Supporting Information for

Efficient Amide Bond Formation via Tropylium Ion Organocatalysis

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General experimental information

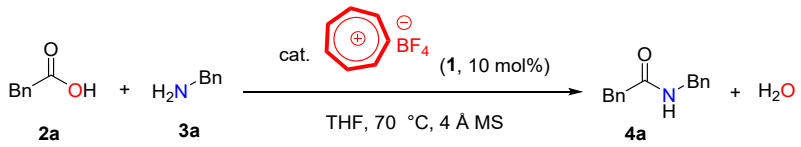
All reagents and solvents were purchased and used as received from commercial suppliers or synthesized according to cited procedures. Oxygen and moisture sensitive reactions were carried out in dried glassware under nitrogen atmosphere. Flash chromatography was performed using 15-45 μm silica gel cartridges (60 Å mesh) on a Teledyne ISCO Combiflash Rf. SiliaSep. SiO2 cartridges used for all the purifications were provided by SiliCycle. Analytical thin layer chromatography (TLC) was performed on E. Merck silica gel 60 F254 plates and the spots were visualized by UV light (254 nm). NMR spectra for the characterization of compounds were recorded at room temperature on a Bruker instrument 400 MHz (^{1}H) and at 101 MHz (^{13}C), or 500 MHz (^{1}H) and at 126 MHz (^{13}C). All the NMR data were collected for $CDCl_3$ and DMSO-d6 solutions at ambient temperature. Chemical shifts (δ) are reported in parts per million (ppm) relative to CHCl3 (δ (H) =7.26 ppm and δ(C) = 77.2 ppm) and DMSO solvent peaks (δ (H) = 2.50 ppm and δ(C) = 39.5 ppm). Data for ^{1}H-NMR are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz), and integration. High resolution mass spectroscopy (HRMS) measurements were carried out on a Bruker microTOF/ESI mass spectrometer, and HRMS data analysis was performed using the software “Bruker Daltonics DataAnalysis”, version 4.0 SP5.

General Procedure - Substrate Scope

Procedure A for substrates in Scheme 1

To a 5 mL Schlenk tube loaded with a stirring bar containing the phenylacetic acid or benzoic acid derivatives (1mmol, 1Equiv.) and activated molecular sieves 4 Å pellets (0.5 g) tropylium tetrafluoroborate (catalyst) **1** (0.2 mmol, 10 mol%) and dry THF (5 mL) was added through the septa, primary or secondary amine 3a (1 mmol, 1Equiv) was added slowly through the septa and the resulting mixture was then heated to 70-90 °C for 15 hours. The crude reaction mixture was filtered through a pad of silica eluted with 100 mL EtOAc:Et3N (100:1) and the target product was isolated from the crude mixture by column chromatography (silica-gel, hexane/ethyl acetate).

Table S1. Optimization of the tropylium-catalyzed reaction between 2a and 3aa



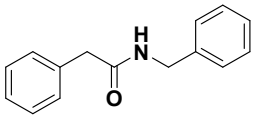
Entry[a]	cat.	mol (%)	solvent	*T* (°C)	*t* (h)	4a[b] (%)
1	1	no cat.	THF	70°C	15	<10%
2	1	5 mol%	DCM	rt	15	30
3	1	5 mol%	DCM	50 °C	15	37
4	1	5 mol%	DCM	70 °C	15	46
5	1	10 mol%	THF	45°C	7	49
6	**1**	**10 mol%**	**THF**	**70 °C**	**15 h**	**89**
7	1	10 mol%	DCE	70 °C	15 h	55
8	1	10 mol%	DMF	70 °C	15 h	62
9	1	10 mol%	toluene	70 °C	15 h	37
10	1	10 mol%	MeCN	70 °C	15 h	55
11	1	10 mol%	1,4-Dioxan	70 °C	15 h	45
12	1	10 mol%	MeOH	70 °C	15 h	61
13[c]	1	10 mol%	THF	150 °C	1 h *mw*	51
14	1	5 mol%	THF	70°C	15	69
15	1	1 mol%	THF	70°C	15	35
16[d]	HBF_4	10 mol%	THF	70°C	15	15
17[d]	TfOH	10 mol%	THF	70°C	15	18

[a] Reaction conditions: 1 mmol **2a** in the indicated solvent, 1 mmol **3a** and catalyst **1** in microwave vial at the indicated temperature for the indicated time. [b]Yield of the isolated **4a**.[c] Reaction was run with 150 °C. [d]10 mol% of a Brønsted acid catalyst was used instead of tropylium catalyst **1**.

Characterization data

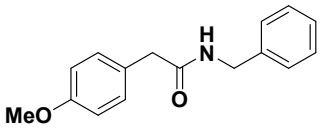
Substrate synthesis

***N*-benzyl-2-phenylacetamide** (**4a**) Prepared by general procedure A using phenylacetic acid and benzylamine. Compound 4a was obtained as a white solid (200 mg, 89% yield).



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.27 (m, 8H), 7.21 – 7.17 (m, 2H), 5.90 (s, 1H), 4.41 (d, J = 5.8 Hz, 2H), 3.62 (s, 2H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 171.1, 138.3, 134.1, 129.6, 129.2, 128.8, 127.6, 127.5, 127.5, 43.9, 43.7.
Characterization data was in accordance with previously reported[1]

***N*-benzyl-2-(4-methoxyphenyl)acetamide** (**4b**) Prepared by procedure A from 4-methoxyphenylacetic acid, tropylium tetrafluoroborate and benzylamine as amine group source to give compound 4b as a white crystal (209 mg, 82% yield).

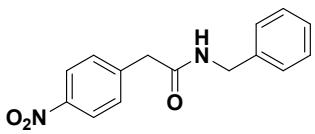


^{1}H NMR (400 MHz, $CDCl_3$) δ 3.40 (s, 2H), 3.72 (s, 3H), 4.26 (d, J =5.9, 2H), 6.84-6.89 (m, 2H), 7.17-7.24 (m, 5H), 7.28-7.33 (m, 2H), 8.47 (t, J = 5.3, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 41.5, 42.3, 55.0, 113.7, 126.8,127.2, 128.3, 128.4, 130.0, 139.5, 158.0, 170.6.

Characterization data matches the literature report[1]

***N*-benzyl-2-(4-nitrophenyl)acetamide** (**4c**) Prepared by general procedure A using 4-nitrophenylacetic acid and benzylamine. Compound 4c was obtained as a bile solid (213 mg, 79 % yield).

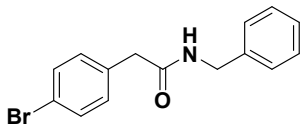


^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 – 8.14 (m, 2H), 7.49 – 7.44 (m, 2H), 7.35 – 7.27 (m, 3H), 7.24 – 7.20 (m, 2H), 5.79 (s, 1H), 4.44 (d, J = 5.7 Hz, 2H), 3.67 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.1, 147.4, 142.3, 137.8, 130.4, 128.9, 127.9, 124.1, 44.1, 43.4.

Characterization data was in accordance with previously reported[2]

***N*-benzyl-2-(4-bromophenyl)acetamide** (**4d**) Prepared by general procedure A using 4-bromophenylacetic acid and benzylamine. Compound 4d was obtained as a colorless crystal (205 mg, 68% yield).

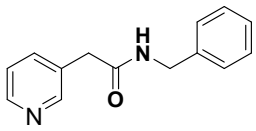


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.40 (m, 2H), 7.29 (ddd, J = 12.5, 7.7, 6.0 Hz, 3H), 7.17 (ddd, J = 17.4, 7.3, 1.9 Hz, 4H), 5.77 (s, 1H), 4.40 (d, J = 5.8 Hz, 2H), 3.54 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 138.1, 133.9, 132.2, 131.2, 128.8, 127.7, 127.7, 121.5, 43.8, 43.2.

Characterization data was in accordance with previously reported[3]

***N*-benzyl-2-(pyridin-3-yl)acetamide** (**4e**) Prepared by general procedure A using 2-(pyridin-3-yl)acetic acid and benzylamine. Compound 4e was obtained as a colorless crystal (164 mg, 73 % yield).

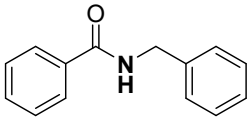


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 7.40 (m, 2H), 7.29 (ddd, J = 12.5, 7.7, 6.0 Hz, 3H), 7.17 (ddd, J = 17.4, 7.3, 1.9 Hz, 4H), 5.77 (s, 1H), 4.40 (d, J = 5.8 Hz, 2H), 3.54 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 138.1, 133.9, 132.2, 131.2, 128.8, 127.7, 127.7, 121.5, 43.8, 43.2.

Characterization data was in accordance with previously reported[3]

***N*-benzylbenzamide** (**4f**) Prepared by general procedure A using benzoic acid and benzylamine. Compound 4f was obtained as a colorless oil (162 mg, 75% yield).

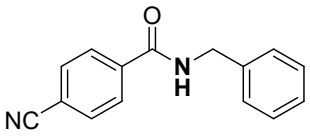


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (dt, J = 8.5, 1.9, 1.9 Hz, 2H), 7.63 – 7.22 (m, 8H), 6.49 (s, 1H), 4.65 (d, J = 5.7 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 167.5, 138.3, 134.5, 131.7, 128.9, 128.7, 128.1, 127.8, 127.1, 44.3.

Characterization data was in accordance with previously reported[4]

***N*-benzyl-4-cyanobenzamide** (**4g**) Prepared by general procedure A using 4-cyanobenzoic acid and benzylamine. Compound 4g was obtained as a yellowish oil (189 mg, 81% yield).

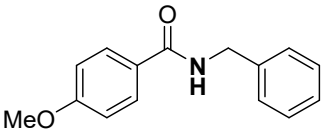


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.9 (d, J = 8.1 Hz, 2H), 7.7 (d, J = 8.0 Hz, 2H), 7.4 – 7.2 (m, 5H), 6.6 (s, 1H), 4.6 (d, J = 5.6 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.0, 137.6, 133.5, 133.3, 133.2, 133.0, 128.8, 127.8, 127.7, 127.3, 125.6, 125.5, 125.4, 44.2.

Characterization data was in accordance with previously reported[4]

***N*-benzyl-4-methoxybenzamide** (**4h**) Prepared by general procedure A using 4-methoxybenzoic acid and benzylamine. Compound 4h was obtained as a colorless oil (185 mg, 77 % yield).

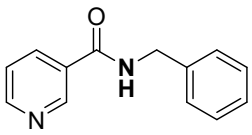


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.74 (m, 2H), 7.36 (d, *J* = 4.3 Hz, 5H), 6.92 (d, *J* = 8.8 Hz, 2H), 6.33 (s, 1H), 4.64 (d, *J* = 5.6 Hz, 2H), 3.84 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 166.9, 162.3, 138.4, 128.8, 128.7, 127.9, 127.6, 126.7, 113.8, 55.4, 44.1.

Characterization data was in accordance with previously reported[4]

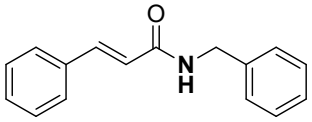
***N*-benzylnicotinamide** (**4i**) Prepared by procedure A from isonicotinic acid, tropylium tetrafluoroborate and benzylamine as amine group source to give compound 4i as a yellowish oil (116 mg, 55 % yield).



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.79 (m, 1H), 7.52 – 7.48 (m, 1H), 7.46 – 7.41 (m, 2H), 7.38 – 7.32 (m, 5H), 6.36 (s, 1H), 4.66 (d, *J* = 5.6 Hz, 2H).

Characterization data matches the literature report[4]

***N*-benzylcinnamamide** (**4j**) Prepared by general procedure A using cinnamic acid and benzylamine. Compound 4j was obtained as a white solid (175 mg, 74% yield).

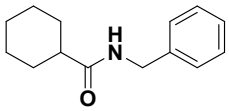


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 15.6 Hz, 1H), 7.51 – 7.48 (m, 2H), 7.39 – 7.31 (m, 8H), 6.41 (d, *J* = 15.6 Hz, 1H), 5.90 (s, 1H), 4.58 (d, *J* = 5.7 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9, 141.6, 138.3, 134.9, 129.9, 128.9, 128.9, 128.1, 127.9, 127.8, 120.5, 44.1.

Characterization data was in accordance with previously reported[5]

***N*-benzylcyclohexanecarboxamide** (**4k**) Prepared by general procedure A using cyclohexanecarboxylic acid and benzylamine. Compound 4k was obtained as a white powder (154 mg, 71 % yield).

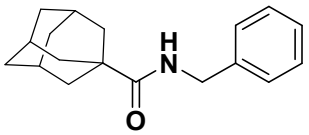


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.26 (m, 5H), 6.67 (tt, *J* = 3.8, 3.8, 1.8, 1.8 Hz, 1H), 5.95 (s, 1H), 4.50 (d, *J* = 5.7 Hz, 2H), 2.25 (dddd, *J* = 8.6, 6.2, 2.6, 1.6 Hz, 2H), 2.16 (dddd, *J* = 8.8, 6.2, 3.9, 2.6 Hz, 2H), 1.83 – 1.39 (m, 5H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 168.6, 138.7, 133.9, 133.1, 128.9, 127.9, 127.6, 43.8, 25.5, 24.5, 22.7, 21.7.

Characterization data was in accordance with previously reported[6]

***N*-benzyladamantane-1-carboxamide** (**4l**) Prepared by general procedure A using 1-adamantanecarboxylic acid and benzylamine. Compound 4l was obtained as a yellowish oil (177 mg, 66% yield).

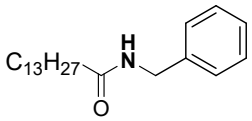


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.26 (m, 4H), 7.26 – 7.23 (m, 1H), 5.85 (s, 1H), 4.44 (d, *J* = 5.6 Hz, 2H), 2.05 (p, *J* = 3.2, 3.2, 3.2, 3.2 Hz, 3H), 1.89 (d, *J* = 2.9 Hz, 6H), 1.79 – 1.60 (m, 7H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 128.9, 127.8, 127.6, 43.5, 40.8, 39.5, 36.7, 28.8.

Characterization data was in accordance with previously reported[7]

***N*-benzyltetradecanamide** (**4m**) Prepared by general procedure A using myristic acid and benzylamine. Compound 4m was obtained as a white powder (264 mg, 85% yield).

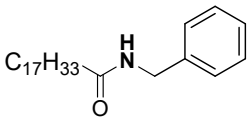


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.31 (m, 2H), 7.27 (dd, *J* = 7.1, 3.4 Hz, 3H), 5.77 (s, 1H), 4.43 (d, *J* = 5.6 Hz, 2H), 2.22 – 2.18 (m, 2H), 1.65 (t, *J* = 7.3, 7.3 Hz, 2H), 1.25 (s, 18H), 0.90 – 0.86 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) ***δ*** 173.1, 138.6, 128.8, 127.9, 127.6, 43.7, 36.9, 32.1, 29.8, 29.8, 29.7, 29.6, 29.5, 29.5, 25.9, 22.8, 14.3.

Characterization data was in accordance with previously reported[8]

(*E*)-*N*-benzyloctadec-9-enamide (**4n**) Prepared by general procedure A using oleic acid and benzylamine. Compound 4n was obtained as a colorless crystal (273 mg, 73 % yield).

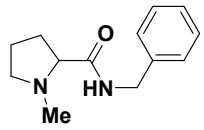


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.26 (m, 5H), 5.67 (s, 1H), 5.36 – 5.31 (m, 2H), 4.45 (d, *J* = 5.7 Hz, 2H), 2.24 – 2.18 (m, 2H), 2.04 – 1.97 (m, 4H), 1.66 (td, *J* = 7.5, 7.1, 3.3 Hz, 2H), 1.33 – 1.26 (m, 18H), 0.89 – 0.86 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 138.6, 130.2, 129.9, 128.9, 128.0, 127.7, 43.8, 36.9, 32.1, 29.9, 29.9, 29.7, 29.5, 29.4, 29.4, 29.3, 27.4, 27.3, 25.9, 22.8, 14.3.

Characterization data was in accordance with previously reported[9]

***(R)-N*-benzyl-1-methylpyrrolidine-2-carboxamide** (**4o**) Prepared by general procedure A using *N*-methyl-L-proline and benzyl amine. Compound 4o was obtained as a yellowish oil (133mg, 61 % yield).

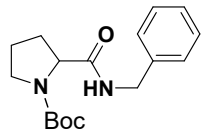


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (s, 1H), 7.35 – 7.25 (m, 5H), 4.50 – 4.42 (m, 2H), 3.11 – 3.02 (m, 1H), 2.95 (dd, *J* = 10.2, 5.4 Hz, 1H), 2.35 (s, 3H), 2.34 – 2.16 (m, 2H), 1.92 – 1.83 (m, 1H), 1.80 – 1.71 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.7, 138.8, 128.8, 127.6, 127.4, 69.1, 56.8, 42.9, 41.9, 31.3, 24.5.

Characterization data was in accordance with previously reported[10]

***tert*-butyl-2-(benzylcarbamoyl)pyrrolidine-1-carboxylate** (**4p**) Prepared by general procedure B using *N*-Boc-*L*-proline and benzyl amine. Compound 4p was obtained as a yellow oil (163 mg, 54 %yield).

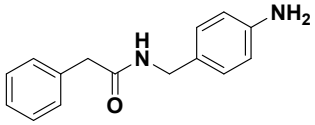


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.23 (m, 5H), 4.63 – 4.21 (m, 3H), 3.51 – 3.26 (m, 2H), 2.46 – 1.77 (m, 4H), 1.49 – 1.27 (m, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.4, 172.1, 138.3, 128.7, 127.5, 80.6, 61.4, 60.1, 47.2, 43.4, 31.1, 28.4, 24.7, 23.8.

Characterization data was in accordance with previously reported[11]

***N*-(4-aminobenzyl)-2-phenylacetamide** (**4q**) Prepared by general procedure A using phenylacetic acid and 4-aminobenzylamine. Compound 4q was obtained as a colorless oil (206 mg, 86% yield).

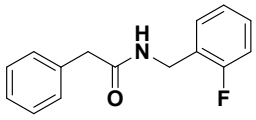


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.22 (m, 7H), 7.09 – 6.98 (m, 2H), 5.94 (s, 1H), 4.45 (d, *J* = 6.0 Hz, 2H), 3.59 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.1, 134.8, 130.1, 130.0, 129.5, 129.3, 129.3, 129.1, 127.5, 125.2, 124.4, 124.3, 115.5, 115.3, 43.8, 37.7, 37.7.

Characterization data was in accordance with previously reported[12]

***N*-(2-fluorobenzyl)-2-phenylacetamide** (**4r**) Prepared by general procedure A using phenylacetic acid and 2-fluorobenzylamine. Compound 4r was obtained as a colorless crystal (168 mg, 69 % yield).

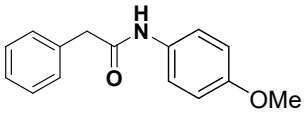


^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.39 – 7.22 (m, 7H), 7.13 – 6.96 (m, 2H), 5.80 (s, 1H), 4.45 (d, *J* = 6.1 Hz, 2H), 3.61 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 171.1, 134.8, 130.1, 130.1, 129.6, 129.4, 129.3, 129.2, 127.6, 125.3, 124.4, 124.4, 115.6, 115.4, 43.9, 37.8, 37.8.

Characterization data was in accordance with previously reported[13]

***N*-(4-methoxyphenyl)-2-phenylacetamide** (**4s**) Prepared by general procedure A using phenylacetic acid and 4-methoxyaniline. Compound 4s was obtained as a white solid (155 mg, 64 % yield).

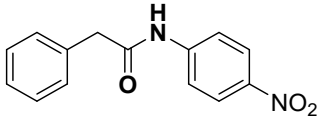


^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.50 (d, *J* = 11.5 Hz, 1H), 8.33 (d, *J* = 1.8 Hz, 1H), 7.44 (d, *J* = 9.0 Hz, 2H), 7.03 (d, *J* = 8.9 Hz, 2H), 6.91 – 6.86 (m, 4H), 3.81 (s, 2H), 3.80 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 152.9, 137.9, 131.2, 128.8, 125.5, 124.6, 117.4, 113.8, 112.7, 55.8, 40.9.

Characterization data was in accordance with previously reported[14]

***N*-(4-nitrophenyl)-2-phenylacetamide** (**4t**) Prepared by general procedure A using phenylacetic acid and 4-nitroaniline. Compound 4t was obtained as a yellow solid (172 mg, 67 % yield).

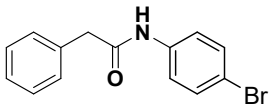


^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.09 – 8.03 (m, 5H), 7.36 – 7.26 (m, 3H), 6.67 – 6.58 (m, 5H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 152.66, 129.60, 128.89, 127.55, 126.60, 113.63, 41.13.

Characterization data was in accordance with previously reported[15]

***N*-(4-bromophenyl)-2-phenylacetamide** (**4u**) Prepared by general procedure A using phenylacetic acid and 4-bromoaniline. Compound 4u was obtained as a white solid (153 mg, 61 % yield).

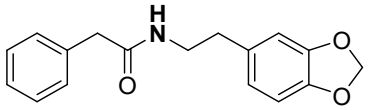


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.37 (m, 4H), 7.32 (td, *J* = 6.3, 5.9, 2.0 Hz, 5H), 7.08 (s, 1H), 3.73 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.2, 136.8, 134.3, 132.1, 129.7, 129.5, 127.9, 121.5, 117.2, 44.9.

Characterization data was in accordance with previously reported[16]

***N*-(2-(benzo[d][1,3]dioxol-5-yl)ethyl)-2-phenylacetamide** (**4v**) Prepared by general procedure A using phenylacetic acid and homopiperonylamine. Compound 4v was obtained as a bile solid (171 mg, 72% yield).

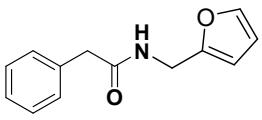


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.25 (m, 3H), 7.21 – 7.14 (m, 2H), 6.65 (d, *J* = 7.8 Hz, 1H), 6.53 (d, *J* = 1.7 Hz, 1H), 6.44 (dd, *J* = 7.9, 1.7 Hz, 1H), 5.88 (s, 2H), 5.71 (s, 1H), 3.50 (s, 2H), 3.38 (td, *J* = 6.8, 6.8, 5.8 Hz, 2H), 2.62 (t, *J* = 6.9, 6.9 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 147.7, 146.1, 134.9, 132.4, 129.4, 128.9, 127.2, 121.5, 108.9, 108.2, 100.8, 43.7, 40.8, 35.1.

Characterization data was in accordance with previously reported[17]

***N*-(furan-2-ylmethyl)-2-phenylacetamide** (**4w**) Prepared by general procedure A using phenylacetic acid and furfuryl amine. Compound 4w was obtained as a yellowish oil (159 mg, 74 % yield).

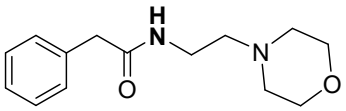


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.16 (m, 5H), 6.19 (dd, J = 3.2, 1.9 Hz, 1H), 6.04 (dq, J = 3.2, 0.8, 0.8, 0.8 Hz, 1H), 6.01 (d, J = 5.9 Hz, 1H), 4.28 (dd, J = 5.6, 0.8 Hz, 2H), 3.47 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 151.3, 142.1, 134.8, 129.4, 128.9, 127.3, 110.4, 107.26, 43.6, 36.7.

Characterization data was in accordance with previously reported[18]

***N*-(2-morpholinoethyl)-2-phenylacetamide** (**4x**) Prepared by general procedure A using phenylacetic acid and 4-(2-Aminoethyl)morpholine). Compound 4x was obtained as a brown viscous oil (185 mg, 75 % yield).

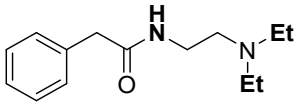


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.18 (m, 5H), 6.21 (s, 1H), 3.50 – 3.45 (m, 6H), 3.24 – 3.20 (m, 2H), 2.33 (t, J = 6.1, 6.1 Hz, 2H), 2.26 (t, J = 4.7, 4.7 Hz, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.1, 135.2, 129.6, 129.1, 127.4, 66.8, 56.4, 53.1, 43.9, 35.7.

HRMS (ESI+) m/z [M+Na]: Calc. for $C_{11}H_{12}O_2$+Na 248.1500; Found 248.1211.

***N*-benzyl-4-cyanobenzamide** (**4y**) Prepared by general procedure A using 3-isopropoxypropylamine and benzylamine. Compound 4y was obtained as a white crystal (140 mg, 60 % yield).

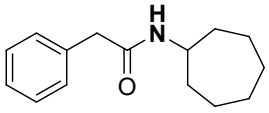


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.18 (m, 5H), 6.54 (s, 1H), 3.48 (s, 2H), 3.21 – 3.17 (m, 2H), 2.45 – 2.35 (m, 6H), 0.82 (t, J = 7.2, 7.2 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 135.1, 129.2, 128.6, 126.9, 50.9, 46.5, 43.5, 36.6, 11.5.

Characterization data was in accordance with previously reported[19]

***N*-cycloheptyl-2-phenylacetamide** (**4z**) Prepared by general procedure A using phenylacetic acid and cycloheptylamine. Compound 4z was obtained as a white powder (175 mg, 76 % yield).

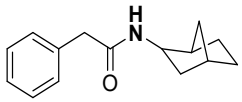


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.25 (m, 5H), 5.26 (s, 1H), 3.98 – 3.89 (m, 1H), 3.54 (s, 2H), 1.85 – 1.78 (m, 2H), 1.60 – 1.52 (m, 4H), 1.50 – 1.43 (m, 4H), 1.34 – 1.27 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 135.3, 129.5, 129.1, 127.4, 52.9, 44.0, 42.4, 40.5, 35.7, 35.6, 28.2, 26.5.

Characterization data was in accordance with previously reported[20]

***N*-((1R,4S)-bicyclo[2.2.1]heptan-2-yl)-2-phenylacetamide** (**4za**) Prepared by general procedure A using phenylacetic acid and exo-2-aminonorbornane. Compound 4za was obtained as a brown solid (158 mg, 69 % yield).

