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Supplementary information

Aziridine synthesis by coupling amines and alkenes via an electrogenerated dication

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Aziridine synthesis by coupling amines and alkenes via an electrochemically generated dication

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SUPPORTING INFORMATION

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1. General Methods and Materials

Unless otherwise noted, reactions were performed under an inert N_2 atmosphere in an anhydrous solvent. MeCN, THF, DMF, and DCM were dried by passing through activated alumina columns. Tetrabutylammonium hexafluorophosphate was recrystallized three times from EtOAc prior to use. Lithium tetrafluoroborate was dried at 50 °C under vacuum prior to use. All liquid amines were distilled from CaH_2 prior to use. Thianthrene was recrystallized from acetone prior to use. Unless otherwise noted, other commercially-available reagents were used as received. Crude mixtures were evaluated by thin-layer chromatography using EMD/Merck silica gel 60 F254 pre-coated plates (0.25 mm) and were visualized by UV, Seebach, p-anisaldehyde, ninhydrin, or $KMnO_4$ staining. Flash chromatography was performed with a Biotage Isolera One automated chromatography system with re-packed silica columns (technical grade silica, pore size 60 Å, 230-400 mesh particle size, 40-63 particle size) or pre-packed Biotage SNAP Ultra columns unless otherwise noted. Purified materials were dried in vacuo (0.050 Torr) to remove trace solvent. ^{1}H, ^{13}C, ^{19}F Spectra were taken using a Bruker Avance-400 with a BBFO Probe, a Bruker Avance-500 with a DCH Cryoprobe, Bruker Avance III HD-500 with a TXO Cryoprobe, or a Bruker Avance-600 with a TCI-F cryoprobe. NMR data are reported relative to residual $CHCl_3$ (^{1}H, δ = 7.26 ppm), $CDCl_3$ (^{13}C, δ = 77.16 ppm) or residual C_6H_6 (^{1}H, δ = 7.16), C_6D_6 (^{13}C, δ = 128.06 ppm). Data for ^{1}H NMR spectra are reported as follows: chemical shift (δ ppm) (multiplicity, coupling constant (Hz), integration). Multiplicity and qualifier abbreviations are as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. All NMR yields were determined via reference against an internal standard (dibromomethane or mesitylene for ^{1}H, trifluorotoluene for ^{19}F). GC traces were taken on an Agilent 7890A GC with dual DB-5 columns (20 m ×180 μμm × 0.18 μm), dual FID detectors, and hydrogen as the carrier gas. A sample volume of 1 μL was injected at a temperature of 300 °C and a 100:1 split ratio. The initial inlet pressure was 20.3 psi but varied as the column flow was held constant at 1.8 mL/min for the duration of the run, FID temperature was 325 °C. Mass spectrometry data was collected on a Thermo Scientific Q Exactive Plus Mass Spectrometer. The crystal evaluation and data collections were performed on a Bruker D8 VENTURE PhotonIII four-circle diffractometer with Cu Kα (λ = 1.54178 Å) radiation with the detector to crystal distance of 4.0 cm (Bruker-AXS (2018). APEX3. Version 2018.1-0. Madison, Wisconsin, USA.). The reflections were indexed by an automated indexing routine built in the APEX3 program. Mercury was used for structural visualization[1].

Abbreviations: Boc—tert-butyl carbamate, tBu—tert-butyl, CV—cyclic voltammetry, DCM—dichloromethane, DMF—dimethyl formamide, EtOAc—ethyl acetate, MeCN—acetonitrile, MeOH—methanol, RVC—reticulated vitreous carbon, Ph—phenyl, *n*-Hex—hexyl, *n*-Pr—propyl, DMSO—dimethylsulfoxide, THF— tetrahydrofuran, TEA—triethylamine, TFA—trifluoroacetic acid, GC— gas chromatography

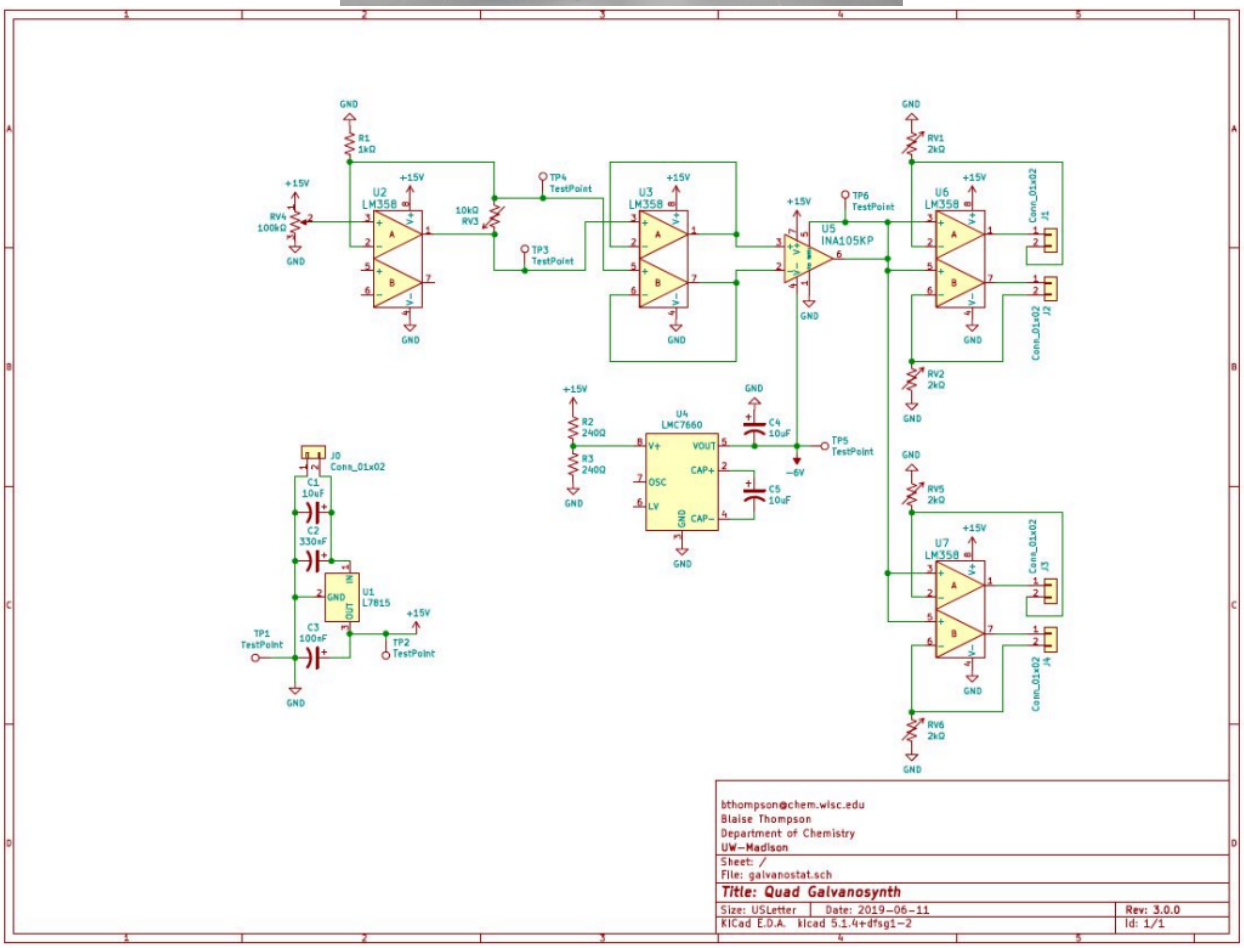
Electrochemical Methods and Materials

All chronoamperometric, chronopotentiometric, and cyclic voltammetry measurements were performed at room temperature using a Pine WaveNowXV. The CV experiments were carried out in a three-electrode cell configuration with a glassy carbon (GC) working electrode (3 mm diameter, unless otherwise stated) and a platinum wire counter electrode. Chronoamperometric and chronopotentiometric measurements were carried out in divided cells with RVC (8 × 6 × 6 mm, Ultramet, 80 ppi) as working and counter electrodes affixed to stainless steel wire or a graphite pencil/silver wire assembly (see below). The potentials were measured versus an $Ag/AgNO_3$ (0.01 M in MeCN with 0.1 M n-Bu_4N•PF_6) reference electrode (all electrodes from Pine Research) and externally referenced via the ferrocene/ferrocenium couple. Bulk constant current electrolysis experiments were driven with a Dr. Meter HY3005M-L DC Power Supply or a custom–made low current power supply (see Scheme below) which was externally calibrated with a multimeter using a 10 or 1–Ohm resistor.

Divided cell fabricated in house. Glass frit purchased from Ace Glass (7176-36). Anode electrode assembled via affixing end of the silver wire (Belden Hook-Up wire, item no. 83005 007100) around the pencil (JuneGold 2B graphite 2 mm) using conductive graphite adhesive (Alfa Aesar, 42465), wrapping in teflon tape to prevent exposure, then piercing RVC with pencil. Solvent exposed electrode surface area (2.1 cm^2) was calculated via manufacturer-supplied surface area/volume ratio measurements. PTFE tubing (Cole-Parmer; 1/32” ID, 1/16” OD, item number EW-06407-41) connects both sides of the divided cell to normalize pressure. Septa inner

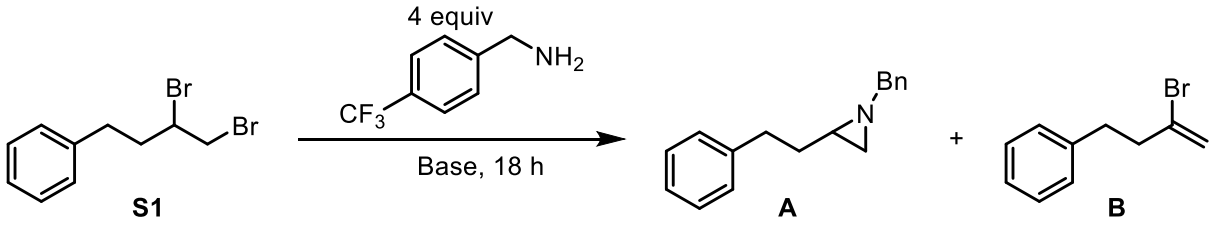
diameter 16 mm. Stainless steel purchased from Grainger; stainless steel lockwire, 0.025" diameter, item number 16Y043. Average cell resistance: 0.9 kΩ.

Low-current Power Supply [2]**:** Original design and fabrication by Dr. Blaise J. Thompson. Provides an operational range of ±0.01–9.99 mA, tunable by analog input, delivering power to multiple banana socket pairs. The power supply is limited to ±15 V for bulk electrolysis and is powered by an 18 V wall wart. Circuitry is housed within an aluminum enclosure.



Dibromide substitution with a primary amine:

A literature survey revealed that the only examples of aziridine formation from vicinal dibromides were restricted to substitution of activated α-carbonyl vicinal dibromides. Reactivity of vicinal dibromides to form aziridines with primary amines was not found outside of these examples. We adapted a selection of precedent conditions from α-carbonyl vicinal dibromides[3–5] to the substitution reaction, as well as conditions similar to our scope procedures to probe aziridine formation directly from a 4-phenylbutene-derived dibromide. For comparison, substitution of the 4-phenylbutene-derived dicationic adduct results in 91% yield of the desired aziridine product.



entry	Base (equiv)	Solvent	Temp (°C)	Conc. (M)	**A** (%)	**B** (%)	Dibromide Conv. (%)	Amine Conv. (%)	Source
1	Cs_2CO_3 (4)	MeCN*	20	0.05	0	51	100	12	this work
2	Cs_2CO_3 (6)	MeCN*	20	0.05	0	54	100	25	this work
3	TEA (3)	MeOH	20, 50	0.4	0	0	0	0	ref. 3
4	TEA (4)	toluene	80	0.35	0	0	0	0	ref. 4
5	TEA (2)	THF	20, 50	0.125	0	0	0	0	ref. 5

Table S1.

*0.2 M *n*-Bu_4NPF_6. Concentrations are in reference to the dibromide starting material. Entries 3 and 5 were heated to 50 °C following stirring at rt for 18 h and stirred for an additional 18 h. No change in the amount of dibromide or amine was observed upon heating. Under these conditions, substitution of a vicinal dibromide using a primary amine results in exclusively vinyl bromide or no reactivity.

Limiting Alkene and Amine Conditions:

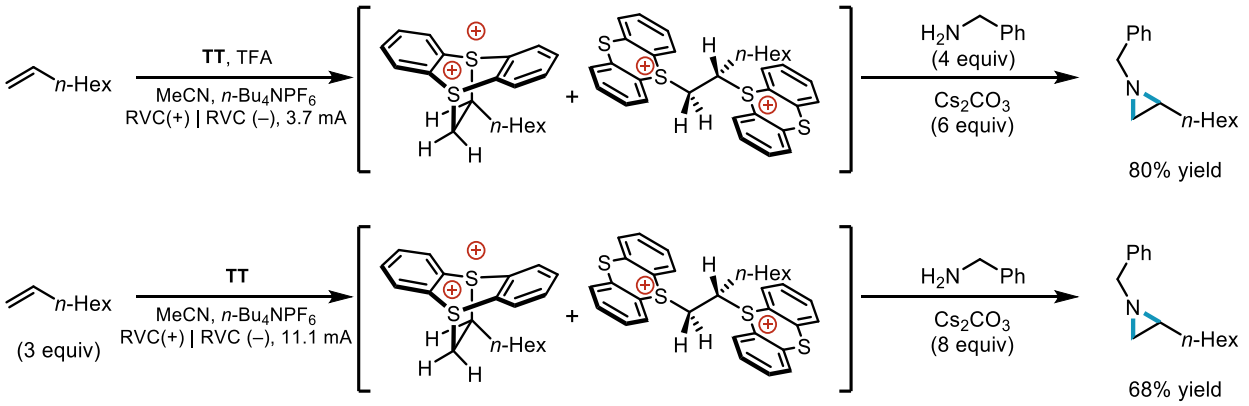


Fig. S1.

Limiting alkene (top, General Procedure E, NMR yield) and limiting amine (bottom, General Procedure D, isolated yield) conditions for aziridine formation

Internal Alkene Adduct Formation and Attempted Aziridination

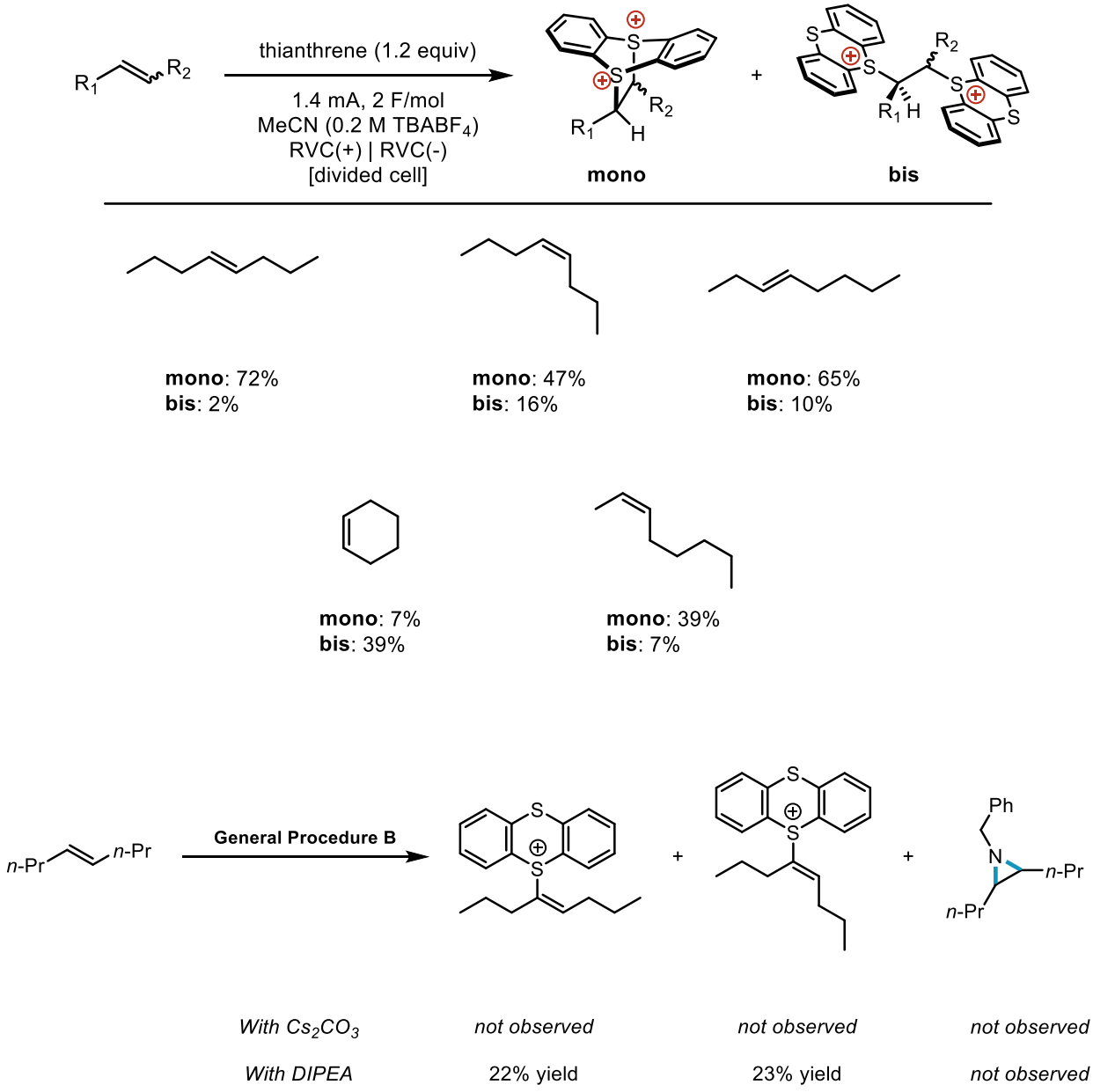


Fig. S2.

1,2-Disubstituted alkenes, which can form both mono- and bis- adduct under electrolysis in the presence of thianthrene, give intractable mixtures of products or eliminate to the internal vinyl thianthrenium salt but do not react further when subjected to standard aziridination conditions. Reactions performed on 0.15 mmol scale.

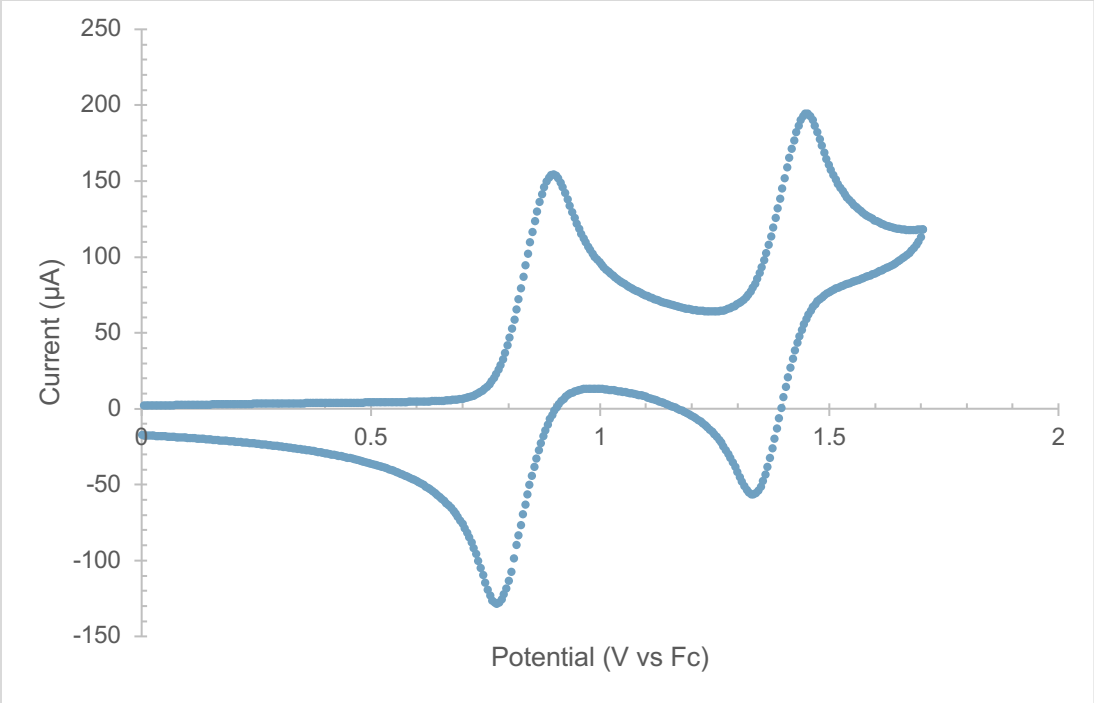


Fig. S3.

Cyclic voltammetry of thianthrene (5 mM) in MeCN (0.1 M BuN_4PF_6). Sweep rate: 100 mV/s. Externally referenced to the ferrocene/ferrocenium couple. 2% trifluoroacetic anhydride by volume was added to the solution as a dessicant before the CV measurement was taken to render the second oxidation peak reversible.

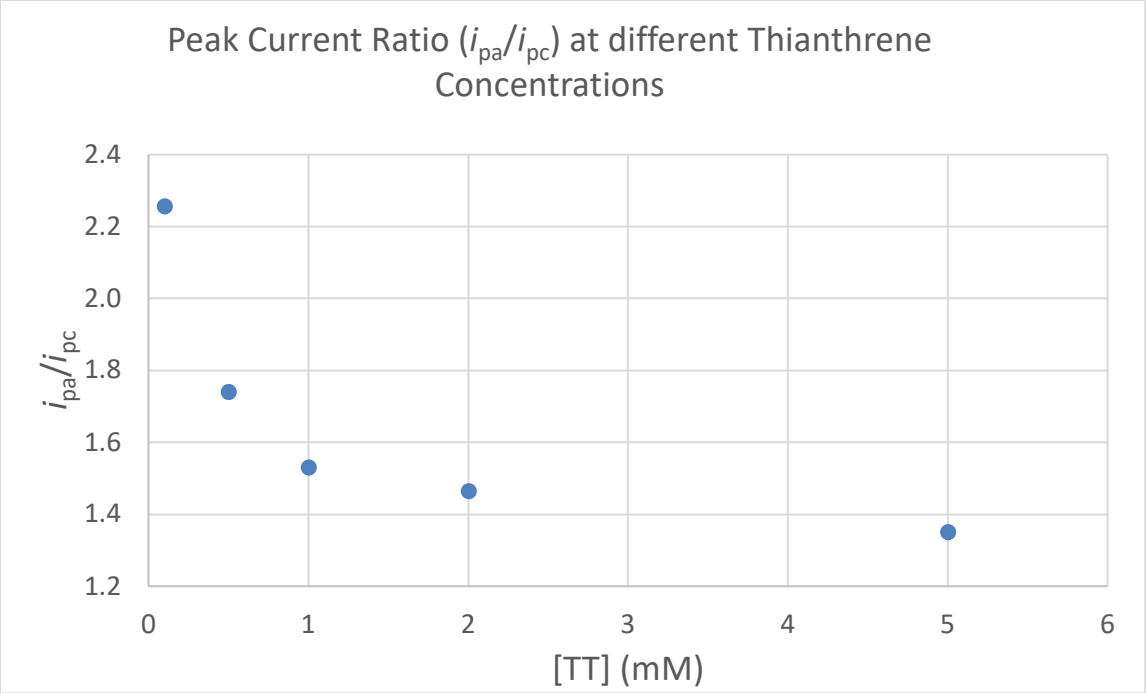


Fig. S4.
Peak current ratios (anodic over cathodic, i_{pa}/i_{pc}) from cyclic voltammetry of different concentrations of thianthrene (0.1 – 5 mM) in MeCN (0.1 M *n*-BuN_4PF_6). Sweep rate: 100 mV/s. Externally referenced to the ferrocene/ferrocenium couple. 2% trifluoroacetic anhydride by volume was added to the solution as a desiccant. As the thianthrene concentration is increased, disproportionation becomes disfavored relative to comproportionation, which should lower the ratio of peak currents since more thianthrene radical cation should remain in solution at cathodic peak.

3. Mechanistic Investigations

Conversion Time Courses Procedure

To an oven-dried divided electrochemical cell equipped with magnetic stir bars was added thianthrene (130 mg, 0.6 mmol, 1.5 equiv or 217 mg, 1.0 mmol, 2.5 equiv) to the anode compartment and *n*-Bu_4NPF_6 (620 mg, 1.6 mmol, 4 equiv) to both compartments. The cell was equipped with two septa containing a stainless steel wire/RVC cathode assembly and a pencil/RVC anode assembly connected together with a teflon tubing to equalize pressure. MeCN (8 mL) was added to the cathode compartment and the glass frit was allowed to become saturated (<1 min). MeCN (8 mL) was added to the anode compartment, followed by 4-phenylbutene (0.4 mmol, 1 equiv, 60 µL), benzonitrile (0.4 mmol, 1 equiv, 41 µL) and trifluoroacetic acid (61 µL, 0.8 mmol, 2 equiv). Trifluoroacetic acid (153 µL, 2.0 mmol, 5 equiv) was added to the cathode compartment and both sides of the cell were stirred and electrolyzed under a constant current of 3.7 mA (1.8 mA/cm^2) for 7.2 h (2.5 F/mol). At varying times, ~10 µL aliquots of the reaction mixture were removed via syringe and immediately diluted with a small amount of Et_2O and quenched by passing through a short pad of silica. The solution was transferred to a GC vial and the concentration of the 4-phenylbutene starting material was determined via GC using benzonitrile as the internal standard.

Adduct Yield Time Course Procedure

To an oven-dried divided electrochemical cell equipped with magnetic stir bars was added thianthrene (130 mg, 0.6 mmol, 1.5 equiv or 217 mg, 1.0 mmol, 2.5 equiv) to the anode compartment and n-Bu_4NPF_6 (620 mg, 1.6 mmol, 4 equiv) to both compartments. The cell was equipped with two septa containing a stainless steel wire/RVC cathode assembly and a pencil/RVC anode assembly connected together with a teflon tubing to equalize pressure. MeCN (8 mL) was added to the cathode compartment and the glass frit was allowed to become saturated (<1 min). MeCN (8 mL) was added to the anode compartment, followed by 4-phenylbutene (0.4 mmol, 1 equiv, 60 µL), dibromomethane (0.4 mmol, 1 equiv, 28 µL) and trifluoroacetic acid (61 µL, 0.8 mmol, 2 equiv). Trifluoroacetic acid (153 µL, 2.0 mmol, 5 equiv) was added to the cathode compartment and both sides of the cell were stirred and electrolyzed under a constant current of 3.7 mA (1.8 mA/cm^2) for 7.2 h (2.5 F/mol). At varying times, aliquots of the reaction mixture were removed via syringe (~50 µL for time points before 3 h, then ~10 µL afterwards) and transferred to an NMR tube and diluted with CD_3CN. The concentration of monoadduct **1** and bisadduct **2** were determined via NMR using dibromomethane as an internal standard.

Constant Potential Electrolysis at Potential of Second Oxidation of Thianthrene

To an oven-dried divided electrochemical cell equipped with magnetic stir bars was added thianthrene (66 mg, 0.3 mmol, 1.5 equiv or 109mg, 0.5 mmol, 2.5 equiv) to the anode compartment and Bu_4NPF_6 (775 mg, 2.0 mmol, 10 equiv) to both compartments. The cell was equipped with two septa containing a stainless steel wire/RVC cathode assembly and a pencil/RVC, reference electrode anode assembly connected together with a teflon tubing to

equalize pressure. MeCN (4 mL) was added to the cathode compartment and the glass frit was allowed to become saturated (<1 min). MeCN (4 mL) was added to the anode compartment, followed by 4-phenylbutene (0.2 mmol, 1 equiv, 30 μL), benzonitrile (0.2 mmol, 1 equiv, 21 μL) and trifluoroacetic acid (31 μL, 0.4 mmol, 2 equiv). Trifluoroacetic acid (77 μL, 1.0 mmol, 5 equiv) was added to the cathode compartment and both sides of the cell were stirred and electrolyzed under a constant potential of 1.4 V (vs. $Ag/AgNO_3$) until no starting material remained as monitored by GC. At varying times, ~10 μL aliquots of the reaction mixture were removed via syringe and immediately diluted with a small amount of Et_2O and quenched by passing through a short pad of silica. The solution was transferred to a GC vial and the concentration of the 4-phenylbutene starting material was determined via GC using benzonitrile as the internal standard.

Time Course Full Data

Figure 4A/Figure 4B 1.5 equiv thianthrene conversion:

	Time (h)	Conv (%)
t1	0.7	0.9
t2	1.4	5.3
t3	2.2	4.4
t4	2.9	12.6
t5	3.6	16.5
t6	4.3	24.6
t7	4.7	27.9
t8	5.0	41.1
t9	5.4	53.4
t10	5.8	69.0
t11	6.1	82.1
t12	6.5	94.5
t13	6.9	100.0
t14	7.3	100.0

Figure 4B 2.5 equiv thianthrene conversion:

	Time (h)	Conv (%)
t1	1.2	2.4
t2	2.4	10.2
t3	3.6	18.4
t4	4.8	30.4
t5	6.1	41.1
t6	7.3	51.6
t7	7.9	56.4
t8	8.5	68.7
t9	9.1	90.3
t10	9.7	100.0

Figure 4C monoadduct/bisadduct yield:

	time (h)	bisadduct (%)	monoadduct (%)
t1	0.5	1	0
t2	1	3	0
t3	1.5	4	0
t4	2	6	0.5
t5	2.5	7	1
t6	3	9	0
t7	4	12	2
t8	5	16	16
t9	5.5	15	30
t10	6	19	48
t11	6.5	17	64
t12	6.9	19	70

Constant Potential electrolysis at second oxidation potential of thianthrene conversion:

Figure 4D 1.5 equiv. thianthrene conversion:

	time (min)	Conv (%)
t1	2	0.3
t2	5	0.7
t3	9	0.2
t4	12	9.9
t5	15	24.1
t6	19	47.9
t7	23	73
t8	27	96.3
t9	32	100

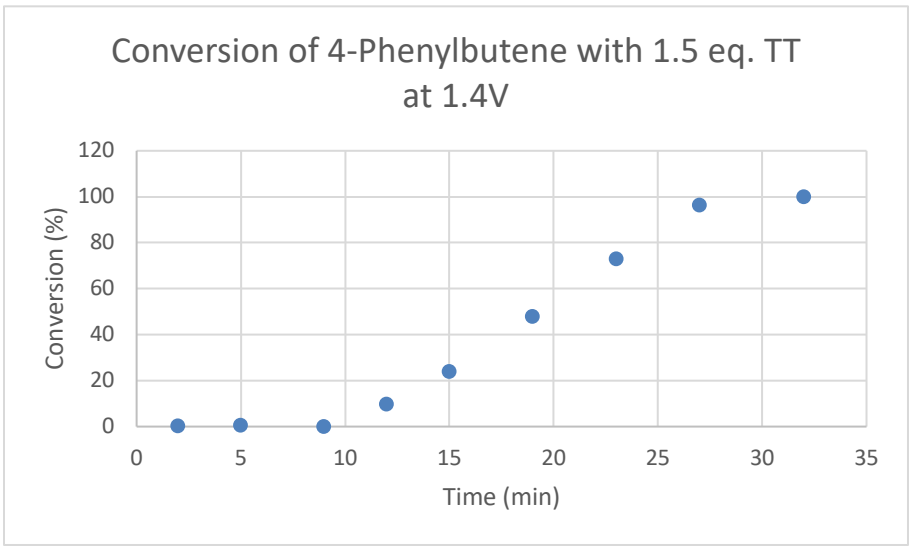
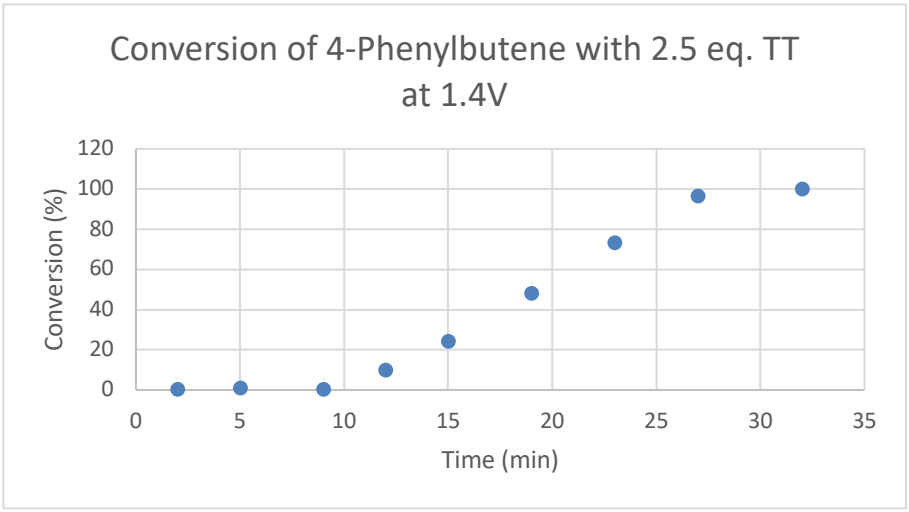
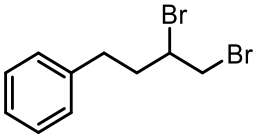


Figure 4D 2.5 equiv. thianthrene conversion:

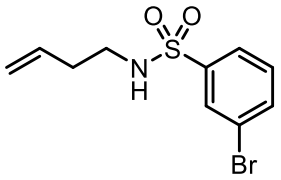
	time (min)	Conv (%)
t1	2	2.3
t2	5	1.1
t3	9	3.5
t4	12	9.5
t5	15	14.5
t6	19	26.2
t7	23	39
t8	27	46.4
t9	32	66.7
t10	37	82.5
t11	42	95.8
t12	48	100



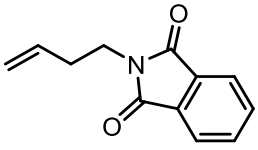
4. Substrate Preparation



(3,4-dibromobutyl)benzene (S1): 4-phenylbutene (0.75 mL, 5.0 mmol, 1 equiv), DMSO (0.43 mL, 6.0 mmol, 1.2 equiv), and EtOAc (20 mL) were combined. The mixture was heated to 60 °C, and 48% HBr (1.4 mL, 12 mmol, 2.4 equiv) was added and the mixture was stirred for 1.5 h. After cooling to room temperature, the mixture was diluted with ~20 mL EtOAc and washed with water (20 mL x3). The organic layer was dried using anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified via flash column chromatography (0-20% EtOAc/hexanes) to yield 1.5 g (quant.) of **S1** as an oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.37 – 7.21 (m, 5H), 4.14 (tdd, J = 9.6, 4.4, 2.9 Hz, 1H), 3.89 (dd, J = 10.3, 4.4 Hz, 1H), 3.68 (t, J = 10.0 Hz, 1H), 2.97 (ddd, J = 13.9, 9.3, 4.7 Hz, 1H), 2.78 (ddd, J = 13.7, 9.1, 7.2 Hz, 1H), 2.56 – 2.45 (m, 1H), 2.12 (dtd, J = 14.3, 9.3, 4.7 Hz, 1H). ^{13}C NMR Consistent with reported spectra[6].



3-bromo-N-(but-3-en-1-yl)benzenesulfonamide (S2): To a solution of 3-bromobenzenesulfonyl chloride (1.41 g, 5.5 mmol, 1.1 equiv.) in DCM (5 mL) at 0 °C was added triethylamine (0.77 mL, 5.5 mmol, 1.1 equiv) followed by 3-buten-1-amine (0.46 mL, 5.0 mmol, 1 equiv). The mixture was allowed to warm to room temperature overnight. ~10 mL 1 M HCl was added to the reaction mixture and the layers were separated. The aqueous layer was extracted with DCM (~20 mL x3). The combined organic layers were dried with anhydrous Na_2SO_4, filtered, and evaporated under reduced pressure to give 1.44 g (99 % yield) of **S2** as a white fluffy solid. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.94 (t, *J* = 1.8 Hz, 1H), 7.73 (dt, *J* = 8.1, 1.3 Hz, 1H), 7.65 (ddd, *J* = 8.0, 2.0, 1.0 Hz, 1H), 7.34 (t, *J* = 7.9 Hz, 1H), 5.56 (ddt, *J* = 17.1, 10.2, 6.9 Hz, 1H), 5.07 – 4.97 (m, 2H), 4.47 (t, *J* = 6.1 Hz, 1H), 2.99 (q, *J* = 6.5 Hz, 2H), 2.20 – 2.13 (m, 2H), 1.54 (brs, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 142.12, 135.85, 134.04, 130.79, 130.17, 125.72, 123.27, 118.69, 42.26, 33.82; **HRMS** (ESI+) **Calc:** [M+Na]+ (C10H12BrNO2SNa) 311.96643; measured: 311.9660; 1.4 ppm difference.



2-(but-3-en-1-yl)isoindoline-1,3-dione (S3): To a mixture of potassium phthalimide (741 mg, 4.0 mmol, 1 equiv) in DMF (8 mL) was added 4-bromo-1-butene (406 µL, 4 mmol, 1 equiv). The reaction mixture was heated to 60 °C and stirred overnight (16 h). At completion, the mixture was cooled to rt and poured into a saturated aqueous NaCl solution (~50 mL). The aqueous layer was extracted with Et_2O (3 x 100 mL). The combined organic layers were washed with aqueous 10% LiCl solution (2 x 10 mL), dried over anhydrous $MgSO_4$, filtered, and

concentrated under reduced pressure. The residue was purified via flash column chromatography (0-45% EtOAc/hexanes) to give 492 mg (61% yield) of **S3** as a solid.
^{1}H NMR (500MHz, $CDCl_3$) δ 7.84 (dd, J = 5.4, 3.1 Hz, 2H), 7.71 (dd, J = 5.4, 3.0, 2H), 5.79 (ddt, J = 17.2, 10.2, 6.9 Hz, 1H), 5.07 (dd, J = 17.1, 1.7 Hz, 1H), 5.02 (dd, J = 10.3, 1.7 Hz, 1H), 3.77 (t, J = 7.1 Hz, 2H), 2.45 (q, J = 7.0 Hz, 2H); ^{13}C NMR consistent with reported spectra[7].

5. General Experimental Procedures

CAUTION: Although there is no known toxicology data on these dicationic adducts and no issues were encountered during these experiments, we suspect, based on analogy to other dielectrophiles[8], that these adducts are extremely toxic. Isolation or storage of the adducts was avoided, and all substitutions were carried out *in situ*.

Preparation of Basified Silica (Silica 9):

Following reported procedure[9], Silica gel (100 g) was added to 1 L of saturated aqueous $NaHCO_3$. The resulting slurry was stirred vigorously for 2 h. After stirring, the mixture was diluted with 100 mL acetone and filtered. The pad of silica gel was washed two times with 100 mL 1:1 water/acetone and once with 100 mL acetone. The filtrate was dried overnight under reduced pressure before use. Silica plates for crude mixture evaluation can be similarly basified.

General Procedure A: Limiting Amine

To an oven-dried divided electrochemical cell equipped with magnetic stir bars was added thianthrene (390 mg, 1.8 mmol, 4.5 equiv) to the anode compartment and n-Bu_4NPF_6 (310 mg, 0.8 mmol, 2 equiv) to both compartments. The cell was equipped with two septa containing a stainless steel wire/RVC cathode assembly and a pencil/RVC anode assembly connected together with a teflon tubing to equalize pressure. MeCN (4 mL) was added to the cathode compartment and the glass frit was allowed to become saturated (<1 min). MeCN (4 mL) was added to the anode compartment, followed by 1-octene (188 µL, 1.2 mmol, 3 equiv). (*Electrode depth: 2 cm).* Trifluoroacetic acid (460 µL, 6.0 mmol, 15 equiv) was added to the cathode compartment and both sides of the cell were stirred and electrolyzed under a constant current of 11.1 mA (5.4 mA/cm^2) for 7.2 h (2.5 F/mol alkene). At completion of electrolysis, the electrode leads were disconnected, septa removed, and the anode RVC was pushed off the pencil into the reaction mixture. Cs_2CO_3 (1.04 g, 3.2 mmol, 8 equiv) was added to the anode compartment followed by amine (0.4 mmol, 1 equiv). To the anode compartment was added a septum pierced with a needle to prevent pressurizing. After pressure equilibration, the needle was removed, and the cathode solution was removed from the cell via pipette. The anode solution was stirred in the cell for 16 h. At completion, the mixture was diluted with DCM (~60 mL) and water (150 mL). The aqueous layer was extracted with DCM (50 mL x 3). The combined organic layers were washed with saturated NaCl solution (40 mL), dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified via flash column chromatography using basified silica gel to yield the pure aziridine product.

General Procedure B: Limiting Alkene

To an oven-dried divided electrochemical cell equipped with magnetic stir bars was added thianthrene (130 mg, 0.6 mmol, 1.5 equiv) to the anode compartment and *n*-Bu_4NPF_6 (620 mg, 1.6 mmol, 4 equiv) to both compartments. The cell was equipped with two septa containing a stainless steel wire/RVC cathode assembly and a pencil/RVC anode assembly connected together with a teflon tubing to equalize pressure. MeCN (8 mL) was added to the cathode compartment and the glass frit was allowed to become saturated (<1 min). MeCN (8 mL) was

added to the anode compartment, followed by the alkene (0.4 mmol, 1 equiv) and trifluoroacetic acid (61 μL, 0.8 mmol, 2 equiv). (*Electrode depth: 2 cm).* Trifluoroacetic acid (153 μL, 2.0 mmol, 5 equiv) was added to the cathode compartment and both sides of the cell were stirred and electrolyzed under a constant current of 3.7 mA (1.8 mA/cm^2) for 7.2 h (2.5 F/mol). At completion of electrolysis, the electrode leads were disconnected, septa removed, and the anode RVC was pushed off the pencil into the reaction mixture. Cs_2CO_3 (782 mg, 2.4 mmol, 6 equiv) was added to the anode compartment followed by benzylamine (175 μL, 1.6 mmol, 4 equiv). To the anode compartment was added a septum pierced with a needle to prevent pressurizing. After pressure equilibration, the needle was removed, and the cathode solution was removed from the cell via pipette. The anode solution was stirred in the cell for 16 h. At completion, the mixture was diluted with DCM (~60 mL) and water (150 mL). The aqueous layer was extracted with DCM (50 mL x 3). The combined organic layers were washed with saturated NaCl solution (40 mL), dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified via flash column chromatography using basified silica gel to yield the pure aziridine product.

General Procedure C: Propene Aziridination Procedure

To an oven-dried divided electrochemical cell equipped with magnetic stir bars was added thianthrene (390 mg, 1.8 mmol, 4.5 equiv) to the anode compartment and *n*-Bu_4NPF_6 (310 mg, 0.8 mmol, 2 equiv) to both compartments. The cell was equipped with two septa containing a stainless steel wire/RVC cathode assembly and a pencil/RVC anode assembly connected together with a teflon tubing to equalize pressure. In a separate 25 mL-round bottom flask, MeCN (12mL) was sparged with a balloon of propene for 12 mins. Propene-saturated MeCN (4mL) was delivered to cathode compartment via Teflon cannula and the glass frit was allowed to become saturated (<1). Propene-saturated MeCN (4 mL) was delivered to the anode compartment via Teflon cannula. (*Electrode depth: 2 cm).* The Teflon cannulae in both compartments were left attached to the 25-mL round bottom flask in order to maintain 1 atm atmosphere of propene. 1-octene (188 μL, 1.2 mmol, 3 equiv) was then added to the anode compartment. Trifluoroacetic acid (460 μL, 6.0 mmol, 15 equiv) was added to the cathode compartment and both sides of the cell were stirred and electrolyzed under a constant current of 11.1 mA (5.4 mA/cm^2) for 7.2 h. At completion of electrolysis, the electrode leads were disconnected, septa removed, and the anode RVC was pushed off the pencil into the reaction mixture. Cs_2CO_3 (1.04 g, 3.2 mmol, 8 equiv) was added to the anode compartment followed by amine (0.4 mmol, 1 equiv). To the anode compartment was added a septum pierced with a needle to prevent pressurizing. After pressure equilibration, the needle was removed, and the cathode solution was removed from the cell via pipette. The anode solution was stirred in the cell for 16 h. At completion, the mixture was diluted with DCM (~60 mL) and water (150 mL). The aqueous layer was extracted with DCM (50 mL x 3). The combined organic layers were washed with saturated NaCl solution (40 mL), dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified via flash column chromatography using basified silica gel to yield the pure aziridine product.

General Procedure D: Limiting Amine NMR Yield

Following General Procedure A, but with the following modification: following stirring with benzylamine and Cs_2CO_3 for 16 h, aziridine product yield was determined via NMR using mesitylene or dibromomethane as an internal standard. Presence of aziridine product was further validated via HRMS analysis.

General Procedure E: Limiting Alkene NMR Yield

Following General Procedure B, but with the following modification: following stirring with benzylamine and Cs_2CO_3 for 16 h, aziridine product yield was determined via NMR using mesitylene or dibromomethane as an internal standard. Presence of aziridine product was further validated via HRMS analysis.

General Procedure F: Propene Aziridination Procedure NMR Yield

Following General Procedure C, but with the following modification: following stirring with amine and Cs_2CO_3 for 16 h, aziridine product yield was determined via 19F NMR using trifluorotoluene as an internal standard. Presence of aziridine product was further validated via HRMS analysis.

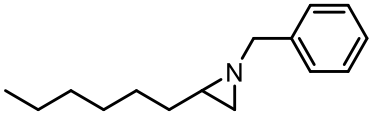
General Procedure G: Adduct Derivatization Procedure

To an oven-dried divided electrochemical cell equipped with magnetic stir bars was added thianthrene (130 mg, 0.6 mmol, 1.5 equiv) to the anode compartment and n-Bu_4NPF_6 (620 mg, 1.6 mmol, 4 equiv) to both compartments. The cell was equipped with two septa containing a stainless steel wire/RVC cathode assembly and a pencil/RVC anode assembly connected together with a teflon tubing to equalize pressure. MeCN (8 mL) was added to the cathode compartment and the glass frit was allowed to become saturated (<1 min). MeCN (8 mL) was added to the anode compartment, followed by 4-phenyl-butene (60 μL, 0.4 mmol, 1 equiv) and trifluoroacetic acid (61 μL, 0.8 mmol, 2 equiv). (*Electrode depth: 2 cm).* Trifluoroacetic acid (153 μL, 2.0 mmol, 5 equiv) was added to the cathode compartment and both sides of the cell were stirred and electrolyzed under a constant current of 3.7 mA (1.8 mA/cm^2) for 7.2 h (2.5 F/mol). At completion of electrolysis, the electrode leads were disconnected, septa removed, and the anode RVC was pushed off the pencil into the reaction mixture. The nucleophile was added to the anode compartment and the cell was capped with a septum pierced with a needle to prevent pressurizing. After pressure equilibration, the needle was removed, and the cathode solution was removed from the cell via pipette. The anode solution was stirred in the cell for 16 h. At completion, the mixture was diluted with DCM (~60 mL) and water (150 mL). The aqueous layer was extracted with DCM (50 mL x 3). The combined organic layers were washed with saturated NaCl solution (40 mL), dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified via flash column chromatography to yield the pure difunctionalized product.

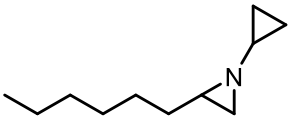
General Procedure H: Adduct Derivatization NMR Yield

Following General Procedure G, but with the following modification: following stirring with nucleophile for 16 h, product yield was determined via NMR using mesitylene or dibromomethane as an internal standard.

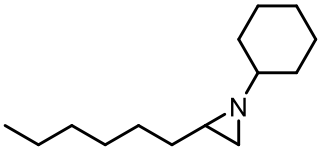
6. Aziridine Product Isolation and Characterization



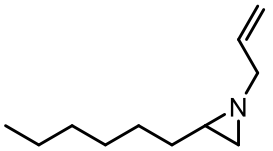
1-Benzyl-2-hexylaziridine (4): Following General Procedure B with 0-14% acetone/hexanes gradient, 60.7 mg (70% yield) obtained as an oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.14 (m, 5H), 3.41 (d, *J* = 13.3 Hz, 1H), 3.24 (d, *J* = 13.3 Hz, 1H), 1.53 (d, *J* = 3.3 Hz, 1H), 1.42 – 1.06 (m, 12H), 0.78 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR consistent with reported spectra[10].



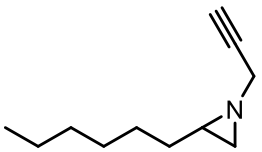
1-cyclopropyl-2-hexylaziridine (5): Following General Procedure D with the following modification: after stirring for 16 h, the mixture was diluted with DCM (~60 mL) and water (150 mL). The aqueous layer was extracted with DCM (50 mL x 3). The combined organic layers were washed with saturated NaCl solution (40 mL), dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. Electrolyte was removed via flash column chromatography on basified silica (0-15% diethyl ether/hexanes gradient). Obtained 50% yield. **HRMS** (ESI+) Calc: [M+H]+ (C11H22N) 168.1747; measured: 168.1745; 1.2 ppm difference.



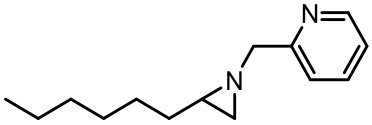
1-cyclohexyl-2-hexylaziridine (6): Following General Procedure A except with non-basified silica, 0-20% acetone/hexanes gradient, 60% yield obtained as a mixture with thianthrene S-oxide (127.7 mg, 1:1.4 pdt:S-oxide). **^{1}H NMR** (500 MHz, CDCl3) δ 1.81 – 1.63 (m, 4H), 1.58 – 1.51 (m, 1H), 1.44 – 1.02 (m, 18H), 0.93 (tt, J = 10.8, 3.8 Hz, 1H), 0.81 (t, J = 6.7 Hz, 3H). **^{13}C NMR** (126 MHz, CDCl3) δ 69.07, 38.42, 33.46, 33.08, 32.48, 32.44, 31.89, 29.24, 27.83, 26.14, 25.07, 25.05, 22.63, 14.09. **HRMS** (ESI+) Calc: [M+H]+ (C14H28N) 210.22163; measured: 210.2216; 0.1 ppm difference.



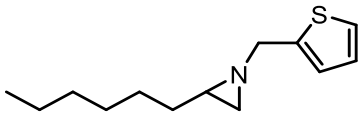
1-allyl-2-hexylaziridine (7): Following General Procedure B except with allylamine (120 µL, 1.6 mmol, 4 equiv) and non-basified silica with 0-15% acetone/hexanes gradient, 59% yield obtained as a mixture with thianthrene S-oxide (76.8 mg, 1:1 pdt:S-oxide). **^{1}H NMR** (500 MHz, CDCl3) δ 5.86 (ddt, J = 16.4, 10.3, 5.8 Hz, 1H), 5.12 (dd, J = 17.2, 1.8 Hz, 1H), 5.03 (dd, J = 10.3, 1.7 Hz, 1H), 2.77 (qd, J = 13.9, 6.0 Hz, 2H), 1.46 (d, J = 3.4 Hz, 1H), 1.40 – 1.18 (m, 12H), 1.17 (d, J = 6.3 Hz, 1H), 0.81 (t, J = 6.8 Hz, 3H). ^{13}C NMR consistent with reported spectra[11].



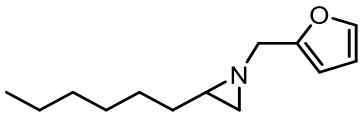
2-hexyl-1-(prop-2-yn-1-yl)aziridine (8): Following General Procedure D with the following modification: after stirring for 16 h, the mixture was diluted with DCM (~60 mL) and water (150 mL). The aqueous layer was extracted with DCM (50 mL x 3). The combined organic layers were washed with saturated NaCl solution (40 mL), dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. Electrolyte was removed via flash column chromatography on basified silica (0-10% acetone/hexanes gradient). obtained 52% yield. **HRMS** (ESI+) Calc: [M+H]+ (C11H20N) 166.1590; measured: 166.1590; <0.1 ppm difference.



2-((2-hexylaziridin-1-yl)methyl)pyridine (9): Following General Procedure A with 0-50% acetone/diethyl ether gradient, 65.4mg (75% yield) obtained as an oil. **^{1}H NMR** (500MHz, $CDCl_3$) δ 8.45 (d, J = 2.3Hz, 2H), 8.42 (d, J = 4.8Hz, 1H), 7.63 (d, J = 7.7, 2.5Hz, 1H), 7.17 (m, 1H), 3.40 (d, J = 13.6Hz, 1H), 3.22 (d, J = 13.5Hz, 1H), 1.54 (d, J = 3.5Hz, 1H), 1.41-1.35 (m, 1H), 1.34-1.25 (m, 3H), 1.23-1.07 (m, 8H), 0.76 (t, J = 7.0Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 149.46, 148.49, 135.75, 134.83, 123.28, 62.22, 40.02, 34.18, 32.84, 31.71, 28.96, 27.32, 22.49, 14.00; **HRMS** (ESI+) Calc: [M+H]+ (C14H23N2) 219.1856; measured: 219.1854; 0.9 ppm difference.

