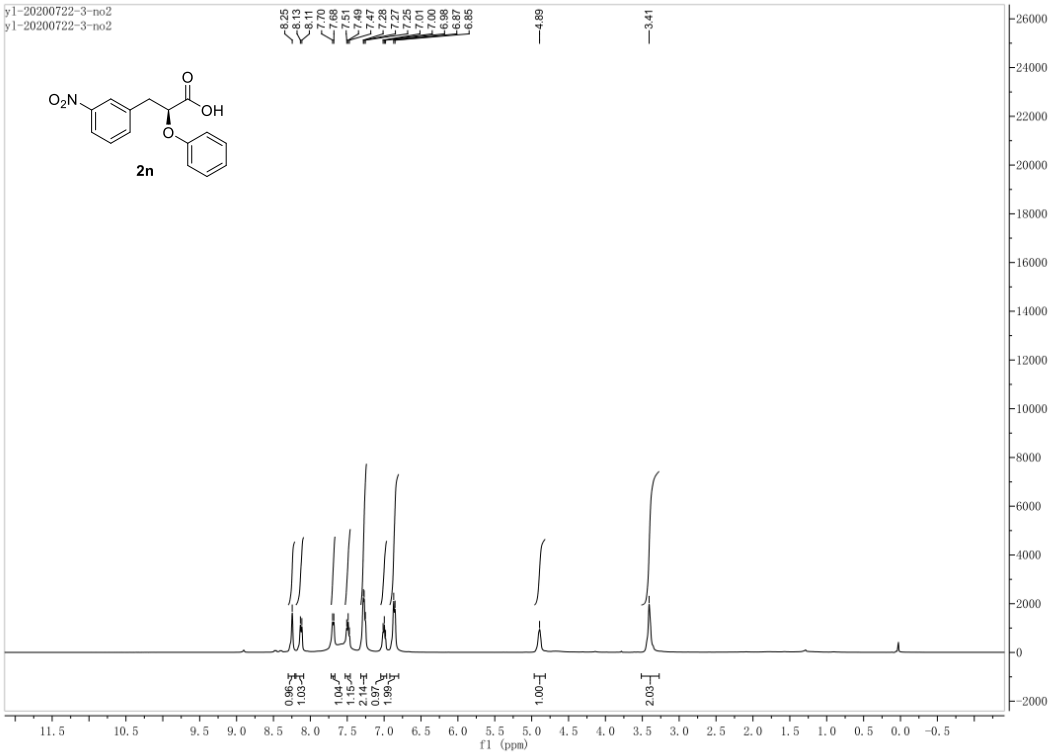
149.85
133.56
132.99
131.13
129.60
128.35
124.90
122.03
115.16
77.37
77.05
76.73
35.91
NO2
O
OH
O
2m
f1 (ppm)


yl-20200722-3-no2
yl-20200722-3-no2
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7.47
7.28
7.27
7.25
7.01
7.00
6.98
6.87
6.85
4.89
3.41
O2N
O
OH
O
2n
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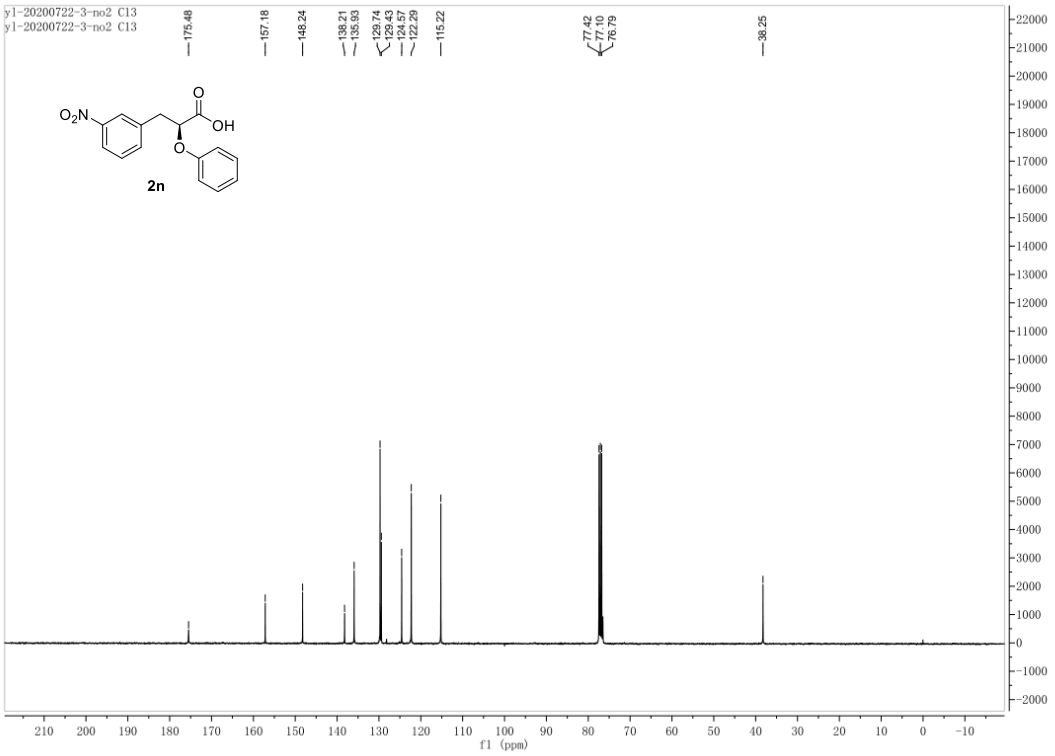
1.03
1.04
1.15
2.14
0.97
1.99
1.00
2.03
f1 (ppm)


yl-20200722-3-no2 C13
yl-20200722-3-no2 C13
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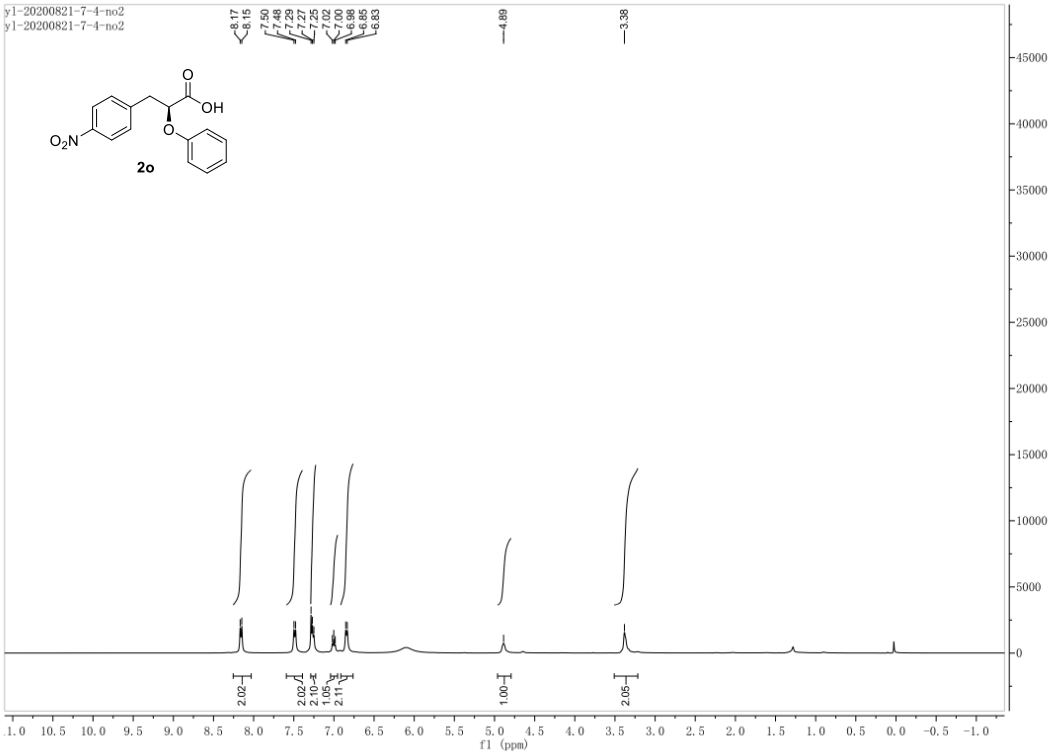
157.18
148.24
138.21
135.93
129.74
129.43
124.57
122.29
115.22
77.42
77.10
76.79
38.25
O2N
OH
O
2n
f1 (ppm)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yl-20200821-7-4-no2
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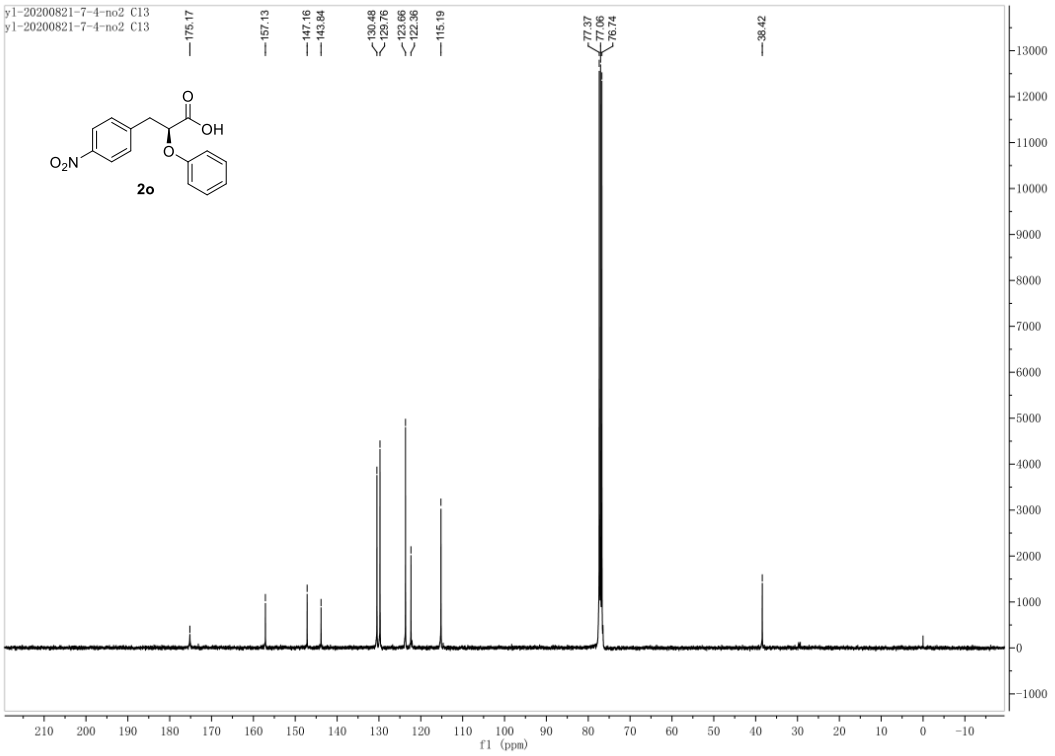
8.15
7.50
7.48
7.29
7.27
7.25
7.02
7.00
6.98
6.85
6.83
4.89
3.38
O2N
OH
O
2o
2.02
2.02
2.10
1.05
2.11
1.00
2.05
f1 (ppm)


yl-20200821-7-4-no2 C13
yl-20200821-7-4-no2 C13
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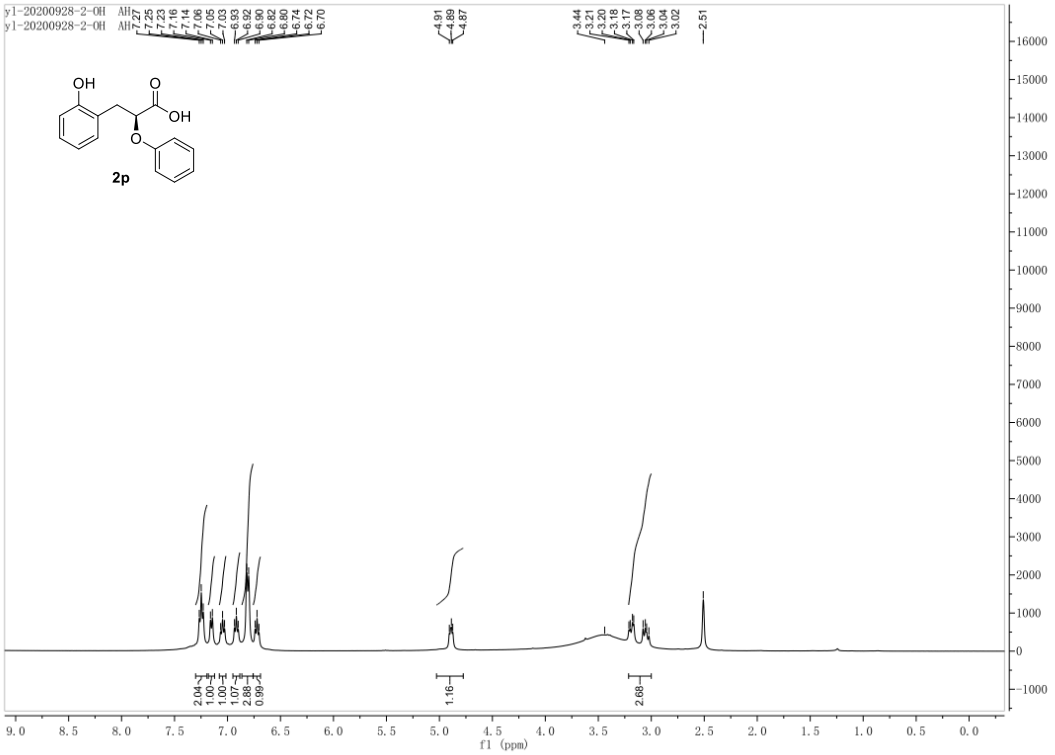
157.13
147.16
143.84
130.48
129.76
123.66
122.36
115.19
77.37
77.06
76.74
38.42
O
OH
O
O2N
2o
f1 (ppm)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yl-20200928-2-OH
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7.25
7.23
7.16
7.14
7.06
7.05
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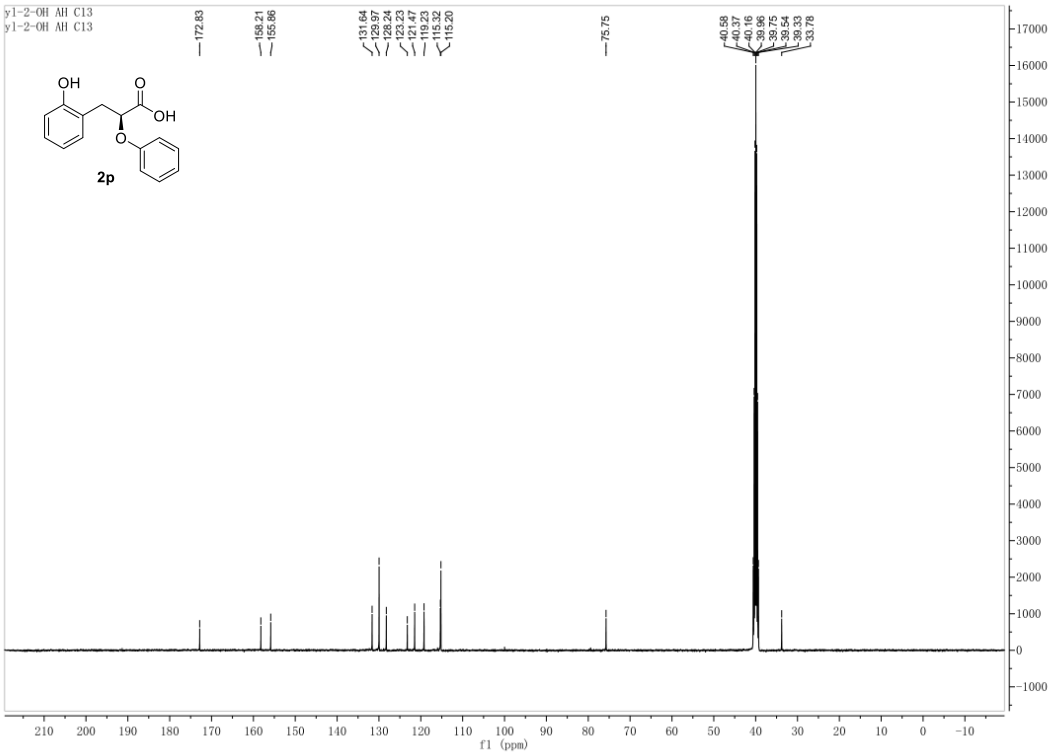
6.93
6.92
6.90
6.82
6.80
6.74
6.72
6.70
4.91
4.89
4.87
3.44
3.21
3.20
3.18
3.17
3.08
3.06
3.04
3.02
2.51
OH
O
OH
O
2p
2.04
1.00
1.00
1.07
2.88
0.99
1.16
2.68
f1 (ppm)