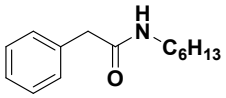


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.24 (m, 5H), 5.20 (s, 1H), 3.71 – 3.66 (m, 1H), 3.53 (s, 2H), 2.20 – 2.11 (m, 2H), 1.73 (ddd, J = 13.2, 8.0, 2.3 Hz, 1H), 1.49 – 1.38 (m, 2H), 1.24 – 1.18 (m, 1H), 1.11 – 0.96 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 169.83, 135.31, 129.53, 129.13, 127.41, 50.50, 44.19, 35.00, 27.96, 24.12.

Characterization data was in accordance with previously reported[21]

***N*-hexyl-2-phenylacetamide** (**4zb**) Prepared by general procedure A using phenylacetic acid and hexylamine. Compound 4zb was obtained as a white solid (177 mg, 81 % yield).

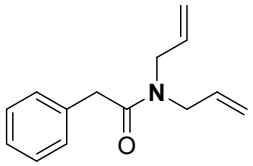


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.24 (m, 5H), 5.48 (s, 1H), 3.56 (s, 2H), 3.19 (td, J = 7.3, 7.2, 5.8 Hz, 2H), 1.44 – 1.36 (m, 2H), 1.27 – 1.19 (m, 6H), 0.88 – 0.83 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 135.2, 129.6, 129.1, 127.4, 44.0, 39.8, 31.5, 29.5, 26.5, 22.6, 14.1.

Characterization data was in accordance with previously reported[22]

***N,N*-diallyl-2-phenylacetamide** (**4zc**) Prepared by general procedure A using phenylacetic acid and diallylamine. Compound 4zc was obtained as a yellow liquid (165 mg, 77 % yield).

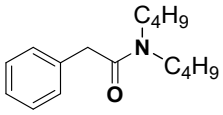


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.20 (m, 5H), 5.82 – 5.61 (m, 2H), 5.22 – 5.05 (m, 4H), 4.00 (dt, *J* = 6.0, 1.5, 1.5 Hz, 2H), 3.86 (dt, *J* = 5.0, 1.8, 1.8 Hz, 2H), 3.70 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.1, 135.3, 133.2, 132.9, 128.9, 128.8, 126.9, 117.4, 116.9, 49.5, 47.9, 40.9.

Characterization data was in accordance with previously reported[23]

***N,N*-dibutyl-2-phenylacetamide** (**4zd**) Prepared by general procedure A using phenylacetic acid and dibutyl amine. Compound 4zd was obtained as a colorless oil (173 mg, 70 % yield).

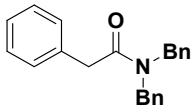


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, *J* = 3.5 Hz, 5H), 3.54 (s, 2H), 2.50 – 2.40 (m, 4H), 1.49 – 1.38 (m, 4H), 1.21 (dq, *J* = 14.8, 7.4, 7.4, 7.3 Hz, 4H), 0.86 (t, *J* = 7.3, 7.3 Hz, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 177.1, 137.6, 129.4, 128.2, 126.1, 47.2, 44.3, 27.9, 19.9, 13.6.

Characterization data was in accordance with previously reported[24]

***N,N*-dibenzyl-2-phenylacetamide** (**4ze**) Prepared by general procedure A using phenylacetic acid and dibenzylamine. Compound 4ze was obtained as a colorless oil (173 mg, 55 % yield).

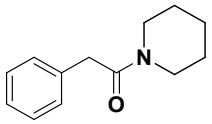


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.27 (m, 11H), 7.21 – 7.17 (m, 2H), 7.13 – 7.09 (m, 2H), 4.62 (s, 2H), 4.44 (s, 2H), 3.80 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 137.4, 136.5, 135.1, 129.1, 128.9, 128.9, 128.7, 128.5, 127.8, 127.5, 127.0, 126.6, 50.3, 48.4, 41.1.

Characterization data was in accordance with previously reported[25]

2-phenyl-1-(piperidin-1-yl)ethan-1-one (**4zf**) Prepared by general procedure A using phenylacetic acid and piperidine. Compound 4zf was obtained as a yellow oil (138mg, 68 % yield).

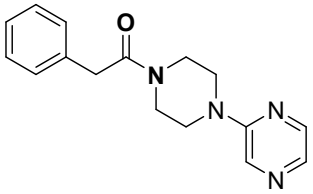


^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.34 – 7.20 (m, 5H), 3.73 (s, 2H), 3.63 – 3.49 (m, 2H), 3.45 – 3.30 (m, 2H), 1.62 – 1.47 (m, 4H), 1.39 – 1.30 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 169.4, 135.6, 128.8, 128.7, 126.8, 47.4, 43.0, 41.3, 26.3, 25.6, 24.6.

Characterization data was in accordance with previously reported[26]

2-phenyl-1-(4-(pyrazin-2-yl)piperazin-1-yl)ethan-1-one (**4zg**) Prepared by general procedure A using phenylacetic acid and 1-(2-pyridyl)piperazine. Compound 4zg was obtained as a bile powder (179 mg, 64 % yield).



^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.07 (d, *J* = 23.3 Hz, 2H), 7.97 – 7.76 (m, 1H), 7.36 – 7.19 (m, 5H), 3.77 (d, *J* = 9.8 Hz, 4H), 3.56 (q, *J* = 5.3, 5.2, 5.2 Hz, 4H), 3.46 – 3.34 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) *δ* 169.8, 154.7, 141.8, 134.8, 133.6, 131.1, 128.9, 128.6, 127.1, 45.6, 44.4, 44.3, 41.3, 41.2.

HRMS (ESI+) m/z [M+Na]: Calc. for $C_{11}H_{12}O_2$+Na 283.15; Found: 283.3.

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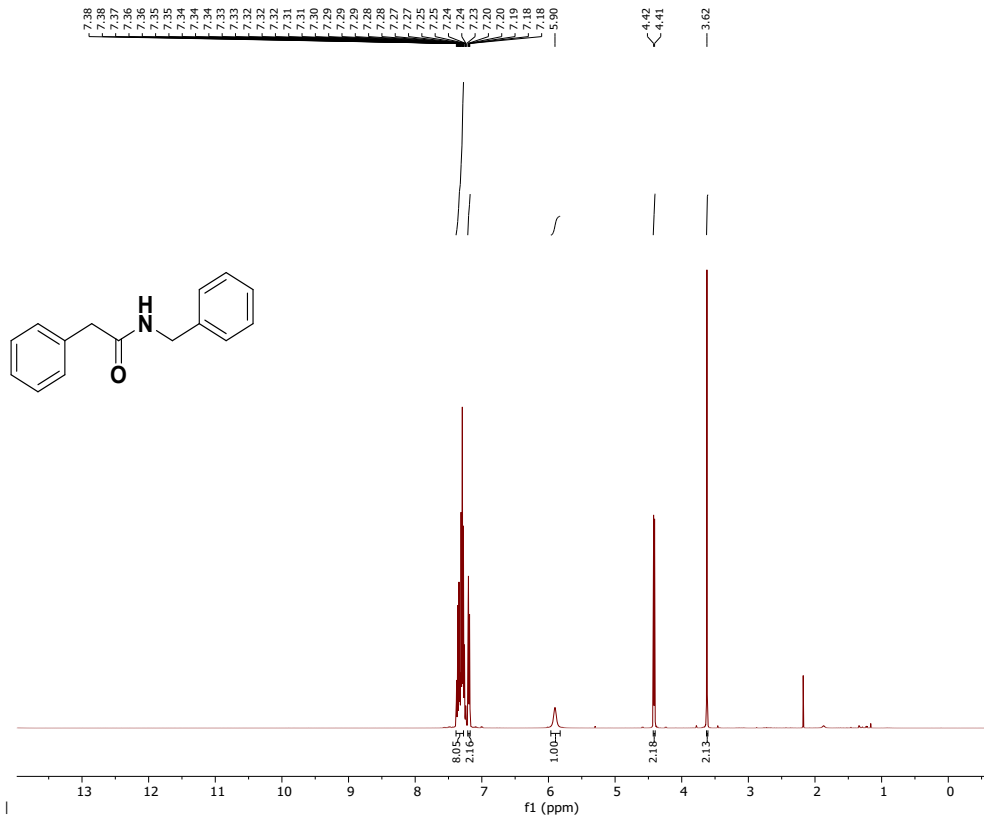
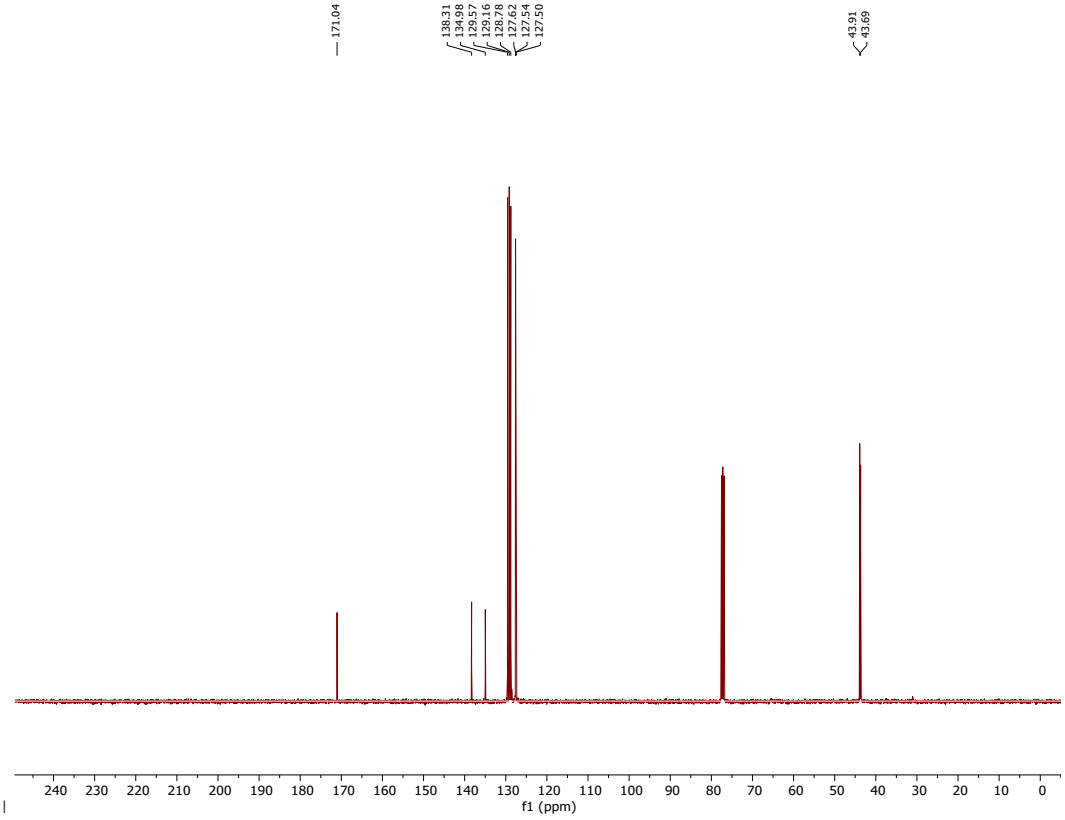
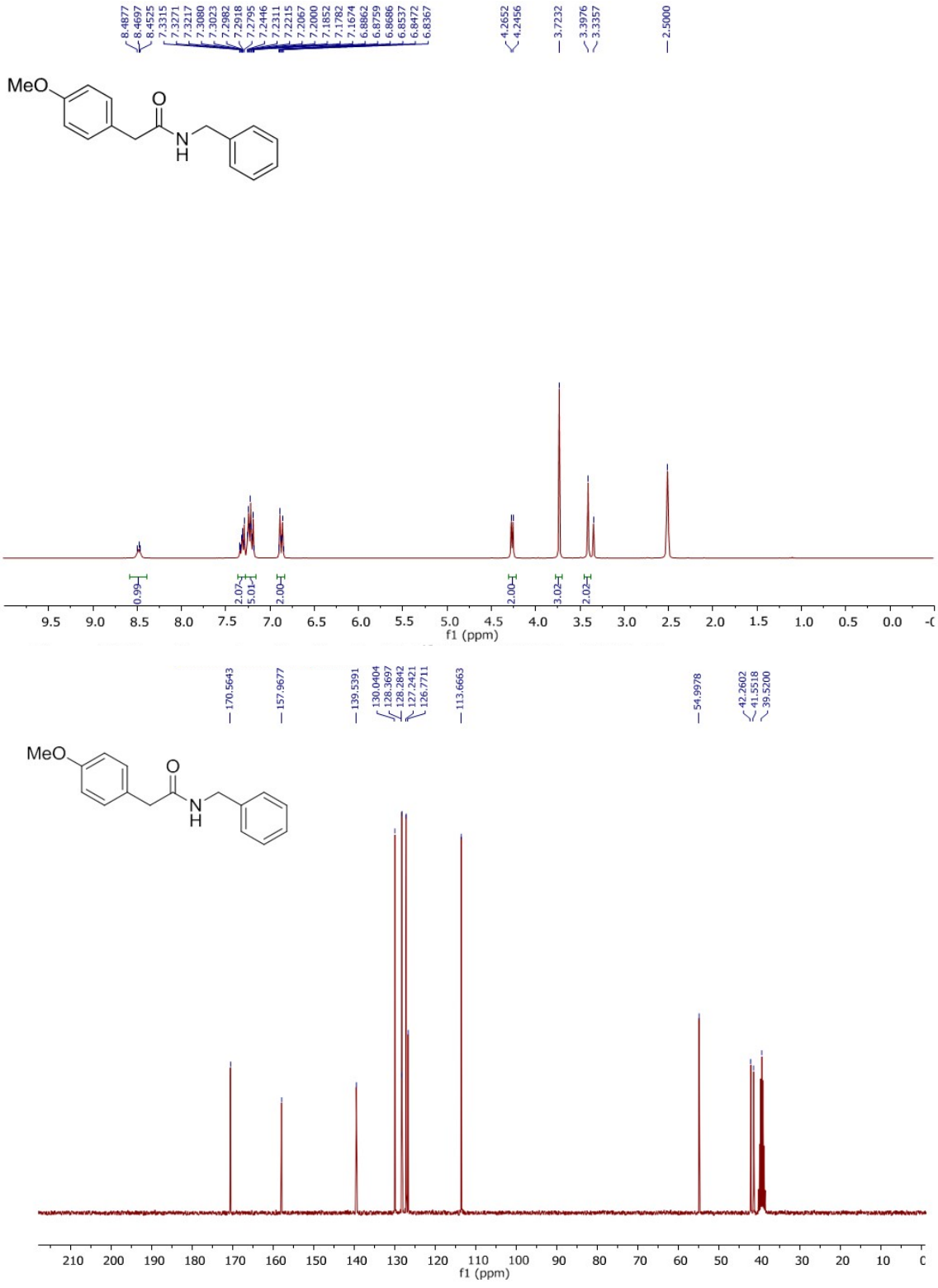
NMR Data

N-benzyl-2-phenylacetamide (4a); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**

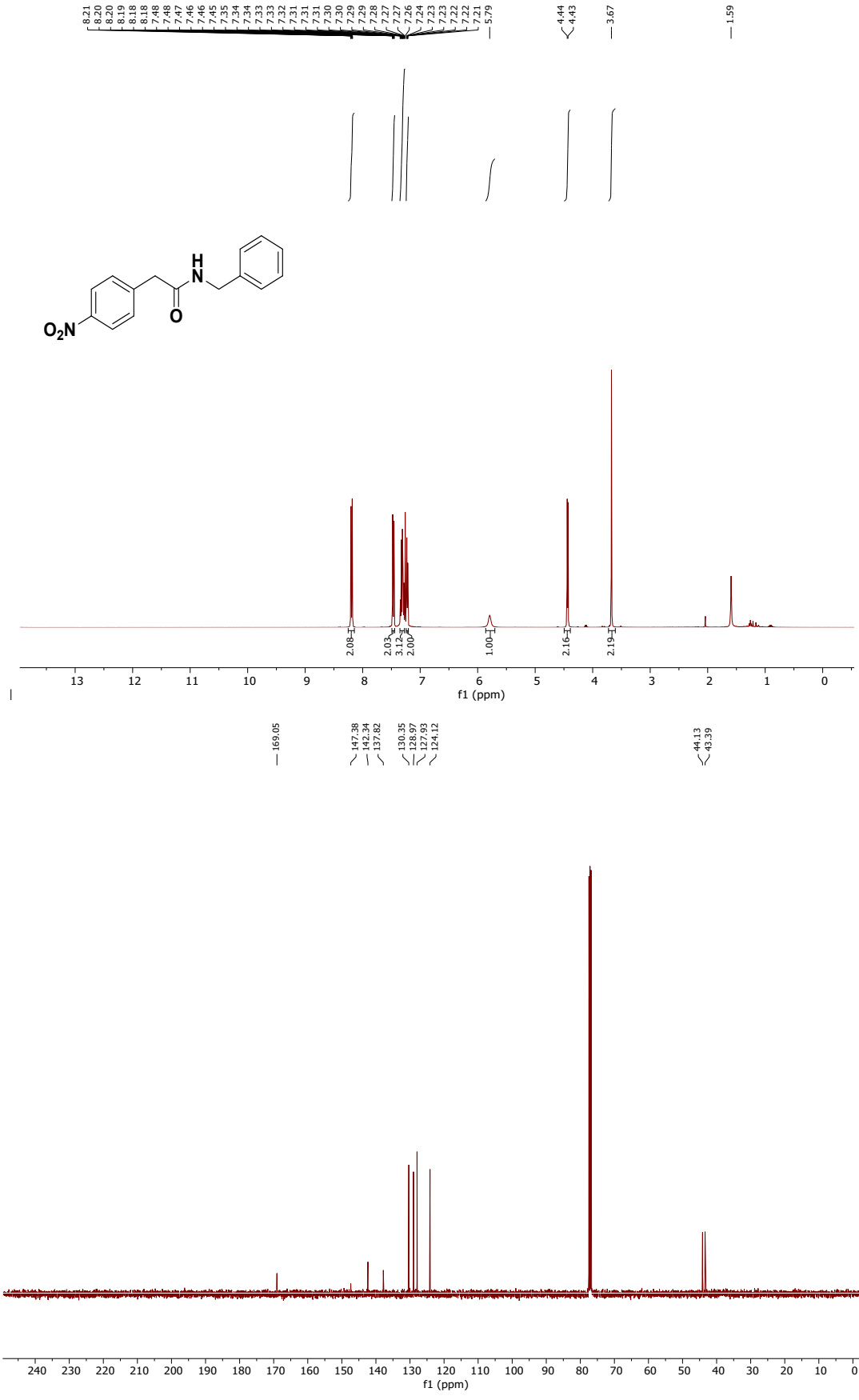




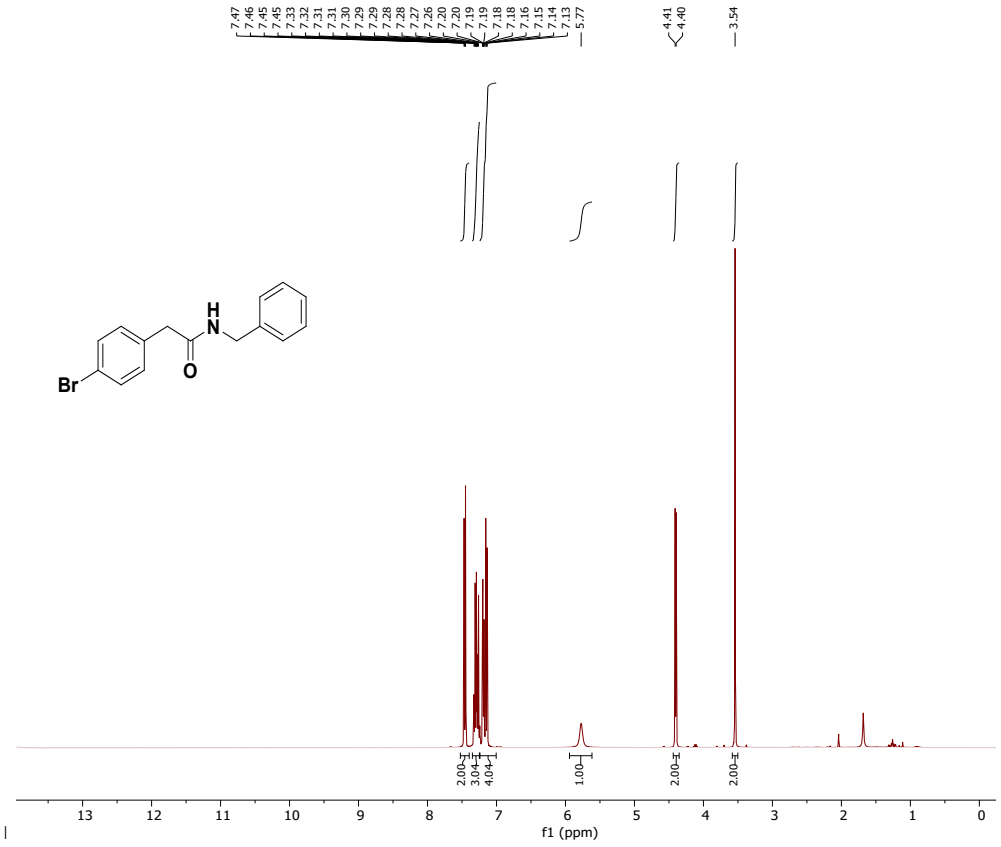
N-benzyl-2-(4-methoxyphenyl)acetamide (4b); **1H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**

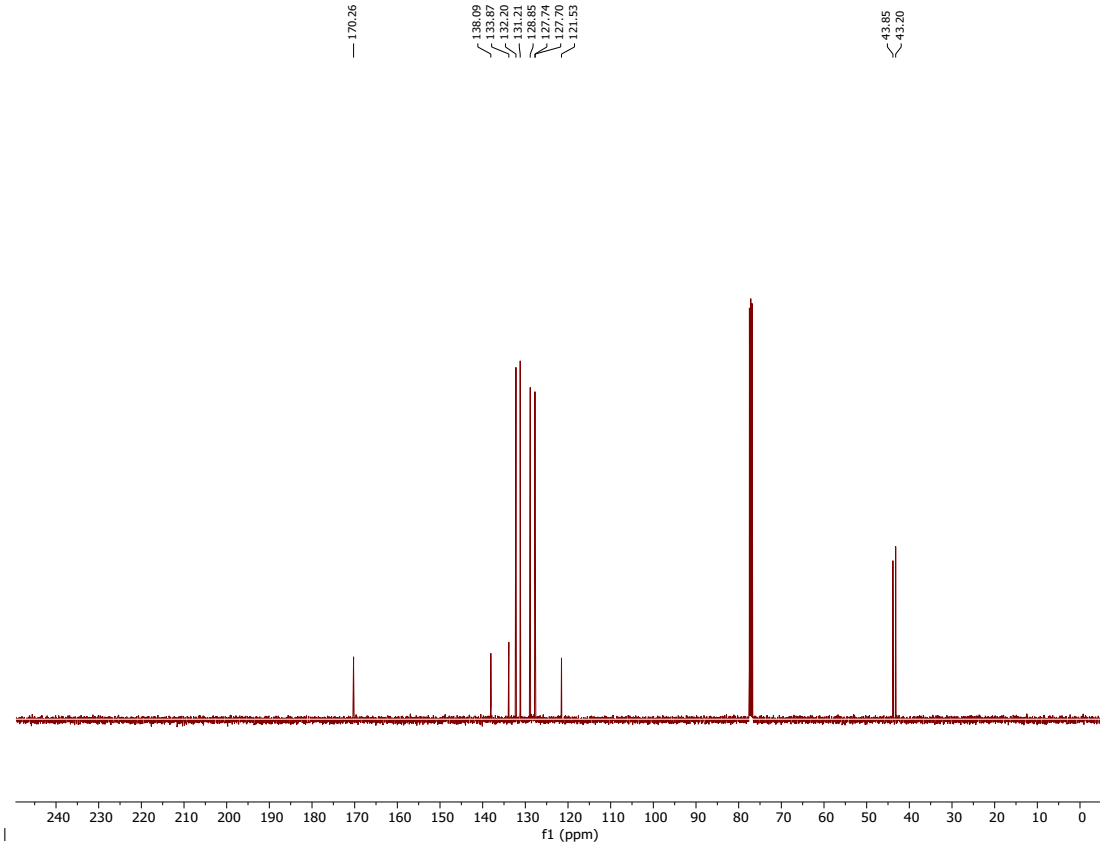


N-benzyl-2-(4-nitrophenyl)acetamide (4c); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



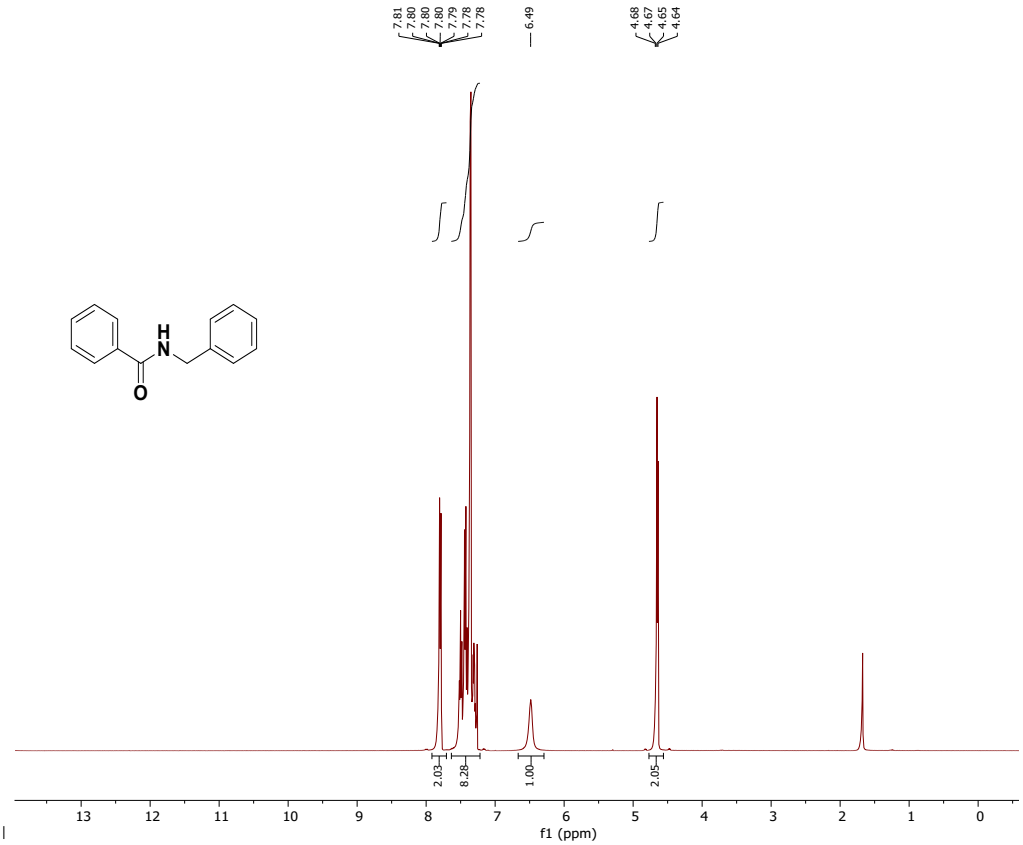
N-benzyl-2-(4-bromophenyl)acetamide (4d); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**

