Supporting Information

Direct Decarboxylative C−N Coupling with Dioxazolones Mediated by a Base

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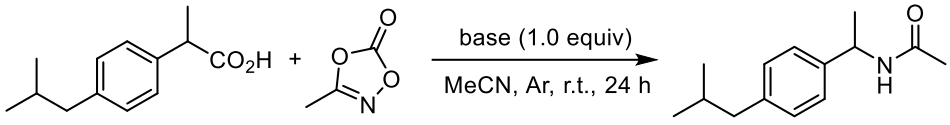
1. General information

All reactions were carried out in oven-dried Schlenk tubes under argon atmosphere(purity≥99.999%) unless otherwise mentioned. Commercial reagents were purchased from Adamas, TCI and Aldrich. Organic solutions were concentrated under reduced pressure on Buchi rotary evaporator. Flash column chromatographic purification of products was accomplished using forced-flow chromatography on Silica Gel (200-300 mesh).

^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded on a Bruker Avance 600 spectrometer at ambient temperature. Data for ^{1}H NMR are reported as follows: chemical shift (ppm, scale), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet and/or multiplet resonances, br = broad), coupling constant (Hz), and integration. Data for ^{13}C NMR are reported in terms of chemical shift (ppm, scale), multiplicity, and coupling constant (Hz). Gas chromatographic (GC) analysis was acquired on a Shimadzu GC-2014 Series GC System equipped with a flame-ionization detector. HRMS analysis was performed on Finnigan LCQ advantage Max Series MS System.

2. Reaction Optimization

Table S1. Different bases in the decarboxylative amidation

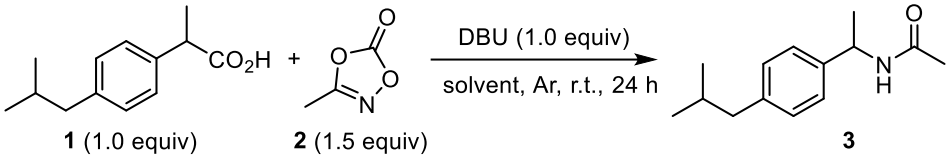


1 (1.0 equiv) **2** (1.5 equiv) **3**

entry	base	yield (%)[a]
1	None	0
2	**DBU**	**97**
3	DBU (0.2 equiv)	62
4	Et_3N	75
5	DMAP	8
6	DABCO	60
7	**DBN**	**97**
8	DIPEA	27
9	TMG	5
10	Pyridine	0
11	2,6-Lutidine	0
12	**Cs_2CO_3**	**92**
13	K_2CO_3	65
14	KO*t*Bu	62
15	KOMe	31
16	K_3PO_4	55
17	CsOPiv	27
18	NaOAc	12
19	K_2HPO_4	40
20	$NaHCO_3$	0
21	DBU	85[b]
22	DBU	92[c]
23	DBU	95[d]

[a]Reaction conditions: **1** (0.2 mmol), **2** (0.3 mmol), base (0.2 mmol), MeCN (2 mL), Ar, r.t., 24 h. Yield determined by GC using tridecane as internal standard. DBU = 1,8-Diazabicyclo[5.4.0]-7-undecene, DMAP = 4-Dimethylaminopyridine, DABCO = Triethylenediamine, DBN = 1,5-Diazabicyclo[4.3.0]non-5-ene, DIPEA = *N*,*N*-Diisopropylethylamine, TMG = Tetramethylguanidine. [b]5 h; [c]10 h; [d]20 h.

Table S2. Different solvents in the decarboxylative amidation



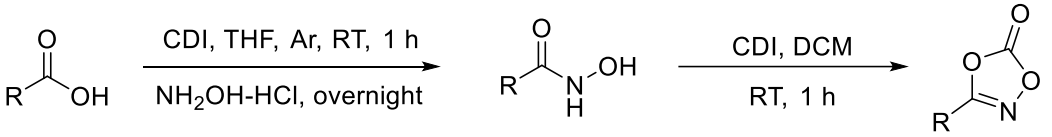
1 (1.0 equiv) **2** (1.5 equiv) **3**

entry	solvent	yield (%)[a]
1	THF	85
2	toluene	72
3	DCM	88
4	EtOAc	5
5	DMF	80
6	acetone	10
7	MeCN	97
8	MeCN (1 mL)	72
9	MeCN (3 mL)	84
10	MeCN (4 mL)	85

[a]Reaction conditions: **1** (0.2 mmol), **2** (0.3 mmol), DBU (0.2 mmol), solvent (2 mL), Ar, r.t., 24 h. Yield determined by GC using tridecane as internal standard. THF = Tetrahydrofuran, DCM = Dichloromethane, DMF = *N*,*N*-Dimethylformamide.

3. Experimental Procedures and Characterization Data

3.1 General procedure for the synthesis of dioxazolones[1]

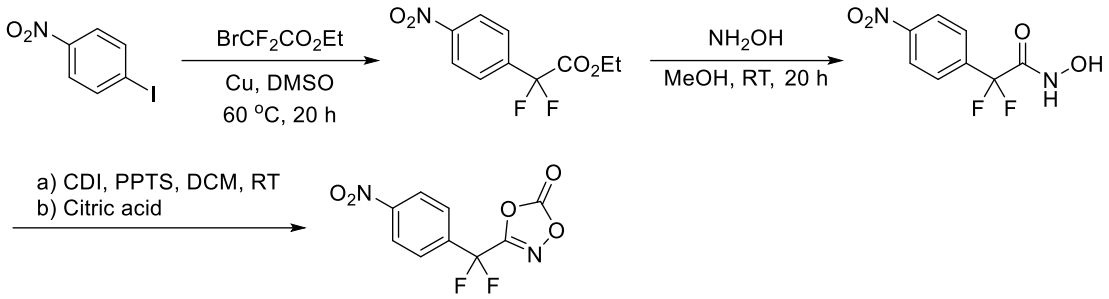


In a flame-dried Schlenk flask, 1,1'-carbonyldiimidazole (CDl, 45 mmol, 1.5 equiv.) was added to a solution of carboxylic acid (30 mmol, 1 equiv,) in dry THF (80 mL). After stirring for 1 h under an argon atmosphere at room temperature, hydroxylamine hydrochloride (60 mmol, 2 equiv.) was added and the resulting solution was stirred under Ar overnight. Subsequently, the solution was diluted with aqueous potassium bisulfate (5%, 100 mL) and extracted with ethyl acetate (3 × 80 mL). The combined organic phase was washed with brine (3 × 60 mL), dried over anhydrous Na_2SO_4, and concentrated in vacuo. lf necessary, the formed hydroxamic acid was further recrystallized from EtOAc/hexane mixtures.

CDI (25 mmol, 1.25 equiv.) was added to a stirred solution of hydroxamic acid (20 mmol, 1.0 equiv.) in DCM (100 mL) in one portion at room temperature. After stirring for 1 h, the reaction mixture was quenched with 1 N HCI (100 mL), extracted with DCM three times (3 × 80 mL) and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure to afford the corresponding dioxazolone, which could be purified by filtration over a plug of silica with DCM, if necessary.

The dioxazolones used in the reaction, except 3-(difluoro(4-nitrophenyl)methyl)-1,4,2-dioxazol-5-one, were all prepared by the above method, and their characterization data are consistent with the literatures.

3.2 Preparation of 3-(difluoro(4-nitrophenyl)methyl)-1,4,2-dioxazol-5-one[2]



A 250 mL round bottom flask was charged with anhydrous DMSO (80 mL), *p*-nitroiodobenzene (40 mmol, 1 equiv.), ethyl bromodifluoroacetate (50 mmol, 1.25 equiv.) and activated Cu powder (112 mmol, 2.8 equiv.). The reaction mixture was then stirred vigorously at 60 °C for 20 h under argon atmosphere. Upon completion, a saturated aqueous solution of NH_4Cl (80 mL) was added to quench the reaction. Ethyl ether (80 mL) was then added to the mixture, and stirring was continued for 1 h. The mixture was transferred to a separating funnel, further diluted with water (80 mL) and ethyl ether (60 mL), and the organic layer was separated. The aqueous layer was extracted with ethyl ether (2 × 100 mL). The combined organic layers were washed with a saturated aqueous solution of NH_4Cl (200 mL), water (200 mL), and brine (200 mL). The organic solution was dried over anhydrous Na_2SO_4, concentrated in vacuo, and purified by flash column chromatography on silica gel to yield the ethyl 2,2-difluoro-2-(4-nitrophenyl)acetate as a colorless oil (8.04g, 32.8 mmol, 82%).

A freshly prepared solution of hydroxylamine in methanol (1.8M, 37.5 mmol, 1.25 equiv.) was added to a round bottom flask containing ethyl 2,2-difluoro-2-(4-nitrophenyl)acetate (30 mmol, 1 equiv.) and a magnetic stirrer under argon atmosphere. The mixture was stirred at room temperature for 20 h, then diluted with ethyl acetate (150 mL) and stirred for 10 minutes. The sodium chloride precipitate was filtered off over Celite®. The filtrate was concentrated in vacuo, and the resulting solid was crushed and suspended in $CHCl_3$ (300 mL). The mixture was refluxed for 30 minutes until completely dissolved, then cooled to 0 °C under stirring. The resulting white solid was collected by filtration. Pentane (100 mL) was added to the filtrate at 0 °C, and the mixture was stirred for 15 minutes. A second white solid was recovered by filtration. Both solids were combined and dried under high vacuum to yield the corresponding hydroxamic acid (5.57g, 24 mmol, 80%).

A finely crushed suspension of the corresponding hydroxamic acid (20 mmol, 1 equiv.) in DCM (190 mL) was vigorously stirred while Pyridinium *p*-toluenesulfonate (22 mmol, 1.1 equiv.) was added. The mixture was stirred until dissolution was complete, then stirred further for 10 minutes to allow a white crystalline solid to precipitate. A solution of CDI (24 mmol, 1.2 equiv.) in DCM (80 mL) was added dropwise to the stirred suspension at room temperature over 30 minutes. The reaction

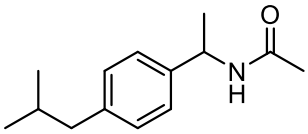
mixture was further stirred for 45 minutes, then quenched by adding an aqueous solution of citric acid (2M, 100 mL). The aqueous layer was separated, and the organic layer was washed with water (3 × 70 mL), brine/water (8:2, 70 mL), dried over Na_2SO_4, and concentrated in vacuo to yield pure 3-(difluoro(4-nitrophenyl)methyl)-1,4,2-dioxazol-5-one (4.13g, 16 mmol, 80%).

The characterization data was in agreement with the literature[2].

3.3 General procedure for decarboxylative amination

Carboxylic acid (0.2 mmol, 1.0 equiv) (if solid) and dioxazolone (0.3 mmol, 1.5 equiv) (if solid) were placed in a transparent Schlenk tube equipped with a stirring bar. The tube was evacuated and filled with argon (repeated for three times). Then DBU (0.2 mmol, 1.0 equiv), carboxylic acid (0.2 mmol, 1.0 equiv) (if liquid), dioxazolone (0.3 mmol, 1.5 equiv) (if liquid), and MeCN (2 mL) was added using a syringe under argon atmosphere. The reaction mixture was stirred at room temperature for 24 h, Then, the reaction mixture was quenched with saturated brine and extracted with ethyl acetate (3 x 10 mL). The combined organic phases were dried over anhydrous Na_2SO_4, and concentrated under vacuo. The residue was purified by flash column chromatography on silica gel to afford the product.

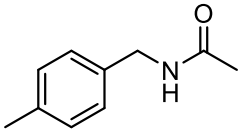
3.4 Characterization data



***N*-(1-(4-isobutylphenyl)ethyl) acetamide (3):** According to the general procedure, obtained as white solid in 95% yield (41.7 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *ACS Catal.* **2022**, *12*, 809-817).

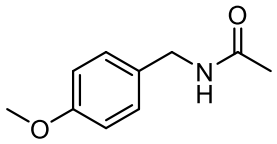
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.22 (d, J = 8.0 Hz, 2H), 7.11 (d, J = 8.1 Hz, 2H), 5.68 (br s, 1H), 5.11 (p, J = 7.1 Hz, 1H), 2.45 (d, J = 7.2 Hz, 2H), 1.98 (s, 3H), 1.88-1.81 (m, 1H), 1.48 (d, J = 6.9 Hz, 3H), 0.90 (d, J = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.3, 141.1, 140.5, 129.6, 126.2, 48.7, 45.2, 30.4, 23.7, 22.6, 21.8.

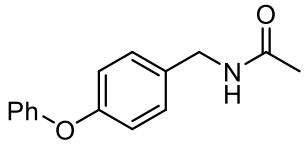


***N*-(4-methylbenzyl) acetamide (4):** According to the general procedure, obtained as white solid in 95% yield (31.0 mg, eluent: petroleum ether/ethyl acetate = 3/1). The

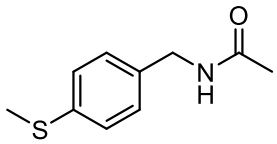
compound data was in agreement with the literature (Ref: *Chem. Pap.* **2020**, *74*, 3259-3268).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.17-7.11 (m, 4H), 5.91 (s, 1H), 4.36 (d, J = 5.6 Hz, 2H), 2.33 (s, 3H), 1.99 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.1, 137.4, 135.4, 129.5, 128.0, 43.7, 23.4, 21.3.



***N*-(4-methoxybenzyl) acetamide (5):** According to the general procedure, obtained as white solid in 90% yield using Cs_2CO_3 as base (32.3 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *J. Mol. Catal. A-Chem.* **2015**, *403*, 15-26).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.19 (d, J = 8.6 Hz, 2H), 6.85 (d, J = 8.6 Hz, 2H), 5.88 (s, 1H), 4.33 (d, J = 5.6 Hz, 2H), 3.78 (s, 3H), 1.98 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-d) δ 170.1, 159.2, 130.5, 129.4, 114.2, 55.5, 43.4, 23.4.

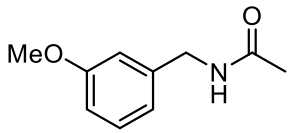


***N*-(4-phenoxybenzyl) acetamide (6):** According to the general procedure, obtained as yellow solid in 66% yield (31.9 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 97-99 °C.
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.35-7.32 (m, 2H), 7.26-7.23 (m, 2H), 7.11 (t, J = 7.4 Hz, 1H), 7.01-6.96 (m, 4H), 5.73 (s, 1H), 4.41 (d, J = 5.7 Hz, 2H), 2.03 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.9, 157.1, 156.8, 133.0, 129.8, 129.4, 123.4, 119.1, 118.9, 43.2, 23.3.
HRMS (ESI): ([M+H]$^{+}$) calcd for $C_{15}H_{16}NO_2^{+}$: 242.1176; found: 242.1178.



***N*-(4-(methylthio)benzyl)acetamide (7):** According to the general procedure, obtained as white solid in 74% yield using Cs_2CO_3 as base (28.9 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: Biomacromolecules **2022**, *23*, 77-88).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.23-7.18 (m, 4H), 5.85 (s, 1H), 4.38 (d, J = 4.7 Hz, 2H), 2.47 (s, 3H), 2.02 (s, 3H).

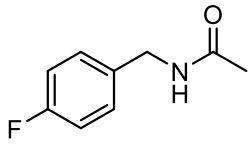
^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.2, 138.0, 135.2, 128.7, 127.1, 43.5, 23.6, 16.1.



***N*-(3-methoxybenzyl) acetamide (8):** According to the general procedure, obtained as colorless liquid in 71% yield (25.4 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *RSC Adv.* **2015**, *5*, 95313-95317).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.28-7.22 (m, 1H), 6.87-6.85 (m, 1H), 6.83- 6.80 (m, 2H), 5.88 (s, 1H), 4.40 (d, J = 5.7 Hz, 2H), 3.80 (s, 3H), 2.02 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.1, 160.0, 140.0, 129.9, 120.2, 113.6, 113.1, 55.4, 43.9, 23.5.

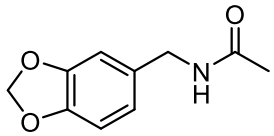


***N*-(4-fluorobenzyl) acetamide (9):** According to the general procedure, obtained as white solid in 91% yield using Cs_2CO_3 as base (30.4 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *Chem. Commun.* **2021**, *57*, 5266-5269).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.25-7.23 (m, 2H), 7.02-6.99 (m, 2H), 5.96 (s, 1H), 4.38 (d, J = 5.3 Hz, 2H), 2.01 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.0, 161.2 (d, J = 245.7 Hz), 133.0 (d, J = 3.3 Hz), 128.5 (d, J = 7.9 Hz), 114.5 (d, J = 21.5 Hz), 42.0, 22.3.

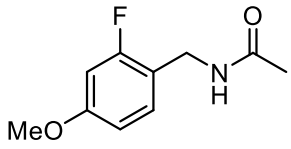
^{19}F NMR (565 MHz, Chloroform-*d*) δ -114.96.



***N*-(benzo[d][1,3]dioxol-5-ylmethyl) acetamide (10):** According to the general procedure, obtained as white solid in 77% yield (29.8 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *Synth. Commun*. **2014**, *44*, 2364-2376).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 6.77-6.67 (m, 3H), 5.95 (s, 1H), 5.92 (s, 2H), 4.30 (d, J = 5.7 Hz, 2H), 1.98 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.0, 147.9, 147.0, 132.2, 121.1, 108.4, 108.3, 101.1, 43.5, 23.2.



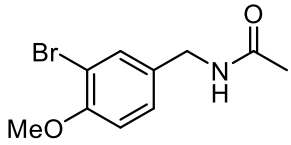
***N*-(2-fluoro-4-methoxybenzyl) acetamide (11):** According to the general procedure, obtained as white solid in 76% yield (30.0 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 68-70 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.25 (t, J = 8.6 Hz, 1H), 6.67-6.64 (m, 1H), 6.63-6.59 (m, 1H), 5.82 (s, 1H), 4.40 (d, J = 5.8 Hz, 2H), 3.79 (s, 3H), 1.99 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.9, 161.6 (d, J = 245.5 Hz), 160.5 (d, J = 11.0 Hz), 131.1 (d, J = 6.4 Hz), 117.2 (d, J = 15.7 Hz), 109.8 (d, J = 3.2 Hz), 101.7 (d, J = 25.2 Hz), 55.6, 37.3 (d, J = 3.2 Hz), 23.3.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -117.05.

HRMS (ESI): ([M+H]$^{+}$) calcd for $C_{10}H_{13}FNO_2^{+}$: 198.0925; found: 198.0922.

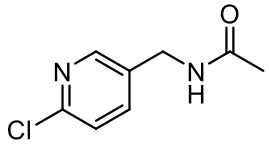


***N*-(3-bromo-4-methoxybenzyl) acetamide (12):** According to the general procedure, obtained as white solid in 64% yield (33.0 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 101-103 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.46 (d, J = 2.2 Hz, 1H), 7.20 (dd, J = 8.4, 2.2 Hz, 1H), 6.85 (d, J = 8.4 Hz, 1H), 5.82 (s, 1H), 4.34 (d, J = 5.8 Hz, 2H), 3.88 (s, 3H), 2.02 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.9, 155.3, 132.8, 132.0, 128.2, 112.0, 111.8, 56.3, 42.6, 23.3.

HRMS (ESI): ([M+H]$^{+}$) calcd for $C_{10}H_{13}BrNO_2^{+}$: 258.0130; found: 258.0132.

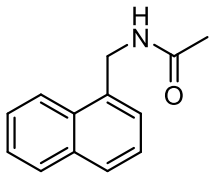


***N*-((6-chloropyridin-3-yl)methyl) acetamide (13):** According to the general procedure, obtained as light yellow liquid in 74% yield (27.3 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *Tetrahedron Lett*. **2000**, *41*, 3513-3516).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.13 (d, J = 2.5 Hz, 1H), 7.51 (dd, J = 8.2, 2.5 Hz, 1H), 7.37-7.29 (m, 1H), 7.18 (d, J = 8.2 Hz, 1H), 4.27 (d, J = 6.0 Hz, 2H), 1.90 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-d) δ 169.8, 149.1, 147.7, 137.6, 132.5, 123.2, 39.2, 21.9.

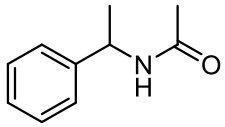
HRMS (ESI): ([M+H]$^{+}$) calcd for $C_8H_{10}ClN_2O^{+}$: 185.0477; found: 185.0477.



***N*-(naphthalen-1-ylmethyl) acetamide (14):** According to the general procedure, obtained as white solid in 84% yield (33.5 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *Synth. Commun.* **2013**, *43*, 3224-3232).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.01 (d, J = 8.3 Hz, 1H), 7.88 (dd, J = 8.0, 1.5 Hz, 1H), 7.82 (t, J = 6.4, 3.1 Hz, 1H), 7.58-7.50 (m, 2H), 7.44-7.42 (m, 2H), 5.77 (s, 1H), 4.87 (d, J = 5.3 Hz, 2H), 2.00 (s, 3H).

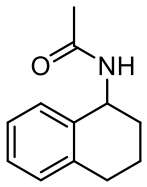
^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.0, 134.1, 133.7, 131.6, 129.0, 128.9, 127.1, 126.9, 126.3, 125.6, 123.7, 42.1, 23.4.



***N*-(1-phenylethyl) acetamide (15):** According to the general procedure, obtained as white solid in 90% yield (29.4 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *Synth. Commun.* **2020**, *50*, 3326-3336).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.36-7.30 (m, 4H), 5.86 (s, 1H), 5.15-5.08 (m, 1H), 1.97 (s, 3H), 1.48 (d, J = 6.9 Hz, 3H).

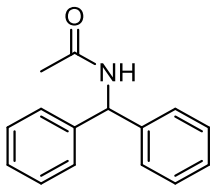
^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.2, 143.2, 128.7, 127.4, 126.2, 48.8, 23.5, 21.7.



***N*-(1,2,3,4-tetrahydronaphthalen-1-yl) acetamide (16):** According to the general procedure, obtained as white solid in 80% yield (30.3 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *Angew. Chem. Int. Ed.* **2022**, *61*, e202200638).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.26-7.23 (m, 1H), 7.18-7.13 (m, 2H), 7.10-7.07 (m, 1H), 5.93 (br, 1H), 5.21-5.09 (m, 1H), 2.88-2.68 (m, 2H), 2.03-1.99 (m, 4H), 1.84-1.78 (m, 3H).

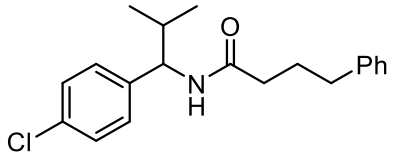
^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.4, 137.6, 136.7, 129.2, 128.7, 127.3, 126.3, 47.5, 30.1, 29.2, 23.5, 19.9.



***N*-benzhydrylacetamide (17):** According to the general procedure, obtained as white solid in 70% yield (31.5 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *Chem. Commun.* **2021**, *57*, 8901-8904).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.34-7.32 (m, 4H), 7.29-7.27 (m, 2H), 7.24-7.21 (m, 4H), 6.25 (d, J = 8.0 Hz, 1H), 6.06 (br, 1H), 2.07 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.1, 140.4, 127.7, 126.5, 126.4, 56.0, 22.4.

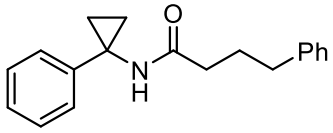


***N*-(1-(4-chlorophenyl)-2-methylpropyl)-4-phenylbutanamide (18):** According to the general procedure, obtained as white solid in 70% yield (46.2 mg, eluent: petroleum ether/ethyl acetate = 5/1), m.p. = 115-116 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.28-7.24 (m, 4H), 7.20-7.16 (m, 1H), 7.16-7.10 (m, 4H), 5.89-5.80 (m, 1H), 4.71 (t, J = 8.4 Hz, 1H), 2.60 (t, J = 7.5 Hz, 2H), 2.23-2.11 (m, 2H), 1.99-1.91 (m, 3H), 0.94 (d, J = 6.7 Hz, 3H), 0.80 (d, J = 6.7 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.1, 141.4, 140.4, 132.8, 128.6, 128.5, 128.4, 128.4, 126.0, 58.6, 35.9, 35.2, 33.2, 27.2, 19.8, 18.9.

HRMS (ESI): ([M+H]$^+$) calcd for $C_{20}H_{25}ClNO^+$: 330.1625; found: 330.1625.

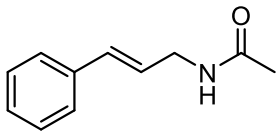


4-phenyl-*N*-(1-phenylcyclopropyl) butanamide (19): According to the general procedure, obtained as solid in 69% yield (38.6 mg, eluent: petroleum ether/ethyl acetate = 5/1), m.p. = 74-76 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.27-7.24 (m, 4H), 7.20-7.12 (m, 6H), 6.34 (s, 1H), 2.60 (t, J = 7.6 Hz, 2H), 2.14 (t, J = 7.6 Hz, 2H), 1.96-1.93 (m, 2H), 1.23-1.16 (m, 4H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.9, 142.4, 141.5, 128.6, 128.4, 128.4, 126.4, 126.0, 125.6, 35.9, 35.2, 35.0, 27.0, 17.8.

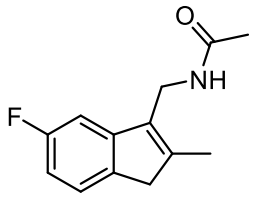
HRMS (ESI): ([M+H]$^+$) calcd for $C_{19}H_{22}NO^+$: 280.1696; found: 280.1699.



***N*-cinnamylacetamide (20):** According to the general procedure, obtained as white solid in 75% yield (26.3 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *Adv. Synth. Catal*. **2013**, *355*, 1570-1578).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.36-7.29 (m, 4H), 7.24 (t, J = 7.0 Hz,1H), 6.52 (d, J = 15.8 Hz, 1H), 6.22-6.17 (m, 1H), 5.64 (s, 1H), 4.04 (td, J = 6.1, 1.5 Hz, 2H), 2.03 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.0, 136.5, 132.3, 128.6, 127.8, 126.4, 125.5, 41.7, 23.4.



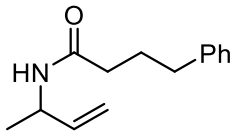
***N*-((5-fluoro-2-methyl-1*H*-inden-3-yl)methyl) acetamide (21):** According to the general procedure, obtained as light yellow solid in 46% yield (20.2 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 137-139 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.28-7.25 (m, 1H), 6.99-6.94 (m, 1H), 6.84-6.78 (m, 1H), 5.51 (s, 1H), 4.32 (d, *J* = 5.4 Hz, 2H), 3.28 (s, 2H), 2.14 (s, 3H), 1.97 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.1, 162.5 (d, J = 242.2 Hz), 147.0 (d, J = 8.8 Hz), 145.4, 137.2 (d, J = 2.6 Hz), 132.9 (d, J = 3.1 Hz), 124.0 (d, J = 8.9 Hz), 110.7 (d, J = 23.0 Hz), 105.8 (d, J = 23.3 Hz), 42.3, 34.4, 23.2, 14.2.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -116.70.

HRMS (ESI): ([M+H]$^+$) calcd for $C_{13}H_{15}FNO^+$: 220.1133; found: 220.1129.

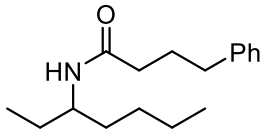


***N*-(but-3-en-2-yl)-4-phenylbutanamide (22):** According to the general procedure, obtained as viscous liquid in 62% yield (26.9 mg, eluent: petroleum ether/ethyl acetate = 3/1).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.29-7.24 (m, 2H), 7.20-7.15 (m, 3H), 5.84-5.77 (m, 1H), 5.34 (s, 1H), 5.13 (d, J = 17.3 Hz, 1H), 5.07 (d, J = 10.3 Hz, 1H), 4.62-4.54 (m, 1H), 2.65 (t, J = 7.4 Hz, 2H), 2.17 (t, J = 7.3 Hz, 2H), 2.01-1.95 (m, 2H), 1.21 (d, J = 6.7 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 171.8, 141.5, 139.6, 128.5, 128.4, 126.0, 114.1, 46.6, 36.0, 35.2, 27.2, 20.3.

HRMS (ESI): ([M+H]$^+$) calcd for $C_{14}H_{20}NO^+$: 218.1540; found: 218.1543.

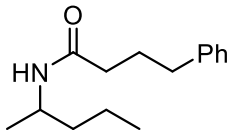


***N*-(heptan-3-yl)-4-phenylbutanamide (23):** According to the general procedure, obtained as white solid in 78% yield (40.8 mg, eluent: petroleum ether/ethyl acetate = 5/1), m.p. = 46-48 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.23-7.18 (m, 2H), 7.14-7.09 (m, 3H), 5.15 (d, J = 8.8 Hz, 1H), 3.85-3.68 (m, 1H), 2.58 (t, J = 7.6 Hz, 2H), 2.10 (t, J = 7.5 Hz, 2H), 1.95-1.83 (m, 2H), 1.49-1.38 (m, 2H), 1.32-1.13 (m, 6H), 0.90-0.85 (m, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.3, 141.6, 128.5, 128.4, 126.0, 50.4, 36.3, 35.3, 34.5, 28.1, 28.0, 27.4, 22.7, 14.1, 10.3.

HRMS (ESI): ([M+H]$^+$) calcd for $C_{17}H_{28}NO^+$: 262.2166; found: 262.2164.

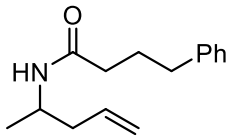


***N*-(pentan-2-yl)-4-phenylbutanamide (24):** According to the general procedure, obtained as viscous liquid in 68% yield (31.7 mg, eluent: petroleum ether/ethyl acetate = 5/1).

^{1}HNMR (600 MHz, Chloroform-*d*) δ 7.30-7.26 (m, 2H), 7.21-7.16 (m, 3H), 5.22 (br, 1H), 4.02-3.96 (m, 1H), 2.65 (t, J = 7.5 Hz, 2H), 2.14 (t, J = 7.5 Hz, 2H), 1.98-1.94 (m, 2H), 1.40-1.36 (m, 2H), 1.35-1.30 (m, 2H), 1.10 (d, J = 6.5 Hz, 3H), 0.90 (t, J = 7.1 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 171.9, 141.6, 128.5, 128.4, 126.0, 44.9, 39.2, 36.2, 35.2, 27.3, 21.1, 19.3, 14.0.

HRMS (ESI): ([M+H]$^+$) calcd for $C_{15}H_{24}NO^+$: 234.1853; found: 234.1852.

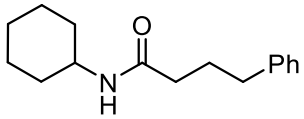


***N*-(pent-4-en-2-yl)-4-phenylbutanamide (25):** According to the general procedure, obtained as viscous liquid in 62% yield (28.7 mg, eluent: petroleum ether/ethyl acetate = 5/1).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.30-7.26 (m, 2H), 7.21-7.16 (m, 3H), 5.81-5.73 (m, 1H), 5.24 (d, J = 8.3 Hz, 1H), 5.12-4.97 (m, 2H), 4.12-4.05 (m, 1H), 2.64 (t, J = 7.5 Hz, 2H), 2.21 (t, J = 7.5 Hz, 2H), 2.13 (t, J = 8.3 Hz, 2H), 1.99-1.92 (m, 2H), 1.13 (d, J = 6.6 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.9, 140.5, 133.4, 127.5, 127.4, 124.9, 116.8, 43.4, 39.9, 35.1, 34.1, 26.2, 19.3.

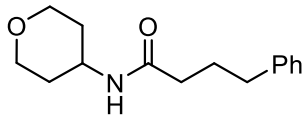
HRMS (ESI): ([M+H]$^+$) calcd for $C_{15}H_{22}NO^+$: 232.1696; found: 232.1696.



***N*-cyclohexyl-4-phenylbutanamide (26):** According to the general procedure, obtained as white solid in 75% yield (36.8 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *Angew. Chem. Int. Ed.* **2022**, *61*, e202200638).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.28 (t, J = 7.5 Hz, 2H), 7.22-7.14 (m,3H), 5.37 (d, J = 8.2 Hz, 1H), 3.79-3.72 (m, 1H), 2.64 (t, J = 7.6 Hz, 2H), 2.14 (t, J = 7.5 Hz, 2H), 1.92-1.98 (m, 2H), 1.86-1.92 (m, 2H), 1.66-1.72 (m, 2H), 1.57-1.63 (m, 1H), 1.3-1.39 (m, 2H), 1.17-1.03 (m, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 171.8, 141.6, 128.5, 128.4, 126.0, 48.1, 36.2, 35.2, 33.3, 27.3, 25.6, 24.9.

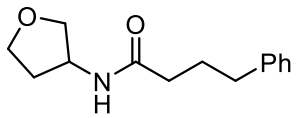


4-phenyl-*N*-(tetrahydro-2*H*-pyran-4-yl) butanamide (27): According to the general procedure, obtained as white solid in 56% yield (27.7 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 93-94 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.27 (t, J = 7.6 Hz, 2H), 7.20-7.14 (m, 3H), 5.56 (d, J = 8.4 Hz, 1H), 4.01-3.96 (m, 1H), 3.95-3.91 (m, 2H), 3.46-3.42 (m, 2H), 2.63 (t, J = 7.5 Hz, 2H), 2.14 (t, J = 7.6 Hz, 2H), 1.98-1.92 (m, 2H), 1.88-1.82 (m, 2H), 1.46-1.37 (m, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 171.0, 140.4, 127.5, 127.4, 125.0, 65.8, 44.5, 34.9, 34.1, 32.1, 26.1.

HRMS (ESI): ([M+H]$^+$) calcd for $C_{15}H_{22}NO_2^+$: 248.1646; found: 248.1647.

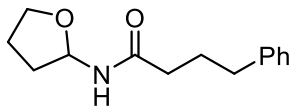


4-phenyl-*N*-(tetrahydrofuran-3-yl) butanamide (28): According to the general procedure, obtained as viscous liquid in 50% yield (23.3 mg, eluent: petroleum ether/ethyl acetate = 5/1).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.28 (t, *J* = 7.6 Hz, 2H), 7.22-7.15 (m, 3H), 5.73 (s, 1H), 3.95-3.88 (m, 1H), 3.87-3.84 (m, 2H), 3.82-3.75 (m, 1H), 3.29 (td, *J* = 7.1, 5.8 Hz, 2H), 2.86-2.77 (m, 1H), 2.65 (t, *J* = 7.6 Hz, 2H), 2.13-2.09 (m, 2H), 1.84 (p, *J* = 7.3 Hz, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.5, 140.4, 127.5, 127.3, 125.1, 69.9, 7.14, 44.6, 38.3, 32.3, 30.1, 29.5.

HRMS (ESI): ([M+H]$^+$) calcd for $C_{14}H_{20}NO_2^+$: 234.1489; found: 234.1485.

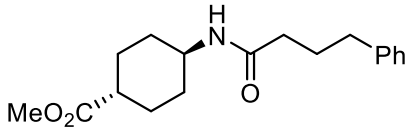


4-phenyl-*N*-(tetrahydrofuran-2-yl) butanamide (29): According to the general procedure, obtained as white solid in 52% yield (24.3 mg, eluent: petroleum ether/ethyl acetate = 5/1), m.p. = 58-60 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.28-7.25 (m, 2H), 7.20-7.13 (m, 3H), 5.86 (d, J = 8.2 Hz, 1H), 5.72-5.68 (m, 1H), 3.92-3.87 (m, 1H), 3.80-3.75 (m, 1H), 2.64 (t, J = 7.5 Hz, 2H), 2.19-2.13 (m, 3H), 1.99-1.93 (m, 2H), 1.93-1.88 (m, 2H), 1.70-1.62 (m, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.6, 141.5, 128.5, 128.4, 126.0, 81.0, 67.4, 35.9, 35.1, 32.1, 26.8, 24.7.

HRMS (ESI): ([M+H]$^+$) calcd for $C_{14}H_{20}NO_2^+$: 234.1489; found: 234.1487.

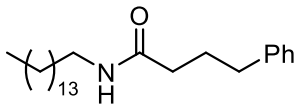


trans-methyl 4-(4-phenylbutanamido)cyclohexane-1-carboxylate (30): According to the general procedure using trans-4-(methoxycarbonyl)cyclohexanecarboxylic acid as substrate, obtained as white solid in 66% yield (40.0 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 113-115 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.29-7.26 (m, 2H), 7.21-7.14 (m, 3H), 5.27 (d, J = 8.8 Hz, 1H), 3.79-3.71 (m, 1H), 3.66 (s, 3H), 2.64 (t, J = 7.5 Hz, 2H), 2.25-2.19 (m, 1H), 2.13 (t, J = 7.5 Hz, 2H), 2.06-1.97 (m, 4H), 1.97-1.94 (m, 2H), 1.59-1.50 (m, 2H), 1.14-1.05 (m, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.7, 170.9, 140.5, 127.5, 127.4, 125.0, 50.7, 46.6, 41.4, 35.0, 34.1, 31.2, 26.7, 26.1.

HRMS (ESI): ([M+H]$^+$) calcd for $C_{18}H_{26}NO_3^+$: 304.1913; found: 304.1907.

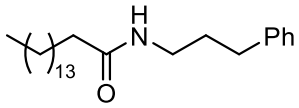


***N*-pentadecyl-4-phenylbutanamide (31)**: According to the general procedure, obtained as white solid in 22% yield (16.4 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 67-69 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.28 (t, J = 7.5 Hz, 2H), 7.22-7.16 (m, 3H), 5.37 (s, 1H), 3.23 (td, J = 7.4, 5.9 Hz, 2H), 2.65 (t, J = 7.5 Hz, 2H), 2.16 (t, J = 7.5 Hz, 2H), 1.97 (t, J = 7.5 Hz, 2H), 1.47 (t, J = 7.2 Hz, 2H), 1.30-1.23 (m, 24H), 0.88 (t, J = 7.0 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.6, 141.5, 128.5, 128.4, 125.9, 39.5, 36.0, 35.2, 31.9, 29.7 – 29.6 (m), 29.6, 29.6, 29.4, 29.3, 27.2, 26.9, 22.7, 14.1.

HRMS (ESI): ([M+H]$^+$) calcd for $C_{25}H_{44}NO^+$: 374.3418; found: 374.3417.

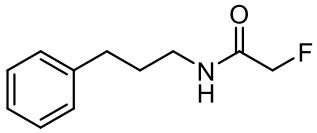


***N*-(3-phenylpropyl)palmitamide (31′):** According to the general procedure, obtained as white solid in 34% yield (25.4 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 63-65 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.28 (t, J = 7.6 Hz, 2H), 7.22-7.16 (m, 3H), 5.44 (s, 1H), 3.32-3.26 (m, 2H), 2.68-2.63 (m, 2H), 2.14-2.08 (m, 2H), 1.84 (p, J = 7.4 Hz, 2H), 1.61-1.56 (m, 2H), 1.30-1.23 (m, 24H), 0.88 (t, J = 7.0 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.1, 141.5, 128.5, 128.4, 126.0, 39.2, 36.9, 33.9, 33.4, 31.9, 31.3, 29.7, 29.7, 29.7, 29.6, 29.5, 29.4, 29.3, 25.8, 25.6, 24.9, 22.7, 14.2.

HRMS (ESI): ($[M+H]^+$) calcd for $C_{25}H_{44}NO^+$: 374.3418; found: 374.3419.

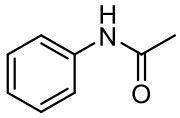


2-fluoro-*N*-(3-phenylpropyl) acetamide (32): According to the general procedure, obtained as white solid in 45% yield using cyclohexane as solvent (17.6 mg, eluent: petroleum ether/ethyl acetate = 5/1). The compound data was in agreement with the literature (Ref: *Angew. Chem. Int. Ed.* **2019**, *58*, 12211-12215).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.29 (t, J = 7.6 Hz, 2H), 7.20-7.17 (m, 3H), 6.28 (s, 1H), 4.81 (s, 1H), 4.73 (s, 1H), 3.38 (q, J = 6.8 Hz, 2H), 2.68 (t, J = 7.7 Hz, 2H), 1.90 (p, J = 7.4 Hz, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) *δ* 167.6 (d, J = 17.0 Hz), 141.1, 128.5, 128.3, 126.1, 80.3 (d, J = 186.0 Hz), 38.5, 33.2, 31.0.

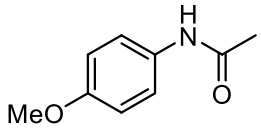
^{19}F NMR (565 MHz, Chloroform-*d*) *δ* -103.59.



***N*-phenylacetamide (34):** According to the general procedure, obtained as white solid in 50% yield (13.5 mg, eluent: petroleum ether/ethyl acetate = 2/1). The compound data was in agreement with the literature (Ref: *Chem. Commun.* **2008**, 1115-1117).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.50 (d, J = 7.3Hz, 2H), 7.40 (s, 1H), 7.31 (t, J = 7.4 Hz, 2H), 7.10 (t, J = 7.3Hz, 1H), 2.17 (s, 3H).

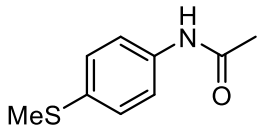
^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.5, 137.9, 129.0, 124.4, 119.9, 24.7.



***N*-(4-methoxyphenyl) acetamide (35):** According to the general procedure, obtained as white solid in 70% yield (23.1 mg, eluent: petroleum ether/ethyl acetate = 2/1). The compound data was in agreement with the literature (Ref: *Chem. Commun.* **2021**, *57*, 1955-1958).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.38 (d, J = 8.9 Hz, 2H), 7.21 (s, 1H), 6.85 (d, J = 8.9 Hz, 2H), 3.78 (s, 3H), 2.15 (s, 3H).

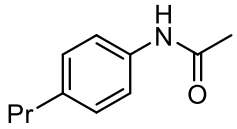
^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.3, 155.4, 129.9, 120.9, 113.1, 54.5, 23.3.



***N*-(4-(methylthio)phenyl) acetamide (36):** According to the general procedure, obtained as white solid in 65% yield (23.6 mg, eluent: petroleum ether/ethyl acetate = 2/1). The compound data was in agreement with the literature (Ref: *Org. Lett.* **2016**, *18*, 2758-2761).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.43 (d, J = 8.4 Hz, 2H), 7.31 (s, 1H), 7.22 (d, J = 8.5 Hz, 2H), 2.46 (s, 3H), 2.16 (s, 3H).

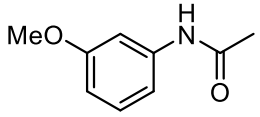
^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.5, 135.4, 133.6, 127.8, 120.6, 24.6, 16.6.



N*-(4-propylphenyl)acetamide (37):** According to the general procedure, obtained as white solid in 72% yield (25.5 mg, eluent: petroleum ether/ethyl acetate = 5/1). The compound data was in agreement with the literature (Ref: *J. Org. Chem.* **2022, 87*, 11958-11967).

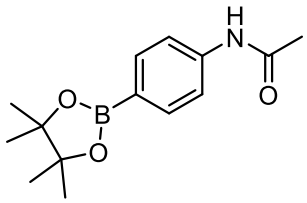
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.48 (s, 1H), 7.39 (d, J = 8.4 Hz, 2H), 7.10 (d, J = 8.4 Hz, 2H), 2.53 (t, J = 7.7 Hz, 2H), 2.15 (s, 3H), 1.60 (q, J = 7.5 Hz, 2H), 0.93 (t, J = 7.5 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.5, 138.9, 135.5, 128.9, 120.1, 37.5, 24.6, 24.5, 13.8.

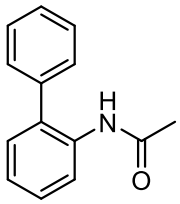


***N*-(3-methoxyphenyl) acetamide (38):** According to the general procedure, obtained as white solid in 68% yield (22.5 mg, eluent: petroleum ether/ethyl acetate = 2/1). The

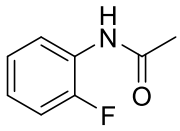
compound data was in agreement with the literature (Ref: *RSC Adv.* **2015**, *5*, 95313-95317).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.41 (s, 1H), 7.27 (s, 1H), 7.20 (t, J = 8.1 Hz, 1H), 6.96 (d, J = 8.1 Hz, 1H), 6.65 (dd, J = 8.2, 2.5 Hz, 1H), 3.79 (s, 3H), 2.16 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.5, 160.1, 139.1, 129.7, 112.0, 110.0, 105.7, 55.3, 24.7.



***N*-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl) acetamide (39):** According to the general procedure, obtained as light yellow solid in 58% yield (30.3 mg, eluent: petroleum ether/ethyl acetate = 2/1). The compound data was in agreement with the literature (Ref: *Org. Lett.* **2016**, *18*, 2758-2761).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.76 (d, J = 8.0 Hz, 2H), 7.51 (d, J = 8.0 Hz, 2H), 7.27 (s, 1H), 2.18 (s, 3H), 1.33 (s, 12H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.3, 139.5, 134.8, 117.5, 82.7, 28.7, 23.8. The carbon directly attached to the boron atom was not detected due to quadrupolar broadening.

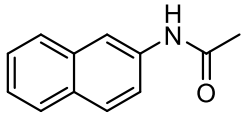


***N*-([1,1'-biphenyl]-2-yl) acetamide (40):** According to the general procedure, obtained as light yellow solid in 52% yield (22.0 mg, eluent: petroleum ether/ethyl acetate = 2/1). The compound data was in agreement with the literature (Ref: *Synth. Commun.* **2020**, *50*, 3326-3336).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.25 (d, J = 8.2 Hz, 1H), 7.49 (t, J = 7.5 Hz, 2H), 7.42 (t, J = 7.5 Hz, 1H), 7.39-7.35 (m, 3H), 7.25 (t, J = 7.5 Hz, 1H), 7.18 (t, J = 7.5 Hz, 2H), 2.02 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.4, 138.2, 134.7, 132.3, 130.1, 129.3, 129.1, 128.5, 128.0, 124.5, 121.8, 24.6.

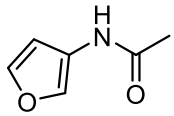


***N*-(2-fluorophenyl) acetamide (41):** According to the general procedure, obtained as white solid in 55% yield (16.9 mg, eluent: petroleum ether/ethyl acetate = 2/1). The

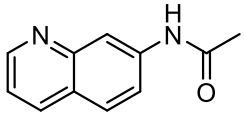
compound data was in agreement with the literature (Ref: *Chem. Commun.* **2021**, *57*, 1955-1958).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.29 (td, J = 8.1, 1.7 Hz, 1H), 7.39 (s, 1H), 7.12-7.01 (m, 3H), 2.22 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.5, 152.5 (d, J = 243.3 Hz), 126.6 (d, J = 10.0 Hz), 124.8 (d, J = 3.8 Hz), 124.5 (d, J = 7.6 Hz), 122.0, 114.9 (d, J = 19.3 Hz), 24.9.
^{19}F NMR (565 MHz, Chloroform-*d*) δ -131.55.



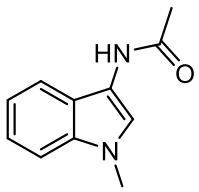
***N*-(naphthalen-2-yl) acetamide (42):** According to the general procedure, obtained as white solid in 65% yield (24.1 mg, eluent: petroleum ether/ethyl acetate = 2/1). The compound data was in agreement with the literature (Ref: *ACS Sustain Chem. Eng*. **2021**, *9*, 2100-2114).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.18 (s, 1H), 7.78-7.75 (m, 3H), 7.66 (s, 1H), 7.46-7.38 (m, 3H), 2.22 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.8, 135.4, 133.8, 130.6, 128.8, 127.7, 127.6, 126.5, 125.1, 119.9, 116.7, 24.7.



***N*-(furan-3-yl)acetamide (43):** According to the general procedure, obtained as brown solid in 44% yield (11.0 mg, eluent: petroleum ether/ethyl acetate = 2/1). The compound data was in agreement with the literature (Ref: *J. Org. Chem.* **2020**, *85*, 4583-4593).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.00 (s, 1H), 7.29 (s, 1H), 7.26 (s, 1H), 6.30 (s, 1H), 2.15 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.5, 141.5, 132.6, 124.1, 104.5, 23.4.



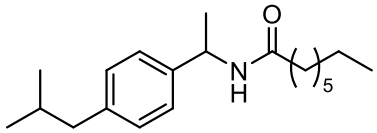
***N*-(quinolin-7-yl) acetamide (44):** According to the general procedure, obtained as white solid in 47% yield (17.5 mg, eluent: petroleum ether/ethyl acetate = 2/1). The compound data was in agreement with the literature (Ref: *Chem. Eur. J.* **2019**, *25*, 14972-14982).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.27 (s, 1H), 8.79 (dd, J = 4.3, 1.7 Hz, 1H), 8.07 (d, J = 2.1 Hz, 1H), 8.04 (d, J = 8.9 Hz, 1H), 7.97 (dd, J = 8.9, 2.1 Hz, 1H), 7.66 (d, J = 8.9 Hz, 1H), 7.29-7.26 (m, 1H), 2.15 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.4, 150.4, 148.3, 140.0, 136.1, 128.5, 125.2, 120.9, 120.0, 116.4, 24.5.



***N*-(1-methyl-1*H*-indol-3-yl) acetamide (45):** According to the general procedure, obtained as red solid in 51% yield (19.2 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *Org. Biomol. Chem.* **2017**, *15*, 576-580).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.66 (s, 1H), 7.49-7.47 (m, 1H), 7.32-7.29 (m, 1H), 7.26-7.22 (m, 2H), 7.14-7.10 (m, 1H), 3.76 (s, 3H), 2.25 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.5, 134.4, 122.1, 120.9, 120.6, 118.9, 116.5, 113.5, 109.5, 32.8, 23.8.

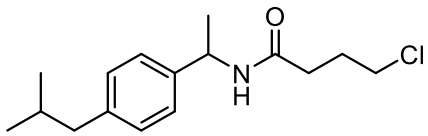


***N*-(1-(4-isobutylphenyl)ethyl)octanamide (46):** According to the general procedure, obtained as viscous liquid in 76% yield (48.6 mg, eluent: petroleum ether/ethyl acetate = 3/1).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.22 (d, J = 7.8 Hz, 2H), 7.11 (d, J = 7.8 Hz, 2H), 5.71 (s, 1H), 5.12 (q, J = 7.0 Hz, 1H), 2.45 (d, J = 7.2 Hz, 2H), 2.17 (t, J = 7.6 Hz, 2H), 1.88-1.80 (m, 1H), 1.62 (t, J = 7.3 Hz, 2H), 1.48 (d, J = 6.8 Hz, 3H), 1.36-1.21 (m, 8H), 0.91-0.85 (m, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.2, 140.9, 140.4, 129.4, 126.0, 48.3, 45.0, 37.0, 31.7, 30.2, 29.3, 29.0, 25.8, 22.6, 22.4, 21.6, 14.1.

HRMS (ESI): ($[M+H]^+$) calcd for $C_{20}H_{34}NO^+$: 304.2635; found: 304.2633.

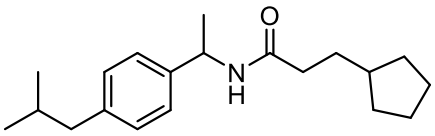


4-chloro-*N*-(1-(4-isobutylphenyl)ethyl)butanamide (47): According to the general procedure, obtained as white solid in 66% yield (37.2 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 98-101 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.21 (d, J = 8.1 Hz, 2H), 7.12 (d, J = 8.1 Hz, 2H), 5.71 (d, J = 7.2 Hz, 1H), 5.12-5.09 (m, 1H), 3.61-3.57 (m, 2H), 2.45 (d, J = 7.2 Hz, 2H), 2.40-2.32 (m, 2H), 2.15-2.09 (m, 2H), 1.88-1.81 (m, 1H), 1.49 (d, J = 6.9 Hz, 3H), 0.89 (d, J = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.6, 141.0, 140.3, 129.4, 125.9, 48.6, 45.0, 44.6, 33.4, 30.2, 28.1, 22.4, 21.7.

HRMS (ESI): ($[M+H]^+$) calcd for $C_{16}H_{25}ClNO^+$: 282.1625; found: 282.1625.

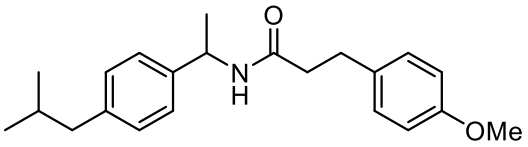


3-cyclopentyl-*N*-(1-(4-isobutylphenyl)ethyl)propanamide (48): According to the general procedure, obtained as white solid in 50% yield (30.1 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 49-51 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.21 (d, J = 8.1 Hz, 2H), 7.11 (d, J = 8.0 Hz, 2H), 5.66 (d, J = 7.9 Hz, 1H), 5.12 (p, J = 7.1 Hz, 1H), 2.45 (d, J = 7.2 Hz, 2H), 2.20-2.16 (m, 2H), 1.84 (hept, J = 6.8 Hz, 1H), 1.76-1.71 (m, 3H), 1.66-1.57 (m, 4H), 1.52-1.46 (m, 5H), 1.11-1.03 (m, 2H), 0.89 (d, J = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.3, 140.9, 140.5, 129.4, 126.0, 48.3, 45.0, 39.8, 36.3, 32.5, 32.0, 30.2, 25.1, 22.4, 21.6.

HRMS (ESI): ([M+H]$^+$) calcd for $C_{20}H_{32}NO^+$: 302.2479; found: 302.2478.

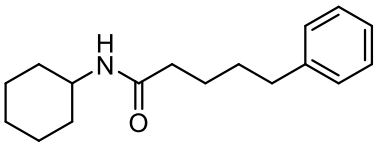


***N*-(1-(4-isobutylphenyl)ethyl)-3-(4-methoxyphenyl) propanamide (49):** According to the general procedure, obtained as white solid in 54% yield (36.7 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 107-109 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.13-7.06 (m, 6H), 6.81 (d, J = 8.6 Hz, 2H), 5.48 (d, J = 8.0 Hz, 1H), 5.10-5.02 (m, 1H), 3.78 (s, 3H), 2.91 (t, J = 7.5 Hz, 2H), 2.46-2.41 (m, 4H), 1.87-1.80 (m, 1H), 1.40 (d, J = 6.9 Hz, 3H), 0.89 (d, J = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.2, 157.0, 139.8, 139.1, 131.8, 128.4, 128.3, 124.9, 112.9, 54.2, 47.3, 44.0, 38.0, 29.9, 29.2, 21.4, 20.4.

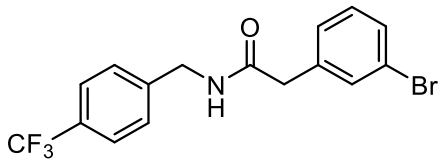
HRMS (ESI): ([M+H]$^+$) calcd for $C_{22}H_{30}NO_2^+$: 340.2272; found: 340.2273.



***N*-cyclohexyl-5-phenylpentanamide (50):** According to the general procedure, obtained as white solid in 70% yield (36.3 mg, eluent: petroleum ether/ethyl acetate = 5/1). The compound data was in agreement with the literature (Ref: *RSC Adv.* **2015**, *5*, 25789-25793).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.30-7.26 (m, 2H), 7.20-7.15 (m, 3H), 5.25 (br, 1H), 3.80-3.72 (m, 1H), 2.63 (t, J = 7.1 Hz, 2H), 2.16 (t, J = 7.1 Hz, 2H), 1.89 (dd, J = 12.7, 4.0 Hz, 2H), 1.71-1.62 (m, 8H), 1.38-1.33 (m, 2H), 1.13-1.03 (m, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 171.9, 142.3, 128.4, 128.3, 125.8, 48.1, 37.0, 35.7, 33.3, 31.1, 25.6, 24.9. (one carbon signal is overlapped)



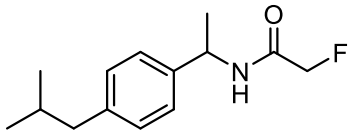
2-(3-bromophenyl)-N-(4-(trifluoromethyl)benzyl) acetamide (51): According to the general procedure, obtained as white solid in 71% yield (25.5 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 103-106 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.52 (d, J = 8.0 Hz, 2H), 7.41-7.38 (m, 2H), 7.25 (d, J = 8.0 Hz, 2H), 7.21-7.15 (m, 2H), 6.27 (d, J = 6.0 Hz, 1H), 4.39 (d, J = 6.0 Hz, 2H), 3.51 (s, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.4, 142.2, 136.9, 132.3, 130.6, 130.5, 129.7 (q, J = 32.3 Hz), 127.9, 127.7, 125.6 (q, J = 3.8 Hz), 124.0 (q, J = 272.0 Hz), 122.9, 43.1, 43.0.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -62.49.

HRMS (ESI): ([M+H]$^{+}$) calcd for $C_{16}H_{14}BrF_3NO^{+}$: 372.0211; found: 372.0209.



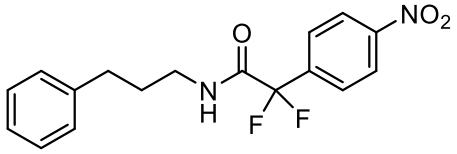
2-fluoro-N-(1-(4-isobutylphenyl)ethyl) acetamide (52): According to the general procedure, obtained as white solid in 50% yield (23.3 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 46-48 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.25-7.22 (m, 2H), 7.15-7.11 (m, 2H), 6.48 (br, 1H), 5.19 (q, J = 7.2 Hz, 1H), 4.87-4.80 (m, 1H), 4.79-4.72 (m, 1H), 2.46 (d, J = 7.2 Hz, 2H), 1.89-1.81 (m, 1H), 1.54 (d, J = 6.9 Hz, 3H), 0.90 (d, J = 6.6 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 166.6 (d, J = 17.1 Hz), 141.2, 139.6, 129.5, 126.0, 80.3 (d, J = 186.1 Hz), 48.1, 45.0, 30.2, 22.4, 21.7.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -224.32.

HRMS (ESI): ([M+Na]$^{+}$) calcd for $C_{14}H_{20}FNNaO^{+}$: 260.1427; found: 260.1426.

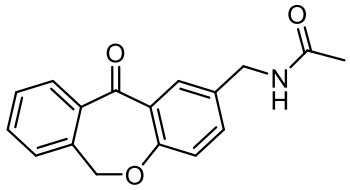


2,2-difluoro-2-(4-nitrophenyl)-N-(3-phenylpropyl)acetamide (53): According to the general procedure, obtained as white solid in 40% yield with 2 equivalents of DBU (26.7 mg, eluent: petroleum ether/ethyl acetate = 5/1), m.p. = 115-117 °C.

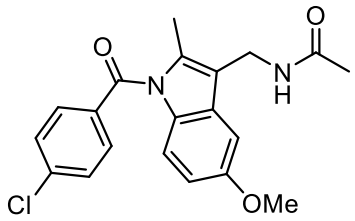
^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.29 (d, *J* = 8.6 Hz, 2H), 7.79 (d, J = 8.6 Hz, 2H), 7.30 (t, J = 7.6 Hz, 2H), 7.22 (t, J = 7.4 Hz, 1H), 7.17 (d, J = 8.6 Hz, 2H), 6.55 (s, 1H), 3.38 (q, J = 6.7 Hz, 2H), 2.67 (t, J = 7.5 Hz, 2H), 2.00-1.73 (m, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 161.9 (t, J = 30.0 Hz), 148.4, 139.7, 137.9 (t, J = 25.9 Hz), 127.6, 127.3, 126.1 (t, J = 6.0 Hz), 125.3, 122.7, 112.7 (t, J = 254.8 Hz), 38.5, 32.2, 29.6.

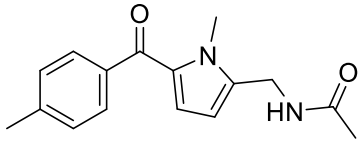
^{19}F NMR (565 MHz, Chloroform-*d*) δ -103.62.
HRMS (ESI): ([M+Na]$^+$) calcd for $C_{17}H_{16}F_2N_2NaO_3^+$: 357.1022; found: 357.1025.



***N*-((11-oxo-6,11-dihydrodibenzo[b,e]oxepin-2-yl)methyl)acetamide (54):** According to the general procedure, obtained as white solid in 50% yield (28.1 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 170-172 °C.
^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.04 (s, 1H), 7.83-7.79 (m, 1H), 7.54 (t, J = 7.5 Hz, 1H), 7.44 (t, J = 7.6 Hz, 1H), 7.39 (d, J = 8.2 Hz, 1H), 7.33 (d, J = 7.6 Hz, 1H), 6.98-6.95 (m, 1H), 6.37 (br, 1H), 5.12 (d, J = 3.8 Hz, 2H), 4.37 (t, J = 4.9 Hz, 2H), 2.01 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 191.1, 170.4, 160.8, 140.4, 135.6, 135.3, 133.0, 132.3, 130.8, 129.5, 129.4, 128.0, 125.1, 121.4, 73.7, 42.9, 23.4.
HRMS (ESI): ([M+H]$^+$) calcd for $C_{17}H_{16}NO_3^+$: 282.1130; found: 282.1126.

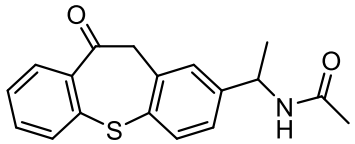


***N*-((1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl)methyl)acetamide (55):** According to the general procedure, obtained as yellow solid in 60% yield (44.5 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 155-157 °C.
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.62 (d, J = 8.5 Hz, 2H), 7.45 (d, J = 8.5 Hz, 2H), 6.99 (d, J = 2.5 Hz, 1H), 6.80 (d, J = 9.0 Hz, 1H), 6.65 (dd, J = 9.0, 2.5 Hz, 1H), 5.81 (br, 1H), 4.50 (d, J = 5.1 Hz, 2H), 3.81 (s, 3H), 2.38 (s, 3H), 1.98 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.4, 156.1, 139.5, 136.2, 133.6, 131.2, 130.8, 130.0, 129.2, 115.8, 115.0, 112.0, 101.1, 55.7, 33.5, 23.2, 13.1. (one carbon signal is overlapped)
HRMS (ESI): ([M+H]$^+$) calcd for $C_{20}H_{20}ClN_2O_3^+$: 371.1162; found: 371.1163.

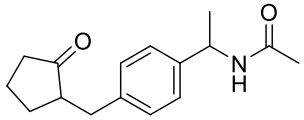


***N*-((1-methyl-5-(4-methylbenzoyl)-1*H*-pyrrol-2-yl)methyl) acetamide (56):** According to the general procedure, obtained as white solid in 51% yield (27.6 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 190-192 °C.

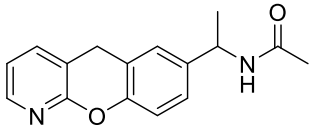
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.70 (d, J = 8.1 Hz, 2H), 7.25 (d, J = 7.9 Hz, 2H), 6.64 (d, J = 4.0 Hz, 1H), 6.11 (d, J = 4.0 Hz, 1H), 5.67 (s, 1H), 4.51 (d, J = 5.5 Hz, 2H), 3.93 (s, 3H), 2.42 (s, 3H), 2.04 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 186.1, 169.7, 142.3, 137.8, 137.0, 131.9, 129.5, 128.8, 121.8, 108.8, 35.5, 33.3, 23.2, 21.6.
HRMS (ESI): ([M+H]$^+$) calcd for $C_{16}H_{19}N_2O_2^+$: 271.1442; found: 271.1444.



***N*-(1-(10-oxo-10,11-dihydrodibenzo[b,f]thiepin-2-yl)ethyl) acetamide (57):** According to the general procedure, obtained as white solid in 55% yield (34.3 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 178-180 °C.
^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.19 (dd, J = 8.0, 1.6 Hz, 1H), 7.62-7.57 (m, 2H), 7.43 (t, J = 7.5 Hz, 1H), 7.38 (s, 1H), 7.34-7.29 (m, 1H), 7.15 (d, J = 7.8 Hz, 1H), 5.77 (s, 1H), 5.10 (br, 1H), 4.43-4.30 (m, 2H), 1.99 (s, 3H), 1.45 (d, J = 6.6 Hz, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 191.5, 169.4, 145.6, 140.2, 138.0, 136.1, 133.4, 132.6, 131.6, 131.5, 130.9, 126.9, 126.8, 125.4, 51.2, 48.5, 23.5, 21.9.
HRMS (ESI): ([M+H]$^+$) calcd for $C_{18}H_{18}NO_2S^+$: 312.1053; found: 312.1050.

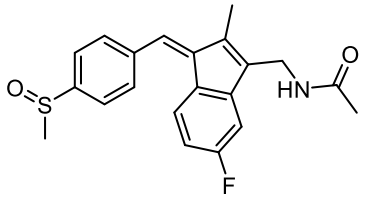


N-(1-(4-((2-oxocyclopentyl)methyl)phenyl)ethyl) acetamide (58): According to the general procedure, obtained light yellow liquid in 74% yield (38.4 mg, eluent: petroleum ether/ethyl acetate = 3/1).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.22 (d, J = 8.0 Hz, 2H), 7.13 (d, J = 7.9 Hz, 2H), 5.73 (d, J = 7.4 Hz, 1H), 5.13-5.07 (m, 1H), 3.11 (dd, J = 14.0, 4.3 Hz, 1H), 2.52 (dd, J = 13.9, 9.4 Hz, 1H), 2.38-2.29 (m, 2H), 2.15-2.04 (m, 2H), 1.97 (s, 3H), 1.78- 1.69 (m, 2H), 1.56-1.52 (m, 1H), 1.46 (d, J = 6.9 Hz, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.3, 141.2, 139.3, 129.4, 126.5, 51.2, 48.7, 38.4, 35.3, 29.4, 23.7, 21.9, 20.7.
HRMS (ESI): ([M+H]$^+$) calcd for $C_{16}H_{22}NO_2^+$: 260.1645; found: 260.1648.

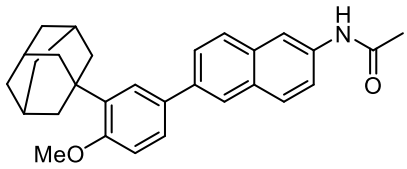


***N*-(1-(5*H*-chromeno[2,3-b]pyridin-7-yl)ethyl) acetamide (59):** Following the general procedure, obtained as white solid in 86% yield (46.2 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 197-199 °C.

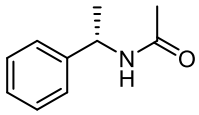
^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.13 (d, J = 4.5 Hz, 1H), 7.55-7.49 (m, 1H), 7.20-6.98 (m, 4H), 6.58 (d, J = 7.8 Hz, 1H), 5.06 (p, J = 7.0 Hz, 1H), 4.04 (s, 2H), 2.00 (s, 3H), 1.46 (d, J = 7.0 Hz, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.6, 160.3, 150.6, 146.5, 138.8, 134.7, 126.7, 125.6, 119.9, 119.4, 117.2, 115.3, 48.1, 28.0, 23.3, 21.7.
HRMS (ESI): ([M+H]$^+$) calcd for $C_{16}H_{17}N_2O_2^+$: 269.1285; found: 269.1286.



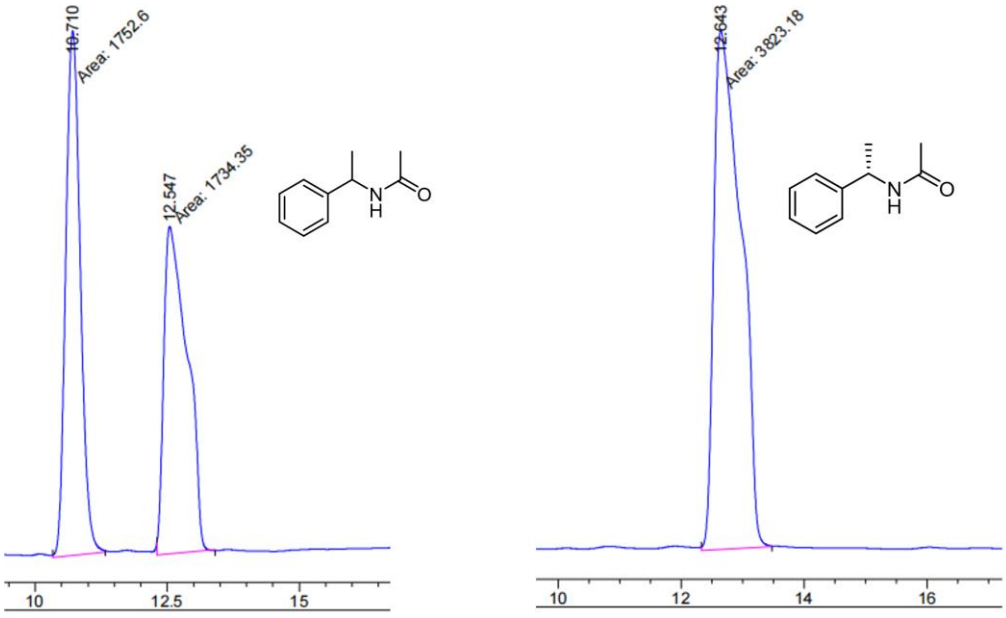
(*Z*)-*N*-((5-fluoro-2-methyl-1-(4-(methylsulfinyl)benzylidene)-1*H*-inden-3-yl)methyl) acetamide (60): Following the general procedure, obtained white solid in 45% yield (33.3 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 177-179 °C.
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.72 (d, J = 8.3 Hz, 2H), 7.65 (d, J = 8.1 Hz, 2H), 7.19-7.14 (m, 2H), 6.92 (dd, J = 8.8, 2.4 Hz, 1H), 6.60-6.58 (m, 1H), 5.56 (s, 1H), 4.41 (d, J = 5.3 Hz, 2H), 2.81 (s, 3H), 2.23 (s, 3H), 2.02 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.1, 162.4 (d, J = 247.1 Hz), 144.9, 144.8, 144.5, 140.6, 138.5, 137.5, 133.8 (d, J = 2.5 Hz), 129.2, 128.5 (d, J = 2.9 Hz), 127.9, 122.9, 110.0 (d, J = 22.6 Hz), 105.2 (d, J = 23.8 Hz), 42.8, 33.4, 22.2, 9.4.
^{19}F NMR (565 MHz, Chloroform-*d*) δ -112.21.
HRMS (ESI): ([M+H]$^+$) calcd for $C_{21}H_{21}FNO_2S^+$: 370.1272; found: 370.1272.



