Supporting Information for the manuscript:

Stereo-selective synthesis of non-canonical *γ*-hydroxy-*α*-amino acids by enzymatic carbon-carbon bond formation

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Content

Supplementary Figure S1-S6

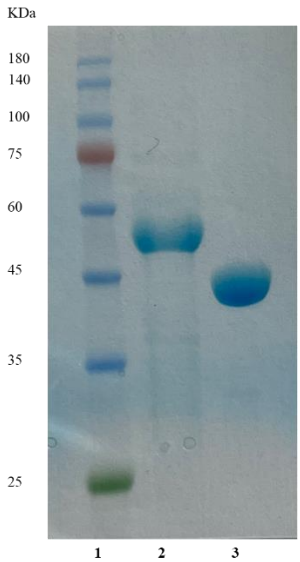


Figure S1. SDS PAGE of ApUstD and PfK. Lane **1**: protein markers, lane **2**: purified ApUstD, lane **3**: purified PfK.

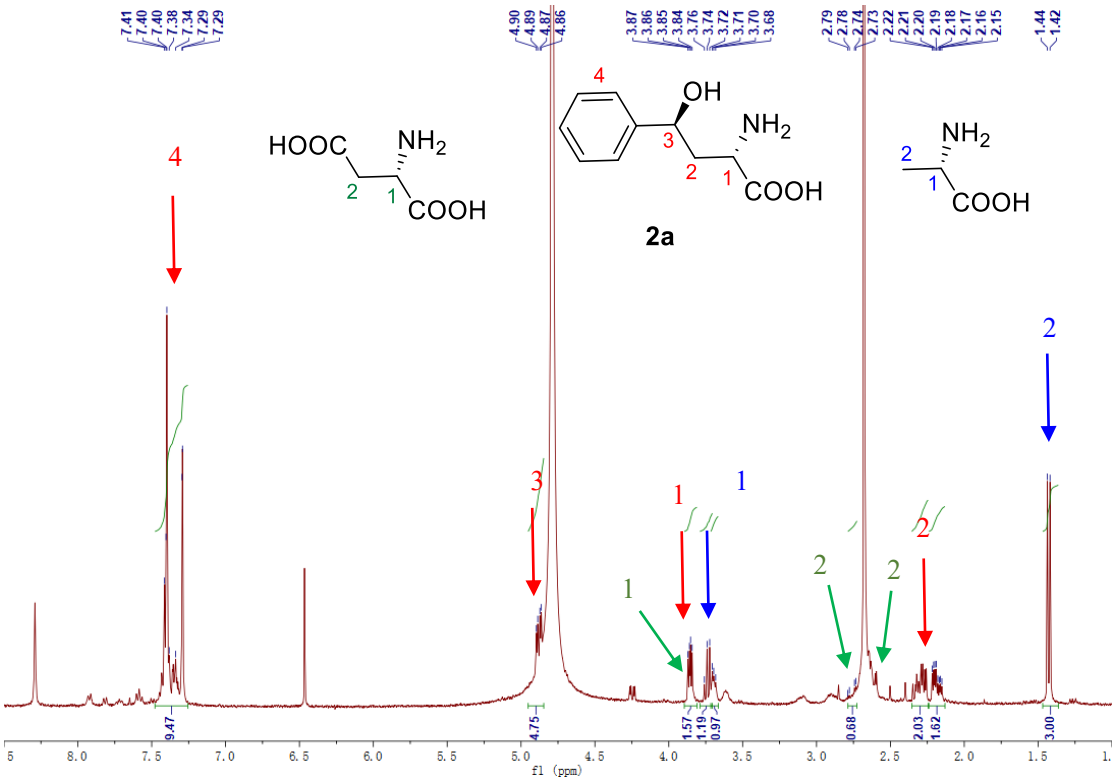


Figure S2. ApUstD reaction with L-Asp and benzaldehyde. 1 ml reaction containing 4 mM L-aspartic acid, 5 mM benzaldehyde (**1a**), 1mM dithiothreitol, 100 µM PLP and 0.3 mg/ml ApUstD in 50 mM phosphate buffer, at pH 7.4 were run at 25 °C for 24 hours. Reaction mixture was lyophilized, and then was dissolved in 600 µl D_2O. ^1H NMR was recorded thereafter. Resonances of different compound were assigned.

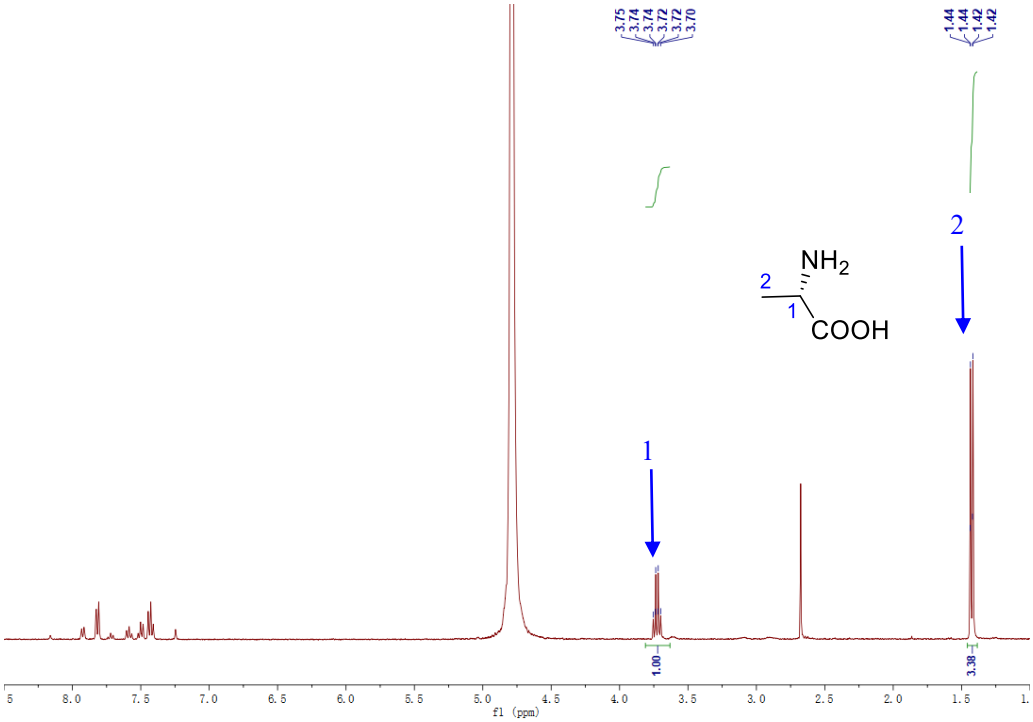


Figure S3. ApUstD reaction with L-Alanine and benzaldehyde. 1 ml reaction containing 4 mM L-alanine, 5 mM benzaldehyde (**1a**), 1mM dithiothreitol, 100 µM PLP and 0.3 mg/ml ApUstD in 50 mM phosphate buffer, at pH 7.4 were run at 25 °C for 24 hours. Reaction mixture was lyophilized, and then was dissolved in 600 µl D_2O. ^1H NMR was recorded thereafter. No product was observed.

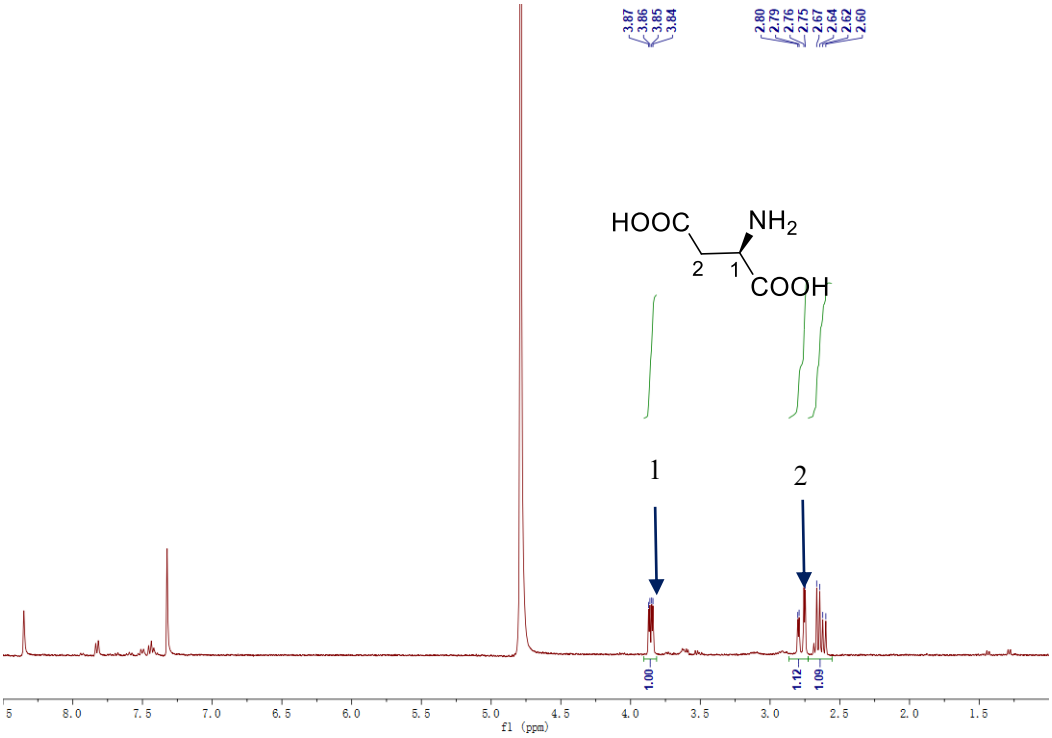


Figure S4. ApUstD reaction with D-Asp and benzaldehyde. 1 ml reaction containing 4 mM D-aspartic acid, 5 mM benzaldehyde (**1a**), 1mM dithiothreitol, 100 µM PLP and 0.3 mg/ml ApUstD in 50 mM phosphate buffer, at pH 7.4 were run at 25 °C for 24 hours. Reaction mixture was lyophilized, and then was dissolved in 600 µl D_2O. ^1H NMR was recorded thereafter. No product

was observed.

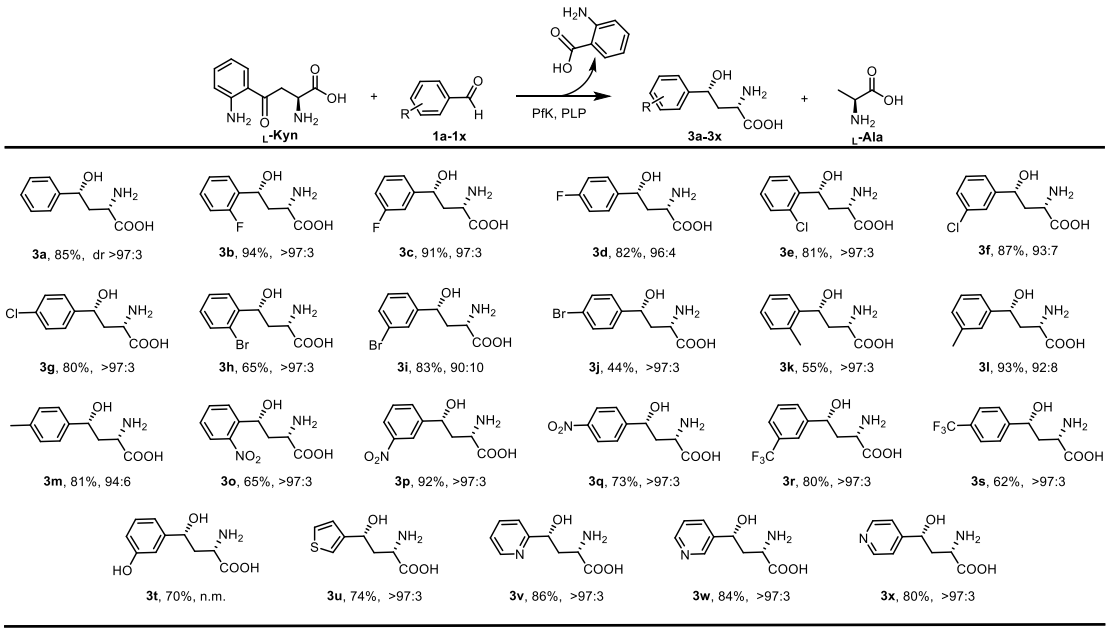


Figure S5. Conversion and diastereoisomeric ratio (d.r.) of **3a-3x** from PfK reaction. Reaction details were indicated in the method section.

X-ray crystallographic analyses of 2c

Colorless needle crystals of **2c** were obtained by recrystallization from methanol. The crystal data was collected on a Bruker D8 VENTURE diffractometer by CuKα radition (λ = 1.54178). Integration and scaling of intensity data was performed using the SAINT program. Data were corrected for the effects of absorption using SADABS. The structures were solved by direct method and refined with full-matrix least-squares technique using SHELX-2014 software. Non-hydrogen atoms were refined with anisotropic displacement parameters, and hydrogen atoms were placed in calculated positions and refined with a riding model. The crystallographic data have been deposited at the Cambridge Crystallographic Data Center (deposition no. CCDC 2084340), which can be obtained free of charge from the CCDC via https://www.ccdc.cam.ac.uk/data_request/cif.

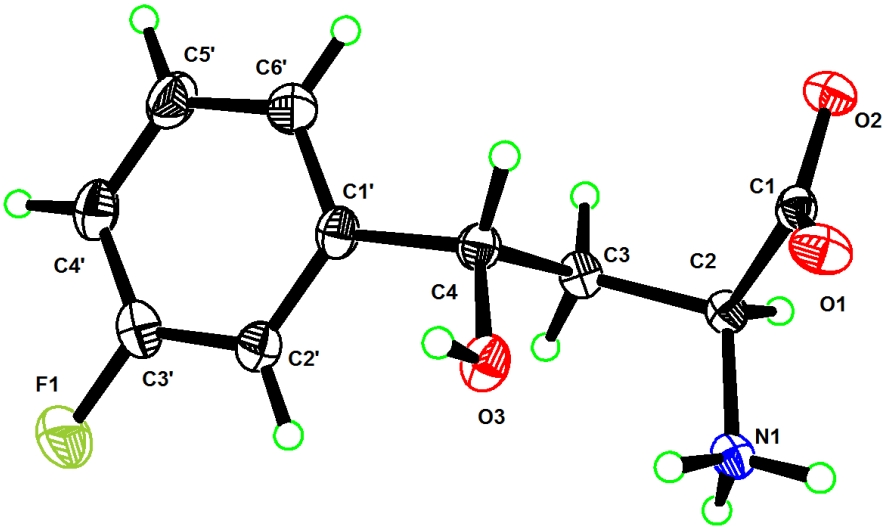


Figure S6. Perspective ORTEP drawing for **2c**

Supplementary Tables

Table S1. ApUstD reaction with L-Asp and benzaldehyde.

	Enzyme	L-Asp	1a	time	temp	2a	L-Ala	L-Asp
1	0.3 mg/ml	4 mM	5 mM	24 h	25 ℃	49.1 %	30.3 %	20.6 %
2	0.3 mg/ml	4 mM	10 mM	24 h	25 ℃	75.9 %	24.1 %	<0.1 %
3	0.3 mg/ml	4 mM	20 mM	24 h	25 ℃	84.4 %	12.2 %	3.4 %
4	0.3 mg/ml	4 mM	40 mM	24 h	25 ℃	84.9 %	6.1 %	9.0 %
5	0.3 mg/ml	8 mM	40 mM	24 h	25 ℃	76.9 %	6.7 %	16.4 %

1 ml reaction containing both substrates, 1mM dithiothreitol, 100 μM PLP and 0.4 mg/ml ApUstD in 50 mM phosphate buffer, at pH 7.4 were run at 25 °C. Substrate concentration was indicated in different entries. Relatvie content of different compounds were determined based on the integrals from ^{1}H NMR.

Table S2. X-ray crystallographic data for **2c**

Identification code	cu_2021524_0m
Empirical formula	$C_{10}H_{12}FNO_3$
Formula weight	213.21
Temperature/K	170.0
Crystal system	monoclinic
Space group	$P2_1$
a/Å	5.93840(10)
b/Å	5.30530(10)
c/Å	15.9518(4)
α/°	90
β/°	93.2890(10)
γ/°	90
Volume/Å^3	501.734(18)
Z	2
ρ_{calc}g/cm^3	1.411
μ/mm^{-1}	0.993
F(000)	224.0
Crystal size/mm^3	0.15 × 0.08 × 0.05
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	5.55 to 127.37
Index ranges	-6 ≤ h ≤ 6, -6 ≤ k ≤ 6, -18 ≤ l ≤ 18
Reflections collected	5180
Independent reflections	1596 [R_{int} = 0.0275, R_{sigma} = 0.0272]
Data/restraints/parameters	1596/1/149
Goodness-of-fit on F^2	1.095
Final R indexes [I>=2σ (I)]	R_1 = 0.0260, wR_2 = 0.0656
Final R indexes [all data]	R_1 = 0.0268, wR_2 = 0.0676
Largest diff. peak/hole / e Å^{-3}	0.15/-0.13
Flack parameter	0.13(8)

Table S3. Kinetic parameters of ApUstD with different substrates.

Substrate	k_{cat} (min^{-1})	K_M (μM)	k_{cat}/K_M ($M^{-1}min^{-1}$)
3-F (**1c**)	5.0 ± 0.1	3400 ± 200	1400
2-Br (**1h**)	3.5 ± 0.1	1700 ± 200	2000
4-NO_2 (**1q**)	6.9 ± 0.3	400 ± 40	17000

200 μl reaction containing 12 mM L-aspartic acid, 100 μM PLP, 0.3 mg/ml ApUstD and varied aldehyde concentration in 50 mM phosphate buffer at pH 7.4 were run at 25 °C. 40 μl of reaction mixture were quenched by 20 μl of 1M HCl after 1, 2, 3, 4, 5 minutes respectively. The product formation was monitored by HPLC-UV.

Supplementary Methods

General

All enzyme-encoding pET-28a(+) based expression plasmids were purchased from GenScript and expression strain *E. coli* BL21 (DE3) were purchased from Sangon Biotech. Proteins were analyzed by sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE) under denaturing conditions. The gels were stained with Coomassie brilliant blue.

The crystal data was collected on a Bruker D8 VENTURE diffractometer. Semi-Preparative HPLC was performed on a Waters 1525 instrument with a Waters 2489 UV detector using a DAICEL CHIRALPAK IF column (S-5 μm, 250 × 10 mml) and a Water SunFire column (S-5 μm, 100 × 19 mm). HRESIMS spectra were recorded on an Angilent G6520 Q-Tof mass detector. NMR spectra were recorded using the Bruker AVANCE III 400, 500 and 600 MHz instrument. Standard abbreviations indicating multiplicity were used as follows: s (singlet), d (doublet), t (triplet), and m (multiplet). Chemical shifts were reported in ppm (δ), coupling constants (J) in hertz. Econosep C18 60A (50 μm, DIKMA, China) was used for column chromatography (CC).

Antibiotics, isopropyl β-D-thiogalactoside (IPTG) and dithiothreitol (DTT) were purchased from Sangon Biotech. L-Aspartic acid was purchased from RHAWN. Aldehyde substrates were purchased from *J & K* SCIENTIFIC LTD. and bidephamarmatech. PLP and L-kynurenine were from *J & K*. Deuterated solvents were purchased from *J & K* SCIENTIFIC LTD. High pressure cell disrupter and Ni-NTA unionrose 6FF agarose were purchased from Union Biotech.

Protein expression and purification

E. coli BL21 (DE3) cells were transformed with pET-28a(+) expression plasmids by heat shock. Transformed cells were first cultivated on solid medium (LB-AGAR plates with 50 μg/ml kanamycin) and then in liquid medium (LB with 50 μg/ml kanamycin). After incubation at 37°C overnight, 15 ml of pre-culture was used to inoculate fresh Terrific Broth (TB) medium (1L) with kanamycin (50 μg/ml). The cells were grown in 3L shaking flask at 37 °C (170 rpm) until OD600 reached 1.0. The culture was cooled to 18 °C and supplemented with 100 μM isopropyl β-D-thiogalactoside (IPTG). This culture was incubated at 18 °C for 20 hours. Cells were harvested by centrifugation at 13000 g for 15 minutes and stored at -20 °C.

For purification of ApUstD, cell pellets (10 g) were suspended in 50 ml lysis buffer (50 mM sodium phosphate, 300 mM NaCl, pH 8.0). Cells were disrupted by high pressure

cell disrupter for 3 times. Lysates were centrifuged at 42000 g for 15 min at 4 °C. The cleared lysate was loaded onto a Ni-NTA unionrose 6FF agarose column. The agarose beads were washed with 150 ml lysis buffer containing 100 mM, 150 mM and 200 mM imidazole respectively. The protein was eluted in a lysis buffer solution containing 500 mM imidazole. Protein containing fractions were collected and dialyzed against dialysis buffer (50 mM sodium phosphate, 50 mM NaCl, 1 mM dithiothreitol, 100 μM PLP, pH 7.4). Protein was used directly after dialysis (yield, 2.3 mg/L).

For purification of PfK, cell pellets (10 g) were suspended in 50 ml lysis buffer (50 mM sodium phosphate, 300 mM NaCl, pH 8.0). Cells were disrupted by high pressure cell disrupter for 3 times. Lysates were centrifuged at 42000 g for 20 min at 4 °C. The cleared lysate was loaded onto a Ni NTA unionrose 6FF agarose column. The agarose beads were washed with 100 ml lysis buffer containing 10 mM and 20 mM imidazole respectively. The protein was eluted in a lysis buffer solution containing 250 mM imidazole. Protein containing fractions were collected and dialyzed against dialysis buffer (50 mM sodium phosphate, 50 mM NaCl, 100 μM PLP, pH 7.4), aliquoted and stored at -80 °C.

Protein sequence:

ApUstD

MGSSHHHHHHSSGLVPGSHMKSVANSSLHDVDKDSVPLSSGTNGTTQAETPLDNVID
VESVRSHFPVLEGETAAFNNASGTVVLKEAIESTSKFMFSFPFPPGVDAKSMEAITA
YTGNKGKVATFINALPDEITFGQSTTCLFRLLGLSLKPMLNSDCEIVCSTLCHEAAA
SAWIHLSRDLGITIKWWSPTTTPNSPDDPVLTTDSLKPLLSPKTRLVTCNHVSNVVG
TIHPIREIADVVHAIPGCMLIVDGVACVPHRPVDVKELDVDFYCFSWYKLFGPHMGT
LYASRKAQDRYMTSINHYFLSSSSLDGKLALGMPSFELQLMCSPIVSYLQDIVGWDR
IVRQETVLVKILLQYLLSKPGVYRVFGRRNSDPSQRVSIVTFEVVGRSSGDVAMRVN
TRNRFRITSGICLAPRPTWDVLKPVSADGLIRVSFVHYNTVEEVREFCNELDEIVTQ
DT

PfK

MGSSHHHHHHSSGLVPGSHMGTTRNDCLALDAQDSLAPLRQQFALPEGVIYLDGNSL
GARPVAALARAQAVIAEEWGNGLIRSWNSAGWRDLSERLGNRLATLIGARDGEVVVT
DTTSINLFKVLSAALRVQATRSPERRVIVTETSNFPTDLYIAEGLADMLQQGYTLRL
VDSPEELPQAIDQDTAVVMLTHVNYKTGYMHDMQALTALSHECGALAIWDLAHSAGA
VPVDLHQAGADYAIGCTYKYLNGGPGSQAFVWVSPQLCDLVPQPLSGWFGHSRQFAM
EPRYEPSNGIARYLCGTQPITSLAMVECGLDVFAQTDMASLRRKSLALTDLFIELVE
QRCAAHELTLVTPREHAKRGSHVSFEHPEGYAVIQALIDRGVIGDYREPRIMRFGFT
PLYTTFTEVWDAVQILGEILDRKTWAQAQFQVRHSVT

Time dependent Progress of ApUstD reaction

Reaction containing 12 mM L-aspartic acid, 80 mM benzaldehyde (**1a**), 100 μM PLP and 0.3 mg/ml ApUstD in 50 mM phosphate buffer, at pH 7.4 were run at 25 °C. 1 ml reaction mixture was lyophilized at different time point (12h, 24h, 48h, 72h, 96h). After lyophilization, the mixture was dissolved in 600 μl D_2O and submitted to ^1H NMR measurement. Relative content of different compounds was calculated based on integrals of key ^1H NMR resonances and shown in Figure 2b.

Determination of conversion and diastereoisomeric ratio (d.r.)

Products of **2a-2f, 2h, 2i, 2r, 2s, 2u-2aa and 2ad**: 1 ml reactions containing 0.4 mg ApUstD, 12 mM L-Aspartic acid, 80 mM aldehyde, 1 mM DTT, 100 μM PLP and 50 mM sodium phosphate, 50 mM NaCl, at pH 7.4 were run at 25 °C. After 72 hours, the reaction mixtures were centrifugated and lyophilized. After lyophilization, the mixtures were dissolved in 600 μl of D_2O. ^1H NMR were recorded. Conversion efficiency (% of consumed amino acid) and ratio of different products were determined by integration of characteristic ^1H NMR resonances from different compounds.

Products of **2g, 2j, 2o-2q and 2t**: 1 ml reactions containing 0.4 mg ApUstD, 12 mM L-Aspartic acid, 80 mM aldehyde, 4% DMSO (v/v), 1 mM DTT, 100 μM PLP and 50 mM sodium phosphate, 50 mM NaCl, at pH 7.4 were run at 25 °C. After 72 hours, the reaction mixtures were centrifugated and lyophilized. After lyophilization, the mixtures were dissolved in 600 μl of D_2O. ^1H NMR were recorded. Conversion efficiency (% of consumed amino acid) and ratio of different products were determined by integration of characteristic ^1H NMR resonances from different compounds.

Products of **2k-2n, 2ab and 2ac**: 1 ml reactions containing 0.4 mg ApUstD, 12 mM L-Aspartic acid, 16 mM aldehyde, 2% DMSO (v/v), 1 mM DTT, 100 μM PLP and 50 mM sodium phosphate, 50 mM NaCl, at pH 7.4 were run at 25 °C. After 72 hours, the reaction mixtures were centrifugated and lyophilized. After lyophilization, the mixtures were dissolved in 600 μl of D_2O. ^1H NMR were recorded. Conversion efficiency (% of consumed amino acid) and ratio of different products were determined by integration of characteristic ^1H NMR resonances from different compounds.

Products of **3a-3x**: 1 ml reactions containing 0.5 mg PfK, 24 mM L-kynurenine, 180 mM aldehyde, 100 μM PLP and 50 mM sodium phosphate, 50 mM NaCl, at pH 7.4 were run at 25 °C. After 12 hours, the reaction mixtures were centrifugated and lyophilized. After lyophilization, the mixtures were dissolved in 600 μl of D_2O. ^1H NMR were recorded. Conversion efficiency (% of consumed L-kynurenine) and ratio of different products were determined by integration of characteristic ^1H NMR resonances from different compounds.

The diastereoisomeric ratio of ApUstD and PfK reactions were determined by

integration of ^{1}H NMR resonances of γ-H of the products and their diastereo-isomers (Figure S58-S85).

Determination of Kinetic Parameters

200 µl reaction containing 12 mM L-aspartic acid, 100 µM PLP, 0.3 mg/ml ApUstD and varied aldehyde concentration in 50 mM phosphate buffer at pH 7.4 were run at 25 °C. 40 µl of reaction mixture were quenched by 20 µl of 1M HCl after 1, 2, 3, 4, 5 minutes respectively. The product formation was monitored by HPLC-UV. Product concentration were calculated based on the respective calibration curve. Velocities were calculated and plotted against substrate concentrations. The velocity was fitted to equation of $v = v_{max} * [s] / (K_M + [s])$ and values of k_{cat}, K_M and k_{cat}/K_M were obtained thereafter.

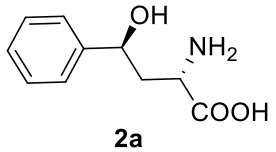
Semi-preparative reaction and characterization of Compounds

For the structural characterization of products **2a-2x** and **2ab**, 15 ml reactions were incubated for 72 h, lyophilized. Products of **2a-2x** were loaded on C18 chromatography eluted with methanol in water in a stepwise manner (0%, 20%, 40%, 60%, 95%). The purification was monitored with HPLC. Fractions containing products were collected and the solvent was removed by rotavapor to yield products.

Product of **2ab** was purified by semi-preparative HPLC using a DAICEL CHIRALPAK IF HPLC column (methanol: 20 mM ammonium bicarbonate in water = 1:99, 4 ml/min). The purified compounds were dissolved in methanol to detect the HRESIMS, and dissolved in NaOD/D_2O analyzed by ^{1}H NMR and ^{13}C NMR.

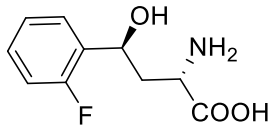
For the structural characterization of products **3a-3x**, 5 ml reactions were incubated for 12 h, lyophilized. Products of **3a-3g, 3o-3q** and **3u** were purified by semi-preparative HPLC using a Water sunfire column eluted with MeOH/H_2O (0-30 min, 5-95%, 10 ml/min). Products of **3h-3m** were purified by semi-preparative HPLC using a Water sunfire column eluted with MeOH/H_2O (0-30 min, 25-95%, 10 ml/min). Products of **3r** and **3s** were purified by semi-preparative HPLC using a Water sunfire column eluted with MeOH/H_2O (0-30 min, 40-95%, 10 ml/min). Products of **3t** and **3v-3x** were purified by semi-preparative HPLC using a Water sunfire column eluted with MeOH/H_2O (0-30 min, 2-50%, 10 ml/min). The solvent was removed by rotavapor to yield products.

All reported chemical shifts was adjusted with reference of D_2O (4.79). Raw NMR Data of all compounds has been deposited on Zendo.org (DOI: https://doi.org/10.5281/zenodo.5205646)



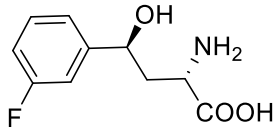
2a

^{1}H NMR (400 MHz, D_2O, pD = 7.0) δ 7.44 – 7.33 (m, 5H), 4.89 (dd, J = 9.5, 3.7 Hz, 1H), 3.86 (dd, J = 7.0, 4.2 Hz, 1H), 2.30 (ddd, J = 14.8, 9.5, 4.2 Hz, 1H), 2.19 (ddd, J = 14.8, 7.0, 3.7 Hz, 1H) ppm. ^{13}C NMR (125 MHz, pD = 7.0) δ 174.3, 143.0, 128.9, 128.9, 128.1, 125.8, 125.8, 70.9, 52.9, 37.9 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{14}NO_3$ calculated 196.0968, observed 196.0968.



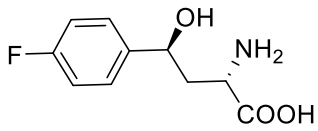
2b

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.46 (t, J = 7.6 Hz, 1H), 7.33 (q, J = 6.8 Hz, 1H), 7.22 (m, 1H), 7.11 (m, 1H), 5.12 (dd, J = 9.1, 4.6 Hz, 1H), 3.34 (dd, J = 8.6, 4.8 Hz, 1H), 2.16 (ddd, J = 14.0, 9.1, 4.8 Hz, 1H), 1.87 (ddd, J = 14.0, 8.6, 4.6 Hz, 1H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 8.0) δ 182.8, 159.7 (d, $^{1}J_{C\text{-}F}$ = 244.3 Hz), 130.2 (d, $^{2}J_{C\text{-}F}$ = 13.2 Hz), 127.5 (d, $^{3}J_{C\text{-}F}$ = 8.5 Hz), 127.5 (d, $^{3}J_{C\text{-}F}$ = 4.4 Hz), 124.6 (d, $^{4}J_{C\text{-}F}$ = 3.3 Hz), 115.6 (d, $^{2}J_{C\text{-}F}$ = 21.7 Hz), 65.4 (d, $^{3}J_{C\text{-}F}$ = 2.6 Hz), 53.5, 41.7 ppm. ^{19}F NMR (471 MHz, D_2O, pD = 8.0) δ -119.7 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}FNO_3$ calculated 214.0874, observed 214.0874.



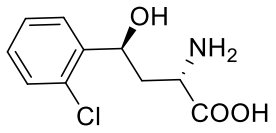
2c

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.37 (td, J = 8.0, 6.0 Hz, 1H), 7.15 (m, 2H), 7.03 (m, 1H), 4.81 (m, 1H, partially overlapped with solvent), 3.31 (m, 1H, partially overlapped with solvent), 2.08 (ddd, J = 14.0, 9.1, 5.0 Hz, 1H), 1.80 (ddd, J = 14.0, 8.5, 4.6 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 182.8, 162.6 (d, $^{1}J_{C\text{-}F}$ = 243.4 Hz), 146.4 (d, $^{3}J_{C\text{-}F}$ = 6.8 Hz), 130.3 (d, $^{3}J_{C\text{-}F}$ = 8.2 Hz), 121.7 (d, $^{4}J_{C\text{-}F}$ = 2.8 Hz), 114.3 (d, $^{2}J_{C\text{-}F}$ = 21.1 Hz), 112.7 (d, $^{2}J_{C\text{-}F}$ = 21.9 Hz), 70.7, 53.4, 43.0 ppm. ^{19}F NMR (376 MHz, D_2O, pD = 8.0) δ -113.7 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}FNO_3$ calculated 214.0874, observed 214.0870. $[\alpha]_D^{20}$ = -30.0 (c = 0.10, Methanol).



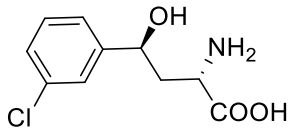
2d

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.38 (m, 2H), 7.11 (t, J = 8.0 Hz, 2H), 4.81 (m, 1H, partially overlapped with solvent), 3.38 (m, 1H), 2.14 (ddd, J = 14.4, 8.7, 5.0 Hz, 1H), 1.89 (m, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 180.4, 162.0 (d, $^{1}J_{C\text{-}F}$ = 243.0 Hz), 139.2 (d, $^{4}J_{C\text{-}F}$ = 3.1 Hz), 127.8 (d, $^{3}J_{C\text{-}F}$ = 8.3 Hz), 127.8 (d, $^{3}J_{C\text{-}F}$ = 8.3 Hz), 115.3 (d, $^{2}J_{C\text{-}F}$ = 21.4 Hz), 115.3 (d, $^{1}J_{C\text{-}F}$ = 21.4 Hz), 70.5, 53.3, 41.6 ppm. ^{19}F NMR (471 MHz, D_2O, pD = 8.0) δ -115.5 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}FNO_3$ calculated 214.0874, observed 214.0873.



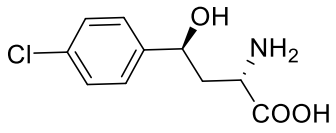
2e

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.55 (d, J = 7.7 Hz, 1H), 7.41 (d, J = 7.7 Hz, 1H), 7.37 (t, J = 7.7 Hz, 1H), 7.28 (t, J = 7.7 Hz, 1H), 5.28 (dd, J = 9.6, 3.6 Hz, 1H), 3.41 (dd, J = 9.1, 4.2 Hz, 1H), 2.04 (ddd, J = 14.0, 9.6, 4.2 Hz, 1H), 1.86 (ddd, J = 14.0, 9.1, 3.6 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 182.8, 140.8, 131.5, 129.5, 128.9, 127.4, 126.9, 67.5, 53.5, 41.5 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}ClNO_3$ calculated 230.0578, observed 230.0574.



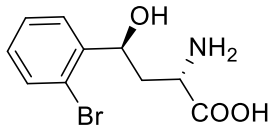
2f

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.41 (s, 1H), 7.33 (m, 3H), 4.79 (m, 1H, partially overlapped with solvent), 3.32 (m, 1H), 2.07 (m, 1H), 1.81 (m, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 182.8, 145.9, 133.7, 130.1, 127.6, 125.9, 124.3, 70.6, 53.3, 43.0 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}ClNO_3$ calculated 230.0578, observed 230.0580.



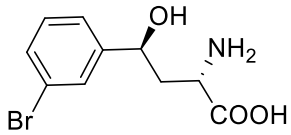
2g

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.39 (d, J = 8.4 Hz, 2H), 7.34 (d, J = 8.4 Hz, 2H), 4.81 (m, 1H, partially overlapped with solvent), 3.36 (dd, J = 8.1, 5.0 Hz, 1H), 2.11 (ddd, J = 14.2, 9.1, 5.0 Hz, 1H), 1.84 (ddd, J = 14.2, 8.1, 4.5 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 181.6, 142.2, 132.7, 128.5, 128.5, 127.5, 127.5, 70.5, 53.3, 42.3 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}ClNO_3$ calculated 230.0578, observed 230.0575.



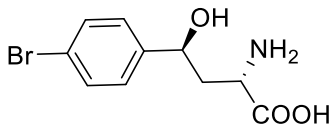
2h

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.60 (d, J = 8.0 Hz, 1H), 7.54 (d, J =8.0 Hz, 1H), 7.41 (t, J = 8.0 Hz, 1H), 7.21 (t, J = 8.0 Hz, 1H), 5.23 (dd, J = 10.3, 2,4 Hz, 1H), 3.43 (dd, J = 9.2, 4.2 Hz, 1H), 2.00 (m, 1H), 1.87 (m, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 182.8, 142.4, 132.7, 129.2, 128.0, 127.1, 121.5, 69.8, 53.5, 41.6 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}BrNO_3$ calculated 274.0073, observed 274.0066.



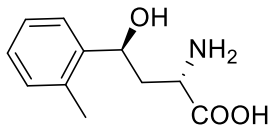
2i

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.56 (s, 1H), 7.46 (d, J = 7.6 Hz, 1H), 7.33 (d, J = 7.6 Hz, 1H), 7.28 (t, J = 7.6 Hz, 1H), 4.76 (m, 1H, partially overlapped with solvent), 3.32 (m, 1H, partially overlapped with solvent), 2.08 (ddd, J = 14.0, 9.2, 4.9 Hz, 1H), 1.78 (ddd, J = 14.0, 8.5, 4.5 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 182.6, 146.2, 130.6, 130.4, 128.8, 124.8, 122.0, 70.6, 53.3, 43.0 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}BrNO_3$ calculated 274.0073, observed 274.0072.



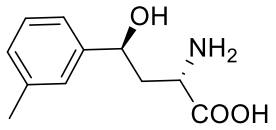
2j

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.54 (d, J = 8.4 Hz, 2H), 7.29 (d, J = 8.4 Hz, 2H), 4.77 (m, 1H, partially overlapped with solvent), 3.31 (m, 1H), 2.09 (ddd, J = 14.0, 9.1, 5.0 Hz, 1H), 1.80 (ddd, J = 14.0, 8.3, 4.7 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 182.4, 142.8, 131.5, 131.5, 127.9, 127.9, 120.8, 70.6, 53.4, 42.8 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}BrNO_3$ calculated 274.0073, observed 274.0072.



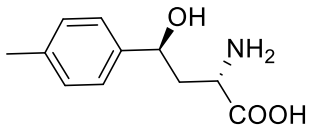
2k

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.45 (d, J = 7.6 Hz, 1H), 7.26 (m, 1H), 7.21 (m, 2H), 5.10 (dd, J = 9.5, 3.9 Hz, 1H), 3.36 (dd, J = 8.7, 4.5 Hz, 1H), 2.30 (s, 3H), 2.05 (ddd, J = 14.2, 9.5, 4.5 Hz, 1H), 1.76 (ddd, J = 14.2, 8.7, 3.9 Hz, 1H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 8.0) δ 184.4, 143.3, 136.6, 131.9, 129.0, 127.9, 126.6, 68.7, 55.1, 43.6, 19.5 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{11}H_{16}NO_3$ calculated 210.1125, observed 210.1122.



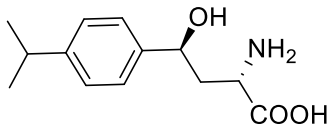
2l

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.30 (t, J = 7.8 Hz, 1H), 7.23 (s, 1H), 7.17 (t, J = 7.8 Hz, 2H), 4.76 (m, 1H, partially overlapped with solvent), 3.30 (q, J = 5.0 Hz, 1H), 2.31 (s, 3H), 2.10 (ddd, J = 14.0, 8.8, 5.0 Hz, 1H), 1.78 (ddd, J = 14.0, 8.8, 5.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 182.9, 143.8, 138.8, 128.7, 128.4, 126.6, 123.0, 71.2, 53.5, 43.2, 20.4 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{11}H_{16}NO_3$ calculated 210.1125, observed 210.1124.



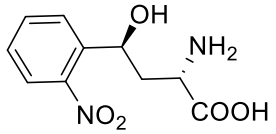
2m

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.28 (d, J = 8.0 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 4.76 (m, 1H, partially overlapped with solvent), 3.34 (dd, J = 8.2, 4.9 Hz, 1H), 2.29 (s, 3H), 2.12 (ddd, J = 14.0, 9.1, 4.9 Hz, 1H), 1.82 (ddd, J = 14.0, 8.2, 4.7 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 182.0, 140.6, 138.0, 129.2, 129.2, 126.0, 126.0, 71.0, 53.4, 42.6, 20.1 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{11}H_{16}NO_3$ calculated 210.1125, observed 210.1119.



2n

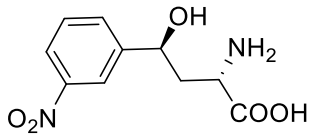
^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.32 (s, 4H), 4.79 (m, 1H, partially overlapped with solvent), 3.30 (dd, J = 8.1, 5.1 Hz, 1H), 2.89 (m, 1H), 2.10 (m, 1H), 1.78 (m, 1H), 1.20 (d, J = 7.1, 6H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 8.0) δ 183.0, 149.1, 141.4, 126.7, 126.7, 126.2, 126.2, 71.1, 53.5, 43.3, 33.3, 23.2, 23.2 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{13}H_{20}NO_3$ calculated 238.1438, observed 238.1438.



2o

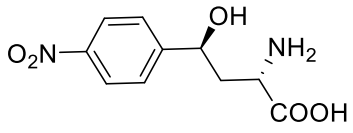
^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.95 (d, J = 7.7 Hz, 1H), 7.79 (d, J = 7.7 Hz, 1H), 7.72 (t, J = 7.7 Hz, 1H), 7.48 (t, J = 7.7 Hz, 1H), 5.40 (dd, J = 9.6, 3.1 Hz, 1H), 3.44 (dd, J = 9.6, 4.2 Hz, 1H), 2.07 (ddd, J = 14.0, 9.6, 4.2 Hz, 1H), 1.90 (ddd, J = 14.0, 9.5, 3.1 Hz, 1H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 8.0) δ 184.4, 148.6, 140.6, 135.5,

129.9, 129.2, 125.9, 67.6, 55.0, 44.0 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}N_2O_5$ calculated 241.0819, observed 241.0812.



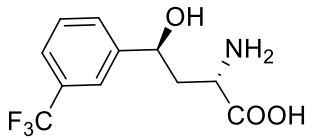
2p

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 8.24 (s, 1H), 8.15 (d, J = 7.9 Hz, 1H), 7.77 (d, J = 7.9 Hz, 1H), 7.59 (t, J =7.9 Hz, 1H), 4.94 (dd, J = 9.3, 4.4 Hz, 1H), 3.27 (m, 1H, partially overlapped with solvent), 2.12 (ddd, J = 14.0, 9.3, 4.9 Hz, 1H), 1.86 (ddd, J = 14.0, 8.5, 4.4 Hz, 1H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 8.0) δ 182.7, 148.0, 145.9, 132.8, 129.8, 122.7, 120.9, 70.4, 53.4, 43.0 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}N_2O_5$ calculated 241.0819, observed 241.0813.



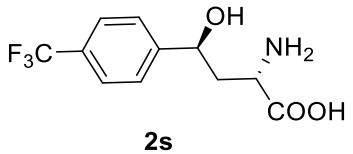
2q

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 8.15 (d, J = 8.5 Hz, 2H), 7.51 (d, J = 8.5 Hz, 2H), 4.88 (dd, J = 9.4, 4.4 Hz, 1H), 3.28 (dd, J = 8.6, 4.8 Hz, 1H), 2.02 (ddd, J = 14.0, 9.4, 4.8 Hz, 1H), 1.77 (ddd, J = 14.0, 8.6, 4.4 Hz, 1H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 8.0) δ 184.2, 153.3, 148.4, 128.3, 128.3, 125.3, 125.3, 72.0, 64.0, 44.5 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}N_2O_5$ calculated 241.0819, observed 241.0814.



2r

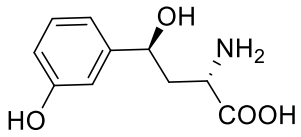
^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.71 (s, 1H), 7.62 (m, 2H), 7.54 (m, 1H), 4.89 (m, 1H), 3.35 (dd, J = 7.8, 4.8 Hz, 1H), 2.12 (m, 1H), 1.84 (m, 1H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 8.0) δ 182.4, 144.9, 130.1 (q, $^2J_{C\text{-}F}$ = 32.0 Hz), 129.7, 129.3, 124.5 (q, $^3J_{C\text{-}F}$ = 3.9 Hz), 124.2 (q, $^1J_{C\text{-}F}$ = 273.5 Hz), 122.7 (q, $^3J_{C\text{-}F}$ = 3.9 Hz), 70.8, 53.4, 42.9 ppm. ^{19}F NMR (376 MHz, D_2O, pD = 8.0) δ -62.4 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{11}H_{13}F_3NO_3$ calculated 264.0842, observed 264.0844.



2s

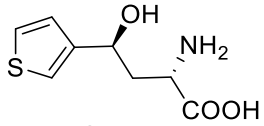
^{1}H NMR (400 MHz, D_2O, pD = 7.0) δ 7.79 (d, J = 8.1 Hz, 2H), 7.63 (d, J = 8.1 Hz, 2H), 5.05 (dd, J = 9.1, 4.1 Hz, 1H), 3.94 (dd, J = 6.8, 4.3 Hz, 1H), 2.24 (m, 2H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 7.0) δ 174.0, 147.2, 129.3 (q, $^2J_{C\text{-}F}$ = 32.1 Hz), 126.2,

126.2, 125.6 (q, $^{3}J_{C\text{-}F}$ = 3.8 Hz), 125.6 (q, $^{3}J_{C\text{-}F}$ = 3.8 Hz), 124.2 (q, $^{1}J_{C\text{-}F}$ = 271.3 Hz), 70.4, 52.9, 37.7 ppm. ^{19}F NMR (376 MHz, D_2O, pD = 7.0) δ -62.3 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{11}H_{13}F_3NO_3$ calculated 264.0842, observed 264.0840.



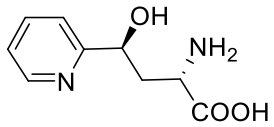
2t

^{1}H NMR (500 MHz, D_2O, pD = 7.0) δ 7.28 (m, 1H), 6.94 (d, J = 7.6 Hz, 1H), 6.89 (s, 1H), 6.82 (d, J = 8.1 Hz, 1H), 4.83 (m, 1H, partially overlapped with solvent), 3.84 (d, J = 6.2 Hz, 1H), 2.23 (m, 2H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 7.0) δ 174.3, 155.8, 145.1, 130.3, 117.7, 114.9, 112.6, 70.7, 52.9, 37.9 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{14}NO_4$ calculated 212.0917, observed 212.0915.



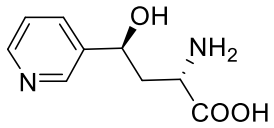
2u

^{1}H NMR (400 MHz, D_2O, pD = 7.0) δ 7.45 (m, 1H), 7.36 (s, 1H), 7.14 (d, J = 5.3 Hz, 1H), 4.99 (dd, J = 9.2, 4.1 Hz, 1H), 3.85 (m, 1H), 2.30 (m, 2H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 7.0) δ 174.2, 144.1, 127.1, 125.5, 121.8, 67.1, 52.8, 37.2 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_8H_{12}NO_3S$ calculated 202.0532, observed 202.0530.



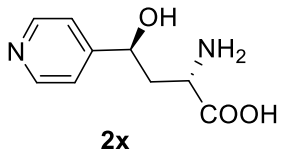
2v

^{1}H NMR (600 MHz, D_2O, pD = 7.0) δ 8.44 (m, 1H), 7.86 (td, J = 7.7, 1.8 Hz, 1H), 7.51 (d, J = 7.8 Hz, 1H), 7.34 (m, 1H), 4.95 (t, J = 6.5 Hz, 1H), 3.88 (t, J = 6.0 Hz, 1H), 2.29 (m, 2H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 7.0) δ 174.1, 160.5, 148.3, 138.4, 123.5, 120.9, 71.2, 52.7, 36.5 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_9H_{13}N_2O_3$ calculated 197.0921, observed 197.0919.



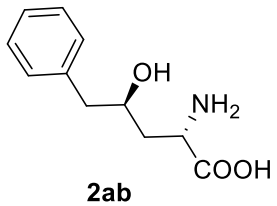
2w

^{1}H NMR (400 MHz, D_2O, pD = 7.0) δ 8.51 (s, 1H), 8.44 (d, J = 5.0, 1H), 7.86 (d, J = 8.2 Hz, 1H), 7.44 (dd, J = 8.2, 5.0 Hz, 1H), 4.95 (dd, J = 9.3, 3.6 Hz, 1H), 3.89 (dd, J = 6.9, 4.2 Hz, 1H), 2.26 (m, 2H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 7.0) 174.0, 148.2, 146.4, 139.0, 135.0, 124.4, 68.7, 52.8, 37.5 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_9H_{13}N_2O_3$ calculated 197.0921, observed 197.0924.



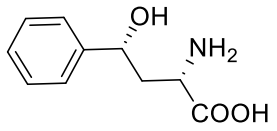
2x

^{1}H NMR (400 MHz, D_2O, pD = 7.0) δ 8.49 (d, J = 5.5, 2H), 7.45 (d, J = 5.5, 2H), 4.94 (t, J = 6.6 Hz, 1H), 3.89 (t, J = 5.7 Hz, 1H), 2.24 (m, 2H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 7.0) 174.0, 153.6, 148.8, 148.8, 121.2, 121.2, 69.5, 52.8, 37.3 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_9H_{13}N_2O_3$ calculated 197.0921, observed 197.0918.



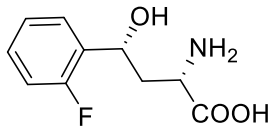
2ab

^{1}H NMR (400 MHz, D_2O, pD = 7.0) δ 7.35 (m, 2H), 7.27 (m, 3H), 4.11 (m, 1H), 3.70 (m, 1H), 2.88 (dd, J = 13.8, 4.8 Hz, 1H), 2.72 (m, 1H), 2.11 (d, J = 14.9 Hz, 1H), 1.76 (m, 1H) ppm. ^{13}C NMR (150 MHz, D_2O, pD = 7.0) δ 196.2, 138.1, 129.5, 129.5, 128.6, 128.6, 126.6, 71.5, 54.3, 43.2, 37.2 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{11}H_{16}NO_3$ calculated 210.1125, observed 210.1128.



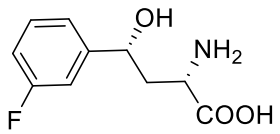
3a

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.42 (m, 5H), 4.88 (dd, J = 8.4, 5.3 Hz, 1H), 3.48 (dd, J = 8.4, 5.3 Hz, 1H), 2.19 (dt, J = 14.4, 5.3 Hz, 1H), 2.03 (dt, J = 14.4, 8.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 178.9, 143.0, 128.8, 128.8, 128.0, 126.0, 126.0, 72.2 54.0, 40.9 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{14}NO_3$ calculated 196.0968, observed 196.0965.



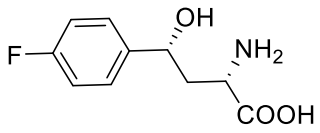
3b

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.47 (m, 1H), 7.34 (m, 1H), 7.23 (t, J = 7.5 Hz, 1H), 7.13 (m, 1H), 5.15 (dd, J = 8.0, 5.9 Hz, 1H), 3.39 (m, 1H), 2.20 (m, 1H), 2.04 (dt, J = 14.9, 8.0 Hz, 1H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 8.0) δ 180.2, 159.8 (d, $^{1}J_{C\text{-}F}$ = 244.5 Hz), 129.8 (d, $^{3}J_{C\text{-}F}$ = 8.1 Hz), 129.7 (d, $^{2}J_{C\text{-}F}$ = 12.6 Hz), 127.6 (d, $^{3}J_{C\text{-}F}$ = 4.6 Hz), 124.6 (d, $^{4}J_{C\text{-}F}$ = 3.5 Hz), 115.6 (d, $^{2}J_{C\text{-}F}$ = 21.8 Hz), 66.4 (d, $^{3}J_{C\text{-}F}$ = 2.9 Hz), 54.0, 40.6 ppm. ^{19}F NMR (376 MHz, D_2O, pD = 8.0) δ -119.6 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}FNO_3$ calculated 214.0874, observed 214.0872.



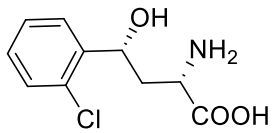
3c

^{1}H NMR (400 MHz, D_2O, pD = 7.0) δ 7.40 (m, 1H), 7.19 (m, 2H), 7.07 (t, J = 8.9 Hz, 1H), 4.99 (d, J = 9.4 Hz, 1H), 3.87 (m, 1H), 2.32 (m, 1H), 2.09 (dt, J = 16.5, 9.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 7.0) δ 174.2, 162.7 (d, $^{1}J_{C\text{-}F}$ = 234.1 Hz), 145.7 (d, $^{3}J_{C\text{-}F}$ = 7.0 Hz), 130.4 (d, $^{3}J_{C\text{-}F}$ = 8.3 Hz), 121.5 (d, $^{4}J_{C\text{-}F}$ = 2.6 Hz), 114.7 (d, $^{2}J_{C\text{-}F}$ = 21.2 Hz), 112.5 (d, $^{2}J_{C\text{-}F}$ = 22.3 Hz), 71.6, 53.8, 38.4 ppm. ^{19}F NMR (376 MHz, D_2O, pD = 7.0) δ -113.4 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}FNO_3$ calculated 214.0874, observed 214.0875. $[\alpha]_D^{20}$ = + 4.667 (c = 0.05, Methanol).



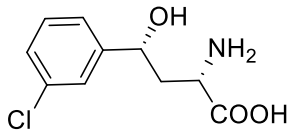
3d

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.40 (dd, J = 8.8, 5.6 Hz, 2H), 7.13 (t, J = 8.8 Hz, 1H), 4.85 (dd, J = 8.1, 5.7 Hz, 2H), 3.38 (m, 1H), 2.14 (dt, J = 14.3, 5.7 Hz, 1H), 2.00 (dt, J = 14.3, 8.1 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 179.9, 162.1 (d, $^{1}J_{C\text{-}F}$ = 234.1 Hz), 138.9 (s), 128.0 (d, $^{3}J_{C\text{-}F}$ = 8.4 Hz), 128.0 (d, $^{3}J_{C\text{-}F}$ = 8.4 Hz), 115.3 (d, $^{2}J_{C\text{-}F}$ = 21.6 Hz), 115.3 (d, $^{2}J_{C\text{-}F}$ = 21.6 Hz), 71.5, 54.0, 41.4 ppm. ^{19}F NMR (376 MHz, D_2O, pD = 8.0) δ -115.3 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}ClNO_3$ calculated 214.0874, observed 214.0868.



3e

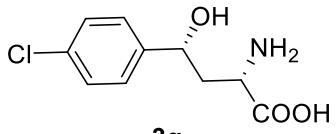
^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.56 (m, 1H), 7.40 (m, 2H), 7.29 (td, J = 7.8, 1.4 Hz, 1H), 5.31 (dd, J = 9.0, 4.0 Hz, 1H), 3.59 (t, J = 6.5 Hz, 1H), 2.22 (ddd, J = 14.5, 6.5, 4.0 Hz, 1H), 1.93 (m, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 178.6, 140.4, 131.4, 129.5, 129.1, 127.5, 126.9, 68.4, 53.9, 39.8 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}ClNO_3$ calculated 230.0578, observed 230.0575.



3f

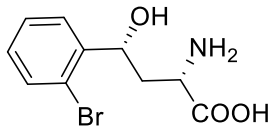
^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.43 (s, 1H), 7.34 (m, 3H), 4.79 (m, partially overlapped by solvent, 1H), 3.19 (m, 1H), 2.05 (dt, J = 14.0, 6.1 Hz, 1H), 1.92 (dt, J = 14.0, 7.8 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 182.5, 145.4, 133.8,

130.2, 127.8, 126.1, 124.6, 71.5, 54.0, 42.9 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}ClNO_3$ calculated 230.0578, observed 230.0584.



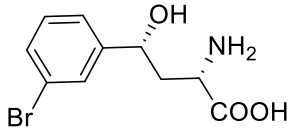
3g

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.41 (d, J = 8.3 Hz, 2H), 7.36 (d, J = 8.3 Hz, 2H), 4.85 (dd, J = 8.4, 5.5 Hz, 1H), 3.43 (m, 1H), 2.14 (dt, J = 14.0, 5.5 Hz, 1H), 1.99 (dt, J = 14.0, 8.4 Hz, 1H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 8.0) δ 179.3, 141.8, 133.0, 128.7, 128.7, 127.7, 127.7, 71.6, 54.0, 41.2 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}ClNO_3$ calculated 230.0578, observed 230.0580.



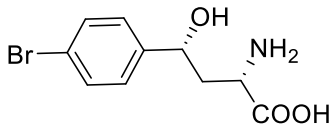
3h

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.60 (d, J = 8.0 Hz, 1H), 7.54 (m, 1H), 7.42 (t, J = 7.6 Hz, 1H), 7.22 (m, 1H), 5.23 (dd, J = 8.9, 4.4 Hz, 1H), 3.42 (t, J = 6.8 Hz, 1H), 2.13 (ddd, J = 14.2, 6.8, 4.4 Hz, 1H), 1.86 (m, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ181.1, 142.1, 132.7, 129.4, 128.1, 127.2, 121.6, 70.6, 54.0, 41.5 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}BrNO_3$ calculated 274.0073, observed 274.0074.



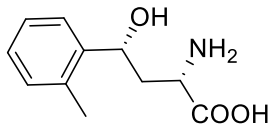
3i

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.59 (s, 1H), 7.51 (d, J = 7.7 Hz, 1H), 7.33 (m, 2H), 4.79 (m, 1H, partially overlapped with solvent), 3.24 (m, 1H), 2.07 (m, 1H), 1.93 (m, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 181.9, 145.7, 130.8, 130.5, 129.1, 125.0, 122.0, 71.6, 54.0, 42.6 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}BrNO_3$ calculated 274.0073, observed 274.0078.



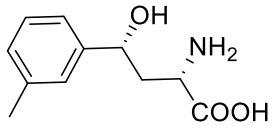
3j

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.56 (d, J = 8.8 Hz, 2H), 7.30 (d, J = 8.8 Hz, 2H), 4.75 (m, 1H, partially overlapped with solvent), 3.16 (dd, J = 7.7, 5.7 Hz, 1H), 2.04 (dt, J = 14.4, 5.7 Hz, 1H), 1.92 (dt, J = 14.4, 7.7 Hz, 1H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 8.0) δ 182.7, 142.4, 131.6, 131.6, 128.2, 128.2, 121.0, 71.6, 54.1, 42.9. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}BrNO_3$ calculated 274.0073, observed 274.0080.



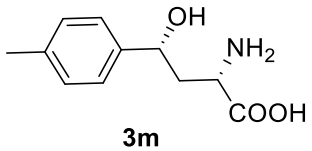
3k

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.47 (d, J = 7.5 Hz, 1H), 7.25 (m, 3H), 5.19 (dd, J = 9.0, 3.3 Hz, 1H), 3.73 (m, 1H), 2.31(s, 3H), 2.12 (m, 1H), 1.97 (dt, J = 15.2, 9.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 176.9, 141.4, 134.9, 130.5, 127.7, 126.4, 125.0, 68.4, 54.1, 39.3, 18.0 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{11}H_{16}NO_3$ calculated 210.1125, observed 210.1120.



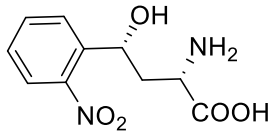
3l

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.32 (t, J = 7.6 Hz, 1H), 7.25 (s, 1H), 7.20 (m, 2H), 4.75 (m, 1H, partially overlapped with solvent), 3.20 (t, J = 6.9 Hz, 1H), 2.33 (s, 3H), 2.06 (m, 1H), 1.95 (m, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 8.0) δ 182.4, 143.2, 138.8, 128.7, 128.5, 126.8, 123.2, 72.1, 54.0, 42.8, 20.4 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{11}H_{16}NO_3$ calculated 210.1125, observed 210.1122.



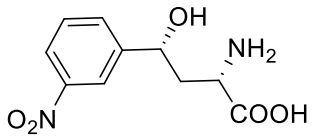
3m

^{1}H NMR (400 MHz, D_2O, pD = 9.0) δ 7.30 (d, J = 8.1, 2H), 7.25 (d, J = 8.1 Hz, 2H), 4.76 (m, partially overlapped with solvent, 1H), 3.15 (dd, J = 8.0, 5.7 Hz, 1H), 2.31 (s, 3H), 2.05 (m, 1H), 1.94 (dt, J = 13.5, 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 9.0) δ 182.7, 140.0, 138.1, 129.2, 129.2, 126.3, 126.3, 71.9, 54.0, 42.9, 20.1 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{11}H_{16}NO_3$ calculated 210.1125, observed 210.1130.



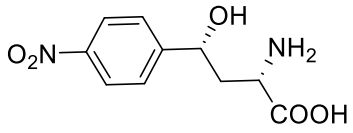
3o

^{1}H NMR (400 MHz, D_2O, pD = 7.0) δ 8.01 (d, J = 8.3 Hz, 1H), 7.83 (m, 1H), 7.75 (m, 1H), 7.52 (m, 1H), 5.51 (d, J = 9.9 Hz, 1H), 3.96 (m, 1H), 2.46 (m, 1H), 2.08 (m, 1H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 7.0) δ 174.1, 146.9, 138.8, 134.4, 128.9, 127.7, 124.7, 67.7, 54.2, 38.2 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}N_2O_5$ calculated 241.0819, observed 241.0825.



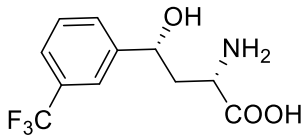
3p

^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 8.26 (s, 1H), 8.17 (m, 1H), 7.79 (d, J = 7.7 Hz, 1H), 7.61 (t, J = 8.0 Hz, 1H), 5.01 (dd, J = 8.8, 4.9 Hz, 1H), 3.49 (m, 1H), 2.19 (dt, J = 14.3, 4.9 Hz, 1H), 2.02 (dt, J = 14.3, 8.4 Hz, 1H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 8.0) δ 179.5, 148.0, 145.3, 132.8, 129.8, 122.9, 121.0, 71.4, 54.0, 41.3 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}N_2O_5$ calculated 241.0819, observed 241.0822.



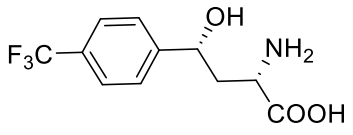
3q

^{1}H NMR (400 MHz, D_2O, pD = 9.0) δ 8.23 (d, J = 8.4 Hz, 2H), 7.59 (d, J = 8.4 Hz, 2H), 4.93 (m, 1H), 3.24 (t, J = 6.9 Hz, 1H), 2.07 (dt, J = 13.8, 6.9 Hz, 1H), 1.94 (dt, J = 13.8, 6.9 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 9.0) 182.5, 151.2, 147.0, 127.0, 127.0, 123.9, 123.9, 71.3, 54.0, 43.0 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{13}N_2O_5$ calculated 241.0819, observed 241.0823.



3r

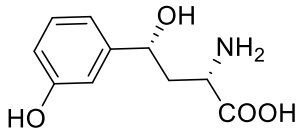
^{1}H NMR (400 MHz, D_2O, pD = 9.0) δ 7.72 (s, 1H), 7.64 (m, 2H), 7.56 (t, J = 7.8 Hz, 1H), 4.92 (t, J = 6.6 Hz, 1H), 3.36 (t, J = 6.6 Hz, 1H), 2.13 (m, 1H), 1.98 (m, 1H) ppm. ^{13}C NMR (125 MHz, D_2O, pD = 9.0) δ 180.7, 144.3, 130.1 (q, $^{2}J_{C\text{-}F}$ = 32.0 Hz), 129.8, 129.4, 124.7 (q, $^{3}J_{C\text{-}F}$ = 4.0 Hz), 124.2 (q, $^{1}J_{C\text{-}F}$ = 271.6 Hz), 122.8 (q, $^{3}J_{C\text{-}F}$ = 4.0 Hz), 71.7, 54.1, 42.0 ppm. ^{19}F NMR (376 MHz, D_2O, pD = 9.0) δ -62.4 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{11}H_{13}F_3NO_3$ calculated 264.0842, observed 264.0846.



3s

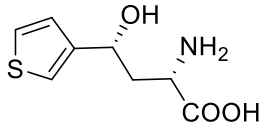
^{1}H NMR (400 MHz, D_2O, pD = 8.0) δ 7.72 (d, J = 8.0 Hz, 2H), 7.55 (d, J = 8.0 Hz, 2H), 4.88 (t, J = 7.0 Hz, 1H), 3.19 (t, J = 7.0 Hz, 1H), 2.06 (dt, J = 14.2, 7.0 Hz, 1H), 1.94 (dt, J = 14.2, 7.0 Hz, 1H). ^{13}C NMR (125 MHz, D_2O, pD = 8.0) δ 182.6, 147.5, 129.2 (q, $^{2}J_{C\text{-}F}$ = 32.1 Hz), 126.6, 126.6, 125.6 (q, $^{3}J_{C\text{-}F}$ = 3.9 Hz), 125.6 (q, $^{3}J_{C\text{-}F}$ = 3.9 Hz), 124.2 (q, $^{1}J_{C\text{-}F}$ = 271.3 Hz), 71.6, 54.1, 43.0 ppm. ^{19}F NMR (376 MHz, D_2O, pD =

8.0) δ -62.3 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{11}H_{13}F_3NO_3$ calculated 264.0842, observed 264.0845.



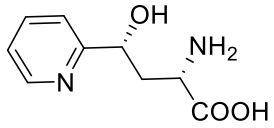
3t

^{1}H NMR (400 MHz, D_2O, pD = 7.0) δ 7.28 (t, J = 7.9 Hz, 1H), 6.95 (d, J = 7.9 Hz, 1H), 6.89 (s, 1H), 6.82 (m, 1H), 4.90 (m, 1H), 3.84 (dd, J = 8.6, 4.7 Hz, 1H), 2.28 (dt, J = 15.0, 4.7 Hz, 1H), 2.08 (dt, J = 15.0, 8.6 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 7.0) δ 174.2, 155.6, 145.1, 130.2, 117.7, 114.9, 112.5, 71.9, 53.8, 38.5 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_{10}H_{14}NO_4$ calculated 212.0917, observed 212.0913.



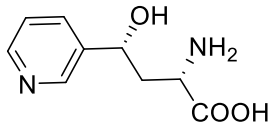
3u

^{1}H NMR (400 MHz, D_2O, pD = 7.0) δ 7.47 (m, 1H), 7.39 (s, 1H), 7.17 (m, 1H), 5.06 (dd, J = 9.1, 3.7 Hz, 1H), 3.84 (m, 1H), 2.41 (m, 1H), 2.18 (dt, J = 14.9, 9.1 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 7.0) δ 174.2, 144.0, 127.1, 125.5, 121.9, 68.1, 53.7, 37.8 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_8H_{12}NO_3S$ calculated 202.0532, observed 202.0530.



3v

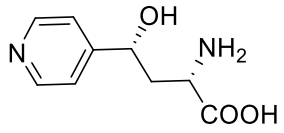
^{1}H NMR (400 MHz, D_2O, pD = 7.0) δ 8.46 (d, J = 4.9 Hz, 1H), 7.88 (td, J = 7.9, 2.0 Hz, 1H), 7.54 (d, J = 7.9 Hz, 1H), 7.37 (m, 1H), 5.04 (m, 1H), 3.92 (dd, J = 9.1, 4.4 Hz, 1H), 2.40 (dt, J = 14.6, 4.4 Hz, 1H), 2.12 (dt, J = 14.6, 9.1 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 7.0) δ 174.2, 160.7, 148.2, 138.6, 123.5, 120.9, 72.4, 53.7, 37.1 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_9H_{13}N_2O_3$ calculated 197.0921, observed 197.0919.



3w

^{1}H NMR (400 MHz, D_2O, pD = 7.0) δ 8.53 (s, 1H), 8.45 (d, J = 4.8 Hz, 1H), 7.89 (d, J = 8.0, 1H), 7.46 (dd, J = 8.0, 4.8 Hz, 1H), 5.07 (dd, J = 10.2, 4.0 Hz, 1H), 3.91 (dd, J = 8.5, 4.0 Hz, 1H), 2.33 (dt, J = 14.9, 4.0 Hz, 1H), 2.14 (ddd, J = 14.9, 10.2, 8.5 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 7.0) δ 174.1, 148.4, 146.2, 139.1, 135.1, 124.3,

70.0, 53.9, 38.2 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_9H_{13}N_2O_3$ calculated 197.0921, observed 197.0918.



3x

^{1}H NMR (400 MHz, D_2O, pD = 7.0) δ 8.49 (d, *J* = 4.9 Hz, 2H), 7.45 (d, *J* = 4.9 Hz, 2H), 5.04 (m, 1H), 3.91 (dd, *J* = 8.3, 5.2 Hz, 1H), 2.33 (m, 1H), 2.04 (dt, *J* = 14.8, 8.3 Hz, 1H) ppm. ^{13}C NMR (100 MHz, D_2O, pD = 7.0) 174.1, 153.5, 148.8, 148.8, 121.1, 121.1, 70.8, 53.8, 38.1 ppm. HRMS (ESI) (m/z) for $[M+H]^+$ $C_9H_{13}N_2O_3$ calculated 197.0921, observed 197.0916.

Preparative scale of ApUstD

For preparative scale product of ApUstD, 62.5 ml reactions containing 0.4 mg/ml ApUstD, 100 mg L-Aspartic acid, 80 mM **1c**, 1 mM DTT, 100 μM PLP and 50 mM sodium phosphate, 50 mM NaCl, at pH 7.4 were run at 25 °C. After 72 hours, the reaction mixture was centrifugated (800 g), and then the supernatant loaded on C18 chromatography eluted with methanol in water in a stepwise manner (0%, 20%, 40%, 60%, 95%) and Fractions containing product were collected and the solvent was evaporated under vacuum to yield **2c** (134 mg, 84%).