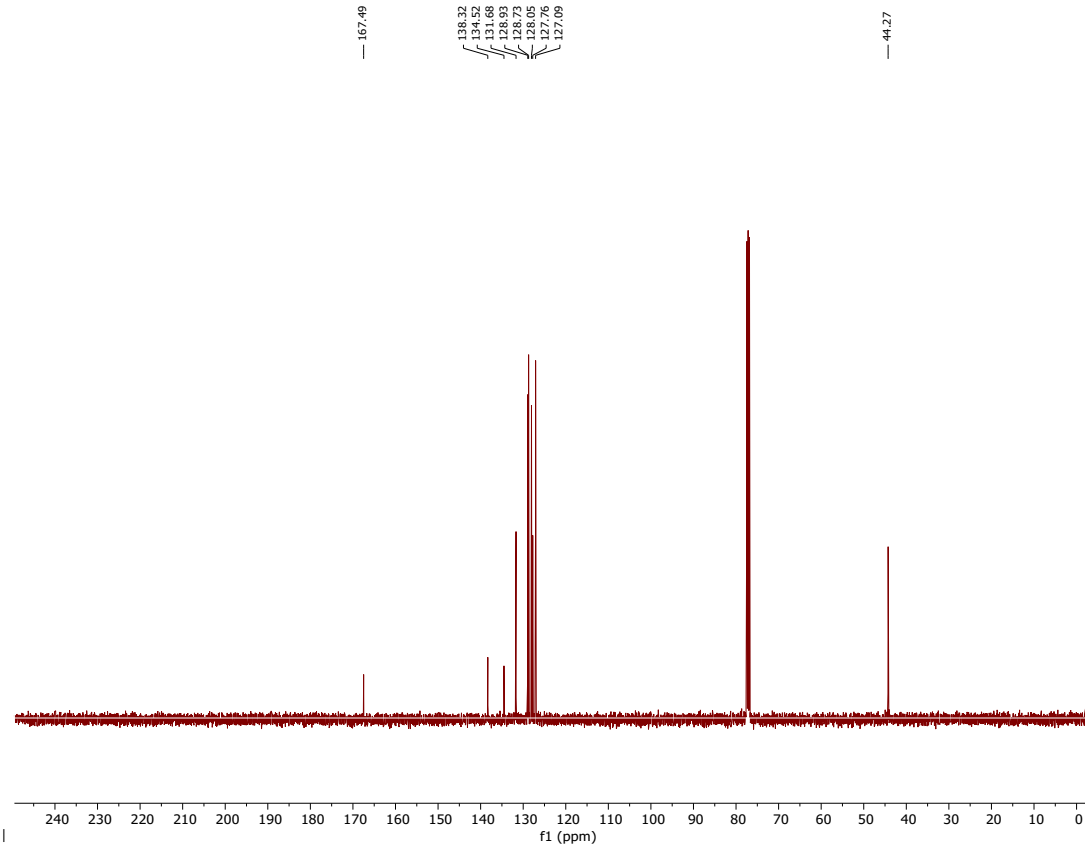




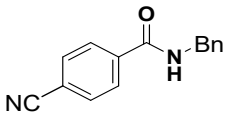
N-benzyl-2-(pyridin-3-yl)acetamide **(4e) 1H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**

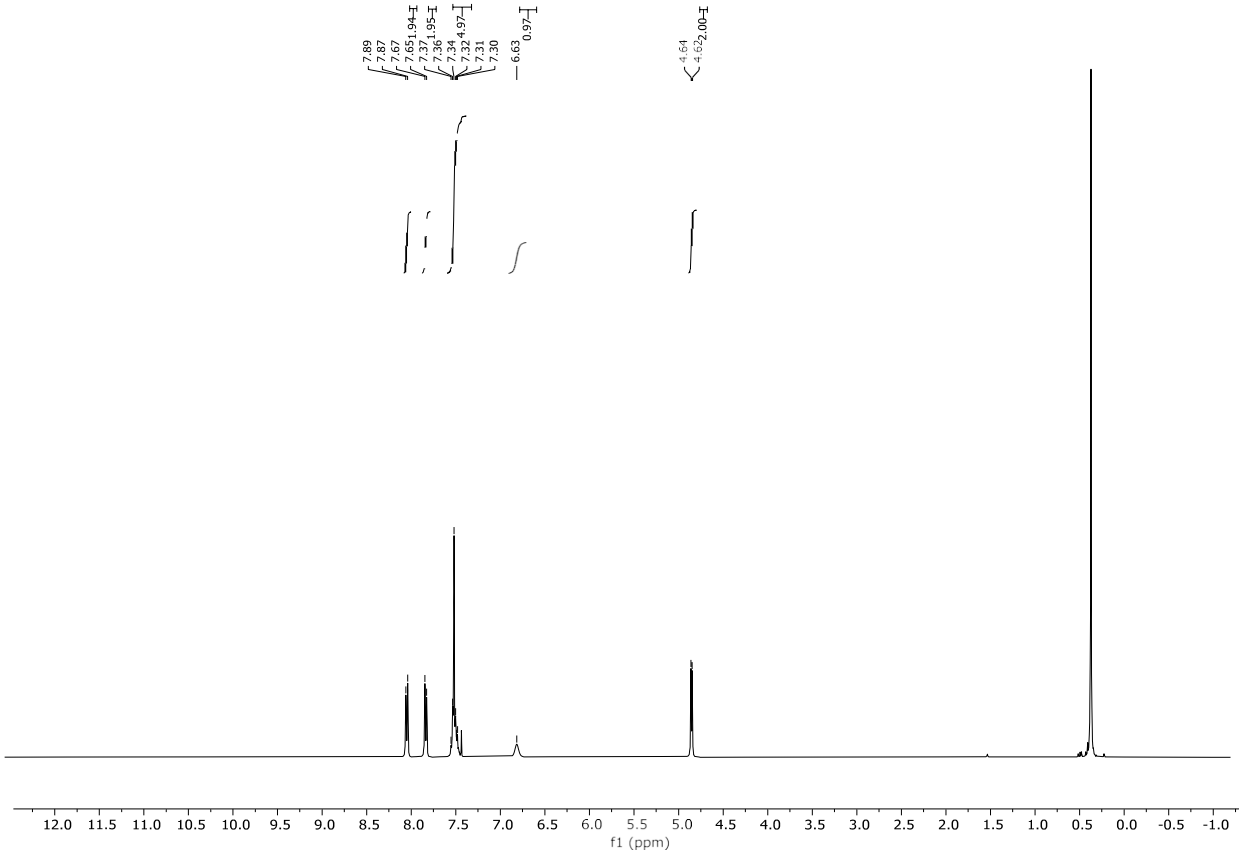
N-benzylbenzamide (4f); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**

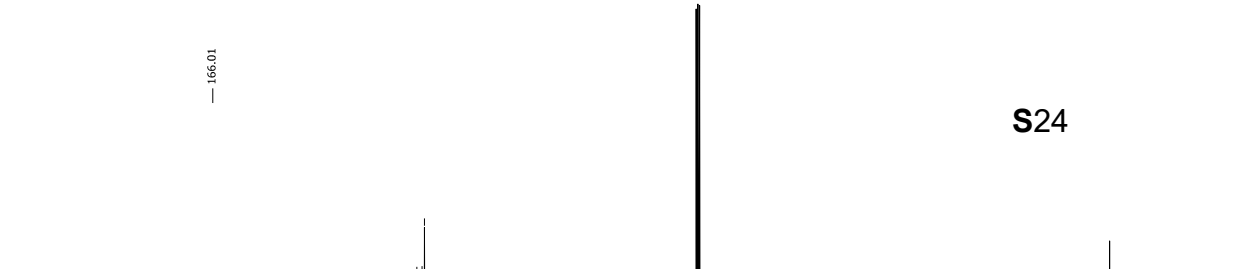


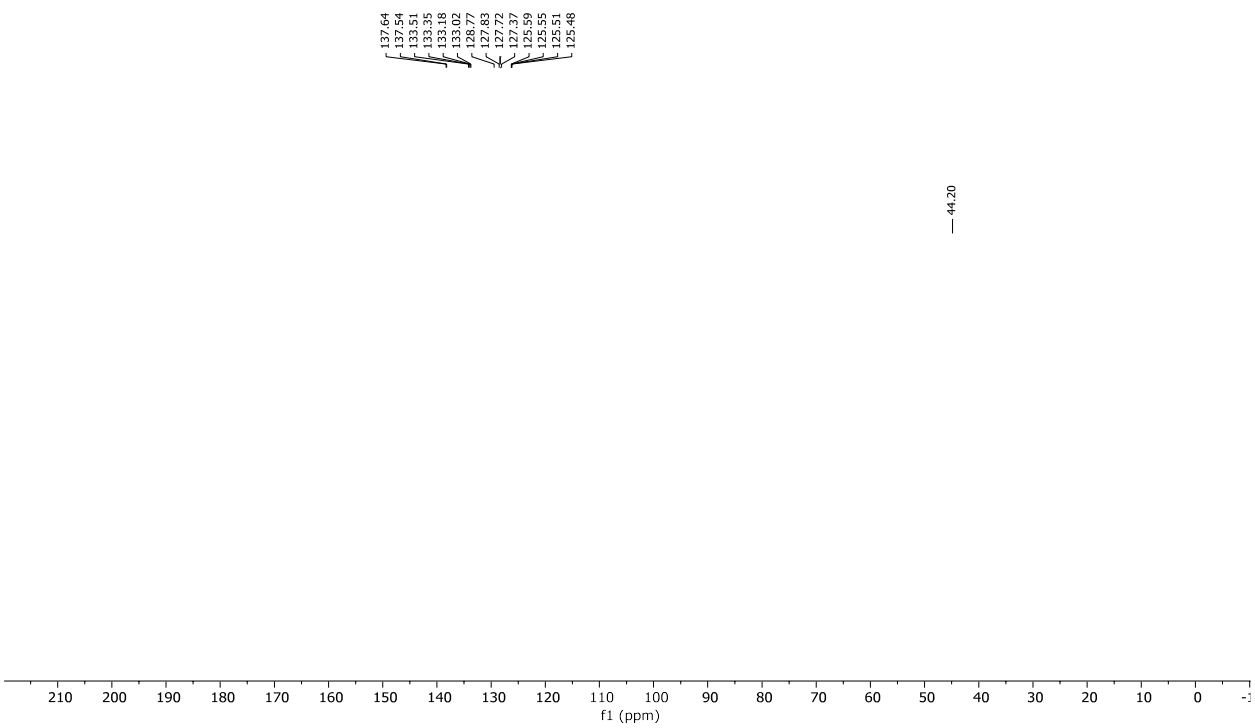


N-benzyl-4-cyanobenzamide (4g); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**

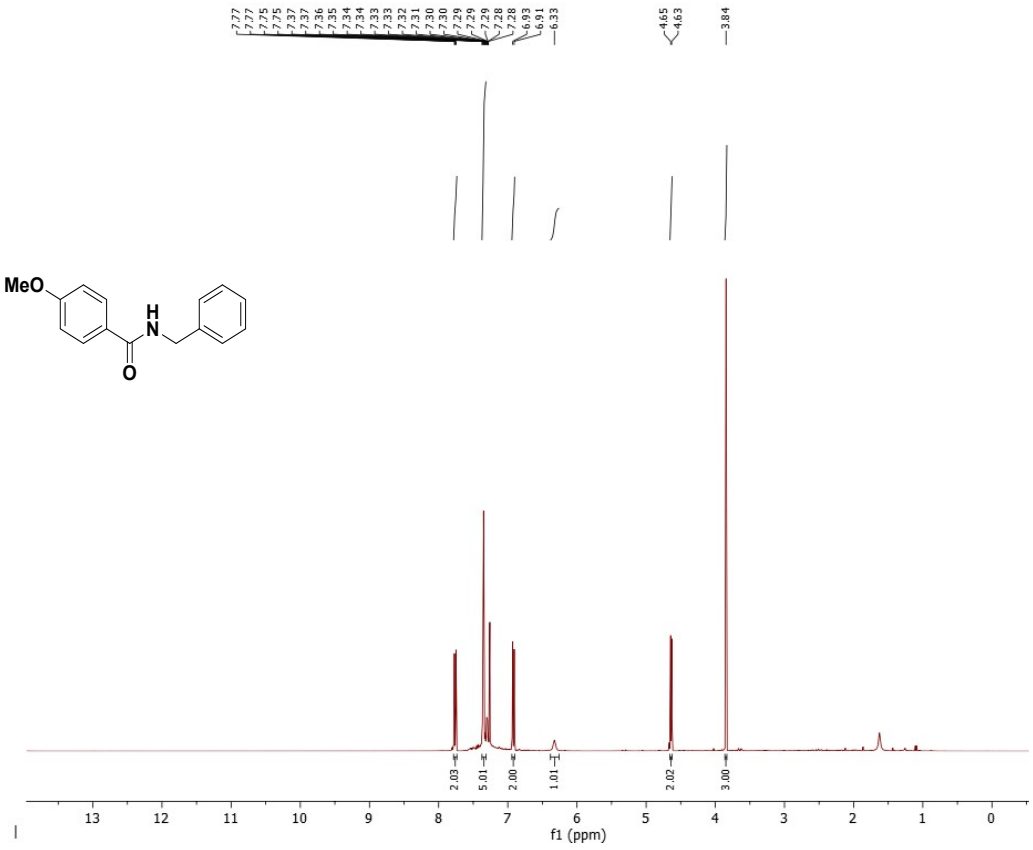


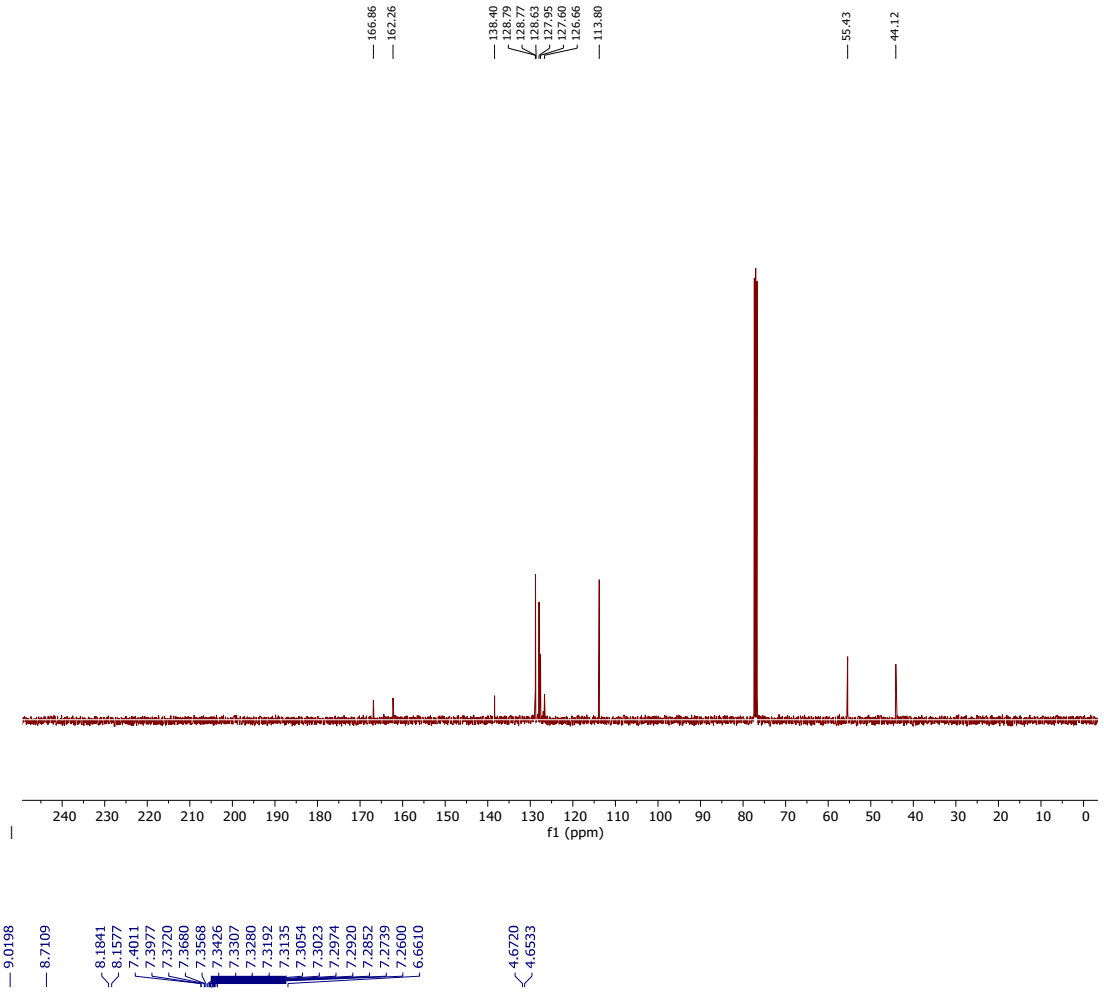




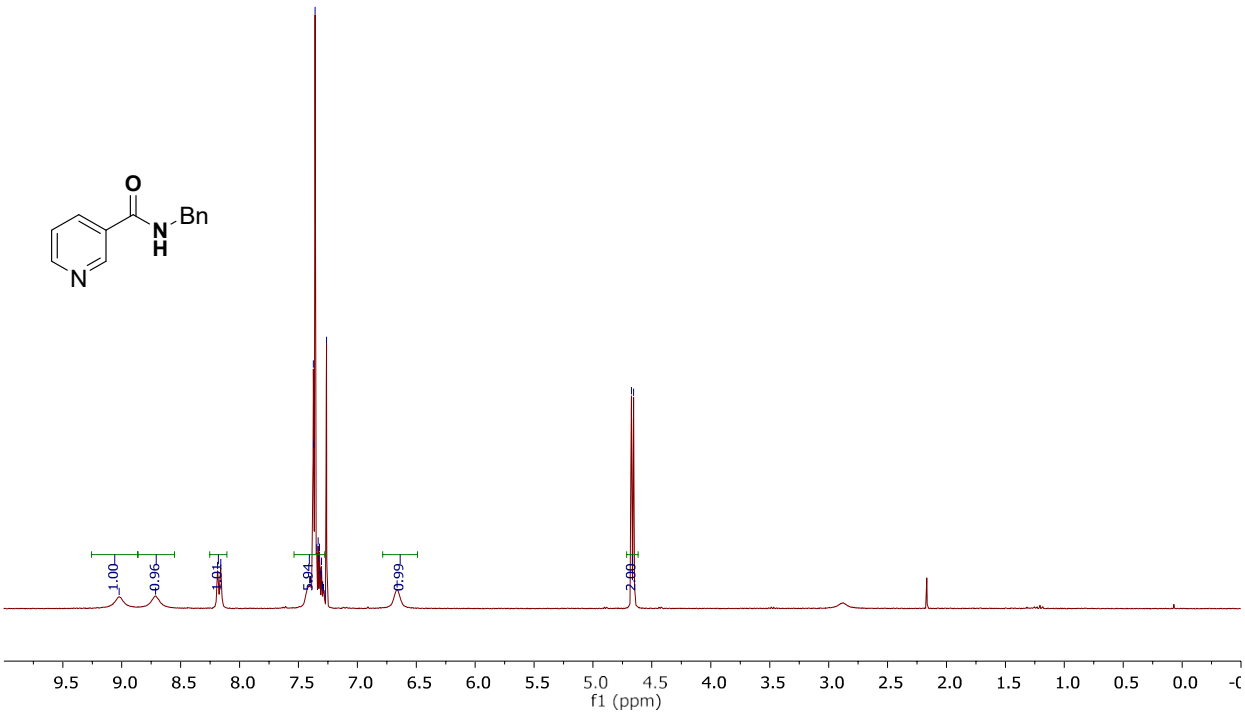


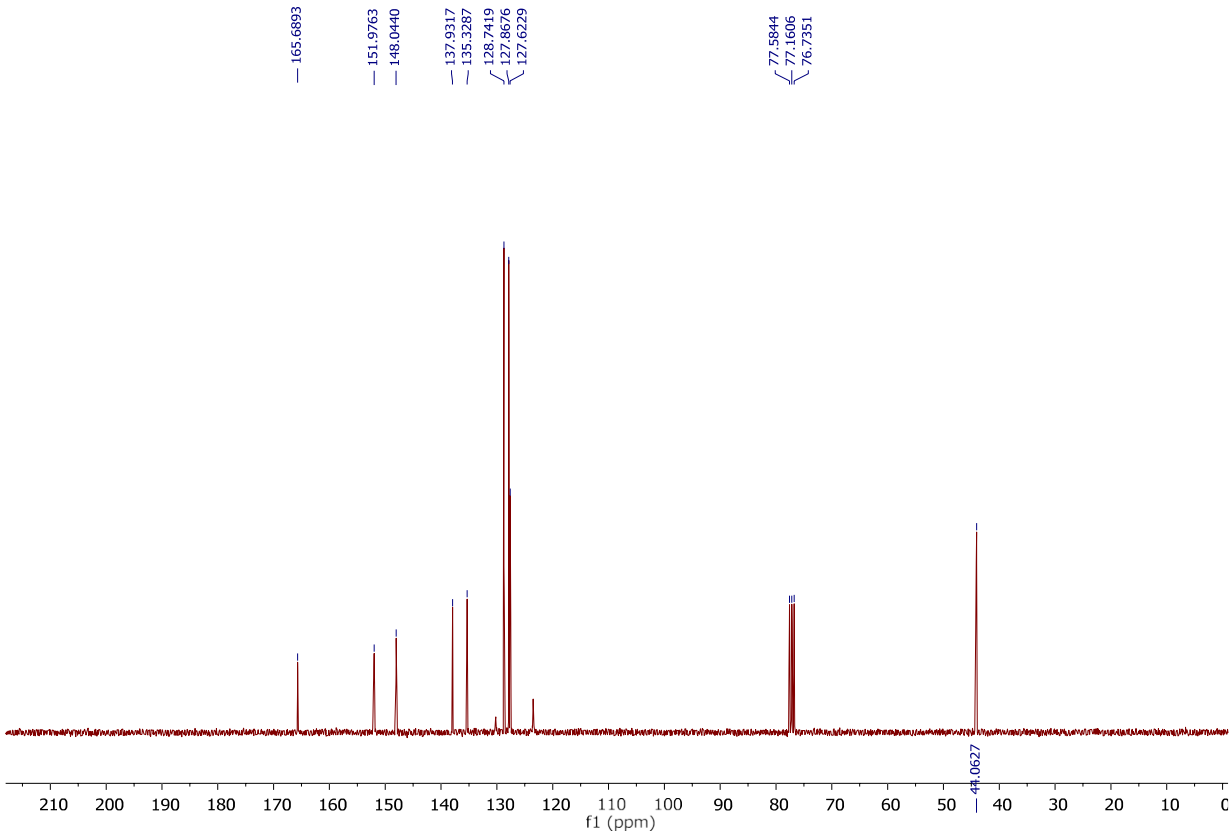
N-benzyl-4-methoxybenzamide (4h); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



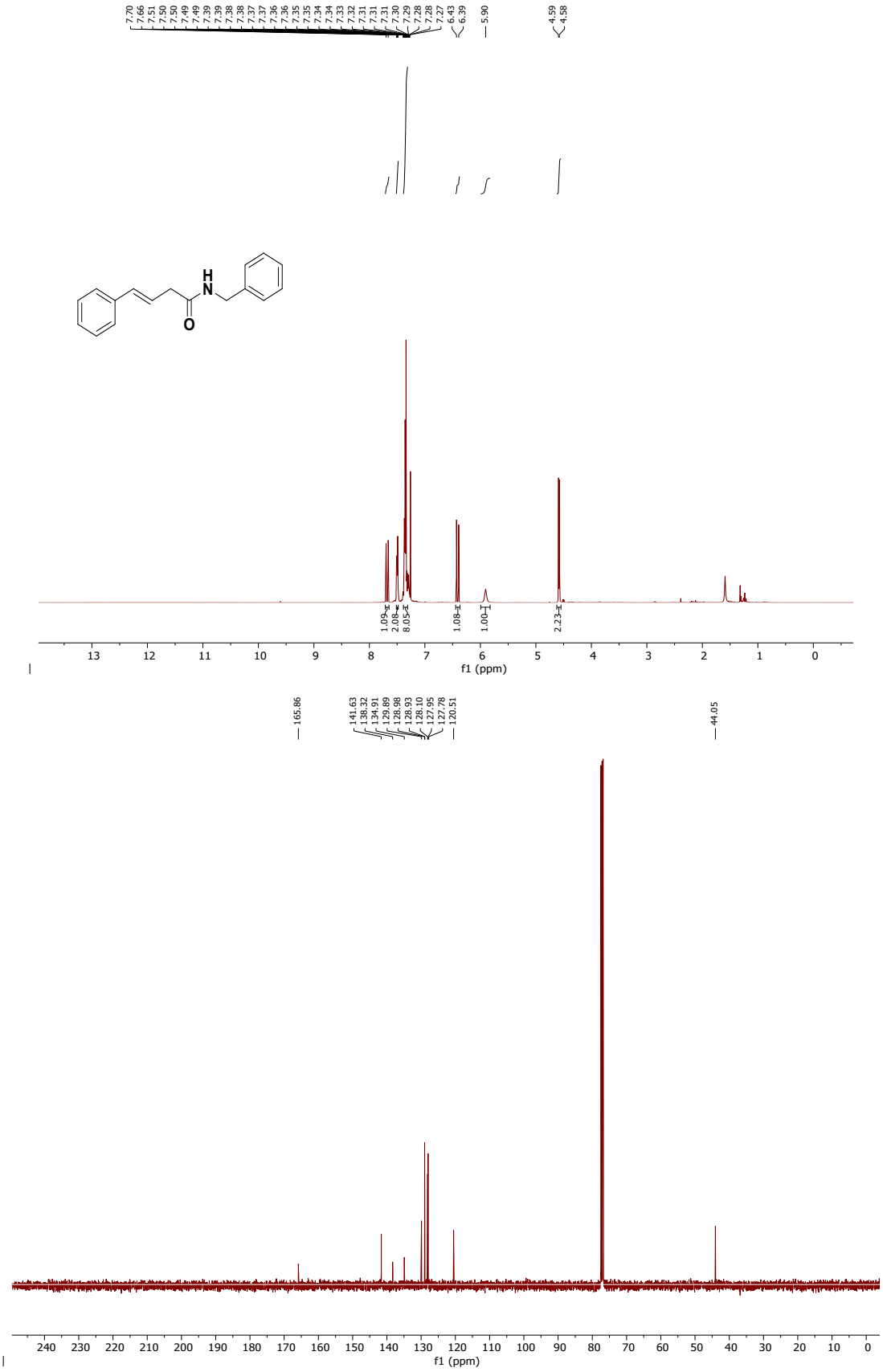


N-benzylnicotinamide (4i); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**

