Electronic Supplementary Material (ESI) for Chemical Communications.

Supplementary Information

Iron-catalyzed dual decarboxylative coupling of α-amino acids and dioxazolones under visible light to access amide derivatives

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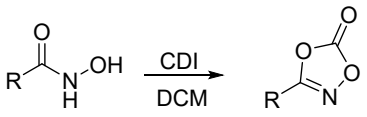
1. General Information

The commercially available reagents were used without further purification unless otherwise noted. Dry solvents were distilled over CaH_2 and stored under argon in Schlenk tubes. The available acids were obtained commercially. All reactions involving air- or moisture-sensitive reagents or intermediates were carried out in preheated glassware under an argon atmosphere using standard Schlenk techniques. Flash column chromatography was performed with silica gel (300–400 mesh). NMR spectra were recorded on Varian Inova–600 MHz, Inova–400 MHz, Bruker DRX–400 spectrometer. Data were reported as chemical shifts in ppm relative to TMS (0.00 ppm) for ^{1}H and $CDCl_3$ (77.0 ppm) for ^{13}C, respectively. The abbreviations used for explaining the multiplicities were as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. ^{19}F-NMR spectra were recorded on a BRUKER AVANCE III HD (376 MHz) spectrometer. Mass spectra were measured with an Agilent Technologies 6120 Quadrupole LC/MS. High resolution mass spectrometry (HRMS) were measured with a GCT PremierTM and BRUKERmicrOTF-Q III. Melting points were measured using INESA WRR and values were uncorrected.

2. Experimental Section

2.1 General procedure for the synthesis of dioxazolones

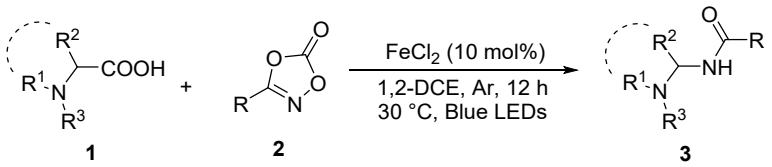
Dioxazolones (1) were prepared by reported methods.[1,2]



1

To a stirred solution of hydroxamic acid (10.0 mmol) in dichloromethane (DCM), was added 1,1'-carbonyldiimidazole (CDI 1.62 g, 10.0 mmol) at room temperature. The reaction mixture was stirred for 30 min until a high conversion of hydroxamic acid was reached (detected by TLC). Then, the reaction mixture was quenched with 1 N HCl (50 mL), and the mixture was extracted with DCM, dried over $MgSO_4$ and concentrated under reduced pressure to give the dioxazolone **1**. Product was recrystallized with acetone/hexane, if necessary.

2.2 General procedure for visible-light induced iron-catalyzed synthesis of amide derivatives

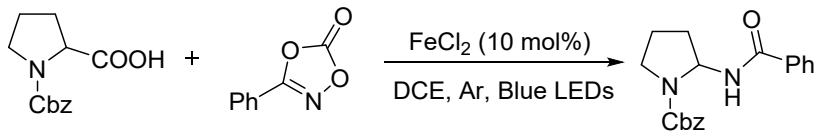


1 **2** **3**

A reaction tube was charged with the $FeCl_2$ (0.12 mg, 10 mol %), α-amino acids **1** (0.1 mmol, 1.0 equiv), dioxazolone **2** (0.12 mmol, 1.2 equiv) and 1,2-DCE (1 mL). The mixture was stirred under irradiation of 6 W Blue LEDs under an argon atmosphere at 30°C for 12 hours. The organic layers were washed with brine, dried ($MgSO_4$), and filtered. The filtrate was concentrated under reduced pressure. The residue was purified by chromatography on silica gel.

3. Optimization of Reaction Conditions

Table S1. Optimization of reaction conditions



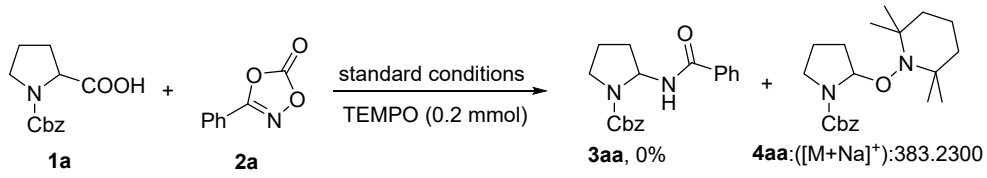
1a **2a** **3aa**

Entry[a]	Catalyst	Solvent	Yield(%)[b]
1	$FeCl_2$	1,2-DCE	88
2	$NiCl_2$	1,2-DCE	n.r.
3	$CoCl_2$	1,2-DCE	n.r.
4	$CuCl_2$	1,2-DCE	n.r.
5	$PdCl_2$	1,2-DCE	n.r.
6	$Pd(PPh_3)_4$	1,2-DCE	n.r.
7	$FeCl_2$	Dry 1,2-DCE	60
8	$FeCl_2$	DCM	58
9	$FeCl_2$	CH_3CN	56
10	$FeCl_2$	THF	44
11	$FeCl_2$	PhMe	52
12[b]	$FeCl_2$	1,2-DCE	trace
13[c]	$FeCl_2$	1,2-DCE	n.r.

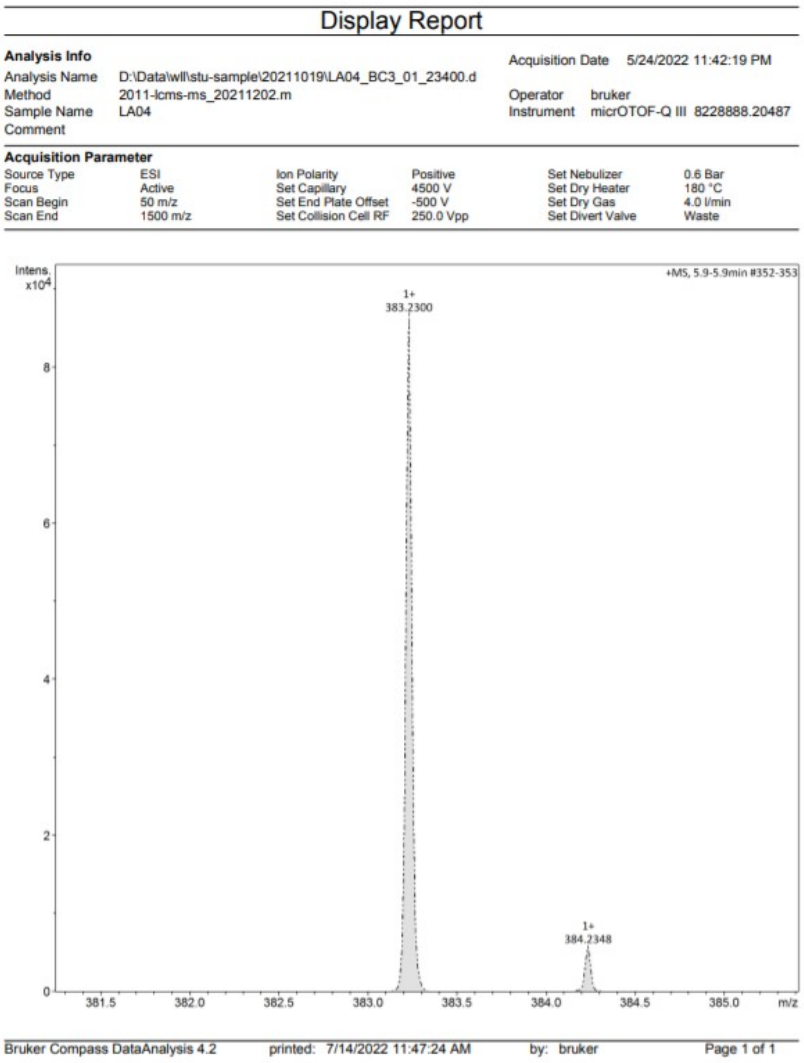
[a] Reaction conditions: **1a** (0.1 mmol), **2a** (0.12 mmol), $FeCl_2$ (10 mol%), 1,2-DCE (1 mL), Ar atmosphere, irradiation with 6 W blue LEDs (450~465 nm), 30°C , 12 h. [b] ^1H NMR yield determined using dibromomethane as an internal standard.

4. Mechanistic Experiments

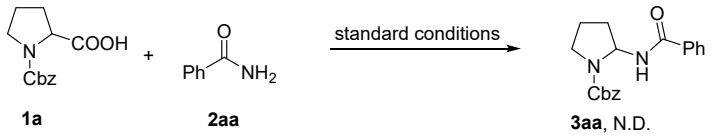
4.1 Radical trapping experiment



General procedure: A flame-dried Schlenk-tube equipped with a magnetic stir bar was charged with **1a** (0.1 mmol) in 1 mL 1,2-DCE was added **2a** (0.12 mmol), TEMPO (2,2,6,6-tetramethyl-1-piperidinyloxy) (0.2 mmol, 2 equiv.), $FeCl_2$ (10 mol%) at 30°C under an argon atmosphere, 6W Blue LEDs. The reaction mixture was then stirred for 12 hours. According to the detected result by ESI-HRMS, the *α*-amino radical could be trapped by TEMPO produce the benzyl 2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)pyrrolidine-1-carboxylate, [M+Na^+] 383.2305, found: 383.2300.



4.2 The reaction of *N*-benzyloxycarbonyl-proline with 2aa



1a **2aa** **3aa**, N.D.

A flame-dried Schlenk-tube equipped with a magnetic stir bar was charged with **1a** (0.1 mmol) in 1 mL 1,2-DCE was added **2aa** (0.12 mmol), $FeCl_2$ (10 mol%) at 30°C under an argon atmosphere, 6W Blue LEDs. The reaction mixture was then stirred for 12 hours. The solvent was then removed under reduced pressure with the aid of a rotary evaporator. The crude residue was purified by silica gel column chromatography. The desired **3aa** could not be obtained.

4.3 Light on-off experiments

Following the standard procedure, the reaction between **1a** (0.1 mmol) and **2a** (0.12 mmol) was conducted for light on-off experiment.

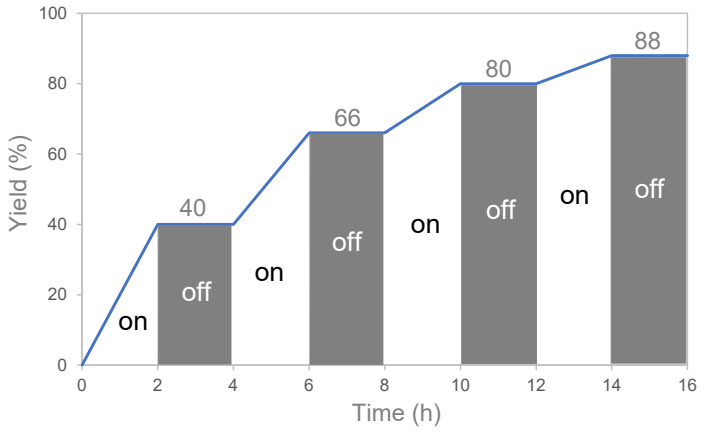


Fig. S1 Profile of the yield with light on-off over time. The yield was determined by ^{1}H NMR.

4.4 UV-Vis spectra

Agilent Technologies Carry 60 UV-Vis spectrophotometer was employed to collect the spectra.

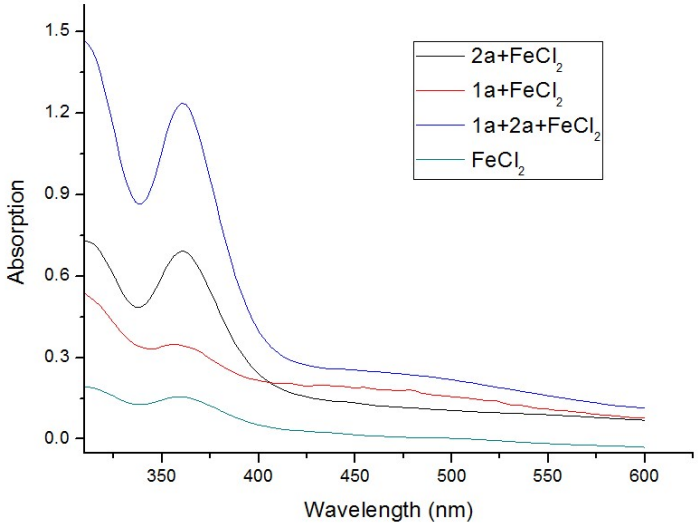


Fig. S2 UV–Vis spectra of mixed solution under standard reaction concentration.

5. Computational Studies

The B3LYP density functional method with Grimme-D3 correction[3] was employed to carry out the computational studies. To consider the solvent effect, the SMD[4] continuum model was used for geometry optimizations. The LANL2DZ basis set in conjunction with the LANL2DZ pseudopotential[5] was used for Fe atom and the 6-31G(d) basis set was used for other atoms for geometry optimizations. Vibrational frequency analyses at the same level of theory were performed on all the optimized geometries to characterize stationary points as local minima (no imaginary frequency) or transition states (one imaginary frequency). In addition, intrinsic reaction coordinate (IRC) calculations[6] were performed to verify that the transition state connects with appropriate reactant and product. The basis sets, LANL2DZ for Fe atom and 6-311++G(d,p) for the remaining atoms, were utilized for single-point energy calculations. Solution–phase Gibbs energy was determined by the sum of solvation single-point energy and thermal correction to Gibbs energy via frequency calculation. All calculations were carried out with the Gaussian 09 suite of programs[7]. The 3D structures of optimized intermediates or transition states were demonstrated using the software of CYLView.[8]

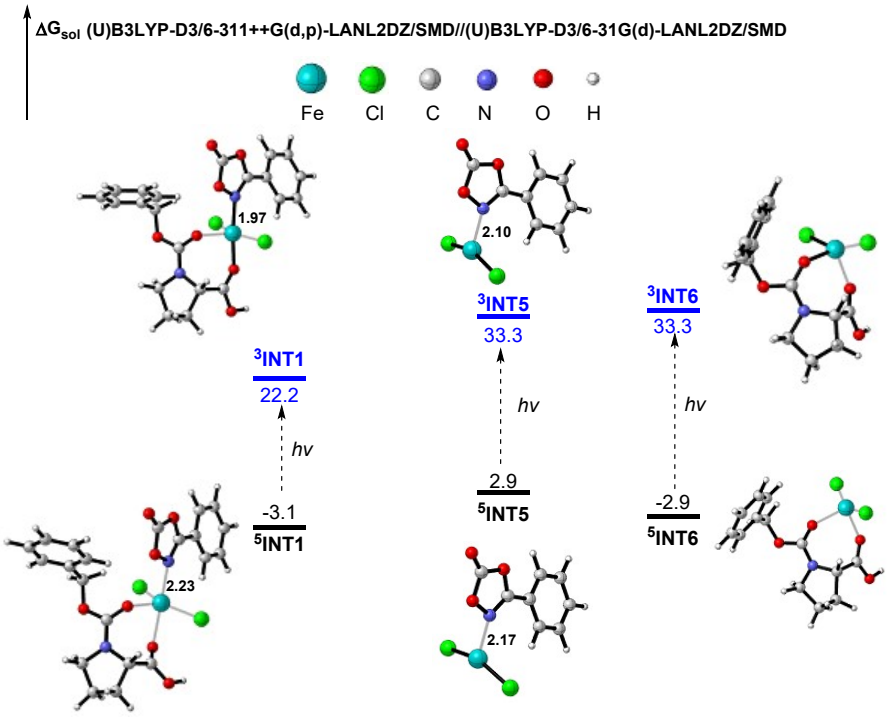


Fig. S3 Energy profiles (in kcal/mol) for different coordination forms of the iron catalyst with α-amino acids and dioxazolones. Bond lengths are shown in Å.

6. Cartesian Coordinates and Energies

1a

C	-2.82181600	-0.94715700	1.01979200
C	-2.04907200	0.62256400	-0.69639300
C	-3.31957500	1.17490200	-0.00944900
C	-3.34077700	0.45750700	1.34825000
H	-3.63646100	-1.62437200	0.73561300
H	-2.26326800	-1.40716300	1.83766200
H	-2.15694900	0.59298300	-1.78190900
H	-3.30321600	2.26492400	0.06931900
H	-4.19003800	0.88976700	-0.60910700
H	-2.65895600	0.95250900	2.04666600
H	-4.33729900	0.43619600	1.79669600
N	-1.93117600	-0.72067500	-0.12841200
C	-0.86658100	-1.52785200	-0.36000700
O	-0.60835500	-2.54900400	0.26289300
O	-0.12885200	-1.05381400	-1.40482200
C	1.24318400	-1.52484600	-1.47456500
H	1.26914400	-2.58598200	-1.22302100
H	1.52243100	-1.38734600	-2.52049300
C	2.10226600	-0.70039800	-0.55301400
C	2.38028200	-1.13888000	0.74673200
C	2.53519000	0.56967600	-0.95371300
C	3.07588200	-0.31768400	1.63550500
H	2.03004300	-2.11620700	1.06427800
C	3.22635200	1.39514300	-0.06607000
H	2.31086800	0.91854600	-1.95816800
C	3.49509200	0.95262100	1.23312600
H	3.28490300	-0.66593000	2.64321200
H	3.55525400	2.37997200	-0.38610000
H	4.03311500	1.59390400	1.92584100
C	-0.83072400	1.49815800	-0.41598000
O	-0.46438000	2.39221000	-1.14980700
O	-0.23478600	1.20592900	0.75541100
H	0.57141300	1.75782900	0.82370900

Zero-point correction= 0.270317 (Hartree/Particle)
Thermal correction to Energy= 0.286196
Thermal correction to Enthalpy= 0.287140
Thermal correction to Gibbs Free Energy= 0.225188
Sum of electronic and zero-point Energies= -859.917899
Sum of electronic and thermal Energies= -859.902020
Sum of electronic and thermal Enthalpies= -859.901076
Sum of electronic and thermal Free Energies= -859.963028
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -860.4388043

2a

C	2.74703400	-0.31163300	0.00023700
O	3.74816600	-0.96434200	-0.00018600
O	1.46177800	-0.80408200	0.00002100
O	2.65135200	1.03860300	-0.00012400
N	1.27222400	1.40951200	-0.00005400
C	0.63690100	0.28320900	0.00004600
C	-0.80461300	0.09096300	0.00003500
C	-1.65296900	1.21079900	0.00012300
C	-1.34046500	-1.20535800	-0.00006700
C	-3.03081400	1.02699100	0.00011200
H	-1.22956600	2.20972300	0.00020500
C	-2.72289200	-1.37657100	-0.00007200
H	-0.68260600	-2.06758800	-0.00013600
C	-3.56747200	-0.26483600	0.00001600
H	-3.68828900	1.89080700	0.00018200
H	-3.13916000	-2.37908600	-0.00014600
H	-4.64456700	-0.40326000	0.00001100

Zero-point correction= 0.120109 (Hartree/Particle)
Thermal correction to Energy= 0.128838
Thermal correction to Enthalpy= 0.129782
Thermal correction to Gibbs Free Energy= 0.084895
Sum of electronic and zero-point Energies= -588.173686
Sum of electronic and thermal Energies= -588.164958
Sum of electronic and thermal Enthalpies= -588.164013
Sum of electronic and thermal Free Energies= -588.208900
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -588.4545019

$FeCl_2$

Fe	0.00000000	0.09247700	0.00000000
Cl	2.29145700	-0.09419600	0.00000000
Cl	-2.29145700	-0.04724000	0.00000000

Zero-point correction= 0.001988 (Hartree/Particle)
Thermal correction to Energy= 0.006159

Thermal correction to Enthalpy= 0.007103
Thermal correction to Gibbs Free Energy= -0.026892
Sum of electronic and zero-point Energies= -1043.981601
Sum of electronic and thermal Energies= -1043.977430
Sum of electronic and thermal Enthalpies= -1043.976486
Sum of electronic and thermal Free Energies= -1044.010481
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -1044.054105

^{5}INT1

Fe	-0.51477200	-1.26514300	-0.04225500
Cl	-0.89876600	-0.76728300	2.23942500
Cl	-1.09397800	-2.53245900	-1.95329600
C	4.34483000	-1.42800500	0.98910400
C	2.92316600	-2.31256200	-0.79952400
C	4.31744600	-2.96238800	-0.87318700
C	4.84259500	-2.81381900	0.56176800
H	5.05415000	-0.63631400	0.72643000
H	4.12062800	-1.35796100	2.05517600
H	2.60925600	-1.88794700	-1.75923000
H	4.27488300	-3.99472400	-1.22162600
H	4.93115500	-2.38448800	-1.57086600
H	4.40121600	-3.58433400	1.20419100
H	5.92995000	-2.89484400	0.62620100
N	3.10893900	-1.26005900	0.19597800
C	2.24512700	-0.25091600	0.34058200
O	1.20459800	-0.12717800	-0.35176000
O	2.60810100	0.61819300	1.27914500
C	1.70887400	1.73950600	1.56726800
H	0.69344800	1.43713300	1.31859700
H	1.79528600	1.86634100	2.64676700
C	2.13822700	2.97705100	0.83141900
C	1.72186800	3.20054900	-0.48811700
C	2.95899300	3.92094900	1.46015300
C	2.11702900	4.35445900	-1.16491400
H	1.08986400	2.46796400	-0.97737700
C	3.35669200	5.07533800	0.78335500
H	3.27987600	3.75195700	2.48511900
C	2.93479400	5.29385400	-0.53029200
H	1.77939200	4.52373900	-2.18352200
H	3.98977600	5.80423900	1.28167200
H	3.23812200	6.19498100	-1.05609000
C	1.80866200	-3.26443100	-0.37418300
O	0.95162200	-2.99591400	0.45961100
O	1.83221100	-4.41145600	-1.03956300
H	1.03014900	-4.92245600	-0.79493900
C	-1.87913600	2.52379600	-1.63808700
O	-1.62322500	3.55355300	-2.18262500
O	-3.08608500	2.18112800	-1.06743100
O	-1.05021700	1.46508800	-1.46358400
N	-1.74543200	0.46187000	-0.74126200
C	-2.93994100	0.93015300	-0.55345200
C	-4.06121600	0.28936500	0.10383100
C	-4.03115400	-1.08938800	0.37590900
C	-5.17803300	1.06138100	0.46638500
C	-5.11222300	-1.68468000	1.01521500
H	-3.18312100	-1.69120300	0.07202200
C	-6.25312800	0.45316500	1.10713700
H	-5.19755600	2.12458400	0.25392700
C	-6.22113100	-0.91634800	1.38308400
H	-5.09160600	-2.74995800	1.22190000
H	-7.11555200	1.04789700	1.39075100
H	-7.06318100	-1.38742100	1.88126600

Zero-point correction= 0.396356 (Hartree/Particle)
Thermal correction to Energy= 0.428319
Thermal correction to Enthalpy= 0.429263
Thermal correction to Gibbs Free Energy= 0.325276
Sum of electronic and zero-point Energies= -2492.099865
Sum of electronic and thermal Energies= -2492.067903
Sum of electronic and thermal Enthalpies= -2492.066958
Sum of electronic and thermal Free Energies= -2492.170946
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -2492.994502

^{5}TS1

Fe	-0.74467600	-1.11943300	-0.38783100
Cl	-1.10268500	-1.01297100	1.89776700
Cl	-1.18869000	-2.36214800	-2.30780500
C	3.78467000	-1.75380600	1.45619400
C	2.68949300	-2.62967700	-0.55989300
C	4.00560100	-3.38658000	-0.30423800
C	4.23014000	-3.19762900	1.20259200

H	4.59580300	-1.03636100	1.29644200
H	3.36065900	-1.59361100	2.44894400
H	2.63176300	-2.22350900	-1.57575000
H	3.94689200	-4.43056100	-0.61247100
H	4.80002100	-2.89868500	-0.87665300
H	3.59599600	-3.88977400	1.76786500
H	5.26824600	-3.36083200	1.49963400
N	2.74418800	-1.54545400	0.42487400
C	1.95700300	-0.47837700	0.35740700
O	1.07984500	-0.34034500	-0.55192600
O	2.17219600	0.42664300	1.29195500
C	1.39517500	1.67921000	1.26209500
H	0.48591000	1.51042800	0.68919900
H	1.14749700	1.85338500	2.30883700
C	2.24018400	2.77790800	0.68713500
C	2.26660400	2.99948400	-0.69640500
C	3.03201600	3.56971300	1.52757200
C	3.07509200	4.00395200	-1.22943100
H	1.64285700	2.39538700	-1.34733700
C	3.84051400	4.57420400	0.99414700
H	3.00926100	3.39885000	2.60093500
C	3.86314000	4.79154400	-0.38586800
H	3.08430600	4.17662500	-2.30192500
H	4.44823000	5.18782600	1.65318000
H	4.48900700	5.57607300	-0.80209200
C	1.42572300	-3.45930600	-0.36559300
O	0.40629800	-3.04204500	0.17088700
O	1.51605700	-4.67686700	-0.87729800
H	0.64037300	-5.11449500	-0.79236600
C	-1.18756900	3.02273100	-1.58086800
O	-1.16504300	4.21309700	-1.55088900
O	-2.67426700	2.49768100	-0.75205400
O	-0.63030200	2.00496700	-1.94999600
N	-1.73906100	0.40221300	-0.83741700
C	-2.69370400	1.24048300	-0.52014000
C	-3.86694600	0.65070100	0.18221500
C	-4.25705800	-0.67458400	-0.06112100
C	-4.56381900	1.44122800	1.10644900
C	-5.34717800	-1.20601500	0.62387300
H	-3.72551900	-1.27194700	-0.79499900
C	-5.64876000	0.89825400	1.79012800
H	-4.25007700	2.46423400	1.28234500
C	-6.03944100	-0.42337300	1.55161700
H	-5.65774900	-2.22826200	0.43067300
H	-6.19062100	1.50595300	2.50849100
H	-6.88733000	-0.84119500	2.08646900

Zero-point correction= 0.391553 (Hartree/Particle)
Thermal correction to Energy= 0.424070
Thermal correction to Enthalpy= 0.425014
Thermal correction to Gibbs Free Energy= 0.319361
Sum of electronic and zero-point Energies= -2492.053567
Sum of electronic and thermal Energies= -2492.021051
Sum of electronic and thermal Enthalpies= -2492.020106
Sum of electronic and thermal Free Energies= -2492.125760
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -2492.954157

^{3}INT1

Fe	0.83012500	0.91131200	-0.34151300
Cl	1.08542300	0.83661700	1.99796700
Cl	1.41797900	1.26943500	-2.58467900
C	-3.46326700	2.47967400	1.24960400
C	-2.06359500	2.79474400	-0.73924200
C	-3.25133600	3.76483600	-0.78199700
C	-3.64552000	3.89916100	0.69658200
H	-4.37430500	1.88107100	1.15016800
H	-3.14232800	2.45842800	2.29329700
H	-1.94574600	2.21188100	-1.65789200
H	-3.00611500	4.71291000	-1.26095300
H	-4.05476200	3.28593400	-1.35038100
H	-2.96893300	4.59363800	1.20589300
H	-4.66814500	4.25851200	0.83123400
N	-2.41273700	1.91154700	0.37817700
C	-1.99402400	0.63653400	0.42301200
O	-1.17376300	0.15308100	-0.38451400
O	-2.54771900	-0.05622900	1.41583300
C	-2.13837300	-1.45502400	1.55832600
H	-1.09425900	-1.53963500	1.26062700
H	-2.23219900	-1.63783600	2.62927900
C	-3.03992900	-2.35745600	0.76175300
C	-2.69813000	-2.74662600	-0.54006200

C	-4.25030900	-2.79805100	1.31268800
C	-3.55418100	-3.56638900	-1.27712700
H	-1.76449800	-2.40377300	-0.97081000
C	-5.10843400	-3.61464200	0.57534500
H	-4.51624400	-2.50120000	2.32434400
C	-4.76050000	-4.00039800	-0.72197300
H	-3.27737100	-3.86800300	-2.28353700
H	-6.04341300	-3.95341500	1.01288400
H	-5.42534600	-4.63978400	-1.29621600
C	-0.70788700	3.44227400	-0.46755300
O	0.31977700	2.81676500	-0.20853100
O	-0.69186900	4.76202100	-0.52690700
H	0.22616000	5.07510900	-0.36619000
C	1.29296600	-3.13267300	-0.86405400
O	0.85238400	-4.20546300	-1.14084900
O	2.57034000	-2.86197500	-0.42974300
O	0.63662000	-1.94623800	-0.92035800
N	1.52107200	-0.93018200	-0.48017300
C	2.64879100	-1.51767400	-0.22946100
C	3.89743600	-0.93073100	0.21341600
C	4.16380200	0.43136000	-0.00720700
C	4.83696100	-1.74252100	0.87133400
C	5.35897700	0.97668800	0.44838300
H	3.45997800	1.04474600	-0.55944100
C	6.02780500	-1.18314100	1.32434600
H	4.62795000	-2.79407200	1.03512100
C	6.28783300	0.17437500	1.11793500
H	5.56875000	2.02730500	0.27422100
H	6.75203600	-1.80645200	1.83910000
H	7.21867500	0.60646300	1.47293400

Zero-point correction= 0.398049 (Hartree/Particle)
Thermal correction to Energy= 0.429063
Thermal correction to Enthalpy= 0.430007
Thermal correction to Gibbs Free Energy= 0.330875
Sum of electronic and zero-point Energies= -2492.064363
Sum of electronic and thermal Energies= -2492.033350
Sum of electronic and thermal Enthalpies= -2492.032406
Sum of electronic and thermal Free Energies= -2492.131538
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -2492.959663

^{3}TS1

Fe	0.76076000	-0.47146200	0.44841800
Cl	0.95234500	-0.20983800	-1.84424200
Cl	0.80951800	-0.91565500	2.71791800
C	-3.01406600	-2.63806500	-1.66045900
C	-1.70960500	-2.96633500	0.39458800
C	-2.67862300	-4.13942300	0.19316300
C	-2.93429000	-4.13004000	-1.32104300
H	-4.02789700	-2.24317400	-1.54223700
H	-2.65508700	-2.39604300	-2.66264000
H	-1.79027900	-2.50279500	1.38325800
H	-2.28128400	-5.08254300	0.56803600
H	-3.59904700	-3.90943200	0.73838800
H	-2.09523700	-4.59429100	-1.85047500
H	-3.84904200	-4.65805400	-1.59841800
N	-2.13416100	-2.01782000	-0.64438600
C	-1.95646300	-0.69951400	-0.51423300
O	-1.24775900	-0.19935500	0.40156400
O	-2.59294900	0.02434000	-1.41495000
C	-2.45695300	1.48677900	-1.31887000
H	-1.41741800	1.72843600	-1.10408100
H	-2.71663200	1.81410800	-2.32637000
C	-3.39597900	2.03795800	-0.28241500
C	-2.89621400	2.64246000	0.87644800
C	-4.78191600	1.93538800	-0.46469200
C	-3.77407900	3.14352700	1.84046900
H	-1.82308400	2.72536500	1.01020000
C	-5.65788400	2.42805400	0.50188600
H	-5.17153200	1.46725500	-1.36535000
C	-5.15399200	3.03431900	1.65703400
H	-3.37869300	3.61567600	2.73559700
H	-6.73102300	2.34584600	0.35320700
H	-5.83602000	3.42239000	2.40862900
C	-0.23244800	-3.30469200	0.21688800
O	0.66222800	-2.45807800	0.14234100
O	0.05193300	-4.58730800	0.16133200
H	1.02534700	-4.70306200	0.07385500
C	1.08624000	3.36674900	-0.76847400
O	1.11232700	4.20826100	-1.62333500
O	2.59839700	2.72017500	-0.59994600

O	0.32753000	2.82971200	0.03413300
N	1.64846400	1.11813600	0.74993800
C	2.65955400	1.61646000	0.05717600
C	3.95834200	0.90385900	0.08693900
C	4.18614900	-0.13878400	1.00103700
C	4.94812600	1.25785700	-0.84269400
C	5.39435800	-0.82881700	0.97252400
H	3.43072700	-0.39259100	1.73737300
C	6.15321900	0.56059200	-0.86338200
H	4.76094400	2.06203400	-1.54474800
C	6.37692100	-0.48265900	0.03998900
H	5.57212300	-1.63105100	1.68213500
H	6.91728300	0.82904600	-1.58635900
H	7.31824100	-1.02395900	0.01942100

Zero-point correction= 0.392656 (Hartree/Particle)
Thermal correction to Energy= 0.424460
Thermal correction to Enthalpy= 0.425404
Thermal correction to Gibbs Free Energy= 0.323462
Sum of electronic and zero-point Energies= -2492.037343
Sum of electronic and thermal Energies= -2492.005539
Sum of electronic and thermal Enthalpies= -2492.004594
Sum of electronic and thermal Free Energies= -2492.106537
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -2492.934458

^{3}INT2

Fe	-0.56617500	0.91628000	0.32802700
Cl	-0.89120300	0.81044200	-1.97603600
Cl	-1.15768500	1.83729000	2.38058600
C	4.03278100	1.17369300	-1.38968100
C	2.86816800	2.03890900	0.59085800
C	4.27426200	2.64904800	0.50190200
C	4.60869100	2.53796800	-0.99280500
H	4.75157300	0.36288300	-1.23405700
H	3.67299500	1.13321000	-2.41955200
H	2.65577800	1.58838600	1.56646400
H	4.31466600	3.66741500	0.88777200
H	4.95136200	2.02563100	1.09387200
H	4.10775600	3.33592600	-1.55202700
H	5.68042800	2.60003400	-1.19319700
N	2.90306800	1.00519600	-0.45005600
C	2.08040100	-0.04497800	-0.43236500
O	1.16259600	-0.18031500	0.41802200
O	2.32173900	-0.93635500	-1.38281800
C	1.42769100	-2.09503900	-1.44812800
H	0.39514800	-1.74903600	-1.40760900
H	1.63487200	-2.49374700	-2.44312200
C	1.72916900	-3.09684500	-0.36734800
C	0.69884500	-3.58097100	0.44536000
C	3.03556000	-3.56681100	-0.18024700
C	0.97095400	-4.53165400	1.43167300
H	-0.31171900	-3.21123000	0.29947700
C	3.30861100	-4.50777200	0.81230500
H	3.83768500	-3.19081500	-0.81019100
C	2.27524500	-4.99388400	1.61928300
H	0.16499000	-4.90384100	2.05811600
H	4.32459900	-4.86629900	0.95308200
H	2.48734800	-5.72953400	2.39019000
C	1.71794000	3.00474100	0.31545400
O	0.58651800	2.65028000	-0.00892200
O	2.01966500	4.28137000	0.46610600
H	1.20959000	4.81717300	0.31110200
O	-2.30121800	-2.14676500	-0.84976900
N	-1.60477900	-0.64616600	0.63165600
C	-2.60128600	-1.13662100	-0.20194000
C	-3.94392400	-0.51923000	-0.19251600
C	-4.22825500	0.59123200	0.61701100
C	-4.94160600	-1.06785400	-1.01258800
C	-5.50326600	1.15269700	0.59714500
H	-3.46034200	1.00921900	1.25962400
C	-6.21161400	-0.50034400	-1.03095300
H	-4.70508000	-1.92913800	-1.62846600
C	-6.49311000	0.61005400	-0.22633400
H	-5.72427900	2.01125500	1.22415500
H	-6.98367400	-0.91952600	-1.66916800
H	-7.48604200	1.05034800	-0.24118700

Zero-point correction= 0.379018 (Hartree/Particle)
Thermal correction to Energy= 0.408500
Thermal correction to Enthalpy= 0.409444
Thermal correction to Gibbs Free Energy= 0.313907
Sum of electronic and zero-point Energies= -2303.491964

Sum of electronic and thermal Energies= -2303.462482
Sum of electronic and thermal Enthalpies= -2303.461538
Sum of electronic and thermal Free Energies= -2303.557075
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -2304.310665

