Supporting Information

Redox-Neutral Remote Amidation of Alkenyl Alcohols *via* Long-Range Isomerization/Transformation

Na Bai,[†,‡] Xuchao Wang,[†,‡] Zhenchao Wang,[*,‡] Feipeng Liu,[†] Zi-Qiang Rong[*,†]

[†]Frontiers Science Center for Flexible Electronics (FSCFE), Shaanxi Institute of Flexible Electronics (SIFE) & Shaanxi Inst-itute of Biomedical Materials and Engineering (SIBME), Northwestern Polytechnical University (NPU), 127 West Youyi Road, Xi'an 710072, China. E-mail: iamzqrong@nwpu.edu.cn

[‡]College of Pharmacy, Guizhou University, Guiyang, Guizhou 550025, China. E-mail: wzc.4884@163.com

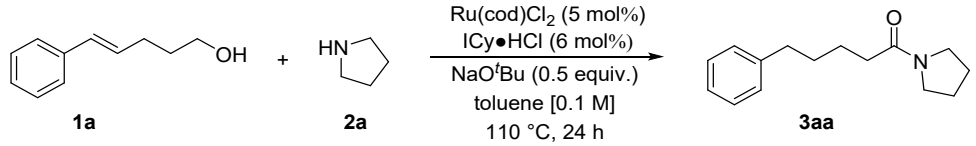
Table of Contents

1. General considerations

Unless noted otherwise, all solvents were dried by filtration through a Pure–Solv MD–5 Solvent Purification System (Innovative Technology). Toluene was carefully freeze–pump–thawed and dried by 4A molecular sieves (activated at 350 °C for 8h). Reaction temperatures were reported as the temperatures of the bath surrounding the flasks or cylindrical pressure vessel. Sensitive reagents and solvents were transferred under nitrogen into a nitrogen–filled glovebox with standard techniques. Analytical thin–layer chromatography (TLC) was carried out using 0.2 mm commercial silica gel plates (silica gel 60, F254, Leyan chemical). Cylindrical pressure vessel (26 x 109 mm (15 mL) with PTFE lined cap attached) were purchased from Synthware. Nuclear magnetic resonance spectra (^{1}H NMR, ^{13}C NMR and ^{19}F NMR) were recorded with a Bruker Model DMX 500 (500 MHz, ^{1}H at 500 MHz, ^{13}C at 126 MHz, ^{19}F at 471 MHz). Chemical shifts were reported in parts per million (ppm, δ), downfield from tetramethylsilane (TMS, δ=0.00ppm) and were referenced to residual solvent ($CDCl_3$, δ=7.26 ppm (^{1}H) and 77.0 ppm (^{13}C)). All the ^{19}F chemical shifts were not referenced. Coupling constants were reported in Hertz (Hz). Data for ^{1}H NMR spectra were reported as follows: chemical shift (ppm, referenced to protium, s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, dd = doublet of doublets, td = triplet of doublets, ddd = doublet of doublet of doublets, m = multiplet, coupling constant (Hz), and integration). All other materials were obtained from Rhawn Corporation, Aladdin Bio–Chem Technology or Energy chemical and were used as received.

2. Supplementary table

Optimization of Reaction Conditions [a]

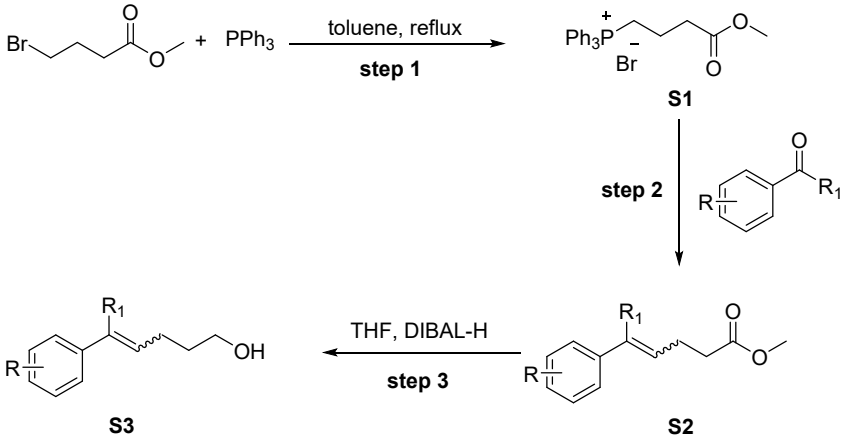


1a 2a 3aa

entry	Variation	Yield[b]
1	Bis(dichloro(1,3,5-trimethylbenzene)ruthenium) instead of $Ru(cod)Cl_2$	50%
2	Chloro(pentamethylcyclopentadienyl)(cyclooctadiene)ruthenium instead of $Ru(cod)Cl_2$	trace
3	Sphos instead of ICy•HCl	trace
4	Xantphos instead of ICy•HCl	trace
5	X-phos instead of ICy•HCl	29%
6	Cphos instead of ICy•HCl	32
7	Dppbz instead of ICy•HCl	trace
8	SIPr•HCl instead of ICy•HCl	18%
9	Johnphos instead of ICy•HCl	trace
10	Triphos instead of ICy•HCl	trace
11	Dppf instead of ICy•HCl	trace
12	K_2CO_3 instead of NaO^tBu	trace
13	CH_3COONa instead of NaO^tBu	trace
14	CF_3COONa instead of NaO^tBu	trace
15	K_2HPO_4 instead of NaO^tBu	trace
16	KH_2PO_4 instead of NaO^tBu	trace
17	K_3PO_4 instead of NaO^tBu	trace
18	DBU instead of NaO^tBu	trace
19	4-Methylpiperidine instead of NaO^tBu	trace
20	1-Methylpiperidine instead of NaO^tBu	trace
21	Cyclopentyl methyl ether instead of Toluene	65%
22	0.1 equiv. NaO^tBu instead of 0.5 equiv. NaO^tBu	trace
23	0.2 equiv. NaO^tBu instead of 0.5 equiv. NaO^tBu	31%
24	0.3 equiv. NaO^tBu instead of 0.5 equiv. NaO^tBu	61%
25	0.4 equiv. NaO^tBu instead of 0.5 equiv. NaO^tBu	82%
26	1.0 equiv. NaO^tBu instead of 0.5 equiv. NaO^tBu	65%

[a]All the reactions were run with 0.2 mmol of 1a, 0.2 mmol of 2a in a 2 mL toluene at 110 °C for 24 h. [b]Determined by ^{1}H NMR using 1,1,2,2-tetrachloroethane as the internal standard. Abbreviations: DABCO, 1,4-diazabicyclo[2.2.2]octane; DBU, 1,8-Diazabicyclo[5.4.0]undec-7-ene.

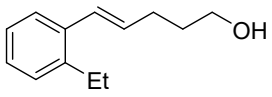
3. General procedure for the preparation of alkenyl alcohol



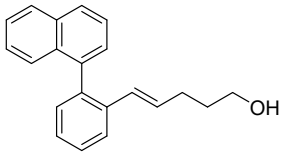
Step 1: To a 100 mL flask charged with a solution of methyl 4-bromobutyrate (30 mmol) in toluene (50 mL) was added triphenylphosphine (60 mmol) at room temperature. Then the reaction mixture was stirred at 130 °C overnight and cooled to room temperature. The white precipitate was filtered, washed with petroleum ether and dried under vacuum to afford phosphonium salt **S1**.

Step 2: NaH (21.6 mmol, 1.5 equiv.) was added to a suspension of phosphonium salt **S1** (15.8 mmol, 1.1 equiv.) in anhydrous THF (30 mL) at 0 °C under N_2 and further stirred for 30 min. The reaction mixture was then cooled to -78 °C and benzaldehyde or acetophenone (14.4 mmol, 1.0 equiv.) was slowly added. After stirred at room temperature for 24 h, the reaction was quenched by H_2O (10mL) and extracted by ethyl acetate (3 × 20 mL) and washed with brine. The organic phase was dried over anhydrous Na_2SO_4 then filtered and concentrated in *vacuo*. The residue was purified by flash column chromatography to afford **S2**.

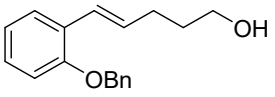
Step 3: To a suspension of $LiAlH_4$ (3.5 equiv.) in anhydrous THF (25 mL) was slowly added **S2** (1.0 equiv.) in THF at -20°C. Then the reaction was stirred at room temperature for overnight. The reaction mixture was cooled to 0 °C and quenched carefully by methanol. Potassium sodium tartrate solution was added and stirred vigorously for 2 h until the solution was clear. Then the aqueous phase extracted with ethyl acetate (3 × 15 mL) and washed with brine. The combined organic extracts were dried over Na_2SO_4, filtered and concentrated in vacuo. The residue was purified by flash column chromatography.



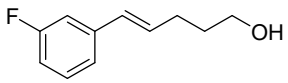
1c: Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) (*E:Z* = 9:1) δ 7.21 – 7.10 (m, 4H), 6.54 (dt, *J* = 11.4, 1.8 Hz, 1H), 5.72 (dt, *J* = 11.4, 7.4 Hz, 1H), 3.60 (t, *J* = 6.6 Hz, 2H), 2.61 (q, *J* = 7.6 Hz, 2H), 2.25-2.20 (m, 2H), 1.69 – 1.62 (m, 2H), 1.31 (s, 1H),1.16 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 142.4, 136.0, 132.0, 129.3, 128.5, 128.2, 127.2, 125.4, 62.5, 32.7, 26.5, 24.7, 14.9. **HRMS** (ESI): Calculated for $C_{13}H_{19}O$ [M+H]: 191.1436, found: 191.1438.



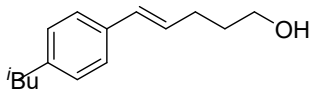
1d: White oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.90 – 7.79 (m, 2H), 7.53 – 7.39 (m, 5H), 7.38 – 7.29 (m, 4H), 6.00 (dt, *J* = 11.6, 1.8 Hz, 1H), 5.39 – 5.28 (m, 1H), 3.57 (t, *J* = 6.5 Hz, 2H), 2.33-2.27 (m, 2H), 1.61 – 1.54 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 134.0, 139.3, 136.8, 131.8, 130.8, 129.2, 128.8, 128.2, 127.6, 127.2, 127.2, 126.7, 126.4, 125.8, 125.7, 125.3,62.6, 32.7, 24.9. **HRMS** (ESI): Calculated for $C_{21}H_{21}O$ [M+H]: 289.1592, found: 289.1588.



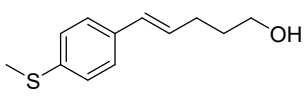
1f: White oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.18 (m, 7H), 6.96-6.91 (m, 2H), 6.63 (d, *J* = 11.6 Hz, 1H), 5.80 – 5.64 (m, 1H), 5.09 (d, *J* = 2.4 Hz, 2H), 3.65-3.61 (m, 2H), 2.37 – 2.28 (m, 2H), 1.70 (td, *J* = 8.7, 4.5 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 156.2, 137.3, 131.9, 130.1, 128.5, 128.1, 127.8, 127.2, 125.1, 120.5, 112.3, 70.2, 62.6, 32.8, 25.0. **HRMS** (ESI): Calculated for $C_{18}H_{21}O_2$ [M+H]: 269.1542, found: 269.1544.



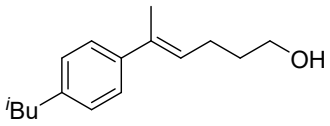
1j: Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.32 – 7.23 (m, 1H), 7.06 – 7.02 (m, 1H), 7.00-6.96 (m, 1H), 6.95 – 6.88 (m, 1H), 6.40 (dt, *J* = 11.7, 1.9 Hz, 1H), 5.71 (dt, *J* = 11.6, 7.3 Hz, 1H), 3.66 (t, *J* = 6.5 Hz, 2H), 2.43-2.37 (m, 2H), 1.75-1.68 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.7 (d, *J* = 244.7 Hz), 139.7(d, *J* = 7.5 Hz), 133.3, 129.6 (d, *J* = 8.3 Hz), 128.4, 124.5(d, *J* = 2.8 Hz), 115.4(d, *J* = 21.8 Hz), 113.5(d, *J* = 21.2 Hz), 62.4, 32.7, 24.9. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -113.6. **HRMS** (ESI): Calculated for $C_{11}H_{13}FONa$ [M+Na]: 203.0848, found: 203.0848.



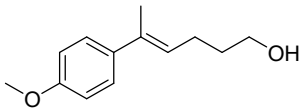
1l: White oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.21 – 7.17 (m, 2H), 7.12 – 7.07 (m, 2H), 6.41 (d, *J* = 11.6 Hz, 1H), 5.61 (d, *J* = 11.6 Hz, 1H), 3.65 (t, *J* = 6.5 Hz, 2H), 2.62 – 2.24 (m, 4H), 1.86 (s, 1H), 1.69-1.74 (m, 2H), 0.90 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.2, 134.9, 131.3, 129.4, 129.0, 128.5, 62.5, 45.2, 32.9, 30.2, 25.0, 22.4. **HRMS** (ESI): Calculated for $C_{15}H_{23}O$ [M+H]: 219.1749, found: 219.1746.



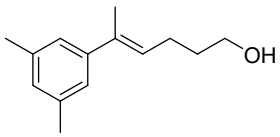
1n: Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.28 – 7.17 (m, 5H), 6.40-6.35 (m, 1H), 5.67-5.59 (m, 1H), 3.65 (t, *J* = 6.5 Hz, 2H), 2.48 (s, 3H), 2.44 – 2.37 (m, 2H), 1.73 – 1.68 (m, 2H), 1.52 (s, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 136.6, 134.5, 131.9, 129.2, 128.8, 126.4, 62.4, 32.8, 25.0, 16.0. **HRMS** (ESI): Calculated for $C_{12}H_{17}OS$ [M+H]: 209.1000, found: 209.1000.



1u: Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.13 – 7.05 (m, 4H), 5.45-5.41(m, 1H), 3.56 (t, *J* = 6.5 Hz, 2H), 2.46 (d, *J* = 7.1 Hz, 2H), 2.10 – 2.04 (m, 2H), 2.02 (t, *J* = 1.4 Hz, 3H), 1.90 – 1.83 (m, 1H), 1.62 – 1.55 (m, 2H), 0.91 (d, *J* = 6.5 Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 134.0, 139.1, 136.9, 128.9, 127.6, 126.5, 62.5, 45.2, 33.0, 30.2, 25.8, 25.3, 22.5. **HRMS** (ESI): Calculated for $C_{16}H_{25}O$ [M+H]: 233.1905, found: 233.1900.

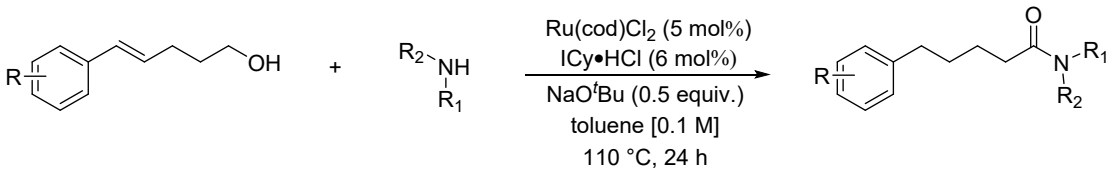


1v: Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.11 (d, *J* = 8.3 Hz, 2H), 6.89 – 6.83 (m, 2H), 5.47 – 5.36 (m, 1H), 3.80 (s, 3H), 3.59– 3.54 (m, 2H), 2.06 (t, *J* = 7.5 Hz, 2H), 2.00 (s, 3H), 1.63 – 1.55 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.2, 136.5, 134.2, 129.0, 126.4, 113.5, 62.5, 55.2, 33.0, 25.7, 25.3. **HRMS** (ESI): Calculated for $C_{13}H_{19}O_2$ [M+H]: 207.1385, found: 207.1389.



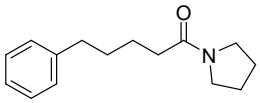
1x: Yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.93 – 6.85 (m, 1H), 6.78 (d, J = 1.5 Hz, 2H), 5.43-5.39 (m, 1H), 3.58 (t, J = 6.5 Hz, 2H), 2.31 (s, 6H), 2.08 – 2.03 (m, 2H), 2.01-1.98(m, 3H), 1.68 – 1.54 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 142.0, 137.6, 137.3, 128.2, 126.3, 125.6, 62.5, 33.0, 25.8, 25.3, 21.4. **HRMS** (ESI): Calculated for $C_{14}H_{21}O$ [M+H]: 205.1592, found: 205.1593.

4. General procedures for the redox neutral ruthenium catalysis cross–coupling reactions

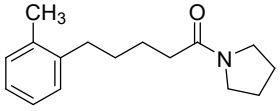


A flame–dried 15 mL cylindrical pressure vessel was charged with alkenyl alcohol (0.2 mmol, 1.0 equiv.), tetrahydropyrrole (0.2 mmol, 1.0 equiv.), $Ru(cod)Cl_2$ (2.8 mg, 0.01 mmol, 5 mol%), ICy•HCl (3.2mg, 0.012 mmol, 6 mol%), NaO^tBu (9.6 mg, 0.01 mmol, 0.5 equiv.) and 2.0 mL dry toluene in a nitrogen-filled glovebox. Then the cylindrical pressure vessel was tightly sealed, transferred out of the glovebox and stirred at 110 °C for 24 h. After the completion of the reaction, the solvent was removed in vacuo and the residue was purified by flash column chromatography on silica gel to give the desired amide products.

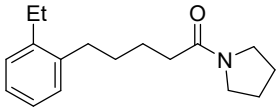
5. Characterization data for the products



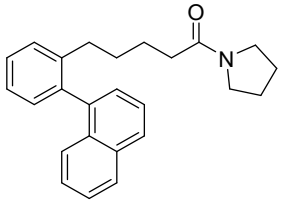
3aa (**CAS**:89414-46-0)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.29 – 7.24 (m, 2H), 7.22 – 7.13 (m, 3H), 3.45 (t, *J* = 6.9 Hz, 2H), 3.37 (t, *J* = 6.8 Hz, 2H), 2.64 (t, *J* = 7.2 Hz, 2H), 2.27 (t, *J* = 7.0 Hz, 2H), 1.92 (q, *J* = 6.8 Hz, 2H), 1.83 (q, *J* = 6.8 Hz, 2H), 1.74 – 1.65 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.6, 142.4, 128.4, 128.3, 125.7, 46.6, 45.6, 35.8, 34.7, 31.3, 26.1, 24.7, 24.4.



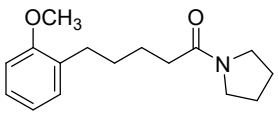
3ab: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.13-7.07 (m, 4H), 3.46 (t, *J* = 6.9 Hz, 2H), 3.39 (t, *J* = 6.8 Hz, 2H), 2.66 – 2.59 (m, 2H), 2.30 (s, 3H), 2.27 (t, *J* = 7.8 Hz, 2H), 1.96-1.90 (m, 2H), 1.87-1.82 (m, 2H), 1.79-1.72 (m, 2H), 1.66-1.59 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.5, 140.6, 130.1, 128.8, 125.9, 46.6, 45.6, 33.2, 30.1, 26.1, 25.0, 19.3. **HRMS** (ESI): Calculated for $C_{16}H_{24}NO$ [M+H]: 246.1858, found: 246.1860.



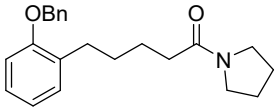
3ac: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.17 (m, 4H), 3.48 (t, *J* = 6.9 Hz, 2H), 3.42 (t, *J* = 6.8 Hz, 2H), 2.71 – 2.64 (m, 4H), 2.31 (t, *J* = 7.5 Hz, 2H), 1.97-1.93 (m, 2H), 1.89 – 1.84 (m, 2H), 1.81 – 1.75 (m, 2H), 1.70-1.64 (m, 2H), 1.24 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.5, 129.1, 128.3, 126.0, 125.8, 46.6, 45.6, 32.5, 31.1, 26.1, 25.5, 25.1, 24.4, 15.4. **HRMS** (ESI): Calculated for $C_{17}H_{26}NO$ [M+H]: 260.2014, found: 260.2012.



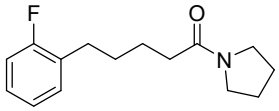
3ad: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.89-7.85 (m, 2H), 7.53 – 7.43 (m, 3H), 7.40 – 7.32 (m, 4H), 7.30-7.27 (m, 1H), 7.21 (d, *J* = 7.3 Hz, 1H), 3.36 (t, *J* = 6.8 Hz, 2H), 3.14-3.09 (m, 2H), 2.41 (d, *J* = 7.7 Hz, 1H), 2.32 – 2.25 (m, 1H), 1.95 – 1.82 (m, 4H), 1.81-1.75 (m, 2H), 1.44-1.38 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.5, 141.1, 139.8, 133.5, 130.7, 129.0, 128.1, 127.7, 127.4, 127.0, 126.3, 125.9, 125.7, 125.6, 125.2, 45.5, 34.2, 32.9, 30.7, 26.1, 24.4, 24.3. **HRMS** (ESI): Calculated for $C_{25}H_{28}NO$ [M+H]: 358.2171, found: 358.2173.



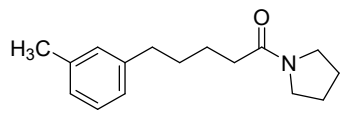
3ae: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.22 – 7.09 (m, 2H), 6.92 – 6.78 (m, 2H), 3.81 (s, 3H), 3.46 (t, *J* = 6.9 Hz, 2H), 3.34 (d, *J* = 13.5 Hz, 2H), 2.66 (s, 2H), 2.31 – 2.23 (m, 2H), 1.99 – 1.89 (m, 4H), 1.83 (d, *J* = 13.7 Hz, 2H), 1.44 – 1.38 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.7, 157.5, 130.3, 127.1, 110.2, 55.2, 46.5, 45.6, 34.4, 24.8, 24.4. **HRMS** (ESI): Calculated for $C_{16}H_{24}NO_2$ [M+H]: 262.1807, found: 262.1805.



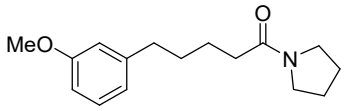
3af: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.47 (m, 2H), 7.41 (m, 2H), 7.34 (m, 1H), 7.22 – 7.15 (m, 2H), 6.95-6.92 (m, 2H), 5.10 (s, 2H), 3.47 (t, *J* = 6.8 Hz, 2H), 3.34 (t, *J* = 6.8 Hz, 2H), 2.74 (t, *J* = 7.1 Hz, 2H), 2.28 (t, *J* = 7.2 Hz, 2H), 1.95-1.89 (m, 2H), 1.87-1.83 (m, 2H), 1.77 – 1.69 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.8, 156.6, 130.0, 128.5, 127.7, 127.1, 126.9, 120.7, 111.7, 69.8, 46.6, 45.6, 34.7, 30.0, 29.8, 26.1, 24.8, 24.4. **HRMS** (ESI): Calculated for $C_{22}H_{28}NO_2$ [M+H]: 338.2120, found: 338.2122.



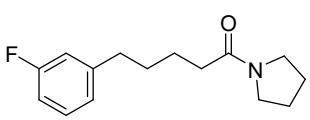
3ag: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.20=7.14 (m, 2H), 7.06 – 6.95 (m, 2H), 3.45 (t, *J* = 6.9 Hz, 2H), 3.39 (t, *J* = 6.8 Hz, 2H), 2.67 (t, *J* = 7.2 Hz, 2H), 2.28 (t, *J* = 7.2 Hz, 2H), 1.96-1.90 (m, 2H), 1.86-1.81 (m, 2H), 1.74 – 1.65 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.5, 160.2 (d, *J* = 244.3 Hz), 130.7 (d, *J* = 5.4 Hz), 129.1(d, *J* = 15.7 Hz), 127.4(d, *J* = 7.5 Hz), 123.9(d, *J* = 3.6 Hz), 115.1 (d, *J* = 22.1 Hz), 46.6, 45.6, 34.5, 29.9, 28.8, 26.1, 24.6, 24.4. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -114.1. **HRMS** (ESI): Calculated for $C_{15}H_{21}FNO$ [M+H]: 250.1607, found: 250.1608.



3ah: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.15 (t, J = 7.5 Hz, 1H), 6.99 (d, *J* = 4.9 Hz, 2H), 6.97 (s, 1H), 3.45 (t, *J* = 6.9 Hz, 2H), 3.38 (t, *J* = 6.8 Hz, 2H), 2.60 (t, *J* = 7.3 Hz, 2H), 2.32 (s, 3H), 2.27 (t, *J* = 7.2 Hz, 2H), 1.95-1.90 (m, 2H), 1.87-1.82 (m, 2H), 1.73 – 1.63 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$ δ 171.7, 142.4, 129.3, 128.2, 126.4, 125.4, 46.6, 45.6, 35.8, 34.7, 31.4, 26.1, 24.7, 24.4, 21.4. **HRMS** (ESI): Calculated for $C_{16}H_{24}NO$ [M+H]: 246.1858, found: 246.1861.

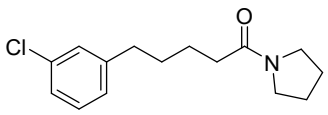


3ai: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.18-7.12 (m, 2H), 6.92 – 6.77 (m, 2H), 3.81 (s, 3H), 3.45 (t, *J* = 6.9 Hz, 2H), 3.39 (t, *J* = 6.8 Hz, 2H), 2.67 – 2.58 (m, 2H), 2.28 (t, *J* = 7.5 Hz, 2H), 1.94-1.90 (q, *J* = 6.7 Hz, 2H), 1.86 – 1.81 (m, 2H), 1.74-1.69 (m, 2H), 1.66-1.60 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.8, 157.4, 130.8, 129.8, 126.9, 120.4, 110.2, 55.3, 46.6, 45.6, 34.8, 30.0, 29.7, 26.1, 24.9, 24.4. **HRMS** (ESI): Calculated for $C_{16}H_{24}NO_2$ [M+H]: 262.1807, found: 262.1808.

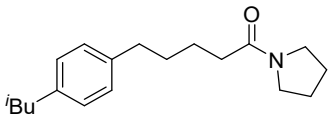


3aj: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.25 – 7.17 (m, 1H), 6.95 (d, *J* = 7.6 Hz, 1H), 6.93 – 6.75 (m, 2H), 3.46 (t, *J* = 6.9 Hz, 2H), 3.38 (t, *J* = 6.8 Hz, 2H), 2.64 (t, *J* = 7.2 Hz, 2H), 2.27 (t, *J* = 7.0 Hz, 2H), 1.97-1.91 (m, 2H), 1.87-1.81 (m, 2H), 1.74 – 1.65 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.4, 162.9 (d, J = 244.7 Hz), 145.0 (d, J = 7.3 Hz), 129.6 (d, J = 8.3 Hz), 124.1(d, J = 20.5 Hz),

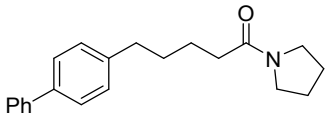
115.2(d, J = 20.5 Hz), 112.6 (d, J = 21.1 Hz), 46.6, 45.6, 35.6, 34.6, 31.0, 26.1, 24.5, 24.4. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -114.1. **HRMS** (ESI): Calculated for $C_{15}H_{21}FNO$ [M+H]: 250.1607, found: 250.1611.



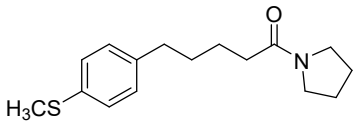
3ak: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.24 – 7.13 (m, 3H), 7.06 (d, J = 7.4 Hz, 1H), 3.45 (t, J = 6.9 Hz, 2H), 3.38 (t, J = 6.8 Hz, 2H), 2.62 (t, J = 7.1 Hz, 2H), 2.27 (t, J = 7.0 Hz, 2H), 1.96-1.91 (m, 2H), 1.87 – 1.80 (m, 2H), 1.69-1.64 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) 171.4, 144.4, 134.0, 129.5, 128.5, 126.7, 125.9, 46.6, 45.6, 35.5, 34.5, 31.0, 26.1, 24.5, 24.4. **HRMS** (ESI): Calculated for $C_{15}H_{21}ClNO$ [M+H]: 266.1312, found: 266.1313.



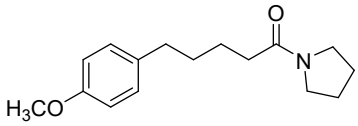
3al: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.10 – 7.02 (m, 4H), 3.45 (t, *J* = 6.9 Hz, 2H), 3.37 (t, *J* = 6.8 Hz, 2H), 2.61 (t, *J* = 7.3 Hz, 2H), 2.43 (d, *J* = 7.2 Hz, 2H), 2.27 (t, *J* = 7.2 Hz, 2H), 1.96 – 1.90 (m, 2H), 1.84 (d, *J* = 7.1 Hz, 2H), 1.69-1.63 (m, 4H), 0.89 (d, *J* = 6.6 Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ171.6, 139.6, 139.0, 129.0, 128.1, 46.6, 45.6, 45.1, 35.4, 34.7, 31.4, 30.3, 26.1, 24.7, 24.4, 22.4. **HRMS** (ESI): Calculated for $C_{19}H_{30}NO$ [M+H]: 288.2327, found: 288.2323.



3am: White solid. Melting point: 87–88 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) 7.60 – 7.54 (m, 2H), 7.53 – 7.46 (m, 2H), 7.45 – 7.38 (m, 2H), 7.35 – 7.29 (m, 1H), 7.27 – 7.22 (m, 2H), 3.45 (t, *J* = 6.9 Hz, 2H), 3.37 (t, *J* = 6.8 Hz, 2H), 2.68 (t, *J* = 7.1 Hz, 2H), 2.28 (t, *J* = 7.1 Hz, 2H), 1.93-1.90 (m, 2H), 1.86-1.80 (m, 2H), 1.75-1.69 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) 171.5, 141.6, 141.2, 138.7, 128.9, 128.7, 127.1, 127.0, 46.6, 45.6, 35.5, 34.7, 31.3, 26.2, 24.7, 24.4. **HRMS** (ESI): Calculated for $C_{21}H_{26}NO$ [M+H]: 308.2014, found: 308.2017.

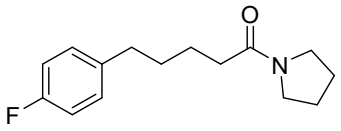


3an: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.26 – 7.00 (m, 4H), 3.45 (t, *J* = 6.9 Hz, 2H), 3.37 (t, *J* = 6.8 Hz, 2H), 2.60 (t, *J* = 7.3 Hz, 2H), 2.46 (s, 3H), 2.26 (t, *J* = 7.2 Hz, 2H), 1.94-1.90 (m 2H), 1.86-1.81 (m, 2H), 1.75 – 1.59 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.5, 139.2, 135.1, 129.0, 127.1, 46.7, 45.6, 35.3, 34.6, 31.3, 26.1, 24.6, 24.4, 16.4. **HRMS** (ESI): Calculated for $C_{16}H_{24}NOS$ [M+H]: 278.1579, found: 278.1584.

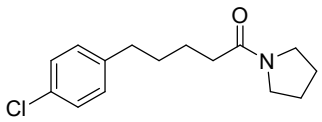


3ao: Brown oil.**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.13 – 7.07 (m, 2H), 6.84 – 6.80 (m, 2H), 3.78 (s, 3H), 3.45 (t, *J* = 6.9 Hz, 2H),

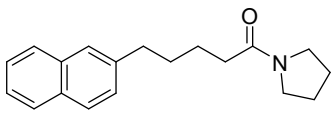
3.38 (t, *J* = 6.8 Hz, 2H), 2.58 (t, *J* = 7.4 Hz, 2H), 2.27 (t, *J* = 7.3 Hz, 2H), 1.96 – 1.91 (m, 2H), 1.86 – 1.81 (m, 2H), 1.70 – 1.64 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.6, 157.7, 134.5, 129.3, 113.7, 55.3, 46.6, 45.6, 34.9, 34.7, 31.6, 26.1, 24.6, 24. **HRMS** (ESI): Calculated for $C_{16}H_{24}NO_2$ [M+H]: 262.1807, found: 262.1803.



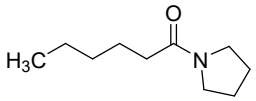
3ap (**CAS**:1215696-45-9)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.14 – 7.11 (m, 2H), 6.95 (t, *J* = 8.4 Hz, 2H), 3.45 (t, *J* = 6.9 Hz, 2H), 3.38 (t, *J* = 6.8 Hz, 2H), 2.61 (t, *J* = 7.2 Hz, 2H), 2.27 (t, *J* = 7.0 Hz, 2H), 1.97 – 1.91 (m, 2H), 1.87 – 1.81 (m, 2H), 1.71 – 1.64 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.4, 161.2 (d, *J* = 243.4 Hz), 137.98 (d, *J* = 3.4 Hz), 129.69 (d, *J* = 7.5 Hz), 114.96 (d, *J* = 21.1 Hz), 46.59, 45.60, 35.01, 34.59, 31.43, 26.13, 24.49, 24.41. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -118.09.



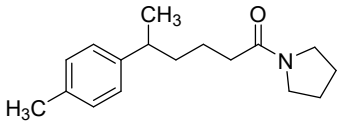
3aq: Brown oil.**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.23 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 8.1 Hz, 2H), 3.45 (t, *J* = 6.9 Hz, 2H), 3.37 (t, *J* = 6.8 Hz, 2H), 2.61 (t, *J* = 7.2 Hz, 2H), 2.26 (t, *J* = 7.0 Hz, 2H), 1.94 (p, *J* = 6.8 Hz, 2H), 1.84 (p, *J* = 6.8 Hz, 2H), 1.72 – 1.64 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.4, 140.8, 131.4, 129.8, 128.4, 46.6, 45.6, 35.2, 34.6, 31.2, 26.1, 24.5, 24.4. **HRMS** (ESI): Calculated for $C_{15}H_{21}ClNO$ [M+H]: 266.1312, found: 266.1311.



3ar: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.80 – 7.74 (m, 3H), 7.61 (s, 1H), 7.45 – 7.38 (m, 2H), 7.33 (d, *J* = 8.4 Hz, 1H), 3.44 (t, *J* = 6.9 Hz, 2H), 3.35 (t, *J* = 6.8 Hz, 2H), 2.81 (t, *J* = 6.8 Hz, 2H), 2.28 (t, *J* = 6.7 Hz, 2H), 1.93 – 1.88 (m, 2H), 1.84 – 1.80 (m, 2H), 1.78 – 1.72 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.5, 140.0, 133.6, 132.0, 127.8, 127.6, 127.4, 127.4, 126.4, 125.8, 125.1, 46.6, 45.6, 36.0, 34.7, 31.2, 26.1, 24.7, 24.4. **HRMS** (ESI): Calculated for $C_{19}H_{24}NO$ [M+H]: 282.1858, found: 282.1858.

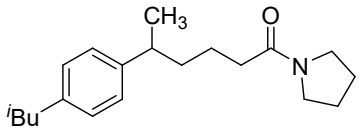


3as (**CAS**:3389-56-8)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ 3.46 (t, *J* = 6.9 Hz, 2H), 3.41 (t, *J* = 6.8 Hz, 2H), 2.25 (t, *J* = 7.6 Hz, 2H), 1.98 – 1.92 (m, 2H), 1.88 – 1.82 (m, 2H), 1.68 – 1.62 (m, 2H), 1.35 – 1.31 (m, 4H), 0.92 – 0.88 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.9, 46.6, 45.6, 34.8, 31.7, 26.1, 24.7, 24.4, 22.5, 14.0.

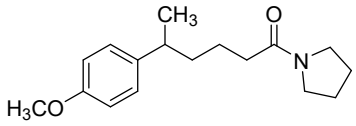


3at: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.10 – 7.06 (m, 4H), 3.43 (t, *J* = 6.9 Hz, 2H), 3.33 (t, *J* = 6.8 Hz, 2H), 2.71 – 2.64 (m,

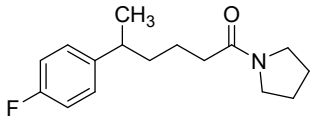
1H), 2.31 (s, 3H), 2.22 – 2.17 (m, 2H), 1.94 – 1.88 (m, 2H), 1.85 – 1.79 (m, 2H), 1.65 – 1.58 (m, 3H), 1.55 – 1.48 (m, 1H), 1.23 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.6, 144.5, 135.3, 129.0, 126.9, 46.6, 45.6, 39.5, 38.2, 34.8, 26.1, 24.4, 23.2, 22.4, 21.0. **HRMS** (ESI): Calculated for $C_{17}H_{26}NO$ [M+H]: 260.2014, found: 260.2010.



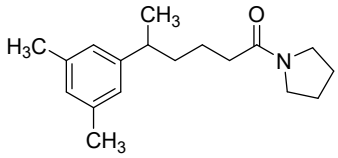
3au: Brown oil.**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.09 – 7.03 (m, 4H), 3.43 (t, *J* = 6.9 Hz, 2H), 3.32 (t, *J* = 6.8 Hz, 2H), 2.71 – 2.64 (m, 1H), 2.43 (d, *J* = 7.2 Hz, 2H), 2.26 – 2.19 (m, 2H), 1.93 – 1.87 (m, 2H), 1.84 – 1.80 (m, 2H), 1.70 – 1.56 (m, 4H), 1.54 – 1.49 (m, 1H), 1.23 (d, *J* = 7.0 Hz, 3H), 0.89 (d, *J* = 6.7 Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.7, 144.7, 139.1, 129.0, 126.7, 46.6, 45.6, 45.1, 39.5, 38.2, 34.9, 30.2, 26.1, 24.4, 23.2, 22.4, 22.4. **HRMS** (ESI): Calculated for $C_{20}H_{32}NO$ [M+H]: 302.2484, found: 302.2487.



3av: Brown oil.**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.13 – 7.07 (m, 2H), 6.86 – 6.79 (m, 2H), 3.78 (s, 3H), 3.43 (t, *J* = 6.9 Hz, 2H), 3.33 (t, *J* = 6.8 Hz, 2H), 2.70 – 2.63 (m, 1H), 2.21 – 2.19 (m, 2H), 1.94 – 1.89 (m, 2H), 1.85 – 1.80 (m, 2H), 1.62 – 1.50 (m, 4H), 1.22 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.6, 157.7, 139.6, 127.8, 113.7, 55.3, 46.6, 45.6, 39.1, 38.3, 34.9, 26.1, 24.4, 23.1, 22.5. **HRMS** (ESI): Calculated for $C_{17}H_{26}NO_2$ [M+H]: 276.1964, found: 276.1962.

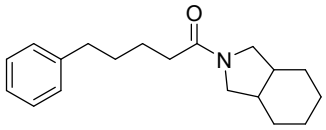


3aw: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.16 – 7.10 (m, 2H), 7.00 – 6.92 (m, 2H), 3.43 (t, *J* = 6.9 Hz, 2H), 3.33 (t, *J* = 6.8 Hz, 2H), 2.73 – 2.66 (m, 1H), 2.20 (t, *J* = 6.9 Hz, 2H), 1.95 – 1.89 (m, 2H), 1.85 – 1.80 (m, 2H), 1.63 – 1.58 (m, 3H), 1.53 – 1.47 (m, 1H), 1.22 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.43, 161.14 (d, *J* = 243.1 Hz), 143.01 (d, *J* = 3.2 Hz), 128.22 (d, *J* = 7.8 Hz), 114.95 (d, *J* = 20.8 Hz), 46.52, 45.54, 39.25, 38.20, 34.71, 26.08, 24.36, 22.99, 22.43.**^{19}F NMR** (471 MHz, $CDCl_3$) δ -117.87. **HRMS** (ESI): Calculated for $C_{16}H_{22}FNO$ [M+H]: 264.1764, found: 264.1768.

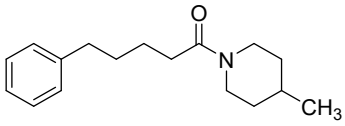


3ax: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 6.81 – 6.79 (m, 3H), 3.43 (t, *J* = 6.9 Hz, 2H), 3.34 (t, *J* = 6.9 Hz, 2H), 3.33 (d, *J* = 7.0 Hz, 2H), 2.30 – 2.28 (m, 3H), 2.22 – 2.19 (m, 1H), 1.91 (p, *J* = 6.8, 2H), 1.82 (p, *J* = 6.8 Hz, 2H), 1.67 – 1.53 (m, 9H), 1.22 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz,

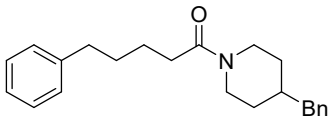
$CDCl_3$) δ 171.7, 147.5, 137.7, 127.5, 124.8, 46.6, 45.6, 39.8, 38.2, 34.9, 29.7, 26.1, 24.4, 23.2, 22.3, 21.4. **HRMS** (ESI): Calculated for $C_{18}H_{28}NO$ [M+H]: 274.2171, found: 274.2171.



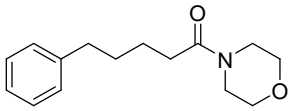
3ba: Brown oil.**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.26 (t, *J* = 7.5 Hz, 2H), 7.20 – 7.14 (m, 3H), 3.44 – 3.34 (m, 3H), 3.22 (dd, *J* = 9.9, 5.9 Hz, 1H), 2.64 (t, *J* = 7.1 Hz, 2H), 2.27 – 2.21 (m, 3H), 2.17 (p, *J* = 6.1 Hz, 1H), 1.73 – 1.64 (m, 4H), 1.61 – 1.55 (m, 2H), 1.54 – 1.45 (m, 2H), 1.44 – 1.35 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.3, 142.4, 128.4, 128.3, 125.7, 50.8, 49.4, 37.6, 35.9, 35.8, 34.5, 31.3, 25.8, 25.8, 24.7, 22.8, 22.6. **HRMS** (ESI): Calculated for $C_{19}H_{28}NO$ [M+H]: 286.2171, found: 286.2175.



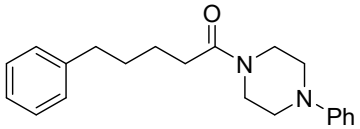
3ca(CAS:872815-54-8)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.28 – 7.25 (m, 2H), 7.18 – 7.15 (m, 3H), 4.57 (d, *J* = 13.2 Hz, 1H), 3.76 (d, *J* = 13.4 Hz, 1H), 2.95 (td, *J* = 13.2, 2.4 Hz, 1H), 2.65 – 2.63 (m, 2H), 2.51 (td, *J* = 12.9, 2.5 Hz, 1H), 2.34 – 2.31 (m, 2H), 1.73 – 1.64 (m, 6H), 1.61 – 1.53 (m, 1H), 1.09 – 1.02 (m, 2H), 0.94 (d, *J* = 6.5 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.3, 142.3, 128.4, 128.3, 125.7, 46.0, 42.0, 35.7, 34.7, 33.8, 33.4, 31.2, 31.1, 25.1, 21.7.