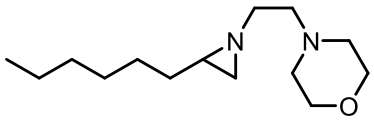


2-((2-hexylaziridin-1-yl)methyl)thiophene (10): Following General Procedure A with 0-15% EtOAc/hexanes gradient, 70% yield obtained as a mixture with thianthrene S-oxide (76.1 mg, 1:0.2 pdt:S-oxide). **1H NMR** (400 MHz, CDCl3) δ 7.21 (dd, J = 5.1, 1.3 Hz, 1H), 6.97-6.90 (m, 2H), 3.67 (d, J = 13.7 Hz, 1H), 3.47 (d, J = 13.7 Hz, 1H), 1.62 (d, J = 3.3 Hz, 1H), 1.51-1.18 (m, 12H), 0.86 (t, J = 6.8 Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.18, 126.44, 124.94, 124.37, 59.32, 40.05, 34.05, 32.89, 31.78, 29.00, 27.30, 2.54, 14.05; **HRMS** (ESI+) Calc: [M+H]+ (C13H22NS) 224.14675; measured: 224.1467; 0.2 ppm difference.

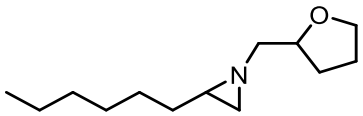


1-(furan-2-ylmethyl)-2-hexylaziridine (11): Following General Procedure A with 0-10% acetone/DCM gradient, 44.2mg (53% yield) obtained as an oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.29 (d, J = 1.8 Hz, 1H), 6.24 (dd, J = 3.1, 1.9 Hz, 1H), 6.13 (d, J = 3.1 Hz, 1H), 3.35 (d, J = 13.9Hz, 1H), 3.28 (d, J = 13.9 Hz, 1H), 1.51 (d, J = 3.6 Hz, 1H), 1.44-1.38 (m, 11H), 0.80 (5, J = 6.9 Hz, 3H); **^{13}C NMR** (101 MHz, C_6D_6) δ 154.70, 142.42, 111.02, 107.75, 57.82, 40.16,

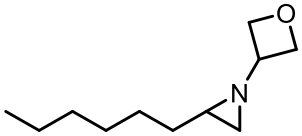
34.12, 33.94, 32.83, 30.07, 28.25, 23.59, 14.92 ; **HRMS** (ESI+) Calc: [M+H]+ (C13H22NO) 208.16959; measured: 208.1693; 1.4 ppm difference.



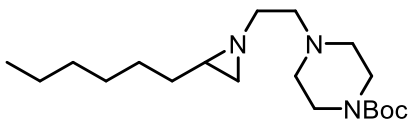
4-(2-(2-hexylaziridin-1-yl)ethyl)morpholine (12): Following General Procedure A with 10-40% acetone/hexanes gradient, 47 mg (49%) obtained as an oil. **1H NMR** (600 MHz, C_6D_6) δ 3.61 (t, *J* = 4.7 Hz, 4H), 2.48 (t, *J* = 6.9 Hz, 2H), 2.34 – 2.23 (m, 5H), 2.19 (dt, *J* = 11.5, 6.9 Hz, 1H), 1.51 – 1.23 (m, 11H), 1.07 (qd, *J* = 6.0, 3.3 Hz, 1H), 0.95 (d, *J* = 6.2 Hz , 1H), 0.90 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (101 MHz, C_6D_6) δ 66.82, 59.07, 58.74, 54.28, 39.47, 33.21, 33.19, 31.92, 29.28, 27.51, 22.69, 13.98. **HRMS** (ESI+) Calc: [M+H]+ (C14H29N2O) 241.22744; measured: 241.2269; 2.2 ppm difference.



2-hexyl-1-((tetrahydrofuran-2-yl)methyl)aziridine (13): Following General Procedure A with 15-35% EtOAc/hexanes gradient, 55.4mg (66% yield) obtained as 1:1 mixture of diastereomers. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.04-3.93 (m, 1H), 3.89-3.81 (m, 1H), 3.78-3.70 (m, 1H), 2.40-2.26 (m, 2H), 2.08-1.96 (m, 1H), 1.93-2.82 (m, 2H), 1.66-1.55 (m, 1H), 1.53 (dd, J = 6.0 2.4 Hz, 1H), 1.48-1.19 (m, 13H), 0.87 (t, J = 6.7 Hz, 3H); **^{13}C NMR** (101 MHz, C_6D_6) δ 79.04, 68.01, 67.69, 65.96, 65.86, 39.63, 39.59, 33.62, 33.57, 33.54, 32.32, 32.30, 30.19, 30.08, 29.66, 27.79, 27.78, 25.93, 23.07 14.37; **HRMS** (ESI+) Calc: [M+H]+ (C13H26NO) 212.20089; measured: 212.2007; 0.9 ppm difference.

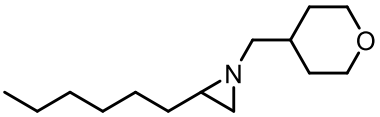


2-hexyl-1-(oxetan-3-yl)aziridine (14): Following General Procedure A with 35-75% EtOAc/hexanes gradient, 40.2mg (55% yield) obtained as an oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 4.70 (dt, J = 13.4, 6.6 Hz, 2H), 4.61 (td, J = 5.9, 4.2 Hz, 2H), 3.02 (ddd, J = 12.2, 6.7, 5.5 Hz, 1H), 1.57 (d, J = 3.3 Hz, 1H), 1.49-1.41 (m, 2H), 1.38-1.24 (m, 10H), 0.88 (t, J = 7.0 Hz)z ; **^{13}C NMR** (151 MHz, $CDCl_3$) δ 67.93, 67.89, 67.84, 39.56, 36.22, 34.17, 33.09, 31.84, 31.64, 31.49, 29.13, 27.45, 22.59, 14.07 ; **HRMS** (ESI+) Calc: [M+H]+ (C11H22NO) 184.1696; measured: 184.1694; 1.1 ppm difference.

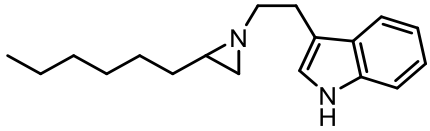


tert-butyl 4-(2-(2-hexylaziridin-1-yl)ethyl)piperazine-1-carboxylate (15): Following General Procedure A with 5-40% acetone/hexanes gradient, 87.6mg (63% yield) obtained as an oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.36 (t, J = 5.1Hz, 4H), 2.50 (t, J = 7.0Hz, 2H), 2.44-2.31 (m, 5H), 2.22 (dt, J = 11.7, 7.1Hz, 1H), 1.45 (d, J = 3.0Hz, 1H), 1.42-1.13 (m, 22H), 0.81 (t, J = 6.6Hz, 3H) ; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.56, 79.40, 58.38, 58.07, 53.31, 52.48, 39.69, 33.68,

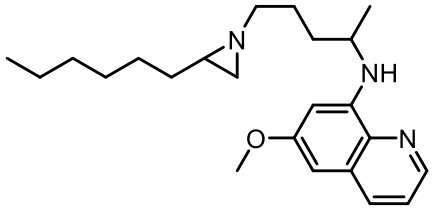
32.93, 31.69, 28.99, 28.26, 27.39, 22.45, 13.94; **HRMS** (ESI+) Calc: [M+H]+ (C19H38N3O2) 340.29585; measured: 340.2958; 0.1 ppm difference.



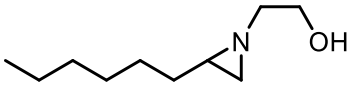
1-(tetrahydropyran-4-ylmethyl)-2-hexylaziridine (16): Following General Procedure A with 30-50% EtOAc/hexanes gradient followed by an additional flash column chromatography purification using 0-15% acetone/hexanes gradient, 86.4mg (75% yield) obtained as an oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 4.00-3.92 (m, H), 3.44-3.35 (m, 2H), 2.19 (ddd, J = 11.8, 5.7, 1.7 Hz, 1H), 2.04 (ddd, J = 11.6, 5.7, 1.7 Hz, 1H), 1.86-1.73 (m, 2H), 1.66-1.59 (m, 1H), 1.51 (dd, J = 3.3, 1.9 Hz, 1H), 1.46-1.17 (m, 14H), 0.88 (t, J = 5.9Hz, 3H) ; **^{13}C NMR** (126 MHz, $CDCl_3$) δ 67.93, 67.89, 67.84, 39.56, 36.22, 34.17, 33.09, 31.84, 31.64, 31.49, 29.13, 27.45, 22.59, 14.07 ; **HRMS** (ESI+) Calc: [M+H]+ (C14H28NO) 226.21654; measured: 226.2162; 1.5 ppm difference.



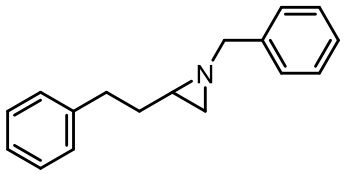
3-(2(2-hexylaziridin-1-yl)ethyl)-1H-indole (17): Following General Procedure A with 20-40% EtOAc/hexanes gradient, 60.8mg (56% yield) obtained as an oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.38 (br s, 1H), 7.60 (d, J = 7.8Hz, 1H), 7.33 (d, J = 8.0Hz, 1H), 7.19 (t, J = 7.5 Hz, 1H), 7.19 (t, J = 7.5 Hz, 1H), 6.97 (d, J = 2.3 Hz, 1H), 3.13-2.99 (m, 2H), 2.67 (ddd, J = 11.4, 8.8, 6.8 Hz, 1H), 2.52 (ddd, J = 11.4, 9.2, 6.5 Hz, 1H), 1.57 (d, J = 3.2 Hz, 1H), 1.53-1.22 (m, 14H), 0.90 (t, J = 6.6 Hz, 3H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 136.41, 127.58, 122.00, 121.72, 119.27, 118.92, 114.30, 111.23, 62.14, 39.92, 33.98, 33.31, 32.00, 29.31, 27.70, 25.93, 22.76, 14.24; **HRMS** (ESI+) Calc: [M+H]+ (C18H27N2) 271.2166; measured: 271.2166; 1.1ppm difference.



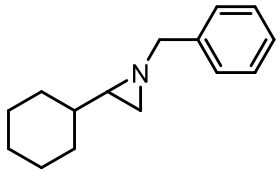
N-(5-(2-hexylaziridin-1-yl)pentan-2-yl)-6-methoxyquinolin-8-amine (18): Following General Procedure A using Primaquine phosphate (0.4 mmol, 1.0 equiv.) with 0-20% acetone/hexanes gradient followed by an additional flash column chromatography purification on non-basified silica using 0-10% MeOH/DCM gradient, 90.2 mg (61% yield) obtained as an 1:1 mixture of diastereomers. **^{1}H NMR** (600MHz, $CDCl_3$) δ 8.52 (dt, J = 4.1, 1.5 Hz, 1H), 7.91 (dd, J = 8.2, 1.7 Hz, 1H), 7.29 (dd, J = 8.2, 4.2 Hz, 1H), 6.32 (d, J = 2.5 Hz, 1H), 6.28 (d, J = 2.5Hz), 6.09-5.95 (m, 1H), 3.89 (s, 3H), 3.67-3.57 (m, 1H), 2.34-2.26 (m, 1H), 2.22-2.13 (m, 1H), 1.82-1.61 (m, 4H), 1.50 (d, J = 3.5 Hz), 1.46-1.20 (m, 14H), 1.17 (dd, J = 6.4, 4.0 Hz), 0.87 (5, J = 6.9 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 159.61, 145.27, 144.38, 135.57, 134.85, 130.03, 121.93, 96.75, 91.64, 61.59, 61.52, 55.34, 48.30, 48.16, 39.81, 39.76, 34.78, 34.69, 33.25, 31.97, 29.29, 27.69, 27.68, 26.77, 26.64, 22.76, 20.64, 14.22; **HRMS** (ESI+) Calc: [M+H]+ (C23H36N3O) 370.2853; measured: 370.2850; 0.8ppm difference.



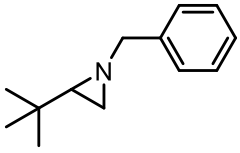
2-(2-hexylaziridin-1-yl)ethan-1-ol (19): Following General Procedure A except with the following purification modification: following flash column chromatography on basified silica (0-40% acetone/DCM), the product containing fractions were concentrated under reduced pressure, and the residue was dissolved into 5 mL pentane and filtered to yield 48.5 mg (71% yield) of **18** as an oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 3.73 (t, J = 5.3Hz, 2H), 2.59-2.34 (m, 3H), 1.57 (d, J = 2.3Hz, 1H), 1.50-1.25 (m, 12H), 0.90 (t, J = 6.6Hz, 3H); **^{13}C NMR** (101 MHz, $CDCl_3$) δ 62.87, 62.16, 39.68, 33.80, 33.22, 31.99, 29.32, 27.62, 22.78, 14.25; **HRMS** (ESI+) Calc: [M+H]+ ($C_{10}H_{22}NO$) 172.1696; measured: 172.1696; <0.1 ppm difference. Connectivity confirmed by edited HSQC and HMBC.



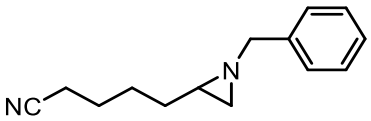
1-benzyl-2-phenethylaziridine (3): Following General Procedure B with 0-20% acetone/hexanes gradient, 73% yield obtained as a mixture with thianthrene-S-oxide (83 mg, 1:0.2 pdt:S-oxide). **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.30 – 7.22 (m, 4H), 7.20 – 7.13 (m, 3H), 7.11 – 7.05 (m, 1H), 7.04 – 7.00 (m, 2H), 3.41 (d, J = 13.2 Hz, 1H), 3.21 (d, J = 13.2 Hz, 1H), 2.57 (ddd, J = 14.9, 9.1, 6.1 Hz, 1H), 2.50 (ddd, J = 13.8, 9.0, 6.9 Hz, 1H), 1.64 (m, 2H), 1.55 (d, J = 3.5 Hz, 1H), 1.43 – 1.38 (m, 1H), 1.31 (d, J = 6.4 Hz, 1H). **^{13}C NMR** (151 MHz, CDCl3) δ 141.93, 139.41, 128.48, 128.40, 128.32, 128.27, 127.11, 125.78, 64.97, 39.23, 34.78, 34.13, 33.74.. **HRMS** (ESI+) Calc: [M+H]+ ($C_{17}H_{20}N$) 238.1590; measured: 238.1588; 0.8 ppm difference.



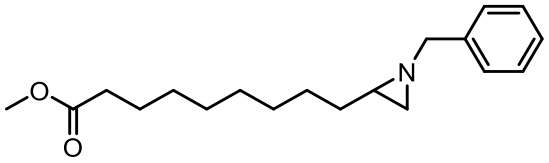
1-Benzyl-2-cyclohexylaziridine (20): Following General Procedure B with 0-10% acetone/hexanes, 63.4 mg (74% yield) obtained as an oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.36-7.30 (m, 4H), 7.27-7.23 (m, 1H), 3.50 (d, J = 13.0Hz, 1H), 3.25 (d, J = 13.0Hz, 1H), 1.71-1.56 (m, 6H), 1.36 (d, J = 6.5Hz, 1H), 1.25 (ddd, J = 7.6, 6.4, 3.6Hz), 1.03-0.87 (m, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 139.44, 128.45, 128.25, 127.00, 65.42, 45.24, 41.10, 33.09, 31.24, 30.29, 26.44, 25.96, 25.78; **HRMS** (ESI+) Calc: [M+H]+ ($C_{15}H_{22}N$) 216.1747; measured: 216.1747; < 0.1 ppm difference.



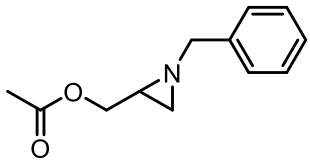
1-Benzyl-2-*t*-butylaziridine (21): Following General Procedure B with 0-20% acetone/hexanes, 24.5 mg (32% yield) obtained as an oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.38-7.29 (m, 4H), 7.27-7.22 (m, 1H), 3.66 (d, J = 13.0Hz, 1H), 3.13 (d, J = 13.0Hz), 1.74 (d, J = 3.7Hz, 1H), 1.28 (dd, J = 6.6, 3.7Hz, 1H), 1.23 (d, J = 6.6Hz, 1H), 0.76 (s, 9H); ^{13}C NMR consistent with reported spectra[12].



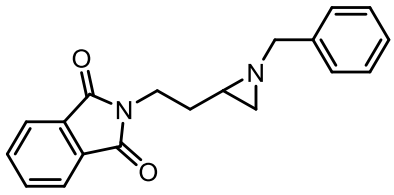
5-(1-benzylaziridin-2-yl)pentanenitrile (22): Following General Procedure E, obtained 77% yield. **HRMS** (ESI+) Calc: [M+H]+ (C14H19N2) 215.1543; measured: 215.1542; 0.5 ppm difference.



methyl 9-(1-benzylaziridin-2-yl)nonanoate (23): Following General Procedure B with 0-15% acetone/hexanes gradient, 81% yield obtained as a mixture with thianthrene-S-oxide (110.7 mg, 1:0.1 pdt:S-oxide). **^{1}H NMR** (500 MHz, CDCl3) δ 7.28 – 7.14 (m, 5H), 3.58 (s, 3H), 3.42 (d, *J* = 13.3 Hz, 1H), 3.22 (d, *J* = 13.3 Hz, 1H), 2.21 (t, *J* = 7.6 Hz, 2H), 1.57 – 1.48 (m, 3H), 1.40 – 1.10 (m, 14H).**; ^{13}C NMR** (126 MHz, $CDCl_3$) δ 174.27, 139.46, 128.27, 128.18, 126.95, 65.03, 51.40, 39.76, 34.09, 34.07, 32.99, 29.36, 29.26, 29.12, 29.10, 27.39, 24.93; **HRMS** (ESI+) Calc: [M+H]+ (C19H30NO2) 304.22711; measured: 304.2266; 1.7 ppm difference.

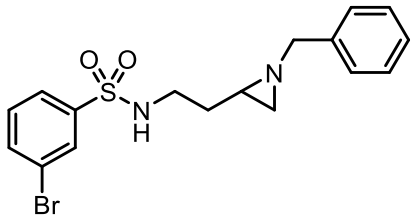


1-Benzyl-2-acetoxymethylaziridine (24): Following General Procedure B except with 12.0 mA (5.8 mA/cm^2), with 20-40% EtOAc/hexanes gradient, 57.3 mg (70% yield) obtained as an oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.37-7.31 (m, 4H), 7.29-7.24 (m, 1H), 4.19 (dd, J = 11.7, 4.5Hz, 1H), 3.82 (dd, J = 11.7, 7.5 Hz, 1H), 3.60 (d, J = 13.4Hz, 1H), 3.32 (d, J = 13.4Hz, 1H), 1.97 (s, 3H), 1.87 (dddd, J = 7.7, 6.6, 4.5, 3.4 Hz, 1H), 1.53 (d, J = 6.5Hz, 1H); ^{13}C NMR consistent with reported spectra[13].

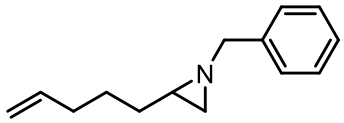


1-Benzyl-2-ethylpthalimidoaziridine (25): Following General Procedure B except with 12.0 mA (5.8 mA/cm^2), with 30-50% EtOAc/hexanes gradient, 75.4 mg (62% yield) obtained as an oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.86-7.82 (m, 2H), 7.73-7.68 (m, 2H), 7.31-7.26 (m, 4H), 7.24-7.20 (m, 1H), 3.75 (t, J = 6.9Hz, 2H), 3.55 (d, J = 13.3Hz, 1H), 3.24 (d, J = 13.3Hz, 1H),

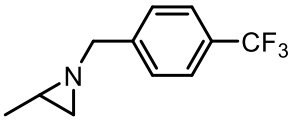
1.86-1.74 (m, 2H), 1.60 (d, J = 3.4Hz, 1H), 1.58-1.52 (m, 1H), 1.38 (d, J = 6.3Hz); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.49, 139.33, 134.04, 132.30, 128.46, 128.22, 127.13, 123.34, 64.81, 37.23, 36.37, 33.64, 31.08; **HRMS** (ESI+) Calc: [M+H]+ (C19H19N2O2) 307.1441; measured: 307.1438; 1.0 ppm difference.



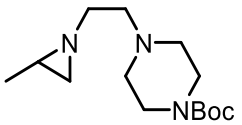
N-(2-(1-benzylaziridin-2-yl)ethyl)-3-bromobenzenesulfonamide (26): Following General Procedure B except with 12.0 mA (5.8 mA/cm^2), with 0-40% acetone/hexanes gradient, 99.2 mg (63% yield) obtained as a powder. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.91 (t, J = 1.8 Hz, 1H), 7.69-7.63 (m, 2H), 7.40-7.29 (m, 6H), 5.71 (t, J = 4.9Hz, 1H), 3.50 (d, J = 12.9 Hz, 1H), 3.23 (d, J = 12.9 Hz, 1H), 2.98 (ddd, J = 12.6, 10.9, 5.9Hz, 1H), 2.79 (ddt, J = 13.0, 8.8, 4.2 Hz, 1H), 1.92 (ddt, J = 13.4, 8.6, 4.1 Hz, 1H), 1.67-1.59 (m, 2H), 1.44-1.32 (m, 2H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 142.28, 138.79 135.51, 130.62, 130.07, 128.87, 128.47, 127.72, 125.65, 123.08, 64.85, 41.16, 37.20, 32.51, 29.68; **HRMS** (ESI+) Calc: [M+H]+ (C17H20BrN2O2S) 395.04234; measured: 395.0420; 0.9 ppm difference.



1-Benzyl-2-pent-4-eneaziridine (27): Following General Procedure B with 0-20% acetone/hexanes gradient, 55.3mg (67% yield) obtained as an oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.36-7.30 (m, 4H), 7.28-7.24 (m, 1H), 5.75 (ddt, J = 16.9, 10.2, 6.6Hz, 1H), 4.98-4.89 (m, 2H), 3.50 (d, J = 13.3Hz, 1H), 3.32 (d, J = 13.2Hz, 1H), 2.04-1.97 (m, 2H), 1.62 (d, J = 3.3Hz), 1.48-1.35 (m, 6H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 139.44, 138.75, 128.32, 128.19, 126.99, 114.41, 65.00, 39.58, 34.09, 33.44, 32.49, 26.70; **HRMS** (ESI+) Calc: [M+H]+ (C14H20N) 202.1590.; measured: 202.1589; 0.5 ppm difference.

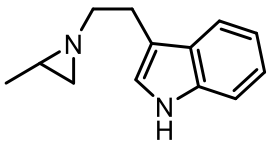


1-Trifluoromethylbenzyl-2-methylaziridine (28): Following General Procedure F, 71% yield obtained. **HRMS** (ESI+) Calc: [M+H]+ (C11H13F3N) 216.09946; measured: 216.0994; 0.3 ppm difference.

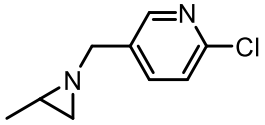


tert-butyl 4-(2-(2-methylaziridin-1-yl)ethyl)piperazine-1-carboxylate (29): Following General Procedure C with 10-50% acetone/hexanes gradient, 76.2 mg (71% yield) obtained as an oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 3.45-3.37 (m, 4H), 2.60-2.51 (m, 2H), 2.45-2.32 (m, 6H),

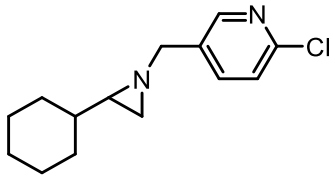
1.47 (d, J = 3.6 Hz, 1H), 1.44 (s, 9H), 1.38-1.32 (m, 1H), 1.21 (d, J = 6.3 Hz, 1H), 1.16 (d, J = 5.5 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 154.91, 79.73, 58.75, 58.43, 53.66, 34.86, 34.82, 29.45, 28.59, 18.51; **HRMS** (ESI+) Calc: [M+H]+ ($C_{14}H_{28}N_3O_2$) 270.21760; measured: 270.2175; 0.4 ppm difference.



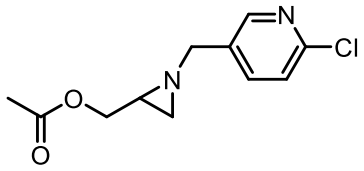
3-(2-(2-methylaziridin-1-yl)ethyl)-1H-indole (30): Following General Procedure C with 0-30% acetone/hexanes gradient followed by an additional flash column chromatography purification using 0-30% acetone/DCM gradient, 52.3 mg (65% yield) obtained as an oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.06 (br s, 1H), 7.60 (dd, J = 7.9, 1.1 Hz, 1H), 7.35 (d, J = 8.1 Hz, 1H), 7.18 (ddd, J = 8.2, 6.9Hz, 1.2 Hz, 1H), 7.11 (ddd, J = 8.0, 7.0, 1.0 Hz, 1H), 7.01 (d, J = 2.3 Hz, 1H), 3.04 (t, J = 7.7 Hz, 2H), 2.62-2.52 (m, 2H), 1.50 (d, J = 3.5 Hz, 1H), 1.36-1.29 (m, 1H), 1.23 (d, J = 6.3 Hz, 1H), 1.15 (d, J = 5.4 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 136.44, 127.61, 122.05, 121.79, 119.32, 118.99, 114. 46, 111.24, 62.02, 34.78, 34.73, 26.02, 18.62; **HRMS** (ESI+) Calc: [M+H]+ ($C_{13}H_{17}N_2$) 201.13863; measured: 201.1386; 0.1 ppm difference.



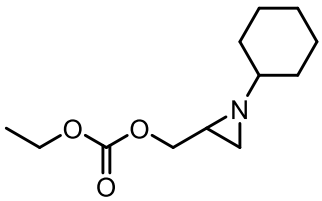
2-chloro-5-((2-methylaziridin-1-yl)methyl)pyridine (31): Following General Procedure C with 20-50% 1:3 acetone:DCM/hexanes gradient, 60.1 mg (82% yield) obtained as an oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.31 (d, J = 2.5 Hz, 1H), 7.69 (dd, J = 8.2, 2.5 Hz, 1H), 7.29 (d, J = 8.1 Hz, 1H), 3.37 (d, J = 14.0 Hz, 1H), 3.41 (d, J = 14.0 Hz, 1H), 1.59 (d, J = 3.6 Hz, 1H), 1.55-1.49 (m, 1H), 1.37 (d, J = 6.4 Hz, 1H), 1.19 (d, J = 5.5 Hz, 3H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 150.21, 149.05, 138.53, 134.13, 124.15, 61.26, 35.37, 35.11, 18.31; **HRMS** (ESI+) Calc: [M+H]+ ($C_9H_{11}ClN_2$) 183.06835; measured: 183.0684; 0.3 ppm difference.



2-chloro-5-((2-cyclohexylaziridin-1-yl)methyl)pyridine (32): Following General Procedure B except with (6-chloropyridin-3-yl)methanamine (228 mg, 1.6 mmol, 4 equiv) and isolated using 0-50% EtOAc/hexanes, followed by an additional flash column chromatography purification using 0-45% acetone/hexanes gradient, 61.9 mg (62% yield) obtained as an oil. **^{1}H NMR** (500 MHz, C_6D_6) δ 8.19 (d, J = 2.4 Hz, 1H), 7.20 (dd, J = 8.2, 2.5 Hz, 1H), 6.85 (d, J = 8.1 Hz, 1H), 2.84 (d, J = 13.5 Hz, 1H), 2.69 (d, J = 13.5 Hz, 1H), 1.65 – 1.51 (m, 5H), 1.38 (d, J = 3.1 Hz, 1H), 1.08 (m, 3H), 0.90 – 0.78 (m, 5H).; **^{13}C NMR** (126 MHz, C_6D_6) δ 150.91, 149.85, 138.85, 134.65, 124.13, 61.78, 45.60, 41.07, 32.71, 31.47, 30.64, 26.97, 26.50, 26.36.; **HRMS** (ESI+) Calc: [M+H]+ ($C_{14}H_{20}ClN_2$) 251.13095; measured: 251.1309; 0.2 ppm difference.



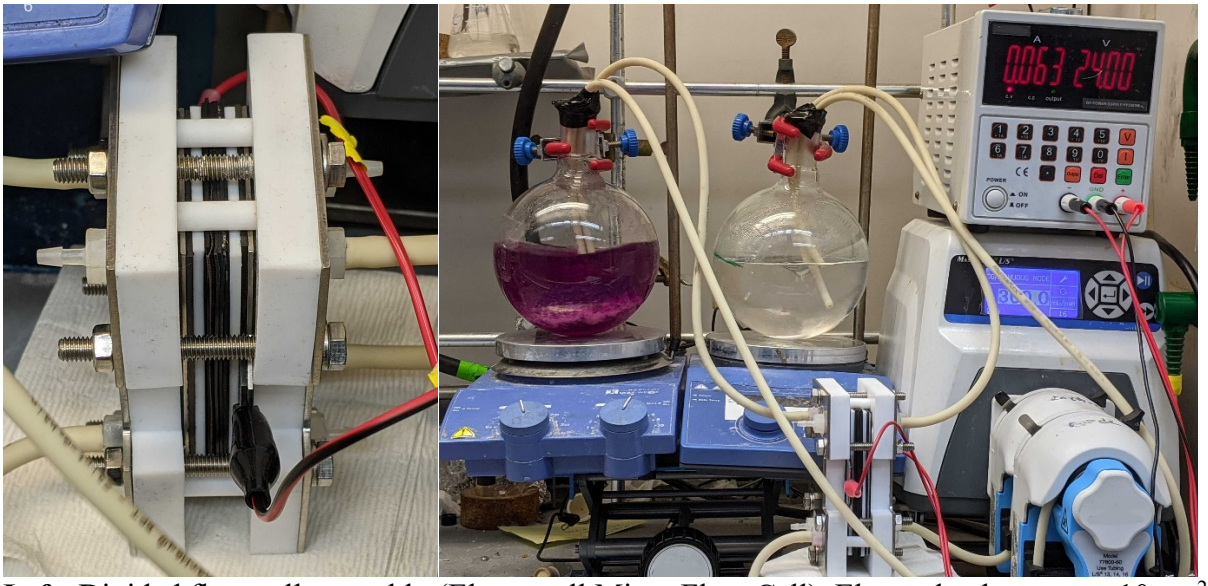
(1-((6-chloropyridin-3-yl)methyl)aziridin-2-yl)methyl acetate (33): Following General Procedure A except with 35 mA (17 mA/cm^2), Bu_4NPF_6 (620 mg, 1,6 mmol, 4 equiv), allyl acetate (129 µL, 1.2 mmol, 3 equiv), and the following purification modification: following flash column chromatography on basified silica (35-75% EtOAc/hexanes), the product containing fractions were concentrated under reduced pressure, and the residue was dissolved into 5 mL 1:1 EtOAc/hexanes and filtered to yield 64 mg (66%) as an oil. **^{1}H NMR** (500 MHz, C_6D_6) δ 8.15 (d, *J* = 2.4 Hz, 1H), 7.13 (dd, *J* = 8.2, 2.5 Hz, 1H), 6.84 (d, *J* = 8.2 Hz, 1H), 4.01 (dd, *J* = 11.6, 4.3 Hz, 1H), 3.60 (dd, *J* = 11.6, 7.4 Hz, 1H), 2.81 (d, *J* = 13.9 Hz, 1H), 2.55 (d, *J* = 13.9 Hz, 1H), 1.64 (s, 3H), 1.34 – 1.27 (m, 2H), 0.77 (d, *J* = 6.4 Hz, 1H).; **^{13}C NMR** (126 MHz, C_6D_6) δ 170.17, 150.89, 149.62, 138.49, 134.03, 124.07, 66.66, 60.47, 37.57, 31.64, 20.53. **HRMS** (ESI+) Calc: [M+H]+ (C11H14ClN2O2) 241.0738; measured: 241.0737; 0.4 ppm difference.



(1-cyclohexylaziridin-2-yl)methyl ethyl carbonate (38): Following General Procedure B except with 12 mA (5.8 mA/cm^2) and cyclohexylamine (183 µL, 1.6 mmol, 4 equiv), with 0-30% acetone/hexanes gradient followed by an additional flash column chromatography purification on non-basified silica using 40-70% 1:11 acetone:DCM/hexanes gradient, 60.6mg (67% yield) obtained as an oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 4.20 (q, J = 7.1 Hz, 2H), 4.11 (dd, J = 11.4, 5.0 Hz, 1H), 3.95 (dd, J = 11.4, 7.2 Hz, 1H), 1.87-1.64 (m, 6H), 1.63-1.54 (m, 1H), 1.41-1.05 (m, 11H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.29, 70.33, 68.74, 64.15, 35.59, 32.88, 32.58, 30.57, 26.17 24.99, 24.92, 14.44; **HRMS** (ESI+) Calc: [M+H]+ (C12H22NO3) 228.1594*;* measured: 228.1591; 1.3 ppm difference.

7. Scale-Up Flow Electrolysis Set-Up and Procedure

Electrochemical flow reactor and setup:



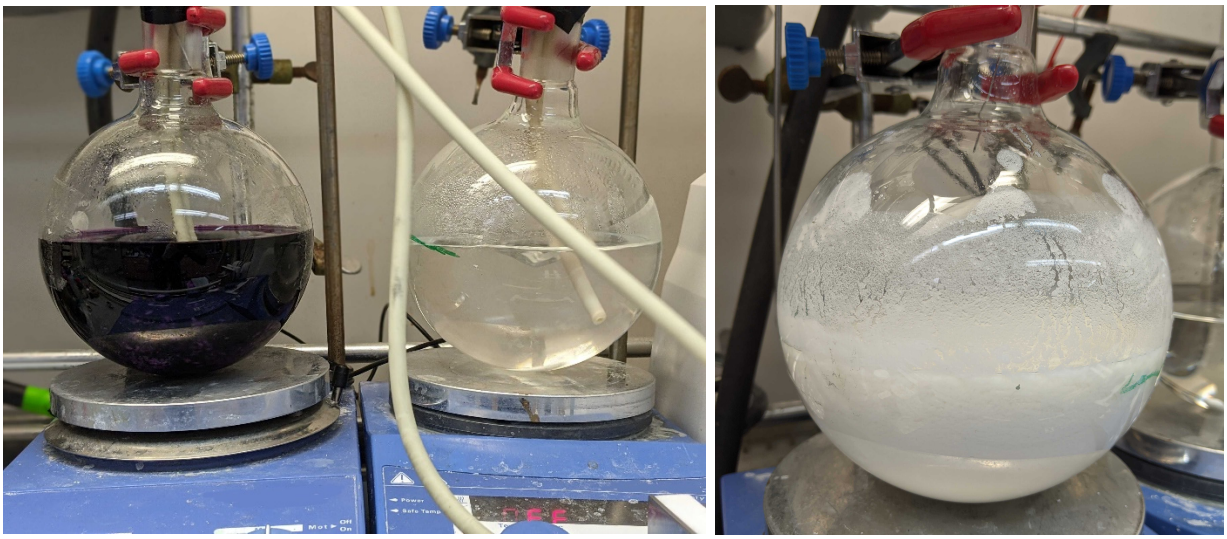
Left: Divided flow cell assembly (Electrocell Micro Flow Cell). Electrode plates area: 10 cm^2. In addition to the plates, a 32 x 32 x 8 mm graphite felt electrode (AvCarb Style G600A) was placed in each electrode compartment. The anode and cathode chambers were separated using a Nafion frit and the entire system sealed using rubber gaskets.

Right: Full flow assembly (pictured during first 30 mins of electrolysis). Cole Parmer Masterflex L/S digital peristaltic pump (2x Masterflex Easy-Load 3 pump heads, item no. 77800-60, PharMed® BPT, L/S 16 tubing item no. 06508-16), flow rate: 250 mL/min. Driven using DC power supply (see above). For each electrode compartment, the solution is pumped from the bulk, through the pump head and into the bottom inlet of the flow cell, through the flow cell making contact with the electrode, then flows out of the top outlet and back into the bulk solution.

Scale-Up Flow Electrolysis Procedure

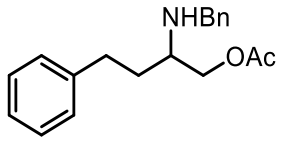
To an oven-dried 1 L round-bottom flask was added thianthrene (6.5 g, 30 mmol, 1.5 equiv), $LiBF_4$ (7.5 g, 80 mmol, 4 equiv), and MeCN (400 mL), followed by 4-phenylbutene (3.0 mL, 20 mmol, 1 equiv) and trifluoroacetic acid (3.0 mL, 40 mmol, 2 equiv). Both ends of the anode pump tubing were submerged in the solution (see picture). To a separate oven-dried 1 L round-bottom flask was added *n*-Bu_4NPF_6 (15.5 g, 40 mmol, 2 equiv) and MeCN (400 mL) followed by trifluoroacetic acid (7.65 mL, 100 mmol, 5 equiv). Both ends of the cathode pump tubing were submerged into the solution. An argon balloon was added to the anode flask. Both flasks were stirred, a flow rate of 250 mL/min was applied using the peristaltic pump, and the reaction was electrolyzed at 60 mA (4.2 mA/cm^2) for 24 h (2.7 F/mol). Following electrolysis, the balloon was removed, and the pump tubing was held above the solution while pumping to expel solution from the flow cell. Once the cell was emptied, Cs_2CO_3 (39.1 g, 120 mmol, 6 equiv) was added to the anode solution, followed by benzylamine (8.75 mL, 80 mmol, 4 equiv). The solution was

vigorously stirred for an additional 22 h. After this time, the mixture was diluted with DCM (500 mL) and divided into two portions. Water (500 mL) was added to each individual portion, and the organic layer was separated and washed with additional water (500 mL). Each aqueous portion was individually extracted with DCM (100 mL x 3). The combined organic layers were dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was divided into two portions, and each portion was filtered onto a silica column to remove thianthrene and purified individually using flash column chromatography (0-60% EtOAc/hexanes). Mixed fractions from both portions were combined and repurified (0-45% EtOAc/hexanes). All pure fractions were combined to obtain 3.2 g (67% yield, 13.4 mmol) of **3** as an oil.

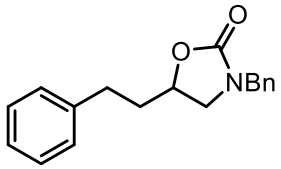


Left: anode solution (left) and cathode solution (right) after 2 h of electrolysis. **Right:** anode solution after complete substitution of dicationic adduct.

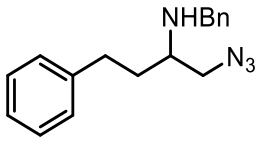
8. Aziridine and Adduct Derivatization Reactions



2-(benzylamino)-4-phenylbutyl acetate (34): To an oven-dried septum capped 2 dram vial equipped with a stir bar under nitrogen atmosphere was added aziridine **20 (**95 mg, 0.4 mmol, 1 equiv) via syringe, followed by DCM (0.8 mL). Acetic acid (114 µL, 2 mmol, 5 equiv) was added dropwise to the solution. The reaction was stirred at rt for 72 h before being quenched by addition of saturated aqueous $NaHCO_3$ (10 mL) and diluted with EtOAc (10 mL). The aqueous layer was separated and extracted with EtOAc (20 mL x 3). The combined organic layers were washed with saturated aqueous NaCl solution (10 mL), dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified via flash column chromatography (10-60% EtOAc to yield 89 mg (75% yield) as an oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.30 – 7.17 (m, 7H), 7.15 – 7.09 (m, 3H), 4.13 (dd, J = 11.2, 4.4 Hz, 1H), 4.02 (dd, J = 11.2, 5.7 Hz, 1H), 3.77 (d, J = 13.1 Hz, 1H), 3.73 (d, J = 13.1 Hz, 1H), 2.79 (qd, J = 6.1, 4.5 Hz, 1H), 2.70 – 2.60 (m, 2H), 2.01 (s, 3H), 1.78 – 1.71 (m, 2H), 1.47 (bs, 1H); **^{13}C NMR** (151 MHz, $CDCl_3$) δ 171.12, 141.95, 140.45, 128.46, 128.44, 128.38, 128.18, 127.04, 125.92, 65.98, 55.09, 51.09, 33.63, 32.09, 20.99. **HRMS** (ESI+) Calc: [M+H]+ (C19H24NO2) 298.1802; measured: 298.1800; 0.7 ppm difference.

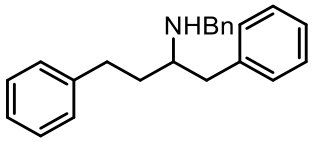


3-benzyl-5-phenethyloxazolidin-2-one (35): An oven-dried 2 dram vial equipped with a stir bar was transferred into a nitrogen-filled glovebox and anhydrous LiI (54 mg, 0.4 mmol, 1 equiv) was added. The vial was sealed with septum cap and transferred out of the glovebox. The atmosphere was immediately evacuated and replaced with 1 atm CO_2 using two balloons filled with CO_2. Aziridine **20** (95 mg, 0.4 mmol, 1 equiv) was added via syringe followed by THF (2 mL). The reaction mixture was warmed to 40 °C and stirred for 24 h, at which point the deflated balloon was replaced with an additional balloon of CO_2. The reaction mixture was stirred for an additional 20 h. The reaction mixture was cooled to rt and diluted with EtOAc (10 mL) and water (10 mL). The aqueous layer was separated and extracted with EtOAc (10 mL x 3). The combined organic layers were washed with saturated aqueous NaCl solution (10 mL), dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified via flash column chromatography (0-50% acetone/hexanes) to yield 97 mg (86% yield) as a 16:1 mixture of regioisomers (major isomer depicted). **^{1}H NMR** (500 MHz, CDCl3) δ 7.31 – 7.18 (m, 7H), 7.15 – 7.07 (m, 3H), 4.42 – 4.34 (m, 2H), 4.32 (d, *J* = 14.8 Hz, 1H), 3.37 (t, *J* = 8.5 Hz, 1H), 2.94 (dd, *J* = 8.6, 7.0 Hz, 1H), 2.73 (ddd, *J* = 14.4, 9.3, 5.3 Hz, 1H), 2.64 (ddd, *J* = 13.8, 8.9, 7.3 Hz, 1H), 1.98 (dtd, *J* = 14.0, 8.7, 5.3 Hz, 1H), 1.79 (dddd, *J* = 13.9, 9.2, 7.3, 4.6 Hz, 1H).; **^{13}C NMR** (126 MHz, $CDCl_3$) δ 158.07, 140.47, 135.78, 128.86, 128.58, 128.46, 128.13, 127.99, 126.27, 72.60, 49.23, 48.33, 36.87, 30.95. **HRMS** (ESI+) Calc: [M+H]+ (C18H20NO2) 282.14886; measured: 282.1484; 1.6 ppm difference. Connectivity confirmed by edited HSQC and HMBC.



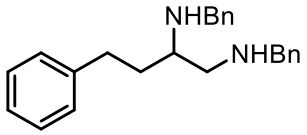
1-azido-N-benzyl-4-phenylbutan-2-amine (36):
CAUTION: Organic azides and hydrazoic acid are known to be potentially explosive compounds. While no issue was encountered during this synthesis, proper precautions were taken. All azidation reactions should be performed behind a blast shield, and aqueous layers should be kept basic. Once isolated, organic azides should be stored below room temperature and away from sources of heat, light, pressure and shock.

To an oven-dried septum capped 2 dram vial equipped with a stir bar under nitrogen atmosphere was added $TMSN_3$ (265 µL, 2.0 mmol, 5 equiv), followed by DCM (1 mL). Acetic acid (114 µL, 2 mmol, 5 equiv) was added dropwise. The reaction mixture was stirred at rt for 20 min. A solution of aziridine **20 (**95 mg, 0.4 mmol, 1 equiv) in DCM (1 mL) was added via syringe, and the reaction mixture was stirred at rt for 48 h. At completion, the reaction mixture was quenched using slow addition of saturated aqueous $NaHCO_3$ solution (10 mL). The aqueous layer was separated and extracted with EtOAc (10 mL x 3). The combined organic layers were dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified via flash column chromatography (0-45% EtOAc/hexanes) to yield 83.8 mg (75% yield) as an oil. **^{1}H NMR** (500 MHz, CDCl3) δ 7.26 (dd, *J* = 4.4, 1.3 Hz, 3H), 7.23 – 7.17 (m, 4H), 7.14 – 7.07 (m, 3H), 3.76 (d, *J* = 13.0 Hz, 1H), 3.70 (d, *J* = 12.7 Hz, 1H), 3.39 (dd, *J* = 12.3, 4.5 Hz, 1H), 3.22 (dd, *J* = 12.3, 5.5 Hz, 1H), 2.71 (p, *J* = 5.4 Hz, 1H), 2.61 (t, *J* = 7.9 Hz, 2H), 1.82 – 1.67 (m, 2H), 1.37 (bs, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 141.73, 140.29, 128.49, 128.35, 128.17, 127.10, 125.98, 56.15, 54.32, 51.15, 34.20, 32.11. **HRMS** (ESI+) Calc: [M+H]+ (C17H21N4) 281.17607; measured: 281.1759; 0.6 ppm difference.

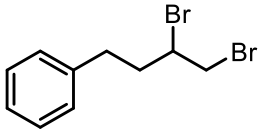


N-benzyl-1,4-diphenylbutan-2-amine (37): An oven-dried 50 mL three-necked round bottom flask equipped with a stir bar was charged with CuI (230 mg, 1.2 mmol, 3 equiv). The atmosphere was evacuated and refilled with nitrogen three times. THF (5 mL) was added and the flask was cooled to -40 °C. PhLi (1.9 M in dibutyl ether, 1.25 mL, 2.4 mmol, 6 equiv) was added via syringe and the reaction mixture was stirred at -40 °C for 30 min. The resulting black mixture was then cooled to -78 °C and a solution of aziridine **20** (95 mg, 0.4 mmol, 1 equiv) in THF (1 mL) was added, followed by dropwise addition of BF_3OEt_2 (152 µL, 1.2 mmol, 3 equiv). The reaction mixture was stirred at -78 °C for 30 min, then removed from the bath and allowed to warm to rt while stirring for 4 h. The reaction mixture was then quenched via addition of NH_4OH (10 mL) and saturated aqueous NH_4Cl (10 mL) and diluted with Et_2O (10 mL). The dark blue aqueous layer was separated, basified via the addition of 10% aqueous Na_2CO_3 (~20 mL), and extracted with Et_2O (20 mL x 3). The combined organic layers were washed with saturated aqueous NaCl (20 mL), dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced

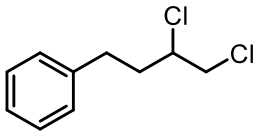
pressure. The residue was purified via flash column chromatography (0-45% acetone/hexanes followed by 0-35% acetone/hexanes on basified silica) to yield 63.5 mg (50% yield) as an oil. **^{1}H NMR** (500 MHz, CDCl3) δ 7.24 – 7.03 (m, 15H), 3.71 (d, *J* = 13.2 Hz, 1H), 3.67 (d, *J* = 13.2 Hz, 1H), 2.84 – 2.57 (m, 5H), 1.70 (td, *J* = 8.1, 5.8 Hz, 2H), 1.35 – 1.26 (bs, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$) δ 142.51, 140.67, 139.36, 129.33, 128.42, 128.40, 128.35, 128.09, 126.82, 126.18, 125.72, 57.69, 51.09, 40.67, 35.63, 32.04. **HRMS** (ESI+) Calc: [M+H]+ (C23H26N) 316.2060; measured: 316.2058; 0.6 ppm difference. Connectivity confirmed by edited HSQC and HMBC.



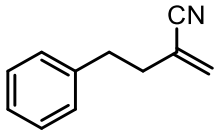
N^{1},N^{2}-dibenzyl-4-phenylbutane-1,2-diamine (39): Following General Procedure H with benzylamine (310 µL, 2.8 mmol, 7 equiv) as the nucleophile, 53% yield obtained.



(3,4-dibromobutyl)benzene (40): Following General Procedure G with *n*-Bu_4NBr (645 mg, 2.0 mmol, 5 equiv) as the nucleophile, with 0-5% acetone/hexanes gradient, 89.9 mg (77% yield) obtained as an oil. **^{1}H NMR** (500 MHz, CDCl3) δ 7.42 – 7.29 (m, 5H), 4.18 (tdd, *J* = 9.8, 4.5, 2.9 Hz, 1H), 3.93 (dd, *J* = 10.3, 4.3 Hz, 1H), 3.72 (t, *J* = 10.0 Hz, 1H), 3.02 (ddd, *J* = 13.7, 9.2, 4.6 Hz, 1H), 2.83 (ddd, *J* = 13.7, 9.2, 7.2 Hz, 1H), 2.60 – 2.50 (m, 1H), 2.16 (dtd, *J* = 14.5, 9.4, 4.7 Hz, 1H). ^{13}C NMR Consistent with reported spectra[6].



(3,4-dichlorobutyl)benzene (41): Following General Procedure H with $BnMe_3NCl$ (371 mg, 2.0 mmol, 5 equiv) as the nucleophile, 72% yield obtained.



2-methylene-4-phenylbutanenitrile (42): Following General Procedure G with KCN (130 mg 2.0 mmol, 5 equiv) as the nucleophile, with 0-5% acetone/hexanes gradient, 38.8 mg (61% yield) obtained as an oil. **^{1}H NMR** (500 MHz, CDCl3) δ 7.36 (dd, *J* = 8.2, 6.8 Hz, 2H), 7.27 (m, 3H), 5.88 (s, 1H), 5.69 (s, 1H), 2.97 – 2.88 (m, 2H), 2.62 (t, *J* = 7.8 Hz, 2H). ^{13}C NMR consistent with reported spectra[14].

9. X-Ray Crystallography Data

Data Collection for 1

A colorless crystal with approximate dimensions 0.09 × 0.05 × 0.04 mm^3 was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker D8 VENTURE PhotonIII four-circle diffractometer with Cu Kα (λ = 1.54178 Å) radiation and the detector to crystal distance of 4.0 cm[15].

The initial cell constants were obtained from a 180° φ scan conducted at a 2θ = 50° angle with the exposure time of 1 second per frame. The reflections were successfully indexed by an automated indexing routine built in the APEX3 program. The final cell constants were calculated from a set of 9088 strong reflections from the actual data collection.

The data were collected by using the full sphere data collection routine to survey the reciprocal space to the extent of a full sphere to a resolution of 0.78 Å. A total of 136275 data were harvested by collecting 44 sets of frames with 1.0º scans in ω and φ with an exposure time 1–3 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements[16].

Structure Solution and Refinement

The systematic absences in the diffraction data were consistent for the space groups $P\bar{1}$ and $P1$. The *E*-statistics strongly suggested the centrosymmetric space group $P\bar{1}$ that yielded chemically reasonable and computationally stable results of refinement[17–22].

A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients unless indicated otherwise. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

There are two sulfur-containing dications and four BF_4^- anions in the asymmetric unit. The crystallized compound is a racemate. The chiral dications have identical chemical composition and connectivity, but different handedness – chiral center C13 is *S*, whereas C13A is *R*.

Two BF_4^- anions exhibit positional disorder. Tetrafluroborate B3 is disordered over three positions in a 0.718(3) : 0.147(2) : 0.135(2) ratio. Tetrafluroborate B4 is disordered over three positions in a 0.699(3) : 0.154(3) : 0.147(3) ratio. The four minor disorder components were refined isotropically with an idealized geometry[23] and atomic displacement parameter constraints.

The final least-squares refinement of 897 parameters against 13706 data resulted in residuals R (based on F2 for I≥2σ) and wR (based on F2 for all data) of 0.0399 and 0.1037, respectively. The final difference Fourier map was featureless.

Data Collection for 2

Two separate data collections were carried out on two different colorless crystals with approximate dimensions of 0.07 x 0.06 x 0.05 mm^3 and 0.04 x 0.04 x 0.04 mm^3 in a similar fashion. Unless otherwise specified, the data collection parameters were similar for both crystals and therefore we report only the procedural details for the first.

The crystal was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount©. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collections were performed on a Bruker D8 VENTURE PhotonIII four-circle diffractometer with Cu Kα (λ = 1.54178 Å) radiation with the detector to crystal distance of 4.0 cm[15].

The initial cell constants were obtained from a 180° φ scan conducted at a 2θ = 50° angle with an exposure time of 1 second per frame. The reflections were successfully indexed by an automated indexing routine built in the APEX3 program. The final cell constants were calculated from a set of 8035 strong reflections from the actual data collection.

The data were collected by using a full sphere data collection routine to survey reciprocal space to the extent of a full sphere to a resolution of 0.79 Å. For the crystal with dimensions of 0.07 x 0.06 x 0.05 mm^3, a total of 25205 data were harvested by collecting 14 sets of frames with 0.9º scans in ω and φ with exposure times of 3 – 22 sec per frame; for the crystal with dimensions of 0.04 x 0.04 x 0.04 mm^3, a total of 22269 data were harvested by collecting 13 sets of frames with 0.9º scans in ω and φ with exposure times of 1-15 sec per frame. The two datasets were then merged and corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements[16].

Structure Solution and Refinement

The diffraction data were consistent with the space groups $P\bar{1}$ and $P1$. The *E*-statistics strongly suggested the centrosymmetric space group $P\bar{1}$ which yielded chemically reasonable and computationally stable results of refinement[17–22].