^{5}INT2

Fe	0.36865300	-0.81275600	-0.64988500
Cl	0.04254400	-0.96085400	-2.86588500
Cl	0.44677300	-2.85126900	0.30643400
C	-4.77902900	0.51727600	0.02477700
C	-3.37626900	-1.11388900	1.21230300
C	-4.80854200	-1.13637800	1.78658400
C	-5.65683200	-0.58367400	0.63175700
H	-4.93721100	1.48744900	0.50687600
H	-4.90861600	0.63209500	-1.05254400
H	-2.61567300	-0.99099100	1.98612400
H	-5.10424700	-2.13709500	2.10628200
H	-4.84856600	-0.46867300	2.65264400
H	-5.83876600	-1.36654700	-0.11177400
H	-6.62175400	-0.19497100	0.96443700
N	-3.40880000	0.04869500	0.32473100
C	-2.30737600	0.54810200	-0.21242900
O	-1.15787700	0.11839500	0.10612900
O	-2.50206300	1.54647500	-1.05928300
C	-1.34373200	2.31302600	-1.51241300
H	-0.63658000	1.64221400	-2.00270500
H	-1.78154000	2.96804600	-2.26831500
C	-0.69843000	3.08671000	-0.39386600
C	0.69544900	3.18446000	-0.34182400
C	-1.47381700	3.72938200	0.57918300
C	1.31058300	3.91632600	0.67582700
H	1.30342400	2.67662300	-1.08364200
C	-0.85728500	4.45178800	1.60120700
H	-2.55741300	3.65770200	0.54178400
C	0.53669800	4.54799500	1.65117400
H	2.39471300	3.97862400	0.71026800
H	-1.46445600	4.94247800	2.35681700
H	1.01511900	5.11039600	2.44808400
C	-3.05311400	-2.37019800	0.40644200
O	-2.96282800	-2.41545000	-0.80104700
O	-2.89903200	-3.42675400	1.21732400
H	-2.66561800	-4.19783500	0.65922100
O	3.27339300	1.28931100	-1.42004700
N	1.84277900	0.14939200	-0.18976700
C	3.11940200	0.42234900	-0.54132000
C	4.22465700	-0.27978800	0.15092200
C	3.96394100	-1.29216300	1.08536900
C	5.54380100	0.08503300	-0.14837600
C	5.02443200	-1.93789400	1.71692800
H	2.93978300	-1.57575000	1.30848600
C	6.60007500	-0.56342500	0.48647200
H	5.72374600	0.87112900	-0.87445100
C	6.34095500	-1.57383600	1.41844100
H	4.82580900	-2.72445800	2.43862900
H	7.62397400	-0.28354200	0.25727400
H	7.16650300	-2.07879700	1.91185200

Zero-point correction= 0.378381 (Hartree/Particle)
Thermal correction to Energy= 0.408650
Thermal correction to Enthalpy= 0.409594
Thermal correction to Gibbs Free Energy= 0.309134
Sum of electronic and zero-point Energies= -2303.504072
Sum of electronic and thermal Energies= -2303.473803
Sum of electronic and thermal Enthalpies= -2303.472859
Sum of electronic and thermal Free Energies= -2303.573319
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy =-2304.328095

^{5}TS2

Fe	1.70137400	0.65007600	0.78869300
Cl	0.90363600	-0.53906200	2.48859400
Cl	2.90540300	2.41922400	1.42938800
C	-2.84702400	3.03207200	-0.07173500
C	-1.51227900	1.87138000	-1.76291200
C	-1.42055000	3.39990500	-1.98434000
C	-1.77411800	3.98734300	-0.60965700
H	-3.85338800	3.33193700	-0.38718300
H	-2.83654700	2.94445300	1.01596400
H	-1.82448500	1.33841300	-2.66333500
H	-0.43896600	3.70831200	-2.35339600
H	-2.16888700	3.68031000	-2.73199400
H	-0.89755600	3.96808600	0.04557400

H	-2.13228300	5.01782400	-0.67569200
N	-2.48660300	1.74501600	-0.69087400
C	-2.68171300	0.51452100	-0.14837300
O	-2.14642800	-0.50272600	-0.58108500
O	-3.51649800	0.55889000	0.91090500
C	-3.80771500	-0.72083100	1.53615800
H	-2.88535600	-1.29933400	1.60774800
H	-4.14222000	-0.44409200	2.53774200
C	-4.87727100	-1.47184100	0.78758000
C	-6.20790000	-1.03575700	0.84273800
C	-4.55861600	-2.59555900	0.01692900
C	-7.20460500	-1.71285700	0.13997000
H	-6.46011100	-0.16281600	1.43995300
C	-5.55573500	-3.28000600	-0.68102800
H	-3.52595400	-2.92544700	-0.03911100
C	-6.87962700	-2.83890000	-0.62220000
H	-8.23353700	-1.36743000	0.19053400
H	-5.29817100	-4.15400400	-1.27294300
H	-7.65578300	-3.37016900	-1.16624800
C	-0.17169400	1.28693700	-1.34384700
O	0.17129800	1.41603600	-0.11253200
O	0.55757500	0.75335600	-2.22855000
H	1.55371500	0.27585900	-1.68143700
O	2.35142500	-2.22555500	-1.45922000
N	2.38071600	-0.15193200	-0.82105800
C	3.07835700	-1.32401800	-1.02024300
C	4.49475100	-1.44660900	-0.67211400
C	5.19934300	-0.34955800	-0.15216800
C	5.13615500	-2.68132500	-0.85930500
C	6.54170700	-0.49264400	0.18717900
H	4.70119200	0.60485500	-0.01421700
C	6.47711700	-2.81679900	-0.51675000
H	4.57629000	-3.51809500	-1.26422700
C	7.17834800	-1.72433100	0.00677300
H	7.08987700	0.35221300	0.59203600
H	6.97824700	-3.76979800	-0.65448400
H	8.22519000	-1.83413300	0.27446400

Zero-point correction= 0.373507 (Hartree/Particle)
Thermal correction to Energy= 0.402835
Thermal correction to Enthalpy= 0.403779
Thermal correction to Gibbs Free Energy= 0.305158
Sum of electronic and zero-point Energies= -2303.490499
Sum of electronic and thermal Energies= -2303.461171
Sum of electronic and thermal Enthalpies= -2303.460227
Sum of electronic and thermal Free Energies= -2303.558849
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy =-2304.308328

^{5}INT3

Fe	-1.73775100	0.66737100	-0.55497600
Cl	-1.06337800	-0.93387200	-1.94960700
Cl	-2.76239300	2.31661300	-1.67026500
C	2.70099200	2.80398400	-0.58495800
C	1.60271100	2.21896100	1.52451500
C	1.61909200	3.75447200	1.35479900
C	1.77150400	3.94951600	-0.16145000
H	3.75664600	3.09602900	-0.53572400
H	2.49188800	2.43588300	-1.59114700
H	2.01101300	1.90068300	2.48573100
H	0.72406100	4.22565700	1.76911900
H	2.49047500	4.15130500	1.88571300
H	0.80050000	3.84081000	-0.65441400
H	2.18055100	4.92968100	-0.41972900
N	2.42164600	1.75673300	0.41281100
C	2.53918400	0.42044900	0.20874300
O	2.08990200	-0.42366700	0.98073700
O	3.20214000	0.14808500	-0.93729000
C	3.43774800	-1.25724200	-1.22472400
H	2.59752200	-1.83691500	-0.83986400
H	3.44928400	-1.30905500	-2.31458400
C	4.75012700	-1.71596000	-0.64454700
C	5.91219200	-1.68862700	-1.42529300
C	4.83272300	-2.14638000	0.68732700
C	7.13854200	-2.08452000	-0.88809000
H	5.85284800	-1.35745800	-2.45925600
C	6.05777500	-2.54085500	1.22625200
H	3.93395100	-2.15917700	1.29540100
C	7.21303400	-2.51072600	0.43998800
H	8.03285200	-2.06184800	-1.50477600
H	6.11109000	-2.87455700	2.25898700
H	8.16611500	-2.82044000	0.85997200

C	0.18080700	1.66448200	1.44121400
O	-0.25144900	1.48472300	0.20467700
O	-0.49858700	1.46647000	2.44403900
H	-2.01795600	0.56153200	1.96469100
O	-2.76075300	-1.64898900	2.42829000
N	-2.56481700	0.12887300	1.18577600
C	-3.30393800	-0.98961400	1.52640700
C	-4.48973500	-1.37026400	0.77114200
C	-5.05498500	-0.47642200	-0.15296800
C	-5.05927500	-2.63743500	0.98062800
C	-6.17970200	-0.85875600	-0.87755700
H	-4.62964000	0.51172000	-0.29554800
C	-6.18161200	-3.01123600	0.25131900
H	-4.61181000	-3.31508200	1.70020500
C	-6.73874900	-2.12457100	-0.67815800
H	-6.61968300	-0.17215000	-1.59352600
H	-6.62345400	-3.99110200	0.40139200
H	-7.61502600	-2.42150800	-1.24672900

Zero-point correction= 0.377961 (Hartree/Particle)
Thermal correction to Energy= 0.407543
Thermal correction to Enthalpy= 0.408487
Thermal correction to Gibbs Free Energy= 0.309791
Sum of electronic and zero-point Energies= -2303.493426
Sum of electronic and thermal Energies= -2303.463844
Sum of electronic and thermal Enthalpies= -2303.462899
Sum of electronic and thermal Free Energies= -2303.561596
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -2304.314478

^{5}TS3

Fe	1.87844000	-0.04330400	0.70258000
Cl	1.15332800	-2.18148900	0.44739200
Cl	1.44142800	0.58524300	2.86134500
C	-2.42450200	2.47914700	1.11048000
C	-1.77387500	2.38718900	-1.15902900
C	-1.62192900	3.82334000	-0.75163000
C	-1.58787800	3.73048200	0.78801700
H	-3.47236900	2.70824900	1.32520000
H	-2.01770600	1.87504700	1.92186000
H	-1.90408400	2.02694300	-2.17367300
H	-0.74770400	4.30243900	-1.19527900
H	-2.51264700	4.36369800	-1.10524600
H	-0.55823300	3.58561800	1.12928600
H	-1.98873700	4.62191200	1.27284200
N	-2.37084900	1.71165300	-0.15891000
C	-2.72431900	0.35411800	-0.29890700
O	-2.56210600	-0.25527300	-1.33446600
O	-3.22165300	-0.10323000	0.84480900
C	-3.68415100	-1.49522800	0.83139300
H	-2.93457800	-2.10205300	0.32180200
H	-3.70944800	-1.75315100	1.89039800
C	-5.03879800	-1.60325700	0.18838300
C	-6.16637900	-1.09103900	0.84470200
C	-5.18609000	-2.18978700	-1.07344100
C	-7.42374200	-1.16347300	0.24612300
H	-6.05486200	-0.63598600	1.82573400
C	-6.44596900	-2.27119100	-1.66976600
H	-4.31142400	-2.57731600	-1.58684500
C	-7.56512800	-1.75576500	-1.01252200
H	-8.29305700	-0.76478700	0.76145800
H	-6.55212800	-2.73215300	-2.64771600
H	-8.54519800	-1.81671900	-1.47742100
C	0.24472500	1.68859100	-1.12335400
O	0.26112200	0.90031700	-0.18113700
O	0.85768000	2.23012300	-1.98735800
H	2.87964600	2.16677300	-0.04120300
O	4.77734800	1.86917800	-1.45941200
N	3.18065000	1.19298800	0.03389100
C	4.32206800	0.99935400	-0.71336600
C	4.99691500	-0.32769900	-0.56452100
C	4.94456500	-1.05409700	0.63395900
C	5.74666300	-0.82580400	-1.63928000
C	5.60439400	-2.27848500	0.74622300
H	4.39556100	-0.65209400	1.48229100
C	6.39750200	-2.05219400	-1.53000500
H	5.80150500	-0.24650700	-2.55518900
C	6.32702700	-2.78084800	-0.33723200
H	5.55885800	-2.83266300	1.67909700
H	6.96240200	-2.44183400	-2.37194300
H	6.83958700	-3.73486400	-0.25275500

Zero-point correction= 0.377362 (Hartree/Particle)

Thermal correction to Energy= 0.406875
Thermal correction to Enthalpy= 0.407819
Thermal correction to Gibbs Free Energy= 0.310252
Sum of electronic and zero-point Energies= -2303.500943
Sum of electronic and thermal Energies= -2303.471430
Sum of electronic and thermal Enthalpies= -2303.470486
Sum of electronic and thermal Free Energies= -2303.568052
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -2304.328488

^{5}INT4

Fe	-1.90044100	1.43122300	-0.71450500
Cl	0.19909000	2.46854300	-1.25977100
Cl	-3.05842100	2.82852700	0.75512500
C	0.83925000	0.92588400	2.05901300
C	0.02302600	-0.97286300	0.96292800
C	-0.86306000	-0.82965200	2.13856700
C	-0.52401300	0.57651500	2.68538500
H	1.68852900	0.74831300	2.72235400
H	0.89625500	1.93328700	1.64910900
H	0.01800600	-1.78558400	0.24128300
H	-1.91299900	-0.97973600	1.87072400
H	-0.60191800	-1.63991100	2.83618000
H	-1.27960500	1.29535600	2.35943500
H	-0.47881000	0.59481400	3.77489800
N	0.93462800	-0.04849700	0.93258200
C	1.93859600	-0.00704100	-0.10538400
O	1.87966200	-0.73670400	-1.06513400
O	2.84650400	0.88467600	0.21731900
C	3.96871100	1.05680800	-0.72408400
H	3.58406700	0.91780100	-1.73441100
H	4.25713400	2.09655800	-0.57403200
C	5.07539900	0.10156500	-0.38419100
C	5.98200600	0.41981400	0.63566700
C	5.19222800	-1.12403000	-1.05205100
C	6.99202800	-0.47598200	0.98565100
H	5.89345800	1.37231100	1.15195700
C	6.20482600	-2.01946200	-0.70403500
H	4.48827000	-1.37288700	-1.84020000
C	7.10400700	-1.69744900	0.31549200
H	7.69251200	-0.22099400	1.77577100
H	6.29237500	-2.96655000	-1.22869200
H	7.89255800	-2.39438200	0.58516100
H	-0.59191100	-0.56771400	-1.69250900
O	-1.48272200	-2.70953600	-1.08465400
N	-1.52294200	-0.42756000	-1.29801300
C	-2.09610400	-1.62675300	-1.02212300
C	-3.51818100	-1.60265700	-0.54031400
C	-4.42021900	-0.59294100	-0.90216700
C	-3.95378200	-2.63934000	0.29743900
C	-5.72811600	-0.60434500	-0.41591000
H	-4.10363200	0.19235000	-1.58322400
C	-5.25705000	-2.64749100	0.79119400
H	-3.25497500	-3.42842200	0.55489900
C	-6.14685600	-1.62855700	0.43646700
H	-6.41898500	0.18150200	-0.70739200
H	-5.58169300	-3.44832000	1.44964600
H	-7.16407100	-1.63700200	0.81768000

Zero-point correction= 0.365687 (Hartree/Particle)
Thermal correction to Energy= 0.392877
Thermal correction to Enthalpy= 0.393821
Thermal correction to Gibbs Free Energy= 0.301825
Sum of electronic and zero-point Energies= -2114.996473
Sum of electronic and thermal Energies= -2114.969284
Sum of electronic and thermal Enthalpies= -2114.968339
Sum of electronic and thermal Free Energies= -2115.060336
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -2115.748129

^{5}TS4

Fe	-1.77143600	1.50105300	-0.48892000
Cl	0.26233800	2.46277500	-1.19478000
Cl	-2.92088800	3.05173100	0.81023600
C	0.73579600	0.54869400	1.89519700
C	-0.14163700	-1.22185000	0.62046800
C	-0.98976100	-1.16377800	1.84156900
C	-0.67590200	0.23060200	2.41654300
H	1.52850400	0.27829800	2.59689200
H	0.86823900	1.58081600	1.57308200
H	-0.07845800	-2.04716400	-0.07755600
H	-2.04491500	-1.35108000	1.63937500
H	-0.63480900	-1.97106300	2.50043600

H	-1.39068100	0.95709700	2.02032900
H	-0.72349400	0.25893600	3.50607600
N	0.84317800	-0.34820200	0.70957800
C	1.86600100	-0.28021900	-0.27754300
O	1.81325700	-0.94066600	-1.29249400
O	2.80444100	0.55889600	0.11572700
C	3.92351100	0.79270200	-0.80722500
H	3.60375500	0.48943300	-1.80435800
H	4.07353500	1.87165300	-0.77827500
C	5.13680900	0.04405000	-0.33535400
C	6.19068200	0.72919900	0.27840700
C	5.21533100	-1.34800400	-0.48595800
C	7.31362600	0.03581200	0.73474400
H	6.13013600	1.80807500	0.39539800
C	6.33184700	-2.04205700	-0.02149500
H	4.40106100	-1.88273300	-0.96708000
C	7.38346200	-1.35081100	0.58855500
H	8.12918200	0.57727800	1.20557200
H	6.38587800	-3.12055100	-0.14009400
H	8.25493700	-1.89223300	0.94587400
H	-0.68325600	-0.52512300	-1.69513400
O	-1.85802000	-2.60491500	-1.64088800
N	-1.50335900	-0.40848700	-1.09677200
C	-2.28125300	-1.53828200	-1.17672500
C	-3.64849900	-1.46599500	-0.56805800
C	-4.45558400	-0.32492900	-0.66387400
C	-4.13610500	-2.59612600	0.10562200
C	-5.71919300	-0.30109500	-0.07228500
H	-4.10772200	0.53899600	-1.22523100
C	-5.39017400	-2.56671100	0.71228800
H	-3.51475900	-3.48442100	0.15744200
C	-6.18357300	-1.41811000	0.62542500
H	-6.33831400	0.58689800	-0.15915200
H	-5.75157200	-3.43827800	1.25062800
H	-7.16300000	-1.39706700	1.09473400

Zero-point correction= 0.367358 (Hartree/Particle)
Thermal correction to Energy= 0.393038
Thermal correction to Enthalpy= 0.393983
Thermal correction to Gibbs Free Energy= 0.306016
Sum of electronic and zero-point Energies= -2114.993282
Sum of electronic and thermal Energies= -2114.967602
Sum of electronic and thermal Enthalpies= -2114.966658
Sum of electronic and thermal Free Energies= -2115.054624
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -2115.746081

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C	-0.24362500	-2.22693100	-0.24769500
C	0.88574900	-0.11706500	0.29757900
C	1.56767600	-1.28393400	1.01646700
C	1.21210000	-2.49937500	0.15160000
H	-0.95082600	-2.64785000	0.47617000
H	-0.49883700	-2.60995800	-1.23870400
H	0.60010400	0.68444900	0.98403900
H	2.63409600	-1.14103800	1.16857200
H	1.09448600	-1.37385100	2.00086600
H	1.84829900	-2.52733000	-0.73905100
H	1.32347500	-3.44744900	0.68340100
N	-0.31769800	-0.75580500	-0.22412100
C	-1.34792500	-0.01078200	-0.69152100
O	-1.33503900	1.21740900	-0.75252400
O	-2.37524600	-0.79372300	-1.09401500
C	-3.56414900	-0.10341500	-1.56837400
H	-3.25746500	0.81802200	-2.06516500
H	-3.99586600	-0.78839900	-2.30003200
C	-4.52512600	0.16219600	-0.43976900
C	-5.52765300	-0.76704100	-0.13732600
C	-4.41419500	1.32364600	0.33679500
C	-6.40813400	-0.54206900	0.92194200
H	-5.61869900	-1.66851900	-0.73846400
C	-5.29301100	1.54989100	1.39638800
H	-3.63108200	2.03970600	0.10900800
C	-6.29157200	0.61787100	1.69096800
H	-7.18480200	-1.26854900	1.14450300
H	-5.20104500	2.45494300	1.99060800
H	-6.97757400	0.79640200	2.51446900
H	0.92595700	1.02040700	-1.39996800
O	2.88527800	2.26157000	-1.45710700
N	1.60489400	0.48545300	-0.85893000
C	2.78233900	1.20661400	-0.82941100
C	3.97620100	0.64187200	-0.12617800

C	4.41992400	-0.66223700	-0.38169600
C	4.72885300	1.47883700	0.70664900
C	5.59525200	-1.12925400	0.20693300
H	3.84915900	-1.30221400	-1.04725400
C	5.88925000	1.00198700	1.31415200
H	4.39440200	2.49724800	0.87912400
C	6.32524800	-0.30196600	1.06344900
H	5.93960900	-2.13796600	-0.00261400
H	6.45807400	1.64905800	1.97575100
H	7.23500700	-0.66977700	1.52955100

Zero-point correction= 0.364238 (Hartree/Particle)
Thermal correction to Energy= 0.385114
Thermal correction to Enthalpy= 0.386058
Thermal correction to Gibbs Free Energy= 0.309025
Sum of electronic and zero-point Energies= -1071.027883
Sum of electronic and thermal Energies= -1071.007007
Sum of electronic and thermal Enthalpies= -1071.006062
Sum of electronic and thermal Free Energies= -1071.083095
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -1071.688483

CO_2

C	0.00000000	0.00000000	-0.00000100
O	0.00000000	0.00000000	1.16886400
O	0.00000000	0.00000000	-1.16886300

Zero-point correction= 0.011532 (Hartree/Particle)
Thermal correction to Energy= 0.014185
Thermal correction to Enthalpy= 0.015129
Thermal correction to Gibbs Free Energy= -0.009844
Sum of electronic and zero-point Energies= -188.569859
Sum of electronic and thermal Energies= -188.567205
Sum of electronic and thermal Enthalpies= -188.566261
Sum of electronic and thermal Free Energies= -188.591234
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -188.6475876

^{5}INT5

C	-0.16090400	3.11537700	-0.23003800
O	-0.16843800	4.30536900	-0.25601200
O	-1.26930700	2.29362900	-0.17459300
O	0.92682700	2.30167200	-0.25643800
N	0.47897500	0.95967200	-0.19212900
C	-0.82105400	1.01524400	-0.16161400
C	-1.77396000	-0.07628700	-0.10688100
C	-1.38880100	-1.38765500	-0.43960100
C	-3.09753400	0.19420800	0.28350500
C	-2.31592900	-2.41922800	-0.35902000
H	-0.39049900	-1.59581200	-0.80359800
C	-4.01778000	-0.84720000	0.35490600
H	-3.39656500	1.20586600	0.53400700
C	-3.62899200	-2.15187100	0.04000900
H	-2.01704900	-3.42873200	-0.62225000
H	-5.03959300	-0.64029500	0.65578300
H	-4.35118500	-2.96074800	0.09576300
Fe	1.90458300	-0.64647600	0.13253700
Cl	2.22194900	-1.43809100	-2.00929100
Cl	1.87452000	-0.81782000	2.43564300

Zero-point correction= 0.124717 (Hartree/Particle)
Thermal correction to Energy= 0.138834
Thermal correction to Enthalpy= 0.139778
Thermal correction to Gibbs Free Energy= 0.080194
Sum of electronic and zero-point Energies= -1632.161543
Sum of electronic and thermal Energies= -1632.147426
Sum of electronic and thermal Enthalpies= -1632.146482
Sum of electronic and thermal Free Energies= -1632.206067
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -1632.526249

^{3}INT5

C	0.05427900	3.07511200	-0.22008600
O	0.13033300	4.26193300	-0.25204300
O	-1.11094600	2.33352900	-0.17494500
O	1.08256200	2.18696100	-0.22896000
N	0.53504800	0.87961700	-0.16387000
C	-0.75908300	1.02703500	-0.15070800
C	-1.78579100	0.00733100	-0.10497000
C	-1.48785400	-1.32658300	-0.43683200
C	-3.08986200	0.36904900	0.27834200
C	-2.48321800	-2.29255900	-0.36063600
H	-0.49941600	-1.59973400	-0.78696900
C	-4.07814900	-0.60769700	0.34688200
H	-3.31966600	1.39888900	0.52813200
C	-3.77647400	-1.93596500	0.03387000

H	-2.25275500	-3.32057300	-0.62075300
H	-5.08454100	-0.33277500	0.64518300
H	-4.55168100	-2.69423600	0.08917600
Fe	1.83964000	-0.73472200	0.12805800
Cl	2.14635400	-1.48362500	-2.00099100
Cl	1.83914000	-0.90813000	2.40659300

Zero-point correction= 0.124926 (Hartree/Particle)
Thermal correction to Energy= 0.138817
Thermal correction to Enthalpy= 0.139761
Thermal correction to Gibbs Free Energy= 0.081626
Sum of electronic and zero-point Energies= -1632.114858
Sum of electronic and thermal Energies= -1632.100967
Sum of electronic and thermal Enthalpies= -1632.100022
Sum of electronic and thermal Free Energies= -1632.158158
B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -1632.39759

^{5}INT6

C	-0.55798300	3.12046100	-0.75984700
C	-1.63450500	1.53589900	0.78005700
C	-1.89058600	2.97429000	1.24555600
C	-1.72245300	3.80504700	-0.03557000
H	0.41110100	3.52696600	-0.45361900
H	-0.63180400	3.17176100	-1.84796900
H	-1.21560200	0.89749200	1.56301100
H	-2.86505600	3.09228800	1.72078000
H	-1.11606700	3.23409100	1.97381400
H	-2.63078100	3.75204400	-0.64381000
H	-1.50801000	4.85636400	0.16869300
N	-0.65632000	1.71451100	-0.30583700
C	0.23634300	0.76426400	-0.62284500
O	0.23326400	-0.39193100	-0.15283800
O	1.15394800	1.17963300	-1.49387100
C	2.21738400	0.22834900	-1.82257500
H	1.76554100	-0.73306300	-2.06895400
H	2.66026600	0.66506900	-2.71886300
C	3.21288200	0.11288600	-0.70052900
C	3.36004000	-1.08752400	0.00245600
C	3.98925700	1.22138800	-0.33726600
C	4.27632400	-1.18300200	1.05162000
H	2.75002700	-1.94377300	-0.27041200
C	4.89778900	1.13080500	0.71699900
H	3.87649500	2.15636200	-0.88039900
C	5.04371700	-0.07328400	1.41241500
H	4.38459600	-2.11989600	1.59076000
H	5.49481800	1.99544800	0.99328200
H	5.75303600	-0.14524100	2.23225800
C	-2.84794500	0.79446200	0.22108100
O	-2.80804100	-0.37269700	-0.16487200
O	-3.96290600	1.50154700	0.16059100
H	-4.67491100	0.93765800	-0.21635500
Fe	-1.24166500	-1.85519700	0.07233100
Cl	-1.32962500	-2.06907000	2.39135600
Cl	-1.25789400	-2.78426400	-2.07273100

Zero-point correction= 0.274961 (Hartree/Particle)
Thermal correction to Energy= 0.296117
Thermal correction to Enthalpy= 0.297061
Thermal correction to Gibbs Free Energy= 0.220363
Sum of electronic and zero-point Energies= -1903.917434
Sum of electronic and thermal Energies= -1903.896279
Sum of electronic and thermal Enthalpies= -1903.895334
Sum of electronic and thermal Free Energies= -1903.972033
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD//(U)B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -1904.51954

^{3}INT6

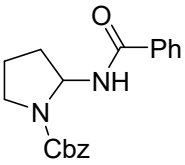
C	-1.19862500	2.92043400	-0.78169300
C	-1.95040400	1.18639400	0.79018700
C	-2.43270100	2.56453100	1.25641400
C	-2.44781900	3.39643600	-0.03386500
H	-0.31082500	3.49422800	-0.49976700
H	-1.30279300	2.94338200	-1.86821300
H	-1.41530400	0.63160600	1.56565500
H	-3.39795100	2.51817700	1.76190300
H	-1.69204600	2.95982200	1.95855200
H	-3.34773000	3.17774600	-0.61657300
H	-2.41526300	4.47124100	0.15747200
N	-1.03138300	1.52083200	-0.31527400
C	0.04955400	0.78748000	-0.61068200
O	0.28849400	-0.36626400	-0.17469400
O	0.90713600	1.40244800	-1.41330400
C	2.09091400	0.63960600	-1.82525200

H	1.76499900	-0.33847200	-2.18123000
H	2.46872500	1.22897300	-2.66201800
C	3.09718400	0.52682900	-0.71343500
C	3.46571200	-0.72807800	-0.21775200
C	3.66929200	1.68023000	-0.16138800
C	4.40126200	-0.83187600	0.81305900
H	3.01132500	-1.62138100	-0.63684600
C	4.59499200	1.57866500	0.87700700
H	3.38369200	2.65725700	-0.54309000
C	4.96424400	0.32136100	1.36425800
H	4.68233000	-1.81085800	1.19078100
H	5.03208700	2.47761300	1.30266200
H	5.68750300	0.24180500	2.17108400
C	-3.04099800	0.25041200	0.26825100
O	-2.82061200	-0.90897900	-0.07527200
O	-4.25323600	0.77453800	0.20603400
H	-4.87450500	0.09545000	-0.13996000
Fe	-0.87733300	-1.86909600	0.06928200
Cl	-0.65145500	-1.96613200	2.37954200
Cl	-0.63053300	-2.63059700	-2.08822400

Zero-point correction= 0.275259 (Hartree/Particle)
Thermal correction to Energy= 0.296336
Thermal correction to Enthalpy= 0.297280
Thermal correction to Gibbs Free Energy= 0.220751
Sum of electronic and zero-point Energies= -1903.861214
Sum of electronic and thermal Energies= -1903.840137
Sum of electronic and thermal Enthalpies= -1903.839193
Sum of electronic and thermal Free Energies= -1903.915722
(U)B3LYP-D3/6-311++G(d,p)-LANL2DZ SMD/(U)/B3LYP-D3/6-31G(d)-LANL2DZ SMD energy = -1904.462267

7. Characterization of Compounds

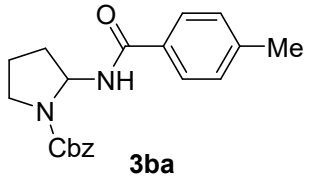
Benzyl 2-benzamidopyrrolidine-1-carboxylate (3aa)



3aa

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2a** (0.12 mmol) provided the product **3aa** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (82% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 133-134 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.3 Hz, 2H), 7.47 (t, J = 7.4 Hz, 1H), 7.37 (dd, J = 8.3, 6.9 Hz, 4H), 7.21 (d, J = 22.1 Hz, 3H), 6.66 (br s, 1H), 5.84 (br s, 1H), 5.24 – 4.99 (m, 2H), 3.63 – 3.28 (m, 2H), 2.14 – 1.86 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 154.5, 136.2, 134.0, 131.3, 128.3, 128.0, 127.8, 127.7, 126.9, 66.8, 64.6, 46.5, 33.7, 22.2. HRMS (ESI): calcd. for $C_{19}H_{20}N_2NaO_3$([M+Na]$^+$): 347.1366, found: 347.1373.

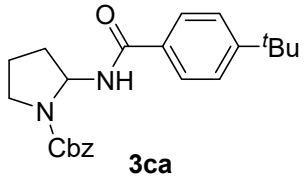
Benzyl 2-(4-methylbenzamido)pyrrolidine-1-carboxylate (3ba)



3ba

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2b** (0.12 mmol) provided the product **3ba** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (88% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 124-125 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, J = 7.7 Hz, 2H), 7.35 – 7.13 (m, 7H), 6.67 (br s, 1H), 5.83 (br s 1H), 5.20 – 5.00 (m, 2H), 3.46 (m, 2H), 2.36 (s, 3H), 2.15 – 1.85 (m, 4H).^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 154.7, 141.9, 136.5, 131.4, 129.1, 128.4, 127.9, 127.8, 127.1, 66.9, 64.8, 46.7, 33.9, 21.4. HRMS (APCI): calcd. for $C_{20}H_{22}N_2NaO_3$ ([M+Na]$^+$): 361.1523, found: 361.1518.

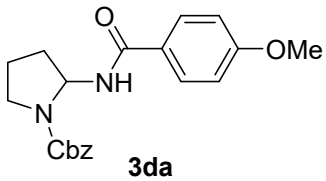
Benzyl 2-(4-(tert-butyl)benzamido)pyrrolidine-1-carboxylate(3ca)



3ca

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2c** (0.12 mmol) provided the product **3ca** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (90% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 161-162 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, J = 8.4 Hz, 2H), 7.43 – 7.29 (m, 4H), 7.26 – 7.09 (m, 3H), 6.54 (br s, 1H), 5.84 (br s, 1H), 5.22 – 5.03 (m, 2H), 3.62 – 3.34 (m, 2H), 2.17 – 1.89 (m, 4H), 1.32 (s, 9H).^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 154.7, 145.3, 136.5, 128.4, 128.0, 127.3, 126.9, 125.4, 107.6, 67.0, 55.2, 46.7, 34.9, 32.8, 31.2. HRMS (APCI): calcd. for $C_{23}H_{28}N_2NaO_3$ ([M+Na]$^+$): 403.1992, found: 403.1989.

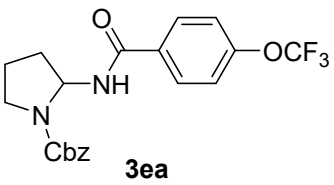
Benzyl 2-(4-methoxybenzamido)pyrrolidine-1-carboxylate(3da)



3da

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2d** (0.12 mmol) provided the product **3da** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (84% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 143-144 °C. R_f = 0.70 (10 vol % EtOAc in petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (s, 2H), 7.37 – 7.15 (m, 5H), 6.86 (p, J = 7.4, 6.5 Hz, 2H), 6.47 (br s, 1H), 5.83 (br s, 1H), 5.25 – 4.99 (m, 2H), 3.81 (s, 3H), 3.48 (m, 2H), 2.16 – 1.87 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2, 154.7, 136.5, 128.9, 128.4, 127.8, 126.5, 122.0, 114.2, 113.6, 66.9, 64.8, 55.4, 46.7, 34.0. HRMS (APCI): calcd. for $C_{20}H_{22}N_2NaO_4$ ([M+Na]$^+$): 377.1472, found: 377.1465.

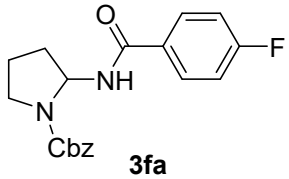
Benzyl 2-(4-(trifluoromethoxy)benzamido)pyrrolidine-1-carboxylate(3ea)



3ea

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2e** (0.12 mmol) provided the product **3ea** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (64% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 149-150 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 8.3 Hz, 2H), 7.33 (d, J = 4.9 Hz, 2H), 7.16 (d, J = 8.4 Hz, 5H), 6.89 (br s, 1H), 5.84 (br s, 1H), 5.24 – 5.00 (m, 2H), 3.64 – 3.30 (m, 2H), 2.16 – 1.84 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.7, 151.5, 136.3, 132.6, 129.0, 128.4, 128.1, 127.9, 121.6, 120.5, 119.0 (q, *J* = 258.2 Hz), 67.0, 64.9, 46.7, 33.9, 22.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.74. HRMS (APCI): calcd. for $C_{20}H_{19}F_3N_2NaO_4$ ([M+Na]$^+$): 431.1189, found: 431.1193.

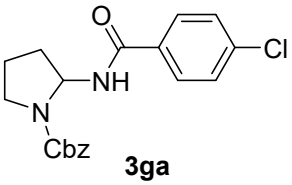
Benzyl 2-(4-fluorobenzamido)pyrrolidine-1-carboxylate(3fa)



3fa

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2f** (0.12 mmol) provided the product **3fa** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (70% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 121-122 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (s, 2H), 7.38 – 7.18 (m, 5H), 7.05 – 6.98 (m, 2H), 6.76 (br s, 1H), 5.82 (br s, 1H), 5.22 – 4.99 (m, 2H), 3.44 (m, 2H), 2.15 – 1.87 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8(d, *J* = 251.8 Hz), 165.3, 154.5, 136.2, 130.2, 129.4(d, *J* = 9.0 Hz), 128.3, 128.3, 127.8(d, *J* = 22.1 Hz), 115.3(d, *J* = 21.9 Hz), 66.8, 64.7, 46.5, 33.7, 22.1. ^{19}F NMR (376 MHz, $CDCl_3$) δ -108.1. HRMS (APCI): calcd. for $C_{19}H_{19}FN_2NaO_3$ ([M+Na]$^+$): 365.1272, found: 365.1279.

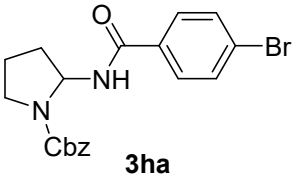
Benzyl 2-(4-chlorobenzamido)pyrrolidine-1-carboxylate (3ga)



3ga

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2g** (0.12 mmol) provided the product **3ga** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (82% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 152-153 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 8.4 Hz, 2H), 7.36 – 7.17 (m, 7H), 6.83 (br s, 1H), 5.82 (br s, 1H), 5.23 – 4.99 (m, 2H), 3.60 – 3.27 (m, 2H), 2.13 – 1.87 (m, 4H).^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 154.6, 137.7, 136.3, 132.5, 128.7, 128.6, 128.5, 128.1, 127.9, 67.0, 64.9, 46.7, 33.9, 22.3. HRMS (APCI): calcd. for $C_{19}H_{19}ClN_2NaO_3$ ([M+Na]$^+$): 381.0976, found: 381.0978.

