Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

Selective Synthesis of Functionalized Linear Aliphatic Primary Amines via Decarboxylative Radical Polar Crossover Process

Robin Cauwenbergh[a‡], Prakash Kumar Sahoo[a‡], Rakesh Maiti[a‡], Abra Mathew[b], Rositha Kuniyil[b], and Shoubhik Das[a]*

[‡]*Authors contributed equally*

[a]Department of Chemistry, Organic Synthesis Division, University of Antwerp, 2020 Antwerp, Belgium.

[b]Department of Chemistry, CompCat group, Indian Institute of Technology Palakkad, 678557, Kerala, India.

Correspondance: Shoubhik Das. E-mail: shoubhik.das@uantwerpen.be

1. Table of Contents

2. General Considerations

Materials. Chemicals and solvents were obtained from commercial suppliers (Sigma Aldrich, TCI, Thermo Fisher Scientific, J&K Scientific, Fluorochem and ABCR) and used without further purification. Non-commercial starting materials were prepared as described below according to literature procedures. All reactions were carried out under Nitrogen atmosphere using Schlenck techniques.

Analytical Methods. Thin Layer Chromatography (TLC) was performed using TLC plates from Merck (SiO_2, Kieselgel 60 F254 neutral, on aluminum with fluorescence indicator) and compounds were visualized by UV detection (254 nm). Flash column chromatographic purification of products was accomplished using an automated chromatography system with on-line UV and ELSD detection using Grace® Silica flash Cartridges.

Gas chromatography-mass spectrometry (GC-MS) samples were prepared by dissolving 0.1-5 mg of the compound in acetone (GC-MS quality) and further diluted to a concentration of 10^{-5} - 10^{-6} M. The samples were subsequently filtered using a CHROMAFIL® PET-20/25 syringe filter and 3 µL were injected. The apparatus was an Agilent Technologies 7890 A GC System coupled to an Agilent Technologies 5975 C inert MSD with triple-axis detector. As column an Optima 725820.30 30 m × 250 µm × 0.25 µm was selected. Carrier gas was helium. Inlet temperature heater: 225 °C. Oven program: 70 °C for 3 min, then heating 5 °C min^{-1} to 160 °C and heating at 160 °C for 2 min. A one-minute post-run at 280 °C ends the oven program.

Nuclear Magnetic Resonance (NMR) spectra were recorded on a Bruker Avance III 400 (101 MHz for ^{13}C and 376 MHz for ^{19}F) Fourier Transform NMR spectrometer at 300 K, using the non or partly deuterated solvent as internal standard (^1H: δ = 7.26 ppm, ^{13}C: δ = 77.16 ppm for $CDCl_3$; ^1H: δ = 2.50 ppm, ^{13}C: δ = 39.52 ppm for DMSO-d6). Chemical shifts (δ) are given in ppm and coupling constants (J) are reported in Hertz (Hz). Multiplicities are described as s (singlet), d (doublet), t (triplet), q (quartet), p (pentet), br s (broad singlet) and m (multiplet) or combinations thereof. ^{13}C NMR spectra were recorded with complete proton decoupling. ^1H NMR yields were determined by addition of a known amount of an internal standard and dissolving everything in a suitable deuterated solvent, followed by ^1H NMR analysis.

High resolution mass spectrometry (HRMS) samples were prepared by dissolving 0.1-5 mg of the compound in DMSO or CH_3CN/H_2O and further diluted to a concentration of 10^{-5} - 10^{-6} M. Formic acid (0.1%) was added prior to injection. 10 µL of each sample was injected using the CapLC system (Waters, Manchester, UK) and electrosprayed using a standard electrospray source. Samples were injected with an interval of 3 minutes. Positive ion mode accurate mass spectra were acquired using a Q-TOF II instrument (Waters, Manchester, UK). The MS was calibrated prior to use with a 0.1% H_3PO_4 solution. The spectra were lock mass corrected using the known mass of the nearest H_3PO_4 cluster or a known background ion. Analytes were detected as protonated or as a sodium adduct. All measured masses are within a difference of 5 ppm compared to the calculated mass unless specified otherwise.

Computational Details. All calculations were carried out using Gaussian 16 software.[1] All the structures were optimized using PBE0 functional[2] along with Grimme's D3 dispersion correction[3] and Becke Jhonson damping scheme[4] in the gas phase. A 6-31g(d) basis set was used for all the atoms.[5] Frequency calculations were performed on the optimized geometries to make sure that they are the equilibrium geometries. Transition states were characterized by a single imaginary frequency and all the intermediates were characterized by no imaginary frequency.

The single point energy calculation and spin natural orbital analysis on the optimized geometries were performed using the def2-TZVPP basis set and the same functional.[6] The solvation effects were considered in these single point calculations by using the SMD solvation model[7] for the solvent DMSO (dielectric constant, ε = 46.826). Spin natural orbitals were visualized using the Chemcraft program.[8] The 3D images of the transition state structures were generated using CYLView software.[9] All the reported energies are in Gibbs free energies (kcal mol^{-1}).

Photocatalytic setup. The reaction setup is depicted in Figure S1. The reaction setup consists of a 456 nm Kessil lamp, cooling of the setup was performed by two commercially available 120 mm computer fans to keep the temperature around 30 ℃. The light intensity was measured by Ophir StarLite power meter with 3A probe head. The light intensity of Kessil lamp (λ = 456 nm) was 0.34 W/cm^2 and the distance between tube and light was maintained between 3 to 4 cm.

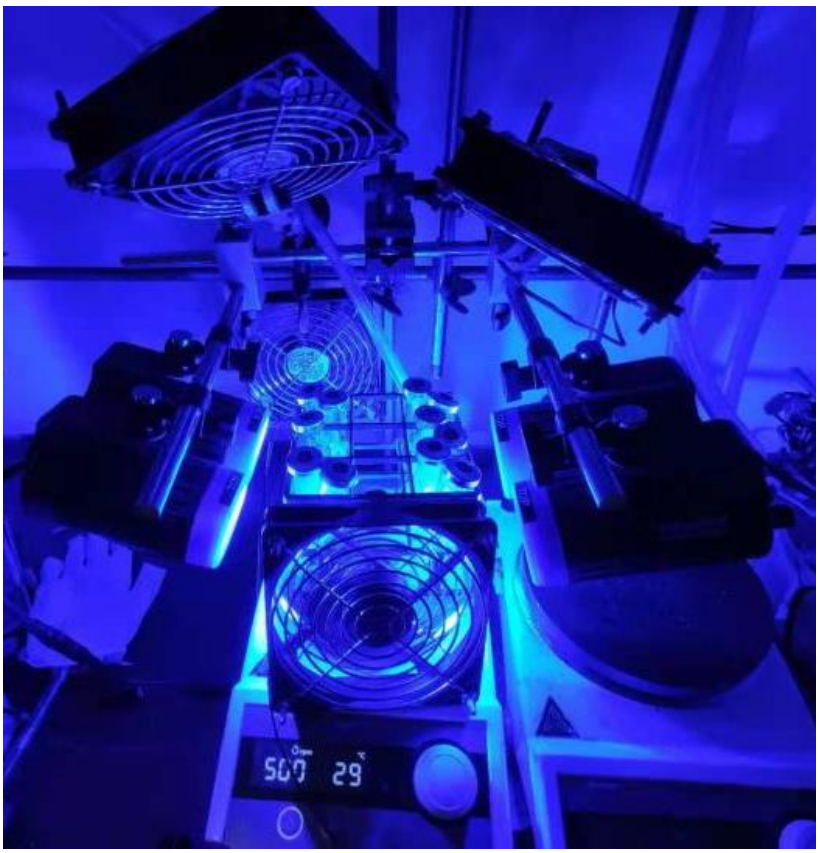


Figure S1: Photocatalytic set up for the hydroaminoalkylation reactions.

3. Experimental Section

3.1. Hydroaminomethylation and hydroamination protocols

Condition A. An oven dried 20 mL Schlenk Tube was charged with olefin (if solid, 0.2 mmol), 4CzIPN (0.02 equiv.), NaOH (1.0 equiv.), protected amino acid (1.0 equiv.) and a magnetic stirring bar. The reaction mixture was degassed by three freeze/pump/thaw cycles (3 min) using Schlenck techniques and refilled with nitrogen. After, olefin (if liquid, 0.2 mmol) and dry DMSO (1 ml) were added. After, the reaction was allowed to stirr under 456 nm blue KESSIL light at room temperature. The mixture was monitored via TLC, quenched with water and extracted with EtOAc (3 times). Lastly, the solvent was removed under reduced pressure. NMR yield was determined by adding 1,3,5-trimethoxybenzene as the internal standard. The pure compound was obtained using Flash column chromatography using heptane:EtOAc (0-50 %) as the eluent.

Condition B. An oven-dried 20 mL Schlenk Tube was charged with olefin (if solid, 0.2 mmol), 4CzIPN (0.02 equiv.), NaOH (1 equiv.), boc-anhydride (1.5 equiv.), unprotected amino acid (1.5 equiv.) and a magnetic stirring bar. The reaction mixture was degassed by three freeze/pump/thaw cycles (3 min) and refilled with nitrogen. After, olefin (if liquid, 0.2 mmol) and dry DMSO (2 ml) were added. After, the reaction was allowed to stir in the dark for 4 hours and subsequently under 456 nm blue KESSIL light at room temperature. The mixture was monitored via TLC, quenched with water and extracted with EtOAc (3 times). Lastly, the solvent was removed under reduced pressure. NMR yield was determined by adding 1,3,5-trimethoxybenzene as the internal standard. The pure compound was obtained using Flash column chromatography using heptane:EtOAc (0-50 %) as the eluent.

Condition C. An oven dried 20 mL Schlenk Tube was charged with 4CzIPN (0.02 equiv.), NaOH (1.0 equiv.), protected amino acid (1.0 equiv.) and a magnetic stirring bar. The reaction mixture was degassed by three freeze/pump/thaw cycles (3 min) using Schlenck techniques and refilled with nitrogen. After, olefin (0.2 mmol) and dry DMSO (2 ml) were added. Next, the reaction was allowed to stirr under 456 nm blue KESSIL light at 70 °C. The mixture was monitored via TLC, quenched with water and extracted with EtOAc (3 times). Lastly, the solvent was removed under reduced pressure. NMR yield was determined by adding 1,3,5-trimethoxybenzene as the internal standard. The pure compound was obtained using Flash column chromatography using heptane:EtOAc (0-50 %) as the eluent.

3.2. Literature protocols

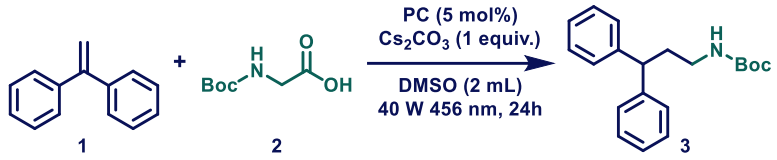
Procedure D. Modification from Ahmad *et al.*[10]: Unprotected amino acid (0.03 mol) was dissolved in 25 mL of 10% sodium hydroxide solution (2.5g in 25 mL) and benzoyl chloride (4,14 ml, 0,038 mol) was added in five equal portions and stirred vigorously after each addition until all the benzoyl chloride has reacted. The reaction mixture was neutralized carefully with concentrated hydrochloric acid and the precipitate was washed with methylene chloride to remove any little benzoic acid formed and was then recrystallised in boiling water. The pure solid was allowed to dry for 24 hours in vacuo at 25 °C.

Procedure E. A slurry of unprotected amino acid (25 mmol) in 70 mL methylene chloride was treated with chlorotrimethylsilicane (2 equiv.) and was allowed to reflux for 140 minutes. The reaction mixture was cooled to 0 °C and was then treated with Triethylamine (1.5 equiv.). After this mixture stirred for about 20 min, a solution of benzoyl chloride (1 equiv.) in 10 mL of methylene chloride was added dropwise to the reaction mixture over a period of 15 min. The reaction mixture was allowed to stir for 30 min. at 0 °C and then for 18 hours at 25 °C. Methylene chloride was removed in vacuo and 100 mls of NaOH solution (2N) was added to the residue. This mixture was allowed to stir for 1 hour before the mixture was acidified to pH = 1 with hydrochloric acid solution (2M). The acidified mixture was then extracted with ethyl acetate (2 × 100 mls), dried over sodium sulfate, and concentrated in vacuo. The resulting white solid was recrystallized from a 50% ethanol/water mixture yielding a white solid, which was allowed to dry for 24 hours in vacuo at 25 °C.

3.3. Reaction Optimization

3.3.1. Optimization Using Boc-Glycine

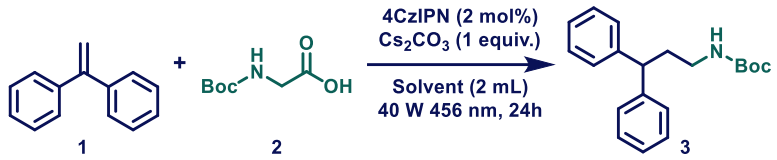
Table S1. Screening of different catalysts.[a]



Entry	Photocatalyst (PC)	Yield (%)[b]
1	$Ir[dF(CF_3)ppy]_2(dtbpy))PF_6$	93
2	DPZ[c]	12
3	Mes-Acr[c]	0
4	Fluorenone[c]	0
5	4CzIPN	98
6	4CzIPN (4 mol%)	91
7	4CzIPN (3 mol%)	95
8	4CzIPN (2 mol%)	94
9	4CzIPN (1 mol%)	65
10	No PC	0
11	No light	0

[a]Reaction conditions: **1** (0.2 mmol), **2** (0.2 mmol, 1 equiv.), Cs_2CO_3 (0.2 mmol, 1 equiv.) and PC (10 µmol, 0.05 equiv. unless stated otherwise) in DMSO (2mL) under N_2 atmosphere and light irradiation (456 nm 40 W KESSIL) at room temperature for 24h. [b]Yield determined by ^1H NMR using 1,3,5-trimethoxybenzene as internal standard. [c]Reaction performed with 40W 390 nm KESSIL light irradiation.

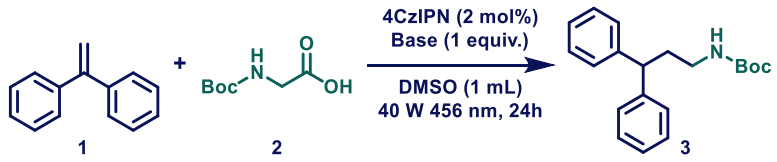
Table S2. Screening of different solvents.[a]



Entry	Solvent	Yield (%)[b]
1	DMSO	94
2	DMA	95
3	DMF	95
4	MeCN	61
5	Toluene	0
6	$CHCl_3$	0
7	Dioxane	83
8	MeOH	0
9	DCM	0
10	THF	86
11	2-Me THF	35
12	DMSO (1 mL)	94

[a]Reaction conditions: **1** (0.2 mmol), **2** (0.2 mmol, 1 equiv.), Cs_2CO_3 (0.2 mmol, 1 equiv.) and 4CzIPN (4 µmol, 0.02 equiv.) in solvent (2 mL, unless stated otherwise) under N_2 atmosphere and light irradiation (456 nm 40 W KESSIL) at room temperature for 24h. [b]Yield determined by ^1H NMR using 1,3,5-trimethoxybenzene as internal standard.

Table S3. Screening of different bases.[a]

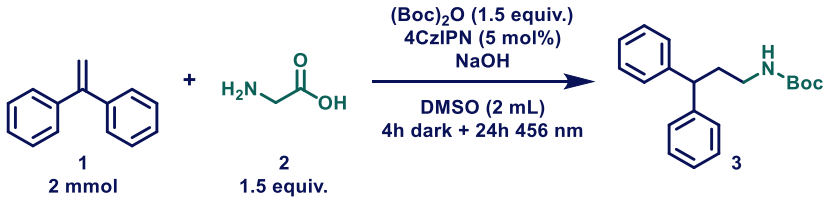


Entry	Base	Yield (%)[b]
1	Cs_2CO_3	94
2	Li_2CO_3	93
3	Na_2CO_3	80
4	K_2CO_3	66
5	KOAc	56
6	NaOH	95
7	K_3PO_4	92
8	DIPEA	0
9	No base	0

[a]Reaction conditions: **1** (0.2 mmol), **2** (0.2 mmol, 1 equiv.), Base (0.2 mmol, 1 equiv.) and 4CzIPN (4 µmol, 0.02 equiv.) in DMSO (1 mL) under N_2 atmosphere and light irradiation (456 nm 40 W KESSIL) at room temperature for 24h. [b]Yield determined by ^1H NMR using 1,3,5-trimethoxybenzene as internal standard.

3.3.2. Optimization Using Free Amines

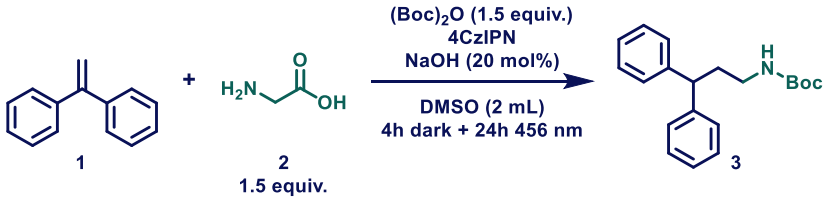
Table S4. Screening of base amount.[a]



Entry	Amount of NaOH (mol%)	Yield (%)[b]
1	0	81
2	5	83
3	10	82
4	20	95
5	50	88
6	100	90

[a]Reaction conditions: **1** (0.2 mmol), **2** (0.3 mmol, 1.5 equiv.), Boc-anhydride (0.3 mmol, 1.5 equiv.), NaOH (x mmol, x equiv.) and 4CzIPN (10 µmol, 0.05 equiv.) in DMSO (2 mL) under N_2 atmosphere in the dark for 4h and subsequently under light irradiation (456 nm 40 W KESSIL) at room temperature for 24h. [b]Yield determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard.

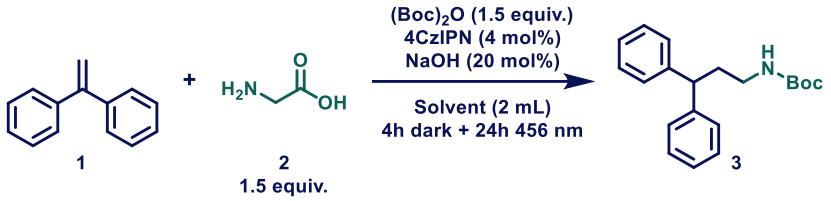
Table S5. Screening of catalyst loading.[a]



Entry	Amount of 4CzIPN (mol%)	Yield (%)[b]
1	1.0	72
2	2.0	88
3	3.0	89
4	4.0	93
5	5.0	93

[a]Reaction conditions: **1** (0.2 mmol), **2** (0.3 mmol, 1.5 equiv.), Boc-anhydride (0.3 mmol, 1.5 equiv.), NaOH (0.04 mmol, 0.2 equiv.) and 4CzIPN (x mmol, x equiv.) in DMSO (2 mL) under N_2 atmosphere in the dark for 4h and subsequently under light irradiation (456 nm 40 W KESSIL) at room temperature for 24h. [b]Yield determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard.

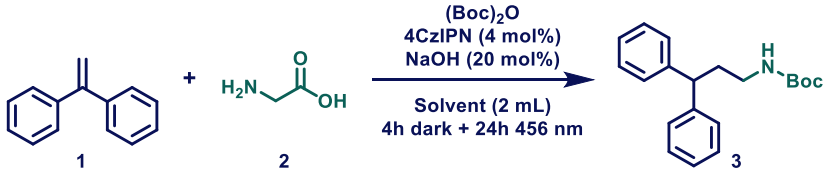
Table S6. Screening of solvent.[a]



Entry	Solvent	Yield (%)[b]
1	DMSO	96
2	DMA	95
3	DMF	95
4	MeCN	43
5	Dioxane	73
6	THF	82
7	DMSO (1 mL)	86

[a]Reaction conditions: **1** (0.2 mmol), **2** (0.3 mmol, 1.5 equiv.), Boc-anhydride (0.3 mmol, 1.5 equiv.), NaOH (0.04 mmol, 0.2 equiv.) and 4CzIPN (8 µmol, 0.04 equiv.) in solvent (2 mL, unless stated otherwise) under N_2 atmosphere in the dark for 4h and subsequently under light irradiation (456 nm 40 W KESSIL) at room temperature for 24h. [b]Yield determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard.

Table S7. Screening of glycine and boc-anhydride ratio.[a]

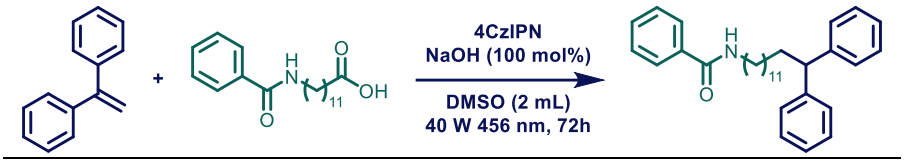


Entry	Glycine:boc-anhydride (equivalents)	Yield (%)[b]
1	1.0:1.0	70
2	1.1:1.1	72
3	1.2:1.2	72
4	1.3:1.3	75
5	1.4:1.4	86
6	1.5:1.5	93
7	1.0:1.1	60
8	1.0:1.2	63
9	1.0:1.3	54
10	1.0:1.4	50
11	1.0:1.5	56

[a]Reaction conditions: **1** (0.2 mmol), **2** (x mmol, x equiv.), Boc-anhydride (x mmol, x equiv.), NaOH (0.04 mmol, 0.2 equiv.) and 4CzIPN (8 µmol, 0.04 equiv.) in solvent (2 mL, unless stated otherwise) under N_2 atmosphere in the dark for 4h and subsequently under light irradiation (456 nm 40 W KESSIL) at room temperature for 24h. [b]Yield determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard.

3.3.3. Optimization Using Long Chain Amino Acids

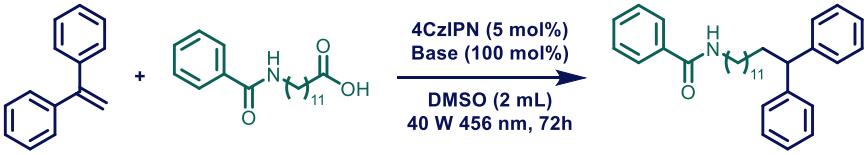
Table S8. Screening of catalyst loading.[a]



Entry	Loading	Yield (%)[b]
1	0 mol%	0
2	1 mol%	0
3	2 mol%	Trace
4	3 mol%	5
5	4 mol%	15
6	5 mol%	20

[a]Reaction conditions: **1** (0.2 mmol), **2** (0.2 mmol, 1 equiv.), NaOH (0.2 mmol, 1 equiv.) and 4CzIPN (x mmol, x equiv.) in DMSO (2 mL) under N_2 atmosphere and light irradiation (456 nm 40 W KESSIL) at room temperature for 72h. [b]Yield determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard.

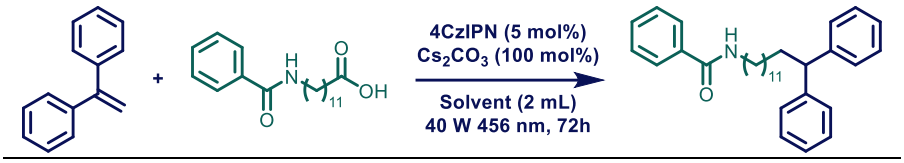
Table S9. Screening of base.[a]



Entry	Base	Yield (%)[b]
1	Cs_2CO_3	43
2	Li_2CO_3	16
3	Na_2CO_3	10
4	NaOH	20
5	K_3PO_4	17
6	DIPEA	0
7	No base	0

[a]Reaction conditions: **1** (0.2 mmol), **2** (0.2 mmol, 1 equiv.), Base (0.2 mmol, 1 equiv.) and 4CzIPN (10 µmol, 0.05 equiv.) in DMSO (2 mL) under N_2 atmosphere and light irradiation (456 nm 40 W KESSIL) at room temperature for 72h. [b]Yield determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard.

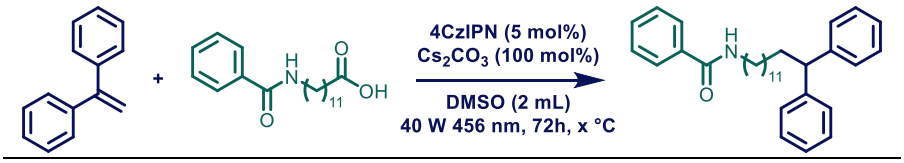
Table S10. Screening of solvent.[a]



Entry	Solvent	Yield (%)[b]
1	DMSO	43
2	DMF	40
3	DMA	38
4	MeCN	10
5	THF	16
6	DMSO (1 mL)	19

[a]Reaction conditions: **1** (0.2 mmol), **2** (0.2 mmol, 1 equiv.), Cs_2CO_3 (0.2 mmol, 1 equiv.) and 4CzIPN (10 µmol, 0.05 equiv.) in solvent (2 mL) under N_2 atmosphere and light irradiation (456 nm 40 W KESSIL) at room temperature for 72h. [b]Yield determined by ^1H NMR using 1,3,5-trimethoxybenzene as internal standard.

Table S11. Screening of temperature.[a]

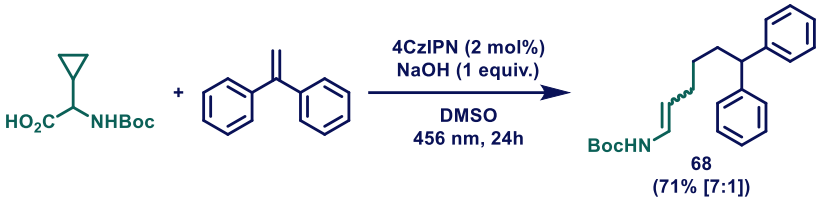


Entry	Temperature (°C)	Yield (%)[b]
1	r.t.	43
2	50	48
3	70	62

[a]Reaction conditions: **1** (0.2 mmol), **2** (0.2 mmol, 1 equiv.), Cs_2CO_3 (0.2 mmol, 1 equiv.) and 4CzIPN (10 µmol, 0.05 equiv.) in DMSO (2 mL) under N_2 atmosphere and light irradiation (456 nm 40 W KESSIL) at a given temperature for 72h. [b]Yield determined by ^1H NMR using 1,3,5-trimethoxybenzene as internal standard.

3.4. Mechanistic studies

3.4.1. Radical clock experiment



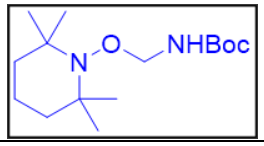
An oven dried 20 mL Schlenk Tube was charged with 4CzIPN (0.01 equiv.), NaOH (1 equiv.), 2-((tert-butoxycarbonyl)amino)-2-cyclopropylacetic acid (1.0 equiv.) and a magnetic stirring bar. The reaction mixture was degassed by three freeze/pump/thaw cycles (3 min) using Schlenck techniques and refilled with nitrogen. After, 1,1-diphenyl ethylene (0.2 mmol) and dry DMSO (1 ml) were added. After, the reaction was allowed to stir under 456 nm blue KESSIL light at room temperature. The mixture was monitored via TLC, quenched with water and extracted with EtOAc (3 times). Lastly, the solvent was removed under reduced pressure. NMR yield was determined by adding 1,3,5-trimethoxybenzene as the internal standard. The pure compounds were obtained using Flash column chromatography using heptane:EtOAc (0-50 %) as the eluent.

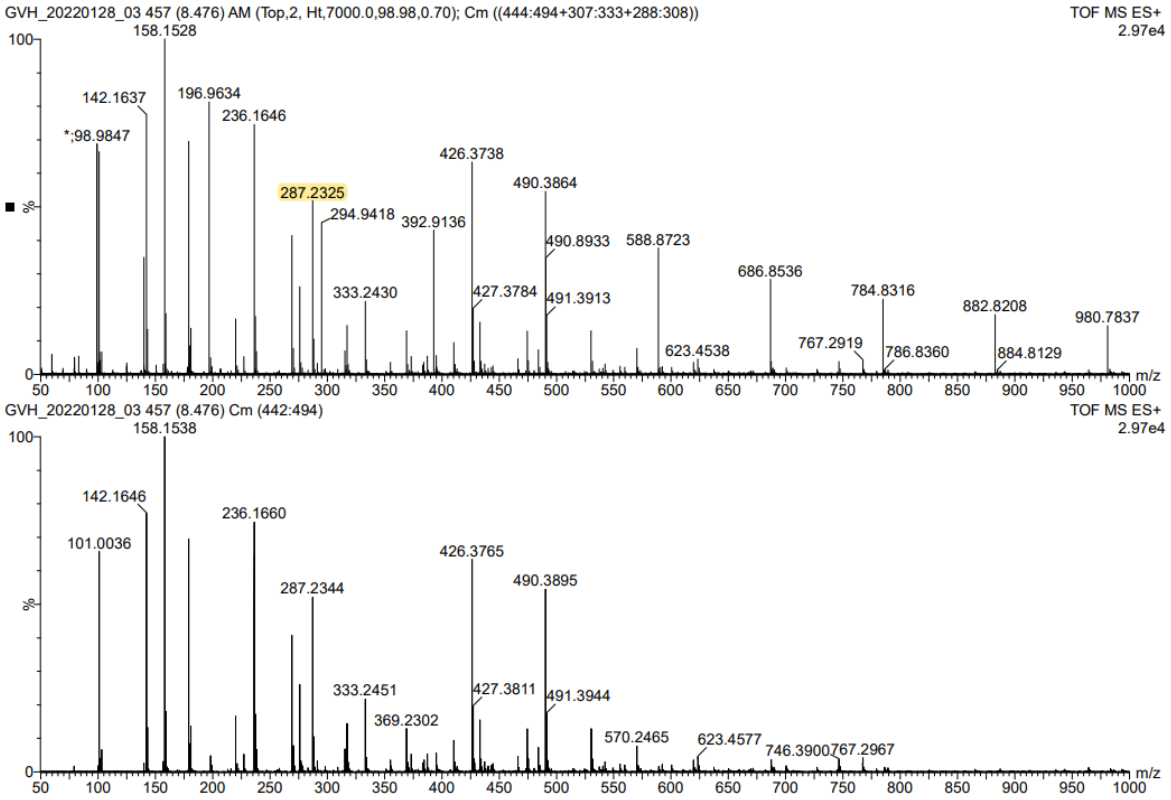
3.4.2. α-Aminomethyl radical capturing by TEMPO

An oven dried 20 mL Schlenk Tube was charged with 4,4'-(ethene-1,1-diyl)bis(fluorobenzene) (0.2 mmol, 1 equiv.) , boc-glycine (1.0 equiv.) or 12-benzoyldodecanoic acid (1.0 equiv.), 4CzIPN (0.02 equiv. for boc-glycine or 0.05 equiv. for 12-benzoyldodecanoic acid), NaOH (1 equiv., for boc-glycine), Cs_2CO_3 (1 equiv., for 12-benzoyldodecanoic acid), TEMPO (1.0 equiv.) and a magnetic stirring bar. The reaction mixture was degassed by three freeze/pump/thaw cycles (3 min) using Schlenck techniques and refilled with nitrogen. After that, dry DMSO (1 mL boc-glycine or 2 mL for 12-benzoyldodecanoic acid) was added. The boc-glycine reaction mixture was allowed to stir under 456 nm blue KESSIL light at room temperature for 24 h and the 12-benzoydodecanoic acid reaction mixture was allowed to stir under 456 nm blue KESSIL light at 70 °C for 60 h. The mixture was monitored via TLC, quenched with water and extracted with EtOAc (3 times). Lastly, the solvent was removed under reduced pressure and the formation of the hydroaminomethylation was detected using NMR where 1,3,5-trimethoxybenzene was used as the internal standard to calculate the yield. However, no desired product peaks were detected in the NMR spectra. The formation of 69 was confirmed by HRMS analysis using the crude reaction mixture.

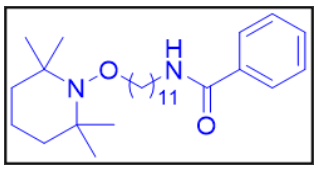
3.4.2.1. HRMS spectra

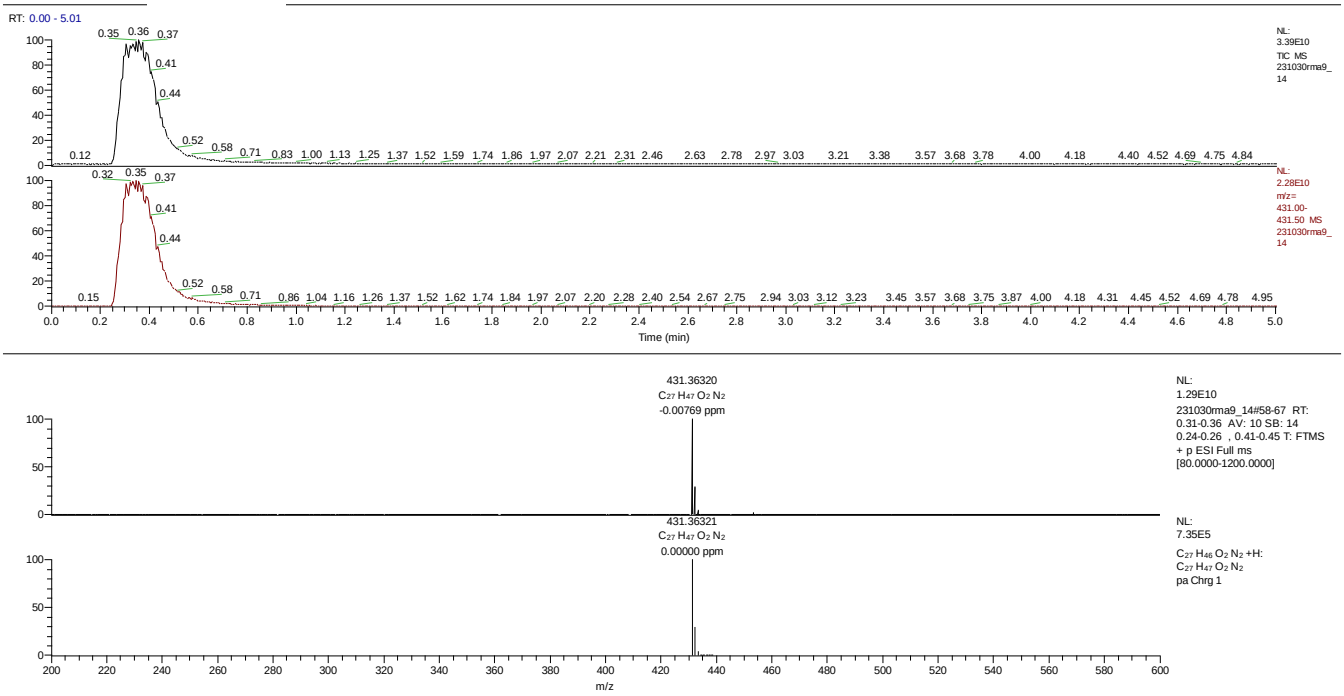
3.4.2.1.1. TEMPO trapping with boc-glycine (crude HRMS spectrum)

				(M+H)+	
Mol weight	(M+H)+	(M+Na)+	Structure	**measured**	**error (ppm)**
286.225643	287.2329	309.214863		**287.2325**	-1.45



3.4.2.1.2. TEMPO trapping with 12-benzoyldodecanoic acid (purified spectrum)

Mol weight	(M+H)+	(M+Na)+	Structure	(M+H)+ measured	error (ppm)
430.355929	431.3632	753.345149		**431.3632**	-0.01



3.4.3. Radical quenching by BHT

An oven dried 20 mL Schlenk Tube was charged with 4,4'-(ethene-1,1-diyl)bis(fluorobenzene) (0.2 mmol, 1 equiv.), 4CzIPN (0.02 equiv.), NaOH (1.0 equiv.), boc-glycine (1.0 equiv.), BHT (1.0 equiv.) and a magnetic stirring bar. The reaction mixture was degassed by three freeze/pump/thaw cycles (3 min) using Schlenck techniques and refilled with nitrogen. After that, dry DMSO (1 ml) was added. The reaction was allowed to stir under 456 nm blue KESSIL light at room temperature for 24 h. The mixture was monitored via TLC, quenched with water and extracted with EtOAc (3 times). Lastly, the solvent was removed under reduced pressure and the formation of the hydroaminomethylation was detected using NMR where 1,3,5-trimethoxybenzene was used as the internal standard to calculate the yield. In this case, the desired HAM product was detected in 83% yield.

3.4.4. H-source

An oven-dried 20 mL Schlenk Tube was charged with 4CzIPN (0.04 equiv.), boc-anhydride (1.5 equiv.), glycine (1.5 equiv.) and a magnetic stirring bar. The reaction mixture was degassed by three freeze/pump/thaw cycles (3 min) and refilled with nitrogen. After, 1,1-diphenyl ethylene (0.2 mmol) and dry DMSO (2 ml) were added. After, the reaction was allowed to stir in the dark for 4 hours and subsequently under 456 nm blue KESSIL light at room temperature for 24h. The mixture was monitored via TLC, quenched with water and extracted with EtOAc (3 times). Lastly, the solvent was removed under reduced pressure. The yield and the percentage of deuteration in the desired HAM product were determined by NMR analysis using 1,3,5-trimethoxybenzene as the internal standard.

3.5. Stern-Volmer Experiments

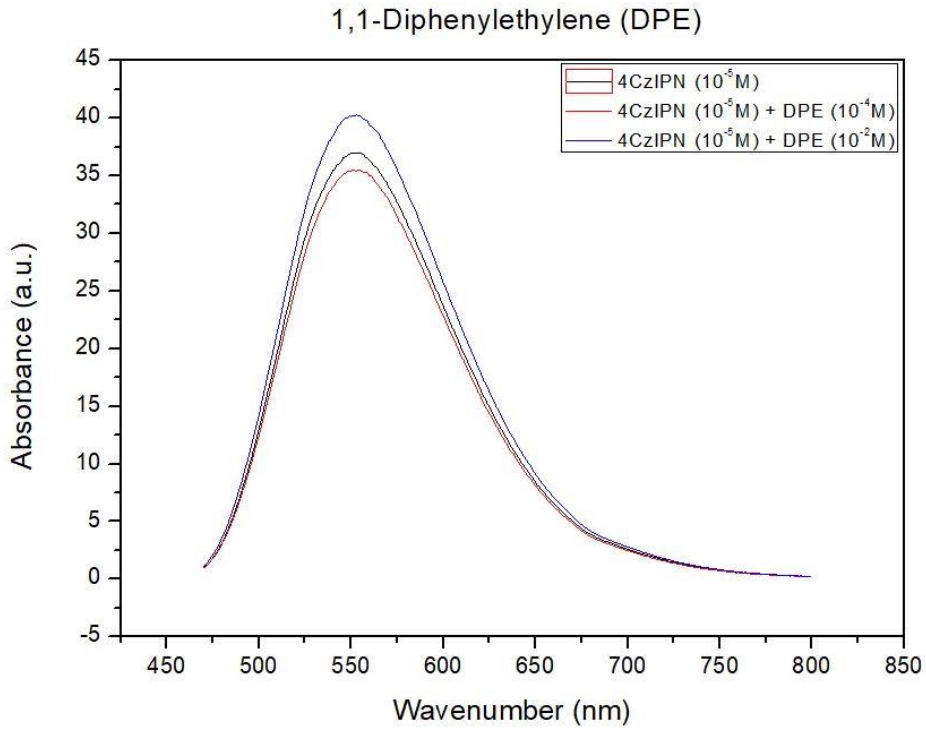


Figure S2. Stern-Volmer experiment between 4CzIPN and DPE.

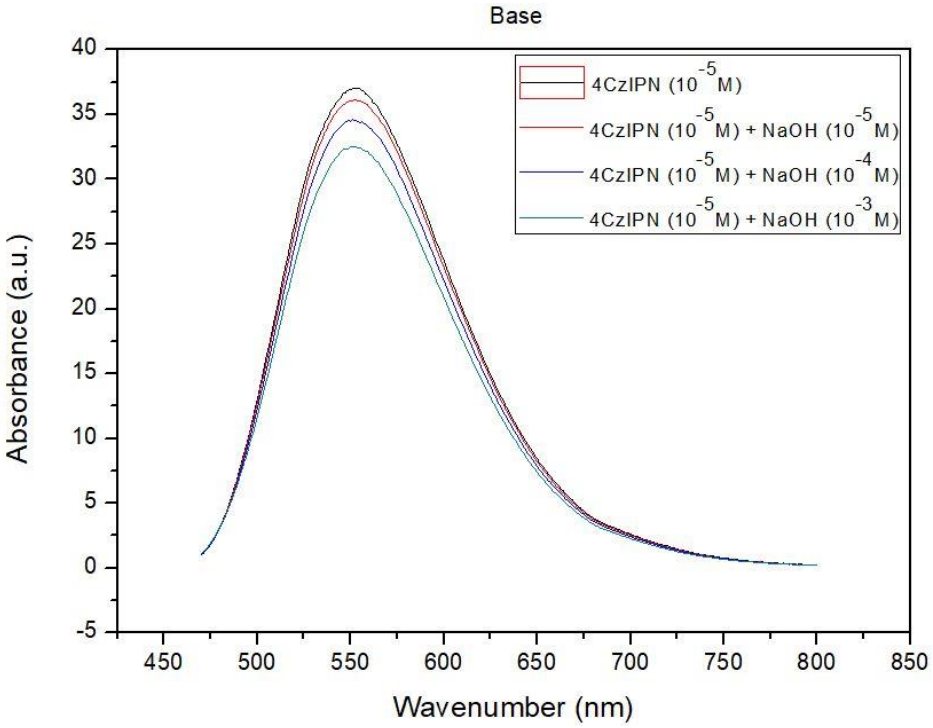


Figure S3. Stern-Volmer experiment between 4CzIPN and NaOH.

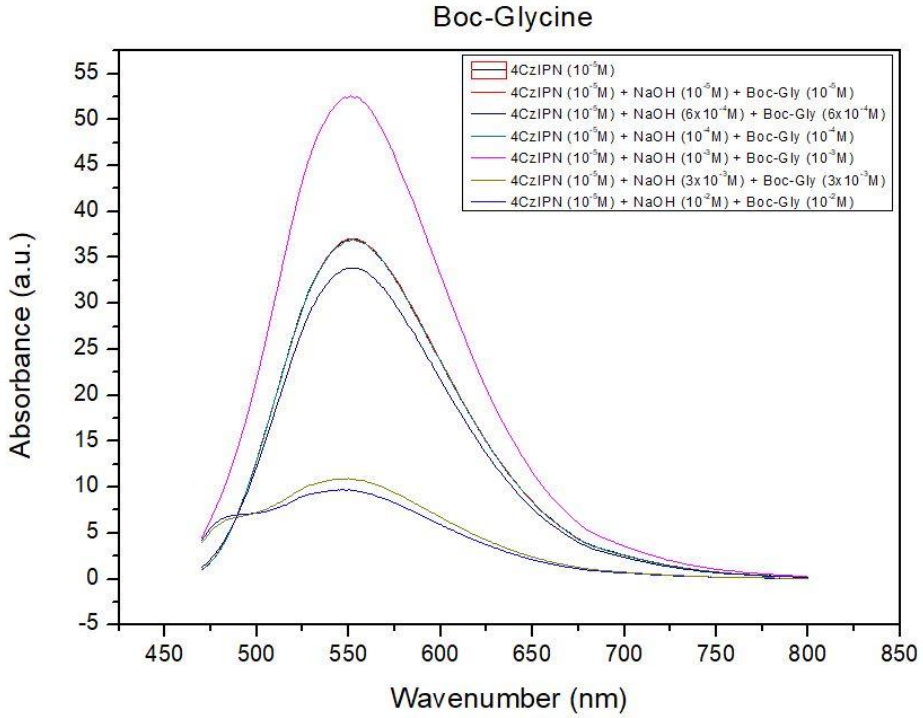


Figure S4. Stern-Volmer experiment between 4CzIPN and deprotonated boc-glycine.

4. Computational Methods

4.1. Estimation of the Activation Barrier for the Single Electron Transfer Process

Marcus-Hush theory is employed to calculate the activation barrier for the single electron transfer (SET) processes.[11-18] The expression for the activation barrier of SET process is given by,

$$\Delta G^{\ddagger} = \frac{(\Delta G_r + \lambda)^2}{4\lambda} \qquad [Eq.(1)]$$

$\Delta G^{\ddagger}$ = Activation energy barrier

ΔG_r = Free energy change for the SET process

λ = Total reorganisation energy for the SET process

The total reorganisation energy (λ) has two components; internal reorganisation energy (λ_i) and solvent reorganisation energy (λ_s).

$$\lambda = \lambda_i + \lambda_s \qquad [Eq.(2)]$$

To estimate the internal reorganisation energy, Nelsen's four-point method was used.[19,20] The method is as follows,

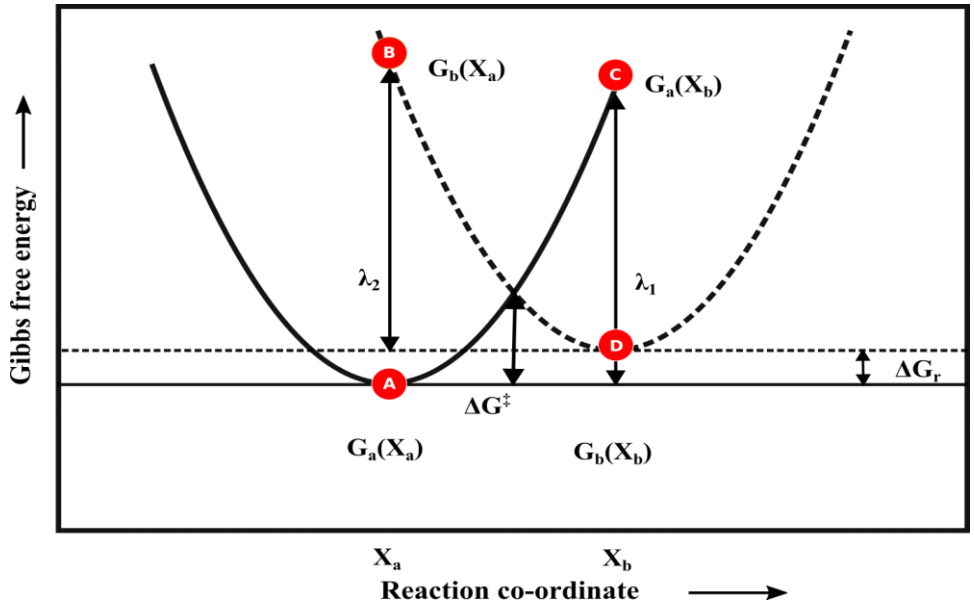


Figure S5. Schematic representation of Marcus-Hush theory parameters.

$G_a(X_a)$ = Sum of Gibbs free energies of reactants in equilibrium geometries.

$G_b(X_b)$ = Sum of Gibbs free energies of products in equilibrium geometries.

$G_a(X_b)$ = Sum of Gibbs free energies of reactants in products' geometries.

$G_b(X_a)$ = Sum of Gibbs free energies of products in reactants' geometries.

$$\Delta G_r = G_b(X_b) - G_a(X_a) \qquad [Eq.(3)]$$

$$\lambda_1 = G_a(X_b) - G_a(X_a) \qquad [Eq.(4)]$$

$$\lambda_2 = G_b(X_a) - G_b(X_b) \qquad [Eq.(5)]$$

For calculating λ_{in} , arithmetic mean is widely applied

$$\lambda_i = \frac{\lambda_1 + \lambda_2}{2} \qquad [Eq.(6)]$$

The solvent contribution to the total reorganisation energy is given by,

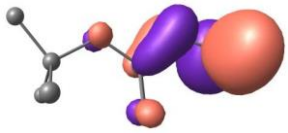
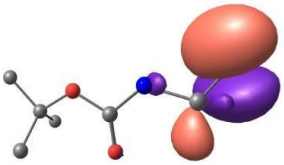
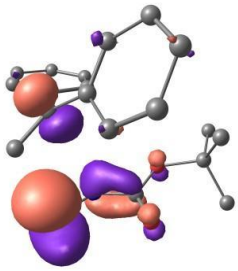
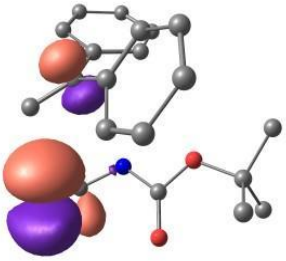
$$\lambda_s = (332\ kcal/mol)\left(\frac{1}{2r_D} + \frac{1}{2r_A} - \frac{1}{r_{DA}}\right)\left(\frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon_s}\right) \qquad [Eq.(7)]$$

ε_{op} and ε_s are optical and static dielectric constants of solvent (DMSO) (ε_{op}= 2.0 and ε_s= 46.83). r_D, r_A, and r_{DA} are hard-sphere radii of electron donor and acceptor species, and the distance between them ($r_{DA} = r_D + r_A$).

Table S12: Calculated parameters for the calculations of SET barriers

	λ_i(kcal mol^{-1})	λ_s(kcal mol^{-1})	ΔG_r(kcal mol^{-1})	r_A (Å)	r_D(Å)	$\Delta G^{\ddagger}$(kcal mol^{-1})
SET 1	49.7	11.7	-20.6	8.6	5.8	6.7
SET 2	8.6	11.3	6.5	6.1	8.6	8.8
SET 3	16.8	11.5	-2.6	8.6	6	5.8
SET 4	7.2	11.1	6.7	6.3	8.6	8.6

Table S13: Spin natural orbitals for various species involved in the reaction (isovalue = 0.05)

Species	Spin natural orbitals
F	
F'	
TS1	
TS3	

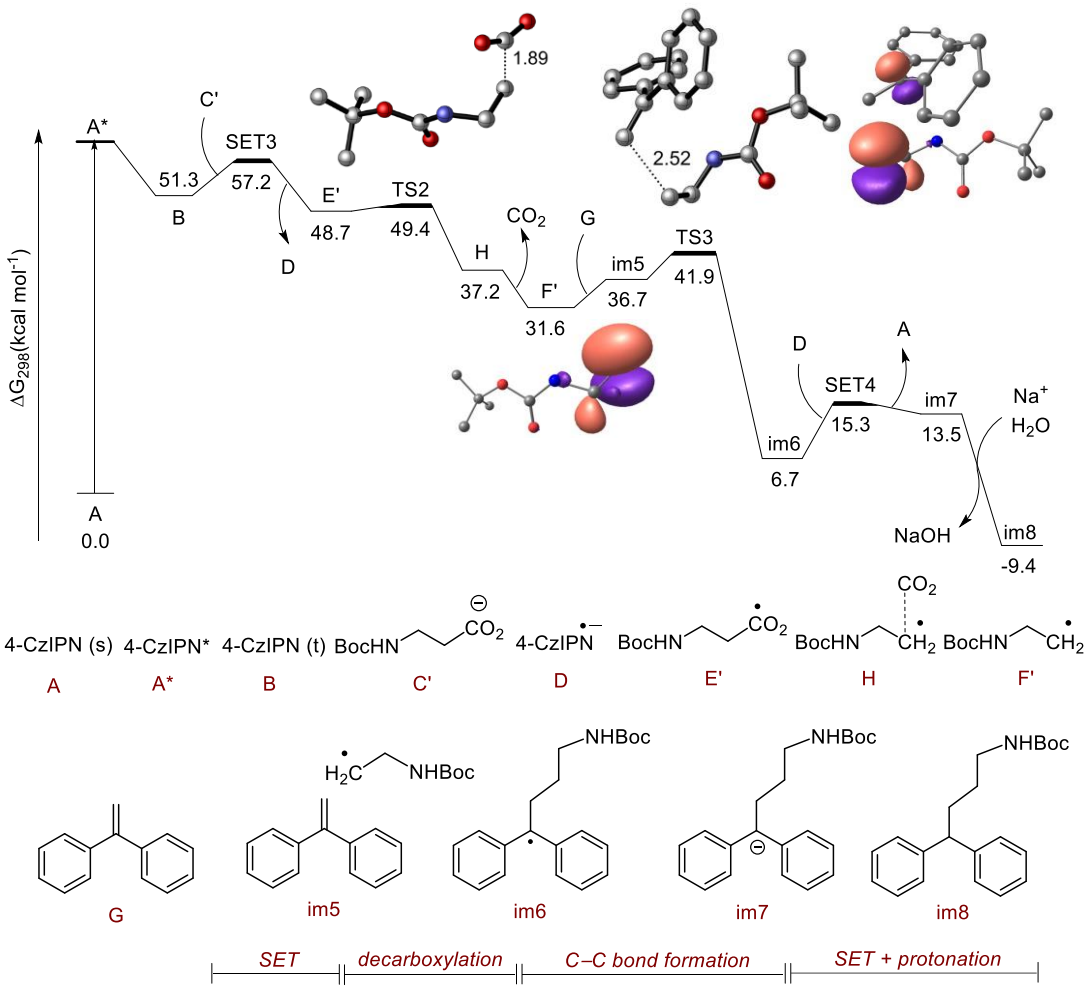


Figure S6: Computed Gibbs free energy profile diagram for the hydroaminoalkylation reaction involving boc-3-aminopropanoic acid and 1,1-diphenylethylene at the PBE0-D3(BJ)/Def2-TZVPP+SMD(DMSO)//PBE0-D3(BJ)/6-31G(d) level of theory. The spin natural orbitals of the species **F'** and transition state **TS3** are visualized using an isovalue of 0.05. The bond lengths are given in Å.

4.2. Cartesian Coordinates of the Optimized Geometries

A

SCF Energy = -2479.976298

Thermal correction to Gibbs Free Energy = 0.651965

Charge = 0, Multiplicity = 1

C	0.51801900	0.00010200	0.00000500
C	-0.19491500	1.15680600	0.38534100
C	-1.60361300	1.13803400	0.41044900
C	-2.31275200	0.00024300	0.00009200
C	-1.60374600	-1.13760000	-0.41036900
C	-0.19505200	-1.15652300	-0.38534700
C	-2.31661000	2.23977100	0.97029100
C	-2.31687300	-2.23924300	-0.97023200
N	-2.90095600	3.12510800	1.44129800
N	-2.90131400	-3.12449400	-1.44128400
C	-5.86877200	0.52387600	-0.49858500
C	-4.52062800	0.82567000	-0.78156900
C	-4.15668100	1.77190200	-1.73220300
C	-5.17967800	2.44416800	-2.38955100
C	-6.52545300	2.17177000	-2.11280800
C	-6.87720600	1.21097600	-1.17423200
C	-5.86870800	-0.52418400	0.49833400
C	-4.52052700	-0.82544000	0.78170000
C	-4.15646800	-1.77151200	1.73245400
C	-5.17937900	-2.44419400	2.38950700

C	-6.52518500	-2.17233600	2.11237800
C	-6.87705700	-1.21167800	1.17370600
H	-3.11507200	1.97394300	-1.96238000
H	-4.92720900	3.19405500	-3.13345700
H	-7.30080200	2.71579400	-2.64366400
H	-7.92182800	0.99247000	-0.97105300
H	-3.11483900	-1.97309300	1.96295400
H	-4.92682300	-3.19397200	3.13349400
H	-7.30046700	-2.71666800	2.64301500
H	-7.92171100	-0.99358900	0.97023700
N	-3.70754600	0.00029900	0.00021300
C	4.07914800	-0.55285900	0.46571300
C	2.73097800	-0.86657600	0.73462500
C	2.37349200	-1.85176600	1.64734900
C	3.39784700	-2.56413700	2.25972300
C	4.74237300	-2.28571000	1.98599400
C	5.08973400	-1.27537900	1.09842600
C	4.07925900	0.55201300	-0.46616800
C	2.73115300	0.86630800	-0.73473100
C	2.37386000	1.85165900	-1.64735700
C	3.39836800	2.56354800	-2.26003700
C	4.74284700	2.28451900	-1.98668500
C	5.08999600	1.27406500	-1.09917500
H	1.33666900	-2.07160900	1.87648300
H	3.14194500	-3.35391500	2.95982600
H	5.51989300	-2.86142200	2.47922100

H	6.13336400	-1.04667600	0.90101500
H	1.33707800	2.07196300	-1.87622300
H	3.14262700	3.35341900	-2.96009400
H	5.52048800	2.85986500	-2.48014600
H	6.13357600	1.04489700	-0.90204300
N	1.91489800	0.00003600	0.00005300
C	2.09090800	3.66938900	1.65235200
C	1.49769700	2.39388000	1.72895200
C	1.89496500	1.45040100	2.66752900
C	2.95412300	1.78351300	3.50245400
C	3.57775200	3.03485700	3.42234600
C	3.14341000	3.98737400	2.51000500
C	1.39089100	4.40178800	0.62053600
C	0.39101400	3.54879900	0.11025700
C	-0.43887000	3.93357800	-0.93673900
C	-0.26208600	5.20852700	-1.46282000
C	0.71815300	6.07341200	-0.96270500
C	1.54835000	5.67576200	0.07718900
H	1.40767700	0.48525500	2.74787800
H	3.30025300	1.05423300	4.22869800
H	4.40246900	3.26510500	4.09016700
H	3.61352500	4.96568500	2.46411000
H	-1.20491900	3.27451900	-1.33190300
H	-0.90471700	5.53731600	-2.27420200
H	0.82834800	7.06416600	-1.39313300
H	2.31694900	6.34249700	0.45794800

N	0.46866500	2.31810600	0.78173900
C	1.39071000	-4.40151500	-0.62025400
C	0.39070500	-3.54854600	-0.11019100
C	-0.43929500	-3.93328500	0.93672500
C	-0.26246900	-5.20816300	1.46297000
C	0.71791100	-6.07301900	0.96308500
C	1.54820400	-5.67541600	-0.07675000
C	2.09081000	-3.66917700	-1.65205800
C	1.49751100	-2.39372500	-1.72887600
C	1.89480300	-1.45032800	-2.66752200
C	2.95411700	-1.78343100	-3.50225300
C	3.57785400	-3.03470500	-3.42190400
C	3.14346100	-3.98716500	-2.50952500
H	-1.20548000	-3.27427200	1.33169700
H	-0.90518900	-5.53691900	2.27429600
H	0.82813300	-7.06371600	1.39363700
H	2.31690700	-6.34212800	-0.45734100
H	1.40742300	-0.48524300	-2.74805400
H	3.30028800	-1.05419700	-4.22852300
H	4.40269300	-3.26495200	-4.08957600
H	3.61365600	-4.96542900	-2.46345800
N	0.46835200	-2.31790700	-0.78179900

B

SCF Energy = -2479.888411

Thermal correction to Gibbs Free Energy = 0.645943

Charge = 0, Multiplicity = 3

C	-0.50079800	0.02839200	-0.07950600
C	0.14465200	-1.22575300	0.21441500
C	1.58454300	-1.26478900	0.28039400
C	2.32138800	-0.12583300	-0.00104200
C	1.67777700	1.11576700	-0.34108900
C	0.23337900	1.16821000	-0.35143600
C	2.22839600	-2.42897900	0.77488700
C	2.41673200	2.17193300	-0.89651700
N	2.73694700	-3.39587200	1.17601700
N	3.02818000	3.06509800	-1.33952000
C	5.87024000	-0.72913000	-0.48954200
C	4.51635700	-1.02665900	-0.75428800
C	4.14104700	-1.98688600	-1.68789500
C	5.15556800	-2.67255700	-2.34497700
C	6.50358900	-2.40279000	-2.08361900
C	6.86895200	-1.42723200	-1.16094700
C	5.88515900	0.34225700	0.48523700
C	4.53981100	0.66045200	0.76466800
C	4.18555100	1.61781600	1.70984600
C	5.21576500	2.29512000	2.34981400
C	6.55727200	2.00891600	2.06999400
C	6.90053700	1.02776700	1.14454600
H	3.09676300	-2.19308500	-1.89511200
H	4.89321100	-3.43401300	-3.07323600
H	7.27266200	-2.95839000	-2.61166200

H	7.91622100	-1.20785700	-0.97355000
H	3.14568200	1.82569800	1.93671400
H	4.97276500	3.05777900	3.08344800
H	7.33947300	2.55417700	2.58949800
H	7.94299000	0.79641400	0.94523800
N	3.71428100	-0.17172800	0.00711200
C	-4.07526600	0.53211700	0.37538600
C	-2.72999500	0.87645500	0.63863700
C	-2.38847900	1.84178700	1.58225100
C	-3.42504600	2.50672700	2.22506900
C	-4.76281200	2.19734000	1.95543400
C	-5.09564500	1.20122500	1.04010000
C	-4.05279300	-0.55023100	-0.58719700
C	-2.69733900	-0.81766700	-0.86655700
C	-2.31169500	-1.74682300	-1.82600500
C	-3.31619500	-2.47128900	-2.45973300
C	-4.66468000	-2.24468800	-2.16904400
C	-5.04212400	-1.27379800	-1.24366700
H	-1.35529900	2.07891000	1.80427600
H	-3.18442200	3.28243600	2.94550200
H	-5.55132300	2.73440700	2.47408300
H	-6.13513300	0.94702700	0.85385000
H	-1.26726800	-1.90112100	-2.07193000
H	-3.04027300	-3.22345700	-3.19237600
H	-5.42747300	-2.82203500	-2.68269100
H	-6.09212800	-1.07976700	-1.04408600

N	-1.89981900	0.04454800	-0.10715500
C	-2.23447500	-3.44136200	1.84727500
C	-1.49777400	-2.23941500	1.79212400
C	-1.66072100	-1.22879800	2.73232100
C	-2.63270100	-1.41283100	3.71019500
C	-3.39585100	-2.58423600	3.76224600
C	-3.19341800	-3.60972000	2.84193500
C	-1.74198100	-4.27875700	0.77311600
C	-0.73277700	-3.54050700	0.11190600
C	-0.05575600	-4.04191300	-0.99879300
C	-0.40192900	-5.31117800	-1.44081900
C	-1.39983000	-6.05669000	-0.79762800
C	-2.07479900	-5.54672900	0.30770400
H	-1.04728900	-0.33468300	2.70779000
H	-2.79590100	-0.63085000	4.44560900
H	-4.14544400	-2.70021300	4.53922900
H	-3.77086100	-4.52800400	2.90304900
H	0.71906500	-3.46255000	-1.49064500
H	0.11417800	-5.73479100	-2.29719900
H	-1.64744400	-7.04716100	-1.16758000
H	-2.85323300	-6.12720600	0.79474700
N	-0.61277100	-2.29418000	0.71156900
C	-1.22682800	4.48652900	-0.56583500
C	-0.31272000	3.56281700	-0.01321800
C	0.45996000	3.87033300	1.10356900
C	0.30674000	5.13288800	1.66303000

C	-0.59248000	6.06426600	1.12661200
C	-1.36037700	5.74801400	0.01340000
C	-1.87053800	3.82455100	-1.67752700
C	-1.32232300	2.52580600	-1.75367300
C	-1.69472900	1.62913600	-2.74901600
C	-2.66580100	2.03850800	-3.65373600
C	-3.23891200	3.31517300	-3.58049000
C	-2.83907100	4.21566700	-2.60222600
H	1.16545700	3.15472100	1.51320800
H	0.90454900	5.40362600	2.52867400
H	-0.68431600	7.04458800	1.58475600
H	-2.06018300	6.47000900	-0.39863100
H	-1.24135300	0.64665600	-2.82131200
H	-2.98221100	1.35174000	-4.43354600
H	-3.99594800	3.60457500	-4.30337400
H	-3.27070400	5.21189800	-2.55734700
N	-0.39015500	2.36758500	-0.72743900

C

SCF Energy = -629.382926

Thermal correction to Gibbs Free Energy = 0.154843

Charge = -1, Multiplicity = 1

C	-3.47145100	0.28721300	0.00020000
O	-4.60353300	-0.22312500	0.00066100
O	-3.11753400	1.49503700	0.00023700
C	-2.28584100	-0.73927100	-0.00033800

H	-2.36016400	-1.38627700	0.88266300
H	-2.36166900	-1.38727400	-0.88245900
N	-1.05925700	0.01351000	-0.00179000
H	-1.27424200	1.01627000	-0.00129200
C	0.17008000	-0.49141800	-0.00064800
O	0.47372100	-1.67996500	0.00048100
O	1.09043800	0.53362400	-0.00111000
C	2.49180800	0.23315300	0.00015500
C	2.88399200	-0.52958500	1.26384300
C	2.88577500	-0.53182300	-1.26162500
C	3.13954400	1.61369400	-0.00061200
H	2.56755900	0.03224500	2.14980200
H	2.40059600	-1.50753800	1.27547000
H	3.97260500	-0.65720800	1.30580900
H	2.57065200	0.02846700	-2.14902400
H	3.97444200	-0.65957600	-1.30179200
H	2.40233400	-1.50976500	-1.27222300
H	4.23190500	1.52528900	0.00022400
H	2.83192500	2.17644400	-0.88800900
H	2.83068800	2.17801000	0.88535900

D

SCF Energy = -2480.088033

Thermal correction to Gibbs Free Energy = 0.645650

Charge = -1, Multiplicity = 2

C	0.53396900	0.00003100	0.00000400

C	-0.15270300	1.16394300	0.36787400
C	-1.60513500	1.14687700	0.42281000
C	-2.28577200	-0.00007100	-0.00001300
C	-1.60504700	-1.14696800	-0.42282900
C	-0.15261500	-1.16393100	-0.36787400
C	-2.31228800	2.23057800	0.98637700
C	-2.31211500	-2.23072100	-0.98640200
N	-2.88749600	3.13794200	1.44414400
N	-2.88725100	-3.13812100	-1.44418700
C	-5.85976700	0.51088800	-0.50987000
C	-4.50594900	0.80245500	-0.79327000
C	-4.14178000	1.74141800	-1.75398300
C	-5.16133300	2.39981900	-2.42723600
C	-6.51077800	2.13004200	-2.15660300
C	-6.86544600	1.18721400	-1.20165300
C	-5.85973300	-0.51133400	0.50977500
C	-4.50589600	-0.80277400	0.79321100
C	-4.14166500	-1.74169900	1.75393800
C	-5.16117300	-2.40019400	2.42716500
C	-6.51063600	-2.13054400	2.15649500
C	-6.86536700	-1.18775100	1.20153300
H	-3.09738500	1.94988400	-1.96037700
H	-4.90473700	3.14300500	-3.17742300
H	-7.28392700	2.66592700	-2.70046800
H	-7.91143800	0.97409000	-0.99547600
H	-3.09725500	-1.95006400	1.96036300

H	-4.90452800	-3.14335400	3.17736100
H	-7.28375000	-2.66650000	2.70034100
H	-7.91137400	-0.97472500	0.99532900
N	-3.69738900	-0.00012200	-0.00001800
C	4.11368500	-0.51312700	0.50724000
C	2.75994700	-0.80169900	0.79340900
C	2.40007500	-1.72876100	1.76696900
C	3.42008400	-2.39395900	2.43363300
C	4.76845000	-2.13282400	2.15264300
C	5.12033700	-1.18999100	1.19606600
C	4.11366200	0.51325100	-0.50734300
C	2.75991200	0.80183100	-0.79344500
C	2.39999900	1.72888400	-1.76699900
C	3.41998000	2.39406100	-2.43372600
C	4.76835900	2.13291800	-2.15280200
C	5.12028600	1.19009600	-1.19623000
H	1.35918400	-1.93519800	1.98822900
H	3.15973400	-3.13741000	3.18200300
H	5.54314700	-2.67286000	2.69025200
H	6.16565400	-0.97813900	0.98530400
H	1.35909900	1.93532700	-1.98821100
H	3.15959900	3.13750200	-3.18209600
H	5.54303300	2.67293700	-2.69046200
H	6.16561100	0.97823300	-0.98552200
N	1.94886300	0.00007700	0.00001100
C	2.01612900	3.79848500	1.66246900

C	1.45084800	2.50419600	1.73726800
C	1.81874000	1.60115200	2.73001800
C	2.79225400	1.99928100	3.63528200
C	3.37762100	3.27224400	3.56712100
C	2.98867100	4.17727600	2.58881800
C	1.38338600	4.46160400	0.54714600
C	0.46892800	3.53643500	-0.00628400
C	-0.30557900	3.84759000	-1.12146200
C	-0.15053600	5.10841100	-1.68206800
C	0.75279800	6.03916300	-1.14862500
C	1.52000300	5.72179600	-0.03531400
H	1.36503200	0.61822300	2.78659600
H	3.10783700	1.30342900	4.40790500
H	4.14061700	3.55102200	4.28895900
H	3.43459700	5.16785900	2.54186700
H	-1.00984800	3.12839900	-1.52725900
H	-0.74834800	5.37885700	-2.54850700
H	0.84833100	7.01850300	-1.60975100
H	2.22316200	6.44238800	0.37526600
N	0.52757900	2.34811000	0.71105600
C	1.38382200	-4.46143200	-0.54705000
C	0.46922200	-3.53636600	0.00631800
C	-0.30530100	-3.84759600	1.12146300
C	-0.15012800	-5.10838700	1.68210100
C	0.75334700	-6.03903700	1.14872000
C	1.52056600	-5.72159600	0.03544000

C	2.01654500	-3.79825400	-1.66235000
C	1.45111000	-2.50403500	-1.73719800
C	1.81895000	-1.60095800	-2.72993700
C	2.79256800	-1.99897800	-3.63513800
C	3.37808400	-3.27186900	-3.56692700
C	2.98918600	-4.17693800	-2.58863800
H	-1.00968000	-3.12848600	1.52721200
H	-0.74794900	-5.37889100	2.54851500
H	0.84897900	-7.01835600	1.60986900
H	2.22383600	-6.44210800	-0.37509300
H	1.36512600	-0.61808500	-2.78655300
H	3.10811300	-1.30309500	-4.40774800
H	4.14115800	-3.55056300	-4.28871600
H	3.43523000	-5.16746600	-2.54164800
N	0.52776000	-2.34804800	-0.71104500

E

SCF Energy = -629.209337

Thermal correction to Gibbs Free Energy = 0.148299

Charge = 0, Multiplicity = 2

C	-2.67905700	1.20478500	-0.20014000
O	-2.00085500	1.32757000	-1.14148600
O	-3.39089900	1.11155500	0.71698800
C	-2.11419200	-2.10005900	-0.10179300
H	-2.49910100	-1.64007200	0.79628200
H	-2.56740700	-2.97108600	-0.55144500

N	-0.80591700	-1.82401000	-0.43132700
H	-0.36745700	-2.29708900	-1.20735500
C	-0.08261200	-0.82215700	0.16168500
O	-0.51378400	-0.12514800	1.06157200
O	1.13023300	-0.76107000	-0.40858400
C	2.08389900	0.26147400	0.00515500
C	1.50921600	1.64879200	-0.25056000
C	2.46530300	0.05445900	1.46500700
C	3.27261500	-0.00439300	-0.90680100
H	1.16626500	1.73273800	-1.28679500
H	0.66959900	1.85531000	0.41435600
H	2.28740600	2.40082400	-0.08267100
H	2.84020200	-0.96302700	1.61846600
H	3.26023900	0.75633600	1.73846600
H	1.60762300	0.22050900	2.11907100
H	4.07844700	0.70233300	-0.68624200
H	3.65116100	-1.02076200	-0.75935000
H	2.98585500	0.11139700	-1.95672500

F

SCF Energy = -440.734688

Thermal correction to Gibbs Free Energy = 0.143782

Charge = 0, Multiplicity = 2

C	3.41782200	0.19917500	-0.04308100
H	4.22727300	0.89274000	0.12978300
H	3.53063000	-0.87058600	0.04498600

N	2.13254100	0.69212700	0.00909900
H	1.96932700	1.68747200	-0.01492600
C	1.02028200	-0.11010300	0.00263200
O	1.06033900	-1.32384700	0.00404900
O	-0.07566900	0.67293500	-0.00248800
C	-1.40147100	0.07156500	-0.00021800
C	-1.60132100	-0.75878900	-1.26179700
C	-1.60152700	-0.75012900	1.26698700
C	-2.31997600	1.28498100	-0.00439000
H	-1.40844200	-0.14860900	-2.15059600
H	-0.93328000	-1.62152400	-1.27089900
H	-2.63718900	-1.11132100	-1.30775900
H	-1.40857800	-0.13400900	2.15168300
H	-2.63749100	-1.10204800	1.31529500
H	-0.93386500	-1.61309200	1.28183800
H	-3.36592000	0.96301300	-0.00364300
H	-2.14548000	1.90301500	0.88202100
H	-2.14499700	1.89715600	-0.89475500

G

SCF Energy = -540.277444

Thermal correction to Gibbs Free Energy = 0.179323

Charge = 0, Multiplicity = 1

C	-0.00010400	1.15590100	-0.00028400
C	0.00009800	2.49836800	-0.00054800
H	0.92296800	3.06401900	-0.08728100

H	-0.92242500	3.06457500	0.08603600
C	1.27159000	0.39505500	-0.04157700
C	1.38161800	-0.77302300	-0.80729500
C	2.39611300	0.83686100	0.66566800
C	2.58573700	-1.46337800	-0.88123700
H	0.51497100	-1.13174600	-1.35539300
C	3.59996300	0.14506800	0.59426000
H	2.31143300	1.71975800	1.29328300
C	3.70010500	-1.00655900	-0.18180600
H	2.65447300	-2.36172500	-1.48878300
H	4.45965000	0.50016900	1.15619800
H	4.63931100	-1.55030700	-0.23441500
C	-1.27168100	0.39498300	0.04137900
C	-1.38082900	-0.77417200	0.80556400
C	-2.39712900	0.83759700	-0.66398500
C	-2.58476800	-1.46484100	0.87978700
H	-0.51355500	-1.13365300	1.35220200
C	-3.60082100	0.14560000	-0.59219000
H	-2.31331000	1.72121100	-1.29072000
C	-3.70001000	-1.00719200	0.18233300
H	-2.65259100	-2.36414900	1.48602600
H	-4.46112500	0.50136700	-1.15276500
H	-4.63909000	-1.55113800	0.23520000

im1

SCF Energy = -981.023422

Thermal correction to Gibbs Free Energy = 0.342545

Charge = 0, Multiplicity = 2

C	0.40039900	0.31297000	3.29998300
H	-0.52687300	0.24736500	3.84855900
H	1.31695200	0.67972100	3.73737200
N	0.52008600	-0.45821500	2.16708000
H	-0.30561300	-0.86390300	1.74762700
C	1.68617600	-0.54254100	1.45090500
O	2.72565100	-0.00944600	1.78317400
O	1.47416100	-1.30781900	0.36253000
C	2.55001400	-1.55461800	-0.58637600
C	3.01799400	-0.24357700	-1.20143000
C	3.68026800	-2.31198300	0.09844700
C	1.87566600	-2.42702500	-1.63619500
H	2.17086400	0.29588200	-1.63597900
H	3.48994400	0.39302700	-0.45150100
H	3.74134800	-0.45237900	-1.99725300
H	3.29795900	-3.22931400	0.55886400
H	4.43699200	-2.59032100	-0.64269600
H	4.14863600	-1.69616800	0.86803900
H	2.60010700	-2.71704200	-2.40351700
H	1.47055400	-3.33548300	-1.17866000
H	1.05821500	-1.88430200	-2.12249400
C	-1.86512400	1.23598700	0.52318900
C	-2.28491400	1.82036400	1.65725600
H	-3.06426200	1.37523000	2.26920500