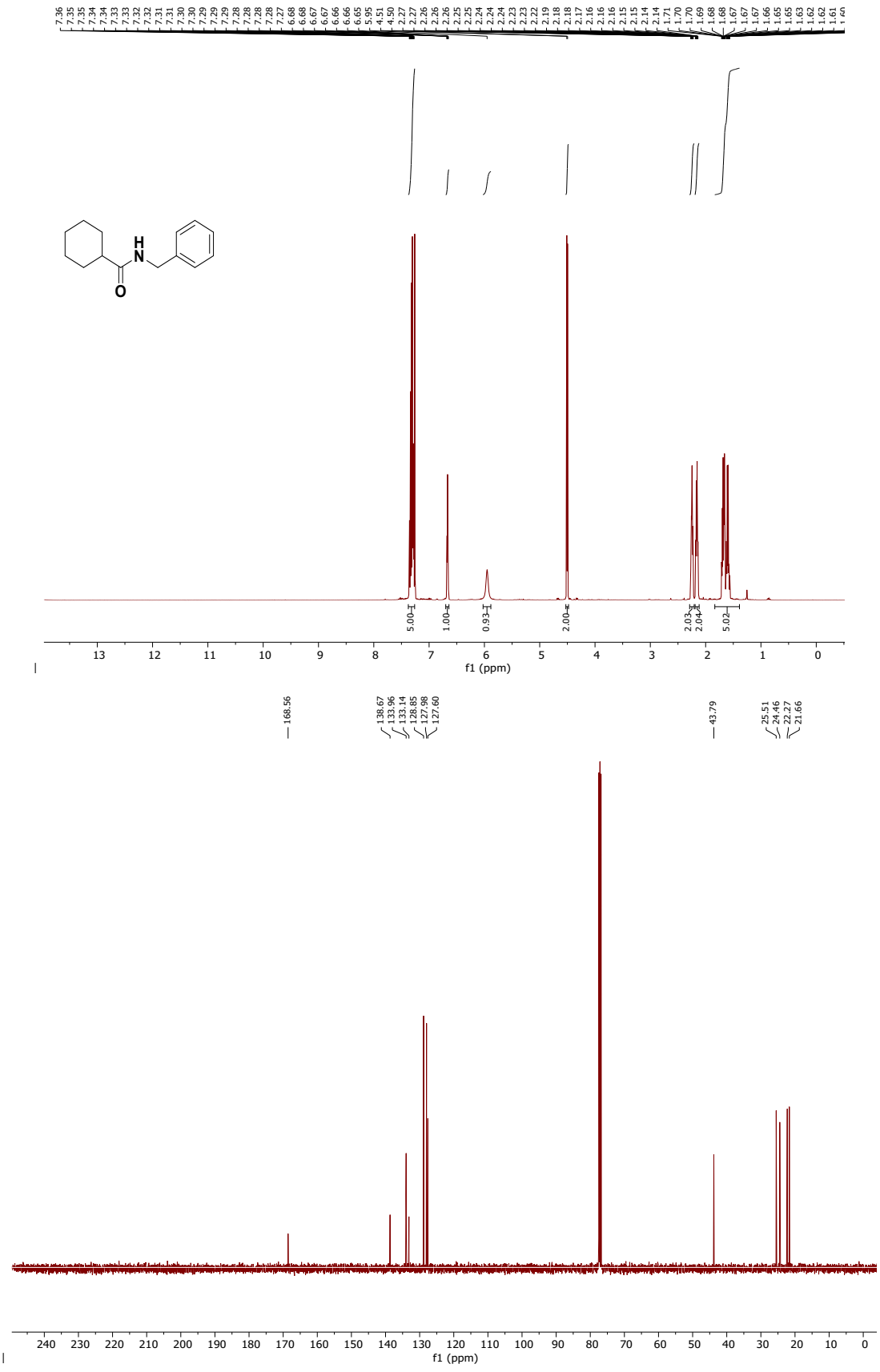




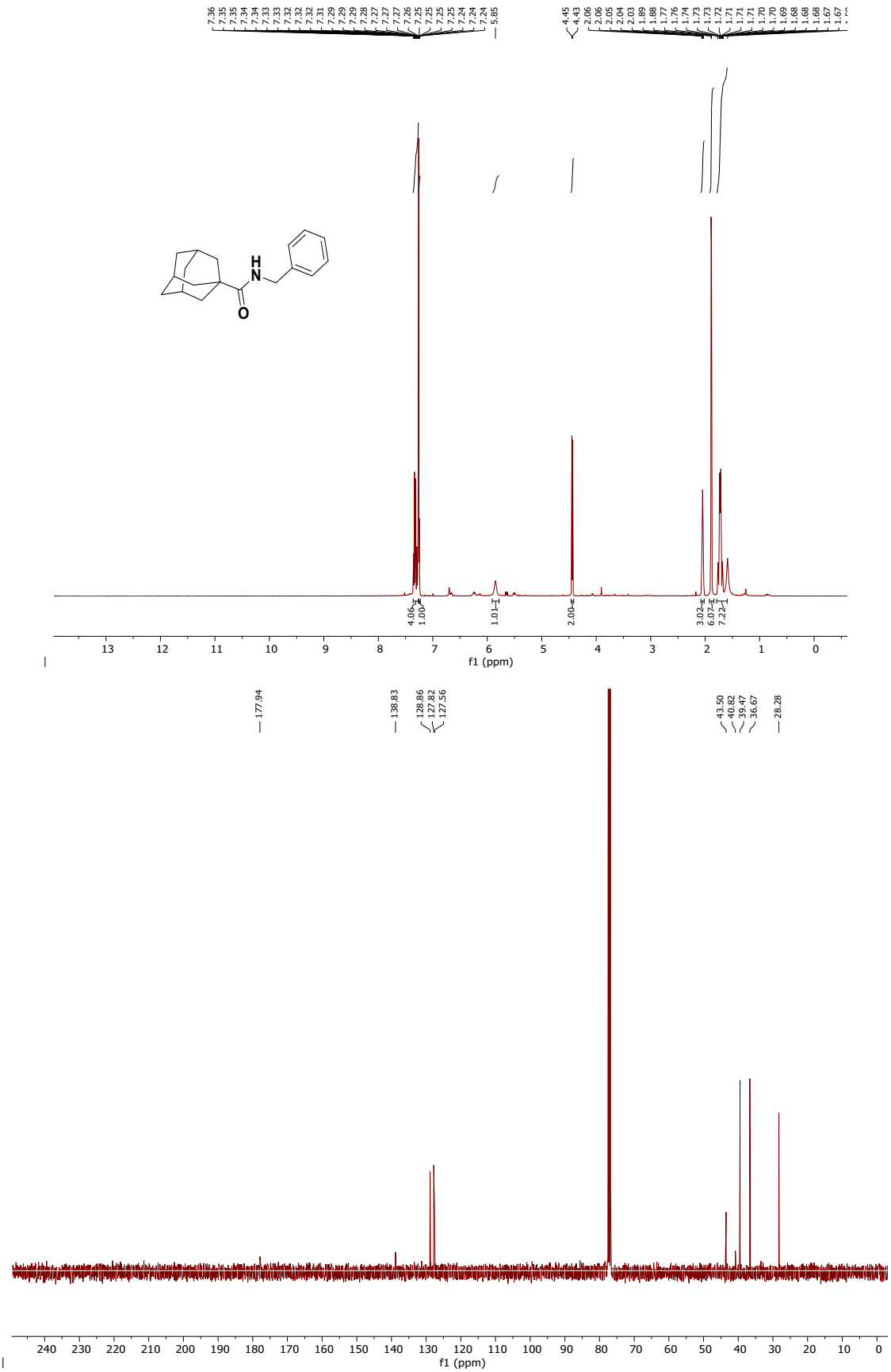
N-benzylcinnamamide (4j); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



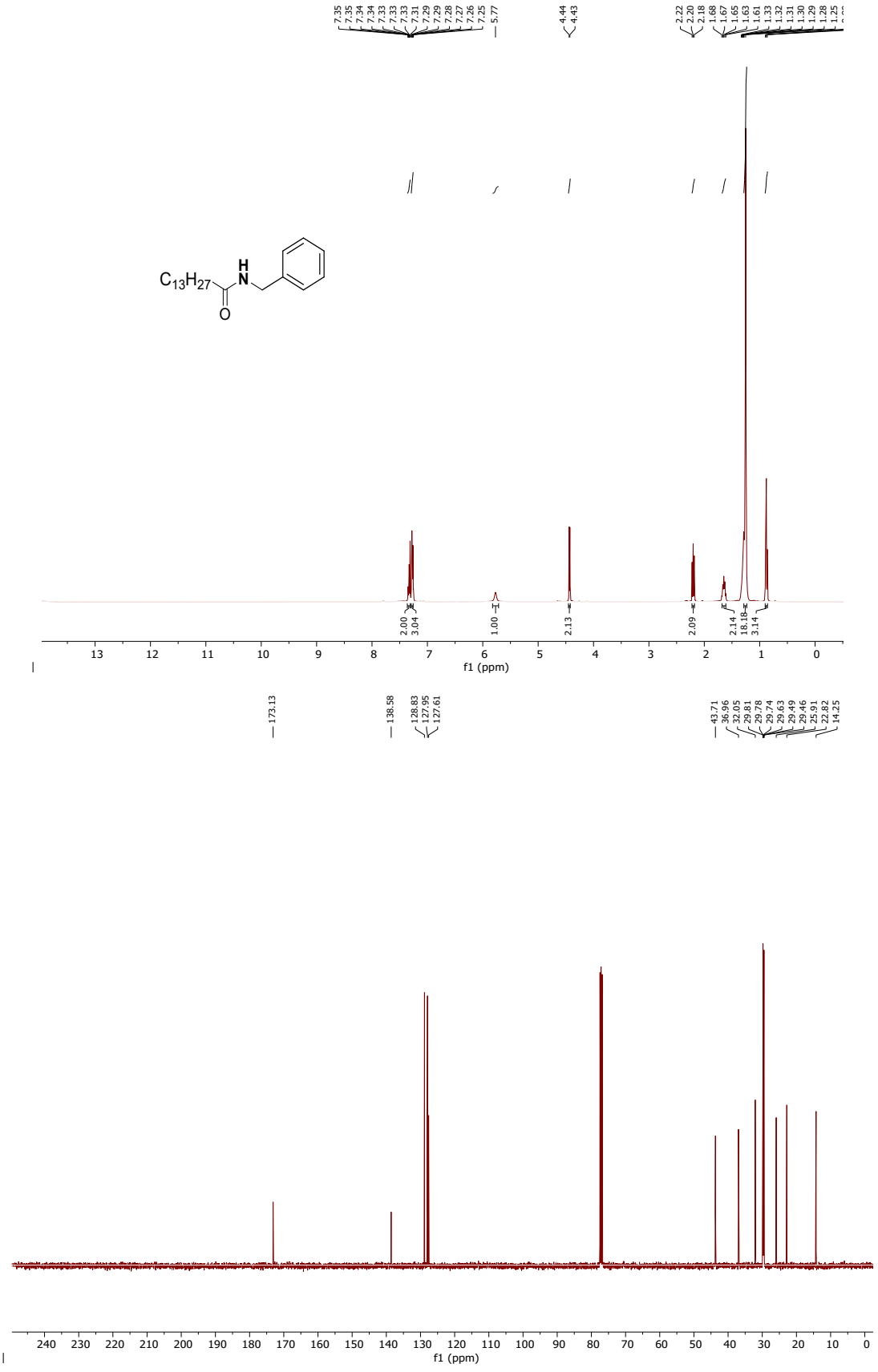
N-benzylcyclohexanecarboxamide (4k); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



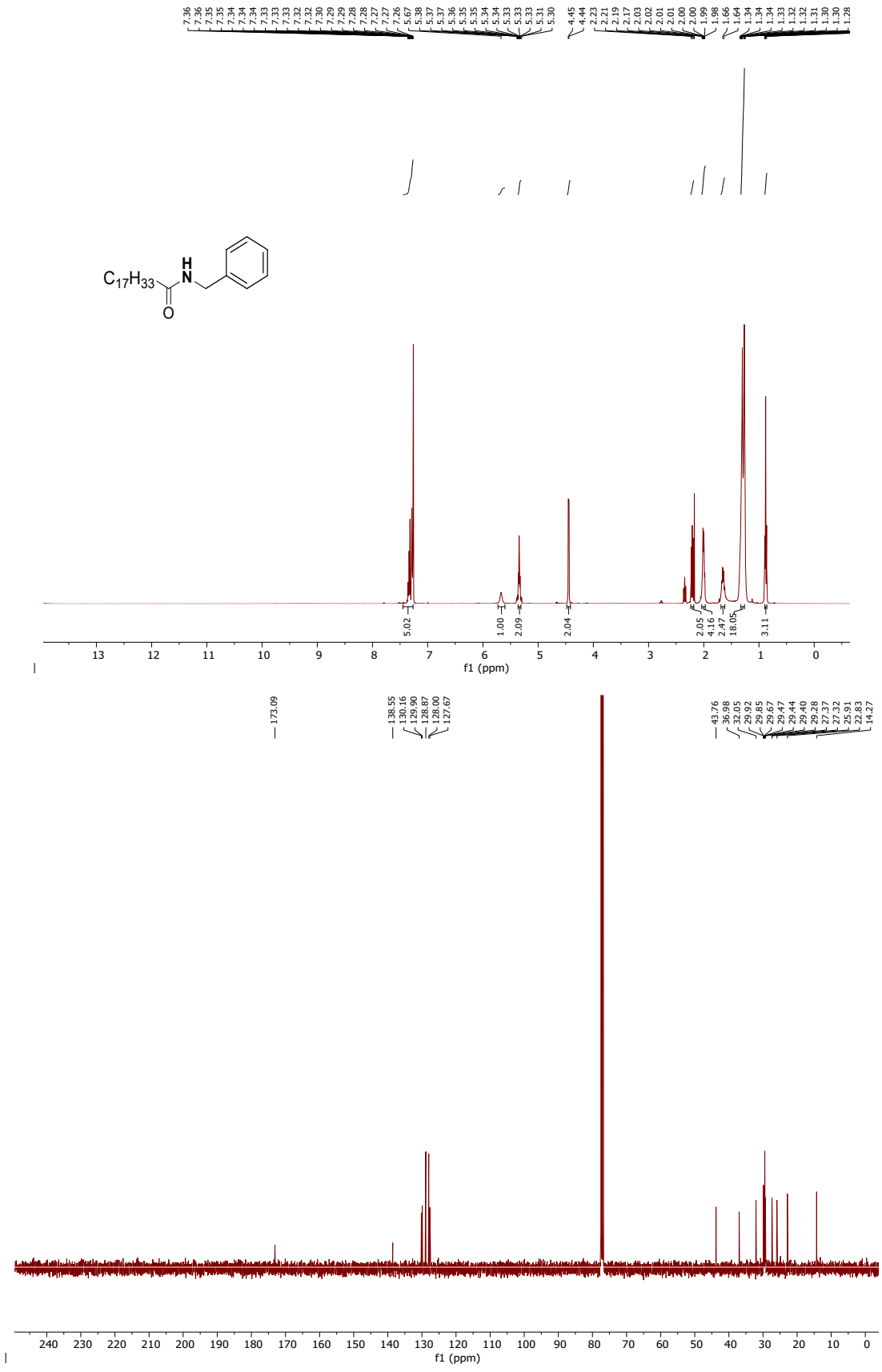
N-benzyladamantane-1-carboxamide (4l); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



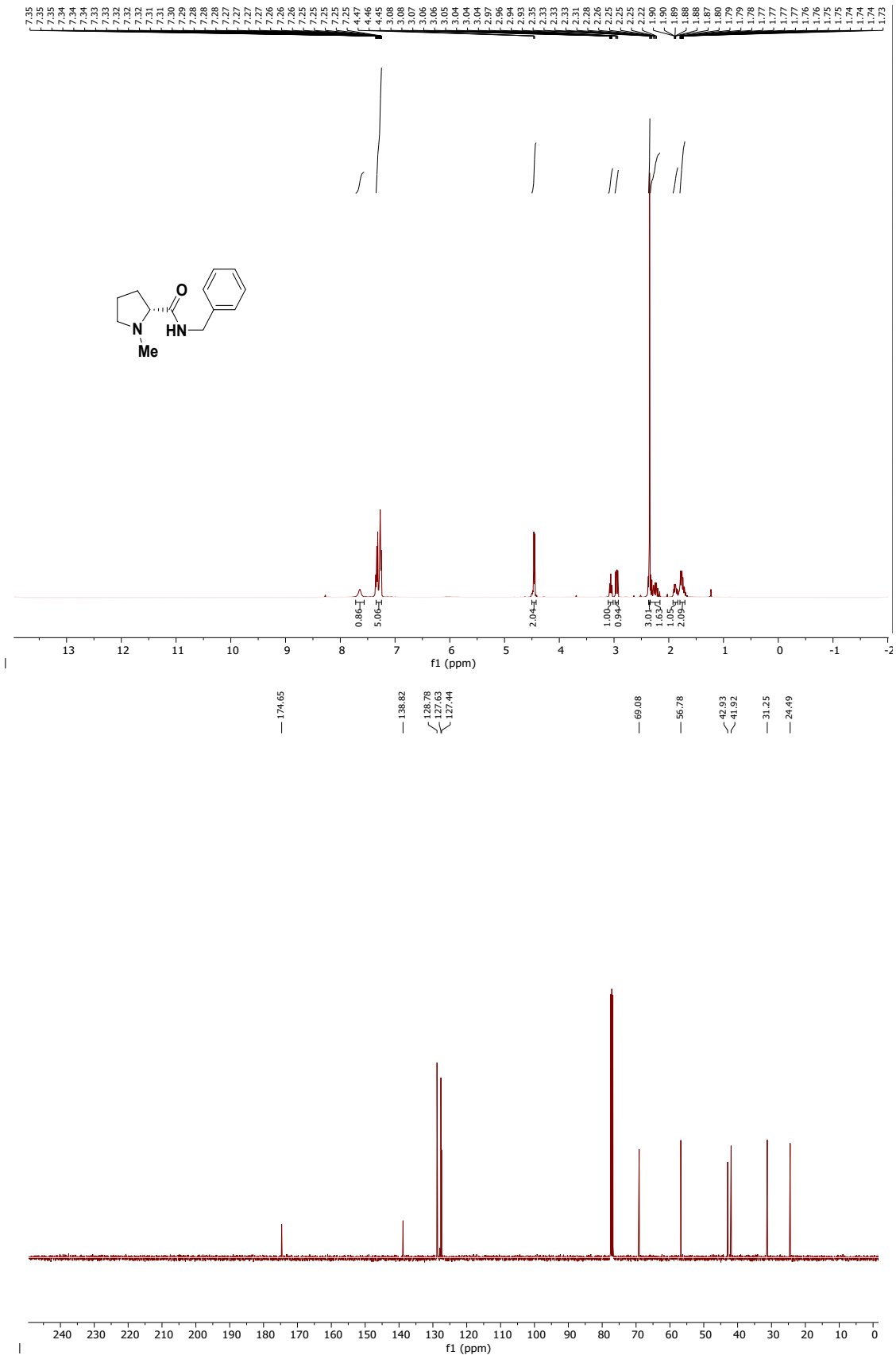
N-benzyltetradecanamide (4m); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



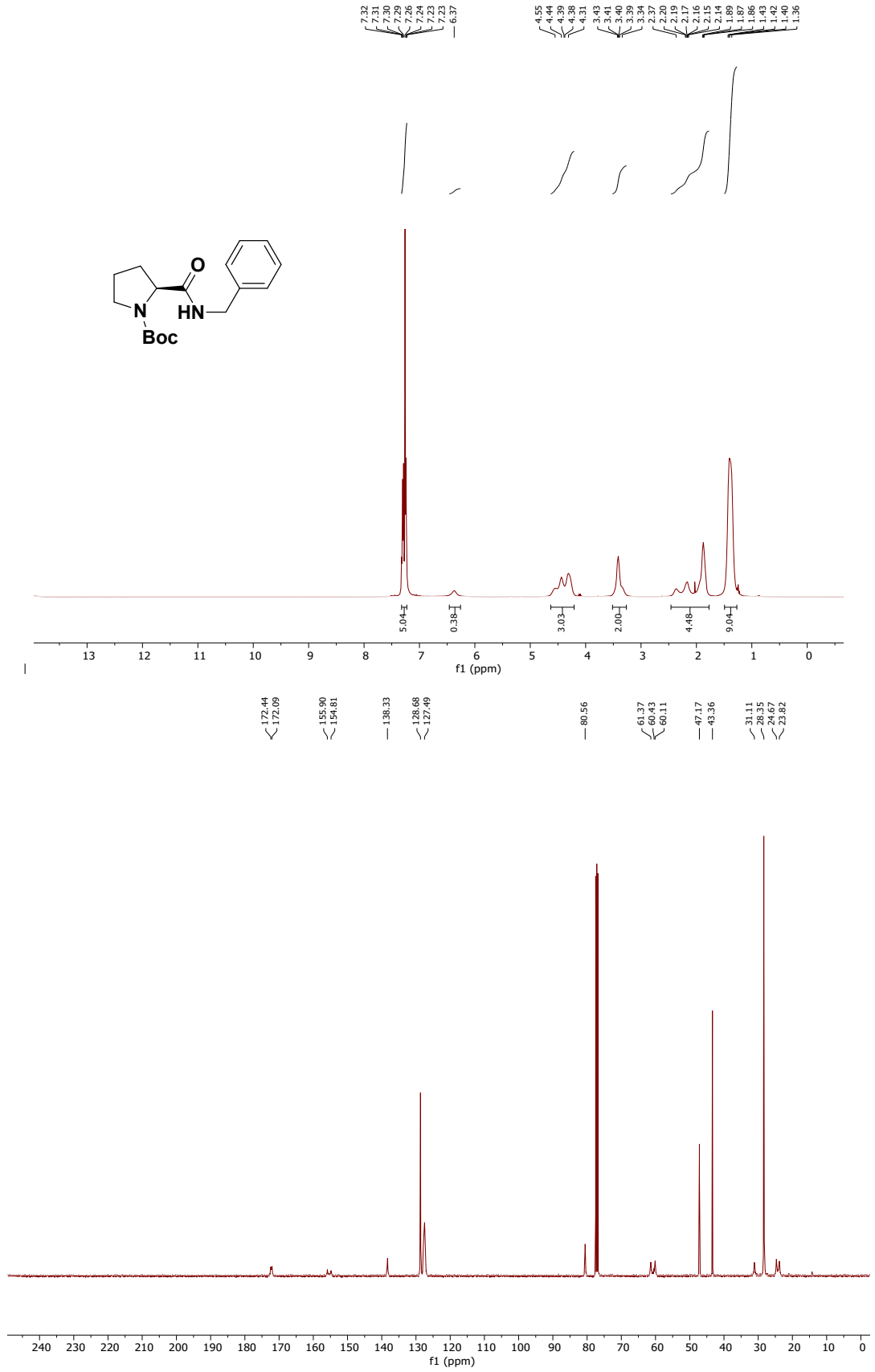
(*E*)-*N*-benzyloctadec-9-enamide (4n); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



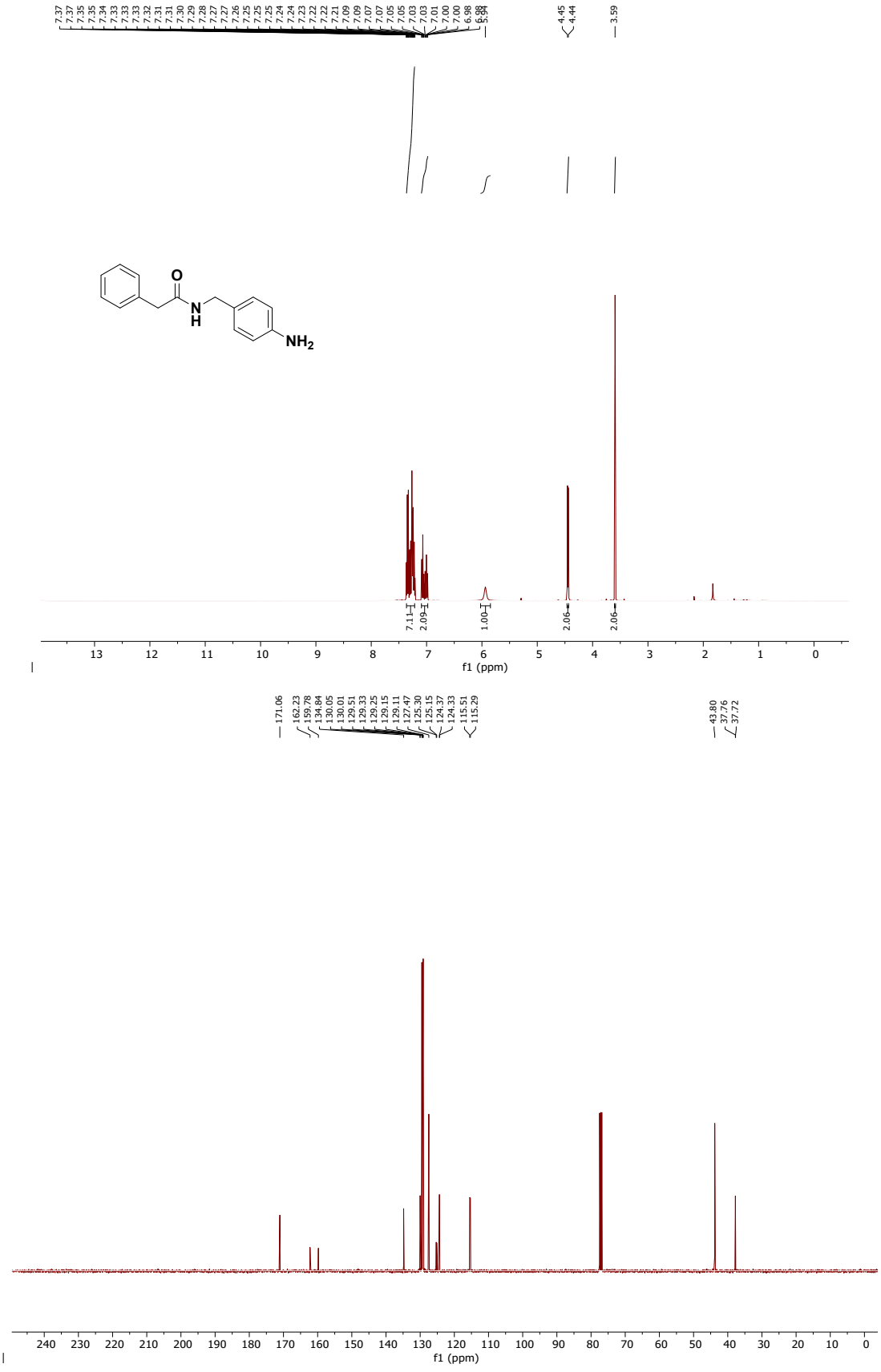
(R)-N-benzyl-1-methylpyrrolidine-2-carboxamide (4o); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