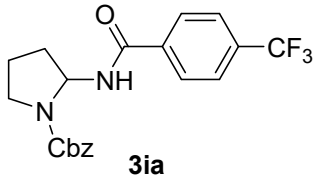
Benzyl 2-(4-bromobenzamido)pyrrolidine-1-carboxylate (3ha)



3ha

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2h** (0.12 mmol) provided the product **3ha** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (84% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 158-159 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (s, 2H), 7.49 (d, J = 8.5 Hz, 2H), 7.36 – 7.17 (m, 5H), 6.68 (br s, 1H), 5.81 (br s, 1H), 5.23 – 4.97 (m, 2H), 3.61 – 3.28 (m, 2H), 2.17 – 1.87 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 154.5, 136.3, 133.0, 131.7, 128.7, 128.5, 128.1, 127.9, 126.2, 67.1, 64.9, 46.7, 33.9, 22.4. HRMS (APCI): calcd. for $C_{19}H_{19}BrN_2NaO_3$ ([M+Na]$^+$): 425.0471, found: 425.0474.

Benzyl 2-(4-(trifluoromethyl)benzamido)pyrrolidine-1-carboxylate (3ia)

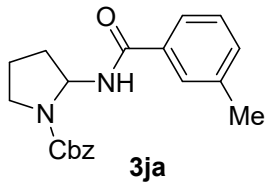


3ia

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2i** (0.12 mmol) provided the product **3ia** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (84% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 137-138 °C. ^{1}H NMR (400

MHz, $CDCl_3$) δ 7.79 (s, 2H), 7.59 (d, J = 8.2 Hz, 2H), 7.34 (s, 2H), 7.23 (d, J = 28.5 Hz, 3H), 6.90 (br s, 1H), 5.84 (br s, 1H), 5.22 – 5.02 (m, 2H), 3.46 (m, 2H), 2.16 – 1.88 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 154.6, 136.8 (q, *J* = 118.2 Hz), 133.1 (d, *J* = 32.6 Hz), 128.46, 127.58, 125.4 (q, *J* = 3.6 Hz), 123.6 (q, *J* = 272.5 Hz), 77.4, 64.9, 46.7, 33.8, 22.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.9. HRMS (APCI): calcd. for $C_{20}H_{19}F_3N_2NaO_3$ ($[M+Na]^+$): 415.1240, found: 415.1236.

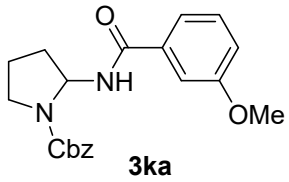
Benzyl 2-(3-methylbenzamido)pyrrolidine-1-carboxylate (3ja)



3ja

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2j** (0.12 mmol) provided the product **3ja** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (90% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 136-137 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.41 (m, 2H), 7.35 – 7.17 (m, 7H), 6.52 (br s, 1H), 5.84 (br s, 1H), 5.12 (m, 2H), 3.63 – 3.35 (m, 2H), 2.36 (s, 3H), 2.02 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 138.3, 136.4, 134.2, 132.3, 128.4, 128.4, 128.0, 127.7, 124.1, 67.0, 64.9, 46.7, 34.0, 21.3. HRMS (APCI): calcd. for $C_{20}H_{22}N_2NaO_3$ ($[M+Na]^+$): 361.1523, found: 361.1514.

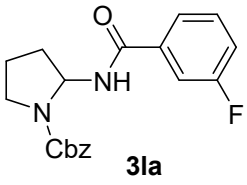
Benzyl 2-(3-methoxybenzamido)pyrrolidine-1-carboxylate (3ka)



3ka

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2k** (0.12 mmol) provided the product **3ka** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a colorless oil (80% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (dtd, J = 26.5, 19.0, 18.1, 10.4 Hz, 8H), 7.01 (dd, J = 8.3, 3.3 Hz, 1H), 6.63 (br s, 1H), 5.83 (br s, 1H), 5.23 – 4.98 (m, 2H), 3.80 (s, 3H), 3.48 (m, 2H), 2.03 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 159.8, 154.7, 136.4, 129.5, 128.6, 128.4, 128.2, 127.9, 118.9, 117.9, 112.3, 67.0, 55.4, 46.7, 33.9, 22.4, 17.5. HRMS (APCI): calcd. for $C_{20}H_{22}N_2NaO_4$ ($[M+Na]^+$): 377.1472, found: 377.1480.

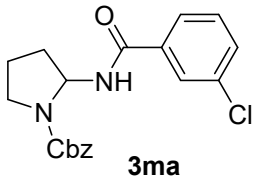
Benzyl 2-(3-fluorobenzamido)pyrrolidine-1-carboxylate (3la)



3la

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2l** (0.12 mmol) provided the product **3la** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (80% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 106-107 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (dd, J = 15.0, 8.7 Hz, 2H), 7.32 (td, J = 7.9, 5.4 Hz, 3H), 7.19 (dd, J = 19.1, 12.1 Hz, 4H), 6.79 (br s, 1H), 5.83 (br s, 1H), 5.24 – 5.01 (m, 2H), 3.62 – 3.27 (m, 2H), 2.17 – 1.86 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 162.5 (q, *J* = 247.6 Hz), 154.5, 130.0 (d, *J* = 7.9 Hz), 128.3, 127.9, 127.7, 122.5, 118.3 (d, *J* = 21.2 Hz), 114.3 (d, *J* = 23.0 Hz), 66.9, 64.7, 46.5, 33.7, 22.2. ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.9. HRMS (APCI): calcd. for $C_{19}H_{19}FN_2NaO_3$ ($[M+Na]^+$): 365.1272, found: 365.1280.

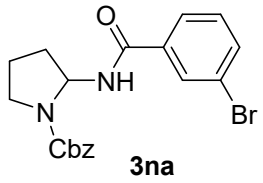
Benzyl 2-(3-chlorobenzamido)pyrrolidine-1-carboxylate (3ma)



3ma

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2m** (0.12 mmol) provided the product **3ma** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (78% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 143-144 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.46 (m, 2H), 7.46 – 7.37 (m, 1H), 7.37 – 7.17 (m, 6H), 6.52 (br s, 1H), 5.82 (br s, 1H), 5.26 – 4.98 (m, 2H), 3.70 – 3.29 (m, 2H), 2.18 – 1.79 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 154.6, 136.3, 134.6, 131.6, 129.8, 128.7, 128.5, 128.1, 128.0, 127.4, 125.2, 67.1, 64.9, 46.7, 33.9, 22.4. HRMS (APCI): calcd. for $C_{19}H_{19}ClN_2NaO_3$ ($[M+Na]^+$): 381.0976, found: 381.0982.

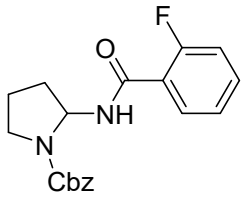
Benzyl 2-(3-bromobenzamido)pyrrolidine-1-carboxylate(3na)



3na

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2n** (0.12 mmol) provided the product **3na** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (81% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 156-157 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.99 – 8.75 (m, 1H), 8.02 (d, J = 7.8 Hz, 1H), 7.83 (d, J = 8.2 Hz, 1H), 7.73 (d, J = 8.0 Hz, 1H), 7.47 – 7.30 (m, 3H), 7.22 (d, J = 7.0 Hz, 2H), 7.15 (br s, 1H), 5.90 – 5.68 (br s, 1H), 5.22 – 4.89 (m, 2H), 3.51 – 3.30 (m, 2H), 1.94 (m, 4H).^{13}C NMR (100 MHz, DMSO-d_6) δ 164.2, 154.0, 137.4, 136.8, 134.5, 130.9, 130.4, 128.9, 128.5, 127.4, 127.1, 122.0, 66.1, 64.4, 46.9, 34.2, 22.1. HRMS (APCI): calcd. for $C_{19}H_{19}BrN_2NaO_3$ ([M+Na]$^+$): 425.0471, found: 425.0479.

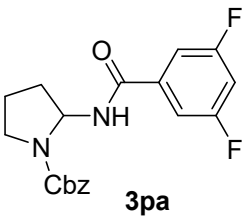
Benzyl 2-(2-fluorobenzamido)pyrrolidine-1-carboxylate (3oa)



3oa

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2o** (0.12 mmol) provided the product **3oa** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (75% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 112-113 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 – 8.01 (m, 1H), 7.51 – 7.45 (m, 1H), 7.36 (d, J = 4.3 Hz, 2H), 7.26 – 7.20 (m, 2H), 7.15 – 7.03 (m, 2H), 6.91 (m, 1H), 6.50 (br s, 1H), 5.92 (br s, 1H), 5.15 (m, 2H), 3.66 – 3.37 (m, 2H), 2.24 – 1.94 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 160.7 (q, J = 248.5 Hz), 154.4, 136.3, 133.7 (d, J = 9.3 Hz), 133.2 (d, J = 9.4 Hz), 132.1, 132.0, 131.7, 127.9 (q, J = 51.0 Hz), 124.6, 120.1 (d, J = 11.6 Hz), 115.9 (d, J = 24.8 Hz), 66.8, 64.5, 46.5, 33.7, 22.2. ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.8. HRMS (APCI): calcd. for $C_{19}H_{19}FN_2NaO_3$ ([M+Na]$^+$): 365.1272, found: 365.1274.

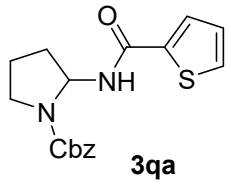
Benzyl 2-(3,5-difluorobenzamido)pyrrolidine-1-carboxylate (3pa)



3pa

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2p** (0.12 mmol) provided the product **3pa** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (76% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 163-164 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.20 (m, 7H), 6.92 (d, J = 8.4 Hz, 1H), 6.89 – 6.67 (br s, 1H), 6.07 – 5.58 (br s, 1H), 5.21 – 4.99 (m, 2H), 3.61 – 3.32 (m, 2H), 2.18 – 1.89 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9 (d, J = 11.9 Hz), 161.5 (d, J = 12.1 Hz), 154.5, 136.7 (q, J = 146.8 Hz), 128.3, 128.0, 127.8, 110.3 (d, J = 11.6 Hz), 110.3 (d, J = 26.5 Hz), 107.0, 106.7 (t, J = 25.2 Hz), 67.0, 64.8, 46.6, 33.7, 22.2. ^{19}F NMR (376 MHz, $CDCl_3$) δ -108.2. HRMS (APCI): calcd. for $C_{19}H_{18}F_2N_2NaO_3$ ([M+Na]$^+$): 383.1178, found: 383.1174.

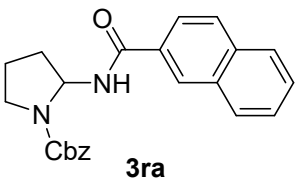
Benzyl 2-(thiophene-2-carboxamido)pyrrolidine-1-carboxylate (3qa)



3qa

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2q** (0.12 mmol) provided the product **3qa** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (71% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 132-133 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J = 20.8 Hz, 2H), 7.38 – 7.08 (m, 5H), 7.01 (t, J = 4.4 Hz, 1H), 6.72 (br s, 1H), 5.81 (br s, 1H), 5.26 – 4.98 (m, 2H), 3.71 – 3.24 (m, 2H), 2.19 – 1.81 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 154.7, 139.0, 136.4, 130.3, 128.4, 128.3, 128.0, 127.7, 127.6, 67.0, 64.7, 46.7, 33.9, 22.3. HRMS (APCI): calcd. for $C_{17}H_{18}N_2NaO_3S$([M+Na]$^+$): 353.0930, found: 353.0938.

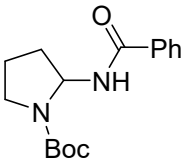
Benzyl 2-(2-naphthamido)pyrrolidine-1-carboxylate (3ra)



3ra

With general procedure 2.2, reaction of **1a** (0.1 mmol) and **2r** (0.12 mmol) provided the product **3ra** after flash column chromatography (50 vol % EtOAc in petroleum ether) as a white solid (80% yield). R_f = 0.20 (20 vol % EtOAc in petroleum ether). M.P. 161-162 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, J = 18.5 Hz, 1H), 7.89 – 7.77 (m, 4H), 7.55 (p, J = 7.1 Hz, 2H), 7.38 – 7.11 (m, 5H), 6.86 (br s, 1H), 5.93 (br s, 1H), 5.27 – 5.04 (m, 2H), 3.68 – 3.36 (m, 2H), 2.20 – 1.93 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.7, 136.4, 134.8, 132.6, 131.5, 129.0, 128.5, 128.4, 128.0, 128.0, 127.7, 127.7, 127.6, 126.7, 123.7, 67.0, 64.9, 46.8, 34.0, 22.4. HRMS (APCI): calcd. for $C_{23}H_{22}N_2NaO_3$ ([M+Na]$^+$): 397.1523, found: 397.1532.

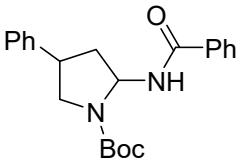
Tert-butyl 2-benzamidopyrrolidine-1-carboxylate (3ab)[9]



3ab

With general procedure 2.2, reaction of **1b** (0.1 mmol) and **2a** (0.12 mmol) provided the product **3ab** after flash column chromatography (10 vol % EtOAc in petroleum ether) as a white solid (80% yield). R_f = 0.50 (10 vol % EtOAc in petroleum ether). M.P. 156-157 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.68 (m, 2H), 7.48 (t, J = 7.4 Hz, 1H), 7.41 (t, J = 7.5 Hz, 2H), 6.53 (br s, 1H), 5.86 (s, 1H), 3.56 – 3.30 (m, 2H), 2.19 – 1.88 (m, 4H), 1.41 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 154.0, 134.3, 131.2, 128.3, 126.8, 79.9, 64.4, 45.9, 33.7, 28.2, 22.3. HRMS (APCI): calcd. for $C_{16}H_{22}N_2NaO_3$ ([M+Na]$^+$): 313.1523, found: 313.1530.

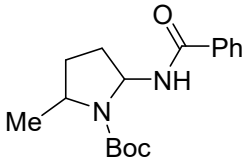
Tert-butyl 2-benzamido-4-phenylpyrrolidine-1-carboxylate (3ac)



3ac

With general procedure 2.2, reaction of **1c** (0.1 mmol) and **2a** (0.12 mmol) provided the product **3ac** after flash column chromatography (10 vol % EtOAc in petroleum ether) as a colorless oil (82% yield, 1:1 dr). R_f = 0.50 (10 vol % EtOAc in petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 7.3 Hz, 2H), 7.56 – 7.37 (m, 3H), 7.32 (t, J = 7.3 Hz, 2H), 7.27 – 7.18 (m, 3H), 6.68 (br s, 1H), 5.95 (br s, 1H), 3.92 (m, 1H), 3.68 – 3.30 (m, 2H), 2.51 – 2.04 (m, 2H), 1.43 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.0, 140.7, 140.0, 134.5, 131.6, 129.0, 128.8, 128.7, 128.6, 127.1, 127.1, 127.0, 126.8, 80.5, 64.9, 53.2, 40.8, 28.4, 28.0. HRMS (APCI): calcd. for $C_{22}H_{26}N_2NaO_3$ ([M+Na]$^+$): 389.1836, found: 389.1831.

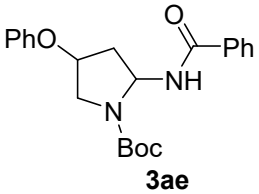
Tert-butyl 2-benzamido-5-methylpyrrolidine-1-carboxylate (3ad)



3ad

With general procedure 2.2, reaction of **1d** (0.1 mmol) and **2a** (0.12 mmol) provided the product **3ad** after flash column chromatography (10 vol % EtOAc in petroleum ether) as a colorless oil (80% yield, 1:1 dr). R_f = 0.50 (10 vol % EtOAc in petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.71 (m, 2H), 7.48 – 7.38 (m, 3H), 6.33 (br s, 1H), 5.84 (br s, 1H), 3.88 (br s, 1H), 2.29 – 1.97 (m, 4H), 1.43 (s, 9H), 1.19 (d, J = 6.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 154.5, 134.6, 131.5, 128.6, 126.9, 80.2, 80.1, 64.5, 54.3, 53.1, 31.3, 29.2, 28.4, 22.0. HRMS (APCI): calcd. for $C_{17}H_{24}N_2NaO_3$ ([M+Na]$^+$): 327.1679, found: 327.1676.

Tert-butyl 2-benzamido-4-phenoxypyrrolidine-1-carboxylate (3ae)

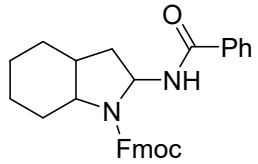


3ae

With general procedure 2.2, reaction of **1e** (0.1 mmol) and **2a** (0.12 mmol) provided the product **3ae** after flash column chromatography (10 vol % EtOAc in petroleum ether) as a colorless oil (76% yield, 1:1 dr). R_f = 0.50 (10 vol % EtOAc in petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, J = 7.5 Hz, 2H), 7.54 – 7.41 (m, 3H), 7.31 (t, J = 7.9 Hz, 2H), 7.00 (t, J = 7.4 Hz, 1H), 6.91 (d, J = 17.1 Hz, 2H), 6.87 (br s, 1H), 6.24 (br s, 1H), 5.00 (m, 1H), 3.94 – 3.60 (m, 2H), 2.39 (q, J = 16.3, 14.3 Hz, 2H), 1.42 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ

165.5, 156.4, 154.0, 134.7, 131.5, 129.9, 128.7, 126.8, 121.8, 115.3, 80.7, 75.5, 62.7, 51.9, 39.1, 28.4. HRMS (APCI): calcd. for $C_{22}H_{26}N_2NaO_3$ ($[M+Na]^+$): 405.1785, found: 405.1772.

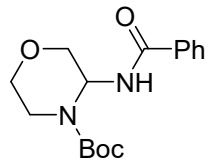
(9H-fluoren-9-yl)methyl 2-benzamidooctahydro-1H-indole-1-carboxylate(3af)



3af

With general procedure 2.2, reaction of **1f** (0.1 mmol) and **2a** (0.12 mmol) provided the product **3af** after flash column chromatography (10 vol % EtOAc in petroleum ether) as a colorless oil (63% yield, 1:1 dr). R_f = 0.50 (10 vol % EtOAc in petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (s, 3H), 7.62 (s, 1H), 7.56 (s, 2H), 7.46 – 7.18 (m, 6H), 7.03 (m, 1H), 6.36 (br s, 1H), 5.79 (br s, 1H), 4.54 – 4.21 (m, 2H), 4.12 (m, 1H), 3.67 (m, 1H), 2.48 (m, 1H), 2.04 (m, 2H), 1.72 (m, 2H), 1.52 (m, 2H), 1.25 (m, 2H), 0.87 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 154.4, 154.3, 143.9, 141.2, 134.0, 131.7, 128.6, 127.7, 127.1, 125.1, 119.9, 67.9, 64.8, 57.6, 47.1, 35.5, 33.9, 27.1, 25.6, 23.6, 20.7. HRMS (APCI): calcd. for $C_{30}H_{30}N_2NaO_3$($[M+Na]^+$): 489.2149, found: 489.2146.

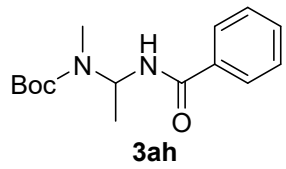
Tert-butyl 3-benzamidomorpholine-4-carboxylate(3ag)



3ag

With general procedure 2.2, reaction of **1g** (0.1 mmol) and **2a** (0.12 mmol) provided the product **3ag** after flash column chromatography (10 vol % EtOAc in petroleum ether) as a colorless oil (52% yield). R_f = 0.50 (10 vol % EtOAc in petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$)) δ 7.79 – 7.76 (m, 2H), 7.51 (d, J = 7.3 Hz, 1H), 7.45 (t, J = 7.4 Hz, 2H), 7.00 (br s, 1H), 6.19 (br s, 1H), 3.98 – 3.90 (m, 2H), 3.85 – 3.72 (m, 2H), 3.62 – 3.32 (m, 2H), 1.49 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 134.2, 131.8, 128.7, 127.1, 81.2, 70.7, 67.0, 57.2, 38.7, 28.2. HRMS (APCI): calcd. for $C_{16}H_{22}N_2NaO_4$ ($[M+Na]^+$): 329.1472, found: 329.1479.

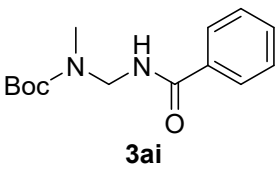
Tert-butyl (1-benzamidoethyl)(methyl)carbamate (3ah)



3ah

With general procedure 2.2, reaction of **1h** (0.1 mmol) and **2a** (0.12 mmol) provided the product **3ah** after flash column chromatography (10 vol % EtOAc in petroleum ether) as a colorless oil (62% yield). R_f = 0.50 (10 vol % EtOAc in petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 7.0 Hz, 2H), 7.51 – 7.49 (m, 1H), 7.45 – 7.42 (m, 2H), 7.39 (br s, 1H), 5.58 (s, 1H), 2.94 (s, 3H), 1.55 (d, J = 6.7 Hz, 3H), 1.49 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 155.3, 134.2, 131.7, 129.0, 128.6, 127.6, 127.0, 80.3, 28.5, 18.9. HRMS (APCI): calcd. for $C_{15}H_{22}N_2NaO_3$ ($[M+Na]^+$): 301.1523, found: 301.1529.

Tert-butyl (benzamidomethyl)(methyl)carbamate (3ai)



3ai

With general procedure 2.2, reaction of **1i** (0.1 mmol) and **2a** (0.12 mmol) provided the product **3ai** after flash column chromatography (10 vol % EtOAc in petroleum ether) as a colorless oil (70% yield). R_f = 0.50 (10 vol % EtOAc in petroleum ether). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 7.7 Hz, 2H), 7.48 (dd, J = 22.7, 7.5 Hz, 3H), 7.28 (s, 1H), 4.89 (d, J = 6.5 Hz, 2H), 3.02 (s, 3H), 1.47 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9, 156.4, 133.9, 131.8, 128.6, 127.1, 80.4, 53.7, 35.0, 28.4. HRMS (APCI): calcd. for $C_{14}H_{20}N_2NaO_3$ ($[M+Na]^+$): 287.1366, found: 287.1365.

8. References

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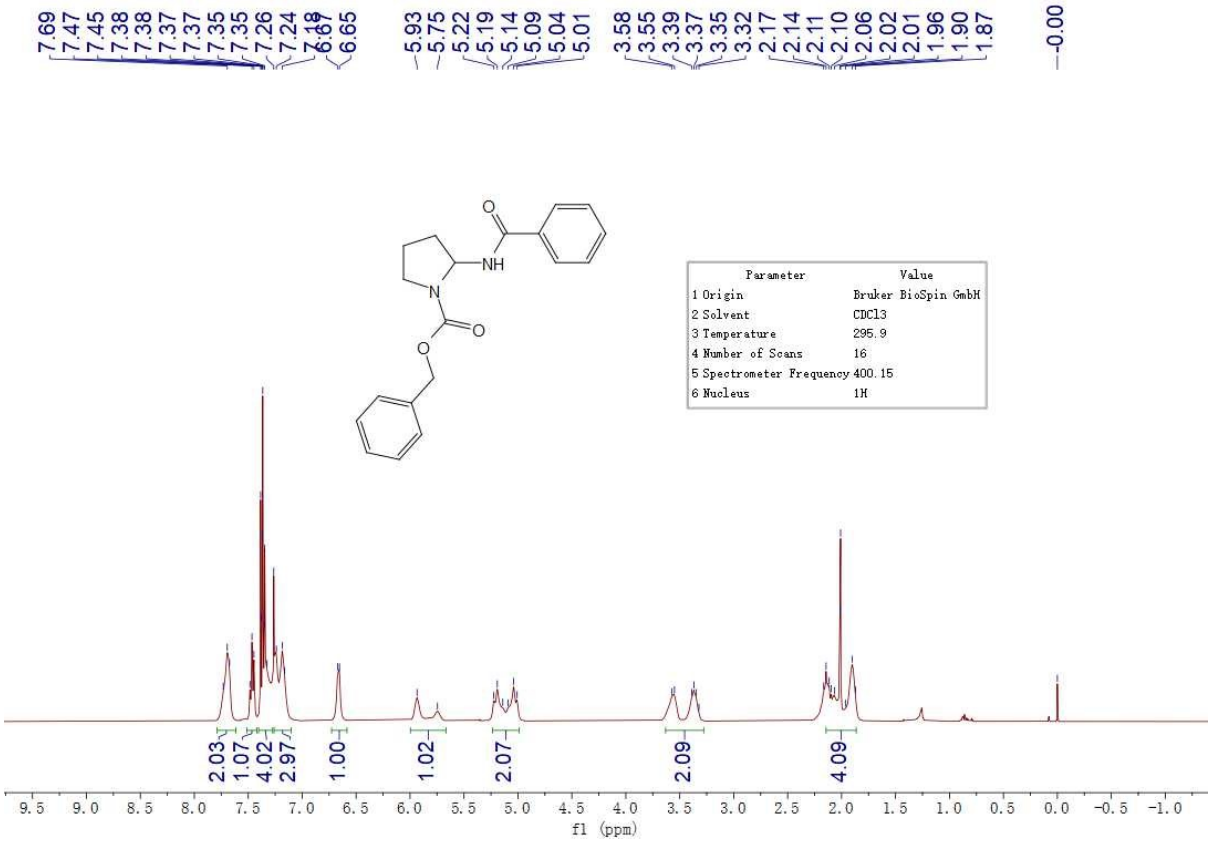
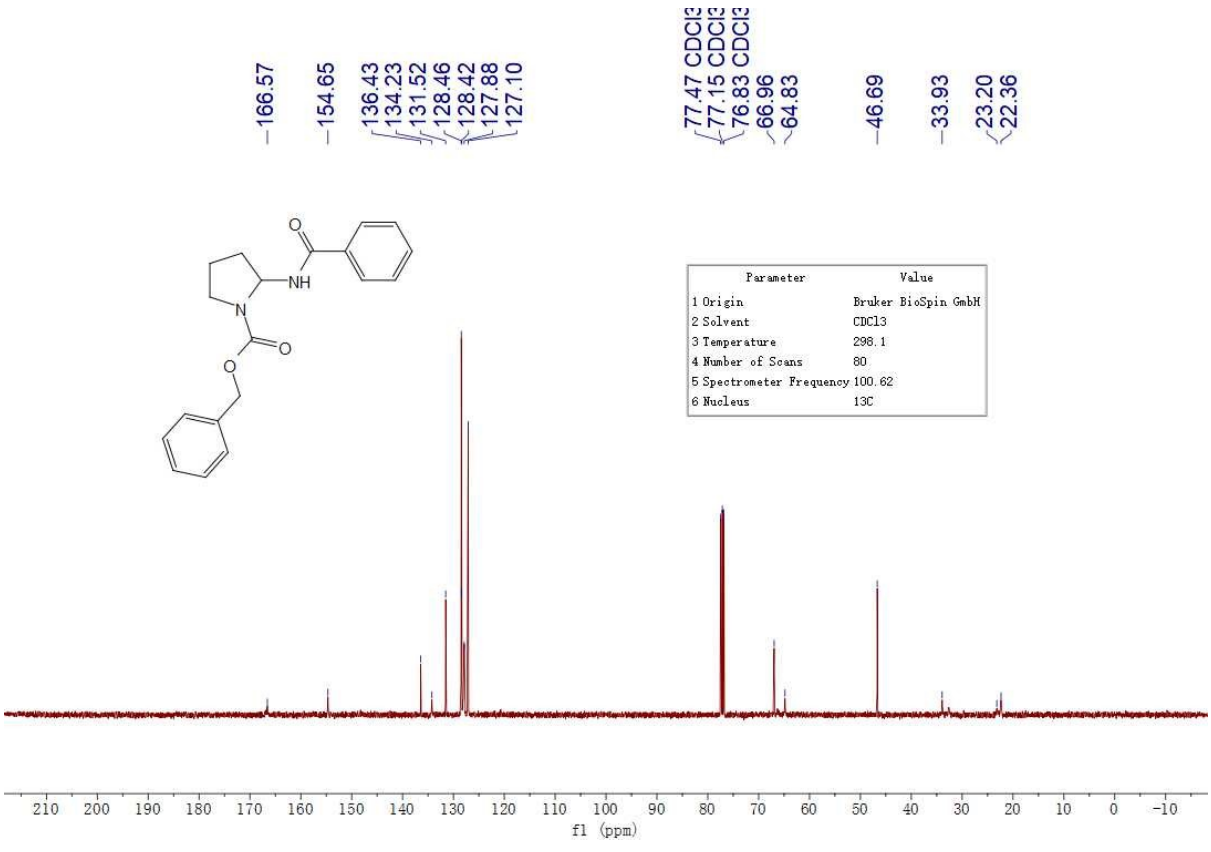
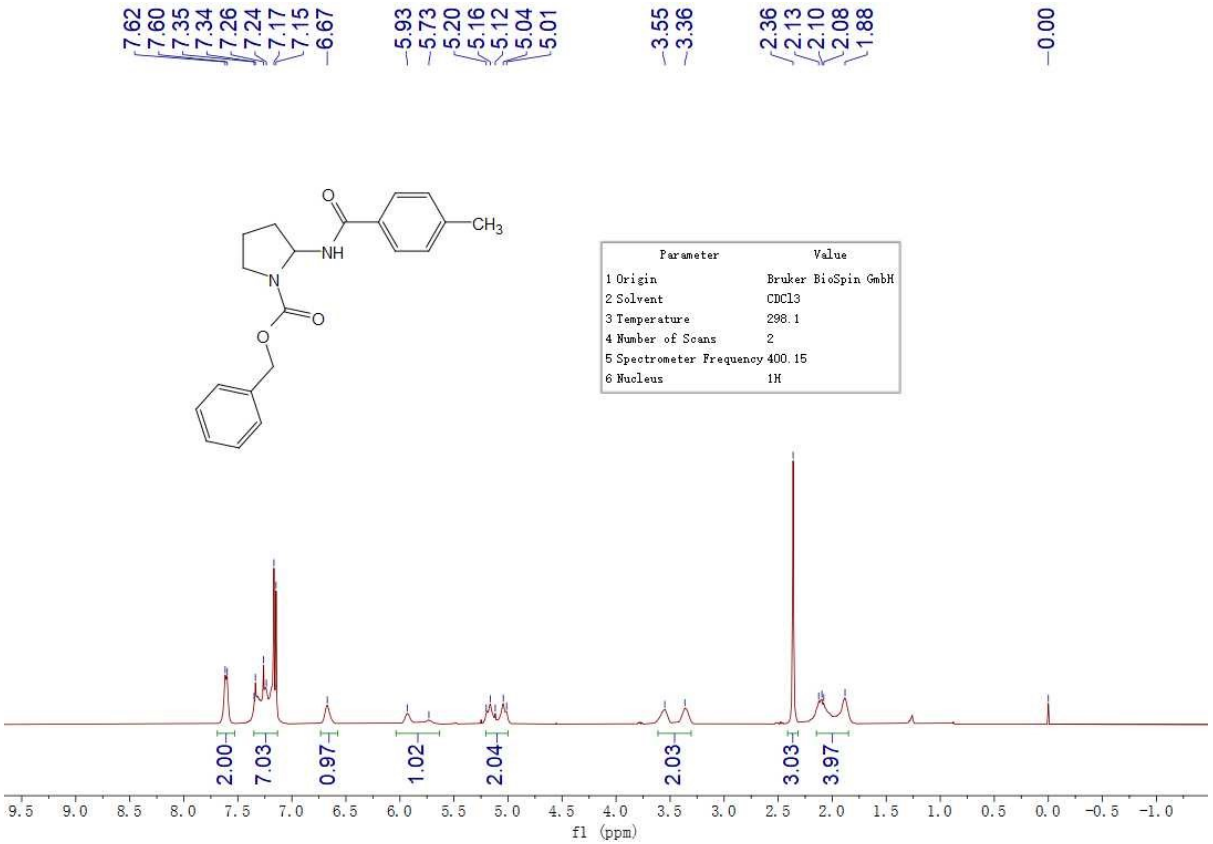
9. NMR spectra



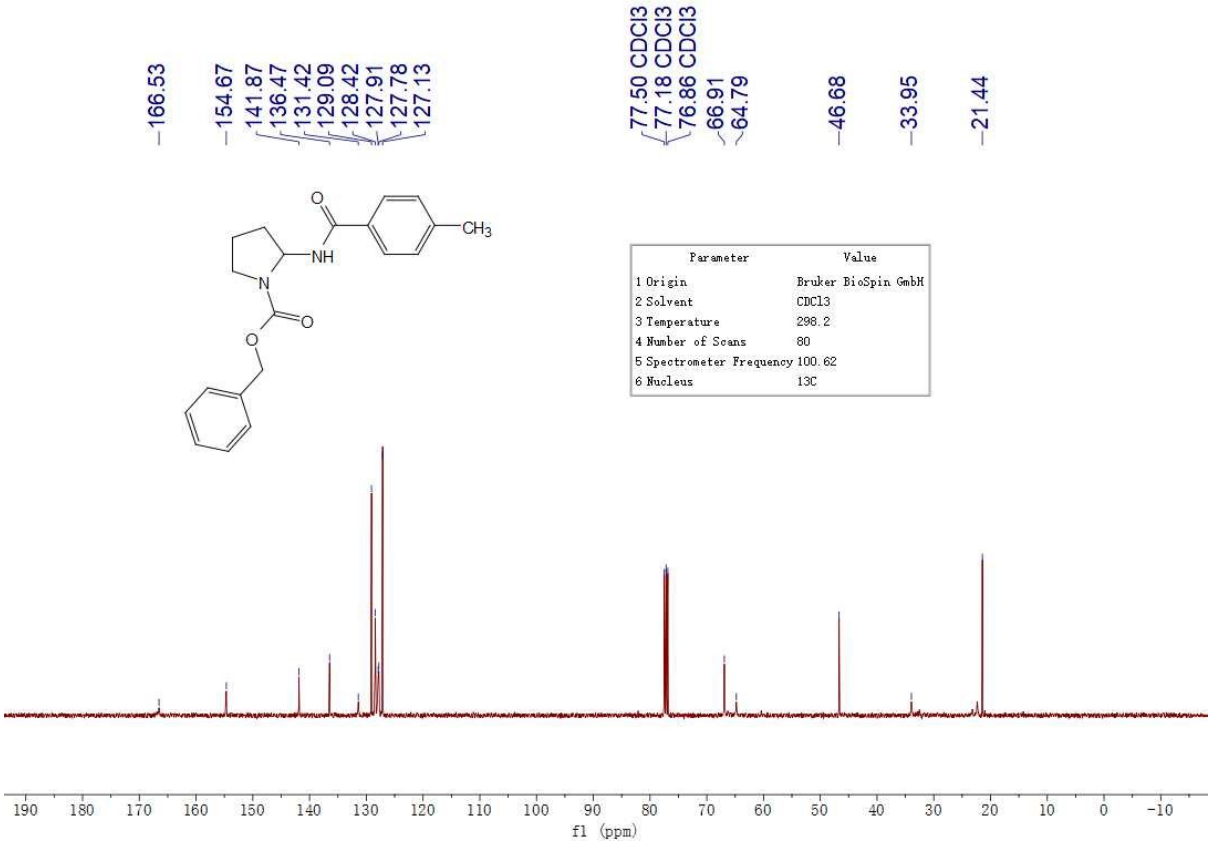
^{1}H NMR spectrum of **3aa** (400 MHz, $CDCl_3$)



