Selectivity Emerges from Indiscriminate Photoreduction

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SUPPORTING INFORMATION

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1. Reaction Optimization

General Methods and Materials

Unless otherwise noted, reactions were performed under an inert N_2 atmosphere in anhydrous solvent (MeCN or DMF) thoroughly degassed by freeze-pump-thaw. 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, CAM, p- anisaldehyde, 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 υm particle size). Purified materials were dried in vacuo (0.050 Torr) to remove trace solvent. ^{1}H, ^{13}C Spectra were taken using a Bruker Avance-400 with a BBFO Probe or a Bruker Avance-500 with a DCH Cryoprobe. NMR data are reported relative to residual CHCl3 (^{1}H, δ = 7.26 ppm), CDCl3 (^{13}C, δ = 77.16 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. GC traces were taken on an Agilent 7890A GC with dual DB-5 columns (20 m × 180 μm × 0.18 μm), dual FID detectors, and hydrogen as the carrier gas.

Experimental set up

Electrode fabrication and assembly

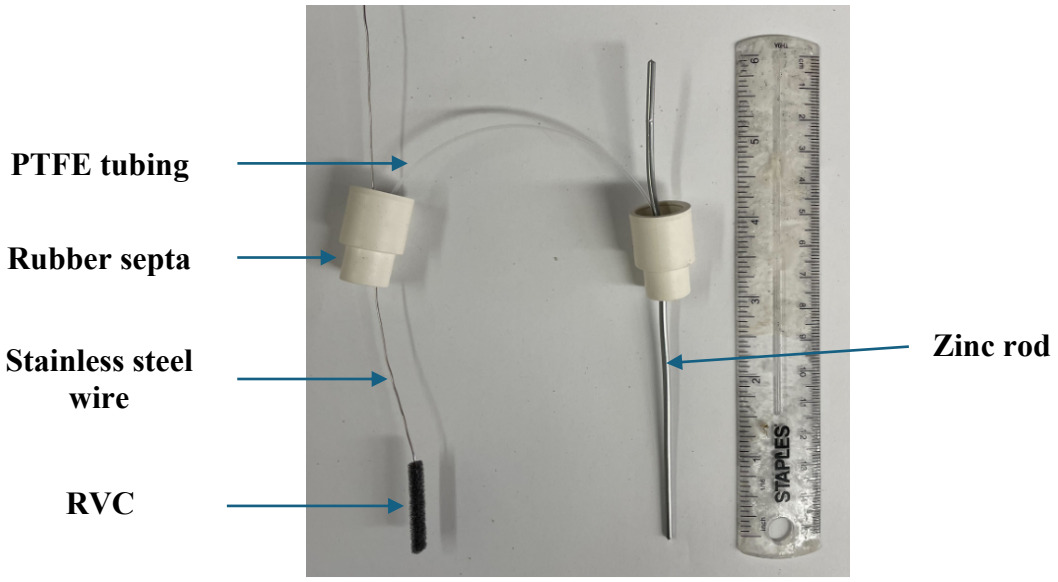


Figure S1.1 Polytetrafluoroethylene (PTFE) tubing purchased from Cole-Parmer; 1/32” ID, 1/16” OD, item number EW-06407-41. 14/20 Rubber septa purchased from VWR, item number 89064-940. Stainless steel wire purchased from Grainger; stainless steel lockwire, 0.025" diameter, item number 16Y043. Reticulated vitreous carbon (RVC) purchased from SELEE Corporation; 80 ppi, 0.4-0.7 g/cc, cut into 15×3×5 mm pieces. Zinc rod was purchased from RotoMetals; 99.9% pure; item number ZINCWIRE-0002.

H-Cell fabrication:



Figure S1.2 Electrochemical cell. (left) Divided cell fabricated in-house (FUSION, Journal of the ASGS, 2020, 67, 4, 19-26). Porosity E glass filter disc purchased from Ace Glass; 8 mm diameter, part number 7176-21. (right) Divided H–cells were constructed at the University of Wisconsin Madison Chemistry Department glass-blowing facility from two Ace glass 7646-06 O-ring seal joints (9 mm) and two 14/20 joints. Nafion 117 was purchased from Fuel Cell Store as a 30 cm x 30 cm sheet and cut to size (SKU: 591539).

Reaction set up:

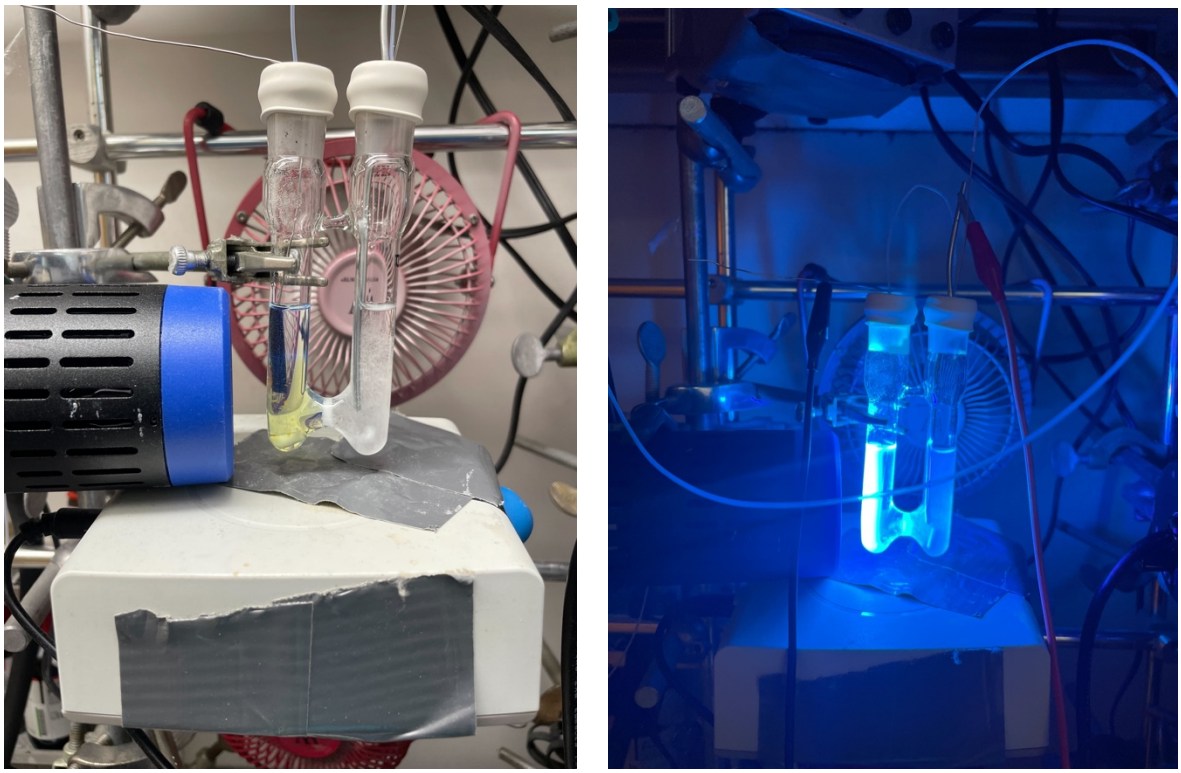
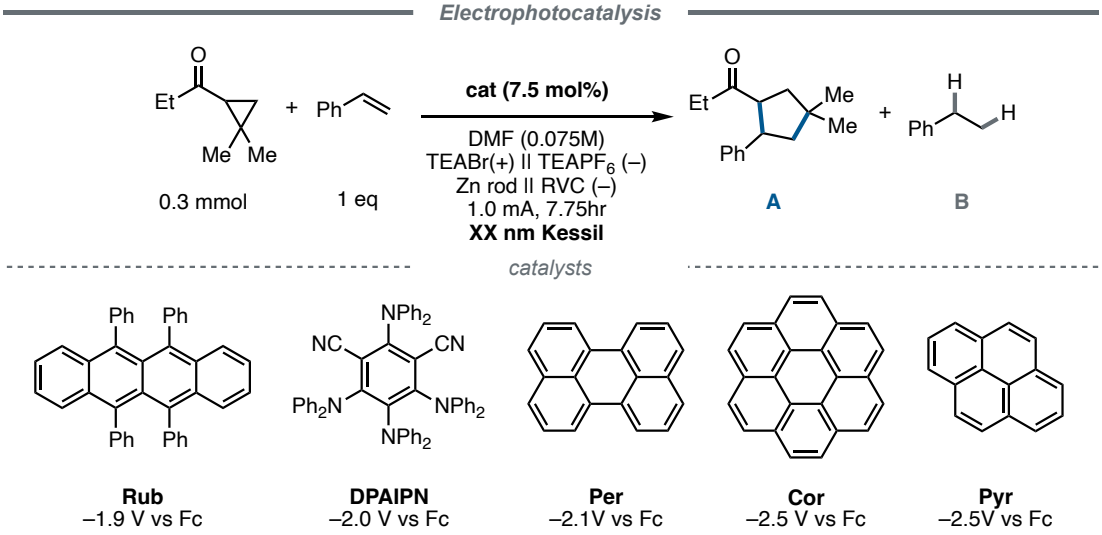


Figure S1.3a Reaction set up

General procedure 1: To an oven-dried divided cell, catalyst and electrolyte (TEAPF6, 0.4 M) were added to the cathode and electrolyte (TEABr, 0.4 M) was added to the anode. In cases when the substrates were solid, they were also added to the cathode chamber at this stage. The electrode assembly was added to the cell and the system was purged with nitrogen (purge needle in cathode, vent needle in anode) for 5 minutes. Solvent (0.075 M) was added to each compartment, and the purge needle was lowered into the solution for an additional 5 minutes. The purge needle was removed to the headspace and all liquid reagents were added. The cell walls were rinsed with an additional 1 mL of solvent and the vent needle was removed from the anode. Electrical leads were connected and a Kessil lamp was placed ½ inch from the cathode. Electrolysis and irradiation were initiated simultaneously (1 F/mol; 1 mA, unless otherwise noted). For GC analysis, mesitylene (1 eq) was added to the crude reaction. A 0.2 mL aliquot was diluted with 20% ethyl acetate in hexanes (2.0 mL). The mixture was then filtered through a silica plug to remove precipitated electrolyte and solvent. When workup was required to isolate the products, the reaction was diluted in brine (100 mL) and extracted with diethyl ether (3 × 100 mL). The combined organic layers were washed with brine and dried with sodium sulfate, concentrated, and subjected to silica column purification (acetone/hexanes eluent). TEABr is added to the anodic chamber of the divided cell to prevent passivation of the zinc anode by promoting the formation of $ZnBr_2$ (Li, Chemical Engineering Science 310 (2025) 121527).

Reaction Screening

Electrophotocatalysis



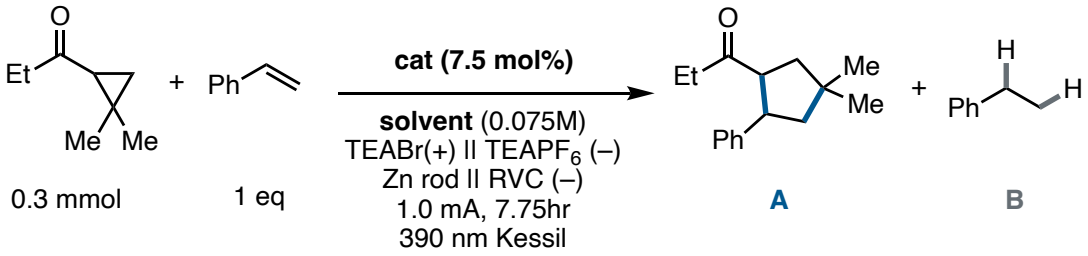
Entry	Catalyst	wavelength (nm)	Remaining Ketone	Remaining Styrene	A	B
1	Rub	370	5	6	51	7
2	Rub	390	2	2	61	9
3	Rub	427	19	4	48	23
4	Rub	456	25	13	44	18
5	Rub	467	46	20	37	30
6	Rub	525	92	55	1	38
7	DPAIPN	370	1	0	37	5
8	DPAIPN	390	1	0	32	4
9	DPAIPN	427	3	1	48	11
10	DPAIPN	456	57	27	21	29
11	DPAIPN	467	68	32	15	30
12	DPAIPN	525	85	49	5	34
13	Per	370	2	0	72	14
14	Per	390	1	8	70	7
15	Per	427	32	28	43	16
16	Per	456	55	45	24	19
17	Per	467	68	64	15	14
18	Per	525	88	81	1	10

Electrophotocatalysis (*cont.*)

Entry	Catalyst	wavelength (nm)	Remaining Ketone	Remaining Styrene	A	B
19	Cor	370	0	1	46	0
20	Cor	390	1	0	41	0
21	Cor	427	4	3	53	8
22	Cor	456	40	40	30	18
23	Cor	467	57	55	15	17
24	Cor	525	70	70	3	14
25	Pyr	370	0	0	40	1
26	Pyr	390	3	1	47	5
27	Pyr	427	3	11	49	18
28	Pyr	456	3	9	45	7
29	Pyr	467	3	5	50	7
30	Pyr	525	0	0	61	19

Table S1.1 Evaluation of select electrophotocatalysis. Reactions are conducted according to general procedure 1. Yields determined by GC with mesitylene (1 eq) as an internal standard

Electrophotocatalysis (*cont.*)



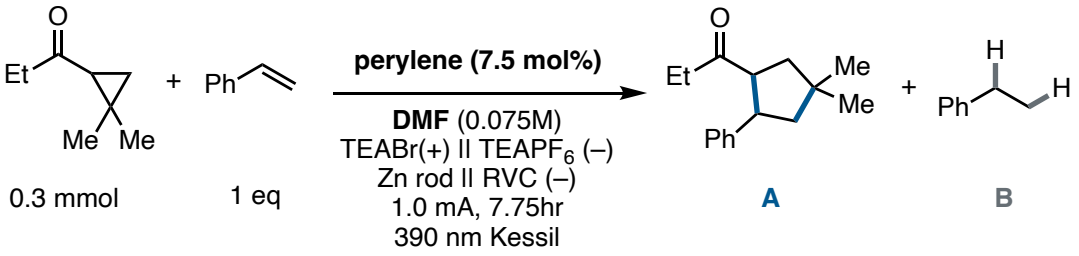
Entry	Catalyst	Solvent	Remaining Ketone	Remaining Styrene	A	B
1	Rub	MeCN	59	39	20	25
2	DPAIPN	MeCN	17	17	42	6
3	Per	MeCN	9	22	54	5
4	Cor	MeCN	6	4	64	3
5	Pyr	MeCN	3	5	69	3
6	Rub	DMF	2	2	61	9
7	DPAIPN	DMF	1	0	32	4
8	Per	DMF	1	8	70	7
9	Cor	DMF	1	0	41	0
10	Pyr	DMF	3	1	47	5

Table S1.2. Probing the role of solvent Reactions are conducted according to general procedure 1. Yields determined by GC with mesitylene (1 eq) as an internal standard

Discussion

Electrophotocatalytic conditions were broadly found to promote the reaction in both MeCN and DMF. We elected to perform transient absorption measurements in MeCN, as the absorption spectrum of solvated electrons is well documented in this solvent.

Controls – role of Per$^{\bullet-}$ in catalysis

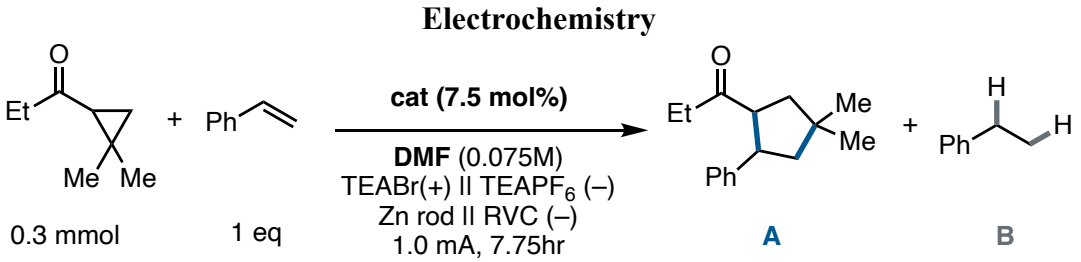


Entry	Variation	Remaining Ketone	Remaining Styrene	A	B
1	none	1	8	70	7
2	constant potential	10	28	49	2
3	constant potential, dark	92	93	0	0
4	constant potential, no styrene	37	-	-	-
5	constant potential, no styrene, dark	96	-	-	-
6	constant potential, no ketone	-	76	-	16
7	constant potential, no ketone, dark	-	95	-	4

Table S1.3. Role of Per$^{\bullet-}$. Reactions were conducted according to general procedure 1. Yields were determined by GC with mesitylene (1 eq) as an internal standard. Constant potential experiments performed at –2.1 V vs $Ag/AgNO_3$, a potential sufficient to reduce **Per** to **Per$^{\bullet-}$**

Discussion

The reaction is selectively promoted with both constant current and constant working potential modes of electrolysis (entries 1 and 2). In the dark under constant potential, low conversion of both coupling partners is observed (entry 3). These data indicate **Per$^{\bullet-}$** is not sufficiently potent to thermally reduce either substrate to a meaningful extent, with light serving as a supplemental driving force to drive substrate conversion. Consistent with our model, light was found to independently promote the reduction of both the ketone (entries 4 and 5) and styrene (entries 6 and 7).

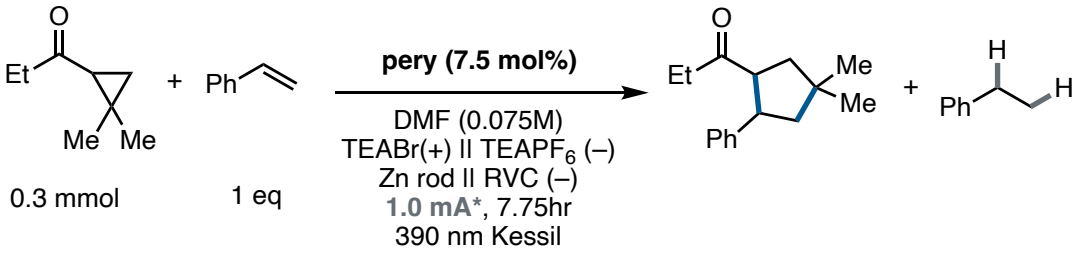


Entry	Catalyst	variation	Remaining Ketone	Remaining Styrene	A	B
1	none	constant current	93	55	0	38
2	none	constant potential[a]	90	86	0	9
3	Rub	constant current	98	54	0	47
4	DPAIPN	constant current	96	57	0	38
5	Per	constant current	96	84	0	12
6	Cor	constant current	95	57	0	37
7	Pyr	constant current	92	52	0	42
8	Pyr	constant potential[b]	82	32	0	55

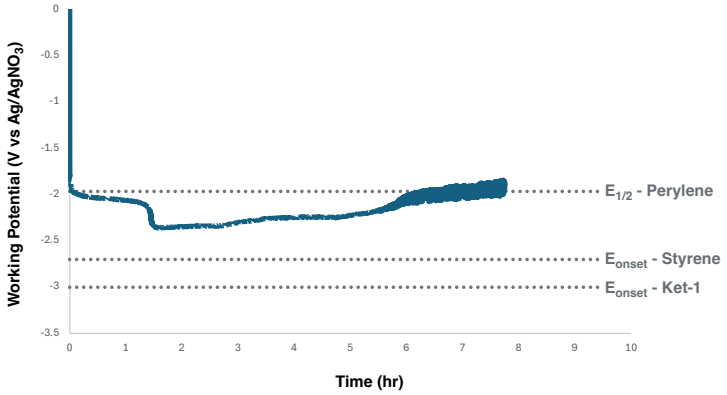
Table S1.4. Probing the efficacy of direct and mediated electrolysis. Reactions were conducted according to general procedure 1, with following modification: The reactions were performed in the dark, wrapped in foil and heated to 40 °C to recapitulate the heat from irradiation. Yields were determined by GC with mesitylene (1 eq) as an internal standard. [a]Constant potential experiment performed with at –3.2 V vs $Ag/AgNO_3$, a potential sufficient to reduce Ket-1 at the electrode. [b]Constant potential experiment performed with at –2.5 V vs $Ag/AgNO_3$, a potential sufficient to reduce pyrene.

Discussion

These data reflect the dominant influence of redox potentials on the selectivity of both direct and mediated electrolysis. Under constant current without a mediator, the RVC cathode selectively reduces styrene (entry 1). In principle, the inclusion of a mediator can promote coupling by catalyzing reversible SET to both substrates. If accessible, selectivity out of this pre-equilibrium could arise from a fast chemical step (i.e. β-scission of the ketyl radical). However, a range of mediators tested afford only styrene hydrogenation, demonstrating that the difference in redox potentials of the two substrates is sufficiently large to preclude such a mechanistic scenario (entries 3–7). Finally, control experiments with pyrene under constant potential, which prevents any contribution from direct electrolysis, fail to deliver any product (entry 8).



**reaction performed on a potentiostat to monitor the working potential*



Electrolysis Trace 1: working potential of the cathode measured during the course of constant current electrolysis. Superimposed lines represent the half-wave potential for perylene and onset potentials for styrene and Ket-1 measured by cyclic voltammetry.

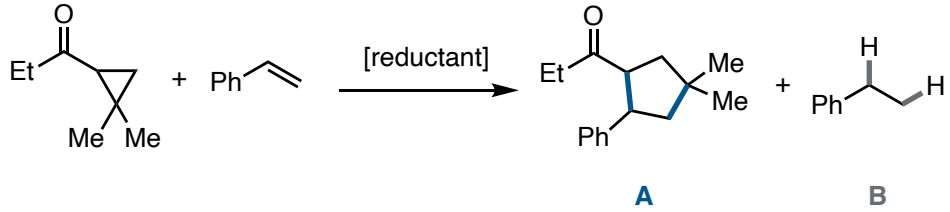
Discussion:

Monitoring the working potential under our optimal constant current electrolysis illustrates that the working potential shifts to more reducing potentials during the course of electrolysis.

Accordingly, we next evaluated potential contributions from direct electrolysis. Since direct electrolysis of either substrate requires more negative potentials than those accessed during electrophotocatalysis, the observed [3+2] annulation is unlikely to arise from direct electrolysis as it would require significantly uphill cathodic SET. Moreover, the onset for cathodic styrene reduction occurs ~300 mV positive of ketone reduction, suggesting that any direct electrolysis contribution would selectively reduce the olefin rather than drive product formation via ketone reduction. Consistent with this supposition, performing the reaction under constant current in the absence of perylene or irradiation results in exclusive styrene hydrogenation with minimal ketone conversion (93% RSM), confirming this prediction. These data indicate that contributions from direct electrolysis cannot account for the observed [3+2] annulation reactivity under electrophotocatalytic conditions. Of note, these data do suggest other catalyst redox states could also promote the observed reactivity (e.g., perylene dianion). While such possibilities can never be fully excluded, we performed the reaction under constant working potential at the half-wave

potential of perylene to verify that the catalytic system that was the subject of our mechanistic studies is appropriate. Under these conditions, perylene effectively promotes the desired reaction (49% yield) with minimal styrene hydrogenation (2%). These data unambiguously illustrate that perylene anion is competent to unlock the selective [3+2] chemistry and confirm that it is an appropriate subject for our detailed mechanistic study, even if the optimal constant current conditions result in a more complex scenario.

Additional Strategies to Drive SET



Entry	Reductant/Catalyst	Remaining Ketone	Remaining Styrene	A	B
1	sodium metal/no catalyst	21	65	0	1
2	sodium naphthalide/no catalyst	98	54	0	47
3	DIPEA/Mes-Acr-BF_4[a]	42	0	2	5
4	Cathode/Mes-Acr-BF_4[b]	40	10	23	10
5	Cathode/Mes-Acr-BF_4[c]	87	2	0	0
6	Tributyl amine/PTH	96	84	0	12
7	Formate/1-methylindoline-2-thione[d]	0	0	44	6
8	No reductant/1-methylindoline-2-thione[e]	53	30	13	5

Table S1.5. Probing Additional SET Reductants. Reactions were conducted according to the procedure listed below, with yields determined by GC with mesitylene (1 eq) as an internal standard. [a]DIPEA reductant [b]electrophotocatalysis (constant current) [b]electrophotocatalysis (constant potential) [d]1 equiv. sodium formate added [e]no sodium formate added

Procedure for sodium metal reduction (Entry 1)

35 mg of Na was added to a flame-dried 25 mL round bottom flask. 5 mL of dry Et_2O was added and the solution was chilled to −78 °C. The flask was covered with a rubber septum and pierced with a nitrogen needle. While the reaction was cooling, styrene (104 mg, 115 µL, 1 eq, 1.00 mmol) and 1-(2,2-dimethylcyclopropyl)propan-1-one (126 mg, 140 µL, 1 eq, 1.00 mmol) were dissolved in 5 mL of ether and stored in a flame-dried 2-dram vial. The solution containing the starting materials was added to the sodium mixture slowly and the reaction was allowed to stir at −78 °C for a few minutes before transferring to a salty ice bath for the remainder of the reaction. The reaction was allowed to stir for 3 h. The light-yellow mixture was quenched with glacial acetic acid and water. A white precipitate formed with addition of the acid but dissolved when the water was added. The reaction mixture went clear. The reaction mixture was added to a separatory funnel. Ether was added to the organic layer and the organic layer was washed 3 times with sat. $NaHCO_3$ and then twice with brine.

Comment on mass balance for entry 1.

By using a potent thermal reductant such as sodium metal, SET can be rendered indiscriminate and therefore unlock activation of the ketone. However, this alone is insufficient to promote the desired [3+2] reaction for several reasons. Unfortunately, we were not able to identify specific byproducts under these conditions. The ketyl radical likely does form and fragment under these conditions, but productive annulation is precluded by several downstream problems:

- There is no mechanism to protect styrene from decomposition. Under a regime where both substrates are reduced, SET to styrene will result in perspicuous decomposition unless there is a mechanistic to reoxidize styrene radical anion. By leveraging a photoreductant, BET is rendered fast and favorable. However, with a thermal reductant BET is highly endergonic and thus no recovery of styrene is expected.
- The accumulation of styrene radical anion can lead to additional side reactions. Styrene radical anion is both basic and nucleophilic, which likely contributes to side reactions with the ketone in the absence of proton source. We anticipate this side reactivity contributes to the poor mass balance of the reaction.
- Sodium can drive the pernicious overreduction of carbon radicals. For example, we observe up to 10% of the linear ketone byproduct derived from ketone reduction followed by premature reduction of the nascent radical. Thus, even when the ketone is reduced, we anticipate intermediates on-path to product can be intercepted.

Procedure for sodium naphthalide reduction (Entry 2)

To a flame-dried 2-dram vial with a stir bar was added sodium metal (34.5 mg, 5 eq). The atmosphere was purged and backfilled with nitrogen (×3). 2 mL of anhydrous THF was added and allowed to stir before naphthalene (154 mg, 4 eq) dissolved in 2 mL of anhydrous THF was added slowly. The resultant mixture was allowed to stir at room temperature for one hour. To another flame-dried 2-dram vial with a stir bar was added anhydrous THF. The THF was sparged with nitrogen for 5 minutes before adding 1-(2,2-dimethylcyclopropyl)propan-1-one (37.9 mg, 0.300 mmol) and styrene (31.2 mg, 34.5 μL, 0.300 mmol). Sodium naphthalide solution was then added and the reactions were stirred for 9 h at room temperature. DI water was added to quench the reaction.

Procedure for consecutive photoinduced electron transfer (Entry 3)

To a flame-dried 2-dram vial equipped with a stir bar and septum cap was added 3,6-di-tert-butyl-9-mesityl-10-phenylacridin-10-ium tetrafluoroborate (5.74 mg, 0.05 eq, 10.0 μmol), N-ethyl-N-isopropylpropan-2-amine (77.6 mg, 105 μL, 3 eq, 600 μmol), and acetonitrile (4 mL, 50 mM). The reaction mixture was sparged with nitrogen for 5 minutes. Styrene (20.8 mg, 23.0 μL, 1.00 eq, 0.200 mmol) and 1-(2,2-dimethylcyclopropyl)propan-1-one (25.2 mg, 1 eq, 0.200 mmol) were then added and the vial was sealed with parafilm and placed in front of a 390 nm Kessil lamp for 16 hours. To the crude reaction mixture, mesitylene (24.0 mg, 27.8 μL, 1 eq, 200 μmol) was added. A small aliquot of the mixture was diluted with EtOAc:hexanes (1:4) for GC analysis.

Procedure for electrophotocatalysis with the acridinium photocatalysts (Entries 4 and 5)

Constant current electrolysis was performed according to general procedure 1. Constant working potentials electrolysis was performed at -1.14 V vs Fc for 12 hours, a potential sufficiently reducing to access the catalyst neutral radical.

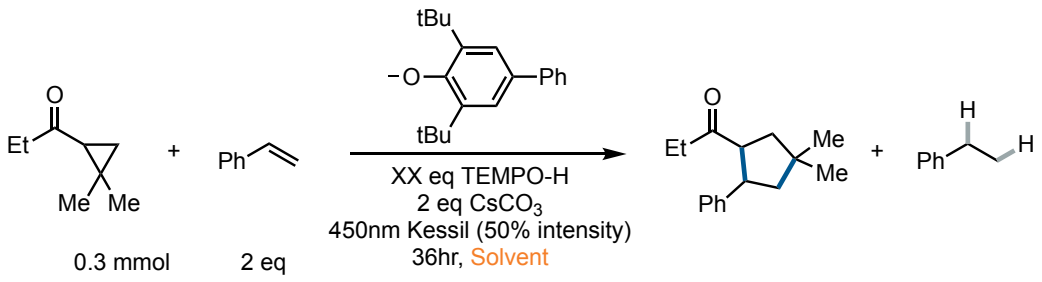
Procedure for PTH photoredox (Entry 6)

To a flame-dried 1-dram vial equipped with a stir bar was added 10-phenyl-10H-phenothiazine (1.38 mg, 0.05 eq, 5.00 μmol), tributylamine (92.7 mg, 119 μL, 5 eq, 500 μmol), 1-(2,2-dimethylcyclopropyl)propan-1-one (12.6 mg, 1 eq, 0.100 mmol), and DMSO (1.0 mL). The solution was sparged with argon for 10 min before styrene (10.4 mg, 11.5 μL, 1 eq, 100 μmol) was added. The vial was placed next to the 390 nm light under vigorous stirring while cooling with a fan for 24 h. Mesitylene (12.0 mg, 13.9 μL, 1 eq, 100 μmol) was added to the crude reaction mixture. A small aliquot of the mixture was diluted with EtOAc:hexanes (1:4) for GC analysis.

Procedure for super potent photoredox (entries 7 and 8)

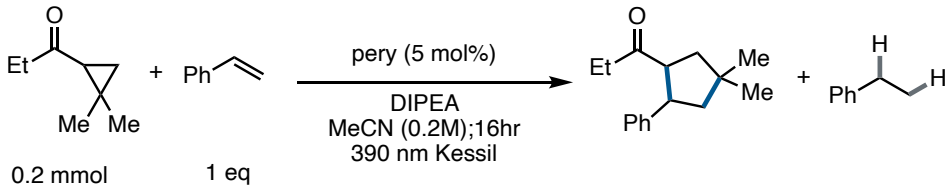
Reactions were performed under identical conditions reported by the Melchiorre lab (Angew. Chem. Int. Ed. 2023, 62, e202306364)

We evaluated the efficacy of a potent phenolate catalyst recently reported by the Xia group (Chem. Sci., 2020, 11, 6996) however no productive coupling was observed.



Remaining SM		*TEMPO-H eq*	*Solvent*		
92%	1.4 eq	1.2 eq	DMSO	**0%**	0%
65%	0.9 eq	0 eq	DMSO	**0%**	0%
0%	1.2 eq	0 eq	MeCN	**0%**	0%

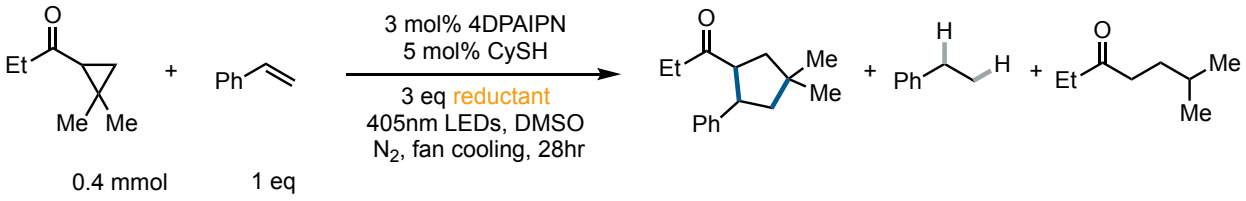
We evaluated the efficacy of perylene a potent photoreductants under ConPET conditions, however only trace product is observed.



Remaining SM

100%	65%	0.1 eq DIPEA	**0%**	1%
73%	0%	1.0 eq DIPEA	**1%**	1%

Finally, we evaluated the efficacy of our previously reported photoredox conditions leveraging formate as a terminal reductant (J. Am. Chem. Soc. 2021, 143, 10882−10889). Intriguingly, when DIPEA was used as a terminal reductant under these conditions, the product derived from the addition of styrene radical anion into the ketone was observed in approximately 30% yield.



		Reductant			
84% RSM	8% RSM	NaCHO	**0%**	2%	**10%**
50% RSM	0% RSM	DIPEA	**0%**	4%	**21%**

Summary of Conditions Evaluated in Section 1.

Mediated Electrolysis: A mediator that is sufficiently reducing to activate both substrates could, in principle, drive productive annulation since SET to the ketone would be followed by rapid β-scission. However, even a comparatively mild reductant (pyrene radical anion) efficiently catalyzes styrene hydrogenation before SET to the ketone is even thermodynamically accessible (the barrier to SET from pyrene radical anion to Ket-1 was calculated to be 34 kcal/mol). This outcome confirms that the difference in substrate reduction potentials is large enough to preclude access to the requisite ketyl radical in the presence of styrene under a mediated electrolysis manifold.

Direct Electrolysis: If reversible SET between two substrates is thermodynamically accessible, selective activation of the harder to reduce substrate can be achieved via a Curtin-Hammett scenario. By cyclic voltammetry styrene is observed to be reduced approximately 300mV more positive than Ket-1, indicating that styrene radical anion will be preferentially generated under direct electrolysis. Therefore, these conditions test whether styrene radical anion itself is a competent SET reductant to promote the model reaction. Notably, the barrier for SET from styrene radical anion to the ketone was computed to be 27.5 kcal/mol, suggesting this pathway may be accessible under the reaction conditions, which are heated to 40 °C. However, direct electrolysis affords exclusively hydrogenated styrene with minimal ketone conversion.

Sodium Metal: While thermal reductants like sodium metal are sufficiently potent to reduce both substrates, they nonetheless are ineffective at promoting the desired annulation reaction. This is because SET from potent thermal reductants is intrinsically irreversible, preventing recovery of styrene radical anion. We further suspect that the accumulation of styrene radical anion can lead to addition side reactions, contributing to the poor mass balance of this reaction.

Conventional Photoredox: Since photoinduced SET is followed by fast and favorable BET, photoreductants can be selective for the activation of substrates that fragment upon SET reduction. However, despite the rapid downstream fragmentation step, classic photoreductants such as PTH do not promote the annulation because they are insufficiently reducing to access the ketyl radical.

Super-potent Photoredox: Our mechanistic proposal is that the observed selectivity for annulation over styrene hydrogenation should not be tied specifically to polycyclic aromatic hydrocarbon electrophotocatalysts. Rather, any photoreductant sufficiently potent to indiscriminately reduce both substrates while retaining fast and favorable back electron transfer could, in principle, circumvent redox potential control. The Melchiorre thiolate system supports this hypothesis and shows that radical coupling is feasible, even without extensive optimization. This result is particularly notable given the difference in active reductant between our system (solvated electrons) and Melchiorre's (the thiolate excited state), which indicates these design principles will be conserved across various potent photoreductant systems.

2. Cyclic Voltammetry Studies

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) and a platinum wire counter electrode. The potentials were measured versus an $Ag/AgNO_3$ (0.01 M in MeCN with 0.1 M n-Bu_4NPF_6) reference electrode (all electrodes from Pine Research) and internally referenced via the ferrocene/ferrocenium couple.

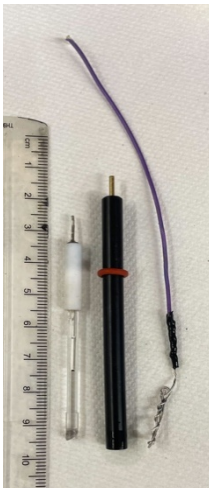


Figure S1.4 Electrodes for CV studies. (left) Reference electrode (middle) working electrode (right) counter electrode



Figure S1.5 Experimental set up for CV studies.

Comment on CV setup.

The setup used mirrors a recent report in the literature from Boucher and coworkers (https://chemrxiv.org/doi/full/10.26434/chemrxiv-2025-7h38h-v2). To mitigate the effects of heating, the cell was placed in a room-temperature water bath. The Kessil lamp (390 nm) was turned on as the measurement was initiated. The working electrode was placed 3 mm above the bottom of the cell, and the light was placed 3 mm below the bottom the cell. Placing the working electrode ~30 mm above the bottom of the cell led to minimal changes in current upon irradiation.

Data Analysis

The following voltammograms were collected either in the dark or upon irradiation with 390 nm LEDs. Upon irradiation with 390 nm, there is a slight increase in the cathodic current and decrease in the anodic current. These changes are consistent with the impact of convection due to heating from the lamp. In this process, a finite diffusion layer has been used to describe the voltammogram of the photocatalyst. For an extended discussion of the underlying theoretical treatment see: *J. Phys. Chem. Lett*. 2020, 11, 6097−6104. Moreover, our interpretation of these data draws on prior reports using CV to probe the photoactivity of radical anions. For more details see: *ACS Catal.* 2025, 15, 16938−16952.

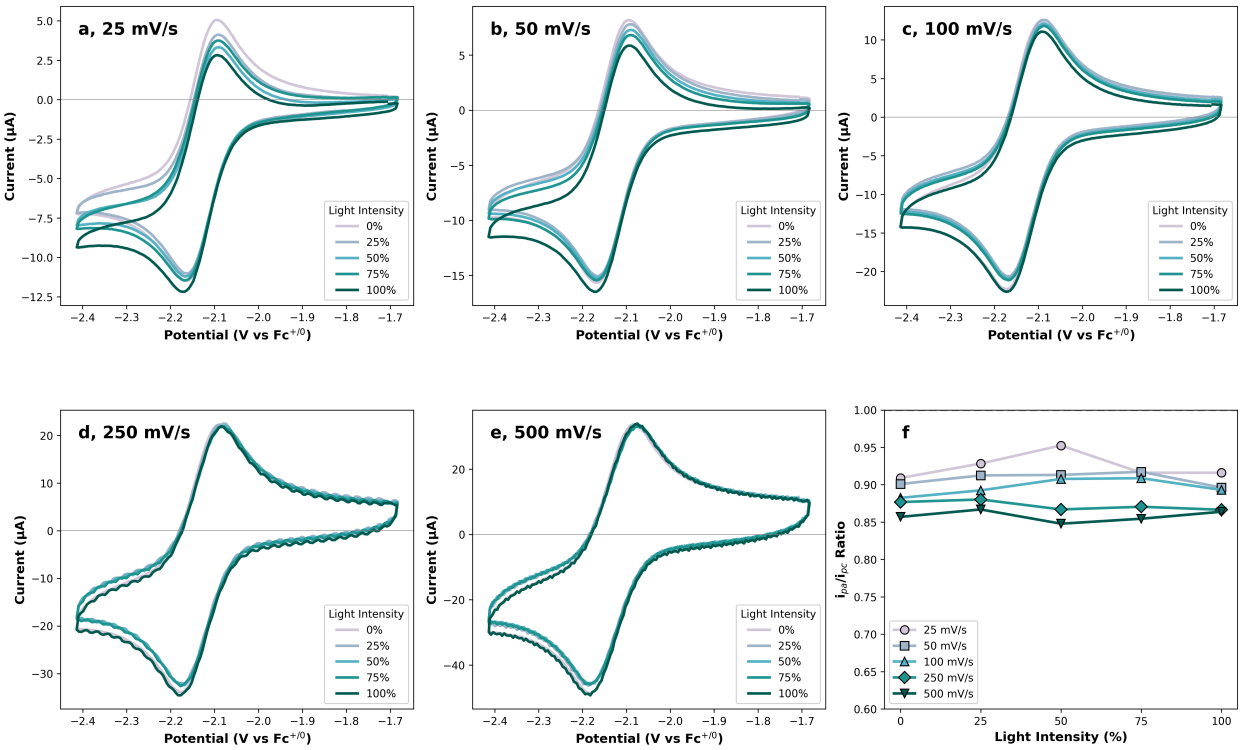


Figure S1.6 CV of **Per** (1 mM) in DMF containing 0.1 M $TEAPF_6$ at various light intensities (0%, 25%, 50%, 75%, 100%) with a 390 nm Kessil lamp. (a) 25 mV/s; (b) 50 mV/s; (c) 100 mV/s; (d) 250 mV/s; (e) 500 mV/s; (f) impact of light intensity on the ratio of peak anodic to peak cathodic current (i_pa/i_pc) for all scan rates. Different marker shapes in panel (f) represent different scan rates: circles (25 mV/s), squares (50 mV/s), upward triangles (100 mV/s), diamonds (250 mV/s), and downward triangles (500 mV/s). Lines are drawn to guide the eyes.

Discussion: Perylene exhibits a reversible reduction feature centered at –2.1 V vs Fc/Fc^+, representing the one electron reduction of **Per** to **Per**$^{\bullet-}$**.** Upon irradiation, the CV remains reversible despite the propensity of **Per**$^{\bullet-}$ to eject an electron into solvent upon irradiation (as indicated by TA spectroscopy.) In principle, formation of a solvated electron generates neutral perylene, which could be then reduced at the electrode, leading to catalytic current. However, no significant catalytic current is observed, with the slight loss of reversibility being attributed to convection due to heating from the light. These data therefore indicate that recombination of the solvated electron with **Per** is fast at the scan rate used for this study.