***N*-(6-(3-(adamantan-1-yl)-4-methoxyphenyl)naphthalen-2-yl) acetamide (61):** Following the general procedure, obtained in 42% yield as yellow solid (35.8 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 225-227 °C.
^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.18 (s, 1H), 7.91 (d, J = 1.9 Hz, 1H), 7.84-7.81 (m, 2H), 7.71 (dd, J = 8.5, 1.9 Hz, 1H), 7.57 (d, J = 2.4 Hz, 1H), 7.51 (dd, J = 8.4, 2.4 Hz, 1H), 7.45 (dd, J = 8.8, 2.2 Hz, 1H), 7.35 (s, 1H), 6.98 (d, J = 8.4 Hz, 1H), 3.89 (s, 3H), 2.24 (s, 3H), 2.20-2.08 (m, 9H), 1.82-1.79 (m, 6H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 168.4, 158.5, 138.9, 138.2, 135.0, 133.1, 132.6, 131.0, 128.9, 128.0, 126.4, 125.8, 125.5, 124.7, 120.1, 116.4, 112.1, 55.2, 40.6, 37.2, 37.2, 29.7, 24.9.
HRMS (ESI): ([M+H]$^+$) calcd for $C_{29}H_{32}NO_2^+$: 426.2433; found: 426.2428.

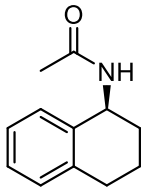


(*S*)-*N*-(1-phenylethyl) acetamide (62): Following the general procedure with (*S*)-2-phenylpropanoic acid as substrate, obtained in 92% yield (30.0 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the compound **15**. HPLC: 99% ee, Daicel Chiralpak AD-H column, 5% *i*-PrOH in *n*-hexane, 0. 5 mL/min, 210 nm, t_r (minor) = 10.7 min, t_r (major) = 12.6 min.



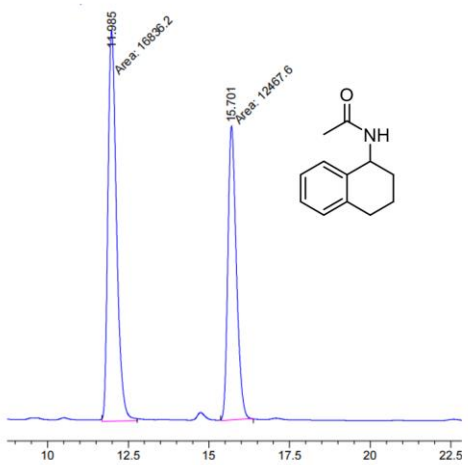
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.710	MM	0.3206	1752.59900	91.09795	50.2617
2	12.547	MM	0.5092	1734.34912	56.76305	49.7383

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.643	MM	0.5081	3823.18457	125.40464	100.0000

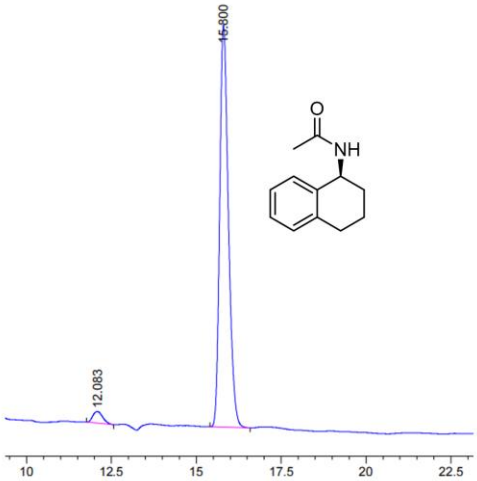


(*S*)-*N*-(1,2,3,4-tetrahydronaphthalen-1-yl) acetamide (63): Following the general procedure with (*S*)-1,2,3,4-tetrahydronaphthalene-1-carboxylic acid as substrate, obtained as white solid in 76% yield (28.7 mg, eluent: petroleum ether/ethyl acetate = 3/1). The NMR data was in agreement with the compound **16**.

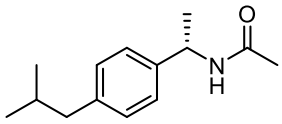
HPLC: 94% ee, Daicel Chiralpak AD-H column, 5% *i*-PrOH in *n*-hexane, 0.5 mL/min, 210 nm, t_r (minor) = 12.0 min, t_r (major) = 15.8 min.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.985	MM	0.3091	1.68362e4	907.72034	57.4541
2	15.701	MM	0.3040	1.24676e4	683.59515	42.5459

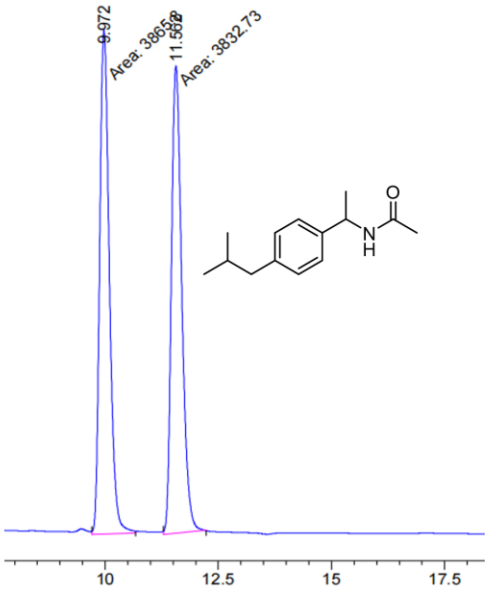


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.083	BB	0.3242	39.91629	1.98012	3.1139
2	15.800	BB	0.2721	1241.97583	69.63890	96.8861



(*S*)-*N*-(1-(4-isobutylphenyl)ethyl) acetamide (64): Following the general procedure with (*S*)-Ibuprofen as substrate, obtained as light yellow viscous liquid in 90% yield (39.5 mg, eluent: petroleum ether/ethyl acetate = 3/1). The NMR data was in agreement with the compound **3**.

HPLC: 91% ee, Daicel Chiralpak AD-H column, 10% *i*-PrOH in *n*-hexane, 0.75 mL/min, 210 nm, t_r (minor) = 9.9 min, t_r (major) = 11.5 min.



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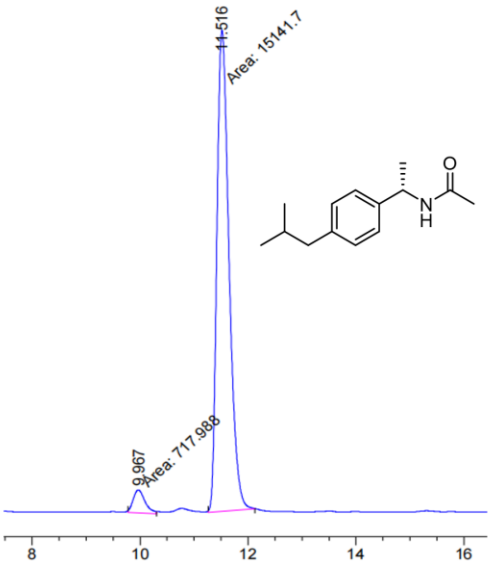
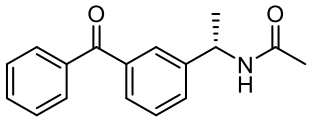


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.967	MM	0.2567	717.98773	46.61342	4.5271
2	11.516	MM	0.2600	1.51417e4	970.80261	95.4729

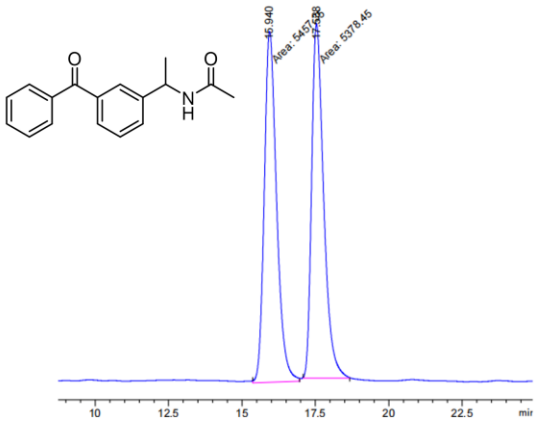


(*S*)-*N*-(1-(3-benzoylphenyl)ethyl) acetamide (65): Following the general procedure with (*S*)-Ketoprofen as substrate, obtained as white solid in 75% yield (40.1 mg, eluent: petroleum ether/ethyl acetate = 3/1). The compound data was in agreement with the literature (Ref: *ACS Catal.* **2022**, *12*, 809-817).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.80-7.75 (m, 3H), 7.66-7.52 (m, 3H), 7.48 (t, J = 7.7 Hz, 2H), 7.42 (t, J = 7.6 Hz,1H), 6.08 (d, J = 7.6 Hz, 1H), 5.16 (p, J = 7.2 Hz, 1H), 1.98 (s, 3H), 1.48 (d, J = 6.9 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 196.7, 169.4, 144.0, 137.9, 137.5, 132.6, 130.7, 130.1, 129.3, 128.5, 128.4, 127.2, 48.7, 23.4, 22.1.

HPLC: 90% ee, Daicel Chiralpak OD-H column, 10% *i*-PrOH in *n*-hexane, 0.75 mL/min, 210 nm, t_r (minor) = 16.0 min, t_r (major) = 17.5 min.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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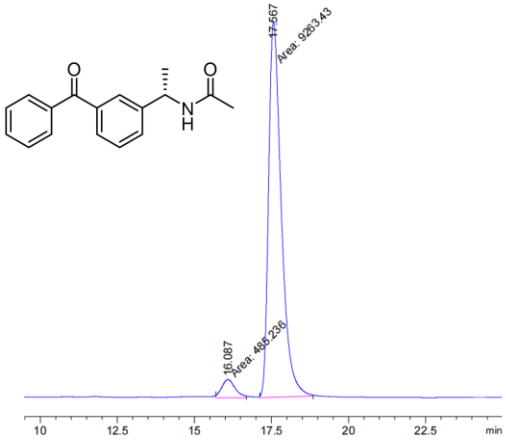
2	17.538	MM	0.4747	5378.45410	188.82851	49.6359



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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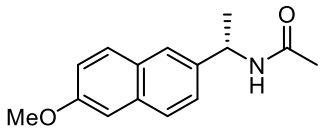
2	17.567	MM	0.4773	9263.42578	323.44333	95.0225



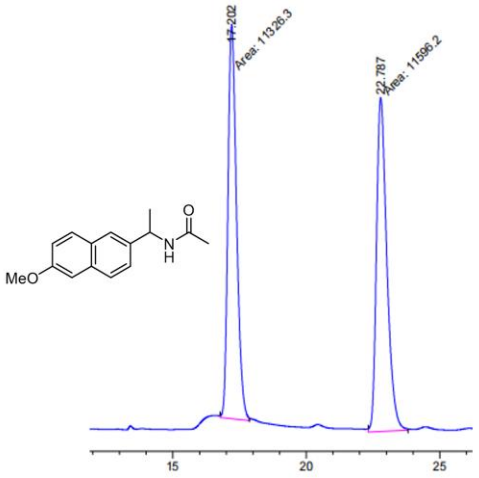
(*S*)-*N*-(1-(6-methoxynaphthalen-2-yl)ethyl) acetamide (66): Following the general procedure with (*S*)-Naproxen as substrate, obtained as white solid in 82% yield (39.9 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 146-148 °C.

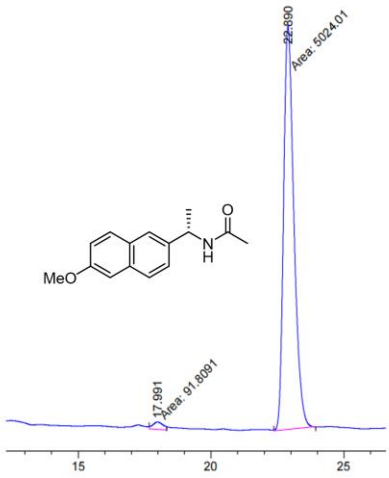
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.71-7.68 (m, 2H), 7.67 (s, 1H), 7.39 (d, J = 8.5 Hz,1H), 7.14 (dd, J = 8.9, 2.5 Hz, 1H), 7.10 (d, J = 2.6 Hz,1H), 5.93 (d, J = 7.6 Hz,1H), 5.30-5.23 (m, 1H), 3.91 (s, 3H), 1.99 (s, 3H), 1.55 (d, J = 6.8 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.3, 157.7, 138.2, 133.8, 129.3, 128.7, 127.3, 125.3, 124.4, 119.1, 105.6, 55.3, 48.7, 23.5, 21.5.

HRMS (ESI): ([M+H]$^{+}$) calcd for $C_{15}H_{18}NO_2^{+}$: 244.1332; found: 244.1332.

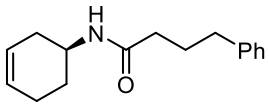
HPLC: 96% ee, Daicel Chiral pak AD-H column, 10% *i*-PrOH in *n*-hexane, 0.5 mL/min, 210 nm, t_r (minor) = 17.9 min, t_r (major) = 22.8 min.





Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.202	MM	0.3726	1.13263e4	506.69989	49.4113
2	22.787	MM	0.4506	1.15962e4	428.90424	50.5887

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.991	MM	0.4537	91.80907	3.37292	1.7946
2	22.890	MM	0.4490	5024.00732	186.50471	98.2054



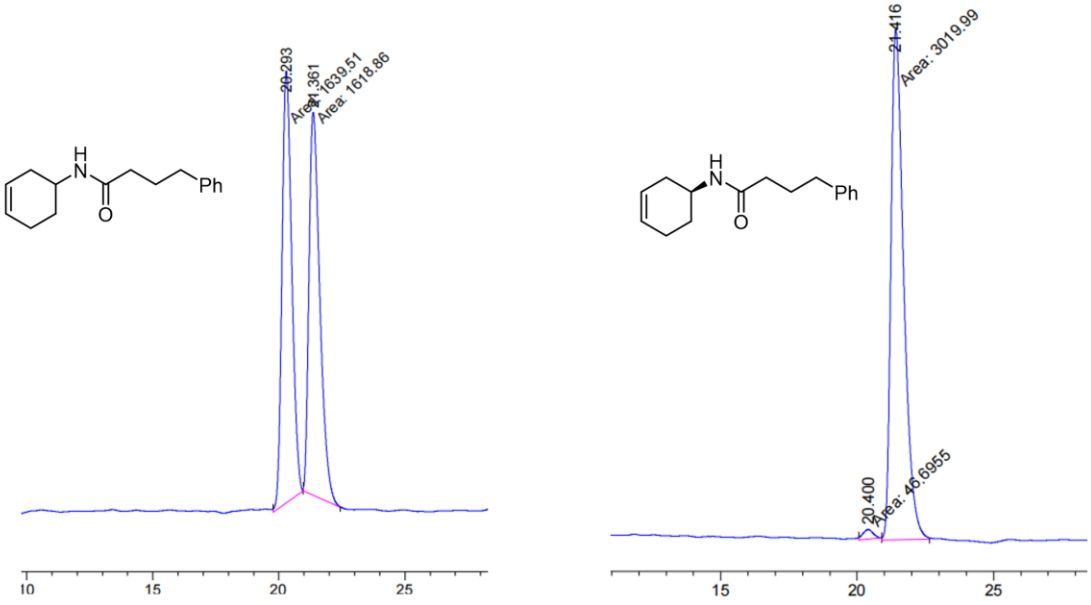
(*S*)-*N*-(cyclohex-3-en-1-yl)-4-phenylbutanamide (67): Following the general procedure with (*S*)-cyclohex-3-ene-1-carboxylic acid as substrate, obtained as white solid in 54% yield (26.3 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 57-59 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.30-7.26 (m, 2H), 7.22-7.16 (m, 3H), 5.72-5.64 (m, 1H), 5.63-5.58 (m, 1H), 5.37 (s, 1H), 4.22-4.04 (m, 1H), 2.66 (t, J = 7.5 Hz, 2H), 2.42-2.36 (m, 1H), 2.18-2.14 (m, 2H), 2.11-2.05 (m, 1H), 1.98 (p, J = 7.5 Hz, 2H), 1.88-1.82 (m, 2H), 1.62-1.57 (m, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.0, 141.6, 128.6, 128.4, 127.1, 126.0, 124.4, 44.3, 36.1, 35.2, 31.7, 27.9, 27.2, 23.4.

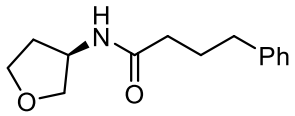
HRMS (ESI): ([M+H]$^{+}$) calcd for $C_{16}H_{22}NO^{+}$: 244.1696; found: 244.1699.

HPLC: 97% ee, Daicel Chiralpak OD-H column, 5% ^{i}PrOH in ^{n}hexane, 0.75 mL/min, 210 nm, t_r (minor) = 20.4 min, t_r (major) = 21.4 min.



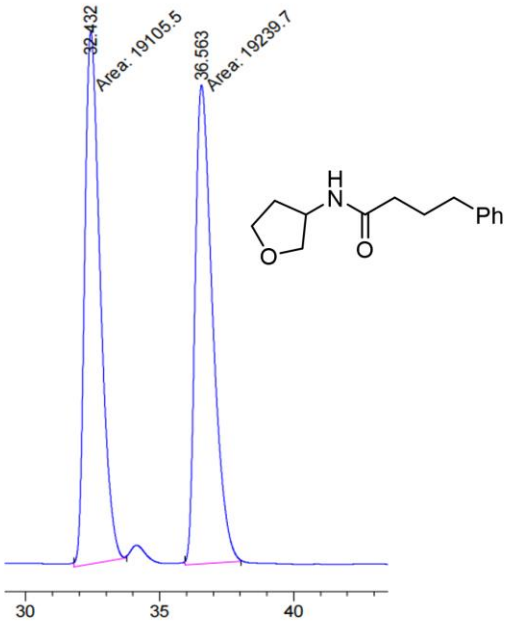
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.293	MM	0.4480	1639.50525	60.99278	50.3168
2	21.361	MM	0.4984	1618.86328	54.13635	49.6832

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	20.400	MM	0.4383	46.69549	1.77564	1.5227
2	21.416	MM	0.5408	3019.99341	93.06693	98.4773

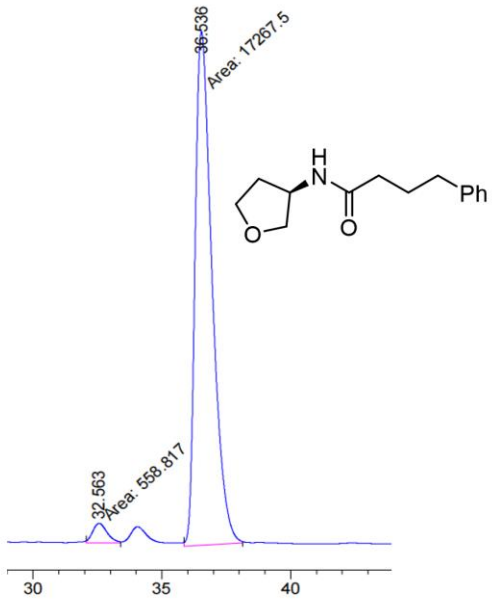


(*R*)-4-phenyl-*N*-(tetrahydrofuran-3-yl)butanamide (68): Following the general procedure with (*R*)-tetrahydrofuran-3-carboxylic acid as substrate, obtained in 65% yield as white solid (30.3 mg, eluent: petroleum ether/ethyl acetate = 3/1). The NMR data was in agreement with the compound **28**.

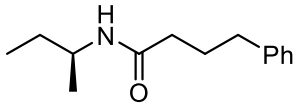
HPLC: 94% ee, Daicel Chiralpak AD-3 column, 5% ^{i}PrOH in ^{n}hexane, 0.5 mL/min, 210 nm, t_r (minor) = 32.5 min, t_r (major) = 36.5 min.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	32.432	MM	0.6762	1.91055e4	470.88531	49.8250
2	36.563	MM	0.7565	1.92397e4	423.86307	50.1750



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	32.563	MM	0.6485	558.81689	14.36134	3.1348
2	36.536	MM	0.7612	1.72675e4	378.06952	96.8652



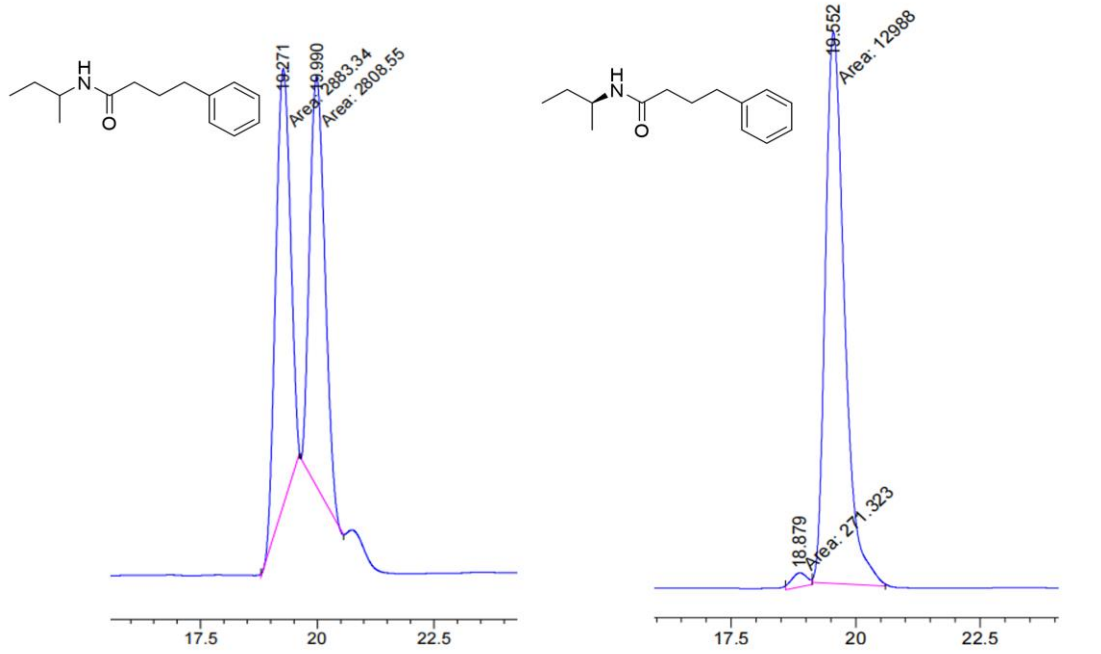
(*S*)-*N*-(sec-butyl)-4-phenylbutanamide (69): Following the general procedure with (S)-2-methylbutanoic acid as substrate, obtained in 50% yield as colorless liquid (21.9 mg, eluent: petroleum ether/ethyl acetate = 5/1).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.29-7.26 (m, 2H), 7.20-7.16 (m, 3H), 5.26 (d, J = 8.2 Hz, 1H), 3.95-3.88 (m, 1H), 2.65 (t, J = 7.6 Hz, 2H), 2.15 (t, J = 7.6 Hz, 2H), 2.04-1.92 (m, 2H), 1.52-1.40 (m, 2H), 1.10 (d, J = 6.6 Hz, 3H), 0.89 (t, J = 7.5 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 172.0, 141.6, 128.5, 128.4, 126.0, 46.5, 36.2, 35.2, 29.7, 27.3, 20.5, 10.4.

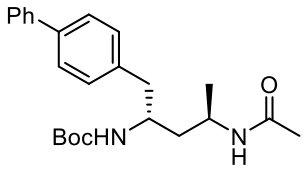
HRMS (ESI): ([M+H]$^{+}$) calcd for $C_{14}H_{22}NO^{+}$: 220.1696; found: 220.1695.

HPLC: 96% ee, Daicel Chiralpak AD-3 column, 5% ^{i}PrOH in ^{n}hexane, 0.5 mL/min, 210 nm, t_r (minor) = 18.8 min, t_r (major) = 19.5 min.



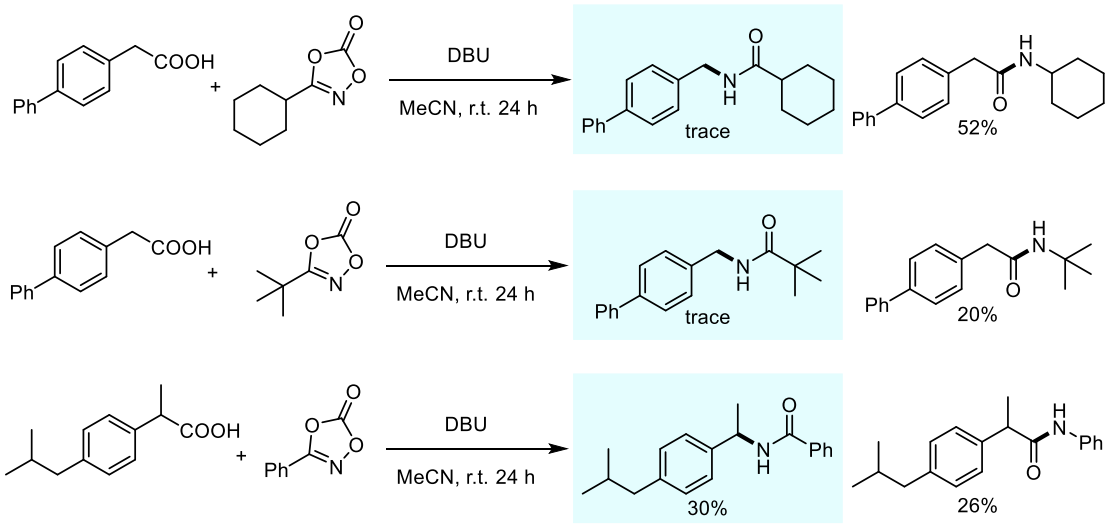
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.271	MM	0.3622	2883.34253	132.69296	50.6570
2	19.990	MM	0.3764	2808.55322	124.37435	49.3430

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.879	MM	0.3646	271.32266	12.40335	2.0463
2	19.552	MM	0.4468	1.29880e4	484.51312	97.9537



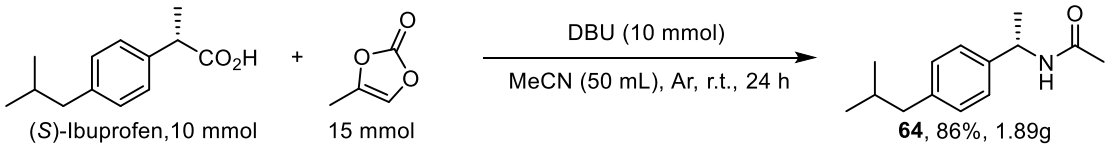
tert-butyl (2*R*,4*R*)-1-([1,1'-biphenyl]-4-yl)-4-acetamidopentan-2-yl)carbamate (70): Following the general procedure with (2*R*,4*S*)-5-([1,1'-biphenyl]-4-yl)-4-((tert-

butoxycarbonyl)amino)-2-methylpentanoic acid as substrate, obtained in 68% yield as white solid (53.9 mg, eluent: petroleum ether/ethyl acetate = 3/1), m.p. = 171-173 °C.
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.59-7.56 (m, 2H), 7.53 (d, J = 8.1 Hz, 2H), 7.43 (t, J = 7.7 Hz, 2H), 7.33 (t, J = 7.2 Hz, 1H), 7.28-7.24 (m, 2H), 5.60 (s, 1H), 4.62 (d, J = 8.4 Hz, 1H), 4.09 (s, 1H), 3.87 (s, 1H), 2.95-2.76 (m, 2H), 1.93 (s, 3H), 1.69-1.59 (m, 2H), 1.40 (s, 9H), 1.16 (d, J = 6.7 Hz, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.7, 155.5, 140.9, 139.4, 137.1, 129.9, 128.8, 127.2, 127.2, 127.0, 79.4, 48.9, 42.8, 41.1, 40.3, 28.4, 23.6, 21.0.
HRMS (ESI): ([M+H]$^+$) calcd for $C_{24}H_{33}N_2O_3^+$: 397.2491; found: 397.2493.

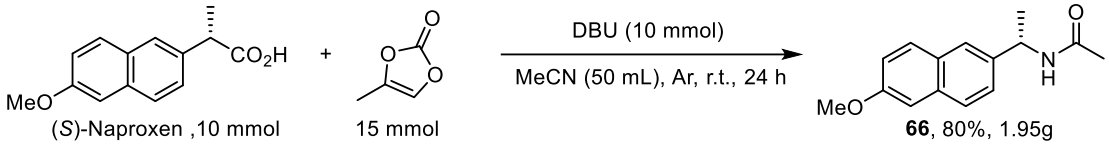


Scheme S1. Unsuccessful examples

3.5 Gram-scale reactions



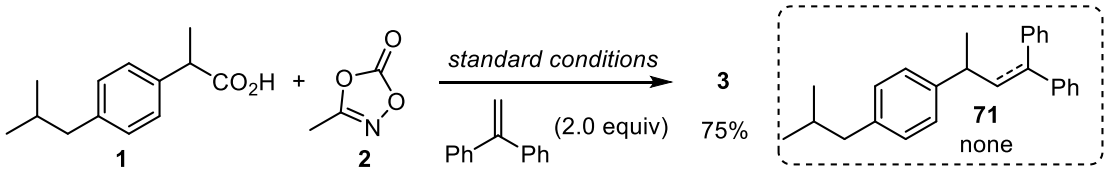
(*S*)-Ibuprofen (2.06 g, 10 mmol, 1.0 equiv) was placed in a transparent Schlenk tube equipped with a stirring bar. The tube was evacuated and filled with argon (repeated for three times). Then DBU (1.52 g, 10 mmol, 1.0 equiv), methyl dioxazolone (1.00 g, 15 mmol, 1.5 equiv), and MeCN (50 mL) was added using a syringe under argon atmosphere. The reaction mixture was stirred at room temperature for 24 h, Then, the reaction mixture was quenched with saturated brine (80 mL) and extracted with ethyl acetate (3 x 50 mL). The combined organic phases were dried over anhydrous Na_2SO_4, and concentrated under vacuo. The residue was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate = 3/1) to afford the product **64** as a white solid (1.89 g, 86%). The *ee* value was determined to be 92%.



(*S*)-Naproxen (2.30 g, 10 mmol, 1.0 equiv) was placed in a transparent Schlenk tube equipped with a stirring bar. The tube was evacuated and filled with argon (repeated for three times). Then DBU (1.52 g, 10 mmol, 1.0 equiv), methyl dioxazolone (1.00 g, 15 mmol, 1.5 equiv), and MeCN (50 mL) was added using a syringe under argon atmosphere. The reaction mixture was stirred at room temperature for 24 h, Then, the reaction mixture was quenched with saturated brine (80 mL) and extracted with ethyl acetate (3 x 50 mL). The combined organic phases were dried over anhydrous Na_2SO_4, and concentrated under vacuo. The residue was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate = 3/1) to afford the product **66** as a white solid (1.95 g, 80%). The *ee* value was determined to be 97%.

4. Mechanistic experiments

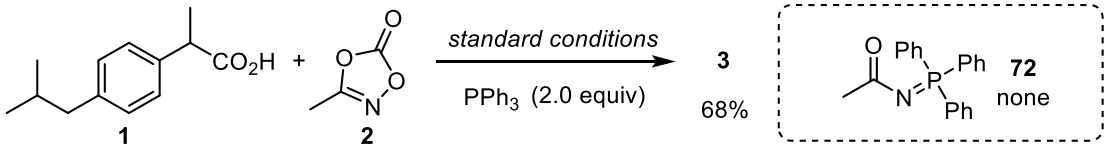
4.1 Control experiments



Control experiment utilizing 1,1-diphenylethylene as a radical scavenger was conducted. 2 equivalents of 1,1-diphenylethylene were added to the model reaction under the standard conditions.

Ibuprofen **1** (0.2 mmol, 1.0 equiv) was placed in a transparent Schlenk tube equipped with a stirring bar. The tube was evacuated and filled with argon (repeated for three times). Then DBU (0.2 mmol, 1.0 equiv), methyl dioxazolone **2** (0.3 mmol, 1.5 equiv), 1,1-diphenylethylene (0.4 mmol, 2.0 equiv) and MeCN (2 mL) was added using a syringe under argon atmosphere. The reaction mixture was stirred at room temperature for 24 h, Then, the reaction mixture was quenched with saturated brine and extracted with ethyl acetate (3 x 10 mL). The combined organic phases were dried over anhydrous Na_2SO_4 and tridecane was added as an internal standard.

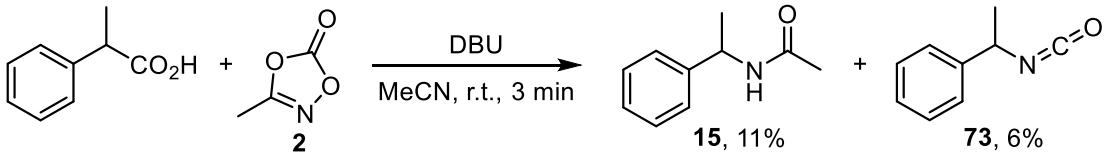
GC analysis showed that the yield of the decarboxylative amidation product **3** was 75%. And no decarboxylated adduct **71** of ibuprofen and 1,1-diphenylethylene was observed in the GC-MS test. These results indicate that the reaction is unlikely to undergo a radical decarboxylation process.



Dioxazolone, as a convenient class of acyl nitrene transfer reagent, can easily generate acyl nitrene under the action of metal.[3] In order to explore whether acyl nitrene was produced during the reaction, triphenylphosphine was added to the reaction under the standard conditions.

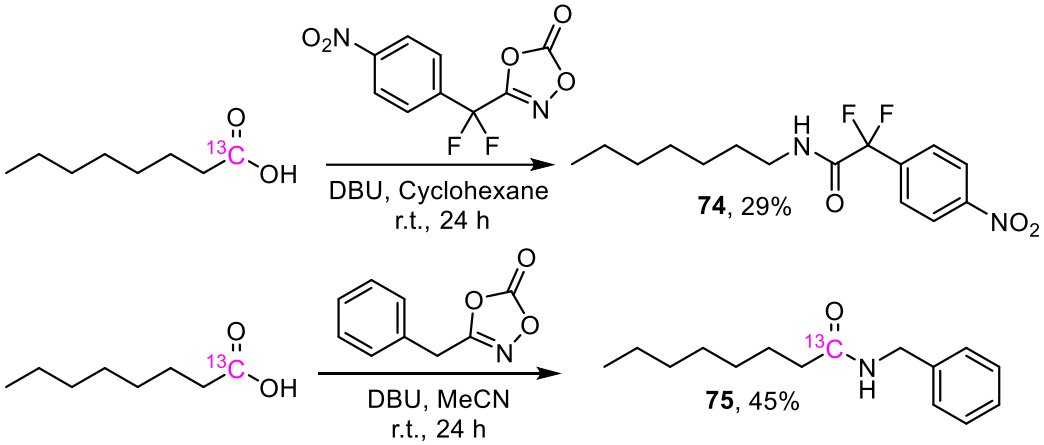
Ibuprofen **1** (0.2 mmol, 1.0 equiv) and PPh_3 (0.4 mmol, 2.0 equiv) were placed in a transparent Schlenk tube equipped with a stirring bar. The tube was evacuated and filled with argon (repeated for three times). Then DBU (0.2 mmol, 1.0 equiv), methyl dioxazolone **2** (0.3 mmol, 1.5 equiv), and MeCN (2 mL) was added using a syringe under argon atmosphere. The reaction mixture was stirred at room temperature for 24 h, Then, the reaction mixture was quenched with saturated brine and extracted with ethyl acetate (3 x 10 mL). The combined organic phases were dried over anhydrous Na_2SO_4 and tridecane was added as an internal standard.

GC analysis showed that the yield of the decarboxylative amidation product **3** was 68%. And no iminophosphorane **72** was observed in the GC-MS test. These results indicate that the reaction may not involve acyl nitrene intermediate.



2-Phenylpropionic acid (0.2 mmol, 1.0 equiv) was placed in a transparent Schlenk tube equipped with a stirring bar. The tube was evacuated and filled with argon (repeated for three times). Then DBU (0.2 mmol, 1.0 equiv), methyl dioxazolone **2** (0.3 mmol, 1.5 equiv), and MeCN (2 mL) was added using a syringe under argon atmosphere. The reaction mixture was stirred at room temperature for 3 minutes, Then, the reaction mixture was diluted rapidly with ethyl acetate (20 mL). The corresponding product **15** and (1-isocyanatoethyl)benzene **73** could been observed by GC-MS analysis.

4.2 Isotopic labelling examples



3-(difluoro(4-nitrophenyl)methyl)-1,4,2-dioxazol-5-one (0.3 mmol, 1.5 equiv) was placed in a transparent Schlenk tube equipped with a stirring bar. The tube was evacuated and filled with argon (repeated for three times). Then DBU (0.2 mmol, 1.0 equiv), commercially available octanoic acid-1-^{13}C (0.2 mmol, 1.0 equiv), and MeCN (2 mL) was added using a syringe under argon atmosphere. The reaction mixture was stirred at room temperature for 24 h, Then, the reaction mixture was quenched with saturated brine and extracted with ethyl acetate (3 x 10 mL). The combined organic phases were dried over anhydrous Na_2SO_4, and concentrated under vacuo. The residue was purified by flash column chromatography on silica gel to afford the product **74** in 29% yield (18.2 mg).

2,2-difluoro-*N*-heptyl-2-(4-nitrophenyl)acetamide (74), colorless oil.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.31 (d, J = 8.5 Hz, 2H), 7.83 (d, J = 8.8 Hz, 2H), 6.54 (br s, 1H), 3.34 (q, J = 7.0 Hz, 2H), 1.57 (p, J = 7.2 Hz, 2H), 1.34-1.23 (m, 8H), 0.88 (t, J = 6.9 Hz, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 162.9 (t, J = 29.8 Hz), 149.4, 139.1 (t, J = 25.8 Hz), 127.1 (t, J = 6.1 Hz), 123.7, 113.9 (t, J = 254.8 Hz), 39.9, 31.6, 29.2, 28.8, 26.7, 22.5, 14.0.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -103.49.

HRMS (ESI): ([M+H]$^+$) calcd for $C_{15}H_{21}F_2N_2O_3^+$: 315.1515; found: 315.1512.

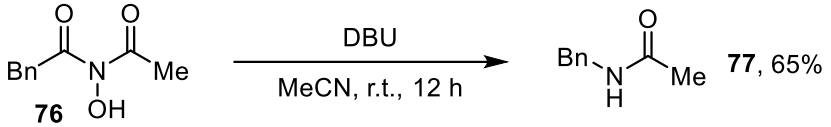
3-benzyl-1,4,2-dioxazol-5-one (0.3 mmol, 1.5 equiv) was placed in a transparent Schlenk tube equipped with a stirring bar. The tube was evacuated and filled with argon (repeated for three times). Then DBU (0.2 mmol, 1.0 equiv), commercially available octanoic acid-1-^{13}C (0.2 mmol, 1.0 equiv), and MeCN (2 mL) was added using a syringe under argon atmosphere. The reaction mixture was stirred at room temperature for 24 h, Then, the reaction mixture was quenched with saturated brine and extracted with ethyl acetate (3 x 10 mL). The combined organic phases were dried over anhydrous Na_2SO_4, and concentrated under vacuo. The residue was purified by flash column chromatography on silica gel to afford the product **75** in 45% yield as white solid (21.1 mg).

***N*-benzyloctanamide-1-^{13}C (75)**, m.p. = 63-64 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.35-7.31 (m, 2H), 7.30-7.24 (m, 3H), 5.92 (br s,

1H), 4.42 (dd, J = 5.8, 3.0 Hz, 2H), 2.23-2.17 (m, 2H), 1.68-1.60 (m, 2H), 1.34-1.22 (m, 8H), 0.87 (t, J = 6.9 Hz, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 173.1 (^{13}C enriched), 138.5, 128.7, 127.8, 127.5, 43.6, 36.8 (d, *J* = 50.1 Hz), 31.7, 29.3 (d, *J* = 3.3 Hz), 29.0, 25.8 (d, *J* = 1.9 Hz), 22.6, 14.1.
HRMS (ESI): ([M+H]$^+$) calcd for $C_{14}{}^{13}CH_{24}NO^+$: 235.1886; found: 235.1890.

4.3 Intermediate verification experiment

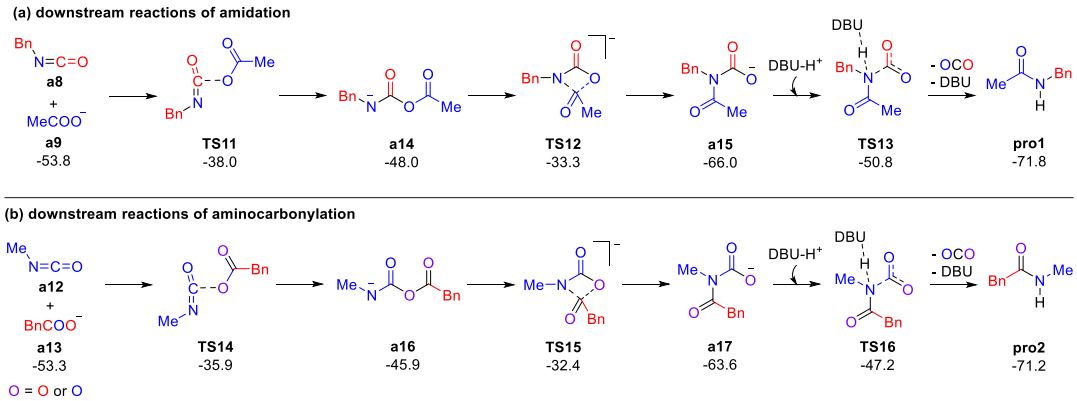


N-acetyl-*N*-hydroxy-2-phenylacetamide **76** was prepared following reported procedure.[4] **76** (0.2 mmol), DBU (0.3 mmol), and MeCN (2 mL) was placed in a transparent Schlenk tube equipped with a stirring bar. The reaction mixture was stirred at room temperature for 12 h, Then, the reaction mixture was quenched with saturated brine and extracted with ethyl acetate (3 x 10 mL). The combined organic phases were dried over anhydrous Na_2SO_4, and concentrated under vacuo. The residue was purified by flash column chromatography on silica gel to afford the product **77** in 65% yield as white solid (19.4 mg). The compound data was in agreement with the literature (Ref: *ACS Catal.* **2022**, *12*, 809-817).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.35-7.32 (m, 2H), 7.30-7.27 (m, 3H), 5.77 (br s, 1H), 4.43 (d, J = 5.6 Hz, 2H), 2.03 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.0, 138.2, 128.8, 127.9, 127.6, 43.8, 23.3.

5. DFT studies

All density functional theory (DFT) calculations were performed with Gaussian09 program,[5] M06-2X method,[6] SMD solvation model[7] (solvent = acetonitrile) associated with a (99,590) grid. Geometry optimization, frequency analysis and intrinsic reaction coordinate (IRC) analysis[8] were performed with 6-31G(d) basis set while solution-phase single-point energy calculation was performed with 6-311++G(d,p) basis set based on the solution-phase optimized structures. No imaginary frequency was found for energetic minima while only one imaginary frequency was found for transition states. IRC analysis was performed to ensure that the optimized transition states connect with correct intermediates. The thermodynamic correction to Gibbs free energy (ΔG_{cor}), solution-phase single-point energy (ΔE_{sol}) and an extra 1.89 kcal/mol which accounts for the standard state change from 1 atm. to 1 M at 298.15 K[9] were added up to get the solution-phase Gibbs free energy of every species (ΔG_{sol}) referring to 1 M and 298.15 K except for CO_2. Natural population atomic (NPA) charge was calculated at the level of M06-2X/6-31G(d) with the NBO 3.1 implemented in Gaussian 09.[10]

The mole fraction of CO_2 in propanenitrile (data in acetonitrile was not available) is $1.69*10^{-2}$ at 298.15 K and a partial CO_2 pressure of 101.3 kPa,[11] and was used to estimate the concentration of CO_2 in acetonitrile. Assuming that the partial pressure of CO_2 in the atmosphere is 0.03 atm. and the Henry's law is obeyed, the mole fraction of CO_2 should be $5.07*10^{-4}$ ($1.69*10^{-2}*0.03$). Based on the density of acetonitrile 0.777g/cm^3 at 298 K,[12] the concentration of CO_2 should be $9.59*10^{-3}$ M. Considering the standard state change from 1 M to $9.59*10^{-3}$ M at 298.15 K and the equation $\Delta G = \Delta G^o + RTln(C/C^o)$, an extra energy of 2.75 kcal/mol was subtracted from the calculated standard Gibbs free energy of CO_2 ($\Delta G_{cor} + \Delta E_{sol}$ + 1.89 kcal/mol − 2.75 kcal/mol).



Scheme S2. Calculated relative solution-phase Gibbs free energies for the downstream transformations of (a) benzyl isocyanate and acetate, and (b) that of methyl isocyanate and phenylacetate (in kcal/mol).

Table S3. Calculated thermodynamic corrections to Gibbs free energy (ΔG_{cor}), solution-phase single-point energies (ΔE_{sol}), solution-phase Gibbs free energies

(ΔG_{sol}) and imaginary frequencies (ImF, in cm^{-1}). All ΔG_{sol} refer to 1 M and 298.15 K except the ΔG_{sol} of CO_2 refers to $9.59*10^{-3}$ M and 298.15 K (in Hartree).

species	ΔG_{cor}	ΔE_{sol}	ΔG_{sol}	ImF
a1	0.110185	-460.092551	-459.979354	N.A.
DBU	0.214295	-462.017797	-461.800490	N.A.
a2	0.097860	-459.616662	-459.515790	N.A.
DBU-H^+	0.228420	-462.500129	-462.268697	N.A.
2	0.038671	-396.487413	-396.445730	N.A.
TS1	0.156012	-856.103533	-855.944509	-167.13
a3	0.156619	-856.105820	-855.946189	N.A.
TS2	0.156535	-856.099082	-855.939535	-214.59
a4	0.152278	-856.108637	-855.953347	N.A.
TS3	0.148221	-856.071539	-855.920306	-663.90
TS4	0.159639	-856.100420	-855.937769	-171.31
a5	0.155830	-856.140984	-855.982143	N.A.
TS5	0.153387	-856.106514	-855.950115	-27.84
CO_2	-0.008937	-188.575220	-188.585528	N.A.
a6	0.147216	-667.527955	-667.377727	N.A.
TS6	0.144880	-667.501738	-667.353846	-224.73
a7	0.145272	-667.544297	-667.396013	N.A.
TS7	0.139472	-667.496019	-667.353535	-666.86
a8	0.098501	-438.987387	-438.885874	N.A.
a9	0.022533	-228.596821	-228.571276	N.A.
TS8	0.144863	-667.502662	-667.354787	-217.40
a10	0.145154	-667.505399	-667.357233	N.A.
TS9	0.145127	-667.505466	-667.357328	-68.43
a11	0.147064	-667.545713	-667.395637	N.A.
TS10	0.140983	-667.493042	-667.349047	-687.77
a12	0.024264	-207.967822	-207.940547	N.A.
a13	0.097860	-459.616662	-459.515790	N.A.
TS11	0.141252	-667.576209	-667.431945	-206.74
a14	0.145707	-667.596498	-667.447779	N.A.
TS12	0.148115	-667.575572	-667.424445	-237.24
a15	0.149105	-667.628661	-667.476544	N.A.
TS13	0.389820	-1130.113877	-1129.721045	-230.37
pro1	0.149066	-479.520606	-479.368528	N.A.
TS14	0.142294	-667.573846	-667.428541	-243.09
a16	0.145121	-667.592554	-667.444421	N.A.
TS15	0.146113	-667.572087	-667.422962	-220.49
a17	0.148563	-667.624240	-667.472665	N.A.
TS16	0.393470	-1130.111822	-1129.715340	-241.23
pro2	0.147807	-479.518357	-479.367538	N.A.

Cartesian coordinates of calculated stationary points (in angstrom)

a1

C	2.14737900	-0.10636900	-0.17288900
O	1.89500500	-0.92646800	-1.02205100
C	1.15201500	0.60640800	0.71661200
H	1.38413900	0.30495700	1.74576700
H	1.35857600	1.67971500	0.65512600
C	-0.28253900	0.30536600	0.37463300
C	-0.79812300	-0.98145600	0.56135500
C	-1.12088400	1.30303600	-0.12458400
C	-2.12591100	-1.26359000	0.25454100
H	-0.15138200	-1.76374200	0.95064500
C	-2.45271300	1.02418800	-0.43227200
H	-0.72845800	2.30619000	-0.27120400
C	-2.95798800	-0.25973100	-0.24358900
H	-2.51389200	-2.26658700	0.40567000
H	-3.09331700	1.81167200	-0.81805500
H	-3.99458300	-0.47907400	-0.48104100
O	3.40109900	0.28260400	0.10884100
H	4.00267300	-0.20933600	-0.48407700

DBU

C	0.92579800	1.47001300	-0.40771500
C	-0.36857700	0.71987600	-0.13690600
C	2.07891800	1.15805500	0.55617300
C	0.84974200	-1.45486000	0.27519400
C	2.94821500	-0.00239700	0.06783500
C	2.11239900	-1.13957700	-0.52556800
H	1.24744900	1.28603400	-1.44091800
H	1.06194000	-1.39735100	1.35502900
H	1.66835800	0.92969400	1.54734200
H	3.55032400	-0.38304600	0.90117800
H	0.65174000	2.52431800	-0.34522400
H	2.69755100	2.05253500	0.68121700
H	0.56528200	-2.49097300	0.07162700
H	3.65169400	0.35788300	-0.69210000
H	2.72033600	-2.04922900	-0.57139400
H	1.81854100	-0.91233300	-1.55639200
N	-0.33994600	-0.66177000	-0.05966100
C	-1.58391600	-1.34771200	0.29109300
H	-1.52570800	-2.36731200	-0.10295800
H	-1.68395600	-1.42343200	1.38511600
C	-2.77649700	-0.61273700	-0.29260700
H	-3.70597700	-1.09824600	0.01897700
H	-2.72574400	-0.65042100	-1.38701000
C	-2.72061000	0.83294900	0.17679300
H	-2.95533500	0.88292700	1.24978900
H	-3.48307600	1.43322700	-0.33273900
N	-1.42380500	1.45663500	-0.05566700

a2

C	-2.26628200	-0.09008000	0.14922400
O	-2.11731300	-1.29872900	0.43852900
C	-1.21251000	0.50308200	-0.85010300
H	-1.39886000	0.02055900	-1.81895100
H	-1.39323200	1.57473100	-0.96883100
C	0.21351400	0.25931800	-0.43888200
C	0.74601500	-1.03780300	-0.41868100
C	1.04150900	1.31667100	-0.04646400
C	2.06136600	-1.26537700	-0.02390900
H	0.10277700	-1.86554000	-0.69794300
C	2.35972600	1.09321700	0.35284300
H	0.64715900	2.33038800	-0.05681200
C	2.87657600	-0.20017900	0.36408100
H	2.45494000	-2.27829700	-0.01868600
H	2.98227300	1.93204900	0.65165600
H	3.90342600	-0.37841600	0.66957900
O	-3.15993300	0.69765800	0.52538800

DBU-H^+

C	0.93665900	1.50297500	-0.25076000
C	-0.30623500	0.66632900	-0.05207200
C	2.13705500	1.09481800	0.60859100
C	0.90858800	-1.49997600	0.22762800
C	2.96376300	-0.01007100	-0.04784400
C	2.07466900	-1.08976900	-0.66516300
H	1.19508000	1.47836800	-1.31615900
H	1.21758800	-1.56610600	1.27793100
H	1.78321400	0.77342600	1.59496400
H	3.62746100	-0.45862200	0.69916300
H	0.65030200	2.53235200	-0.02501000
H	2.75780100	1.97924900	0.77618100
H	0.56671400	-2.49113400	-0.07299000
H	3.60114200	0.41871000	-0.82903200
H	2.66762000	-1.98862800	-0.85946600
H	1.67748500	-0.76760600	-1.63445500

N	-0.29672700	-0.64392600	0.14360200
C	-1.56746600	-1.33349000	0.44210300
H	-1.44322400	-2.38008500	0.16379800
H	-1.74813700	-1.28265800	1.52178600
C	-2.71351700	-0.70634500	-0.33300600
H	-3.64904700	-1.20362200	-0.06947900
H	-2.54264200	-0.83598000	-1.40614500
C	-2.79192200	0.76763600	0.01045300
H	-3.17253400	0.91606800	1.02570200
H	-3.43370500	1.31202200	-0.68444700
N	-1.44956700	1.33964900	-0.08371000
H	-1.38061700	2.34154400	-0.22117000

2

C	0.98144400	0.01976000	0.00014500
O	-0.02208100	-0.89556600	-0.00004200
C	-1.18372300	-0.18177700	0.00012400
O	-0.84355600	1.11999800	0.00002900
N	0.56244300	1.22937100	-0.00009900
C	2.38290900	-0.44332100	-0.00001800
H	2.56845100	-1.05292800	0.88836400
H	2.56820600	-1.05306600	-0.88835800
H	3.04738200	0.42097700	-0.00018600
O	-2.28497600	-0.63550200	-0.00006500

TS1

C	-3.76317000	-0.44521500	0.33996900
O	-3.37119700	-0.16883700	-0.91071000
C	-2.41555500	0.87349500	-0.77326100
O	-2.60823400	1.33816000	0.51634600
N	-3.35224000	0.38162900	1.22856800
C	-4.61440400	-1.63122300	0.59148400
H	-5.52967300	-1.56725100	-0.00368700
H	-4.07946600	-2.53983600	0.30054500
H	-4.87102800	-1.68138900	1.65052000
O	-2.09619400	1.57335500	-1.69962300
C	0.08408200	0.08135400	0.01843300
O	0.37766500	1.25579900	0.23256700
C	1.10886200	-1.04088800	0.31820600
H	0.89403400	-1.37241100	1.34302000
H	0.90232400	-1.88894100	-0.33975500
C	2.54614500	-0.61490900	0.20533100
C	3.09647600	0.29780600	1.11375600
C	3.36225300	-1.10930200	-0.81576700
C	4.42469600	0.70012200	1.00539800
H	2.46916100	0.69456300	1.90632300
C	4.69362900	-0.70775500	-0.93037500
H	2.94895800	-1.81869800	-1.52896600
C	5.22978000	0.19877400	-0.01909300
H	4.83509000	1.40636900	1.72172500
H	5.31044900	-1.10576000	-1.73116800
H	6.26639100	0.51153900	-0.10289800
O	-1.03531400	-0.38138200	-0.40556000

a3

C	-3.75512400	0.63097800	0.06323600
O	-3.33578100	-0.41680900	0.76513700
C	-2.22073200	-1.00794300	-0.04163200
O	-2.46446900	-0.38265400	-1.31284600
N	-3.28814100	0.74285400	-1.12662900
C	-4.72367100	1.57742000	0.67481400
H	-5.63183400	1.04330700	0.97015600
H	-4.29292700	2.03083700	1.57239200
H	-4.98104500	2.36034500	-0.04045400
O	-2.06563400	-2.22134900	0.01012000
C	0.11189300	-0.23236400	0.02703700
O	0.41078100	-0.85511000	-0.96939900
C	1.09770800	0.63761600	0.81009100
H	0.79232000	1.67807300	0.64008300
H	0.95278200	0.44164500	1.87659400
C	2.53508600	0.43654400	0.41535400
C	2.98449700	0.82520300	-0.85163900
C	3.44657500	-0.14130900	1.30116900
C	4.31392000	0.64353600	-1.22145000
H	2.28214600	1.27352000	-1.54931000
C	4.78025800	-0.32568500	0.93518500
H	3.10864800	-0.44796300	2.28807900
C	5.21752300	0.06642800	-0.32753200
H	4.64744600	0.95332700	-2.20764900
H	5.47567600	-0.77466500	1.63837900
H	6.25536500	-0.07390200	-0.61472600
O	-1.08479500	-0.16745800	0.58262000

TS2

C	-3.54198300	-0.82907900	-0.07825900
O	-3.55263900	0.16435700	-0.87427700
C	-2.16237300	1.18805700	0.09372700
O	-2.50415200	0.57493600	1.25240600

N	-2.94162900	-0.78841500	1.08770200
C	-4.19648800	-2.12830400	-0.45897900
H	-5.25813900	-1.95686200	-0.66130400
H	-3.74296600	-2.51516000	-1.37653100
H	-4.09710200	-2.87016400	0.33623600
O	-2.25397800	2.37609700	-0.07470200
C	0.07665000	0.46172300	-0.06053900
O	0.37438300	1.08592800	0.92819400
C	1.00465200	-0.44277400	-0.85225600
H	0.61412400	-1.46112800	-0.72949900
H	0.89504000	-0.19498900	-1.91249400
C	2.44429400	-0.36307600	-0.42072100
C	2.82516000	-0.78442600	0.85790900
C	3.42289700	0.12161000	-1.28995900
C	4.15716100	-0.72286700	1.25664100
H	2.06922400	-1.16250700	1.54121600
C	4.75931000	0.18357500	-0.89443000
H	3.13575700	0.45005100	-2.28573900
C	5.12939600	-0.23846400	0.38002600
H	4.43906800	-1.05436100	2.25170000
H	5.50894900	0.56085900	-1.58371400
H	6.16905800	-0.19256000	0.69006800
O	-1.14532200	0.45366600	-0.61697300

a4

C	0.44951300	0.70815900	0.16244100
O	-0.58112300	1.40973300	0.69962500
C	-1.77725200	1.37177100	-0.03799700
O	0.35381100	0.11499700	-0.87975100
O	-2.41791600	0.29065600	0.29174100
O	-2.07080700	2.27497900	-0.76925100
C	1.66701100	0.80392000	1.05173700
H	1.38610300	0.36297100	2.01613100
H	1.85814200	1.86566900	1.23848800
C	2.87738600	0.12250800	0.47132600
C	2.91438700	-1.27086200	0.35744900
C	3.97569500	0.86675900	0.03922300
C	4.03019400	-1.90735600	-0.17808100
H	2.06155900	-1.85639800	0.69218700
C	5.09633100	0.23183200	-0.49653900
H	3.95394500	1.95025100	0.12459500
C	5.12563400	-1.15622200	-0.60653000
H	4.04702700	-2.99011000	-0.25969600
H	5.94510700	0.82336900	-0.82655200
H	5.99732100	-1.65222300	-1.02268400
N	-3.70216900	0.16157300	-0.39616700
C	-4.25666800	-0.96423200	0.05625400
C	-5.61167500	-1.18643800	-0.61134900
H	-5.86561500	-0.40238200	-1.32848200
H	-5.60361000	-2.15317200	-1.12473100
H	-6.38752400	-1.23134100	0.15980000
O	-3.83654100	-1.78619900	0.88970100

TS3

C	-0.59166100	-0.55616900	0.23756600
O	0.41255300	-1.26235900	0.74537500
C	1.69487000	-1.14195600	0.00806500
O	-0.50663800	0.12376300	-0.76163800
O	2.35699400	-0.17932400	0.44132100
O	1.88282300	-2.01119400	-0.81735500
C	-1.84187300	-0.70769500	1.09047100
H	-1.61655400	-0.23152100	2.05311600
H	-1.98339600	-1.77280300	1.29718500
C	-3.07491500	-0.10613200	0.47180900
C	-3.17903600	1.27877700	0.30298600
C	-4.13426000	-0.91579400	0.05889800
C	-4.31862600	1.84065700	-0.26499500
H	-2.35793500	1.91642000	0.62016900
C	-5.27887800	-0.35662400	-0.51011000
H	-4.06269000	-1.99314100	0.18637700
C	-5.37358400	1.02310900	-0.67363600
H	-4.38569200	2.91759100	-0.38863200
H	-6.09512600	-1.00065500	-0.82388300
H	-6.26360200	1.46129300	-1.11528300
N	4.14988000	-0.07368900	-0.52809700
C	4.71682500	0.83052300	0.14233100
C	6.00192000	0.61758300	-0.89025600
H	5.97912600	-0.11725800	-1.69182700
H	6.11140000	1.62008600	-1.30754700
H	6.80172000	0.37623500	-0.18784600
O	4.74163000	1.64185300	1.04430600

TS4

C	-0.43469700	-0.93389000	0.06641900
O	-1.72257800	-1.32319300	-0.54757600
C	-2.76362600	-1.03825400	0.22868200
O	-0.08261200	-1.59611400	1.02074900
O	-2.54922600	0.01519500	1.03954300

O	-3.81228700	-1.63105400	0.22098300
C	0.49204800	-0.45672700	-1.04046400
H	0.08731000	0.43935900	-1.51389600
H	0.50132800	-1.26144800	-1.78588300
C	1.88905600	-0.22308900	-0.52360000
C	2.22222900	0.98010200	0.10730500
C	2.86432600	-1.21673900	-0.64020700
C	3.50763500	1.18335400	0.60626300
H	1.45893500	1.74968000	0.19145600
C	4.15128100	-1.01446000	-0.14406300
H	2.61227600	-2.15580800	-1.12725900
C	4.47672800	0.18803000	0.48157300
H	3.75508700	2.12308600	1.09219000
H	4.89933900	-1.79541000	-0.24655700
H	5.47906100	0.34893600	0.86754800
N	-1.30825500	0.66058400	0.72634000
C	-1.54984500	1.76289600	-0.04496000
C	-2.97972900	2.16265300	-0.35751100
H	-3.56904900	2.28314700	0.55484500
H	-2.95786700	3.10044400	-0.91362100
H	-3.47240100	1.39483200	-0.96440100
O	-0.60382200	2.43325900	-0.46894900

a5

C	-0.21298000	0.67756700	0.01012300
N	-1.57344800	0.56010200	0.31017600
O	0.25428700	1.65688800	-0.52765400
C	0.61888100	-0.52591500	0.43924700
H	0.39811900	-0.74011500	1.48987200
H	0.26817900	-1.38929600	-0.13679100
C	2.09218700	-0.30548400	0.22445600
C	2.79574300	0.59899100	1.02698200
C	2.78294200	-1.00103600	-0.76886200
C	4.16017500	0.80088300	0.84210800
H	2.26545200	1.14576000	1.80316200
C	4.15112800	-0.80274400	-0.95743000
H	2.24589500	-1.70692000	-1.39753600
C	4.84306000	0.09865400	-0.15248200
H	4.69306800	1.50490000	1.47454600
H	4.67438300	-1.35450200	-1.73285300
H	5.90820300	0.25368200	-0.29605900
C	-2.59004300	1.40539900	-0.15468000
O	-2.35750900	2.43818100	-0.74503000
C	-3.98810500	0.92965000	0.15570600
H	-4.10531100	0.70470900	1.21793300
H	-4.68101100	1.71602700	-0.14403800
H	-4.20229200	0.01743600	-0.40916500
O	-1.97442800	-0.60129300	0.92295600
C	-2.28165200	-1.71229900	-0.03618800
O	-2.62821200	-2.70277200	0.59353500
O	-2.12895900	-1.42280500	-1.22058000

TS5

C	0.76474800	-0.95727100	0.17981800
N	2.01897600	-0.49068800	0.54592500
O	0.49663200	-1.51183900	-0.87728500
C	-0.28227100	-0.69742100	1.26433800
H	-0.20559200	-1.51570600	1.99264600
H	0.01289500	0.20713100	1.79980100
C	-1.67399500	-0.60082000	0.70292000
C	-2.33241200	-1.72534900	0.19201200
C	-2.33455200	0.63077200	0.66811000
C	-3.61674800	-1.62109500	-0.33496900
H	-1.82761700	-2.68702200	0.21004600
C	-3.62101900	0.74131200	0.13932800
H	-1.83793900	1.51325100	1.06707000
C	-4.26611700	-0.38565700	-0.36392700
H	-4.11416200	-2.50471500	-0.72467200
H	-4.11772800	1.70718700	0.12461400
H	-5.26863800	-0.30494000	-0.77350200
C	3.05178400	-0.31892800	-0.36793800
O	3.00227400	-0.62117300	-1.55390800
C	4.27317800	0.31541900	0.25594500
H	4.65952800	-0.31330700	1.06225400
H	5.02946300	0.45317200	-0.51872800
H	4.00466400	1.27127700	0.71332200
O	2.22033300	-0.09815700	1.82324000
C	0.41675300	1.88971600	-0.75838300
O	0.78930700	2.33115000	0.25223800
O	0.03414300	1.48422000	-1.77906200

CO_2

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16286800
O	0.00000000	0.00000000	-1.16286800

a6

C	-0.83951000	-1.09687100	0.18648900

N	-1.68206300	-0.00692100	0.34178600
O	-0.99257500	-1.99967100	-0.62506800
C	0.35912300	-1.08492100	1.13012500
H	0.06836700	-0.60059300	2.06363400
H	0.63146200	-2.12882200	1.30545700
C	1.52582300	-0.35666200	0.49642100
C	1.42226100	1.00464700	0.17533400
C	2.70999900	-1.03379900	0.19385900
C	2.48987600	1.66713600	-0.42531000
H	0.48661000	1.50801000	0.41917700
C	3.77937800	-0.36782200	-0.40607500
H	2.79659300	-2.09129300	0.43151100
C	3.67305700	0.98574400	-0.71698000
H	2.40070400	2.72252900	-0.66879300
H	4.69376400	-0.90940500	-0.63148600
H	4.50385300	1.50599700	-1.18462800
C	-2.82731600	0.17823000	-0.42588500
O	-3.20512300	-0.56847300	-1.31869500
C	-3.58695800	1.42764200	-0.04472600
H	-3.86266800	1.39585500	1.01226200
H	-2.95286100	2.30895500	-0.17044900
H	-4.47578400	1.49970900	-0.67374600
O	-1.39605000	0.93034000	1.28439300

TS6

C	0.80812500	-1.18120600	-0.01943600
N	1.58847100	-0.21500200	0.54137400
O	0.67875400	-2.31828500	0.41591200
C	-0.06567100	-0.64699500	-1.15232400
H	0.45636200	0.15228300	-1.68545300
H	-0.23746400	-1.47763700	-1.84285300
C	-1.37755800	-0.14601200	-0.59506200
C	-1.60249600	1.22085700	-0.41104200
C	-2.36994400	-1.05146400	-0.20533500
C	-2.79982000	1.67669500	0.13819700
H	-0.83218100	1.93085100	-0.70346100
C	-3.56672700	-0.59912700	0.34554800
H	-2.19443800	-2.11621800	-0.33521200
C	-3.78629800	0.76762700	0.51740900
H	-2.96209100	2.74262000	0.26946000
H	-4.32982600	-1.31385300	0.63987200
H	-4.72052400	1.12154700	0.94286700
C	2.56214000	0.54662100	-0.15902700
O	3.02232300	0.21194200	-1.24903200
C	2.81845700	1.91163200	0.43658000
H	2.44132600	1.98384700	1.45632500
H	3.89151300	2.12157200	0.42592700
H	2.32654500	2.66620100	-0.18890600
O	2.71395300	-0.55590200	1.31546700

a7

C	-0.79252100	-1.65487800	0.11047600
N	-1.03956300	-0.36808500	-0.10095600
O	-1.56810400	-2.62550500	0.19067800
C	0.71747300	-1.93256300	0.28358800
H	0.82705000	-2.38262100	1.27767900
H	0.97024100	-2.71501700	-0.44081200
C	1.65613100	-0.76503300	0.13554200
C	1.86844200	0.12246600	1.19743800
C	2.32294200	-0.52715400	-1.06966000
C	2.72030200	1.21498100	1.05940300
H	1.35382400	-0.04819700	2.14056500
C	3.17913800	0.56431500	-1.21386600
H	2.17011800	-1.20835800	-1.90370200
C	3.38015600	1.44091400	-0.14955600
H	2.87226700	1.89098900	1.89615600
H	3.69023600	0.72827400	-2.15837800
H	4.04763500	2.29054300	-0.25828500
C	-2.90814000	1.03097000	-0.14562300
O	-4.09333700	1.25165800	-0.31557500
C	-1.91228800	2.11287400	0.18678000
H	-1.39040300	1.88034800	1.11840100
H	-1.14871200	2.18096400	-0.59221900
H	-2.44806500	3.05833800	0.27411300
O	-2.47069100	-0.21865400	-0.25184500

TS7

C	0.39205100	1.15949200	0.23678300
N	1.07607100	0.27567600	0.79673200
O	0.12960800	2.02423800	-0.56365400
C	-0.78635000	0.67392300	1.44221800
H	-0.49482500	0.02284500	2.26248600
H	-0.97008800	1.68089200	1.82609800
C	-1.91174500	0.11706400	0.64141400
C	-2.06207600	-1.26795200	0.50428500
C	-2.80671600	0.96672500	-0.01824300
C	-3.09648700	-1.79388000	-0.26400300
H	-1.36074500	-1.93095900	1.00516500