3da: Brown oil.**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.29 – 7.24 (m, 4H), 7.21 – 7.15 (m, 4H), 7.12 – 7.11 (m, 2H), 4.59 (d, *J* = 13.1 Hz, 1H), 3.76 (d, *J* = 13.3 Hz, 1H), 2.88 (t, *J* = 12.9 Hz, 1H), 2.63 (t, *J* = 6.6 Hz, 2H), 2.56 – 2.42 (m, 3H), 2.31 – 2.29 (m, 2H), 1.75 – 1.69 (m, 1H), 1.68 – 1.64 (m, 6H), 1.16 – 1.04 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.2, 142.3, 140.0, 129.1, 128.5, 128.3, 126.1, 125.7, 45.9, 43.0, 42.0, 38.3, 35.8, 33.3, 32.7, 31.8, 31.3, 25.1. **HRMS** (ESI): Calculated for $C_{23}H_{30}NO$ [M+H]: 336.2327, found: 336.2325.

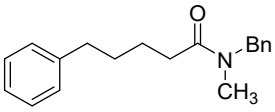


3ea (CAS:1071001-86-9)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.29 – 7.25 (m, 2H), 7.19 – 7.16 (m, 3H), 3.66 – 3.59 (m, 6H), 3.41 (t, *J* = 4.8 Hz, 2H), 2.67 – 2.62 (m, 2H), 2.33 – 2.30 (m, 2H), 1.70 – 1.66 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 1171.6, 142.2, 128.4, 128.3, 125.8, 67.0, 66.7, 46.0, 41.9, 35.7, 33.0, 31.1, 24.8.

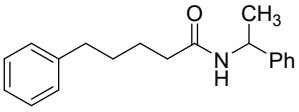


3fa (CAS:1215790-81-0)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.30 – 7.24 (m, 4H), 7.19 – 7.15 (m, 3H), 6.95 – 6.87 (m, 3H), 3.80 – 3.71 (t, *J* = 5.1 Hz, 2H), 3.61 – 3.52 (t, *J* = 5.0 Hz, 2H), 3.13 (q, *J*

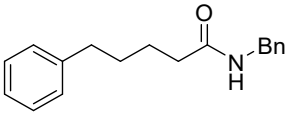
= 4.2 Hz, 4H), 2.65 (t, *J* = 6.9 Hz, 2H), 2.38 (t, *J* = 7.1 Hz, 2H), 1.70 (p, *J* = 3.7 Hz, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.5, 151.0, 142.2, 129.3, 128.4, 128.3, 125.8, 120.6, 116.7, 49.8, 49.5, 45.6, 41.5, 35.7, 33.2, 31.2, 24.9.



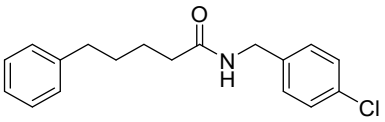
3ga (**CAS**:1216410-52-4)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.41 – 7.15 (m, 10H), 4.61 – 4.53 (m, 2H), 2.97 – 2.91 (m, 3H), 2.71 – 2.62 (m, 2H), 2.41 (q, *J* = 6.6 Hz, 2H), 1.80 – 1.73 (m, 3H), 1.70 – 1.65 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.4, 173.0, 142.4, 142.3, 137.6, 136.8, 128.9, 128.6, 128.4, 128.4, 128.3, 128.2, 128.0, 127.6, 127.3, 126.3, 125.7, 125.6, 53.4, 50.8, 35.8, 35.8, 34.8, 33.9, 33.4, 33.0, 31.3, 31.2, 25.1, 24.9.



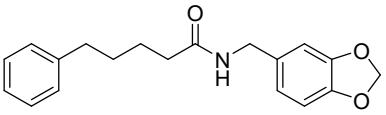
3ha (**CAS**:1215457-69-4)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 – 7.25 (m, 8H), 7.19 – 7.12 (m, 3H), 5.60 (d, *J* = 6.6 Hz, 1H), 5.17 – 5.10 (m, 1H), 2.61 (t, *J* = 7.3 Hz, 2H), 2.18 (t, *J* = 7.1 Hz, 2H), 1.70 – 1.64 (m, 4H), 1.47 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.8, 143.3, 142.2, 128.7, 128.4, 128.3, 127.4, 126.2, 125.8, 48.6, 36.7, 35.7, 31.0, 25.4, 21.7.



3ia (**CAS**:144146-84-9): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.34 – 7.30 (m, 2H), 7.29 – 7.24 (m, 5H), 7.19 – 7.13 (m, 3H), 5.71 (s, 1H), 4.42 (d, *J* = 5.7 Hz, 2H), 2.62 (t, *J* = 7.3 Hz, 2H), 2.22 (t, *J* = 7.2 Hz, 2H), 1.73 – 1.64 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.7, 142.2, 138.4, 128.7, 128.4, 128.3, 127.9, 127.5, 125.8, 43.6, 36.6, 35.7, 31.1, 25.4.

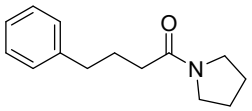


3ja: White solid. Melting point: 87-88 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.29 – 7.25 (m, 4H), 7.22 – 7.11 (m, 5H), 5.72 (s, 1H), 4.38 (d, *J* = 5.8 Hz, 2H), 2.62 (t, *J* = 7.3 Hz, 2H), 2.22 (t, *J* = 7.2 Hz, 2H), 1.74 – 1.63 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.7, 142.1, 137.0, 133.3, 129.2, 128.8, 128.4, 128.4, 125.8, 42.9, 36.6, 35.7, 31.1, 25.3. **HRMS** (ESI): Calculated for $C_{18}H_{21}ClNO$ [M+H]: 302.1312, found: 302.1318.

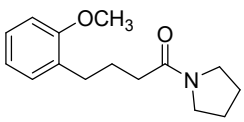


3ka (**CAS**:1215514-45-6)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.31 – 7.23 (m, 2H), 7.18 – 7.14 (m, 3H), 6.84 – 6.59 (m, 3H), 5.93 (s, 2H), 5.70 (s, 1H), 4.31 (d, *J* = 5.7 Hz, 2H), 2.62 (t, *J* = 7.3 Hz, 2H), 2.20 (t, *J* = 7.2 Hz, 2H), 1.73 – 1.61 (m, 4H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.6,

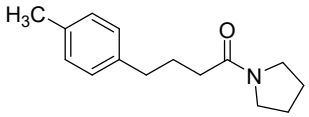
147.9, 147.0, 142.2, 132.3, 128.4, 128.3, 125.8, 121.1, 108.4, 108.3, 101.1, 43.4, 36.6, 35.7, 31.1, 25.4.



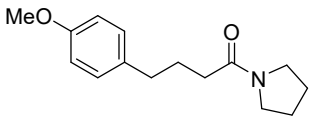
4aa (**CAS**:100420-10-8)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.29 – 7.26 (m, 2H), 7.20 – 7.16 (m, 3H), 3.46 (t, *J* = 6.9 Hz, 2H), 3.32 (t, *J* = 6.8 Hz, 2H), 2.69 (t, *J* = 7.6 Hz, 2H), 2.26 (t, *J* = 7.5 Hz, 2H), 2.00 (p, *J* = 6.7 Hz, 2H), 1.92 (p, *J* = 6.7 Hz, 2H), 1.83 (p, *J* = 6.8 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ171.4, 141.9, 128.5, 128.3, 125.8, 46.5, 45.6, 35.4, 33.9, 26.3, 26.1, 24.4.



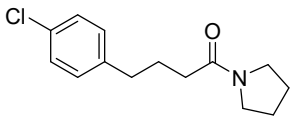
4ab: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ7.22 – 7.09 (m, 2H), 6.87 (t, *J* = 7.4 Hz, 1H), 6.83 (d, *J* = 8.1 Hz, 1H), 3.81 (s, 3H), 3.46 (t, *J* = 6.9 Hz, 2H), 3.34 (t, *J* = 6.8 Hz, 2H), 2.68 (t, *J* = 7.5 Hz, 2H), 2.27 (t, *J* = 7.6 Hz, 2H), 1.99 – 1.89 (m, 4H), 1.87 – 1.80 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.7, 157.5, 130.3, 123.0, 127.1, 120.3, 110.2, 55.2, 46.5, 45.6, 34.4, 29.8, 26.1, 24.8, 24.4. **HRMS** (ESI): Calculated for $C_{15}H_{22}NO_2$ [M+H]: 248.1651, found: 248.1648.



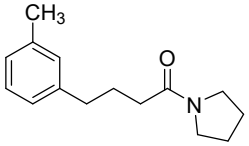
4ac:(**CAS:**1216738-01-0)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.08 (s, 4H), 3.45 (t, *J* = 6.9 Hz, 2H), 3.32 (t, *J* = 6.8 Hz, 2H), 2.64 (t, *J* = 7.5 Hz, 2H), 2.31 (s, 3H), 2.25 (t, *J* = 7.5 Hz, 2H), 2.00 – 1.94 (m, 2H), 1.92 – 1.89 (m, 2H), 1.85 – 1.81 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.4, 138.8, 135.2, 129.0, 128.4, 46.5, 45.6, 34.9, 33.9, 26.4, 26.1, 24.4, 21.0.



4ad (**CAS**:2340760-34-9)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.11 – 7.09 (m, 2H), 6.86 – 6.77 (m, 2H), 3.78 (s, 3H), 3.45 (t, *J* = 6.9 Hz, 2H), 3.32 (t, *J* = 6.8 Hz, 2H), 2.62 (t, *J* = 7.5 Hz, 2H), 2.25 (t, *J* = 7.5 Hz, 2H), 1.99 – 1.94 (m, 2H), 1.93 – 1.89 (m, 2H), 1.83 (p, *J* = 6.6 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.4, 157.8, 134.0, 129.4, 113.7, 55.3, 46.5, 45.6, 34.4, 33.9, 26.5, 26.1, 24.4.

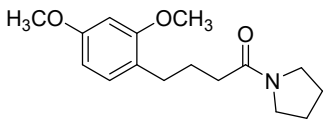


4ae (**CAS**:1215665-98-7)**: ^{1}H NMR** (500 MHz, $CDCl_3$) 7.27 – 7.22 (m, 2H), 7.12 (d, *J* = 8.3 Hz, 2H), 3.46 (t, *J* = 6.9 Hz, 2H), 3.33 (t, *J* = 6.8 Hz, 2H), 2.65 (t, *J* = 7.6 Hz, 2H), 2.25 (t, *J* = 7.4 Hz, 2H), 2.00 – 1.90 (m, 4H), 1.84 (p, *J* = 6.7 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.1, 140.3, 131.5, 129.9, 128.4, 46.5, 45.6, 34.7, 33.7, 26.2, 26.1, 24.4.

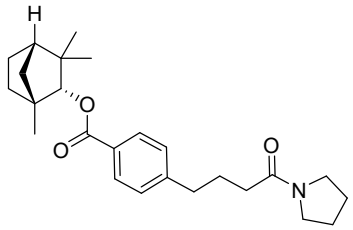


4af: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.16 (t, *J* = 7.4 Hz, 1H), 7.03 – 6.97 (m, 4H), 3.46 (t, *J* = 6.8 Hz, 2H), 3.33 (t, *J* = 6.7 Hz, 2H), 2.64 (t, *J*

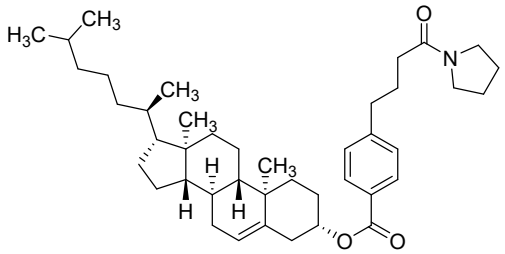
= 7.5 Hz, 2H), 2.32 (s, 3H), 2.26 (t, *J* = 7.5 Hz, 2H), 2.01 – 1.97 (m, 2H), 1.91 (q, *J* = 6.8 Hz, 2H), 1.86 – 1.81 (m, 2H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.5, 141.8, 137.9, 129.3, 128.2, 126.6, 125.5, 46.5, 45.6, 35.3, 33.9, 26.3, 26.1, 24.4, 21.4. **HRMS** (ESI): Calculated for $C_{15}H_{22}NO$ [M+H]: 232.1701, found: 2 32.1702.



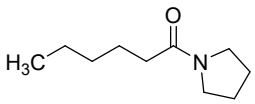
4ag: White solid. Melting point: 51-52 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.04 (d, *J* = 8.1 Hz, 1H), 6.51 – 6.40 (m, 2H), 3.86 – 3.75 (m, 6H), 3.47 (t, *J* = 6.8 Hz, 2H), 3.36 (t, *J* = 6.7 Hz, 2H), 2.62 (t, *J* = 7.6 Hz, 2H), 2.27 (t, *J* = 7.6 Hz, 2H), 1.99 – 1.91 (m, 4H), 1.90 – 1.78 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.7, 159.1, 158.4, 130.1, 122.7, 103.7, 98.4, 55.4, 55.2, 46.5, 45.6, 34.3, 29.1, 26.1, 25.0, 24.4. **HRMS** (ESI): Calculated for $C_{16}H_{24}NO_3$ [M+H]: 278.1756, found: 278.1757.



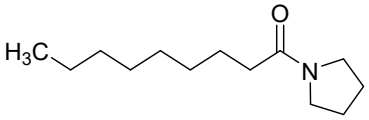
4ah: Brown oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.0 Hz, 2H), 7.29 – 7.26 (m, 3H), 4.61 (d, *J* = 1.9 Hz, 1H), 3.46 (t, *J* = 6.9 Hz, 2H), 3.33 (t, *J* = 6.8 Hz, 2H), 2.75 (t, *J* = 7.6 Hz, 2H), 2.27 (t, *J* = 7.4 Hz, 2H), 2.02 (t, *J* = 7.5 Hz, 2H), 1.94 – 1.91 (m, 2H), 1.85 (q, *J* = 6.8 Hz, 2H), 1.79 – 1.76 (m, 2H), 1.72 – 1.63 (m, 2H), 1.55 – 1.48 (m, 2H), 1.18 (s, 3H), 1.10 (s, 3H), 0.84 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.0, 166.9, 147.3, 129.7, 128.6, 128.5, 86.5, 48.6, 48.5, 46.5, 45.6, 41.5, 39.8, 35.4, 33.7, 29.8, 26.9, 26.1, 25.9, 25.9, 24.4, 20.3, 19.5. **HRMS** (ESI): Calculated for $C_{25}H_{36}NO_3$[M+H]: 398.2695, found: 398.2691.



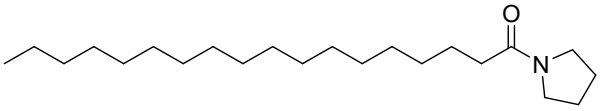
4ai: Yellow solid**.** Melting point: 132-133 °C.**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.97 – 7.94 (m, 2H), 7.27 – 7.25 (m, 3H), 5.42 (s, 1H), 4.88 – 4.82 (m, 1H), 3.48 – 3.44 (m, 2H), 3.35 – 3.31 (m, 2H), 2.76 – 2.73 (m, 2H), 2.46 (d, *J* = 8.3 Hz, 2H), 2.27 – 2.24 (m, 2H), 2.03 – 1.98 (m, 6H), 1.94 – 1.89 (m, 3H), 1.87 – 1.82 (m, 4H), 1.76 – 1.69 (m, 2H), 1.64 – 1.42 (m, 8H), 1.29 – 1.23 (m, 2H), 1.22 – 1.20 (m, 1H) 1.19 – 1.17 (m, 1H) 1.17 – 1.09 (m, 3H), 1.07 (d, *J* = 3.0 Hz, 3H), 1.05 – 0.96 (m, 3H), 0.93 (dd, J = 6.5, 3.0 Hz, 3H), 0.88 – 0.86 (m, 6H), 0.69 (d, J = 3.0 Hz, 3H). **^{13}C NMR** (126 MHz, CDCl3) δ 171.0, 166.0, 147.3, 139.7, 129.7, 128.6, 128.5, 122.7, 74.4, 56.7, 56.2, 50.1, 46.5, 45.6, 42.3, 39.8, 39.5, 38.3, 37.1, 36.7, 36.2, 35.8, 35.4, 33.7, 32.0, 31.9, 28.3, 28.0, 27.9, 26.1, 25.9, 24.4, 24.3, 23.8, 22.8, 22.6, 21.1, 19.4, 18.7, 11.9. **HRMS** (ESI): Calculated for $C_{42}H_{64}NO_3$ [M+H]: 630.4886, found: 630.4890.



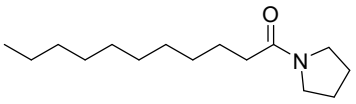
5aa (**CAS**:3389-56-8)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ 3.46 (t, *J* = 6.9 Hz, 2H), 3.41 (t, *J* = 6.8 Hz, 2H), 2.25 (t, *J* = 7.7 Hz, 2H), 1.95 (p, *J* = 6.6 Hz, 1H), 1.85 (p, *J* = 6.6 Hz, 1H), 1.69 – 1.62 (m, 2H), 1.35 – 1.31 (m, 4H), 0.92 – 0.88 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.9, 46.6, 45.6, 34.8, 31.7, 26.1, 24.7, 24.4, 22.5, 14.0.



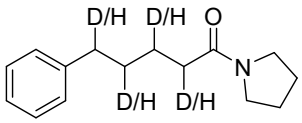
6aa (**CAS**:20308-70-7)**: ^{1}H NMR** (500 MHz, $CDCl_3$) δ3.47 (t, *J* = 6.9 Hz, 2H), 3.42 (t, *J* = 6.8 Hz, 2H), 2.26 (t, *J* = 7.7 Hz, 2H), 1.98 – 1.92 (m, 2H), δ 1.85 (p, *J* = 6.8 Hz, 1H), 1.68 – 1.62 (m, 2H), 1.31 – 1.27 (m, 10H), 0.89 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.9, 46.6, 45.6, 34.9, 31.9, 29.6, 29.6, 29.5, 29.5, 29.3, 26.2, 25.0, 24.4, 22.7, 14.1.



7aa: White solid. Melting point: 46-47 °C.**^{1}H NMR** (500 MHz, $CDCl_3$) δ 3.46 (t, *J* = 6.9 Hz, 2H), 3.41 (t, *J* = 6.8 Hz, 2H), 2.25 (t, *J* = 7.6 Hz, 2H), 1.95 (q, *J* = 6.6 Hz, 2H), 1.85 (q, *J* = 6.6 Hz, 2H), 1.66 – 1.63 m, 2H), 1.26 (s, 28H), 0.88 (t, *J* = 6.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.9, 46.6, 45.6, 34.9, 31.9, 29.7, 29.7, 29.6, 29.5, 29.4, 26.2, 25.0, 24.4, 22.7, 14.1. **HRMS** (ESI): Calculated for $C_{22}H_{44}NO$ [M+H]: 338.3423, found: 338.3424.

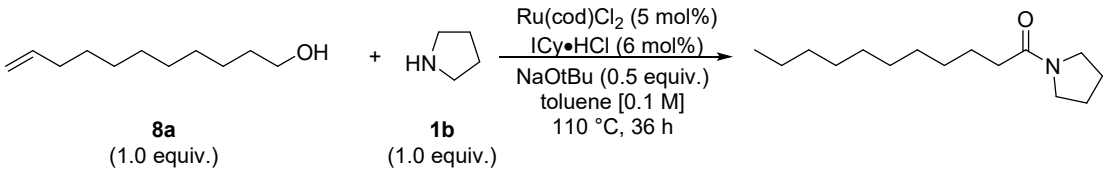


8aa: (**CAS**:70974-44-6)**: ^{1}H NMR** (500 MHz, $CDCl_3$) 3.46 (t, *J* = 6.9 Hz, 2H), 3.41 (t, *J* = 6.8 Hz, 2H), 2.25 (t, *J* = 7.6 Hz, 2H), 1.95 (p, *J* = 6.8 Hz, 2H), 1.84 (p, *J* = 6.8 Hz, 2H), 1.67 – 1.61 (m, 2H), 1.32 – 1.21 (m, 14H), 0.88 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.9, 46.6, 45.6, 34.9, 31.9, 29.6, 29.6, 29.5, 29.5, 29.3, 26.2, 25.0, 24.4, 22.7, 14.1.



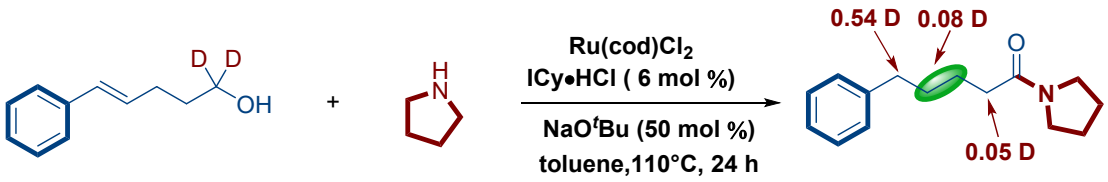
3aa-d_2: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 – 7.24 (m, 2H), 7.19 – 7.15 (m, 3H), 3.45 (t, *J* = 6.9 Hz, 2H), 3.37 (t, *J* = 6.8 Hz, 2H), 2.65 – 2.61 (m, 1.46H + 0.54D), 2.28 – 2.26 (m, 1.95H + 0.05D), 1.96 – 1.89 (m, 1H), 1.87 – 1.80 (m, 1H), 1.77 – 1.59 (m, 1.92H + 0.08D).

6. Gram-scale preparation



A flame–dried 150 mL cylindrical pressure vessel was charged with 10-Undecen-1-ol **8a** (6.8 mmol, 1.0 equiv.) and Pyrrolidine **1b** (6.8 mmol, 1.0 equiv), $Ru(cod)Cl_2$ (95.1 mg, 0.34 mmol, 5 mol%), ICy·HCl (110.2 mg, 0.41mmol, 6 mol%), NaO^tBu (326.7 mg, 3.4 mmol, 0.5 equiv.) and 34 mL dry toluene in a nitrogen-filled glovebox. Then the cylindrical pressure vessel was tightly sealed, transferred out of the glovebox and stirred at 110 °C for 36 h. After the completion of reaction, the solvent was removed in vacuo and the residue was purified by flash column chromatography on silica gel to give the desired amide products with 84% isolated yield (1.37 g).

7. Mechanism studies



1.0 equiv. (0.2 mmol) | 1.0 equiv. | Yield: 85 %

In order to determine the source and transfer route of hydrogen during the reaction, an isotopic labeling experiment was carried out. When deuterated alkenyl **1a-*d*$_2$** reacted with pyrrolidine **2a** under standard reaction conditions, the corresponding amide product **3aa-*d*$_2$** was obtained in 85% yield. ^{1}H NMR analysis showed that deuterium was scrambling at the alkyl chain including α (0.54D), internal β/γ (0.08 D), and terminal δ (0.05 D) position, thus indicating that the transfer route of hydrogen during the reaction was a chain-walking process.

In addition, hydrogen gas signal was detected by gas chromatography after the end of the reaction (**Figure S1**), suggesting a dehydrogenative process involved in this cross-coupling of alcohols and amines.

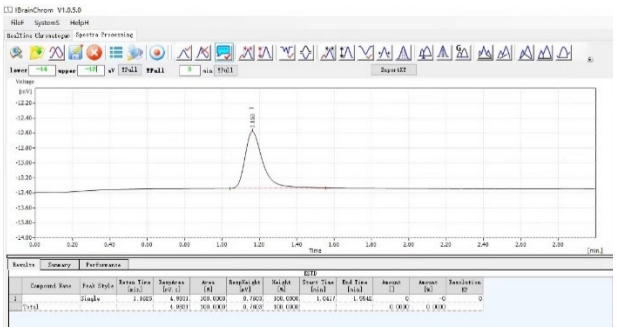
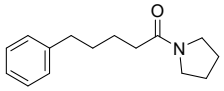
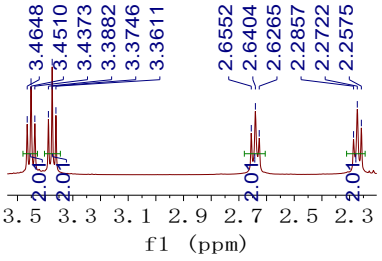


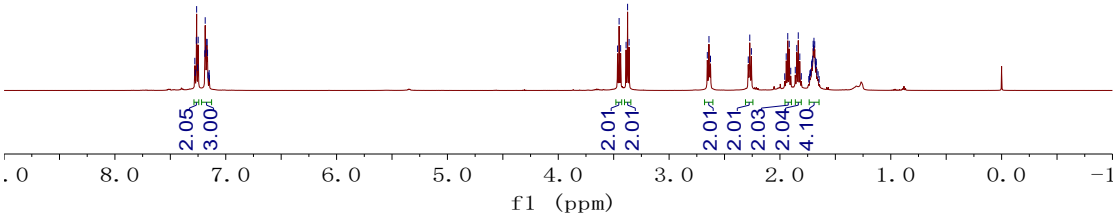
Figure S1 Hydrogen detection of reaction

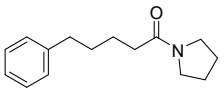
8. ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra



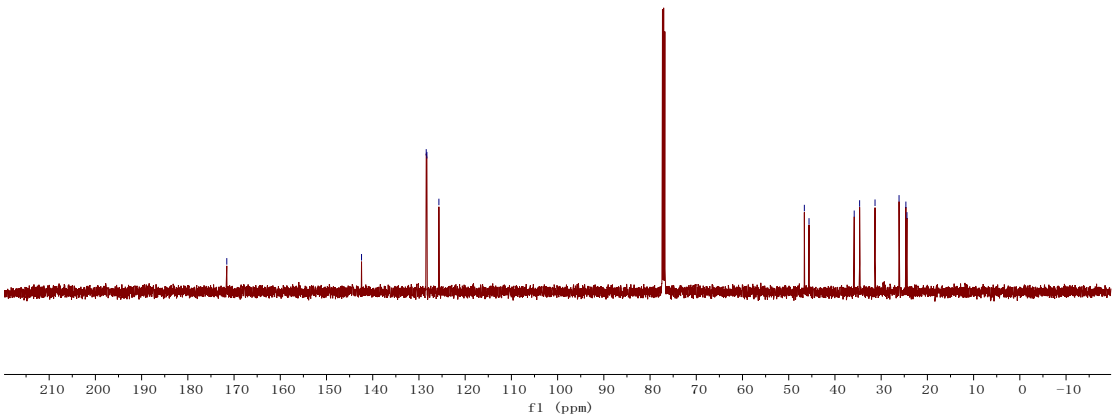
3aa

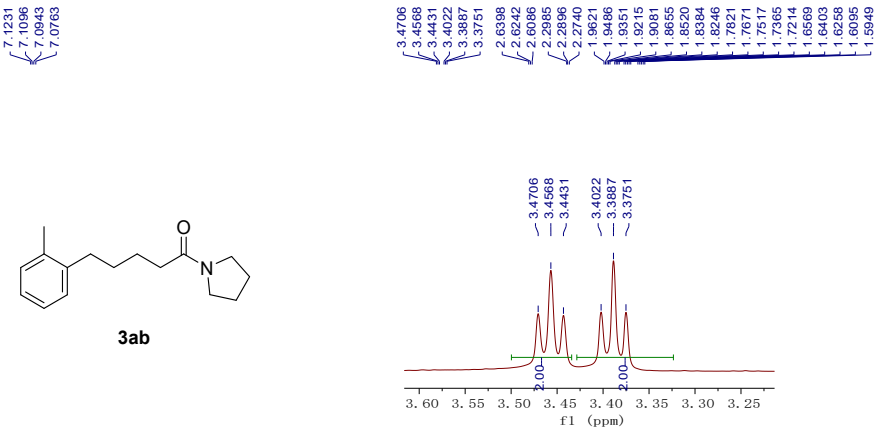


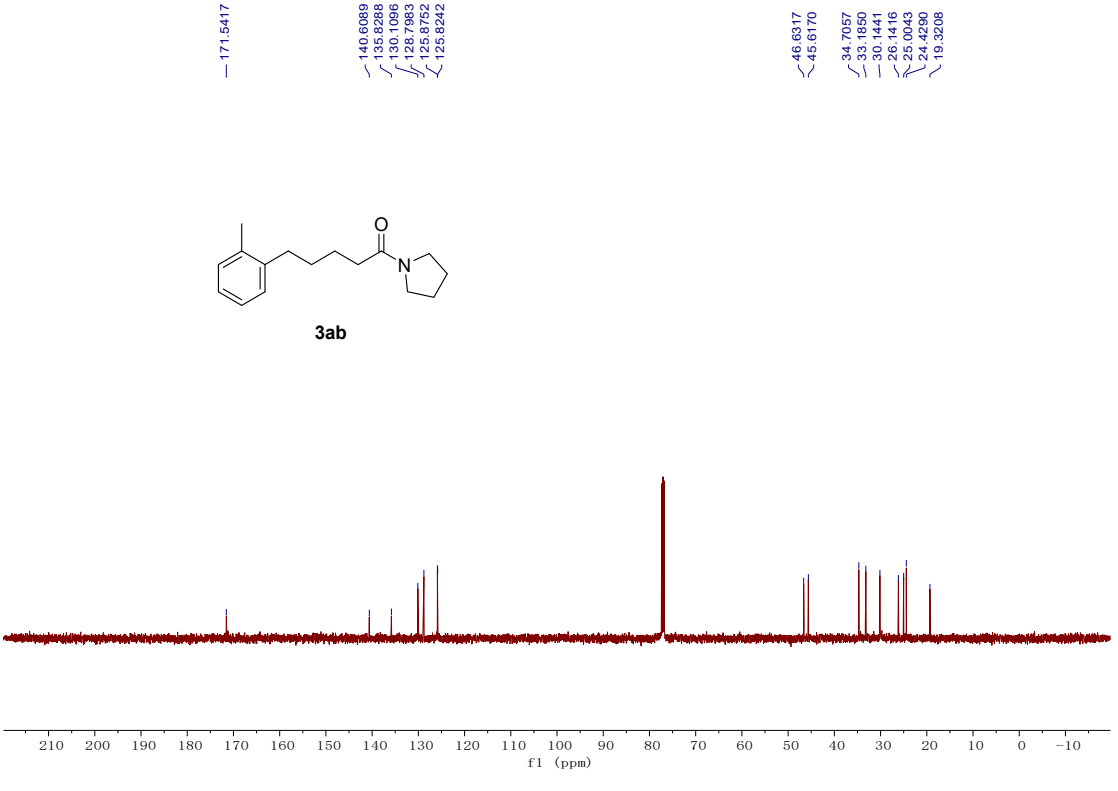




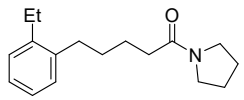
3aa



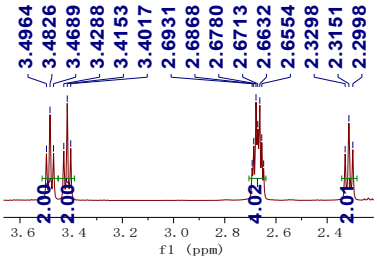

7.1231
7.1096
7.0943
7.0763
3.4706
3.4568
3.4431
3.4022
3.3887
3.3751
2.6398
2.6242
2.6086
2.2985
2.2896
2.2740
1.9621
1.9486
1.9351
1.9215
1.9081
1.8655
1.8520
1.8384
1.8246
1.7821
1.7671
1.7517
1.7365
1.7214
1.6569
1.6403
1.6258
1.6095
1.5949
O
N
3ab
3.4706
3.4568
3.4431
3.4022
3.3887
3.3751
2.00
2.00
3.60 3.55 3.50 3.45 3.40 3.35 3.30 3.25
f1 (ppm)
4.00
2.00
2.01
2.00
5.00
2.02
2.02
2.03
2.06
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)

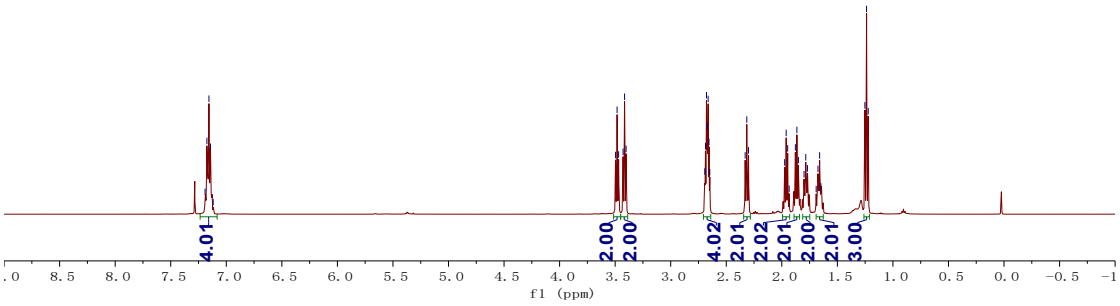

171.5417
140.6089
135.8288
130.1086
128.7983
125.8752
125.8242
46.6317
45.6170
34.7057
33.1850
30.1441
26.1416
25.0043
24.4290
19.3208
O
N
3ab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


7.1909
7.1745
7.1560
7.1420
7.1180
3.4964
3.4826
3.4689
3.4288
3.4153
3.4017
2.6868
2.6780
2.6713
2.6632
2.6554
2.3298
2.3151
2.2998
1.9607
1.9471
1.8781
1.8642
1.8506
1.7843
1.6595
1.2523
1.2371

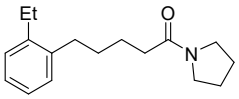

Et
O
N

3ac


3.4964
3.4826
3.4689
3.4288
3.4153
3.4017
2.6931
2.6868
2.6780
2.6713
2.6632
2.6554
2.3298
2.3151
2.2998
2.00
2.00
4.02
2.01
3.6 3.4 3.2 3.0 2.8 2.6 2.4
f1 (ppm)

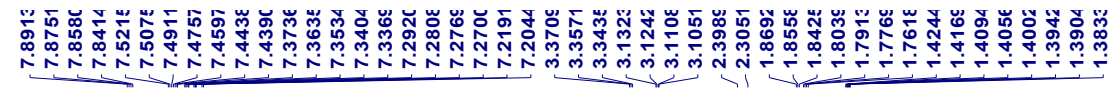

4.01
2.00
2.00
4.02
2.01
2.02
2.01
2.00
2.01
3.00
f1 (ppm)

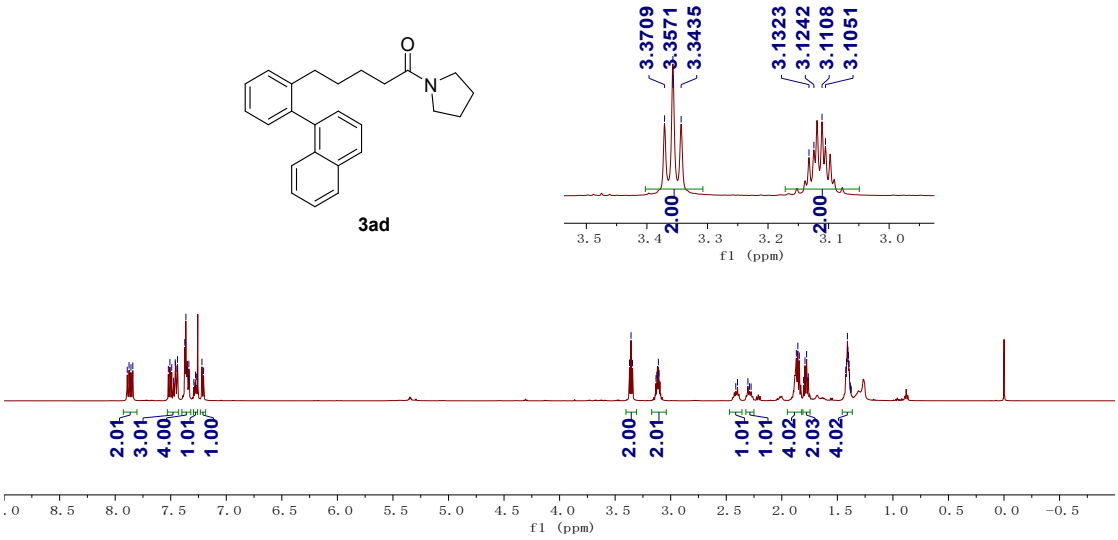

171.5436
141.8013
139.9456
129.0748
128.3431
126.0173
125.7737
46.6384
45.6188
34.7203
32.5293
31.0834
26.1448
25.5178
25.1085
24.4309
15.3718

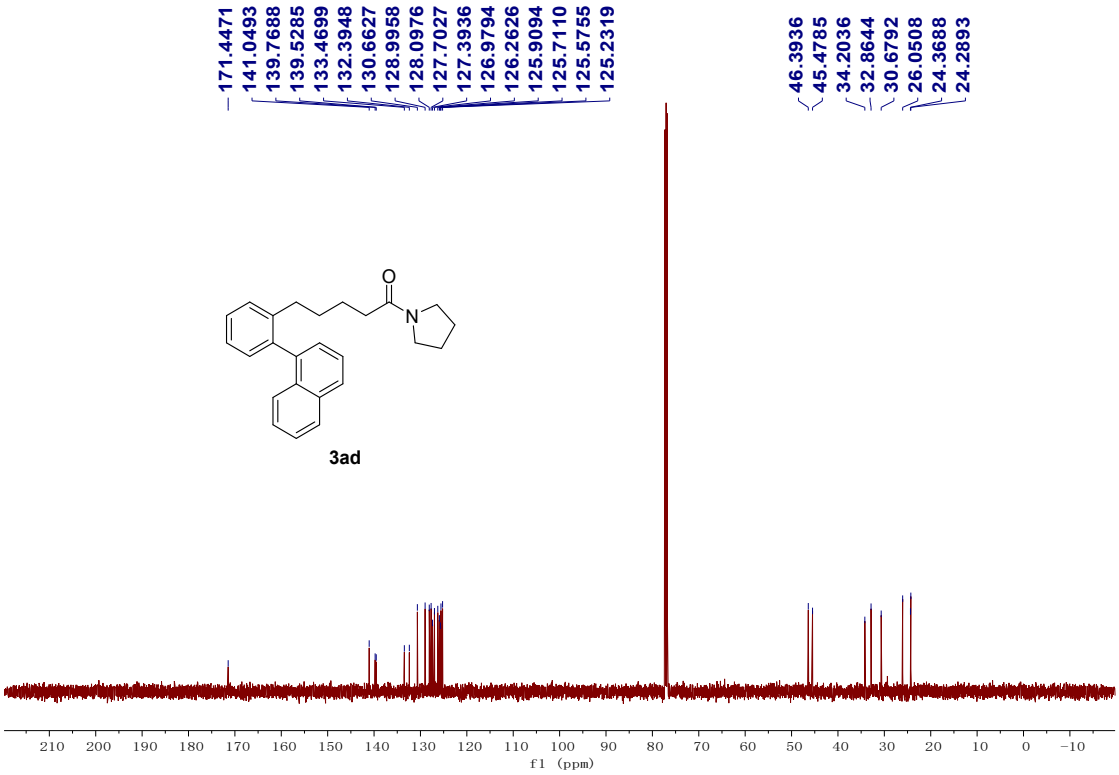

Et
O
N

3ac

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

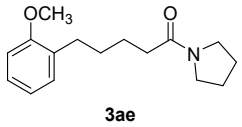



3ad
3.3709
3.3571
3.3435
3.1323
3.1242
3.1108
3.1051
2.00
2.00
f1 (ppm)
2.01
3.01
4.00
1.01
1.00
2.00
2.01
1.01
1.01
4.02
2.03
4.02
f1 (ppm)

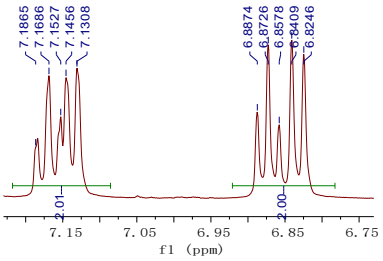

171.4471
141.0493
139.7688
139.5285
133.4699
132.3948
130.6627
128.9958
128.0976
127.7027
127.3936
126.9794
126.2626
125.9094
125.7110
125.5755
125.2319
46.3936
45.4785
34.2036
32.8644
30.6792
26.0508
24.3688
24.2893
3ad
f1 (ppm)

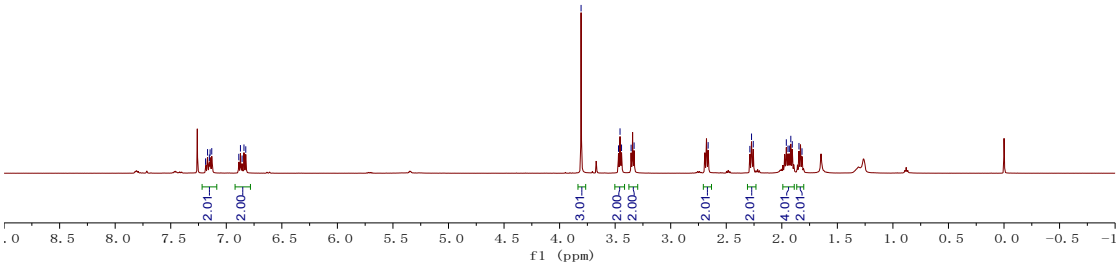

7.1865
7.1686
7.1527
7.1456
7.1308
6.8874
6.8726
6.8578
6.8409
6.8246


3.8067
3.4699
3.4561
3.4424
3.3565
3.3294
2.6630
2.2875
2.2725
2.2569
1.9594
1.9444
1.9323
1.9190
1.9056
1.8456
1.8183

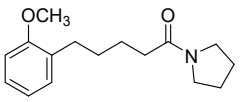

OCH3
O
N

3ae


7.1865
7.1686
7.1527
7.1456
7.1308
6.8874
6.8726
6.8578
6.8409
6.8246
2.01
2.00
7.15
7.05
6.95
6.85
6.75
f1 (ppm)