yl-2-OH AH C13
yl-2-OH AH C13
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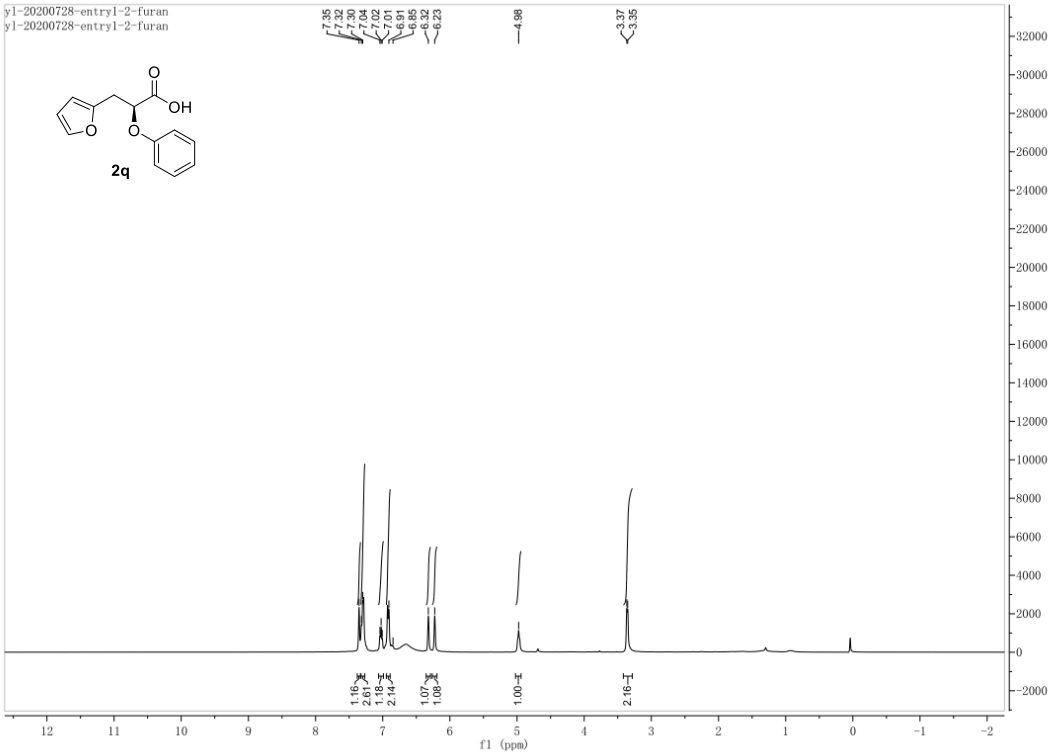
158.21
155.86
131.64
129.97
128.24
123.23
121.47
119.23
115.32
115.20
75.75
40.58
40.37
40.16
39.96
39.75
39.54
39.33
33.78
OH
O
OH
O
2p
f1 (ppm)


yl-20200728-entryl-2-furan
yl-20200728-entryl-2-furan
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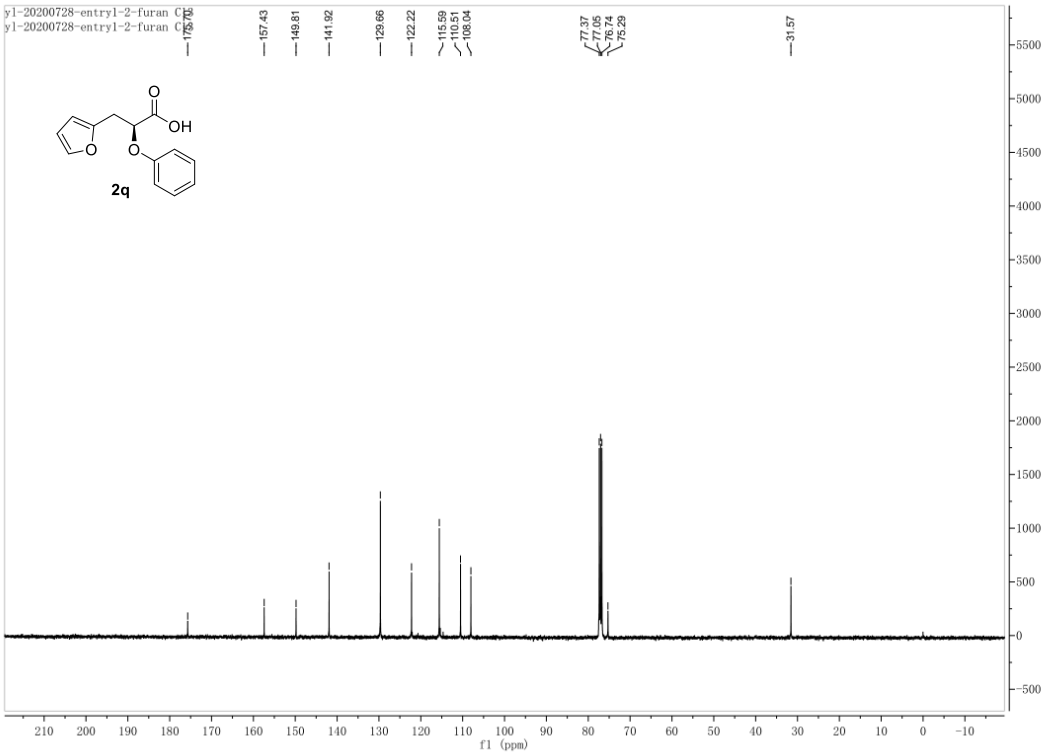
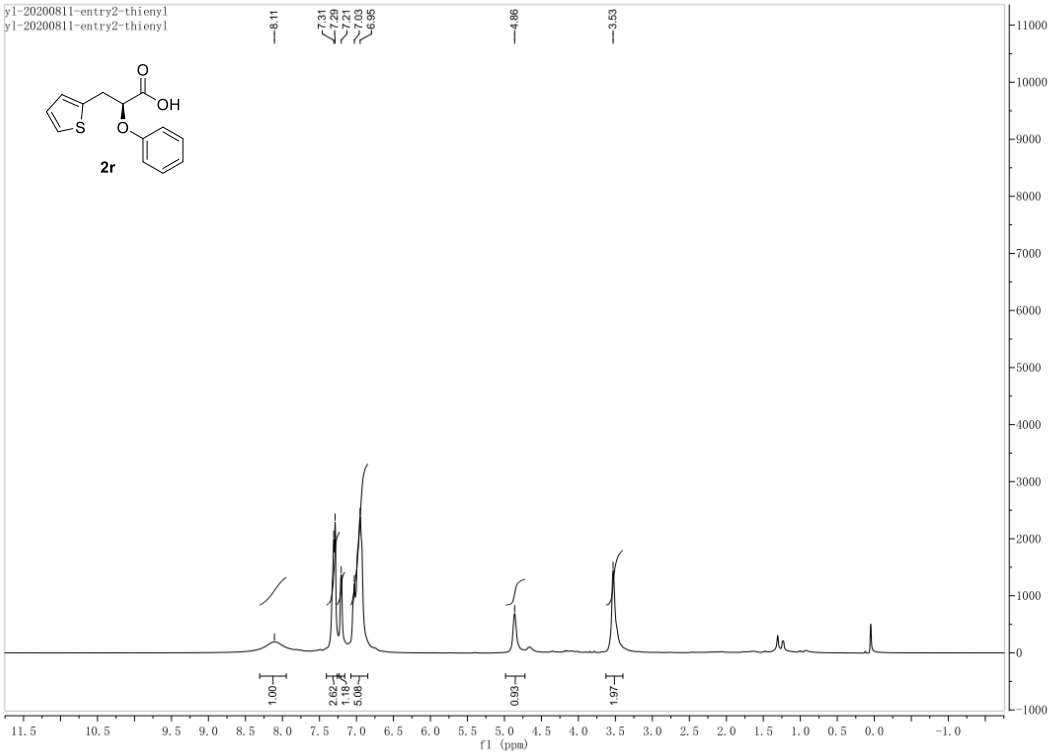
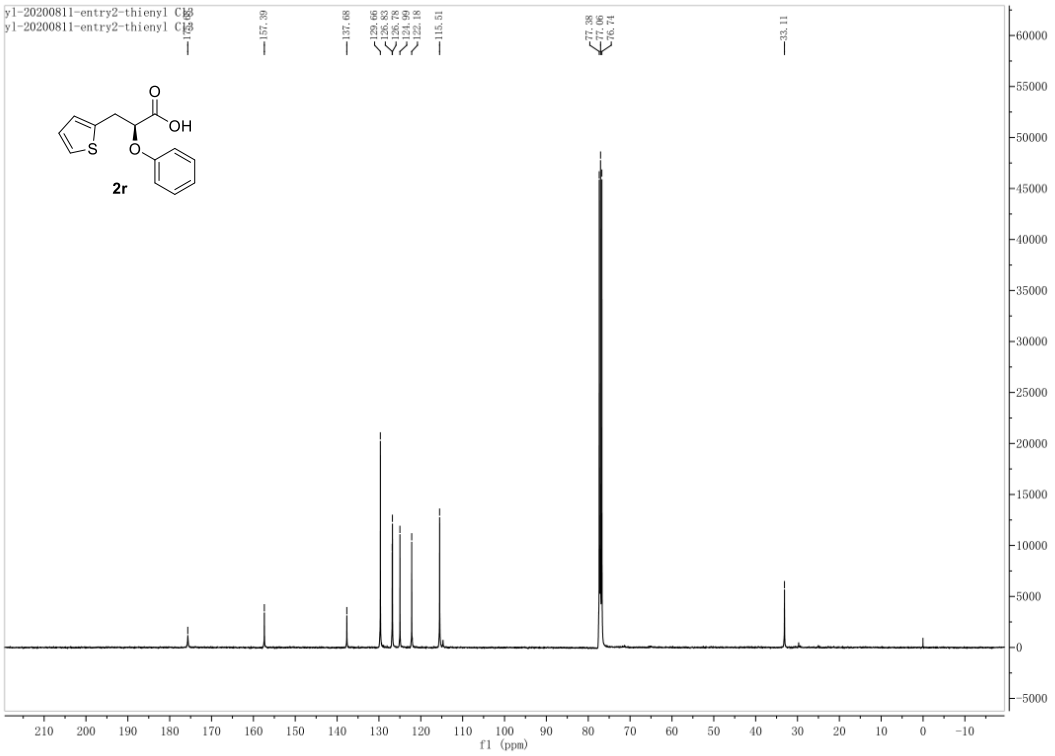
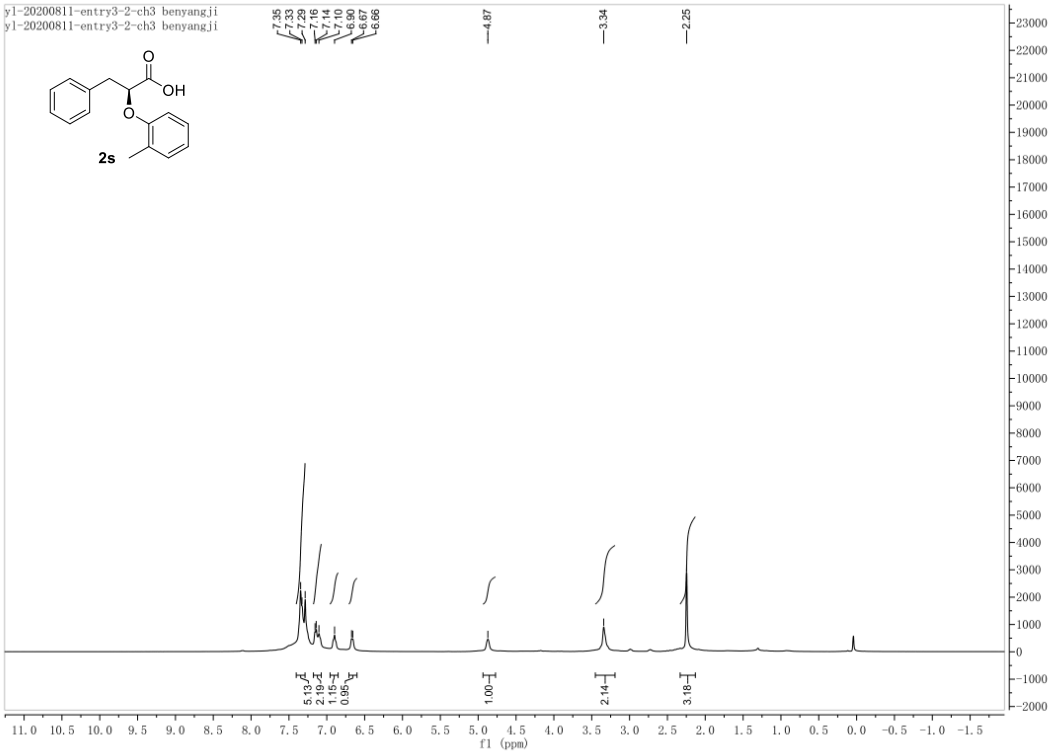
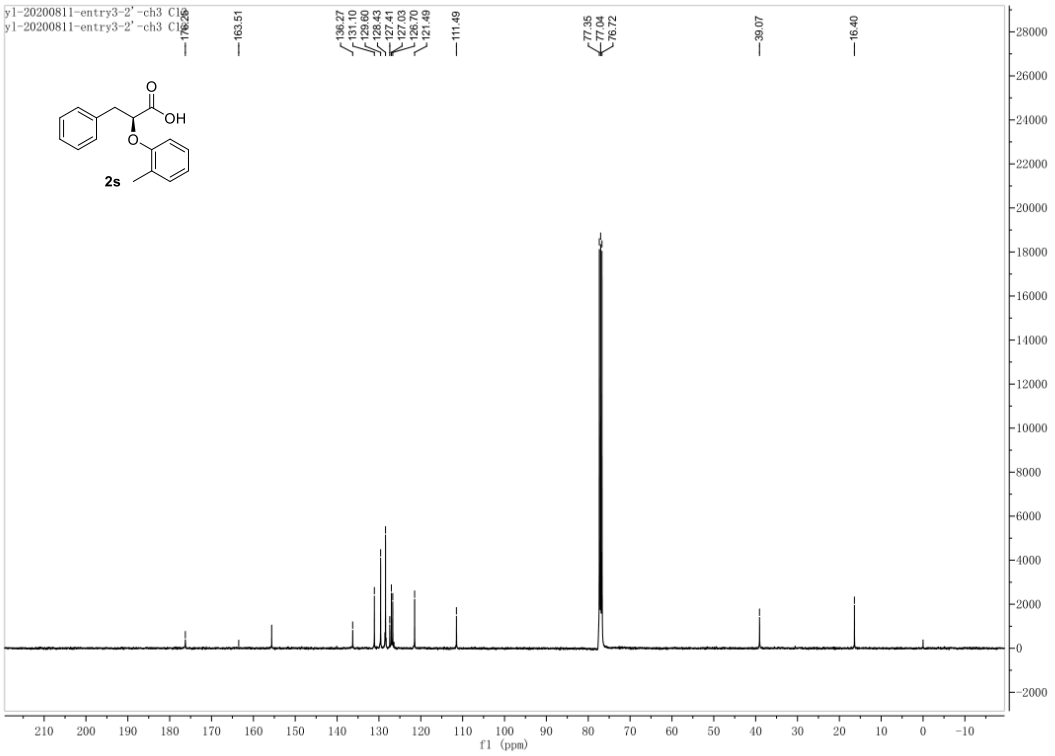
7.32
7.30
7.04
7.02
7.01
6.91
6.85
6.32
6.23
4.98
3.37
3.35
O
OH
O
O
2q
1.16
2.61
1.18
2.14
1.07
1.08
1.00
2.16
f1 (ppm)

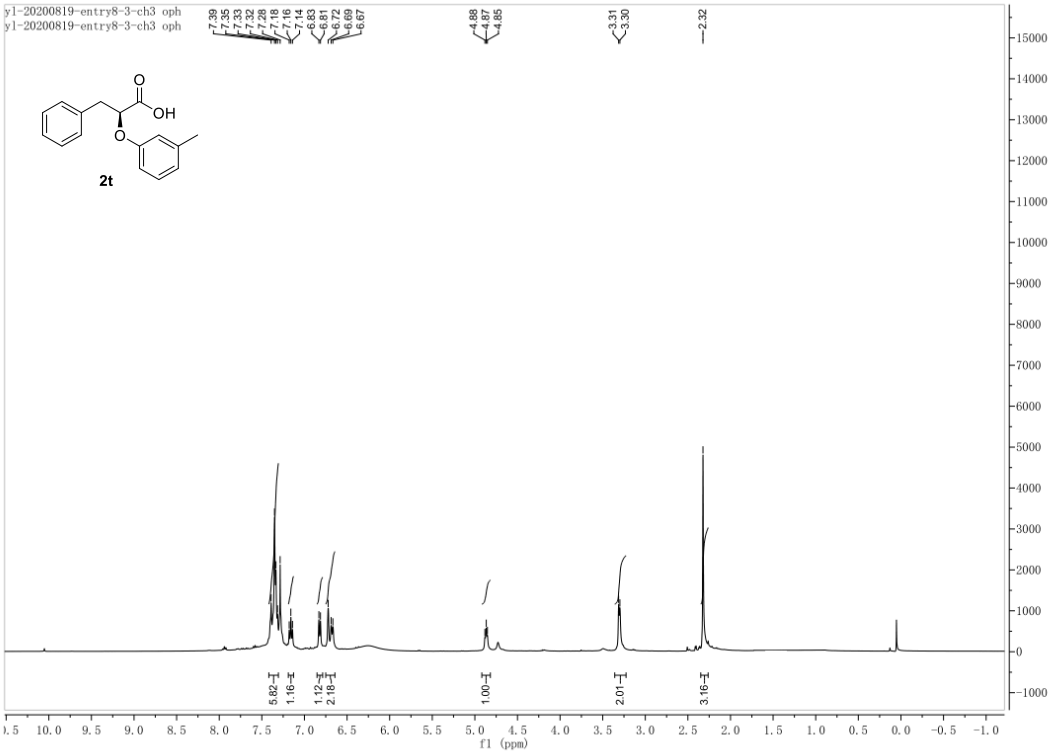

yl-20200728-entryl-2-furan C
yl-20200728-entryl-2-furan C
175.70
157.43
149.81
141.92
129.66
122.22
115.59
110.51
108.04
77.37
77.05
76.74
75.29
31.57
O
OH
O
O
2q
f1 (ppm)