Supplementary Figure S7-S88

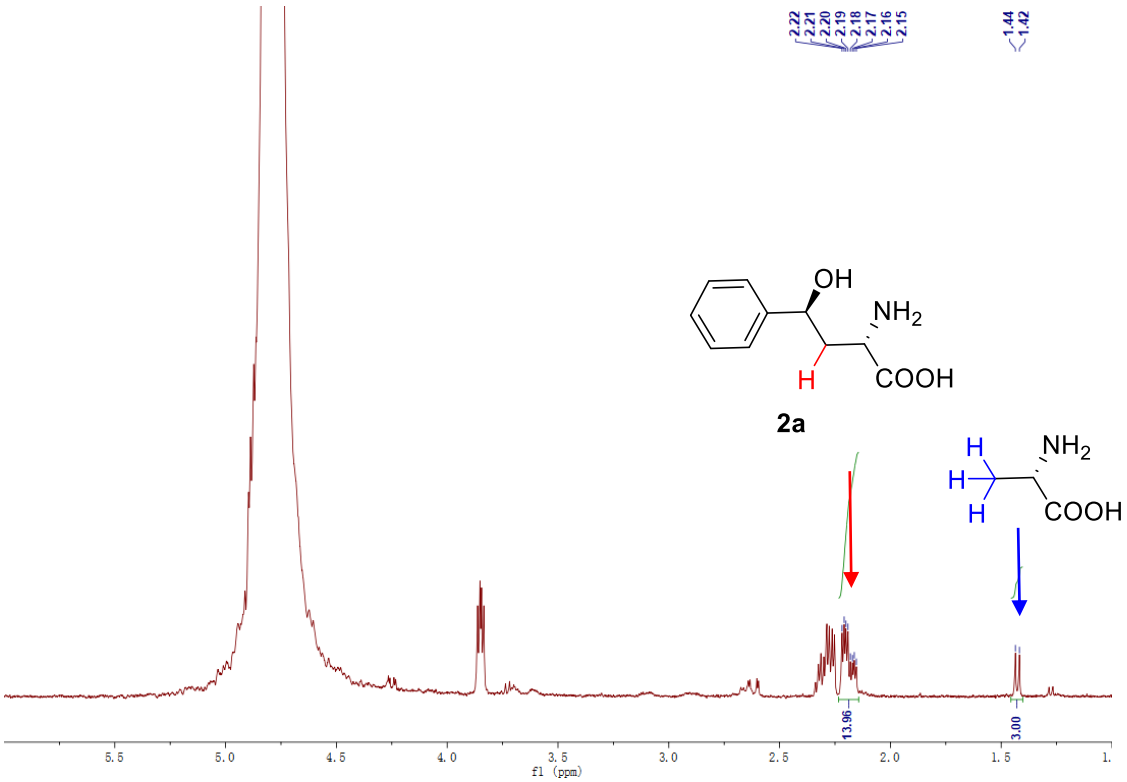


Figure S7. Conversion of **2a**

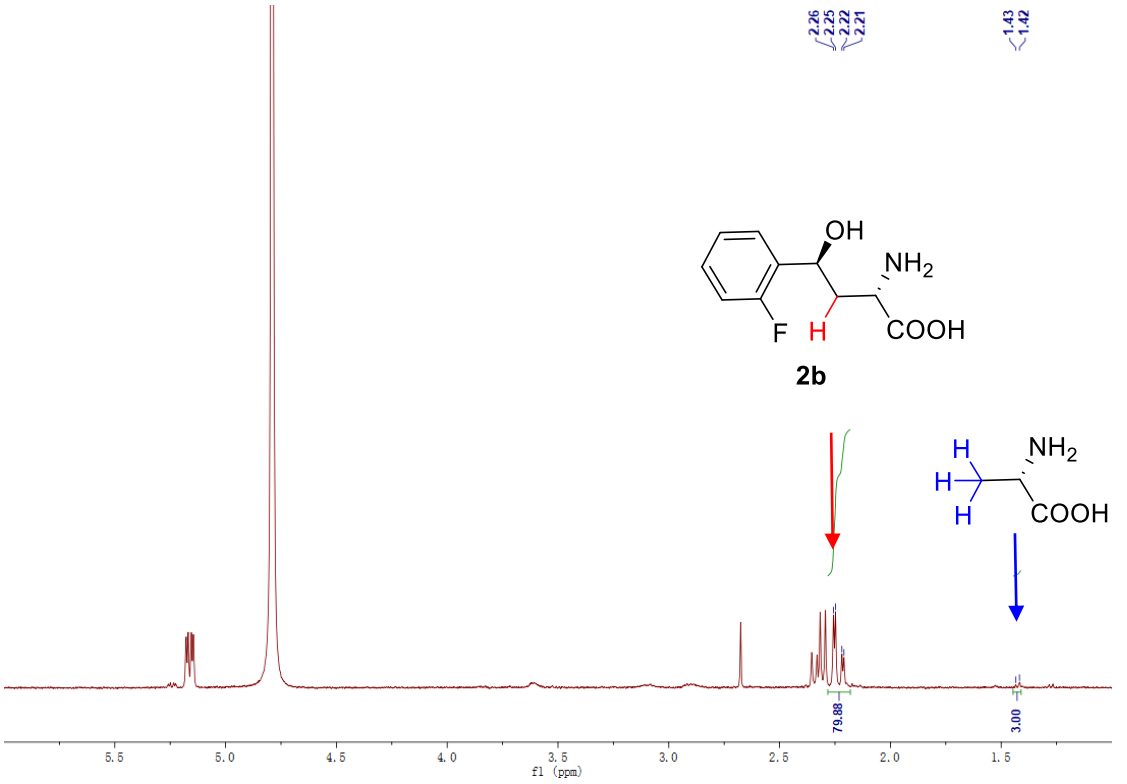


Figure S8. Conversion of **2b**

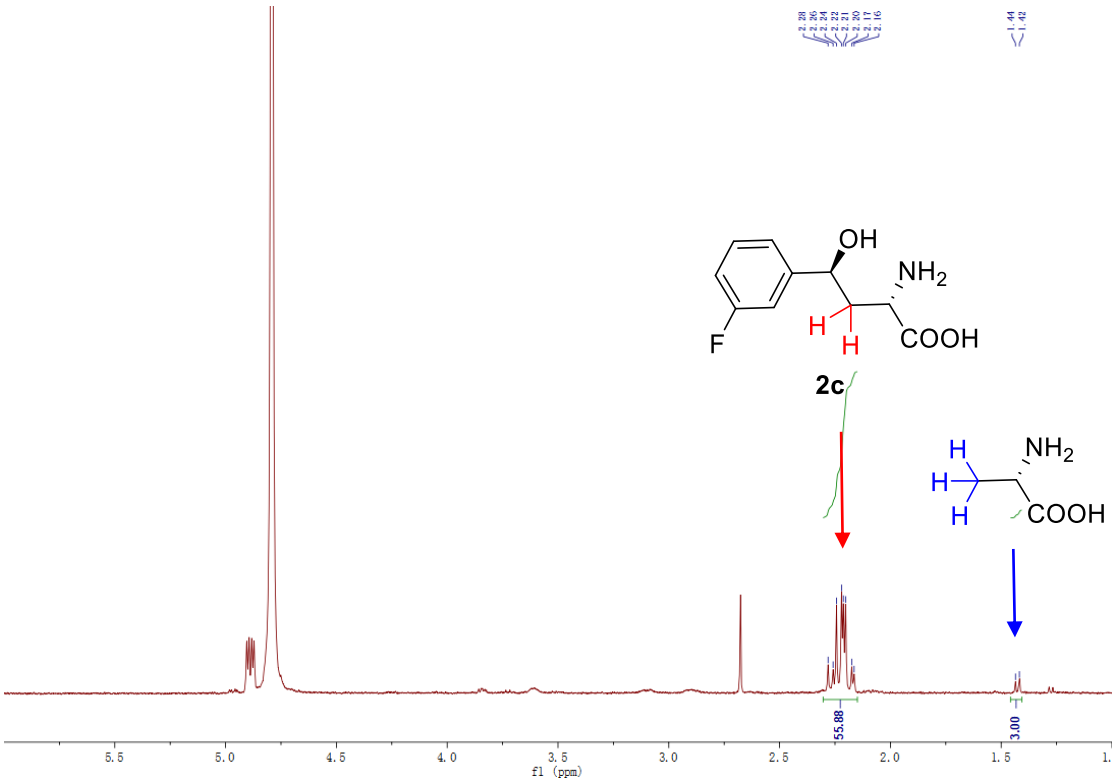


Figure S9. Conversion of **2c**

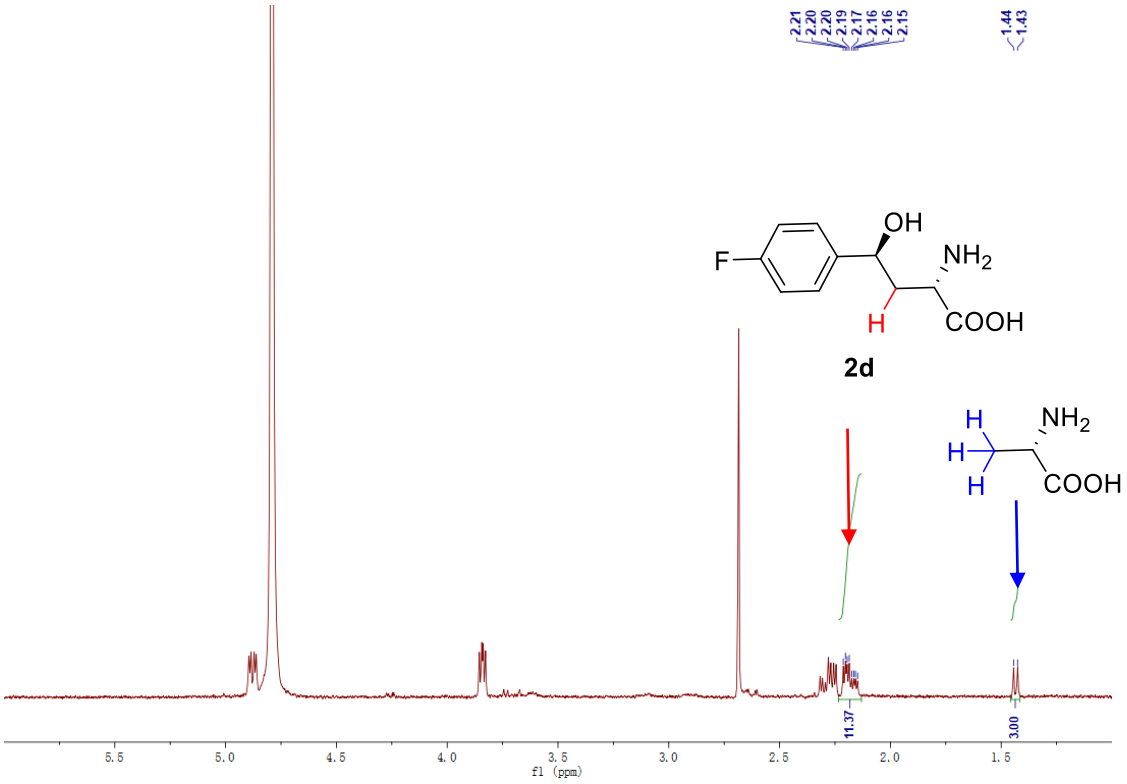


Figure S10. Conversion of **2d**

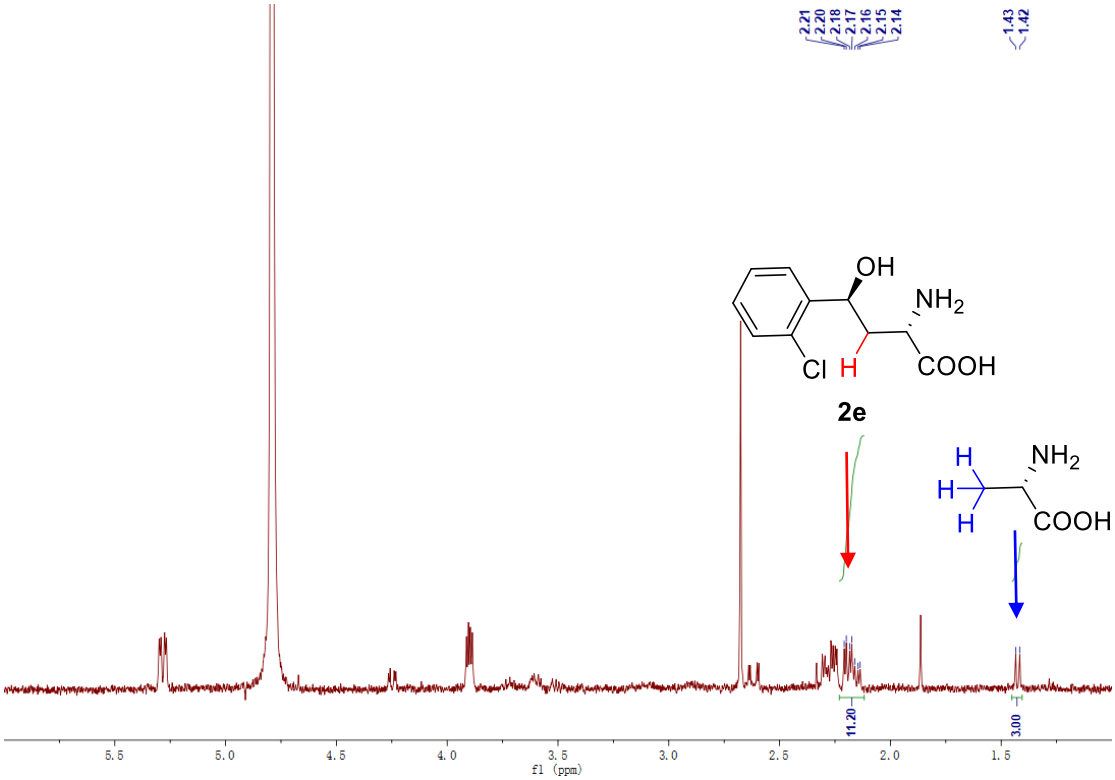


Figure S11. Conversion of **2e**

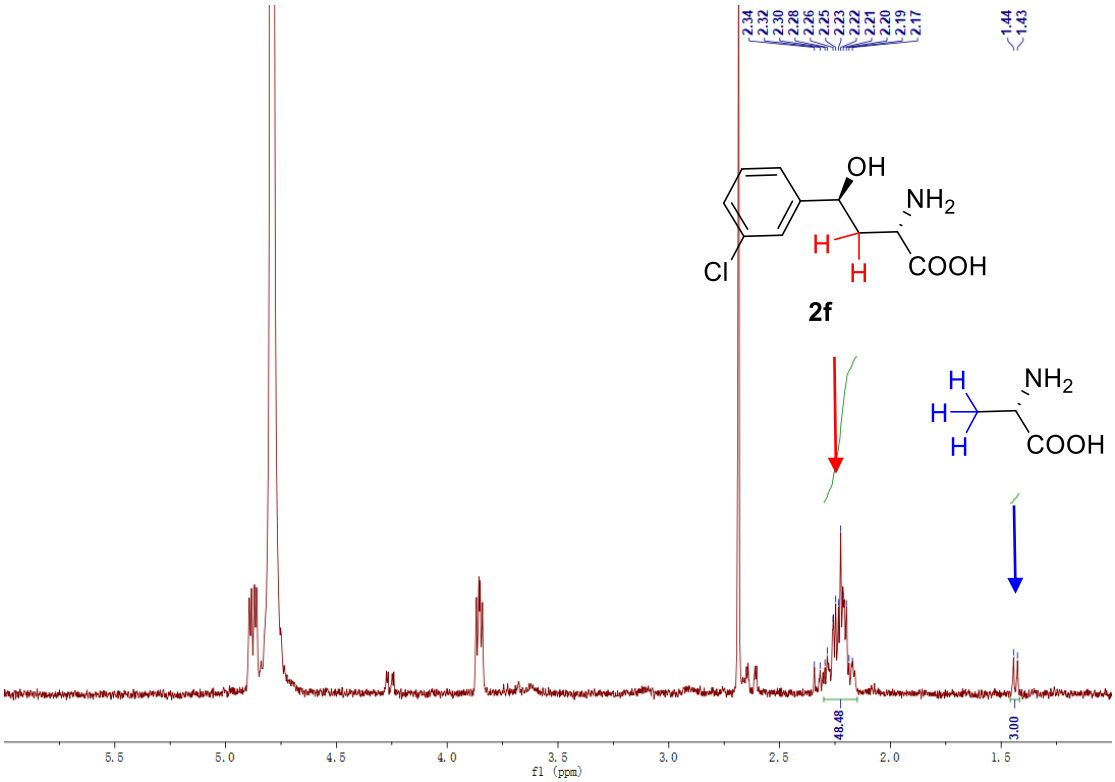


Figure S12. Conversion of **2f**

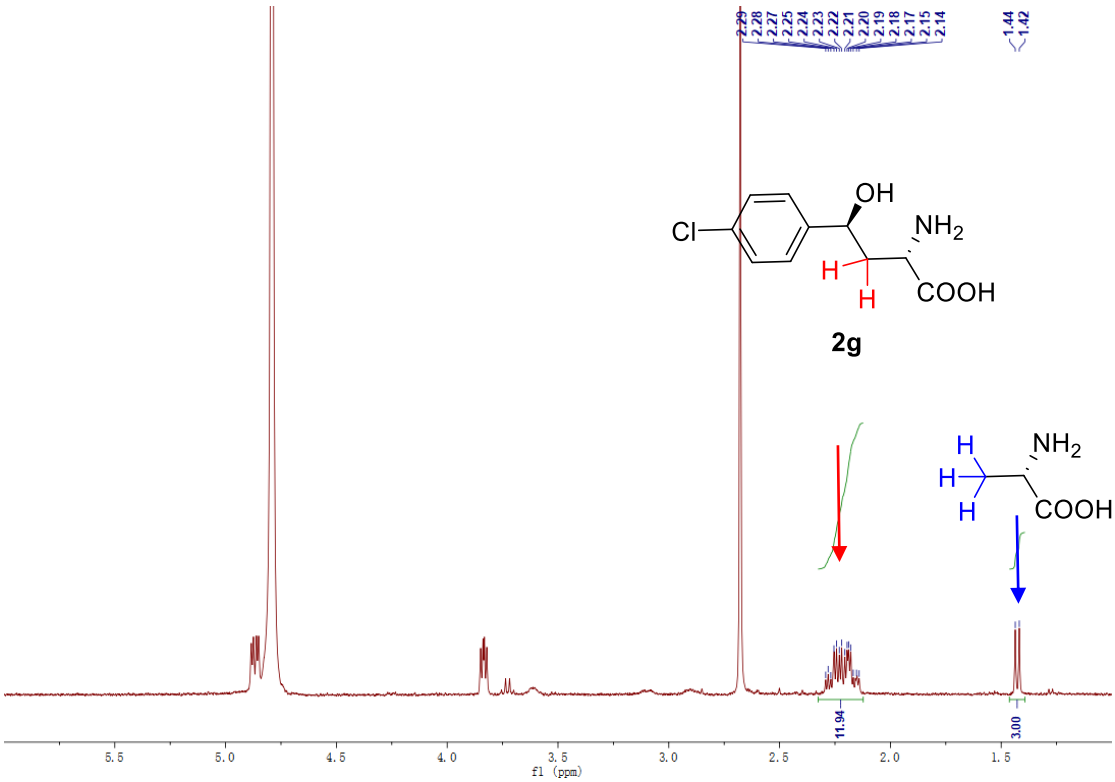


Figure S13. Conversion of **2g**

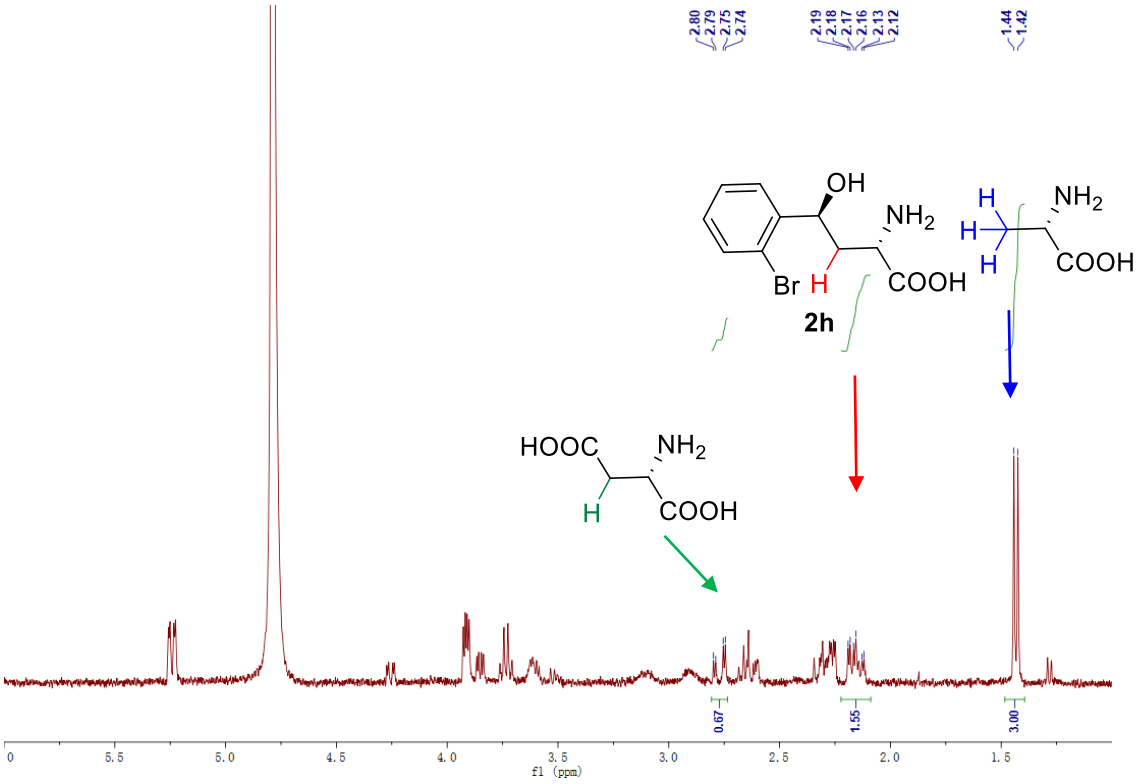


Figure S14. Conversion of **2h**

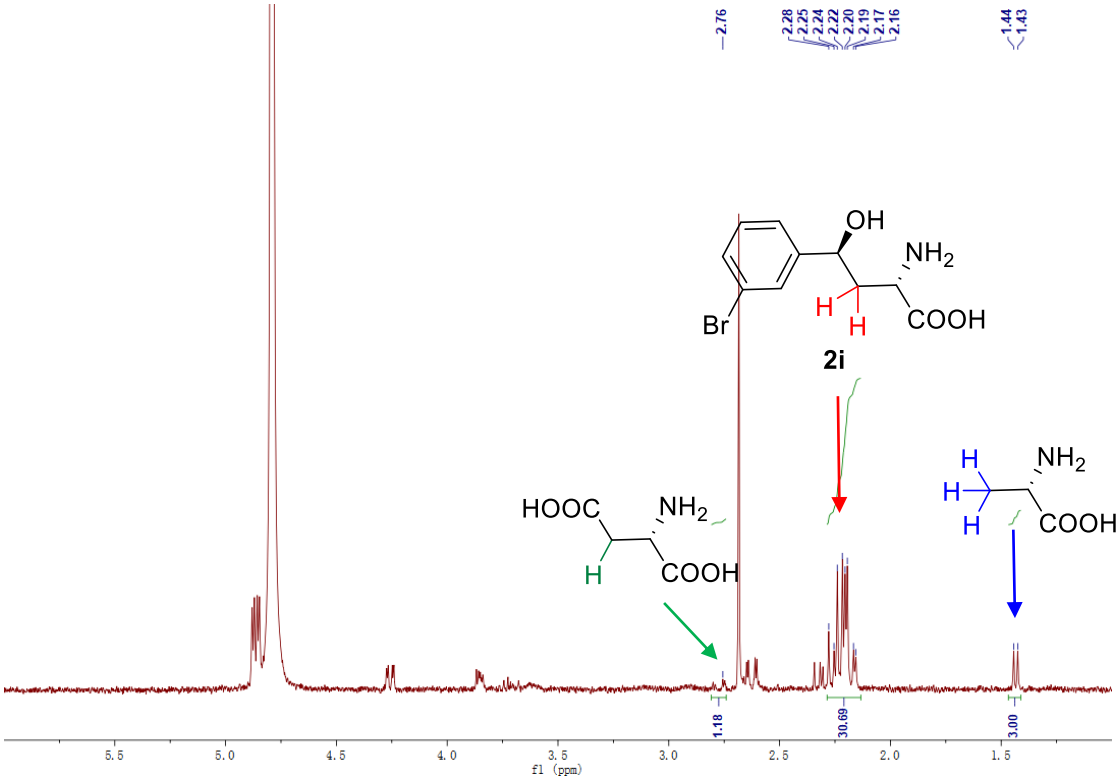


Figure S15. Conversion of **2i**

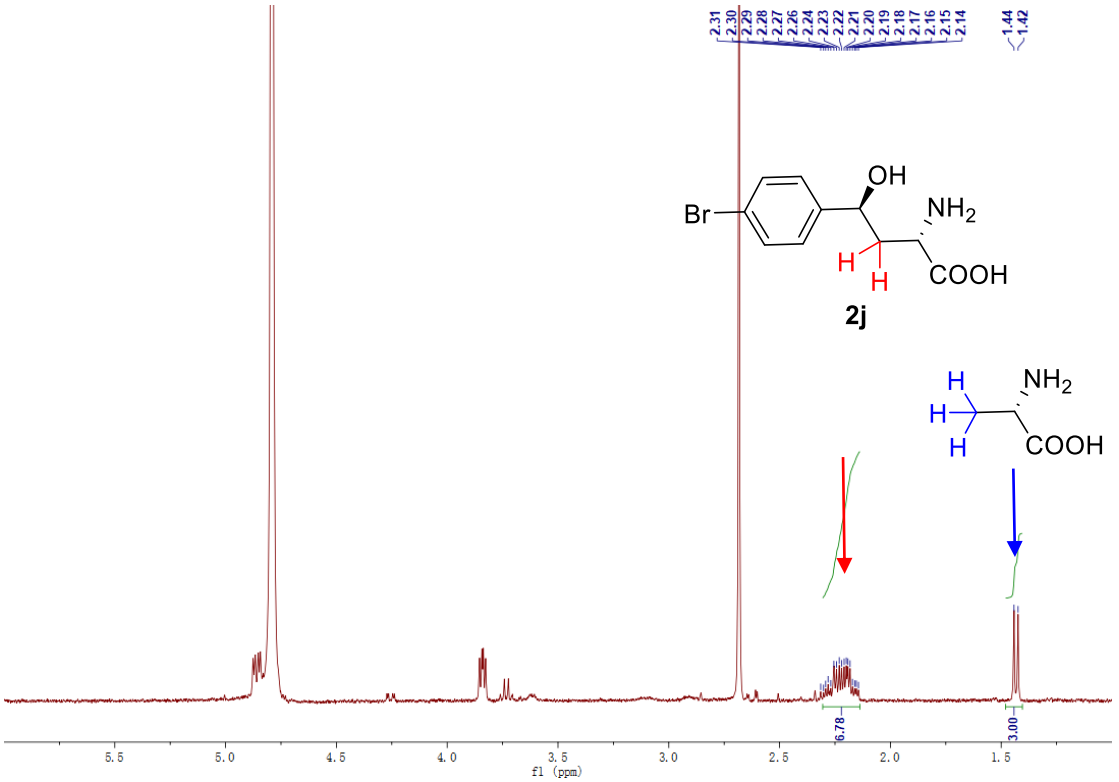


Figure S16. Conversion of **2j**

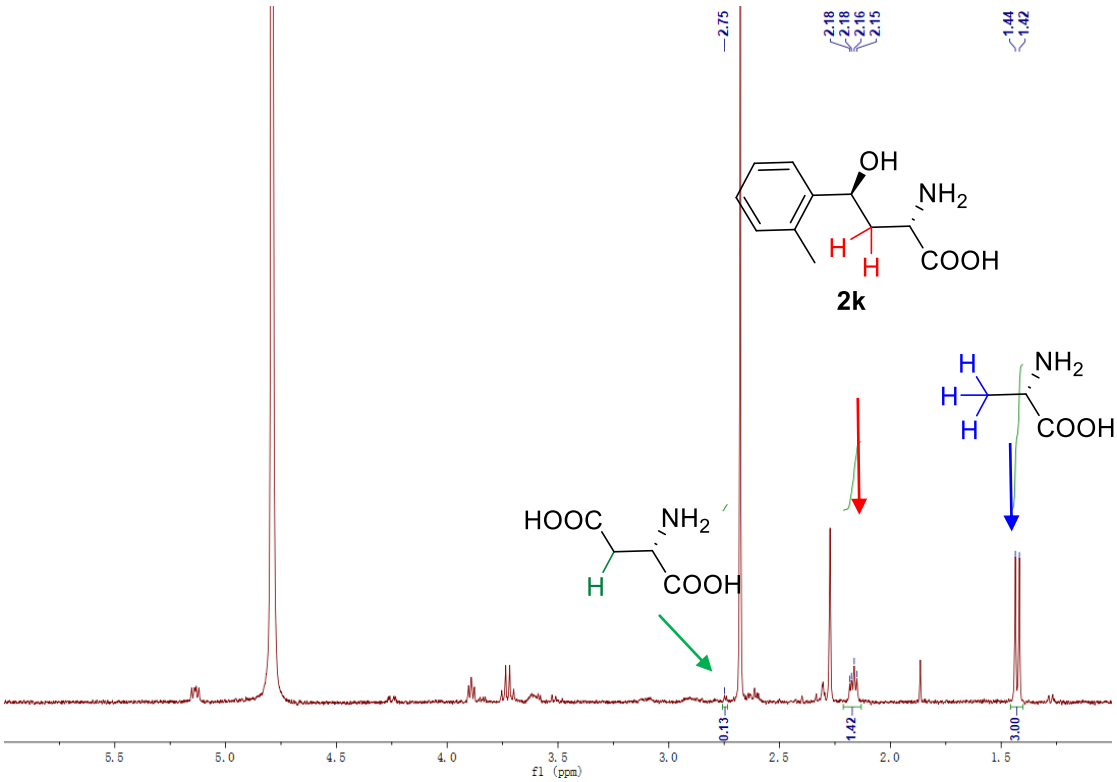


Figure S17. Conversion of **2k**

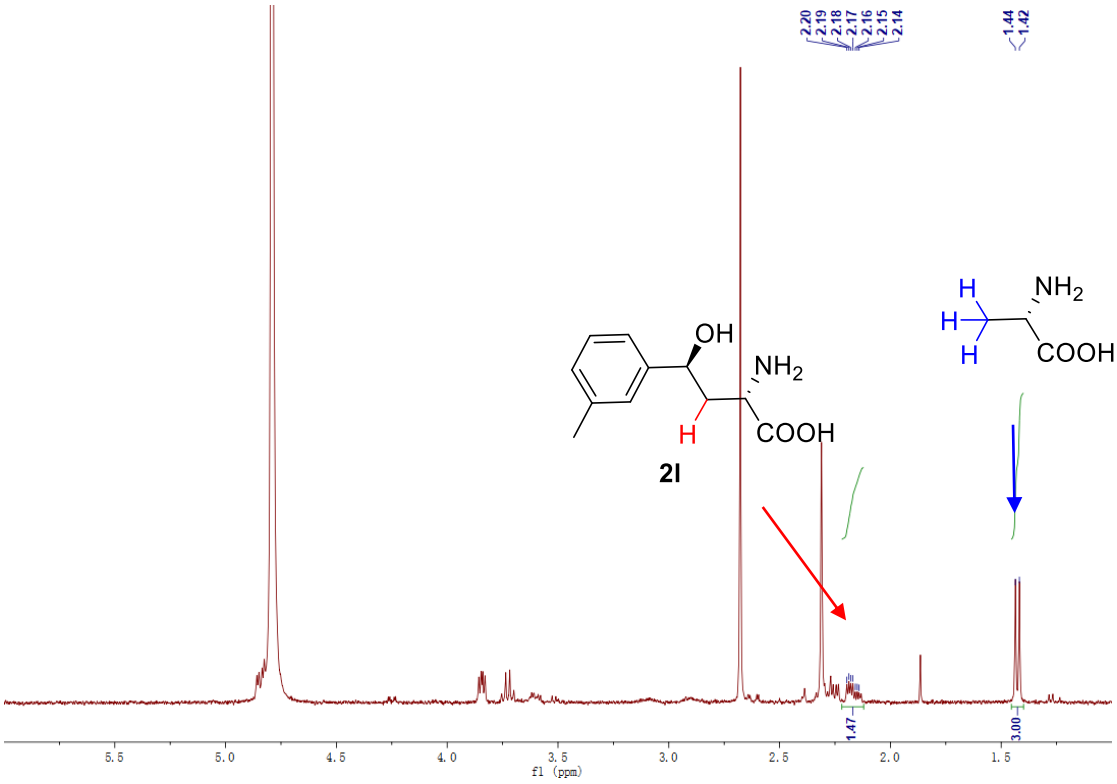


Figure S18. Conversion of **2l**

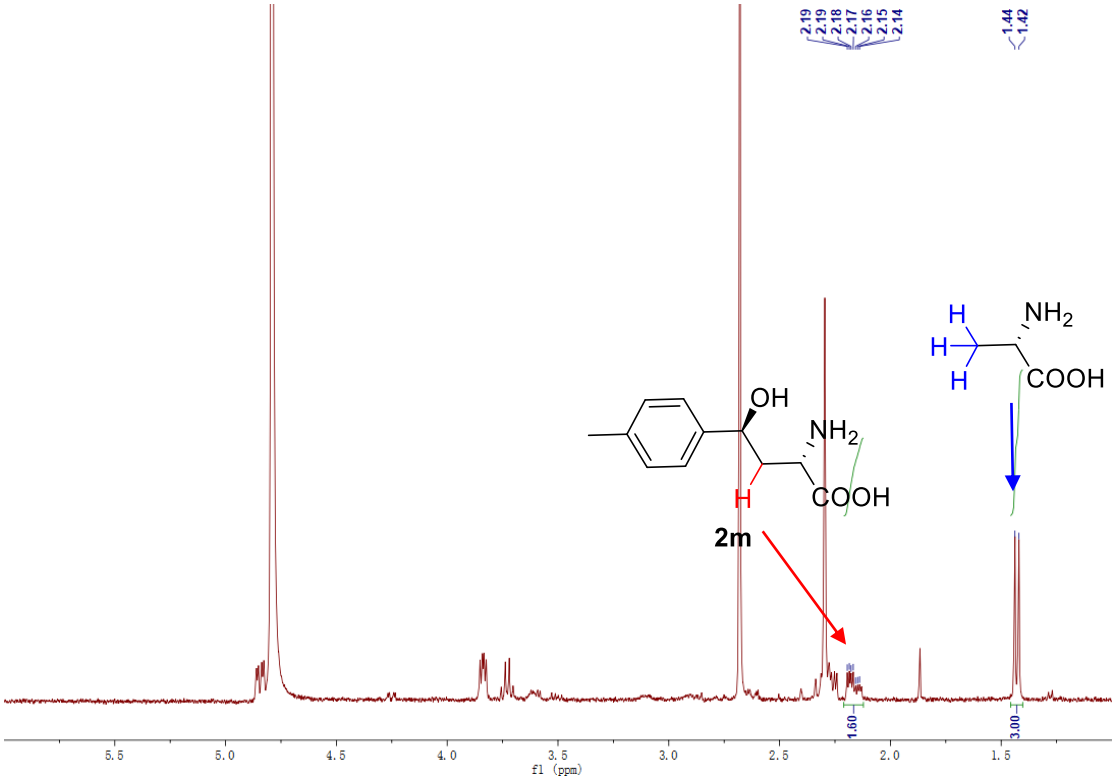


Figure S19. Conversion of **2m**

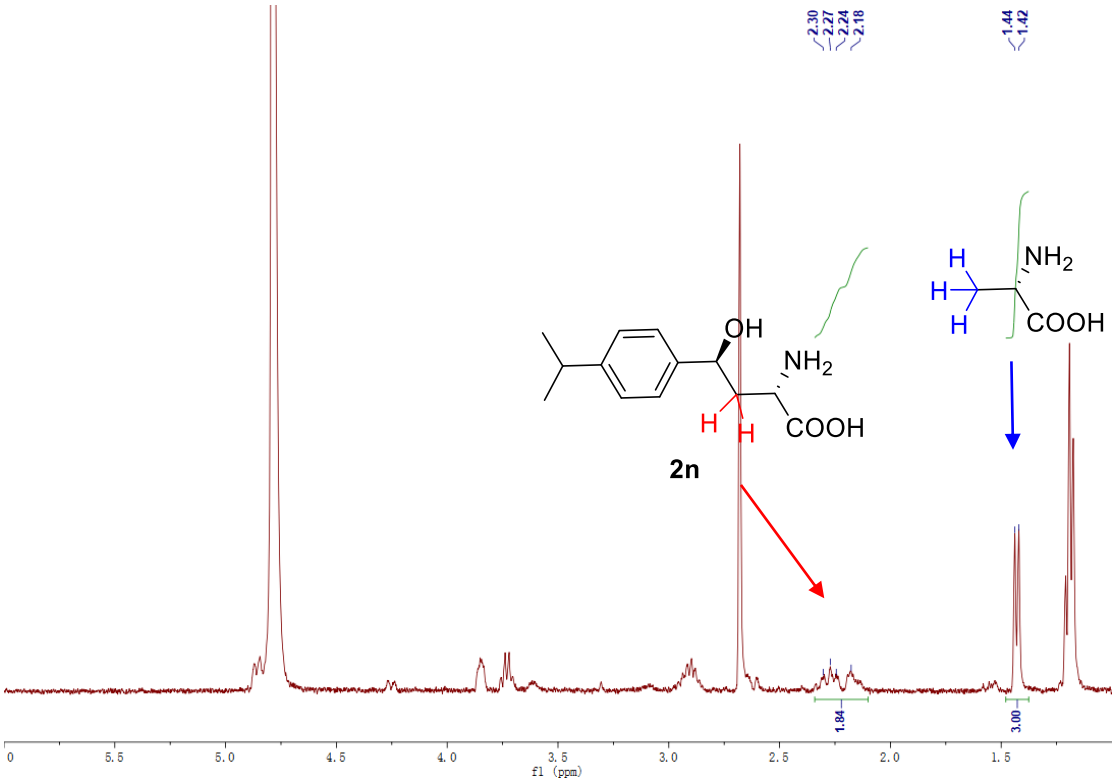


Figure S20. Conversion of **2n**

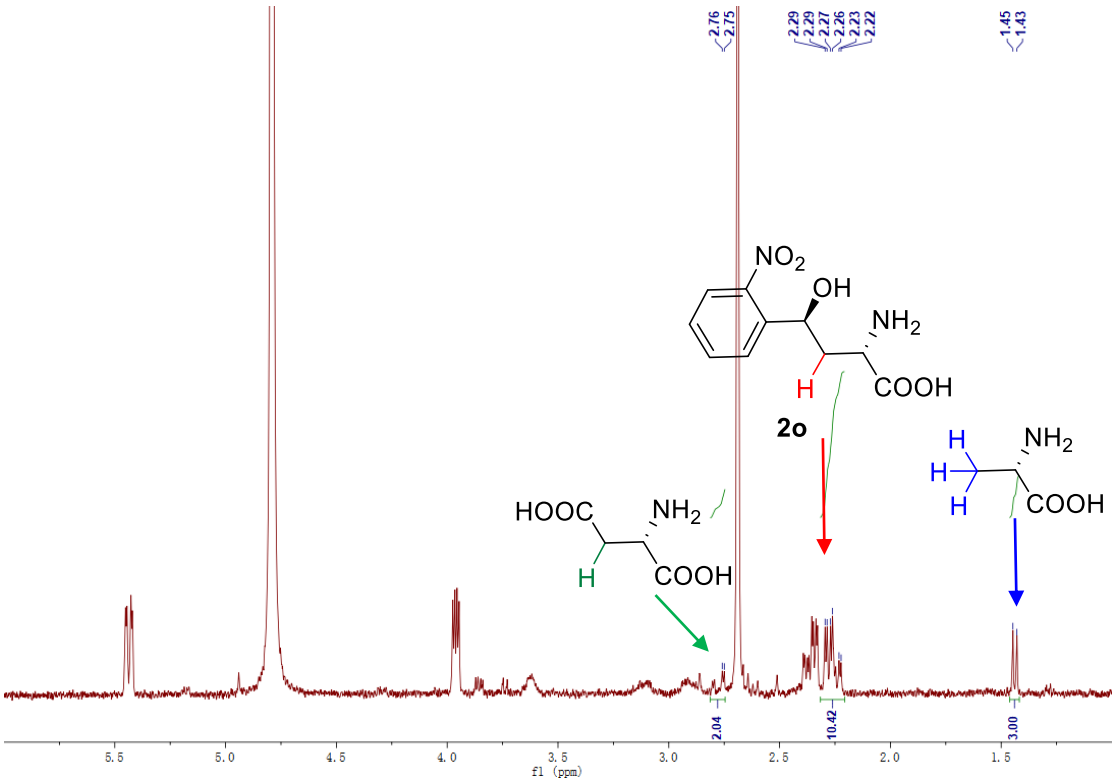


Figure S21. Conversion of **2o**

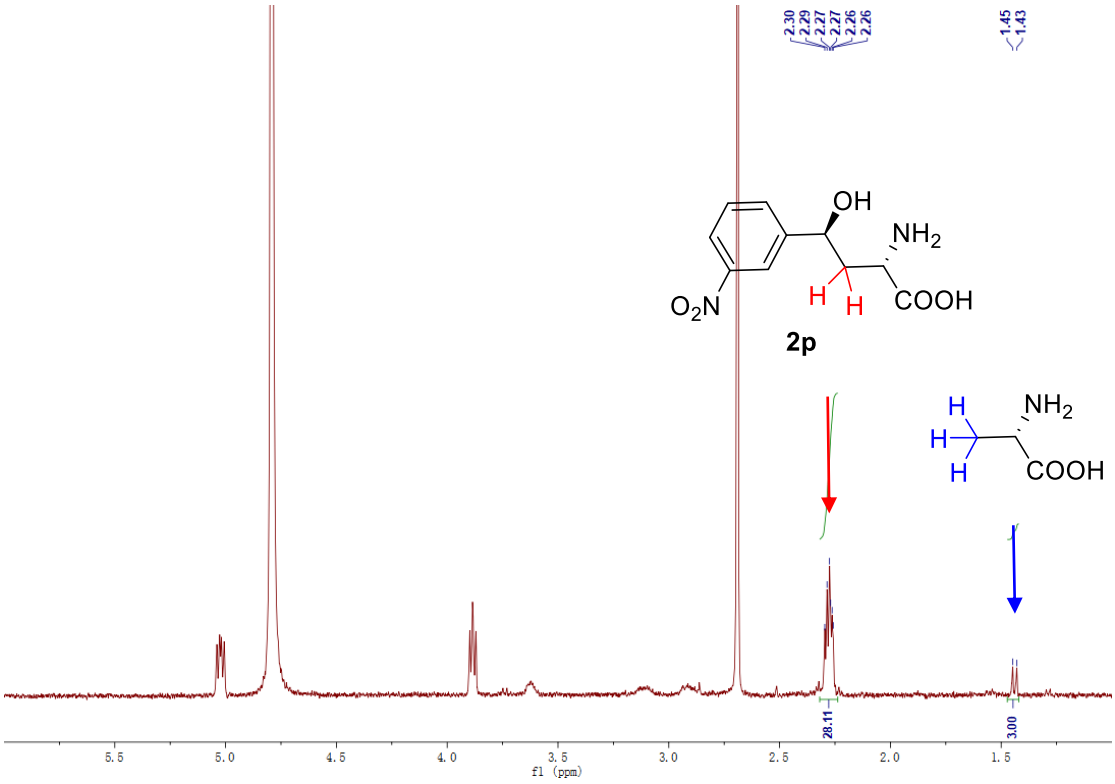


Figure S22. Conversion of **2p**

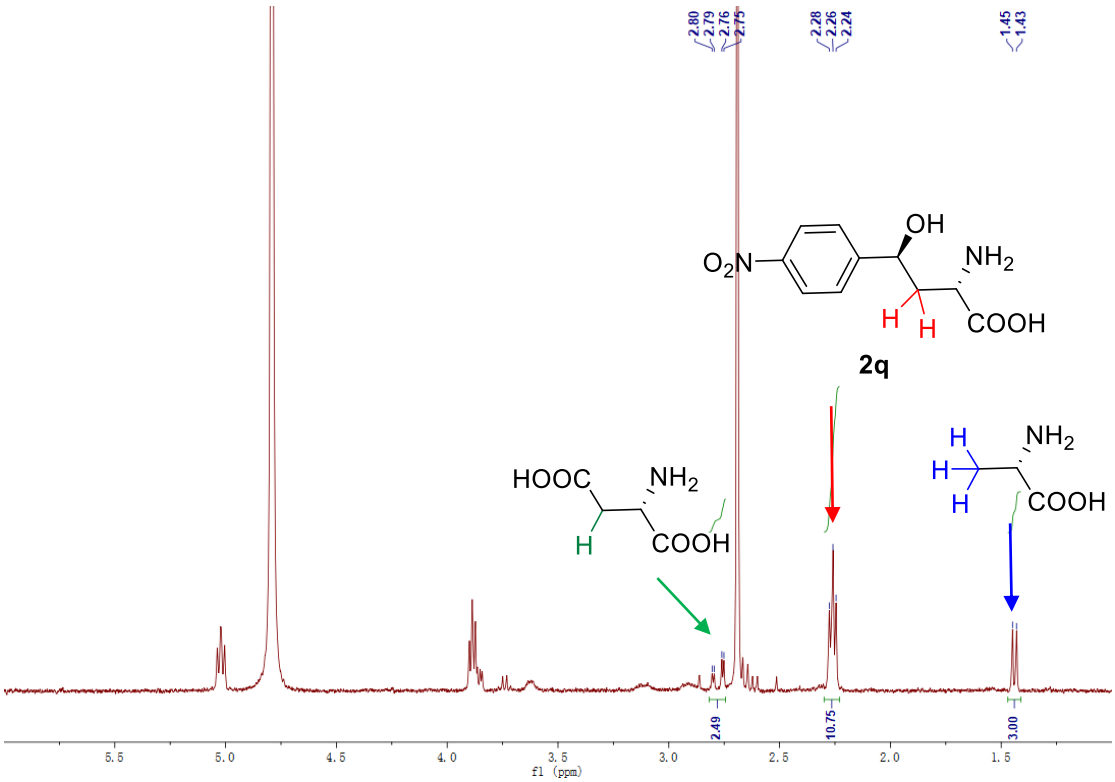


Figure S23. Conversion of **2q**

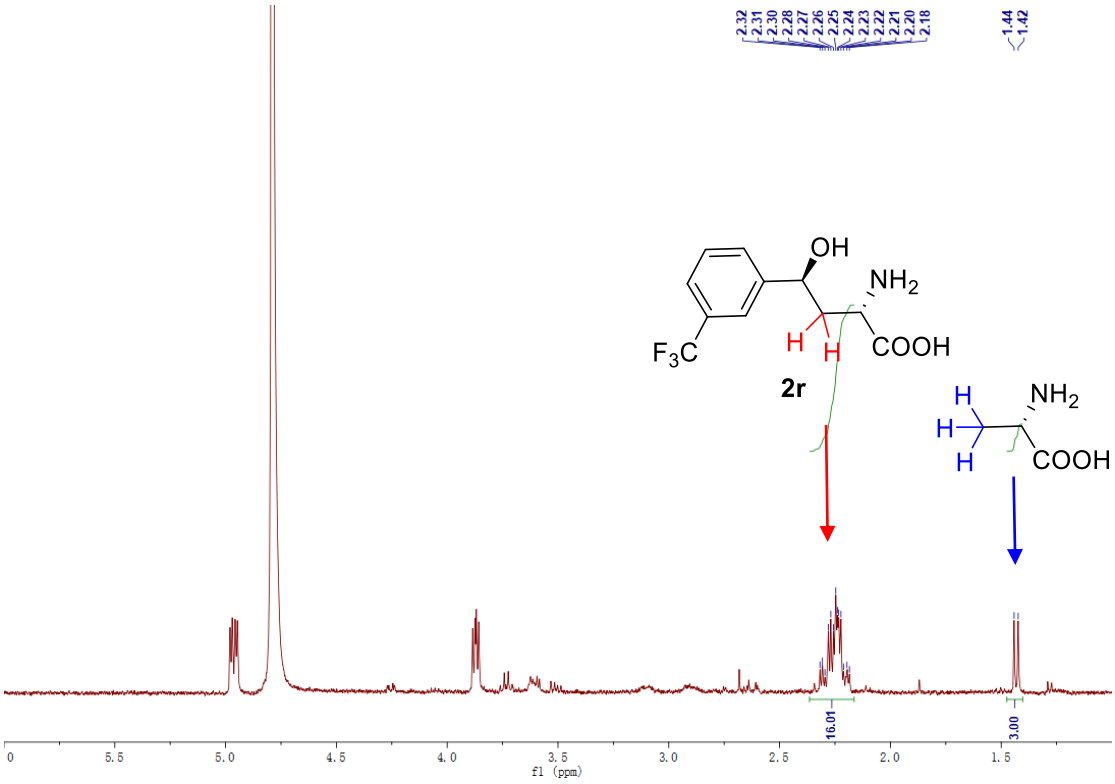


Figure S24. Conversion of **2r**

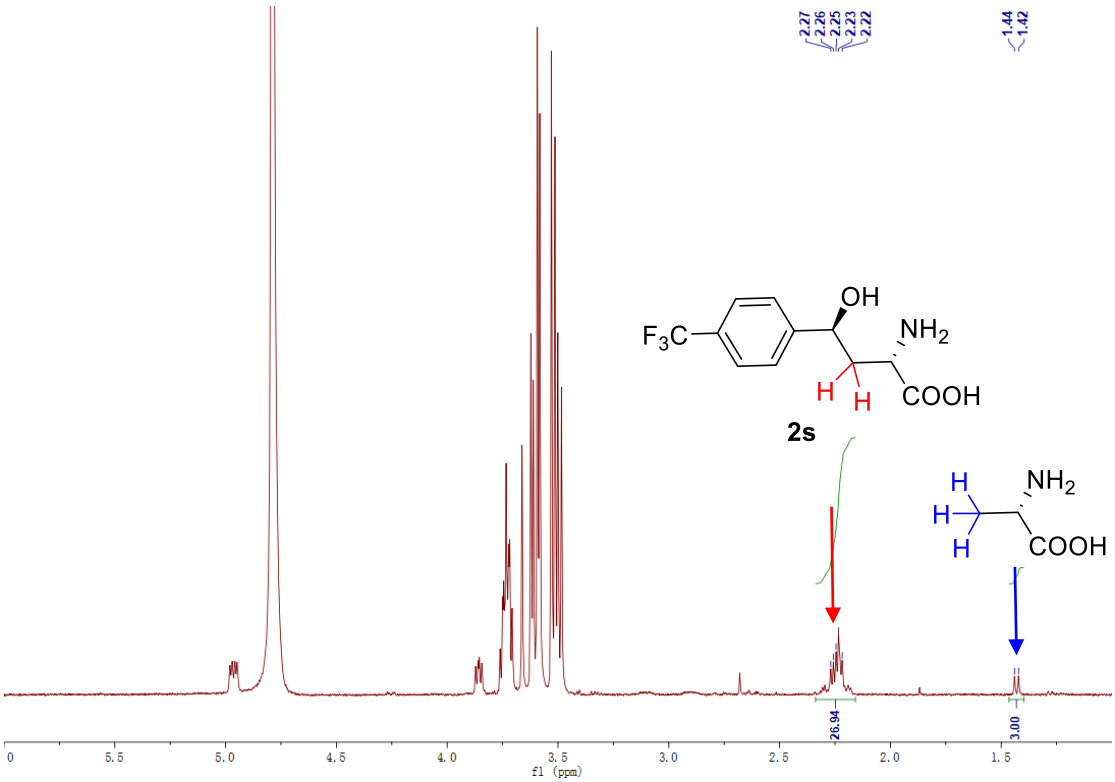


Figure S25. Conversion of **2s**

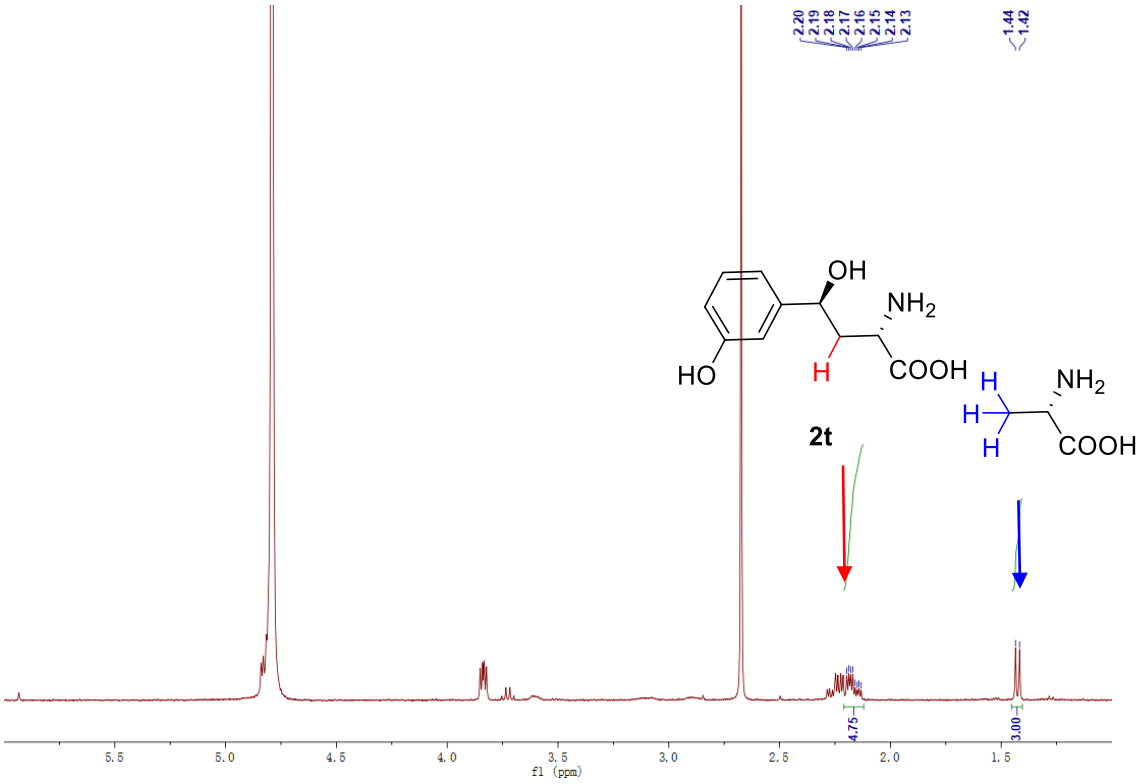


Figure S26. Conversion of **2t**

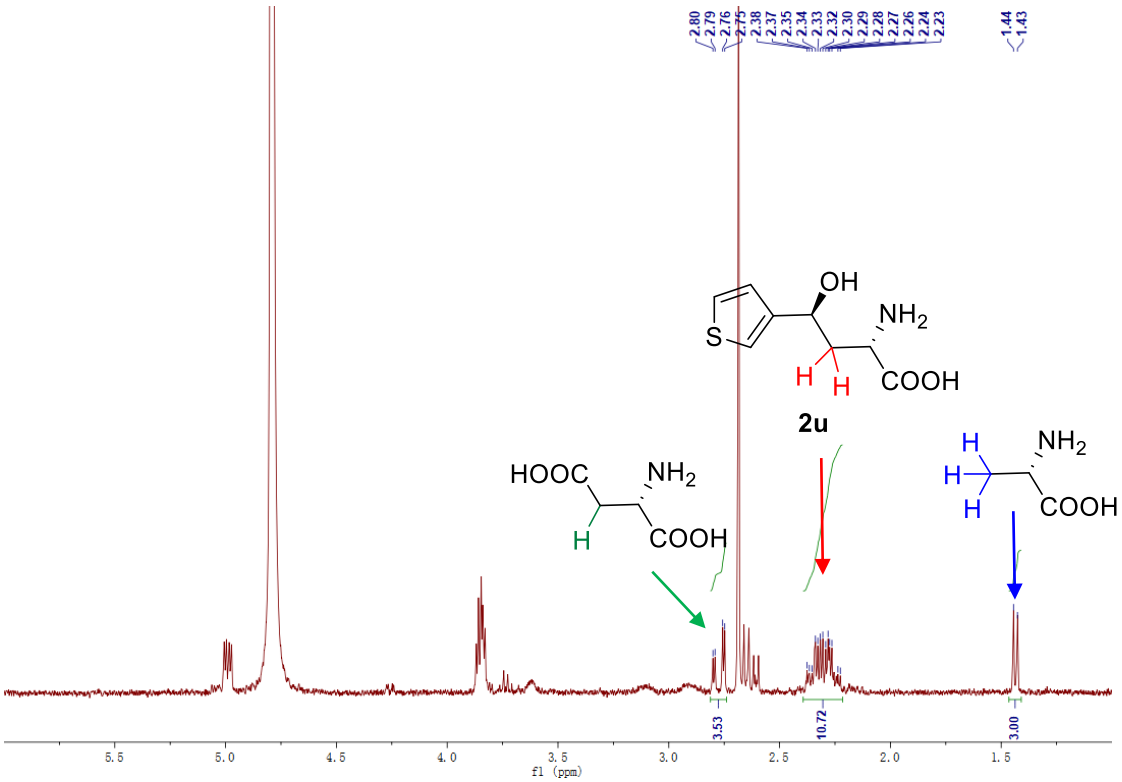


Figure S27. Conversion of **2u**

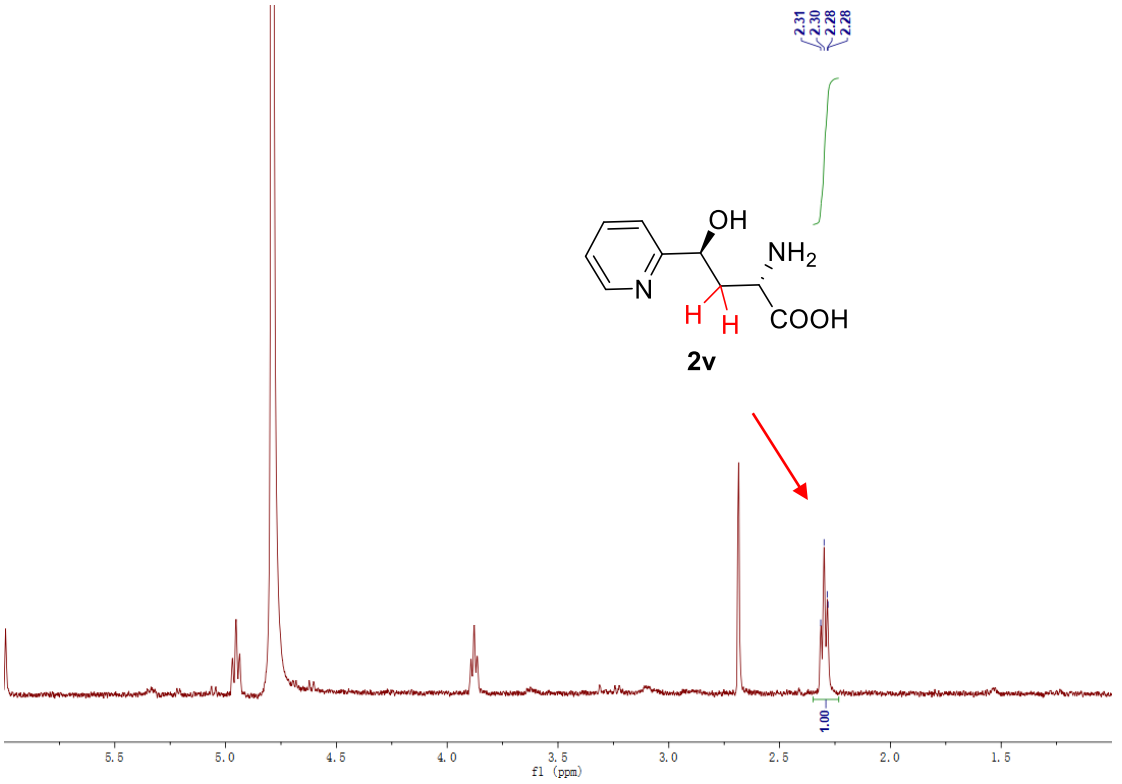


Figure S28. Conversion of **2v**

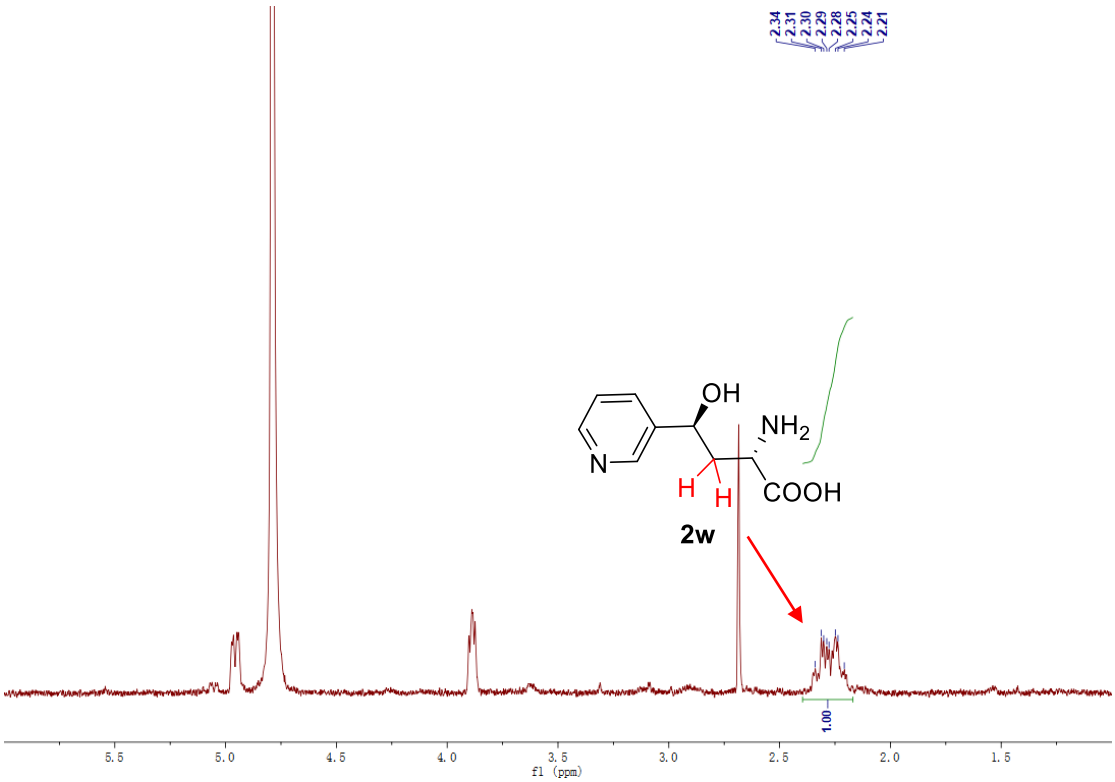


Figure S29. Conversion of **2w**

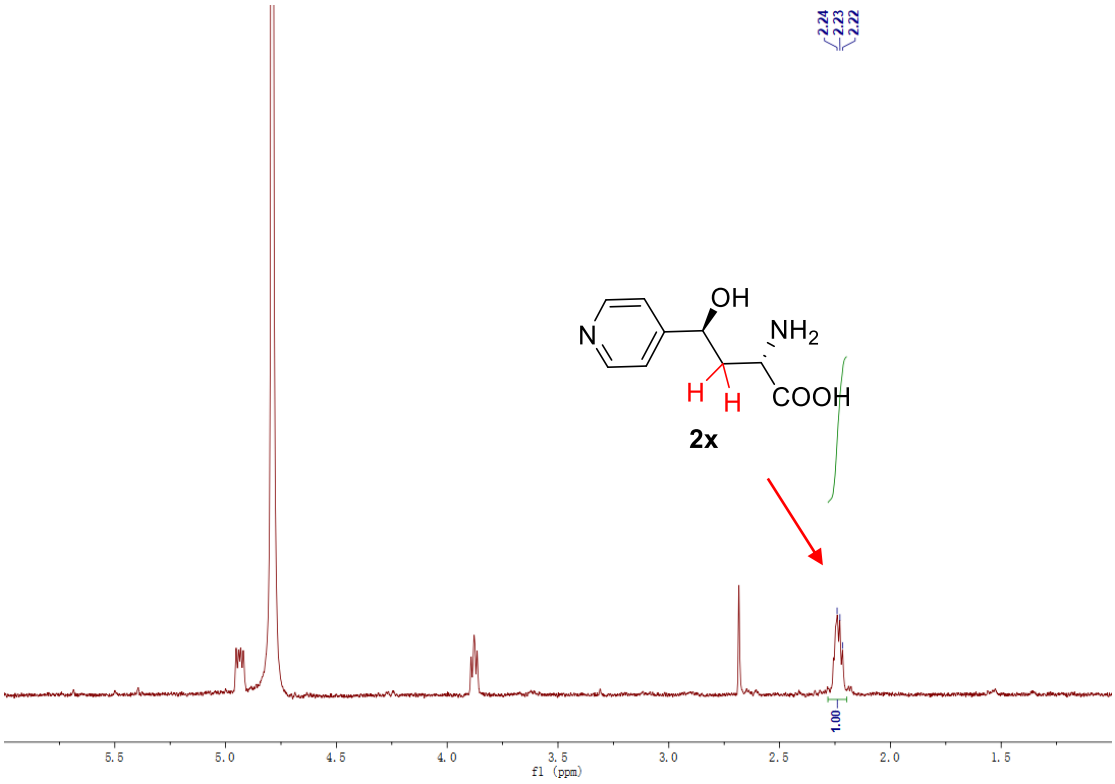


Figure S30. Conversion of **2x**

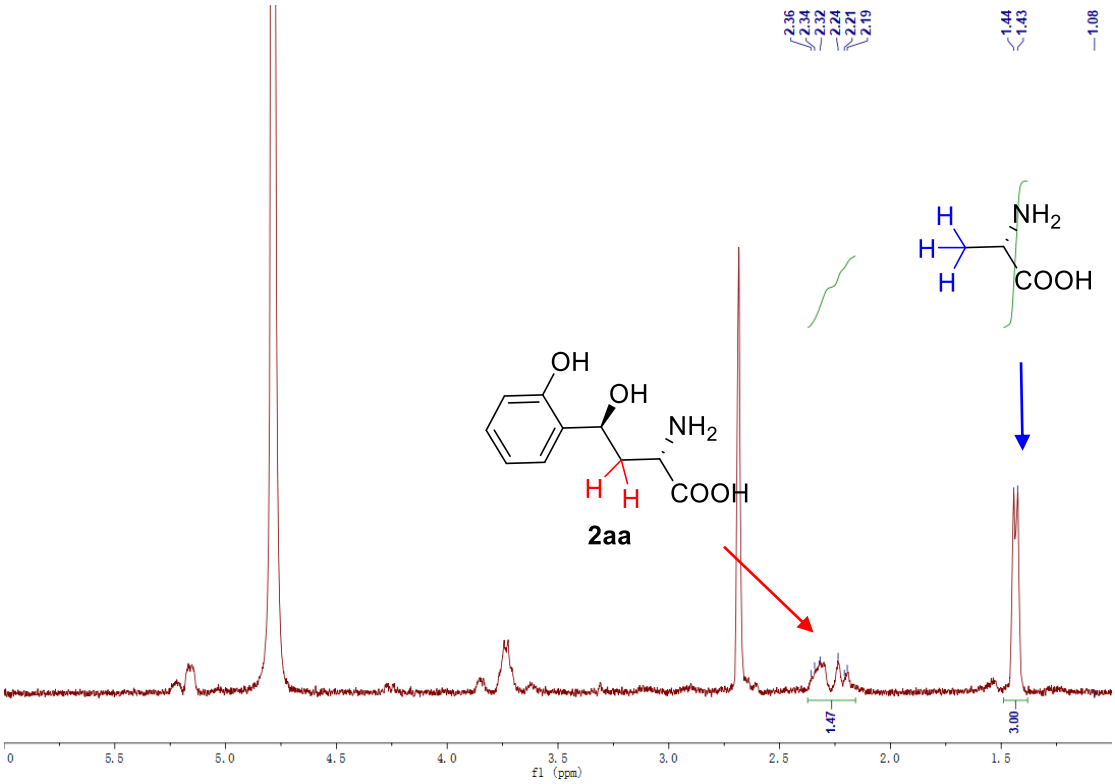


Figure S31. Conversion of **2aa**

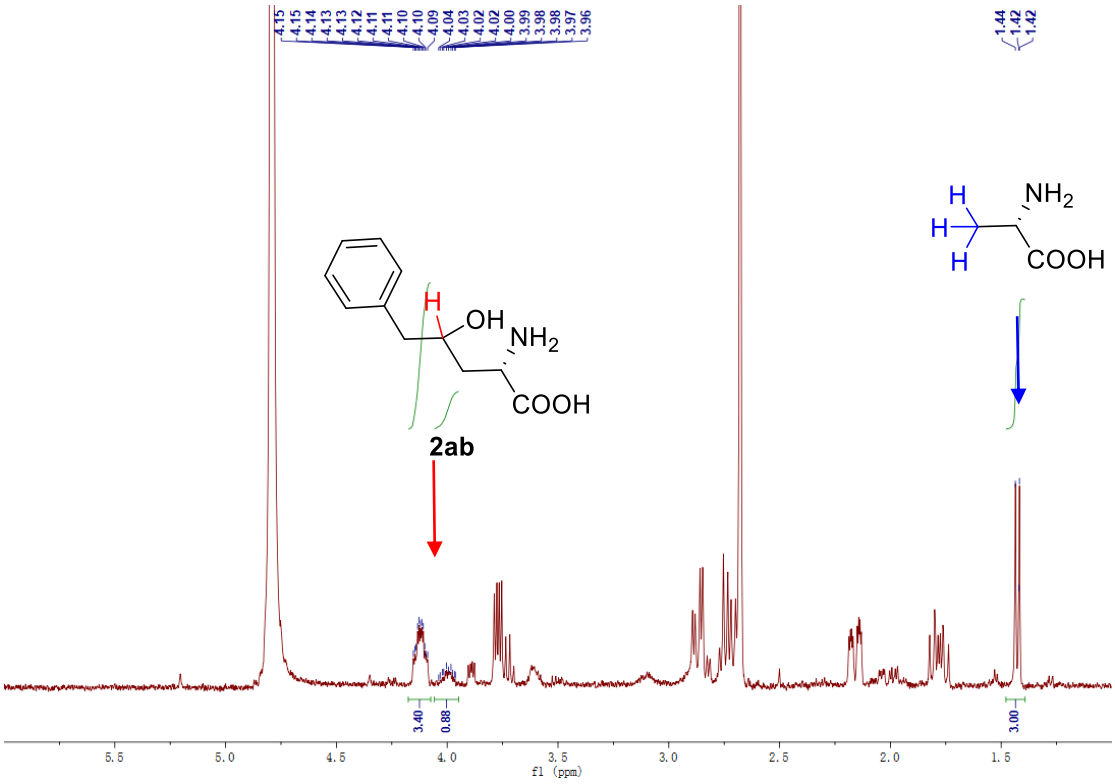


Figure S32. Conversion of **2ab**

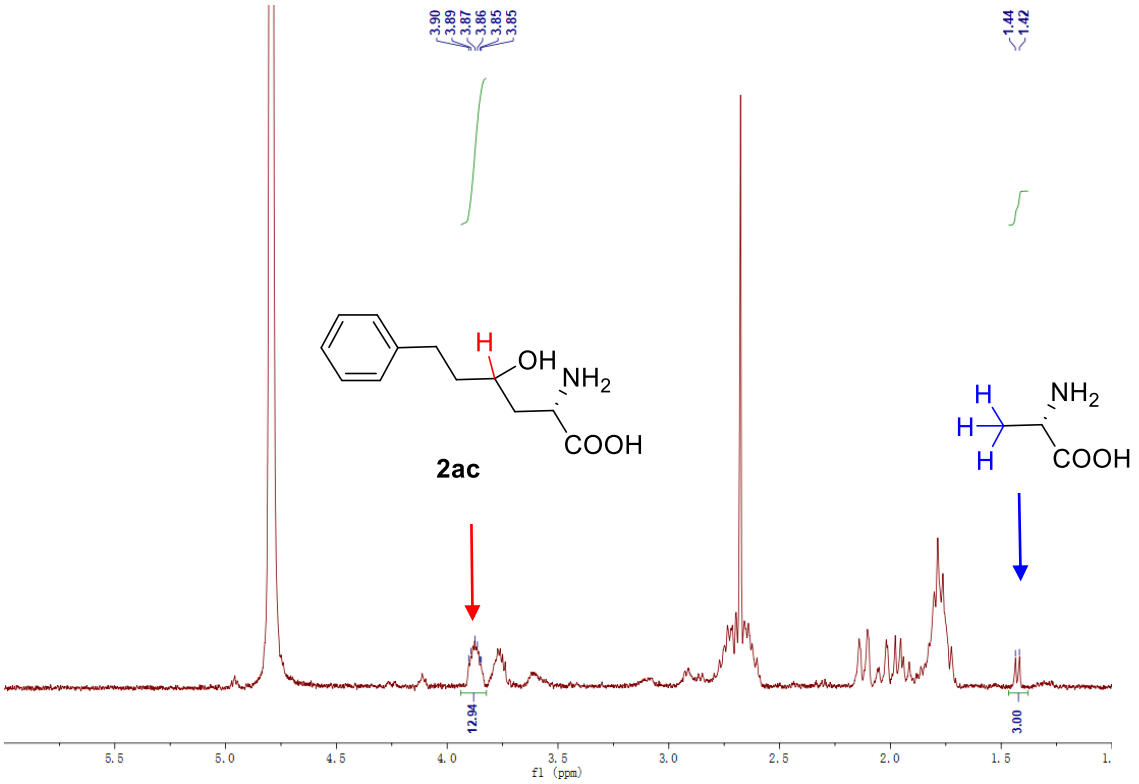


Figure S33. Conversion of **2ac**

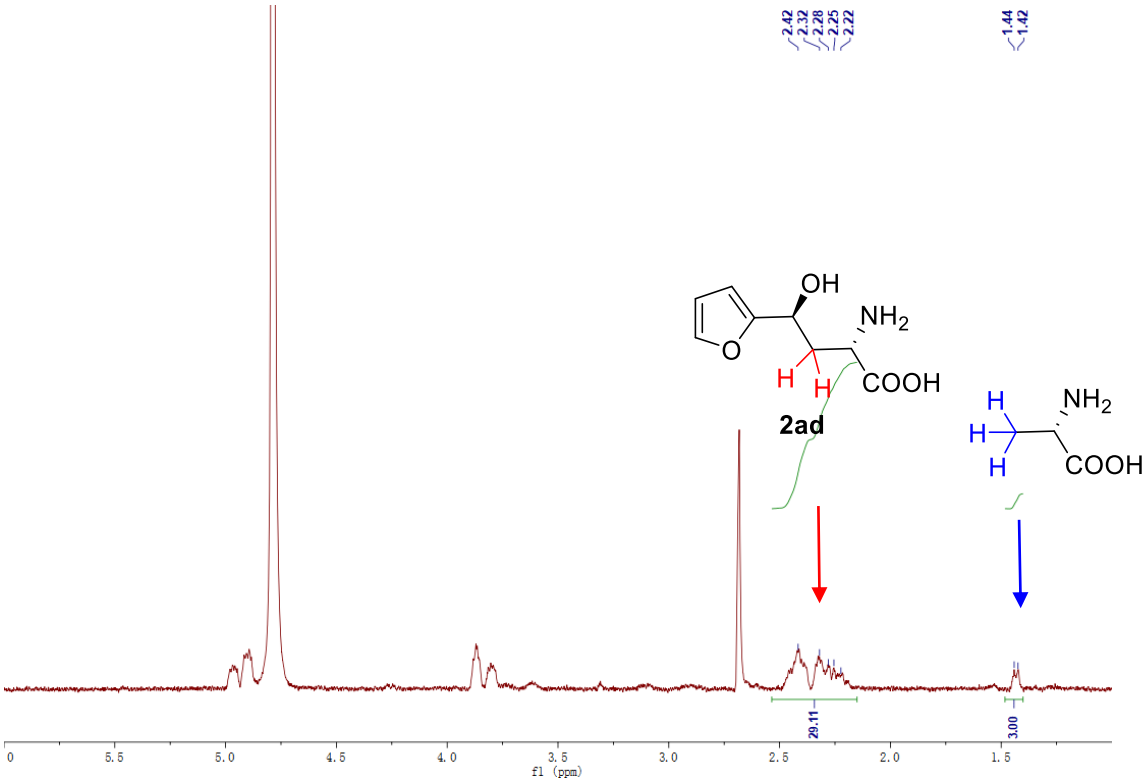


Figure S34. Conversion of **2ad**

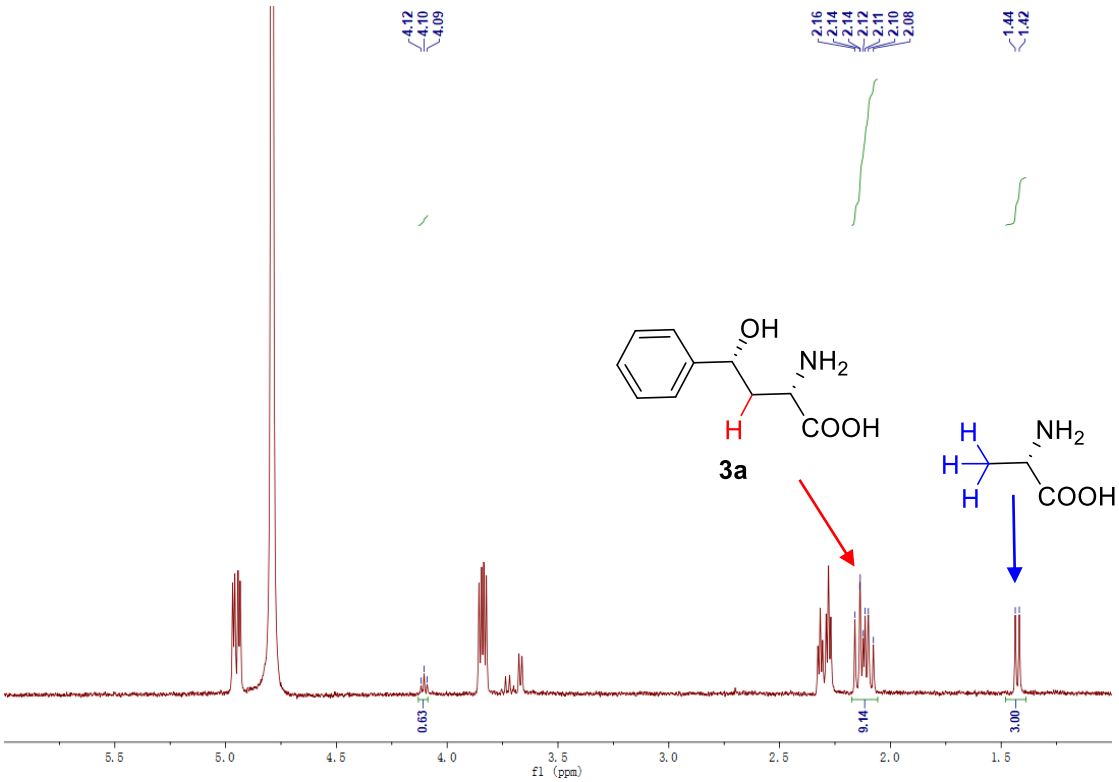


Figure S35. Conversion of **3a**

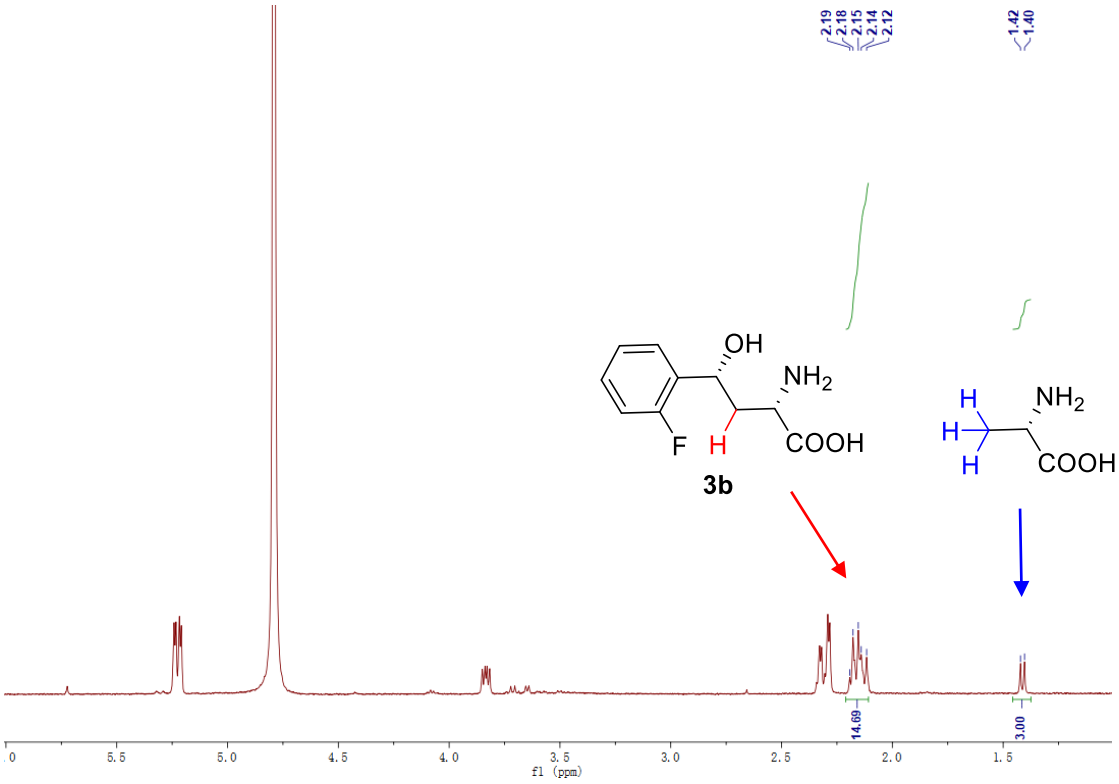


Figure S36. Conversion of **3b**

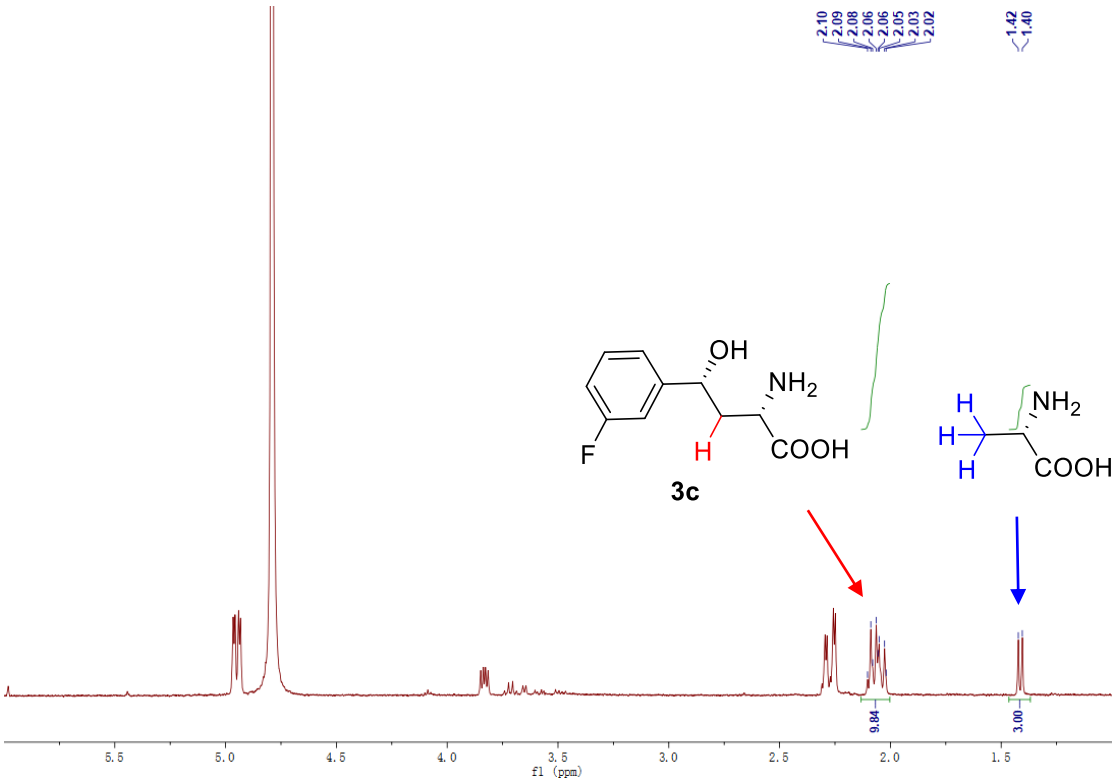


Figure S37. Conversion of **3c**

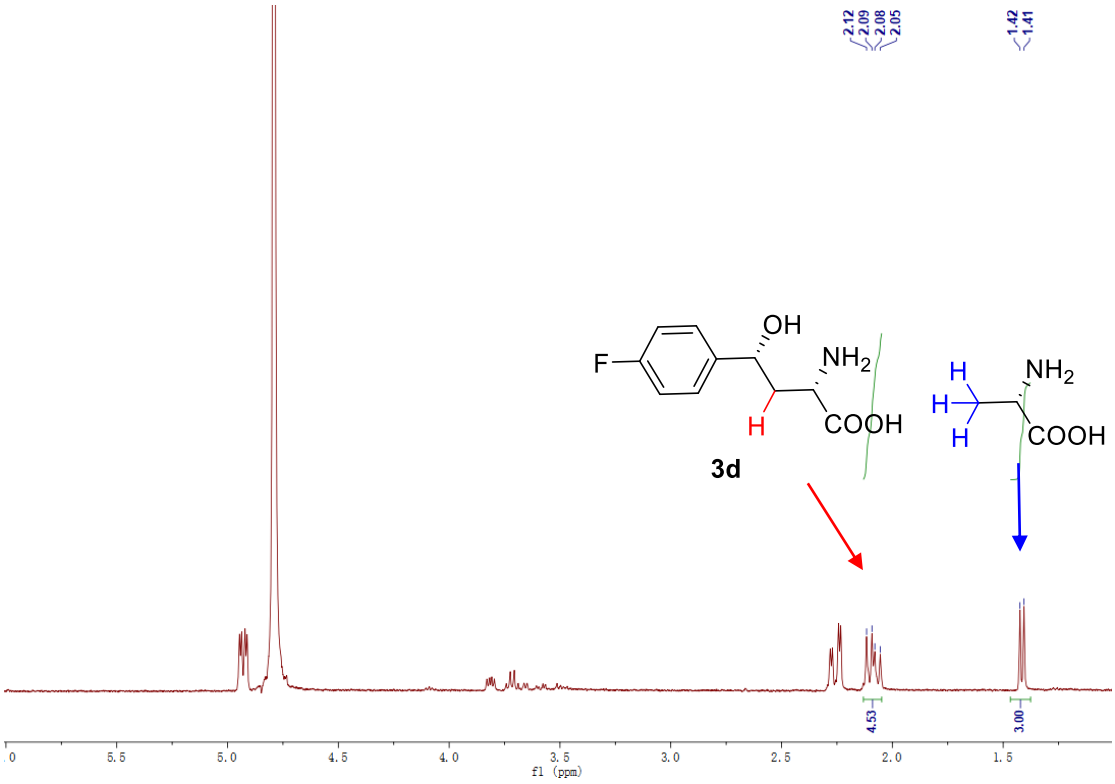


Figure S38. Conversion of **3d**

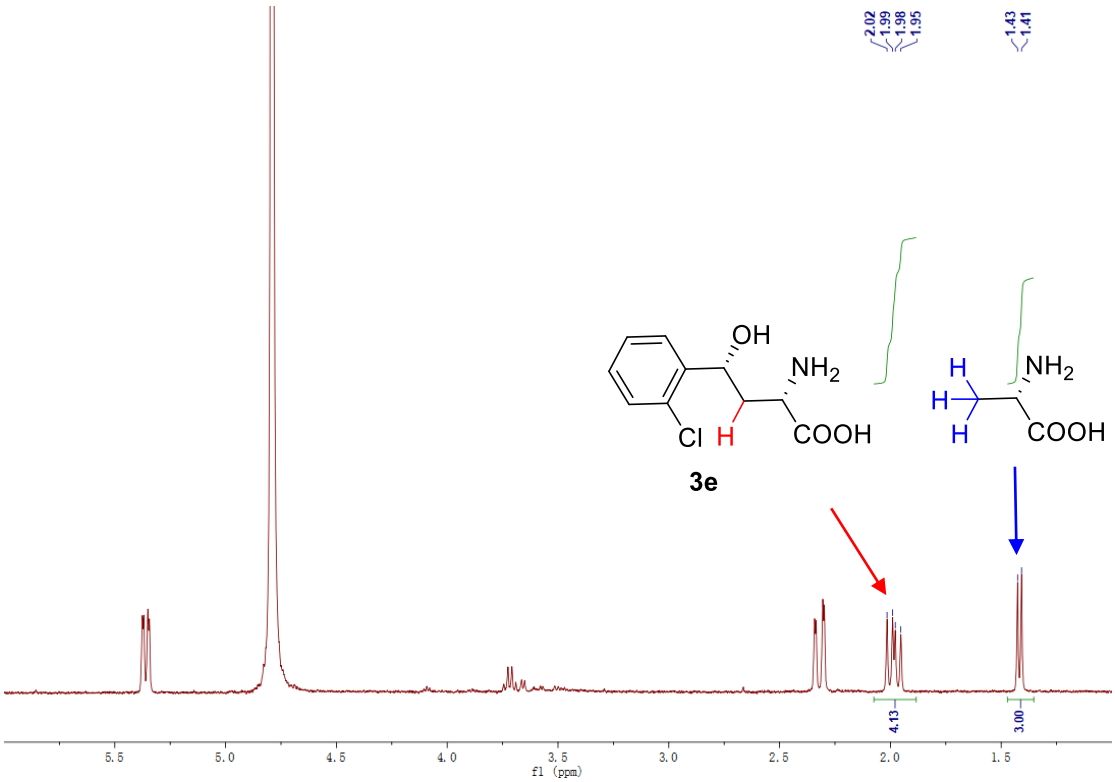


Figure S39. Conversion of **3e**

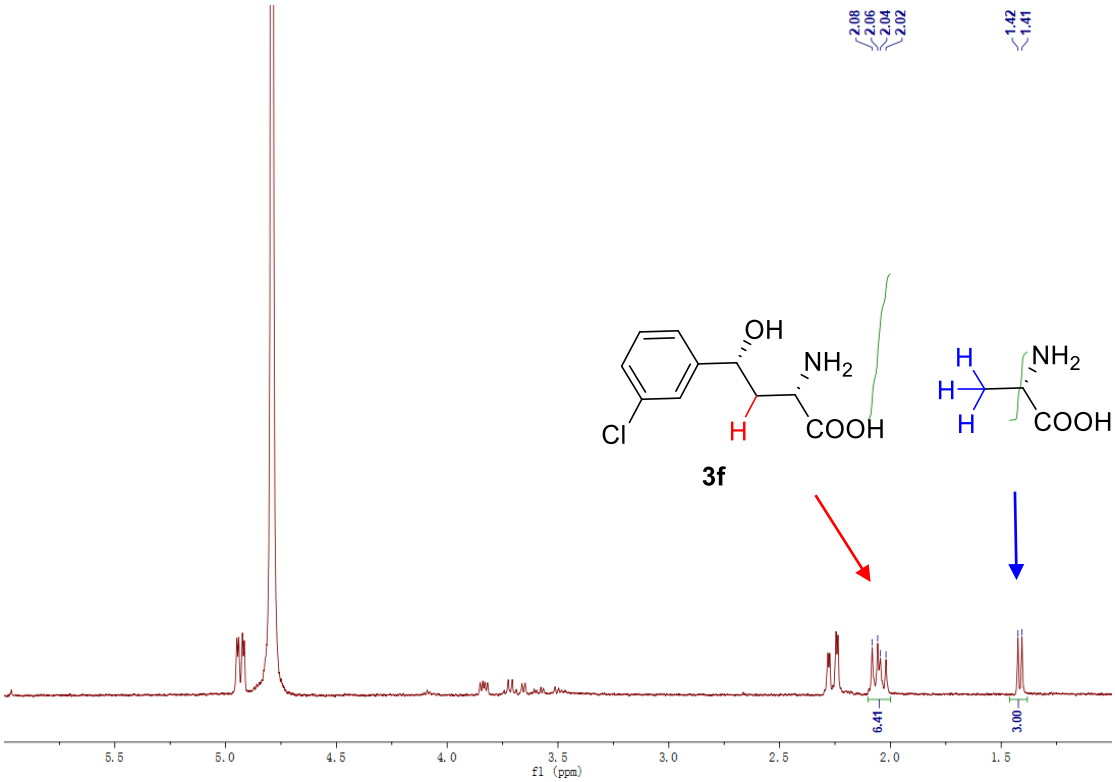


Figure S40. Conversion of **3f**

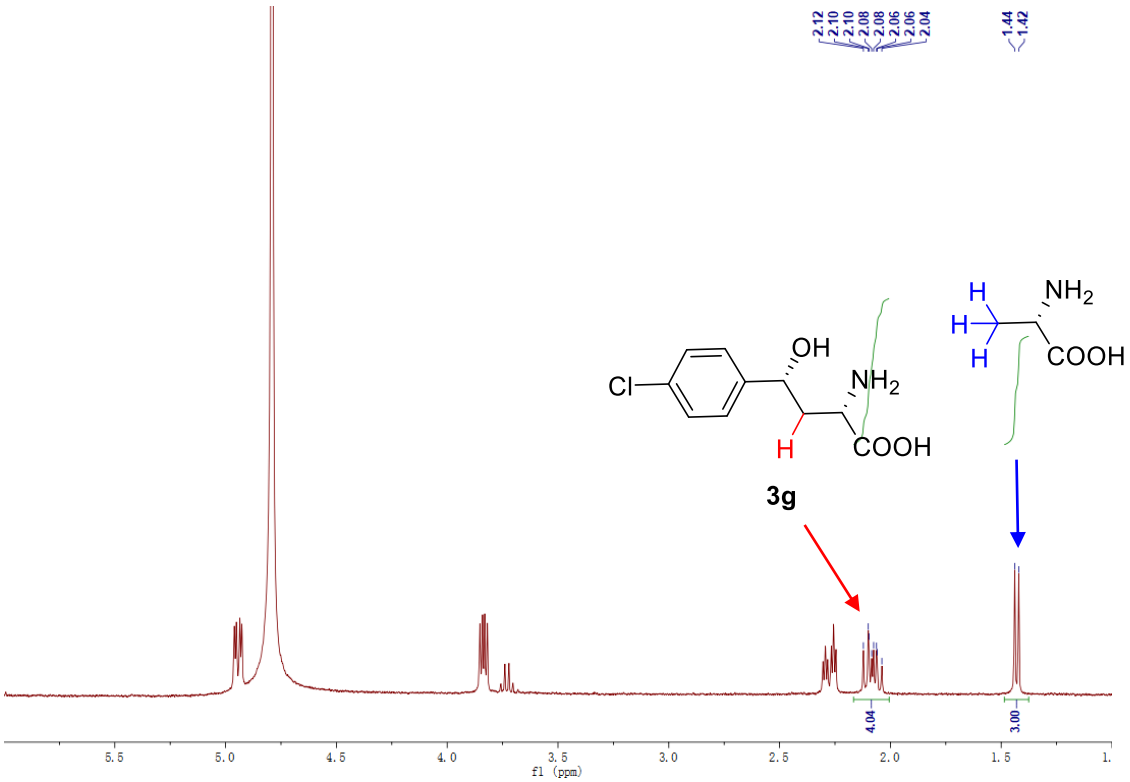


Figure S41. Conversion of **3g**

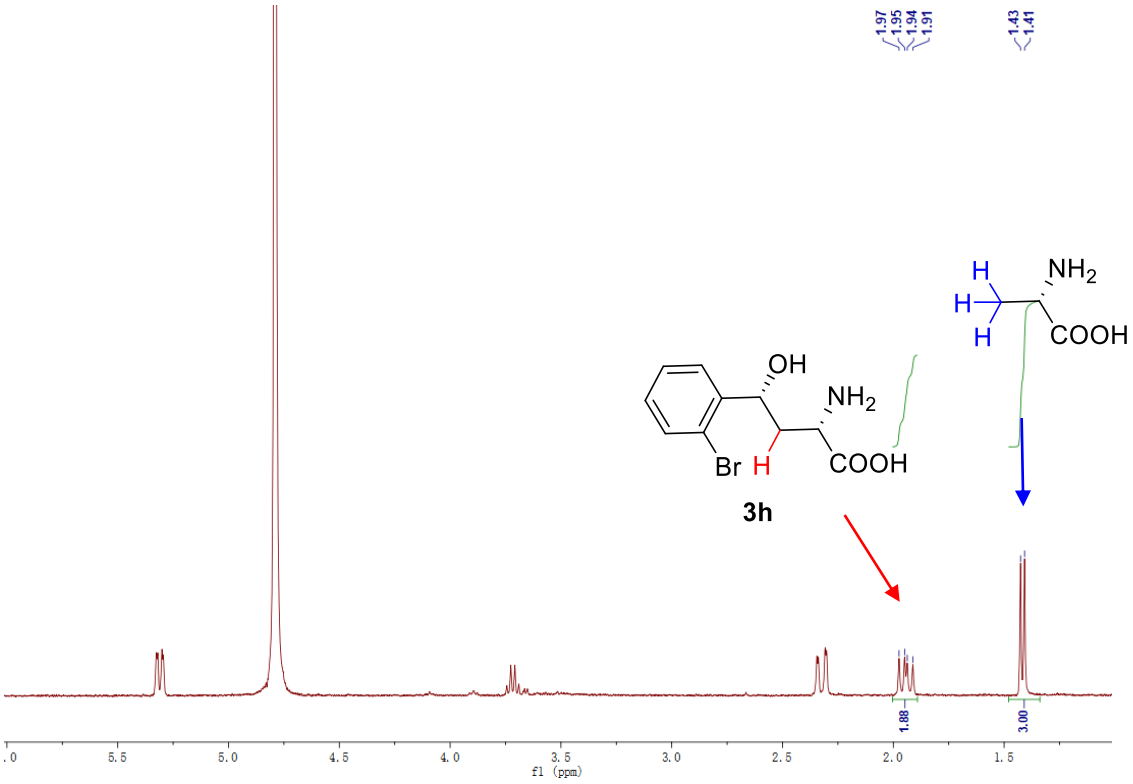


Figure S42. Conversion of **3h**

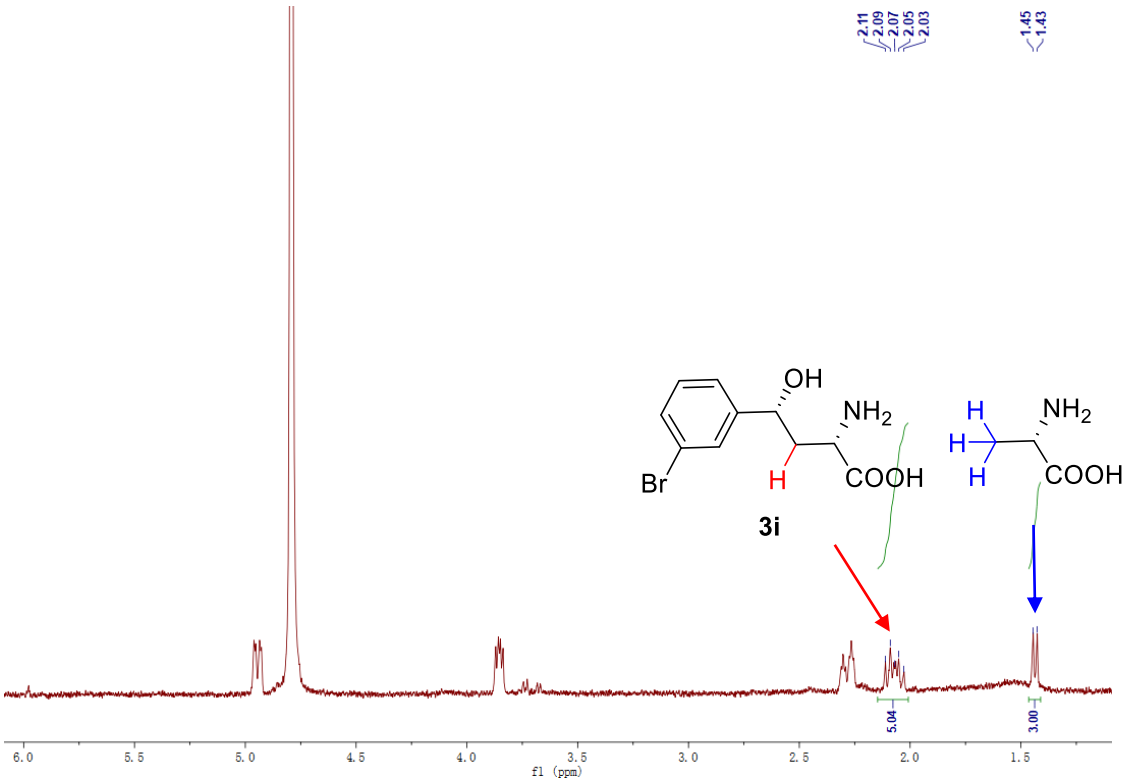


Figure S43. Conversion of **3i**

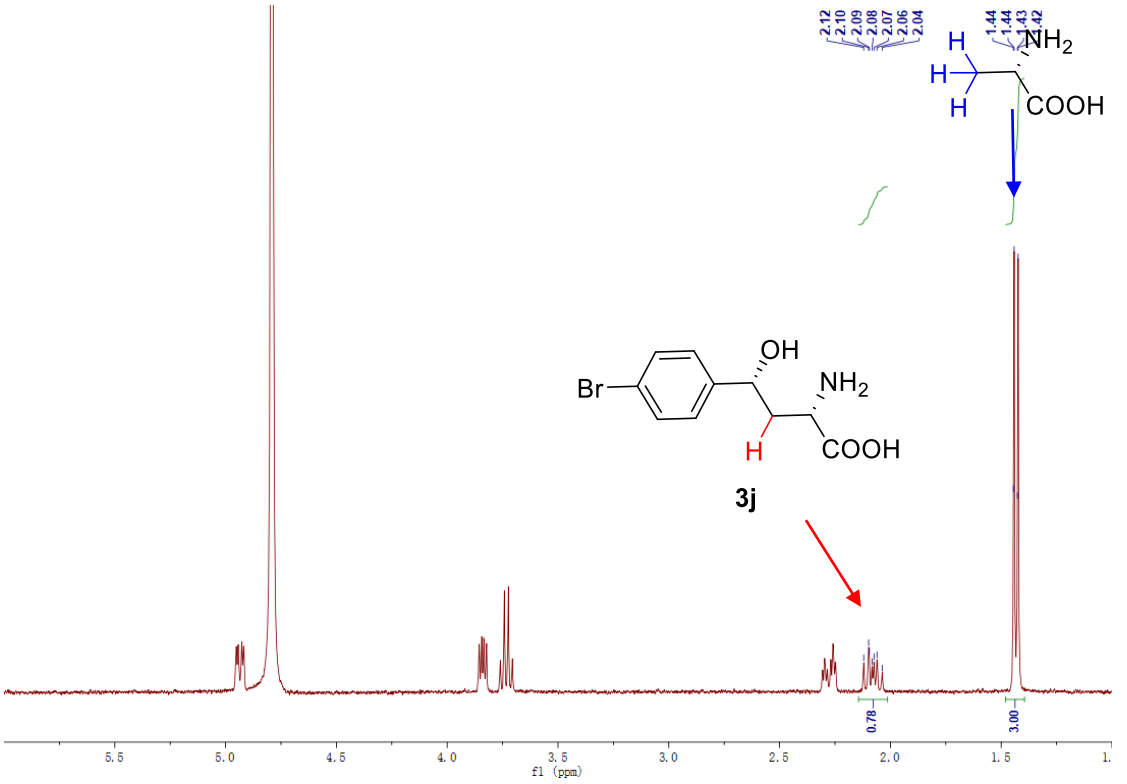


Figure S44. Conversion of **3j**

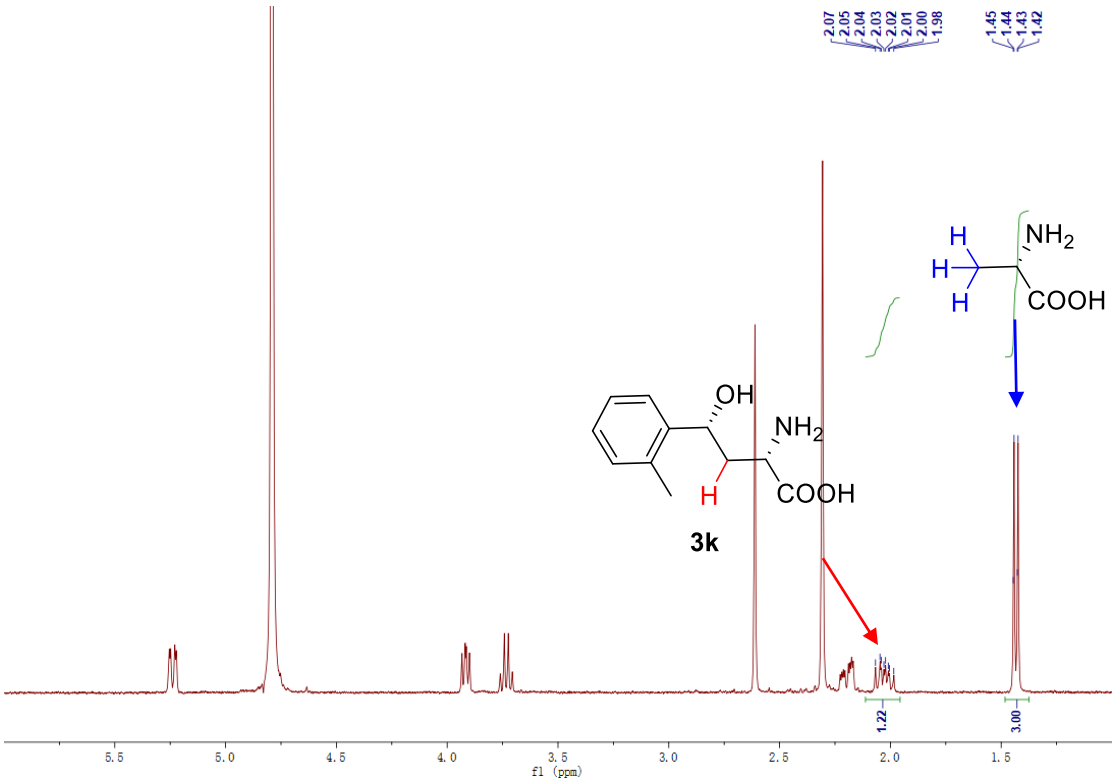


Figure S45. Conversion of **3k**

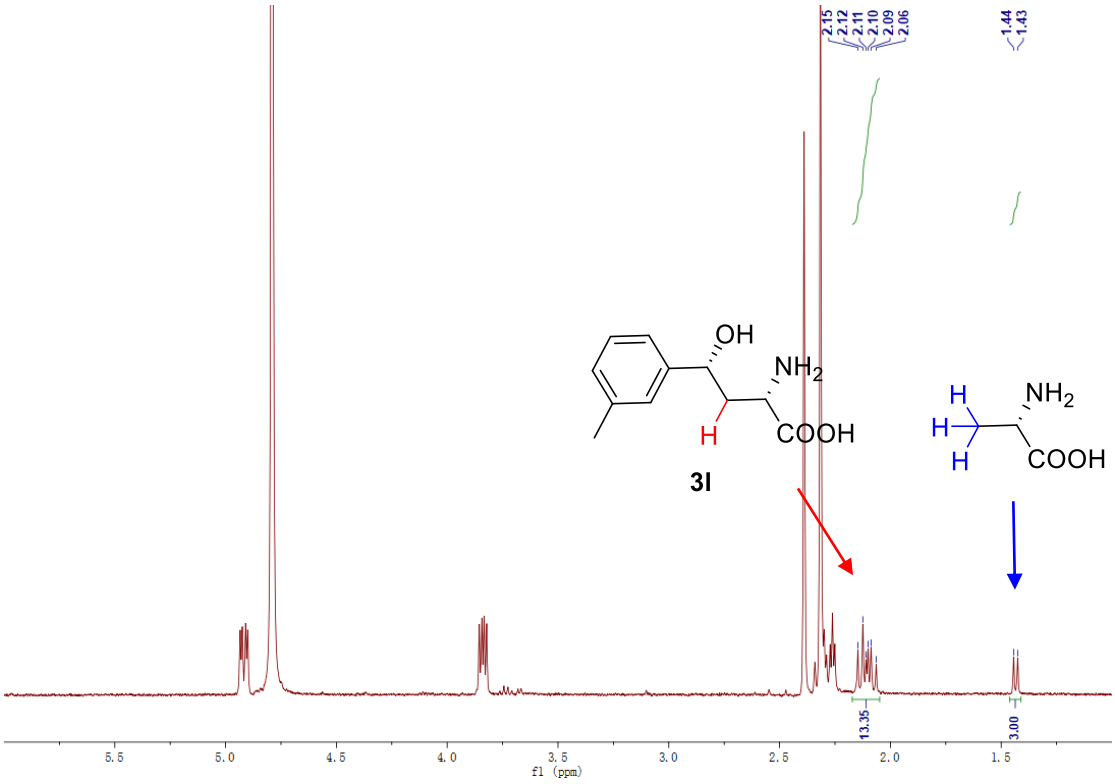


Figure S46. Conversion of **3l**

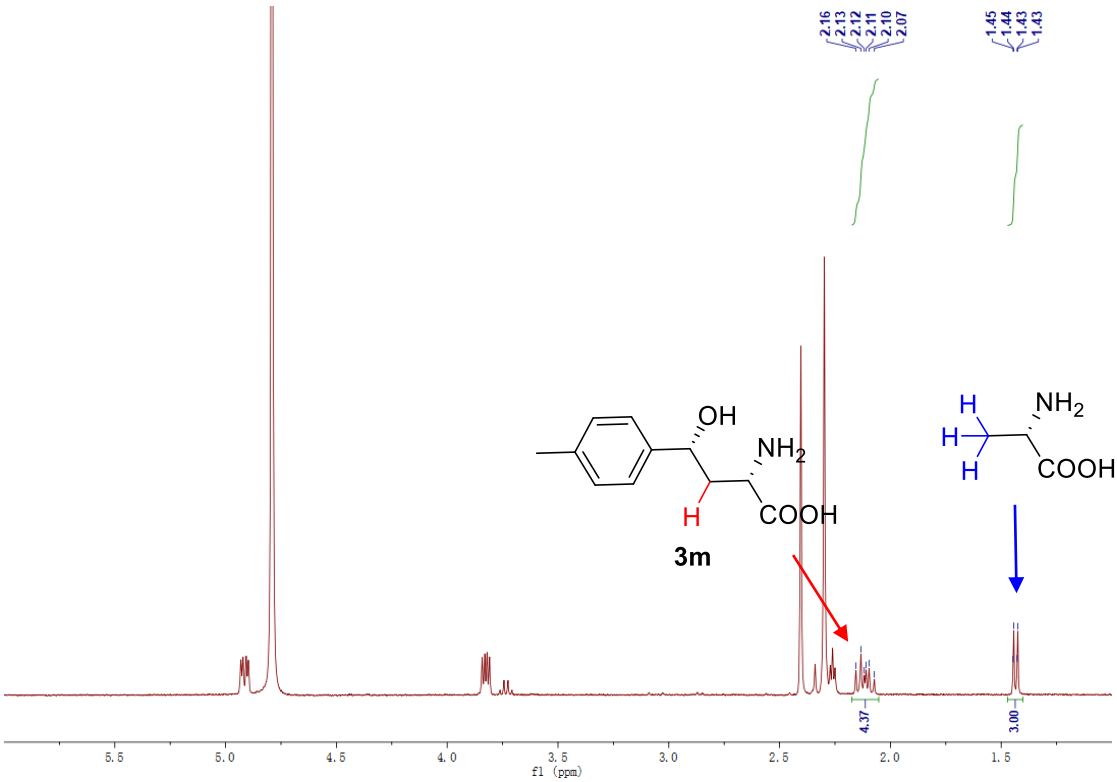


Figure S47. Conversion of **3m**

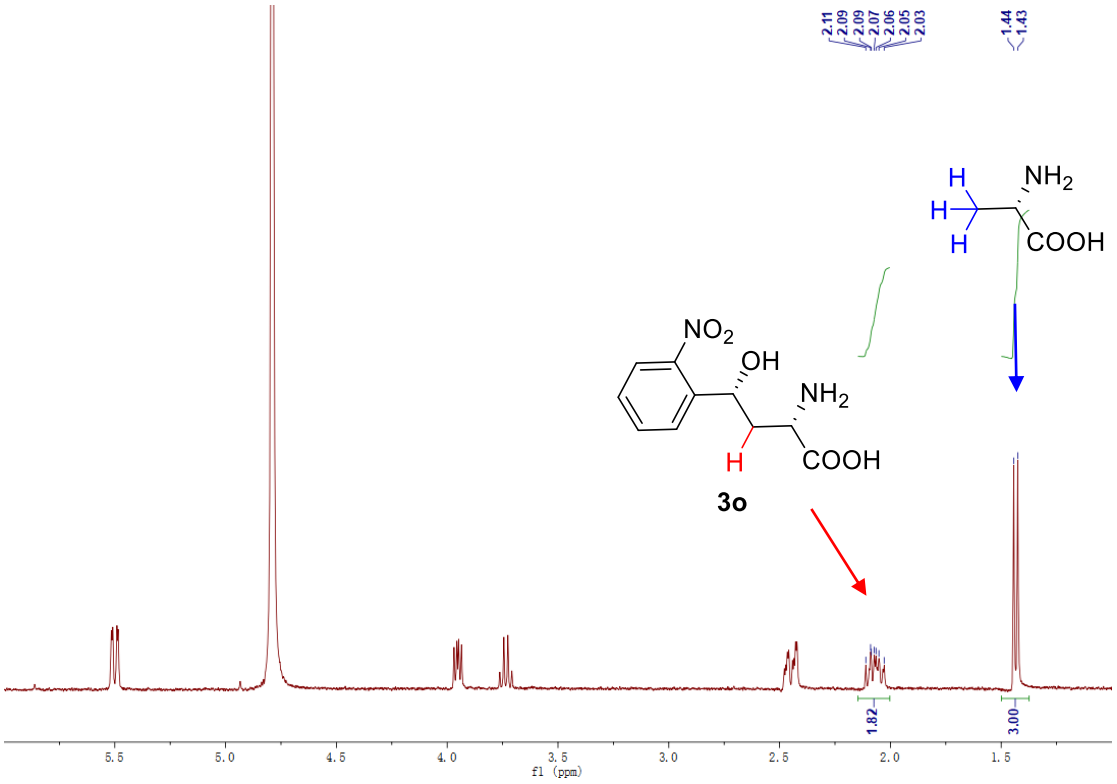


Figure S48. Conversion of **3o**

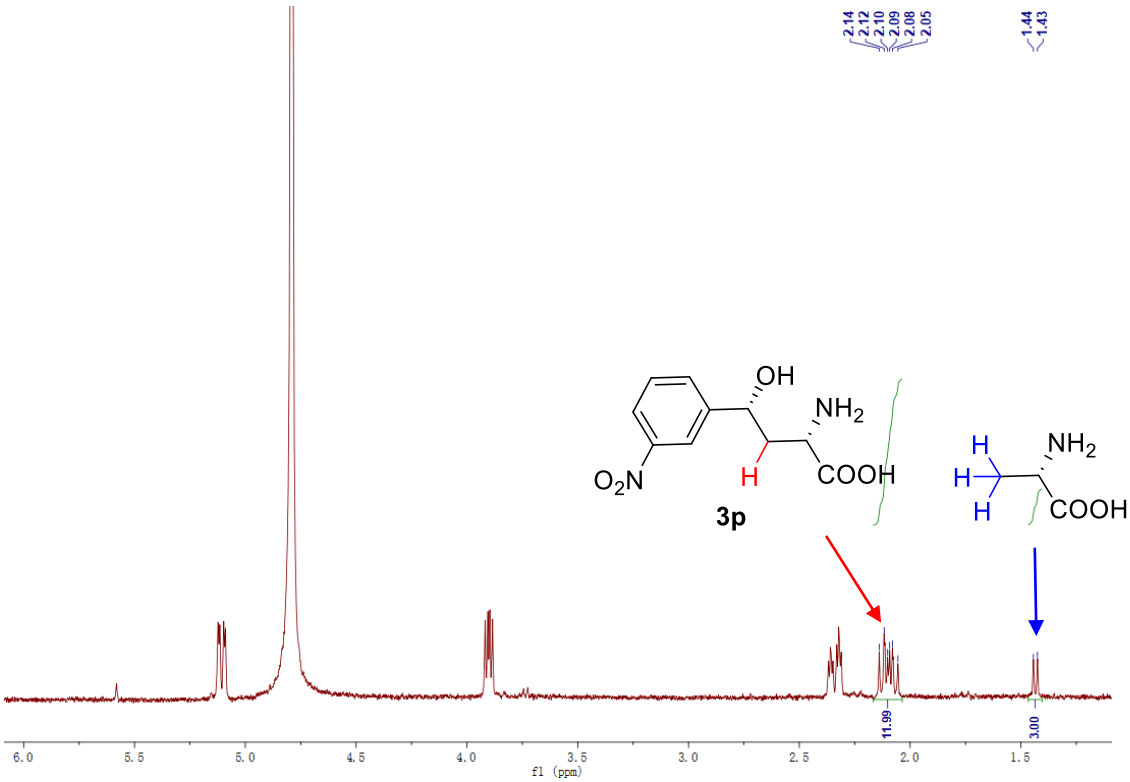


Figure S49. Conversion of **3p**

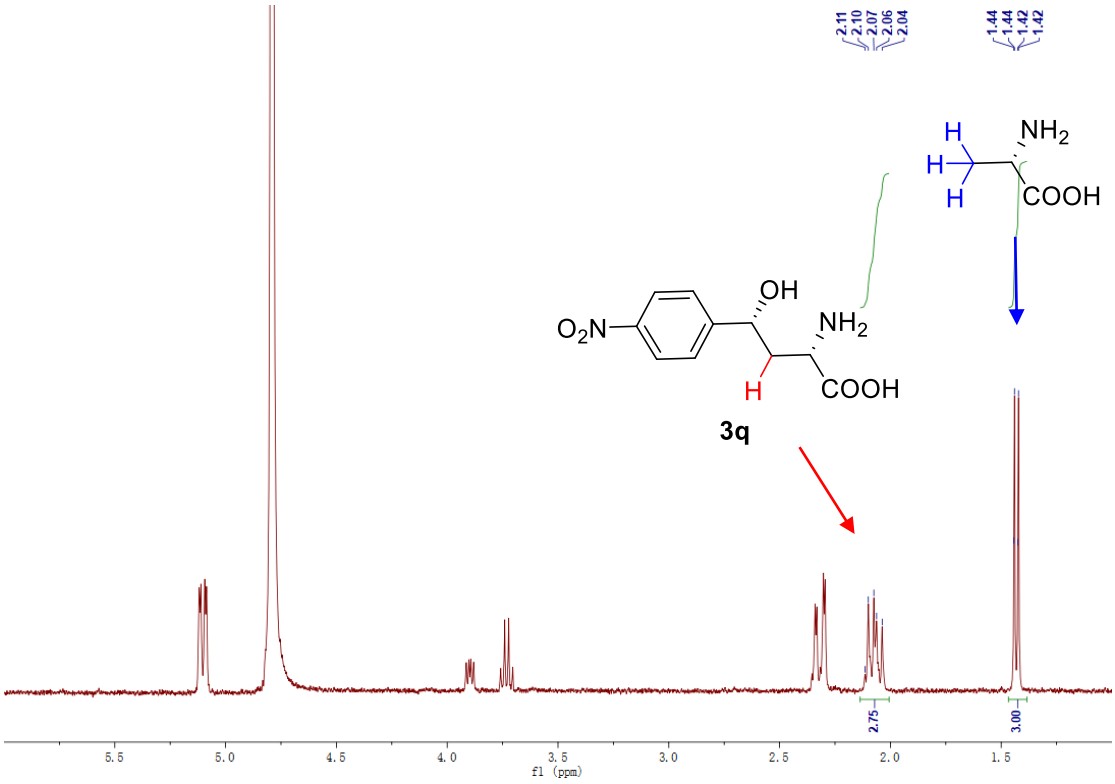


Figure S50. Conversion of **3q**

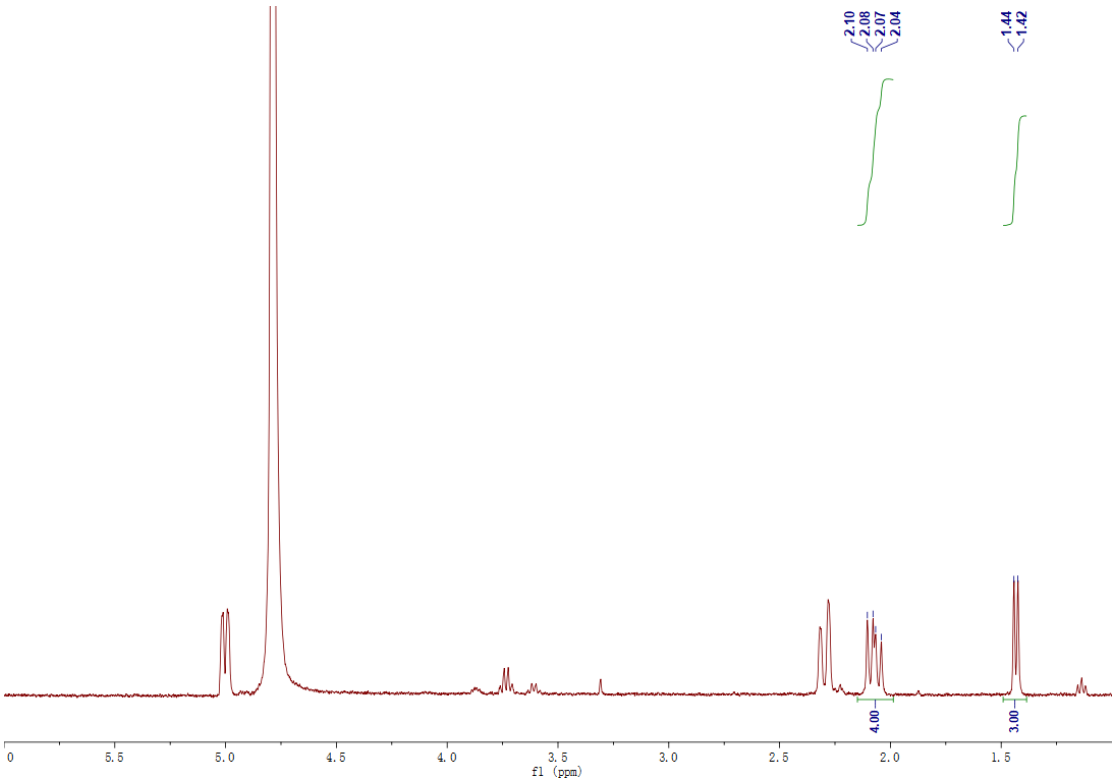


Figure S51. Conversion of **3r**

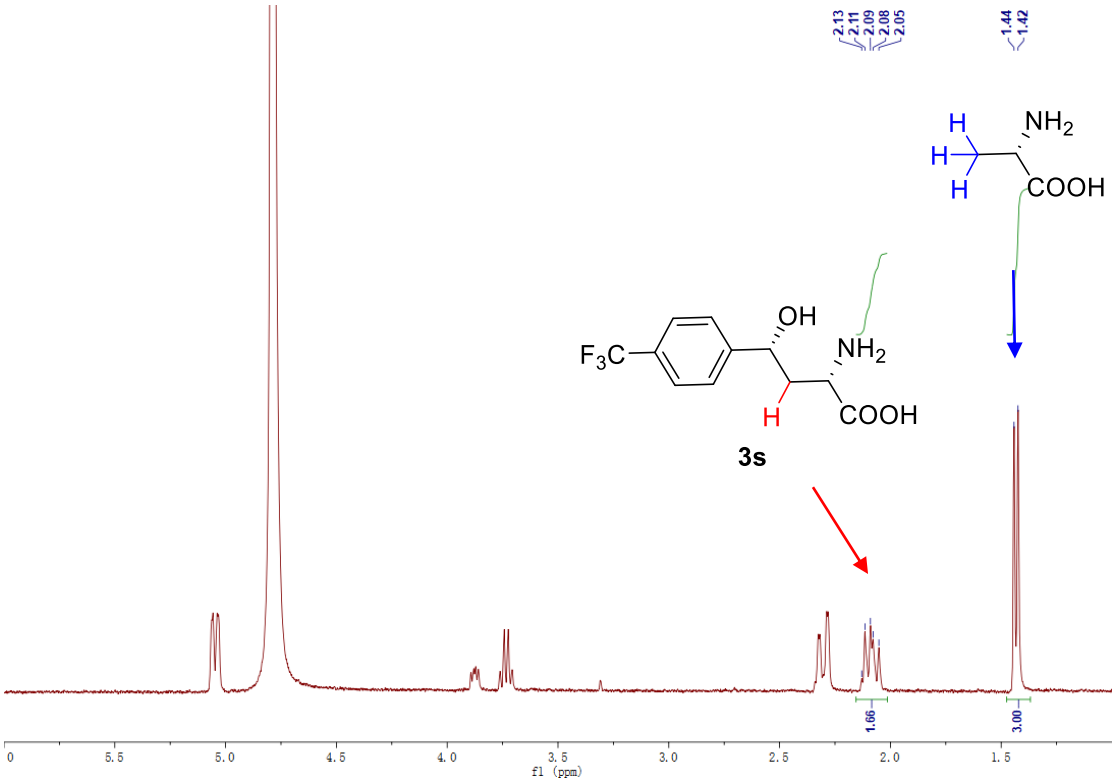


Figure S52. Conversion of **3s**

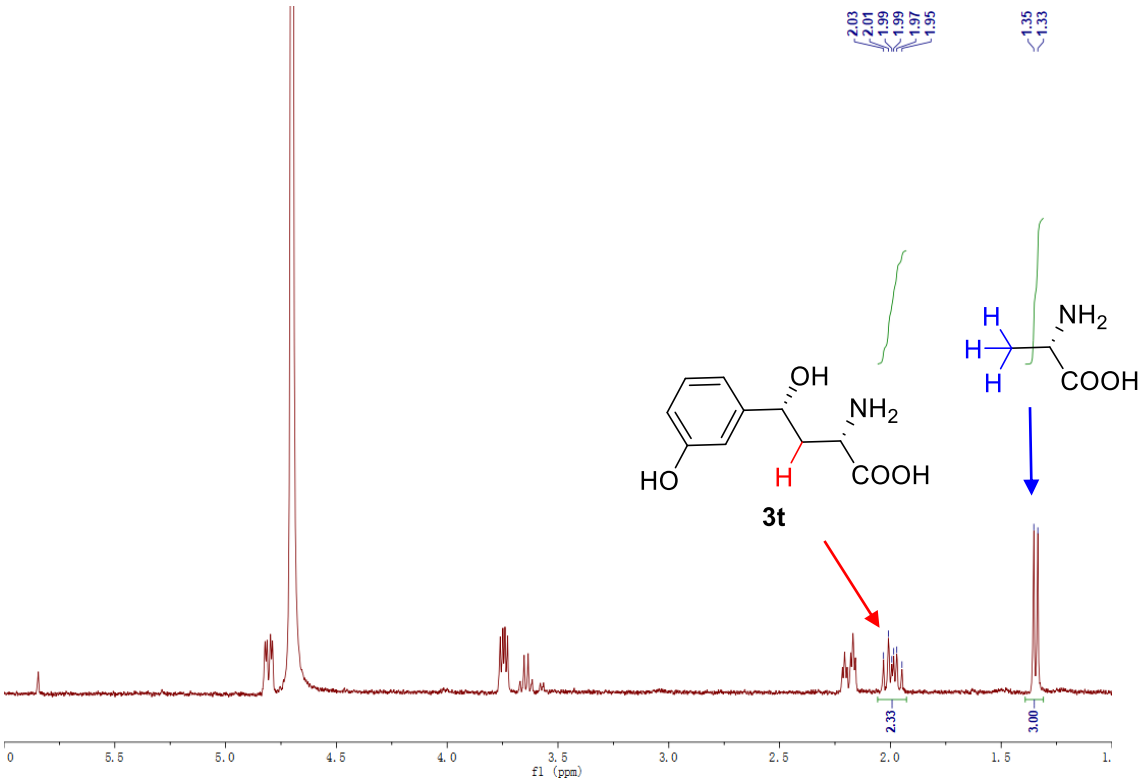


Figure S53. Conversion of **3t**

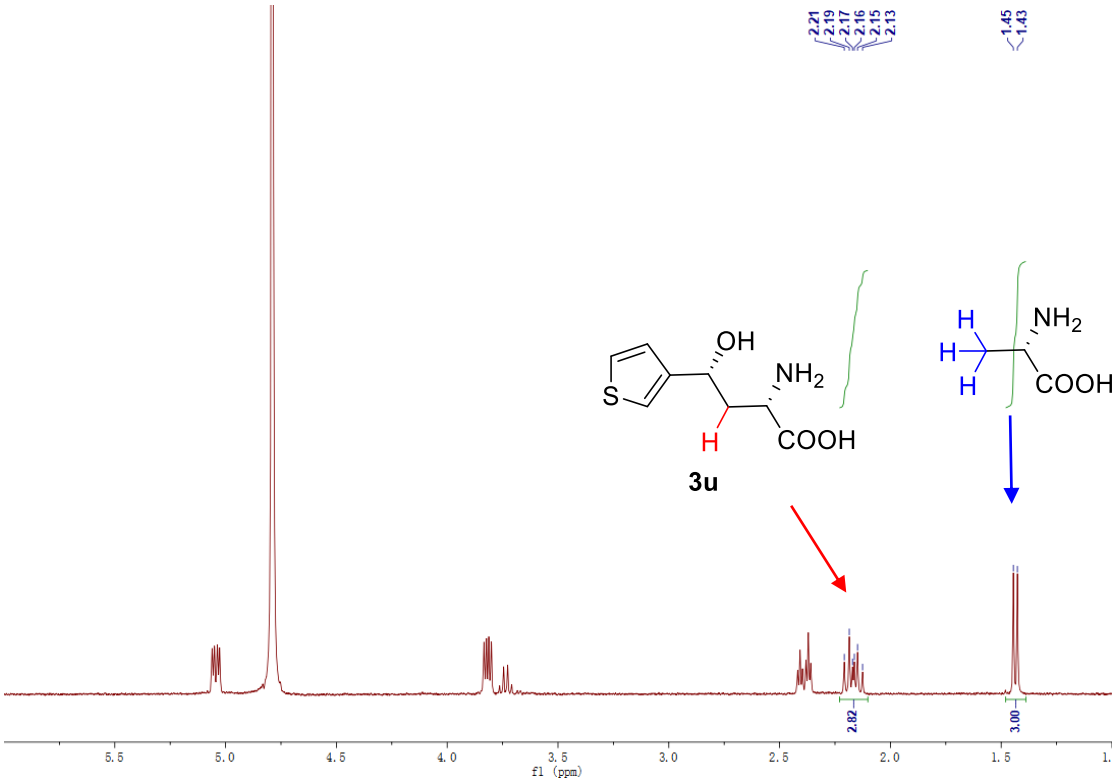


Figure S54. Conversion of **3u**

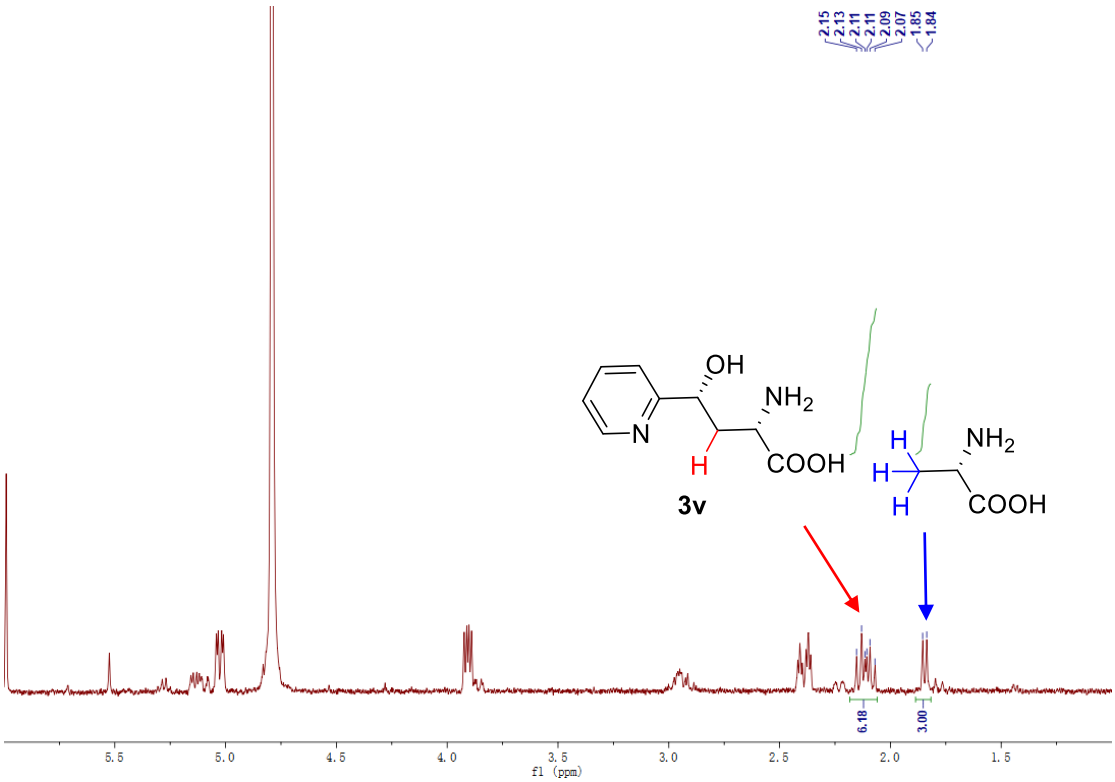


Figure S55. Conversion of **3v**

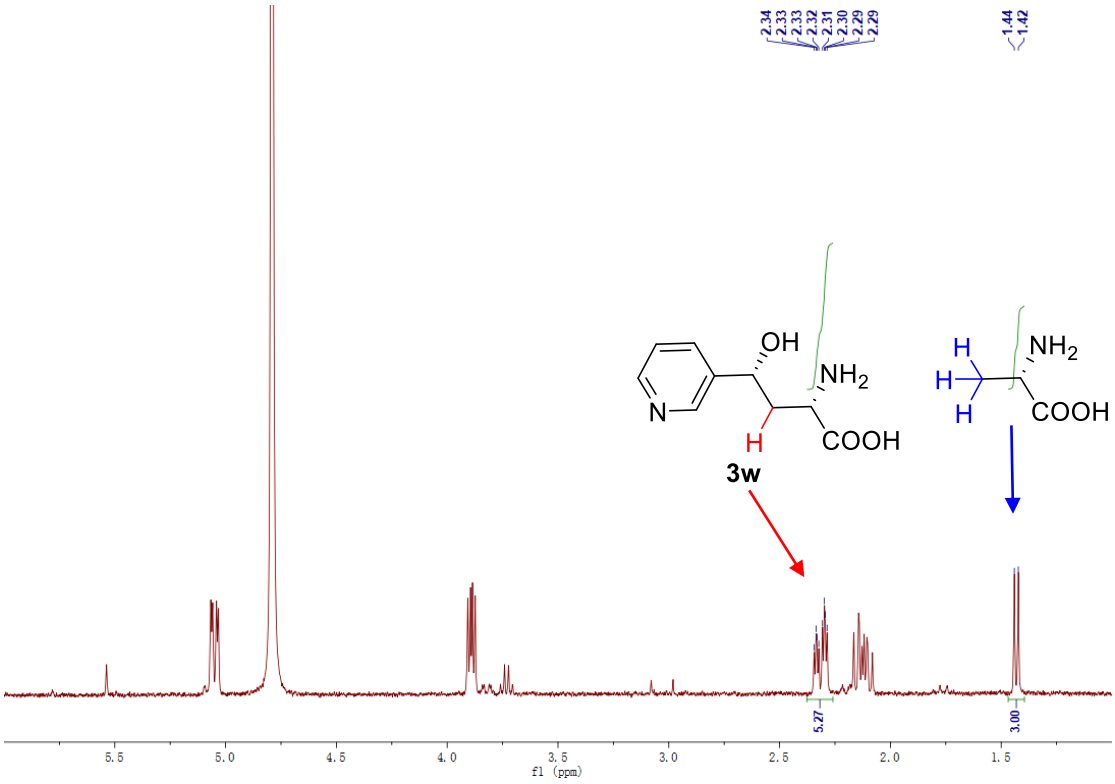


Figure S56. Conversion of **3w**

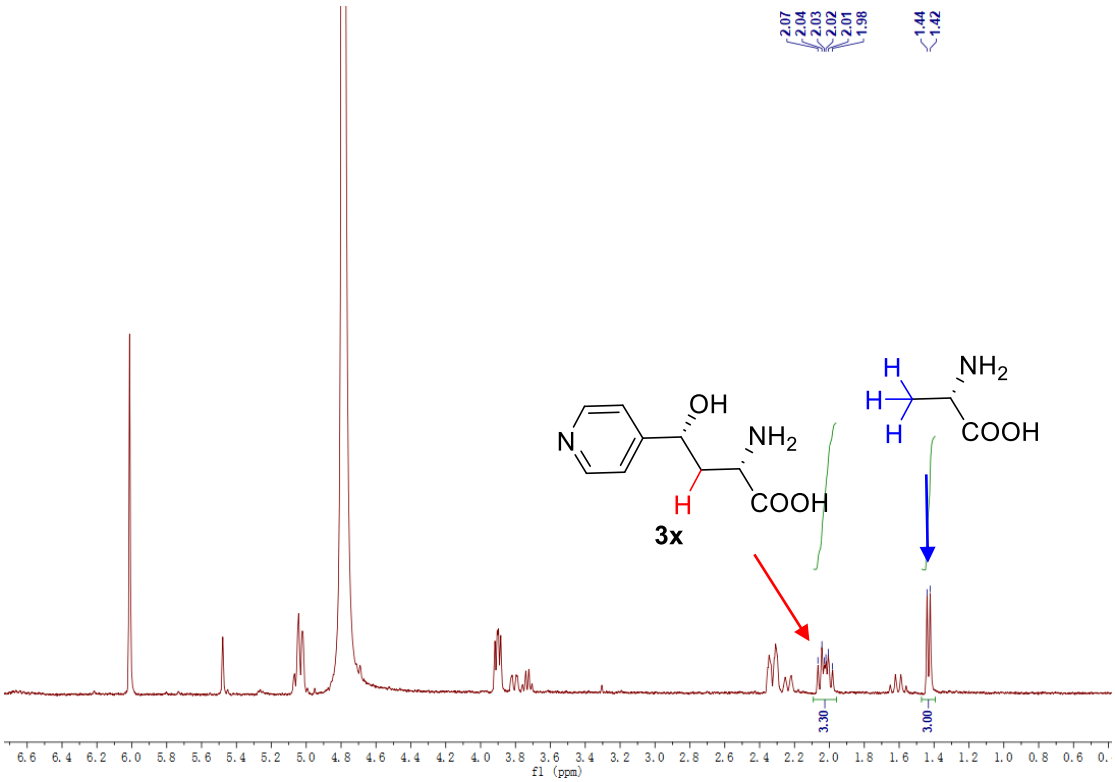


Figure S57. Conversion of **3x**

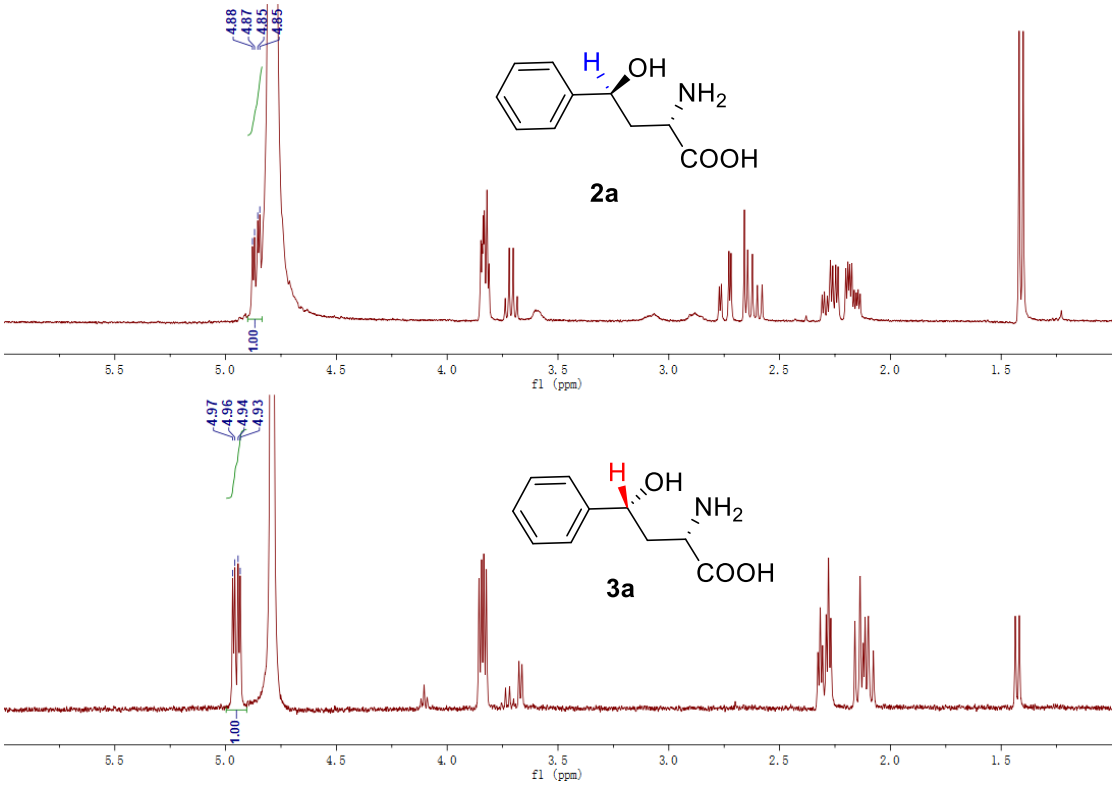


Figure S58. Diastereoisomeric ratio of **2a** and **3a**

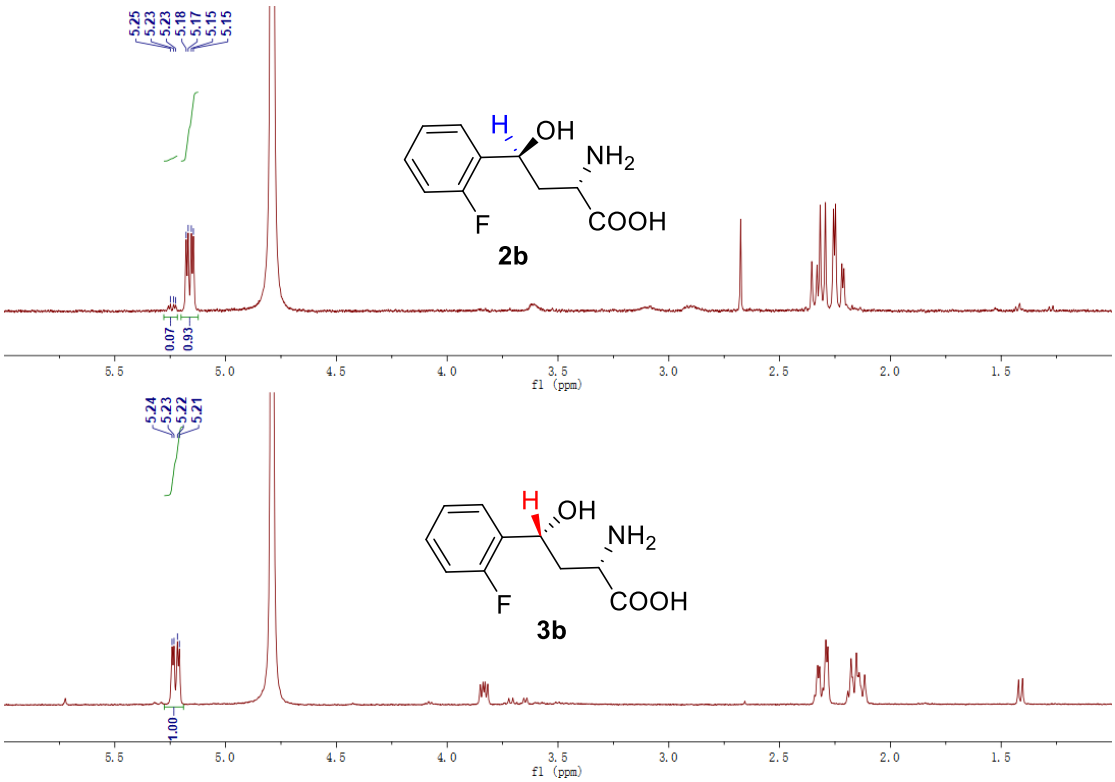


Figure S59. Diastereoisomeric ratio of **2b** and **3b**

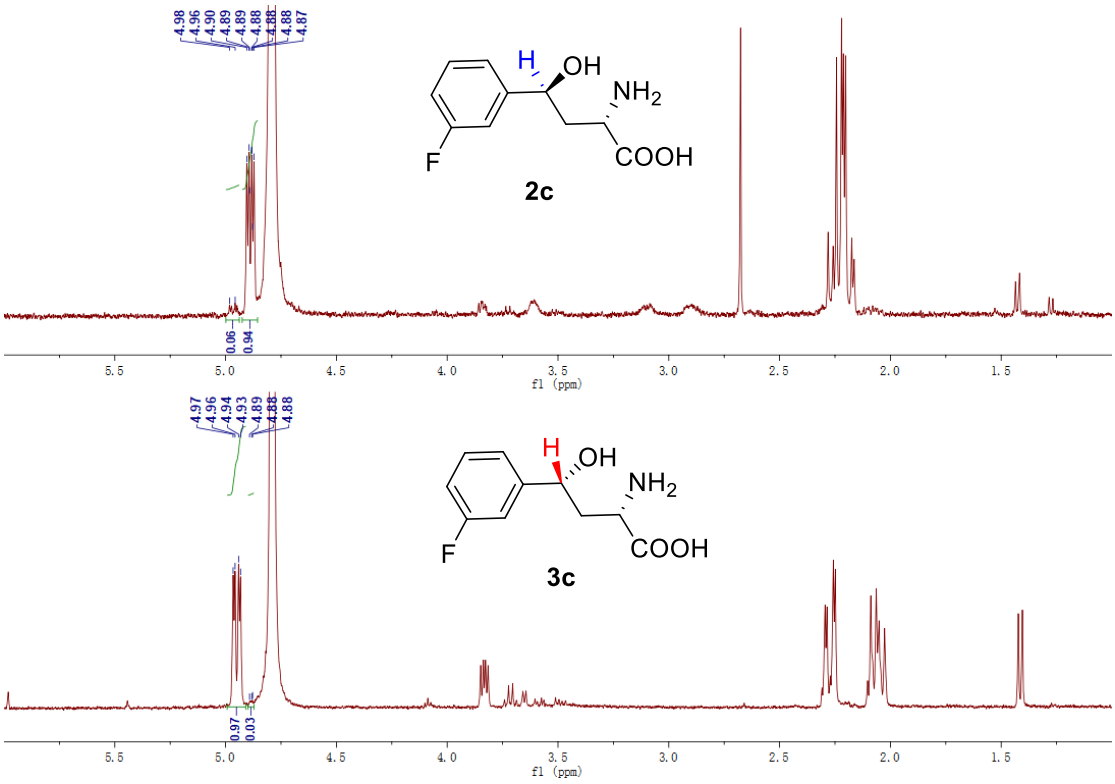


Figure S60. Diastereoisomeric ratio of **2c** and **3c**

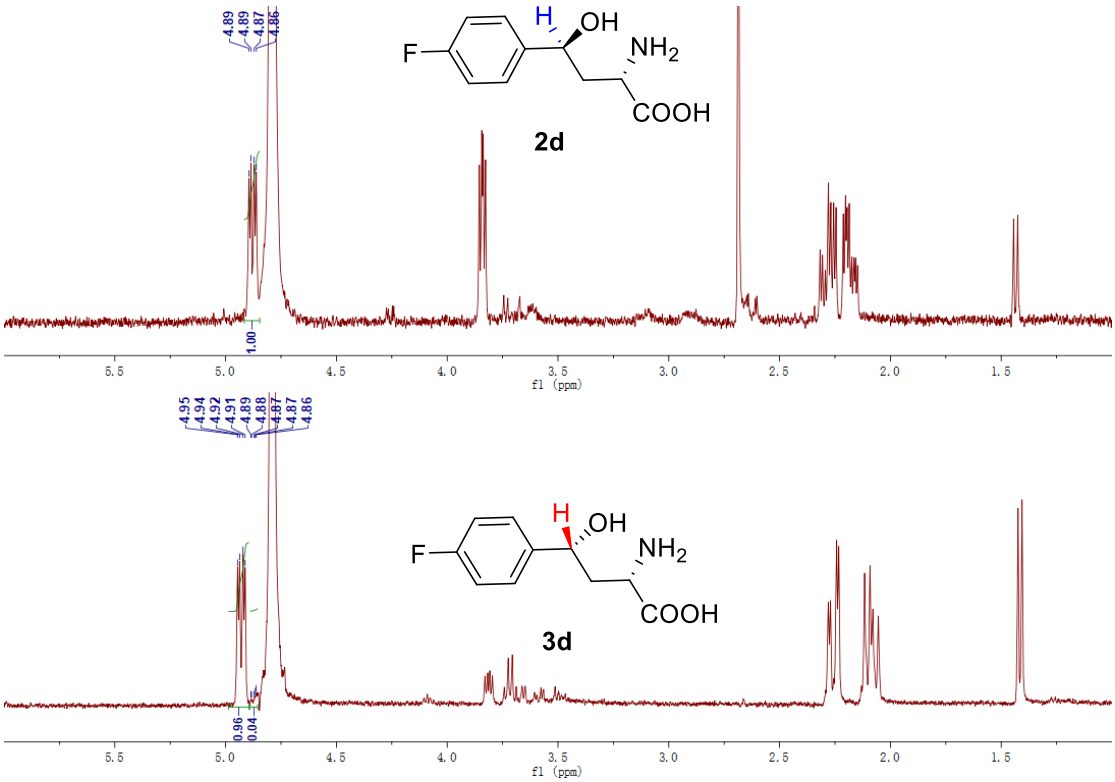


Figure S61. Diastereoisomeric ratio of **2d** and **3d**

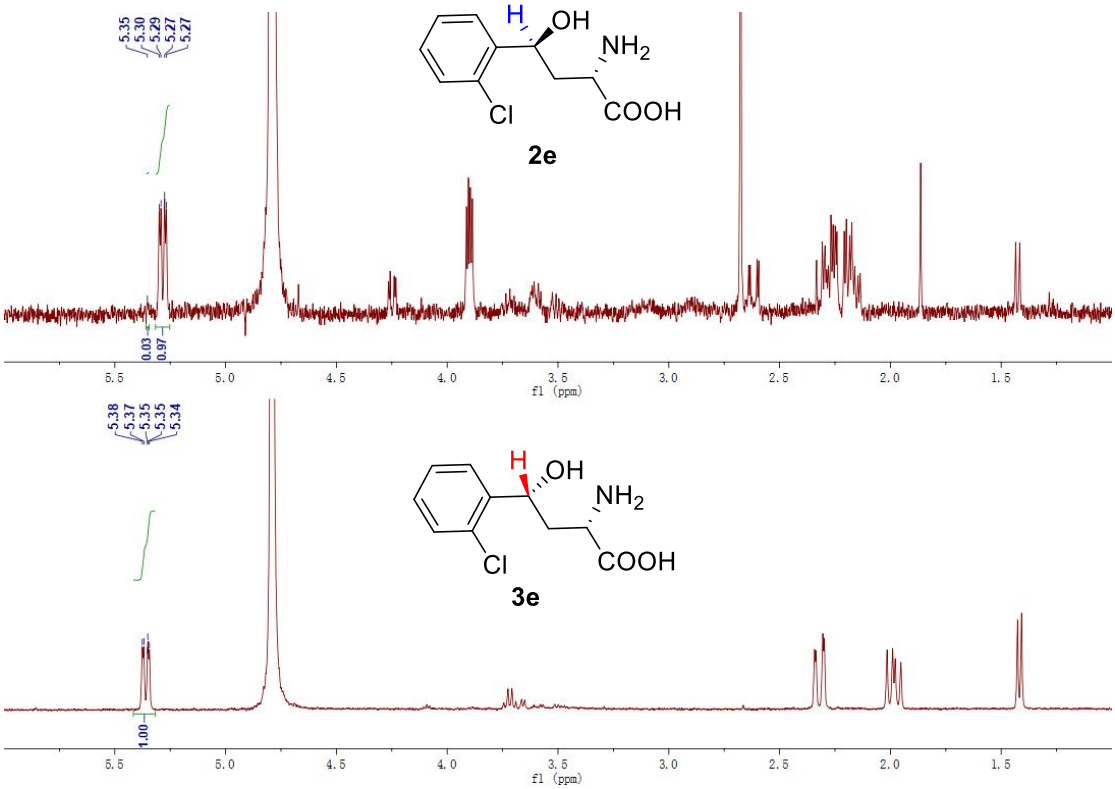


Figure S62. Diastereoisomeric ratio of **2e** and **3e**