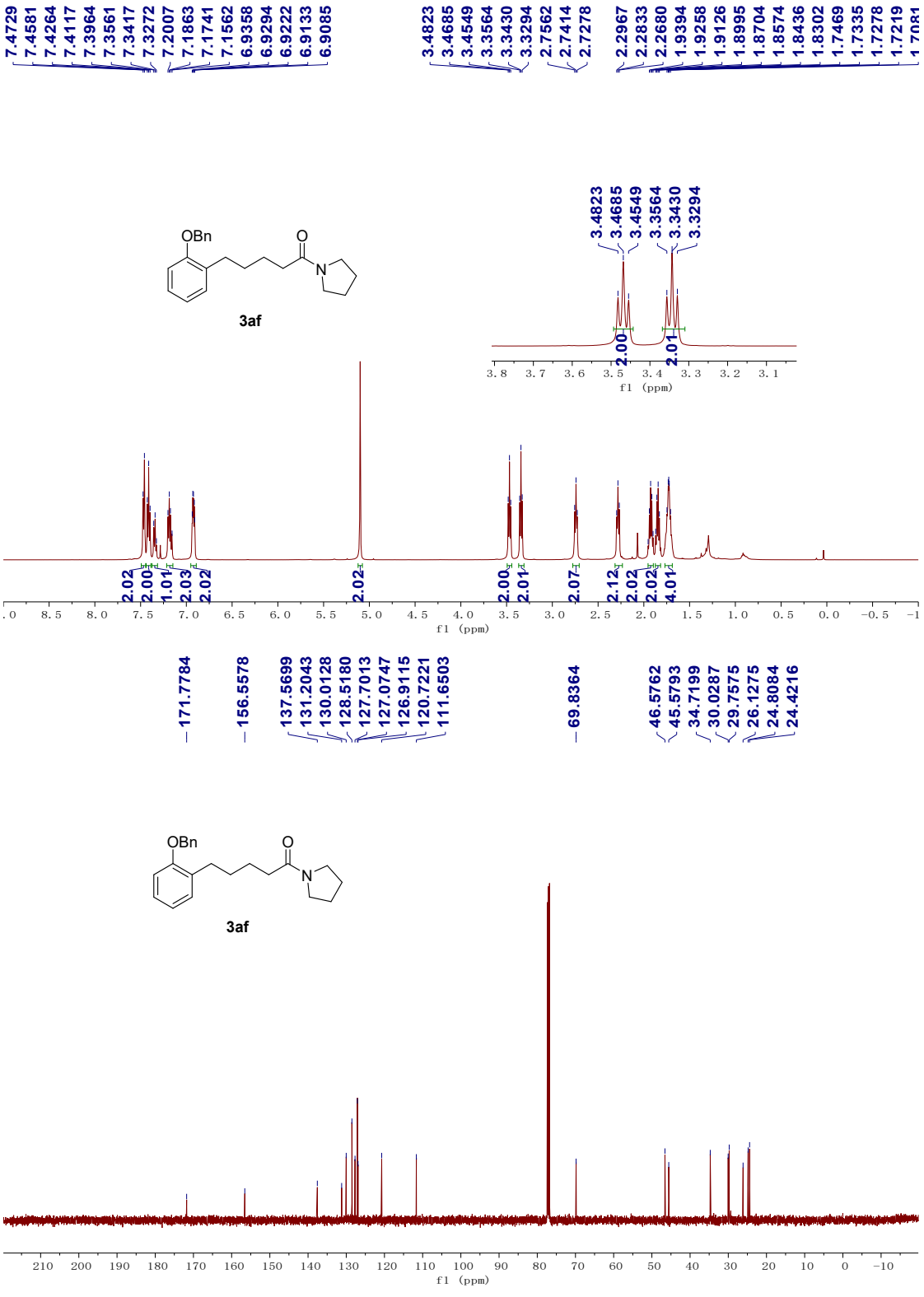

2.01
2.00
3.01
2.00
2.00
2.01
2.01
4.01
2.01
f1 (ppm)

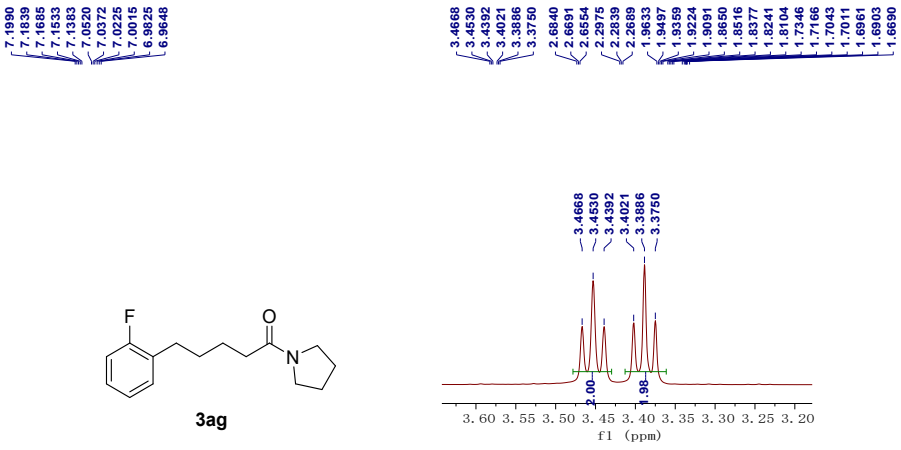

171.6606
157.5178
130.2459
129.9537
127.0666
120.3416
110.1839
55.2221
46.5033
45.5680
34.3483
29.7645
26.1389
24.7805
24.4386

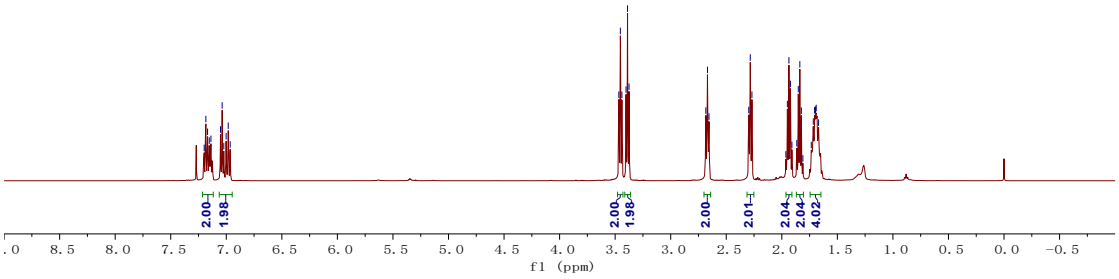

OCH3
O
N

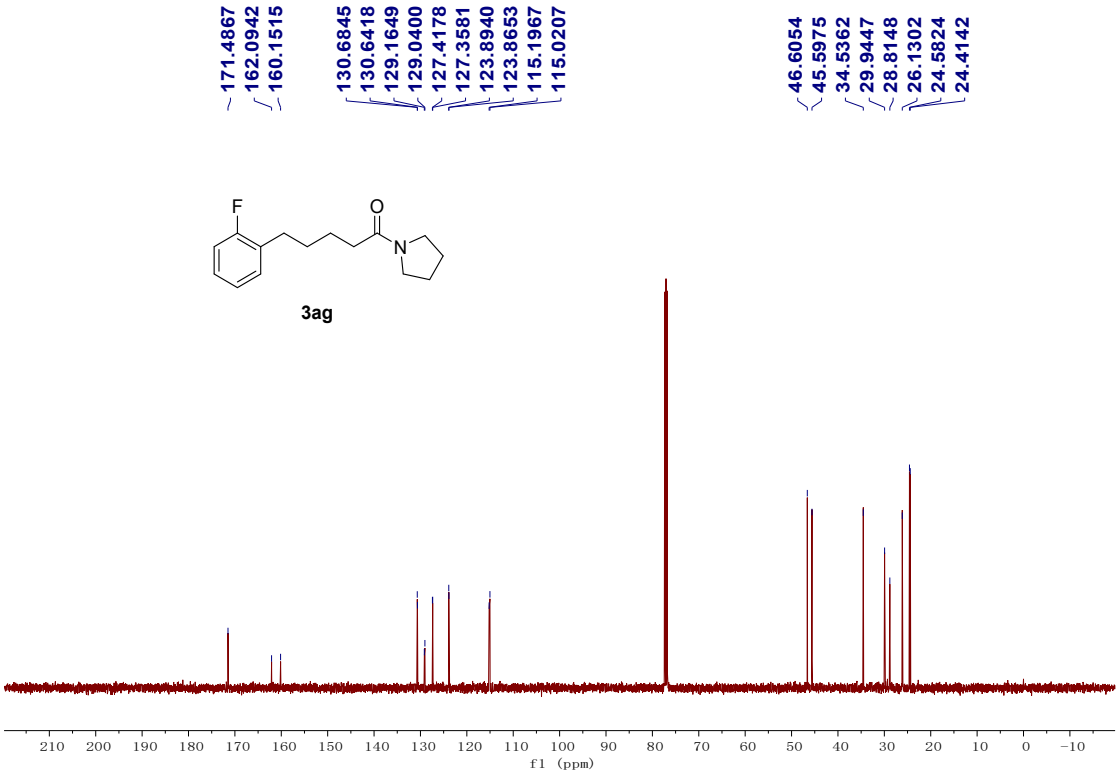
3ae

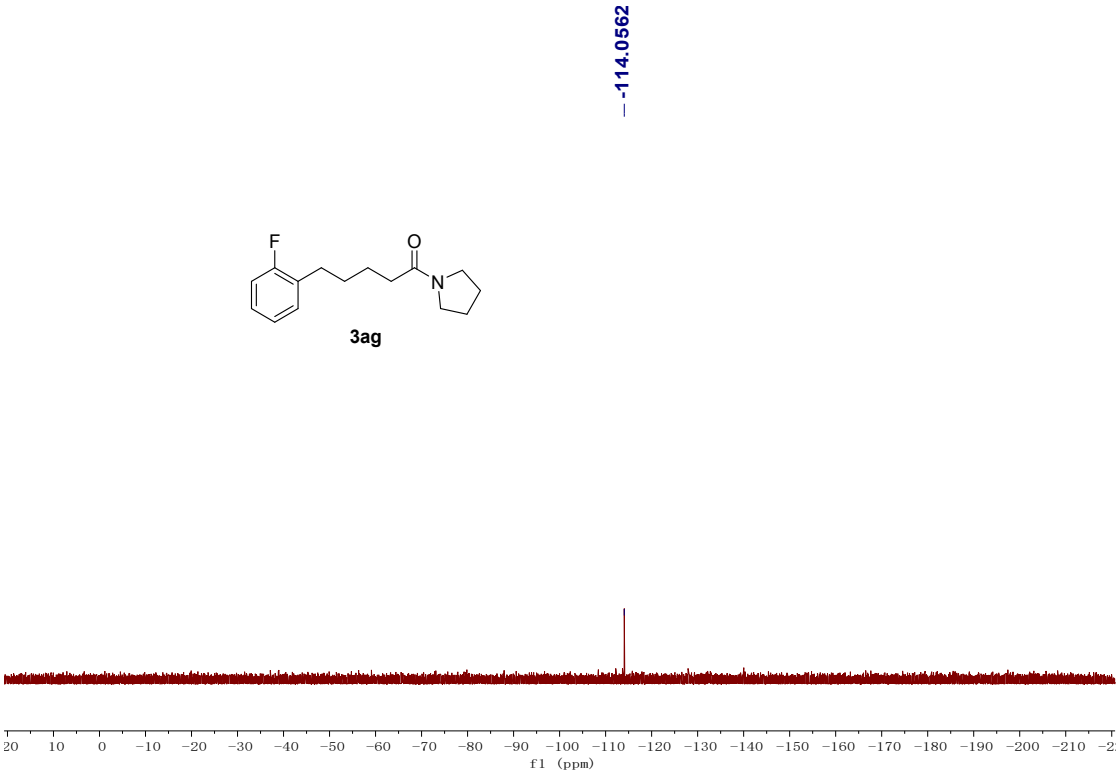
f1 (ppm)

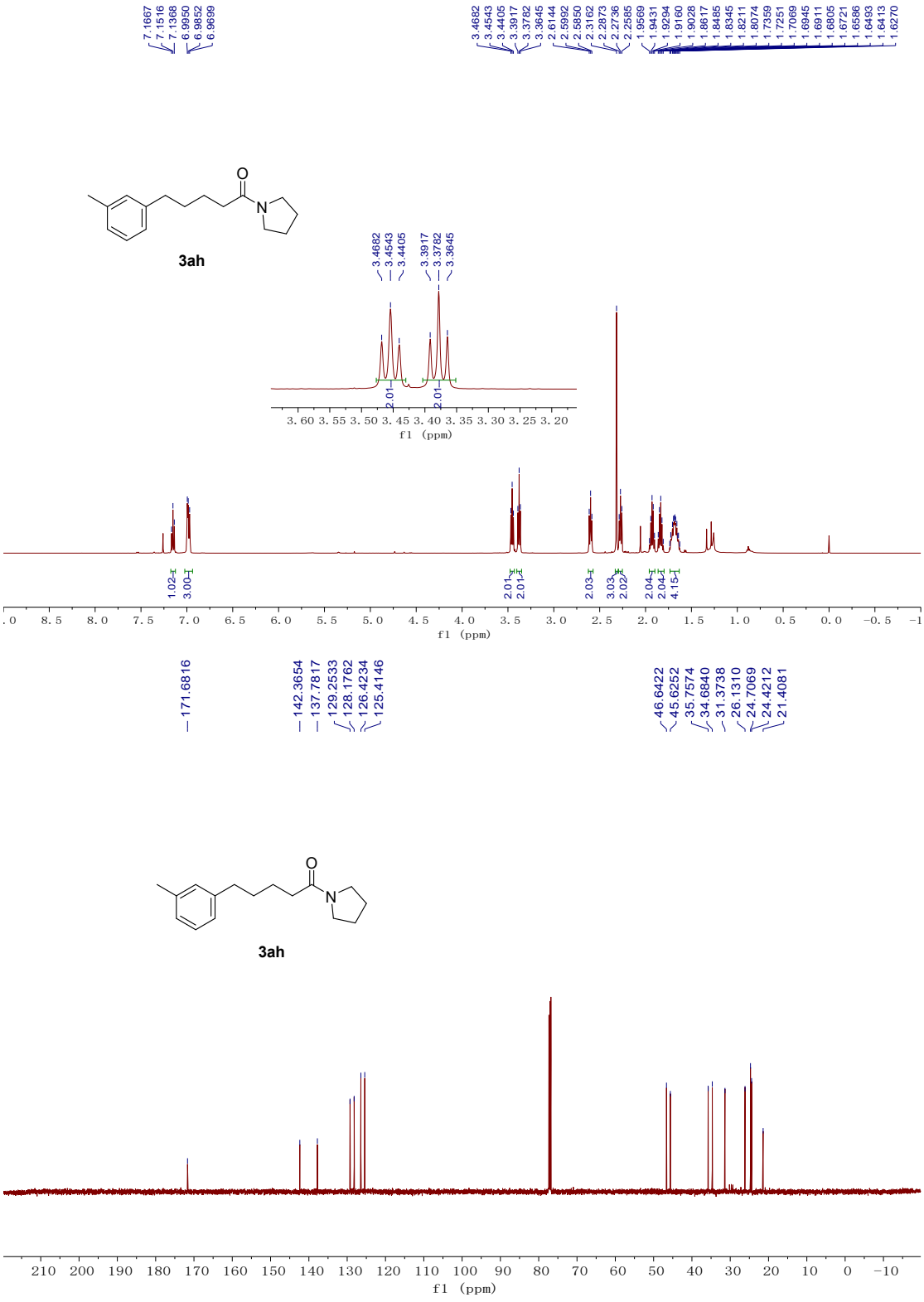

7.4729
7.4581
7.4264
7.4117
7.3964
7.3561
7.3417
7.3272
7.2007
7.1863
7.1741
7.1562
6.9358
6.9294
6.9222
6.9133
6.9085
3.4823
3.4685
3.4549
3.3564
3.3430
3.3294
2.7562
2.7414
2.7278
2.2967
2.2833
2.2680
1.9394
1.9258
1.9126
1.8995
1.8704
1.8574
1.8436
1.8302
1.7469
1.7335
1.7278
1.7219
OBn
O
N
3af
f1 (ppm)
2.02
2.00
1.01
2.03
2.02
2.02
2.00
2.01
2.07
2.12
2.02
2.02
4.01
171.7784
156.5578
137.5699
131.2043
130.0128
128.5180
127.7013
127.0747
126.9115
120.7221
111.6503
69.8364
46.5762
45.5793
34.7199
30.0287
29.7575
26.1275
24.8084
24.4216

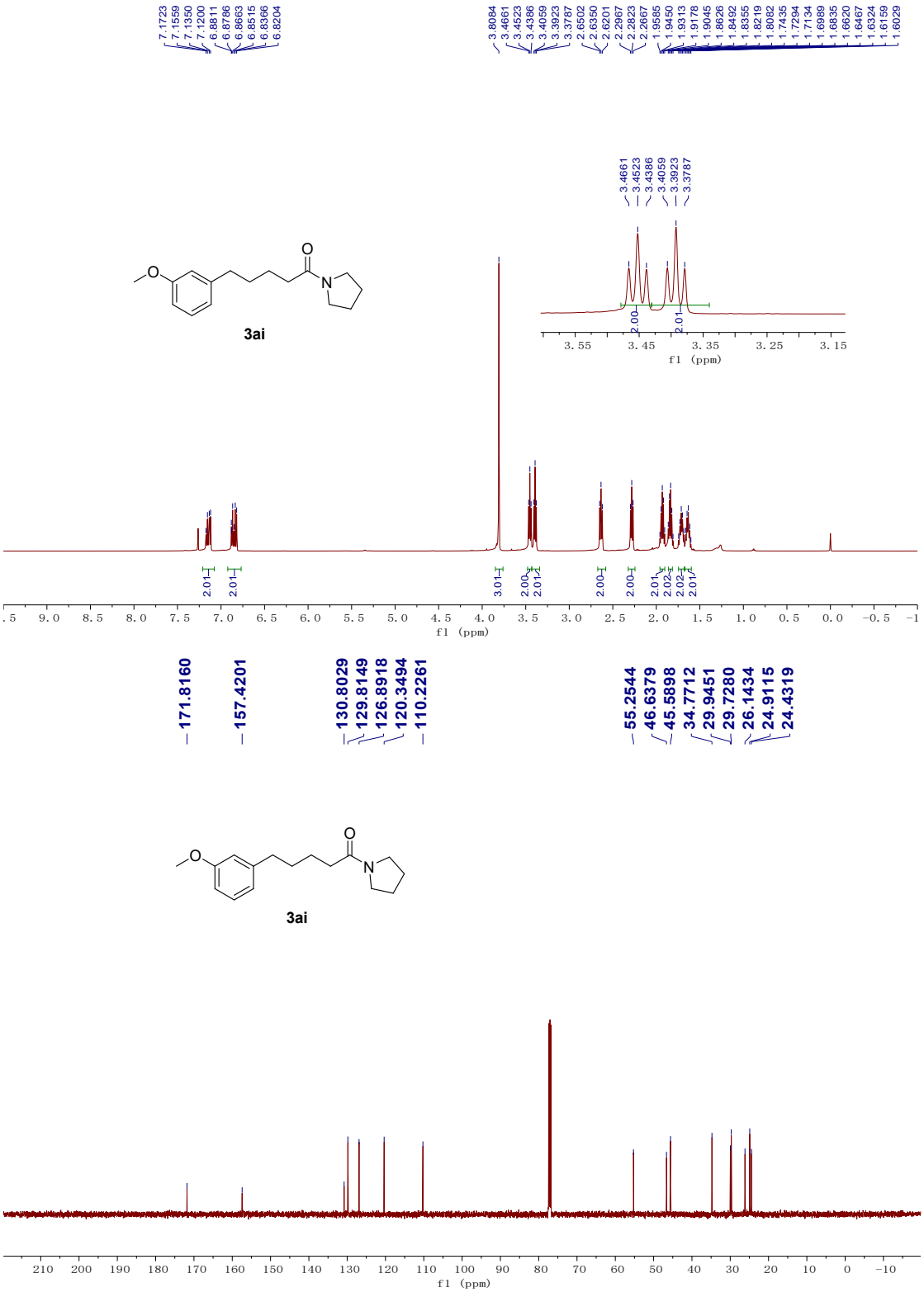

7.1990
7.1839
7.1685
7.1533
7.1383
7.0520
7.0372
7.0225
7.0015
6.9825
6.9648
3.4668
3.4530
3.4392
3.4021
3.3886
3.3750
2.6840
2.6691
2.6554
2.2975
2.2839
2.2689
1.9633
1.9497
1.9359
1.9224
1.9091
1.8650
1.8516
1.8377
1.8241
1.8104
1.7346
1.7166
1.7043
1.7011
1.6961
1.6903
1.6890
F
O
N
3ag
2.00
1.98
3.60 3.55 3.50 3.45 3.40 3.35 3.30 3.25 3.20
f1 (ppm)

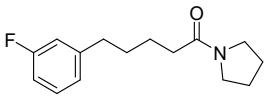

2.00
1.98
2.00
1.98
2.00
2.01
2.04
2.04
4.02
f1 (ppm)


171.4867
162.0942
160.1515
130.6845
130.6418
129.1649
129.0400
127.4178
127.3581
123.8940
123.8653
115.1967
115.0207
46.6054
45.5975
34.5362
29.9447
28.8148
26.1302
24.5824
24.4142
F
O
N
3ag
f1 (ppm)

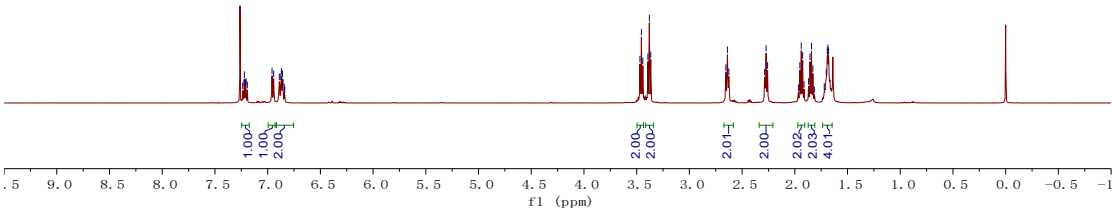

-114.0562
F
O
N
3ag
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

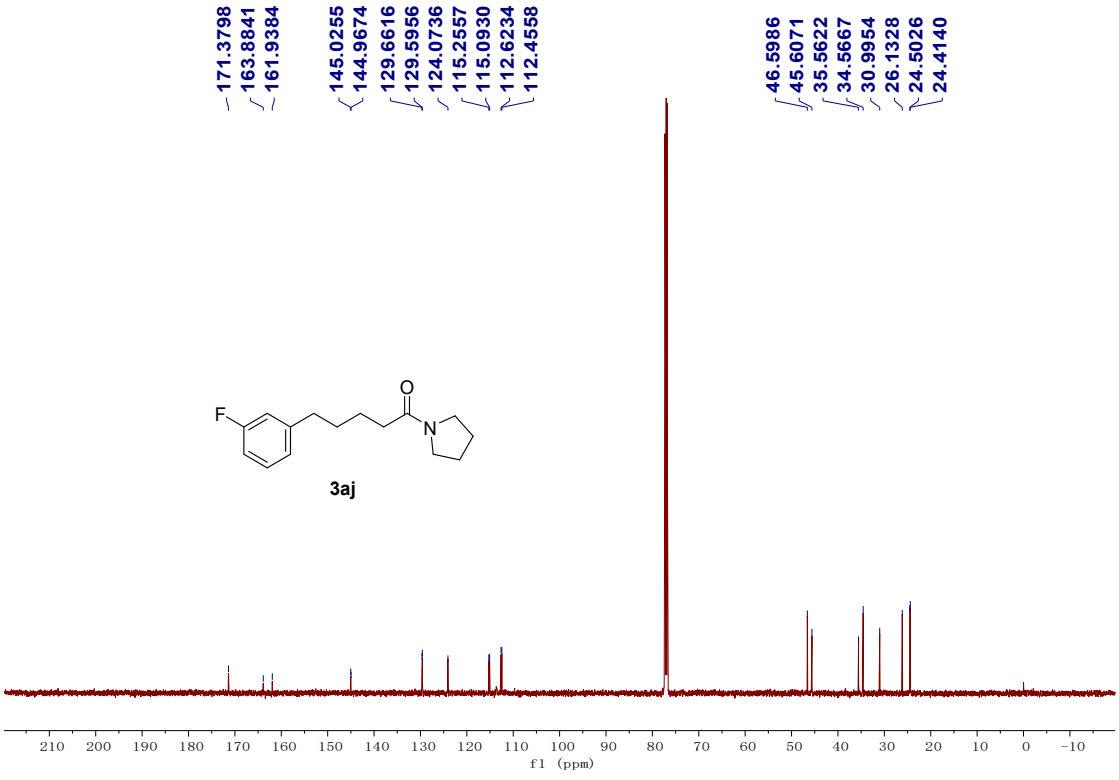

7.1667
7.1516
7.1368
6.9950
6.9852
6.9699
3.4682
3.4543
3.4405
3.3917
3.3782
3.3645
2.6144
2.5992
2.5850
2.3162
2.2873
2.2736
2.2585
1.9569
1.9431
1.9294
1.9160
1.9028
1.8617
1.8485
1.8345
1.8211
1.8074
1.7359
1.7251
1.7069
1.6945
1.6911
1.6805
1.6721
1.6586
1.6493
1.6413
1.6270
O
N
3ah
3.4682
3.4543
3.4405
3.3917
3.3782
3.3645
2.01
2.01
3.60 3.55 3.50 3.45 3.40 3.35 3.30 3.25 3.20
f1 (ppm)
1.02
3.00
2.01
2.01
2.03
3.03
2.02
2.04
2.04
4.15
f1 (ppm)
171.6816
142.3654
137.7817
129.2533
128.1762
126.4234
125.4146
46.6422
45.6252
35.7574
34.6840
31.3738
26.1310
24.7069
24.4212
21.4081
O
N
3ah
f1 (ppm)


7.1723
7.1559
7.1350
7.1200
6.8811
6.8786
6.8663
6.8515
6.8366
6.8204
3.8084
3.4661
3.4523
3.4386
3.4059
3.3923
3.3787
2.6502
2.6350
2.6201
2.2967
2.2823
2.2667
1.9585
1.9450
1.9313
1.9178
1.9045
1.8826
1.8492
1.8355
1.8219
1.8082
1.7435
1.7294
1.7134
1.6989
1.6835
1.6620
1.6467
1.6324
1.6159
1.6029
O
N
O
3ai
3.4661
3.4523
3.4386
3.4059
3.3923
3.3787
2.00
2.01
3.55
3.45
3.35
3.25
3.15
f1 (ppm)
2.01
2.01
3.01
2.00
2.01
2.00
2.00
2.01
2.02
2.02
2.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1
f1 (ppm)
171.8160
157.4201
130.8029
129.8149
126.8918
120.3494
110.2261
55.2544
46.6379
45.5898
34.7712
29.9451
29.7280
26.1434
24.9115
24.4319
O
N
O
3ai
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

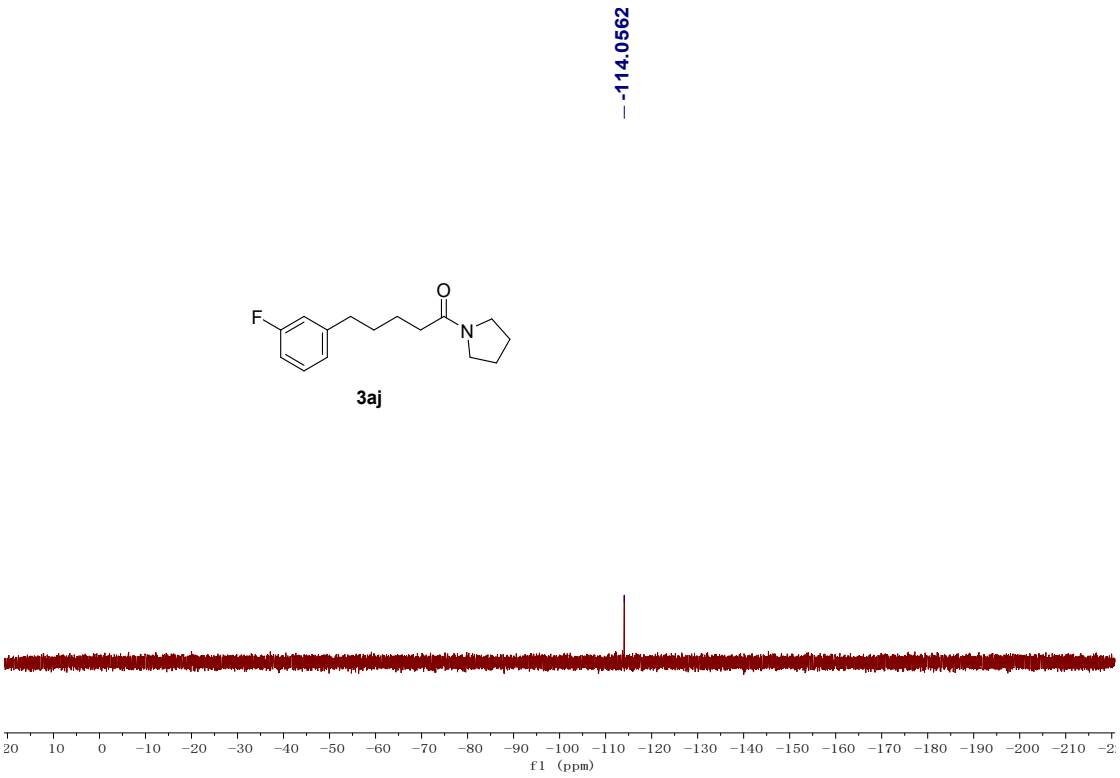


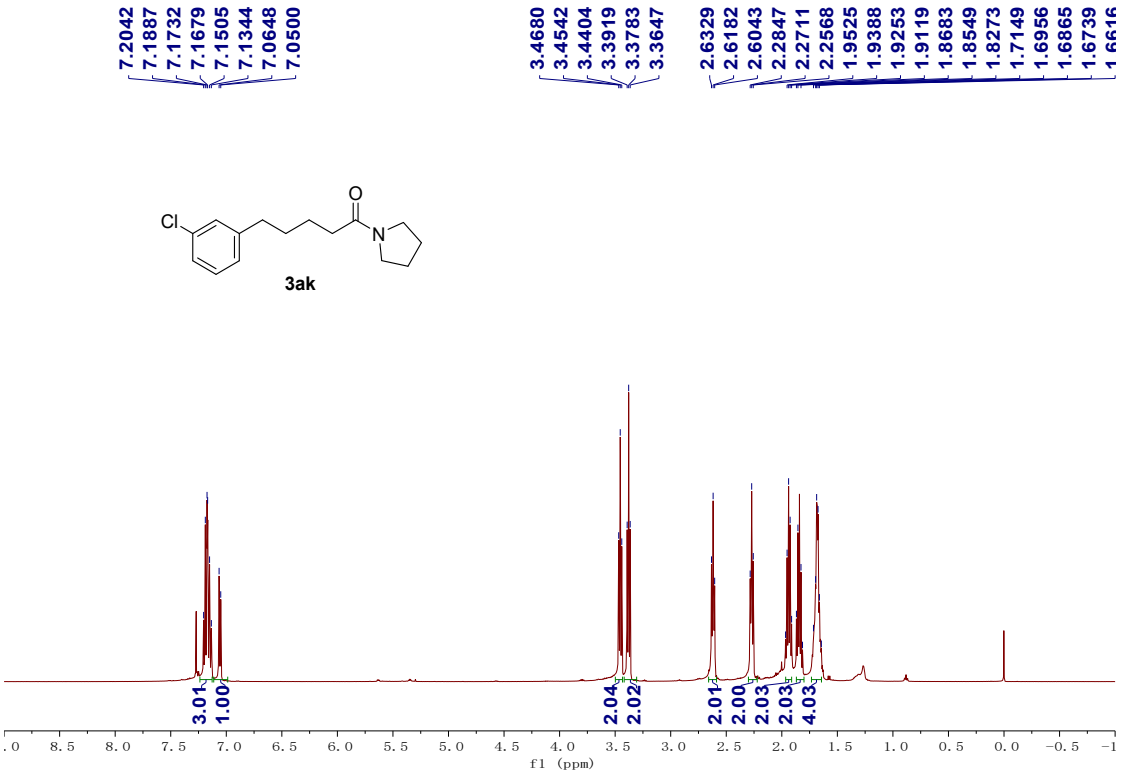
3aj

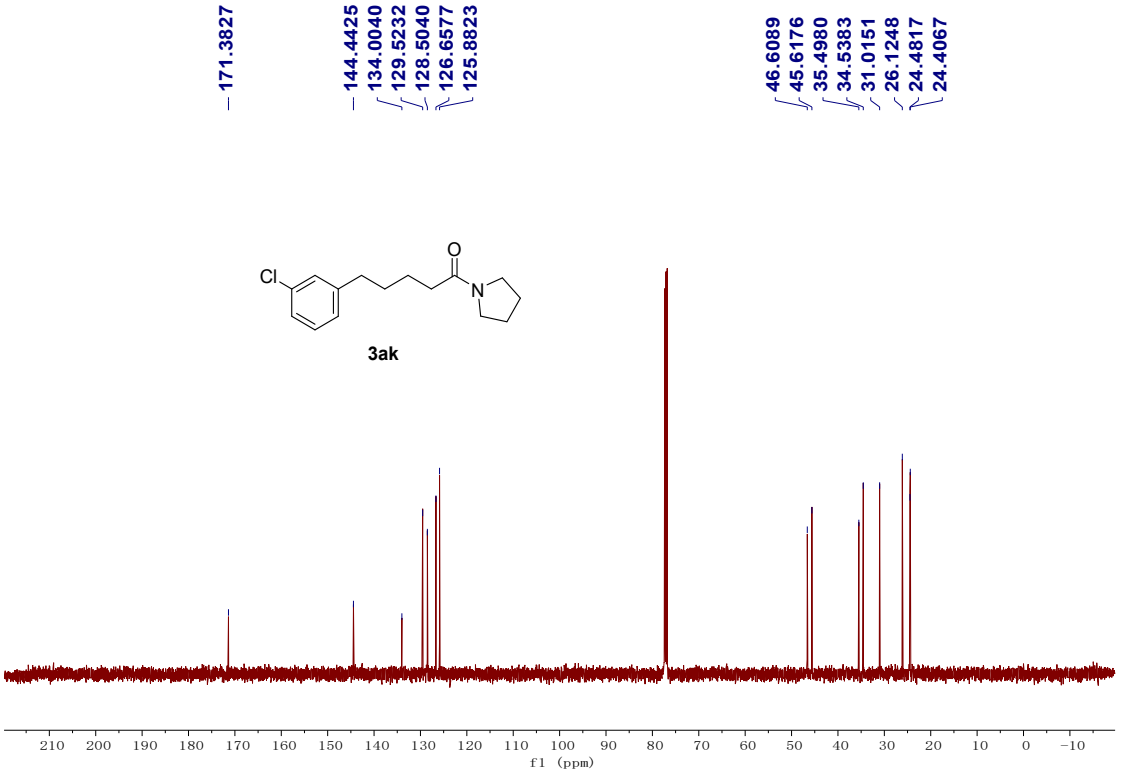


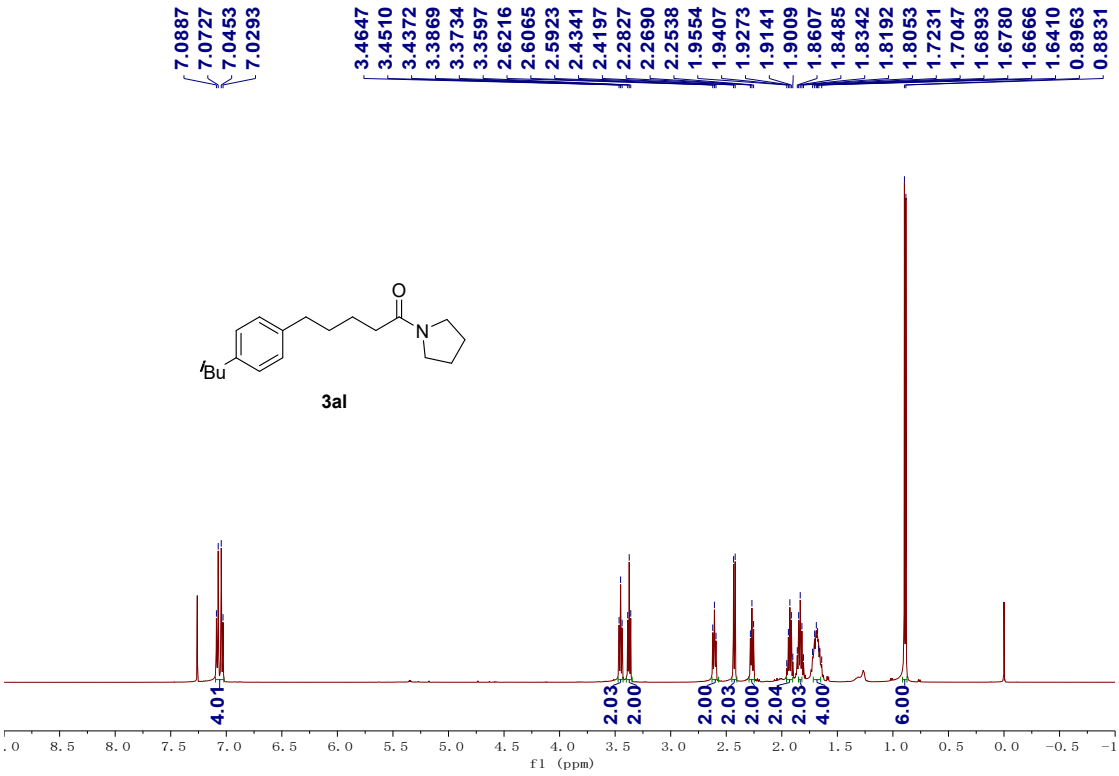


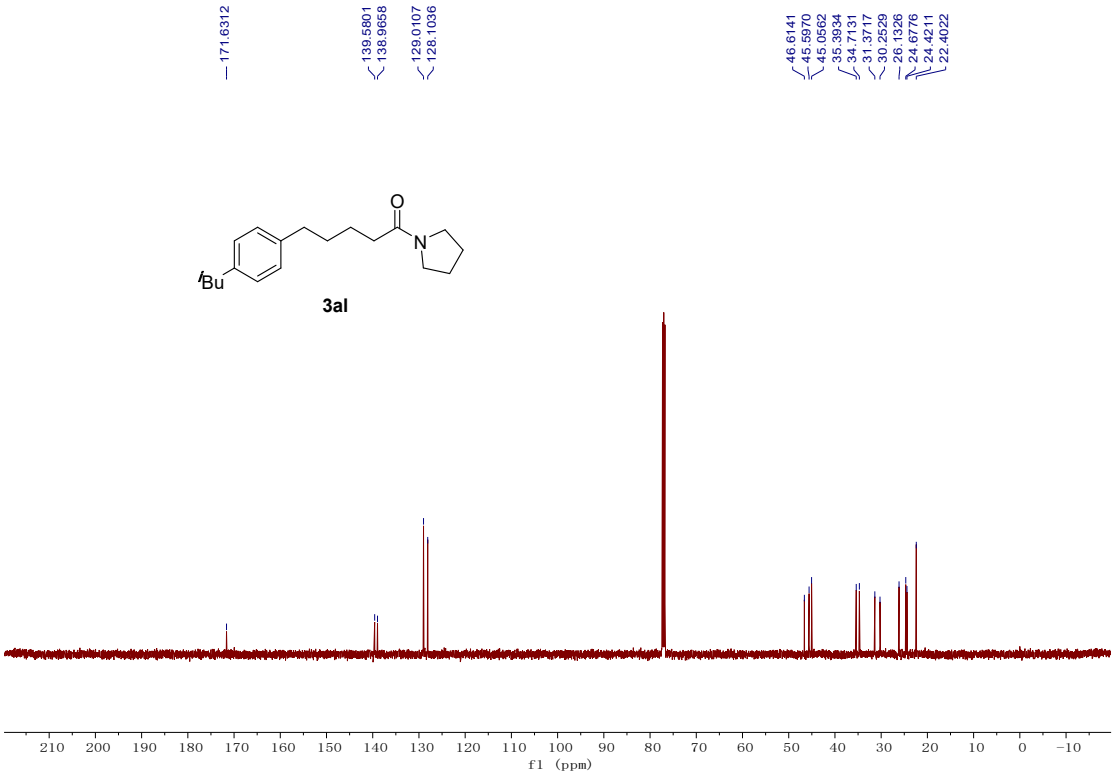
3aj


-114.0562
F
O
N
3aj
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)


7.2042
7.1887
7.1732
7.1679
7.1505
7.1344
7.0648
7.0500
3.4680
3.4542
3.4404
3.3919
3.3783
3.3647
2.6329
2.6182
2.6043
2.2847
2.2711
2.2568
1.9525
1.9388
1.9253
1.9119
1.8683
1.8549
1.8273
1.7149
1.6956
1.6865
1.6739
Cl
O
N
3ak
3.01
1.00
2.04
2.02
2.01
2.00
2.03
2.03
4.03
f1 (ppm)

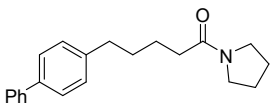

171.3827
144.4425
134.0040
129.5232
128.5040
126.6577
125.8823
46.6089
45.6176
35.4980
34.5383
31.0151
26.1248
24.4817
24.4067
Cl
O
N
3ak
f1 (ppm)


7.0887
7.0727
7.0453
7.0293
3.4647
3.4510
3.4372
3.3869
3.3734
3.3597
2.6216
2.6065
2.5923
2.4341
2.4197
2.2827
2.2690
2.2538
1.9554
1.9407
1.9273
1.9141
1.9009
1.8607
1.8485
1.8342
1.8192
1.8053
1.7231
1.7047
1.6893
1.6780
1.6666
1.6410
0.8963
0.8831
O
N
tBu
3al
4.01
2.03
2.00
2.00
2.03
2.00
2.04
2.03
4.00
6.00
f1 (ppm)

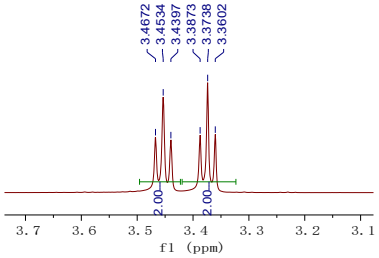

171.6312
139.5801
138.9658
129.0107
128.1036
46.6141
45.5970
45.0562
35.3934
34.7131
31.3717
30.2529
26.1326
24.6776
24.4211
22.4022
O
N
tBu
3al
f1 (ppm)

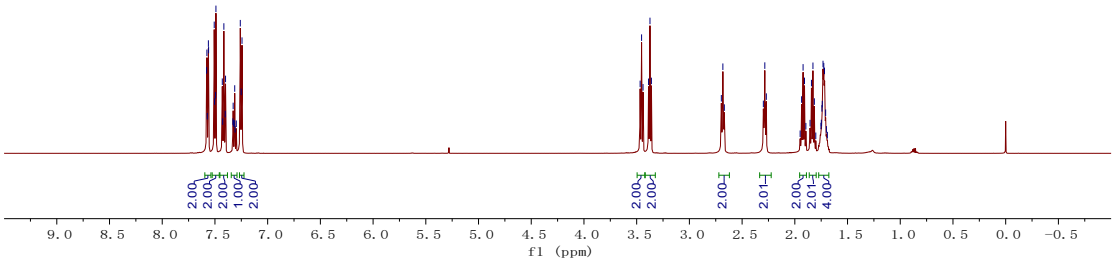

7.5791
7.5763
7.5727
7.5623
7.5602
7.5069
7.5035
7.4940
7.4906
7.4303
7.4265
7.4154
7.4026
7.3995
7.3295
7.3272
7.3247
7.3157
7.3124
7.3089
7.2977
7.2596
7.2510
7.2433


3.4672
3.4534
3.4397
3.3873
3.3738
3.3602
2.6970
2.6825
2.6685
2.2985
2.2846
2.2702
1.9496
1.9357
1.9217
1.9083
1.8952
1.8555
1.8422
1.8281
1.8148
1.8011
1.7522
1.7484
1.7428
1.7394
1.7326
1.7253
1.7185
1.7076
1.7005
1.6913