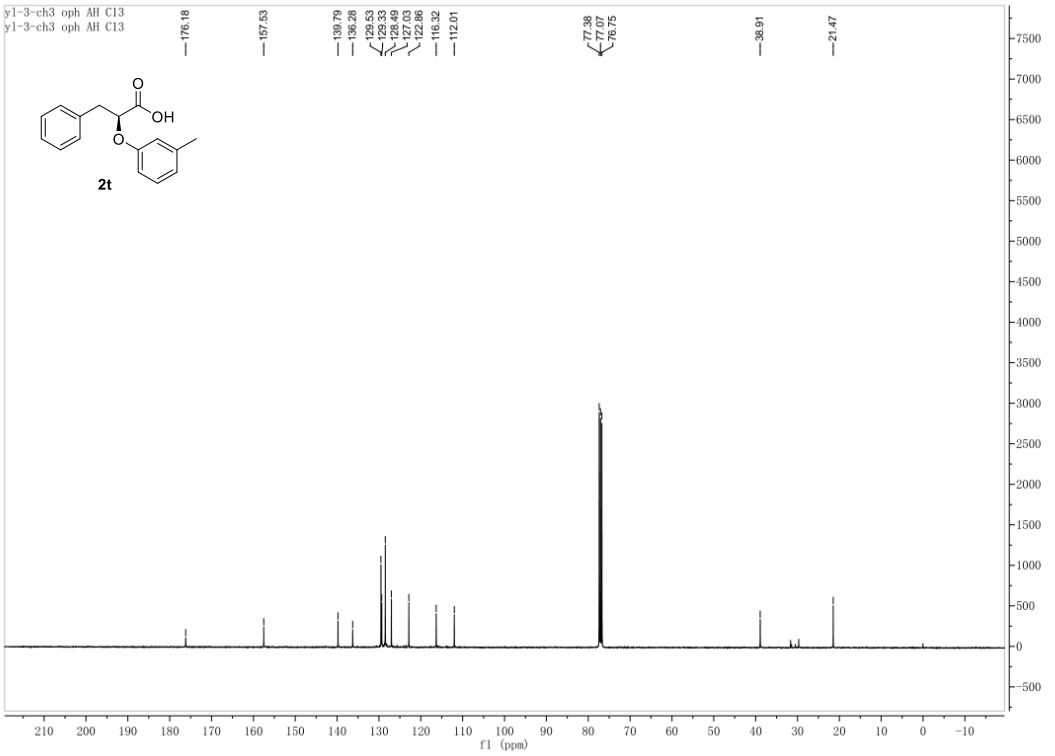

yl-20200811-entry2-thienyl
yl-20200811-entry2-thienyl
8.11
7.31
7.29
7.21
7.03
6.95
4.86
3.53
O
OH
S
O
2r
1.00
2.62
1.18
5.08
0.83
1.97
f1 (ppm)

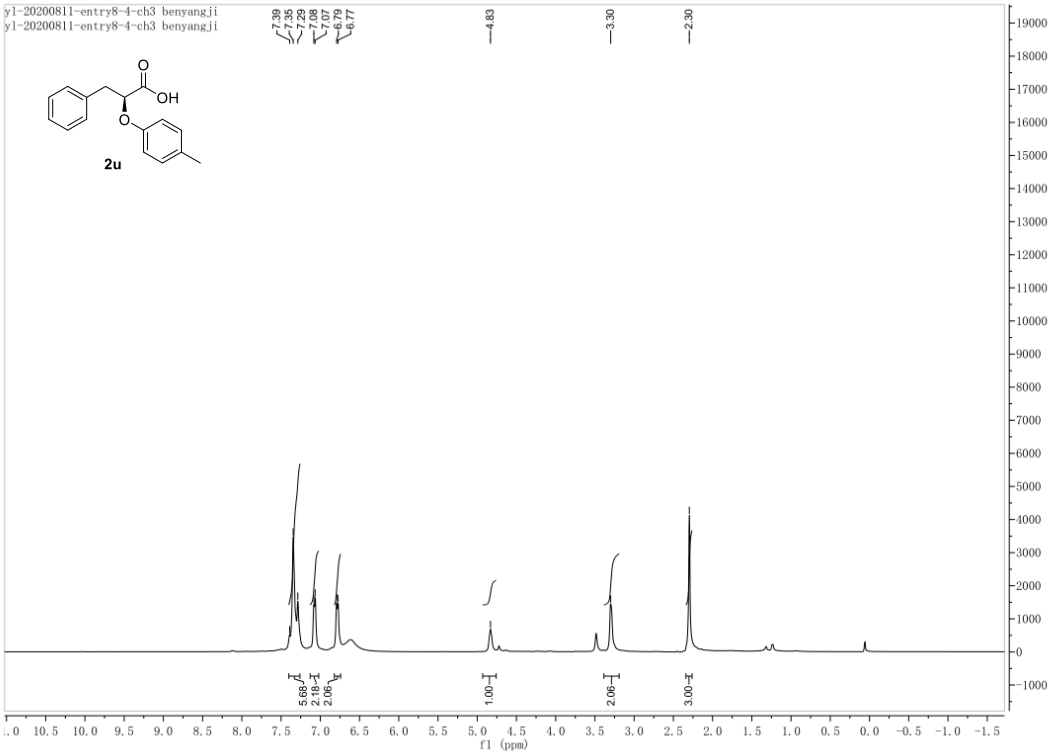

yl-20200811-entry2-thienyl C
yl-20200811-entry2-thienyl C
157.39
137.68
129.66
126.83
126.78
124.99
122.18
115.51
77.38
77.06
76.74
33.11
O
OH
S
O
2r
f1 (ppm)

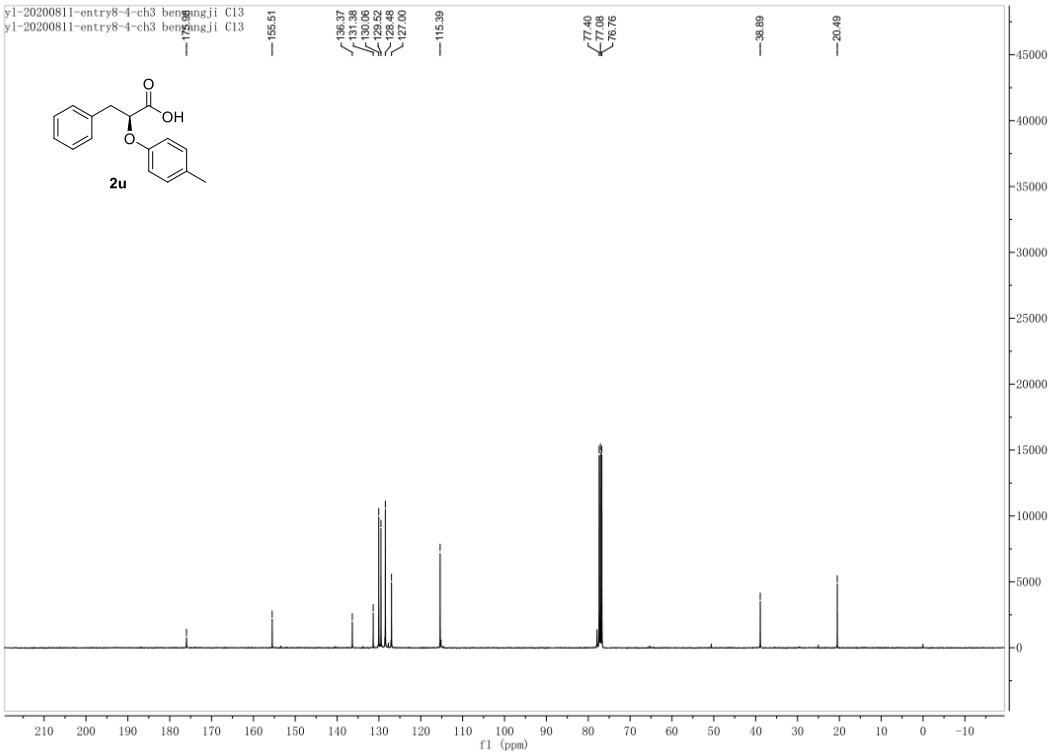

yl-20200811-entry3-2-ch3 benyangji
yl-20200811-entry3-2-ch3 benyangji
7.35
7.33
7.29
7.16
7.14
7.10
6.90
6.87
6.86
4.87
3.34
2.25
O
OH
O
2s
5.13
2.19
1.15
0.95
1.00
2.14
3.18
f1 (ppm)

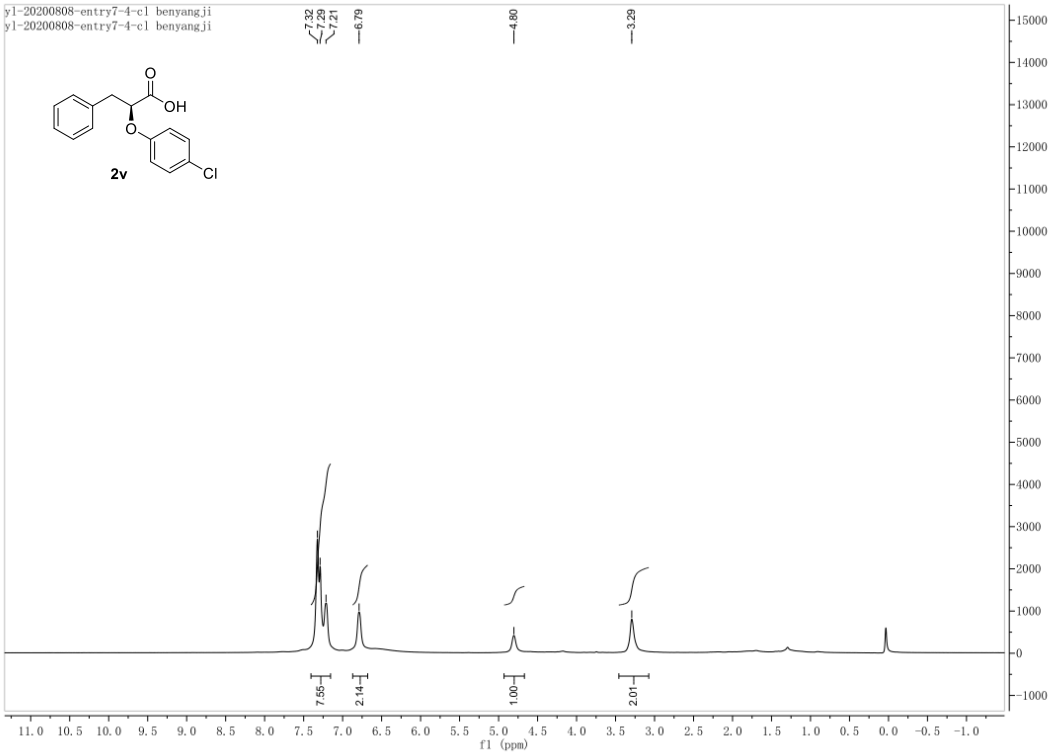

yl-20200811-entry3-2'-ch3 Cl
yl-20200811-entry3-2'-ch3 Cl
176.26
163.51
136.27
131.10
129.60
128.43
127.41
127.03
126.70
121.49
111.49
77.35
77.04
76.72
39.07
16.40
2s
f1 (ppm)

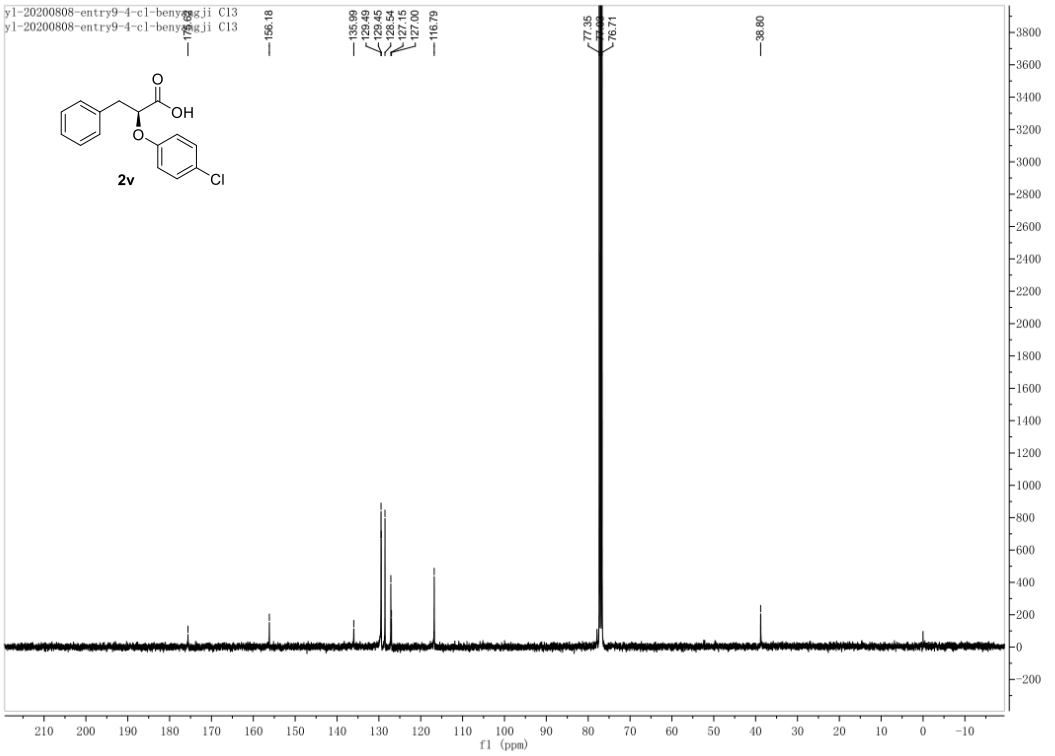

yl-20200819-entry8-3-ch3 oph
yl-20200819-entry8-3-ch3 oph
7.39
7.35
7.33
7.32
7.28
7.18
7.16
7.14
6.83
6.81
6.72
6.69
6.67
4.88
4.87
4.85
3.31
3.30
2.32
5.82
1.16
1.12
2.18
1.00
2.01
3.16
2t
f1 (ppm)

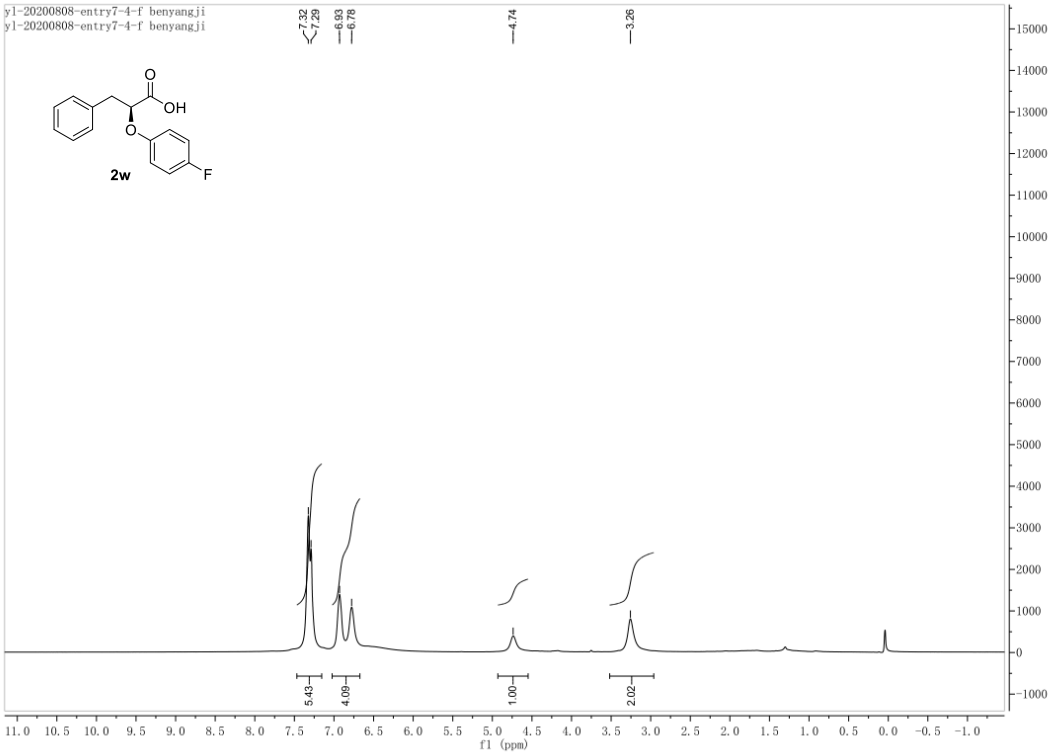

yl-3-ch3 oph AH C13
yl-3-ch3 oph AH C13
176.18
157.53
139.79
136.28
129.53
129.33
128.49
127.03
122.86
116.32
112.01
77.38
77.07
76.75
38.91
21.47
O
OH
O
2t
f1 (ppm)