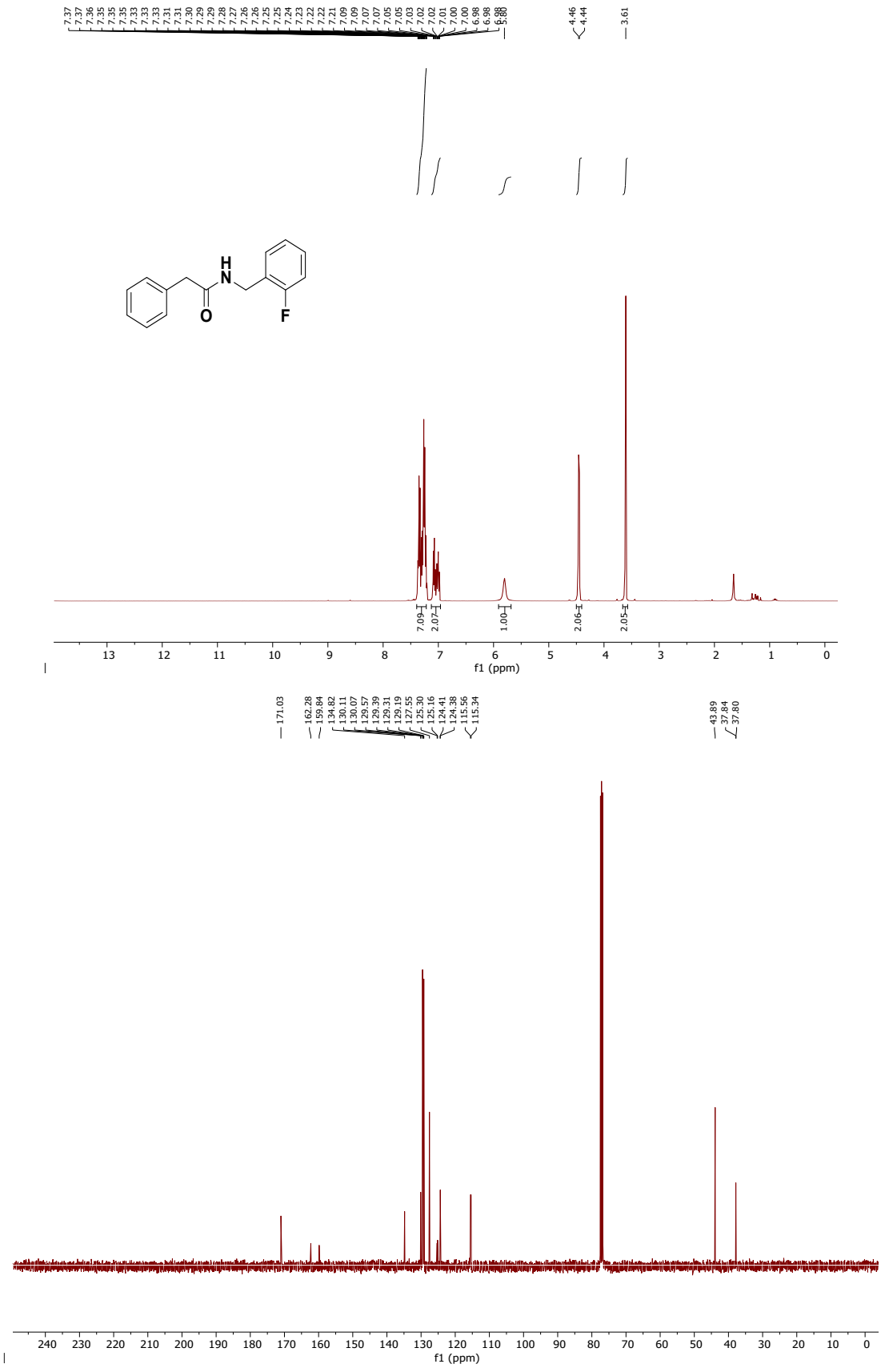
tert-butyl 2-(benzylcarbamoyl)pyrrolidine-1-carboxylate (4p); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



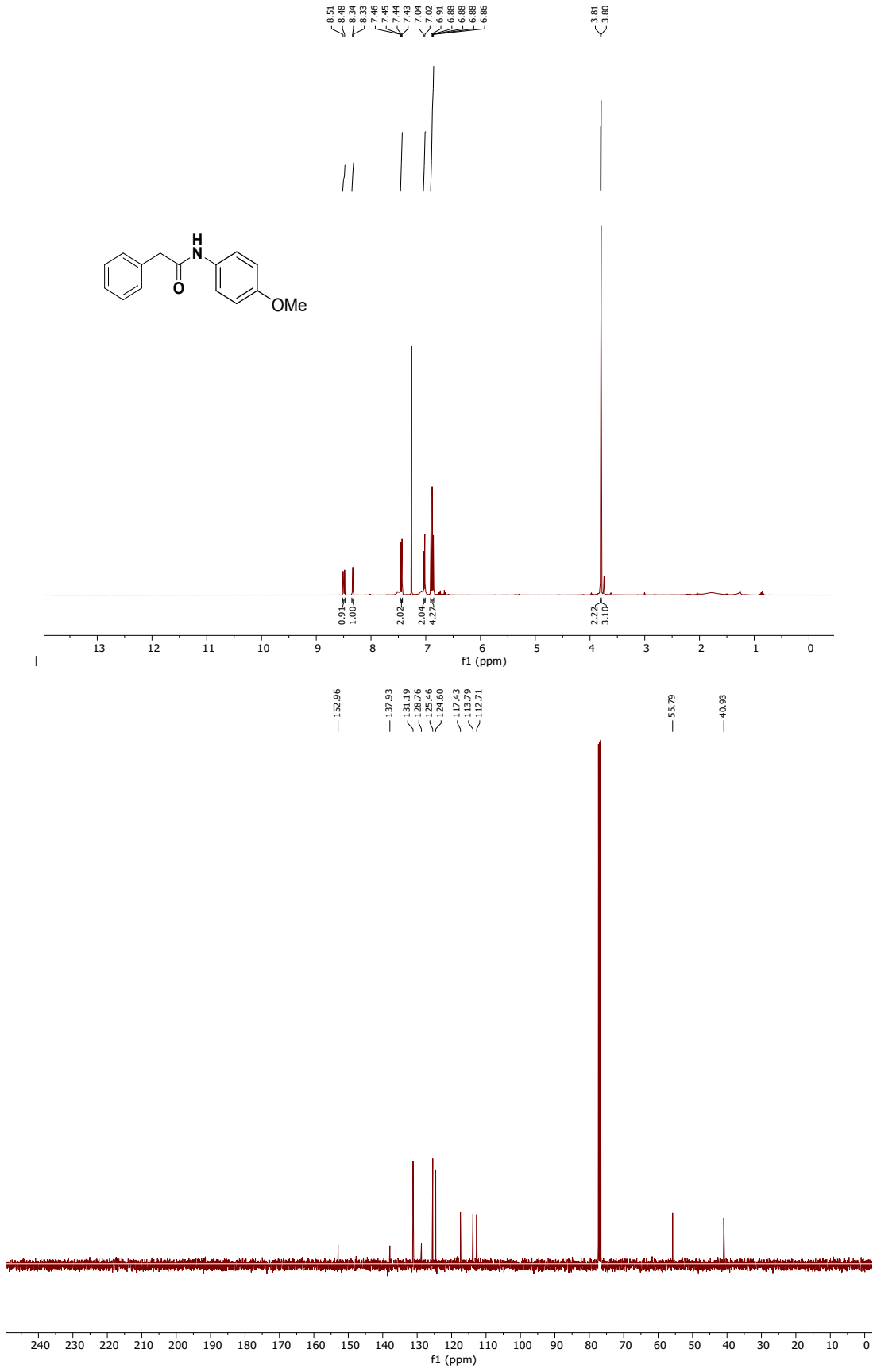
N-(4-aminobenzyl)-2-phenylacetamide (**4q**); **1H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



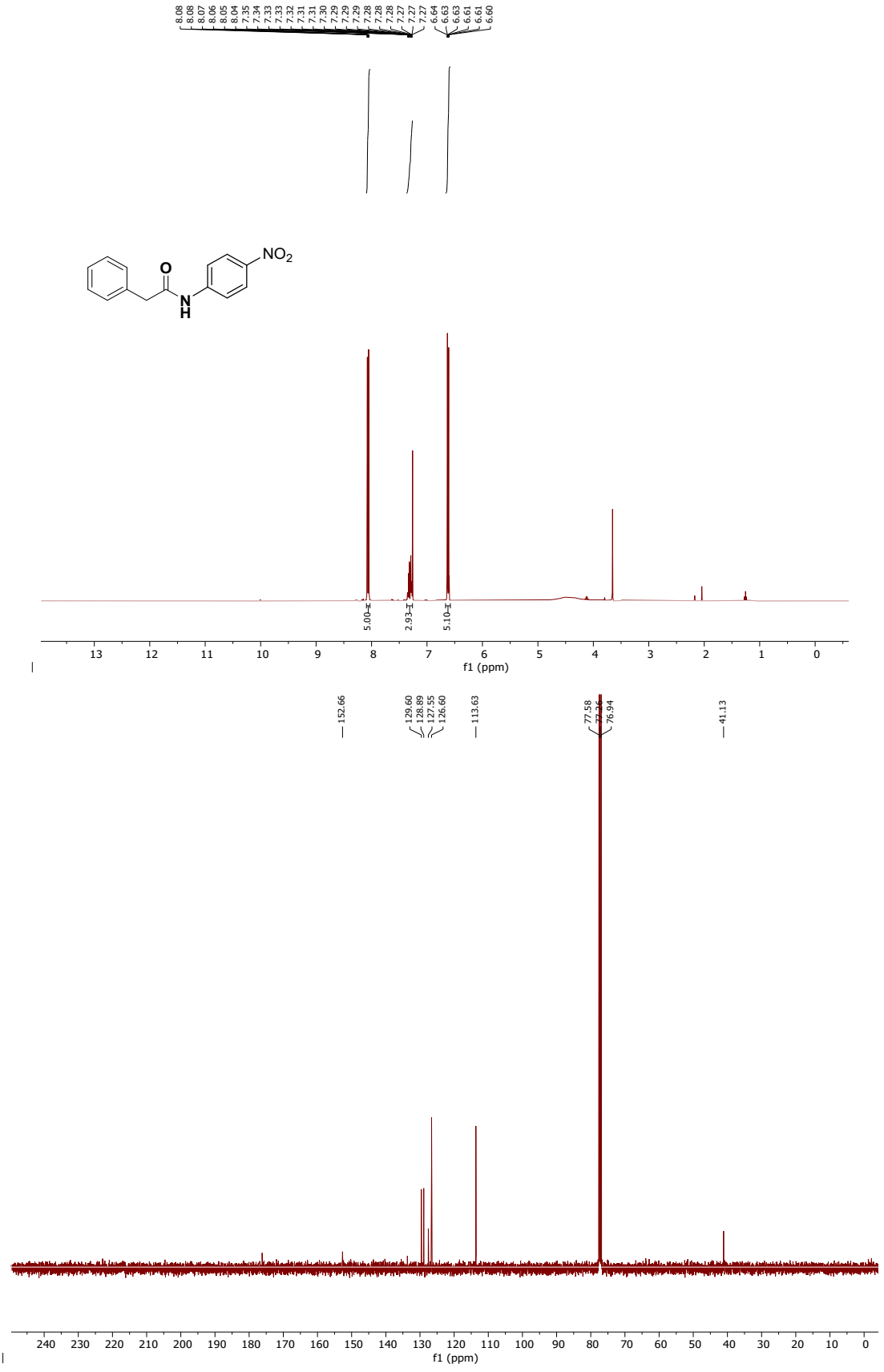
N-(2-fluorobenzyl)-2-phenylacetamide (4r); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, $CDCl_3$).**



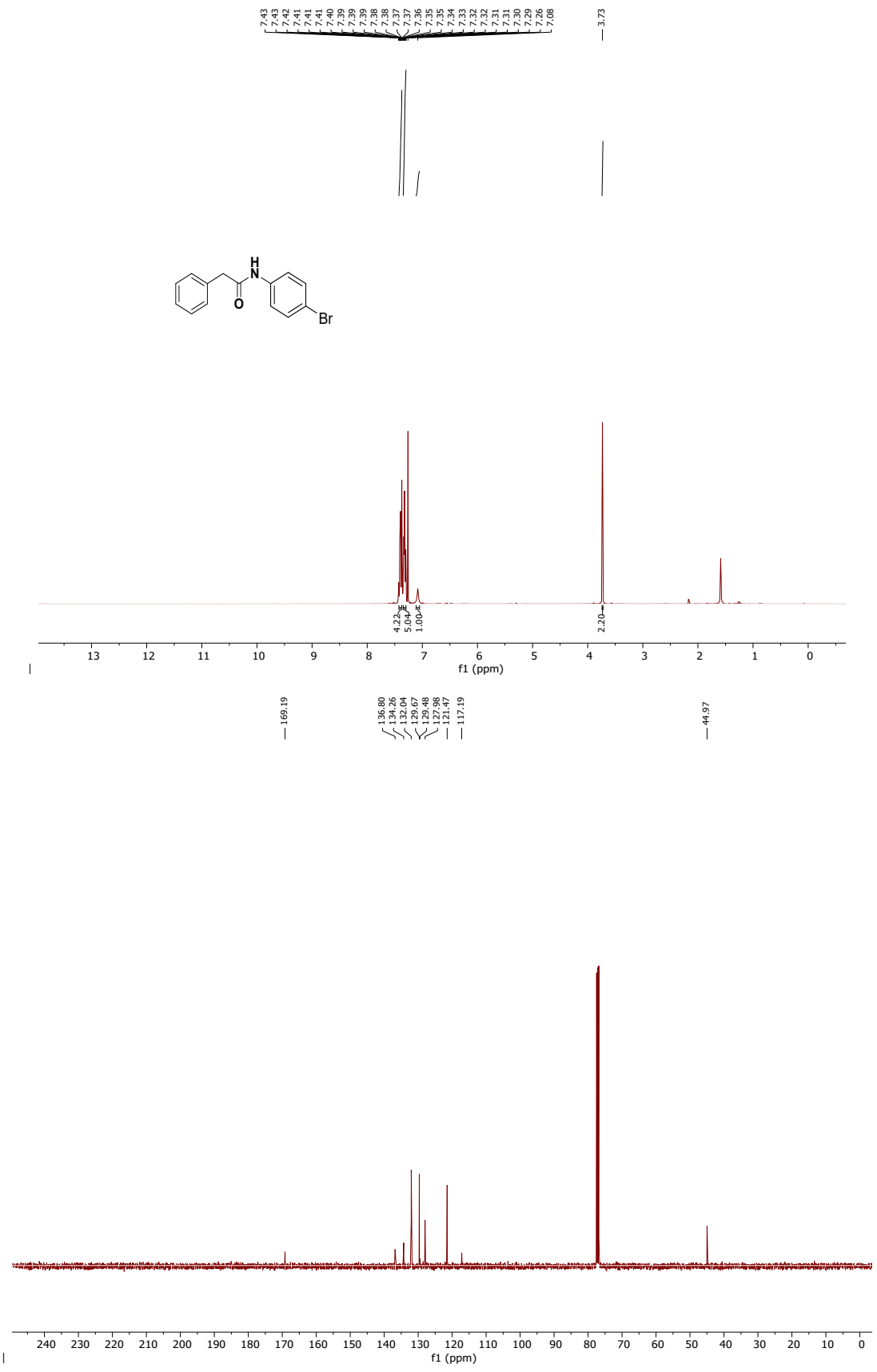
N-(4-methoxyphenyl)-2-phenylacetamide (4s); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



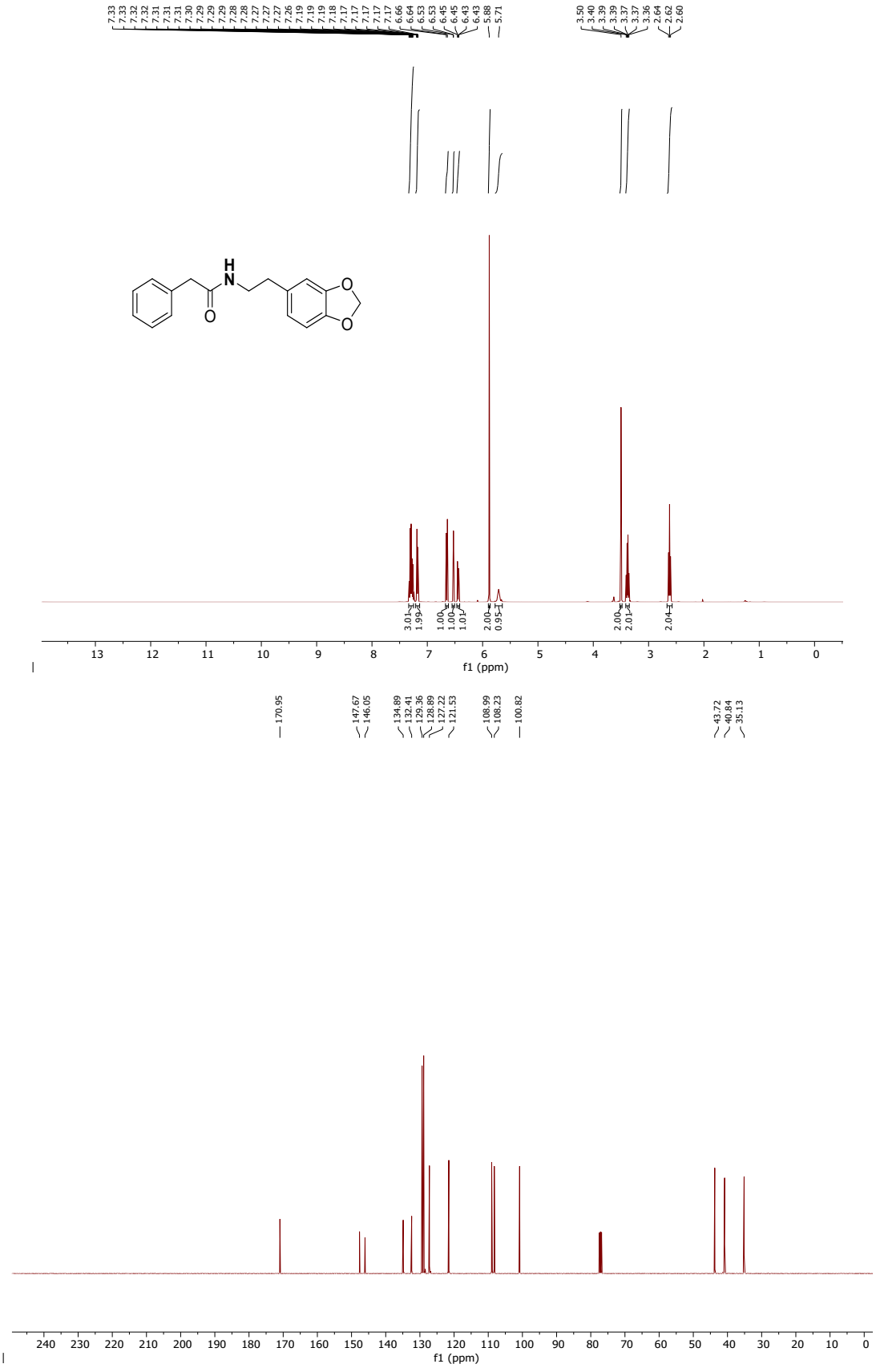
N-(4-nitrophenyl)-2-phenylacetamide (4t); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



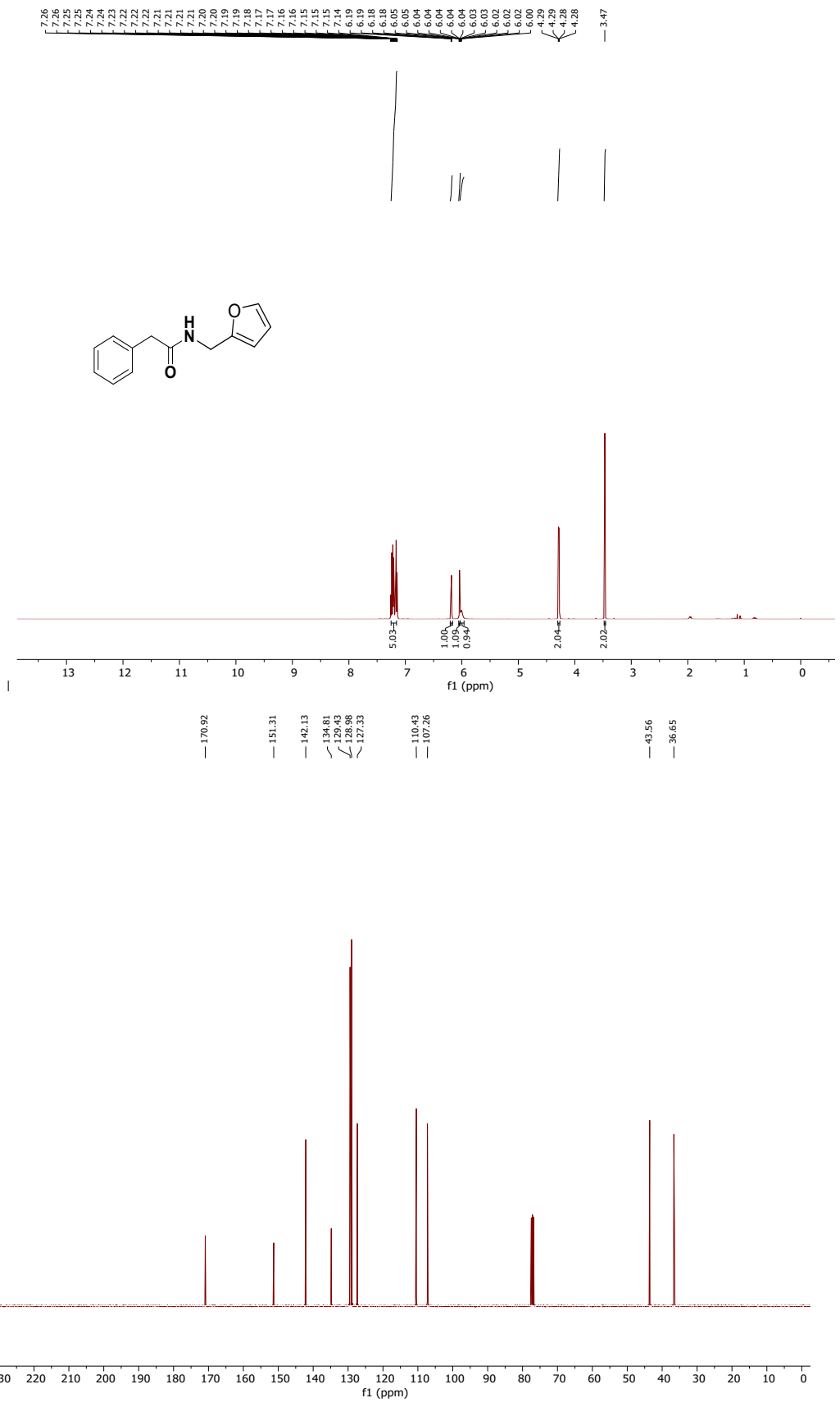
N-(4-bromophenyl)-2-phenylacetamide (4u); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