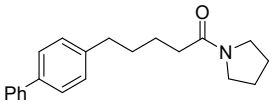

O
N
Ph

3am

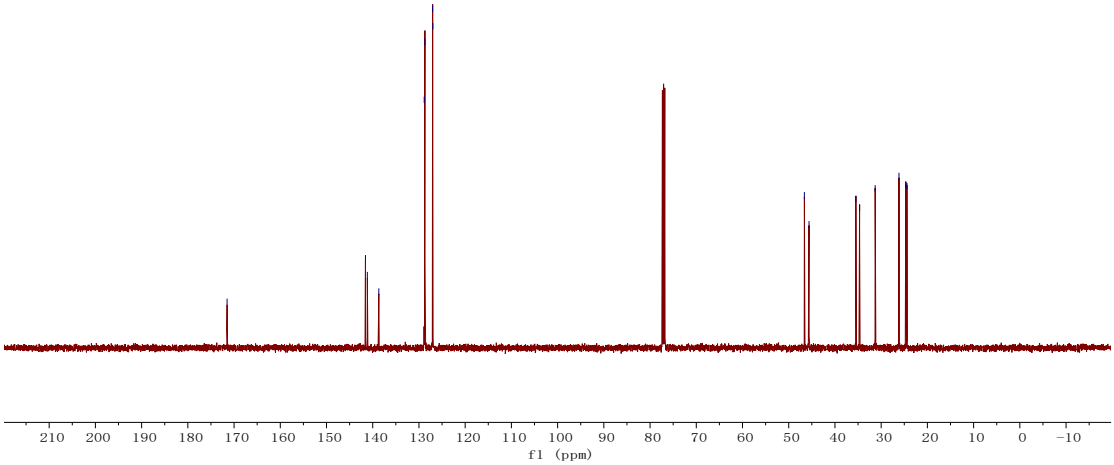

3.4672
3.4534
3.4397
3.3873
3.3738
3.3602
2.00
2.00
3.7
3.6
3.5
3.4
3.3
3.2
3.1
f1 (ppm)

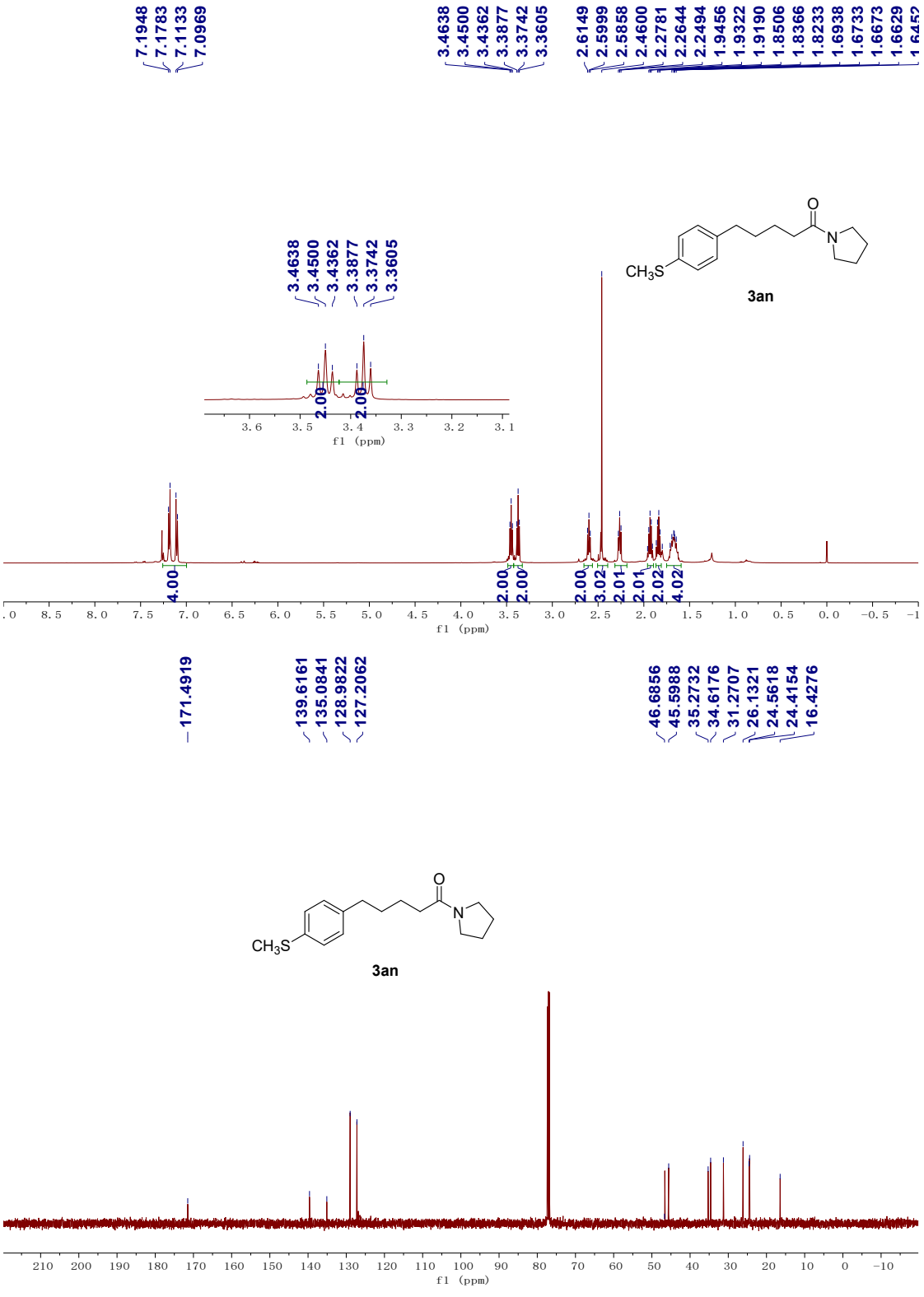

2.00
2.00
2.00
1.00
2.00
2.00
2.00
2.00
1.01
2.00
2.01
4.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

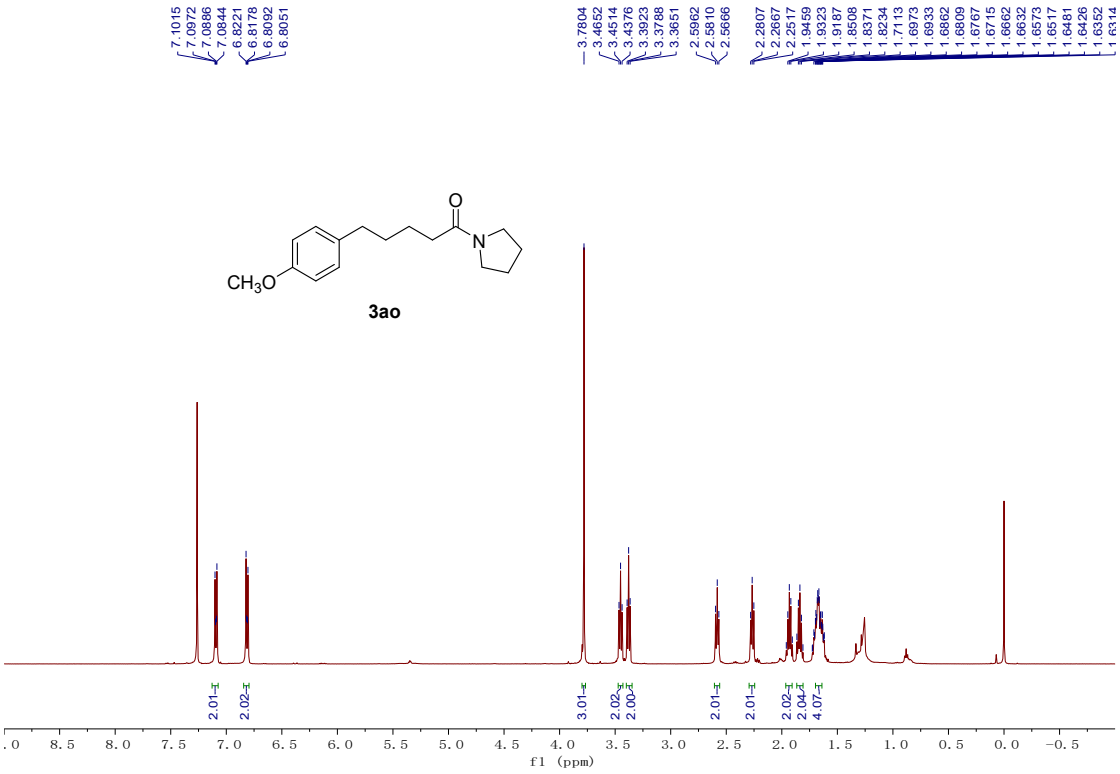

171.5092
141.5757
141.1665
138.6833
128.8610
128.7118
127.0376
126.9942
46.6130
45.6085
35.4721
34.6675
31.2992
26.1464
24.6711
24.4283

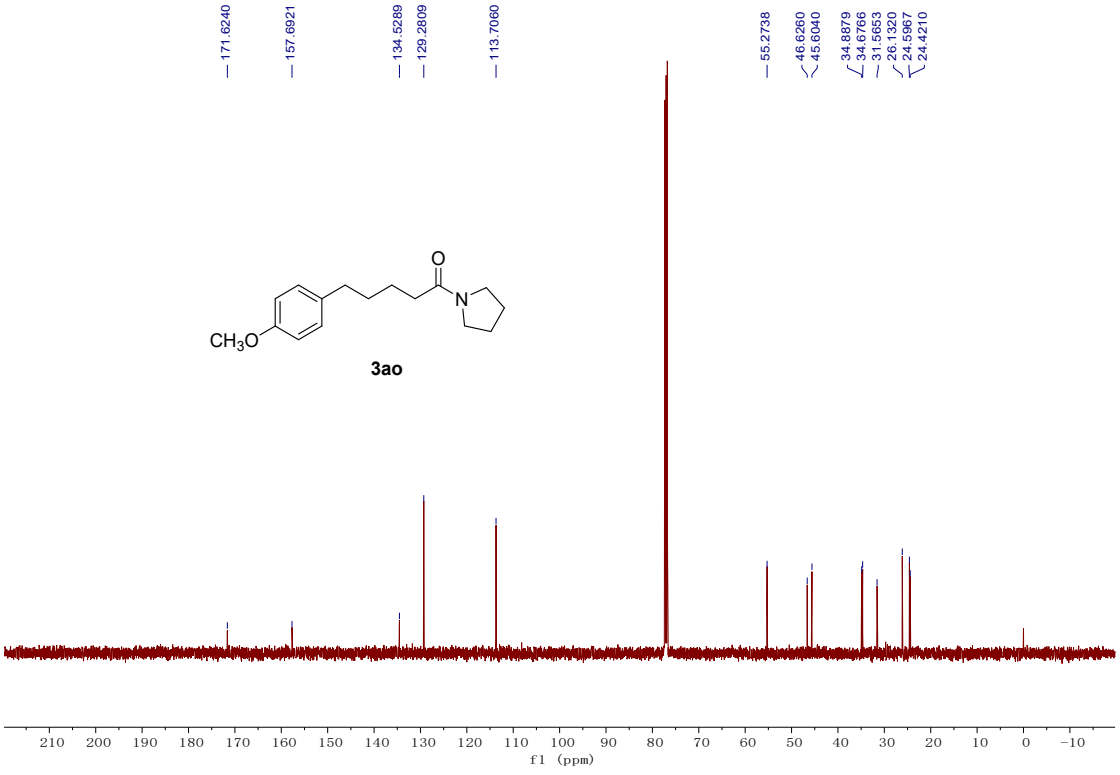

O
N
Ph

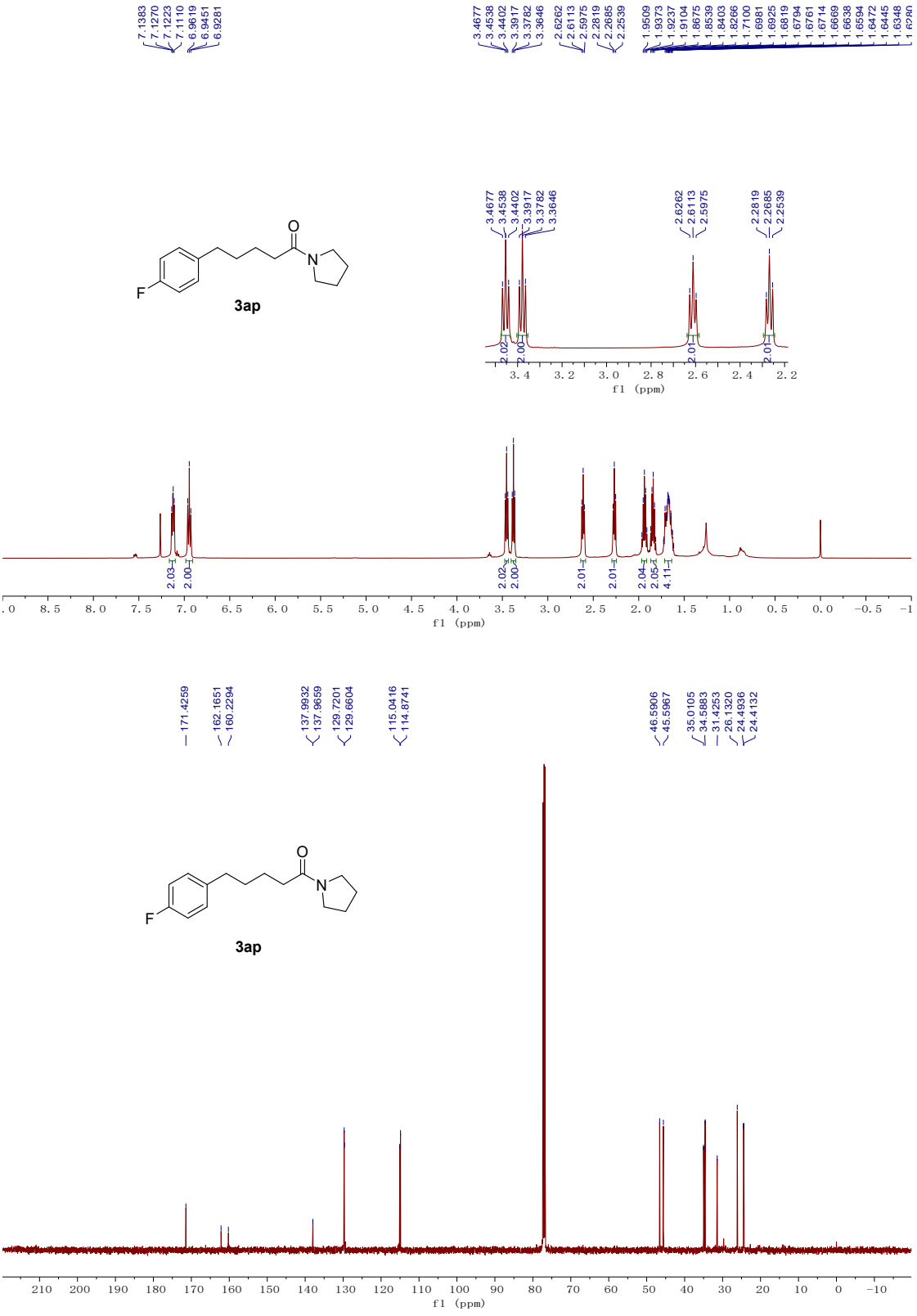
3am

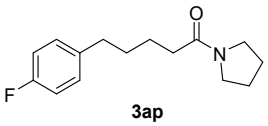

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


7.1948
7.1783
7.1133
7.0969
3.4638
3.4500
3.4362
3.3877
3.3742
3.3605
2.6149
2.5999
2.5858
2.4600
2.2781
2.2644
2.2494
1.9456
1.9322
1.9190
1.8506
1.8366
1.8233
1.6938
1.6733
1.6673
1.6629
1.6452
O
N
CH3S
3an
f1 (ppm)
4.00
2.00
2.00
2.00
3.02
2.01
2.01
2.02
4.02
171.4919
139.6161
135.0841
128.9822
127.2062
46.6856
45.5988
35.2732
34.6176
31.2707
26.1321
24.5618
24.4154
16.4276


7.1015
7.0972
7.0886
7.0844
6.8221
6.8178
6.8092
6.8051
3.7804
3.4652
3.4514
3.4376
3.3923
3.3788
3.3651
2.5962
2.5810
2.5666
2.2807
2.2667
2.2517
1.9459
1.9323
1.9187
1.8508
1.8371
1.8234
1.7113
1.6973
1.6933
1.6862
1.6809
1.6767
1.6715
1.6662
1.6632
1.6573
1.6517
1.6481
1.6426
1.6352
1.6314
O
N
CH3O
3ao
2.01
2.02
3.01
2.02
2.00
2.01
2.01
2.02
2.04
4.07
f1 (ppm)

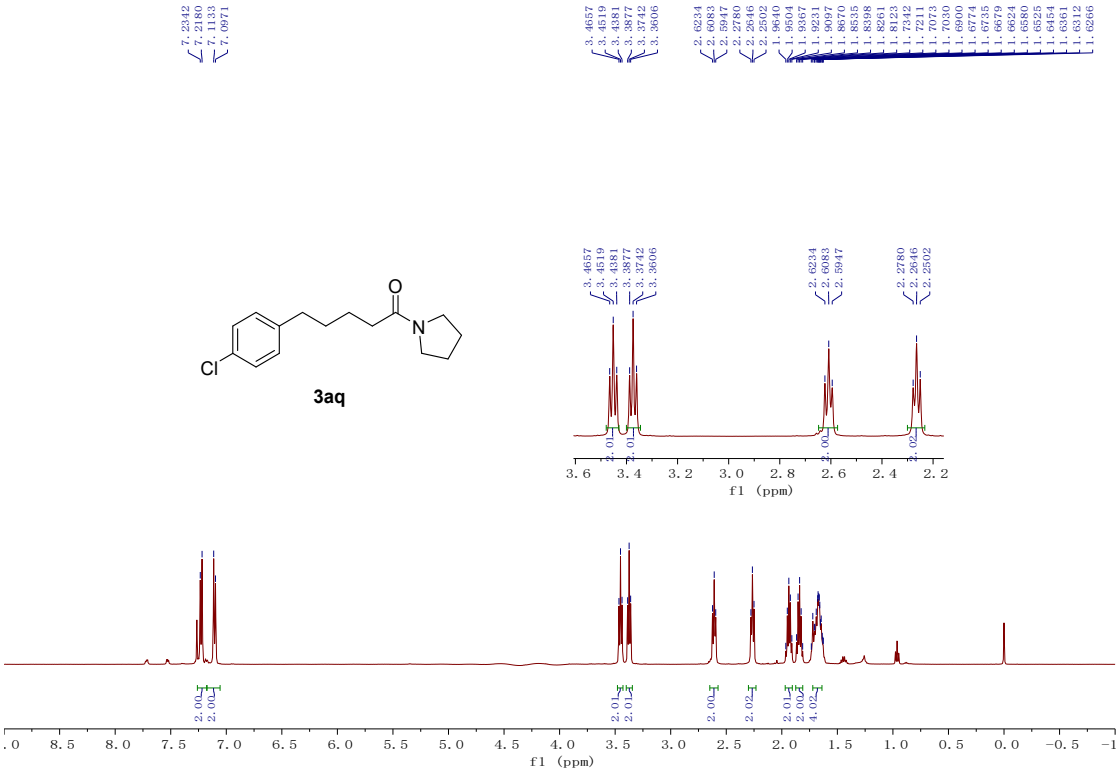

171.6240
157.6921
134.5289
129.2809
113.7060
55.2738
46.6260
45.6040
34.8879
34.6766
31.5653
26.1320
24.5967
24.4210
O
N
CH3O
3ao
f1 (ppm)

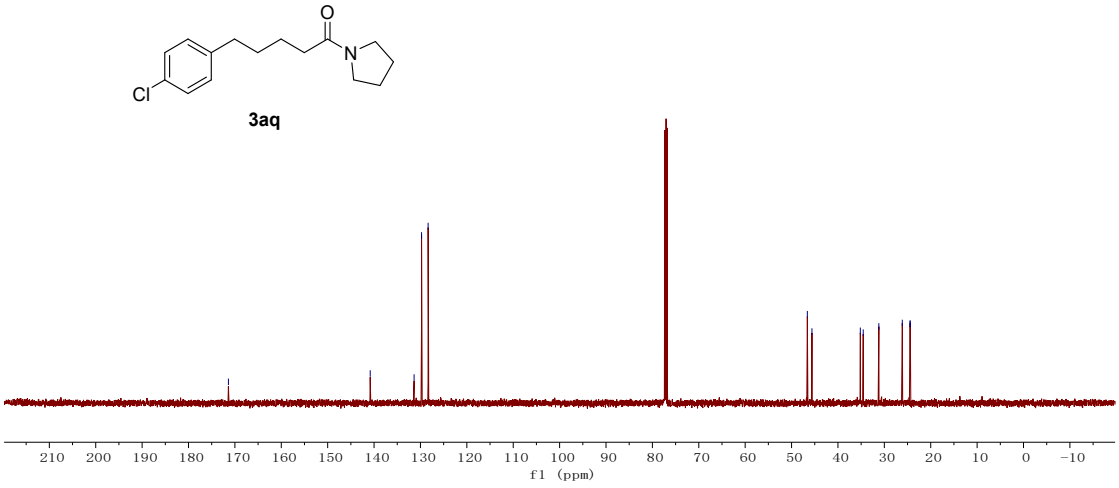

7.1383
7.1270
7.1223
7.1110
6.9619
6.9451
6.9281
3.4677
3.4538
3.4402
3.3917
3.3782
3.3646
2.6262
2.6113
2.5975
2.2819
2.2685
2.2539
1.9509
1.9373
1.9237
1.9104
1.8675
1.8539
1.8403
1.8266
1.7100
1.6981
1.6925
1.6819
1.6794
1.6761
1.6714
1.6669
1.6638
1.6594
1.6472
1.6445
1.6348
O
N
F
3ap
2.02
2.00
2.01
2.01
f1 (ppm)
2.03
2.00
2.02
2.00
2.01
2.01
2.04
2.05
4.11
f1 (ppm)
171.4259
162.1651
160.2294
137.9932
137.9659
129.7201
129.6604
115.0416
114.8741
46.5906
45.5967
35.0105
34.5883
31.4253
26.1320
24.4936
24.4132
O
N
F
3ap
f1 (ppm)


O
N
F

3ap

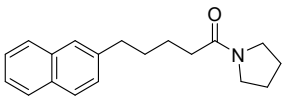
-118.0874
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)


7.2342
7.2180
7.1133
7.0971
3.4657
3.4519
3.4381
3.3877
3.3742
3.3606
2.6234
2.6083
2.5947
2.2780
2.2646
2.2502
1.9640
1.9504
1.9367
1.9231
1.8697
1.8550
1.8535
1.8398
1.8261
1.8123
1.7342
1.7211
1.7073
1.7030
1.6900
1.6774
1.6735
1.6679
1.6624
1.6580
1.6525
1.6454
1.6361
1.6312
1.6266
O
N
Cl
3aq
f1 (ppm)

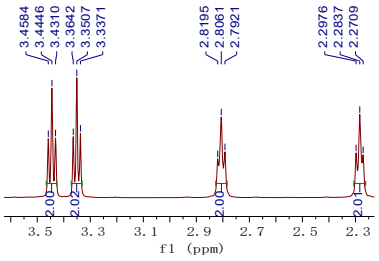

171.3961
140.8272
131.3698
129.7640
128.3458
46.5985
45.6064
35.1764
34.5500
31.1846
26.1267
24.4818
24.4087
O
N
Cl
3aq
f1 (ppm)

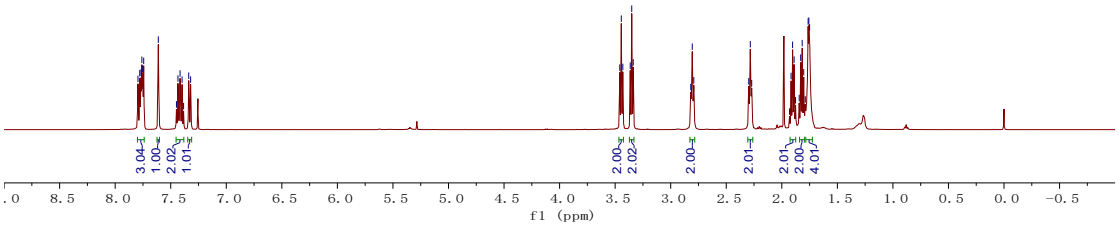

7.7948
7.7790
7.7678
7.7598
7.7521
7.7433
7.6119
7.4484
7.4349
7.4160
7.3979
7.3844
7.3380
7.3212


3.4584
3.4446
3.4310
3.3642
3.3507
3.3371
2.8195
2.8061
2.7921
2.2976
2.2837
2.2709
1.9301
1.9166
1.9029
1.8893
1.8761
1.8435
1.8302
1.8165
1.8029
1.7888
1.7631
1.7565
1.7498

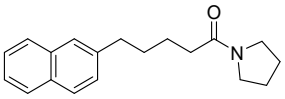

O
N

3ar


3.4584
3.4446
3.4310
3.3642
3.3507
3.3371
2.8195
2.8061
2.7921
2.2976
2.2837
2.2709
2.00
2.02
2.00
2.01
3.5
3.3
3.1
2.9
2.7
2.5
2.3
f1 (ppm)

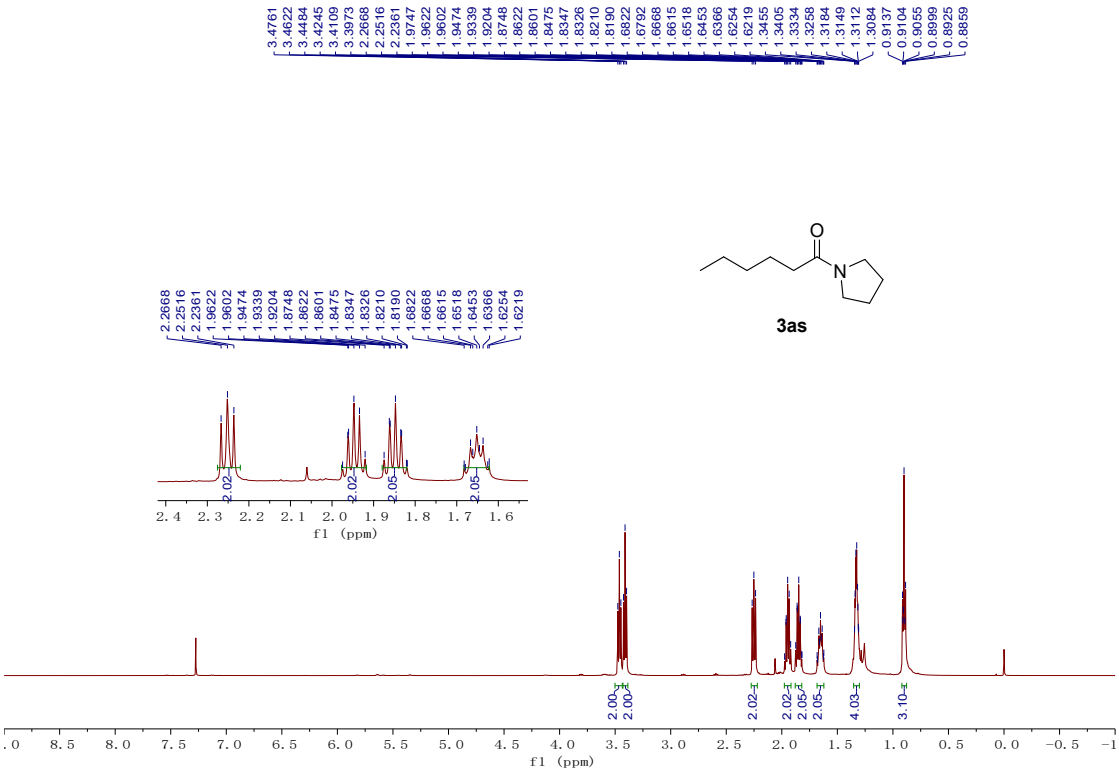

3.04
1.00
2.02
1.01
2.00
2.02
2.00
2.01
2.01
2.00
4.01
f1 (ppm)

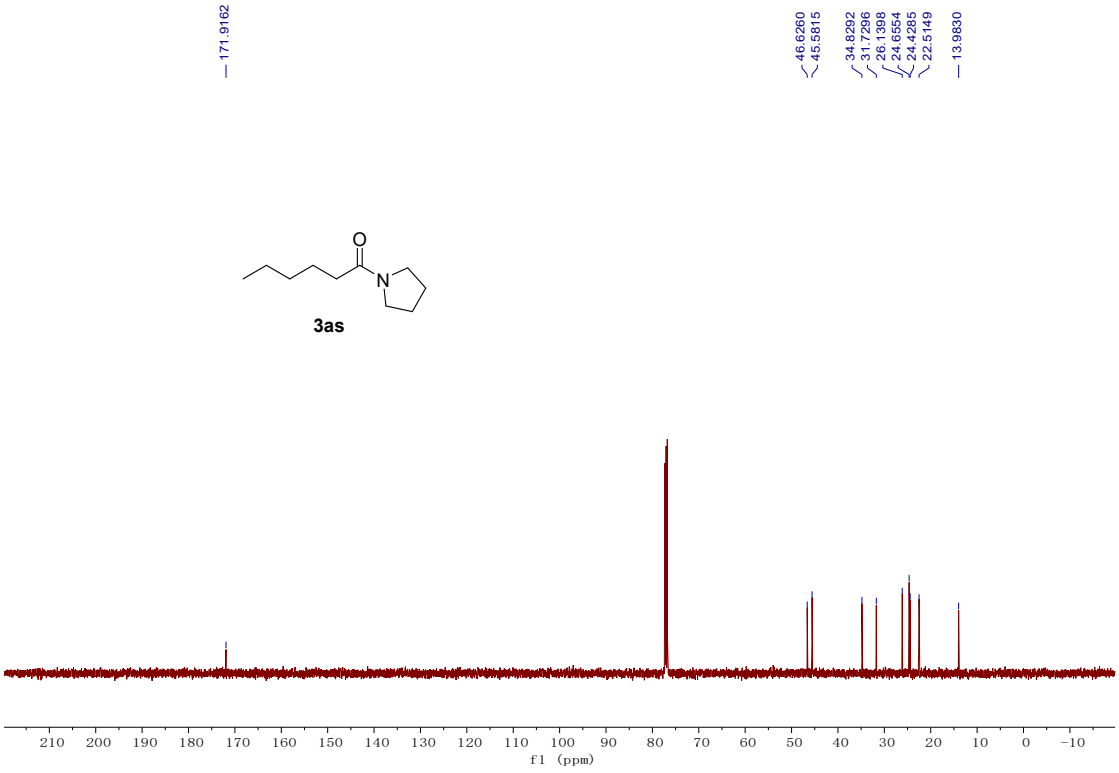

171.5386
139.9513
133.6308
131.9758
127.8057
127.5864
127.4155
127.3885
126.3835
125.8409
125.0504
46.6117
45.6047
35.9993
34.6676
31.2047
26.1167
24.6936
24.4074


O
N

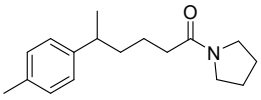
3ar

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)


3.4761
3.4622
3.4484
3.4245
3.4109
3.3973
2.2668
2.2516
2.2361
1.9747
1.9622
1.9602
1.9474
1.9339
1.9204
1.8748
1.8622
1.8601
1.8475
1.8347
1.8326
1.8210
1.8190
1.6822
1.6792
1.6668
1.6615
1.6518
1.6453
1.6366
1.6254
1.6219
1.3455
1.3405
1.3334
1.3258
1.3184
1.3149
1.3112
1.3084
0.9137
0.9104
0.9055
0.8999
0.8925
0.8859
O
N
3as
2.02
2.02
2.05
2.05
2.00
2.00
2.02
2.02
2.05
2.05
4.03
3.10
f1 (ppm)


171.9162
46.6260
45.5815
34.8292
31.7296
26.1398
24.6554
24.4285
22.5149
13.9830
O
N
3as
f1 (ppm)

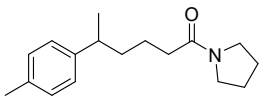

7.0993
7.0886
7.0823
7.0787
7.0728
7.0615
3.4427
3.4290
3.4153
3.3396
3.3259
3.3123
2.6916
2.6776
2.6711
2.6636
2.6572
2.6499
2.3074
2.2137
2.2116
2.2075
2.2037
2.1979
2.1838
1.9386
1.9366
1.9252
1.9229
1.9118
1.9096
1.8968
1.8843
1.8825
1.8483
1.8465
1.8349
1.8324
1.8202
1.8074
1.8051
1.7937
1.7916
1.6615
1.6598
1.6478
1.6453
1.6310
1.6267
1.6230
1.6193
1.6163
1.6103
1.6053
1.6010
1.5967
1.5832
1.5804
1.5487
1.5415
1.5347
1.5322
1.5280
1.5255
1.5125
1.5079
1.5051
1.5020
1.4974
1.4917
1.2349
1.2210


O
N

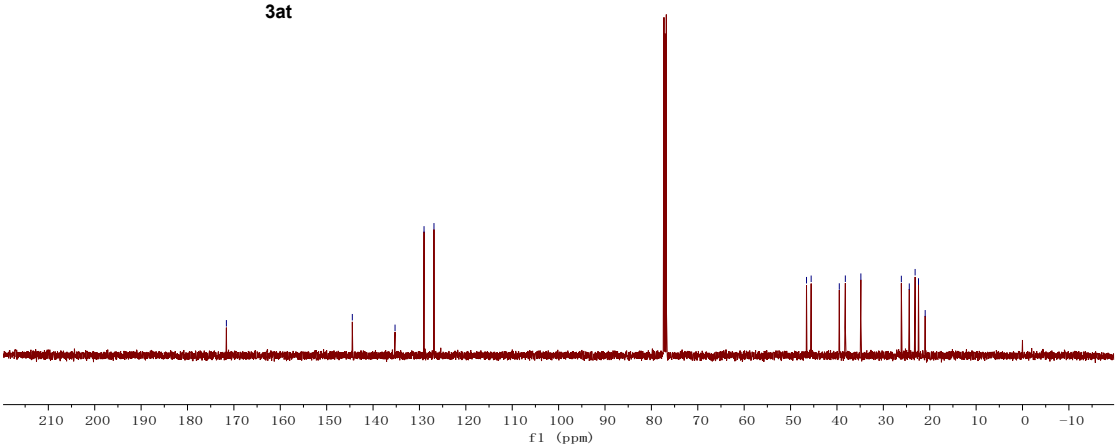
3at

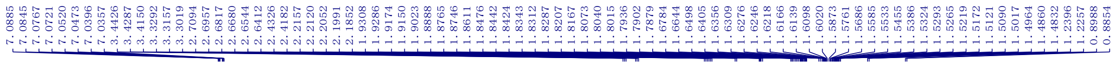
3.4427
3.4290
3.4153
3.3396
3.3259
3.3123
2.01
2.00
3.50 3.45 3.40 3.35 3.30 3.25 3.20
f1 (ppm)
4.00
2.01
2.00
1.00
3.00
2.01
2.01
2.00
3.00
1.00
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5
f1 (ppm)

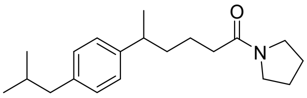

171.6165
144.4700
135.2610
129.0111
126.8689
46.5615
45.5602
39.4939
38.1923
34.8444
26.1175
24.4062
23.1498
22.4184
20.9797


O
N

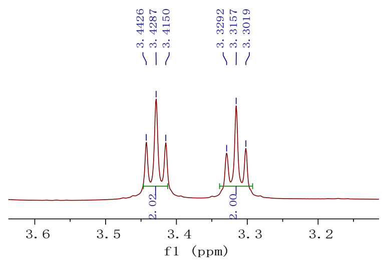
3at

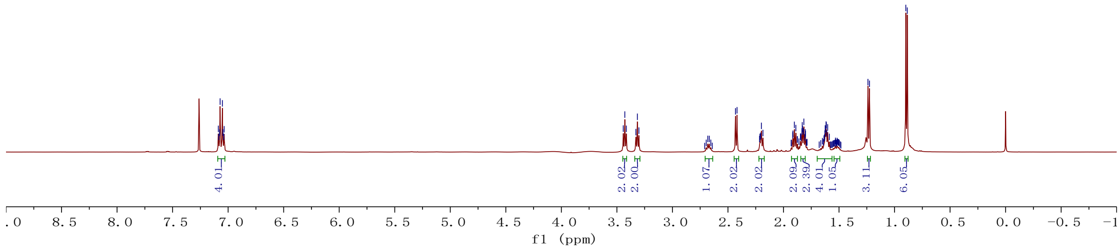

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


7.0885
7.0845
7.0767
7.0721
7.0520
7.0473
7.0396
7.0357
3.4426
3.4287
3.4150
3.3292
3.3157
3.3019
2.7094
2.6957
2.6817
2.6680
2.6544
2.6412
2.4326
2.4182
2.2157
2.2120
2.2052
2.1991
2.1852
1.9308
1.9286
1.9174
1.9150
1.9023
1.8888
1.8765
1.8746
1.8611
1.8476
1.8442
1.8424
1.8343
1.8312
1.8287
1.8207
1.8167
1.8073
1.8040
1.8015
1.7936
1.7902
1.7879
1.6784
1.6644
1.6498
1.6405
1.6356
1.6309
1.6276
1.6246
1.6218
1.6166
1.6139
1.6098
1.6020
1.5873
1.5761
1.5686
1.5585
1.5533
1.5455
1.5386
1.5324
1.5293
1.5265
1.5219
1.5172
1.5121
1.5090
1.5017
1.4964
1.4860
1.4832
1.2396
1.2257
0.8988
0.8854

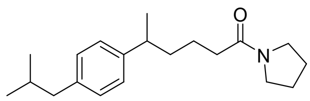

O
N

3au

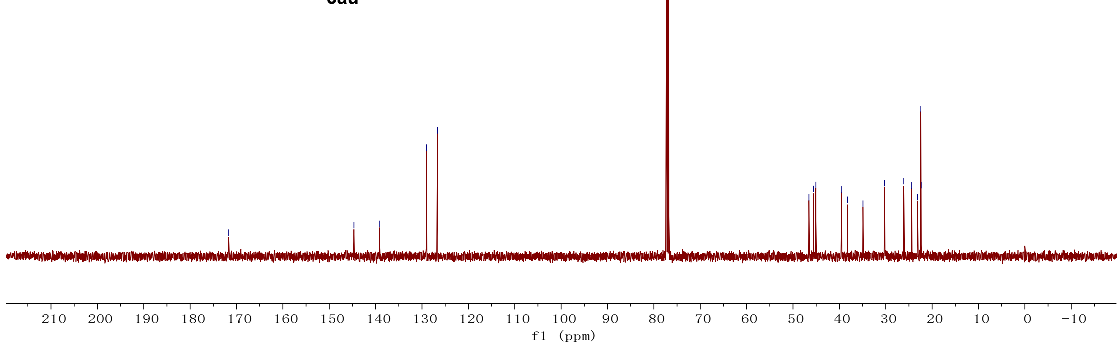

3.4426
3.4287
3.4150
3.3292
3.3157
3.3019
2.02
2.00
3.6
3.5
3.4
3.3
3.2
f1 (ppm)


4.01
2.02
2.00
1.07
2.02
2.02
2.09
2.39
4.01
1.05
3.11
6.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

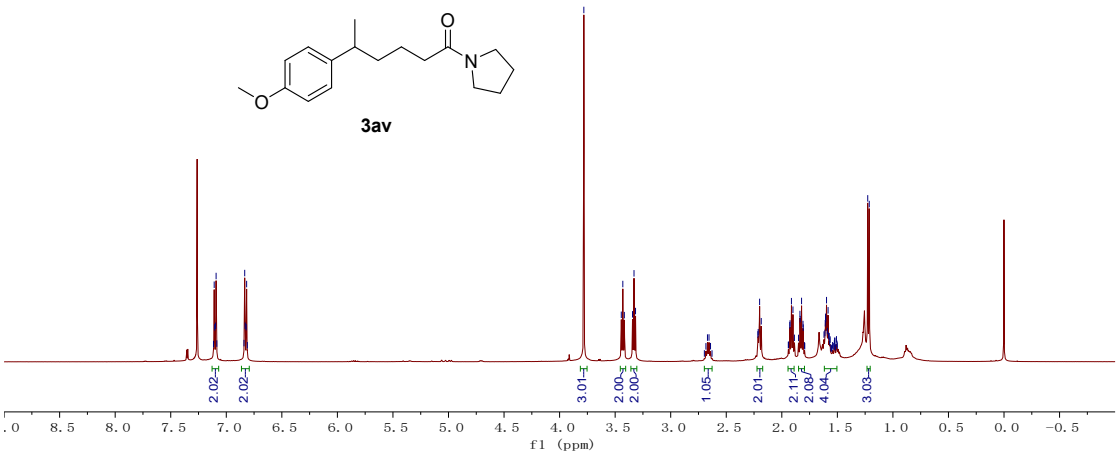

171.6756
144.6742
139.1056
129.0266
126.6575
46.5601
45.5602
45.0628
39.4867
38.2216
34.9091
30.2323
26.1101
24.3992
23.1488
22.4333
22.3602


O
N

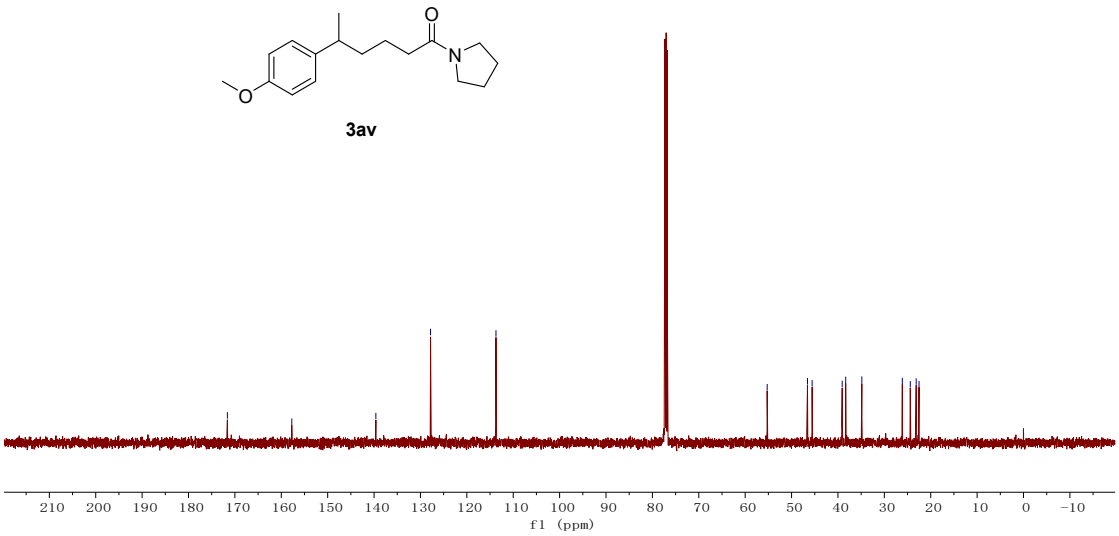
3au

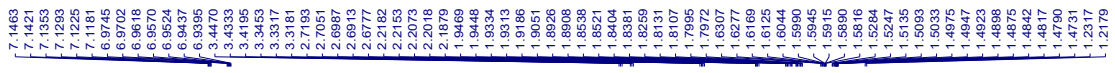

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

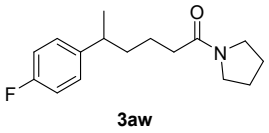

7.1152
7.1089
7.1046
7.0960
7.0917
7.0854
6.8405
6.8342
6.8299
6.8212
6.8169
6.8106
3.7818
3.4448
3.4310
3.4173
3.3438
3.3302
3.3165
2.6970
2.6830
2.6691
2.6553
2.6416
2.6281
2.2155
2.2124
2.1998
2.1850
1.9414
1.9394
1.9280
1.9259
1.9133
1.8997
1.8867
1.8494
1.8368
1.8345
1.8223
1.8093
1.8071
1.7957
1.7935
1.6202
1.6122
1.6090
1.6065
1.6045
1.5975
1.5902
1.5836
1.5789
1.5729
1.5692
1.5647
1.5583
1.5540
1.5492
1.5428
1.5378
1.5301
1.5272
1.5244
1.5219
1.5168
1.5081
1.5032
1.5010
1.2266
1.2129