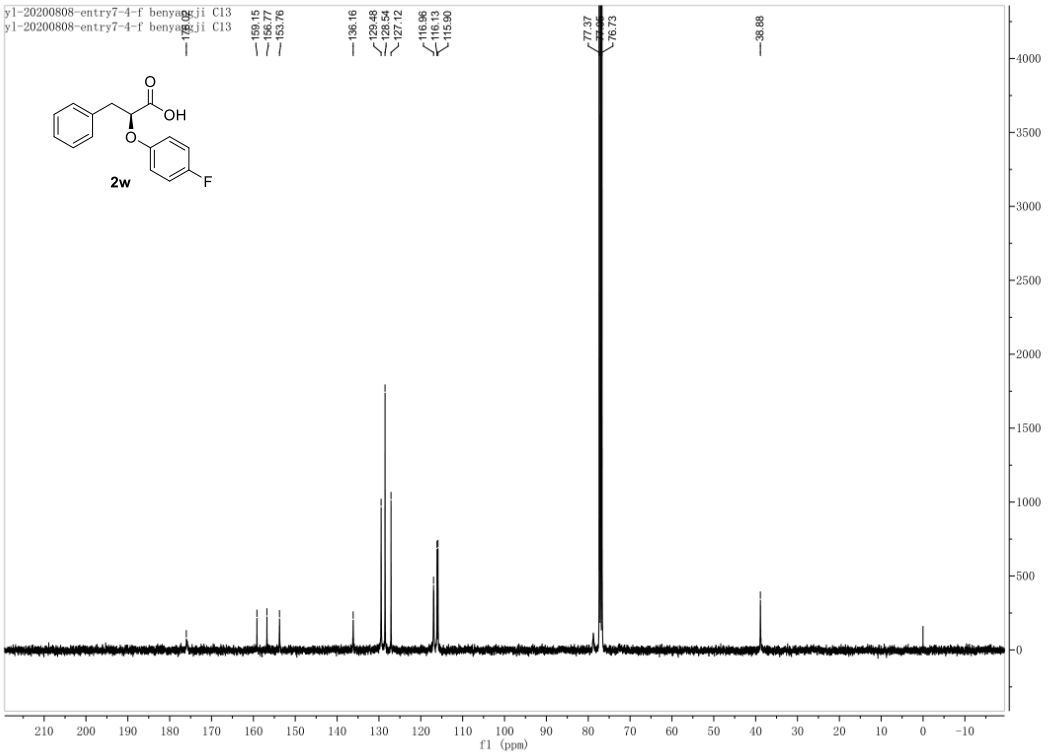

yl-20200811-entry8-4-ch3 benyangji
yl-20200811-entry8-4-ch3 benyangji
7.39
7.35
7.29
7.08
7.07
6.79
6.77
4.83
3.30
2.30
O
OH
O
2u
5.68
2.18
2.06
1.00
2.06
3.00
f1 (ppm)

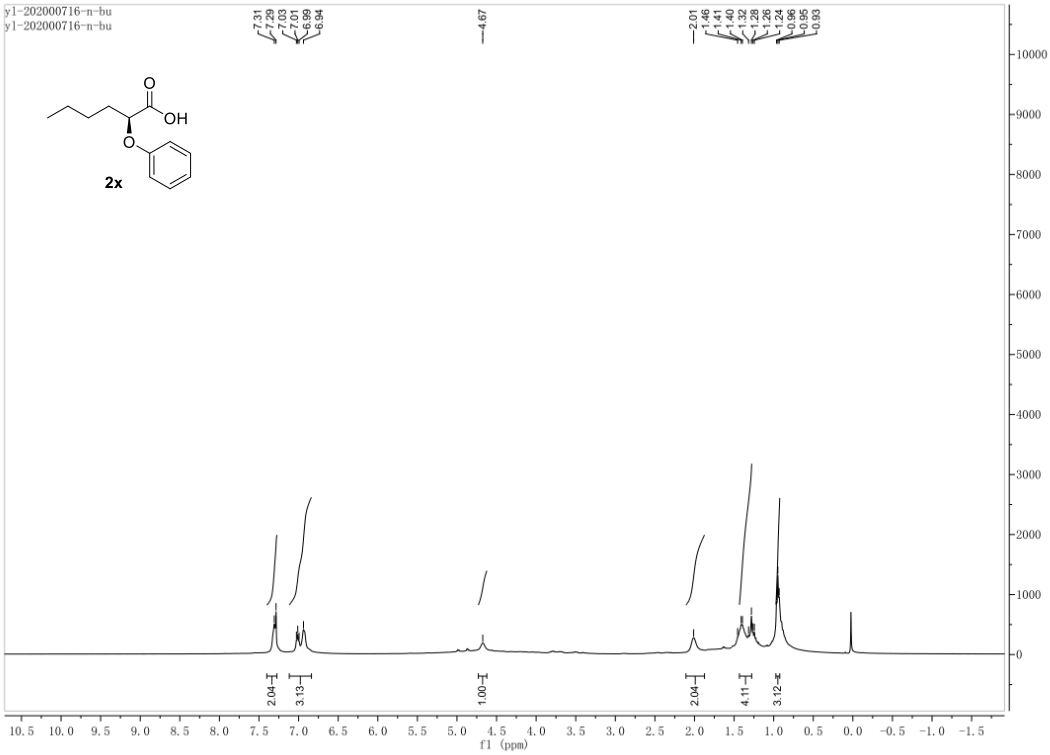

yl-20200811-entry8-4-ch3 benyangji C13
yl-20200811-entry8-4-ch3 benyangji C13
175.98
155.51
136.37
131.38
130.06
129.52
129.48
127.00
115.39
77.40
77.08
76.76
38.89
20.49
O
OH
O
2u
f1 (ppm)

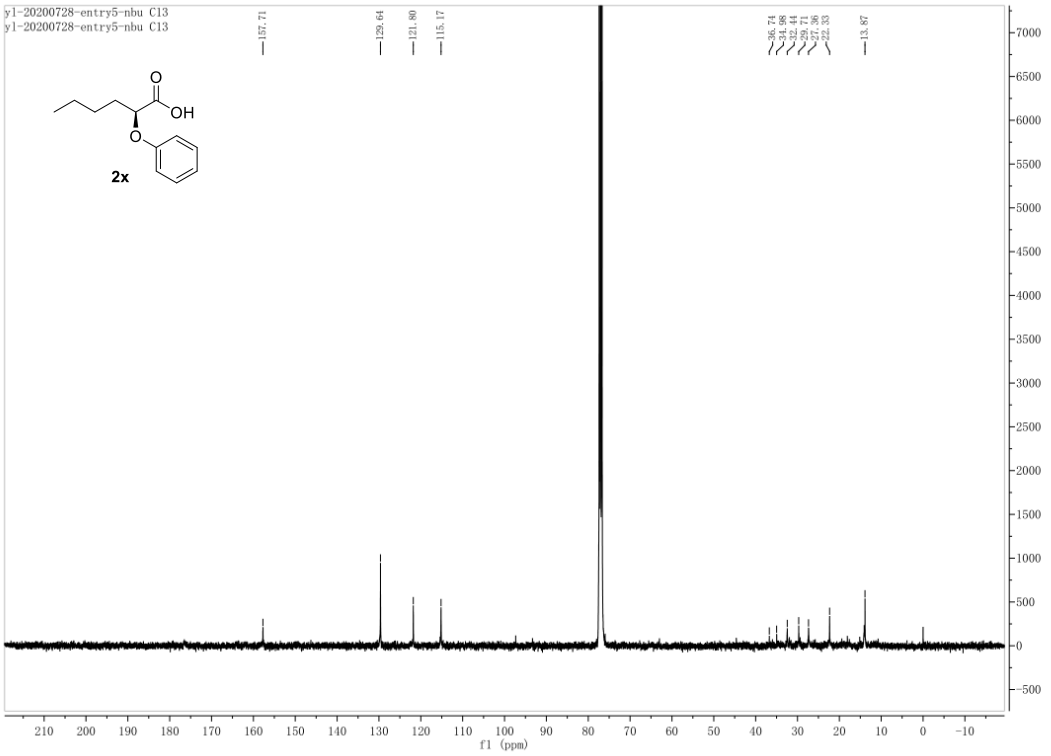

yl-20200808-entry7-4-cl benyangji
yl-20200808-entry7-4-cl benyangji
7.32
7.29
7.21
6.79
4.80
3.29
O
OH
O
Cl
2v
7.55
2.14
1.00
2.01
f1 (ppm)

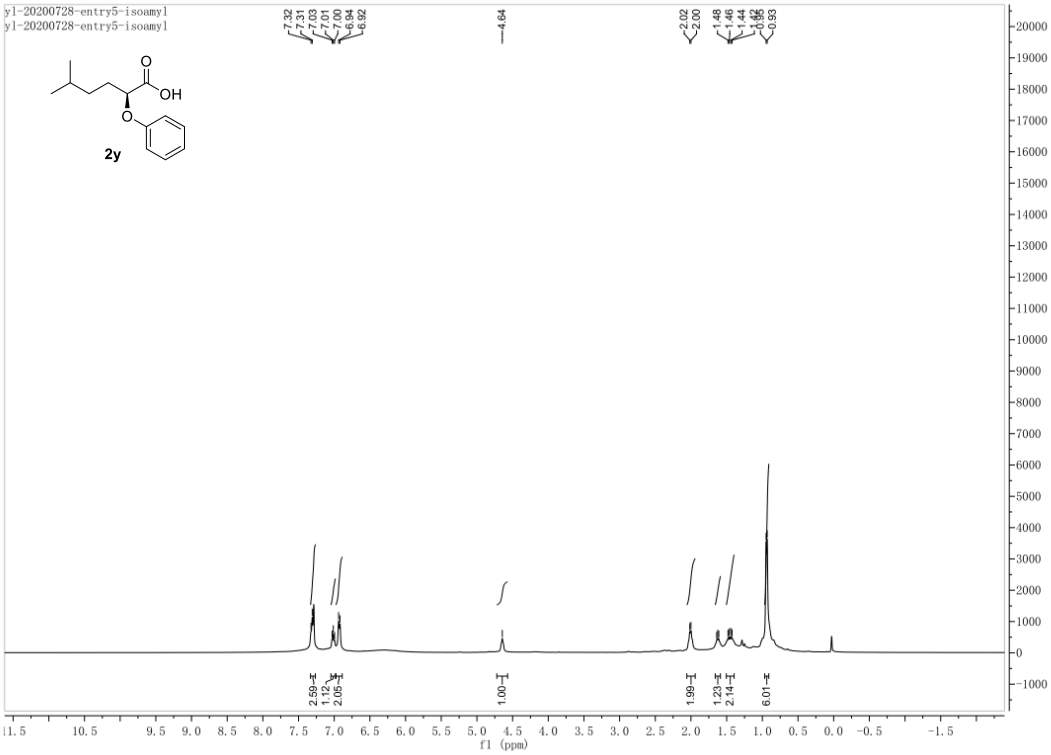

yl-20200808-entry9-4-cl-benyangji C13
yl-20200808-entry9-4-cl-benyangji C13
178.68
156.18
135.99
129.49
129.45
129.54
127.15
127.00
116.79
77.35
77.03
76.71
38.80
O
OH
O
Cl
2v
f1 (ppm)

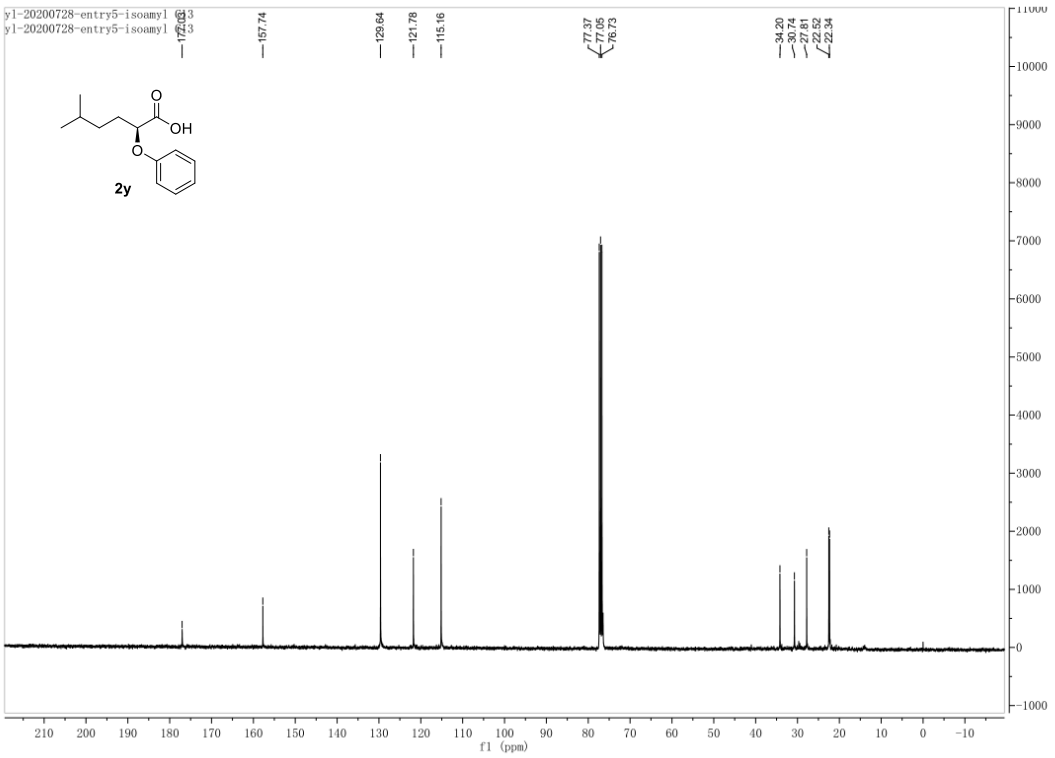

yl-20200808-entry7-4-f benyangji
yl-20200808-entry7-4-f benyangji
7.32
7.29
6.93
6.78
4.74
3.26
O
OH
O
F
2w
5.43
4.09
1.00
2.02
f1 (ppm)

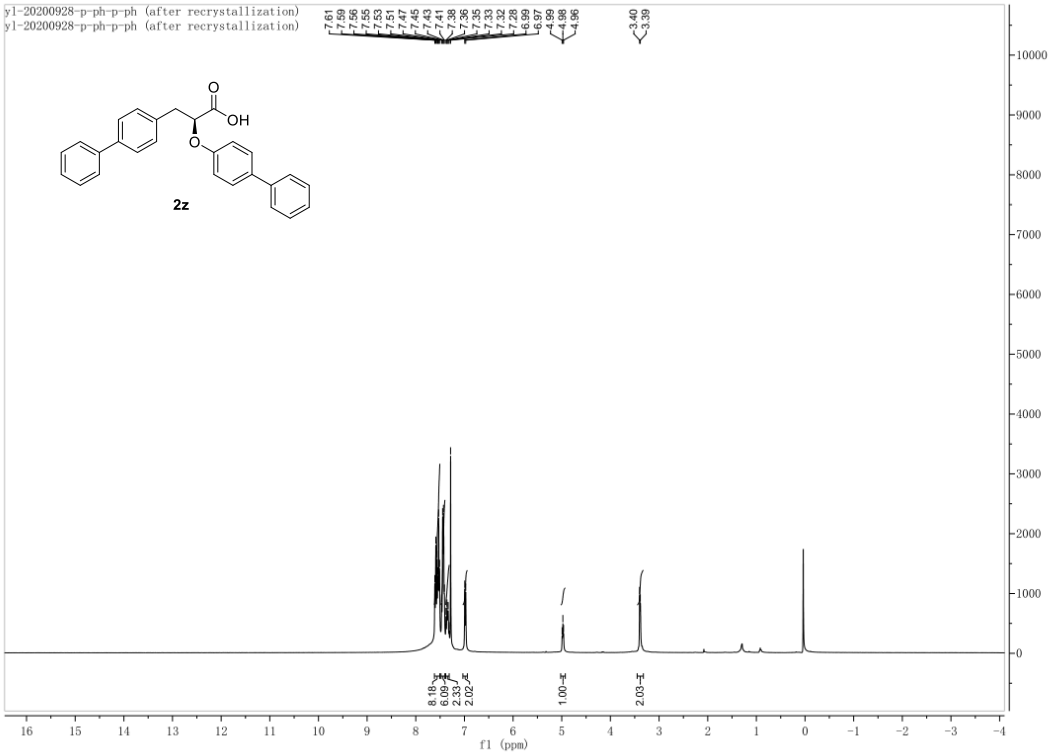

yl-20200808-entry7-4-f benyaoji C13
yl-20200808-entry7-4-f benyaoji C13
178.02
159.15
156.77
153.76
136.16
129.48
128.54
127.12
116.96
116.13
115.90
77.37
77.05
76.73
38.88
O
OH
O
F
2w
f1 (ppm)