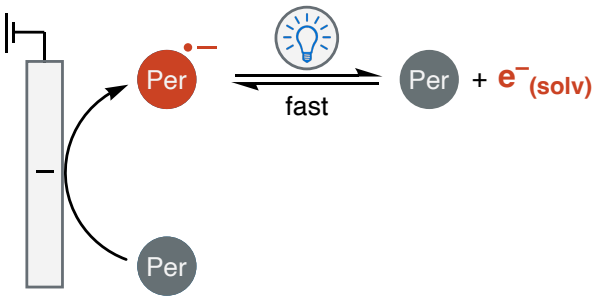


Figure S1.7. Rapid capture of solvated electrons by perylene during CV experiments in the light. Recombination was measured to occur at the diffusion limit by transient absorption spectroscopy ($k_{ET} = 8\times10^{10}\ M^{-1}s^{-1}$)

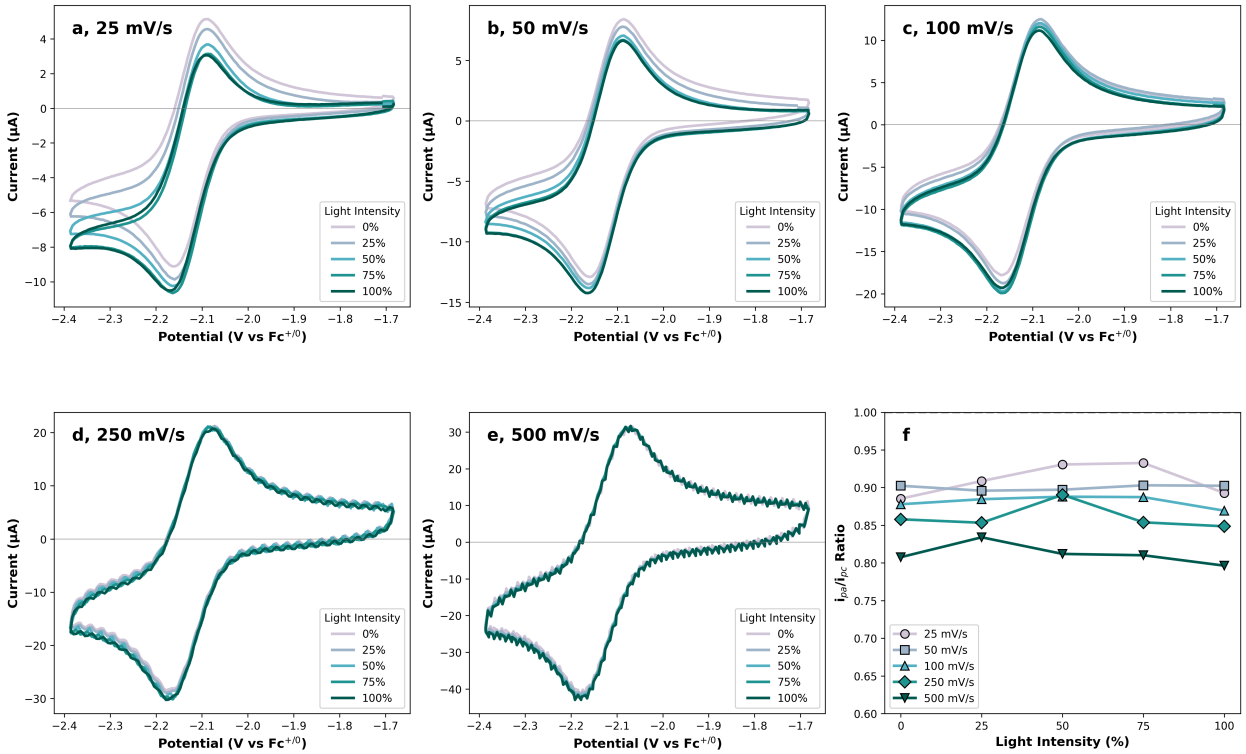


Figure S1.8 CV of **Per** (1 mM) in DMF containing 100 mM styrene and 0.1 M $TEAPF_6$ at various light intensities (0%, 25%, 50%, 75%, 100%) with a 390 nm Kessil lamp. (a) 25 mV/s; (b) 50 mV/s; (c) 100 mV/s; (d) 250 mV/s; (e) 500 mV/s; (f) impact of light intensity on the ratio of peak anodic to peak cathodic current (i_pa/i_pc) for all scan rates. Different marker shapes in panel (f) represent different scan rates: circles (25 mV/s), squares (50 mV/s), upward triangles (100 mV/s), diamonds (250 mV/s), and downward triangles (500 mV/s). Lines are drawn to guide the eyes.

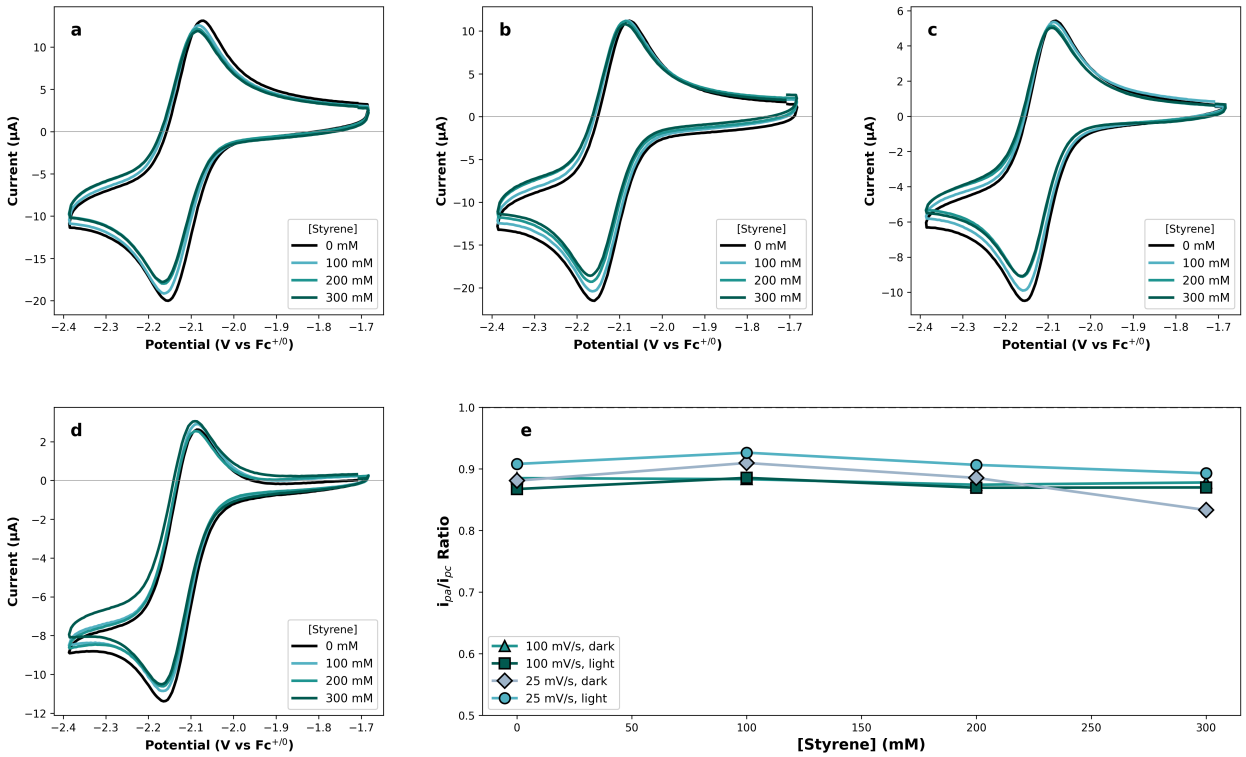


Figure S1.9 CV of **Per** (1 mM) in DMF containing various concentrations of styrene and 0.1 M $TEAPF_6$. (a) 100 mV/s, no irradiation; (b) 100 mV/s, 100% irradiation; (c) 25 mV/s, 0% irradiation; (d) 25 mV/s, 100% irradiation; (e) impact of styrene concentration on the ratio of peak anodic to peak cathodic current. Lines are drawn to guide the eyes.

Discussion: The voltammogram of perylene remains unchanged upon the addition of 50 equivalents of styrene, indicating no background thermal reduction of styrene from Per•–. Upon irradiation, the CV remains reversible. This indicates that either there is no photochemical olefin reduction, or that BET from styrene radical anion is fast relative to the scan rate used for this study, regenerating Per•– before Per can be reduced again at the cathode. Based on quenching studies with styrene, we observed that excitation of Per•– induces fast, diffusion-limited olefin reduction (kset = 3×10^{10} $M^{-1}s^{-1}$). Taken together, these electrochemical and spectroscopic data support our model that the olefinic coupling partner is reduced but then undergoes rapid BET.

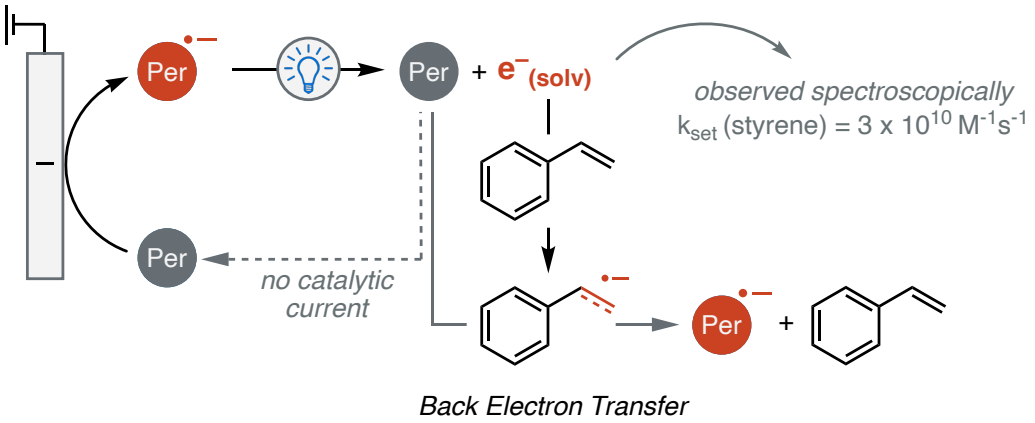


Figure S1.10 Rapid BET from styrene radical anion to perylene prevents catalytic current.

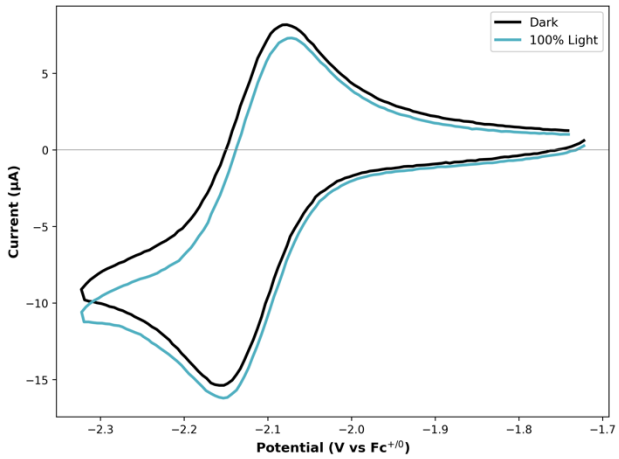


Figure S1.11 CV of Per (1 mM) in DMF containing styrene (50 mM), water (500 mM), and 0.1 M $TEAPF_6$ at 100 mV/s. Black line: dark; cyan line: 100% irradiation with a 390 nm Kessil lamp. Potentials are referenced vs $Fc^{+/0}$.

Discussion: The voltammogram of perylene remains unchanged upon the addition of 50 equivalents of styrene and 500 equivalents of water, indicating that protonation of styrene radical anion does not drive thermal olefin reduction. Upon irradiation, the voltammogram of perylene remains reversible. Transient absorption measurements indicate that styrene radical anion is readily formed under these conditions. The retention of reversibility in the Per voltammogram indicates that BET is faster than protonation of styrene radical anion by water. These observations are consistent with the computed barriers of the two steps (shown below).

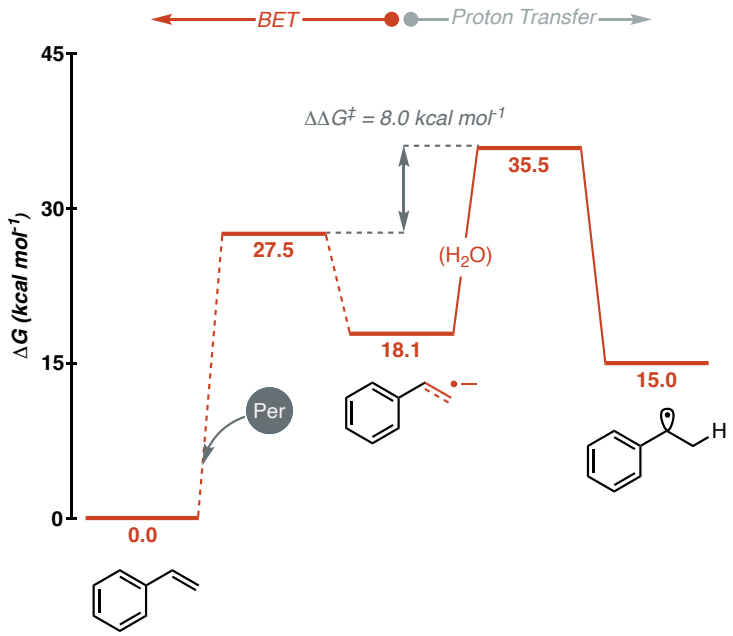


Figure S1.12 Computed barriers for protonation and BET from styrene radical anion.

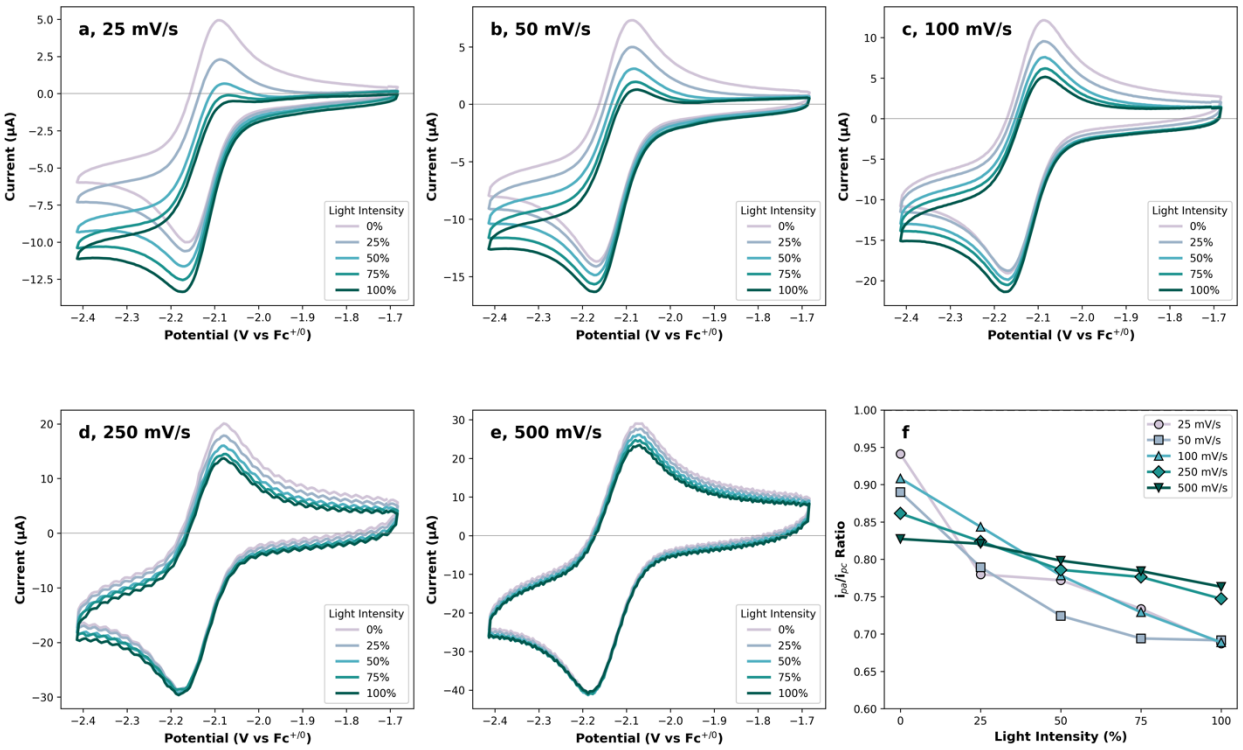


Figure S1.13 CV of **Per** (1 mM) in DMF containing 100mM Ket-1 (1-(2,2-dimethylcyclopropyl)propan-1-one) and 0.1 M $TEAPF_6$ at various light intensities (0%, 25%, 50%, 75%, 100%) with a 390 nm Kessil lamp. (a) 25 mV/s; (b) 50 mV/s; (c) 100 mV/s; (d) 250 mV/s; (e) 500 mV/s; (f) impact of light intensity on the ratio of peak anodic to peak cathodic current (i_pa/i_pc) for all scan rates. Different marker shapes in panel (f) represent different scan rates: circles (25 mV/s), squares (50 mV/s), upward triangles (100 mV/s), diamonds (250 mV/s), and downward triangles (500 mV/s). Lines are drawn to guide the eyes.

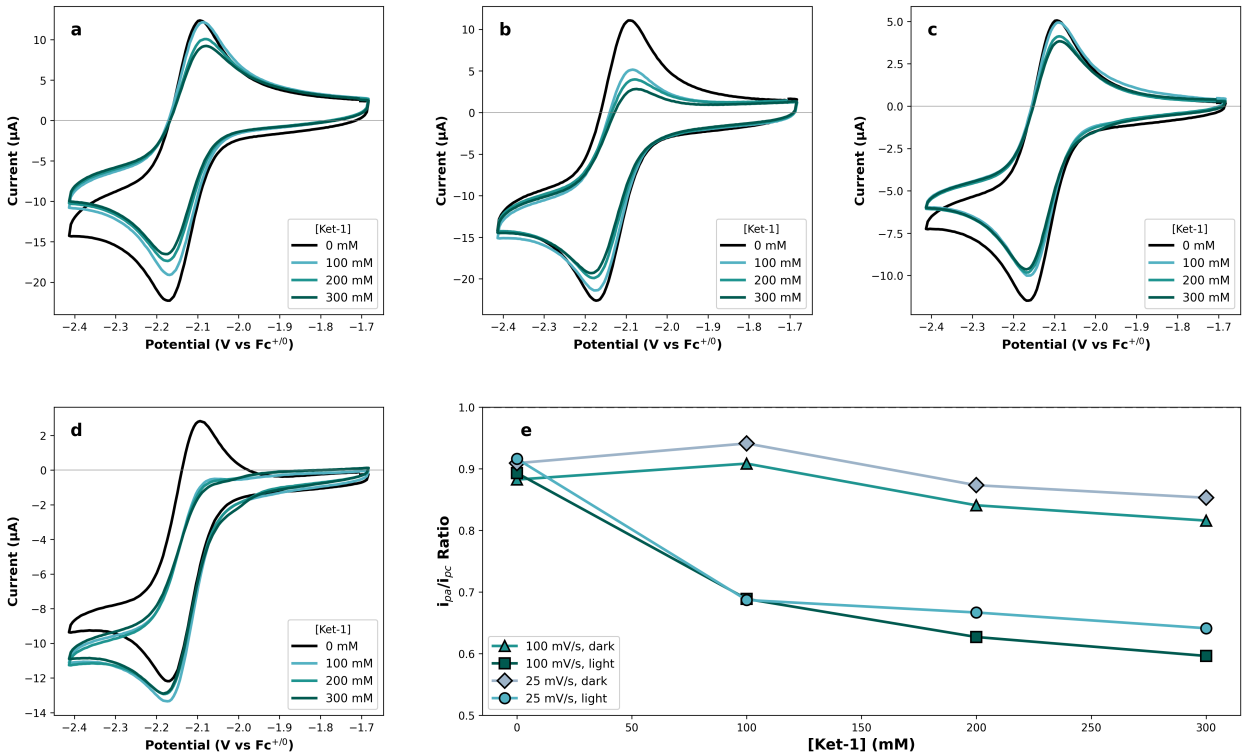


Figure S1.14 CV of **Per** (1 mM) in DMF containing various concentrations of Ket-1 (1-(2,2-dimethylcyclopropyl)propan-1-one) and 0.1 M $TEAPF_6$. (a) 100 mV/s, no irradiation; (b) 100 mV/s, 100% irradiation; (c) 25 mV/s, 0% irradiation; (d) 25 mV/s, 100% irradiation; (e) impact of Ket-1 concentration on the ratio of peak anodic to peak cathodic current. Lines are drawn to guide the eyes.

Discussion: The voltammogram of perylene remains unchanged upon the addition of 50 equivalents of Ket-1, indicating no background thermal reduction of Ket-1 from Per•–. Upon irradiation, the cathodic current increases with loss of the anodic feature. TA studies indicate that photochemically generated solvated electrons rapidly reduce the ketone substrate (kset = 4 × 10^9 $M^{-1}s^{-1}$). These data are consistent with a mechanism in which ketone reduction is followed by rapid β-scission of the nascent ketyl radical anion, which outcompetes BET and turns over perylene. These findings are consistent with the computed barriers for BET and β-scission, which are shown below.

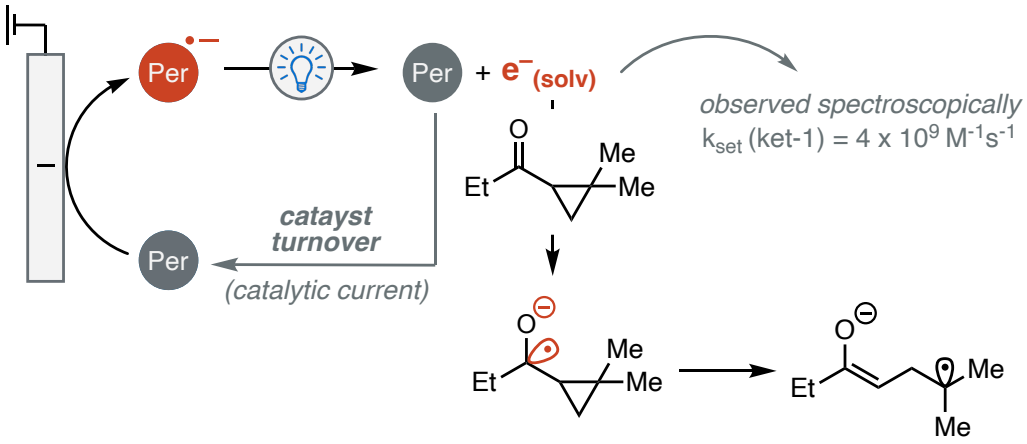


Figure S1.15. β-scission of the ketyl radical outcompetes BET, resulting in catalytic current.

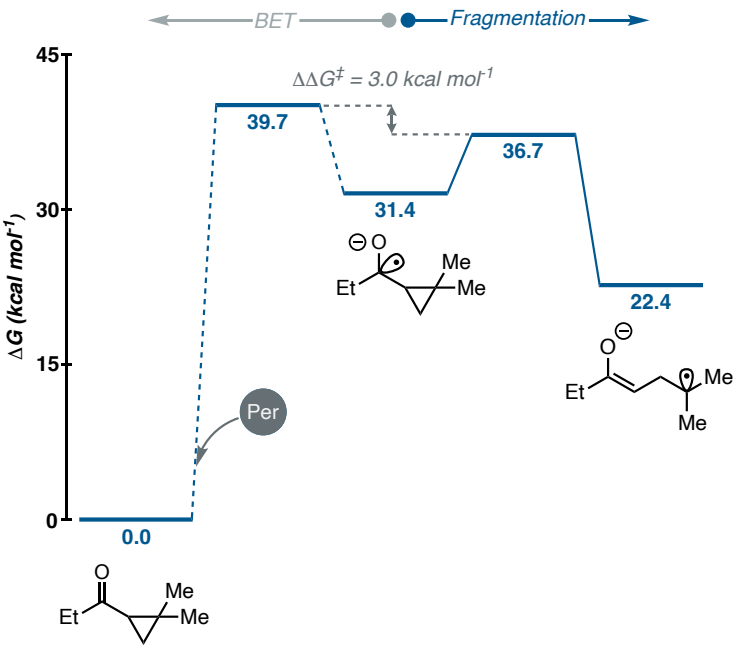


Figure S1.16. Computed barriers for β-scission and BET from the ketyl radical anion.

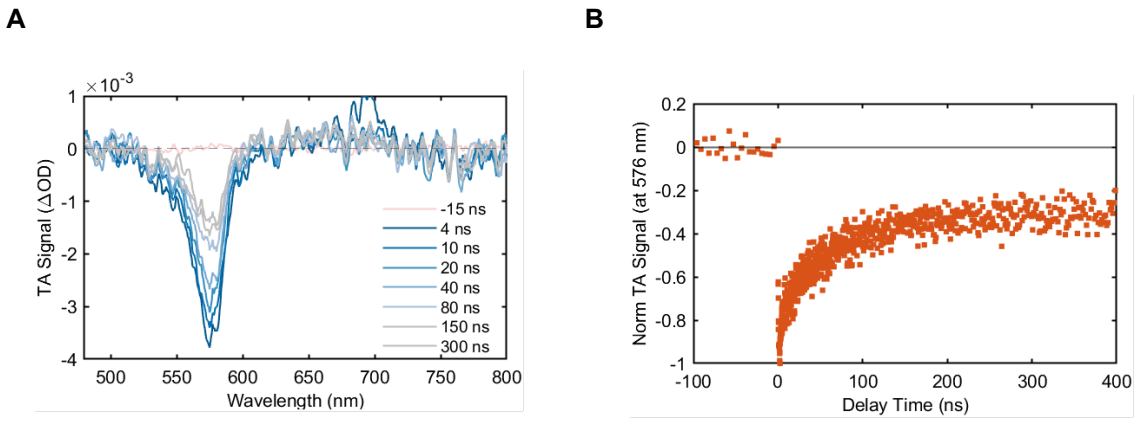


Figure S1.17 (A) Transient absorption spectra at representative delay times as indicated in the legend. Data were acquired following 460 nm excitation of perylene radical anion in the presence of 0.9 mM Ket-1. (B) Normalized transient absorption trace of the ground-state bleach (GSB) of the perylene radical anion at 576 nm. Incomplete recovery of the GSB, reflected by a persistent offset, is consistent with irreversible electron transfer.

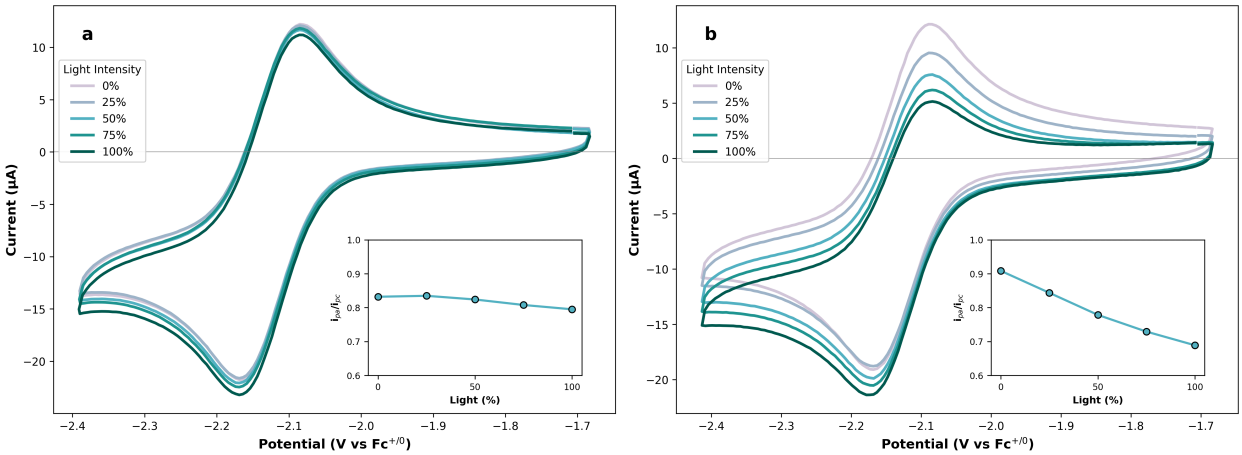


Figure S1.18 CV of **Per** (1 mM) in DMF containing 100 mM ketone substrate and 0.1 M $TEAPF_6$ at 100 mV/s with various light intensities (0%, 25%, 50%, 75%, 100%). (a) Cyclohexylmethyl ketone; (b) Ket-1. Insets show the impact of light intensity on the ratio of peak anodic to peak cathodic current (i_pa/i_pc). Lines are drawn to guide the eyes.

Discussion: The voltammogram of perylene remains unchanged upon the addition of 100 equivalents of cyclohexylmethyl ketone, indicating no background thermal reduction of the ketone from Per•–. Upon irradiation, the voltammogram of perylene remains largely unchanged. The retention of reversibility upon irradiation indicates that the ketyl radical undergoes fast BET with perylene on the time scale of the CV. These data contrast the electrochemical data collected with Ket-1, in which catalytic current is observed upon irradiation. We therefore hypothesize that ring opening of the nascent ketyl radical anion is mechanistically required to drive catalyst turnover. Consistent with our model, no catalytic current is observed with cyclohexylmethyl ketone because it does not undergo fragmentation upon SET reduction.

3. Gas Chromatograph Calibration Curves

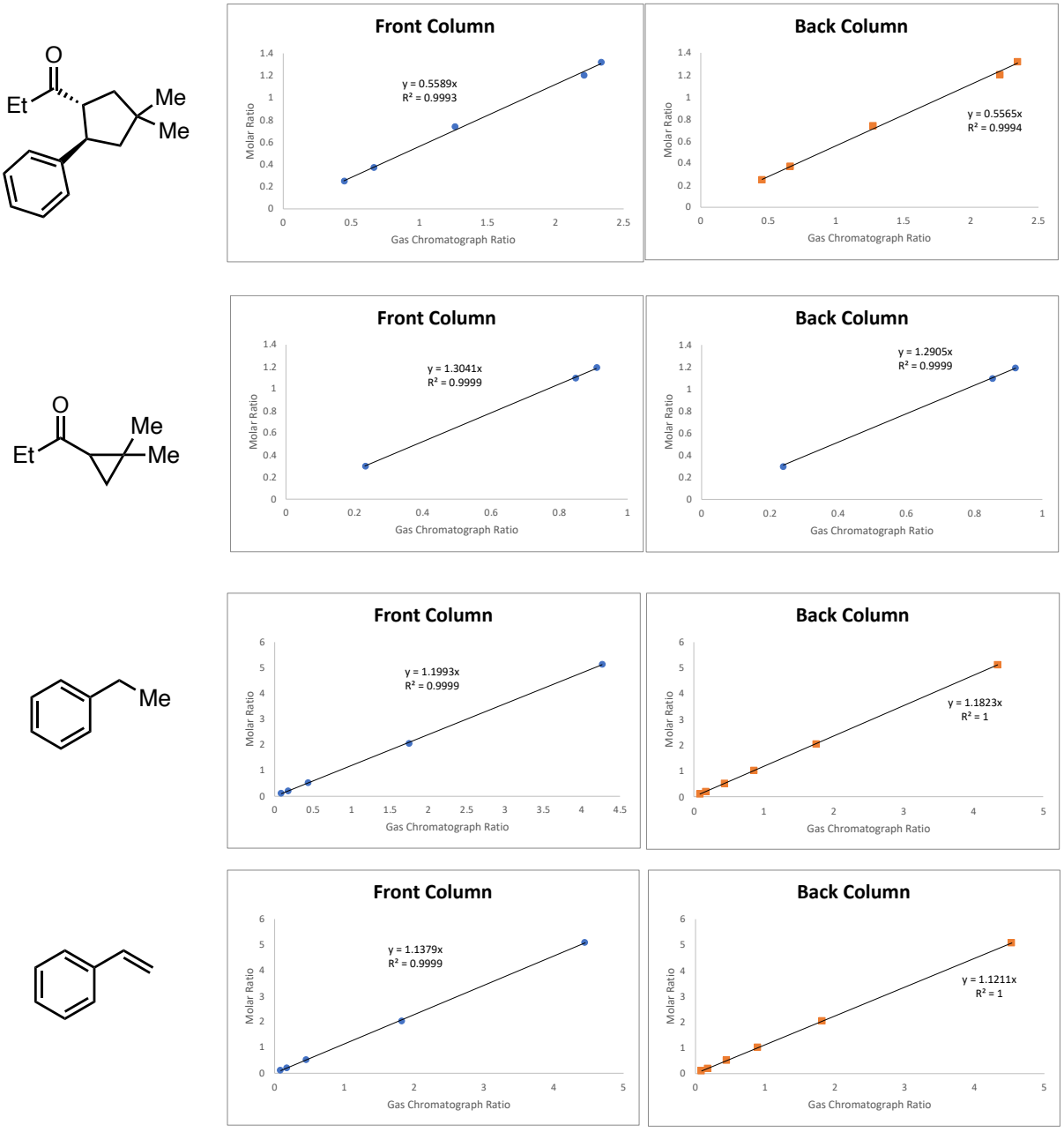
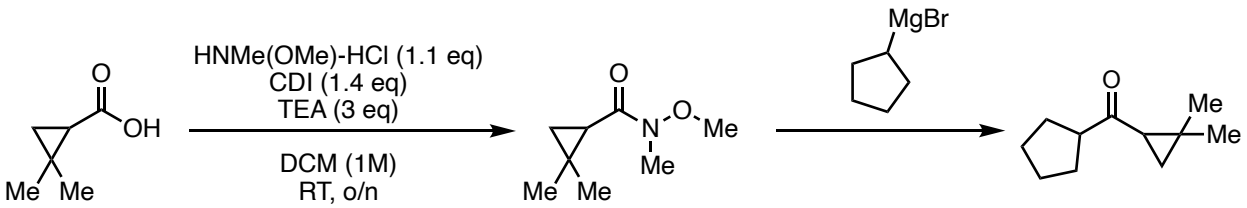


Figure S1.19. GC calibration cures, using mesitylene as in internal standard.

4. Substrate Synthesis

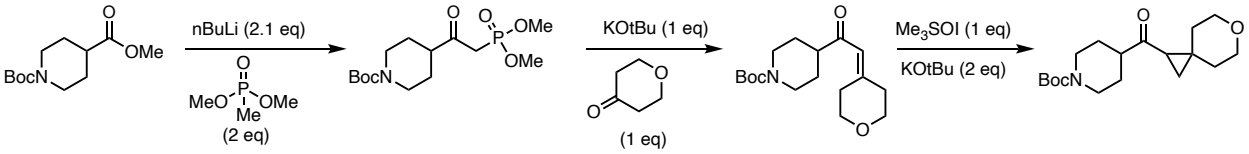
cyclopentyl(2,2-dimethylcyclopropyl)methanone



Step 1: Adapted from a protocol developed by Schoenebeck and co-workers (ACIE 2023, 62 (7), e202211167). 2,2-dimethylcyclopropane-1-carboxylic acid (5 g, 44 mmol) was added to a dry flask in 50 mL DCM. N,O-dimethylhydroxylamine hydrochloride (4.7 g, 48 mmol), CDI (10 g, 62 mmol), and triethylamine (18 mL, 130 mmol) were added dropwise, and the mixture was stirred overnight. The reaction was diluted with brine and extracted with ethyl acetate (3 x 100 mL). The combined organic layers were dried over sodium sulfate and concentrated under reduced pressure. The crude mixture was then used directly in the next step without further purification.

Step 2: Adapted from a protocol developed by Procter and co-workers (JACS 2024, 146, 18, 12799–12807). To a flame-dried flask, N-methoxy-N,2,2-trimethylcyclopropane-1-carboxamide (1.32 g, 8.37 mmol) and THF (50 mL, 0.15 M) were charged under nitrogen. The reaction mixture was chilled to -78 °C and a solution of cyclopentylmagnesium bromide in THF was added (7.53 mmol, 2 M). The reaction was allowed to come to room temperature and stirred overnight. The reaction was quenched with saturated NH_4Cl (50 mL) and extracted with diethyl ether (3 x 100 mL). The combined organic layers were dried over sodium sulfate and concentrated under reduced pressure. The product was purified by flash chromatography (ethyl acetate in hexanes) to provide the title compound as a clear liquid (40% yield over 2 steps). ^1H NMR (500 MHz, $CDCl_3$) δ 2.95 (tt, J = 8.6, 7.3 Hz, 1H), 1.91–1.52 (m, 8H), 1.24 (dd, J = 5.6, 3.9 Hz, 1H), 1.19 (s, 3H), 1.05 (s, 3H), 0.79 (dd, J = 7.5, 3.9 Hz, 1H), consistent with reported spectra.

tert-butyl 4-(6-oxaspiro[2.5]octane-1-carbonyl)piperidine-1-carboxylate

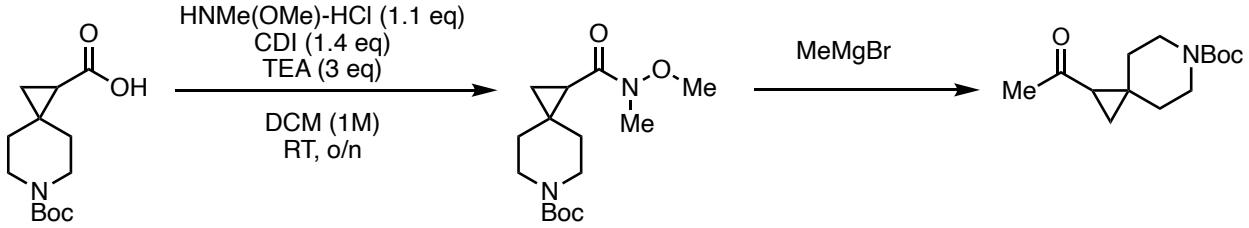


Step 1: Adapted from a protocol developed by Sherer and co-workers (US2016075711A1·2016-03-17). A solution of dimethyl methylphosphonate (40 mmol, 5 g) in THF (30 mL) was added to a dry flask and cooled to –78 °C. A solution of n-butyllithium (42 mmol, 17 mL, 2.5 M) was added and the mixture was stirred for 30 minutes at –78 °C. 1-(tert-butyl) 4-methyl piperidine-1,4-dicarboxylate (4.9 g, 20 mmol) was added and the reaction was stirred overnight at room temperature. The reaction mixture was quenched with water and extracted with ethyl acetate (3 x 100 mL). The combined organic layers were dried over sodium sulfate and concentrated under reduced pressure. The crude mixture was then used directly in the next step without further purification.

Step 2: Adapted from a protocol developed by Procter and co-workers (JACS 2024, 146, 18, 12799–12807). A dry 100 mL flask was charged with potassium tert-butoxide (1.4 g, 12.5 mmol) and THF (25 mL) and flushed with nitrogen. A solution of tert-butyl 4-(2-(dimethoxyphosphoryl)acetyl)piperidine-1-carboxylate (12.5 mmol) in THF was added dropwise, and the mixture was stirred at room temperature for 1 hr. Tetrahydro-4H-pyran-4-one was added in one portion and the mixture was heated to 70 °C and stirred overnight. The reaction mixture was diluted with brine (100 mL) and extracted with ethyl acetate (3 x 100 mL). The combined organic layers were dried over sodium sulfate and concentrated under reduced pressure. The intermediate was then purified by flash chromatography (ethyl acetate in hexanes) before carrying forward to the next step (21% yield over 2 steps). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.03 (t, J = 1.3 Hz, 1H), 4.14–3.96 (m, 2H), 3.71 (t, J = 5.5 Hz, 2H), 3.64 (t, J = 5.6 Hz, 2H), 2.94–2.87 (m, 2H), 2.72 (t, J = 12.5 Hz, 2H), 2.41 (tt, J = 11.3, 3.6 Hz, 1H), 2.28–2.22 (m, 2H), 1.73 (d, J = 13.3 Hz, 2H), 1.46 (dtd, J = 13.5, 11.6, 4.3 Hz, 2H), 1.38 (s, 9H).

Step 3: Adapted from a protocol developed by Procter and co-workers (JACS 2024, 146, 18, 12799–12807). tert-butyl 4-(2-(tetrahydro-4H-pyran-4-ylidene)acetyl)piperidine-1-carboxylate (4.35 mmol), dimethylmethanesulfinic iodide (8.7 mmol, 1.9 g), and potassium tert-butoxide (0.98 g, 8.7 mmol) were added to a vial with DMSO (15 mL) and stirred vigorously overnight at room temperature. The reaction mixture was diluted with brine (100 mL) and extracted with ethyl acetate (3 x 100 mL). The combined organic layers were dried over sodium sulfate and concentrated under reduced pressure. The title compound was purified as a solid by flash chromatography (ethyl acetate in hexanes) (70% yield, 1 g). ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.24–4.06 (m, 3H), 3.76 (ddd, J = 10.4, 6.9, 4.5 Hz, 1H), 3.69 (ddd, J = 11.2, 7.7, 3.3 Hz, 1H), 3.65–3.54 (m, 2H), 2.80 (q, J = 13.7 Hz, 2H), 2.63 (tt, J = 11.5, 3.7 Hz, 1H), 1.97–1.78 (m, 3H), 1.67–1.40 (m, 16H), 1.37–1.32 (m, 1H), 0.94 (dd, J = 7.6, 4.1 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 208.99, 154.68, 79.63, 67.97, 67.30, 50.08, 37.43, 32.25, 31.85, 28.69, 28.45, 27.87, 27.35, 21.43. HRMS (ESI): $[M+Na]^+$ calcd. 346.1989, found 346.1988 (0.3 ppm).

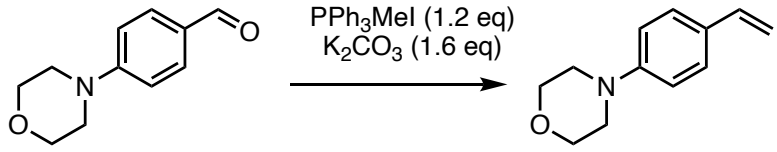
tert-butyl 1-acetyl-6-azaspiro[2.5]octane-6-carboxylate



Step 1: Adapted from a protocol developed by Schoenebeck and co-workers (ACIE 2023, 62 (7), e202211167). 6-(tert-butoxycarbonyl)-6-azaspiro[2.5]octane-1-carboxylic acid (5 g, 19.6 mmol) was added to a dry flask in 20 mL DCM. N,O-dimethylhydroxylamine hydrochloride (2.1 g, 21.5 mmol), CDI (4.45 g, 27 mmol), and triethylamine (8.2 mL, 60 mmol) were added dropwise, and the mixture was stirred overnight. The reaction was diluted with brine and extracted with ethyl acetate (3 x 100 mL). The combined organic layers were dried over sodium sulfate and concentrated under reduced pressure. The crude mixture was then used directly in the next step without further purification.

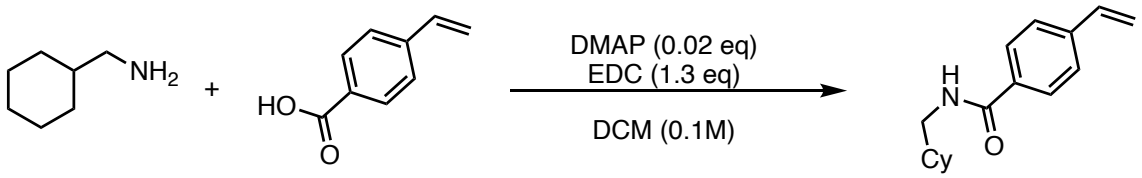
Step 2: Adapted from a protocol developed by Procter and co-workers (JACS 2024, 146, 18, 12799–12807). To a flame-dried flask, tert-butyl 1-(methoxy(methyl)carbamoyl)-6-azaspiro[2.5]octane-6-carboxylate (2.4 g, 8.1 mmol) and THF (40 mL, 0.2 M) were charged under nitrogen. The reaction mixture was chilled to –78 °C and a solution of methylmagnesium bromide in THF was added (11 mmol, 3 M). The reaction was allowed to come to room temperature and stirred overnight. The reaction was quenched with saturated NH_4Cl (50 mL) and extracted with diethyl ether (3 x 100 mL). The combined organic layers were dried over sodium sulfate and concentrated under reduced pressure. The product was purified by flash chromatography (ethyl acetate in hexanes) to provide the title compound as a solid (40% yield over 2 steps). ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.59–3.49 (m, 1H), 3.47–3.38 (m, 2H), 3.23–3.12 (m, 1H), 2.31 (d, J = 1.7 Hz, 3H), 1.96–1.91 (m, 1H), 1.69–1.40 (m, 14H), 1.38–1.32 (m, 1H), 0.92 (dd, J = 7.8, 4.2 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 205.86, 154.85, 79.51, 60.37, 36.57, 33.70, 32.48, 32.02, 28.44, 27.55, 21.05 (d, J = 3.9 Hz), 14.20. HRMS (ESI): $[M+H]^+$ calcd. 254.1751, found 254.1746 (2.0 ppm).