A successful solution by direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located with an alternating series of least-squares cycles and difference Fourier maps. Unless otherwise specified, all non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

The structure consists of one sulfur-containing dication, two PF_6^- anions, and one molecule of solvate acetonitrile. Both PF_6^- anions and the dication were disordered over two positions. However, the position for the minor component for atoms C15-C22 of the dication could not be located in the difference map; thus, atoms C15-C22 (and the H atoms bound to those C atoms)

were refined at a 100 % occupancy to ensure a chemically reasonable structural formula. Atom H14 (bound to atom C14) was refined at a 100 % occupancy while no H atoms were assigned to atom C14A.

The major disorder component has a 90.9(2) % occupancy. The atoms in the minor disorder component were refined isotopically. For the dication, the atoms in the minor disorder component were refined with geometric and atomic displacement parameter constraints, as well as 1,2 and 1,3 distance restraints. For the PF_6^- anions, the atoms in the minor component were refined with geometric and atomic displacement parameter constraints[23].

The structure crystallizes as a racemate. The absolute configuration of the arbitrarily chosen enantiomer shown in Figure 3 is C14 – *R*.

The final least-squares refinement of 413 parameters against 5794 data resulted in residuals *R* (based on F^2 for $I \geq 2\sigma$) and *wR* (based on F^2 for all data) of 0.0378 and 0.1004, respectively. The final difference Fourier map was featureless.

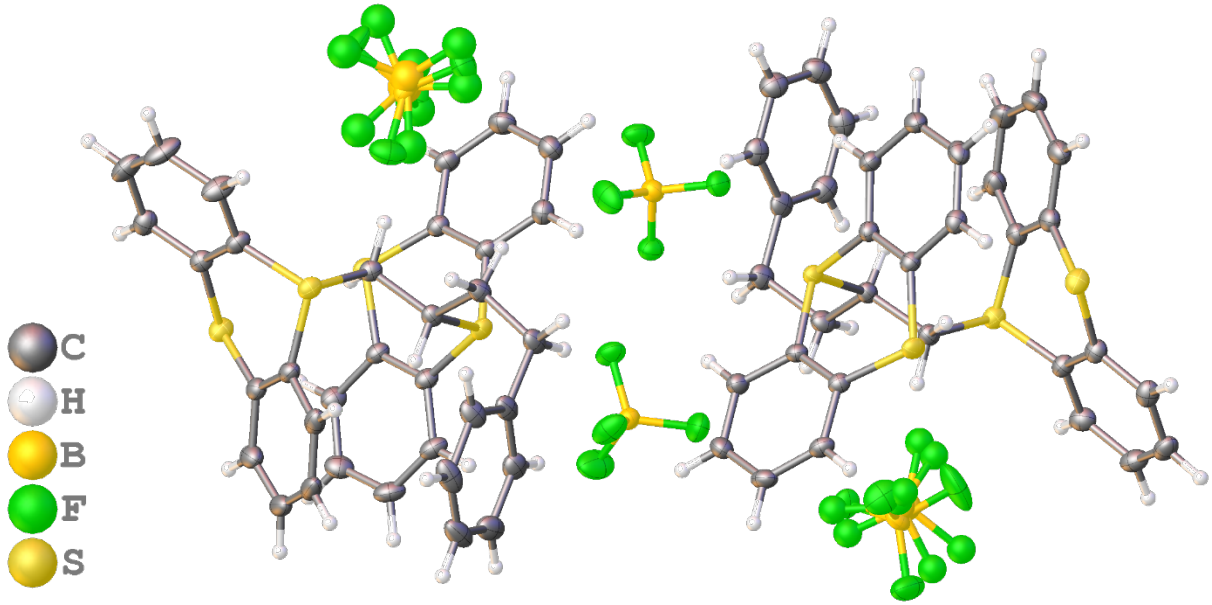


Fig. S5. A molecular drawing of the unit cell content of 1 shown with 50% probability ellipsoids. All disorder components are shown.

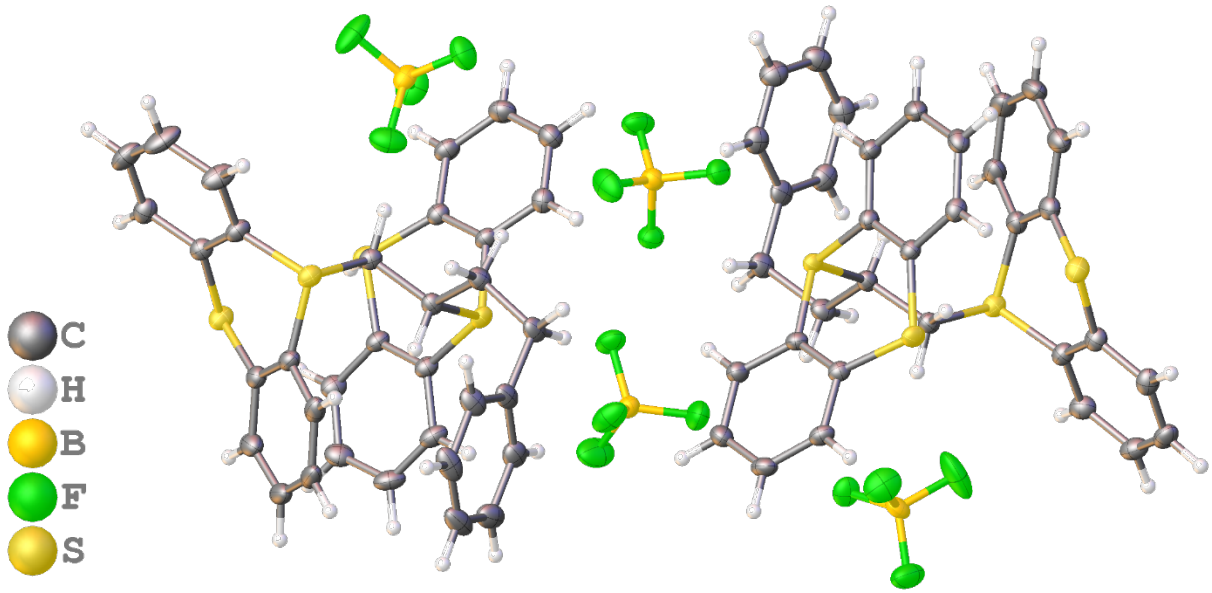


Fig S6. A molecular drawing of the unit cell content of 1 shown with 50% probability ellipsoids. All minor disorder components are omitted.

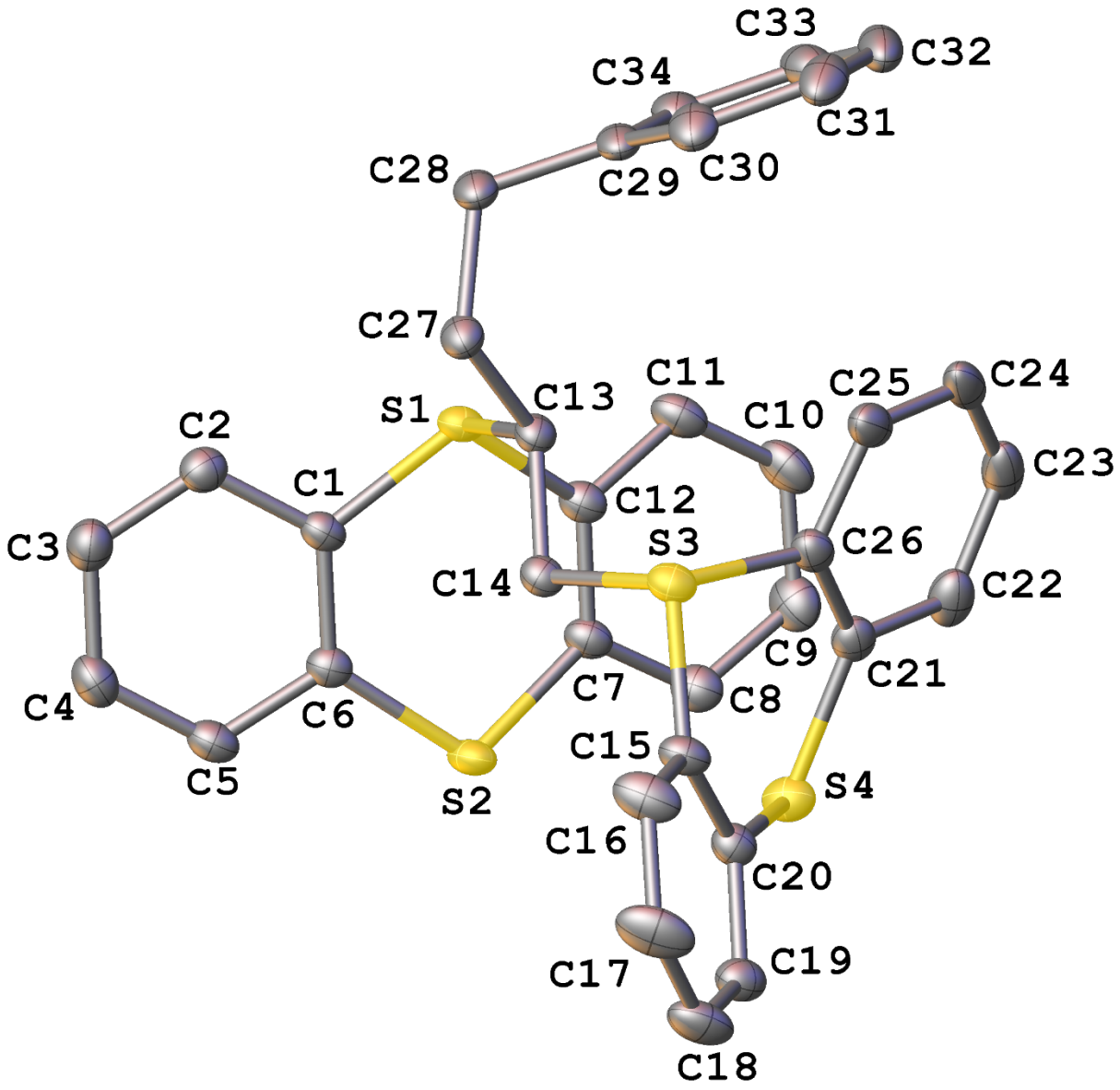


Fig. S7. A molecular drawing of the *S* enantiomer in 1 shown with 50% probability ellipsoids. All H atoms are omitted.

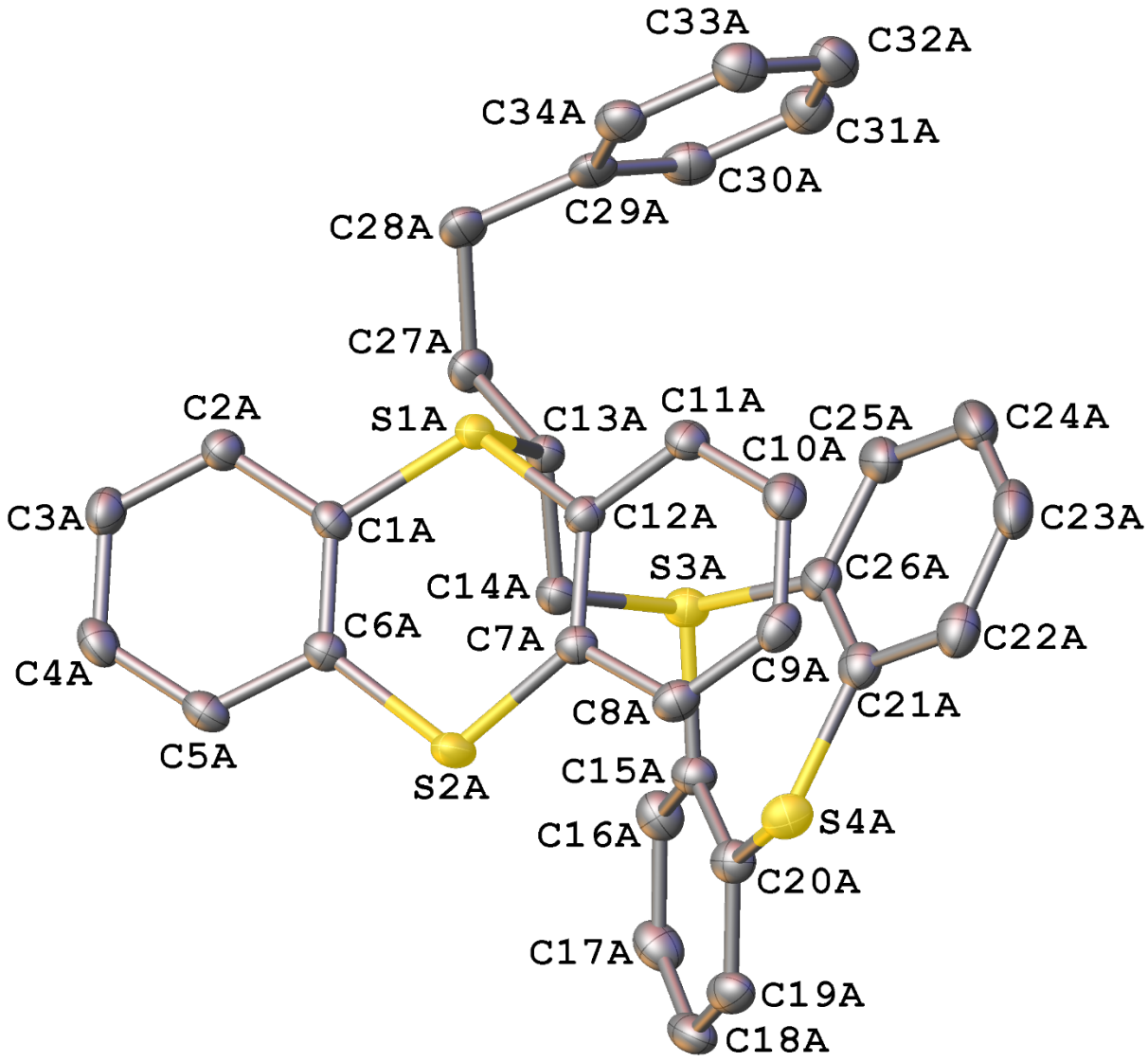


Fig. S8. A molecular drawing of the *R* enantiomer in 1 shown with 50% probability ellipsoids. All H atoms are omitted.

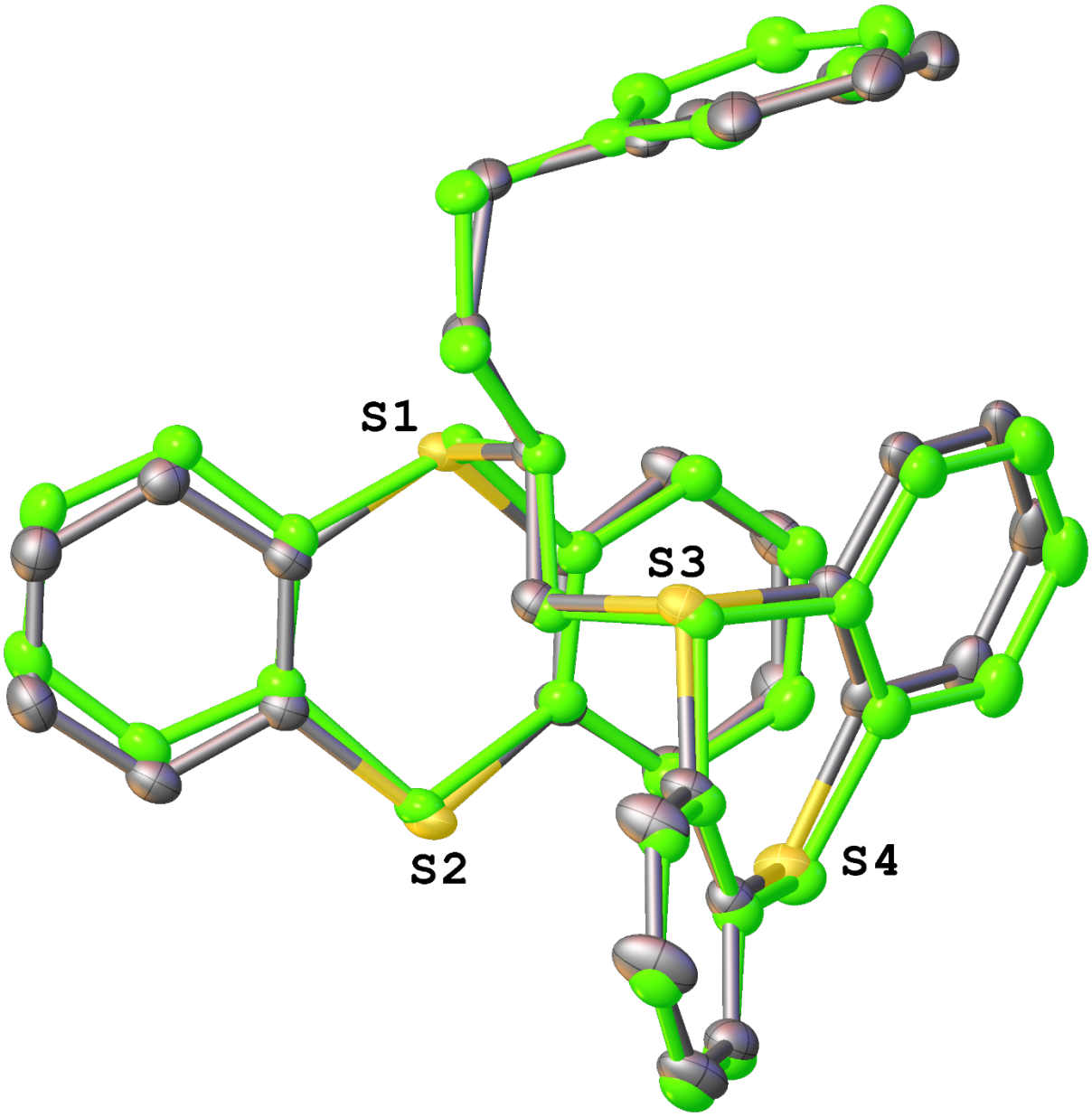


Fig. S9. A superposition of the two enantiomers in 1 shown with 50% probability ellipsoids (one of them is inverted). All H atoms are omitted.

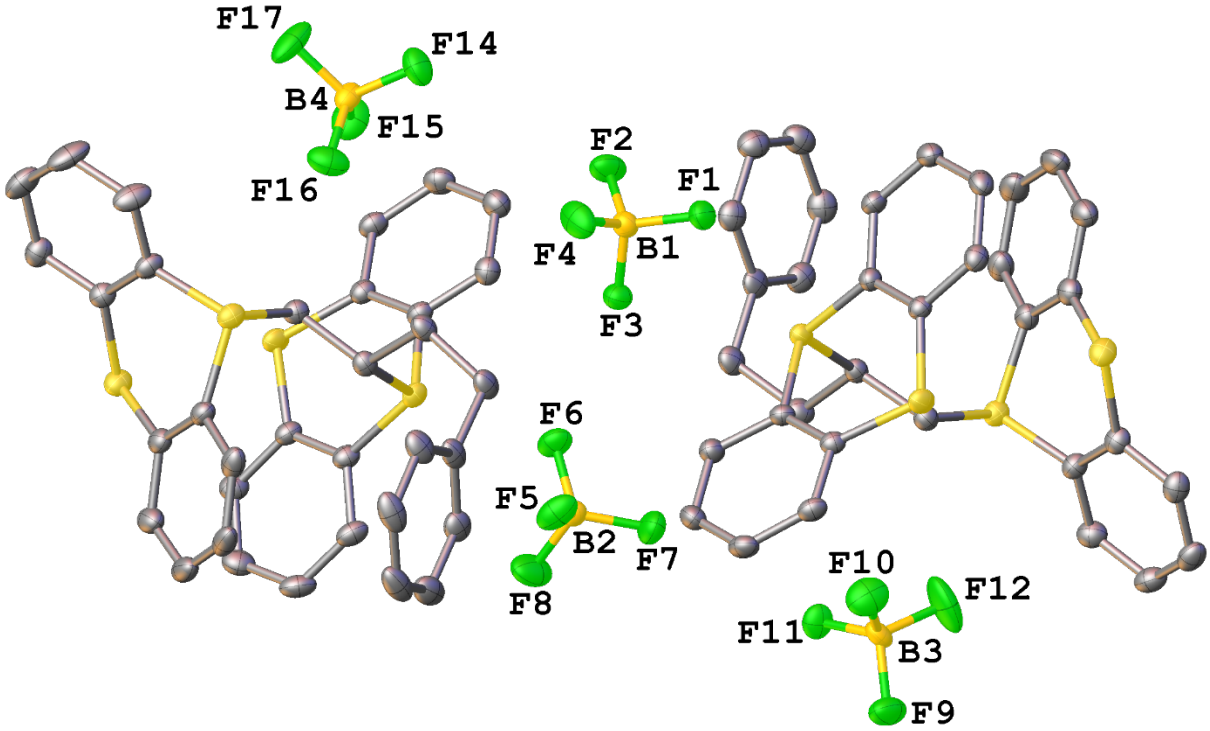


Fig. S10. A molecular drawing of 1 shown with 50% probability ellipsoids. All H atoms and minor disorder components are omitted. Only the B and F atoms are labelled.

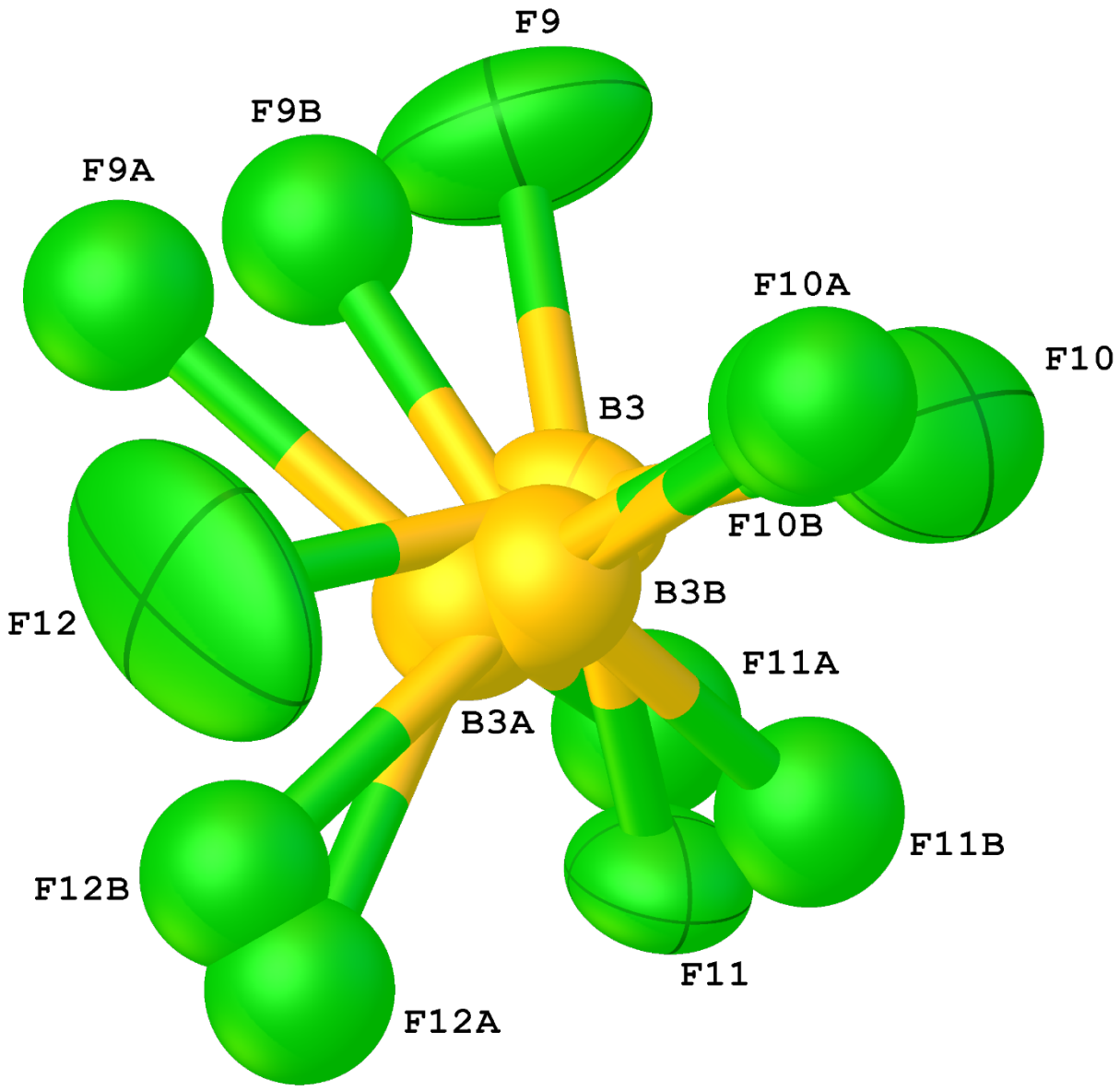


Fig. S11. A molecular drawing of the B3 anion in 1 shown with 50% probability ellipsoids. All disorder positions are shown.

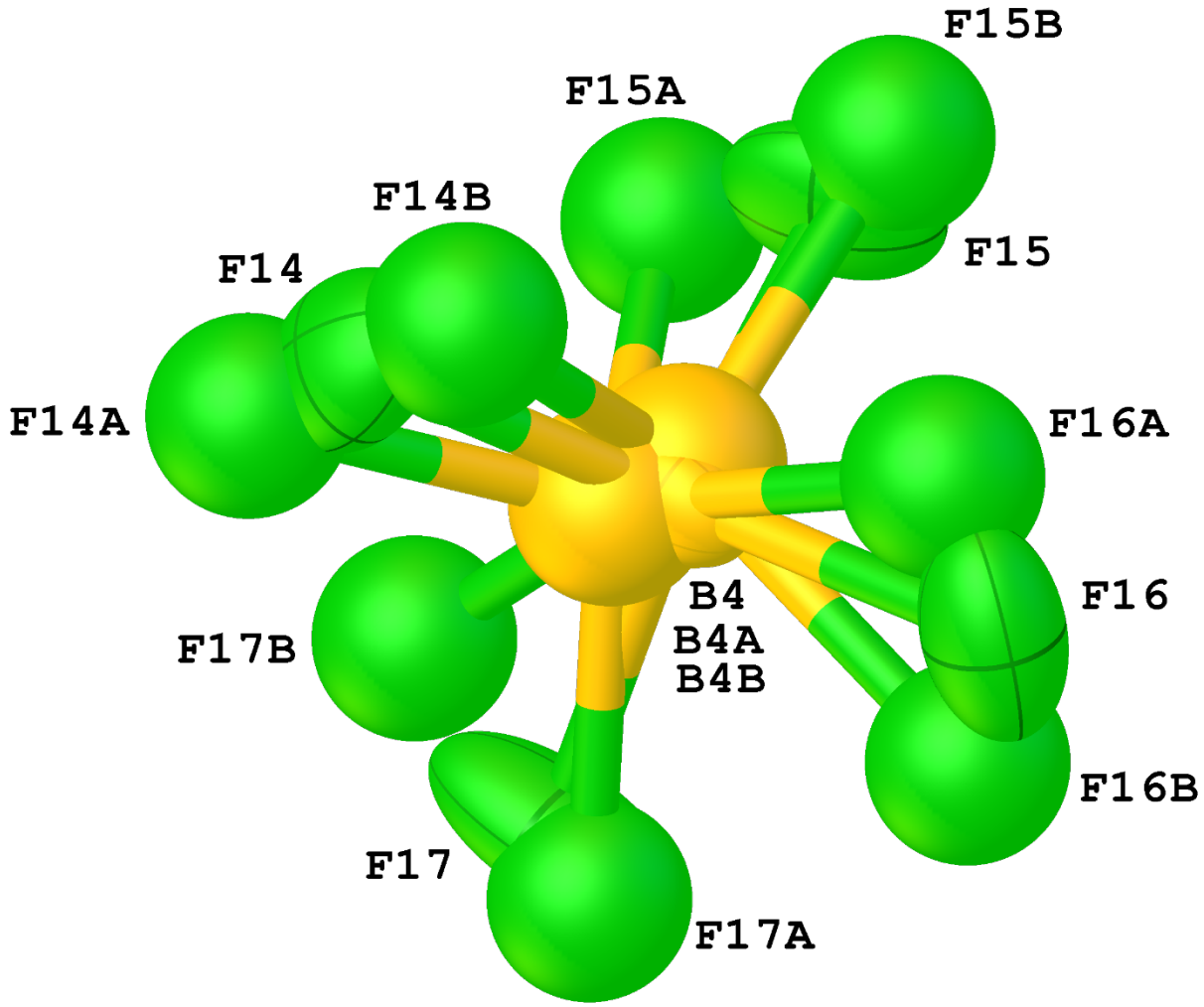


Fig. S12. A molecular drawing of the B4 anion in 1 shown with 50% probability ellipsoids. All disorder positions are shown.

Table S2. Crystal data and structure refinement for 1.

Identification code	1
Empirical formula	$[C_{34}H_{28}S_4][BF_4]_2$
Formula weight	738.42
Temperature/K	100
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	10.334(3)
b/Å	14.268(2)
c/Å	21.678(9)
α/°	87.734(14)
β/°	89.78(4)
γ/°	81.333(16)
Volume/Å^3	3157.3(16)
Z	4
ρ_{calc}g/cm^3	1.553
μ/mm^{-1}	3.423
F(000)	1512.0
Crystal size/mm^3	0.09 × 0.05 × 0.04
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	4.08 to 162.552
Index ranges	$-13 \le h \le 13$, $-18 \le k \le 18$, $-27 \le l \le 27$
Reflections collected	136275
Independent reflections	13706 [R_{int} = 0.0557, R_{sigma} = 0.0259]
Data/restraints/parameters	13706/2/897
Goodness-of-fit on F^2	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0399, wR_2 = 0.1009
Final R indexes [all data]	R_1 = 0.0441, wR_2 = 0.1037
Largest diff. peak/hole / e Å^{-3}	0.76/-0.40

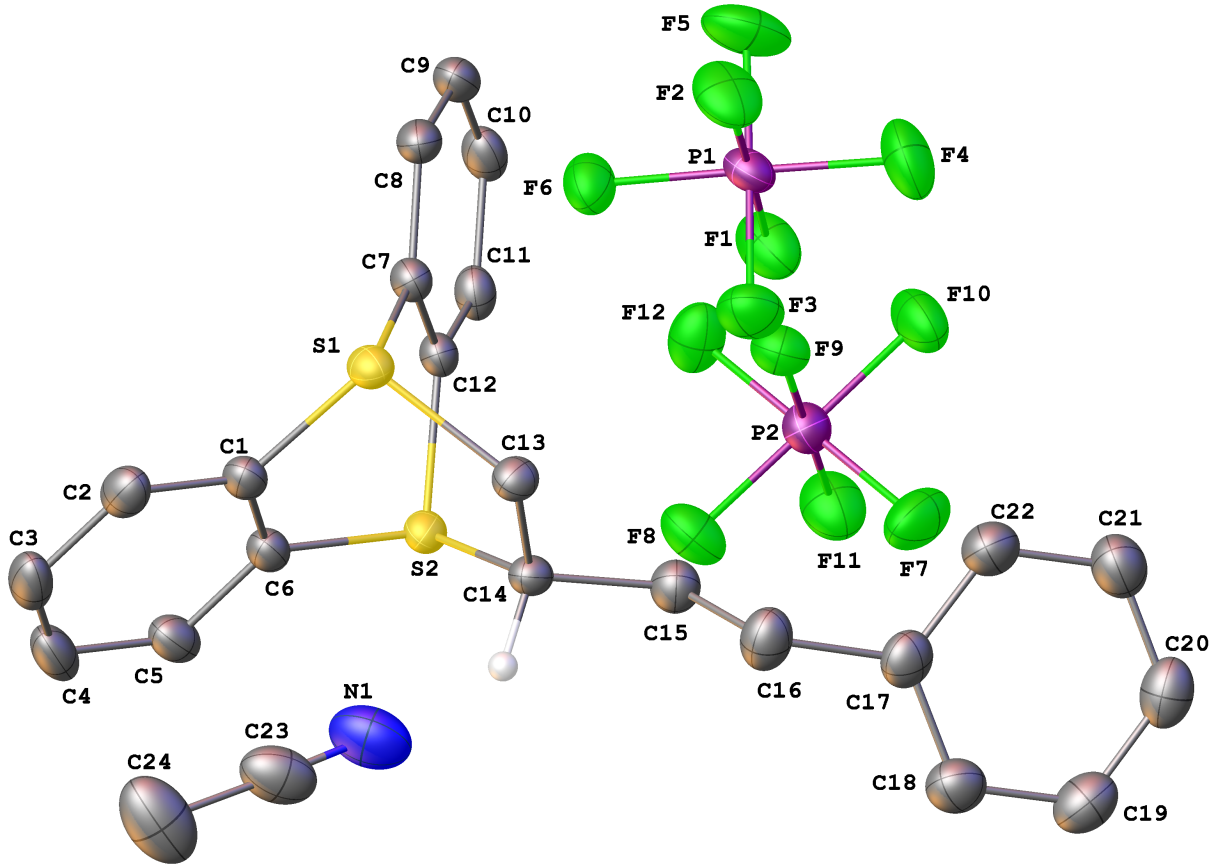


Fig. S13. A molecular drawing of 2 shown with 50% probability ellipsoids. All H atoms (except the H atom bound to C14) and minor disorder components are omitted.

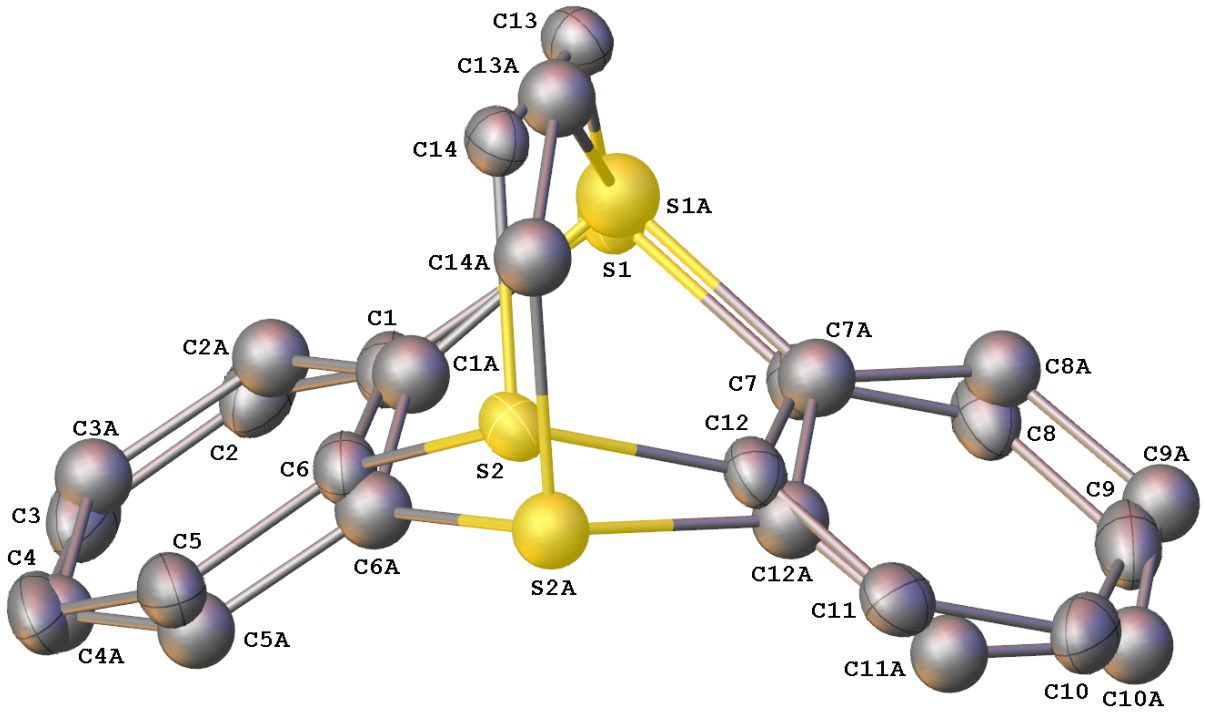


Fig. S14. A molecular drawing of the two disordered components of the sulfur-containing dication in 2 shown with 50 % probability ellipsoids. Atoms C15 – C22 and all H atoms have been omitted for clarity. In addition, the atomic radii of the atoms in the minor disorder component are shown at 80 % of their original value for clarity.

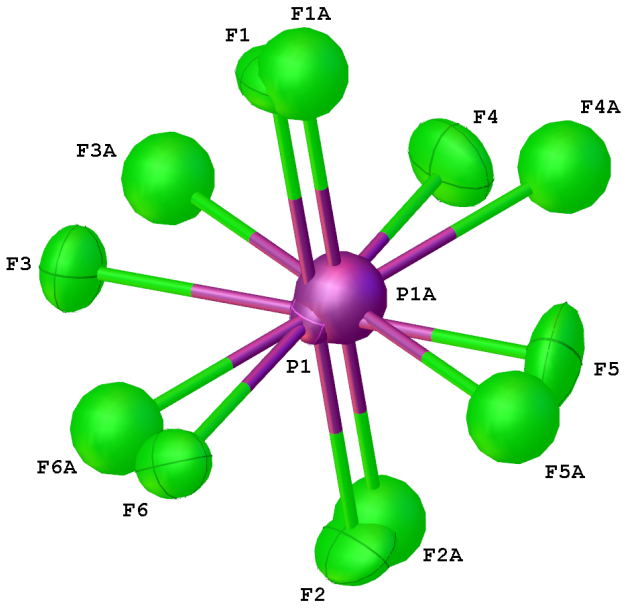


Fig. S15. A molecular drawing of the two disordered components in the first PF_6^- anion in 2 shown with 50 % probability ellipsoids; the atomic radii of the atoms in the minor component are shown at 60 % of their original value for clarity.

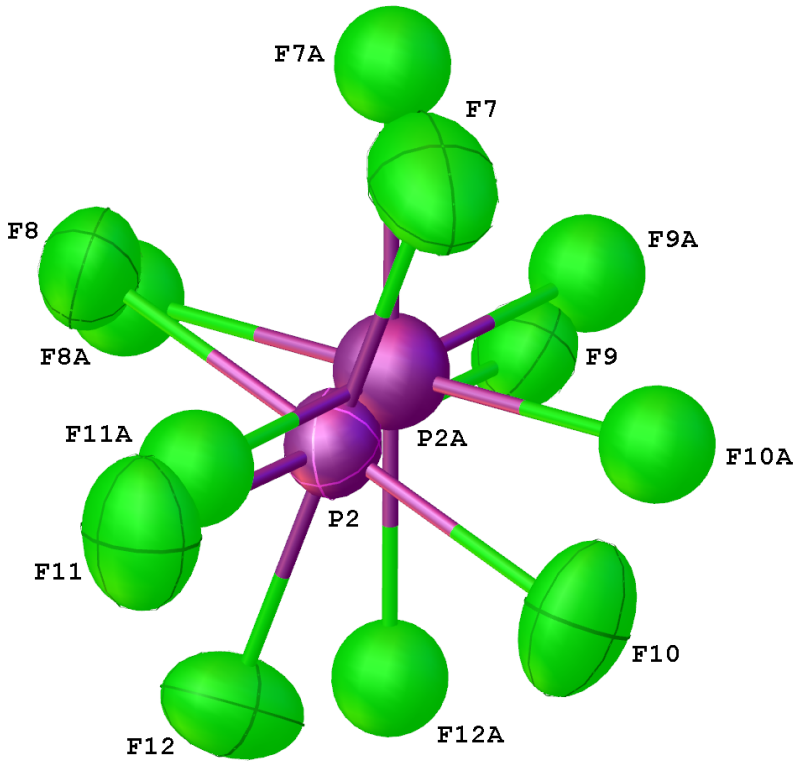


Fig. S16. A molecular drawing of the two disordered components in the second PF_6^- anion in 2 shown with 50 % probability ellipsoids; the atomic radii of the atoms in the minor component are shown at 70 % of their original value for clarity.

Table S3. Crystal data and structure refinement for 2.

Identification code	2
Empirical formula	$[C_{24}H_{23}S_2][PF_6]_2 \bullet CH_3CN$
Formula weight	679.49
Temperature/K	100.0
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	9.4023(15)
b/Å	9.8774(13)
c/Å	16.295(2)
α/°	92.640(8)
β/°	105.034(8)
γ/°	108.174(6)
Volume/Å^3	1375.3(3)
Z	2
ρ_{calc}g/cm^3	1.641
μ/mm^{-1}	3.784
F(000)	688.0
Crystal size/mm^3	0.04 × 0.04 × 0.04
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	5.67 to 157.86
Index ranges	$-11 \le h \le 11$, $-12 \le k \le 12$, $-20 \le l \le 19$
Reflections collected	29750
Independent reflections	5794 [R_{int} = 0.0460, R_{sigma} = 0.0305]
Data/restraints/parameters	5794/47/413
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R_1 = 0.0378, wR_2 = 0.0984
Final R indexes [all data]	R_1 = 0.0405, wR_2 = 0.1004
Largest diff. peak/hole / e Å^{-3}	0.44/-0.34