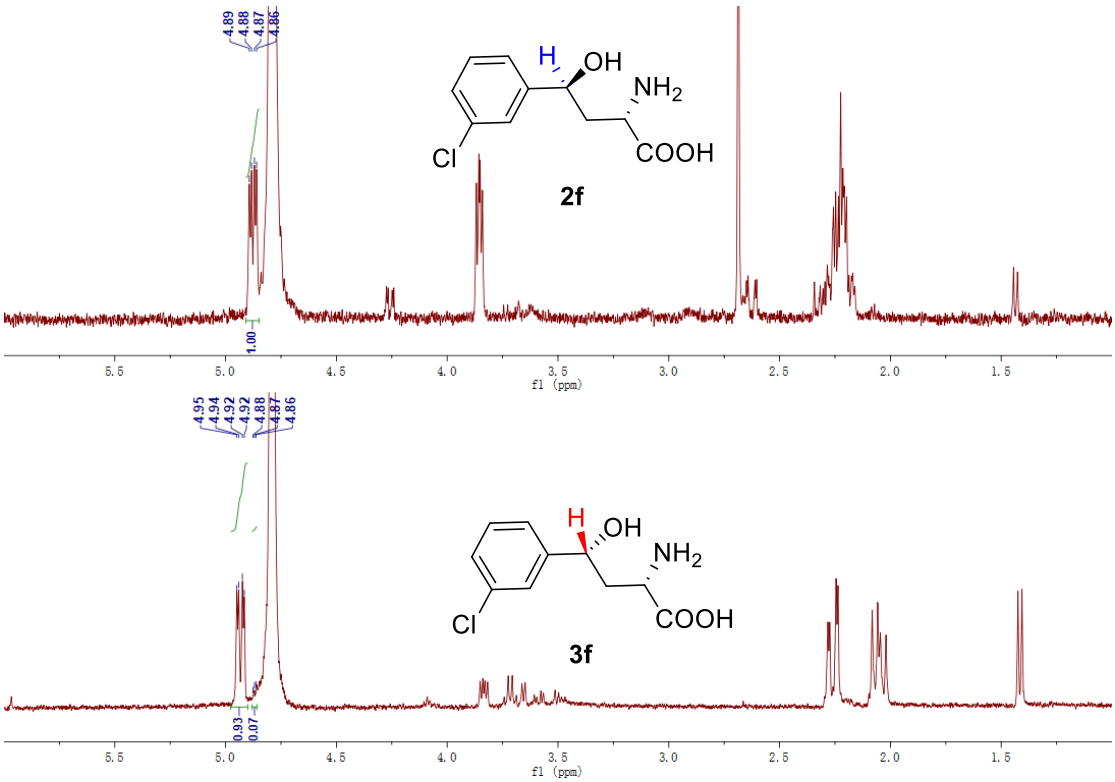


Figure S63. Diastereoisomeric ratio of **2f** and **3f**

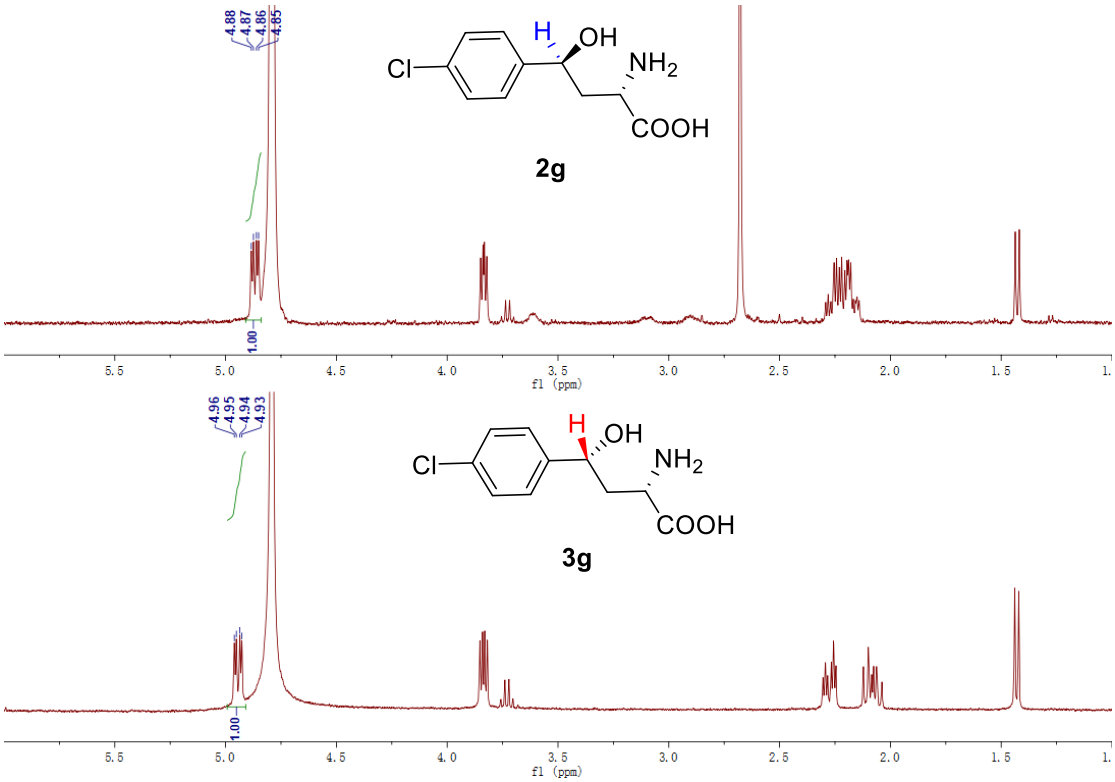


Figure S64. Diastereoisomeric ratio of **2g** and **3g**

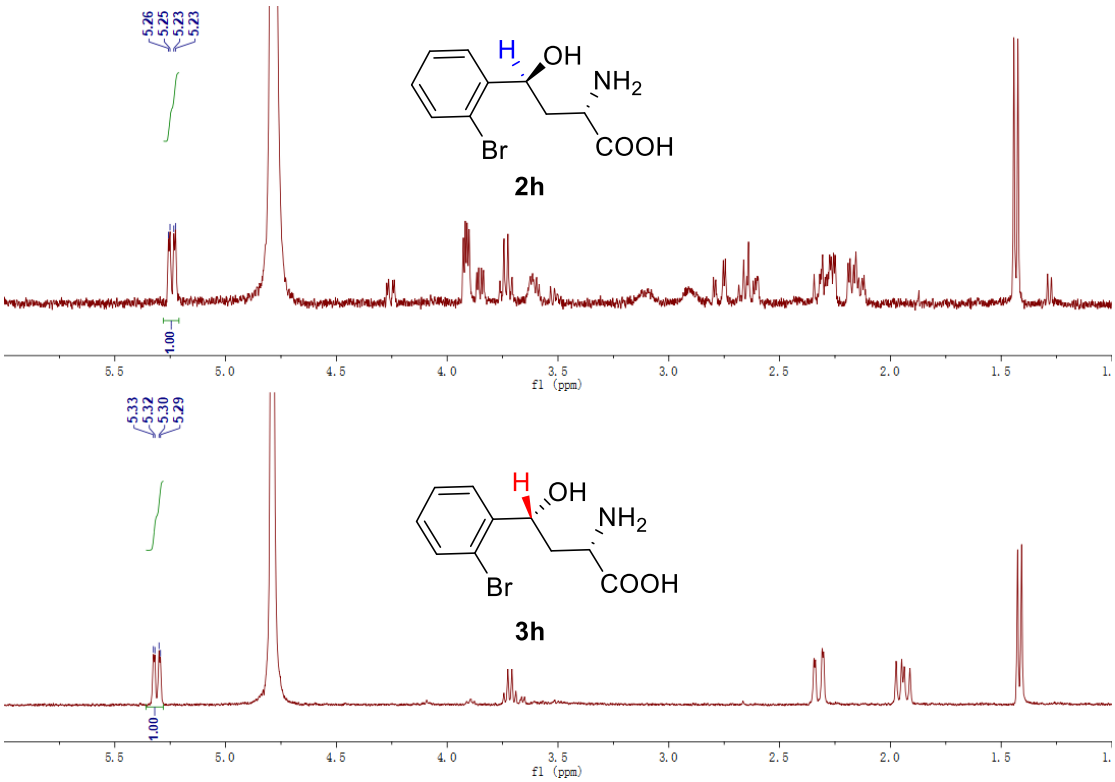


Figure S65. Diastereoisomeric ratio of **2h** and **3h**

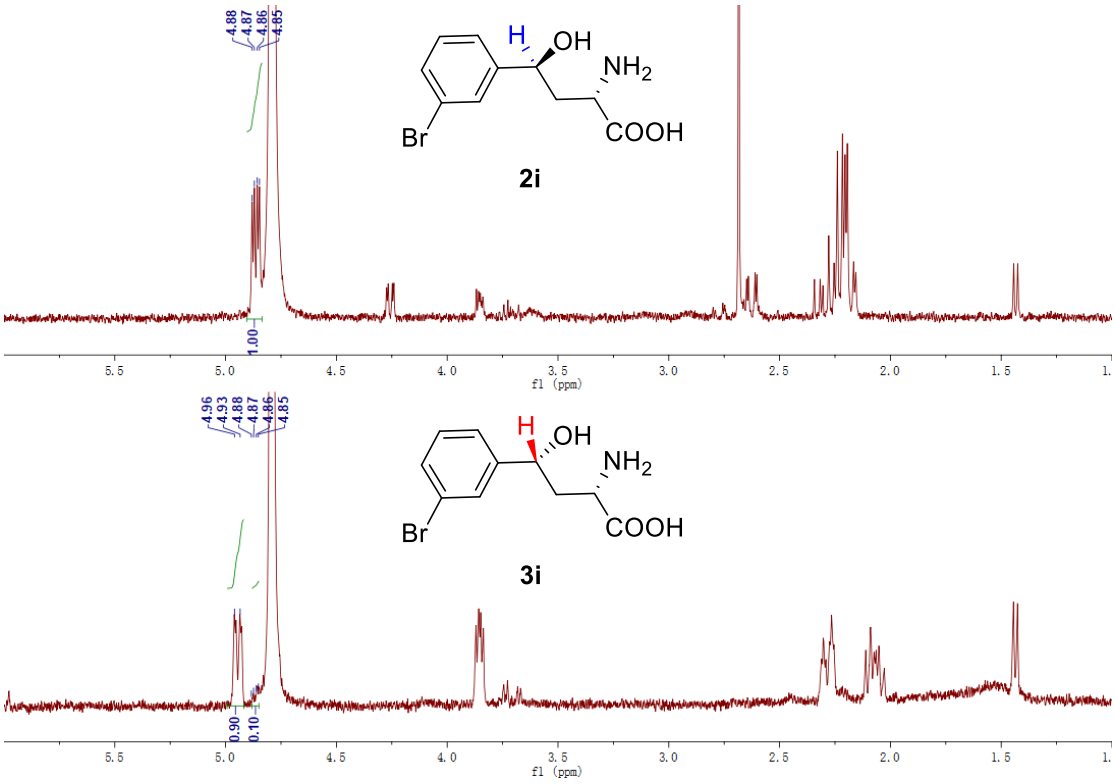


Figure S66. Diastereoisomeric ratio of **2i** and **3i**

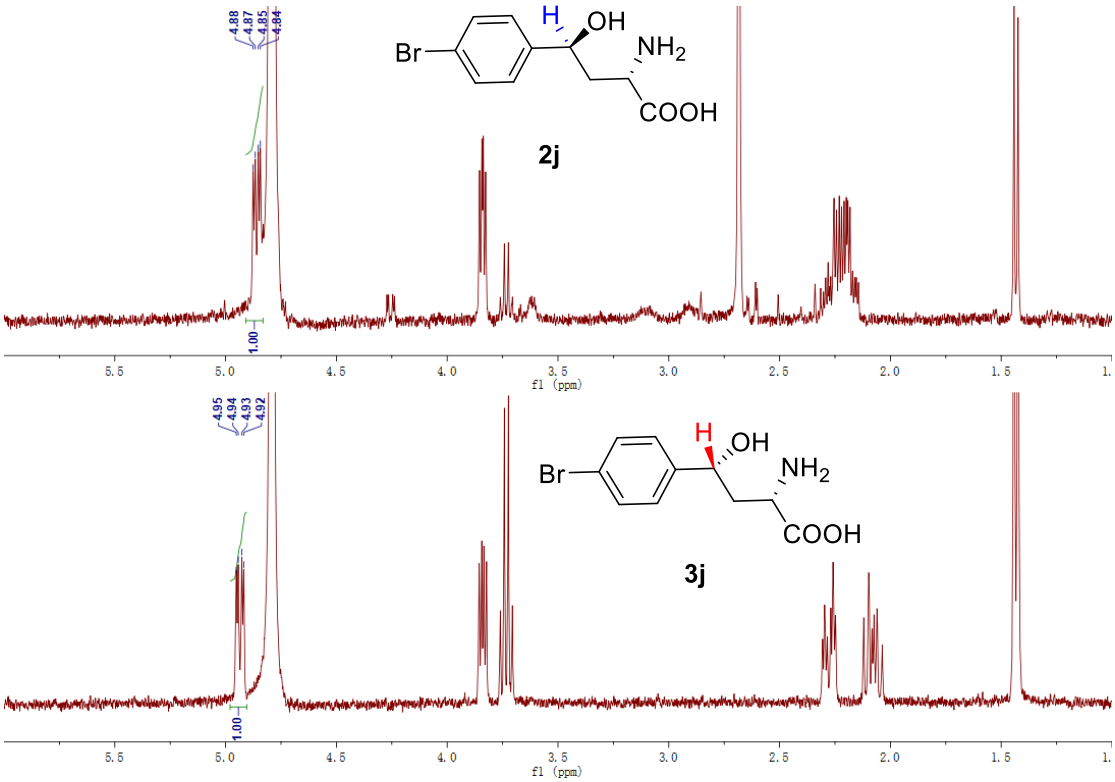


Figure S67. Diastereoisomeric ratio of **2j** and **3j**

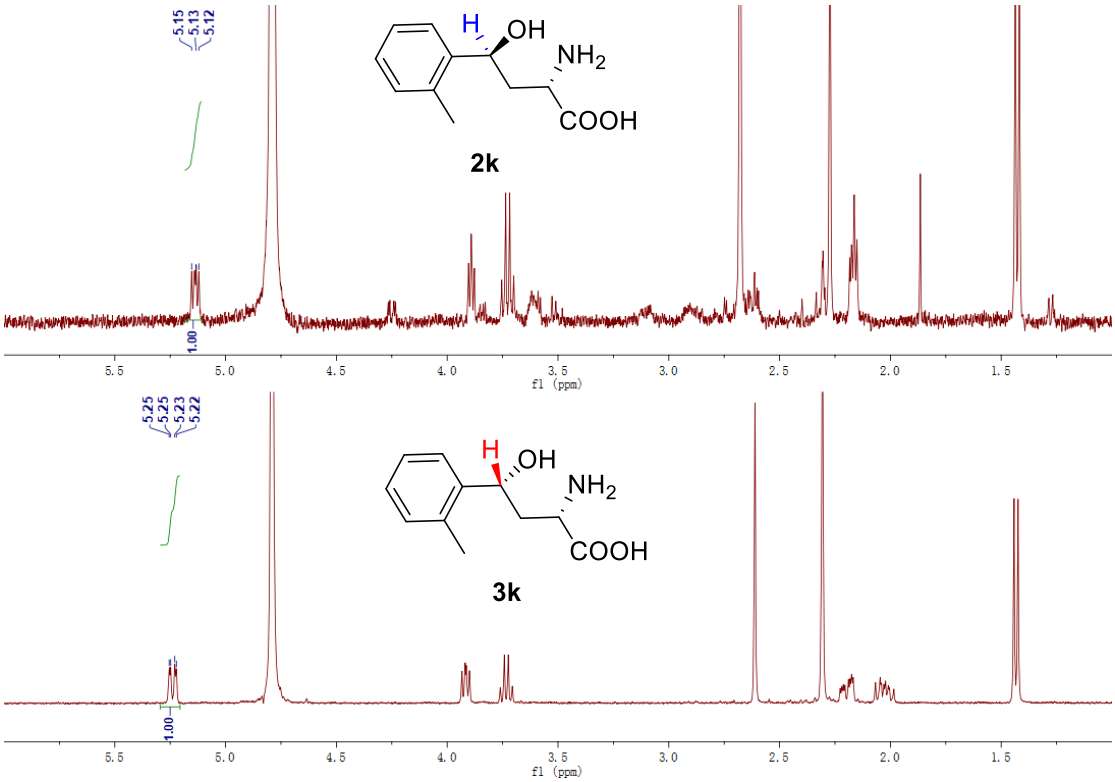


Figure S68. Diastereoisomeric ratio of **2k** and **3k**

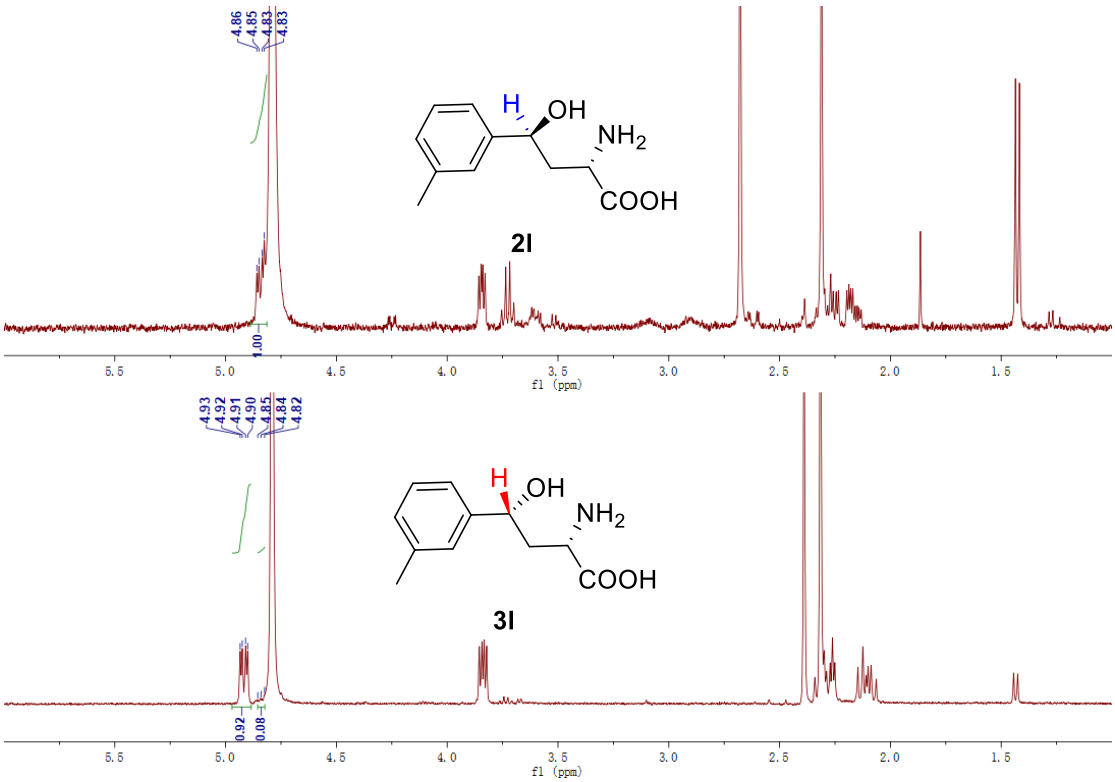


Figure S69. Diastereoisomeric ratio of **2l** and **3l**

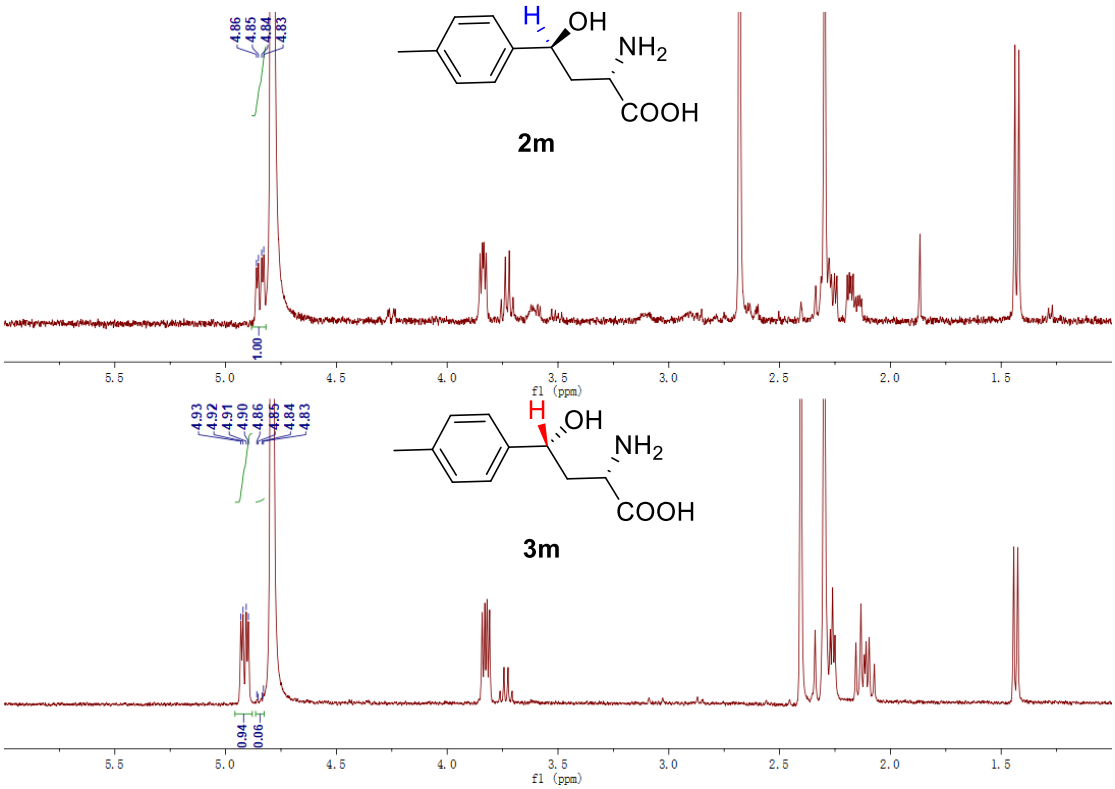


Figure S70. Diastereoisomeric ratio of **2m** and **3m**

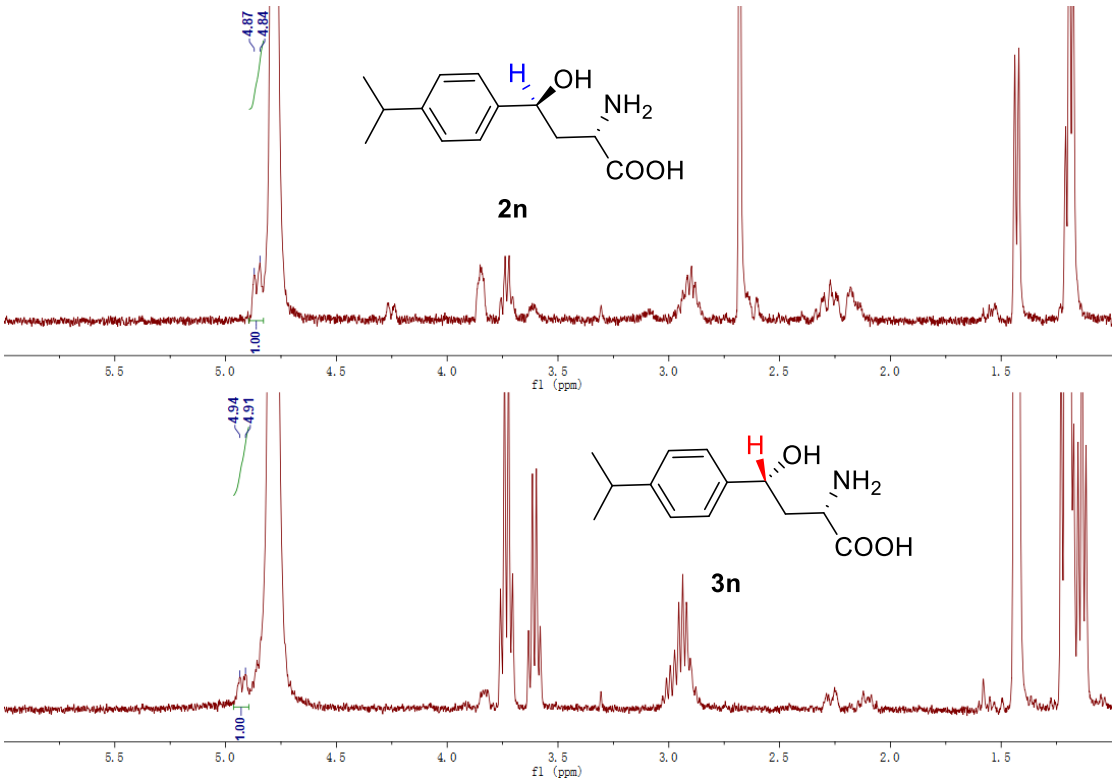


Figure S71. Diastereoisomeric ratio of **2n** and **3n**

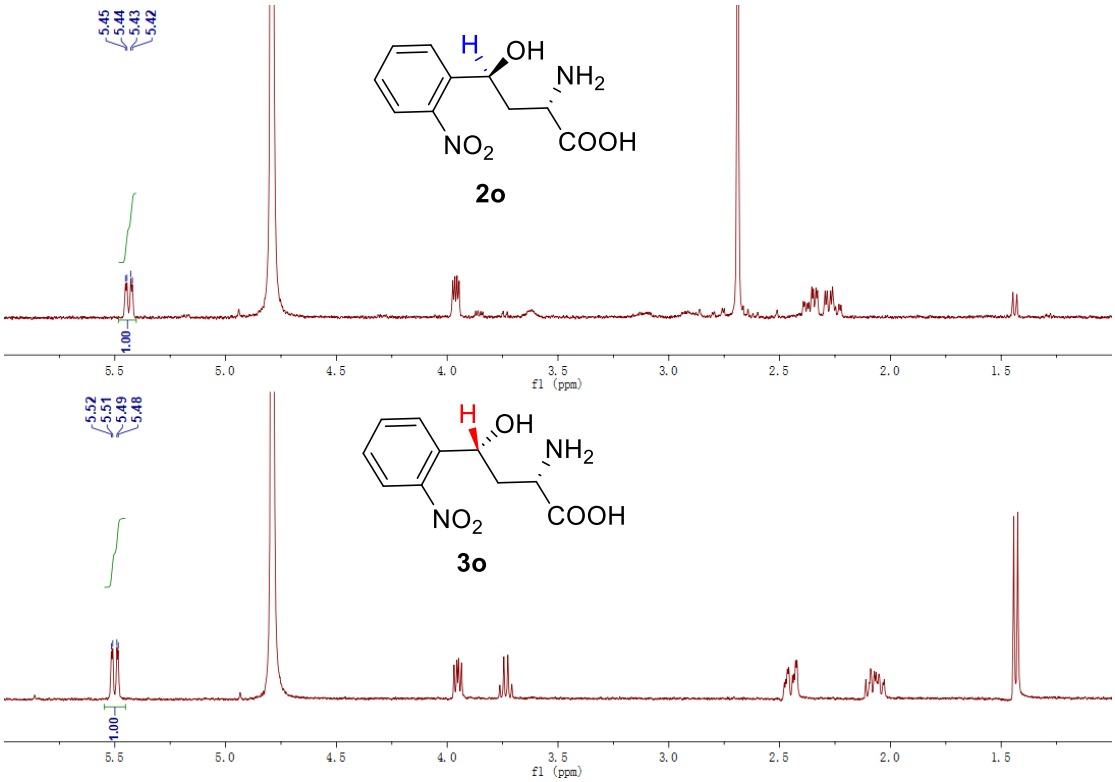


Figure S72. Diastereoisomeric ratio of **2o** and **3o**

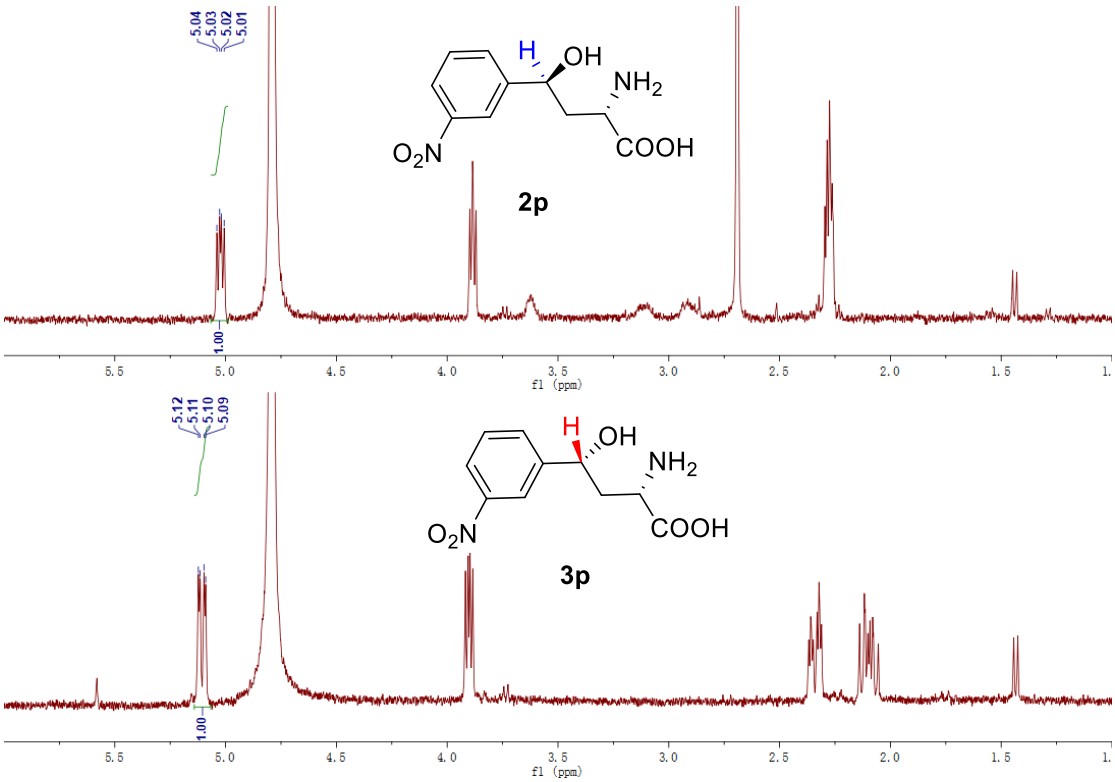


Figure S73. Diastereoisomeric ratio of **2p** and **3p**

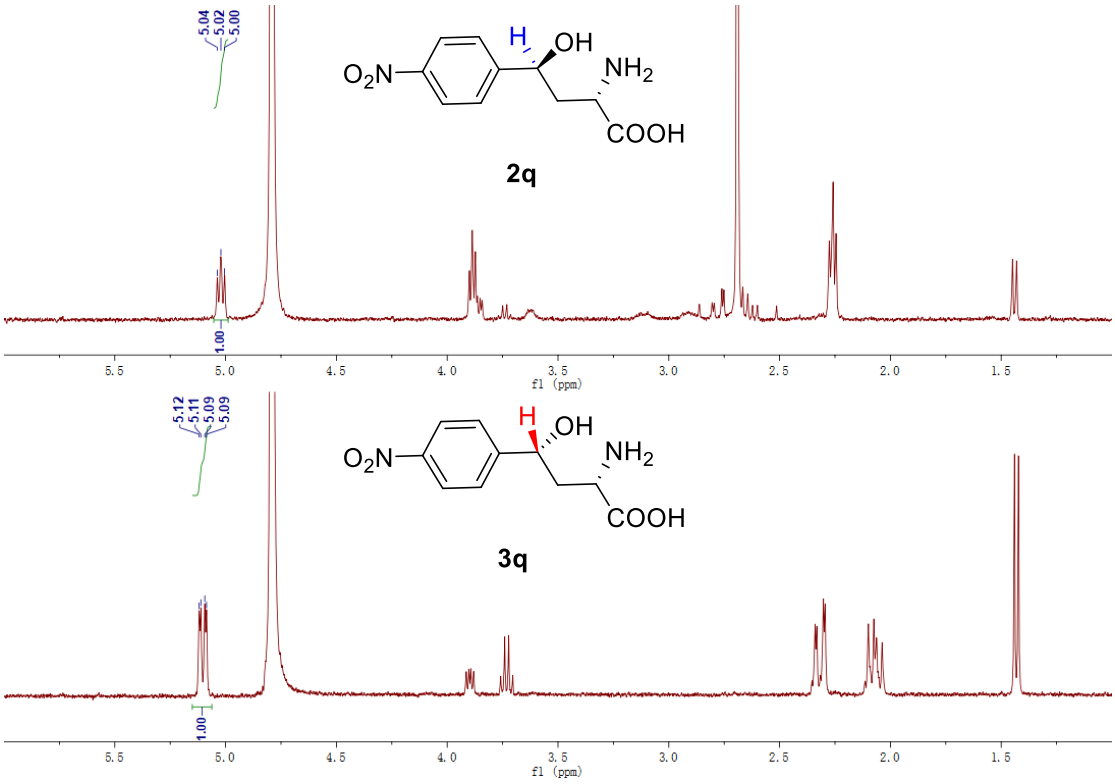


Figure S74. Diastereoisomeric ratio of **2q** and **3q**

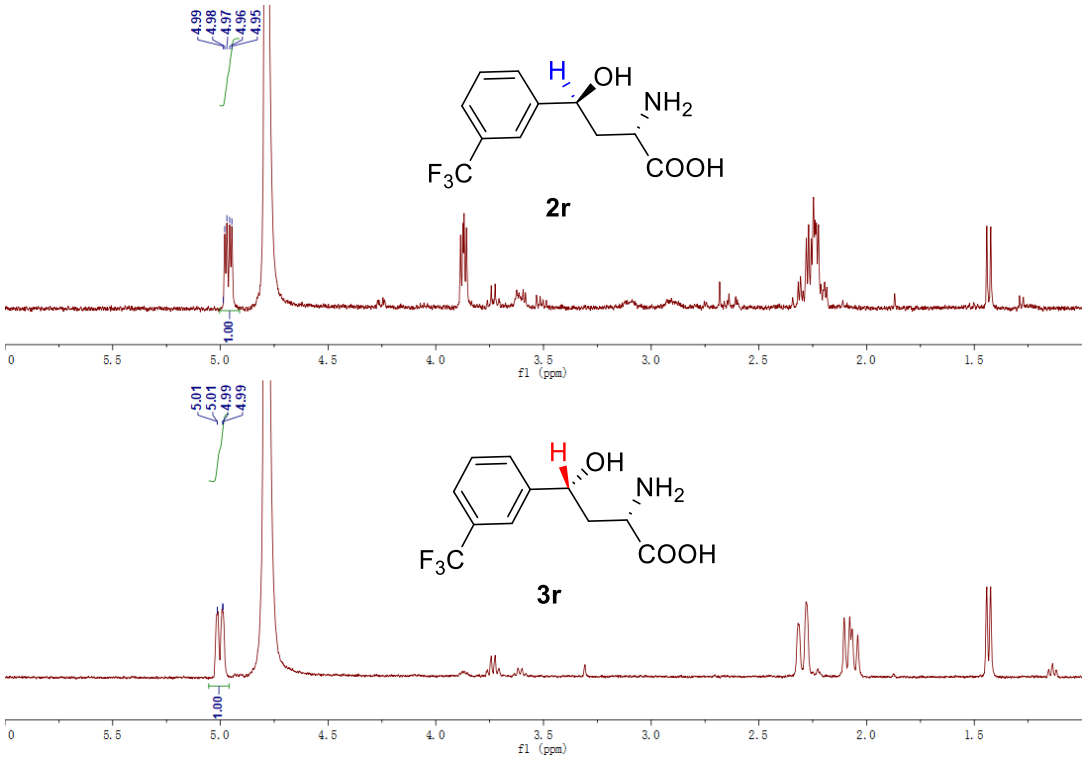


Figure S75. Diastereoisomeric ratio of **2r** and **3r**

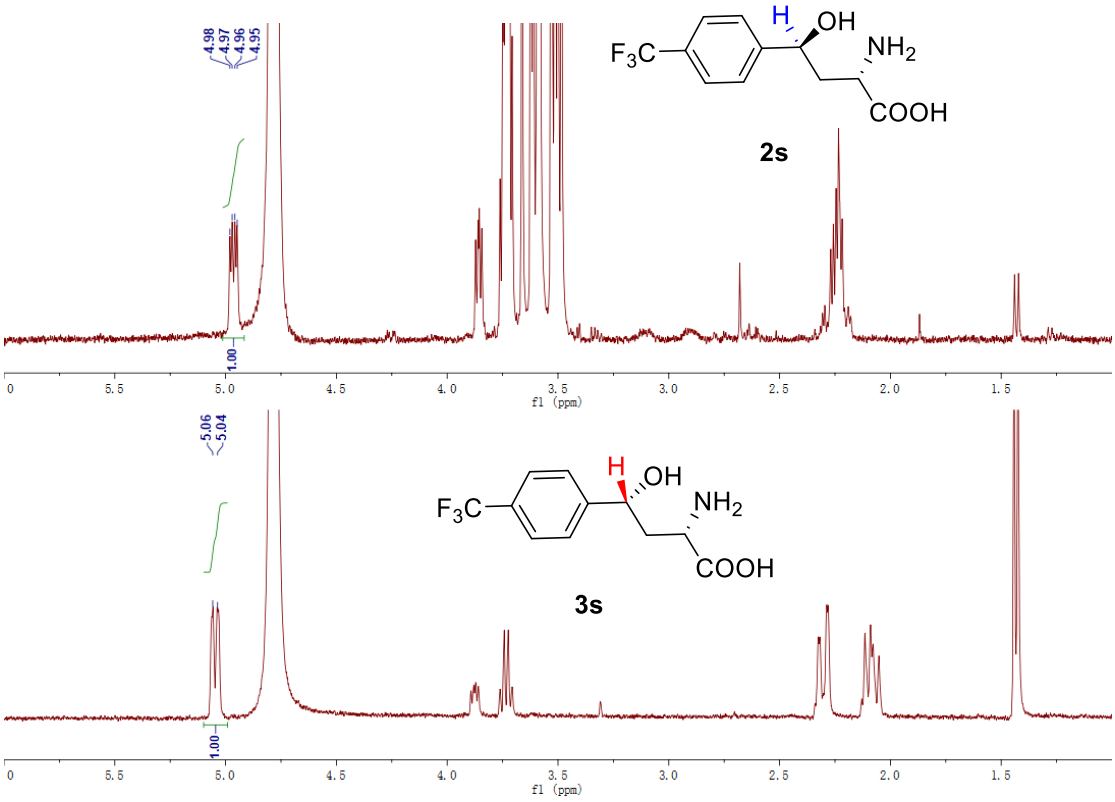


Figure S76. Diastereoisomeric ratio of **2s** and **3s**

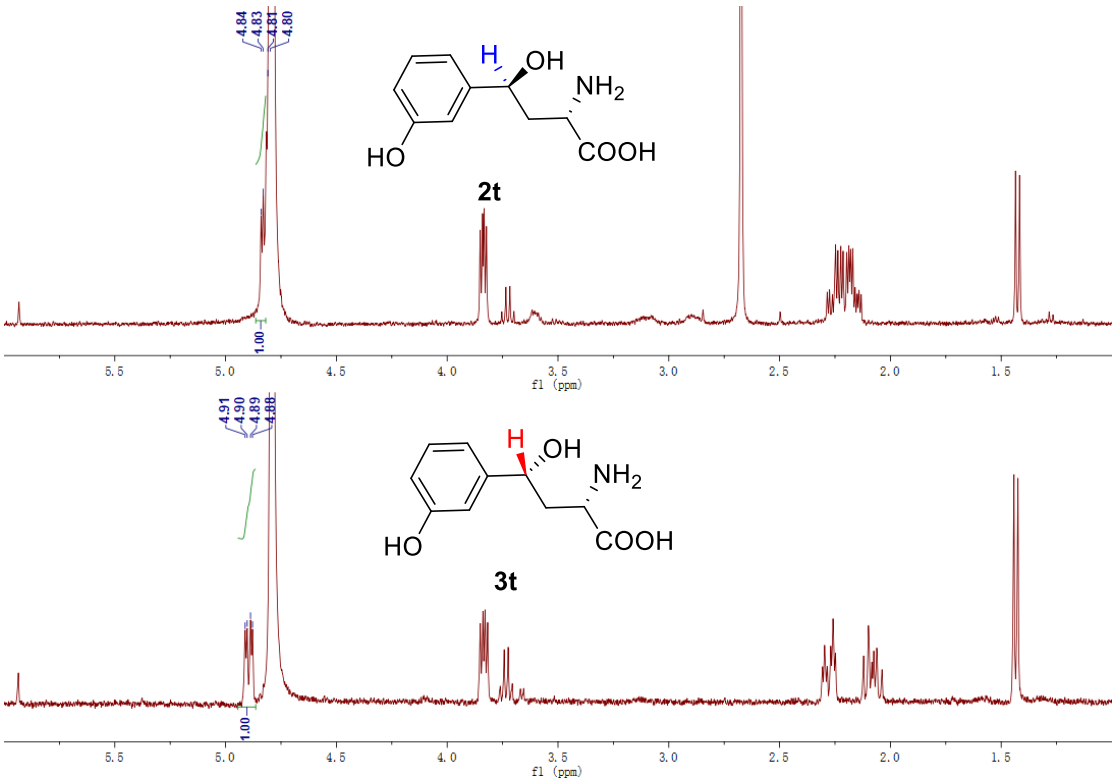


Figure S77. Diastereoisomeric ratio of **2t** and **3t**

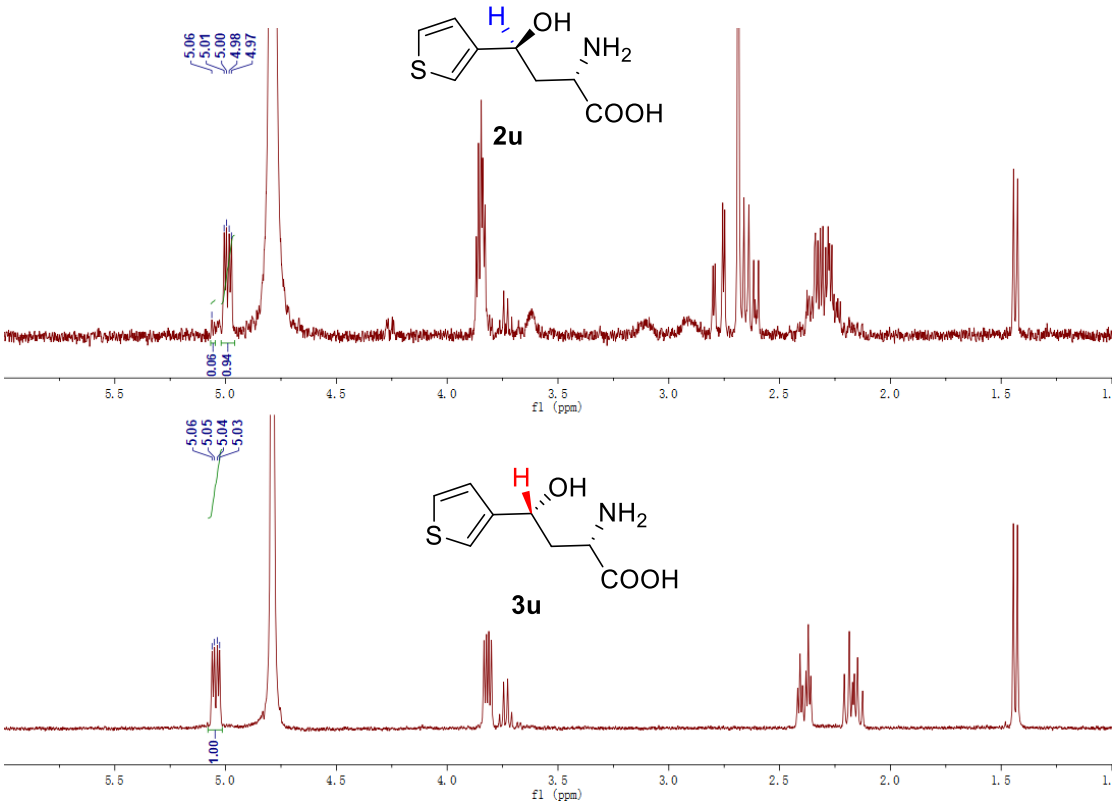


Figure S78. Diastereoisomeric ratio of **2u** and **3u**

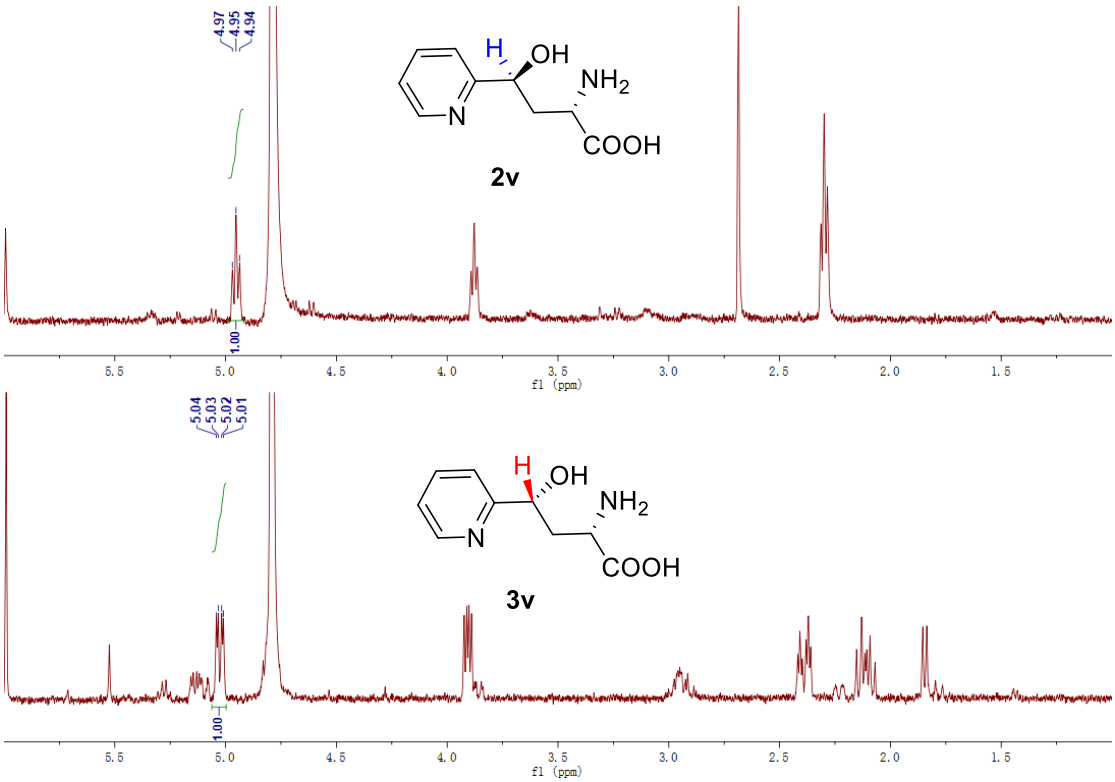


Figure S79. Diastereoisomeric ratio of **2v** and **3v**

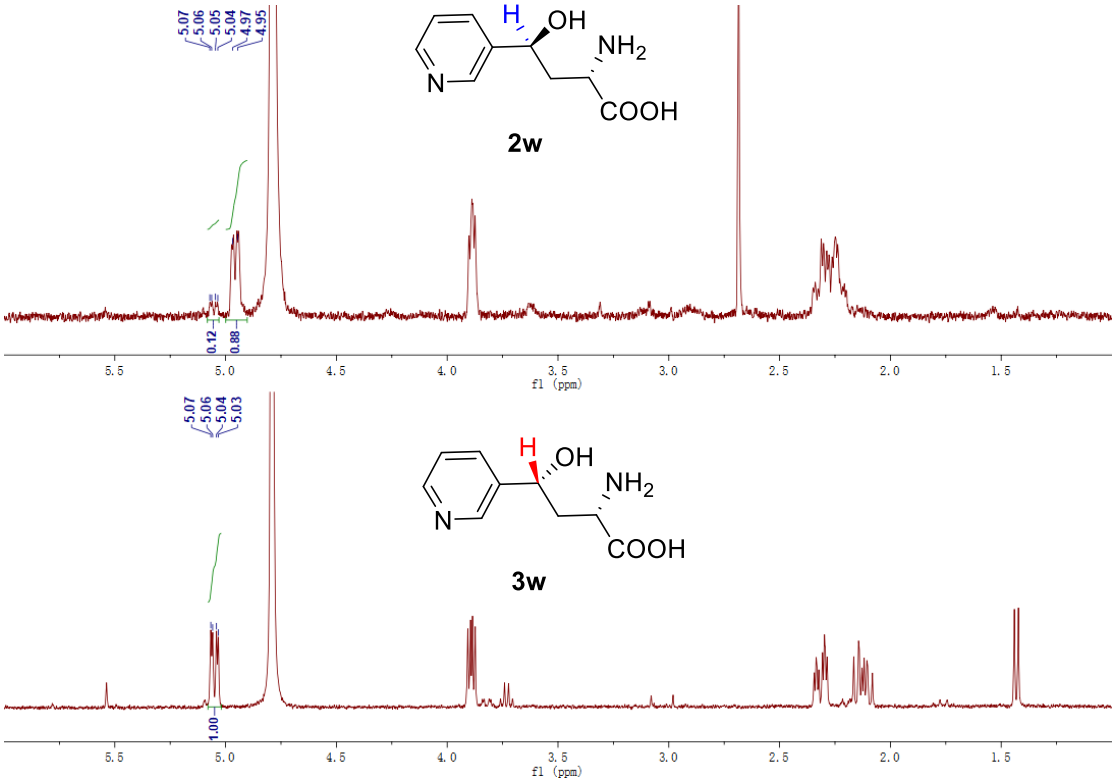


Figure S80. Diastereoisomeric ratio of **2w** and **3w**

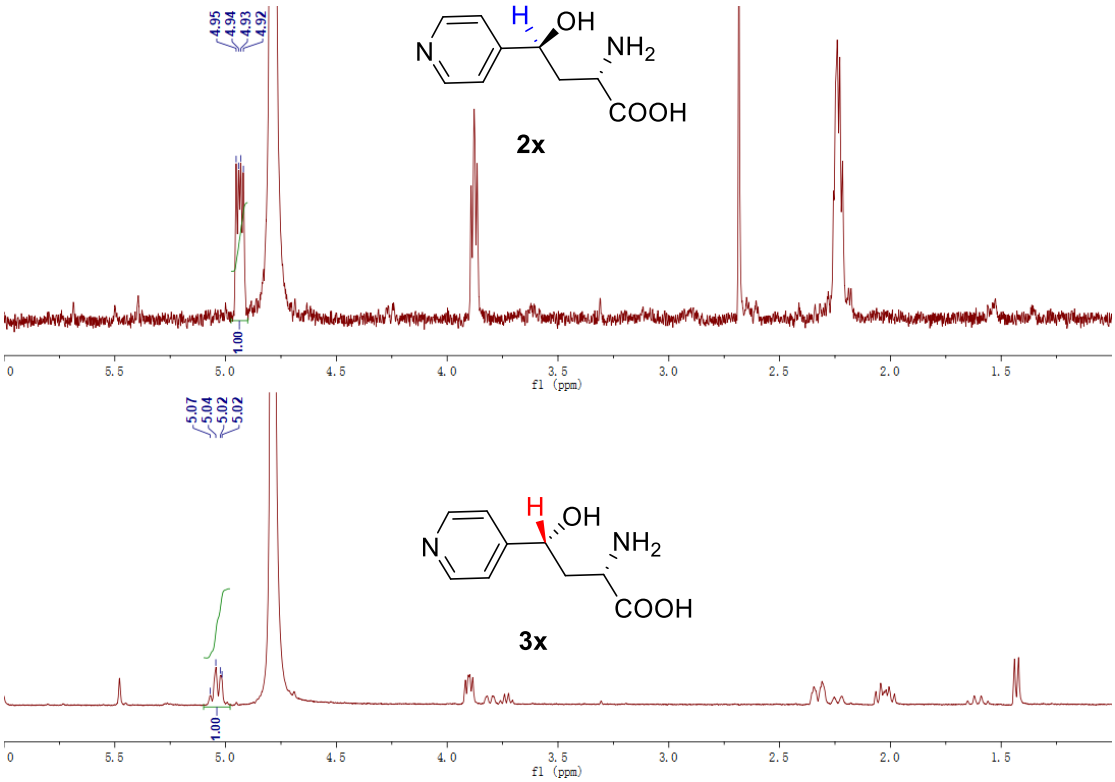


Figure S81. Diastereoisomeric ratio of **2x** and **3x**

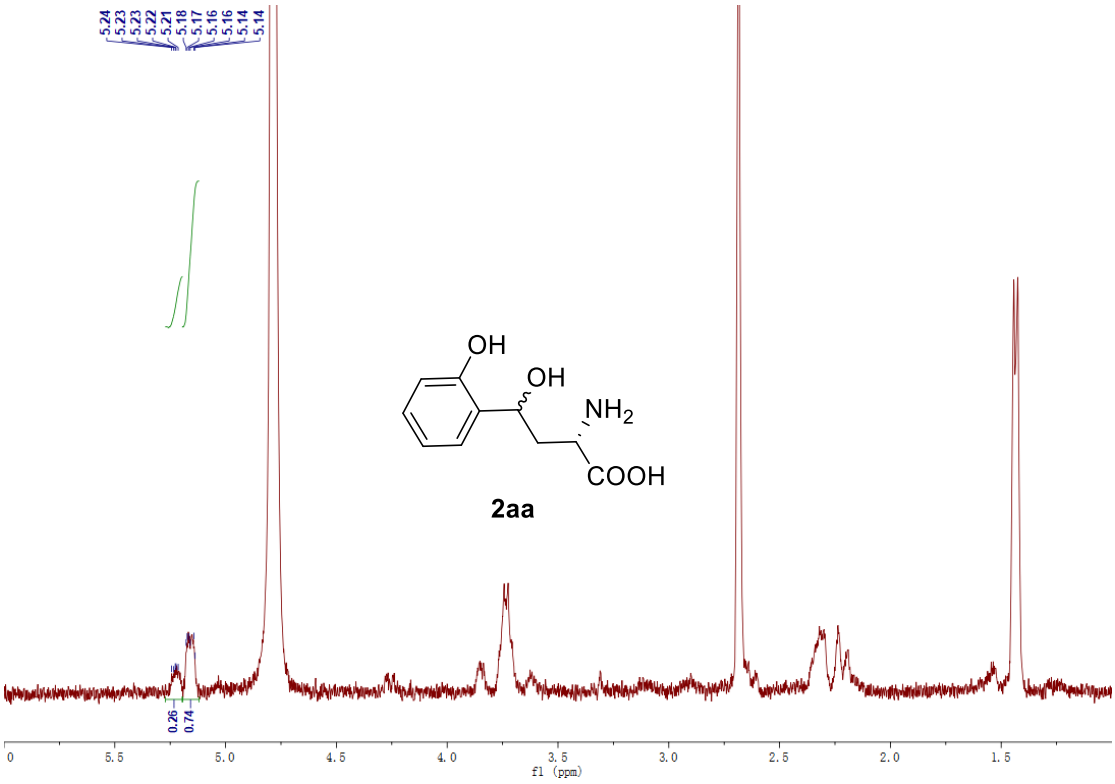


Figure S82. Diastereoisomeric ratio of **2aa**

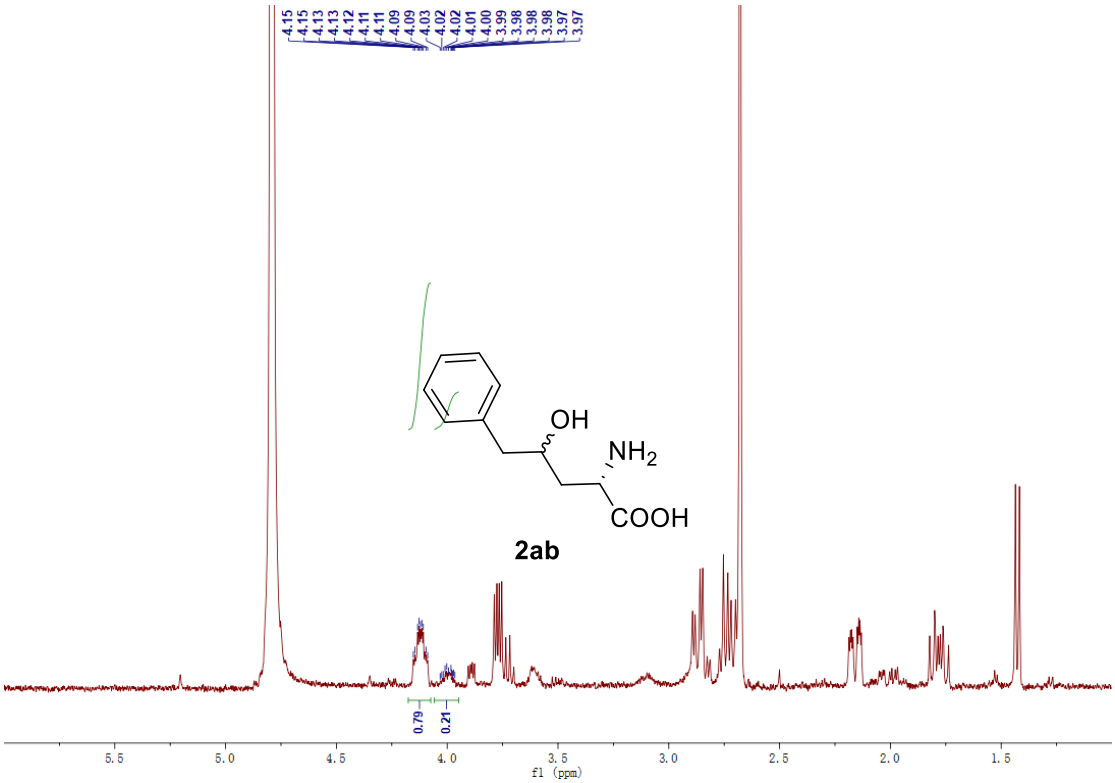


Figure S83. Diastereoisomeric ratio of **2ab**

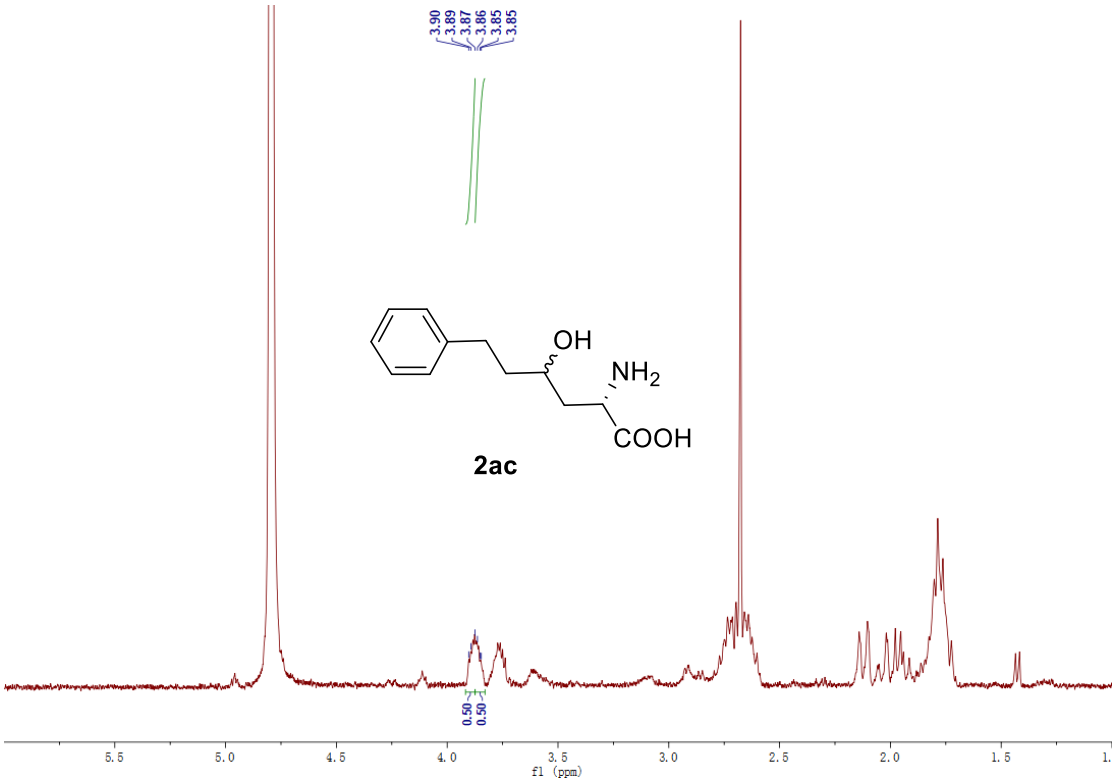


Figure S84. Diastereoisomeric ratio of **2ac**

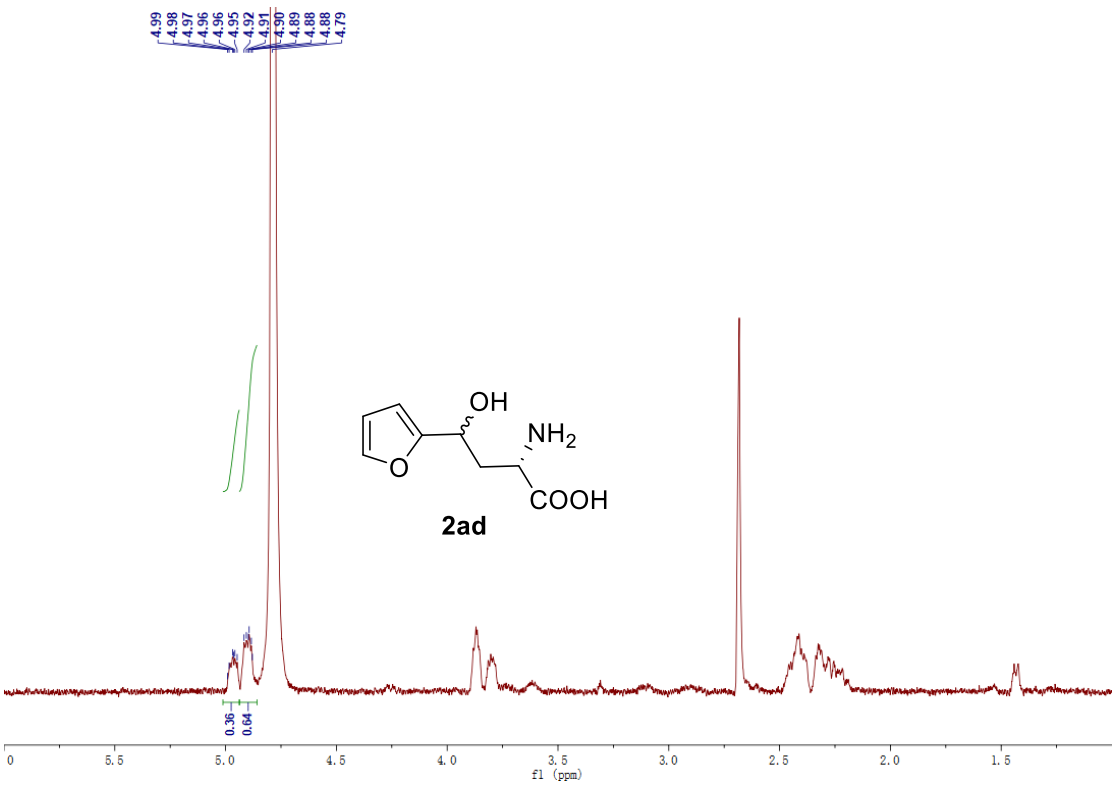


Figure S85. Diastereoisomeric ratio of **2ad**

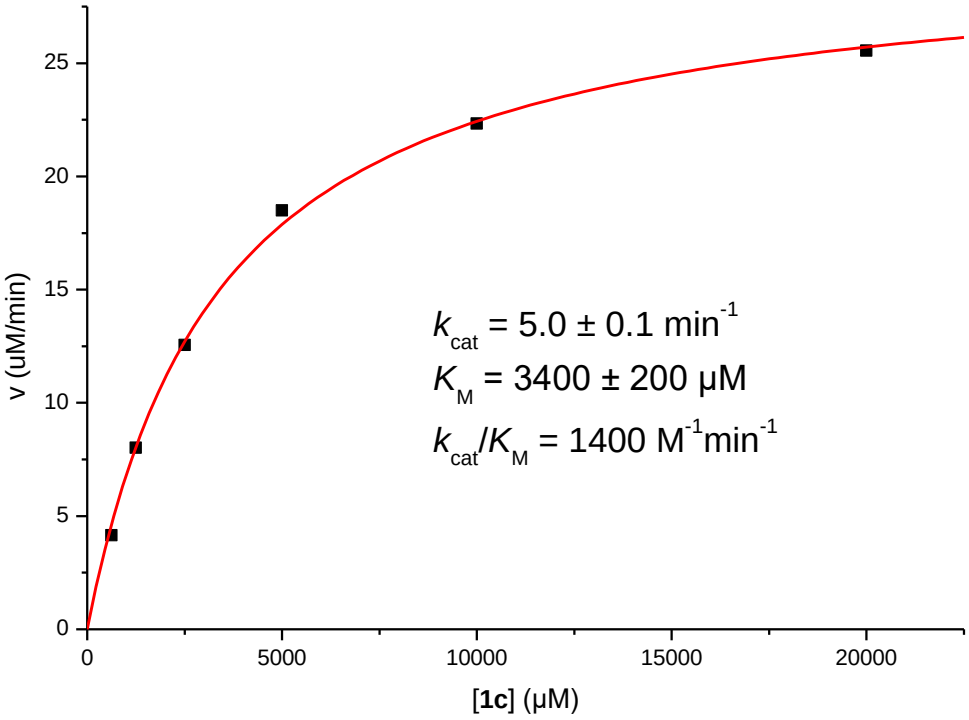


Figure S86. Michaelis-Menten curve and kinetic parameters of **1c**

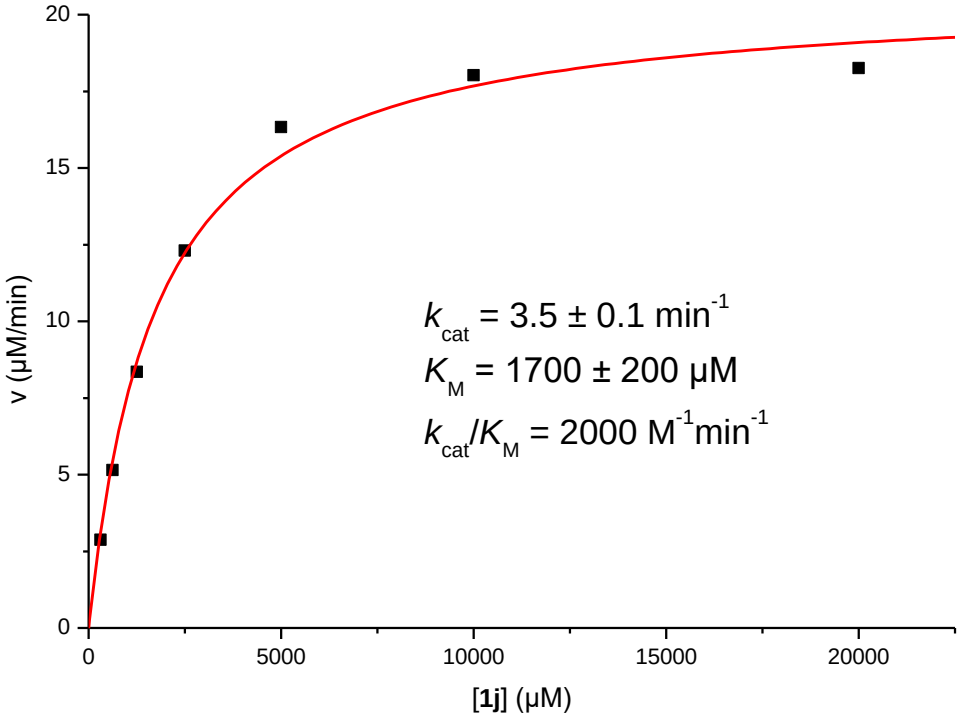


Figure S87. Michaelis-Menten curve and kinetic parameters of **1j**

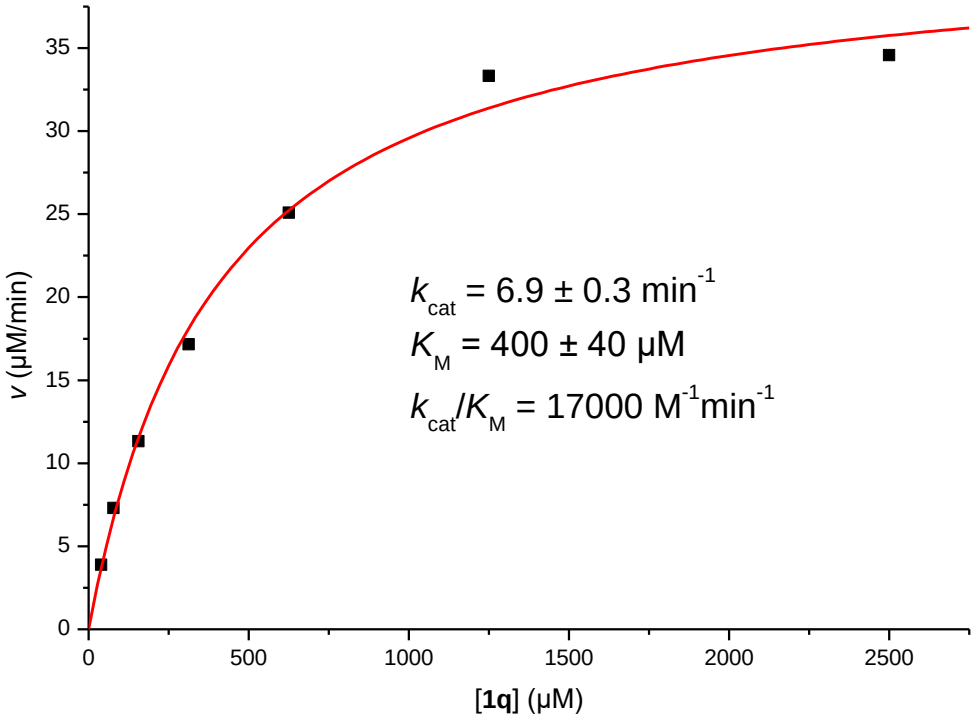


Figure S88. Michaelis-Menten curve and kinetic parameters of **1q**

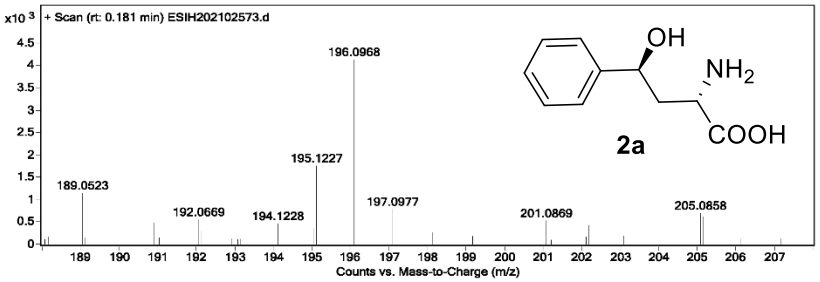
HR-MS and NMR spectra

Qualitative Analysis Report

Data Filename	ESIH202102573.d	**Sample Name**	G5-G5-BJQ
Sample ID		**Position**	P1-B6
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/13/2021 11:47:42	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
196.0968	196.0968	0.05	0.26	C10 H14 N O3	(M+H)+

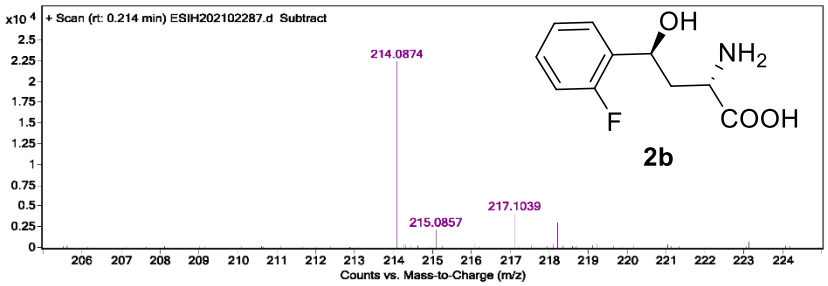
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102287.d	**Sample Name**	G5-AP-2F
Sample ID		**Position**	P2-A3
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:12:47	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
214.0874	214.0874	0.05	0.22	C10 H13 F N O3	(M+H)+

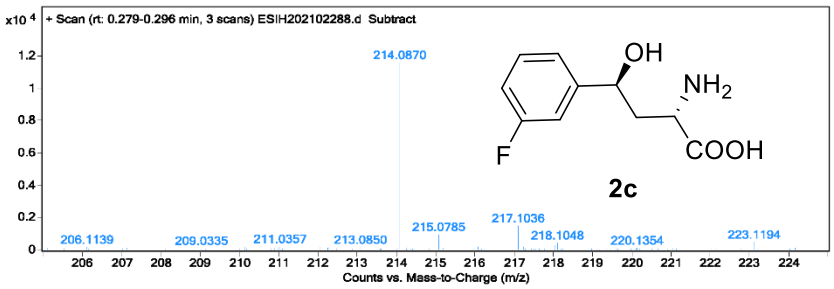
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102288.d	**Sample Name**	G5-AP-3F
Sample ID		**Position**	P2-A4
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:14:14	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



2c

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
214.087	214.0874	0.38	1.77	C10 H13 F N O3	(M+H)+

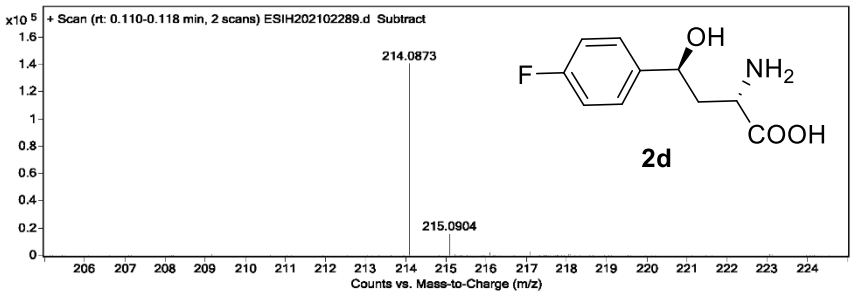
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102289.d	**Sample Name**	G5-AP-4F
Sample ID		**Position**	P2-A5
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:15:42	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



2d

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
214.0873	214.0874	0.08	0.39	C10 H13 F N O3	(M+H)+

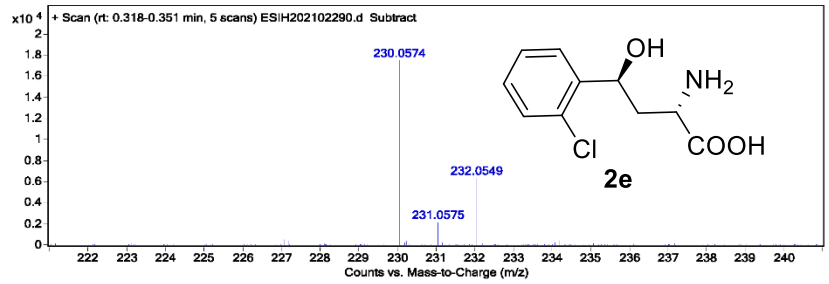
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102290.d	**Sample Name**	G5-AP-2Cl
Sample ID		**Position**	P2-A6
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:17:10	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
230.0574	230.0578	0.42	1.83	C10 H13 Cl N O3	(M+H)+

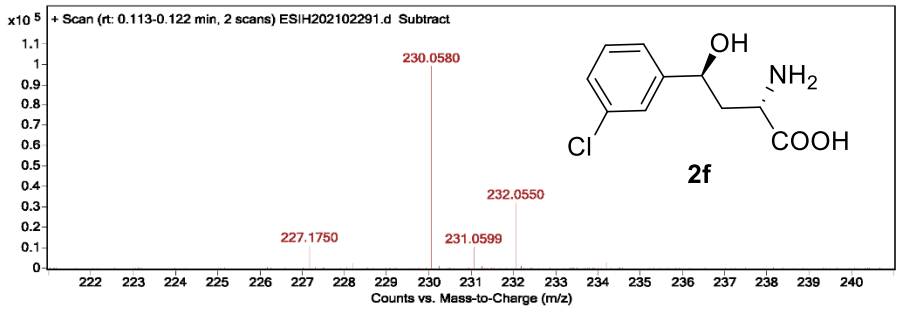