O
N
O
3av
2.02
2.02
3.01
2.00
2.00
1.05
2.01
2.11
2.08
4.04
3.03
f1 (ppm)

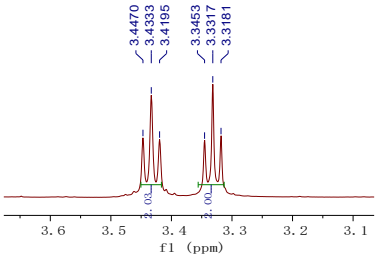

171.6177
157.7324
139.6125
127.8266
113.7202
55.2582
46.5684
45.5668
39.0848
38.3304
34.8510
26.1237
24.4062
23.1335
22.5232

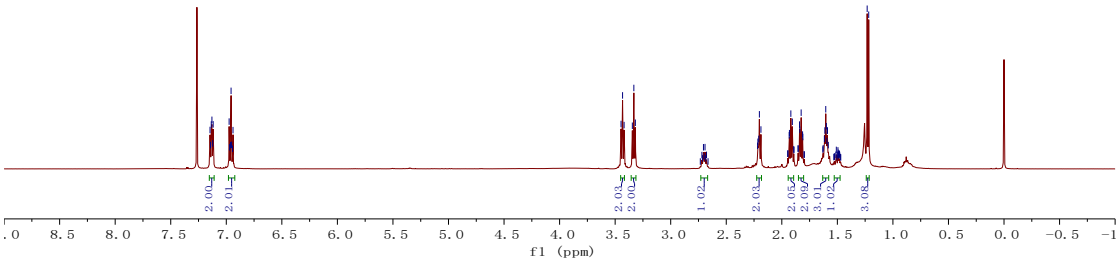

O
N
O
3av
f1 (ppm)




O
N
F

3aw

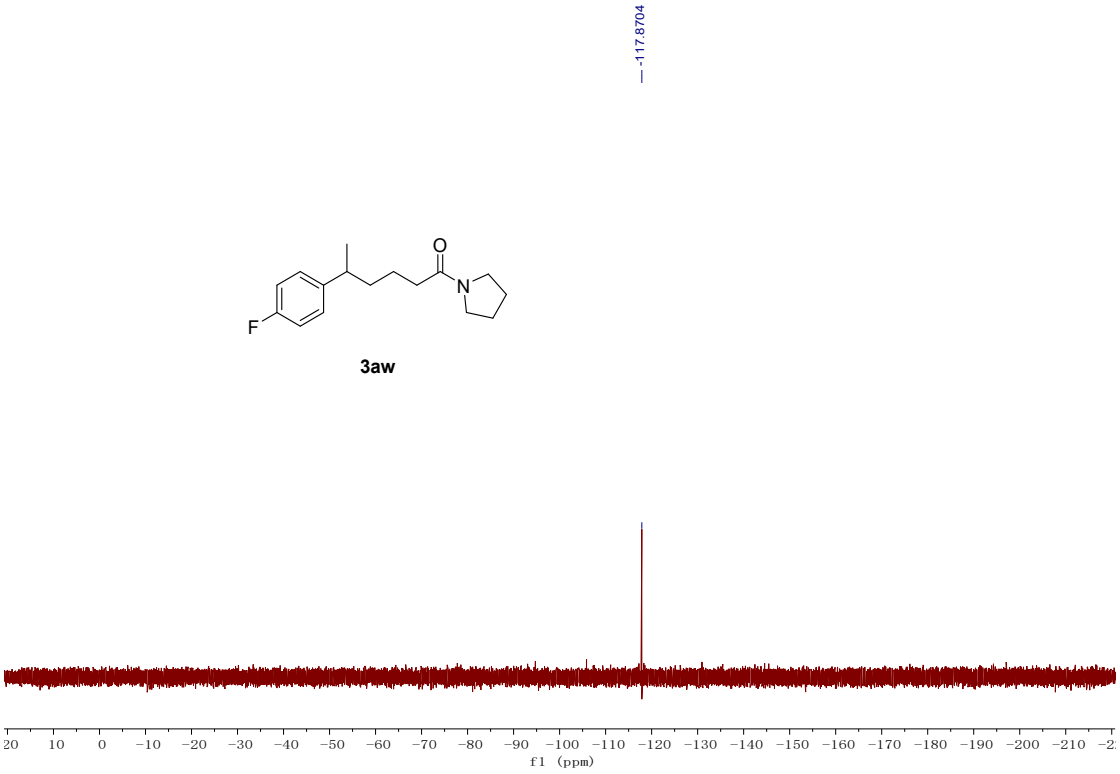

3.4470
3.4333
3.4195
3.3453
3.3317
3.3181
2.03
2.00
3.6
3.5
3.4
3.3
3.2
3.1
f1 (ppm)

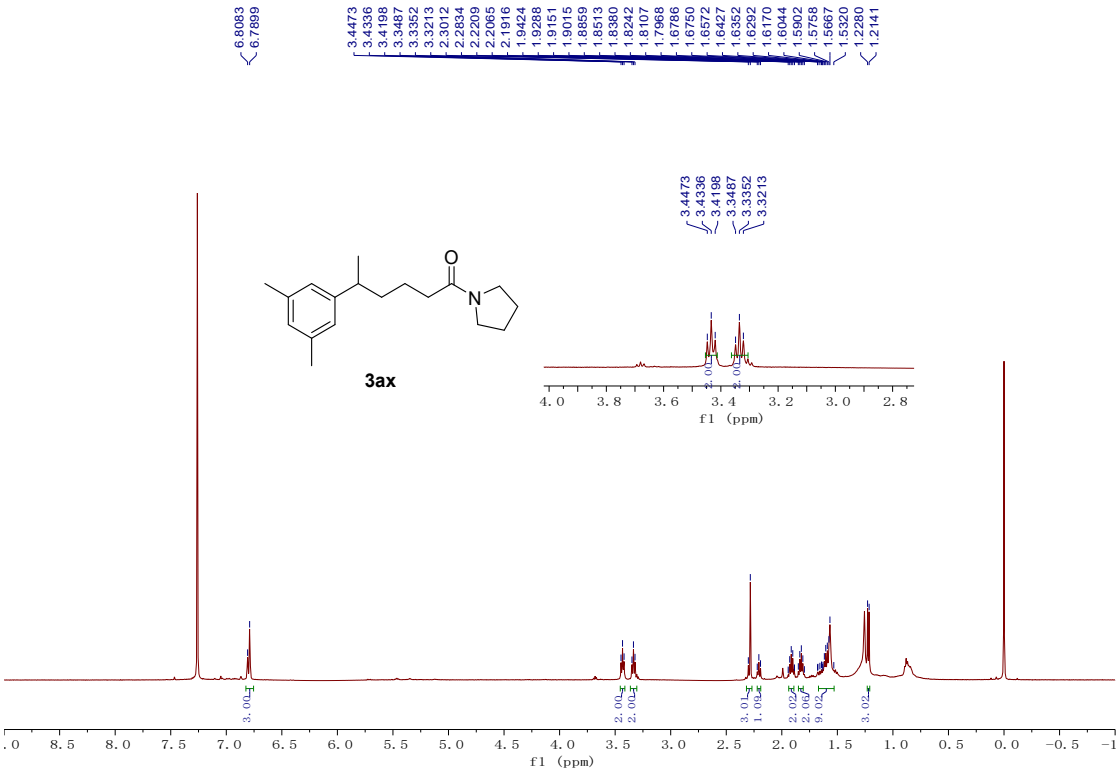

2.00
2.01
2.01
2.00
1.02
2.03
2.05
2.09
3.01
1.02
3.08
f1 (ppm)

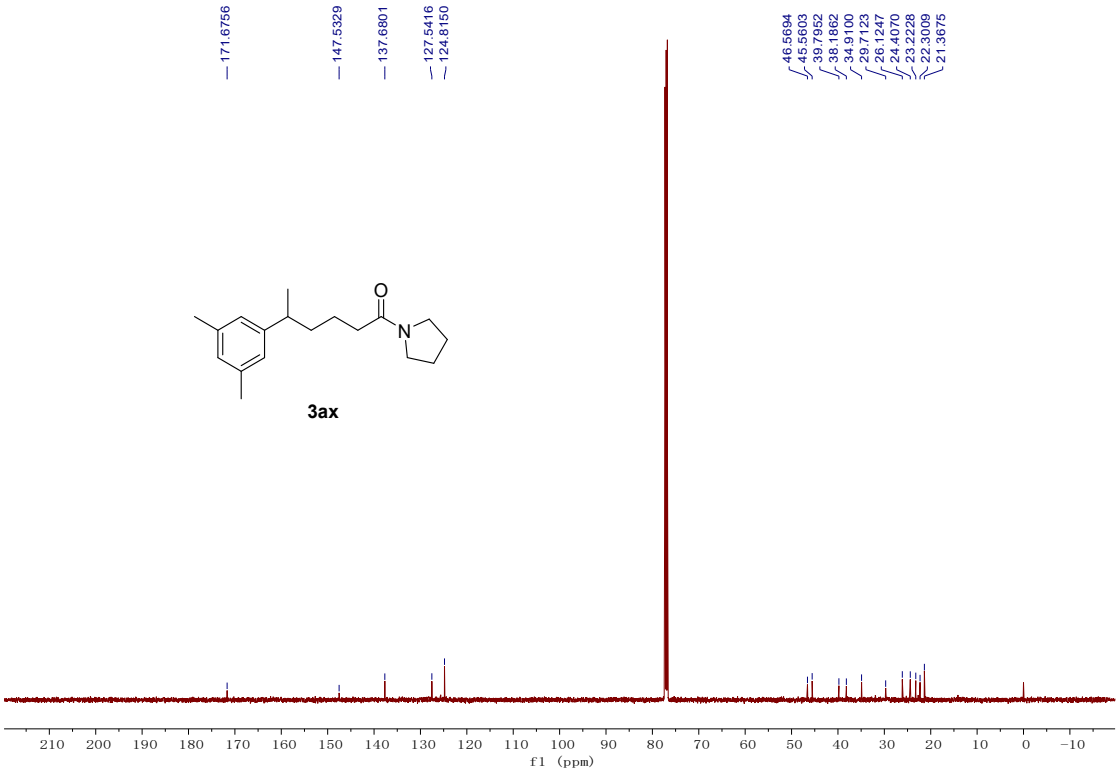

O
N
F

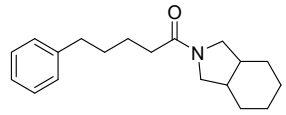
3aw

171.4315
162.1053
160.1722
143.0189
142.9938
128.2502
128.1886
115.0372
114.8718
46.5180
45.5430
39.2538
38.1960
34.7105
26.0750
24.3575
22.9900
22.4338
f1 (ppm)

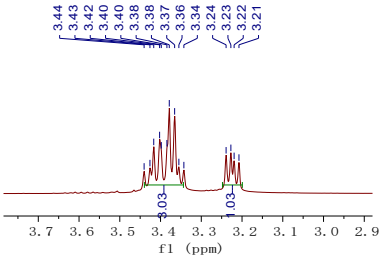

-117.8704
O
N
F
3aw
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)

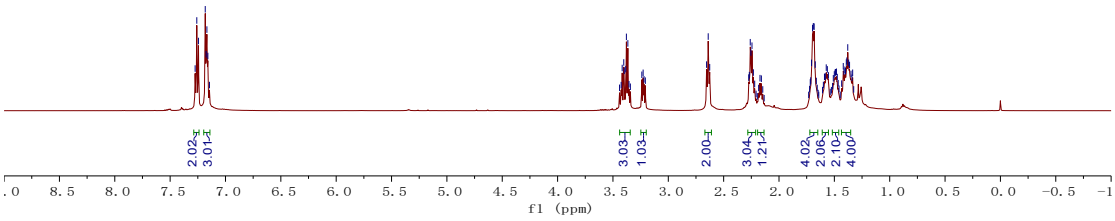

6.8083
6.7899
3.4473
3.4336
3.4198
3.3487
3.3352
3.3213
3.4473
3.4336
3.4198
3.3487
3.3352
3.3213
O
N
3ax
f1 (ppm)
f1 (ppm)

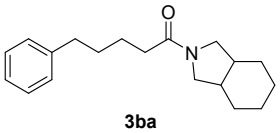

171.6756
147.5329
137.6801
127.5416
124.8150
46.5694
45.5603
39.7952
38.1862
34.9100
29.7123
26.1247
24.4070
23.2228
22.3009
21.3675
O
N
3ax
f1 (ppm)



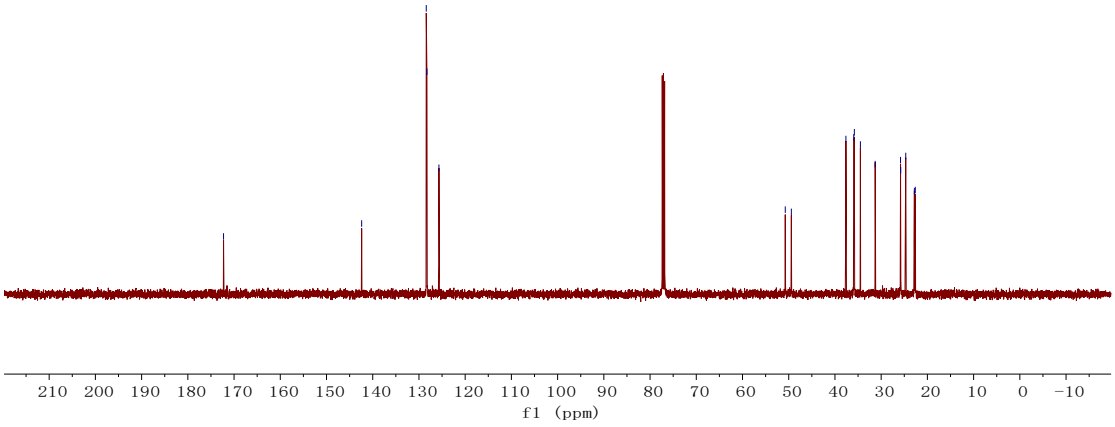
3ba

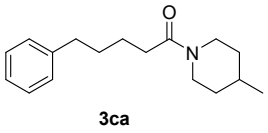




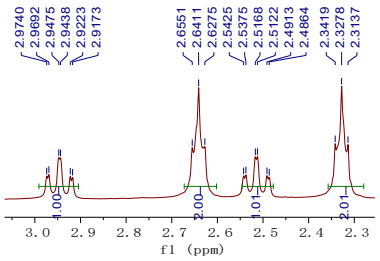


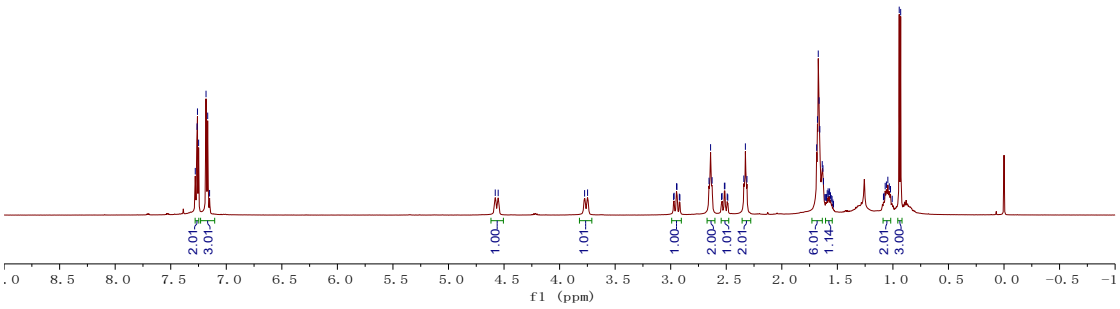
3ba

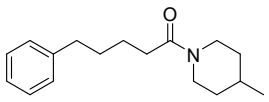




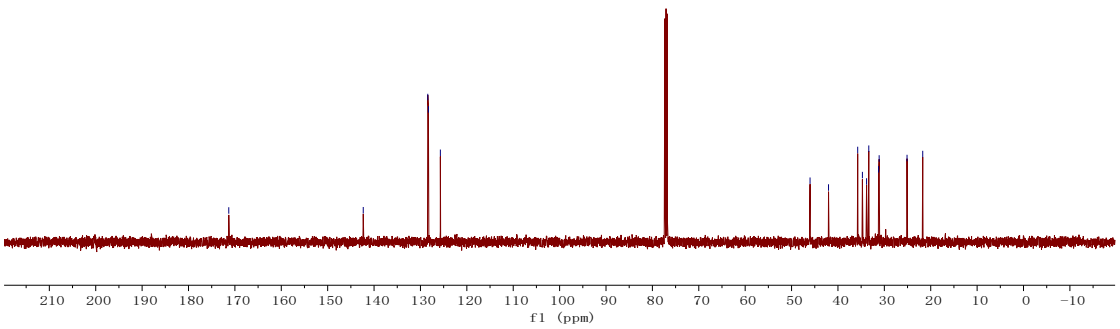
3ca

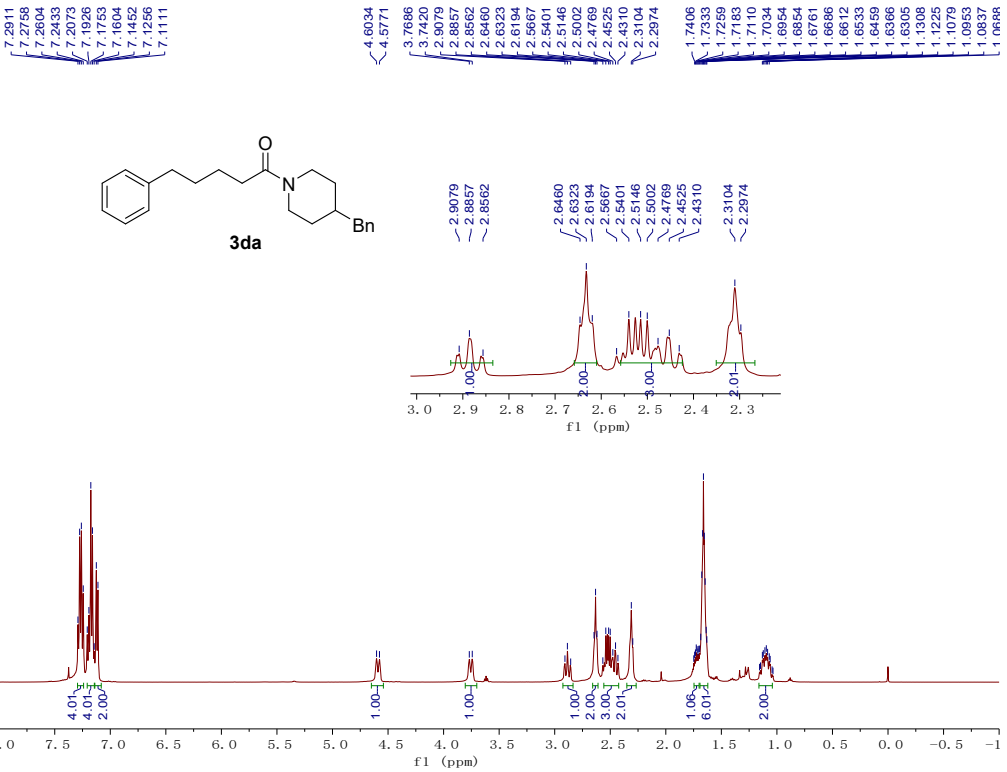


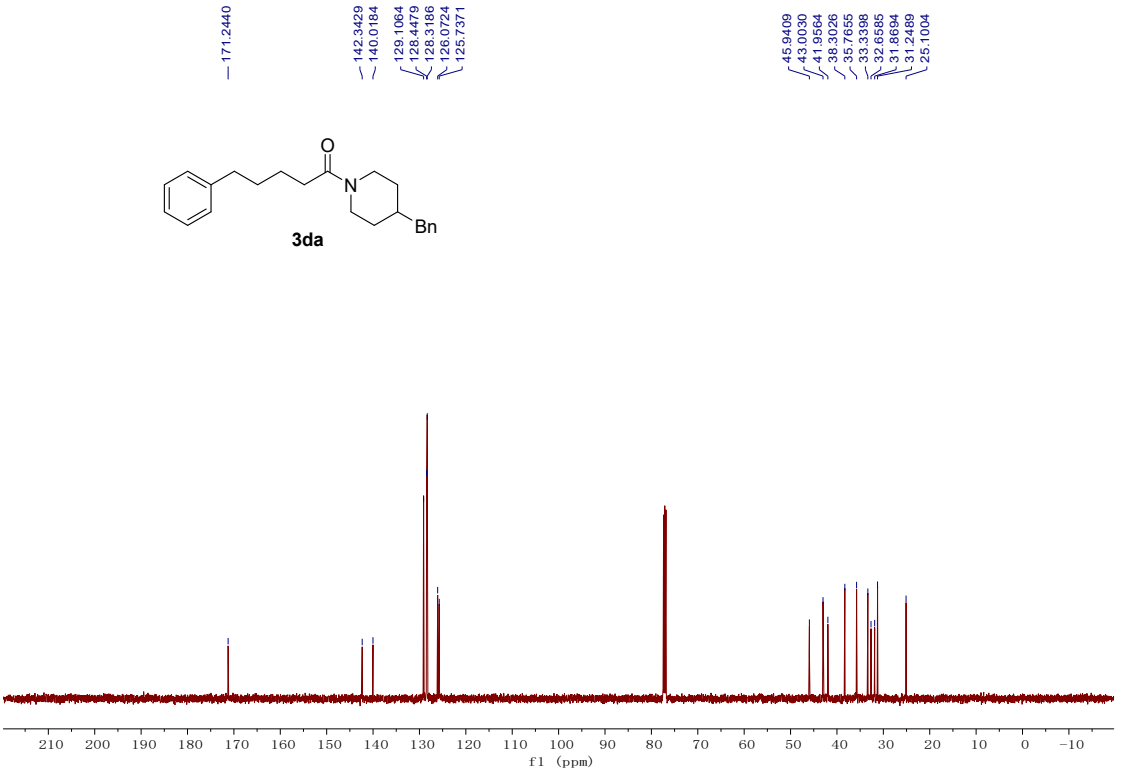


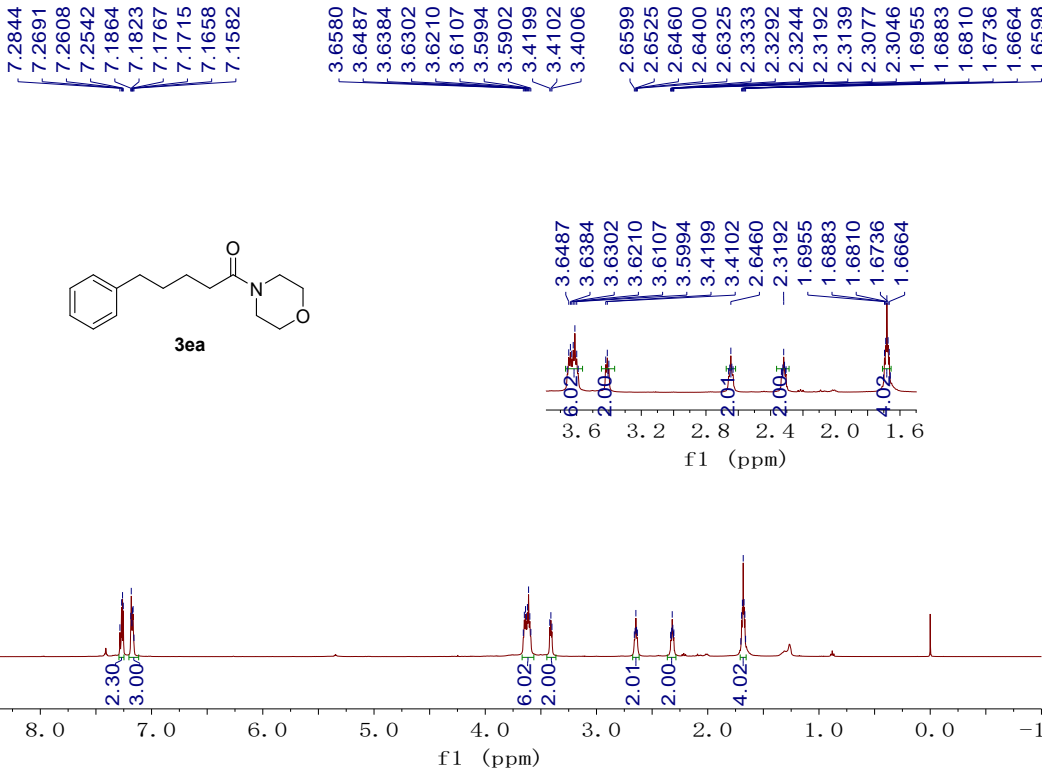


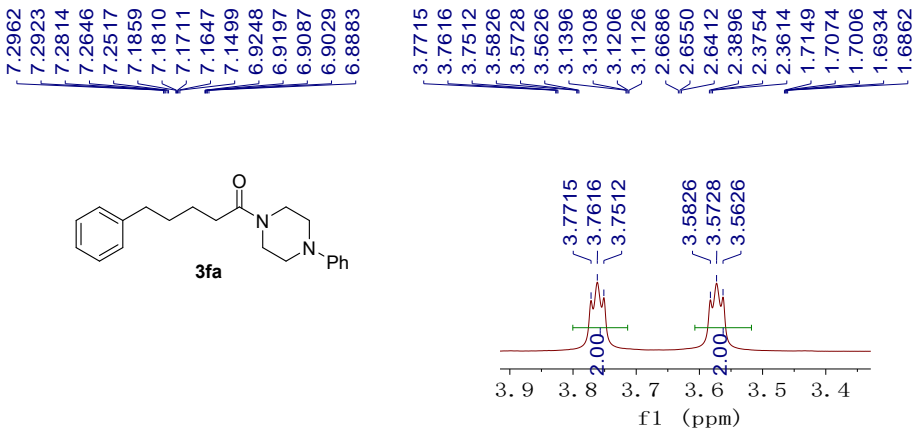
3ca

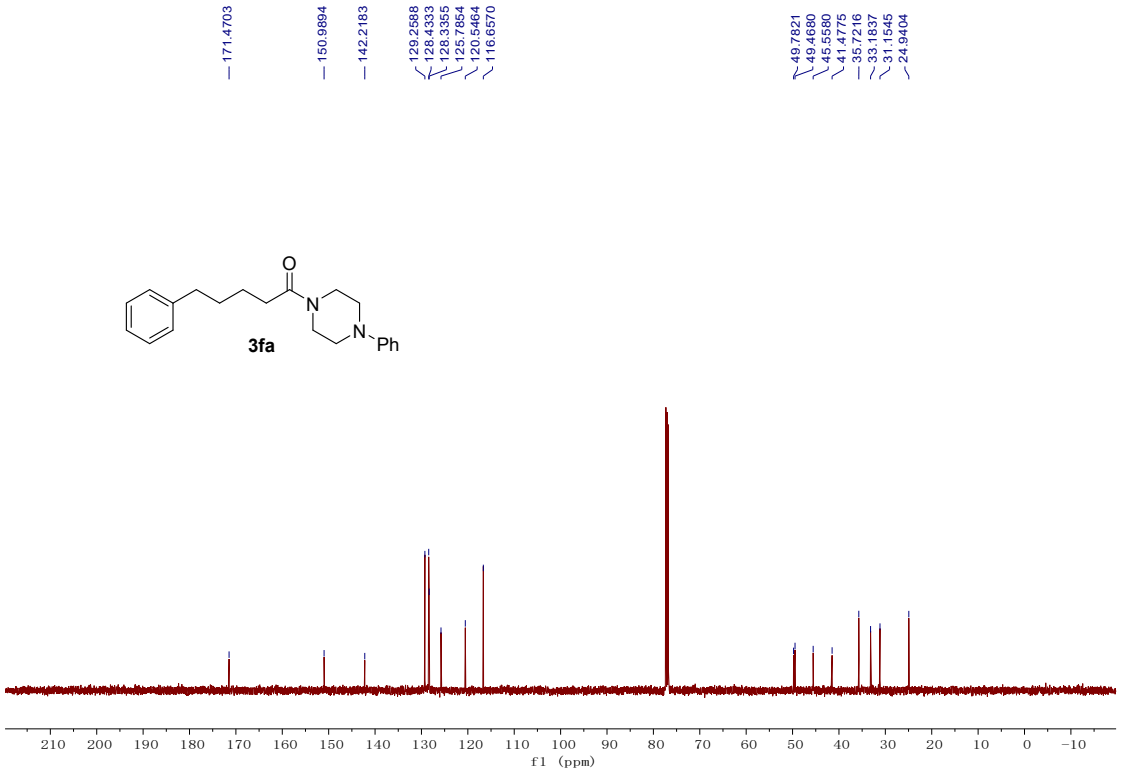



7.2911
7.2758
7.2604
7.2433
7.2073
7.1926
7.1753
7.1604
7.1452
7.1256
7.1111
4.6034
4.5771
3.7686
3.7420
2.9079
2.8857
2.8562
2.6460
2.6323
2.6194
2.5667
2.5401
2.5146
2.5002
2.4769
2.4525
2.4310
2.3104
2.2974
1.7406
1.7333
1.7259
1.7183
1.7110
1.7034
1.6954
1.6854
1.6761
1.6686
1.6612
1.6533
1.6459
1.6366
1.6305
1.1308
1.1225
1.1079
1.0953
1.0837
O
N
Bn
3da
2.9079
2.8857
2.8562
2.6460
2.6323
2.6194
2.5667
2.5401
2.5146
2.5002
2.4769
2.4525
2.4310
2.3104
2.2974
1.00
2.00
3.00
2.01
f1 (ppm)
4.01
4.01
2.00
1.00
1.00
1.00
2.00
3.00
2.01
1.06
6.01
2.00
f1 (ppm)

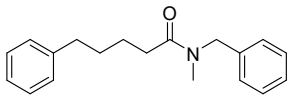

171.2440
142.3429
140.0184
129.1064
128.4479
128.3186
126.0724
125.7371
45.9409
43.0030
41.9564
38.3026
35.7655
33.3398
32.6585
31.8694
31.2489
25.1004
O
N
Bn
3da
f1 (ppm)


7.2844
7.2691
7.2608
7.2542
7.1864
7.1823
7.1767
7.1715
7.1658
7.1582
3.6580
3.6487
3.6384
3.6302
3.6210
3.6107
3.5994
3.5902
3.4199
3.4102
3.4006
2.6599
2.6525
2.6460
2.6400
2.6325
2.3333
2.3292
2.3244
2.3192
2.3139
2.3077
2.3046
1.6955
1.6883
1.6810
1.6736
1.6664
1.6598
O
N
O
3ea
3.6487
3.6384
3.6302
3.6210
3.6107
3.5994
3.4199
3.4102
2.6460
2.3192
1.6955
1.6883
1.6810
1.6736
1.6664
6.02
2.00
2.01
2.00
4.02
3.6 3.2 2.8 2.4 2.0 1.6
f1 (ppm)
2.30
3.00
6.02
2.00
2.01
2.00
4.02
8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)
171.5952
142.1819
128.4121
128.3236
125.7829
66.9602
66.6611
46.0276
41.8840
35.6993
32.9671
31.1248
24.8292
O
N
O
3ea
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

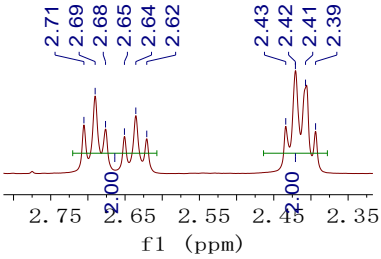

7.2962
7.2923
7.2814
7.2646
7.2517
7.1859
7.1810
7.1711
7.1647
7.1499
6.9248
6.9197
6.9087
6.9029
6.8883
3.7715
3.7616
3.7512
3.5826
3.5728
3.5626
3.1396
3.1308
3.1206
3.1126
2.6686
2.6550
2.6412
2.3896
2.3754
2.3614
1.7149
1.7074
1.7006
1.6934
1.6862
O
N
N
Ph
3fa
3.7715
3.7616
3.7512
3.5826
3.5728
3.5626
2.00
2.00
3.9 3.8 3.7 3.6 3.5 3.4
f1 (ppm)
4.01
3.01
3.00
2.00
2.00
4.00
2.00
2.02
4.02
8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)

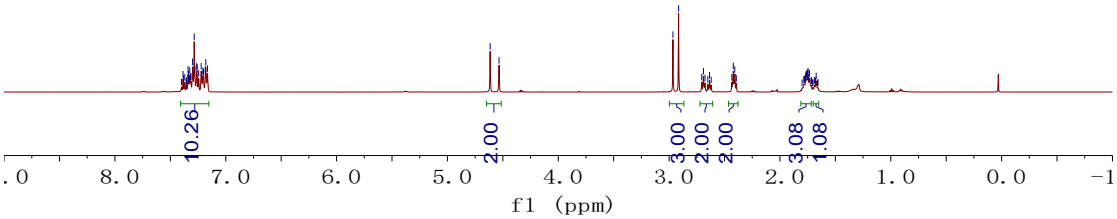

171.4703
150.9894
142.2183
129.2588
128.4333
128.3355
125.7854
120.5464
116.6570
49.7821
49.4680
45.5580
41.4775
35.7216
33.1837
31.1545
24.9404
O
N
N
Ph
3fa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

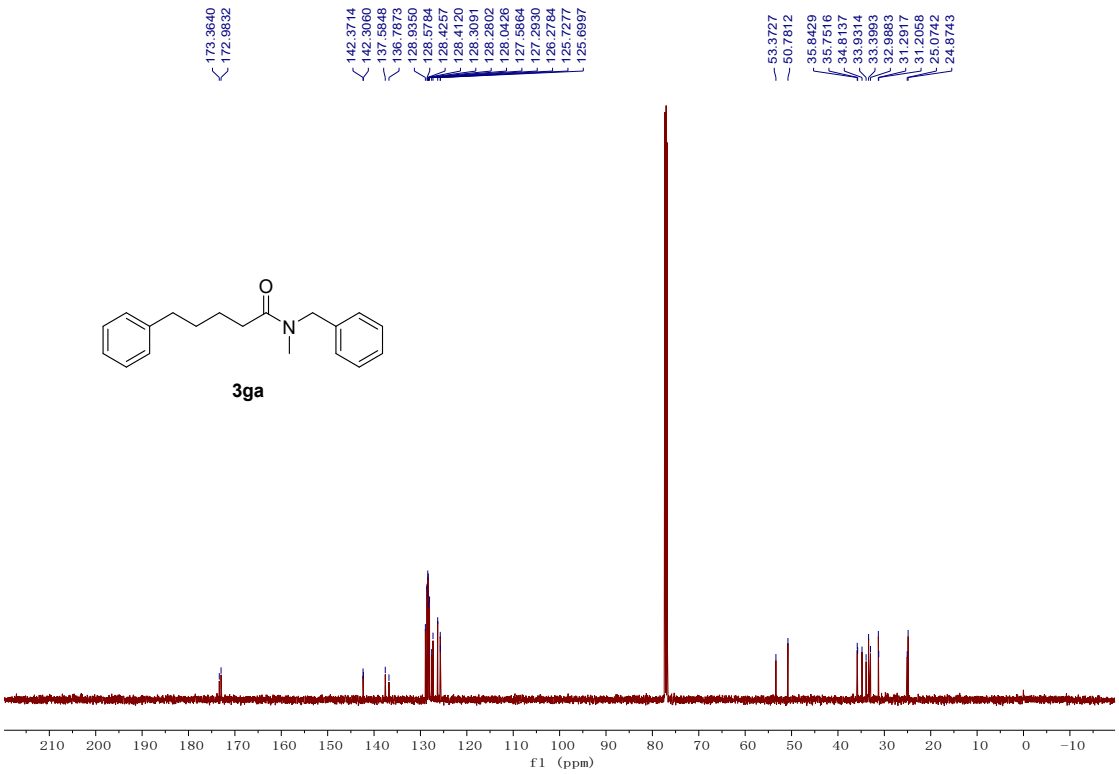

7.39
7.38
7.37
7.34
7.34
7.33
7.33
7.32
7.31
7.30
7.28
7.28
7.26
7.26
7.24
7.22
7.22
7.21
7.20
7.18
7.18
7.17
4.61
4.53
2.97
2.91
2.71
2.69
2.68
2.65
2.64
2.43
2.42
2.41
2.39
1.78
1.77
1.77
1.76
1.76
1.75
1.75
1.74
1.73
1.67


O
N

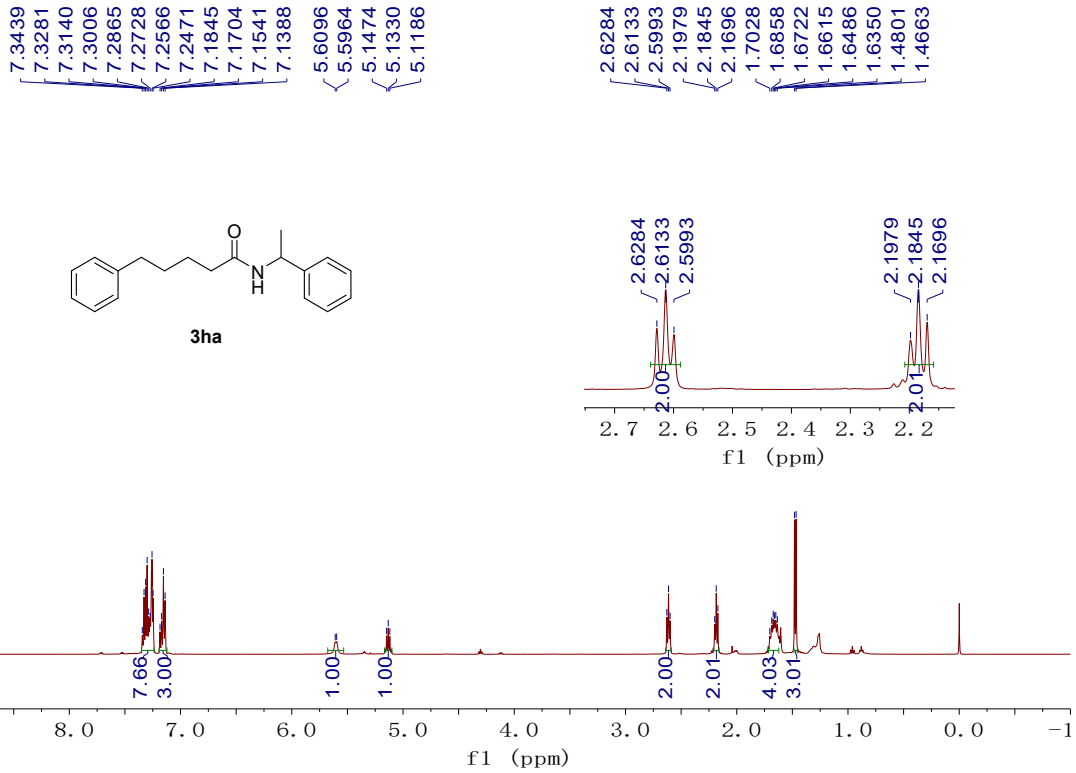
3ga

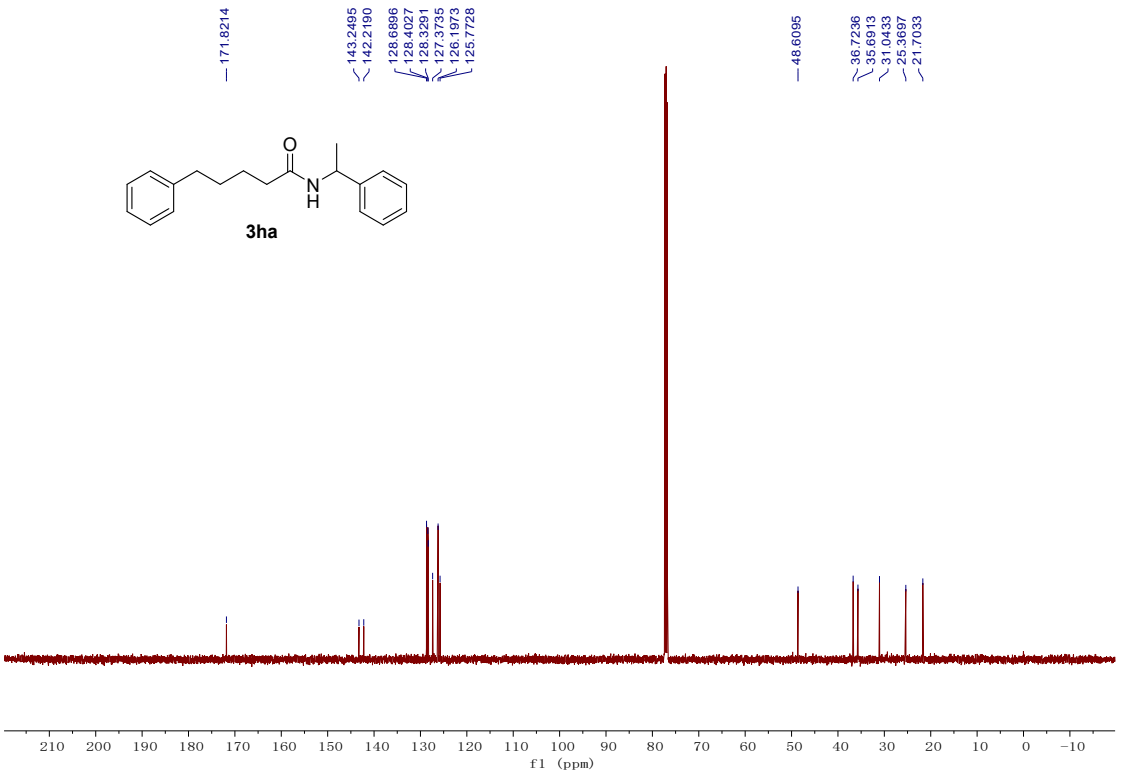

2.71
2.69
2.68
2.65
2.64
2.62
2.43
2.42
2.41
2.39
2.00
2.00
2.75
2.65
2.55
2.45
2.35
f1 (ppm)