4-(4-vinylphenyl)morpholine



Adapted from a protocol developed by Thomas (Adv Synth Catal 2014, 356, 584–590). To a flame-dried flask, a solution of aldehyde (10 mmol), base (16 mmol), and PPh3BnBr (12 mmol) in dioxane was refluxed until complete as determined by TLC. The reaction was quenched with water and extracted with EtOAc (3 x 100 mL). The combined organic fractions were washed with brine. The crude product was purified by flash chromatography to afford the title compound (850 mg, 45%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40–7.33 (m, 2H), 6.90 (d, J = 8.3 Hz, 2H), 6.67 (dd, J = 17.6, 10.9 Hz, 1H), 5.63 (dd, J = 17.6, 1.0 Hz, 1H), 5.16–5.10 (m, 1H), 3.89 (t, J = 4.8 Hz, 4H), 3.25–3.17 (m, 4H), consistent with reported spectra.

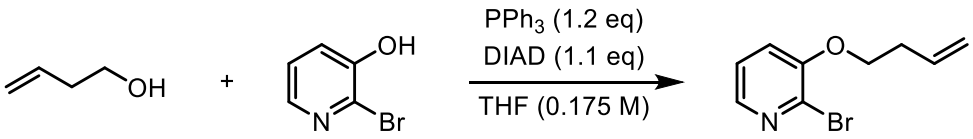
N-(cyclohexylmethyl)-4-vinylbenzamide



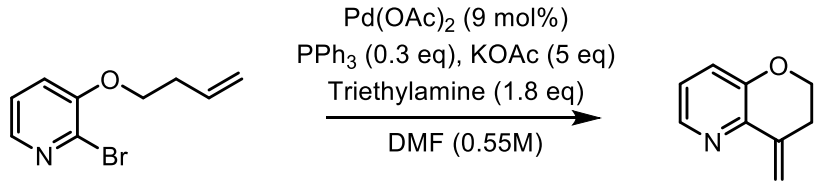
Adapted from a protocol developed by Studer and co-workers (J. Am. Chem. Soc. 2021, 143, 13, 4903–4909). A flame-dried 250-mL round-bottom flask under inert atmosphere was charged with 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDCI) (2.9 g, 1.5 equiv, 15 mmol), DMAP (24 mg, 0.02 equiv, 0.20 mmol), and 4-vinylbenzoic acid (1.5 g, 1 equiv, 10 mmol). Anhydrous DCM (100 mL) was added, followed by cyclohexylmethanamine (1.1 g, 1.3 mL, 1 equiv, 10 mmol). The mixture was allowed to stir for 12 hours at room temperature. The crude mixture was washed with saturated sodium bicarbonate (100 mL), 1 M HCl (100 mL), and brine (100 mL). The organic layer was collected, dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure. The product was purified by recrystallization from dichloromethane to obtain 1.6 g (66% yield, white solid) of the product. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (d, J = 9.2 Hz, 2H), 7.44 (d, J = 9.3 Hz, 2H), 6.73 (dd, J = 17.6, 10.9 Hz, 1H), 6.24 (s, 1H), 5.82 (d, J = 17.6 Hz, 1H), 5.34 (d, J = 10.9 Hz, 1H), 3.29 (t, J = 6.4 Hz, 2H), 1.82–1.70 (m, 4H), 1.70–1.63 (m, 1H), 1.58 (m, 1H), 1.31–1.11 (m, 3H), 0.99 (m, 2H), consistent with reported spectra.

4-methylene-3,4-dihydro-2H-pyrano[3,2-b]pyridine

Step 1:



Step 2:

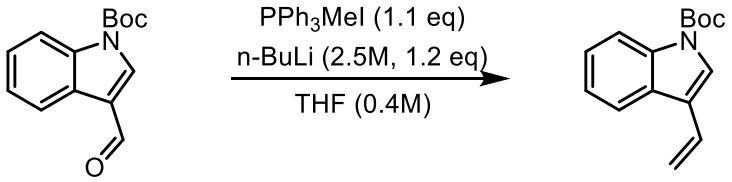


Compound was synthesized via a Mitsunobu reaction (method reported by Bridger US 2004/0019058 A1) and an intramolecular Heck coupling (method reported by Spear and Burdi WO 2022/204150 A1).

Step 1: To a solution of triphenylphosphine (9.44 g, 1.2 equiv, 36.0 mmol), β-vinylethanol (2.16 g, 2.58 mL, 1 equiv, 30.0 mmol), and 3-Pyridinol, 2-bromo- (5.22 g, 1 equiv, 30.0 mmol) in anhydrous THF (170 mL, 0.175 M) at 0 °C was added diisopropyl azodicarboxylate (DIAD) (6.67 g, 6.51 mL, 1.1 equiv, 33.0 mmol) very slowly. The ice bath was removed after addition and the mixture was allowed to stir at 50 °C for 18 hours under nitrogen. The reaction mixture was diluted with EtOAc (100 mL) and washed with sat. $NaHCO_3$ (2 x 50 mL), brine (2 x 50 mL), and dried over Na_2SO_4. The crude product was concentrated in vacuo and purified via flash chromatography (Rf = 0.3 in 15% EtOAc in hexanes) to afford an oil (6.30 g, 92% yield). ^1H NMR (500 MHz, $CDCl_3$) δ 7.98 (dd, J = 4.6, 1.6 Hz, 1H), 7.20 (dd, J = 8.1, 4.6 Hz, 1H), 7.12 (dd, J = 8.1, 1.6 Hz, 1H), 5.94 (ddt, J = 17.0, 10.2, 6.8 Hz, 1H), 5.21 (dq, J = 17.2, 1.7 Hz, 1H), 5.15 (ddt, J = 10.3, 2.2, 1.2 Hz, 1H), 4.08 (t, J = 6.6 Hz, 2H), 2.62 (qt, J = 6.7, 1.4 Hz, 2H).

Step 2: 2-bromo-3-(but-3-en-1-yloxy)pyridine (3.00 g, 1 equiv, 13.2 mmol), triphenylphosphine (1.03 g, 0.3 equiv, 3.95 mmol), potassium acetate (6.45 g, 5 equiv, 65.8 mmol), triethylamine (3.92 g, 3.63 mL, 1.8 equiv, 23.7 mmol), and palladium(II) acetate (266 mg, 0.09 equiv, 1.18 mmol) were added under nitrogen atmosphere to a flame-dried round-bottom flask. The solids were dissolved in DMF (25 mL, 0.55 M). The resulting reaction mixture was stirred at 105 °C for 36 hours. After cooling to room temperature, the mixture was diluted with water (100 mL) and extracted with ethyl acetate (3 × 25 mL). The combined organic layers were washed with brine (3 × 5 mL), dried over sodium sulfate, filtered, and concentrated to dryness in vacuo. The crude product was purified by flash chromatography (5% EtOAc in pentane) to afford the product as an oil (262 mg, 13.5% yield). ^1H NMR (500 MHz, $CDCl_3$) δ 8.20 (dd, J = 4.4, 1.6 Hz, 1H), 7.15 (dd, J = 8.3, 1.6 Hz, 1H), 7.10 (dd, J = 8.3, 4.4 Hz, 1H), 6.20 (q, J = 1.5 Hz, 1H), 5.07 (q, J = 1.7 Hz, 1H), 4.28–4.22 (m, 2H), 2.85–2.79 (m, 2H).

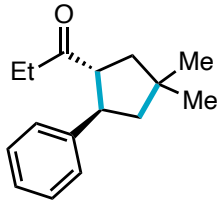
tert-butyl 3-vinyl-1H-indole-1-carboxylate



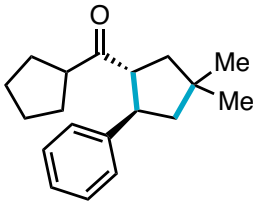
Compound was synthesized via a Wittig olefination (method adapted from Meek ACS Catal. 2019, 9, 7, 5881–5889).

To a flame-dried 250-mL round-bottom flask equipped with a magnetic stir bar, methyltriphenylphosphonium iodide (16.2 g, 1.1 equiv, 40.0 mmol) was added and then suspended in THF (100 mL, 0.4 M). BuLi (2.80 g, 17.5 mL, 2.5 M, 1.2 equiv, 43.6 mmol) was then added slowly and allowed to stir for 10 min. tert-Butyl 3-formyl-1H-indole-1-carboxylate (8.92 g, 1 equiv, 36.4 mmol) was added as a solid and allowed to stir for 18 h. The organics were washed with water three times and the aqueous layers were combined and extracted with Et_2O. The organic layers were combined and dried over $MgSO_4$. Solvents were removed in vacuo. The crude product was purified by flash chromatography (100% hexanes to 20:1 hexanes:Et_2O) to afford a yellow oil (4.83 g, 54% yield). ^1H NMR (500 MHz, $CDCl_3$) δ 8.18 (d, J = 8.2 Hz, 1H), 7.83–7.77 (m, 1H), 7.63 (s, 1H), 7.35 (ddd, J = 8.2, 7.2, 1.3 Hz, 1H), 7.28 (td, J = 7.5, 1.1 Hz, 1H), 6.82 (dd, J = 17.8, 11.3 Hz, 1H), 5.82 (dd, J = 17.8, 1.3 Hz, 1H), 5.33 (dd, J = 11.4, 1.3 Hz, 1H), 1.68 (s, 9H).

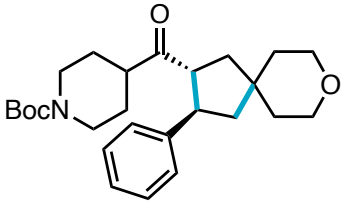
5. Product Characterization



1-(4,4-dimethyl-2-phenylcyclopentyl)propan-1-one (**1**) prepared from styrene (1.2 equiv) and 1-(2,2-dimethylcyclopropyl)propan-1-one; 43 mg (62% yield) obtained as an oil according to general procedure 1 as a single diastereomer. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38–7.13 (m, 5H), 3.54 (td, J = 10.9, 7.8 Hz, 1H), 3.19 (dt, J = 10.3, 9.0 Hz, 1H), 2.32 (dq, J = 17.8, 7.3 Hz, 1H), 2.16 (dq, J = 17.9, 7.2 Hz, 1H), 1.98 (dd, J = 12.7, 7.8 Hz, 1H), 1.90 (dd, J = 12.9, 9.2 Hz, 1H), 1.82–1.68 (m, 2H), 1.19 (s, 3H), 1.14 (s, 3H), 0.94 (t, J = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 212.89, 143.93, 128.50, 127.25, 126.32, 59.27, 50.22, 48.32, 44.80, 38.40, 36.17, 30.65, 29.84, 7.55. HRMS (ESI): $[M+H]^+$ calcd. 231.1743, found 231.1742 (0.4 ppm).

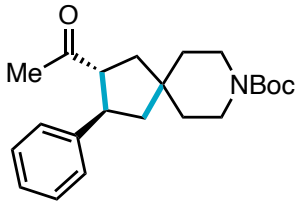


cyclopentyl(4,4-dimethyl-2-phenylcyclopentyl)methanone (**2**) prepared from styrene (1.2 equiv) and cyclopentyl(2,2-dimethylcyclopropyl)methanone as a single diastereomer according to general procedure 1, 81% yield determined by ^{1}H NMR with dibromomethane as an internal standard. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32–7.17 (m, 5H), 3.59 (td, J = 10.9, 7.8 Hz, 1H), 3.26 (dt, J = 10.3, 9.1 Hz, 1H), 2.67 (p, J = 7.4 Hz, 1H), 1.98 (dd, J = 12.7, 7.8 Hz, 1H), 1.90 (dd, J = 12.8, 9.0 Hz, 1H), 1.78–1.69 (m, 2H), 1.68–1.42 (m, 4H), 1.19 (s, 3H), 1.15 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 214.99, 143.90, 128.41, 127.21, 126.25, 59.06, 51.59, 49.83, 48.36, 45.47, 38.53, 30.73, 29.91, 28.61, 28.53, 25.97, 25.87. HRMS (ESI): $[M+H]^+$ calcd. 271.2056, found 271.2053 (1.1 ppm).

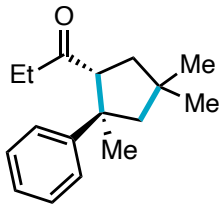


tert-butyl 4-(3-phenyl-8-oxaspiro[4.5]decane-2-carbonyl)piperidine-1-carboxylate (**3**) prepared from styrene (1.2 equiv) and tert-butyl 4-(6-oxaspiro[2.5]octane-1-carbonyl)piperidine-1-carboxylate as a single diastereomer, 92 mg (72% yield) obtained as a solid according to general procedure 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (t, J = 7.6 Hz, 2H), 7.20 (d, J = 7.4 Hz, 3H), 4.12–3.85 (m, 2H), 3.75–3.61 (m, 4H), 3.46 (td, J = 11.0, 7.2 Hz, 1H), 3.27 (q, J = 9.5 Hz, 1H), 2.67–2.48 (m, 2H), 2.29–2.12 (m, 2H), 1.94 (dd, J = 13.1, 8.6 Hz, 1H), 1.86–1.55 (m, 7H), 1.42 (s, 11H), 1.26 (td, J = 14.7, 6.4 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 213.82, 154.57, 142.73, 128.62,

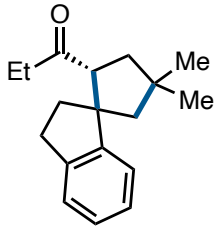
127.06, 126.75, 79.51, 65.37, 65.27, 56.87, 48.97, 48.15, 47.15, 39.85, 39.71, 38.55, 28.40, 27.18, 26.63. HRMS (ESI): $[M+Na]^+$ calcd. 450.2615, found 450.2612 (0.7 ppm).



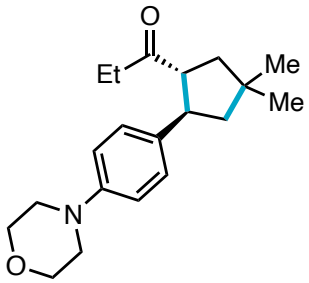
tert-butyl 2-acetyl-3-phenyl-8-azaspiro[4.5]decane-8-carboxylate (**4**) prepared from styrene (1.2 equiv) and tert-butyl 1-acetyl-6-azaspiro[2.5]octane-6-carboxylate as a single diastereomer, 58 mg (54% yield) obtained as an oil according to general procedure 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35–7.20 (m, 5H), 3.41 (q, J = 5.4 Hz, 4H), 3.19 (q, J = 9.4 Hz, 1H), 2.12 (dd, J = 13.0, 7.6 Hz, 1H), 1.99–1.85 (m, 5H), 1.69 (t, J = 12.3 Hz, 1H), 1.56 (ddd, J = 15.7, 10.8, 5.0 Hz, 3H), 1.48 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 209.96, 154.89, 143.06, 128.66, 127.19, 126.66, 79.36, 58.92, 47.69, 47.30, 40.95, 40.38, 38.70, 37.42, 30.20, 28.48. HRMS (ESI): $[M+H]^+$ calcd. 358.2377, found 358.2372 (1.4 ppm).



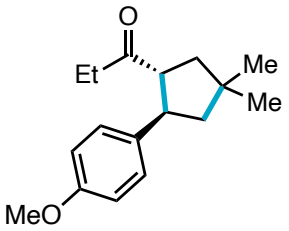
1-(2,4,4-trimethyl-2-phenylcyclopentyl)propan-1-one (**5**) prepared from α-methylstyrene (1.2 equiv) and 1-(2,2-dimethylcyclopropyl)propan-1-one; 43 mg (58% yield) obtained as an oil according to general procedure 1. 5:1 trans:cis diastereomeric mixture determined by crude NMR. **Trans isomer**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49–7.46 (m, 2H), 7.37 (t, J = 7.9 Hz, 2H), 7.29–7.21 (m, 1H), 3.50 (dd, J = 12.6, 6.4 Hz, 1H), 2.30 (t, J = 12.9 Hz, 1H), 2.08 (d, J = 13.8 Hz, 1H), 1.97–1.89 (m, 1H), 1.87–1.77 (m, 2H), 1.74–1.64 (m, 2H), 1.31 (s, 3H), 1.24–1.17 (m), 0.85 (t, J = 7.2 Hz, 3H). **Cis isomer**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31–7.19 (m, 4H), 7.18–7.13 (m, 1H), 3.19 (dd, J = 9.8, 7.0 Hz, 1H), 2.39 (d, J = 13.7 Hz, 1H), 2.15 (dd, J = 13.4, 9.8 Hz, 1H), 2.00 (q, J = 7.3 Hz, 2H), 1.87–1.77 (m), 1.73–1.65 (m), 1.31 (s), 1.25–1.17 (m), 0.66 (t, J = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 212.04, 211.68, 149.11, 148.15, 128.40, 127.99, 126.44, 126.10, 125.97, 125.79, 63.85, 62.16, 59.81, 56.77, 50.31, 50.19, 43.77, 42.52, 37.63, 36.69, 36.00, 35.82, 32.02, 31.75, 31.47, 31.18, 30.86, 23.04, 7.39, 7.31. HRMS (ESI): $[M+H]^+$ calcd. 245.1900, found 245.1900 (<0.1 ppm).



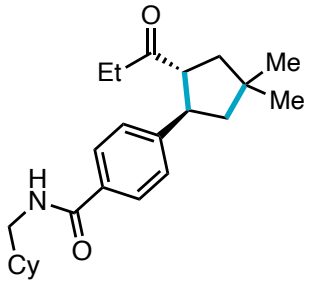
1-(3,3-dimethyl-2',3'-dihydrospiro[cyclopentane-1,1'-inden]-5-yl)propan-1-one (**6**) prepared from 1-methylene-2,3-dihydro-1H-indene (1.2 equiv) and cyclopentyl(2,2-dimethylcyclopropyl)methanone as a single diastereomer according to general procedure 1, 36% yield determined by ^{1}H NMR with dibromomethane as an internal standard.



1-(4,4-dimethyl-2-(4-morpholinophenyl)cyclopentyl)propan-1-one (**7**) prepared from 4-(4-vinylphenyl)morpholine (2 equiv) and 1-(2,2-dimethylcyclopropyl)propan-1-one as a single diastereomer, 43 mg (45% yield) obtained as a solid according to general procedure 1 (0.6 mA, 0.6 F/mol). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (d, J = 8.7 Hz, 2H), 6.84 (d, J = 8.7 Hz, 2H), 3.87–3.82 (m, 4H), 3.42 (td, J = 11.0, 7.7 Hz, 1H), 3.16–3.07 (m, 5H), 2.28 (dq, J = 17.9, 7.3 Hz, 1H), 2.13 (dq, J = 17.9, 7.3 Hz, 1H), 1.90 (dd, J = 12.7, 7.7 Hz, 1H), 1.84 (dd, J = 12.9, 9.1 Hz, 1H), 1.73 (dd, J = 12.9, 9.0 Hz, 1H), 1.65 (dd, J = 12.7, 11.5 Hz, 1H), 1.14 (s, 3H), 1.10 (s, 3H), 0.91 (t, J = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 213.12, 149.72, 127.93, 115.82, 66.97, 59.37, 50.27, 49.52, 47.73, 44.66, 38.22, 36.19, 30.72, 29.90, 7.56. HRMS (ESI): $[M+H]^+$ calcd. 316.2271, found 316.2267 (1.3 ppm).

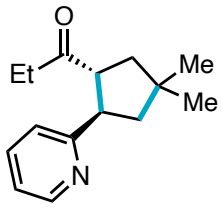


1-(2-(4-methoxyphenyl)-4,4-dimethylcyclopentyl)propan-1-one (**8**) prepared from 4-vinylanisole (1.2 equiv) and 1-(2,2-dimethylcyclopropyl)propan-1-one as a single diastereomer, 52% yield determined by ^{1}H NMR with dibromomethane as an internal standard. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22–7.11 (m, 2H), 6.88–6.77 (m, 2H), 3.78 (s, 3H), 3.44 (td, J = 11.0, 7.7 Hz, 1H), 3.10 (dt, J = 10.4, 9.1 Hz, 1H), 2.28 (dq, J = 17.9, 7.3 Hz, 1H), 2.12 (dq, J = 17.9, 7.3 Hz, 1H), 1.91 (dd, J = 12.8, 7.7 Hz, 1H), 1.85 (dd, J = 12.9, 9.1 Hz, 1H), 1.73 (dd, J = 12.9, 9.0 Hz, 1H), 1.66 (t, J = 12.1 Hz, 1H), 1.15 (s, 3H), 1.10 (s, 3H), 0.91 (t, J = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 213.09, 158.08, 135.88, 128.13, 113.89, 59.46, 55.24, 50.36, 47.74, 44.70, 38.21, 36.22, 30.73, 29.91, 7.54. HRMS (ESI): $[M+H]^+$ calcd. 261.1849, found 261.1850 (0.4 ppm).

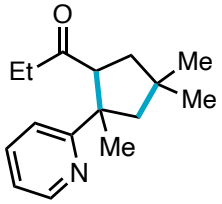


N-(cyclohexylmethyl)-4-(4,4-dimethyl-2-propionylcyclopentyl)benzamide (**9**) prepared from N-(cyclohexylmethyl)-4-vinylbenzamide (3 equiv) and 1-(2,2-dimethylcyclopropyl)propan-1-one; 50 mg (45% yield) obtained as a solid according to a modified general procedure 1 (0.5 mA,

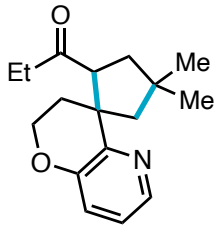
3 F/mol, 8 equiv water) as a single diastereomer. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65–7.56 (m, 2H), 7.23–7.18 (m, 2H), 6.13 (t, J = 6.0 Hz, 1H), 3.50 (td, J = 10.9, 7.8 Hz, 1H), 3.21 (t, J = 6.4 Hz, 2H), 3.08 (dt, J = 10.2, 9.1 Hz, 1H), 2.24 (dq, J = 17.9, 7.3 Hz, 1H), 2.05 (dq, J = 17.9, 7.2 Hz, 1H), 1.86 (ddd, J = 19.8, 12.8, 8.5 Hz, 2H), 1.74–1.57 (m, 8H), 1.50 (tdp, J = 10.4, 6.9, 3.3 Hz, 1H), 1.24–1.11 (m, 3H), 1.09 (s, 3H), 1.04 (s, 3H), 0.92 (tt, J = 12.1, 6.2 Hz, 2H), 0.85 (t, J = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 212.49, 167.36, 147.61, 133.03, 127.43, 127.11, 59.17, 49.92, 47.78, 46.19, 44.88, 38.53, 38.09, 36.16, 30.93, 30.59, 29.81, 26.41, 25.84, 7.55. HRMS (ESI): $[M+H]^+$ calcd. 370.2741, found 370.2738 (0.8 ppm).



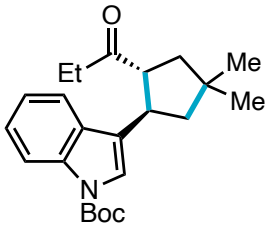
1-(4,4-dimethyl-2-(pyridin-2-yl)cyclopentyl)propan-1-one (10) prepared from 2-vinylpyridine (1.2 equiv) and 1-(2,2-dimethylcyclopropyl)propan-1-one; 61% yield determined by ^{1}H NMR with dibromomethane as an internal standard according to general procedure 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.53 (ddd, J = 4.9, 1.9, 0.9 Hz, 1H), 7.55 (td, J = 7.6, 1.9 Hz, 1H), 7.15 (dt, J = 7.8, 1.1 Hz, 1H), 7.08 (ddd, J = 7.5, 4.9, 1.2 Hz, 1H), 3.70 (ddd, J = 11.0, 9.8, 7.7 Hz, 1H), 3.58 (td, J = 9.7, 8.5 Hz, 1H), 2.37 (dq, J = 17.7, 7.2 Hz, 1H), 2.25 (dq, J = 17.7, 7.3 Hz, 1H), 1.99–1.87 (m, 2H), 1.83 (dd, J = 12.5, 11.0 Hz, 1H), 1.70 (dd, J = 12.8, 8.6 Hz, 1H), 1.14 (s, 3H), 1.09 (s, 3H), 0.94 (t, J = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 213.10, 162.90, 149.32, 136.24, 123.05, 121.31, 56.82, 49.16, 48.95, 44.46, 38.86, 35.66, 30.11, 29.71, 7.64. HRMS (ESI): $[M+H]^+$ calcd. 232.1696, found 232.1693 (1.3 ppm).



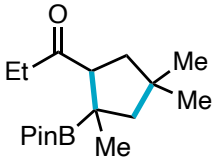
1-(2,4,4-trimethyl-2-(pyridin-2-yl)cyclopentyl)propan-1-one (**11**) prepared from 2-(prop-1-en-2-yl)pyridine (1.2 equiv) and 1-(2,2-dimethylcyclopropyl)propan-1-one; 66% yield determined by ^{1}H NMR with dibromomethane as an internal standard according to general procedure 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (ddd, J = 4.8, 1.9, 0.9 Hz, 1H), 7.64 (td, J = 7.7, 1.9 Hz, 1H), 7.34 (dt, J = 8.0, 1.1 Hz, 1H), 7.13 (ddd, J = 7.5, 4.7, 1.1 Hz, 1H), 4.15 (dd, J = 12.7, 6.6 Hz, 1H), 2.22 (t, J = 12.8 Hz, 1H), 2.15–1.96 (m, 3H), 1.75–1.65 (m, 2H), 1.33 (s, 3H), 1.19 (s, 3H), 1.11 (s, 3H), 0.89 (t, J = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 212.66, 167.46, 148.82, 136.20, 120.91, 120.16, 58.65, 58.02, 52.70, 42.45, 36.47 (d, J = 5.3 Hz), 31.44, 31.20, 23.41, 7.48. HRMS (ESI): $[M+H]^+$ calcd. 246.1852, found 246.1853 (0.4 ppm).



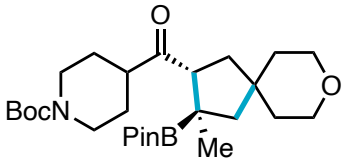
1-(3,3-dimethyl-2',3'-dihydrospiro[cyclopentane-1,4'-pyrano[3,2-b]pyridin]-5-yl)propan-1-one (**12**) prepared from 4-methylene-3,4-dihydro-2H-pyrano[3,2-b]pyridine (1.2 equiv) and 1-(2,2-dimethylcyclopropyl)propan-1-one; 57% yield determined by ^{1}H NMR with dibromomethane as an internal standard. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 (dd, J = 4.1, 1.8 Hz, 1H), 7.10–7.02 (m, 2H), 4.37 (dd, J = 13.3, 6.4 Hz, 1H), 4.19 (dt, J = 11.2, 3.7 Hz, 1H), 4.06 (td, J = 10.9, 3.2 Hz, 1H), 2.18 (t, J = 13.2 Hz, 1H), 2.04 (d, J = 13.4 Hz, 1H), 1.96 (dq, J = 18.2, 7.3 Hz, 1H), 1.89–1.79 (m, 2H), 1.76–1.60 (m, 3H), 1.57 (s, 1H), 1.20 (s, 3H), 1.16 (s, 3H), 0.81 (t, J = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 212.21, 151.13, 147.59, 141.97, 124.04, 122.54, 63.48, 57.90, 57.52, 48.62, 41.54, 36.34, 36.17, 31.97, 31.57, 30.80, 7.32. HRMS (ESI): $[M+H]^+$ calcd. 274.1802, found 274.1798 (1.5 ppm).



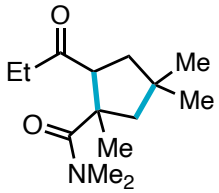
tert-butyl 3-(4,4-dimethyl-2-propionylcyclopentyl)-1H-indole-1-carboxylate (**13**) prepared from tert-butyl 3-vinyl-1H-indole-1-carboxylate (2 equiv) and 1-(2,2-dimethylcyclopropyl)propan-1-one; 55% yield determined by ^{1}H NMR with dibromomethane as an internal standard according to general procedure 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.53 (dt, J = 8.0, 1.0 Hz, 1H), 7.39 (s, 1H), 7.33–7.27 (m, 1H), 7.21 (td, J = 7.5, 1.1 Hz, 1H), 3.78 (td, J = 10.3, 7.8 Hz, 1H), 3.31 (q, J = 9.2 Hz, 1H), 2.38 (dq, J = 17.9, 7.2 Hz, 1H), 2.25 (dq, J = 17.9, 7.2 Hz, 1H), 2.02 (dd, J = 12.7, 7.9 Hz, 1H), 1.94 (dd, J = 12.9, 9.3 Hz, 1H), 1.86–1.73 (m, 2H), 1.67 (s, 11H), 1.16 (s, 3H), 1.14 (s, 3H), 0.94 (t, J = 7.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 213.14, 124.32, 122.31, 121.47, 119.66, 115.29, 57.38, 48.47, 44.87, 38.80, 38.70, 36.15, 30.45, 29.51, 28.22, 7.66. HRMS (ESI): $[M+H]^+$ calcd. 387.2642, found 387.2641 (0.3 ppm).



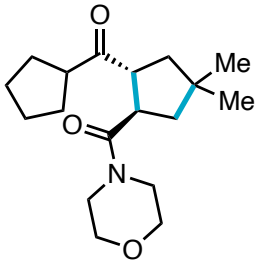
1-(2,4,4-trimethyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)cyclopentyl)propan-1-one (**14**) prepared from 4,4,5,5-tetramethyl-2-(prop-1-en-2-yl)-1,3,2-dioxaborolane (1.2 equiv) and 1-(2,2-dimethylcyclopropyl)propan-1-one as a 1:1 mixture of diastereomers, 60% yield determined by ^{1}H NMR with dibromomethane as an internal standard. **Isomer 1**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.33 (dd, J = 12.2, 6.3 Hz, 1H), 2.52–2.30 (m, 2H), 1.98 (t, J = 12.4 Hz, 1H), 1.83–1.74 (m, 2H), 1.40 (dd, J = 12.7, 6.4 Hz, 1H), 1.27–1.14 (m), 1.10–1.05 (m), 1.05–0.97 (m), 0.95 (s, 3H), 0.82 (s, 3H). **Isomer 2**: ^{1}H NMR (500 MHz, $CDCl_3$) δ 2.69 (dd, J = 11.1, 7.1 Hz, 1H), 2.52–2.30 (m, 2H), 1.92 (t, J = 11.6 Hz, 1H), 1.83–1.74 (m, 2H), 1.27–1.14 (m), 1.10–1.05 (m), 1.05–0.97 (m). ^{13}C NMR (126 MHz, $CDCl_3$) δ 213.58, 212.91, 83.38, 82.54, 63.82, 56.26, 53.28, 51.39, 45.04, 41.50, 38.45, 38.09, 36.19, 34.30, 32.02, 30.67, 30.47, 29.60, 25.41, 24.73, 24.66, 24.62, 20.20, 7.89, 7.63. ^{11}B NMR (128 MHz, $CDCl_3$) δ 34.49. HRMS (ESI): $[M+H]^+$ calcd. 295.2439, found 295.2444 (1.7 ppm).



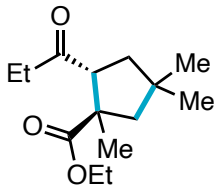
tert-butyl 4-(3-methyl-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-8-oxaspiro[4.5]decane-2-carbonyl)piperidine-1-carboxylate (**15**) prepared from 4,4,5,5-tetramethyl-2-(prop-1-en-2-yl)-1,3,2-dioxaborolane (1.2 equiv) and tert-butyl 4-(6-oxaspiro[2.5]octane-1-carbonyl)piperidine-1-carboxylate as a 2:1 mixture of diastereomers, 81 mg (55% yield) obtained as a solid according to general procedure 1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.11 (s), 3.76–3.50 (m), 3.44 (dd, J = 11.7, 6.5 Hz), 2.85–2.52 (m), 2.03–1.86 (m), 1.73–1.41 (m), 1.40–1.17 (m), 1.03 (s), 0.85 (s). ^{13}C NMR (126 MHz, $CDCl_3$) δ 214.45, 213.57, 154.66 (d, J = 2.2 Hz), 83.61, 82.75, 79.52 (d, J = 3.1 Hz), 65.89, 65.80, 65.33, 64.94, 61.17, 53.11, 50.26, 48.29, 48.06, 46.83, 42.44, 40.87, 40.09, 40.03, 39.66, 39.44, 37.88, 28.71, 28.42, 28.14, 27.30, 26.28, 24.90, 24.79, 24.75, 24.70, 24.67, 20.58. HRMS (ESI): $[M+H]^+$ calcd. 492.3491, found 492.3490 (0.2 ppm).



N,N,1,4,4-pentamethyl-2-propionylcyclopentane-1-carboxamide (**16**) prepared from N,N-dimethylmethacrylamide (3 equiv) and 1-(2,2-dimethylcyclopropyl)propan-1-one according to a modified general procedure 1 (0.5 mA, 3 F/mol, 8 equiv water); 70% yield determined by ^{1}H NMR with dibromomethane as an internal standard. ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.94 (dd, J = 13.5, 6.2 Hz, 1H), 2.98 (s, 6H), 2.82 (dq, J = 18.2, 7.3 Hz, 1H), 2.52 (dq, J = 18.3, 7.3 Hz, 1H), 1.93 (d, J = 12.8 Hz, 1H), 1.83 (t, J = 13.1 Hz, 1H), 1.61 (d, J = 13.1 Hz, 1H), 1.53–1.45 (m, 1H), 1.26 (s, 4H), 1.10 (s, 3H), 0.99 (dd, J = 14.8, 7.6 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 213.48, 177.20, 56.25, 53.89, 53.77, 41.76, 37.22, 37.12, 30.97, 30.37, 22.28, 7.68. HRMS (ESI): $[M+H]^+$ calcd. 240.1958, found 240.1955 (1.3 ppm).



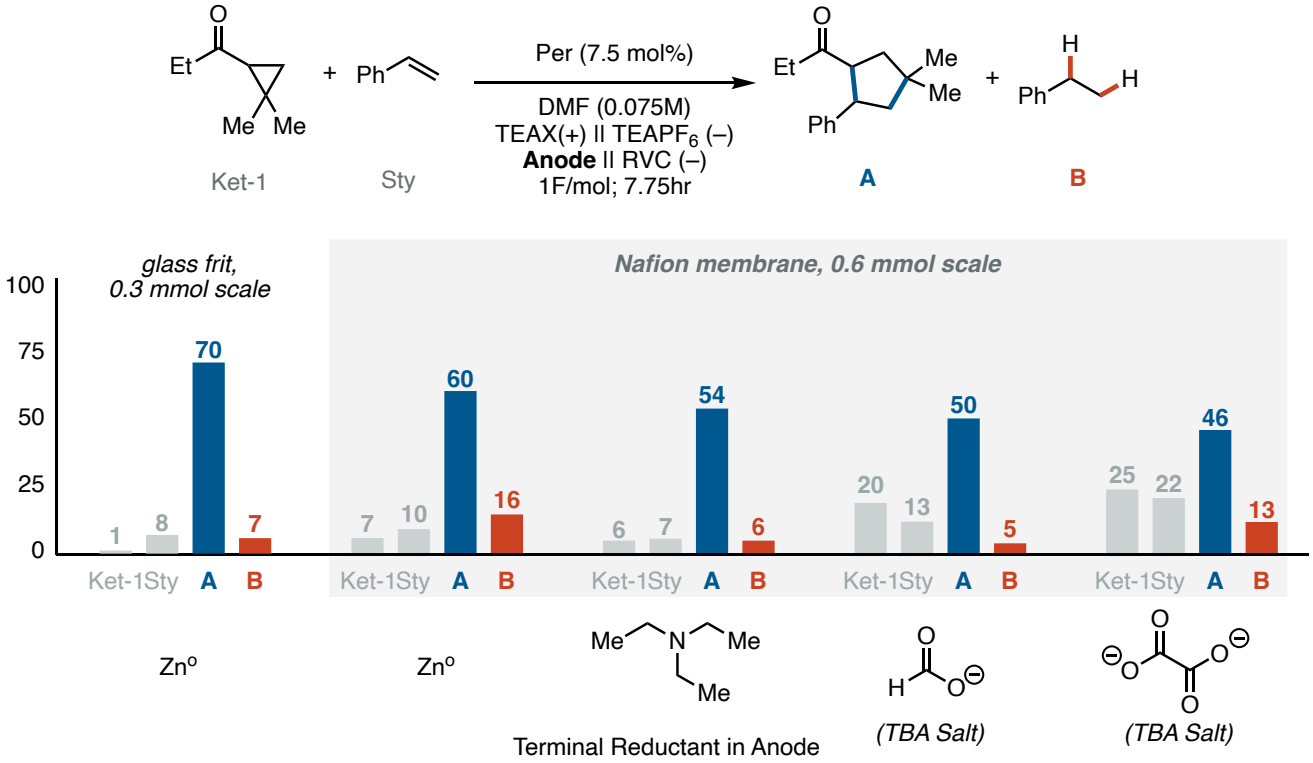
(2-(cyclopentanecarbonyl)-4,4-dimethylcyclopentyl)(morpholino)methanone (**17**) prepared from 1-morpholinoprop-2-en-1-one (3 equiv) and cyclopentyl(2,2-dimethylcyclopropyl)methanone according to a modified general procedure 1 (0.5 mA, 3 F/mol, 8 equiv water); 55% yield determined by ^{1}H NMR with dibromomethane as an internal standard.



ethyl 1,4,4-trimethyl-2-propionylcyclopentane-1-carboxylate (**18**) prepared from ethyl methacrylate (3 equiv) and 1-(2,2-dimethylcyclopropyl)propan-1-one according to a modified general procedure 1 (0.5 mA, 3 F/mol, 8 equiv water) as a 2:1 mixture of diastereomers, 74% yield determined by ^{1}H NMR with dibromomethane as an internal standard. **Trans diastereomer** (major): ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.22 (qd, J = 7.1, 1.4 Hz, 2H), 3.74 (dd, J = 12.6, 6.6 Hz, 1H), 2.58–2.34 (m, 2H), 2.09 (dd, J = 13.4, 1.3 Hz, 1H), 2.01 (t, J = 12.7 Hz, 1H), 1.58 (ddd, J = 12.9, 6.6, 1.3 Hz, 1H), 1.49 (d, J = 14.1 Hz, 1H), 1.32 (d, J = 7.0 Hz, 2H), 1.12 (d, J = 2.8 Hz, 6H), 1.07–1.00 (m, 6H). **Cis diastereomer** (minor): ^{1}H NMR (500 MHz, $CDCl_3$) δ 4.09 (qd, J = 7.1, 1.0 Hz, 2H), 2.86 (dd, J = 11.2, 7.2 Hz, 1H), 2.56–2.32 (m), 2.17 (d, J = 13.7 Hz, 1H), 2.10 (m), 1.90–1.84 (m), 1.49 (m), 1.23 (m), 1.17 (m), 1.12 (m), 1.07–1.01 (m). ^{13}C NMR (126 MHz, $CDCl_3$) δ 211.39, 177.78, 61.50, 60.98, 60.39, 60.20, 56.25, 54.33, 52.92, 52.34, 51.90, 44.14, 42.04, 39.53, 37.55, 37.11, 36.59, 35.02, 31.35, 31.10, 30.54, 29.67, 26.80, 21.69, 14.26, 14.17, 14.03, 7.57, 7.47. HRMS (ESI): $[M+Na]^+$ calcd. 263.1618, found 263.1614 (1.5 ppm).

Excluding contributions from exogenous Lewis Acids

To exclude any potential impact of cationic zinc species that may migrate from the anode across the glass frit, we replaced the glass frit with a Nafion membrane and re-evaluated the reaction. Without any re-optimization for these modified conditions (e.g., changes to resistance, electrode distance, scale, etc.), this change in reaction setup had only a minimal impact on reaction efficiency, selectively promoting the model annulation with comparable performance. While Nafion should preclude Zn migration, we also replaced the zinc anode with a reticulated vitreous carbon (RVC) anode paired with various sacrificial reductants in the anodic chamber. Using triethylamine, tetrabutylammonium formate, or tetrabutylammonium oxalate as the terminal reductant each afforded the desired [3+2] annulation product selectively over hydrogenated styrene. Taken together, these results confirm that a zinc anode is not required to observe selective ketone activation.



6. Transient Absorption Studies

Materials: Anhydrous acetonitrile (MeCN, 99.9+%, Extra Dry, AcroSeal™) was purchased from Fisher Scientific and then dried over 3 Å molecular sieves for three days. All the samples were prepared in an argon-filled glovebox. Chemical reductions were performed using potassium graphite (KC_8) purchased from Strem.

Photophysical experiments: UV-Visible absorption spectra were collected with an HP 8452A diode array spectrophotometer using quartz cuvettes.

Picosecond transient absorption experiments: A home-built pump–probe spectrometer was employed for the picosecond dynamics investigation of perylene radical anion. Details of this setup are published: ACS Catal. 2024, 14, 2252−2263.

Nanosecond transient absorption experiments: Two distinct setups were employed to monitor the nanosecond dynamics of the system. Initially, transient absorption spectra were collected using a commercial EOS broadband pump-probe nanosecond transient absorption spectrometer (Ultrafast Systems), which offers both visible (350–950 nm) and near-infrared (NIR, 800–1600 nm) detection capabilities. Detailed specifications of this instrument are available on the web. While the EOS system is well-suited for spectral acquisition, its relatively slow delay control between the pump and probe pulses necessitates prolonged waiting times. This posed a limitation for kinetic studies involving species sensitive to oxygen, such as the perylene radical anion and solvated electrons, as extended wait times led to significant degradation of the perylene radical anion signal and poor signal-to-noise. To address this limitation, a custom-built setup was employed for kinetic monitoring of solvated electron quenching. In this system, femtosecond laser pulses (796 nm, 150 fs, 1 kHz) were generated using a commercial oscillator and regenerative amplifier (Spectra Physics Solstice Ace). The excitation wavelength (398 nm) was produced via second harmonic generation using a 100 μm thick β-barium borate (Type I, $\theta = 30°$) crystal. Residual 796 nm light was removed using a short-pass filter, which reflected the fundamental beam onto a beam block. A continuous-wave laser-driven light source (LDLS) was used as a probe. The white light was collimated, attenuated, and filtered through a 570 nm long-pass filter before being focused onto the sample using a 50 mm focal length lens. For detection in the NIR region, a second filter (1150 nm long-pass) transmitted wavelengths above 1150 nm, which were then focused onto an InGaAs photodiode using a 100 mm lens. The photodiode output was recorded using a digital oscilloscope (LeCroy). A servo motor-controlled shutter was used to block and unblock the pump beam. A silicon photodiode monitoring scattered pump light provided the trigger signal. Each measurement cycle consisted of an average of 1000 probe pulses with the pump beam blocked, followed by 1000 pulses with the pump beam unblocked. The differential signal (ΔA) was obtained by subtracting the blocked signal from the unblocked signal. 30–40 such cycles were collected and averaged for all the decay traces reported in this work related to probing the rates of electron transfer that involve solvated electrons.