10. References

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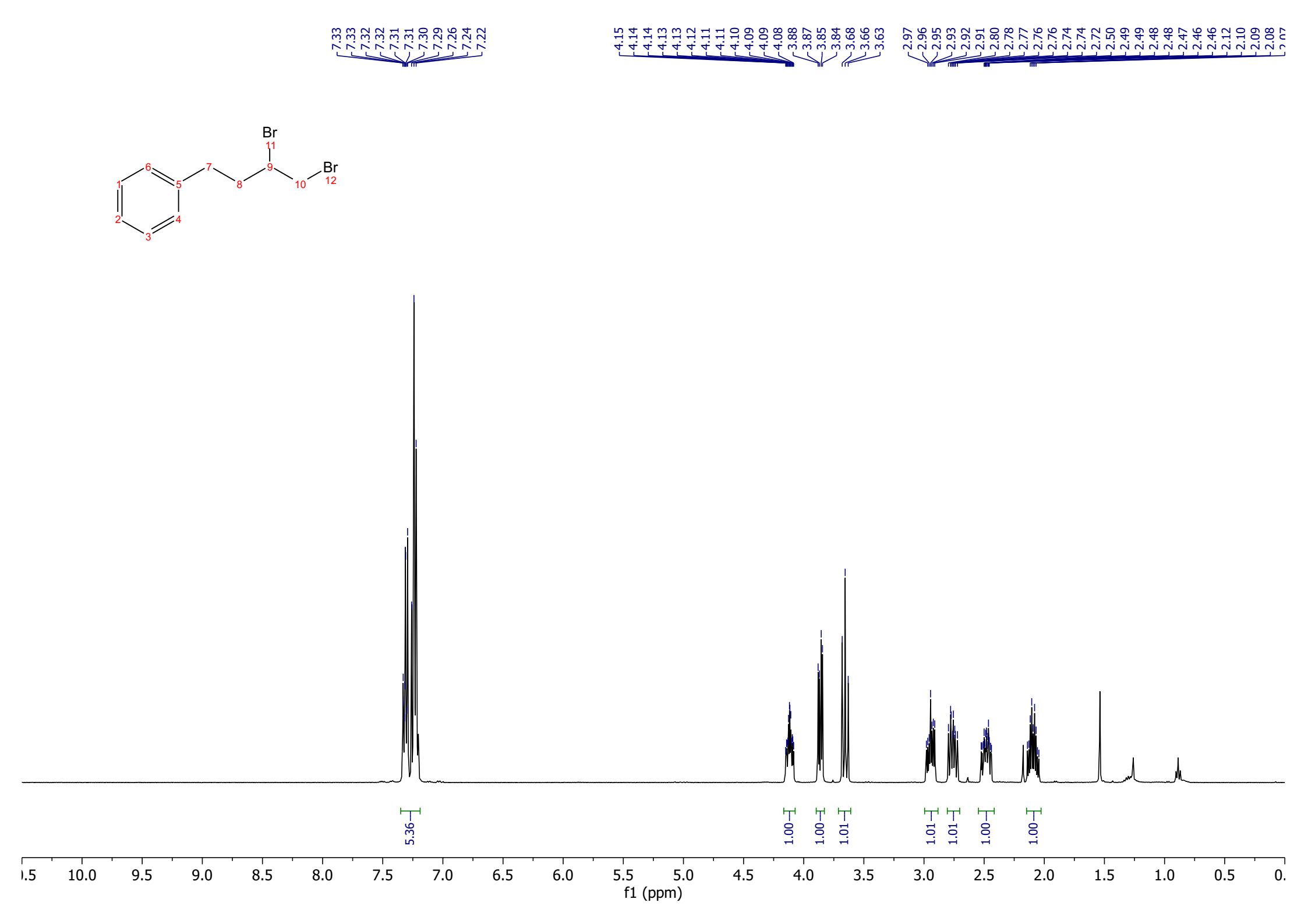
11. NMR Spectra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2.12
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Br
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Br
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2
3
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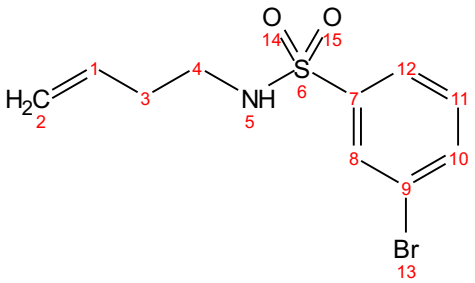
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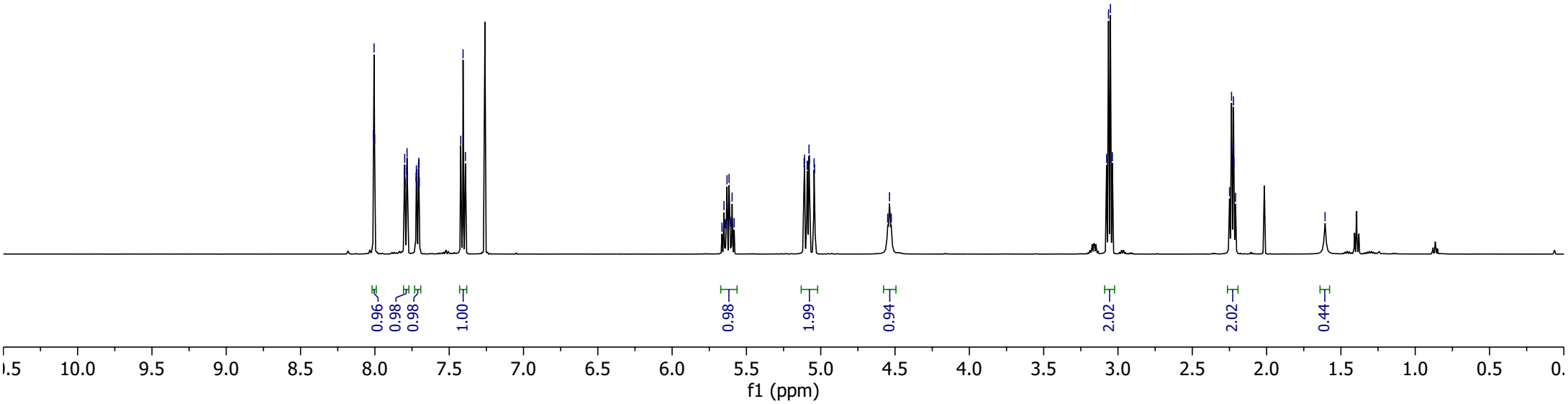
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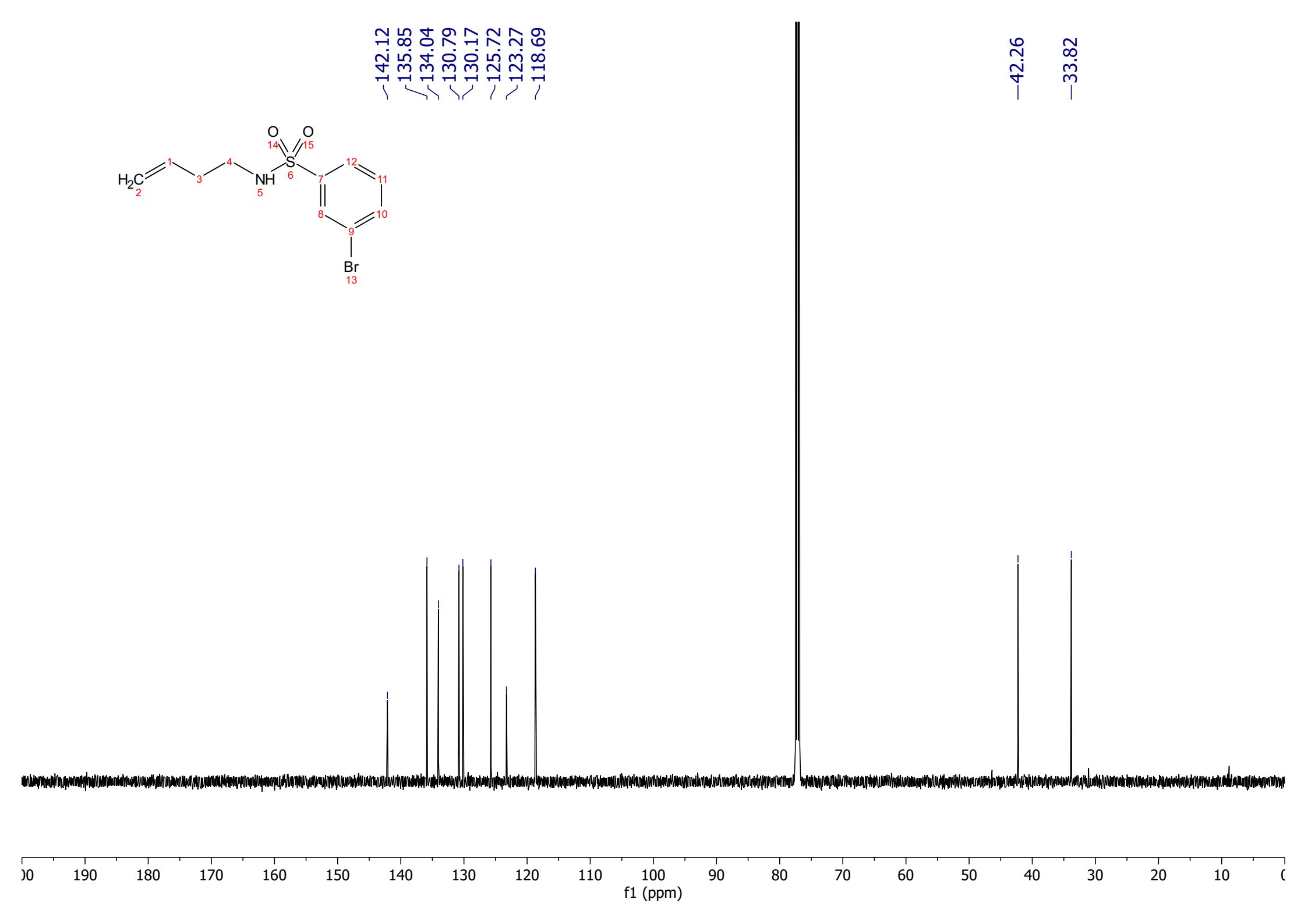
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Br
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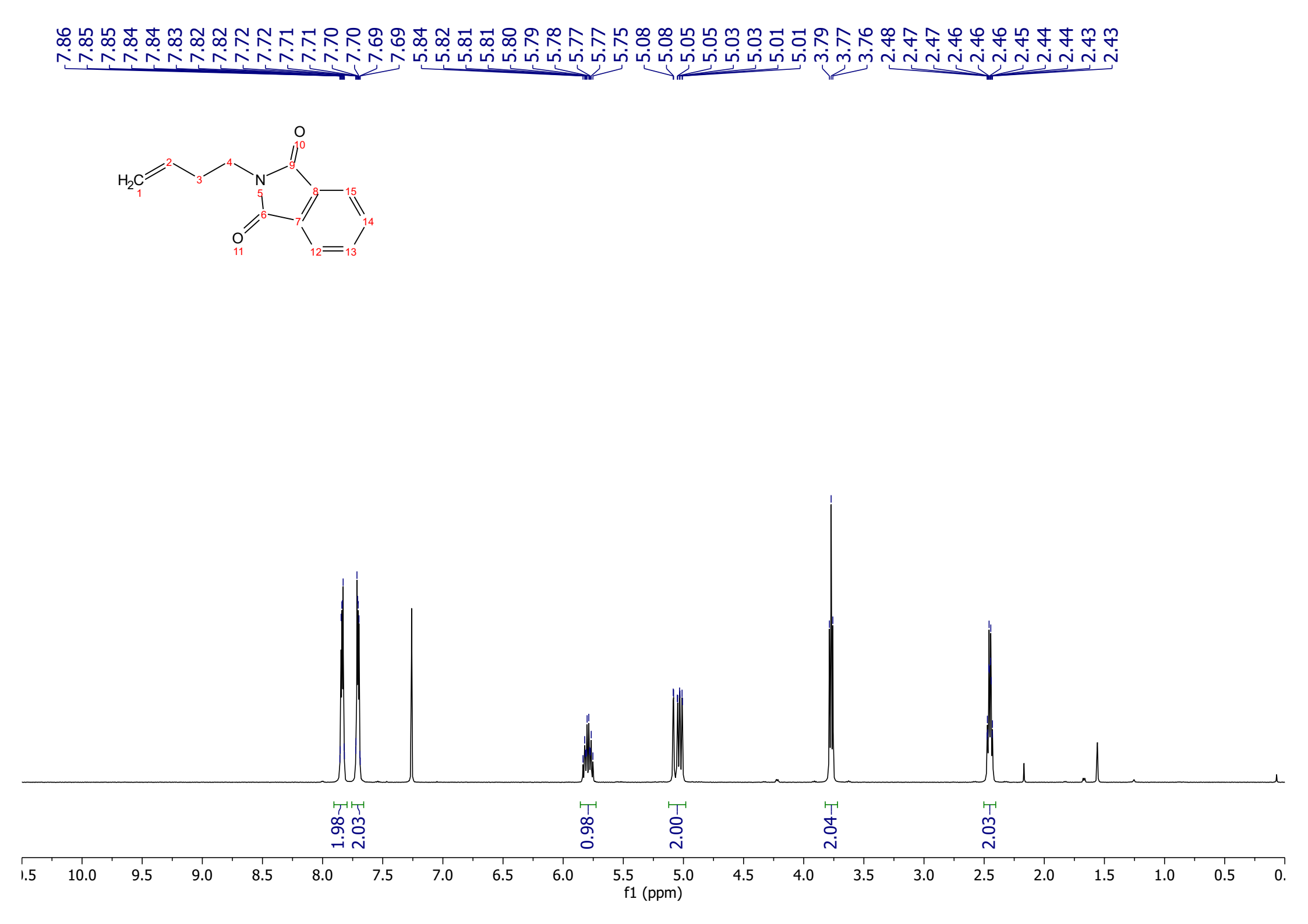
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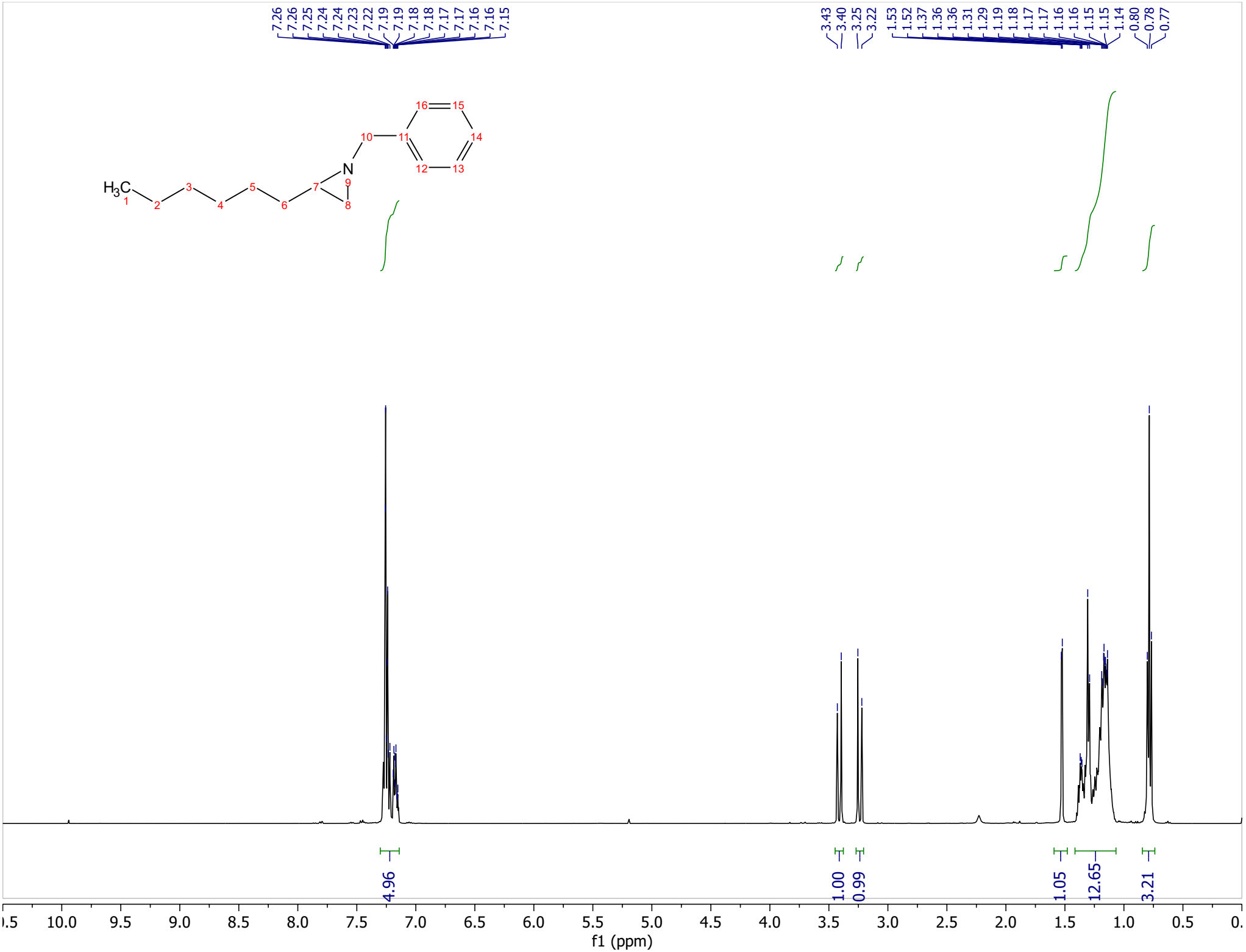
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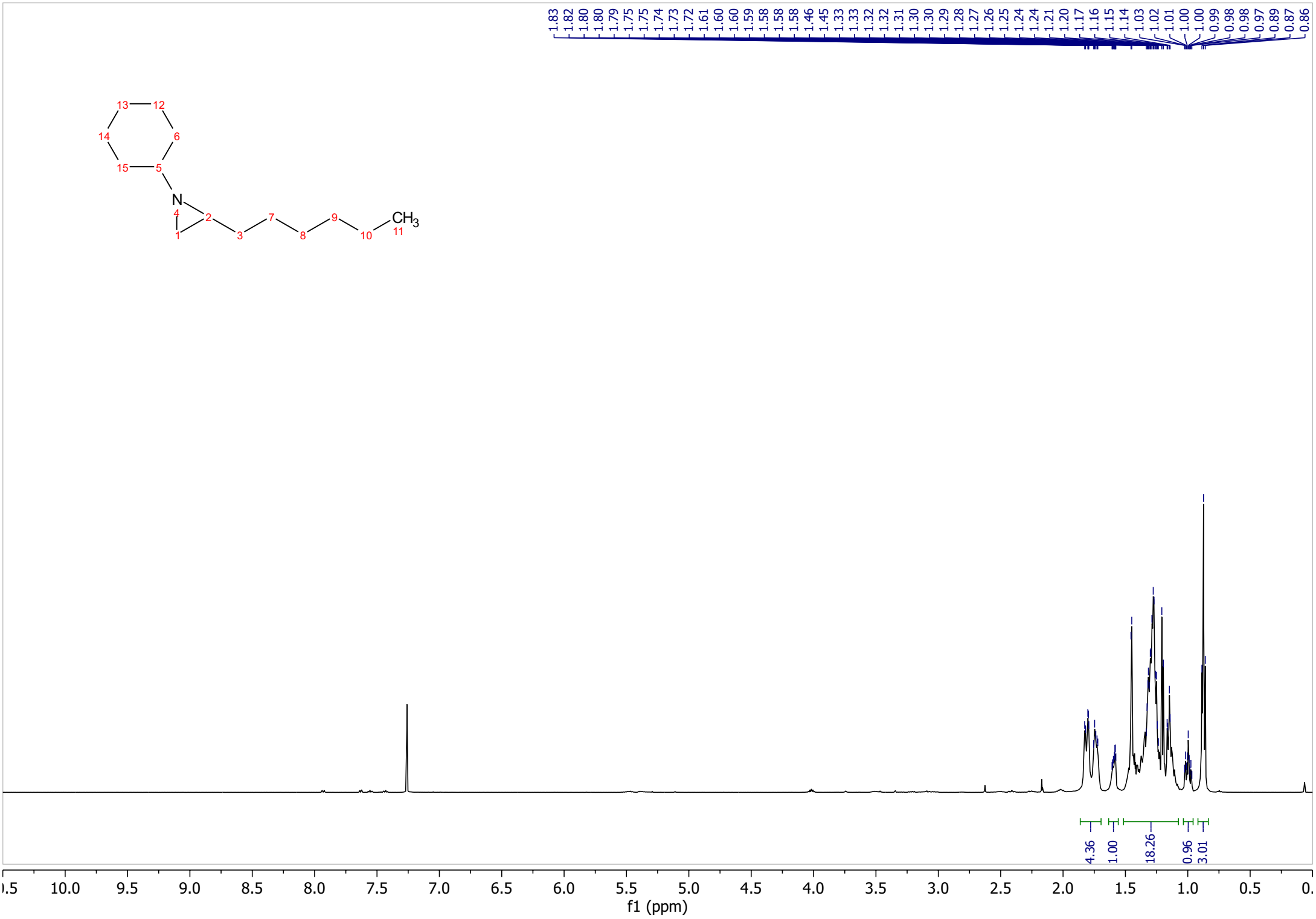
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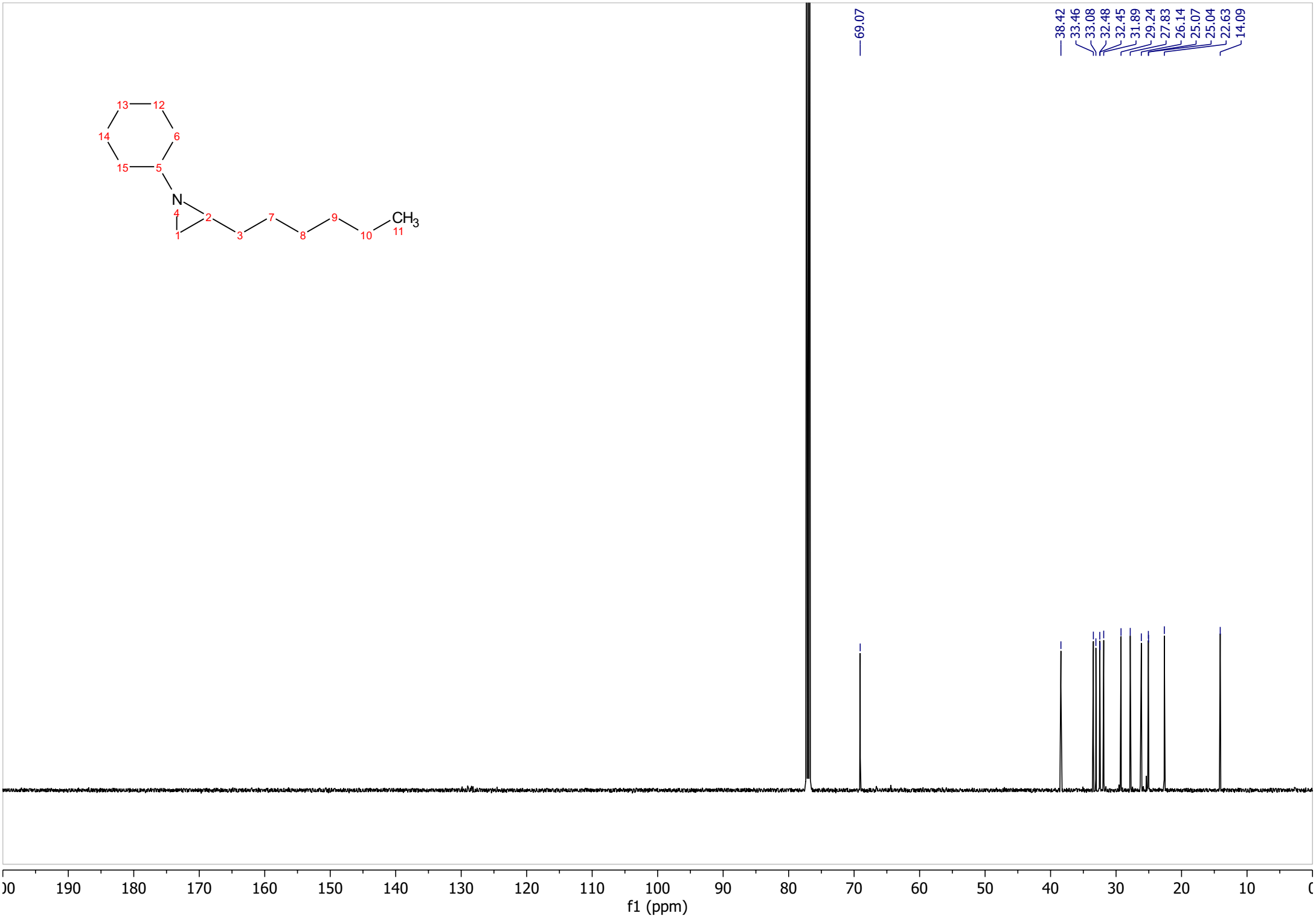
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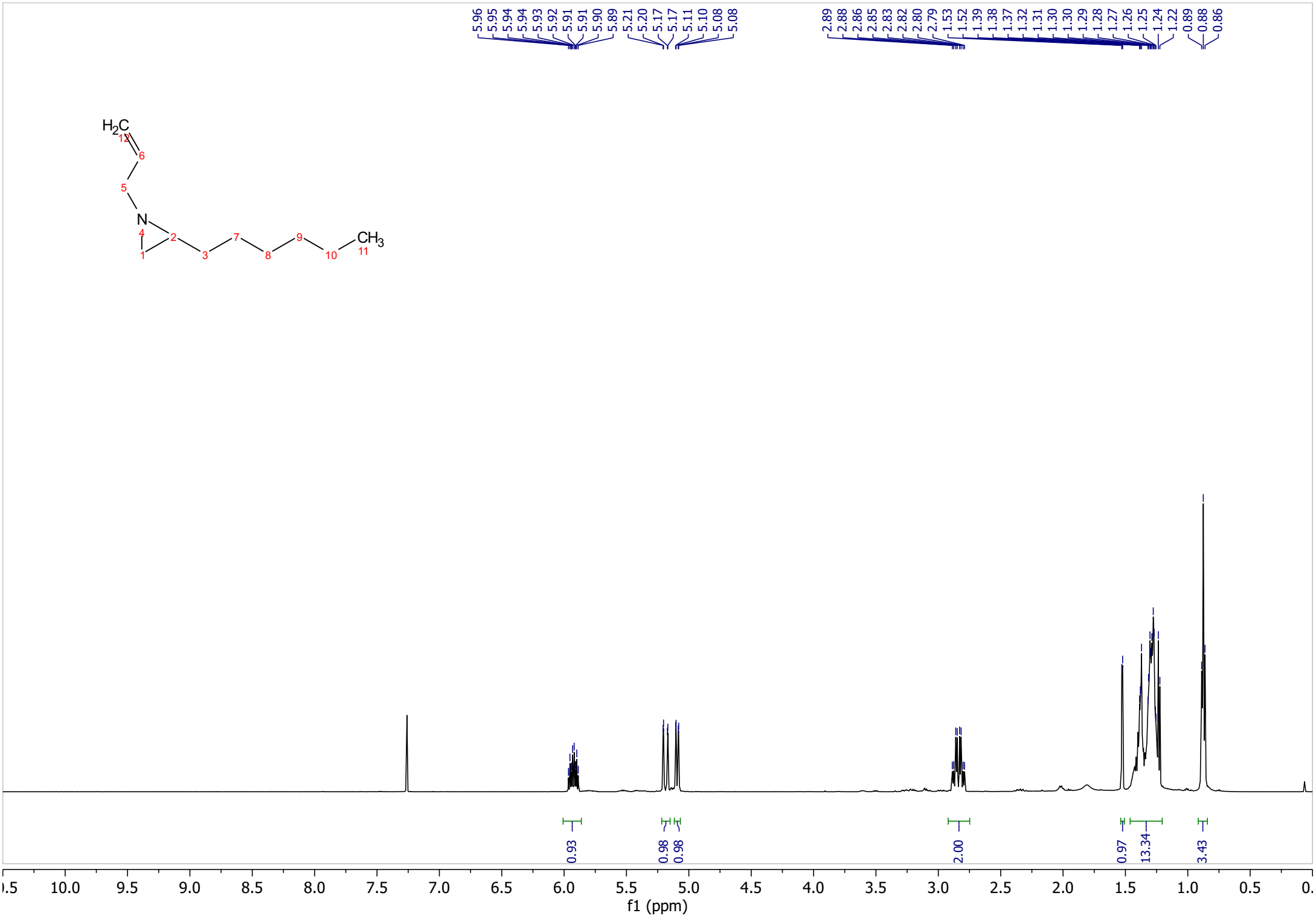
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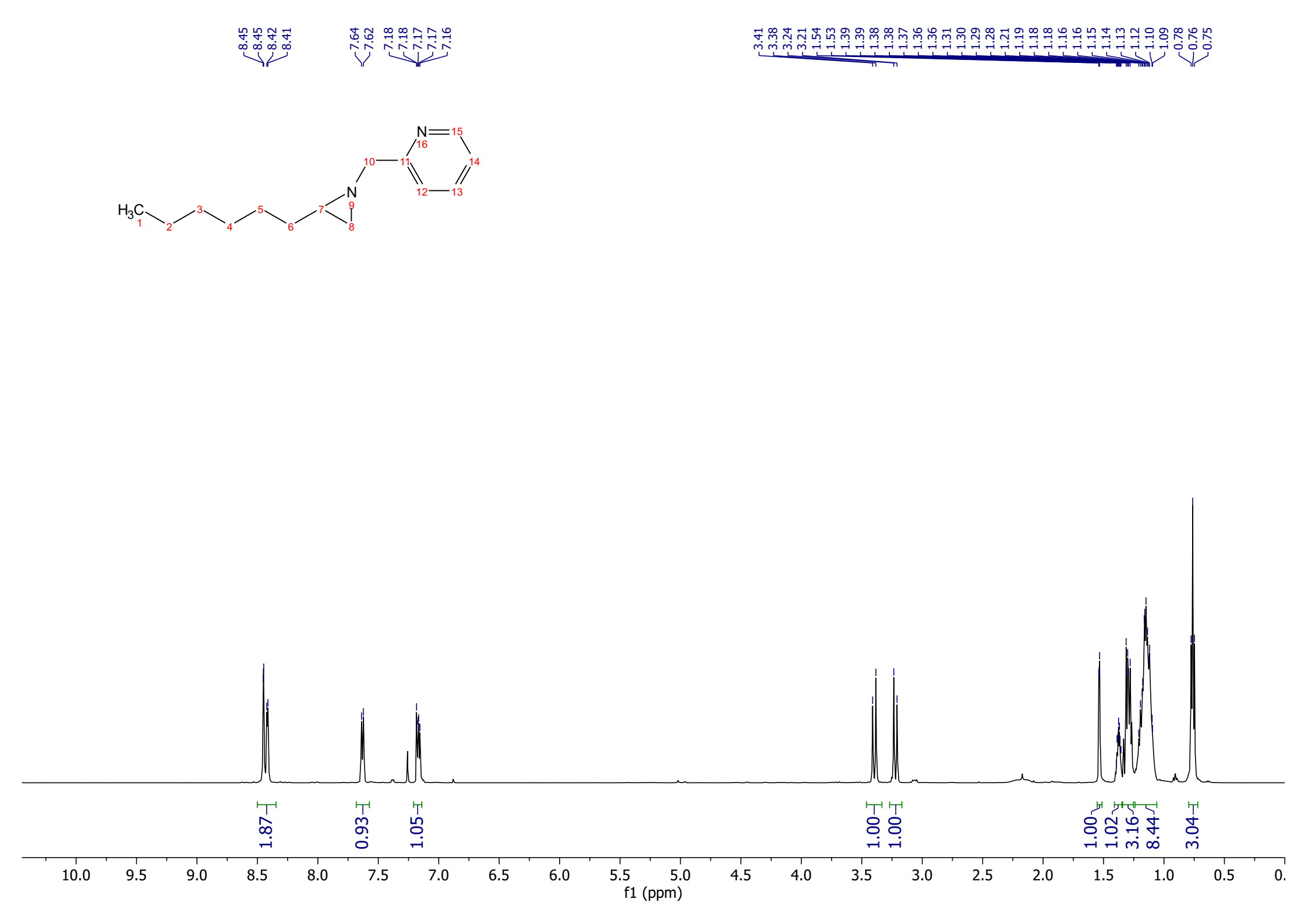
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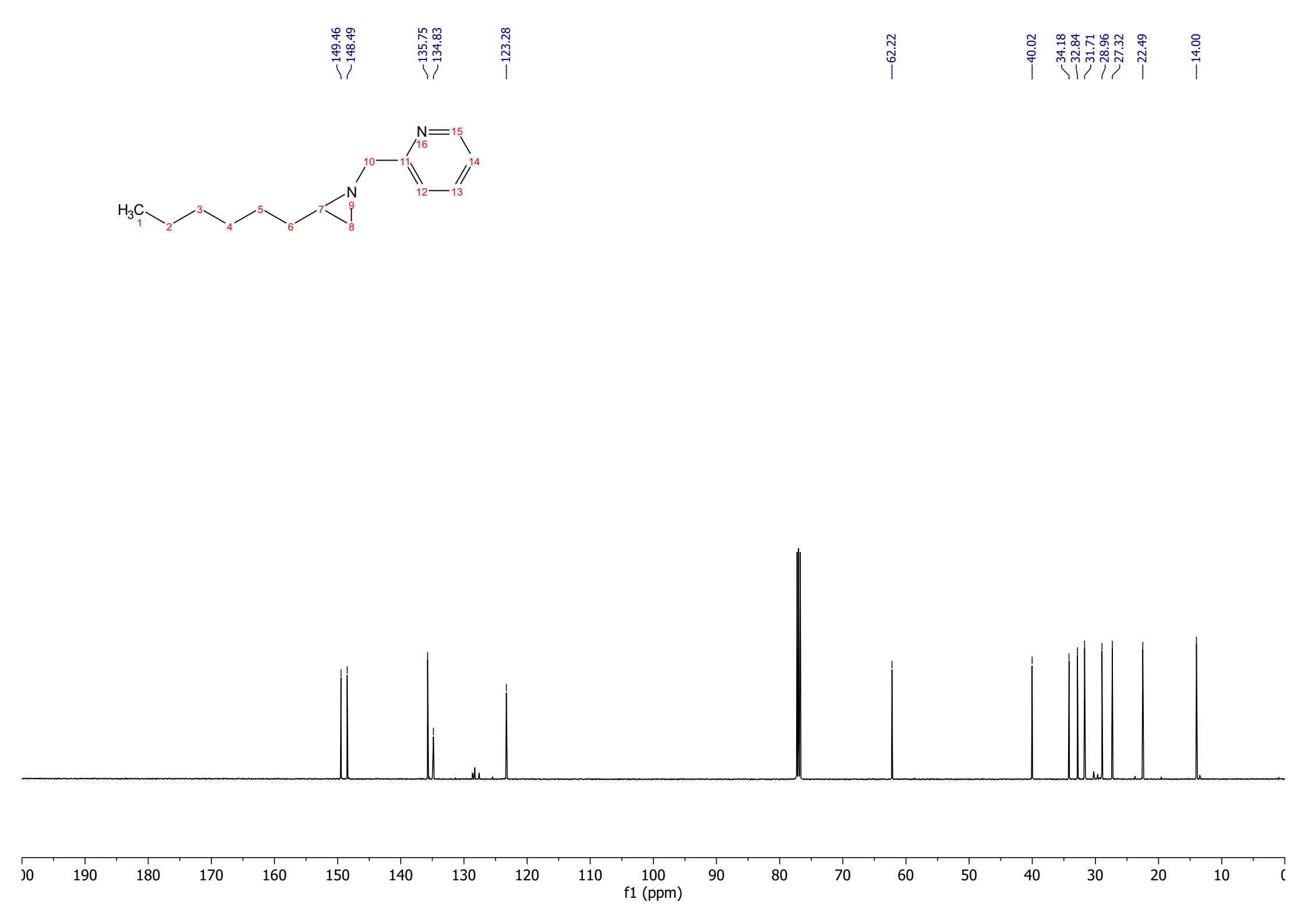
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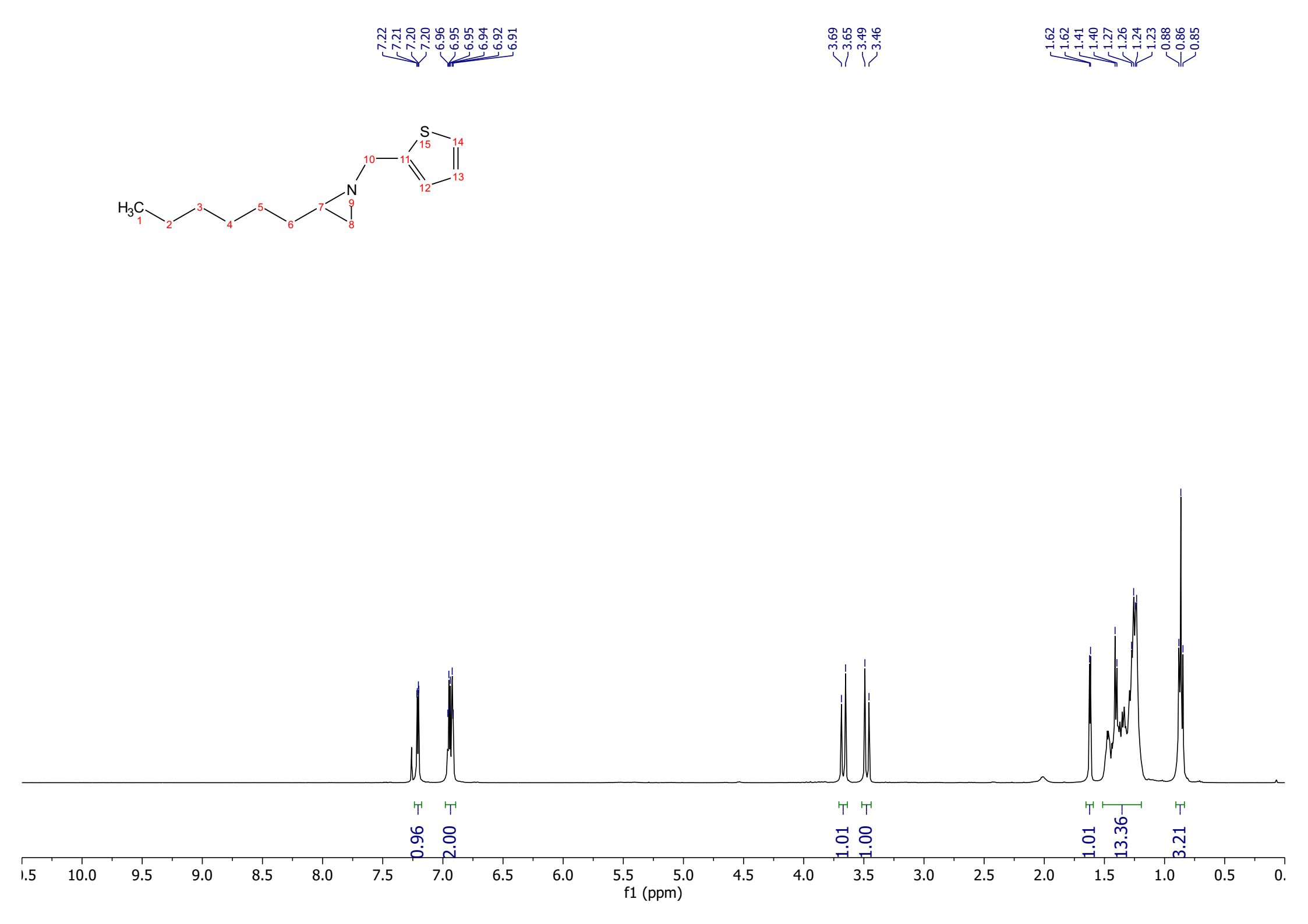
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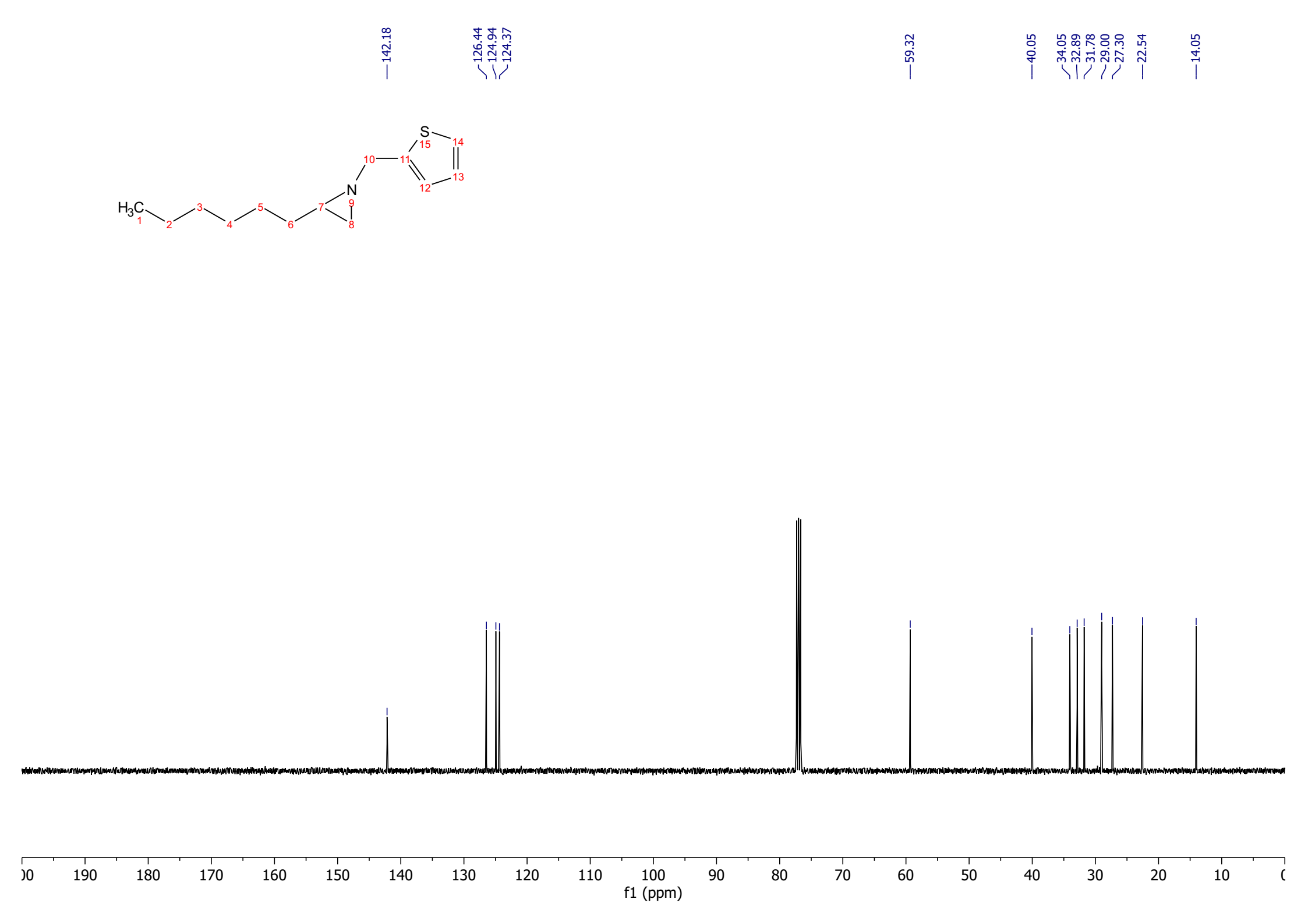
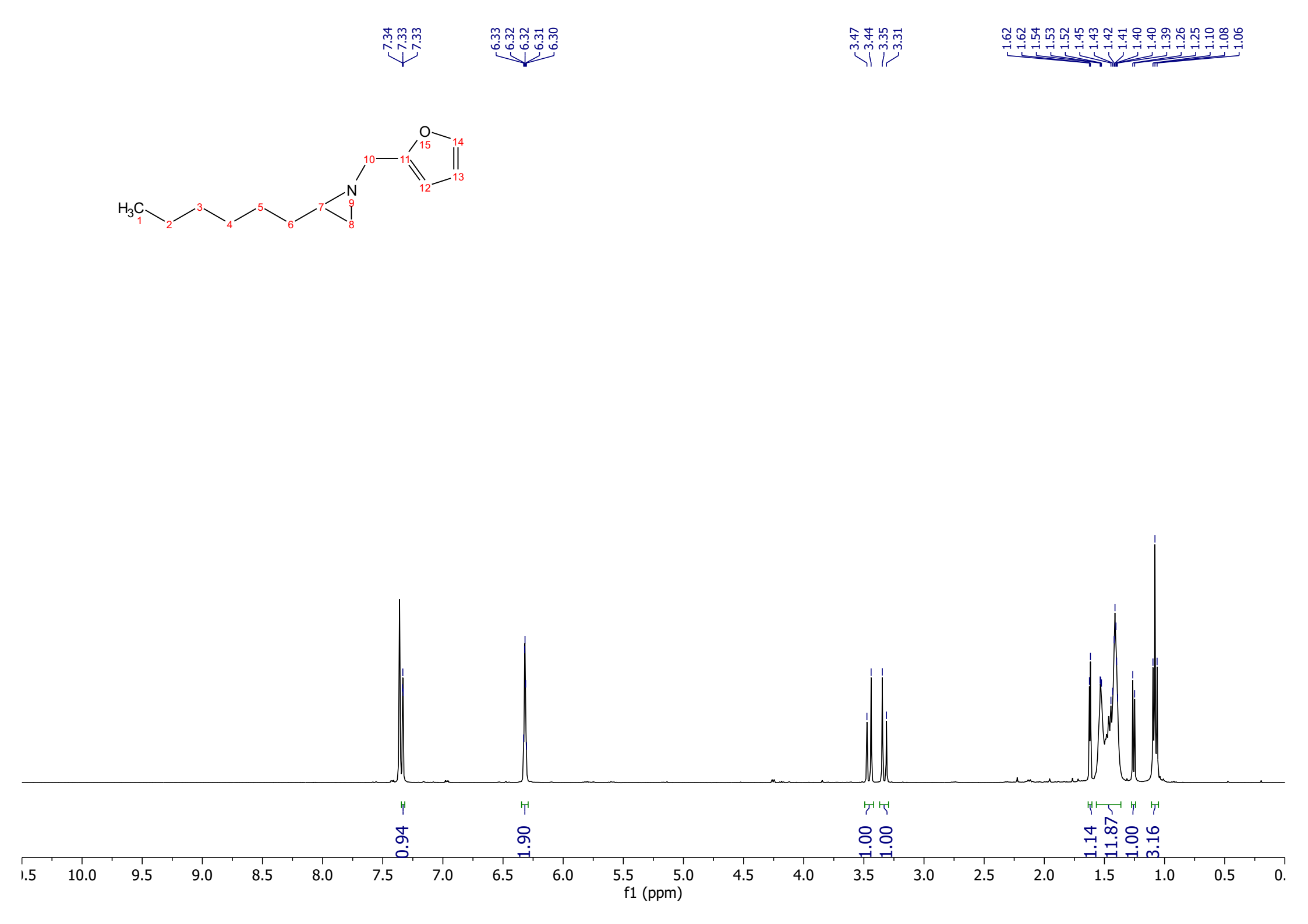
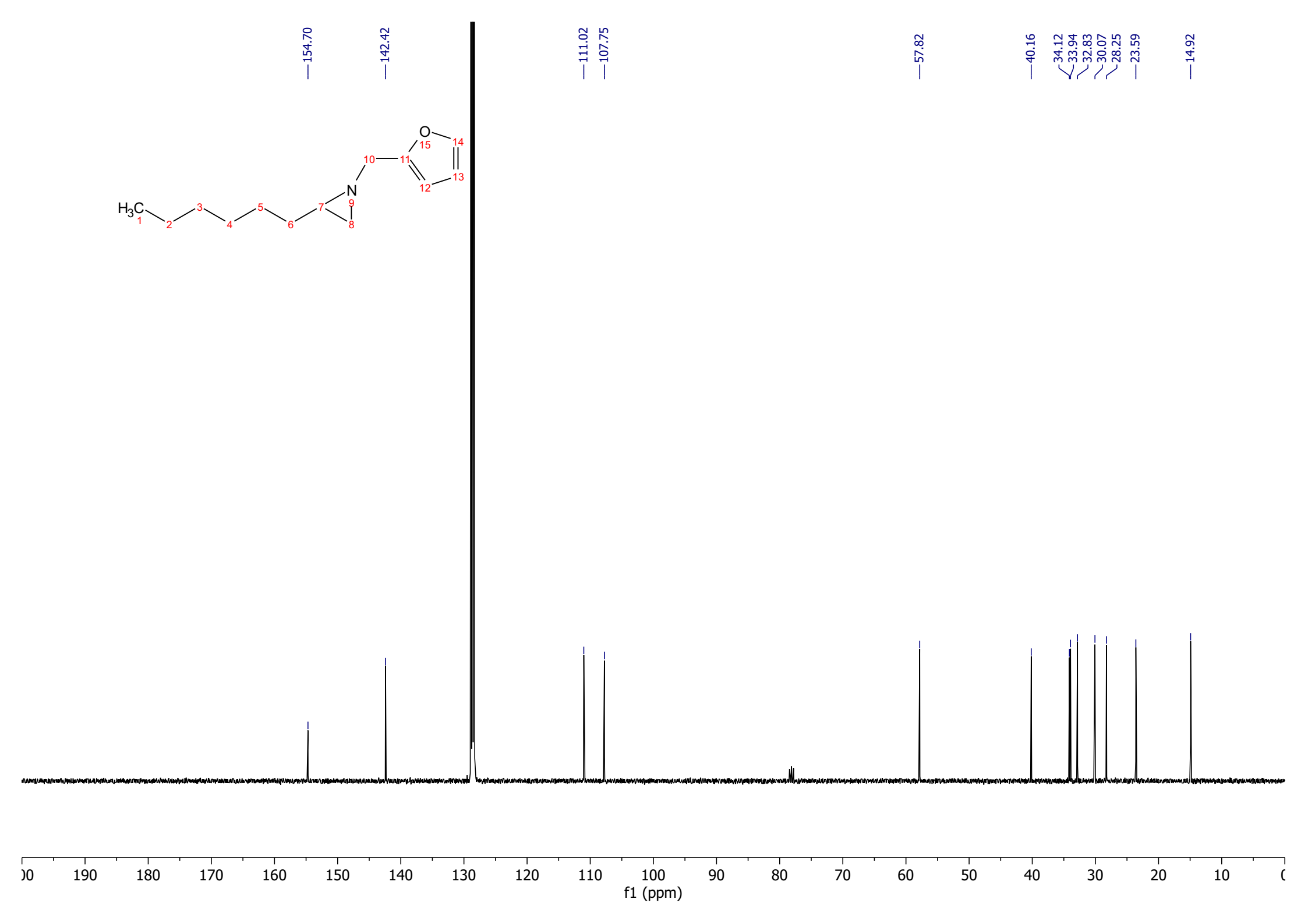
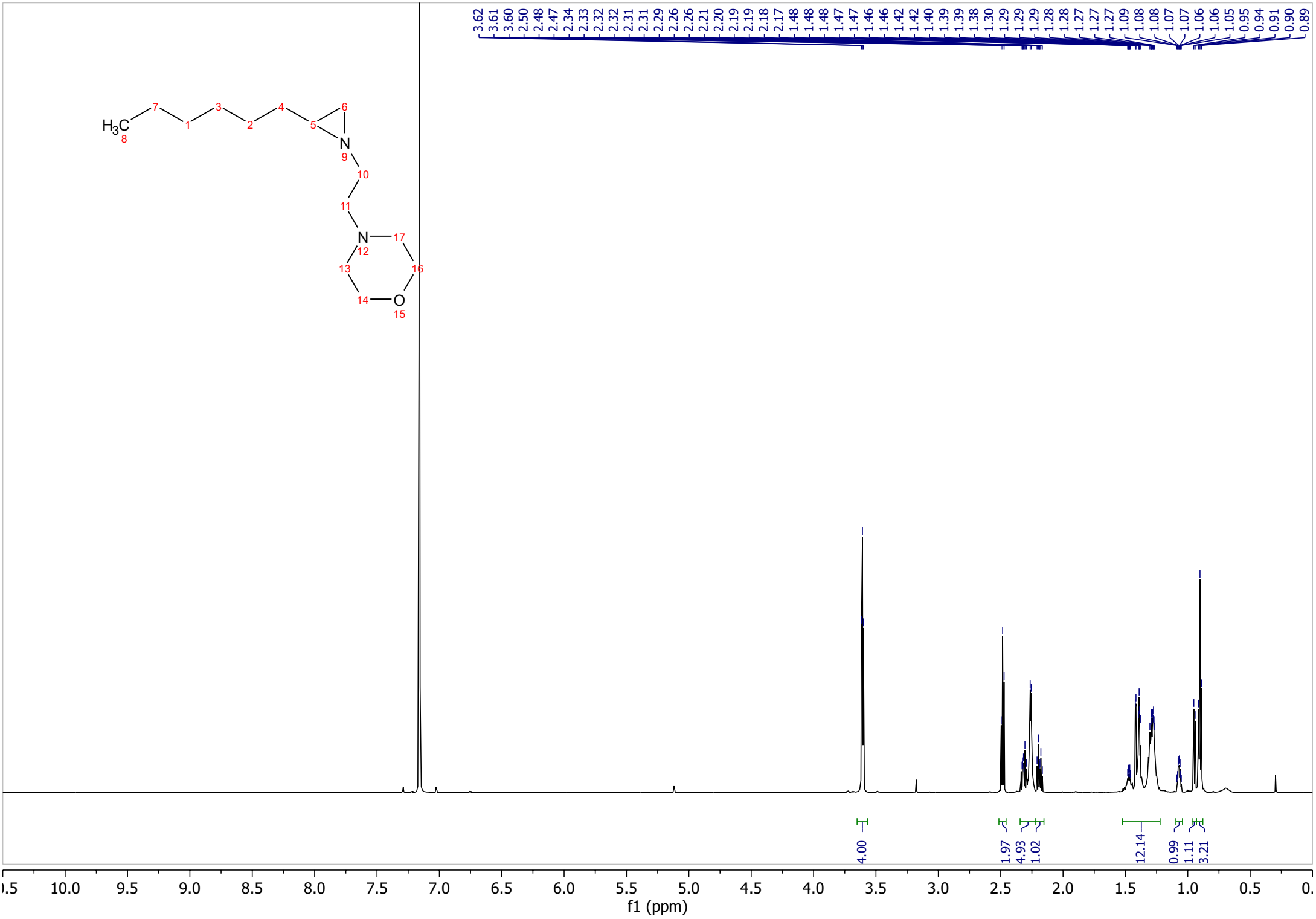
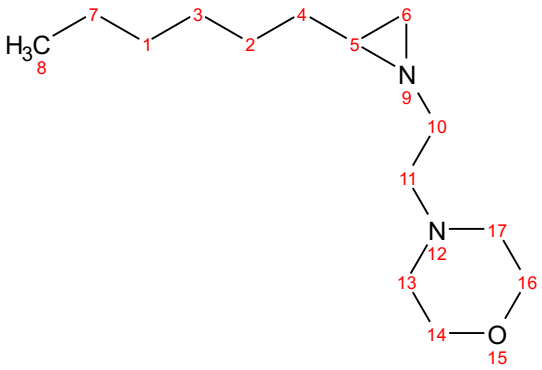
7.21
7.20
7.20
6.96
6.95
6.95
6.94
6.92
6.91
3.69
3.65
3.49
3.46
1.62
1.62
1.41
1.40
1.27
1.26
1.24
1.23
0.88
0.86
0.85
S
15
14
10
11
13
12
N
9
H_3C
1
2
3
4
5
6
7
8
0.96
2.00
1.01
1.00
1.01
13.36
3.21
f1 (ppm)


142.18
126.44
124.94
124.37
59.32
40.05
34.05
32.89
31.78
29.00
27.30
22.54
14.05
S
15
14
10
11
13
12
N
9
H3C
1
2
3
4
5
6
7
8
f1 (ppm)


7.34
7.33
7.33
6.33
6.32
6.32
6.31
6.30
3.47
3.44
3.35
3.31
1.62
1.62
1.54
1.53
1.52
1.45
1.43
1.42
1.41
1.40
1.40
1.39
1.26
1.25
1.10
1.08
1.06
O
15
14
10
11
13
12
N
9
H_3C
1
2
3
4
5
6
7
8
0.94
1.90
1.00
1.00
1.14
11.87
1.00
3.16
f1 (ppm)

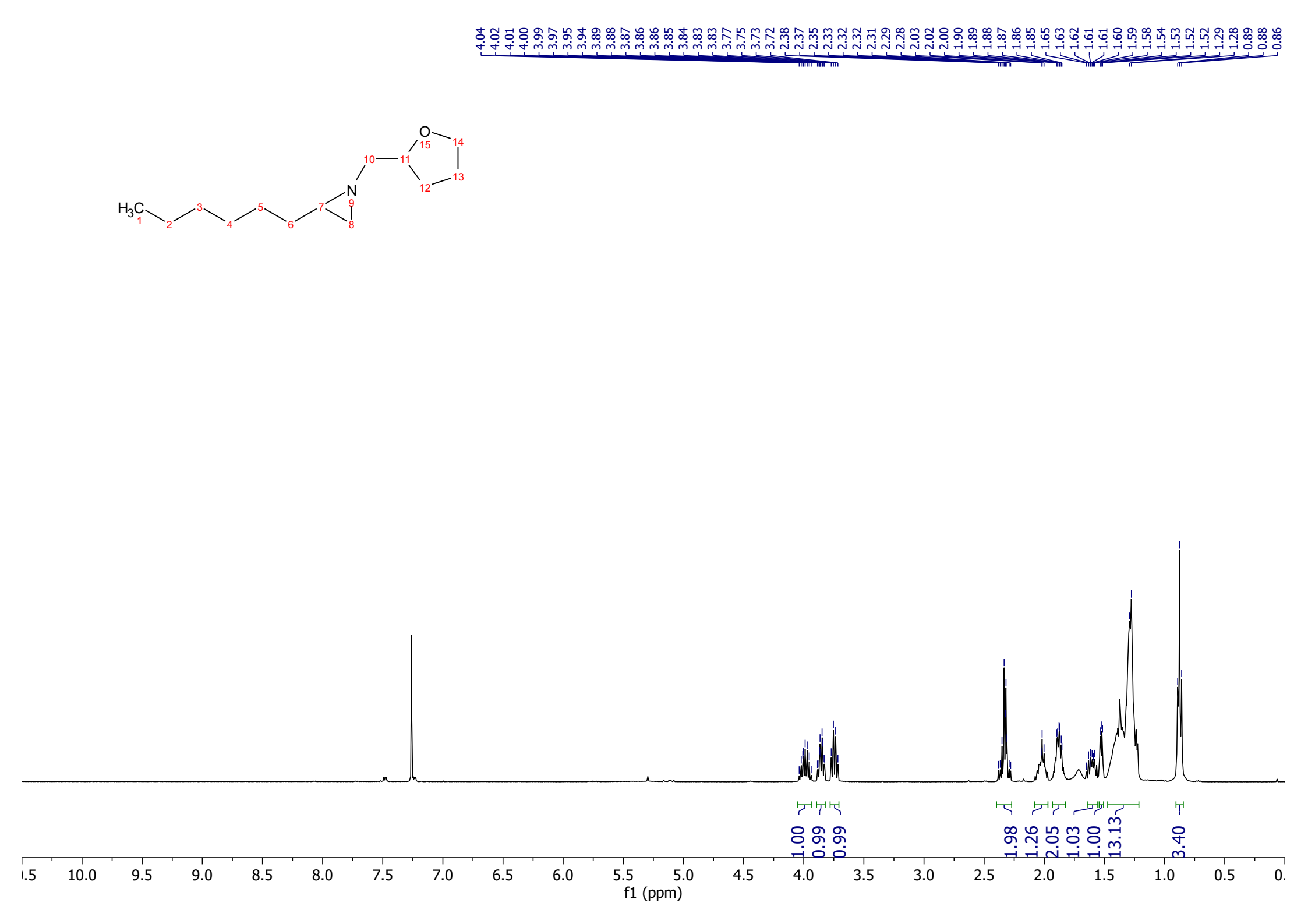

154.70
142.42
111.02
107.75
57.82
40.16
34.12
33.94
32.83
30.07
28.25
23.59
14.92
H3C
1
2
3
4
5
6
7
8
N
9
10
11
12
13
14
O
15
f1 (ppm)

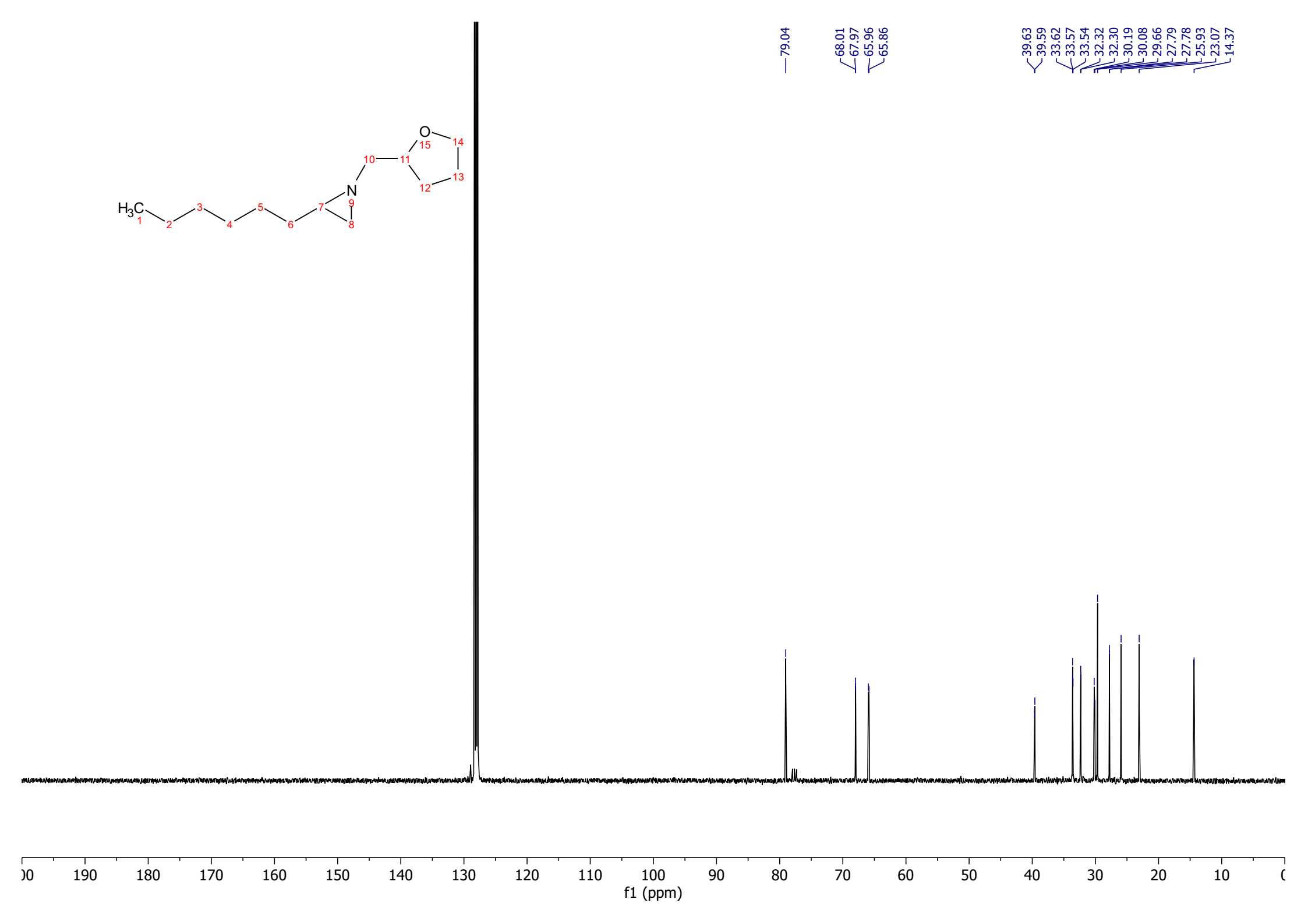

3.62 3.61 3.60 2.50 2.48 2.47 2.34 2.33 2.32 2.32 2.31 2.31 2.29 2.26 2.26 2.21 2.20 2.19 2.19 2.18 2.17 1.48 1.48 1.48 1.47 1.47 1.46 1.46 1.42 1.40 1.39 1.39 1.38 1.30 1.29 1.29 1.29 1.28 1.27 1.27 1.27 1.09 1.08 1.08 1.07 1.07 1.06 1.06 1.05 0.95 0.94 0.91 0.90 0.89
H3C
N
O
4.00
1.97
4.93
1.02
12.14
0.99
1.11
3.21
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