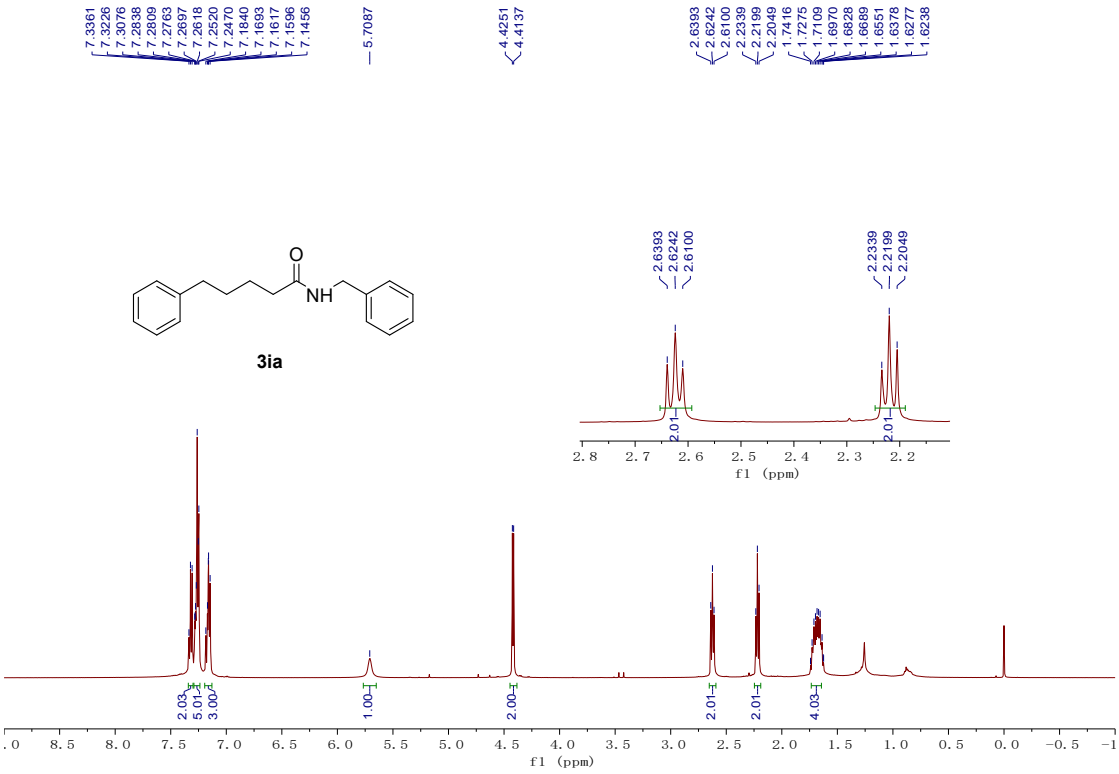

10.26
2.00
3.00
2.00
2.00
3.08
1.08
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

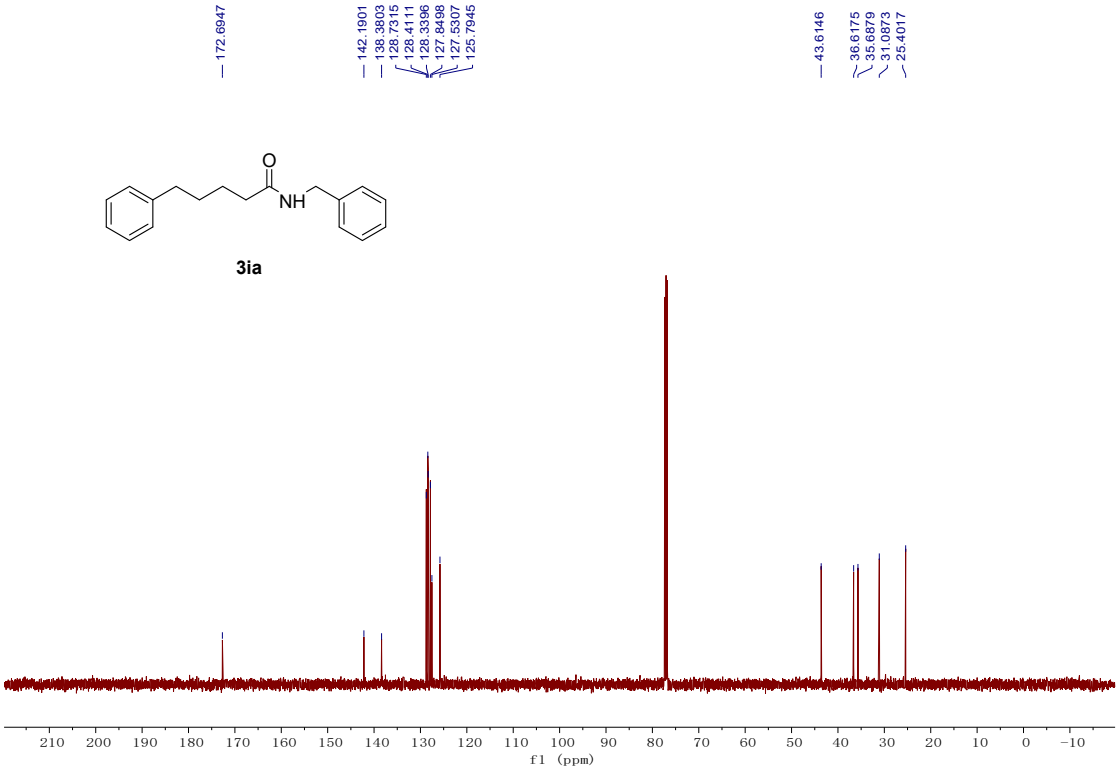

173.3640
172.9832
142.3714
142.3060
137.5848
136.7873
128.9350
128.5784
128.4257
128.4120
128.3091
128.2802
128.0426
127.5864
127.2930
126.2784
125.7277
125.6997
53.3727
50.7812
35.8429
35.7516
34.8137
33.9314
33.3993
32.9883
31.2917
31.2058
25.0742
24.8743
O
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

3ga

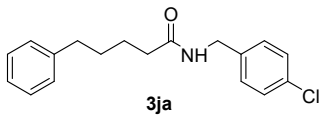

7.3439
7.3281
7.3140
7.3006
7.2865
7.2728
7.2566
7.2471
7.1845
7.1704
7.1541
7.1388
5.6096
5.5964
5.1474
5.1330
5.1186
2.6284
2.6133
2.5993
2.1979
2.1845
2.1696
1.7028
1.6858
1.6722
1.6615
1.6486
1.6350
1.4801
1.4663
3ha
f1 (ppm)
7.66
3.00
1.00
1.00
2.00
2.01
4.03
3.01


171.8214
143.2495
142.2190
128.6896
128.4027
128.3291
127.3735
126.1973
125.7728
48.6095
36.7236
35.6913
31.0433
25.3697
21.7033
3ha
f1 (ppm)

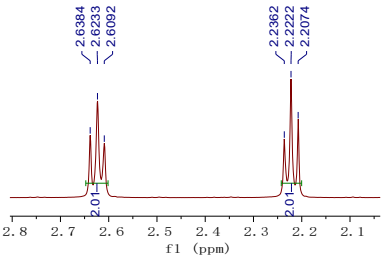

7.3361
7.3226
7.3076
7.2838
7.2809
7.2763
7.2697
7.2618
7.2520
7.2470
7.1840
7.1693
7.1617
7.1596
7.1456
5.7087
4.4251
4.4137
2.6393
2.6242
2.6100
2.2339
2.2196
2.2049
1.7416
1.7275
1.7109
1.6970
1.6828
1.6689
1.6551
1.6378
1.6277
1.6238
O
NH
3ia
2.01
2.01
f1 (ppm)
2.03
5.01
3.00
1.00
2.00
2.01
2.01
4.03
f1 (ppm)

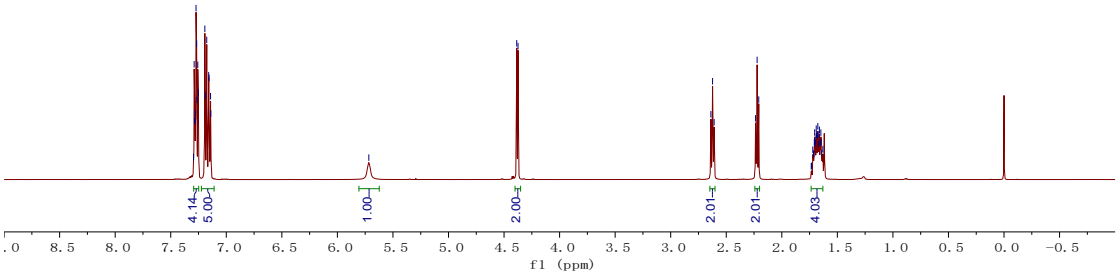

172.6947
142.1901
138.3803
128.7315
128.4111
128.3396
127.8498
127.5307
125.7945
43.6146
36.6175
35.6879
31.0873
25.4017
O
NH
3ia
f1 (ppm)


7.2945
7.2892
7.2851
7.2813
7.2766
7.2723
7.2668
7.2644
7.2565
7.2514
7.1929
7.1893
7.1759
7.1584
7.1552
7.1417
7.1394
5.7171
4.3858
4.3742
2.6384
2.6233
2.6092
2.2362
2.2222
2.2074
1.7351
1.7316
1.7209
1.7152
1.7114
1.7072
1.7042
1.7011
1.6964
1.6903
1.6867
1.6787
1.6758
1.6706
1.6650
1.6616
1.6559
1.6485
1.6451
1.6402
1.6307

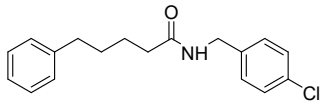

O
NH
Cl

3ja


2.6384
2.6233
2.6092
2.2362
2.2222
2.2074
2.01
2.01
2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1
f1 (ppm)

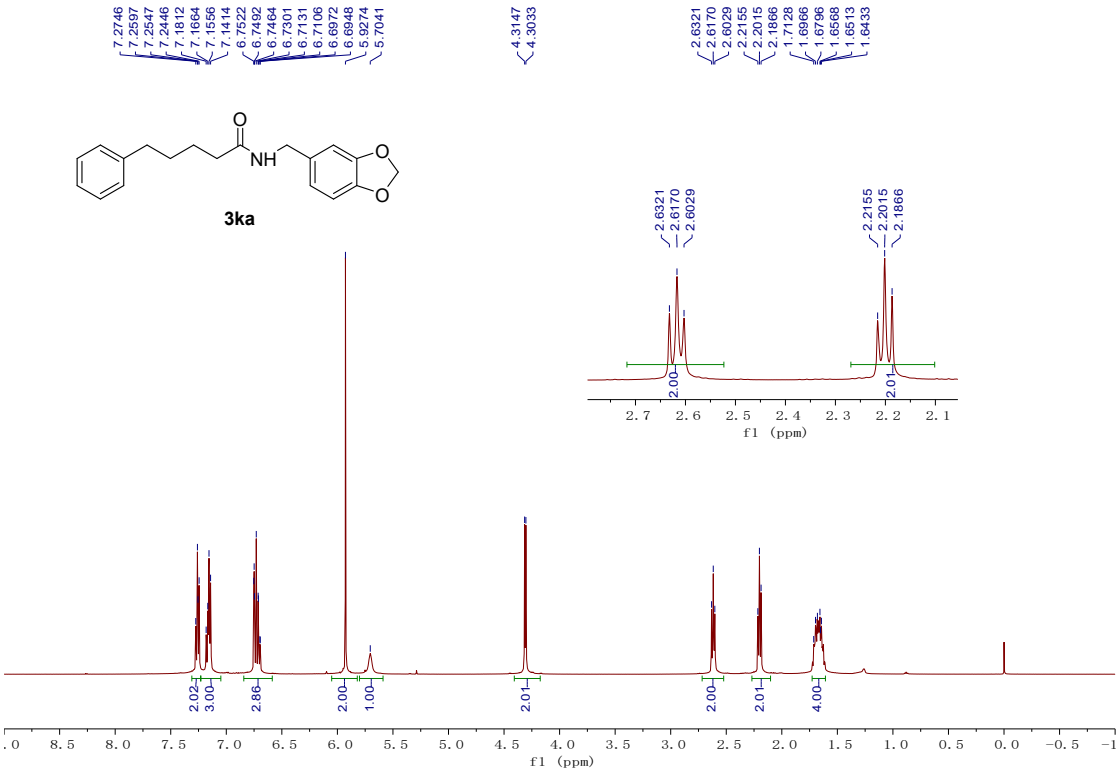

4.14
5.00
1.00
2.00
2.01
2.01
4.03
f1 (ppm)

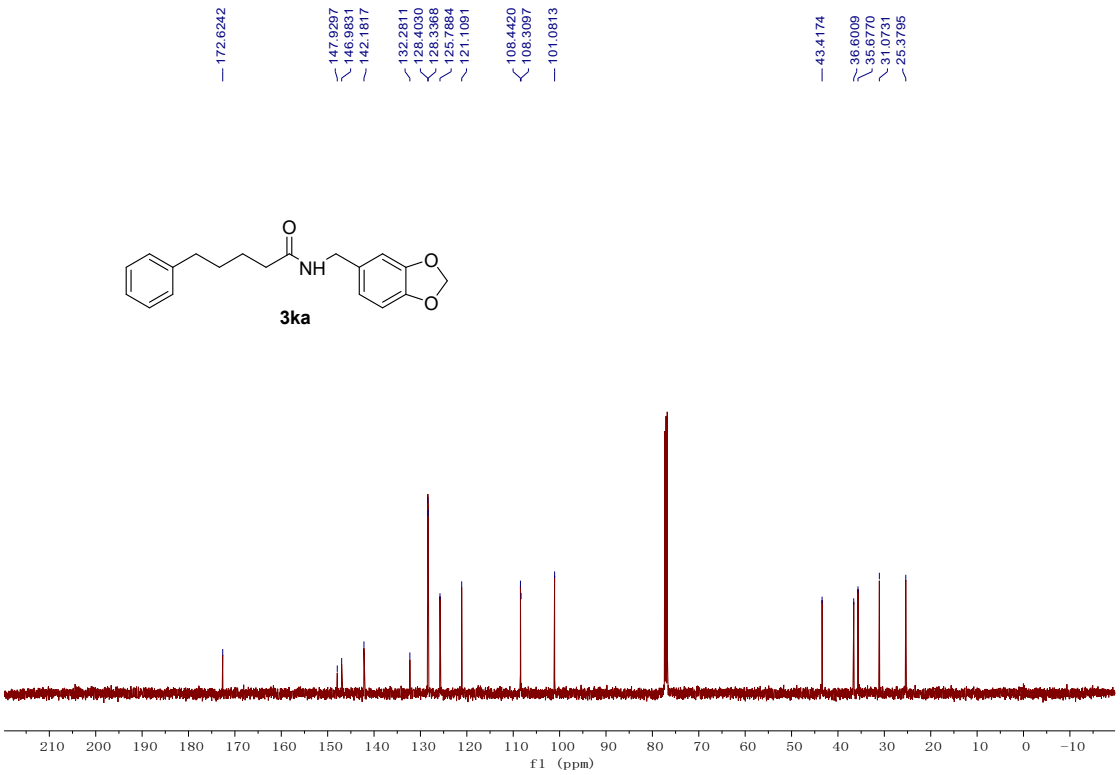

172.7218
142.1310
136.9895
133.3082
129.1575
128.8351
128.3967
128.3530
125.8243
42.8573
36.5693
35.6662
31.0653
25.3439


O
NH
Cl

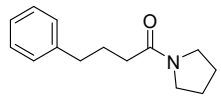
3ja

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

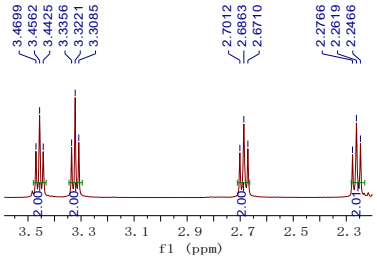

7.2746
7.2597
7.2547
7.2446
7.1812
7.1664
7.1556
7.1414
6.7522
6.7492
6.7464
6.7301
6.7131
6.7106
6.6972
6.6948
5.9274
5.7041
4.3147
4.3033
2.6321
2.6170
2.6029
2.2155
2.2015
2.1866
1.7128
1.6966
1.6796
1.6568
1.6513
1.6433
O
NH
O
O
3ka
2.00
2.01
f1 (ppm)
2.02
3.00
2.86
2.00
1.00
2.01
2.00
2.01
4.00
f1 (ppm)

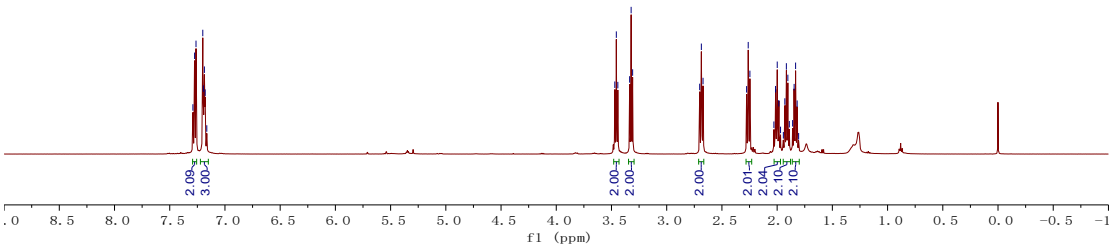

172.6242
147.9297
146.9831
142.1817
132.2811
128.4030
128.3368
125.7884
121.1091
108.4420
108.3097
101.0813
43.4174
36.6009
35.6770
31.0731
25.3795
O
NH
O
O
3ka
f1 (ppm)


7.2903
7.2750
7.2621
7.2007
7.1956
7.1862
7.1792
7.1644
3.4699
3.4562
3.4425
3.3356
3.3221
3.3085
2.7012
2.6863
2.6710
2.2766
2.2619
2.2466
2.0294
2.0145
1.9991
1.9849
1.9692
1.9437
1.9302
1.9165
1.9030
1.8896
1.8598
1.8462
1.8328
1.8189
1.8053

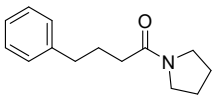

O
N

4aa


3.4699
3.4562
3.4425
3.3356
3.3221
3.3085
2.7012
2.6863
2.6710
2.2766
2.2619
2.2466
2.00
2.00
2.00
2.00
2.01
3.5
3.3
3.1
2.9
2.7
2.5
2.3
f1 (ppm)

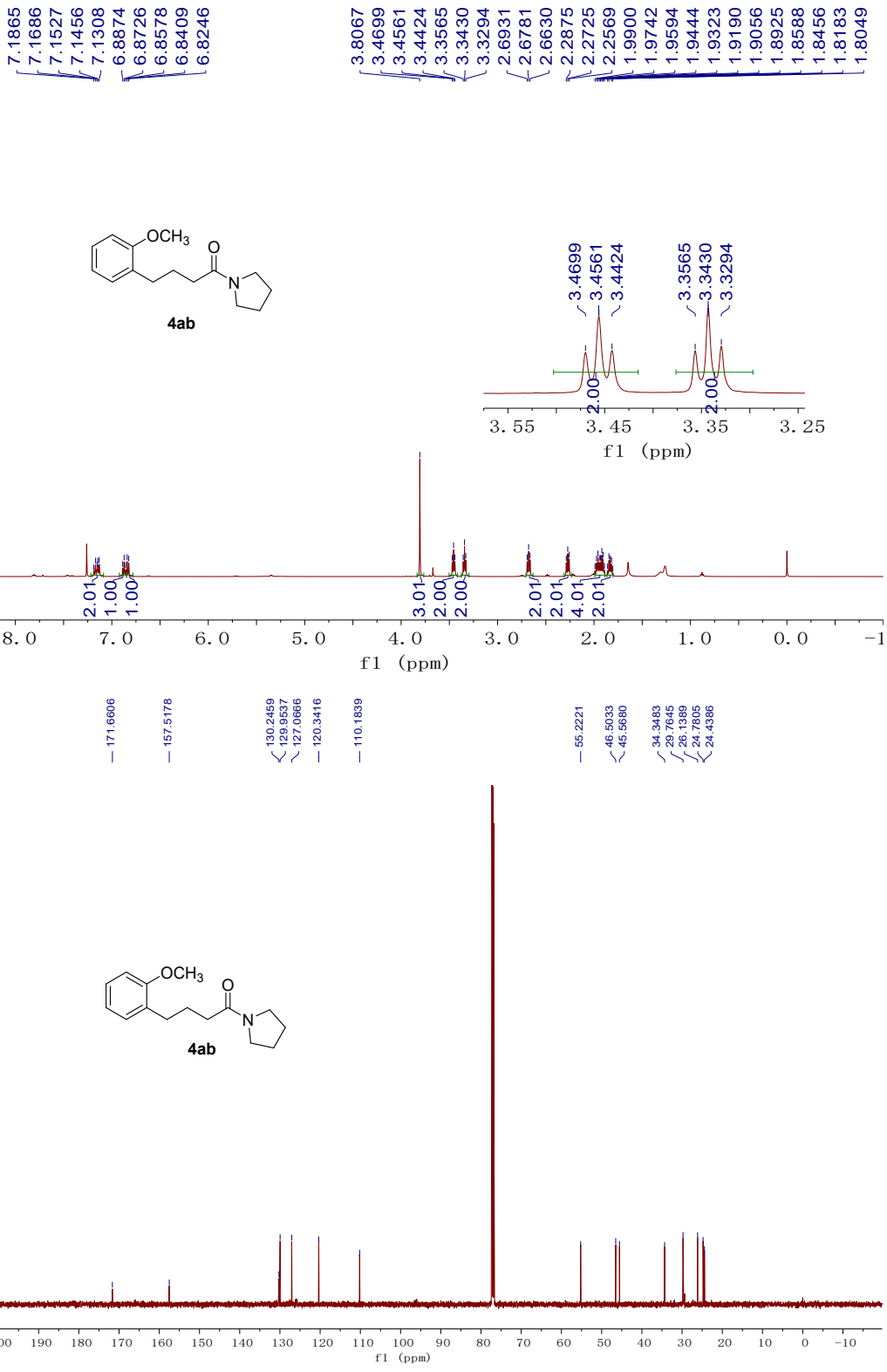

2.09
3.00
2.00
2.00
2.00
2.01
2.04
2.10
2.10
f1 (ppm)

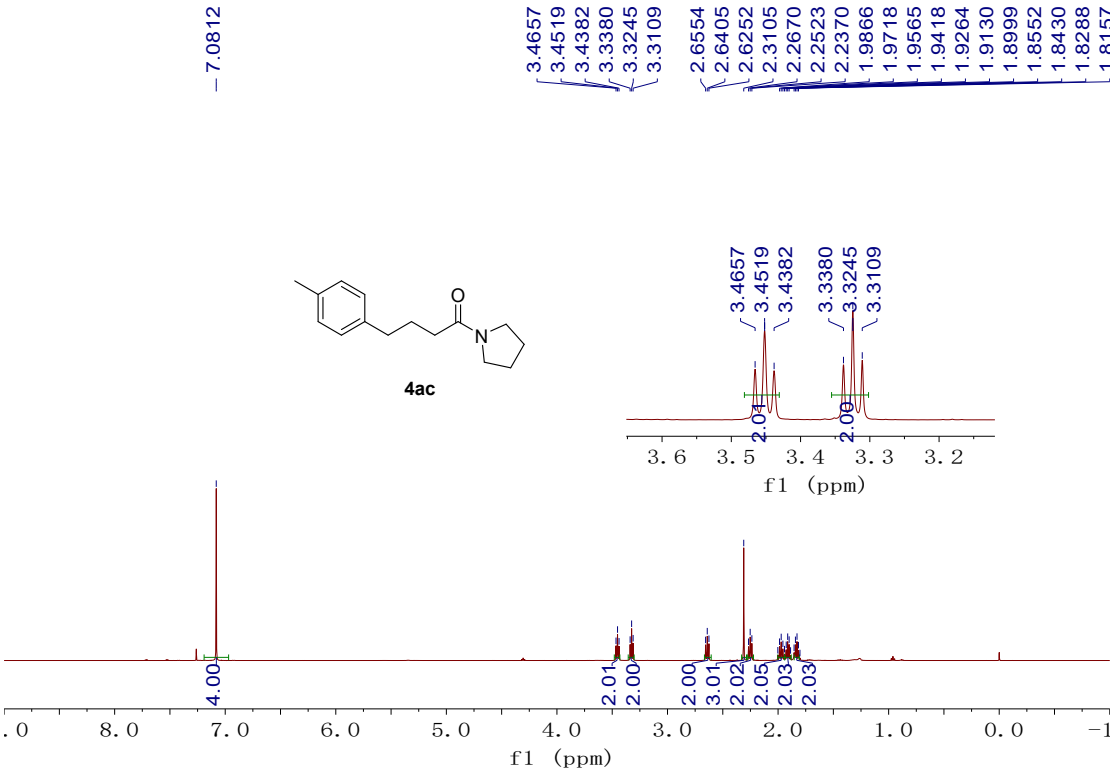

171.3540
141.8830
128.5142
128.3203
125.8389
46.5211
45.6031
35.3625
33.8870
26.2716
26.1087
24.4152

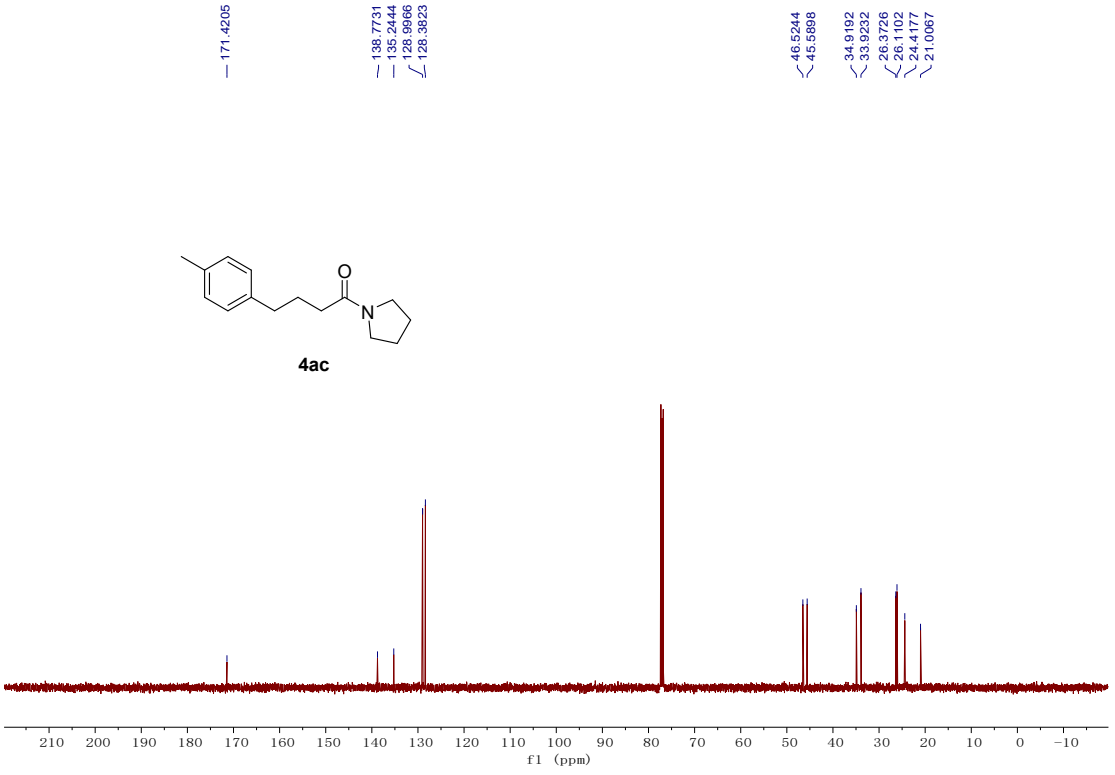

O
N

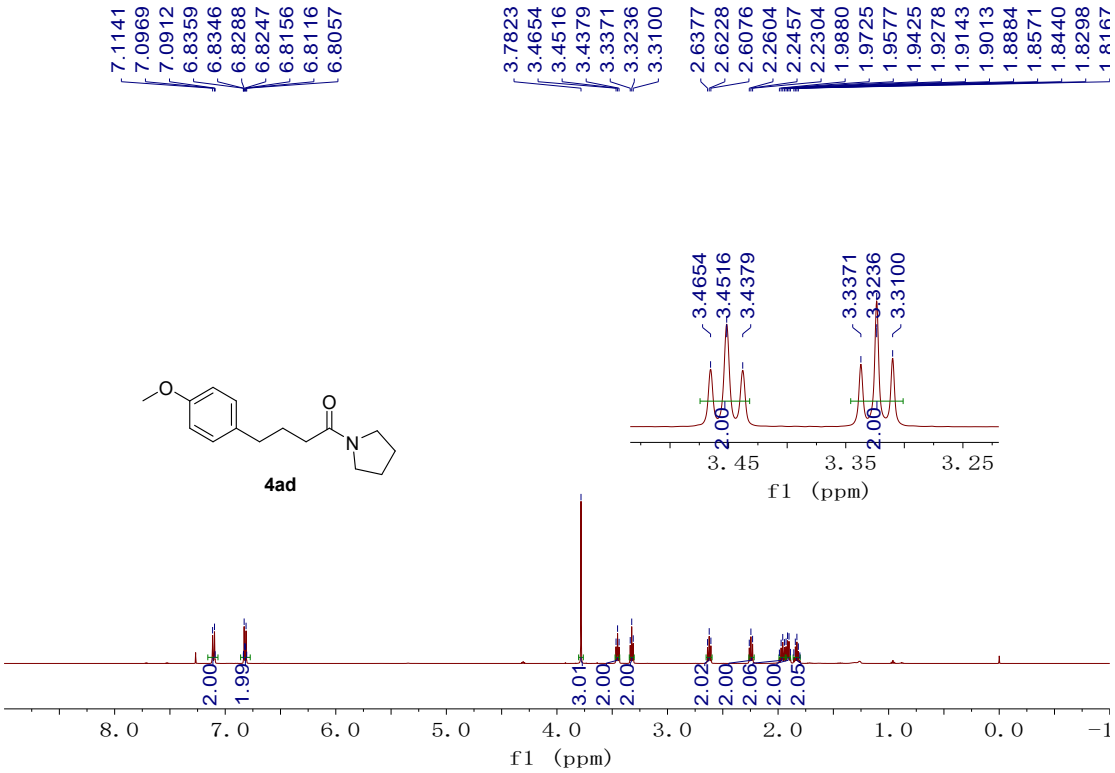
4aa

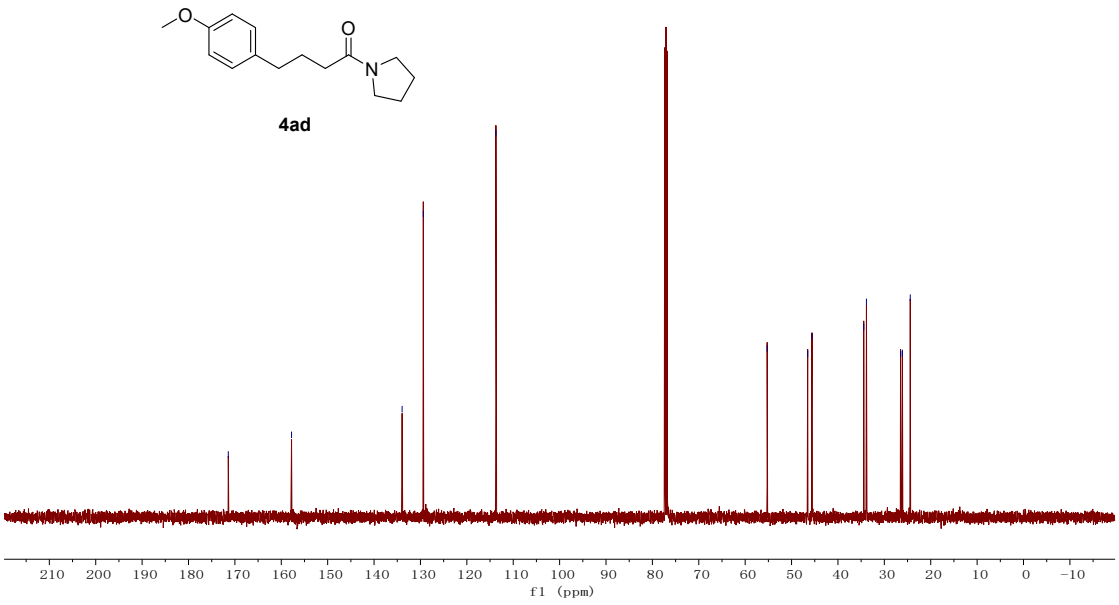
f1 (ppm)


7.1865
7.1686
7.1527
7.1456
7.1308
6.8874
6.8726
6.8578
6.8409
6.8246
3.8067
3.4699
3.4561
3.4424
3.3565
3.3430
3.3294
2.6931
2.6781
2.6630
2.2875
2.2725
2.2569
1.9900
1.9742
1.9594
1.9444
1.9323
1.9190
1.9056
1.8925
1.8588
1.8456
1.8183
1.8049
OCH3
O
N
4ab
3.4699
3.4561
3.4424
3.3565
3.3430
3.3294
2.00
2.00
3.55
3.45
3.35
3.25
f1 (ppm)
2.01
1.00
1.00
3.01
2.00
2.00
2.01
2.01
4.01
2.01
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)
171.6606
157.5178
130.2459
129.9537
127.0666
120.3416
110.1839
55.2221
46.5033
45.5680
34.3483
29.7645
26.1389
24.7805
24.4386
OCH3
O
N
4ab
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

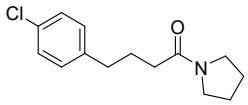

7.0812
3.4657
3.4519
3.4382
3.3380
3.3245
3.3109
2.6554
2.6405
2.6252
2.3105
2.2670
2.2523
2.2370
1.9866
1.9718
1.9565
1.9418
1.9264
1.9130
1.8999
1.8552
1.8430
1.8288
4ac
f1 (ppm)
4.00
2.01
2.00
2.00
3.01
2.02
2.05
2.03
2.03


171.4205
138.7731
135.2444
128.9966
128.3823
46.5244
45.5898
34.9192
33.9232
26.3726
26.1102
24.4177
21.0067
4ac
f1 (ppm)

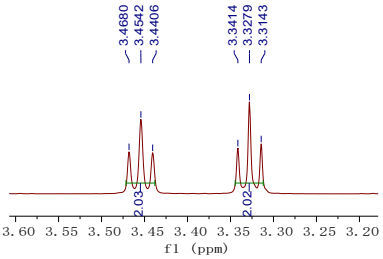

7.1141
7.0969
7.0912
6.8359
6.8346
6.8288
6.8247
6.8156
6.8116
6.8057
3.7823
3.4654
3.4516
3.4379
3.3371
3.3236
3.3100
2.6377
2.6228
2.6076
2.2604
2.2457
2.2304
1.9880
1.9725
1.9577
1.9425
1.9278
1.9143
1.9013
1.8884
1.8571
1.8440
1.8298
4ad
2.00
1.99
3.01
2.00
2.00
2.02
2.00
2.06
2.00
2.05
f1 (ppm)

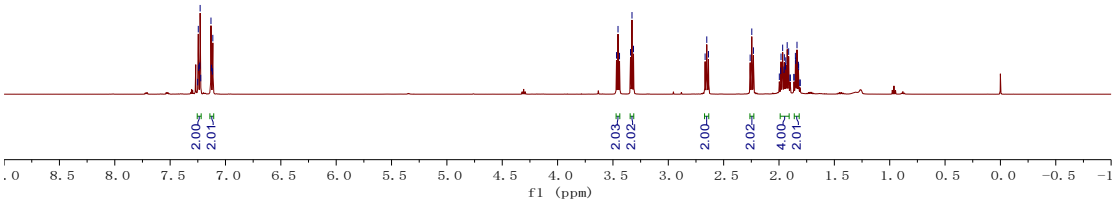

171.4212
157.7875
133.9517
129.3812
113.7338
55.2610
46.5264
45.5887
34.4417
33.8580
26.5067
26.1074
24.4141
4ad
f1 (ppm)


7.2511
7.2457
7.2418
7.2331
7.2290
7.2238
7.1311
7.1268
7.1185
7.1144
3.4680
3.4542
3.4406
3.3414
3.3279
3.3143
2.6675
2.6525
2.6372
2.2606
2.2459
2.2310
1.9972
1.9843
1.9817
1.9669
1.9545
1.9518
1.9413
1.9387
1.9262
1.9127
1.9005
1.8985
1.8654
1.8636
1.8521
1.8498
1.8375
1.8248
1.8225
1.8111
1.8089

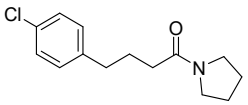

Cl
O
N

4ae

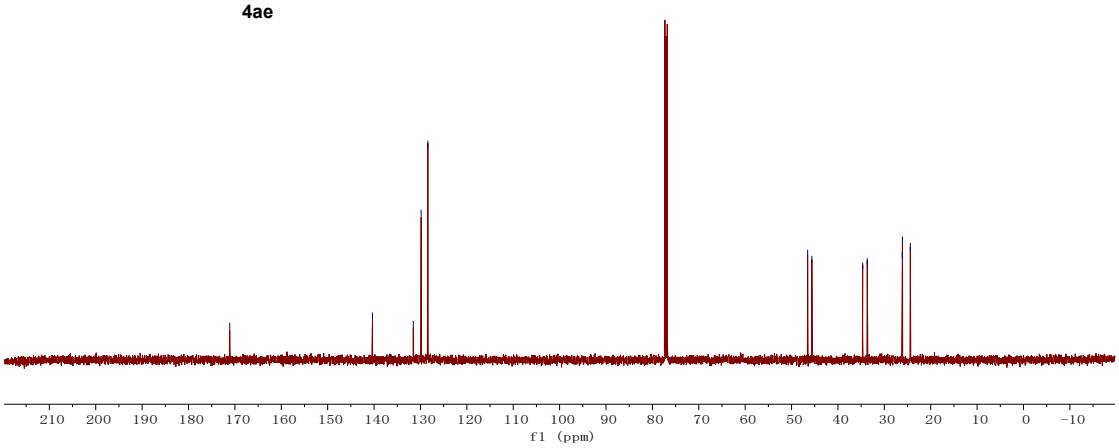

3.4680
3.4542
3.4406
3.3414
3.3279
3.3143
2.03
2.02
3.60 3.55 3.50 3.45 3.40 3.35 3.30 3.25 3.20
f1 (ppm)

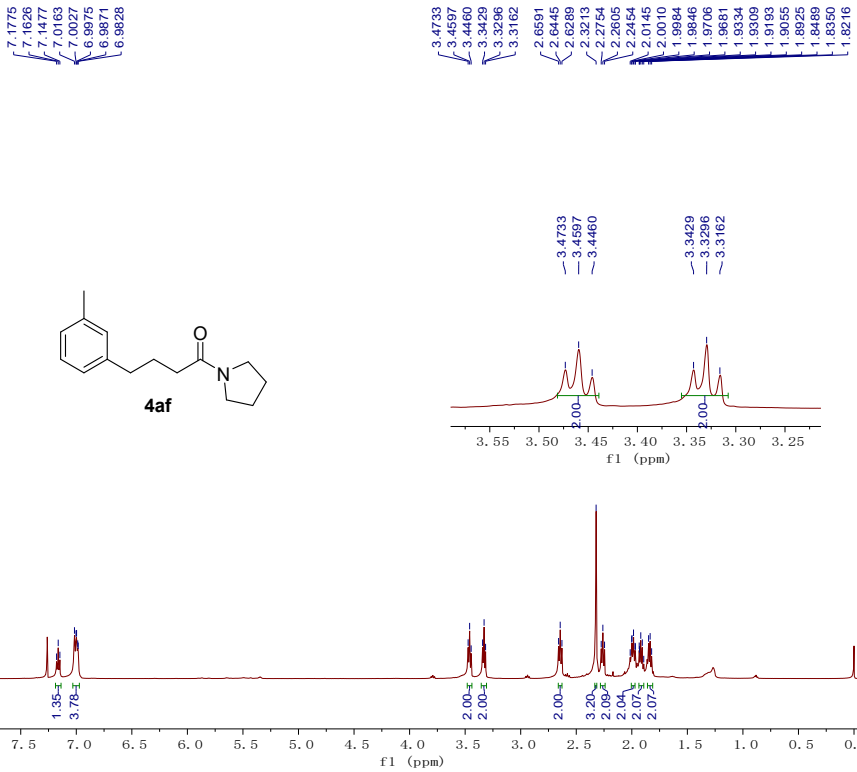

2.00
2.01
2.03
2.02
2.00
2.02
4.00
2.01
f1 (ppm)

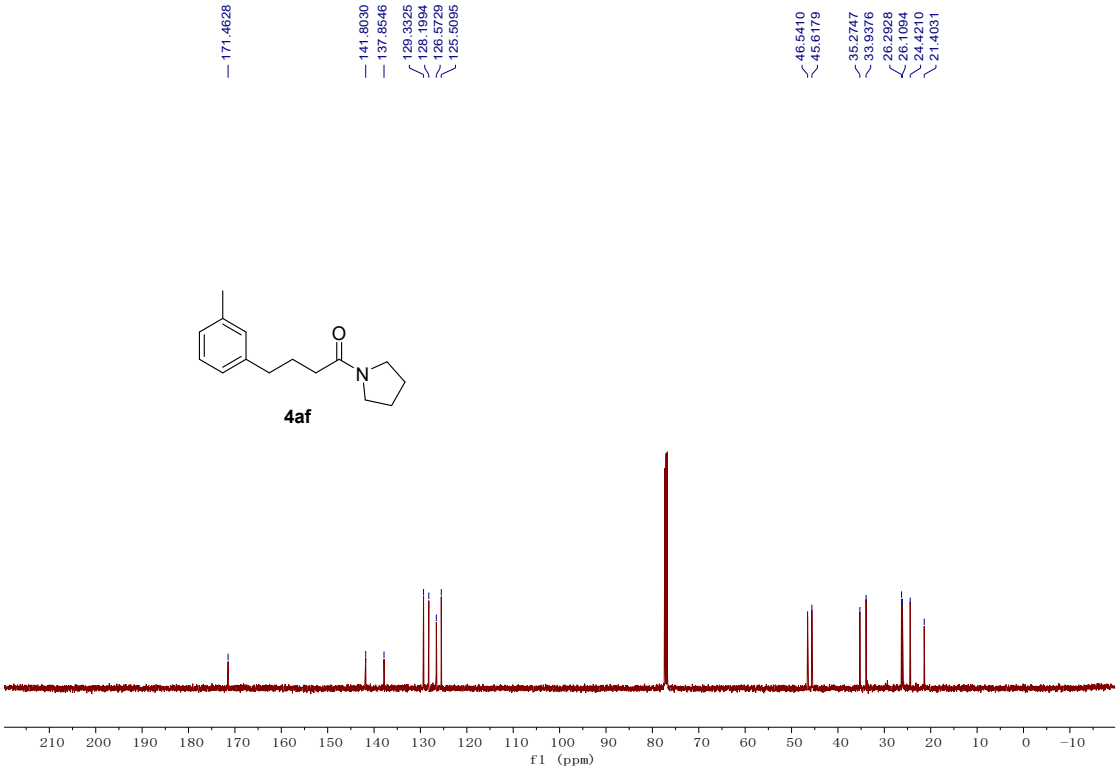

171.1147
140.3415
131.5405
129.8478
128.4037
46.5320
45.6267
34.6708
33.6811
26.1458
26.0959
24.4001