Determination of molar absorptivity of perylene

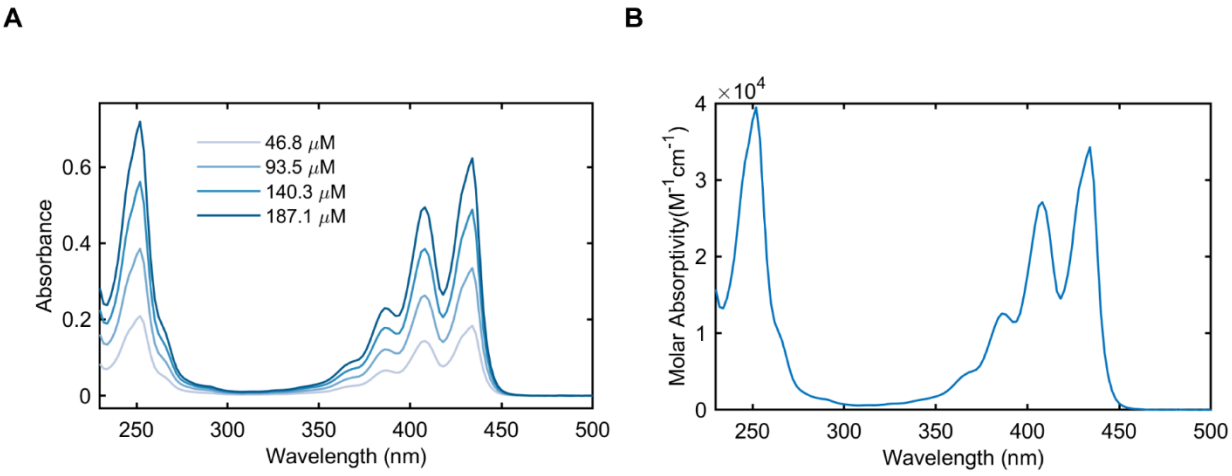


Figure S2.1. (A) UV-Vis absorption spectra of **Per** taken at different concentrations (stated in the legend) in MeCN. The path length is 1 mm. (B) Molar absorption coefficients of **Per** as a function of wavelength calculated using the spectra shown in panel A.

Isolating Per absorption from Per radical anion spectrum

The purpose of this procedure was to isolate the absorption spectrum of **Per** by quantitatively removing contributions from **Per**$^{\bullet-}$.

Procedure:

1. **Electrolysis:** A solution of **Per** (0.6 mM) in MeCN containing $TBAPF_6$ as the supporting electrolyte was electrolyzed at –2.4 V vs $Ag/AgNO_3$ for 30 min inside an Argon-filled glovebox. This potential drives only the first reduction (**Per** → **Per**$^{\bullet-}$), generating a mixture of **Per** and **Per**$^{\bullet-}$.
2. **Sample handling:** An aliquot of the solution was transferred to a 1 mm quartz cuvette and sealed with a Kontes valve to maintain oxygen free conditions.
3. **Initial spectrum:** The absorption spectrum was recorded (**Figure S18**, top panel). Bands at 320 and 575 nm are attributed exclusively to **Per**$^{\bullet-}$, while the region from 360–450 nm shows strong overlap with **Per** absorption.
4. **Reference spectrum:** A normalized absorption spectrum of **Per** is used as a reference for deconvolution.
5. **Constraint:** To avoid overfitting, a smoothness criterion is imposed such that the spectrum of **Per**$^{\bullet-}$ remains featureless between 360–450 nm (i.e., no artificial sharp peaks were permitted in this region). This was based on the literature-reported spectrum of **Per**$^{\bullet-}$ which is characterized by weak and featureless absorption in the 360–450 nm region.
6. **Deconvolution protocol:** The raw spectrum was modeled as a linear combination of neutral and anion contributions by minimizing:

$$\textbf{Minimize } ||\boldsymbol{A_{raw}} - (\boldsymbol{cA_{Pe}} + \boldsymbol{A_{Pe^{\bullet-}}})||^2 \qquad \text{Eq S2.1}$$

where:

   - A_{raw} is the measured absorption spectrum,
   - A_{Pe} is a normalized spectrum of neutral Per (held fixed),
   - $A_{Per^{\bullet-}}$ is the spectrum corresponding to Per anions,
   - c is an adjustable coefficient.

7. **Application:** This method provided a clean separation of Per and Per$^{\bullet-}$ contributions (**Figure S18**, bottom). The same protocol, together with independently determined molar absorptivities for **Per** (**Figure S17**), was subsequently used to determine Per concentrations in solution.

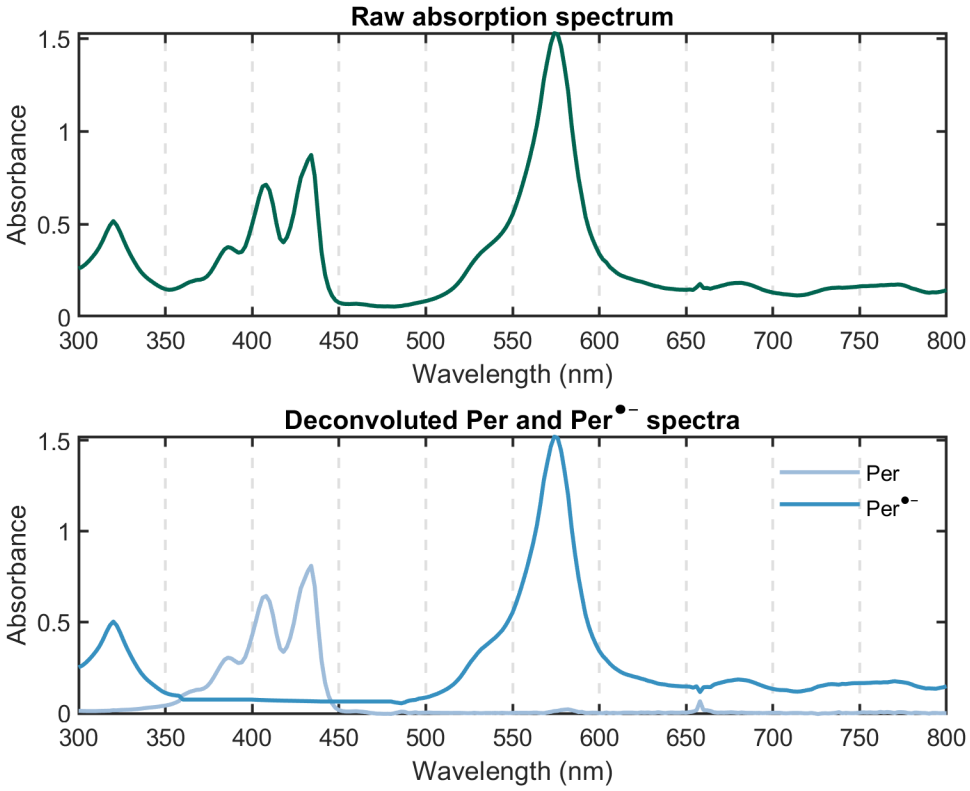


Figure S2.2. (Top) UV-Vis absorption spectrum of electrolyzed **Per** solution in MeCN. The path length is 1 mm. (Bottom) Isolated absorption spectra of **Per** and **Per**$^{\bullet-}$ obtained using the deconvolution procedure described above.

Global modeling of excited state dynamics of Per•– doublet states

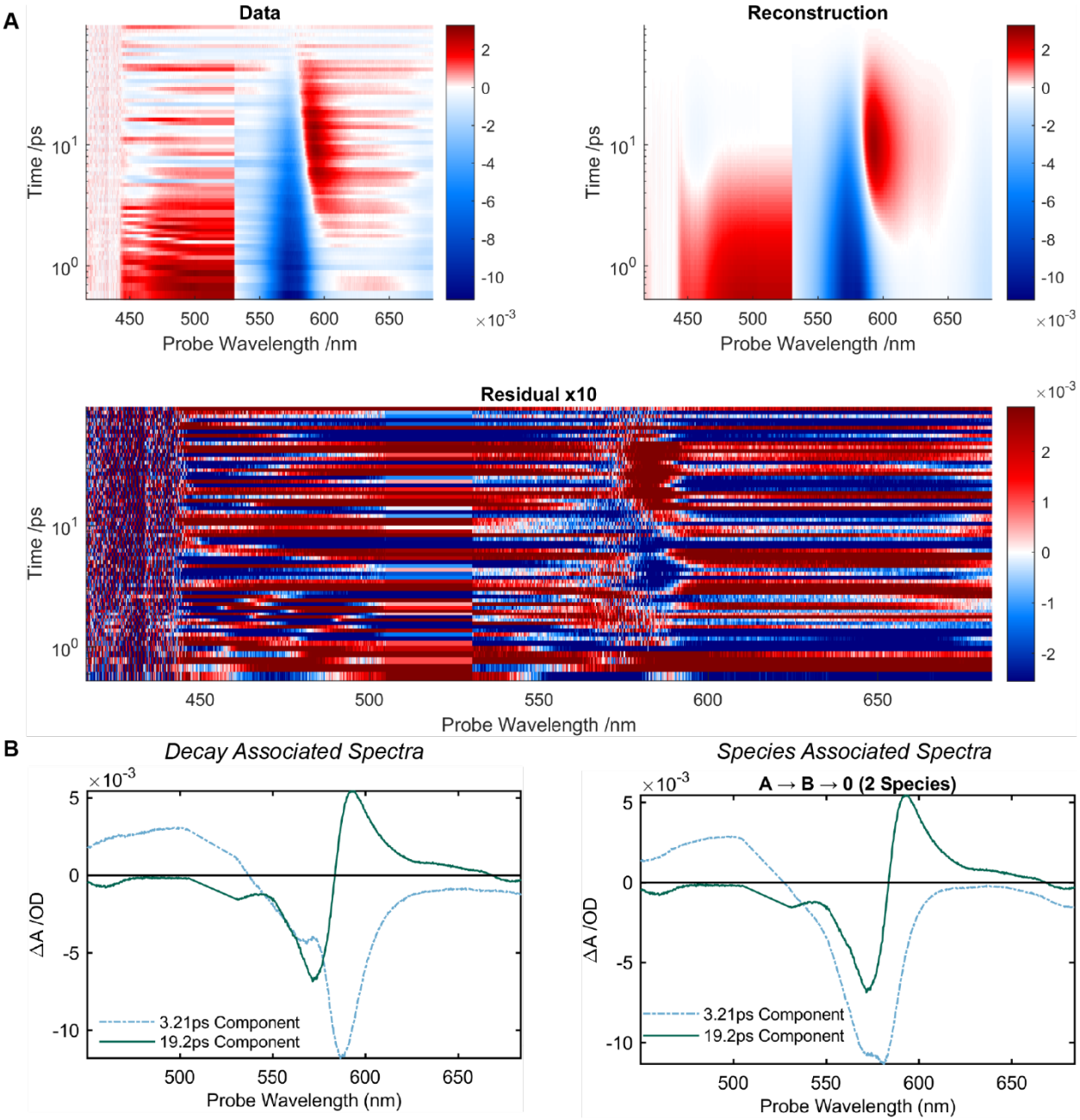


Figure S2.3. (A) The complete set of raw transient absorption data (slices out of this set are shown in manuscript Figure 3B, top) collected for Per•– in room temperature MeCN following an excitation at 520 nm (400 nJ energy per pulse) (left) along with a reconstructed global analysis model (right) comprised of a sequential A→B→0 process. The residuals are shown in the bottom panel. (B) Two-state decay and species-associated spectra retrieved from the global analysis described above.

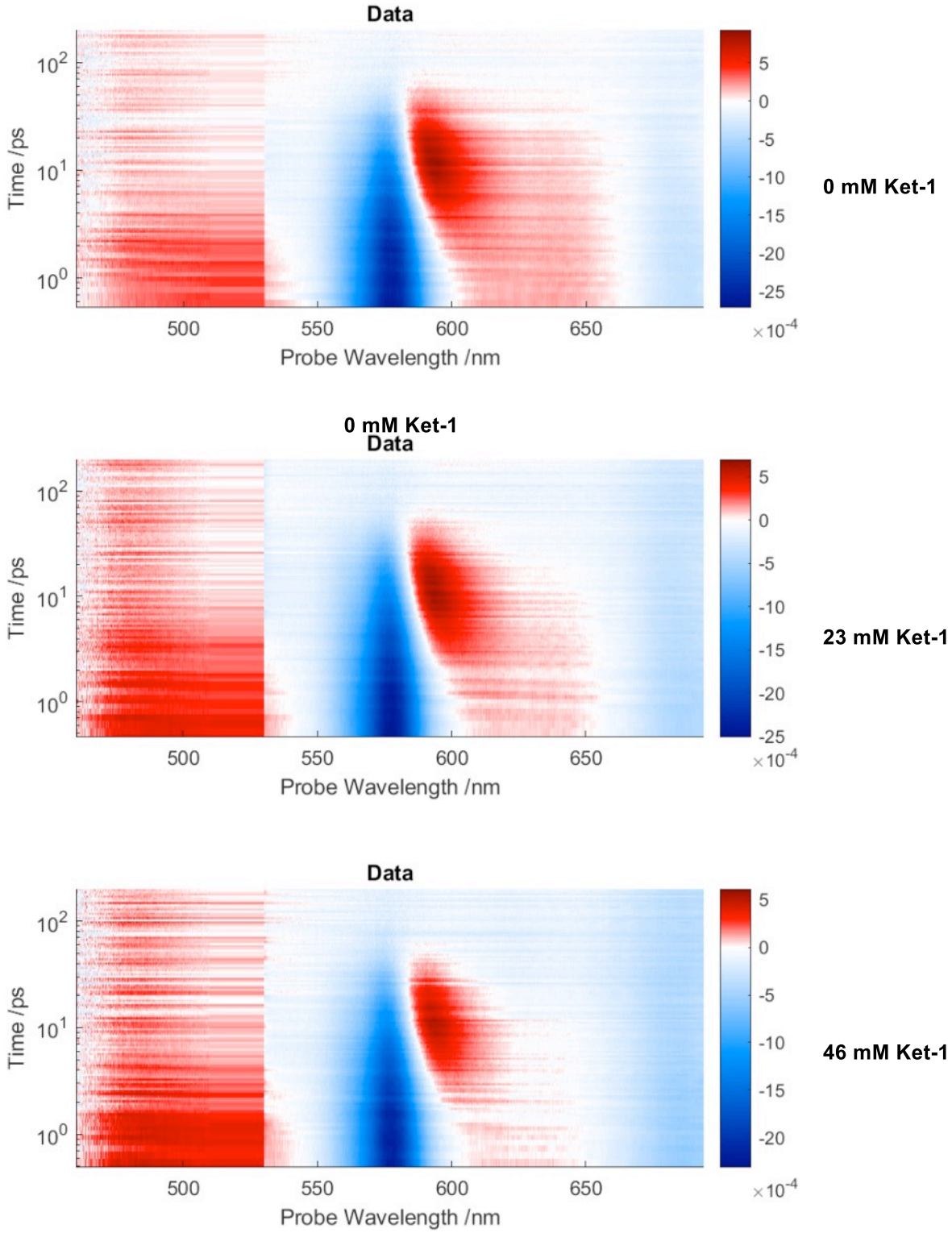


Figure S2.4. Two-dimensional picosecond transient absorption (TA) spectra (wavelength vs. pump–probe delay time) of **Per**$^{\bullet-}$ following 520 nm excitation under three conditions: no Ket-1

(top), 23 mM Ket-1 (middle), and 46 mM Ket-1 (bottom). Within experimental sensitivity, no additional transient absorption features attributable to new species are observed upon addition of Ket-1, and the ground-state bleach (GSB) and excited-state absorption (ESA) dynamics remain unchanged.

Excitation wavelength dependence of solvated electron generation

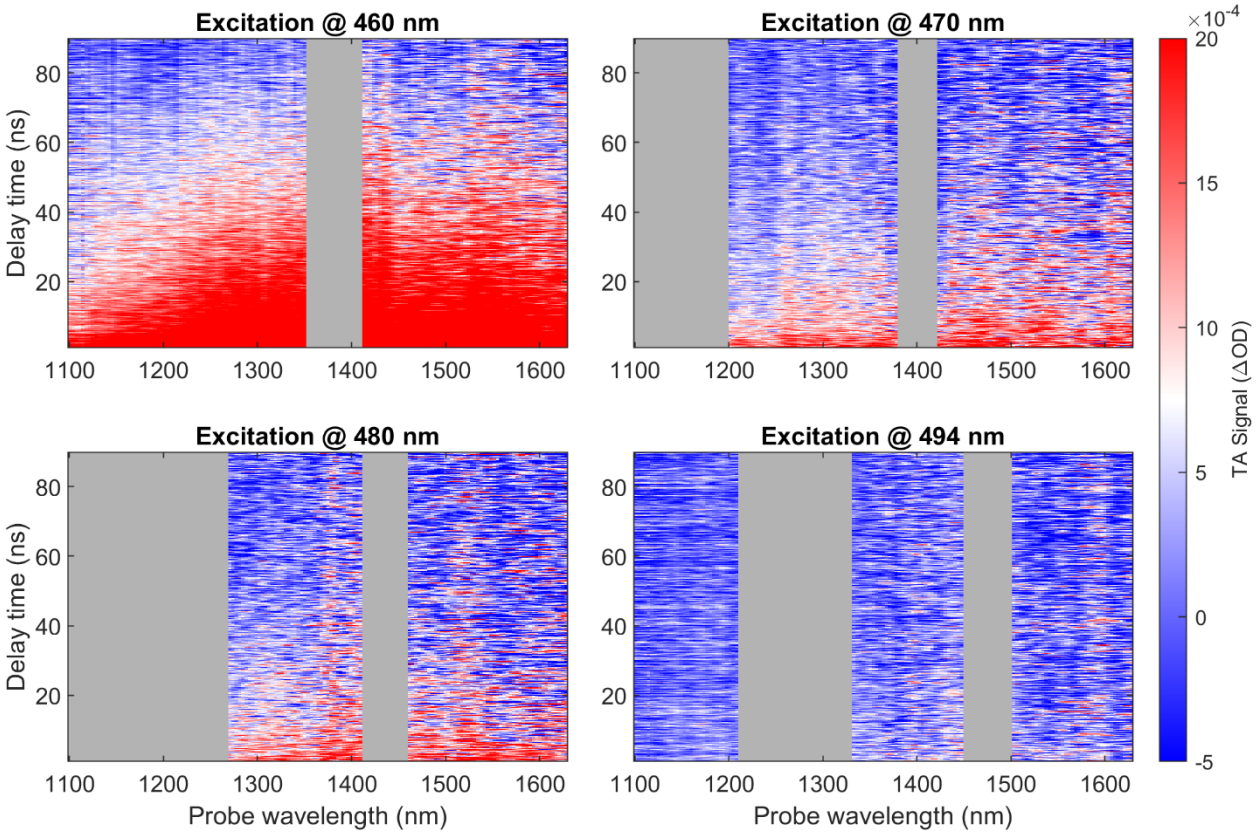


Figure S2.5. Nanosecond transient absorption dynamics in the NIR region following excitation at different wavelengths (specified in subfigure titles), each with 1 mJ energy per pulse. Excitation at 460 nm produces a strong absorptive signal characteristic of solvated electron generation. As the excitation wavelength is shifted to the red, the signal amplitude decreases, reflecting the reduced excitation energy available to drive electron ejection. At 494 nm, no detectable signal is observed, indicating that this was below the energetic threshold for solvated electron formation. The greyed-out regions in the spectra indicate spectral gaps where data could not be collected due to pump scatter. Although excitation was carried out at visible wavelengths (460–494 nm), higher-order diffraction from the detection grating results in apparent pump signal within the near-IR spectral range.

Global Modeling of Nanosecond Dynamics of Solvated Electron Generation

Important note:

Across all datasets, we observe an additional fast component on the 2–3 ns timescale. This can be most readily observed in Figure S2.5 under 470 and 480 nm excitation. Our preliminary interpretation is that this feature may arise from geminate recombination of the initially generated charge-separated pair. Since the present study is focused on the subsequent, slower evolution associated with well-separated solvated electrons and neutral Per, our global analysis emphasizes this longer-timescale behavior. We therefore note the fast component for completeness, but it is not explicitly modeled in the data presented below.

Visible region:

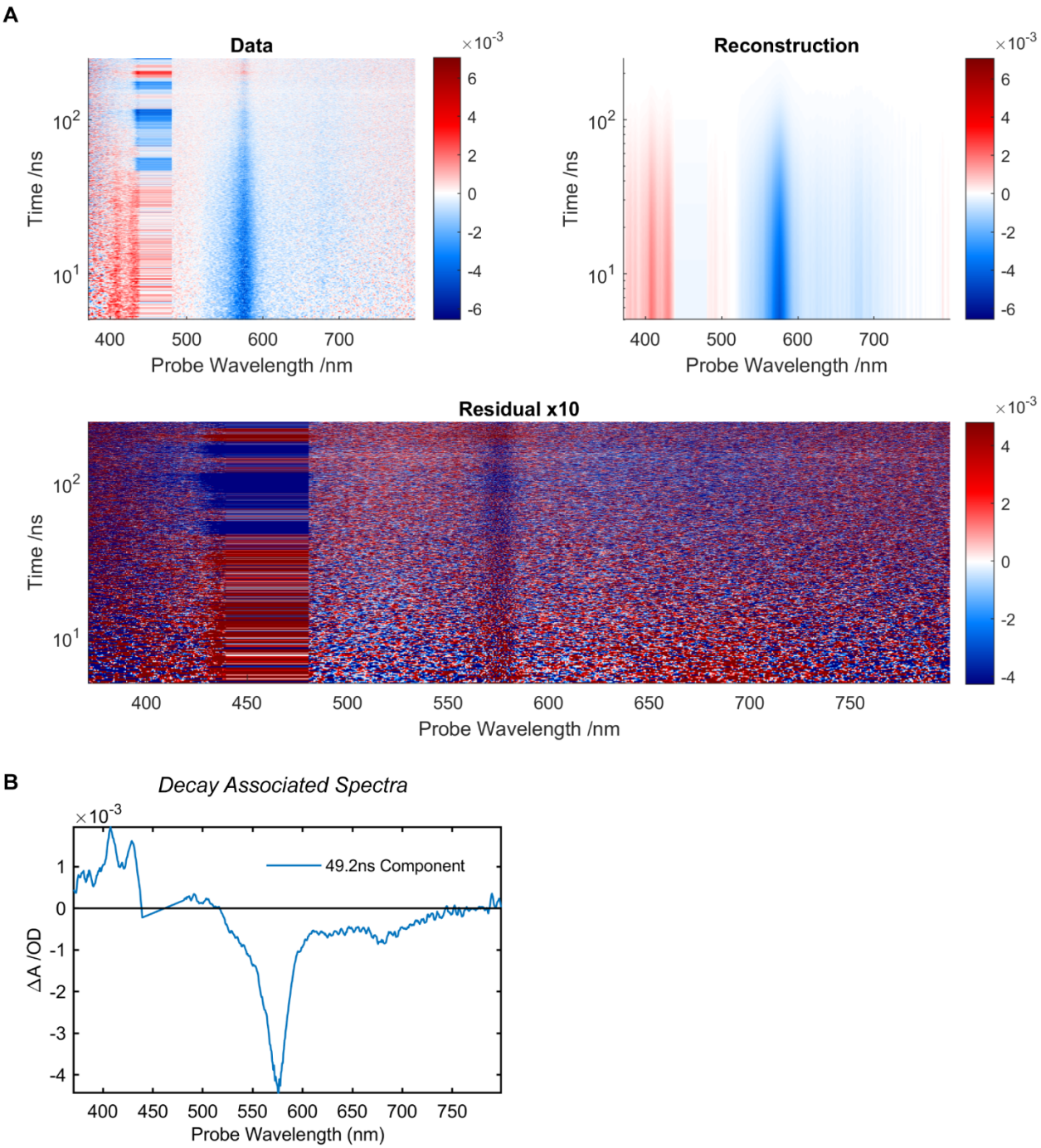


Figure S2.6 (A) The complete set of raw visible transient absorption data (slices out of this set are shown in manuscript Figure 3B, middle) collected for Per•– in room temperature MeCN (left) after excitation with 460 nm (pulse energy of 1 mJ) pump along with a reconstructed global analysis model (right) comprised of a monoexponential A→0 process with an offset. The residuals are shown in the bottom panel. (B) The decay-associated spectrum retrieved from the global analysis described above.

NIR region:

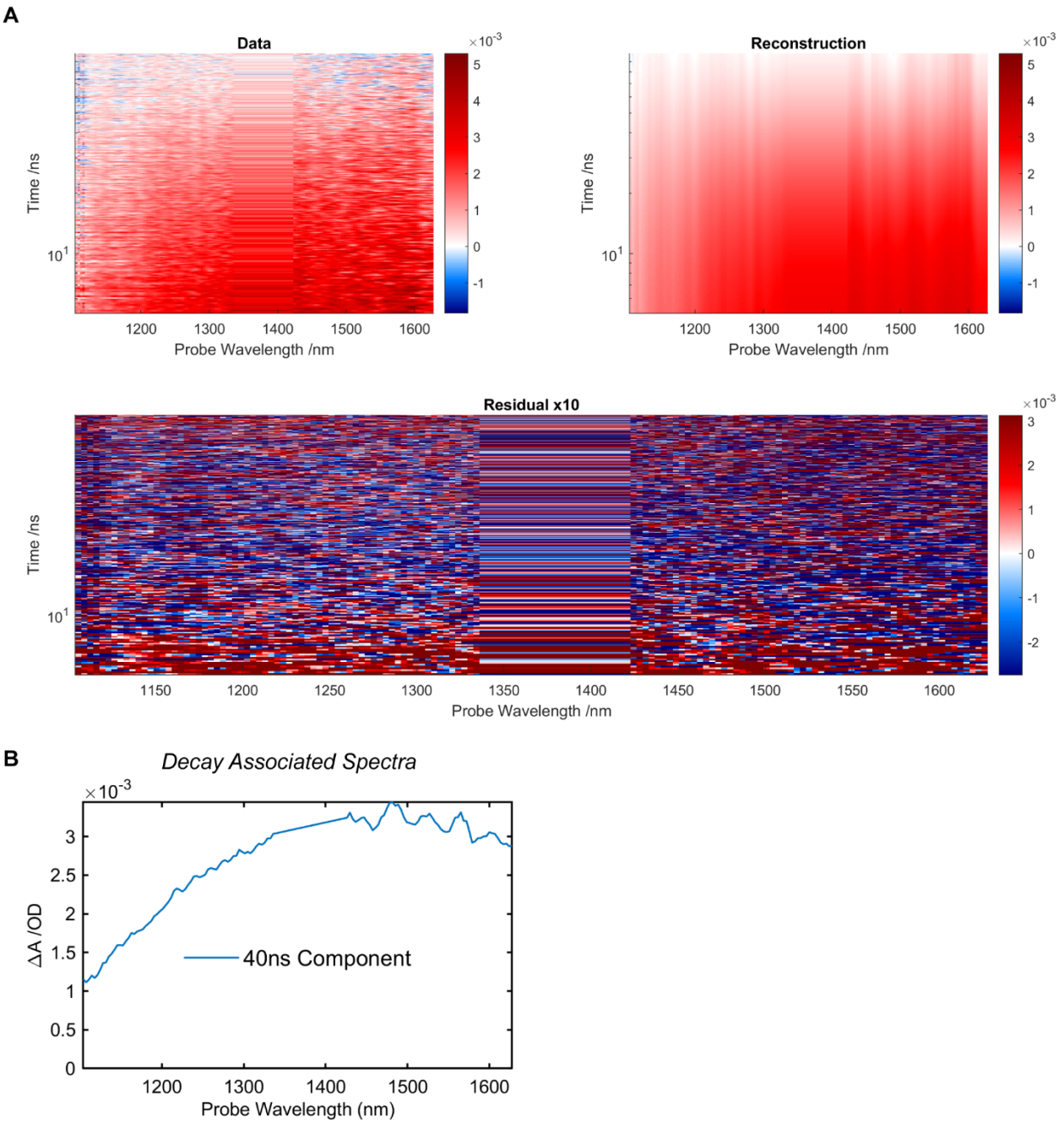


Figure S2.7a. (A) The complete set of raw NIR transient absorption data (slices out of this set are shown in manuscript Figure 3B, bottom) collected for Per•– in room temperature MeCN (left) after excitation with 460 nm (pulse energy of 1 mJ) along with a reconstructed global analysis model (right) comprised of a monoexponential A→0 process with an offset. The residuals are shown in the bottom panel. (B) The decay-associated spectrum retrieved from the global analysis described above.

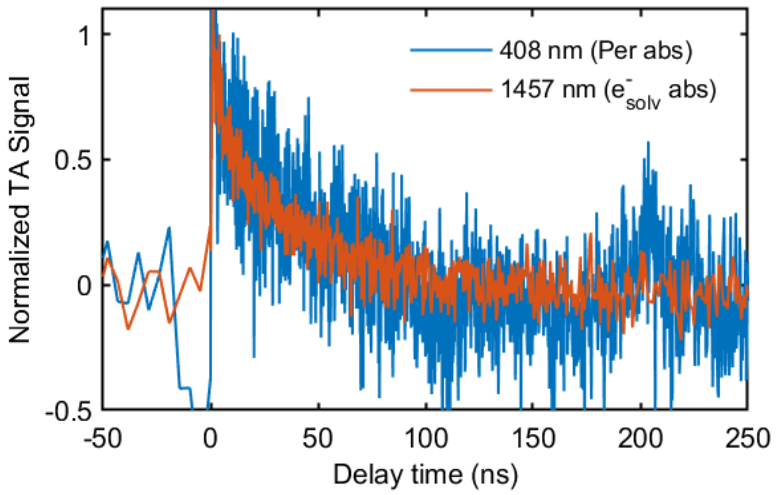


Figure S2.7b. Normalized decay traces at selected wavelengths illustrating the concurrent decay of neutral perylene and the solvated electron following excitation at 460 nm (1 μJ pulse energy).

Discussion: The close correspondence between these decay profiles demonstrates that the loss of solvated electrons occurs on the same timescale as decay of neutral perylene, providing direct experimental evidence for recombination of the solvated electron with its parent chromophore.

Probing rate of electron transfer with solvated electrons

Sample preparation:

1. All sample handling was performed inside an Ar-filled glovebox to avoid exposure to air. Fresh solutions were prepared immediately prior to each quenching study and used within 2 hours.
2. Dissolve 0.3–0.4 mg (1.2–1.6 μmol) of **Per** in 3–4 mL of MeCN in a dram vial equipped with a magnetic stir bar.
3. Add 0.1–0.2 mg (0.7–1.4 μmol) of KC_8 to the **Per** solution. Stir the mixture for 8–9 min until the solution develops a dark blue color, indicative of $\mathbf{Per}^{\bullet-}$ formation. The formation of $\mathbf{Per}^{\bullet-}$ was confirmed spectroscopically (λ_{max} = 578 nm).
4. Avoid prolonged stirring (>10 min), as this promotes over-reduction to $\mathbf{Per}^{2}$–.
5. Use the solution directly for transient absorption or quenching experiments.

Note: These conditions were chosen to generate sufficient $\mathbf{Per}^{\bullet-}$ while retaining an appreciable fraction of neutral **Per**. The presence of neutral **Per** ensures that ejected electrons are preferentially captured by **Per** rather than by impurities. The relative concentration of **Per** was determined by deconvolution of the absorption spectrum as described previously.

Decay trace fitting procedure:

Acquisition. Decay traces were collected on the home-built nanosecond transient spectrometer (see Methods). Excitation at 398 nm populates both **Per** and $\mathbf{Per}^{\bullet-}$; accordingly, the kinetics are well described by a biexponential decay. The faster component ($\tau_1 \approx 5$ ns) corresponds to **Per** S_1 decay ($S_n \leftarrow S_1$ feature centered ~1350 nm).

Model. Each trace was fit to the convolution of a Gaussian instrument response function (IRF) with a sum of two decays ("biexponentially modified Gaussian"). The response is:

$$S(t) = c + [A_1 \exp(-t/\tau_1) + A_2 \exp(-t/\tau_2)] \otimes G(t; t_0, \sigma)$$

where c is a constant offset, t_0 is the time-zero, G is a normalized Gaussian IRF,

$$G(t; t_0, \sigma) = {}^{1}\Big/_{\sqrt{(2\pi)}\sigma} \exp\left(-\frac{(t-t_0)^2}{2\sigma^2}\right)$$

and $\otimes$ denotes convolution.

Using the standard closed form for the convolution of an exponential with a Gaussian, the signal becomes a sum of two terms:

$$S(t) = c + \sum_{i=1}^{2}\left(\frac{A_i}{2}\right) * \exp\left(\frac{\sigma^2}{2\,\tau_i^2} - \frac{t-t_0}{\tau_i}\right) * \operatorname{erfc}\left(\left(\frac{\sigma^2-\tau_i(t-t_0)}{\sqrt{2}\sigma\tau_i}\right)\right) \qquad \text{Eq S2}$$

with amplitudes A_i, lifetimes τ_i and the complementary error function erfc.

Constraints and fixed parameters:

- τ_1 fixed at 5.0 ns (**Per** S1 decay)
- σ constrained ∈ [1.0,1.5] ns. This is based on the rise time of the InGaAs photodiode.
- τ_2 (solvated electron signal) free to change with a lower bound of 10 ns.
- t_0 free to change ($\pm$ few ns around scope trigger)

In all traces reported below, the value of τ_{obs} refers to τ_2 as defined above.

With Per as quencher:

In the absence of competing quenchers, solvated electrons are assumed to be captured predominantly by neutral **Per**. The capture kinetics can be expressed as:

$$\frac{d[e^-]}{dt} = -k_{Per}[Per][e^-]$$

which integrates to:

$$[e^-](t) = A_0 \exp(-k_{Pe}[Per]t) = A_0 \exp\left(-\frac{t}{\tau_{obs}}\right)$$

with the relationship:

$$k_{Per}[Per] = 1/\tau_{obs}$$

Thus, by monitoring the monoexponential decay lifetime τ_{obs} of the solvated electron signal as a function of [**Per**], the bimolecular rate constant k_{Per} can be obtained from the slope of a plot of [**Per**] versus $(1/\tau_{obs})$. From this analysis, k_{Per} was estimated to be 8×10^{10} $M^{-1}s^{-1}$ (see below).

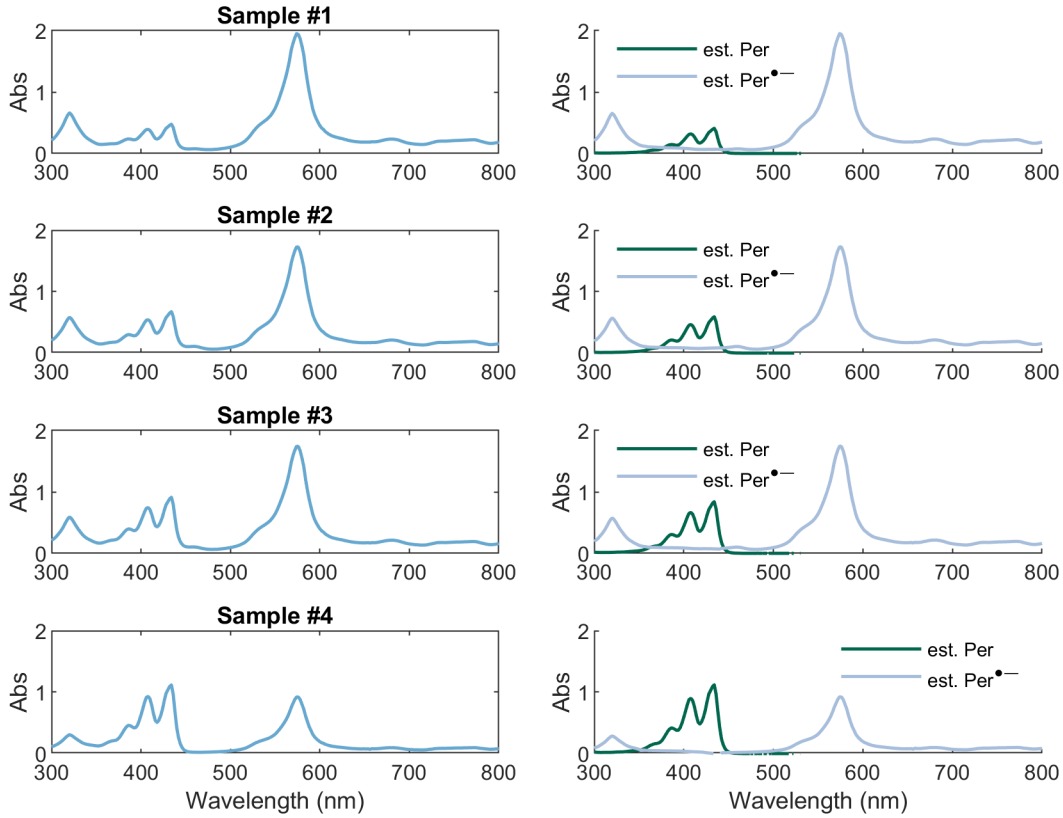


Figure S2.8. (Left panels) Raw absorption spectra of the samples used for collection of decay traces. (Right panels) Corresponding deconvoluted spectra, showing the isolated contribution from **Per**, which was subsequently used to determine the **Per** concentration.

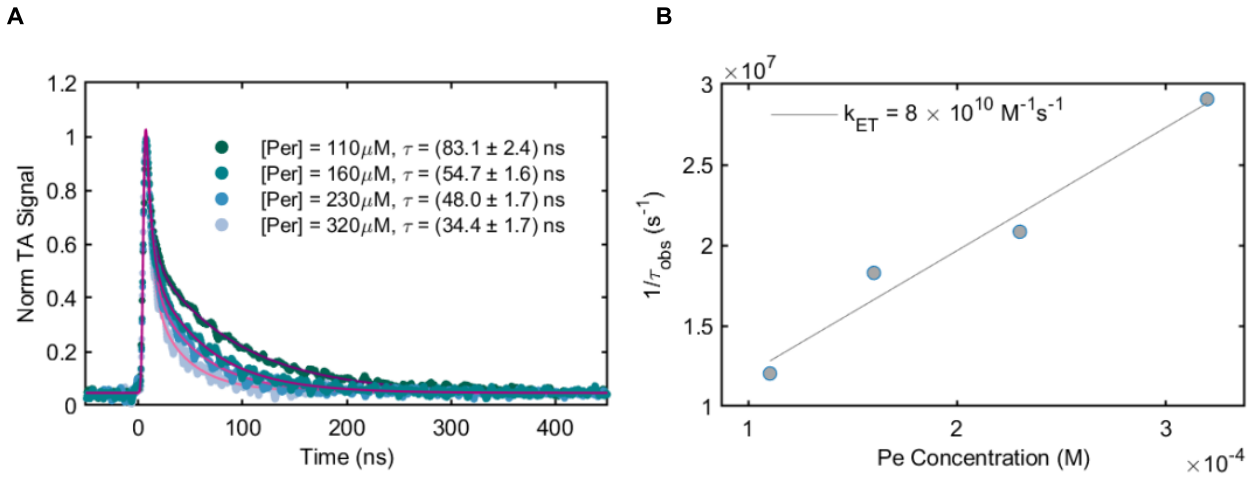


Figure S2.9. (Left panel) NIR nanosecond transient absorption decay traces of samples containing **Per**$^{\bullet-}$ following an excitation at 398 nm (pulse energy of 3μJ). The traces are then fitted to a biexponentially modified Gaussian model (Eq S2) described above (pink lines going through the raw data). The extracted τ value represents the kinetics of solvated electron capture. (Right panel) Plot of **Per** concentration versus $1/\tau_{obs}$ fitted to a straight line. The slope yields the bimolecular rate constant for electron capture by Per, $k_{ET} = 8\times10^{10}\,M^{-1}s^{-1}$.

Sample	Estimated [Per] (mM)	Observed τ_{decay} (ns)
#1	0.11	83.1
#2	0.16	54.7
#3	0.23	48.0
#4	0.32	34.4

Table S2.1. Capture of solvated electrons by Per. Neutral Per concentrations estimated from the isolated Per absorption spectra (**Figure S2.8**), together with the observed lifetimes (τ_{obs}) of the solvated electron decay signal. These values were used to construct the Stern–Volmer–type plot shown above.

Kinetic Equations in presence of an added quencher:

With a quencher the solvated electron dynamics changes in the following way:

$$\frac{d[e^-]}{dt} = -k_{Pe}[Pe][e^-] - k_q[Q][e^-] = -(k_{Pe}[Pe] + k_q[Q])[e^-]$$

which integrates to:

$$[e^-](t) = A_0 \exp((k_{Pe}[Pe] + k_q[Q])t) = A_0 exp\left(-\frac{t}{\tau_{obs}}\right)$$

with the relationship:

$$k_{Pe}[Pe] + k_q[Q] = 1/\tau_{obs}$$

Since, k_{Pe} has been determined already, k_q can be determined by the slope of a plot of

$$[Q] \text{ versus } (1/\tau_{obs} - k_{Pe}[Pe])$$

where $k_{Pe} = 8\times10^{10}\ M^{-1}s^{-1}$

With pyrene as quencher:

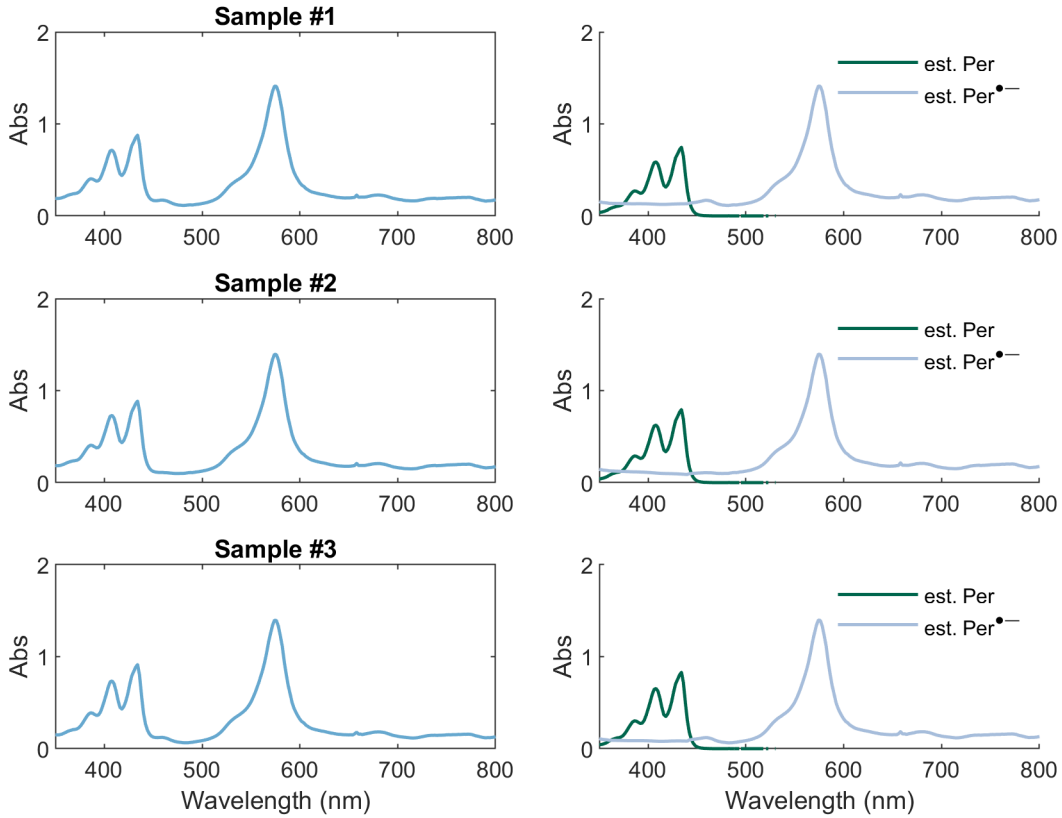


Figure S2.10. (Left panels) Raw absorption spectra of the samples used for collection of decay traces. (Right panels) Corresponding deconvoluted spectra, showing the isolated contribution from **Per**, which was subsequently used to determine the **Per** concentration.