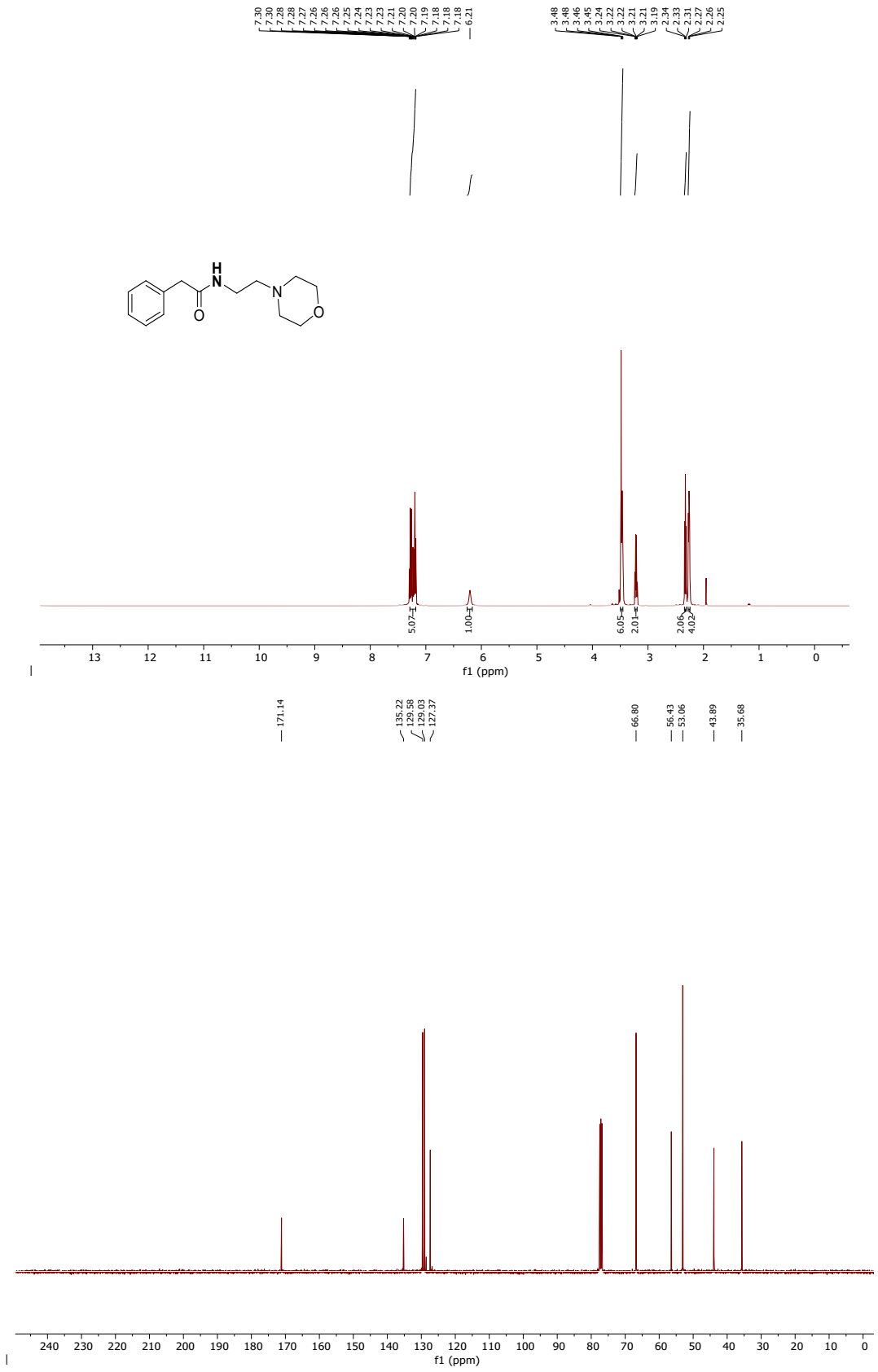
N-(2-(benzo[d][1,3]dioxol-5-yl)ethyl)-2-phenylacetamide (4v); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, CDCl3).**



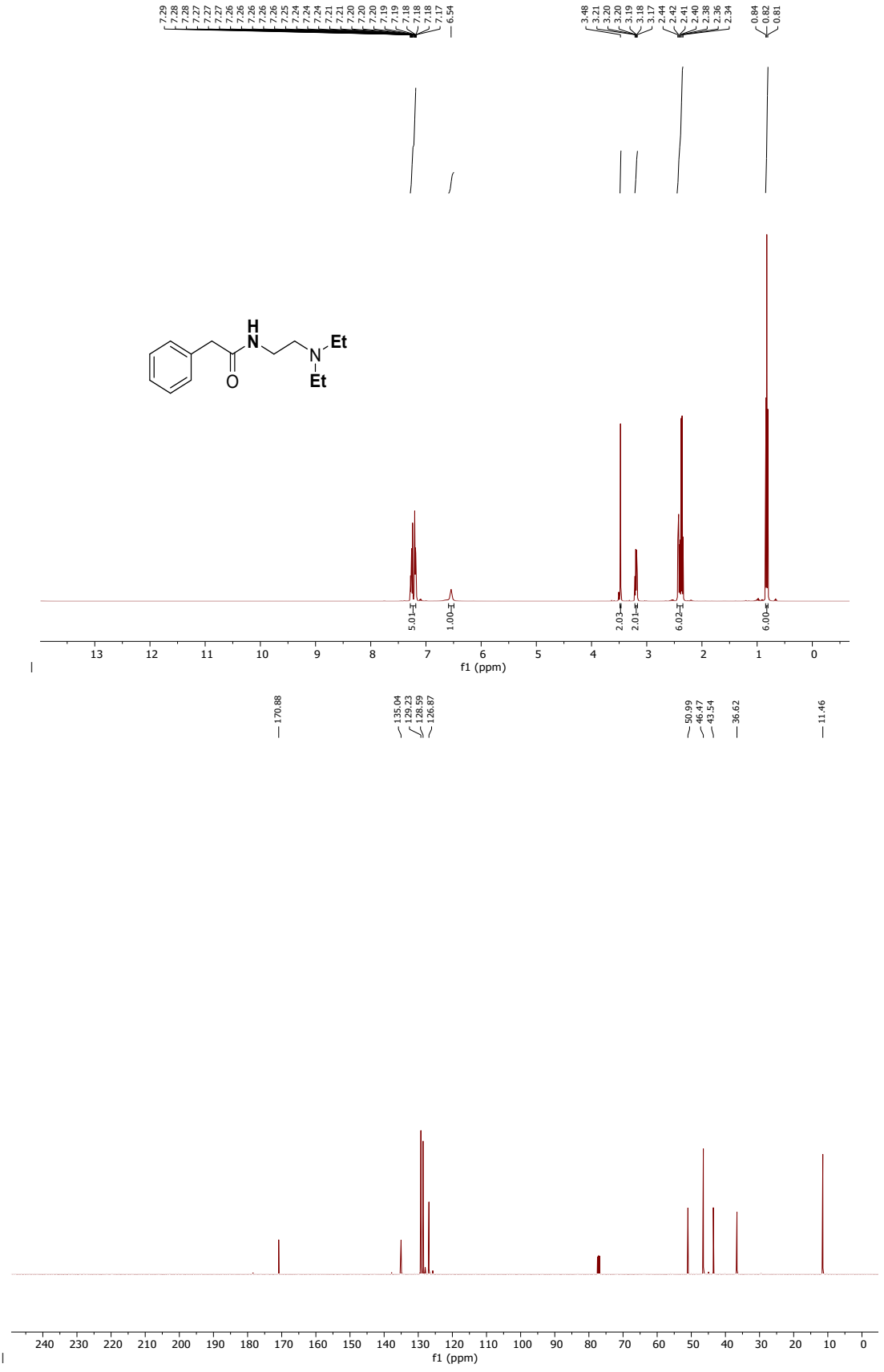
N-(furan-2-ylmethyl)-2-phenylacetamide (4w); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, $CDCl_3$).**



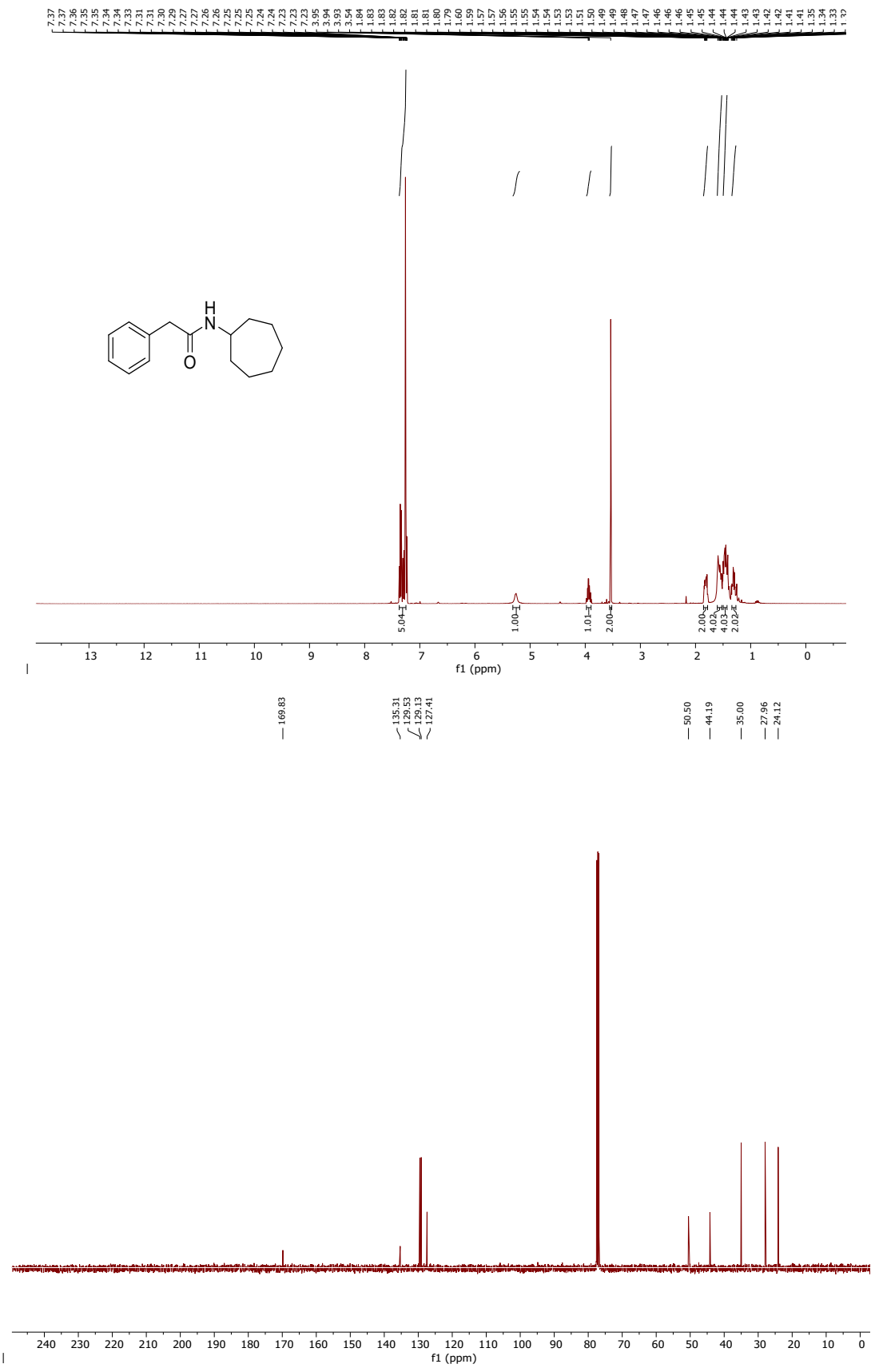
N-(2-morpholinoethyl)-2-phenylacetamide (4x); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, $CDCl_3$).**



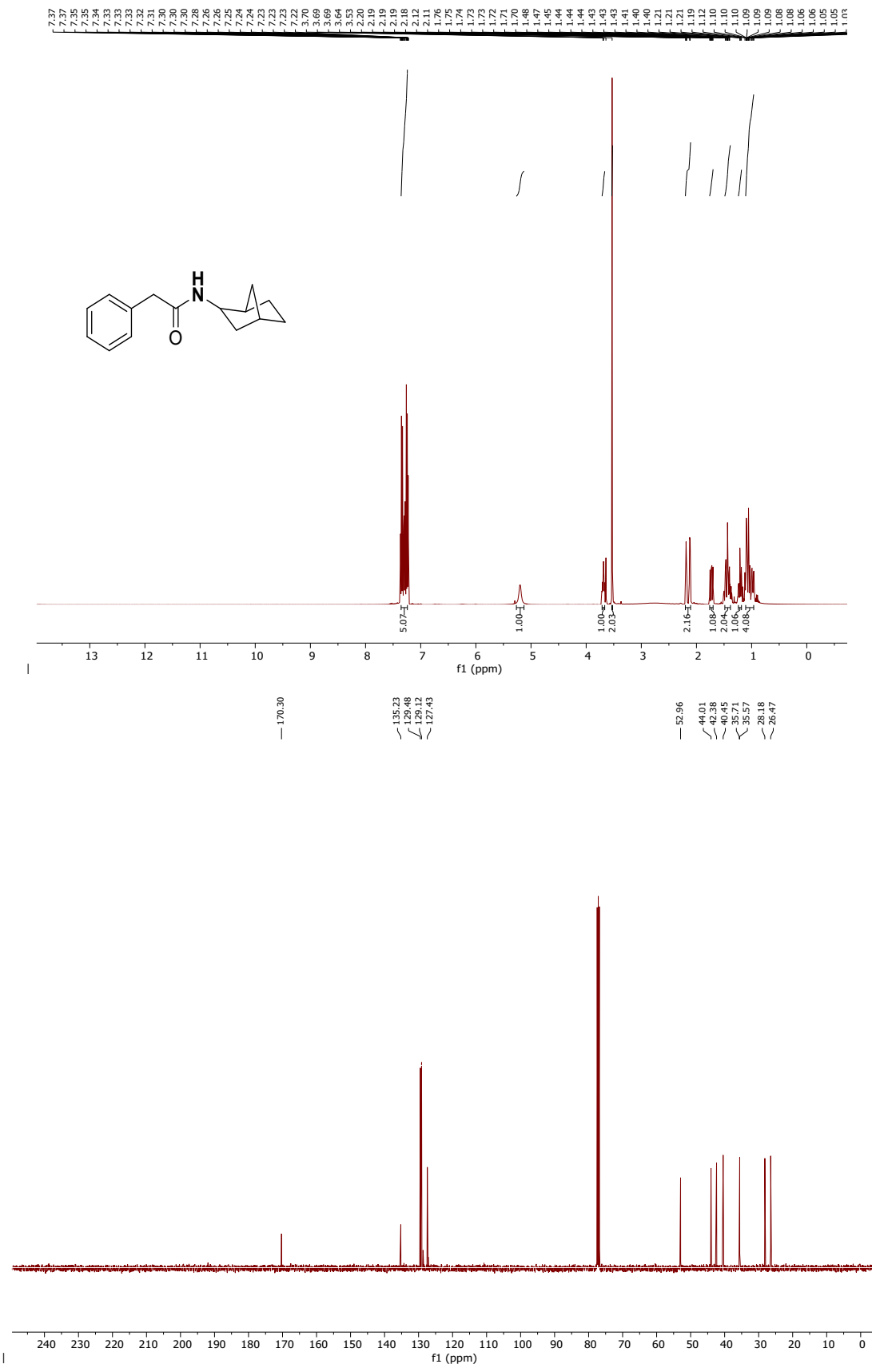
N-(2-(diethylamino)ethyl)benzamide (4y); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, $CDCl_3$).**



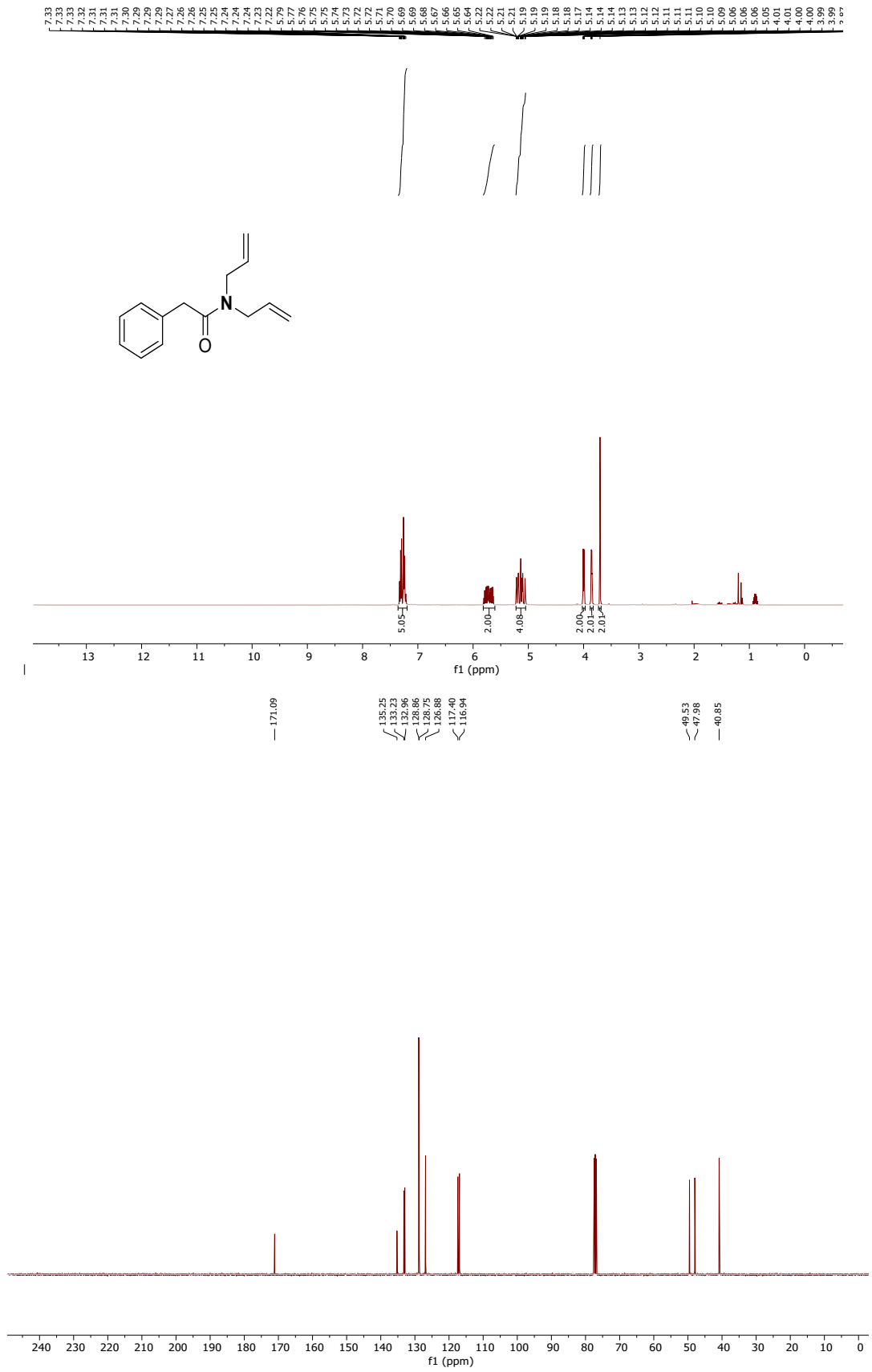
N-cycloheptyl-2-phenylacetamide (4z); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, $CDCl_3$).**



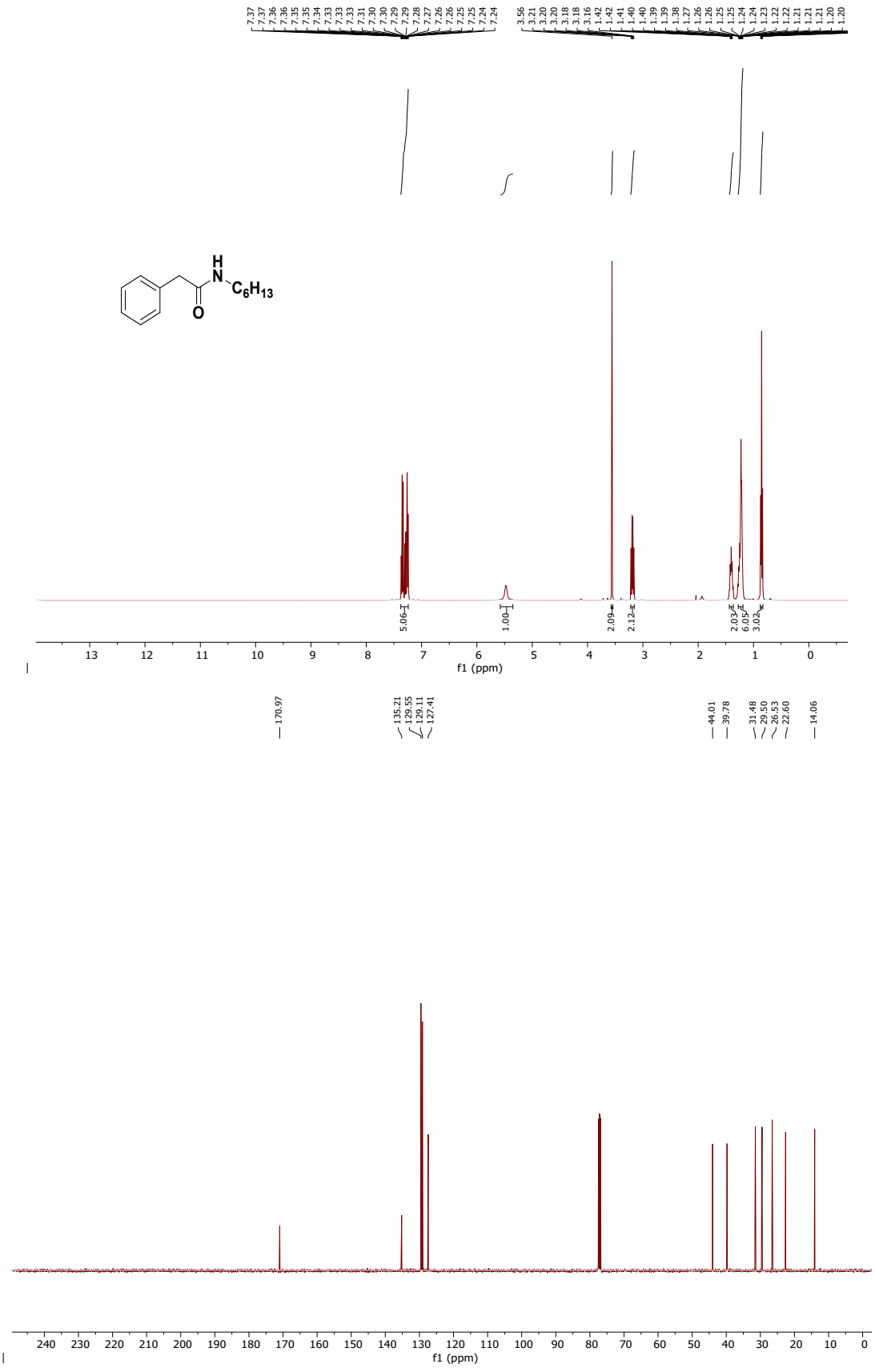
N-((1R,4S)-bicyclo[2.2.1]heptan-2-yl)-2-phenylacetamide (4za); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, $CDCl_3$).**



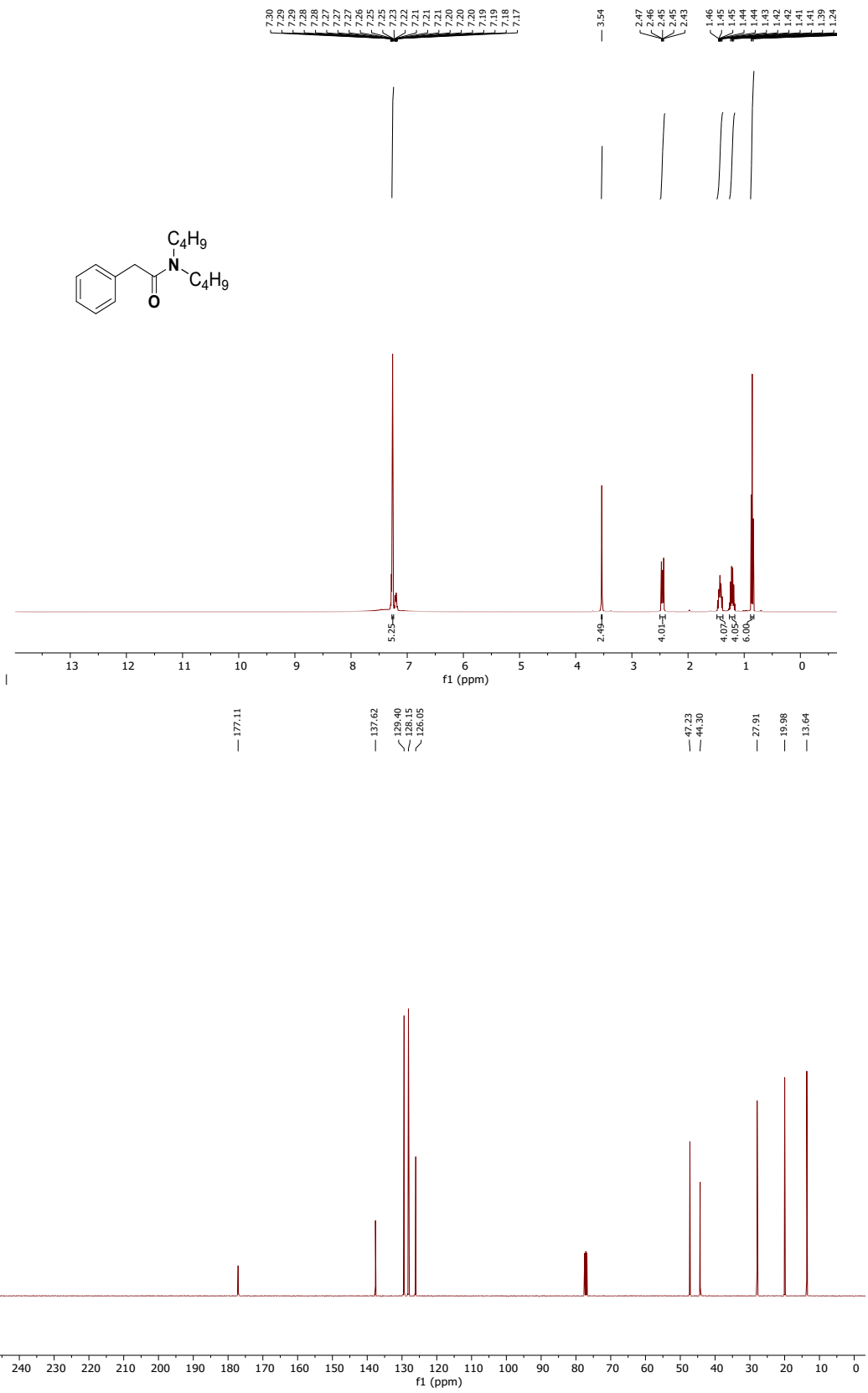
N,N-diallyl-2-phenylacetamide (4zb); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, $CDCl_3$).**