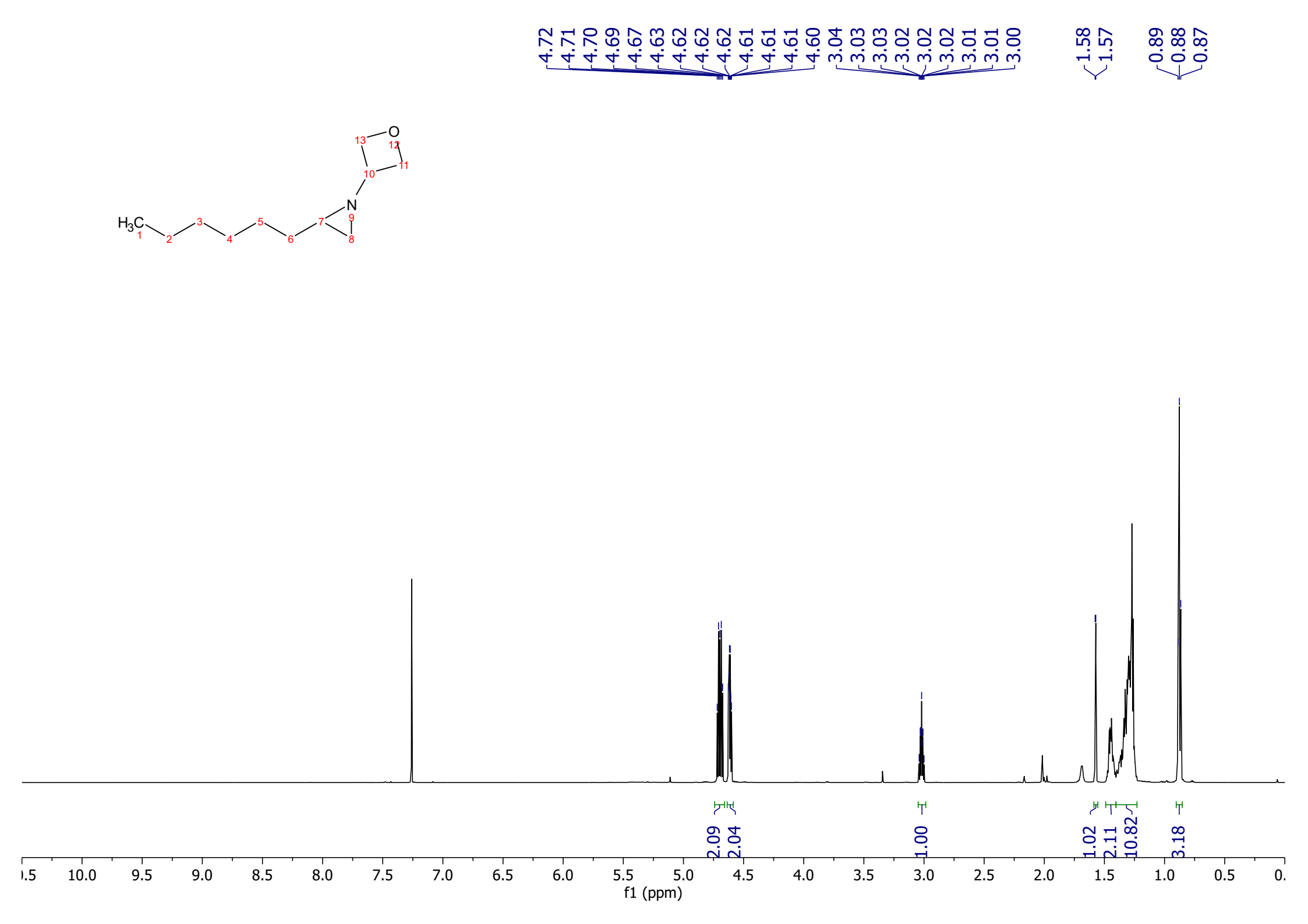


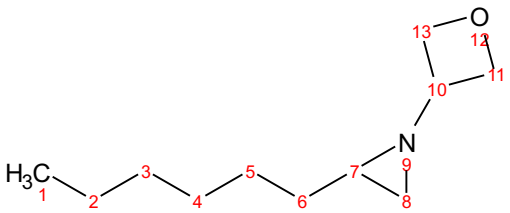
66.82
59.07
58.74
54.28
39.47
33.21
33.19
31.92
29.28
27.51
22.69
13.98

f1 (ppm)


4.04 4.02 4.01 4.00 3.99 3.97 3.95 3.94 3.89 3.88 3.87 3.86 3.86 3.85 3.84 3.83 3.83 3.77 3.75 3.73 3.72 2.38 2.37 2.35 2.33 2.32 2.32 2.31 2.29 2.28 2.03 2.02 2.00 1.90 1.89 1.88 1.87 1.86 1.85 1.65 1.63 1.62 1.61 1.61 1.60 1.59 1.58 1.54 1.53 1.52 1.52 1.29 1.28 0.89 0.88 0.86
H3C
1
2
3
4
5
6
7
N
9
8
10
11
12
13
14
O
15
1.00 0.99 0.99 1.98 1.26 2.05 1.03 1.00 13.13 3.40
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

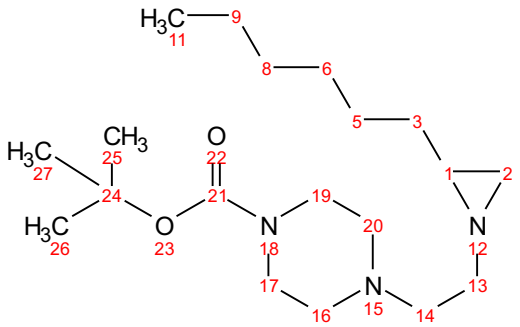

79.04
68.01
67.97
65.96
65.86
39.63
39.59
33.62
33.57
33.54
32.32
32.30
30.19
30.08
29.66
27.79
27.78
25.93
23.07
14.37
H3C
1
2
3
4
5
6
7
8
N
9
10
11
12
13
14
O
15
f1 (ppm)


4.72
4.71
4.70
4.69
4.67
4.63
4.62
4.62
4.62
4.61
4.61
4.61
4.60
3.04
3.03
3.03
3.02
3.02
3.02
3.01
3.01
3.00
1.58
1.57
0.89
0.88
0.87
O
13
12
11
10
N
9
7
8
6
5
4
3
2
1
H3C
2.09
2.04
1.00
1.02
2.11
10.82
3.18
f1 (ppm)

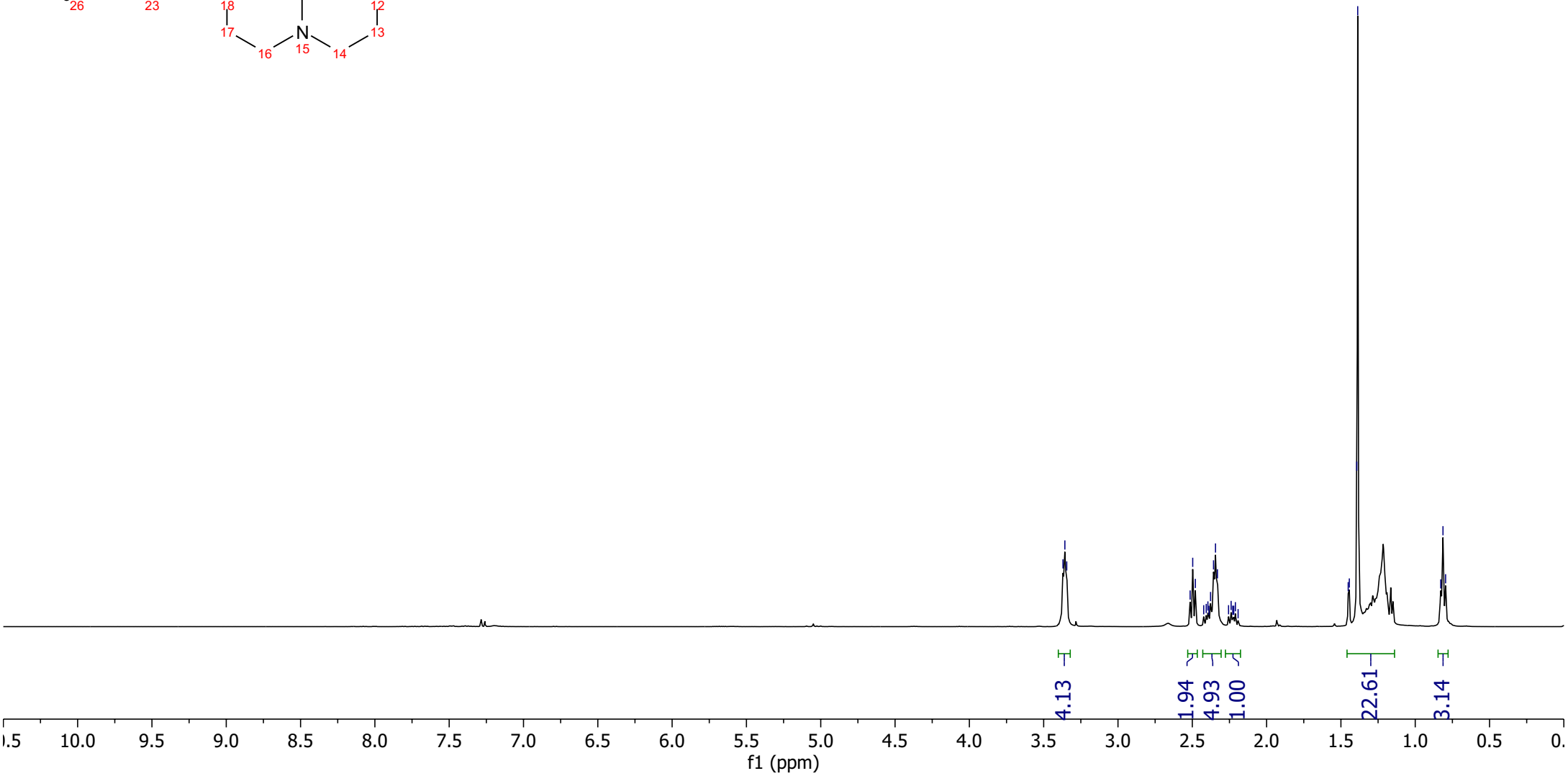


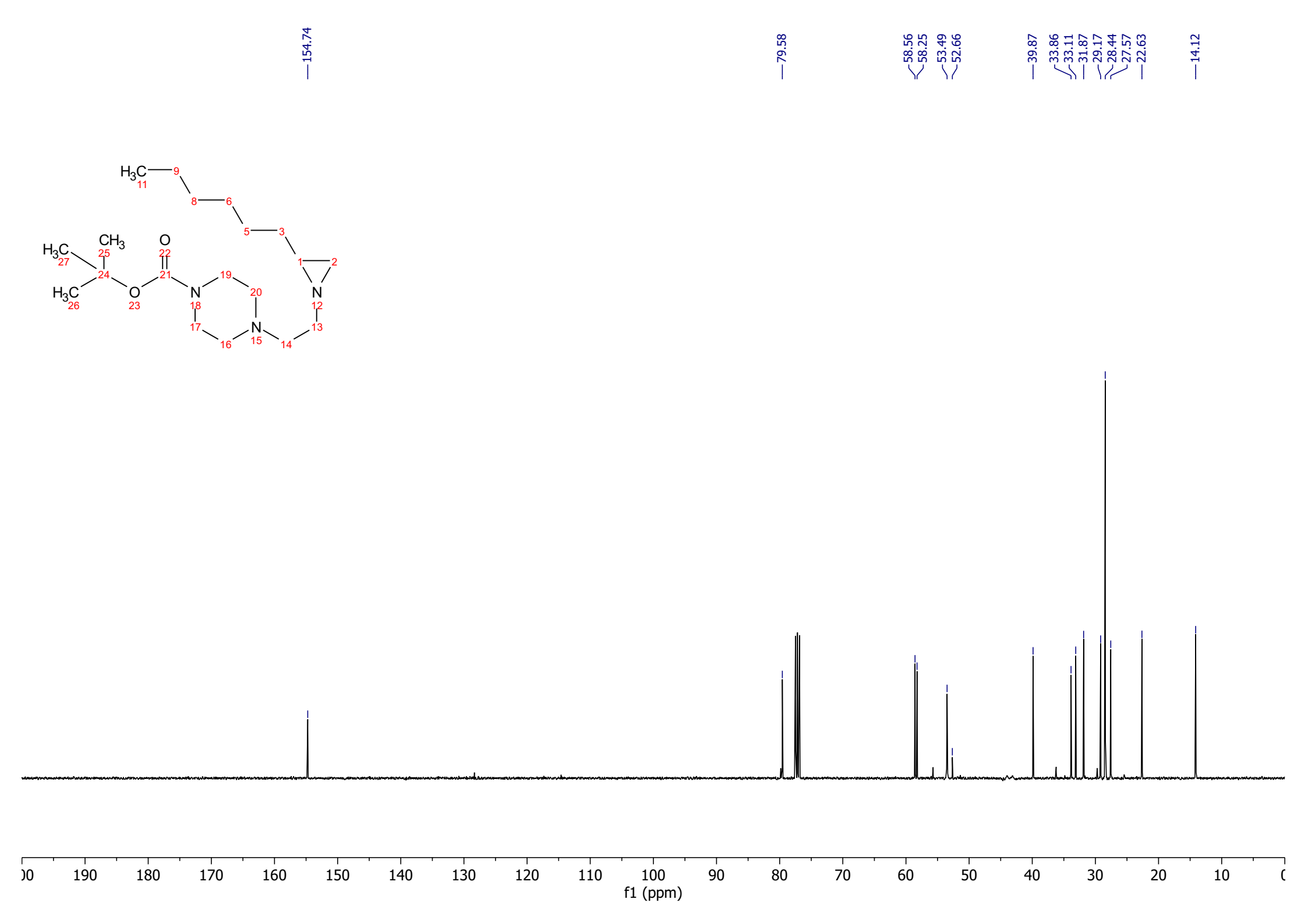
62.97
38.04
32.98
32.22
31.95
29.21
27.83
22.74
14.22

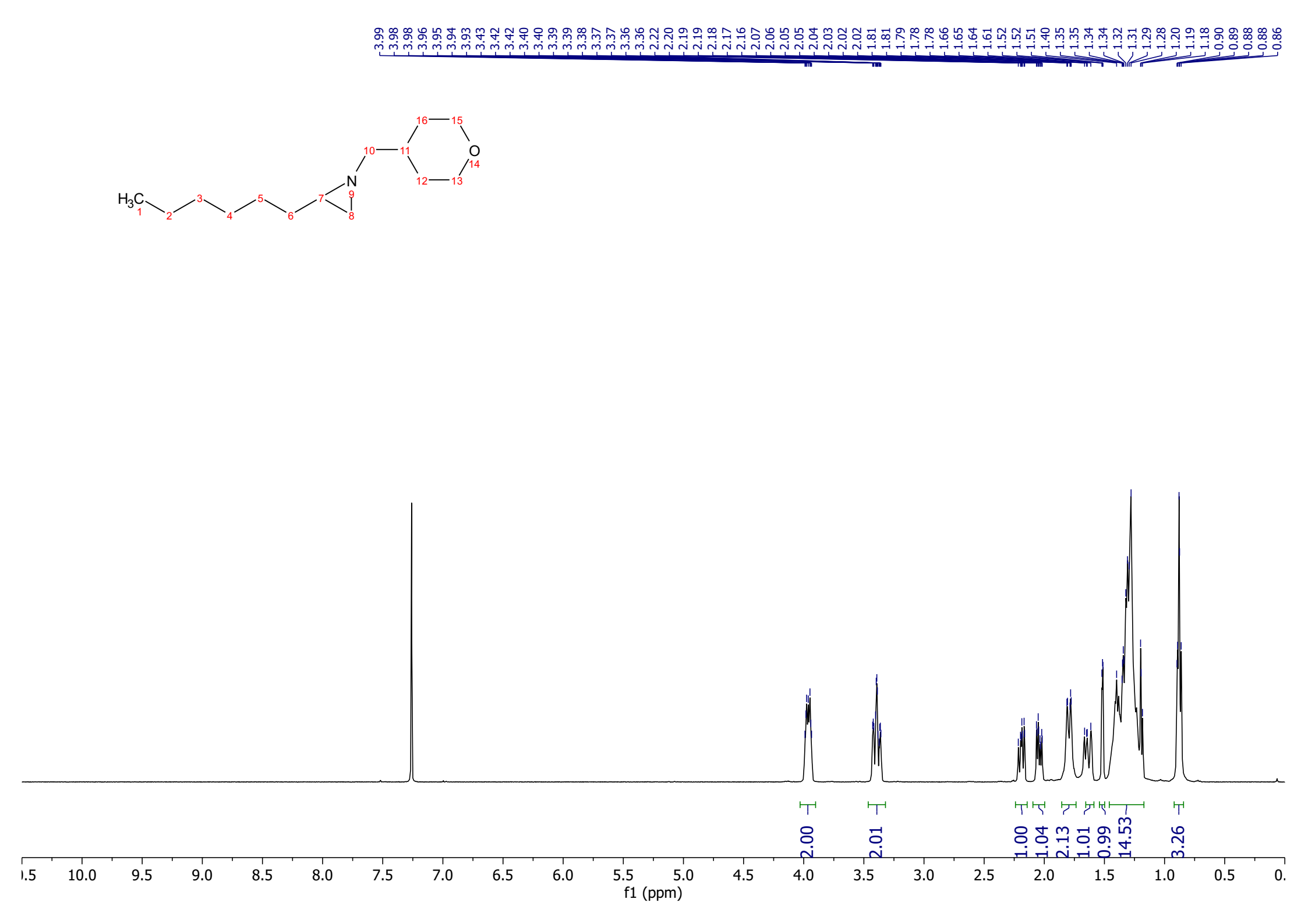
f1 (ppm)

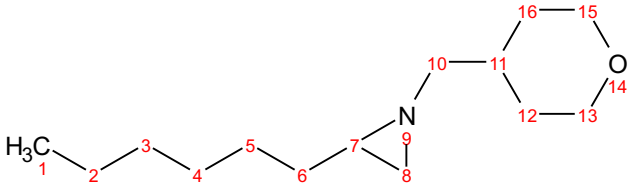

H3C
11
9
8
6
5
3
1
2
CH3
25
O
22
H3C
27
24
21
19
20
H3C
26
O
23
N
18
N
12
17
N
15
16
14
13


3.37
3.36
3.34
2.51
2.50
2.48
2.42
2.41
2.40
2.39
2.38
2.36
2.34
2.33
2.26
2.24
2.23
2.22
2.21
2.19
1.45
1.44
1.39
1.39
0.83
0.81
0.80

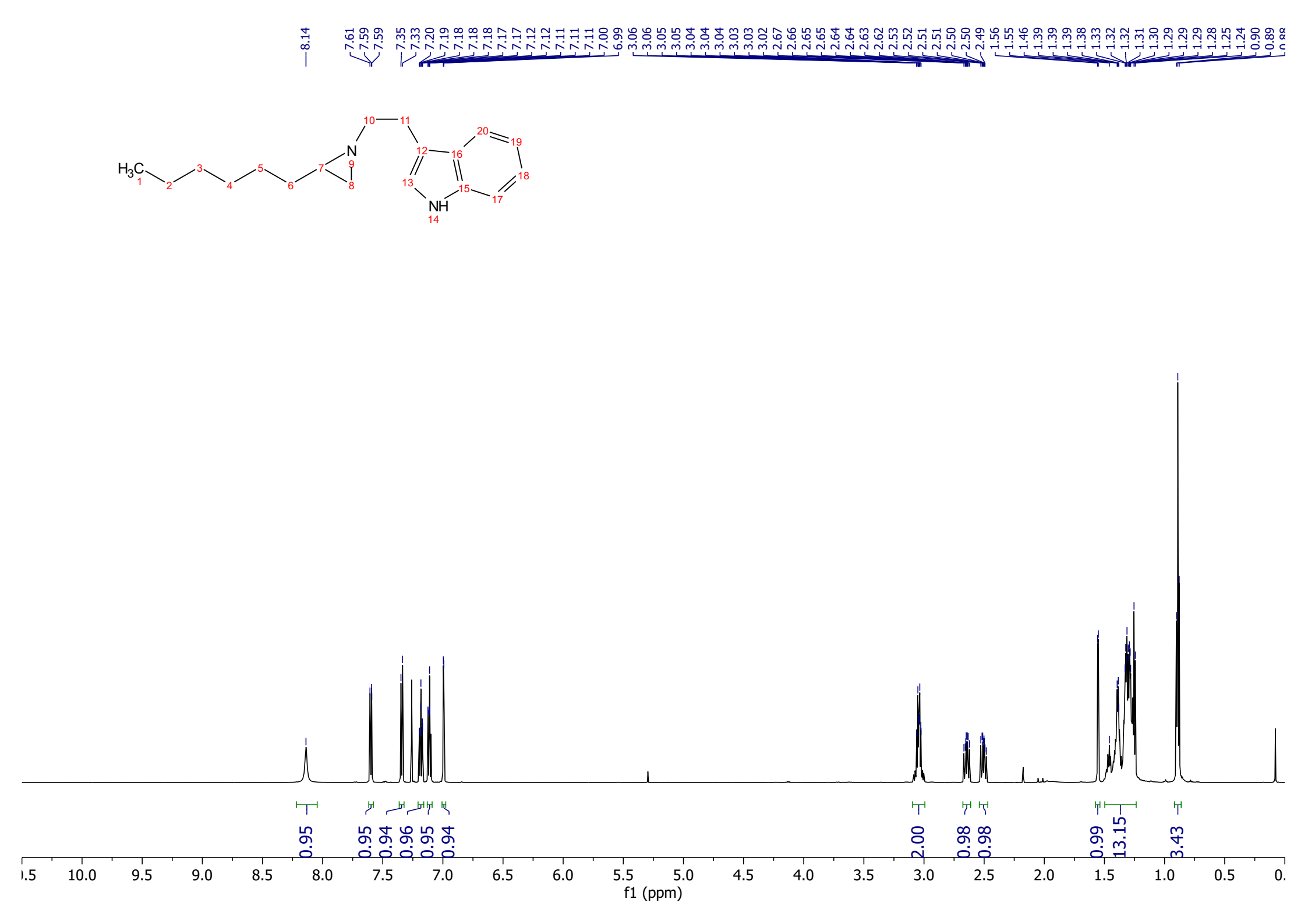

4.13
1.94
4.93
1.00
22.61
3.14
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

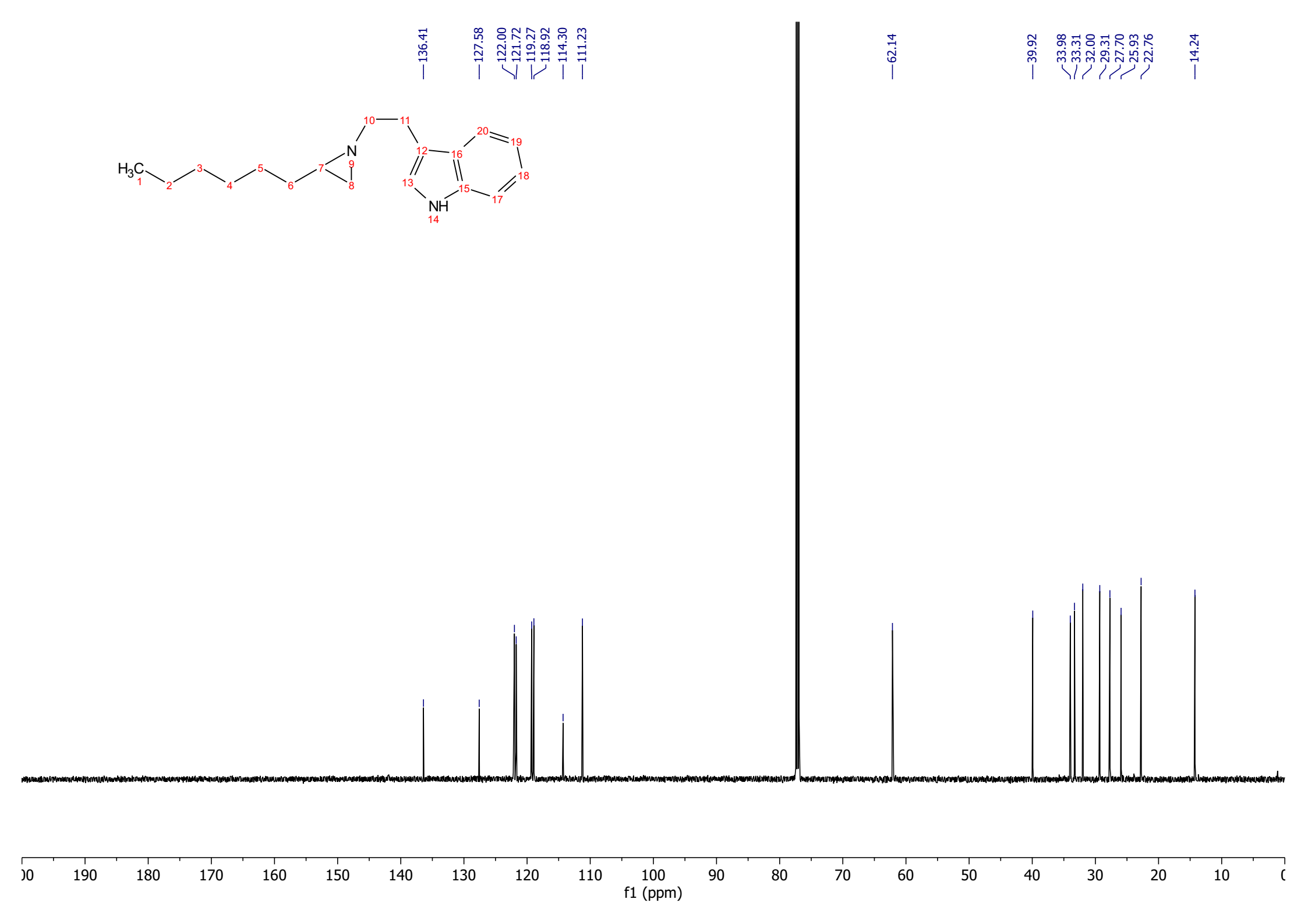

154.74
79.58
58.56
58.25
53.49
52.66
39.87
33.86
33.11
31.87
29.17
28.44
27.57
22.63
14.12
f1 (ppm)

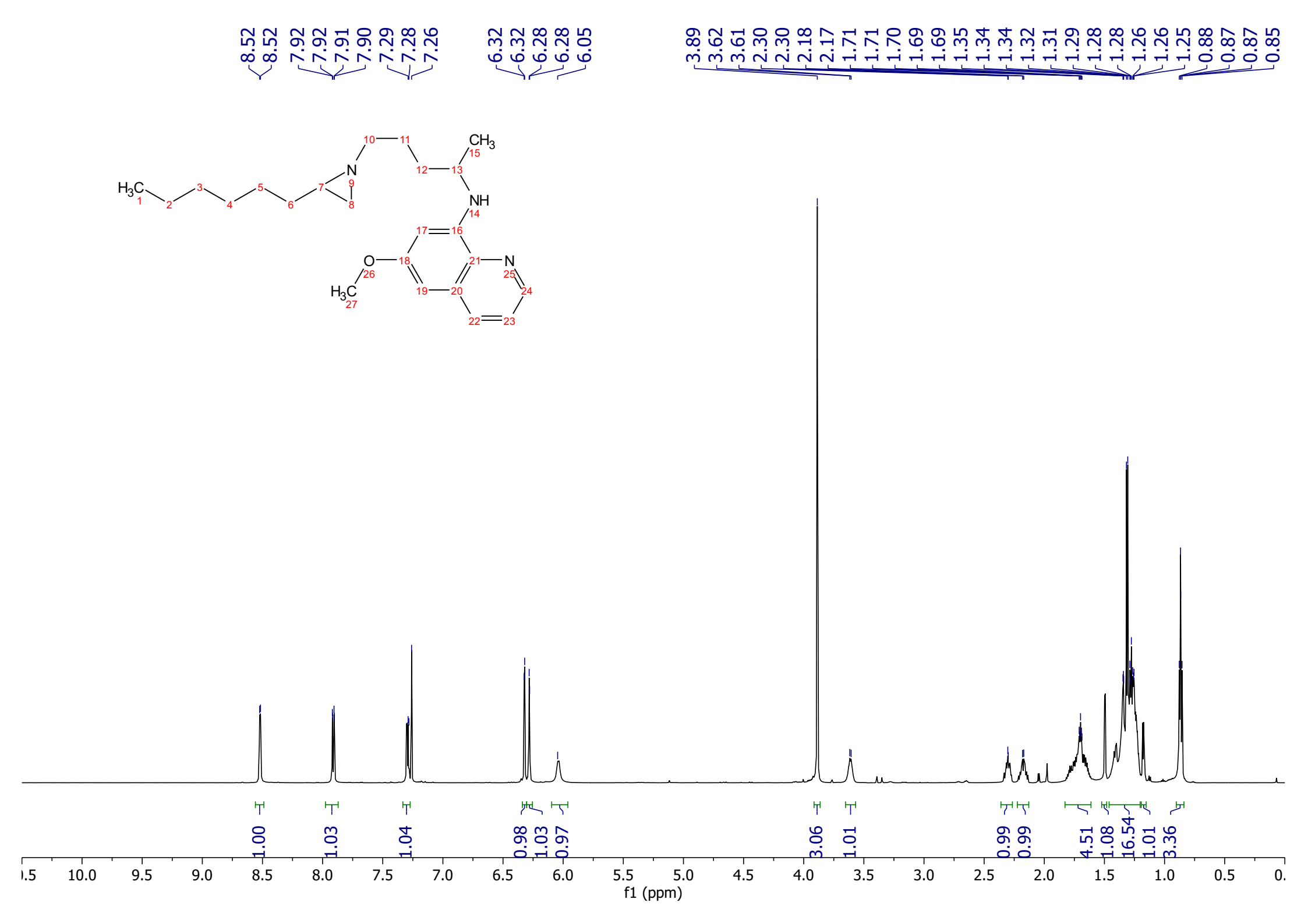

3.99 3.98 3.98 3.96 3.95 3.94 3.93 3.43 3.42 3.42 3.40 3.40 3.39 3.39 3.38 3.37 3.37 3.36 3.36 2.22 2.20 2.19 2.19 2.18 2.17 2.16 2.07 2.06 2.05 2.05 2.04 2.03 2.02 2.02 1.81 1.81 1.79 1.78 1.78 1.66 1.65 1.64 1.61 1.52 1.52 1.51 1.40 1.35 1.35 1.34 1.34 1.32 1.31 1.29 1.28 1.20 1.19 1.18 0.90 0.89 0.88 0.88 0.86
H3C
1
2
3
4
5
6
7
N
9
8
10
11
12
13
O
14
15
16
2.00
2.01
1.00
1.04
2.13
1.01
0.99
14.53
3.26
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

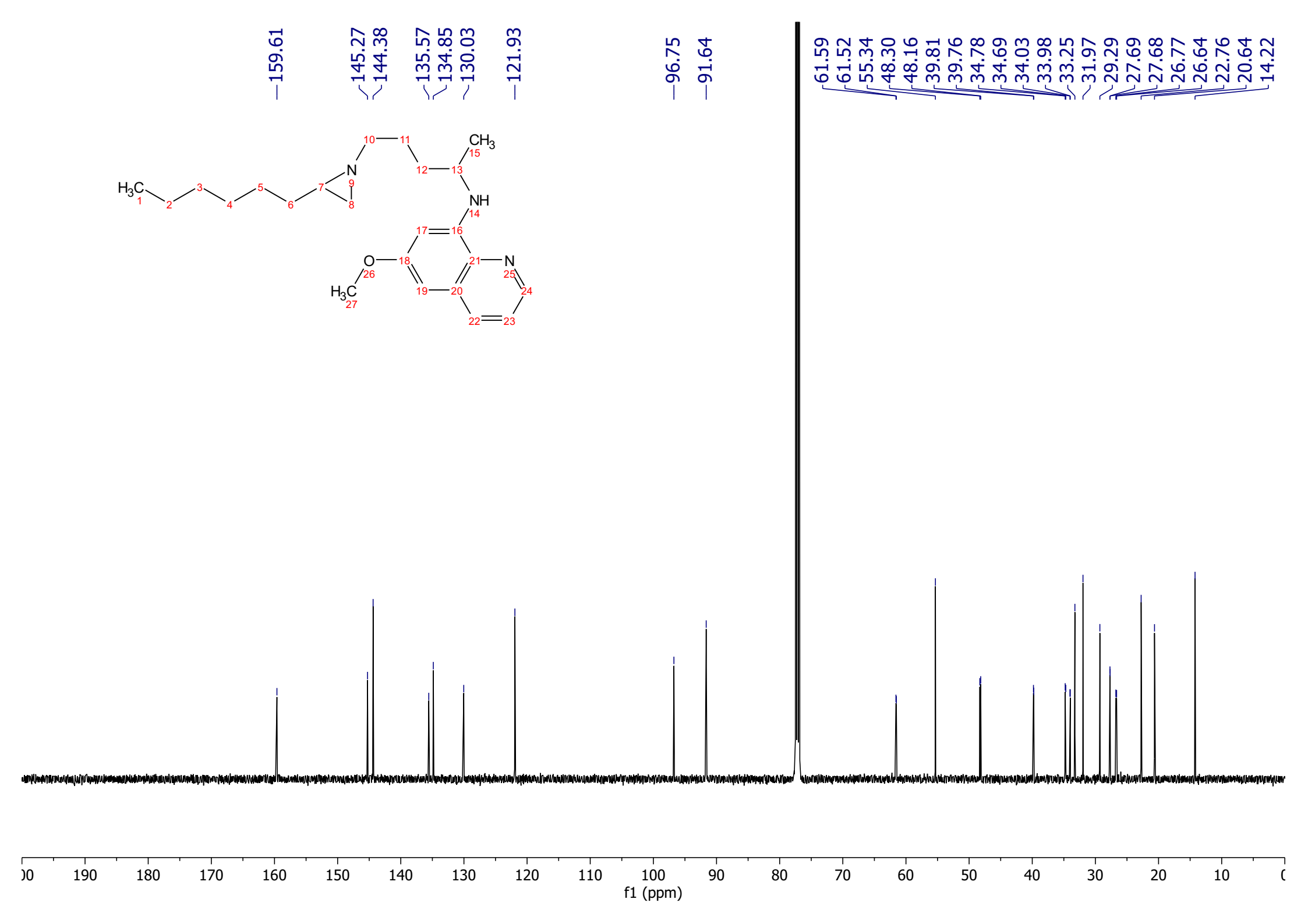

H3C
1
2
3
4
5
6
7
8
N
9
10
11
12
13
14
O
15
16

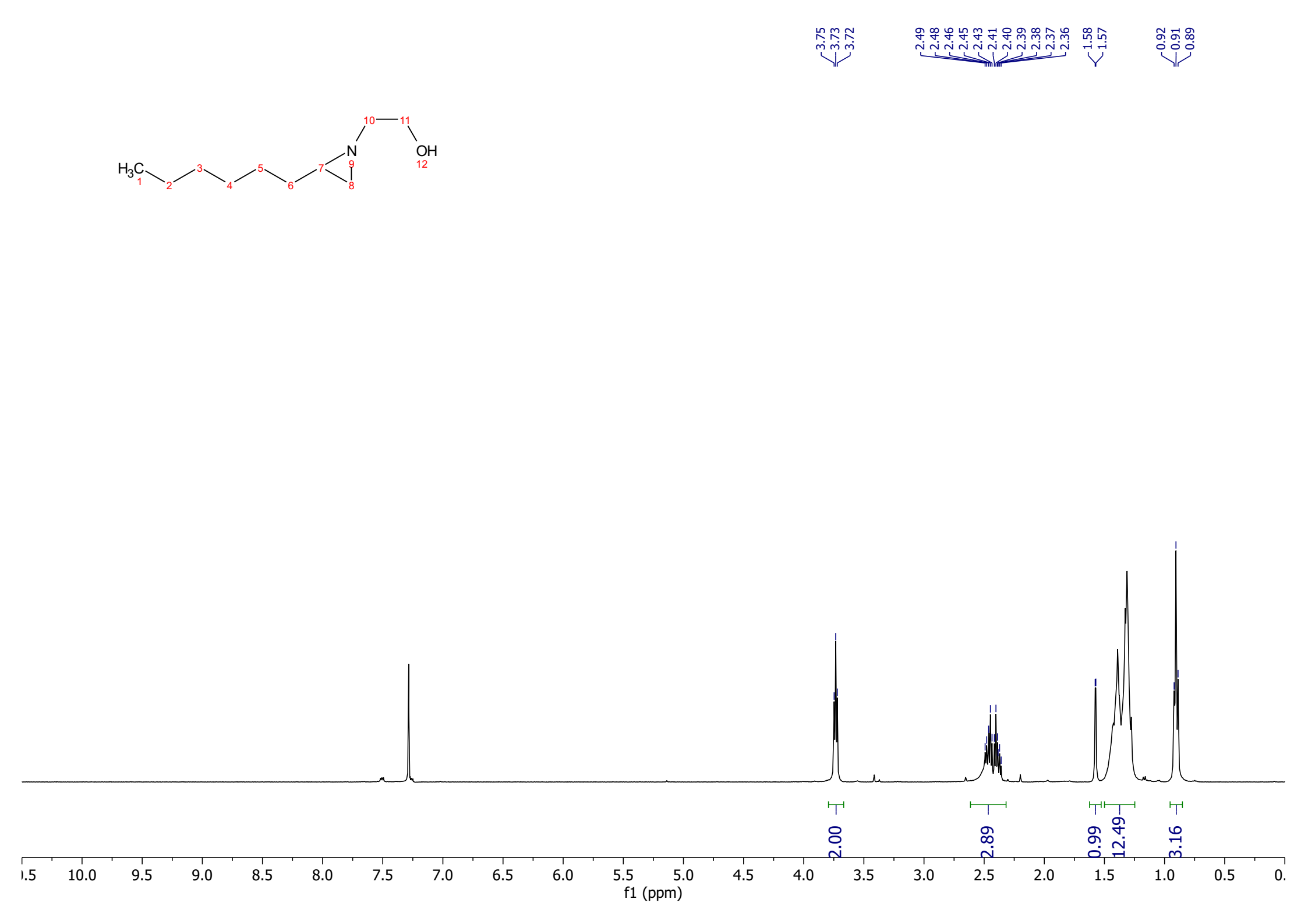
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

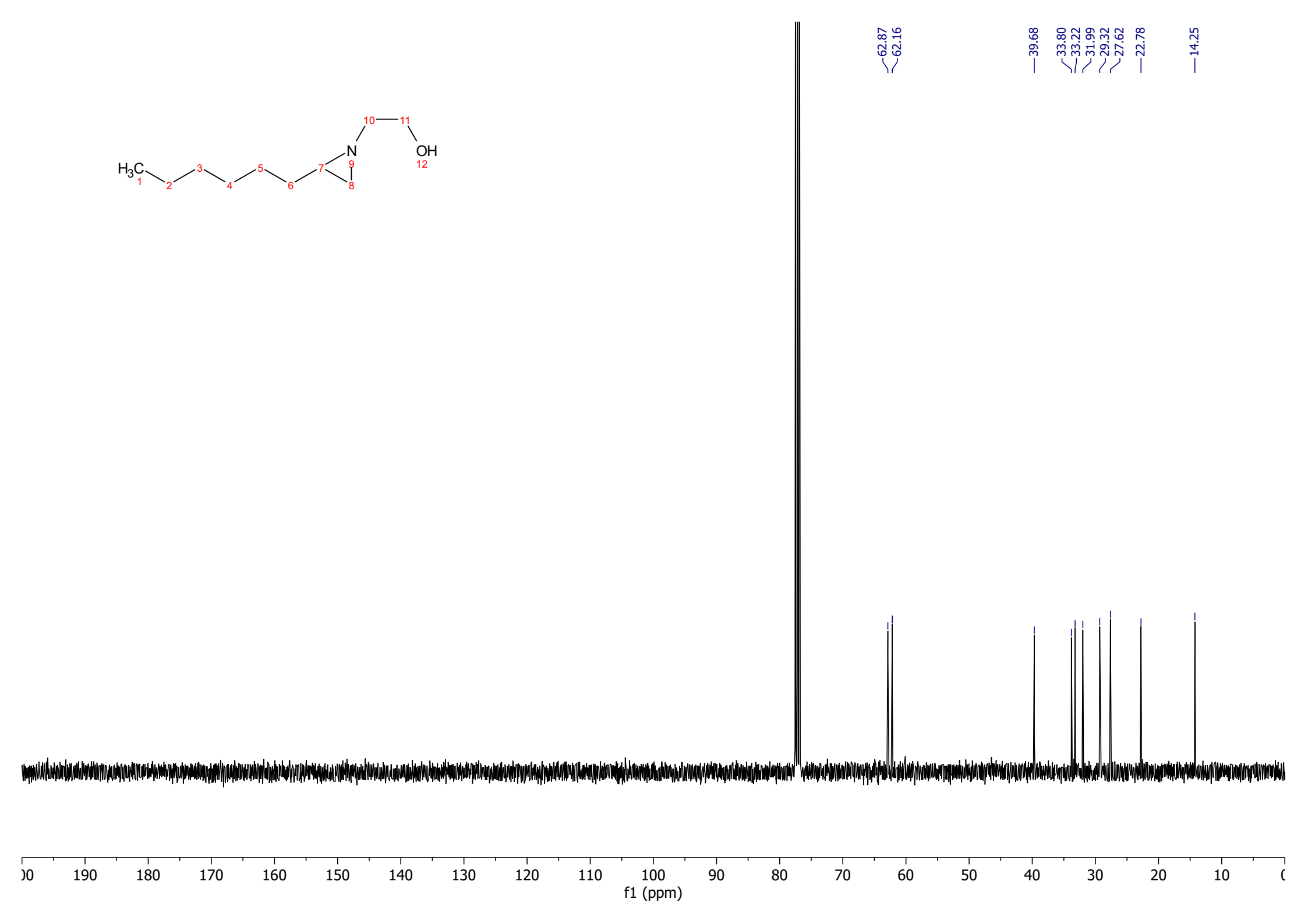

8.14
7.61
7.59
7.59
7.35
7.33
7.20
7.19
7.18
7.18
7.18
7.17
7.17
7.12
7.12
7.11
7.11
7.11
7.00
6.99
3.06
3.06
3.05
3.05
3.04
3.04
3.04
3.03
3.03
3.02
2.67
2.66
2.65
2.65
2.64
2.64
2.63
2.62
2.53
2.52
2.51
2.51
2.50
2.50
2.49
1.56
1.55
1.46
1.39
1.39
1.39
1.38
1.33
1.32
1.32
1.31
1.30
1.29
1.29
1.29
1.28
1.25
1.24
0.90
0.89
H3C
1
2
3
4
5
6
7
N
9
8
10
11
12
13
NH
14
15
16
17
18
19
20
0.95
0.95
0.94
0.96
0.95
0.94
2.00
0.98
0.98
0.99
13.15
3.43
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

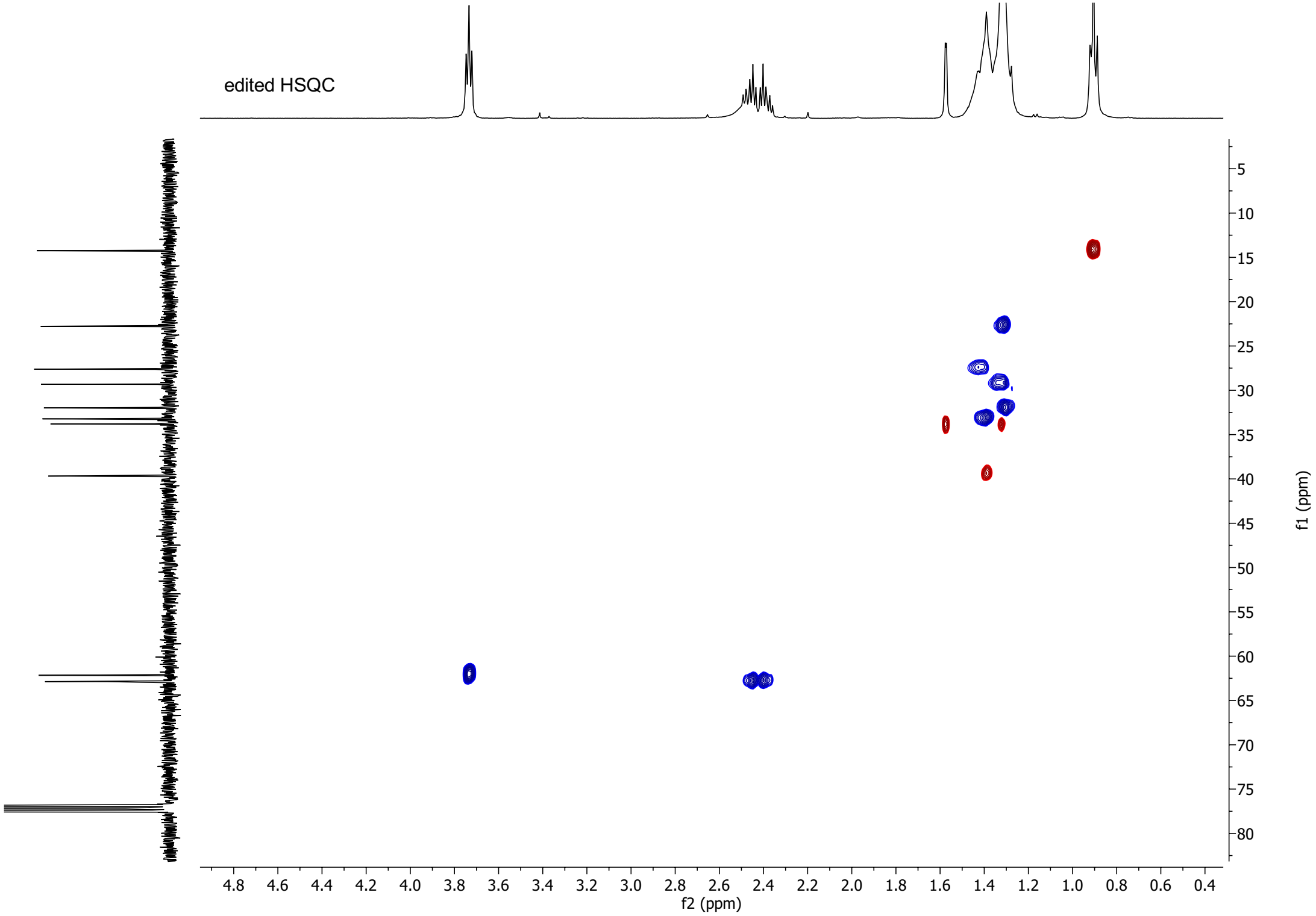

136.41
127.58
122.00
121.72
119.27
118.92
114.30
111.23
62.14
39.92
33.98
33.31
32.00
29.31
27.70
25.93
22.76
14.24
H3C
N
NH
f1 (ppm)

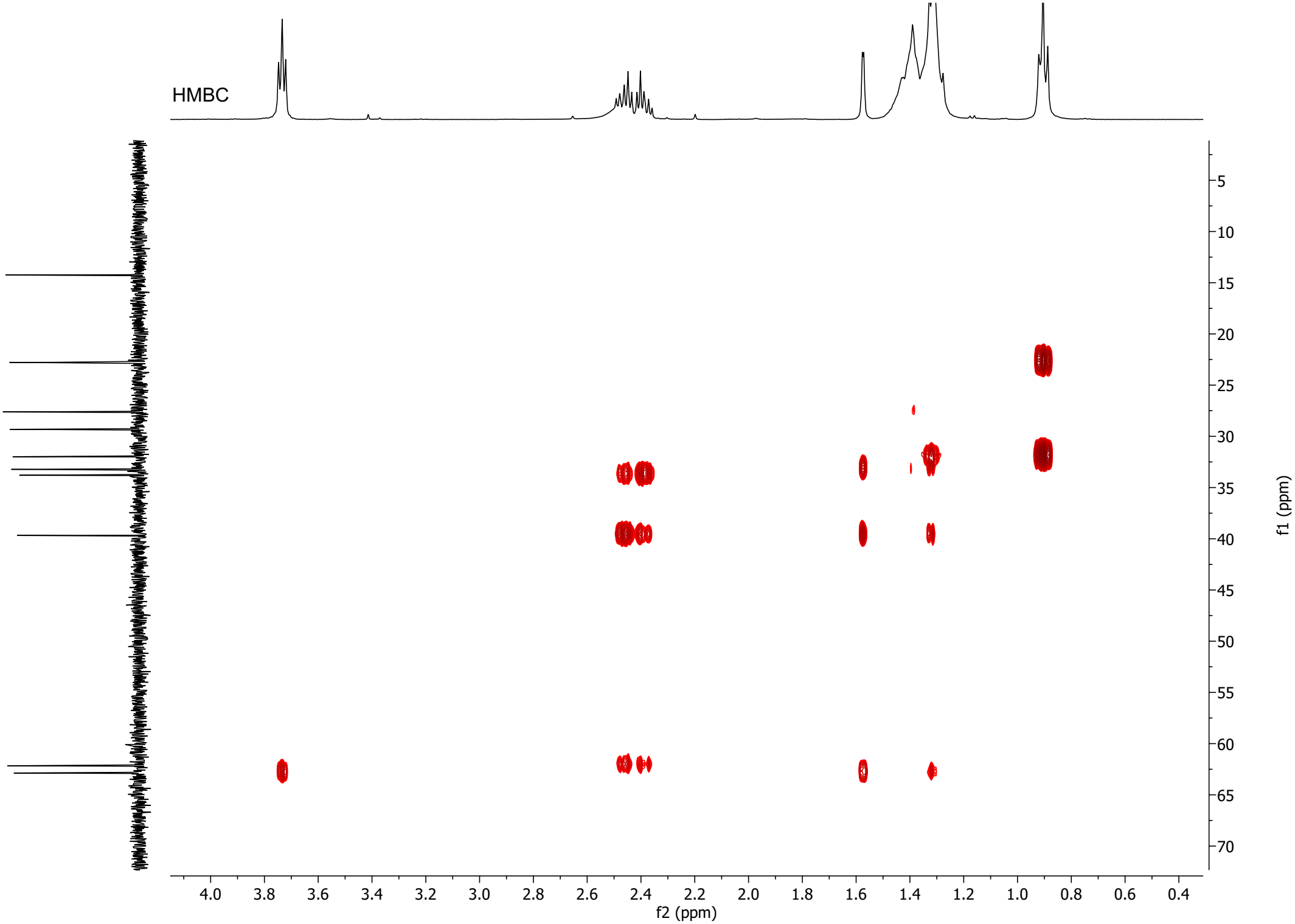

8.52 8.52 7.92 7.92 7.91 7.90 7.29 7.28 7.26 6.32 6.32 6.28 6.28 6.05
3.89 3.62 3.61 2.30 2.30 2.18 2.17 1.71 1.71 1.70 1.69 1.69 1.35 1.34 1.34 1.32 1.31 1.29 1.28 1.28 1.26 1.26 1.25 0.88 0.87 0.87 0.85
H3C 1 2 3 4 5 6 7 N 9 8 10 11 CH3 15 12 13 NH 14 17 16 O 18 26 H3C 27 19 20 21 N 25 24 22 23
1.00 1.03 1.04 0.98 1.03 0.97 3.06 1.01 0.99 0.99 4.51 1.08 16.54 1.01 3.36
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