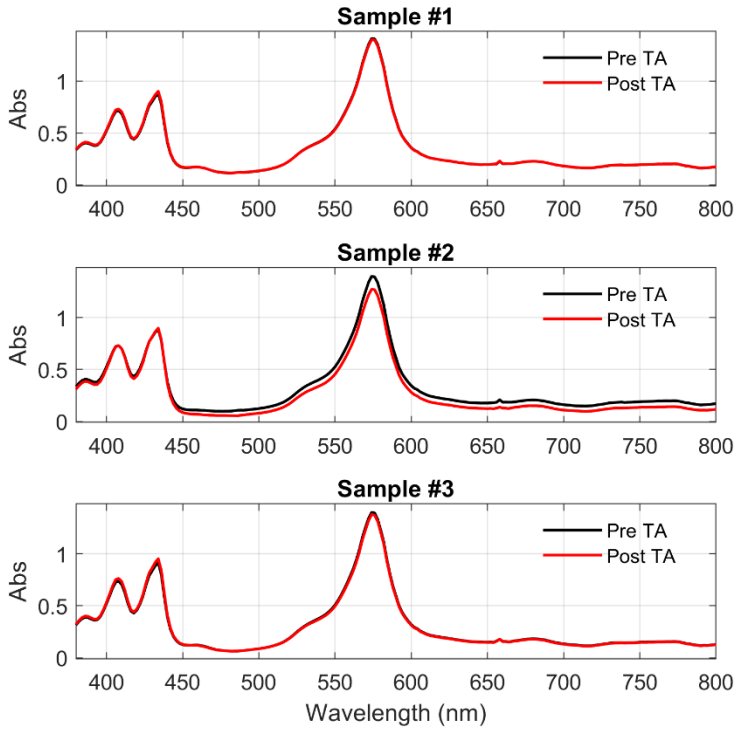


Figure S2.11. Raw absorption spectra of the samples used for collection of decay traces showcasing the stability of the samples and the reversibility of the electron transfer processes.

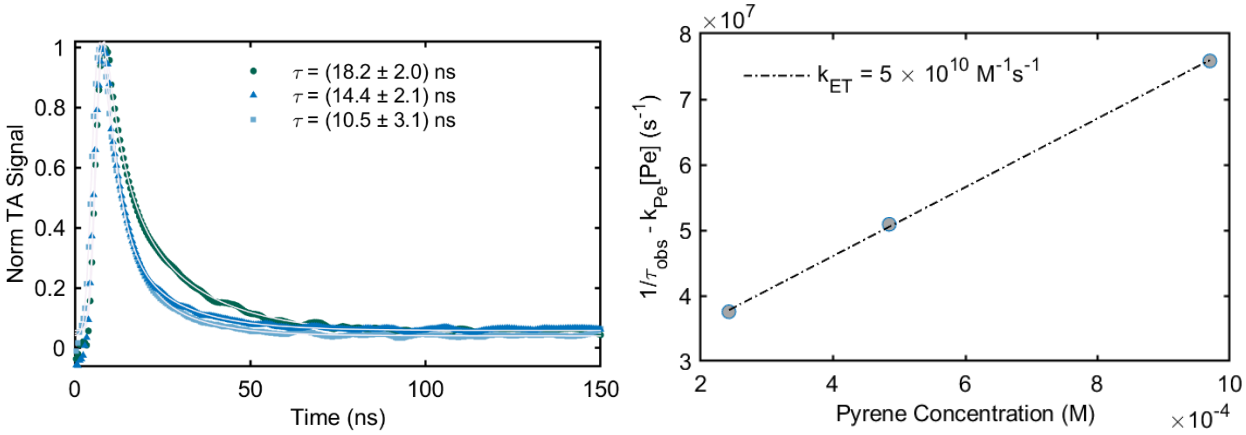


Figure S2.12. (Left panel) NIR nanosecond transient absorption decay traces of samples containing **Per**$^{\bullet-}$ along variable amounts of pyrene as quencher, following an excitation at 398 nm (pulse energy of 3μJ). The traces are then fitted to a biexponentially modified Gaussian model (Eq S2) described above (grey lines going through the raw data). The extracted τ value represents the kinetics of solvated electron capture. (Right panel) Plot of pyrene concentration versus $(1/\tau_{obs} - k_{Pe}[Pe])$ fitted to a straight line. The slope yields the bimolecular rate constant for electron capture by pyrene, $k_{ET} = 5\times10^{10}\ M^{-1}s^{-1}$.

Sample	[Pyrene] (mM)	Estimated [Per](mM)	Observed τ_{decay} (ns)
#1	0.24	0.22	18.2
#2	0.485	0.23	14.4
#3	0.97	0.24	10.5

Table S2.2. Capture of solvated electrons by Pyr. Pyrene concentrations together with the observed lifetimes (τ_{obs}) of the solvated electron decay signal. Neutral **Per** concentrations estimated from the isolated **Per** absorption spectra (**Figure S2.10**) are also tabulated. These values were used to construct the Stern–Volmer–type plot shown above.

With styrene as a quencher:

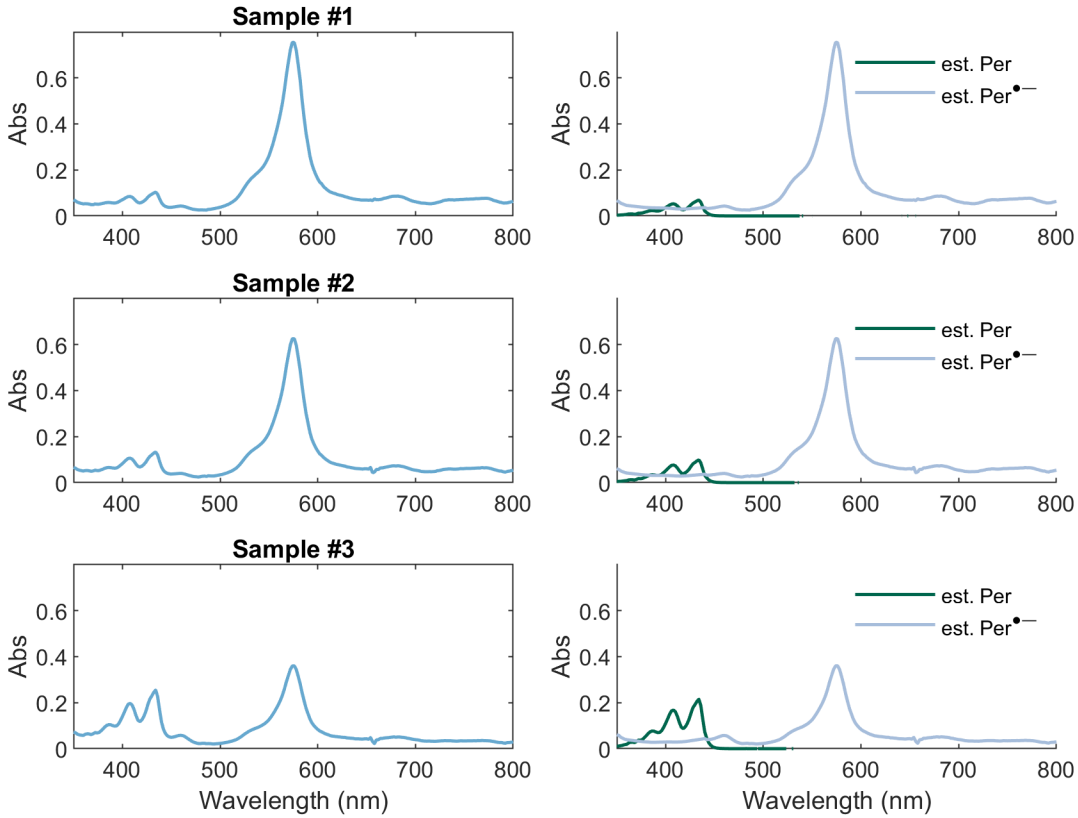


Figure S2.13. (Left panels) Raw absorption spectra of the samples used for collection of decay traces. (Right panels) Corresponding deconvoluted spectra, showing the isolated contribution from Per, which was subsequently used to determine the **Per** concentration.

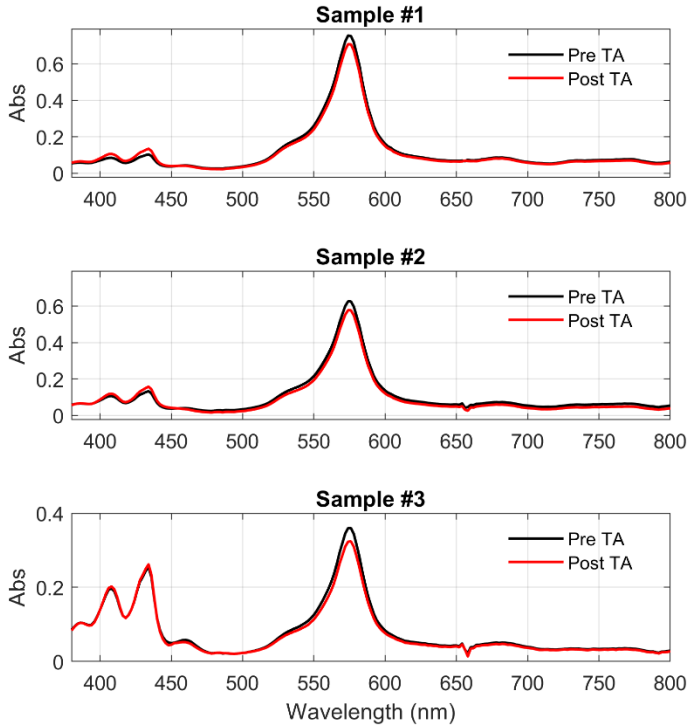


Figure S2.14. Raw absorption spectra of the samples used for collection of decay traces showcasing the stability of the samples and the reversibility of the electron transfer processes.

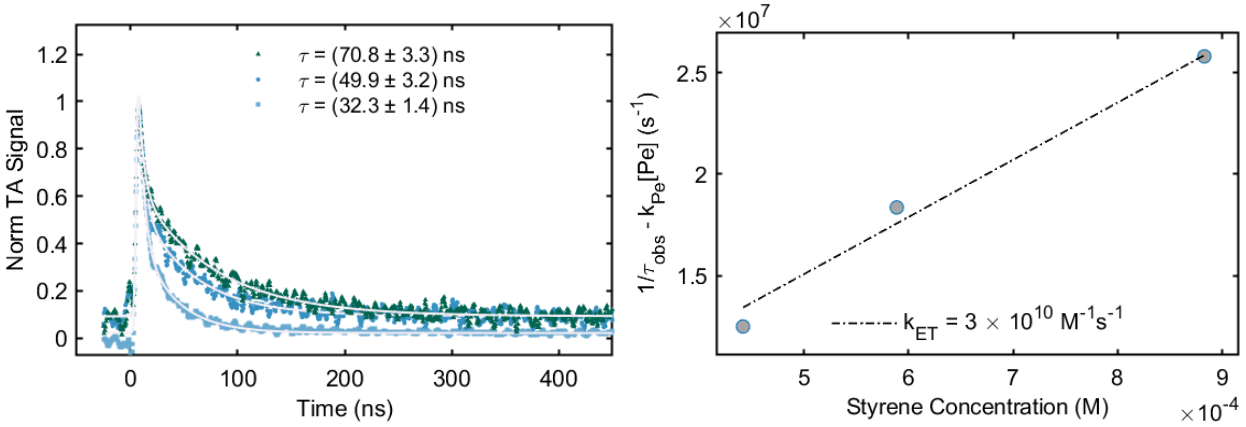


Figure S2.15. (Left panel) NIR nanosecond transient absorption decay traces of samples containing **Per**$^{\bullet-}$ along variable amounts of styrene as quencher, following an excitation at 398 nm (pulse energy of 3µJ). The traces are then fitted to a biexponentially modified Gaussian model (Eq S2) described above (grey lines going through the raw data). The extracted τ value represents the kinetics of solvated electron capture. (Right panel) Plot of pyrene concentration versus $(1/\tau_{obs} - k_{Pe}[Pe])$ fitted to a straight line. The slope yields the bimolecular rate constant for electron capture by pyrene, $k_{ET} = 3\times10^{10}\ M^{-1}s^{-1}$.

Sample	[Styrene] (mM)	Estimated [Per](mM)	Observed τ_{decay} (ns)
#1	0.44	0.02	70.8
#2	0.59	0.03	49.9
#3	0.88	0.06	32.3

Table S2.3. Capture of solvated electrons by styrene. Styrene concentrations together with the observed lifetimes (τ_{obs}) of the solvated electron decay signal. Neutral **Per** concentrations estimated from the isolated **Per** absorption spectra (**Figure S2.13**) are also tabulated. These values were used to construct the Stern–Volmer–type plot shown above.

With 1-(2,2-dimethylcyclopropyl)propan-1-one (**Ket-1**) as a quencher:

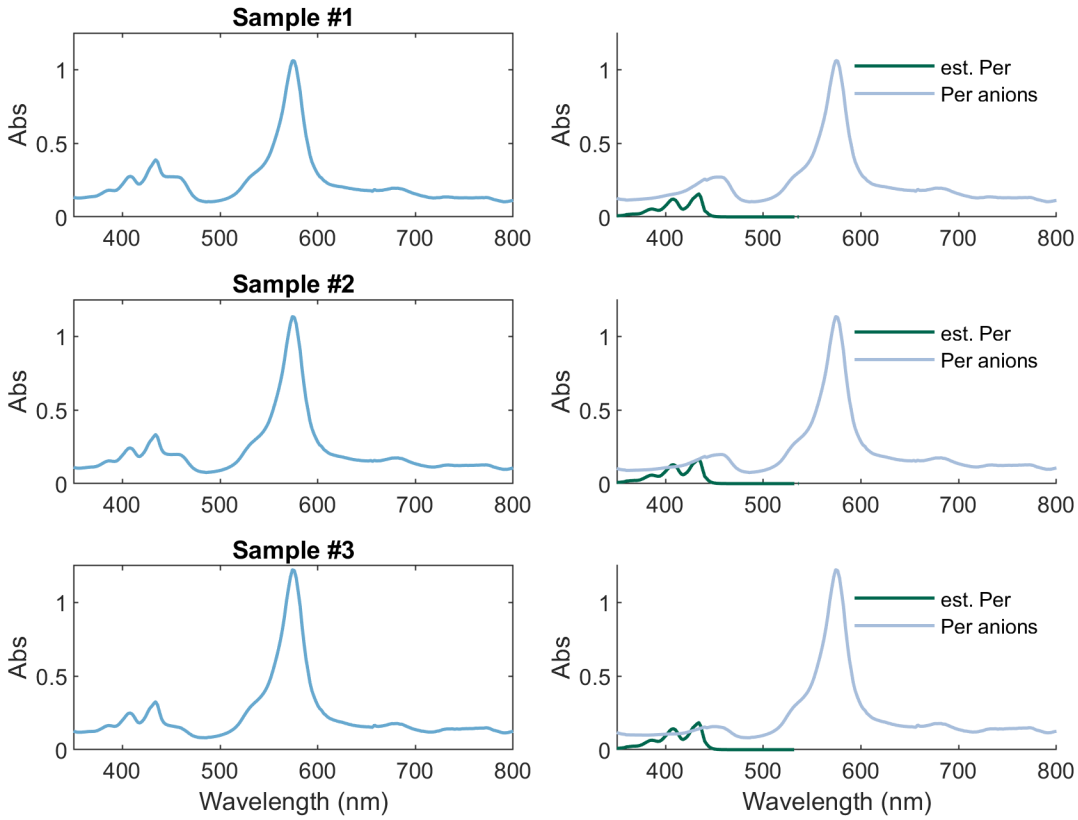


Figure S2.16. (Left panels) Raw absorption spectra of the samples used for collection of decay traces. (Right panels) Corresponding deconvoluted spectra, showing the isolated contribution from **Per**, which was subsequently used to determine the **Per** concentration.

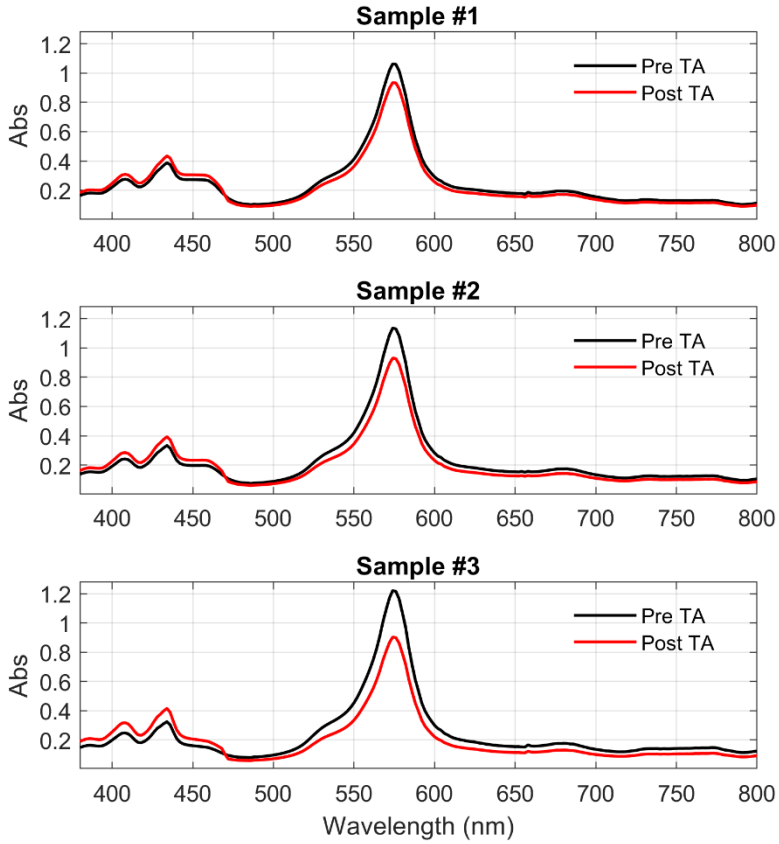


Figure S2.17. Raw absorption spectra of the samples used for collection of decay traces showcasing the stability of the samples and the reversibility of the electron transfer processes.

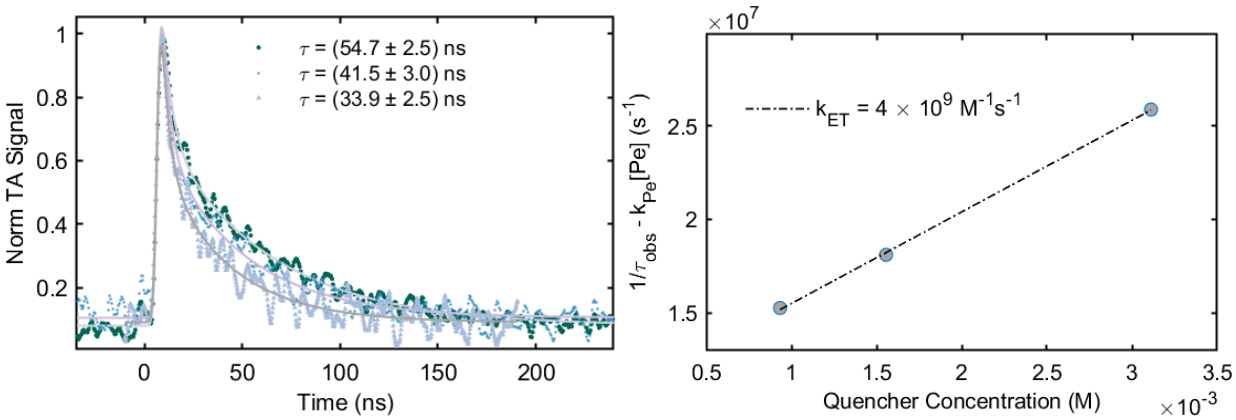


Figure S2.18. (Left panel) NIR nanosecond transient absorption decay traces of samples containing **Per**$^{\bullet-}$ along variable amounts of cyclopropyl ketone (**Ket-1**) as quencher, following an excitation at 398 nm (pulse energy of 3μJ). The traces are then fitted to a biexponentially modified Gaussian model (Eq S2) described above (grey lines going through the raw data). The extracted τ value represents the kinetics of solvated electron capture. (Right panel) Plot of cyclopropylketone (Ket-1) concentration versus $(1/\tau_{obs} - k_{Pe}[Pe])$ fitted to a straight line. The slope yields the bimolecular rate constant for electron capture by pyrene, $k_{ET} = 3\times10^{10}\,M^{-1}s^{-1}$.

Sample	[Ket-1] (mM)	Estimated [Per](mM)	Observed τ_{decay} (ns)
#1	0.93	0.04	54.7
#2	1.56	0.05	41.5
#3	3.11	0.05	33.9

Table S2.4. Capture of solvated electrons by Ket-1. Ket-1 concentrations together with the observed lifetimes (τ_{obs}) of the solvated electron decay signal. Neutral **Per** concentrations estimated from the isolated **Per** absorption spectra (**Figure S2.16**) are also tabulated. These values were used to construct the Stern–Volmer–type plot shown above.

Note: While aryl cyclopropyl ketones are routinely observed via TAS, direct observation of the aliphatic ketyl radicals studied in this work was not feasible due to their much less diagnostic, blue-shifted features that are dwarfed by the perylene absorption features. However, both the concentration-dependent quenching of the solvated electron by Ket-1 and cyclic voltammetry studies are fully consistent with SET reduction of the ketone.

With 4-tert-Butylcyclohexanone (**Ket-2**) as a quencher:

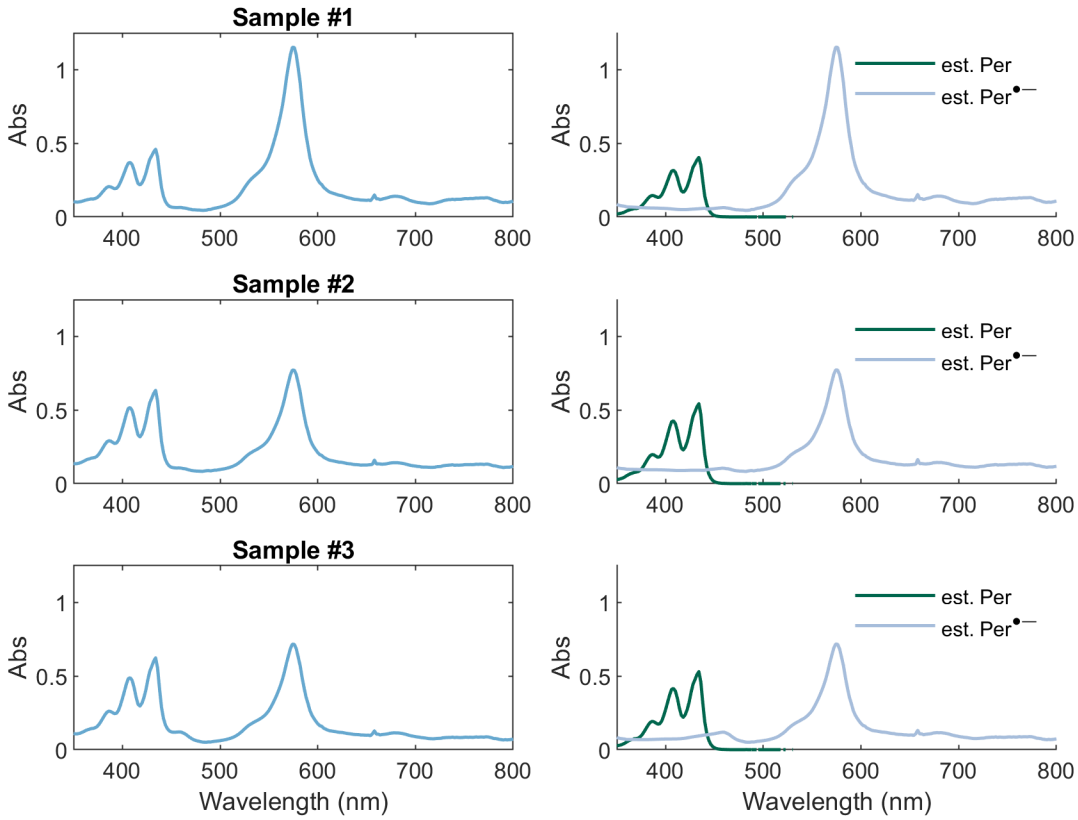


Figure S2.19. (Left panels) Raw absorption spectra of the samples used for collection of decay traces. (Right panels) Corresponding deconvoluted spectra, showing the isolated contribution from **Per**, which was subsequently used to determine the **Per** concentration.

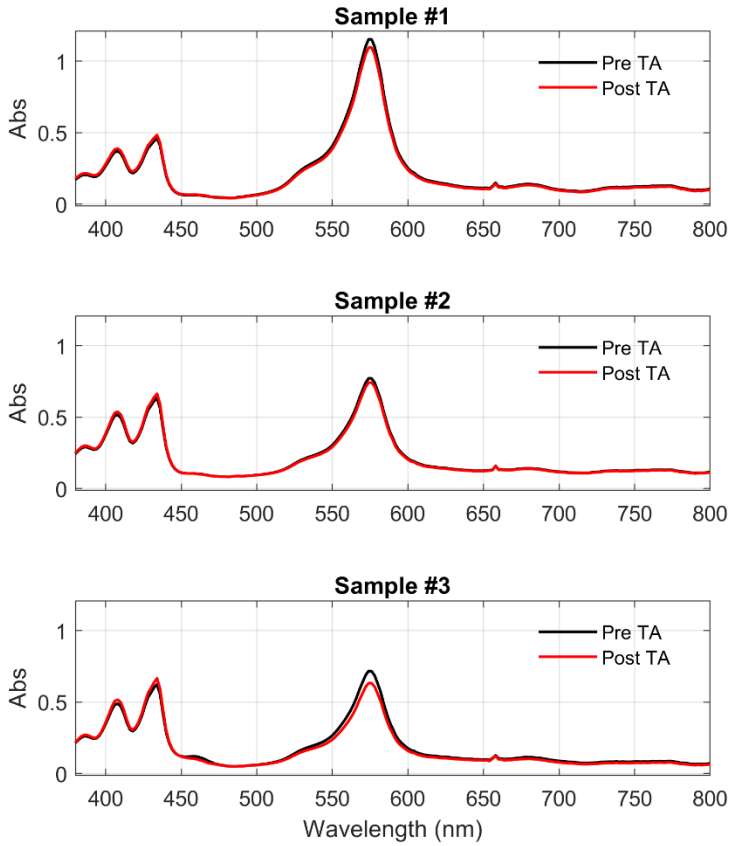


Figure S2.20. Raw absorption spectra of the samples used for collection of decay traces showcasing the stability of the samples and the reversibility of the electron transfer processes.

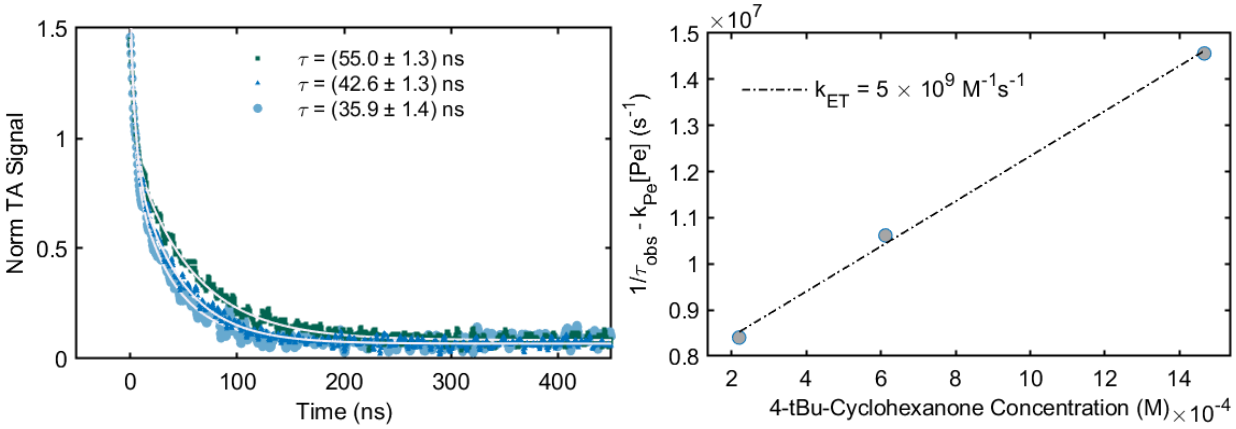


Figure S2.21. (Left panel) NIR nanosecond transient absorption decay traces of samples containing **Per**$^{\bullet-}$ along variable amounts of 4-^{t}butylcyclohexanone as quencher, following an excitation at 398 nm (pulse energy of 3µJ). The traces are then fitted to a biexponentially modified Gaussian model (Eq S2) described above (grey lines going through the raw data). The extracted τ value represents the kinetics of solvated electron capture. (Right panel) Plot of **Ket-2** concentration versus $(1/\tau_{obs} - k_{Pe}[Pe])$ fitted to a straight line. The slope yields the bimolecular rate constant for electron capture by pyrene, $k_{ET} = 3\times10^{10}\ M^{-1}s^{-1}$.

Sample	[4-^{t}Bu-cyclohexanone] (mM)	Estimated [Per](mM)	Observed τ_{decay} (ns)
#1	0.22	0.12	56.3
#2	0.61	0.16	43.0
#3	1.47	0.15	37.2

Table S2.5. Capture of solvated electrons by Ket-2. 4-^{t}Butylcyclohexanone concentrations together with the observed lifetimes (τ_{obs}) of the solvated electron decay signal. Neutral **Per** concentrations estimated from the isolated **Per** absorption spectra (**Figure S2.19**) are also tabulated. These values were used to construct the Stern–Volmer–type plot shown above.

Probing reversible ET dynamics with pyrene

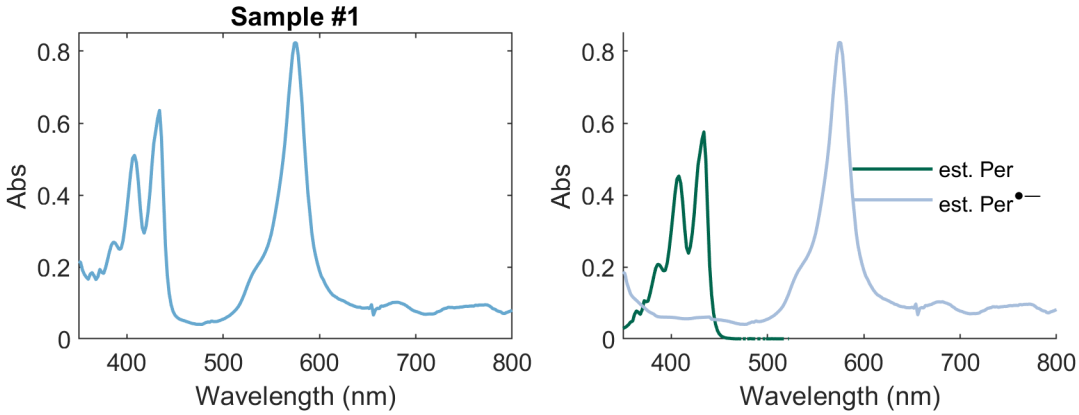


Figure S2.22 (Left panel) Raw absorption spectra of the sample used for collection of transient absorption data. (Right panel) Corresponding deconvoluted spectrum, showing the isolated contribution from **Per**, which was subsequently used to determine the **Per** concentration.

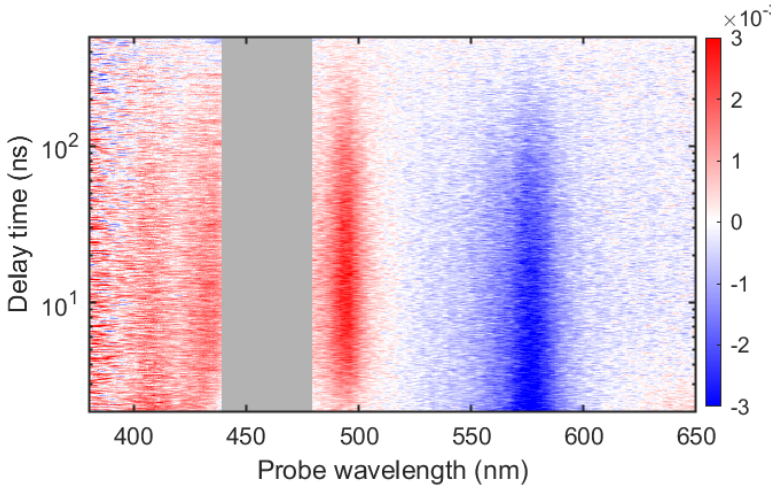


Figure S2.23. Two-dimensional nanosecond transient absorption map in the visible region, obtained by exciting a solution of **Per**$^{\bullet-}$ in the presence of pyrene at 460 nm (1 μJ per pulse).

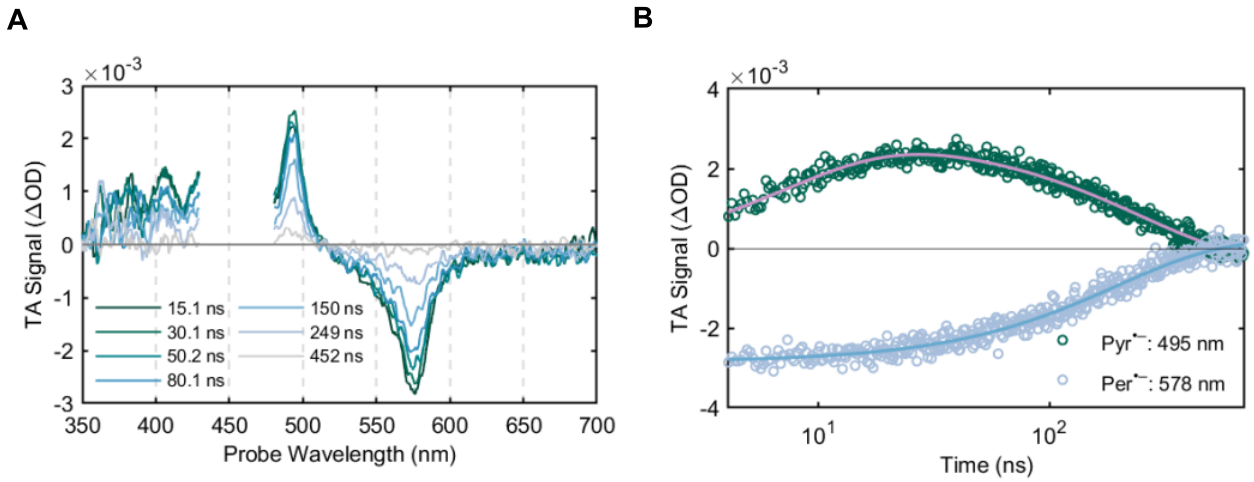


Figure S2.24. (A) Spectral slices at selected delay times (as indicated in the legend); the complete dataset is shown above (**Figure S2.23**). (B) Kinetic traces monitoring the reversible electron transfer between **Per**$^{\bullet-}$ and pyrene: forward electron capture by pyrene produces the pyrene radical anion (**Pyr**$^{\bullet-}$), while subsequent back electron transfer regenerates **Per**$^{\bullet-}$. This process is observed as the growth and decay of the **Pyr**$^{\bullet-}$ absorption at 495 nm and the concurrent recovery of **Per**$^{\bullet-}$ at 578 nm. The 495 nm trace was fit to a biexponential grow–decay model, yielding τ_{grow} = 7.5 ns and τ_{decay} = 243.2 ns. The 578 nm trace was fitted to a monoexponential decay model, yielding a τ = 197.8 ns. The close correspondence between τ_{decay} and the **Per**$^{\bullet-}$ recovery time confirms the reversibility of the electron transfer process.

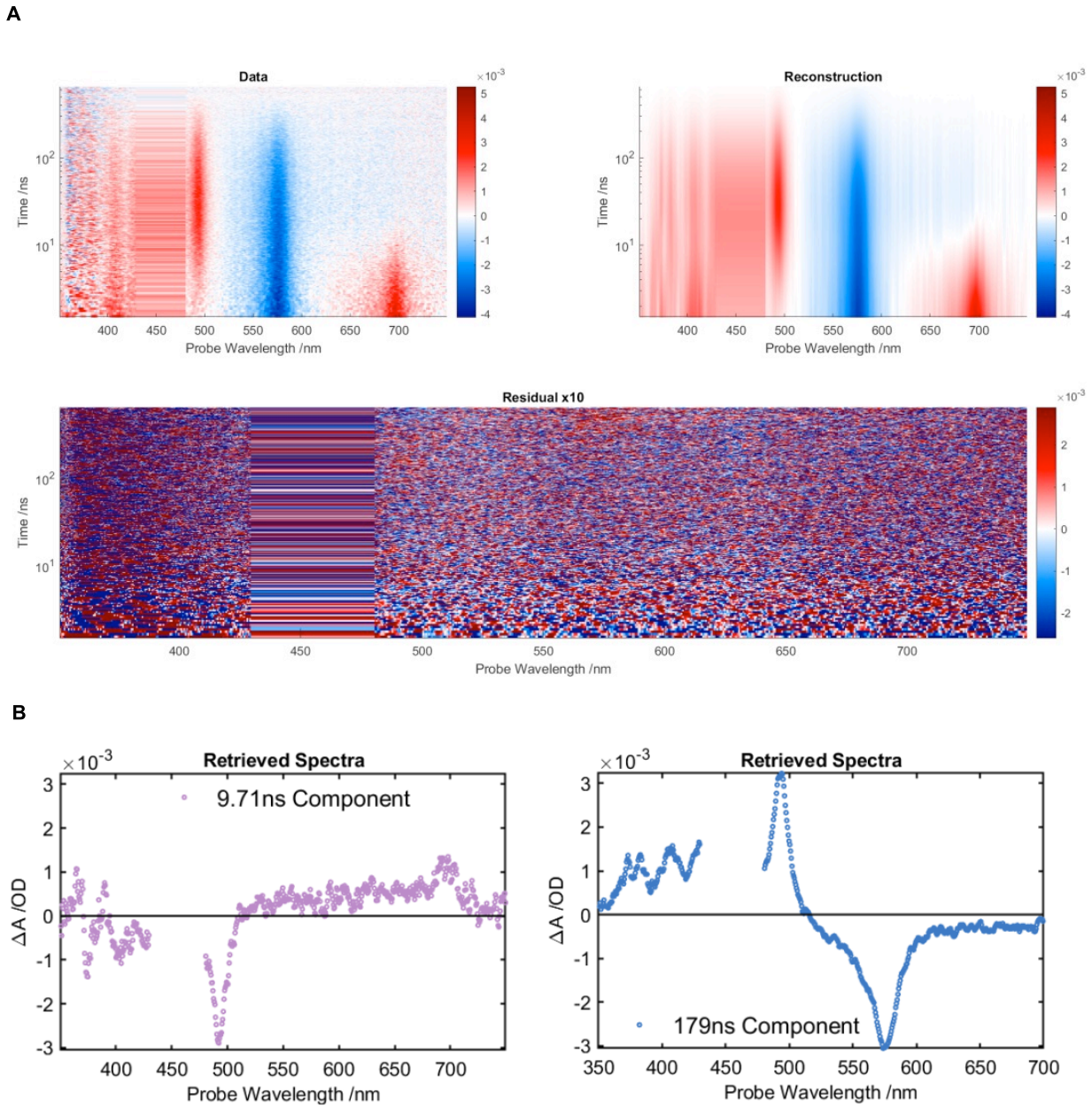


Figure S2.25. (A) The complete set of raw transient absorption data collected for Per•– in room temperature MeCN (left) after excitation with 460 nm (pulse energy of 1 μJ; same data is also presented in **Fig. 2.23**) along with a reconstructed global analysis model (right) comprised of a biexponential decay process. The residuals are shown in the bottom panel. (B) Decay-associated spectra obtained from the global fit corresponding to the two extracted time constants.

Estimating rate of back electron transfer from Pyrene$^{\bullet-}$ to Per

For this we only look at the decay dynamics of pyrene radical anion.

$$\frac{1}{\tau_{decay}} = k_{BET}[Per]$$

[Per] was estimated to be 167 μM which results in a k_{BET} of ~2×10^{10} $M^{-1}s^{-1}$

Note on BET kinetics

Our transient absorption data indicate that recapture of the solvated electrons by neutral perylene is a minor pathway under catalytically relevant conditions. Recombination with neutral perylene occurs at a rate of 8×10^{10} M^{-1} s^{-1}, whereas reduction of styrene and the ketone occur at rates of 3×10^{10} M^{-1} s^{-1} and 4×10^{9} M^{-1} s^{-1}, respectively. After adjusting for concentration differences under catalytically relevant conditions (80 mM for the substrates vs at most 6 mM perylene), substrate reduction becomes the kinetically dominant fate of solvated electrons (krel, (styrene) = 50; krel, (ket-1) = 7). Considering the multistep BET sequence that reoxidizes ketyl radical and inhibits annulation, the low concentration of neutral Per again is relevant. Since styrene is present in much higher concentration than perylene, our calculations indicate styrene mediates BET from the ketyl to Per. Of note, each of these calculations assume all of the catalyst is in its neutral form, while in reality some fraction of perylene is present as the radical anion.

7. Kinetic Modeling

To rationalize the observed product distributions, we developed a simple kinetic framework describing the competition between protonation of reduced styrene and coupling of fragmented cyclopropyl ketone with styrene. The model incorporates forward and back electron transfer steps governed by donor and acceptor redox potentials within a Marcus-theory description, subsequent unimolecular fragmentation and protonation, and bimolecular coupling. This analysis allows us to visualize how varying the driving force of electron transfer (via altering the $E_{1/2}$ of the reductant donor and oxidant acceptor) alters the early-time formation of hydrogenation versus coupling products, and to identify conditions where the desired pathway is favored.

Assumptions:

1. **Excess substrates and redox partners**. Concentrations of styrene [sty], cyclopropyl ketone [ket], reductant donor [D], and acceptor [A] remain constant throughout the reaction window of interest. Only the reactive intermediates ([sty$^{\bullet-}$], [ket$^{\bullet-}$], [ket_frag], [sty_hydrog], [coupling_product]) evolve in time.