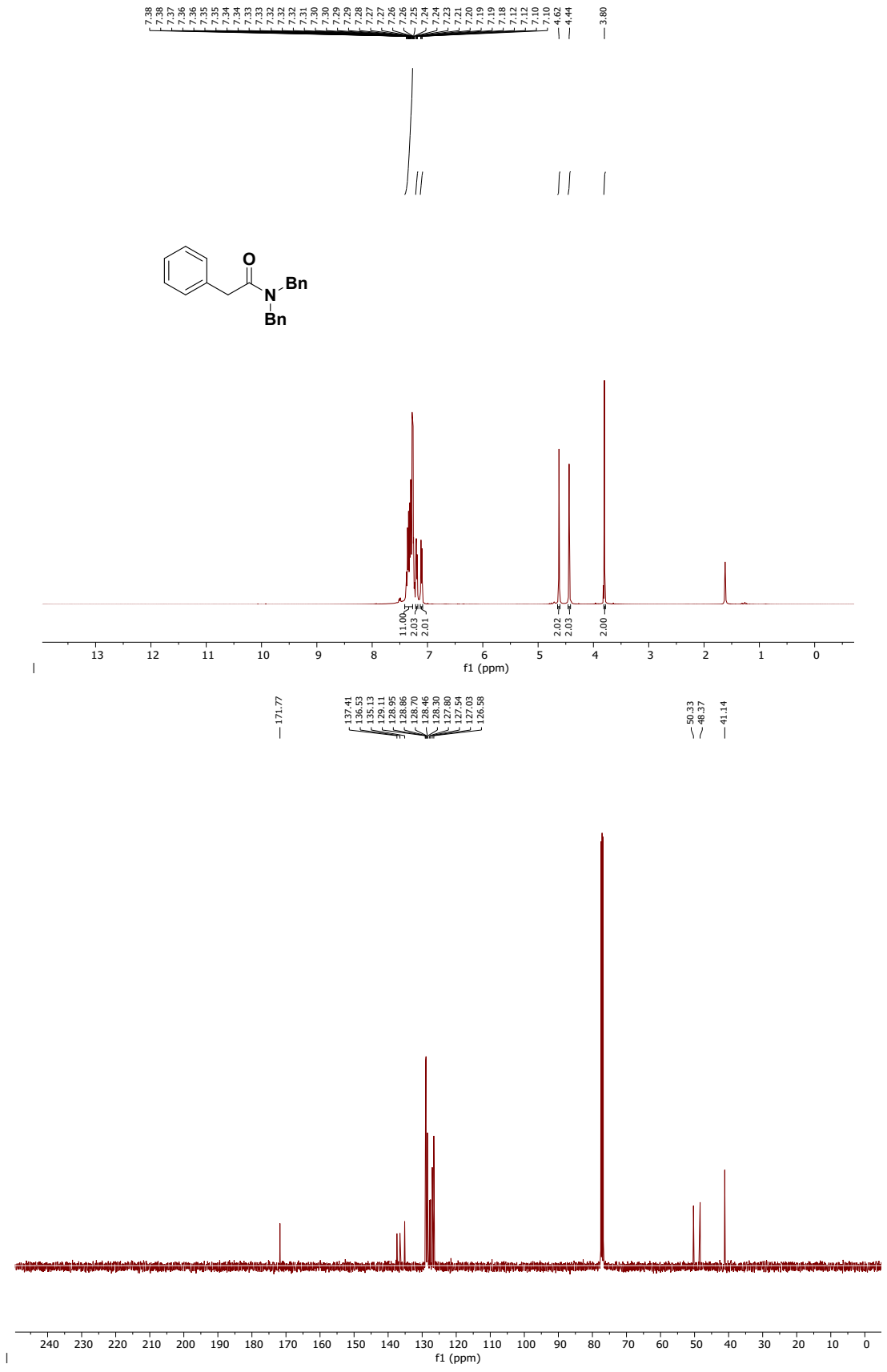
N-hexyl-2-phenylacetamide (4zc); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, $CDCl_3$).**



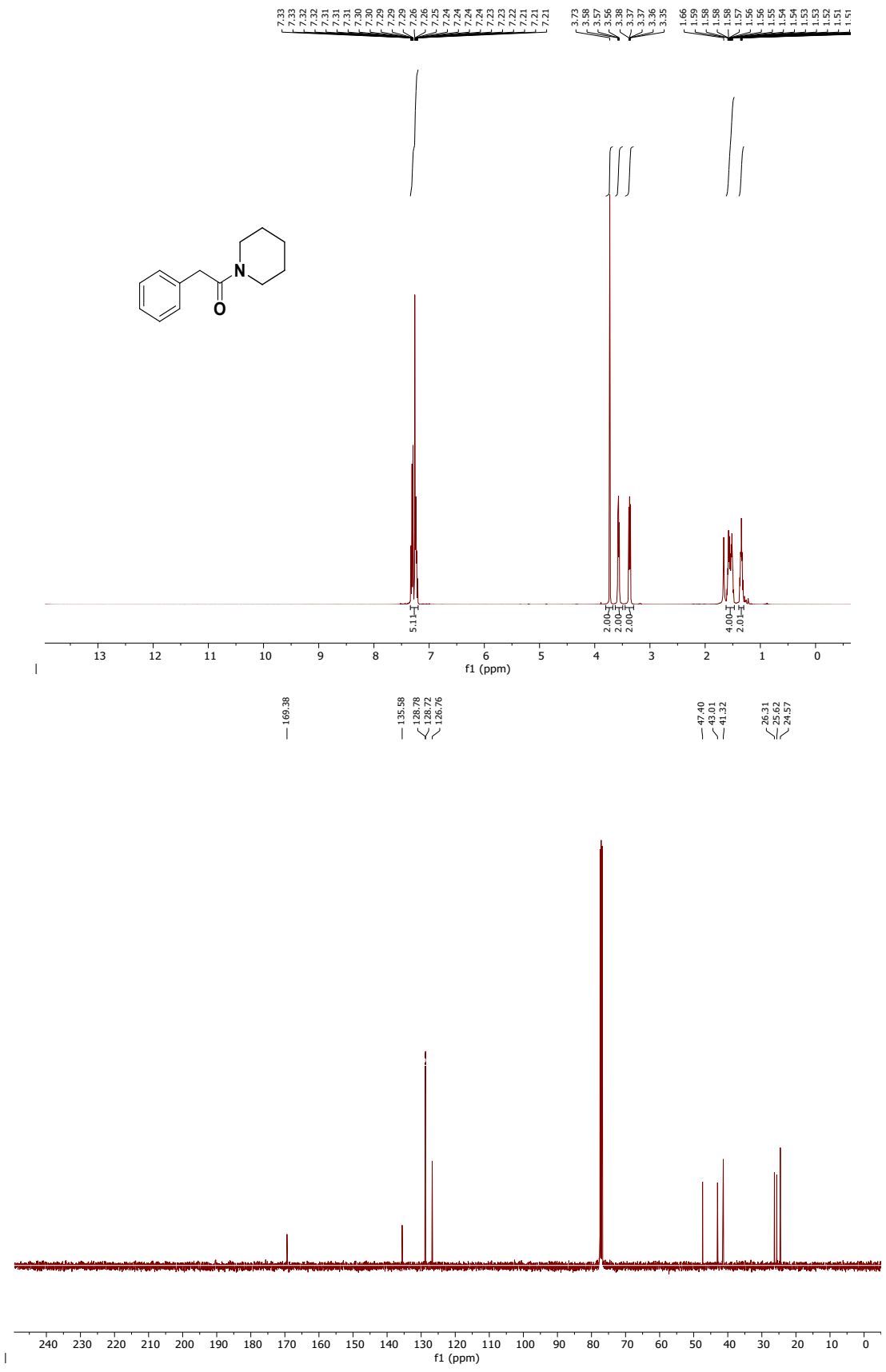
N,N-dibutyl-2-phenylacetamide (4zd); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, $CDCl_3$).**



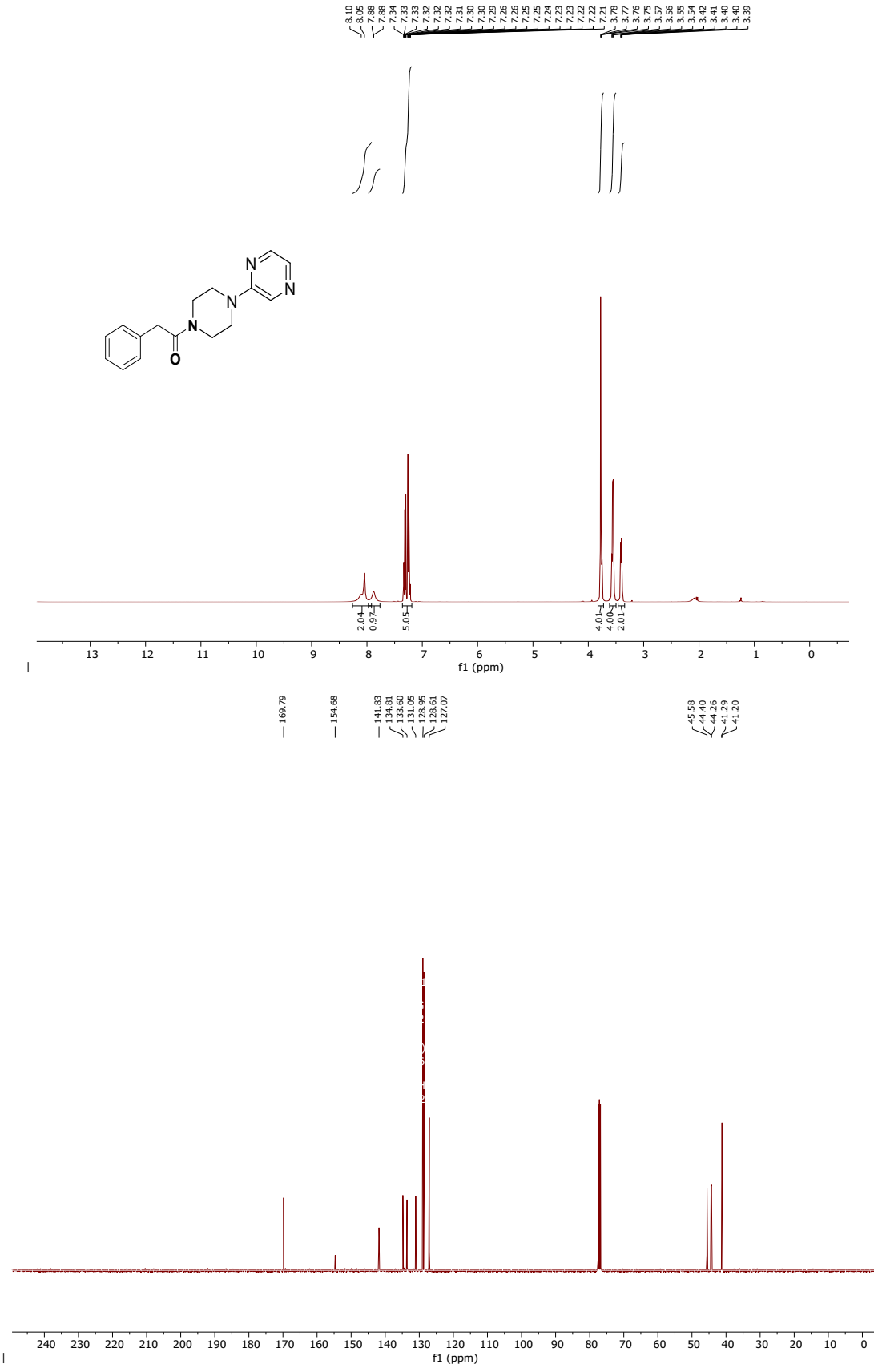
N,N-dibenzyl-2-phenylacetamide (4ze); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, $CDCl_3$).**



2-phenyl-1-(piperidin-1-yl)ethan-1-one (4zf); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, $CDCl_3$).**



2-phenyl-1-(4-(pyrazin-2-yl)piperazin-1-yl)ethan-1-one (4zg); **1 H NMR (400 MHz, CDCl3), 13C NMR (101 MHz, $CDCl_3$).**



Optemized Cartesian coordinates for amid systems labeled alphabatically (a-x), using B3LYP functional and def2-TZVP def2/J basiset.

a

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C	-1.563722000000	3.754934000000	-8.404335000000
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H	-1.633251000000	0.098998000000	-5.306734000000

b

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c

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H	1.776928000000	1.757216000000	-2.925072000000
H	3.051298000000	0.621359000000	-3.367707000000
H	-1.712667000000	0.145887000000	-5.342831000000
N	1.028316000000	-2.260676000000	1.753862000000
O	1.380078000000	-3.429957000000	1.785792000000
O	0.483944000000	-1.674732000000	2.678145000000

d

H	-0.102924000000	1.598219000000	-3.934814000000
O	1.570356000000	-0.956063000000	-4.714452000000
C	1.223846000000	0.055352000000	-4.128357000000
N	0.117796000000	0.771788000000	-4.465655000000
C	-1.579920000000	3.643754000000	-8.273453000000
C	-2.627049000000	3.007656000000	-7.619452000000
C	-0.270569000000	3.229290000000	-8.042344000000
H	-3.648428000000	3.323839000000	-7.792382000000
H	0.550372000000	3.717527000000	-8.552768000000
C	-2.365458000000	1.964181000000	-6.735817000000
C	-0.013532000000	2.186500000000	-7.162482000000
H	-3.187075000000	1.472059000000	-6.227604000000
H	1.006956000000	1.864812000000	-6.989864000000
C	-1.059303000000	1.541429000000	-6.497581000000

H	-1.780301000000	4.457507000000	-8.959563000000
C	1.733686000000	-0.174802000000	-1.665683000000
C	1.115147000000	0.437322000000	-0.577039000000
C	2.088210000000	-1.521465000000	-1.558346000000
H	0.836208000000	1.483573000000	-0.632604000000
H	2.556778000000	-2.016527000000	-2.399574000000
C	0.854178000000	-0.265123000000	0.595447000000
C	1.833327000000	-2.237704000000	-0.396158000000
H	0.377599000000	0.223914000000	1.433891000000
H	2.113259000000	-3.279515000000	-0.323873000000
C	1.217902000000	-1.600415000000	0.673747000000
C	-0.780809000000	0.397002000000	-5.548936000000
C	2.013667000000	0.599841000000	-2.935997000000
H	-0.295309000000	-0.432661000000	-6.064555000000
H	1.801265000000	1.658682000000	-2.776659000000
H	3.068104000000	0.508980000000	-3.204776000000
H	-1.722886000000	0.019990000000	-5.140924000000
Br	0.873260000000	-2.578374000000	2.282200000000

e

H	0.008578000000	1.762047000000	-4.159153000000
O	1.499399000000	-0.936072000000	-4.815645000000
C	1.225994000000	0.122286000000	-4.278758000000
N	0.163814000000	0.892024000000	-4.640791000000
C	-1.515561000000	3.761432000000	-8.452445000000
C	-2.566956000000	3.177038000000	-7.758292000000
C	-0.217329000000	3.297696000000	-8.254262000000
H	-3.579746000000	3.531366000000	-7.905767000000
H	0.606552000000	3.745049000000	-8.796468000000
C	-2.320545000000	2.136168000000	-6.867247000000
C	0.024373000000	2.257443000000	-7.367125000000

H	-3.145349000000	1.684494000000	-6.327668000000
H	1.036016000000	1.897290000000	-7.220304000000
C	-1.025677000000	1.664237000000	-6.661627000000
H	-1.703963000000	4.573061000000	-9.144409000000
C	1.789461000000	-0.058900000000	-1.828077000000
C	1.022297000000	0.508247000000	-0.814780000000
C	2.287526000000	-1.346751000000	-1.608310000000
H	0.618357000000	1.508278000000	-0.928687000000
H	2.886152000000	-1.828283000000	-2.374932000000
C	0.785584000000	-0.213387000000	0.347643000000
N	2.068500000000	-2.048366000000	-0.498772000000
H	0.195968000000	0.202976000000	1.154673000000
C	1.328401000000	-1.486979000000	0.457981000000
H	1.166349000000	-2.080803000000	1.352032000000
C	-0.764164000000	0.525002000000	-5.702759000000
C	2.066244000000	0.672064000000	-3.121322000000
H	-0.311368000000	-0.326013000000	-6.213324000000
H	1.895183000000	1.742173000000	-2.985767000000
H	3.109047000000	0.535520000000	-3.413149000000
H	-1.709601000000	0.180119000000	-5.274286000000

f

H	-0.177503000000	2.170657000000	-4.580001000000
O	0.942959000000	-0.769341000000	-4.704010000000
C	0.864801000000	0.414355000000	-4.411581000000
N	-0.075244000000	1.241664000000	-4.952197000000
C	-1.690163000000	3.525631000000	-9.180773000000
C	-2.768865000000	3.076725000000	-8.429410000000
C	-0.404807000000	3.093749000000	-8.864904000000
H	-3.772189000000	3.408914000000	-8.665979000000
H	0.440731000000	3.436465000000	-9.448653000000

C	-2.562014000000	2.201739000000	-7.366974000000
C	-0.202343000000	2.217593000000	-7.806490000000
H	-3.407385000000	1.857538000000	-6.781732000000
H	0.799550000000	1.881897000000	-7.566590000000
C	-1.280143000000	1.760105000000	-7.044564000000
H	-1.848195000000	4.207774000000	-10.007099000000
C	1.811418000000	1.043567000000	-3.426656000000
C	2.105108000000	2.409067000000	-3.405108000000
C	2.446426000000	0.199178000000	-2.514265000000
H	1.662170000000	3.081208000000	-4.130308000000
H	2.228320000000	-0.859737000000	-2.555364000000
C	3.008709000000	2.921141000000	-2.481006000000
C	3.339436000000	0.712275000000	-1.583969000000
H	3.239177000000	3.979406000000	-2.483373000000
H	3.820534000000	0.048666000000	-0.876047000000
C	3.622512000000	2.074936000000	-1.564647000000
H	4.325147000000	2.474583000000	-0.843505000000
C	-1.069716000000	0.783110000000	-5.909702000000
H	-0.712143000000	-0.178499000000	-6.280034000000
H	-2.024397000000	0.595010000000	-5.408026000000

g

H	0.211376000000	2.266645000000	-4.873895000000
O	0.946317000000	-0.743391000000	-4.324759000000
C	1.002203000000	0.474951000000	-4.263087000000
N	0.264458000000	1.281358000000	-5.071736000000
C	-1.804597000000	3.751667000000	-8.912296000000
C	-2.730980000000	3.291476000000	-7.985022000000
C	-0.514042000000	3.228604000000	-8.916170000000
H	-3.737576000000	3.690753000000	-7.977880000000
H	0.210574000000	3.577837000000	-9.641526000000

C	-2.366772000000	2.315515000000	-7.061688000000
C	-0.155068000000	2.252810000000	-7.995682000000
H	-3.094194000000	1.959174000000	-6.341056000000
H	0.848699000000	1.843761000000	-8.006698000000
C	-1.077285000000	1.786249000000	-7.055087000000
H	-2.085015000000	4.511338000000	-9.631547000000
C	1.909985000000	1.165396000000	-3.279084000000
C	2.404074000000	2.458222000000	-3.464692000000
C	2.293459000000	0.446071000000	-2.145934000000
H	2.156633000000	3.020749000000	-4.356101000000
H	1.923042000000	-0.562765000000	-2.025861000000
C	3.255489000000	3.030023000000	-2.532030000000
C	3.134077000000	1.010548000000	-1.202447000000
H	3.645808000000	4.027066000000	-2.684538000000
H	3.423167000000	0.454490000000	-0.320613000000
C	3.620313000000	2.309900000000	-1.390457000000
C	-0.678619000000	0.737235000000	-6.046388000000
H	-0.192890000000	-0.112392000000	-6.528746000000
H	-1.564686000000	0.344868000000	-5.538620000000
C	4.493721000000	2.898445000000	-0.422345000000
N	5.195750000000	3.375385000000	0.357655000000
		h	
H	-1.356504000000	3.983591000000	-2.082403000000
O	-1.113947000000	0.867660000000	-1.703235000000
C	-0.772671000000	2.039488000000	-1.782460000000
N	-1.639760000000	3.022466000000	-2.167776000000
C	-4.490109000000	5.017861000000	-5.847615000000
C	-5.110988000000	5.133793000000	-4.610602000000
C	-3.389075000000	4.176591000000	-5.988619000000
H	-5.967876000000	5.785435000000	-4.490583000000

H	-2.902222000000	4.078482000000	-6.951301000000
C	-4.632807000000	4.411541000000	-3.520308000000
C	-2.916868000000	3.455846000000	-4.900122000000
H	-5.122860000000	4.505065000000	-2.557568000000
H	-2.061743000000	2.800020000000	-5.016470000000
C	-3.534768000000	3.563440000000	-3.651088000000
H	-4.859864000000	5.577215000000	-6.697970000000
C	0.626590000000	2.471734000000	-1.464041000000
C	1.188670000000	3.688978000000	-1.868054000000
C	1.422952000000	1.590238000000	-0.735972000000
H	0.622141000000	4.388742000000	-2.470906000000
H	0.996092000000	0.641605000000	-0.439558000000
C	2.493114000000	4.014733000000	-1.545945000000
C	2.731825000000	1.905419000000	-0.396575000000
H	2.931659000000	4.950259000000	-1.867149000000
H	3.316249000000	1.197759000000	0.173650000000
C	3.275033000000	3.126422000000	-0.800955000000
C	-3.037078000000	2.757356000000	-2.473195000000
H	-3.105675000000	1.686939000000	-2.673011000000
H	-3.667257000000	2.957314000000	-1.599750000000
O	4.541065000000	3.534780000000	-0.530657000000
C	5.389246000000	2.682552000000	0.225649000000
H	5.558605000000	1.731138000000	-0.286984000000
H	6.334112000000	3.212482000000	0.322152000000
H	4.977968000000	2.490739000000	1.220794000000

i

H	-0.248621000000	2.106746000000	-4.539447000000
O	1.034079000000	-0.766045000000	-4.732890000000
C	0.874096000000	0.398391000000	-4.399060000000
N	-0.098343000000	1.190699000000	-4.927405000000

C	-1.649778000000	3.585393000000	-9.106648000000
C	-2.728150000000	3.129105000000	-8.359718000000
C	-0.368510000000	3.119631000000	-8.822353000000
H	-3.727706000000	3.487279000000	-8.572827000000
H	0.476213000000	3.468388000000	-9.403527000000
C	-2.525574000000	2.212521000000	-7.331693000000
C	-0.170518000000	2.203077000000	-7.798483000000
H	-3.370528000000	1.861149000000	-6.750202000000
H	0.828084000000	1.840879000000	-7.584087000000
C	-1.248296000000	1.738108000000	-7.040667000000
H	-1.804422000000	4.299530000000	-9.906149000000
C	1.761797000000	1.034332000000	-3.365480000000
C	1.957916000000	2.410658000000	-3.235957000000
C	2.468423000000	0.198084000000	-2.502200000000
H	1.472578000000	3.109579000000	-3.910887000000
H	2.353269000000	-0.873591000000	-2.600792000000
N	2.758868000000	2.964991000000	-2.327501000000
C	3.299401000000	0.762697000000	-1.548873000000
H	3.858200000000	0.145450000000	-0.857114000000
C	3.407734000000	2.149211000000	-1.497409000000
H	4.047883000000	2.625300000000	-0.761313000000
C	-1.036654000000	0.724314000000	-5.938996000000
H	-0.622307000000	-0.204408000000	-6.331838000000
H	-1.997887000000	0.476535000000	-5.478359000000

j

H	0.552589000000	3.043251000000	-4.716767000000
O	-0.630364000000	0.553868000000	-3.188741000000
C	0.178587000000	1.407884000000	-3.531459000000
N	-0.153228000000	2.383728000000	-4.435156000000
C	-1.199570000000	2.516987000000	-9.386970000000

C	-1.808838000000	3.566703000000	-8.711833000000
C	-0.669516000000	1.449750000000	-8.665616000000
H	-2.223340000000	4.401503000000	-9.263854000000
H	-0.197437000000	0.625217000000	-9.186171000000
C	-1.884826000000	3.549865000000	-7.321525000000
C	-0.748304000000	1.435615000000	-7.279674000000
H	-2.360407000000	4.373002000000	-6.799260000000
H	-0.336275000000	0.601418000000	-6.723792000000
C	-1.357856000000	2.487212000000	-6.590312000000
H	-1.136785000000	2.527501000000	-10.468398000000
C	2.118000000000	-0.469020000000	-1.458456000000
C	0.900541000000	-1.149659000000	-1.292391000000
C	3.257248000000	-0.991328000000	-0.819040000000
H	0.016026000000	-0.765038000000	-1.775553000000
H	4.205886000000	-0.478294000000	-0.929417000000
C	0.841482000000	-2.303028000000	-0.522744000000
C	3.194558000000	-2.147129000000	-0.056382000000
H	-0.106995000000	-2.813193000000	-0.406151000000
H	4.088981000000	-2.528686000000	0.420148000000
C	1.980953000000	-2.809546000000	0.094946000000
H	1.923762000000	-3.713089000000	0.689576000000
C	-1.452543000000	2.466271000000	-5.080171000000
C	1.577959000000	1.525641000000	-3.055090000000
H	-2.013965000000	1.596904000000	-4.734993000000
H	2.103394000000	2.386462000000	-3.457839000000
H	-1.986717000000	3.357465000000	-4.735104000000
C	2.320195000000	0.755692000000	-2.234050000000
H	3.335695000000	1.127816000000	-2.118565000000

k

H	-0.038593000000	1.837870000000	-4.606403000000

O	1.595883000000	-0.708013000000	-5.483343000000
C	1.302327000000	0.316073000000	-4.886242000000
N	0.123488000000	0.971251000000	-5.091728000000
C	-1.930885000000	3.594805000000	-8.894459000000
C	-2.888732000000	3.102771000000	-8.017406000000
C	-0.633330000000	3.089665000000	-8.851346000000
H	-3.900309000000	3.489039000000	-8.044241000000
H	0.116981000000	3.464474000000	-9.536918000000
C	-2.548904000000	2.113061000000	-7.098691000000
C	-0.298811000000	2.102013000000	-7.935013000000
H	-3.301408000000	1.733109000000	-6.416382000000
H	0.710697000000	1.708659000000	-7.907901000000
C	-1.253491000000	1.602230000000	-7.045165000000
H	-2.190894000000	4.365986000000	-9.609281000000
C	2.228087000000	0.911936000000	-3.828705000000
C	2.335839000000	2.442962000000	-3.815021000000
C	1.840963000000	0.390372000000	-2.417833000000
H	2.475604000000	2.833904000000	-4.825159000000
H	0.752006000000	0.339019000000	-2.329771000000
C	3.503003000000	2.891671000000	-2.908643000000
C	2.407984000000	1.278406000000	-1.290112000000
H	4.420755000000	2.949404000000	-3.500064000000
H	2.548990000000	0.680965000000	-0.386303000000
C	3.721282000000	1.941537000000	-1.711212000000
H	4.439946000000	1.161613000000	-1.980791000000
C	-0.884095000000	0.528737000000	-6.045752000000
H	-0.458309000000	-0.342316000000	-6.544881000000
H	-1.781837000000	0.196893000000	-5.515688000000
H	2.207056000000	-0.632976000000	-2.315322000000
H	1.686211000000	2.058922000000	-1.029435000000