H	-1.85900000	2.75722800	2.00182800
C	-2.49587100	-0.01637000	0.04035500
C	-1.71460700	-1.03261700	-0.52741800
C	-3.87366200	-0.23024400	0.17330700
C	-2.29010300	-2.23623800	-0.92042300
H	-0.64535100	-0.88262900	-0.64202600
C	-4.44913300	-1.43051200	-0.22752400
H	-4.49582300	0.56480700	0.57500800
C	-3.65923300	-2.44057200	-0.77221800
H	-1.66229500	-3.01592300	-1.34381800
H	-5.52121300	-1.57453600	-0.12331200
H	-4.11064200	-3.37753500	-1.08650000
C	-0.74851400	1.81514900	-0.26096600
C	-0.78450800	1.81797600	-1.66152200
C	0.35192200	2.39563600	0.38204200
C	0.23349100	2.41607200	-2.39602900
H	-1.62736600	1.36122500	-2.17293000
C	1.37344400	2.98575800	-0.35307000
H	0.41709200	2.34871700	1.46595900
C	1.31421300	3.00638500	-1.74416600
H	0.18159300	2.42280200	-3.48154300
H	2.22733800	3.41386300	0.16427500
H	2.11422800	3.46530900	-2.31859600

TS1

SCF Energy = -981.018347

Thermal correction to Gibbs Free Energy = 0.346584

Charge = 0, Multiplicity = 2

C	0.39077400	-0.66126600	-2.99408300
H	1.22804700	-1.12720000	-3.49780100
H	-0.36626600	-0.14952500	-3.57361400
N	-0.07460500	-1.30645200	-1.87058900
H	0.58315100	-1.78400500	-1.26882500
C	-1.30422400	-1.03166500	-1.32264700
O	-2.15668700	-0.36327500	-1.87178000
O	-1.38522400	-1.63518300	-0.12457400
C	-2.59096700	-1.51664400	0.68510500
C	-2.84408100	-0.05875700	1.04067500
C	-3.76865700	-2.14646700	-0.04697500
C	-2.23471700	-2.32011500	1.92759500
H	-1.95522000	0.38799300	1.49794000
H	-3.10314000	0.52220600	0.15520500
H	-3.66810400	0.00184600	1.75995100
H	-3.53749800	-3.18178100	-0.31955000
H	-4.64618900	-2.15271100	0.60819500
H	-4.00802100	-1.58483400	-0.95163800
H	-3.07887600	-2.32638100	2.62395600
H	-1.99287800	-3.35419600	1.66248600
H	-1.37074600	-1.87963700	2.43616600
C	1.54503100	1.08879200	-0.75303700
C	1.75439300	1.20008900	-2.09447900
H	2.58403300	0.68656600	-2.56791400

H	1.26113900	1.96729200	-2.68208200
C	2.34179900	0.11194600	0.01995100
C	1.73008900	-0.73249000	0.96136700
C	3.71625300	-0.04449100	-0.20926900
C	2.46266800	-1.70661800	1.63014600
H	0.66426600	-0.63558900	1.14513300
C	4.44955300	-1.01460500	0.46458000
H	4.21241200	0.62112200	-0.91045300
C	3.82639100	-1.85299700	1.38571100
H	1.96287400	-2.35726700	2.34318500
H	5.51554500	-1.11061600	0.27566100
H	4.39986400	-2.61049700	1.91265400
C	0.48062300	1.85078200	-0.07788500
C	0.59002000	2.18735900	1.28185300
C	-0.64809400	2.30582500	-0.77799300
C	-0.37977500	2.95993500	1.90941000
H	1.45803500	1.85287900	1.84264300
C	-1.61401300	3.08149300	-0.15035600
H	-0.79256200	2.00902900	-1.81141700
C	-1.48597600	3.41588600	1.19570300
H	-0.26591700	3.21418400	2.96001500
H	-2.48345300	3.40980800	-0.71357000
H	-2.24550100	4.01819400	1.68639700

im2

SCF Energy = -981.066841

Thermal correction to Gibbs Free Energy = 0.350944

Charge = 0, Multiplicity = 2

C	-0.40937000	0.10341000	2.86477900
H	-0.88268600	-0.29721900	3.76775300
H	0.51346600	0.59877400	3.17314200
N	0.00661400	-0.98397100	2.01236600
H	-0.70755500	-1.49540900	1.51228800
C	1.21305500	-0.90505300	1.37469300
O	2.13254500	-0.19013800	1.72690800
O	1.22040800	-1.75144200	0.32794800
C	2.37810600	-1.81781700	-0.55067000
C	2.63328700	-0.45972200	-1.19387800
C	3.59097100	-2.32641600	0.21799400
C	1.94109700	-2.83336200	-1.59718100
H	1.73320700	-0.09402500	-1.69971100
H	2.93212300	0.27913600	-0.44948900
H	3.42865300	-0.55509800	-1.94107700
H	3.35871100	-3.28134600	0.70142200
H	4.42463300	-2.48666900	-0.47418000
H	3.89529500	-1.60706200	0.97981500
H	2.73799000	-2.98268000	-2.33235600
H	1.71293800	-3.79550800	-1.12793600
H	1.04540600	-2.48419900	-2.12147400
C	-1.32704800	1.08651900	0.67896600
C	-1.37637800	1.12010400	2.18035300
H	-2.39603400	0.89196800	2.50492400

H	-1.15190200	2.12462500	2.55632900
C	-2.19851500	0.12947000	-0.00192200
C	-1.71548900	-0.66880700	-1.06034000
C	-3.52924400	-0.08141300	0.40936400
C	-2.52165300	-1.61675200	-1.67455400
H	-0.67907500	-0.56455600	-1.36320700
C	-4.33770900	-1.02144900	-0.21573300
H	-3.94623500	0.52596000	1.20771300
C	-3.84025400	-1.79687900	-1.26094200
H	-2.11252000	-2.22867700	-2.47425700
H	-5.36574400	-1.14714500	0.11345900
H	-4.47146500	-2.53759200	-1.74345600
C	-0.35987700	1.86579800	-0.04381100
C	-0.48691700	2.10223100	-1.43605900
C	0.74407900	2.46273200	0.61065900
C	0.44703400	2.85543500	-2.12722000
H	-1.34961500	1.70609900	-1.96208000
C	1.67765500	3.21011500	-0.08906800
H	0.89723400	2.29412900	1.67017000
C	1.54277900	3.40952800	-1.46273800
H	0.31541600	3.02354800	-3.19291200
H	2.52665500	3.63236400	0.44143400
H	2.27753300	3.99499800	-2.00788200

im3

SCF Energy = -981.174535

Thermal correction to Gibbs Free Energy = 0.350962

Charge = -1, Multiplicity = 1

C	-0.12939700	0.19054900	2.94923200
H	-0.62239600	0.52481000	3.87215900
H	0.59816800	-0.57586700	3.22945600
N	-1.10396300	-0.48519600	2.11634500
H	-1.72832600	0.13757400	1.61044700
C	-0.65063500	-1.50664300	1.33306000
O	0.31256500	-2.21300800	1.58144300
O	-1.48286600	-1.66411000	0.27991800
C	-1.09639500	-2.50444600	-0.82916700
C	0.26402300	-2.08985800	-1.37847600
C	-1.11783900	-3.96918500	-0.40387100
C	-2.18696300	-2.21599200	-1.85343700
H	0.26485100	-1.02251400	-1.61434300
H	1.06052800	-2.27464100	-0.65653500
H	0.47233900	-2.65249800	-2.29641600
H	-2.09898500	-4.22719500	0.01131500
H	-0.92901200	-4.61413400	-1.27040600
H	-0.35298800	-4.15035500	0.35358600
H	-2.00740900	-2.78747600	-2.77099100
H	-3.16971500	-2.49080700	-1.45463600
H	-2.19681900	-1.14719800	-2.08932200
C	0.58948000	1.39441100	0.73714300
C	0.58162700	1.38933900	2.24524300
H	0.12337300	2.31889700	2.61565200

H	1.61445600	1.41930900	2.61451500
C	-0.59943700	1.79495600	0.06457500
C	-0.83276000	1.63017800	-1.34232900
C	-1.73830800	2.31163500	0.77088100
C	-2.02742400	1.96380700	-1.95109800
H	-0.05173000	1.19497600	-1.95560300
C	-2.92924100	2.64985700	0.14267900
H	-1.67363100	2.46945900	1.84455600
C	-3.10621200	2.49272300	-1.23036100
H	-2.12588300	1.79681700	-3.02420800
H	-3.74230400	3.04681600	0.75125500
H	-4.04209500	2.75315200	-1.71742100
C	1.80446500	0.98811900	0.07734700
C	2.23989500	1.50553400	-1.17446100
C	2.70086500	0.06401800	0.68403000
C	3.42985500	1.11292300	-1.76853400
H	1.64720200	2.27832000	-1.65430800
C	3.89208200	-0.31904400	0.08723300
H	2.41129600	-0.40798800	1.61834300
C	4.27837900	0.19002000	-1.15421000
H	3.71239700	1.55644000	-2.72330700
H	4.52276900	-1.04920000	0.59369200
H	5.20771300	-0.12079400	-1.62565300

im4

SCF Energy = -981.703623

Thermal correction to Gibbs Free Energy = 0.365361

Charge = 0, Multiplicity = 1

C	-0.60753100	0.40609900	2.44227100
H	-0.54032700	0.57639000	3.52630200
H	-0.95191800	1.34282100	1.99887500
N	0.70377000	0.13936200	1.90164300
H	1.07213300	-0.79931100	1.94298700
C	1.32813500	0.98259500	1.04204400
O	0.93028100	2.10011300	0.75261200
O	2.44244800	0.39104500	0.57630700
C	3.30644900	1.08006300	-0.36648800
C	2.54409500	1.44005900	-1.63604500
C	3.92120100	2.30512300	0.29782800
C	4.36736100	0.03007300	-0.66532400
H	2.05271400	0.55022900	-2.04077100
H	1.78941400	2.20204300	-1.43734000
H	3.24607600	1.81958200	-2.38648900
H	4.43818400	2.01670200	1.21926300
H	4.65234900	2.76435300	-0.37616700
H	3.15077700	3.04063800	0.53730500
H	5.09666600	0.42268100	-1.38088100
H	4.89475200	-0.25451300	0.25069600
H	3.90208000	-0.86562700	-1.08908800
C	-1.92971400	-1.12944900	0.74784600
C	-1.60134600	-0.72709200	2.20632100
H	-1.24833700	-1.61881800	2.74140500

H	-2.54320000	-0.44310800	2.69161600
C	-0.74077900	-1.72817300	0.00166700
C	-0.34663600	-1.31028800	-1.26960500
C	-0.04402600	-2.79763600	0.58224300
C	0.72556700	-1.91585700	-1.92335100
H	-0.88403400	-0.50633500	-1.76098800
C	1.03348700	-3.39485200	-0.06070700
H	-0.35455100	-3.17921300	1.55274900
C	1.42990100	-2.95055600	-1.32025800
H	1.00557600	-1.57341900	-2.91637100
H	1.55738400	-4.21809700	0.41793100
H	2.26785600	-3.41812600	-1.82974800
C	-2.68077500	-0.03714900	0.01602900
C	-4.03558500	-0.22494400	-0.27057100
C	-2.08854200	1.17605300	-0.35752300
C	-4.78523400	0.76179900	-0.90368800
H	-4.51138600	-1.16318700	0.00809400
C	-2.83660800	2.16461000	-0.99067100
H	-1.03692800	1.36530400	-0.16244100
C	-4.18624600	1.96407500	-1.26583300
H	-5.83713400	0.58852300	-1.11483100
H	-2.35453600	3.09826700	-1.26764100
H	-4.76628900	2.73851300	-1.76033900
H	-2.64458600	-1.95840400	0.85592400

H_2O

SCF Energy = -76.388438

Thermal correction to Gibbs Free Energy = 0.003875

Charge = 0, Multiplicity = 1

O	0.00000000	0.00000000	0.11901900
H	0.00000000	0.75907100	-0.47607700
H	0.00000000	-0.75907100	-0.47607700

CO_2

SCF Energy = -188.468946

Thermal correction to Gibbs Free Energy = -0.008959

Charge = 0, Multiplicity = 1

C	0.00000000	0.00586300	0.00000000
O	1.15644100	-0.00210200	0.00000000
O	-1.15644100	-0.00229600	0.00000000

C'

SCF Energy = -668.664204

Thermal correction to Gibbs Free Energy = 0.181864

Charge = -1, Multiplicity = 1

C	-3.53539400	0.61390200	0.02609200
O	-4.76396500	0.78290700	0.00413800
O	-2.62404000	1.45698200	-0.23933300
C	-1.80387500	-1.31367400	-0.24215400
H	-1.44635800	-2.26253000	0.17378500
H	-2.04815900	-1.49849500	-1.30093200
N	-0.74607300	-0.33665400	-0.14202300

H	-1.13902100	0.63104800	-0.15993900
C	0.54261200	-0.66098100	-0.10013400
O	1.01460800	-1.79565100	-0.12321100
O	1.30345000	0.47863900	-0.01539900
C	2.73214700	0.38269300	0.04962000
C	3.16950200	1.84123800	0.13016800
C	3.17077700	-0.36718100	1.30562900
C	3.29273400	-0.26444000	-1.21504800
H	4.26176400	1.91189700	0.18568600
H	2.82394400	2.38957400	-0.75206700
H	2.73877600	2.31748100	1.01679200
H	4.26295800	-0.33605000	1.40209700
H	2.73212300	0.10520800	2.19164300
H	2.83753200	-1.40493700	1.25770600
H	4.38897800	-0.23030700	-1.20248000
H	2.96047500	-1.30129100	-1.28453900
H	2.94026300	0.28047300	-2.09789800
C	-3.04292100	-0.79617500	0.48423300
H	-2.81611000	-0.73519600	1.55905000
H	-3.86856900	-1.50560300	0.36526000

E’

SCF Energy = -668.467616

Thermal correction to Gibbs Free Energy = 0.180939

Charge = 0, Multiplicity = 2

C	-3.14430200	0.58898300	0.12667400

O	-3.65469100	1.46893800	0.88037500
O	-3.15177200	0.95639700	-1.06741500
C	-1.85324800	-1.46803500	-0.47400200
H	-1.53744900	-2.43574600	-0.07715400
H	-2.49826500	-1.64765500	-1.33813800
N	-0.68009700	-0.76393700	-0.92752500
H	-0.78188500	-0.05041900	-1.63367300
C	0.42224100	-0.70844900	-0.12754000
O	0.53991400	-1.35660800	0.89766400
O	1.32017100	0.13919300	-0.65317100
C	2.59195800	0.37409400	0.01827900
C	3.27112300	1.38209600	-0.89727000
C	2.35215400	0.97632400	1.39692100
C	3.39413800	-0.91891900	0.08541000
H	4.25545700	1.64630600	-0.49857800
H	3.40207200	0.96347300	-1.89998300
H	2.67149800	2.29419000	-0.97771400
H	3.31049800	1.26231600	1.84305400
H	1.73319700	1.87616400	1.31405100
H	1.85625000	0.26111700	2.05520700
H	4.39298600	-0.70991000	0.48292400
H	2.90278000	-1.64994200	0.72953000
H	3.50786900	-1.34524400	-0.91691000
C	-2.61269300	-0.71608600	0.61879100
H	-1.95220600	-0.53382600	1.47412000
H	-3.45931300	-1.30666000	0.99272800

TS2

SCF Energy = -668.463988

Thermal correction to Gibbs Free Energy = 0.178413

Charge = 0, Multiplicity = 2

C	3.39109700	-0.80796600	0.07906100
O	4.18546000	-0.98767900	0.96211100
O	2.87828100	-1.18391800	-0.94214100
C	1.80905700	1.36892800	-0.61706500
H	1.46990500	2.37367100	-0.32500100
H	2.45480600	1.48212000	-1.49210900
N	0.64862500	0.60681100	-0.98165600
H	0.80205600	-0.25230400	-1.48993800
C	-0.47275100	0.68622400	-0.20532500
O	-0.62945300	1.52040100	0.66817200
O	-1.34216800	-0.26541300	-0.57604300
C	-2.63433800	-0.38218500	0.08756000
C	-3.27190400	-1.56270600	-0.63040000
C	-2.43695200	-0.69439900	1.56550000
C	-3.45023000	0.88540800	-0.13000100
H	-4.26681200	-1.75851700	-0.21871100
H	-3.37202500	-1.35353300	-1.69997200
H	-2.66104100	-2.46270500	-0.50887700
H	-3.40743800	-0.90222300	2.02830500
H	-1.80664300	-1.58241200	1.68330300
H	-1.97173300	0.14551400	2.08403100

H	-4.46052600	0.74305200	0.26801500
H	-2.98910500	1.73753200	0.37195700
H	-3.53232400	1.10264900	-1.20021300
C	2.57541100	0.82792800	0.55342900
H	1.96799500	0.47436100	1.38707300
H	3.43920500	1.41060400	0.87038600

H

SCF Energy = -668.476764

Thermal correction to Gibbs Free Energy = 0.171805

Charge = 0, Multiplicity = 2

C	3.88969100	-1.21974800	-0.03381800
O	4.83323200	-0.97028500	0.59945000
O	2.95538200	-1.49900200	-0.67624200
C	1.58655900	1.70127200	-0.46265500
H	0.97600100	2.59986100	-0.28354100
H	2.01883800	1.81669300	-1.46711800
N	0.65851600	0.59735500	-0.44103600
H	0.99985300	-0.34052200	-0.58844800
C	-0.65859500	0.76762100	-0.15691200
O	-1.18447500	1.84380800	0.06382600
O	-1.26926100	-0.43431300	-0.16319800
C	-2.69623000	-0.53168100	0.09768600
C	-2.95502000	-2.02765800	-0.01286900
C	-3.00915900	-0.03613600	1.50420600
C	-3.47946800	0.22757800	-0.96612700

H	-4.01370600	-2.24010200	0.16592200
H	-2.69013100	-2.39061900	-1.01094500
H	-2.36009200	-2.57611500	0.72430100
H	-4.06360400	-0.22343000	1.73385400
H	-2.39927800	-0.57408400	2.23798900
H	-2.81116700	1.03321100	1.59256500
H	-4.55162700	0.05016700	-0.82949000
H	-3.28602300	1.29941100	-0.90054900
H	-3.19938600	-0.12535300	-1.96444900
C	2.66396800	1.57036400	0.55275100
H	2.42358700	1.18879600	1.54067100
H	3.61761500	2.06926600	0.41222300

F’

SCF Energy = -480.004552

Thermal correction to Gibbs Free Energy = 0.168470

Charge = 0, Multiplicity = 2

C	3.00773900	0.18857400	-0.37087600
H	2.82204500	1.21017700	-0.00507600
H	3.46033900	0.29587300	-1.36731700
N	1.70106500	-0.41856100	-0.47557400
H	1.62267700	-1.39577400	-0.71063800
C	0.56396100	0.24106300	-0.13053700
O	0.52236900	1.40421800	0.22647600
O	-0.48561700	-0.59623900	-0.25474200
C	-1.83187100	-0.13008900	0.03746800

C	-2.67967400	-1.36472100	-0.23459800
C	-1.93993900	0.28239800	1.50027100
C	-2.21431800	1.00161300	-0.90829000
H	-3.73530400	-1.14399800	-0.04805500
H	-2.56935100	-1.68514600	-1.27541200
H	-2.37620500	-2.19062200	0.41654400
H	-2.98246500	0.51821800	1.73942000
H	-1.61853100	-0.53964300	2.14887000
H	-1.32233200	1.15851200	1.70390600
H	-3.26733300	1.26395100	-0.76006200
H	-1.59984700	1.88478300	-0.72674800
H	-2.08462500	0.68415400	-1.94850800
C	3.91602200	-0.56356500	0.53198900
H	3.52761200	-0.99345900	1.44974400
H	4.99033400	-0.53257000	0.38591300

im5

SCF Energy = -1020.293086

Thermal correction to Gibbs Free Energy = 0.367010

Charge = 0, Multiplicity = 2

C	-0.91820700	-3.09058700	-1.58945500
H	-1.82024600	-3.65157200	-1.30579800
H	-0.07113800	-3.78198100	-1.50737800
N	-0.77487600	-2.05067800	-0.59393800
H	0.04385800	-1.46009200	-0.64356000
C	-1.84663300	-1.59269000	0.10461100

O	-2.95130300	-2.10526400	0.09138300
O	-1.48359000	-0.50635000	0.81906100
C	-2.46085000	0.19981000	1.63182900
C	-1.65022700	1.34973000	2.21264800
C	-3.58536900	0.73595400	0.75453100
C	-2.97570200	-0.71125100	2.73875900
H	-2.29256800	1.98382100	2.83216200
H	-0.83558400	0.97133900	2.83960800
H	-1.22122700	1.95988600	1.41198000
H	-4.25614000	1.35664300	1.35838600
H	-3.16875500	1.35701100	-0.04495900
H	-4.15933100	-0.08123200	0.31475200
H	-3.61511400	-0.13840400	3.41913200
H	-3.55028400	-1.54075400	2.32368300
H	-2.13592600	-1.11326200	3.31588500
C	-1.03093900	-2.56049500	-2.97580500
H	-1.72621400	-1.75160600	-3.17907900
H	-0.58704300	-3.08299000	-3.81656800
C	1.76338300	0.19127400	-1.25034400
C	1.91226200	-0.55297800	-2.36037700
H	1.39218000	-0.31307200	-3.28242600
H	2.56687300	-1.41960900	-2.37112000
C	2.54063200	-0.12408700	-0.02621000
C	1.91225500	-0.14662600	1.22581700
C	3.90241400	-0.43602000	-0.10358500
C	2.62769400	-0.49231100	2.36627900

H	0.85199200	0.07887100	1.29296600
C	4.61813500	-0.77361200	1.04009000
H	4.40079400	-0.39126200	-1.06825900
C	3.98230800	-0.80458800	2.27846600
H	2.12290200	-0.52109400	3.32827800
H	5.67718800	-1.00508200	0.96496600
H	4.54153400	-1.06706100	3.17230500
C	0.81984400	1.33363000	-1.20905400
C	1.12503900	2.48162600	-0.46717400
C	-0.38514400	1.29887400	-1.92103300
C	0.26214300	3.57195700	-0.45832100
H	2.05165400	2.51767000	0.09830900
C	-1.24879900	2.38750600	-1.91082900
H	-0.65486700	0.39698900	-2.46336400
C	-0.92810600	3.52974300	-1.18058100
H	0.52038500	4.45778200	0.11553300
H	-2.18236200	2.33897700	-2.46501500
H	-1.60608400	4.37860200	-1.16797600

TS3

SCF Energy = -1020.289610

Thermal correction to Gibbs Free Energy = 0.371832

Charge = 0, Multiplicity = 2

C	-0.40039000	-2.40391000	2.13500500
H	0.26417800	-3.21003200	2.48160200
H	-1.40282400	-2.83675600	2.04760500

N	0.03572700	-2.03415200	0.80644400
H	-0.63728600	-1.58566100	0.20084200
C	1.34512600	-1.75628300	0.56967100
O	2.25857300	-2.05517900	1.31733300
O	1.45799800	-1.12421000	-0.61785700
C	2.76345900	-0.79618100	-1.16441000
C	2.40823000	-0.06846900	-2.45385200
C	3.52677900	0.13237100	-0.22878200
C	3.53210500	-2.07890700	-1.45329200
H	3.31939400	0.21937000	-2.98781700
H	1.81117500	-0.71327300	-3.10726100
H	1.83376300	0.83770900	-2.23304700
H	4.44868300	0.46293900	-0.72004600
H	2.92205100	1.01539100	-0.00186100
H	3.78148300	-0.37546500	0.70235800
H	4.47460400	-1.84143600	-1.95816000
H	3.75349100	-2.61054900	-0.52561700
H	2.94650300	-2.73284100	-2.10836000
C	-0.38460500	-1.27827500	3.11428200
H	0.52181600	-0.68226000	3.16367700
H	-0.94759200	-1.38191100	4.03857800
C	-1.63236400	0.85309600	0.94425500
C	-1.90357900	0.52727000	2.23681300
H	-1.49742500	1.10621400	3.05901100
H	-2.69670100	-0.17250400	2.47835300
C	-2.36964600	0.19106600	-0.15558400

C	-1.71758800	-0.19032700	-1.34039100
C	-3.73396700	-0.10817500	-0.02766700
C	-2.40193600	-0.86716300	-2.34456600
H	-0.65849700	0.02187800	-1.45787900
C	-4.41736800	-0.77835500	-1.03485400
H	-4.26423400	0.21452000	0.86399000
C	-3.75386700	-1.16438600	-2.19744400
H	-1.87120100	-1.16621600	-3.24436600
H	-5.47622500	-0.99193900	-0.91594800
H	-4.28893900	-1.68780000	-2.98479200
C	-0.58094900	1.83448600	0.61322600
C	-0.66922000	2.62818200	-0.54089700
C	0.52161700	2.02462500	1.45851700
C	0.30328400	3.57693200	-0.83342900
H	-1.51858600	2.50592600	-1.20639800
C	1.48934100	2.97945700	1.17119600
H	0.63079300	1.39828600	2.33785100
C	1.38785400	3.75904200	0.02141000
H	0.20840600	4.18336400	-1.73020600
H	2.33718400	3.10170000	1.83994800
H	2.14943400	4.49895000	-0.20822200

im6

SCF Energy = -1020.353824

Thermal correction to Gibbs Free Energy = 0.380073

Charge = 0, Multiplicity = 2

C	-0.78438400	-1.45354800	2.54479100
H	-0.23768700	-2.02599100	3.30149700
H	-1.81255100	-1.83133200	2.52492700
N	-0.19971900	-1.74289800	1.25401700
H	-0.80094800	-1.76951500	0.44349800
C	1.11965600	-1.51576800	1.02668300
O	1.93852600	-1.28815000	1.89946600
O	1.36516300	-1.59634100	-0.29859600
C	2.70261600	-1.35800100	-0.81604000
C	2.50837800	-1.50426100	-2.31892300
C	3.15712800	0.05499700	-0.47618100
C	3.66084000	-2.41875800	-0.28973000
H	3.46376000	-1.37157100	-2.83626100
H	2.11430800	-2.49623500	-2.56196900
H	1.80759000	-0.74835700	-2.68918700
H	4.11363600	0.25908200	-0.96998100
H	2.42443700	0.78550300	-0.83218400
H	3.28123000	0.17712800	0.60068800
H	4.63918500	-2.30186700	-0.76824100
H	3.78122700	-2.32708500	0.79098000
H	3.28257900	-3.41994800	-0.52280900
C	-0.75392100	0.02256500	2.93465400
H	0.28804300	0.35158300	2.87760100
H	-1.05109600	0.10162600	3.98885100
C	-1.41092500	1.01294100	0.63783100
C	-1.67484400	0.95176300	2.11936900

H	-1.60101600	1.95988000	2.54817100
H	-2.70570900	0.62225800	2.28994800
C	-2.24042300	0.20205400	-0.25268100
C	-1.67961800	-0.49994000	-1.34241400
C	-3.62228300	0.04521600	-0.02950900
C	-2.46050000	-1.30781500	-2.15896600
H	-0.60759200	-0.44506300	-1.50782600
C	-4.40252000	-0.75113500	-0.85741100
H	-4.09793600	0.58488600	0.78416200
C	-3.82847200	-1.43517600	-1.92677900
H	-1.99214900	-1.85057300	-2.97575600
H	-5.46910600	-0.83623100	-0.66714500
H	-4.43894400	-2.06479300	-2.56760700
C	-0.35992500	1.85464800	0.12969100
C	-0.26196400	2.19168700	-1.24479100
C	0.59021800	2.45009800	0.99652800
C	0.73419400	3.03069200	-1.71587700
H	-1.00581200	1.81338300	-1.93757400
C	1.58472600	3.28794800	0.51822200
H	0.55527300	2.23953600	2.05890300
C	1.67340100	3.58140000	-0.84212200
H	0.77083800	3.27138300	-2.77514800
H	2.30305300	3.71273700	1.21413500
H	2.45564300	4.23615900	-1.21483500

im7

SCF Energy = -1020.459476

Thermal correction to Gibbs Free Energy = 0.378440

Charge = -1, Multiplicity = 1

C	-0.96685900	-1.53571900	2.31966300
H	-0.51066900	-2.25175400	3.01134000
H	-2.03545700	-1.77026800	2.24727000
N	-0.39168800	-1.77524500	1.01146600
H	-0.89647500	-1.37692400	0.22645200
C	0.95491000	-1.79727000	0.86826600
O	1.75830200	-1.99235800	1.76809000
O	1.26575500	-1.61292600	-0.43688200
C	2.63224600	-1.38194100	-0.84242700
C	2.48397400	-1.01691100	-2.31418500
C	3.24061500	-0.21134200	-0.07994800
C	3.44033700	-2.66404300	-0.67198400
H	3.46954700	-0.85915900	-2.76619800
H	1.97028500	-1.81732600	-2.85764400
H	1.90117400	-0.09491300	-2.40904400
H	4.21654900	0.03574200	-0.51486300
H	2.59529700	0.66849600	-0.15764000
H	3.37215500	-0.45883100	0.97458100
H	4.45641300	-2.52283400	-1.05921100
H	3.49277500	-2.93400400	0.38479200
H	2.96985500	-3.48441900	-1.22607900
C	-0.76385500	-0.11403800	2.84979500
H	0.30789300	0.10611000	2.78303000

H	-1.01609700	-0.11562500	3.92272700
C	-1.36034900	1.11279600	0.65393200
C	-1.59112300	0.97863800	2.14220700
H	-1.39035300	1.93191500	2.65747800
H	-2.64565200	0.76262200	2.35125100
C	-2.25132500	0.41953100	-0.23630600
C	-1.83693000	-0.13181400	-1.49066200
C	-3.60981400	0.12875900	0.09907900
C	-2.69189100	-0.84538300	-2.31769500
H	-0.79433600	-0.04208200	-1.77818400
C	-4.45628400	-0.58031200	-0.73576200
H	-4.01762000	0.51212900	1.03036000
C	-4.02219500	-1.07761000	-1.96805600
H	-2.29727800	-1.25006000	-3.24942300
H	-5.48703300	-0.74282300	-0.42051500
H	-4.69000700	-1.63595800	-2.61897600
C	-0.21483000	1.84971100	0.22481200
C	0.02870000	2.25050500	-1.12866000
C	0.75629300	2.34656500	1.15232700
C	1.12616300	3.00607300	-1.50242700
H	-0.70383800	2.00010200	-1.88862800
C	1.84731900	3.11023600	0.76606400
H	0.64935500	2.11893400	2.20763900
C	2.07270400	3.44477200	-0.56951600
H	1.23659500	3.27757200	-2.55257300
H	2.54904400	3.43959900	1.53243400

H	2.94041200	4.02553200	-0.87140800

im8

SCF Energy = -1020.986134

Thermal correction to Gibbs Free Energy = 0.389275

Charge = 0, Multiplicity = 1

C	0.95213400	-0.34093300	2.79979900
H	1.70514600	-0.05932500	3.54324600
H	0.50868700	-1.28754900	3.12702400
N	1.64164800	-0.60211200	1.55539400
H	1.29310700	-1.32395100	0.94317400
C	2.44570100	0.33541000	0.99717500
O	2.79720000	1.36335600	1.55063000
O	2.79008500	-0.05783400	-0.24857400
C	3.57526300	0.81261500	-1.10153800
C	3.67776300	0.01156400	-2.39220800
C	2.83099000	2.12110700	-1.34213700
C	4.95623500	1.04079700	-0.49940500
H	4.25981200	0.56481200	-3.13592400
H	4.16794300	-0.94945600	-2.20779900
H	2.68129800	-0.18298500	-2.80220400
H	3.37009000	2.72385200	-2.08073900
H	1.82851000	1.91714200	-1.73580100
H	2.74032500	2.69182500	-0.41643700
H	5.57867200	1.60294000	-1.20404700
H	4.88243900	1.59851200	0.43541800

H	5.44358100	0.07991200	-0.30294900
C	-0.10259100	0.76545800	2.74413700
H	0.37132600	1.65314900	2.30766700
H	-0.34069000	1.03125800	3.78288900
C	-1.37180700	0.30905100	0.50134200
C	-1.42683800	0.48324100	2.03274400
H	-2.08101900	1.34197800	2.22530700
H	-1.93836100	-0.37230300	2.49320100
C	-0.91232600	-1.04644700	0.00186400
C	-0.23847300	-1.11657800	-1.22229000
C	-1.14777300	-2.23933400	0.69134000
C	0.20645100	-2.32995900	-1.73216700
H	-0.04537600	-0.19720200	-1.76960800
C	-0.70589100	-3.46007400	0.18257400
H	-1.66801000	-2.22376500	1.64472300
C	-0.02325700	-3.51031200	-1.02826400
H	0.74450500	-2.35326700	-2.67584700
H	-0.89290400	-4.37325700	0.74124200
H	0.33024900	-4.46000800	-1.41942100
C	-2.71512000	0.67922200	-0.10848200
C	-3.76733600	-0.23568200	-0.18439500
C	-2.93070600	1.98201900	-0.56355300
C	-5.00454600	0.14511600	-0.69450200
H	-3.61198000	-1.26018500	0.14307200
C	-4.16552700	2.36595900	-1.07730500
H	-2.11773300	2.70387400	-0.51352500

C	-5.20894300	1.44714500	-1.14312400
H	-5.81094200	-0.58161500	-0.74777600
H	-4.31057500	3.38338400	-1.43083400
H	-6.17363300	1.74212700	-1.54667300
H	-0.64471500	1.04438900	0.12878500

Na^+

SCF Energy = -162.092324

Thermal correction to Gibbs Free Energy = -0.014429

Charge = 1, Multiplicity = 1

Na	0.00000000	0.00000000	0.00000000

NaOH

SCF Energy = -237.999918

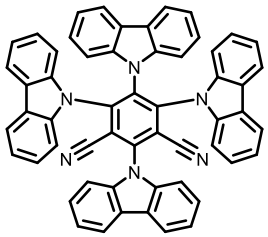
Thermal correction to Gibbs Free Energy = -0.012063

Charge = 0, Multiplicity = 1

Na	0.03578200	-0.91653900	0.00000000
O	0.03578200	1.04888200	0.00000000
H	-0.67985200	1.69087900	0.00000000

5. Characterisations

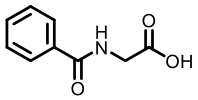
Synthesis of 2,4,5,6-tetrakis(carbazol-9-yl)-4,6-dicyanobenzene (4CzIPN). 4CzIPN was synthesized according to previous literature.[21]



NaH (60% in oil, 1.2 g, 30 mmol) was added slowly to a stirred solution of carbazole (3.34 g, 20.0 mmol) in dry THF (80 mL) under a nitrogen atmosphere at r.t. After 30 min, tetrafluoroisophthalonitrile (0,800 g, 4 mmol) was added. After, the mixture was stirred at r.t. for 12 h and 4 mL water was added to the reaction mixture to quench the excess NaH. The resulting mixture was then concentrated under reduced pressure and purified by column chromatography (gradient towards hexane/DCM 1:1).

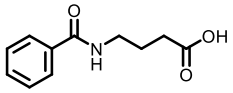
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 7.7 Hz, 2H), 7.76 – 7.60 (m, 8H), 7.51 – 7.45 (m, 2H), 7.38 – 7.29 (m, 2H), 7.21 (dd, *J* = 6.6, 2.0 Hz, 4H), 7.12 – 7.02 (m, 8H), 6.82 (t, *J* = 7.6 Hz, 4H), 6.71 – 6.57 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 145.3 (s), 144.7 (s), 140.0 (s), 138.2 (s), 137.0 (s), 134.8 (s), 127.0 (s), 125.8 (s), 125.0 (s), 124.8 (s), 124.6 (s), 123.9 (s), 122.4 (s), 122.0 (s), 121.4 (s), 121.0 (s), 120.4 (s), 119.7 (s), 116.4 (s), 111.6 (s), 110.0 (s), 109.5 (s), 109.5 (s). Characterization of compound 4CzIPN is in accordance with previous literature.[21]

Benzoylglycine. Benzoylglycine was prepared using Procedure D.



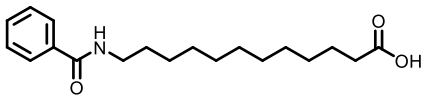
^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ 8.82 (t, *J* = 5.7 Hz, 1Hz), δ 7.89-7.87 (m, 2H), δ 7.57-7.47 (m, 3H), δ 3.95 (d, *J* = 5.9 Hz, 2H), δ 3.39 (br, 1H). **^{13}C NMR** (101 MHz, $(CD_3)_2SO$) δ 171.8, 167.0, 134.3, 131.9, 128.8, 127.7, 41.7. Characterization of compound benzoylglycine is in accordance with previous literature.[22]

4-(Benzoylamino)butanoic acid. 4-(Benzoylamino)butanoic acid was prepared using procedure D.



^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ 8.47 (t, *J* = 5.2 Hz, 1H), 7.86 – 7.84 (m, 2H), 7.52 – 7.42 (m, 3H), 3.30 (dd, *J* = 12.7, 6.8 Hz, 2H), 2.29 (t, *J* = 7.4 Hz, 2H), 1.81 – 1.74 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) 174.7, 166.8, 135.1, 131.5, 128.7, 127.6, 39.1, 31.7, 25.0. Characterization of compound 4-(Benzoylamino)butanoic acid is in accordance with previous literature.[23]

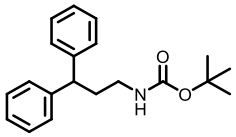
12-(Benzoylamino)dodecanoic acid. 12-(Benzoylamino)dodecanoic acid was prepared using procedure E.



^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ 8.40 (br, 1H), δ 7.84-7.82 (m, 2H), δ 7.53-7.43 (m, 3H), δ 3.25 (dd, *J* = 13.0, 6.8 Hz, 2H), δ 2.18 (t, *J* = 7.4 Hz, 2H), δ 2.2 (dt, *J* = 14.0, 6.8 Hz, 4H), δ 1.29-1.25 (m, 14H). **^{13}C NMR** (101 MHz, $(CD_3)_2SO$) δ 174.9, ^{16}6.5, 135.2, 131.4, 128.7, 127.6, 39.7, 34.1, 29.6, 29.4, 29.4, 29.4, 29.2, 29.2, 29.0, 27.0, 25.0. Characterization of compound 12-(Benzoylamino)dodecanoic acid is in accordance with previous literature.[24]

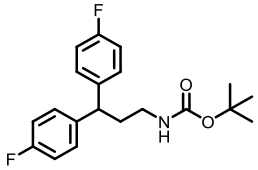
Synthesis of hydroaminoalkylated products

Tert-butyl (3,3-diphenylpropyl)carbamate (from 3). The compound was synthesized according to Condition A, using 1,1-diphenylethylene and boc-glycine.



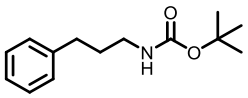
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29-7.15 (m, 10H), δ 4.47 (br, 1H), δ 3.95 (t, *J* = 7.9 Hz, 1H), δ 3.07 (dd, *J* = 12.9, 6.2 Hz, 2H), δ 2.25 (dd, *J* = 14.6, 7.6 Hz, 2H), δ 1.42 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.9, 144.3, 128.6, 127.8, 126.3, 79.1, 48.9, 39.4, 35.8, 28.4. **HRMS (ESI)** $[M+Na]^+$ calcd. 334.1778, found 334.1763.

Tert-butyl (3,3-bis(4-fluorophenyl)propyl)carbamate (from 4). The compound was synthesized according to Condition A, using 4,4'-(ethene-1,1-diyl)bis(fluorobenzene) and boc-glycine.



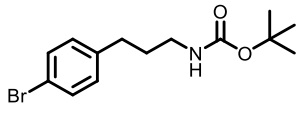
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (dd, *J* = 8.5, 5.4 Hz, 4H), 6.96 (t, *J* = 8.7 Hz, 4H), 4.51 (s, 1H), 3.93 (t, *J* = 7.8 Hz, 1H), 3.05 (dd, *J* = 13.0, 6.3 Hz, 2H), 2.19 (dd, *J* = 14.9, 7.8 Hz, 2H), 1.43 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.8, 160.4, 156.0, 140.0, 139.9, 129.2 (d, *J* = 7.9 Hz), 115.6 (d , *J* = 21.2 Hz), 79.4, 47.4, 39.4, 36.2, 28.5. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -166.7. **HRMS (ESI)** $[M+Na]^+$ calcd. 370.1589, found 370.1594.

Tert-butyl (3-phenylpropyl)carbamate (from 5). The compound was synthesized according to Condition A, using styrene and boc-glycine.



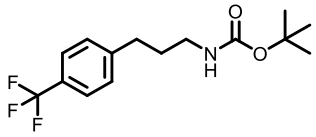
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.21 (m, 2H), 7.18 (t, *J* = 6.8 Hz, 3H), 4.54 (s, 1H), 3.14 (q, *J* = 6.2 Hz, 2H), 2.62 (d, *J* = 7.9 Hz, 2H), 1.86 – 1.73 (m, 2H), 1.44 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.1, 144.5, 142.4, 141.7, 128.7, 128.5, 128.5, 128.4, 127.8, 126.5, 126.0, 125.8, 79.2, 40.4, 33.8, 33.3, 31.9, 28.6. **HRMS (ESI)** $[M+Na]^+$ calcd. 258.1464, found 258.1457.

Tert-butyl (3-(4-bromophenyl)propyl)carbamate (from 6). The compound was synthesized according to Condition A, using *p*-bromostyrene and boc-glycine.



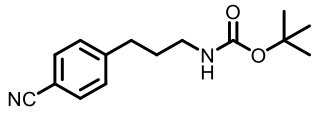
^{1}H NMR (400 MHz, $CDCl_3$) **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.2 Hz, 2H), 7.04 (d, *J* = 8.2 Hz, 2H), 4.55 (s, 1H), 3.13 (q, *J* = 6.2 Hz, 2H), 2.64 – 2.52 (m, 2H), 1.84 – 1.72 (m, 2H), 1.44 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.1, 140.7, 131.6, 130.2, 119.8, 79.3, 40.2, 32.6, 31.7, 28.5. **HRMS (ESI)** $[M+Na]^+$ calcd. 336.0570, found 336.0568.

Tert-butyl (3-(4-(trifluoromethyl)phenyl)propyl)carbamate (from 7). The compound was synthesized according to Condition A, using *p*-trifluoromethylstyrene and boc-glycine.



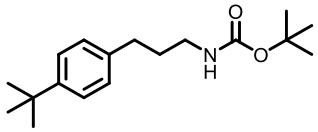
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 4.54 (s, 1H), 3.16 (q, *J* = 6.3 Hz, 1H), 2.75 – 2.64 (m, 1H), 1.83 (dt, *J* = 14.7, 7.4 Hz, 1H), 1.44 (s, 5H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.1, 145.9, 128.8, 126.5 (dd, *J* = 408.6, 152.1 Hz), 125.5 (q, *J* = 3.7 Hz), 79.4, 40.3, 33.1, 31.7, 28.6. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.4. **HRMS (ESI)** $[M+Na]^+$ calcd. 326.1338, found 326.1347.

Tert-butyl (3-(4-cyanophenyl)propyl)carbamate (from 8). The compound was synthesized according to Condition A, using *p*-cyanostyrene and boc-glycine.



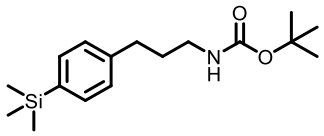
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.1 Hz, 2H), δ 7.28 (d, *J* = 8.1 Hz, 2 H), δ 4.56 (s, 1H), δ 3.15 (m, 2H), δ 2.7 (t, *J* = 7.7 Hz, 2H), δ 1.82 (quint, *J* = 7.6 Hz, 2Hk), δ 1.44 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.0, 147.3, 132.3, 129.2, 119.0, 110.0, 79.4, 41.0, 33.3, 31.4, 28.4. **HRMS (ESI)** $[M+Na]^+$ calcd. 283.1417, found 283.148.

Tert-butyl (3-(4-(tert-butyl)phenyl)propyl)carbamate (from 9). The compound was synthesized according to Condition A, using *p*-^{t}butylstyrene and boc-glycine.

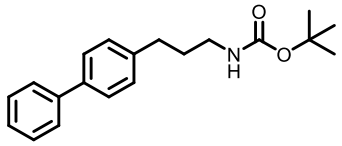


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.2 Hz, 2H), 7.11 (d, *J* = 8.2 Hz, 2H), 4.50 (s, 1H), 3.15 (q, *J* = 6.1 Hz, 2H), 2.68 – 2.51 (m, 2H), 1.89 – 1.71 (m, 2H), 1.44 (s, 9H), 1.30 (s, 9H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.1, 148.9, 138.6, 128.2, 125.4, 79.3, 40.5, 34.5, 32.7, 31.8, 31.5, 28.6. **HRMS (ESI)** $[M+H]^+$ calcd. 292.2271, found 292.2279.

Tert-butyl (3-(4-(trimethylsilyl)phenyl)propyl)carbamate (from 10). The compound was synthesized according to Condition A, using *p*-trimethylsilylstyrene and boc-glycine.

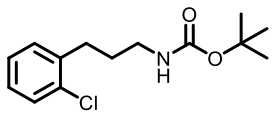


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 7.7 Hz, 2H), 7.17 (d, *J* = 7.7 Hz, 2H), 4.50 (s, 1H), 3.15 (q, *J* = 6.2 Hz, 2H), 2.67 – 2.57 (m, 2H), 1.90 – 1.73 (m, 2H), 1.44 (s, 9H), 0.25 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.1, 142.3, 137.8, 133.7, 128.0, 79.3, 40.5, 33.3, 31.8, 28.6, 0.1. **HRMS (ESI)** $[M+Na]^+$ calcd. 330.2945, found 330.1979.



Tert-butyl (3-([1,1'-biphenyl]-4-yl)propyl)carbamate (from 11). The compound was synthesized according to Condition A, using p-phenylstyrene and boc-glycine. **^{1}H NMR** (400 MHz, CDCl3) δ 7.59 – 7.54 (m, 2H), 7.51 (d, J = 8.1 Hz, 2H), 7.42 (t, J = 7.6 Hz, 1H), 7.31 (t, J = 7.3 Hz, 2H), 7.25 – 7.21 (m, 2H), 4.55 (s, 1H), 3.18 (q, J = 6.2 Hz, 2H), 2.68 (t, 1H), 1.89 – 1.79 (m, 2H), 1.45 (s, 9H). **^{13}C NMR** (101 MHz, CDCl3) δ 156.0, 141.1, 140.7, 139.0, 128.8, 128.7, 127.2, 127.1, 127.0, 79.2, 77.4, 77.0, 76.7, 40.3, 32.8, 31.7, 28.4. **HRMS (ESI)** [M+Na]+ calcd. 334.1777, found 334.1763.

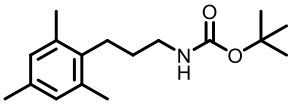
Tert-butyl (3-(2-chlorophenyl)propyl)carbamate (from 12). The compound was synthesized according to Condition A, using *o*-chlorostyrene and boc-glycine.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.27 (m, 1H), 7.24 – 7.07 (m, 3H), 4.57 (br, 1H), 3.17 (q, *J* = 6.4 Hz, 2H), 2.80 – 2.71 (m, 2H), 1.81 (dt, *J* = 14.7, 7.3 Hz, 2H), 1.45 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$)

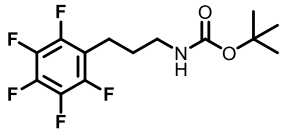
δ 156.0, 139.2, 133.9, 130.4, 129.5, 127.5, 126.8, 79.2, 40.2, 30.8, 30.1, 28.4. **HRMS (ESI)** $[M+H]^+$ calcd. 292.1075, found 292.1088.

Tert-butyl (3-mesitylpropyl)carbamate (from 13). The compound was synthesized according to Condition A, using 2,4,6-trimethylstyrene and boc-glycine.



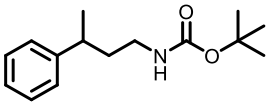
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.82 (s, 2H), 4.55 (s, 1H), 3.20 (q, *J* = 6.1 Hz, 2H), 2.64 – 2.53 (m, 2H), 2.27 (s, 6H), 2.23 (s, 3H), 1.68 – 1.58 (m, 2H), 1.45 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.2, 136.0, 135.6, 135.2, 129.1, 79.3, 41.1, 29.8, 28.6, 26.7, 20.9, 19.8. **HRMS (ESI)** $[M+Na]^+$ calcd. 300.1934, found 300.1945.

Tert-butyl (3-(perfluorophenyl)propyl)carbamate (from 14). The compound was synthesized according to Condition A, using pentafluorostyrene and boc-glycine.



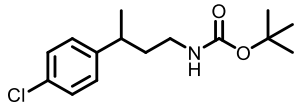
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.58 (s, 1H), 3.16 (q, *J* = 6.3 Hz, 2H), 2.73 (t, *J* = 7.6 Hz, 2H), 1.83 – 1.74 (m, 2H), 1.44 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.0, 144.1, 140.3, 138.6, 114.6, 79.6, 40.0, 29.7, 28.5, 19.8. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -144.2, -157.6, -162.7. **HRMS (ESI)** $[M+H]^+$ calcd. 326.1174, found 326.1159.

Tert-butyl (3-phenylbutyl)carbamate (from 15). The compound was synthesized according to Condition A, using *α*-methylstyrene and boc-glycine.



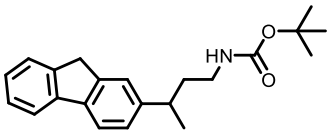
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (dt, *J* = 8.1, 3.3 Hz, 2H), 7.18 (dd, *J* = 7.3, 5.6 Hz, 3H), 4.43 (s, 1H), 3.00 (dt, *J* = 13.2, 6.8 Hz, 2H), 2.84 – 2.62 (m, 1H), 1.77 (ddd, *J* = 14.7, 9.5, 5.4 Hz, 2H), 1.42 (s, 9H), 1.26 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.0, 146.8, 128.6, 127.0, 126.3, 79.2, 39.3, 38.5, 37.8, 28.5, 22.4. **HRMS (ESI)** $[M+H]^+$ calcd. 250.1802, found 250.1813.

Tert-butyl (3-(4-chlorophenyl)butyl)carbamate (from 16). The compound was synthesized according to Condition A, using 1-chloro-4-(prop-1-en-2-yl)benzene and boc-glycine.



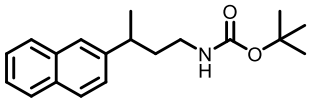
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26-7.24 (m, 2H), δ 7.12-7.10 (m, 2H), δ 4.41 (br, 1H), δ 3.08-2.95 (m, 2H), δ 2.73 (sext, *J* = 7.2 Hz, 1H), δ (1.81-1.67, 2H), δ 1.42 (s, 9H), 1.24, *J* = 7.0 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.9, 145.1, 131.8, 128.6, 128.3, 79.2, 39.1, 38.3, 37.2, 28.4, 22.2. **HRMS (ESI)** $[M+H]^+$ calcd. 306.1231, found 306.1240.

Tert-butyl (3-(9H-fluoren-2-yl)butyl)carbamate (17). The compound was synthesized according to Condition A, using 2-(prop-1-en-2-yl)-9H-fluorene and boc-glycine.



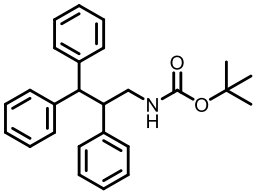
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (dd, *J* = 17.2, 7.6 Hz, 2H), 7.51 (d, *J* = 7.4 Hz, 1H), 7.37 – 7.32 (m, 2H), 7.29 – 7.23 (m, 1H), 7.18 (d, *J* = 7.9 Hz, 1H), 4.43 (s, 1H), 3.86 (s, 2H), 3.03 (dt, *J* = 12.7, 6.4 Hz, 2H), 2.82 (dd, *J* = 14.3, 7.1 Hz, 1H), 1.81 (dt, *J* = 14.4, 7.0 Hz, 2H), 1.42 (s, 9H), 1.31 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.1, 145.6, 143.8, 143.3, 141.8, 140.1, 126.8, 126.5, 125.7, 125.1, 123.6, 120.0, 119.8, 79.2, 39.4, 38.7, 38.0, 37.0, 28.6, 22.6. **HRMS (ESI)** $[M+Na]^+$ calcd. 360.1933, found 360.1939.

Tert-butyl (3-(naphthalen-2-yl)butyl)carbamate (from 18). The compound was synthesized according to Condition A, using 2-(prop-1-en-2-yl)naphthalene and boc-glycine.



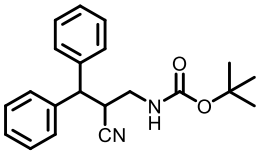
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (dt, *J* = 7.5, 3.8 Hz, 1H), 7.61 (s, 1H), 7.49 – 7.38 (m, 1H), 7.34 (dd, *J* = 8.5, 1.5 Hz, 1H), 4.42 (s, 1H), 3.05 (dd, *J* = 13.3, 6.7 Hz, 1H), 2.93 (dd, *J* = 14.2, 7.1 Hz, 1H), 1.87 (q, *J* = 7.4 Hz, 1H), 1.42 (s, 3H), 1.36 (d, *J* = 6.9 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.1, 144.2, 133.8, 132.5, 128.4, 127.7, 127.7, 126.1, 125.6, 125.4, 125.3, 79.4, 40.5, 38.4, 38.0, 28.6, 22.4. **HRMS (ESI)** $[M+H]^+$ calcd. 322.1777, found 322.1805.

Tert-butyl (2,3,3-triphenylpropyl)carbamate (from 19). The compound was synthesized according to Condition A, using triphenylethylene and boc-glycine.



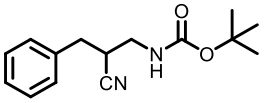
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.4 Hz, 2H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.21 – 7.00 (m, 10H), 6.95 (d, *J* = 7.2 Hz, 1H), 4.12 (d, *J* = 11.4 Hz, 2H), 3.71 (s, 1H), 3.55 (s, 1H), 3.10 – 2.97 (m, 1H), 1.34 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.7, 143.2, 141.2, 129.0, 128.7, 128.5, 128.3, 128.2, 128.2, 126.8, 126.7, 126.0, 79.1, 56.6, 49.7, 45.3, 35.6, 28.5. **HRMS (ESI)** $[M+Na]^+$ calcd. 410.2090, found 410.2091.

Tert-butyl (2-cyano-3,3-diphenylpropyl)carbamate (from 20). The compound was synthesized according to Condition A, using 3,3-diphenylacrylonitrile and boc-glycine.



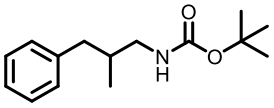
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.23 (m, 10H), 4.93 (s, 1H), 4.12 (d, *J* = 8.9 Hz, 1H), 3.76 (d, *J* = 4.0 Hz, 1H), 3.52 – 3.44 (m, 1H), 3.01-3.08 (m, 1H), 1.44 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.7, 140.20, 140.0, 129.2, 129.1, 128.3, 127.8, 127.7, 127.6, 120.4, 80.3, 51.3, 42.0, 38.1, 35.6, 28.4, 26.6, 26.5, 23.0. **HRMS (ESI)** $[M+Na]^+$ calcd. 359.1730, found 359.1743.

Tert-butyl (2-cyano-3-phenylpropyl)carbamate (from 21). The compound was synthesized according to Condition A, using cinnamonitrile and boc-glycine.



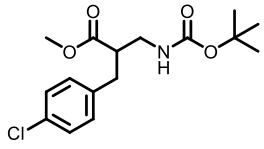
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.24 (m, 5H), δ 4.97 (br, 1H), δ 3.48-3.45 (m, 1H), δ 3.26-3.19 (m, 1H), 3.16-3.10 (m, 1H), δ 2.94-2.83 (m, 2H), δ 1.45 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.7, 136.2, 129.0, 128.9, 127.4, 120.5, 80.3, 42.1, 35.8, 35.0, 28.3. **HRMS (ESI)** $[M+Na]^+$ calcd. 283.1417, found 283.1427.

Tert-butyl (2-methyl-3-phenylpropyl)carbamate (from 22). The compound was synthesized according to Condition A, using *β*-methylstyrene and boc-glycine.



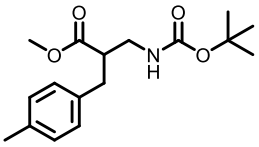
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (dd, *J* = 10.5, 4.1 Hz, 2H), 7.17 (dd, *J* = 20.0, 7.2 Hz, 2H), 4.54 (s, 1H), 3.06 (ddd, *J* = 40.2, 12.9, 6.3 Hz, 1H), 2.69 (dd, *J* = 13.4, 5.7 Hz, 1H), 2.37 (dd, *J* = 13.5, 8.4 Hz, 1H), 1.92 (dq, *J* = 13.4, 6.6 Hz, 1H), 1.44 (s, 9H), 0.87 (d, *J* = 6.7 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.2, 140.6, 129.2, 128.4, 126.1, 79.2, 46.6, 41.1, 36.0, 28.6, 17.5. **HRMS (ESI)** $[M+Na]^+$ calcd. 272.1621, found 272.1610.

Methyl 3-((tert-butoxycarbonyl)amino)-2-(4-chlorobenzyl)propanoate (from 23). The compound was synthesized according to Condition A, using methyl (*E*)-3-(4-chlorophenyl)acrylate and boc-glycine.



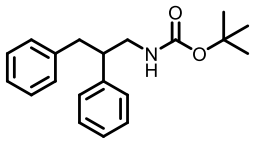
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (d, *J* = 8.4 Hz, 2H), 7.09 (d, *J* = 8.4 Hz, 2H), 4.85 (s, 1H), 3.64 (s, 3H), 3.42 – 3.21 (m, 2H), 2.98 – 2.86 (m, 2H), 2.77 (d, *J* = 6.8 Hz, 1H), 1.43 (s, 9H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 174.5, 155.9, 137.0, 132.6, 130.3, 128.8, 79.7, 77.5, 77.2, 76.8, 52.0, 47.5, 41.7, 35.3, 28.5. **HRMS (ESI)** $[M+Na]^+$ calcd. 350.1130, found 350.1139.

Methyl 3-((tert-butoxycarbonyl)amino)-2-(4-methylbenzyl)propanoate (from 24). The compound was synthesized according to Condition A, using methyl (*E*)-3-(4-methylphenyl)acrylate and boc-glycine.



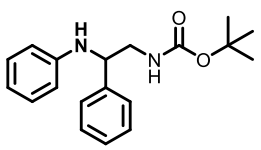
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (dd, *J* = 18.3, 8.0 Hz, 4H), 4.84 (s, 1H), 3.64 (s, 3H), 3.23-3.27 (m, 2H), 2.95 – 2.86 (m, 2H), 2.83 – 2.67 (m, 1H), 2.30 (s, 3H), 1.42 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 174.8, 155.9, 136.2, 135.3, 129.3, 128.8, 79.5, 51.9, 47.6, 41.6, 35.6, 28.5, 21.1. **HRMS (ESI)** $[M+H]^+$ calcd. 308.1856, found 308.1869.

Tert-butyl (2,3-diphenylpropyl)carbamate (from 25). The compound was synthesized according to Condition A, using *trans*-stilbene and boc-glycine.



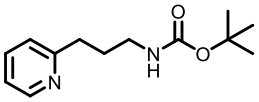
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (dd, *J* = 12.9, 5.3 Hz, 2H), 7.19 (dd, *J* = 12.9, 7.1 Hz, 3H), 7.12 (d, *J* = 7.0 Hz, 3H), 7.02 (d, *J* = 7.1 Hz, 2H), 4.33 (s, 1H), 3.55 (d, *J* = 5.4 Hz, 1H), 3.24 (d, *J* = 8.8 Hz, 1H), 3.06 (s, 1H), 2.91 (qd, *J* = 13.6, 7.4 Hz, 2H), 1.38 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.0, 142.2, 139.7, 129.18, 128.7, 128.4, 128.1, 126.9, 126.2, 79.3, 48.0, 45.5, 40.8, 28.5. **HRMS (ESI)** $[M+Na]^+$ calcd. 334.1777, found 334.1775.

Tert-butyl (2-phenyl-2-(phenylamino)ethyl)carbamate (from 26). The compound was synthesized according to Condition A, using (*E*)-*N*,1-diphenylmethanimine and boc-glycine.



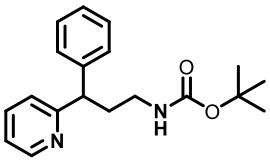
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (dt, *J* = 15.0, 7.5 Hz, 4H), 7.25 (t, *J* = 6.9 Hz, 1H), 7.07 (t, *J* = 7.8 Hz, 2H), 6.63 (t, *J* = 7.2 Hz, 1H), 6.49 (d, *J* = 7.9 Hz, 2H), 4.91 (s, 1H), 4.78 (s, 1H), 4.47 – 4.36 (m, 1H), 3.54 – 3.36 (m, 2H), 1.46 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.3, 147.6, 141.3, 129.2, 129.0, 127.75, 126.7, 117.4, 113.4, 80.1, 60.2, 47.5, 28.5. **HRMS (ESI)** $[M+H]^+$ calcd. 312.1838, found 312.1830.

Tert-butyl (3-(pyridin-2-yl)propyl)carbamate (from 27). The compound was synthesized according to Condition A, using 2-vinylpyridine and boc-glycine.



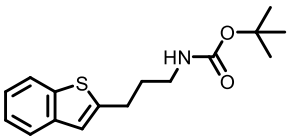
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, *J* = 4.4 Hz, 1H), δ 7.59 (td, *J* = 7.7, 1.7 Hz, 1H), δ 7.15 (d, *J* = 7.8 Hz, 1H), δ 7.10 (dd, *J* = 7.1, 5.3 Hz, 1H), δ 4.77 (br, 1H), δ 3.17 (dd, *J* = 12.6, 6.2 Hz, 2H), δ 2.83 (t, 7.6 Hz, 2H), δ 1.93 (p, *J* = 7.6 Hz, 2H), δ 1.44 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 161.4, 156.0, 149.3, 136.5, 122.9, 121.2, 79.0, 40.1, 35.5, 29.9, 28.5. **HRMS (ESI)** $[M+H]^+$ calcd. 237.1598, found 237.1586.

Tert-butyl (3-phenyl-3-(pyridin-2-yl)propyl)carbamate (from 28). The compound was synthesized according to Condition A, using 2-(1-phenylvinyl)pyridine and boc-glycine.



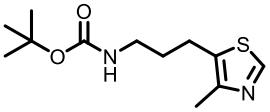
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (dd, *J* = 4.8, 0.8 Hz, 1H), 7.55 (td, *J* = 7.7, 1.9 Hz, 1H), 7.33 – 7.27 (m, 4H), 7.19 (t, *J* = 7.0 Hz, 1H), 7.13 (d, *J* = 7.9 Hz, 1H), 7.09 (ddd, *J* = 7.4, 4.9, 1.0 Hz, 1H), 4.64 (s, 1H), 4.12 (t, *J* = 7.7 Hz, 1H), 3.16 – 3.01 (m, 2H), 2.46 (td, *J* = 14.2, 7.3 Hz, 1H), 2.26 (td, *J* = 14.3, 7.3 Hz, 1H), 1.41 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.29, 156.04, 149.36, 143.35, 136.68, 128.77, 128.11, 126.76, 123.10, 121.59, 79.17, 51.33, 39.40, 35.21, 28.57. **HRMS (ESI)** $[M+H]^+$ calcd. 313.1911, found 313.1919.

Tert-butyl (2-(benzo[b]thiophen-2-yl)ethyl)carbamate (from 29). The compound was synthesized according to Condition A, using 2-vinylbenzo[b]thiophene and boc-glycine.



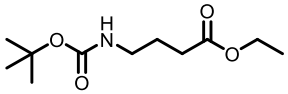
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.9 Hz, 1H), δ 7.65 (d, *J* = 7.6 Hz, 1H), δ 7.31-7.25 (m, 2H), δ 7.01 (s, 1H), δ 4.57 (br, 1H), 3.21 (dd, *J* = 12.9, 7.4 Hz, 2H), δ 2.93 (t, *J* = 7.5 Hz, 2H), δ 1.93 (p, *J* = 7.6 Hz, 2H), δ 1.44 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.0, 145.3, 140.2, 139.3, 124.1, 123.6, 122.8, 122.1, 120.9, 79.3, 40.0, 31.4, 28.4, 28.1. **HRMS (ESI)** $[M+Na]^+$ calcd. 314.1185, found 314.1197.

Tert-butyl (3-(4-methylthiazol-5-yl)propyl)carbamate (from 30). The compound was synthesized according to Condition A, using 4-methyl-5-vinylthiazole and boc-glycine.



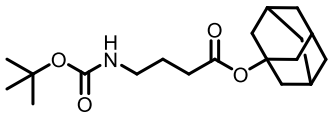
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), δ 4.57 (br, 1H), δ (dd, *J* = 12.5, 6.1 Hz, 2H), δ 2.79 (t, *J* = 7.7 Hz, 2H), δ 2.38 (s, 3H), δ 1.81 (p, *J* = 7.2 Hz, 2H), δ 1.45 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.9; 149.0, 148.7, 130.9, 79.4, 40.0, 32.0, 28.4, 23.6, 14.8. **HRMS (ESI)** $[M+Na]^+$ calcd. 279.1138, found 279.1149.

Ethyl 4-((tert-butoxycarbonyl)amino)butanoate (from 31). The compound was synthesized according to Condition A, using ethyl acrylate and boc-glycine.



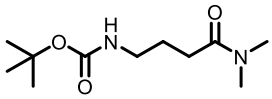
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.63 (s, 1H), 4.13 (q, *J* = 7.1 Hz, 2H), 3.16 (q, *J* = 6.4 Hz, 2H), 2.34 (t, *J* = 7.3 Hz, 2H), 1.81 (p, *J* = 7.1 Hz, 2H), 1.44 (s, 9H), 1.26 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 173.4, 156.1, 79.3, 60.6, 40.1, 31.8, 28.5, 25.5, 14.3. **HRMS (ESI)** $[M+Na]^+$ calcd. 254.1363, found 254.1375.

Adamantan-1-yl 4-((tert-butoxycarbonyl)amino)butanoate (from 32). The compound was synthesized according to Condition A, using adamantyl acrylate and boc-glycine.



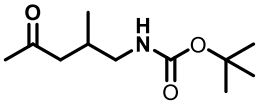
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.62 (br, 1H), δ 3.15 (dd, *J* = 21.2, 5.9 Hz, 1H), δ 2.25 (t, *J* = 7.3 Hz, 1H), δ 2.16-2.10 (m, 9H), δ 1.76 (p, *J* = 6.8 Hz, 2H), δ 1.69-1.63 (m, 6H), δ 1.44 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ172.4, 155.9, 80.6, 79.1, 41.4, 40.1, 36.2, 33.1, 30.9, 28.4, 25.4. **HRMS (ESI)** $[M+H]^+$ calcd. 338.2326, found 338.2327.

Tert-butyl (4-(dimethylamino)-4-oxobutyl)carbamate (from 33). The compound was synthesized according to Condition A, using *N*,*N*-dimethylacrylamide and boc-glycine.



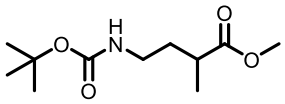
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.84 (br, 1H), δ 3.17 (q, *J* = 6.4 Hz, 2H), δ 3.00 (s, 3H), δ 2.94 (s, 3H), δ 2.36 (t, *J* = 7.1 Hz, 2H), δ 1.83 (p, *J* = 6.9 Hz, 2H), δ 1.44 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 172.5, 156.1, 79.0, 40.3, 37.2, 35.5, 30.6, 28.4, 25.2. **HRMS (ESI)** $[M+H]^+$ calcd. 231.1703, found 231.1709.

Tert-butyl (2-methyl-4-oxopentyl)carbamate (from 34). The compound was synthesized according to Condition A, using (*E*)-pent-3-en-2-one and boc-glycine.



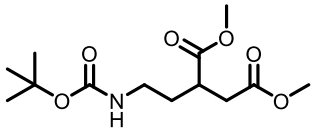
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.57 (br, 1H), δ 3.12 (dd, *J* = 12.9, 6.5 Hz, 2H), δ 2.47-2.40 (m, 4H), δ 1.76 (p, *J* = 7.0 Hz, 2H), δ 1.44 (s, 9H), δ 1.06 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 211.1, 156.0, 79.2, 40.1, 39.4, 36.0, 28.4, 24.2, 7.8. **HRMS (ESI)** $[M+Na]^+$ calcd. 238.1414, found 238.1412.

Methyl 4-((tert-butoxycarbonyl)amino)-2-methylbutanoate (from 35). The compound was synthesized according to Condition A, using methyl methacrylate and boc-glycine.



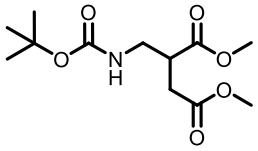
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.57 (s, 1H), 3.68 (s, 3H), 3.15 (s, 2H), 2.51 (dd, *J* = 13.9, 6.9 Hz, 1H), 1.83 (dt, *J* = 14.6, 7.1 Hz, 1H), 1.44 (s, 9H), 1.18 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.9, 156.01, 79.4, 77.5, 77.2, 76.8, 51.8, 38.7, 37.2, 34.0, 28.6, 17.2. **HRMS (ESI)** $[M+Na]^+$ calcd. 254.1363, found 254.1375.

Dimethyl 2-(2-((tert-butoxycarbonyl)amino)ethyl)succinate (from 36). The compound was synthesized according to Condition A, using dimethyl 2-methylenesuccinate and boc-glycine.



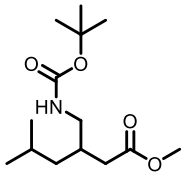
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.74 (s, 1H), 3.71 (s, 3H), 3.67 (s, 3H), 3.16 (ddd, *J* = 26.8, 13.2, 6.7 Hz, 2H), 2.90 (td, *J* = 8.2, 4.2 Hz, 1H), 2.75 (dd, *J* = 16.7, 8.8 Hz, 1H), 2.49 (dd, *J* = 16.6, 5.3 Hz, 1H), 1.88 – 1.69 (m, 2H), 1.44 (s, 9H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.0, 172.2, 155.9, 79.4, 52.1, 51.9, 38.8, 38.3, 35.8, 32.0, 28.5. **HRMS (ESI)** $[M+Na]^+$ calcd. 312.1418, found 312.1416.

Dimethyl 2-(((tert-butoxycarbonyl)amino)methyl)succinate (from 37). The compound was synthesized according to Condition A, using dimethyl maleate and boc-glycine.



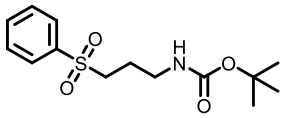
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.91 (br, 1H), δ 3.72 (s, 3H), δ 3.69 (s, 3H), δ 3.46-3.36 (m, 2H), δ 3.03 (p, *J* = 6.8 Hz, 1H), δ 2.64 (ddd, *J* = 22.7, 16.8, 6.8 Hz, 2H), δ 1.43 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 173.7, 172.0, 155.9, 79.6, 52.2, 41.9, 41.8, 41.4, 33.5, 28.4. **HRMS (ESI)** $[M+H]^+$ calcd. 298.1261, found 298.1255.

Methyl 3-(((tert-butoxycarbonyl)amino)methyl)-5-methylhexanoate (from 38). The compound was synthesized according to Condition A, using methyl (E)-5-methylhex-2-enoate and boc-glycine.



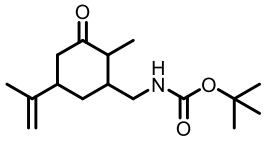
^{1}H NMR (400 MHz, $CDCl_3$)δ 4.67 (s, 1H), 3.67 (s, 3H), 3.27 – 2.91 (m, 2H), 2.28 (d, *J* = 6.6 Hz, 2H), 2.16 – 2.01 (m, 1H), 1.72 – 1.57 (m, 2H), 1.44 (s, 9H), 1.15 (qd, *J* = 13.8, 6.9 Hz, 2H), 0.89 (dd, *J* = 7.7, 6.9 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 173.8, 156.2, 79.2, 51.7, 44.4, 41.7, 37.5, 33.9, 28.5, 25.4, 22.8. **HRMS (ESI)** $[M+Na]^+$ calcd. 296.1832, found 296.1840.

Tert-butyl (3-(phenylsulfonyl)propyl)carbamate (from 39). The compound was synthesized according to Condition A, using (vinylsulfonyl)benzene and boc-glycine.



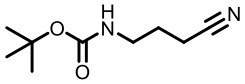
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.4 Hz, 2H), δ 7.62 (dt, *J* = 15.2, 7.4 Hz, 3H), δ 4.68 (br, 1H), δ 3.23 (dd, *J* = 12.7, 6.3 Hz, 2H), δ 3.16-3.12 (m, 2H), δ 1.96-1.89 (m, 2H), δ 1.41 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.9, 139.1, 133.8, 129.4, 128.0, 79.6, 53.7, 38.9, 28.3, 23.6. **HRMS (ESI)** $[M+Na]^+$ calcd. 322.1083, found 322.1095.

Tert-butyl ((2-methyl-3-oxo-5-(prop-1-en-2-yl)cyclohexyl)methyl)carbamate (from 40). The compound was synthesized according to Condition A, using carvone and boc-glycine.