2. **Elementary processes**.
   a. Forward electron transfer (ET):
   $$\mathrm{D} + \mathrm{X} \xrightarrow{k_{f,X}} \mathrm{D}^{\cdot+} + \mathrm{X}^{\cdot-}, X \in \{\mathrm{sty}, \mathrm{ket}\}$$
   b. Back electron transfer (BET):
   $$\mathrm{X}^{\cdot-} + \mathrm{A} \xrightarrow{k_{b,X}} \mathrm{X} + \mathrm{A}^{\cdot-}$$
   c. Subsequent fates: $k_{\mathrm{proto}} = 6\ \mathrm{M^{-1}s^{-1}}$, $k_{frag} = 10^8\ \mathrm{s^{-1}}$, $k_{coup} = 2.4 \times 10^2\ \mathrm{M^{-1}s^{-1}}$, $k_{annul} = 1.7 \times 10^2\ \mathrm{s^{-1}}$ as estimated using DFT calculations (see below)

$$\mathrm{sty}^{\cdot-} + \mathrm{H_2O} \xrightarrow{k_{proto}} \mathrm{sty\_hydrog}$$
$$\mathrm{ket}^{\cdot-} \xrightarrow{k_{frag}} \mathrm{ket\_frag}$$
$$\mathrm{ket\_frag} \xrightarrow{k_{annul}} \mathrm{ket}^{\cdot-}$$
$$\mathrm{ket\_frag} + \mathrm{sty} \xrightarrow{k_{coup}} \mathrm{coupling\_product}$$

3. **Electron transfer kinetics**. Second-order ET rates follow nonadiabatic Marcus theory with a simple "min" diffusion cap. $A = 10^{12}\ \mathrm{M^{-1}s^{-1}}$, $\lambda = 1.2$ eV for styrene and 1.3 eV for cyclopropyl ketone as estimated using DFT calculations. T = 298 K. $k_{diff} = 10^{10}\ \mathrm{M^{-1}s^{-1}}$

$$k_{f,b} = A \exp\left[-\frac{(\Delta G^\circ + \lambda)^2}{4\lambda k_B T}\right], \qquad k_{f,b} \le k_{\mathrm{diff}} \qquad \text{Eq S3}$$

Where the free energies are defined as

$$\Delta G^\circ_{f,X} = E_D - E_X, \qquad \Delta G^\circ_{b,X} = E_X - E_A$$

with redox potentials versus SCE.

Rate equations:

$$\frac{d[sty^{\bullet-}]}{dt} = (k_{f,sty}[D]+k_{sty}^{ET,ketyl}[ketyl\_cyclo]+k_{sty}^{cy\_propyl}[ket^{\bullet-}])[sty] - (k_{b,sty}[A]+k_{proto}[H_2O])[sty^{\bullet-}]$$

$$\frac{d[ket^{\bullet-}]}{dt} = (k_{f,ket}[D]+k_{ket}^{ET,ketyl}[ketyl\_cyclo])[ket] + k_{annul}[ket\_frag] - (k_{b,ket}[A]+k_{frag}+k_{sty}^{cy\_propyl}[sty])[ket^{\bullet-}]$$

$$\frac{d[ket\_frag]}{dt} = k_{frag}[ket^{\bullet-}] - k_{annul}[ket\_frag] - k_{coup}[ket\_frag][sty]$$

$$\frac{d[sty\_hydrog]}{dt} = k_{proto}[sty^{\bullet-}][H_2O]$$

$$\frac{d[ketyl\_linear]}{dt} = k_{coup}[sty][ket\_frag]-k_f^{cyclc}[ketyl\_linear] + k_b^{cyclc}[ketyl\_cyclo]$$

$$\frac{d[ketyl\_cyclo]}{dt} = k_f^{cyclc}[ketyl\_linear] - (k_b^{cyclc} + k_{sty}^{ET,ketyl}[sty] + k_{ket}^{ET,ketyl}[ket] + k_{b,ketyl}[A])[ketyl\_cyclo]$$

$$\frac{d[ox\_cyclo\_adduct]}{dt} = (k_{sty}^{ET,ketyl}[sty] + k_{ket}^{ET,ketyl}[ket] + k_{b,ketyl}[A])[ketyl\_cyclo]$$

Useful composite "loss" terms:

$$L_S = k_{b,sty}[A]+k_{proto}[H_2O]$$

$$L_K = k_{b,ket}[A]+k_{sty}^{cy\_propyl}[sty]$$

$$L_P = k_{sty}^{ET,ketyl}[sty] + k_{ket}^{ET,ketyl}[ket] + k_{b,ketyl}[A]$$

$$L_F = k_{annul} + k_{coup}[sty]$$

We can now estimate the steady-state concentrations of the reactive intermediates by setting

$$\frac{d}{dt} = 0 \text{ for all species except [sty\_hydrog] and [ox\_cyclo\_adduct]}$$

The steady-state concentrations can be written as:

$$\frac{d[ket\_frag]_{SS}}{dt} = 0 \Rightarrow [ket\_frag]_{ss} = \frac{k_{frag}}{L_F}[ket^{\bullet-}]_{SS}$$

$$\frac{d[ketyl\_cyclo]_{SS}}{dt} = 0 \Rightarrow [ketyl\_cyclo]_{ss} = \frac{k_{coup}[sty]}{L_P}[ket\_frag]_{SS}$$

Solving for $[ket^{\bullet-}]_{ss}$:

$$[ket^{\bullet-}]_{ss} = \frac{k_{f,ket}[D][ket]}{L_K - \frac{k_{annul}k_{frag}}{L_F} - k_{ket}^{ET,ketyl}[ket]\left(\frac{k_{coup}[sty]k_{frag}}{L_P L_F}\right)}$$

Solving for $[sty^{\bullet-}]_{ss}$:

$$[sty^{\bullet-}]_{ss} = \frac{k_{f,sty}[D][sty] + [sty](k_{sty}^{ET,ketyl}[ketyl\_cyclo]_{SS} + k_{sty}^{cy\_propyl}[ket^{\bullet-}]_{ss})}{L_S}$$

Rate of product formations under steady-state:

$$r_{hydrogenation} = \frac{d[sty\_hydrog]}{dt} = k_{proto}[sty^{\cdot-}]_{ss}[H_2O] \qquad \text{Eq S4}$$

$$r_{[3+2]addition} = \frac{d[ox\_cyclo\_adduct]}{dt} = (k_{sty}^{ET,ketyl}[sty] + k_{ket}^{ET,ketyl}[ket] + k_{b,ketyl}[A])[ketyl\_cyclo]_{ss} \qquad \text{Eq S5}$$

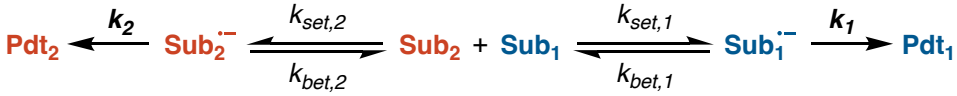
Selectivity:

$$\text{Selectivity} = \frac{r_{[3+2]addition} - r_{hydrogenation}}{r_{[3+2]addition} + r_{hydrogenation}}$$

Selectivity model as a function of reductant strength and relative rates of competing pathways (Fig. 5C)

Derivation:

For the generic case:



Sub_1 is harder to reduce than Sub_2 but reacts as a faster rate. The rate of each product formation is given by

$$\frac{d[Pdt_n]}{dt} = k_n[Sub_n^{\bullet -}]$$

Eq S6

Selectivity is defined as the ratio of rates to form product upon reaching the steady state

$$selectivity = \frac{[Pdt_1]}{[Pdt_2]} = \frac{k_1[Sub_1^{\bullet -}]}{k_2[Sub_2^{\bullet -}]}$$

Eq S7

By applying the steady state model, the concentration of each reduced substrate becomes

$$[Sub_n^{\bullet -}] = \frac{k_{set,n}[D][Sub_n]}{k_{bet,n}[A] + \boldsymbol{k_n}}$$

Eq S8

Where [D] and [A] are the concentrations of the active reductant and the oxidized photocatalyst and $\boldsymbol{k_n}$ is the first-order rate constant for the conversion of the reduced substrate into product. Substituting the expression for the steady-state concentrations of reduced substrates (Eq S8) into the selectivity expression (Eq S7) and simplifying affords the general selectivity expression:

$$\frac{[Pdt_1]}{[Pdt_2]} = \frac{\boldsymbol{k_1}}{\boldsymbol{k_2}} \bullet \frac{k_{set,1}}{k_{set,2}} \bullet \frac{k_{bet,2}[A] + \boldsymbol{k_2}}{k_{bet,1}[A] + \boldsymbol{k_1}}$$

Eq S9

Selectivity profile of super potent reductants

For a reductant that is sufficiently potent to render the forward rates of electron transfer to both substrates diffusion limited, i.e. $k_{set,1} \approx k_{set,2} \approx k_{diff}$, the product selectivity from Eq S9 simplifies to

$$\frac{[Pdt_1]}{[Pdt_2]} = \frac{\boldsymbol{k_1}}{\boldsymbol{k_2}} \bullet \frac{k_{bet,2}[A] + \boldsymbol{k_2}}{k_{bet,1}[A] + \boldsymbol{k_1}}$$

Eq S10

This expression can be further simplified based on 3 chemical scenarios

Scenario 1: BET is fast relative to $\boldsymbol{k_1}$ and $\boldsymbol{k_2}$ ($k_{bet,1}, k_{bet,2} \approx k_{diff}$; $[A]$ is sufficiently large such that $k_{bet,1}[A], k_{bet,2}[A] \gg \mathrm{k_1}, \mathrm{k_2}$)

$$\frac{[Pdt_1]}{[Pdt_2]} = \frac{\boldsymbol{k_1}}{\boldsymbol{k_2}}$$

Eq S11

In this context, both substrates are indiscriminately and reversibly reduced, resulting in a photostationary state that maintains equal concentration of both reduced substrates. Under this scenario, the ratio of products is equal to k_1/k_2.

Scenario 2: $\boldsymbol{k_1}$ is fast relative to BET.

$$\frac{[Pdt_1]}{[Pdt_2]} = \frac{k_{bet,2}[A] + \boldsymbol{k_2}}{\boldsymbol{k_2}}$$

Eq S12

In this context the harder-to-reduce substrate (Sub_1) irreversibly reacts faster than even diffusion-limited BET. As a result, selectivity is determined by the propensity of the easier-to-reduce substrate to either undergo BET or form Pdt_2 upon reduction. When BET is much faster ($k_{bet,2}[A] \gg \mathrm{k_2}$), the easier to reduce substrate is protected from decomposition and the reaction will be highly selective for Pdt_1.

Scenario 3: BET is slow relative to k_1 and k_2.

$$\frac{[Pdt_1]}{[Pdt_2]} = 1$$

Eq S13

In this case, both substrates irreversibly react faster than BET, leading to a completely unselective mixture of products.

Impact of redox potentials on selectivity

For less reducing photoreductants, the rates of SET will no longer be capped by diffusion. In this case the ratio of products for each scenario will be given by Eq S9, wherein the relative rates of SET are determined by redox potentials.

$$\frac{[Pdt_1]}{[Pdt_2]} = \left(\frac{k_1}{k_2}\right)\left(\frac{k_{set,1}}{k_{set,2}}\right)\left(\frac{k_{bet,2}[A] + k_2}{k_{bet,1}[A] + k_1}\right)$$

*impacted by redox potentials for less reducing PC**

The selectivity plots shown in Fig. 5C were generated using Eq S10 in conjunction with forward electron transfer rates calculated using the same diffusion capped Marcus model described in Eq S2. Equal substrate reorganization energies (λ= 1.2 eV) and a preexponential factor of 10^{12} s^{-1} were assumed in this case. Simultaneously, the rate of back electron transfer (BET) for both substrate channels was fixed at the diffusion limit, taken as 10^{10} $M^{-1}s^{-1}$ for acetonitrile. The ratio of k_1 / k_2 was systematically varied to represent the competition between the two competing pathways. Additionally, 2 variables must be fixed. The concentration of the oxidized photocatalyst [A], which impacts the absolute rate of BET, was set to be 1% of the total catalyst concentration. Furthermore, the absolute value of k_2 was set to 100 s^{-1}. This number represents the rate at which the easier to reduce substrate reacts. Below we show the impact are co-varying these parameters on selectivity for each catalyst.

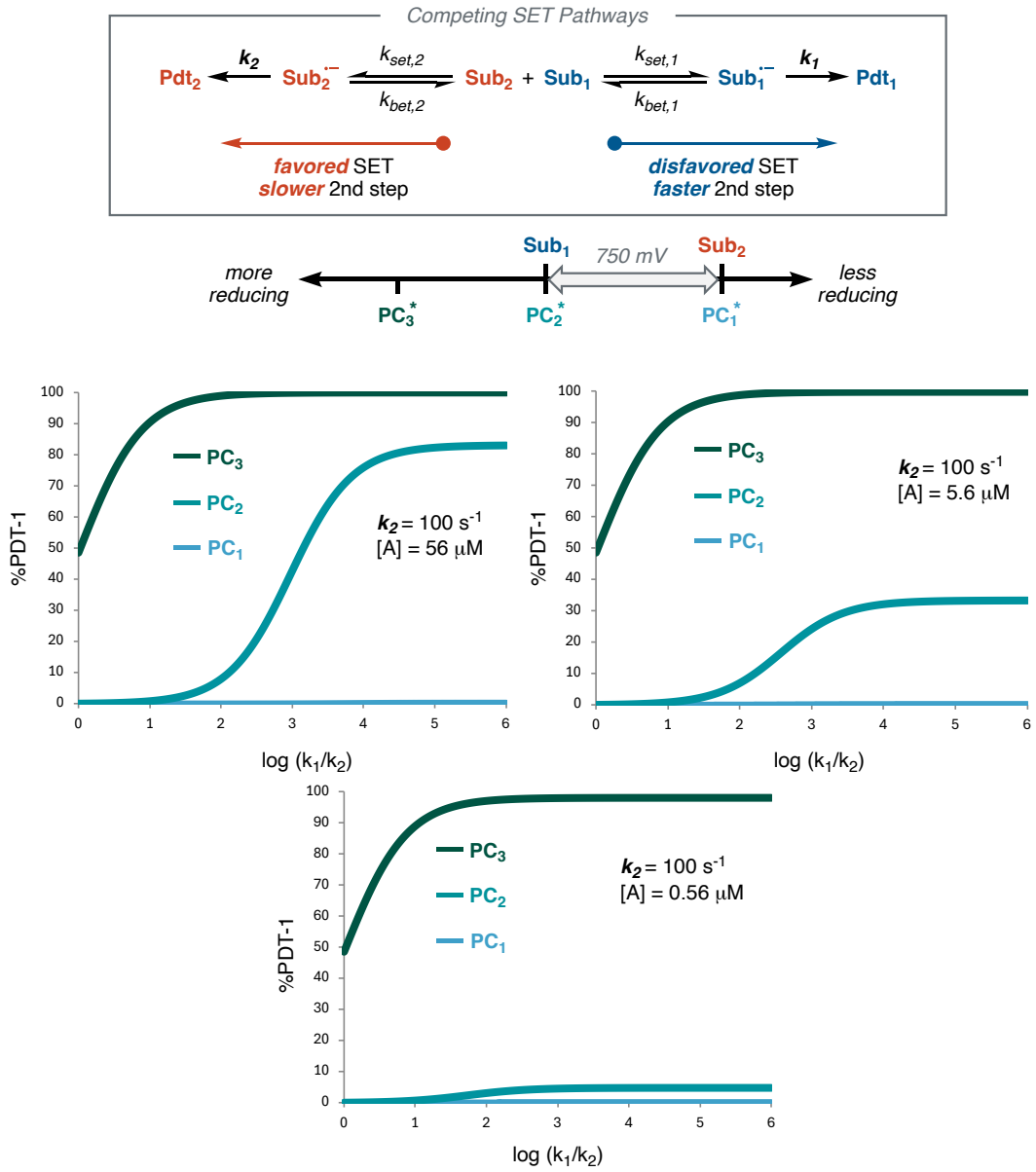


Figure S2.26. Impact of fitting parameters on product selectivity. k_2 represents the rate that easier to reduce substrate reacts upon SET. [A] is the concentration of the oxidized PC, which impacts the absolute rate of BET.

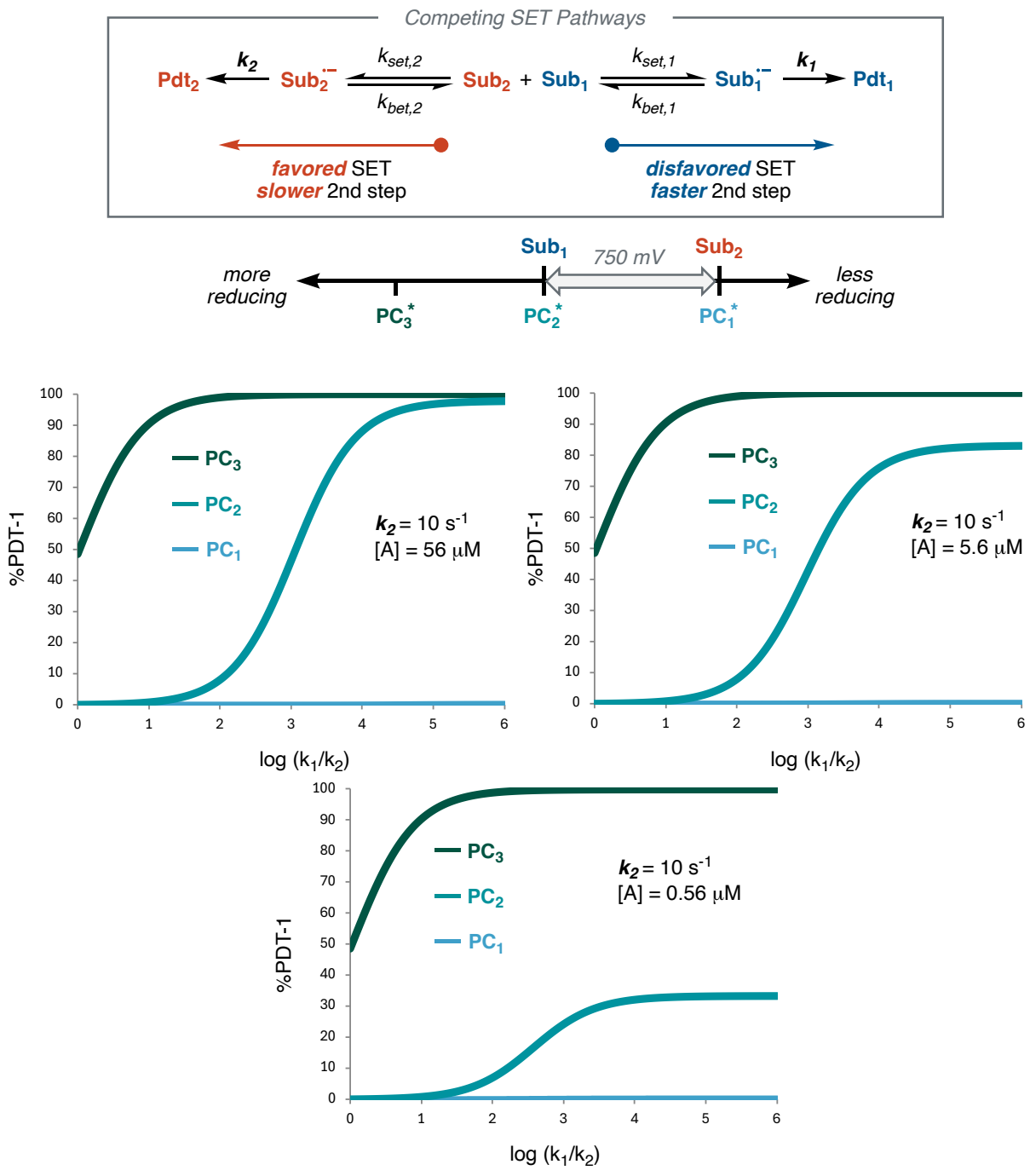


Figure S2.26 (cont.) Impact of fitting parameters on product selectivity. k_2 represents the rate that easier to reduce substrate reacts upon SET. [A] is the concentration of the oxidized PC, which impacts the absolute rate of BET.

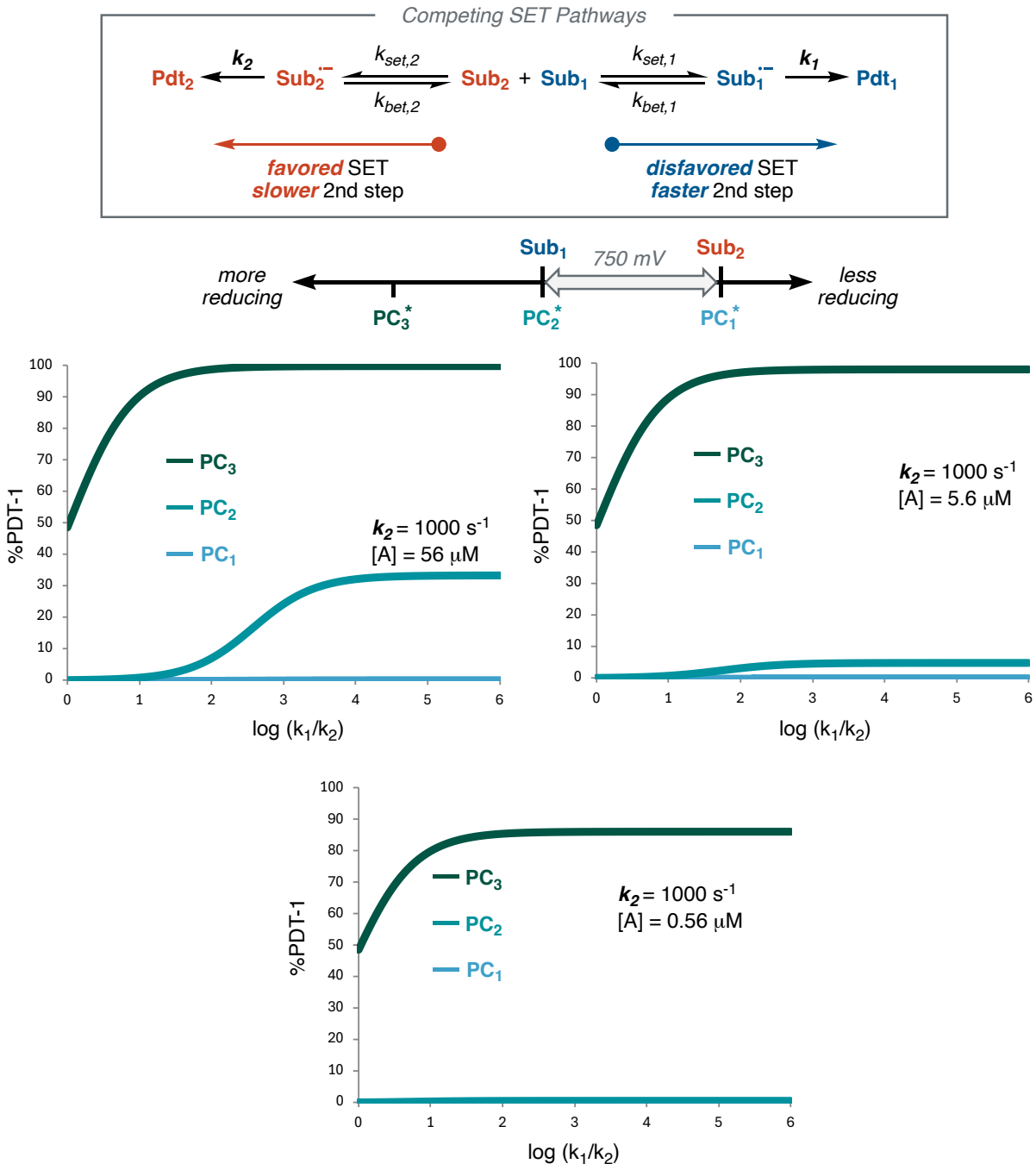


Figure S2.26 (cont.). Impact of fitting parameters on product selectivity. k_2 represents the rate that easier to reduce substrate reacts upon SET. [A] is the concentration of the oxidized PC, which impacts the absolute rate of BET.

Impact of Diffusive BET

We questioned whether the photogeneration of solvated electrons is uniquely well suited to promote radical formation since BET is a bimolecular process that cannot proceed faster than the diffusion limit. In contrast, substrate reduction from an excited state can undergo BET via in-cage charge recombination that will not be limited by diffusion. To probe this hypothesis, we modified our kinetic model in figure 5b to mimic the effects of in-cage charge recombination by removing the diffusion limit on BET (Figure S2.27). However, this change only leads to minor differences in the photocatalyst driving forces needed to elicit the desired selectivity profile, indicating that the diffusive nature of BET is likely not a major origin of selectivity for the model annulation reaction. We suspect that this insensitivity to faster-than-diffusion BET is a consequence of the large differential in rates between styrene radical anion protonation and ketyl β-scission in the present reaction. When we re-evaluate our kinetic model using a slower rate constant for fragmentation, the impact of capping the rate of BET at diffusion becomes far more significant (Figure S2.28 and S2.29).

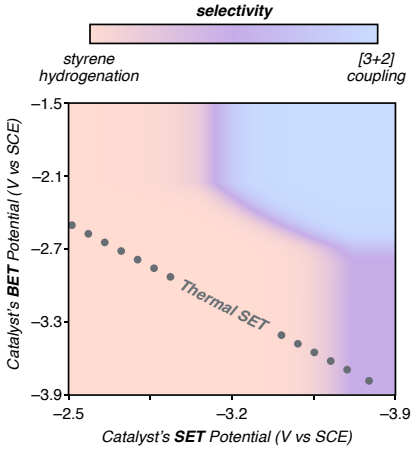


Figure 5c: Kinetic Selectivity model as a function of driving force for SET and BET.

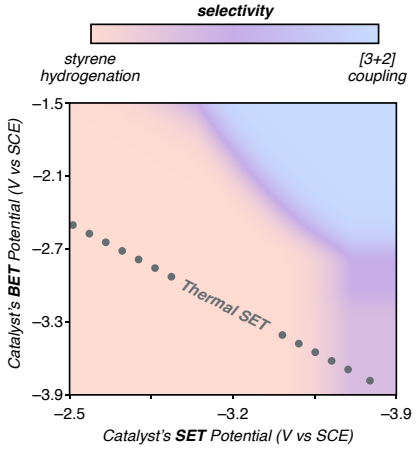


Figure S2.27: Reproduced from Figure 5c. but with no diffusion cap on the rate of BET to mimic the impact of in cage charge recombination

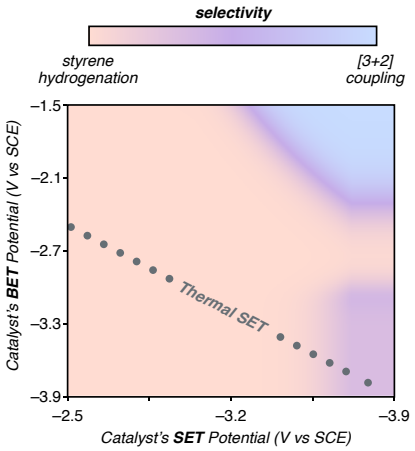


Figure S2.28: Reproduced from Figure 5c. but with no diffusion cap on the rate of BET to mimic the impact of in cage charge recombination and the rate of the radical formation is 100 times slower

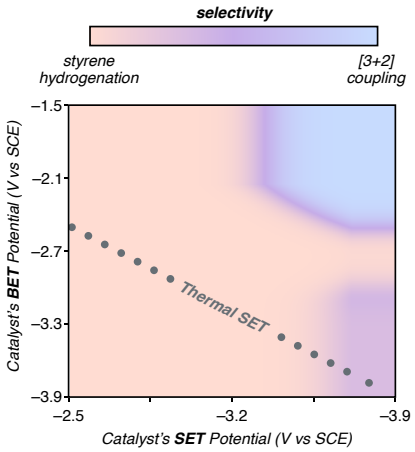


Figure S2.29: Reproduced from Figure 5c. but the rate of the radical formation is 100 times slower

Script for Figure 5b.

```
% New SS selectivity model (H vs [3+2]/cyclization) on (E_D, E_A) grid
% Assumptions: [sty],[ket],[D],[A],[H2O] constants (excess).
% SS for: sty_anion (S-), ket_anion (K-), ket_frag (F),
%         ketyl_adduct_prod (P), ketyl_cyclo_product (C)
% NOT SS for: sty_hydrog, final_cyclo_product (rates only)

clear; clc;

%% ----- CUSTOM COLORMAP -----
rgb_start = [255 220 210];
rgb_mid   = [198 173 233];
rgb_end   = [200 220 255];

rgb_start = rgb_start/255;
rgb_mid   = rgb_mid/255;
rgb_end   = rgb_end/255;

nPoints = 256;
x  = [0, 0.5, 1];
xi = linspace(0,1,nPoints);
cmap = zeros(nPoints,3);
for i = 1:3
    cmap(:,i) = interp1(x, [rgb_start(i), rgb_mid(i), rgb_end(i)], xi,
'linear');
end

%% ---------------- USER SETTINGS ----------------
% Reduction potentials (V vs SCE)
E_S = -2.60;      % styrene
E_K = -3.20;      % ketone (cyclopropyl ketone)
% If ketyl has a different E1/2, set it here; if unknown, reuse E_K
E_ketyl = E_K;

% Bulk concentrations (M)
sty  = 1.0e-3;     % [sty]
ket  = 1.0e-3;     % [ket]
D    = 2.0e-6;     % [D]
A    = 2.0e-5;     % [A]
H2O  = 1;       % [H2O] if solvent water; otherwise set your value

% Chemistry (NON-ET)
k_proto  = 6;      % M^-1s^-1  sty_anion -> sty_hydrog
k_frag   = 1.0e8;  % s^-1  ket_anion -> ket_frag
k_annul  = 1.7e2;  % s^-1  ket_frag -> ket_anion
k_coup   = 2.4e2;  % M^-1 s^-1  ket_frag + sty -> ketyl_adduct_prod

% k_cycl_f = 1.0e3;  % s^-1  ketyl_adduct -> ketyl_cyclo
% k_cycl_b = 1.0e2;  % s^-1  ketyl_cyclo -> ketyl_adduct

k_et_ks  = 4.8e5;   % M^-1 s^-1  ([3+2] ketyl to sty)
```

```
k_et_kk  = 1.3e0;   % M^-1 s^-1  ([3+2] ketyl to ket)
k_et_cks = 2.5e3;   % M^-1 s^-1  (cyclopropyl ketyl to sty)

% Marcus parameters (eV) and prefactors (M^-1 s^-1)
T     = 298;
AfS   = 1e12;  AbS = 1e12;  lambS = 1.2;   % sty forward/back
AfK   = 1e12;  AbK = 1e12;  lambK = 1.3;   % ket forward/back
AfKetyl = 1e12; AbKetyl = 1e12; lambKetyl = 1.2; % ketyl back (to A) if
needed

% Diffusion cap (MIN) for 2nd-order ET
kdiff_cap = 1.0e10;  % M^-1 s^-1

% Grids of potentials (V vs SCE)
E_D_grid = linspace(-3.9, -2.5, 501);  % donor (columns)
E_A_grid = linspace(-3.9, -1.5, 501);  % acceptor (rows)

%% ---------- SURFACES ----------
[ED, EA] = meshgrid(E_D_grid, E_A_grid);  % ED: cols, EA: rows

% Forward ET (2nd order) from donor
k_f_sty_2g = marcus_min_cap(ED, E_S, AfS, lambS, T, kdiff_cap, 'forward'); %
k_f,sty
k_f_ket_2g = marcus_min_cap(ED, E_K, AfK, lambK, T, kdiff_cap, 'forward'); %
k_f,ket

% Back ET (2nd order) to acceptor
k_b_sty_2g   = marcus_min_cap(EA, E_S, AbS, lambS, T, kdiff_cap, 'back');
% k_b,sty
k_b_ket_2g   = marcus_min_cap(EA, E_K, AbK, lambK, T, kdiff_cap, 'back');
% k_b,ket
k_b_ketyl_2g = marcus_min_cap(EA, E_ketyl, AbKetyl, lambKetyl, T, kdiff_cap,
'back'); % k_b,ketyl

%% ---------- Build SS solution analytically ----------
% Define composite loss terms (grids where needed)
B_S = k_b_sty_2g .* A + k_proto .* H2O;                    % s^-1
B_K = k_b_ket_2g .* A + (k_et_cks .* sty) + k_frag;        % s^-1  (k_et_cks
may be scalar)
L   = (k_et_ks .* sty) + (k_et_kk .* ket) + k_b_ketyl_2g.*A; % s^-1
(k_et_ks,k_et_kk may be scalar)

% Sources from forward ET (M/s)
a_S = k_f_sty_2g .* D .* sty;
a_K = k_f_ket_2g .* D .* ket;

% Gamma for frag manifold
Gamma = k_annul + k_coup.*sty;  % s^-1 (scalar)

% ---- Step 1: K- SS ----
% alpha = k_annul*k_frag/Gamma
alpha = (k_annul * k_frag) / Gamma;  % s^-1 scalar

% delta = k_et,kk*[ket] * (k_coup*[sty]*k_frag)/(Gamma*L)
```

```
% Note L is a grid because k_b_ketyl_2g is grid; protect division.
epsL = 1e-300;
delta = (k_et_kk .* ket) .* ( (k_coup.*sty.*k_frag) ./ (Gamma .* max(L,epsL))
); % s^-1 grid if L grid

denK = (B_K - alpha - delta);  % s^-1 grid
K_ss = a_K ./ denK;            % M (grid)

% ---- Step 2: F SS ----
F_ss = (k_frag / Gamma) .* K_ss; % M grid

% ---- Step 3: C SS ----
C_ss = (k_coup.*sty .* F_ss) ./ max(L,epsL);  % M grid

% ---- Step 4: sty anion SS ----
S_ss = ( a_S + sty .* (k_et_ks .* C_ss + k_et_cks .* K_ss) ) ./ B_S; % M grid

%% ---------- Rates (non-SS species) ----------
H_rate = k_proto .* H2O .* S_ss;   % d[sty_hydrog]/dt  (M/s)
P_rate = L .* C_ss;               % d[final_cyclo_product]/dt (M/s)

Sel = P_rate ./ (P_rate + H_rate);   % fraction to cyclo
Sel_ = 2*(Sel - 0.5);                % your centered metric (P-H)/(P+H)

%% ---------- Plot ----------
figure; ax = axes;
imagesc(E_D_grid, E_A_grid, Sel_, 'Parent', ax);
set(gca, 'Color', [1 1 1]);
set(gca, 'XDir','reverse');
set(gca, 'YDir','normal');

colormap(ax, cmap);
caxis([-1 1]);
cb = colorbar(ax);
cb.Label.String = '(P - H) / (P + H)';
xlabel('E_{1/2} (Reductant strength, V vs SCE)');
ylabel('E_{1/2} (Oxidant strength, V vs SCE)');
title('Selectivity surface with ketyl manifold (SS intermediates)');

%% ---------- 2nd-order Marcus with MIN diffusion cap ----------
function k2 = marcus_min_cap(E_donor_or_acceptor, E_X, A, lambda, T,
kdiff_cap, which)
% which='forward' -> dG = (E_D - E_X); which='back' -> dG = (E_X - E_A)
kB = 8.617333262145e-5; % eV/K

switch lower(which)
    case 'forward'
        dG = (E_donor_or_acceptor - E_X);
        k_marcus = A .* exp(-((dG + lambda).^2) ./ (4*lambda*kB*T));
        k2 = min(k_marcus, kdiff_cap);

    case 'back'
        dG = -(E_donor_or_acceptor - E_X);
        k_marcus = A .* exp(-((dG + lambda).^2) ./ (4*lambda*kB*T));
```

```
        k2 = min(k_marcus, kdiff_cap);

    otherwise
        error('which must be ''forward'' or ''back''');
end
```

Script for Figure 5C.

```
%% Parameters
clear;
kB = 8.617e-5;   % eV/K
T  = 298;
lambda = 1.2;    % eV
k0 = 1e12;       % s^-1 pre-exponential
kdiff = 1e10;    % diffusion limit
%%
D = 0.00000012; % does not matter for this plot
A = 5.6e-5;     % Ox PC concentrations
%%
% Driving forces for Sub1 for each donor (example values)
dG2 = [0, -0.75, -1.45];   % donor A, B, C
dG1 = dG2 + 0.75;           % Sub1 is 0.75 V harder to reduce

%% Marcus function
kMarcus = @(dG) k0 .* exp(-(dG + lambda).^2 ./ (4*lambda*kB*T));
kSET_fun = @(dG) 1 ./ (1./kdiff + 1./kMarcus(dG));

%% Compute kSET for each donor
kSET1 = kSET_fun(dG1)*D;
kSET2 = kSET_fun(dG2)*D;

%% Sweep x = k1/k2
x = logspace(0, 6, 400);  % from 10^0 to 10^6
k2 = 1e3;
k1 = k2*x;

%% Compute f1 for each donor
for i = 1:3
    num = kSET1(i) .* k1 ./ (k1 + kdiff*A);
    den = num + (kSET2(i) .* k2 ./ (k2 + kdiff*A));
    f1(:, i) = num ./ den;     % store each donor's curve
end

%%
%% === Ask user for filename ===
[fn, fp] = uiputfile({'*.xlsx','Excel Spreadsheet (*.xlsx)'}, ...
                     'Save data as', 'ProductSelectivityDatasets.xlsx');

if isequal(fn,0) || isequal(fp,0)
    % user cancelled → use default name
    filename = 'ProductSelectivityDatasets.xlsx';
    warning('No file selected. Saving as "%s".', filename);
else
    filename = fullfile(fp, fn);
end

%% === Save datasets to spreadsheet ===
data1 = [log10(x).'  100*f1(:,1)];
data2 = [log10(x).'  100*f1(:,2)];
data3 = [log10(x).'  100*f1(:,3)];
```

```
writematrix(data1, filename, 'Sheet', 'PC1', 'Range', 'A1');
writematrix(data2, filename, 'Sheet', 'PC2', 'Range', 'A1');
writematrix(data3, filename, 'Sheet', 'PC3', 'Range', 'A1');
%% Plot
figure; hold on;
plot(x, 100*f1(:,1), 'LineWidth', 2)
plot(x, 100*f1(:,2), 'LineWidth', 2)
plot(x, 100*f1(:,3), 'LineWidth', 2)
set(gca,'XScale','log')
xlabel('k_1 / k_2')
ylabel('Pdt1 (%)')
legend('PC1*','PC2*','PC3*')
title('Product Selectivity vs k_1/k_2')
grid off
```

8. Evaluation of other selectivity models

Chain Propagation

Product formation requires SET oxidation of the nascent cyclopentyl ketyl radical formed upon cyclization. If another equivalent of ketone starting material acts as the oxidant, this SET step would propagate a radical chain. In principle, such a mechanism would only require initiation via initial ketone reduction, without necessarily requiring facile BET to protect the olefin. To probe the impact of a chain mechanism on selectivity, we introduced new terms into the kinetic model: (1) SET from product•– to styrene; (2) SET from product•– to cyclopropyl ketone; (3) SET from styrene•– to cyclopropyl ketone; (4) SET from product•– to perylene. Marcus barriers were computed for each of these steps (Figure S2.30).

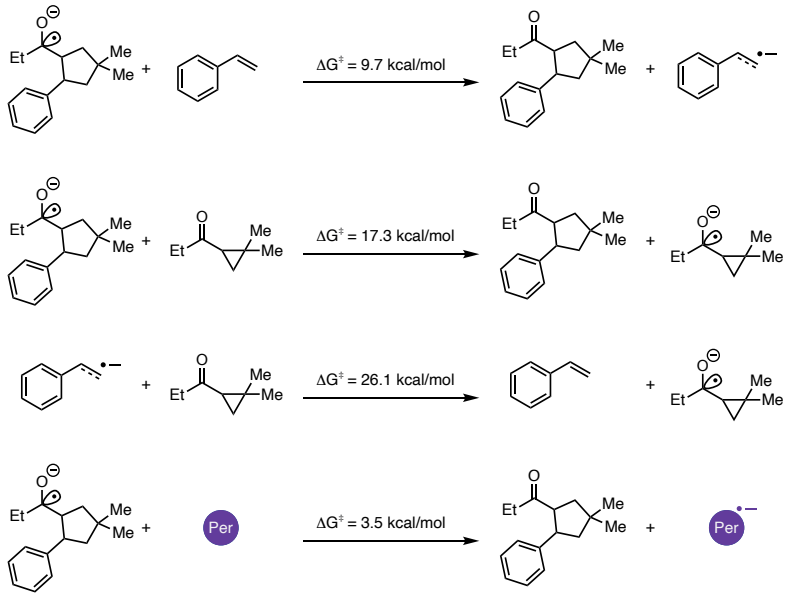


Figure S2.30: Computed barriers for chain termination (top); chain propagation (second); ketone reduction via SET from styrene (third); SET to perylene (bottom)

Kinetic modeling. Introducing these terms has almost no impact on the overall predicted selectivity profile (Figure S2.31). Propagation involves a roughly thermoneutral SET with significant reorganization energy, whereas SET from product•– to styrene is highly exergonic with lower reorganization energy — SET to styrene is predicted to be irreversible and to occur six orders of magnitude faster than propagation. Styrene therefore poses a persistent termination pathway as a direct consequence of its less negative redox potential.

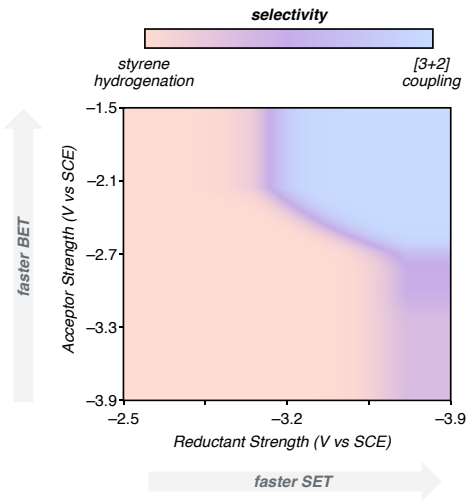


Figure S2.31: Kinetic selectivity model as a function of driving force for SET and BET, accounting for chain propagation and inhibition as predicted computationally

Stress-testing the model. Even if the propagation step were significantly faster than the calculations suggest, persistent reinitiation would still be required to promote coupling. To evaluate this, the barrier for SET from product•– to cyclopropyl ketone was arbitrarily set equal to that of SET to styrene — a 9.7 kcal/mol decrease relative to the calculated value, representing a vast overestimate of the likely propagation rate (Figure S2.32). When that change is made, without modifying the influence of substrate redox potential on any other step, the predicted kinetic selectivity profile remains essentially similar. However, the lower right quadrant – which is the domain of a strong chemical reductant with little to no driving force for BET – becomes entirely unselective. Here there is no kinetic preference for propagation leading to product, versus termination leading to hydrogenation.