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102291.d	**Sample Name**	G5-AP-3Cl
Sample ID		**Position**	P2-A7
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:18:37	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
230.058	230.0578	-0.15	-0.64	C10 H13 Cl N O3	(M+H)+

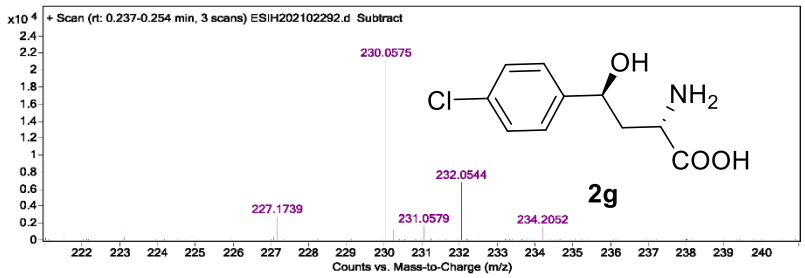
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102292.d	**Sample Name**	G5-AP-4Cl
Sample ID		**Position**	P2-A8
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:21:17	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
230.0575	230.0578	0.38	1.66	C10 H13 Cl N O3	(M+H)+

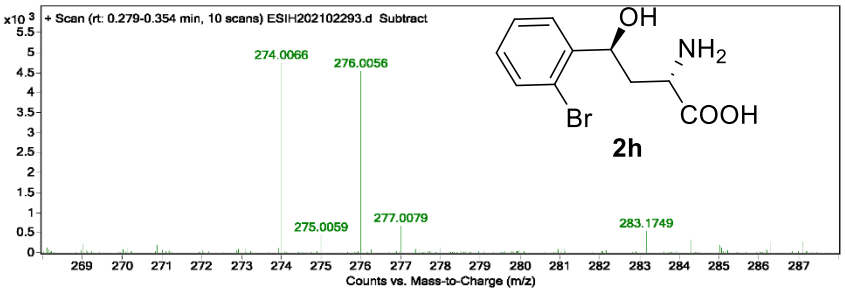
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102293.d	**Sample Name**	G5-AP-2Br
Sample ID		**Position**	P2-A9
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:22:45	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
274.0066	274.0073	0.71	2.6	C10 H13 Br N O3	(M+H)+

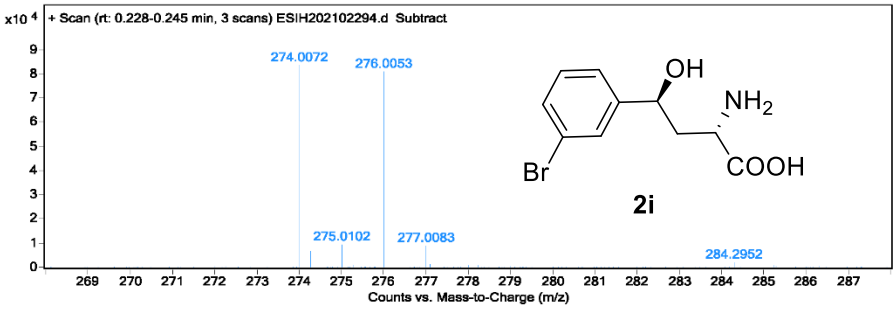
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102294.d	**Sample Name**	G5-AP-3Br
Sample ID		**Position**	P2-B1
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:24:14	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
274.0072	274.0073	0.13	0.48	C10 H13 Br N O3	(M+H)+

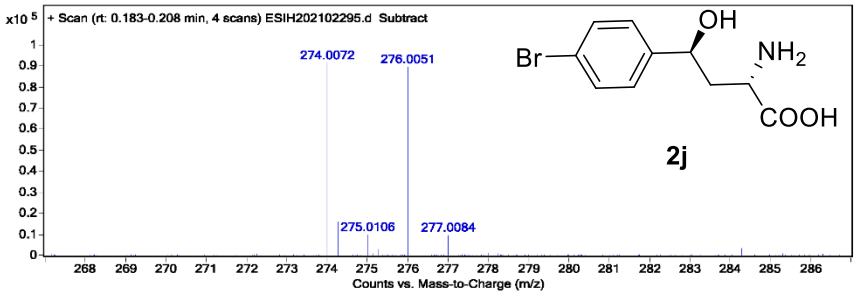
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102295.d	**Sample Name**	G5-AP-4Br
Sample ID		**Position**	P2-B2
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:25:42	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
274.0072	274.0073	0.13	0.48	C10 H13 Br N O3	(M+H)+

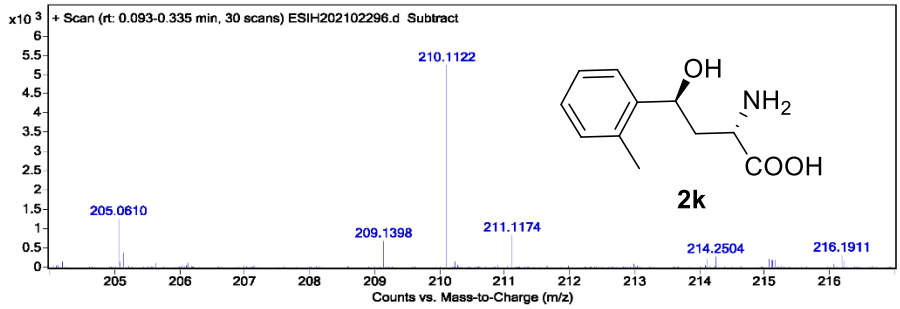
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102296.d	**Sample Name**	G5-AP-2JJ
Sample ID		**Position**	P2-B3
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:27:10	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
210.1122	210.1125	0.23	1.11	C11 H16 N O3	(M+H)+

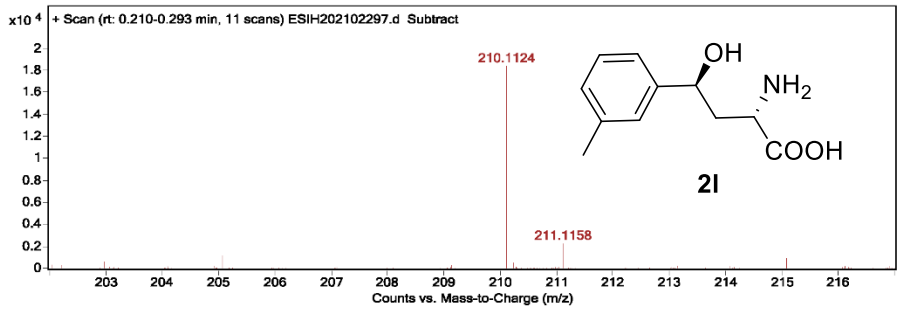
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102297.d	**Sample Name**	G5-AP-3JJ
Sample ID		**Position**	P2-B4
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:28:38	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
210.1124	210.1125	0.02	0.11	C11 H16 N O3	(M+H)+

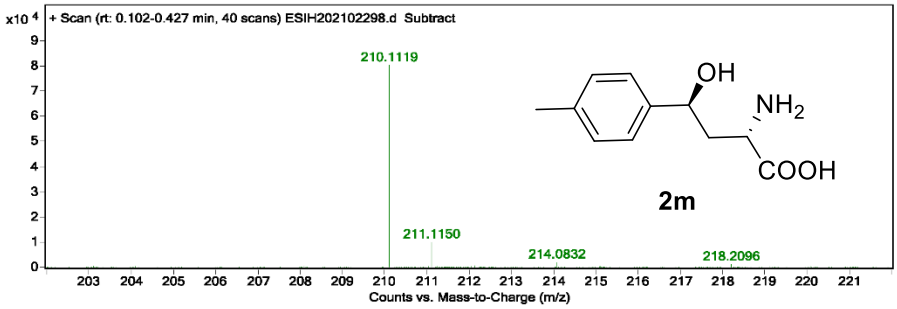
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102298.d	**Sample Name**	G5-AP-4JJ
Sample ID		**Position**	P2-B5
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:30:05	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
210.1119	210.1125	0.55	2.61	C11 H16 N O3	(M+H)+

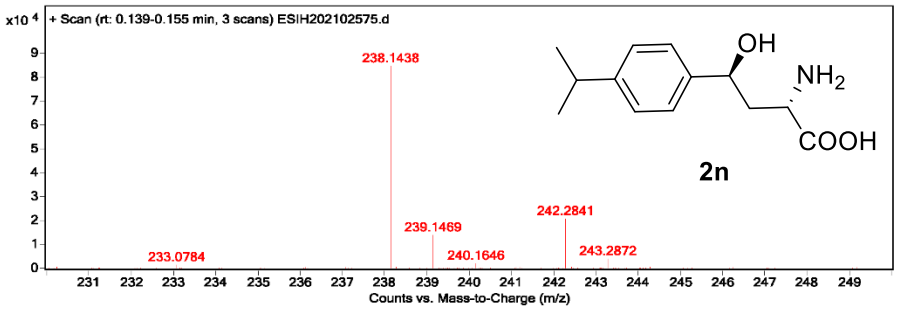
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102575.d	**Sample Name**	G5-G5-4YBJ
Sample ID		**Position**	P1-B8
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/13/2021 11:50:16	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
238.1438	238.1438	-0.04	-0.17	C13 H20 N O3	(M+H)+

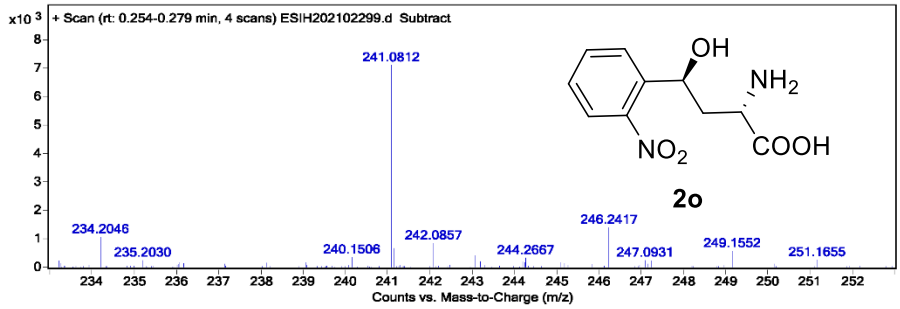
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102299.d	**Sample Name**	G5-AP-2NO2
Sample ID		**Position**	P2-B6
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:31:32	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



2o

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
241.0812	241.0819	0.67	2.79	C10 H13 N2 O5	(M+H)+

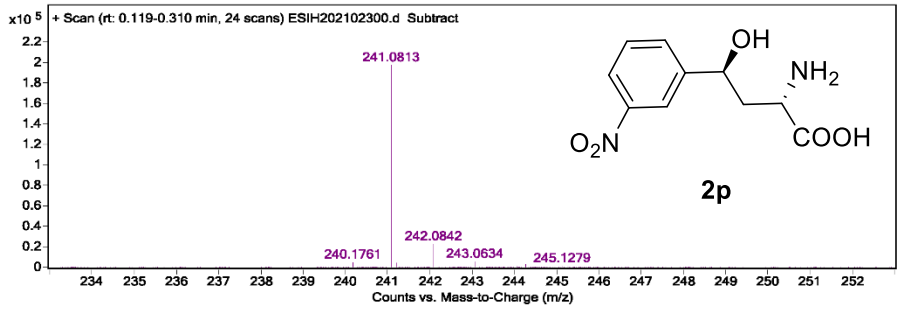
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102300.d	**Sample Name**	G5-AP-3NO2
Sample ID		**Position**	P2-B7
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:33:00	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



2p

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
241.0813	241.0819	0.63	2.61	C10 H13 N2 O5	(M+H)+

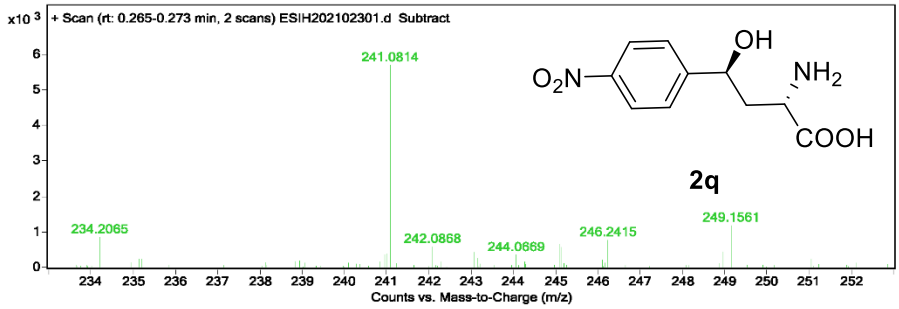
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102301.d	**Sample Name**	G5-AP-4NO2
Sample ID		**Position**	P2-B8
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:34:28	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



2q

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
241.0814	241.0819	0.45	1.88	C10 H13 N2 O5	(M+H)+

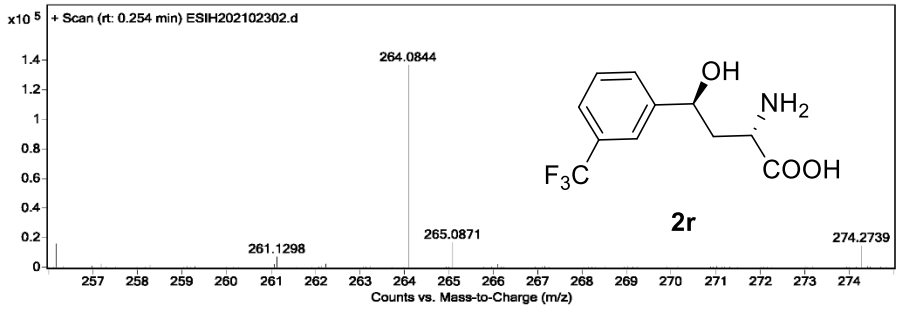
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102302.d	**Sample Name**	G5-AP-3-3F
Sample ID		**Position**	P2-B9
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:35:55	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



2r

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
264.0844	264.0842	-0.17	-0.66	C11 H13 F3 N O3	(M+H)+