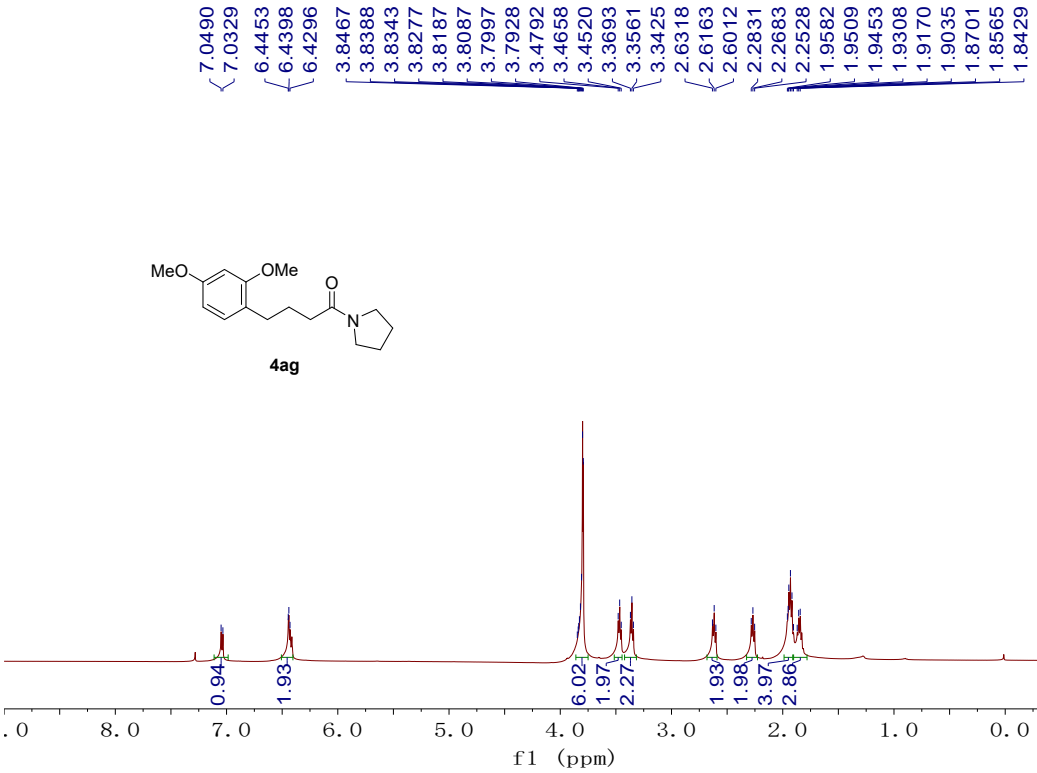

Cl
O
N

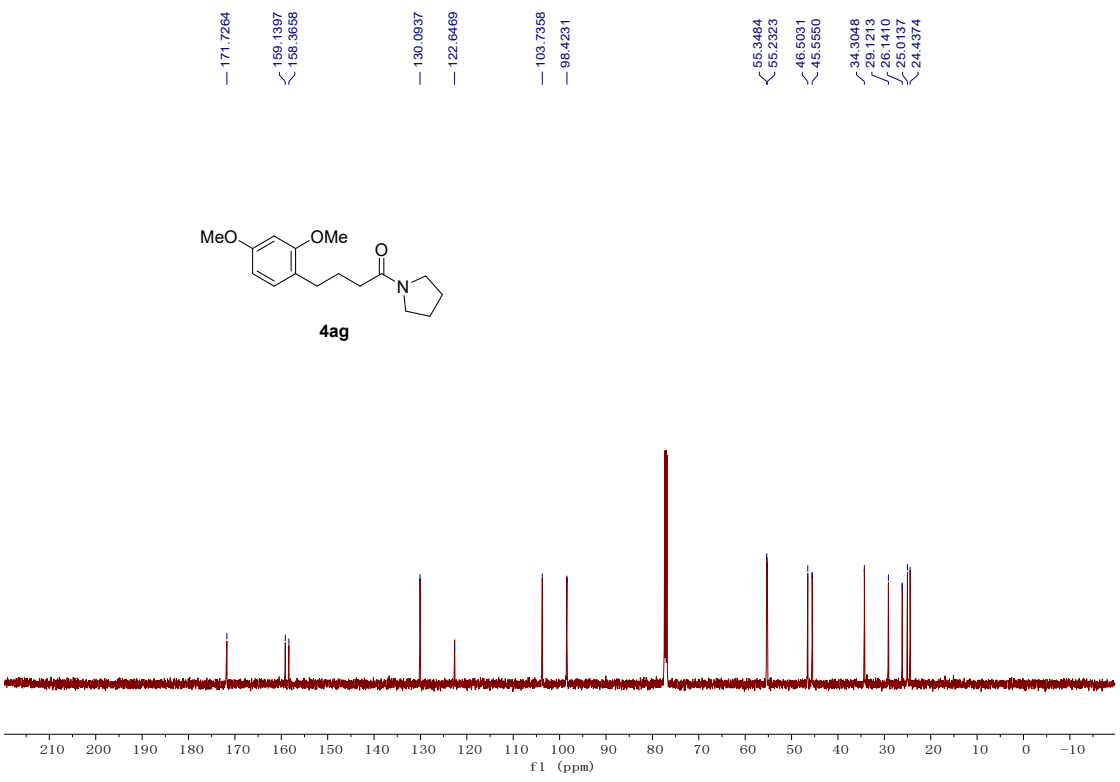
4ae

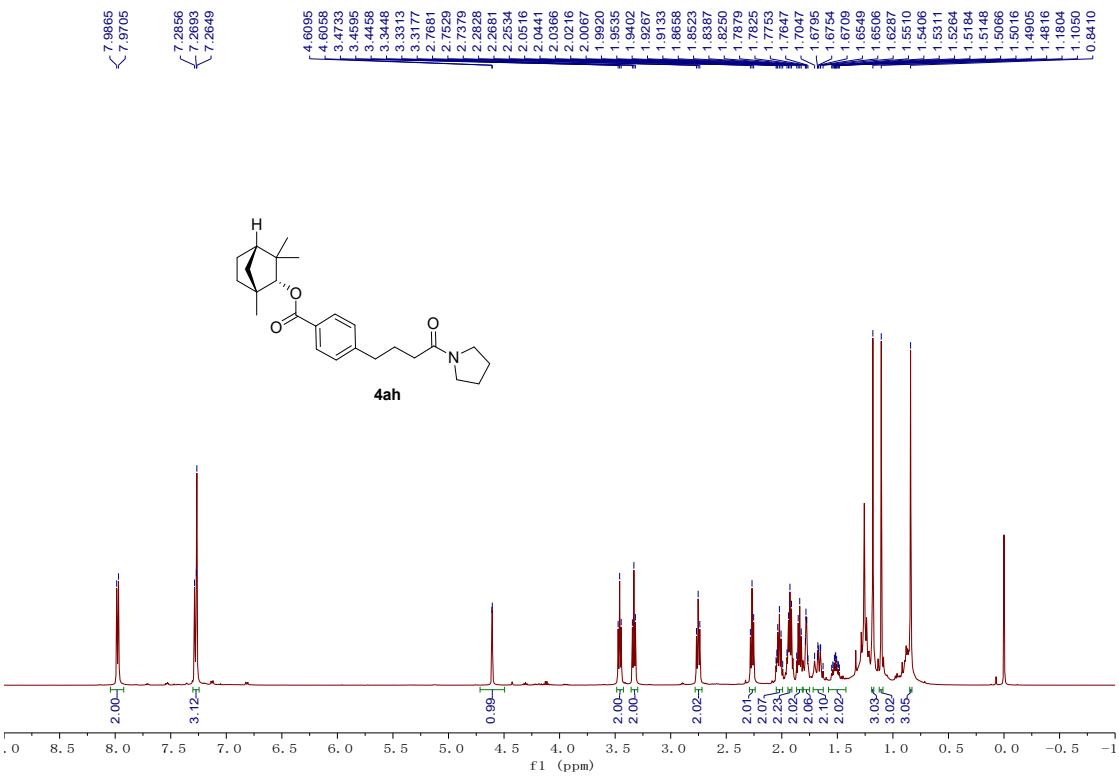

f1 (ppm)

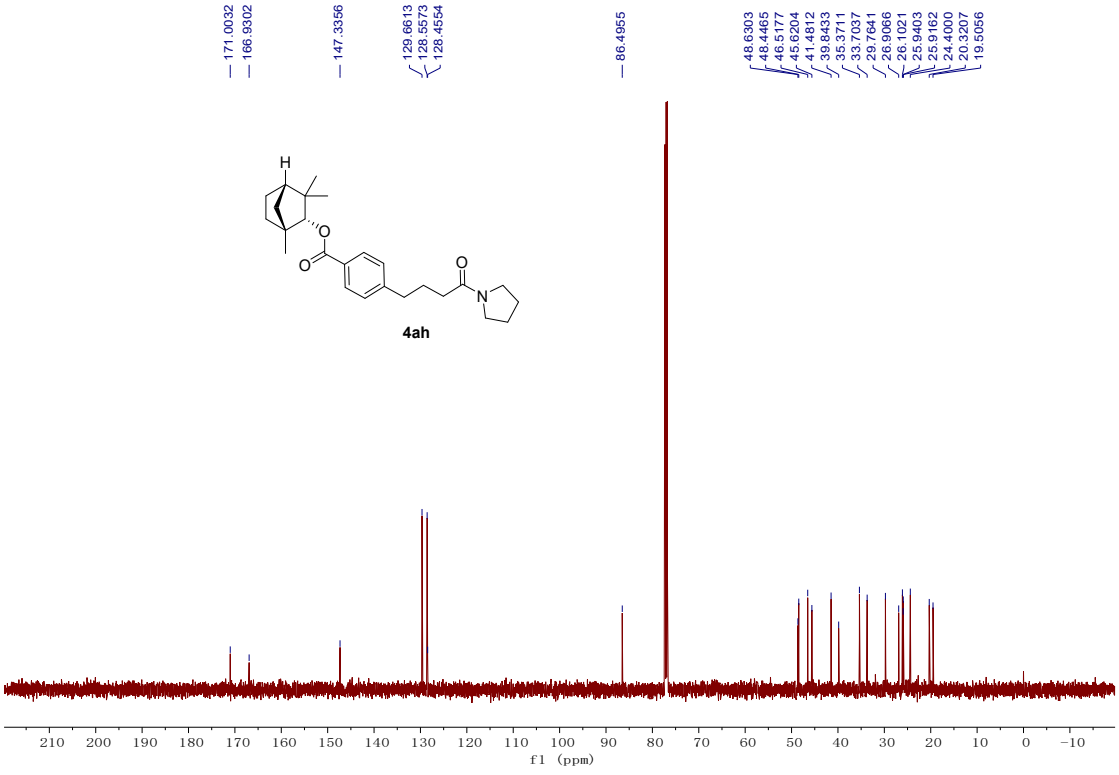

7.1775
7.1626
7.1477
7.0163
7.0027
6.9975
6.9871
6.9828
3.4733
3.4597
3.4460
3.3429
3.3296
3.3162
2.6591
2.6445
2.6289
2.3213
2.2754
2.2605
2.2454
2.0145
2.0010
1.9984
1.9846
1.9706
1.9681
1.9334
1.9309
1.9193
1.9055
1.8925
1.8489
1.8350
1.8216
O
N
4af
2.00
2.00
3.55 3.50 3.45 3.40 3.35 3.30 3.25
f1 (ppm)
1.35
3.78
2.00
2.00
2.00
3.20
2.09
2.04
2.07
2.07
f1 (ppm)

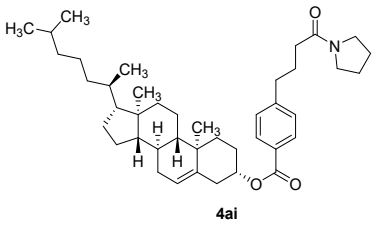

171.4628
141.8030
137.8546
129.3325
128.1994
126.5729
125.5095
46.5410
45.6179
35.2747
33.9376
26.2928
26.1094
24.4210
21.4031
O
N
4af
f1 (ppm)


7.0490
7.0329
6.4453
6.4398
6.4296
3.8467
3.8388
3.8343
3.8277
3.8187
3.8087
3.7997
3.7928
3.4792
3.4658
3.4520
3.3693
3.3561
3.3425
2.6318
2.6163
2.6012
2.2831
2.2683
2.2528
1.9582
1.9509
1.9453
1.9308
1.9170
1.9035
1.8701
1.8565
1.8429
MeO
OMe
O
N
4ag
0.94
1.93
6.02
1.97
2.27
1.93
1.98
3.97
2.86
f1 (ppm)

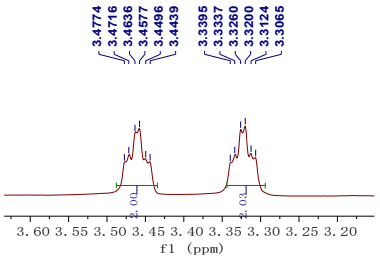

171.7264
159.1397
158.3658
130.0937
122.6469
103.7358
98.4231
55.3484
55.2323
46.5031
45.5550
34.3048
29.1213
26.1410
25.0137
24.4374
MeO
OMe
O
N
4ag
f1 (ppm)

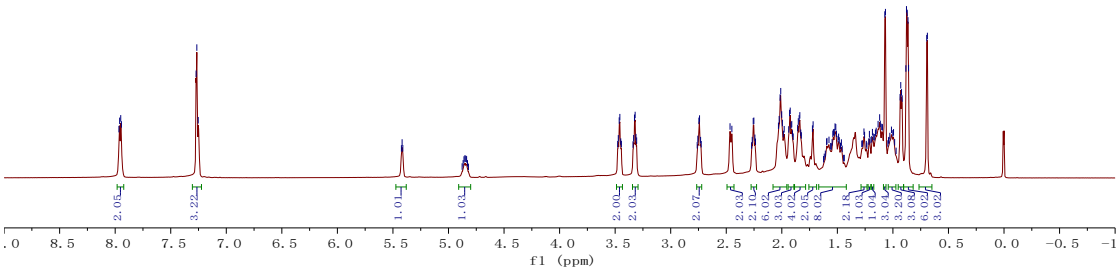

7.9865
7.9705
7.2856
7.2693
7.2649
4.6095
4.6058
3.4733
3.4595
3.4458
3.3448
3.3313
3.3177
2.7681
2.7529
2.7379
2.2828
2.2681
2.2534
2.0516
2.0441
2.0366
2.0216
2.0067
1.9920
1.9535
1.9402
1.9267
1.9133
1.8658
1.8523
1.8387
1.8250
1.7879
1.7825
1.7753
1.7647
1.7047
1.6795
1.6754
1.6709
1.6549
1.6506
1.6287
1.5510
1.5406
1.5311
1.5264
1.5184
1.5148
1.5066
1.5016
1.4905
1.4816
1.1804
1.1050
0.8410
4ah
2.00
3.12
0.99
2.00
2.00
2.02
2.01
2.07
2.23
2.02
2.06
2.10
2.02
3.03
3.02
3.05
f1 (ppm)

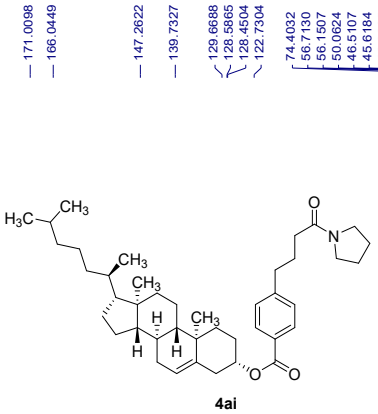

171.0032
166.9302
147.3356
129.6613
128.5573
128.4554
86.4955
48.6303
48.4465
46.5177
45.6204
41.4812
39.8433
35.3711
33.7037
29.7641
26.9066
26.1021
25.9403
25.9162
24.4000
20.3207
19.5056
4ah
f1 (ppm)



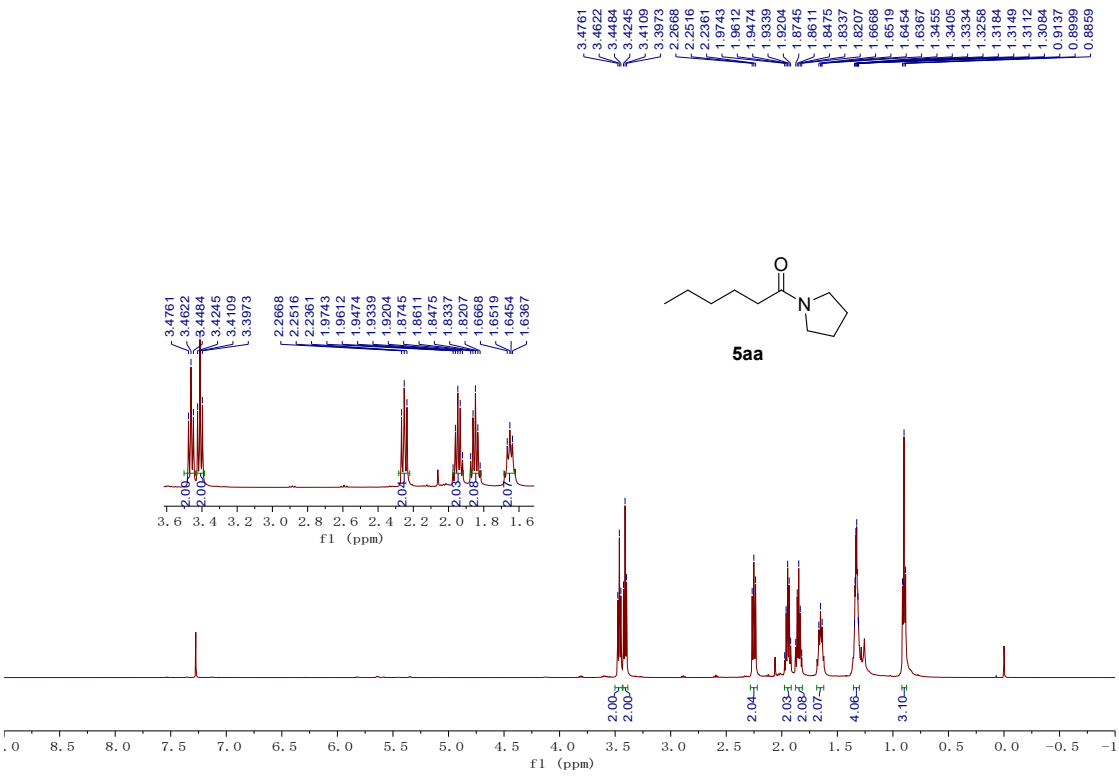
4ai

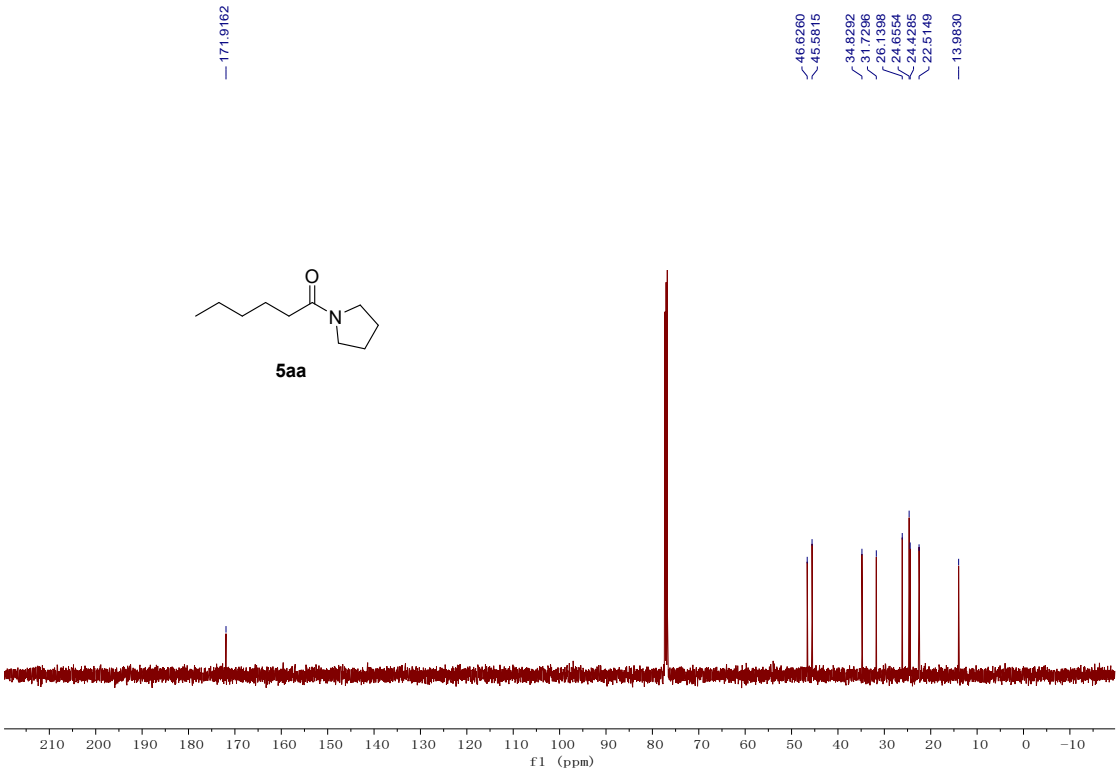


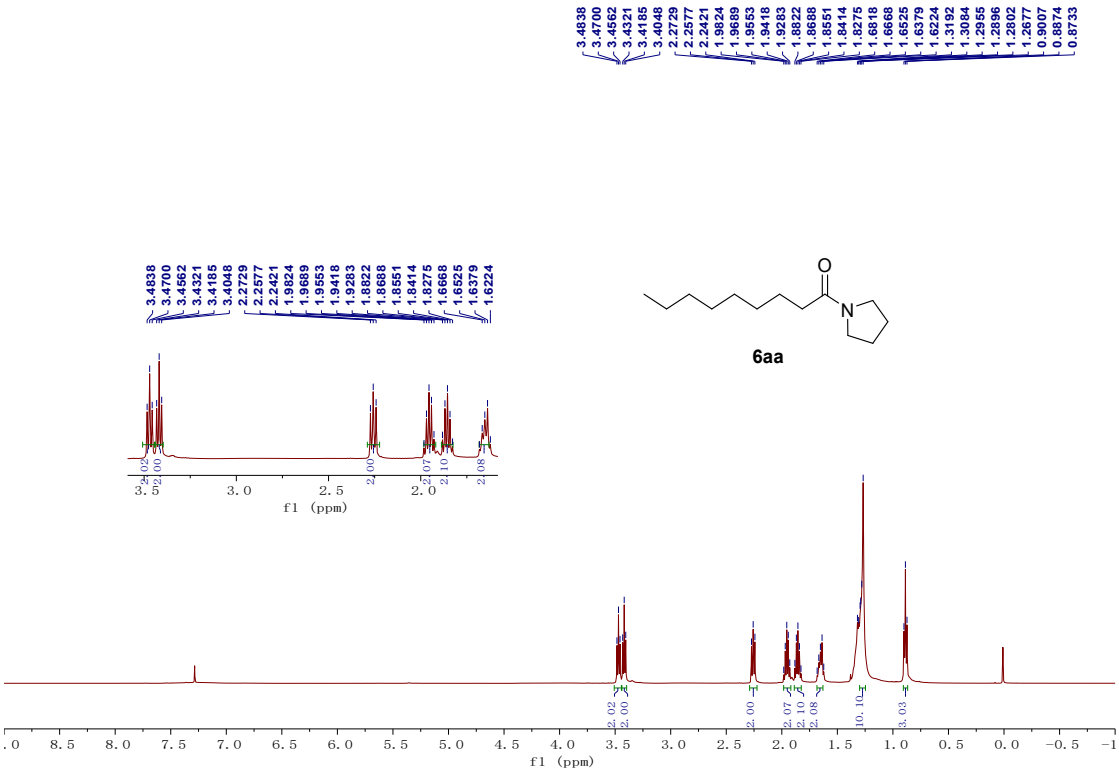


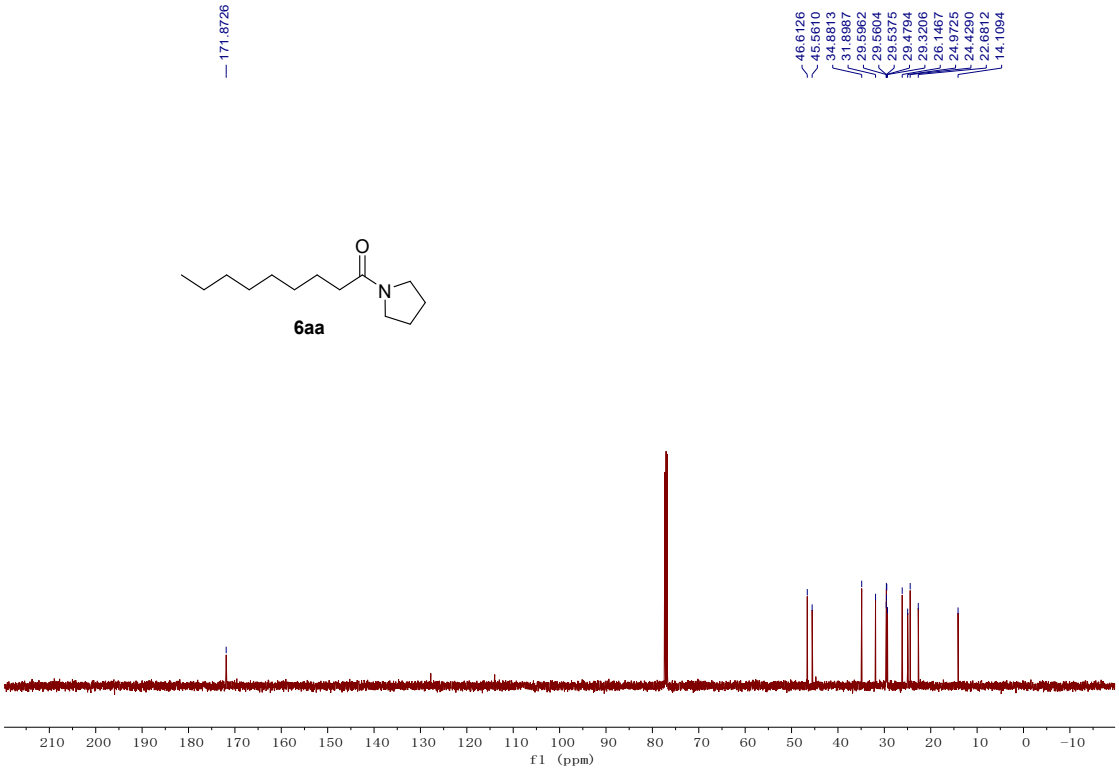


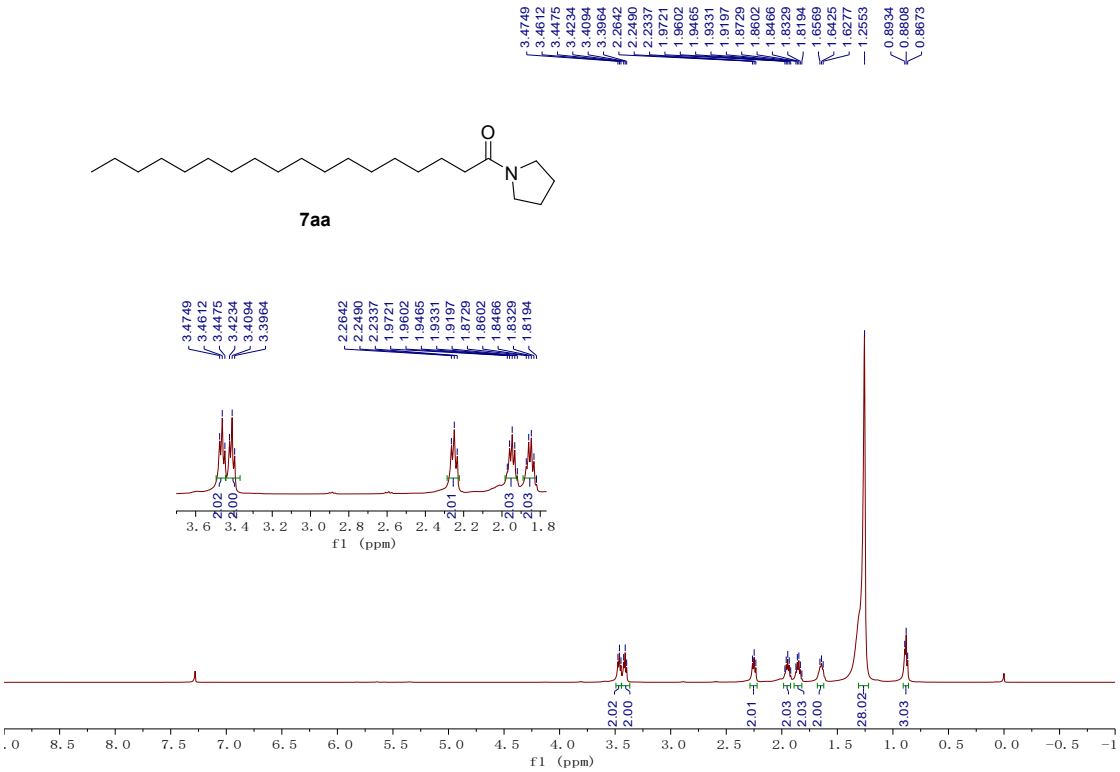
4ai

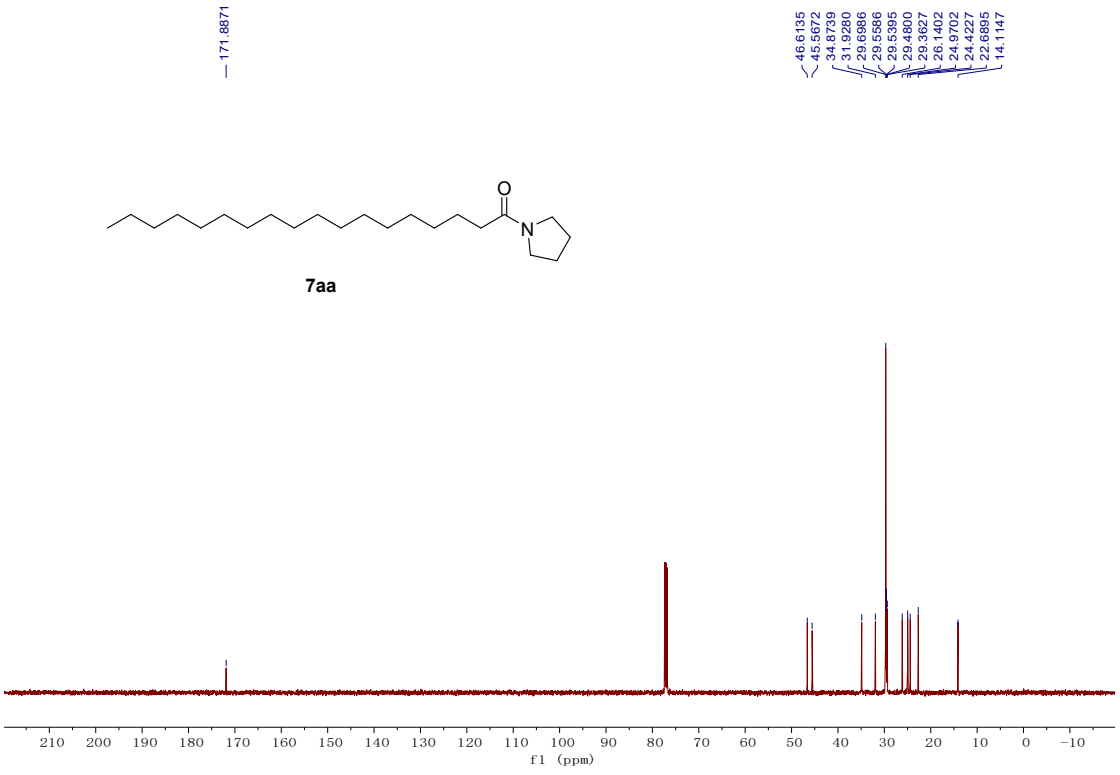

3.4761
3.4622
3.4484
3.4245
3.4109
3.3973
2.2668
2.2516
2.2361
1.9743
1.9612
1.9474
1.9339
1.9204
1.8745
1.8611
1.8475
1.8337
1.8207
1.6668
1.6519
1.6454
1.6367
5aa
f1 (ppm)

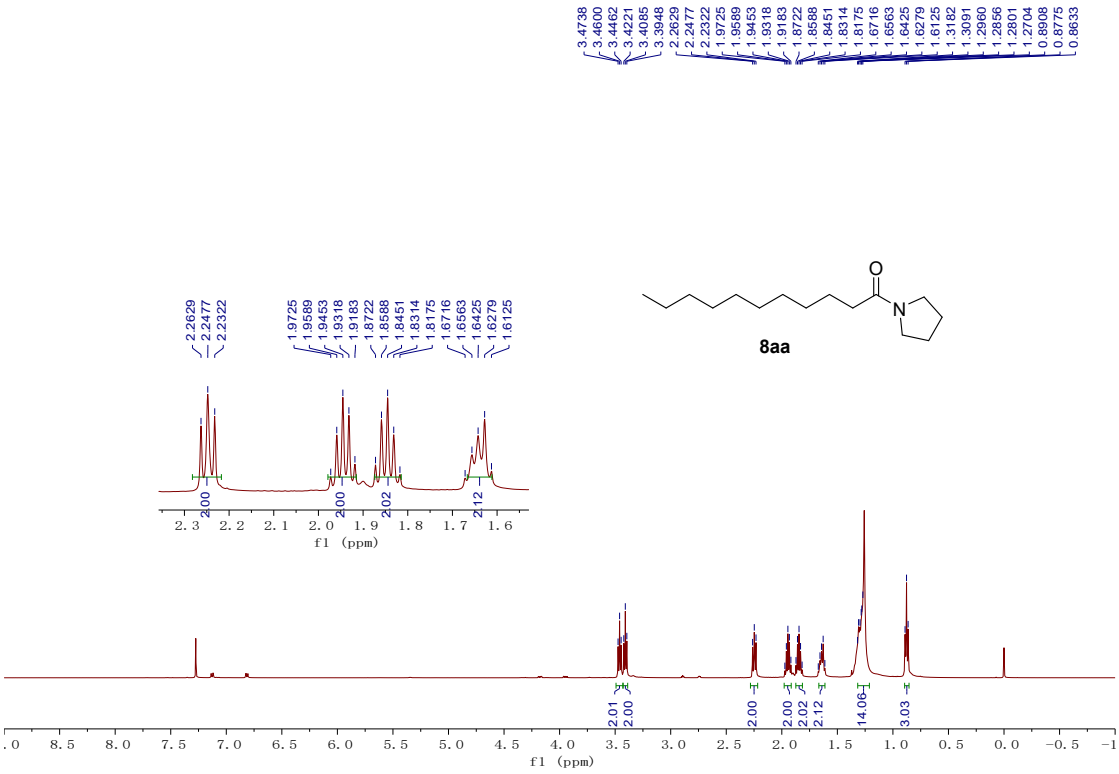

171.9162
46.6260
45.5815
34.8292
31.7296
26.1398
24.6554
24.4285
22.5149
13.9830
5aa
f1 (ppm)

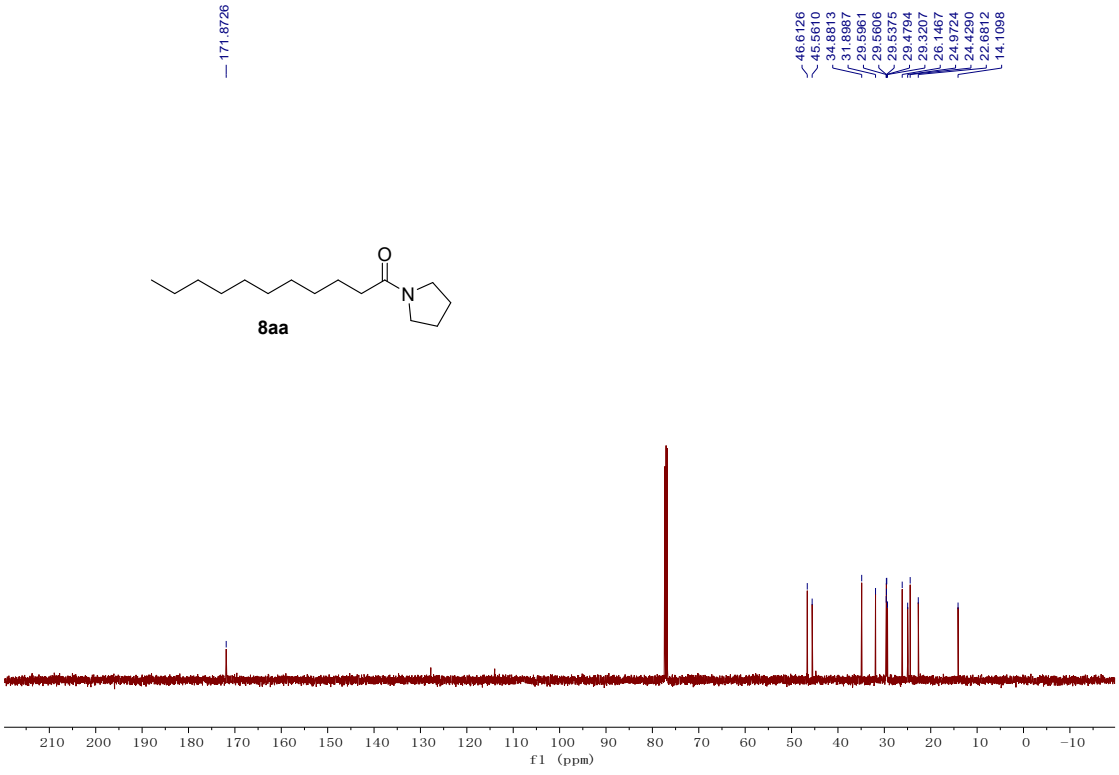

3.4838
3.4700
3.4562
3.4321
3.4185
3.4048
2.2729
2.2577
2.2421
1.9824
1.9689
1.9553
1.9418
1.9283
1.8822
1.8688
1.8551
1.8414
1.8275
1.6818
1.6668
1.6525
1.6379
1.6224
1.3192
1.3084
1.2955
1.2896
1.2802
1.2677
0.9007
0.8874
0.8733
6aa
f1 (ppm)

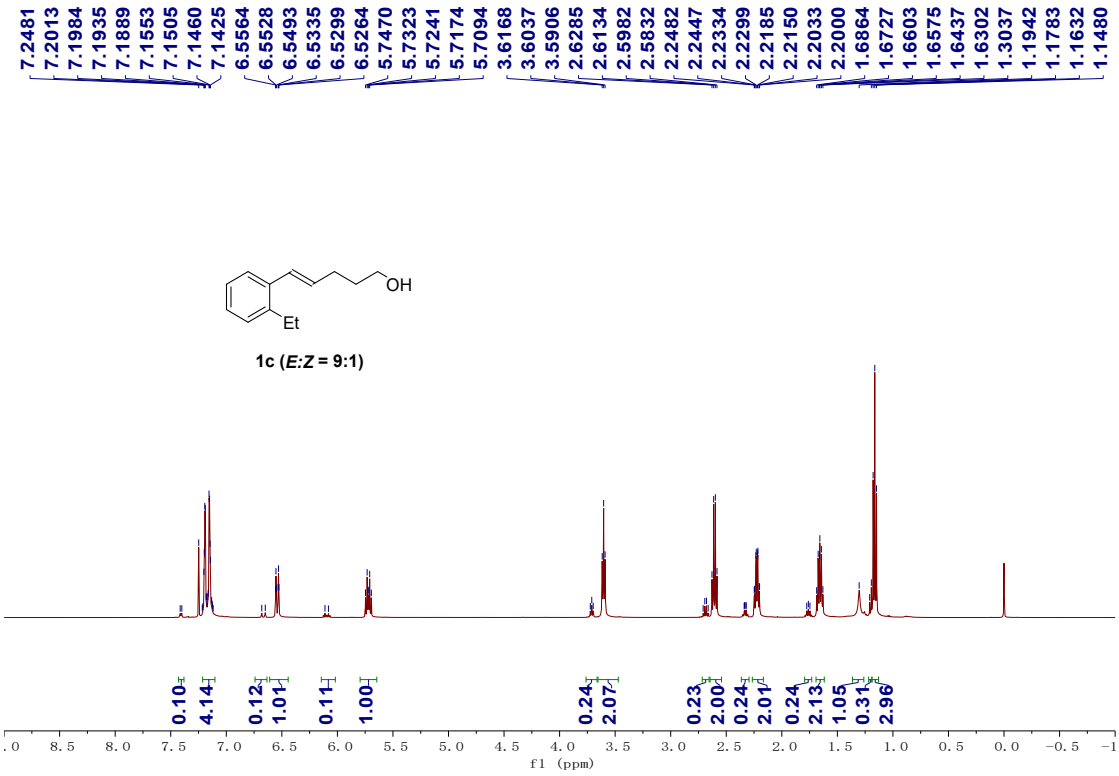

171.8726
46.6126
45.5610
34.8813
31.8987
29.5962
29.5604
29.5375
29.4794
29.3206
26.1467
24.9725
24.4290
22.6812
14.1094
6aa
f1 (ppm)

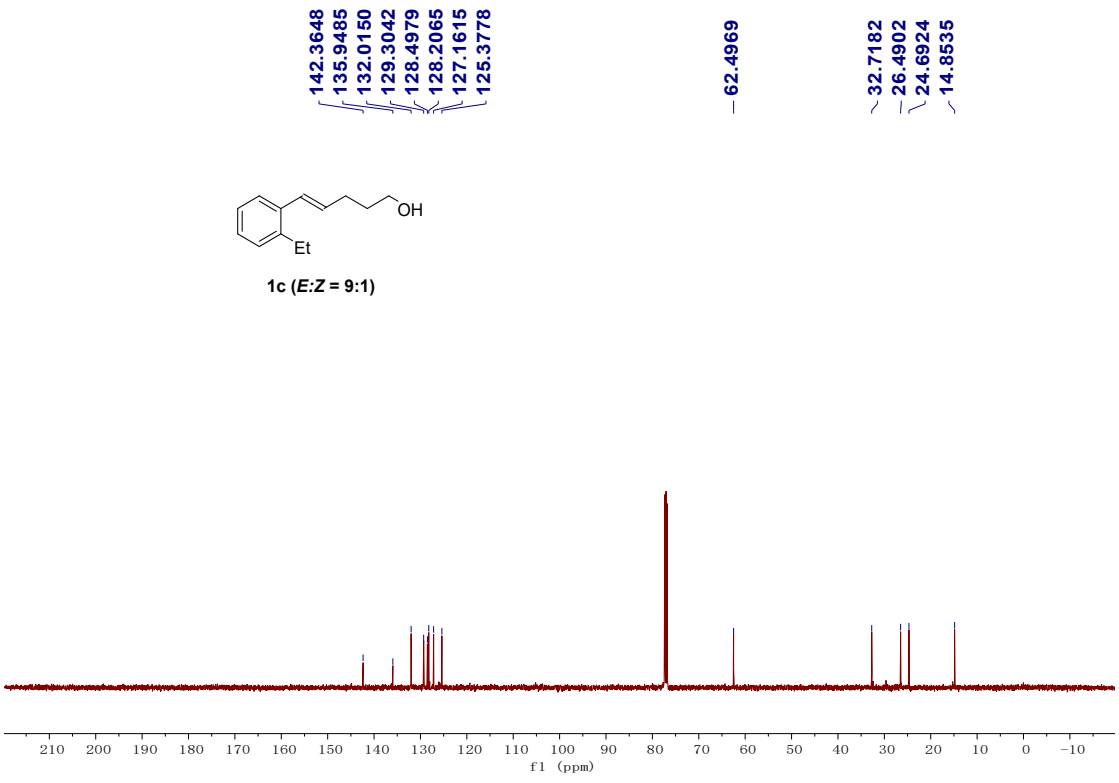

3.4749
3.4612
3.4475
3.4234
3.4094
3.3964
2.2642
2.2490
2.2337
1.9721
1.9602
1.9465
1.9331
1.9197
1.8729
1.8602
1.8466
1.8329
1.8194
1.6569
1.6425
1.6277
1.2553
0.8934
0.8808
0.8673
O
N
7aa
f1 (ppm)