C	-3.84345800	0.44075100	-0.78611300
H	-2.68652200	2.04219500	0.07705900
C	-3.99111600	-0.93999700	-0.91051200
H	-3.20632800	-2.87012300	-0.35824700
H	-4.53656900	1.10970500	-1.28757100
H	-4.79977000	-1.34988700	-1.50812800
C	3.65396400	-0.45346900	-0.13994600
O	3.57364800	-1.39339200	0.66227100
C	4.92091000	-0.32692900	-1.00606600
H	4.65278100	-0.37456500	-2.06667000
H	5.39537200	0.64544700	-0.83820200
H	5.63482300	-1.12178600	-0.77865100
O	2.79993300	0.46442200	-0.36228900

a8

C	-2.52885300	-0.32371300	-0.29614000
N	-2.18322700	0.70380600	0.21404100
O	-2.99297400	-1.29671100	-0.77261900
C	-0.97063700	1.41727700	0.56265200
H	-0.95803800	2.35622800	0.00340200
H	-1.04071000	1.67183700	1.62477900
C	0.29039200	0.62743100	0.28692900
C	1.32713300	1.19782600	-0.45108900
C	0.43765700	-0.67132300	0.78405900
C	2.50036000	0.48186000	-0.69001900
H	1.21440300	2.20548500	-0.84267000
C	1.60547000	-1.38858000	0.54182300
H	-0.36371100	-1.12196200	1.36579900
C	2.64061200	-0.81250600	-0.19606300
H	3.30007200	0.93514000	-1.26792800
H	1.71020200	-2.39669500	0.93136700
H	3.55134200	-1.37261400	-0.38498900

a9

C	-0.20444400	0.00069400	-0.00006500
O	-0.81068900	-1.09563400	0.00001400
C	1.34475000	-0.05615400	-0.00001900
H	1.73716600	0.46980800	-0.87817200
H	1.73674000	0.46688600	0.88008000
H	1.72165900	-1.08257000	-0.00158400
O	-0.69398600	1.15546300	0.00000800

TS8

C	0.88556200	-0.31621700	0.09823200
N	2.03876000	0.08705700	-0.62960300
O	0.84947900	-0.39663700	1.32466400
C	-0.23158500	-0.85340700	-0.77997800
H	-0.03855700	-0.56186500	-1.81565400
H	-0.19416500	-1.94955900	-0.72938200
C	-1.60039900	-0.38262300	-0.34650800
C	-1.80261800	0.94666000	0.04417800
C	-2.69533300	-1.24976700	-0.36193900
C	-3.07050800	1.39376800	0.40645800
H	-0.94570700	1.61433100	0.06720200
C	-3.96785600	-0.80371400	-0.00367500
H	-2.54960400	-2.28651700	-0.65675900
C	-4.15968900	0.52116200	0.38130500
H	-3.21135000	2.42745000	0.71010200
H	-4.80664100	-1.49378500	-0.02164500
H	-5.14815200	0.87098300	0.66409400
C	3.27884700	0.13877600	-0.03899700
O	3.98999200	1.13230600	-0.02952300
C	3.72778100	-1.19158200	0.52566300
H	3.18944300	-2.03154900	0.08038700
H	4.80187600	-1.31387600	0.36986000
H	3.52578900	-1.19112400	1.60179700
O	1.27559600	1.27530400	-0.72154400

a10

C	0.85140800	-0.15365000	-0.07870700
N	2.10000900	0.66750100	-0.42461400
O	0.91950300	-1.22779000	0.56744600
C	-0.20371000	-0.00143100	-1.18260100
H	-0.03688600	0.92635400	-1.73565900
H	-0.07713500	-0.84464400	-1.87131600
C	-1.59098700	-0.01674600	-0.59329400
C	-2.34940600	1.15404900	-0.50888800
C	-2.13118300	-1.20138300	-0.07722900
C	-3.62072300	1.14494000	0.06579800
H	-1.93893900	2.08191700	-0.90027700
C	-3.39975900	-1.21532500	0.49665400
H	-1.53608800	-2.10842100	-0.12082100
C	-4.15095200	-0.04109100	0.56891900
H	-4.19575000	2.06502300	0.11938600
H	-3.80513500	-2.14395100	0.88868100
H	-5.14159200	-0.05223500	1.01378100
C	3.27125700	0.22709800	0.18403200
O	3.72279300	0.64359600	1.23469700

C	3.93856300	-0.83839900	-0.65072900
H	3.92635400	-0.58673000	-1.71421500
H	4.96253500	-1.00646300	-0.31366900
H	3.34934400	-1.75463500	-0.51393900
O	1.12097700	1.13455800	0.54493300

TS9

C	0.82454900	0.19538400	0.04740900
N	2.11259500	-0.65192500	0.41418800
O	0.89544800	1.27438100	-0.57669100
C	-0.20885400	0.03026700	1.16926000
H	-0.02068400	-0.89486200	1.71915900
H	-0.08642100	0.87618100	1.85469400
C	-1.60311600	0.02318000	0.59455800
C	-2.33450200	-1.16392900	0.49978300
C	-2.17442400	1.20190900	0.09946300
C	-3.61045300	-1.17623200	-0.06428500
H	-1.89928300	-2.08723500	0.87473700
C	-3.44805200	1.19453100	-0.46337800
H	-1.60144900	2.12283500	0.15220900
C	-4.17207900	0.00412200	-0.54634300
H	-4.16443500	-2.10859800	-0.12661100
H	-3.87818000	2.11884400	-0.83873300
H	-5.16640400	-0.00149300	-0.98297500
C	3.28663100	-0.23602900	-0.19097100
O	3.68066000	-0.55918200	-1.29888900
C	4.06204100	0.68908800	0.71995400
H	3.99234700	0.38494900	1.76698600
H	5.10738800	0.74138700	0.41079800
H	3.61126100	1.68576500	0.62855000
O	1.11910900	-1.06509700	-0.57095900

a11

C	0.68707100	-1.35762200	0.17683000
N	2.83326100	-0.61078600	-0.45476500
O	0.98476600	-1.41298400	1.34966700
C	-0.68911900	-1.71933900	-0.35716000
H	-0.61018600	-1.97032900	-1.41984300
H	-1.03502900	-2.60896200	0.17663100
C	-1.68436300	-0.59012200	-0.16773600
C	-1.27470000	0.74725000	-0.21298200
C	-3.03841600	-0.88179600	0.01997200
C	-2.21367100	1.76938900	-0.07394500
H	-0.21615000	0.98666600	-0.33087200
C	-3.97471000	0.14173100	0.15264800
H	-3.36016300	-1.91959200	0.06322100
C	-3.56417500	1.47313600	0.10478300
H	-1.88637900	2.80509100	-0.10380600
H	-5.02324800	-0.10156500	0.29832700
H	-4.29100900	2.27297800	0.21167500
C	2.83802500	0.66501900	-0.08075100
O	1.88516300	1.46747700	0.02671200
C	4.24919900	1.14251600	0.24395000
H	4.27782400	1.50873400	1.27523600
H	4.99681500	0.35509300	0.12246900
H	4.50526400	1.98405800	-0.40810300
O	1.47989500	-0.97669900	-0.81828300

TS10

C	0.51408200	-1.59401300	0.00865800
N	3.11633900	-0.41537100	-0.13662000
O	0.76080500	-1.80428900	1.20298100
C	-0.93408000	-1.82481000	-0.48212900
H	-0.92143800	-2.04687100	-1.55503300
H	-1.36705700	-2.68269500	0.04129700
C	-1.78818100	-0.59910200	-0.22844000
C	-1.26144200	0.68917100	-0.39028400
C	-3.12439600	-0.72828900	0.16378500
C	-2.05504100	1.81276000	-0.16863900
H	-0.21619100	0.80571700	-0.66977700
C	-3.92072200	0.39532200	0.38315600
H	-3.54420500	-1.72205300	0.30107500
C	-3.38861900	1.67232800	0.21586000
H	-1.62778100	2.80419300	-0.29245400
H	-4.95576900	0.27149300	0.68913800
H	-4.00453900	2.54965900	0.38992200
C	2.80896800	0.79449100	-0.07141900
O	2.07435200	1.75318200	-0.16948200
C	4.41715700	0.94821200	0.44678400
H	4.26167300	1.42098900	1.41795500
H	5.10103600	0.10901000	0.54806000
H	4.79638300	1.65042200	-0.29769600
O	1.29698700	-1.15498000	-0.89351600

a12

C	-0.74296900	-0.04520200	0.00001100
N	0.40954700	-0.35069900	-0.00003700
O	-1.91172200	0.12874900	0.00000500

C	1.75979300	0.14767600	0.00000100
H	1.93909000	0.75038000	0.89330400
H	2.44972800	-0.69650500	-0.00342700
H	1.93718800	0.75618200	-0.88973300

a13

C	-2.26628200	-0.09008000	0.14922400
O	-2.11731300	-1.29872900	0.43852900
C	-1.21251000	0.50308200	-0.85010300
H	-1.39886000	0.02055900	-1.81895100
H	-1.39323200	1.57473100	-0.96883100
C	0.21351400	0.25931800	-0.43888200
C	0.74601500	-1.03780300	-0.41868100
C	1.04150900	1.31667100	-0.04646400
C	2.06136600	-1.26537700	-0.02390900
H	0.10277700	-1.86554000	-0.69794300
C	2.35972600	1.09321700	0.35284300
H	0.64715900	2.33038800	-0.05681200
C	2.87657600	-0.20017900	0.36408100
H	2.45494000	-2.27829700	-0.01868600
H	2.98227300	1.93204900	0.65165600
H	3.90342600	-0.37841600	0.66957900
O	-3.15993300	0.69765800	0.52538800

TS11

C	-1.16122200	0.49724200	0.81361900
N	-0.44547600	0.48339600	-0.19357800
O	-1.60003700	0.69256400	1.88689600
C	0.76989000	1.30517100	-0.15629800
H	0.77553600	1.94693500	-1.04345700
H	0.78128300	1.97188200	0.71743300
C	2.03442200	0.46944400	-0.15060700
C	3.20941300	0.99656400	-0.69440300
C	2.06751600	-0.80207800	0.42406700
C	4.39758000	0.27065900	-0.65819300
H	3.19004800	1.98274300	-1.15267900
C	3.25486100	-1.53228900	0.45908700
H	1.15584800	-1.22442300	0.83678500
C	4.42383700	-0.99835400	-0.07999800
H	5.30137000	0.69270500	-1.08795500
H	3.26509000	-2.52146200	0.90760800
H	5.34777500	-1.56818700	-0.05446400
C	-3.64530200	-0.28121600	-0.35957100
O	-3.70166800	0.96177000	-0.42150800
C	-4.85560500	-1.08780100	-0.86695100
H	-4.53220200	-1.84013300	-1.59383300
H	-5.31588400	-1.62771600	-0.03175700
H	-5.60563200	-0.43890700	-1.32542000
O	-2.69157600	-0.98061400	0.09183800

a14

C	-1.23428300	0.03915100	-0.38088600
N	-0.54083600	-0.80013700	0.32858100
O	-1.14602400	0.50340700	-1.52244500
C	0.60235900	-1.34548200	-0.39182700
H	0.76317300	-2.38315200	-0.07107600
H	0.42323600	-1.36255400	-1.47813200
C	1.88332300	-0.57150300	-0.13413800
C	3.00488200	-1.18062800	0.43191100
C	1.95050800	0.79291400	-0.44892600
C	4.17033600	-0.45204000	0.67876000
H	2.96486300	-2.23738800	0.68683000
C	3.11043200	1.52253200	-0.20583100
H	1.08039200	1.26691700	-0.89673800
C	4.22643800	0.90233800	0.36101300
H	5.03126900	-0.94340600	1.12347900
H	3.14801700	2.57863700	-0.45876600
H	5.13059500	1.47268200	0.55274900
C	-3.52910400	0.04030000	0.23919400
O	-3.74213000	-0.91249100	-0.48090500
C	-4.59092000	0.74396100	1.04733100
H	-4.31163700	0.75339800	2.10438100
H	-4.67502000	1.78357300	0.71732300
H	-5.54868300	0.23933400	0.92052500
O	-2.33487000	0.59454200	0.41831900

TS12

C	1.76889500	1.10753000	-0.00181500
N	1.25780200	0.20501500	0.84183100
O	1.60689600	2.31535900	-0.15039500
C	0.04974800	0.49121600	1.58730400
H	0.02607100	-0.12496800	2.49337500
H	0.07679200	1.54317700	1.90657700
C	-1.21670600	0.24918100	0.78786000
C	-2.04411200	-0.84355000	1.05055800
C	-1.54044700	1.09999700	-0.27743100
C	-3.17542900	-1.08685000	0.26922100
H	-1.79883000	-1.51205100	1.87281300

C	-2.66751500	0.86067100	-1.05864000
H	-0.88887500	1.94453400	-0.49028500
C	-3.48960100	-0.23547400	-0.78705000
H	-3.80839300	-1.94258300	0.48632900
H	-2.90875400	1.52889100	-1.88051200
H	-4.36909000	-0.42249500	-1.39604000
C	2.13823100	-0.96673300	-0.27165700
O	2.97396300	-1.70370700	0.23611100
C	1.03668200	-1.52123100	-1.16058400
H	0.35618300	-0.74780500	-1.52261800
H	1.50621600	-2.01683300	-2.01866100
H	0.46627100	-2.27174500	-0.60589700
O	2.59155600	0.34562700	-0.78127900

a15

C	2.03746900	1.20215500	0.13647600
N	1.30371600	-0.06120700	0.41496200
O	1.49808000	2.21390200	0.62143800
C	0.15261100	0.00106100	1.31300400
H	0.16489800	-0.87765200	1.96173500
H	0.28294200	0.89982300	1.91415200
C	-1.16884400	0.06564800	0.57610000
C	-2.14092000	-0.92148800	0.74446900
C	-1.42975500	1.13120600	-0.29332700
C	-3.35870800	-0.84438200	0.06807000
H	-1.93606500	-1.76047100	1.40463800
C	-2.64232000	1.20847500	-0.97392900
H	-0.66630700	1.89529700	-0.41858200
C	-3.61236700	0.22108500	-0.79362200
H	-4.10564000	-1.62059700	0.20842200
H	-2.83456600	2.04165900	-1.64419600
H	-4.55857000	0.28171400	-1.32331500
C	1.54360500	-1.29311200	-0.14138300
O	0.82473200	-2.25178000	0.14192200
C	2.68891800	-1.48690200	-1.11061300
H	3.64561800	-1.26179300	-0.63854600
H	2.65629700	-2.52835400	-1.43559700
H	2.59891100	-0.81538200	-1.96552300
O	3.07822900	1.09684400	-0.52828500

TS13

C	1.70192600	2.15623500	0.46791200
N	1.11159300	0.00510800	0.71170800
O	1.37035200	2.28972200	-0.65429000
C	1.73615200	-0.71869400	-0.38963000
H	1.60221200	-1.80173700	-0.25791600
H	1.22866700	-0.42502100	-1.31774900
C	3.21723500	-0.41993400	-0.53995400
C	4.13420800	-0.86273800	0.42362200
C	3.69530500	0.32512900	-1.62165000
C	5.49028200	-0.56970300	0.30205000
H	3.76076800	-1.43737200	1.26663500
C	5.05361500	0.61975900	-1.74677700
H	2.99348000	0.68212800	-2.37123100
C	5.95596000	0.17284300	-0.78447400
H	6.18855100	-0.92318800	1.05575900
H	5.40489700	1.19975100	-2.59560300
H	7.01370000	0.40067000	-0.87844100
C	1.12669800	-0.60984900	1.90356900
O	1.61846800	-1.72497700	2.16524300
C	0.39858400	0.14152500	3.01076700
H	-0.47570800	-0.44225500	3.32161500
H	1.05321400	0.23646600	3.88274600
H	0.07208400	1.13632000	2.69987200
O	2.13768300	2.40631900	1.52998600
C	-1.78925000	-1.61682400	-0.13658400
C	-2.37925000	-0.22276100	-0.08906800
C	-2.65679500	-2.71306700	0.49026800
C	-4.73027300	-0.97109800	-0.52554800
C	-3.66499700	-3.29107800	-0.50203000
C	-4.32418700	-2.19514300	-1.33995600
H	-1.55641600	-1.85919000	-1.18072000
H	-5.14960600	-1.26690800	0.44459000
H	-3.17329300	-2.30739500	1.36811900
H	-4.43176800	-3.85219500	0.04360500
H	-0.83297100	-1.55590800	0.38734200
H	-1.99929100	-3.50520400	0.85964600
H	-5.51381200	-0.43618400	-1.06474500
H	-3.16234700	-3.99945600	-1.17012500
H	-5.22881100	-2.58825400	-1.81394900
H	-3.66567700	-1.87115700	-2.15360400
N	-3.67027900	0.03456000	-0.30151500
C	-4.16857100	1.41111100	-0.12816500
H	-5.05664400	1.51759300	-0.75258500
H	-4.46826800	1.55055400	0.91739000
C	-3.11095100	2.42434500	-0.52878600
H	-3.47882000	3.43405600	-0.33442000
H	-2.90289700	2.33289900	-1.59964500

C	-1.85027300	2.15743200	0.26974400
H	-1.99167400	2.42897700	1.32218400
H	-1.00025200	2.72175300	-0.11820300
N	-1.51663300	0.73922500	0.18110900
H	-0.50647900	0.46605400	0.36701800

pro1

C	0.49732000	-1.24067200	-0.57066100
H	0.81801900	-1.01589700	-1.59155200
H	0.35404700	-2.32148000	-0.48814200
C	-0.80042800	-0.52217200	-0.26216600
C	-0.85004500	0.87628500	-0.29686400
C	-1.95637800	-1.23379400	0.05859900
C	-2.03570400	1.54727800	-0.01358200
H	0.04829500	1.43226800	-0.55470600
C	-3.14761400	-0.56318100	0.34058000
H	-1.92416500	-2.32023700	0.08992600
C	-3.18919900	0.82812900	0.30623100
H	-2.06332200	2.63262100	-0.04455900
H	-4.04001100	-1.12949000	0.59050200
H	-4.11413700	1.35237000	0.52720500
N	1.58939800	-0.84792700	0.30293300
H	1.61622500	-1.23262200	1.23853700
C	2.48751800	0.10850100	-0.03750000
O	2.46650300	0.68263000	-1.12303600
C	3.51536300	0.43974800	1.02112300
H	3.27404000	1.41875400	1.44671800
H	3.55089100	-0.29669500	1.82648900
H	4.49731200	0.51413300	0.54879600

TS14

C	0.60290600	-1.21842200	0.09617900
N	2.72282300	1.21203300	-0.17616900
O	0.89215300	-1.09785600	1.30112700
C	-0.80344000	-1.78115900	-0.23606900
H	-0.80952600	-2.21141200	-1.24087500
H	-1.03453600	-2.57008200	0.48805900
C	-1.84036100	-0.68631700	-0.14284900
C	-2.60335000	-0.31084400	-1.25210100
C	-2.04150200	-0.00559500	1.06577700
C	-3.54810400	0.71203100	-1.15967600
H	-2.45759900	-0.82754700	-2.19767800
C	-2.98415800	1.01383300	1.16196500
H	-1.43230200	-0.28039000	1.92201200
C	-3.74378700	1.37705100	0.04830500
H	-4.13135100	0.98721700	-2.03393900
H	-3.12690100	1.52934100	2.10767100
H	-4.47998700	2.17187600	0.12316000
C	3.12104300	0.04222000	-0.15457900
O	3.81688800	-0.90522500	-0.05107800
C	3.68483000	2.24317400	0.22716900
H	4.70061400	1.85798300	0.37364900
H	3.71738900	3.02165900	-0.54046600
H	3.35376500	2.70853500	1.16085500
O	1.30829500	-0.90098700	-0.90300700

a16

C	0.62616400	-1.18382600	-0.02949800
N	2.50981700	1.29376100	0.25571200
O	0.91812600	-1.53061800	1.09622000
C	-0.66519200	-1.60395700	-0.71441800
H	-0.51074800	-1.64927400	-1.79474200
H	-0.93324900	-2.59583100	-0.34282200
C	-1.74946800	-0.60370900	-0.37601100
C	-2.01355500	0.47731400	-1.22103300
C	-2.46629500	-0.72131100	0.81847300
C	-2.98668400	1.41698800	-0.88537800
H	-1.45511400	0.57869400	-2.14813700
C	-3.43907700	0.21694500	1.15628000
H	-2.25940600	-1.55618700	1.48324900
C	-3.70280100	1.28867400	0.30389400
H	-3.18592500	2.24941600	-1.55384400
H	-3.99232700	0.11033800	2.08475800
H	-4.46292500	2.01889600	0.56465800
C	2.62687200	0.09428200	-0.22277100
O	3.55821300	-0.70037800	-0.36035600
C	3.78137800	1.78838600	0.75433500
H	4.56691600	1.81137100	-0.01829500
H	3.65857900	2.81012500	1.13149900
H	4.18739300	1.17851300	1.57772700
O	1.33867800	-0.36552400	-0.78650700

TS15

C	-0.86422900	0.66661200	0.48634500
N	-2.65237400	0.48165700	-0.10554800
O	-0.60064200	1.60136000	1.22722500
C	-0.09190200	0.44584300	-0.81912100
H	-0.54046300	-0.36751900	-1.39511900

H	-0.17339100	1.36951100	-1.40132600
C	1.35513300	0.13983300	-0.51869800
C	1.82673000	-1.17551300	-0.54160800
C	2.23994800	1.16319700	-0.16034000
C	3.15415700	-1.46419200	-0.22642100
H	1.14561100	-1.97914600	-0.81124700
C	3.56622400	0.87948600	0.15579700
H	1.87720600	2.18681500	-0.12739500
C	4.02849900	-0.43669500	0.12268000
H	3.50451000	-2.49196900	-0.25400100
H	4.24117600	1.68608000	0.42760700
H	5.06327400	-0.65864800	0.36610700
C	-2.47863800	-0.72142200	0.44167700
O	-3.12899500	-1.76087400	0.44042200
C	-3.58445800	0.64937600	-1.19372100
H	-4.33341900	-0.15355700	-1.18914200
H	-4.11332900	1.60697500	-1.12059300
H	-3.08264300	0.62771400	-2.17383000
O	-1.26169900	-0.60011100	1.07463200

a17

C	-0.90471600	-1.12000600	0.23118100
N	-1.91664300	-0.33906500	-0.25775000
O	-0.74077700	-2.26546500	-0.18939400
C	0.07422600	-0.59481200	1.27549300
H	-0.36056900	0.21118300	1.85975800
H	0.30801600	-1.45174200	1.91262400
C	1.33775500	-0.13314800	0.57906400
C	1.37545600	1.09672900	-0.08946500
C	2.47219500	-0.94880300	0.55494500
C	2.52927700	1.50141400	-0.75715500
H	0.48622800	1.72151200	-0.06814800
C	3.62780100	-0.54404400	-0.11289500
H	2.44900400	-1.90810400	1.06606800
C	3.65998600	0.68360800	-0.77104200
H	2.54735600	2.45949500	-1.26921900
H	4.50197800	-1.18884300	-0.11845600
H	4.55858200	1.00119900	-1.29172600
C	-2.37081500	0.99421300	0.23889700
O	-3.51816900	1.29484500	-0.11785400
C	-2.74616900	-0.99384700	-1.26231100
H	-3.41731800	-0.25053800	-1.68177400
H	-2.11301500	-1.42266800	-2.04215200
H	-3.33641100	-1.80822300	-0.82599600
O	-1.55822100	1.64091500	0.92512400

TS16

C	-1.91430000	0.38211400	-1.48309900
N	-0.77265800	-0.32373600	-1.47698400
O	-2.70251600	0.48796700	-2.43795600
C	-2.24643700	1.11284400	-0.17286000
H	-1.42584000	1.01352900	0.54157900
H	-2.35930100	2.17482200	-0.42414800
C	-3.53373200	0.60422600	0.43608900
C	-3.53353500	-0.08262300	1.65379600
C	-4.75664100	0.80403700	-0.21798300
C	-4.72252000	-0.56170000	2.20562900
H	-2.59294300	-0.24326200	2.17333300
C	-5.94393800	0.32628200	0.32991100
H	-4.76002400	1.32518800	-1.16981000
C	-5.93205400	-0.35912900	1.54568500
H	-4.70090700	-1.09186100	3.15353500
H	-6.88285100	0.49108700	-0.19125600
H	-6.85860400	-0.72991500	1.97390700
C	-0.78345600	-1.83125000	0.17978200
O	-1.05700100	-2.78645700	-0.44967400
C	-0.51428100	-1.00391700	-2.73447400
H	0.45433000	-1.51389400	-2.68566100
H	-1.28032100	-1.75758100	-2.96244100
H	-0.49232900	-0.30486400	-3.58137100
O	-0.49006000	-1.17060300	1.11107900
C	2.45609100	-1.17918700	-0.12413100
C	2.51840800	0.33120700	-0.04513800
C	3.73263800	-1.85127400	-0.64116700
C	4.89185500	0.40058800	0.76152500
C	4.72999600	-2.13274700	0.48205400
C	4.83290400	-0.95706800	1.45411900
H	2.18288100	-1.57032300	0.86274600
H	5.53151800	0.35729100	-0.12956300
H	4.19161000	-1.21684600	-1.40838200
H	5.71447100	-2.34278600	0.04951600
H	1.62238200	-1.40879400	-0.79137900
H	3.45640400	-2.78517500	-1.13891300
H	5.34328700	1.12108100	1.44569500
H	4.42355400	-3.02845400	1.03388500
H	5.74238100	-1.05594100	2.05471700
H	3.99586200	-0.95520800	2.16118300
N	3.59180600	0.99615800	0.38816400

C	3.60237400	2.46857500	0.31886500
H	4.28502100	2.82712100	1.09080900
H	4.00038800	2.77447700	-0.65612600
C	2.20976800	3.03488400	0.53691900
H	2.23337300	4.11977200	0.41360600
H	1.87803300	2.81071000	1.55574800
C	1.26441100	2.40636900	-0.46762600
H	1.46900500	2.77565500	-1.47886000
H	0.21940400	2.62396700	-0.23308900
N	1.43021300	0.95760100	-0.44383600
H	0.59415600	0.39106200	-0.78966100

pro2

N	-2.74712200	0.58117800	0.04011100
H	-2.76465500	1.48719600	0.48764100
C	-1.69118900	-0.23709000	0.22728500
O	-1.61393800	-1.33946300	-0.30558400
C	-0.60926000	0.28864200	1.16709300
H	-0.81528800	1.32376000	1.45247700
H	-0.66651900	-0.32423600	2.07439200
C	-3.86006900	0.18336600	-0.79816000
H	-4.60470400	0.97942600	-0.79108800
H	-3.53154700	0.00984700	-1.82761000
H	-4.31754300	-0.73795200	-0.42507500
C	0.76590100	0.17488700	0.55582400
C	1.43533400	1.31063300	0.09458800
C	1.38230100	-1.07366400	0.42080700
C	2.69782000	1.20537500	-0.48849600
H	0.96423200	2.28528300	0.19596700
C	2.64243400	-1.18194700	-0.16185800
H	0.86454100	-1.96057600	0.77348300
C	3.30461700	-0.04192400	-0.61864300
H	3.20613200	2.09863600	-0.83947200
H	3.11093700	-2.15720500	-0.25709600
H	4.28843500	-0.12637800	-1.07036400

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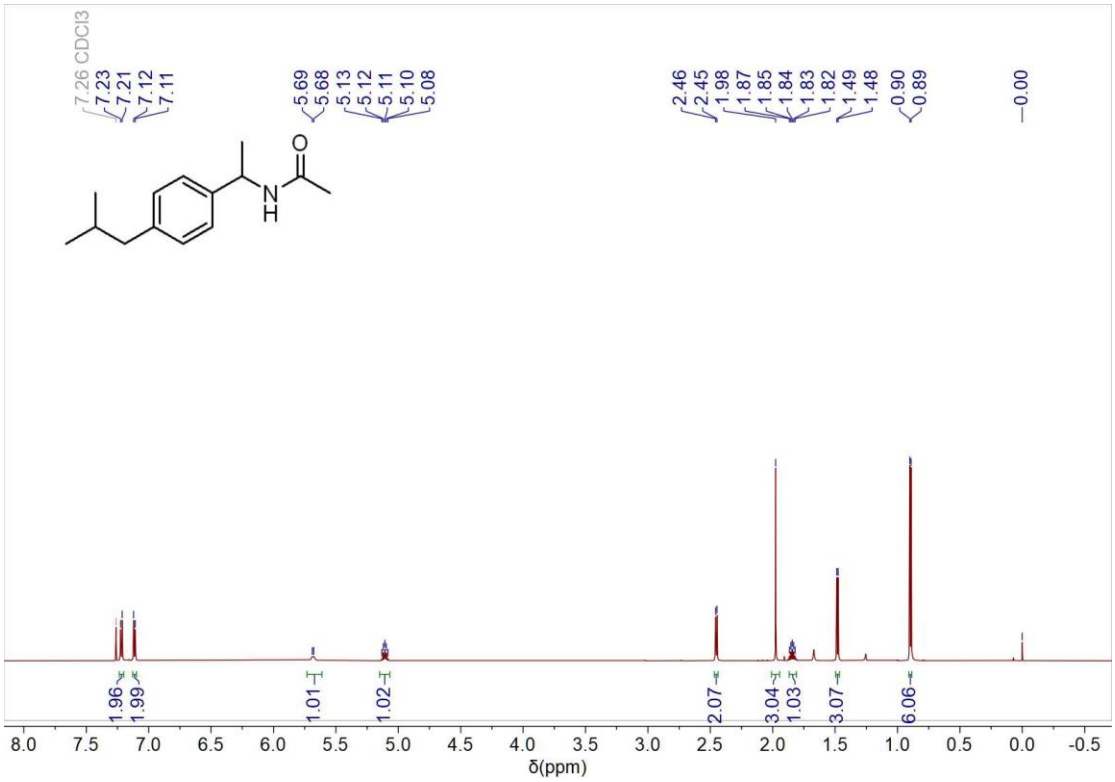
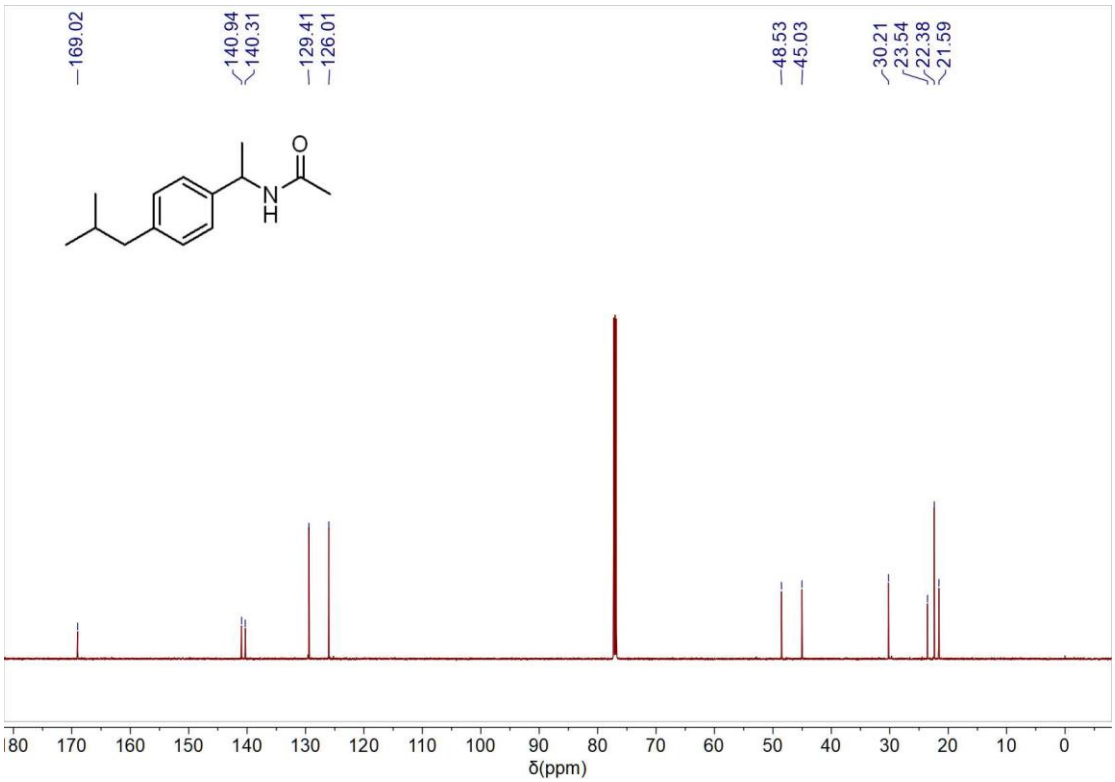
7. NMR Spectra

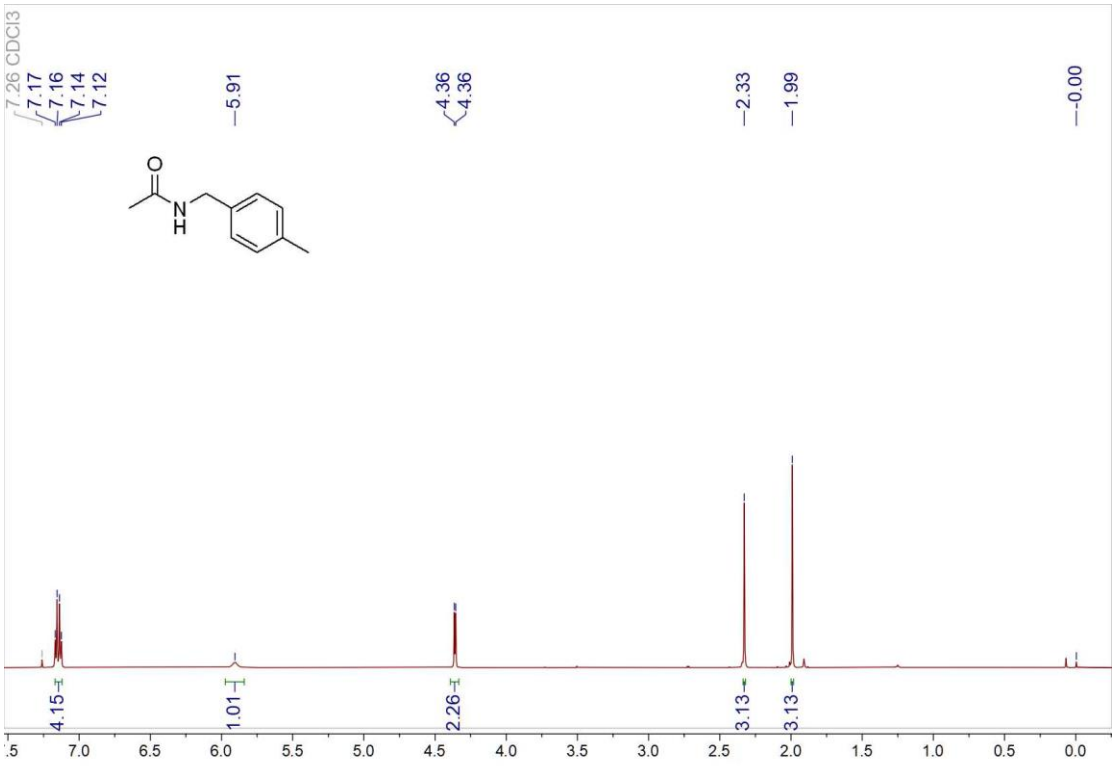
^{1}H NMR of compound 3



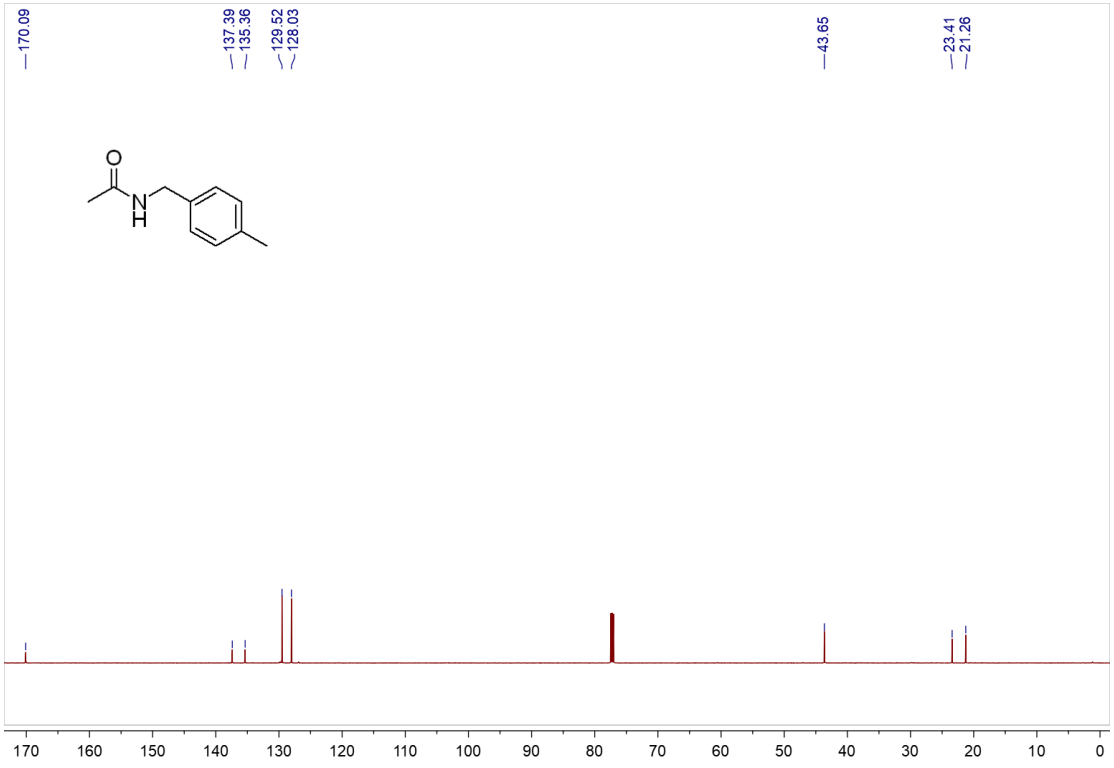
^{13}C NMR of compound 3



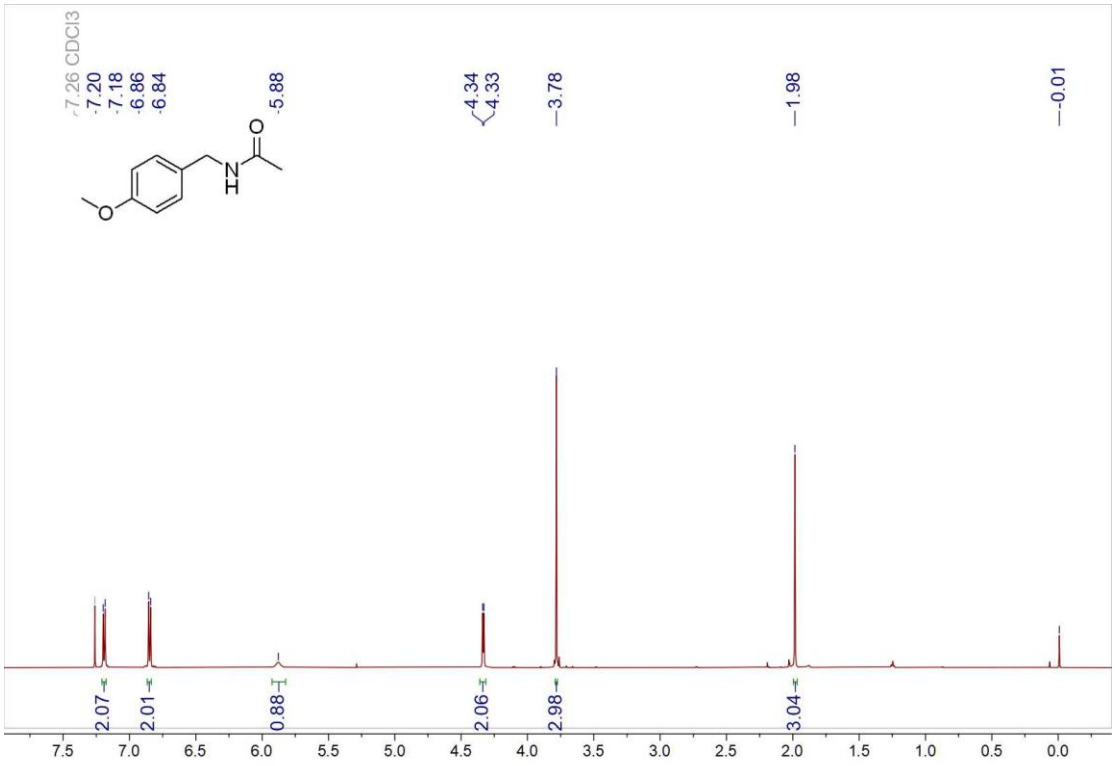
^{1}H NMR of compound 4



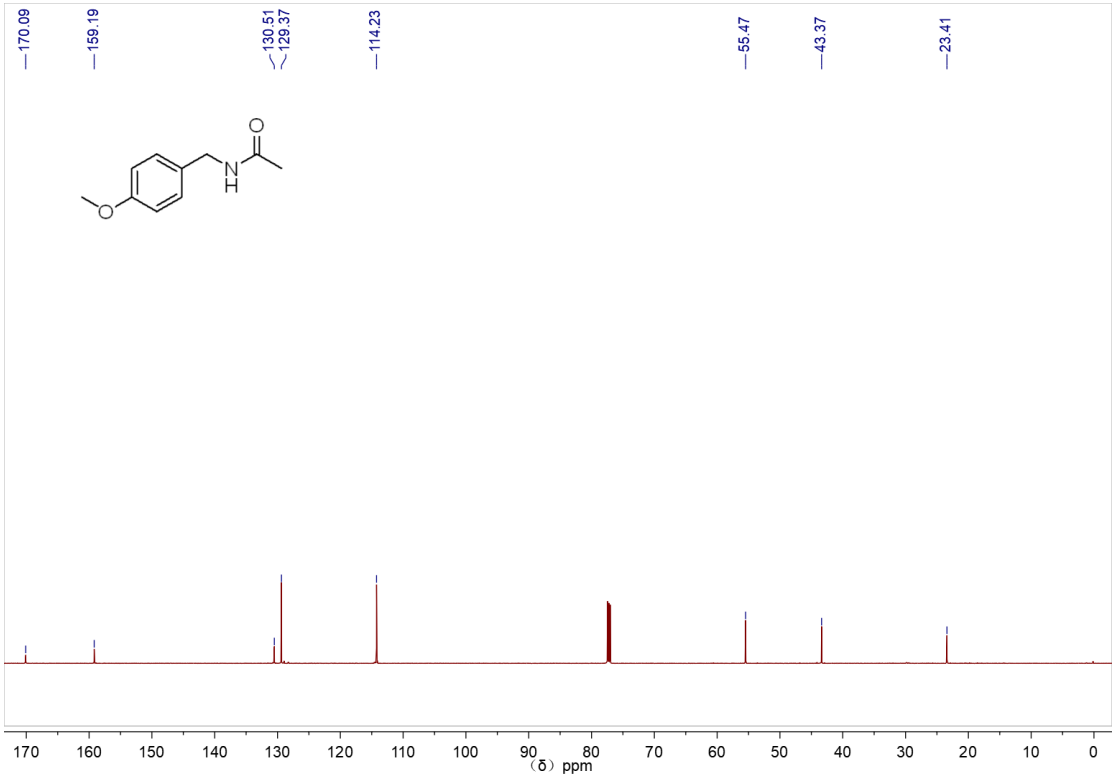
^{13}C NMR of compound 4



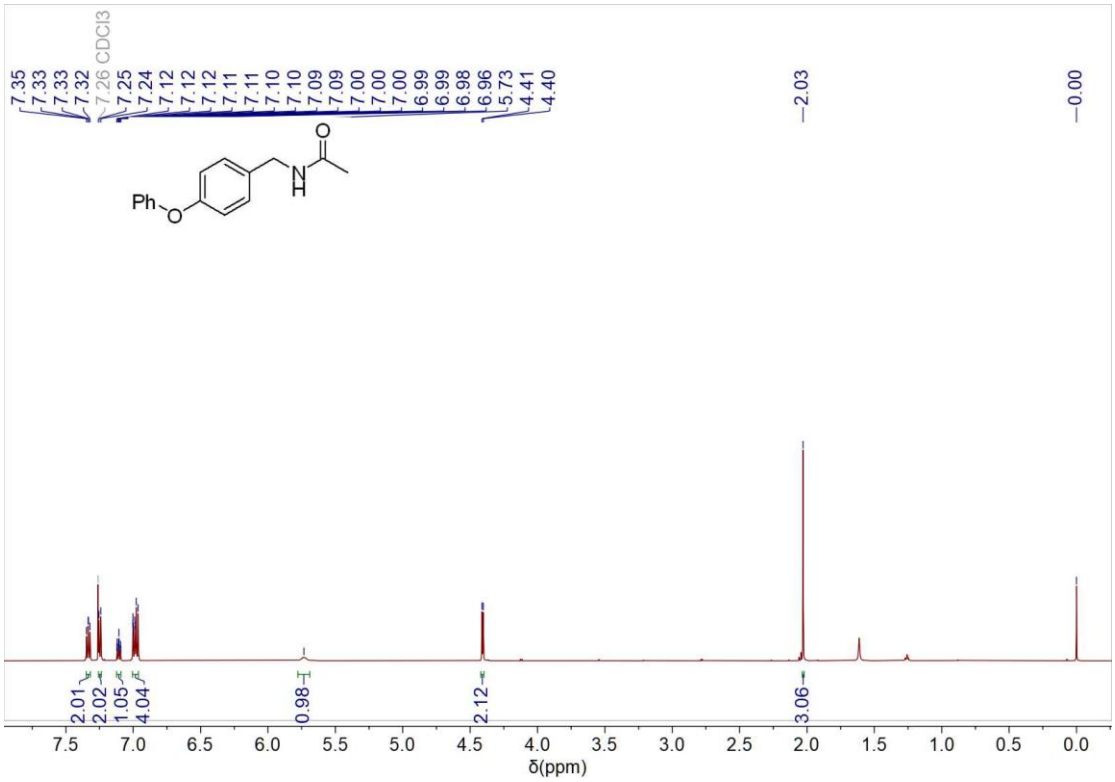
^{1}H NMR of compound 5



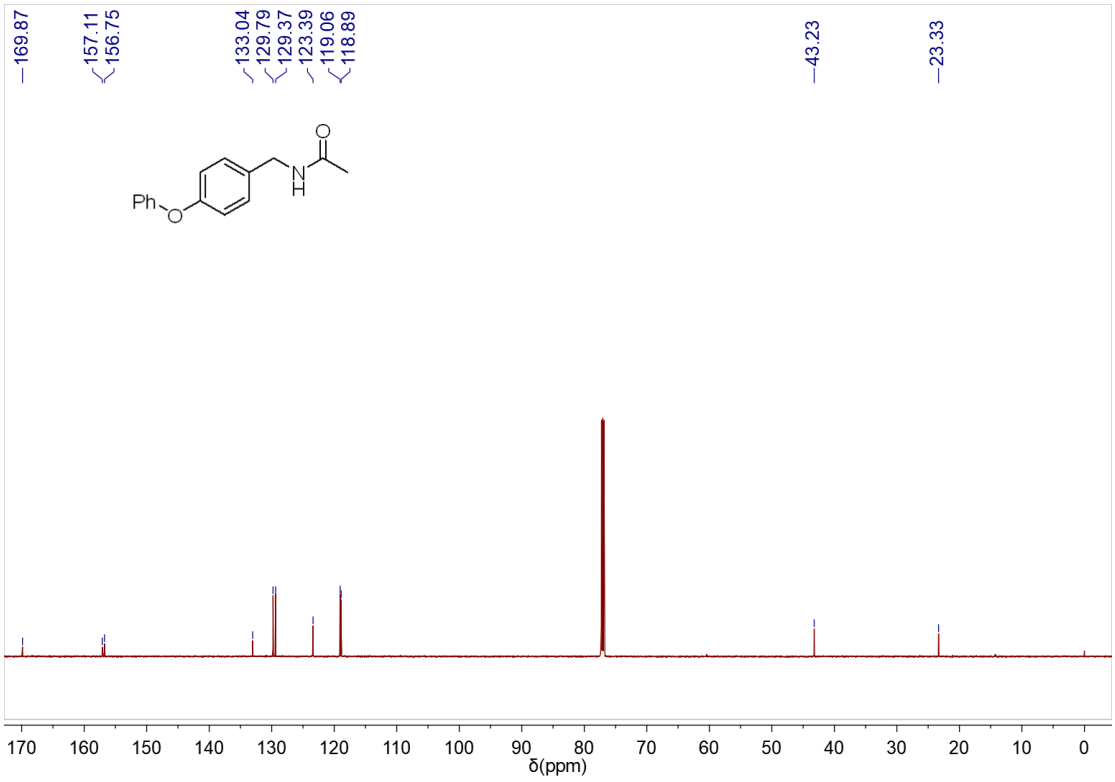
^{13}C NMR of compound 5



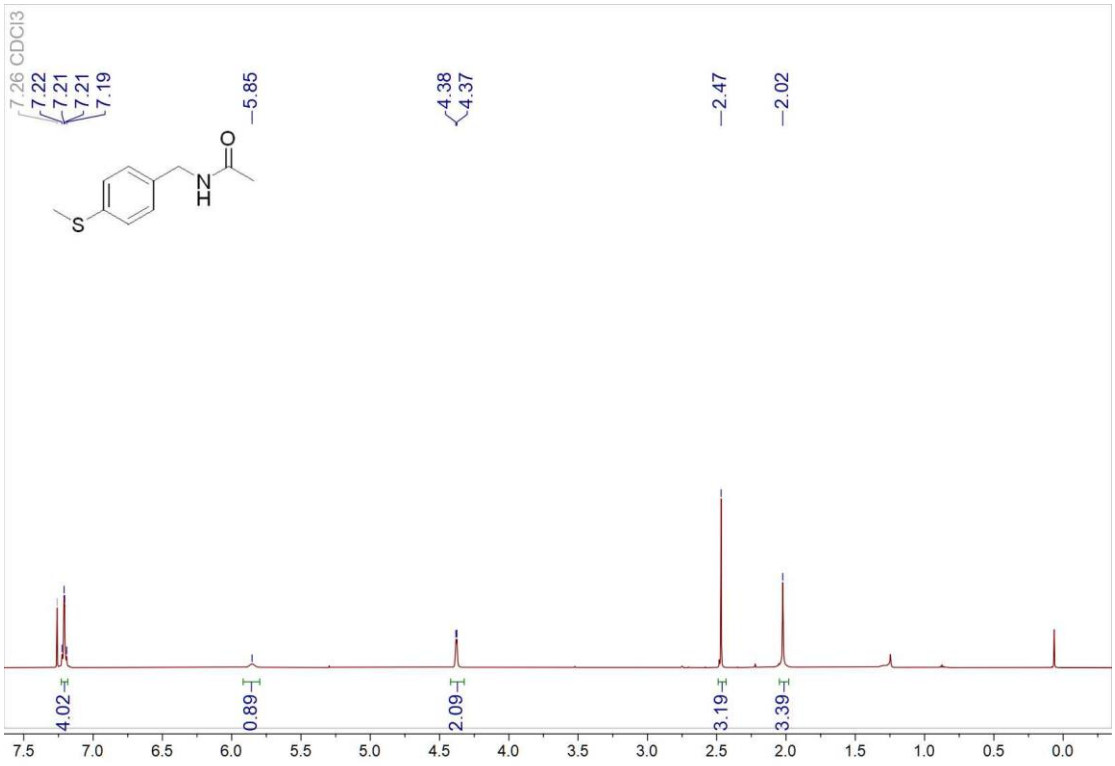
^{1}H NMR of compound 6



^{13}C NMR of compound 6



^{1}H NMR of compound 7



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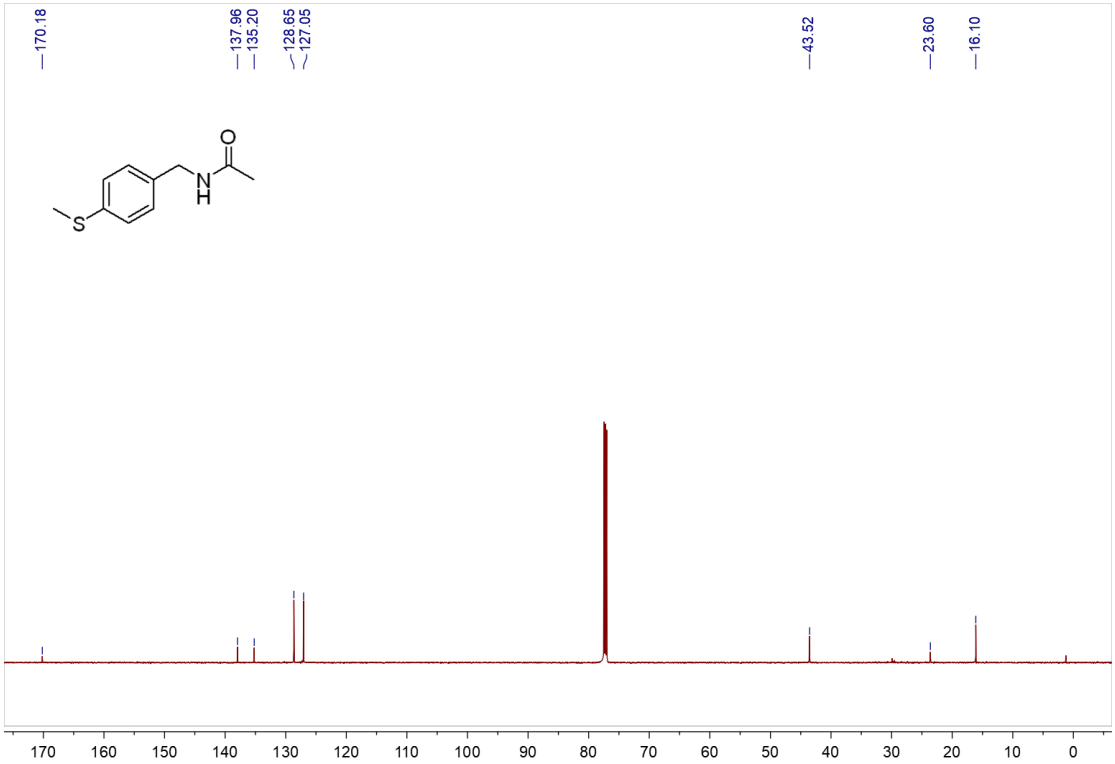
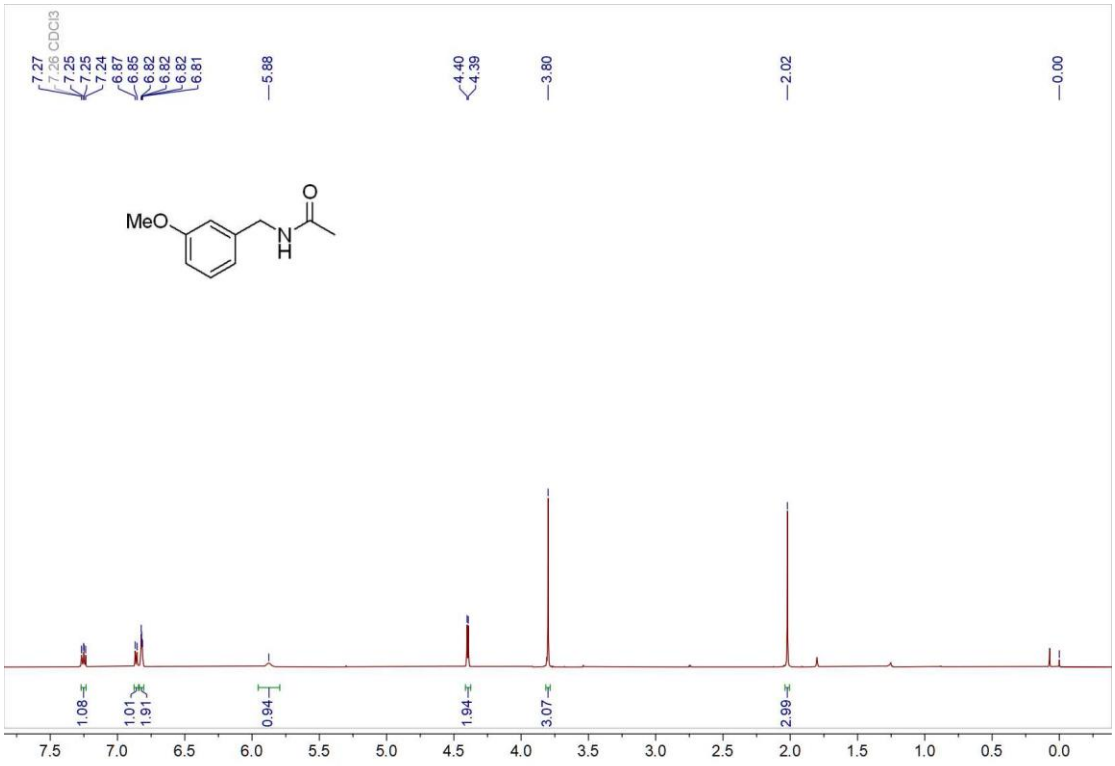


^{1}H NMR of compound 8



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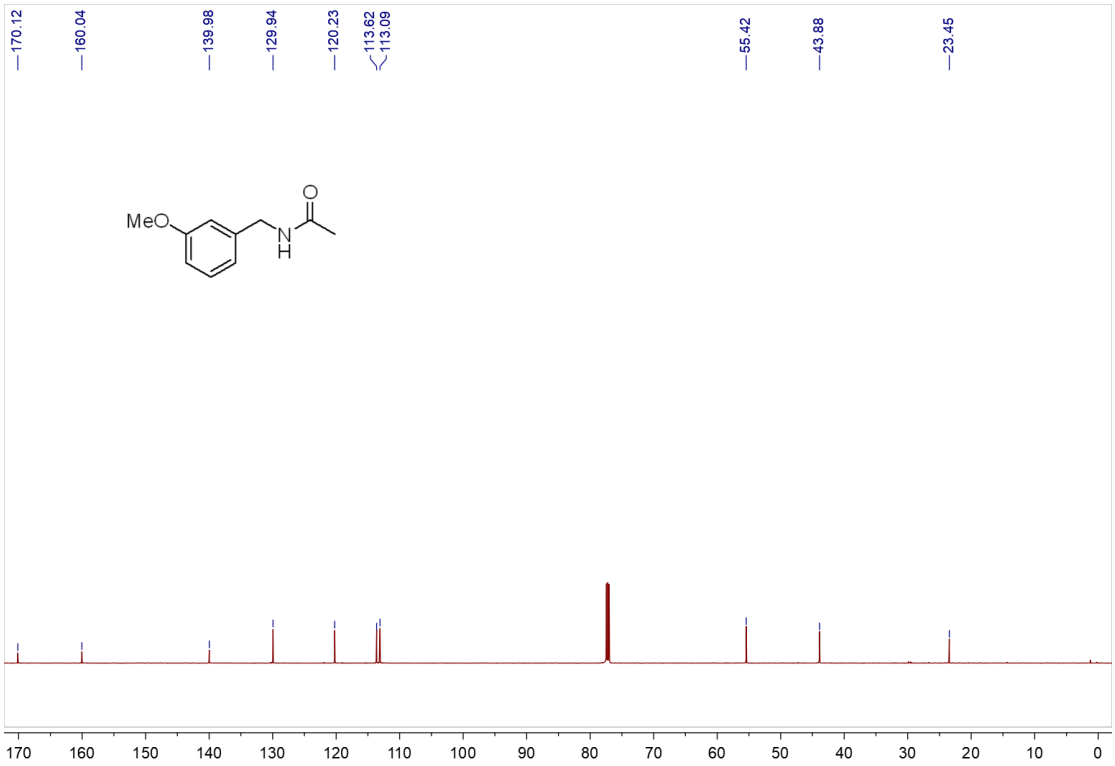
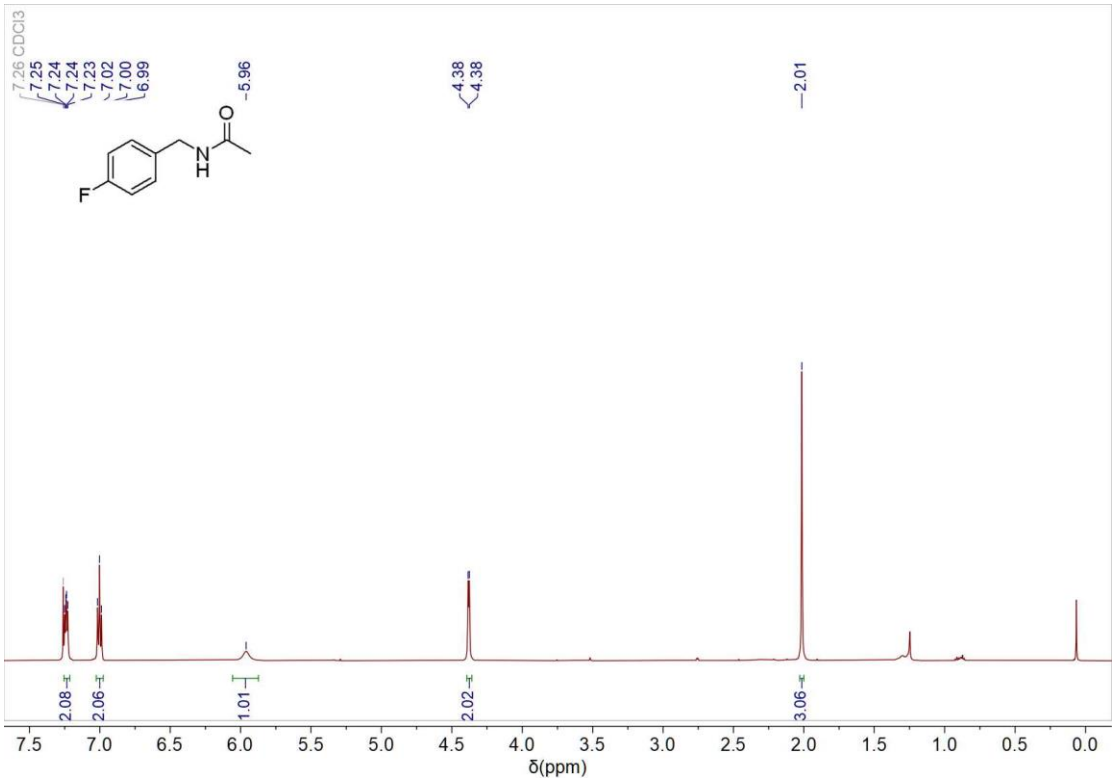


^{1}H NMR of compound 9



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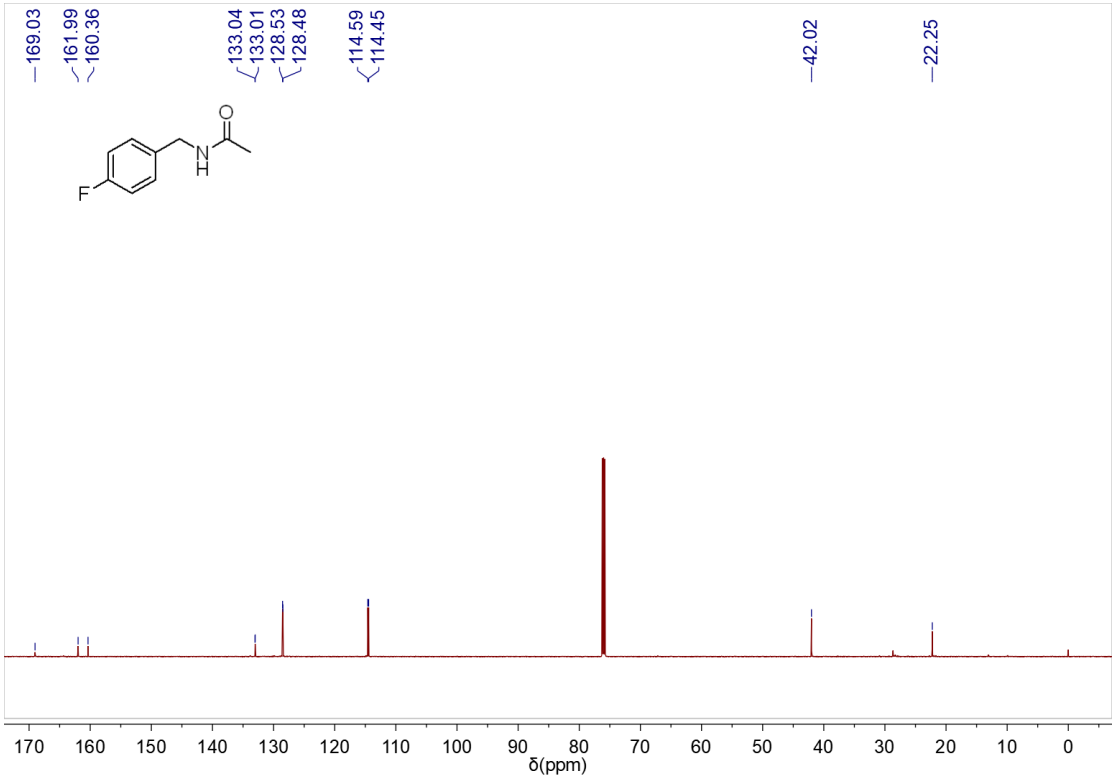
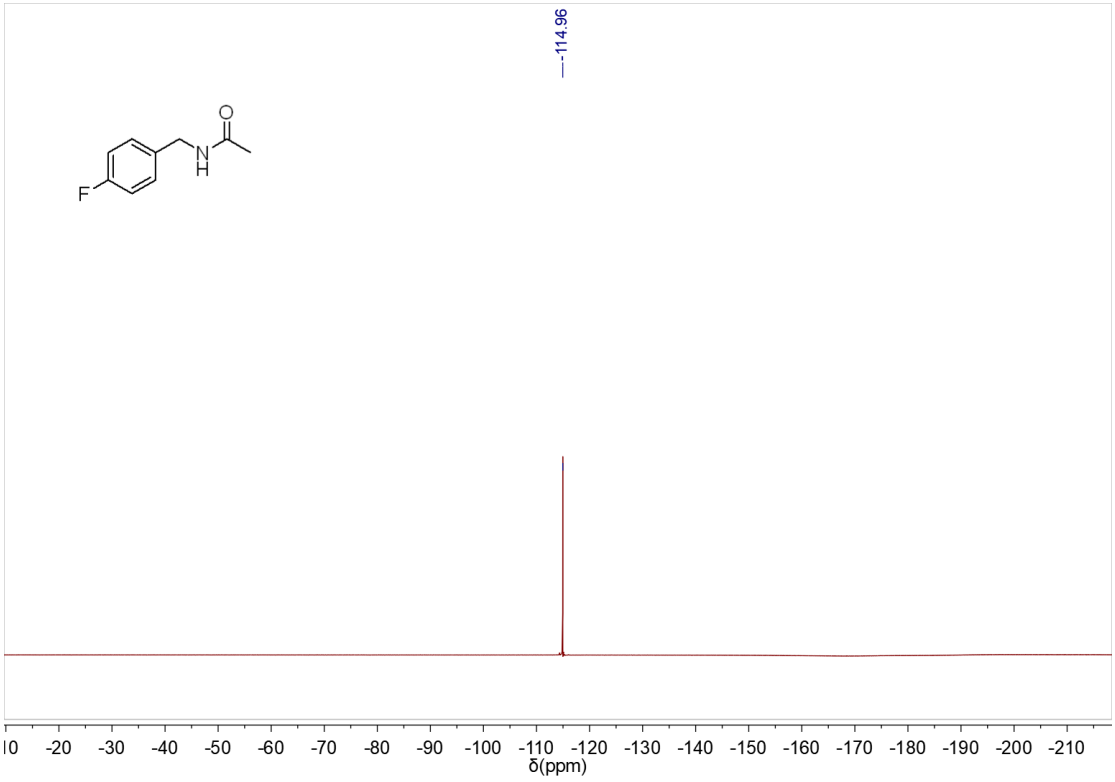


^{19}F NMR of compound 9



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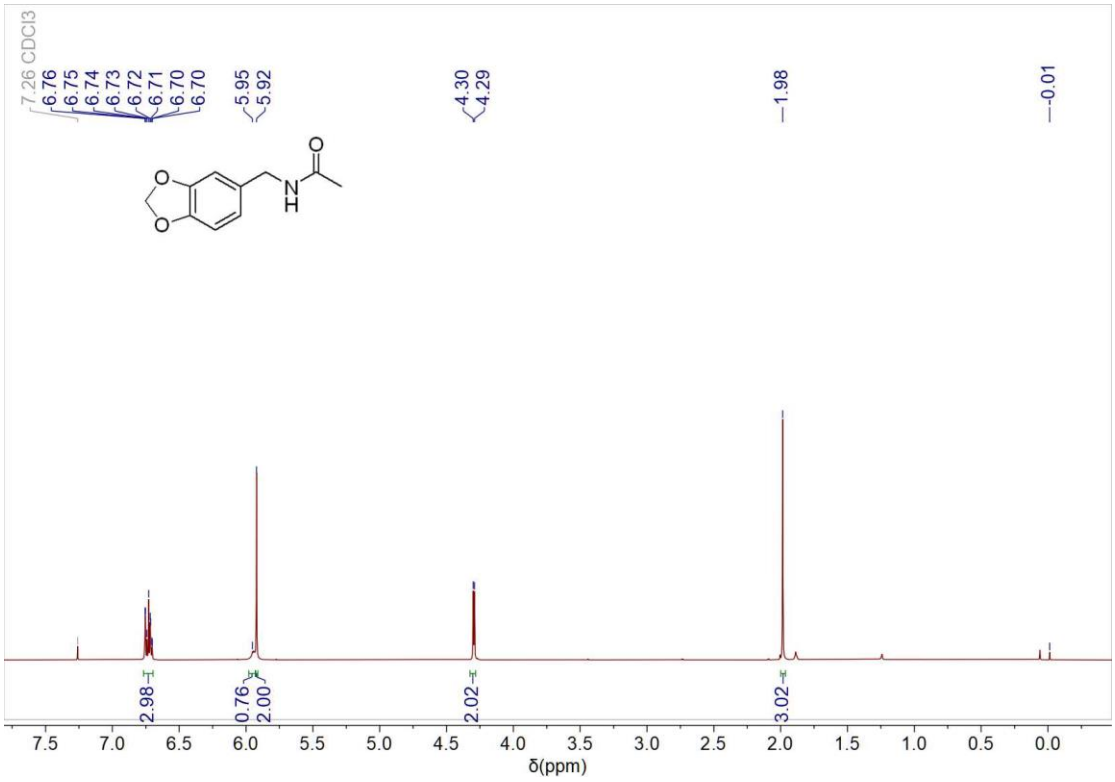