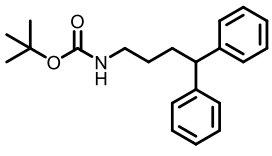
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.79 (s, 1H), 4.75 (s, 1H), 4.48 (br, 1H), 3.22 – 3.14 (m, 1H), 2.90 (s, 1H), 2.71 – 2.58 (m, 2H), 2.53 – 2.41 (m, 1H), 2.31 (dd, *J* = 16.6, 8.4 Hz, 2H), 2.01 (d, *J* = 13.0 Hz, 1H), 1.74 (s, 4H), 1.43 (s, 9H), 1.08 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 212.2, 156.0, 147.4, 110.3, 110.1, 79.6, 47.1, 46.6, 46.1, 44.8, 41.5, 41.0, 39.1, 35.0, 32.0, 28.5, 20.8, 20.5, 11.8, 11.6. **HRMS (ESI)** $[M+Na]^+$ calcd. 304.1883, found 304.1877.

Tert-butyl (3-cyanopropyl)carbamate (from 41). The compound was synthesized according to Condition A, using acrylonitrile and boc-glycine.



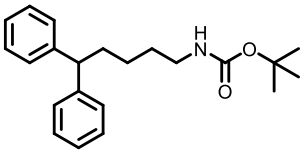
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.69 (br, 1H), δ 3.25 (q, *J* = 6.5 Hz, 2H), δ 2.4 (t, *J* = 7.2 Hz, 2H), δ 1.87 (p, *J* = 6.8 Hz, 2H), δ 1.45 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.0, 119.2, 79.8, 39.4, 28.4, 26.1, 14.6. **HRMS (ESI)** $[M+Na]^+$ calcd. 207.1104, found 207.1094.

Tert-butyl (4,4-diphenylbutyl)carbamate (from 42). The compound was synthesized according to Condition A, using 1,1-diphenylethylene and 3-((Tert-butoxycarbonyl)(methyl)amino)-propanoic acid.



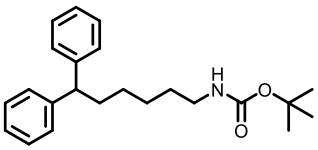
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.21 (m, 8H), δ 7.18-7.14 (m, 2H), δ 4.43 (br, 1H), δ 3.89 (t, *J* = 7.8 Hz, 1H), δ 3.12(dd, *J* = 13, 7.2, 2H), δ 2.08-2.03 (m, 2H), δ 1.47-1.40 (m, 11H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.9, 144.8, 128.5, 127.8, 126.2, 79.1, 51.0, 40.5, 32.8, 28.6, 28.4. **HRMS (ESI)** $[M+Na]^+$ calcd. 348.1934, found 348.1918.

Tert-butyl (5,5-diphenylpentyl)carbamate (from 43). The compound was synthesized according to Condition A, using 1,1-diphenylethylene and 4-((tert-butoxycarbonyl)amino)-butanoic acid.



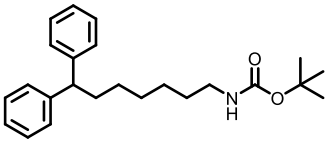
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.12 (m, 10H), 4.42 (s, 1H), 3.87 (t, *J* = 7.8 Hz, 1H), 3.06 (q, *J* = 6.4 Hz, 2H), 2.05 (dd, *J* = 15.6, 7.8 Hz, 2H), 1.49 (dd, *J* = 14.8, 7.4 Hz, 2H), 1.42 (s, 9H), 1.28 (ddd, *J* = 8.0, 6.7, 4.0 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.1, 145.2, 128.6, 128.0, 126.3, 79.2, 51.5, 40.6, 35.5, 30.2, 28.6, 25.4. **HRMS (ESI)** $[M+Na]^+$ calcd. 362.2090, found 362.2096.

Tert-butyl (6,6-diphenylhexyl)carbamate (from 44). The compound was synthesized according to Condition A, using 1,1-diphenylethylene and 5-((tert-butoxycarbonyl)amino)-pentanoic acid.



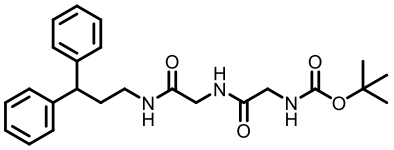
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.06 (m, 10H), 4.44 (s, 1H), 3.87 (t, *J* = 7.8 Hz, 1H), 3.05 (q, *J* = 6.1 Hz, 2H), 2.03 (dd, *J* = 14.9, 7.7 Hz, 2H), 1.42 (d, *J* = 9.2 Hz, 11H), 1.36 – 1.16 (m, 4H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.1, 145.3, 128.5, 128.0, 126.2, 79.2, 51.4, 40.7, 35.8, 30.1, 28.6, 27.9, 26.9. **HRMS (ESI)** $[M+Na]^+$ calcd. 376.2247, found 376.2240.

Tert-butyl (7,7-diphenylheptyl)carbamate (from 45). The compound was synthesized according to Condition A, using 1,1-diphenylethylene and 6-((tert-butoxycarbonyl)-amino)hexanoic acid.



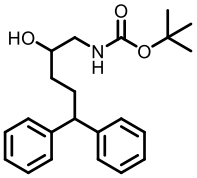
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.20 (m, 8H), 7.19 – 7.11 (m, 2H), 4.45 (s, 1H), 3.87 (t, *J* = 7.8 Hz, 1H), 3.06 (q, *J* = 6.2 Hz, 2H), 2.02 (dd, *J* = 15.0, 7.7 Hz, 2H), 1.43 (s, 10H), 1.36 – 1.12 (m, 5H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.1, 145.4, 128.5, 128.0, 126.2, 79.1, 77.5, 77.2, 76.8, 51.5, 40.7, 35.8, 30.2, 29.4, 28.6, 28.1, 26.8. **HRMS (ESI)** $[M+Na]^+$ calcd. 390.2403, found 390.2389.

Tert-butyl (2-((2-((3,3-diphenylpropyl)amino)-2-oxoethyl)amino)-2-oxoethyl)carbamate (from 46). The compound was synthesized according to Condition B, using 1,1-diphenylethylene and glycylglycylglycine.



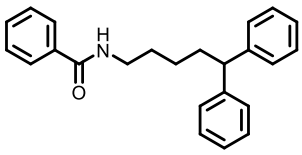
^{1}H NMR (400 MHz, DMSO-d6) δ 8.06 (t, *J* = 5.2 Hz, 1H), 8.8 (t, *J* = 4.4 Hz, 1H), 7.32-7.28 (m, 8H), 7.18-7.14 (m, 2 H), 7.07 (t, *J* = 5.4 Hz, 1H), 3.99 (dd, *J* = 19.2, 8.1 Hz, 1H), 3.72 (d, *J* = 5.6 Hz, 2H), 3.62 (d, *J* = 5.7 Hz, 2H), 3.02 (dd, *J* = 13.7, 5.9 Hz, 2H), 2.21 (dd, *J* = 14.5, 7.6 Hz, 2H), 1.39 (s, 9H). **^{13}C NMR** (101 MHz, DMSO-d6) δ 169.7, 168.6, 156.0, 144.6, 128.4, 127.6, 126.1, 78.2, 47.9, 42.1, 40.4, 37.5, 34.6, 28.2. **HRMS (ESI)** $[M+H]^+$ calcd. 426.2387, found 426.2399.

Tert-butyl (2-hydroxy-5,5-diphenylpentyl)carbamate (from 47). The compound was synthesized according to Condition B, using 1,1-diphenylethylene and 4-amino-3-hydroxybutanoic acid.



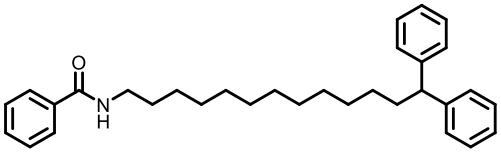
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.20 (m, 8H), 7.15 – 7.11 (m, 2H), 4.99 (s, 1H), 3.85 (t, *J* = 7.8 Hz, 1H), 3.63 (q, *J* = 9.3 Hz, 1H), 3.19 – 3.16 (m, 1H), 2.95 – 2.88 (m, 1H), 2.25 – 2.16 (m, 1H), 2.09 – 2.00 (ddd, *J* = 15.8, 14.4, 7.7 Hz, 1H), 1.41 (s, 9H), 1.39 – 1.33 (m, 2 H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.9, 144.9, 144.8, 128.5, 127.9, 127.9, 126.2, 79.6, 71.5, 51.4, 46.7, 33.3, 31.6, 28.5. **HRMS (ESI)** $[M+Na]^+$ calcd. 378.2040, found 378.2027.

N-(5,5-diphenylpentyl)benzamide (from 48). The compound was synthesized according to Condition C, using 1,1-diphenylethylene and 4-benzamidobutanoic acid.



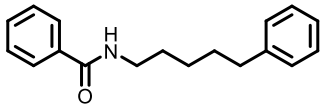
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.62 (m, 2H), 7.46 (dd, *J* = 8.5, 6.2 Hz, 1H), 7.38 (t, *J* = 7.4 Hz, 2H), 7.30 – 7.19 (m, 8H), 7.15 (dd, *J* = 9.1, 4.4 Hz, 2H), 6.09 (s, 1H), 3.89 (t, *J* = 7.8 Hz, 1H), 3.39 (dd, *J* = 13.2, 6.9 Hz, 2H), 2.08 (dd, *J* = 15.6, 7.8 Hz, 2H), 1.63 (dt, *J* = 14.8, 7.4 Hz, 2H), 1.38 – 1.28 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.6, 145.1, 135.0, 131.4, 128.6, 128.6, 127.9, 127.0, 126.3, 51.3, 39.9, 35.3, 29.6, 25.4. **HRMS (ESI)** $[M+H]^+$ calcd. 344.2009, found 344.1991.

N-(12,12-diphenyldodecyl)benzamide (from 49). The compound was synthesized according to Condition C, using 1,1-diphenylethylene and 12-benzamidododecanoic acid acid.



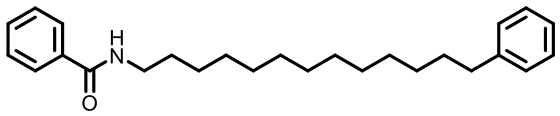
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.767.74 (m, 2H), δ 7.50-7.40 (m, 3H), 7.28-7.13 (m, 10H), δ 6.06 (br, 1H), δ 3.87 (t, *J* = 7.8 Hz, 1H), δ 3.45 (dd, *J* = 13.1, 7.1 Hz, 2H), δ 2.02 (dd, *J* = 14.8, 7.8 Hz, 2H), δ 1.61 (p, *J* = 7.6 Hz, 2H), δ 1.37-1.22 (m, 18H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.5, 145.4, 135.0, 131.3, 128.6, 128.3, 127.9, 126.8, 126.0, 51.4, 40.1, 35.7, 29.7, 29.6, 29.6, 29.5, 29.5, 29.5, 29.3, 28.0, 27.0. **HRMS (ESI)** $[M+Na]^+$ calcd. 456.3261, found 456.3282.

N-(5-phenylpentyl)benzamide (50). The compound was synthesized according to Condition C, using 4-benzamidobutanoic acid and styrene.



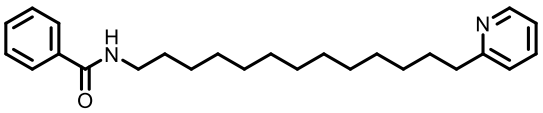
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.70 (m, 1H), 7.50 – 7.35 (m, 2H), 7.31 – 7.12 (m, 3H), 6.22 (s, 1H), 3.47 – 3.39 (m, 1H), 2.66 – 2.57 (m, 1H), 1.72 – 1.58 (m, 2H), 1.46 – 1.36 (m, 1H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.5, 142.4, 134.9, 131.3, 128.5, 128.5, 128.4, 128.4, 128.4, 128.3, 128.3, 126.9, 125.7, 40.0, 35.8, 31.0, 29.5, 26.5. **HRMS (ESI)** $[M+Na]^+$ calcd. 290.1515, found 290.1520.

N-(13-phenyltridecyl)benzamide (from 51). The compound was synthesized according to Condition C, using styrene and 12-benzamidododecanoic acid acid.



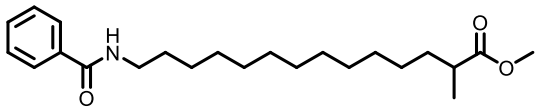
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.74 (m, 1H), 7.45 (ddd, *J* = 26.1, 11.0, 5.9 Hz, 2H), 7.32 – 7.09 (m, 3H), 6.12 (br, 1H), 3.44 (dd, *J* = 13.1, 7.1 Hz, 1H), 2.63 – 2.56 (m, 1H), 1.61 (dt, *J* = 14.7, 7.2 Hz, 2H), 1.35 – 1.19 (m, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.5, 143.0, 135.0, 131.3, 128.5, 128.4, 128.4, 128.3, 128.2, 127.8, 126.8, 125.6, 125.5, 45.6, 40.1, 36.0, 31.5, 29.7, 29.6, 29.6, 29.6, 29.6, 29.5, 29.3, 27.5, 27.0. **HRMS (ESI)** $[M+H]^+$ calcd. 380.2948, found 380.2942.

N-(13-(pyridin-2-yl)tridecyl)benzamide (from 52). The compound was synthesized according to Condition A, using 2-vinylpyridine and 12-benzamidododecanoic acid.



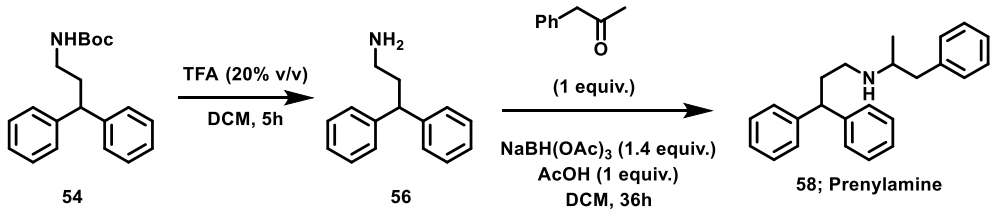
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52-8.50 (m, 1H), δ 7.76-7.74 (m, 2H), δ 7.57 (td, *J* = 7.7, 1.8 Hz, 1H) δ 7.50-7.46 (m, 1H), δ 7.43-7.40 (m, 1H), δ7.14-7.12 (m, 1H), δ 7.10-7.06 (m, 1H), δ 6.16 (br, 1H), δ 3.45 (dd, *J* = 13.1, 7.1 Hz, 2H), δ 2.78 (t, *J* = 7.7 Hz, 2H), δ1.72 (dt, *J* = 15.4, 7.6 Hz, 2H), δ 1.61 (dt, *J* = 14.8, 7.3 Hz, 2H), δ 1.37-1.23 (m, 18H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 167.5, 162.6, 149.2, 136.2, 135.0, 131.3, 128.5, 126.8, 122.7, 120.8, 40.1, 38.5, 29.9, 29.7, 29.6, 29.6, 29.5, 29.5, 29.4, 29.3, 27.0. **HRMS (ESI)** $[M+H]^+$ calcd. 381.2900, found 381.2891.

Methyl 14-benzamido-2-methyltetradecanoate (53). The compound was synthesized according to Condition A, using methyl methacrylate and 12-benzamidododecanoic acid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.75 (m, 2H), 7.48 – 7.39 (m, 3H), 6.28 (br, 1H), 3.66 (s, 3H), 3.46 – 3.41 (m, 2H), 2.47 – 2.38 (m, 1H), 1.67 – 1.57 (m, 3H), 1.42 – 1.25 (m, 19H), 1.14 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 177.4, 167.5, 135.0, 131.3, 128.5, 126.8, 51.4, 40.1, 39.5, 33.8, 29.7, 29.6, 29.5, 29.5, 29.5, 29.5, 29.3, 27.2, 27.0, 17.1. **HRMS (ESI)** $[M+H]^+$ calcd. 376.2846, found 376.2835.

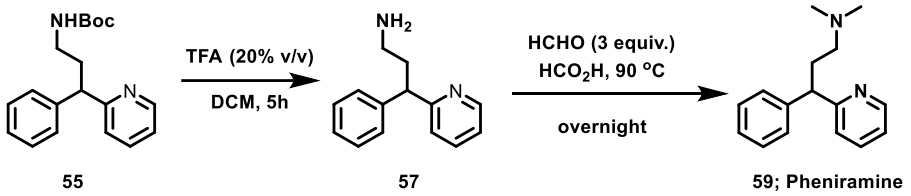
3,3-diphenyl-N-(1-phenylpropan-2-yl)propan-1-amine (Prenylamine, 58)



The compound **54** was synthesized according to Condition A, using 1,1-diphenylethelene and boc-glycin. The pure compound **54** (0.2 mmol) was first disolved in DCM (2 mL). Then trifluoroacetic acid (20% V/V) was added dropwise to to solution and continue stirring for 5 h. After completion of the reaction (monitered with TLC), the solvent was evapored using vaccum. After that, the crude mixture (product **56**) was then used in the next-step without purification. To the solution of **56** in DCM, AcOH (1 equiv.) followed by $NaBH(OAc)_3$ (1.4 equiv.) were added under N_2 atmosphere. The reaction mixture was left to stir for 36h and then the reaction mixture was quenched with H_2O and $NaHCO_3$. The aqueous solution was extracted with 5.0 mL DCM for three times. The organic layer was then dried over Na_2SO_4 and concentrated in vacuo. The reaction mixture was directly loaded onto a short silica gel column, followed by gradient elution with EtOAc/Heptane (20% - 50%). Removing the solvent in vacuo, afforded product prenylamine (**58**).

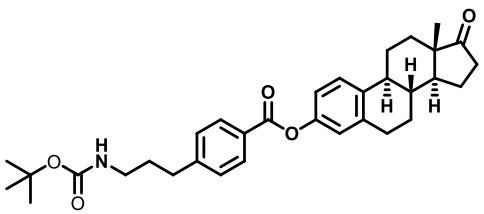
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.26 (ddd, *J* = 9.8, 6.7, 3.4 Hz, 3H), 7.22 – 7.07 (m, 10H), 7.04 (d, *J* = 6.4 Hz, 2H), 3.92 (t, *J* = 8.0 Hz, 1H), 3.22 – 3.13 (m, 1H), 3.10 (dd, *J* = 13.1, 4.1 Hz, 1H), 2.94 – 2.71 (m, 2H), 2.55 (dd, *J* = 12.9, 10.0 Hz, 1H), 2.44 (q, *J* = 7.9 Hz, 2H), 1.06 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.5, 162.2, 143.2, 143.2, 136.6, 129.4, 128.9, 127.6, 127.6, 127.1, 126.8, 126.8, 55.7, 48.8, 44.2, 40.1, 32.1, 16.1. **HRMS (ESI)** $[M+Na]^+$ calcd. 352.2036, found 352.2025.

***N*,*N*-dimethyl-3-phenyl-3-(pyridin-2-yl)propan-1-amine (Pheniramine, 59)**



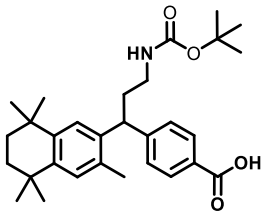
The compound **55** was synthesized according to Condition A, using 2-vinylpyridine and boc-glycin. The pure compound **55** (0.2 mmol) was first disolved in DCM (2 mL). Then trifluoroacetic acid (20% V/V) was added dropwise to to solution and continue stirring for 5h. After completion of the reaction (monitered with TLC), the solvent was evapored using vaccum. The crude product **57** was then without further purification was directly used to synthesize pheniramine following previous reported method.[16] The analytical data of the compound **59** matched with the reported literature data.[16]

(8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl 4-(3-((tert-butoxycarbonyl)amino)propyl)benzoate (60). The compound was synthesized according to Condition A, using estrone derivative and boc-glycine.



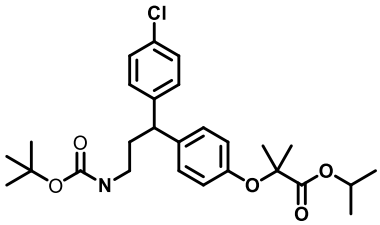
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.2 Hz, 2H), 7.32 (t, *J* = 7.9 Hz, 3H), 6.97 (dd, *J* = 8.4, 2.3 Hz, 1H), 6.94 (s, 1H), 4.54 (s, 1H), 3.17 (d, *J* = 6.4 Hz, 2H), 2.98 – 2.89 (m, 2H), 2.79 – 2.67 (m, 2H), 2.58 – 2.47 (m, 1H), 2.47 – 2.38 (m, 1H), 2.37 – 2.26 (m, 1H), 2.21 – 1.93 (m, 4H), 1.91 – 1.79 (m, 2H), 1.71 – 1.47 (m, 6H), 1.45 (s, 9H), 0.92 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.9, 165.5, 156.1, 149.1, 148.0, 138.2, 137.5, 130.5, 128.7, 127.6, 126.6, 121.9, 119.1, 50.6, 48.1, 44.4, 38.2, 36.0, 33.4, 32.5, 31.7, 31.6, 29.7, 29.6, 28.6, 26.5, 25.9, 21.7, 14.0. **HRMS (ESI)** $[M+Na]^+$ calcd. 554.2877, found 554.2853.

Methyl 4-(3-((tert-butoxycarbonyl)amino)-1-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-yl)propyl)benzoate (61). The compound was synthesized according to Condition A, using bexarotene methyl ester and boc-glycine.



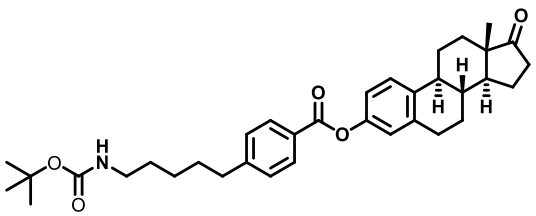
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.3 Hz, 1H), 7.29 (d, *J* = 8.3 Hz, 1H), 7.22 (s, 1H), 7.00 (s, 1H), 4.50 (s, 1H), 4.15 (s, 1H), 3.11 (d, *J* = 6.1 Hz, 1H), 2.23 (d, *J* = 6.8 Hz, 1H), 2.16 (s, 1H), 1.66 (s, 3H), 1.42 (s, 5H), 1.29 (s, 1H), 1.25 (s, 3H), 1.23 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.5, 156.0, 150.6, 143.0, 142.7, 138.01, 133.2, 130.5, 128.7, 128.5, 127.6, 124.6, 79.4, 36.3, 35.6, 35.3, 34.2, 33.9, 32.9, 32.2, 32.1, 32.0, 31.8, 28.5, 26.6, 26.5, 23.0, 19.6. HRMS (ESI) $[M+H]^+$ calcd. 502.2928, found 502.2914. **HRMS (ESI)** $[M+Na]^+$ calcd. 502.2928, found 502.2923.

Isopropyl 2-(4-(3-((tert-butoxycarbonyl)amino)-1-(4-chlorophenyl)propyl)phenoxy)-2-methylpropanoate (62). The compound was synthesized according to Condition A, using protected fenofibrate and boc-glycine.



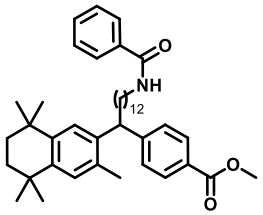
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (d, *J* = 8.4 Hz, 2H), 7.12 (d, *J* = 8.5 Hz, 2H), 7.04 (d, *J* = 8.6 Hz, 2H), 6.76 (d, *J* = 8.6 Hz, 2H), 5.05 (hept, *J* = 6.3 Hz, 1H), 4.47 (s, 1H), 3.86 (t, *J* = 7.8 Hz, 1H), 3.03 (d, *J* = 6.5 Hz, 2H), 2.16 (dd, *J* = 14.5, 7.5 Hz, 2H), 1.42 (s, 9H), 1.19 (d, *J* = 6.3 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 173.8, 156.0, 154.3, 143.2, 137.3, 132.1, 129.2, 128.8, 128.4, 119.3, 79.3, 69.0, 47.5, 39.4, 36.0, 28.5, 25.5, 25.5, 21.7. **HRMS (ESI)** $[M+Na]^+$ calcd. 350.1129, found 350.1122.

(8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl 4-(5-((tert-butoxycarbonyl)amino)pentyl)benzoate (63). The compound was synthesized according to Condition A, using estrone derivative and 4-benzamidobutanoic acid.



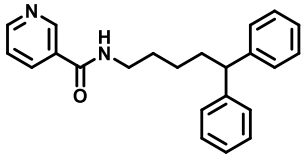
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 8.2 Hz, 2H), 7.31 (dd, J = 14.1, 8.3 Hz, 3H), 7.02 – 6.87 (m, 2H), 4.49 (s, 1H), 3.18 – 3.02 (m, 2H), 3.00 – 2.87 (m, 2H), 2.70 (t, J = 7.6 Hz, 2H), 2.51 (dd, J = 18.8, 8.6 Hz, 1H), 2.47 – 2.38 (m, 1H), 2.37 – 2.25 (m, 1H), 2.21 – 1.92 (m, 4H), δ 1.72 – 1.37 (m, 21H), 0.91 (d, J = 8.5 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.9, 165.6, 156.1, 149.1, 148.9, 138.2, 137.5, 130.4, 128.7, 127.4, 126.6, 121.9, 119.1, 50.6, 48.1, 44.4, 40.6, 38.2, 36.1, 36.0, 35.6, 31.7, 30.9, 30.1, 29.6, 28.6, 26.5, 26.5, 25.9, 21.7, 14.0. **HRMS (ESI)** [M+Na]+ calcd. 582.3190, found 582.3190.

4-(13-benzamido-1-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-yl)tridecyl)benzoic acid (64). The compound was synthesized according to Condition A, using bexarotene methyl ester and 12-benzamidododecanoic acid acid.



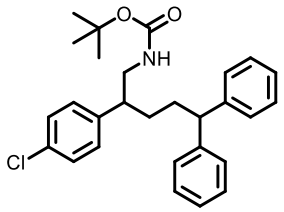
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.3 Hz, 2H), 7.84 – 7.67 (m, 2H), 7.50 – 7.45 (m, 1H), 7.43 – 7.38 (m, 2H), 7.25 (t, *J* = 4.2 Hz, 3H), 6.99 (s, 1H), 6.25 (s, 1H), 4.03 (t, *J* = 7.5 Hz, 1H), 3.44 (dd, *J* = 13.1, 7.1 Hz, 2H), 2.14 (s, 3H), 2.06 – 1.91 (m, 2H), 1.66 – 1.48 (m, 6H), 1.43 – 1.17 (m, 30H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.0, 167.8, 151.9, 142.7, 142.5, 140.0, 139.0, 135.0, 133.3, 131.5, 130.4, 128.7, 128.6, 128.5, 127.1, 127.0, 125.2, 124.7, 120.0, 47.5, 40.4, 36.3, 35.4, 34.2, 34.0, 32.2, 32.2, 32.0, 31.9, 31.1, 29.9, 29.7, 29.7, 29.6, 29.5, 29.5, 28.1, 27.2, 19.7. **HRMS (ESI)** $[M+Na]^+$ calcd. 646.4231, found 646.4231.

***N*-(5,5-diphenylpentyl)nicotinamide (65).** The compound was synthesized according to Condition A, using 1,1-diphenylethylene and picamilon.



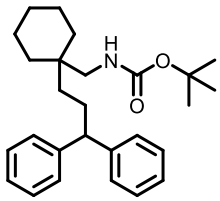
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.88 (s, 1H), 8.66 (d, *J* = 3.4 Hz, 1H), 8.01 (d, *J* = 7.9 Hz, 1H), 7.31 (dd, *J* = 7.7, 4.9 Hz, 1H), 7.28 – 7.19 (m, 8H), 7.18 – 7.12 (m, 2H), 6.37 (s, 1H), 3.88 (t, *J* = 7.8 Hz, 1H), 3.39 (dd, *J* = 13.1, 6.9 Hz, 2H), 2.08 (dd, *J* = 15.5, 7.8 Hz, 2H), 1.71 – 1.56 (m, 2H), 1.42 – 1.25 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 165.7, 152.1, 147.9, 145.0, 135.1, 130.6, 128.6, 127.9, 126.3, 123.5, 51.3, 40.0, 35.2, 29.5, 25.4. **HRMS (ESI)** $[M+H]^+$ calcd. 345.1961, found 345.1949.

Tert-butyl (2-(4-chlorophenyl)-5,5-diphenylpentyl)carbamate (Baclofen, 66). The compound was synthesized according to Condition A, using 1,1-diphenylethylene and 4-((tert-butoxycarbonyl)amino)-3-(4-chlorophenyl)butanoic acid.



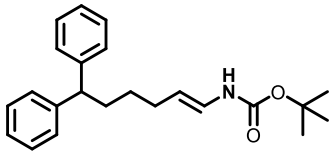
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27-7.20 (m, 6H), δ 7.16-7.10 (m, 6H), 7.02 (d, *J* = 8.3 Hz, 2H), δ 4.29 (br, 1H), δ 3.80 (t, *J* = 7.8 Hz, 1H), δ 3.40-3.32 (m, 1H), δ (ddd, *J* = 13.7, 8.9, 5.1 Hz, 1H), δ 2.79-2.70 (m, 1H), δ 2.03-1.74 (m, 2H), δ 1.66-1.58 (m, 2H), δ 1.37 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 155.8, 144.9, 144.4, 132.4, 129.2, 128.8, 128.4, 127.8, 127.7, 126.2, 126.2, 79.3, 51.5, 46.2, 45.8, 33.3, 31.8, 28.3. **HRMS (ESI)** $[M+H]^+$ calcd. 472.2014, found 472.1998.

Tert-butyl ((1-(3,3-diphenylpropyl)cyclohexyl)methyl)carbamate (from 67). The compound was synthesized according to Condition A, using 1,1-diphenylethylene and boc-protected Gabapentin.



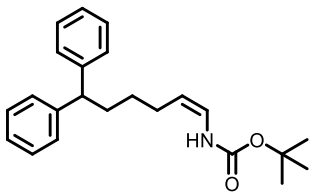
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.20 (m, 8H), 7.18 – 7.12 (m, 2H), 4.25 (s, 1H), 3.78 (t, *J* = 7.7 Hz, 1H), 3.02 (d, *J* = 6.3 Hz, 2H), 2.02 – 1.90 (m, 2H), 1.43 (s, 11H), 1.31 (d, *J* = 6.8 Hz, 4H), 1.25 – 1.12 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.3, 145.2, 128.6, 127.9, 126.3, 79.0, 52.3, 46.8, 36.3, 35.4, 33.6, 29.1, 28.6, 26.5, 26.3, 21.9, 21.5. **HRMS (ESI)** $[M+H]^+$ calcd. 408.2897, found 408.2889.

Tert-butyl (E)-(6,6-diphenylhex-1-en-1-yl)carbamate (68a). The compound was synthesized according to Condition A, using 1,1-diphenylethylene and 2-((*tert*-butoxycarbonyl)amino)-2-cyclopropylacetic acid.



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.20 (m, 8H), 7.19 – 7.12 (m, 2H), 6.38 (t, *J* = 9.6 Hz, 1H), 6.03 (d, *J* = 9.3 Hz, 1H), 4.51 (d, *J* = 7.6 Hz, 1H), 3.88 (t, *J* = 7.8 Hz, 1H), 2.06 (dd, *J* = 15.6, 7.8 Hz, 2H), 1.93 (qd, *J* = 7.3, 1.4 Hz, 2H), 1.47 (s, 9H), 1.41 (t, *J* = 5.0 Hz, 1H), 1.39 – 1.30 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 152.9, 145.2, 128.6, 128.0, 126.3, 122.4, 107.9, 51.4, 35.3, 28.6, 28.4, 28.0, 25.5. **HRMS (ESI)** $[M+Na]^+$ calcd. 374.2090, found 374.2082.

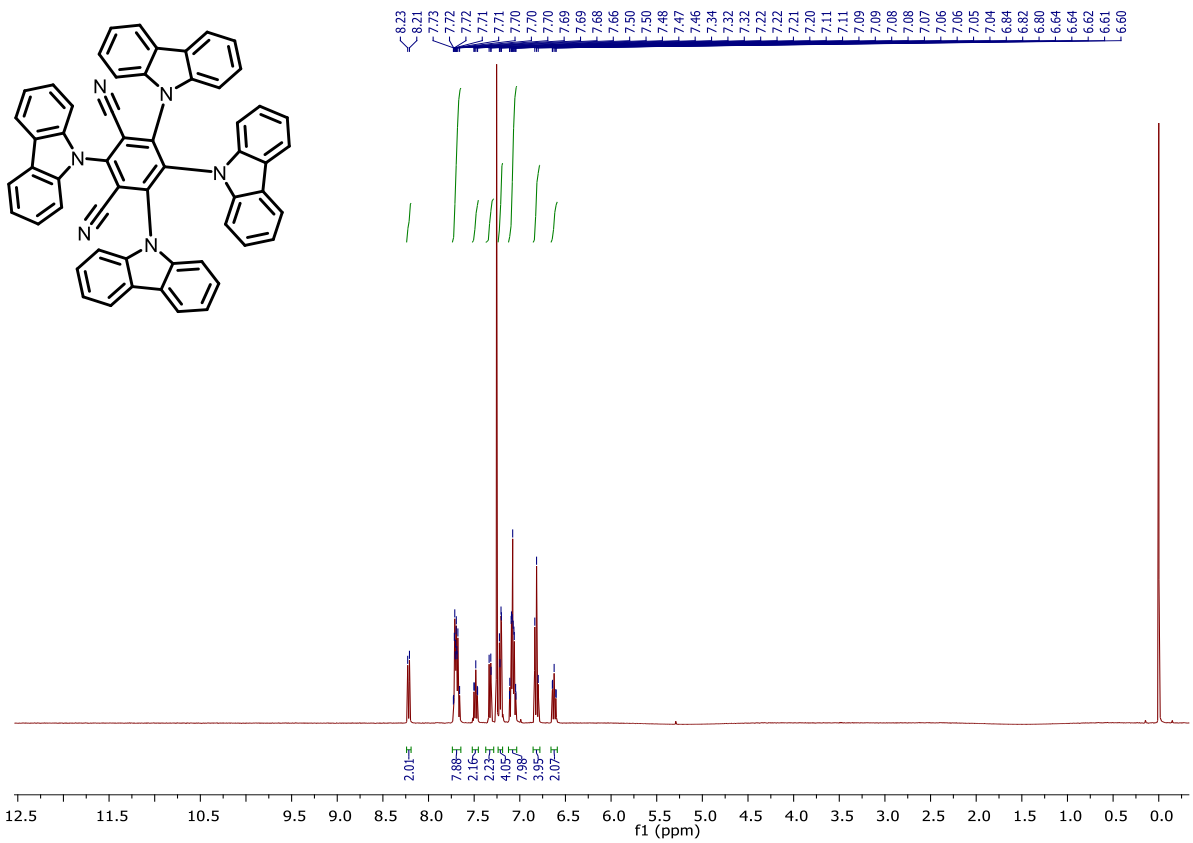
Tert-butyl (Z)-(6,6-diphenylhex-1-en-1-yl)carbamate (68b). The compound was synthesized according to Condition A, using 1,1-diphenylethylene and 2-((*tert*-butoxycarbonyl)amino)-2-cyclopropylacetic acid.

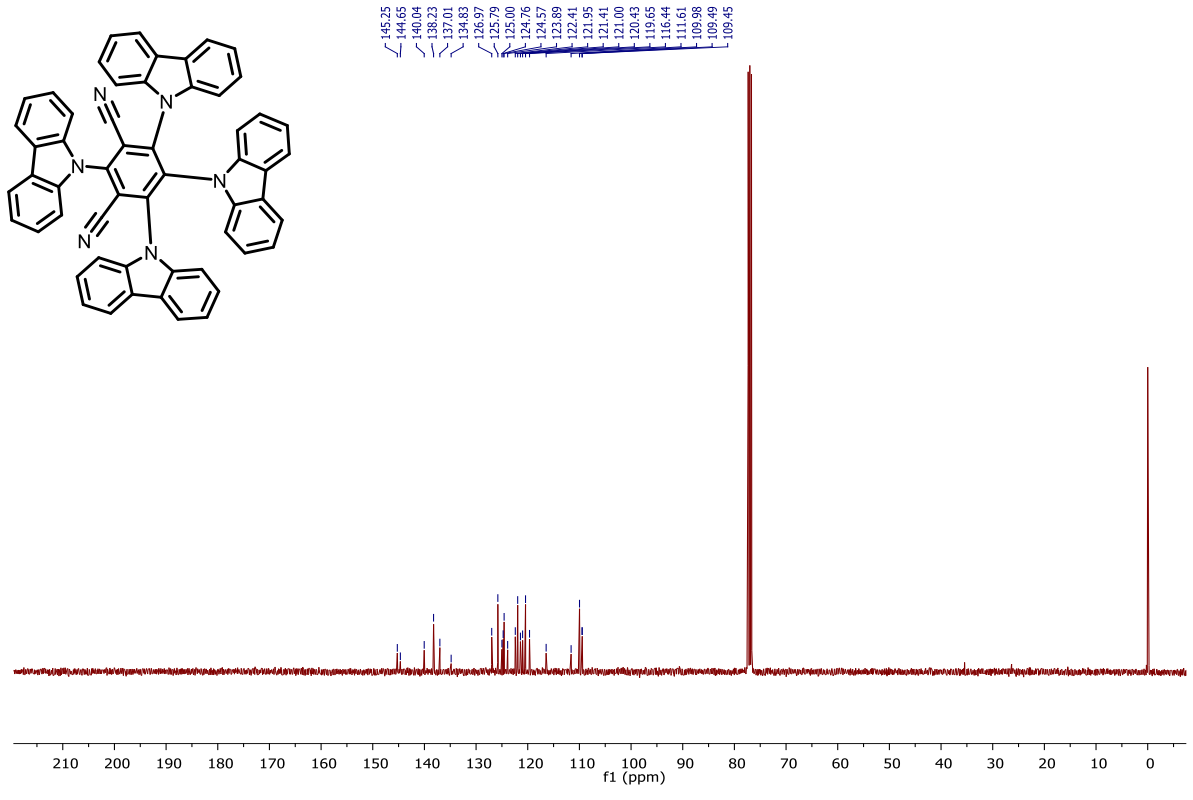


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.18 (m, 8H), 7.18 – 7.11 (m, 2H), 6.40 (t, *J* = 11.8 Hz, 1H), 6.03 (d, *J* = 8.8 Hz, 1H), 4.94 – 4.68 (m, 1H), 3.86 (t, *J* = 7.8 Hz, 1H), 2.02 (tt, *J* = 10.0, 7.5 Hz, 4H), 1.45 (s, 9H), 1.37 – 1.24 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 145.3, 128.5, 128.0, 126.2, 123.9, 109.6, 51.4, 35.3, 29.8, 28.7, 28.4. **HRMS (ESI)** $[M+Na]^+$ calcd. 374.2090, found 374.2082.

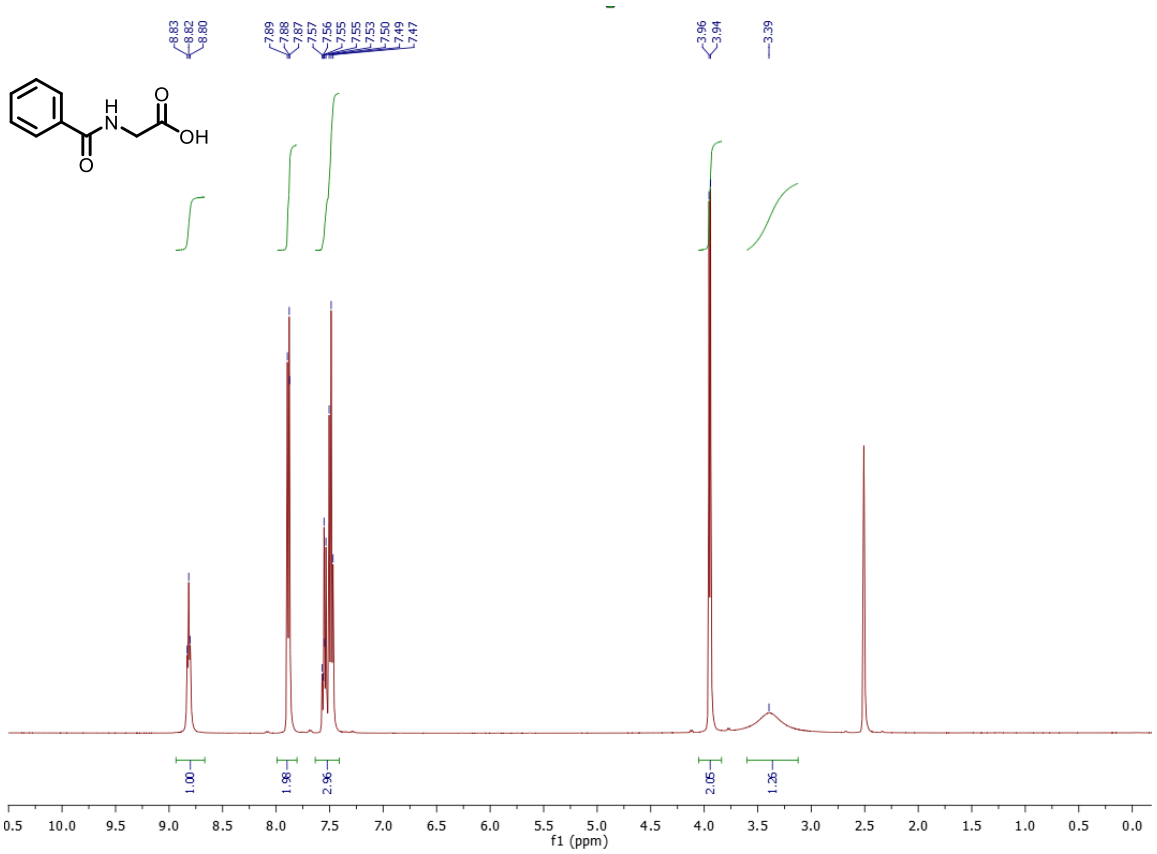
6. Copies of the NMR Spectra

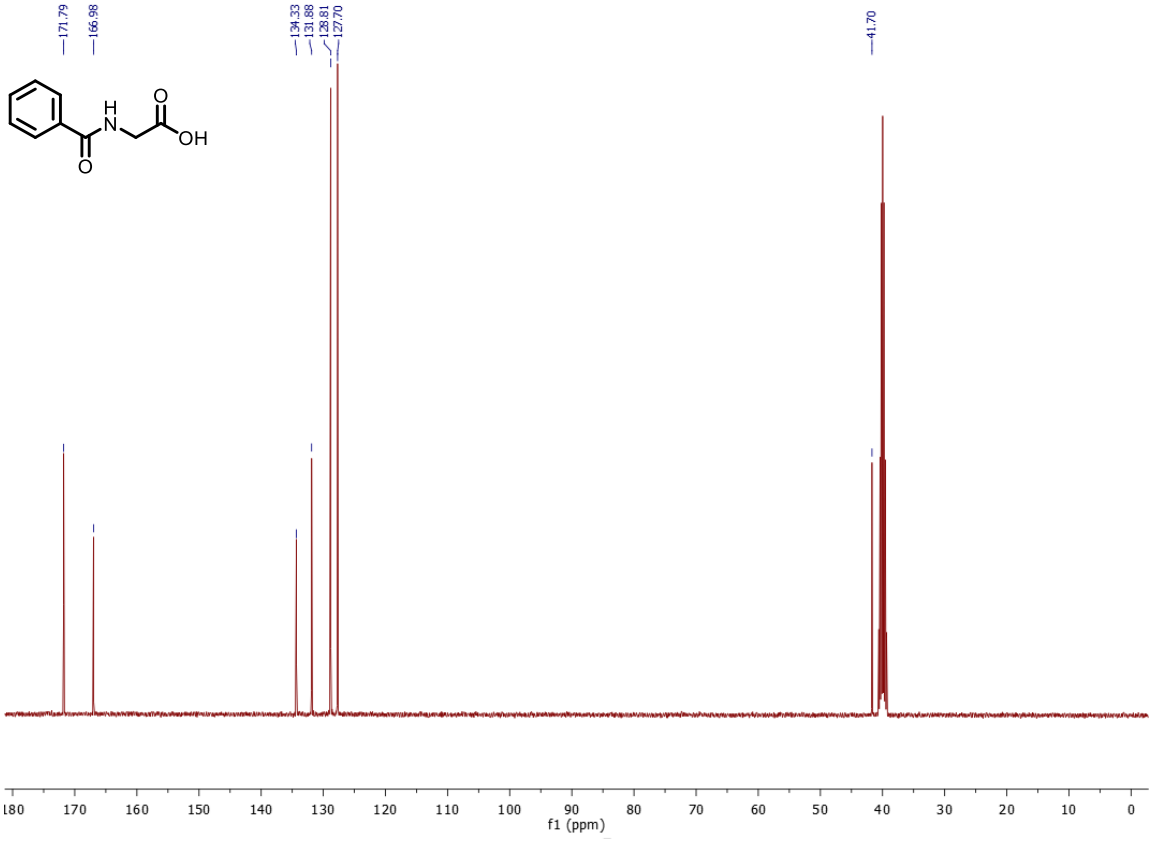
4CzIPN



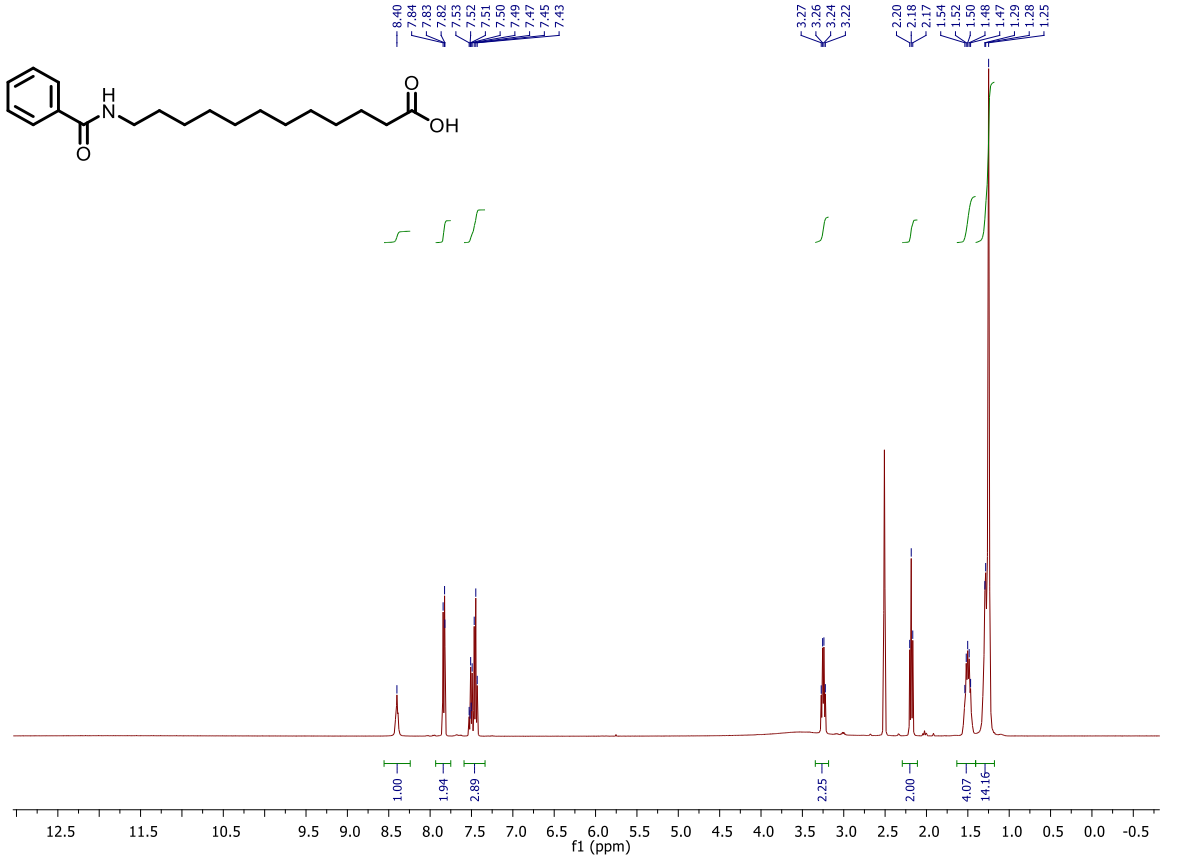


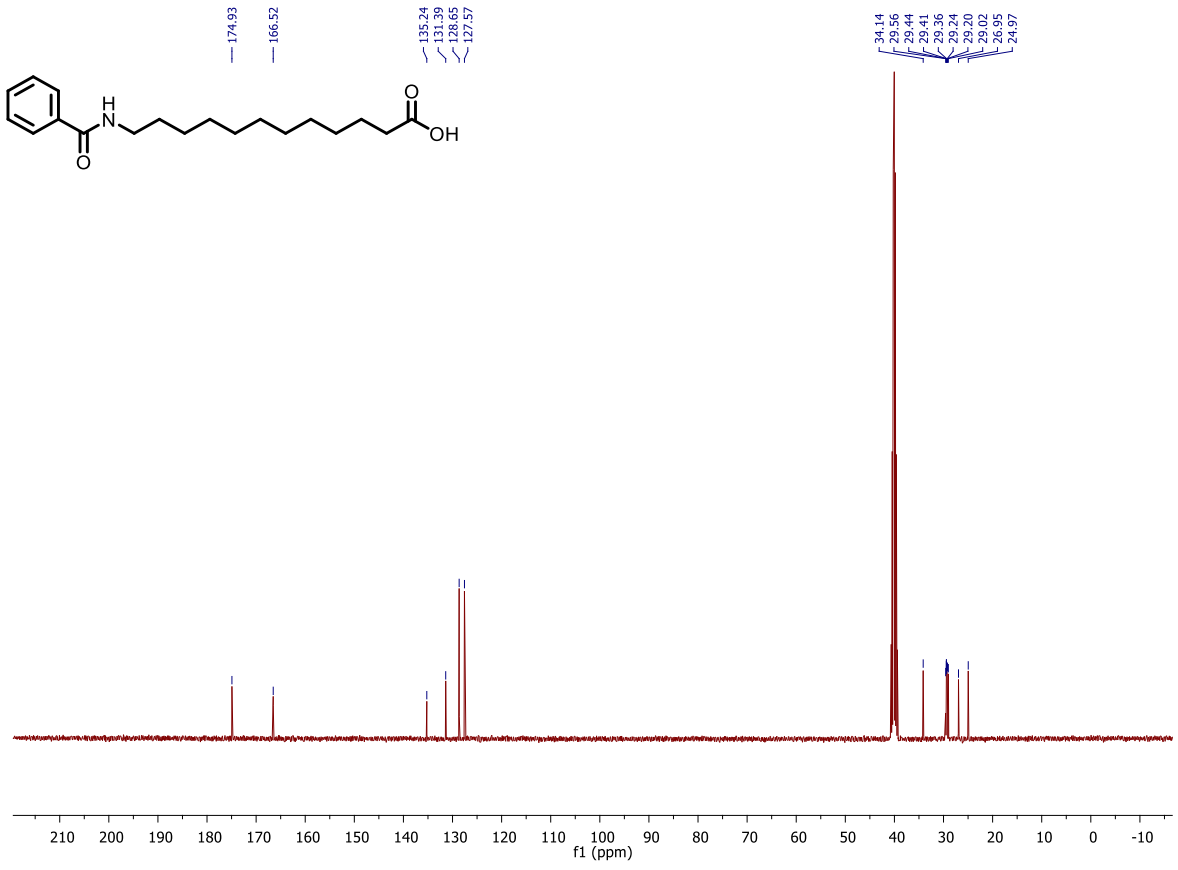
Benzoyl glycine



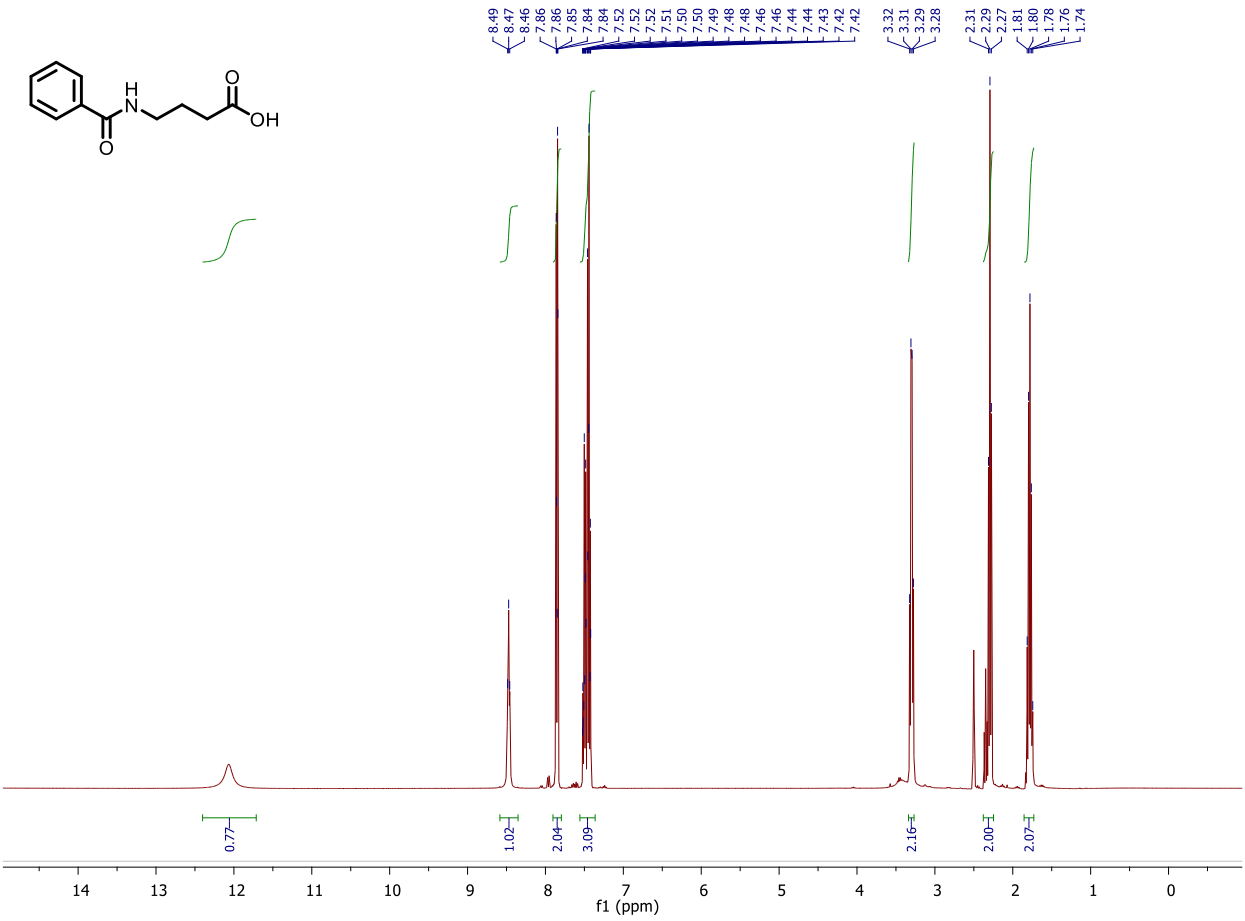


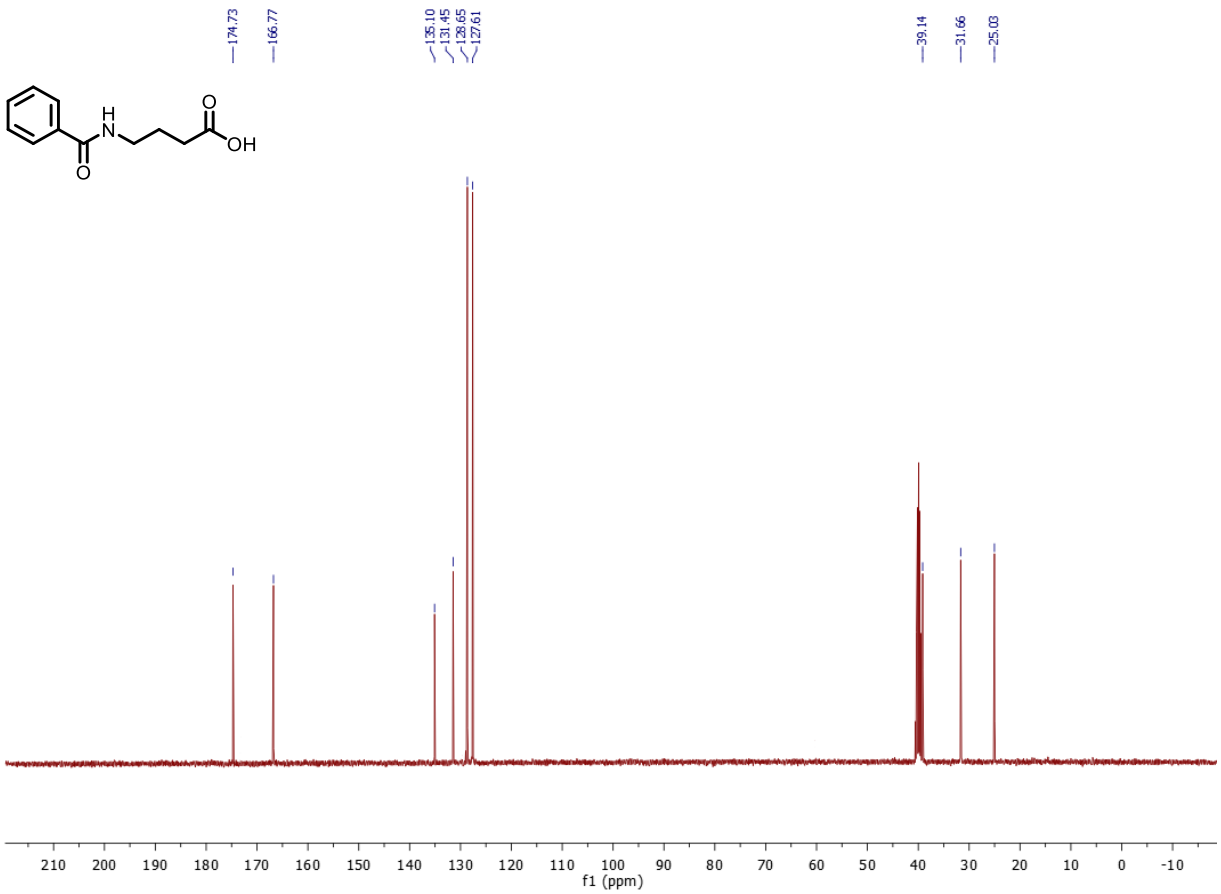
12-(Benzoylamino)dodecanoic acid



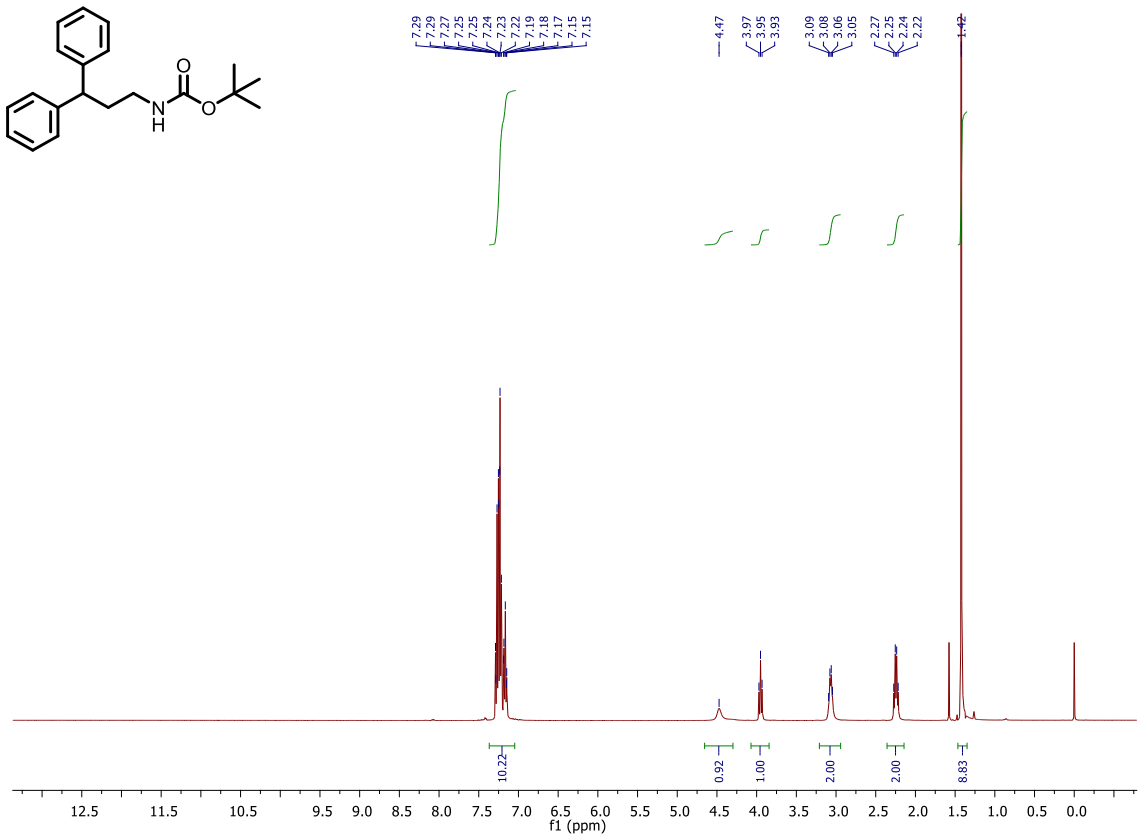


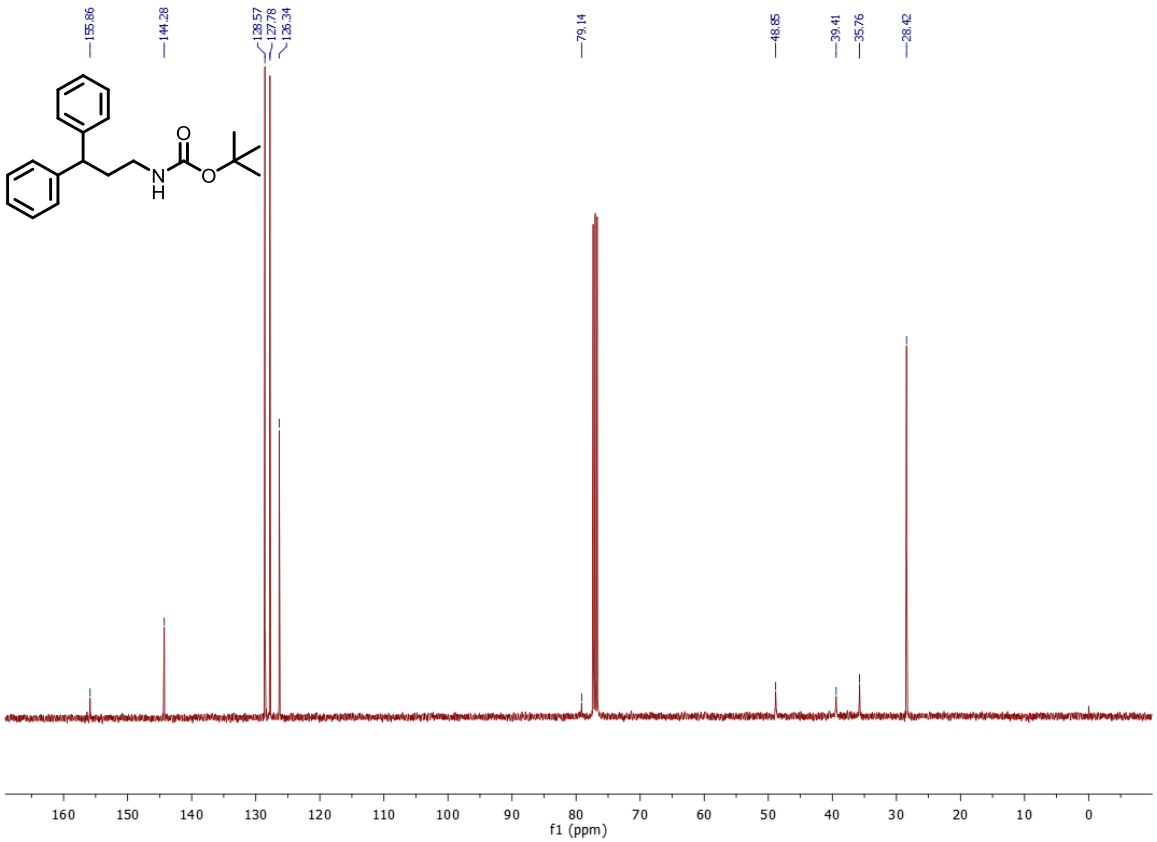
4-(Benzoylamino)butanoic acid



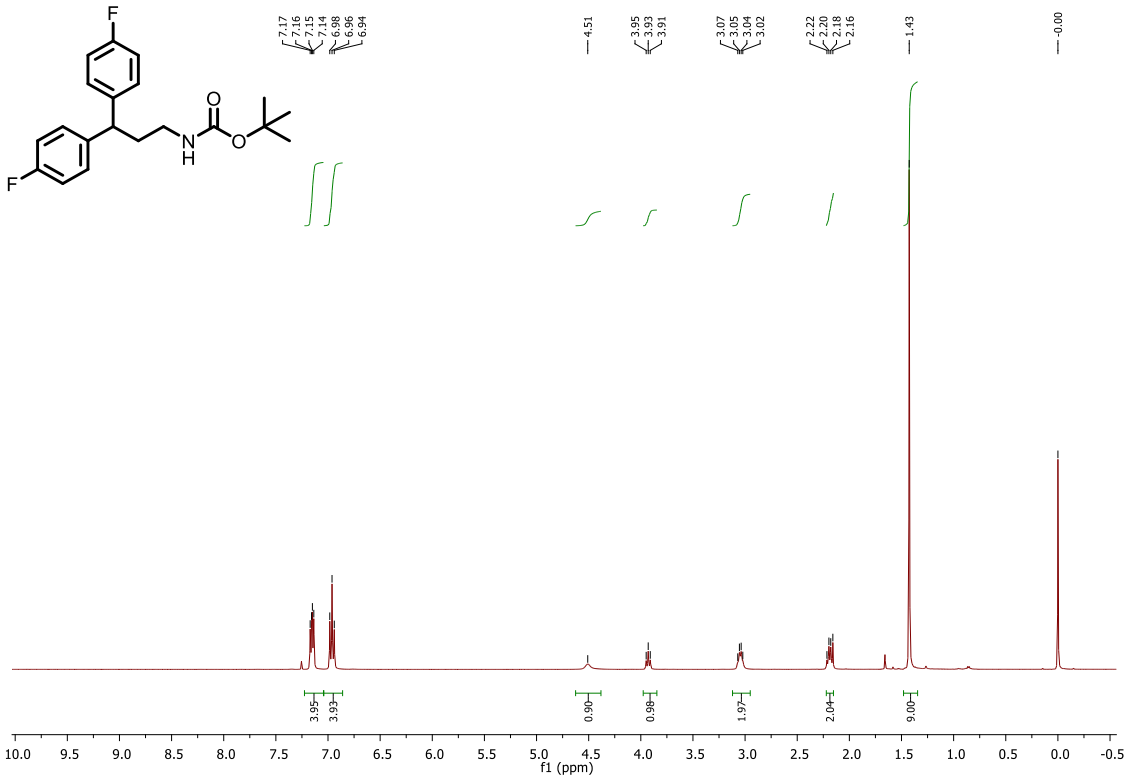


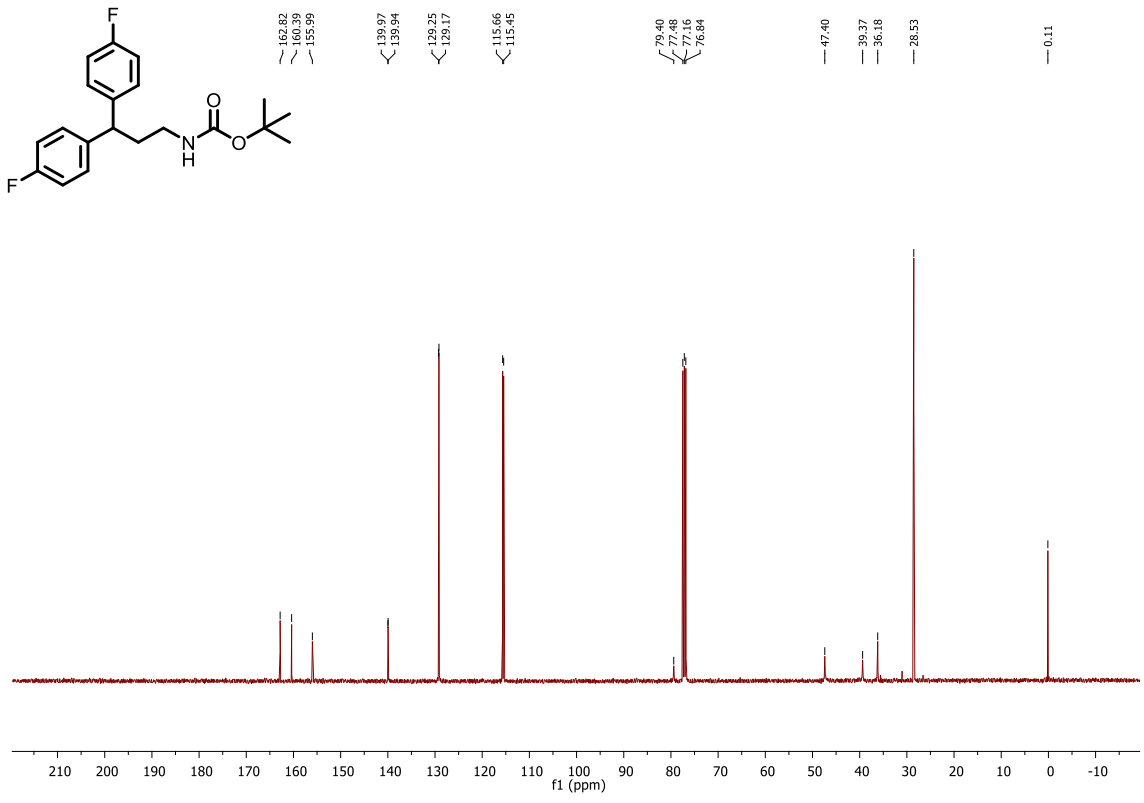
Tert-butyl (3,3-diphenylpropyl)carbamate (from 3)

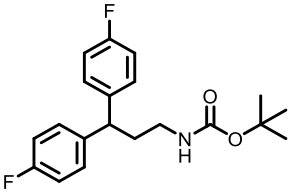




Tert-butyl (3,3-bis(4-fluorophenyl)propyl)carbamate (from 4)