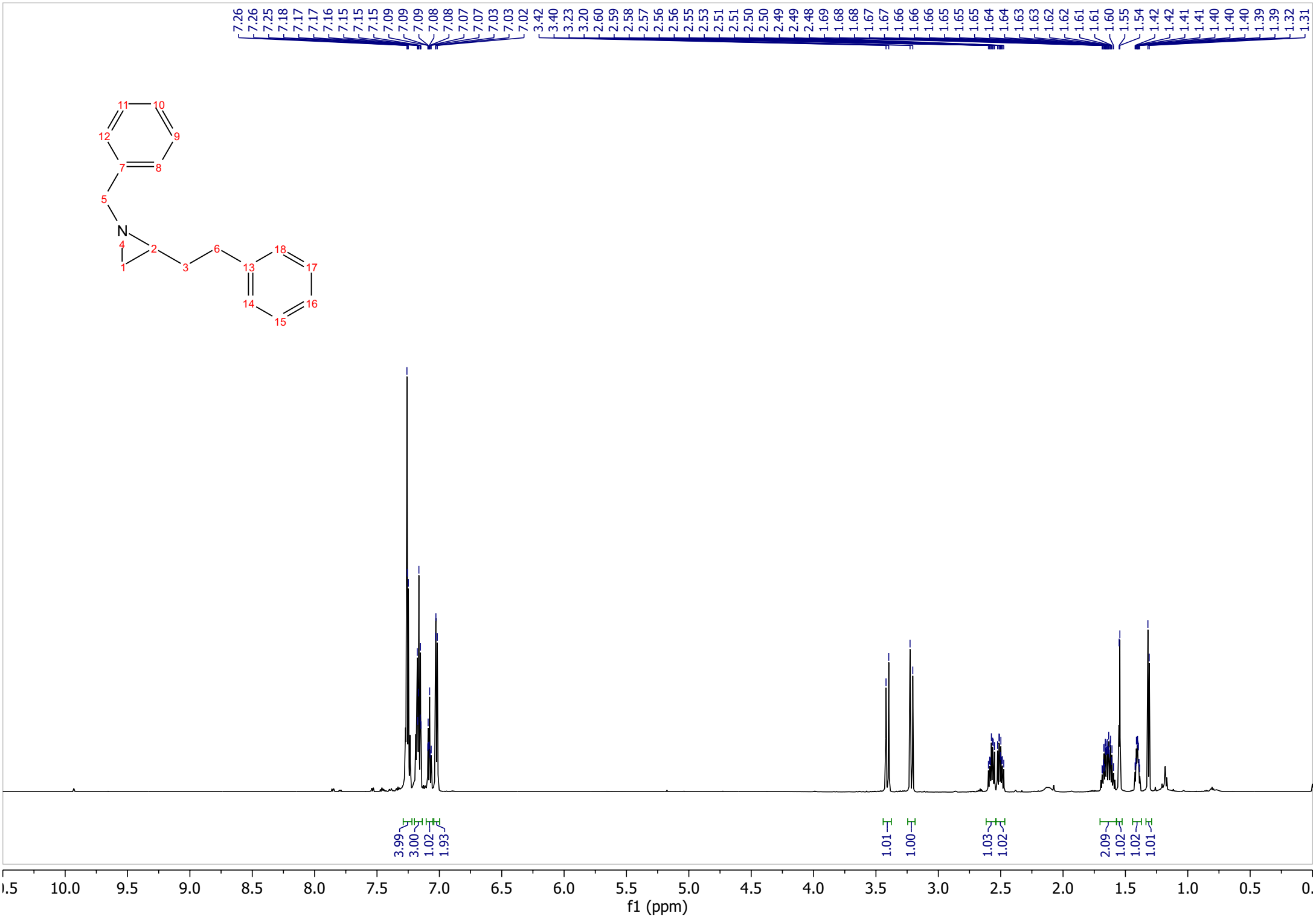

159.61
145.27
144.38
135.57
134.85
130.03
121.93
96.75
91.64
61.59
61.52
55.34
48.30
48.16
39.81
39.76
34.78
34.69
34.03
33.98
33.25
31.97
29.29
27.69
27.68
26.77
26.64
22.76
20.64
14.22
f1 (ppm)

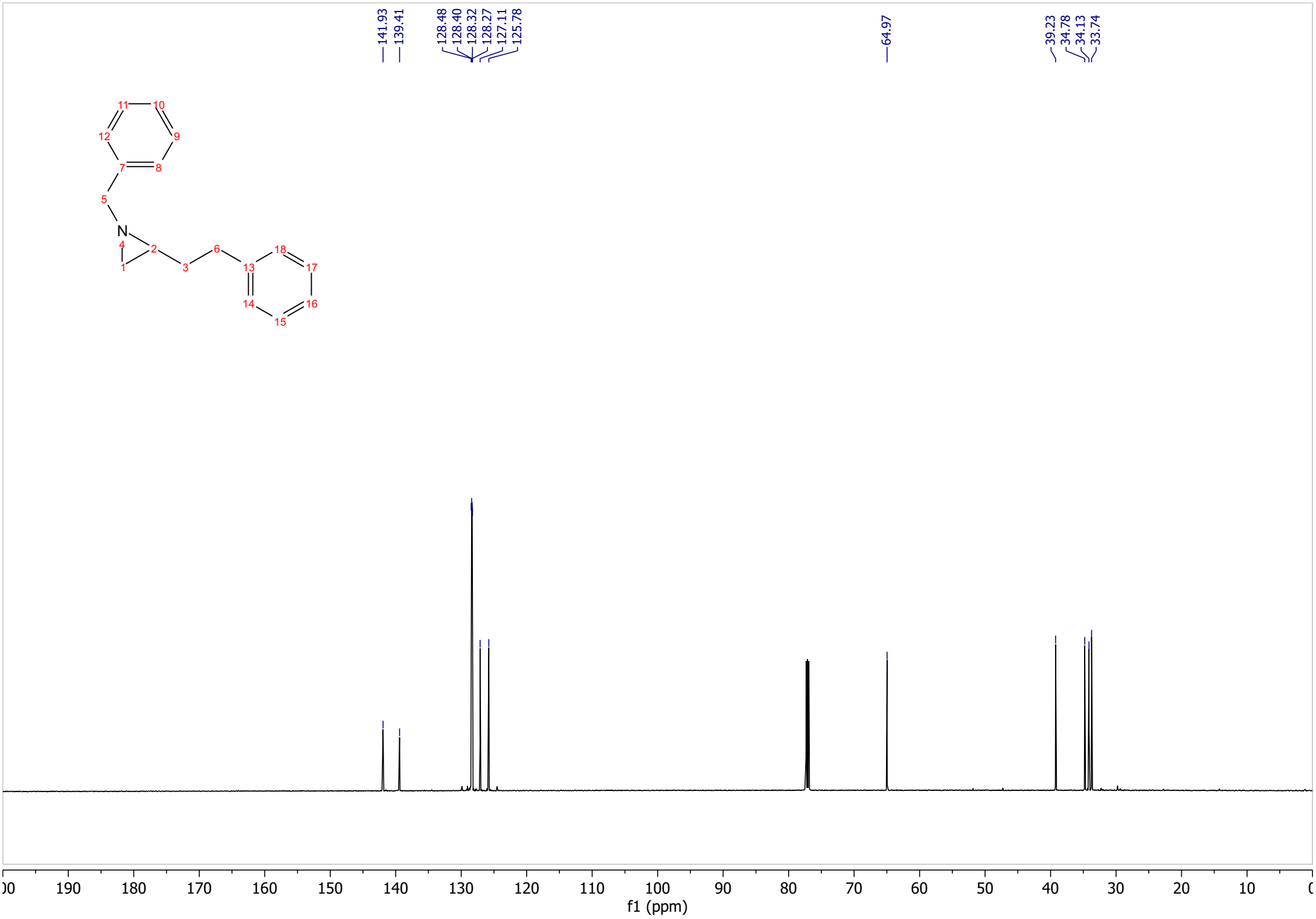

3.75
3.73
3.72
2.49
2.48
2.46
2.45
2.43
2.41
2.40
2.39
2.38
2.37
2.36
1.58
1.57
0.92
0.91
0.89
H3C
1
2
3
4
5
6
7
8
N
9
10
11
OH
12
2.00
2.89
0.99
12.49
3.16
f1 (ppm)


62.87
62.16
39.68
33.80
33.22
31.99
29.32
27.62
22.78
14.25
H3C
1
2
3
4
5
6
7
8
N
9
10
11
OH
12
f1 (ppm)


edited HSQC
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
f2 (ppm)
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
f1 (ppm)


HMBC
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
f2 (ppm)
5
10
15
20
25
30
35
40
45
50
55
60
65
70
f1 (ppm)


7.26 7.26 7.25 7.18 7.17 7.17 7.16 7.15 7.15 7.15 7.09 7.09 7.09 7.08 7.08 7.07 7.07 7.03 7.02
3.42 3.40 3.23 3.20 2.60 2.59 2.58 2.57 2.56 2.56 2.55 2.53 2.51 2.51 2.50 2.50 2.49 2.49 2.48 1.69 1.68 1.68 1.67 1.67 1.66 1.66 1.65 1.65 1.65 1.64 1.64 1.63 1.63 1.62 1.61 1.61 1.60 1.55 1.54 1.42 1.42 1.41 1.41 1.40 1.40 1.40 1.39 1.39 1.32 1.31
N
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
3.99 3.00 1.02 1.93
1.01 1.00
1.03 1.02
2.09 1.02 1.02 1.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)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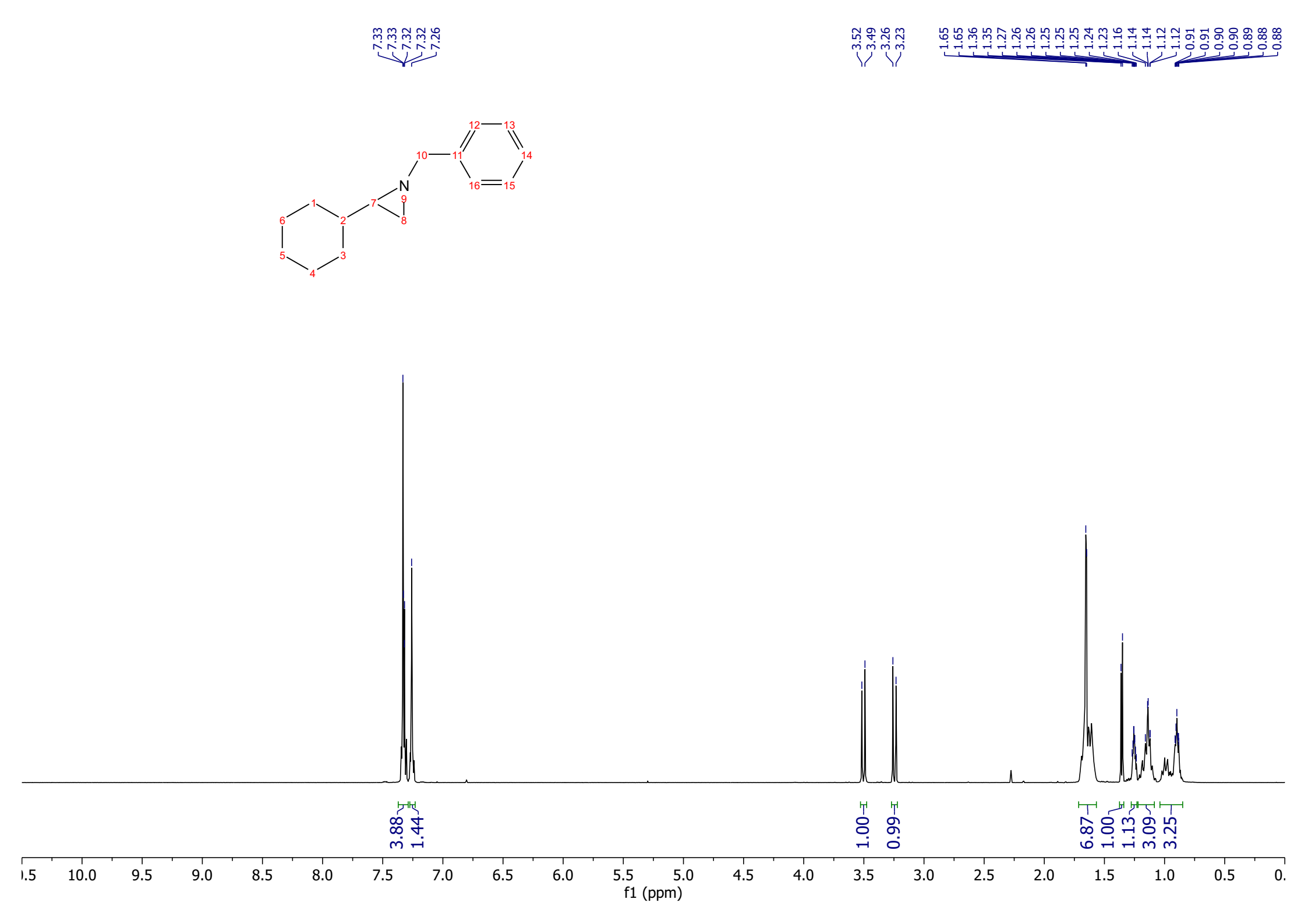
128.32
128.27
127.11
125.78
64.97
39.23
34.78
34.13
33.74
11
10
12
9
7
8
5
N
4
2
6
18
17
1
3
13
14
16
15
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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3.52
3.49
3.26
3.23
1.65
1.65
1.36
1.35
1.27
1.26
1.26
1.25
1.25
1.25
1.24
1.23
1.16
1.14
1.14
1.12
1.12
0.91
0.91
0.90
0.90
0.89
0.88
0.88
N
1
2
3
4
5
6
7
8
9
10
11
12
13
14
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16
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1.44
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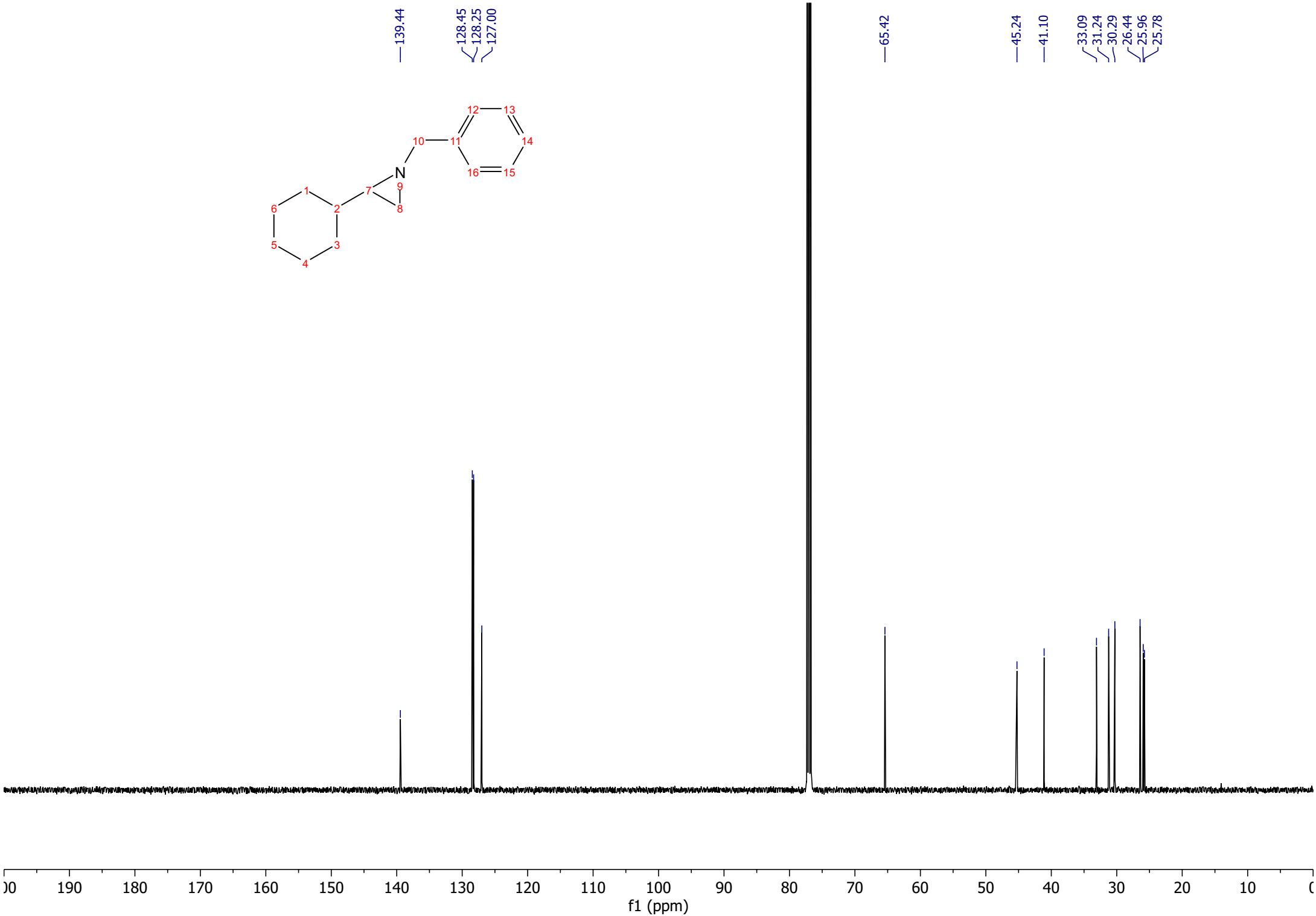
6.87
1.00
1.13
3.09
3.25
f1 (ppm)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128.45
128.25
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45.24
41.10
33.09
31.24
30.29
26.44
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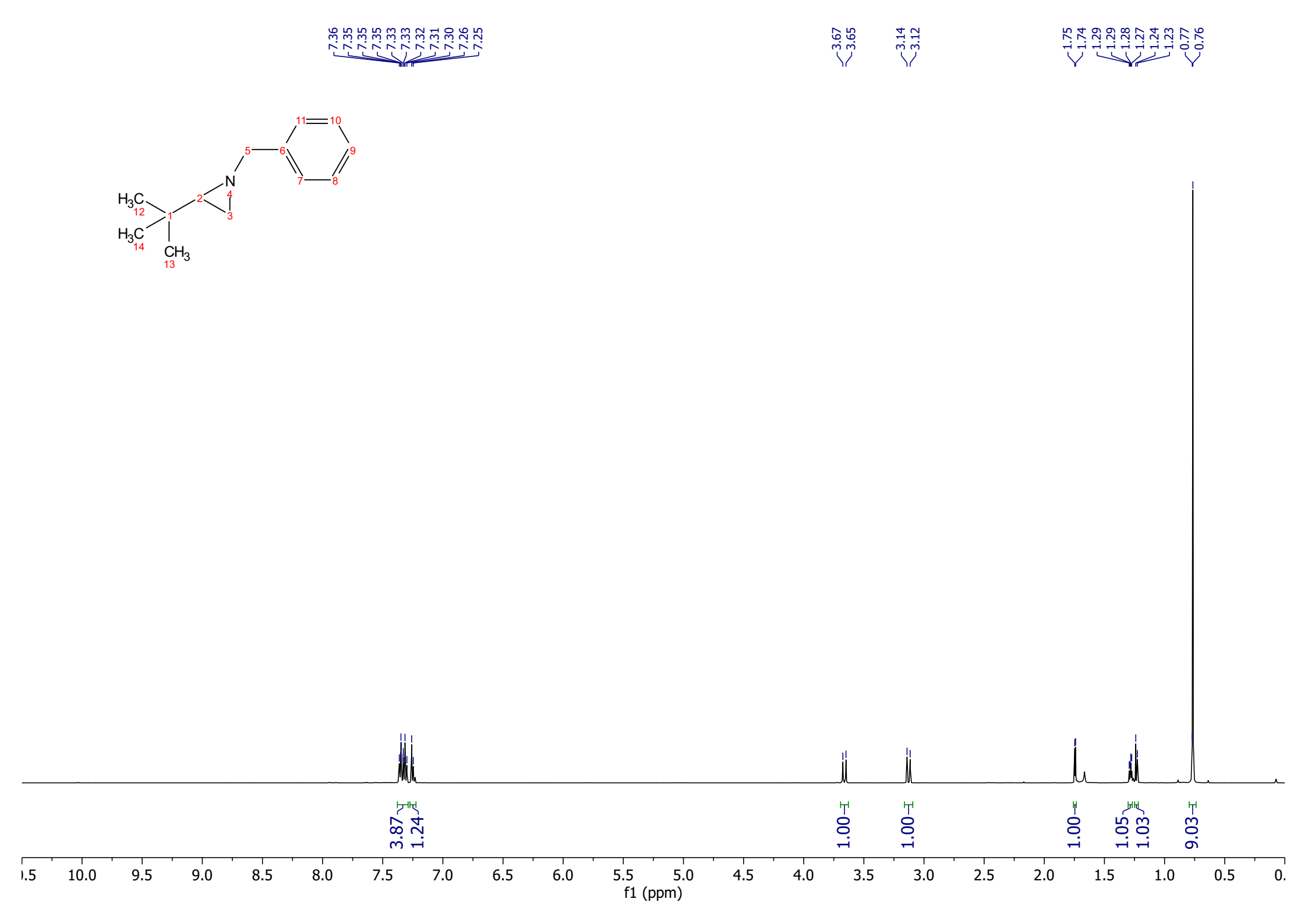
25.78
N
f1 (ppm)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7.31
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7.26
7.25
3.67
3.65
3.14
3.12
1.75
1.74
1.29
1.29
1.28
1.27
1.24
1.23
0.77
0.76
11
10
9
8
7
6
5
N
4
2
3
1
H3C
12
H3C
14
CH3
13
3.87
1.24
1.00
1.00
1.00
1.05
1.03
9.03
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
3.5
3.0
2.5
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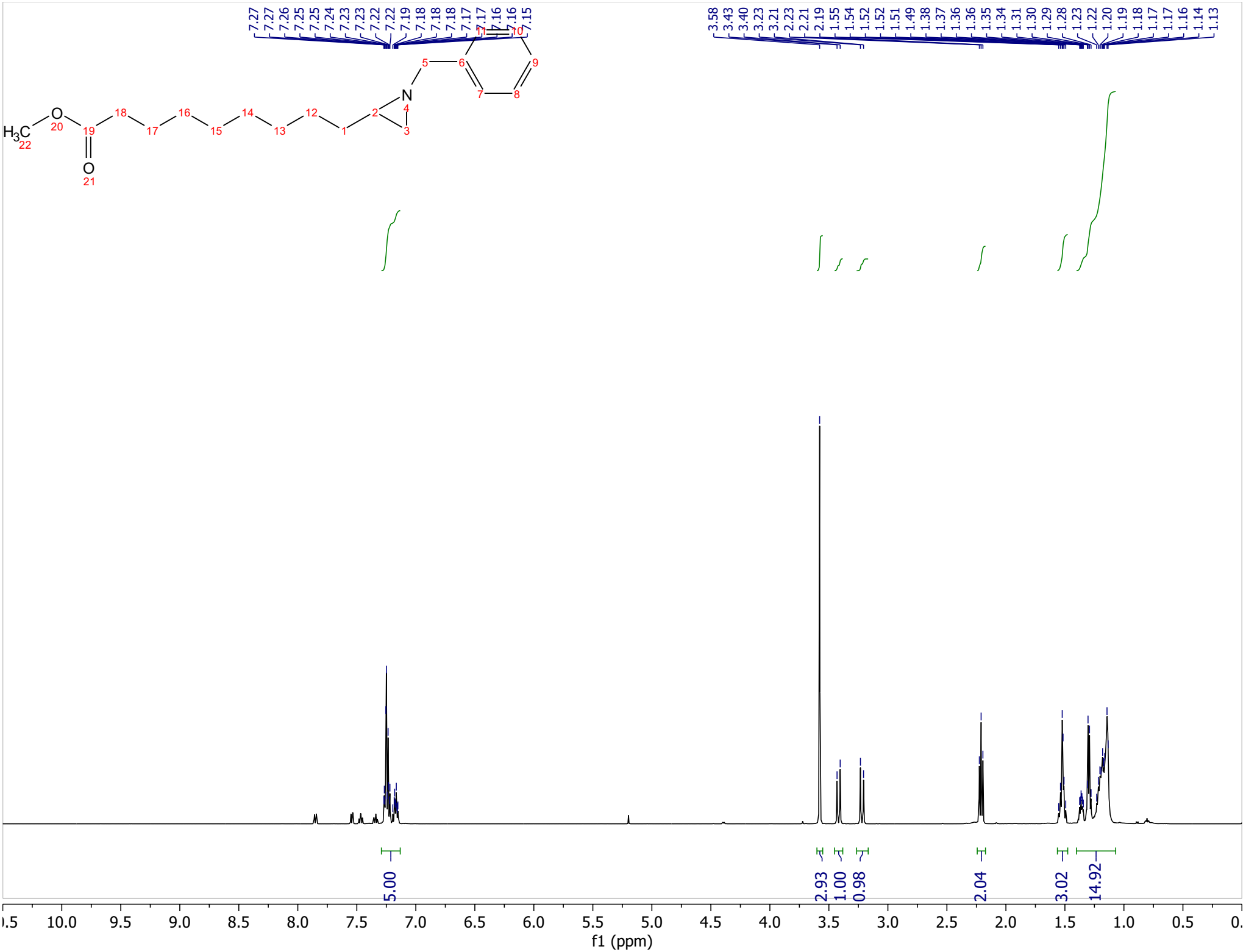
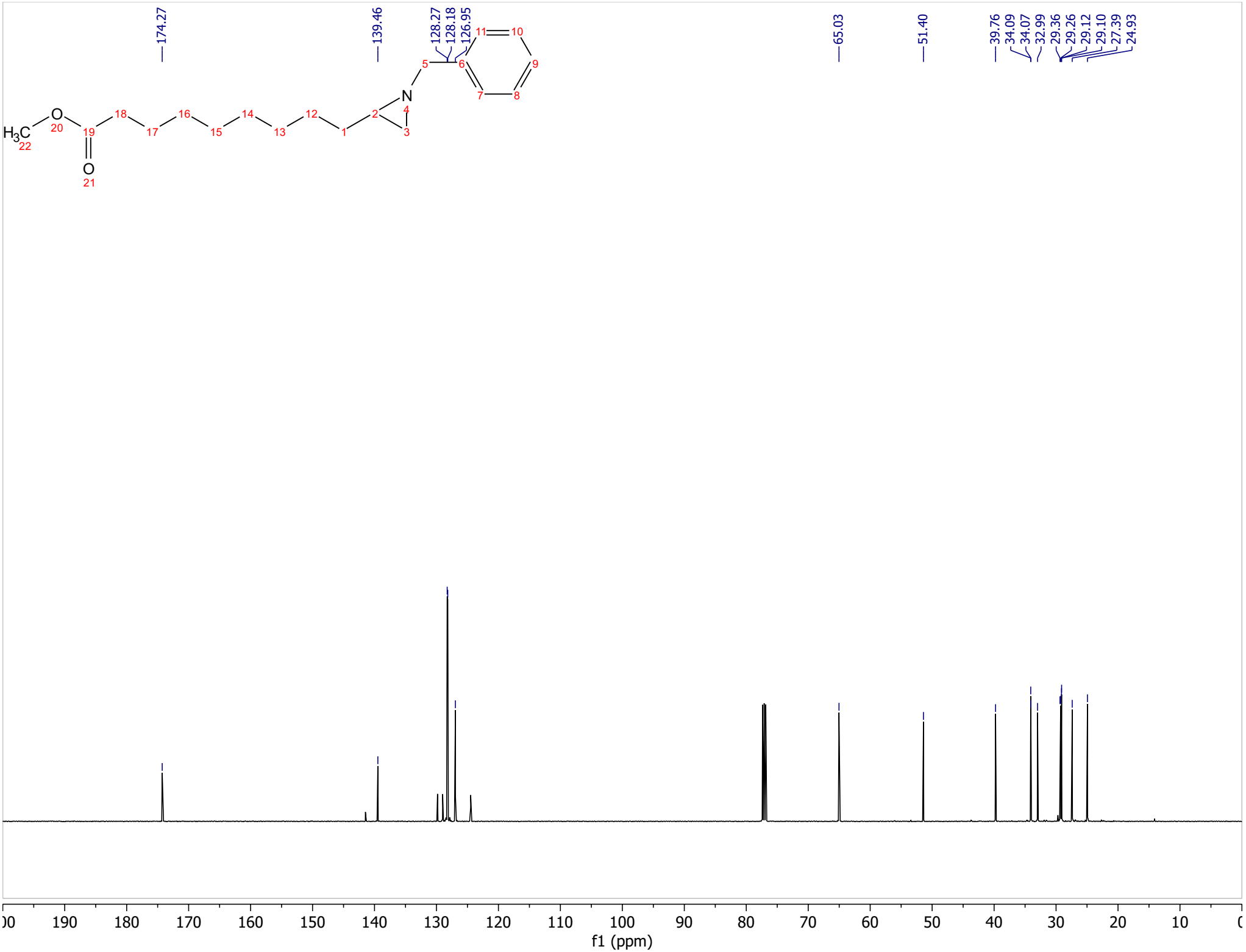
1.5
1.0
0.5
f1 (ppm)


7.27 7.27 7.26 7.25 7.25 7.24 7.23 7.23 7.22 7.22 7.19 7.18 7.18 7.17 7.17 7.16 7.16 7.15
3.58 3.43 3.40 3.23 3.21 2.23 2.21 2.19 1.55 1.54 1.52 1.52 1.51 1.49 1.38 1.37 1.36 1.36 1.35 1.34 1.31 1.30 1.29 1.28 1.23 1.22 1.20 1.19 1.18 1.17 1.17 1.16 1.14 1.13
H3C
O
O
N
5.00
2.93
1.00
0.98
2.04
3.02
14.92
f1 (ppm)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65.03
51.40
39.76
34.09
34.07
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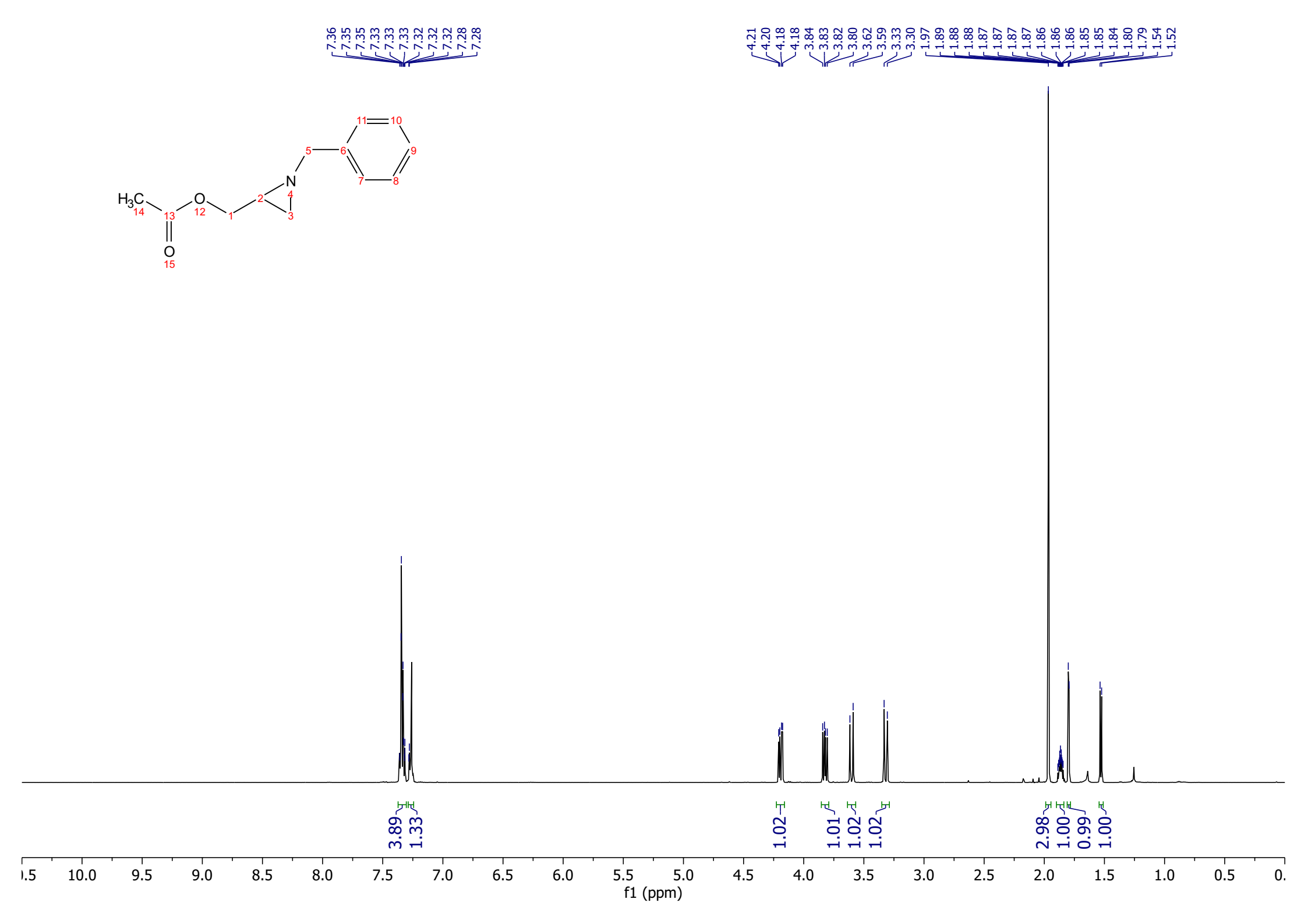
29.36
29.26
29.12
29.10
27.39
24.93
H3C
O
O
N
f1 (ppm)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7.35
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7.33
7.32
7.32
7.32
7.28
7.28
4.21
4.20
4.18
4.18
3.84
3.83
3.82
3.80
3.62
3.59
3.33
3.30
1.97
1.89
1.88
1.88
1.87
1.87
1.87
1.87
1.86
1.86
1.86
1.85
1.85
1.84
1.80
1.79
1.54
1.52
H3C
14
13
O
12
1
2
N
4
3
5
6
11
10
9
7
8
O
15
3.89
1.33
1.02
1.01
1.02
1.02
2.98
1.00
0.99
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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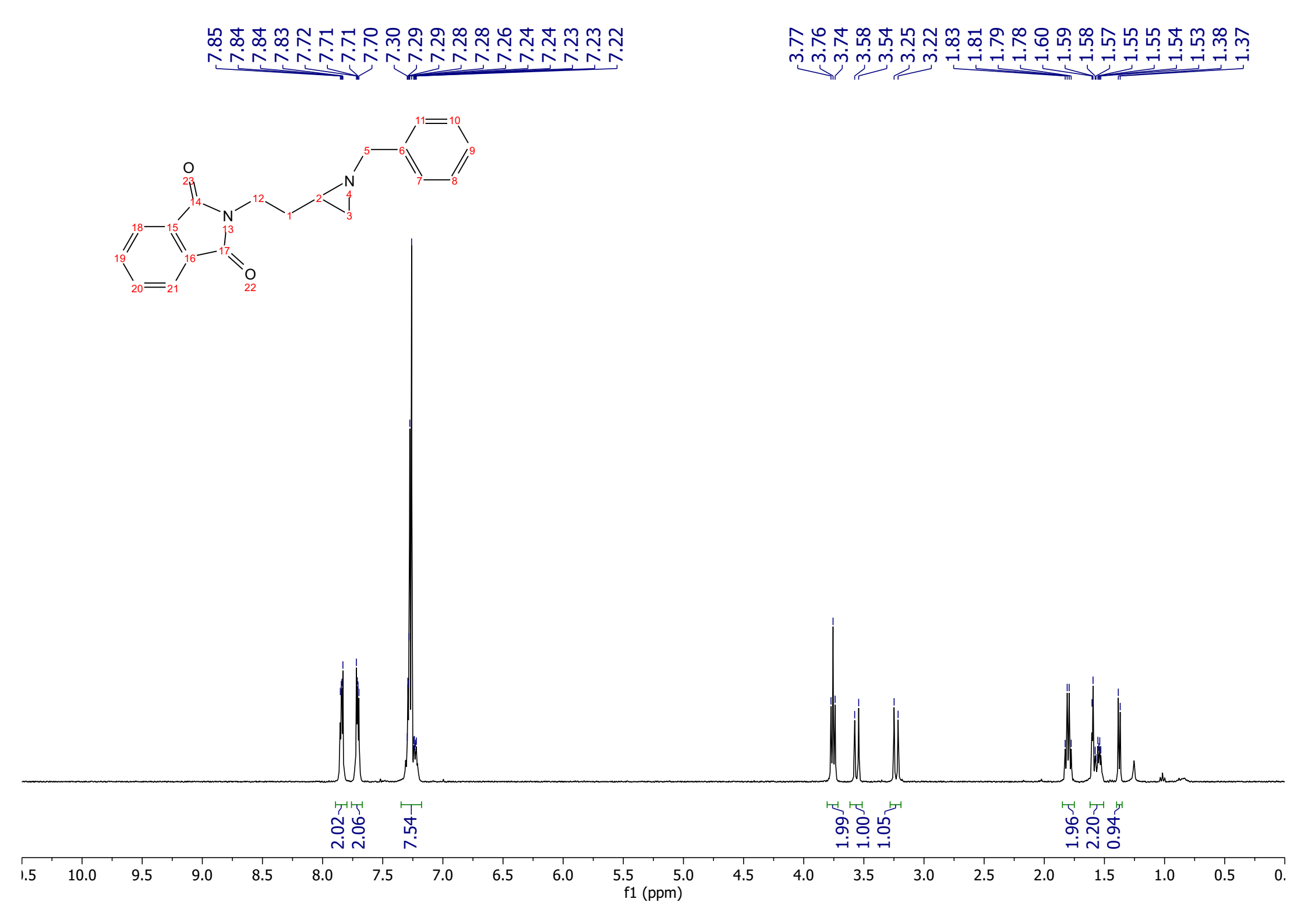
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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7.84
7.84
7.83
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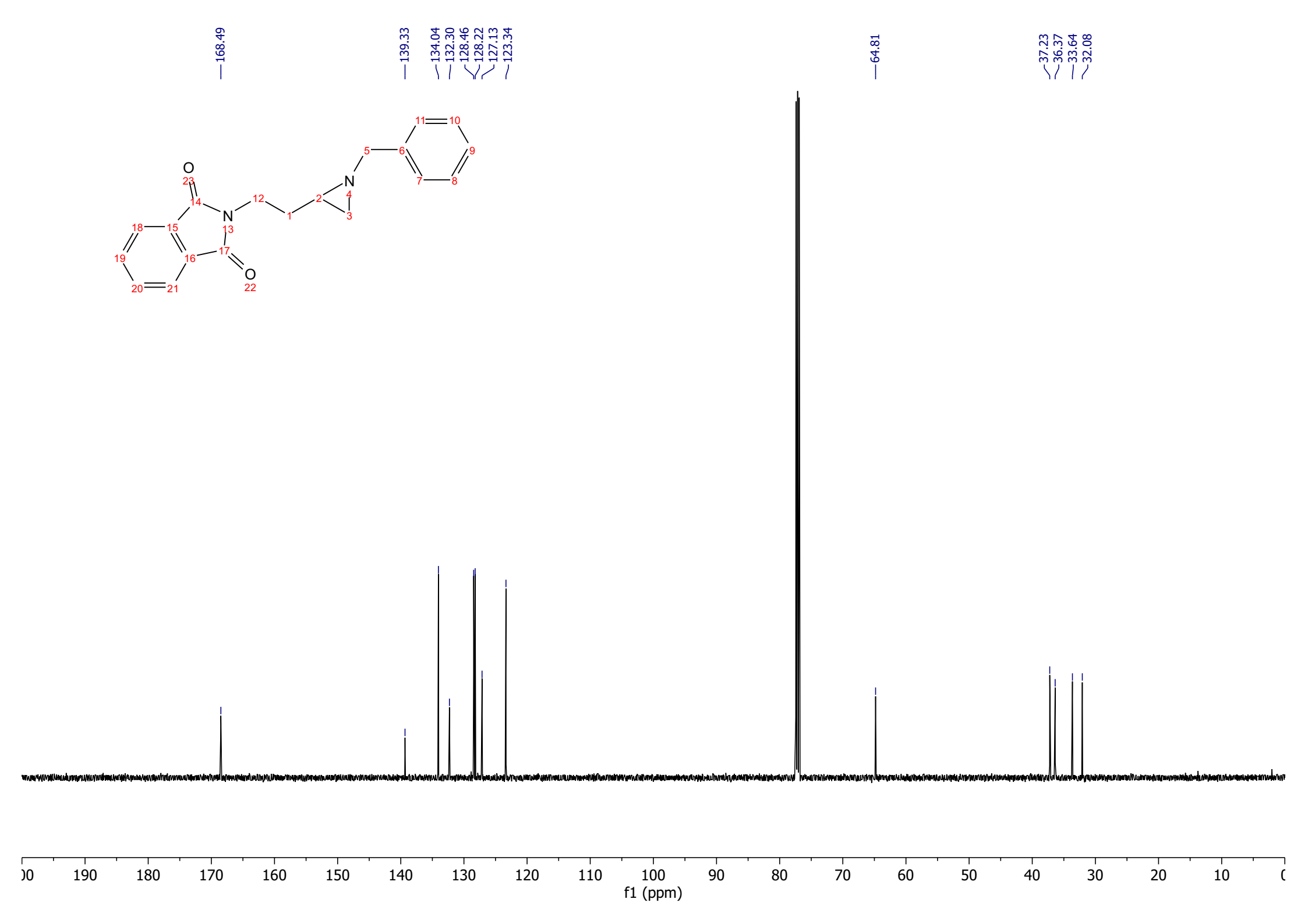
7.71
7.71
7.70
7.30
7.29
7.29
7.28
7.28
7.26
7.24
7.24
7.23
7.23
7.22
3.77
3.76
3.74
3.58
3.54
3.25
3.22
1.83
1.81
1.79
1.78
1.60
1.59
1.58
1.57
1.55
1.55
1.54
1.53
1.38
1.37
O
23
14
N
13
12
1
2
N
4
3
11
10
5
6
9
7
8
18
15
19
16
17
O
22
20
21
2.02
2.06
7.54
1.99
1.00
1.05
1.96
2.20
0.94
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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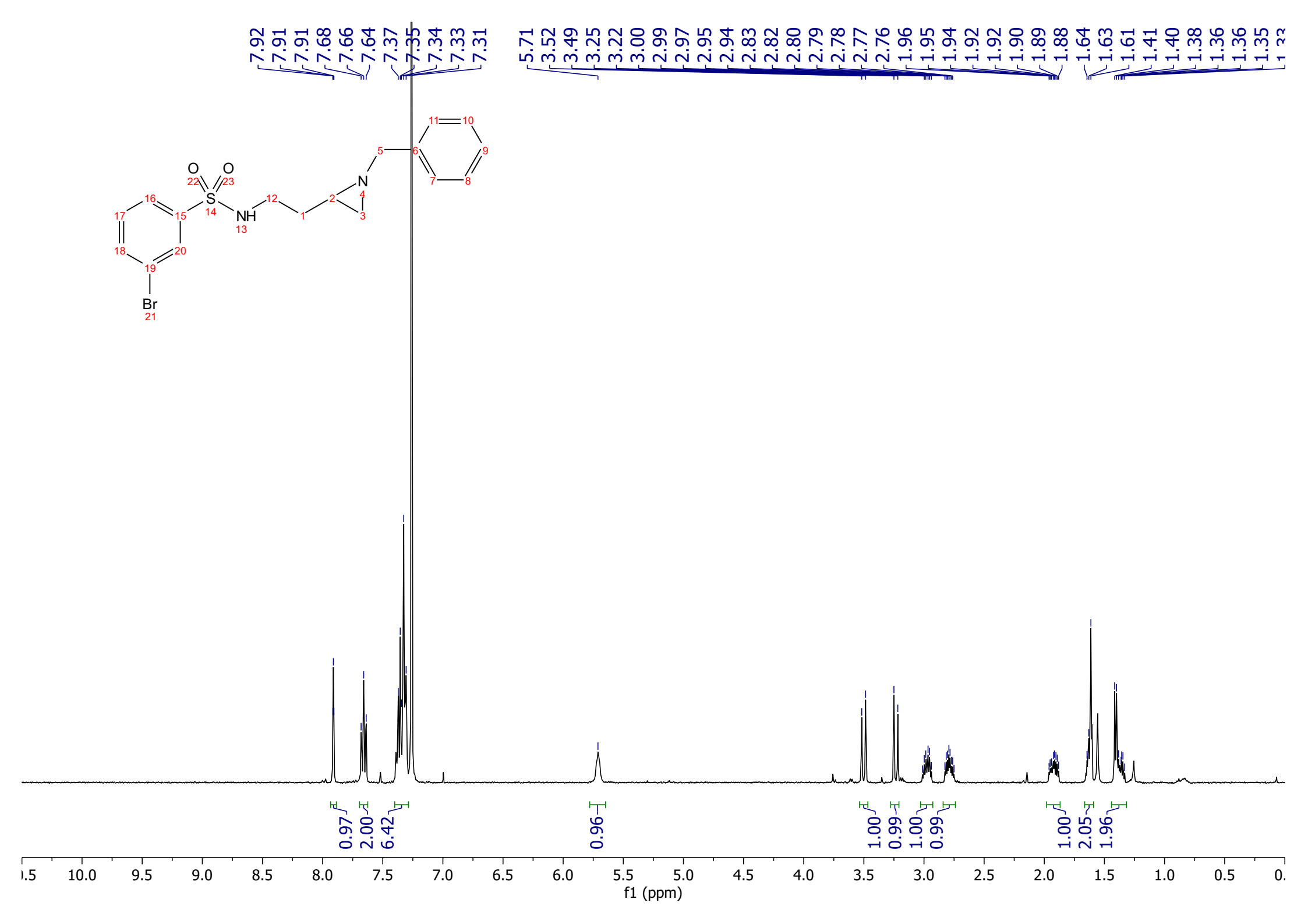
139.33
134.04
132.30
128.46
128.22
127.13
123.34
64.81
37.23
36.37
33.64
32.08
O
23
14
N
13
12
1
2
N
4
3
5
6
11
10
9
7
8
18
15
19
16
17
O
22
20
21
f1 (ppm)


7.92
7.91
7.91
7.68
7.66
7.64
7.37
7.35
7.34
7.33
7.31
5.71
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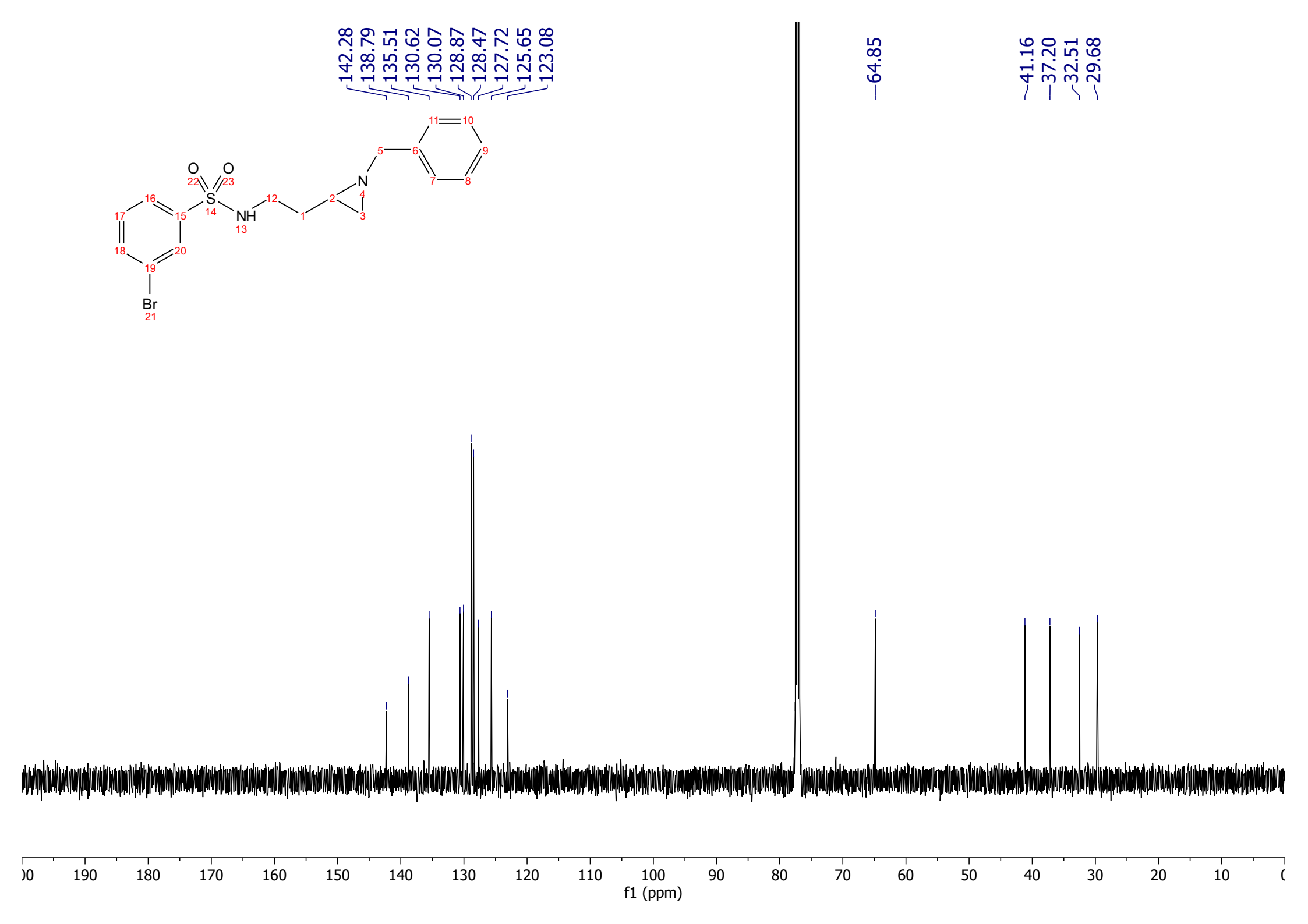
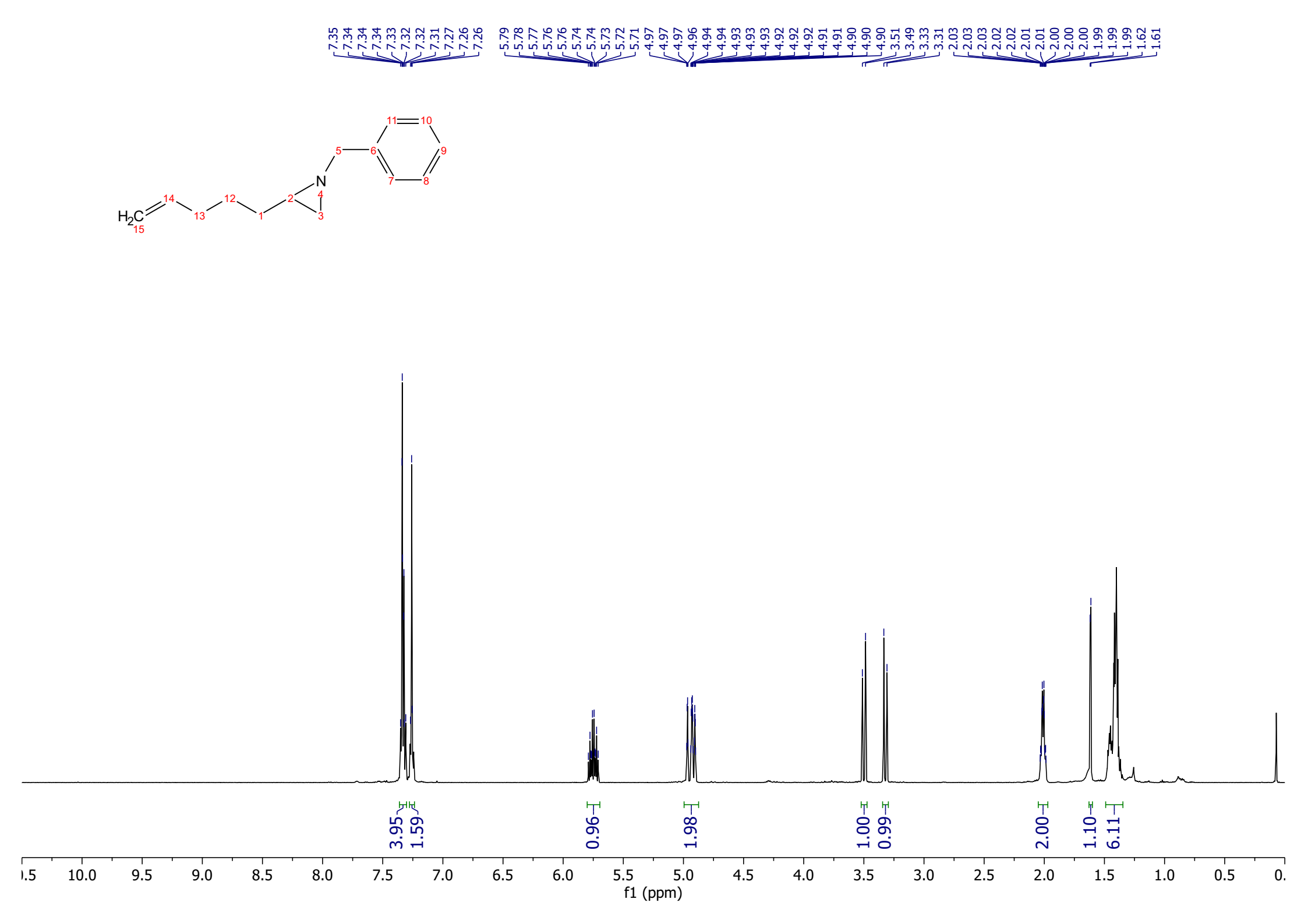
3.49
3.25
3.22
3.00
2.99
2.97
2.95
2.94
2.83
2.82
2.80
2.79
2.78
2.77
2.76
1.96
1.95
1.94
1.92
1.92
1.90
1.89
1.88
1.64
1.63
1.61
1.41
1.40
1.38
1.36
1.36
1.35
O
O
S
NH
N
Br
0.97
2.00
6.42
0.96
1.00
0.99
1.00
0.99
1.00
2.05
1.96
f1 (ppm)