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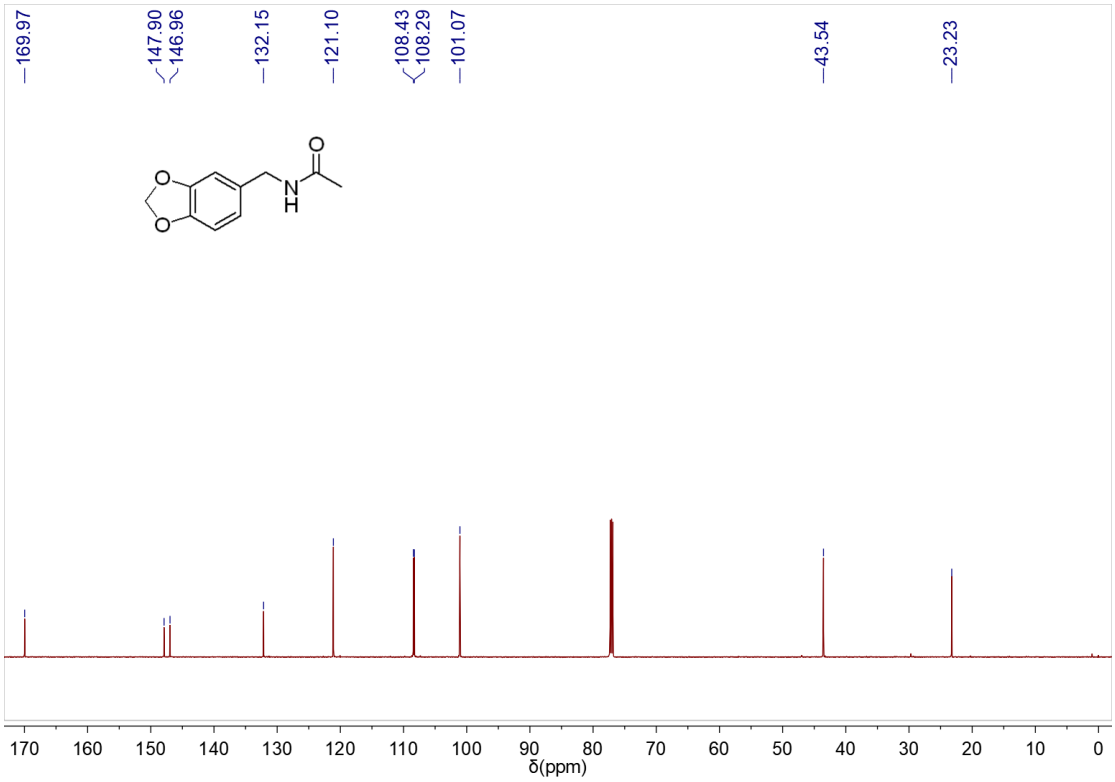
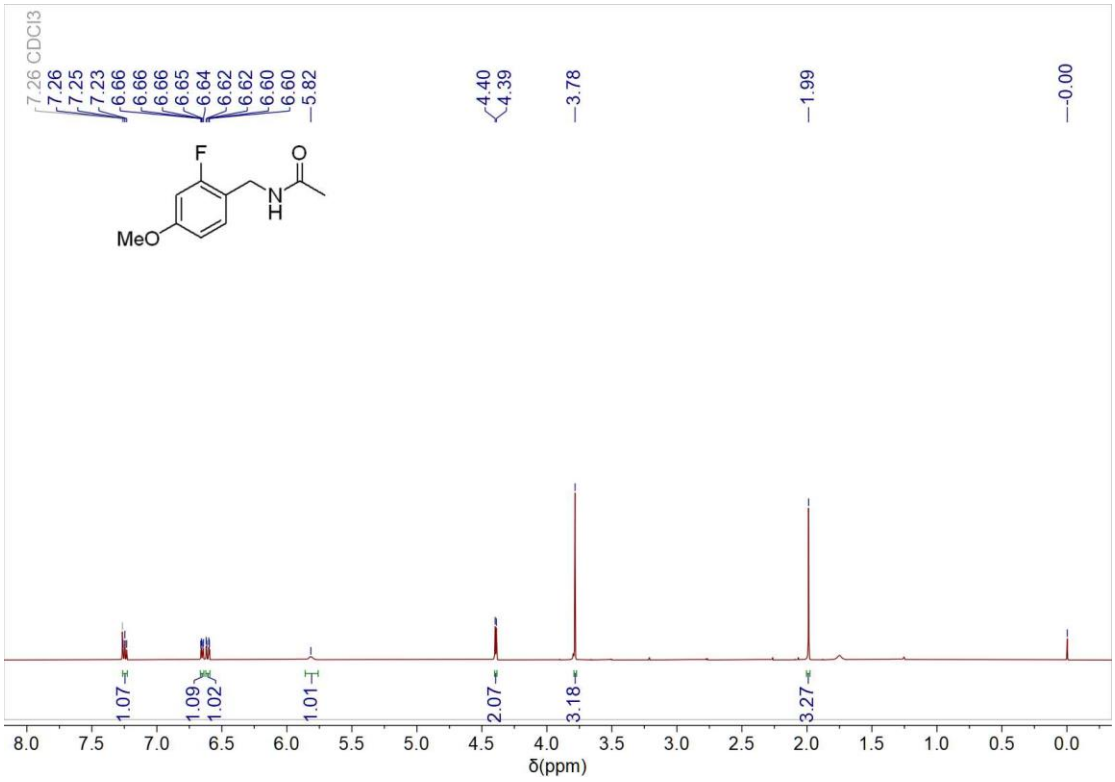


^{1}H NMR of compound 11



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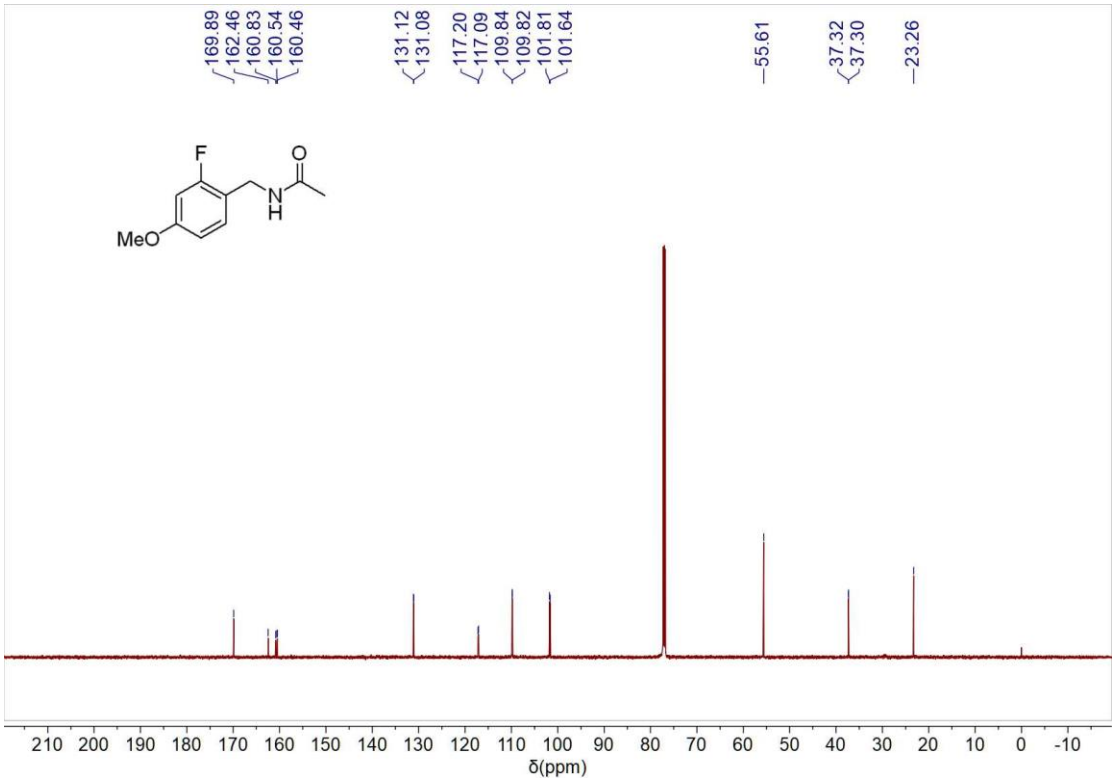

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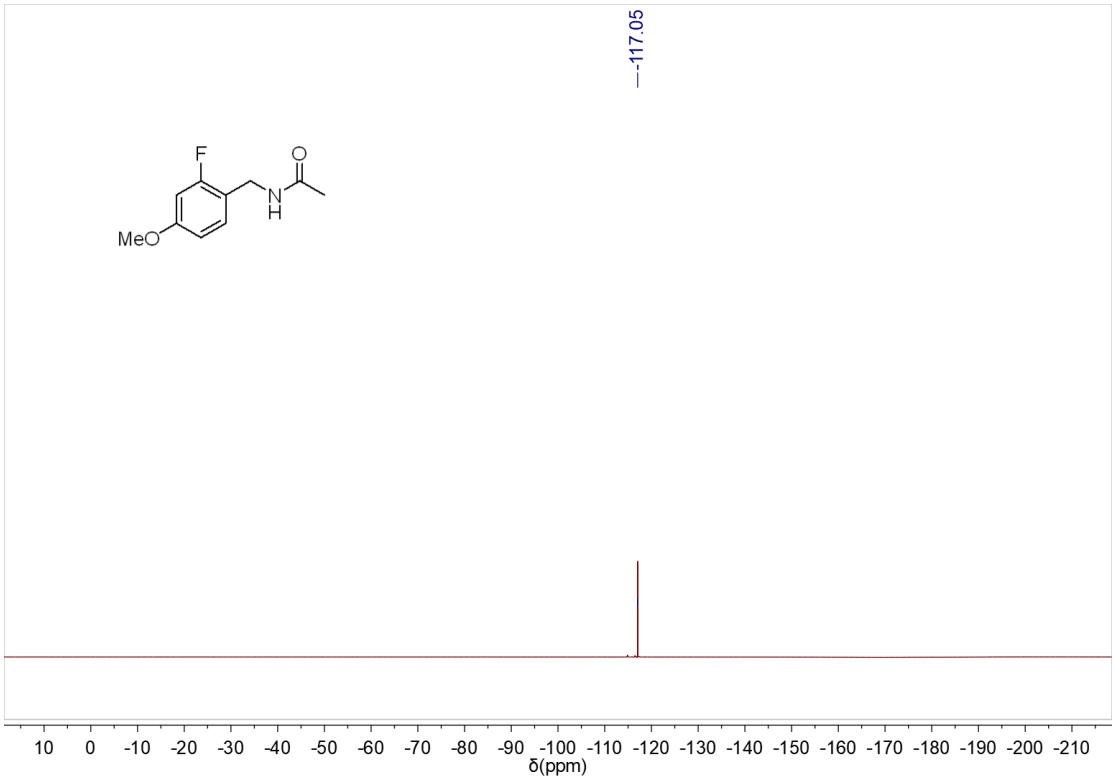

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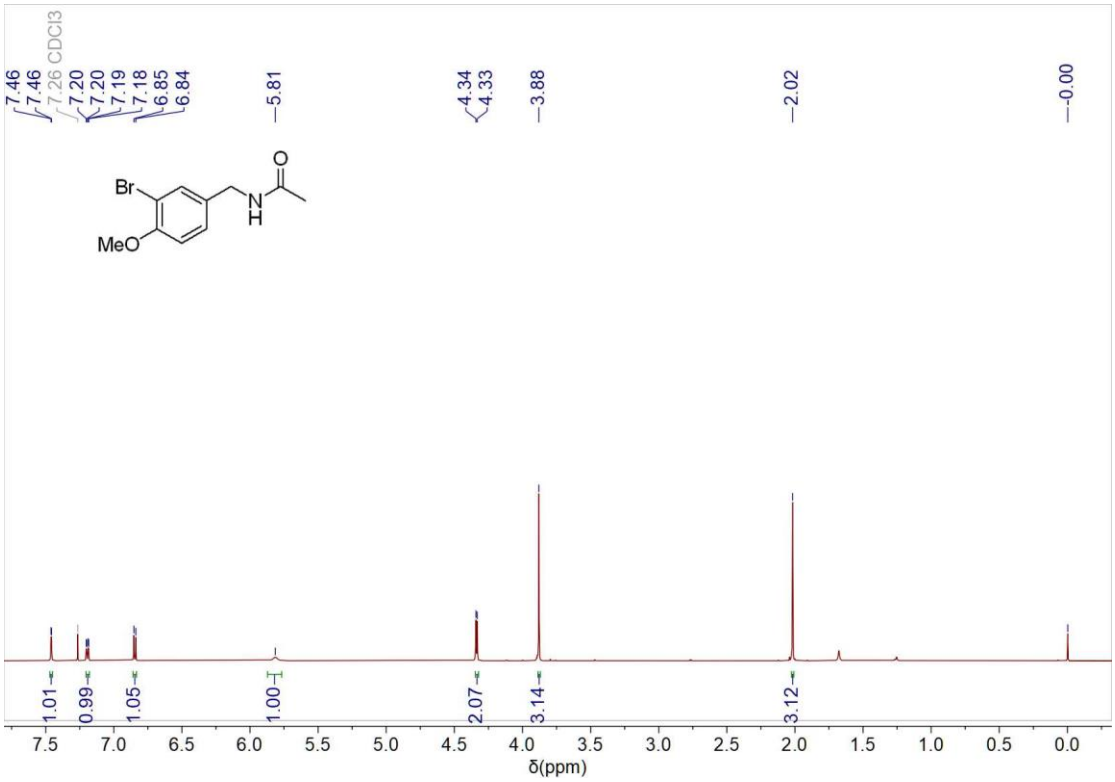

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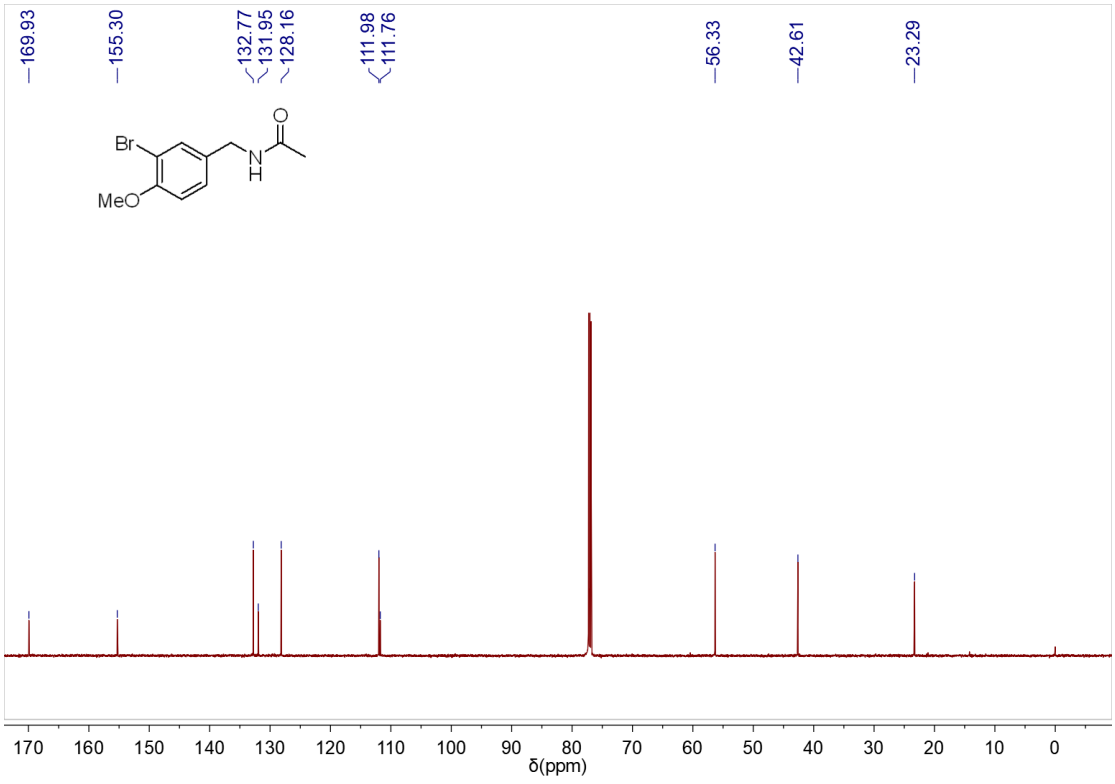

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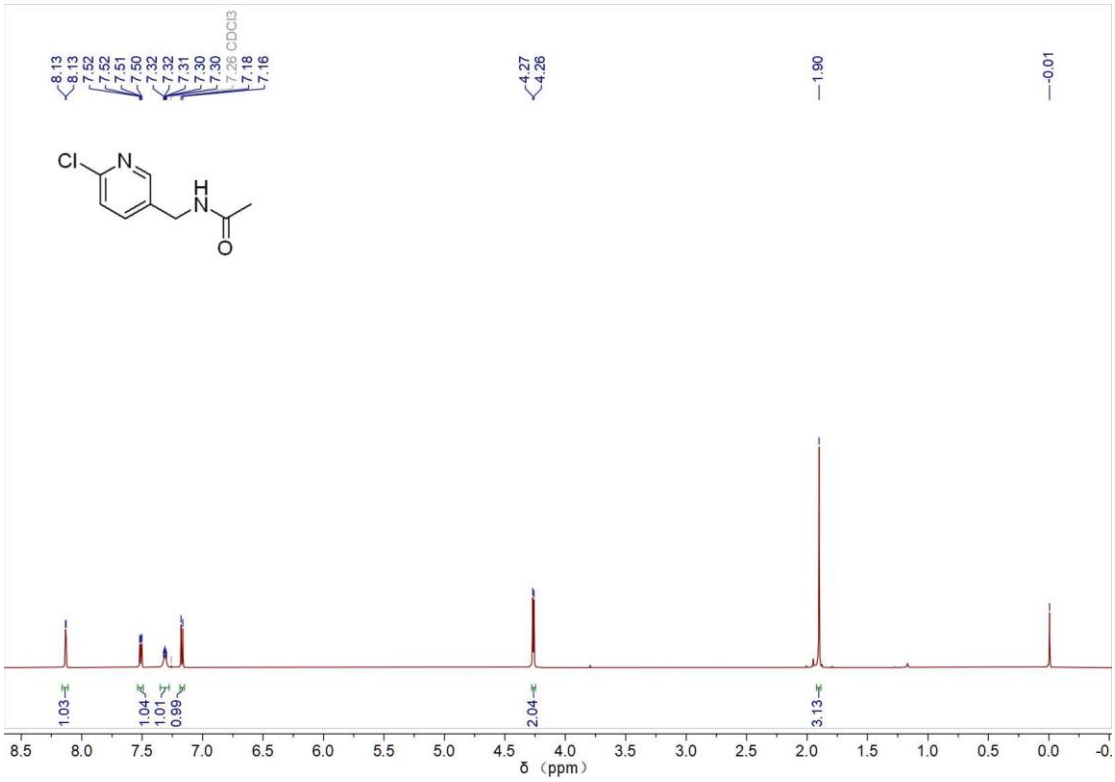

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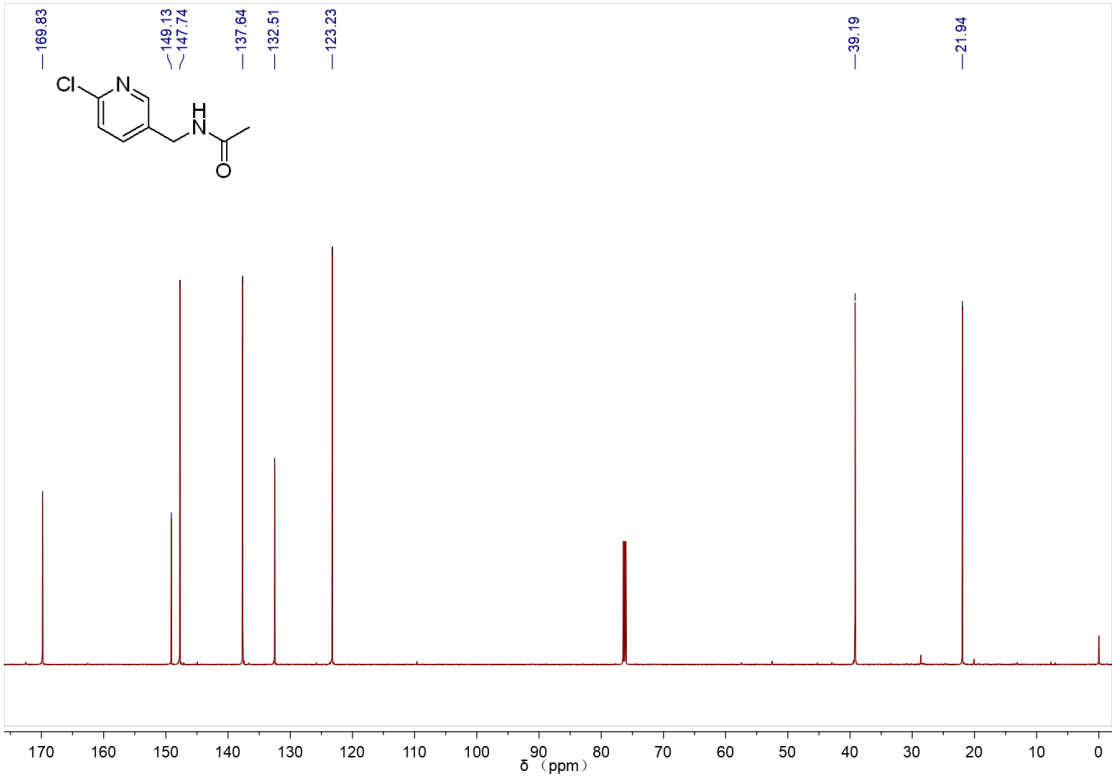

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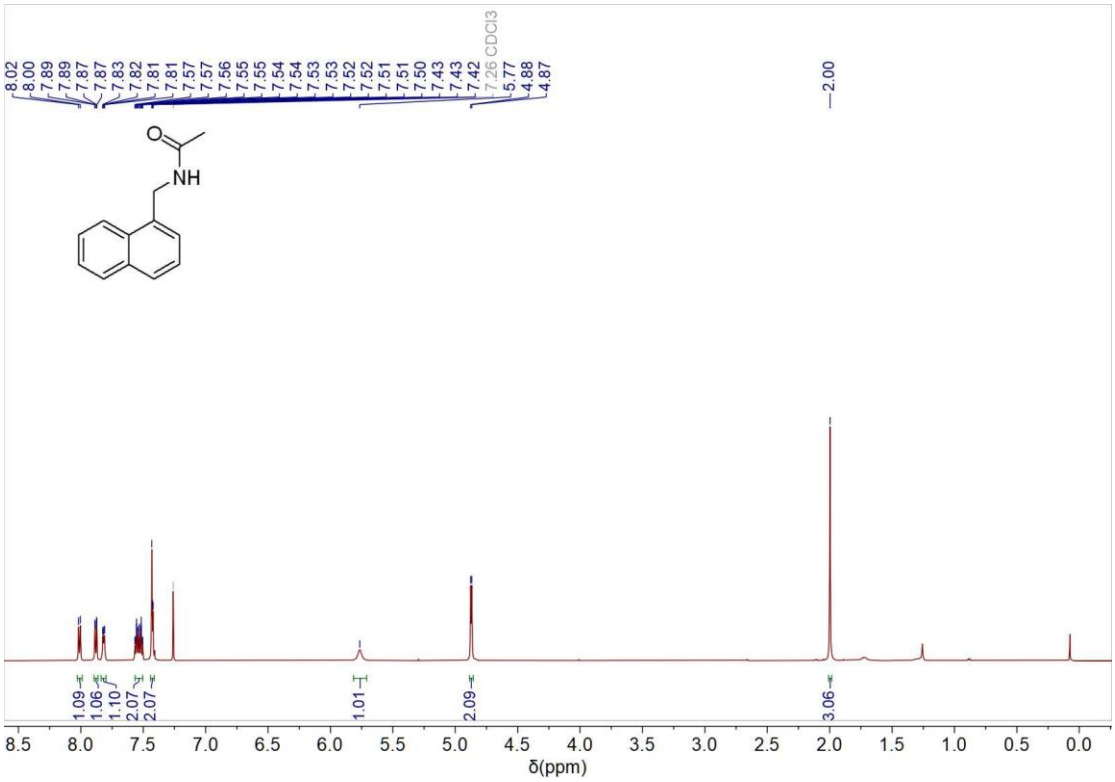
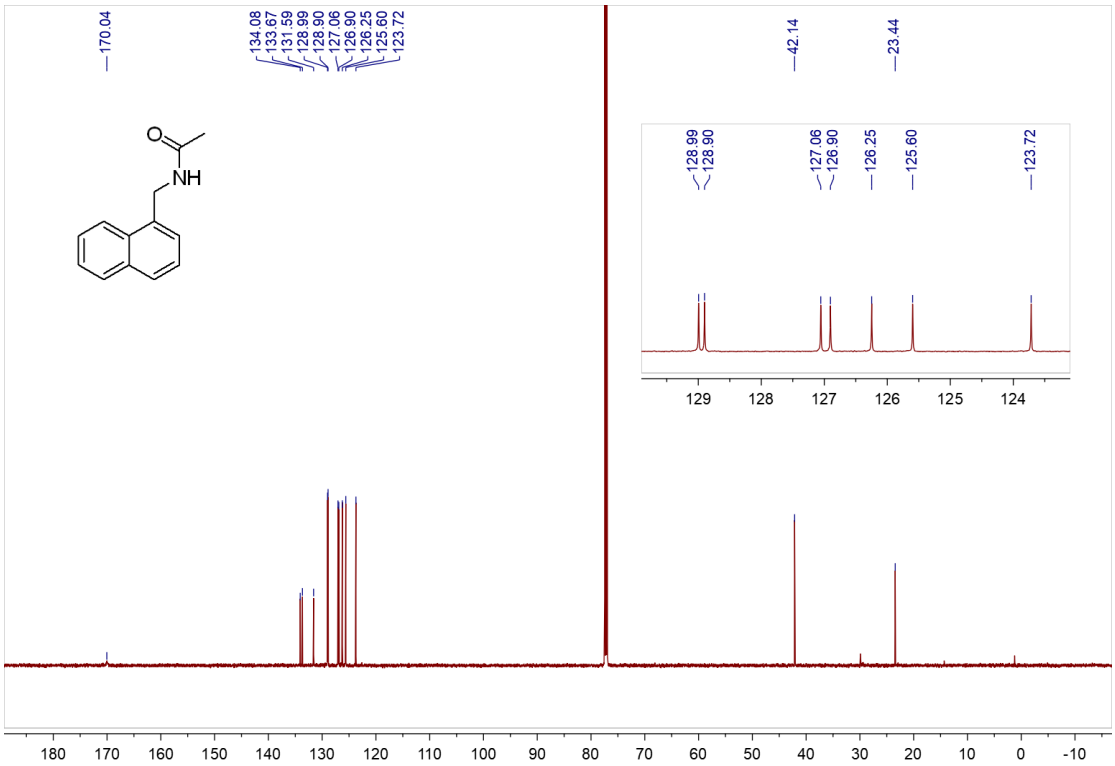


^{13}C NMR of compound 14



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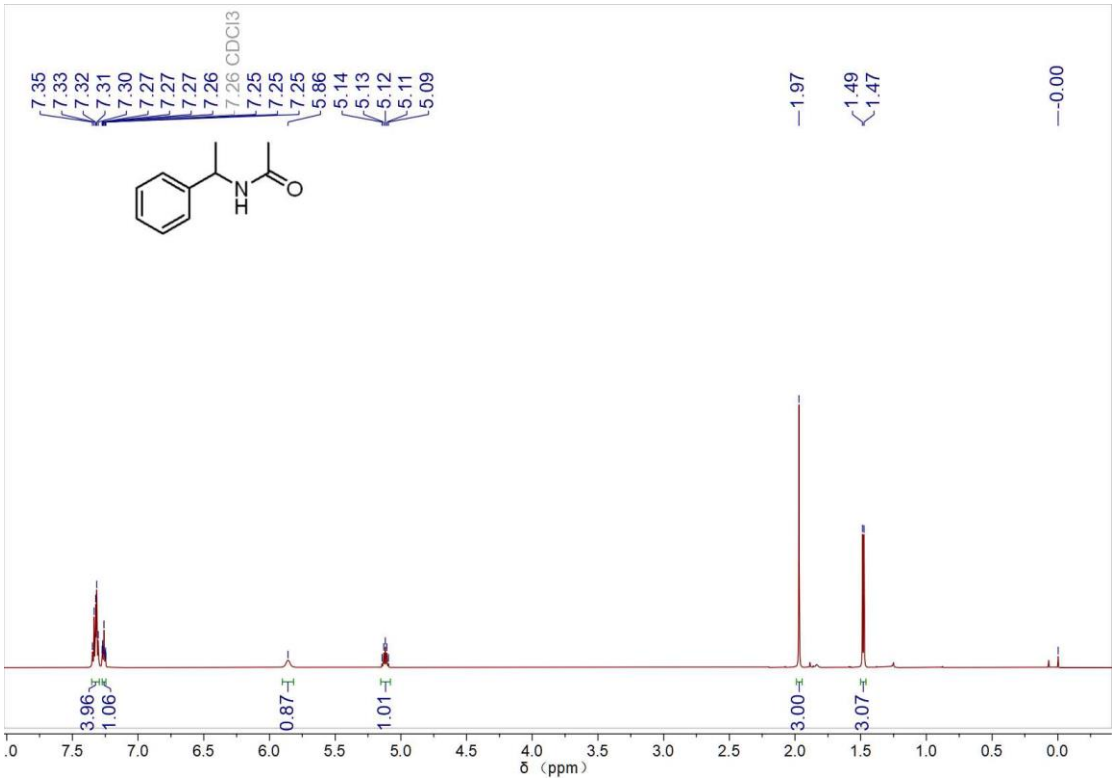

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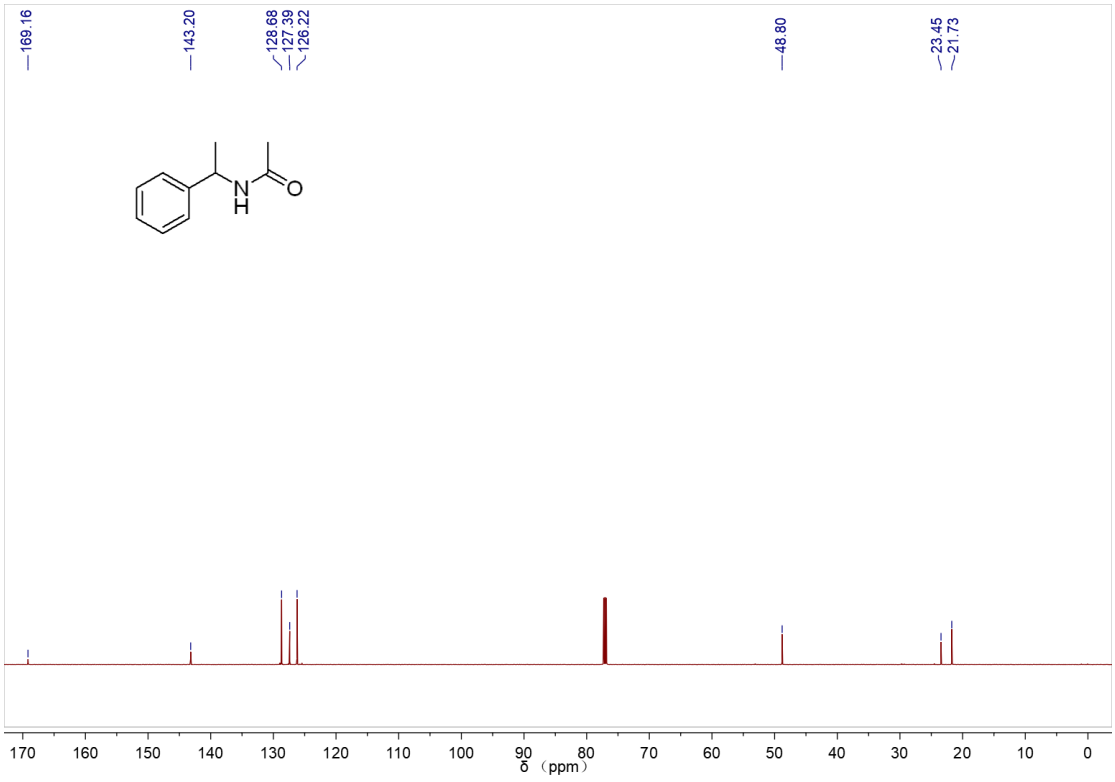
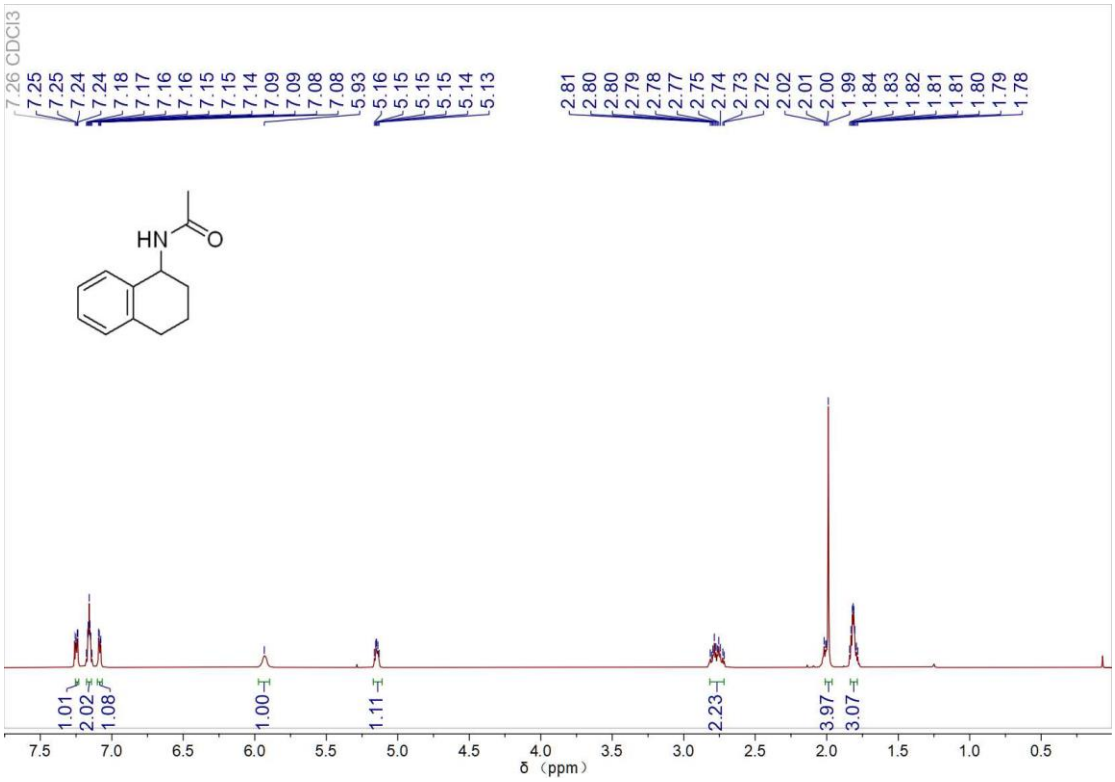


^{1}H NMR of compound 16



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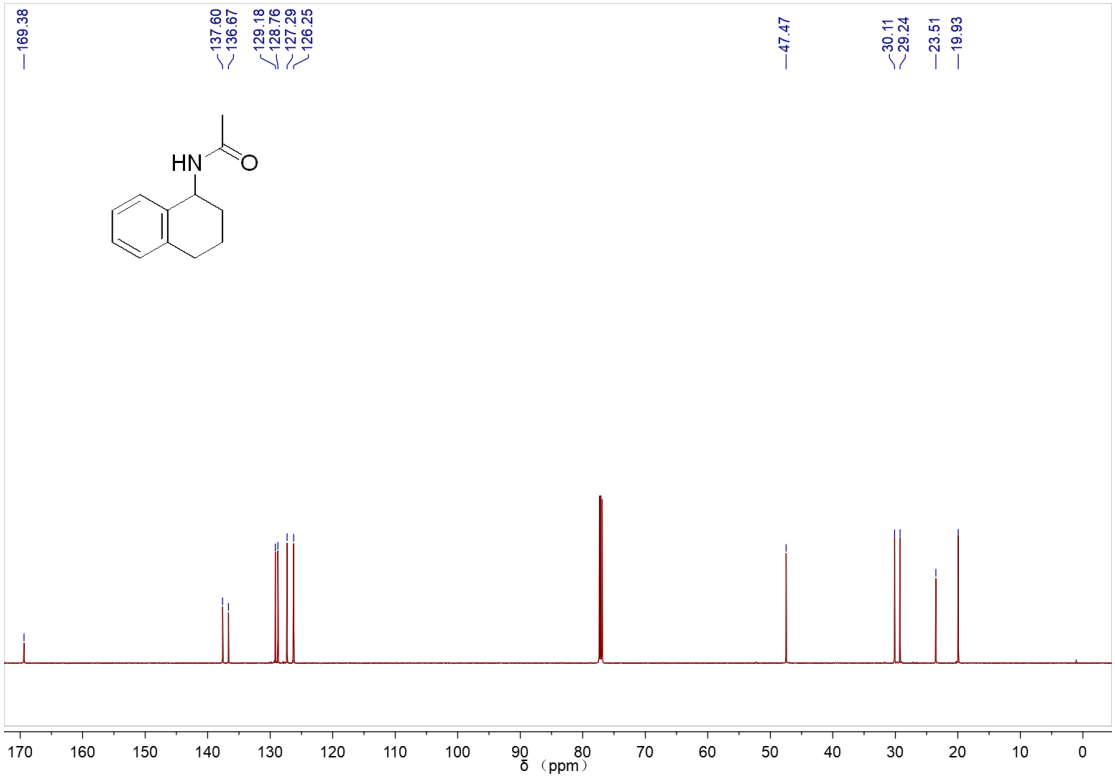

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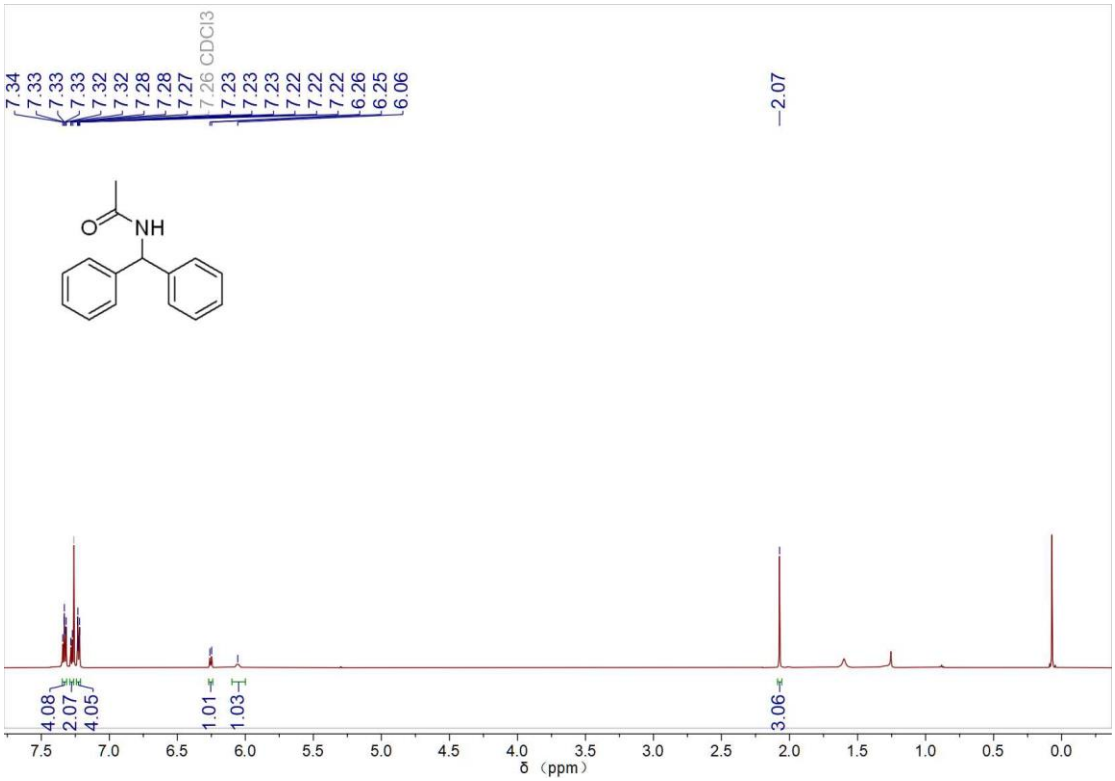

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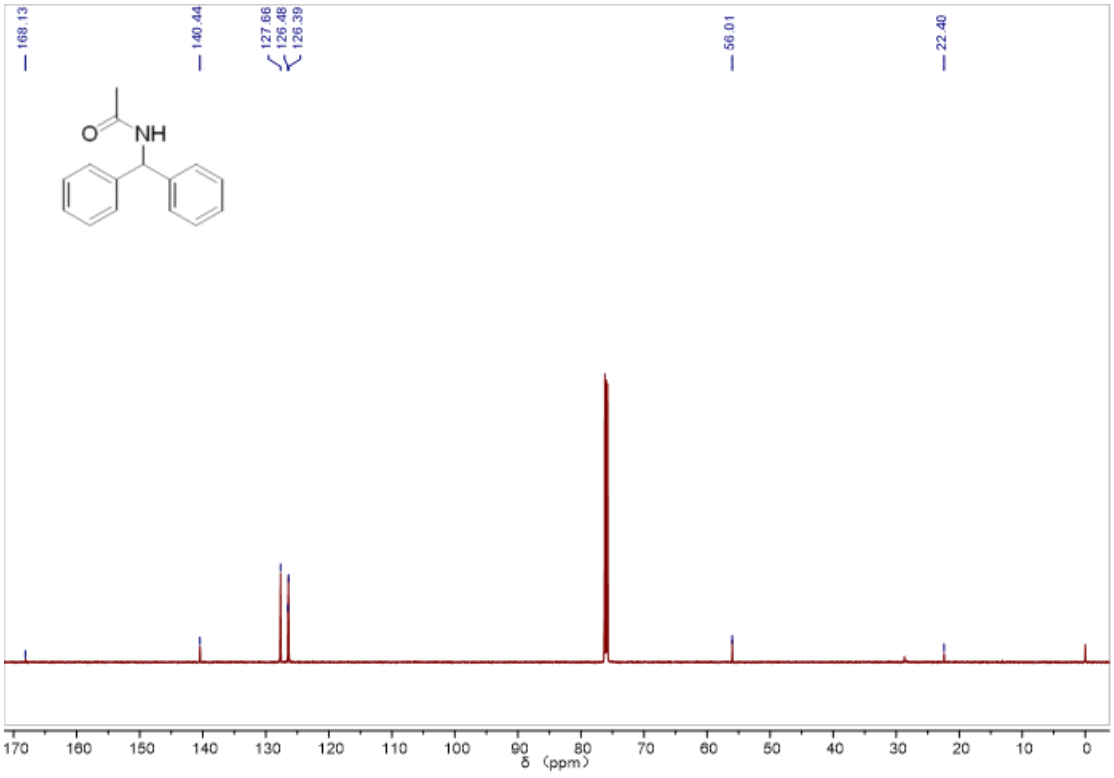
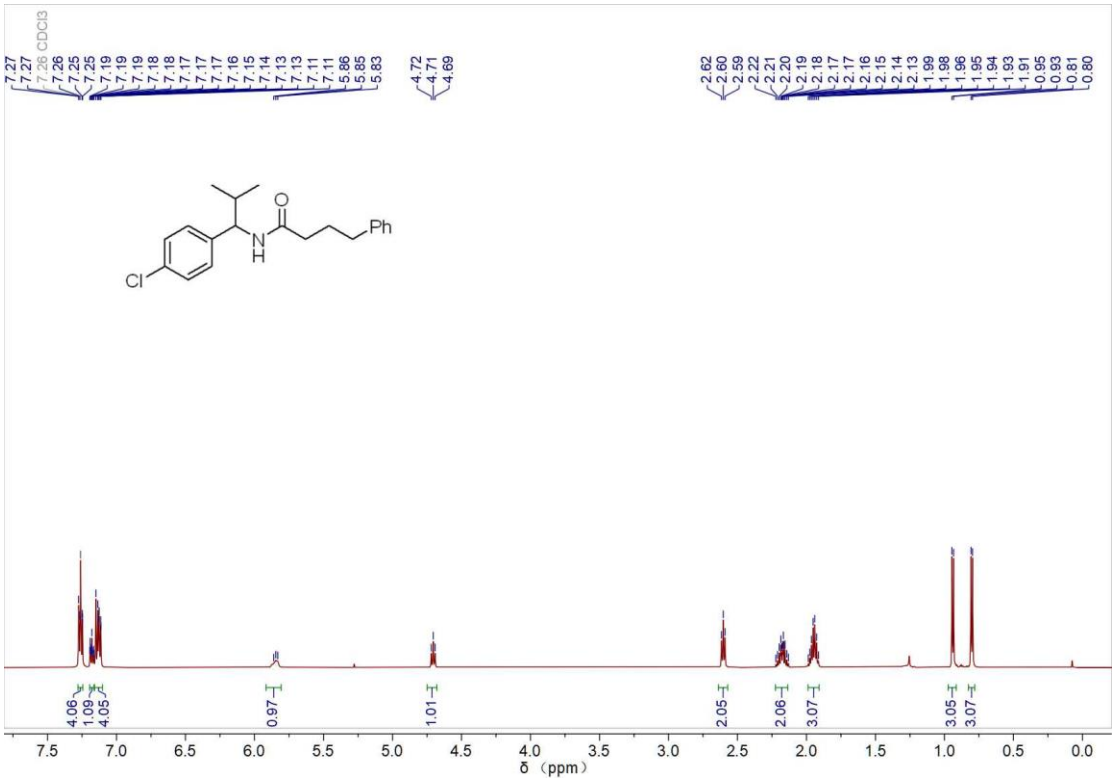


^{1}H NMR of compound 18



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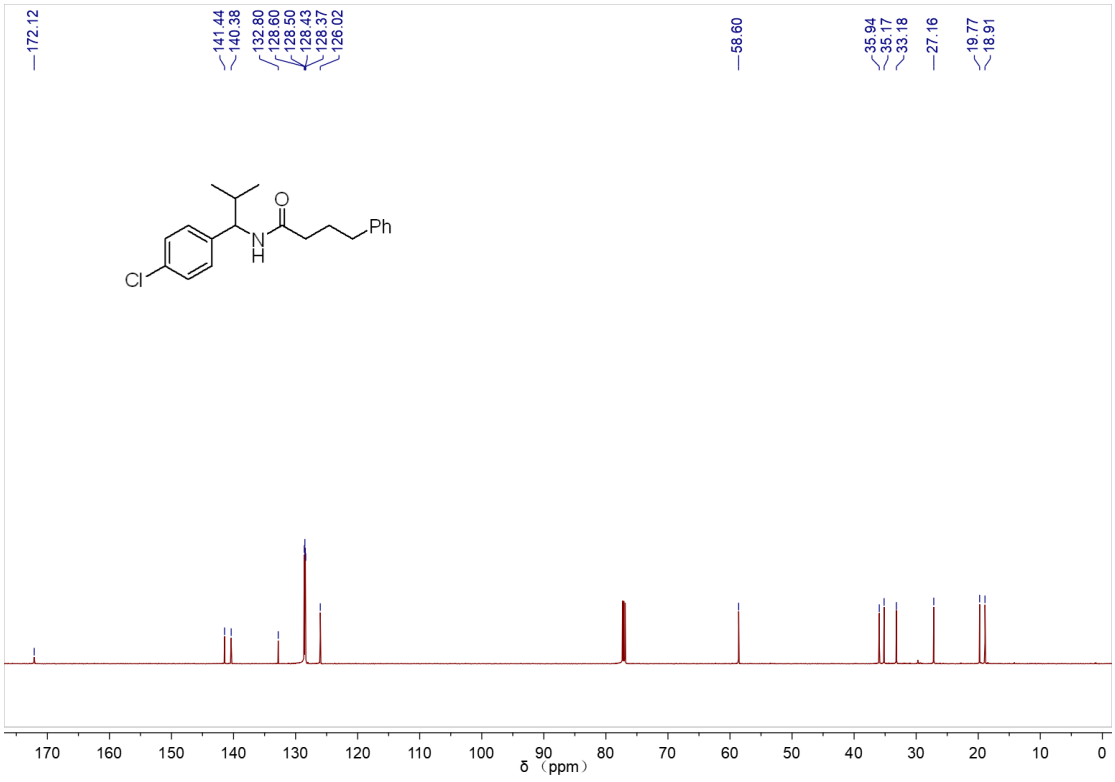
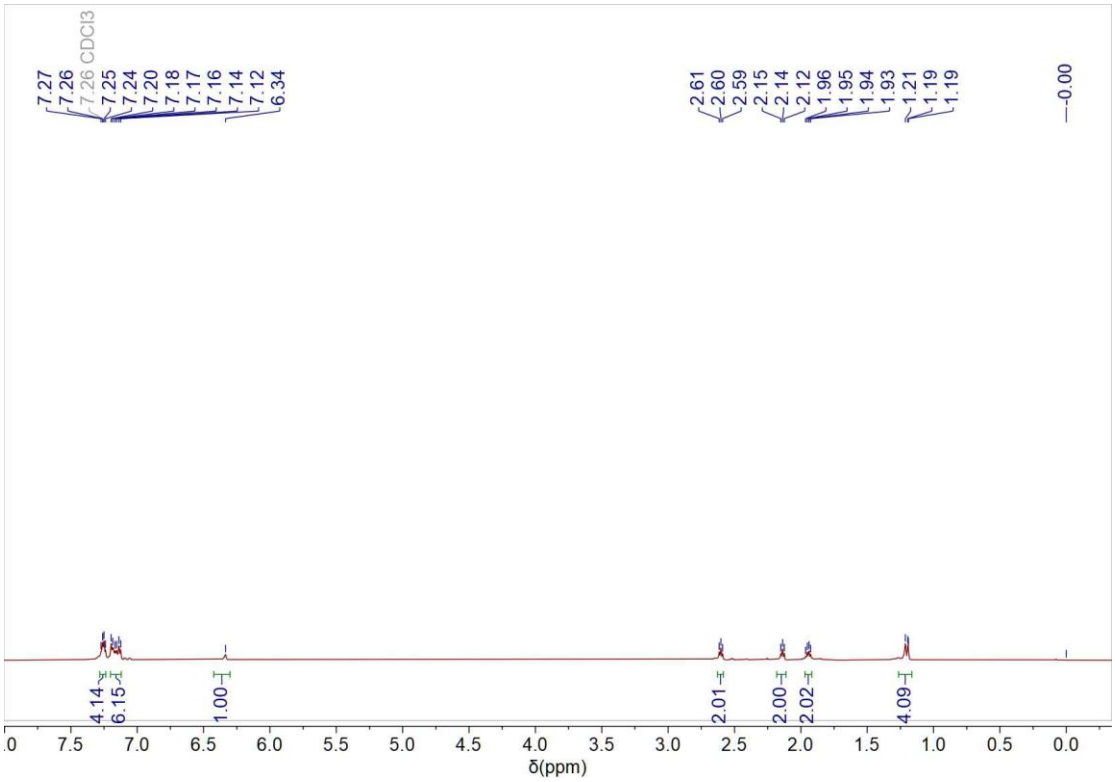


^{1}H NMR of compound 19



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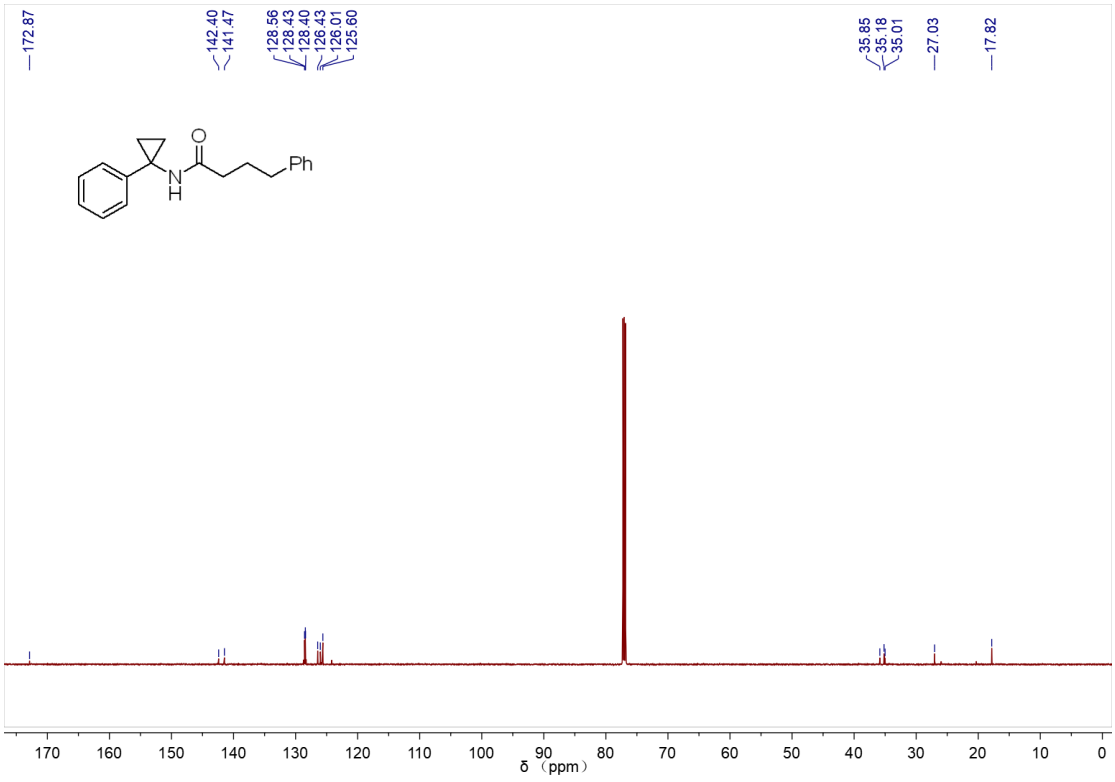

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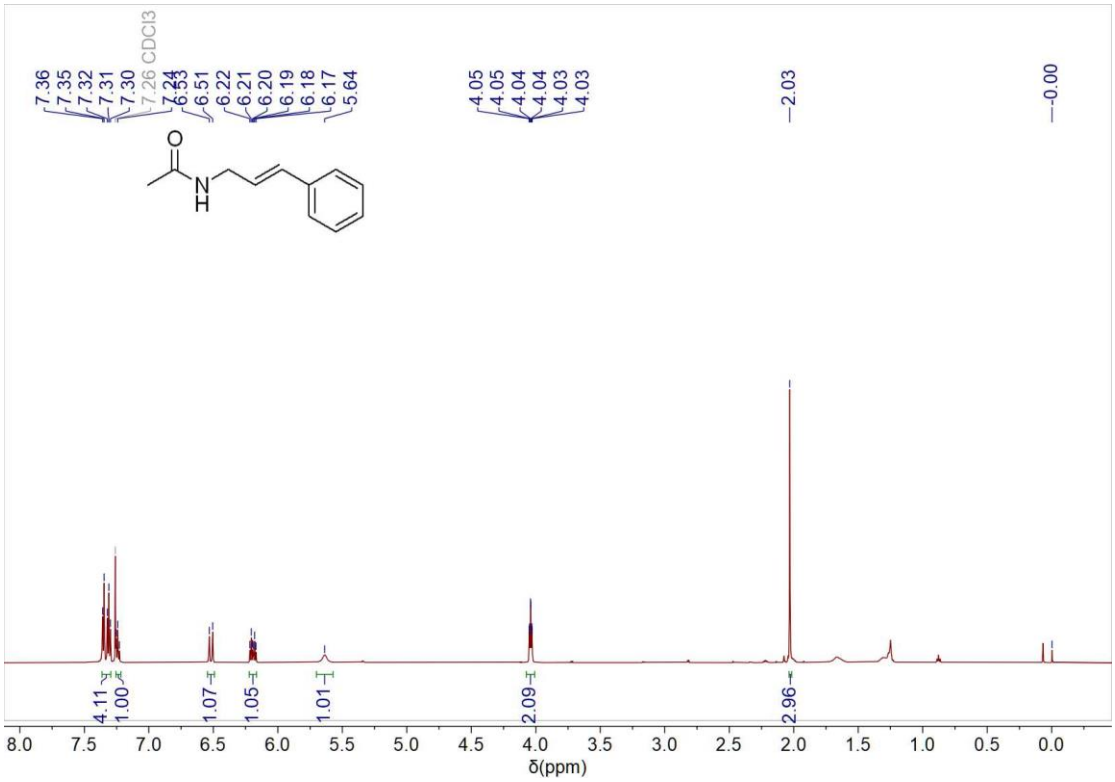

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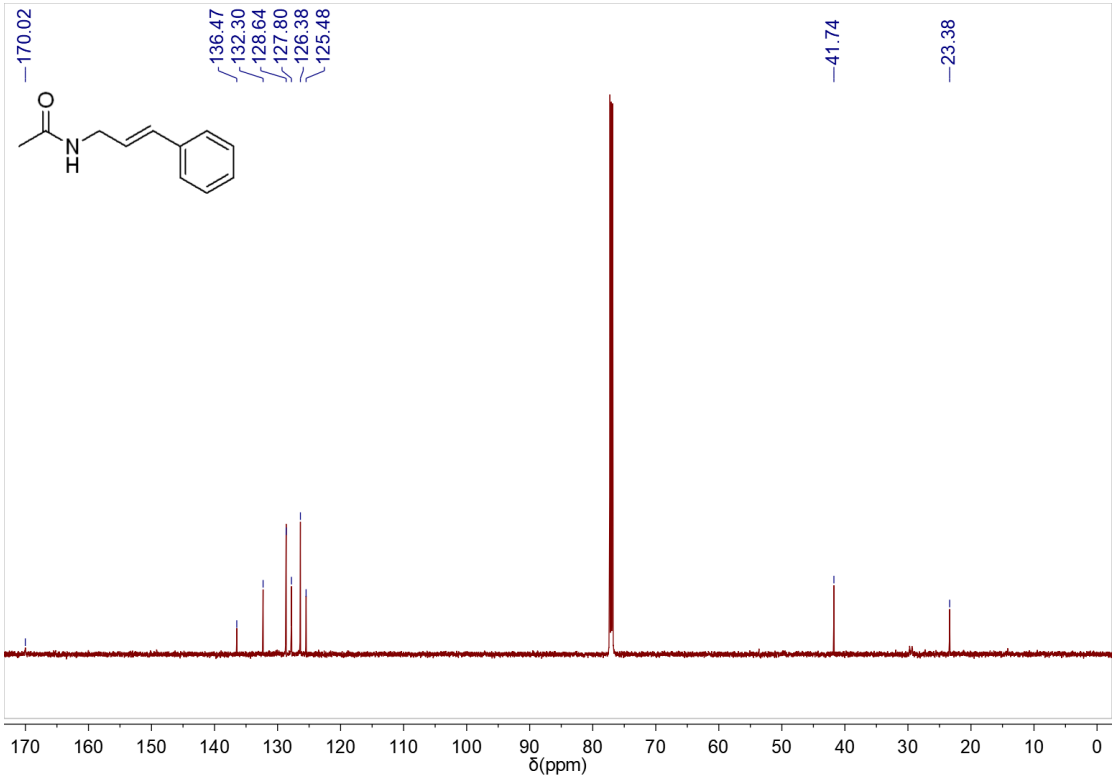

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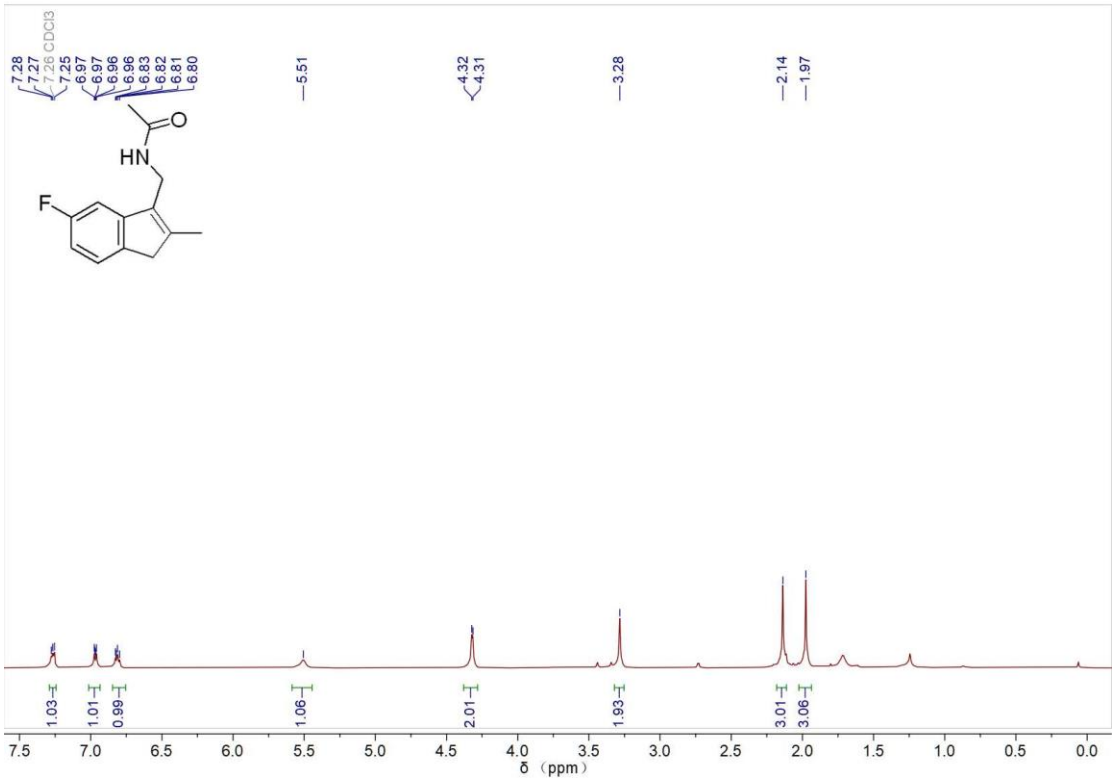

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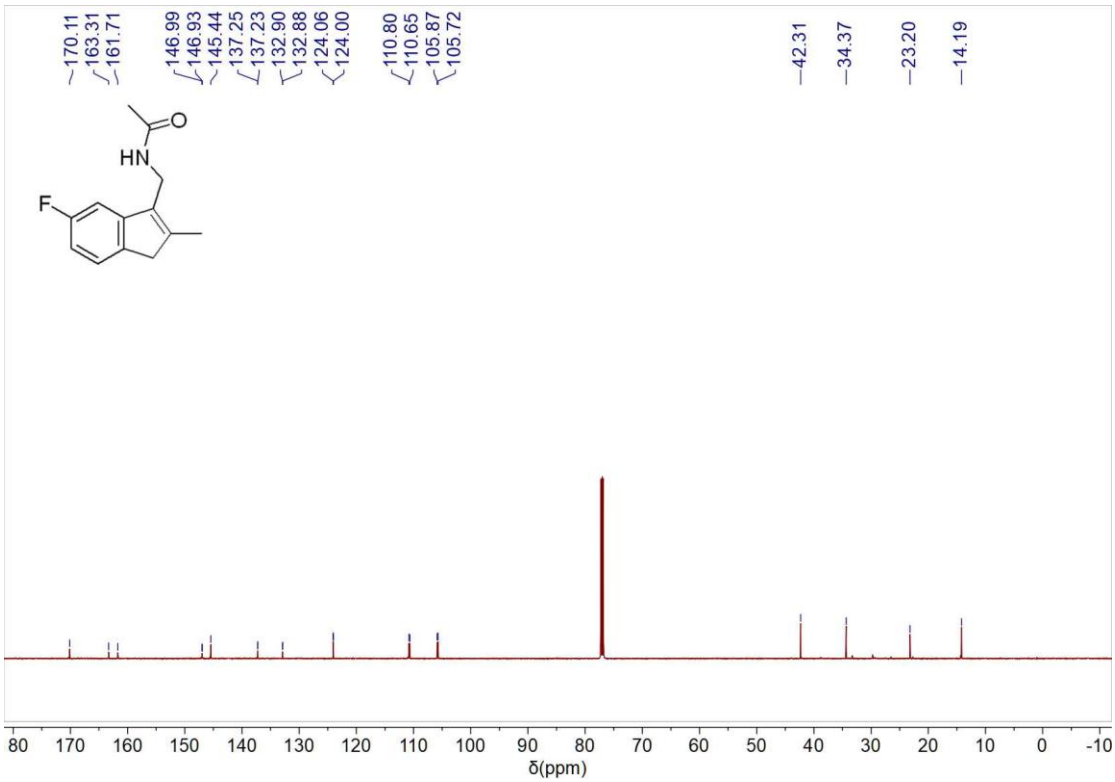
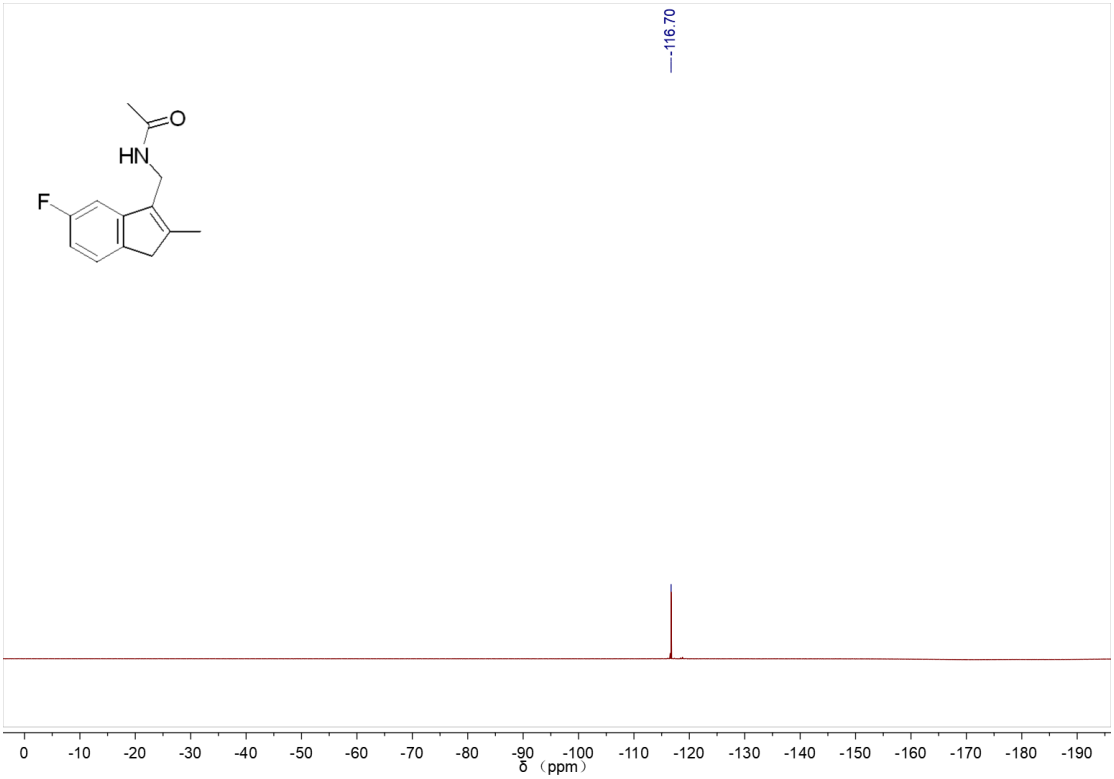
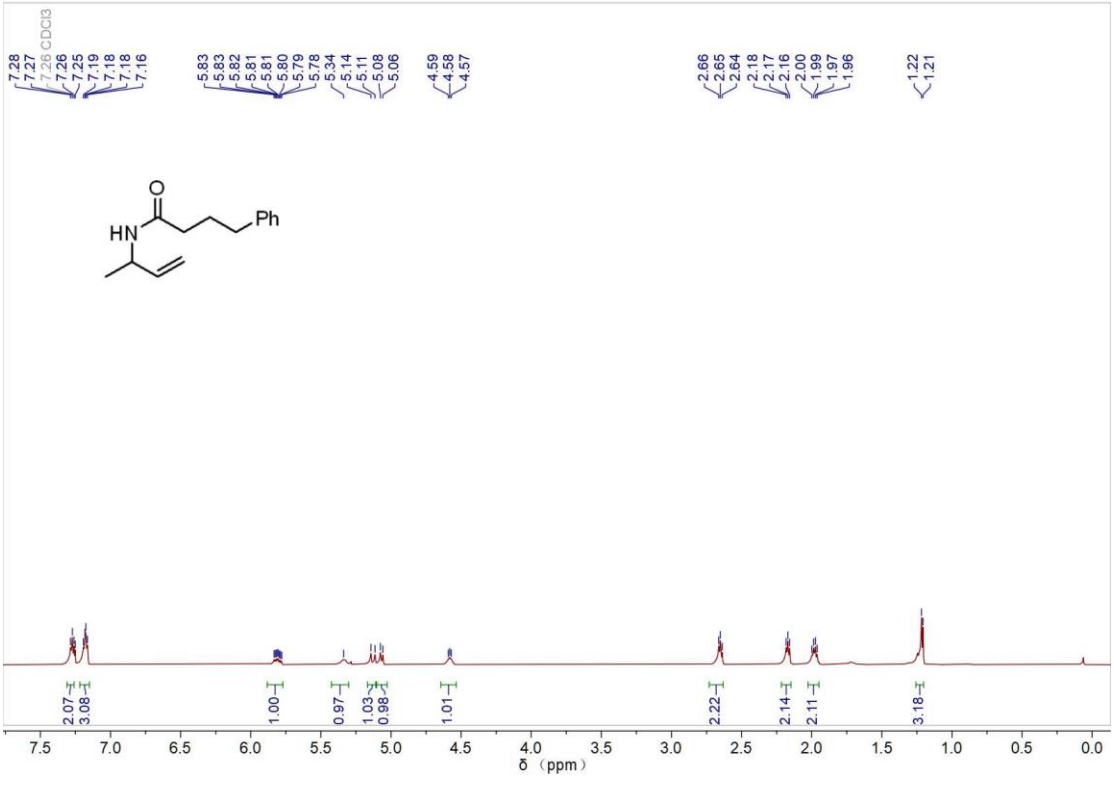