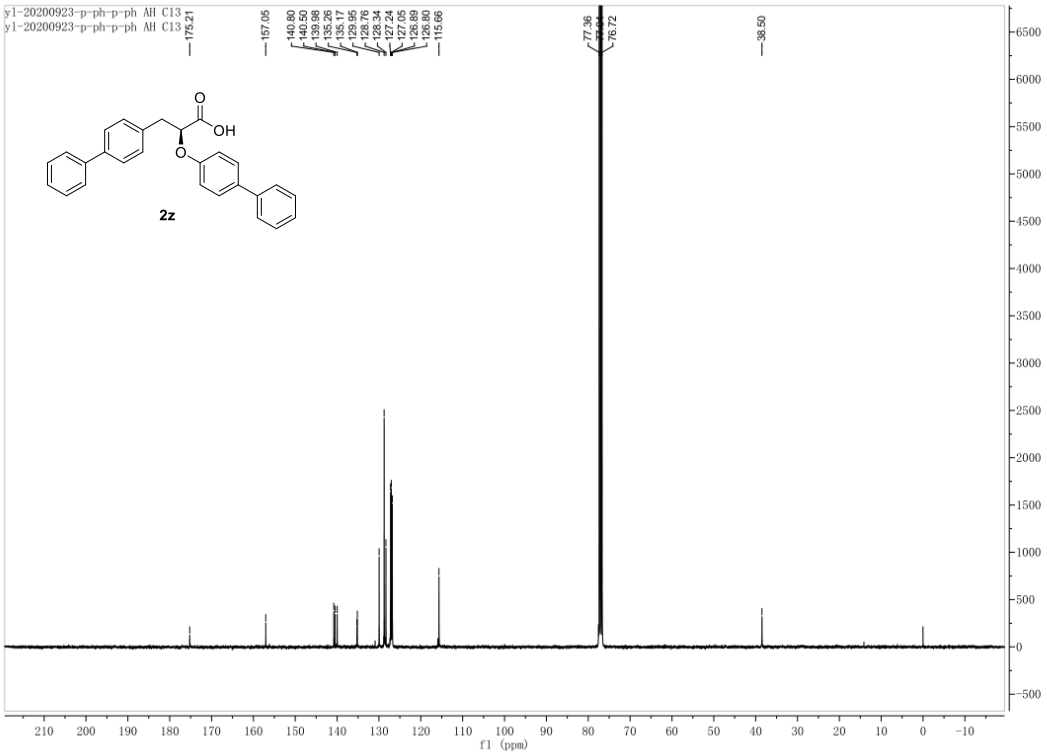

yl-202000716-n-bu
yl-202000716-n-bu
7.31
7.29
7.03
7.01
6.89
6.84
4.67
2.01
1.46
1.41
1.40
1.32
1.28
1.26
1.24
0.96
0.95
0.93
O
OH
O
2x
2.04
3.13
1.00
2.04
4.11
3.12
f1 (ppm)


yl-20200728-entry5-nbu C13
yl-20200728-entry5-nbu C13
157.71
129.64
121.80
115.17
36.74
34.98
32.44
29.71
27.36
22.33
13.87
O
OH
O
2x
f1 (ppm)

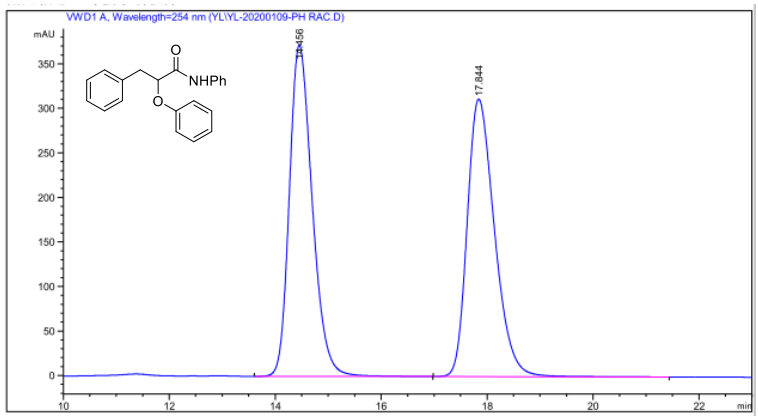

yl-20200728-entry5-isoamyl
yl-20200728-entry5-isoamyl
7.32
7.31
7.03
7.01
7.00
6.94
6.92
4.64
2.02
2.00
1.48
1.46
1.44
0.95
0.93
O
OH
O
2y
2.59
1.12
2.05
1.00
1.99
1.23
2.14
6.01
f1 (ppm)


yl-20200728-entry5-isoamyl
yl-20200728-entry5-isoamyl
157.74
129.64
121.78
115.16
77.37
77.05
76.73
34.20
30.74
27.81
22.52
22.34
O
OH
O
2y
f1 (ppm)

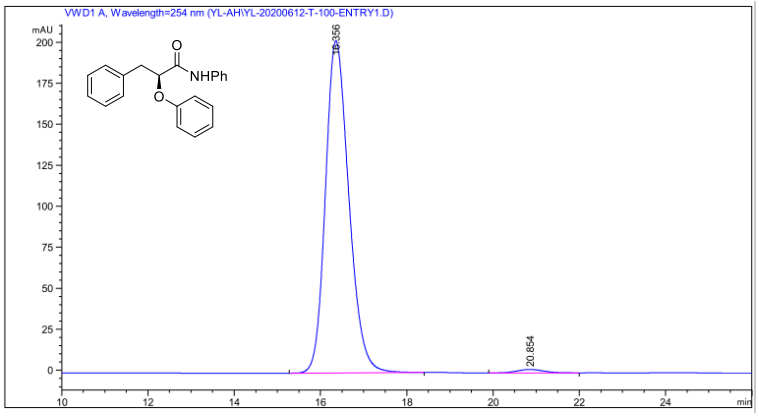

yl-20200928-p-ph-p-ph (after recrystallization)
yl-20200928-p-ph-p-ph (after recrystallization)
7.61
7.59
7.56
7.55
7.53
7.51
7.47
7.45
7.43
7.41
7.38
7.36
7.35
7.33
7.32
7.28
6.99
6.97
4.99
4.98
4.96
3.40
3.39
O
OH
O
2z
8.18
6.09
2.33
2.02
1.00
2.03
f1 (ppm)



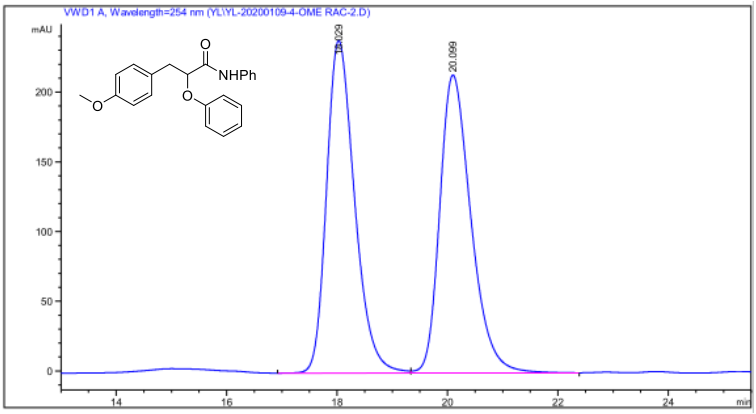
7. HPLC spectra



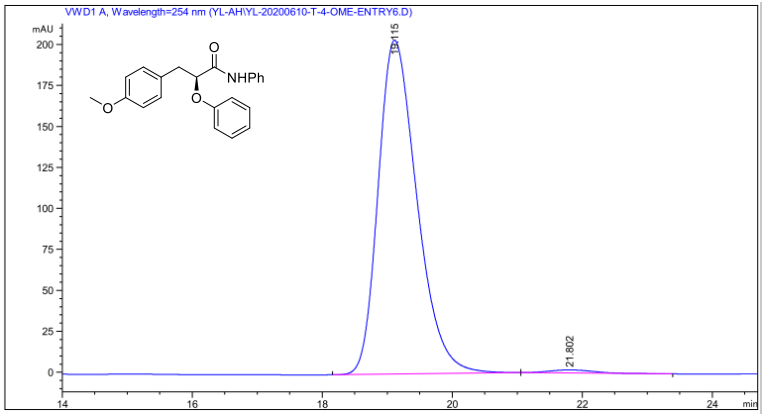
#	[min]			[mAU*s]	[mAU]	%
1	14.456	1	BB	1.11621e4	371.98468	50.0611
2	17.844	1	BB	1.11348e4	311.61880	49.9389



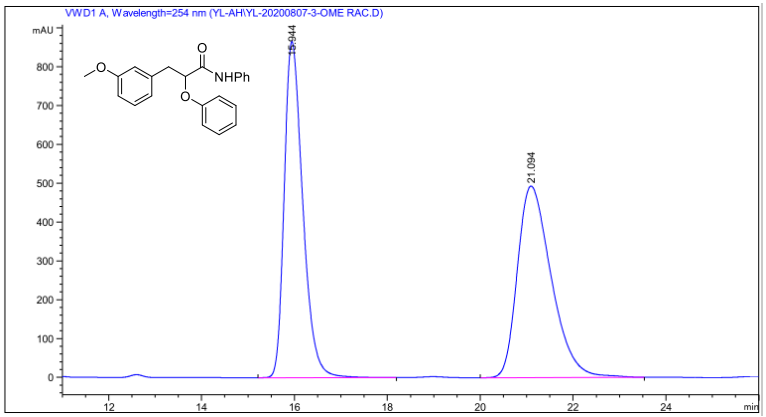
#	[min]			[mAU*s]	[mAU]	%
1	16.356	1	BB	7633.09668	202.41315	98.8278
2	20.854	1	BB	90.53281	2.09149	1.1722



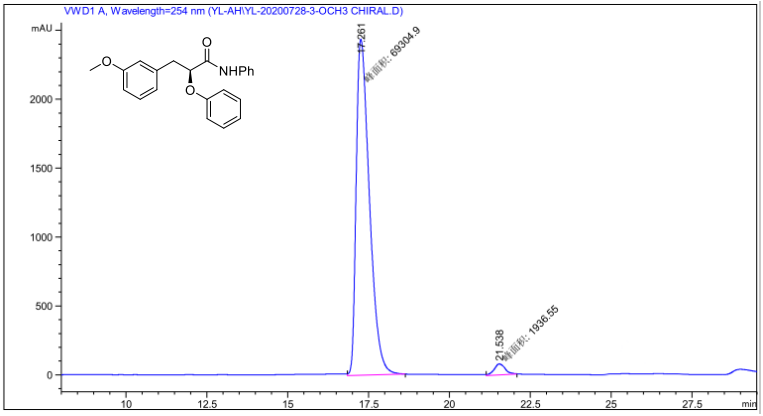
#	[min]			[mAU*s]	[mAU]	%
1	18.029	1	BV	8419.21973	238.53062	50.1058
2	20.099	1	VB	8383.66113	213.67374	49.8942



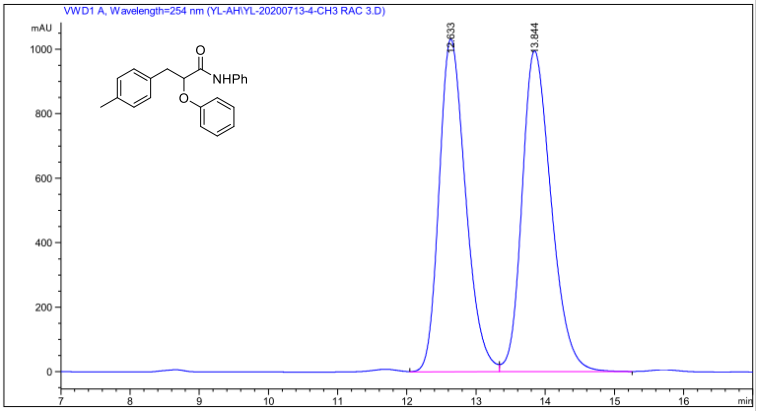
#	[min]			[mAU*s]	[mAU]	%
1	19.115	1	BB	8427.38770	203.73251	98.9535
2	21.802	1	BB	89.12537	1.88190	1.0465



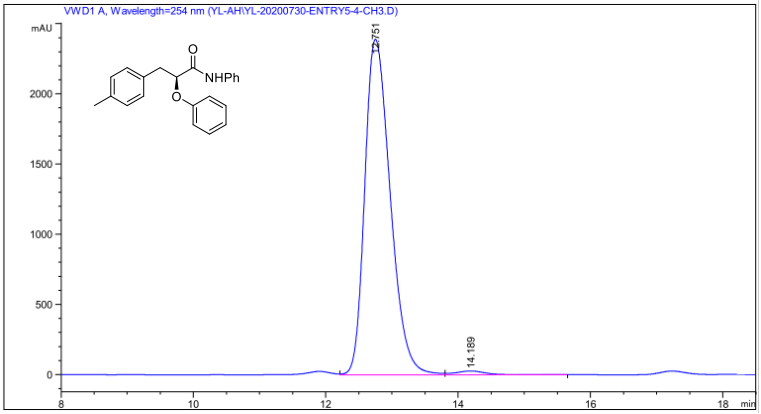
#	[min]		[min]	[mAU*s]	[mAU]	%
1	15.944	BB	0.4260	2.39787e4	866.12836	49.0141
2	21.094	BB	0.7771	2.49433e4	493.16397	50.9859



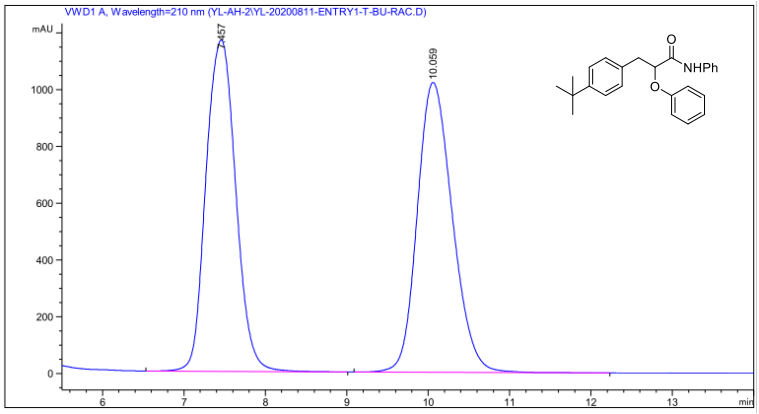
#	[min]			[mAU*s]	[mAU]	%
1	17.261	1	MM	6.93049e4	2438.61694	97.2817
2	21.538	1	MM	1936.55298	80.00856	2.7183



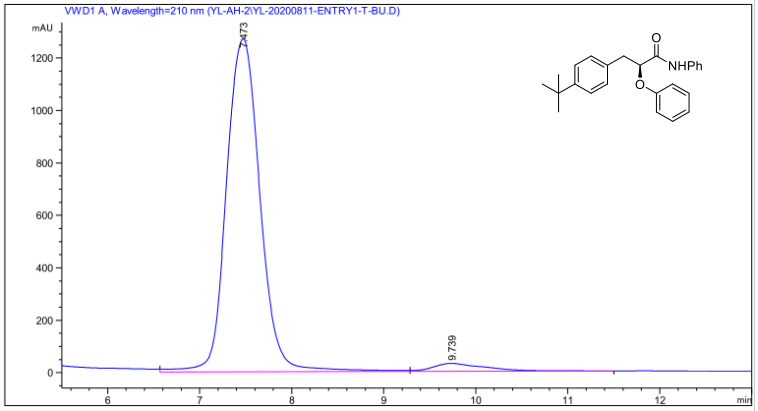
#	[min]			[mAU*s]	[mAU]	%
1	12.633	1	VV	2.75112e4	1032.49316	48.5535
2	13.844	1	VB	2.91504e4	995.45007	51.4465



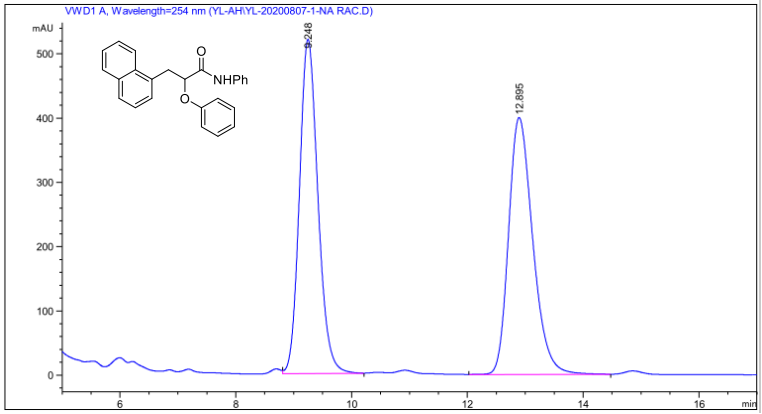
#	[min]			[mAU*s]	[mAU]	%
1	12.751	1	VV	6.39448e4	2390.45239	98.7059
2	14.189	1	VB	838.33112	26.98314	1.2941