H	4.163788000000	2.487610000000	-0.874987000000
H	3.305979000000	3.904544000000	-2.548780000000
H	1.402723000000	2.878852000000	-3.440308000000
H	3.207726000000	0.505106000000	-4.087578000000

m

H	-0.117555000000	1.685011000000	-4.196048000000
O	1.449174000000	-0.840418000000	-5.242942000000
C	1.136777000000	0.102566000000	-4.533727000000
N	0.062278000000	0.901841000000	-4.802342000000
C	-1.252963000000	4.242259000000	-8.384285000000
C	-2.373386000000	3.613824000000	-7.856749000000
C	0.013499000000	3.727960000000	-8.118125000000
H	-3.362450000000	4.007165000000	-8.056933000000
H	0.891559000000	4.210343000000	-8.529576000000
C	-2.227097000000	2.478703000000	-7.064194000000
C	0.155481000000	2.594095000000	-7.329549000000
H	-3.105416000000	1.992732000000	-6.654322000000
H	1.143053000000	2.195333000000	-7.129597000000
C	-0.964728000000	1.955325000000	-6.792146000000
H	-1.363097000000	5.127492000000	-8.998303000000
C	-0.812929000000	0.709190000000	-5.948390000000
C	1.900133000000	0.455679000000	-3.266046000000
H	-0.367515000000	-0.101935000000	-6.526833000000
H	1.841425000000	1.532056000000	-3.078787000000
H	2.946966000000	0.207347000000	-3.448881000000
H	-1.799162000000	0.370218000000	-5.617594000000
C	1.396058000000	-0.303082000000	-2.023165000000
H	0.336152000000	-0.074277000000	-1.865361000000
H	1.925327000000	0.096119000000	-1.151866000000
C	1.589496000000	-1.819250000000	-2.077957000000

H	1.049200000000	-2.229611000000	-2.935190000000
H	2.647002000000	-2.038729000000	-2.261316000000
C	1.140324000000	-2.525508000000	-0.797418000000
H	0.094268000000	-2.270795000000	-0.588839000000
H	1.719611000000	-2.142736000000	0.051301000000
C	1.282889000000	-4.046855000000	-0.862191000000
H	0.666422000000	-4.429916000000	-1.683290000000
H	2.317605000000	-4.301581000000	-1.119062000000
C	0.899116000000	-4.760052000000	0.435184000000
H	-0.123377000000	-4.479971000000	0.715006000000
H	1.543018000000	-4.402732000000	1.247324000000
C	0.997045000000	-6.283705000000	0.346125000000
H	0.326608000000	-6.641059000000	-0.444045000000
H	2.009330000000	-6.562305000000	0.030397000000
C	0.664616000000	-7.002648000000	1.654189000000
H	-0.339307000000	-6.709932000000	1.983980000000
H	1.350859000000	-6.661530000000	2.438088000000
C	0.735917000000	-8.526829000000	1.549957000000
H	0.035899000000	-8.867946000000	0.778421000000
H	1.733695000000	-8.818212000000	1.200993000000
C	0.432109000000	-9.250055000000	2.862496000000
H	-0.562228000000	-8.953606000000	3.217235000000
H	1.138382000000	-8.915409000000	3.631276000000
C	0.493371000000	-10.774012000000	2.752111000000
H	-0.217435000000	-11.110044000000	1.987934000000
H	1.485563000000	-11.070935000000	2.391460000000
C	0.199381000000	-11.499350000000	4.065774000000
H	-0.792349000000	-11.203579000000	4.425375000000
H	0.909702000000	-11.163669000000	4.829141000000
C	0.263706000000	-13.021091000000	3.946167000000

H	-0.459044000000	-13.390742000000	3.214090000000
H	1.255196000000	-13.350798000000	3.624169000000
H	0.047571000000	-13.506601000000	4.900426000000

n

H	-0.081072000000	1.588851000000	-4.036319000000
O	1.463568000000	-0.942807000000	-5.101436000000
C	1.162013000000	0.000314000000	-4.387779000000
N	0.092438000000	0.808786000000	-4.648462000000
C	-1.272036000000	4.185944000000	-8.175795000000
C	-2.384561000000	3.543967000000	-7.647842000000
C	-0.000508000000	3.675955000000	-7.926013000000
H	-3.377513000000	3.933867000000	-7.835241000000
H	0.871450000000	4.168984000000	-8.337842000000
C	-2.225325000000	2.399677000000	-6.871129000000
C	0.154383000000	2.532944000000	-7.153186000000
H	-3.097534000000	1.903167000000	-6.460807000000
H	1.145887000000	2.137820000000	-6.965749000000
C	-0.957757000000	1.880509000000	-6.615458000000
H	-1.392184000000	5.078370000000	-8.777367000000
C	-0.792288000000	0.624905000000	-5.788628000000
C	1.933875000000	0.343976000000	-3.122422000000
H	-0.348602000000	-0.177337000000	-6.380689000000
H	1.904033000000	1.423339000000	-2.945687000000
H	2.973468000000	0.065273000000	-3.301722000000
H	-1.774041000000	0.277225000000	-5.453354000000
C	1.406484000000	-0.388612000000	-1.873495000000
H	0.353130000000	-0.128494000000	-1.720095000000
H	1.944884000000	0.002914000000	-1.004326000000
C	1.556607000000	-1.909881000000	-1.915268000000
H	1.011420000000	-2.311334000000	-2.773743000000

H	2.608789000000	-2.161371000000	-2.088153000000
C	1.076715000000	-2.593494000000	-0.633456000000
H	0.035855000000	-2.309214000000	-0.437320000000
H	1.657899000000	-2.219207000000	0.217739000000
C	1.180269000000	-4.118305000000	-0.685533000000
H	0.562512000000	-4.491668000000	-1.510118000000
H	2.210624000000	-4.401701000000	-0.929772000000
C	0.765746000000	-4.812822000000	0.612714000000
H	-0.252571000000	-4.506422000000	0.879932000000
H	1.409871000000	-4.465574000000	1.429030000000
C	0.829109000000	-6.338755000000	0.533035000000
H	0.155355000000	-6.685239000000	-0.259157000000
H	1.836595000000	-6.641849000000	0.224461000000
C	0.474347000000	-7.044684000000	1.842414000000
H	-0.524333000000	-6.728786000000	2.166693000000
H	1.164671000000	-6.716180000000	2.628126000000
C	0.513229000000	-8.570268000000	1.741821000000
H	-0.194571000000	-8.898097000000	0.971594000000
H	1.504254000000	-8.882904000000	1.391844000000
C	0.197249000000	-9.286688000000	3.055236000000
H	-0.789044000000	-8.968692000000	3.413728000000
H	0.913548000000	-8.968698000000	3.821793000000
C	0.224898000000	-10.811512000000	2.940725000000
H	-0.500064000000	-11.129012000000	2.182177000000
H	1.207005000000	-11.127018000000	2.568717000000
C	-0.070076000000	-11.535862000000	4.254584000000
H	-1.050578000000	-11.219507000000	4.630101000000
H	0.658123000000	-11.222315000000	5.011703000000
C	-0.044944000000	-13.060315000000	4.132419000000
H	-0.776620000000	-13.373650000000	3.378599000000

H	0.933748000000	-13.374971000000	3.750811000000
C	-0.330168000000	-13.789099000000	5.445863000000
H	-1.309414000000	-13.475887000000	5.827344000000
H	0.401380000000	-13.475009000000	6.199559000000
C	-0.301897000000	-15.313013000000	5.321758000000
H	-1.033611000000	-15.628368000000	4.568536000000
H	0.677208000000	-15.626456000000	4.939783000000
C	-0.585456000000	-16.043343000000	6.634847000000
H	-1.565777000000	-15.733725000000	7.013660000000
H	0.143401000000	-15.725563000000	7.388343000000
C	-0.548787000000	-17.564864000000	6.502117000000
H	-1.289613000000	-17.916182000000	5.779023000000
H	0.431538000000	-17.908284000000	6.160703000000
H	-0.757068000000	-18.055035000000	7.455627000000

p

H	-1.070110000000	0.656239000000	-4.025432000000
O	1.476846000000	-1.128398000000	-4.532449000000
C	0.601152000000	-0.515869000000	-3.940550000000
N	-0.396813000000	0.154303000000	-4.580803000000
C	-0.968651000000	4.210266000000	-7.547646000000
C	-1.992951000000	3.287594000000	-7.715901000000
C	0.197395000000	3.831534000000	-6.886187000000
H	-2.902878000000	3.572556000000	-8.229688000000
H	1.002768000000	4.544359000000	-6.756036000000
C	-1.852494000000	1.992952000000	-7.222712000000
C	0.334387000000	2.539441000000	-6.397394000000
H	-2.655002000000	1.276322000000	-7.359242000000
H	1.245125000000	2.248863000000	-5.886758000000
C	-0.690404000000	1.603429000000	-6.559561000000
H	-1.074291000000	5.217709000000	-7.930387000000

C	-0.537027000000	0.195744000000	-6.029922000000
H	0.360239000000	-0.279383000000	-6.428590000000
H	-1.393945000000	-0.409588000000	-6.342166000000
C	0.349249000000	-1.862042000000	-1.805791000000
C	0.554601000000	-0.441321000000	-2.403142000000
N	1.802347000000	0.026135000000	-1.802585000000
C	2.621990000000	-1.131915000000	-1.464021000000
C	1.589044000000	-2.115577000000	-0.921689000000
H	3.142241000000	-1.549626000000	-2.338507000000
H	1.926165000000	-3.151432000000	-0.970996000000
H	0.296619000000	-2.596253000000	-2.609276000000
C	2.478085000000	1.143148000000	-2.427108000000
H	3.294507000000	1.474887000000	-1.781769000000
H	2.899963000000	0.907129000000	-3.416314000000
H	1.784921000000	1.980918000000	-2.539014000000
H	1.368172000000	-1.880835000000	0.121204000000
H	-0.579284000000	-1.921957000000	-1.238135000000
H	3.373558000000	-0.849573000000	-0.721571000000
H	-0.255549000000	0.237494000000	-2.107967000000

q

H	-0.086687000000	1.586735000000	-3.931390000000
O	1.582342000000	-0.973573000000	-4.700025000000
C	1.237425000000	0.040144000000	-4.116459000000
N	0.135541000000	0.760071000000	-4.461208000000
C	-1.588144000000	3.643558000000	-8.246338000000
C	-2.628732000000	3.002721000000	-7.586579000000
C	-0.276306000000	3.229314000000	-8.029099000000
H	-3.651977000000	3.318635000000	-7.748779000000
H	0.539531000000	3.721261000000	-8.544144000000
C	-2.358122000000	1.954659000000	-6.711071000000

C	-0.010340000000	2.182110000000	-7.157200000000
H	-3.174642000000	1.458588000000	-6.198478000000
H	1.011993000000	1.860777000000	-6.995019000000
C	-1.049441000000	1.532127000000	-6.486561000000
H	-1.795462000000	4.460809000000	-8.926206000000
C	1.728654000000	-0.187638000000	-1.649447000000
C	1.103003000000	0.431658000000	-0.568199000000
C	2.076420000000	-1.536492000000	-1.536649000000
H	0.830827000000	1.479065000000	-0.631493000000
H	2.550028000000	-2.033345000000	-2.373731000000
C	0.826179000000	-0.266053000000	0.603610000000
C	1.806829000000	-2.249550000000	-0.376033000000
H	0.344387000000	0.209545000000	1.447596000000
H	2.072708000000	-3.293794000000	-0.279338000000
C	1.185246000000	-1.598413000000	0.676000000000
C	-0.760799000000	0.383946000000	-5.545773000000
C	2.021929000000	0.582412000000	-2.920483000000
H	-0.268858000000	-0.438466000000	-6.066882000000
H	1.812772000000	1.642531000000	-2.764636000000
H	3.077834000000	0.487969000000	-3.182410000000
H	-1.699616000000	-0.003658000000	-5.139876000000
F	0.923832000000	-2.287087000000	1.809872000000

r

H	-0.093220000000	1.594955000000	-3.938557000000
O	1.577374000000	-0.963998000000	-4.708613000000
C	1.232611000000	0.050340000000	-4.126396000000
N	0.128358000000	0.767735000000	-4.467804000000
C	-1.587158000000	3.644995000000	-8.262151000000
C	-2.629905000000	3.005180000000	-7.604803000000
C	-0.275970000000	3.231791000000	-8.039217000000

H	-3.652663000000	3.320305000000	-7.771453000000
H	0.541543000000	3.722948000000	-8.552338000000
C	-2.362110000000	1.959224000000	-6.725949000000
C	-0.012775000000	2.186566000000	-7.164091000000
H	-3.180304000000	1.464034000000	-6.215196000000
H	1.009097000000	1.865930000000	-6.997714000000
C	-1.054087000000	1.537722000000	-6.495823000000
H	-1.792337000000	4.460655000000	-8.944567000000
C	1.732807000000	-0.178361000000	-1.661331000000
C	1.114157000000	0.437199000000	-0.574557000000
C	2.080945000000	-1.526614000000	-1.551558000000
H	0.840179000000	1.484597000000	-0.632213000000
H	2.549516000000	-2.024060000000	-2.391292000000
C	0.846675000000	-0.263157000000	0.596921000000
C	1.819260000000	-2.240051000000	-0.389960000000
H	0.369800000000	0.224706000000	1.436079000000
H	2.092370000000	-3.283412000000	-0.311674000000
C	1.203180000000	-1.600877000000	0.679397000000
C	-0.768732000000	0.391301000000	-5.551800000000
C	2.018765000000	0.594331000000	-2.931659000000
H	-0.278909000000	-0.433836000000	-6.070567000000
H	1.807065000000	1.653561000000	-2.773831000000
H	3.074138000000	0.502399000000	-3.196586000000
H	-1.708546000000	0.007488000000	-5.144796000000
Cl	0.877229000000	-2.493026000000	2.147673000000

s

H	-0.086469000000	1.597536000000	-3.951712000000
O	1.586661000000	-0.960309000000	-4.720219000000
C	1.239914000000	0.053224000000	-4.137937000000
N	0.136105000000	0.770398000000	-4.480698000000

C	-1.597390000000	3.650320000000	-8.263831000000
C	-2.635891000000	3.008732000000	-7.601520000000
C	-0.284670000000	3.237350000000	-8.049567000000
H	-3.659789000000	3.323643000000	-7.761483000000
H	0.529502000000	3.729869000000	-8.566678000000
C	-2.362341000000	1.961173000000	-6.726345000000
C	-0.015737000000	2.190603000000	-7.178030000000
H	-3.177244000000	1.464510000000	-6.211771000000
H	1.007288000000	1.870155000000	-7.018390000000
C	-1.052732000000	1.539957000000	-6.504806000000
H	-1.807015000000	4.467177000000	-8.943454000000
C	1.739251000000	-0.170781000000	-1.672937000000
C	1.121367000000	0.447071000000	-0.587365000000
C	2.085094000000	-1.519095000000	-1.561246000000
H	0.848970000000	1.495056000000	-0.645641000000
H	2.553499000000	-2.019254000000	-2.399695000000
C	0.851791000000	-0.252078000000	0.585578000000
C	1.821118000000	-2.231184000000	-0.398040000000
H	0.374632000000	0.248497000000	1.417012000000
H	2.096961000000	-3.274491000000	-0.330351000000
C	1.204733000000	-1.591512000000	0.672134000000
C	-0.761028000000	0.392340000000	-5.564302000000
C	2.026320000000	0.599632000000	-2.944160000000
H	-0.268553000000	-0.429471000000	-6.085778000000
H	1.815171000000	1.659258000000	-2.788400000000
H	3.081728000000	0.506093000000	-3.208300000000
H	-1.698484000000	0.003490000000	-5.156644000000
I	0.805590000000	-2.667342000000	2.448147000000

t

H	0.018124000000	1.682140000000	-4.123893000000

O	1.652002000000	-0.896351000000	-4.906166000000
C	1.324350000000	0.121813000000	-4.320204000000
N	0.229375000000	0.856114000000	-4.659099000000
C	-1.574276000000	3.768203000000	-8.382503000000
C	-2.599844000000	3.117377000000	-7.709164000000
C	-0.257169000000	3.356164000000	-8.194691000000
H	-3.627059000000	3.431580000000	-7.848275000000
H	0.547058000000	3.855990000000	-8.720361000000
C	-2.309012000000	2.061461000000	-6.849649000000
C	0.028883000000	2.301361000000	-7.338488000000
H	-3.113900000000	1.557565000000	-6.326359000000
H	1.055164000000	1.982118000000	-7.198564000000
C	-0.994916000000	1.641035000000	-6.654452000000
H	-1.797149000000	4.591593000000	-9.049933000000
C	1.788229000000	-0.088339000000	-1.851467000000
C	1.138106000000	0.552198000000	-0.783340000000
C	2.114800000000	-1.452511000000	-1.703445000000
H	0.882777000000	1.603009000000	-0.870032000000
H	2.602761000000	-1.965683000000	-2.523201000000
C	0.818535000000	-0.099409000000	0.383292000000
C	1.819534000000	-2.152780000000	-0.563794000000
H	0.323692000000	0.422025000000	1.191107000000
H	2.082056000000	-3.197957000000	-0.475019000000
C	1.153148000000	-1.492109000000	0.531587000000
C	-0.683951000000	0.485039000000	-5.730806000000
C	2.120203000000	0.651817000000	-3.124351000000
H	-0.196526000000	-0.329234000000	-6.268913000000
H	1.946109000000	1.721263000000	-2.986005000000
H	3.174006000000	0.517567000000	-3.381610000000
H	-1.613833000000	0.087170000000	-5.313803000000

C	0.854977000000	-2.161599000000	1.665150000000
O	0.598048000000	-2.738706000000	2.643595000000

u

H	-0.063151000000	1.734138000000	-4.154348000000
O	1.525649000000	-0.907019000000	-4.814394000000
C	1.206081000000	0.135842000000	-4.270296000000
N	0.134855000000	0.880590000000	-4.650078000000
C	-1.502651000000	3.767280000000	-8.467333000000
C	-2.559148000000	3.146520000000	-7.813661000000
C	-0.199586000000	3.332993000000	-8.237334000000
H	-3.575653000000	3.477935000000	-7.986351000000
H	0.628322000000	3.809025000000	-8.747944000000
C	-2.313183000000	2.098535000000	-6.930968000000
C	0.041924000000	2.285461000000	-7.358703000000
H	-3.141921000000	1.618110000000	-6.423243000000
H	1.057630000000	1.948029000000	-7.187647000000
C	-1.013381000000	1.655995000000	-6.693843000000
H	-1.691031000000	4.584406000000	-9.152756000000
C	1.742546000000	-0.084725000000	-1.812246000000
C	1.140472000000	0.529282000000	-0.713337000000
C	2.101452000000	-1.432566000000	-1.715597000000
H	0.860696000000	1.574808000000	-0.768023000000
H	2.554902000000	-1.921847000000	-2.567614000000
C	0.900263000000	-0.174021000000	0.457492000000
C	1.864912000000	-2.146517000000	-0.553217000000
H	0.435812000000	0.312513000000	1.304985000000
H	2.145126000000	-3.189247000000	-0.485868000000
C	1.262373000000	-1.520960000000	0.545311000000
C	-0.752381000000	0.508097000000	-5.745181000000
C	2.000083000000	0.692327000000	-3.083992000000

H	-0.265420000000	-0.324050000000	-6.255072000000
H	1.780111000000	1.748914000000	-2.922635000000
H	3.053331000000	0.610517000000	-3.361525000000
H	-1.700806000000	0.135368000000	-5.348322000000
C	1.020746000000	-2.253269000000	1.749638000000
N	0.825329000000	-2.842541000000	2.721248000000

v

H	1.613457000000	2.501923000000	-3.109990000000
O	3.325171000000	0.137237000000	-4.296586000000
C	2.918874000000	0.983346000000	-3.517669000000
N	1.899277000000	1.837538000000	-3.810080000000
C	0.974331000000	5.627075000000	-7.044723000000
C	-0.195615000000	4.981176000000	-6.667375000000
C	2.205383000000	5.034094000000	-6.774849000000
H	-1.157773000000	5.434429000000	-6.871949000000
H	3.121916000000	5.529666000000	-7.070527000000
C	-0.134346000000	3.749211000000	-6.021056000000
C	2.262632000000	3.805056000000	-6.131710000000
H	-1.051489000000	3.249631000000	-5.729846000000
H	3.223267000000	3.346763000000	-5.927419000000
C	1.091794000000	3.146694000000	-5.747211000000
H	0.930353000000	6.585677000000	-7.546294000000
C	2.886308000000	0.195611000000	-1.120458000000
C	2.173987000000	0.676964000000	-0.023877000000
C	3.004868000000	-1.187659000000	-1.272128000000
H	2.076962000000	1.747191000000	0.126141000000
H	3.549582000000	-1.583840000000	-2.120516000000
C	1.596114000000	-0.194019000000	0.894161000000
C	2.425150000000	-2.053124000000	-0.355182000000
H	1.054938000000	0.210304000000	1.742540000000

H	2.536096000000	-3.123287000000	-0.493807000000
C	1.707418000000	-1.575062000000	0.744107000000
C	1.155264000000	1.800401000000	-5.060920000000
C	3.516497000000	1.143992000000	-2.119855000000
H	1.664367000000	1.066331000000	-5.686722000000
H	3.408162000000	2.172678000000	-1.768894000000
H	4.583263000000	0.936255000000	-2.219495000000
H	0.141117000000	1.430620000000	-4.882986000000
C	1.058689000000	-2.521909000000	1.720384000000
H	0.050310000000	-2.793197000000	1.393842000000
H	1.628650000000	-3.447359000000	1.814565000000
H	0.970574000000	-2.074404000000	2.711754000000

w

H	0.387707000000	-0.155304000000	-4.067374000000
O	2.906149000000	0.324101000000	-5.889922000000
C	2.223164000000	0.126275000000	-4.897391000000
N	0.880300000000	-0.062735000000	-4.941394000000
C	-2.039084000000	3.690679000000	-6.699590000000
C	-2.731464000000	2.516126000000	-6.433636000000
C	-0.650426000000	3.663928000000	-6.802622000000
H	-3.811995000000	2.527392000000	-6.354016000000
H	-0.105971000000	4.575457000000	-7.017791000000
C	-2.036439000000	1.320844000000	-6.269806000000
C	0.040434000000	2.470496000000	-6.638895000000
H	-2.582047000000	0.406115000000	-6.064445000000
H	1.120641000000	2.448740000000	-6.724789000000
C	-0.646996000000	1.284084000000	-6.367654000000
H	-2.576698000000	4.621909000000	-6.830143000000
C	1.998391000000	-0.196546000000	-2.314891000000
C	1.365705000000	0.841064000000	-1.625300000000

C	1.771069000000	-1.497886000000	-1.859734000000
H	1.523789000000	1.865883000000	-1.943055000000
H	2.251370000000	-2.329509000000	-2.363477000000
C	0.539948000000	0.596682000000	-0.537540000000
C	0.949001000000	-1.757317000000	-0.773193000000
H	0.065721000000	1.425893000000	-0.024631000000
H	0.795623000000	-2.779528000000	-0.445371000000
C	0.316231000000	-0.711075000000	-0.091514000000
C	0.111461000000	-0.012647000000	-6.177882000000
C	2.877288000000	0.075716000000	-3.508106000000
H	0.826474000000	-0.155971000000	-6.988161000000
H	3.391870000000	1.033433000000	-3.398092000000
H	3.665094000000	-0.677041000000	-3.589550000000
H	-0.586534000000	-0.853133000000	-6.189082000000
N	-0.553846000000	-0.967794000000	0.964530000000
H	-0.413100000000	-1.841150000000	1.447524000000
H	-0.714236000000	-0.199964000000	1.597252000000

x

H	-0.794175000000	2.324545000000	-2.908686000000
O	1.211582000000	0.502772000000	-4.517404000000
C	0.760510000000	1.213744000000	-3.634606000000
N	-0.486501000000	1.758785000000	-3.682068000000
C	-3.036736000000	5.168671000000	-6.418476000000
C	-3.885547000000	4.218594000000	-5.865544000000
C	-1.663197000000	4.938214000000	-6.435048000000
H	-4.955236000000	4.389531000000	-5.847760000000
H	-0.995641000000	5.672782000000	-6.868867000000
C	-3.362661000000	3.044404000000	-5.329434000000
C	-1.145777000000	3.765926000000	-5.900965000000
H	-4.030739000000	2.306048000000	-4.899797000000

H	-0.076242000000	3.589552000000	-5.919252000000
C	-1.990415000000	2.803785000000	-5.341105000000
H	-3.440222000000	6.083138000000	-6.835354000000
C	1.452216000000	0.453321000000	-1.326267000000
C	0.914743000000	0.721574000000	-0.070502000000
C	1.889496000000	-0.849081000000	-1.589499000000
H	0.573244000000	1.723263000000	0.165979000000
H	2.300803000000	-1.081583000000	-2.563755000000
C	0.814386000000	-0.269927000000	0.900839000000
C	1.793512000000	-1.846420000000	-0.632872000000
H	0.396165000000	-0.036612000000	1.874449000000
H	2.134180000000	-2.852643000000	-0.839530000000
C	1.254953000000	-1.558663000000	0.620259000000
O	1.188288000000	-2.577255000000	1.529910000000
C	-1.424410000000	1.522665000000	-4.770476000000
C	1.564037000000	1.539895000000	-2.376352000000
H	-0.867126000000	0.969359000000	-5.527722000000
H	1.245614000000	2.494017000000	-1.951147000000
H	2.600660000000	1.650160000000	-2.699808000000
H	-2.240859000000	0.878273000000	-4.430515000000
H	0.804234000000	-2.252711000000	2.352186000000