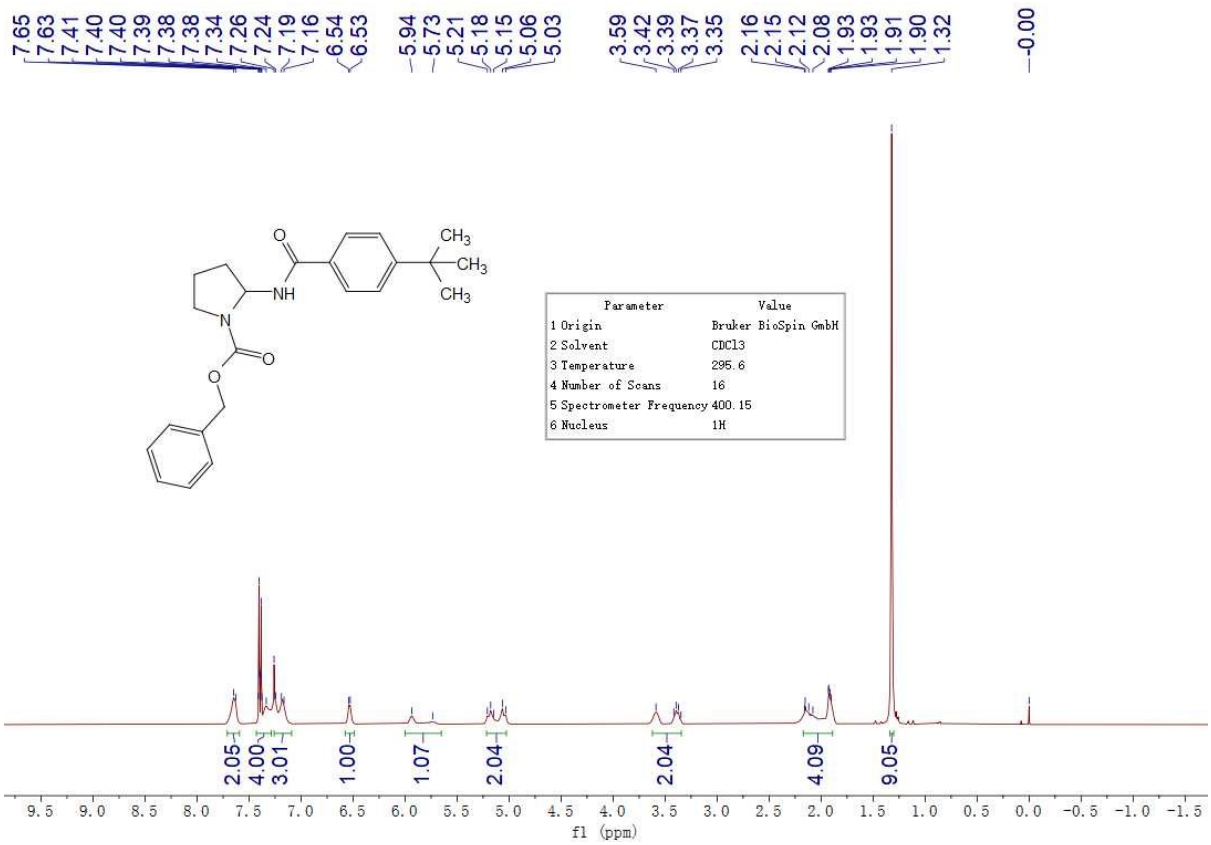
^{13}C NMR spectrum of **3aa** (100 MHz, $CDCl_3$)



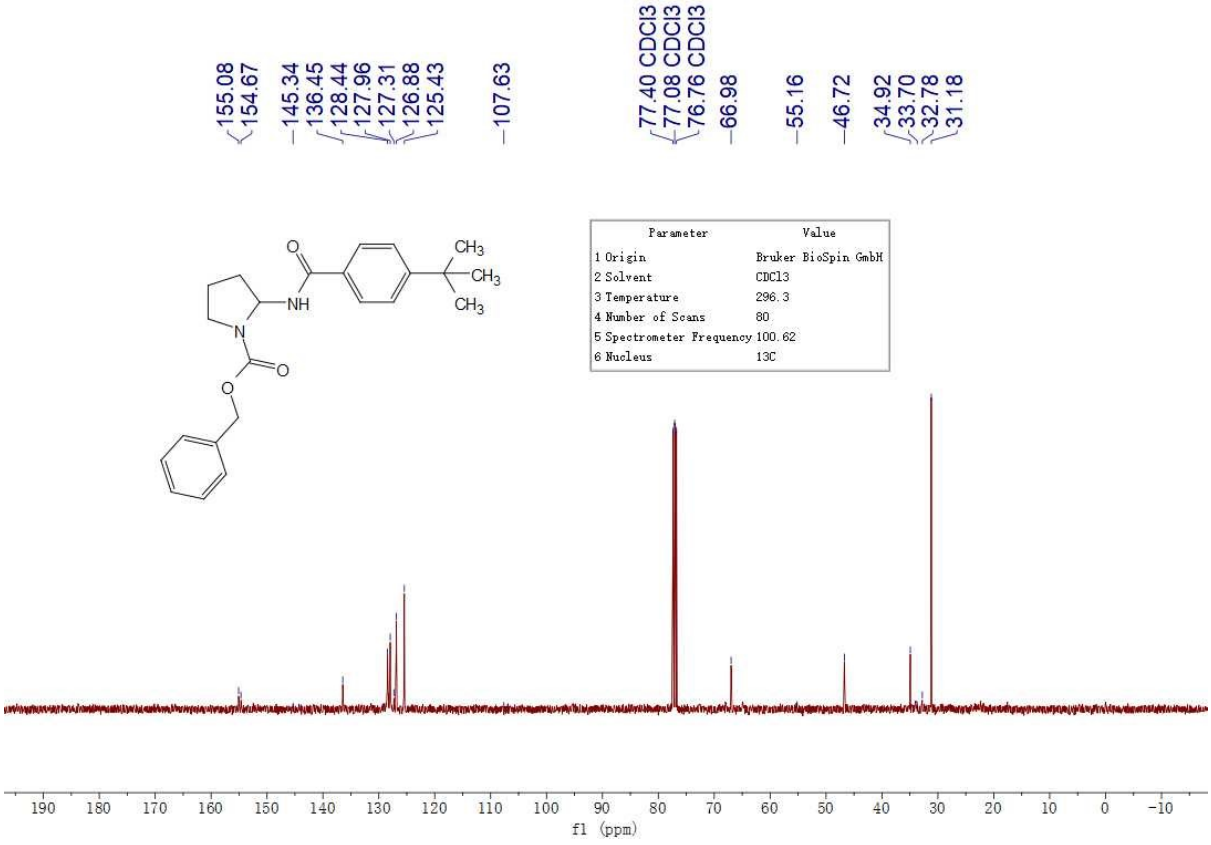
^{1}H NMR spectrum of **3ba** (400 MHz, $CDCl_3$)



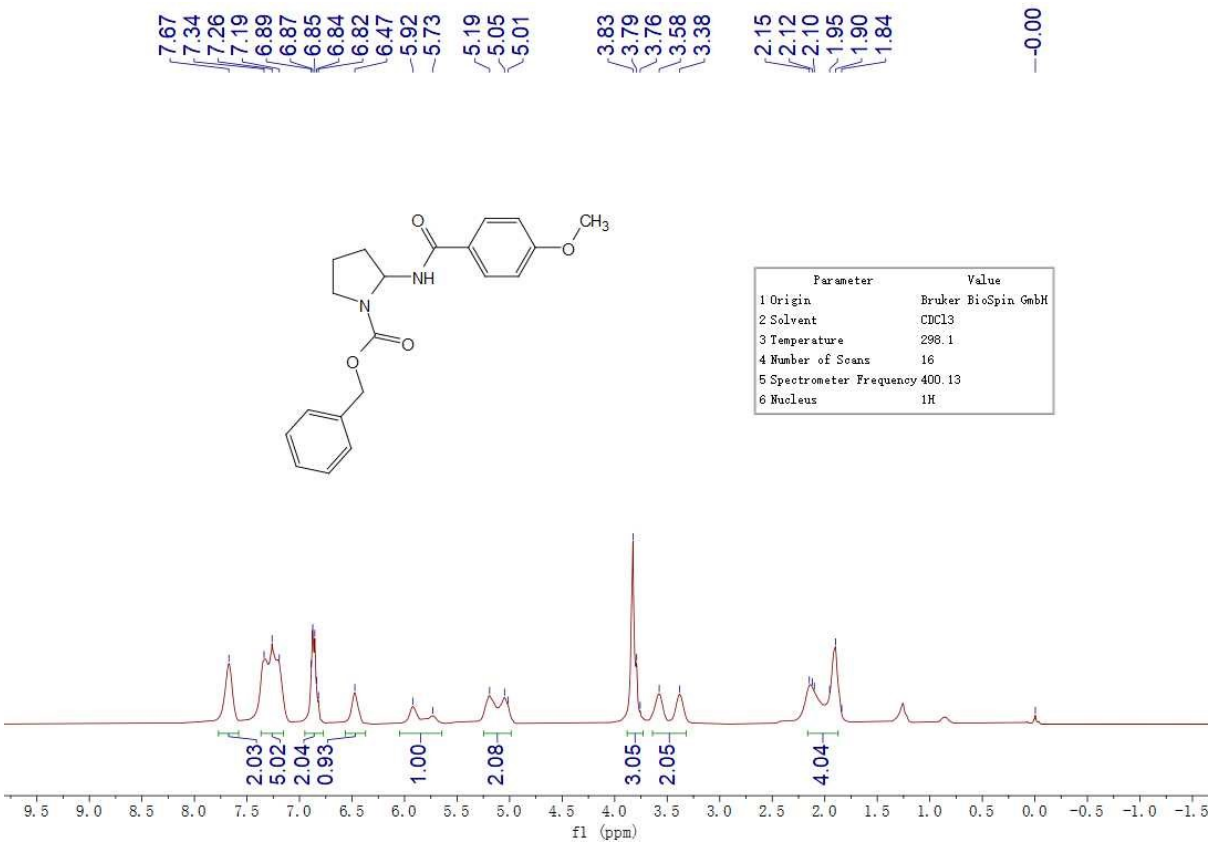
^{13}C NMR spectrum of **3ba** (100 MHz, $CDCl_3$)



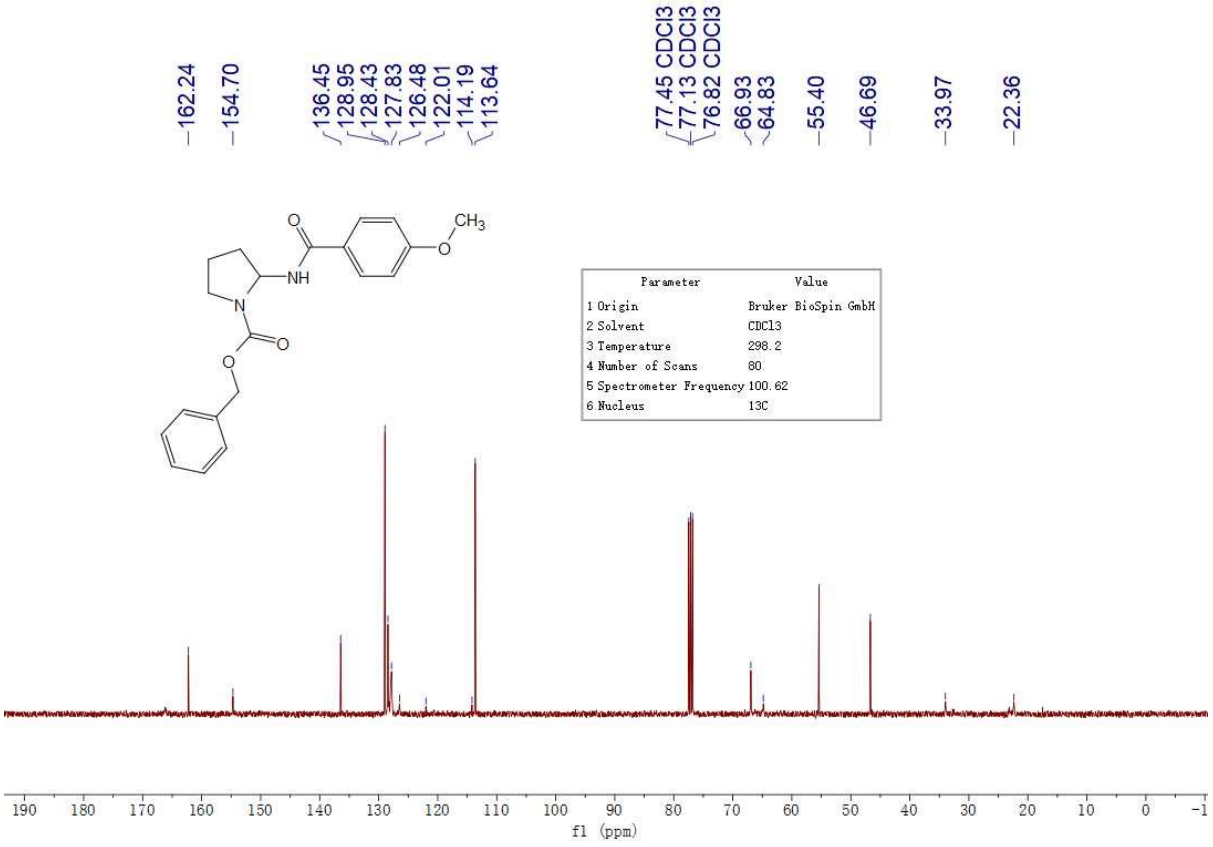
^{1}H NMR spectrum of **3ca** (400 MHz, $CDCl_3$)



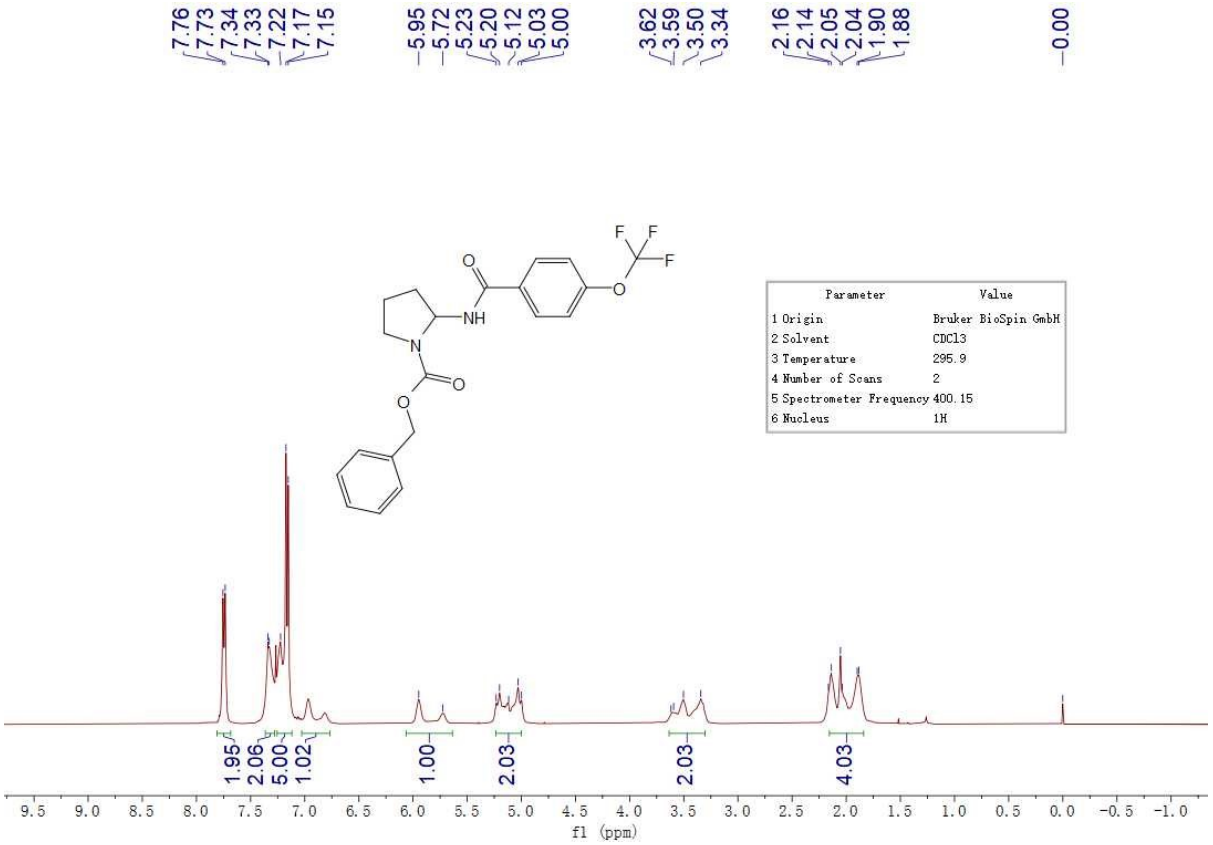
^{13}C NMR spectrum of **3ca** (100 MHz, $CDCl_3$)



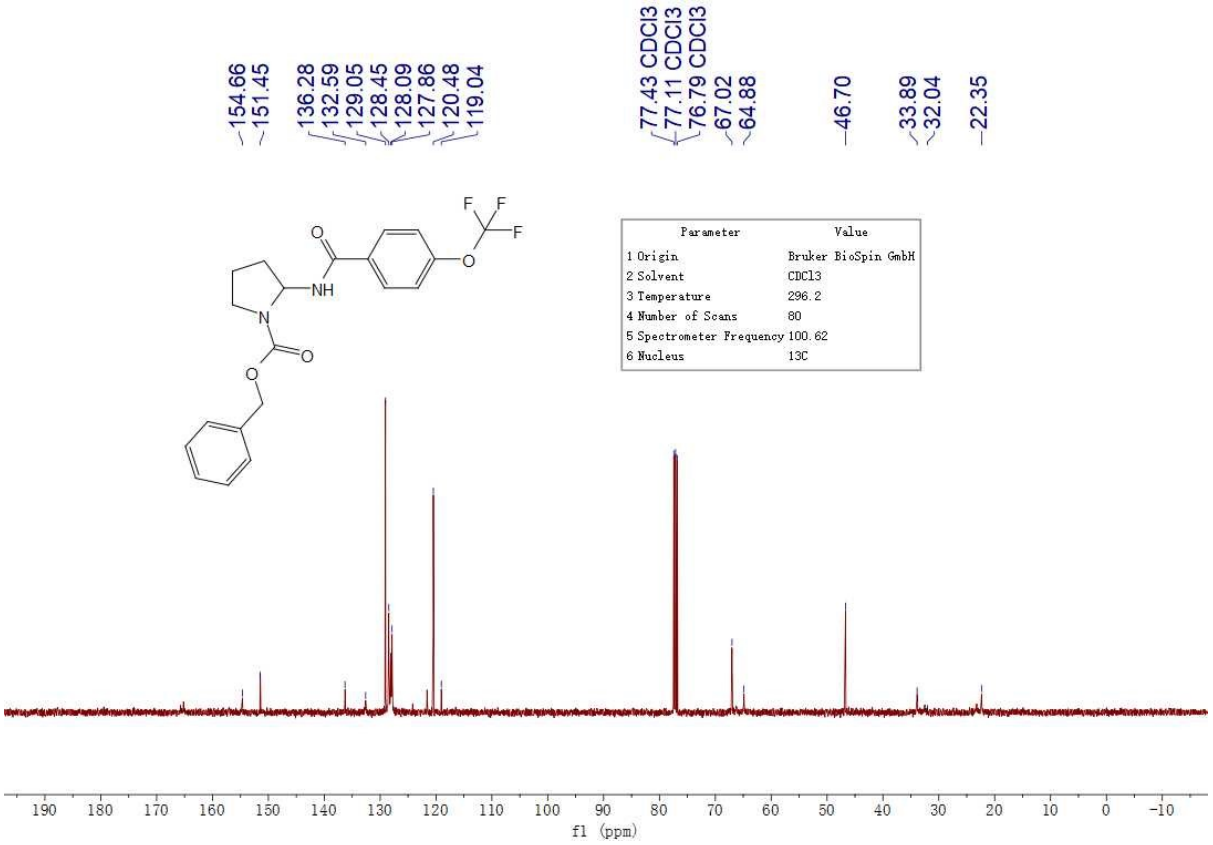
^{1}H NMR spectrum of **3da** (400 MHz, $CDCl_3$)



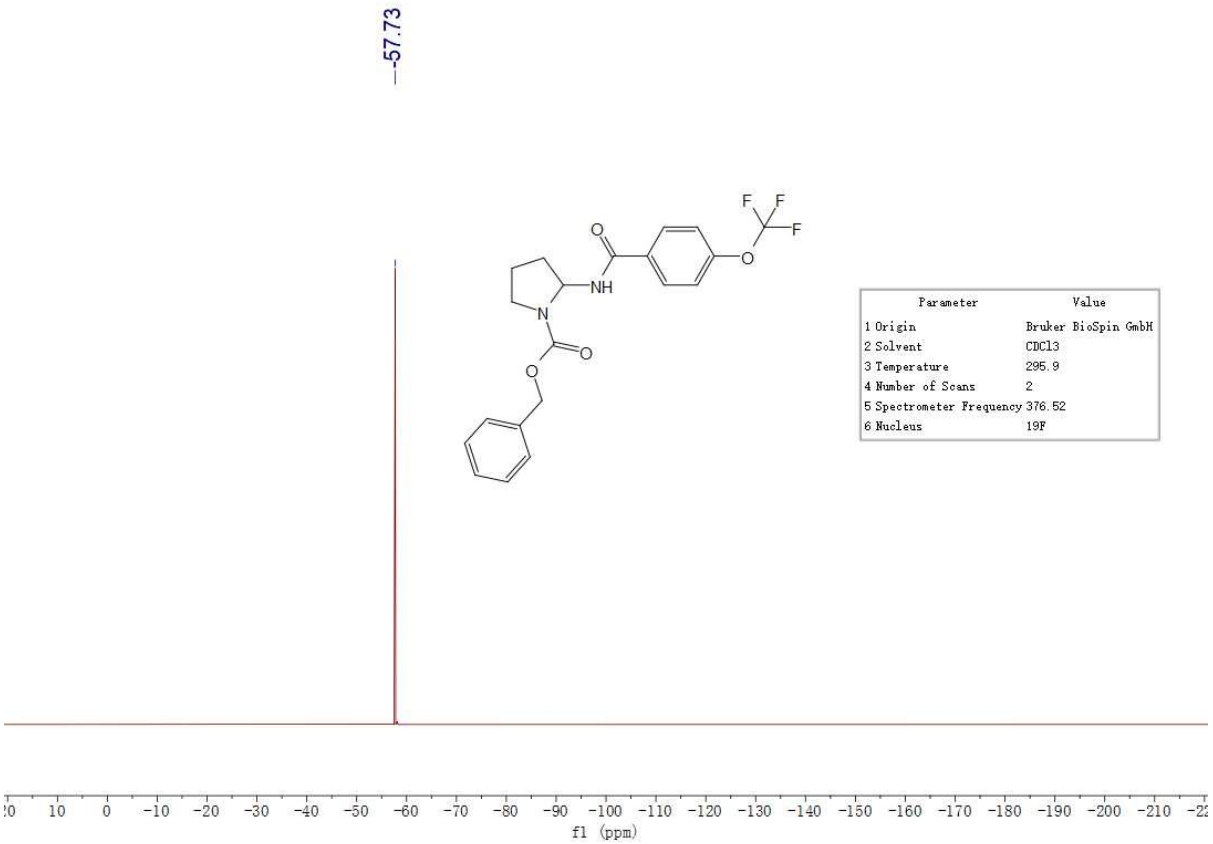
^{13}C NMR spectrum of **3da** (100 MHz, $CDCl_3$)



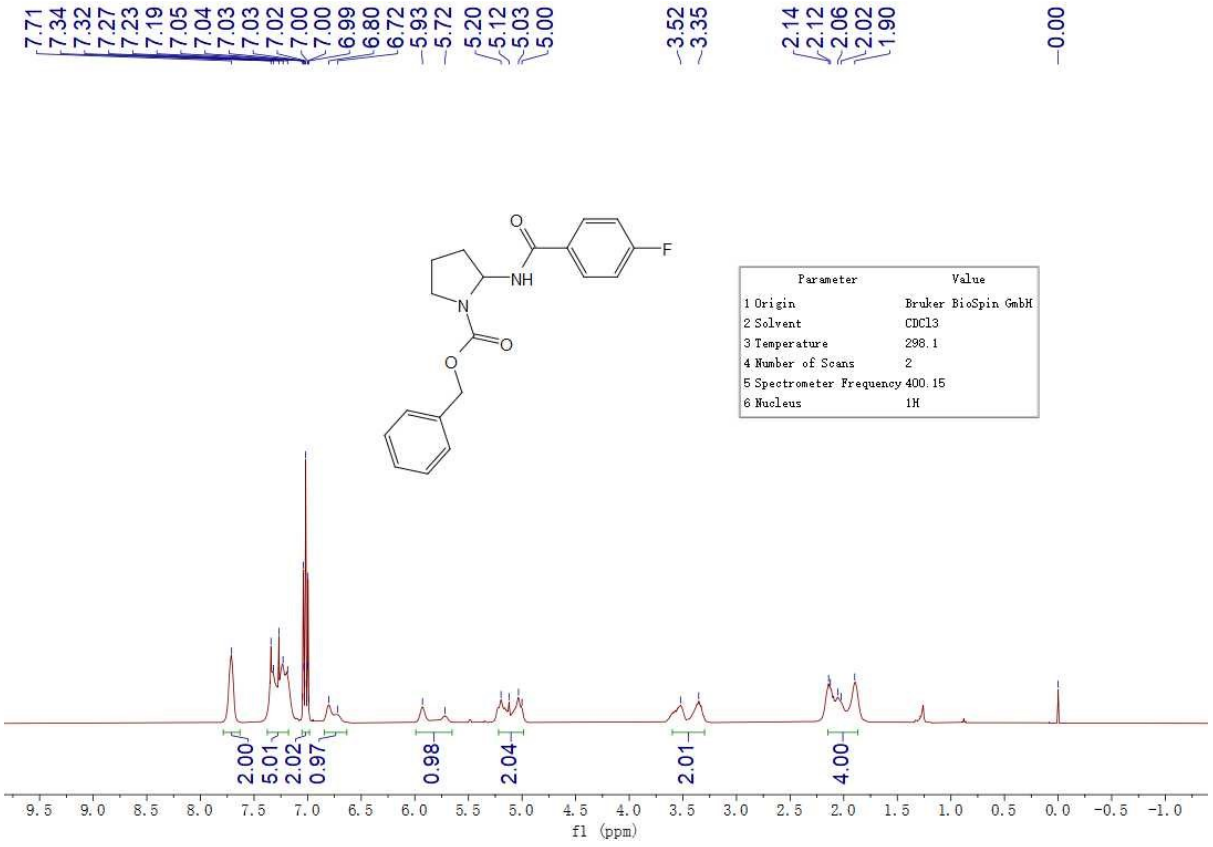
^{1}H NMR spectrum of **3ea** (400 MHz, $CDCl_3$)



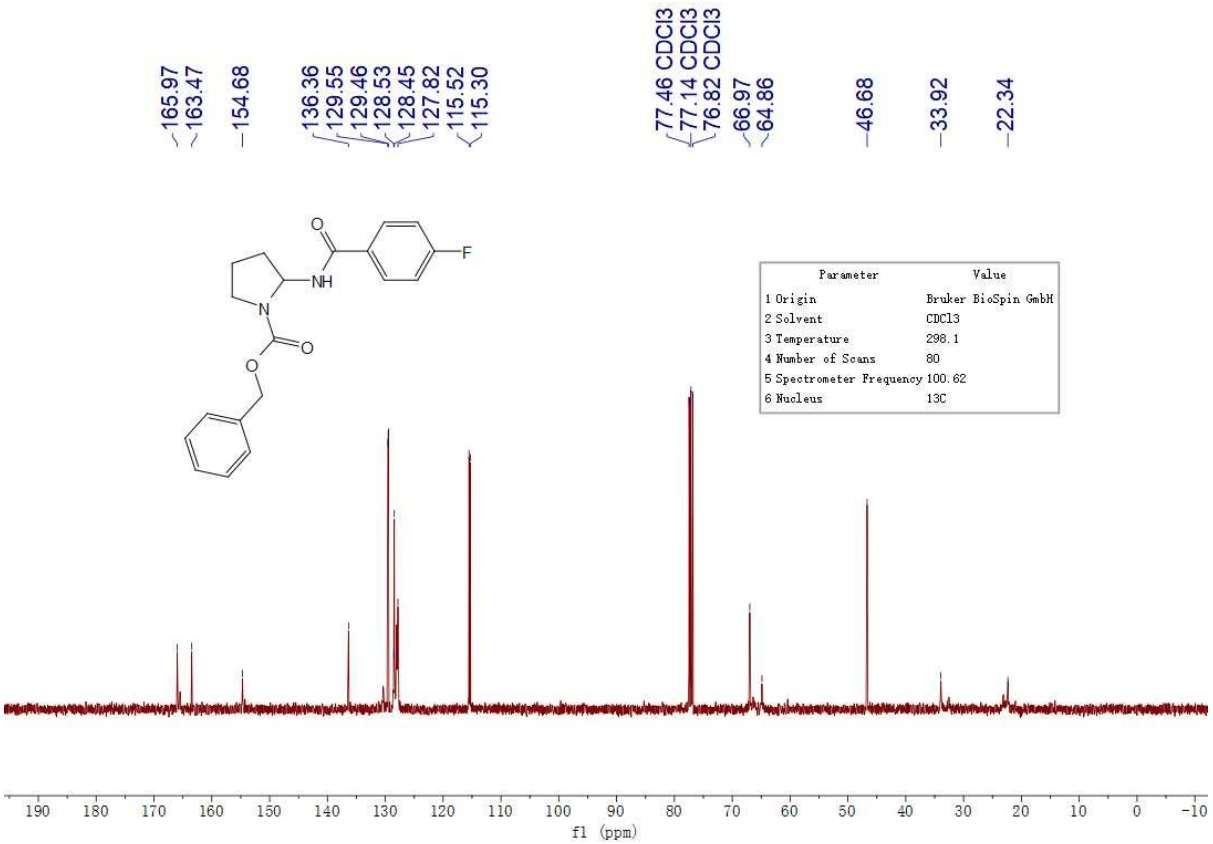
^{13}C NMR spectrum of **3ea** (100 MHz, $CDCl_3$)



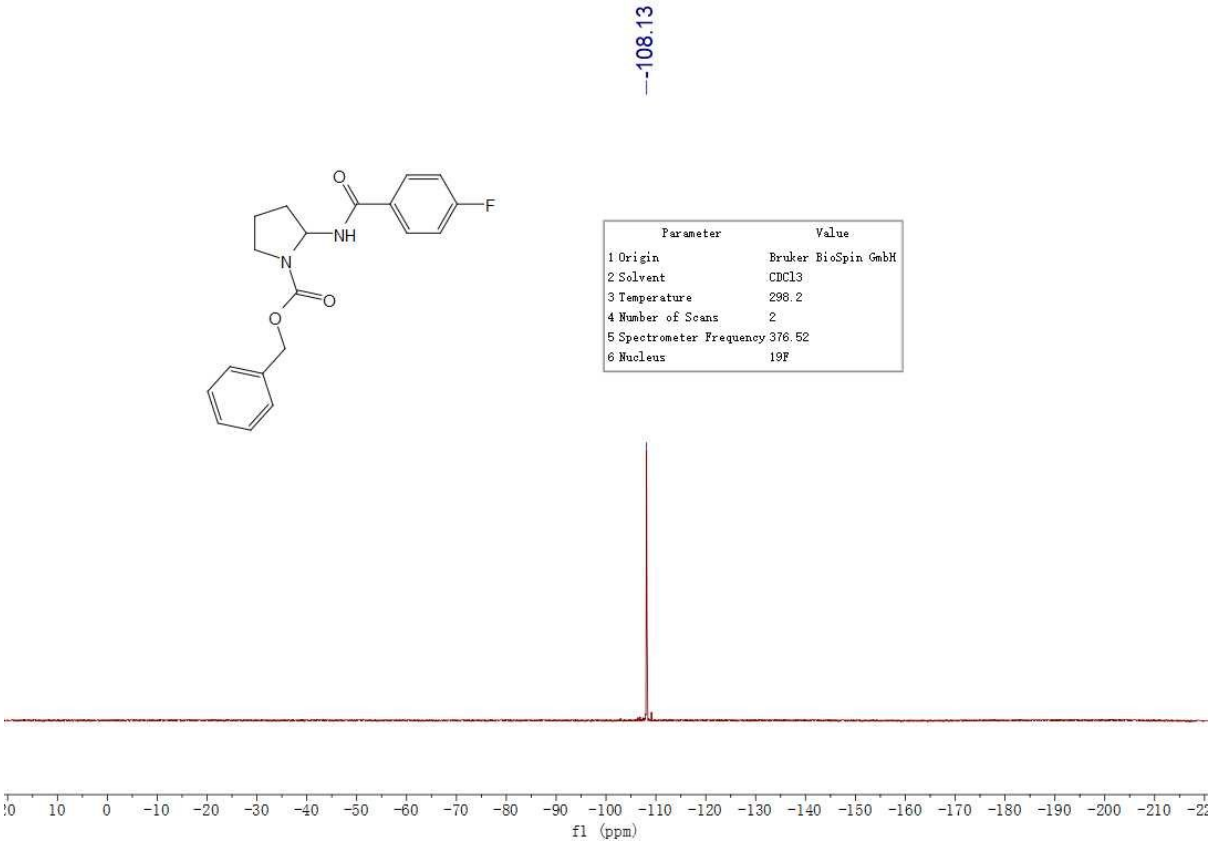
^{19}F NMR spectrum of **3ea** (376 MHz, $CDCl_3$)



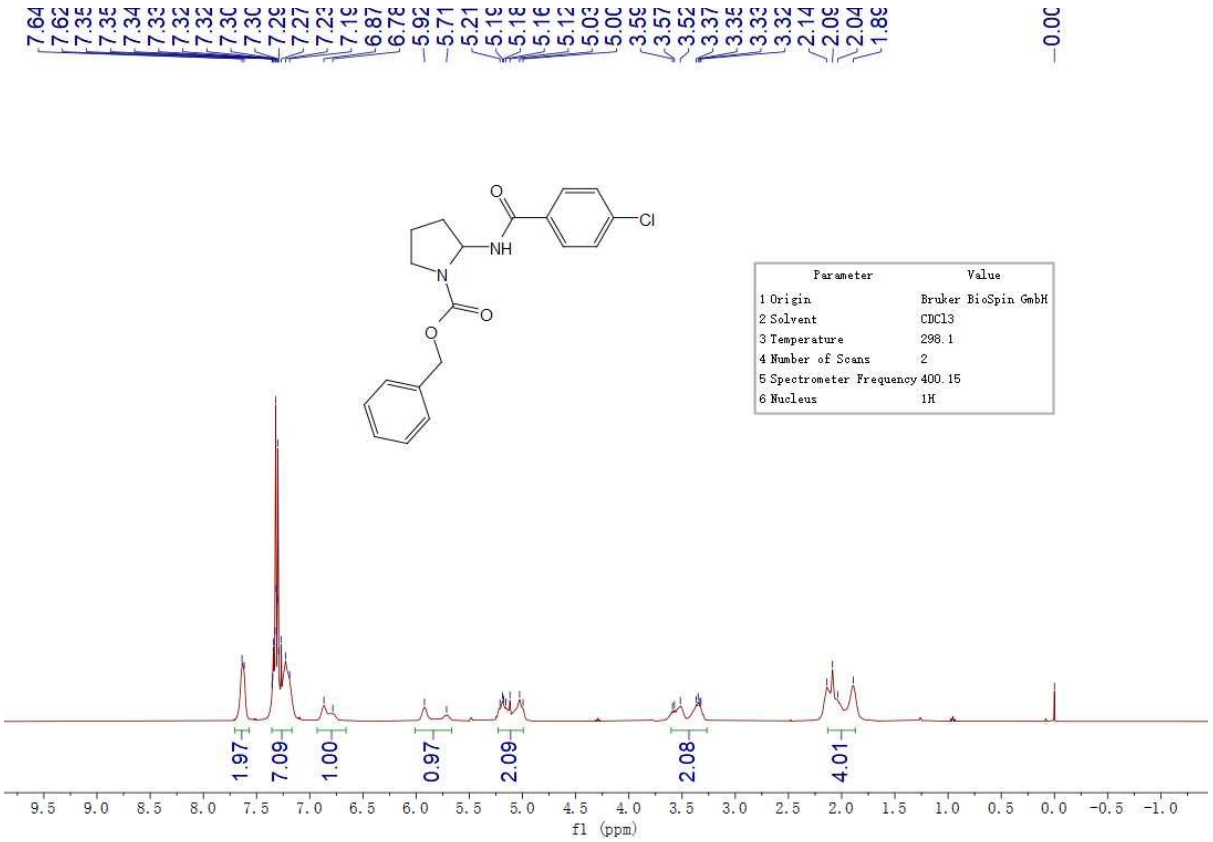
^{1}H NMR spectrum of **3fa** (400 MHz, $CDCl_3$)