^{19}F NMR of compound 21



^{1}H NMR of compound 22



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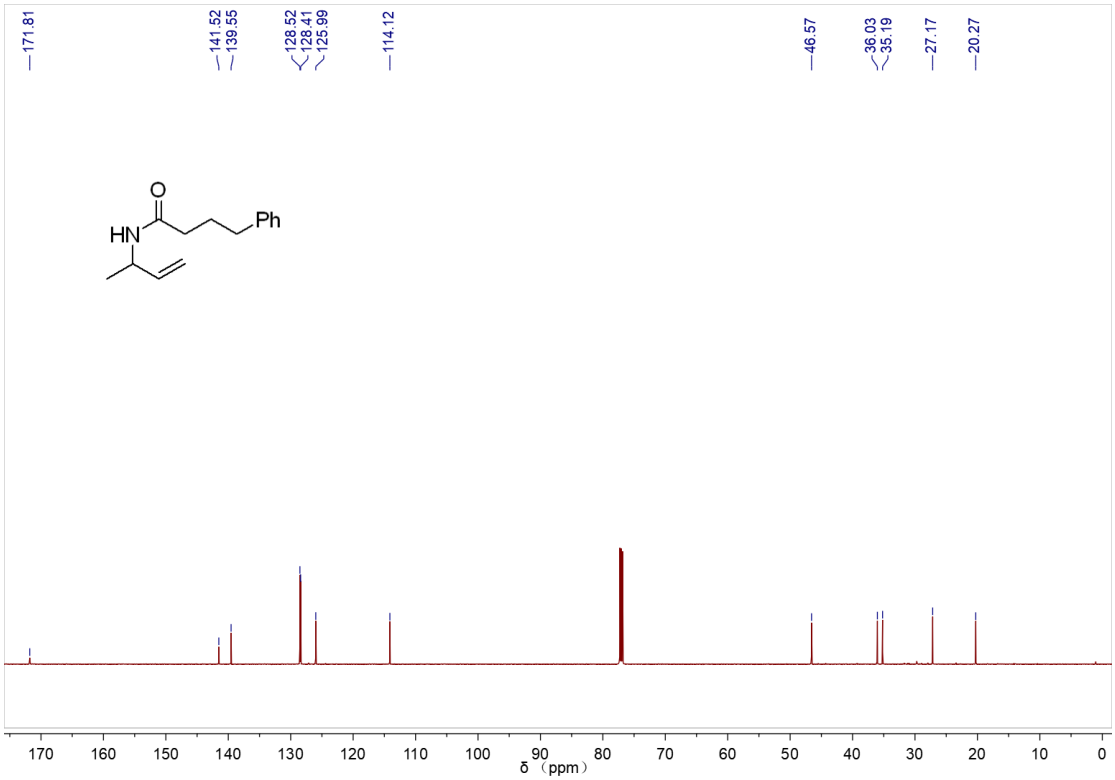
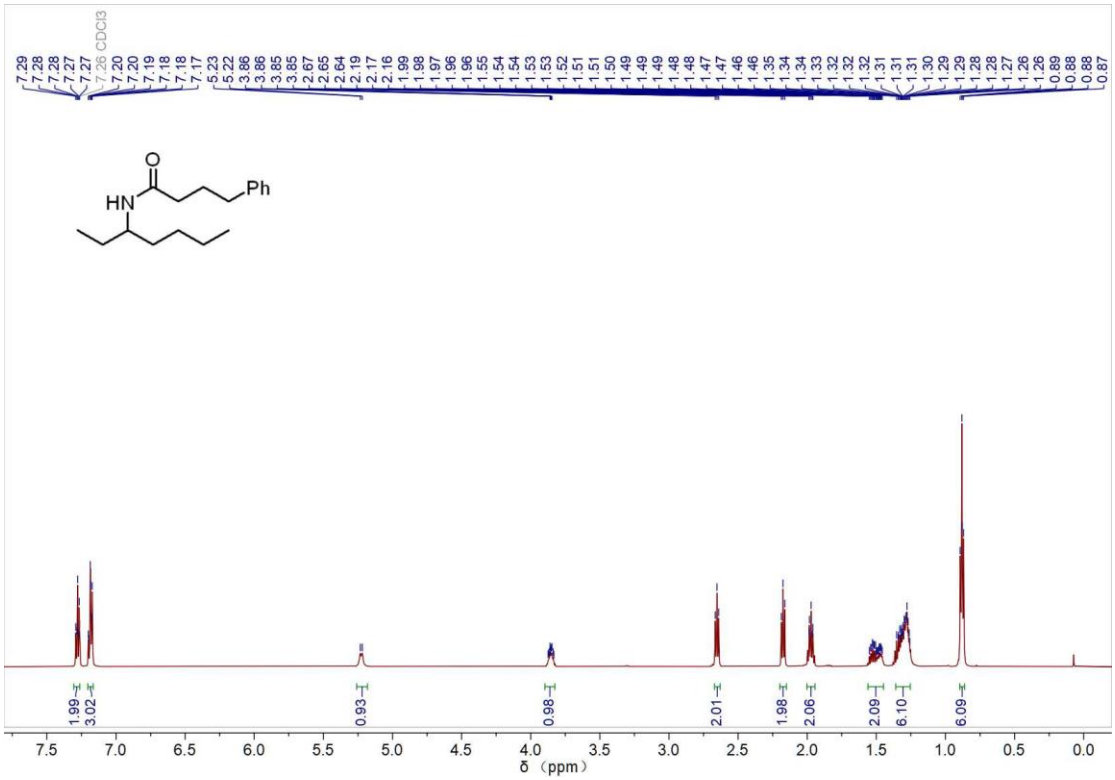


^{1}H NMR of compound 23



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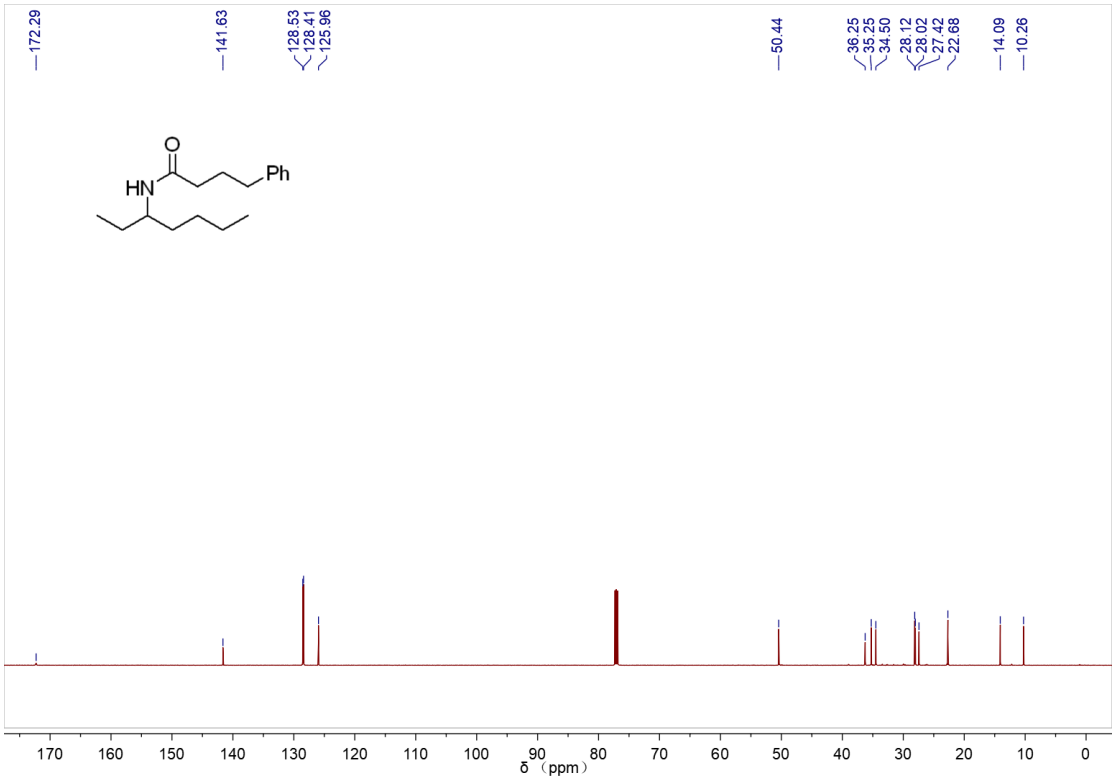
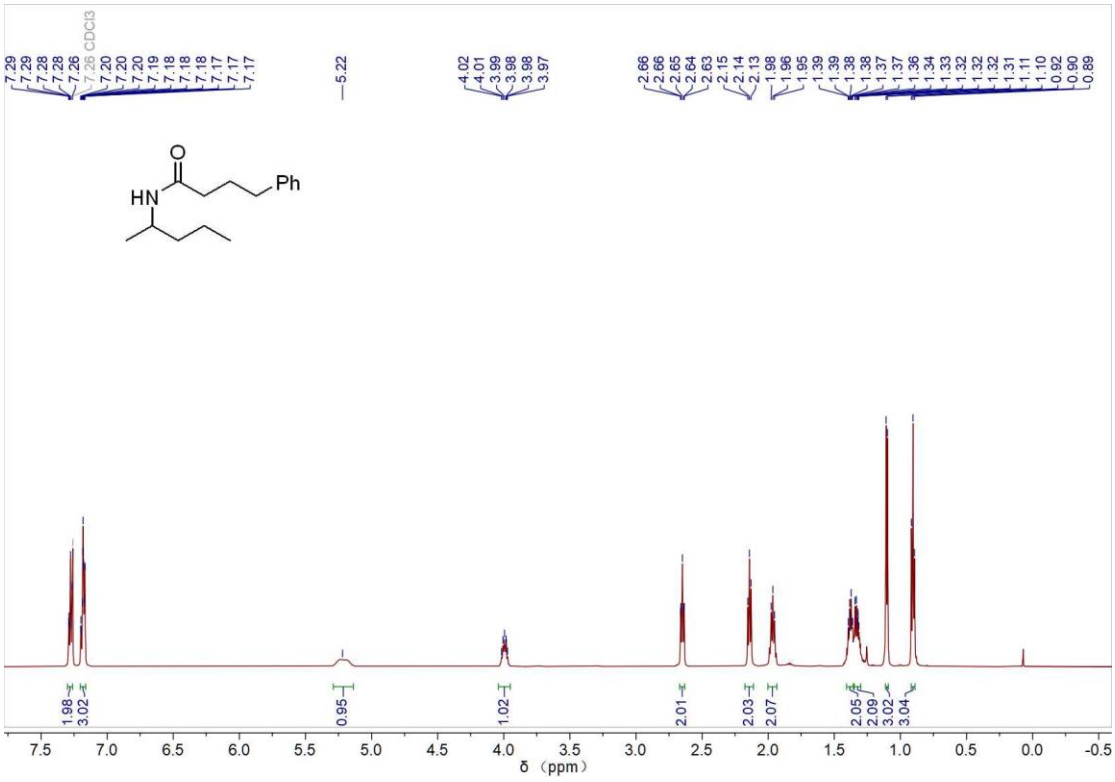


^{1}H NMR of compound 24



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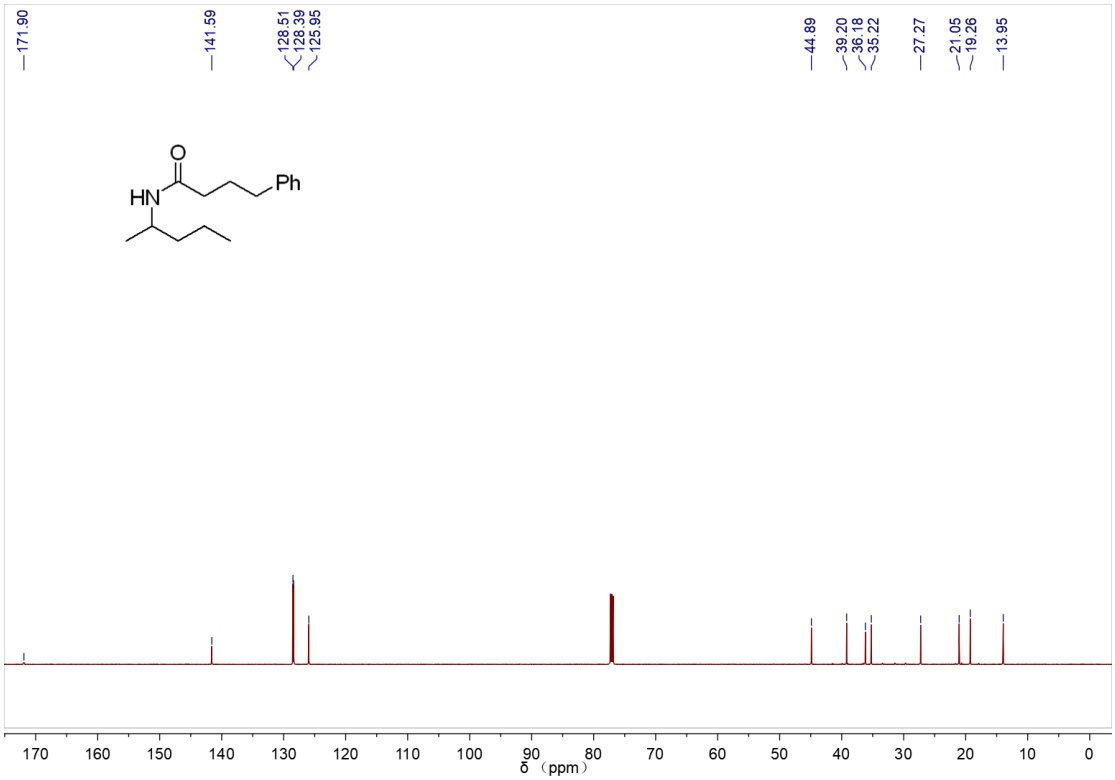

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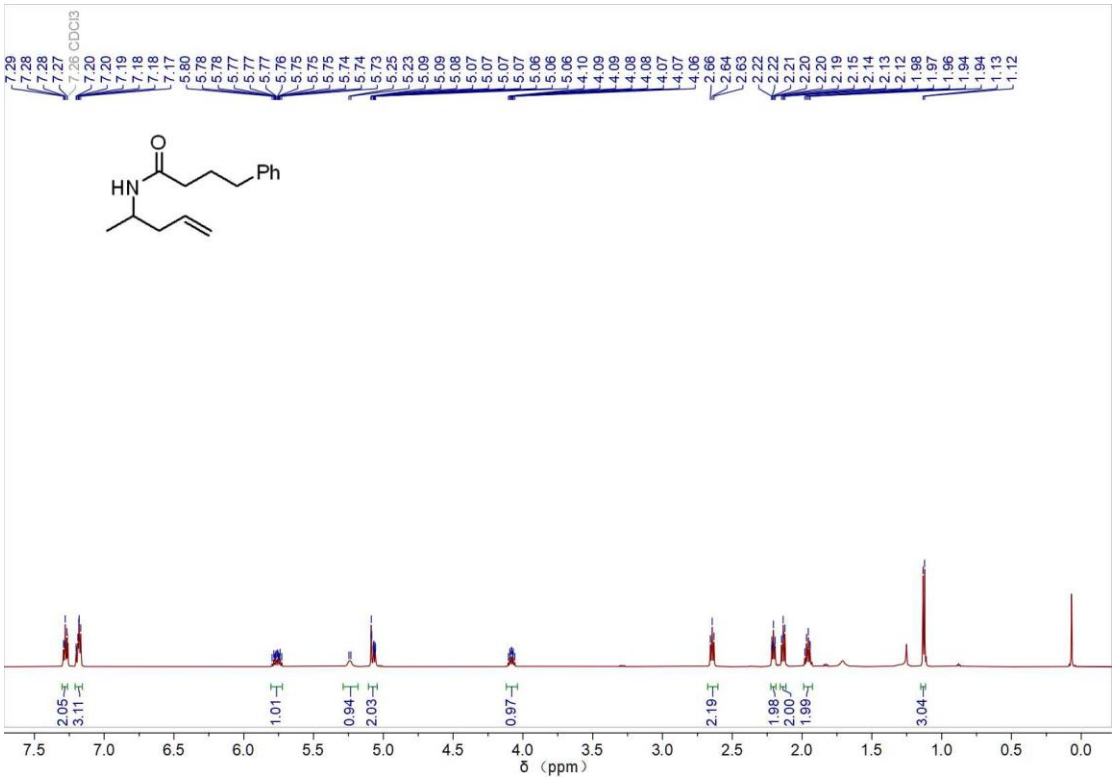

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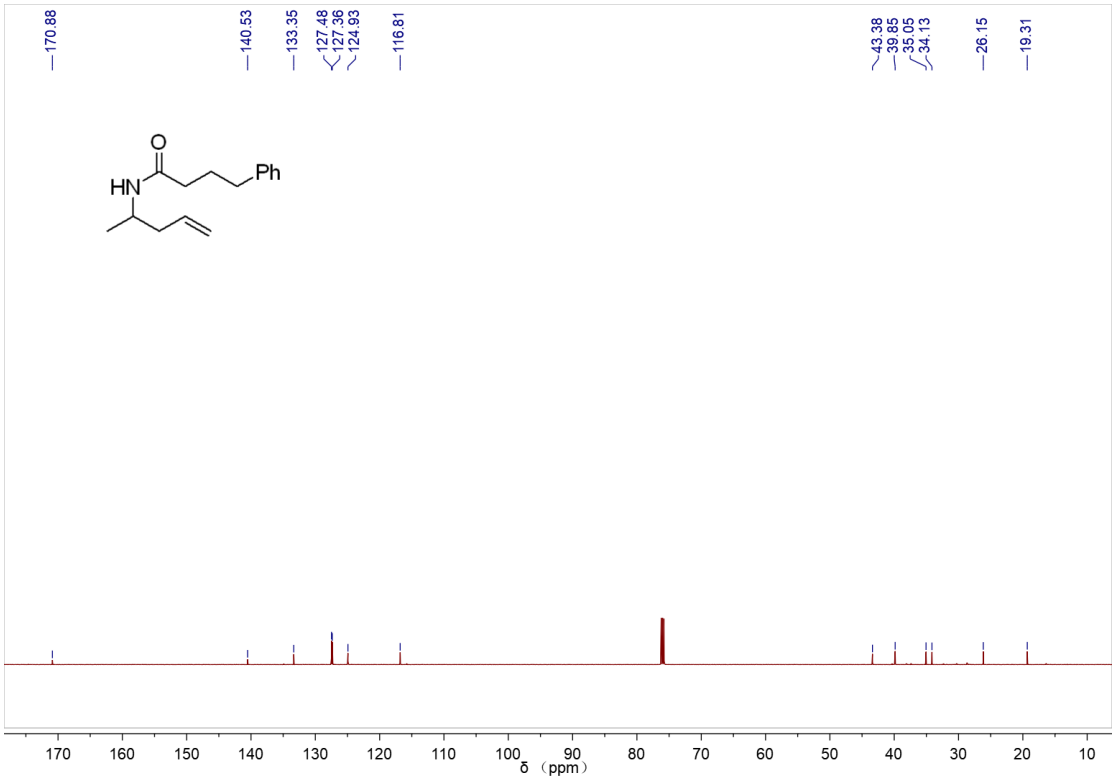

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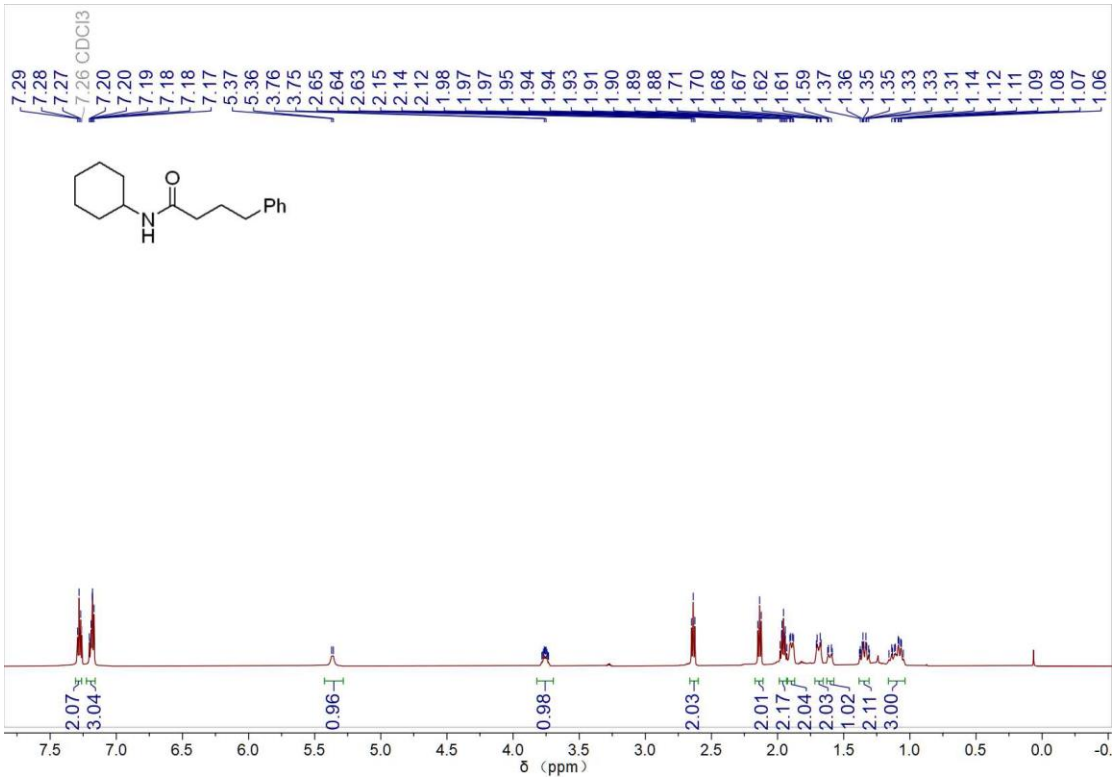

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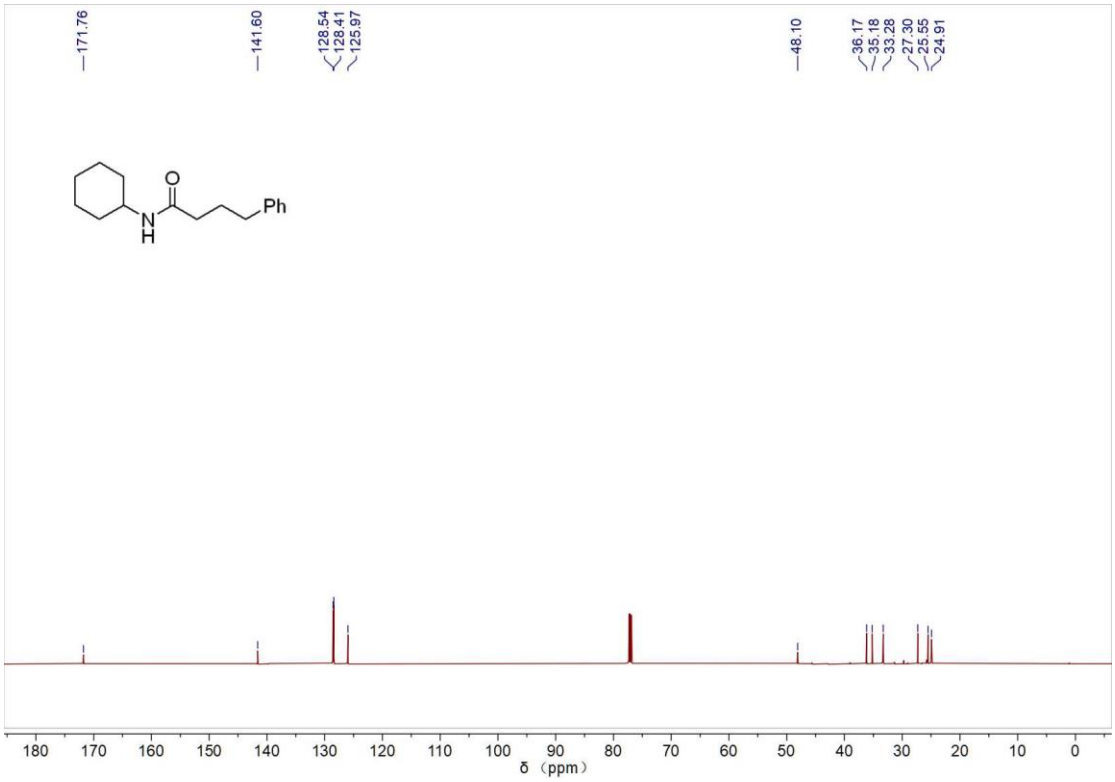
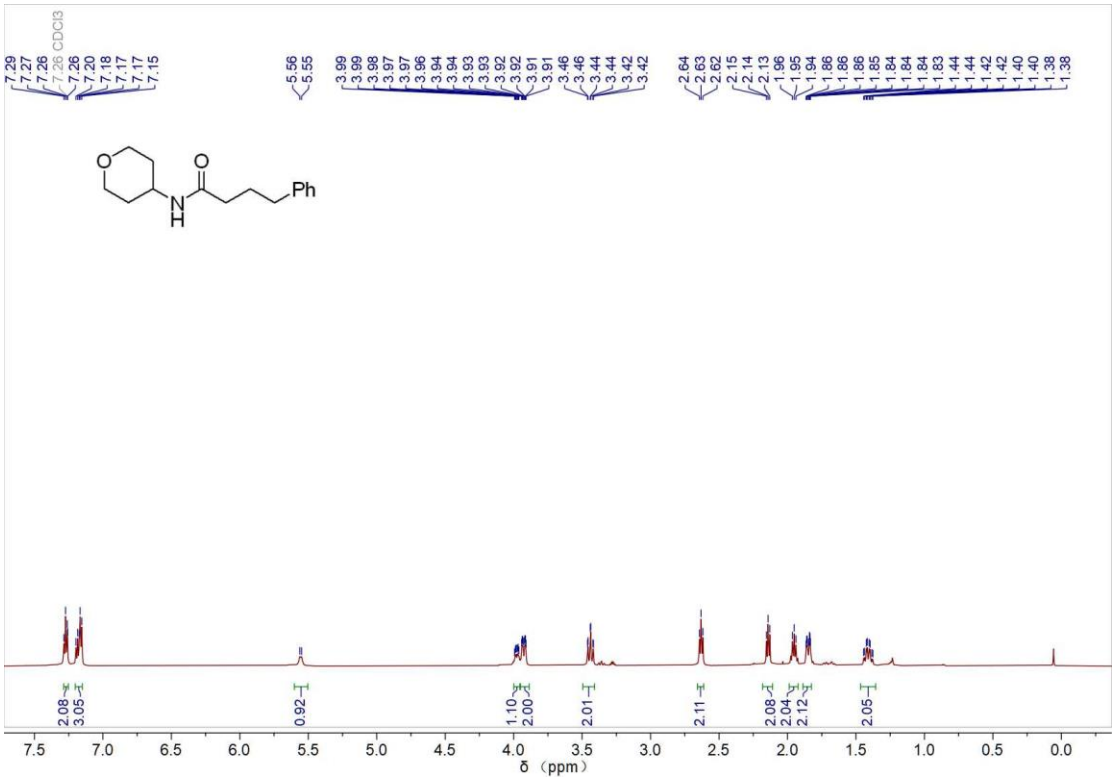
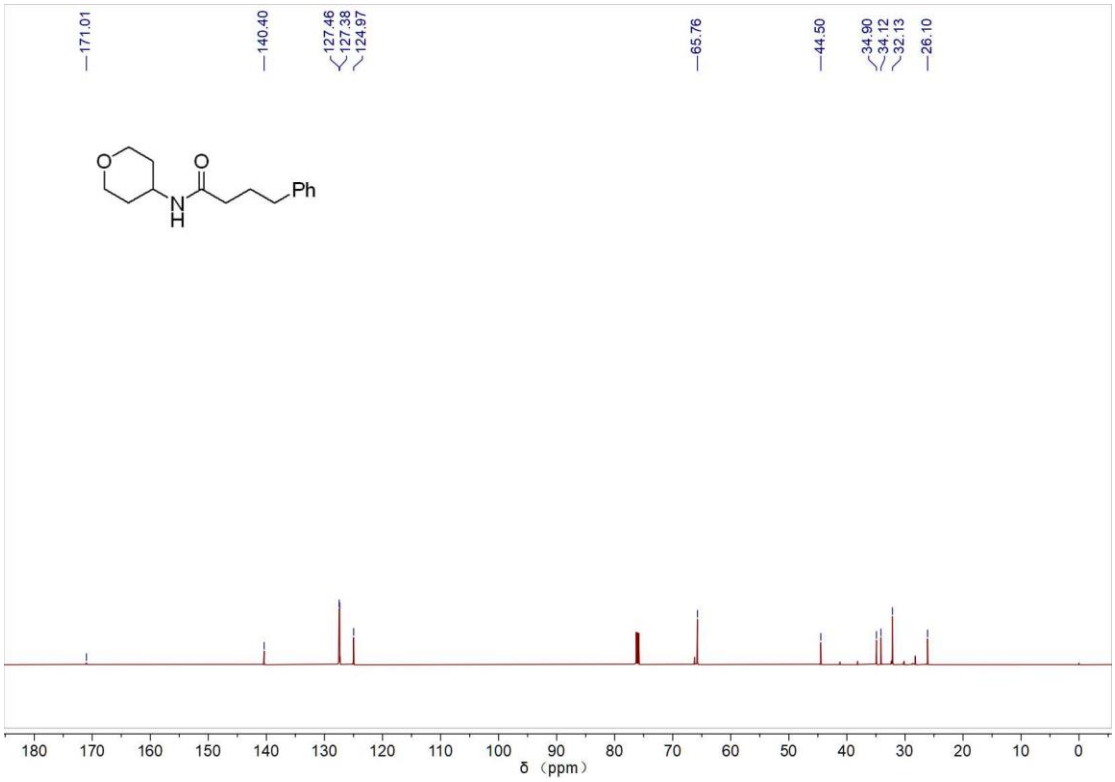