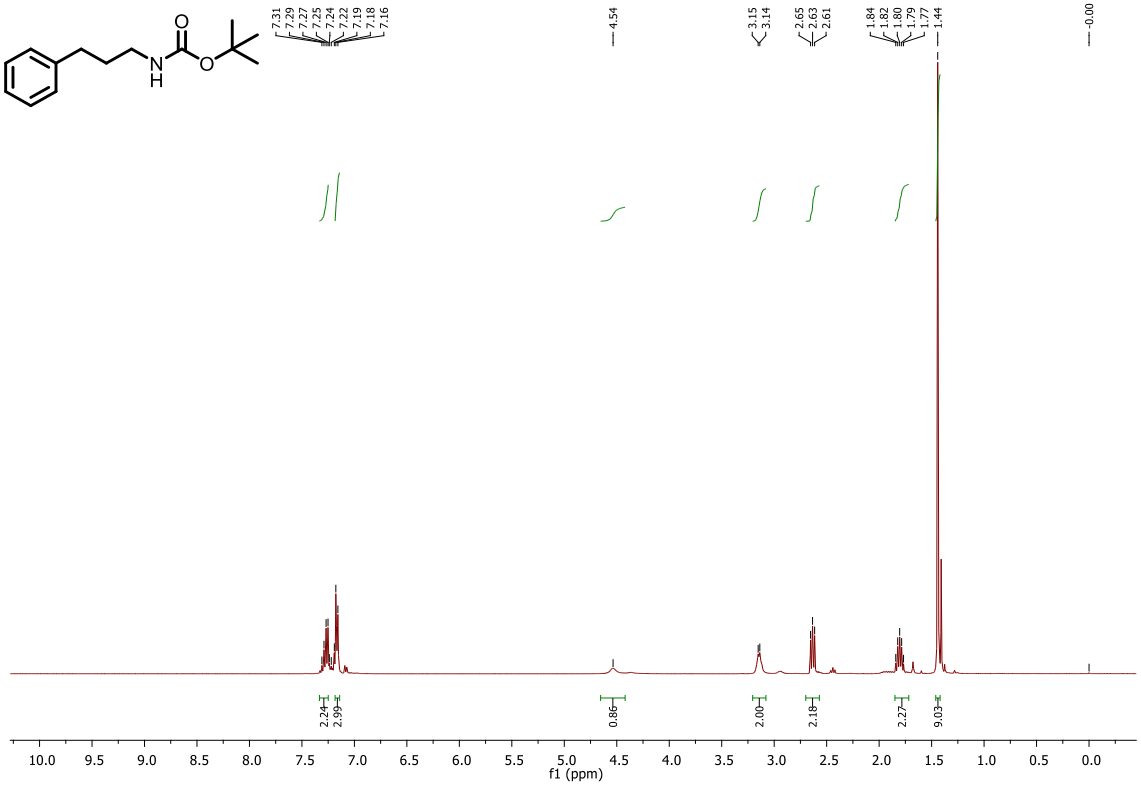


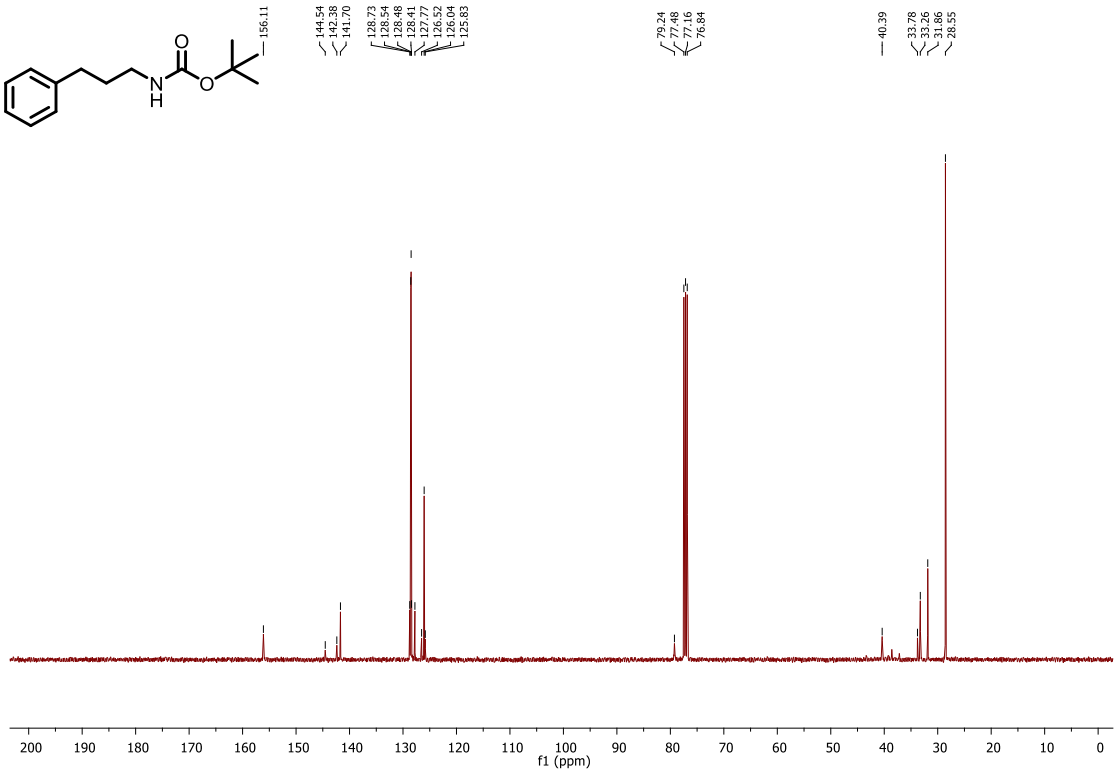



F
O
N
H
O
F

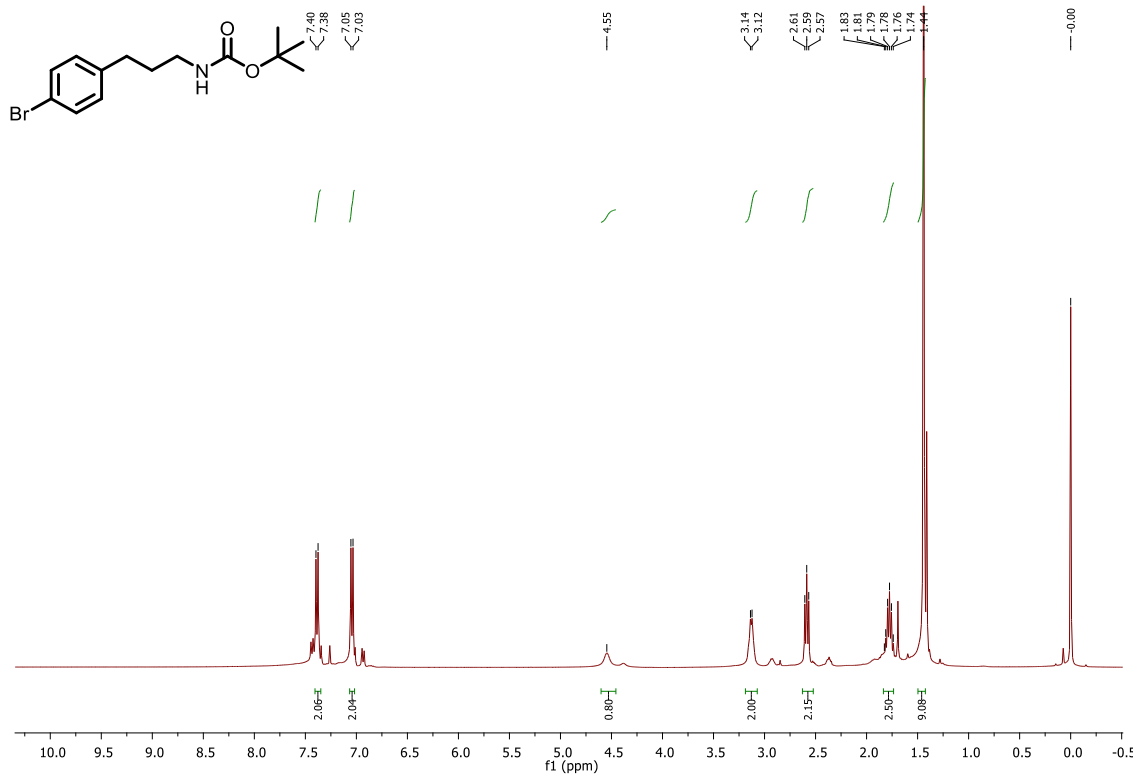
-116.65
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

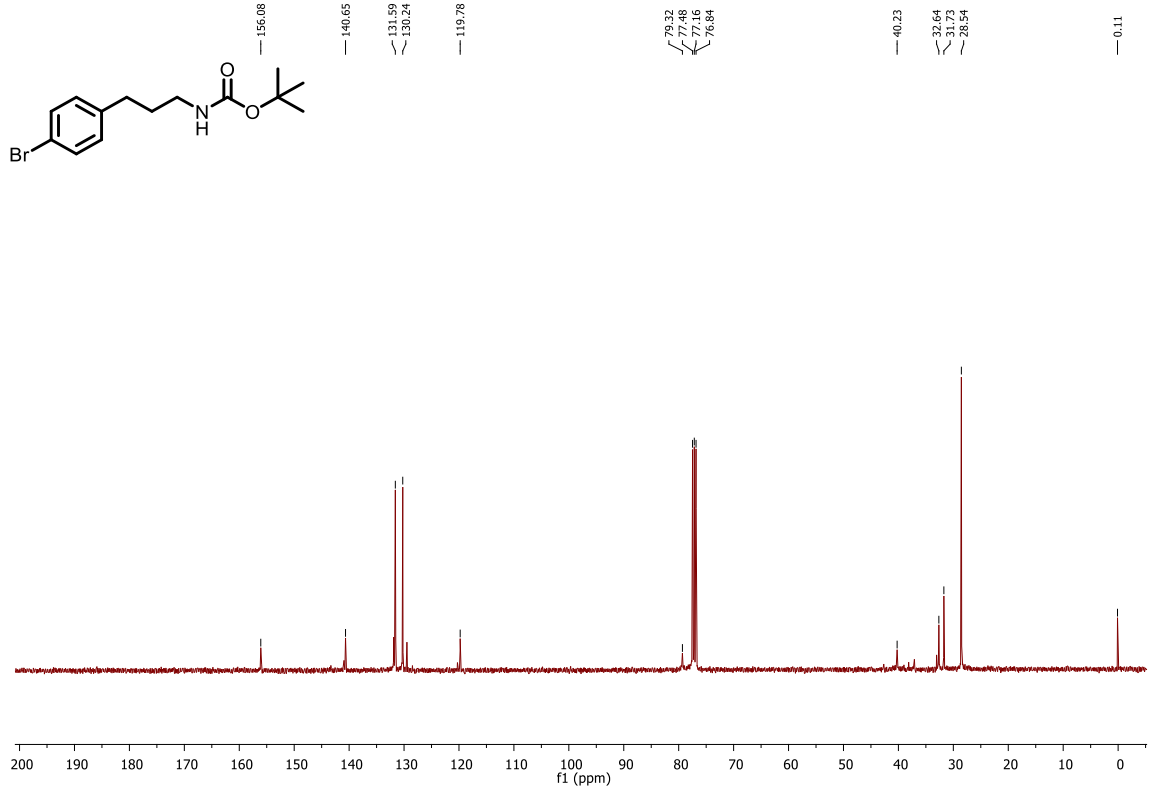
Tert-butyl (3-phenylpropyl)carbamate (from 5)



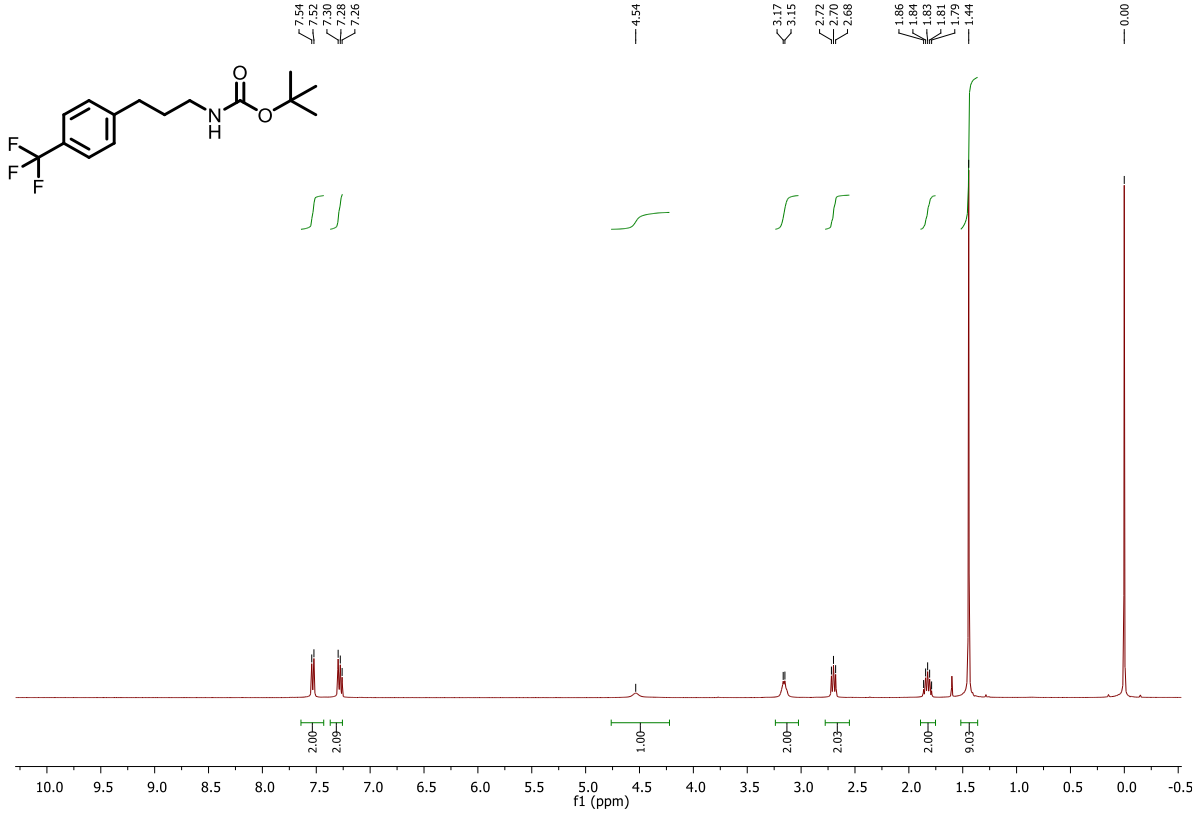


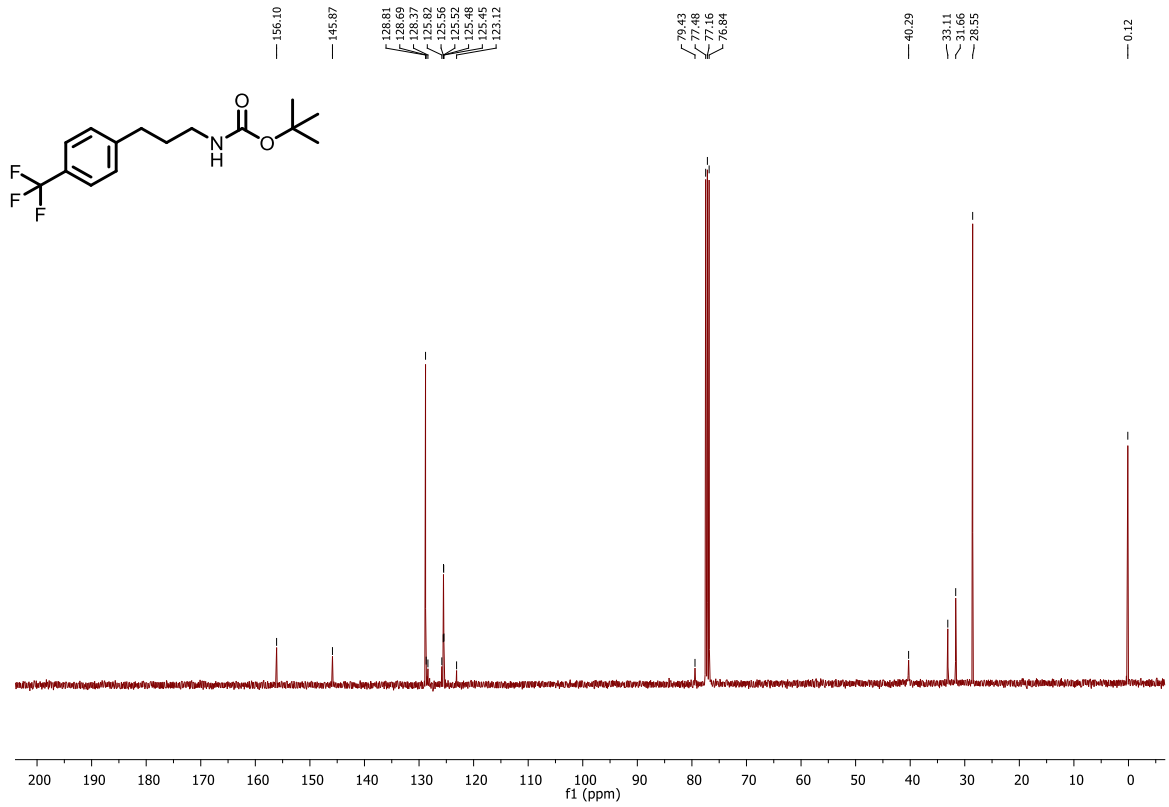
Tert-butyl (3-(4-bromophenyl)propyl)carbamate (from 6)

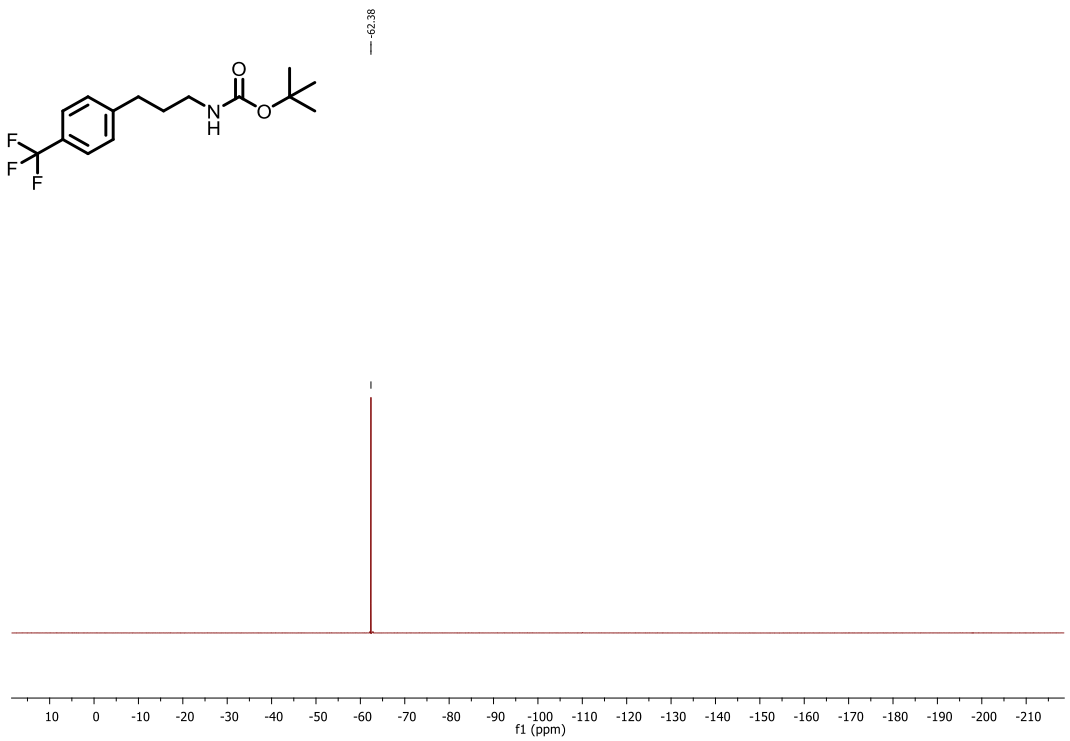




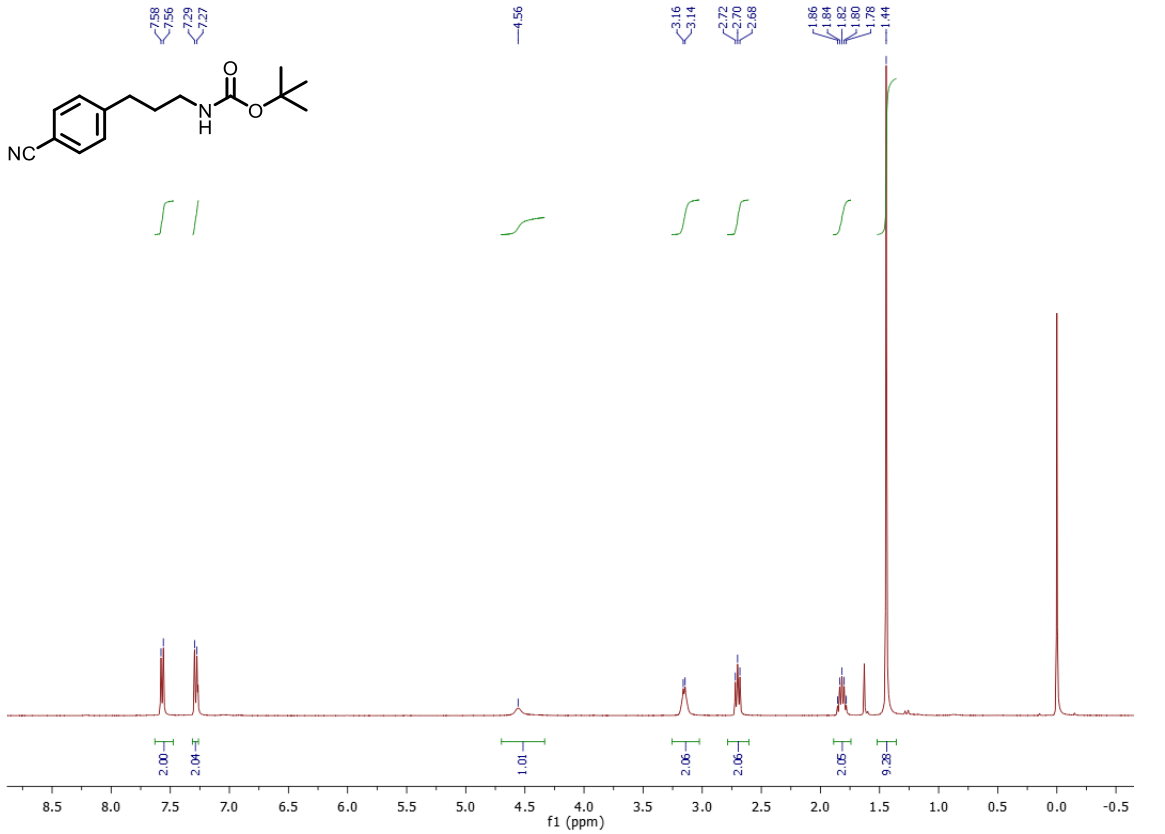
Tert-butyl (3-(4-(trifluoromethyl)phenyl)propyl)carbamate (from 7)

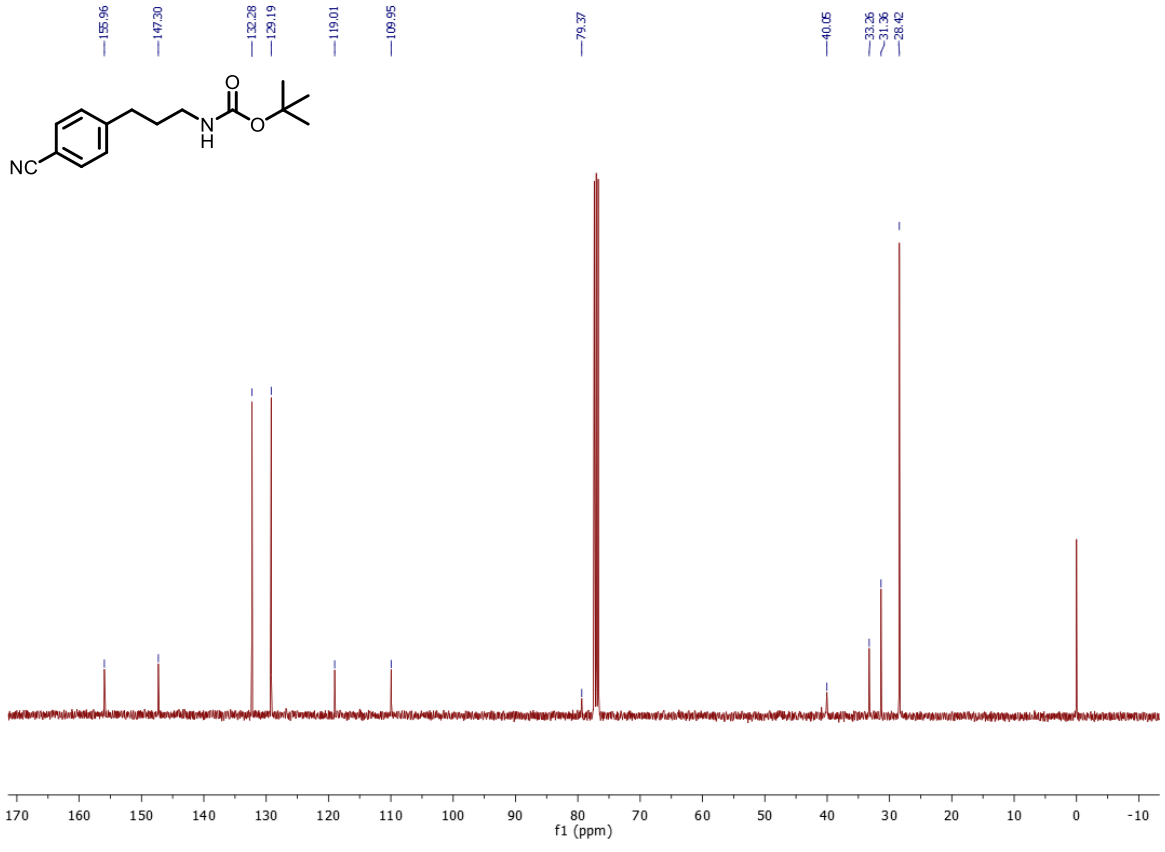




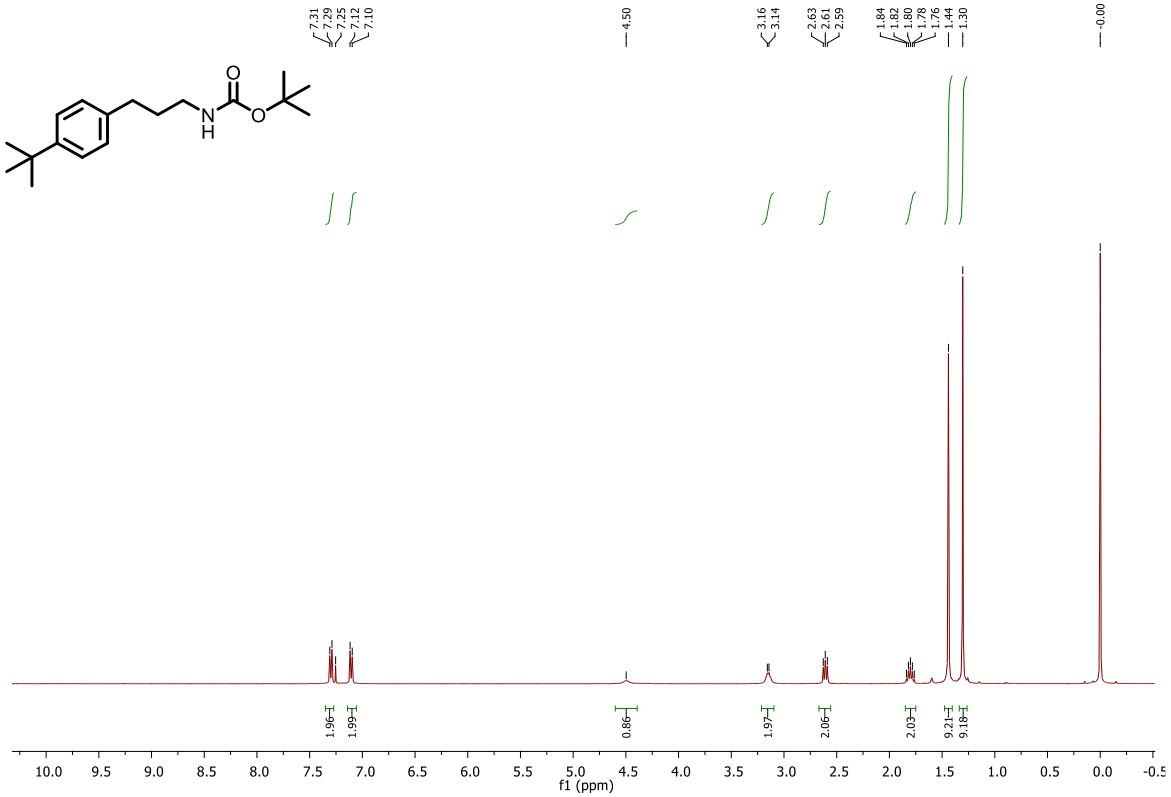

-62.38
O
N
H
O
F
F
F
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

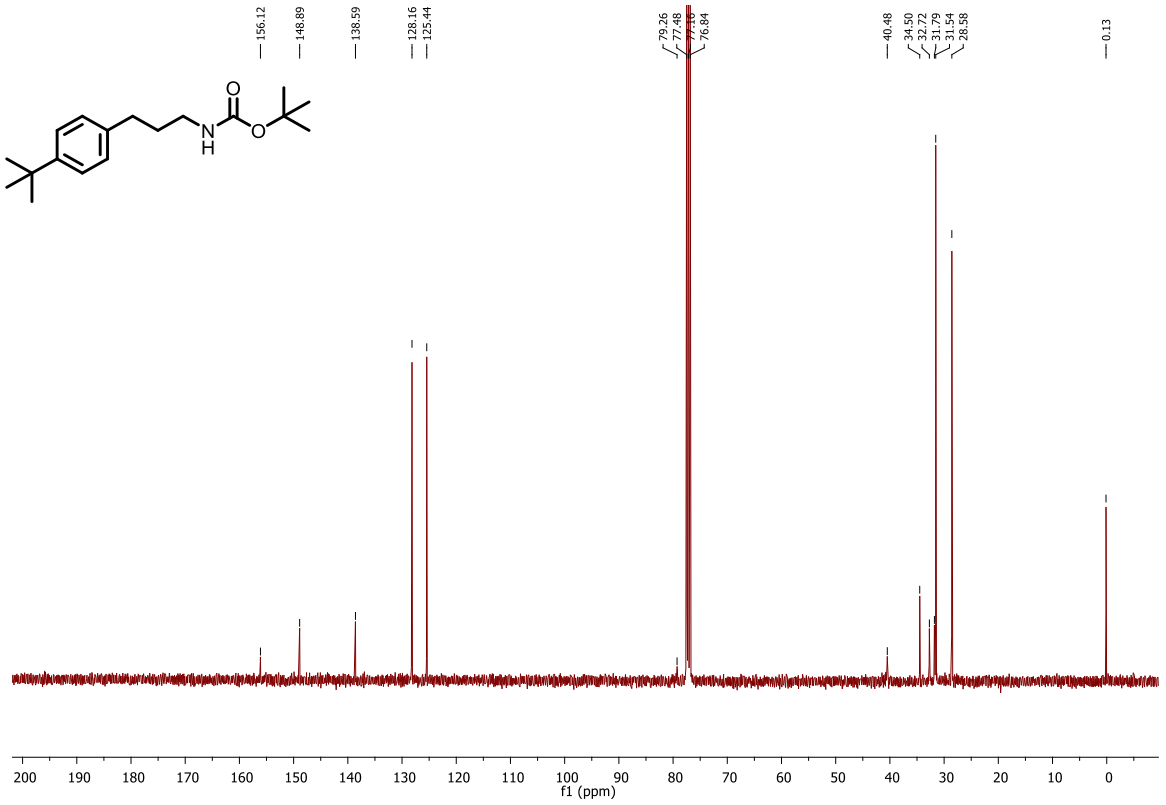
Tert-butyl (3-(4-cyanophenyl)propyl)carbamate (from 8)



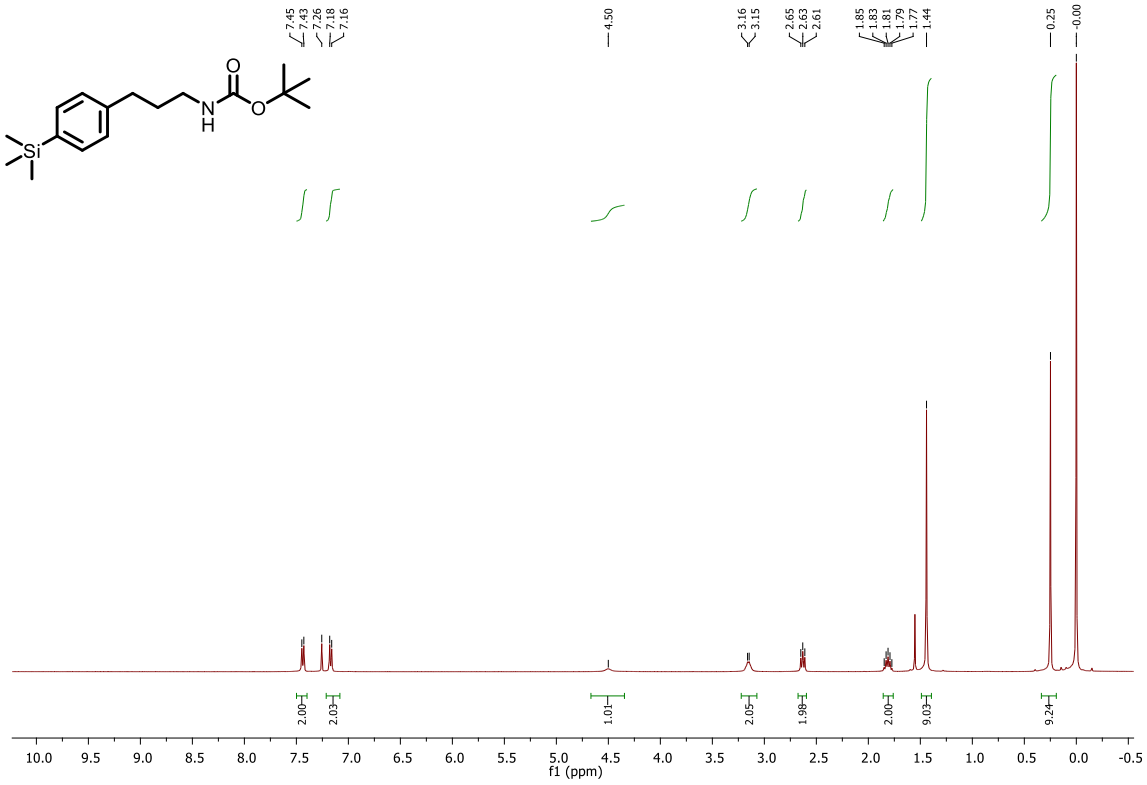


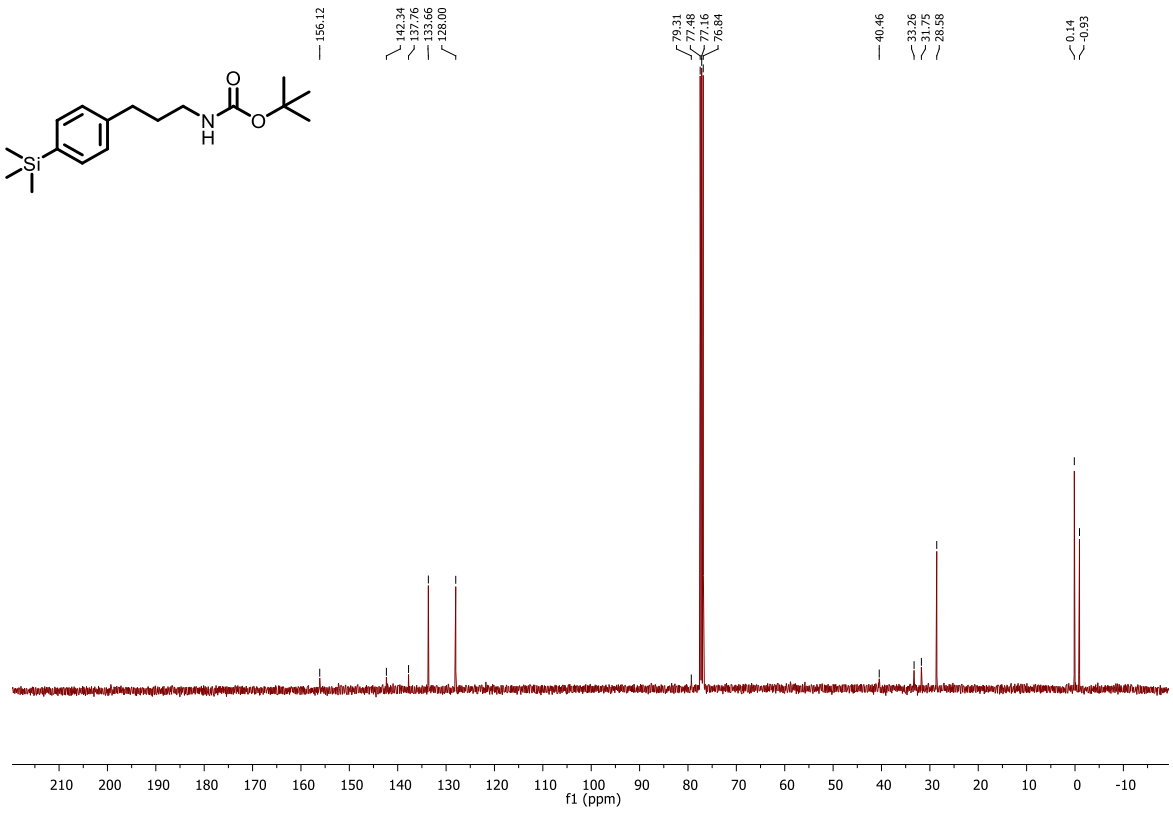
Tert-butyl (3-(4-(tert-butyl)phenyl)propyl)carbamate (from 9)



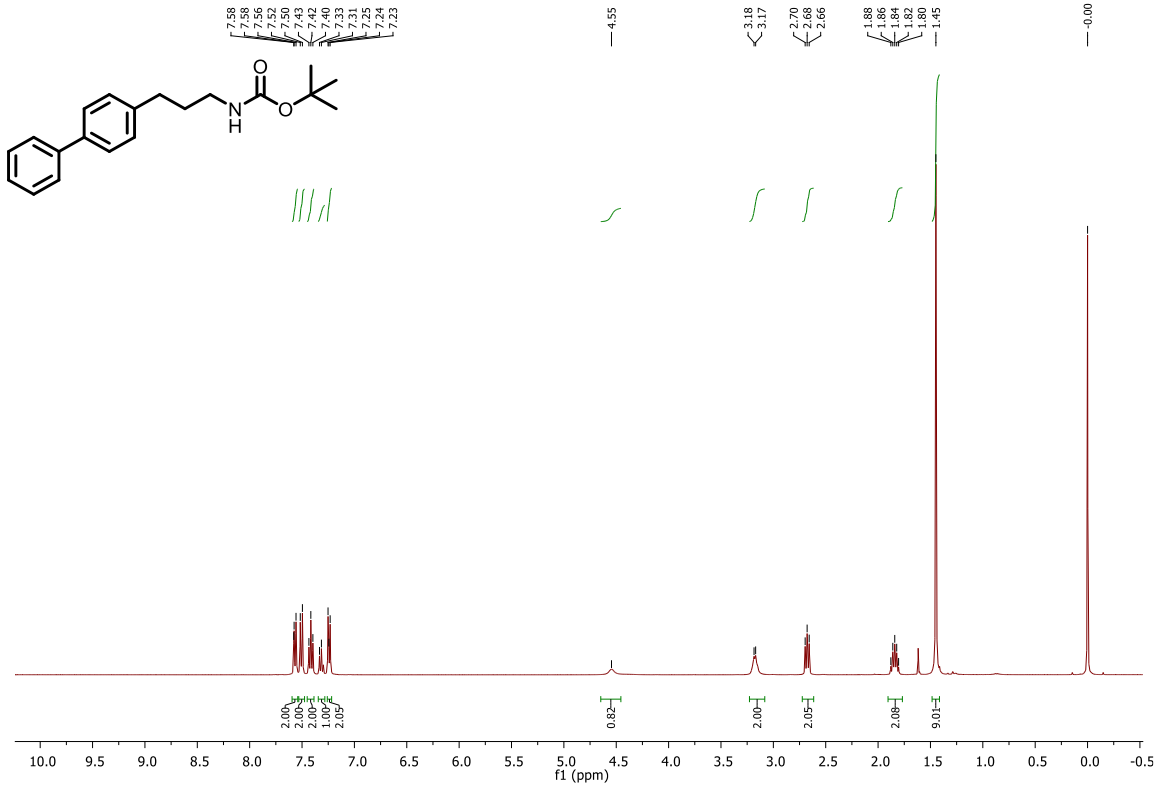


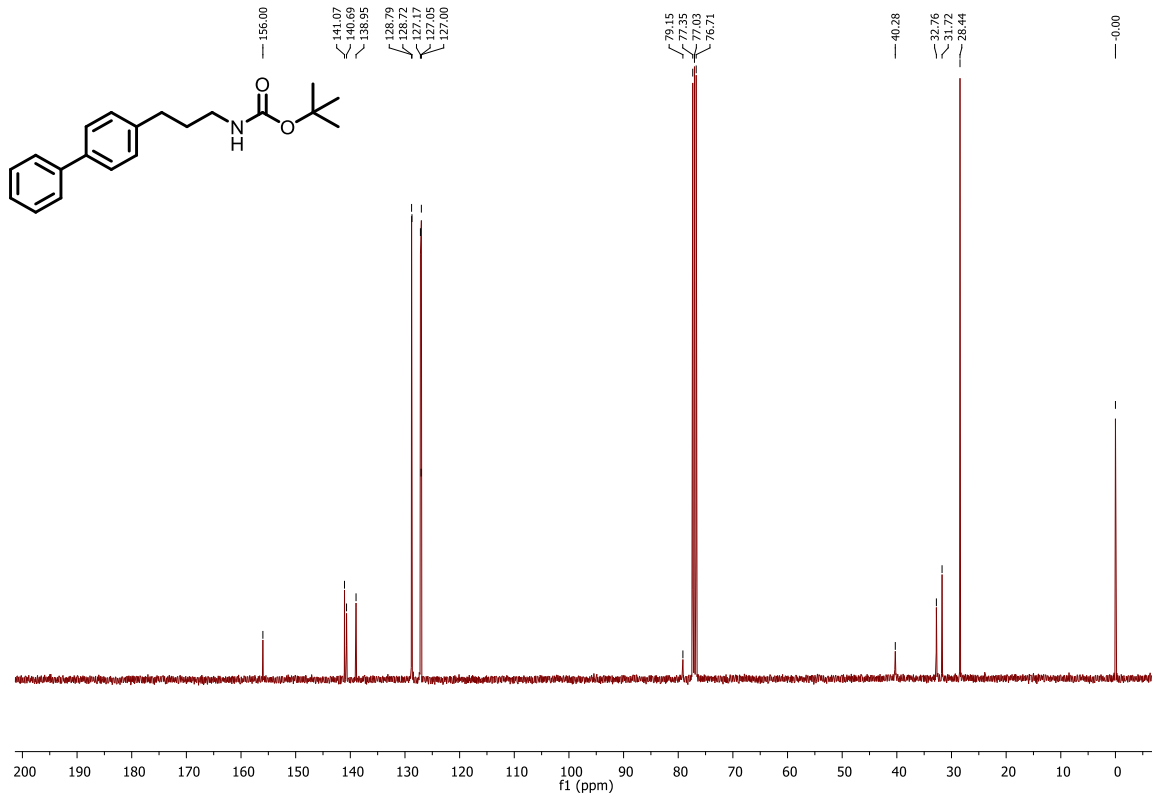
Tert-butyl (3-(4-(trimethylsilyl)phenyl)propyl)carbamate (from 10)



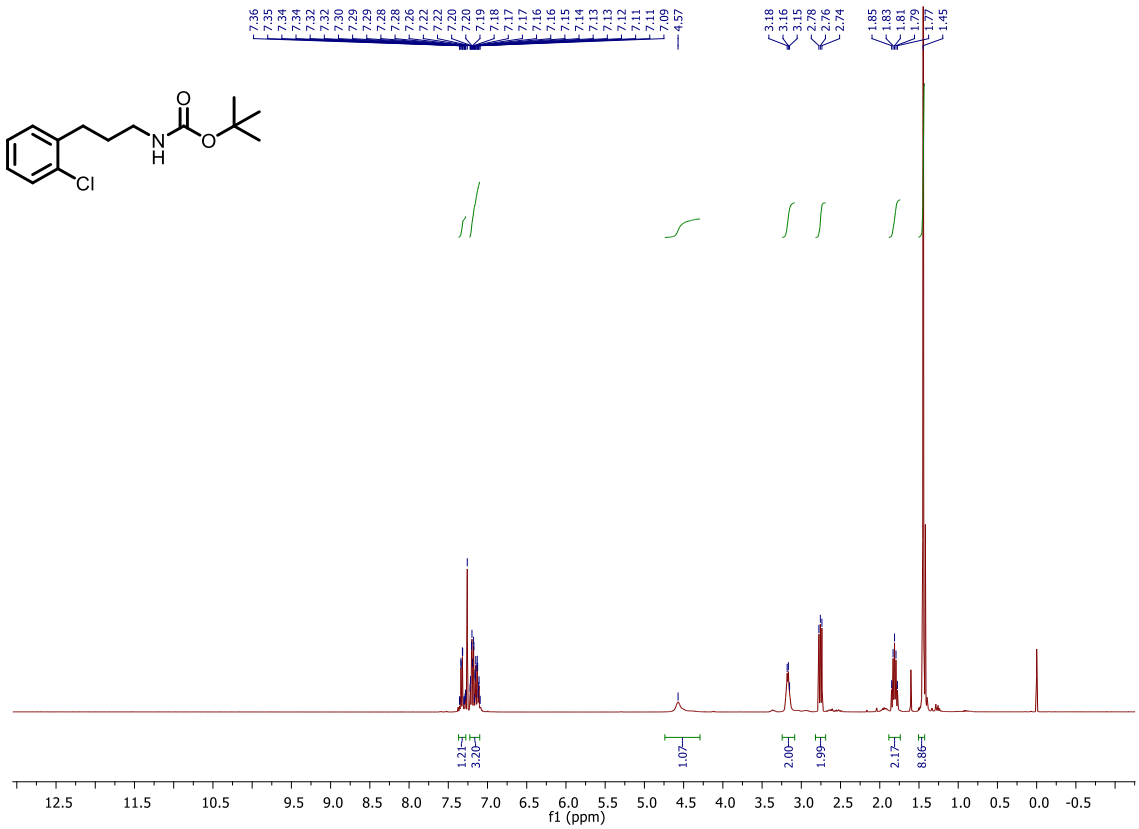


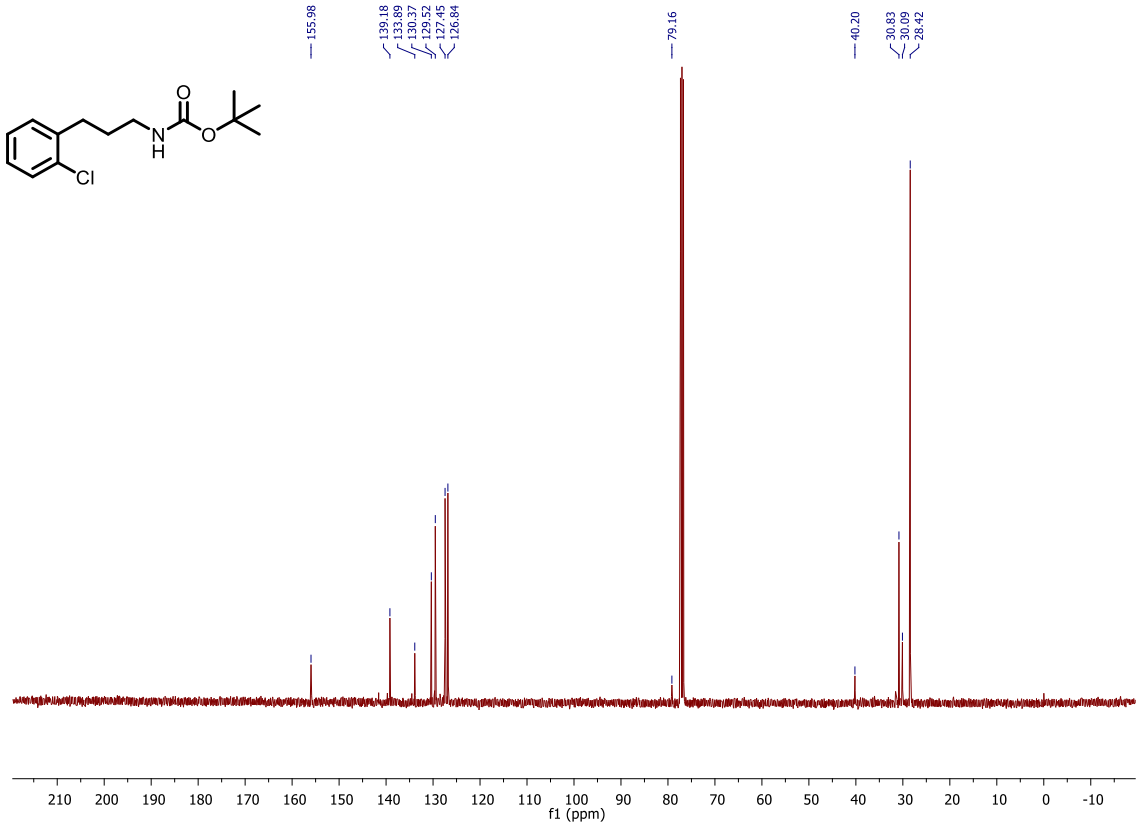
Tert-butyl (3-([1,1'-biphenyl]-4-yl)propyl)carbamate (from 11)



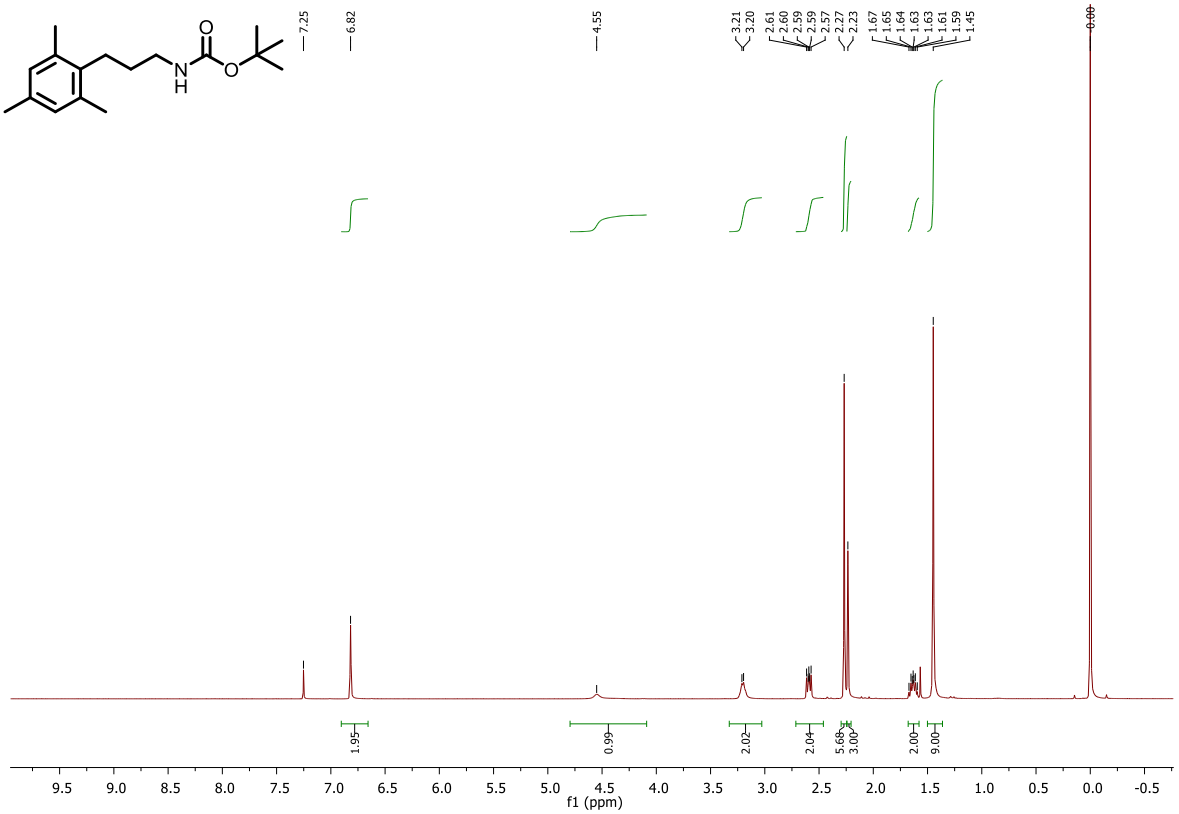


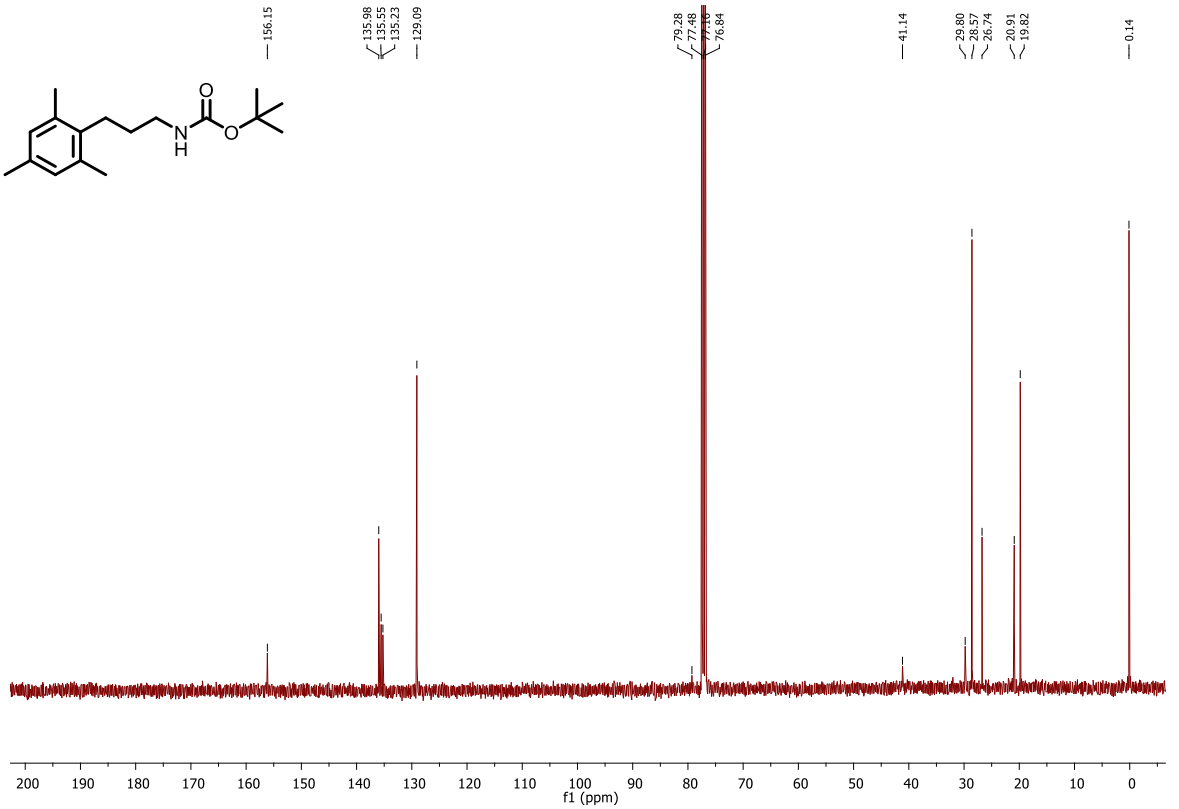
Tert-butyl (3-(2-chlorophenyl)propyl)carbamate (from 12)



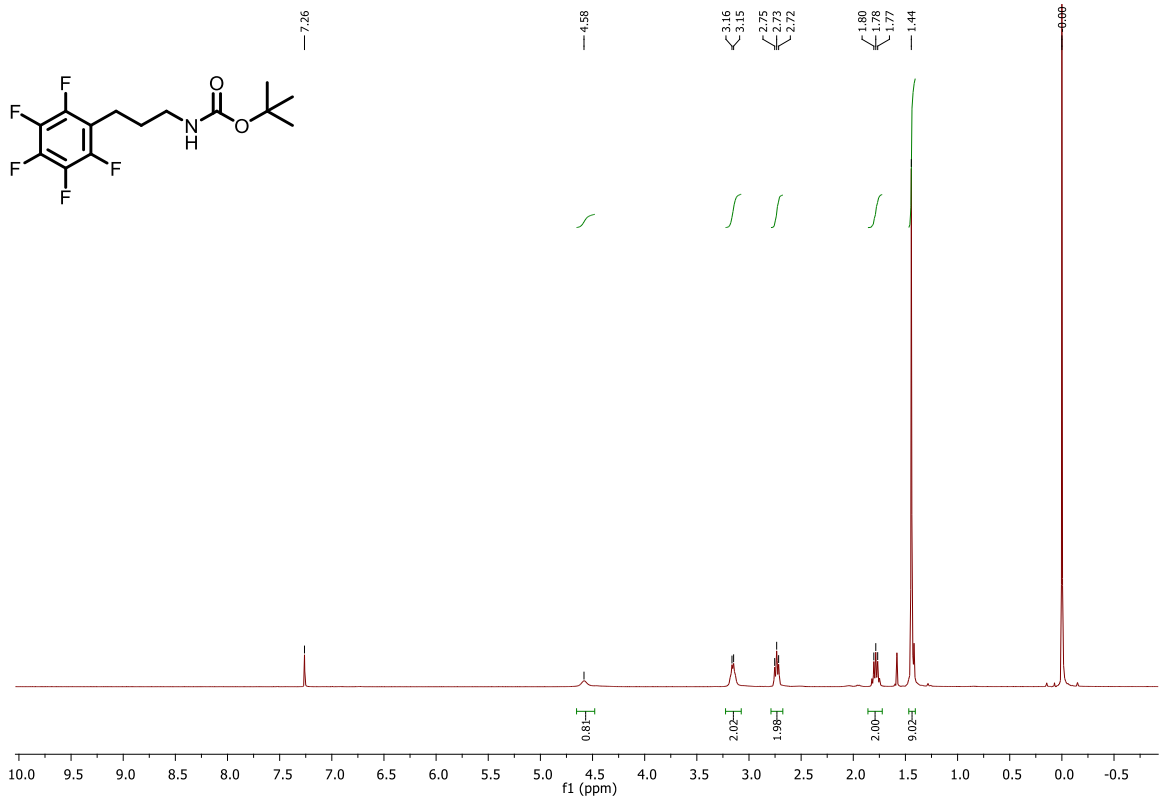


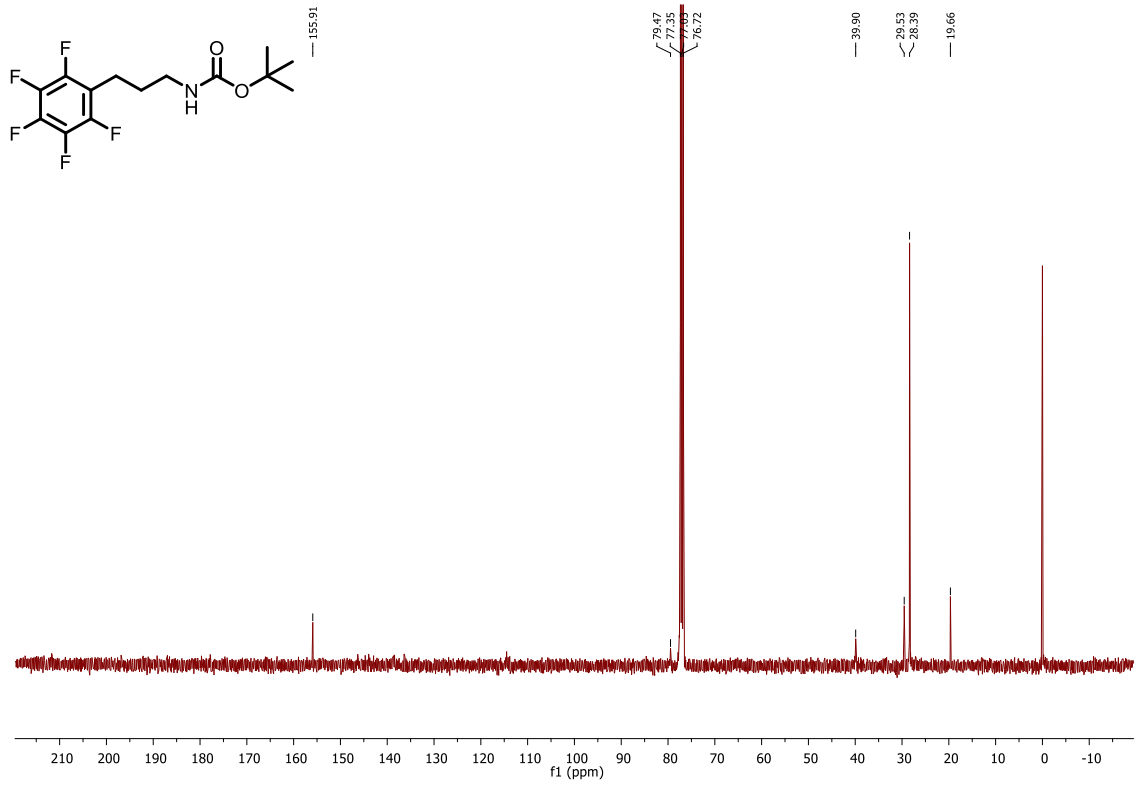
Tert-butyl (3-mesitylpropyl)carbamate (from 13)

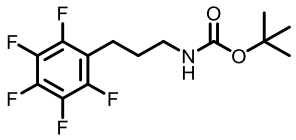




Tert-butyl (3-(perfluorophenyl)propyl)carbamate (from 14)

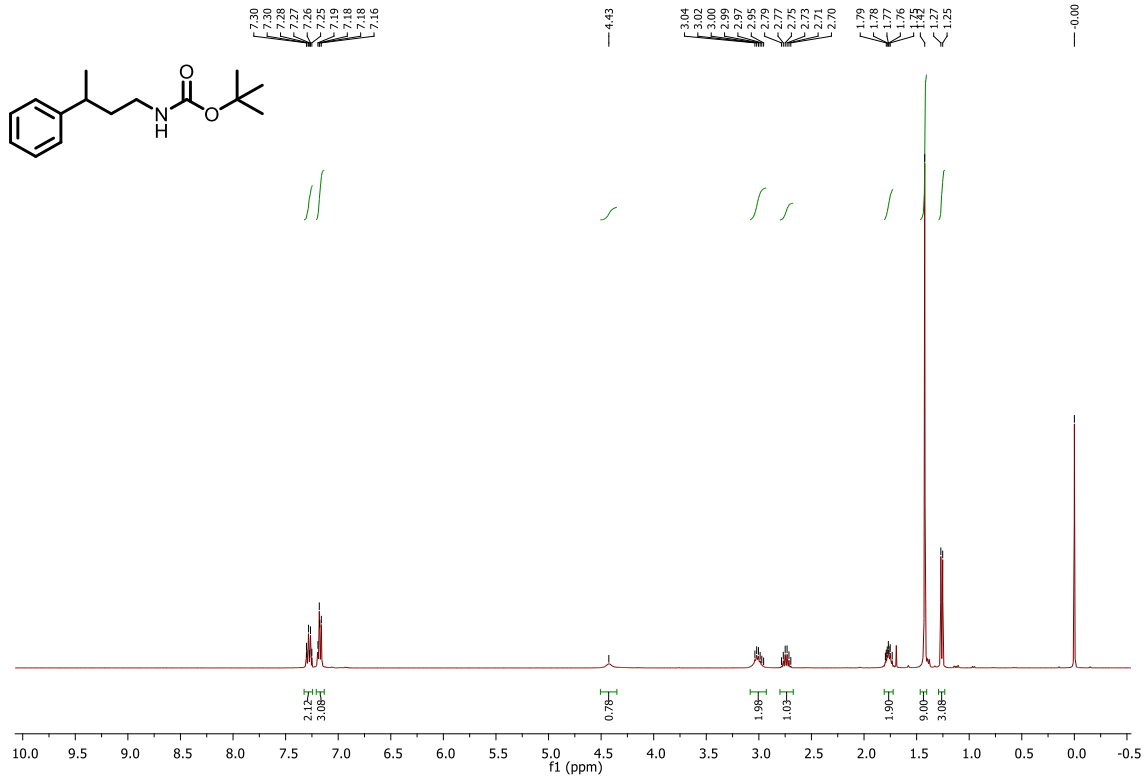


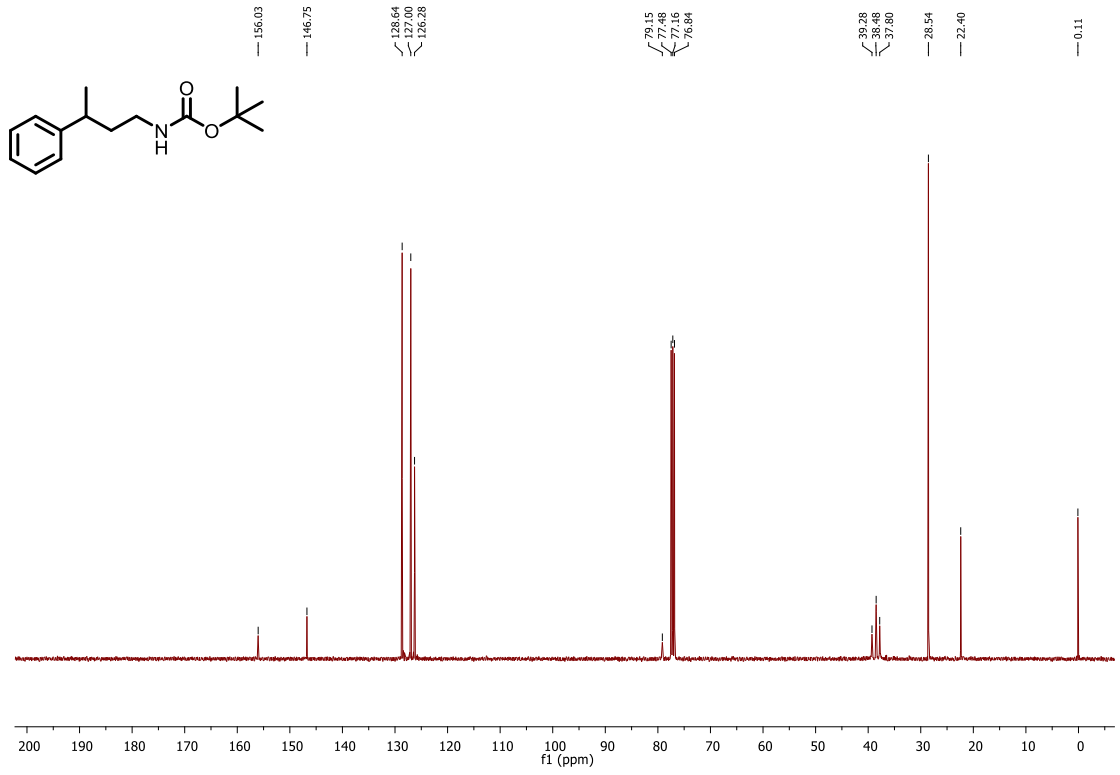



F
F
F
F
F
O
N
H
O

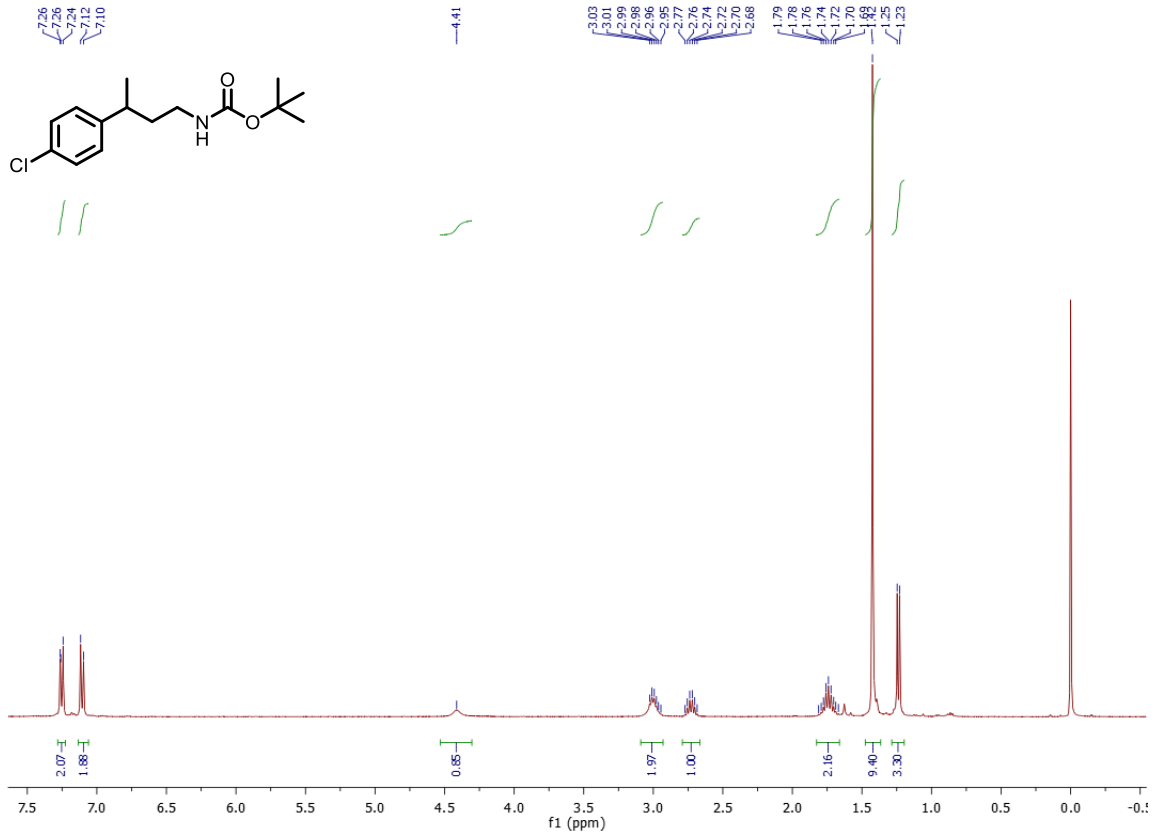
-144.20
-157.60
-162.68
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

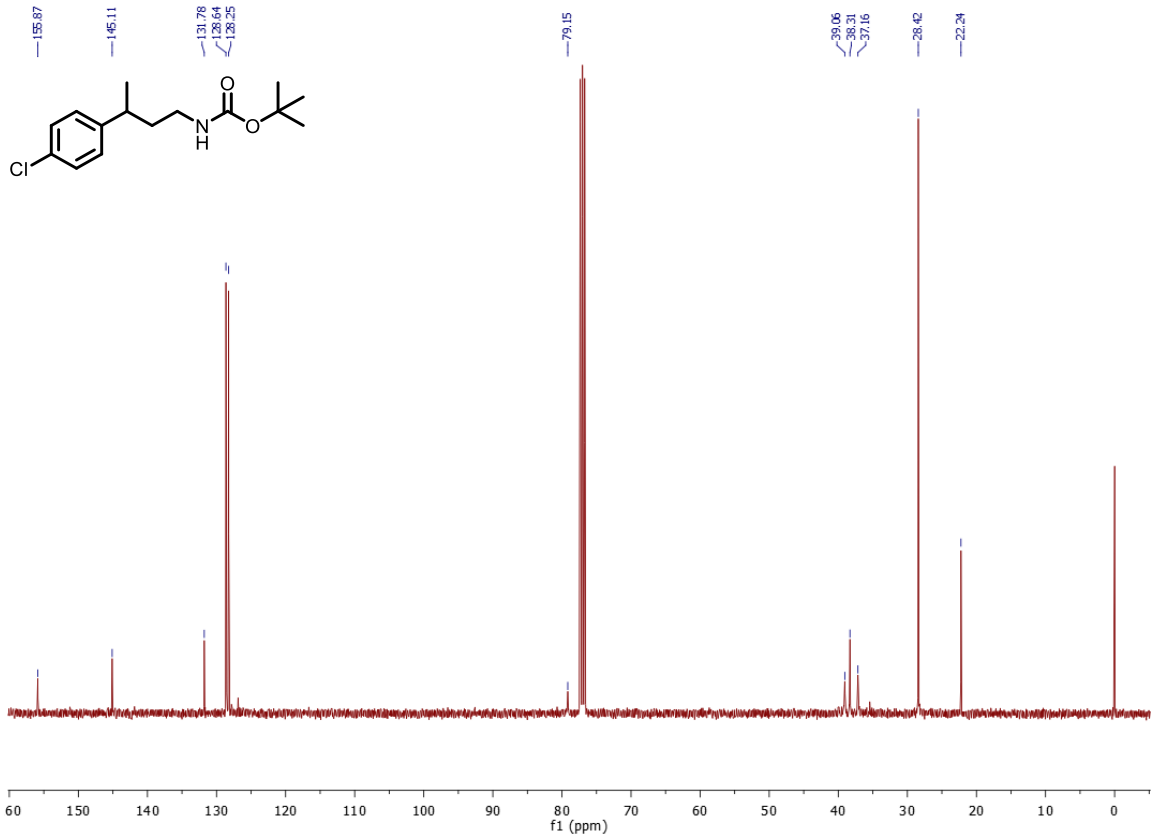
Tert-butyl (3-phenylbutyl)carbamate (from 15)



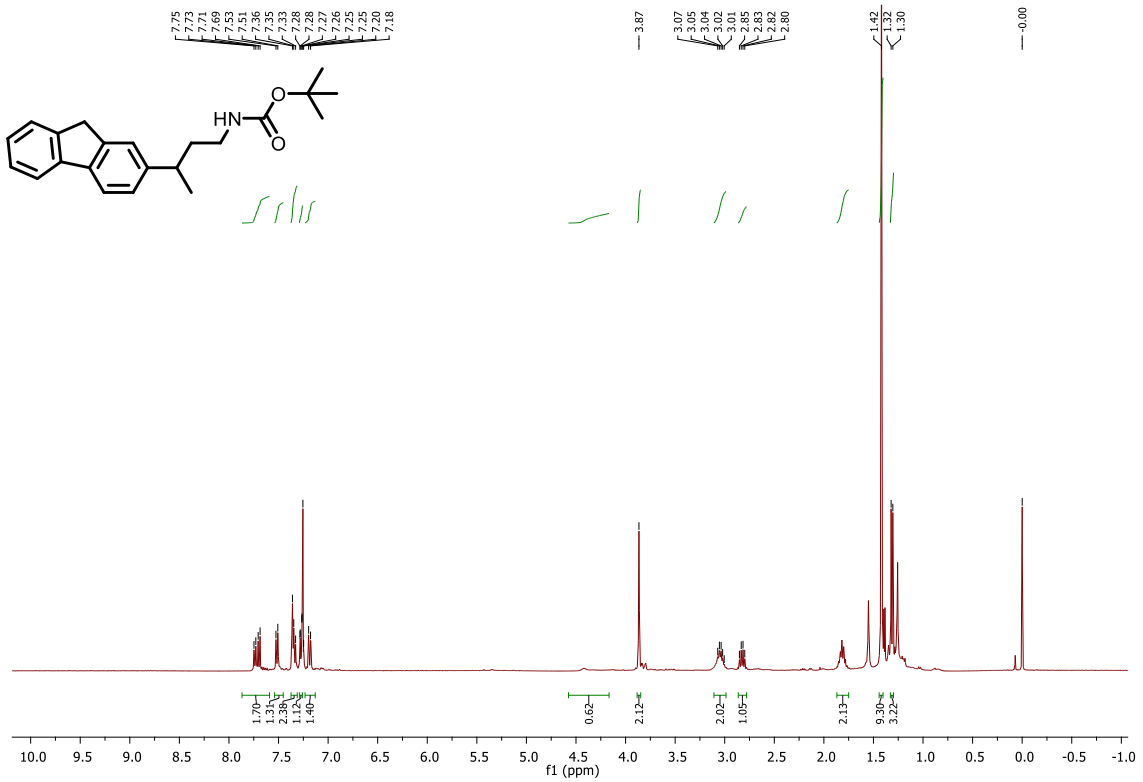


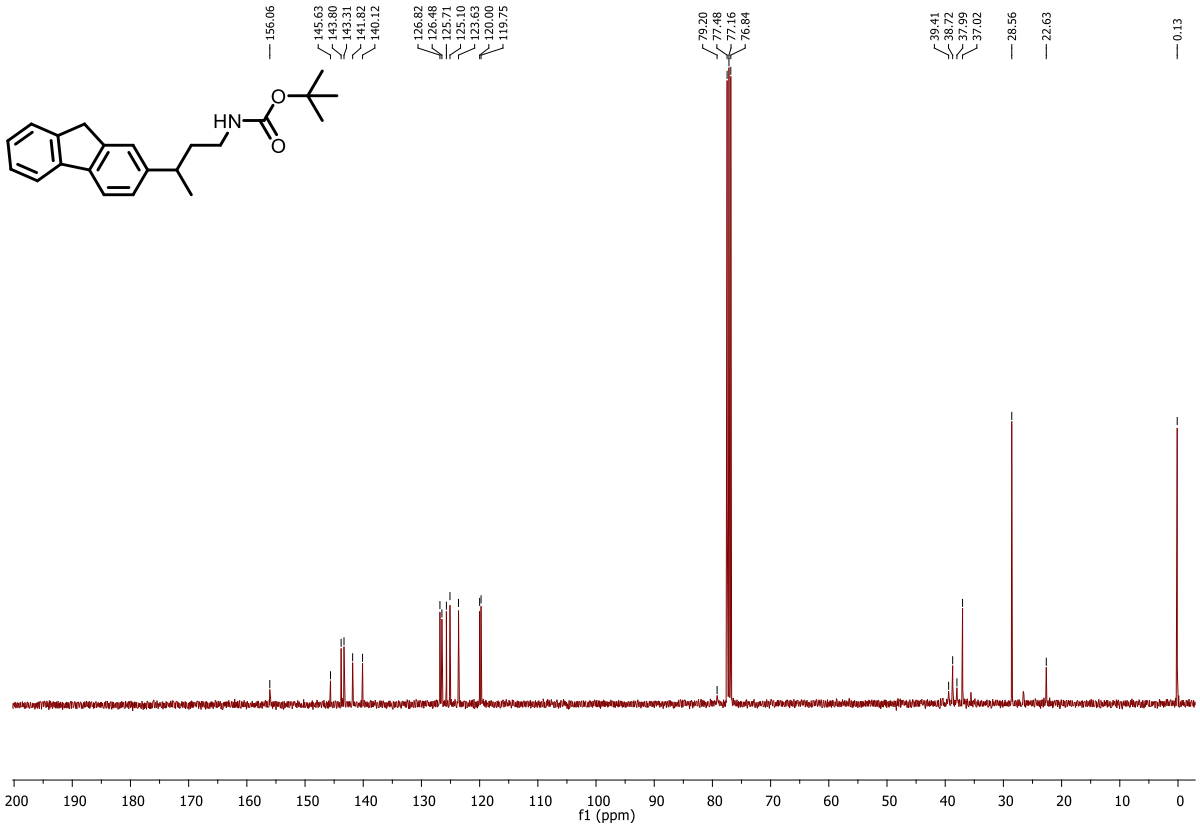
Tert-butyl (3-(4-chlorophenyl)butyl)carbamate (from 16)