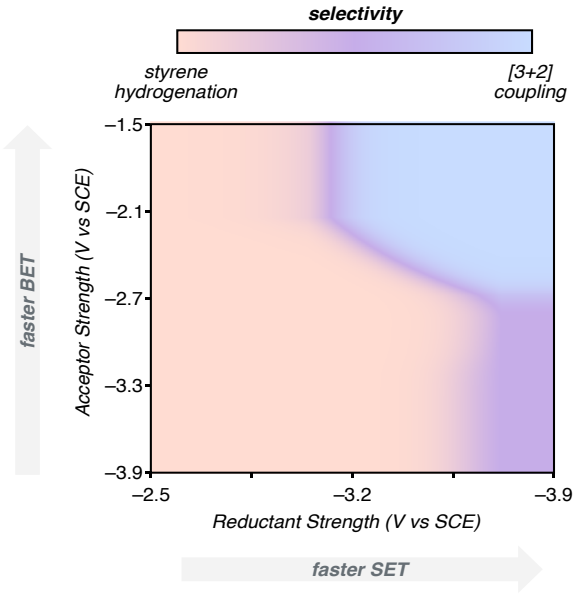


Figure S2.32: Kinetic selectivity model as a function of driving force for SET and BET, accounting for chain propagation and inhibition where propagation rate is intentionally overestimated

Marcus Inverted Back Electron Transfer

BET from the ketyl radical anion to perylene could, in principle, attenuate reoxidation of the ketone-derived radical anion selectively over styrene, enabling chemoselectivity without requiring indiscriminate SET. However, Marcus inverted kinetics in bimolecular systems require not only that the driving force exceed the reorganization energy ($\Delta G > \lambda$), but also that BET remains slower than diffusion ($k_{BET} < k_{diff}$) to be kinetically relevant.

Computational assessment. Marcus theory calculations indicate that BET from the ketyl radical to perylene occurs in the normal region: the reorganization energy (λ = 2.7 eV) far exceeds the driving force (ΔG = 1.4 eV). Furthermore, even if computational uncertainty were sufficient to place BET in the inverted region, computed BET rates exceed the diffusion limit for values of λ as low as 0.7 eV — well beyond any reasonable margin of error (Figure S2.33). Independently, SET from the ketyl radical to styrene, present at approximately equimolar concentration, carries a driving force of only ~0.6 eV and is unambiguously diffusion-limited. Even if BET to perylene were inverted, SET from the ketyl radical to styrene would kinetically mask any such effect.

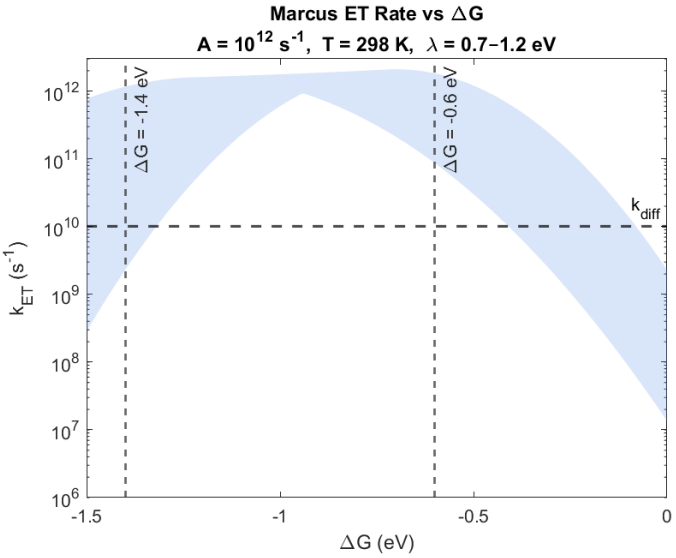


Figure S2.33: Kinetic simulations for the rates of BET and SET from the ketyl radical to perylene (ΔG = –1.4 eV) and styrene (ΔG = –0.6 eV) across a range of reorganization energies (λ).

Experimental assessment. To decouple driving force effects from post-SET fragmentation experimentally, cyclic voltammograms of perylene were recorded under irradiation in the presence of an acyclic dialkyl ketone (1-cyclopentylethan-1-one). This structural analogue maintains the same driving force for BET as the cyclopropyl ketone substrate but cannot undergo ring opening upon SET reduction. The cyclopropyl ketone induces photocatalytic current under these conditions, whereas the acyclic analogue does not (Figure S2.33). These data are consistent with a model in which catalysis arises from rapid fragmentation outcompeting BET, rather than from attenuated BET in the Marcus inverted region.

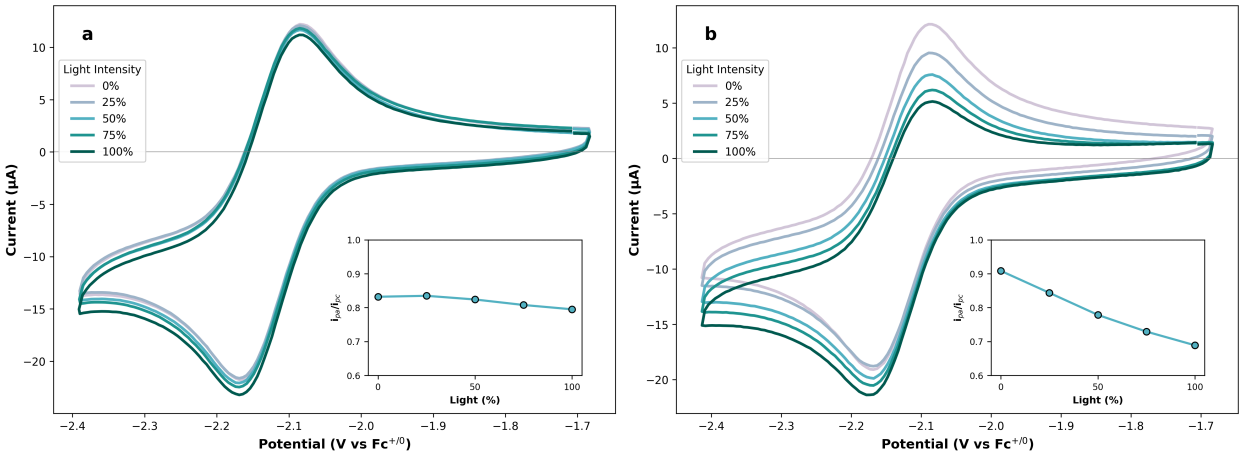


Figure S2.34: CV of **Per** (1 mM) in DMF containing 100 mM ketone substrate and 0.1 M $TEAPF_6$ at 100 mV/s with various light intensities (0%, 25%, 50%, 75%, 100%). (a) Cyclohexylmethyl ketone; (b) Ket-1. Insets show the impact of light intensity on the ratio of peak anodic to peak cathodic current (i_pa/i_pc). Lines are drawn to guide the eyes.

Doublet-to-Triplet Energy Transfer

Upon photoexcitation, the perylene radical anion reaches a doublet excited state that could, in principle, sensitize the cyclopropyl ketone via DTET rather than reducing it via SET. This would generate a triplet-excited ketone capable of ring opening, bypassing the proposed SET mechanism entirely. Two independent lines of evidence are presented below to evaluate this possibility.

Transient absorption spectroscopy. A DTET pathway would require measurable quenching of the doublet excited state by the ketone substrate. Transient absorption spectroscopy on the picosecond timescale revealed no detectable quenching of perylene radical anion doublet features upon addition of the ketone (Figure S2.34). These data are inconsistent with productive energy transfer to the ketone.

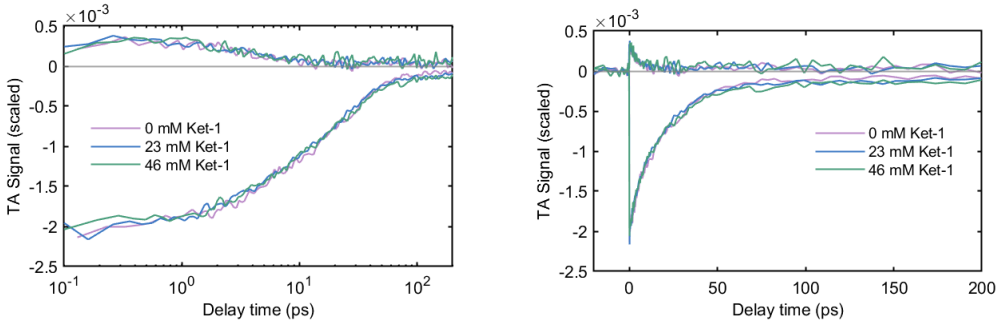


Figure S2.35: Excited state absorption decay and ground-state bleach recovery of Per•– monitored at 505 and 575 nm, respectively, following 520 nm excitation (500 nJ pulse energy). Transient traces were normalized by peak Per•– absorption to enable direct comparison of decay amplitudes. Data are shown on log (left) and linear (right) scales.

Computational assessment of pre-association. The short doublet lifetime (~20 ps) dictates that productive DTET would require ground-state pre-association between catalyst and substrate. Computed free energies of EDA complex formation are endergonic for both styrene (ΔG = +4.1 kcal/mol, $K_{eq} \sim 10^{-4}$) and the ketone (ΔG = +4.2 kcal/mol, $K_{eq} \sim 10^{-4}$), inconsistent with productive doublet reactivity, which typically requires strong pre-association ($K_{eq} > 10^2$, Wegner, Nat. Commun. 2024, 15, 4738).

Ketone reduction via preassociation with perylene radical anion

In principle, preassociation of perylene radical anion to the ketone could result in the formation of an EDA complex that, upon excitation, undergoes SET followed by rapid fragmentation, driving productive radical annulation.

Transient absorption spectroscopy. Transient absorption spectroscopy on the ps timescale found no detectable quenching of perylene radical anion doublet features upon addition of Ket-1. Moreover, we observe complete recovery of the radical anion ground-state bleach — an outcome inconsistent with productive SET, which would consume the radical anion and suppress recovery (Figure S2.34, shown on previous page).

Computational assessment of pre-association. We probed the formation of complexes between the radical anion photocatalyst and both substrates computationally. This analysis indicates that EDA complex formation is endergonic for both the ketone (ΔG = +4.2 kcal/mol, $K_a = 10^{-3}$) and styrene (ΔG = +4.1 kcal/mol, $K_a = 10^{-3}$). In a case where pre-association has been directly quantified for doublet radical anion reactivity, K_a was 185 M^{-1} (Wenger, *Nat. Commun.* 2024), orders of magnitude larger than the computed K_a for our system. While EDA complex formation remains a plausible rationale for the photoactivity of other radical anions, together these spectroscopic and computational analyses indicate that pre-association is not operative in our system.

9. Experimental Details for Figure 3 and Extended data 2

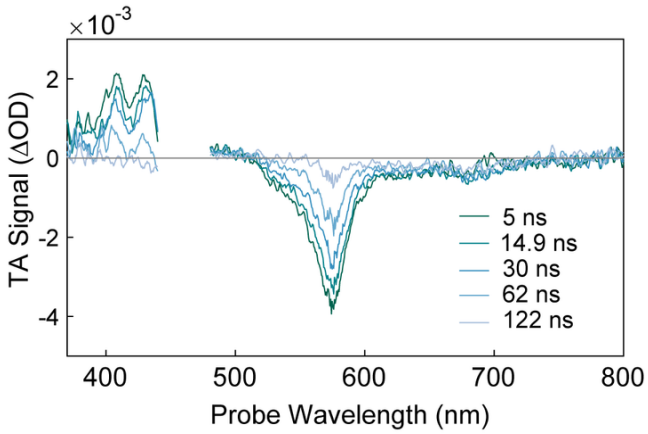


Figure 3b, top: TA spectra of perylene radical anion (Per•–) in acetonitrile: nanosecond dynamics following 460-nm excitation (1 μJ) in the visible region**.** Time delays indicated in the legend.

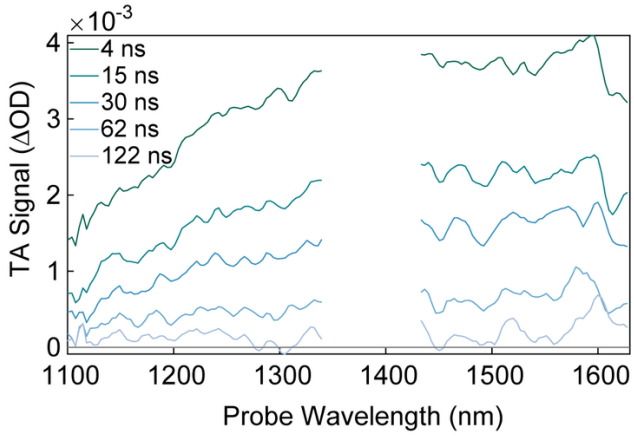


Figure 3b, bottom: TA spectra of perylene radical anion (Per•–) in acetonitrile: nanosecond dynamics following 460-nm excitation (1 μJ) in the near-IR region**.** Time delays indicated in the legend.

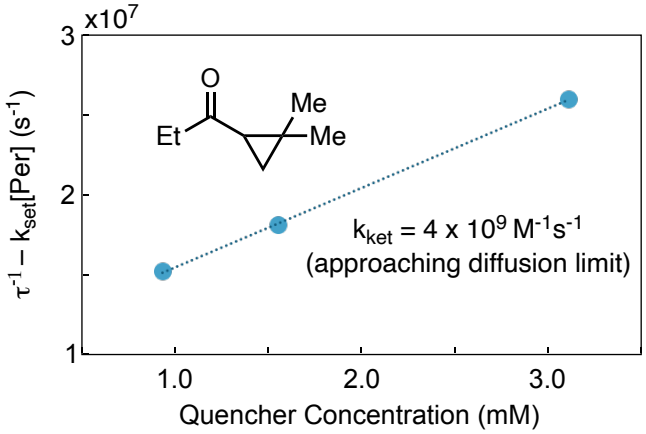


Figure 3c, top: Stern–Volmer–type plot constructed from the time-resolved decay traces of solvated electrons, monitored by averaging the transient absorption signal in the 1200–1700 nm region following an excitation at 398 nm (1 uJ pulse energy), recorded at varying Ket-1 concentrations. The progressive decrease in lifetime with increasing quencher concentration is consistent with Stern–Volmer-type dynamic quenching behavior.

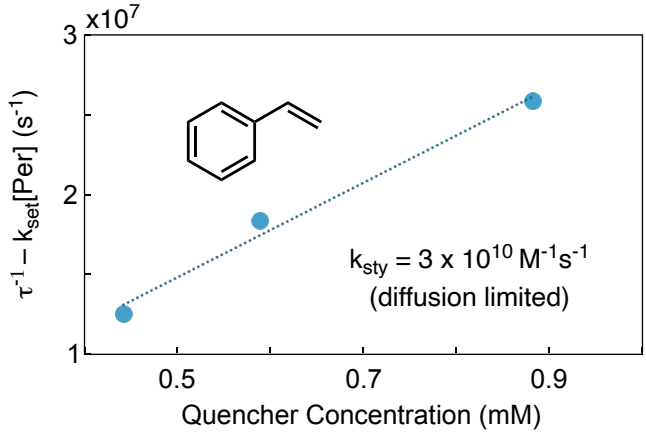


Figure 3c, bottom: Stern–Volmer–type plot constructed from the time-resolved decay traces of solvated electrons, monitored by averaging the transient absorption signal in the 1200–1700 nm region following an excitation at 398 nm (1 uJ pulse energy), recorded at varying styrene concentrations. The progressive decrease in lifetime with increasing quencher concentration is consistent with Stern–Volmer-type dynamic quenching behavior.

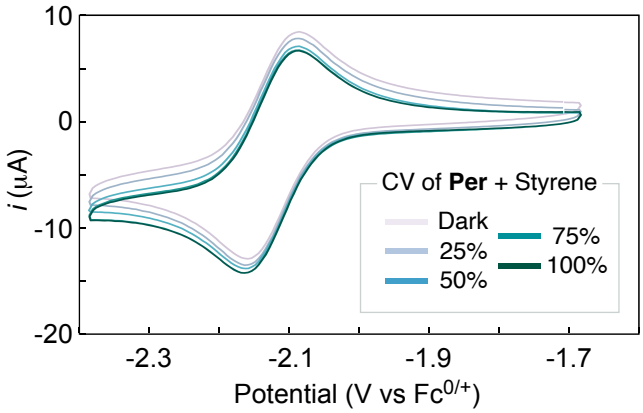


Figure 3d, top: Cyclic voltammogram of perylene (0.001 M) and styrene (0.1 M) in DMF containing 0.1 M tetraethylammonium hexafluorophosphate in the dark and under irradiation with a 390 nm LED light source at various intensities.

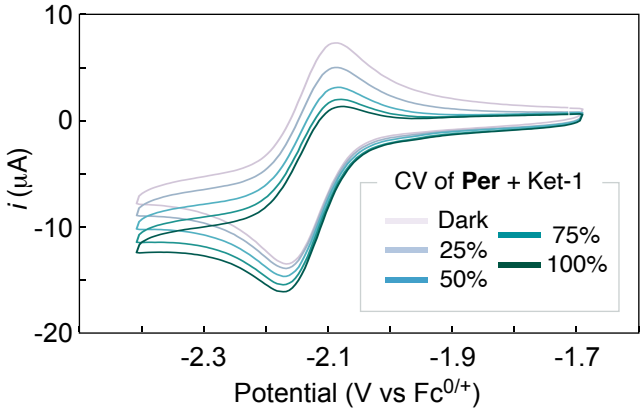
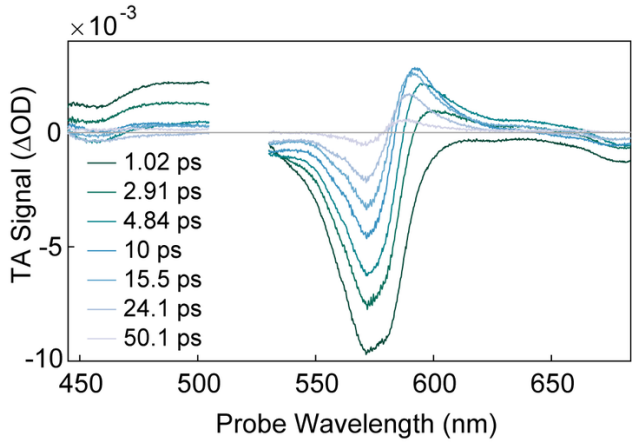
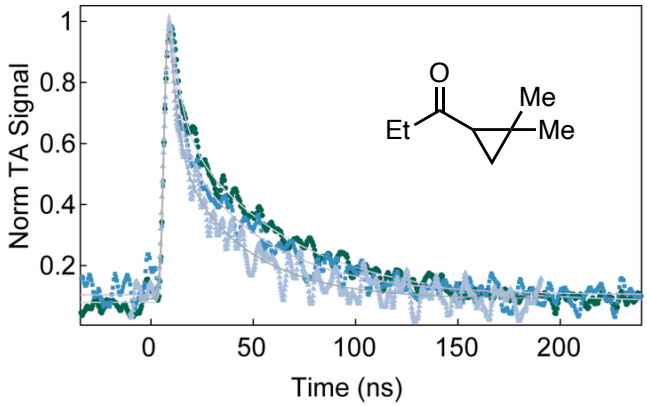


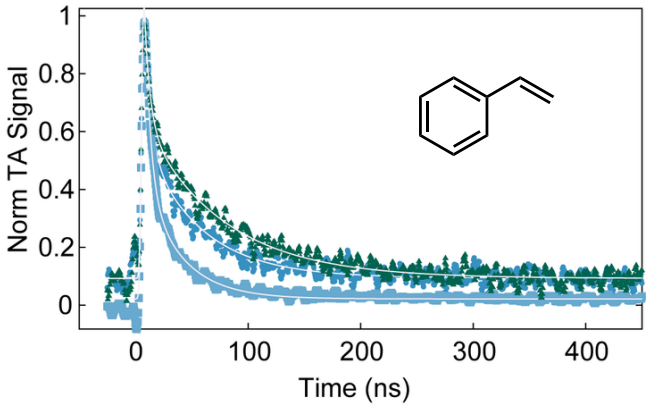
Figure 3d, bottom: Cyclic voltammogram of perylene (0.001 M) and Ket-1 (0.1 M) in DMF containing 0.1 M tetraethylammonium hexafluorophosphate in the dark and under irradiation with a 390 nm LED light source at various intensities.



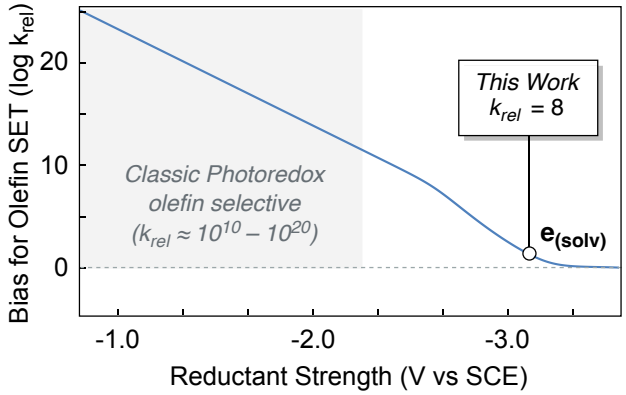
Extended data Figure 2a: TA spectra of perylene radical anion (Per•–) in acetonitrile: picosecond dynamics following 520-nm excitation (400 nJ)**.** Time delays indicated in the legend.



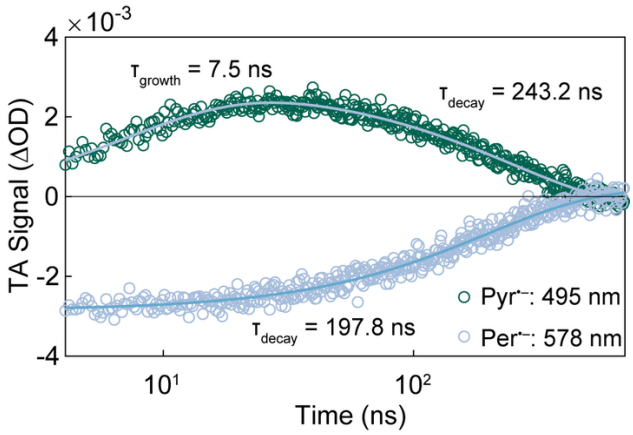
Extended data Figure 2b: Time-resolved decay traces of solvated electrons, monitored by averaging the transient absorption signal in the 1200–1700 nm region following an excitation at 398 nm (1 uJ pulse energy), recorded at varying Ket-1 concentrations. The progressive decrease in lifetime with increasing quencher concentration is consistent with Stern–Volmer-type dynamic quenching behavior.



Extended data Figure 2c: Time-resolved decay traces of solvated electrons, monitored by averaging the transient absorption signal in the 1200–1700 nm region following an excitation at 398 nm (1 uJ pulse energy), recorded at varying styrene concentrations. The progressive decrease in lifetime with increasing quencher concentration is consistent with Stern–Volmer-type dynamic quenching behavior.



Extended data Figure 2d: Predicted relative rate of SET for styrene vs Ket-1 reduction as a function of reductant strength using the Marcus equation. Fitting parameters: $\lambda = 0.6$ eV; $E_{1/2,\ ket\text{-}1} = -3.2$ V vs SCE; $E_{1/2,\ styrene} = -2.6$ V vs SCE; temperature = 298 K; Pre-exponential factor (A) = 10^{13} s^{-1}; $k_d = 10^{11}$ $M^{-1}s^{-1}$.



Extended data Figure 2e: Time-resolved changes in the absorption of pyrene radical anion (λ = 495 nm) and perylene radical anion (λ = 578 nm) following an excitation at 460 nm with pulse energy of 1 μJ.

10. Computation

Gaussian 16 revision C.01 was used for the optimization of stationary points, single-point energy calculations, and non-equilibrium solvation calculations.[1] Geometry optimizations of stationary points were performed using the meta-hybrid M06-2X functional and the Pople split-valence triple-ζ basis set 6-311+G(d).[2, 3] These optimizations were conducted with the integral equation formalism variant of the polarizable continuum model (IEF-PCM) SMD solvation model to simulate solvation by acetonitrile.[4] Single-point energy corrections were performed with the ωB97X-D functional (a range-separated hybrid with D2 empirical nonlocal correlation) and the triple-ζ def2-TZVPD basis set, with the same SMD solvation model.[5,6] For numerical integration of the exchange-correlation functionals, the default "ultrafine" pruned (99,590) grid was utilized. The def2-TZVPD basis set was defined according to the Basis Set Exchange.[7] Harmonic vibrational frequency calculations were performed to obtain thermal corrections to Gibbs energies and to verify the nature of the stationary points. Intermediates and minima have zero imaginary frequencies, while transition structures (TSs) have exactly one imaginary frequency. In the case of an imaginary frequency, Intrinsic Reaction Coordinate (IRC) calculations were performed to verify that the TSs connect the relevant reactants to the products.[8]

Conformational sampling was performed with ORCA 6.0 using the Global Optimization with Adaptation (GOAT) algorithm in combination with the semiempirical GFN2-xTB method.[9,10] These structures were then clustered based on geometry using the CREGEN module of CREST.[11] This workflow was used alongside manual conformer searching to generate the conformer space for all the structures reported.

GoodVibes was used to implement Grimme's quasi-harmonic rigid-rotor approximation using a cutoff frequency of 100 cm^{-1} to correct for errors in vibrational entropy calculations due to low frequencies.[12] The concentrations of all species were adjusted from 1 atm to a 1 M standard state in solution. Boltzmann-weighted Gibbs energies (G_{conf}) were obtained to account for the presence of multiple thermally accessible low-lying conformers and include terms for the entropy of mixing. Reported Gibbs energies (G) correspond to Boltzmann-weighted values.

Input files for single-point energy calculations were generated automatically using the *qprep* function in AQME.[13] 3D molecular graphics were rendered using the PyMOL software.[14]

The following input files and keywords are used to perform the calculations.

a) Gaussian 16 optimization (keywords):

```
# opt freq m062x/6-311+g(d) emp=gd3 scrf=(smd,solvent=acetonitrile)
```

*For TS optimization, the keyword “opt” was replaced with “opt=(ts,calcfc,noeigen).

b) Gaussian 16 single point (example file):

```
# wb97xd/gen scrf=(smd,solvent=acetonitrile)

Title

0 1
 C            -1.77836800   -1.04131400   -0.00006100
 C            -0.40692700   -1.28118800   -0.00001000
 C             0.51073700   -0.22423300    0.00006400
 C             0.01583100    1.08760300    0.00008600
 C            -1.35216900    1.32849900    0.00002600
 C            -2.25617800    0.26552100   -0.00004600
 H            -2.47141000   -1.87569300   -0.00011000
 H            -0.03783400   -2.30241700   -0.00001200
 H             0.70135200    1.92822800    0.00016700
 H            -1.71693400    2.35003400    0.00005300
 H            -3.32347600    0.45788700   -0.00009900
 C             1.95338500   -0.53674800    0.00009800
 H             2.18951900   -1.59906000    0.00034900
 C             2.95842700    0.33997200   -0.00013800
 H             2.80276100    1.41435800   -0.00039100
 H             3.98759600   -0.00201800   -0.00007500

User-defined basis set corresponding to def2-tzvpd for elements C and H
```

c) User-defined basis set for def2-TZVPD (with H atom as example)*:*

```
H    0
S   3   1.00
     34.0613410           0.60251978D-02
      5.1235746           0.45021094D-01
      1.1646626           0.20189726
S   1   1.00
      0.32723041           1.0000000
S   1   1.00
      0.10307241           1.0000000
P   1   1.00
      0.8000000           1.0000000
P   1   1.00
      0.95774129632D-01      1.0000000
****
```

*Basis sets for all the elements in the calculation are appended in this way. These user-defined basis sets are obtained from the Basis Set Exchange.

d) GoodVibes (terminal command):

```
python -m goodvibes *log --spc xd -c 1 --pes pes_vpd.yaml
```

e) AQME (terminal command for generating SPC input files):

```
python -m aqme --qprep --program "gaussian" --files "*log" --qm_input " wb97xd/gen
scrf=(smd,solvent=acetonitrile)” --mem "64GB" --nprocs "32" –suffix sp_xd
```

Choice of Density Functional approximation

The selection of density functionals for geometry optimizations (M06-2X) and single-point energy calculations (ωB97X-D) was informed by prior theoretical benchmarking studies on radical and triplet mechanisms.[16,17] Benchmarks on radical and triplet surface thermochemical values (activation barriers and thermodynamics) indicated that hybrid meta-GGA functionals such as M06-2X provide a good balance between computational cost and reliable geometries and energies. Hence, M06-2X was chosen for geometry optimizations of all structures. For single point energy corrections, we used the range-separated hybrid functional ωB97X-D which have been shown to accurately model open-shell mechanisms[17].

To ensure the consistency of our mechanistic conclusions, we also benchmarked the key selectivity-determining TSs across a range of functionals (see below for results). This showed that the trends and selectivity model are consistent across the functionals and not restricted to the chosen level of theory.

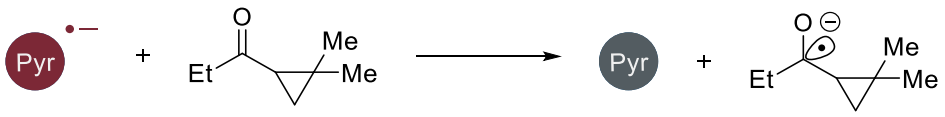
Four-point Marcus calculations for outer-sphere electron transfer barriers

The Marcus–Hush model was used to compute the thermal activation barriers for all outer-sphere electron transfer (ET) steps, with the exception of those involving solvated electrons.[18] The Marcus model requires two terms to calculate the activation barrier of electron transfer: (a) the free energy difference (ΔG^o) between the reactant (pre-SET) and product (post-SET) states, and (b) the total reorganization energy (λ), which is the sum of the internal ($\boldsymbol{\lambda_i}$) and solvent ($\boldsymbol{\lambda_o}$) contributions. These parameters are combined in the expression:

$$\Delta G^{\ddagger} = \frac{(\lambda + \Delta G^{\circ})^2}{4\lambda}$$

DFT calculations were performed on the infinitely separated donor and acceptor species to evaluate both ΔG^o and λ. The free energy difference is obtained directly from the difference between the optimized geometries of the reactant and product states. The reorganization energy is computed by performing a single-point calculation on the optimized product geometry and solvation environment, while constraining the electronic configuration (i.e., charge and spin multiplicity) to that of the reactant state. This procedure yields the total $\lambda = \lambda_i + \lambda_o$. Specifically, computing the product geometry with the reactant electronic state accounts for the internal contribution (λ_i), representing the energetic penalty of distorting the molecular geometry from the reactant's optimized structure toward that of the product while maintaining the reactant's electronic state. Performing this calculation in the solvation environment of the product accounts for the solvent contribution (λ_o), which accounts for the energetic cost of reorganizing the surrounding medium. Computationally, this is achieved using 'Non-Equilibrium' solvation, where the solvation environment of the product is first saved in a checkpoint file using the keyword 'NonEq=Save', and subsequently employed in the single-point calculation with the reactant electronic state using 'NonEq=Read'.

We illustrate this procedure using the example of a thermal SET from pyrene radical anion (**Pyr**$^{\bullet-}$) to neutral cyclopropyl ketone ($\mathbf{A_{ket}}$).



For the calculation of λ, we perform the following four single point calculations:

Reactant (before SET) electronic energy

1) **E_1 : Pyr$^{\bullet-}$** at its optimized geometry and solvation with charge = -1 and multiplicity =2

2) **E_2 : A_{ket}** in its own optimized geometry and solvation with charge = 0 and multiplicity =1

Reactant (after SET) electronic energy

3) **E_3 : Pyr$^{\bullet-}$** with the optimized geometry of neutral **Pyr** with charge = -1 and multiplicity = 2 and non-equilibrium solvation with the solvent environment from charge = 0 and multiplicity =1 saved using Noneq=Save

4) **E_4 : A_{ket}** with the optimized geometry of **B_{ket}** with charge = 0 and multiplicity = 1 and non-equilibrium solvation with the solvent environment from charge = -1 and multiplicity = 2 saved using Noneq=Save

With these four single point energies, λ is calculated as follows:

$\lambda = ((E_3 - E_1) + (E_4 - E_2))$;

where ($E_3 - E_1$) and ($E_4 - E_2$) are the reorganization energies of **Pyr**$^{\bullet-}$ and A_{ket}.

An analogous set of computations can be performed for the products following electron-transfer, and in the event that reactant and product energy surfaces share the same parabolic curvature (an assumption underlying the Marcus model), the value obtained will be identical to that from the reactant side. In practice, the two values of λ differ, and following Nelsen's four-point model, we take the geometric mean of the forward and reverse values of λ to obtain a final prediction. [19] These ΔG^{o} and λ values are used for the calculation of all electron transfer barriers.

Concentration correction for activation barriers

For unimolecular processes (**A** → products), the rate constant is obtained directly from transition state theory (TST) with units of s^{-1}:

$$k_1 = \frac{k_B T}{h} e^{-\Delta G^{\ddagger}/RT}$$

For bimolecular processes (**A** + **B** → products), the corresponding TST expression gives a second-order rate constant with units of $M^{-1}\ s^{-1}$:

$$k_2 = \frac{k_B T}{h} e^{-\Delta G^{\ddagger}/RT} \cdot \frac{1}{C^{\circ}}$$

To compare the kinetics of a bimolecular reaction directly with a unimolecular process (both involving A), the concentration of the other reactant (**B**) must be specified, giving a pseudo–first-order rate constant: $k_{eff} = k_2[B]$, where [B] is the concentration of **B**.

This additional term shows that the kinetics of a bimolecular process, unlike that of a unimolecular one, depends not only on the intrinsic barrier ($\Delta G^{\ddagger}$) but also on the concentration of the reactant partner.
Equivalently, this concentration dependence can be absorbed into an effective activation free energy for bimolecular steps:

$$\Delta G^{\ddagger}_{\text{eff}} = \Delta G^{\ddagger} + RT \ln\left(\frac{1}{[B]}\right)$$

Hence, when comparing the kinetics of unimolecular and bimolecular steps, it is necessary to include this concentration correction to the activation free energy. At [B] = 1 M, the correction vanishes, and the bimolecular expression reduces to the unimolecular form, while at lower concentrations, the effective barrier is increased. This reflects the statistical cost of bringing the two molecules together, which is absent in a unimolecular process. As our study involves the comparison of uni- and bimolecular steps, all the activation barriers for the latter have been corrected by RT ln(1/[B])

Complete mechanistic profile and PES

Competing pathways for [3+2] annulation and styrene hydrogenation were studied computationally using model substrates. The most energetically favorable pathways leading to both products are shown below in **Figure S3.1**, while the corresponding Gibbs energy profile is shown in **Figure S3.2**.

Structures along the styrene hydrogenation pathway are named with the suffix 'sty', while structures along the [3+2] annulation pathway bear the subscript 'ket'. Neutral styrene and cyclopropyl ketone substrates are named $\mathbf{A_{sty}}$ and $\mathbf{A_{ket}}$. As electron transfer processes are naturally described by Marcus theory, which involves intersections of diabatic energy surfaces, we represent them in the energy profile as sharp, intersecting peaks, in contrast to transition state structures (TSs), which are shown as smooth peaks. This visual distinction highlights how the barriers have been modelled computationally. In addition, electron transfer crossing points have been labeled with a suffix such as $\mathbf{TS'\text{-}1_{ket}}$ to distinguish them from the optimized TSSs.

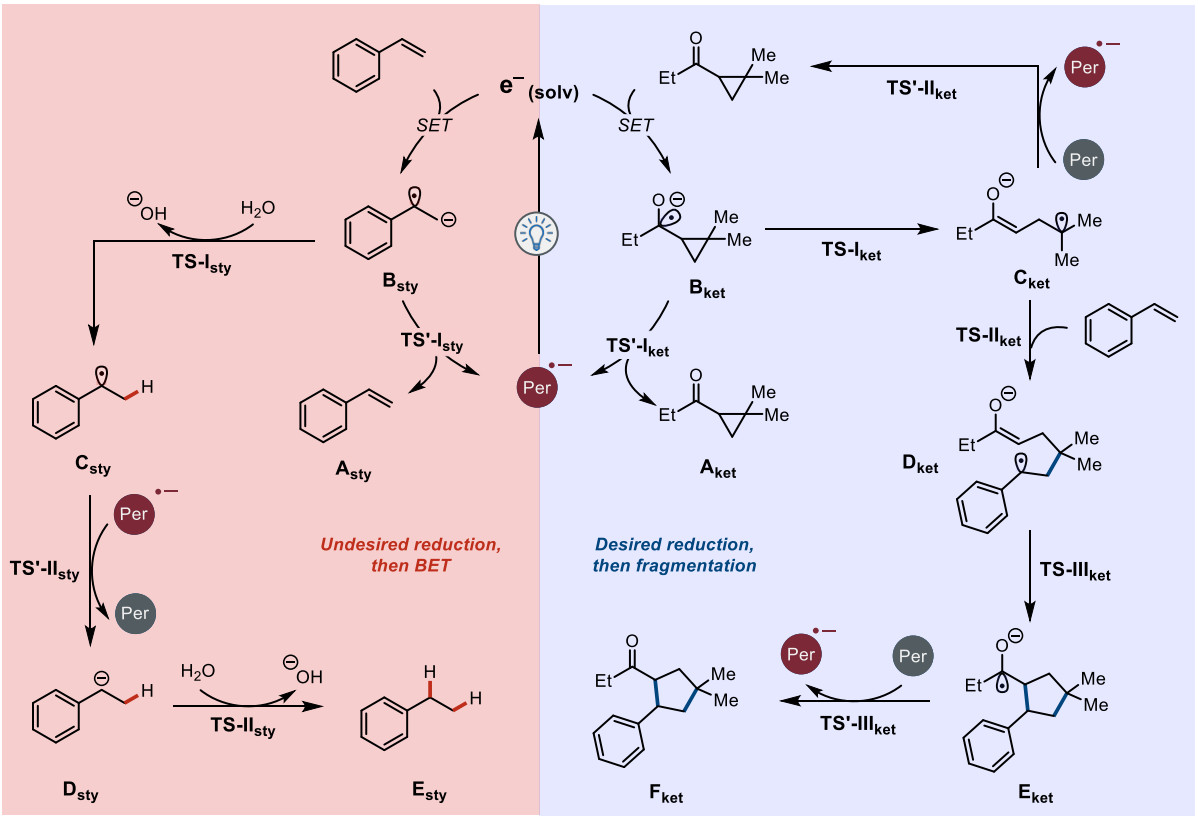


Figure S3.1: Most favored pathways leading to the coupling and styrene hydrogenated products

Following the reduction of the two substrates $\mathbf{A_{sty}}$ and $\mathbf{A_{ket}}$ by a solvated electron, diffusive Back Electron Transfer (BET) to perylene can occur, which is in competition with β-scission of the ketyl radical or protonation of the styrene radical. Calculations show that β-scission of the cyclopropyl ketyl radical anion $\mathbf{B_{ket}}$ to form the open-chain ketyl radical anion $\mathbf{C_{ket}}$ is both thermodynamically favorable ($\Delta G = -10.0$ kcal/mol) and faster than diffusive BET ($\Delta G^{\ddagger} = 5.5$ kcal/mol via **TS-I**). $\mathbf{C_{ket}}$ is the most kinetically persistent against back electron transfer ($\Delta G^{\ddagger} = 20.4$ kcal/mol **via TS'-II$_{ket}$**), orders of magnitude slower than the ensuing radical addition to styrene ($\Delta G^{\ddagger} = 14.3$ kcal/mol via **TS-II$_{ket}$**). This is then followed by a facile ring closure ($\Delta G^{\ddagger} = 9.8$ kcal/mol via **TS-III$_{ket}$**) followed by BET ($\Delta G^{\ddagger} = 3.5$ kcal/mol via **TS'-II$_{ket}$**) to yield the final [3+2] product $\mathbf{F_{ket}}$. The protonated styrene radical $\mathbf{C_{sty}}$ is reduced to its anion ($\Delta G^{\ddagger} = 14.7$ kcal/mol via **TS'-III$_{sty}$**) followed by a facile protonation ($\Delta G^{\ddagger} = 6.5$ kcal/mol via **TS-II$_{sty}$**) to form hydrogenated side product $\mathbf{E_{sty}}$.

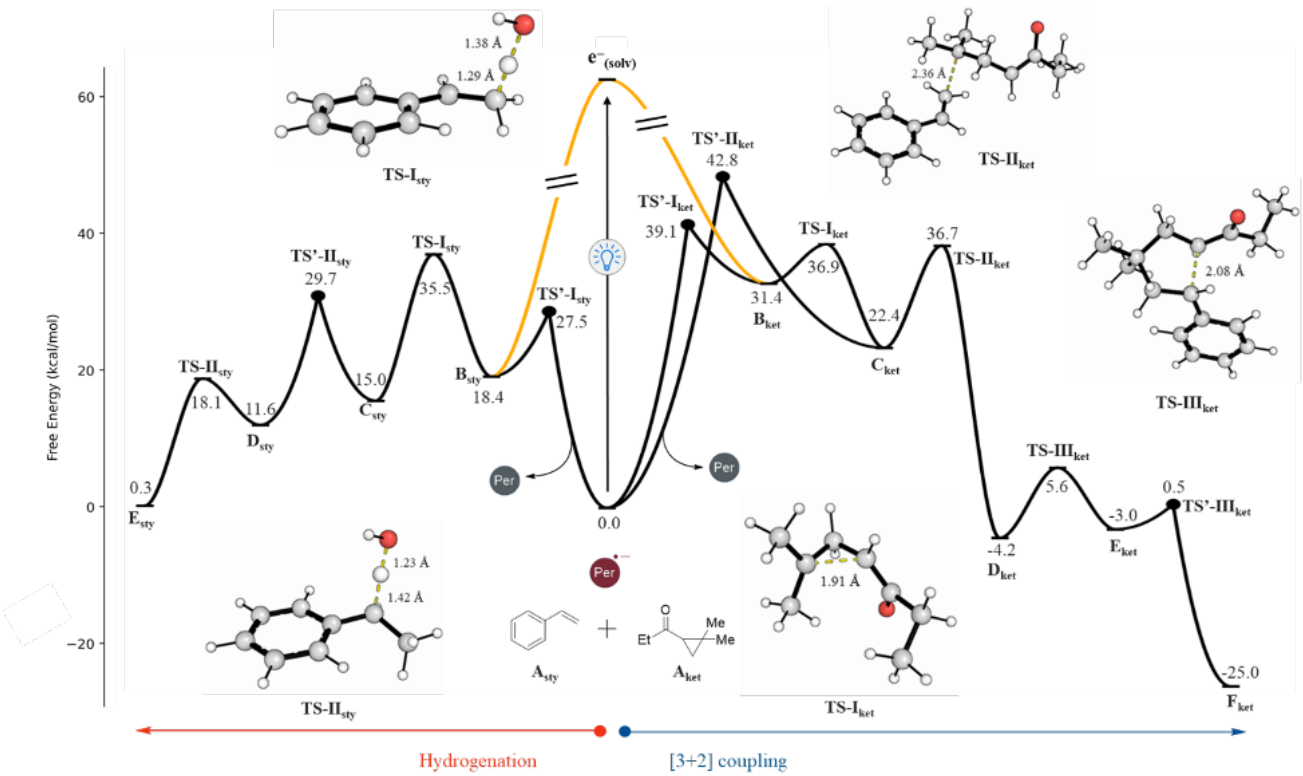


Figure S3.2 Concentration-adjusted Gibbs energy diagram for the most favored pathways leading to coupling and styrene hydrogenated products at 298K (Relative Gibbs energies in kcal/mol). Sharp, intersecting peaks represent electron transfer processes modeled via Marcus theory, while smooth peaks correspond to transition state structures (TSSs) as maxima on the potential energy surface.