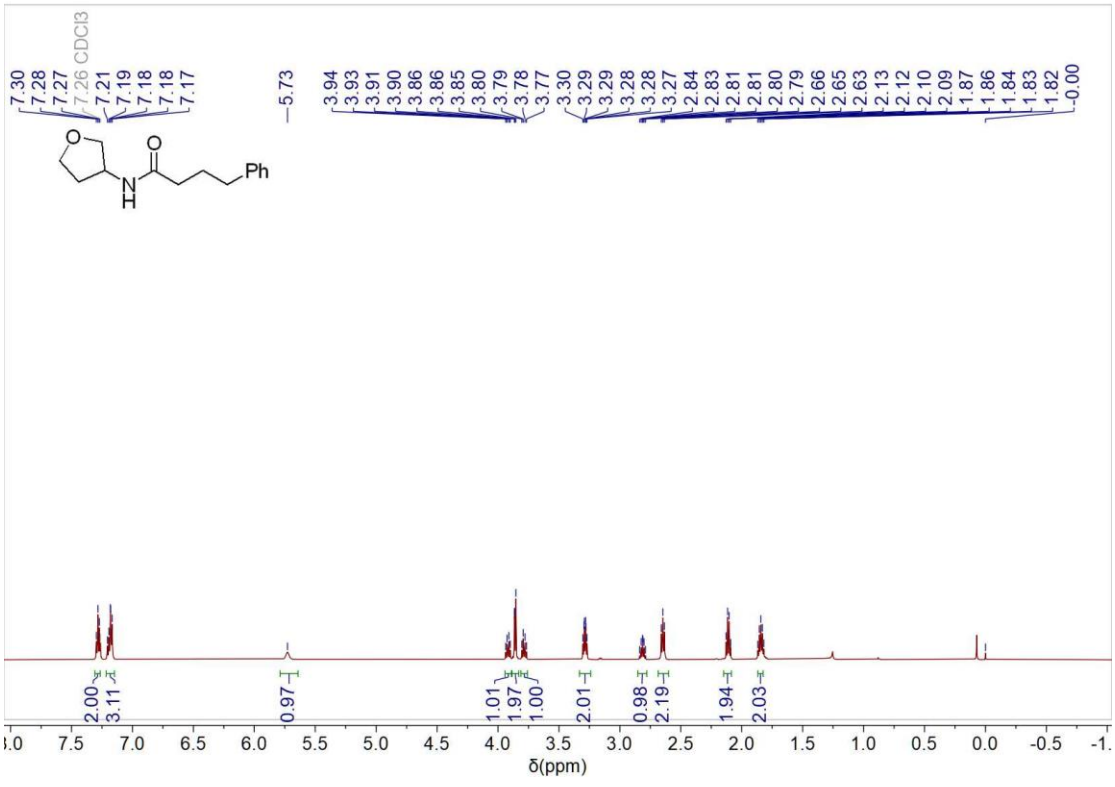
^{1}H NMR of compound 27



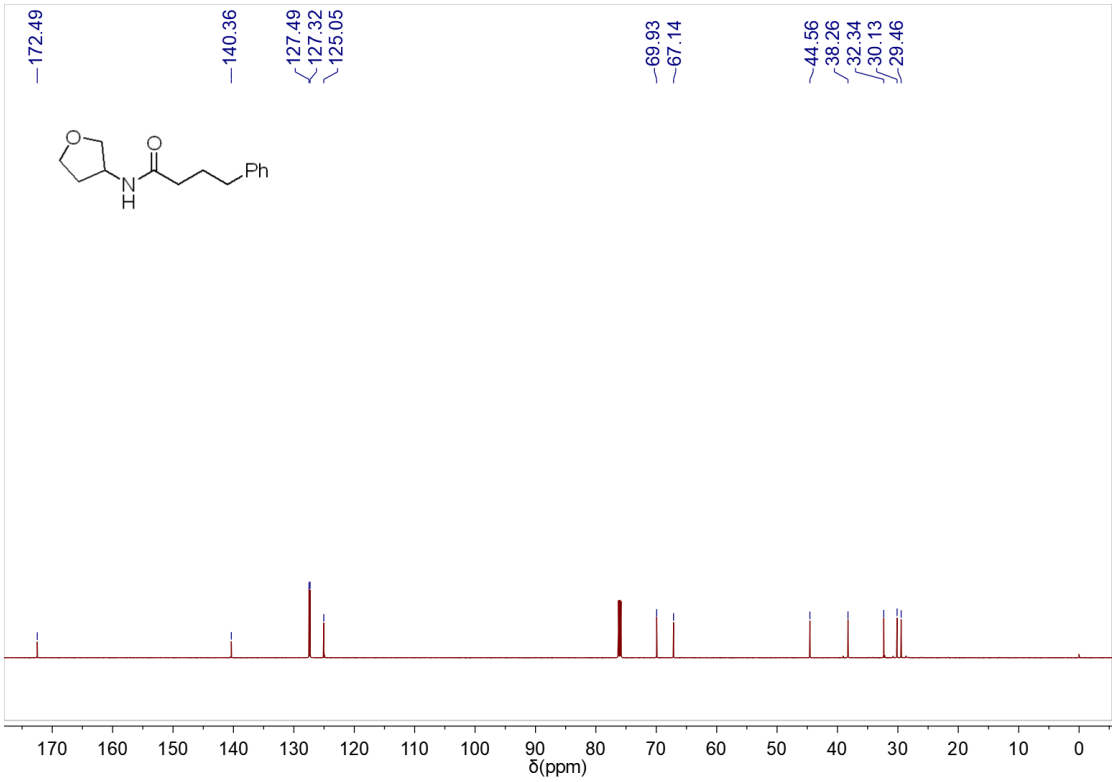
^{13}C NMR of compound 27



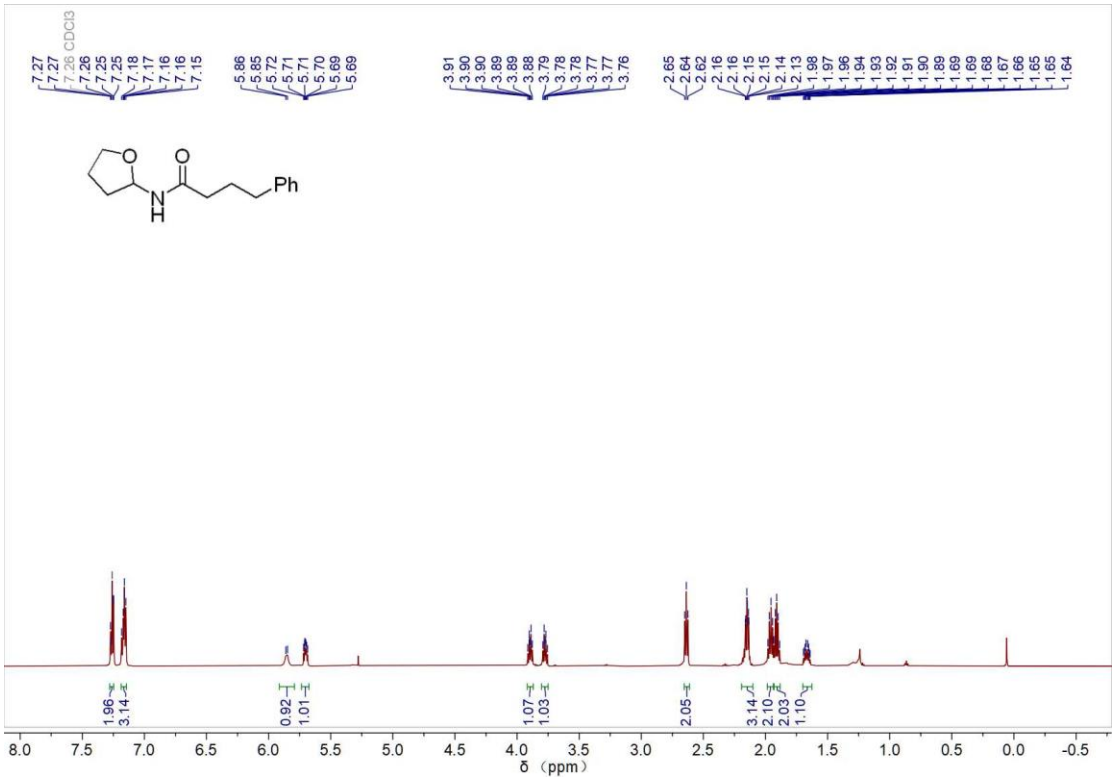
^{1}H NMR of compound 28



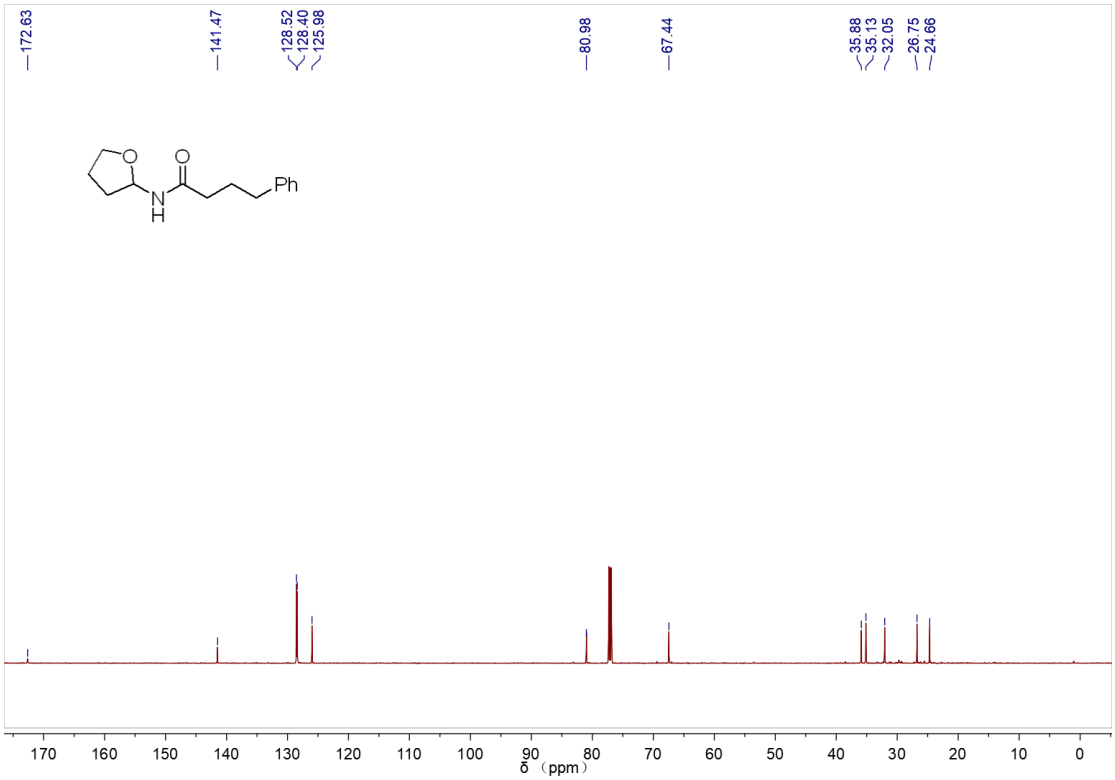
^{13}C NMR of compound 28



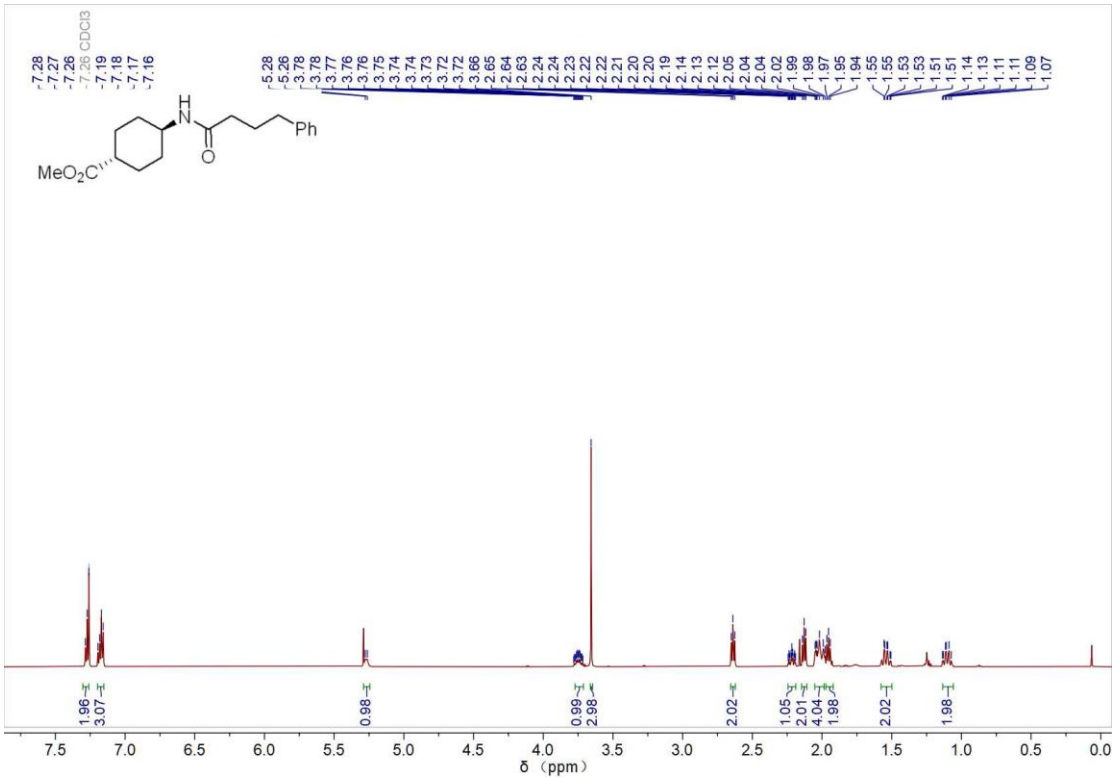
^{1}H NMR of compound 29



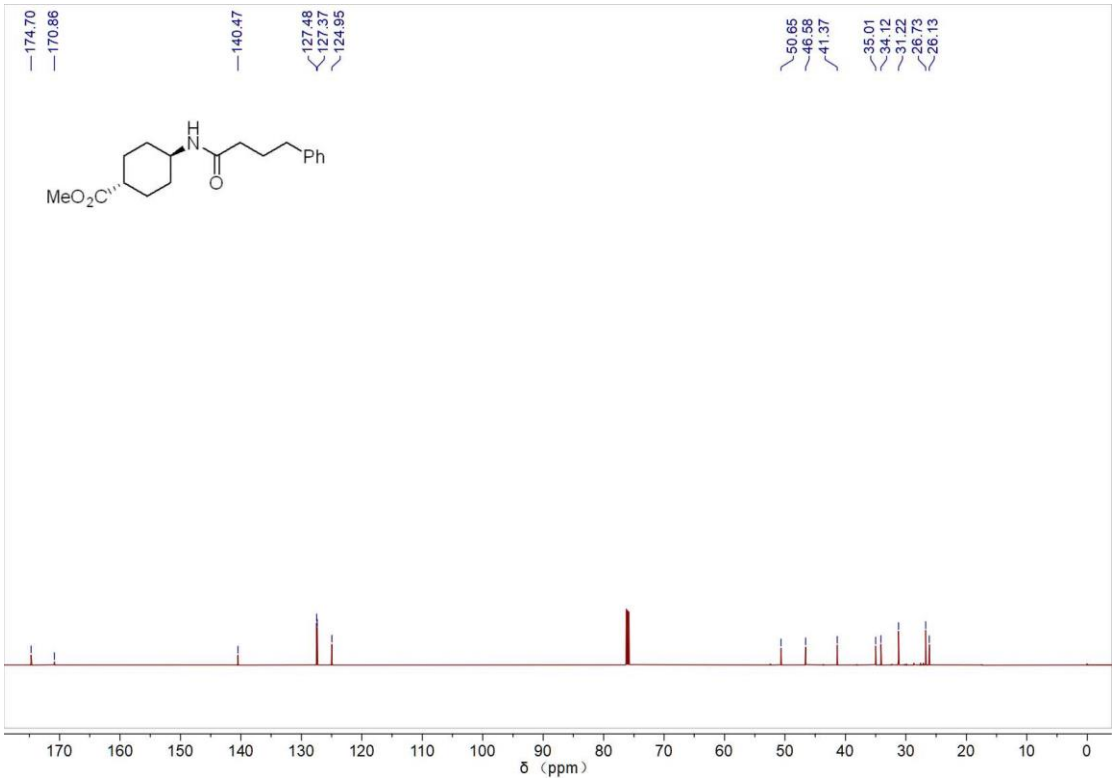
^{13}C NMR of compound 29



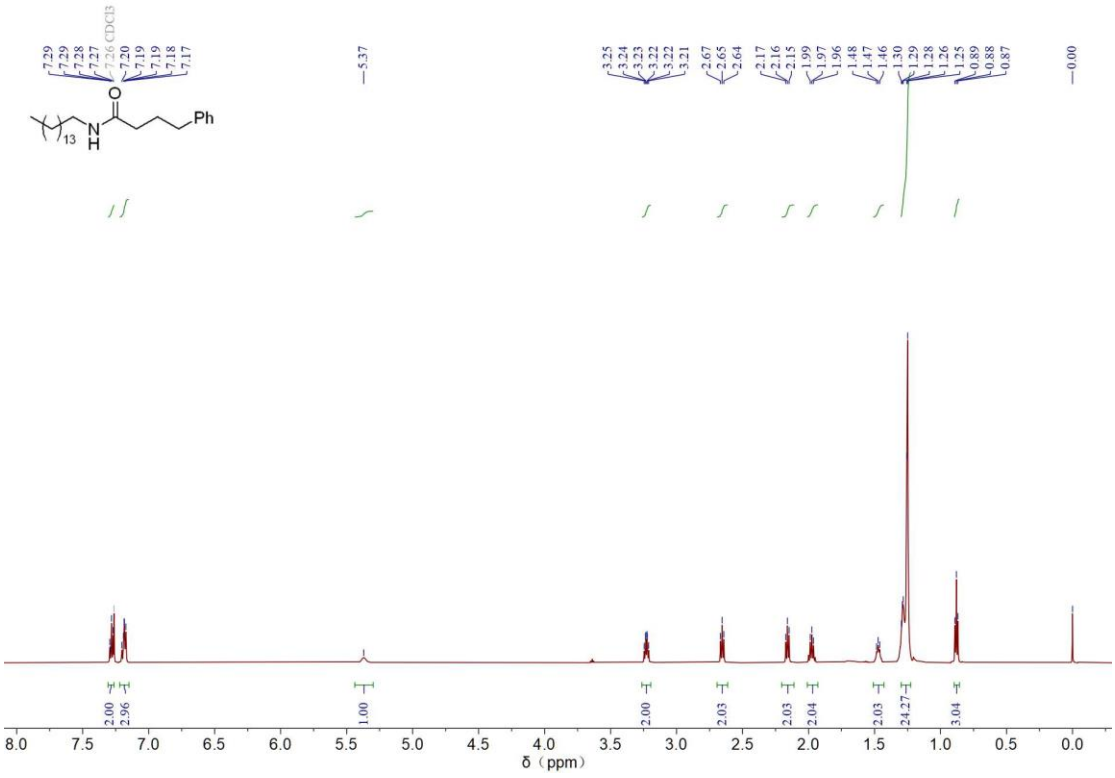
^{1}H NMR of compound 30



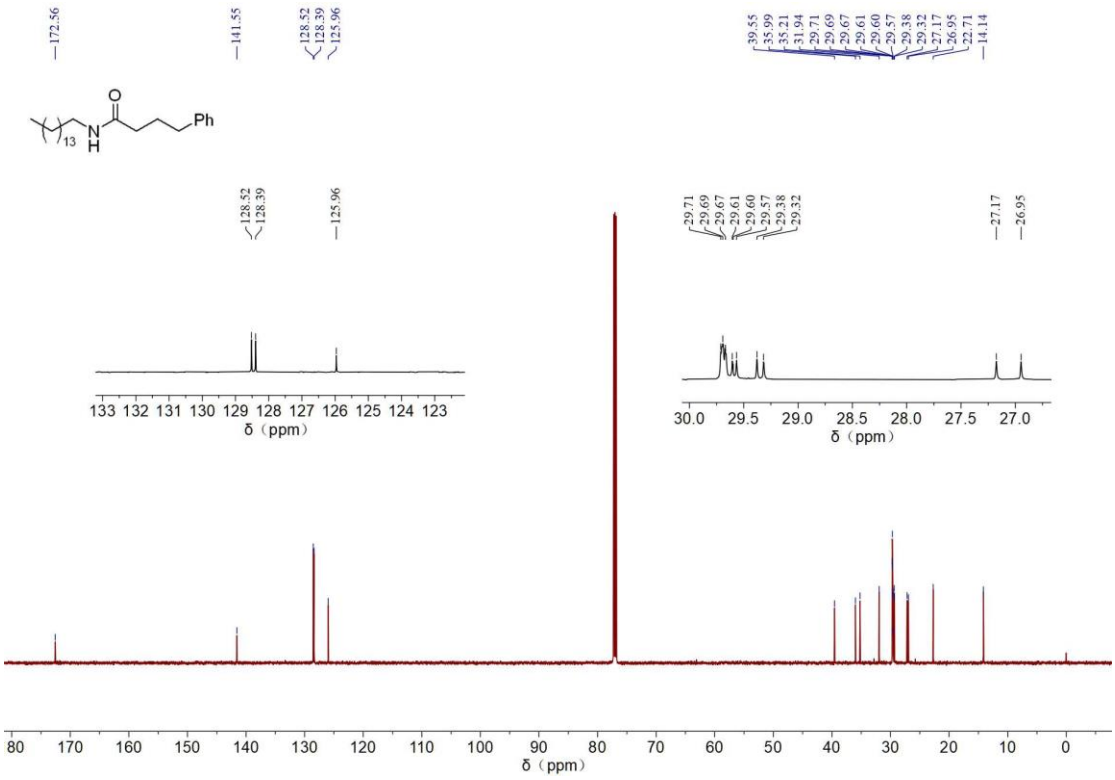
^{13}C NMR of compound 30



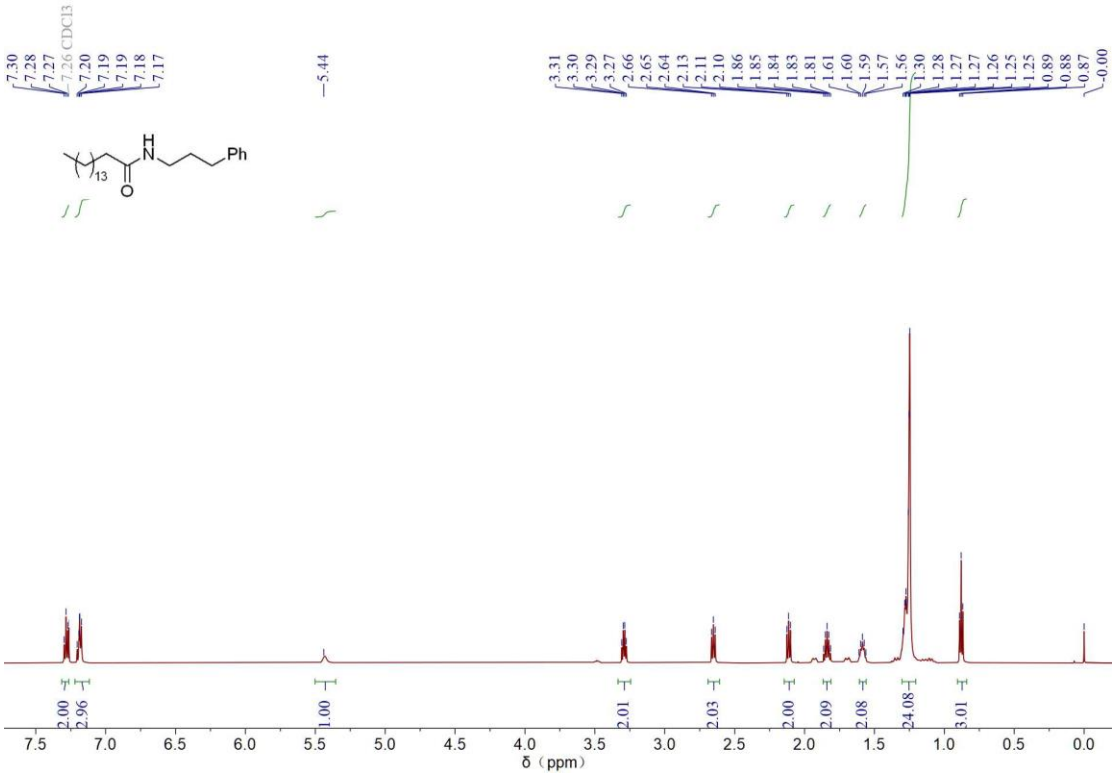
^{1}H NMR of compound 31



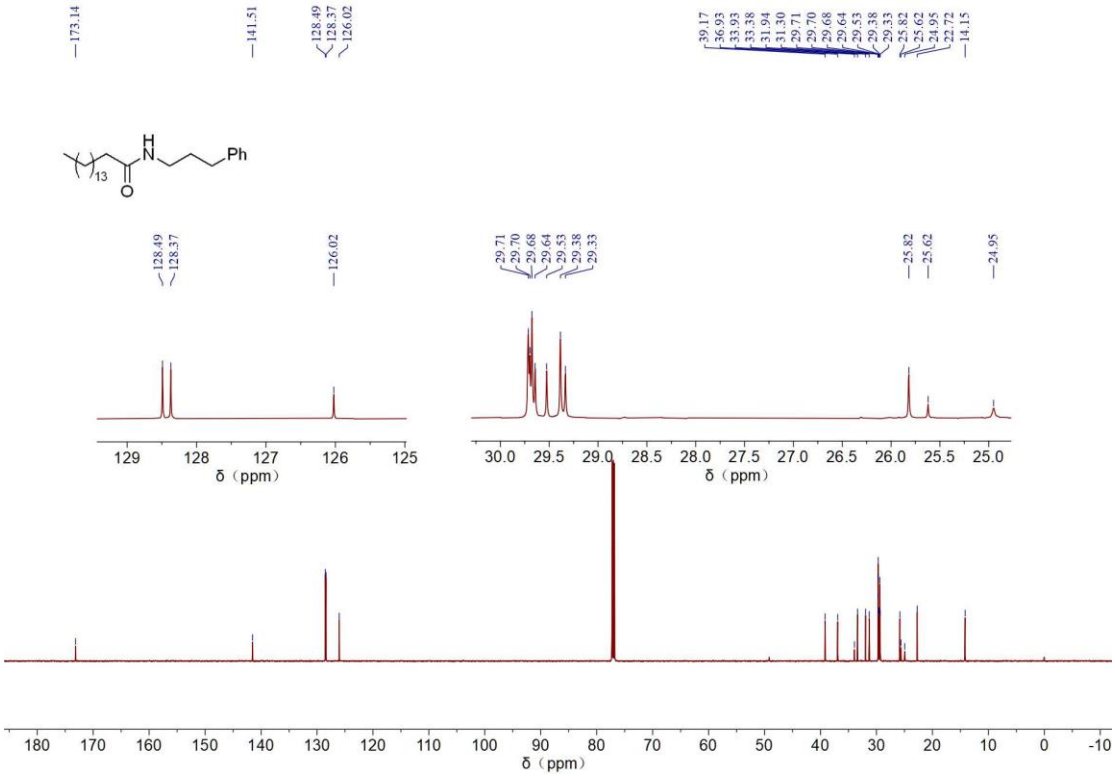
^{13}C NMR of compound 31



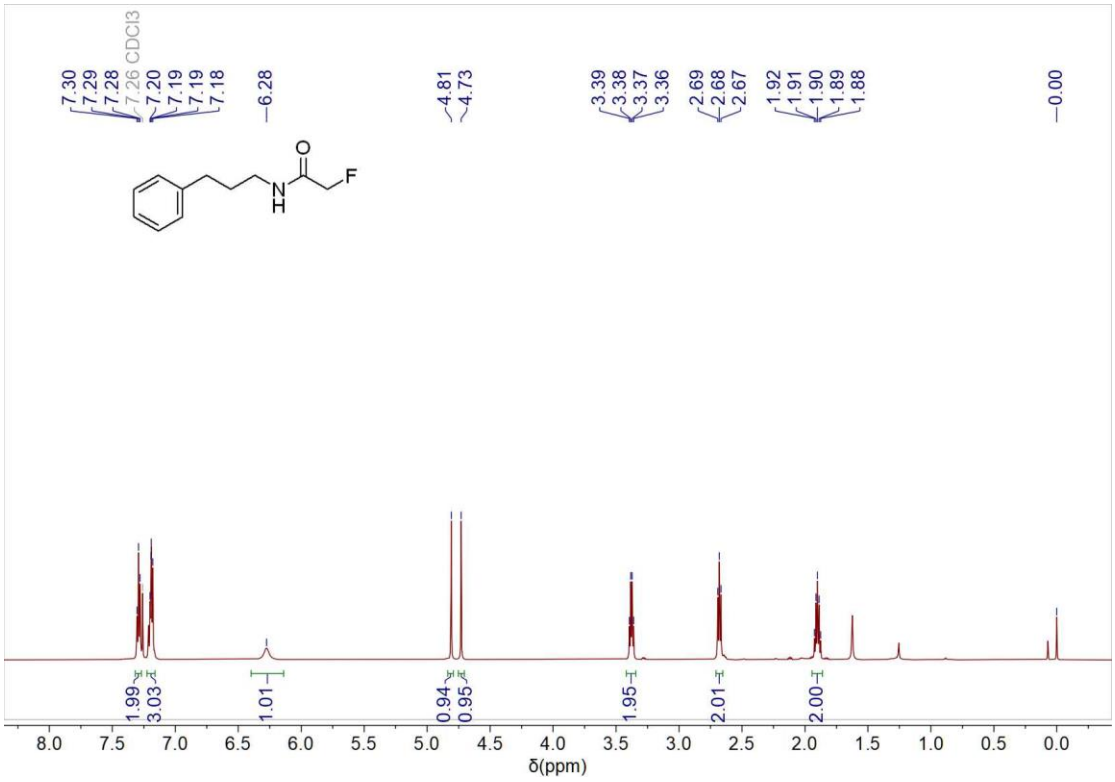
^{1}H NMR of compound 31′



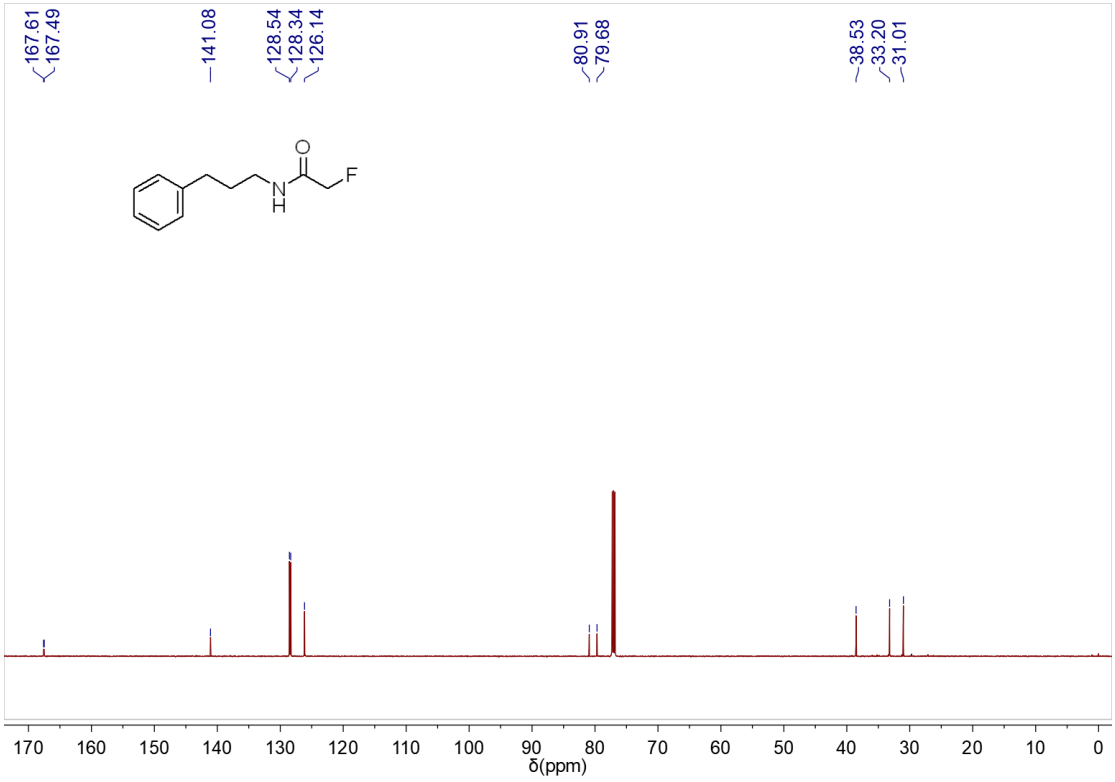
^{13}C NMR of compound 31′



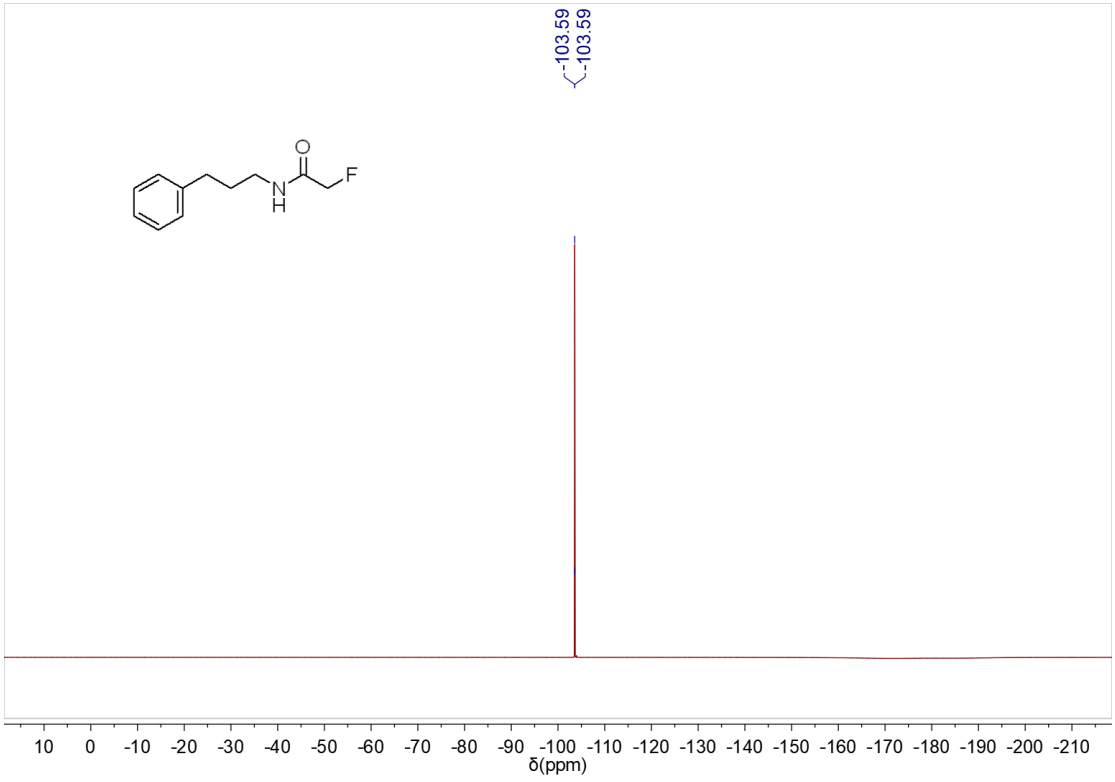
^{1}H NMR of compound 32



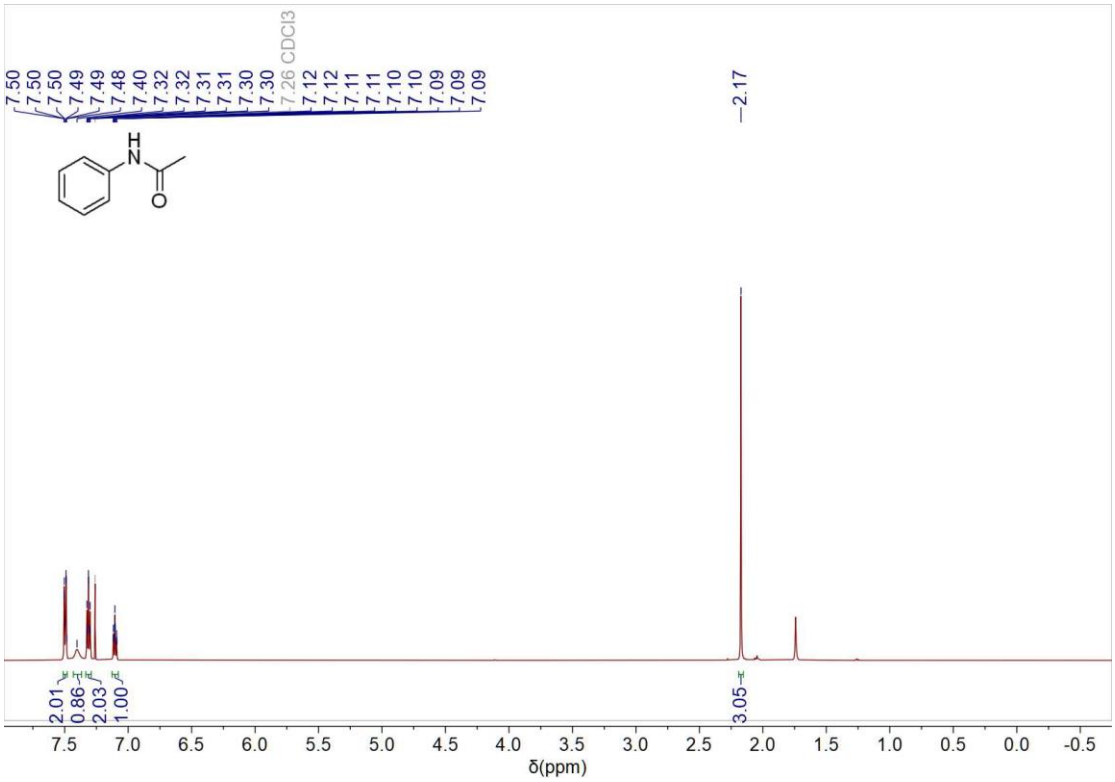
^{13}C NMR of compound 32



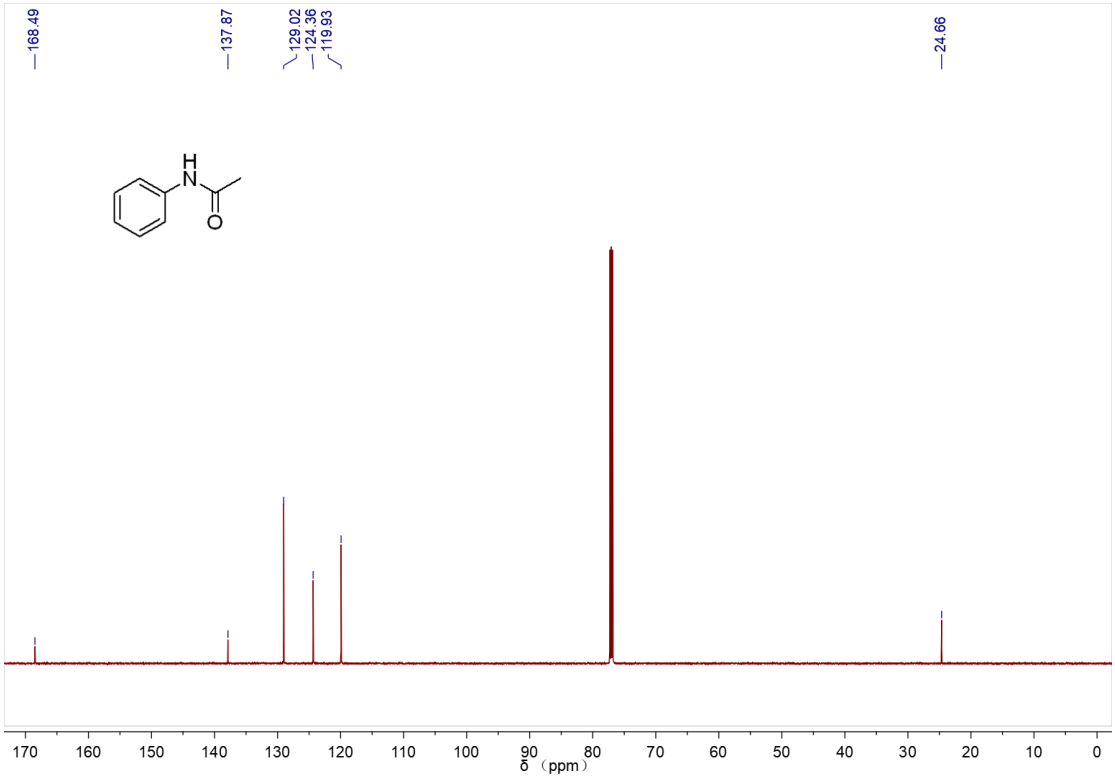
^{19}F NMR of compound 32



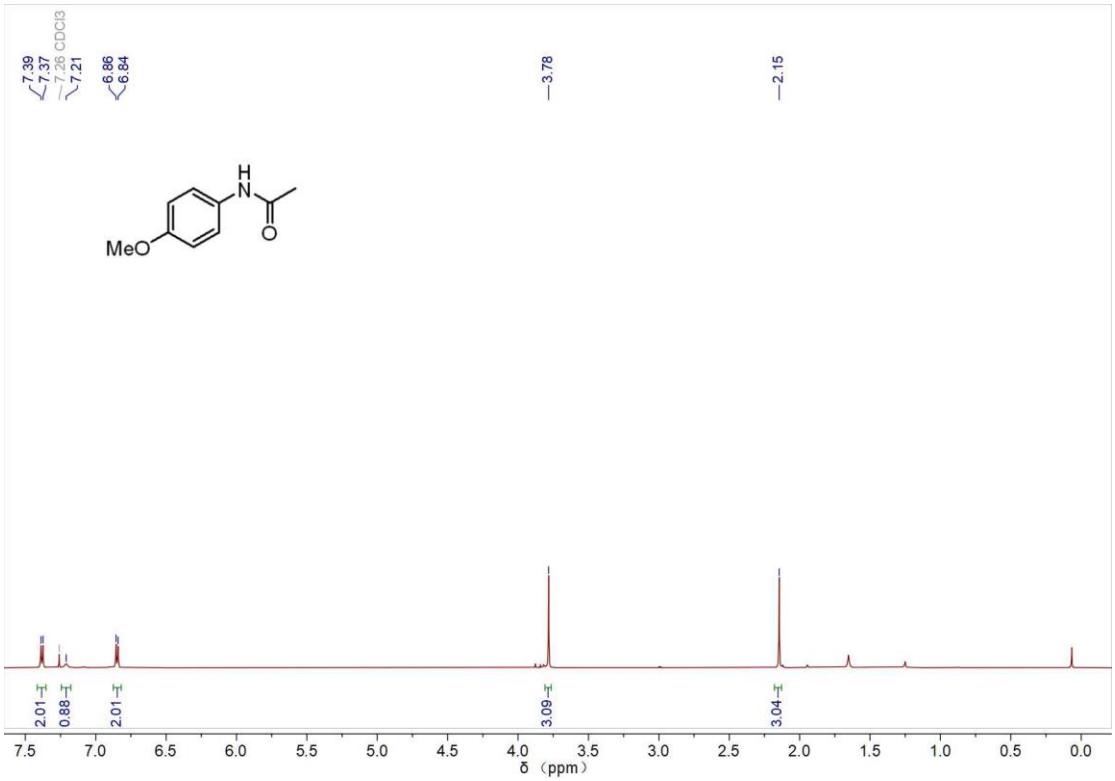
^{1}H NMR of compound 34



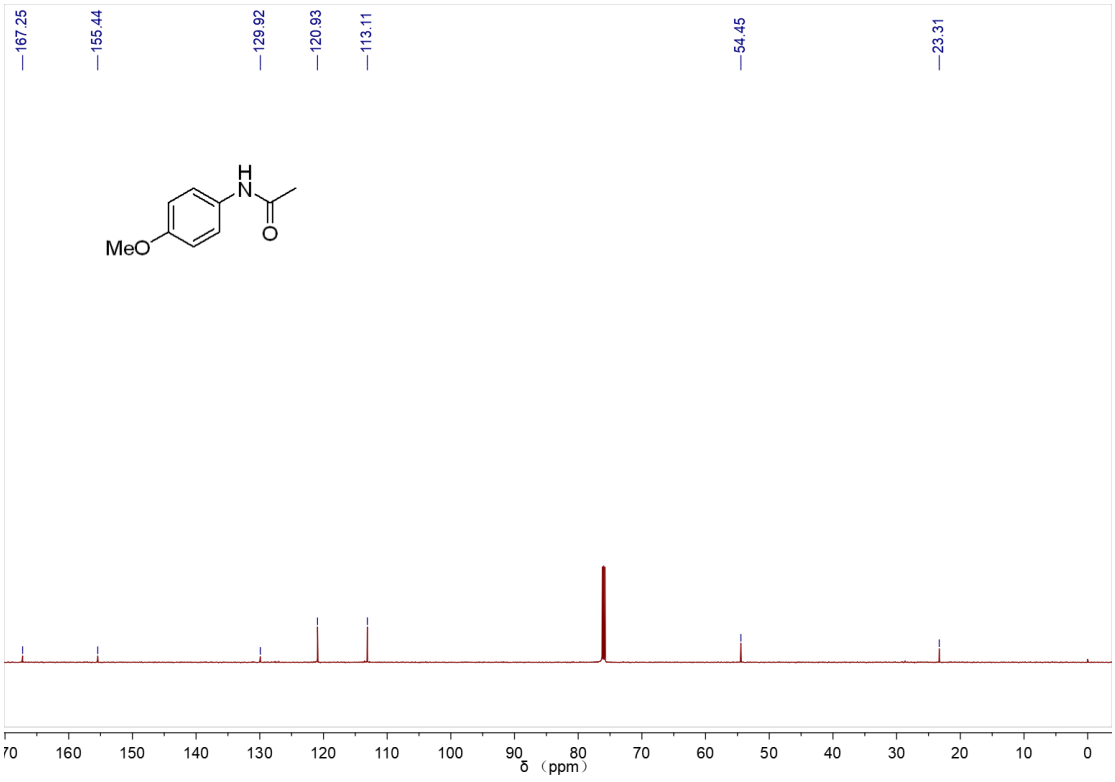
^{13}C NMR of compound 34



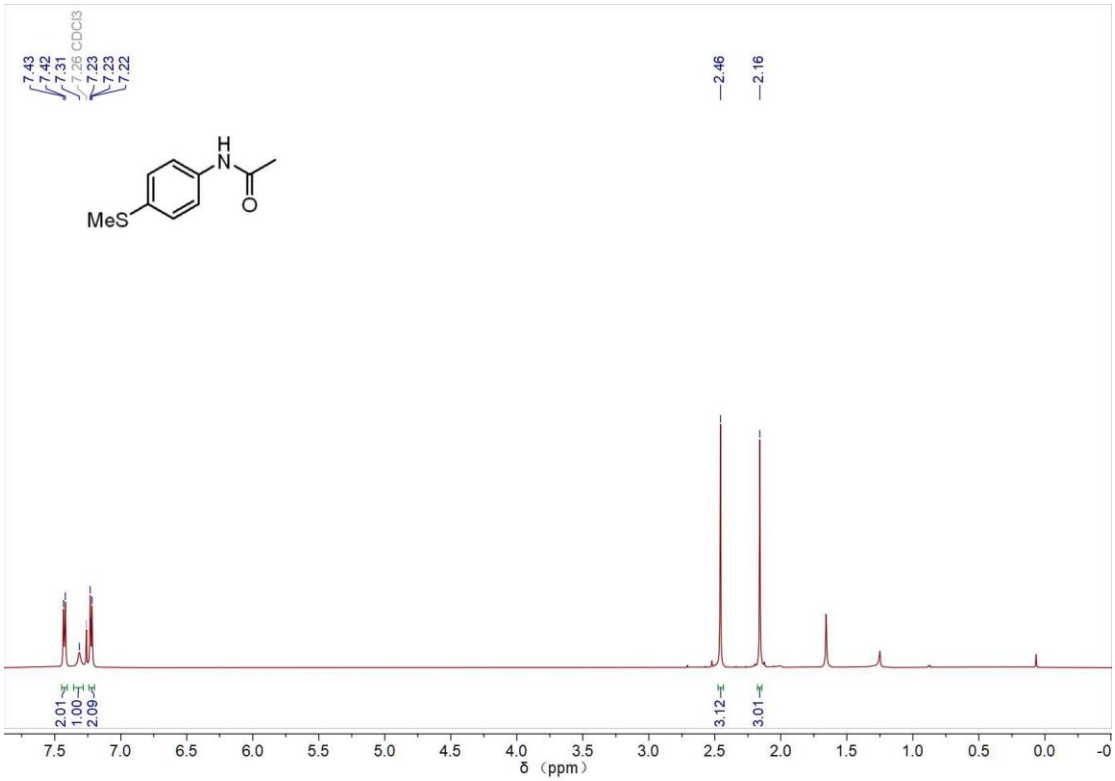
^{1}H NMR of compound 35



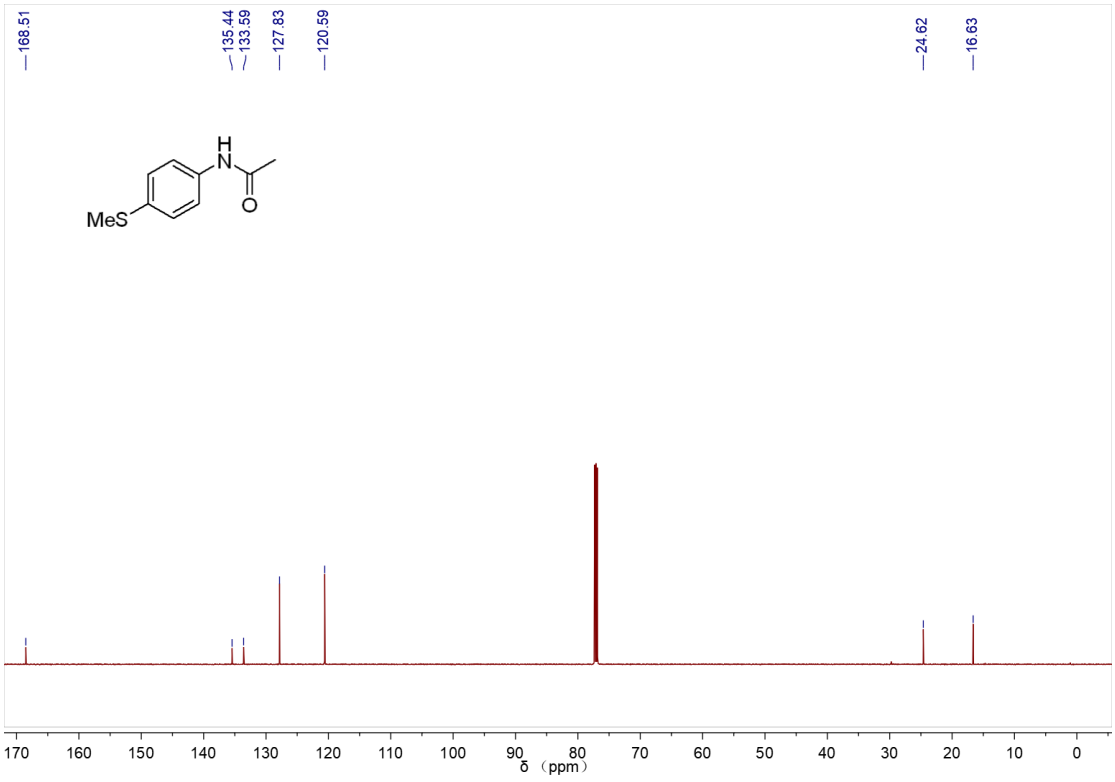
^{13}C NMR of compound 35



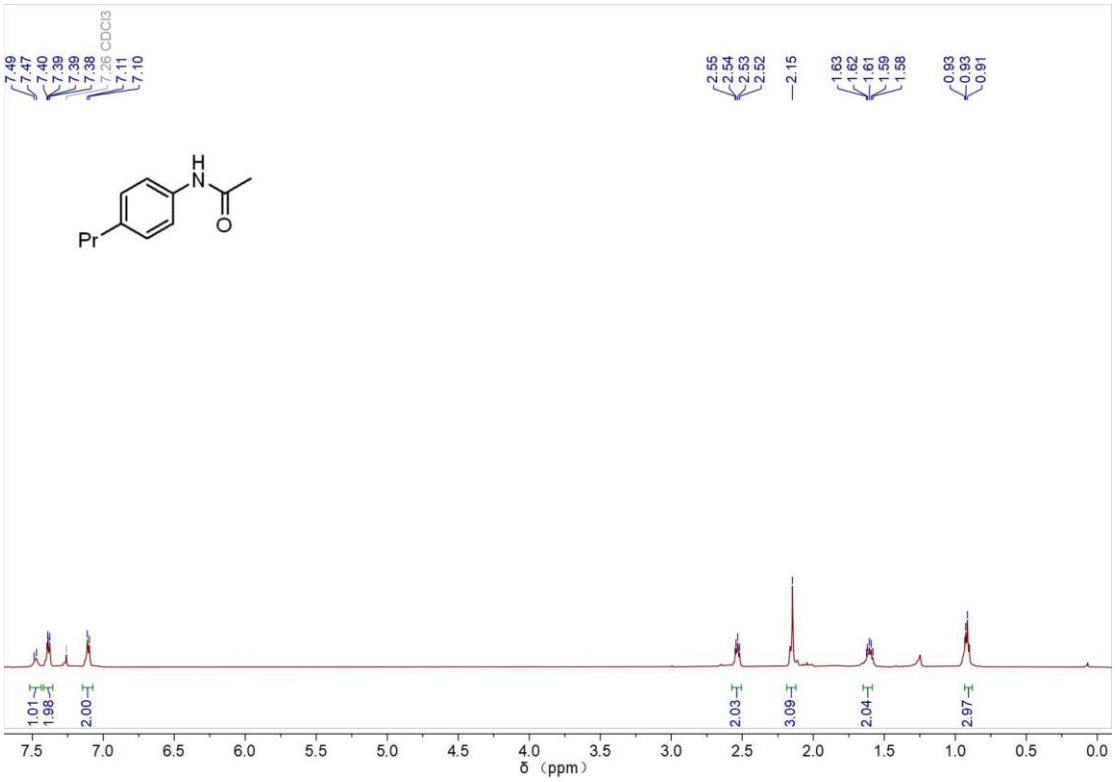
^{1}H NMR of compound 36



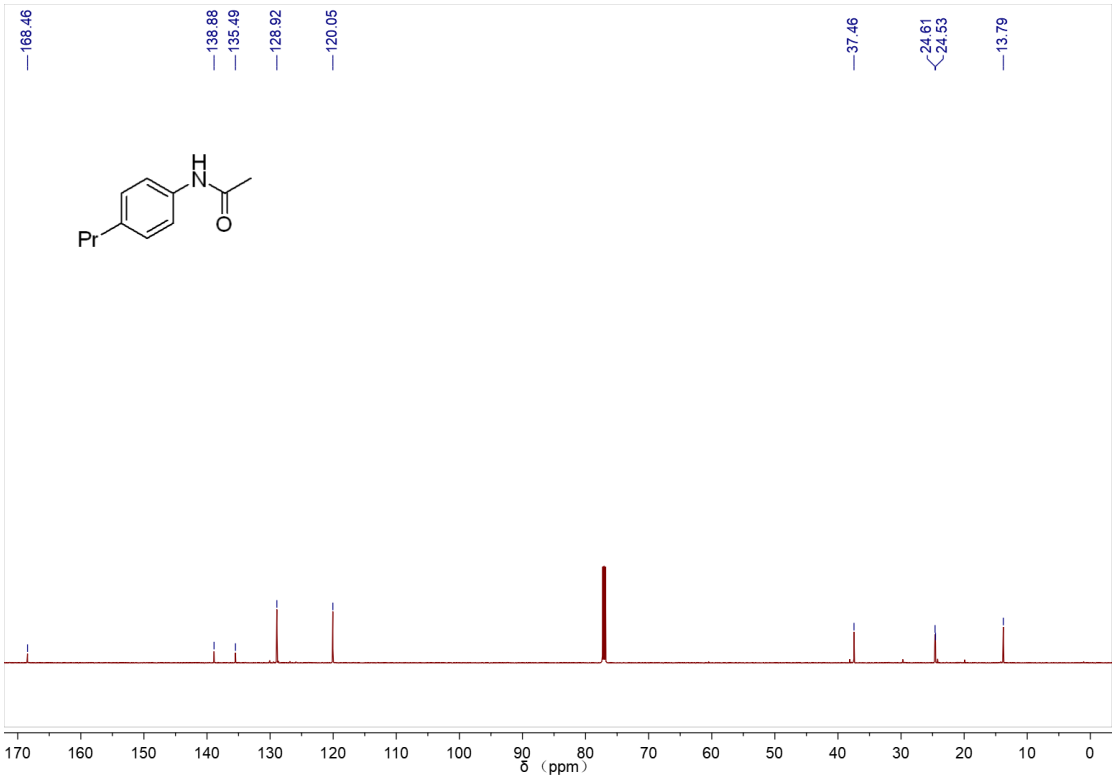
^{13}C NMR of compound 36



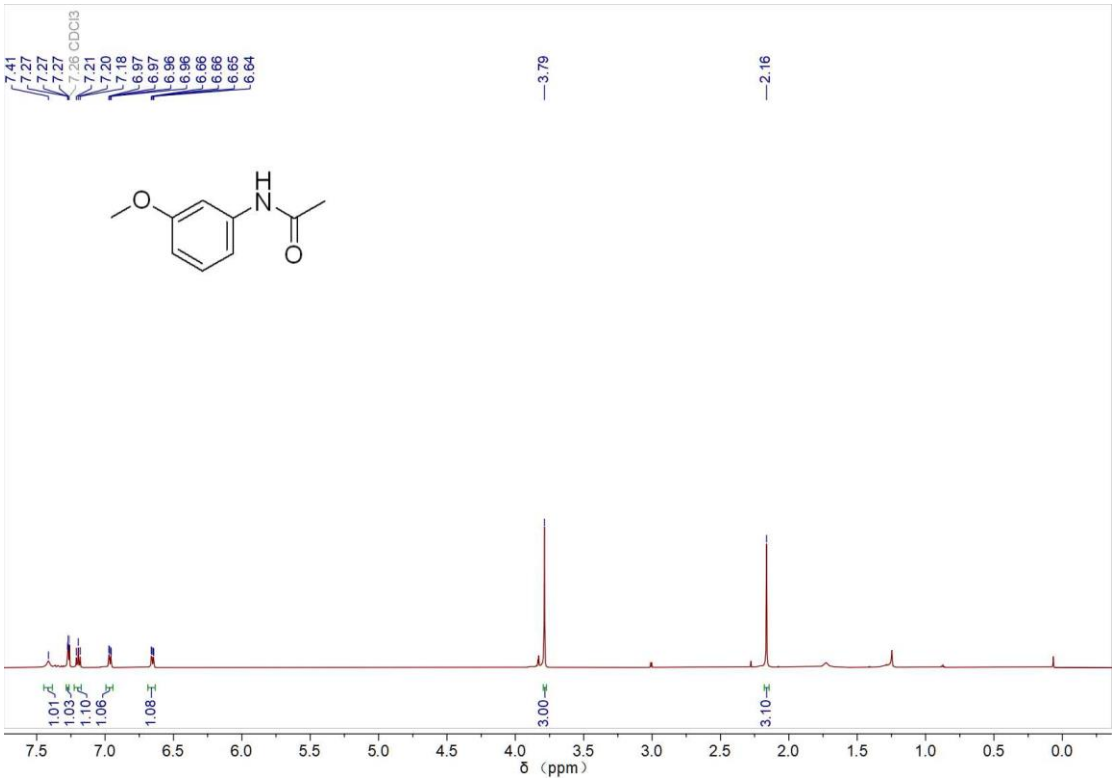
^{1}H NMR of compound 37



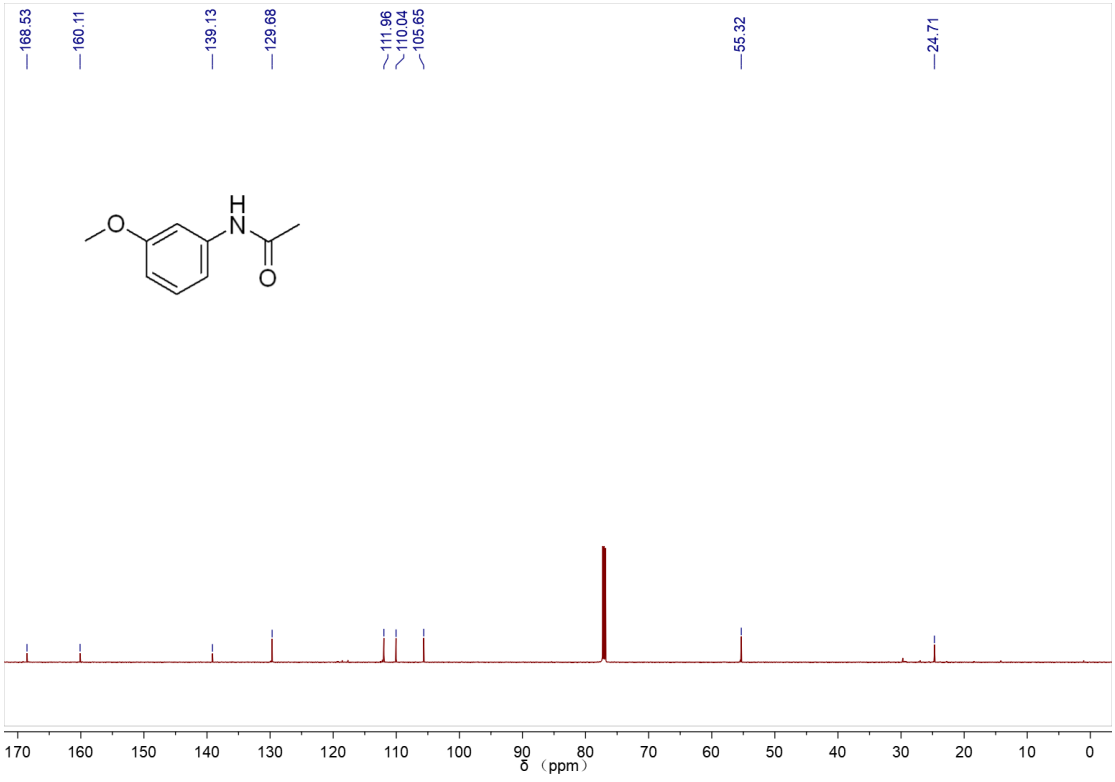
^{13}C NMR of compound 37



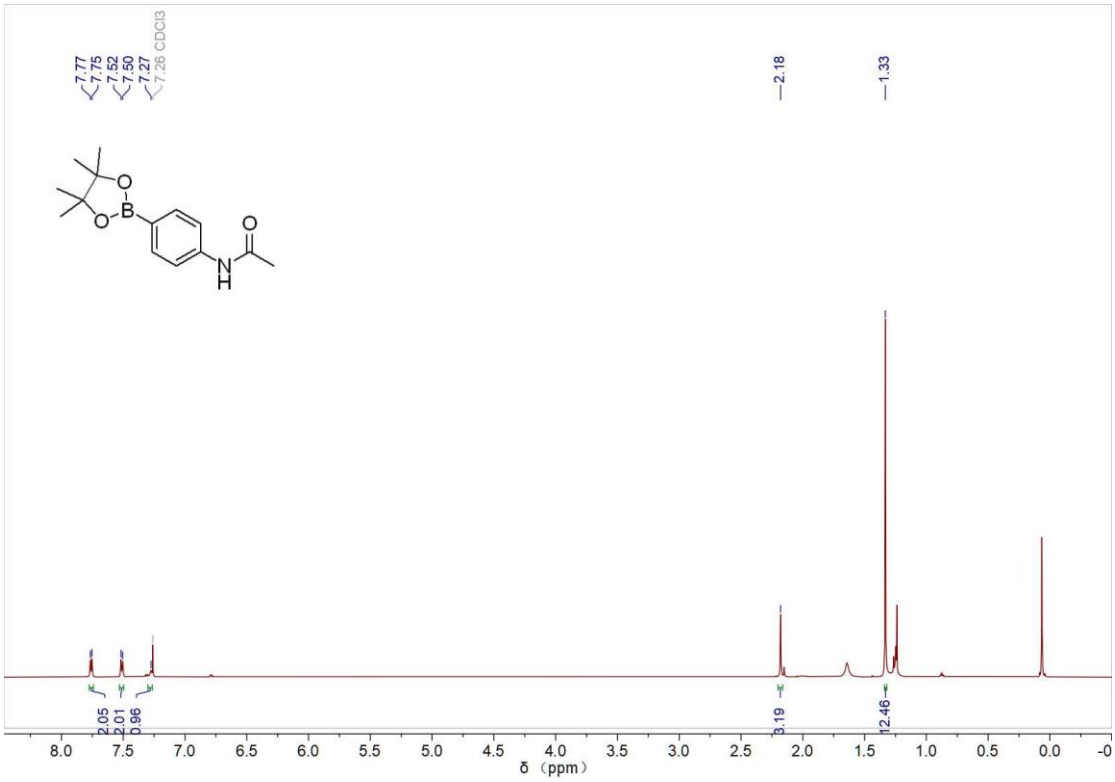
^{1}H NMR of compound 38



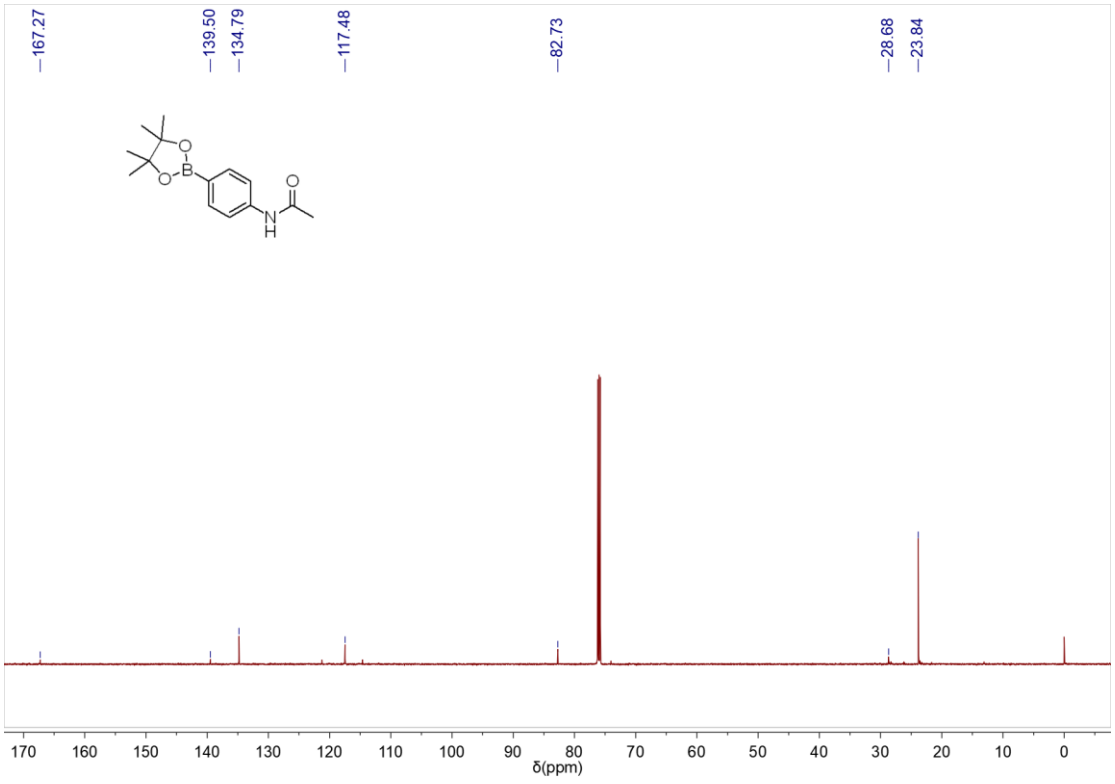
^{13}C NMR of compound 38



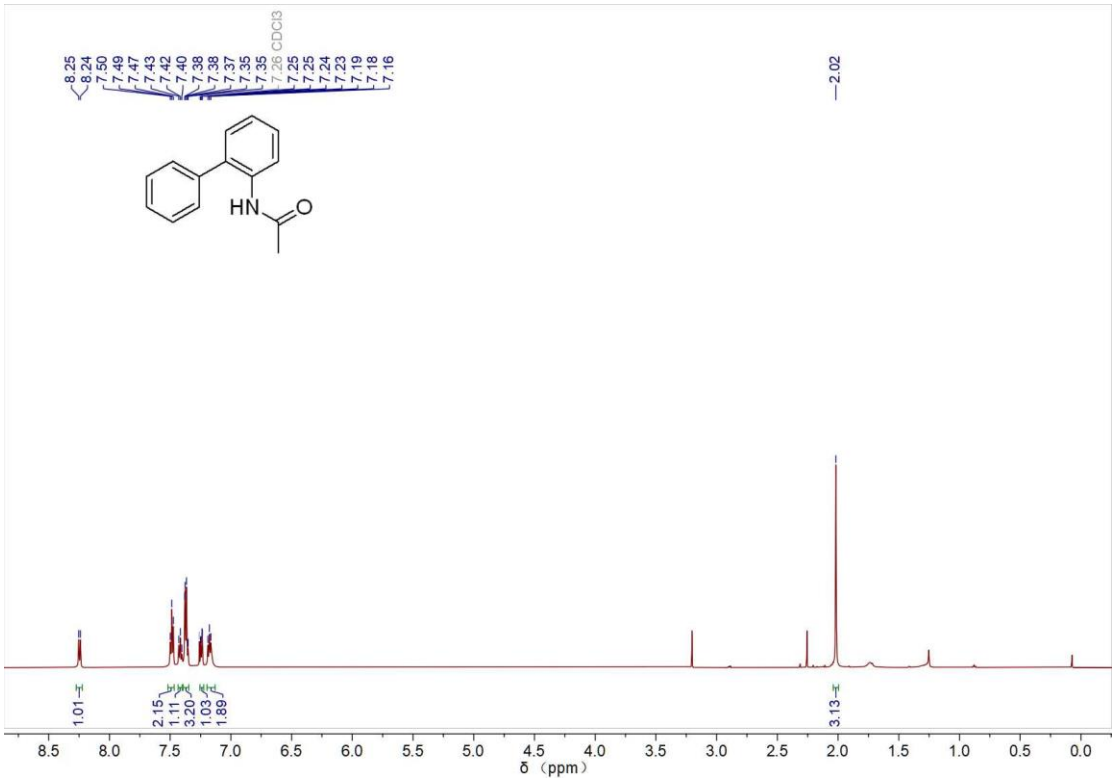
^{1}H NMR of compound 39



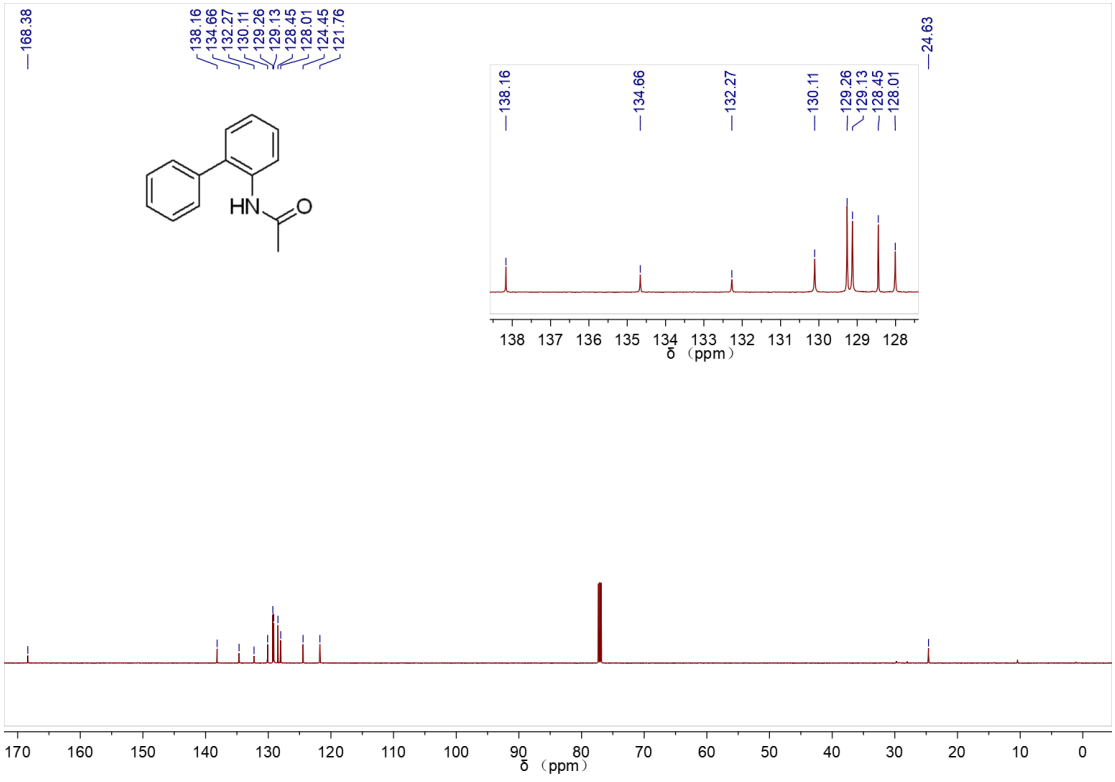
^{13}C NMR of compound 39



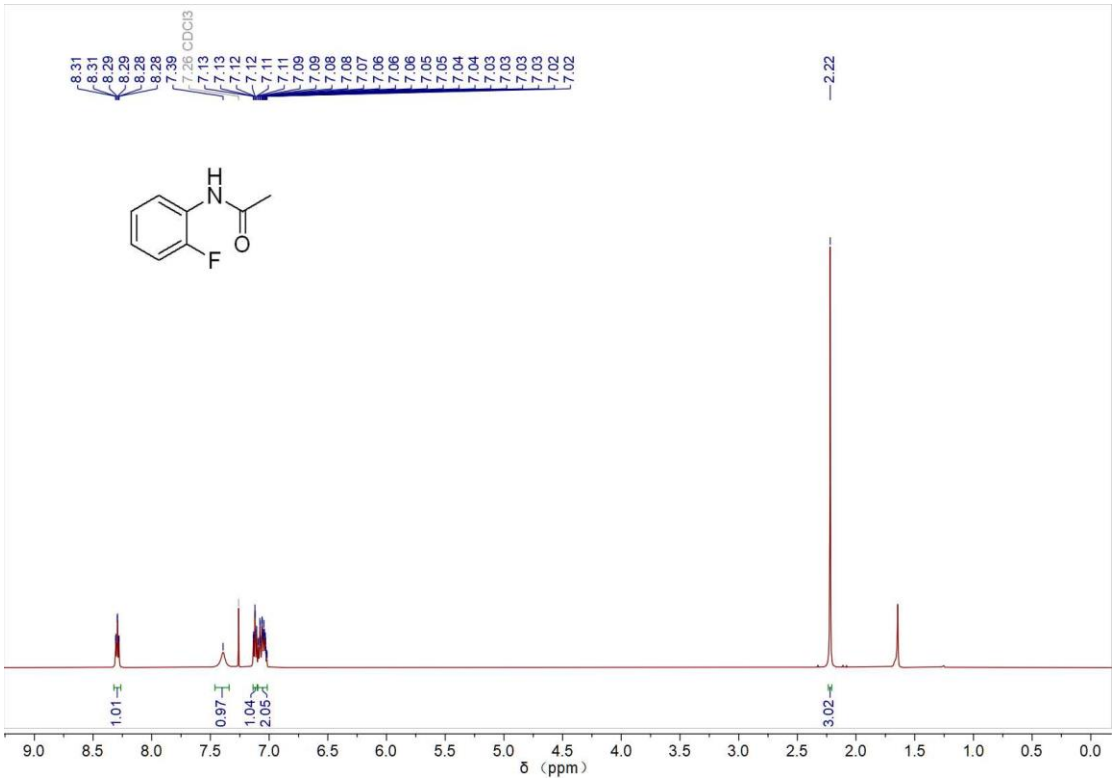
^{1}H NMR of compound 40



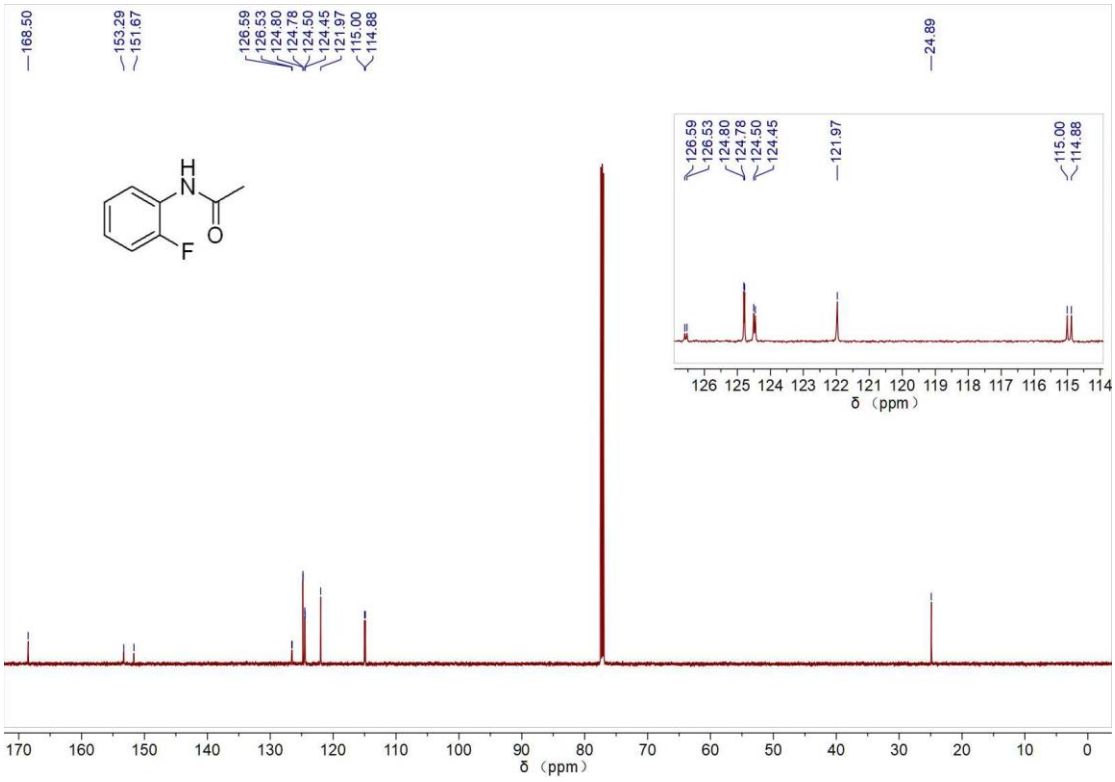
^{13}C NMR of compound 40



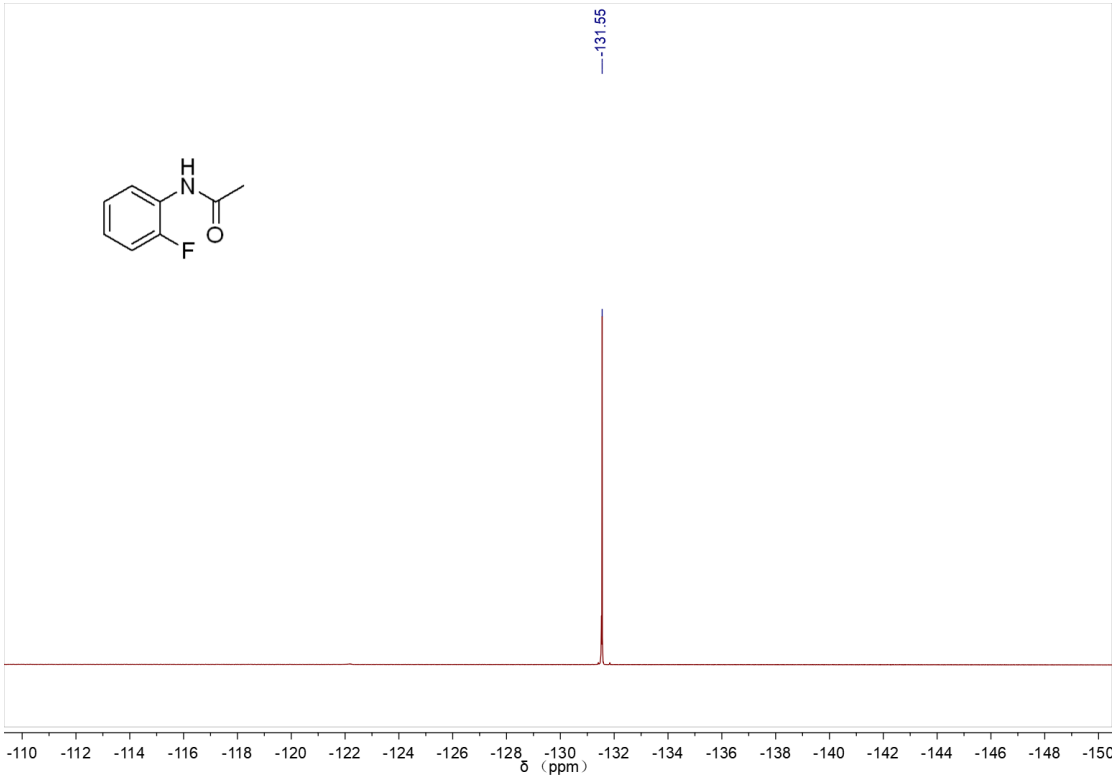
^{1}H NMR of compound 41



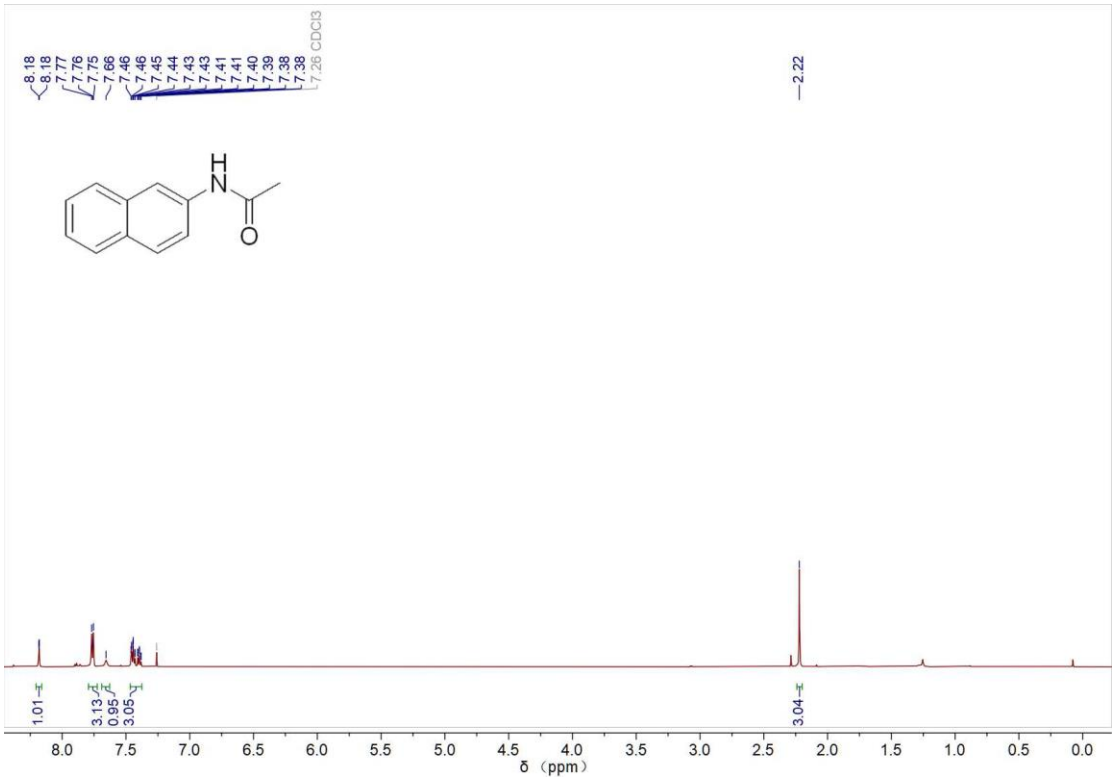