142.28
138.79
135.51
130.62
130.07
128.87
128.47
127.72
125.65
123.08
64.85
41.16
37.20
32.51
29.68
O
O
S
NH
N
Br
f1 (ppm)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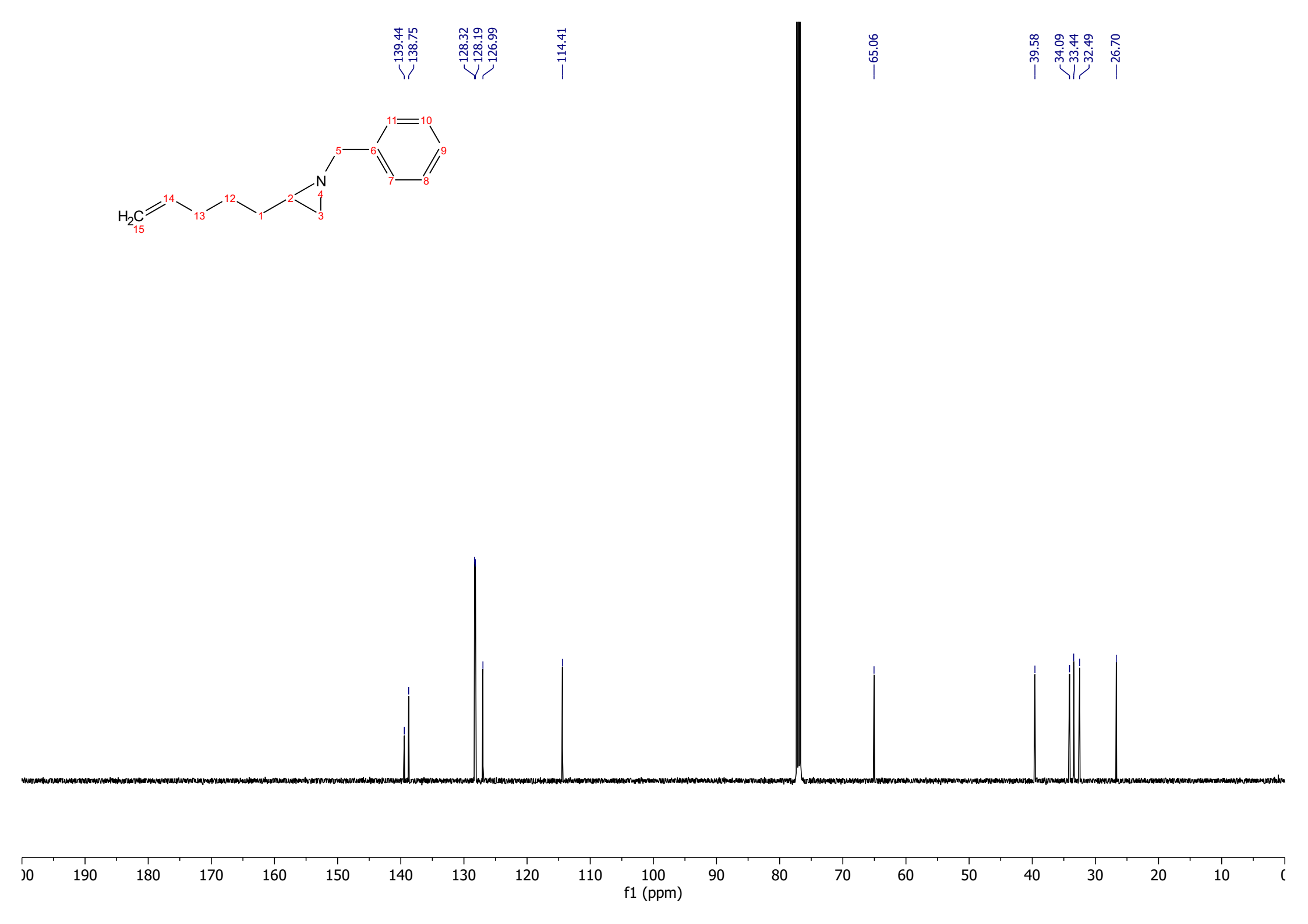
5.79 5.78 5.77 5.76 5.76 5.74 5.74 5.73 5.72 5.71
4.97 4.97 4.97 4.96 4.94 4.94 4.93 4.93 4.93 4.92 4.92 4.92 4.91 4.91 4.90 4.90 4.90
3.51 3.49 3.33 3.31
2.03 2.03 2.03 2.02 2.02 2.01 2.01 2.00 2.00 2.00 1.99 1.99 1.99 1.62 1.61
N
H2C
3.95
1.59
0.96
1.98
1.00
0.99
2.00
1.10
6.11
f1 (ppm)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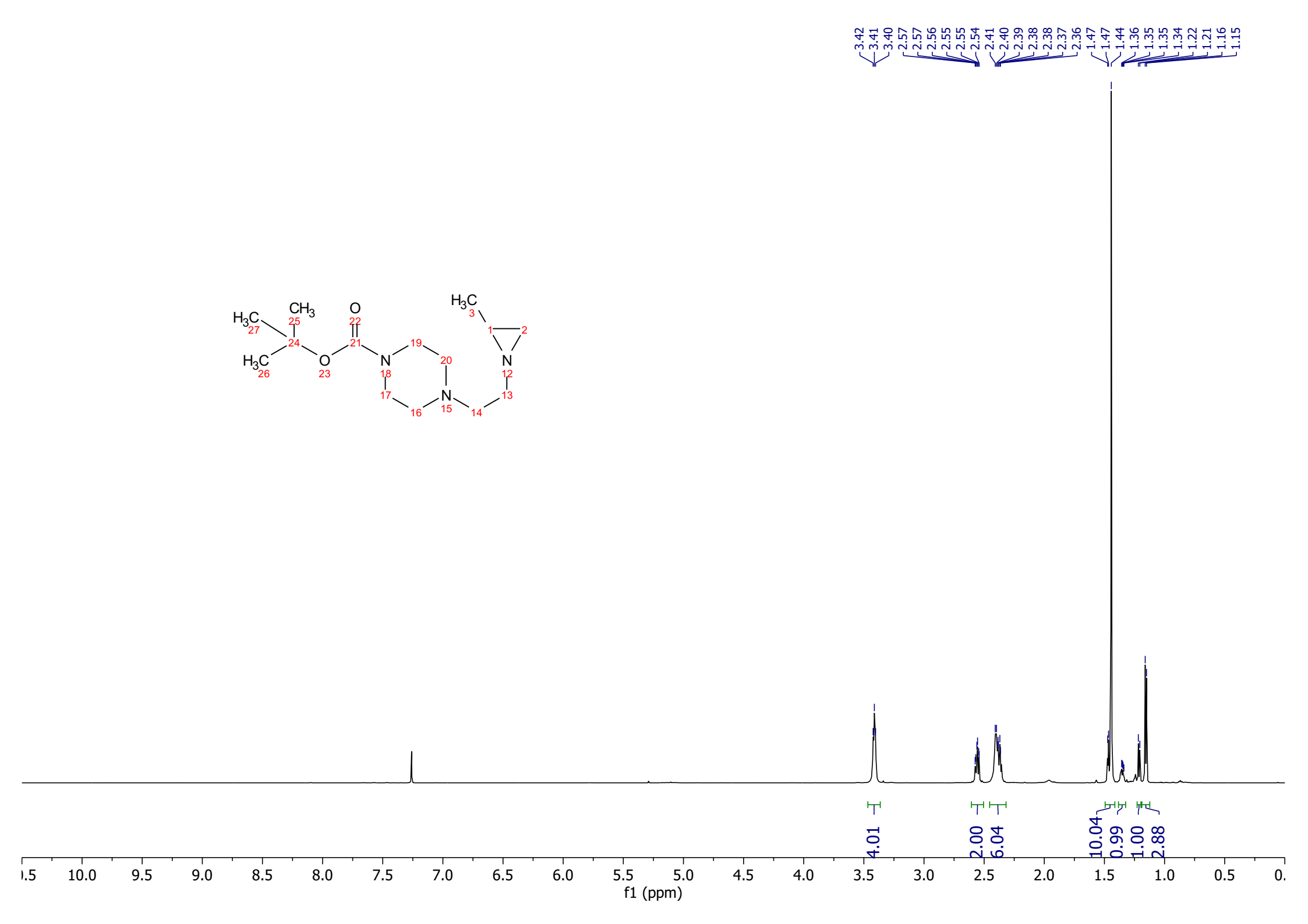
138.75
128.32
128.19
126.99
114.41
65.06
39.58
34.09
33.44
32.49
26.70
N
H_2C
f1 (ppm)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2.57
2.56
2.55
2.55
2.54
2.41
2.40
2.39
2.38
2.38
2.37
2.36
1.47
1.47
1.44
1.36
1.35
1.35
1.34
1.22
1.21
1.16
1.15
H3C
CH3
O
H3C
O
N
N
N
4.01
2.00
6.04
10.04
0.99
1.00
2.88
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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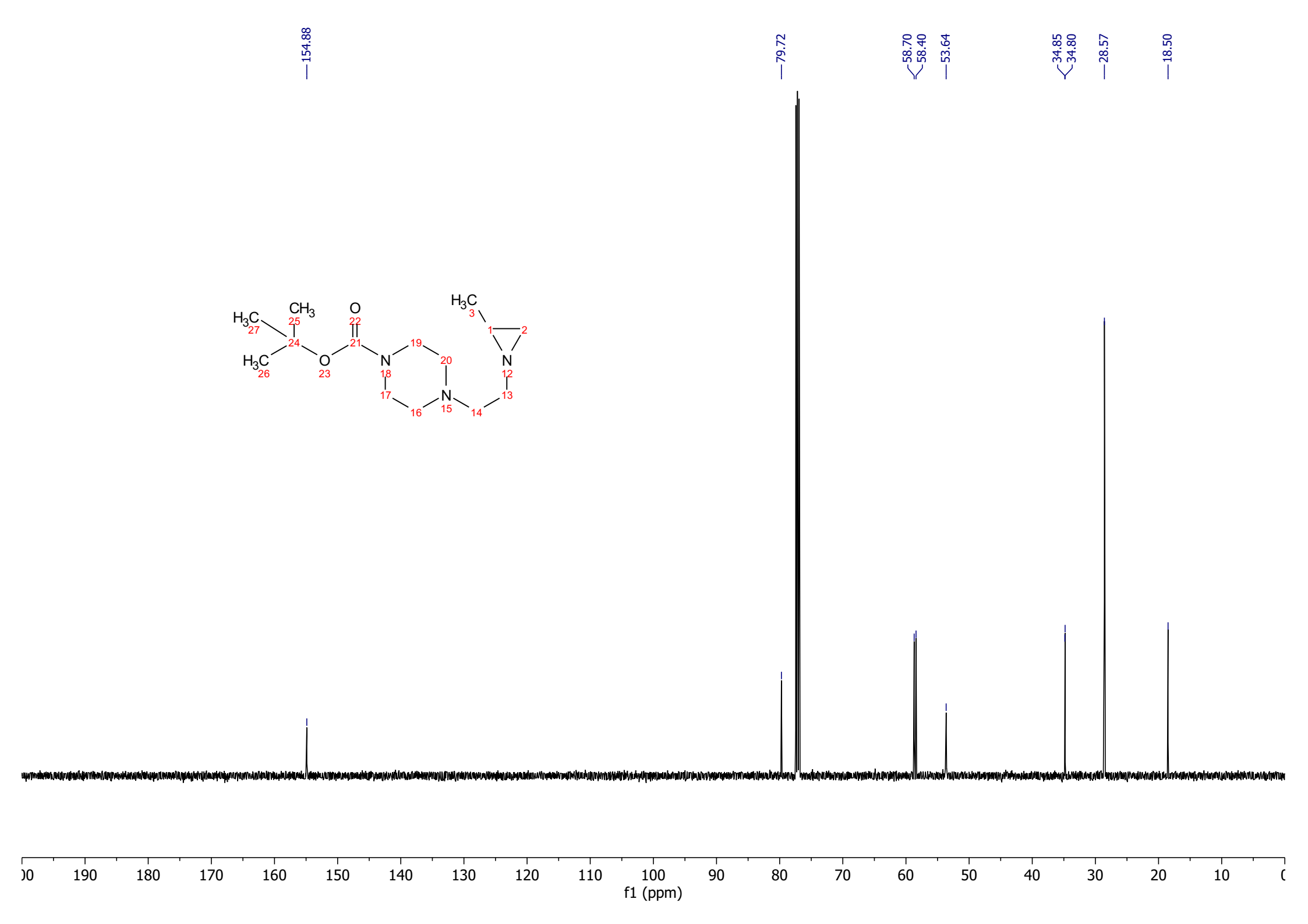
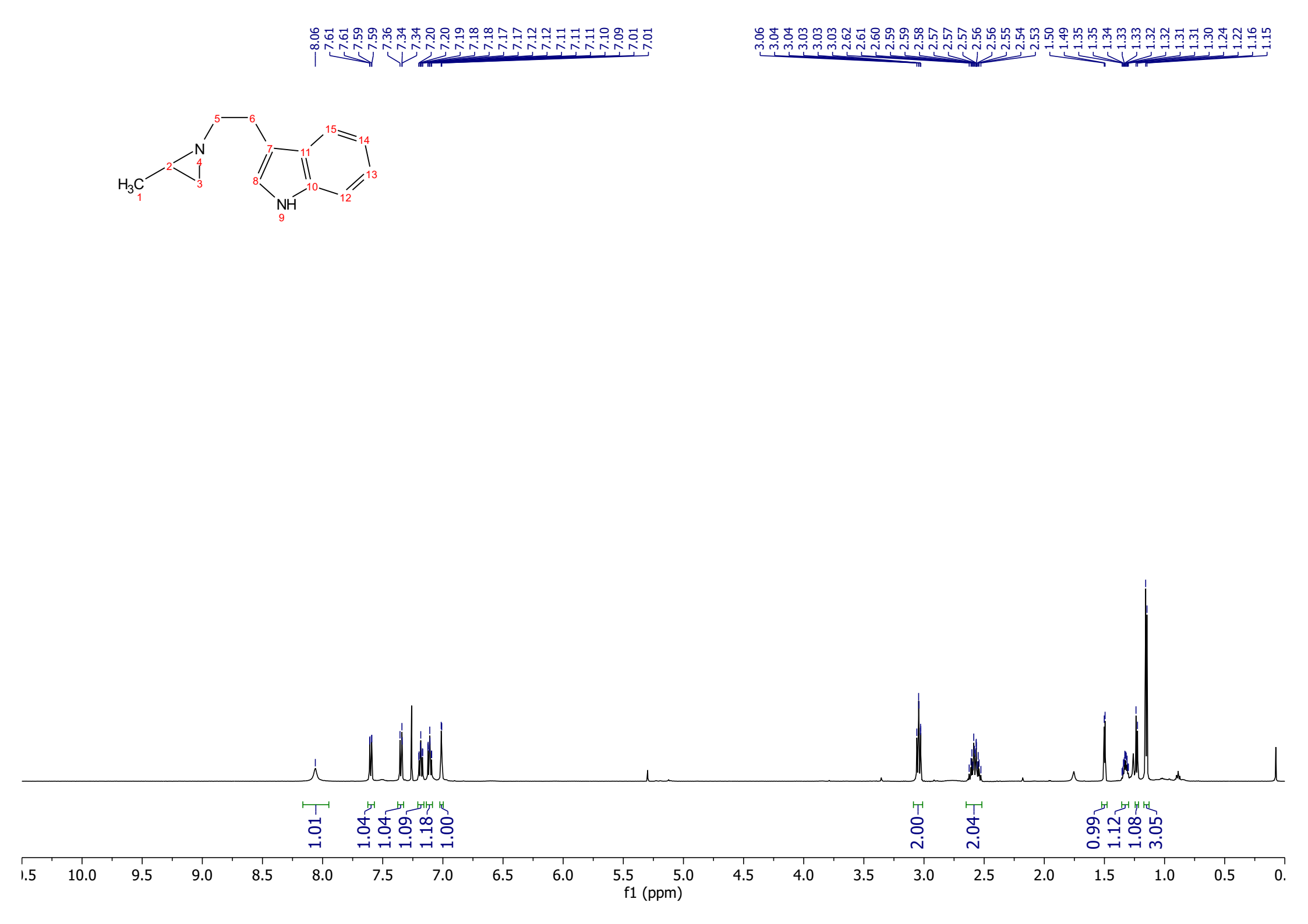
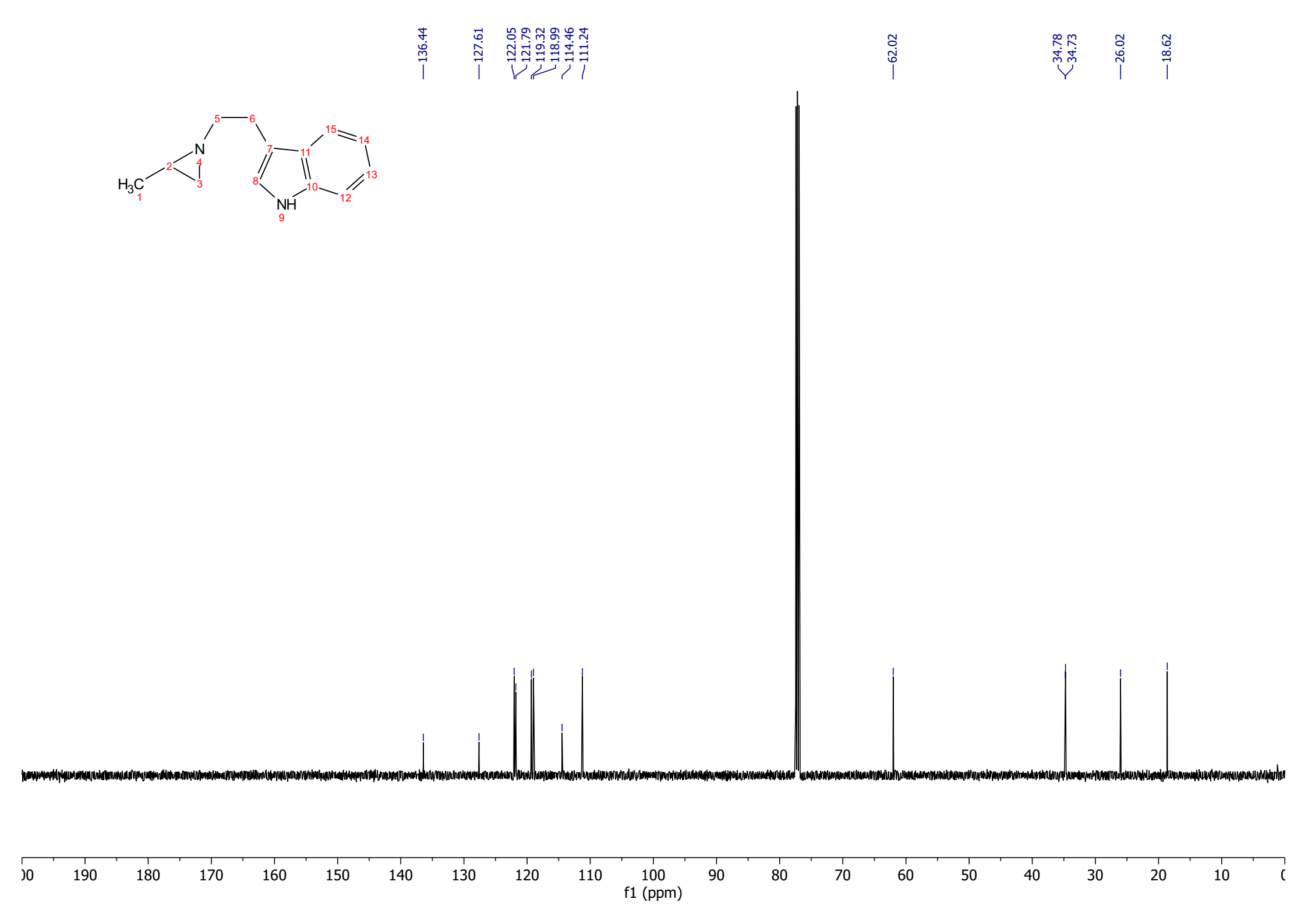
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


154.88
79.72
58.70
58.40
53.64
34.85
34.80
28.57
18.50
f1 (ppm)


8.06 7.61 7.61 7.59 7.59 7.36 7.34 7.34 7.20 7.20 7.19 7.18 7.18 7.17 7.17 7.12 7.12 7.11 7.11 7.11 7.10 7.09 7.01 7.01
3.06 3.04 3.04 3.03 3.03 3.03 2.62 2.61 2.60 2.59 2.59 2.58 2.57 2.57 2.57 2.56 2.56 2.55 2.54 2.53 1.50 1.49 1.35 1.35 1.34 1.33 1.33 1.32 1.32 1.31 1.31 1.30 1.24 1.22 1.16 1.15
H3C
N
NH
1.01 1.04 1.04 1.09 1.18 1.00 2.00 2.04 0.99 1.12 1.08 3.05
f1 (ppm)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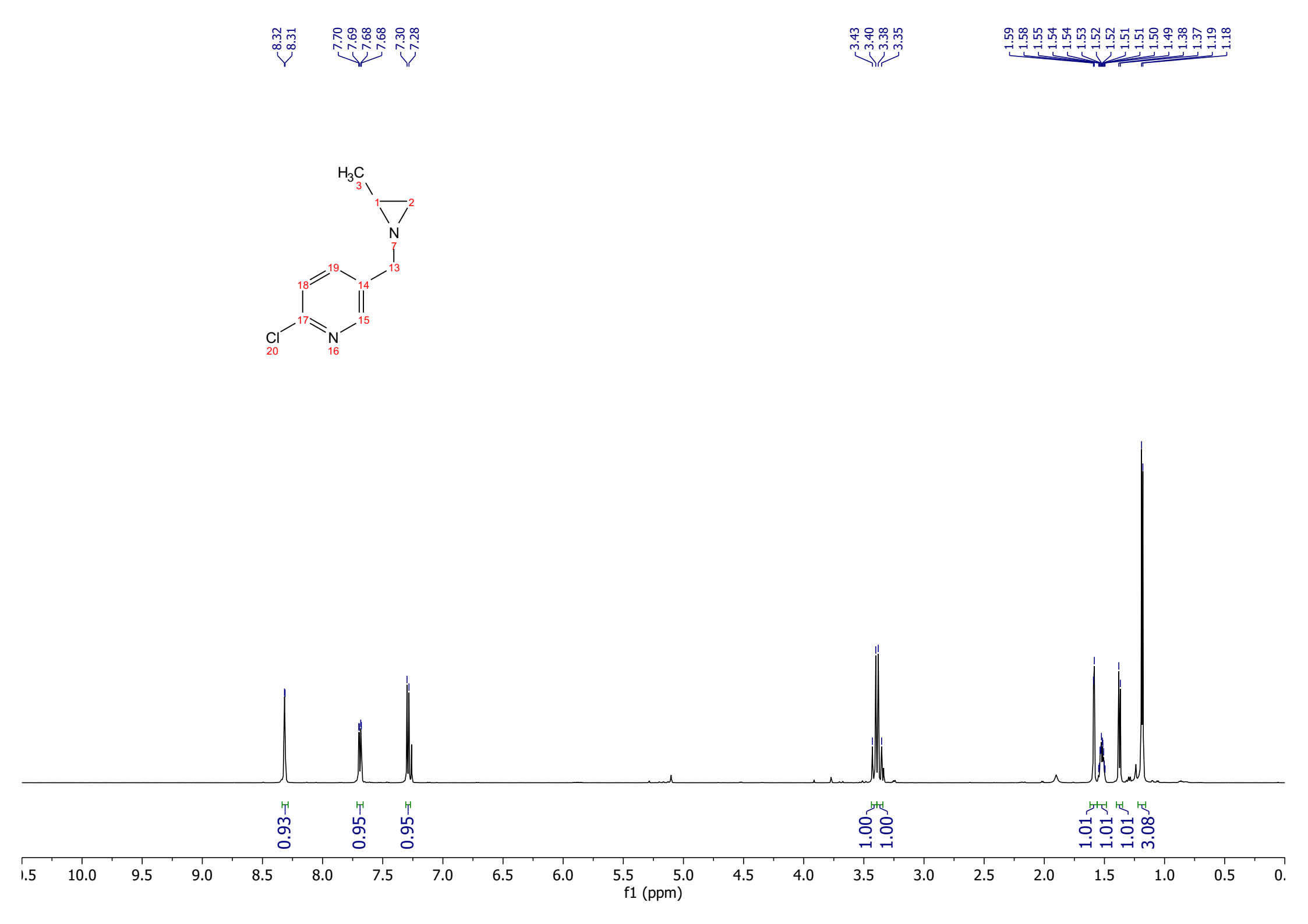
127.61
122.05
121.79
119.32
118.99
114.46
111.24
62.02
34.78
34.73
26.02
18.62
N
NH
H_3C
f1 (ppm)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7.69
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7.68
7.30
7.28
3.43
3.40
3.38
3.35
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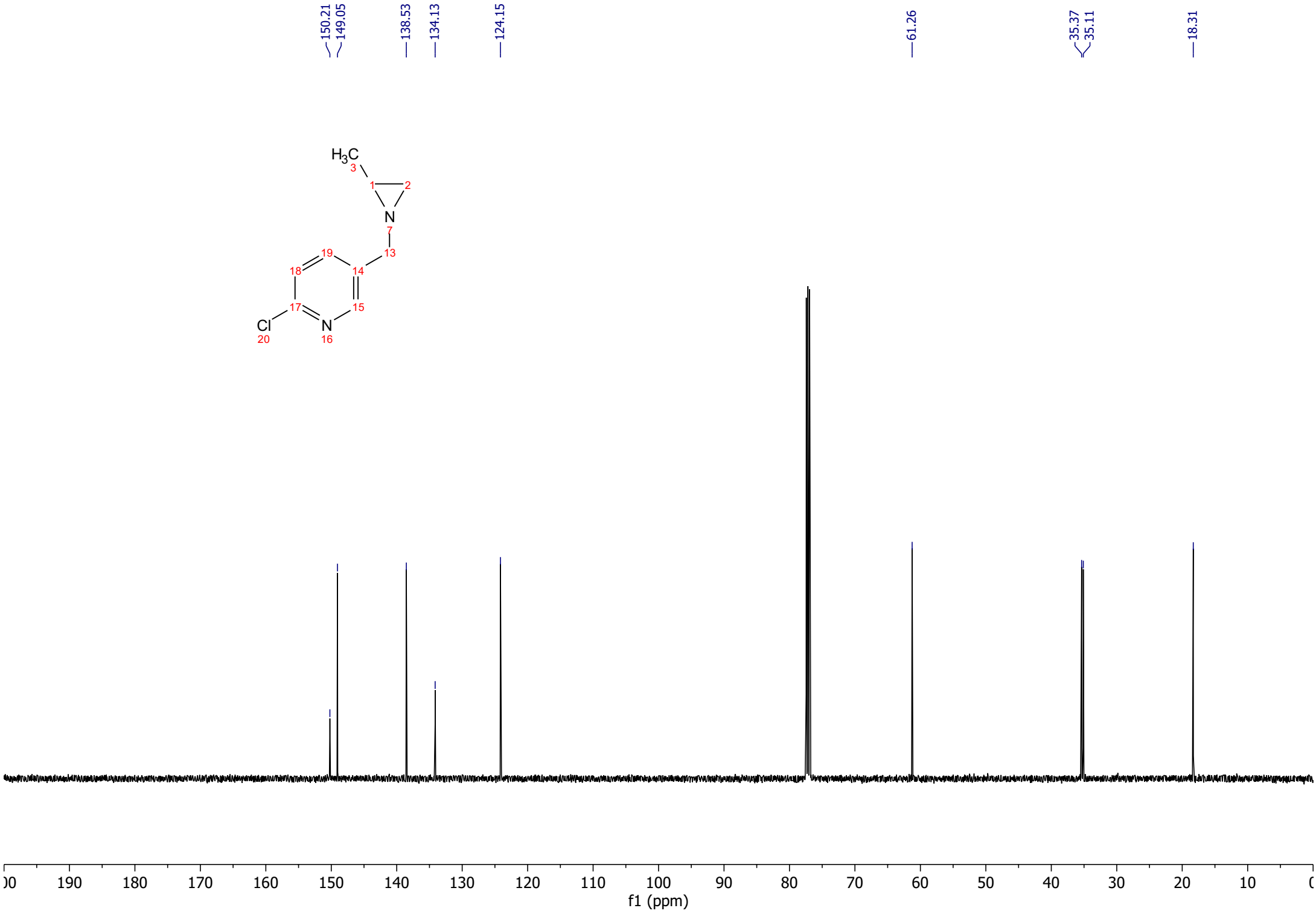
1.58
1.55
1.54
1.54
1.53
1.52
1.52
1.51
1.51
1.50
1.49
1.38
1.37
1.19
1.18
H3C
3
1
2
N
7
13
19
18
14
17
15
Cl
20
N
16
0.93
0.95
0.95
1.00
1.00
1.01
1.01
1.01
3.08
f1 (ppm)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149.05
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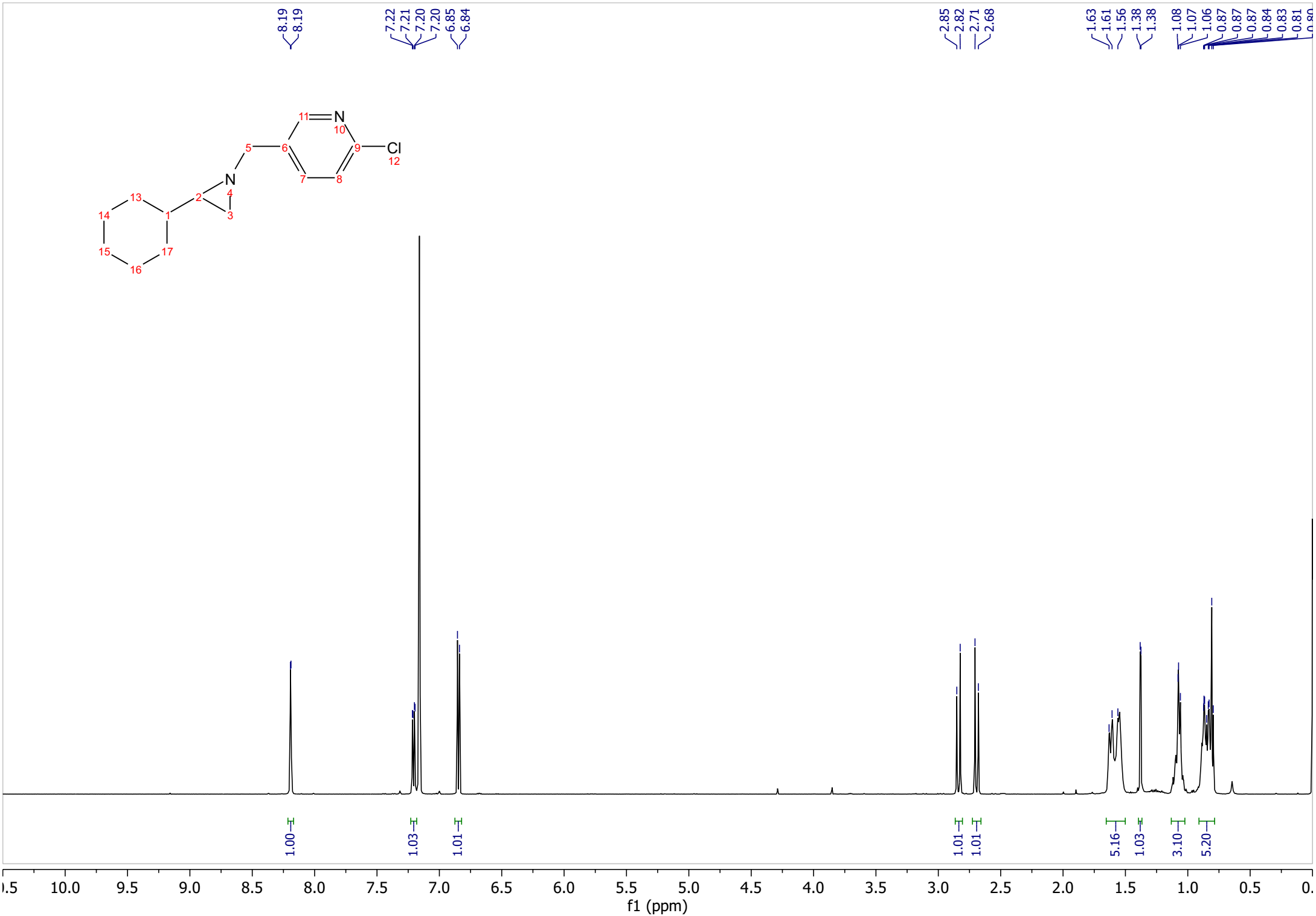
134.13
124.15
61.26
35.37
35.11
18.31
H3C
3
1
2
N
7
13
19
18
14
17
15
Cl
20
N
16
f1 (ppm)


8.19
8.19
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7.20
7.20
6.85
6.84
2.85
2.82
2.71
2.68
1.63
1.61
1.56
1.38
1.38
1.08
1.07
1.06
0.87
0.87
0.87
0.84
0.83
0.81
N
Cl
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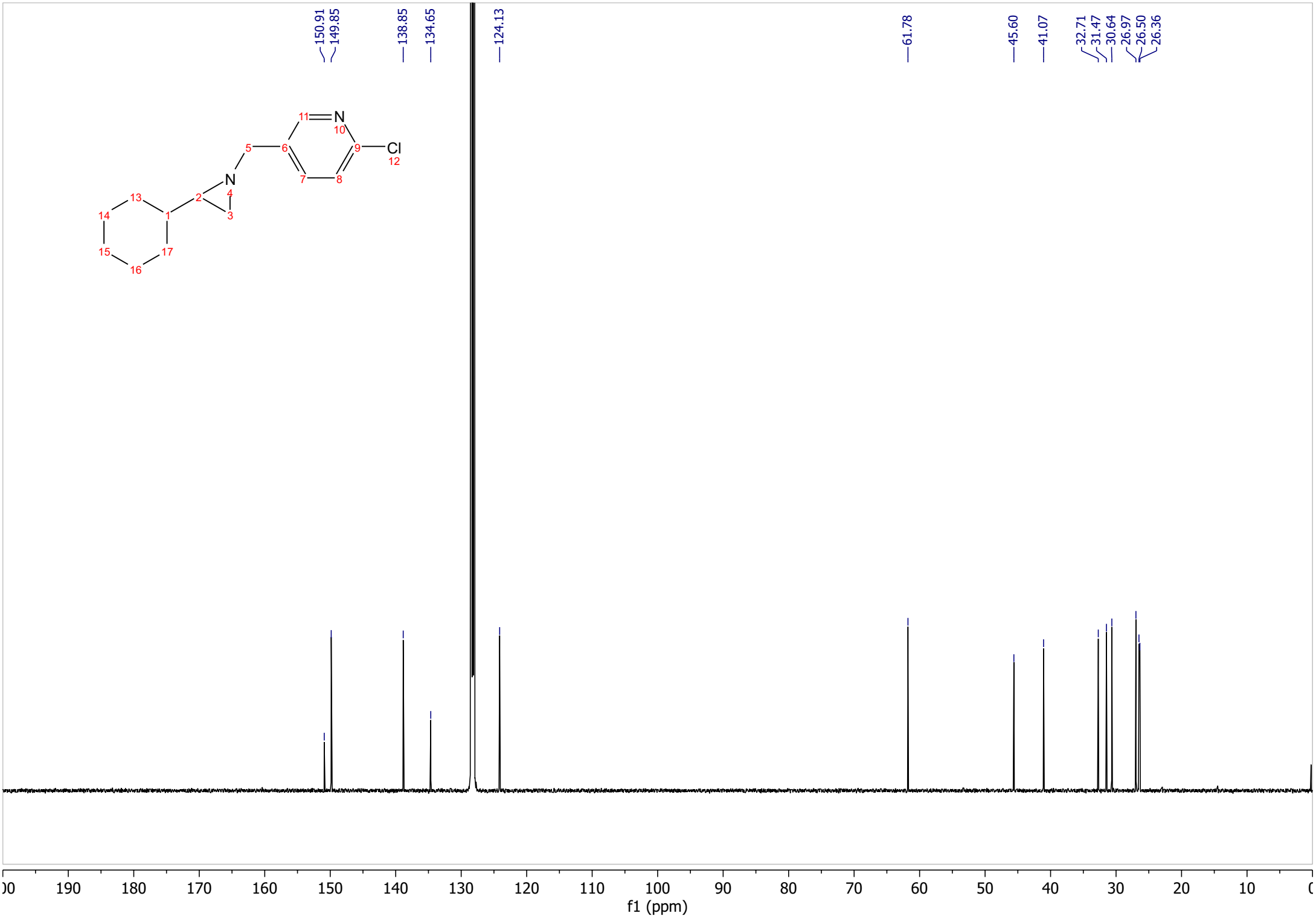
1.03
1.01
1.01
1.01
5.16
1.03
3.10
5.20
f1 (ppm)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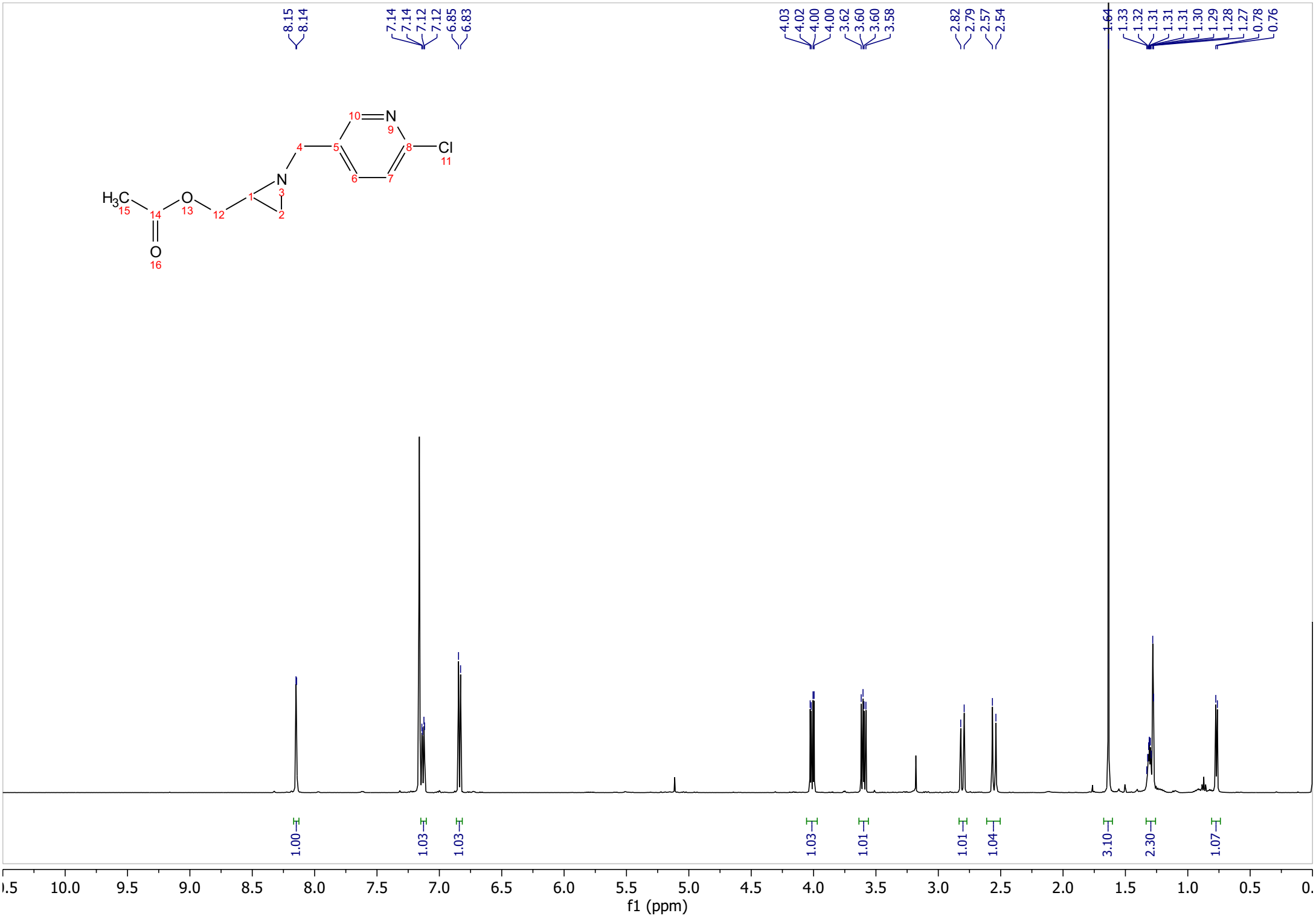
41.07
32.71
31.47
30.64
26.97
26.50
26.36
N
Cl
f1 (ppm)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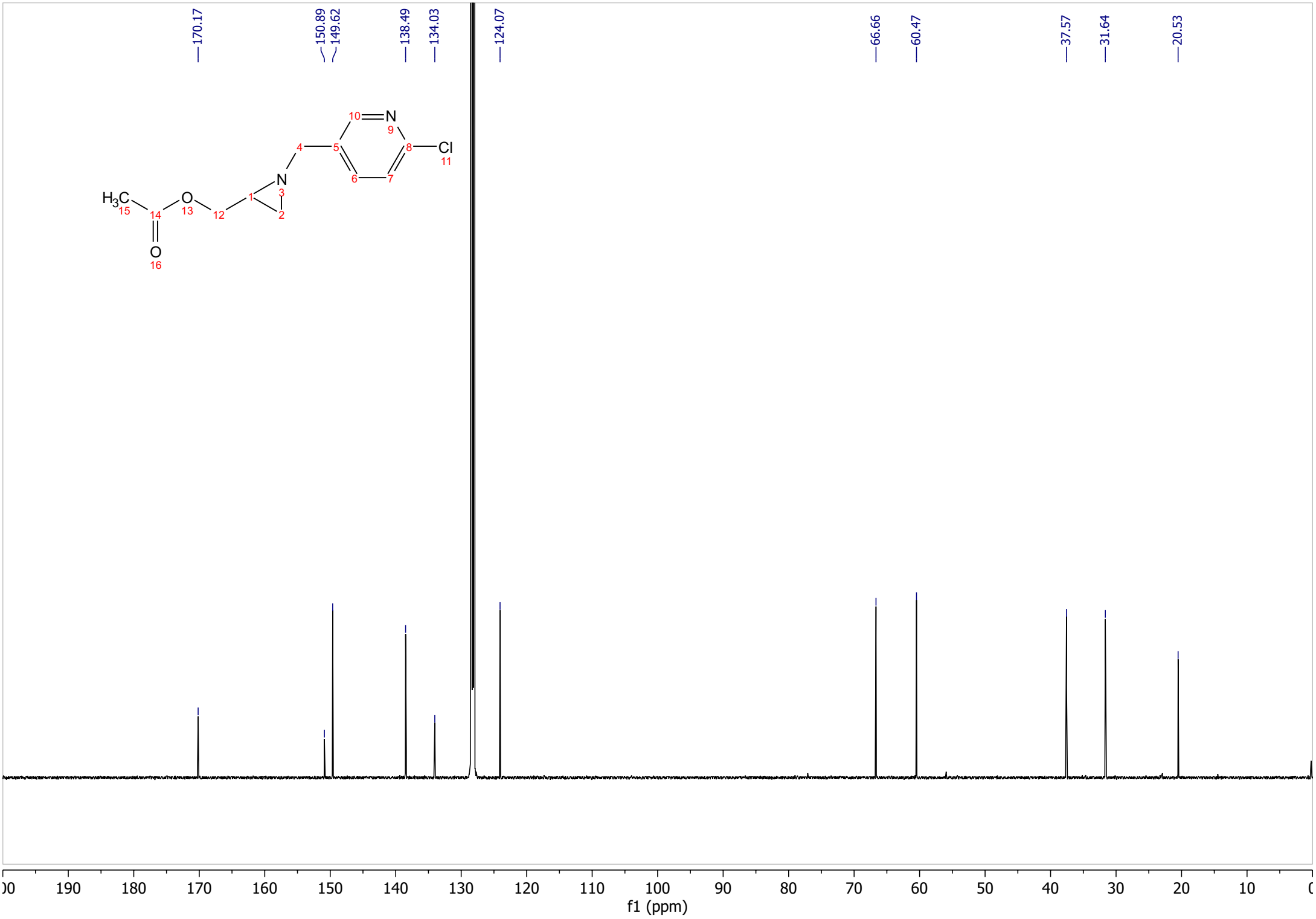
8.14
7.14
7.14
7.12
7.12
6.85
6.83
4.03
4.02
4.00
4.00
3.62
3.60
3.60
3.58
2.82
2.79
2.57
2.54
1.64
1.33
1.32
1.31
1.31
1.31
1.30
1.29
1.28
1.27
0.78
0.76
1.00
1.03
1.03
1.03
1.01
1.01
1.04
3.10
2.30
1.07
f1 (ppm)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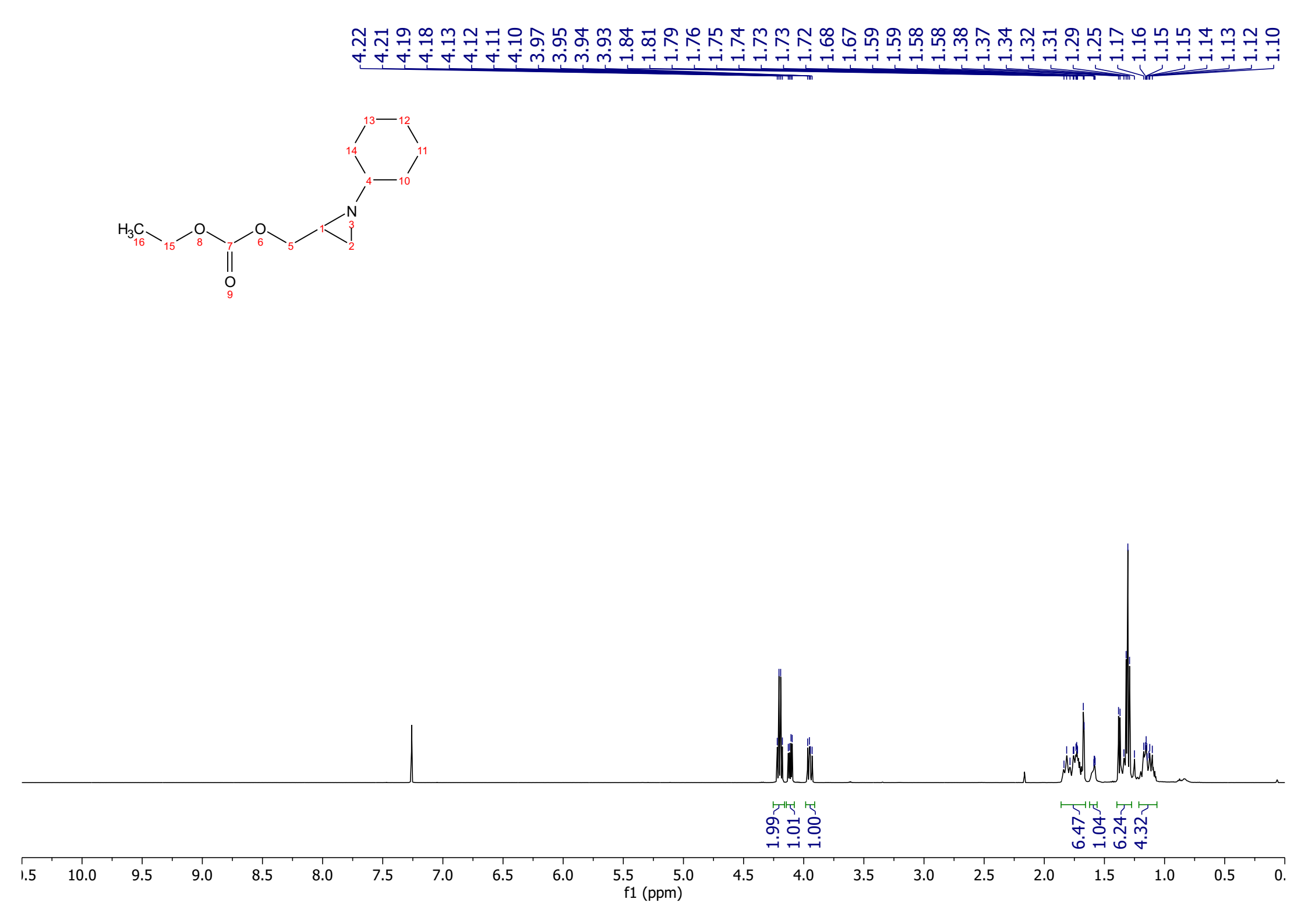
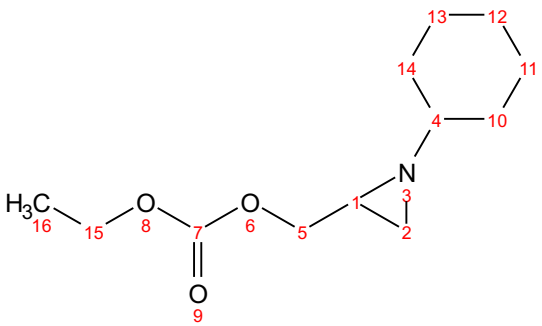
134.03
124.07
66.66
60.47
37.57
31.64
20.53
f1 (ppm)


4.22 4.21 4.19 4.18 4.13 4.12 4.11 4.10 3.97 3.95 3.94 3.93 1.84 1.81 1.79 1.76 1.75 1.74 1.73 1.73 1.72 1.68 1.67 1.59 1.59 1.58 1.58 1.38 1.37 1.34 1.32 1.31 1.29 1.25 1.17 1.16 1.15 1.15 1.14 1.13 1.12 1.10
H3C
O
O
N
O
1.99
1.01
1.00
6.47
1.04
6.24
4.32
f1 (ppm)