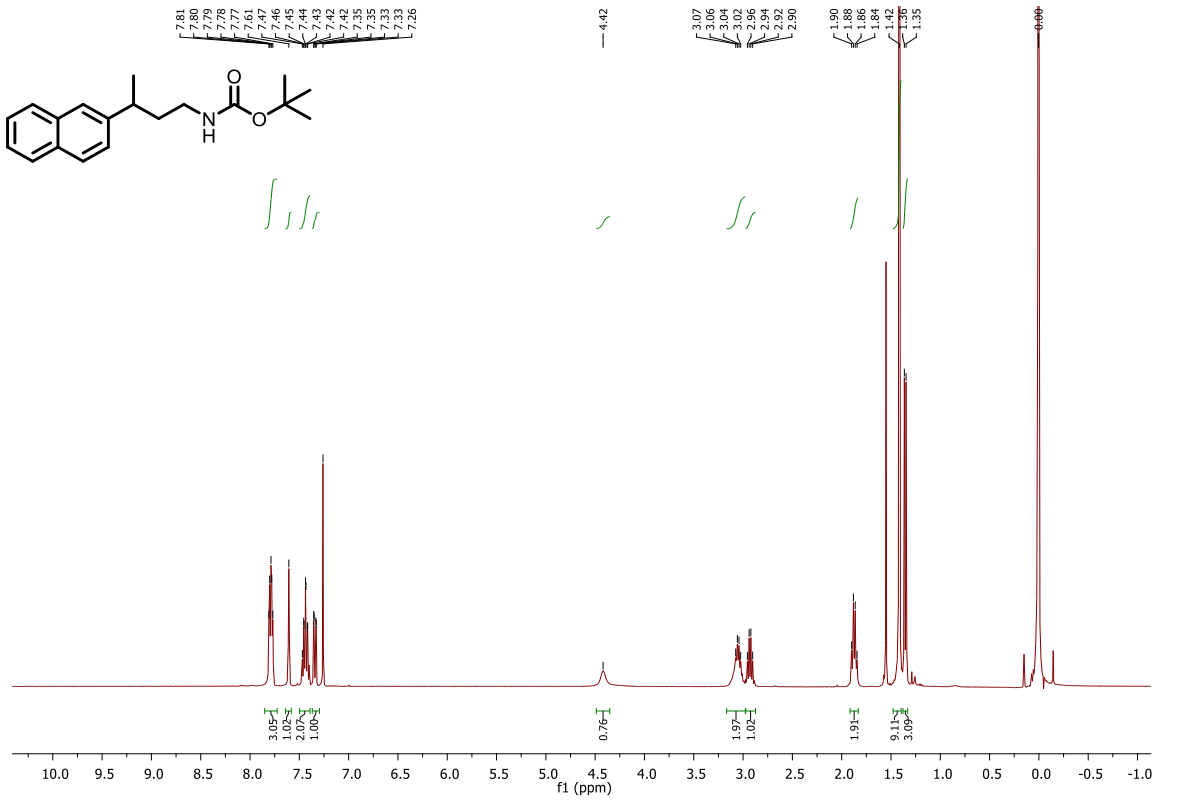


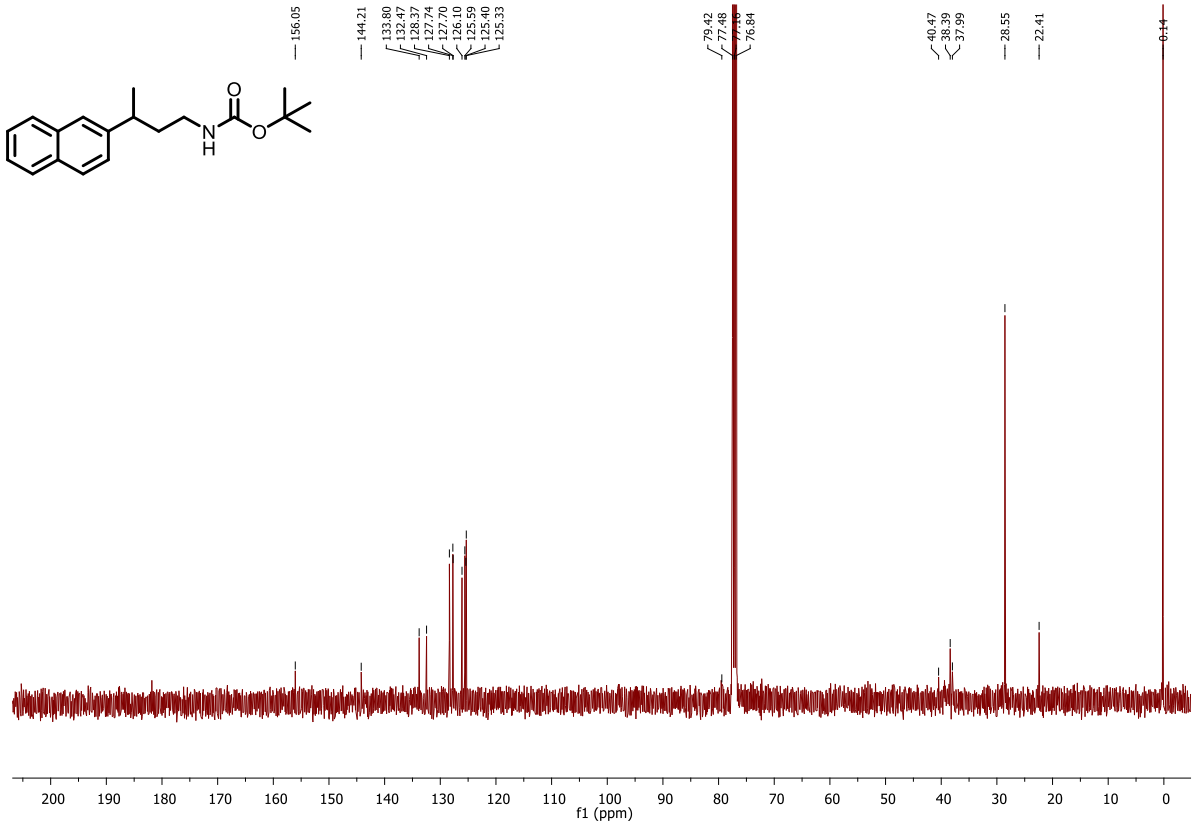
Tert-butyl (3-(9H-fluoren-2-yl)butyl)carbamate (from 17)



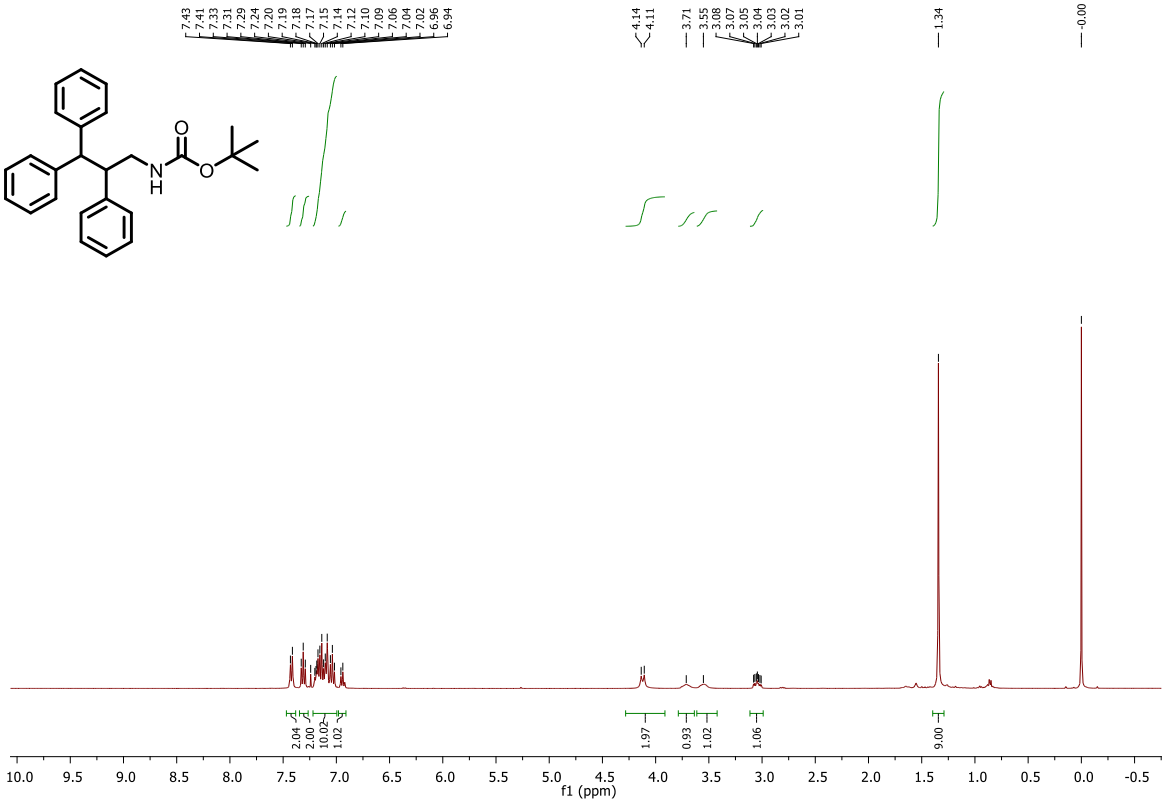


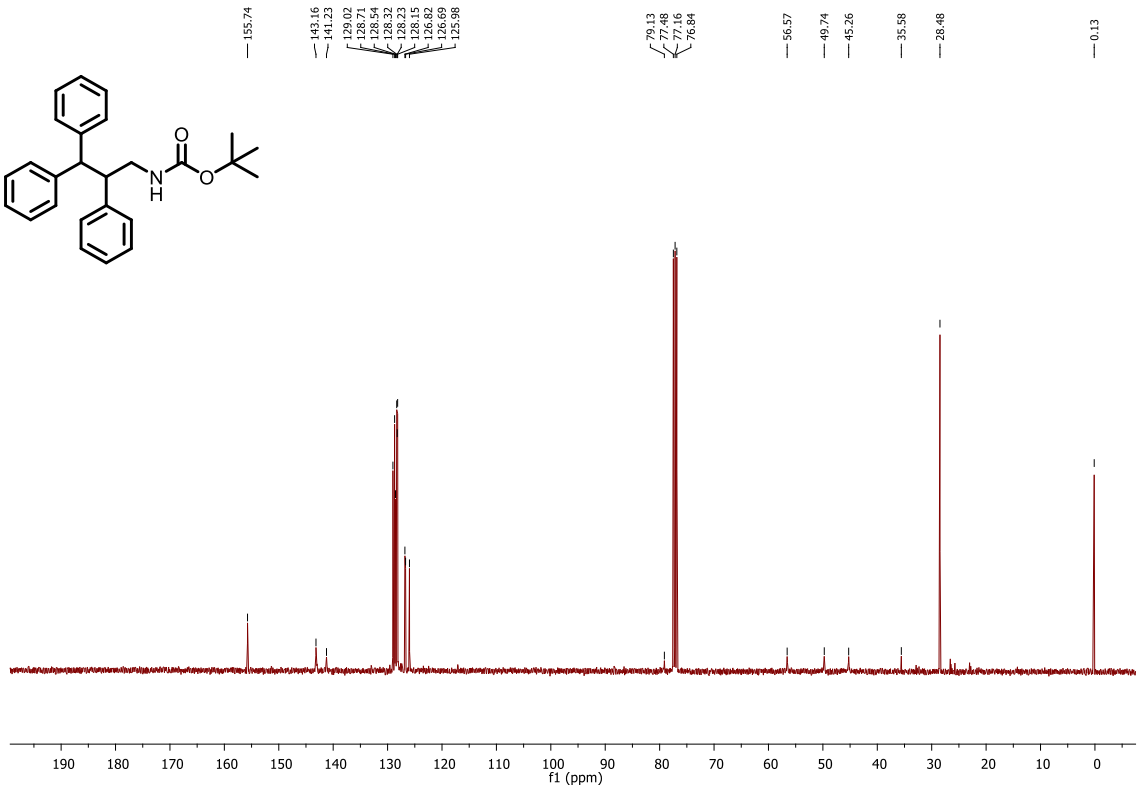
Tert-butyl (3-(naphthalen-2-yl)butyl)carbamate (from 18)



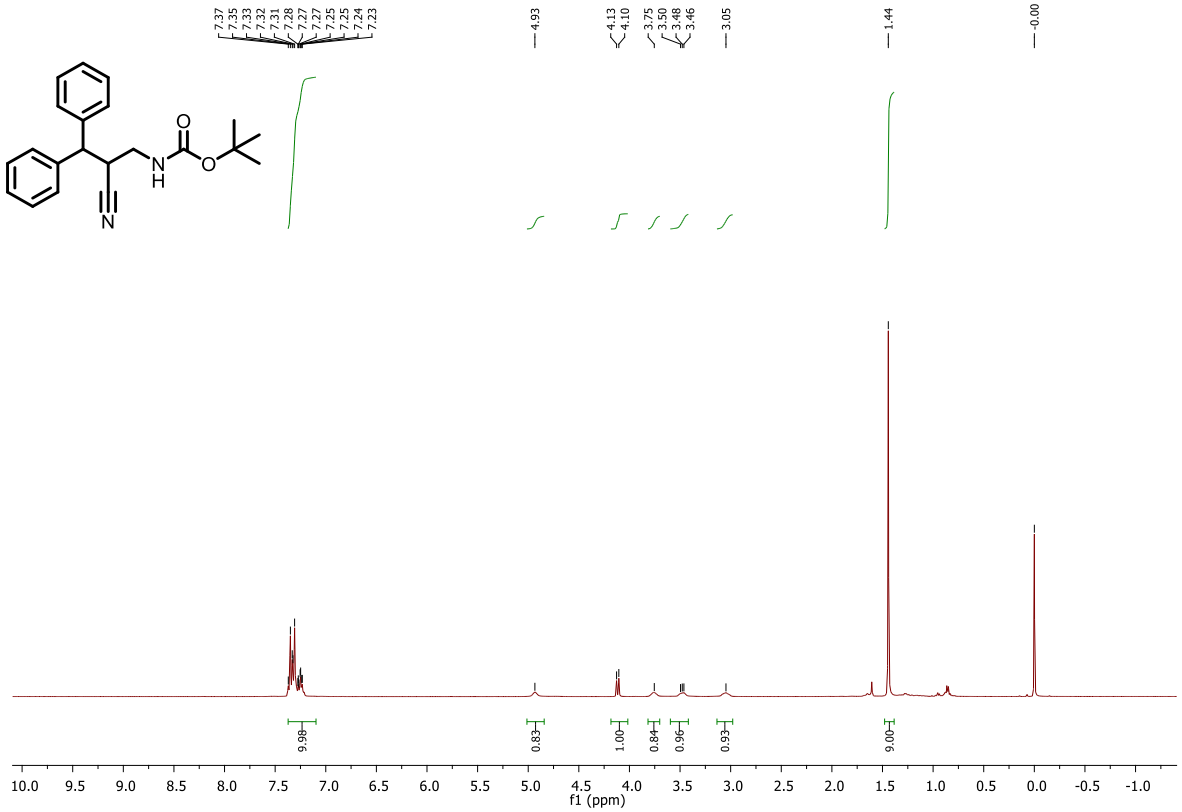


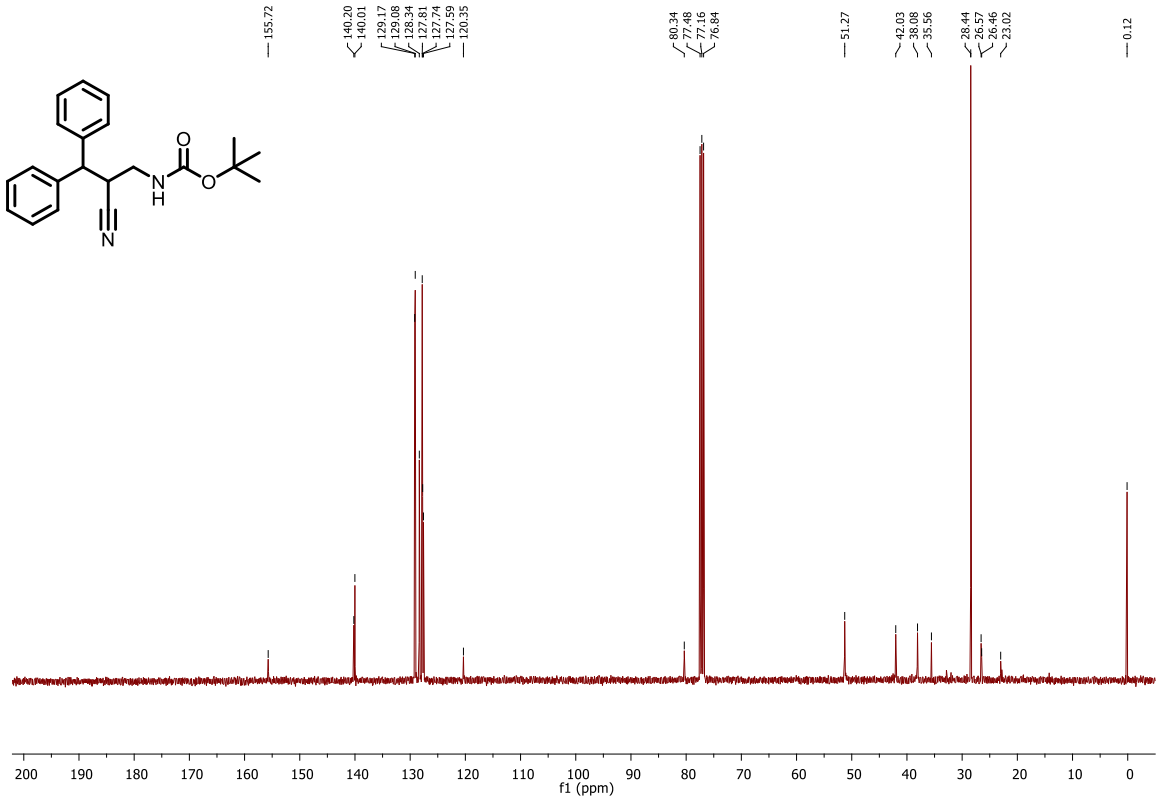
Tert-butyl (2,3,3-triphenylpropyl)carbamate (from 19)



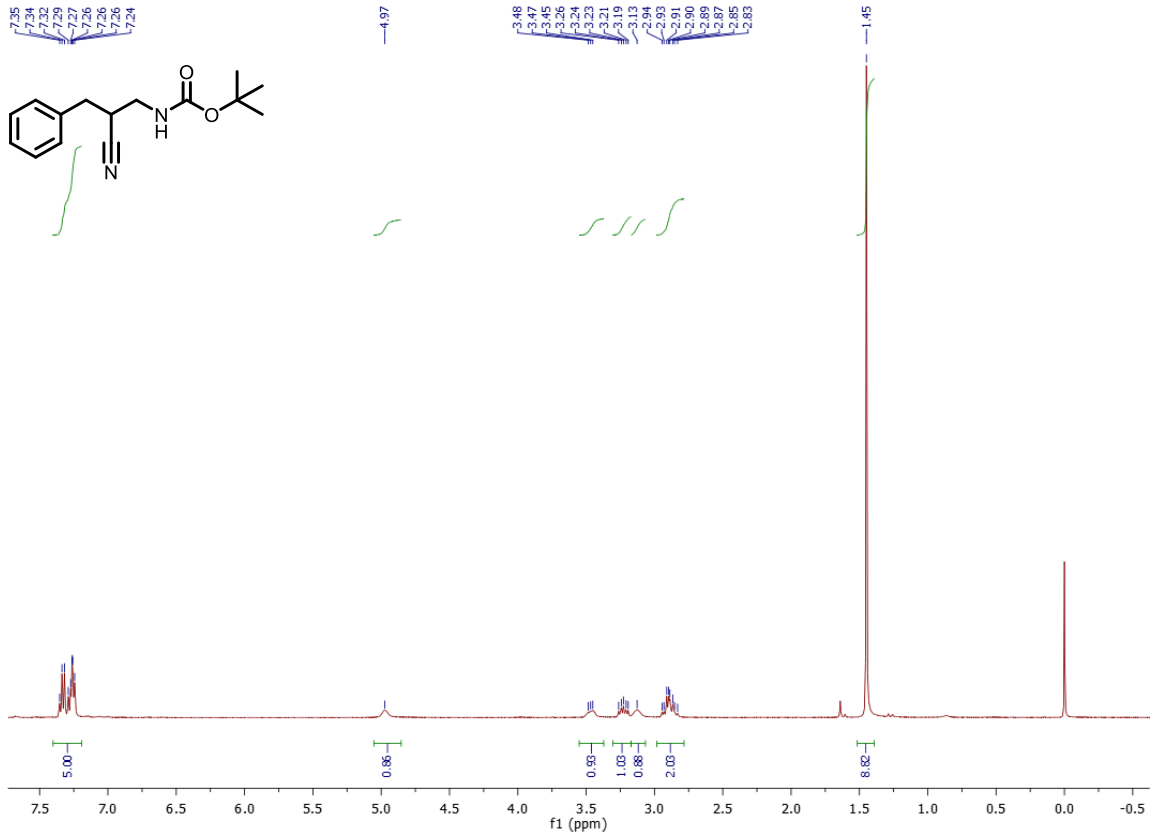


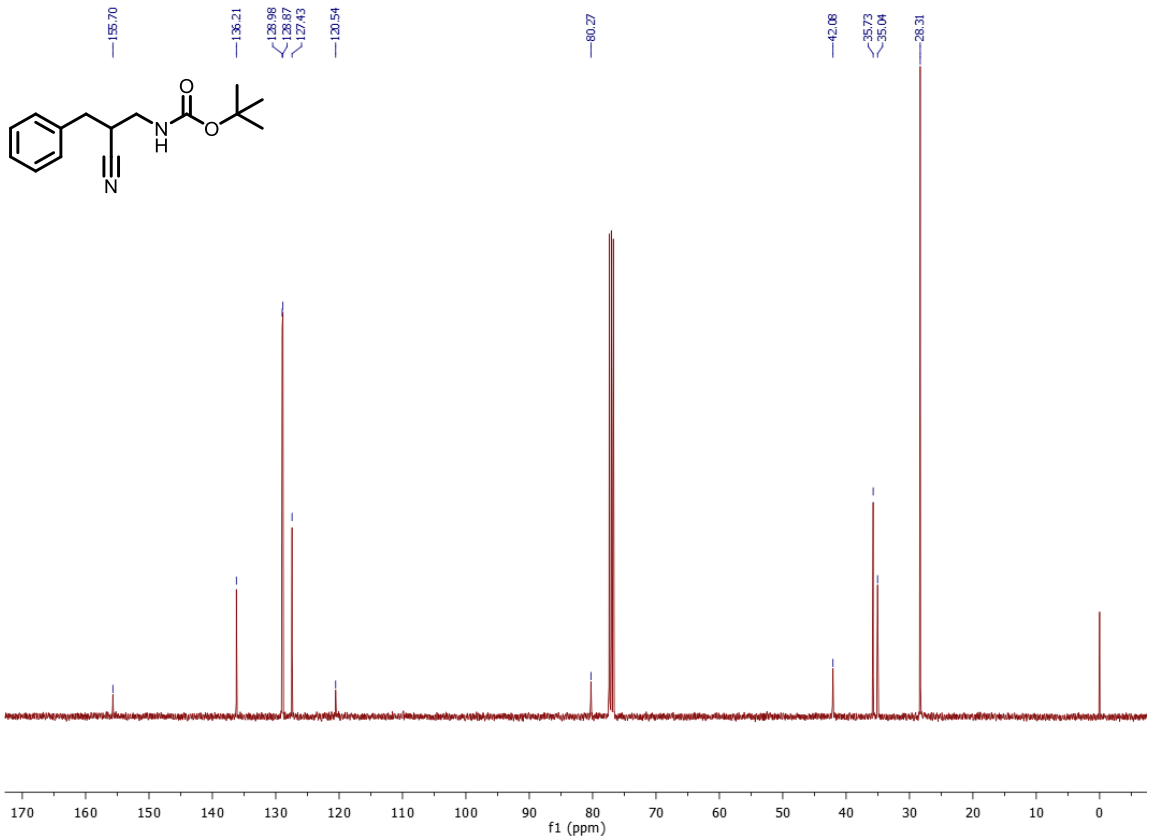
Tert-butyl (2-cyano-3,3-diphenylpropyl)carbamate (from 20)



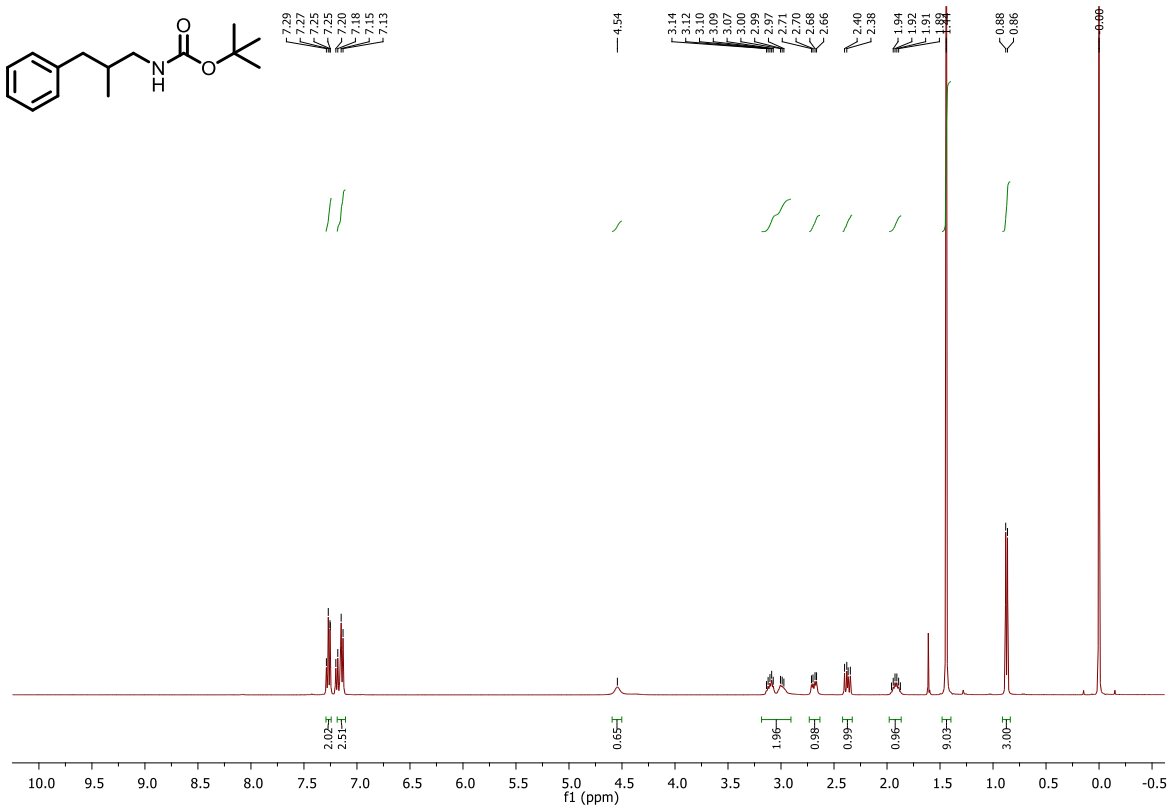


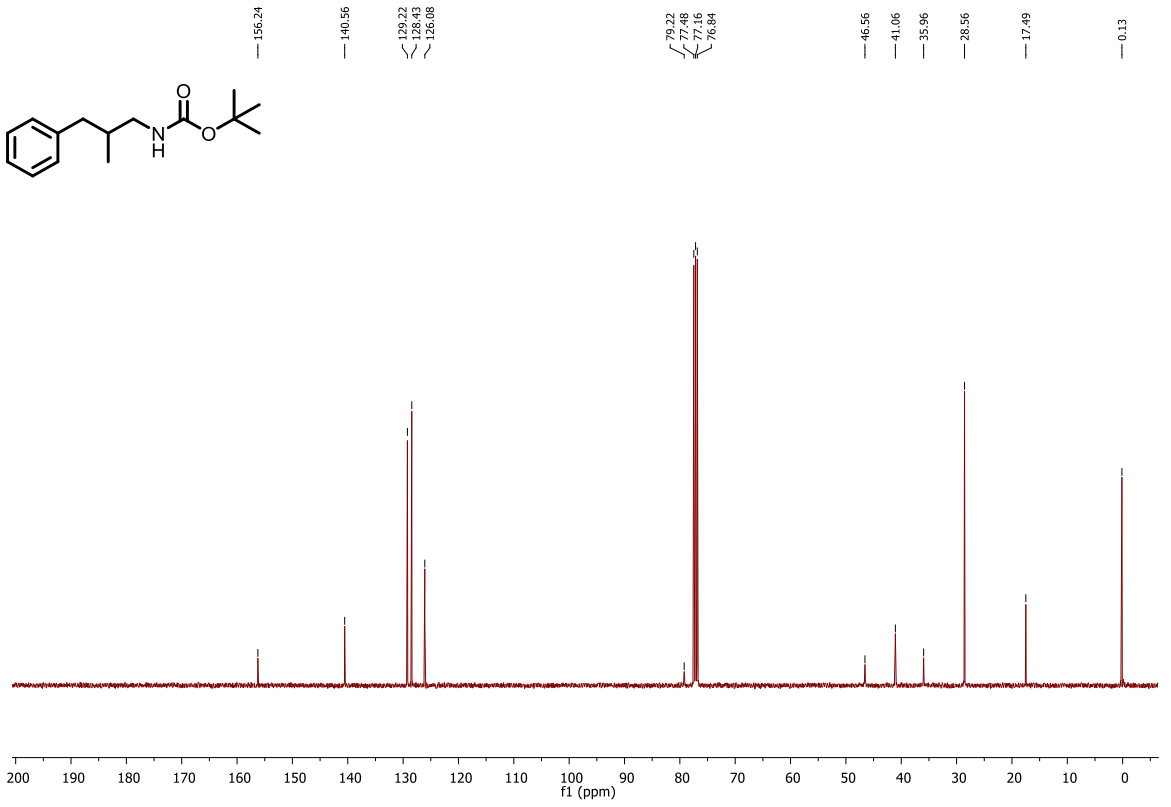
Tert-butyl (2-cyano-3-phenylpropyl)carbamate (from 21)



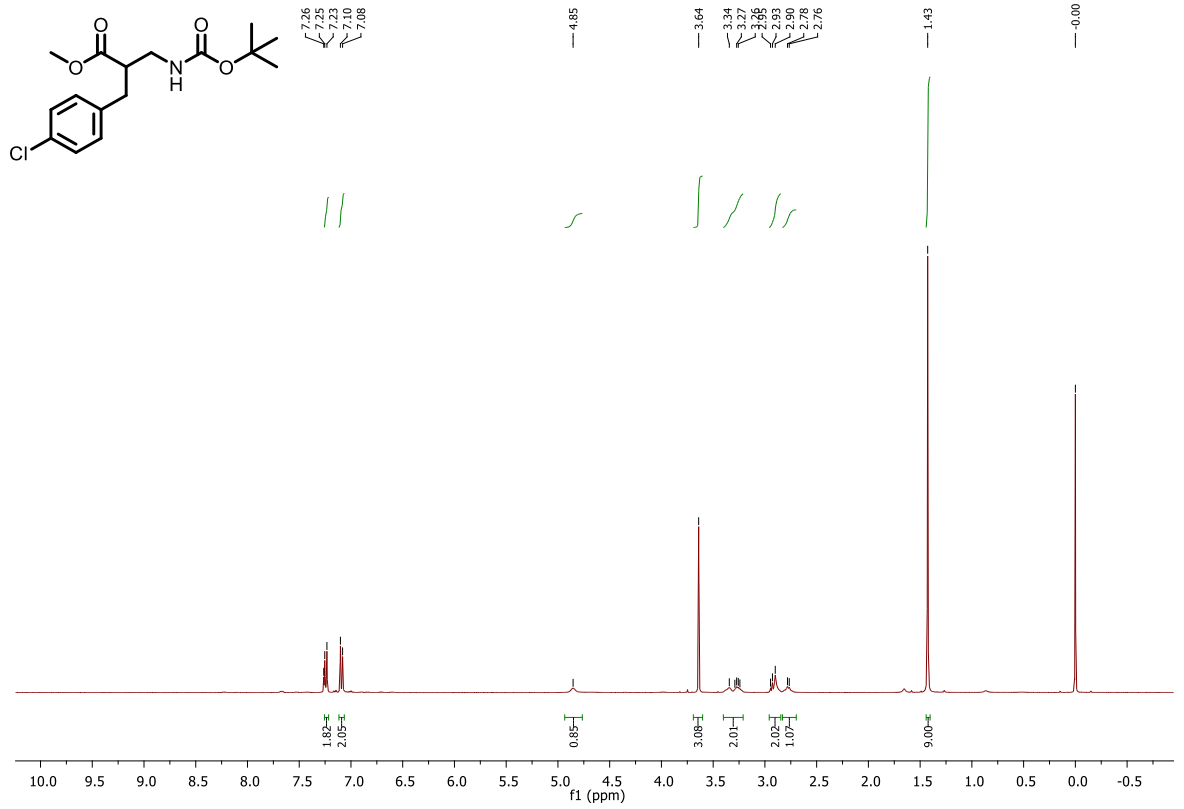


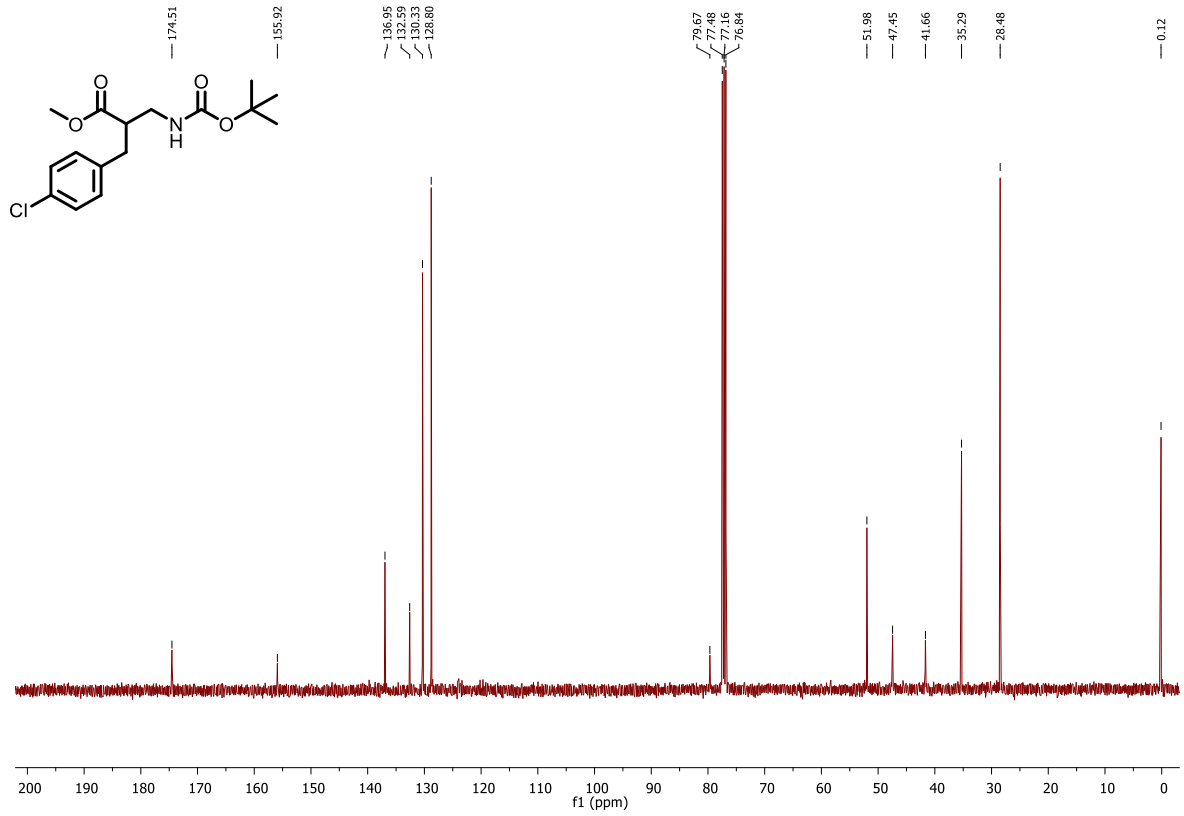
Tert-butyl (2-methyl-3-phenylpropyl)carbamate (from 22)



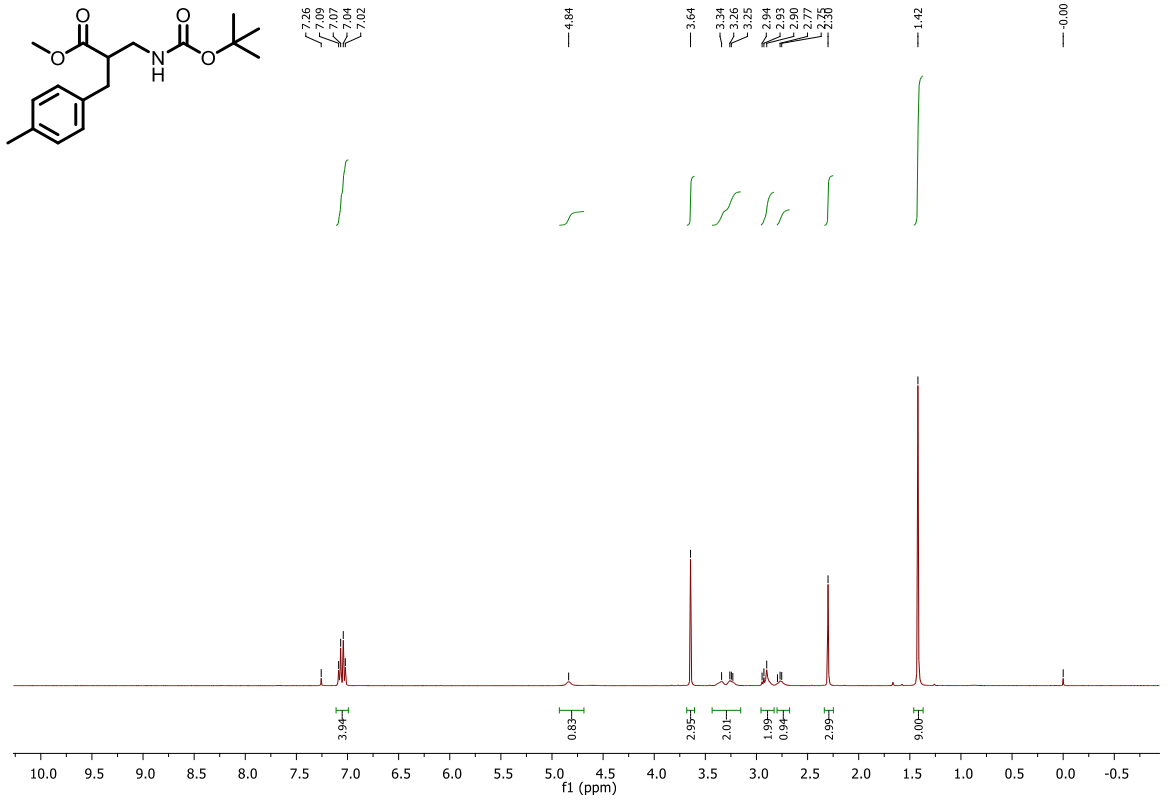


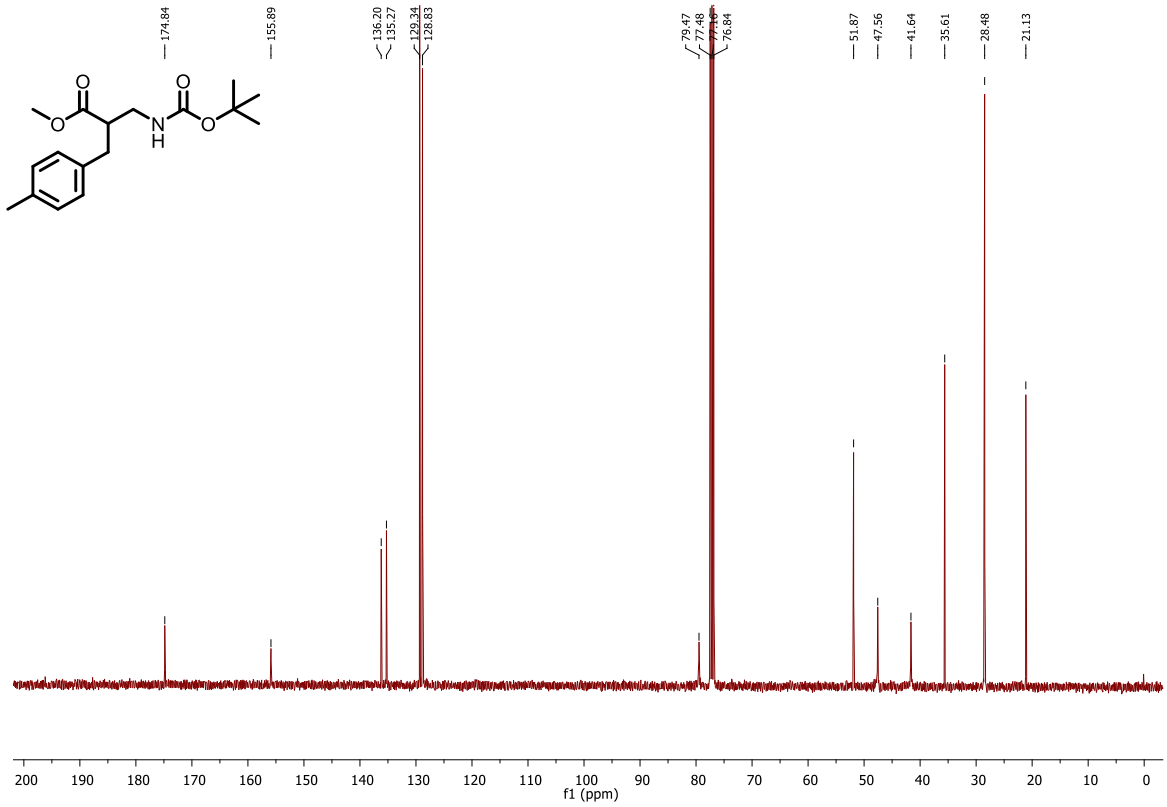
Methyl 3-((tert-butoxycarbonyl)amino)-2-(4-chlorobenzyl)propanoate (from 23)



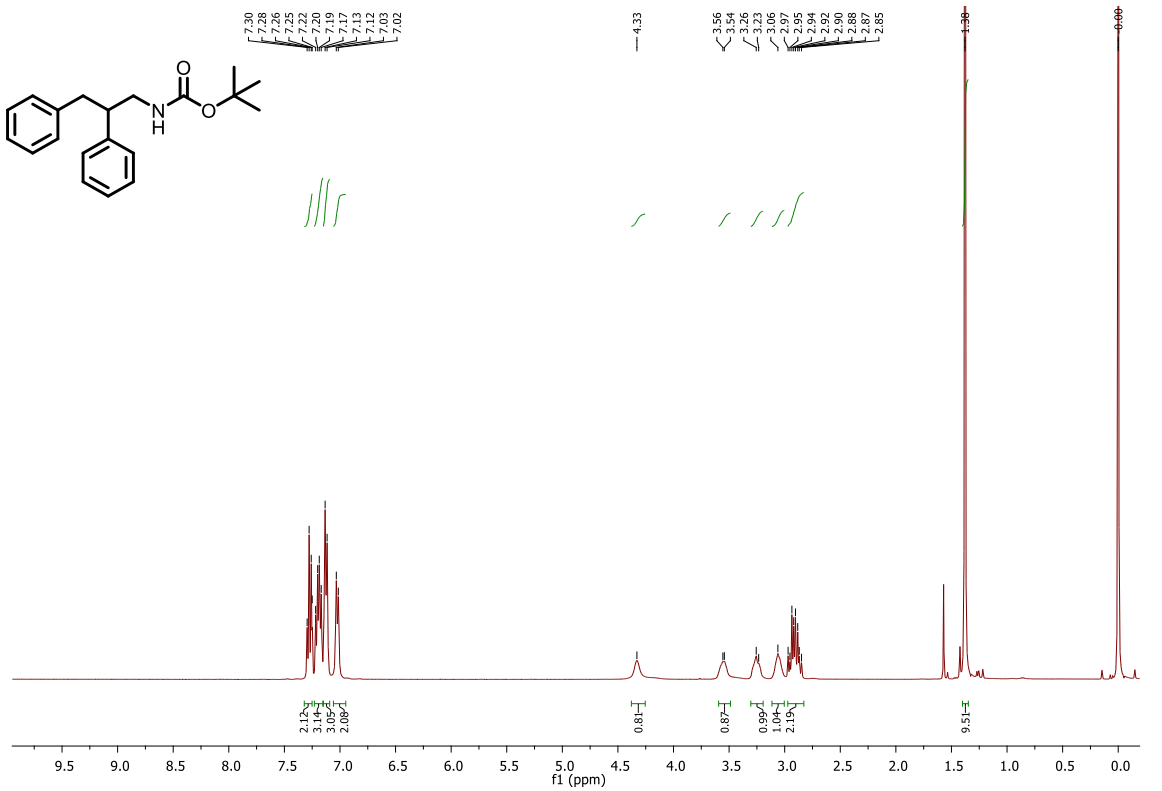


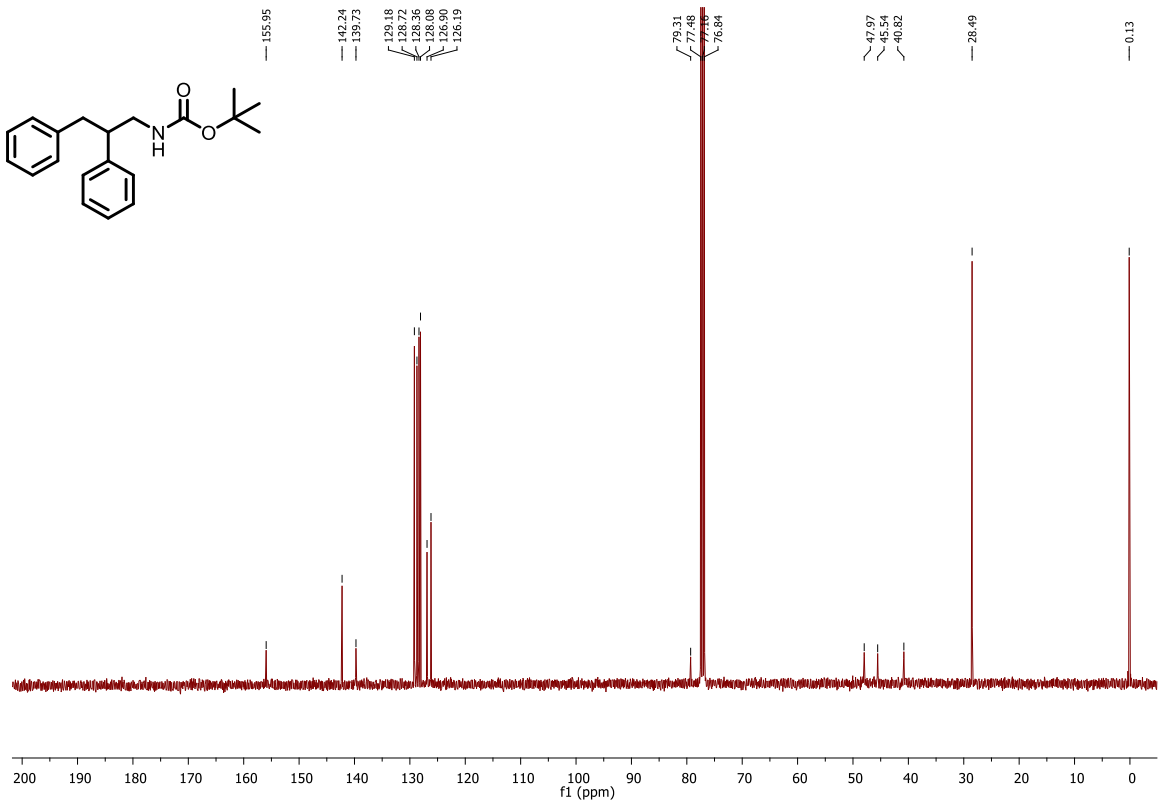
Methyl 3-((tert-butoxycarbonyl)amino)-2-(4-methylbenzyl)propanoate (from 24)



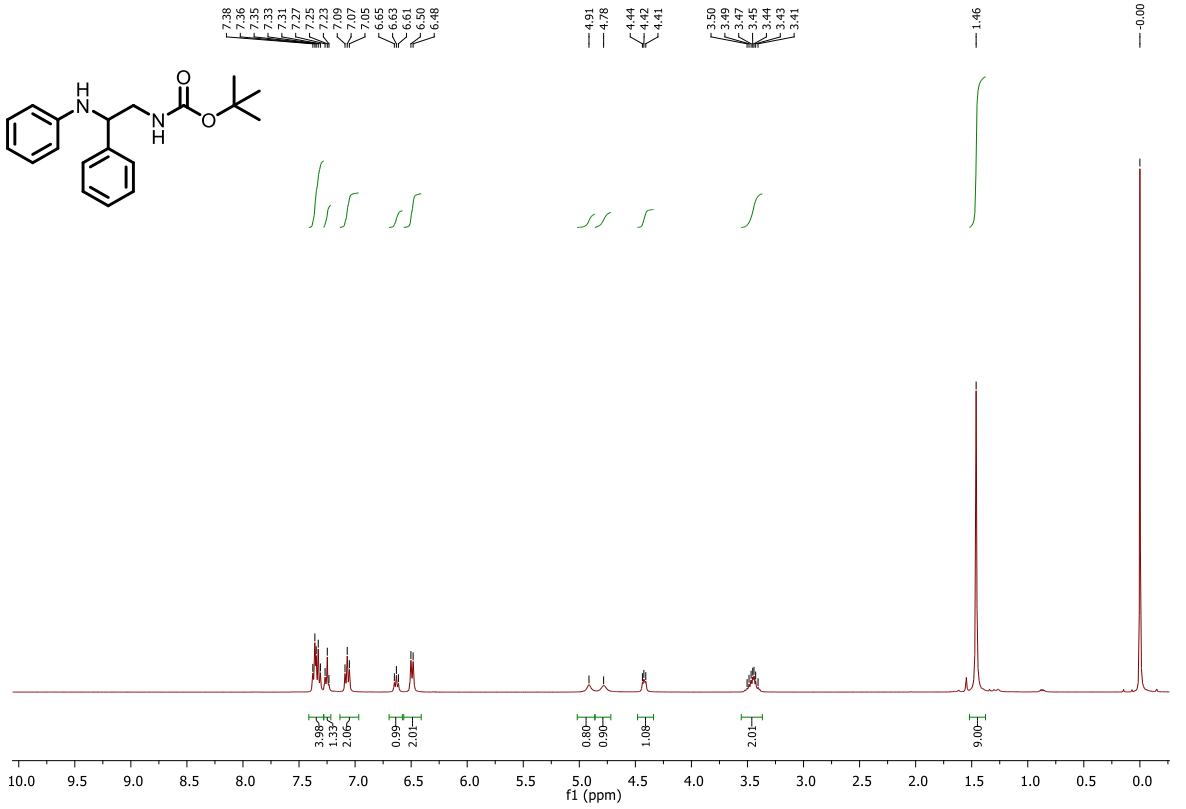


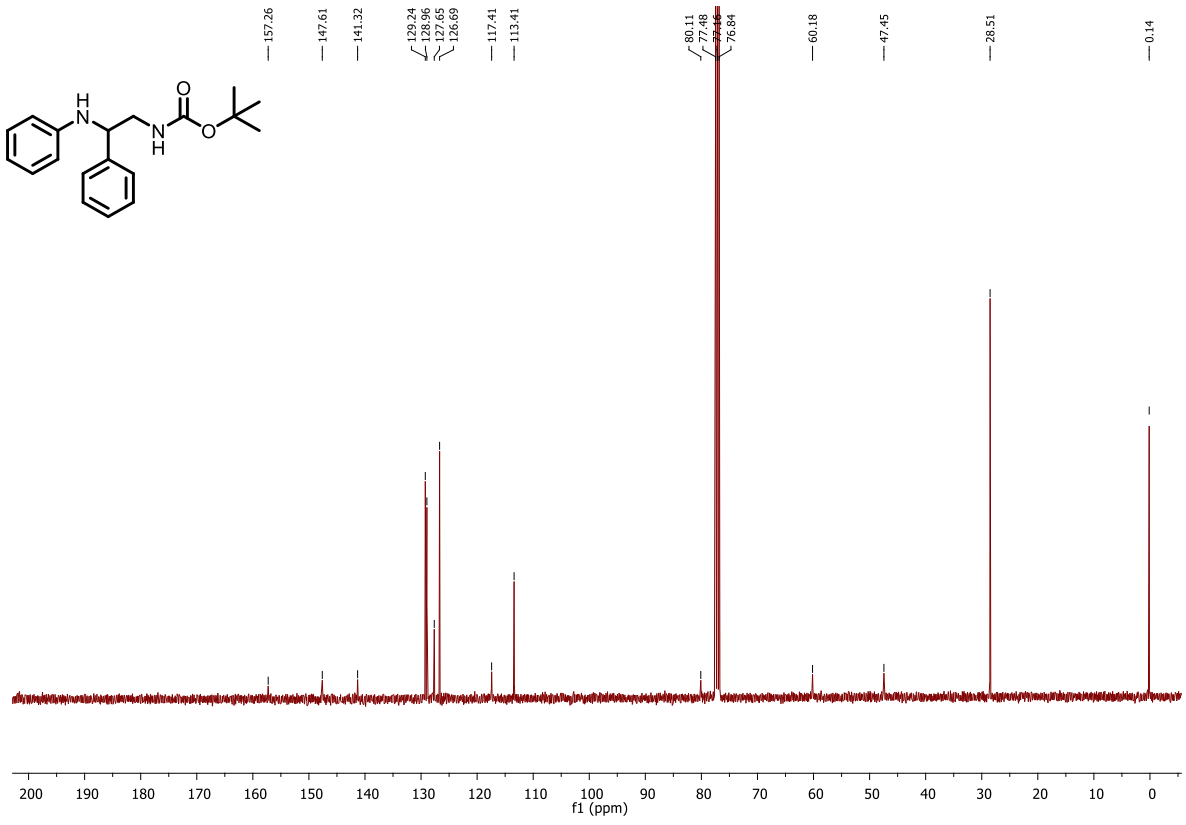
Tert-butyl (2,3-diphenylpropyl)carbamate (from 25)



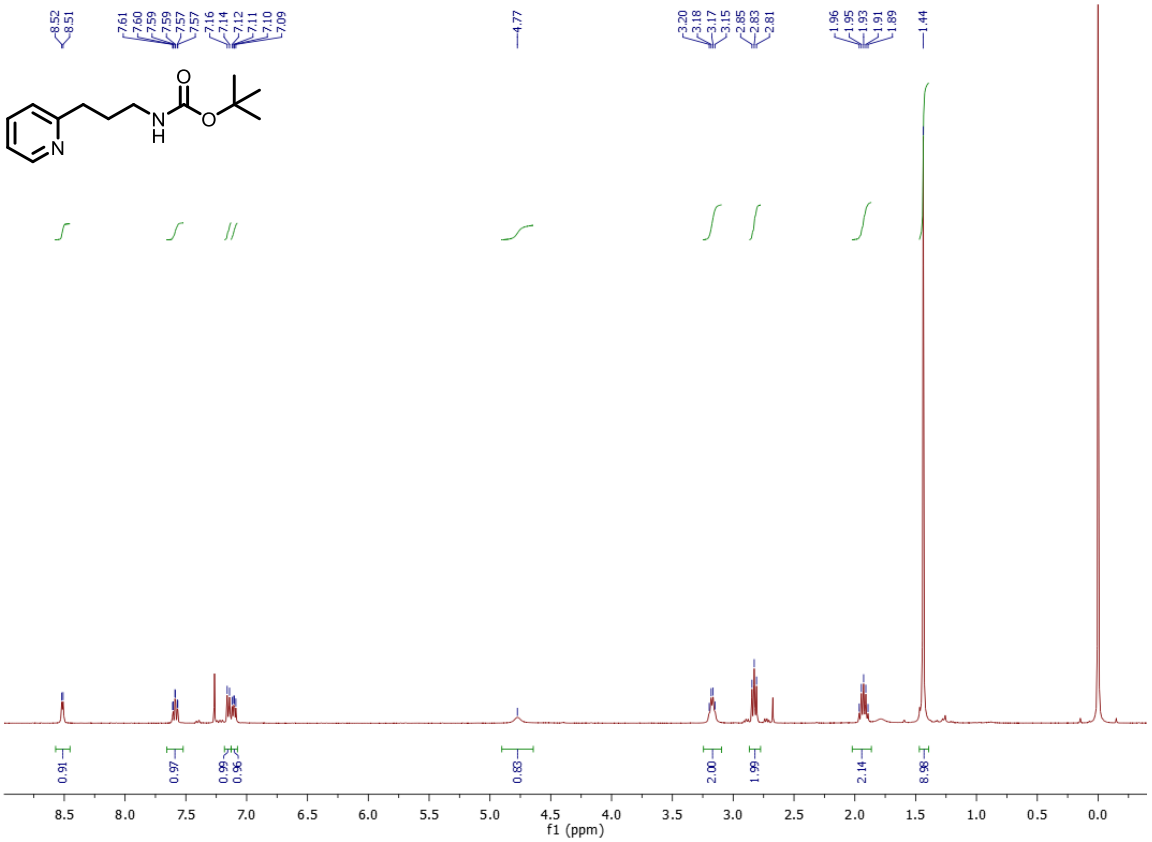


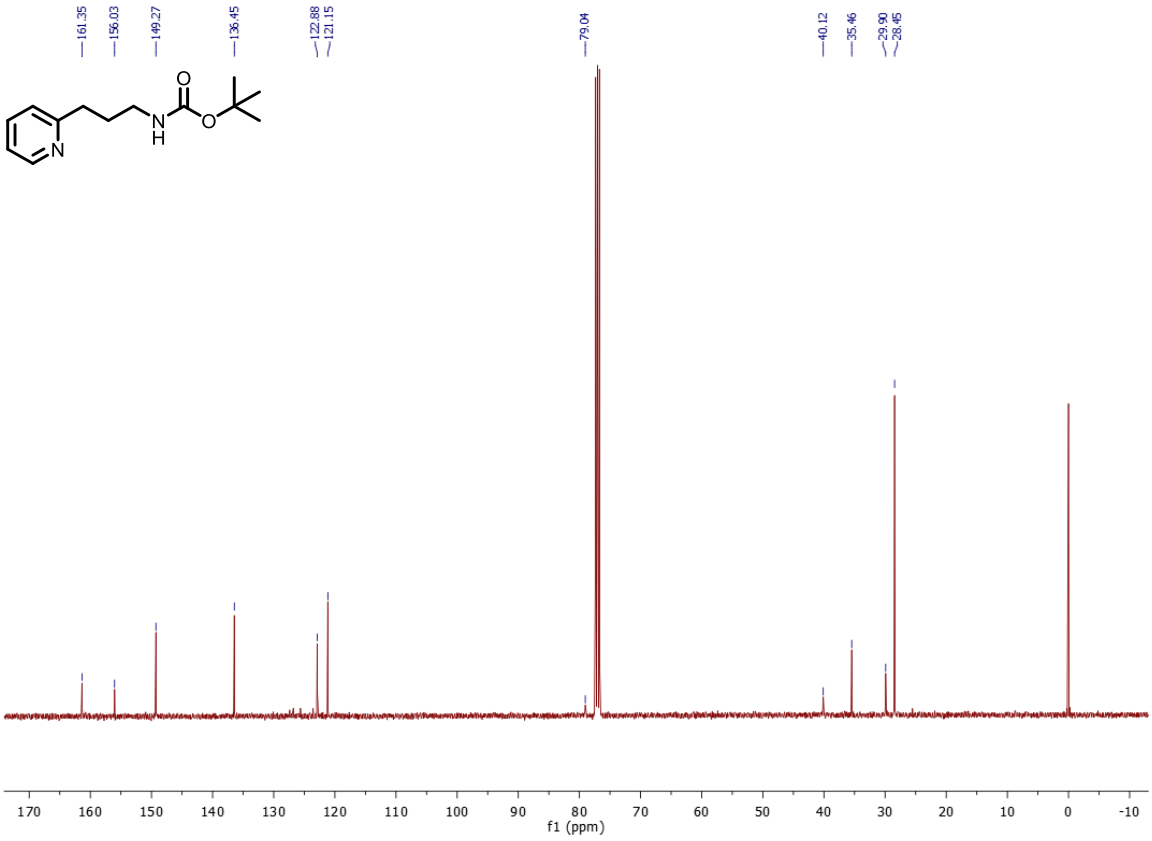
Tert-butyl (2-phenyl-2-(phenylamino)ethyl)carbamate (from 26)



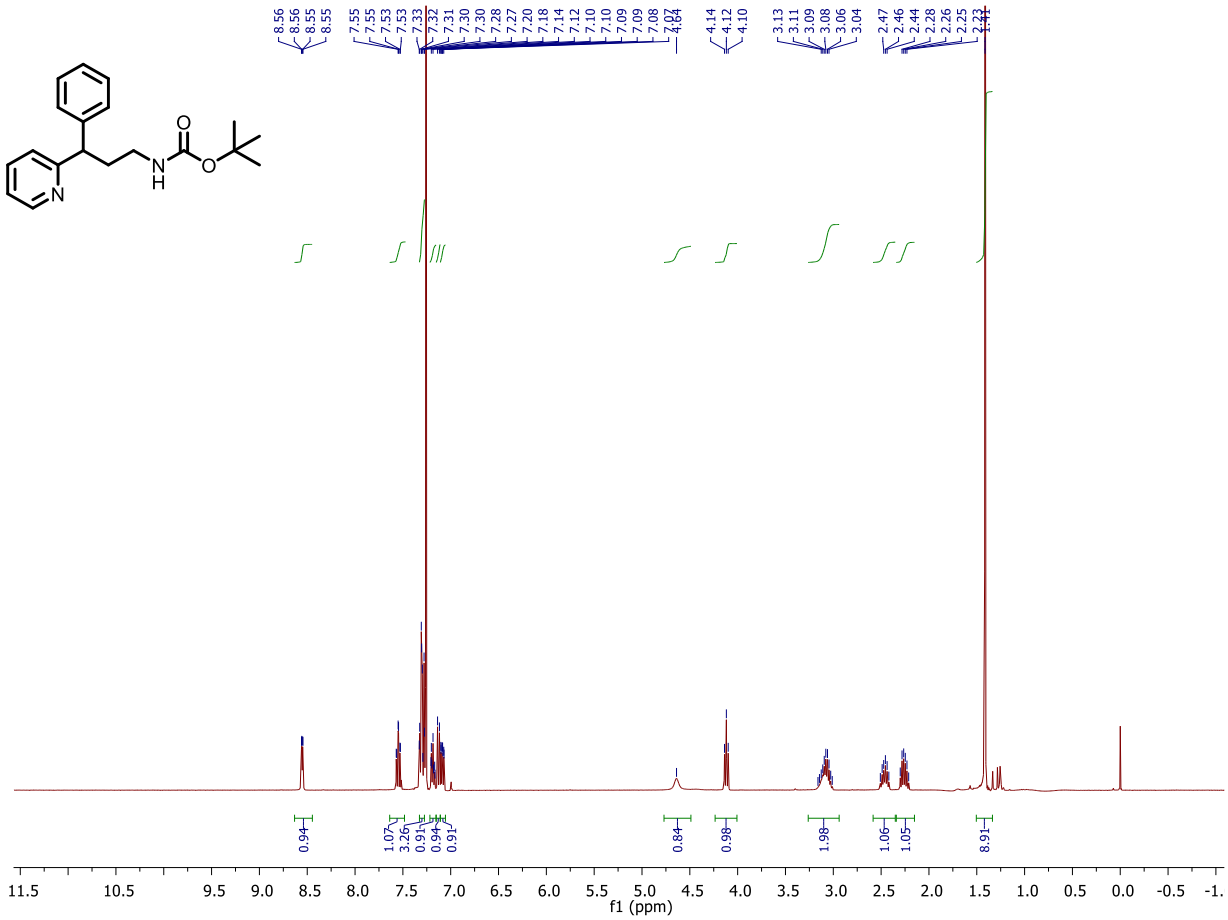


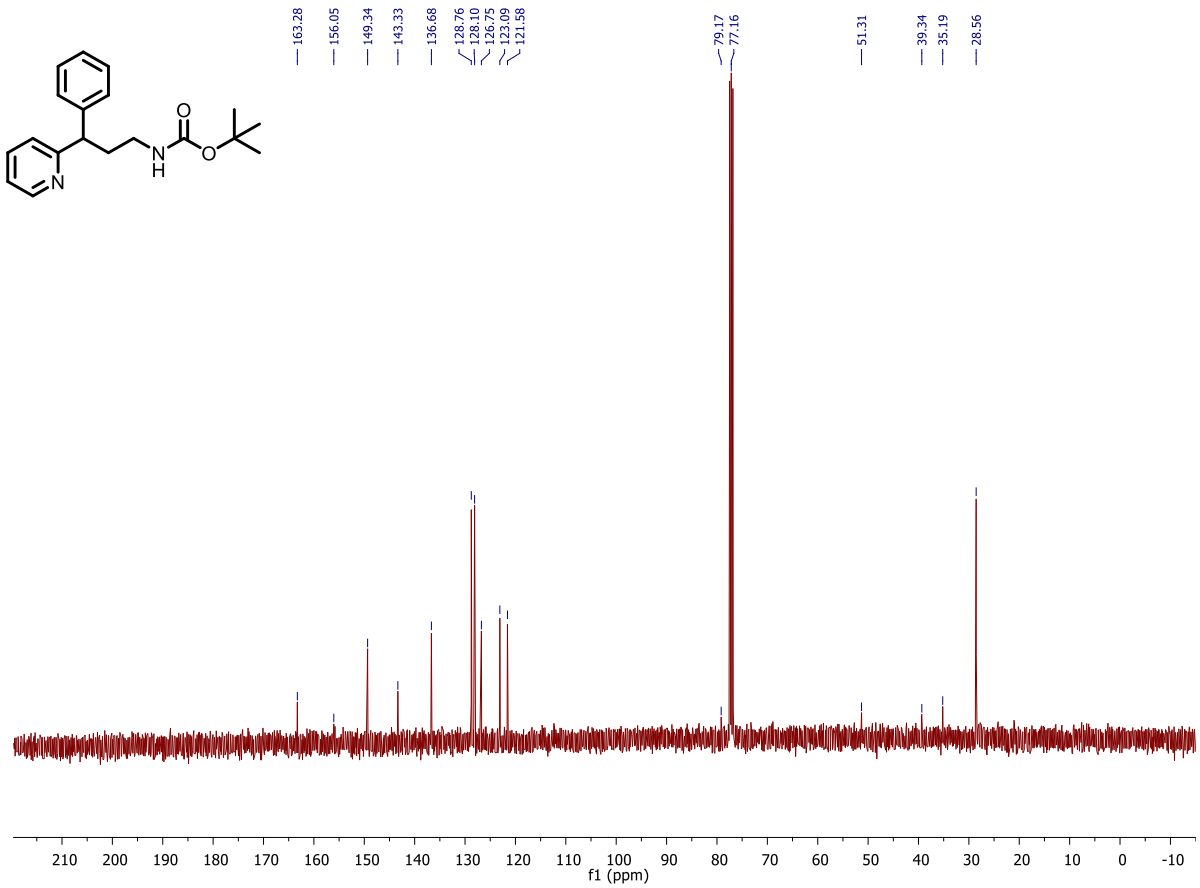
Tert-butyl (3-(pyridin-2-yl)propyl)carbamate (from 27)



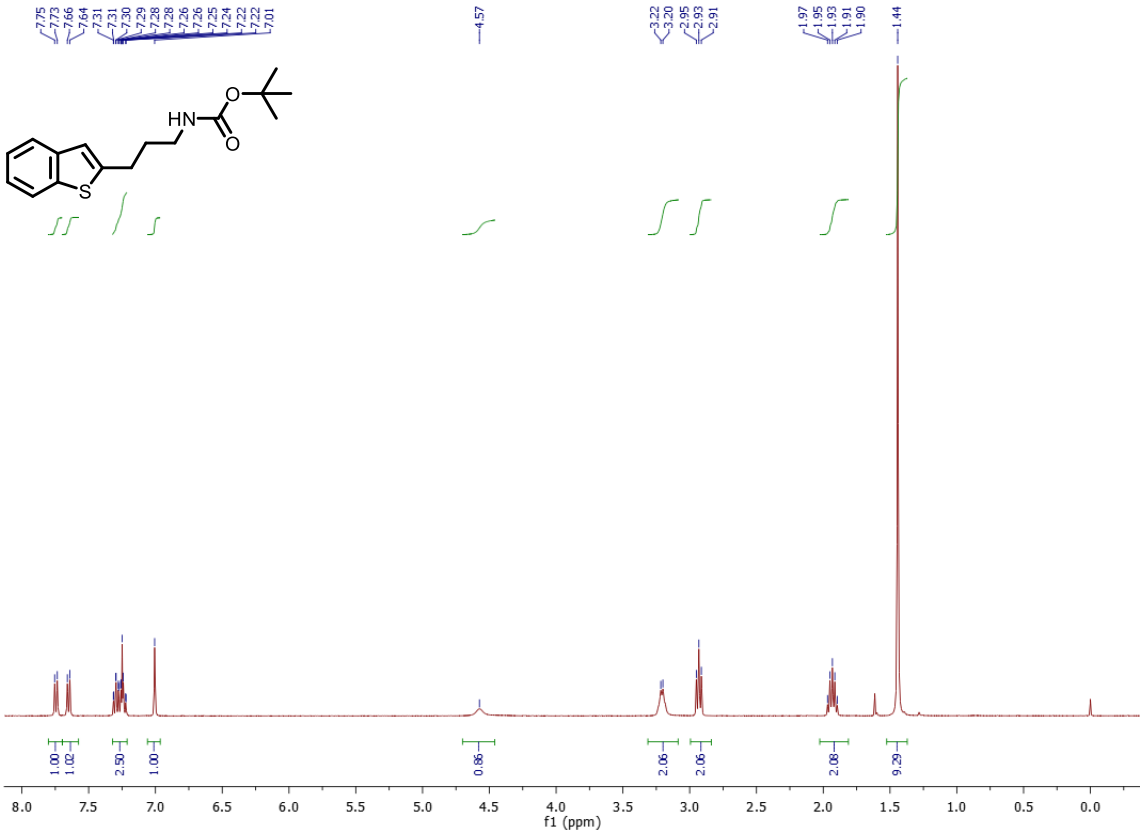


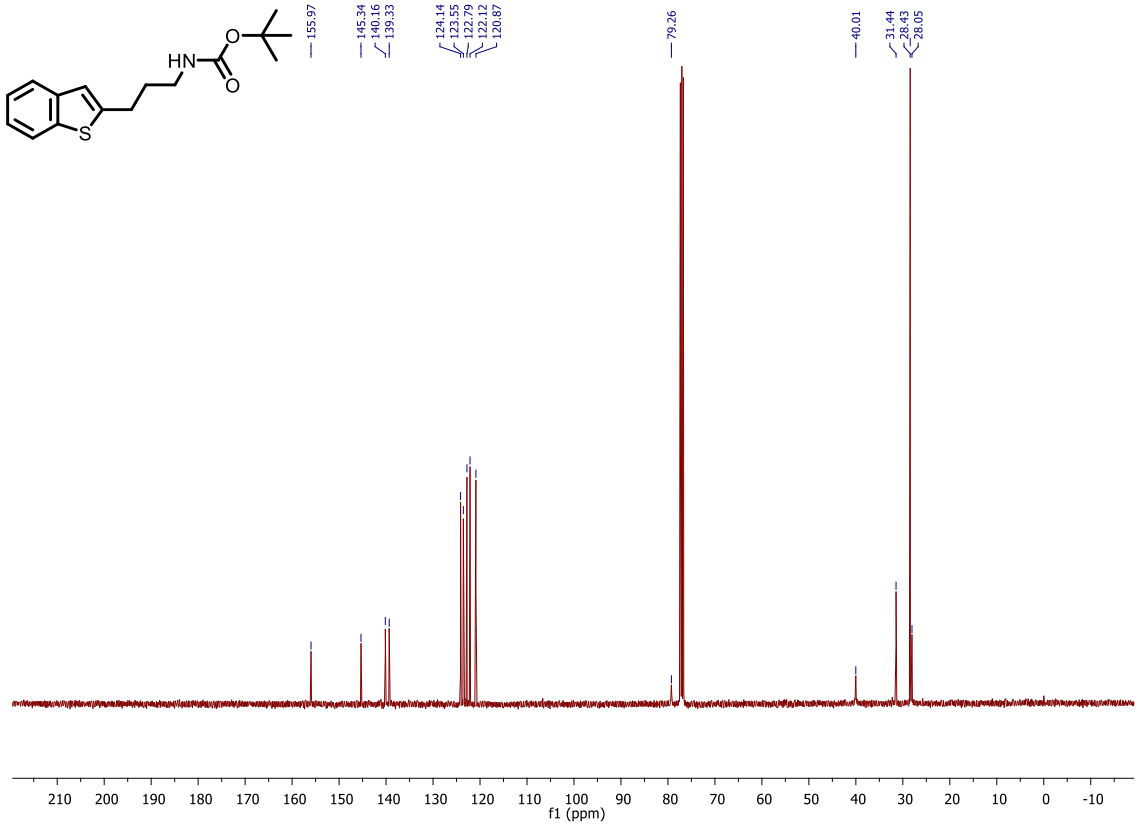
Tert-butyl (3-phenyl-3-(pyridin-2-yl)propyl)carbamate (from 28)