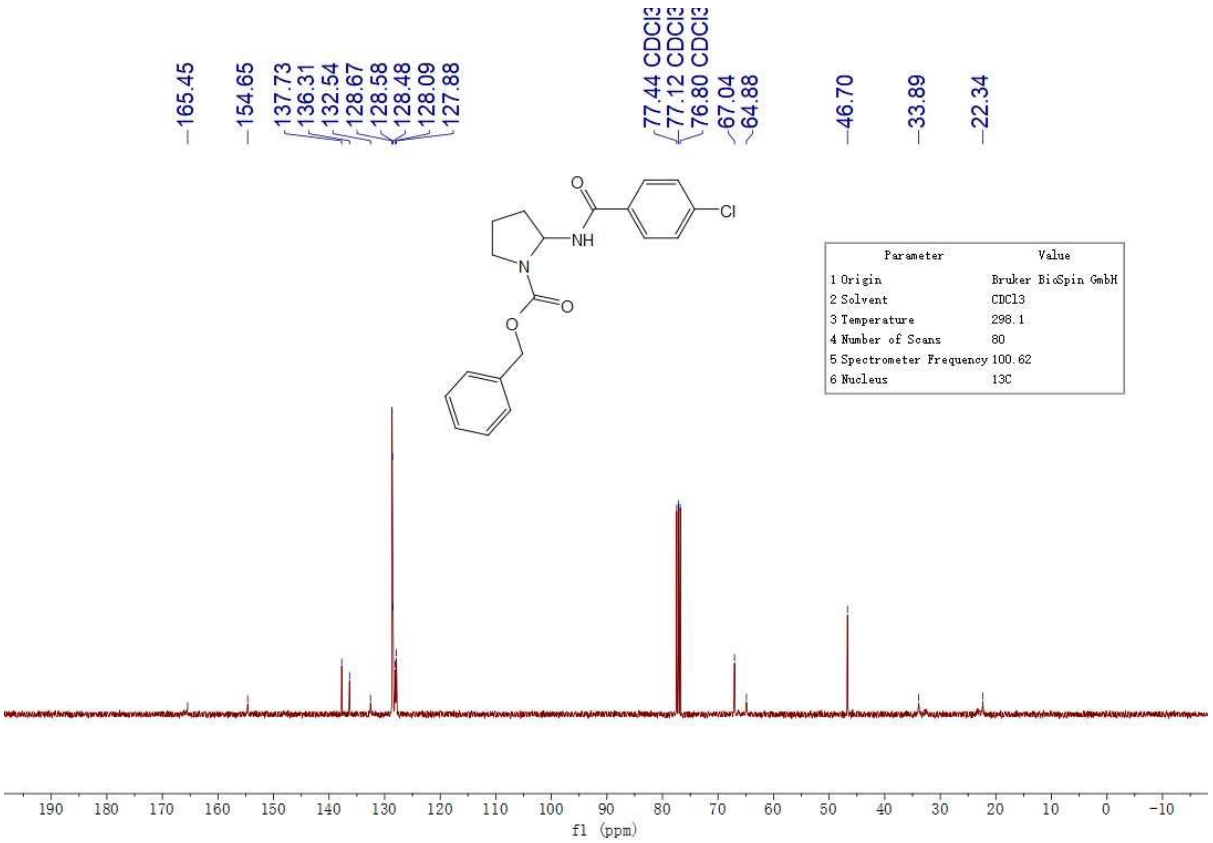
^{13}C NMR spectrum of **3fa** (100 MHz, $CDCl_3$)



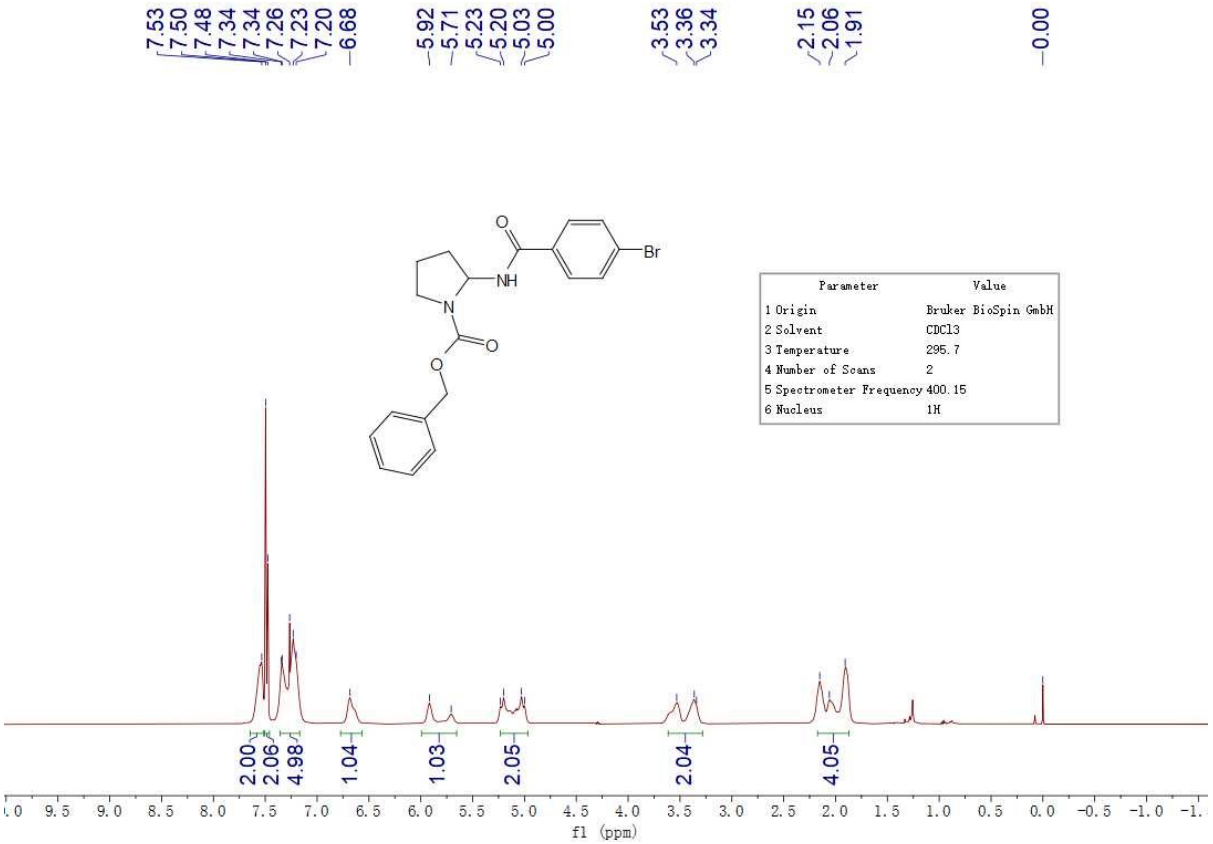
^{19}F NMR spectrum of **3fa** (376 MHz, $CDCl_3$)



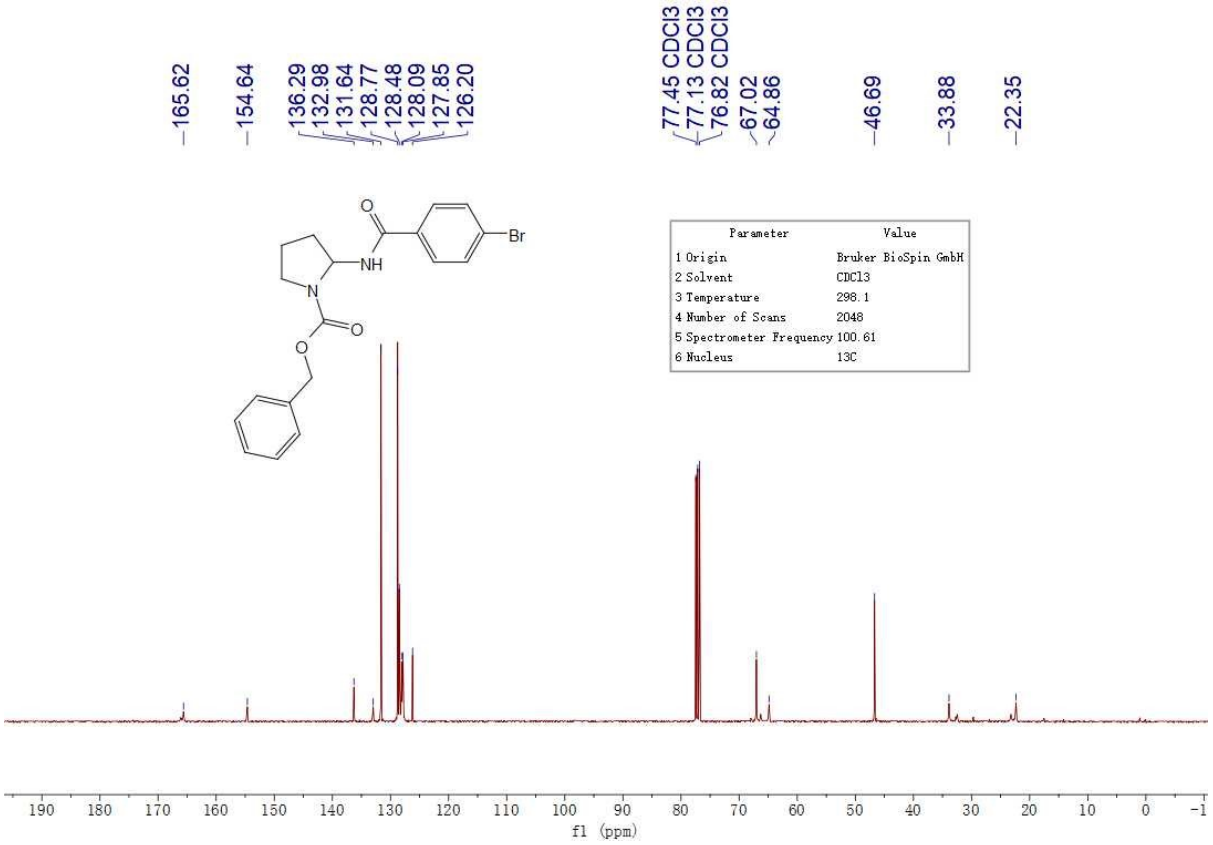
^{1}H NMR spectrum of **3ga** (400 MHz, $CDCl_3$)



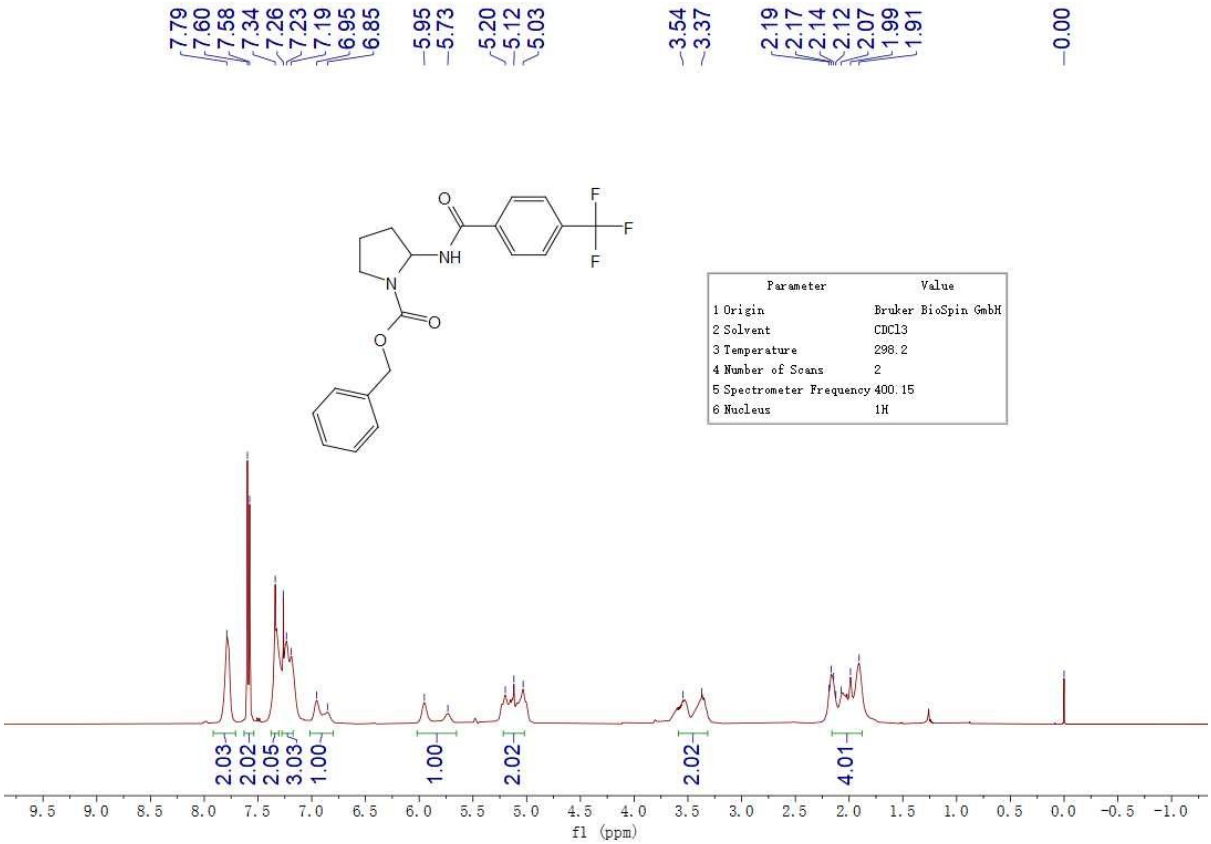
^{13}C NMR spectrum of **3ga** (100 MHz, $CDCl_3$)



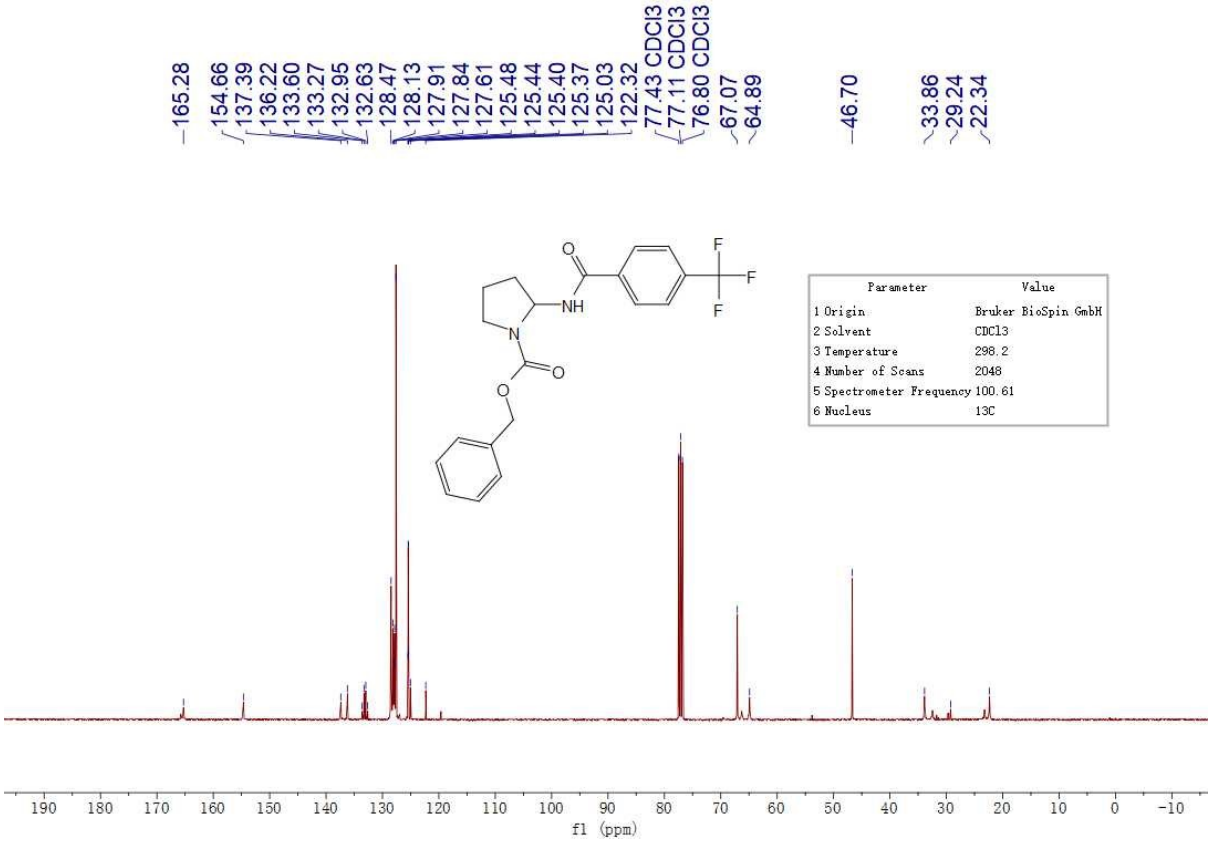
^{1}H NMR spectrum of **3ha** (400 MHz, $CDCl_3$)



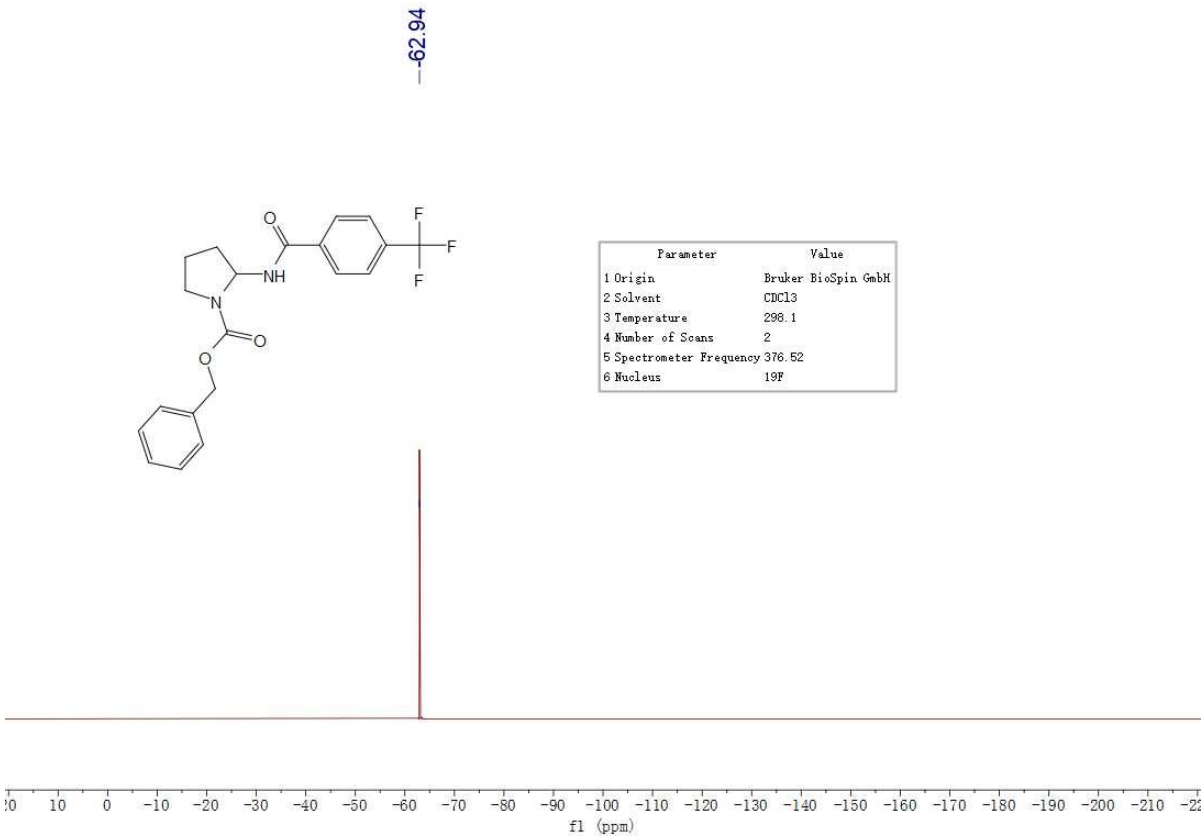
^{13}C NMR spectrum of **3ha** (100 MHz, $CDCl_3$)



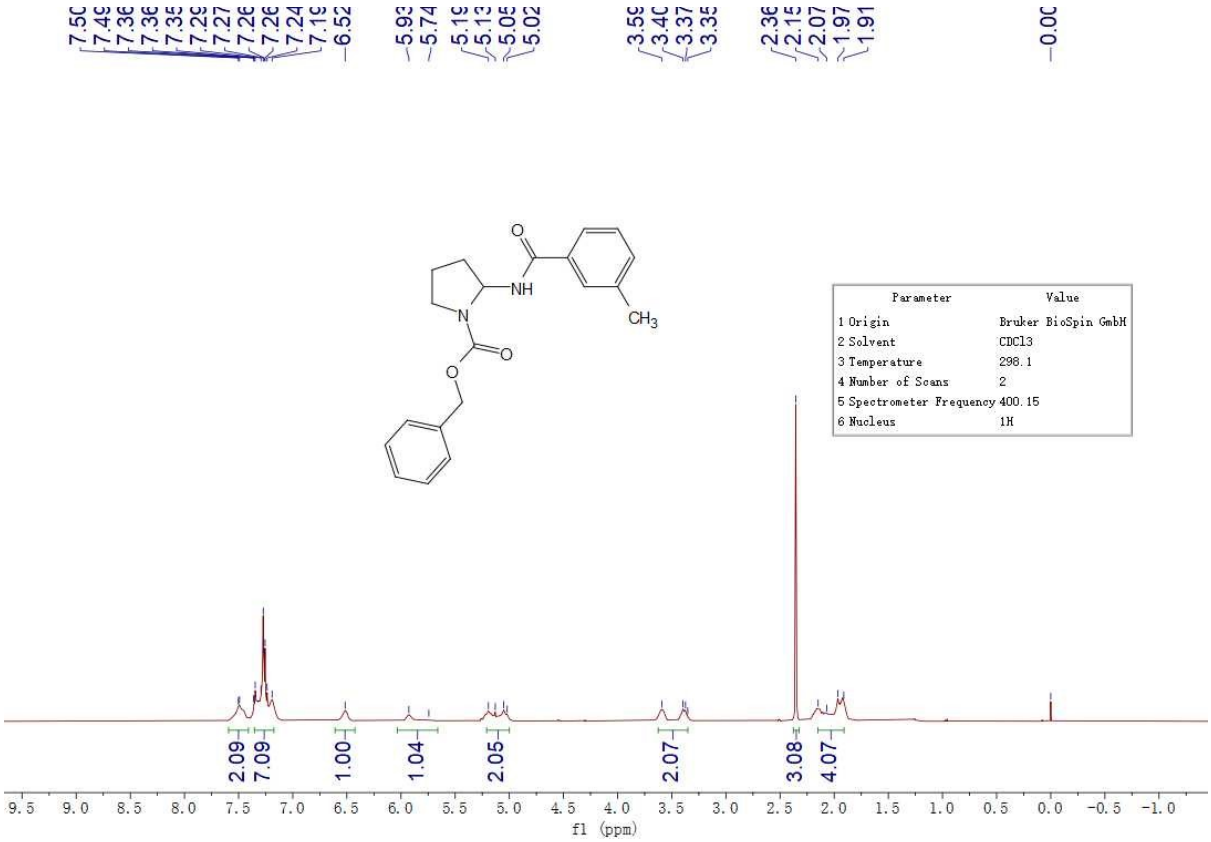
^{1}H NMR spectrum of **3ia** (400 MHz, $CDCl_3$)



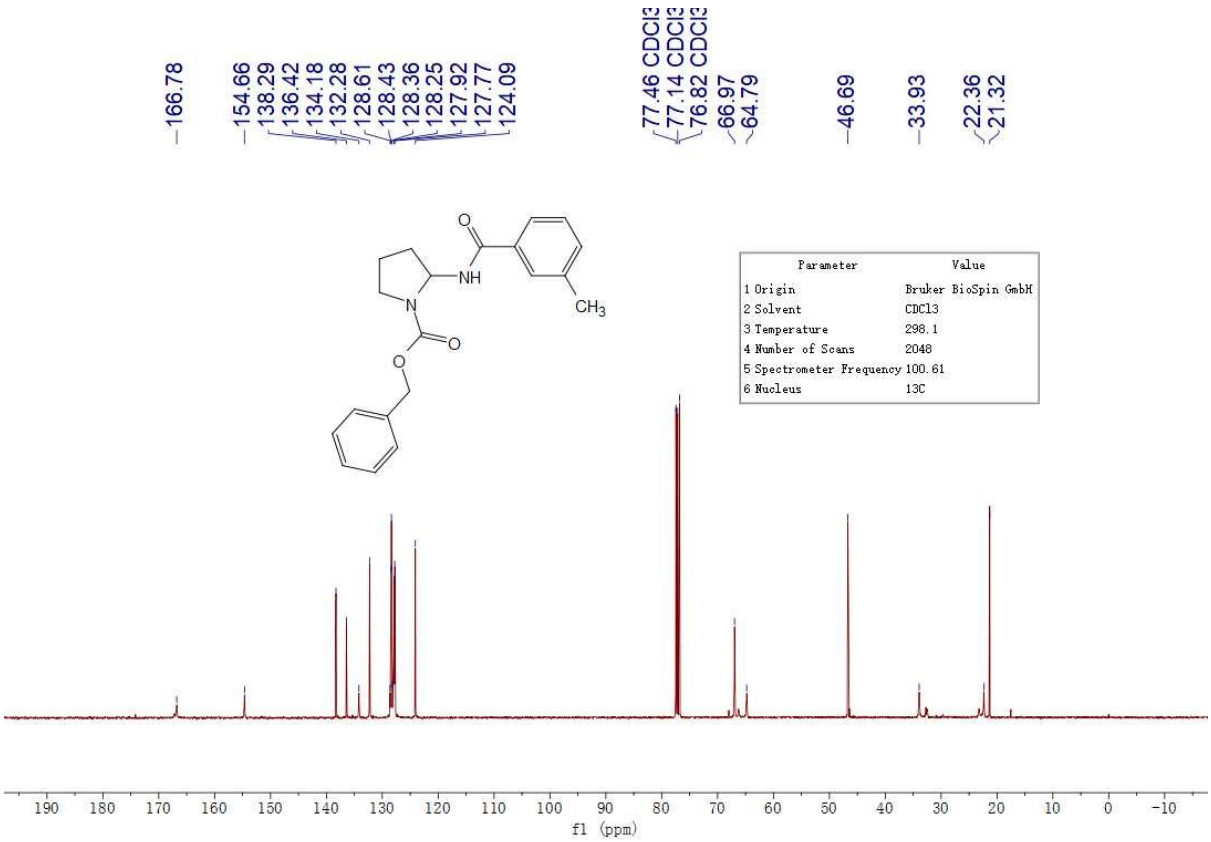
^{13}C NMR spectrum of **3ia** (100 MHz, $CDCl_3$)



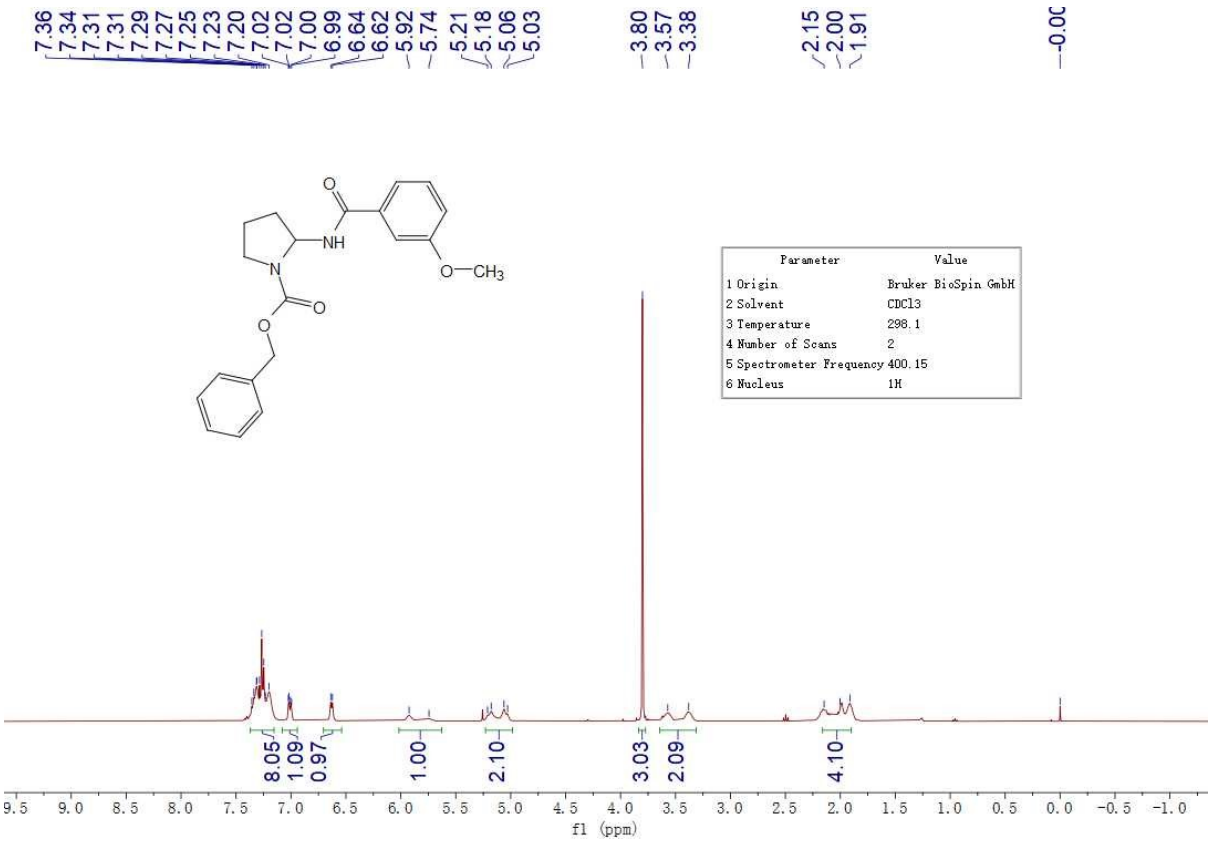
^{19}F NMR spectrum of **3ia** (376 MHz,$CDCl_3$)



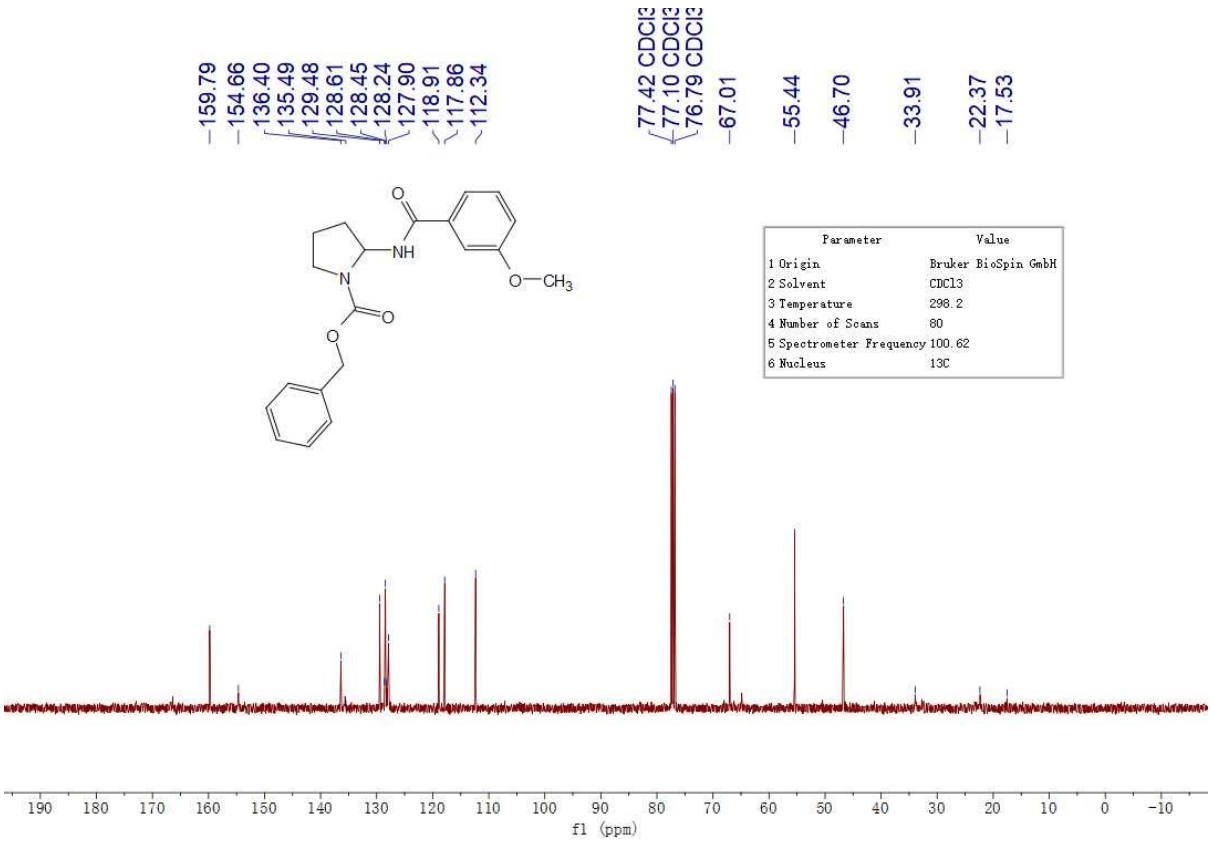
^{1}H NMR spectrum of **3ja** (400 MHz, $CDCl_3$)



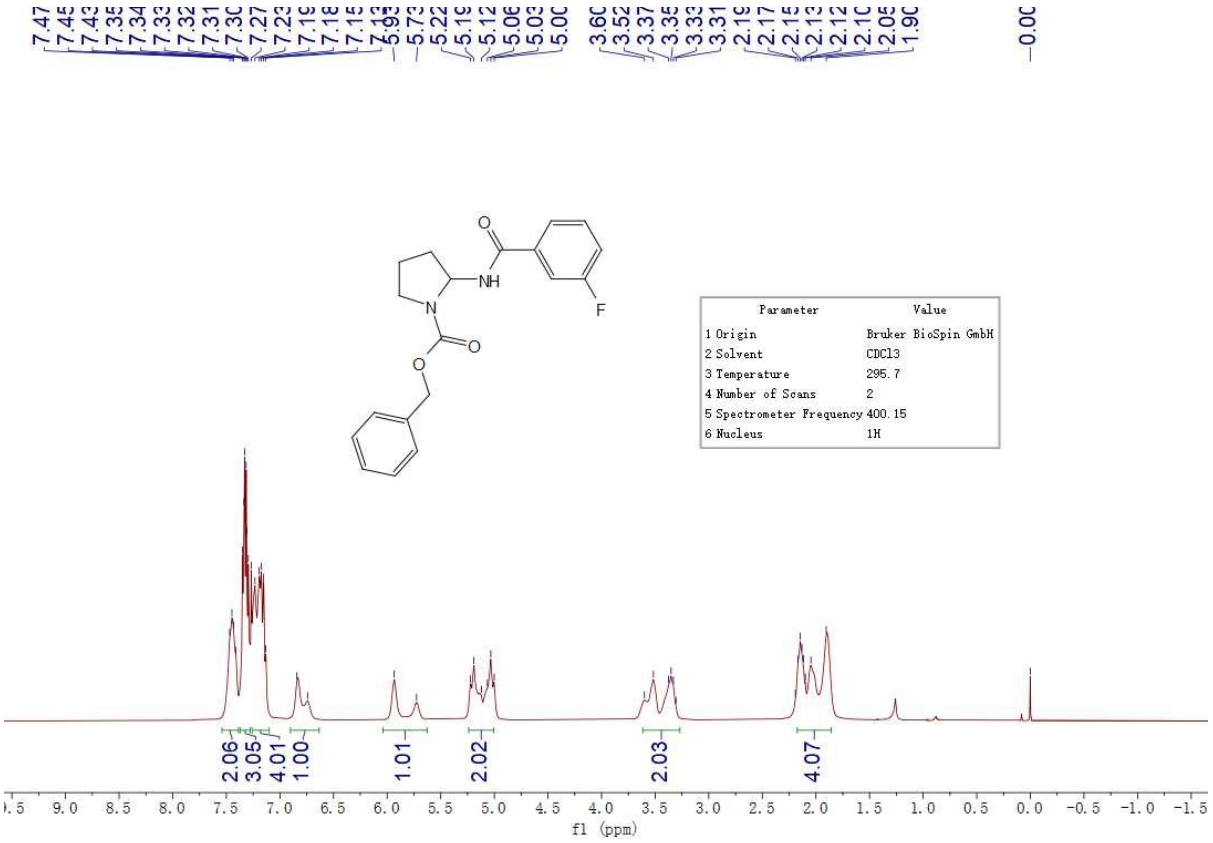
^{13}C NMR spectrum of **3ja** (100 MHz, $CDCl_3$)