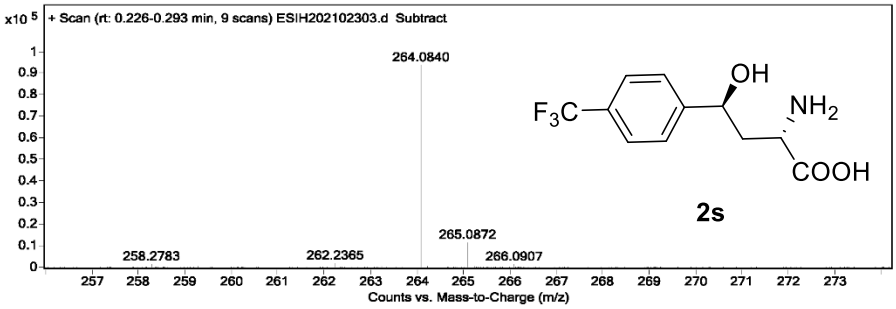
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102303.d	**Sample Name**	G5-AP-4-3F
Sample ID		**Position**	P2-C1
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	4/27/2021 18:37:20	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



2s

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
264.084	264.0842	0.18	0.69	C11 H13 F3 N O3	(M+H)+

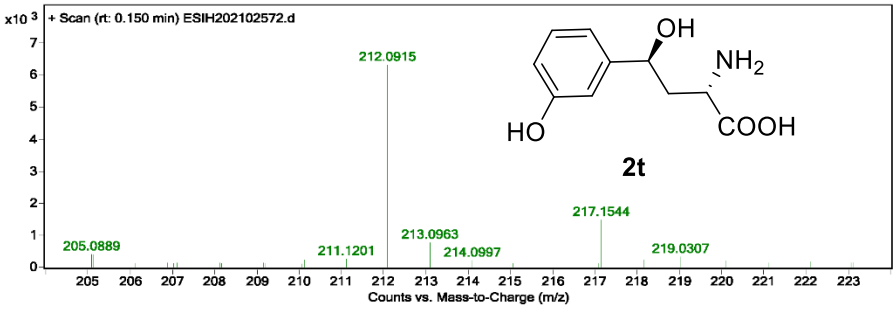
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102572.d	**Sample Name**	G5-G5-3QJ
Sample ID		**Position**	P1-B5
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/13/2021 11:46:25	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



2t

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
212.0915	212.0917	0.23	1.07	C10 H14 N O4	(M+H)+

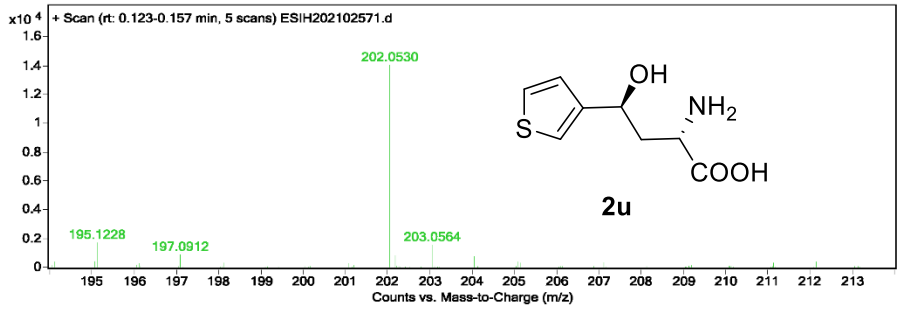
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102571.d	**Sample Name**	G5-G5-3SF
Sample ID		**Position**	P1-B4
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/13/2021 11:45:08	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



2u

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
202.053	202.0532	0.19	0.96	C8 H12 N O3 S	(M+H)+

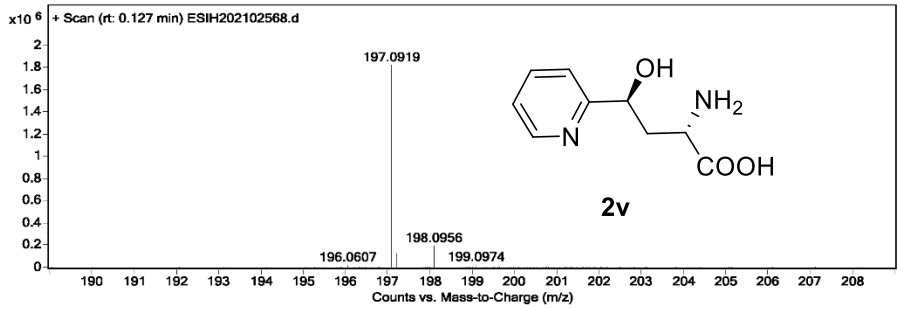
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102568.d	**Sample Name**	G5-2BD
Sample ID		**Position**	P1-B1
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/13/2021 11:41:17	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



2v

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
197.0919	197.0921	0.12	0.61	C9 H13 N2 O3	(M+H)+

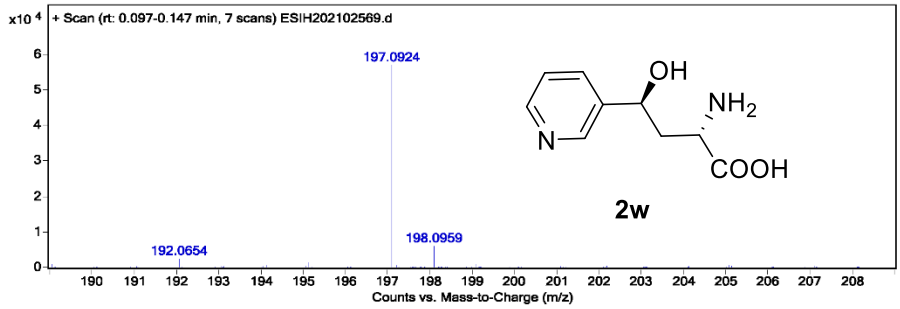
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102569.d	**Sample Name**	G5-3BD
Sample ID		**Position**	P1-B2
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/13/2021 11:42:34	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
197.0924	197.0921	-0.37	-1.88	C9 H13 N2 O3	(M+H)+

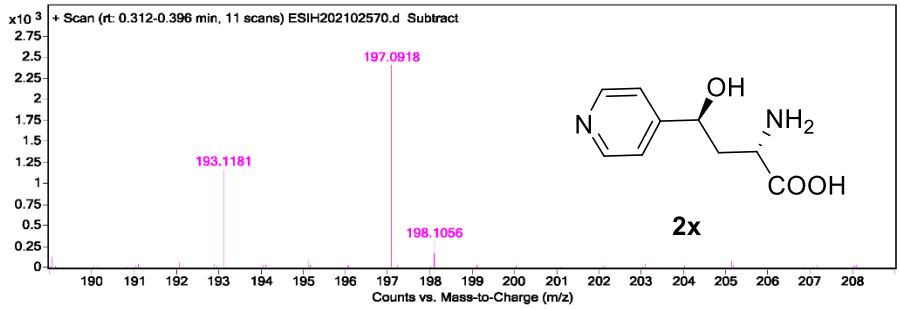
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102570.d	**Sample Name**	G5-4BD
Sample ID		**Position**	P1-B3
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/13/2021 11:43:51	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
197.0918	197.0921	0.23	1.18	C9 H13 N2 O3	(M+H)+

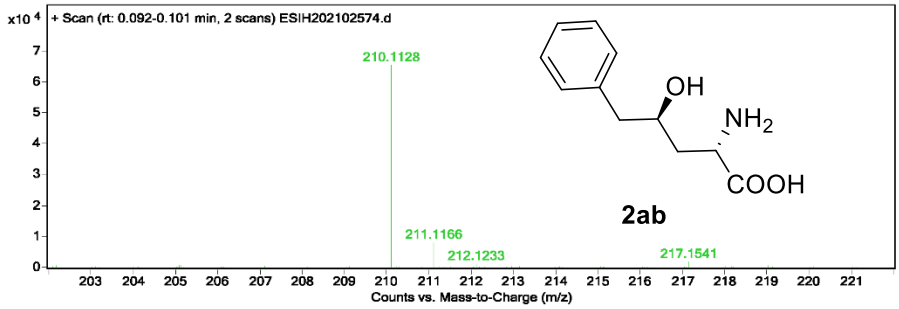
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102574.d	**Sample Name**	G5-G5-BYQ
Sample ID		**Position**	P1-B7
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/13/2021 11:49:00	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
210.1128	210.1125	-0.32	-1.54	C11 H16 N O3	(M+H)+

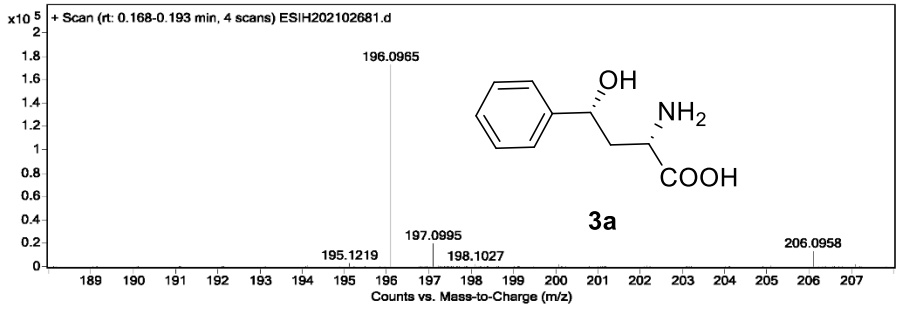
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102681.d	**Sample Name**	G5-G5-PFK-BJQ
Sample ID		**Position**	P1-B5
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:29:24	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
196.0965	196.0968	0.34	1.73	C10 H14 N O3	(M+H)+

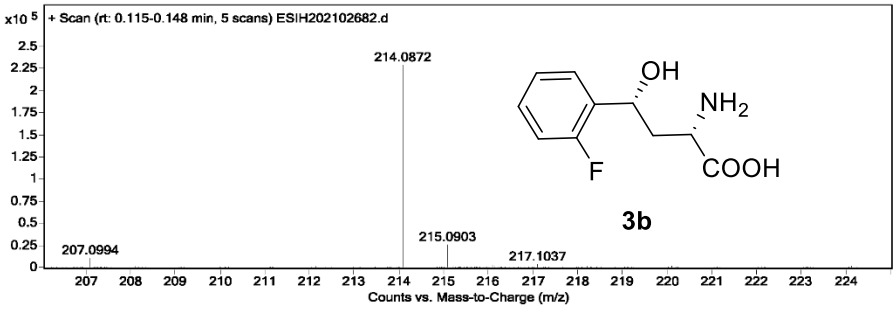
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102682.d	**Sample Name**	G5-G5-PFK-2F
Sample ID		**Position**	P1-B6
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:30:41	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
214.0872	214.0874	0.19	0.87	C10 H13 F N O3	(M+H)+

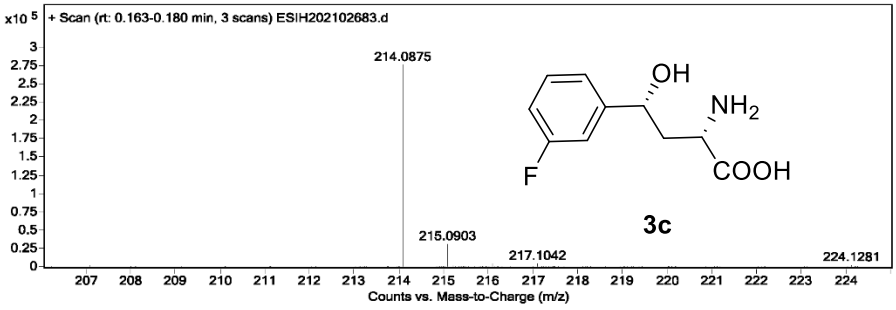
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102683.d	**Sample Name**	G5-G5-PFK-3F
Sample ID		**Position**	P1-B7
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:31:58	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
214.0875	214.0874	-0.14	-0.63	C10 H13 F N O3	(M+H)+

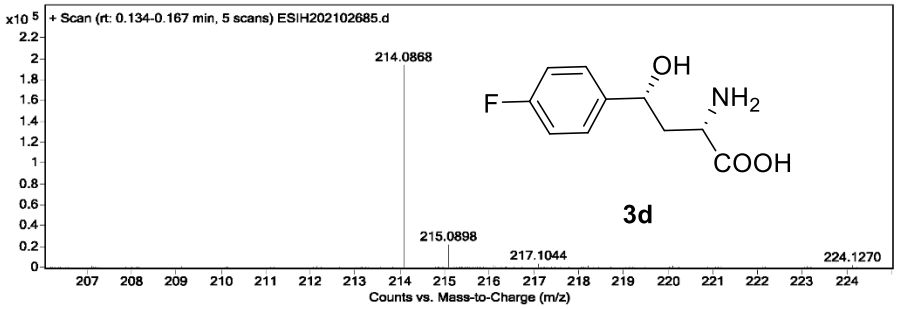
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102685.d	**Sample Name**	G5-G5-PFK-4F
Sample ID		**Position**	P1-B9
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:34:30	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
214.0868	214.0874	0.62	2.89	C10 H13 F N O3	(M+H)+

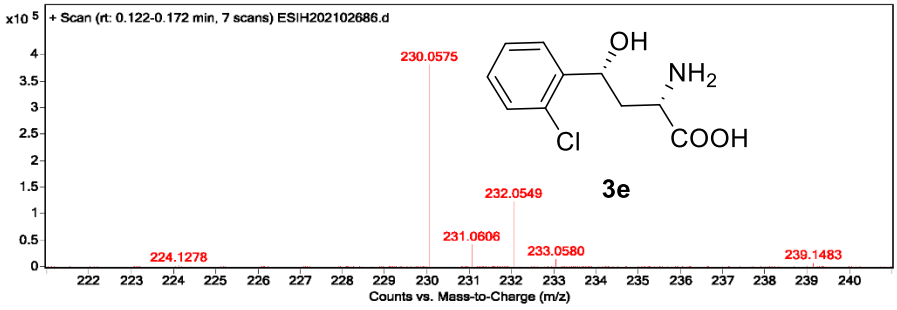
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102686.d	**Sample Name**	G5-G5-PFK-2CL
Sample ID		**Position**	P1-C1
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:35:44	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
230.0575	230.0578	0.31	1.36	C10 H13 Cl N O3	(M+H)+

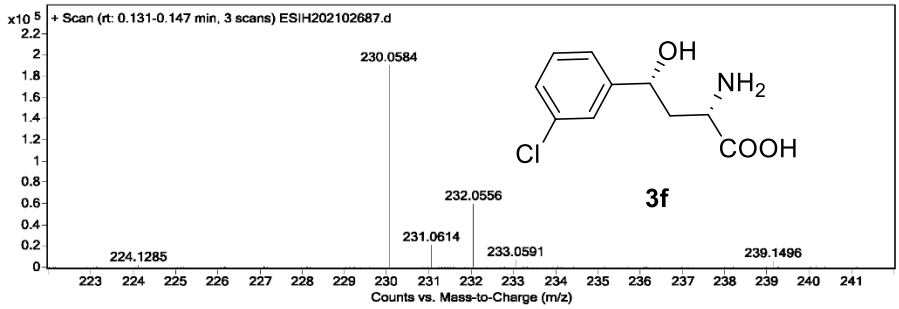
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102687.d	**Sample Name**	G5-G5-PFK-3CL
Sample ID		**Position**	P1-C2
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:37:01	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
230.0584	230.0578	-0.57	-2.47	C10 H13 Cl N O3	(M+H)+

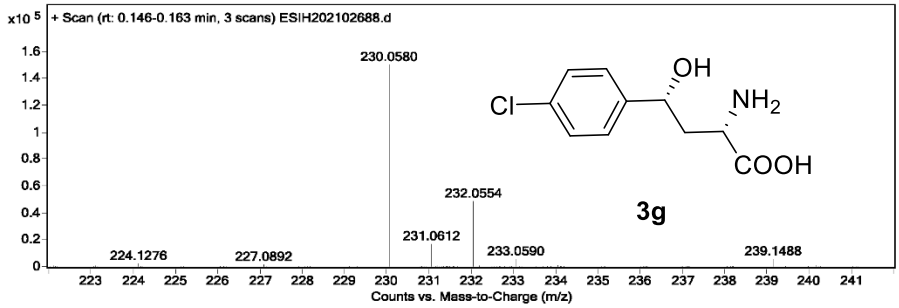
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102688.d	**Sample Name**	G5-G5-PFK-4CL
Sample ID		**Position**	P1-C3
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:38:17	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
230.058	230.0578	-0.18	-0.8	C10 H13 Cl N O3	(M+H)+

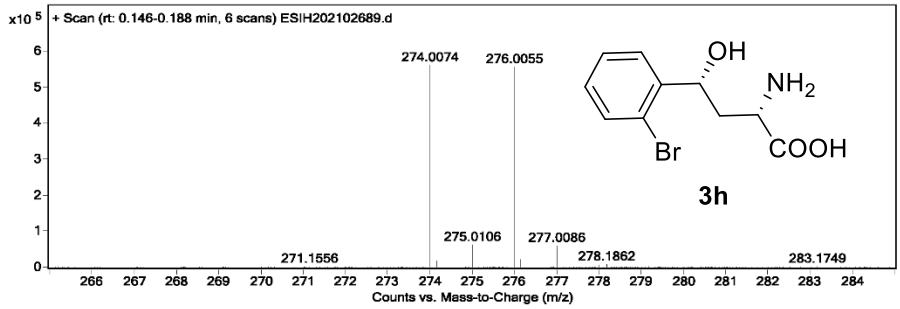
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102689.d	**Sample Name**	G5-G5-PFK-2BR
Sample ID		**Position**	P1-C4
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:39:34	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
274.0074	274.0073	-0.08	-0.28	C10 H13 Br N O3	(M+H)+

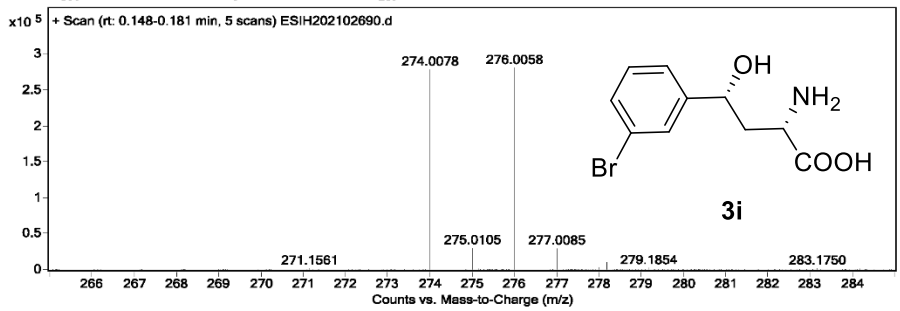
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102690.d	**Sample Name**	G5-G5-PFK-3BR
Sample ID		**Position**	P1-C5
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:40:51	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
274.0078	274.0073	-0.42	-1.53	C10 H13 Br N O3	(M+H)+

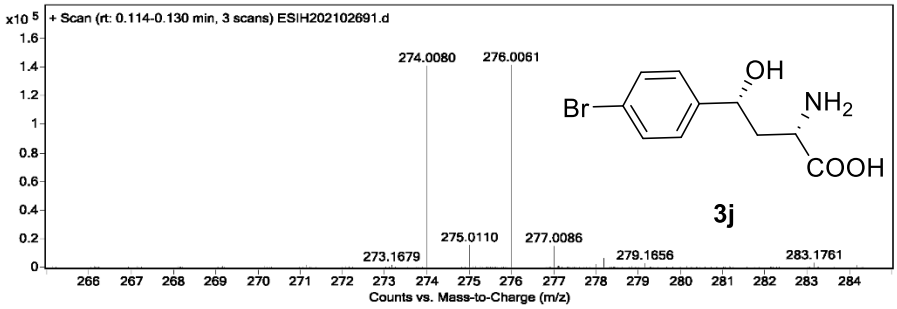
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102691.d	**Sample Name**	G5-G5-PFK-4BR
Sample ID		**Position**	P1-C6
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:42:08	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
274.008	274.0073	-0.66	-2.42	C10 H13 Br N O3	(M+H)+

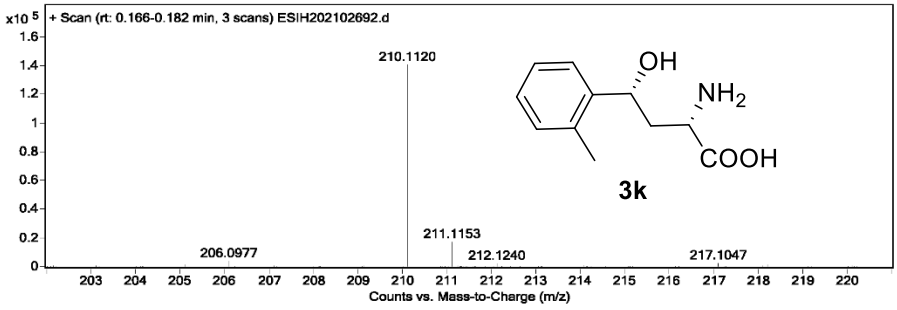
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102692.d	**Sample Name**	G5-G5-PFK-2JJ
Sample ID		**Position**	P1-C7
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:43:26	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
210.112	210.1125	0.52	2.46	C11 H16 N O3	(M+H)+

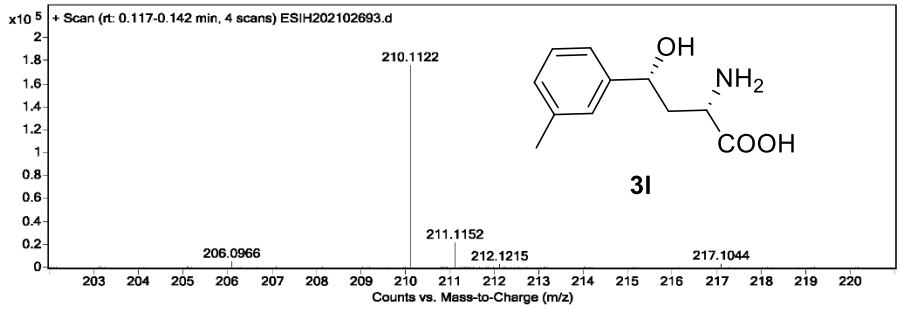
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102693.d	**Sample Name**	G5-G5-PFK-3JJ
Sample ID		**Position**	P1-C8
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:44:43	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
210.1122	210.1125	0.22	1.05	C11 H16 N O3	(M+H)+

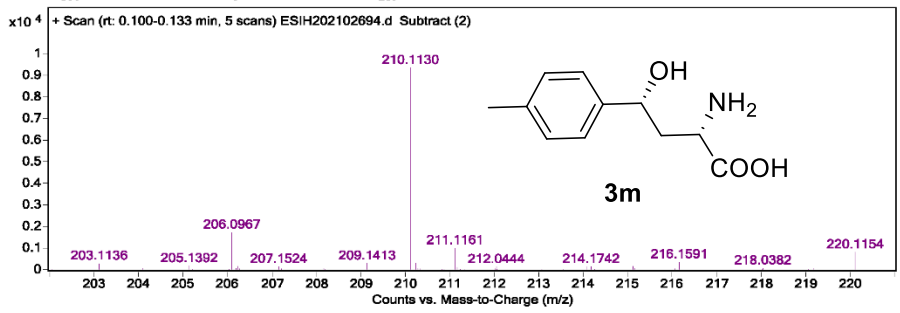
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102694.d	**Sample Name**	G5-G5-PFK-4JJ
Sample ID		**Position**	P1-C9
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:46:00	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
210.113	210.1125	-0.48	-2.31	C11 H16 N O3	(M+H)+

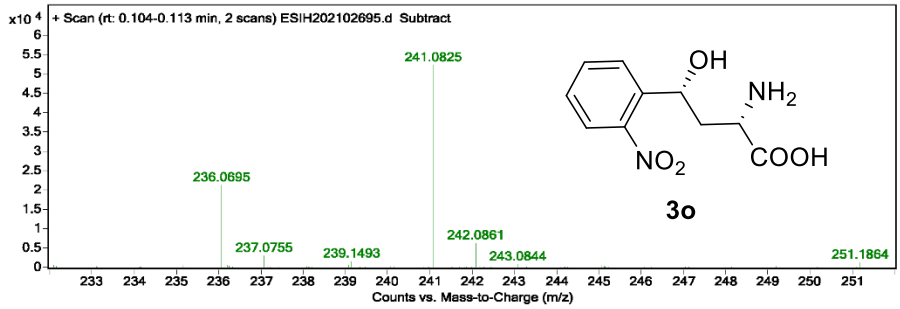
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102695.d	**Sample Name**	G5-G5-PFK-2XJ
Sample ID		**Position**	P1-D1
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:47:16	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
241.0825	241.0819	-0.65	-2.7	C10 H13 N2 O5	(M+H)+

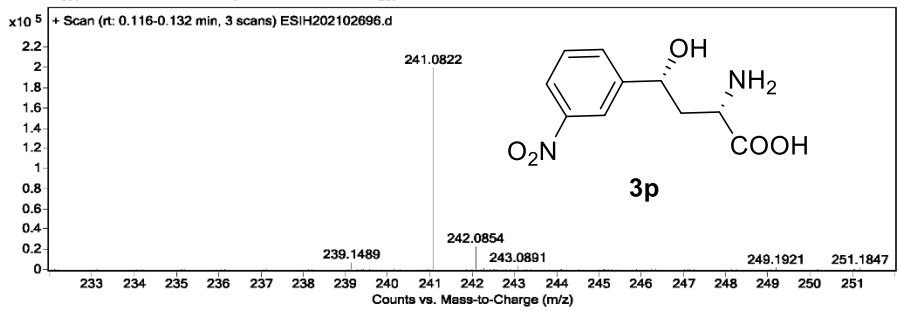
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102696.d	**Sample Name**	G5-G5-PFK-3XJ
Sample ID		**Position**	P1-D2
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:48:33	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
241.0822	241.0819	-0.28	-1.16	C10 H13 N2 O5	(M+H)+

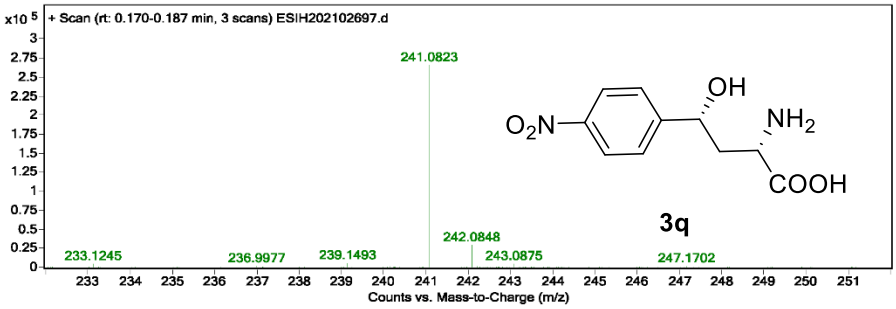
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102697.d	**Sample Name**	G5-G5-PFK-4XJ
Sample ID		**Position**	P1-D3
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:49:49	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



3q

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
241.0823	241.0819	-0.38	-1.57	C10 H13 N2 O5	(M+H)+

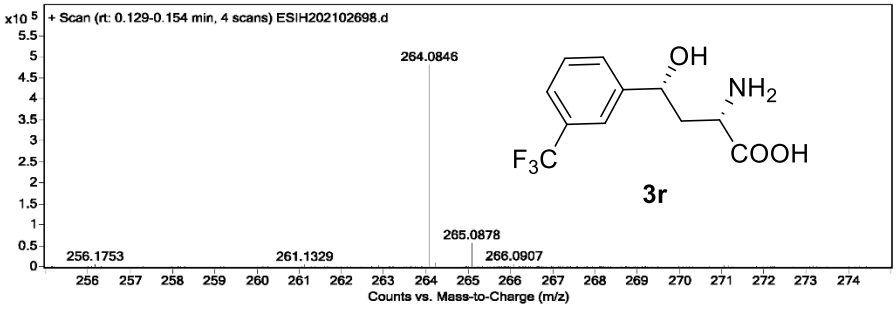
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102698.d	**Sample Name**	G5-G5-PFK-3-3F
Sample ID		**Position**	P1-D4
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:51:07	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



3r

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
264.0846	264.0842	-0.37	-1.4	C11 H13 F3 N O3	(M+H)+

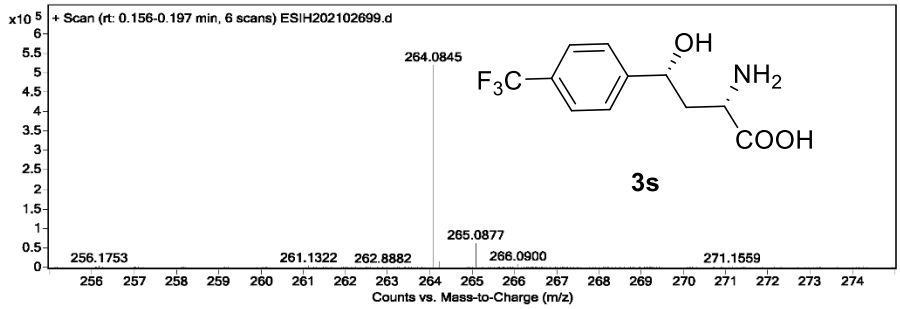
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102699.d	**Sample Name**	G5-G5-PFK-4-3F
Sample ID		**Position**	P1-D5
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:52:24	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



3s

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
264.0845	264.0842	-0.25	-0.96	C11 H13 F3 N O3	(M+H)+

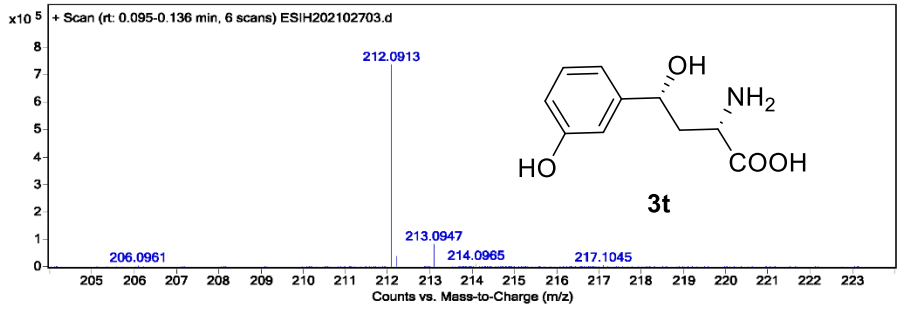
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102703.d	**Sample Name**	G5-G5-PFK-2QJ
Sample ID		**Position**	P1-D9
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:57:32	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



3t

Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
212.0913	212.0917	0.42	1.98	C10 H14 N O4	(M+H)+

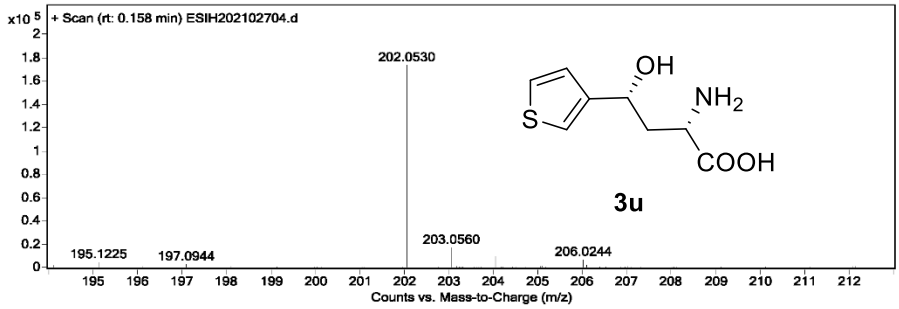
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102704.d	**Sample Name**	G5-G5-PFK-3SF
Sample ID		**Position**	P1-E1
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:58:48	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
202.053	202.0532	0.2	0.98	C8 H12 N O3 S	(M+H)+

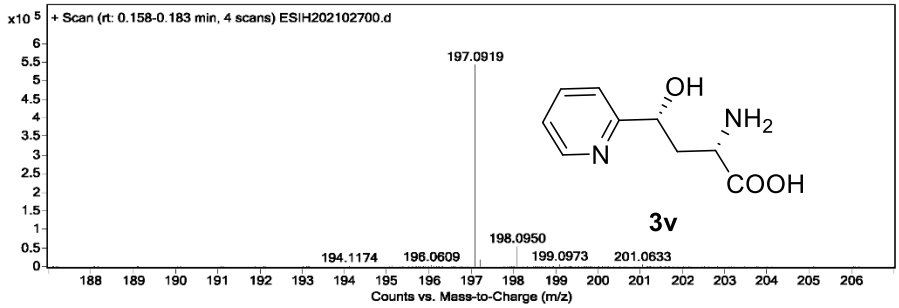
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102700.d	**Sample Name**	G5-G5-PFK-2BD
Sample ID		**Position**	P1-D6
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:53:40	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
197.0919	197.0921	0.13	0.66	C9 H13 N2 O3	(M+H)+

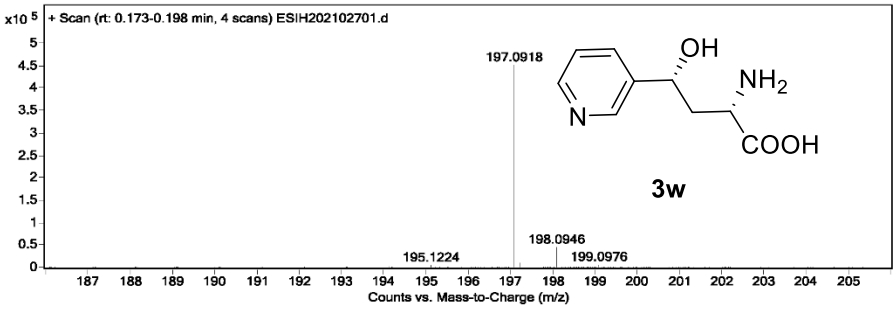
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102701.d	**Sample Name**	G5-G5-PFK-3BD
Sample ID		**Position**	P1-D7
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:54:58	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
197.0918	197.0921	0.28	1.42	C9 H13 N2 O3	(M+H)+

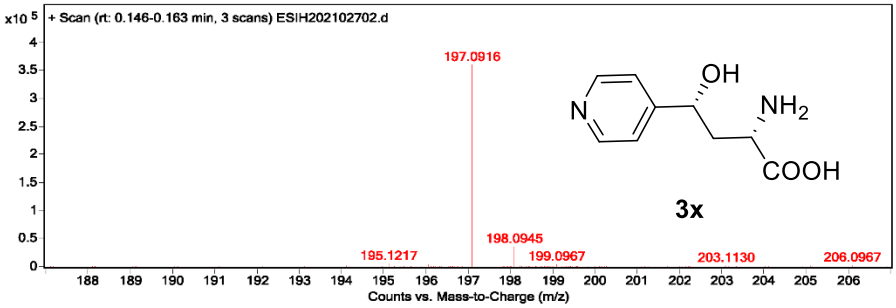
--- End Of Report ---

Qualitative Analysis Report

Data Filename	ESIH202102702.d	**Sample Name**	G5-G5-PFK-4BD
Sample ID		**Position**	P1-D8
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	5/17/2021 19:56:15	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

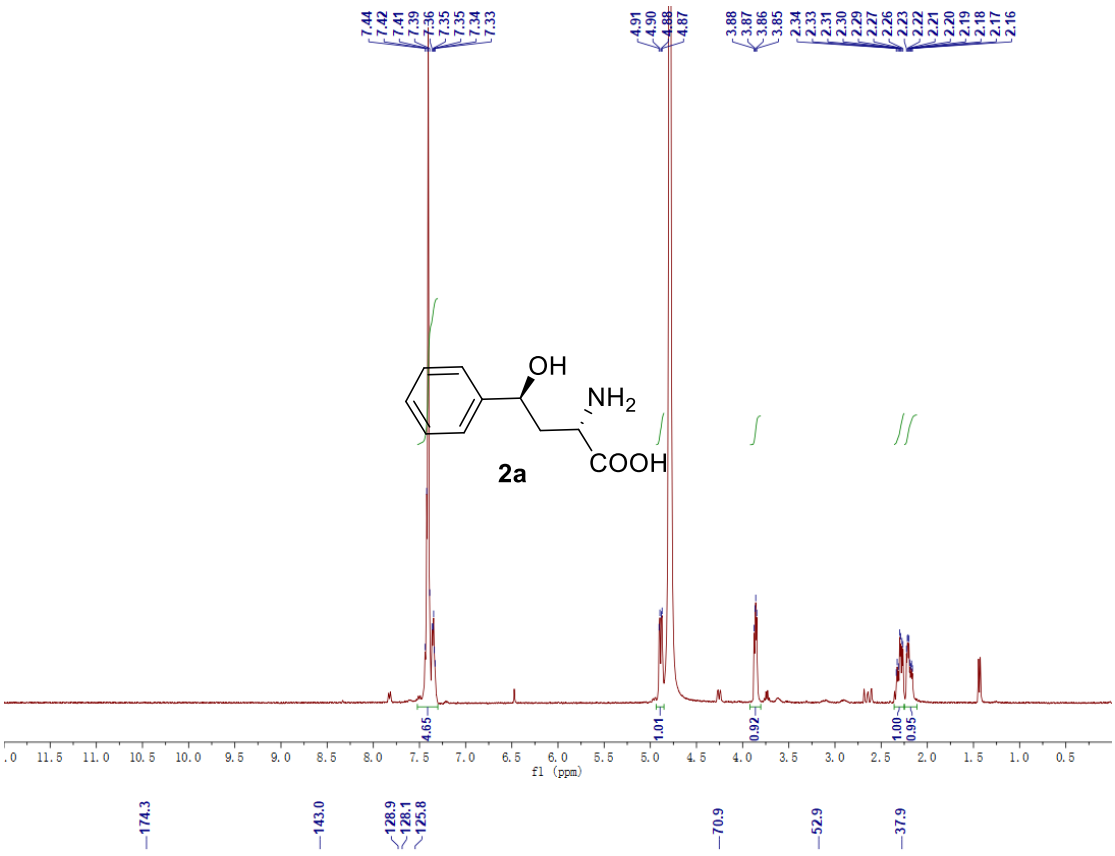
Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
197.0916	197.0921	0.5	2.53	C9 H13 N2 O3	(M+H)+

--- End Of Report ---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7.42
7.41
7.39
7.36
7.35
7.35
7.34
7.33
4.91
4.90
4.88
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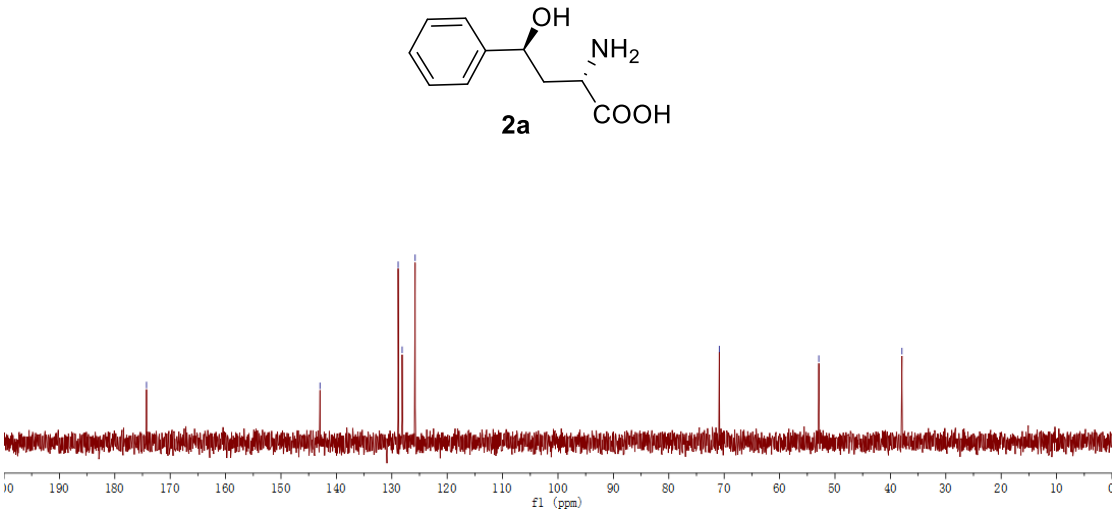
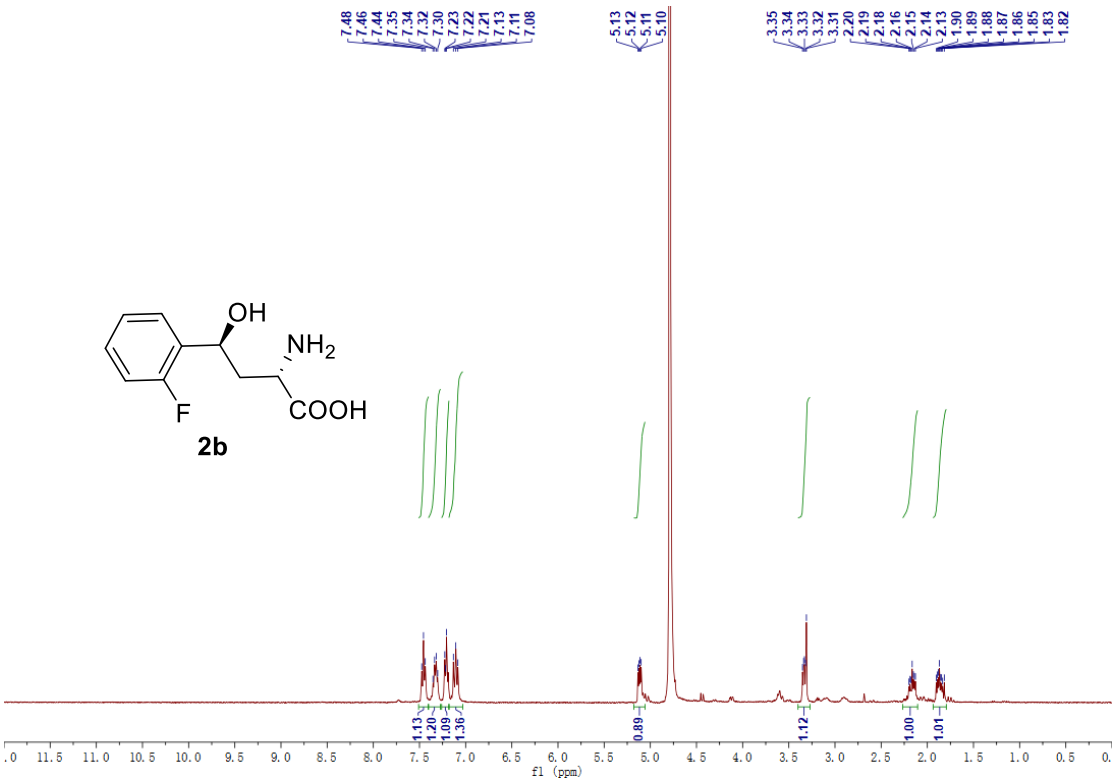
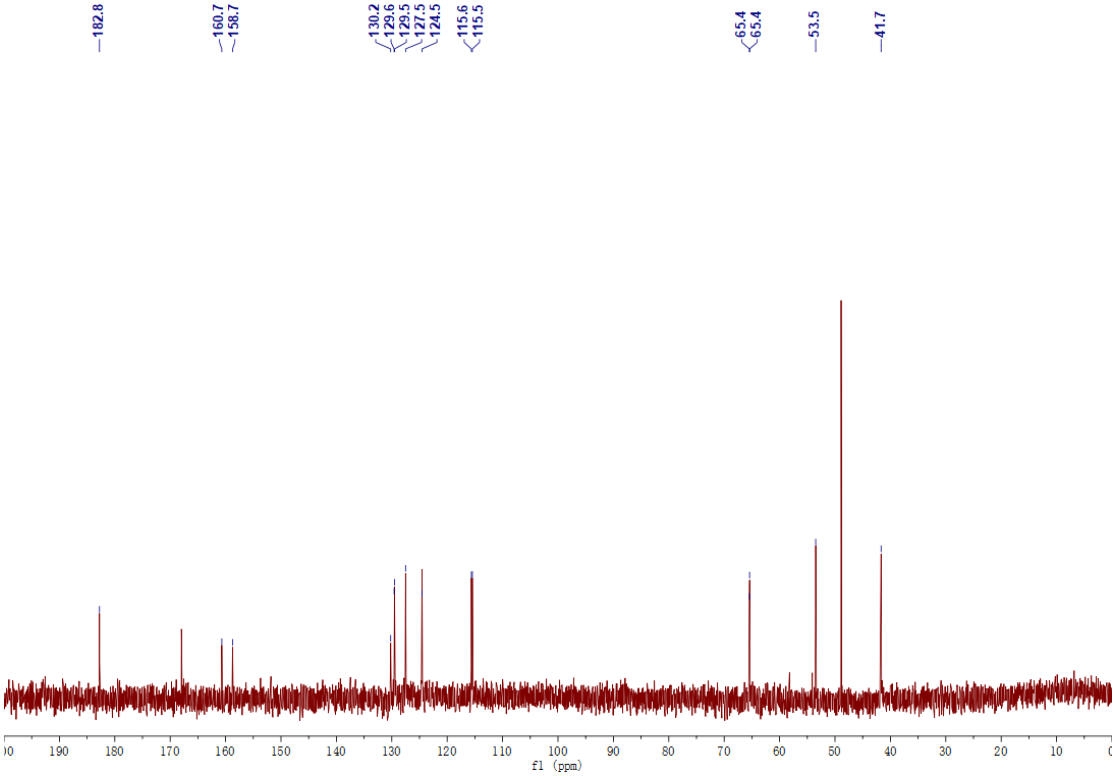
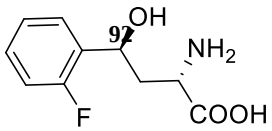
3.88
3.87
3.86
3.85
2.34
2.33
2.31
2.30
2.29
2.27
2.26
2.23
2.22
2.21
2.20
2.19
2.18
2.17
2.16
OH
NH2
COOH
2a
4.65
1.01
0.92
1.00
0.95
f1 (ppm)

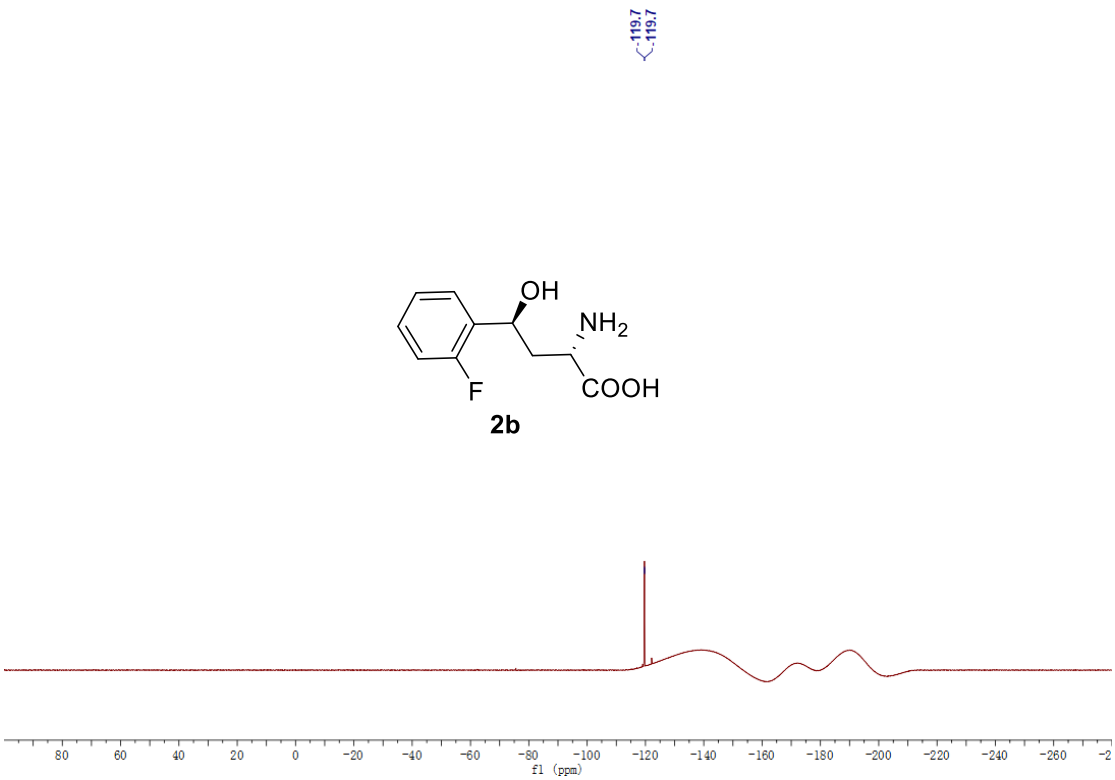

174.3
143.0
128.9
128.1
125.8
70.9
52.9
37.9
OH
NH2
COOH
2a
f1 (ppm)

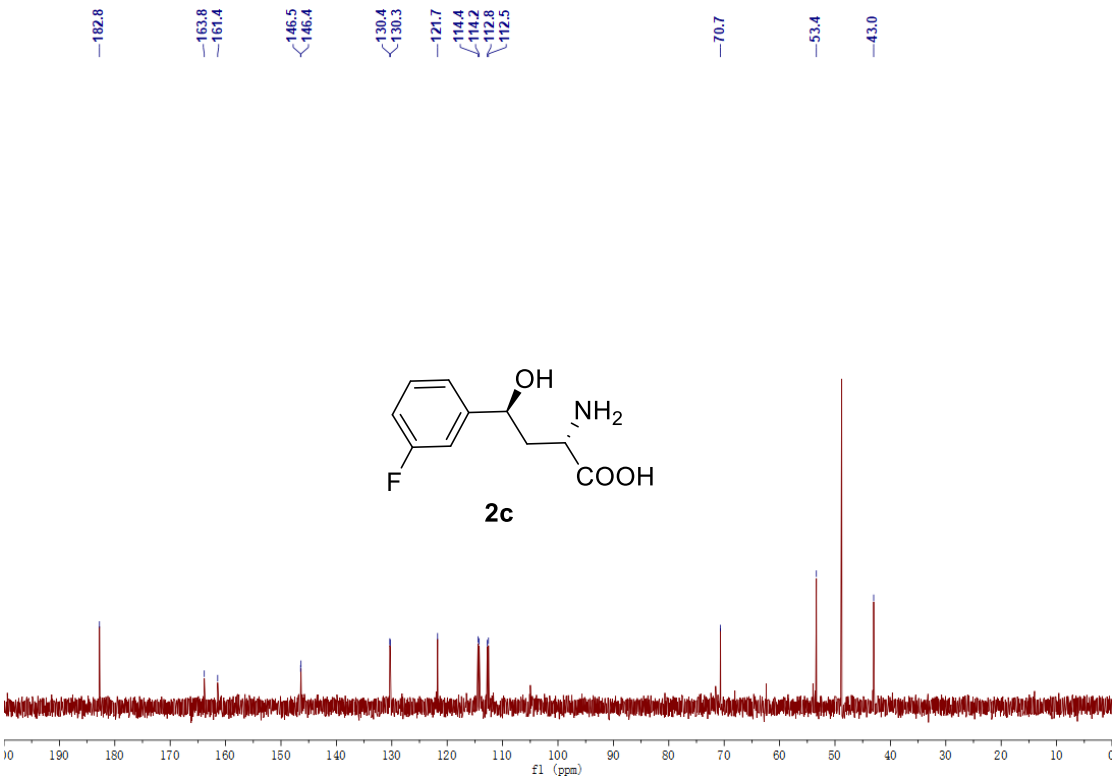

7.48
7.46
7.44
7.35
7.34
7.32
7.30
7.23
7.22
7.21
7.13
7.11
7.08
5.13
5.12
5.11
5.10
3.35
3.34
3.33
3.32
3.31
2.20
2.19
2.18
2.16
2.15
2.14
2.13
1.90
1.89
1.88
1.87
1.86
1.85
1.83
1.82
OH
NH2
F
COOH
2b
1.13
1.20
1.09
1.36
0.89
1.12
1.00
1.01
f1 (ppm)

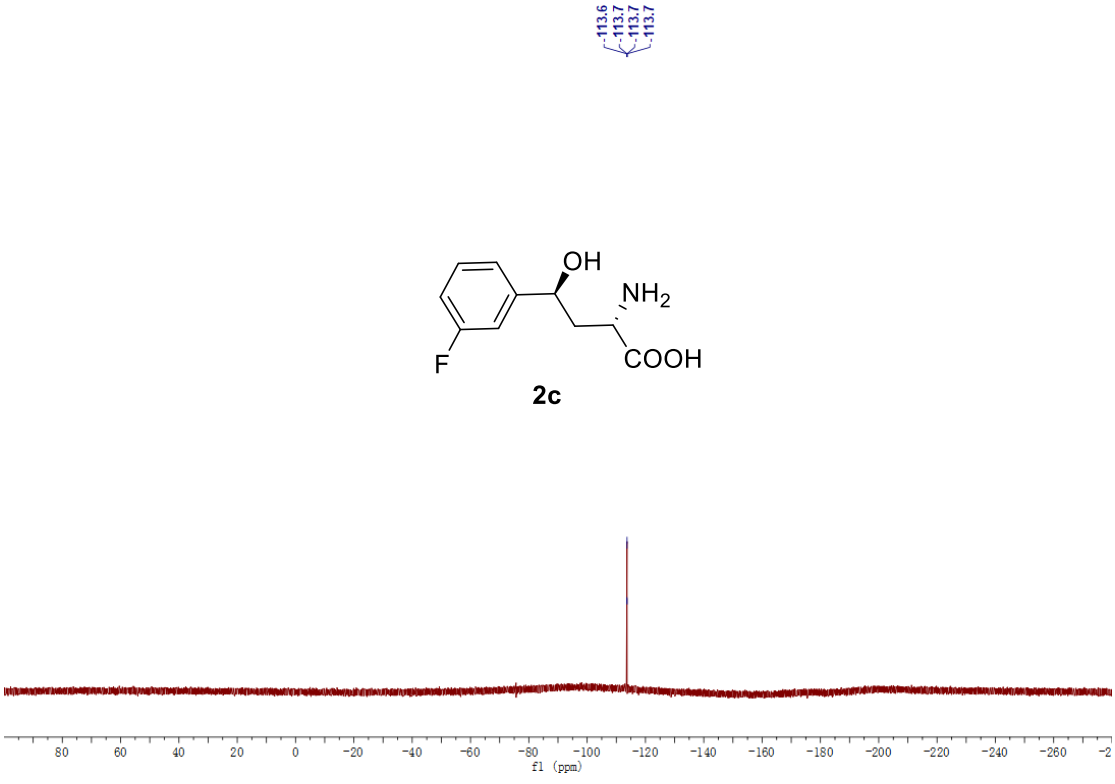

182.8
160.7
158.7
130.2
129.6
129.5
127.5
124.5
115.6
115.5
65.4
65.4
53.5
41.7
f1 (ppm)

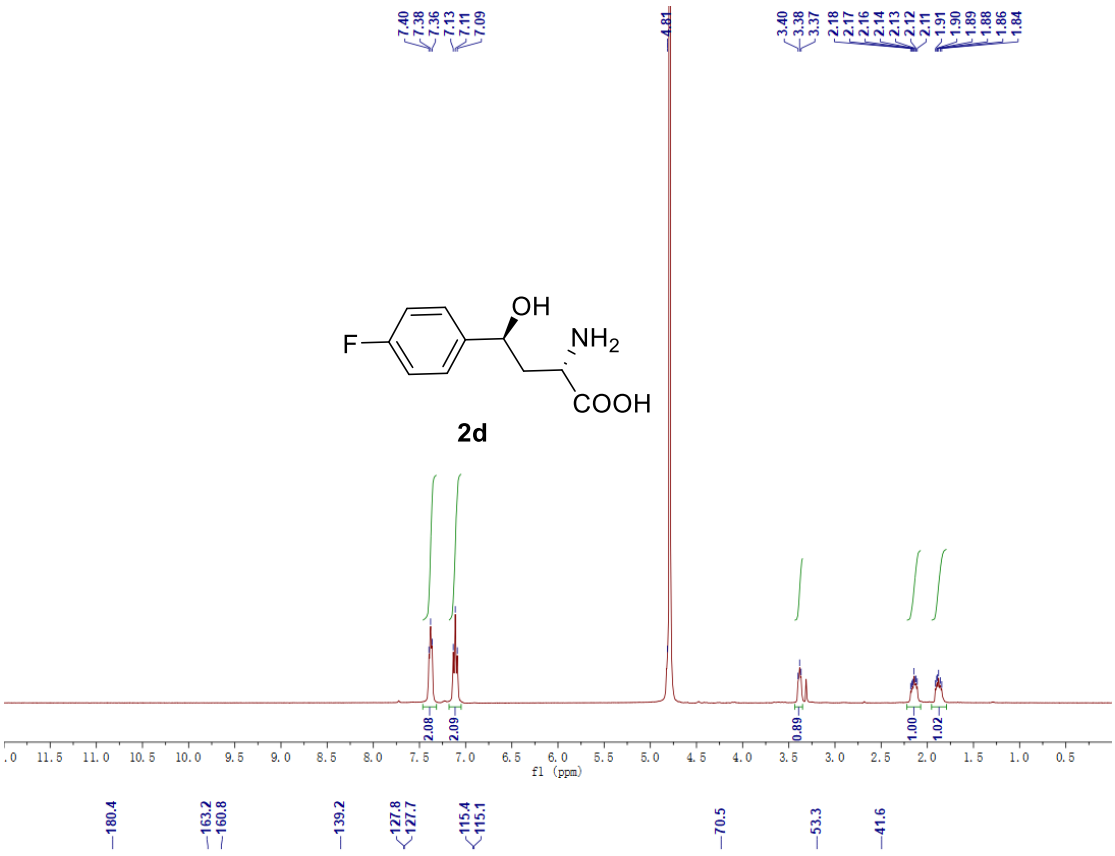

OH
NH2
F
COOH

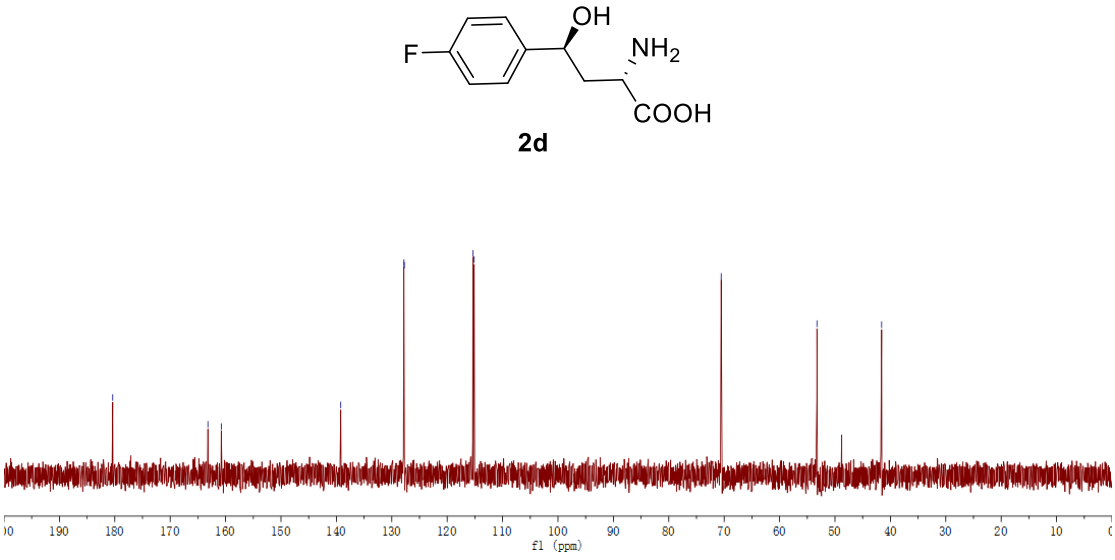
2b

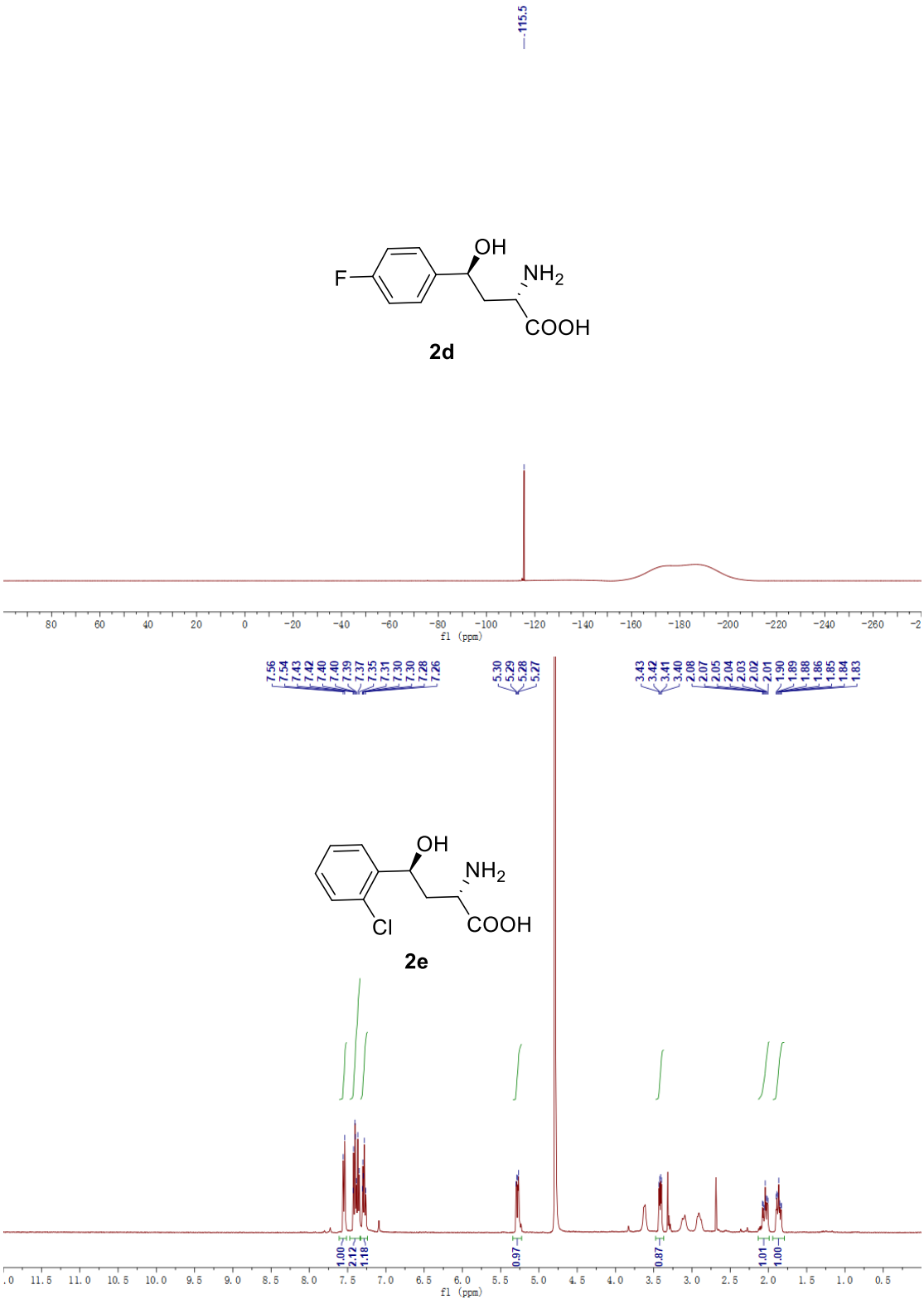

119.7
119.7
OH
NH2
F
COOH
2b
80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -2
f1 (ppm)
7.40 7.38 7.38 7.36 7.36 7.34 7.18 7.16 7.15 7.14 7.12 7.12 7.06 7.05 7.04 7.04 7.03 7.02 7.01
4.82 4.81
3.32 3.30 2.12 2.11 2.10 2.08 2.07 2.06 2.05 2.02 1.84 1.83 1.82 1.80 1.79 1.78 1.77
OH
NH2
F
COOH
2c
1.23 2.12 1.17 1.01 1.00
.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

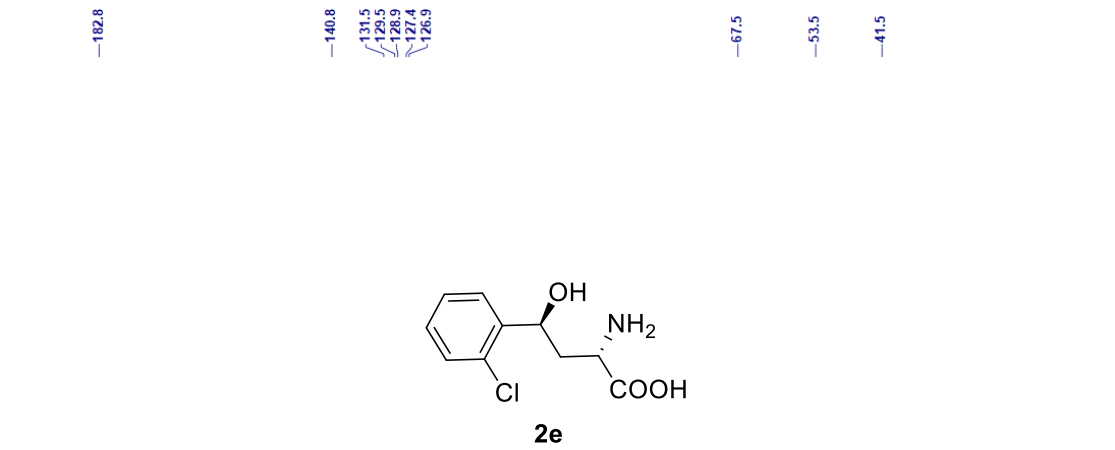

182.8
163.8
161.4
146.5
146.4
130.4
130.3
121.7
114.4
114.2
112.8
112.5
70.7
53.4
43.0
OH
NH2
F
COOH
2c
f1 (ppm)

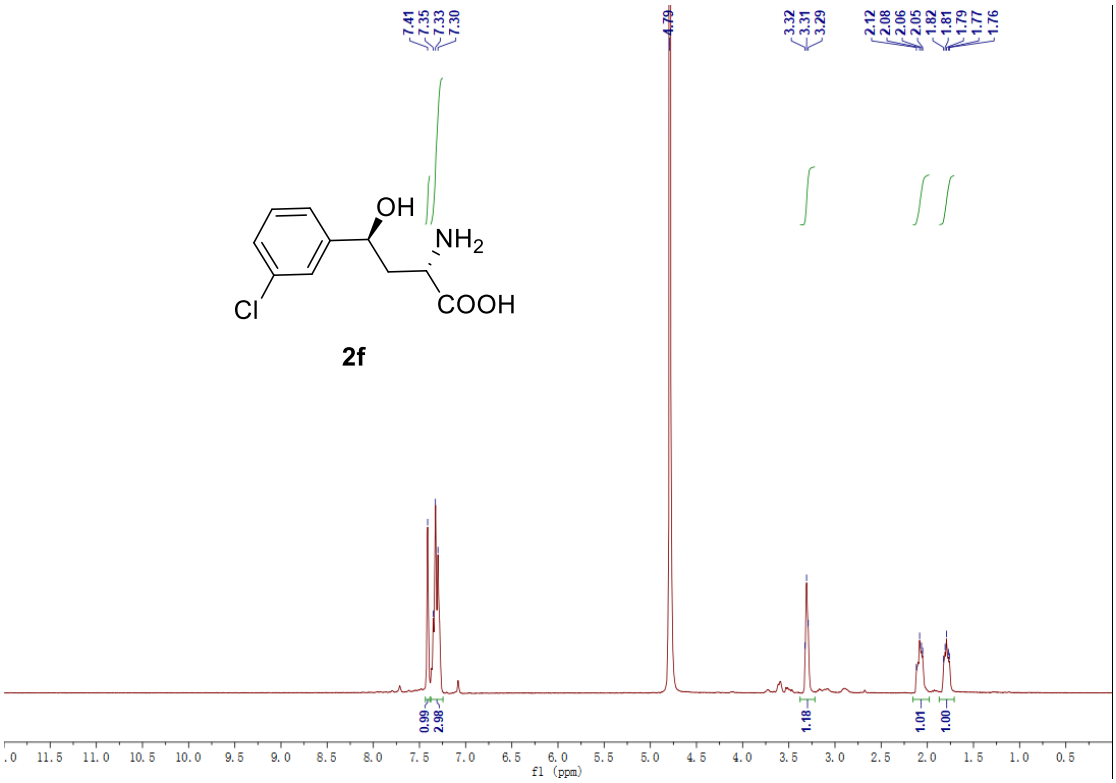

113.6
113.7
113.7
113.7
OH
NH2
F
COOH
2c
f1 (ppm)

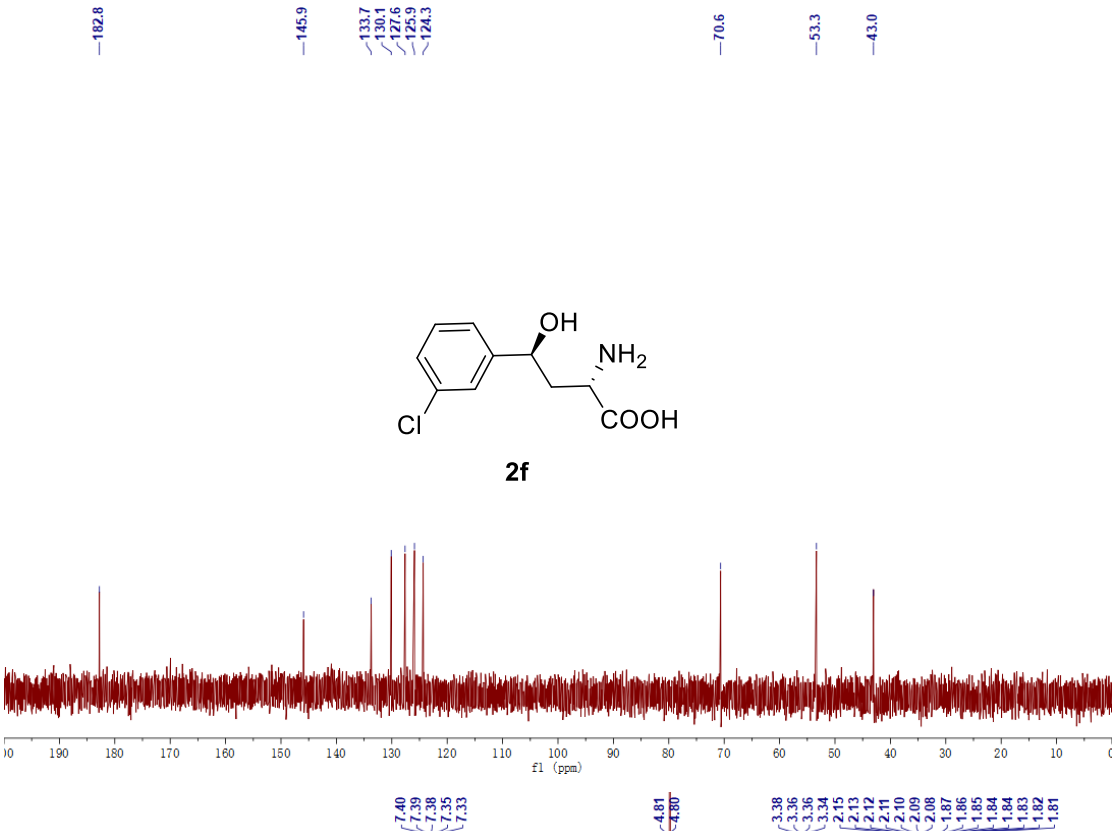

7.40
7.38
7.36
7.13
7.11
7.09
4.81
3.40
3.38
3.37
2.18
2.17
2.16
2.14
2.13
2.12
2.11
1.91
1.90
1.89
1.88
1.86
1.84
OH
NH2
F
COOH
2d
2.08
2.09
0.89
1.00
1.02
f1 (ppm)
180.4
163.2
160.8
139.2
127.8
127.7
115.4
115.1
70.5
53.3
41.6

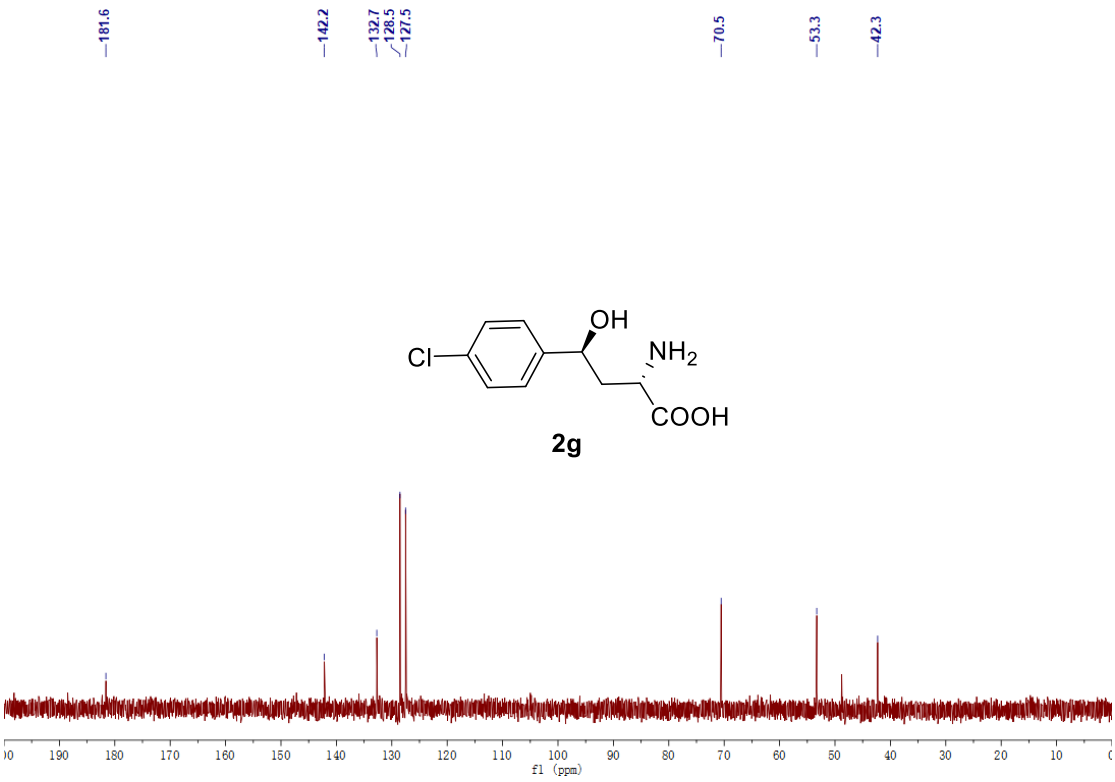

OH
NH2
F
COOH
2d
f1 (ppm)

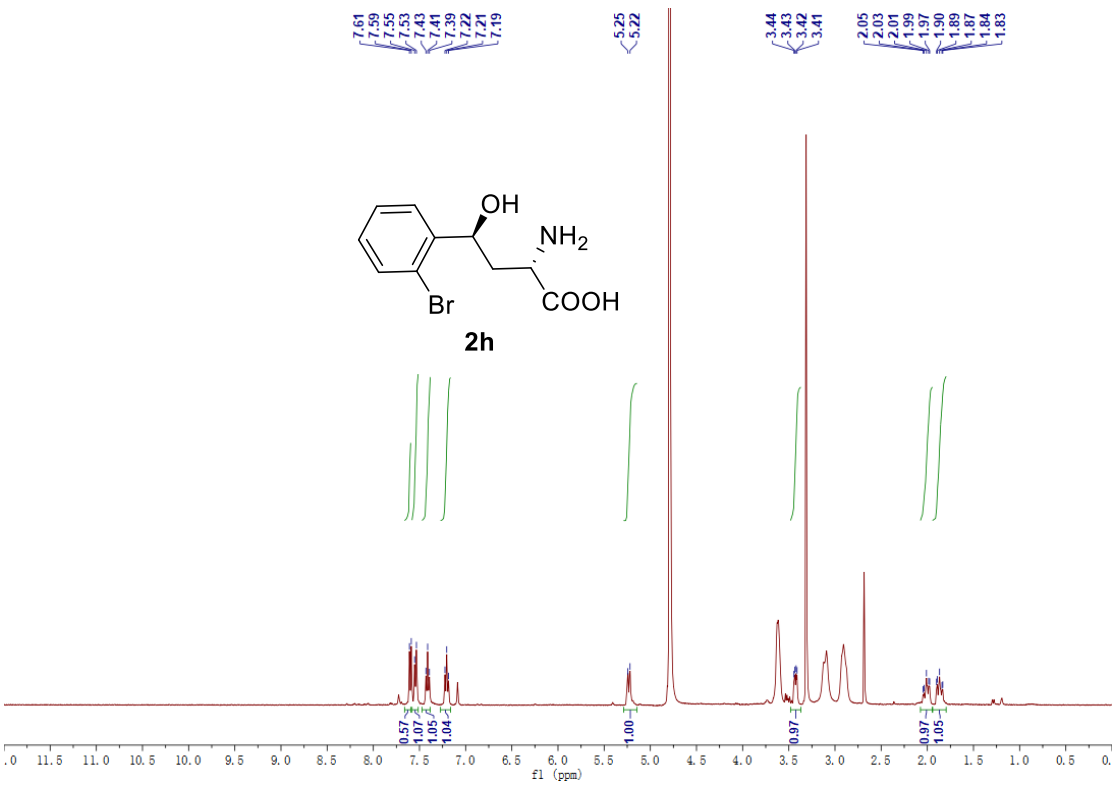

-115.5
OH
F
NH2
COOH
2d
80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -2
f1 (ppm)
7.56 7.54 7.43 7.42 7.40 7.40 7.39 7.37 7.35 7.31 7.30 7.30 7.28 7.26
5.30 5.29 5.28 5.27
3.43 3.42 3.41 3.40 2.08 2.07 2.05 2.04 2.03 2.02 2.01 1.90 1.89 1.88 1.86 1.85 1.84 1.83
OH
NH2
Cl
COOH
2e
1.00 2.12 1.18 0.97 0.87 1.01 1.00
.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