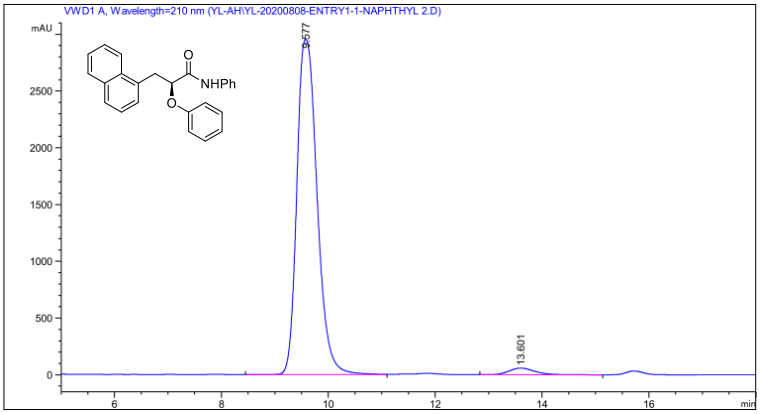
#	[min]			[mAU*s]	[mAU]	%
1	7.457	1	BB	2.97251e4	1167.68933	49.2924
2	10.059	1	BB	3.05786e4	1021.22290	50.7076



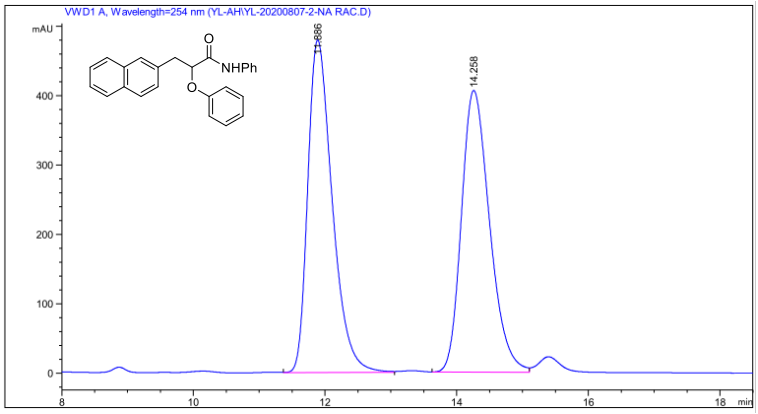
#	[min]			[mAU*s]	[mAU]	%
1	7.473	1	VV	3.23510e4	1270.05847	96.3340
2	9.739	1	VB	1231.11536	30.46997	3.6660



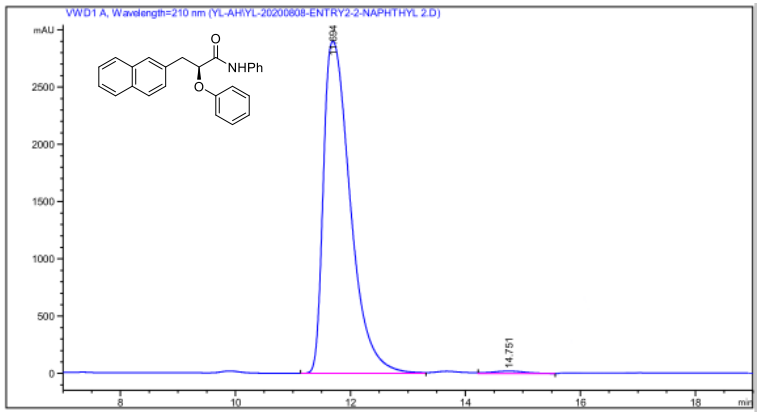
#	[min]		[min]	[mAU*s]	[mAU]	%
1	9.248	VB	0.3408	1.15434e4	520.37146	49.9124
2	12.895	BB	0.4461	1.15839e4	399.75323	50.0876



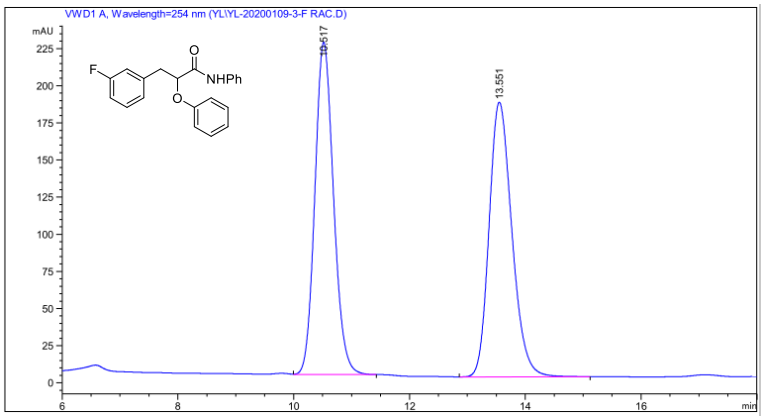
#	[min]			[mAU*s]	[mAU]	%
1	9.577	1	BV	7.77235e4	2954.75293	97.5153
2	13.601	1	BB	1980.39404	58.49048	2.4847



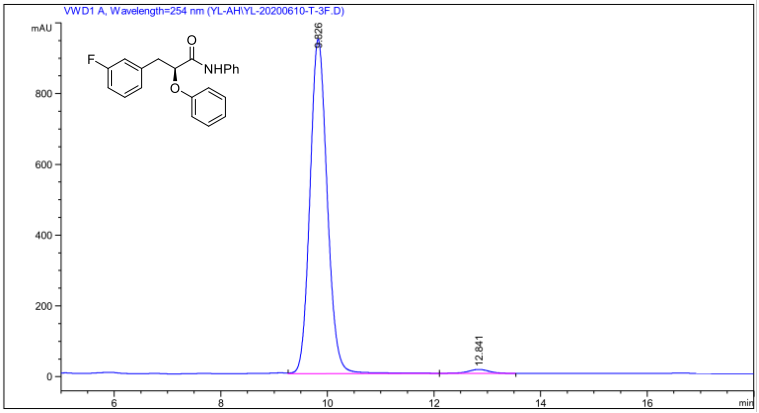
#	[min]		[min]	[mAU*s]	[mAU]	%
1	11.886	VV	0.3948	1.23524e4	479.14896	50.5720
2	14.258	BV	0.4600	1.20730e4	405.90540	49.4280



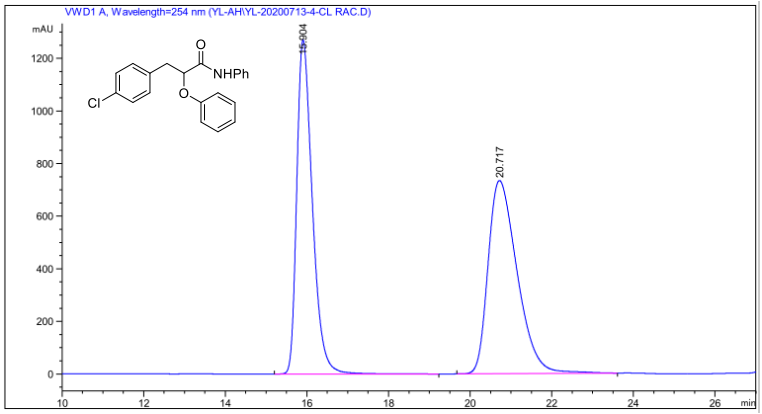
#	[min]			[mAU*s]	[mAU]	%
1	11.694	1	BV	9.42913e4	2900.42627	99.1094
2	14.751	1	VB	847.27905	21.02848	0.8906



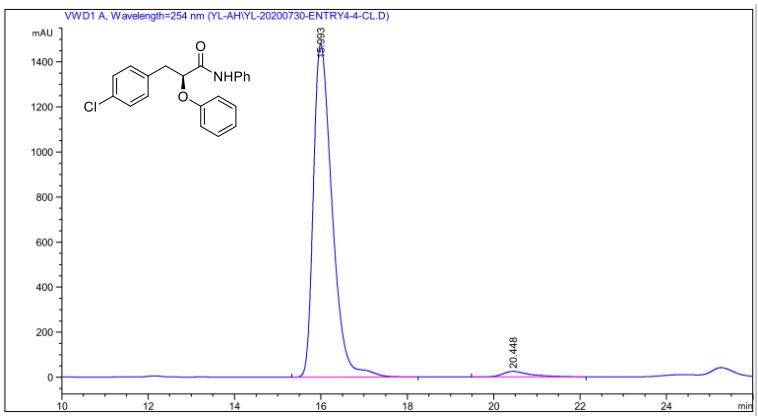
#	[min]			[mAU*s]	[mAU]	%
1	10.517	1	VB	5010.32080	223.72888	49.7766
2	13.551	1	BB	5055.29883	184.92642	50.2234



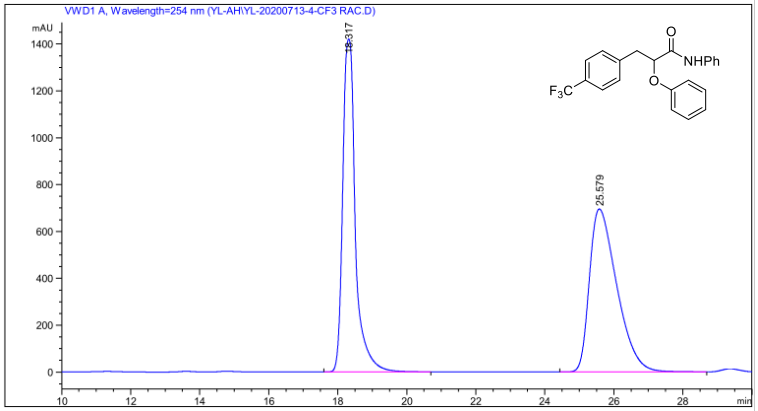
#	[min]			[mAU*s]	[mAU]	%
1	9.826	1	VB	2.12035e4	945.15222	98.6637
2	12.841	1	BB	287.18787	10.94187	1.3363



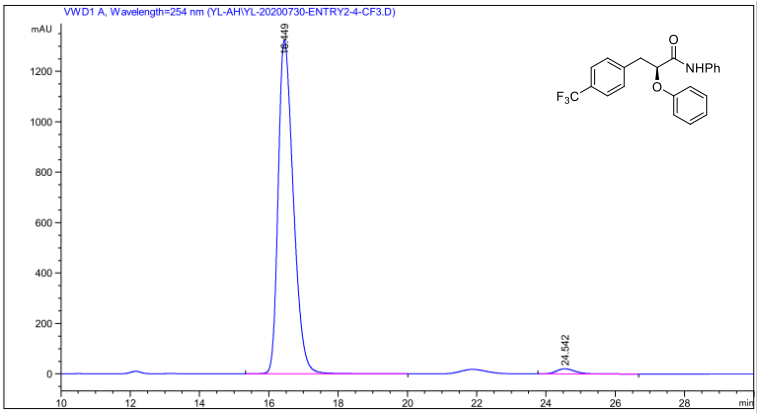
#	[min]			[mAU*s]	[mAU]	%
1	15.904	1	BB	3.36264e4	1269.64490	48.1242
2	20.717	1	BB	3.62478e4	734.32025	51.8758



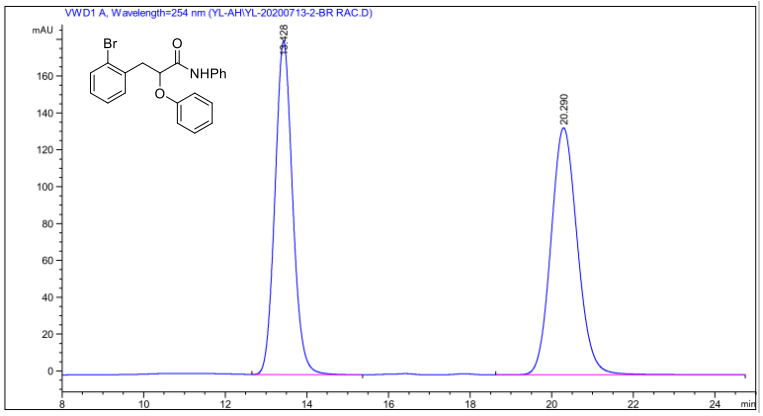
#	[min]			[mAU*s]	[mAU]	%
1	15.993	1	BB	4.43559e4	1478.90100	97.5475
2	20.448	1	BB	1115.17395	24.90404	2.4525



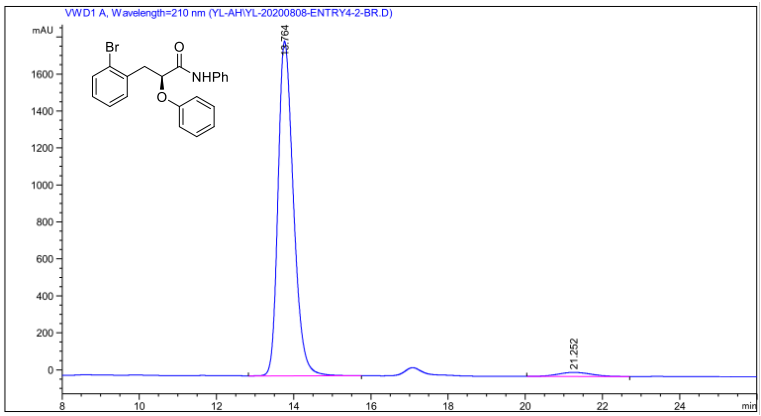
#	[min]			[mAU*s]	[mAU]	%
1	18.317	1	BB	3.60398e4	1421.15356	48.4410
2	25.579	1	BB	3.83596e4	695.75464	51.5590



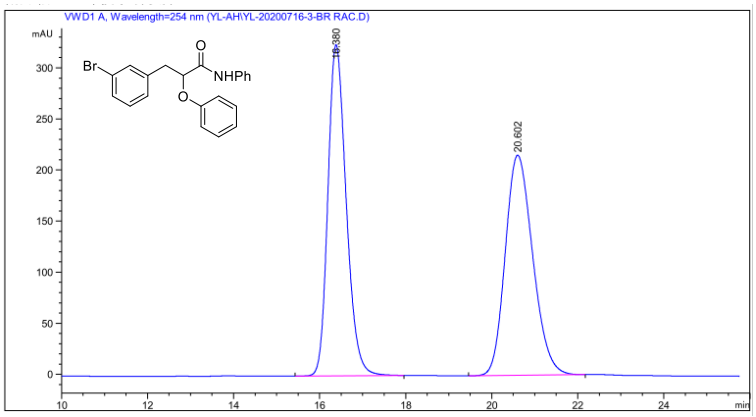
#	[min]			[mAU*s]	[mAU]	%
1	16.449	1	BB	4.01037e4	1323.93127	98.0609
2	24.542	1	BB	793.02222	20.49789	1.9391



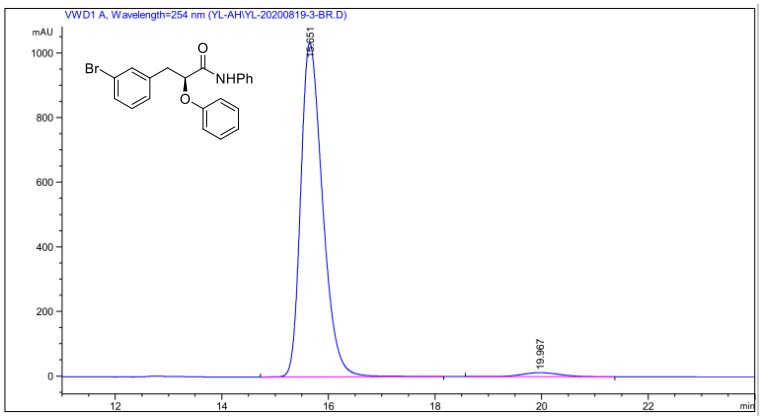
#	[min]			[mAU*s]	[mAU]	%
1	13.428	1	BB	5439.04883	180.97034	47.4403
2	20.290	1	BBA	6025.99072	134.07500	52.5597



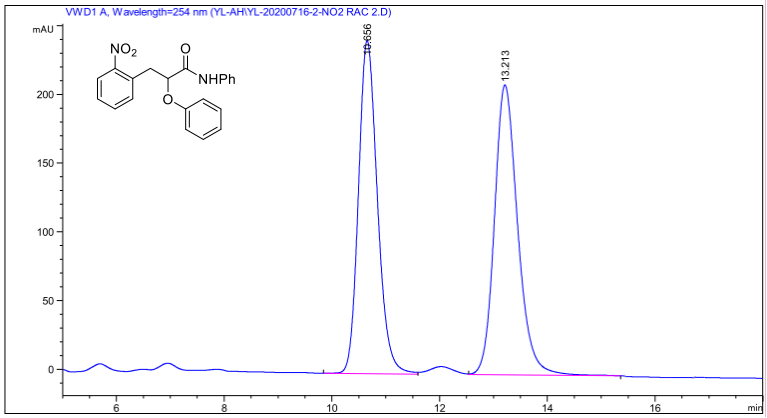
#	[min]			[mAU*s]	[mAU]	%
1	13.764	1	BB	5.01149e4	1809.73901	97.4500
2	21.252	1	BB	1311.37085	21.95840	2.5500