171.8871
46.6135
45.5672
34.8739
31.9280
29.6986
29.5586
29.5395
29.4800
29.3627
26.1402
24.9702
24.4227
22.6895
14.1147
O
N
7aa
f1 (ppm)

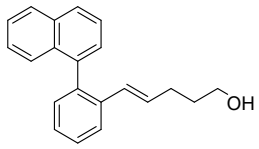

3.4738
3.4600
3.4462
3.4221
3.4085
3.3948
2.2629
2.2477
2.2322
1.9725
1.9589
1.9453
1.9318
1.9183
1.8722
1.8588
1.8451
1.8314
1.8175
1.6716
1.6563
1.6425
1.6279
1.6125
1.3182
1.3091
1.2960
1.2856
1.2801
1.2704
0.8908
0.8775
0.8633
O
N
8aa
f1 (ppm)


171.8726
46.6126
45.5610
34.8813
31.8987
29.5961
29.5606
29.5375
29.4794
29.3207
26.1467
24.9724
24.4290
22.6812
14.1098
O
N
8aa
f1 (ppm)

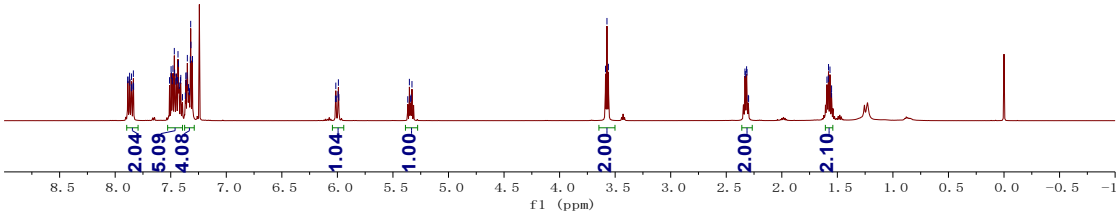

7.2481
7.2013
7.1984
7.1935
7.1889
7.1553
7.1505
7.1460
7.1425
6.5564
6.5528
6.5493
6.5335
6.5299
6.5264
5.7470
5.7323
5.7241
5.7174
5.7094
3.6168
3.6037
3.5906
2.6285
2.6134
2.5982
2.5832
2.2482
2.2447
2.2334
2.2299
2.2185
2.2150
2.2033
2.2000
1.6864
1.6727
1.6603
1.6575
1.6437
1.6302
1.3037
1.1942
1.1783
1.1632
1.1480
OH
Et
1c (E:Z = 9:1)
0.10
4.14
0.12
1.01
0.11
1.00
0.24
2.07
0.23
2.00
0.24
2.01
0.24
2.13
1.05
0.31
2.96
f1 (ppm)

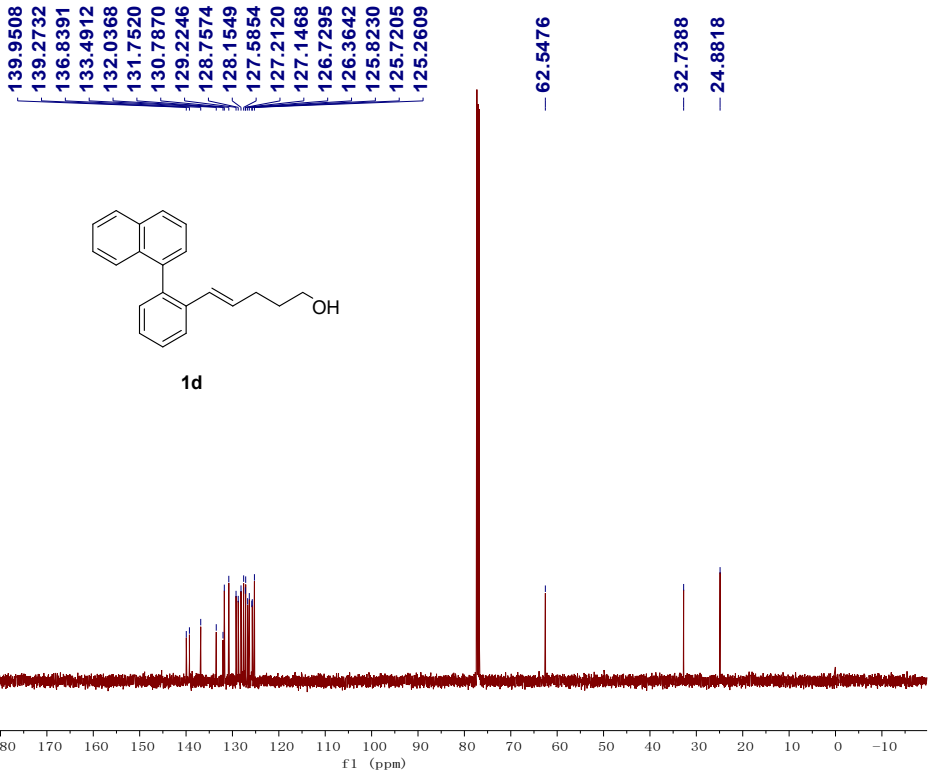

142.3648
135.9485
132.0150
129.3042
128.4979
128.2065
127.1615
125.3778
62.4969
32.7182
26.4902
24.6924
14.8535
OH
Et
1c (E:Z = 9:1)
f1 (ppm)


7.8872
7.8846
7.8702
7.8678
7.8527
7.8384
7.8362
7.8342
7.5107
7.4968
7.4942
7.4863
7.4802
7.4678
7.4651
7.4542
7.4487
7.4378
7.4346
7.4307
7.4233
7.4127
7.4094
7.3645
7.3615
7.3538
7.3505
7.3233
7.3204
7.3182
7.3042
6.0142
5.9910
5.3520
5.3287
3.5867
3.5737
3.5606
2.3317
2.3282
2.3169
2.3133
1.5938
1.5818
1.5794
1.5665


OH

1d

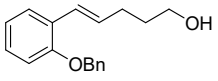

2.04
5.09
4.08
1.04
1.00
2.00
2.00
2.10
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1
f1 (ppm)


139.9508
139.2732
136.8391
133.4912
132.0368
131.7520
130.7870
129.2246
128.7574
128.1549
127.5854
127.2120
127.1468
126.7295
126.3642
125.8230
125.7205
125.2609
62.5476
32.7388
24.8818
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

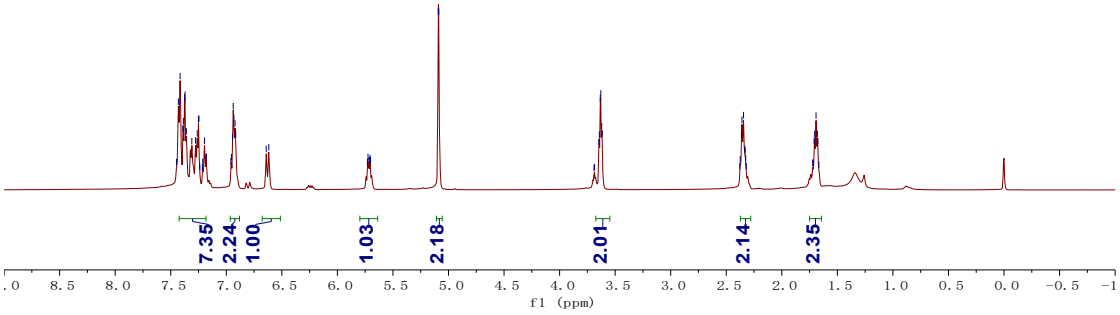
OH

1d

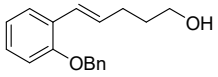

7.4313
7.4155
7.3906
7.3863
7.3755
7.3709
7.3596
7.3103
7.2763
7.2615
7.2506
7.2460
7.1962
7.1842
7.1793
6.9539
6.9436
6.9379
6.9318
6.9214
6.9146
6.6405
6.6173
5.7244
5.7061
5.7016
5.0924
5.0876
3.6469
3.6423
3.6342
3.6291
3.6210
3.6164
2.3741
2.3635
2.3590
2.3445
2.3337
2.3296
2.3250
1.7090
1.7043
1.6919
1.6798
1.6751


OH
OBn

1f


7.35
2.24
1.00
1.03
2.18
2.01
2.14
2.35
f1 (ppm)

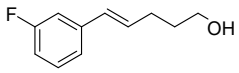

156.1800
137.2679
131.8979
130.1280
128.5209
128.0908
127.7901
127.1615
125.1073
120.4747
112.2958
70.1994
62.5617
32.7692
25.0284


OH
OBn

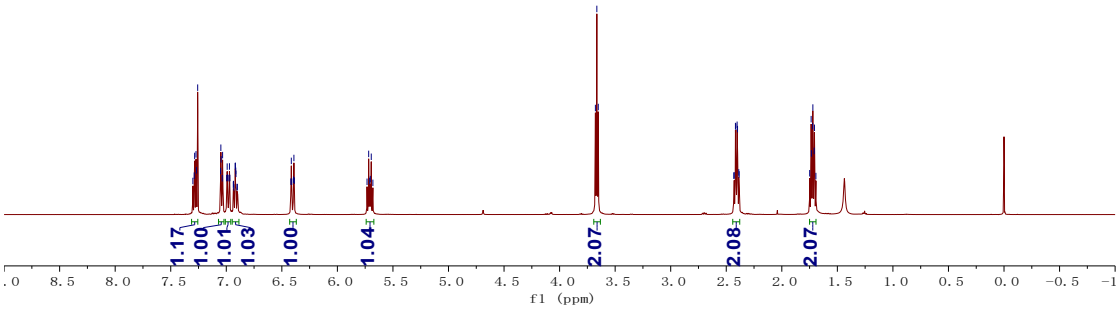
1f

f1 (ppm)

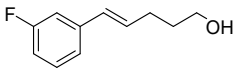

7.2885
7.2848
7.2726
7.2688
7.2575
7.0516
7.0489
7.0466
7.0365
7.0332
6.9965
6.9920
6.9879
6.9760
6.9715
6.9675
6.9199
6.9181
6.9147
6.9129
6.4147
6.3953
6.3913
6.3875
5.7184
5.7038
5.6952
3.6778
3.6648
3.6519
2.4320
2.4283
2.4174
2.4136
2.4023
2.3985
2.3874
2.3837
1.7491
1.7360
1.7335
1.7229
1.7205
1.7082
1.7062
1.6932


F
OH

1j

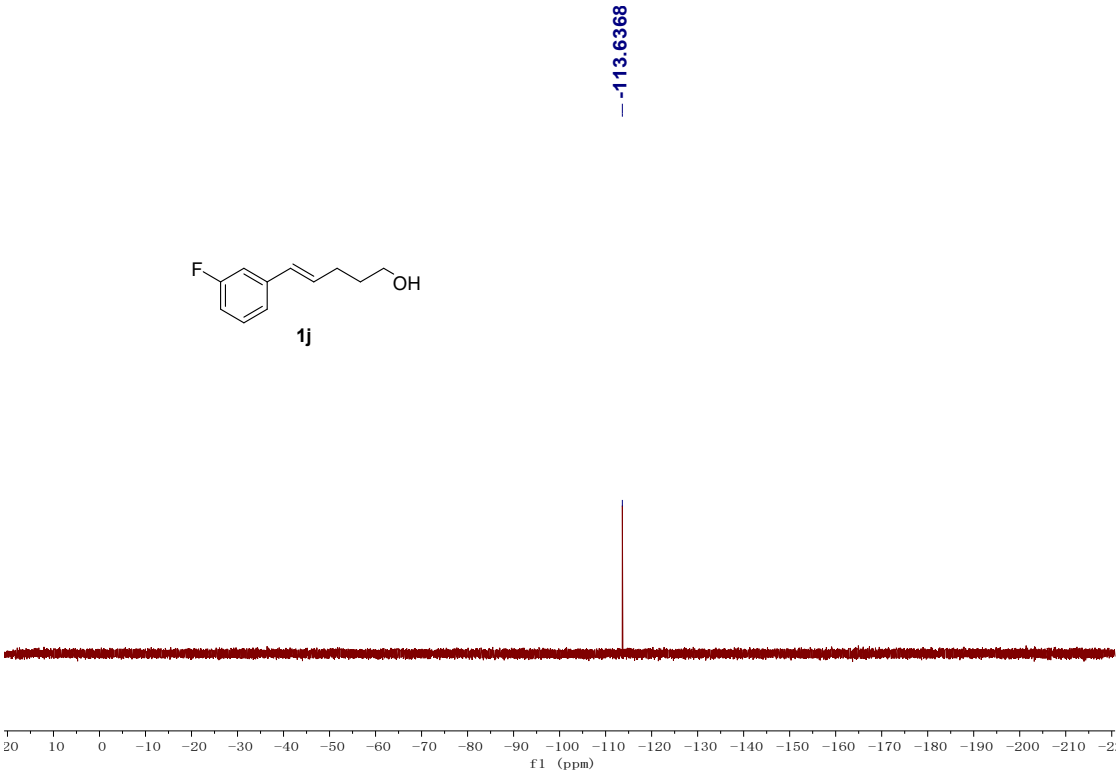

1.17
1.00
1.01
1.03
1.00
1.04
2.07
2.08
2.07
f1 (ppm)

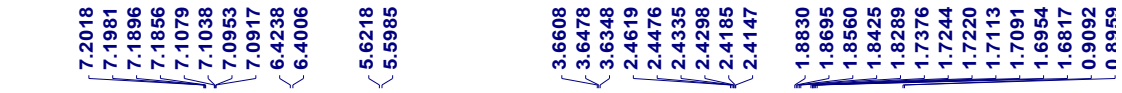

163.6790
161.7335
139.7348
139.6748
133.2572
129.6396
129.5737
128.4398
124.5085
124.4863
115.5019
115.3284
113.5519
113.3836
62.3432
32.7021
24.9178

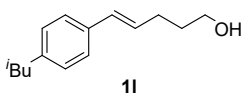

F
OH

1j

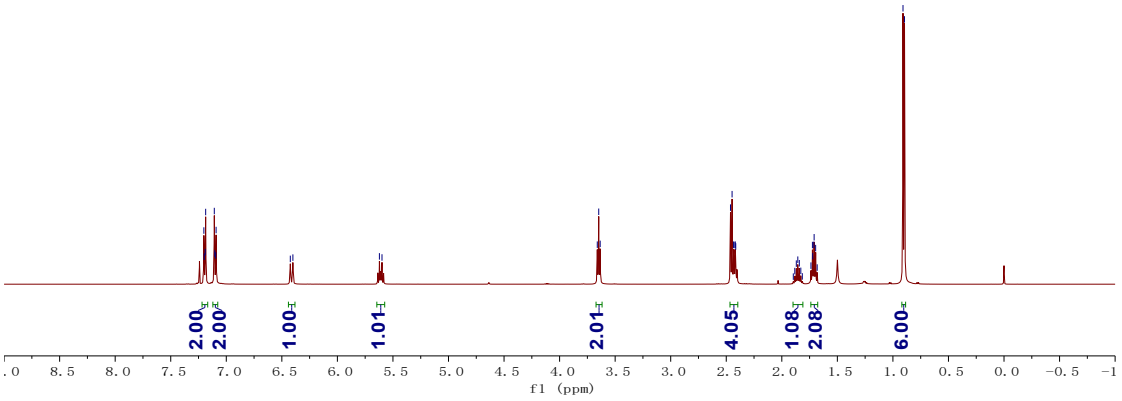
f1 (ppm)


-113.6368
F
OH
1j
20 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −110 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210
f1 (ppm)


7.2018
7.1981
7.1896
7.1856
7.1079
7.1038
7.0953
7.0917
6.4238
6.4006
5.6218
5.5985
3.6608
3.6478
3.6348
2.4619
2.4476
2.4335
2.4298
2.4185
2.4147
1.8830
1.8695
1.8560
1.8425
1.8289
1.7376
1.7244
1.7220
1.7113
1.7091
1.6954
1.6817
0.9092

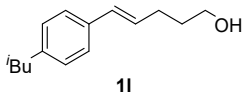

OH
iBu

1l

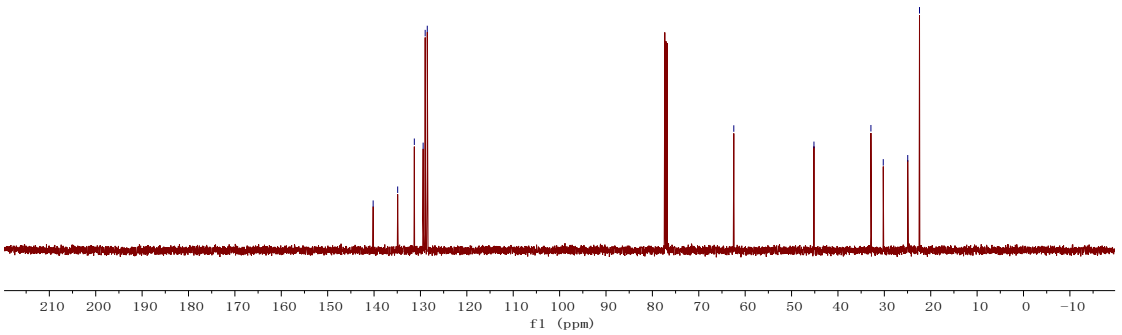

2.00
2.00
1.00
1.01
2.01
4.05
1.08
2.08
6.00
f1 (ppm)

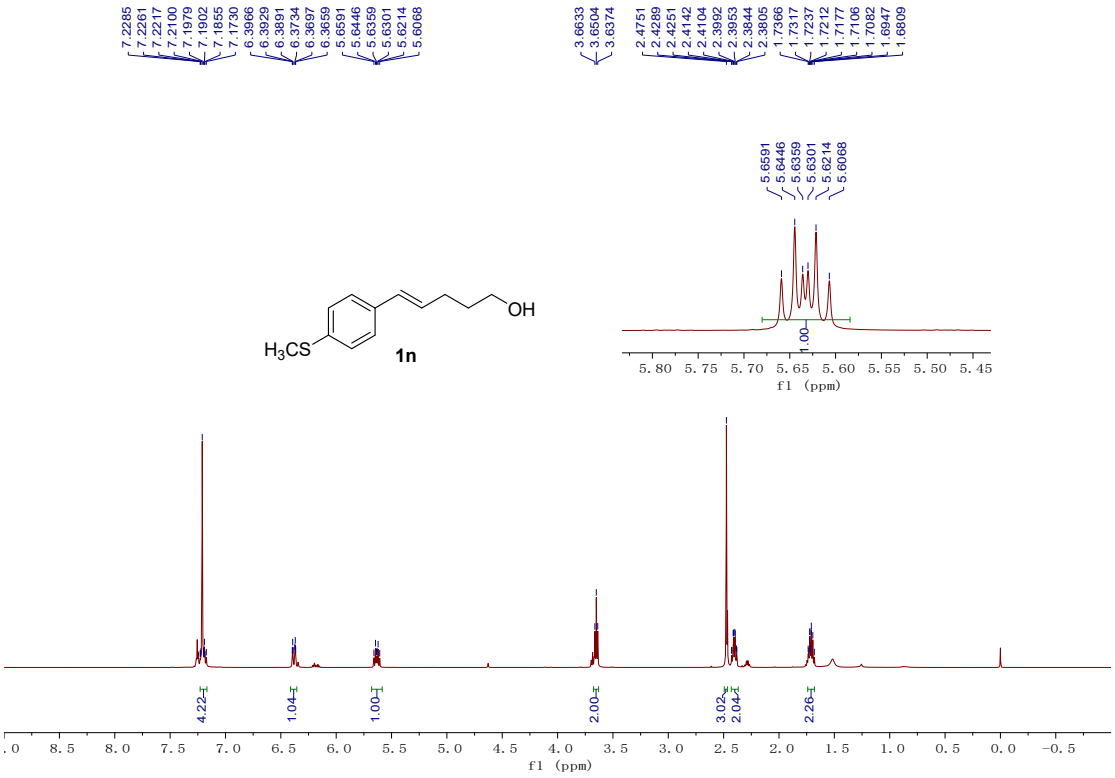

140.1968
134.9093
131.3204
129.4203
128.9814
128.5282

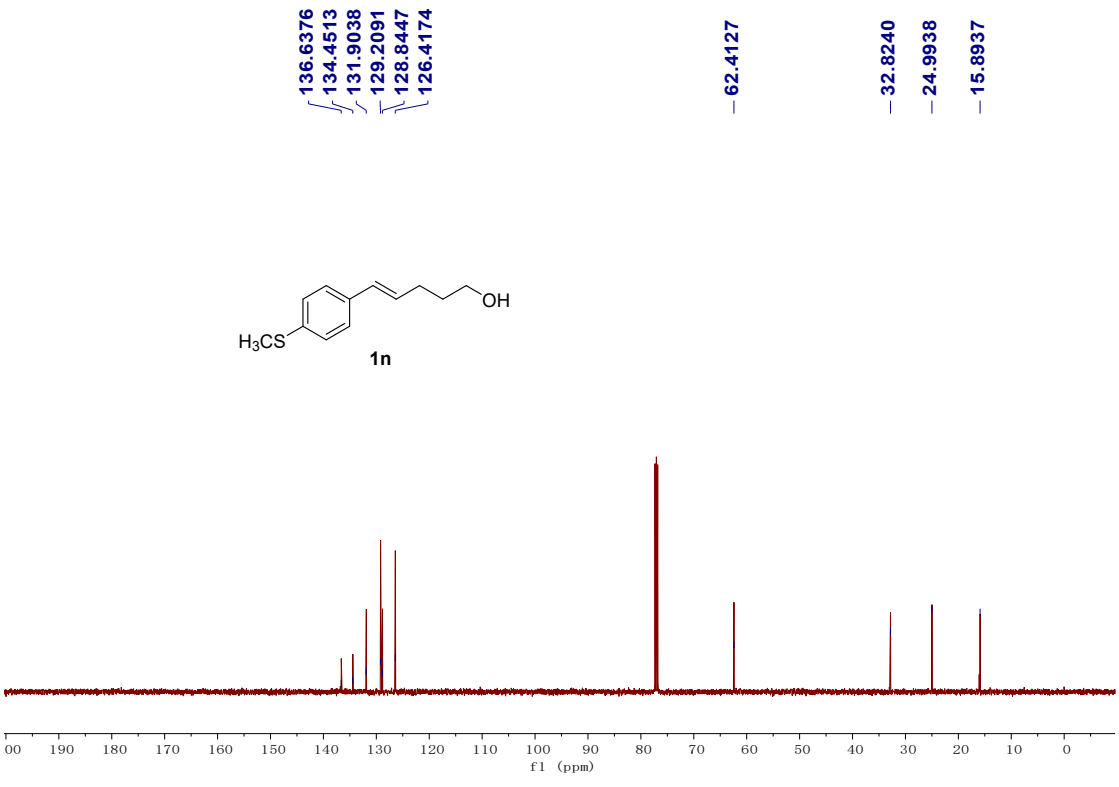

62.4520
45.1722
32.8931
30.2338
24.9569
22.4189

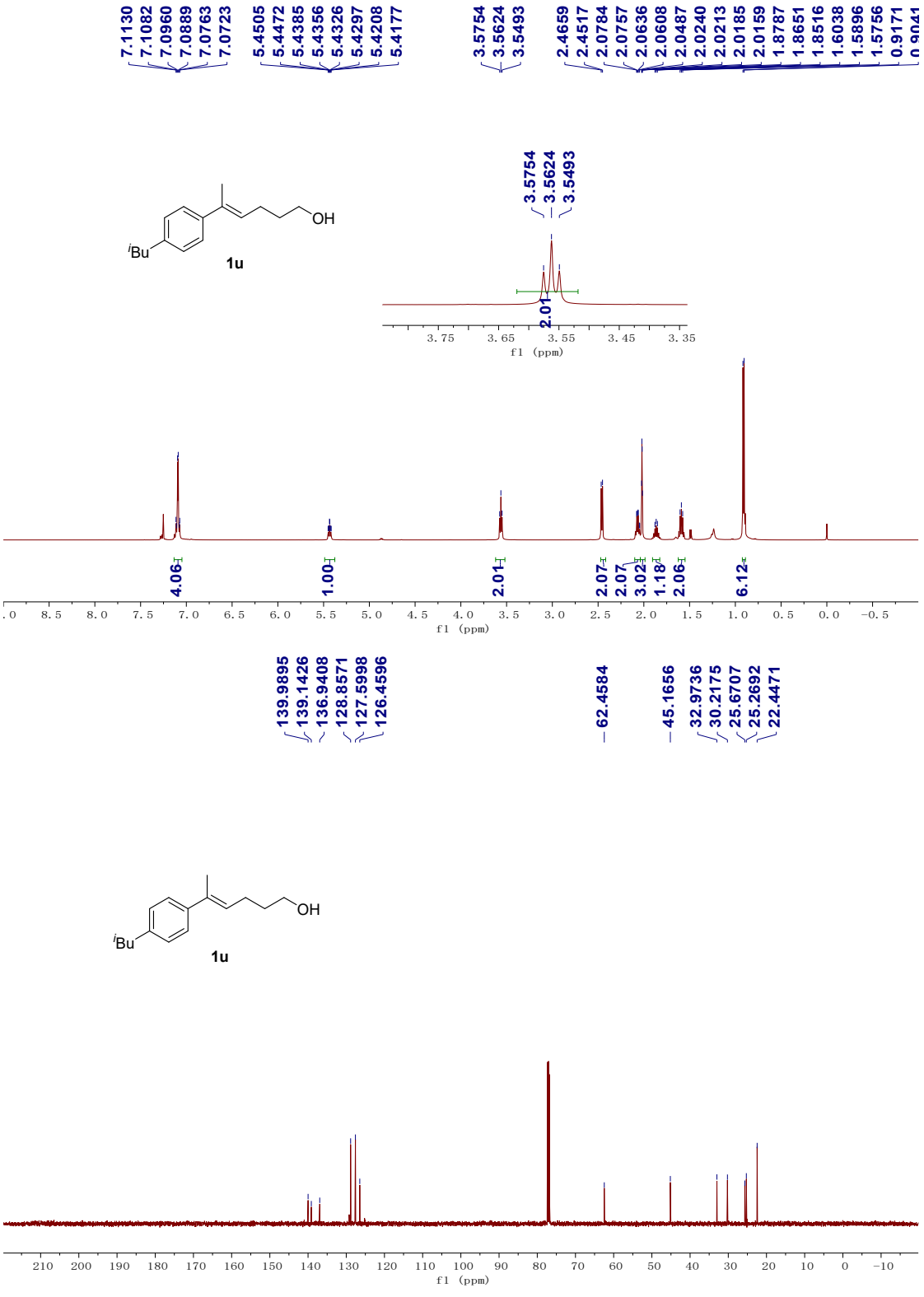

OH
iBu

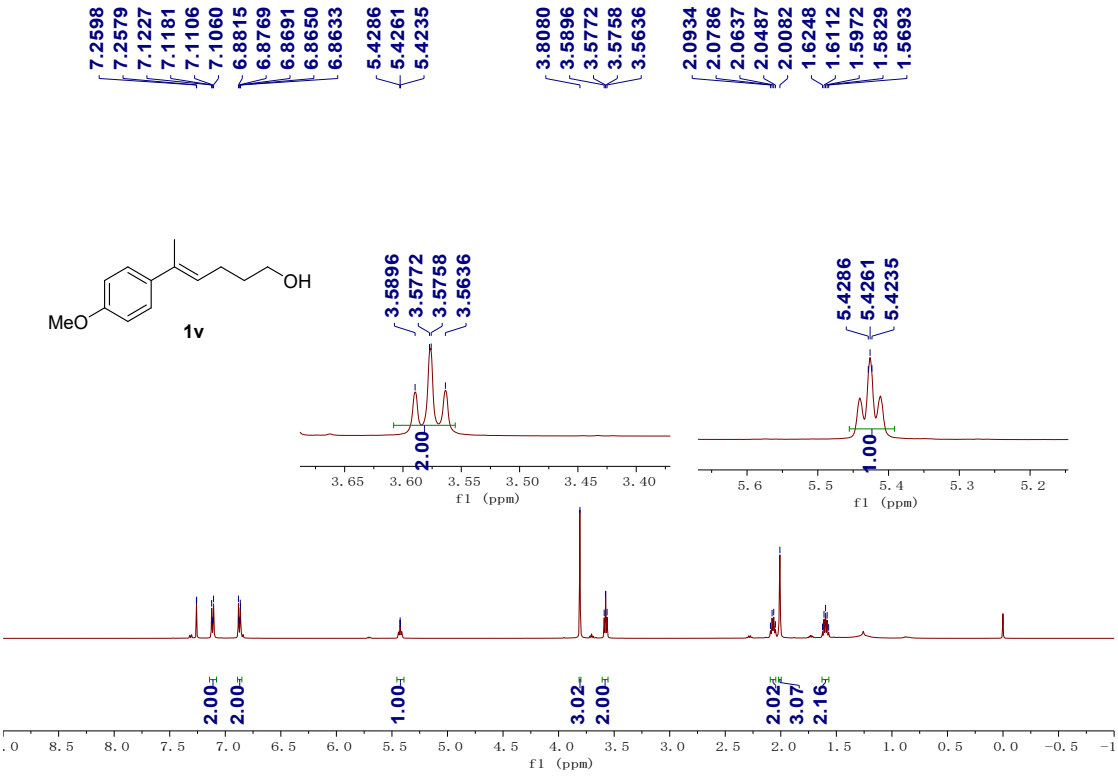
1l

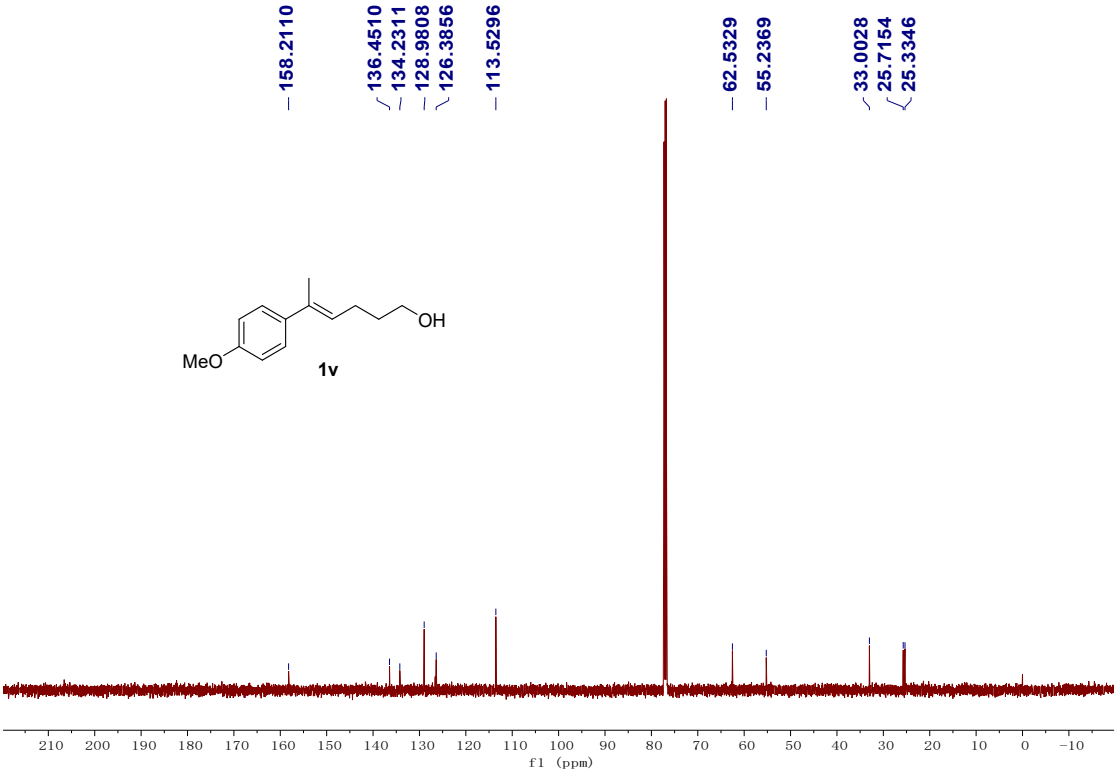

f1 (ppm)

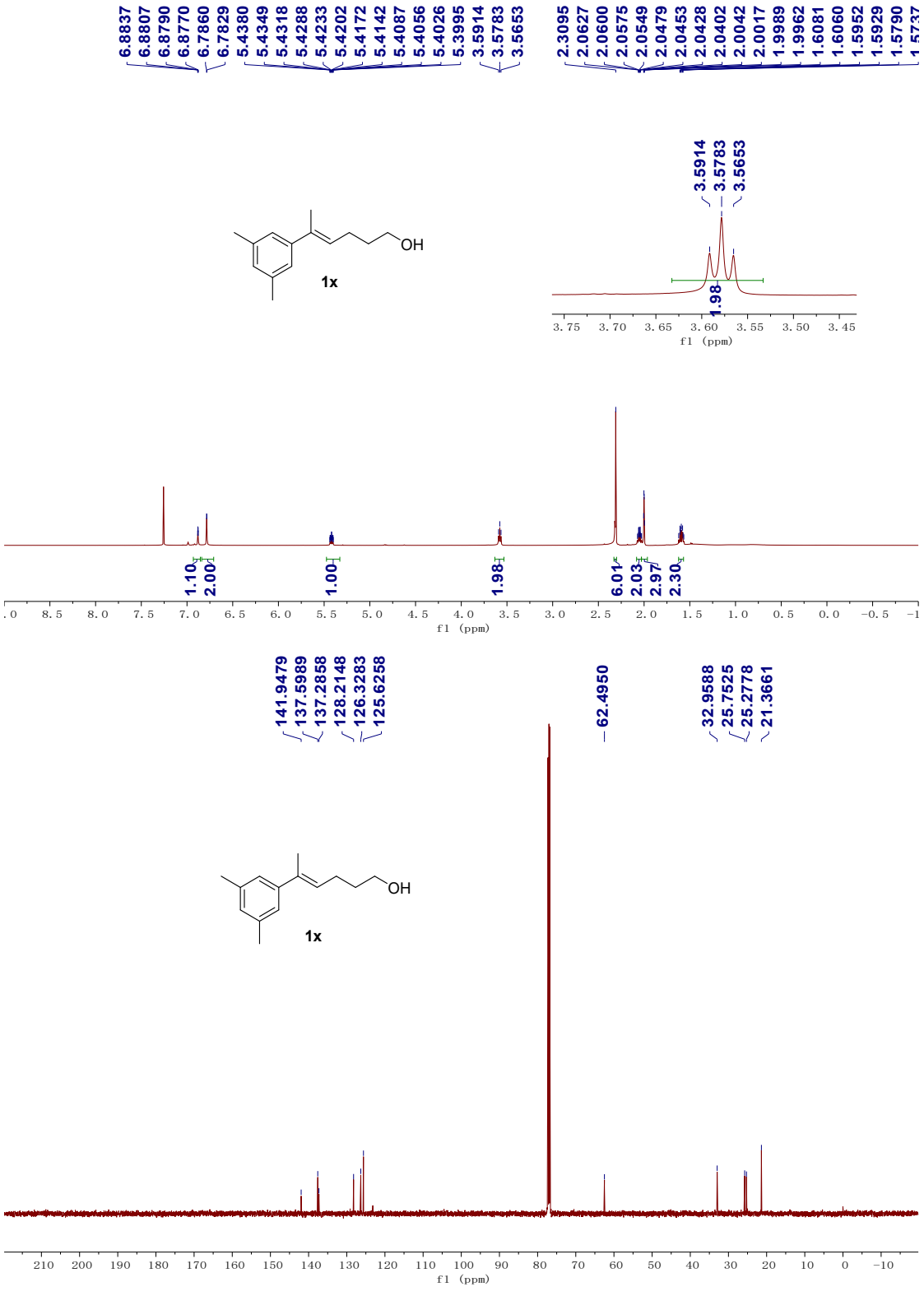

7.2285
7.2261
7.2217
7.2100
7.1979
7.1902
7.1855
7.1730
6.3966
6.3929
6.3891
6.3734
6.3697
6.3659
5.6591
5.6446
5.6359
5.6301
5.6214
5.6068
3.6633
3.6504
3.6374
2.4751
2.4289
2.4251
2.4142
2.4104
2.3992
2.3953
2.3844
2.3805
1.7366
1.7317
1.7237
1.7212
1.7177
1.7106
1.7082
1.6947
1.6809
OH
H3CS
1n
1.00
f1 (ppm)
4.22
1.04
1.00
2.00
3.02
2.04
2.26
f1 (ppm)

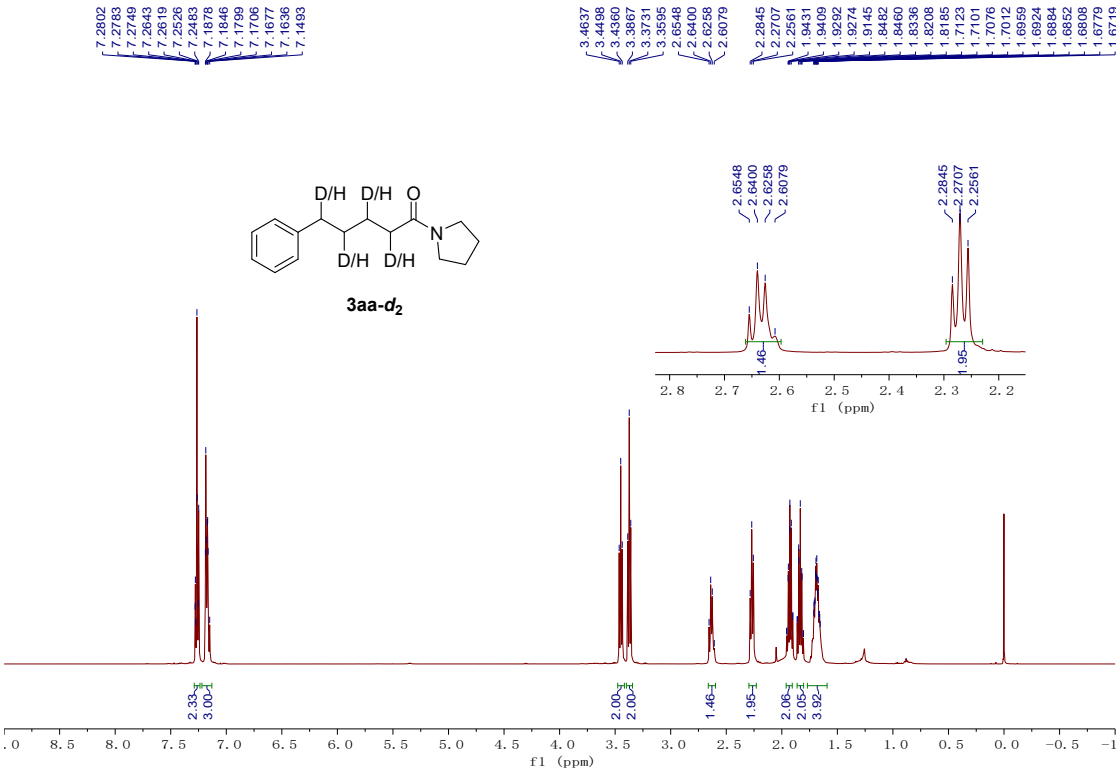

136.6376
134.4513
131.9038
129.2091
128.8447
126.4174
62.4127
32.8240
24.9938
15.8937
OH
H3CS
1n
f1 (ppm)


7.1130
7.1082
7.0960
7.0889
7.0763
7.0723
5.4505
5.4472
5.4385
5.4356
5.4326
5.4297
5.4208
5.4177
3.5754
3.5624
3.5493
2.4659
2.4517
2.0784
2.0757
2.0636
2.0608
2.0487
2.0240
2.0213
2.0185
2.0159
1.8787
1.8651
1.8516
1.6038
1.5896
1.5756
0.9171
OH
iBu
1u
2.01
f1 (ppm)
4.06
1.00
2.01
2.07
2.07
3.02
1.18
2.06
6.12
f1 (ppm)
139.9895
139.1426
136.9408
128.8571
127.5998
126.4596
62.4584
45.1656
32.9736
30.2175
25.6707
25.2692
22.4471
OH
iBu
1u
f1 (ppm)


7.2598
7.2579
7.1227
7.1181
7.1106
7.1060
6.8815
6.8769
6.8691
6.8650
6.8633
5.4286
5.4261
5.4235
3.8080
3.5896
3.5772
3.5758
3.5636
2.0934
2.0786
2.0637
2.0487
2.0082
1.6248
1.6112
1.5972
1.5829
1.5693
MeO
OH
1v
3.5896
3.5772
3.5758
3.5636
2.00
5.4286
5.4261
5.4235
1.00
f1 (ppm)
2.00
2.00
1.00
3.02
2.00
2.02
3.07
2.16
f1 (ppm)


158.2110
136.4510
134.2311
128.9808
126.3856
113.5296
62.5329
55.2369
33.0028
25.7154
25.3346
MeO
OH
1v
f1 (ppm)


6.8837
6.8807
6.8790
6.8770
6.7860
6.7829
5.4380
5.4349
5.4318
5.4288
5.4233
5.4202
5.4172
5.4142
5.4087
5.4056
5.4026
5.3995
3.5914
3.5783
3.5653
2.3095
2.0627
2.0600
2.0575
2.0549
2.0479
2.0453
2.0428
2.0402
2.0042
2.0017
1.9989
1.9962
1.6081
1.6060
1.5952
1.5929
1.5790
OH
1x
3.5914
3.5783
3.5653
1.98
f1 (ppm)
1.10
2.00
1.00
1.98
6.01
2.03
2.97
2.30
f1 (ppm)
141.9479
137.5989
137.2858
128.2148
126.3283
125.6258
62.4950
32.9588
25.7525
25.2778
21.3661
OH
1x
f1 (ppm)


7.2802
7.2783
7.2749
7.2643
7.2619
7.2526
7.2483
7.1878
7.1846
7.1799
7.1706
7.1677
7.1636
7.1493
3.4637
3.4498
3.4360
3.3867
3.3731
3.3595
2.6548
2.6400
2.6258
2.6079
2.2845
2.2707
2.2561
1.9431
1.9409
1.9292
1.9274
1.9145
1.8482
1.8460
1.8336
1.8208
1.8185
1.7123
1.7101
1.7076
1.7012
1.6959
1.6924
1.6884
1.6852
1.6808
1.6779
1.6719
D/H D/H O
N
D/H D/H
3aa-d_2
2.33
3.00
2.00
2.00
1.46
1.95
2.06
2.05
3.92
f1 (ppm)
1.46
1.95
f1 (ppm)