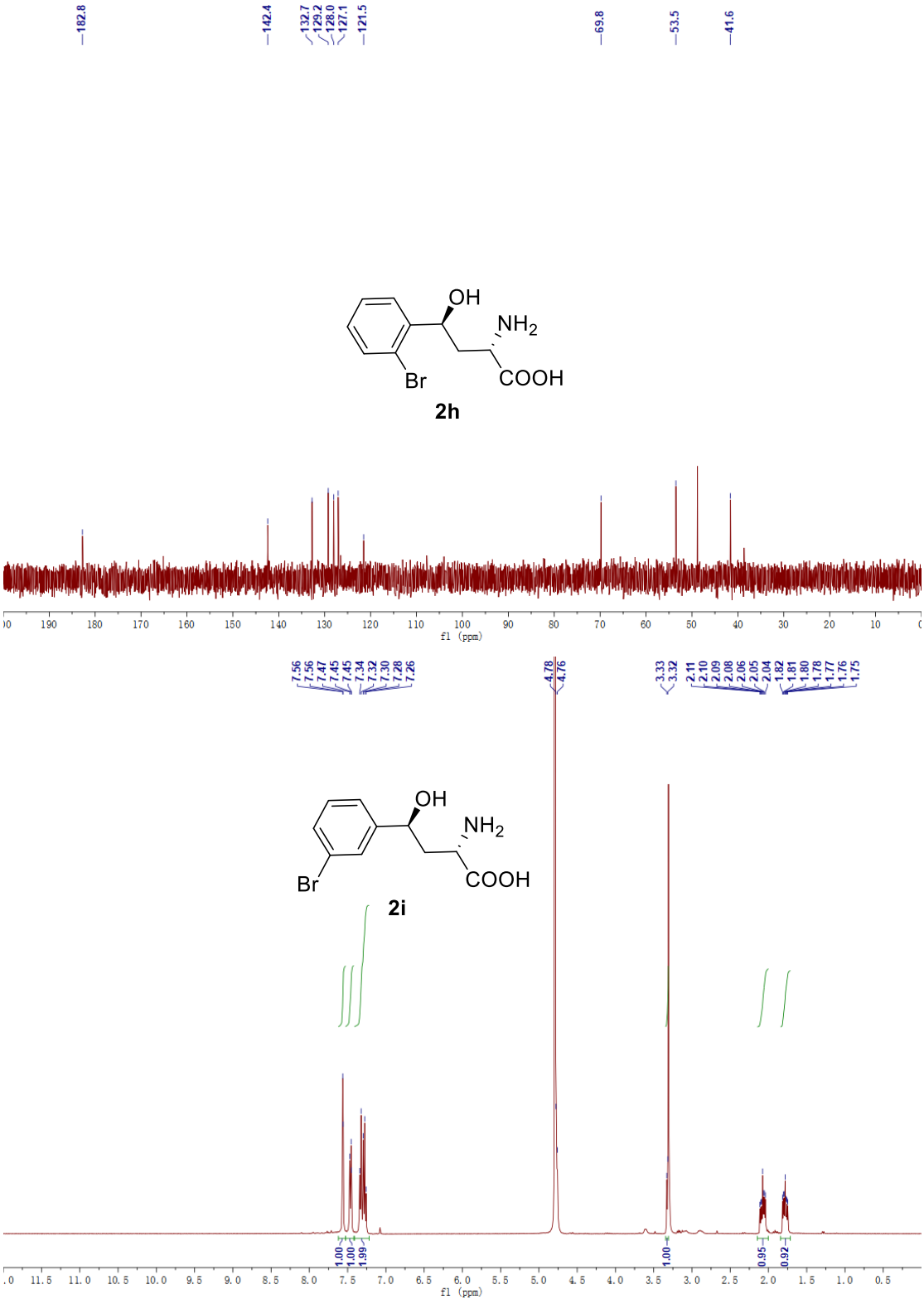

182.8
140.8
131.5
129.5
128.9
127.4
126.9
67.5
53.5
41.5
OH
NH2
Cl
COOH
2e
f1 (ppm)

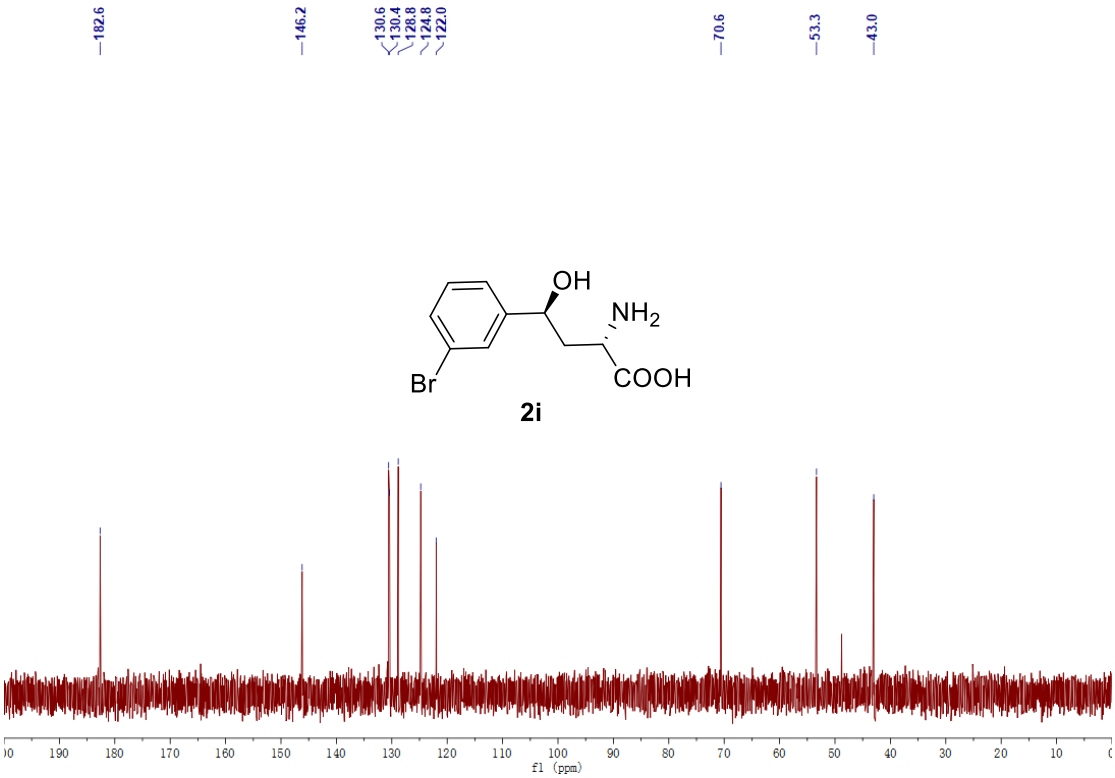

7.41
7.35
7.33
7.30
4.79
3.32
3.31
3.29
2.12
2.08
2.06
2.05
1.82
1.81
1.79
1.77
1.76
OH
NH2
Cl
COOH
2f
0.99
2.98
1.18
1.01
1.00
f1 (ppm)

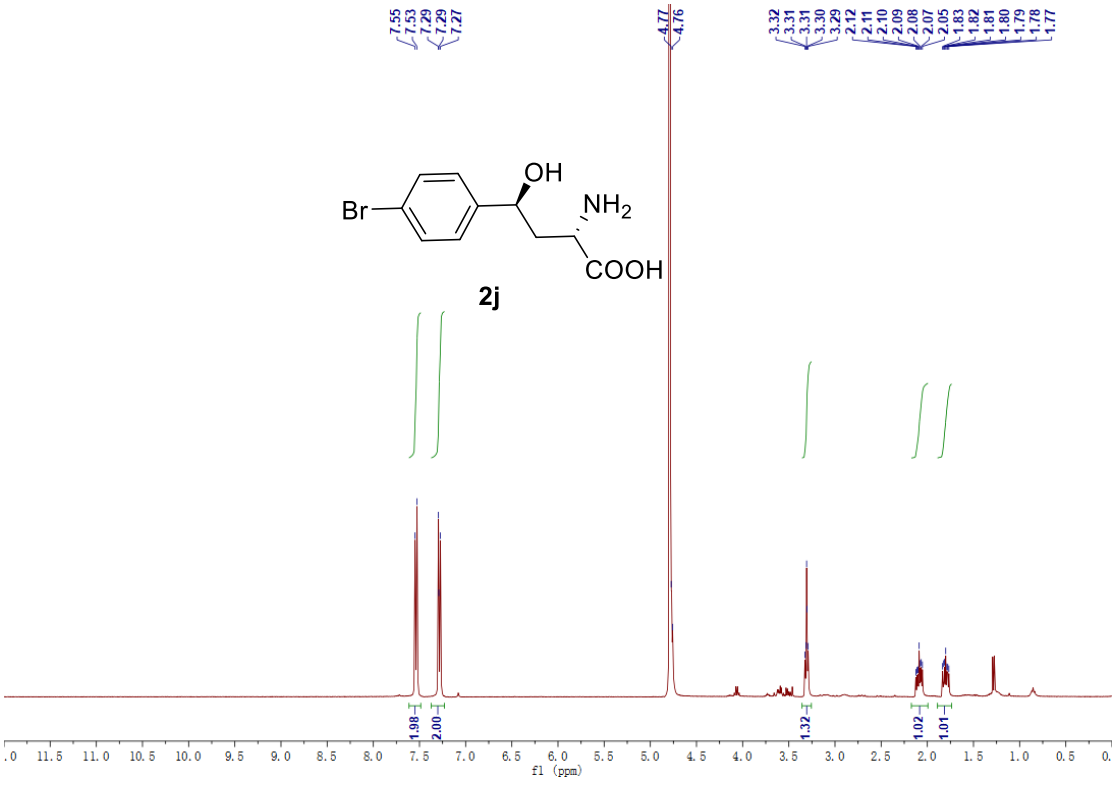

182.8
145.9
133.7
130.1
127.6
125.9
124.3
70.6
53.3
43.0
OH
NH2
Cl
COOH
2f
f1 (ppm)
7.40
7.39
7.38
7.35
7.33
4.81
4.80
3.38
3.36
3.36
3.34
2.15
2.13
2.12
2.11
2.10
2.09
2.08
1.87
1.86
1.85
1.84
1.84
1.83
1.82
1.81
OH
NH2
Cl
COOH
2g
1.95
2.09
0.94
1.00
1.03
f1 (ppm)

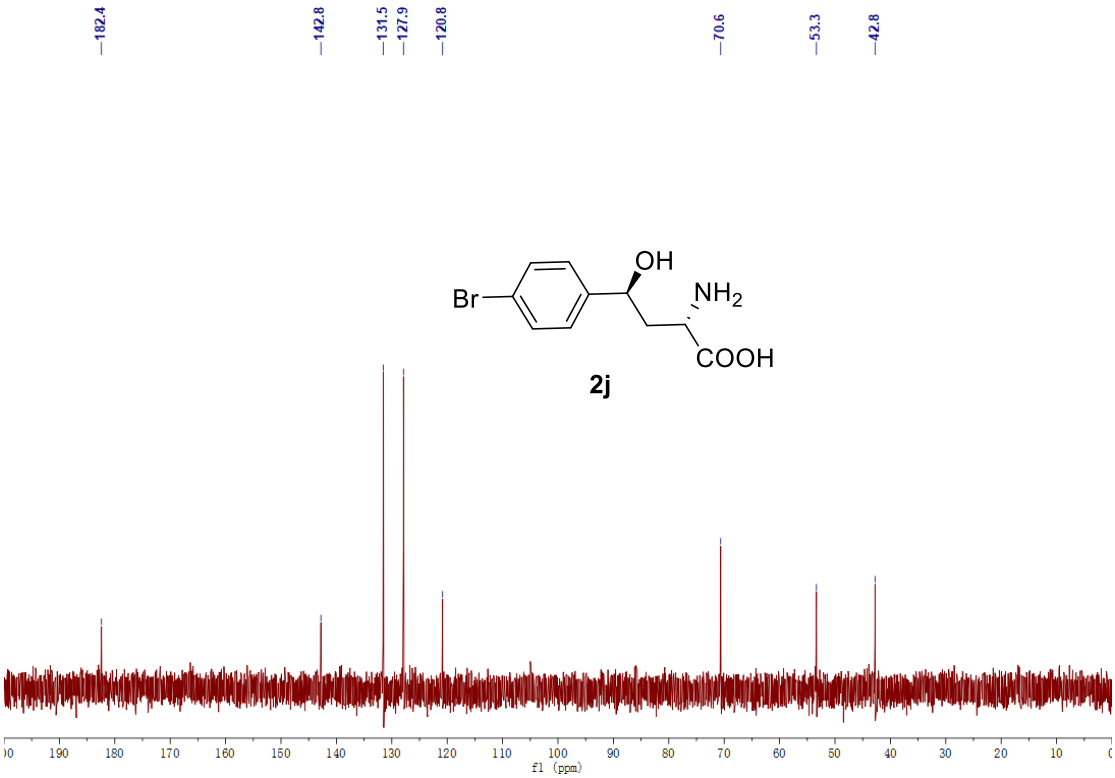

181.6
142.2
132.7
128.5
127.5
70.5
53.3
42.3
Cl
OH
NH2
COOH
2g
f1 (ppm)

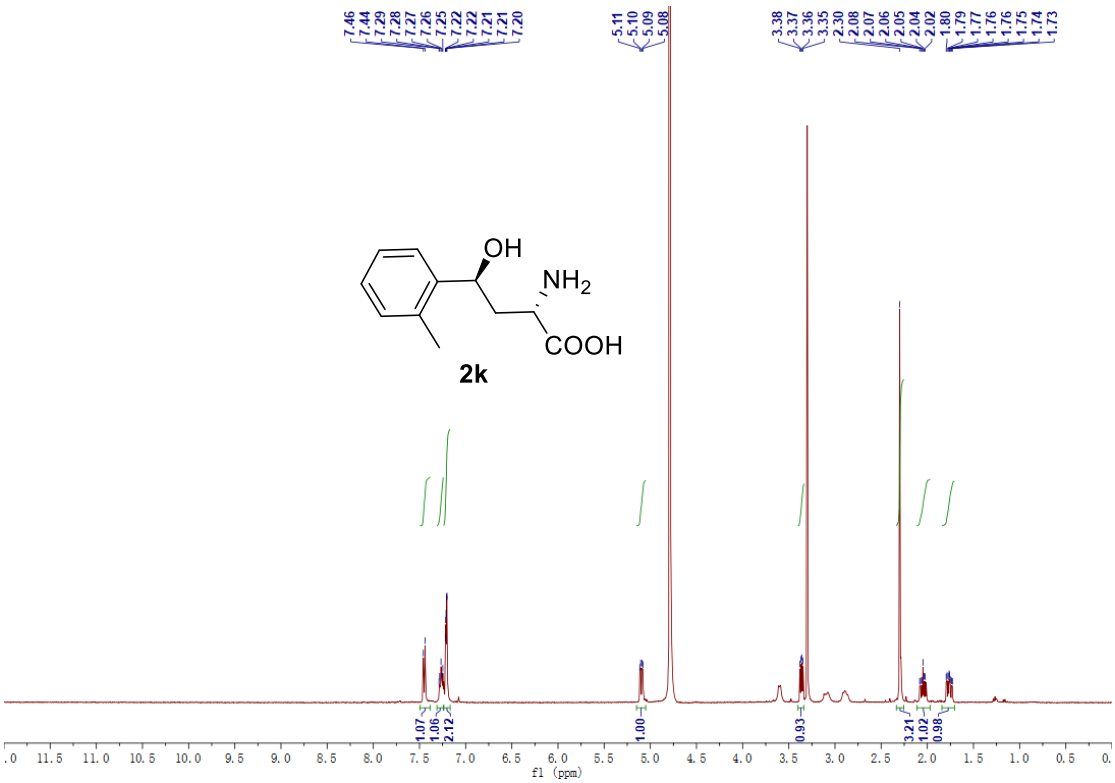

7.61
7.59
7.55
7.53
7.43
7.41
7.39
7.22
7.21
7.19
5.25
5.22
3.44
3.43
3.42
3.41
2.05
2.03
2.01
1.99
1.97
1.90
1.89
1.87
1.84
1.83
OH
NH2
Br
COOH
2h
0.57
1.07
1.05
1.04
1.00
0.97
0.97
1.05
f1 (ppm)

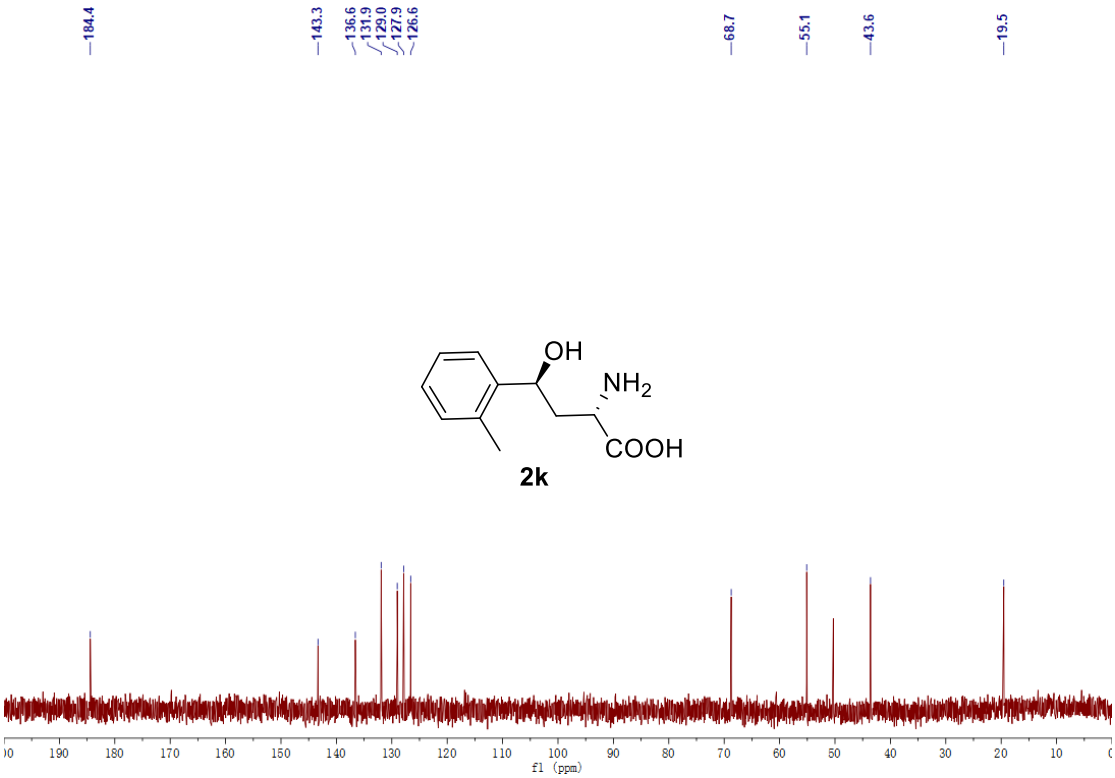

182.8
142.4
132.7
129.2
128.0
127.1
121.5
69.8
53.5
41.6
OH
NH2
Br
COOH
2h
f1 (ppm)
7.56
7.56
7.47
7.45
7.45
7.34
7.32
7.30
7.28
7.26
4.78
4.76
3.33
3.32
2.11
2.10
2.09
2.08
2.06
2.05
2.04
1.82
1.81
1.80
1.78
1.77
1.76
1.75
OH
NH2
Br
COOH
2i
1.00
1.00
1.99
1.00
0.95
0.92
f1 (ppm)

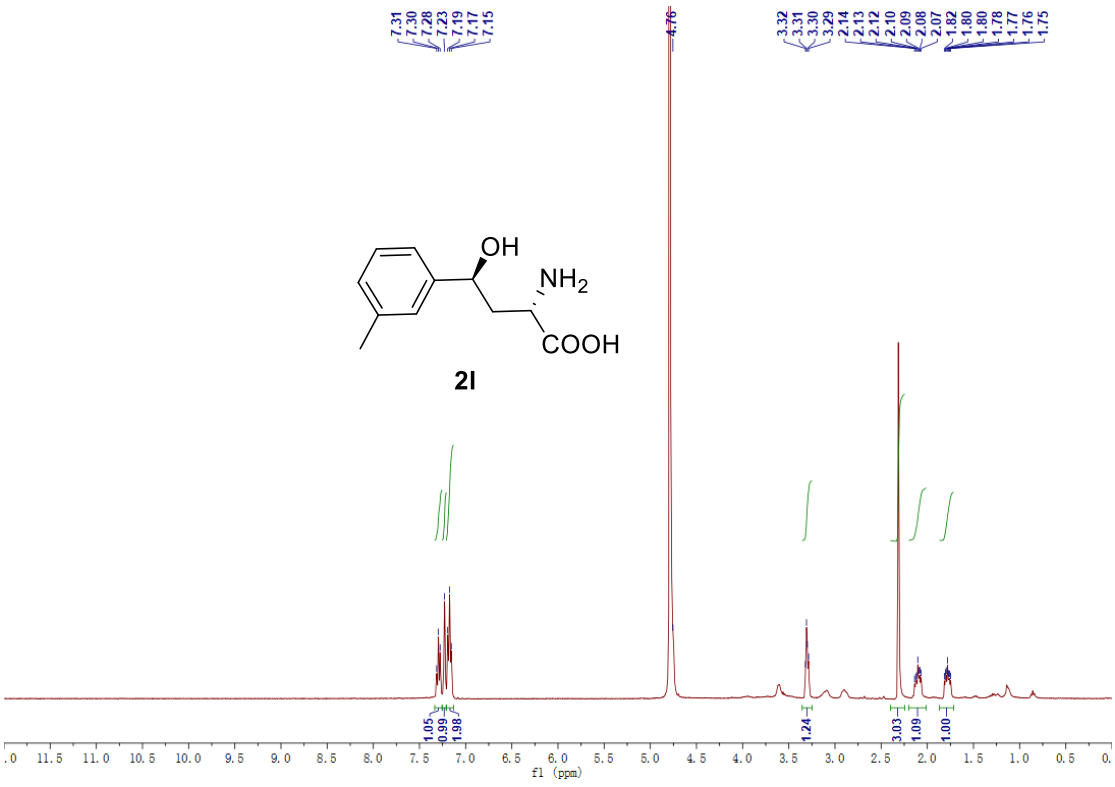

182.6
146.2
130.6
130.4
128.8
124.8
122.0
70.6
53.3
43.0
OH
NH2
Br
COOH
2i
f1 (ppm)

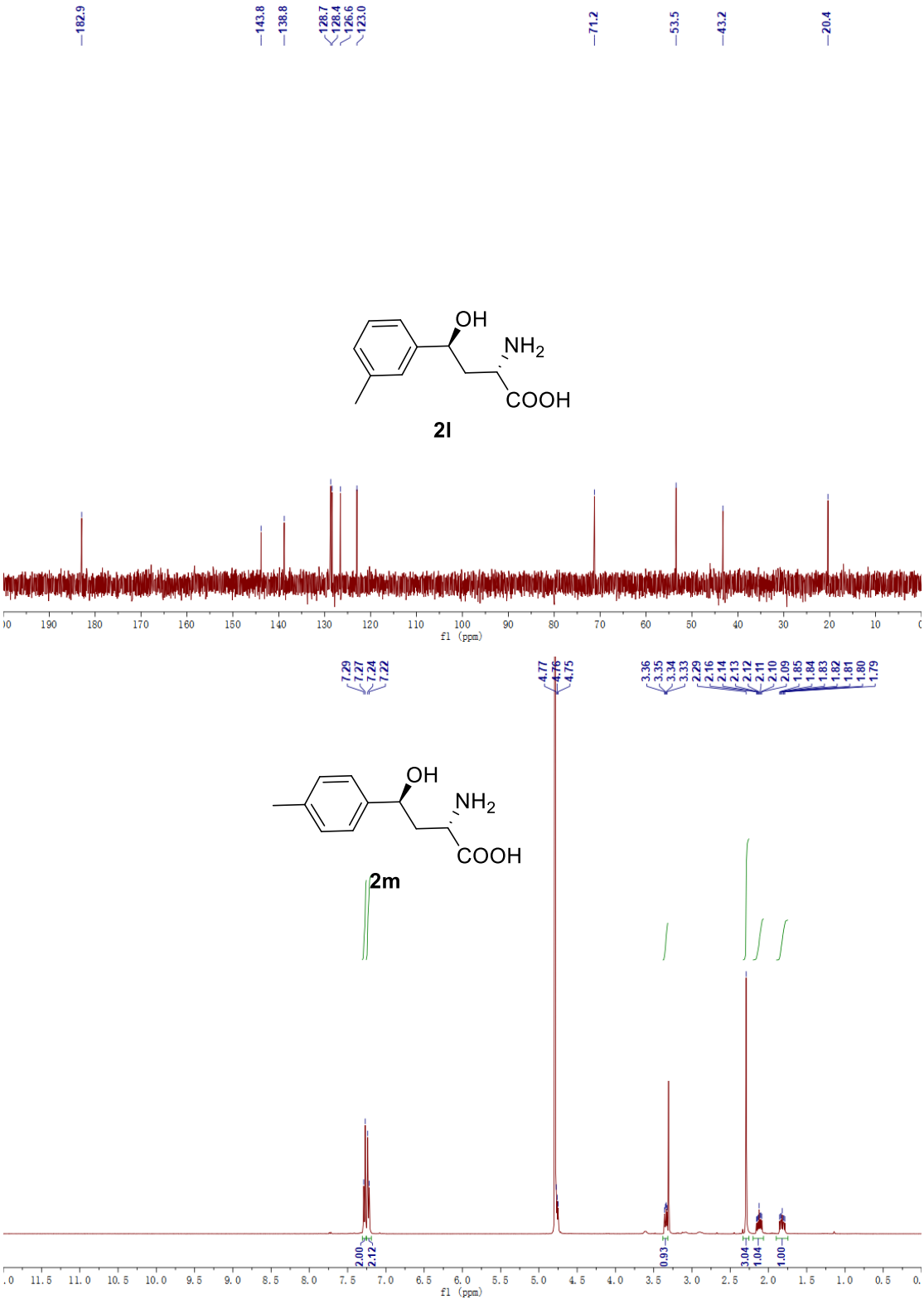

7.55
7.53
7.29
7.29
7.27
4.77
4.76
3.32
3.31
3.31
3.30
3.29
2.12
2.11
2.10
2.09
2.08
2.07
2.05
1.83
1.82
1.81
1.80
1.79
1.78
1.77
OH
NH2
Br
COOH
2j
1.98
2.00
1.32
1.02
1.01
f1 (ppm)

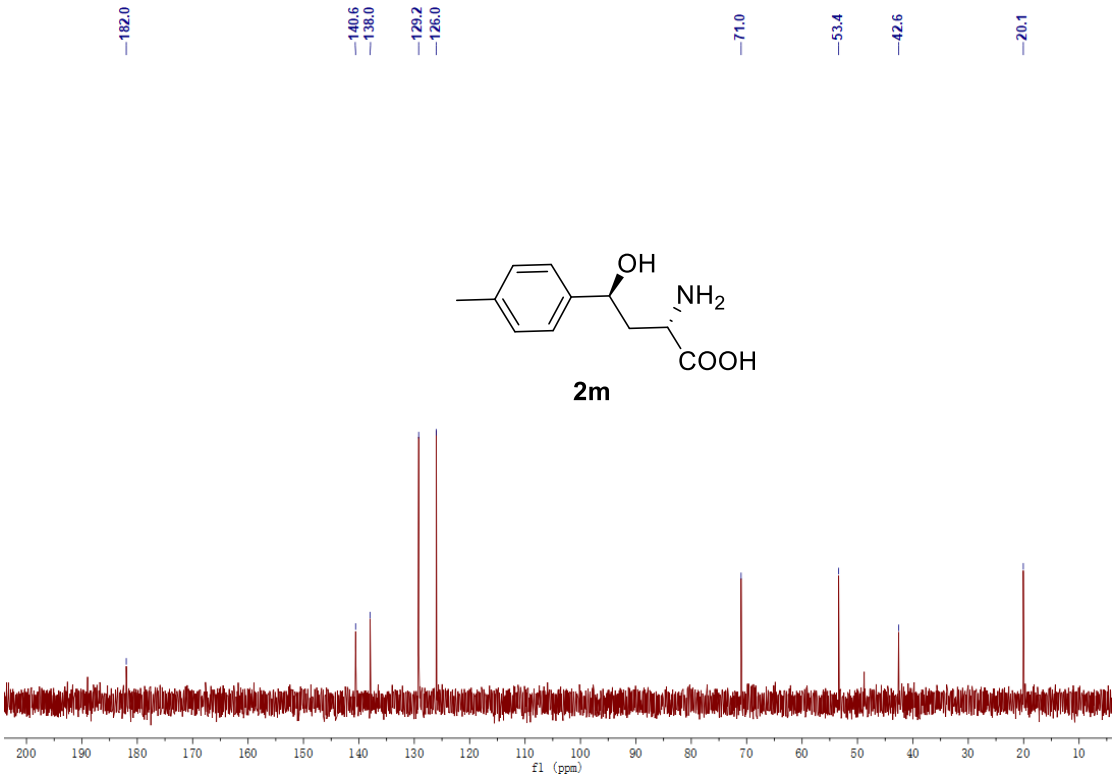

182.4
142.8
131.5
127.9
120.8
70.6
53.3
42.8
Br
OH
NH2
COOH
2j
f1 (ppm)

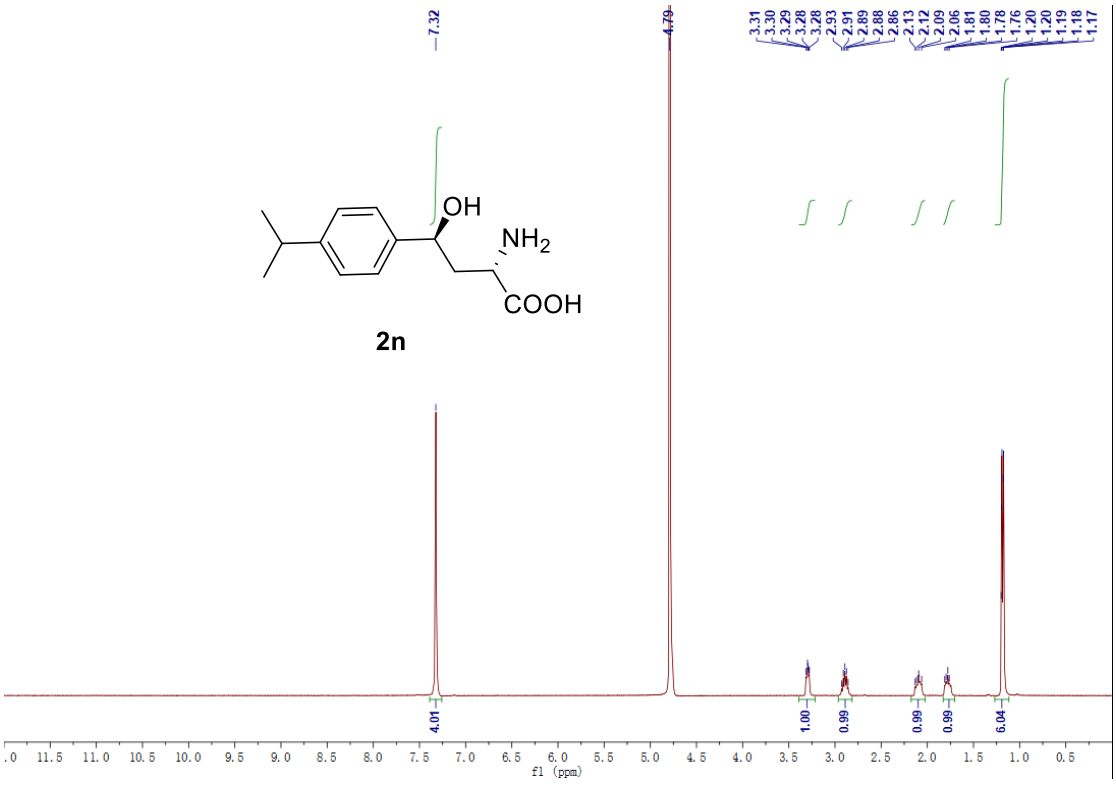

7.46
7.44
7.29
7.28
7.27
7.26
7.25
7.22
7.22
7.21
7.21
7.20
5.11
5.10
5.09
5.08
3.38
3.37
3.36
3.35
2.30
2.08
2.07
2.06
2.05
2.04
2.02
1.80
1.79
1.77
1.76
1.76
1.75
1.74
1.73
OH
NH2
COOH
2k
1.07
1.06
2.12
1.00
0.93
3.21
1.02
0.98
f1 (ppm)

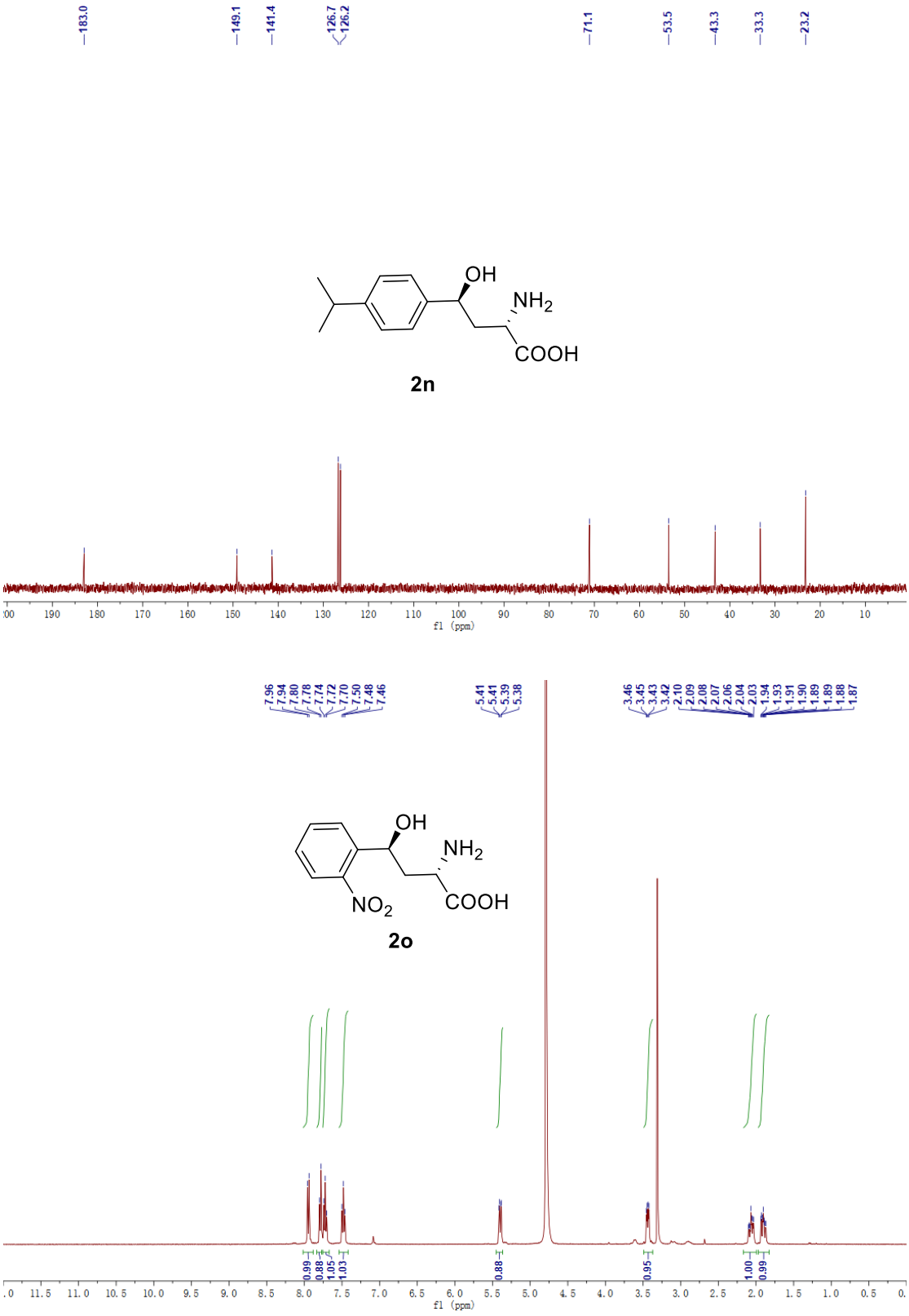

184.4
143.3
136.6
131.9
129.0
127.9
126.6
68.7
55.1
43.6
19.5
OH
NH2
COOH
2k
f1 (ppm)

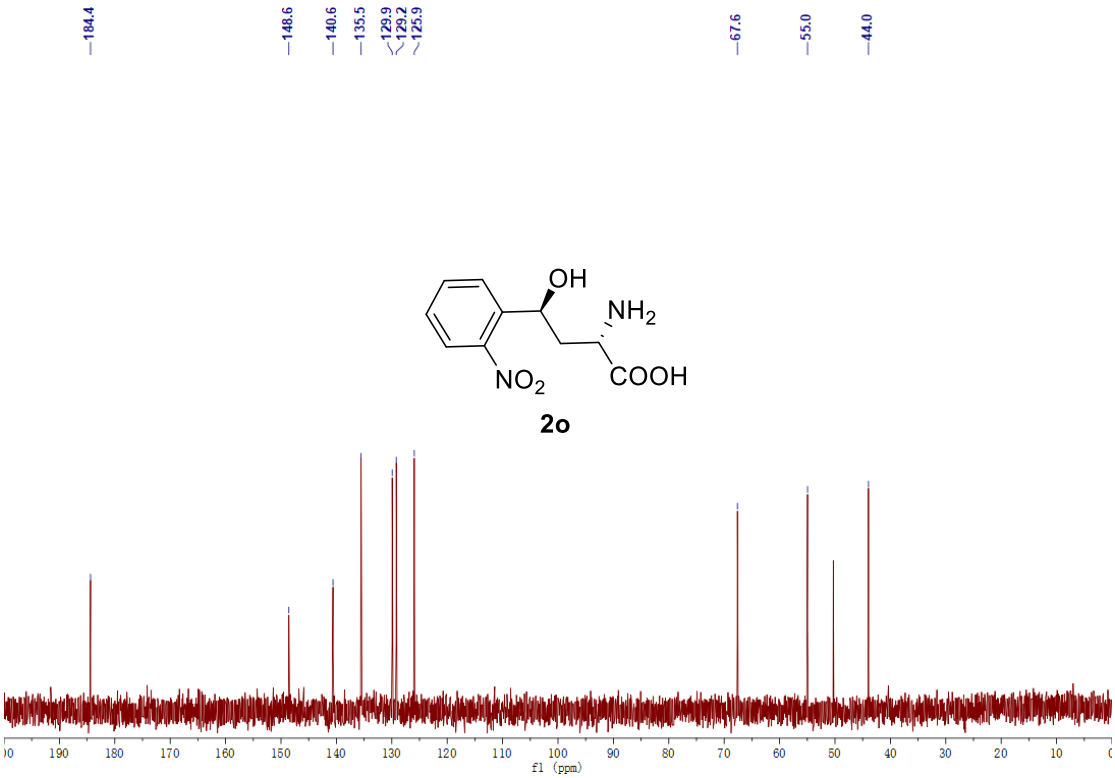

7.31
7.30
7.28
7.23
7.19
7.17
7.15
4.76
3.32
3.31
3.30
3.29
2.14
2.13
2.12
2.10
2.09
2.08
2.07
1.82
1.80
1.80
1.78
1.77
1.76
1.75
OH
NH2
COOH
2l
1.05
0.99
1.98
1.24
3.03
1.09
1.00
f1 (ppm)

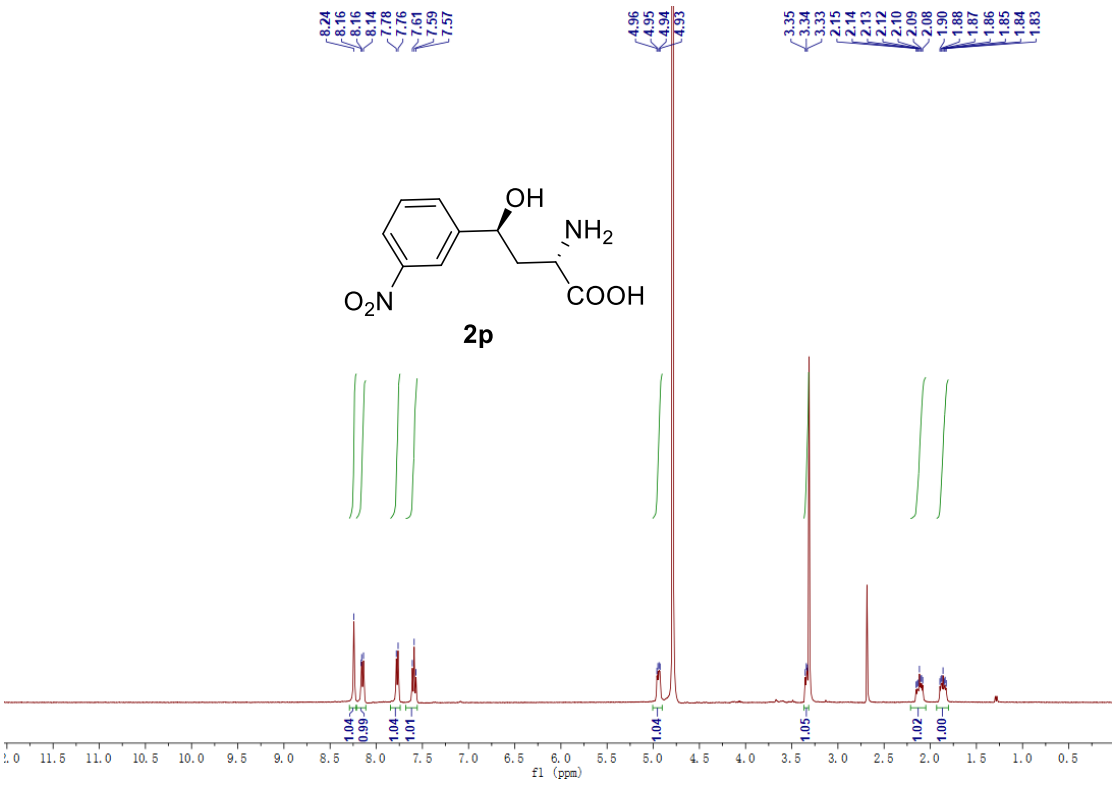

182.9
143.8
138.8
128.7
128.4
126.6
123.0
71.2
53.5
43.2
20.4
OH
NH2
COOH
2l
f1 (ppm)
7.29
7.27
7.24
7.22
4.77
4.76
4.75
3.36
3.35
3.34
3.33
2.29
2.16
2.14
2.13
2.12
2.11
2.10
2.09
1.85
1.84
1.83
1.82
1.81
1.80
1.79
OH
NH2
COOH
2m
2.00
2.12
0.93
3.04
1.04
1.00
f1 (ppm)

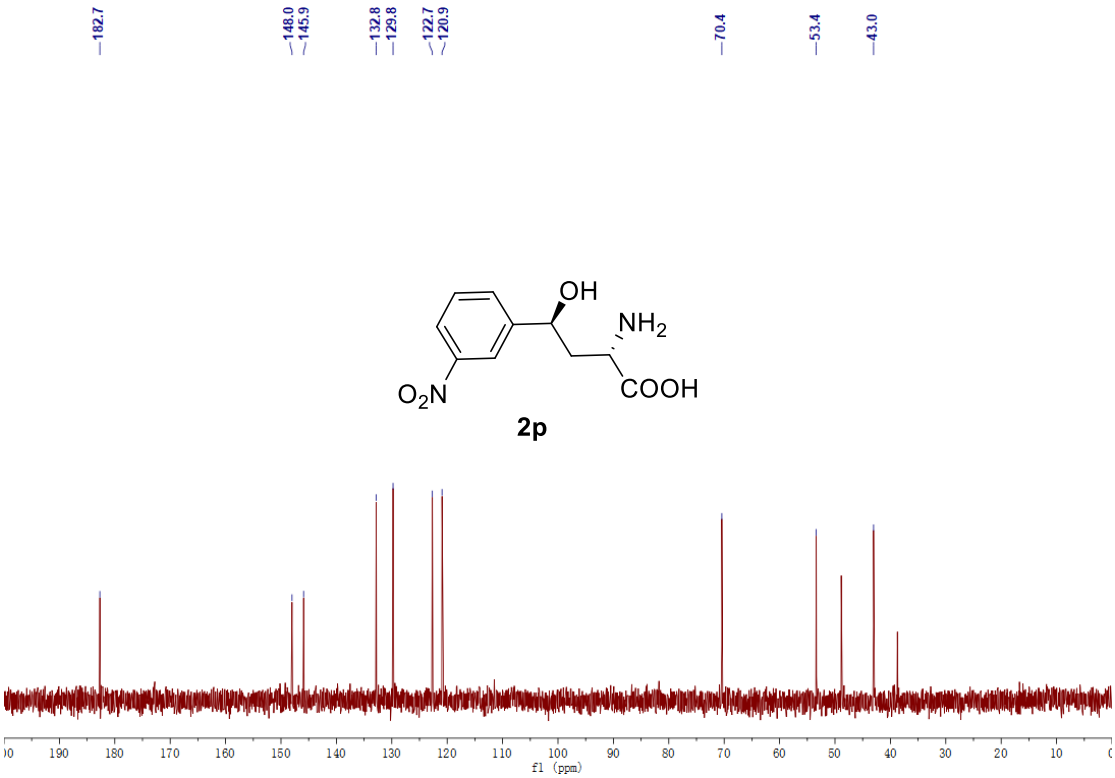

182.0
140.6
138.0
129.2
126.0
71.0
53.4
42.6
20.1
OH
NH2
COOH
2m
f1 (ppm)

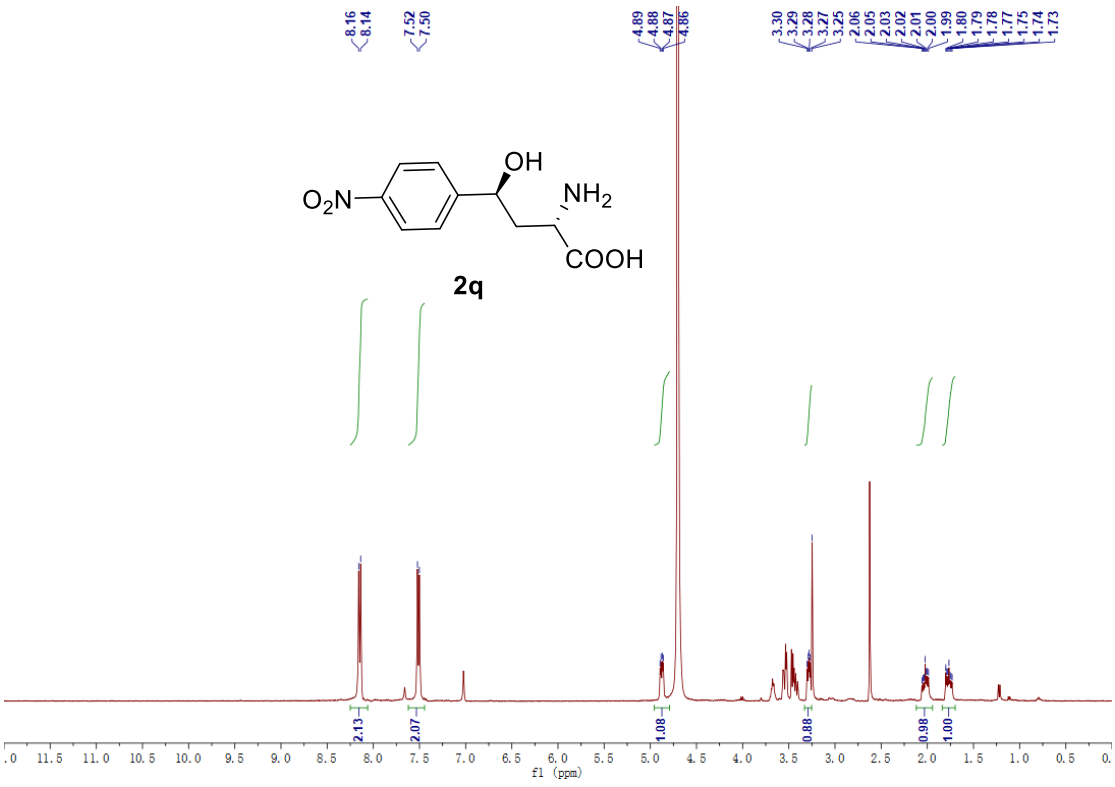

7.32
4.79
3.31
3.30
3.29
3.28
3.26
2.93
2.91
2.89
2.88
2.86
2.13
2.12
2.09
2.06
1.81
1.80
1.78
1.76
1.20
1.20
1.19
1.18
1.17
OH
NH2
COOH
2n
4.01
1.00
0.99
0.99
0.99
6.04
f1 (ppm)

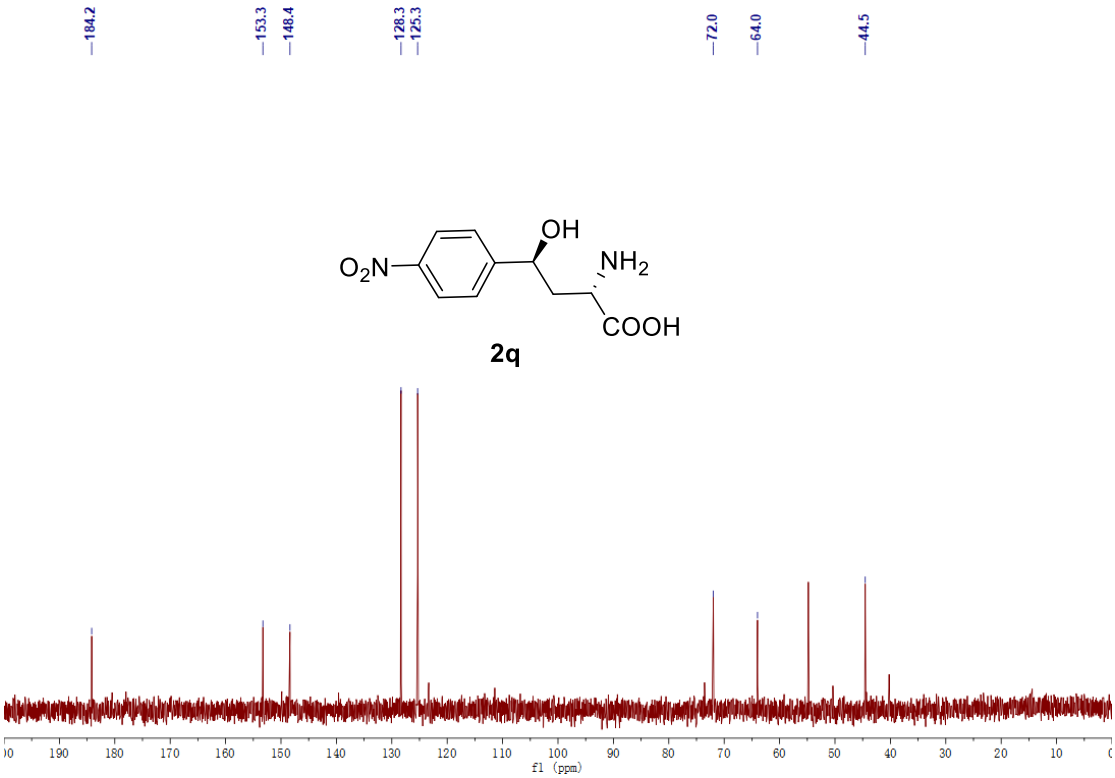

183.0
149.1
141.4
126.7
126.2
71.1
53.5
43.3
33.3
23.2
OH
NH2
COOH
2n
f1 (ppm)
7.96
7.94
7.80
7.78
7.74
7.72
7.70
7.50
7.48
7.46
5.41
5.41
5.39
5.38
3.46
3.45
3.43
3.42
2.10
2.09
2.08
2.07
2.06
2.04
2.03
1.94
1.93
1.91
1.90
1.89
1.89
1.88
1.87
OH
NH2
NO2
COOH
2o
0.99
0.88
1.05
1.03
0.88
0.95
1.00
0.99
f1 (ppm)

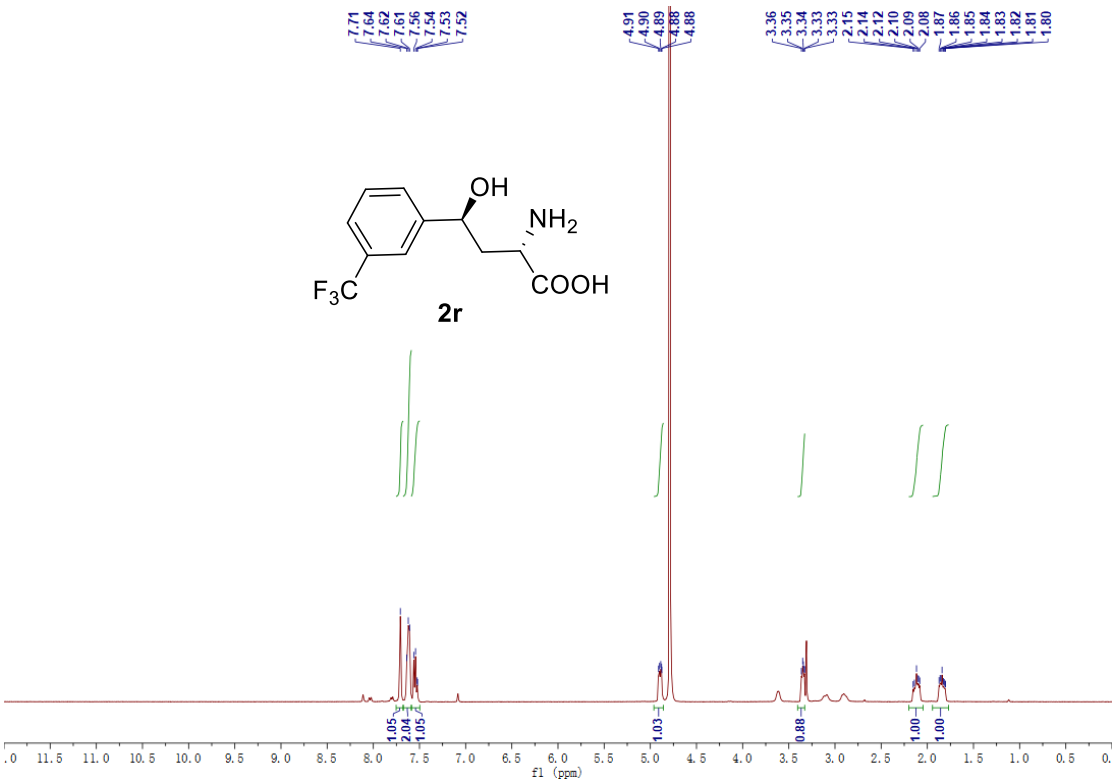

184.4
148.6
140.6
135.5
129.9
129.2
125.9
67.6
55.0
44.0
OH
NH2
NO2
COOH
2o
f1 (ppm)

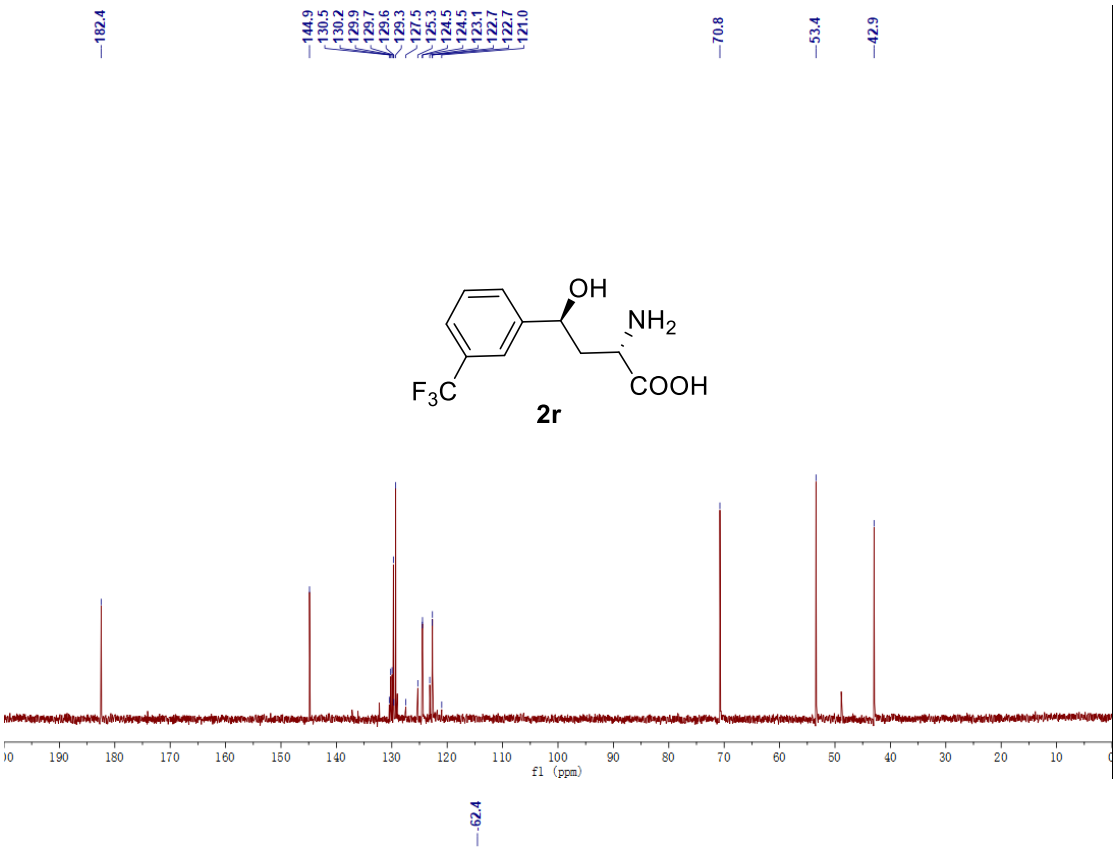

8.24
8.16
8.16
8.14
7.78
7.76
7.61
7.59
7.57
4.96
4.95
4.94
4.93
3.35
3.34
3.33
2.15
2.14
2.13
2.12
2.10
2.09
2.08
1.90
1.88
1.87
1.86
1.85
1.84
1.83
OH
NH2
O2N
COOH
2p
1.04
0.99
1.04
1.01
1.04
1.05
1.02
1.00
f1 (ppm)

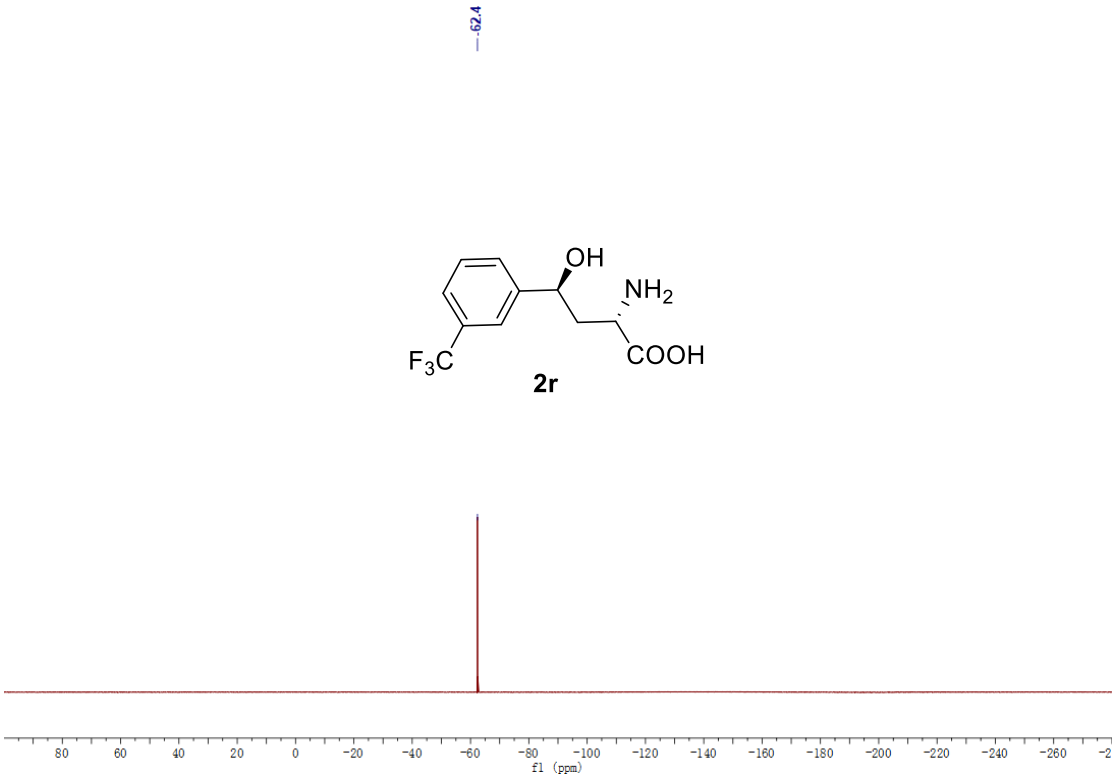

182.7
148.0
145.9
132.8
129.8
122.7
120.9
70.4
53.4
43.0
OH
NH2
O2N
COOH
2p
f1 (ppm)

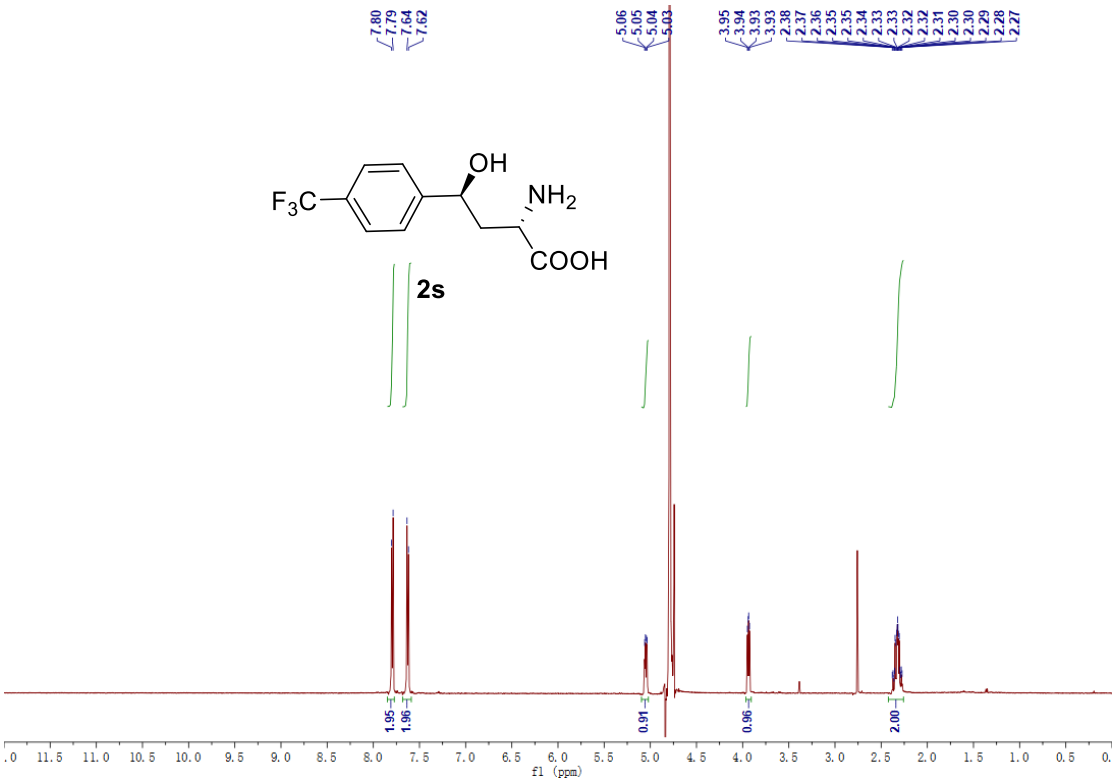

8.16
8.14
7.52
7.50
4.89
4.88
4.87
4.86
3.30
3.29
3.28
3.27
3.25
2.06
2.05
2.03
2.02
2.01
2.00
1.99
1.80
1.79
1.78
1.77
1.75
1.74
1.73
OH
NH2
O2N
COOH
2q
2.13
2.07
1.08
0.88
0.98
1.00
f1 (ppm)

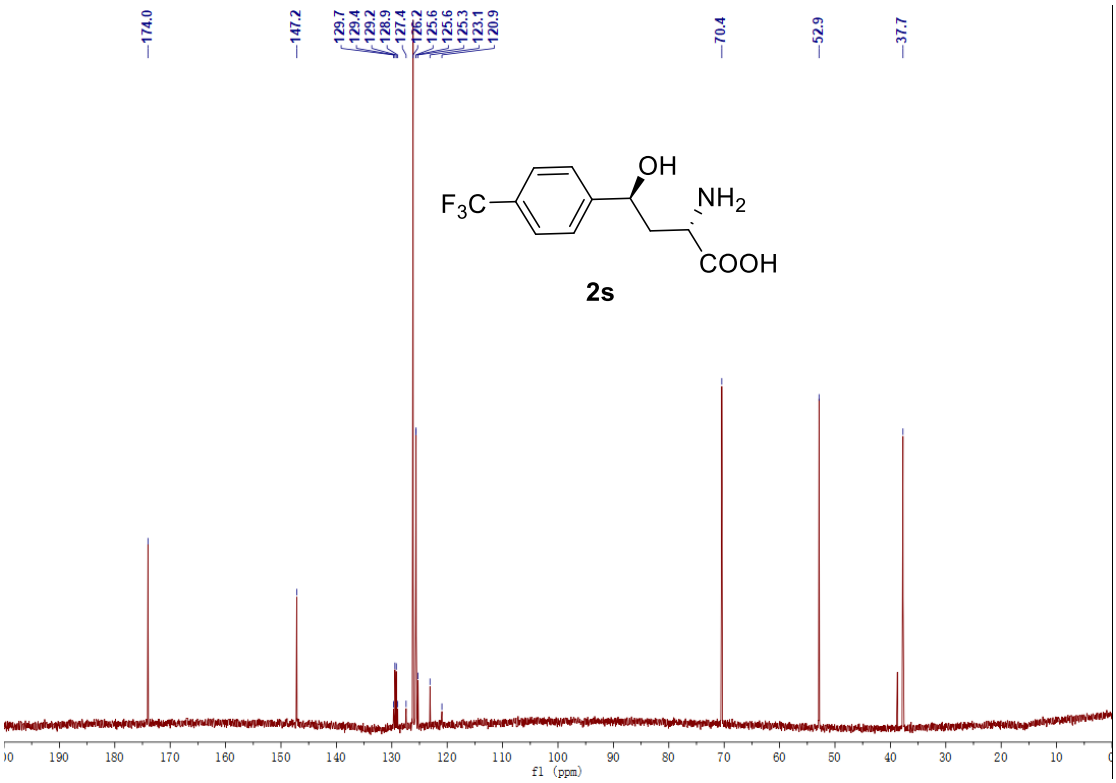

184.2
153.3
148.4
128.3
125.3
72.0
64.0
44.5
OH
O_2N
NH_2
COOH
2q
f1 (ppm)

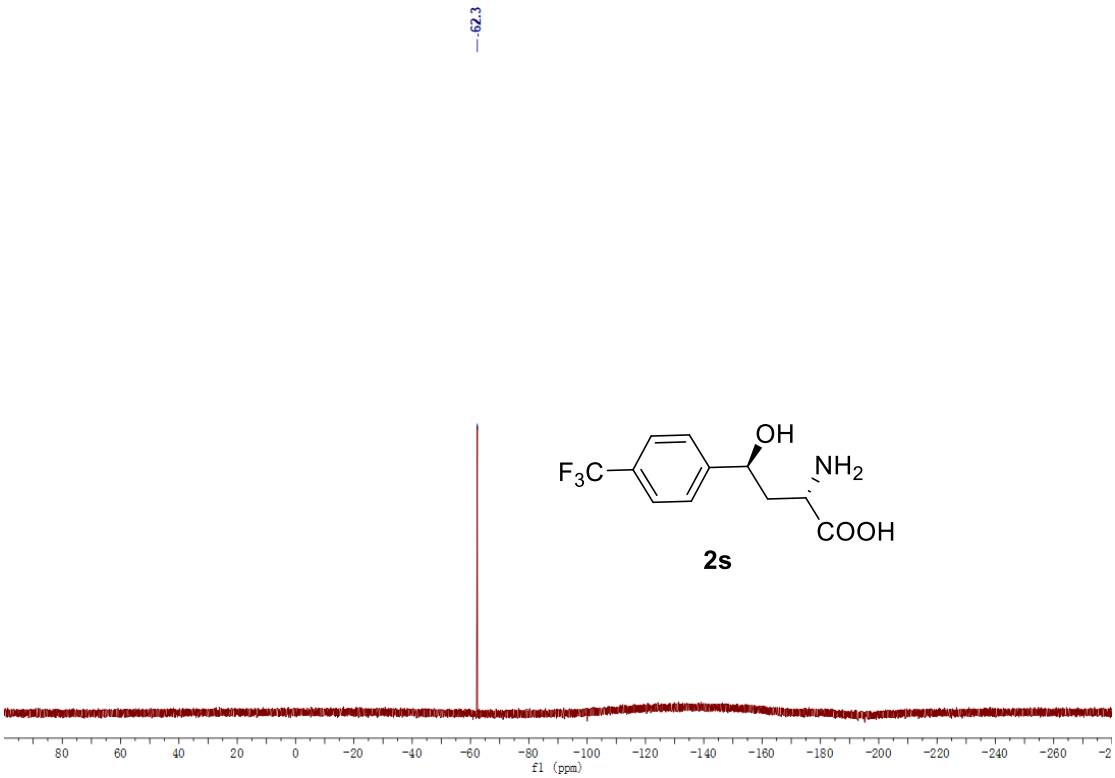

7.71
7.64
7.62
7.61
7.56
7.54
7.53
7.52
4.91
4.90
4.89
4.88
4.88
3.36
3.35
3.34
3.33
3.33
2.15
2.14
2.12
2.10
2.09
2.08
1.87
1.86
1.85
1.84
1.83
1.82
1.81
1.80
OH
NH_2
F_3C
COOH
2r
1.05
2.04
1.05
1.03
0.88
1.00
1.00
f1 (ppm)

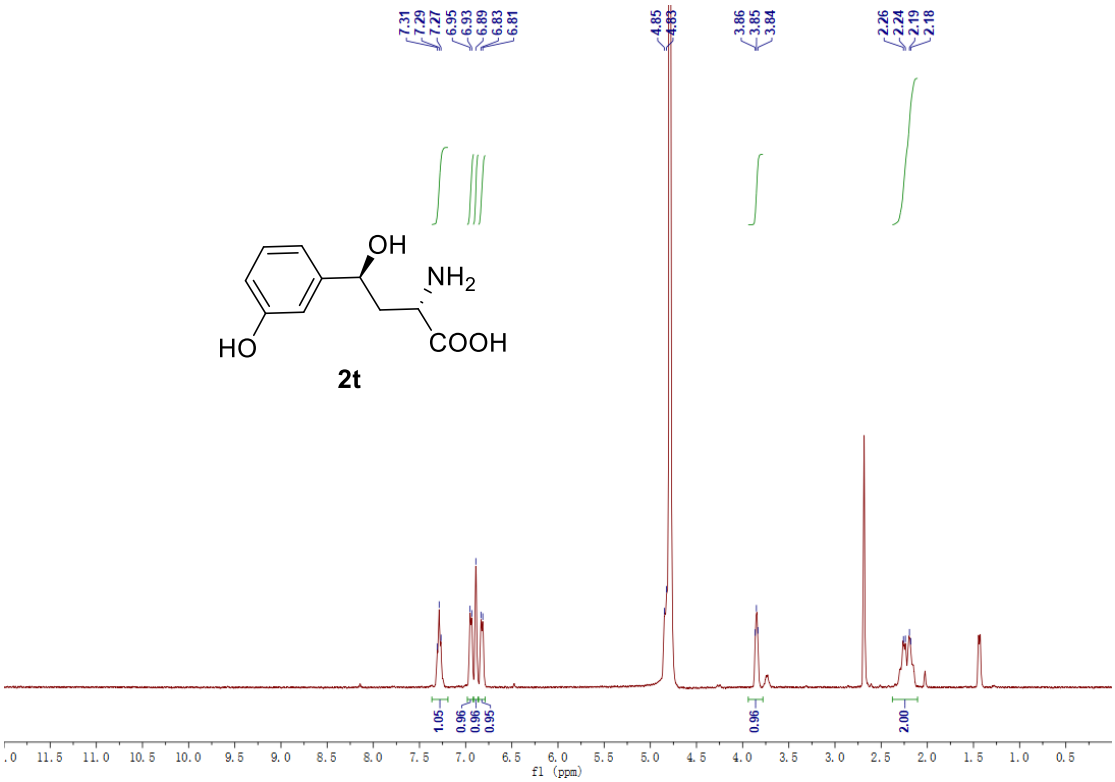

182.4
144.9
130.5
130.2
129.9
129.7
129.6
129.3
127.5
125.3
124.5
124.5
123.1
122.7
122.7
121.0
70.8
53.4
42.9
OH
NH2
F3C
COOH
2r
f1 (ppm)

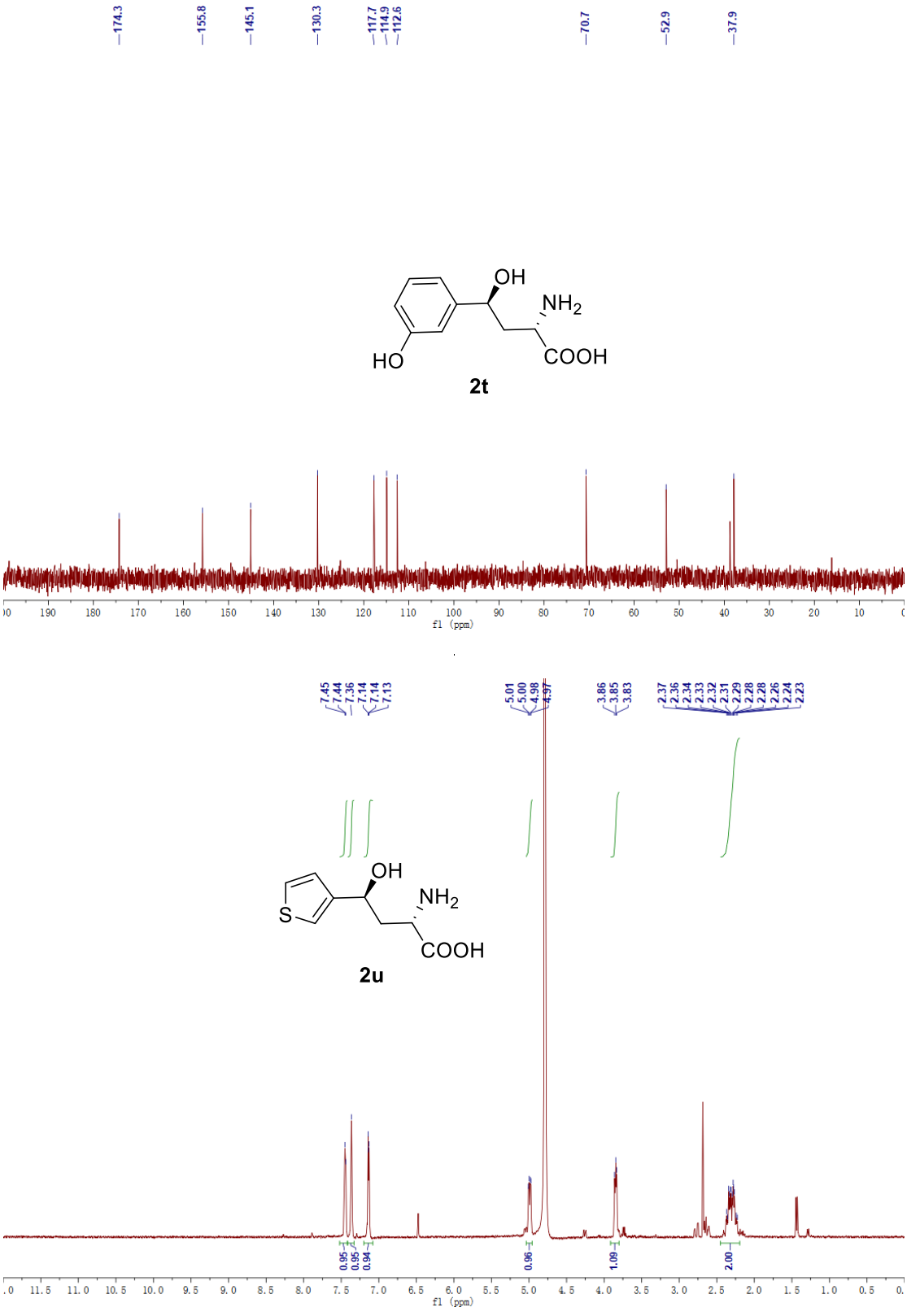

62.4
OH
NH2
F3C
COOH
2r
f1 (ppm)

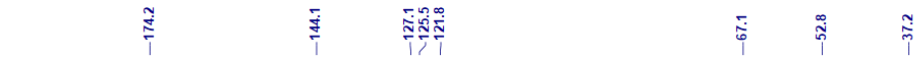

7.80
7.79
7.64
7.62
5.06
5.05
5.04
5.03
3.95
3.94
3.93
3.93
2.38
2.37
2.36
2.35
2.35
2.34
2.33
2.33
2.32
2.32
2.31
2.30
2.30
2.29
2.28
2.27
OH
NH2
F3C
COOH
2s
1.95
1.96
0.91
0.96
2.00
f1 (ppm)

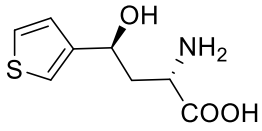

174.0
147.2
129.7
129.4
129.2
128.9
127.4
126.2
125.6
125.6
125.3
123.1
120.9
70.4
52.9
37.7
OH
NH2
F3C
COOH
2s
f1 (ppm)


-62.3
OH
NH2
F3C
COOH
2s
80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -2
f1 (ppm)

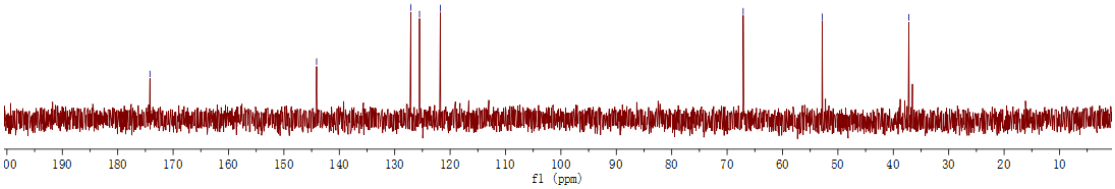

7.31
7.29
7.27
6.95
6.93
6.89
6.83
6.81
4.85
4.83
3.86
3.85
3.84
2.26
2.24
2.19
2.18
OH
NH2
HO
COOH
2t
1.05
0.96
0.96
0.95
0.96
2.00
.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)


174.3
155.8
145.1
130.3
117.7
114.9
112.6
70.7
52.9
37.9
OH
NH2
HO
COOH
2t
f1 (ppm)
7.45
7.44
7.36
7.14
7.14
7.13
5.01
5.00
4.98
4.97
3.86
3.85
3.83
2.37
2.36
2.34
2.33
2.32
2.31
2.29
2.28
2.28
2.26
2.24
2.23
OH
NH2
S
COOH
2u
0.95
0.95
0.94
0.96
1.09
2.00
f1 (ppm)