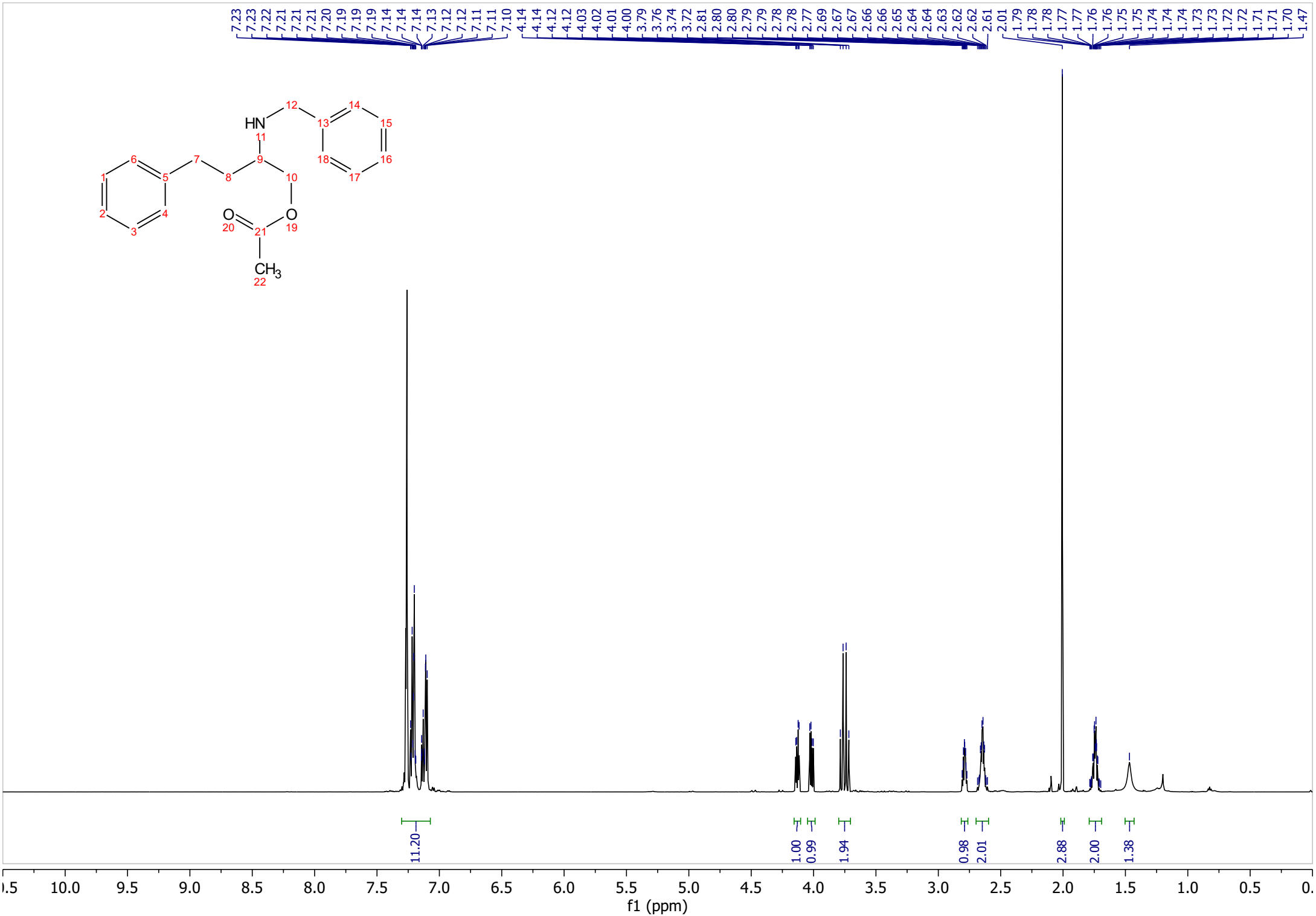


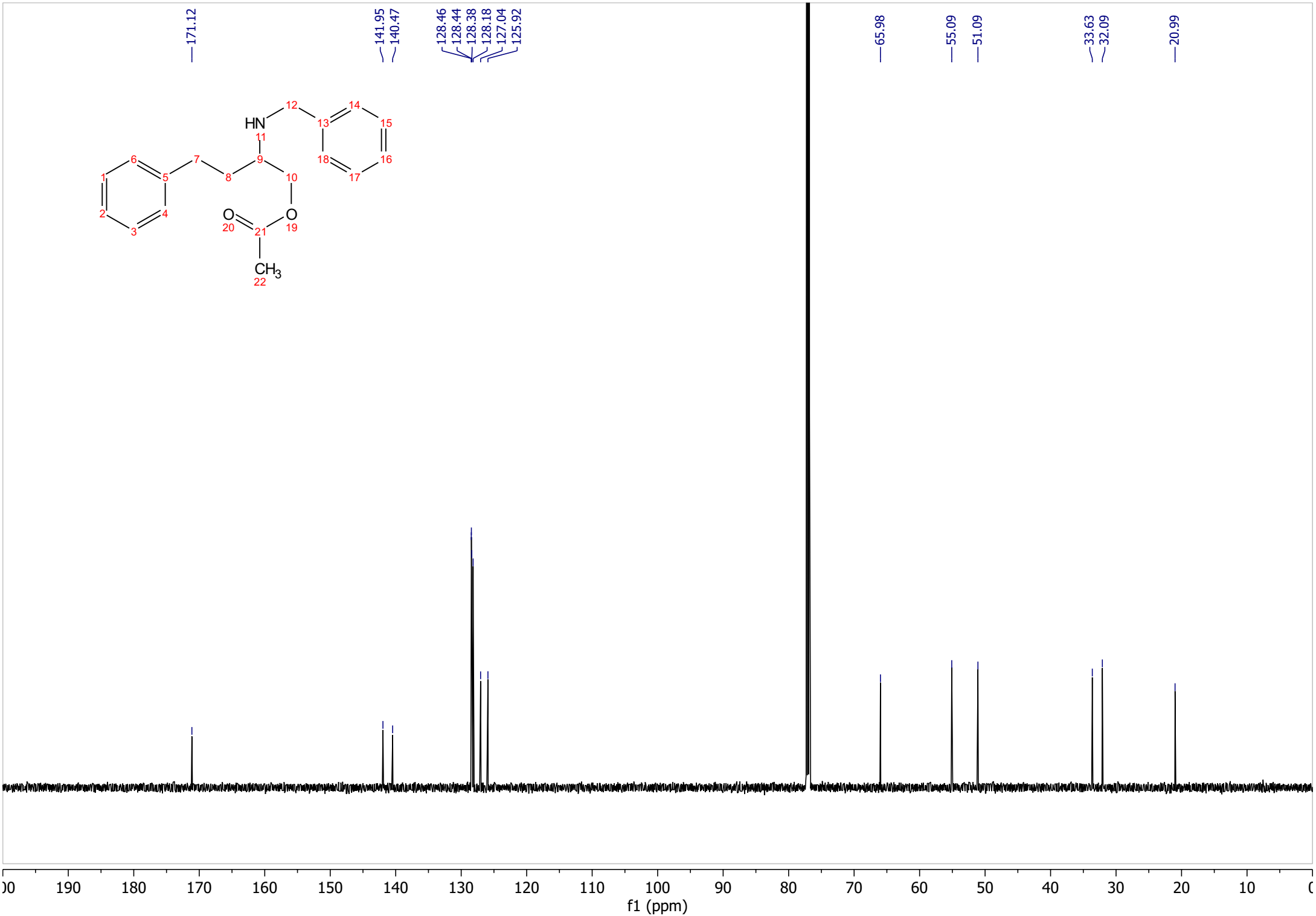
155.29

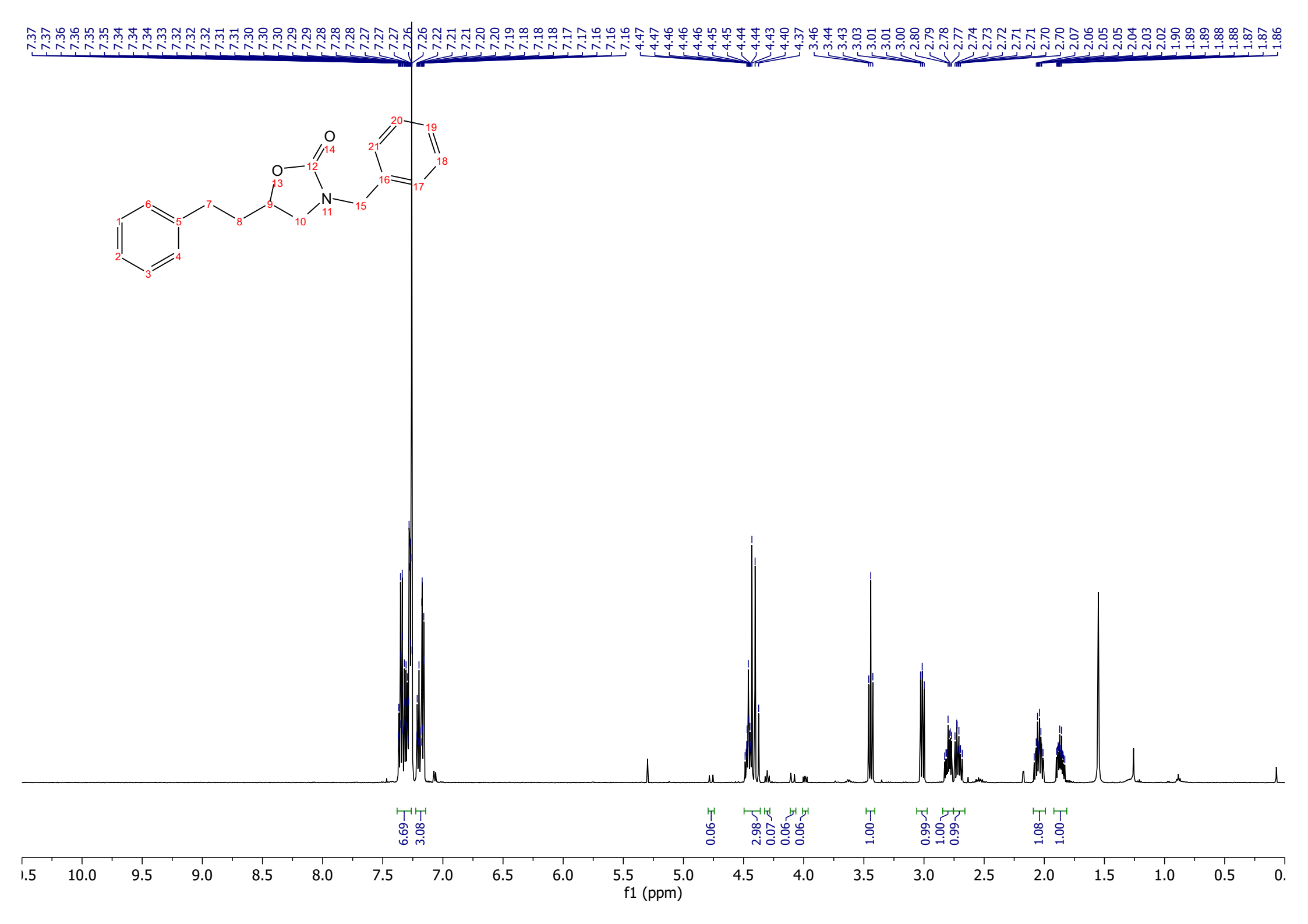
70.33
68.75
64.14

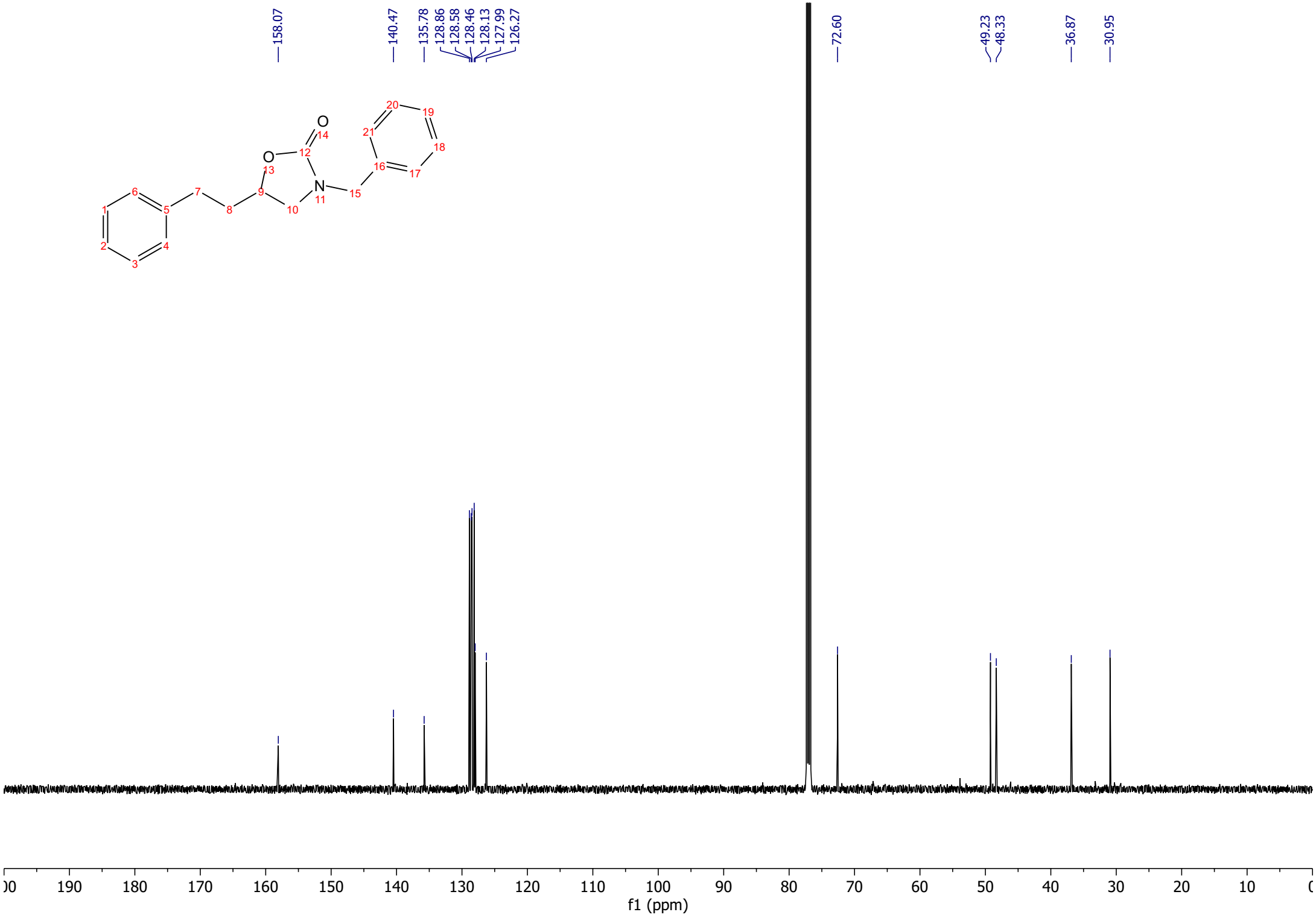
35.60
32.88
32.59
30.57
26.18
24.98
24.92

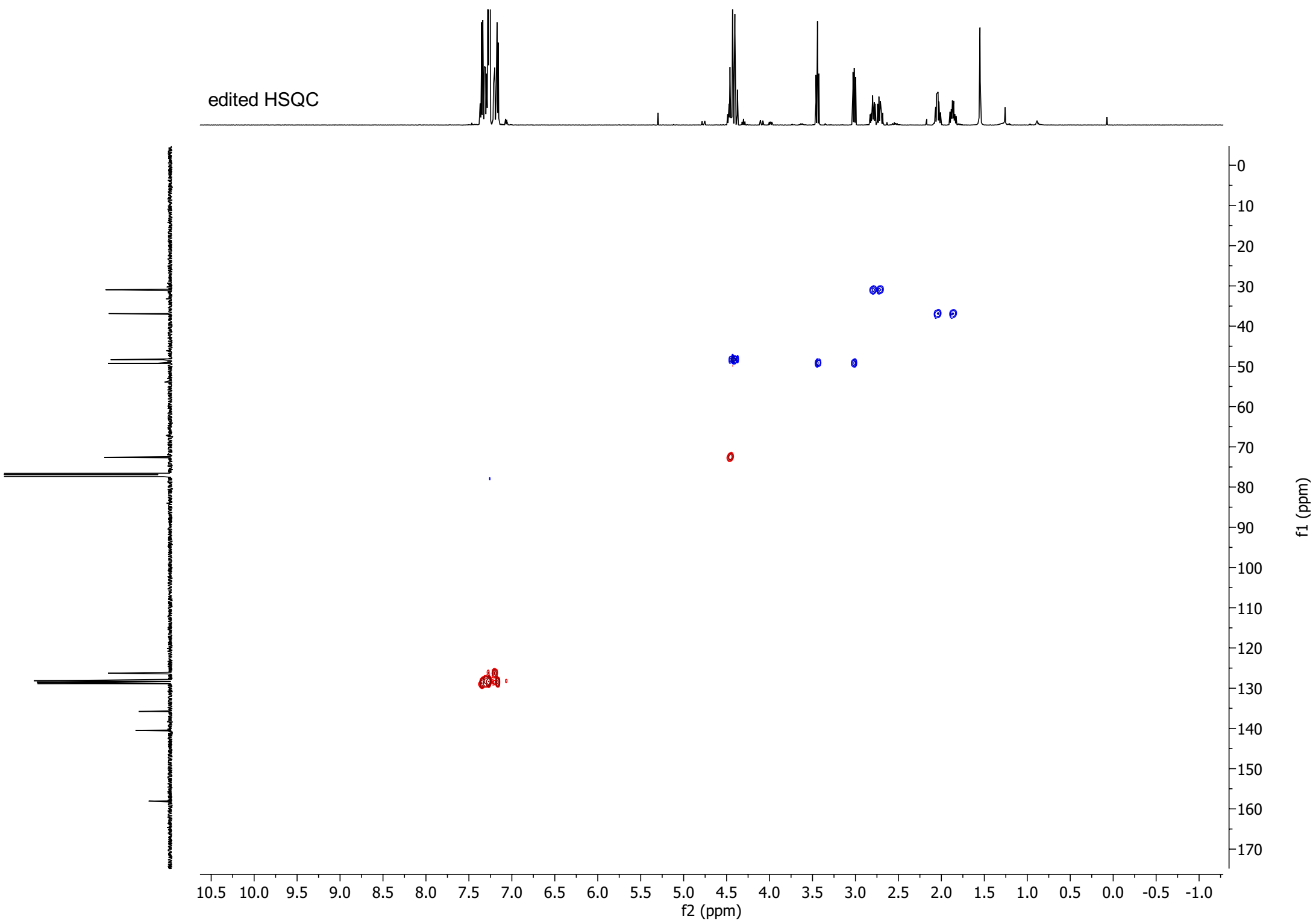
14.44

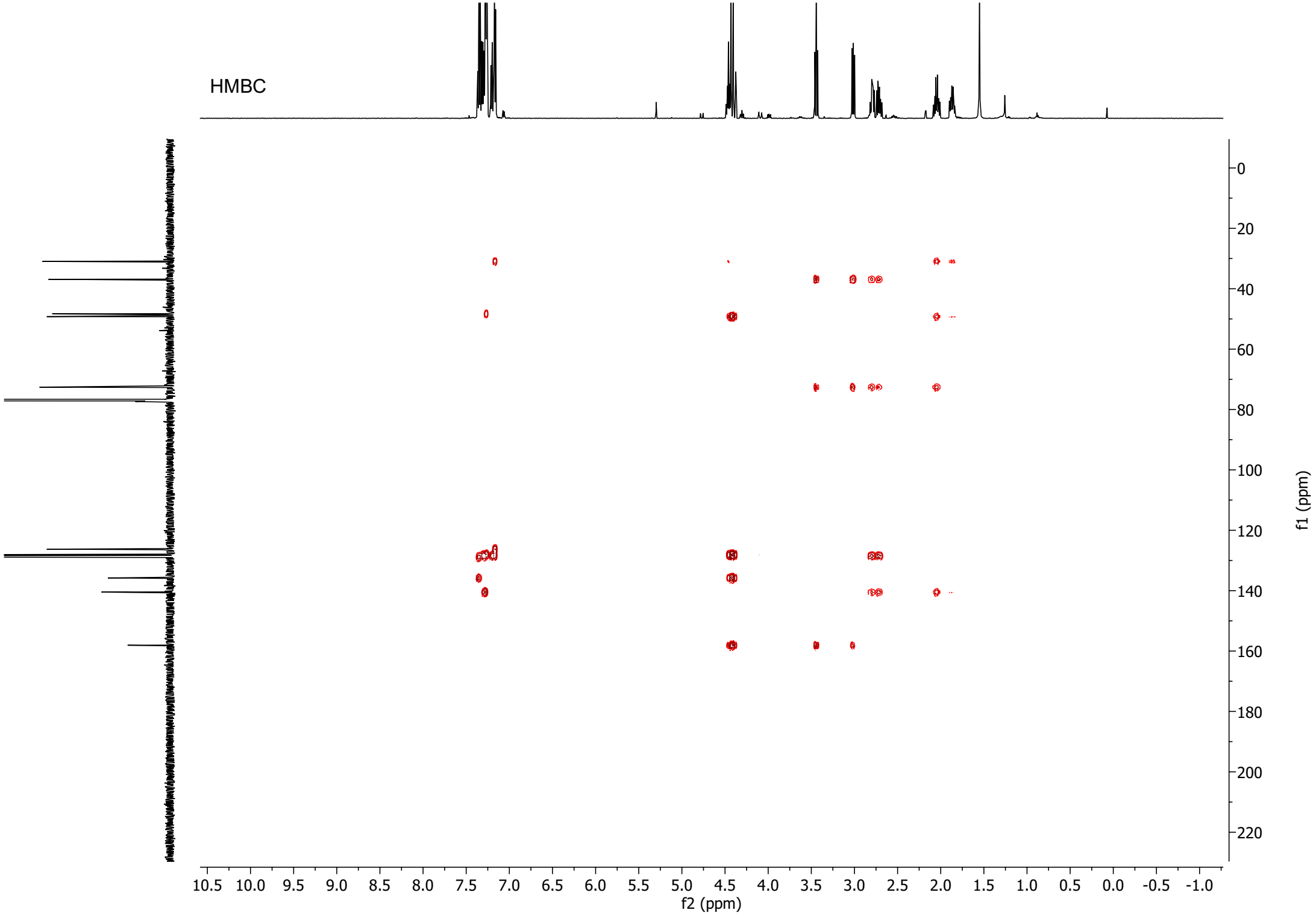

HN
O
O
CH3
f1 (ppm)

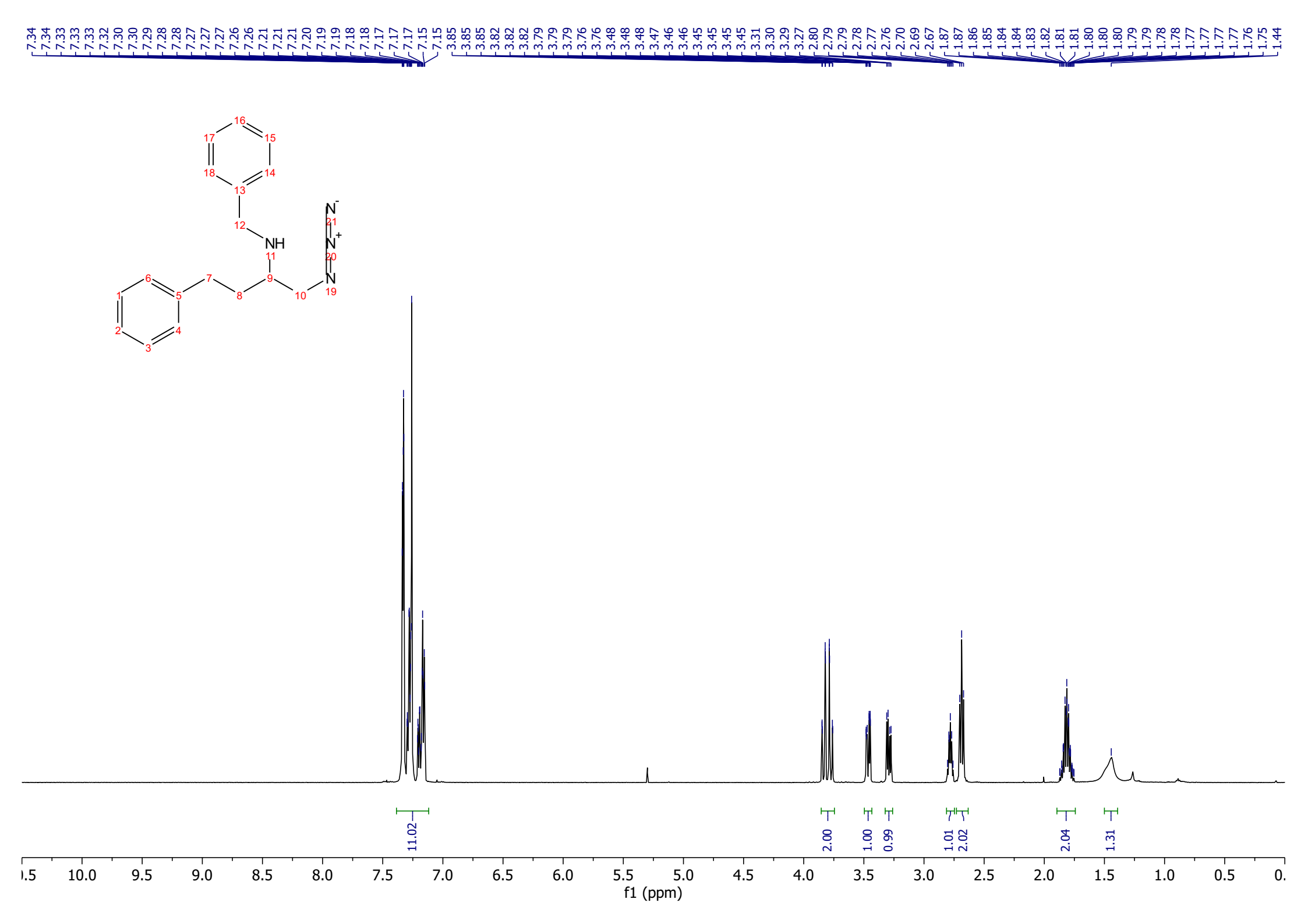

171.12
141.95
140.47
128.46
128.44
128.38
128.18
127.04
125.92
65.98
55.09
51.09
33.63
32.09
20.99
HN
O
O
CH3
f1 (ppm)

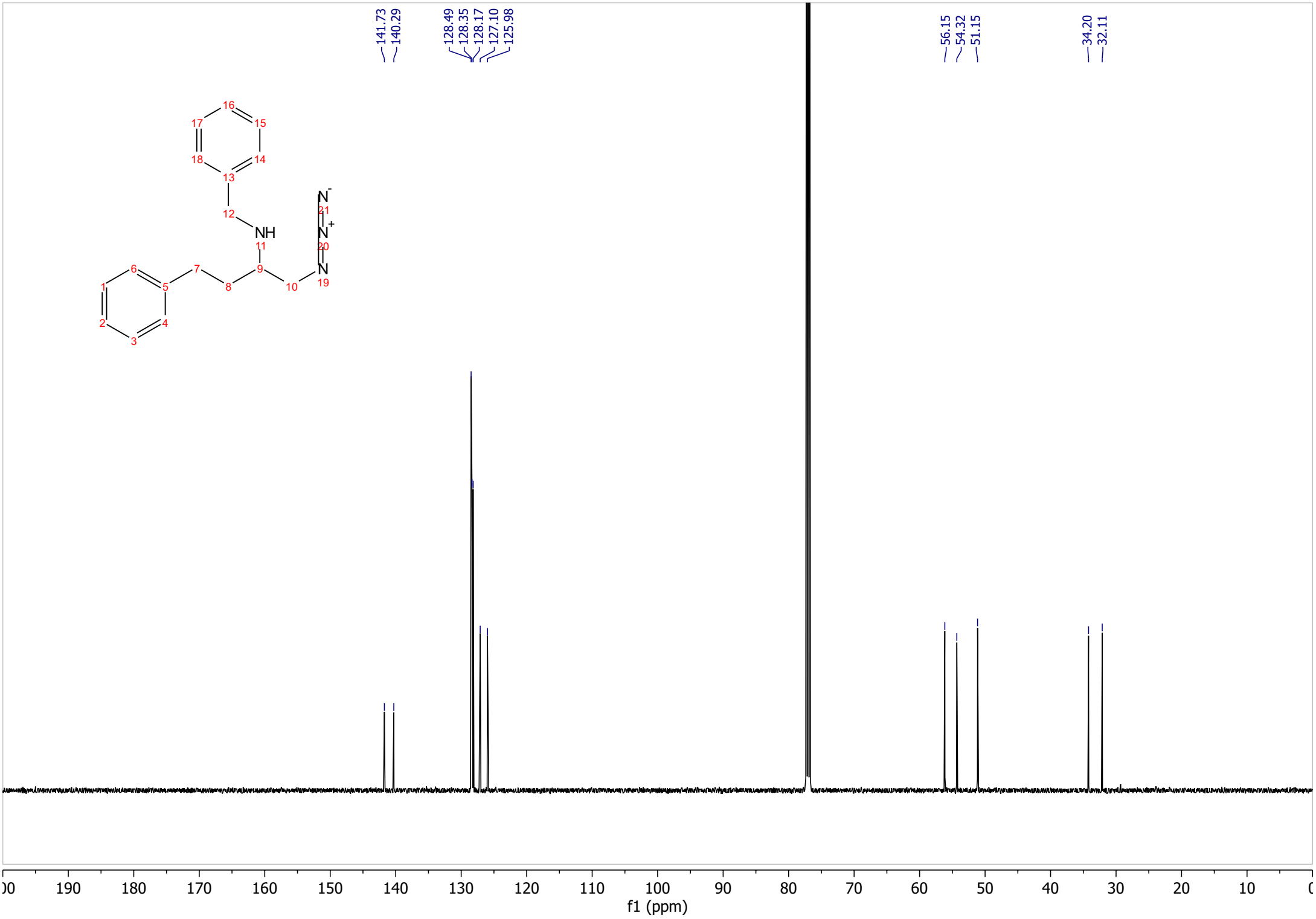

7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.34 7.34 7.33 7.32 7.32 7.32 7.31 7.31 7.30 7.30 7.30 7.29 7.29 7.28 7.28 7.28 7.27 7.27 7.27 7.26 7.26 7.22 7.21 7.21 7.20 7.20 7.19 7.18 7.18 7.17 7.17 7.16 7.16 7.16 4.47 4.47 4.46 4.46 4.46 4.45 4.45 4.44 4.44 4.43 4.40 4.37 3.46 3.44 3.43 3.03 3.01 3.01 3.00 2.80 2.79 2.78 2.77 2.74 2.73 2.72 2.71 2.71 2.70 2.70 2.07 2.06 2.05 2.05 2.04 2.03 2.02 1.90 1.89 1.89 1.88 1.88 1.87 1.87 1.86
O
O
N
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
6.69 3.08 0.06 2.98 0.07 0.06 0.06 1.00 0.99 1.00 0.99 1.08 1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

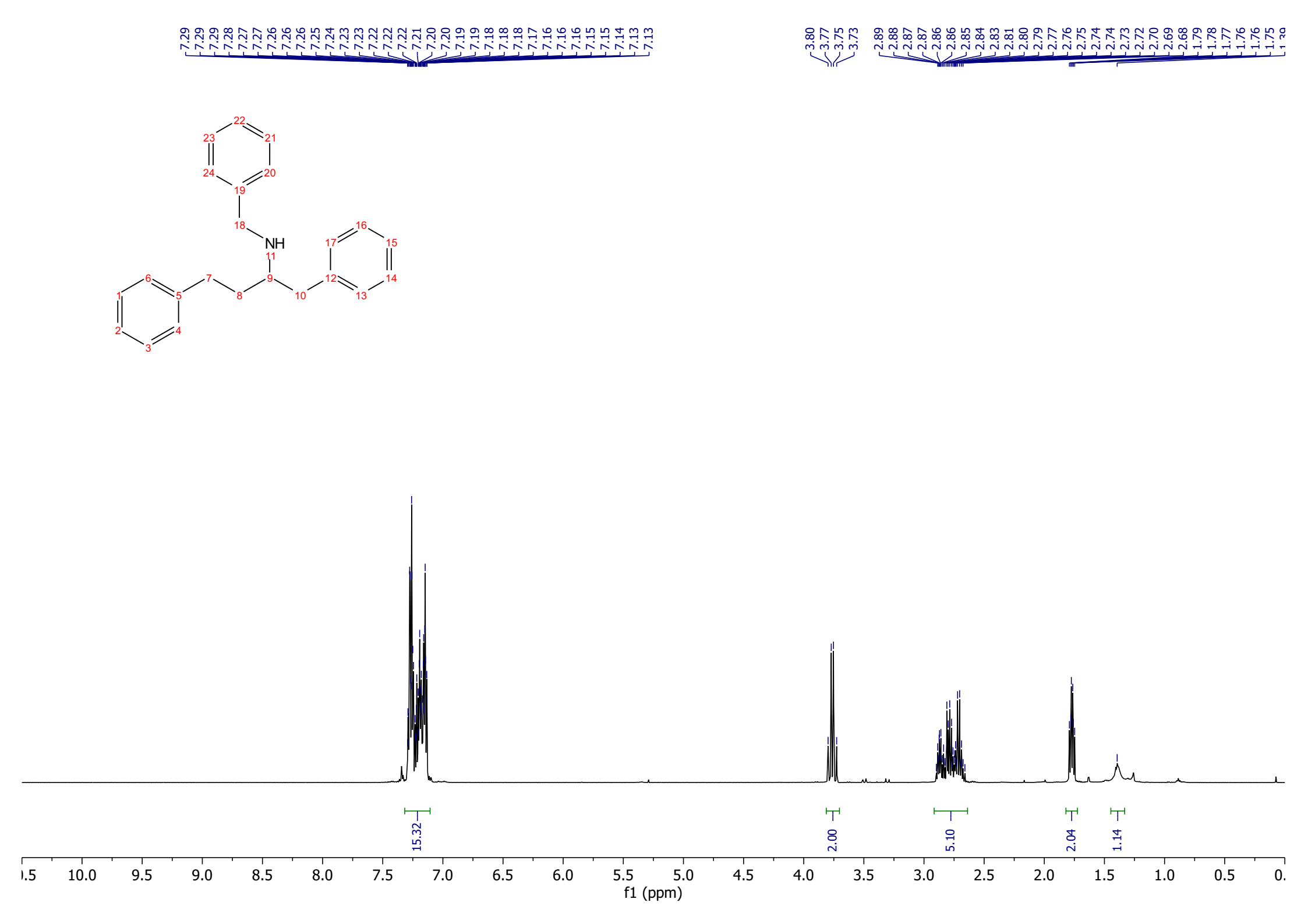

158.07
140.47
135.78
128.86
128.58
128.46
128.13
127.99
126.27
72.60
49.23
48.33
36.87
30.95
O
O
N
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
f1 (ppm)

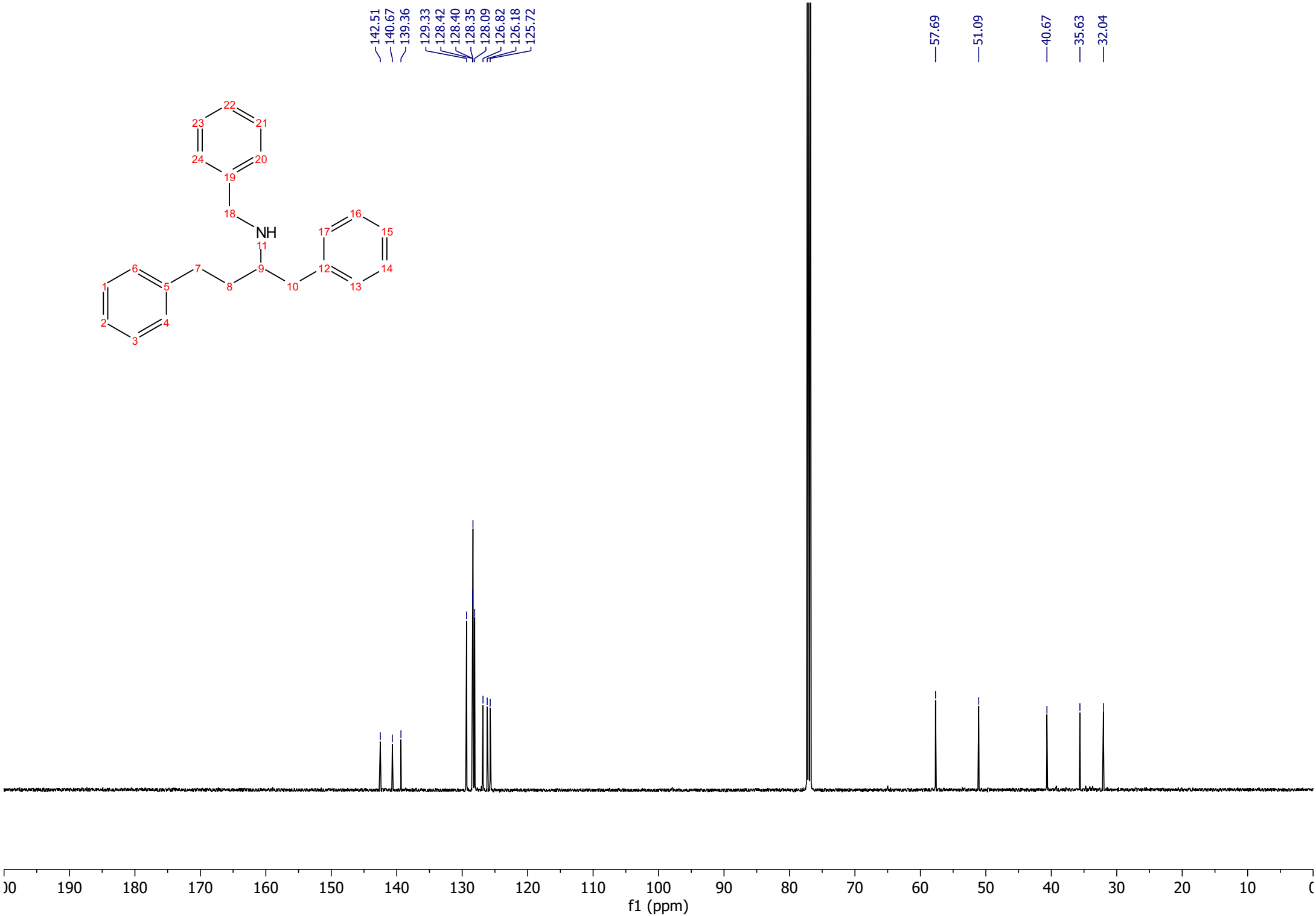

edited HSQC
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
f1 (ppm)
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f2 (ppm)

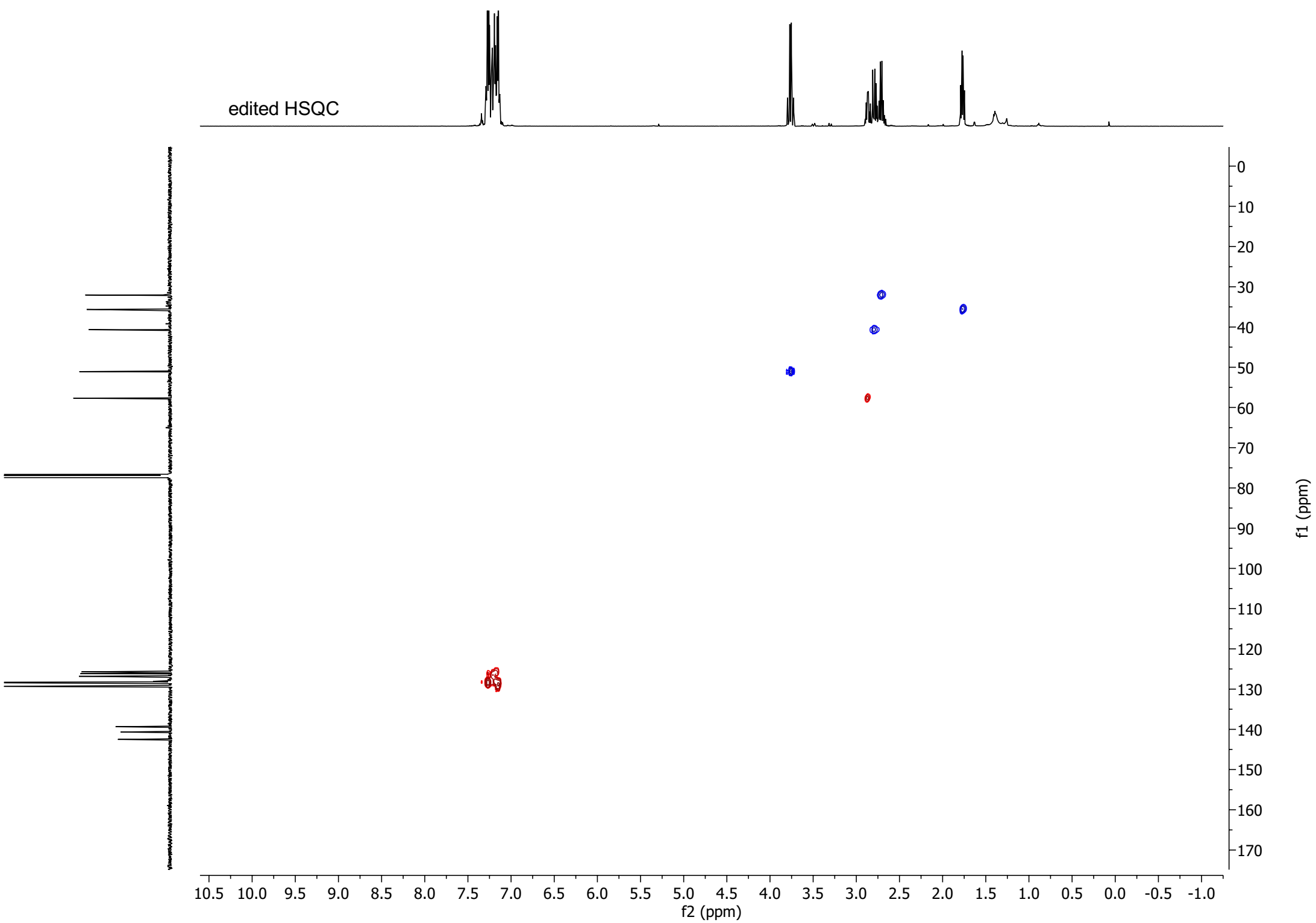

HMBC
0
20
40
60
80
100
120
140
160
180
200
220
f1 (ppm)
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f2 (ppm)

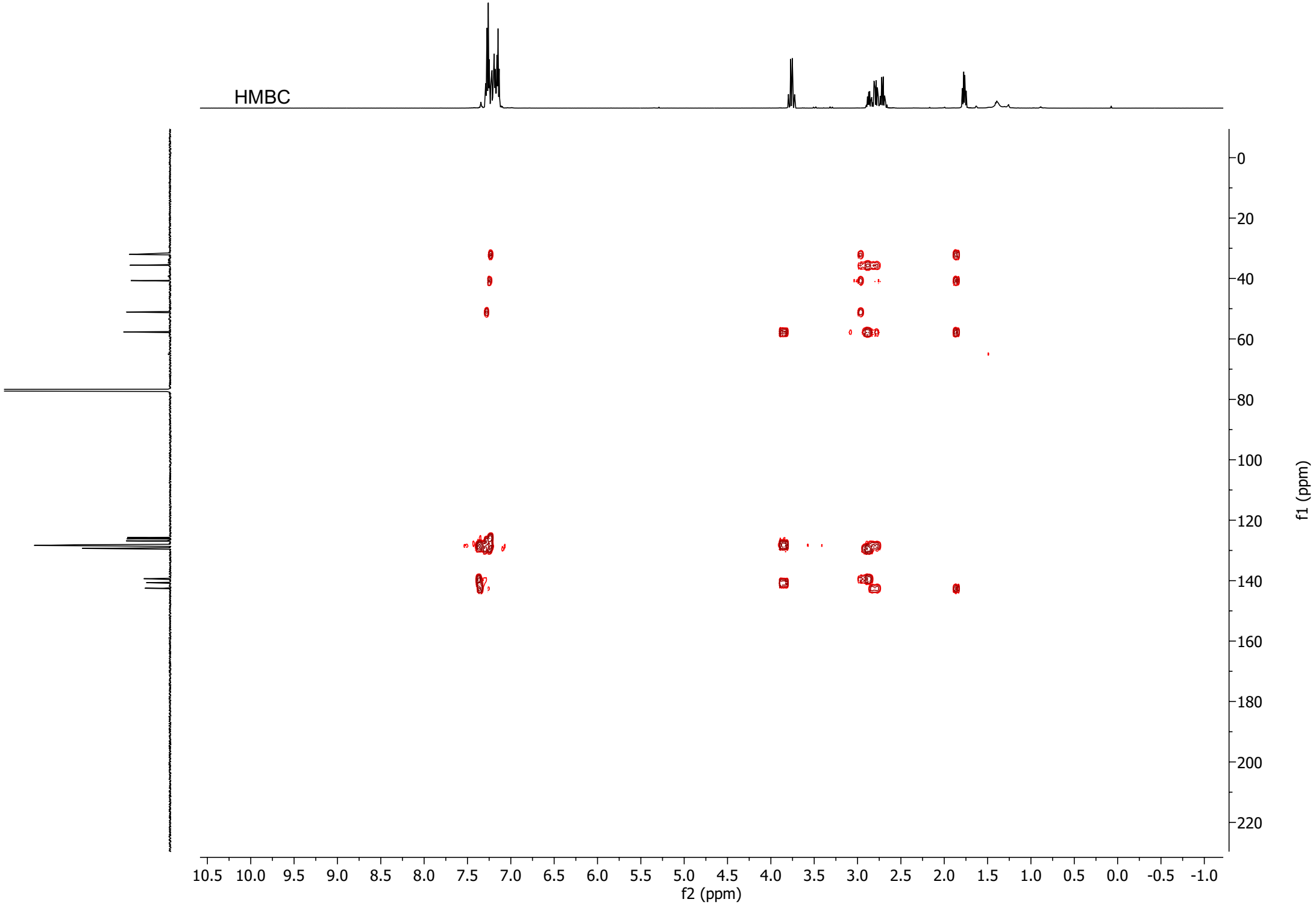

7.34 7.34 7.33 7.33 7.33 7.32 7.30 7.30 7.29 7.28 7.28 7.27 7.27 7.27 7.26 7.26 7.21 7.21 7.21 7.20 7.19 7.19 7.18 7.18 7.17 7.17 7.17 7.15 7.15
3.85 3.85 3.85 3.82 3.82 3.82 3.79 3.79 3.79 3.79 3.76 3.76 3.48 3.48 3.48 3.47 3.46 3.46 3.45 3.45 3.45 3.45 3.31 3.30 3.29 3.27 2.80 2.79 2.79 2.78 2.77 2.76 2.70 2.69 2.67 1.87 1.87 1.86 1.85 1.84 1.84 1.83 1.82 1.81 1.81 1.80 1.80 1.80 1.79 1.79 1.78 1.78 1.77 1.77 1.77 1.77 1.76 1.75 1.44
NH
N
N
N
11.02
2.00
1.00
0.99
1.01
2.02
2.04
1.31
f1 (ppm)

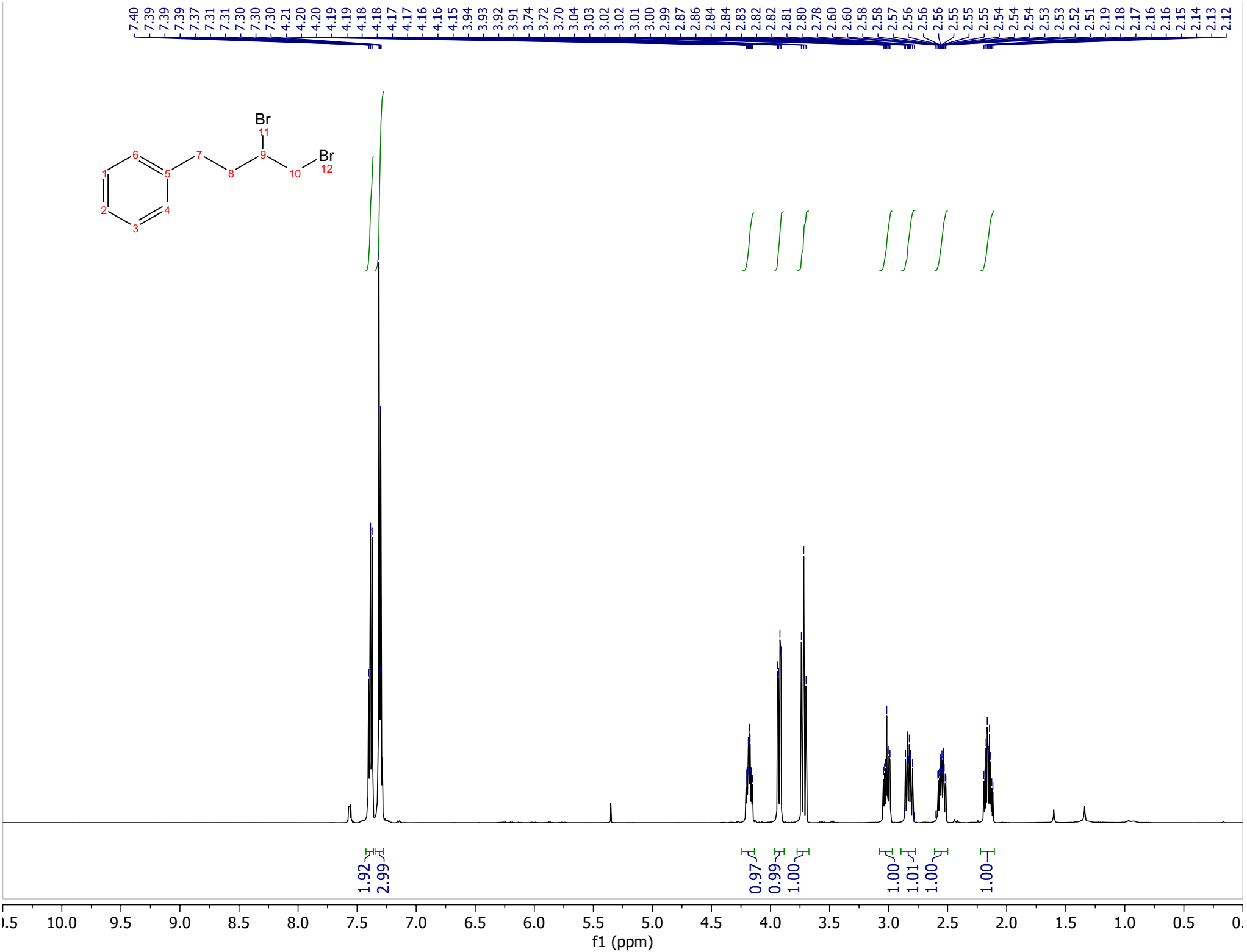

141.73
140.29
128.49
128.35
128.17
127.10
125.98
56.15
54.32
51.15
34.20
32.11
NH
f1 (ppm)

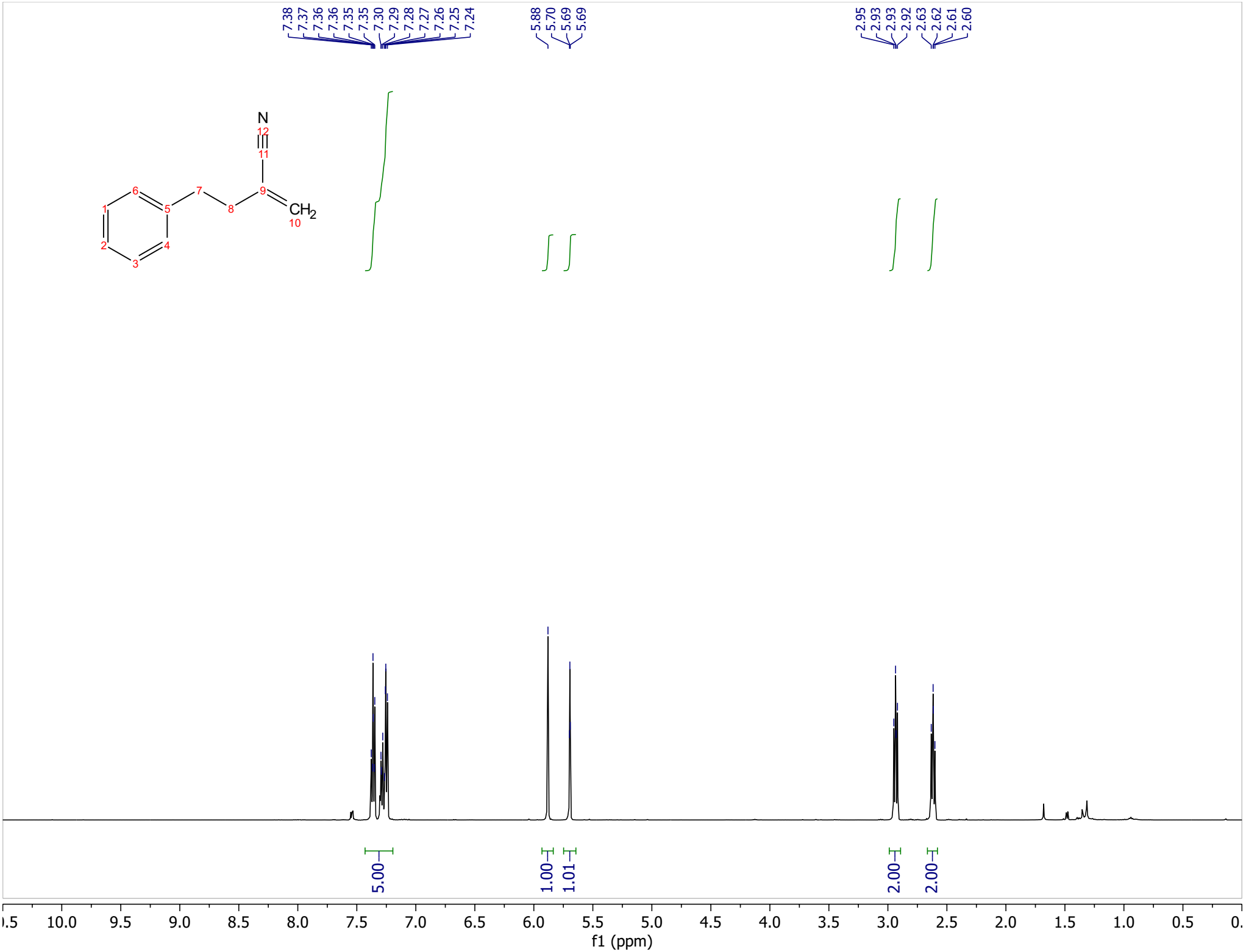

7.29 7.29 7.29 7.28 7.27 7.27 7.26 7.26 7.26 7.25 7.24 7.23 7.23 7.22 7.22 7.22 7.21 7.20 7.20 7.19 7.19 7.18 7.18 7.18 7.17 7.16 7.16 7.16 7.15 7.15 7.14 7.13 7.13
3.80 3.77 3.75 3.73
2.89 2.88 2.87 2.87 2.86 2.86 2.85 2.84 2.83 2.81 2.80 2.79 2.77 2.76 2.75 2.74 2.74 2.73 2.72 2.70 2.69 2.68 1.79 1.78 1.77 1.76 1.76 1.75
NH
15.32
2.00
5.10
2.04
1.14
f1 (ppm)


142.51
140.67
139.36
129.33
128.42
128.40
128.35
128.09
126.82
126.18
125.72
57.69
51.09
40.67
35.63
32.04
NH
f1 (ppm)


edited HSQC
f2 (ppm)
f1 (ppm)


HMBC
0
20
40
60
80
100
120
140
160
180
200
220
f1 (ppm)
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f2 (ppm)


7.40 7.39 7.39 7.39 7.37 7.31 7.31 7.30 7.30 7.30 4.21 4.20 4.20 4.19 4.19 4.18 4.18 4.17 4.17 4.16 4.16 4.15 3.94 3.93 3.92 3.91 3.74 3.72 3.70 3.04 3.03 3.02 3.02 3.01 3.00 2.99 2.87 2.86 2.84 2.84 2.83 2.82 2.82 2.81 2.80 2.78 2.60 2.60 2.58 2.58 2.57 2.56 2.56 2.56 2.55 2.55 2.55 2.54 2.54 2.54 2.53 2.53 2.52 2.51 2.19 2.18 2.17 2.16 2.16 2.15 2.14 2.13 2.12
Br
11
Br
12
1
2
3
4
5
6
7
8
9
10
1.92
2.99
0.97
0.99
1.00
1.00
1.01
1.00
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


7.38
7.37
7.36
7.36
7.35
7.35
7.30
7.29
7.28
7.27
7.26
7.25
7.24
5.88
5.70
5.69
5.69
2.95
2.93
2.93
2.92
2.63
2.62
2.61
2.60
N
12
11
6
7
9
1
5
8
CH2
10
2
4
3
5.00
1.00
1.01
2.00
2.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)