^{13}C NMR of compound 41



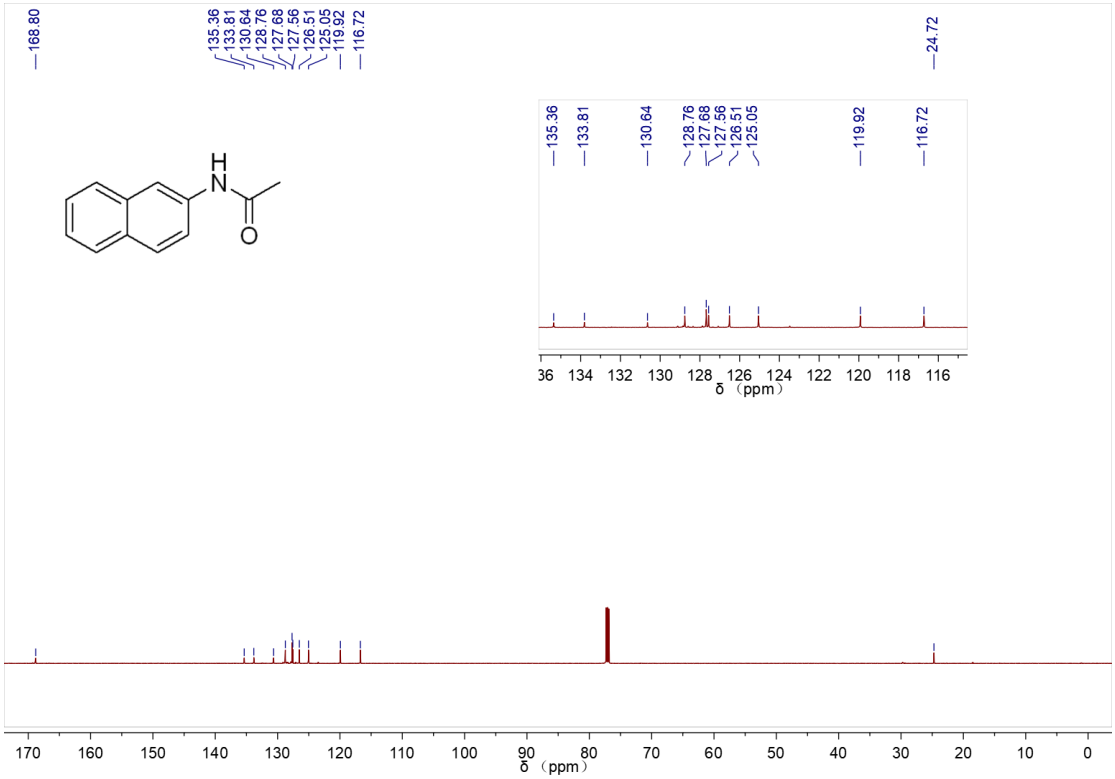
^{19}F NMR of compound 41



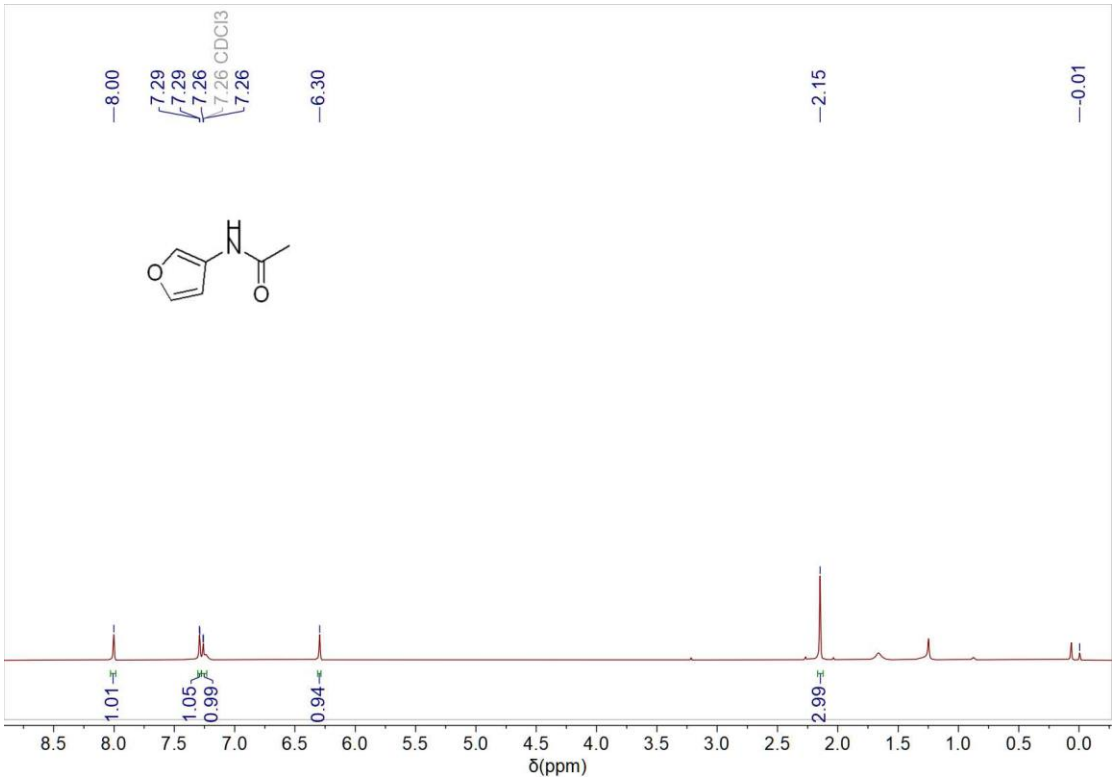
^{1}H NMR of compound 42



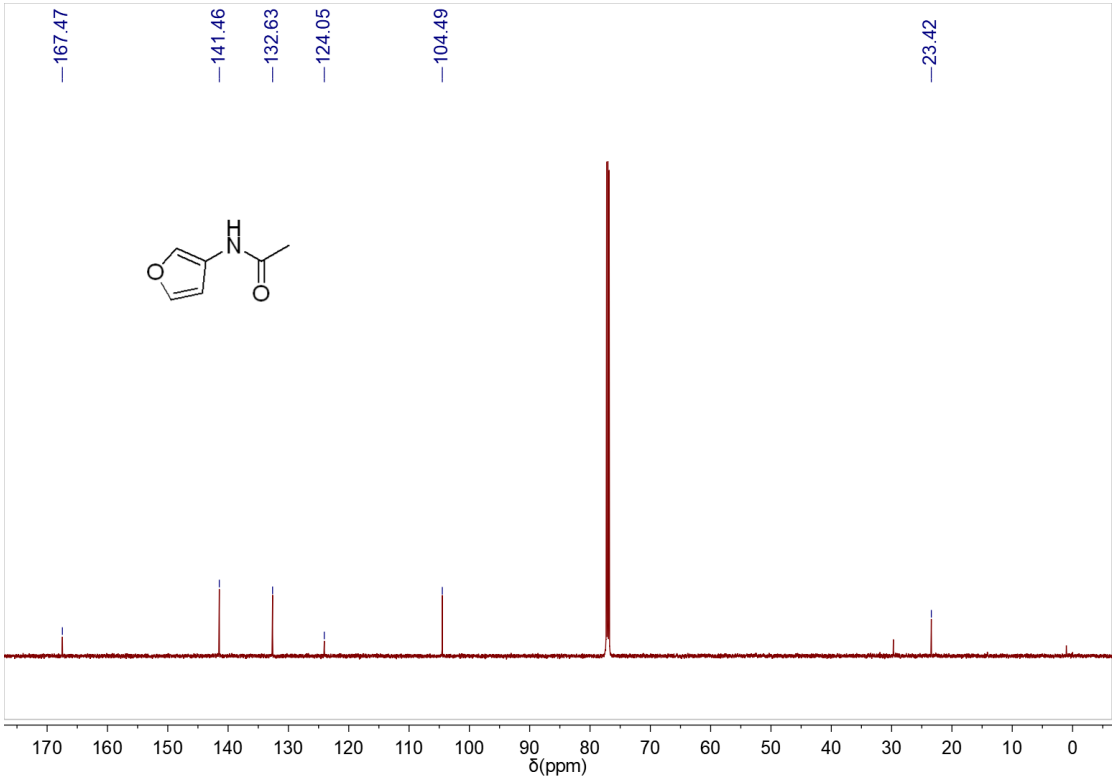
^{13}C NMR of compound 42



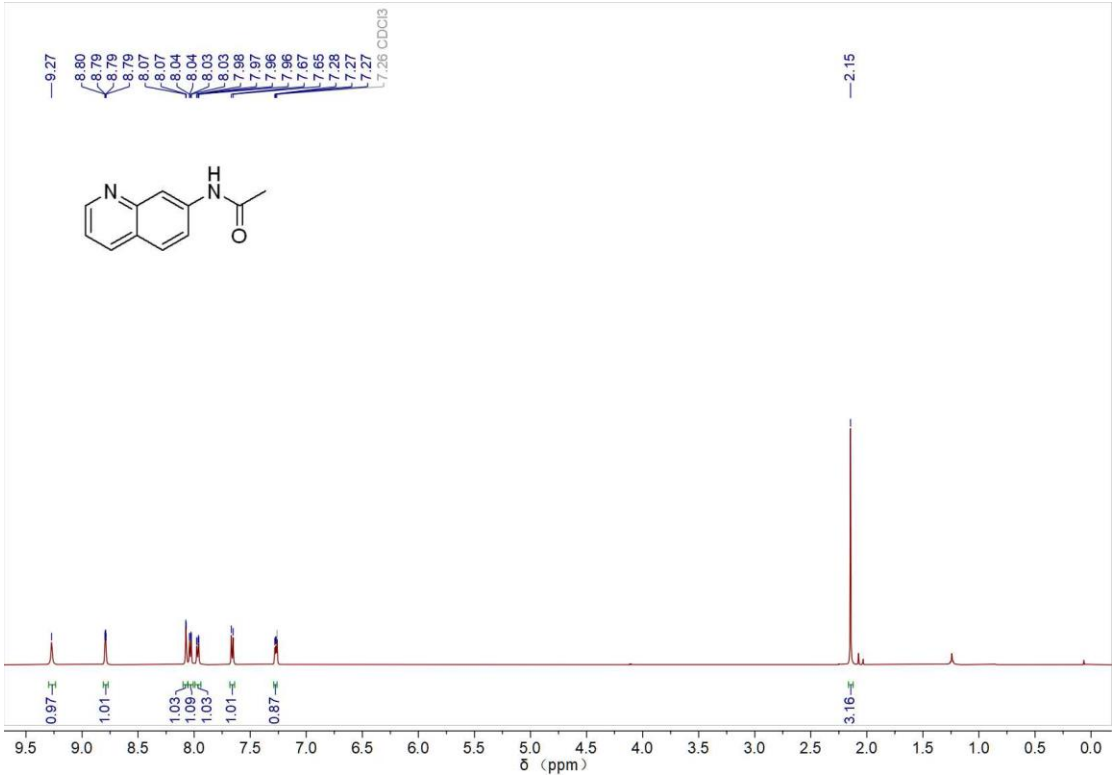
^{1}H NMR of compound 43



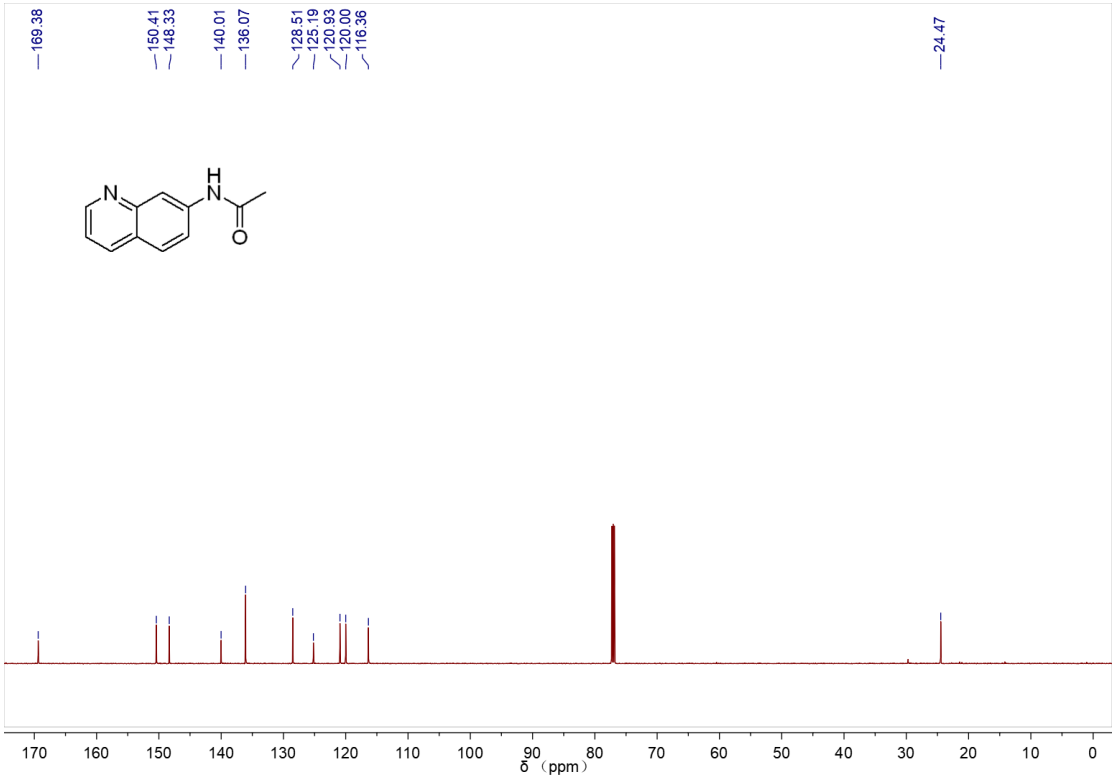
^{13}C NMR of compound 43



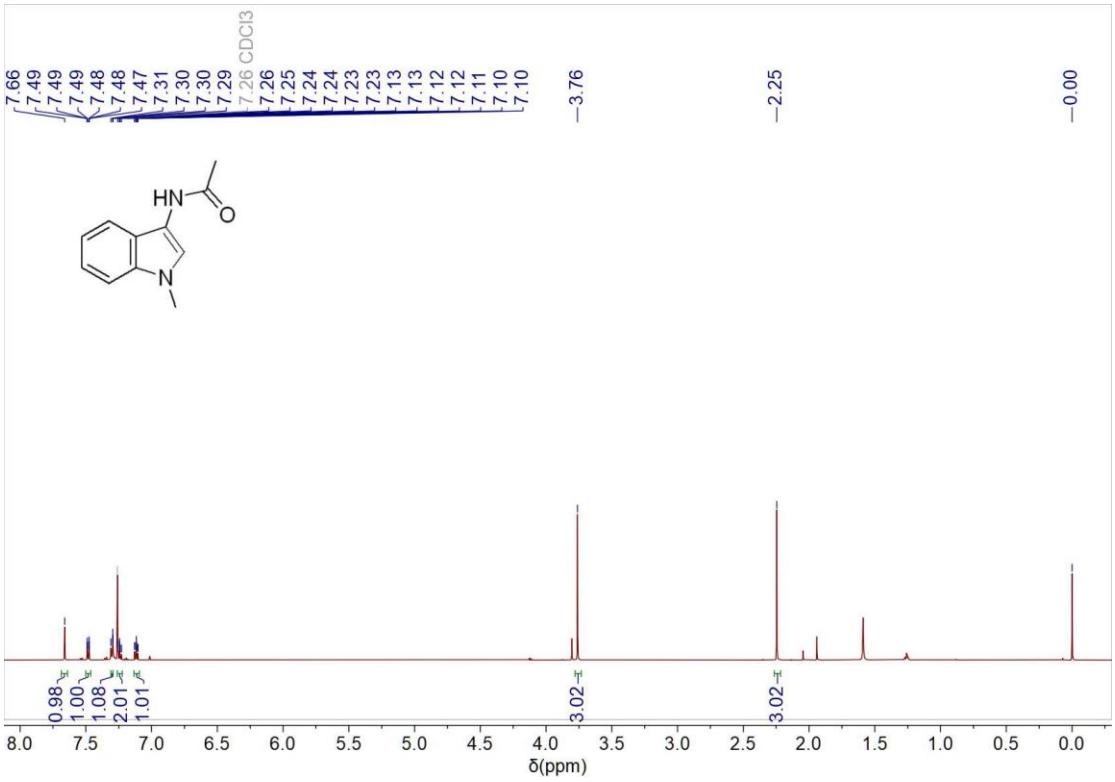
^{1}H NMR of compound 44



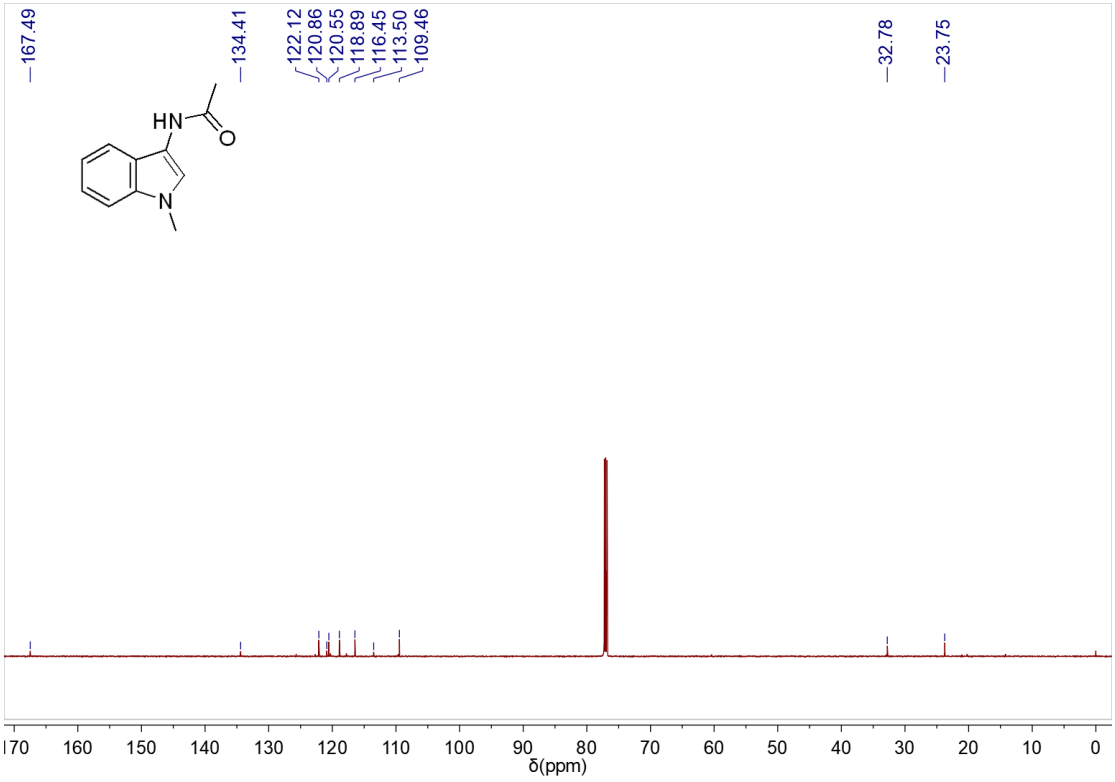
^{13}C NMR of compound 44



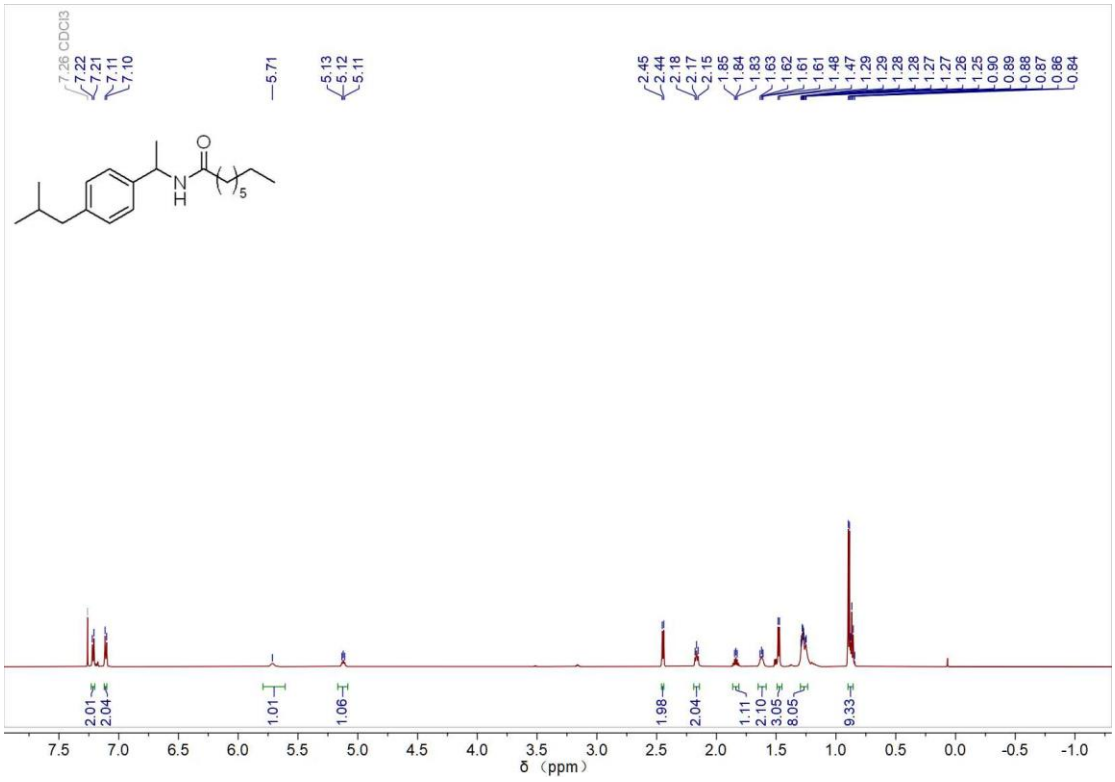
^{1}H NMR of compound 45



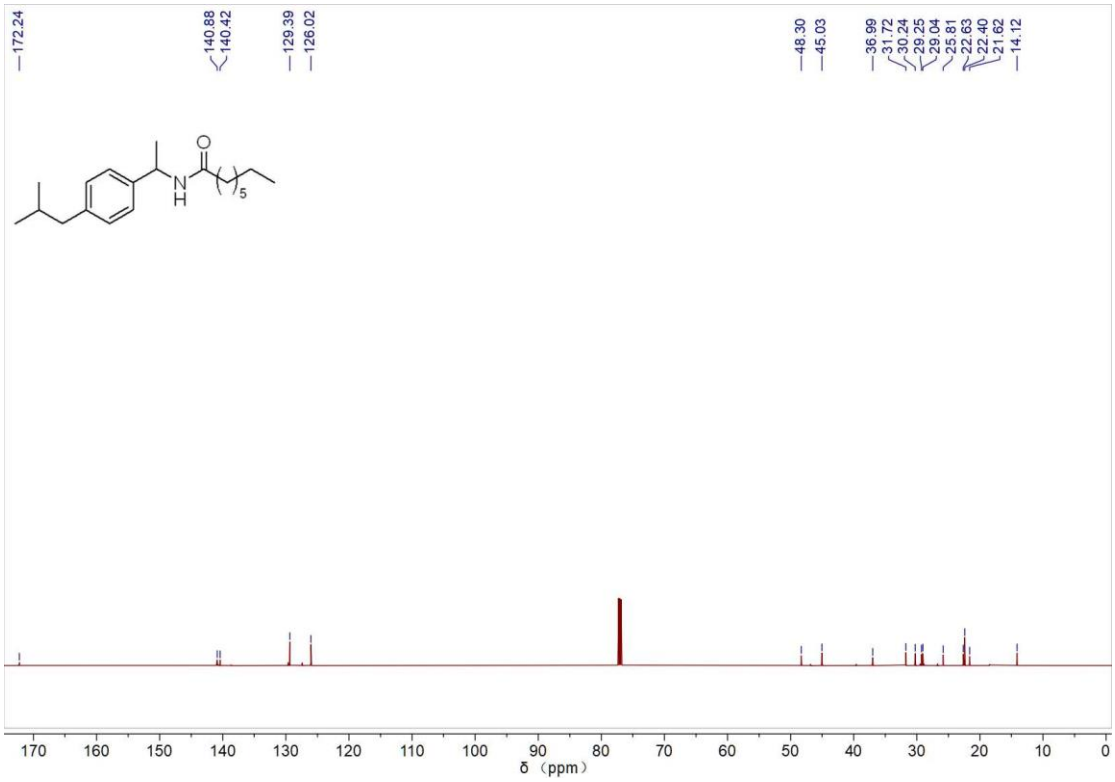
^{13}C NMR of compound 45



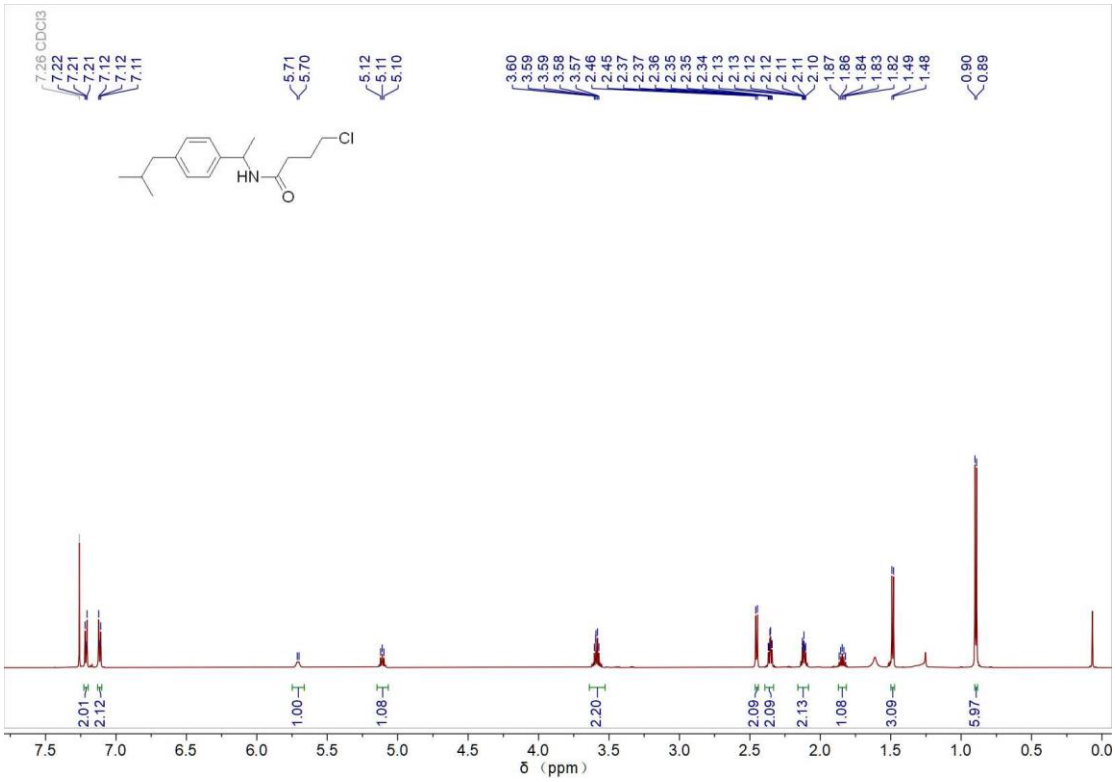
^{1}H NMR of compound 46



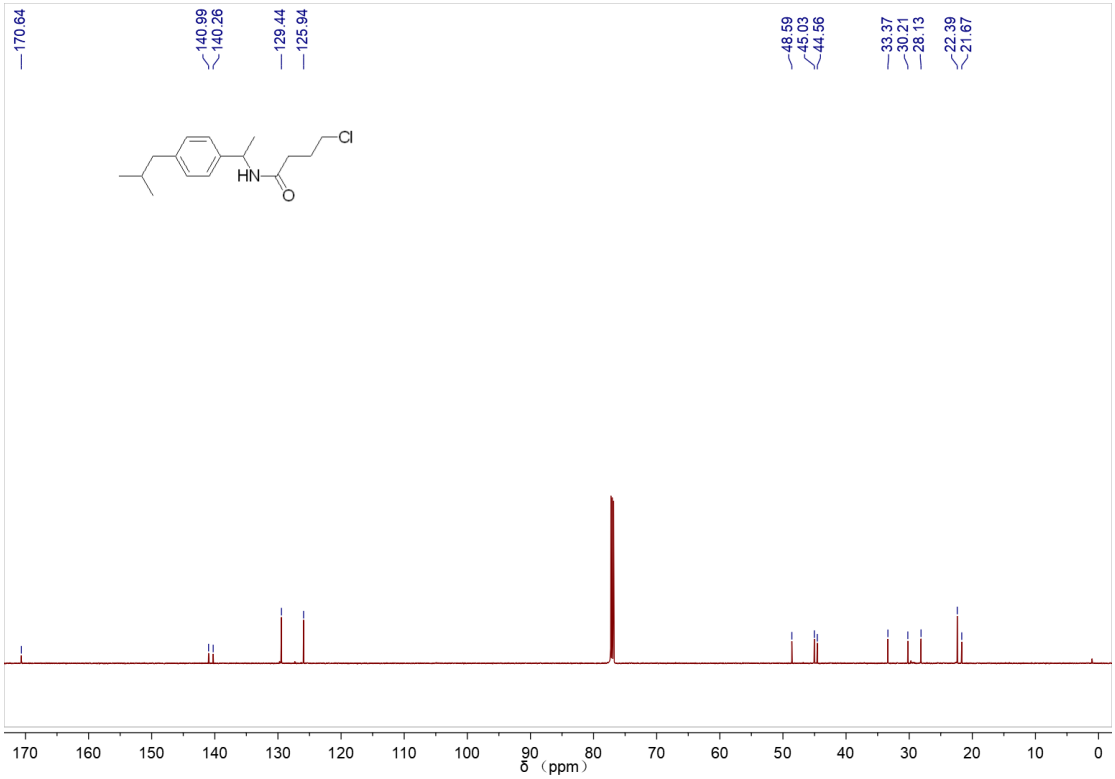
^{13}C NMR of compound 46



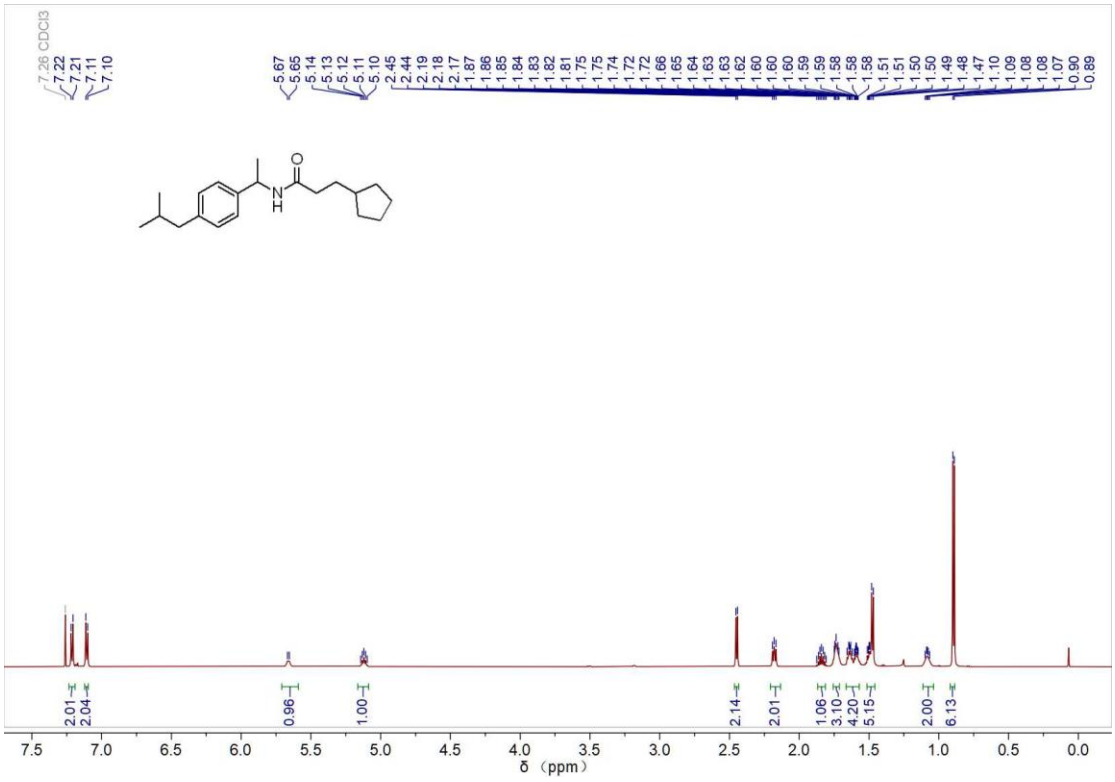
^{1}H NMR of compound 47



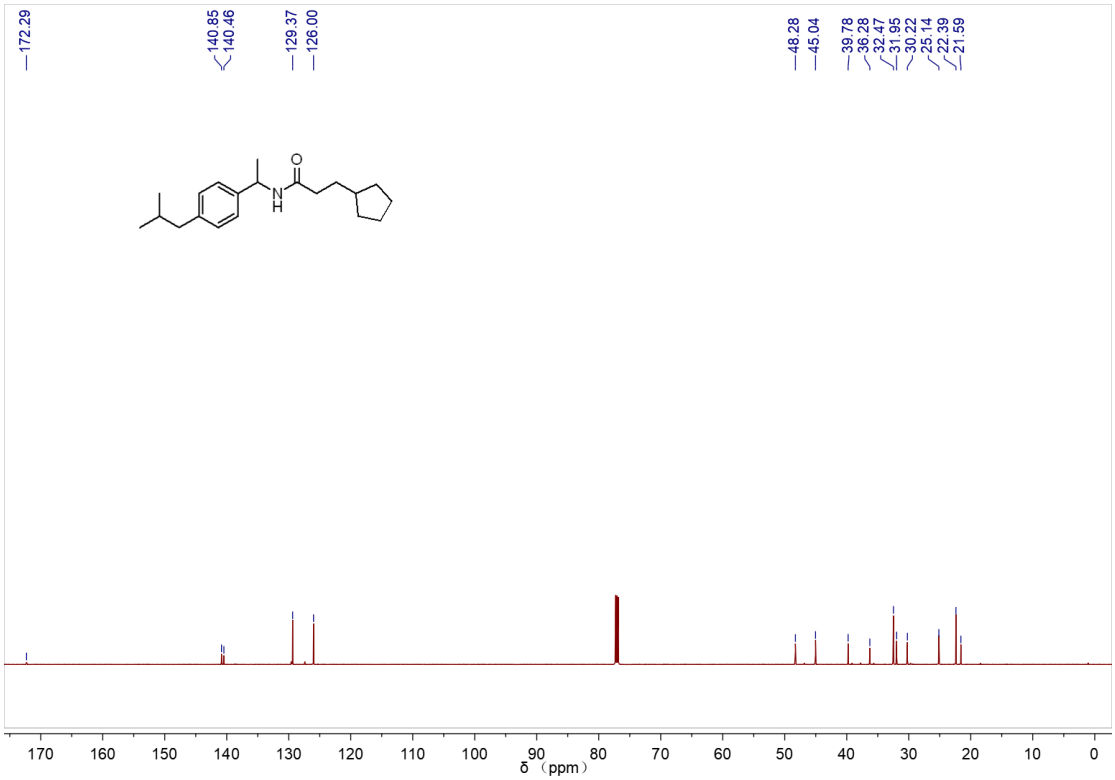
^{13}C NMR of compound 47



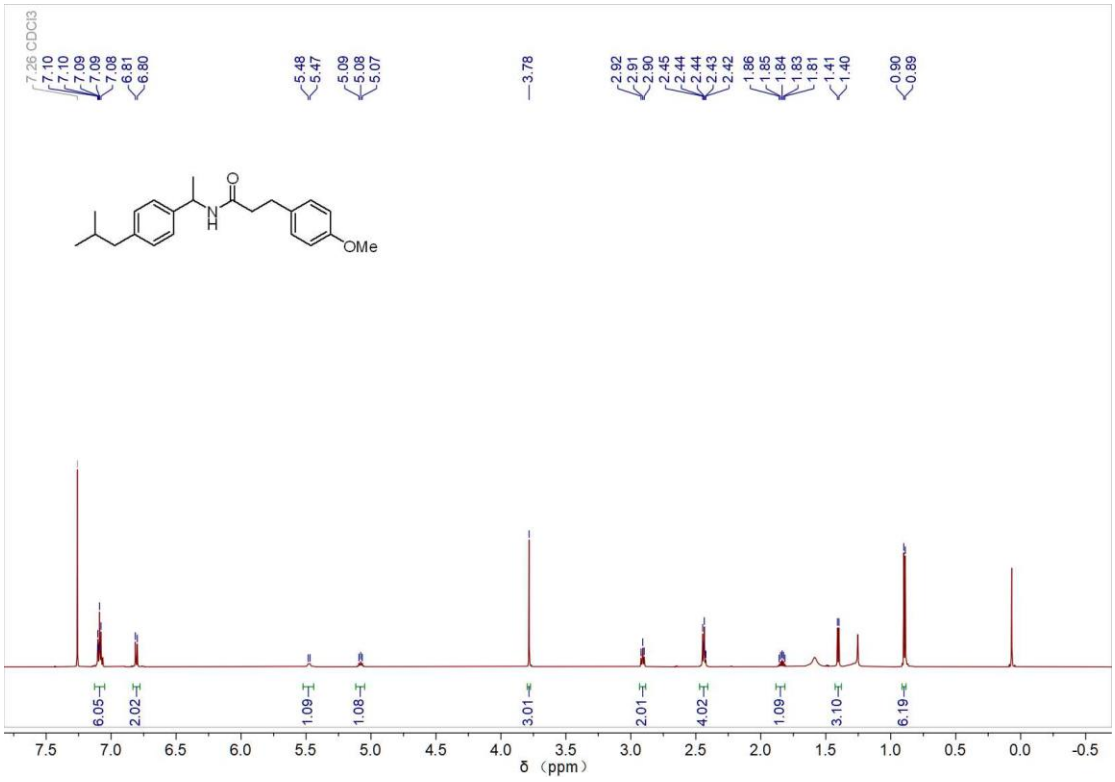
^{1}H NMR of compound 48



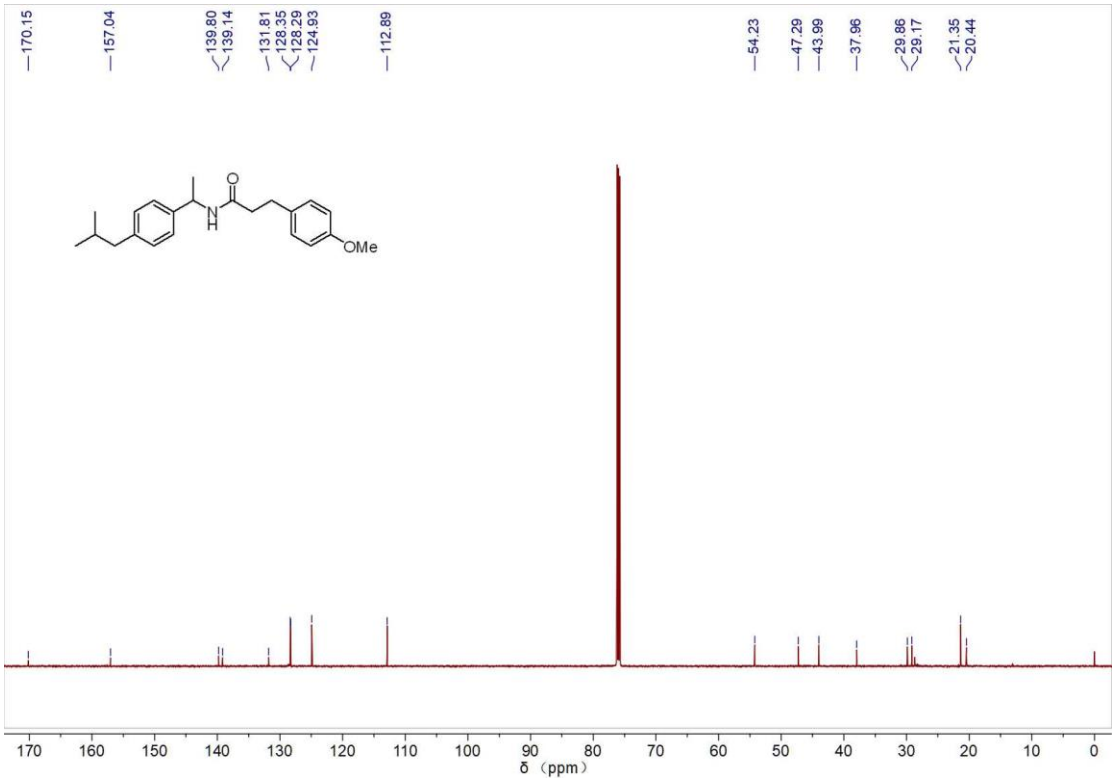
^{13}C NMR of compound 48



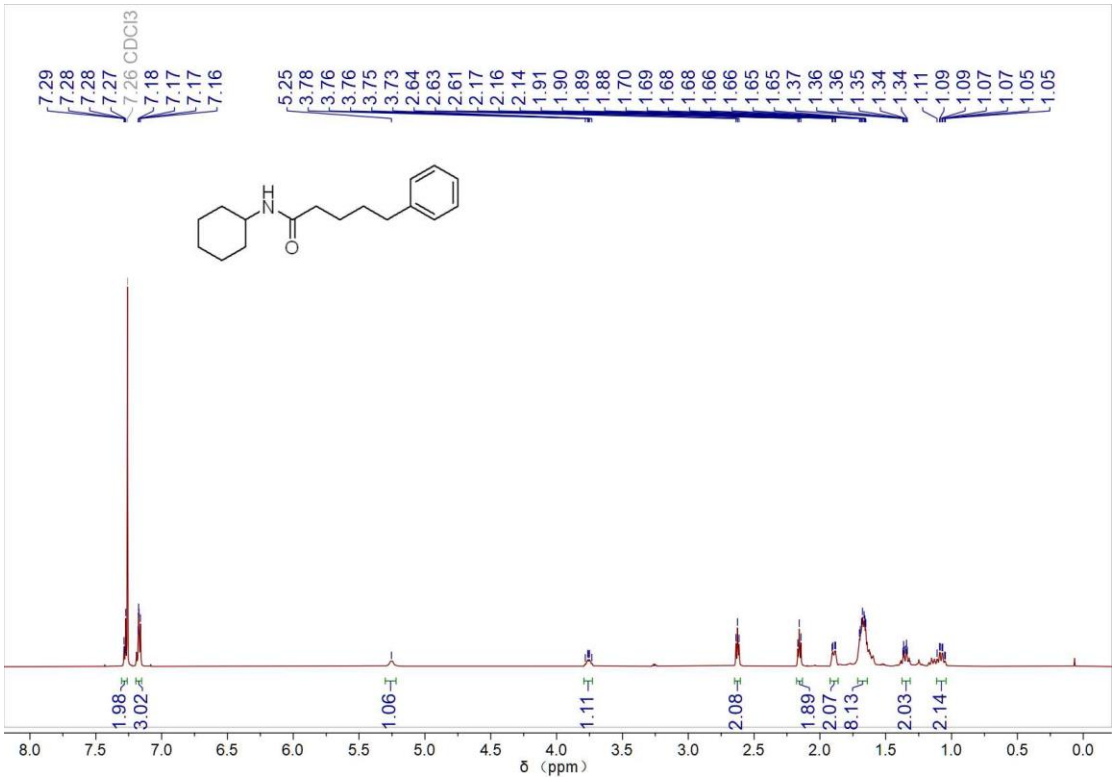
^{1}H NMR of compound 49



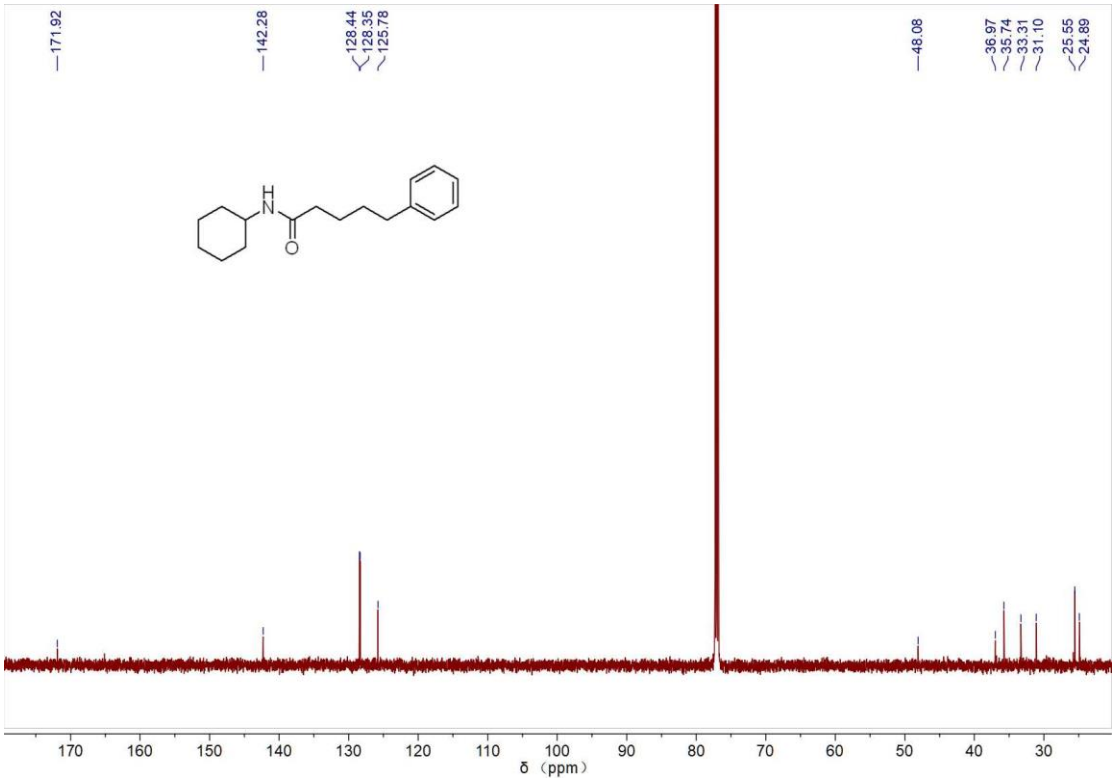
^{13}C NMR of compound 49



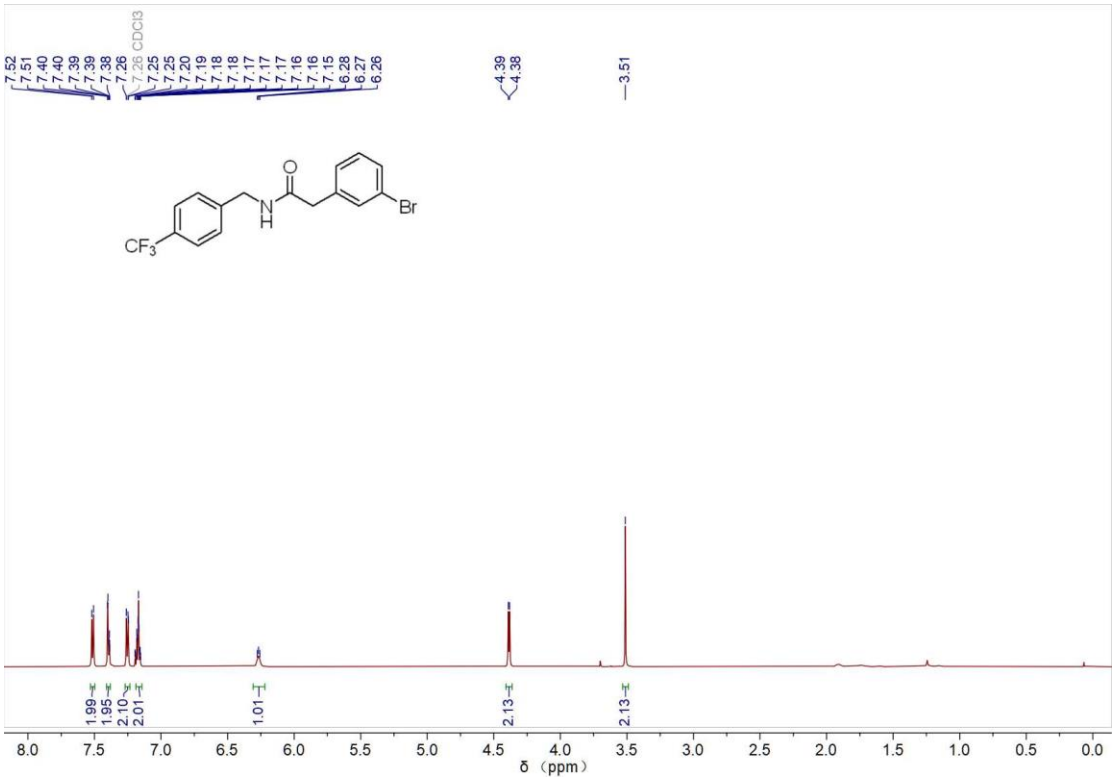
^{1}H NMR of compound 50



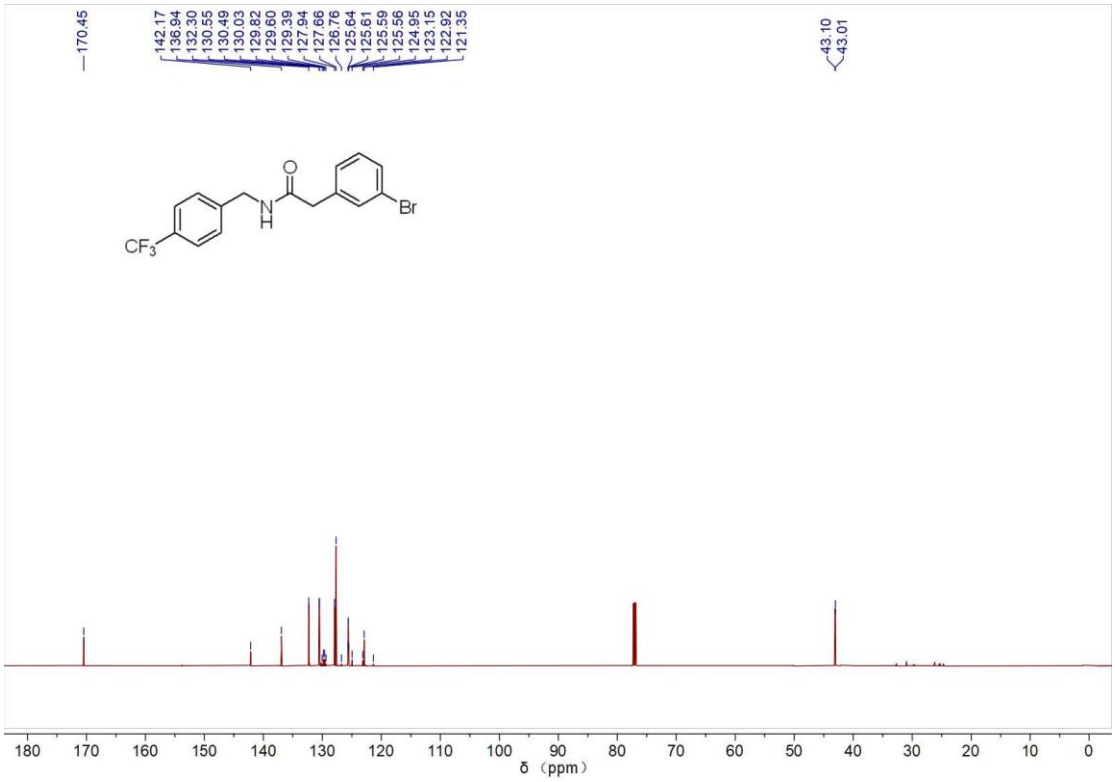
^{13}C NMR of compound 50



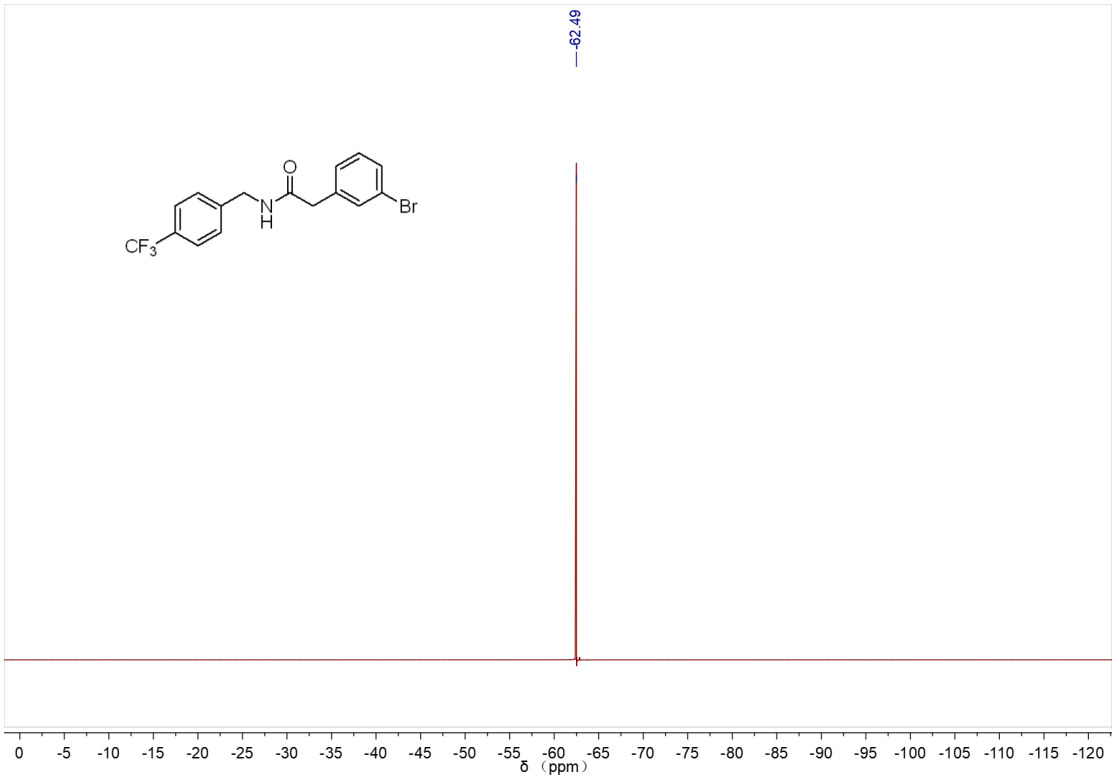
^{1}H NMR of compound 51



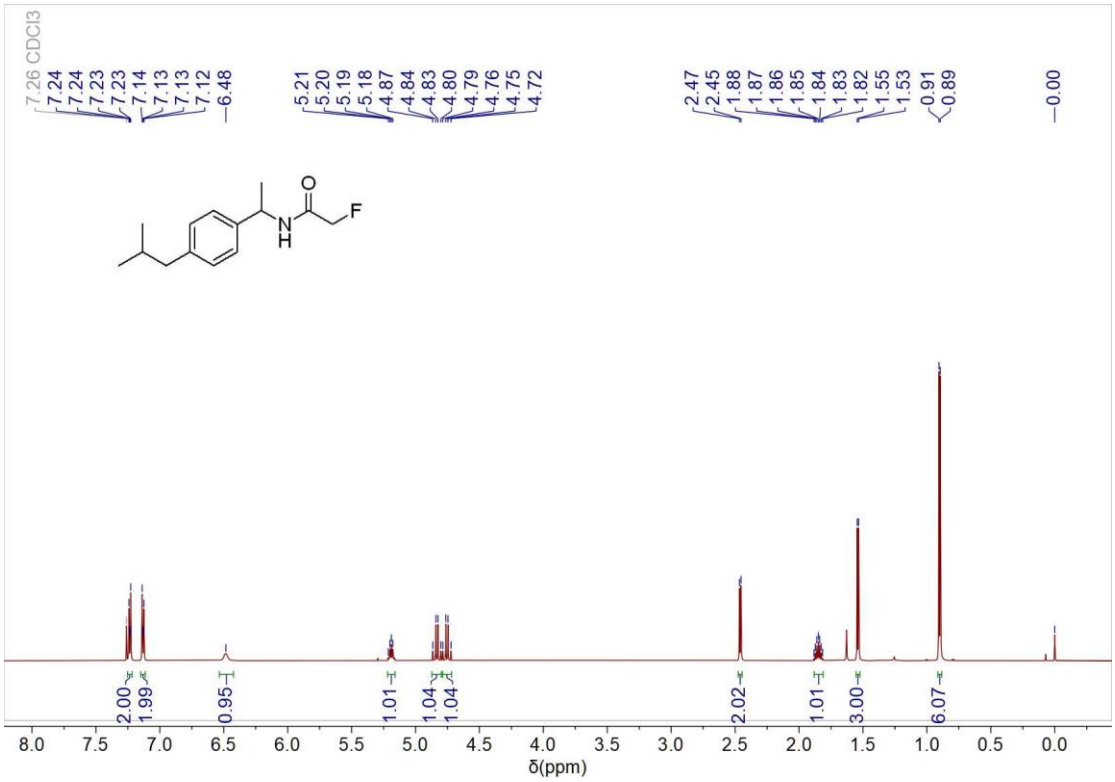
^{13}C NMR of compound 51



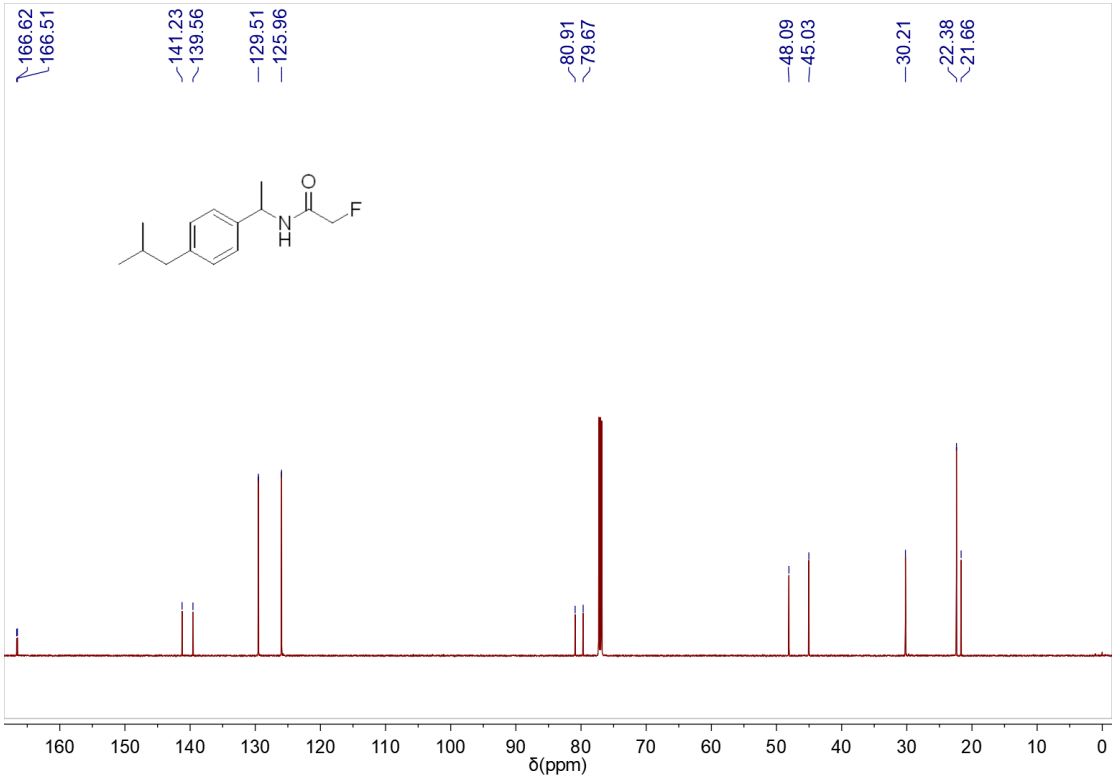
^{19}F NMR of compound 51



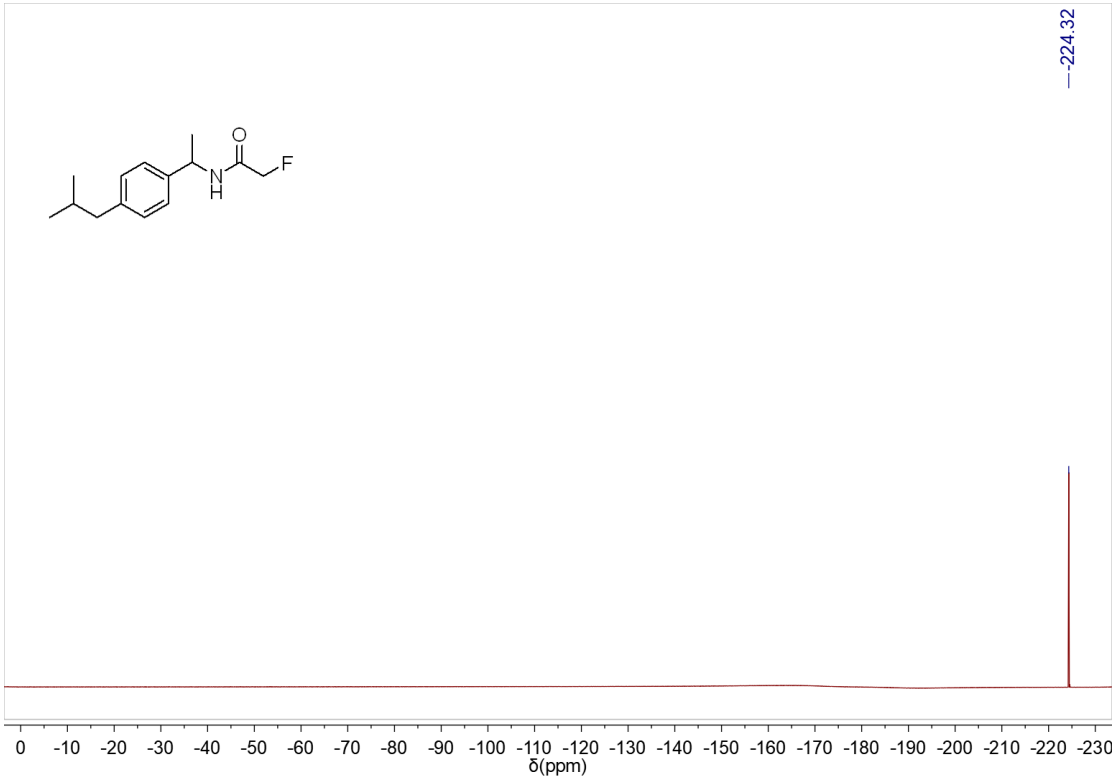
^{1}H NMR of compound 52



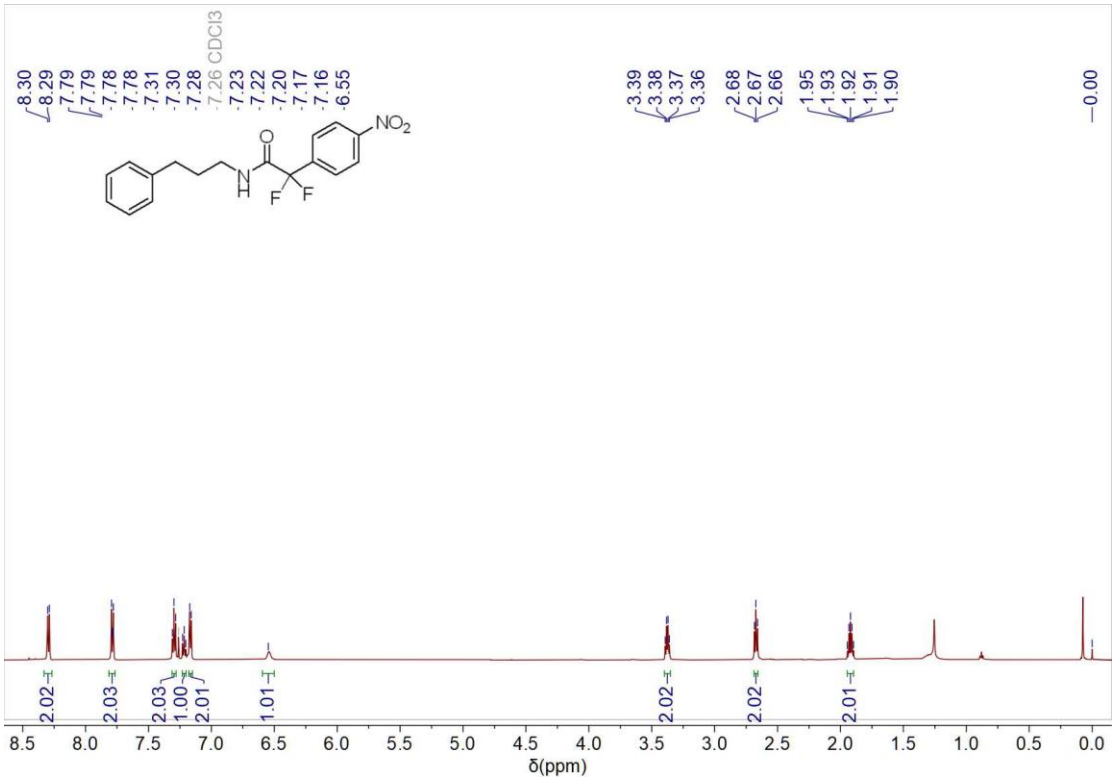
^{13}C NMR of compound 52



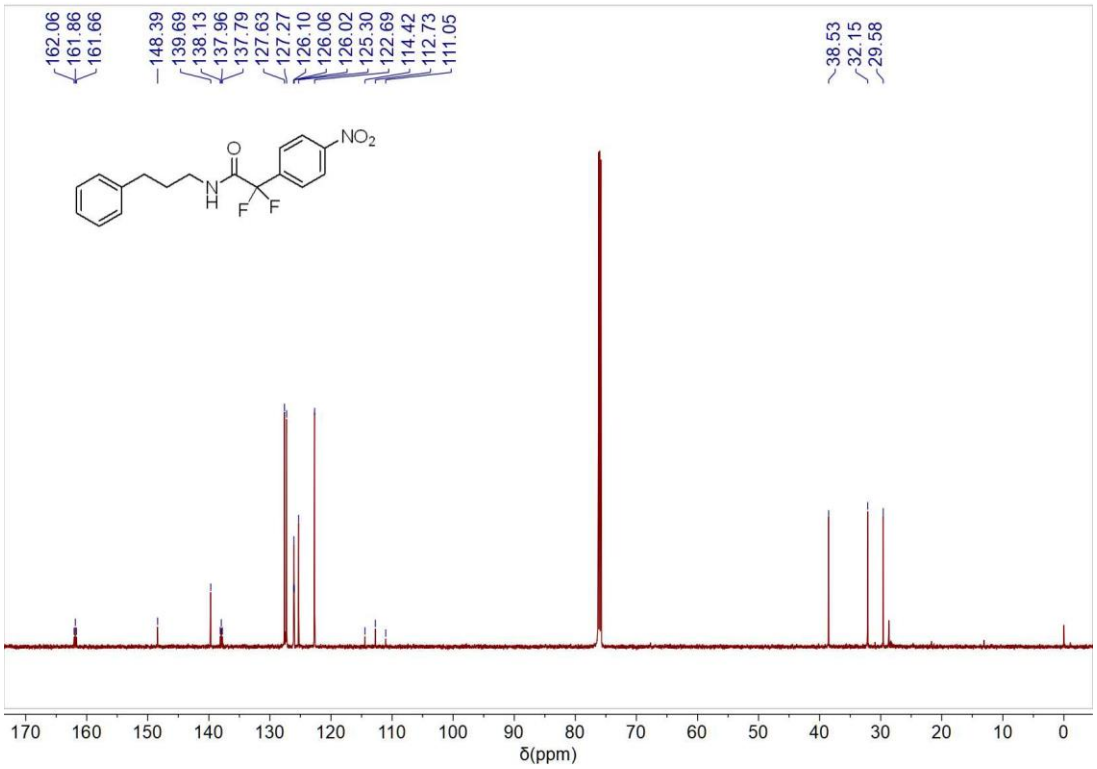
^{19}F NMR of compound 52



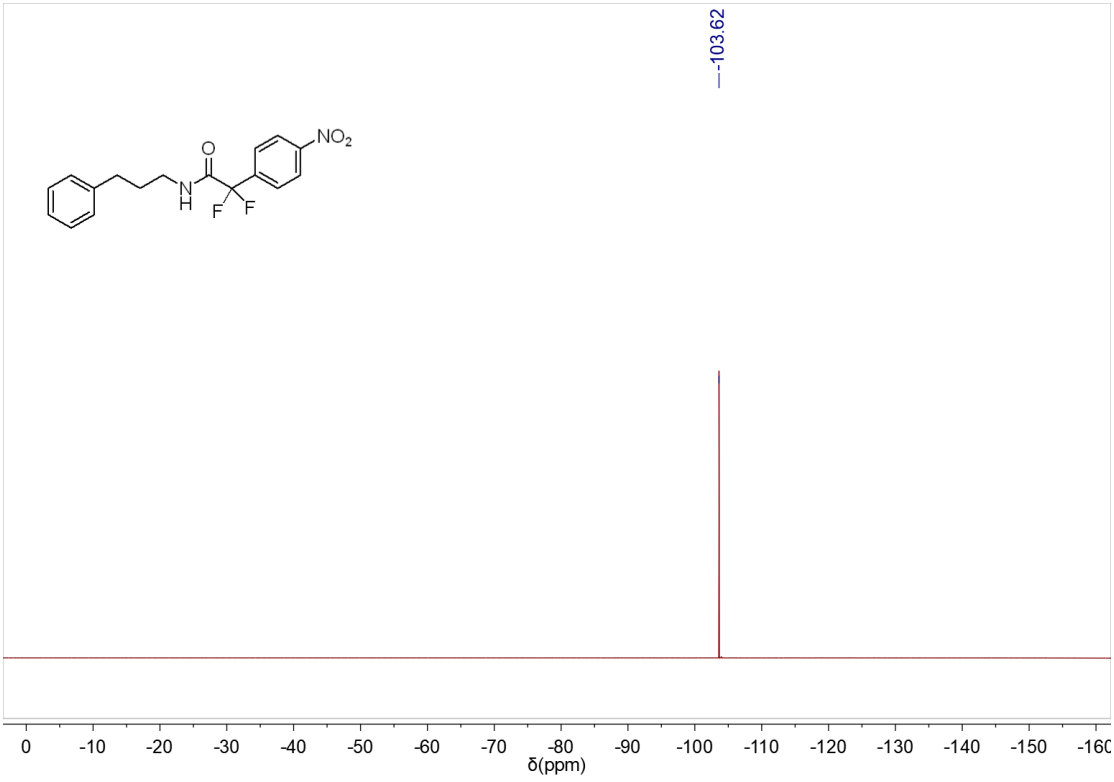
^{1}H NMR of compound 53



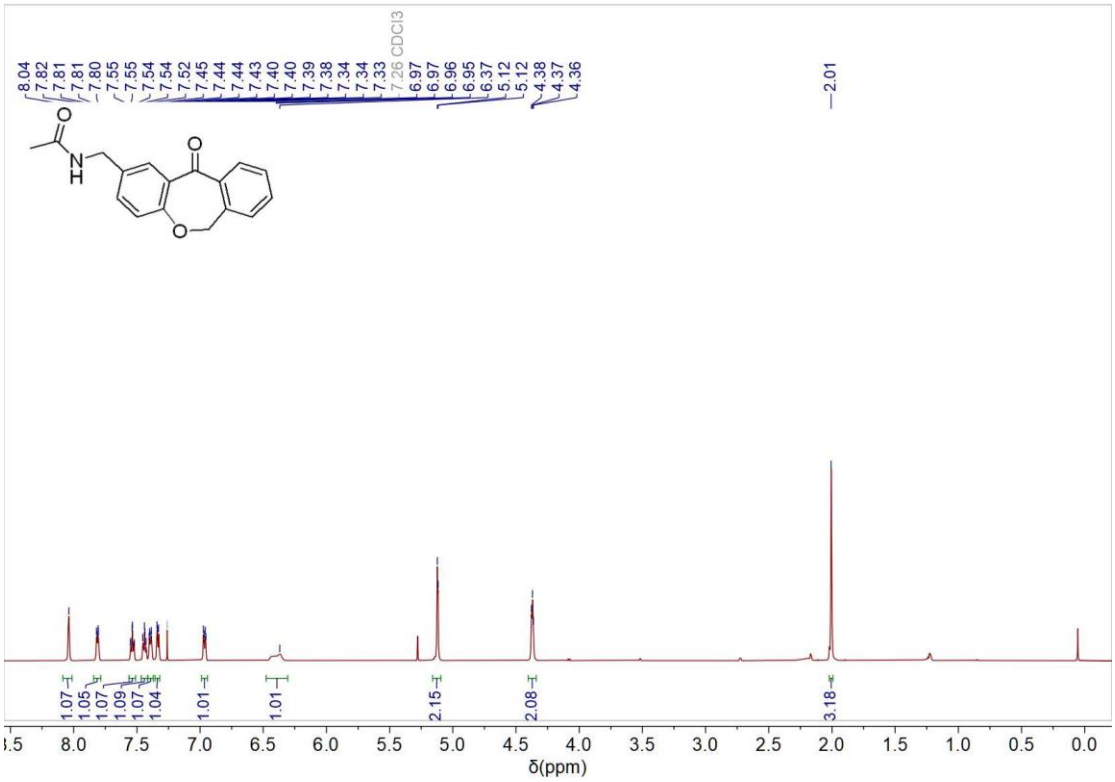
^{13}C NMR of compound 53



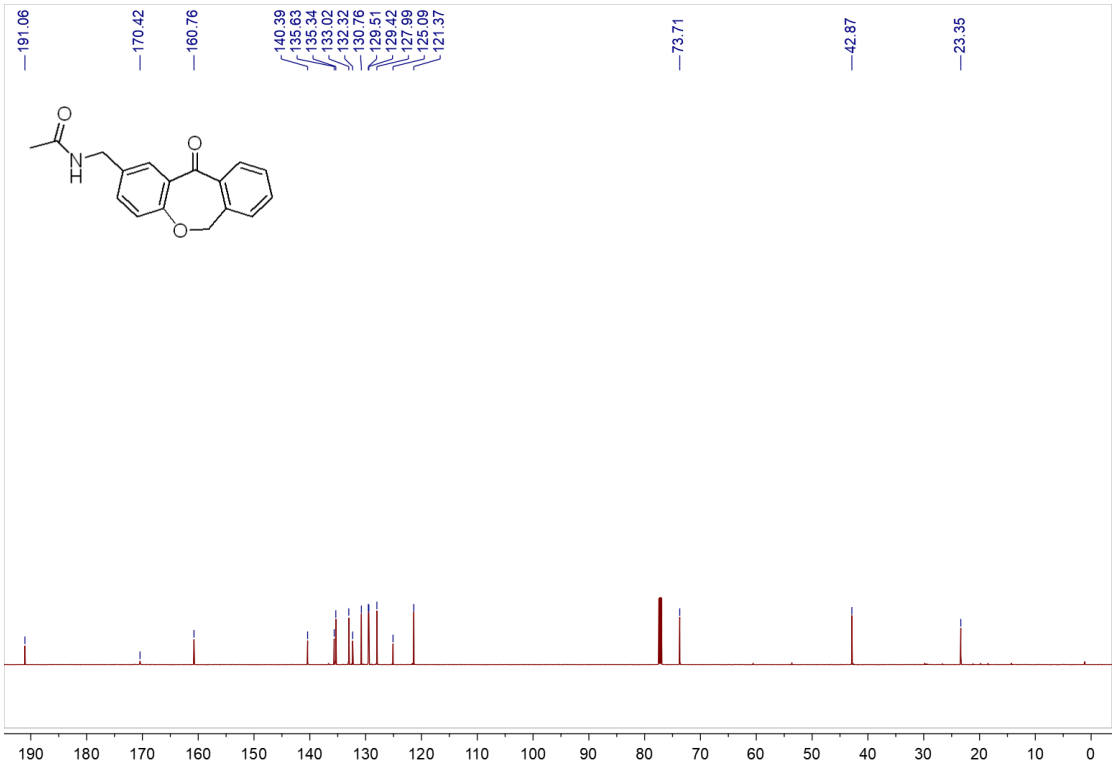
^{19} F NMR of compound 53



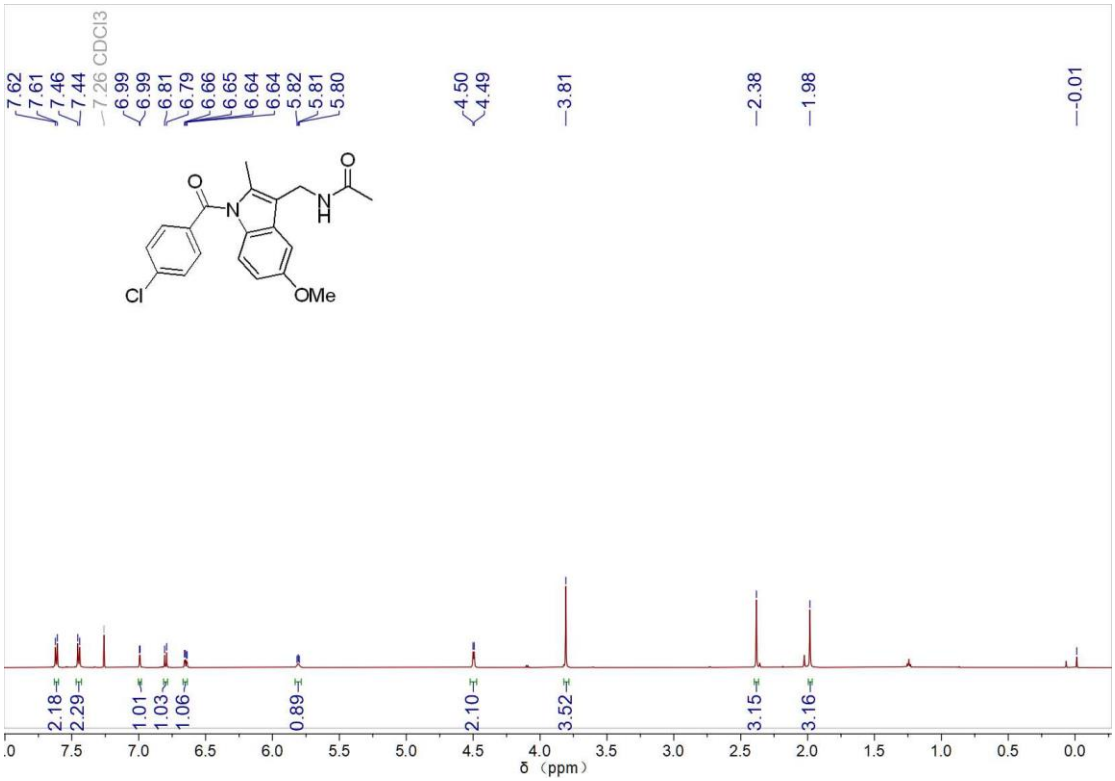
^{1}H NMR of compound 54



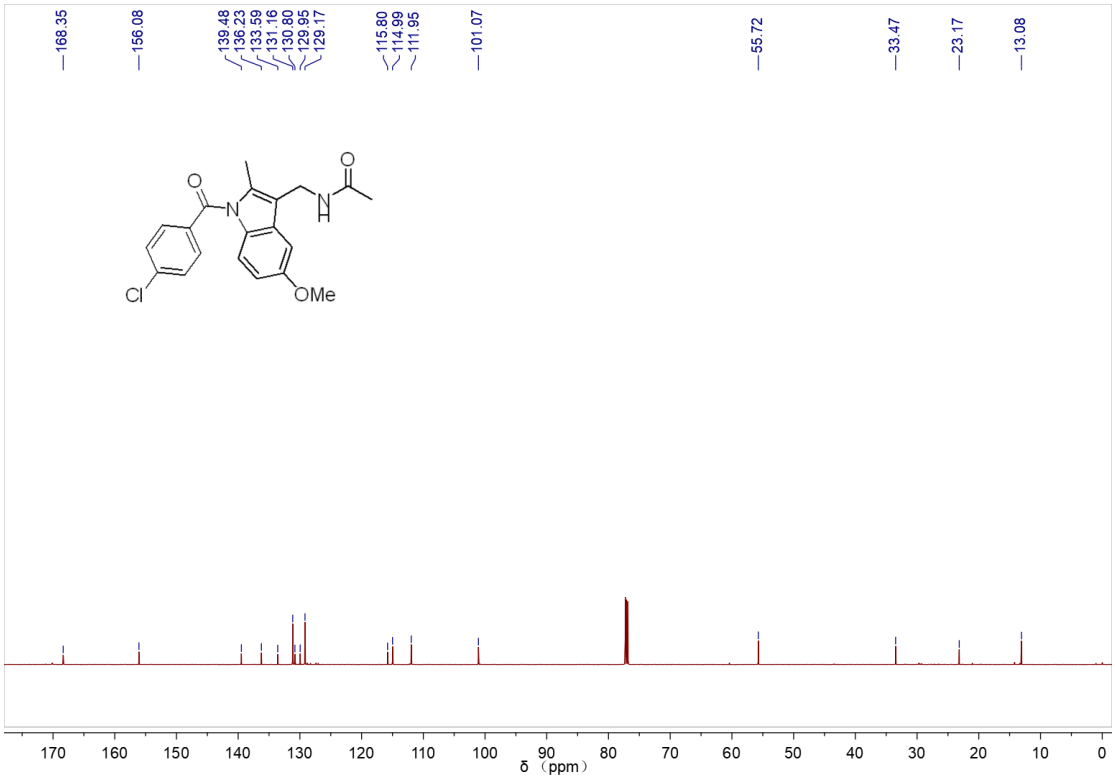
^{13}C NMR of compound 54