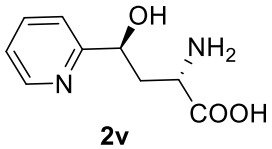

174.2
144.1
127.1
125.5
121.8
67.1
52.8
37.2


OH
NH2
S
COOH

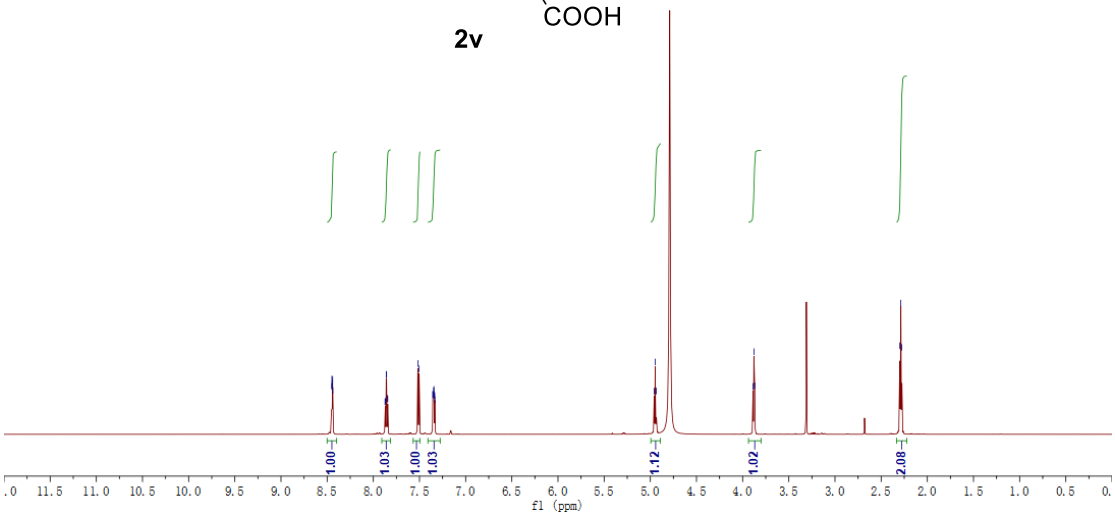
2u

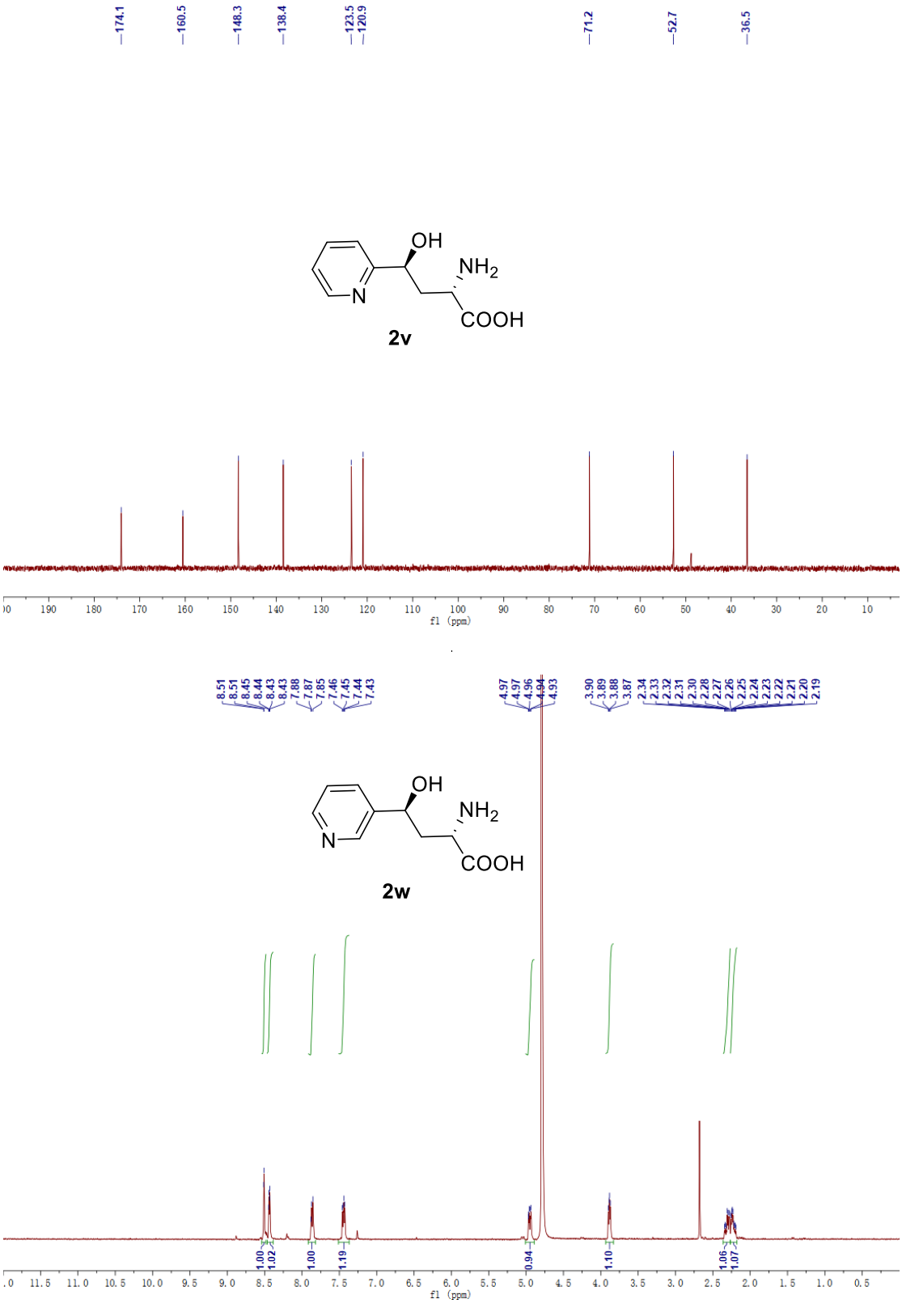

f1 (ppm)

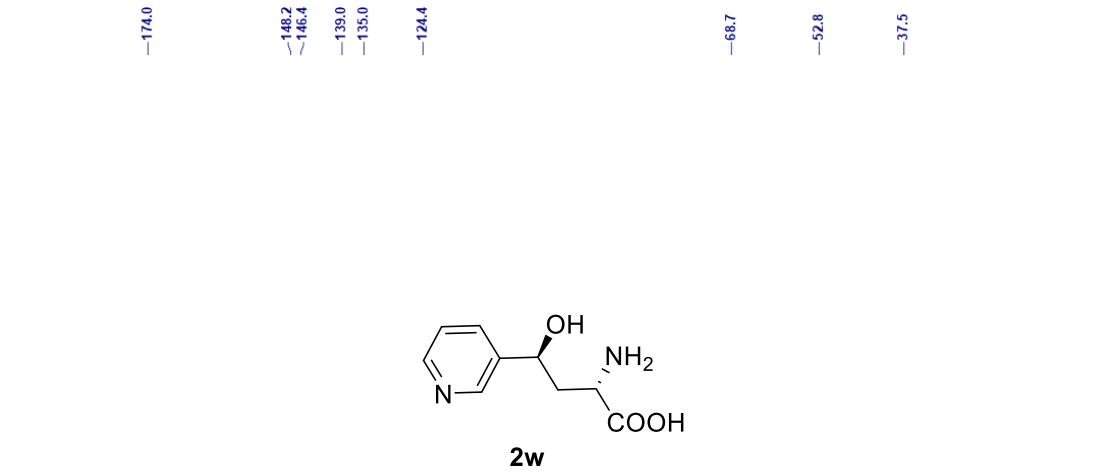

8.45
8.45
8.45
8.44
8.44
8.44
7.87
7.87
7.86
7.86
7.85
7.84
7.52
7.50
7.36
7.35
7.35
7.34
7.34
7.33
7.33
4.96
4.95
4.94
3.89
3.88
3.87
2.30
2.29
2.28

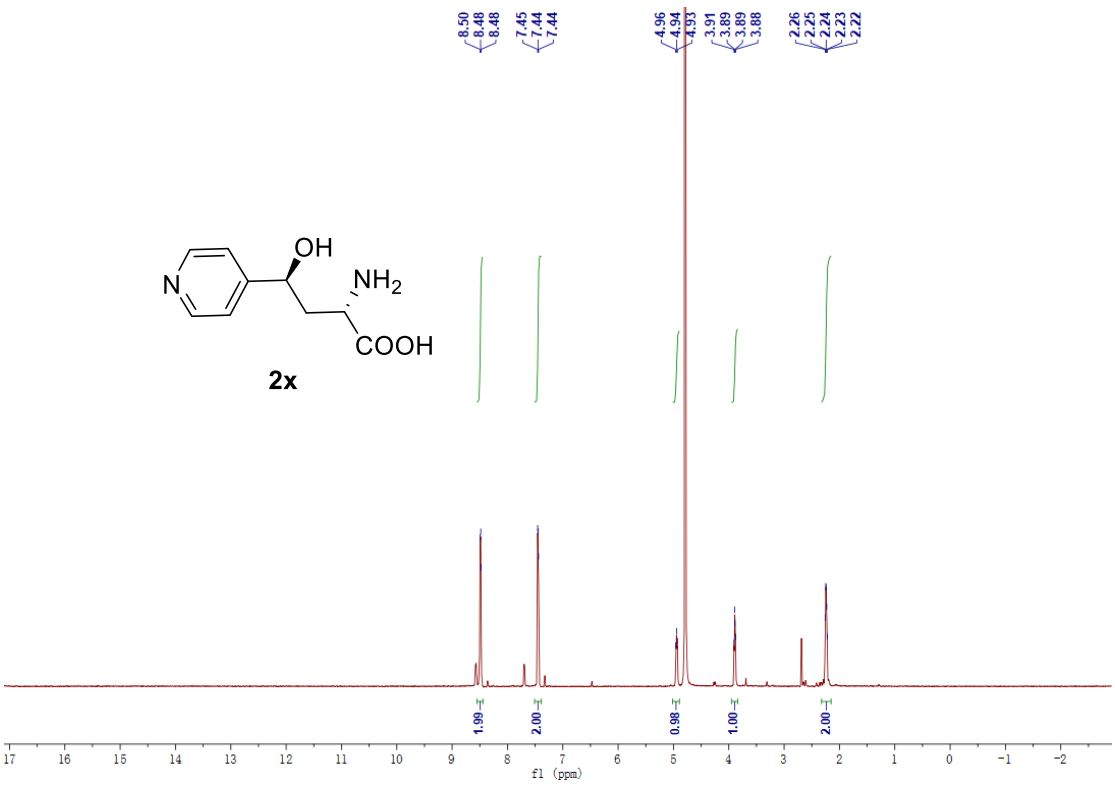

OH
NH2
N
COOH

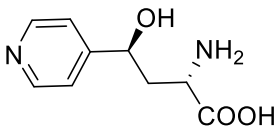
2v

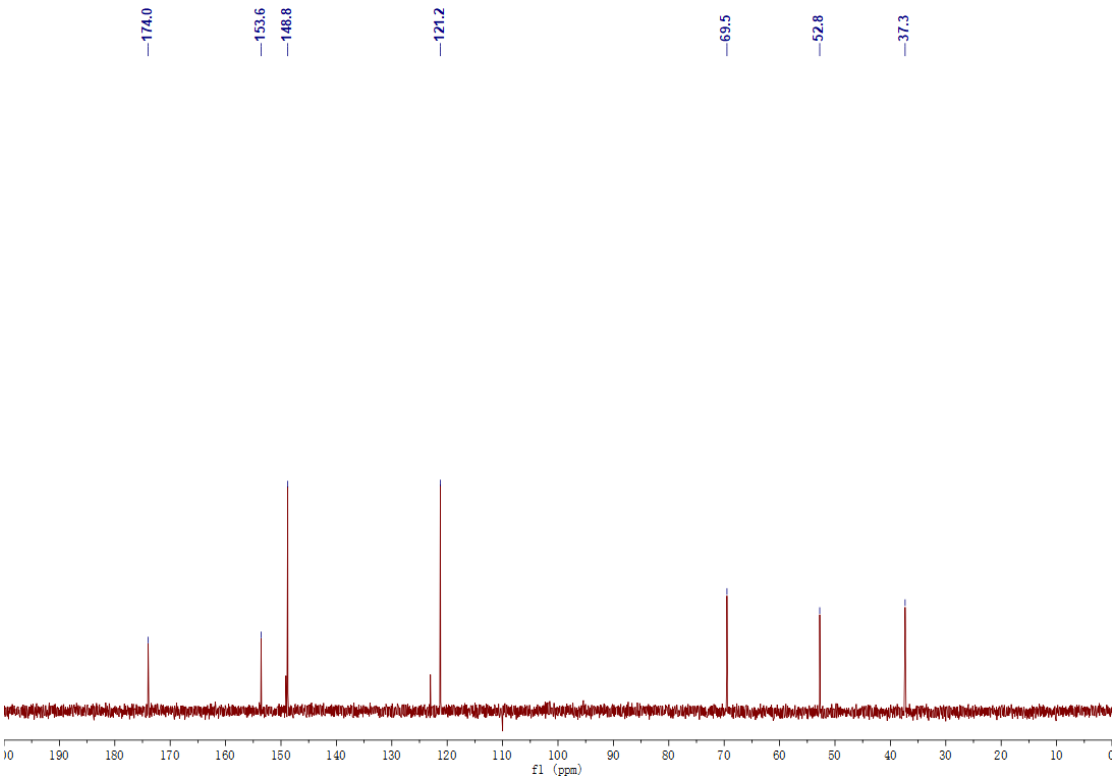

1.00
1.03
1.00
1.03
1.12
1.02
2.08
f1 (ppm)

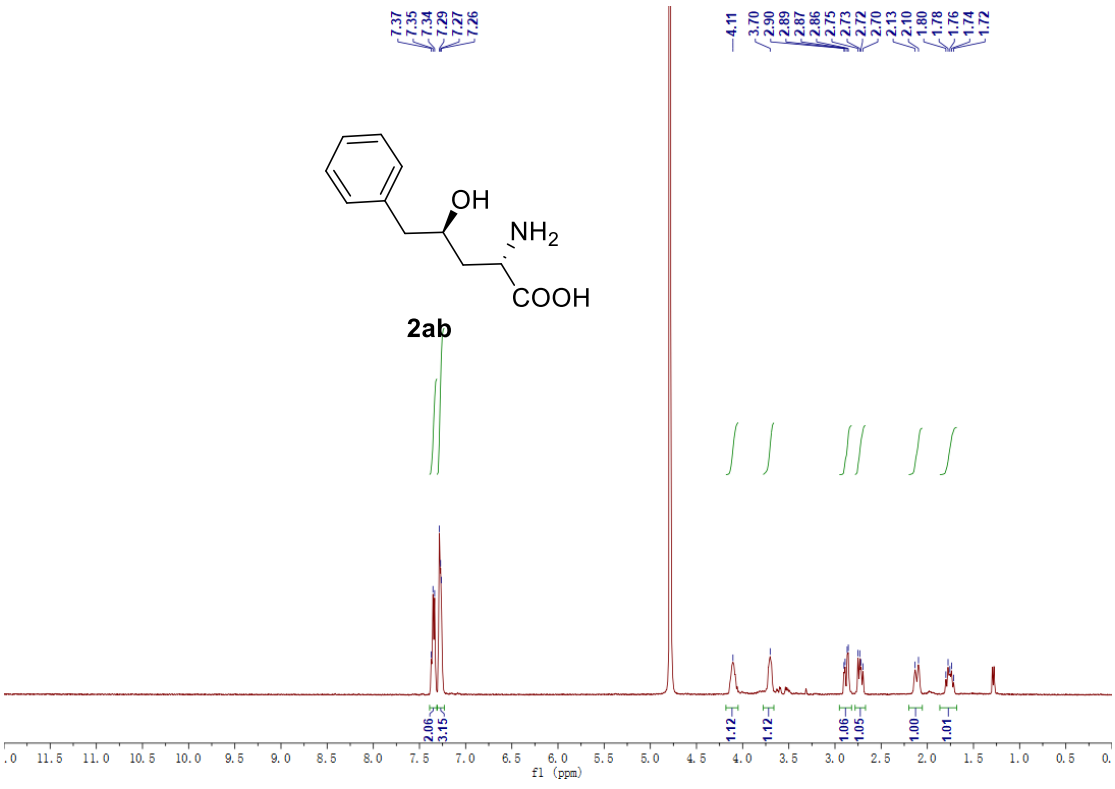

174.1
160.5
148.3
138.4
123.5
120.9
71.2
52.7
36.5
OH
NH2
N
COOH
2v
f1 (ppm)
8.51
8.51
8.45
8.44
8.43
8.43
7.88
7.87
7.85
7.46
7.45
7.44
7.43
4.97
4.97
4.96
4.94
4.93
3.90
3.89
3.88
3.87
2.34
2.33
2.32
2.31
2.30
2.28
2.27
2.26
2.25
2.24
2.23
2.22
2.21
2.20
2.19
OH
NH2
N
COOH
2w
1.00
1.02
1.00
1.19
0.94
1.10
1.06
1.07
f1 (ppm)

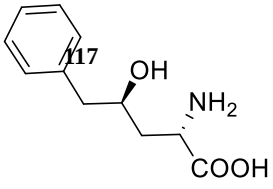

174.0
148.2
146.4
139.0
135.0
124.4
68.7
52.8
37.5
OH
NH2
N
COOH
2w
f1 (ppm)


8.50
8.48
8.48
7.45
7.44
7.44
4.96
4.94
4.93
3.91
3.89
3.89
3.88
2.26
2.25
2.24
2.23
2.22
OH
NH2
N
COOH
2x
1.99
2.00
0.98
1.00
2.00
f1 (ppm)

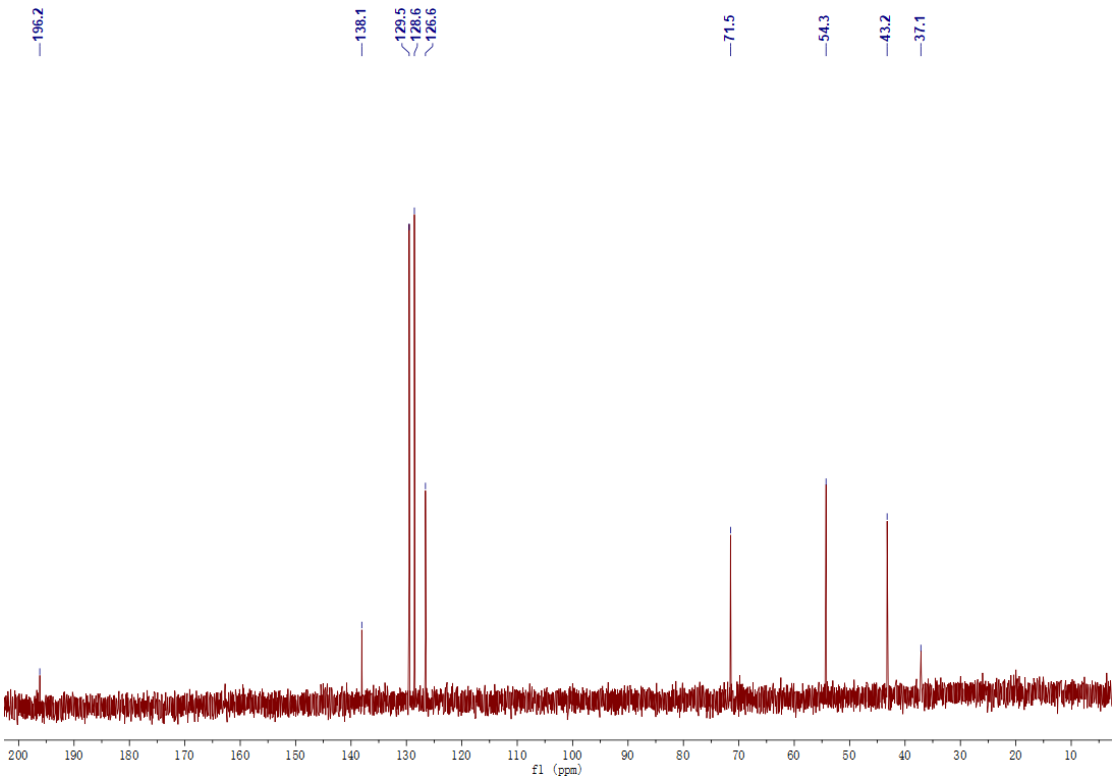

OH
NH2
N
COOH

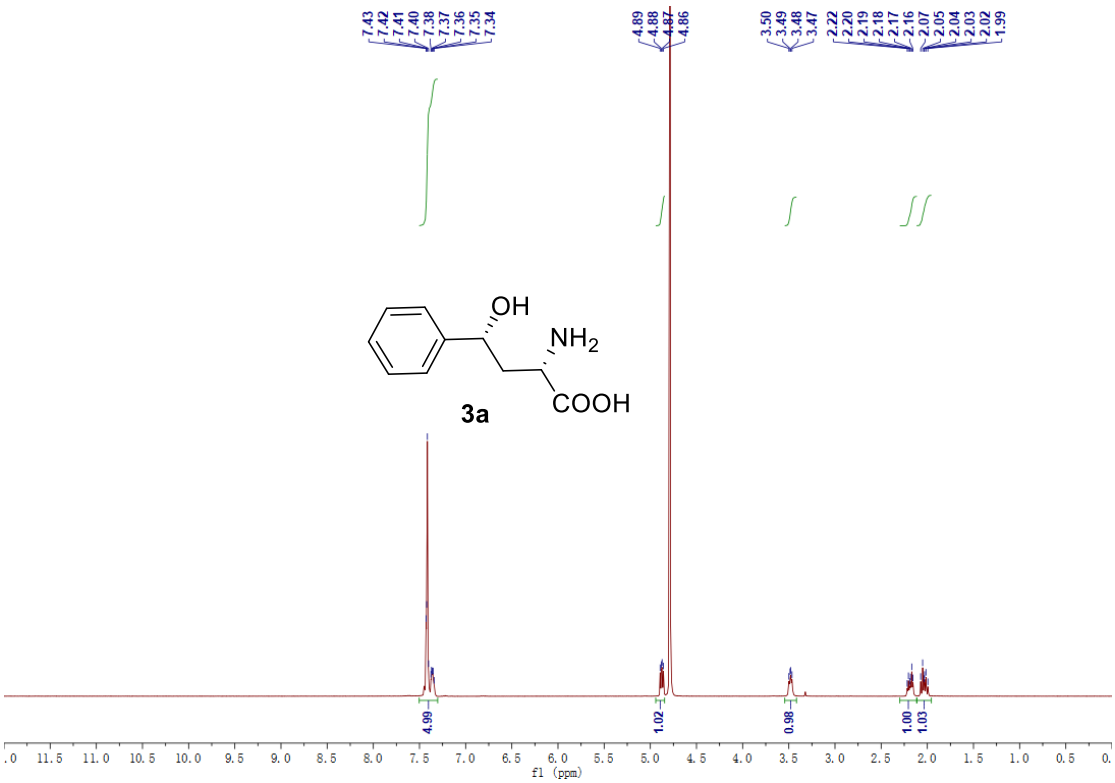

174.0
153.6
148.8
121.2
69.5
52.8
37.3
f1 (ppm)

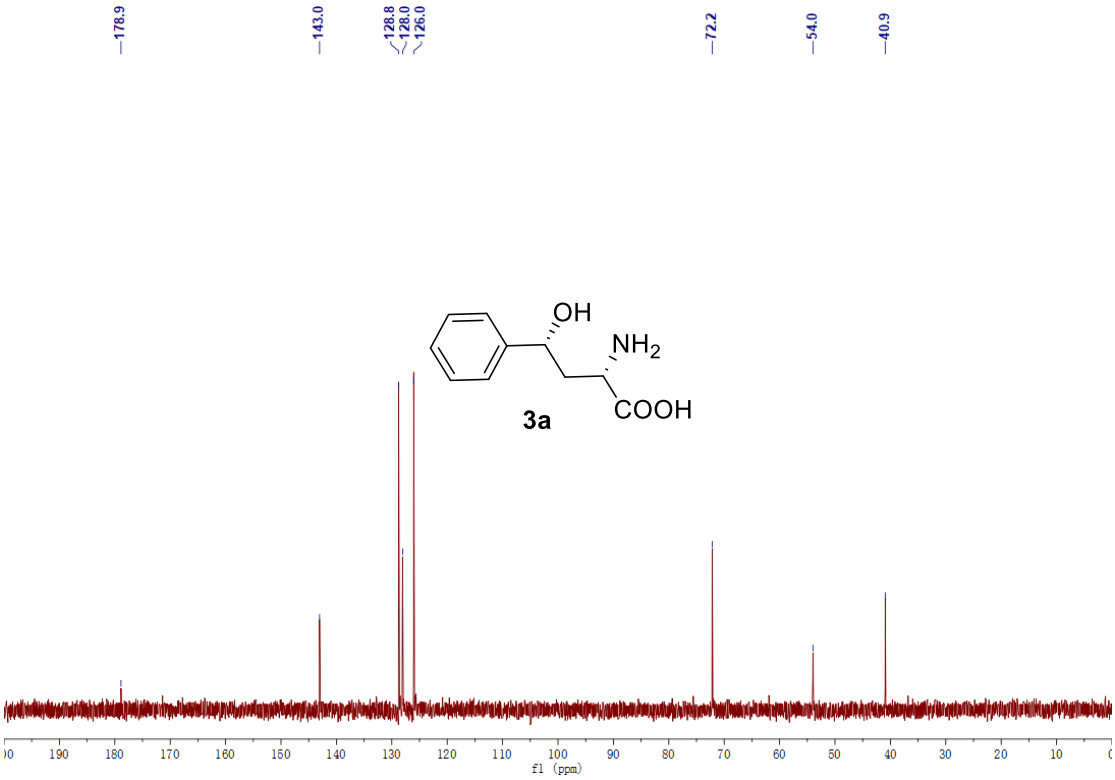

7.37
7.35
7.34
7.29
7.27
7.26
4.11
3.70
2.90
2.89
2.87
2.86
2.75
2.73
2.72
2.70
2.13
2.10
1.80
1.78
1.76
1.74
1.72
OH
NH2
COOH
2ab
2.06
3.15
1.12
1.12
1.06
1.05
1.00
1.01
f1 (ppm)

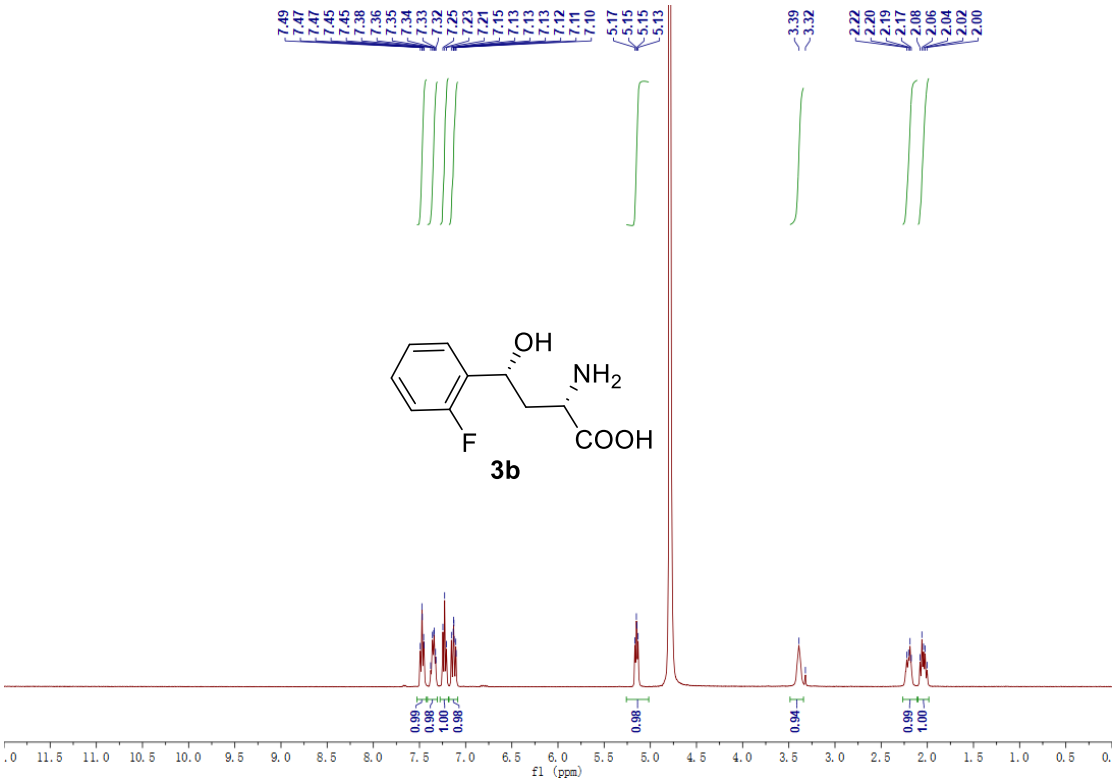

117
OH
NH2
COOH

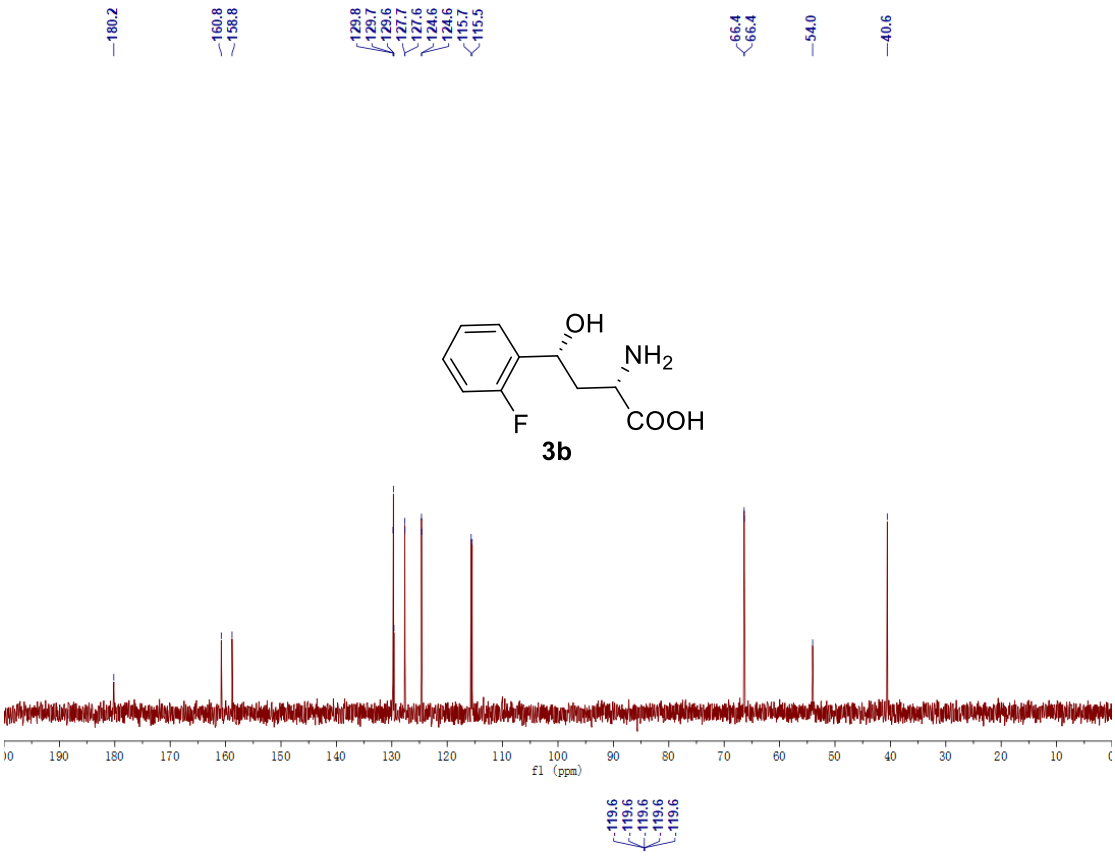
2ab

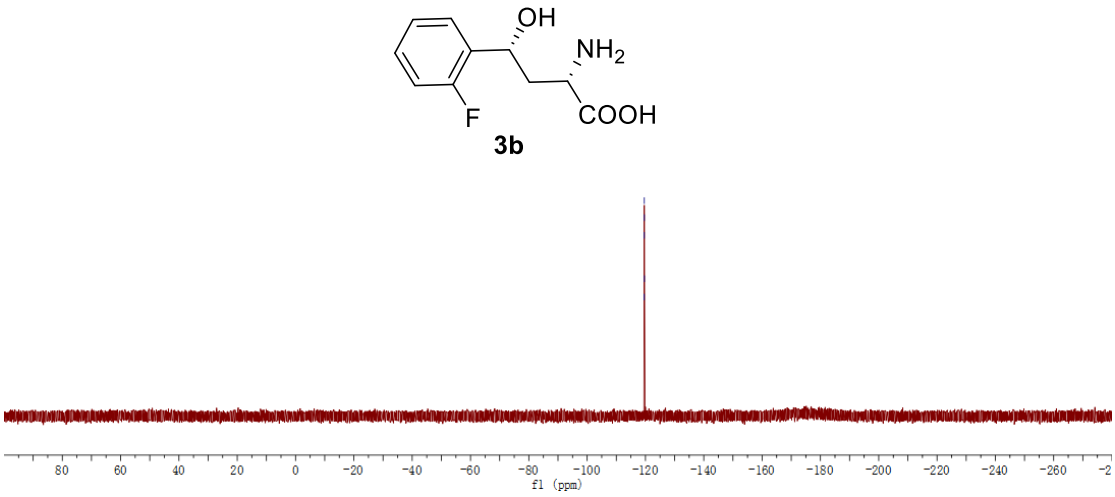

196.2
138.1
129.5
128.6
126.6
71.5
54.3
43.2
37.1
f1 (ppm)

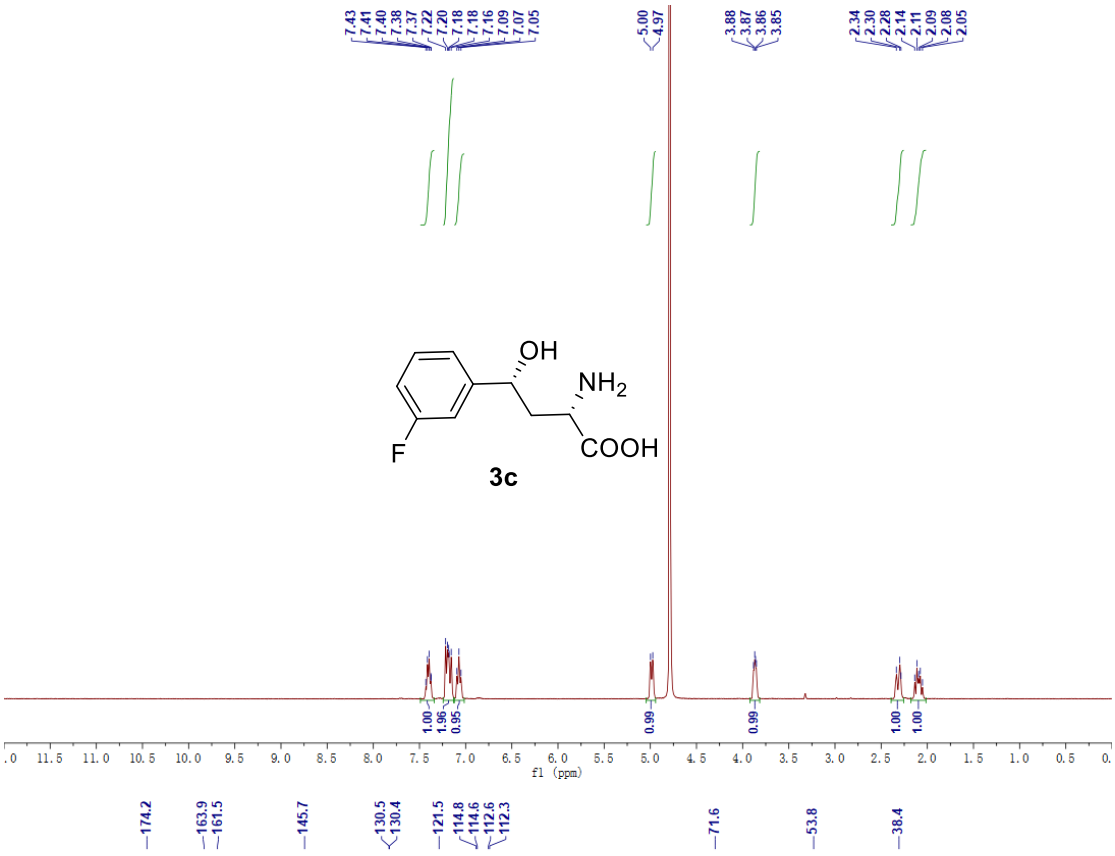

7.43
7.42
7.41
7.40
7.38
7.37
7.36
7.35
7.34
4.89
4.88
4.87
4.86
3.50
3.49
3.48
3.47
2.22
2.20
2.19
2.18
2.17
2.16
2.07
2.05
2.04
2.03
2.02
1.99
OH
NH2
COOH
3a
4.99
1.02
0.98
1.00
1.03
f1 (ppm)

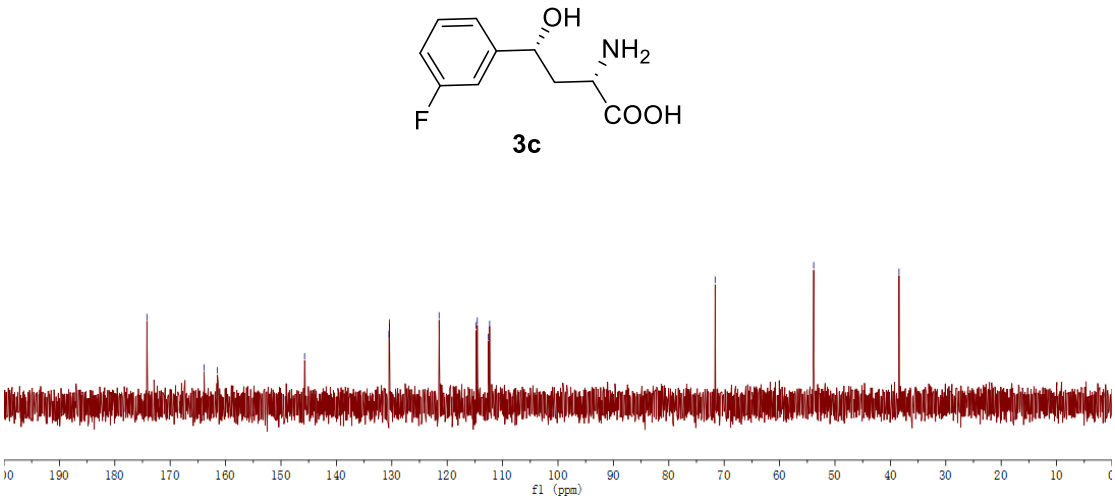

178.9
143.0
128.8
128.0
126.0
72.2
54.0
40.9
OH
NH2
COOH
3a
f1 (ppm)

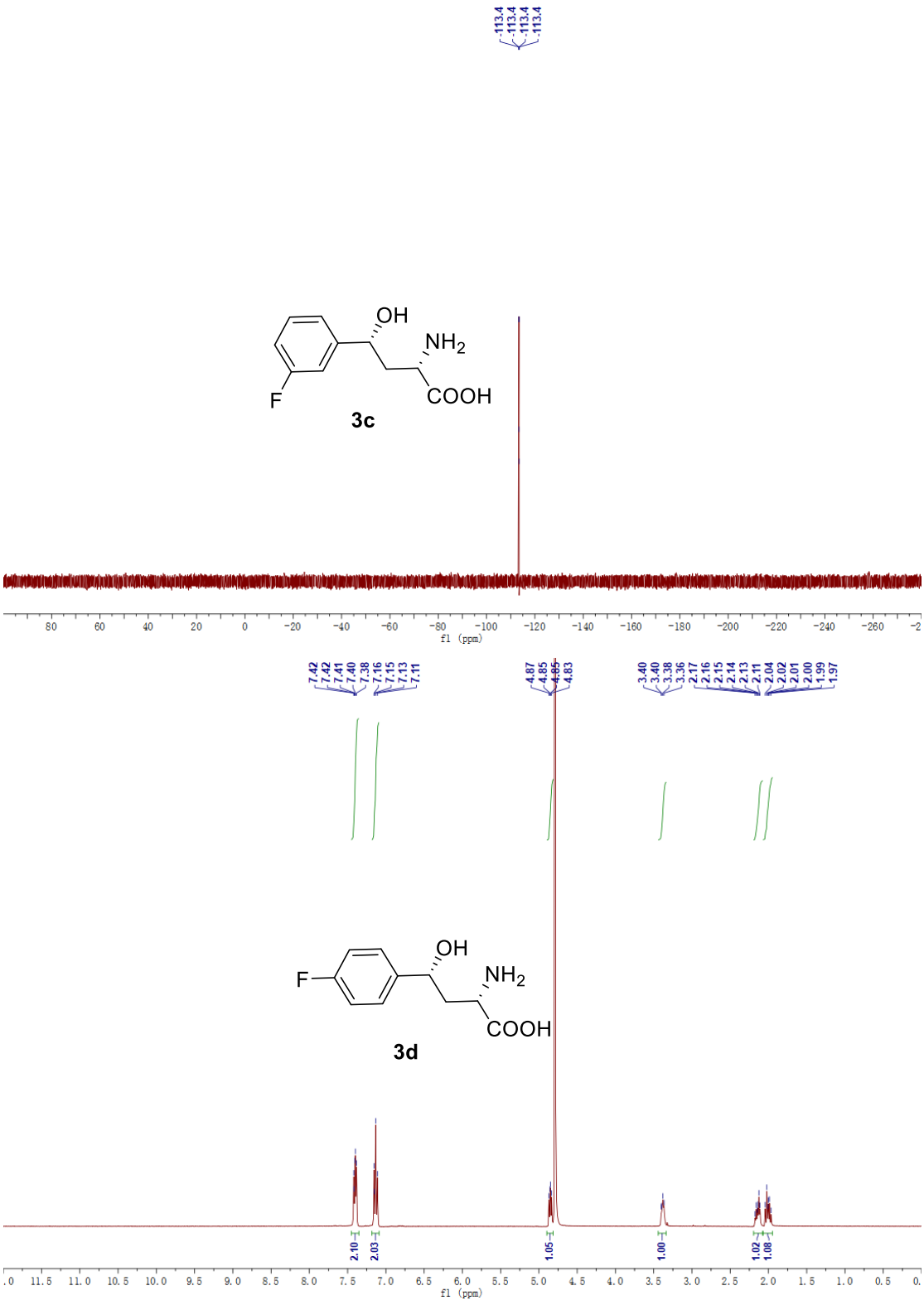

7.49
7.47
7.47
7.45
7.45
7.38
7.36
7.35
7.34
7.33
7.32
7.25
7.23
7.21
7.15
7.13
7.13
7.13
7.12
7.11
7.10
5.17
5.15
5.15
5.13
3.39
3.32
2.22
2.20
2.19
2.17
2.08
2.06
2.04
2.02
2.00
OH
NH2
F
COOH
3b
0.99
0.98
1.00
0.98
0.98
0.94
0.99
1.00
f1 (ppm)

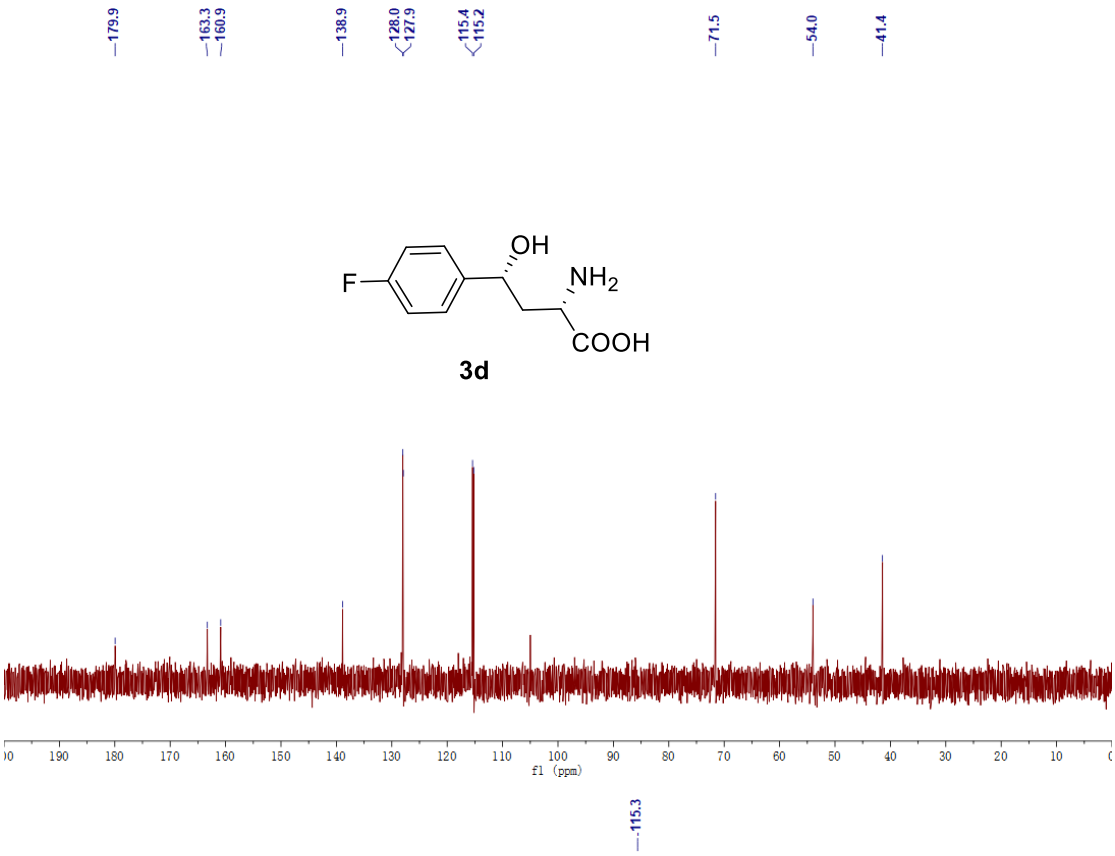

180.2
160.8
158.8
129.8
129.7
129.6
127.7
127.6
124.6
124.6
115.7
115.5
66.4
66.4
54.0
40.6
OH
NH2
F
COOH
3b
f1 (ppm)
119.6
119.6
119.6
119.6
119.6

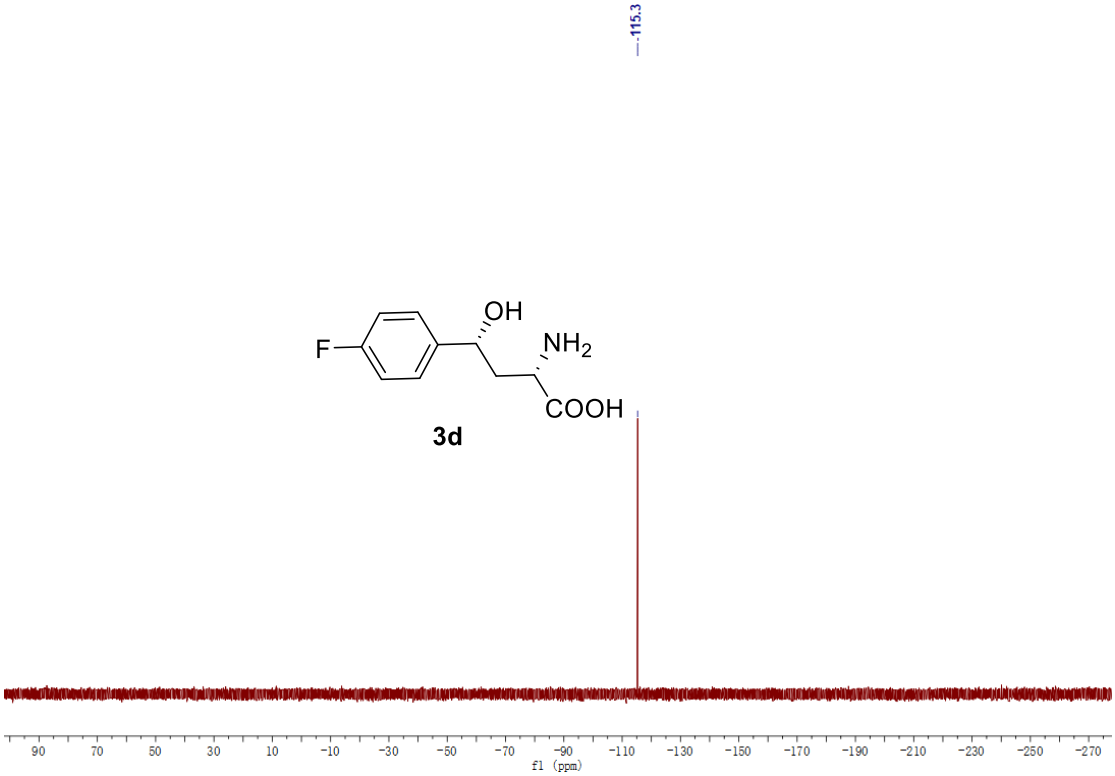

OH
NH2
F
COOH
3b
f1 (ppm)

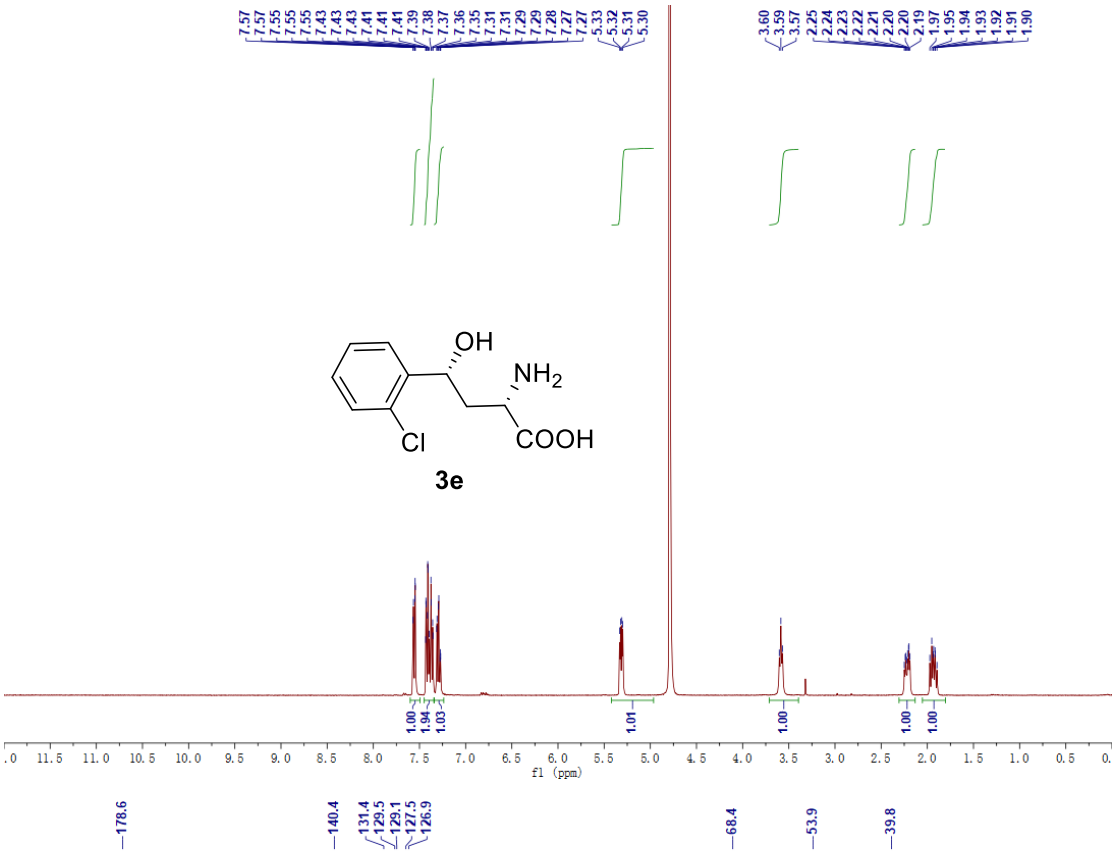

7.43
7.41
7.40
7.38
7.37
7.22
7.20
7.18
7.18
7.16
7.09
7.07
7.05
5.00
4.97
3.88
3.87
3.86
3.85
2.34
2.30
2.28
2.14
2.11
2.09
2.08
2.05
OH
NH2
F
COOH
3c
1.00
1.96
0.95
0.99
0.99
1.00
1.00
f1 (ppm)


174.2
163.9
161.5
145.7
130.5
130.4
121.5
114.8
114.6
112.6
112.3
71.6
53.8
38.4
OH
NH2
F
COOH
3c
f1 (ppm)

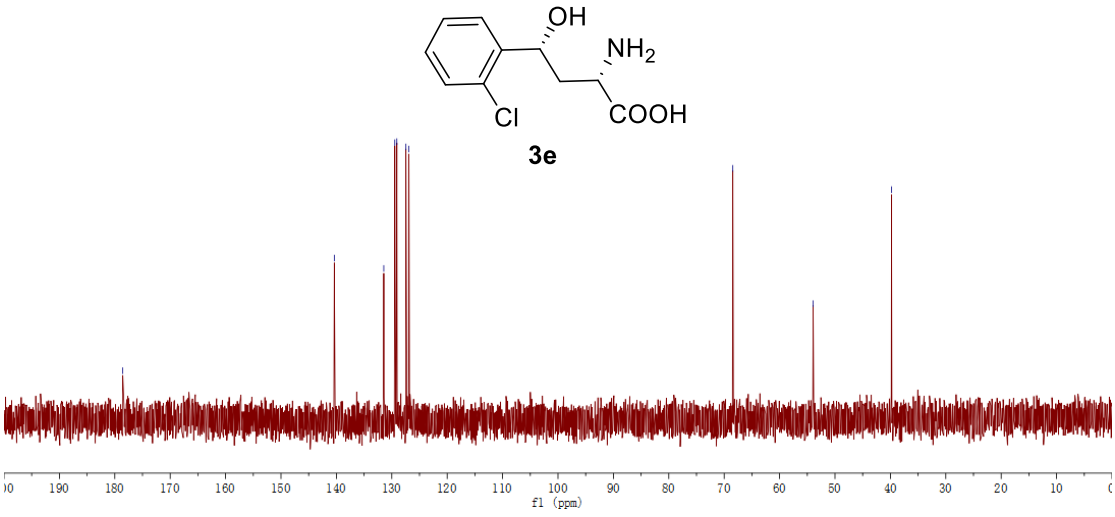

-113.4
-113.4
-113.4
-113.4
OH
NH2
F
COOH
3c
f1 (ppm)
7.42
7.42
7.41
7.40
7.38
7.16
7.15
7.13
7.11
4.87
4.85
4.85
4.83
3.40
3.40
3.38
3.36
2.17
2.16
2.15
2.14
2.13
2.11
2.04
2.02
2.01
2.00
1.99
1.97
OH
NH2
F
COOH
3d
2.10
2.03
1.05
1.00
1.02
1.08
f1 (ppm)

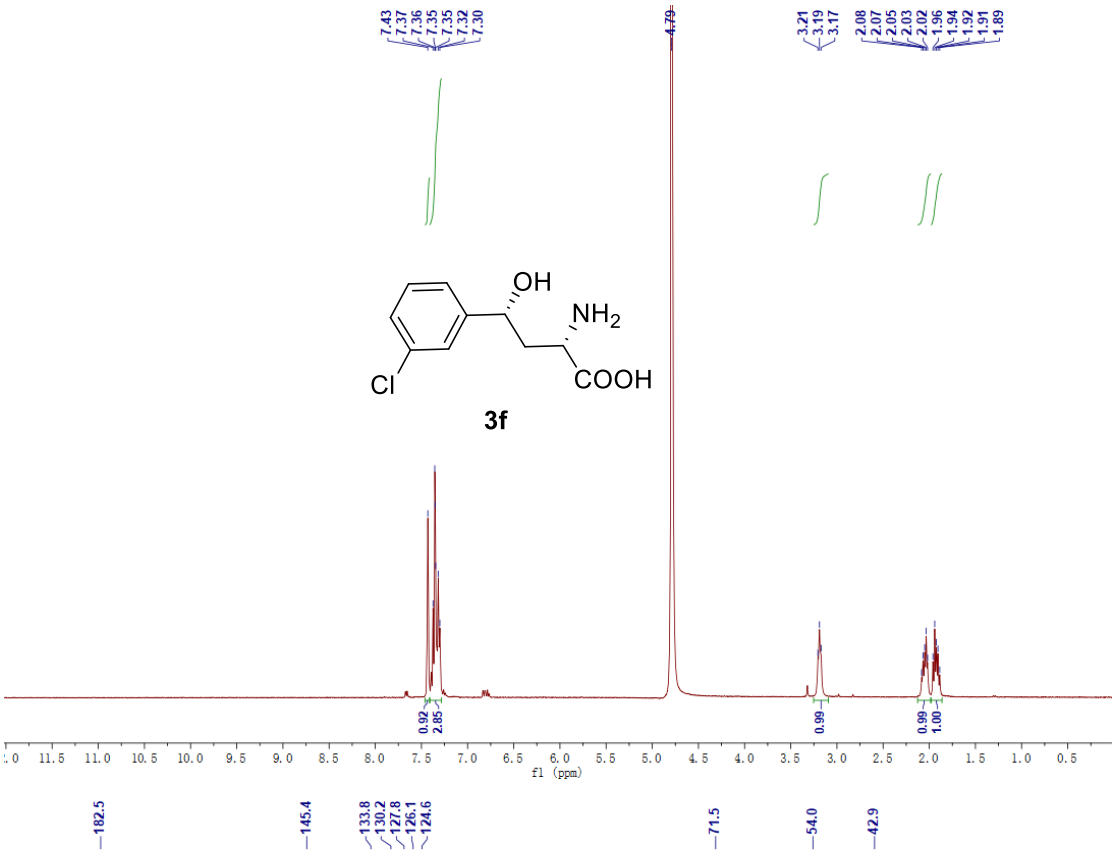

179.9
163.3
160.9
138.9
128.0
127.9
115.4
115.2
71.5
54.0
41.4
OH
NH2
F
COOH
3d
f1 (ppm)

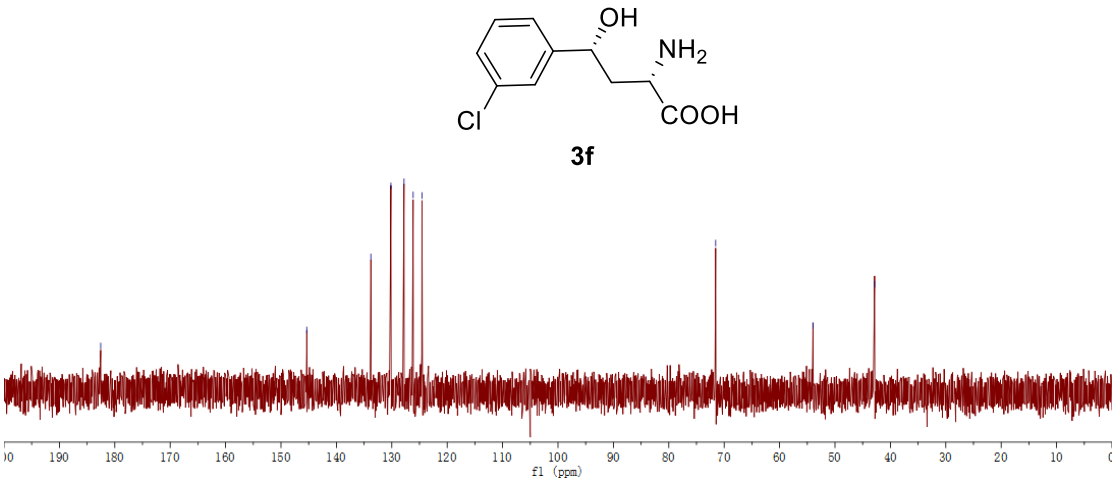

115.3
OH
NH2
F
COOH
3d
f1 (ppm)

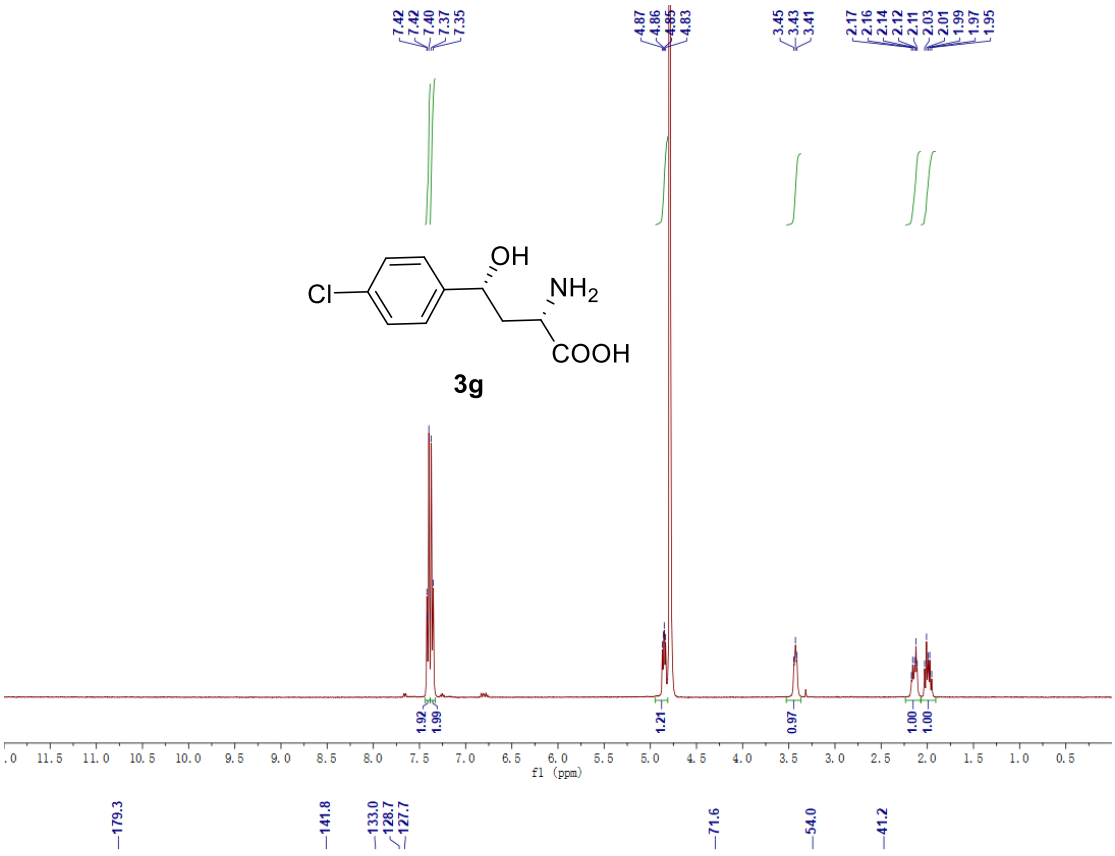

7.57
7.57
7.55
7.55
7.55
7.43
7.43
7.43
7.41
7.41
7.41
7.39
7.38
7.37
7.36
7.35
7.31
7.31
7.29
7.29
7.28
7.27
7.27
5.33
5.32
5.31
5.30
3.60
3.59
3.57
2.25
2.24
2.23
2.22
2.21
2.20
2.20
2.19
1.97
1.95
1.94
1.93
1.92
1.91
1.90
OH
NH2
Cl
COOH
3e
1.00
1.94
1.03
1.01
1.00
1.00
1.00
f1 (ppm)

178.6
140.4
131.4
129.5
129.1
127.5
126.9
68.4
53.9
39.8

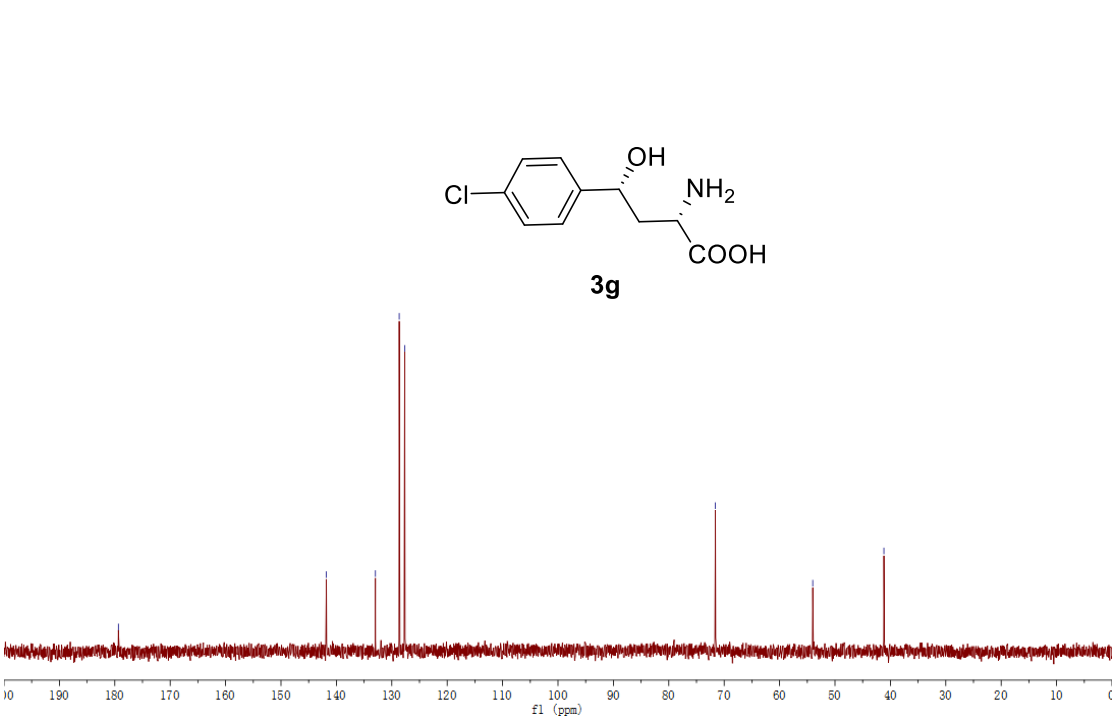

OH
NH2
Cl
COOH
3e
f1 (ppm)


7.43
7.37
7.36
7.35
7.35
7.32
7.30
4.79
3.21
3.19
3.17
2.08
2.07
2.05
2.03
2.02
1.96
1.94
1.92
1.91
1.89
OH
NH2
Cl
COOH
3f
0.92
2.85
0.99
0.99
1.00
f1 (ppm)


182.5
145.4
133.8
130.2
127.8
126.1
124.6
71.5
54.0
42.9
OH
NH2
Cl
COOH
3f
f1 (ppm)

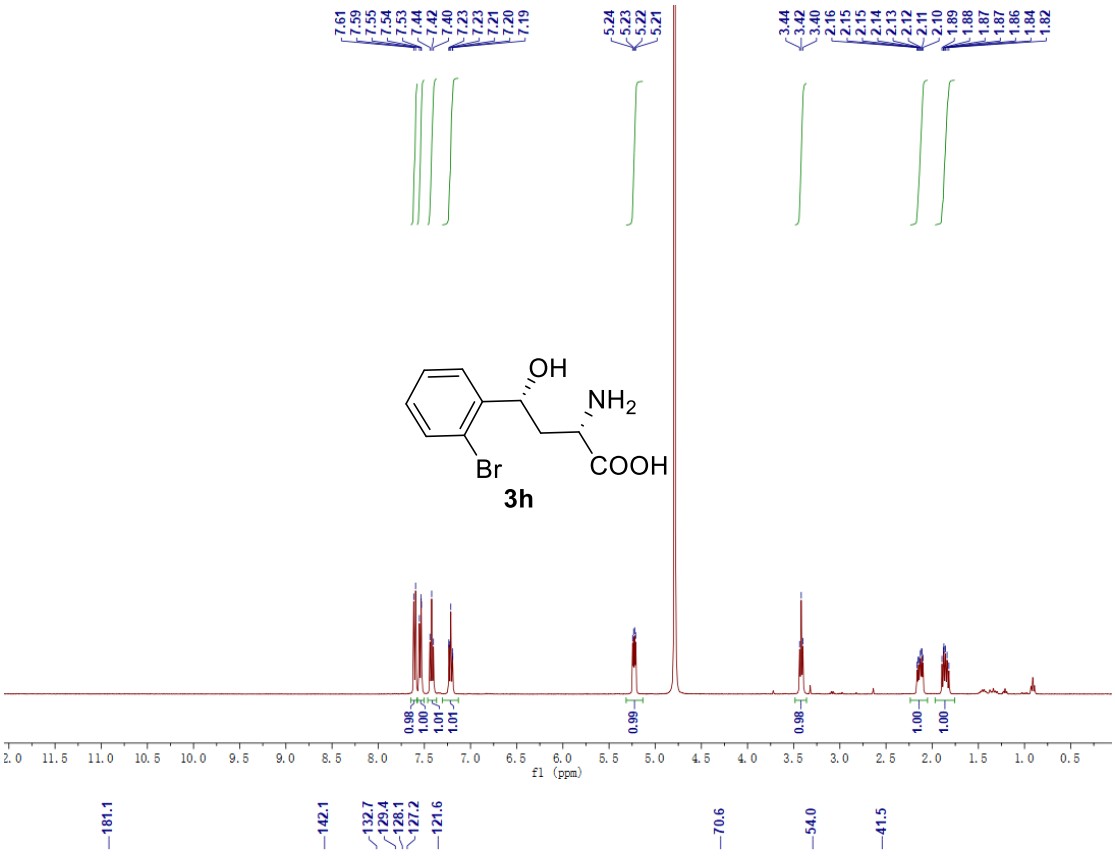

7.42
7.42
7.40
7.37
7.35
4.87
4.86
4.85
4.83
3.45
3.43
3.41
2.17
2.16
2.14
2.12
2.11
2.03
2.01
1.99
1.97
1.95
OH
NH2
Cl
COOH
1.92
1.99
1.21
0.97
1.00
1.00
f1 (ppm)

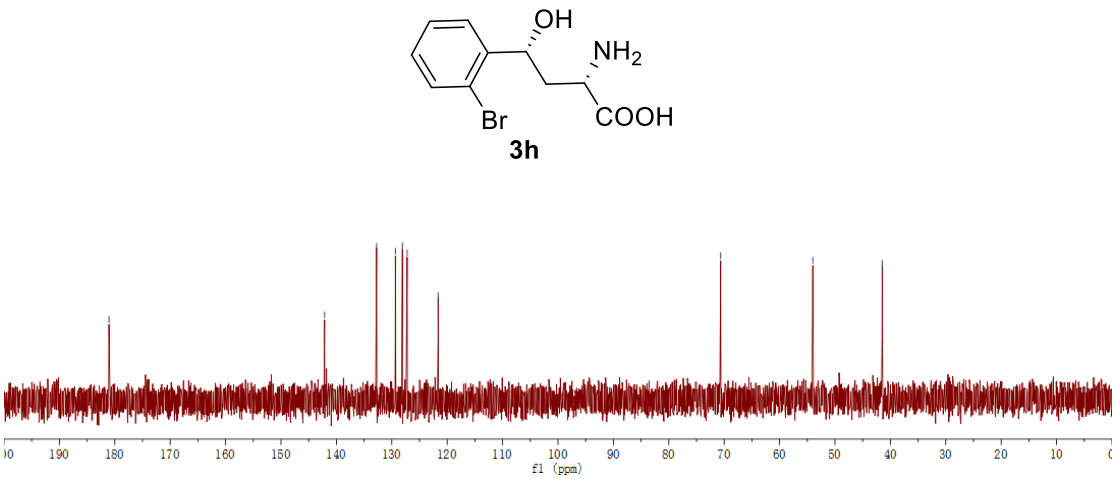
3g

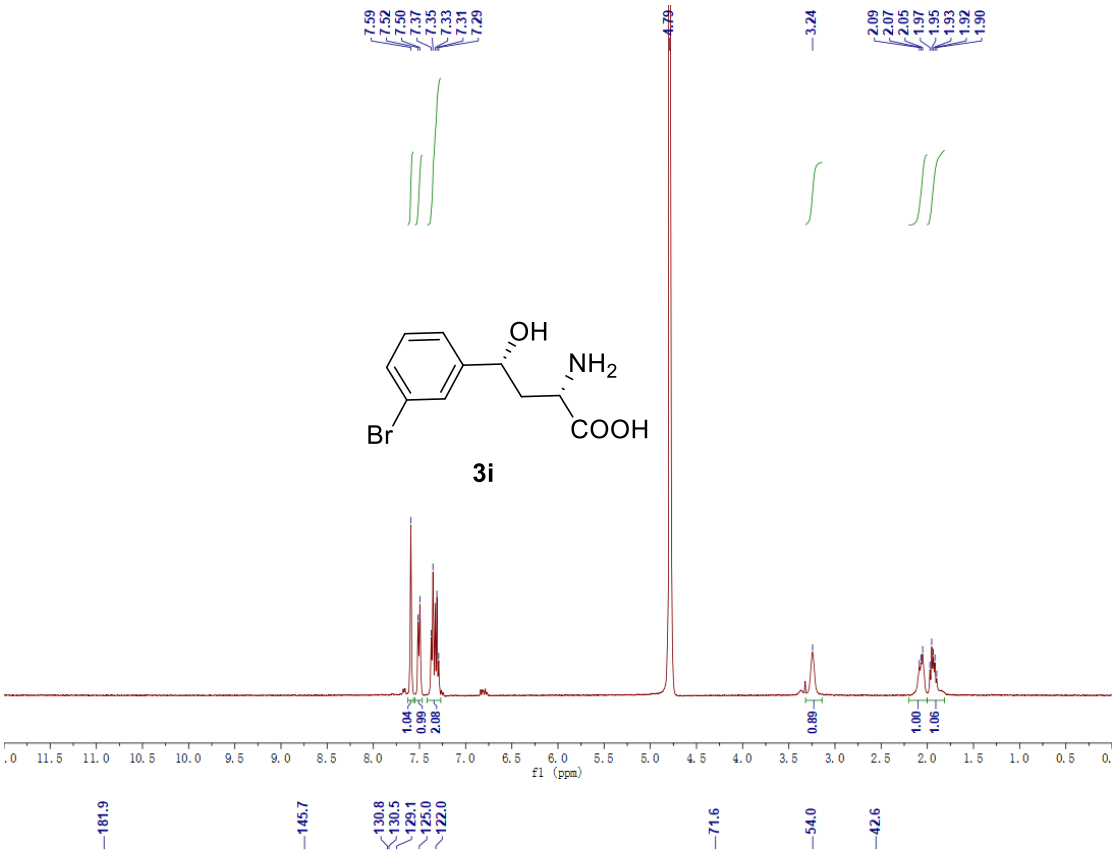

179.3
141.8
133.0
128.7
127.7
71.6
54.0
41.2
f1 (ppm)

OH
NH2
Cl
COOH

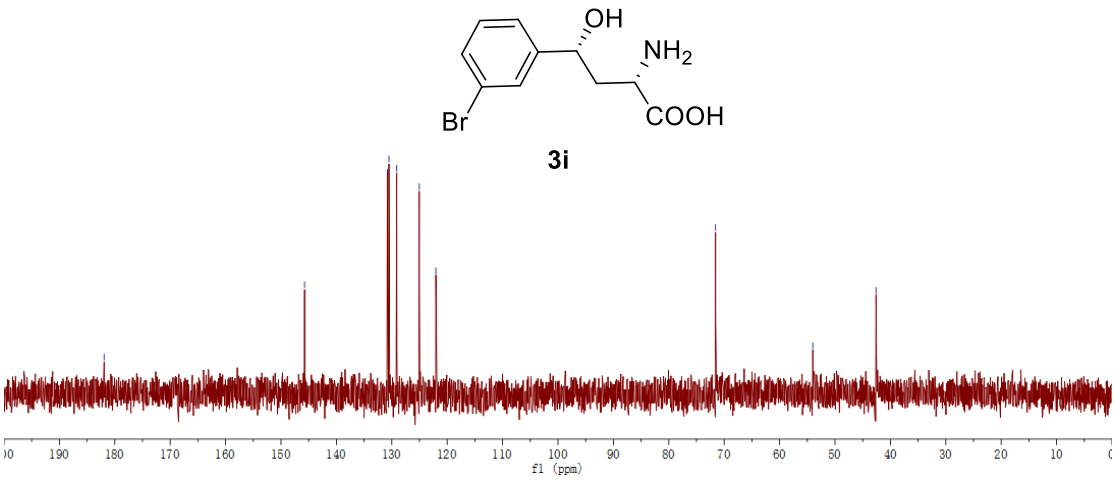
3g


7.61
7.59
7.55
7.54
7.53
7.44
7.42
7.40
7.23
7.23
7.21
7.20
7.19
5.24
5.23
5.22
5.21
3.44
3.42
3.40
2.16
2.15
2.15
2.14
2.13
2.12
2.11
2.10
1.89
1.88
1.87
1.87
1.86
1.84
1.82
OH
NH2
Br
COOH
3h
0.98
1.00
1.01
1.01
0.99
0.98
1.00
1.00
f1 (ppm)

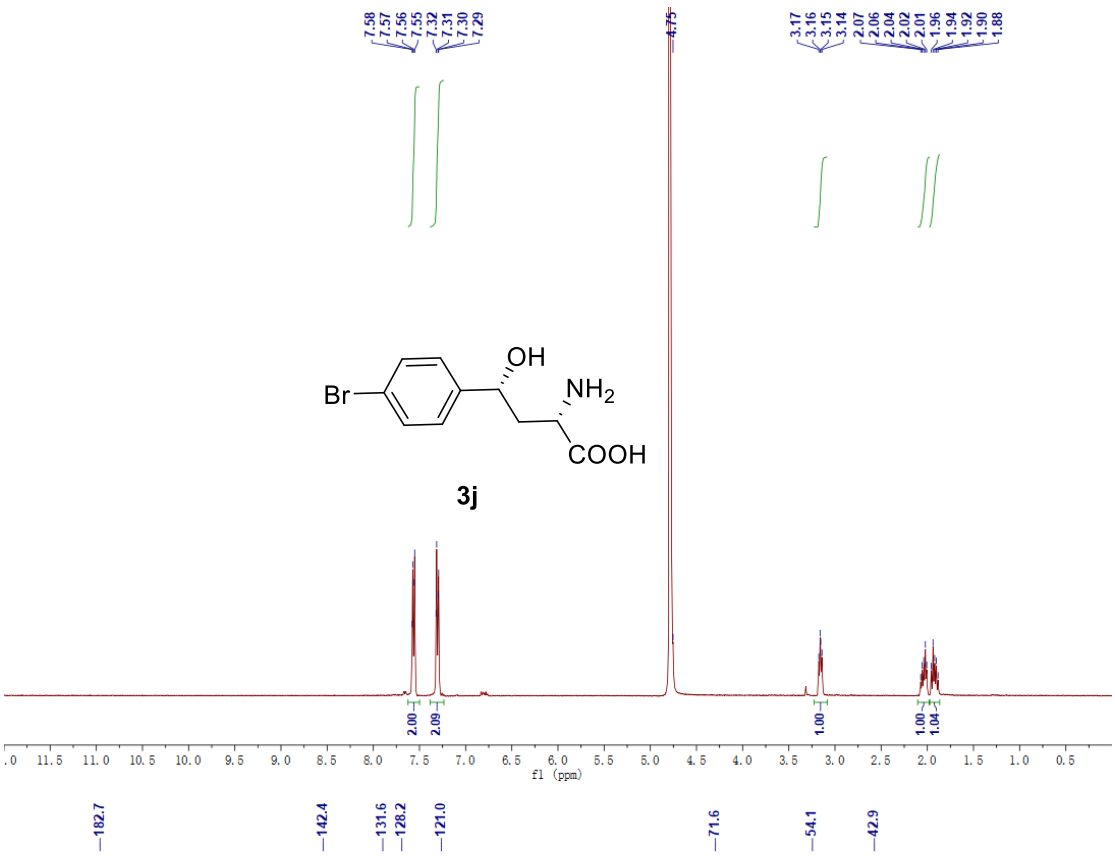

181.1
142.1
132.7
129.4
128.1
127.2
121.6
70.6
54.0
41.5
OH
NH2
Br
COOH
3h
f1 (ppm)