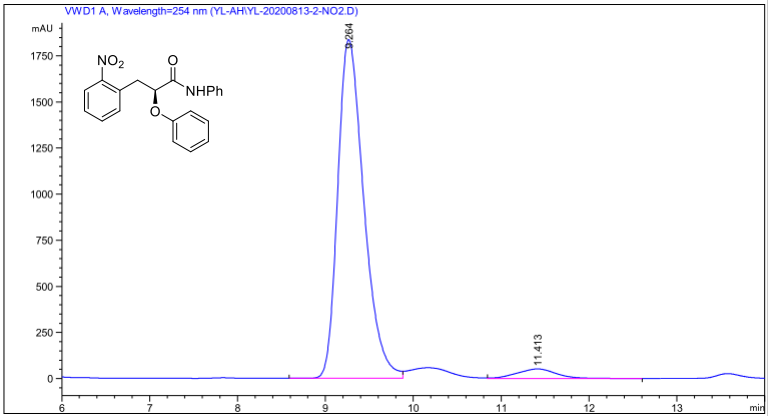
#	[min]			[mAU*s]	[mAU]	%
1	16.380	1	BB	9565.92285	324.09955	49.9932
2	20.602	1	BB	9568.51270	215.48250	50.0068



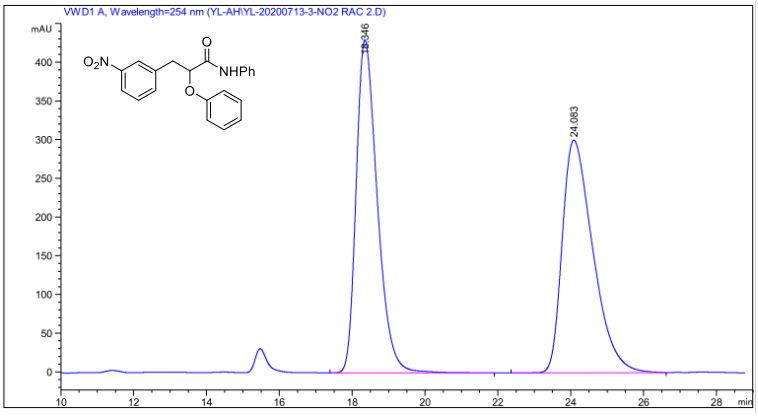
#	[min]		[min]	[mAU*s]	[mAU]	%
1	15.651	BB	0.4379	2.93947e4	1033.24084	97.9238
2	19.967	BB	0.7639	623.23676	12.51628	2.0762



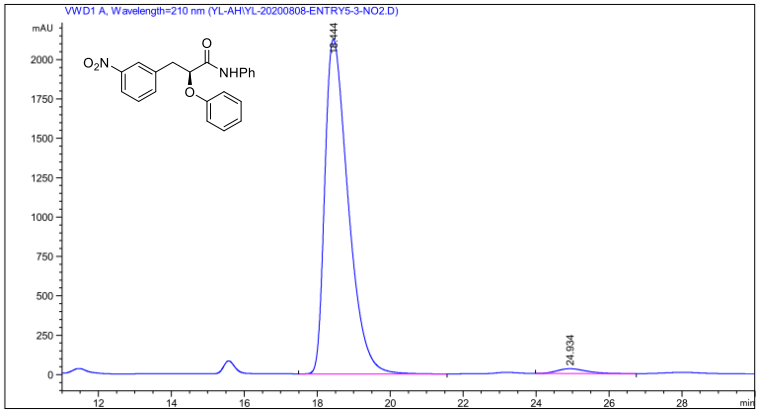
#	[min]			[mAU*s]	[mAU]	%
1	10.656	1	BV	5924.78223	242.27364	48.4093
2	13.213	1	VB	6314.15527	210.75914	51.5907



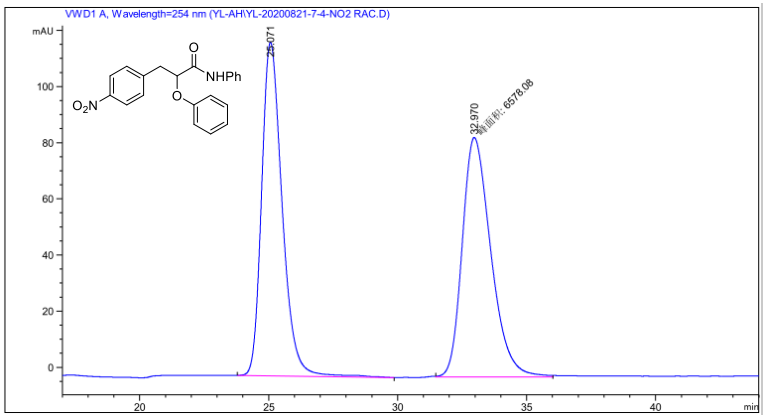
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	9.264	BV	0.3166	3.78936e4	1837.24390	96.0075
2	11.413	VB	0.4571	1575.79480	51.48765	3.9925



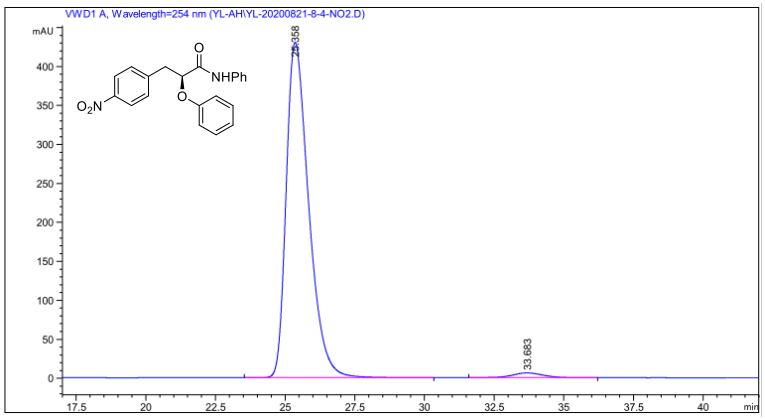
#	[min]			[mAU*s]	[mAU]	%
1	18.346	1	BB	1.73493e4	430.00061	49.6739
2	24.083	1	BB	1.75772e4	300.38028	50.3261



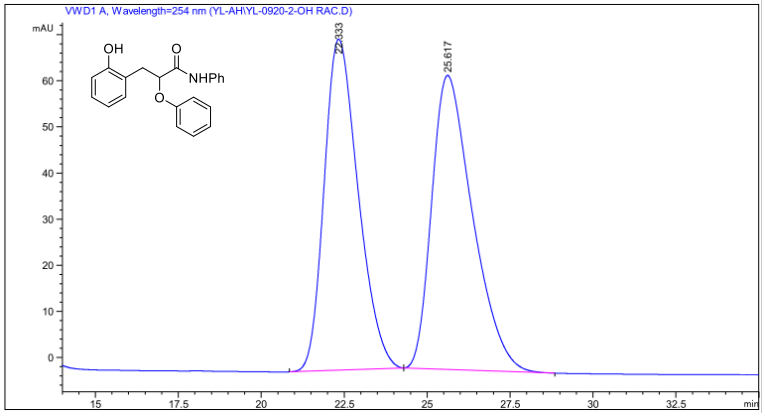
#	[min]			[mAU*s]	[mAU]	%
1	18.444	1	BB	9.42284e4	2125.34717	98.2158
2	24.934	1	BB	1711.75049	30.70453	1.7842



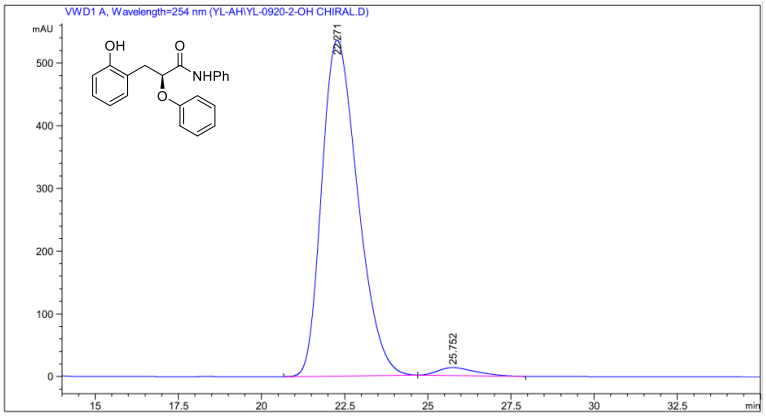
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	25.071	BB	0.8481	6570.88721	118.82989	49.9727
2	32.970	MM	1.2852	6578.07617	85.30623	50.0273



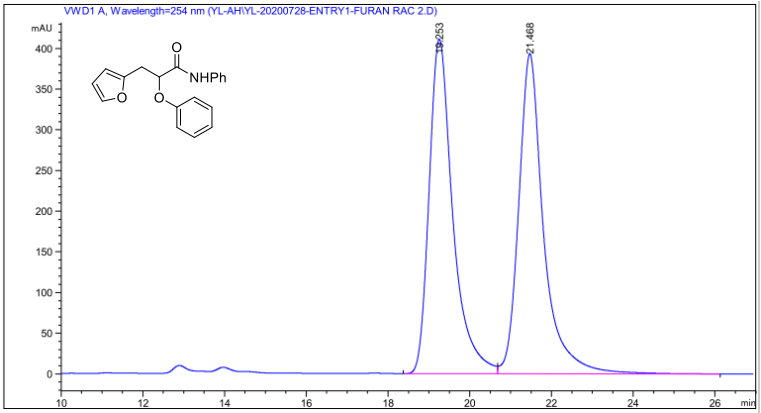
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	25.358	BB	0.8578	2.41147e4	430.29785	98.0319
2	33.683	BB	1.1100	484.12451	6.13918	1.9681



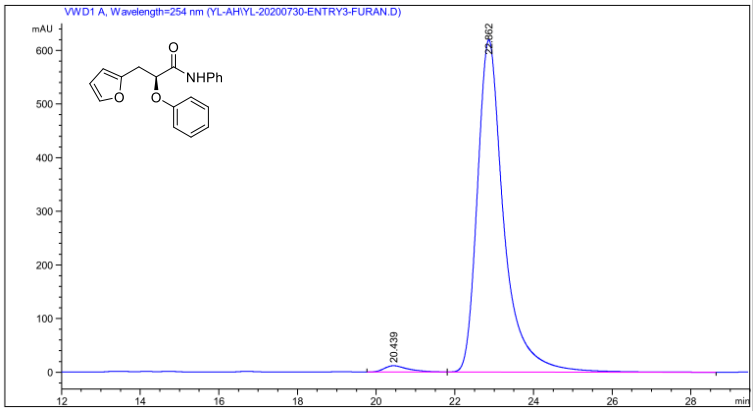
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	22.333	BB	1.0828	5126.80029	71.81991	48.3935
2	25.617	BB	1.2794	5467.18945	63.82139	51.6065



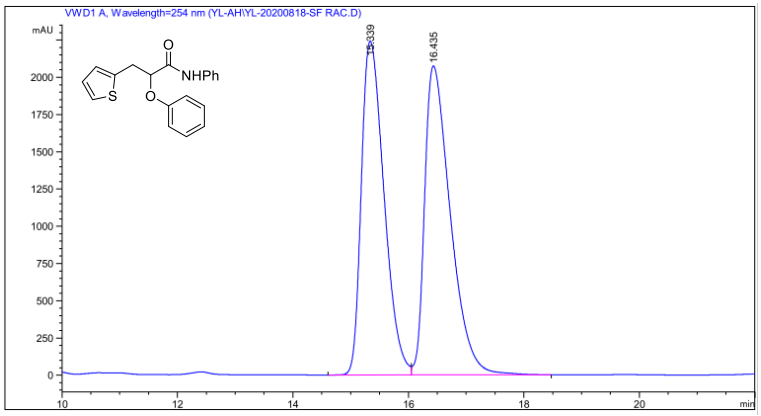
峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	22.271	BB	1.1664	4.02789e4	535.60815	97.6476
2	25.752	BB	1.1390	970.35370	12.55016	2.3524



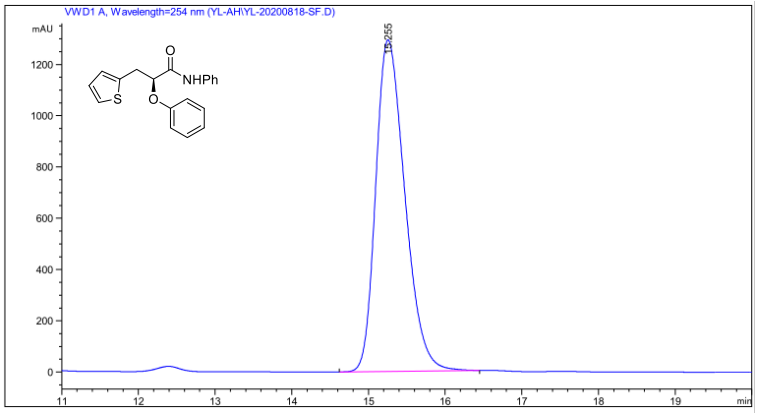
#	[min]			[mAU*s]	[mAU]	%
1	19.253	1	BV	1.65651e4	411.12802	49.8287
2	21.468	1	VB	1.66790e4	393.25052	50.1713



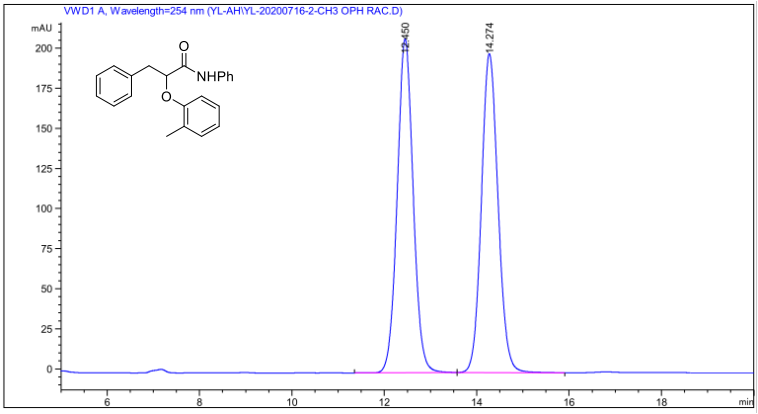
#	[min]			[mAU*s]	[mAU]	%
1	20.439	1	BB	499.55112	11.76875	1.6990
2	22.862	1	BB	2.89036e4	619.23315	98.3010



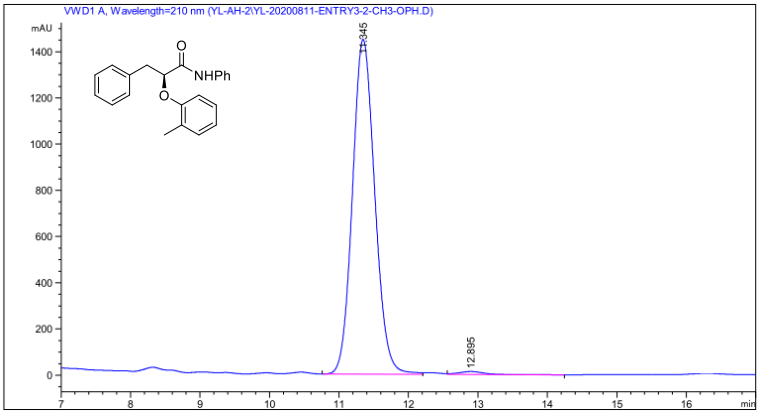
#	[min]			[mAU*s]	[mAU]	%
1	15.339	1	BV	6.10272e4	2241.39893	48.7293
2	16.435	1	VB	6.42101e4	2074.55322	51.2707



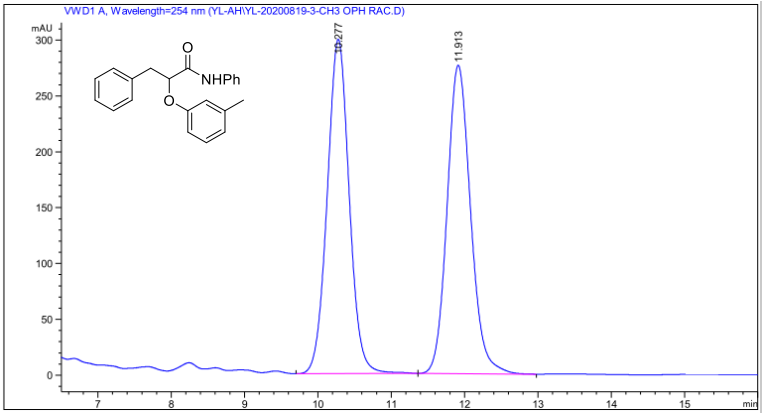
#	[min]			[mAU*s]	[mAU]	%
1	15.255	1	BB	3.41322e4	1293.49548	100.0000