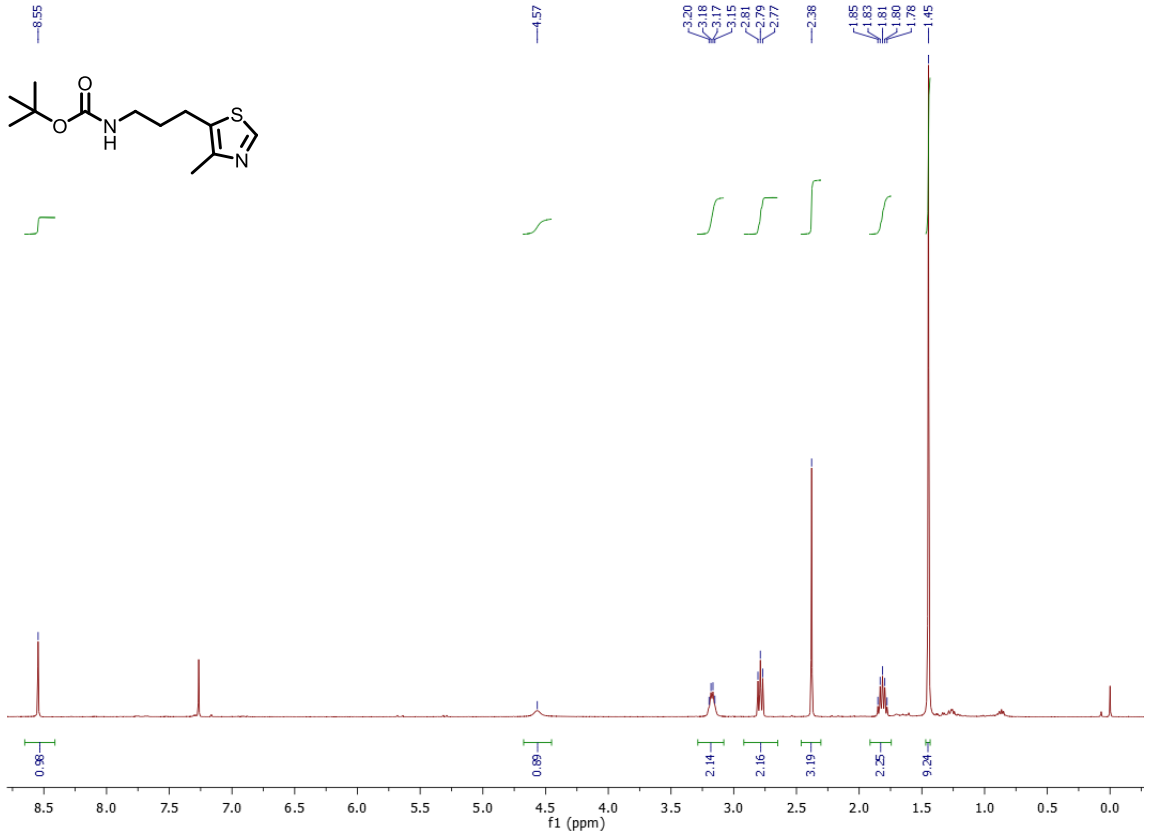


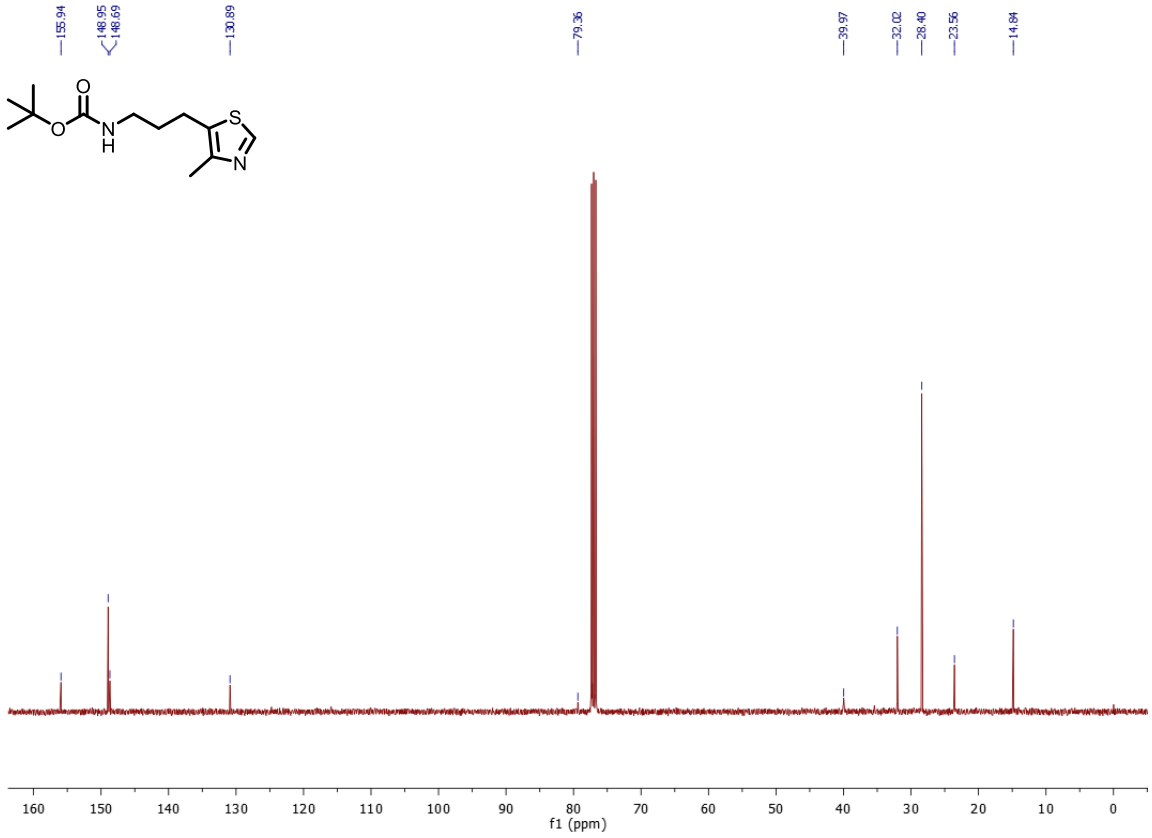
Tert-butyl (2-(benzo[b]thiophen-2-yl)ethyl)carbamate (from 29)



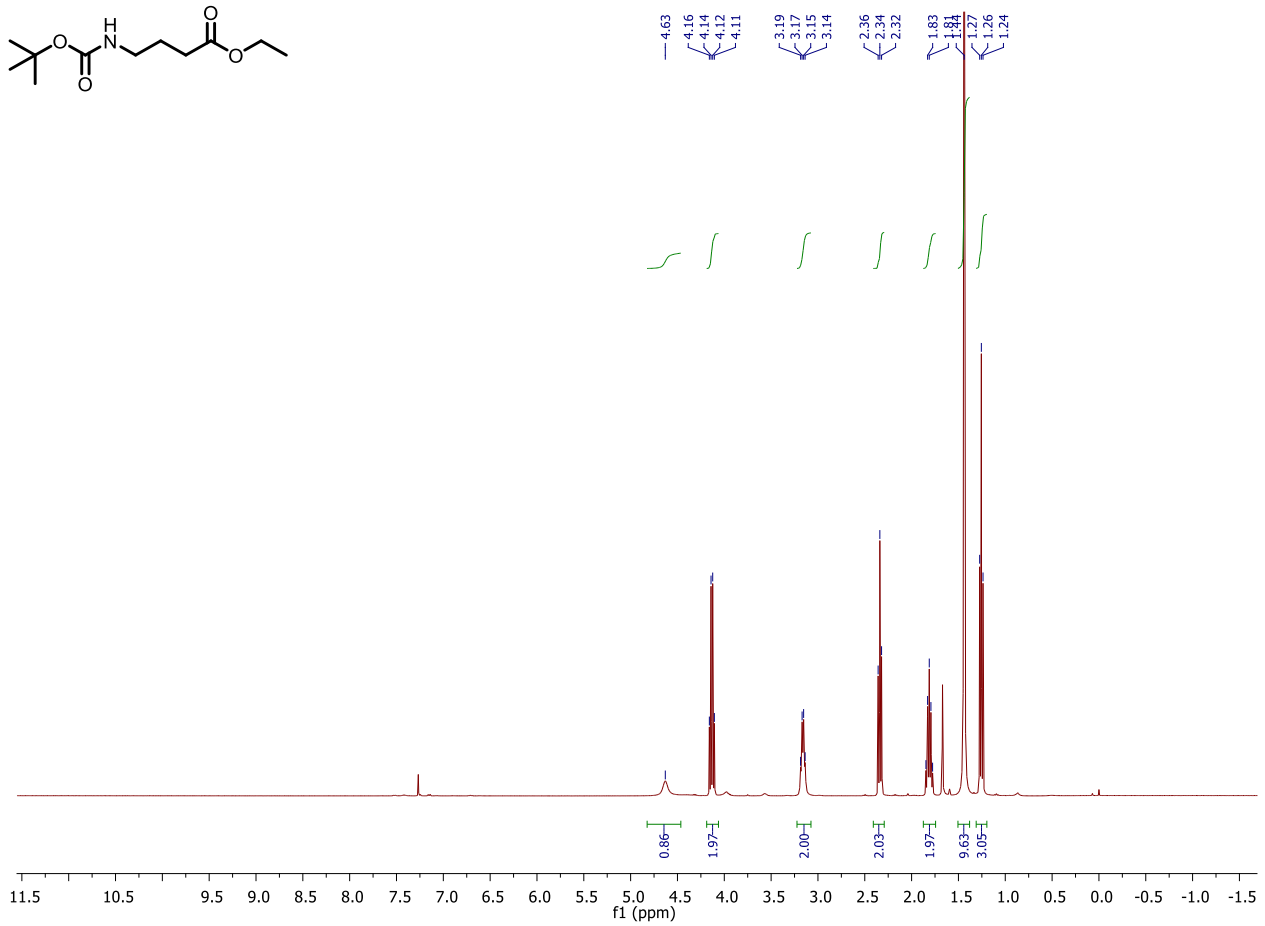


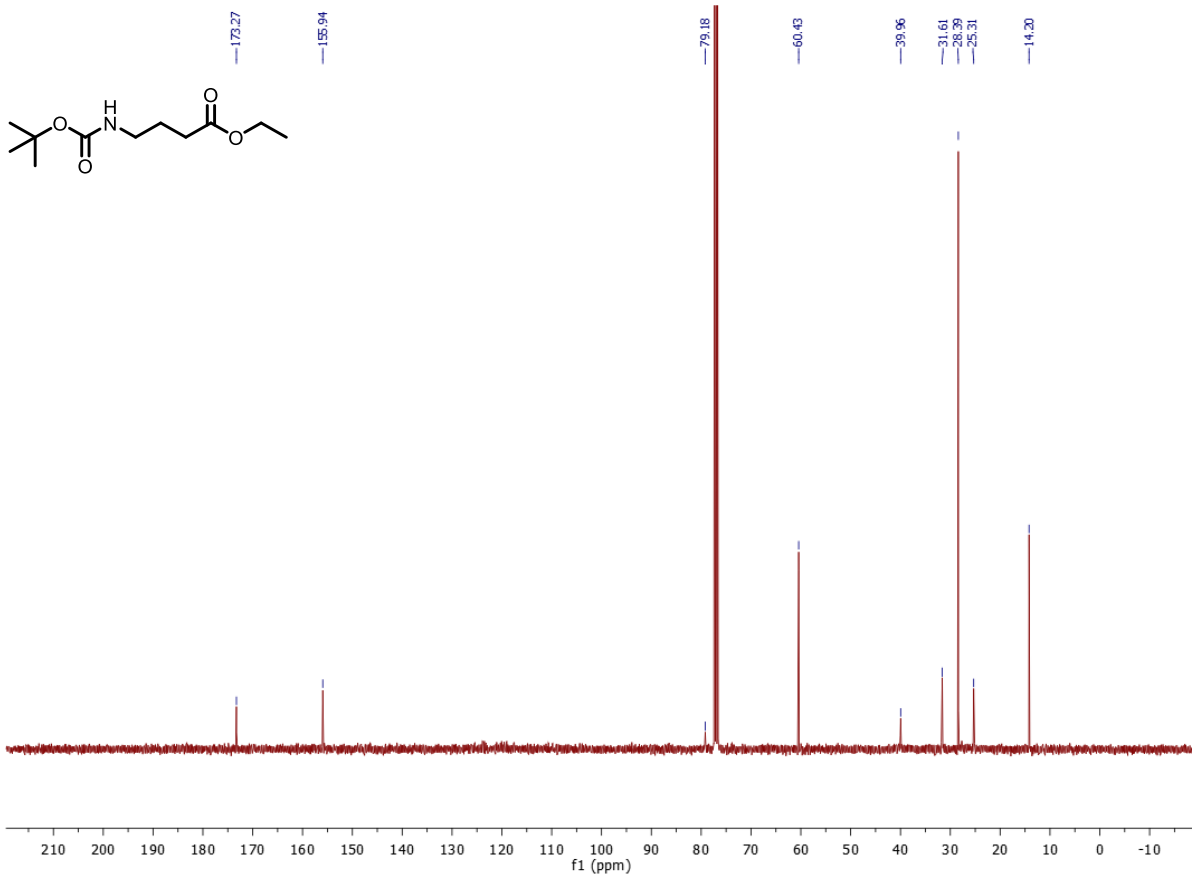
Tert-butyl (3-(4-methylthiazol-5-yl)propyl)carbamate (from 30)



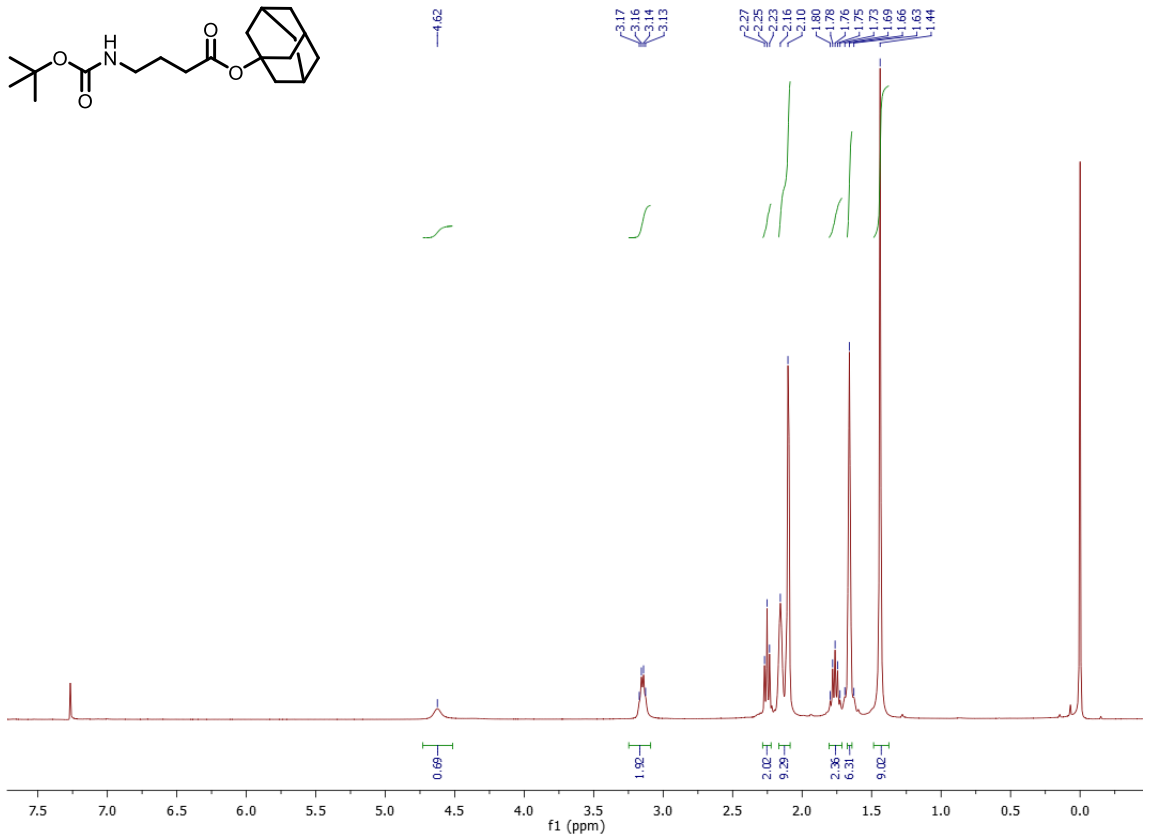


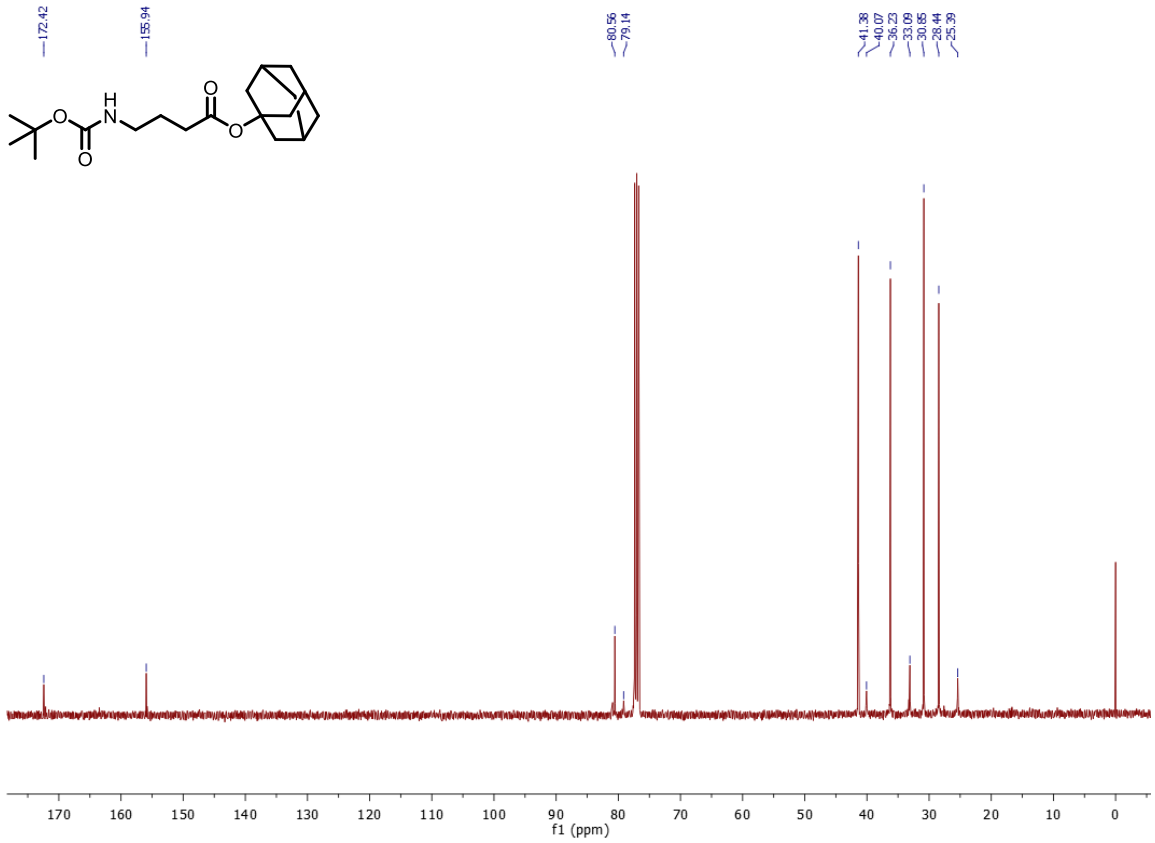
Ethyl 4-((tert-butoxycarbonyl)amino)butanoate (from 31)



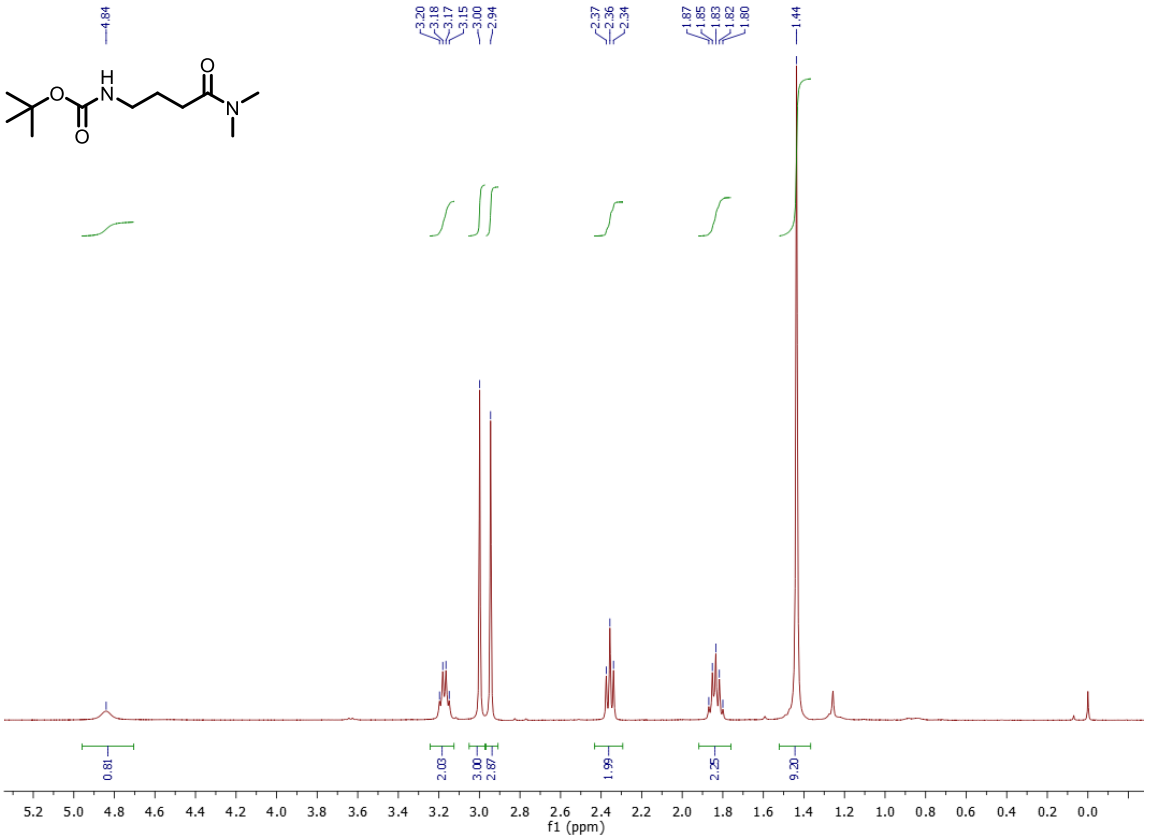


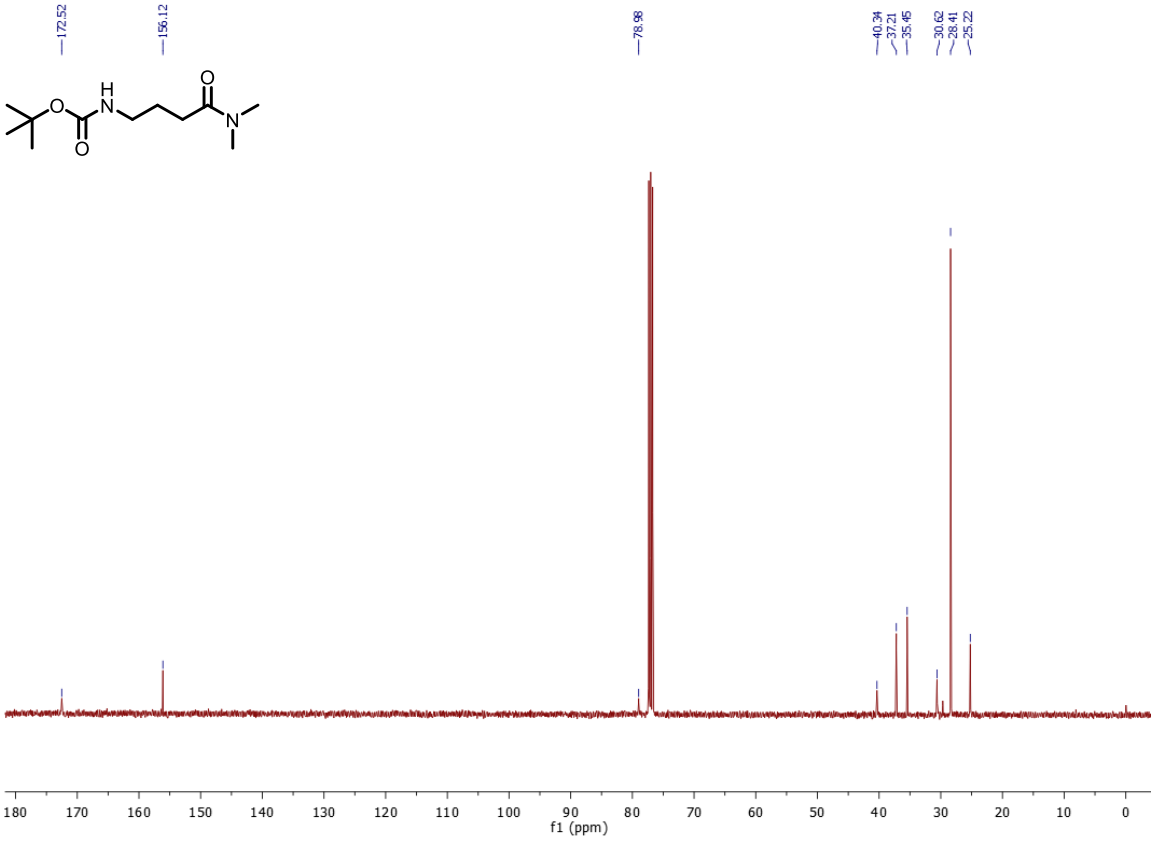
Adamantan-1-yl 4-((tert-butoxycarbonyl)amino)butanoate (from 32)



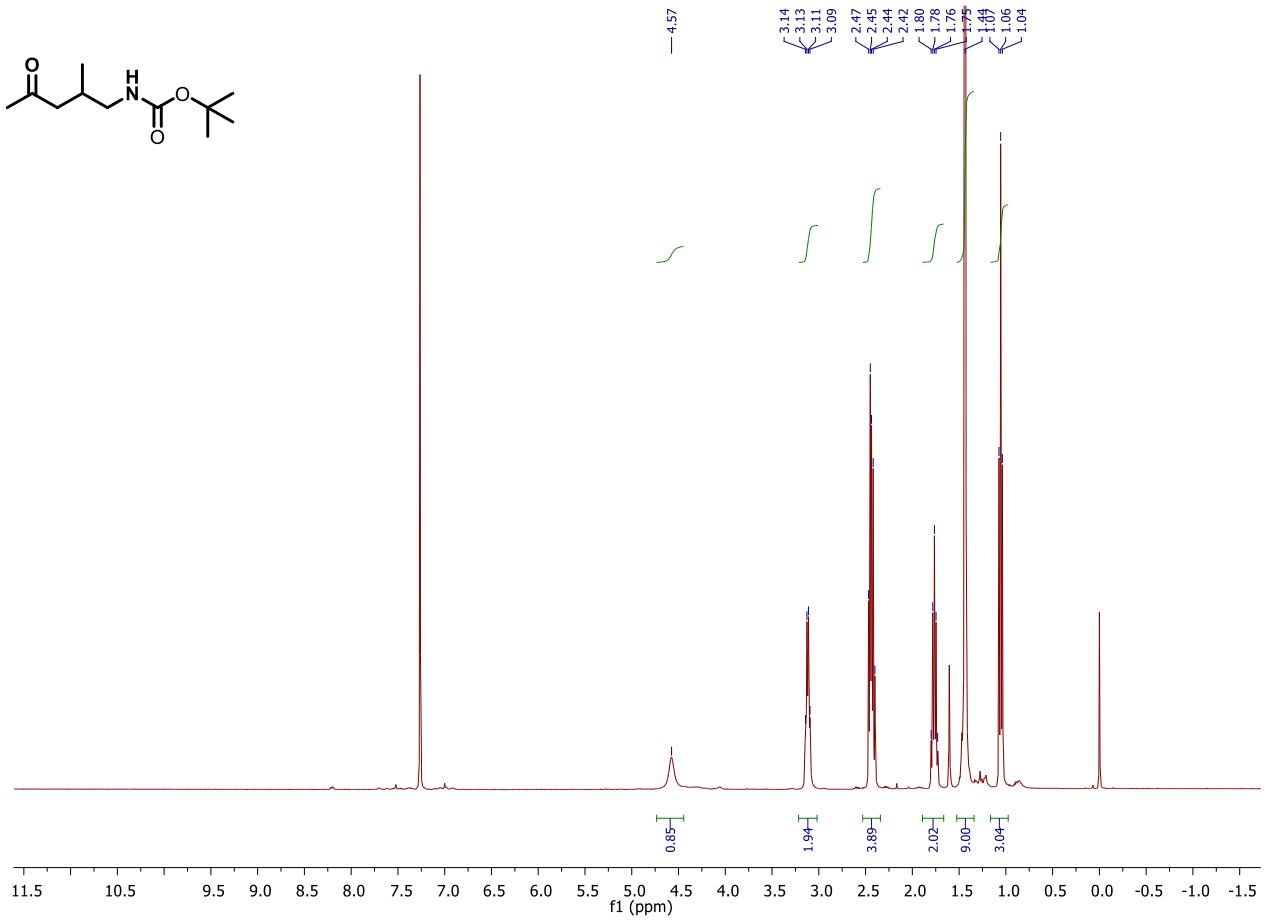


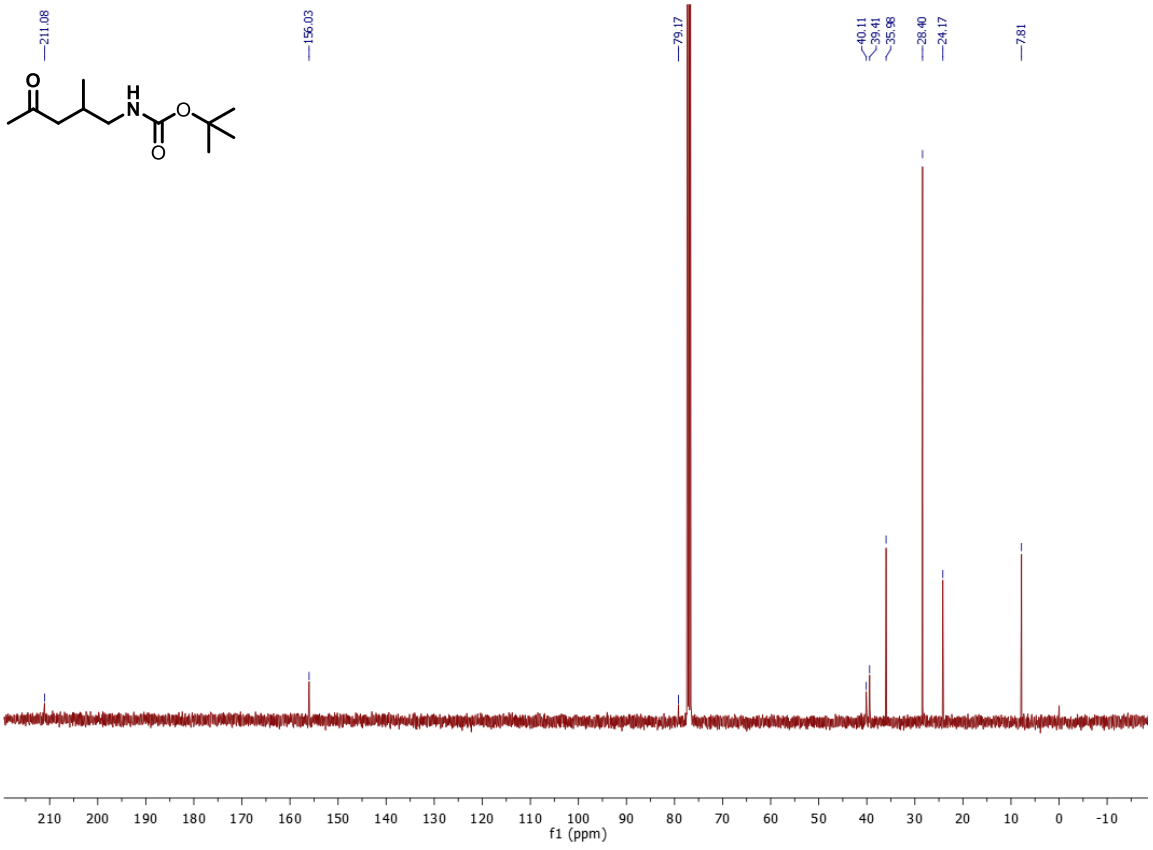
Tert-butyl (4-(dimethylamino)-4-oxobutyl)carbamate (from 33)



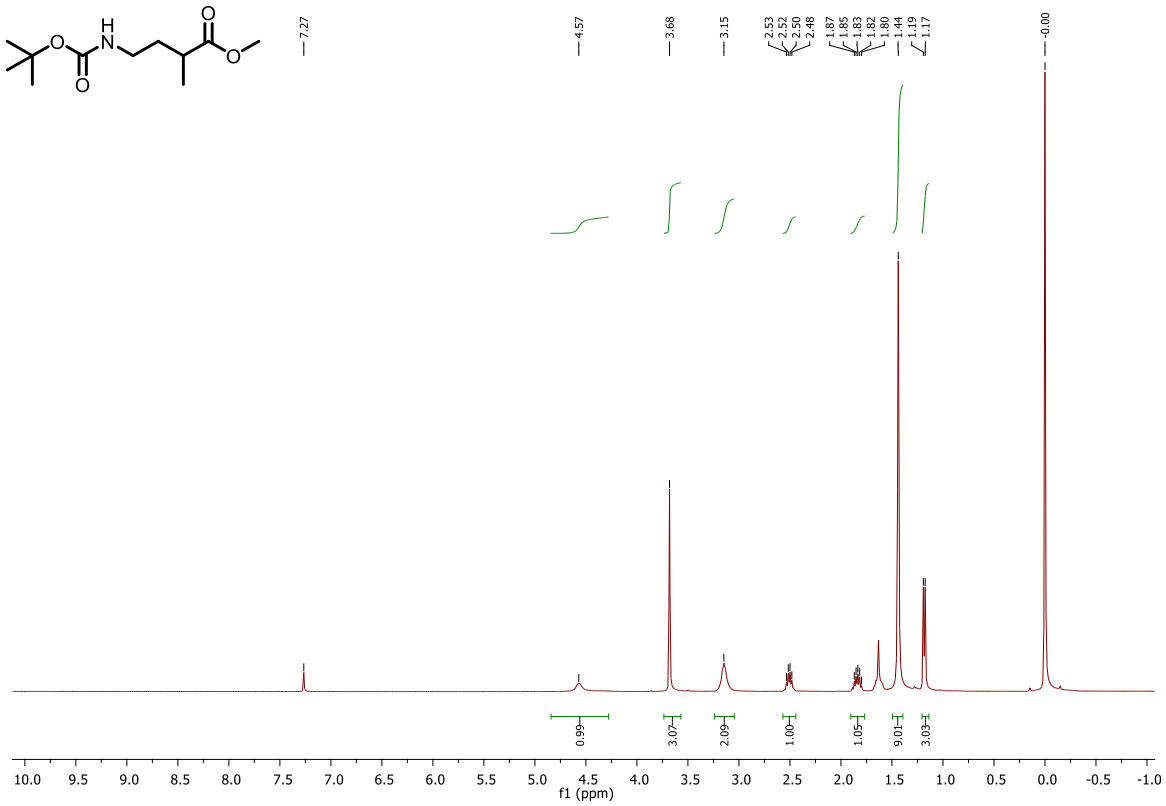


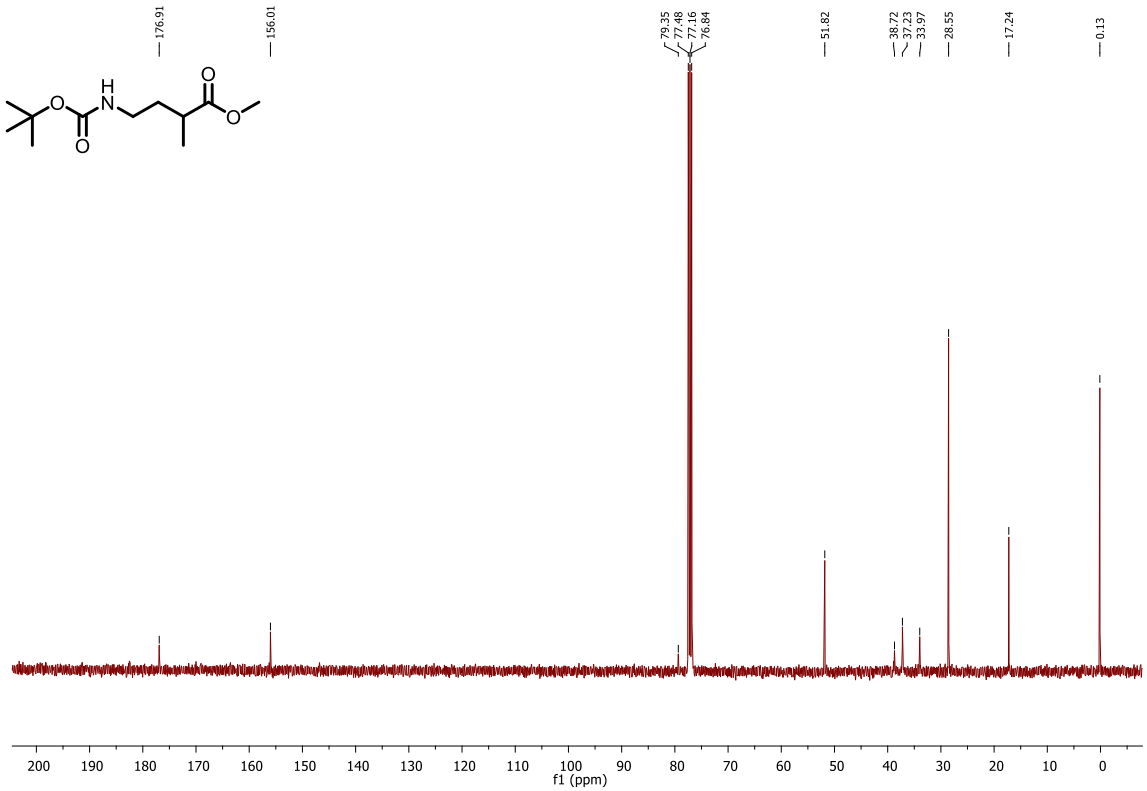
Tert-butyl (2-methyl-4-oxopentyl)carbamate (from 34)



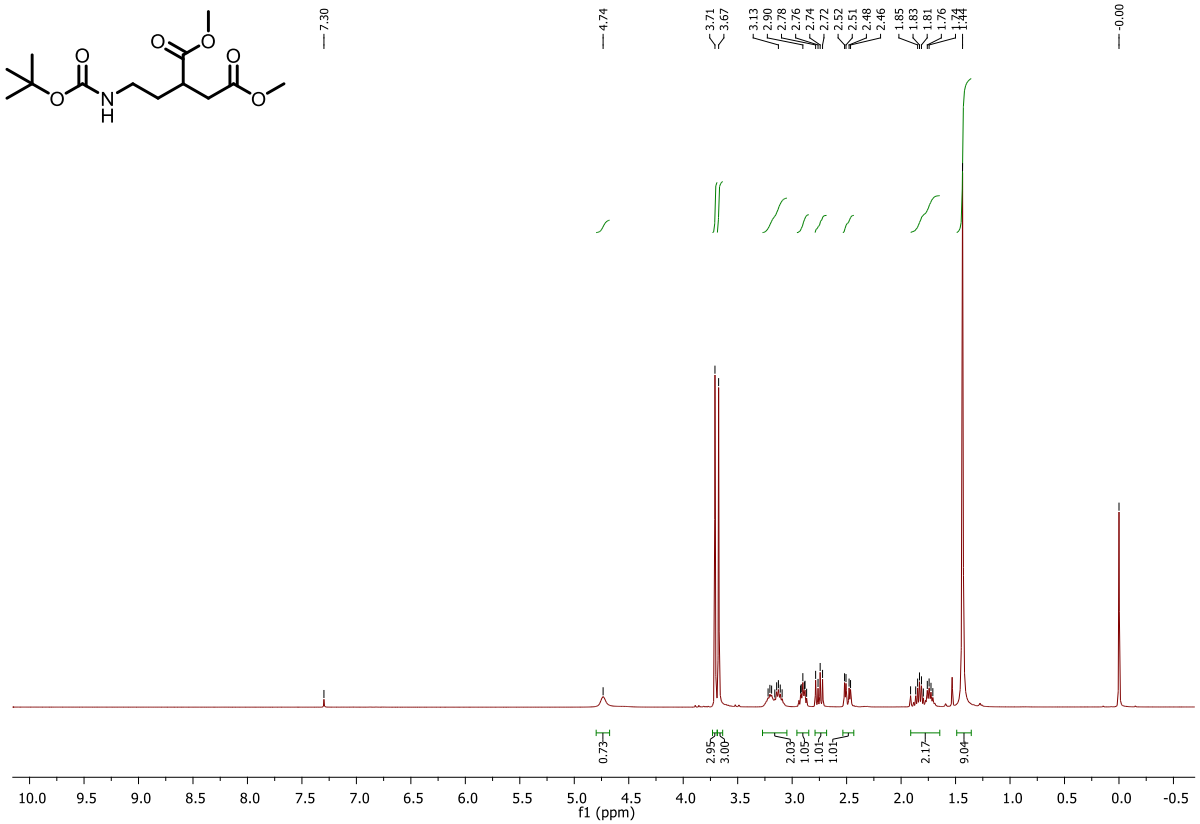


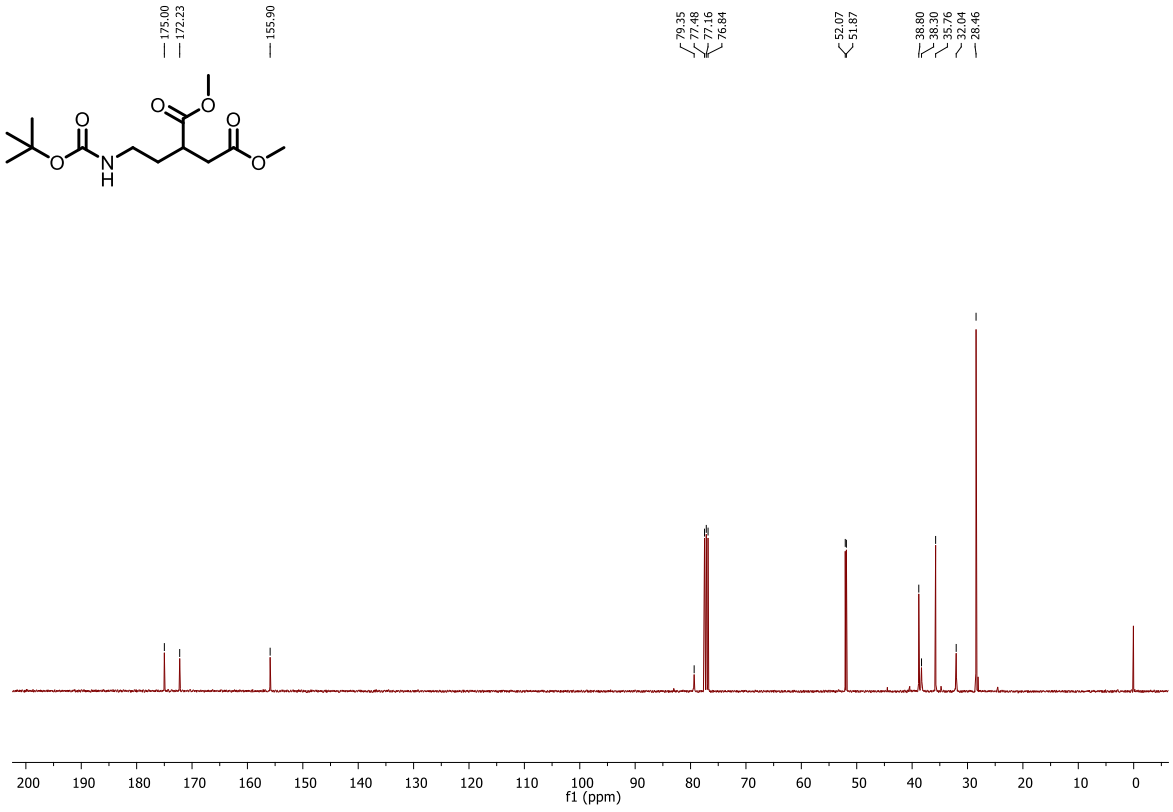
Methyl 4-((tert-butoxycarbonyl)amino)-2-methylbutanoate (from 35)



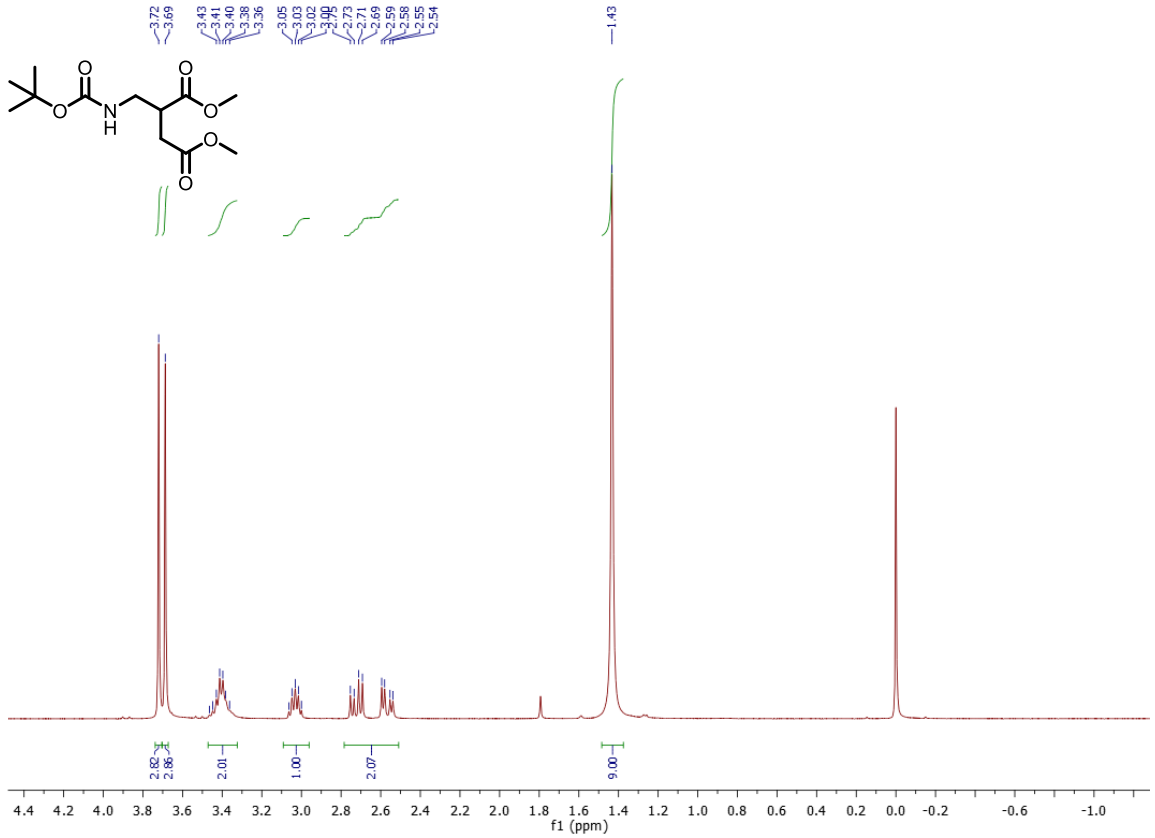


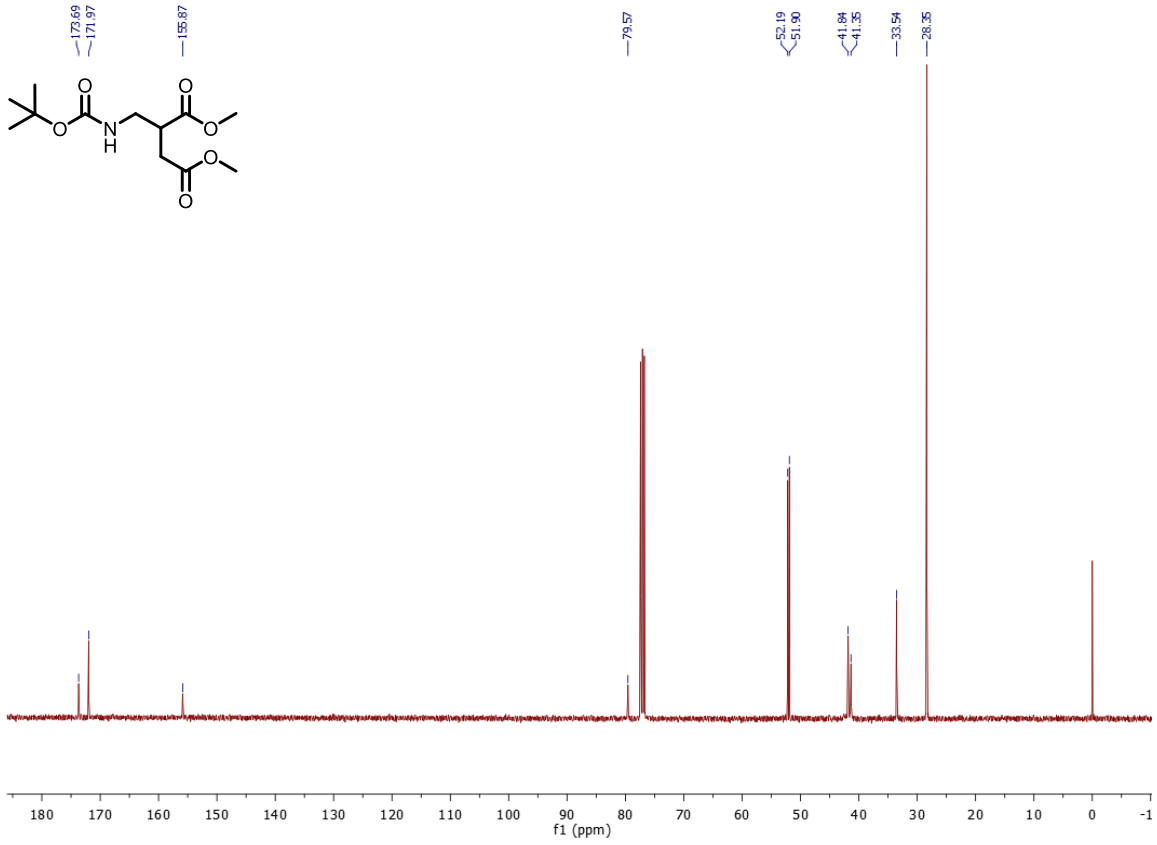
Dimethyl 2-(2-((tert-butoxycarbonyl)amino)ethyl)succinate (from 36)



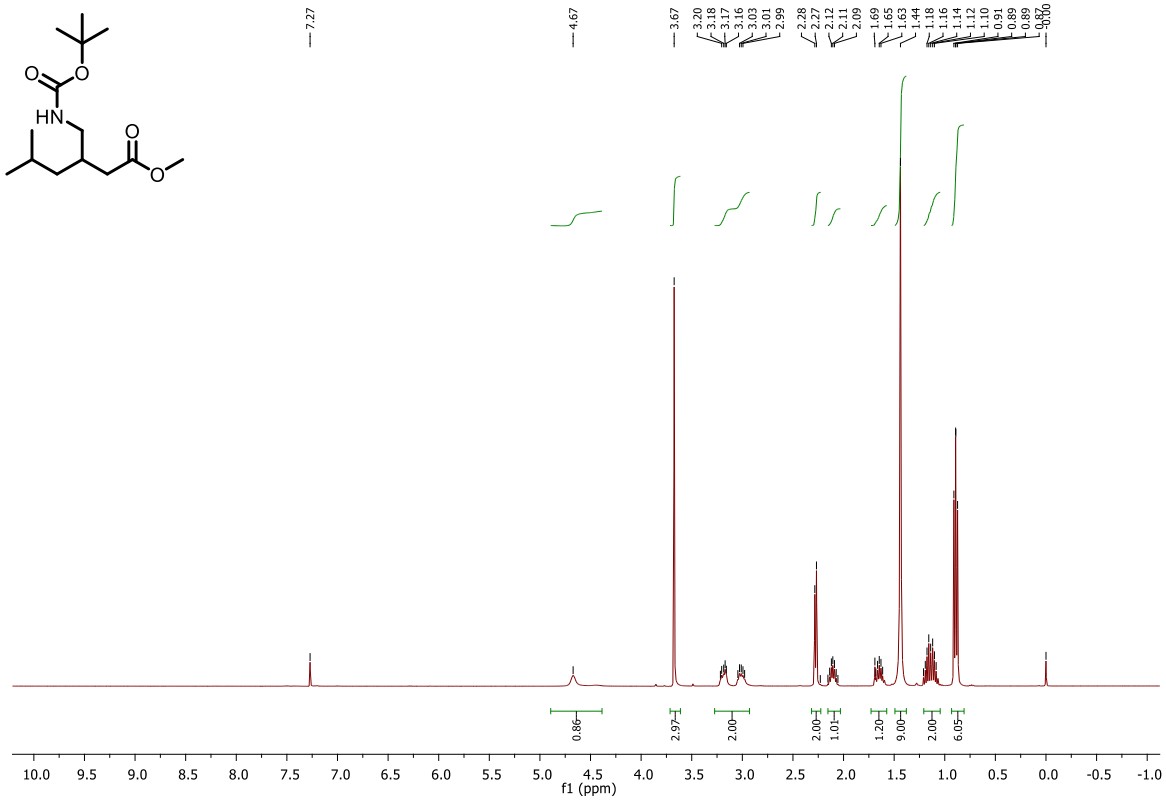


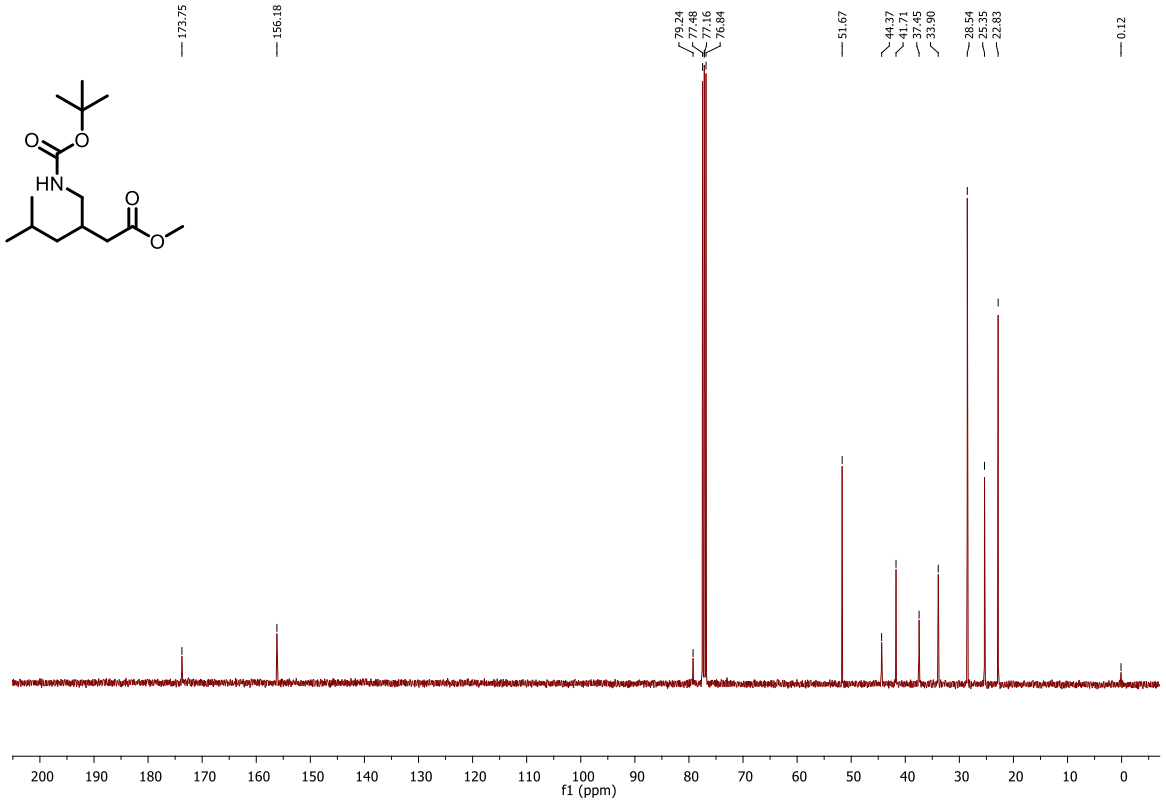
Dimethyl 2-(((tert-butoxycarbonyl)amino)methyl)succinate (from 37)



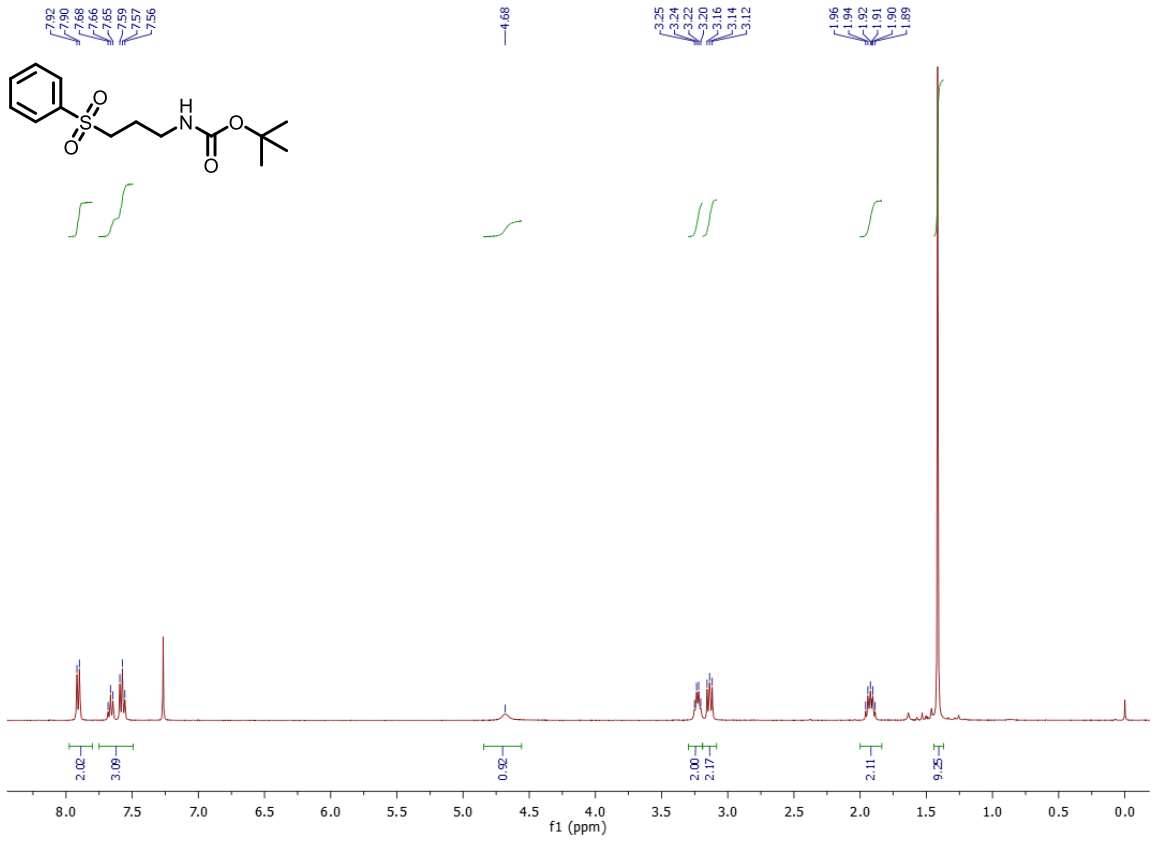


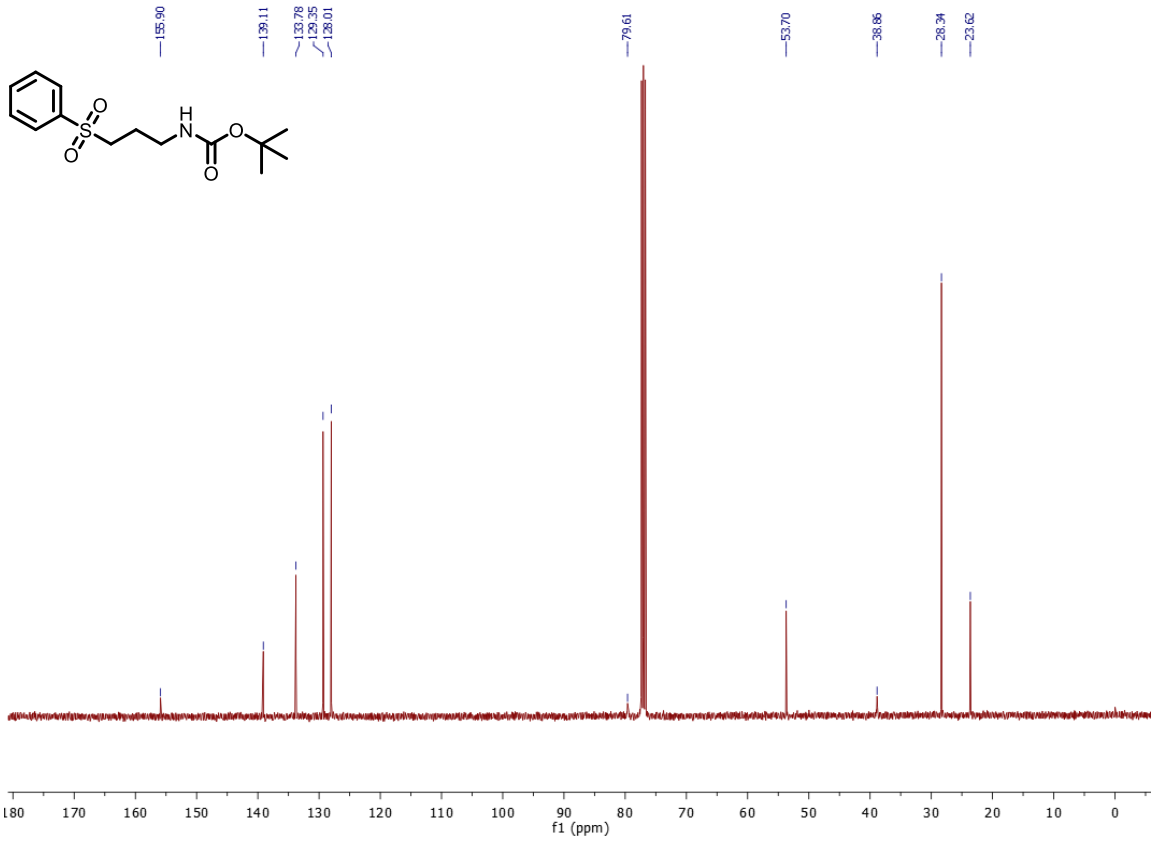
Methyl 3-(((tert-butoxycarbonyl)amino)methyl)-5-methylhexanoate (from 38)



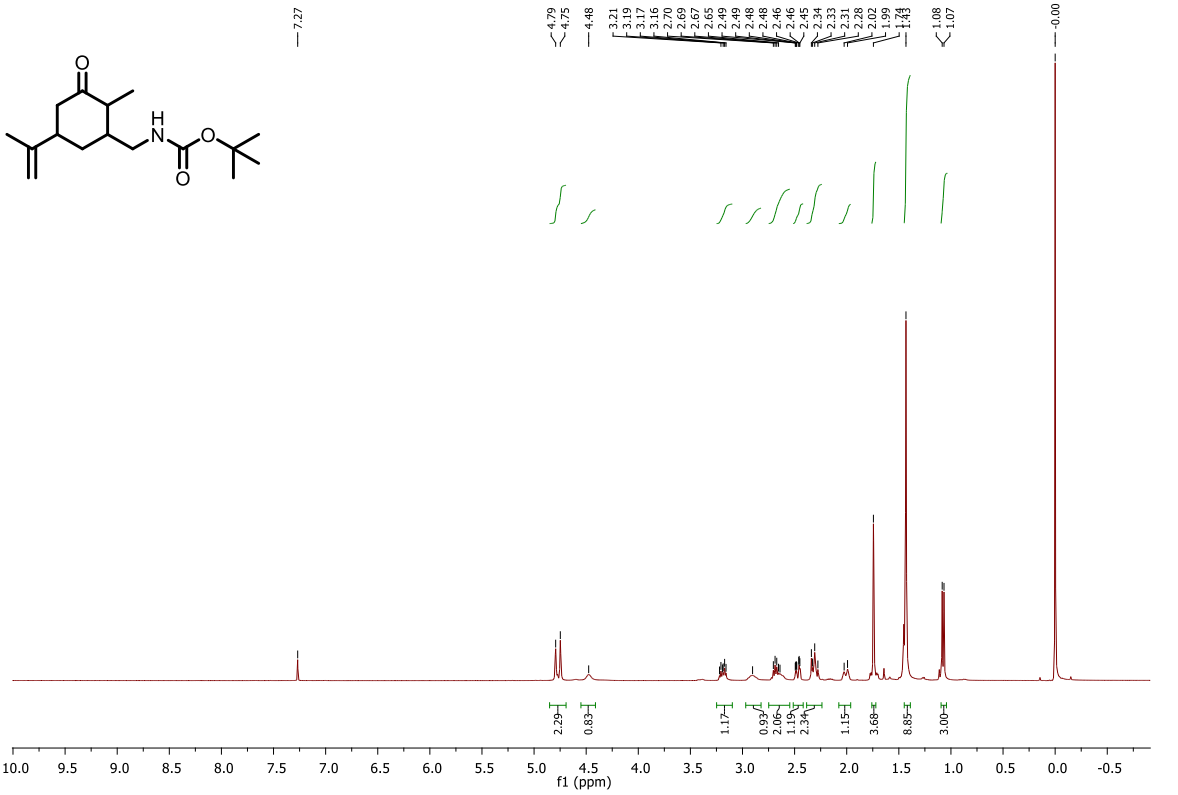


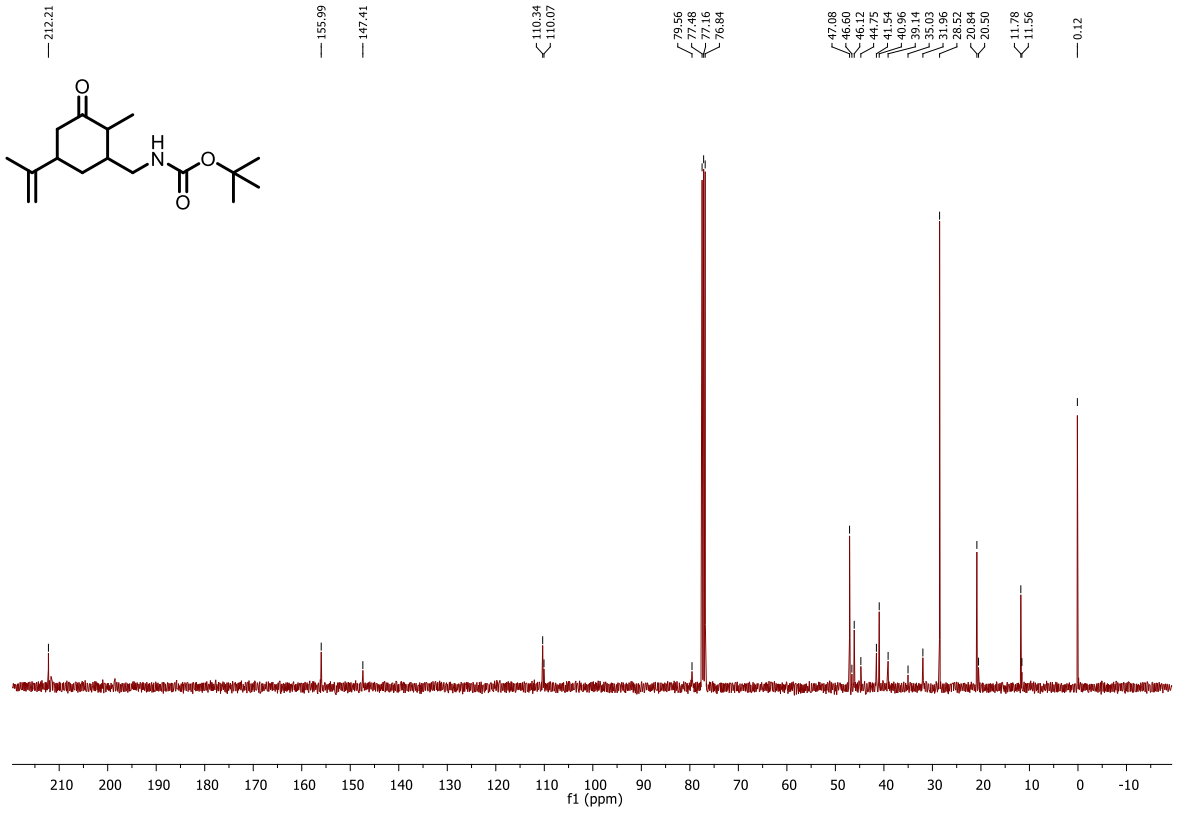
Tert-butyl (3-(phenylsulfonyl)propyl)carbamate (from 39)