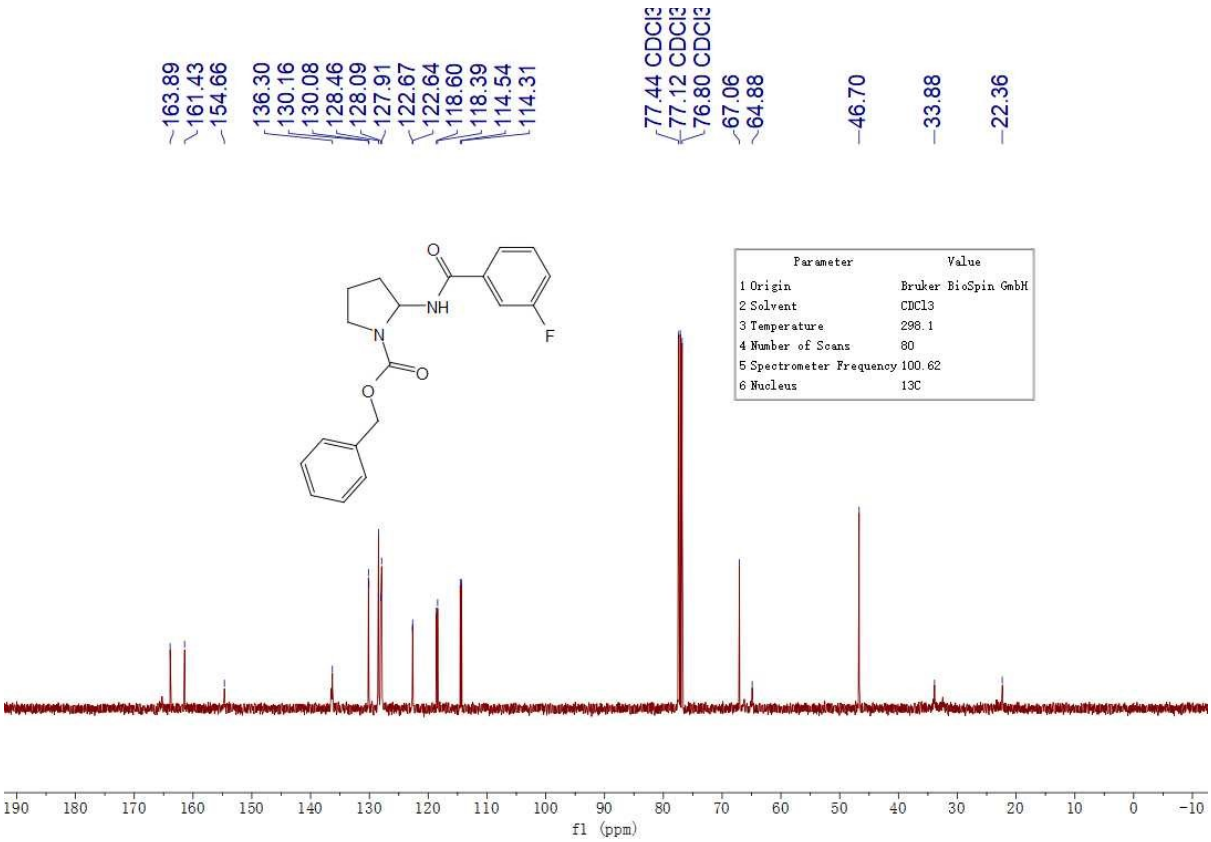
^{1}H NMR spectrum of **3ka** (400 MHz, $CDCl_3$)



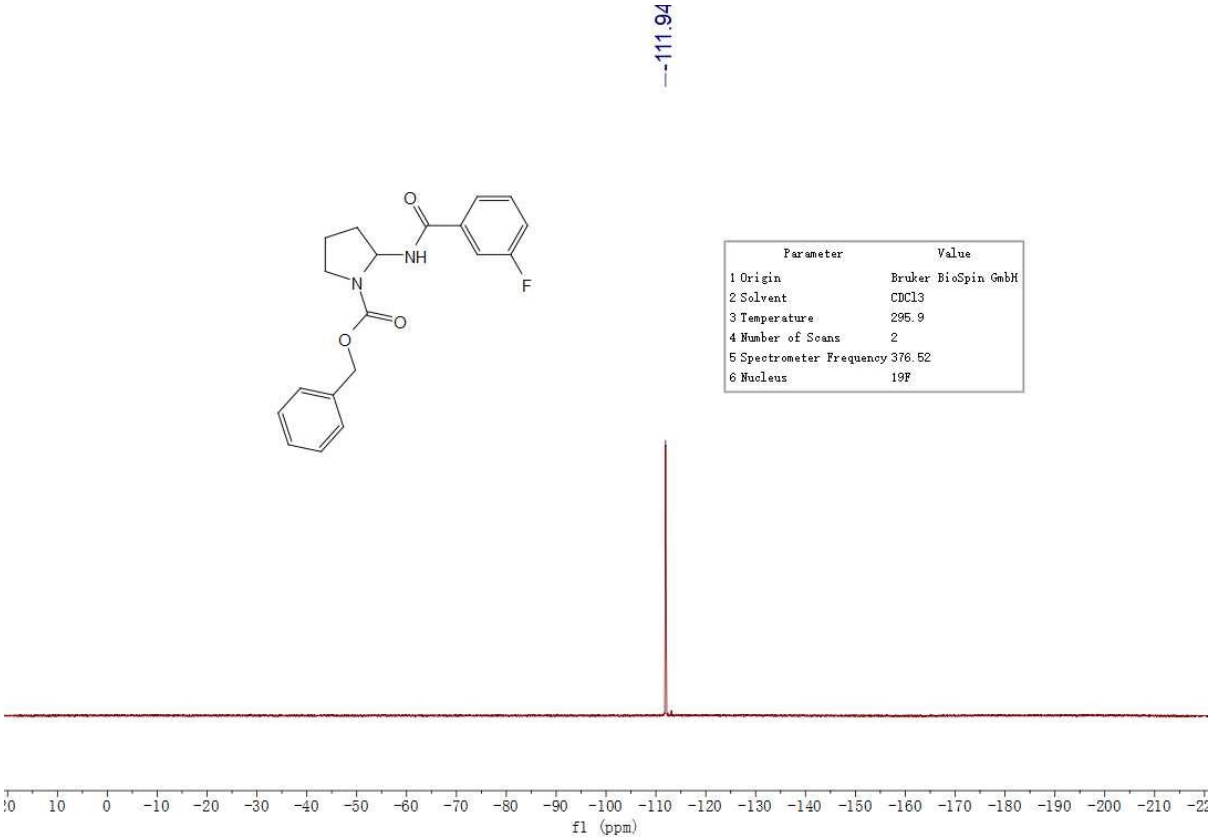
^{13}C NMR spectrum of **3ka** (100 MHz, $CDCl_3$)



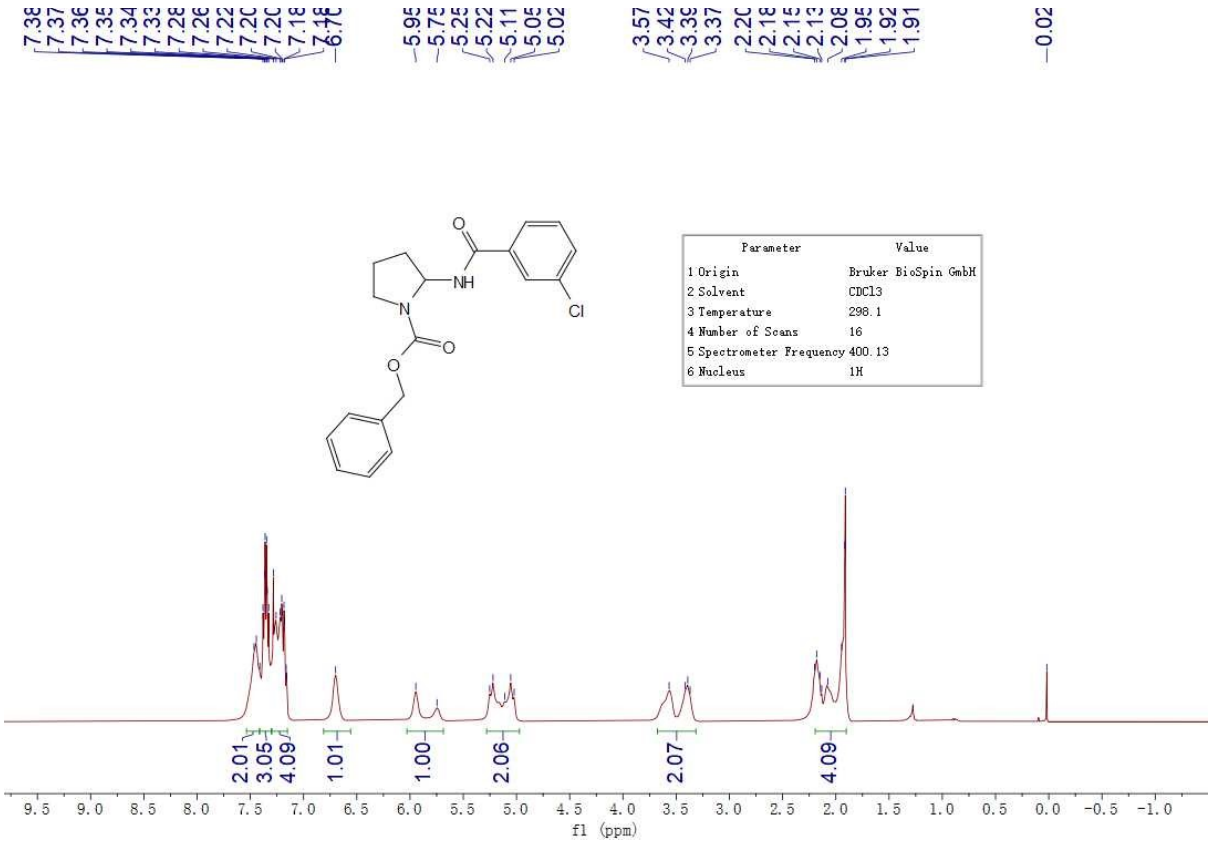
^{1}H NMR spectrum of **3la** (400 MHz, $CDCl_3$)



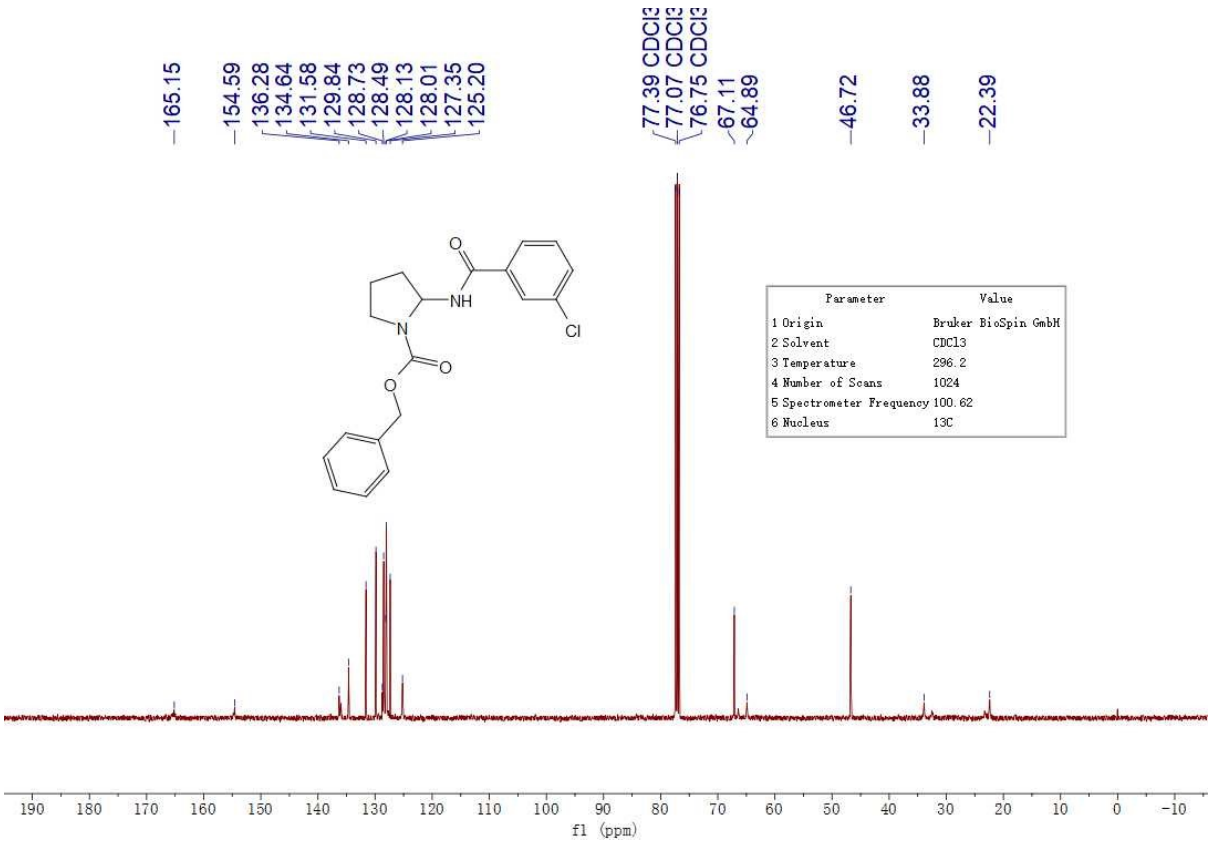
^{13}C NMR spectrum of **3la** (100 MHz, $CDCl_3$)



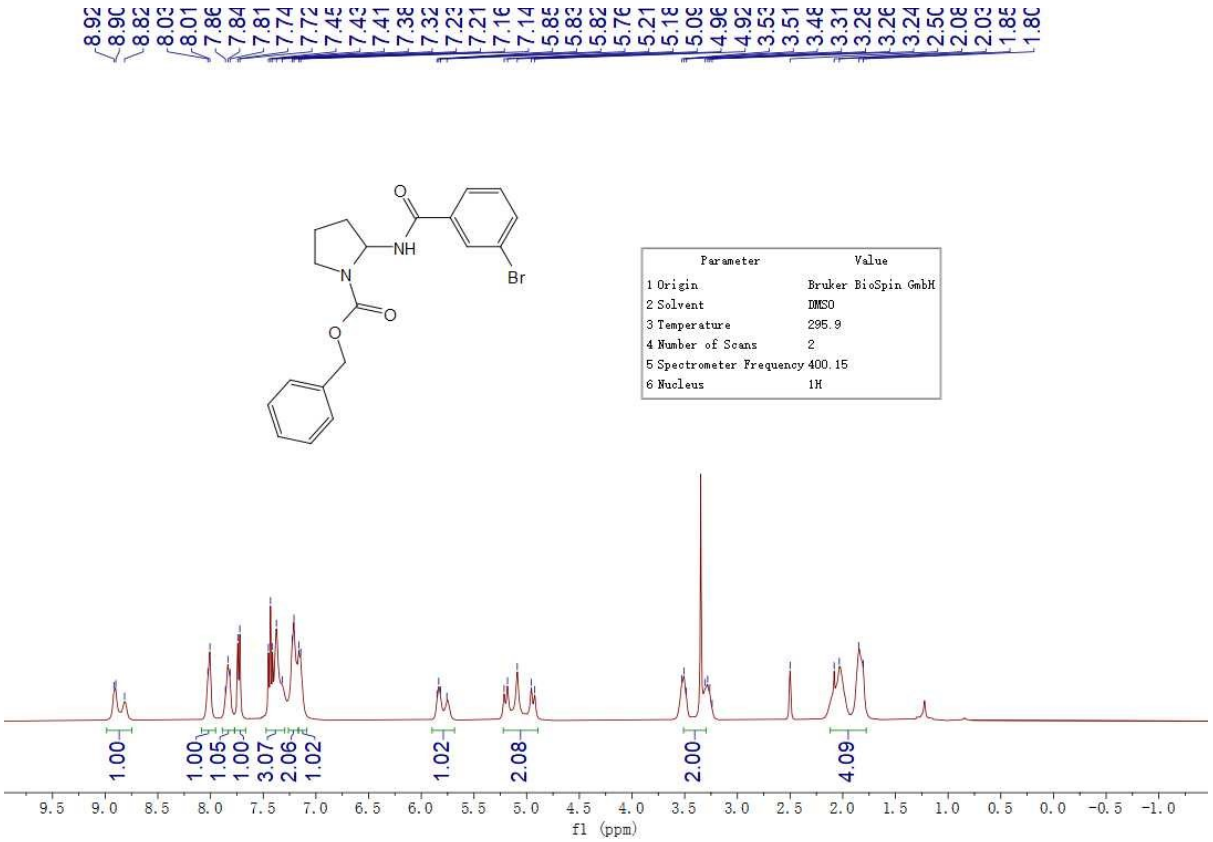
^{19}F NMR spectrum of **3la** (376 MHz, $CDCl_3$)



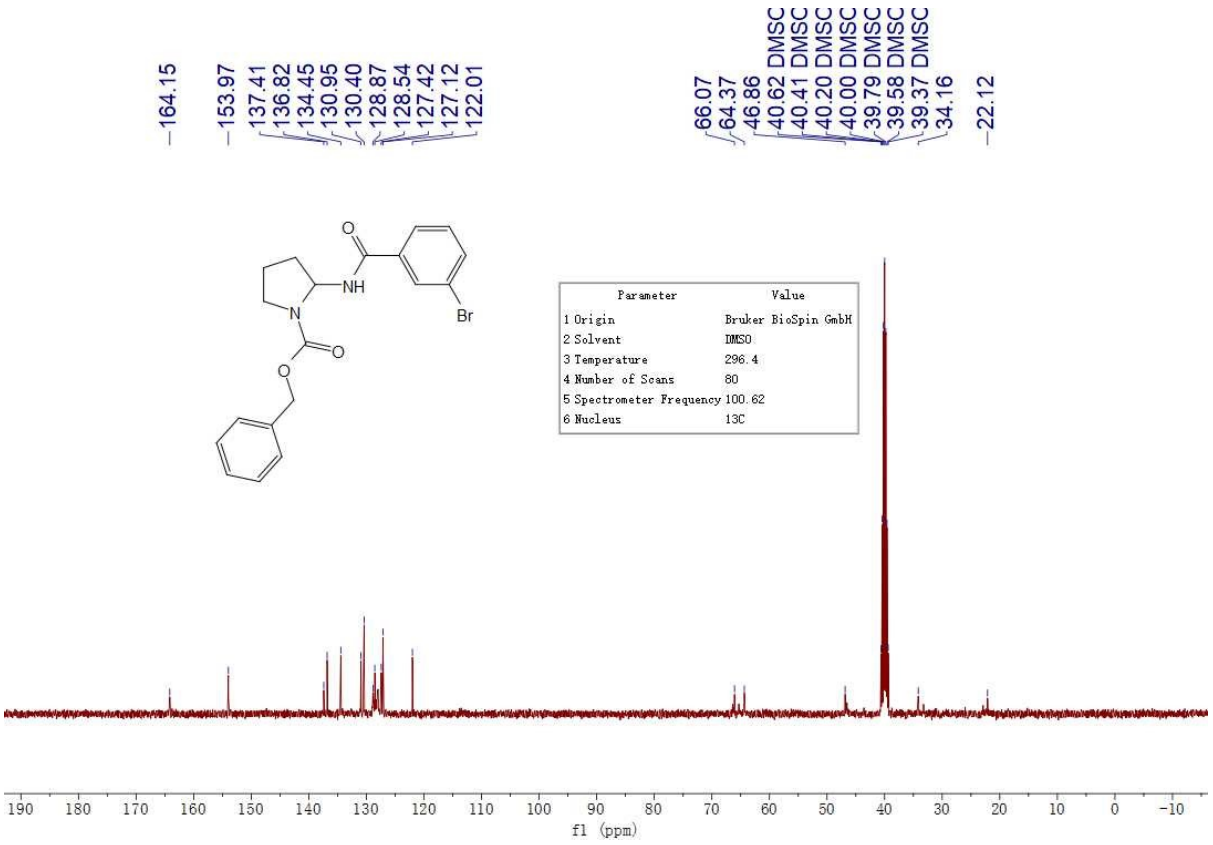
^{1}H NMR spectrum of **3ma** (400 MHz, $CDCl_3$)



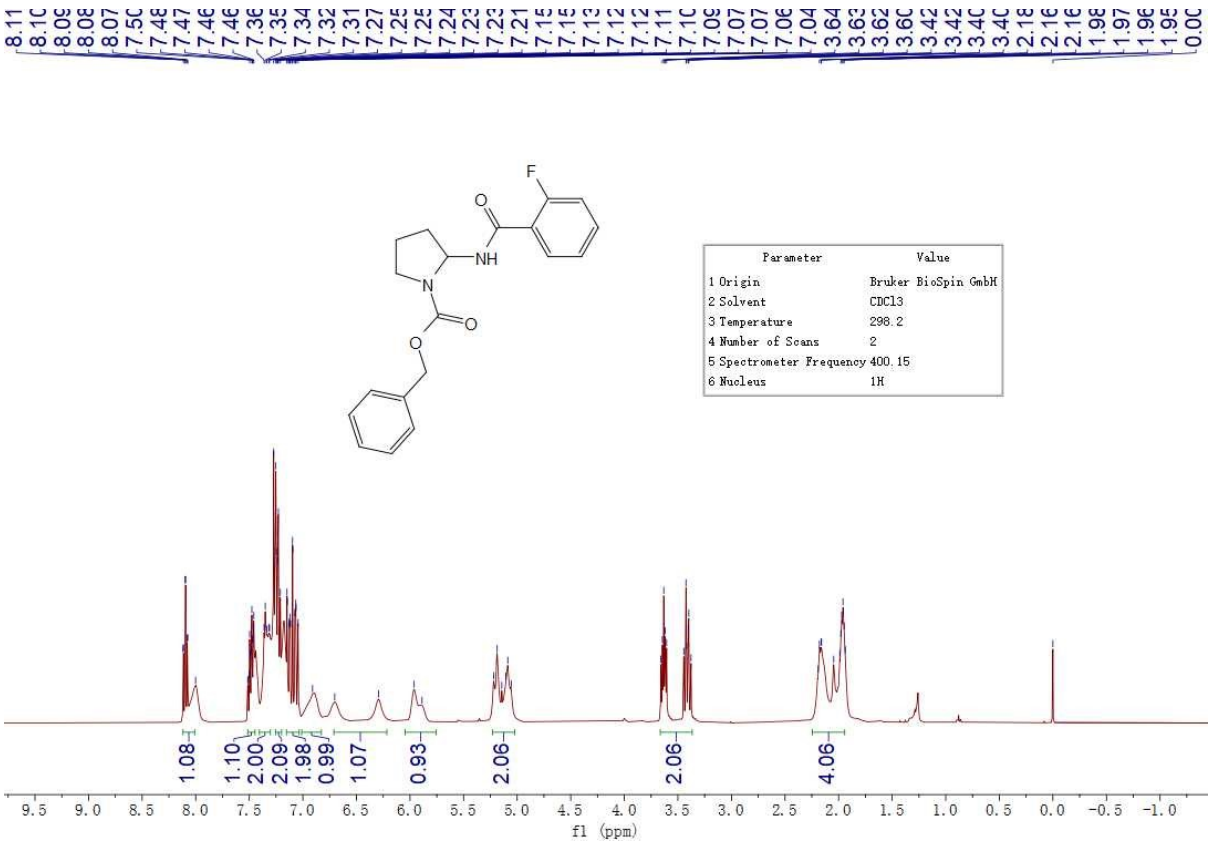
^{13}C NMR spectrum of **3ma** (100 MHz, $CDCl_3$)



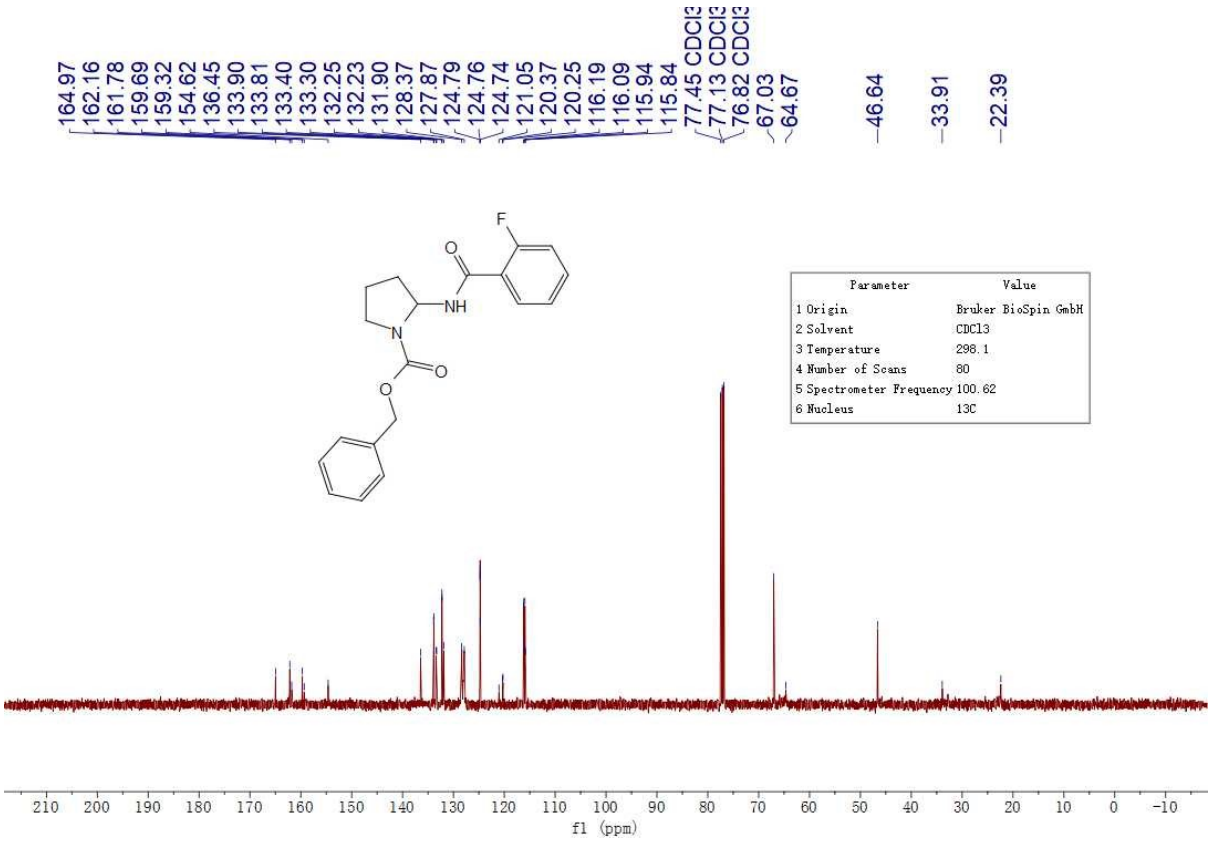
^{1}H NMR spectrum of **3na** (400 MHz, DMSO-d_6)



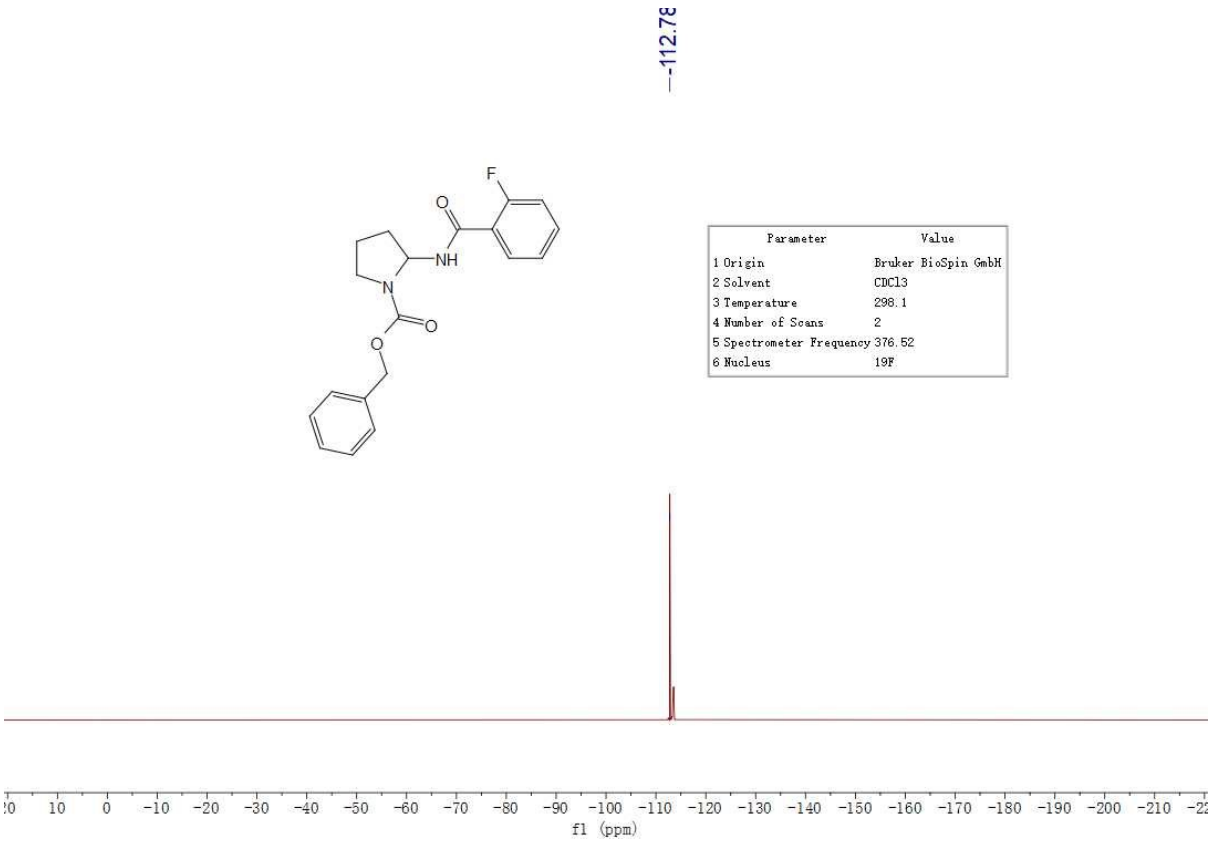
^{13}C NMR spectrum of **3na** (100 MHz, DMSO-d_6)



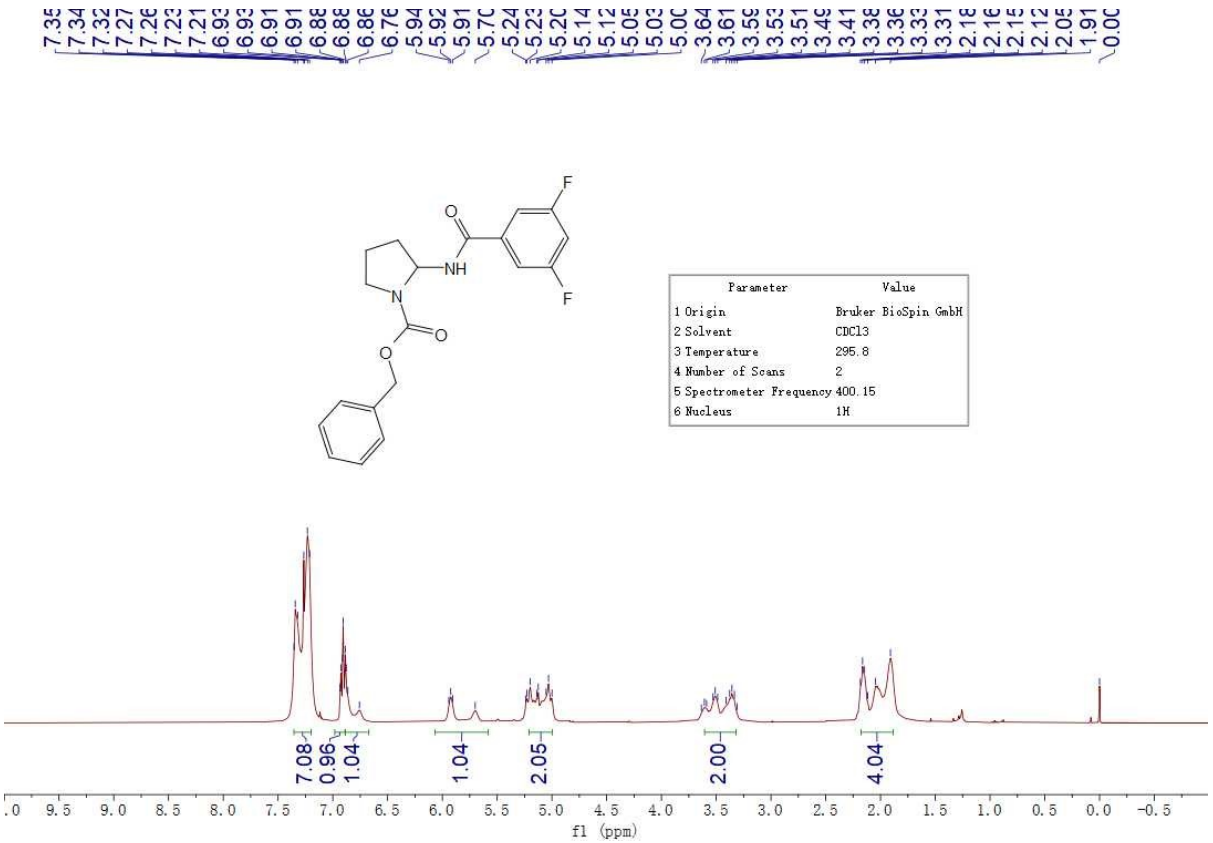
^{1}H NMR spectrum of **3oa** (400 MHz, $CDCl_3$)



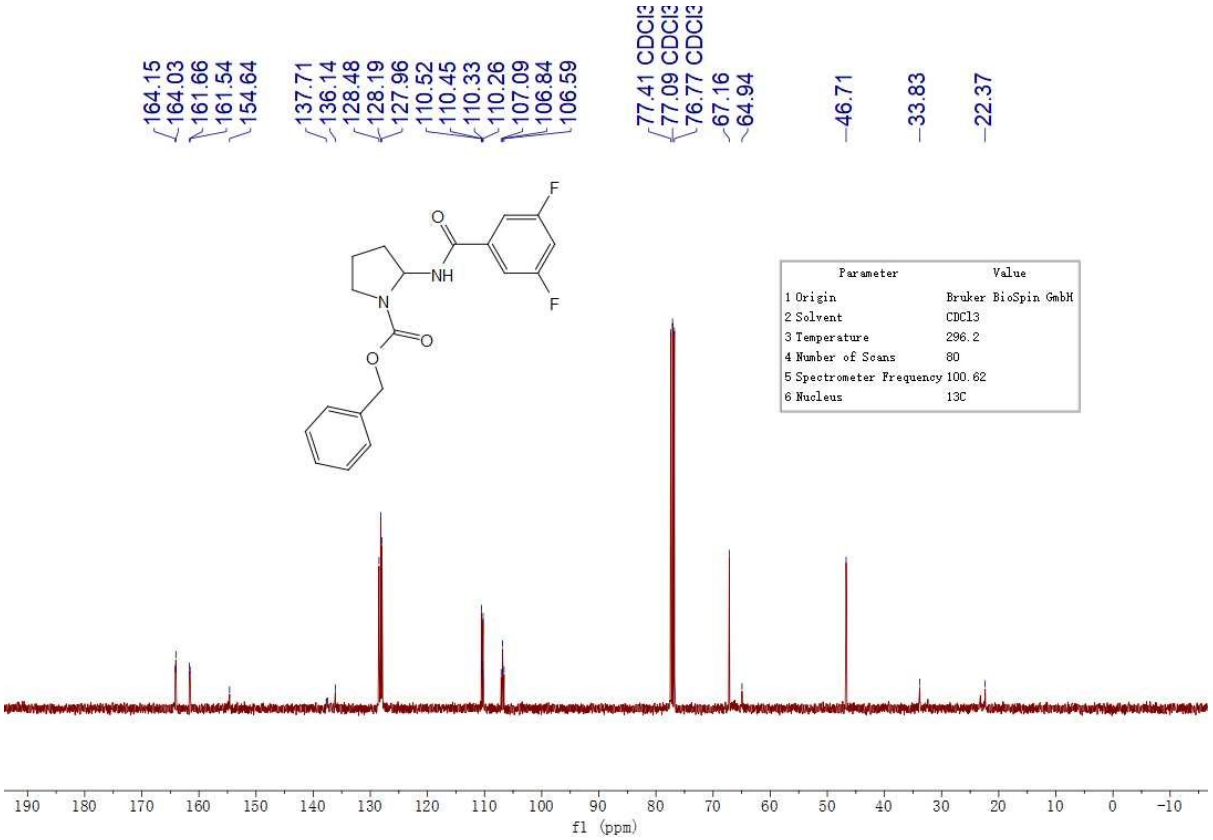
^{13}C NMR spectrum of **3oa** (100 MHz, $CDCl_3$)