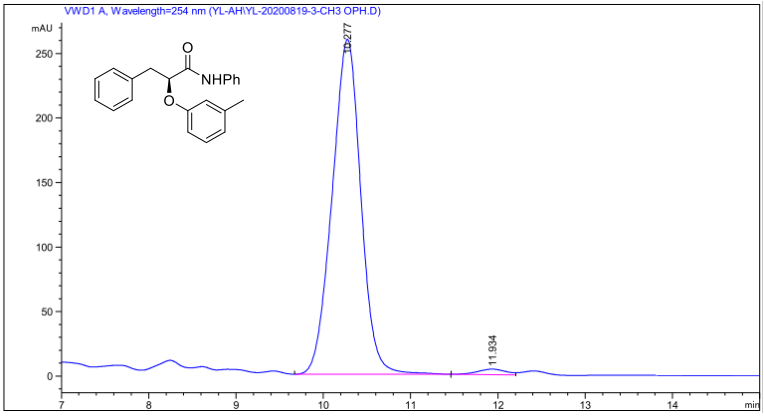
#	[min]			[mAU*s]	[mAU]	%
1	12.450	1	BB	5004.16504	208.01425	50.1476
2	14.274	1	BB	4974.70508	198.77635	49.8524



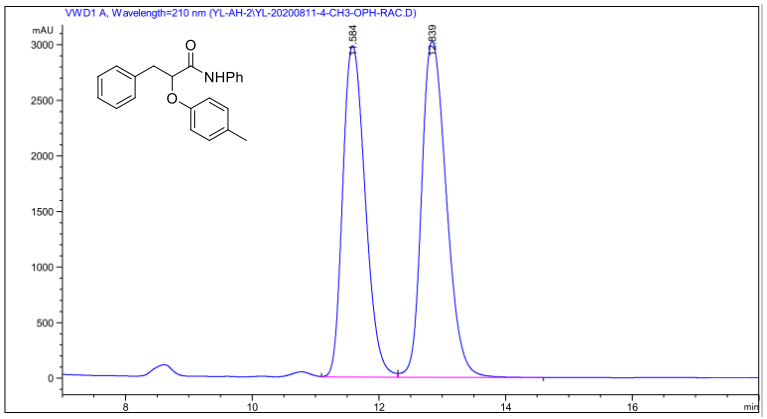
#	[min]			[mAU*s]	[mAU]	%
1	11.345	1	BV	3.23429e4	1449.16553	99.0043
2	12.895	1	VB	325.28265	12.77266	0.9957



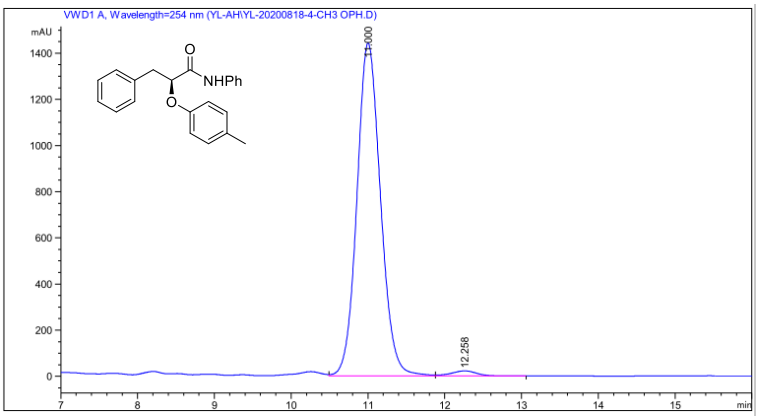
#	[min]		[min]	[mAU*s]	[mAU]	%
1	10.277	BB	0.3200	6236.04785	299.35339	50.3699
2	11.913	BB	0.3436	6144.44824	276.12079	49.6301



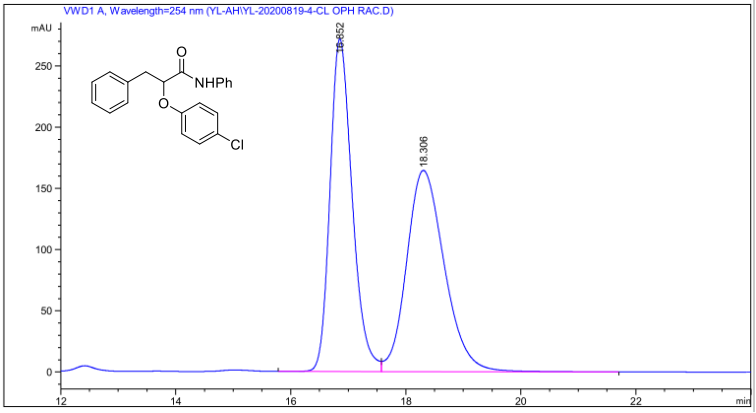
#	[min]		[min]	[mAU*s]	[mAU]	%
1	10.277	BB	0.3466	5932.52295	259.57349	98.4209
2	11.934	BV	0.3417	95.18607	4.24379	1.5791



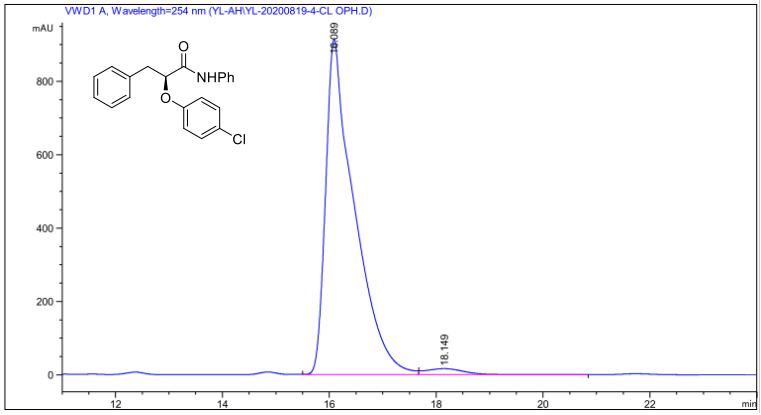
#	[min]			[mAU*s]	[mAU]	%
1	11.584	1	VV	7.34637e4	2982.30029	47.3285
2	12.839	1	VB	8.17572e4	3023.28638	52.6715



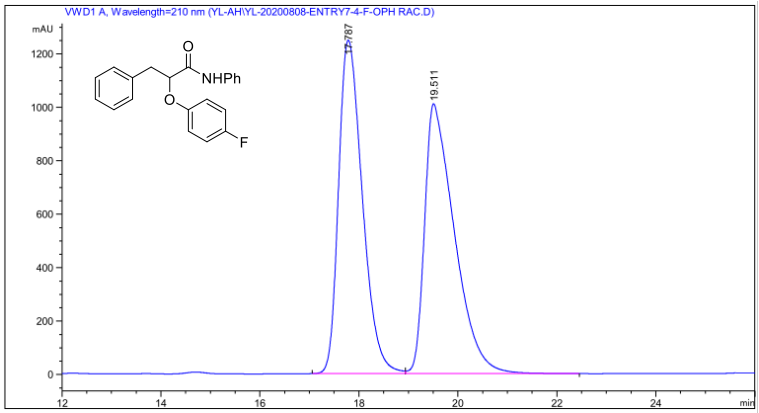
#	[min]			[mAU*s]	[mAU]	%
1	11.000	1	VV	3.07398e4	1442.26489	98.3754
2	12.258	1	VB	507.64709	21.94230	1.6246



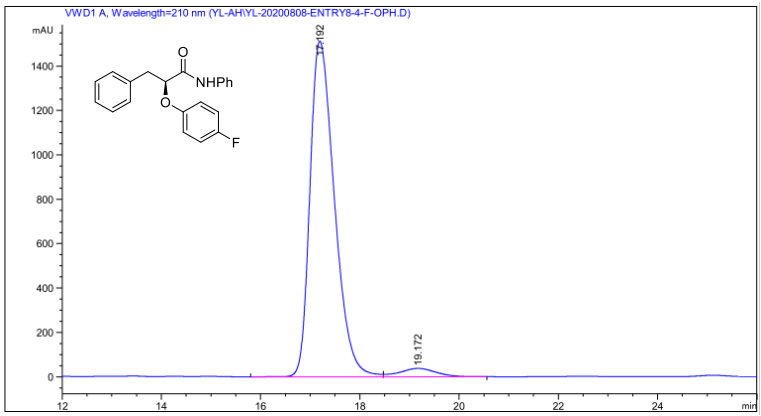
#	[min]		[min]	[mAU*s]	[mAU]	%
1	16.852	BV	0.4140	7286.13916	271.61575	49.2759
2	18.306	VB	0.7035	7500.28711	164.31425	50.7241



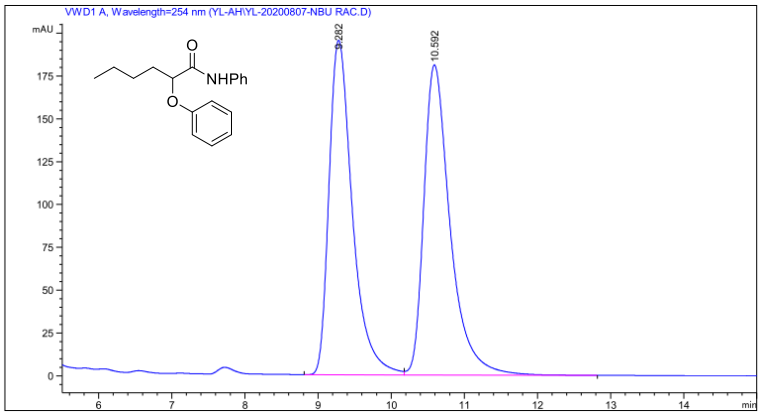
#	[min]		[min]	[mAU*s]	[mAU]	%
1	16.089	VV	0.5005	3.42088e4	914.24762	97.6014
2	18.149	VB	0.7582	840.69275	16.58998	2.3986



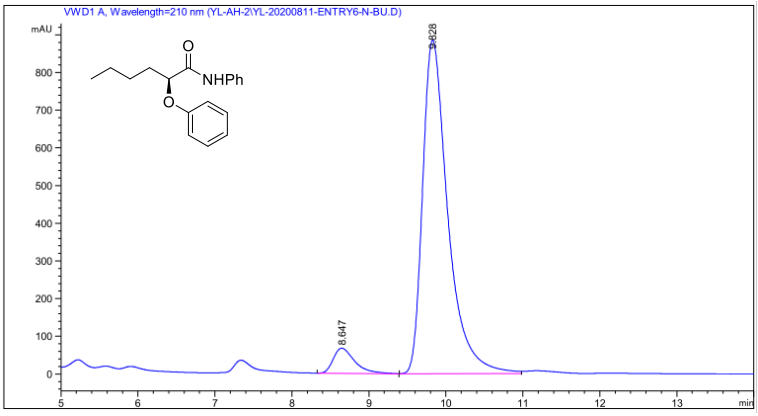
#	[min]			[mAU*s]	[mAU]	%
1	17.787	1	BV	4.16202e4	1248.31604	49.6598
2	19.511	1	VB	4.21905e4	1010.03119	50.3402



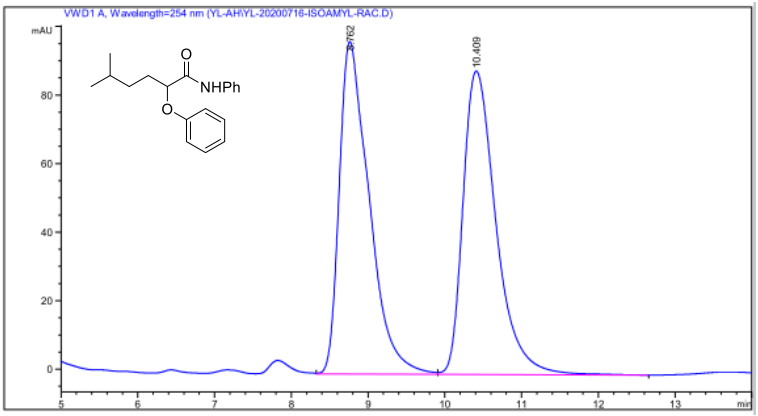
#	[min]			[mAU*s]	[mAU]	%
1	17.192	1	BV	5.16933e4	1511.80249	96.4185
2	19.172	1	VB	1920.15015	37.73603	3.5815



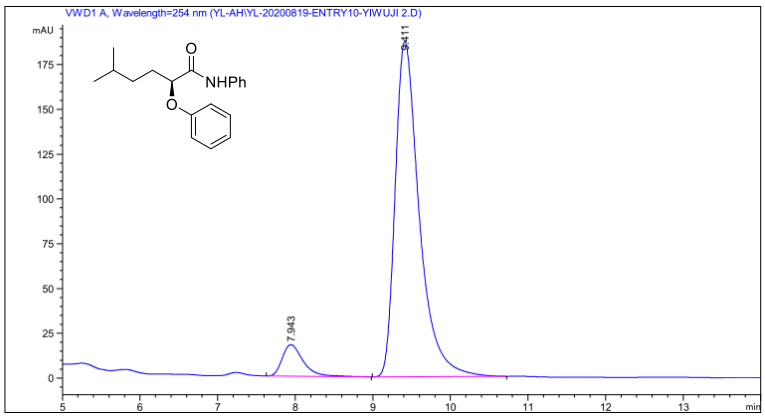
#	[min]		[min]	[mAU*s]	[mAU]	%
1	9.282	BV	0.3391	4334.91016	195.19812	48.9162
2	10.592	VB	0.3778	4527.00049	180.96936	51.0838



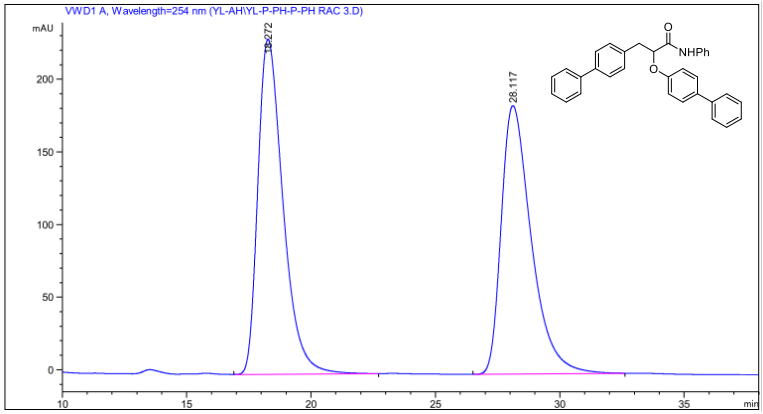
#	[min]			[mAU*s]	[mAU]	%
1	8.647	1	VB	1301.62415	66.89622	6.0664
2	9.828	1	BV	2.01546e4	885.21307	93.9336



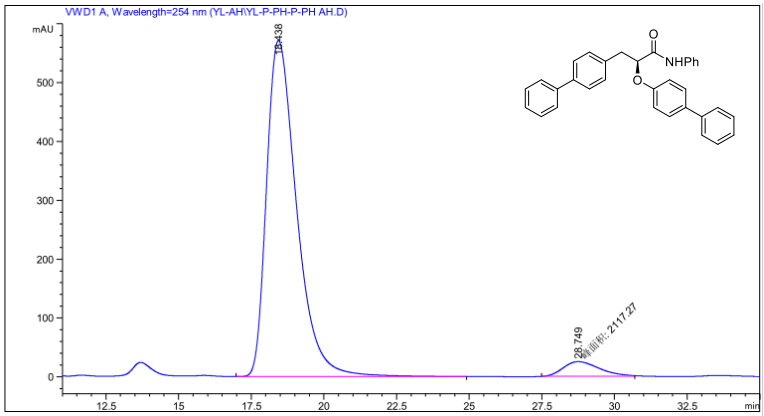
#	[min]			[mAU*s]	[mAU]	%
1	8.762	1	VV	2621.95947	96.99129	49.7918
2	10.409	1	VB	2643.88965	88.54160	50.2082



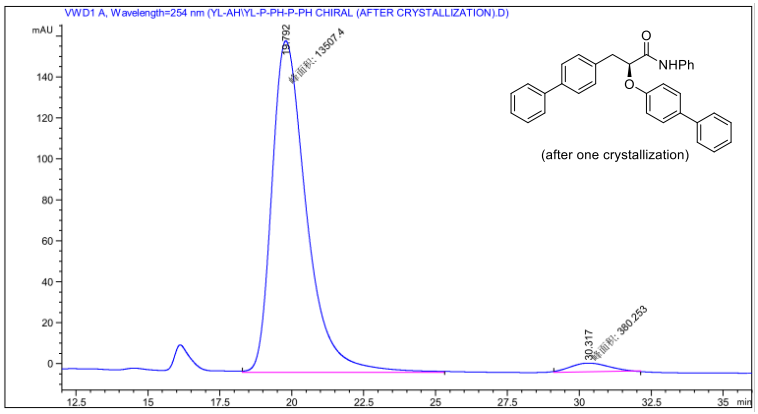
#	[min]		[min]	[mAU*s]	[mAU]	%
1	7.943	BB	0.2874	329.58185	17.52781	7.5501
2	9.411	BB	0.3254	4035.69653	187.25356	92.4499



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.272	BB	1.0744	1.61807e4	230.65280	51.0787
2	28.117	BB	1.2706	1.54973e4	184.76176	48.9213



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	18.438	BB	1.0990	4.09865e4	571.29266	95.0880
2	28.749	MM	1.4293	2117.27295	24.68872	4.9120



峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	19.792	MM	1.3917	1.35074e4	161.76389	97.2619
2	30.317	MM	1.5090	380.25308	4.19992	2.7381