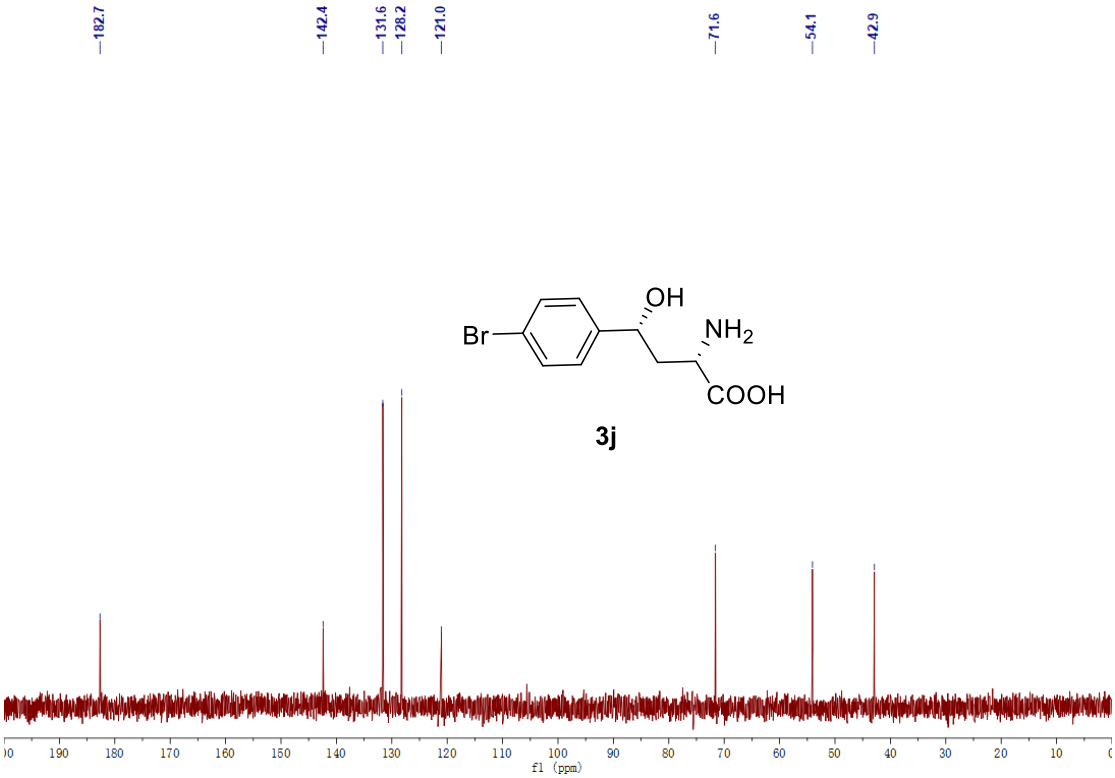

7.59
7.52
7.50
7.37
7.35
7.33
7.31
7.29
4.79
3.24
2.09
2.07
2.05
1.97
1.95
1.93
1.92
1.90
OH
NH2
Br
COOH
1.04
0.98
2.08
0.89
1.00
1.06
f1 (ppm)

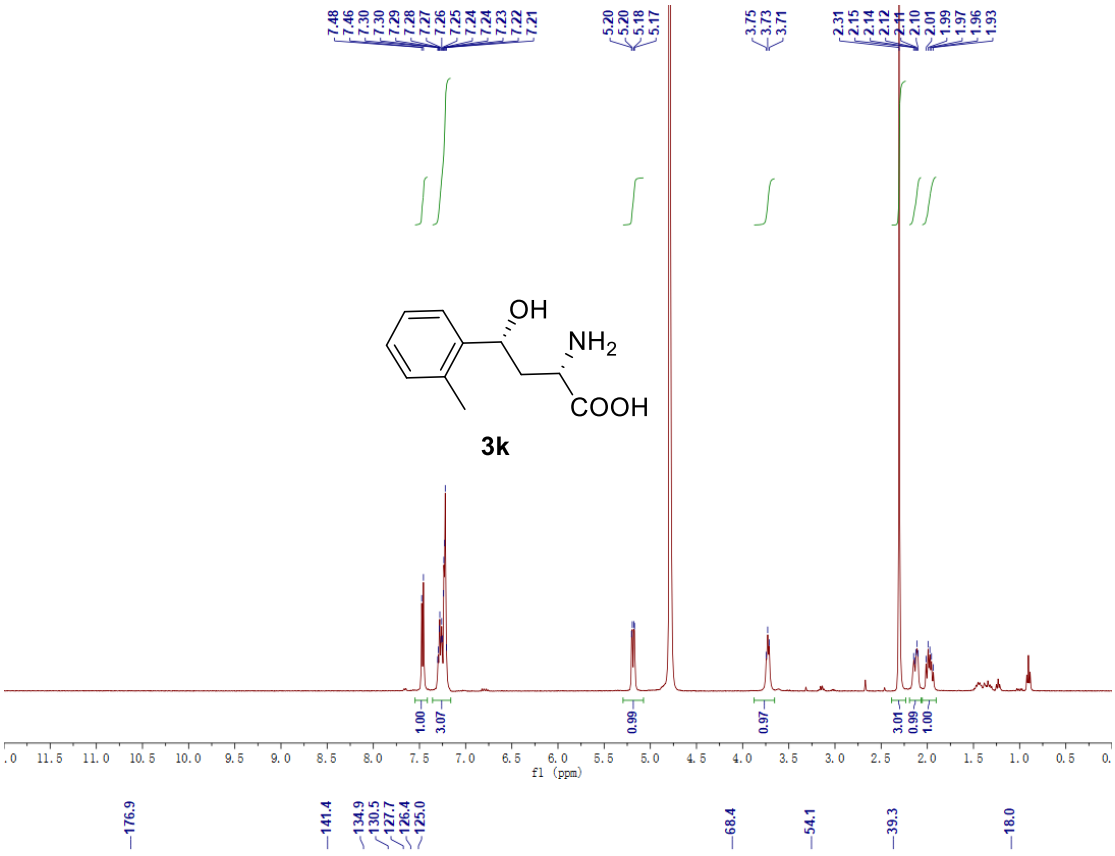
3i

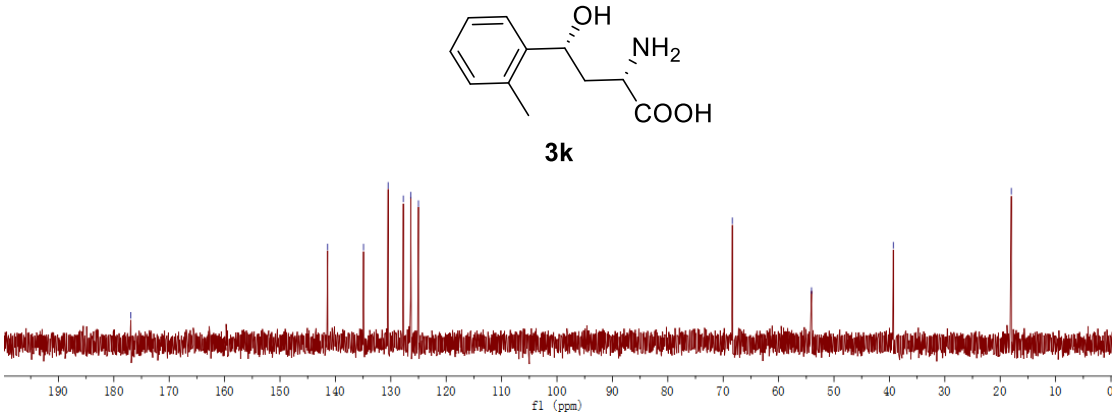

181.9
145.7
130.8
130.5
129.1
125.0
122.0
71.6
54.0
42.6
OH
NH2
Br
COOH
f1 (ppm)

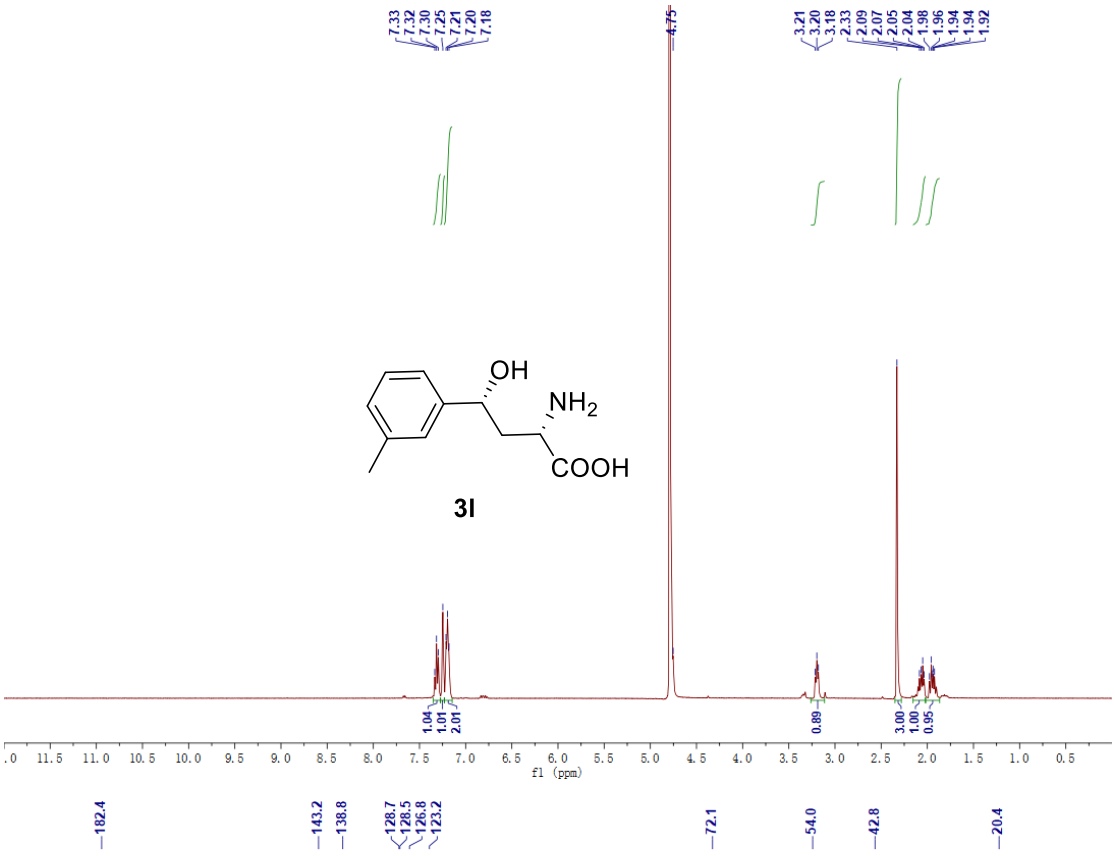
3i


7.58
7.57
7.56
7.55
7.32
7.31
7.30
7.29
4.75
3.17
3.16
3.15
3.14
2.07
2.06
2.04
2.02
2.01
1.96
1.94
1.92
1.90
1.88
Br
OH
NH2
COOH
3j
2.00
2.09
1.00
1.00
1.04
f1 (ppm)

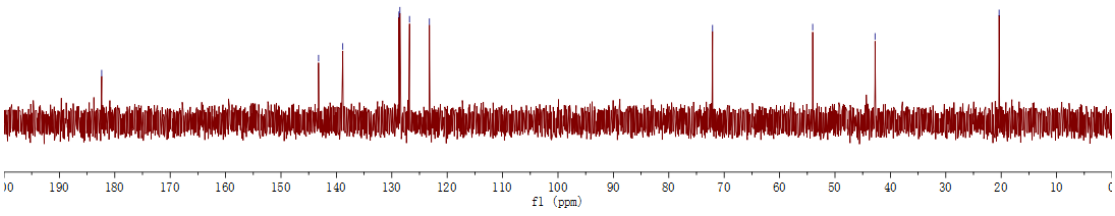

182.7
142.4
131.6
128.2
121.0
71.6
54.1
42.9
Br
OH
NH2
COOH
3j
f1 (ppm)

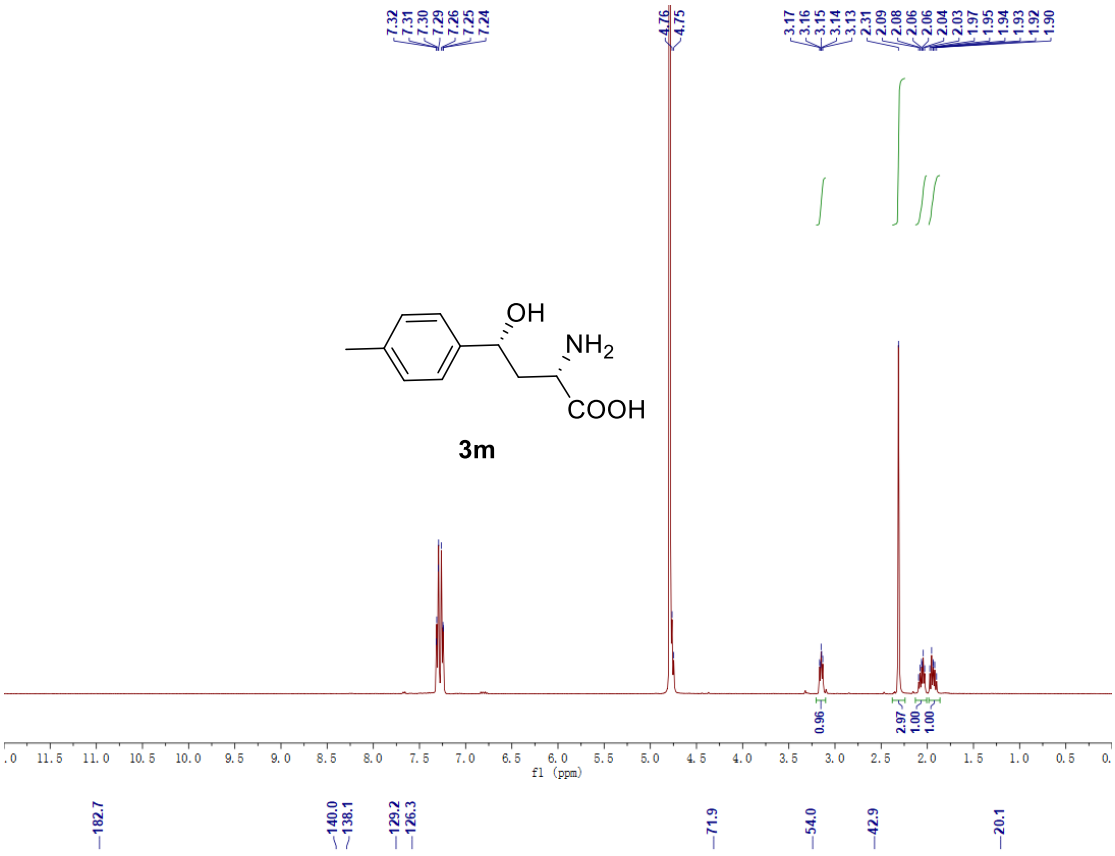

7.48
7.46
7.30
7.30
7.29
7.28
7.27
7.26
7.25
7.24
7.24
7.23
7.22
7.21
5.20
5.20
5.18
5.17
3.75
3.73
3.71
2.31
2.15
2.14
2.12
2.11
2.10
2.01
1.99
1.97
1.96
1.93
OH
NH2
COOH
3k
1.00
3.07
0.99
0.97
3.01
0.99
1.00
f1 (ppm)


176.9
141.4
134.9
130.5
127.7
126.4
125.0
68.4
54.1
39.3
18.0
OH
NH2
COOH
3k
f1 (ppm)

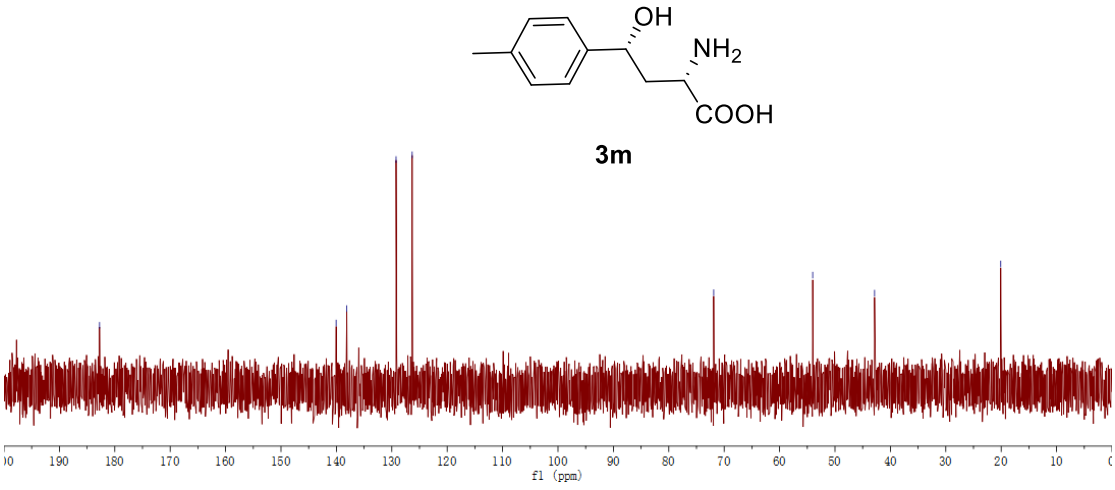

7.33
7.32
7.30
7.25
7.21
7.20
7.18
4.75
3.21
3.20
3.18
2.33
2.09
2.07
2.05
2.04
1.98
1.96
1.94
1.94
1.92
OH
NH2
COOH
1.04
1.01
2.01
0.89
3.00
1.00
0.95
f1 (ppm)

3l


182.4
143.2
138.8
128.7
128.5
126.8
123.2
72.1
54.0
42.8
20.4
f1 (ppm)

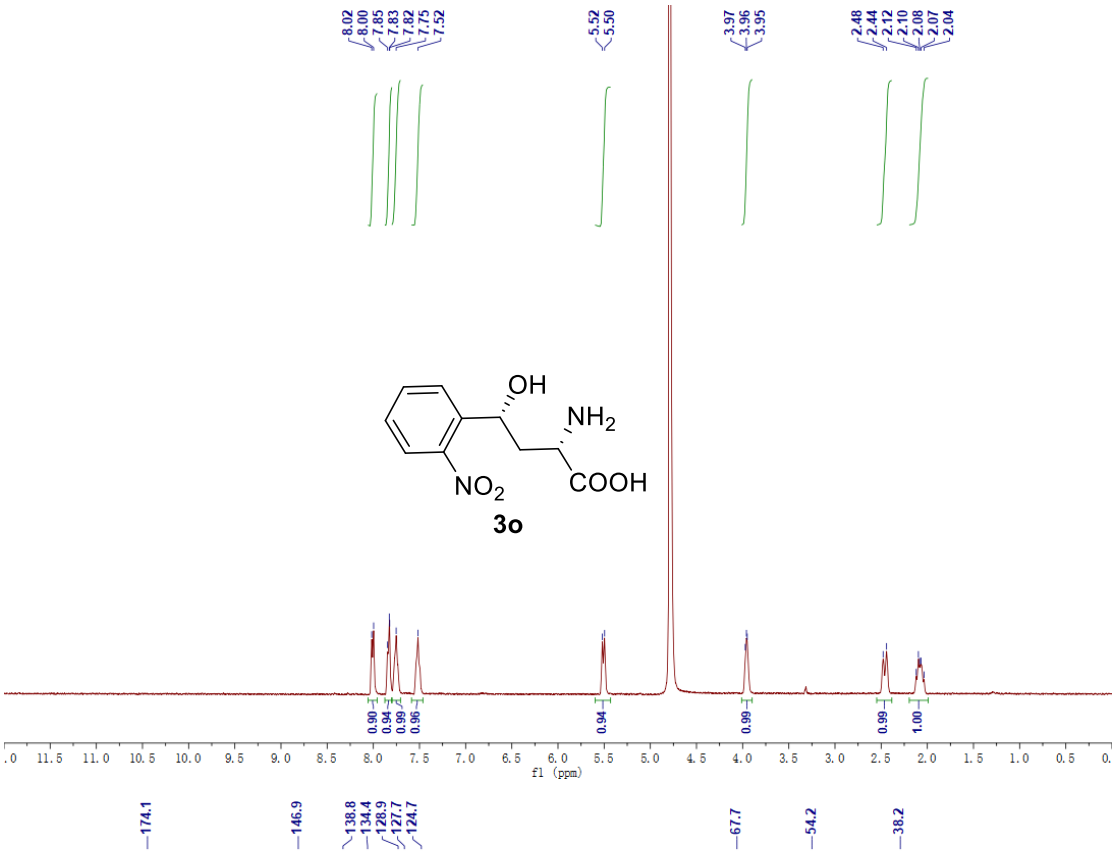

7.32
7.31
7.30
7.29
7.26
7.25
7.24
4.76
4.75
3.17
3.16
3.15
3.14
3.13
2.31
2.09
2.08
2.06
2.06
2.04
2.03
1.97
1.95
1.94
1.93
1.92
1.90
OH
NH2
COOH
0.96
2.97
1.00
1.00
f1 (ppm)

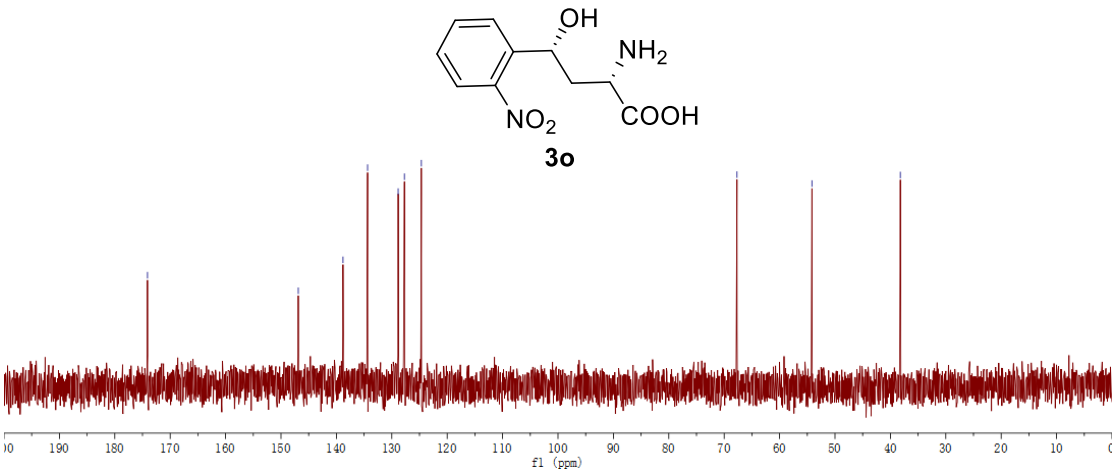
3m

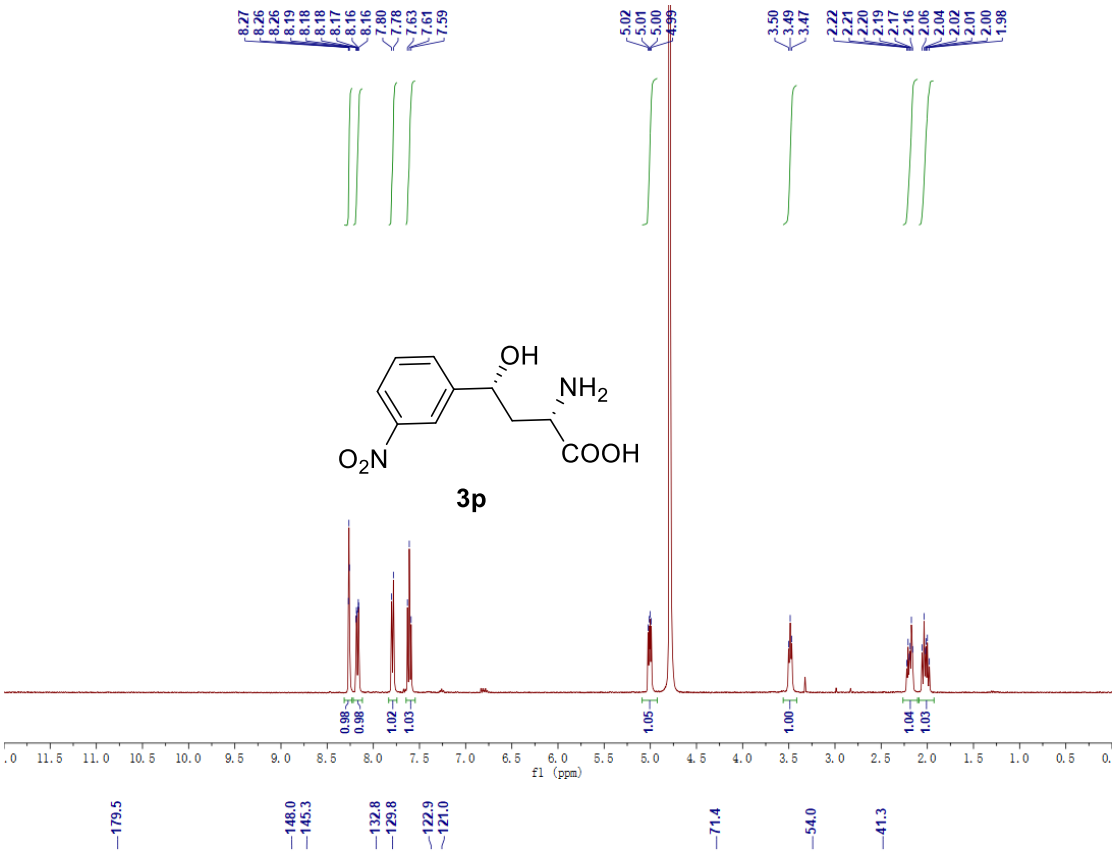

182.7
140.0
138.1
129.2
126.3
71.9
54.0
42.9
20.1
f1 (ppm)

OH
NH2
COOH

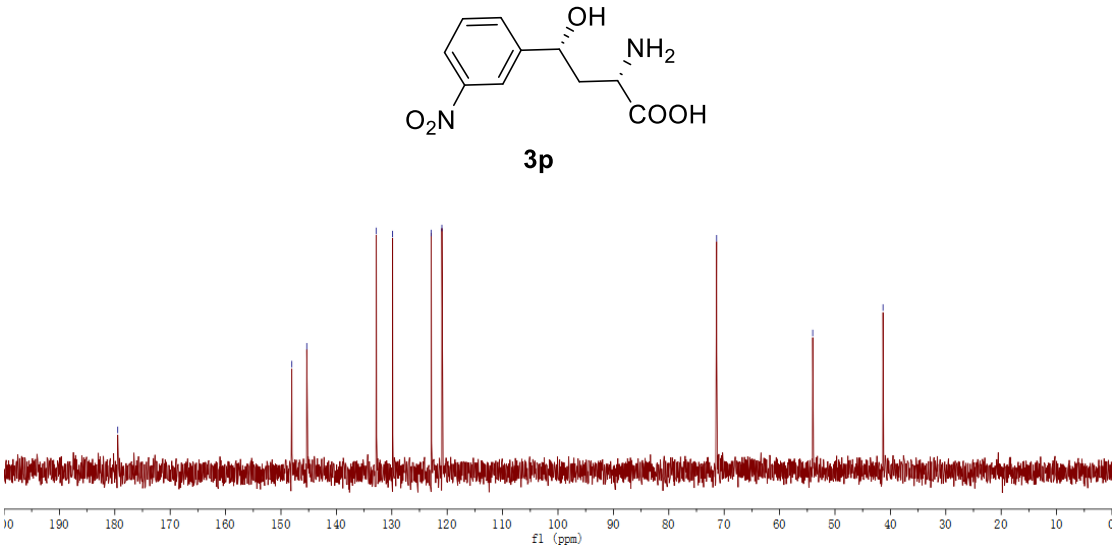
3m


8.02
8.00
7.85
7.83
7.82
7.75
7.52
5.52
5.50
3.97
3.96
3.95
2.48
2.44
2.12
2.10
2.08
2.07
2.04
OH
NH2
NO2
COOH
3o
0.90
0.94
0.99
0.96
0.94
0.99
0.99
1.00
f1 (ppm)


174.1
146.9
138.8
134.4
128.9
127.7
124.7
67.7
54.2
38.2
OH
NH2
NO2
COOH
3o
f1 (ppm)

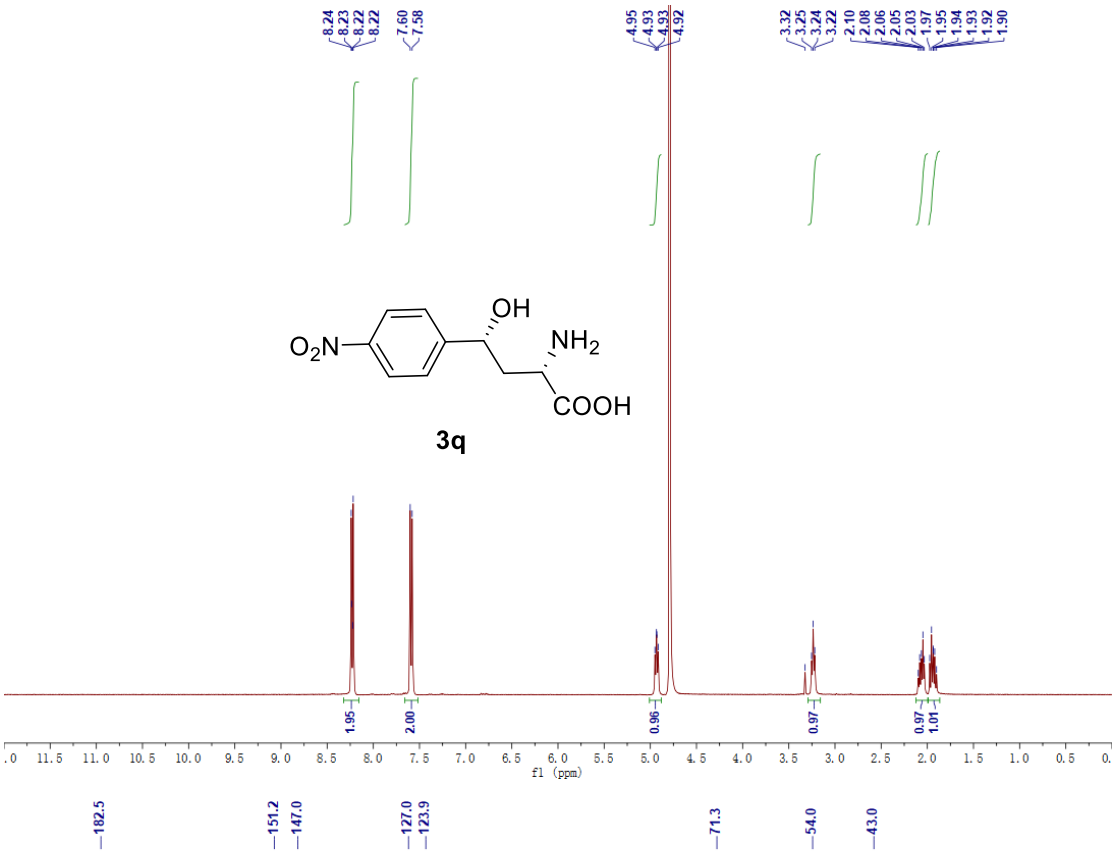

8.27
8.26
8.26
8.19
8.18
8.18
8.17
8.16
8.16
7.80
7.78
7.63
7.61
7.59
5.02
5.01
5.00
4.99
3.50
3.49
3.47
2.22
2.21
2.20
2.19
2.17
2.16
2.06
2.04
2.02
2.01
2.00
1.98
OH
NH2
O2N
COOH
0.98
0.98
1.02
1.03
1.05
1.00
1.04
1.03
f1 (ppm)

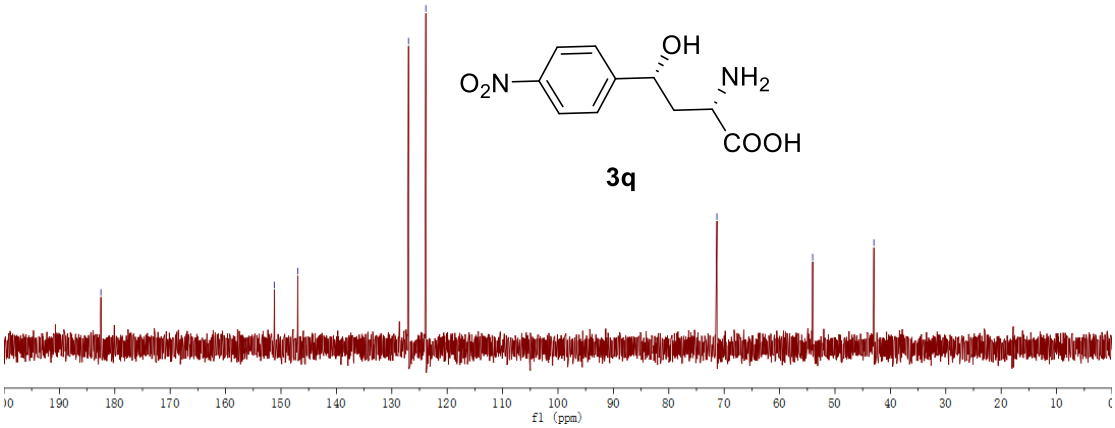
3p

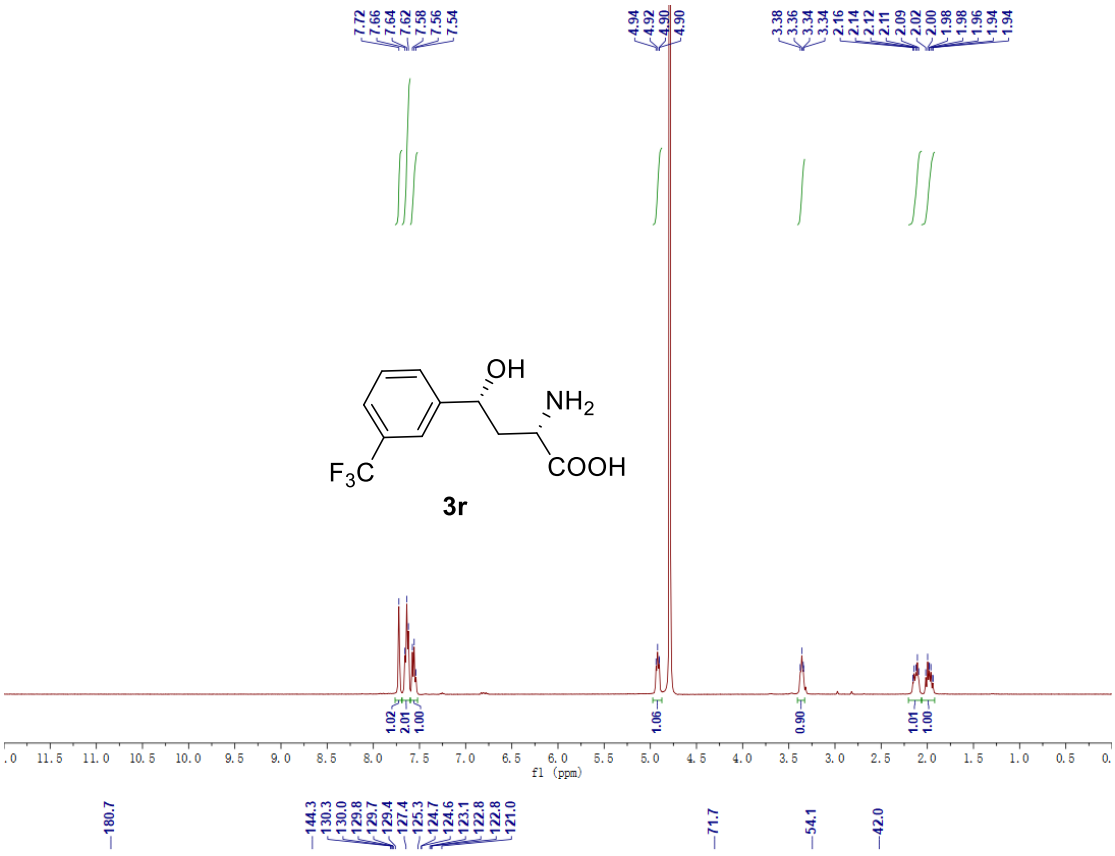

179.5
148.0
145.3
132.8
129.8
122.9
121.0
71.4
54.0
41.3
f1 (ppm)

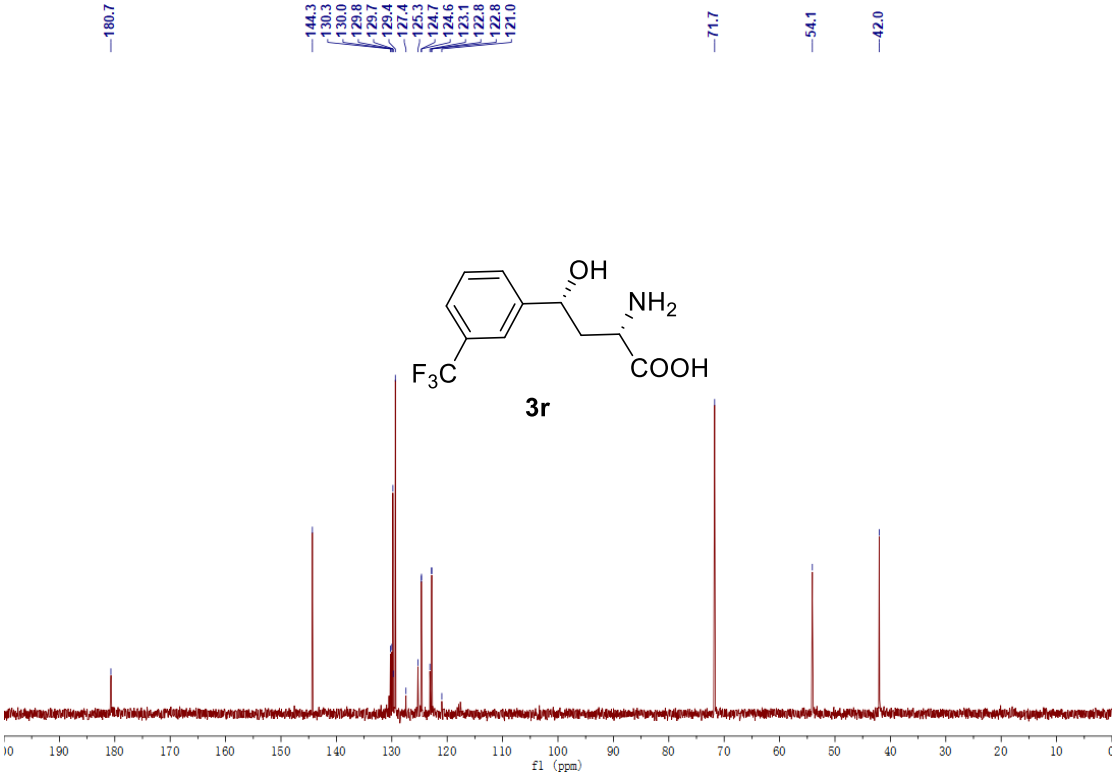
OH
NH2
O2N
COOH

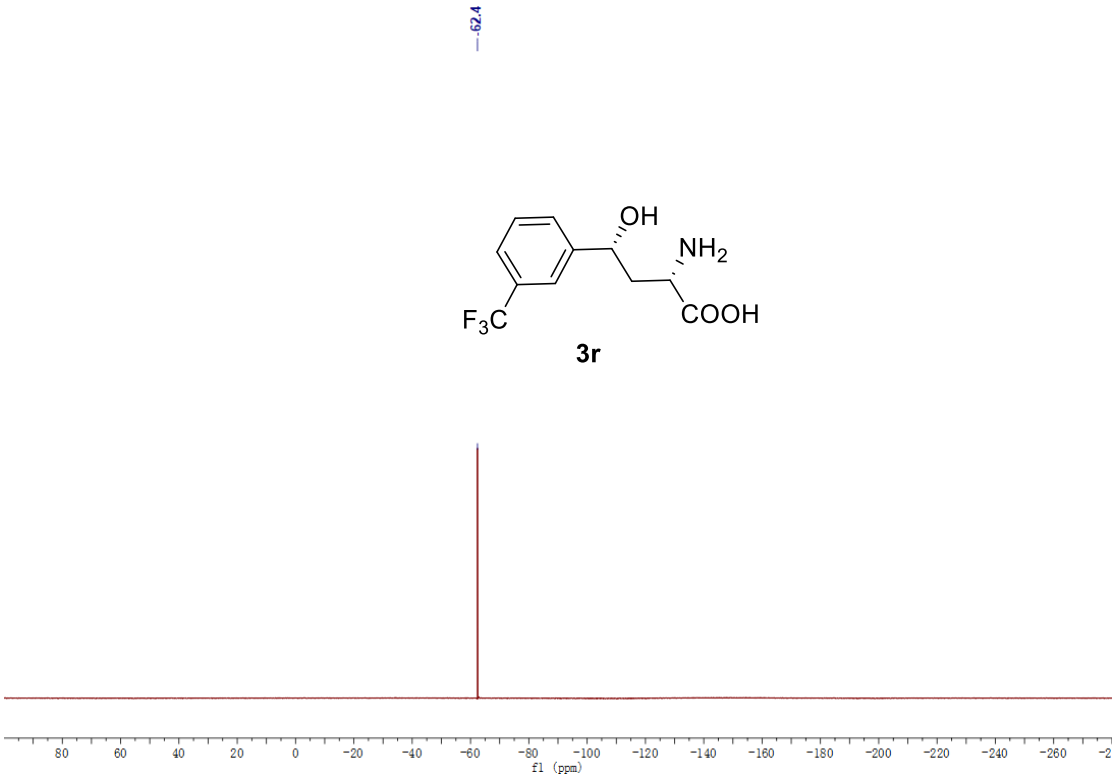
3p

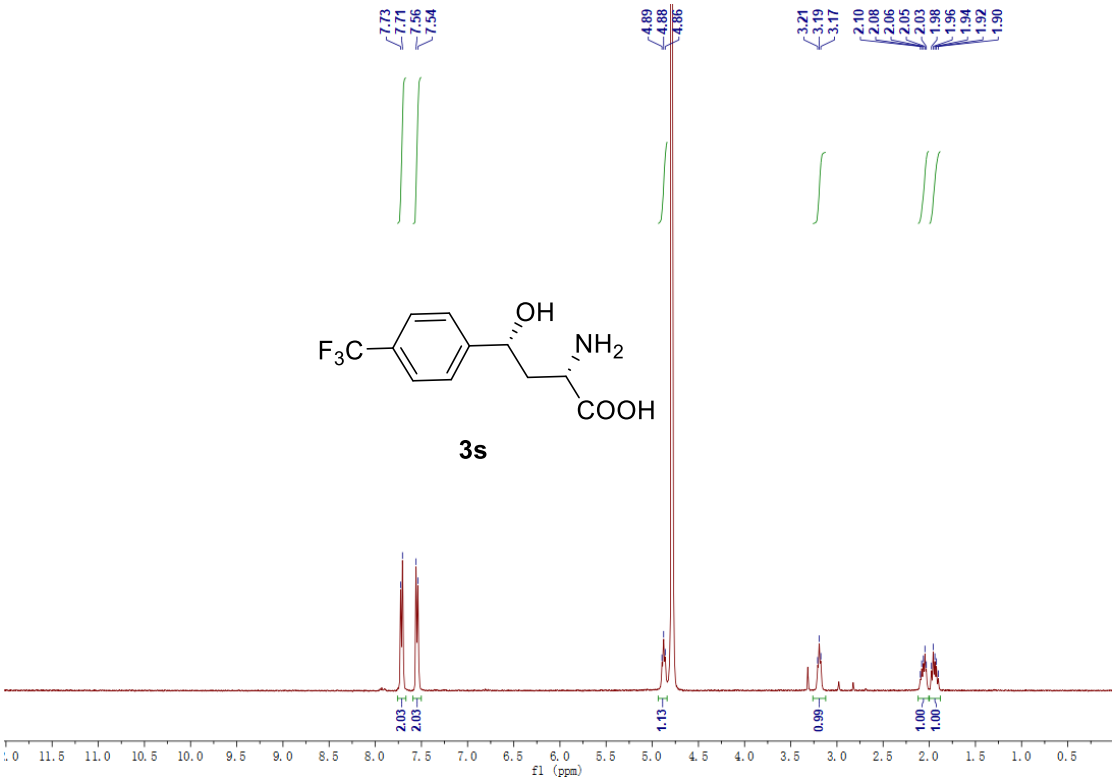

8.24
8.23
8.22
8.22
7.60
7.58
4.95
4.93
4.93
4.92
3.32
3.25
3.24
3.22
2.10
2.08
2.06
2.05
2.03
1.97
1.95
1.94
1.93
1.92
1.90
OH
NH2
O2N
COOH
3q
1.95
2.00
0.96
0.97
0.97
1.01
f1 (ppm)

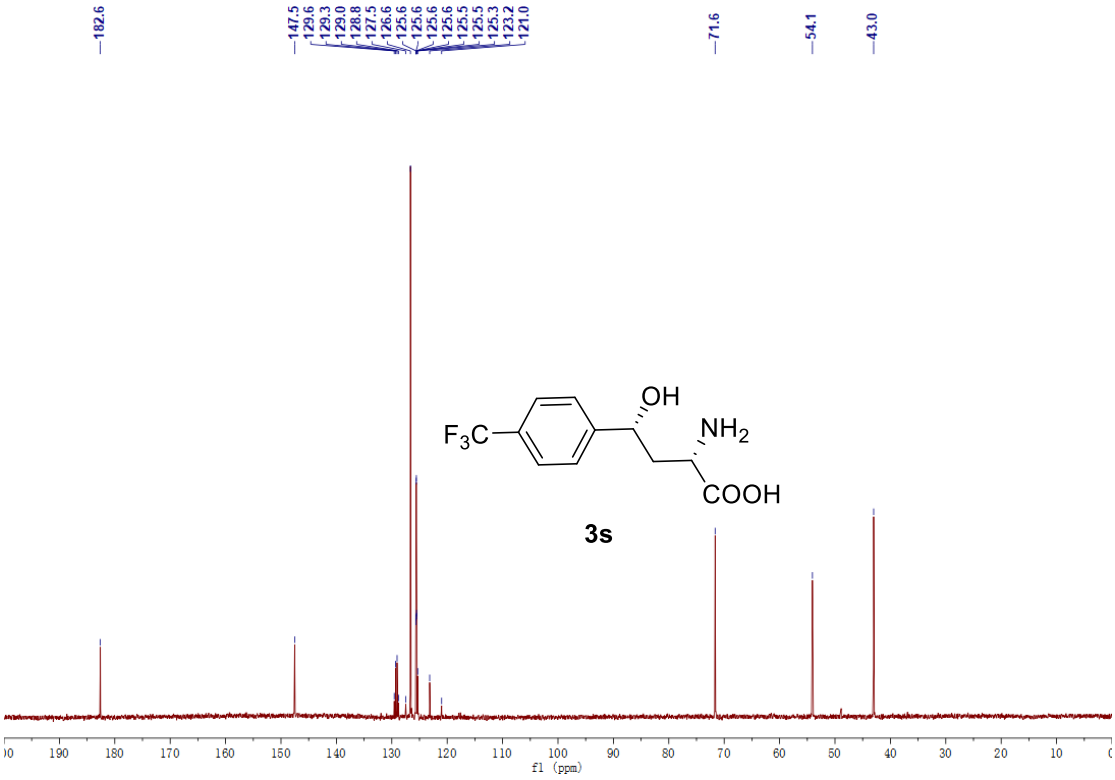

182.5
151.2
147.0
127.0
123.9
71.3
54.0
43.0
OH
NH2
O2N
COOH
3q
f1 (ppm)

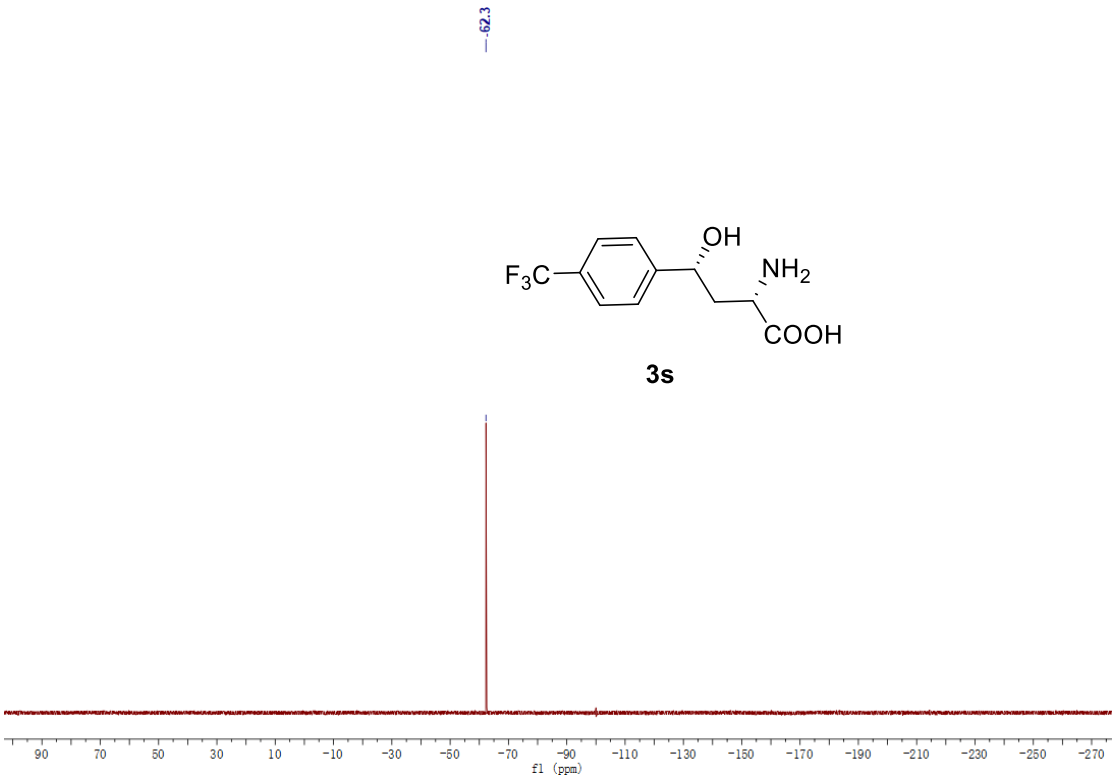

7.72
7.66
7.64
7.62
7.58
7.56
7.54
4.94
4.92
4.90
4.90
3.38
3.36
3.34
3.34
2.16
2.14
2.12
2.11
2.09
2.02
2.00
1.98
1.98
1.96
1.94
1.94
OH
NH2
F3C
COOH
3r
1.02
2.01
1.00
1.06
0.90
1.01
1.00
f1 (ppm)


180.7
144.3
130.3
130.0
129.8
129.7
129.4
127.4
125.3
124.7
124.6
123.1
122.8
122.8
121.0
71.7
54.1
42.0
OH
NH2
F3C
COOH
3r
f1 (ppm)


-62.4
OH
NH2
F3C
COOH
3r
80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -2
f1 (ppm)


7.73
7.71
7.56
7.54
4.89
4.88
4.86
3.21
3.19
3.17
2.10
2.08
2.06
2.05
2.03
1.98
1.96
1.94
1.92
1.90
OH
NH2
F3C
COOH
3s
2.03
2.03
1.13
0.99
1.00
1.00
f1 (ppm)


182.6
147.5
129.6
129.3
129.0
128.8
127.5
126.6
125.6
125.6
125.6
125.6
125.5
125.5
125.3
123.2
121.0
71.6
54.1
43.0
OH
NH2
F3C
COOH
3s
f1 (ppm)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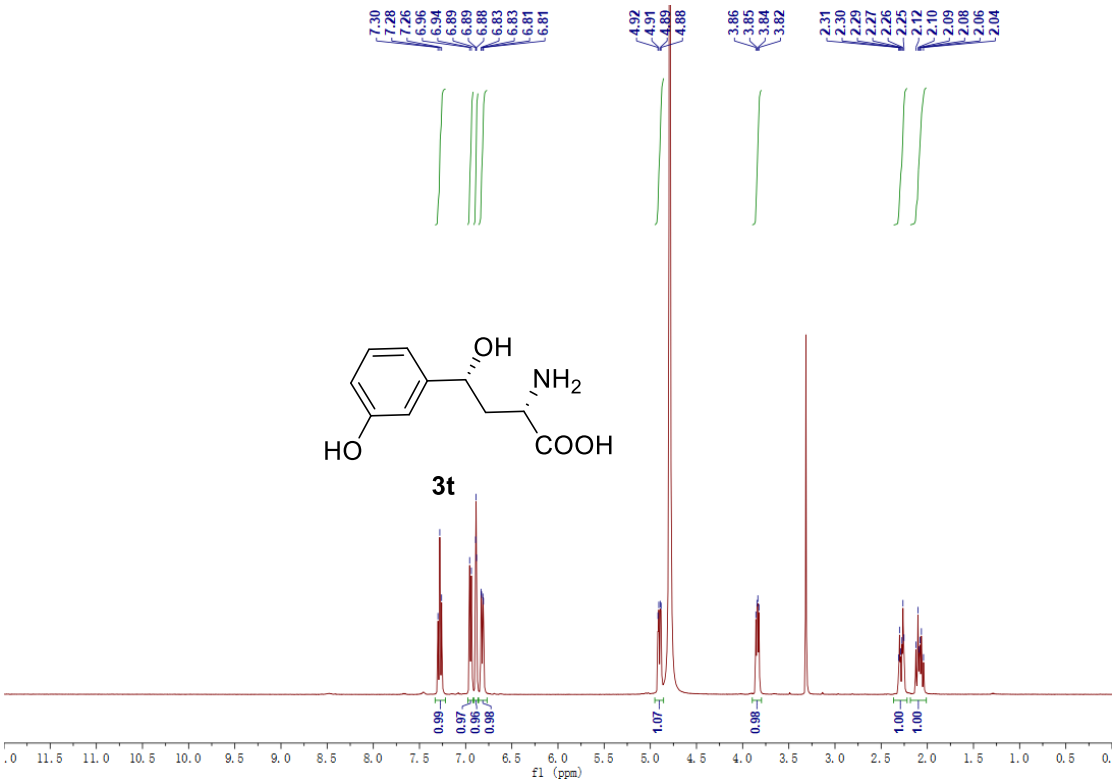
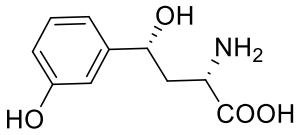
OH
NH2
F3C
COOH
3s
f1 (ppm)

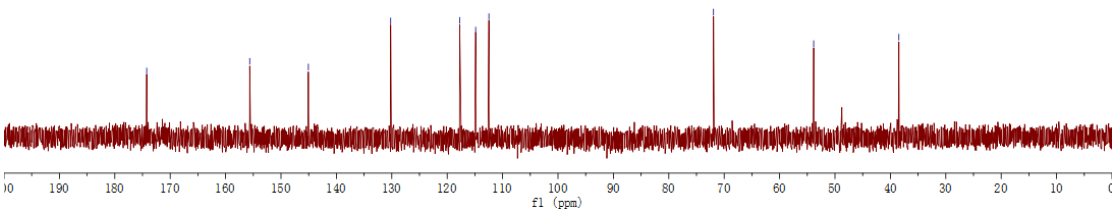

7.30
7.28
7.26
6.96
6.94
6.89
6.89
6.88
6.83
6.83
6.81
6.81
4.92
4.91
4.89
4.88
3.86
3.85
3.84
3.82
2.31
2.30
2.29
2.27
2.26
2.25
2.12
2.10
2.09
2.08
2.06
2.04
OH
NH2
HO
COOH
0.99
0.97
0.96
0.98
1.07
0.98
1.00
1.00
f1 (ppm)

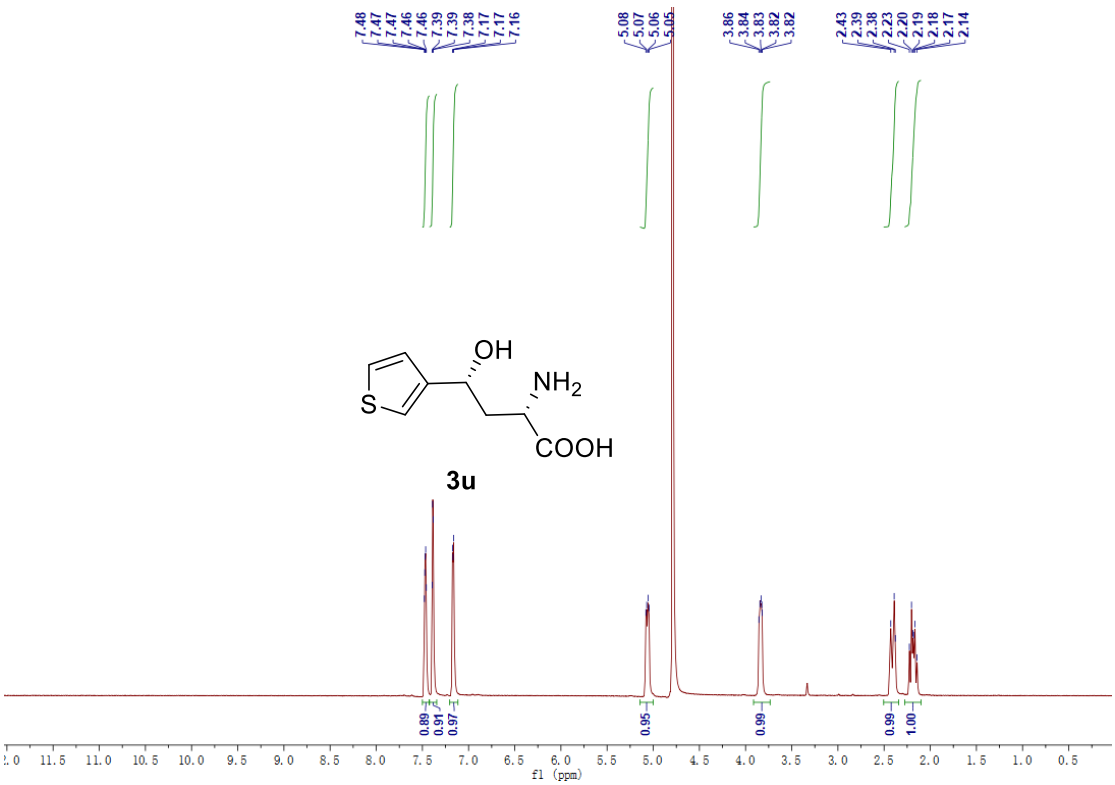
3t


174.2
155.6
145.1
130.2
117.7
114.9
112.5
71.9
53.8
38.5

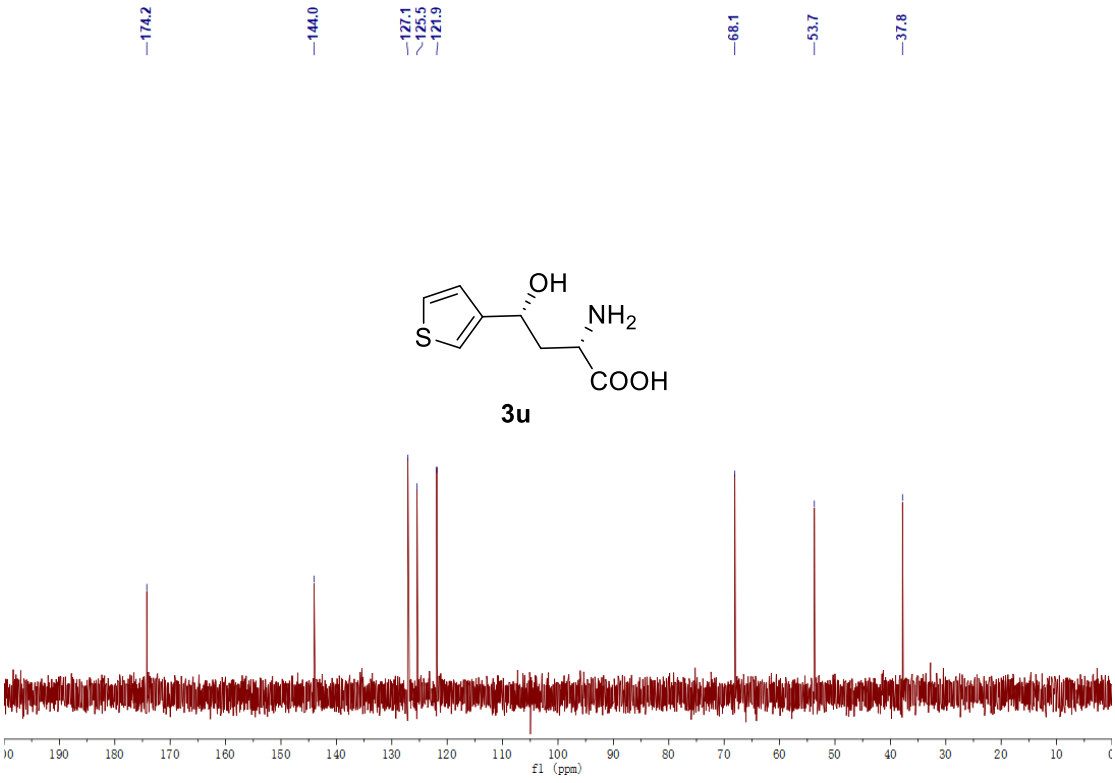

OH
NH2
HO
COOH

3t

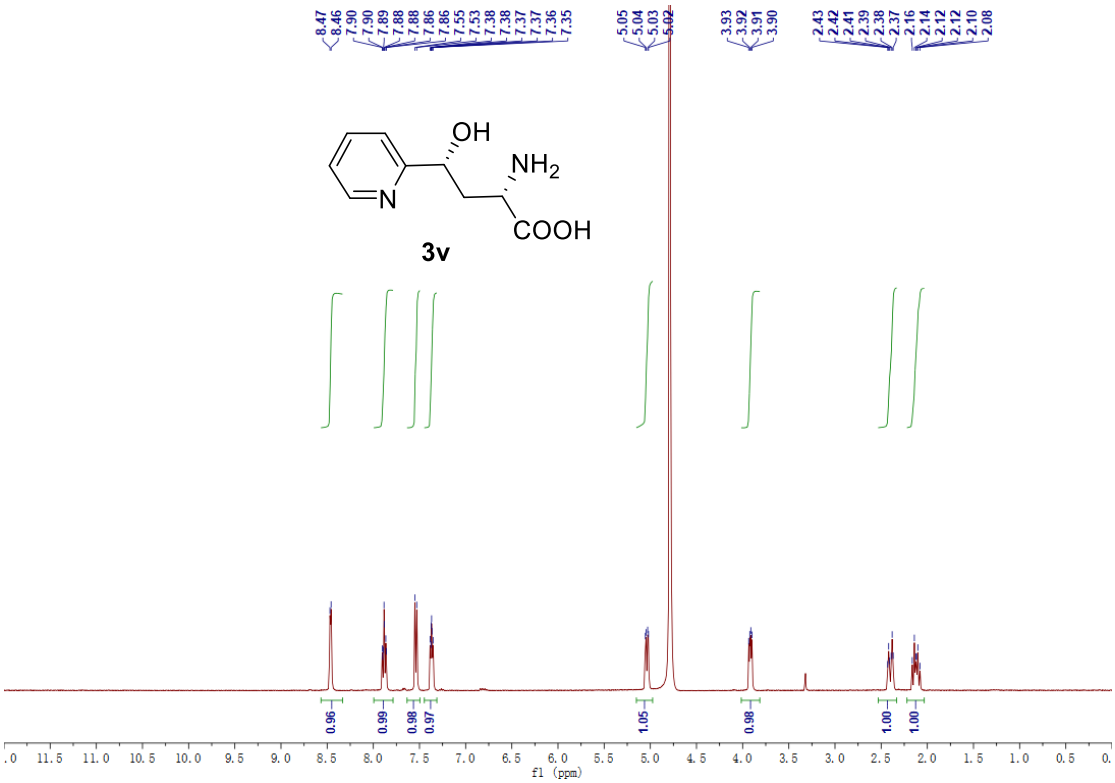

f1 (ppm)


7.48
7.47
7.47
7.46
7.46
7.39
7.39
7.38
7.17
7.17
7.16
5.08
5.07
5.06
5.05
3.86
3.84
3.83
3.82
3.82
2.43
2.39
2.38
2.23
2.20
2.19
2.18
2.17
2.14
OH
NH2
S
COOH
0.89
0.91
0.97
0.95
0.99
0.99
1.00
f1 (ppm)

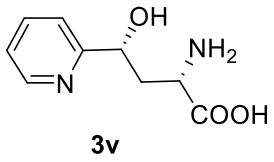
3u

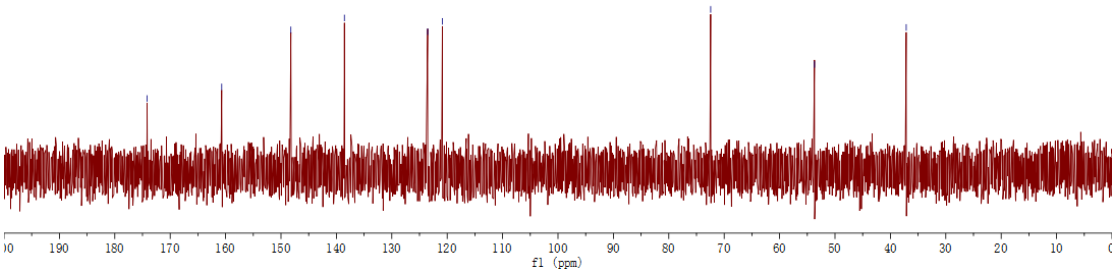

174.2
144.0
127.1
125.5
121.9
68.1
53.7
37.8
OH
NH2
S
COOH
f1 (ppm)

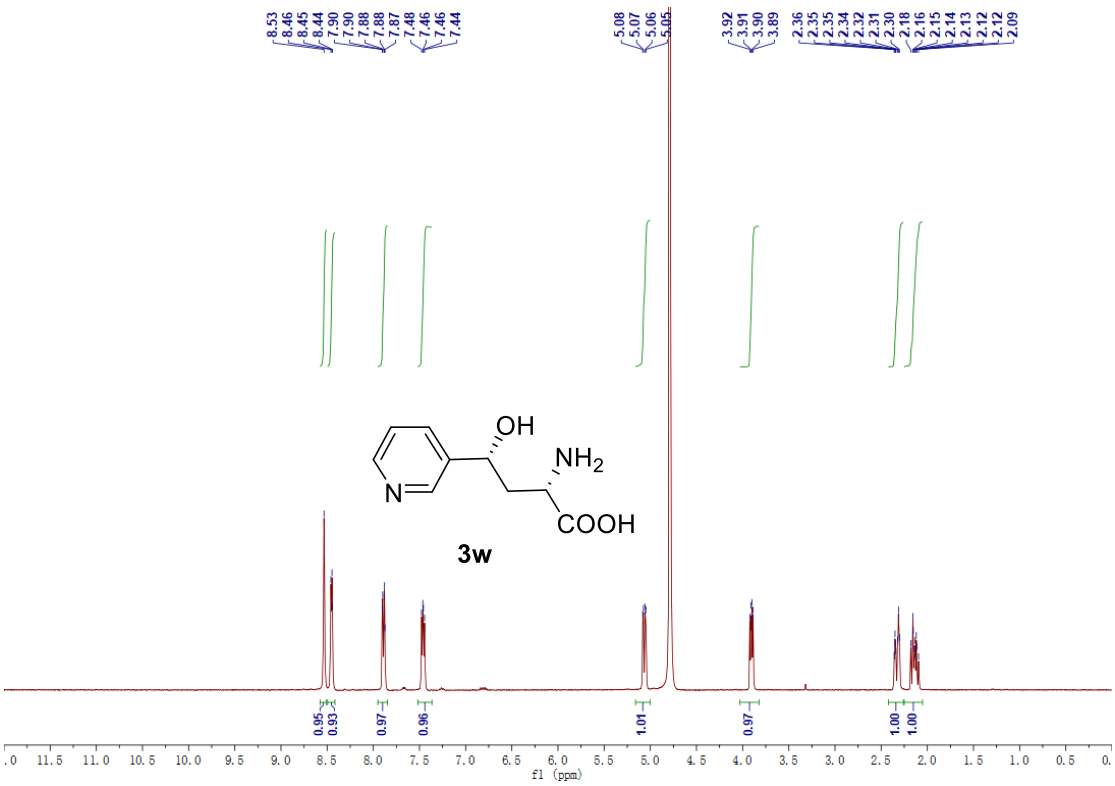
3u

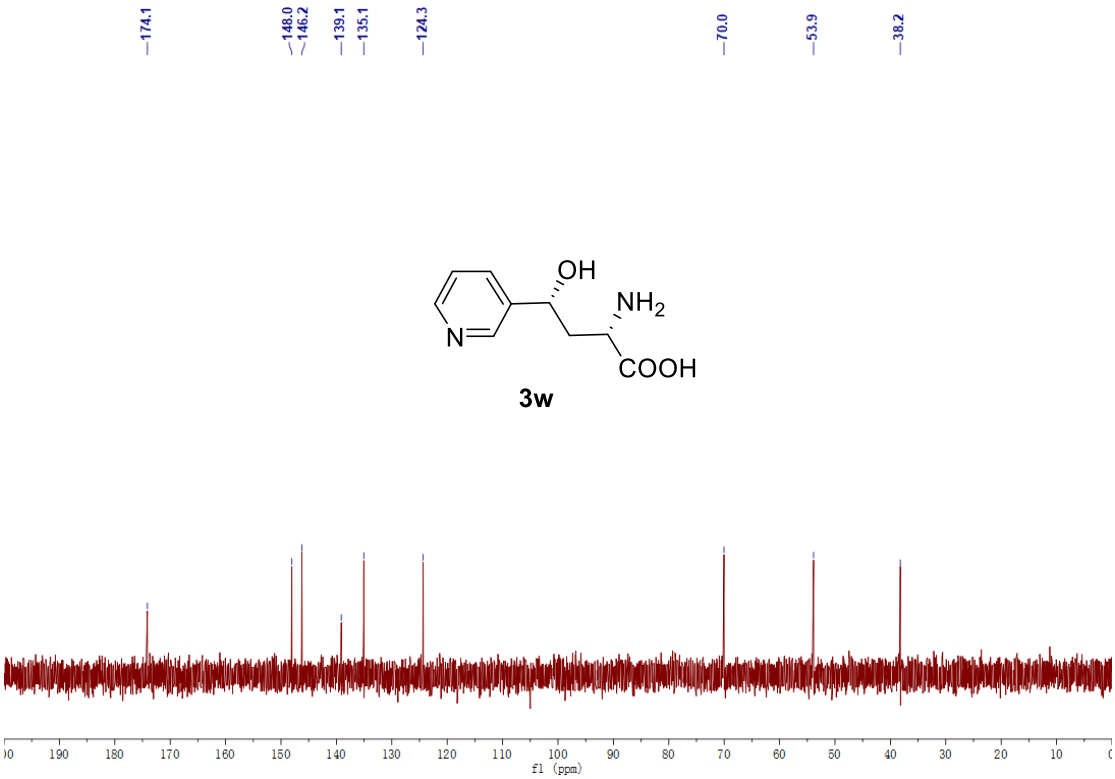

8.47
8.46
7.90
7.90
7.89
7.88
7.88
7.86
7.86
7.55
7.53
7.38
7.38
7.37
7.37
7.36
7.35
5.05
5.04
5.03
5.02
3.93
3.92
3.91
3.90
2.43
2.42
2.41
2.39
2.38
2.37
2.16
2.14
2.12
2.12
2.10
2.08
OH
NH2
N
COOH
3v
0.96
0.99
0.98
0.97
1.05
0.98
1.00
1.00
f1 (ppm)

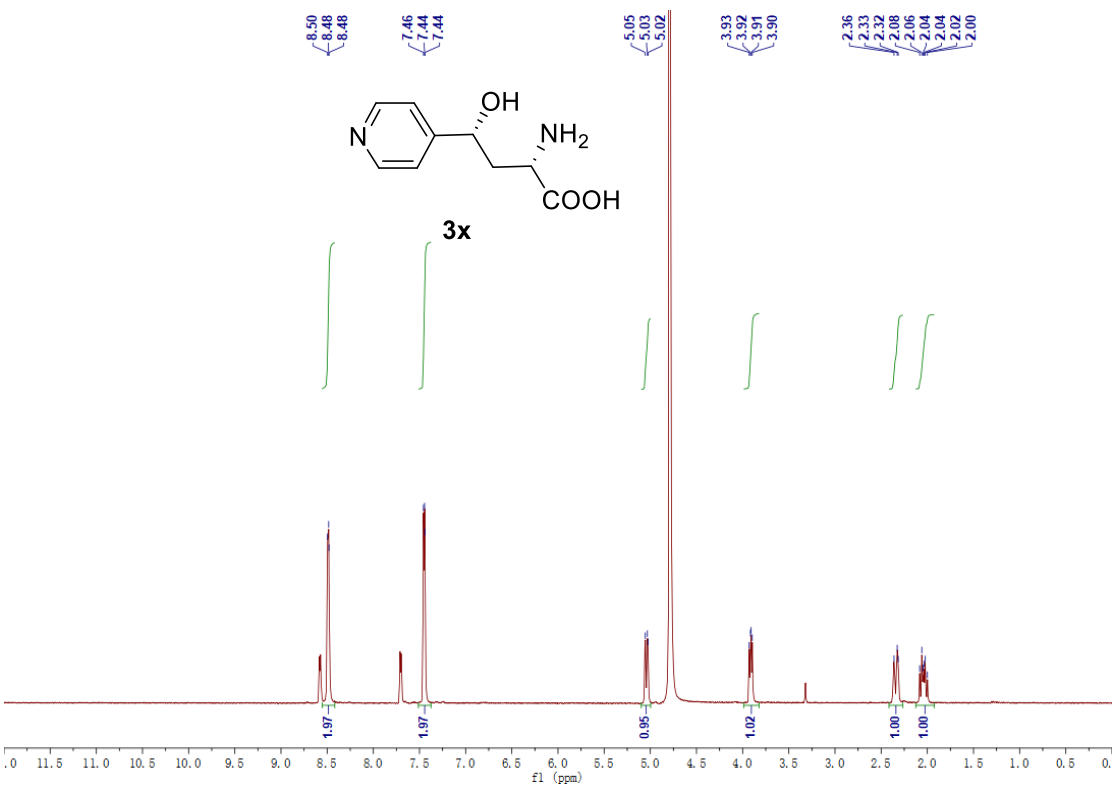

174.2
160.7
148.2
138.6
123.5
120.9
72.4
53.7
37.1

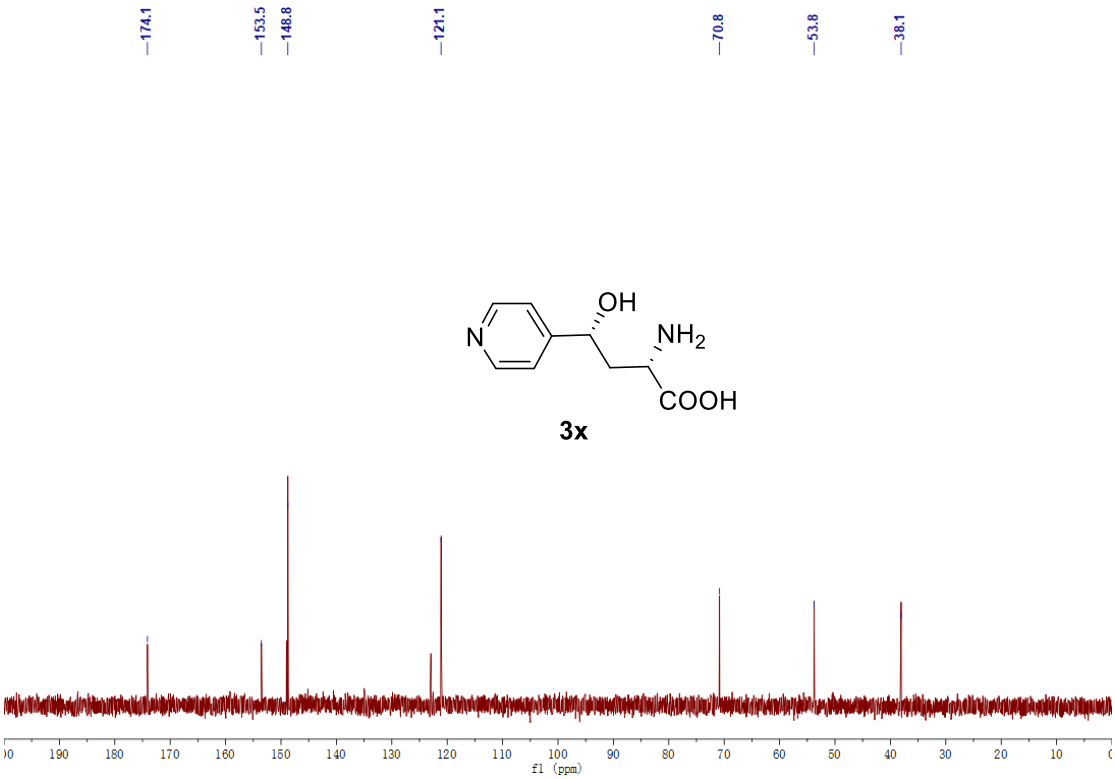

OH
NH2
N
COOH
3v


f1 (ppm)


8.53
8.46
8.45
8.44
7.90
7.90
7.88
7.88
7.87
7.48
7.46
7.46
7.44
5.08
5.07
5.06
5.05
3.92
3.91
3.90
3.89
2.36
2.35
2.35
2.34
2.32
2.31
2.30
2.18
2.16
2.15
2.14
2.13
2.12
2.12
2.09
OH
NH2
N
COOH
3w
0.95
0.93
0.97
0.96
1.01
0.97
1.00
1.00
f1 (ppm)


174.1
148.0
146.2
139.1
135.1
124.3
70.0
53.9
38.2
OH
NH2
N
COOH
3w
f1 (ppm)


8.50
8.48
8.48
7.46
7.44
7.44
5.05
5.03
5.02
3.93
3.92
3.91
3.90
2.36
2.33
2.32
2.08
2.06
2.04
2.04
2.02
2.00
OH
NH2
N
COOH
3x
1.97
1.97
0.95
1.02
1.00
1.00
f1 (ppm)


174.1
153.5
148.8
121.1
70.8
53.8
38.1
OH
NH2
N
COOH
3x
f1 (ppm)