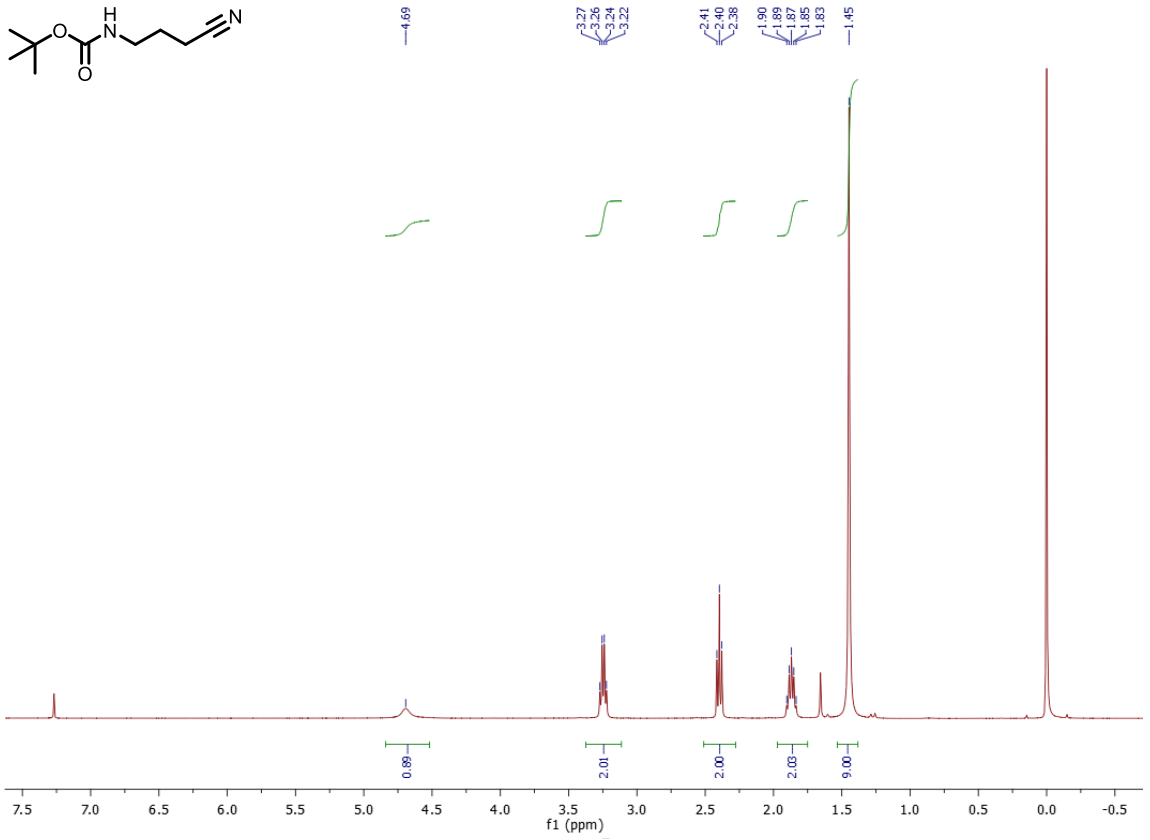


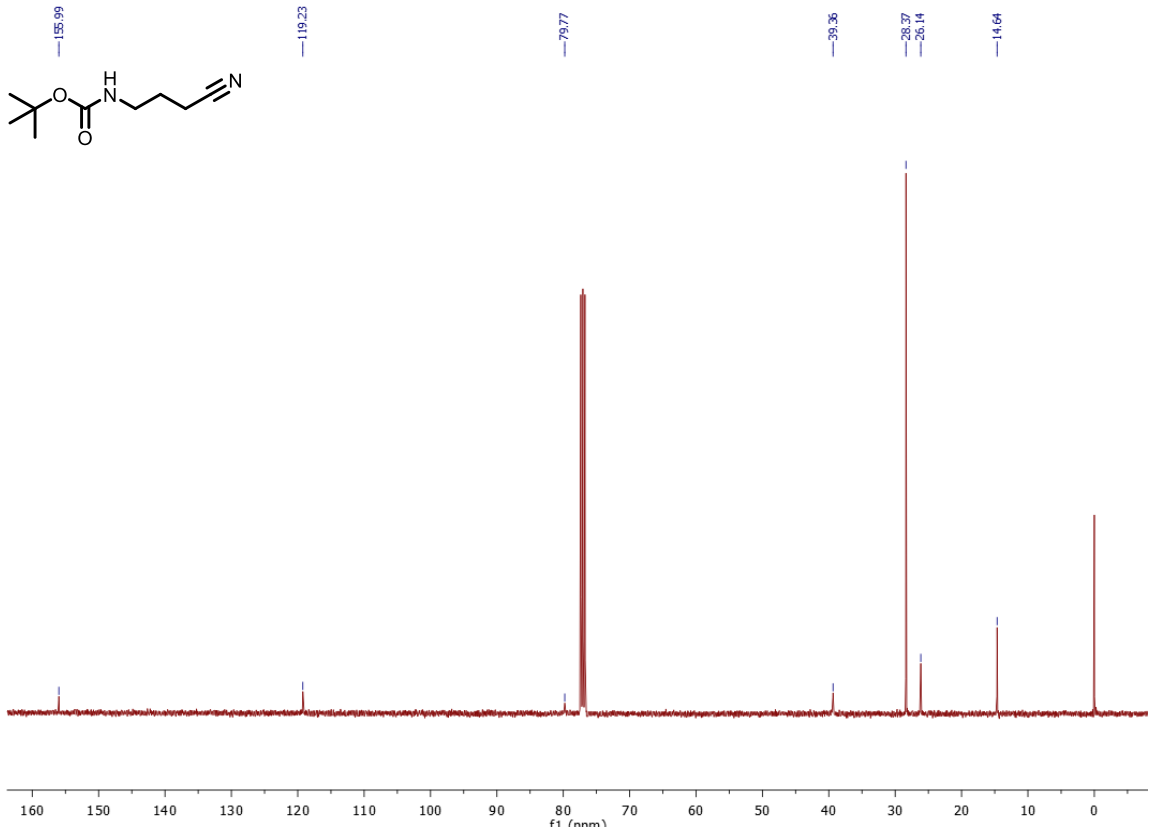
Tert-butyl ((2-methyl-3-oxo-5-(prop-1-en-2-yl)cyclohexyl)methyl)carbamate (from 40)



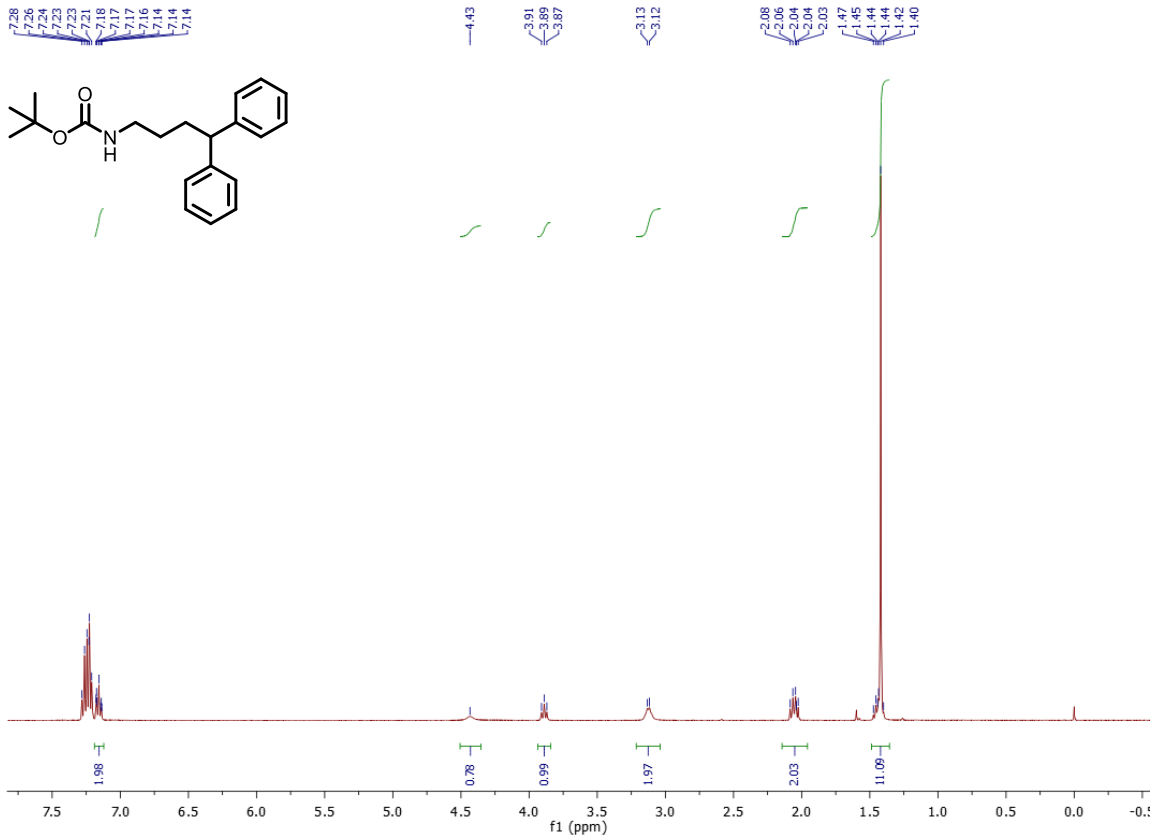


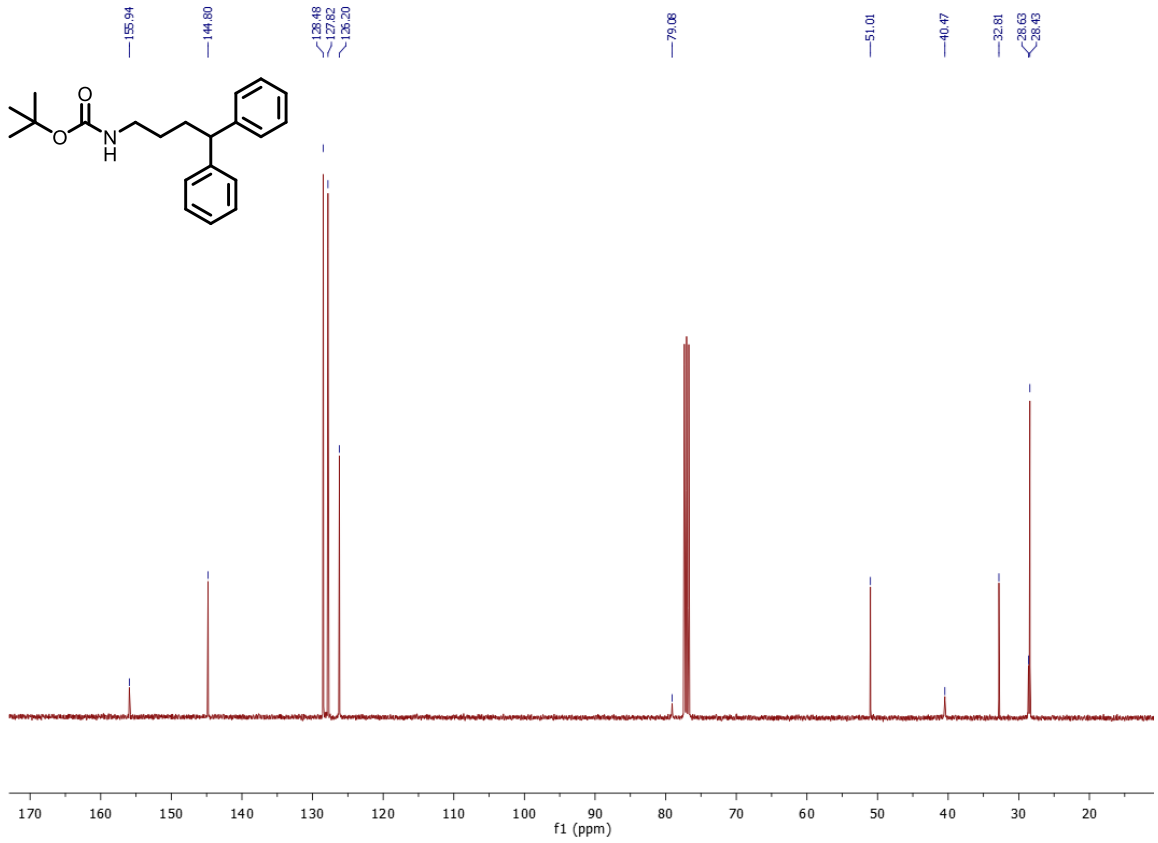
Tert-butyl (3-cyanopropyl)carbamate (from 41)



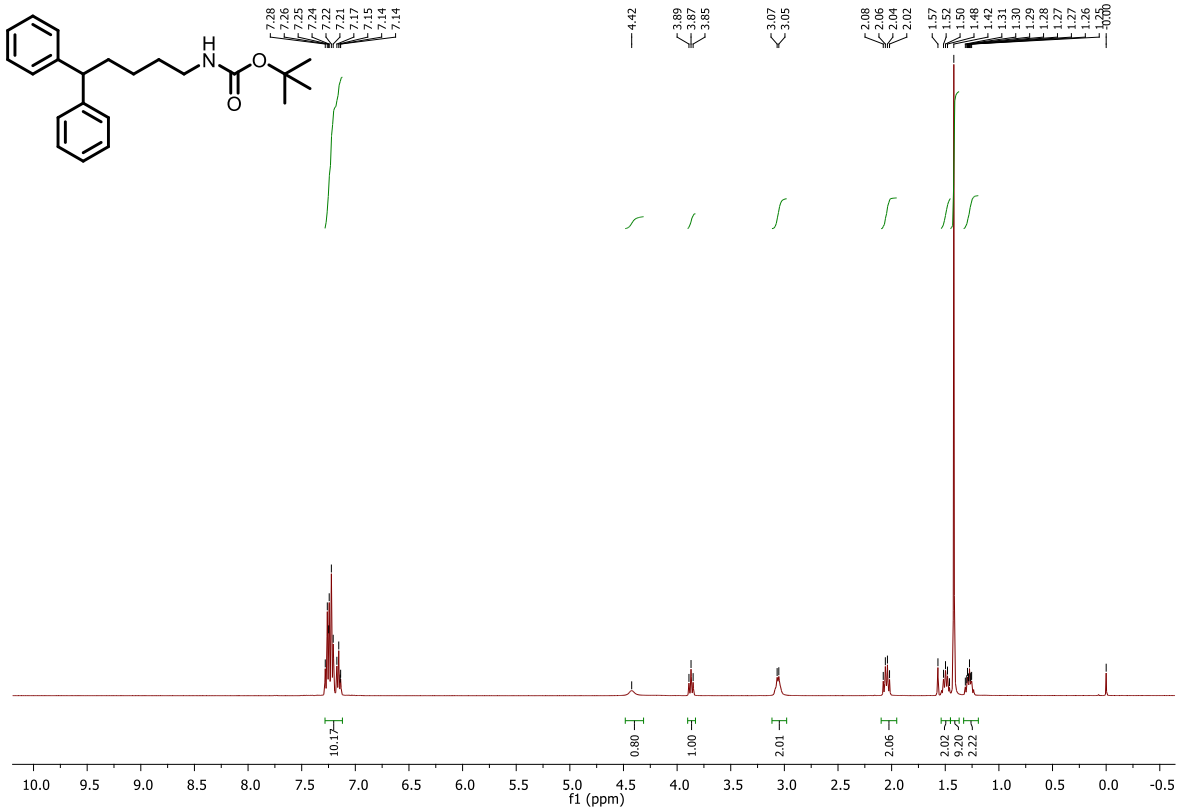


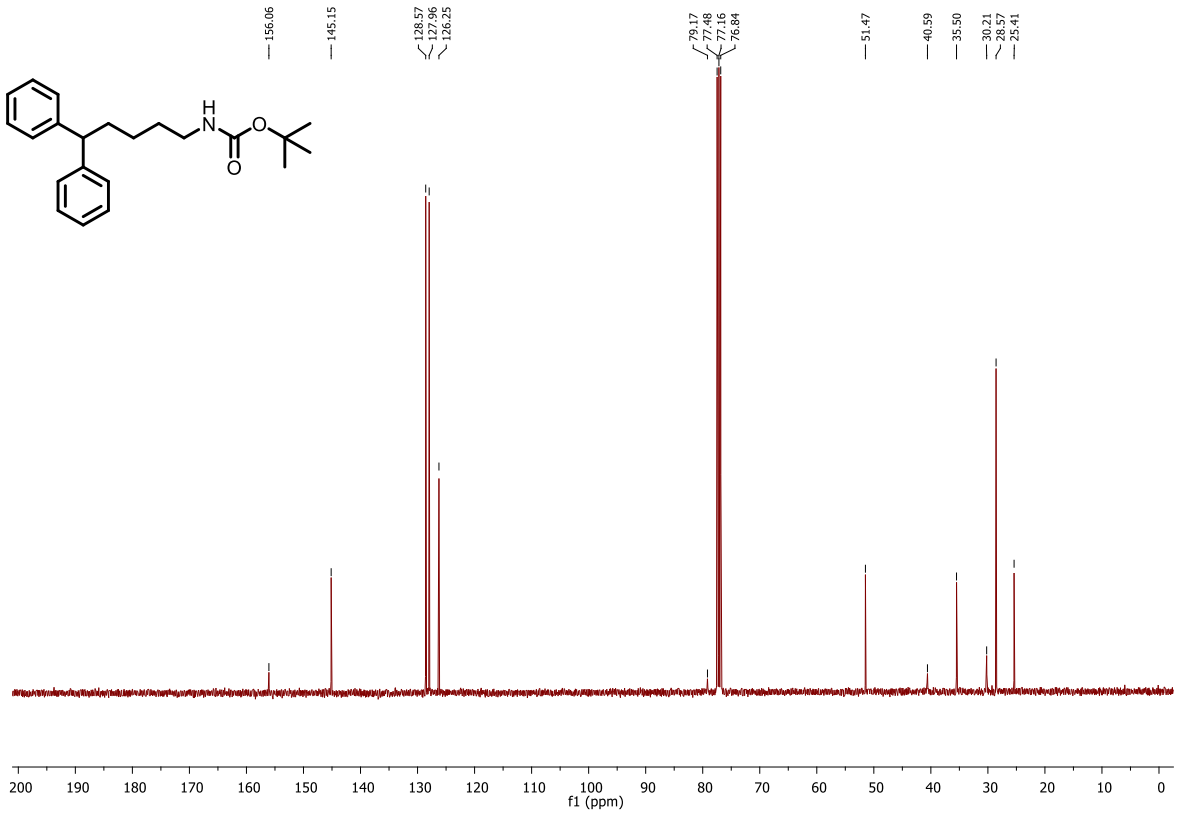
Tert-butyl (4,4-diphenylbutyl)carbamate (from 42)



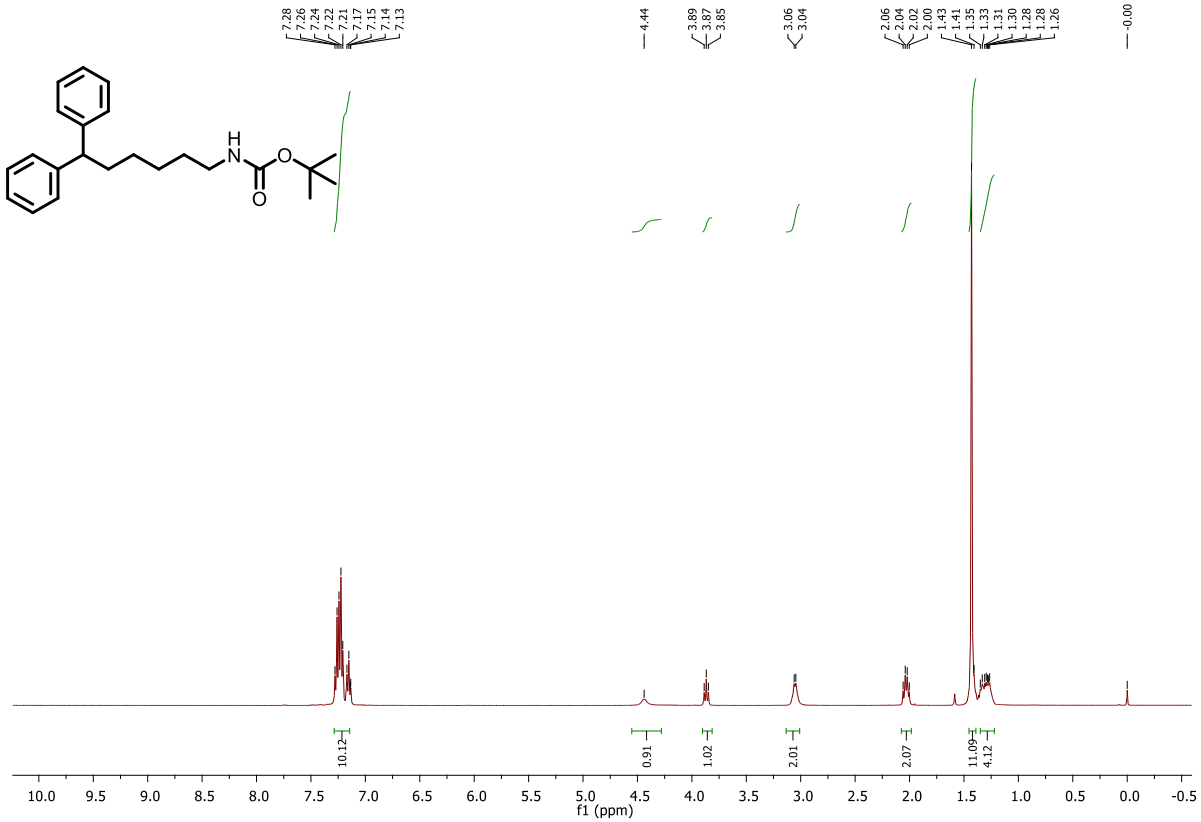


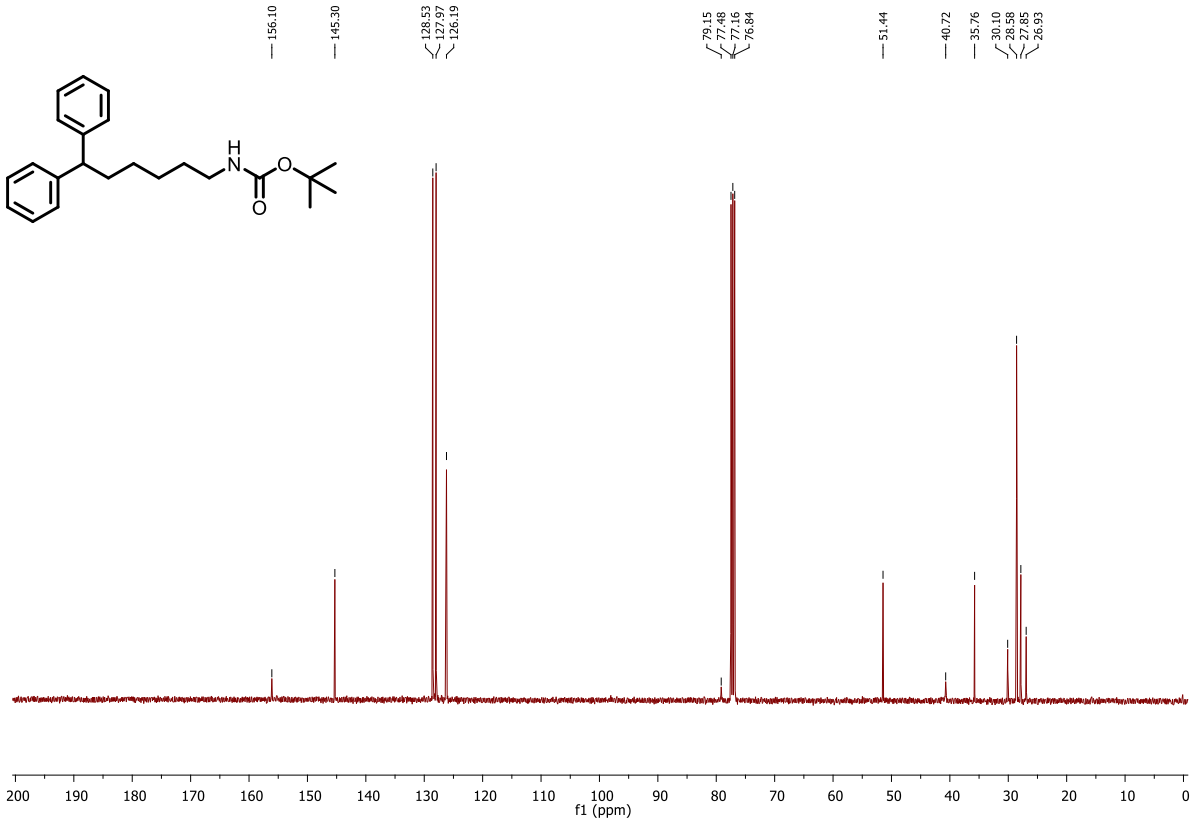
Tert-butyl (5,5-diphenylpentyl)carbamate (from 43)



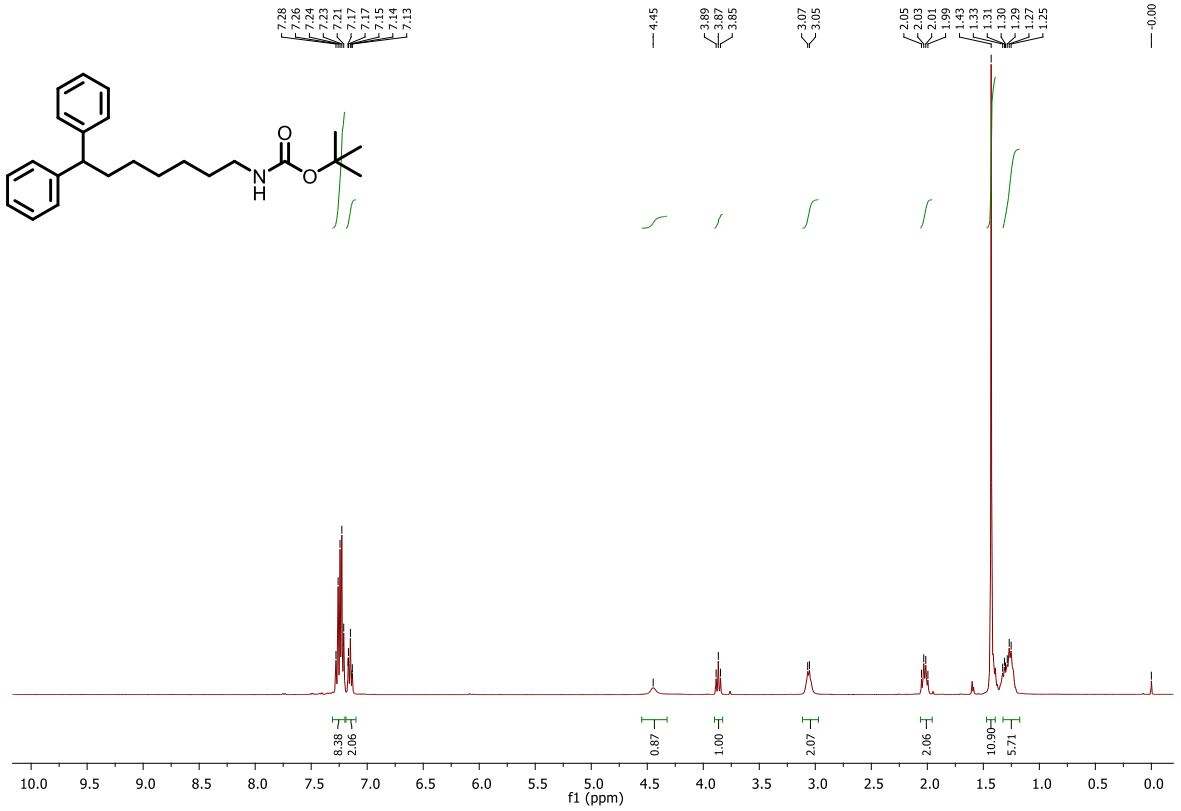


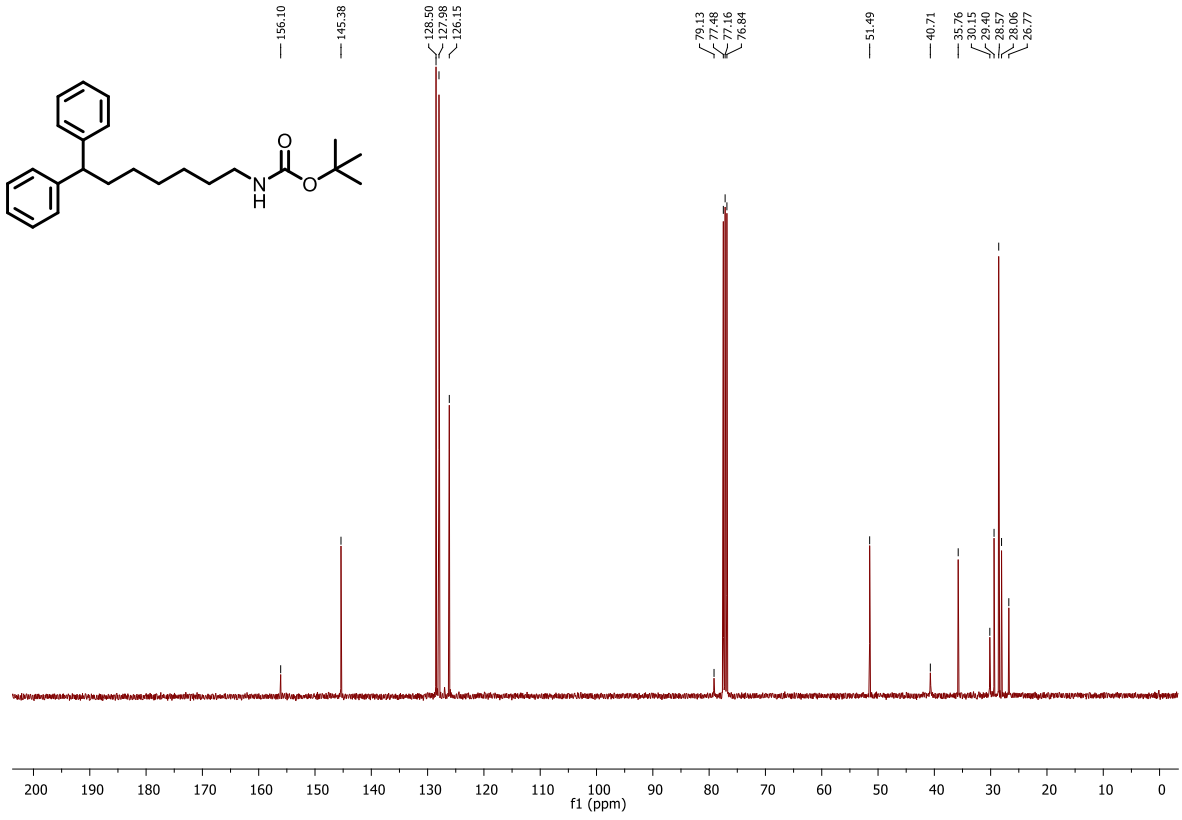
Tert-butyl (6,6-diphenylhexyl)carbamate (from 44)



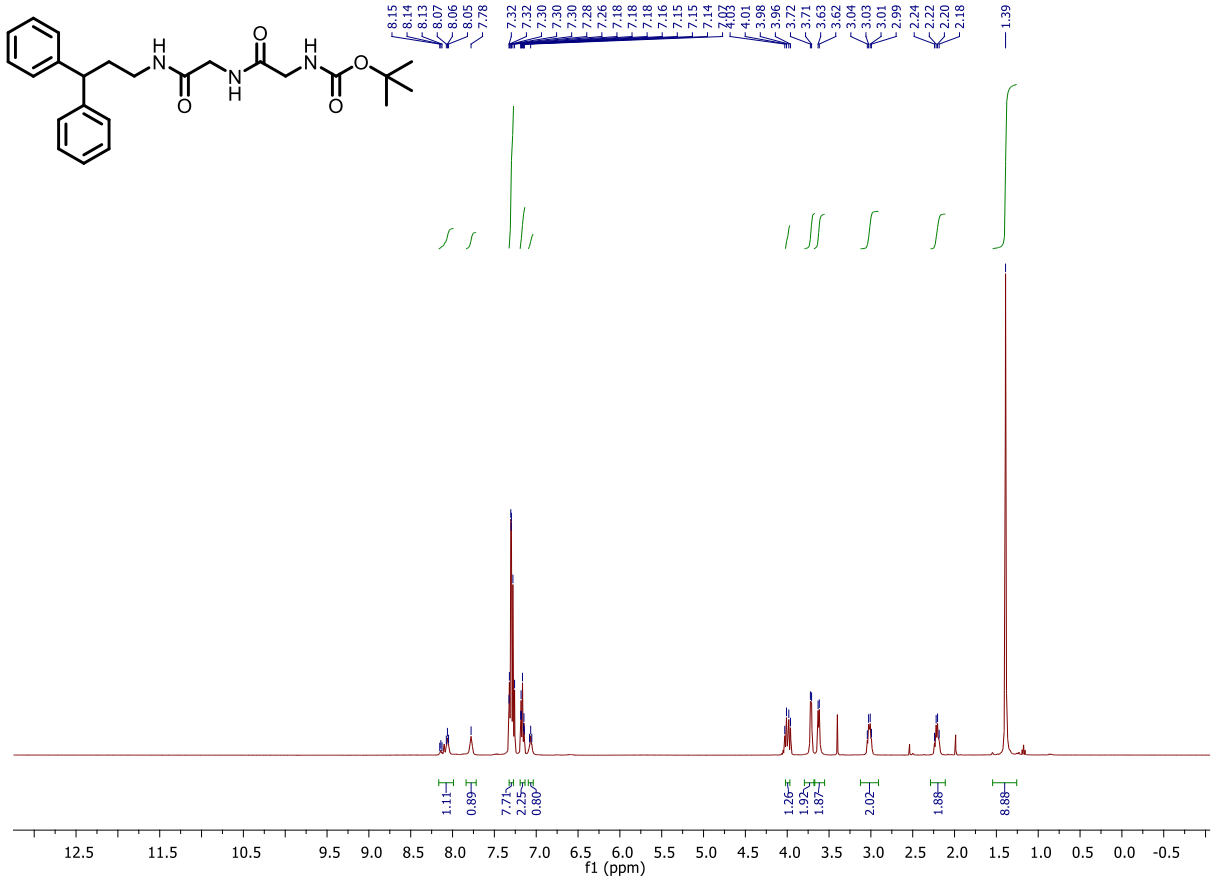


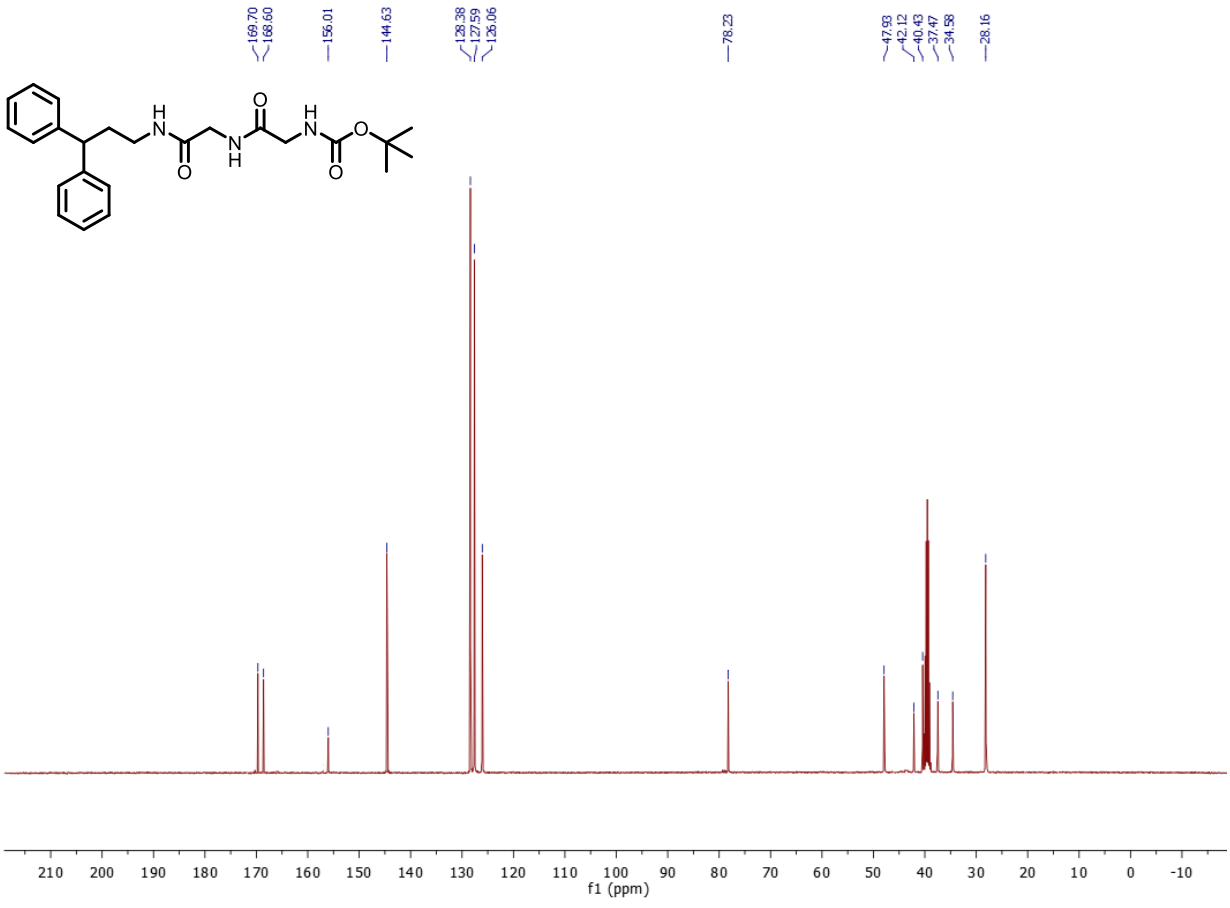
Tert-butyl (7,7-diphenylheptyl)carbamate (from 45)



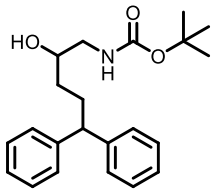


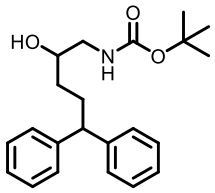
Tert-butyl (2-((2-((3,3-diphenylpropyl)amino)-2-oxoethyl)amino)-2-oxoethyl)carbamate (from 46)



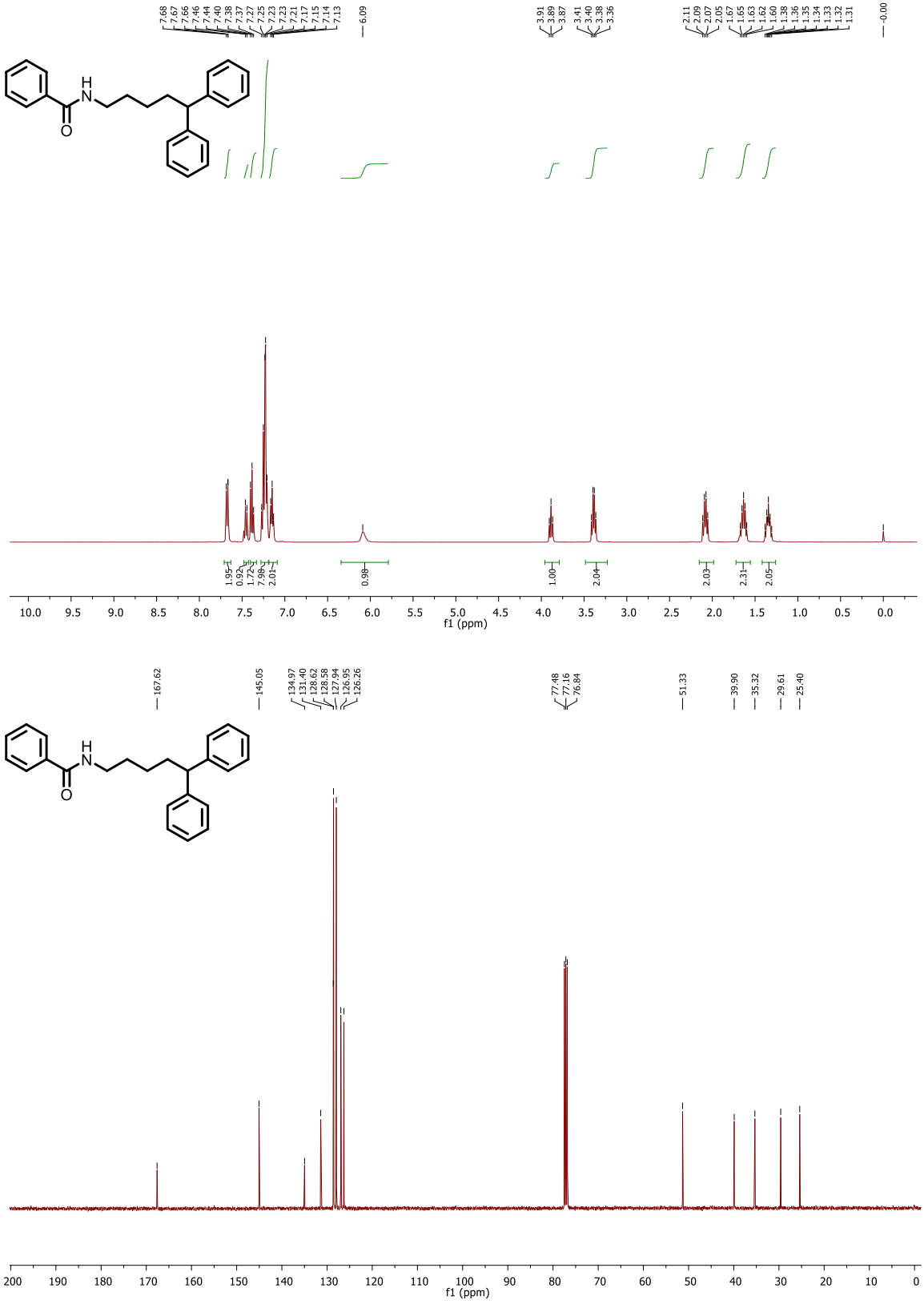


Tert-butyl (2-hydroxy-5,5-diphenylpentyl)carbamate (from 47)

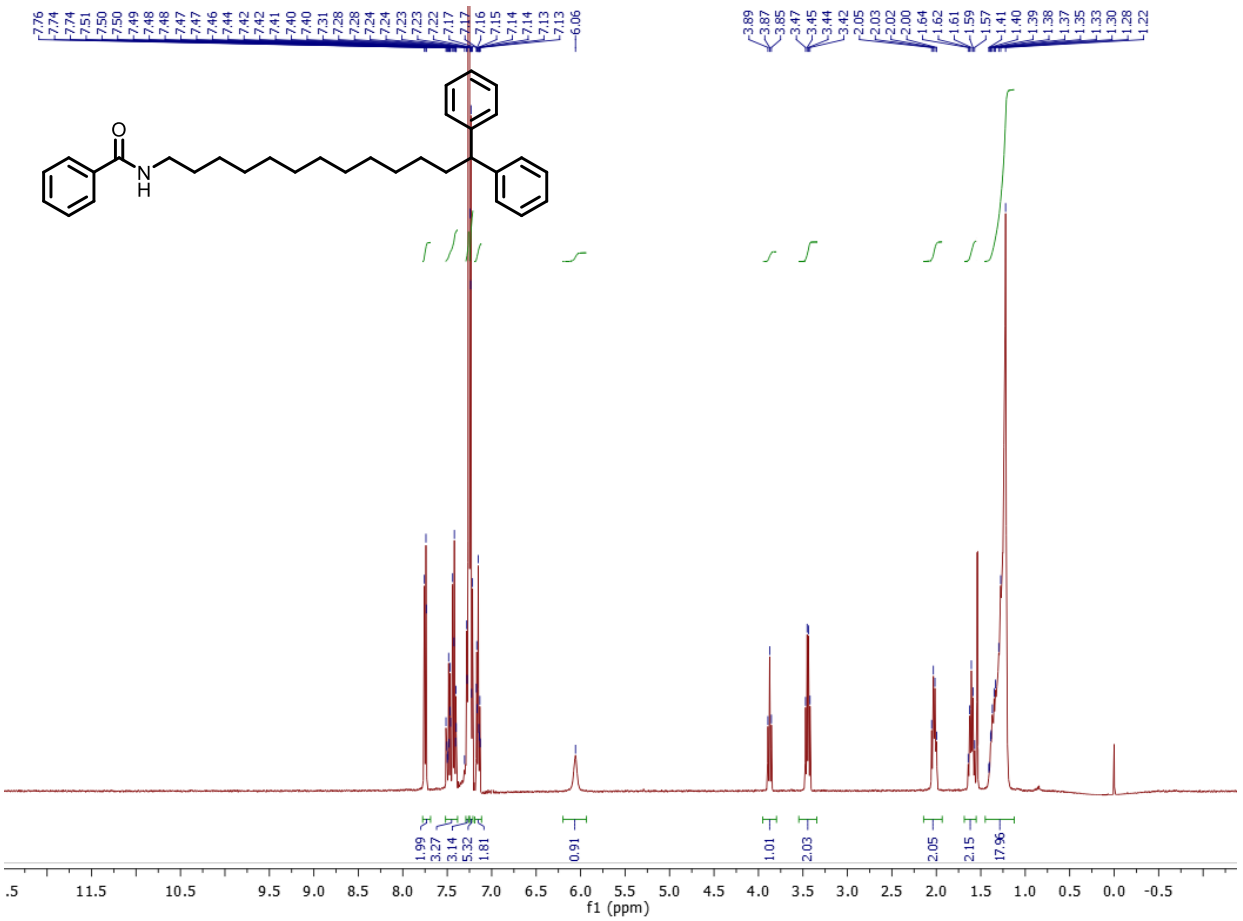


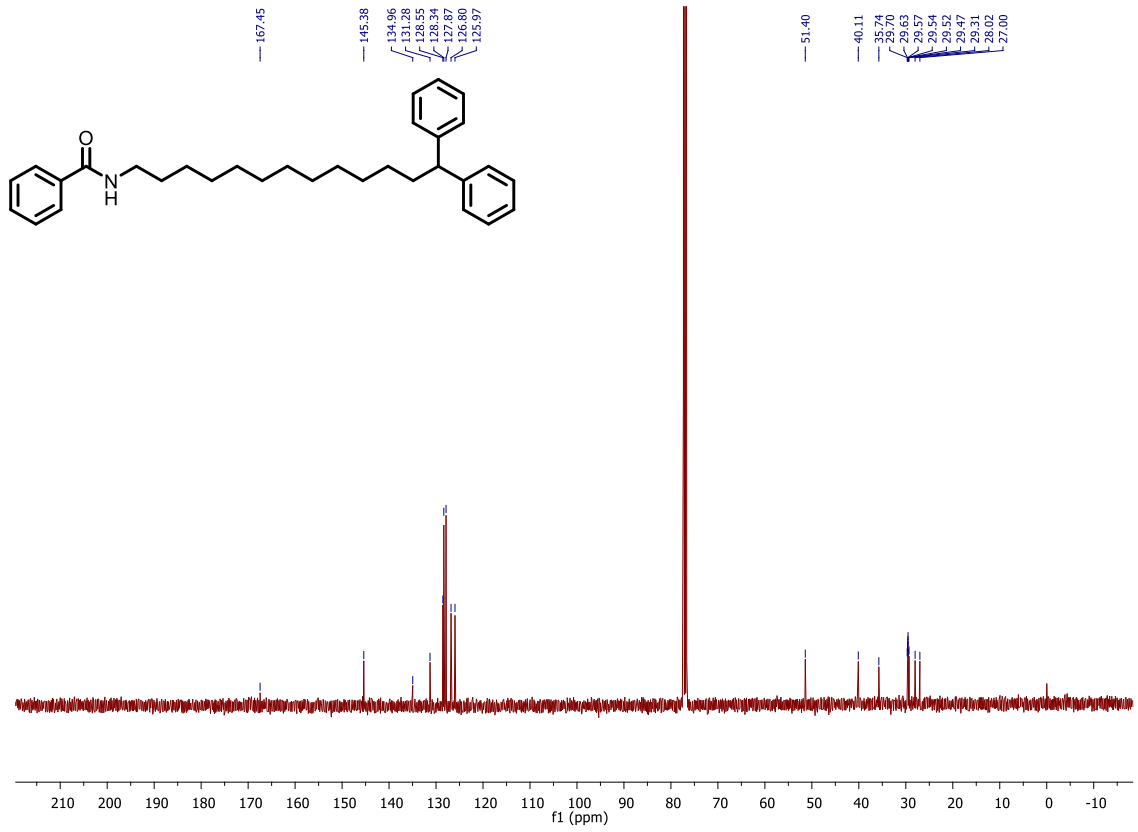


N-(5,5-diphenylpentyl)benzamide (from 48)

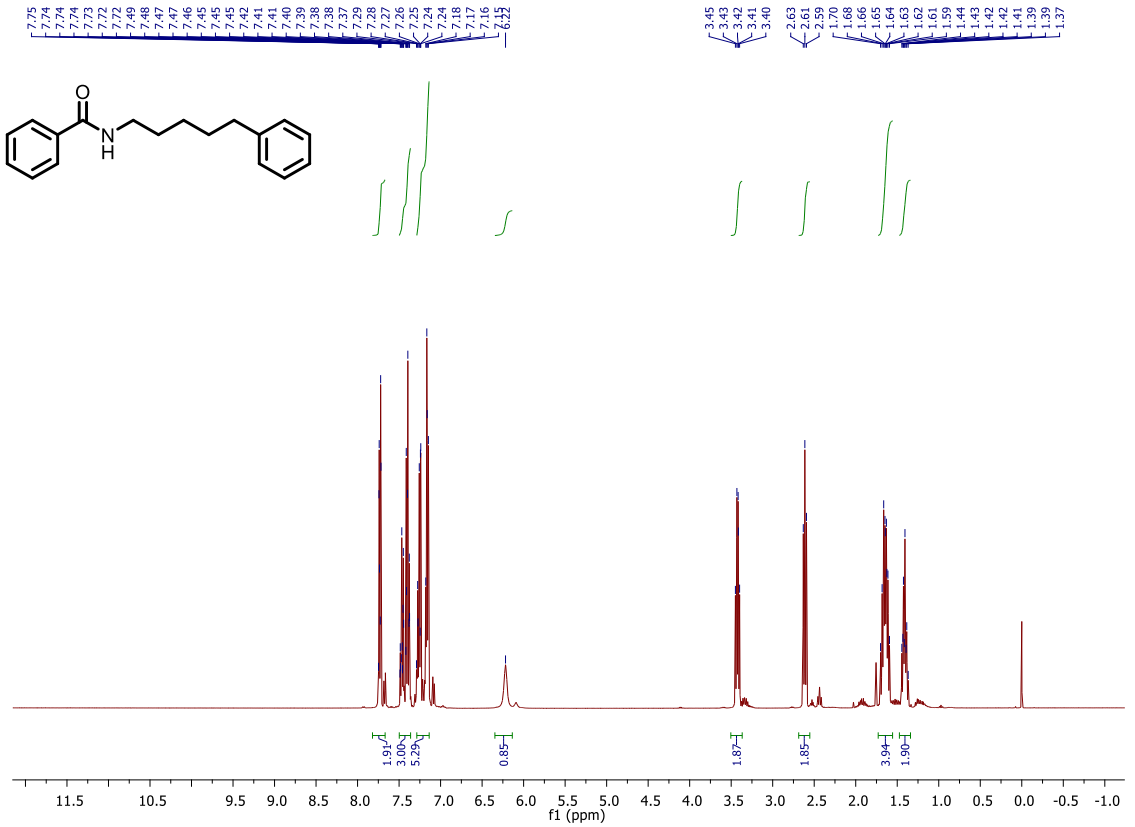


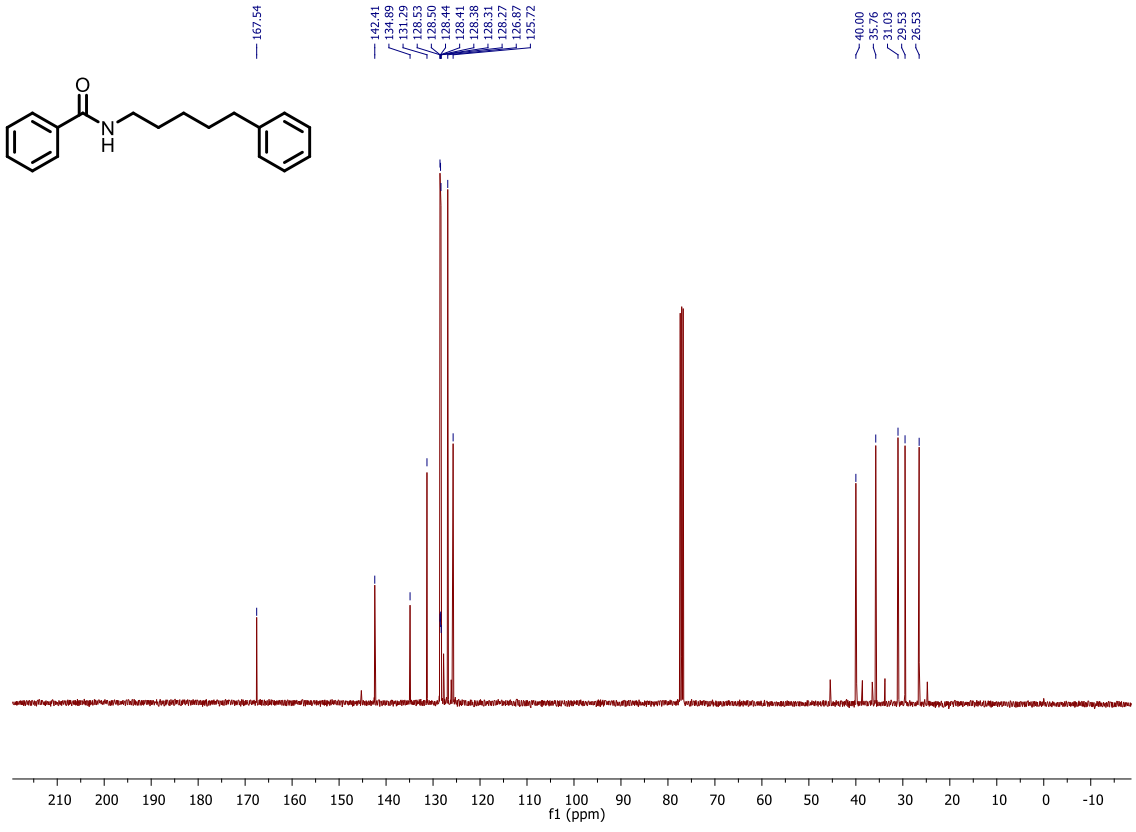
N-(12,12-diphenyldodecyl)benzamide (from 49)



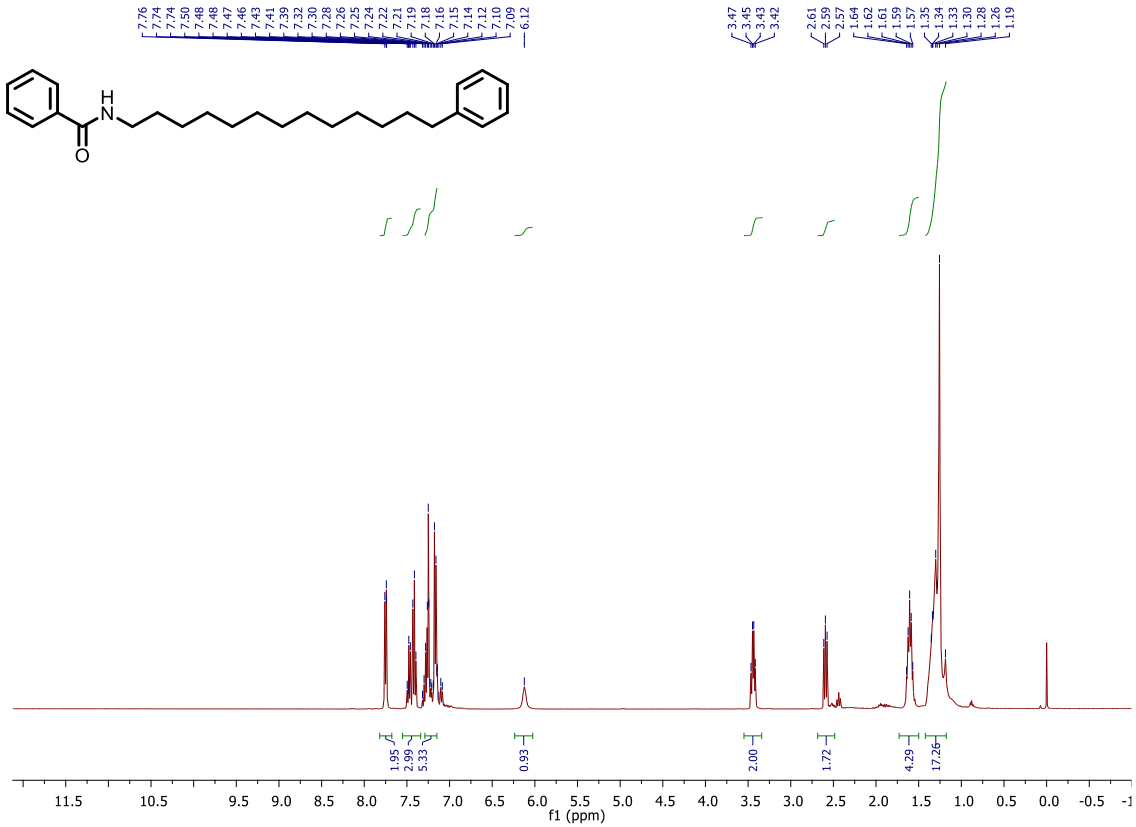


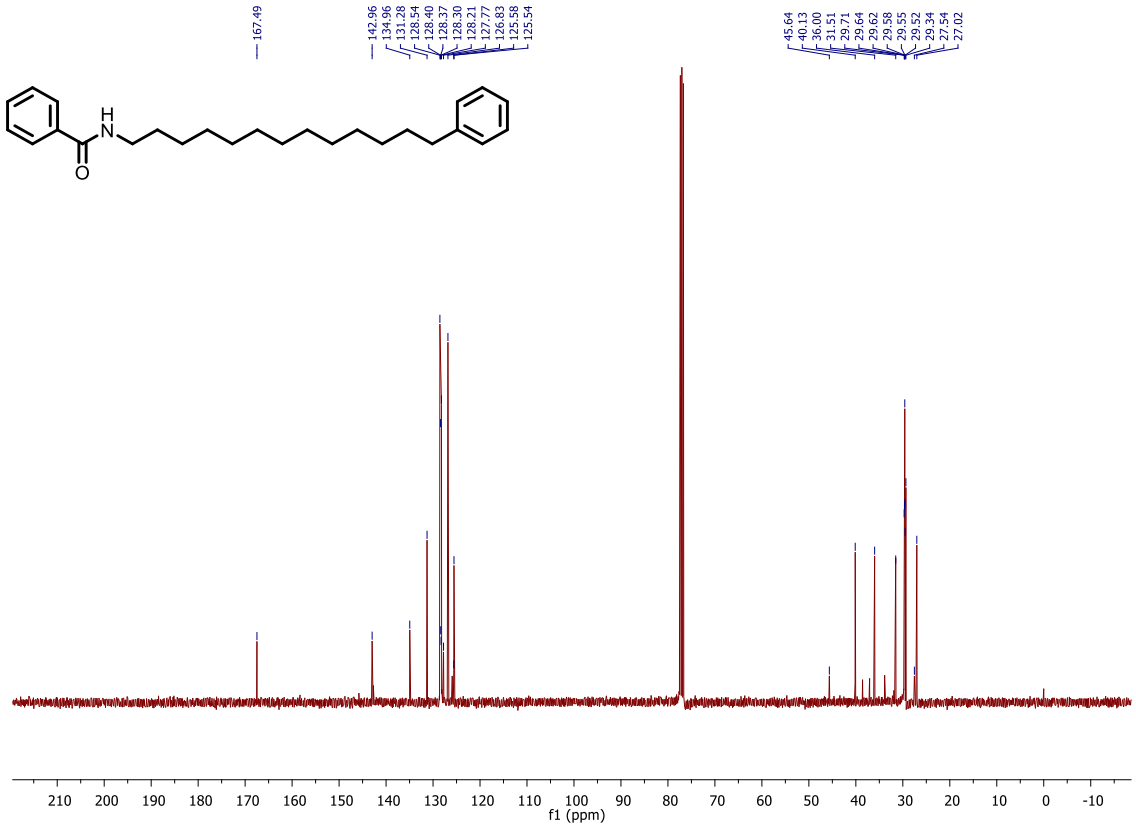
N-(5-phenylpentyl)benzamide (50)



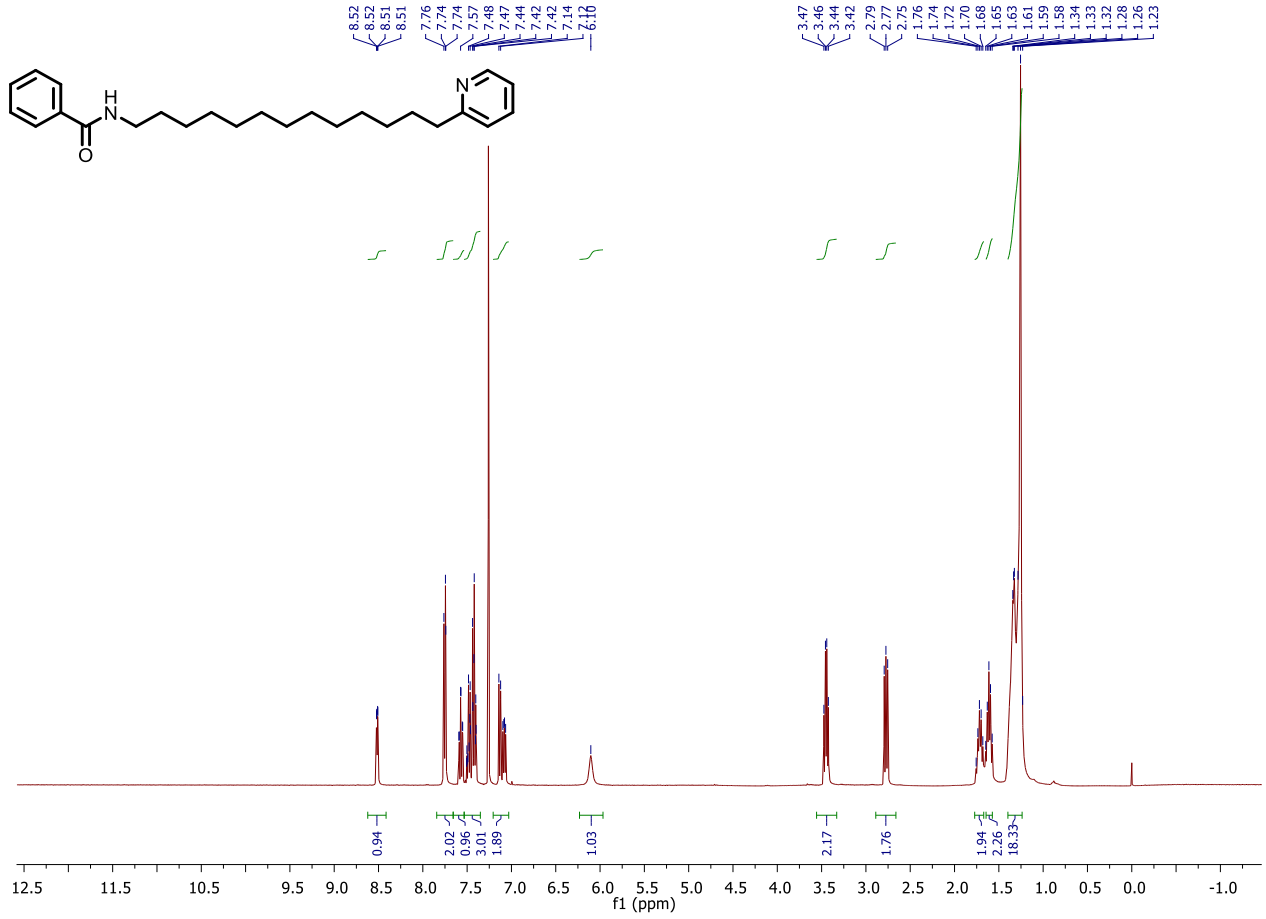


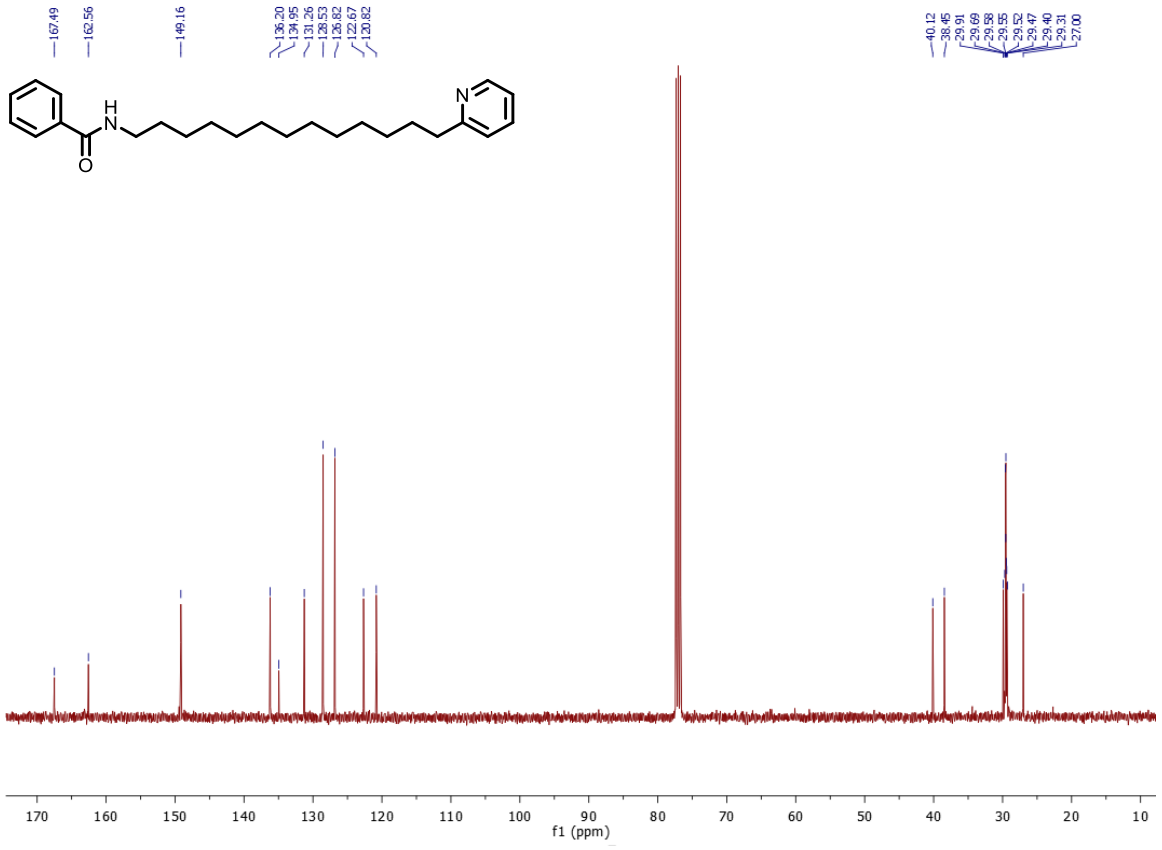
N-(13-phenyltridecyl)benzamide (from 51)



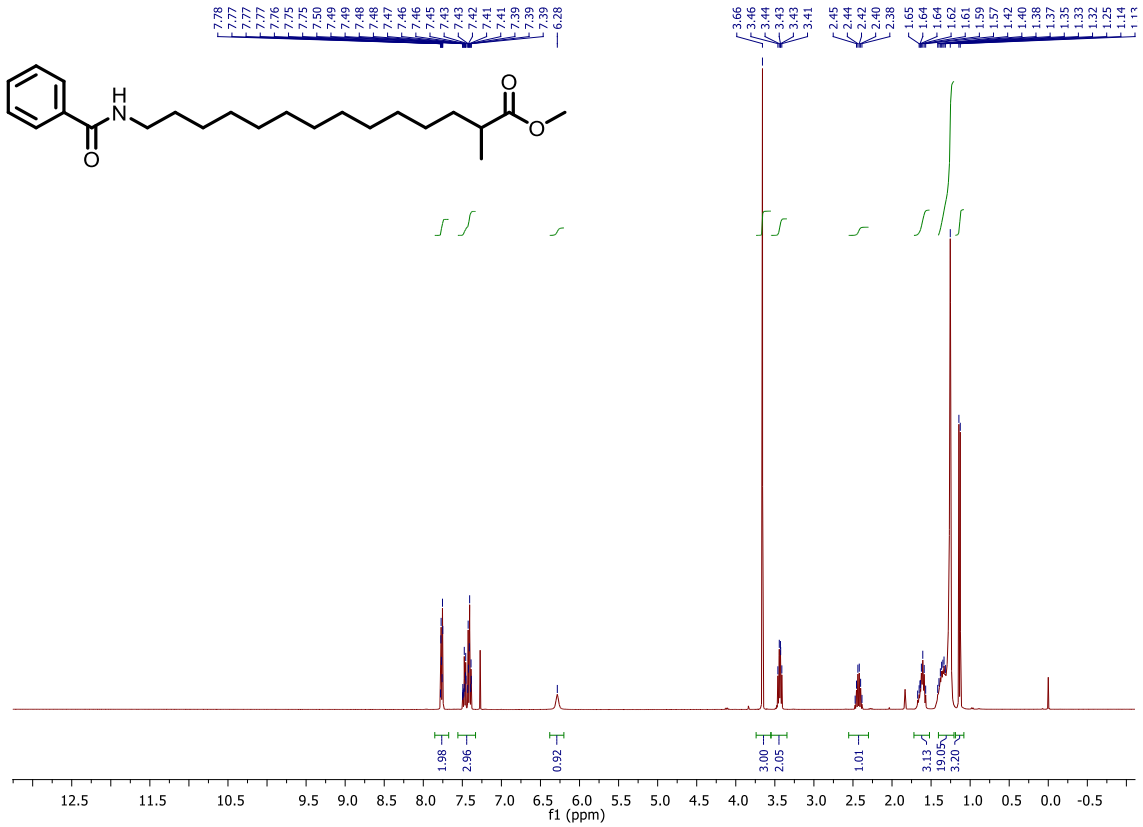


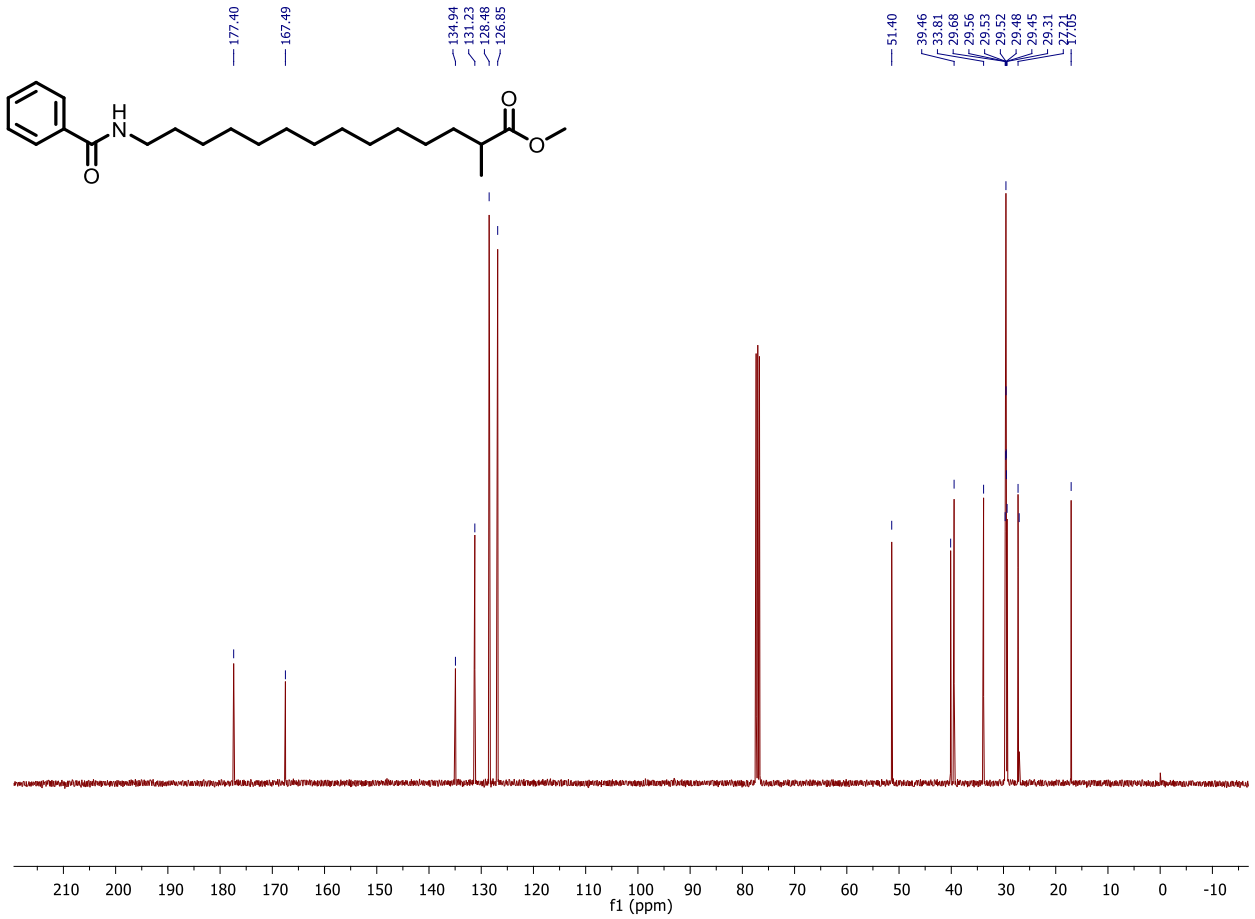
N-(13-(pyridin-2-yl)tridecyl)benzamide (from 52)