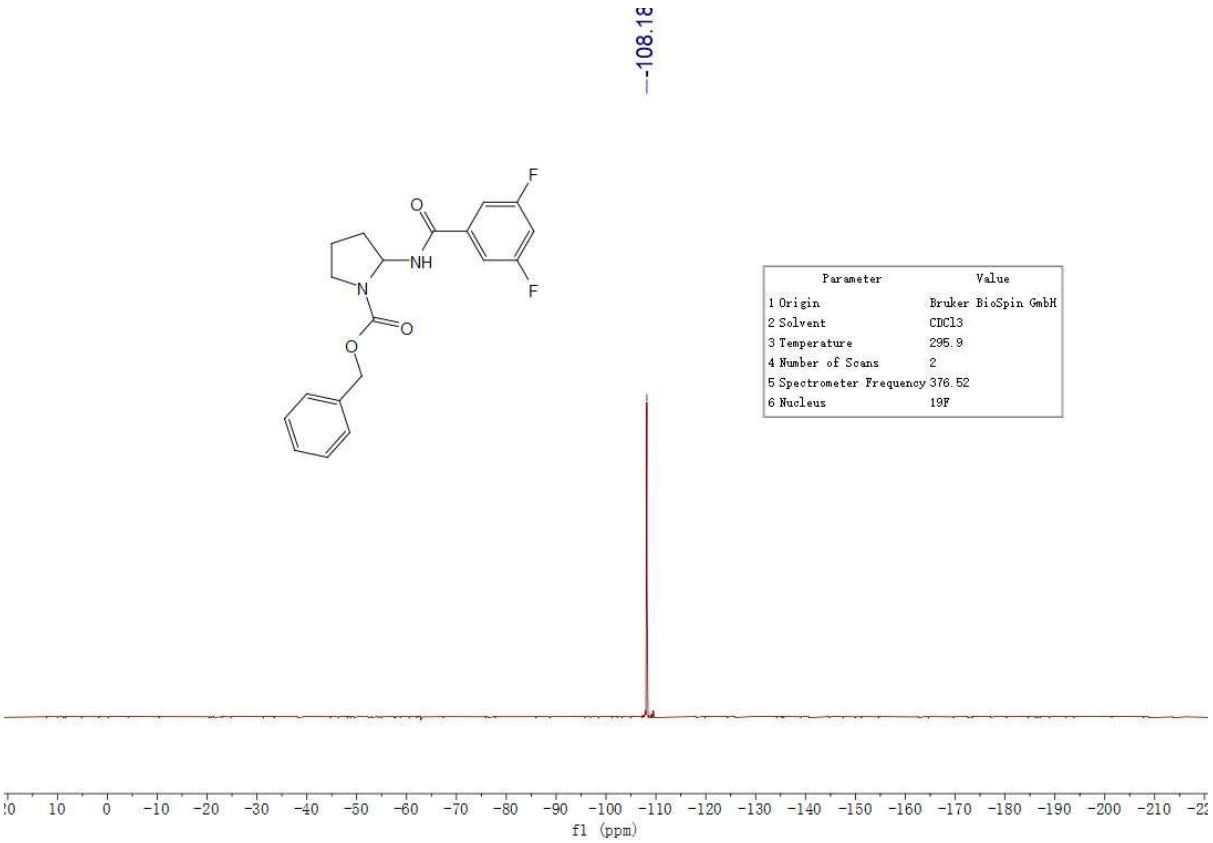
^{19}F NMR spectrum of **3oa** (376 MHz, $CDCl_3$)



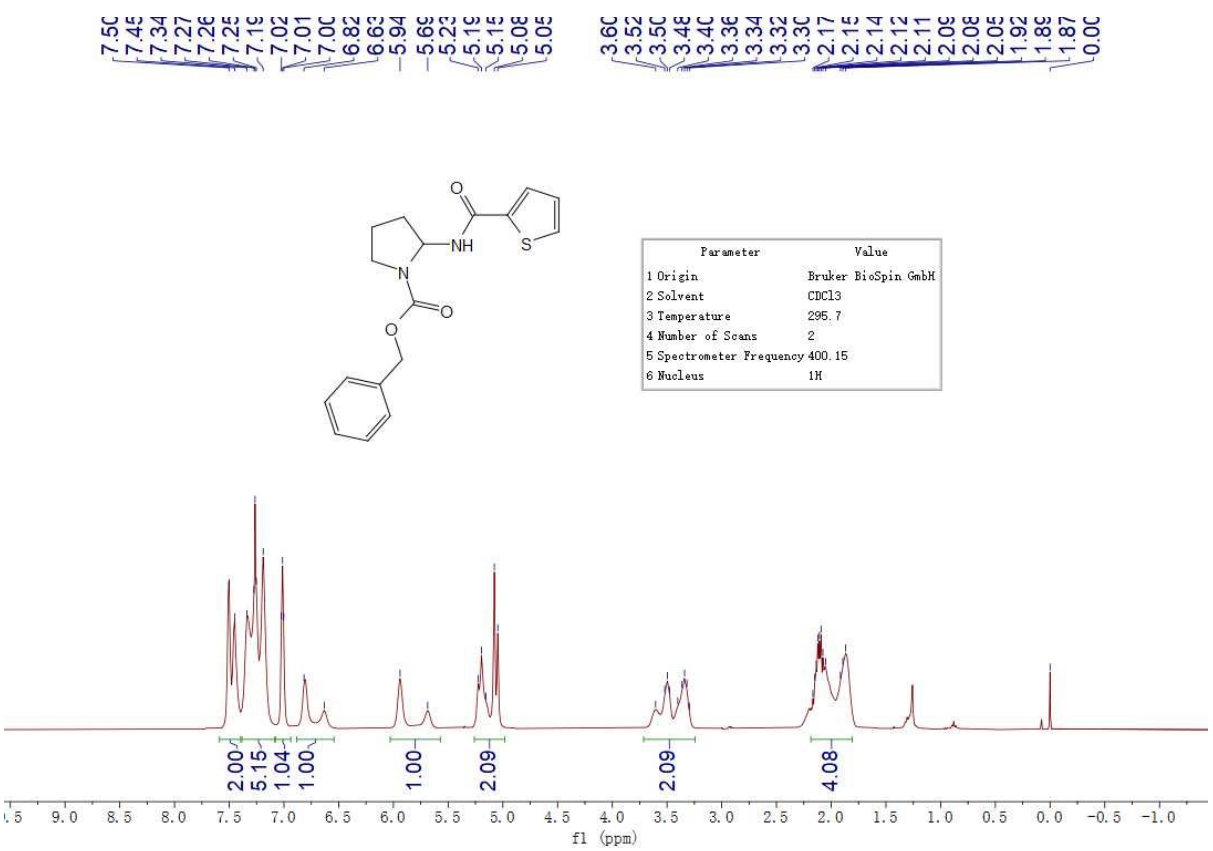
^{1}H NMR spectrum of **3pa** (400 MHz, $CDCl_3$)



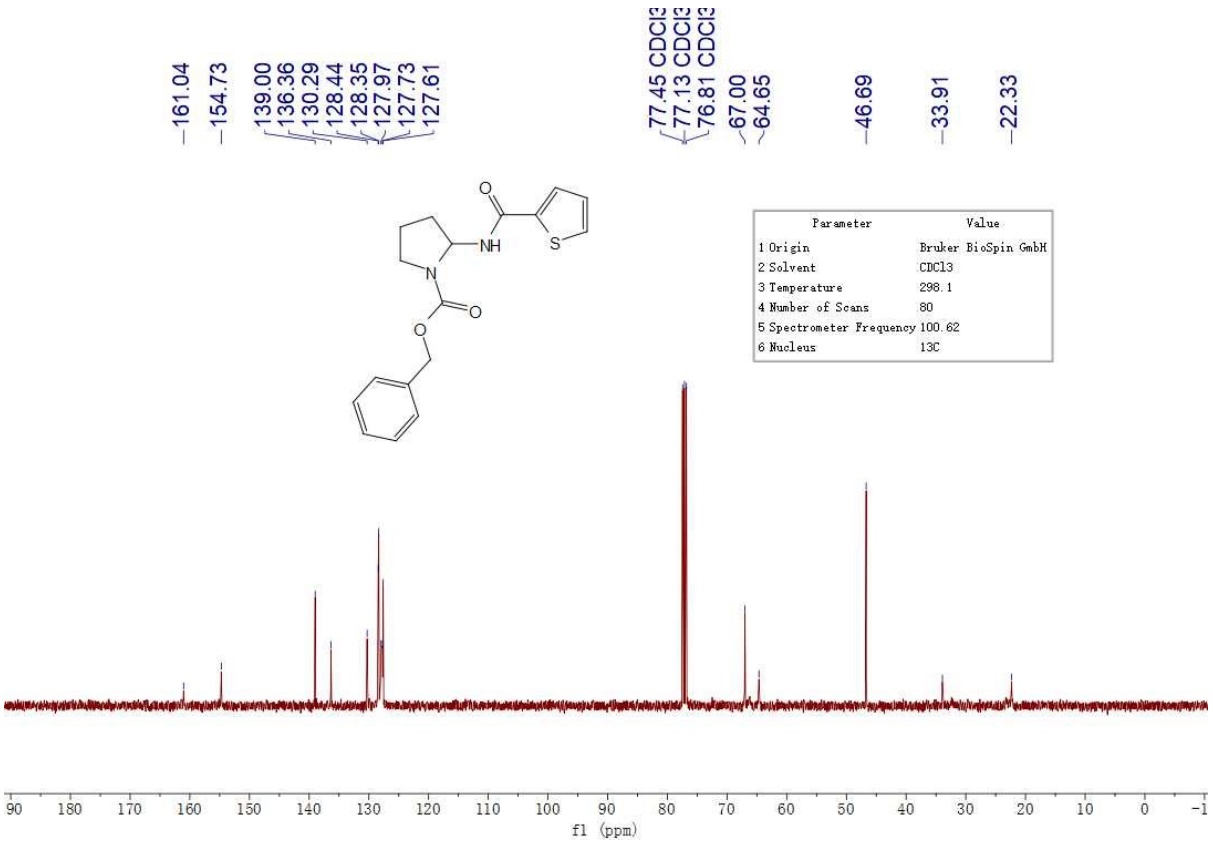
^{13}C NMR spectrum of **3pa** (100 MHz, $CDCl_3$)



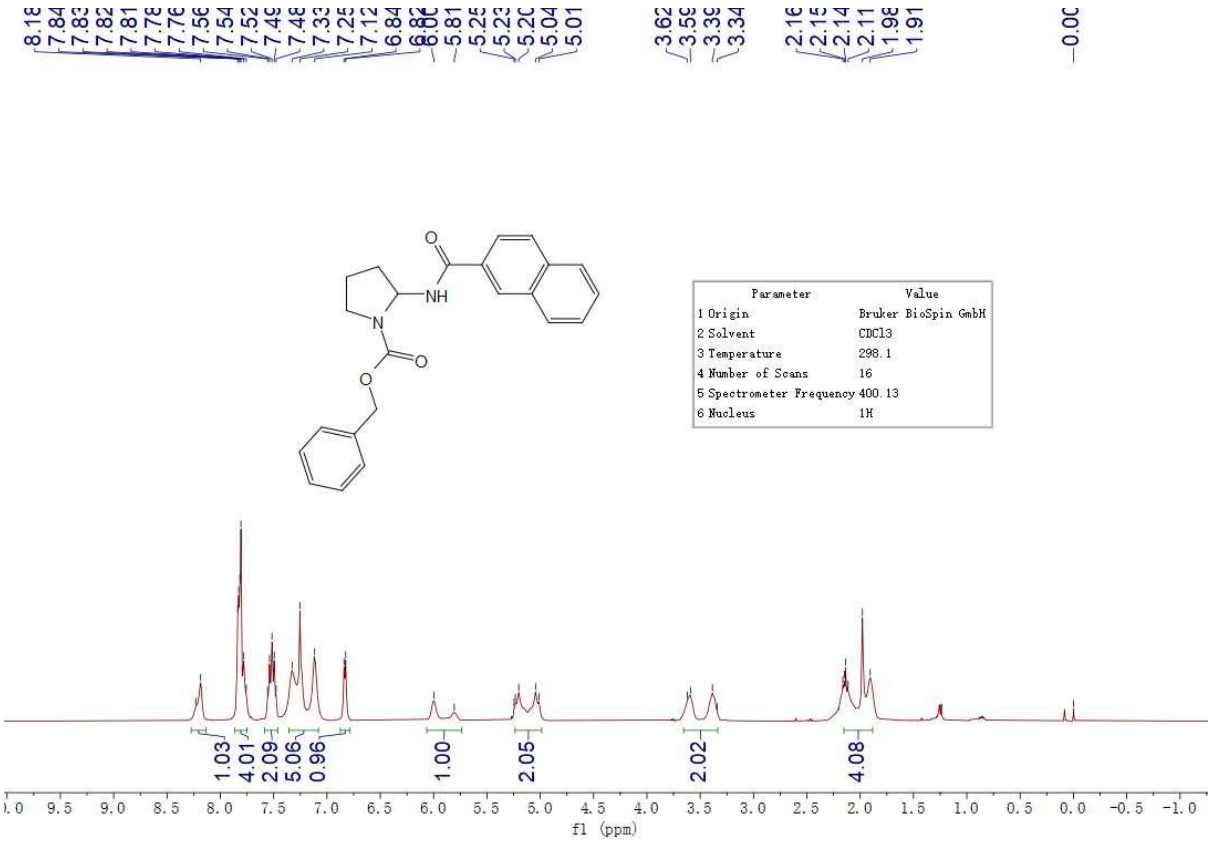
^{19}F NMR spectrum of **3pa** (376 MHz, $CDCl_3$)



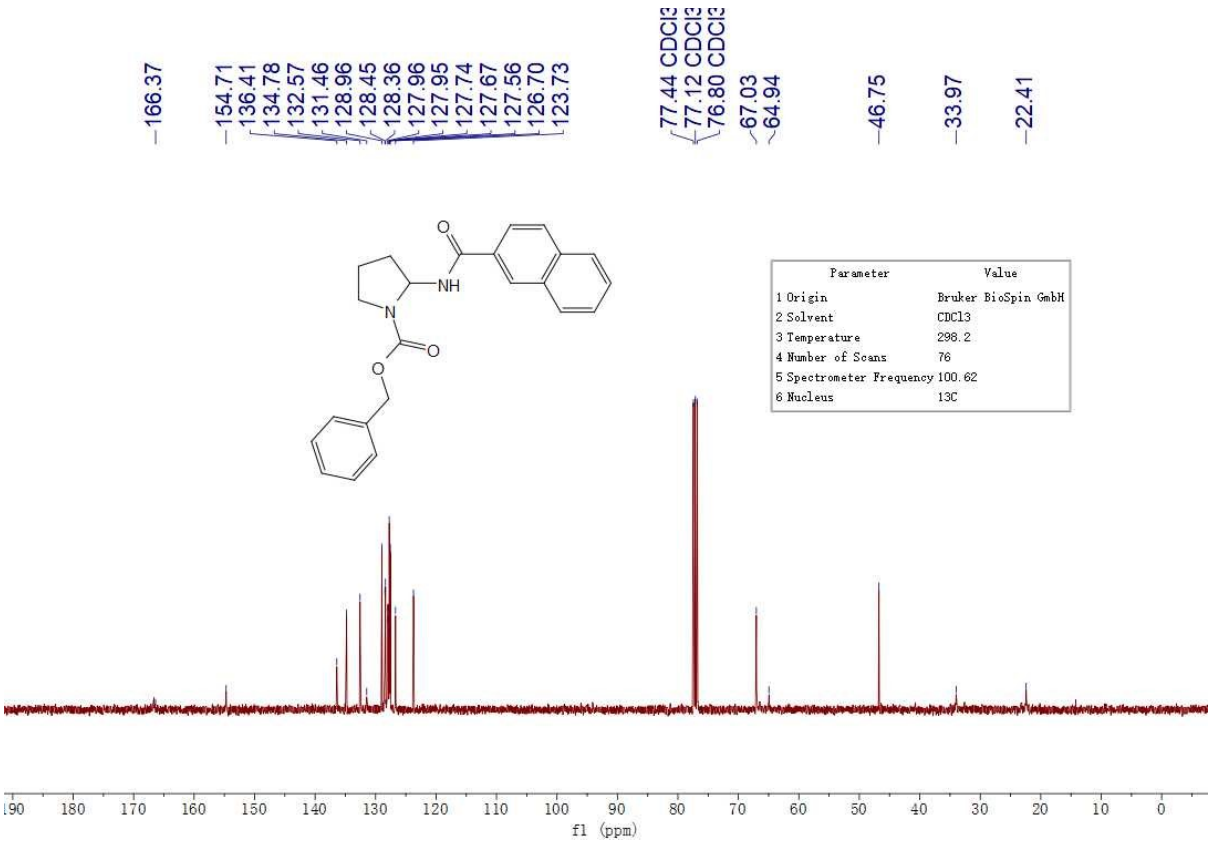
^{1}H NMR spectrum of **3qa** (400 MHz, $CDCl_3$)



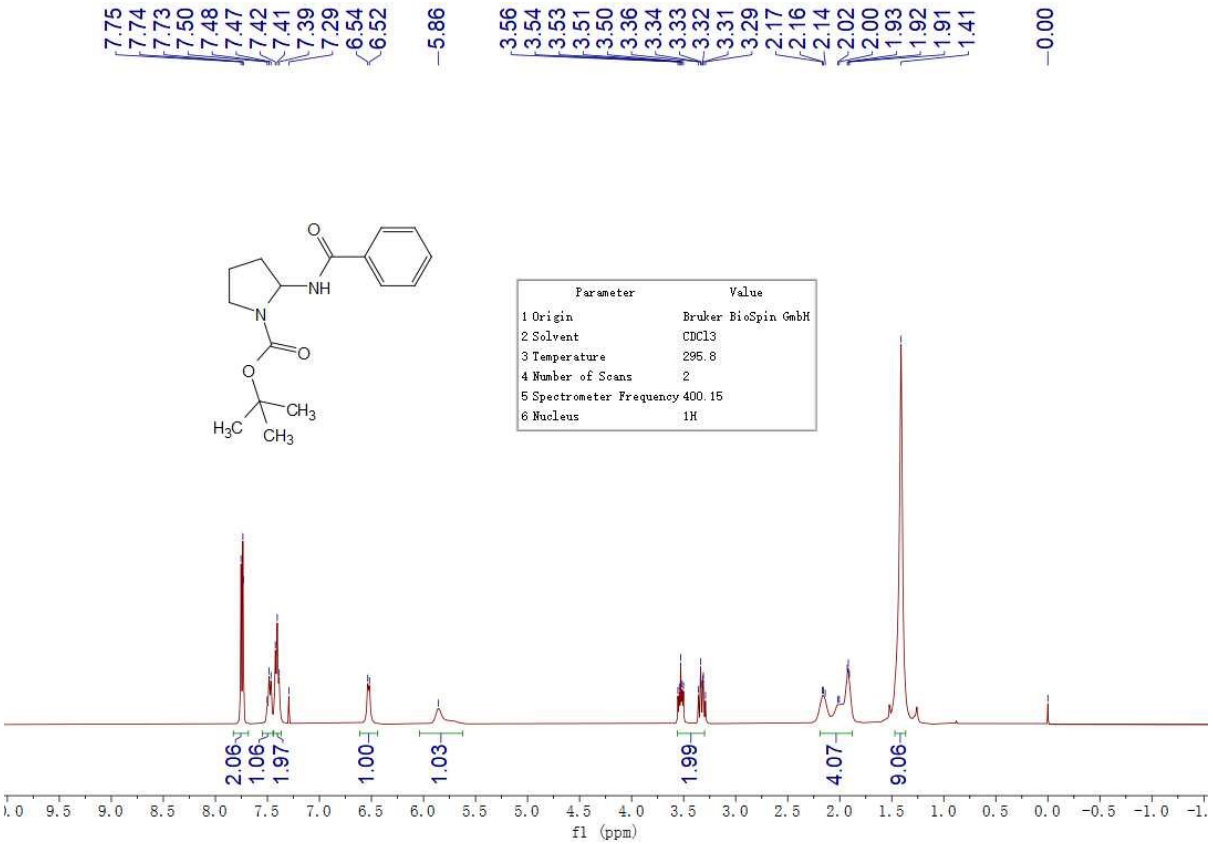
^{13}C NMR spectrum of **3qa** (100 MHz, $CDCl_3$)



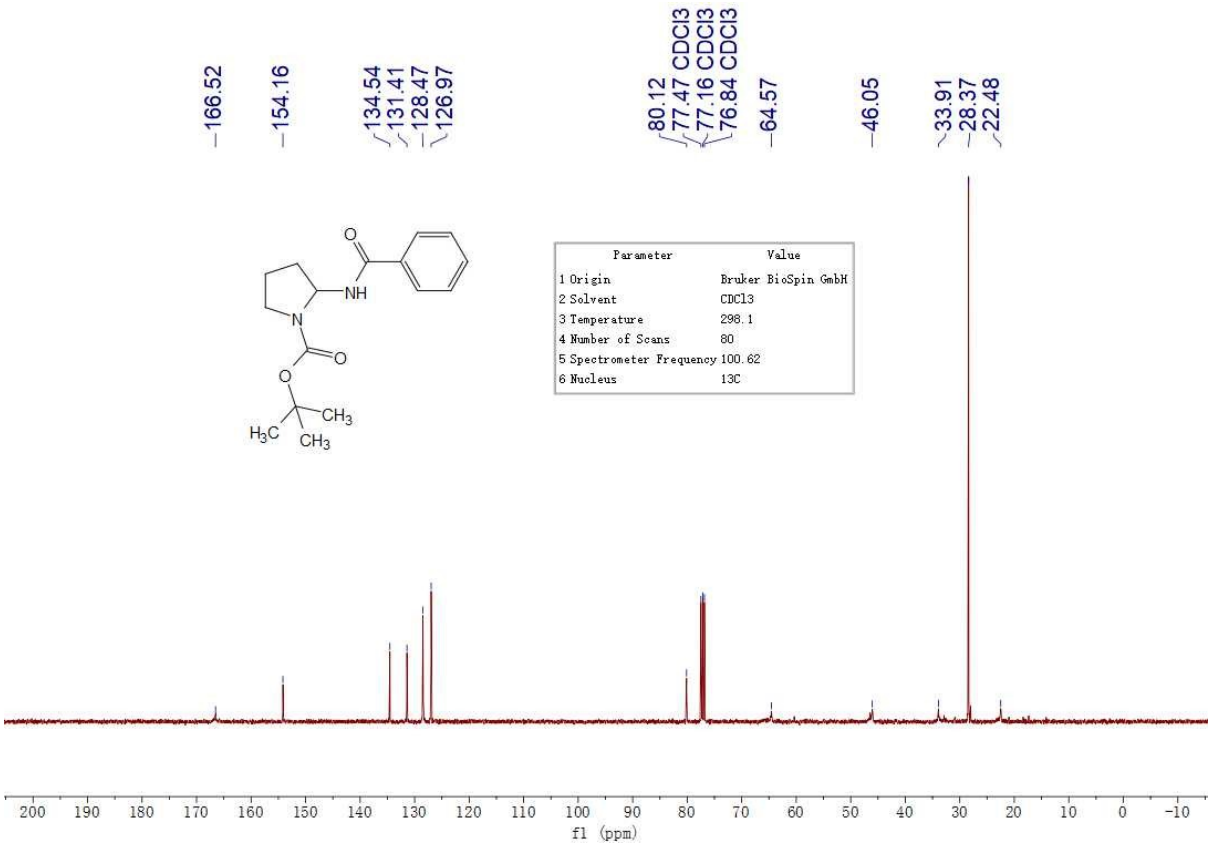
^{1}H NMR spectrum of **3ra** (400 MHz, $CDCl_3$)



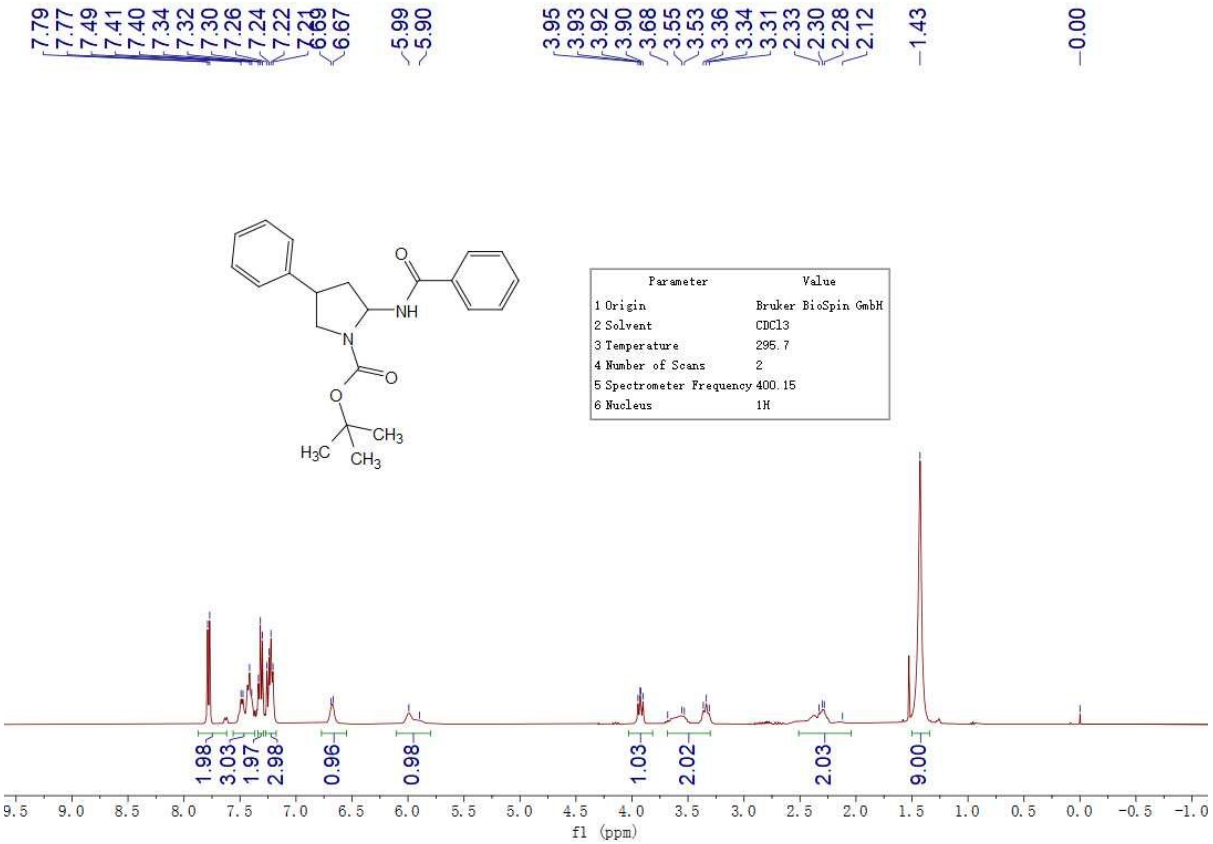
^{13}C NMR spectrum of **3ra** (100 MHz, $CDCl_3$)



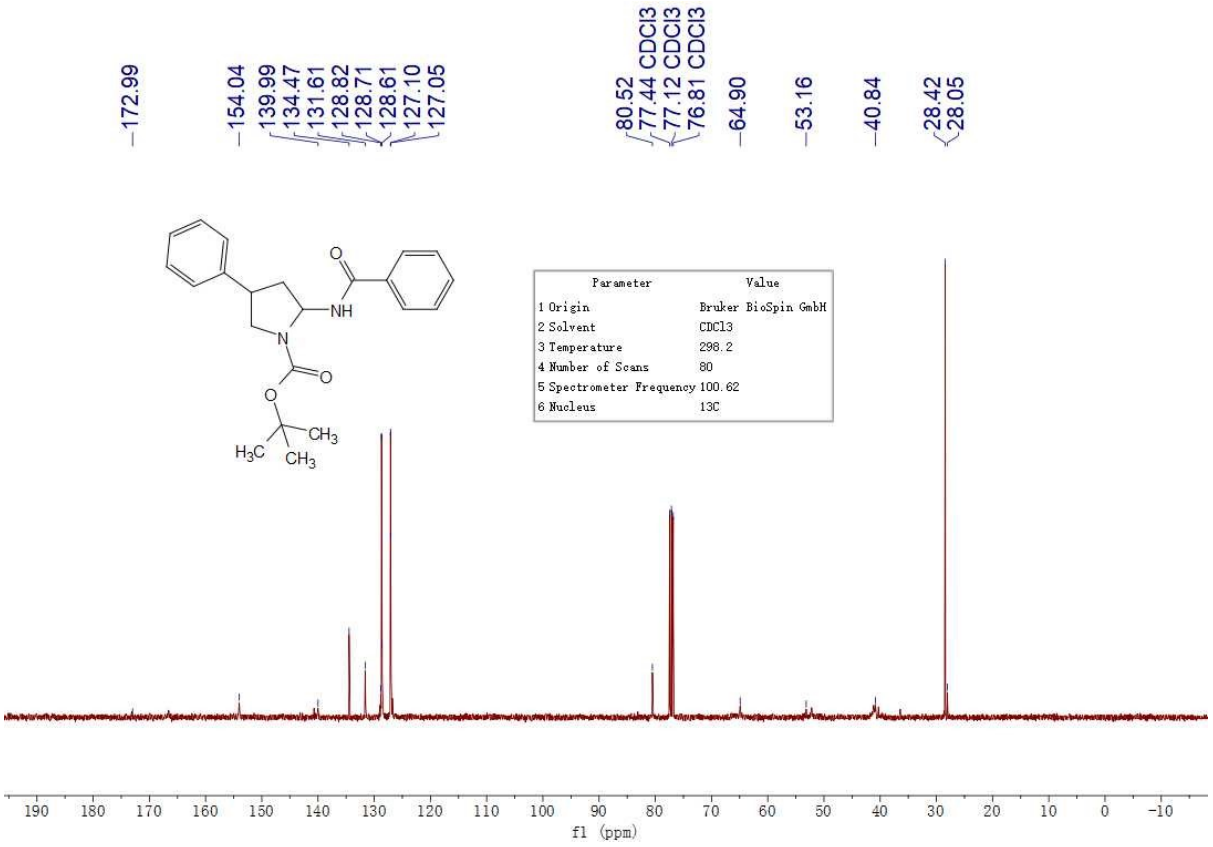
^{1}H NMR spectrum of **3ab** (400 MHz, $CDCl_3$)



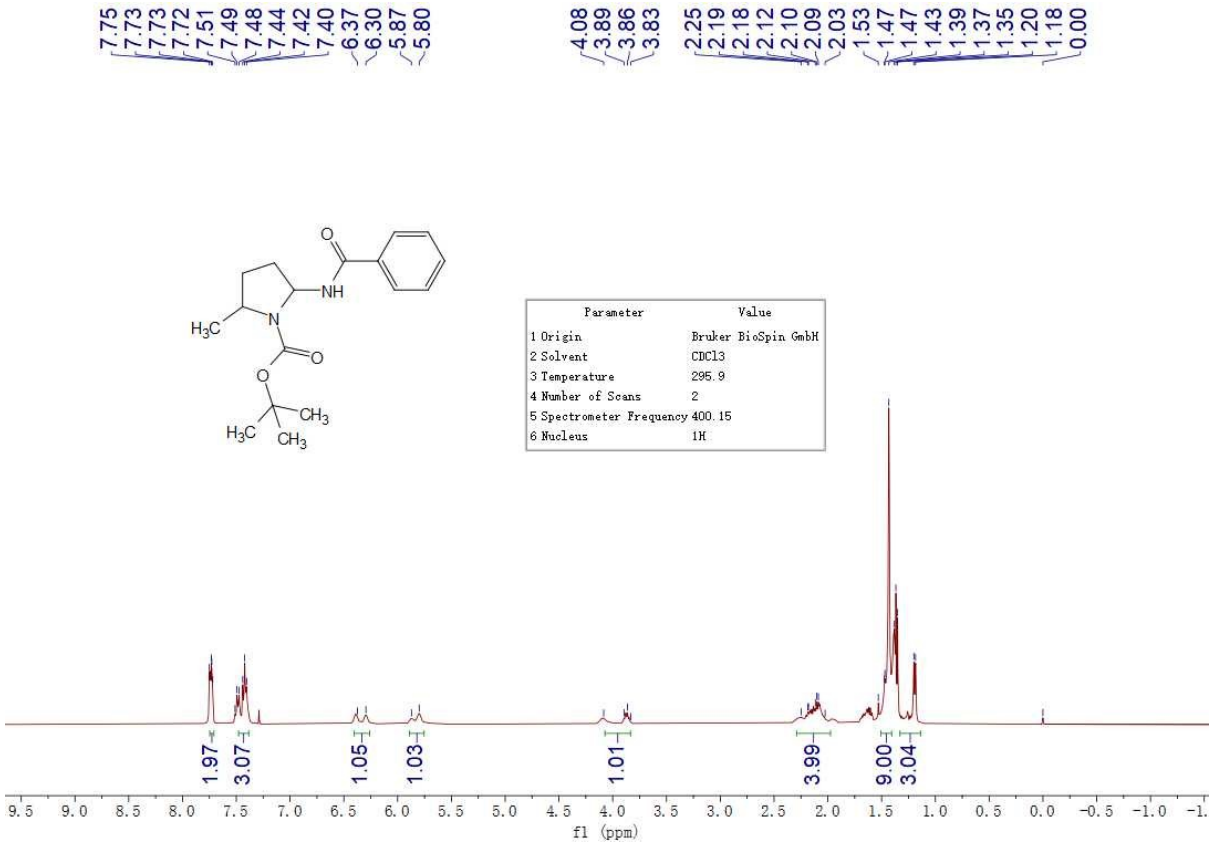
^{13}C NMR spectrum of **3ab** (100 MHz, $CDCl_3$)