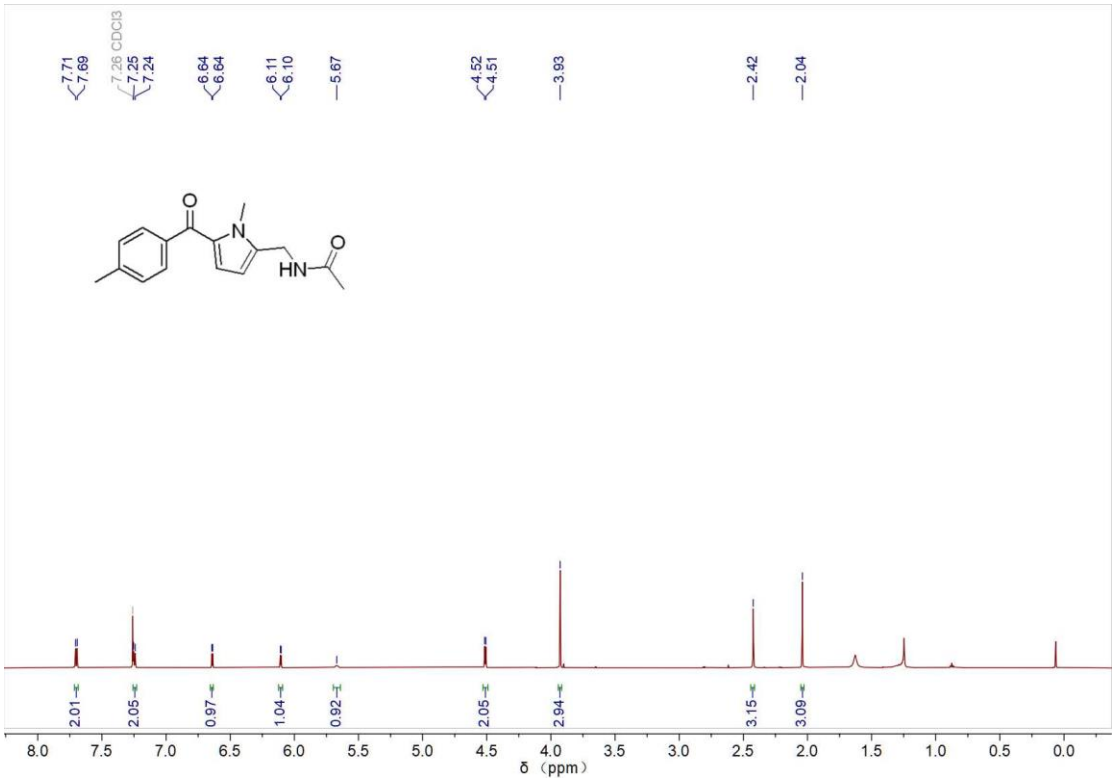
^{1}H NMR of compound 55



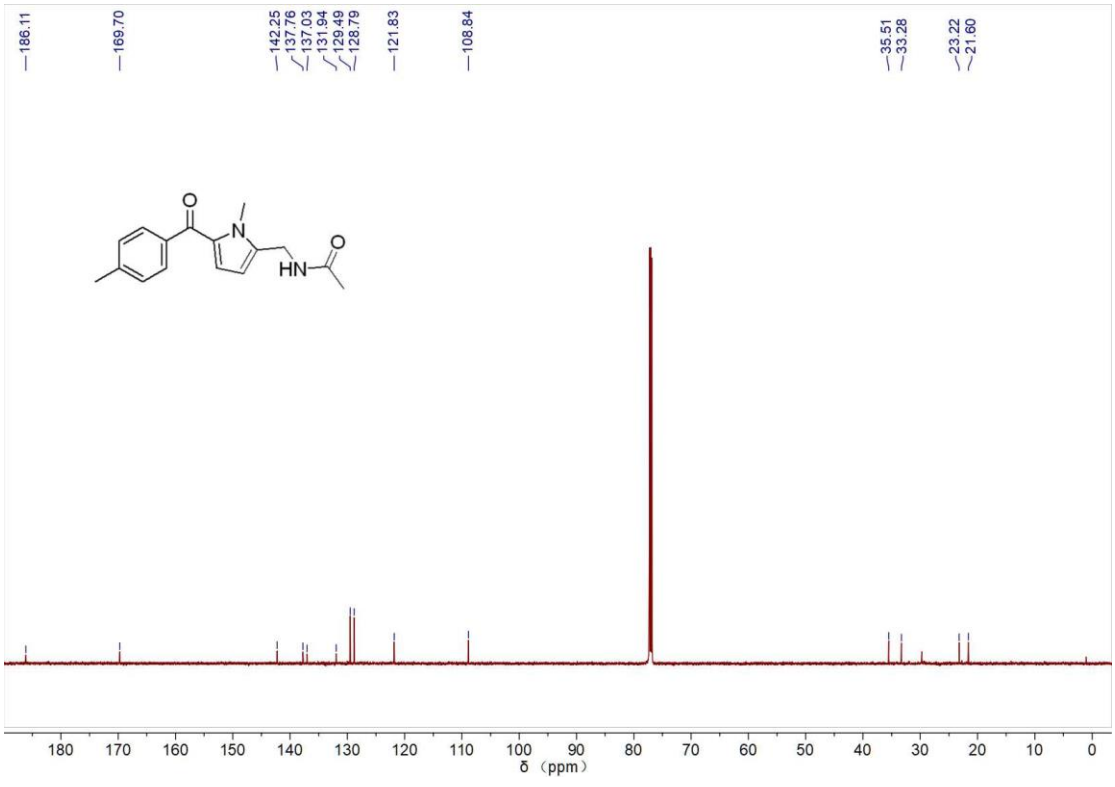
^{13}C NMR of compound 55



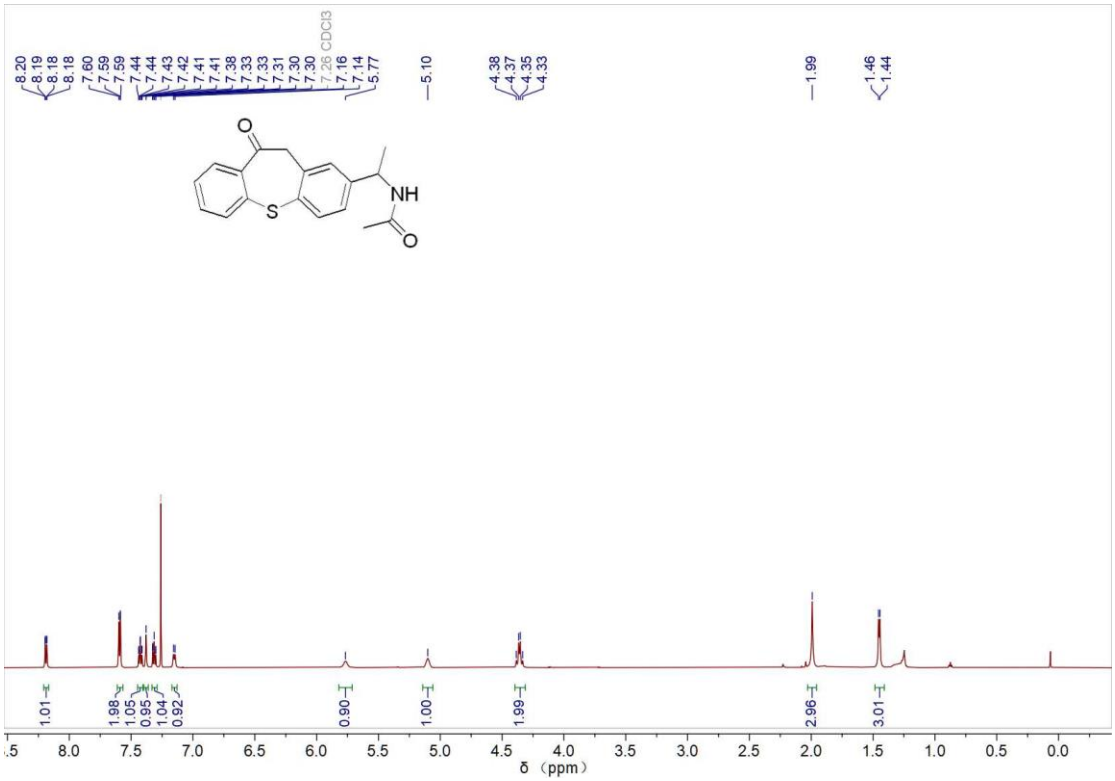
^{1}H NMR of compound 56



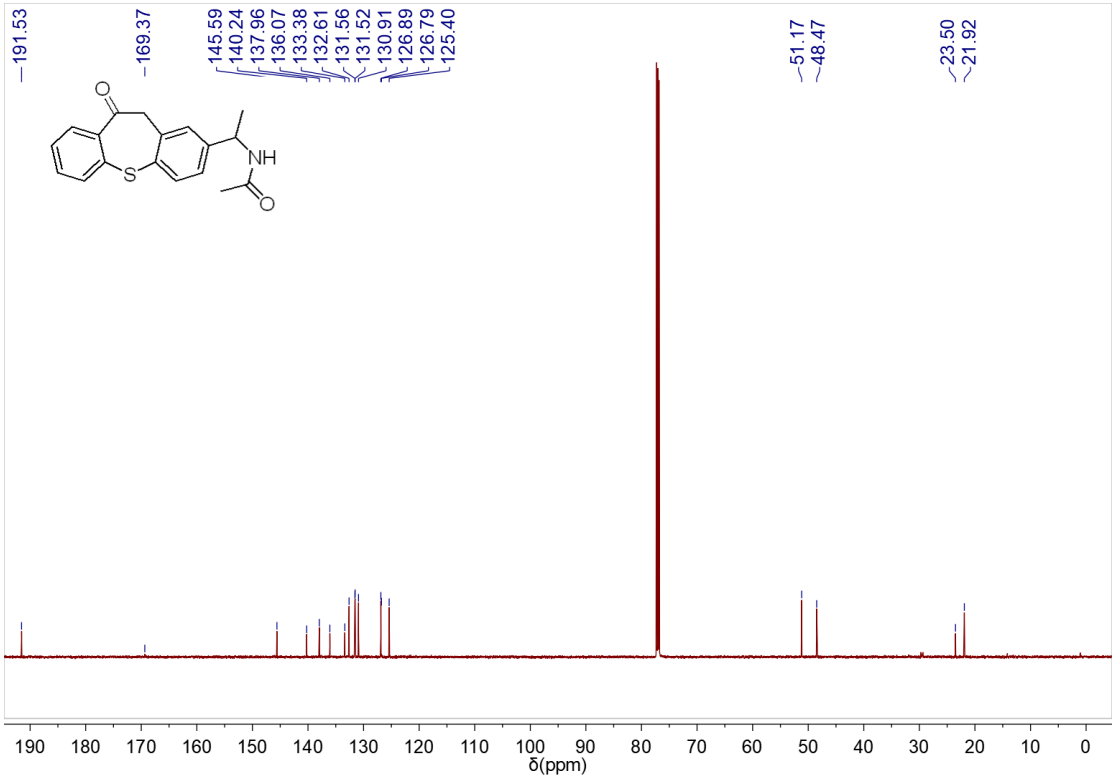
^{13}C NMR of compound 56



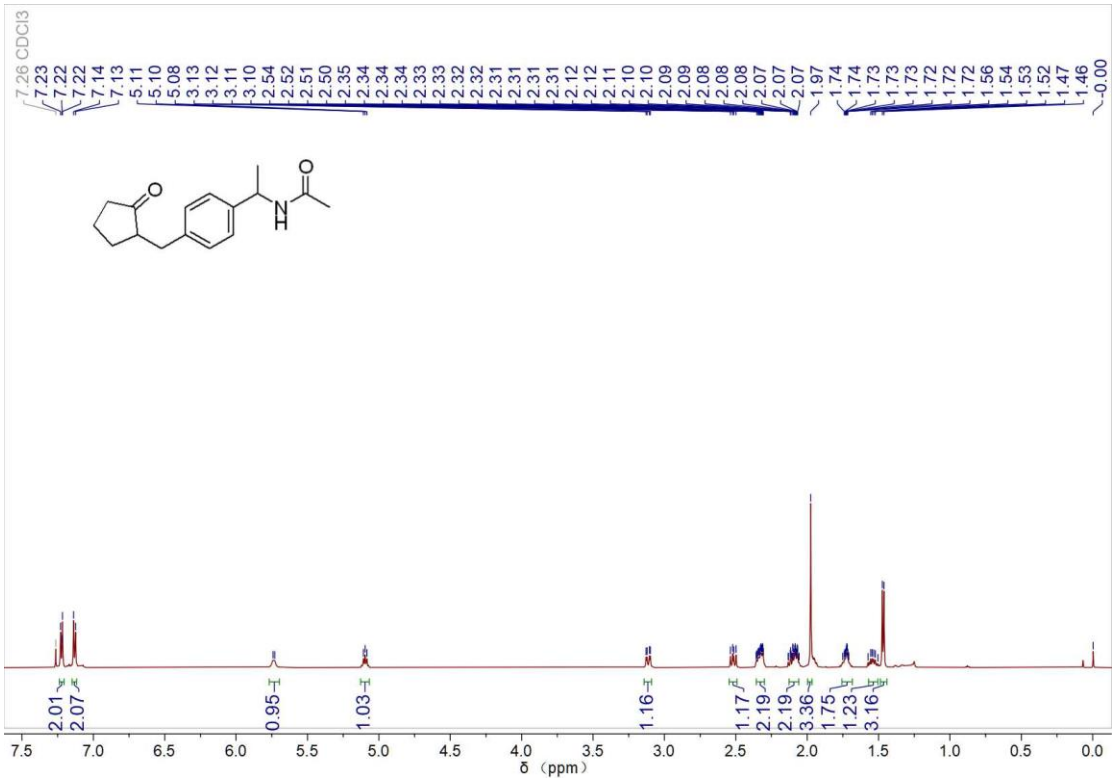
^{1}H NMR of compound 57



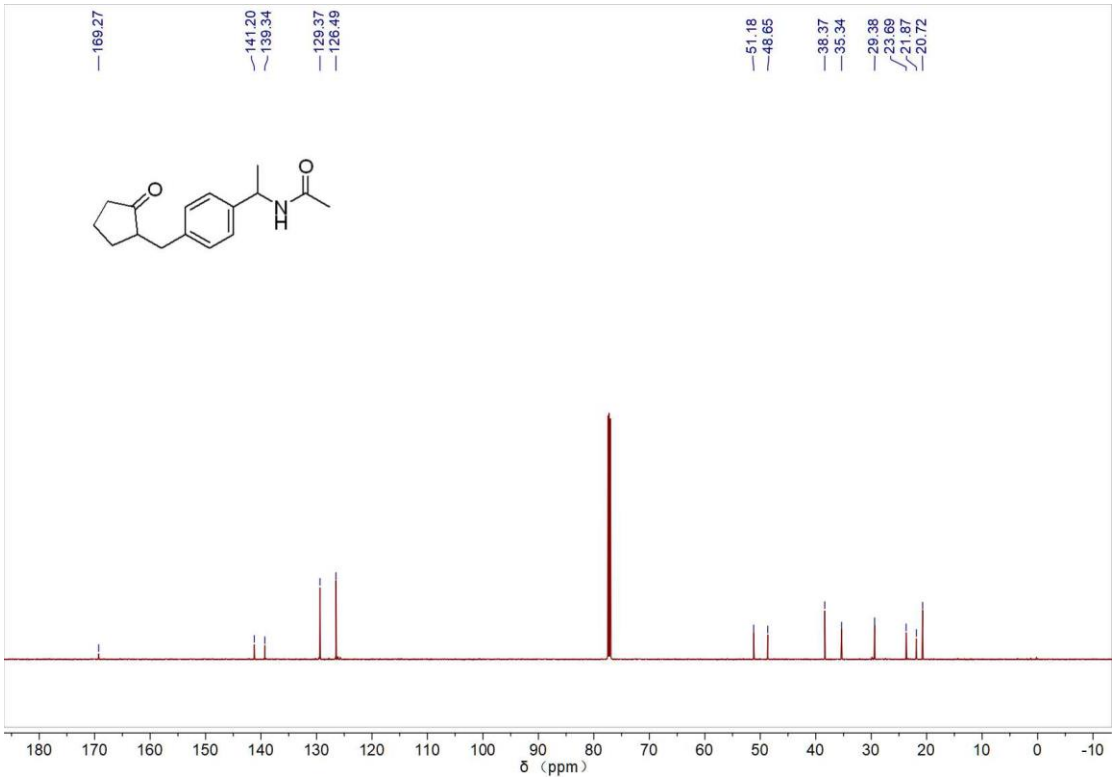
^{13}C NMR of compound 57



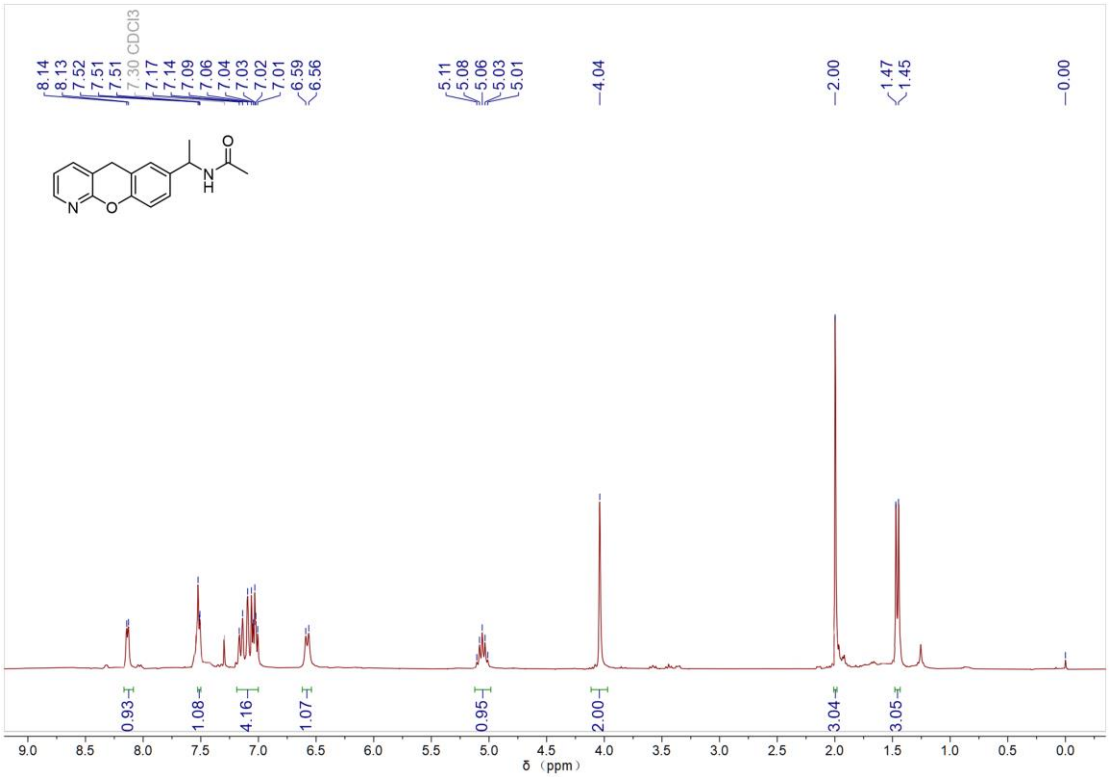
^{1}H NMR of compound 58



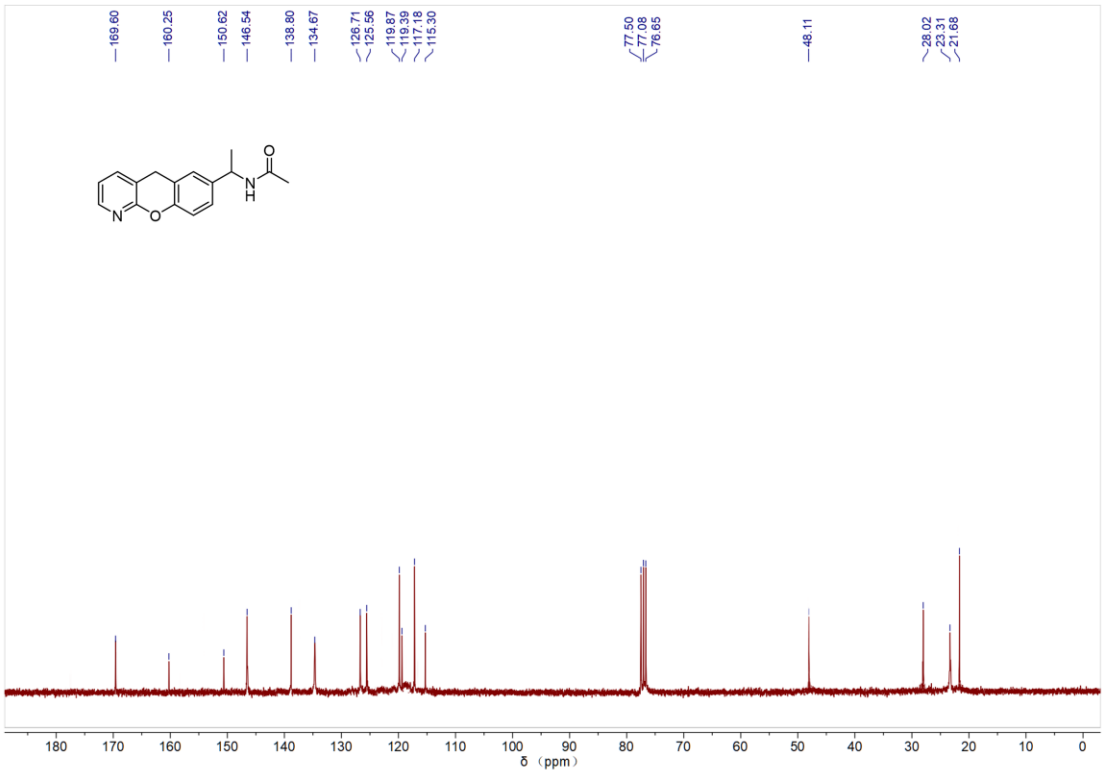
^{13}C NMR of compound 58



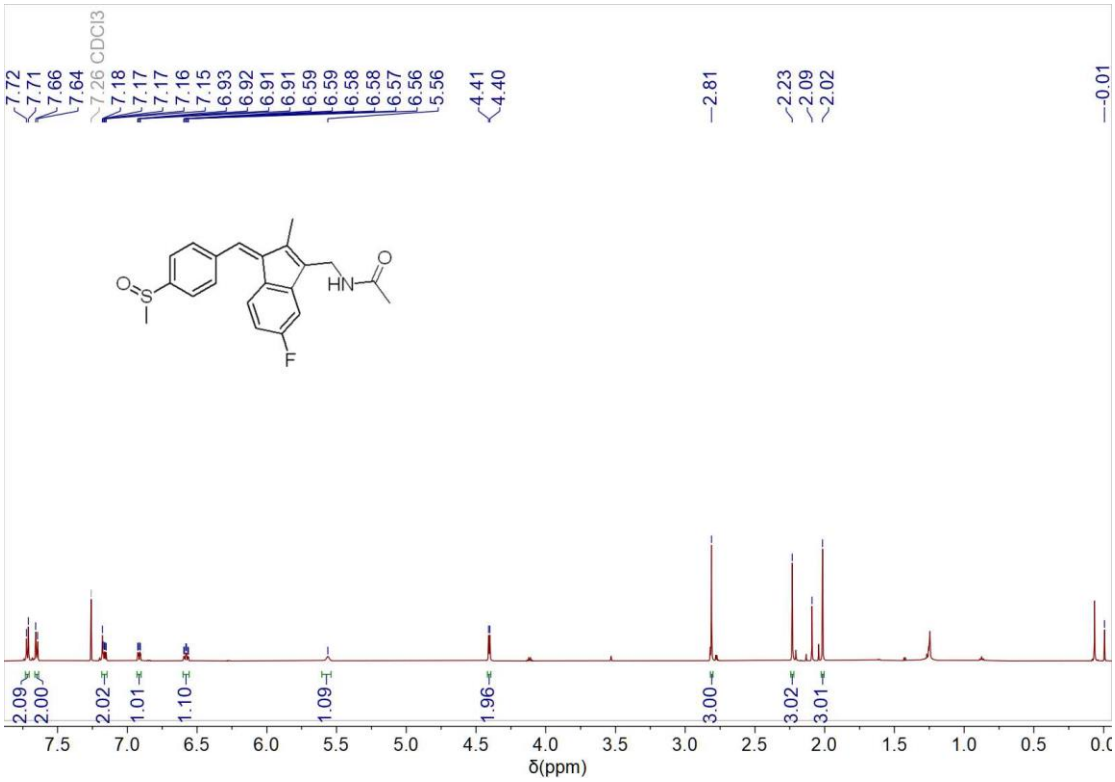
^{1}H NMR of compound 59



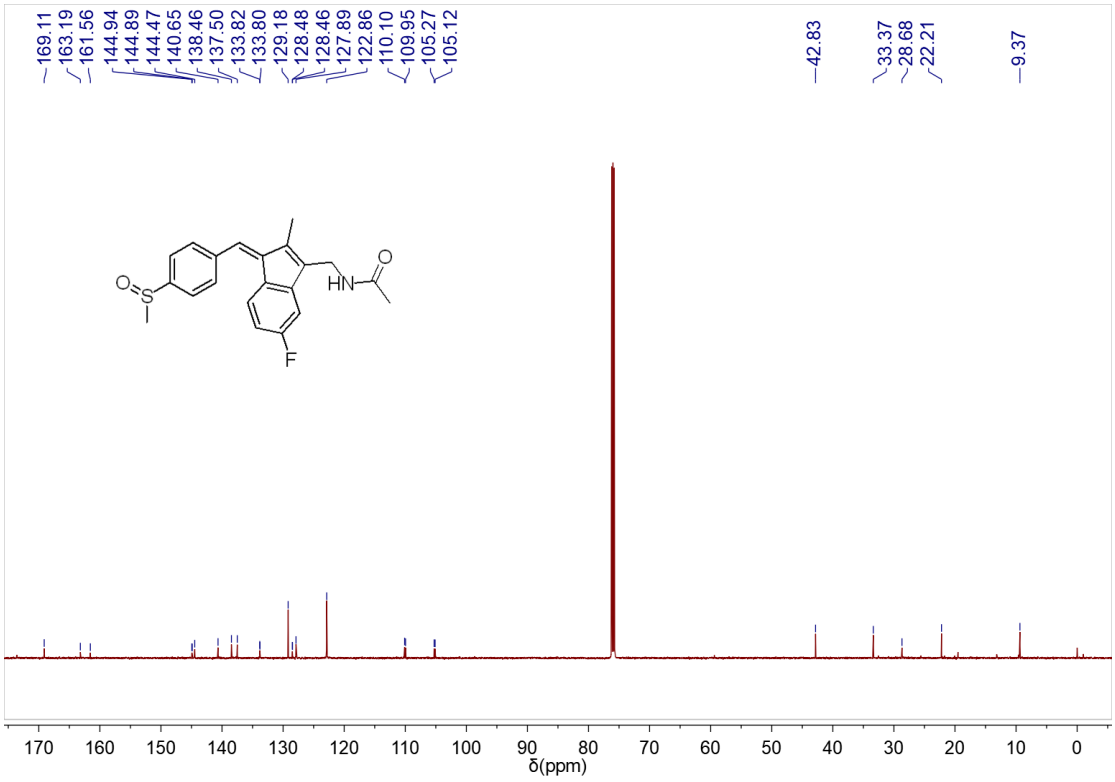
^{13}C NMR of compound 59



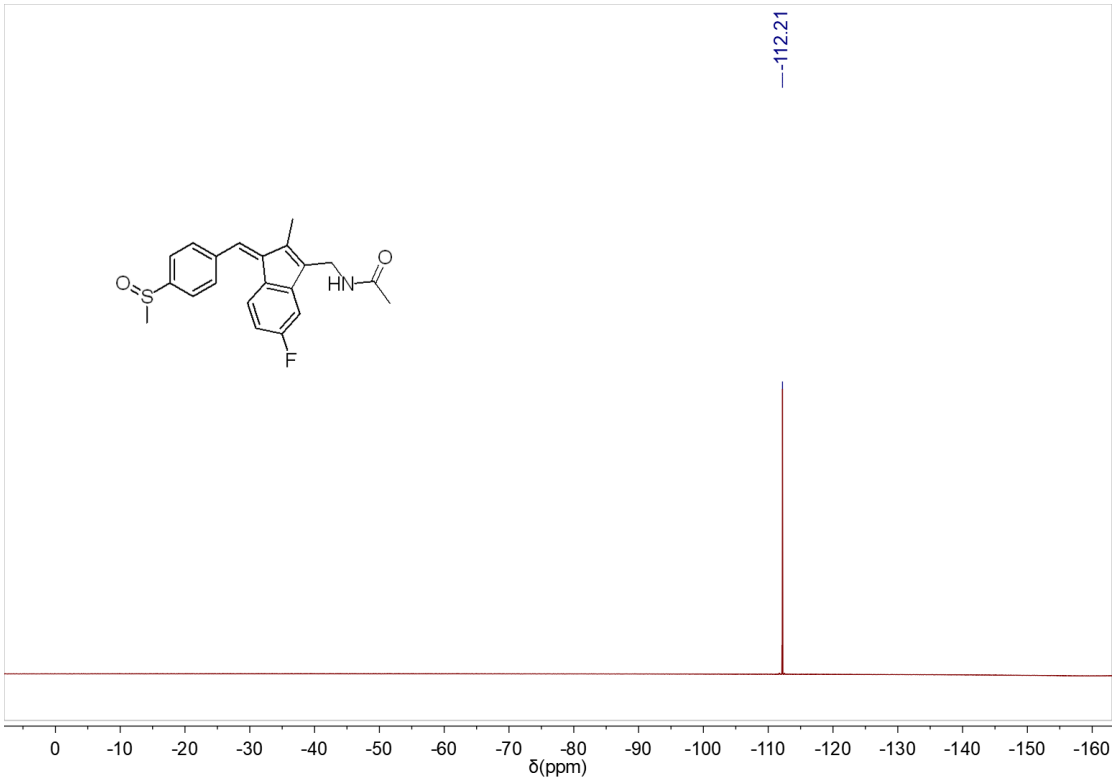
^{1}H NMR of compound 60



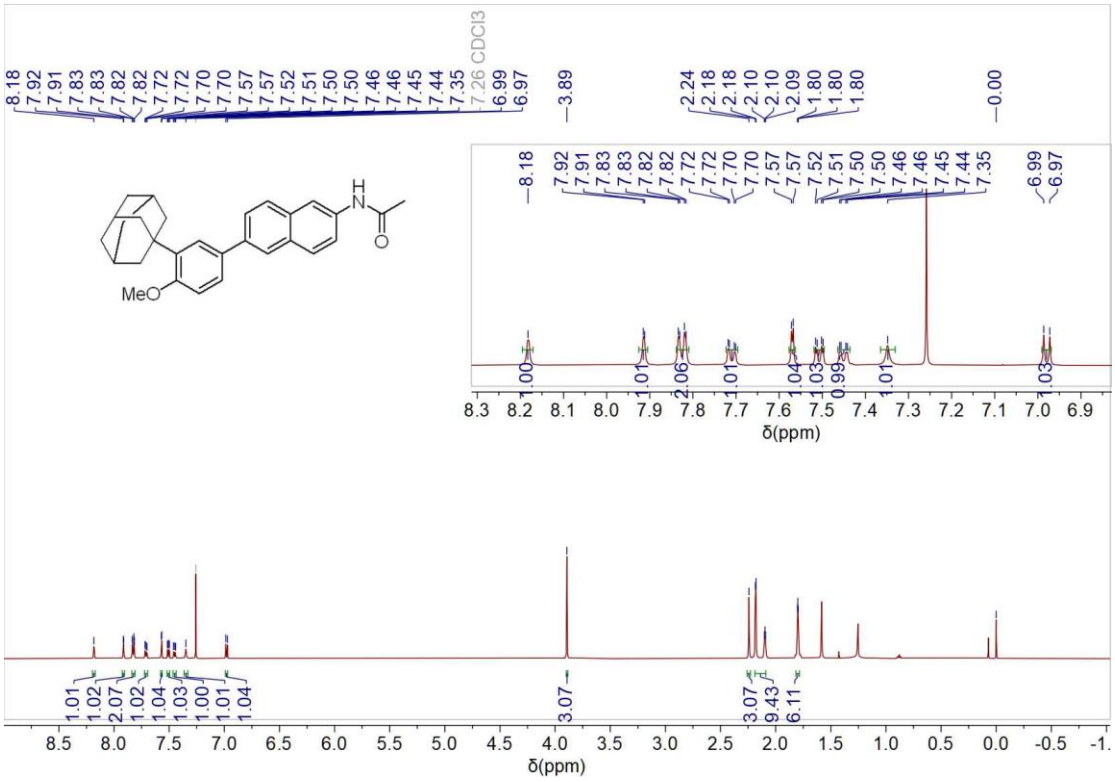
^{13}C NMR of compound 60



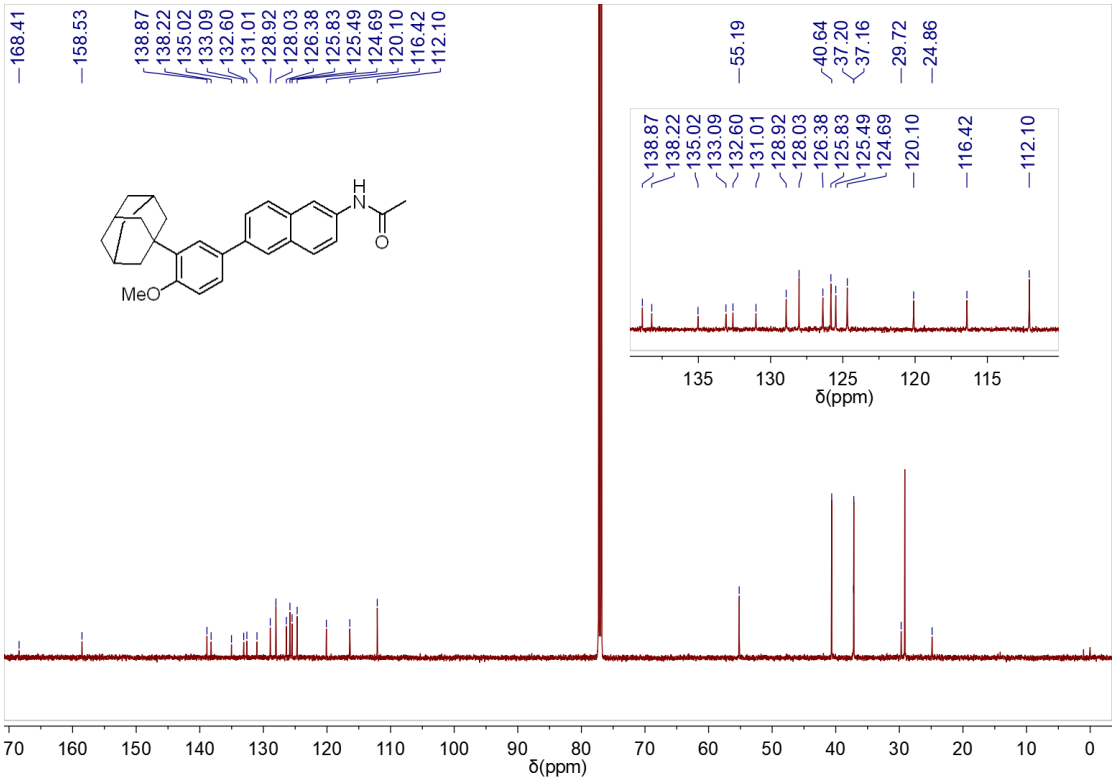
^{19}F NMR of compound 60



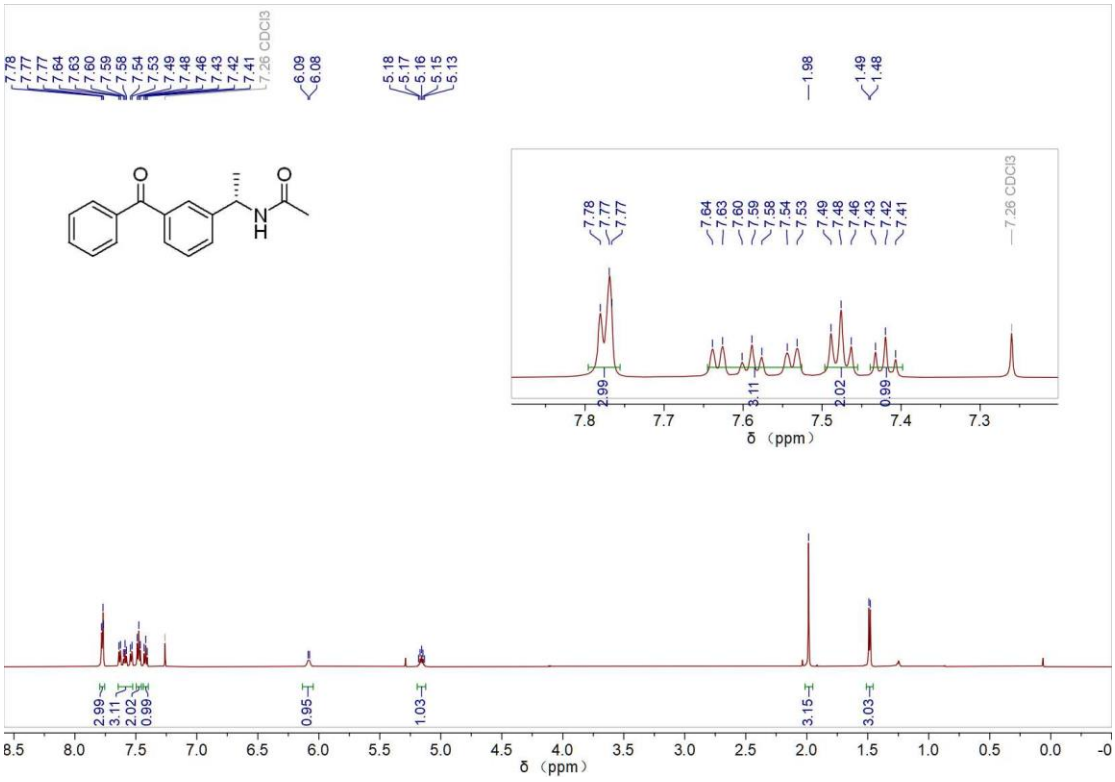
^{1}H NMR of compound 61



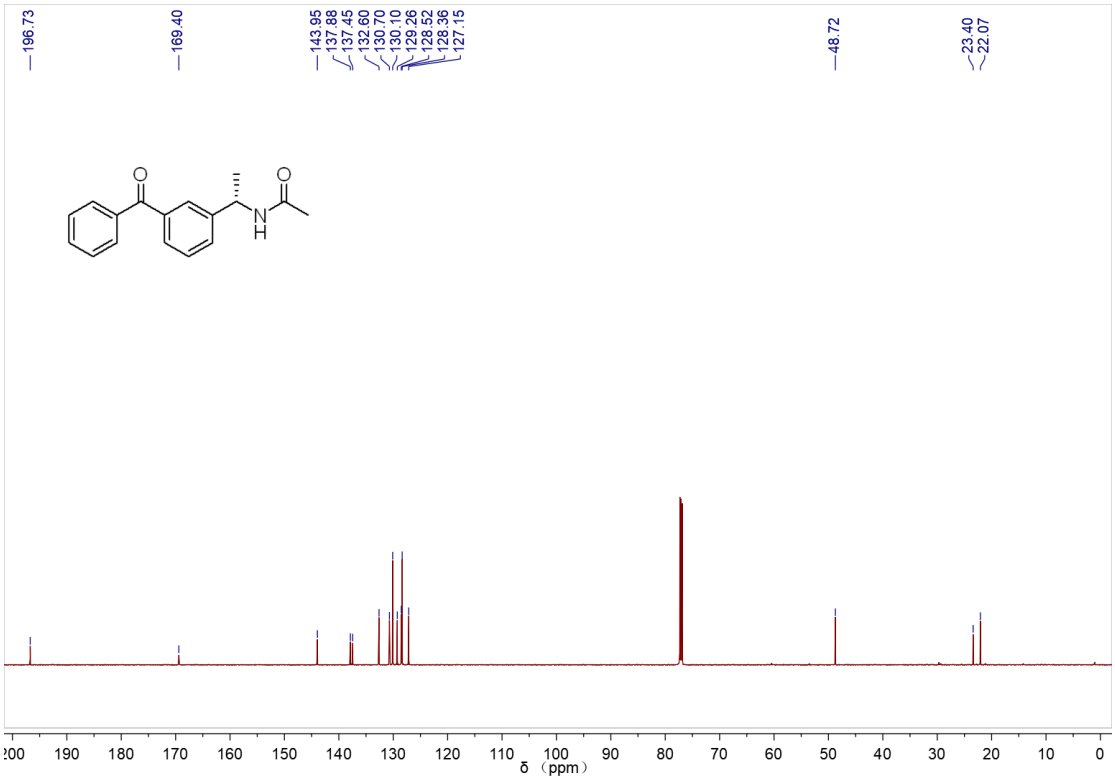
^{13}C NMR of compound 61



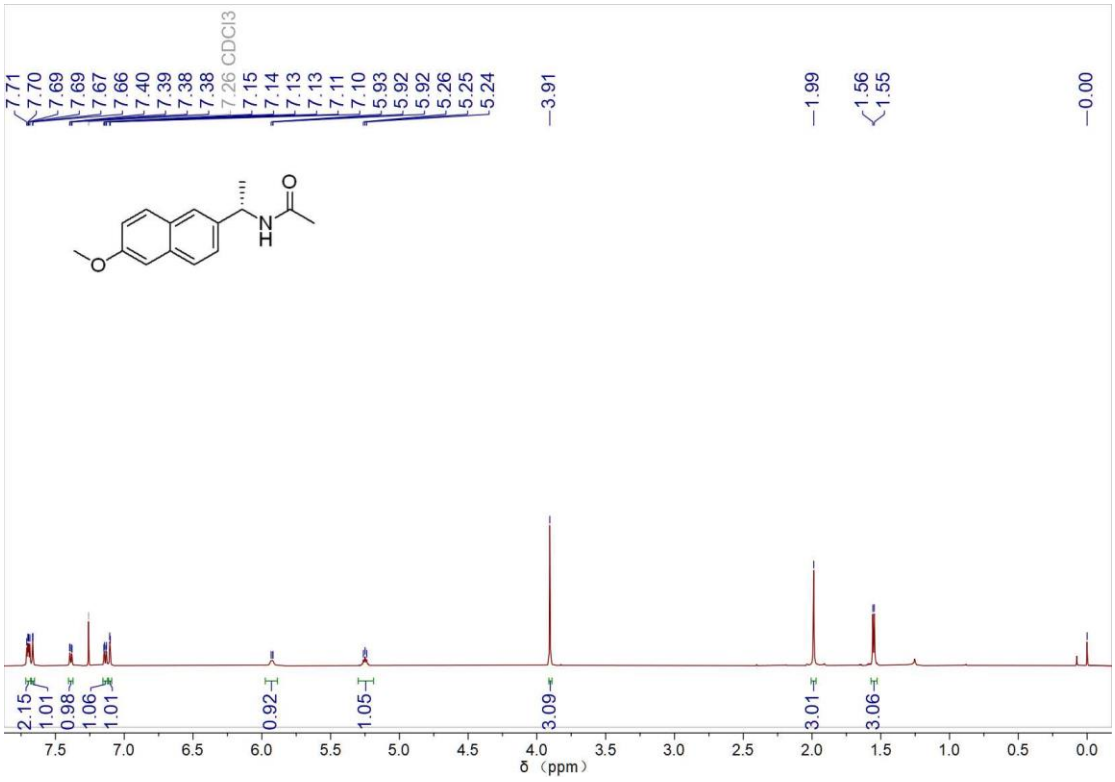
^{1}H NMR of compound 65



^{13}C NMR of compound 65



^{1}H NMR of compound 66



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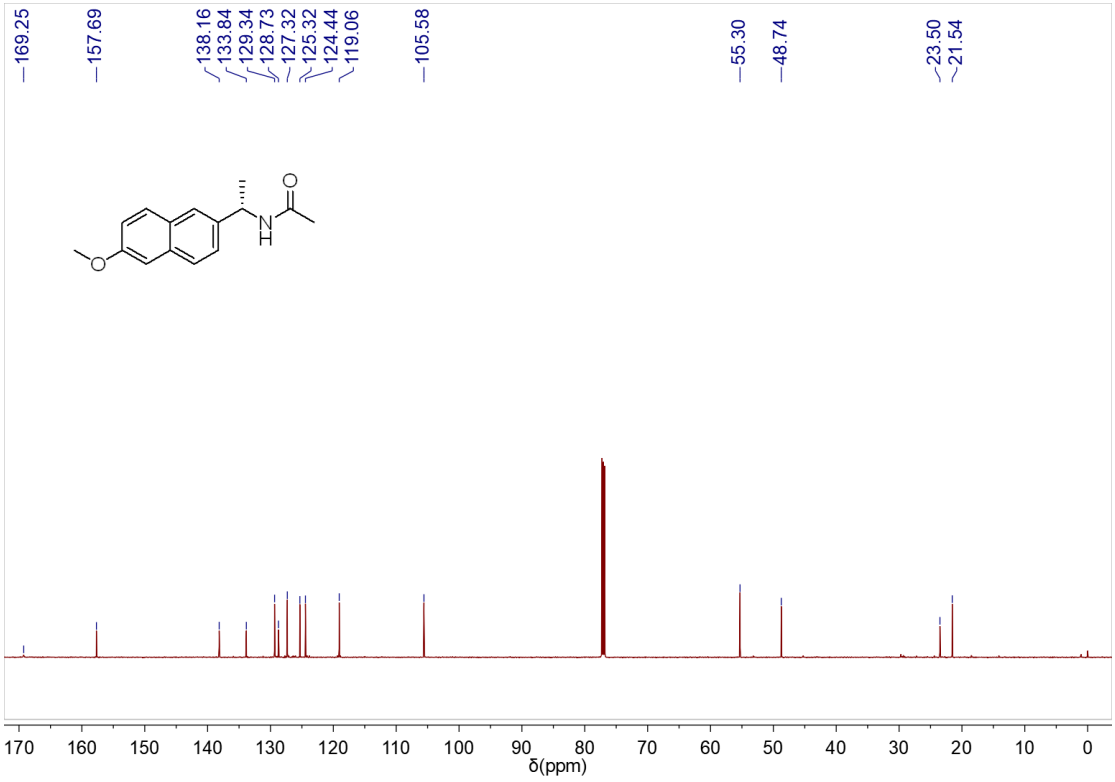
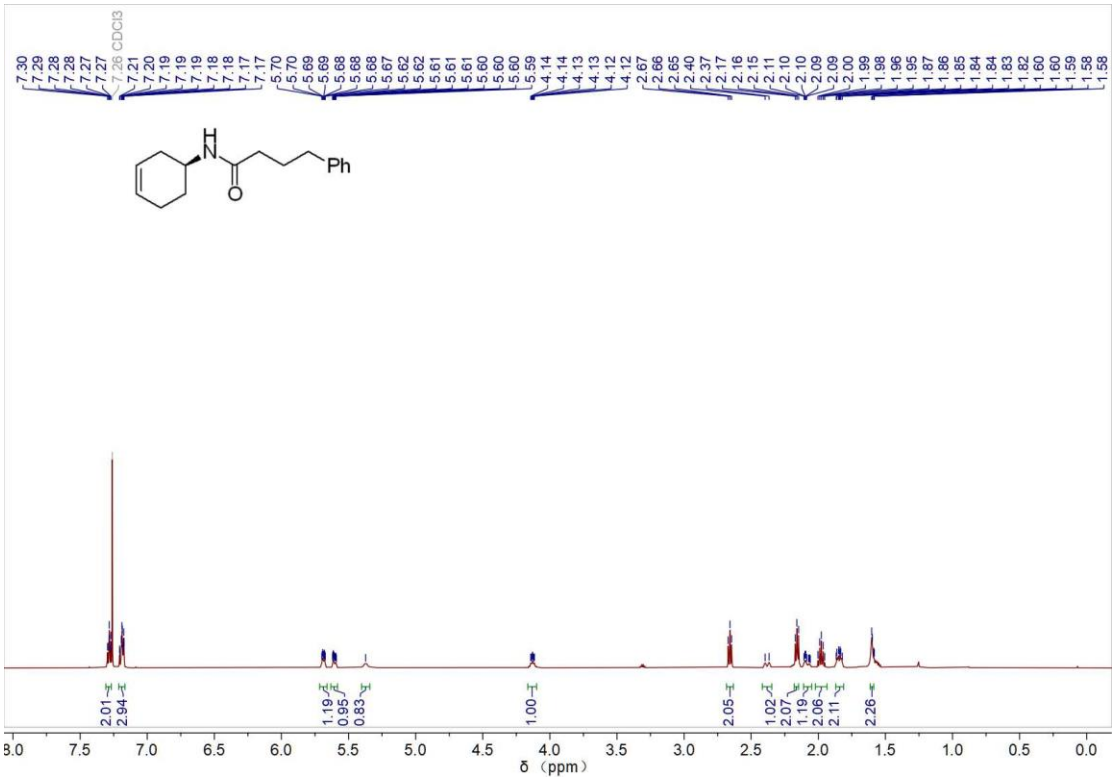
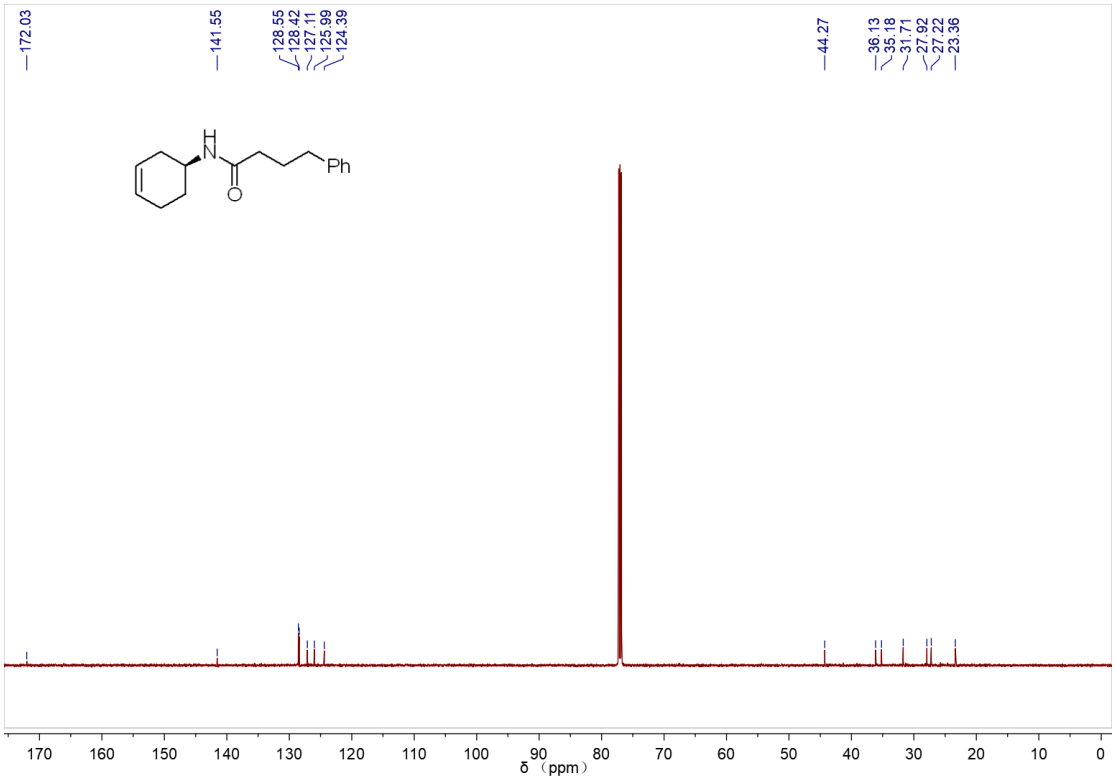


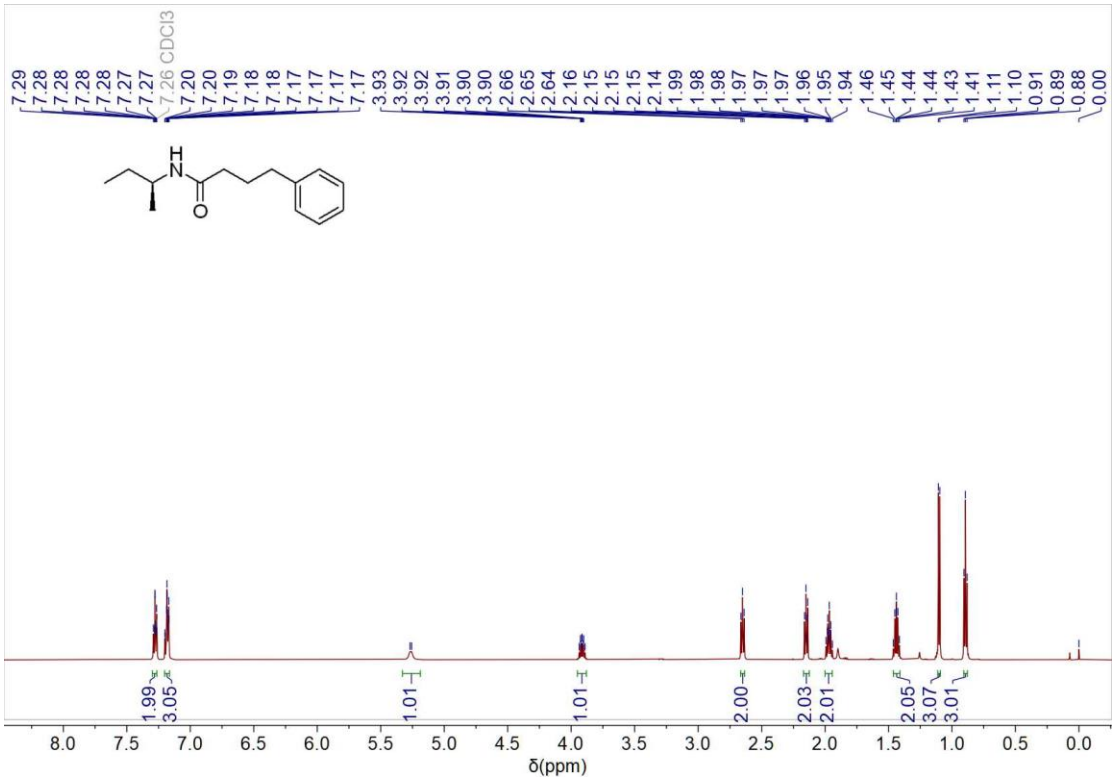
^{1}H NMR of compound 67



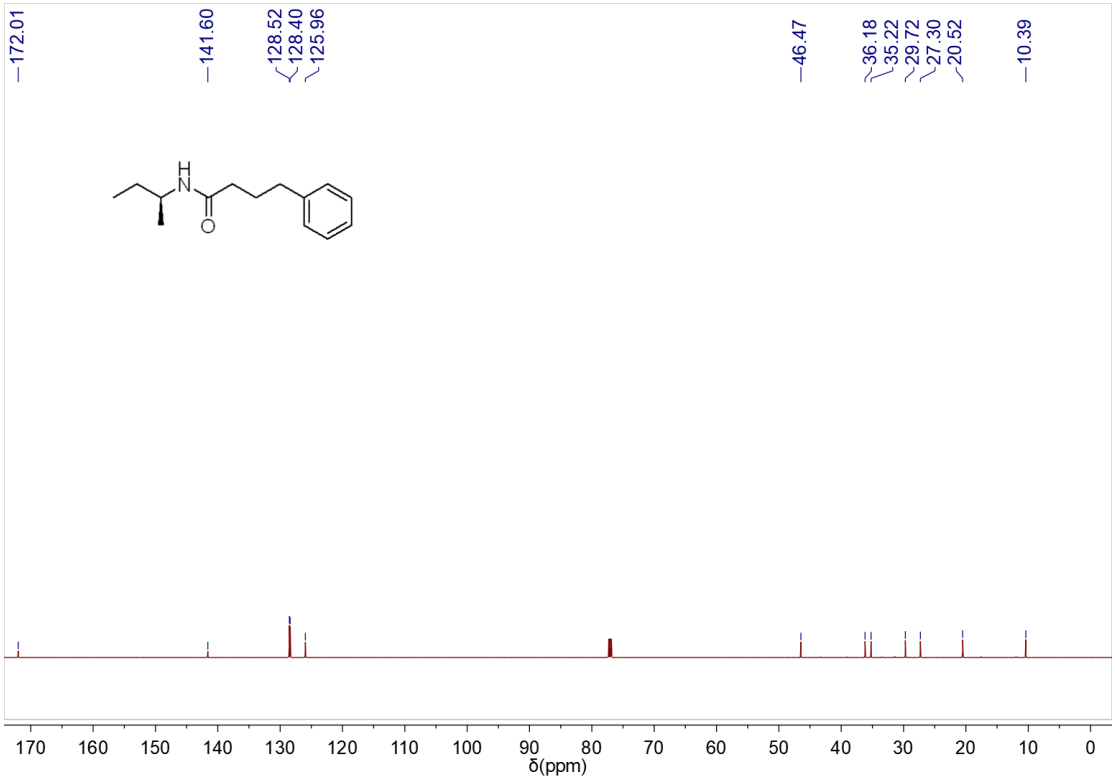
^{13}C NMR of compound 67



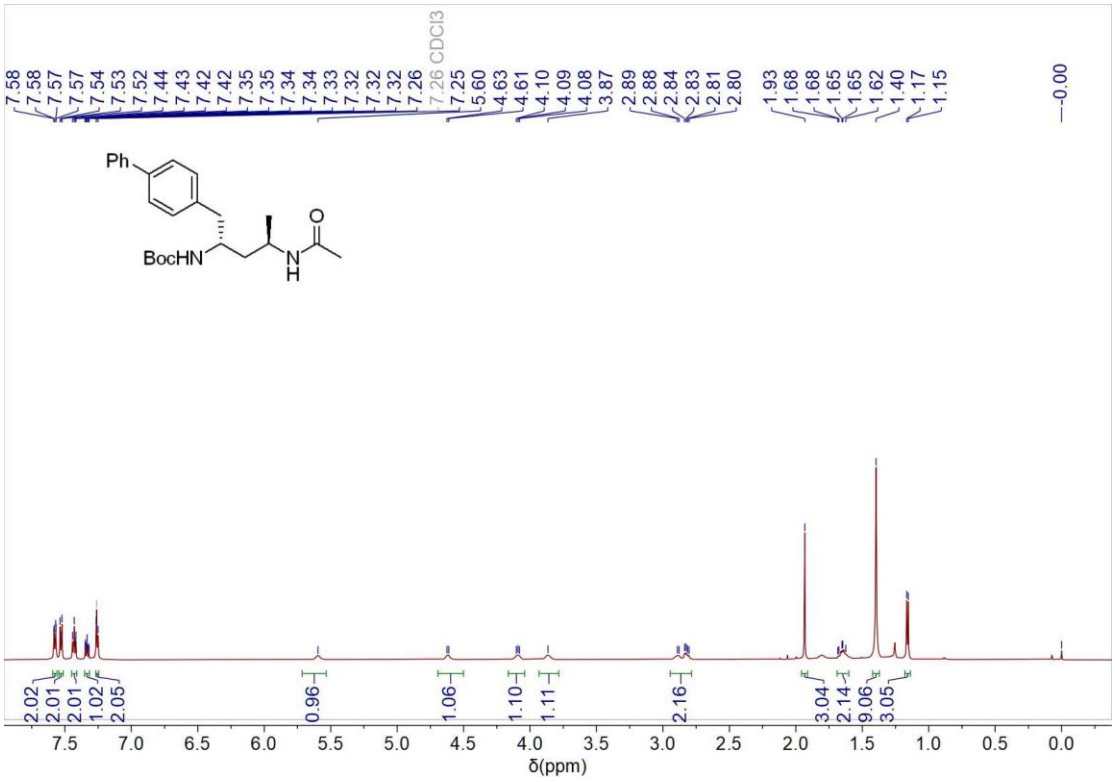
^{1}H NMR of compound 69



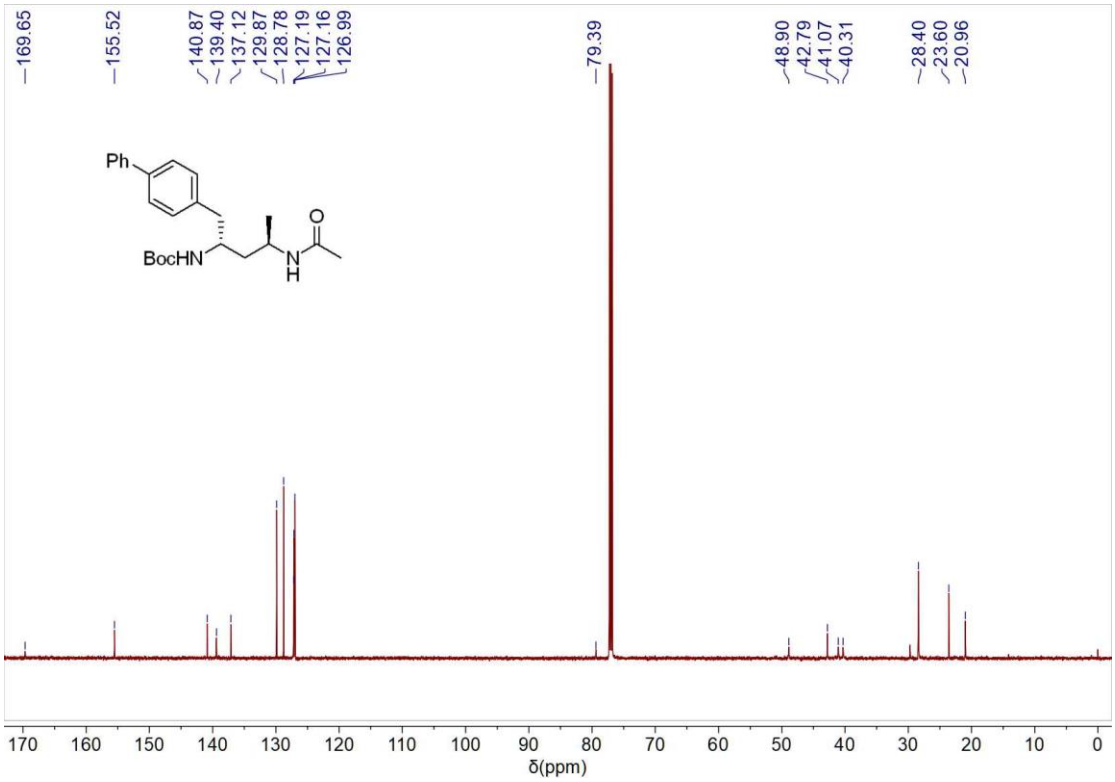
^{13}C NMR of compound 69



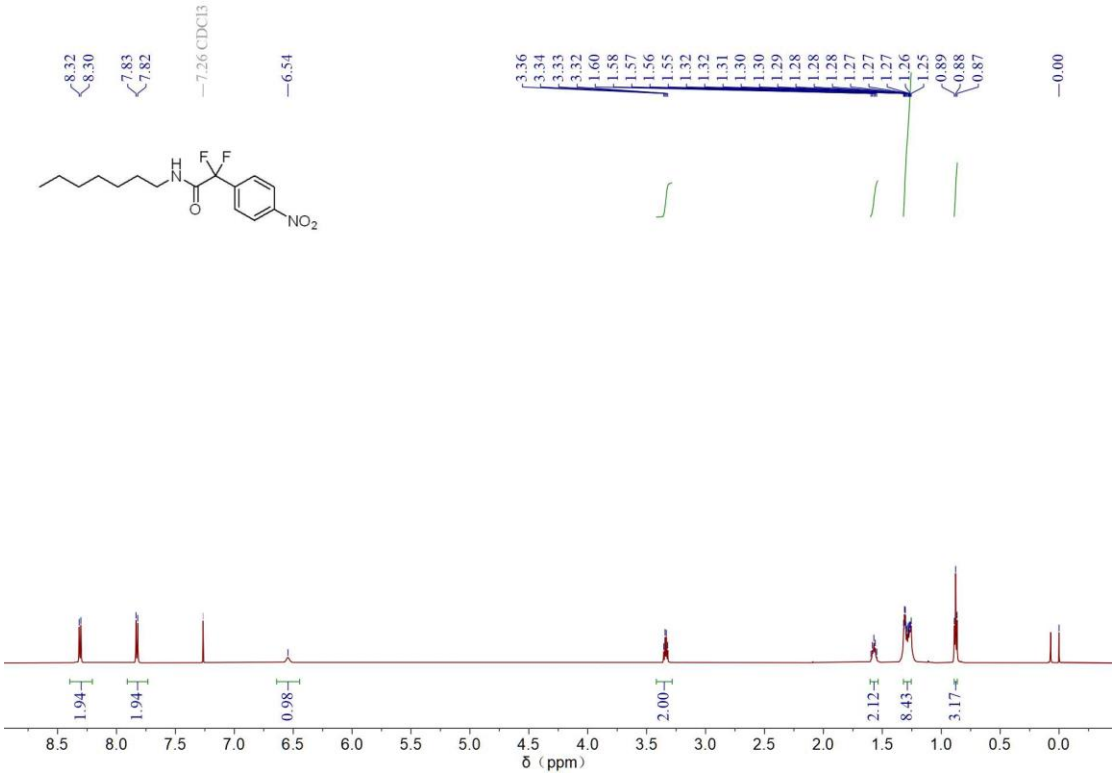
^{1}H NMR of compound 70



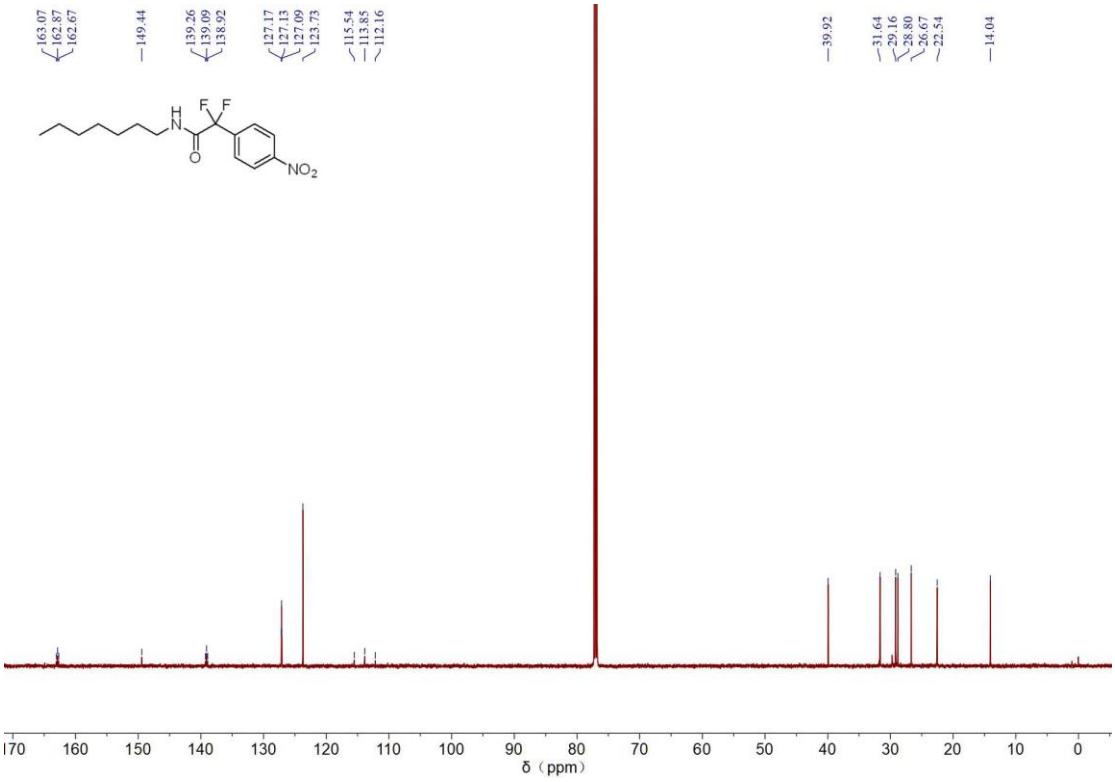
^{13}C NMR of compound 70



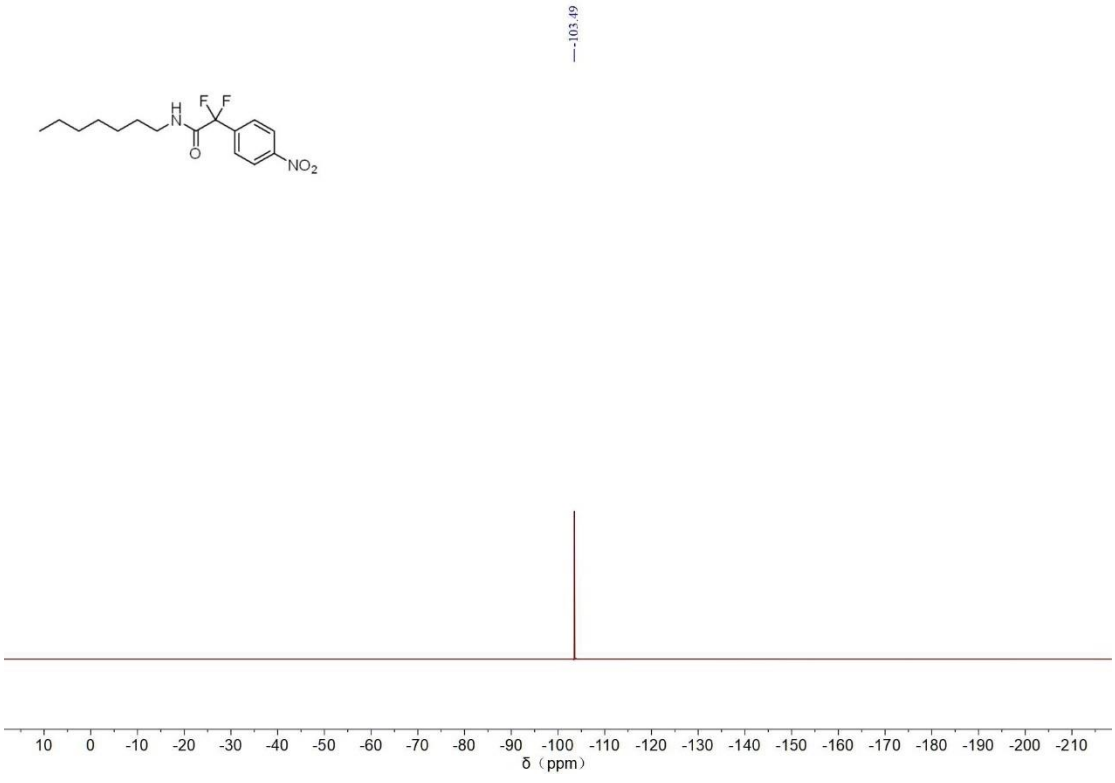
^{1}H NMR of compound 74



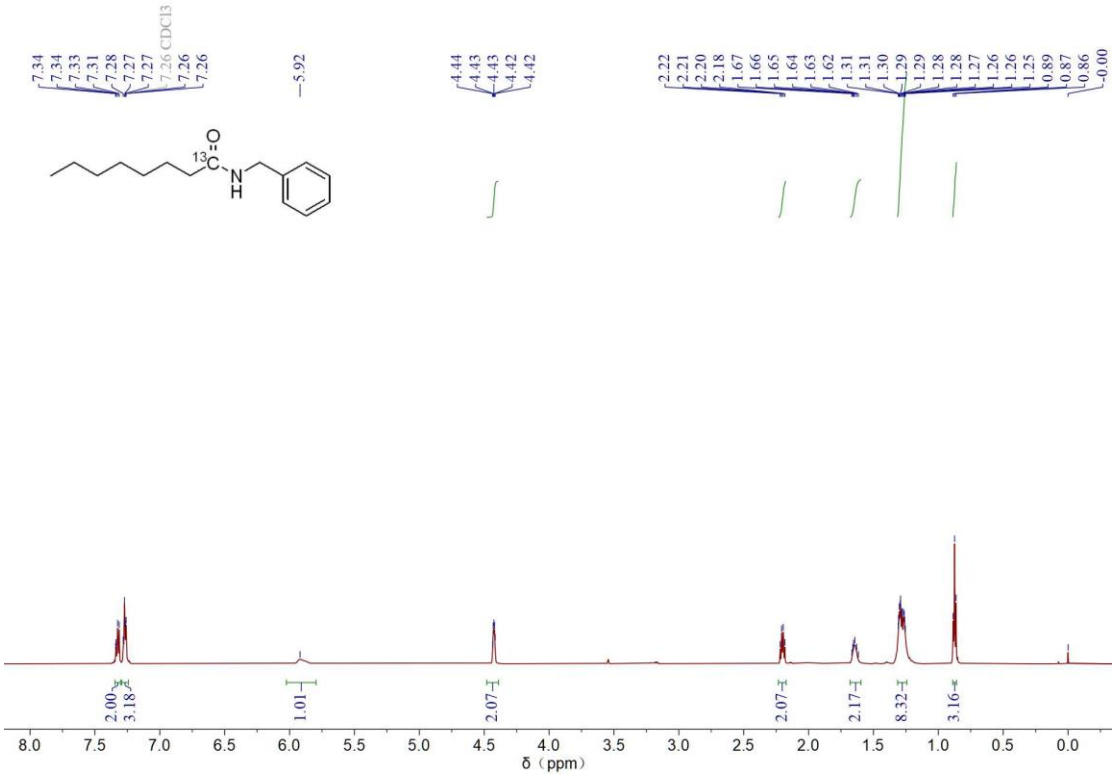
^{13}C NMR of compound 74



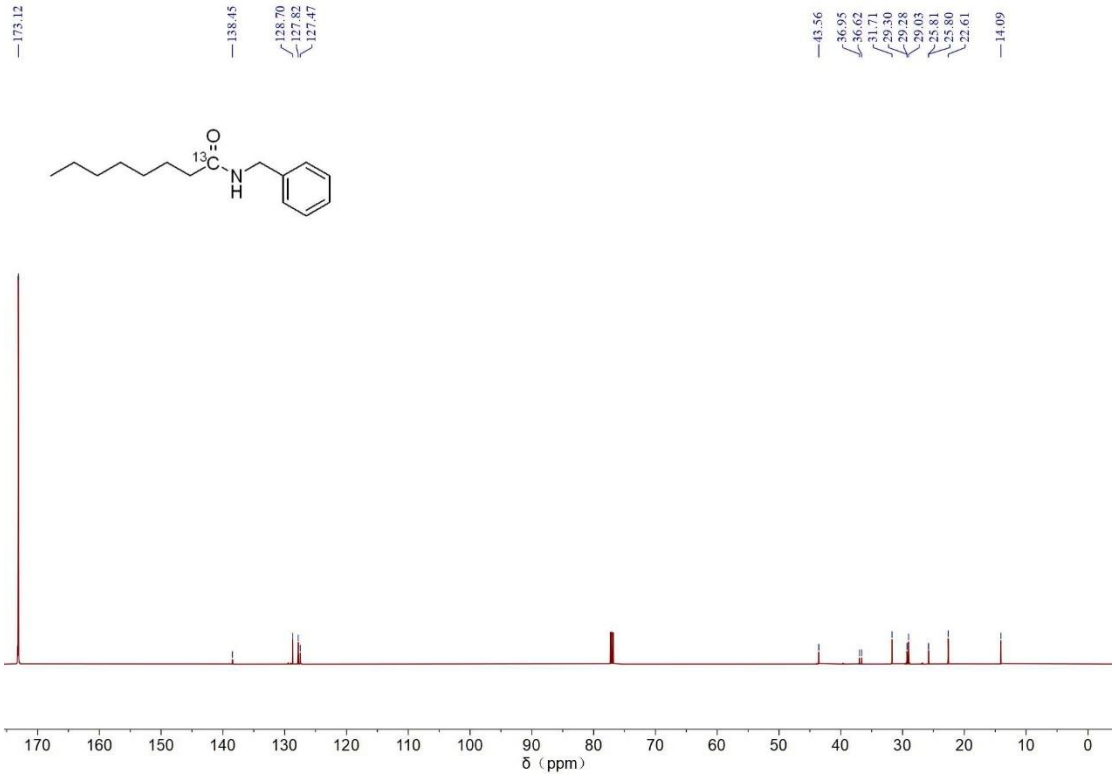
^{19} F NMR of compound 74



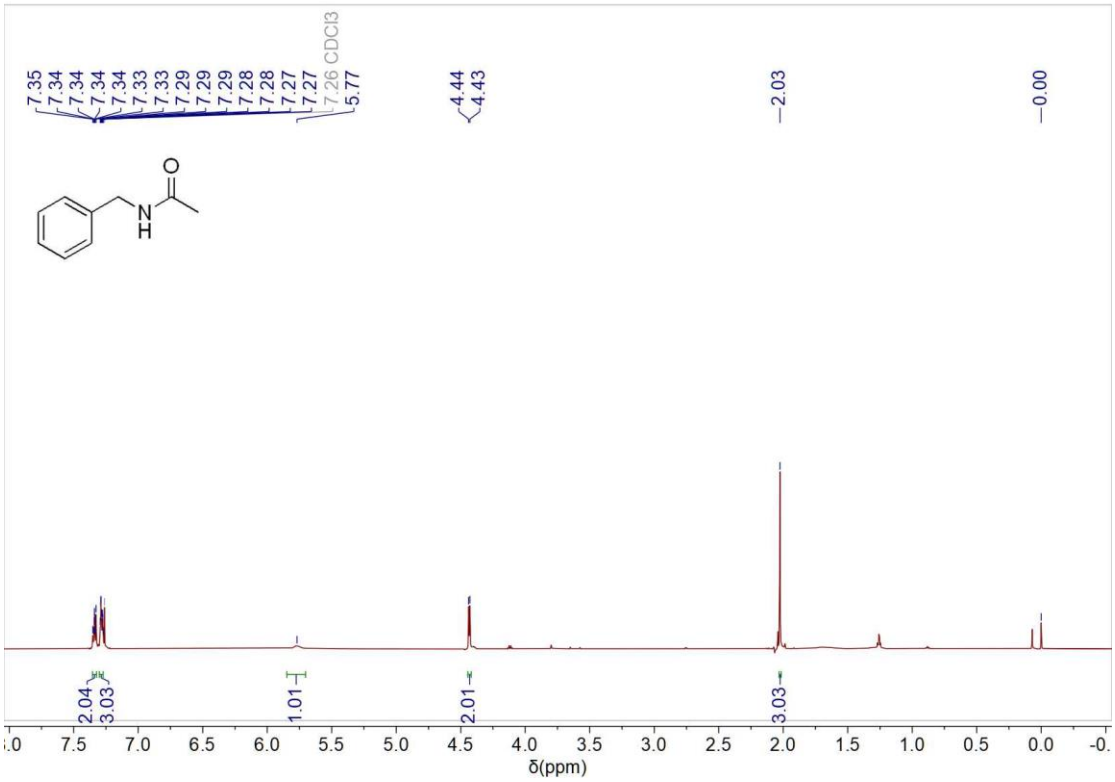
^{1}H NMR of compound 75



^{13}C NMR of compound 75



^{1}H NMR of compound 77



^{13}C NMR of compound 77