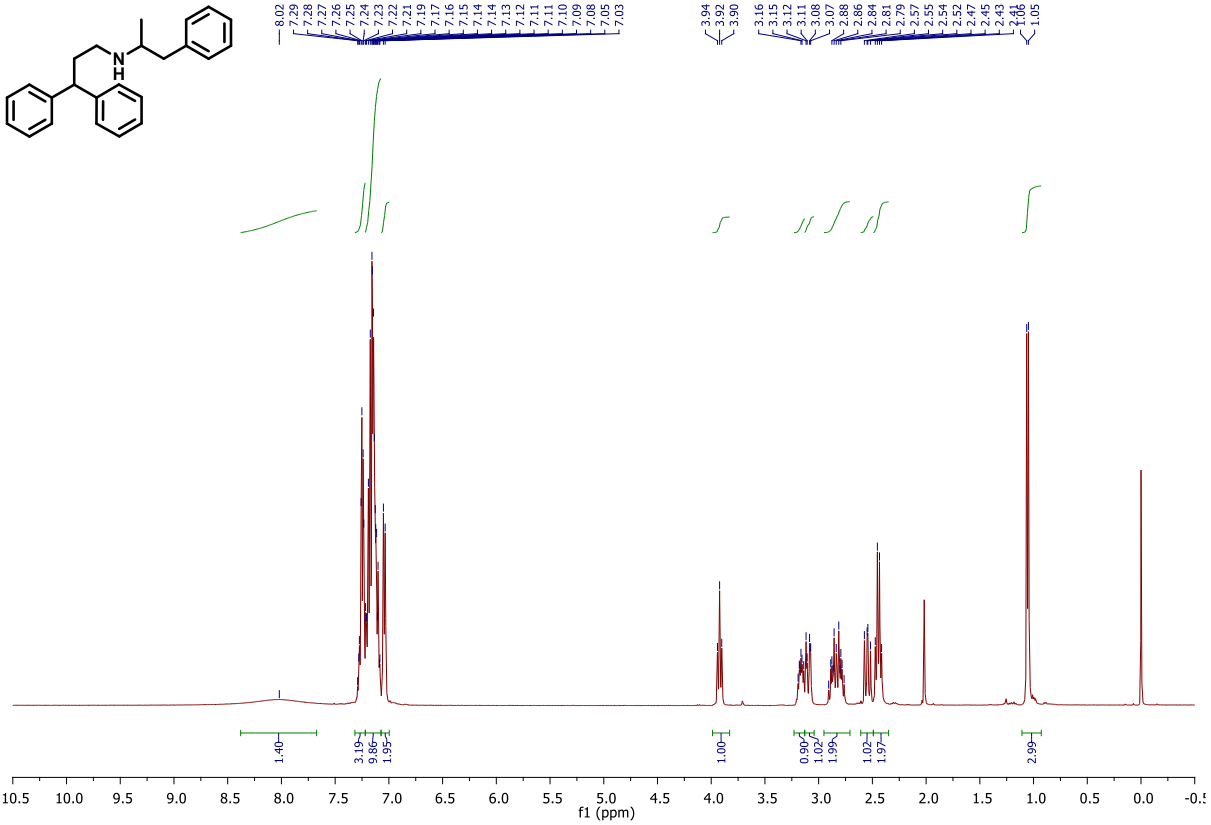


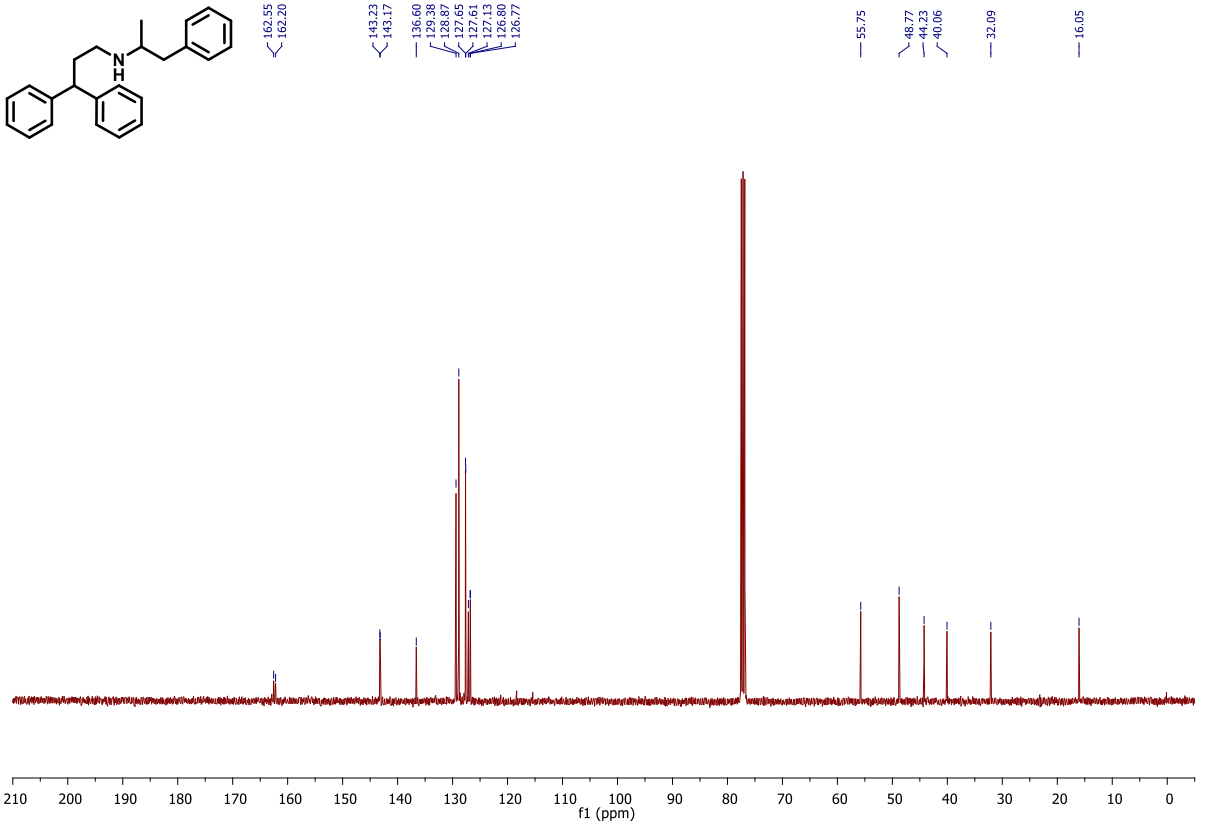
Methyl 14-benzamido-2-methyltetradecanoate (53)



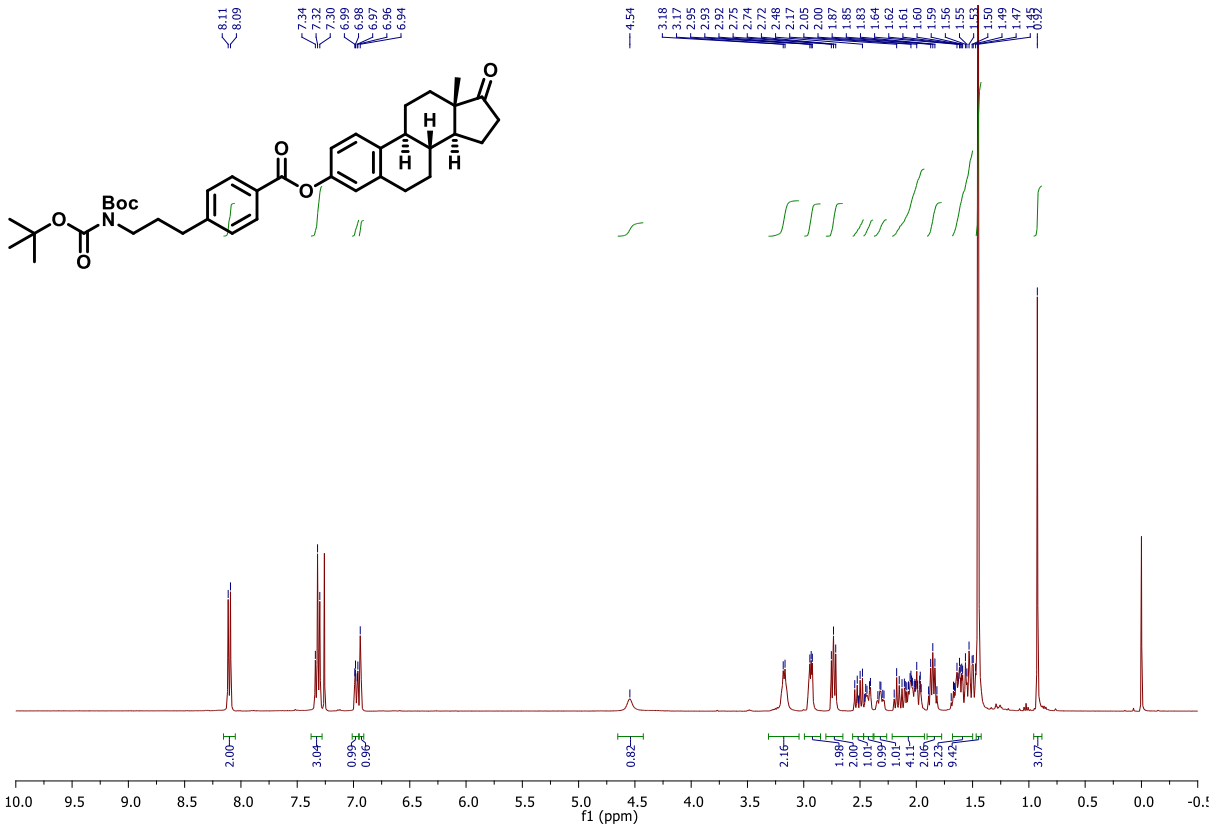


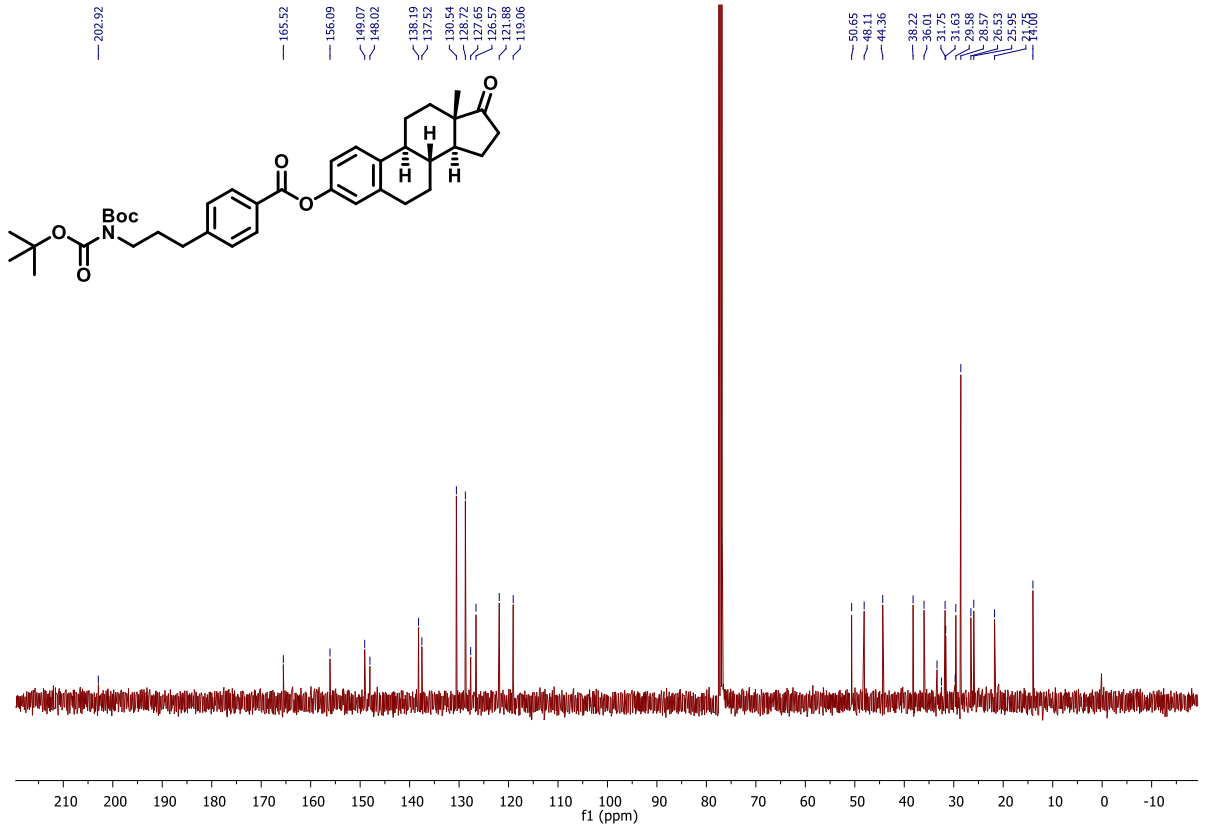
3,3-Diphenyl-N-(1-phenylpropan-2-yl)propan-1-amine (Prenylamine, 58)



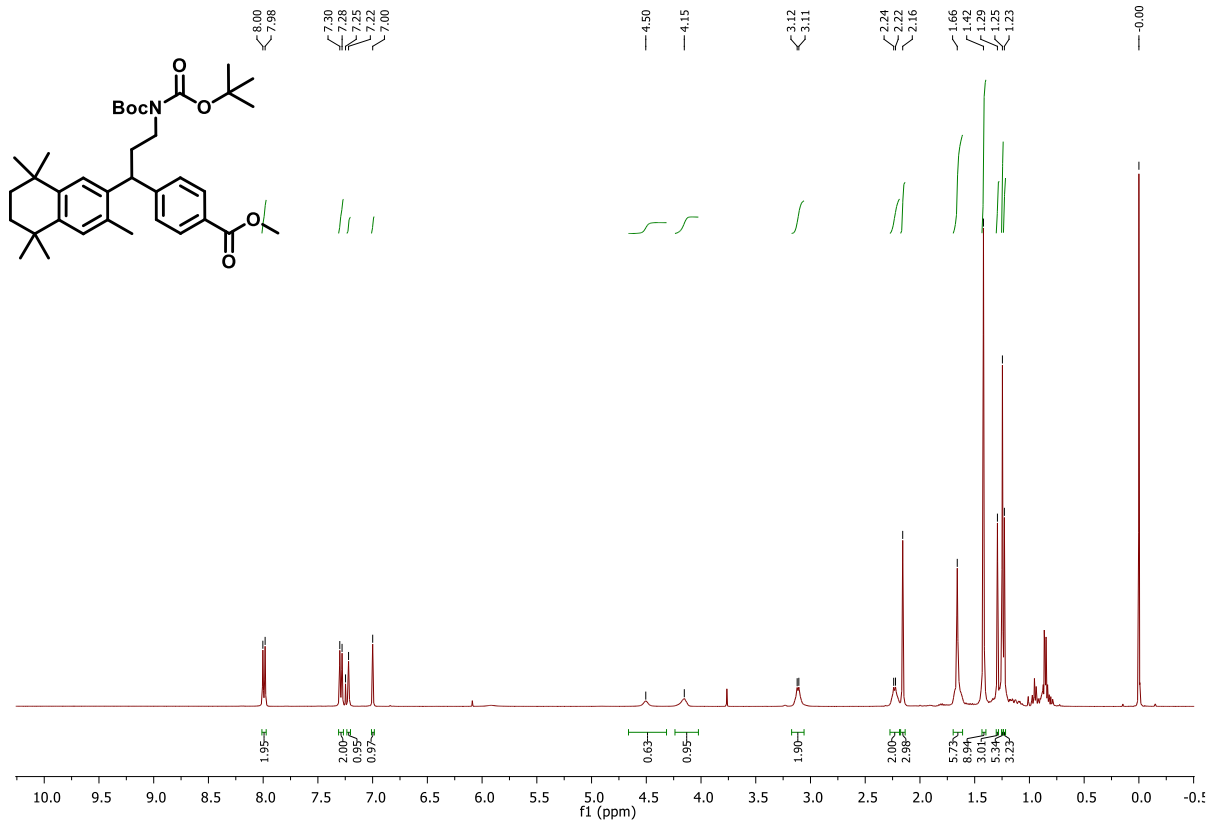


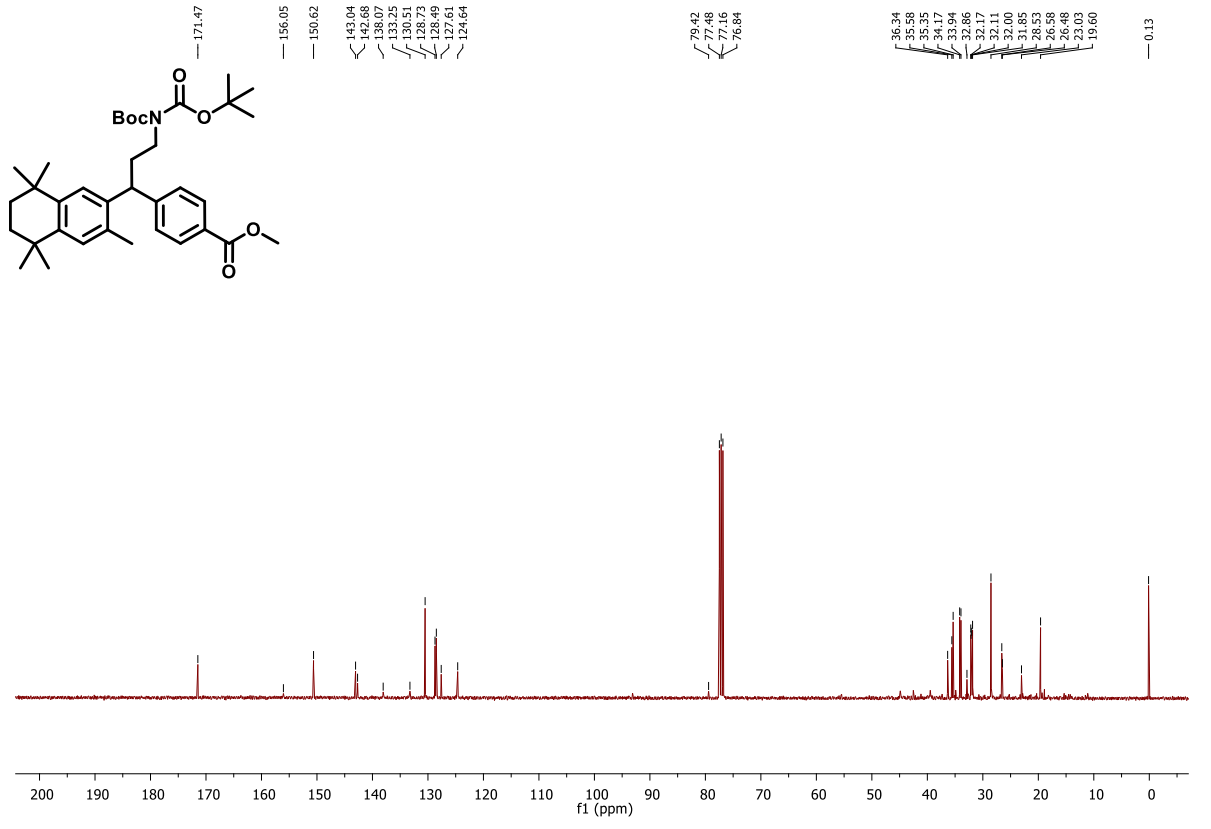
(8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl 4-(3-((tert-butoxycarbonyl)amino)propyl)benzoate (60)



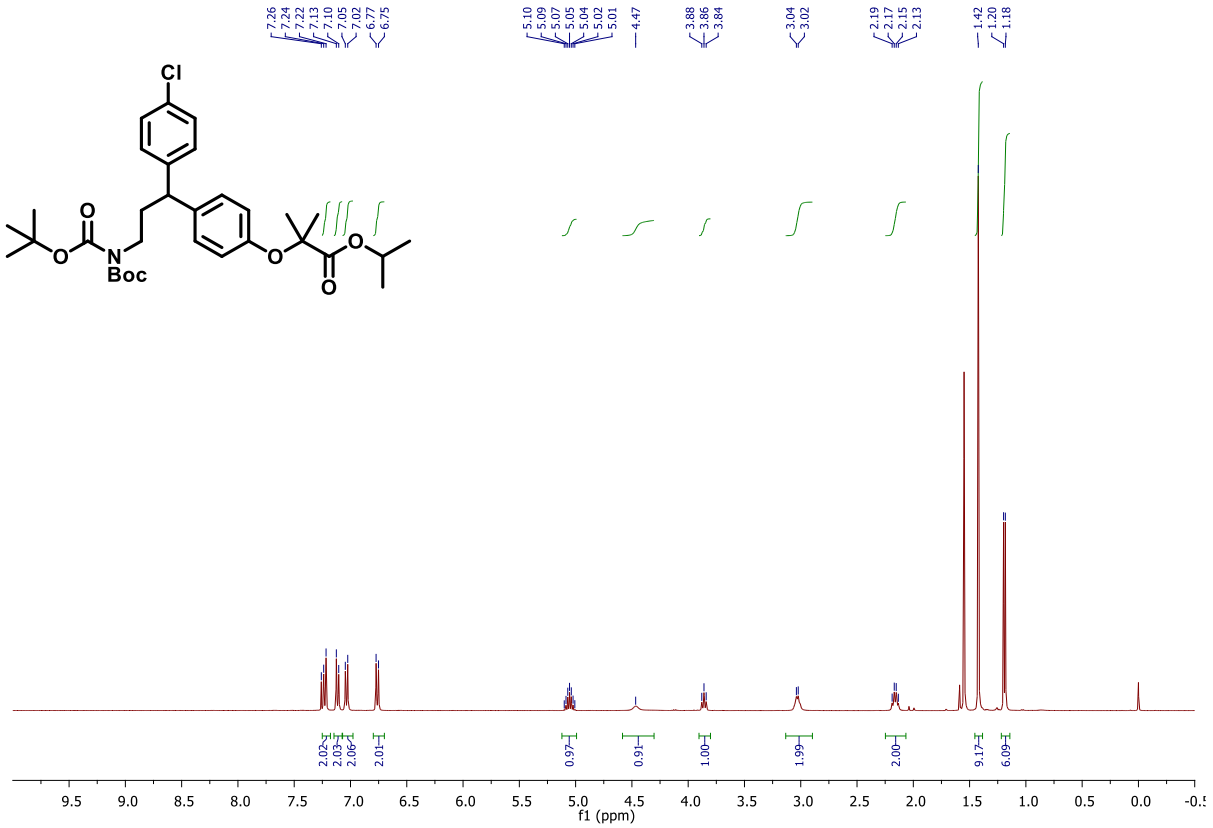


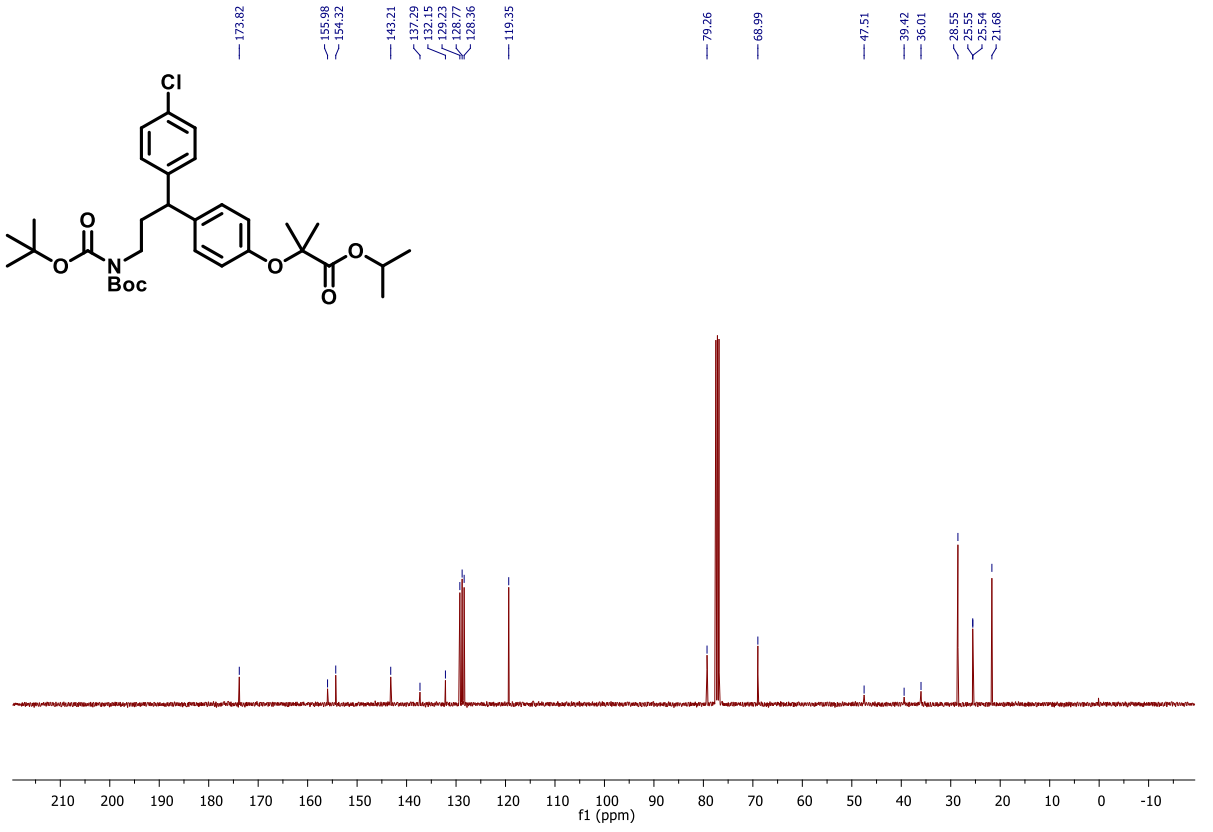
Methyl 4-(3-((tert-butoxycarbonyl)amino)-1-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-yl)propyl)benzoate (61)



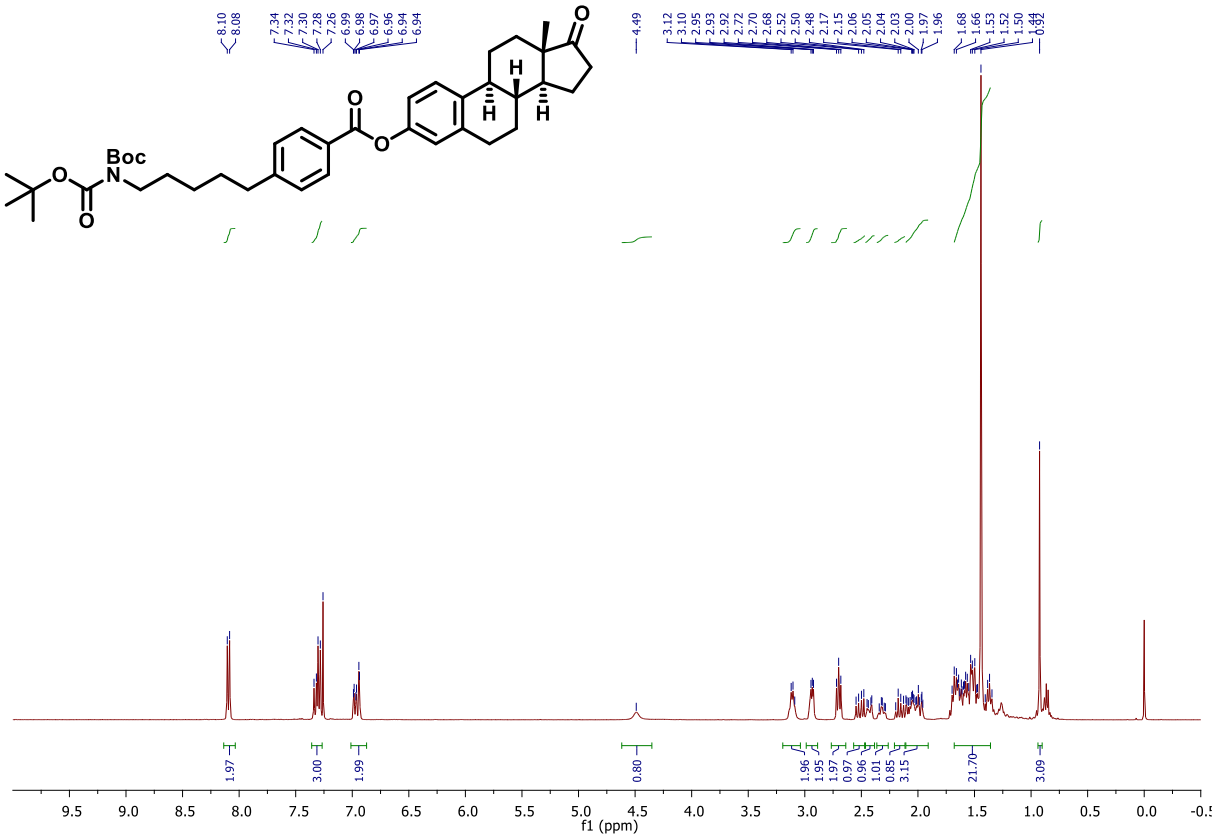


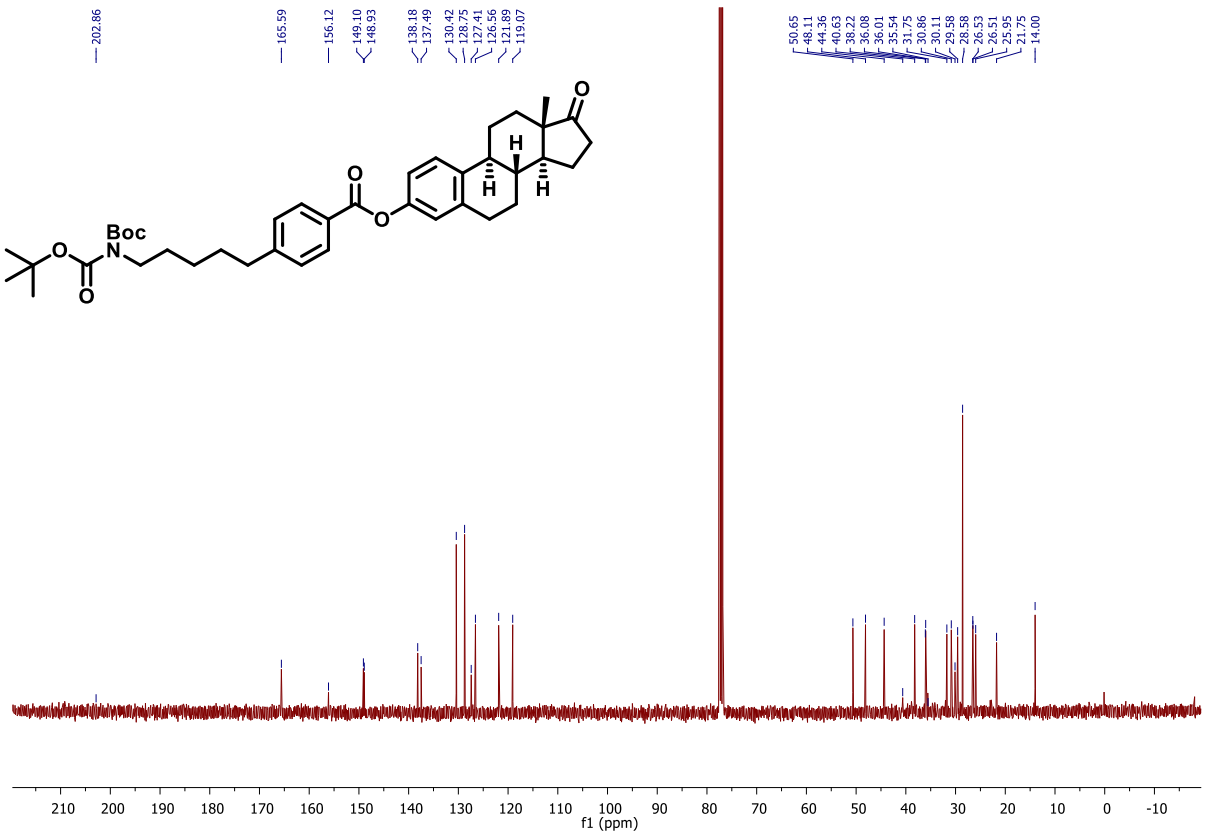
Isopropyl 2-(4-(3-((tert-butoxycarbonyl)amino)-1-(4-chlorophenyl)propyl)phenoxy)-2-methylpropanoate (62)



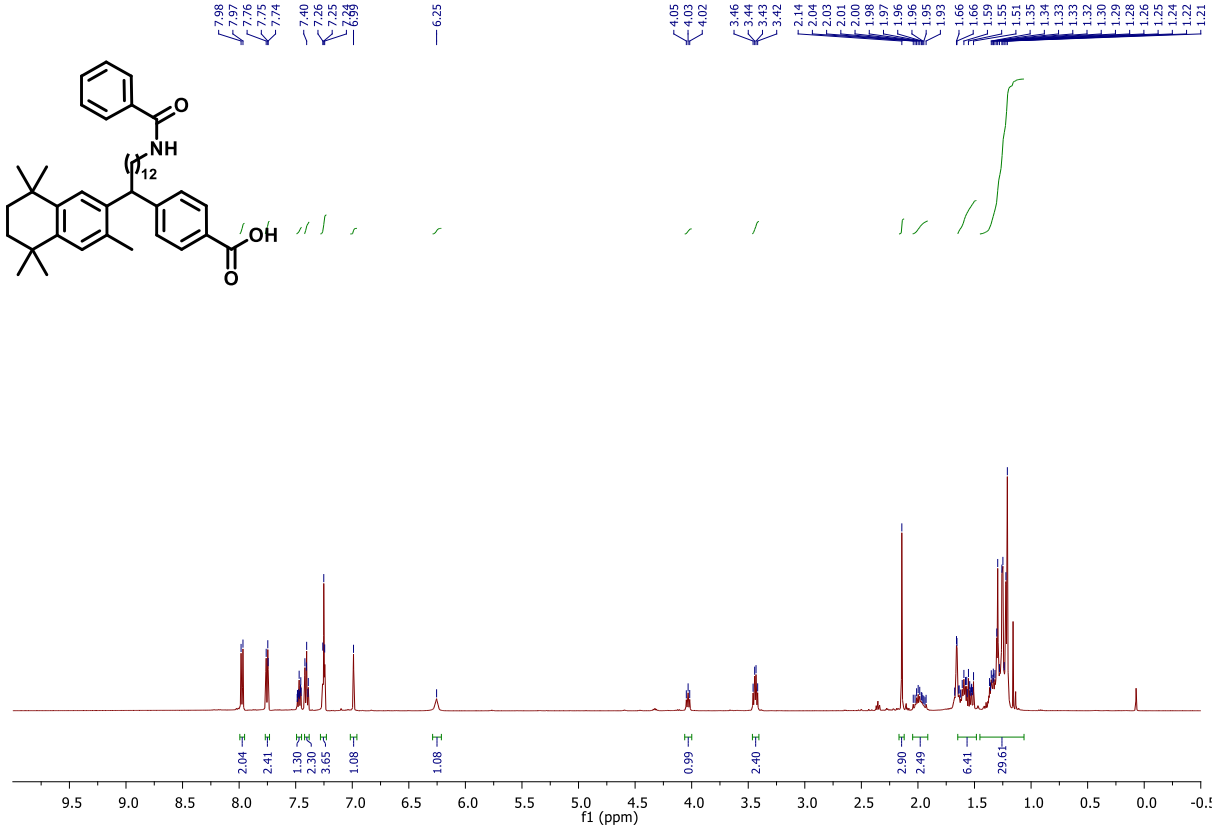


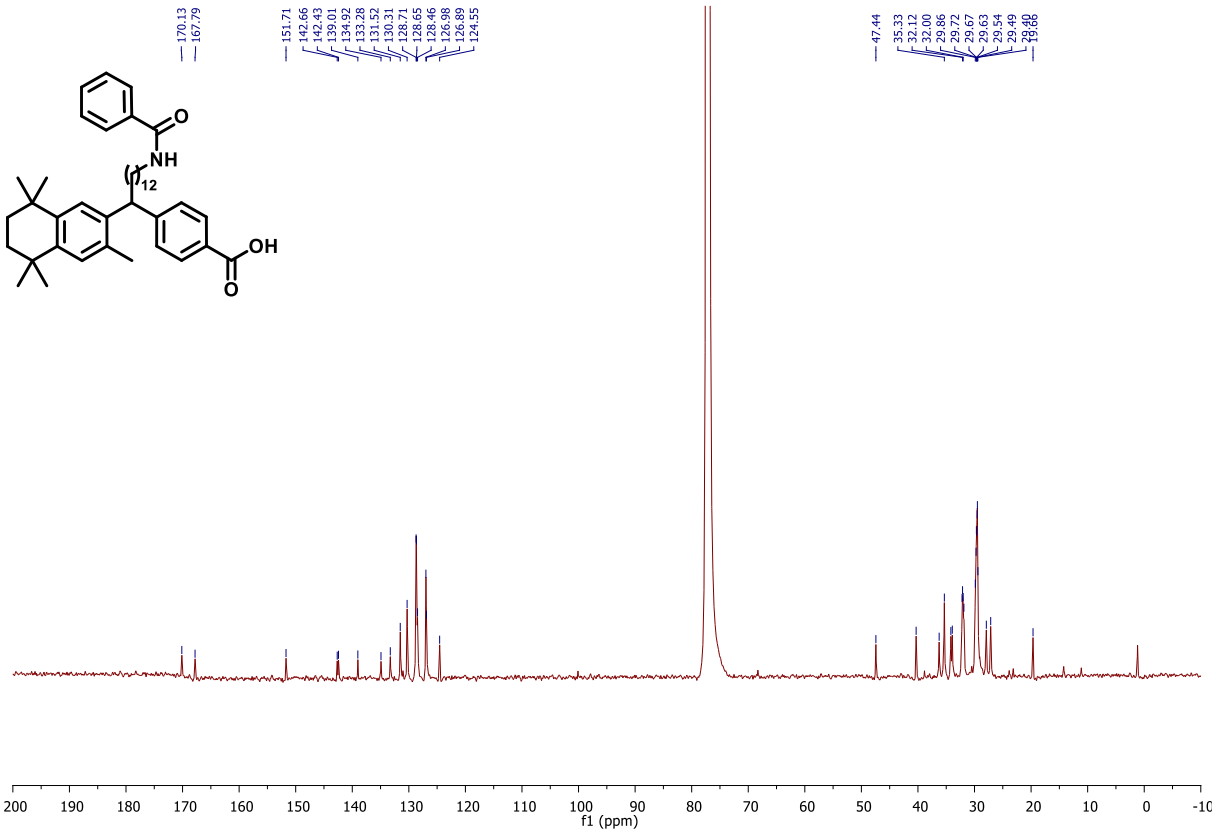
(8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl 4-(5-((tert-butoxycarbonyl)amino)pentyl)benzoate (63)



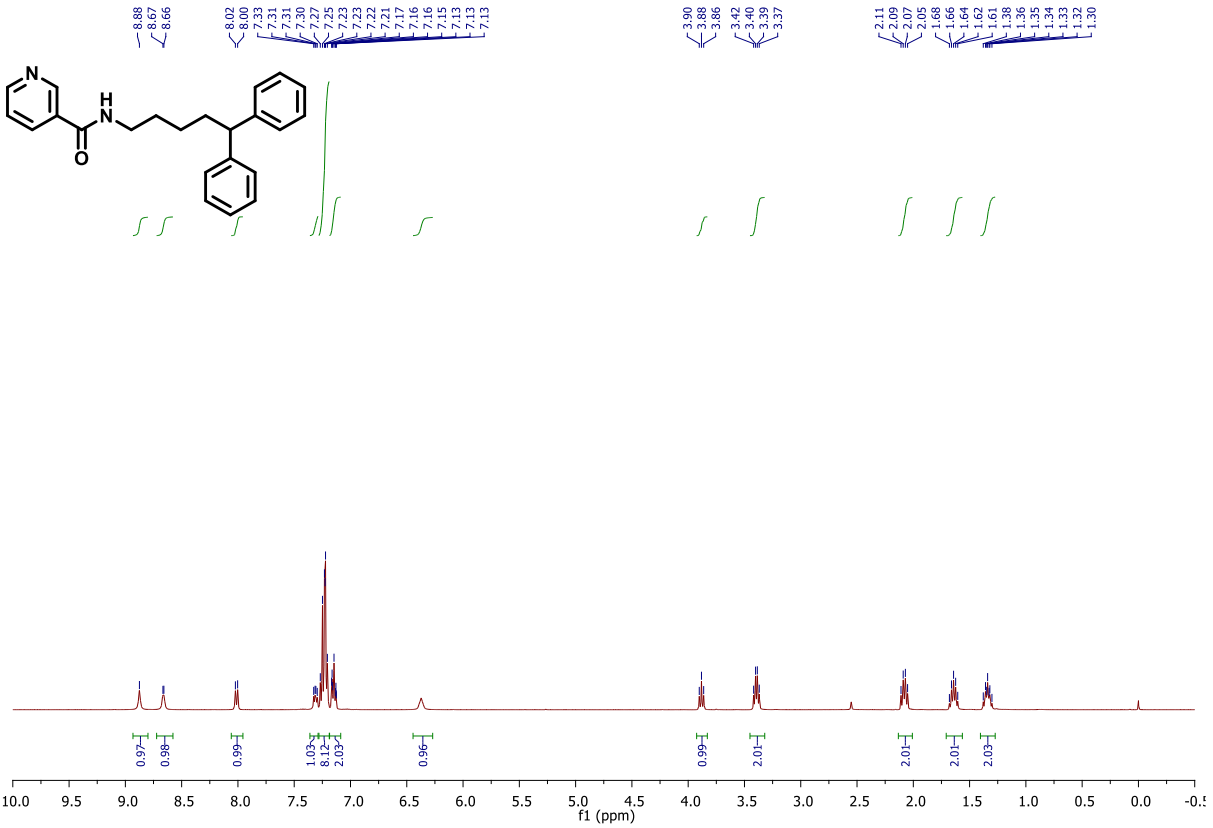


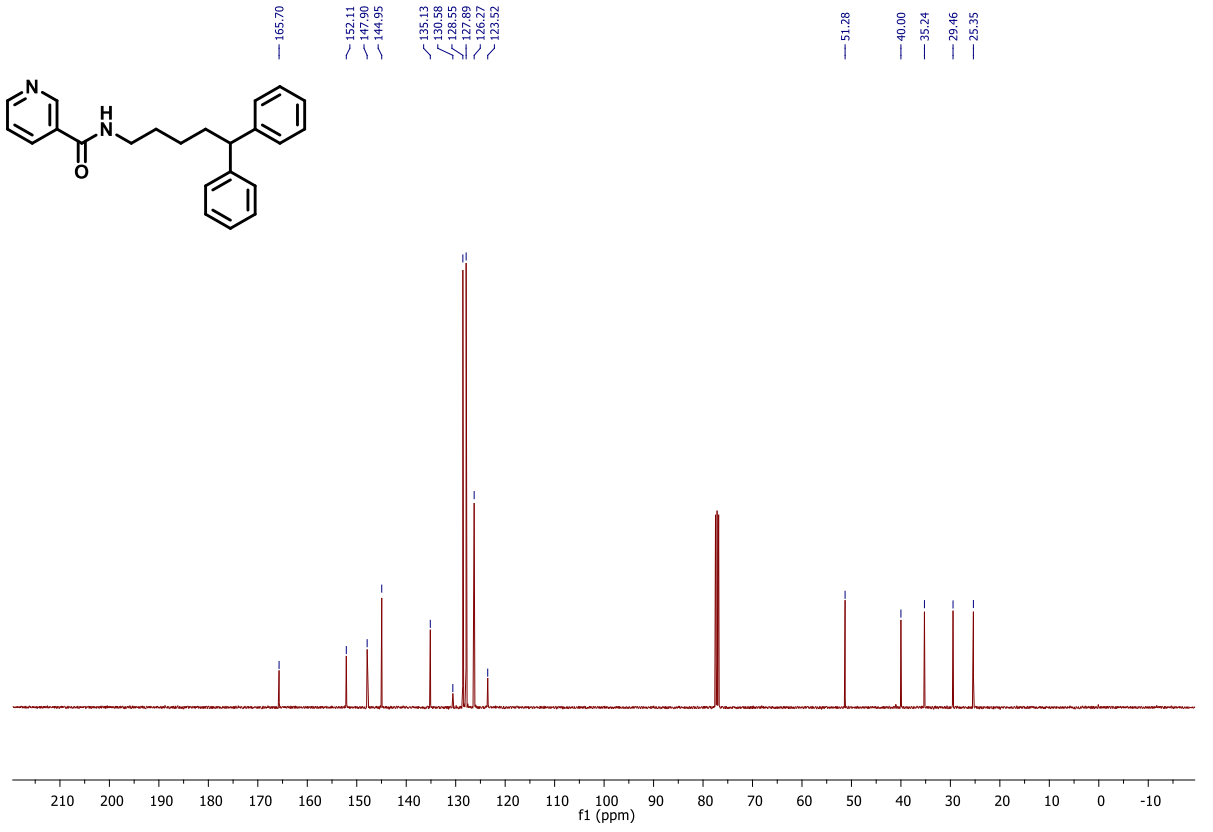
4-(13-benzamido-1-(3,5,5,8,8-pentamethyl-5,6,7,8-tetrahydronaphthalen-2-yl)tridecyl)benzoic acid (64)



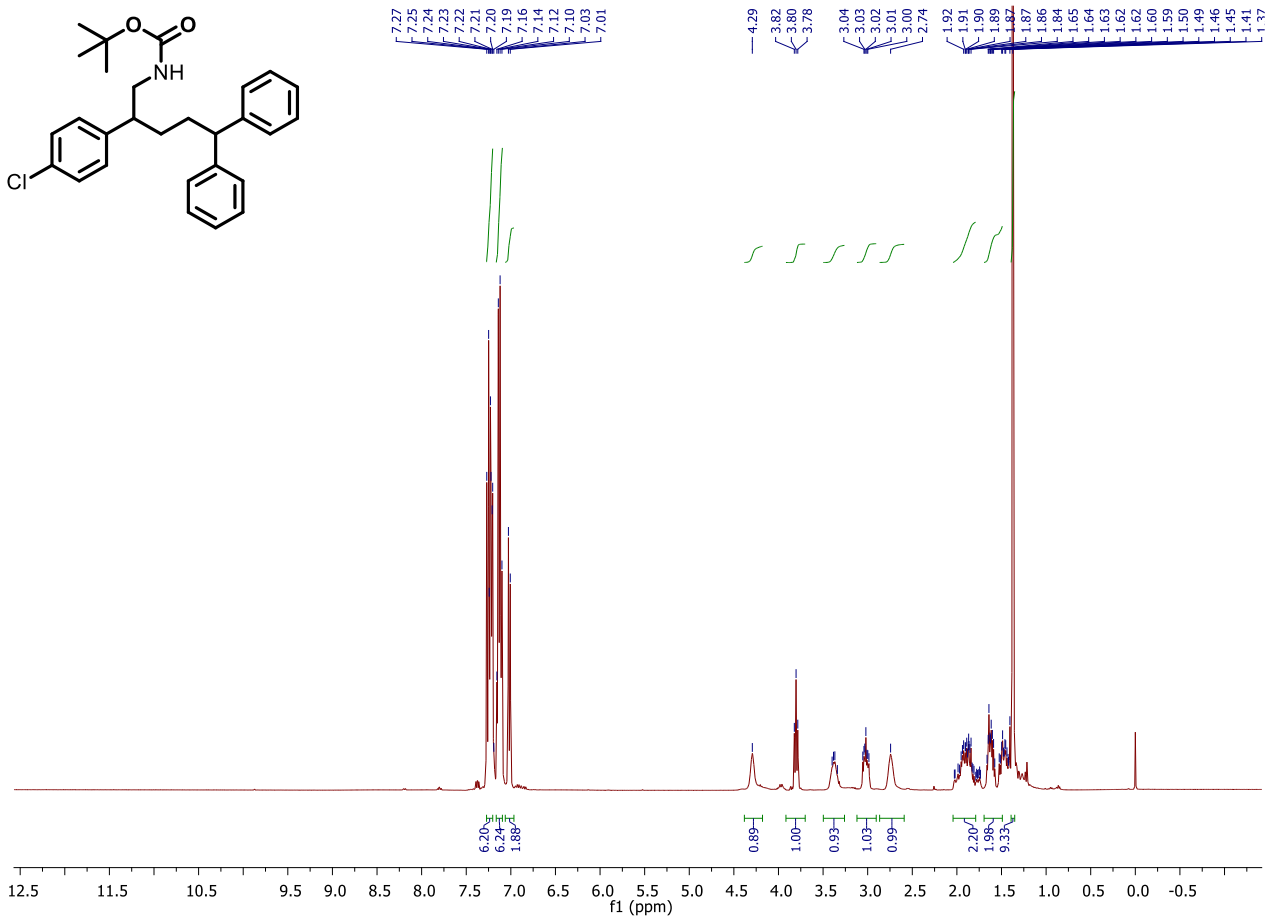


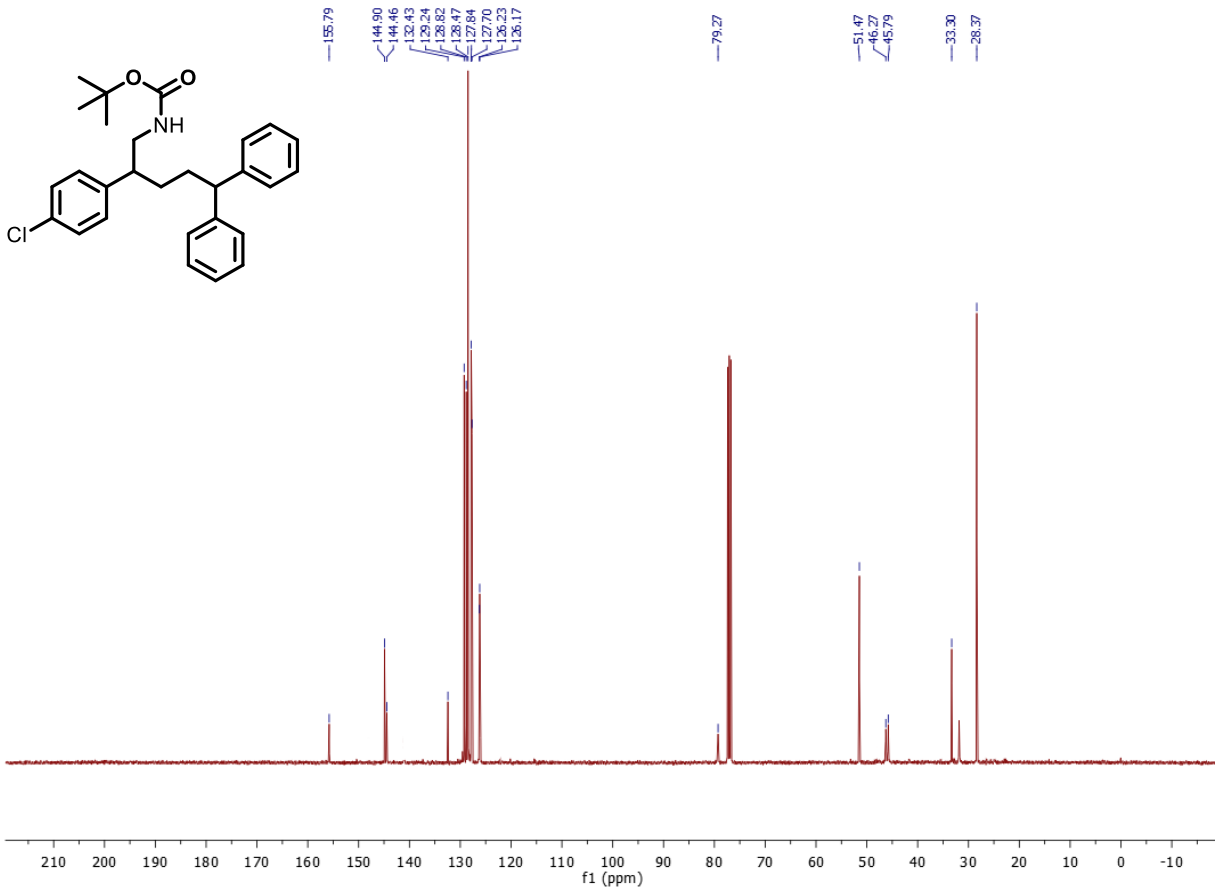
_N_-(5,5-diphenylpentyl)nicotinamide (65)



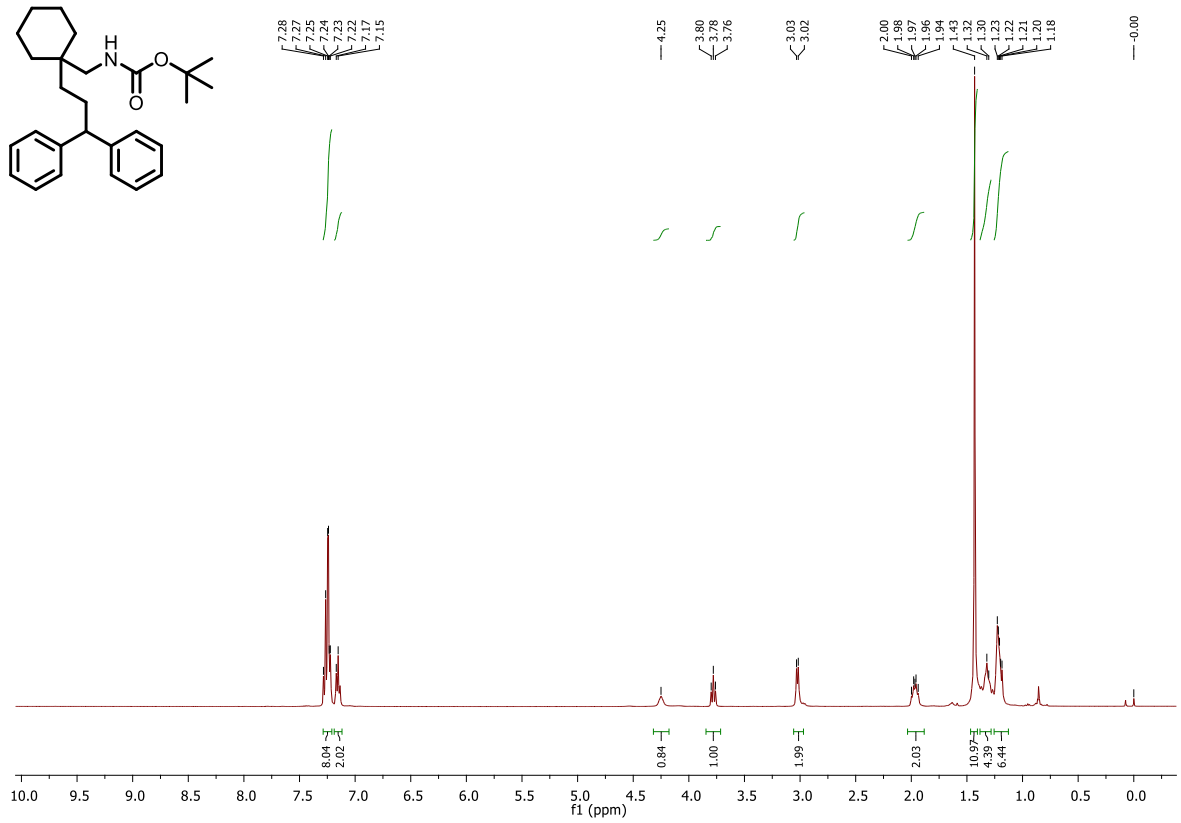


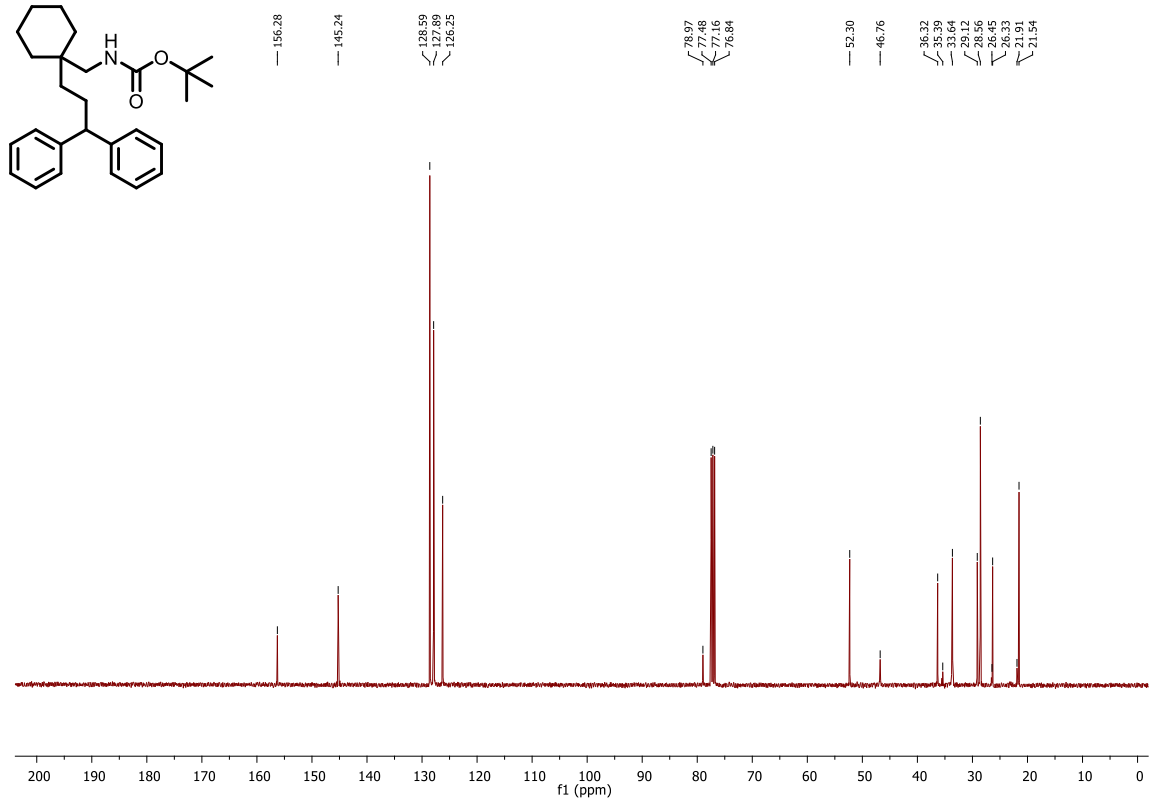
Tert-butyl (2-(4-chlorophenyl)-5,5-diphenylpentyl)carbamate (66)



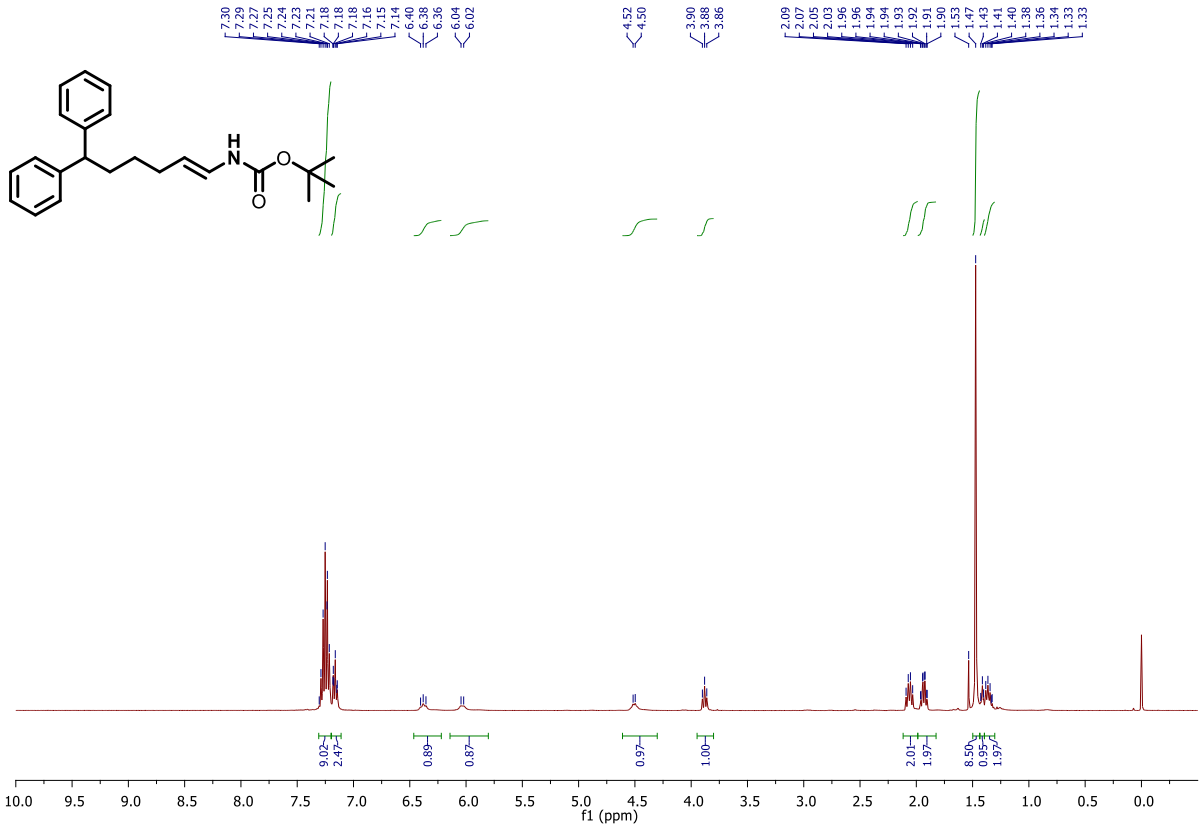


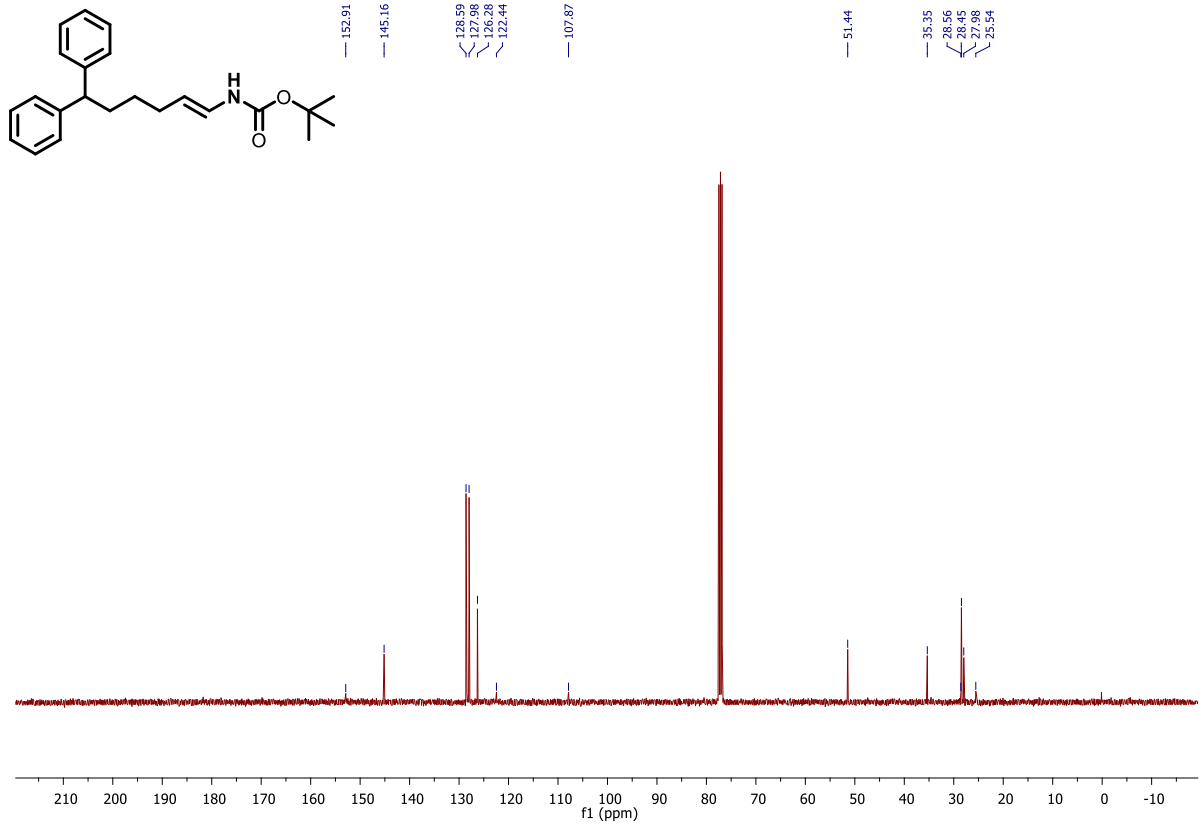
Tert-butyl ((1-(3,3-diphenylpropyl)cyclohexyl)methyl)carbamate (67)



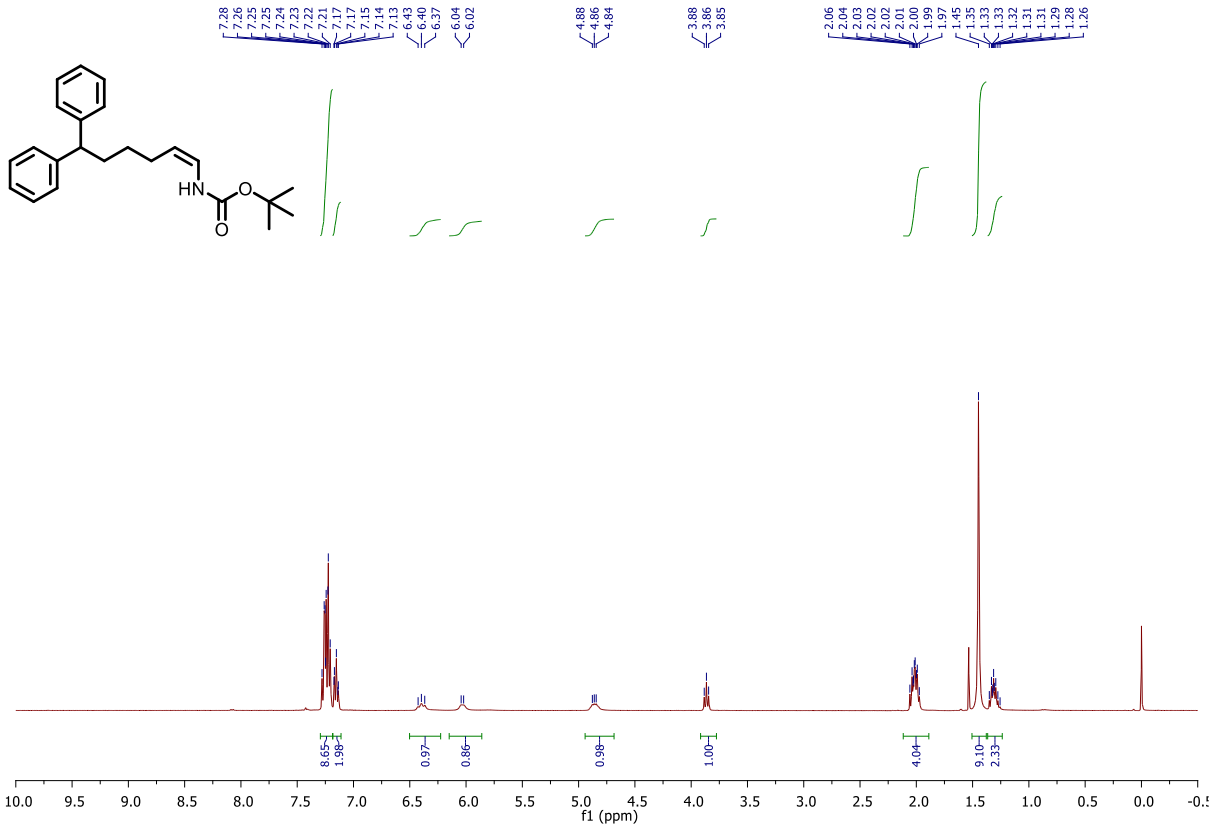


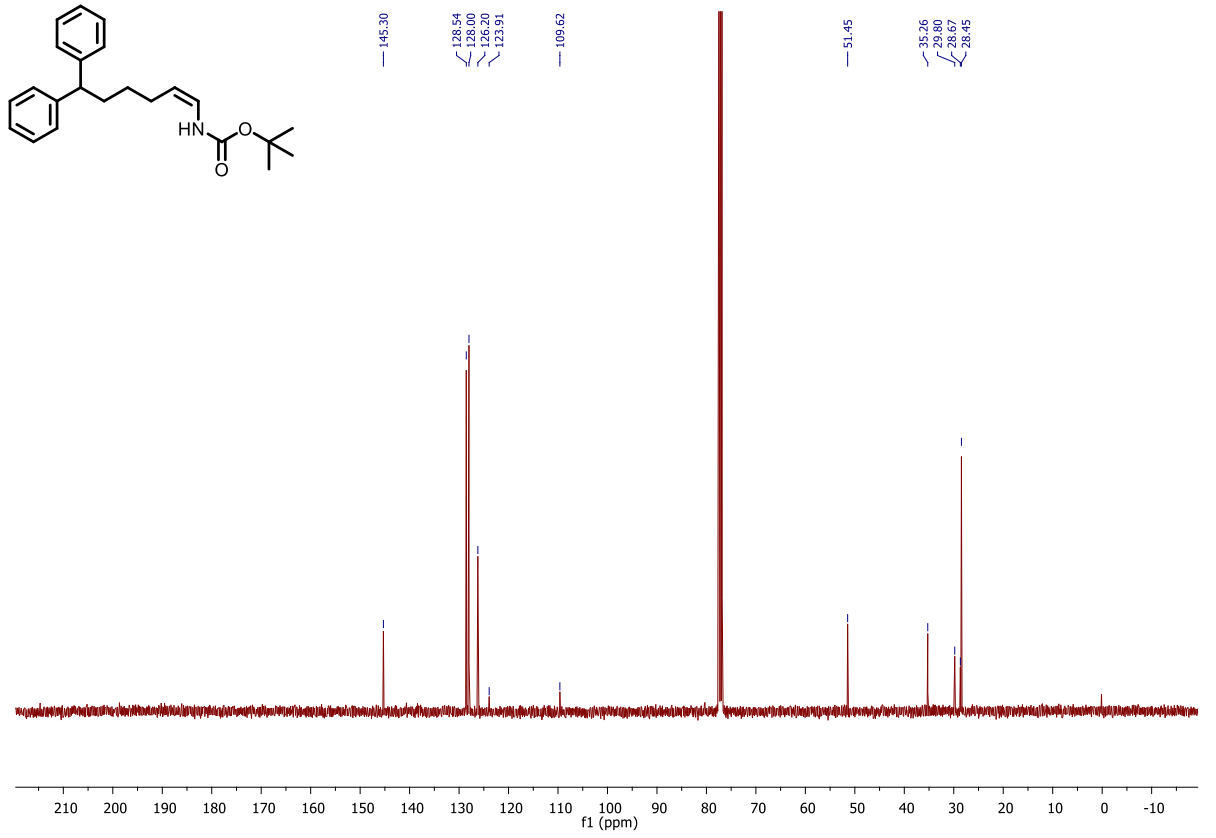
Tert-butyl (E)-(6,6-diphenylhex-1-en-1-yl)carbamate (68a)





Tert-butyl (Z)-(6,6-diphenylhex-1-en-1-yl)carbamate (68b)





7. References

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 16 Rev. C.01*, Wallingford, CT, 2016.
2. Adamo, C.; Barone, V., Toward reliable density functional methods without adjustable parameters: The PBE0 model. *J. Chem. Phys*. **1999**, *110*(13), 6158-6170
3. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H., A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010,** *132* (15), 154104.
4. Grimme, S.; Ehrlich, S.; Goerigk, L., Effect of the damping function in dispersion corrected density functional theory. *J. Comput. Chem.* **2011,** *32* (7), 1456-1465.
5. Hehre, W. J.; Ditchfield, R.; Pople, J. A., Self—Consistent Molecular Orbital Methods. XII. Further Extensions of Gaussian—Type Basis Sets for Use in Molecular Orbital Studies of Organic Molecules. *J. Chem. Phys.* **1972,** *56* (5), 2257-2261.
6. Weigend, F.; Ahlrichs, R., Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **2005,** *7* (18), 3297-3305.
7. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G., Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009,** *113* (18), 6378-6396.
8. *Chemcraft - graphical software for visualization of quantum chemistry computations.* https://www.chemcraftprog.com.
9. Legault, C. Y., *Visualization and analysis software for computational chemistry (http://www.cylview.org/)*.
10. Mesaik, M. A.; Rahat, S.; Khan, K. M.; Zia, U.; Choudhary, M. I.; Murad, S.; Ismail, Z.; Atta ur, R.; Ahmad, A., Synthesis and immunomodulatory properties of selected oxazolone derivatives. *Biorg. Med. Chem.* **2004,** *12* (9), 2049-2057.
11. Marcus, R. A., On the Theory of Oxidation Reduction Reactions Involving Electron Transfer. I. *J. Chem. Phys.* **1956**, 24 (5), 966-78.
12. Marcus, R. A., Electrostatic free energy and other properties of states having nonequilibrium polarization. I. *J. Chem. Phys.* **1956,** *24*(5), 979-989.
13. Marcus, R. A., On the theory of oxidation-reduction reactions involving electron transfer. III. Applications to data on the rates of organic redox reactions. *J. Chem. Phys.* **1957**, *26*(4), 872-877.
14. Hush, N. S, Adiabatic rate processes at electrodes. I. Energy-charge relationships. *J. Chem. Phys.***1958**, *28*(5), 962-972.
15. Marcus, R., On the theory of electrochemical and chemical electron transfer processes. *Can. J. Chem*. **1959**, *37*(1), 155-163.
16. Hush, N. S., Adiabatic theory of outer sphere electron-transfer reactions in solution. *Trans. Faraday Soc.* **1961**, *57*, 557-580.
17. Marcus, R. A., The second RA Robinson memorial lecture. Electron, proton and related transfers. *Faraday Discuss. Chem. Soc.* **1988**, *74*, 7-15.
18. Marcus, R. A.; Sutin, N., Electron transfers in chemistry and biology. *Biochim. Biophys. Act.* **1985**, *811*(3), 265-322.
19. Nelsen, S. F.; Weaver, M. N.; Luo, Y.; Pladziewicz, J. R.; Ausman, L. K.; Jentzsch, T. L.; O'Konek, J. J., Estimation of electronic coupling for intermolecular electron transfer from cross-reaction data. *J. Phys. Chem. A*. **2006**, *110*(41), 11665-11676.
20. Nelson, J.; Kwiatkowski, J. J.; Kirkpatrick, J.; Frost, J. M. Modeling charge transport in organic photovoltaic materials. *Acc. Chem. Res.* **2009**, 42, 11, 1768-1778.21. Yang, H.; Tian, C.; Qiu, D.; Tian, H.; An, G.; Li, G., Organic photoredox catalytic decarboxylative cross-coupling of gem-difluoroalkenes with unactivated carboxylic acids. *Org. Chem. Front.* **2019,** *6* (14), 2365-2370.
22. Harada, N.; Kimura, H.; Ono, M.; Saji, H., Preparation of Asymmetric Urea Derivatives that Target Prostate-Specific Membrane Antigen for SPECT Imaging. *J. Med. Chem.* **2013,** *56* (20), 7890-7901.
23. Cybularczyk-Cecotka, M.; Kamińska, A.; Jopek, Z.; Giedyk, M., Light-Induced Dealkylation of Benzamides in Aqueous Solution. *Eur. J. Org. Chem* **2022,** *2022* (42), e202200913.
24. Leone-Bay, A.; Freeman, J.; O'Toole, D.; Rosado-Gray, C.; Salo-Kostmayer, S.; Tai, M.; Mercogliano, F.; Baughman, R. A., Studies Directed at the Use of a Parallel Synthesis Matrix to Increase Throughput in an in Vivo Assay. *J. Med. Chem.* **2000,** *43* (19), 3573-3576.
25. Yin, Y.; Dai, Y.; Jia, H.; Li, J.; Bu, L.; Qiao, B.; Zhao, X.; Jiang, Z., Conjugate Addition–Enantioselective Protonation of N-Aryl Glycines to α-Branched 2-Vinylazaarenes via Cooperative Photoredox and Asymmetric Catalysis. *Journal of the American Chemical Society* **2018,** *140* (19), 6083-6087.