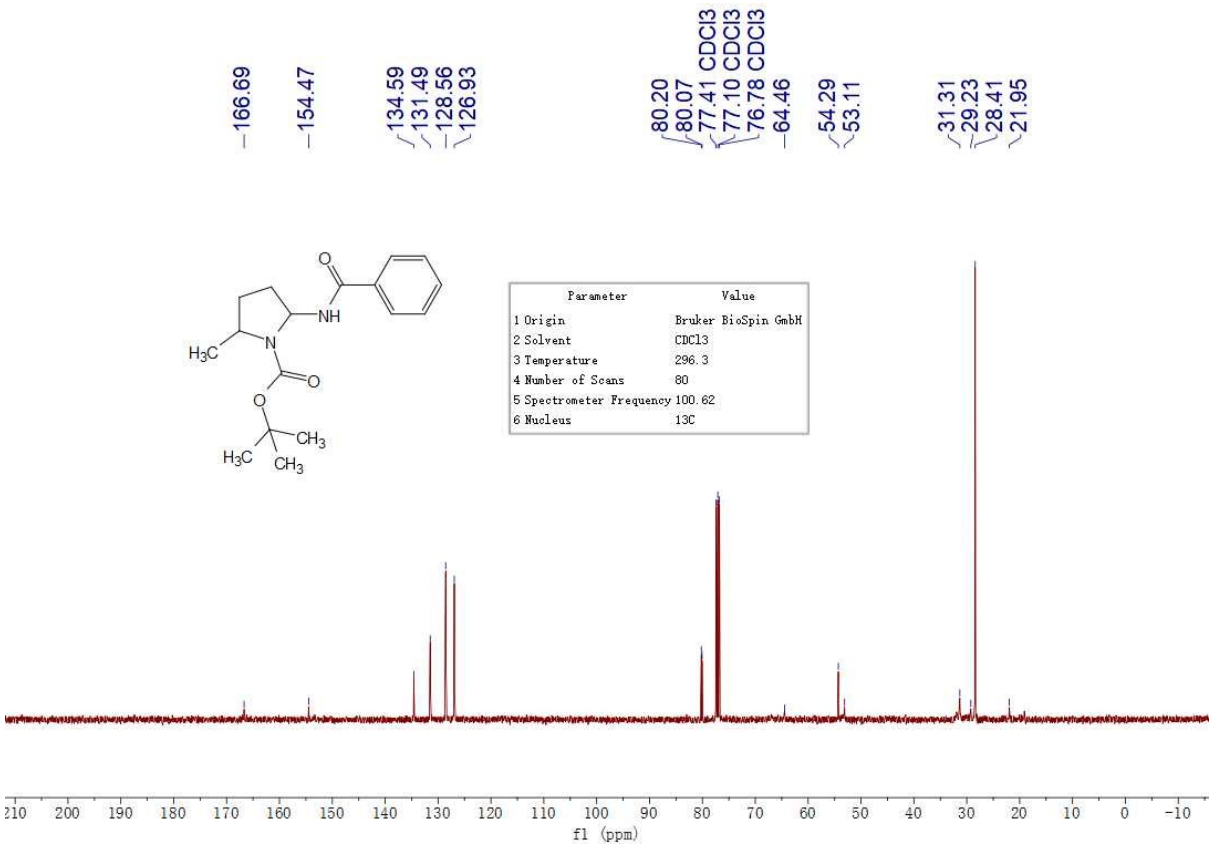
^{1}H NMR spectrum of **3ac** (400 MHz, $CDCl_3$)



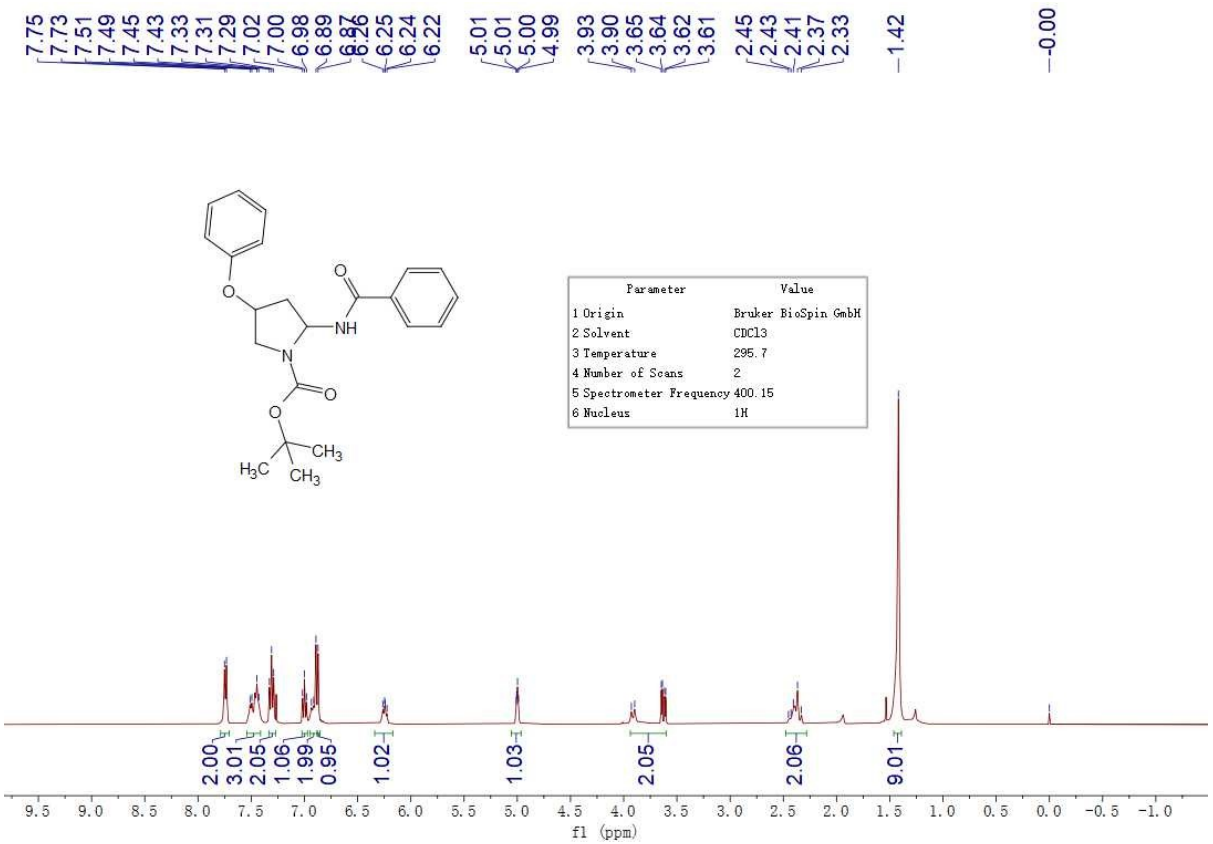
^{13}C NMR spectrum of **3ac** (100 MHz, $CDCl_3$)



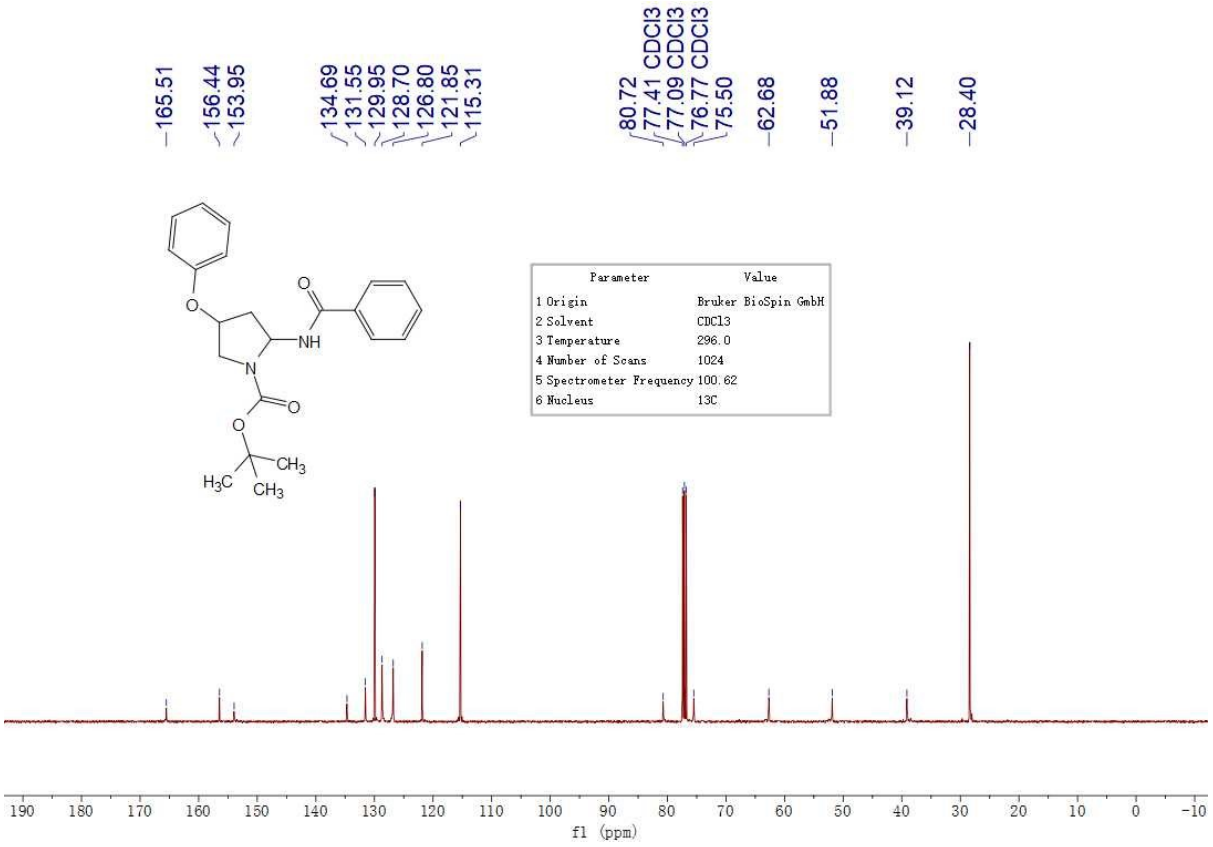
^{1}H NMR spectrum of **3ad** (400 MHz, $CDCl_3$)



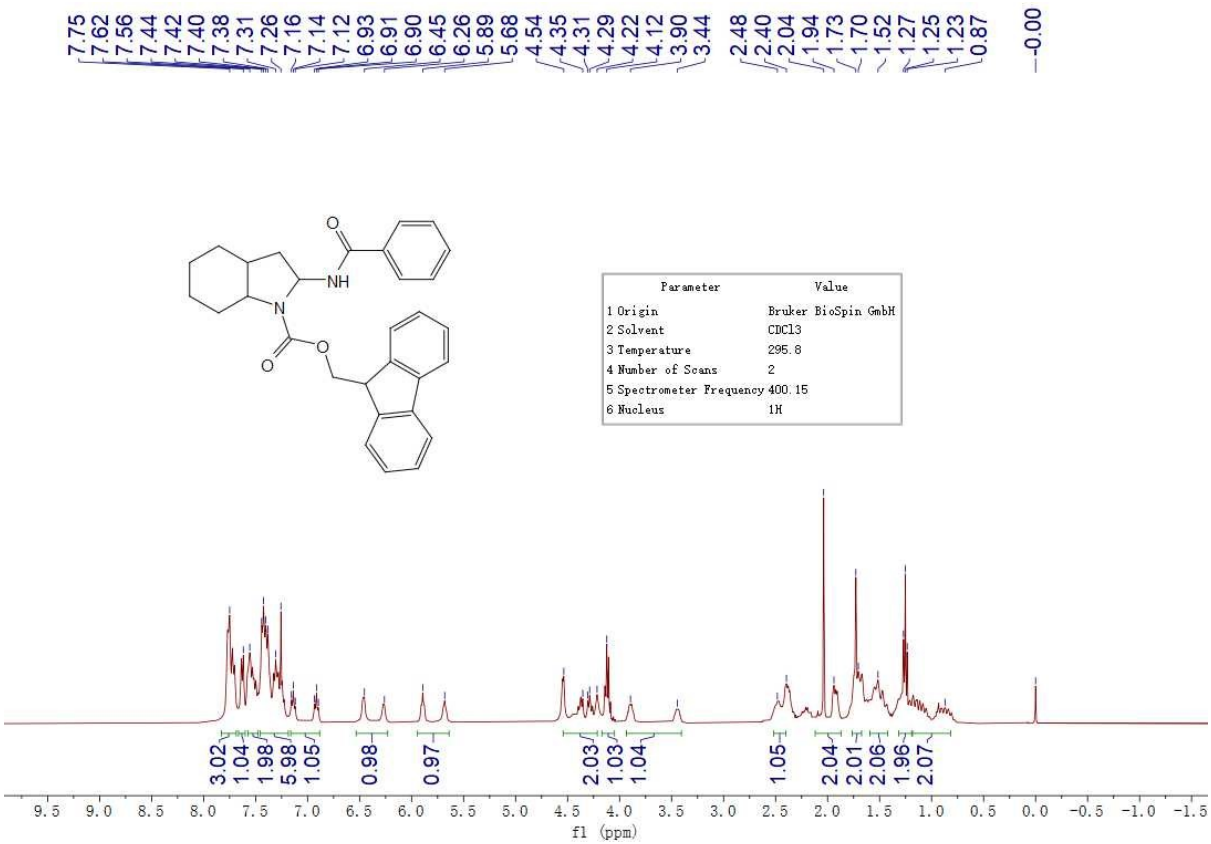
^{13}C NMR spectrum of **3ad** (100 MHz, $CDCl_3$)



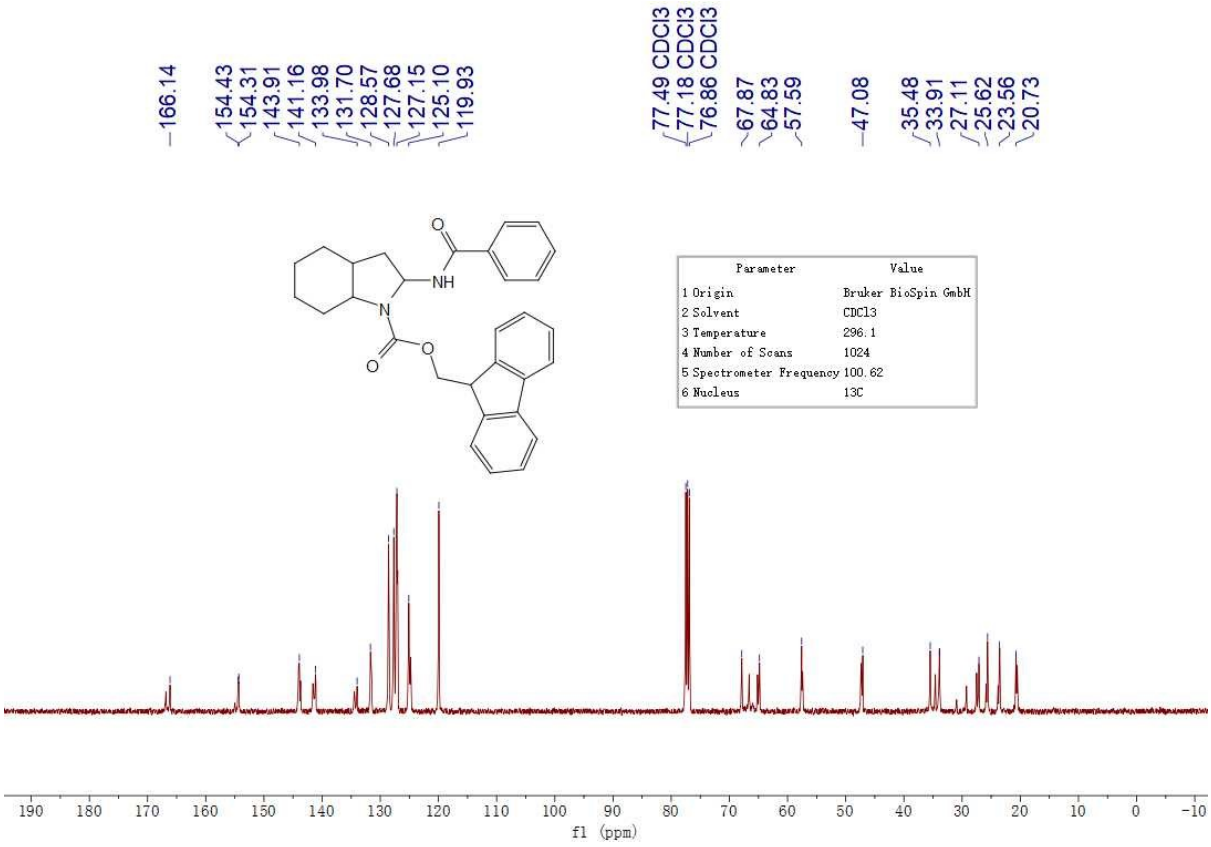
^{1}H NMR spectrum of **3ae** (400 MHz, $CDCl_3$)



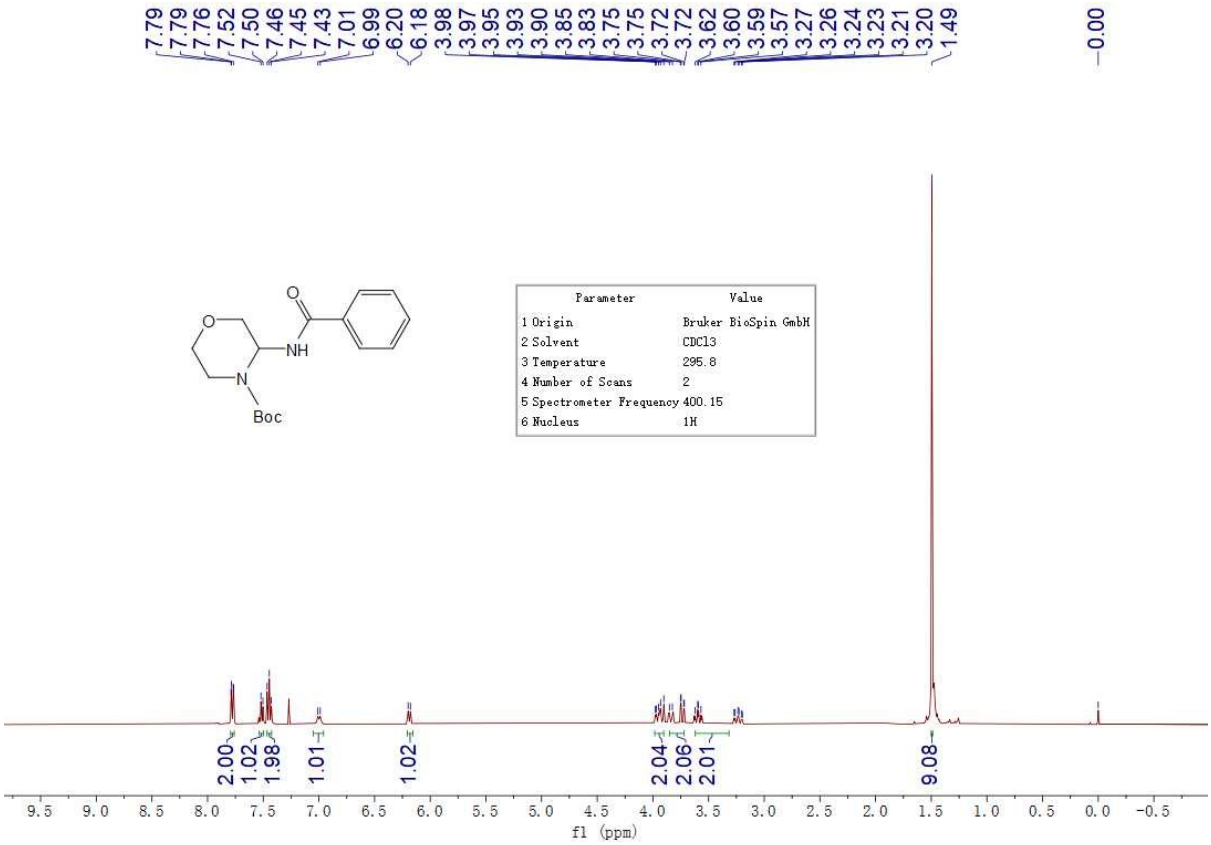
^{13}C NMR spectrum of **3ae** (100 MHz, $CDCl_3$)



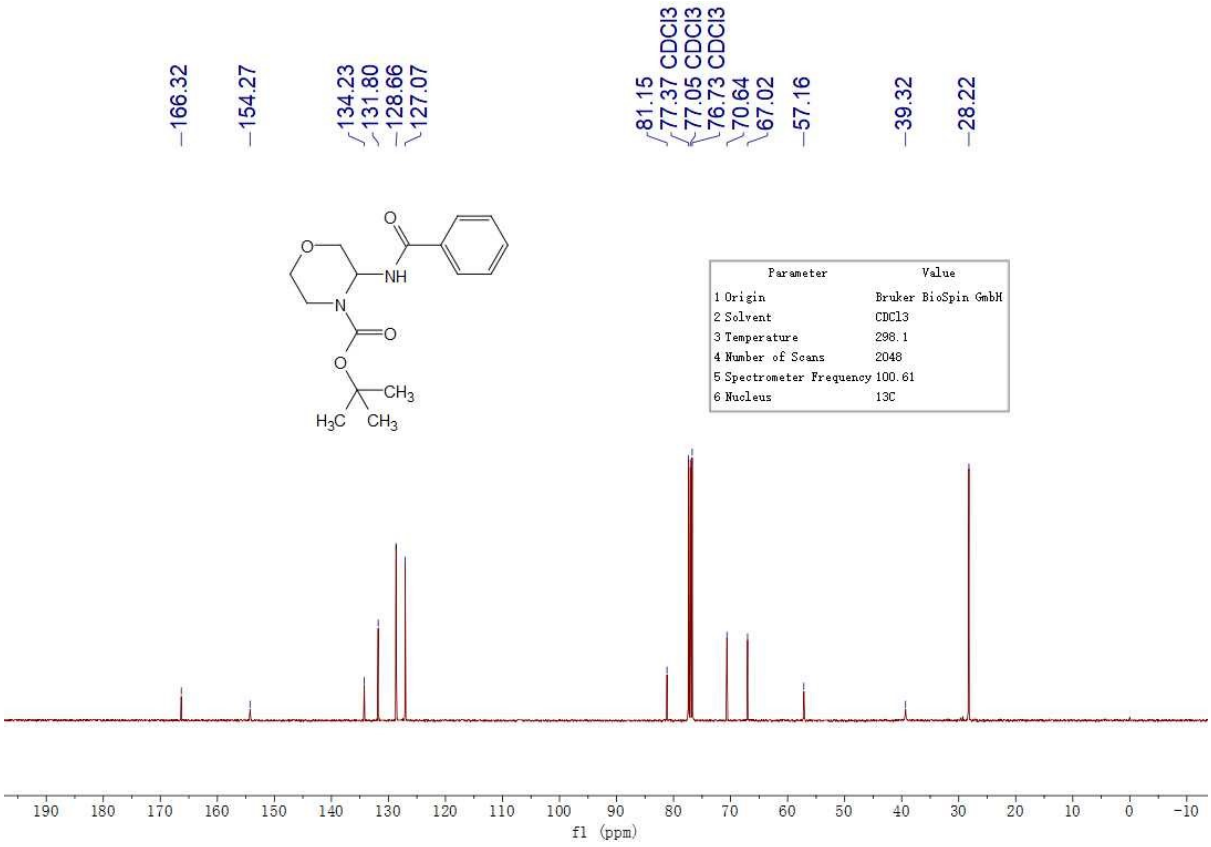
^{1}H NMR spectrum of **3af** (400 MHz, $CDCl_3$)



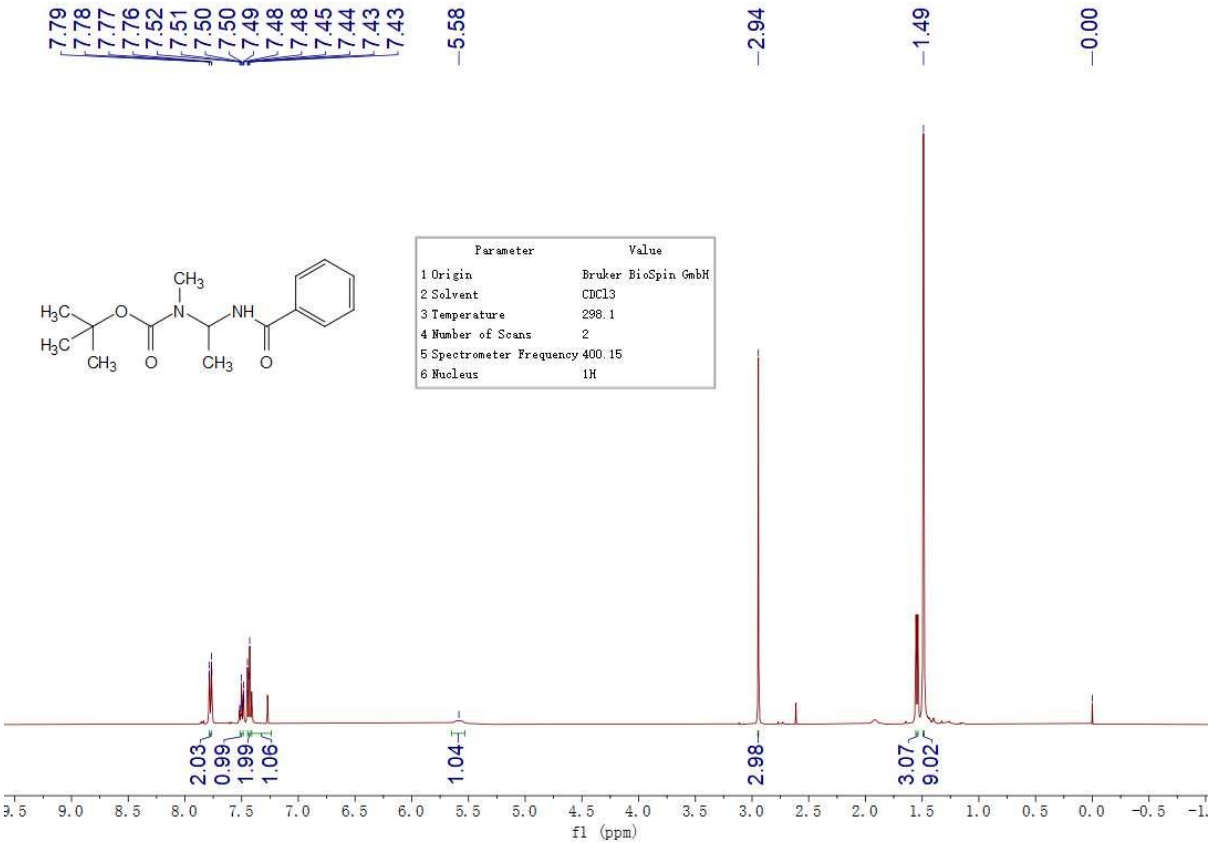
^{13}C NMR spectrum of **3af** (100 MHz, $CDCl_3$)



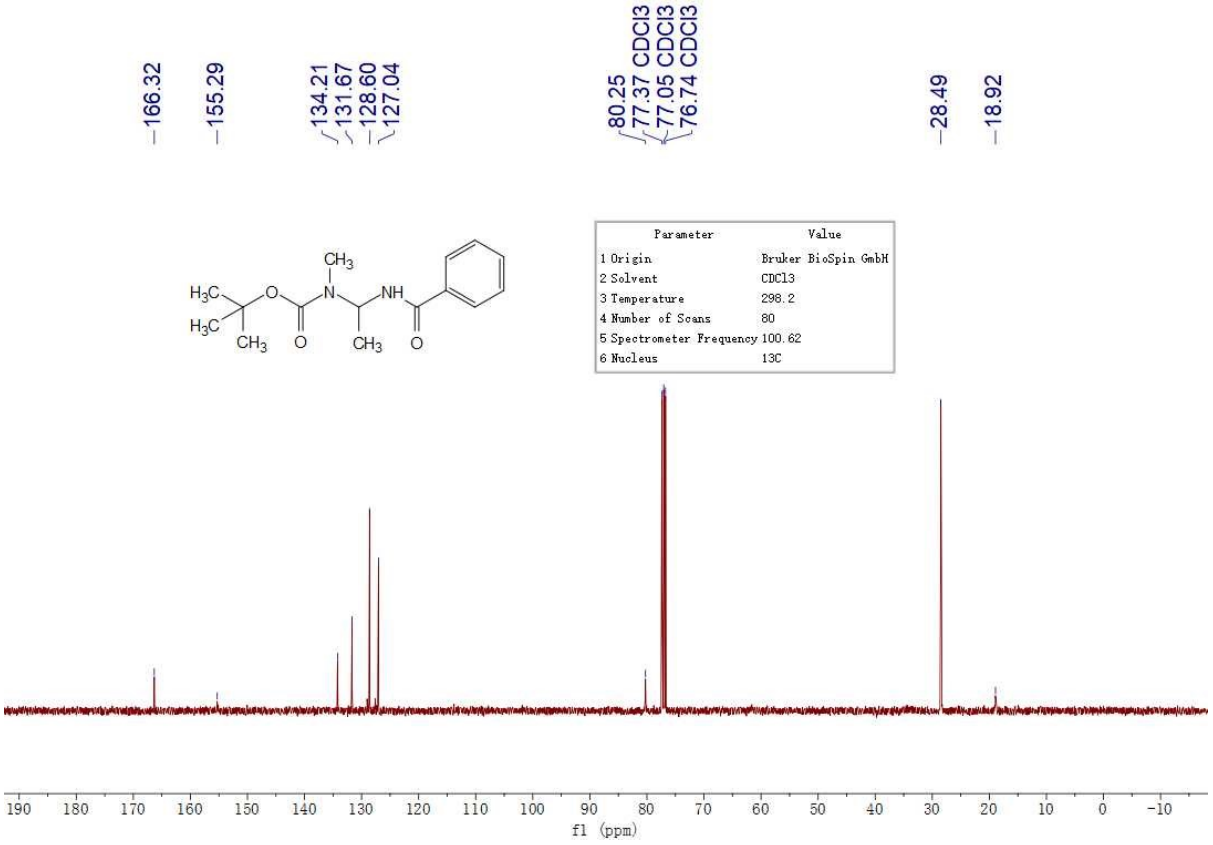
^{1}H NMR spectrum of **3ag** (400 MHz, $CDCl_3$)



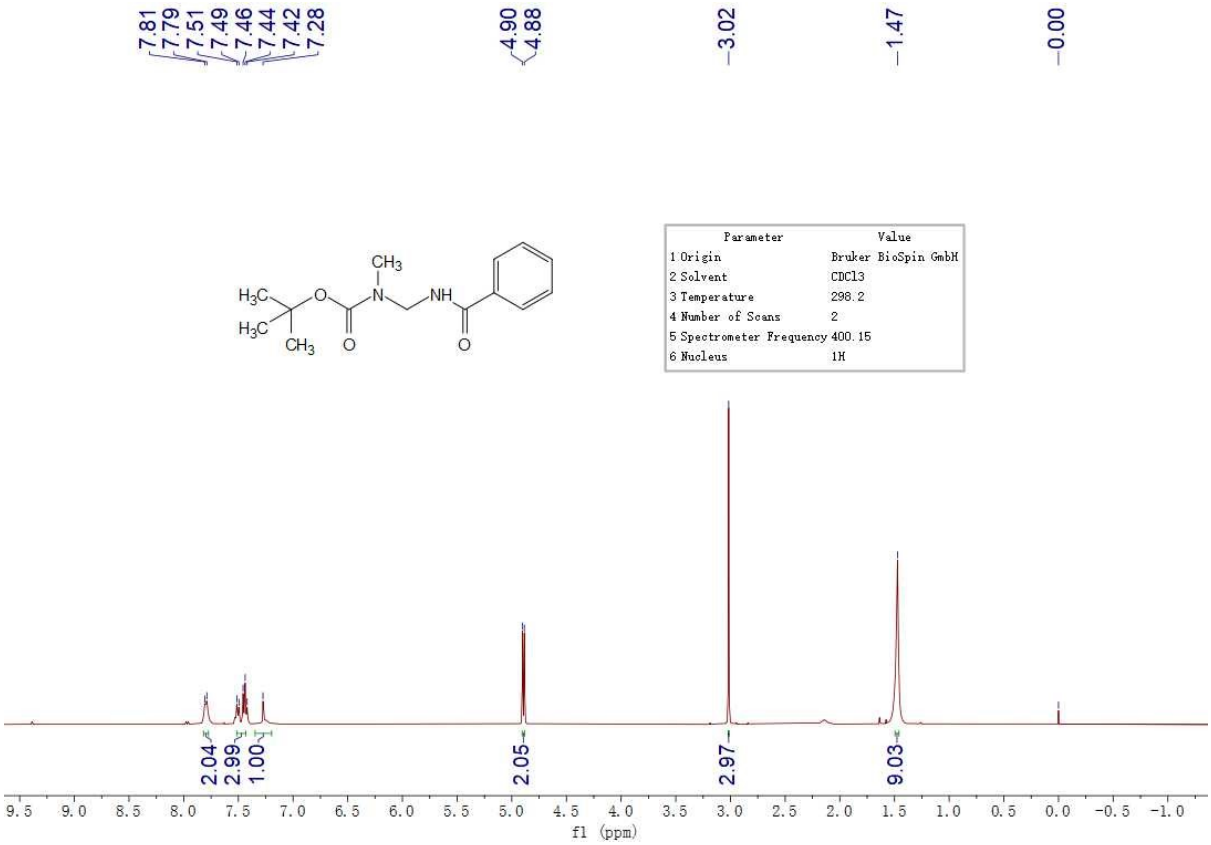
^{13}C NMR spectrum of **3ag** (100 MHz, $CDCl_3$)



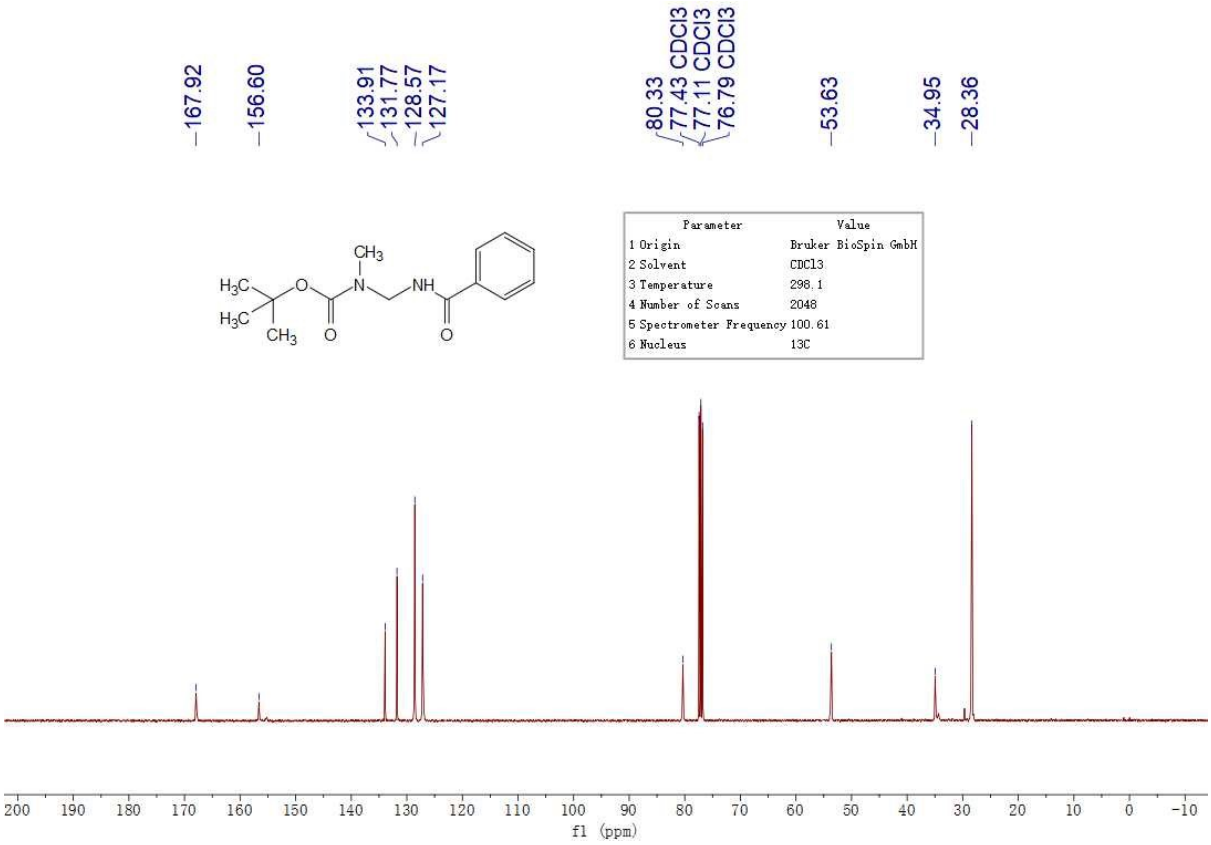
^{1}H NMR spectrum of **3ah** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **3ah** (100 MHz, $CDCl_3$)



^{1}H NMR spectrum of **3ai** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **3ai** (100 MHz, $CDCl_3$)