SET Selectivity under non-photocatalytic conditions

Under electrochemical conditions, which are less strongly reducing, the pyrene radical anion acts as the reductant for both the substrates. The SET barriers are no longer close to diffusion rates and are dictated by the difference in substrate redox potentials, with styrene exhibiting a much lower barrier ($\Delta G^{\ddagger}$ = 22.6 kcal/mol) than the ketone ($\Delta G^{\ddagger}$ = 34.0 kcal/mol) (**Figure S3.3**). According to the Eyring equation, this corresponds to half-lives on the order of minutes for styrene, but ~10^3 years for the ketone. This aligns with the experimental result, where only styrene hydrogenation is observed under mediated electrolysis conditions (**Figure 2**).

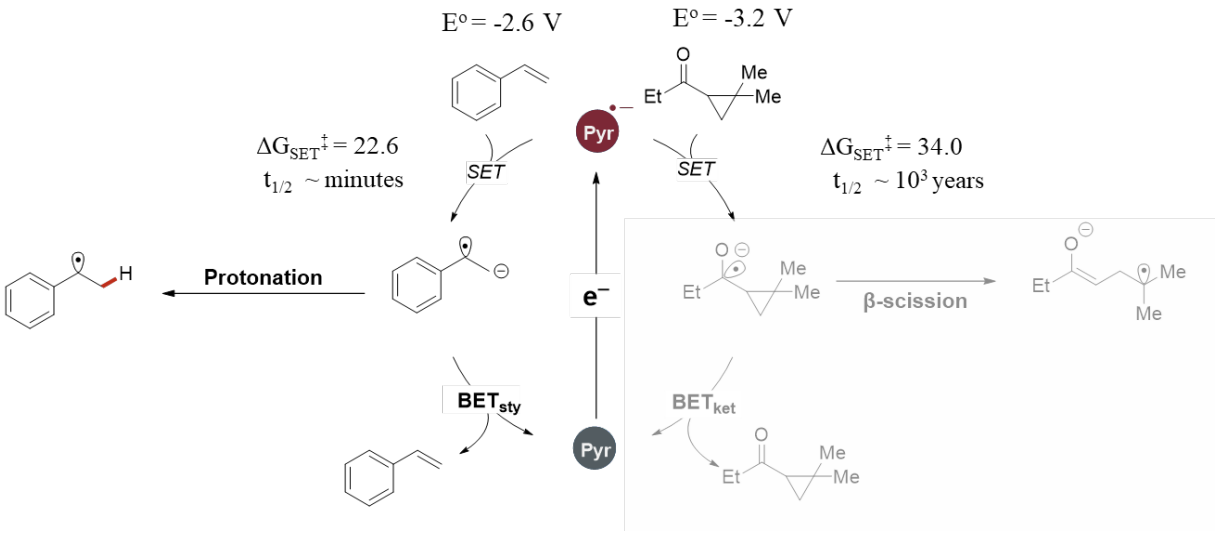


Figure S3.3: Barriers (in kcal/mol) and half-life of styrene and cyclopropyl ketone SET in non-photocatalytic conditions

Selectivity model with pyrene as an electrophotocatalyst

The use of pyrene as an electrophotocatalyst was also found to yield the [3+2] product. The selectivity-determining mechanism was therefore examined computationally with pyrene. The activation barriers and thermodynamics for the following electron transfer processes (**Figure S3.4**) were compared between the photocatalysts perylene and pyrene:
1) **BET$_{sty}$** ($\Delta G°_1$ and $\Delta G^{‡}_1$)
2) **BET$_{ket}$** ($\Delta G°_2$ and $\Delta G^{‡}_2$)
3) **BET$_{open\text{-}ket}$** ($\Delta G°_3$ and $\Delta G^{‡}_3$)

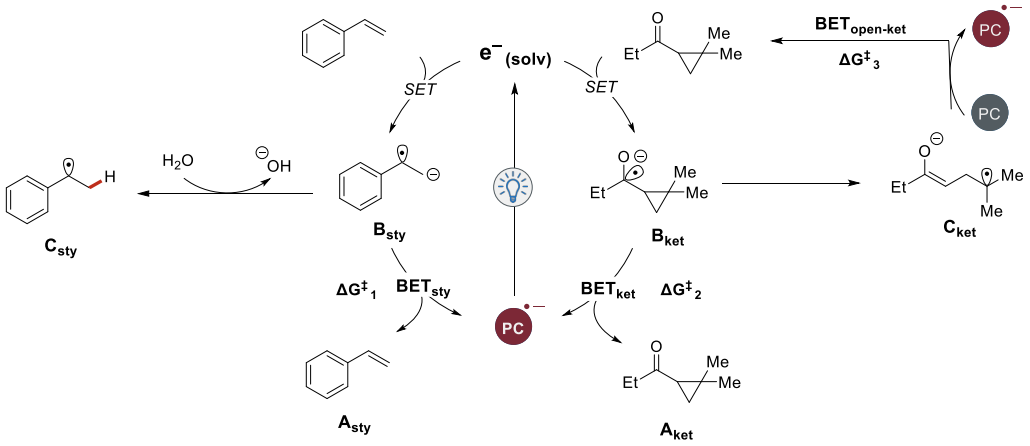


Figure S3.4: Comparison of key selectivity determining steps with photocatalysts pyrene and perylene

The lower computed reduction potential of pyrene (−2.2 V vs SCE) compared to perylene (−1.8 V vs SCE), which implies a weaker driving force for oxidation (i.e., Back Electron Transfer), is reflected in the thermodynamics of BET across the substrates. As the two catalysts have similar reorganization energies, this results in systematically higher BET barriers for pyrene, which translates to less effective olefin recycling. Despite this difference, the overall trends in the barriers (and thus the expected mechanisms) are qualitatively similar to that of perylene (**Table S3.1**).

	$\Delta G°_1$	$\Delta G^{‡}_1$	$\Delta G°_2$	$\Delta G^{‡}_2$	$\Delta G°_3$	$\Delta G^{‡}_3$
Pyrene $E^{o} = -2.2V$	-9.4	13.1	-22.7	11.3	-13.7	24.6
Perylene $E^{o} = -1.8V$	-18.1	9.4	-31.4	8.3	-22.4	20.4

Table S3.1: **Computed SET pathways with pyrene and perylene** Gibbs Free Energy Change ($\Delta G°$) and concentration adjusted activation barriers ($\Delta G^{‡}$) (in kcal/mol) for the key BET steps for pyrene and perylene.

Computed substrate redox potentials

Standard reduction potentials for all the of each redox couples were determined from the Gibbs free energy differences between their optimized structures, calculated at the ωB97X-D3/def2-TZVPD (SMD, MeCN)//M06-2X-D3/6-311+G(d) (SMD, MeCN) level of theory. This difference gives the absolute free energy of reduction, which is converted to volts and then referenced to the saturated calomel electrode (SCE) in MeCN. This is done by subtracting the absolute reduction potential of the SCE couple (4.52 V), yielding reduction potential with respect to the SCE reference (Busch *Phys. Chem. Chem. Phys.* **2021,** *23*, 6849–6870; Isse *Phys. Chem. B* **2010,** *114*, 7894–7899). Using this protocol, the redox potentials were calculated for the following cyclopropyl ketone and olefin substrates (**Figure S3.5**):

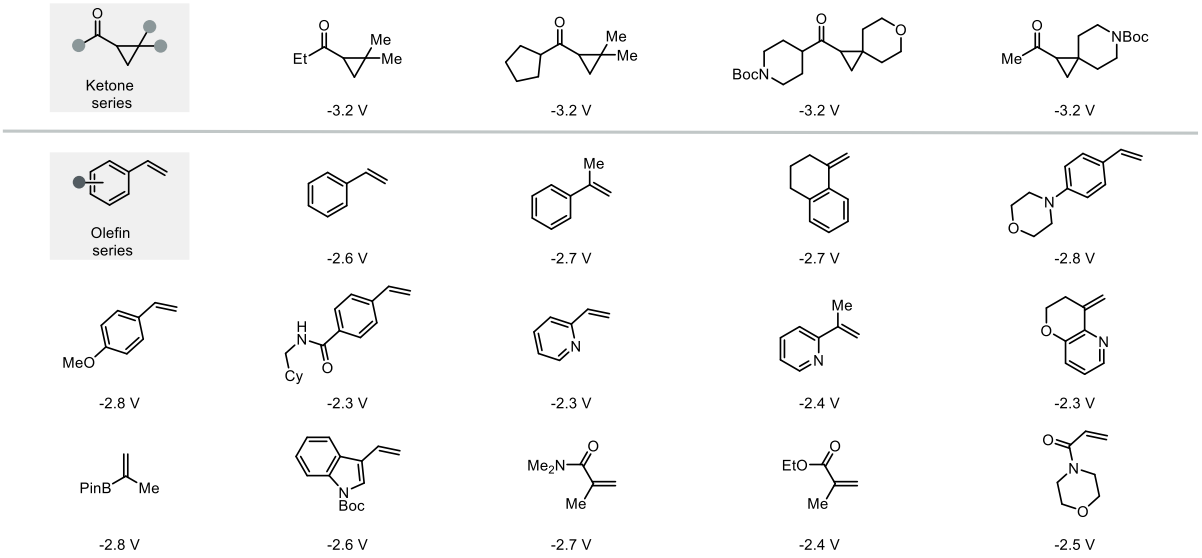


Figure S3.5: Redox potentials (against SCE) across the series of cyclopropyl ketone and olefin substrates

Key TS and electron transfer barriers across functionals

The key selectivity determining steps were benchmarked using single point calculations with different density functional approximations (DFAs) while maintaining the same basis set and solvation model. We examined the thermodynamics (ΔG^{o}) and concentration adjusted activation barriers ($\Delta G^{\ddagger}$) for the following four steps (**Figure S3.6**):

1) BET from styrene radical anion to Per ($\Delta G°_1$ and $\Delta G^{\ddagger}_1$)
2) BET from ketyl radical anion to Per ($\Delta G°_2$ and $\Delta G^{\ddagger}_2$)
3) Protonation of styrene radical anion ($\Delta G°_3$ and $\Delta G^{\ddagger}_3$)
4) β-scission of ketyl radical anion ($\Delta G°_4$ and $\Delta G^{\ddagger}_4$)

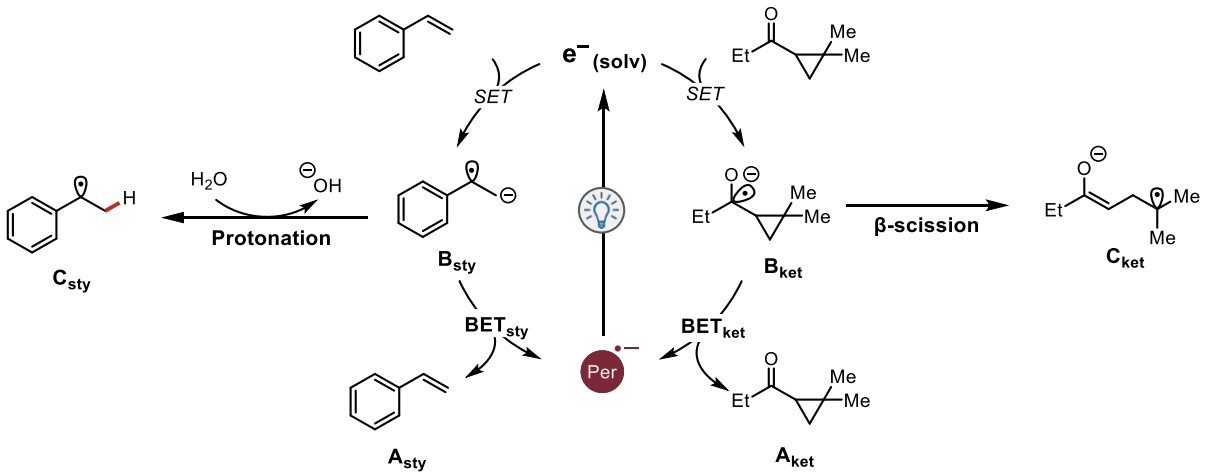


Figure S3.6: Key selectivity determining steps modelled in functional benchmark study

The thermochemical values for these steps show that the emergent selectivity model is consistent across the chosen functionals (**Table S3.2**).

Level of theory (SPC)	$\Delta G°_1$	$\Delta G^‡_1$	$\Delta G°_2$	$\Delta G^‡_2$	$\Delta G°_3$	$\Delta G^‡_3$	$\Delta G°_4$	$\Delta G^‡_4$
ωB97X-D/def2-TZVPD	-18.1	9.4	-31.4	8.3	-3.1	17.4	-9.0	5.5
CAM-B3LYP-D/def2-TZVPD	-17.8	9.5	-31.6	8.2	-4.8	15.9	-10.0	5.9
M062X-D3/def2-TZVPD	-19.3	8.9	-34.0	7.0	2.2	20.6	-6.5	7.3
PW6B95-D3/def2-TZVPD	-19.2	8.8	-34.6	7.0	-0.6	18.6	-9.1	4.6

Table S3.2: Gibbs Free Energy Change ($\Delta G°$) and concentration adjusted activation barriers ($\Delta G^‡$) for the key selectivity determining steps

Sensitivity of SET selectivity to reduction driving force

It is hypothesized that the kinetic bias in thermal electron transfer processes gets attenuated with increasing reduction driving force (i.e. with a stronger reductant). To validate this, we computationally examined the relative kinetics of SET to styrene and cyclopropyl ketone from a series of poly(het)aromatic reductants. The reduction potentials (driving force) for this *in silico* reductant dataset range from -1.2 V (phenazine) to -4.8 V (pyrrole). The SET rate constants for styrene and ketone substrates are plotted on a log scale as a function of the reductant's redox potential (**Figure S3.7**).

We can see that the kinetic selectivity (represented by the line between the styrene and ketone points) decreases as the thermodynamic driving force is increased. Once the diffusion limit is reached there is no selectivity.

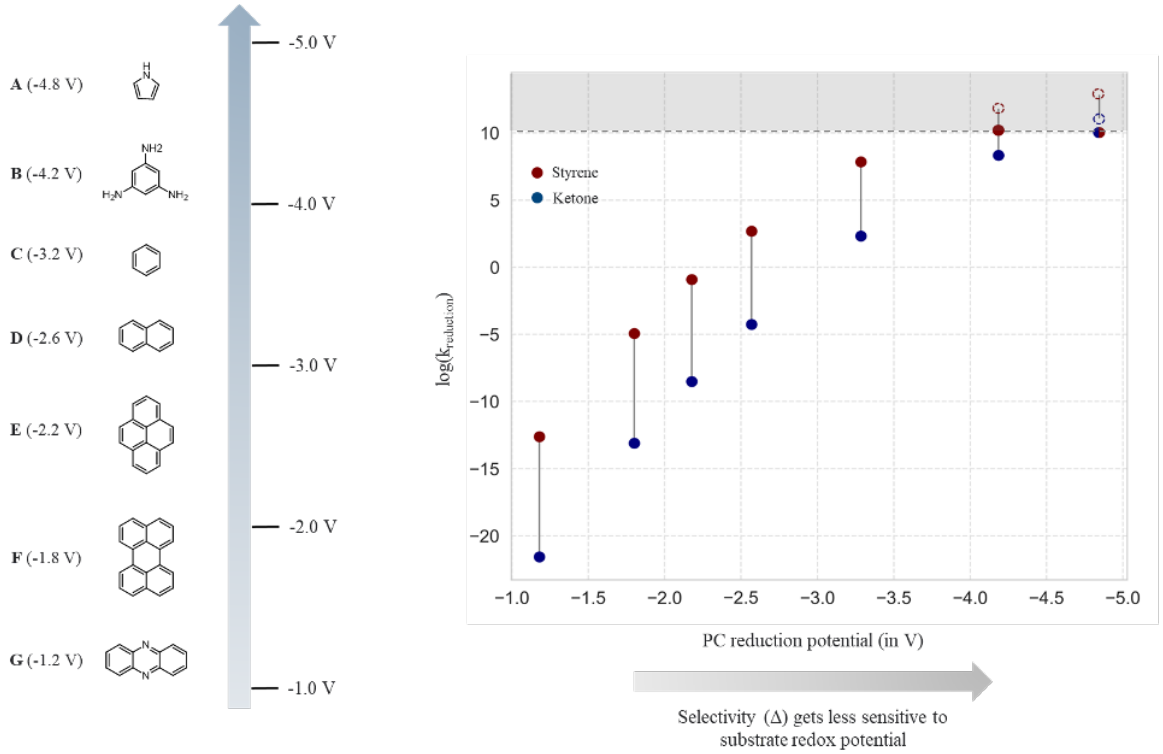


Figure S3.7 Redox potential scale of poly(het)aromatic reductants (left). SET kinetic selectivity as a function of driving force (right)

Alternative post-SET side mechanisms

In addition to the proposed mechanism for the formation of the hydrogenated styrene and [3+2] coupling products, we also considered other side pathways following the reduction of the styrene. Modelling these alternative pathways shows that they have activation barriers significantly higher than those corresponding to the mechanism proposed above (**Figure S3.8**).

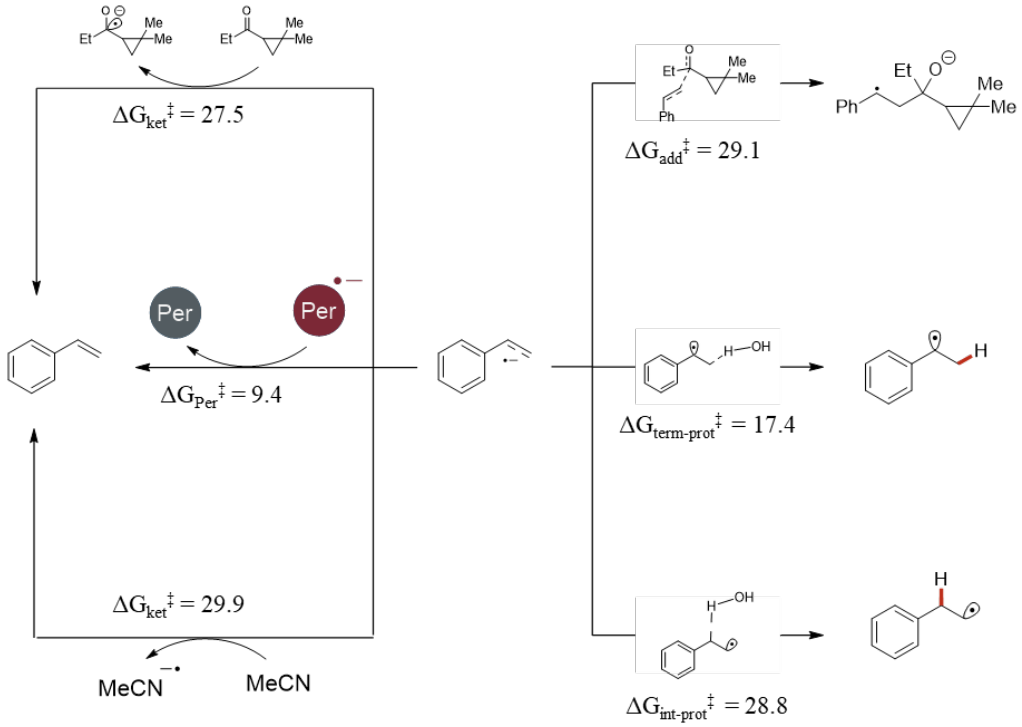


Figure S3.8: Alternative BET (left) and reactive (right) pathways from styrene radical anion. Relative Gibbs energies in kcal/mol

Styrene anion protonation pathways

In the main mechanistic pathway, we modelled protonation of the styrene radical anion using the most acidic plausible available proton source (i.e H_2O) to establish an upper bound for the protonation pathway kinetics and demonstrate that the kinetic paradigm always prefers the [3+2] coupling pathway, even with a reasonable acidic proton source. We also examined activation barriers with other possible proton sources (**Figure S3.9**), which are markedly higher than that of water. We suspect that selectivity for annulation over hydrogenation could be further enhanced by rigorously excluding any reasonable proton source. However, even if styrene does not get hydrogenated, we suspect styrene would operate as an inhibitor for ketone reduction unless initial SET occurs at or near the diffusion limit.

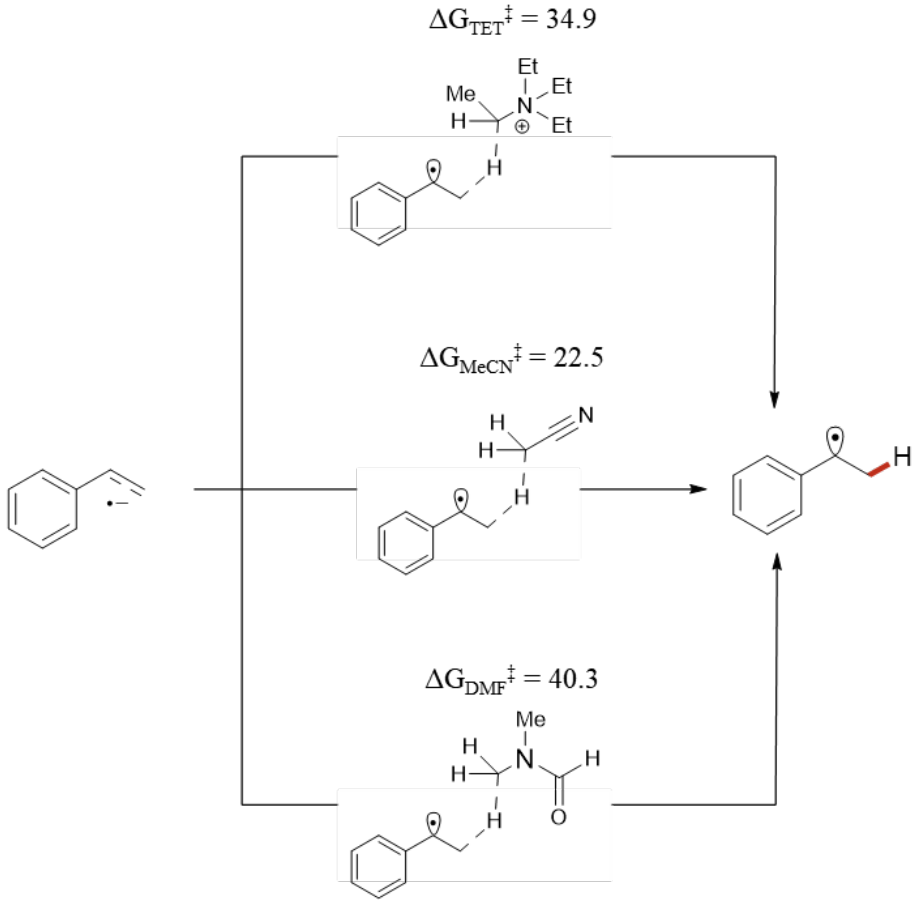


Figure S3.9: Protonation of styrene radical anion with other proton sources in system. Activation gibbs energies in kcal/mol

Pre-association complex formation and thermodynamics

We examined doublet-to-triplet energy transfer (DTET) and donor-acceptor complex-mediated ultrafast SET as alternative substrate activation pathways. Given the picosecond lifetime of the excited state of Per•–, facile formation of a donor–acceptor complex would be required to enable both energy transfer or ultrafast electron transfer on the picosecond timescale. Thus, formation of a ground-state complex between the perylene radical anion (Per•–) and the acceptors (styrene and cyclopropyl ketone) is a prerequisite for these pathways.
To assess this possibility, we computed the free energy of association ($\Delta G°_{sub}$; sub = sty, ket) for the equilibrium:

$$Per^{\cdot-} + \text{substrate} \rightleftharpoons [Per^{\cdot-} \cdots \text{substrate}]$$

In both cases, association is strongly endergonic, with $\Delta G°_{sty}$ = +4.2 kcal mol^{-1} and $\Delta G°_{ket}$ = +4.1 kcal mol^{-1} (**Figure S3.10**). These values correspond to equilibrium constants on the order of 10^{-4} at 298 K, indicating negligible donor–acceptor complex population under typical reaction conditions and lying far outside the regime typically required for efficient donor–acceptor photochemistry. This shows us that ground-state pre-association is thermodynamically inaccessible, effectively excluding ultrafast SET and DTET pathways that depend on such pre-organization.
In addition, this also shows that Per•– has effectively the same affinity for complex formation with styrene and cyclopropyl ketone. Based on the structures, it appears that they are bound by non-covalent interactions (π stacking and C-H---π respectively).

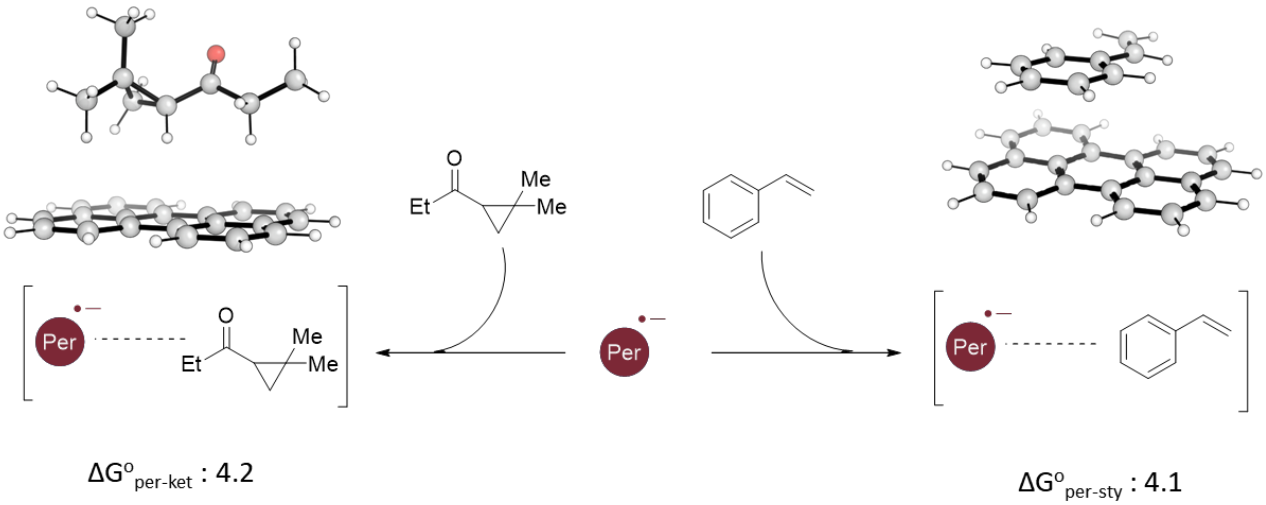


Figure S3.10: Pre-associative complex formation and their respective structures and free energy of association (in kcal/mol)

Radical chain pathway

In addition to the pathways discussed above, we examined the possibility of a radical chain mechanism. In such a scenario, the cyclopentyl radical anion formed via the [3+2] pathway would transfer its electron to another equivalent of the cyclopropyl ketone, rather than undergoing back electron transfer (BET) to the neutral perylene. This intermolecular electron transfer would constitute the propagation step of a radical chain pathway and warrants consideration, given that the concentration of the styrene/ketone substrates is substantially higher than that of the neutral photocatalyst.

To examine this, we computed activation barriers (to account for the low concentration of neutral **Per**) for electron transfer from the cyclopentyl radical anion to styrene and cyclopropyl ketone, and compared these to neutral perylene BET. Despite the lower concentration of the photocatalyst, the barriers for electron transfer to both styrene and ketone are significantly higher than that for BET to **Per**. This pronounced kinetic preference for BET to perylene is therefore inconsistent with a radical chain mechanism.

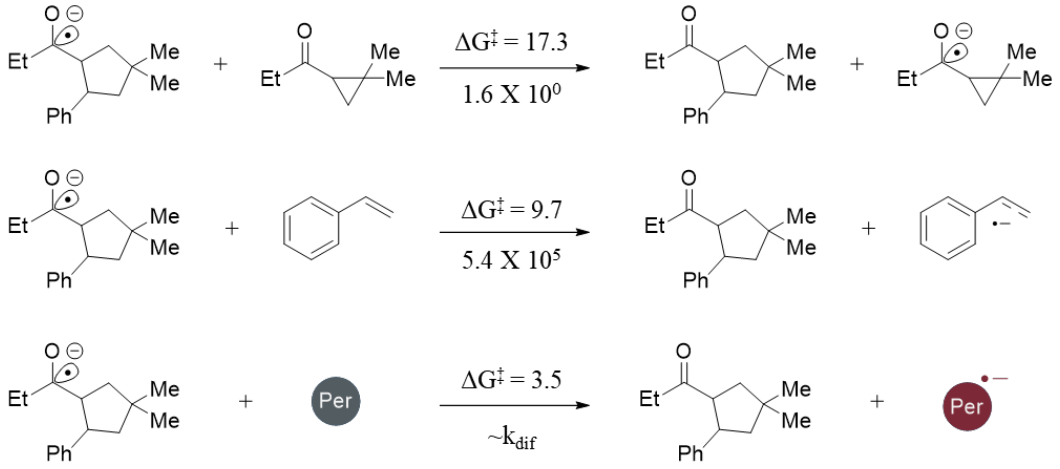


Figure S3.11: Activation barriers for BET (in kcal/mol) and the corresponding rate constant

Error bars for Marcus parameter calculations

To estimate the uncertainty associated with the computed Marcus parameters (ΔG° and λ), we evaluated these quantities across multiple levels of theory (**Figure S3.12**). In addition to employing different density functional approximations, we repeated the calculations using the CPCM (Conductor-like Polarizable Continuum Model) solvation model alongside the default SMD (Solvation Model based on Density) treatment. This approach enables us to quantify the sensitivity of the computed Marcus parameters to both the choice of density functional and the solvation model.

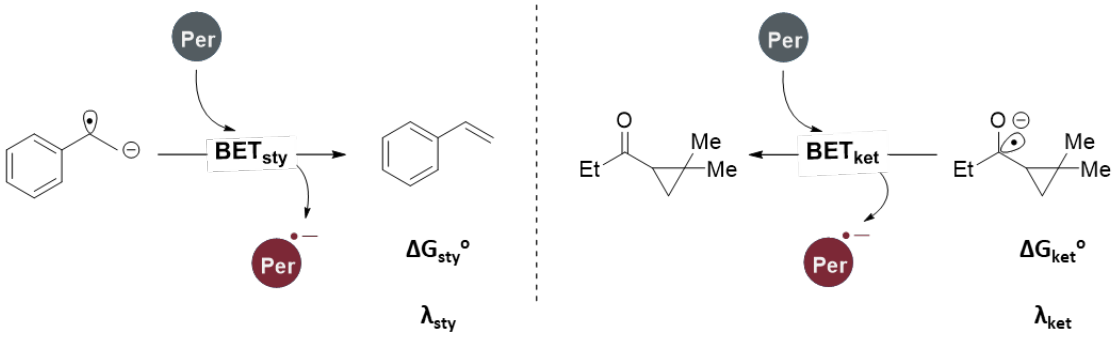


Figure S3.12: Key BET steps and their relevant Marcus parameters: ΔG^{o} and λ

The thermodynamic driving forces (ΔG°) for BET exhibit standard deviations of 1.0 and 1.9 kcal/mol for styrene and ketone, respectively. The corresponding reorganization energies (λ) show greater variability, with standard deviations of 1.4 kcal/mol for styrene and 2.8 kcal/mol for ketone. Propagating these uncertainties conservatively by summing the individual standard deviations yields upper-bound error estimates of 2.4 kcal/mol for styrene and 4.7 kcal/mol for ketone in the composite Marcus term (ΔG° + λ).

Level of theory (SPC)	$\Delta G°_{sty}$	λ_{sty}	$\Delta G°_{ket}$	λ_{ket}
ωB97X-D/def2-TZVPD (SMD)	-18.1	53.7	-31.4	61.9
CAM-B3LYP-D/def2-TZVPD (SMD)	-17.8	53.5	-31.6	61.9
M062X-D3/def2-TZVPD (SMD)	-19.3	53.5	-34.0	61.8
PW6B95-D3/def2-TZVPD (SMD)	-19.2	52.7	-34.6	57.6
ωB97X-D/def2-TZVPD (CPCM)	-19.5	50.9	-30.2	60.5
CAM-B3LYP-D/def2-TZVPD (CPCM)	-19.2	50.7	-28.7	65.9
M062X-D3/def2-TZVPD (CPCM)	-20.8	50.7	-31.7	60.3
PW6B95-D3/def2-TZVPD (CPCM)	-20.5	49.9	-31.8	56.4

Table S3.3: BET thermodynamics (ΔG^o) and reorganization energy (λ) parameters across different levels of theory.

Complexation of product radical anion with cyclopropyl ketone

To further explore an alternative radical chain mechanism involving SET from $\mathbf{E_{ket}}$ to the reactant ketone $\mathbf{A_{ket}}$, we investigated the possibility of donor–acceptor complex formation between these species (Figure S3.13)

Specifically, we probed whether the HOMO or SOMO of the donor ketyl radical anion could interact with the C=O π* orbital of the acceptor ketone, thereby facilitating SET. Three distinct modes of donor–acceptor complexation were considered:

Type 1: interaction between the oxygen lone pair of the ketyl radical anion and the acceptor C=O π* orbital;

Type 2: interaction between the carbon-centered SOMO of the ketyl radical with the acceptor C=O π* orbital;

Type 3: complexes lacking specific orbital interactions, stabilized instead by dispersive interactions.

Association of the donor $\mathbf{E_{ket}}$ with the acceptor $\mathbf{A_{ket}}$ is strongly disfavored, with complex formation being endergonic by 7.8 kcal mol^{-1}.Type 1 complexes were found to be unstable, with optimization leading away from the intended orbital overlap toward Type 3 geometries, likely to relieve steric strain. While Type 2 complexes, which exhibit SOMO–π* interaction, could be optimized, they are less stable than the corresponding Type 3 complexes (by 6.3 kcal mol-1). Type 3 complexes, stabilized by dispersive interactions, are the most stable mode of association, as they avoid the destabilizing steric interactions associated with orbital overlap.

Overall, we see that donor–acceptor complexation between $\mathbf{E_{ket}}$ and $\mathbf{A_{ket}}$ is not only thermodynamically unfavorable, but that the very orbital interactions that could facilitate SET are intrinsically destabilizing. These results are inconsistent a radical chain SET pathway driven by donor-acceptor orbital interactions.

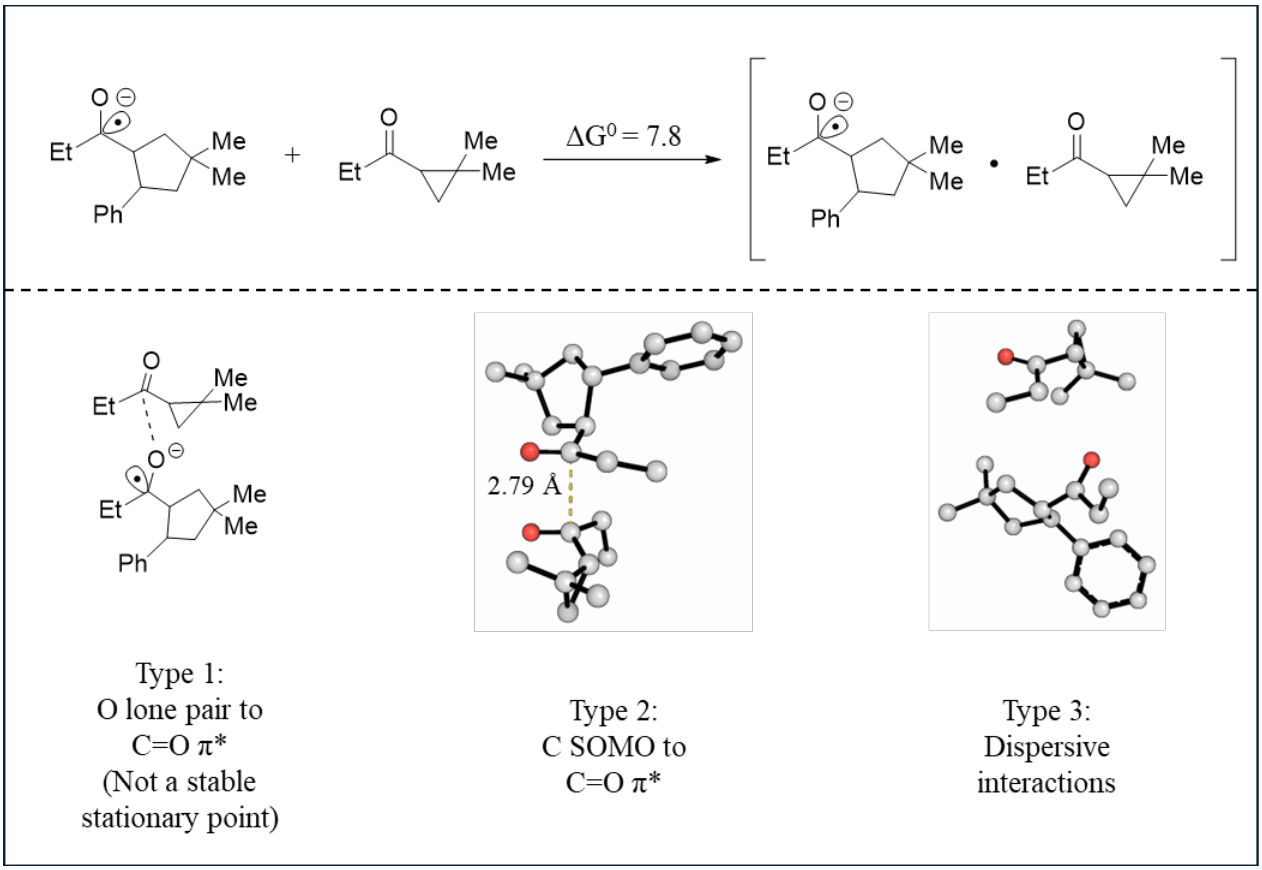


Figure S3.13: (Top) Donor-acceptor complex formation between $\mathbf{A}_{\mathbf{ket}}$ and $\mathbf{E}_{\mathbf{ket}}$ and the free energy of association (in kcal/mol). (Bottom) Different modes of complexation examined.

Structure	E_SPC	E	ZPE	H_SPC	T.S	T.qh-S	G(T)_SPC	qh-G(T)_SPC	im freq
A_ket	-388.52896	-388.41460	0.20471	-388.31270	0.04737	0.04643	-388.36008	-388.35913	
A_ket_conf_1	-388.52837	-388.41407	0.20498	-388.31187	0.04751	0.04636	-388.35938	-388.35823	
A_ket_conf_10	-388.52149	-388.40591	0.20501	-388.30506	0.04701	0.04615	-388.35207	-388.35121	
A_ket_conf_2	-388.52896	-388.41460	0.20471	-388.31270	0.04737	0.04643	-388.36008	-388.35913	
A_ket_conf_3	-388.52740	-388.41286	0.20511	-388.31079	0.04739	0.04636	-388.35818	-388.35715	
A_ket_conf_4	-388.52838	-388.41407	0.20498	-388.31187	0.04752	0.04636	-388.35939	-388.35824	
A_ket_conf_7	-388.52571	-388.41024	0.20471	-388.30944	0.04735	0.04643	-388.35678	-388.35587	
A_ket_conf_8	-388.52478	-388.40934	0.20523	-388.30809	0.04701	0.04626	-388.35509	-388.35435	
A_ket_conf_9	-388.52465	-388.40953	0.20553	-388.30782	0.04664	0.04589	-388.35446	-388.35371	
A_sty	-309.65657	-309.58346	0.13436	-309.51456	0.03895	0.03840	-309.55351	-309.55296	
B_ket_conf_1	-388.56829	-388.45630	0.20151	-388.35525	0.04726	0.04682	-388.40252	-388.40207	
B_ket_conf_2	-388.56611	-388.45452	0.20140	-388.35302	0.04813	0.04726	-388.40115	-388.40028	
B_ket_conf_3	-388.56610	-388.45452	0.20139	-388.35302	0.04814	0.04727	-388.40116	-388.40029	
B_ket_conf_4	-388.56434	-388.45198	0.20130	-388.35131	0.04846	0.04748	-388.39978	-388.39880	
B_ket_conf_5	-388.56444	-388.45201	0.20126	-388.35233	0.04579	0.04556	-388.39812	-388.39789	-11.85
B_ket_conf_6	-388.56465	-388.45264	0.20152	-388.35150	0.04802	0.04718	-388.39952	-388.39868	
B_ket_conf_7	-388.56434	-388.45197	0.20130	-388.35131	0.04846	0.04748	-388.39977	-388.39879	
B_ket_conf_8	-388.56465	-388.45264	0.20152	-388.35150	0.04802	0.04718	-388.39952	-388.39868	
B_ket_conf_9	-388.56704	-388.45508	0.20098	-388.35431	0.04838	0.04749	-388.40268	-388.40179	
B_sty	-309.71758	-309.64751	0.12953	-309.58001	0.03965	0.03956	-309.61966	-309.61957	
C_ket_conf1	-388.58076	-388.46517	0.19998	-388.36824	0.05139	0.04962	-388.41963	-388.41785	
C_ket_conf10	-388.57989	-388.46413	0.20004	-388.36737	0.05090	0.04942	-388.41827	-388.41678	
C_ket_conf11	-388.58063	-388.46504	0.20016	-388.36806	0.05038	0.04915	-388.41844	-388.41721	
C_ket_conf12	-388.58006	-388.46450	0.19967	-388.36780	0.05109	0.04955	-388.41890	-388.41735	
C_ket_conf13	-388.57993	-388.46434	0.19962	-388.36764	0.05155	0.04976	-388.41918	-388.41740	

C_ket_conf14	-388.58007	-388.46450	0.19965	-388.36782	0.05115	0.04958	-388.41897	-388.41740	
C_ket_conf3	-388.57706	-388.46101	0.20016	-388.36447	0.05082	0.04921	-388.41528	-388.41368	
C_ket_conf5	-388.57734	-388.46112	0.20011	-388.36478	0.05066	0.04924	-388.41543	-388.41402	
C_ket_conf6	-388.58080	-388.46515	0.19982	-388.36836	0.05175	0.04987	-388.42010	-388.41823	
C_ket_conf7	-388.58063	-388.46504	0.20016	-388.36806	0.05038	0.04914	-388.41844	-388.41720	
C_ket_conf8	-388.57706	-388.46101	0.20016	-388.36447	0.05081	0.04921	-388.41527	-388.41368	
C_sty	-310.24237	-310.16094	0.14361	-310.09050	0.04040	0.04028	-310.13090	-310.13078	
D_ket_conf_1	-698.28738	-698.10147	0.33937	-697.92911	0.06677	0.06319	-697.99588	-697.99231	
D_ket_conf_10	-698.28743	-698.10155	0.33950	-697.92909	0.06608	0.06294	-697.99517	-697.99203	
D_ket_conf_11	-698.28822	-698.10232	0.33953	-697.92987	0.06620	0.06290	-697.99608	-697.99277	
D_ket_conf_12	-698.28760	-698.10198	0.33931	-697.92940	0.06673	0.06315	-697.99613	-697.99256	
D_ket_conf_13	-698.28408	-698.09753	0.33953	-697.92568	0.06702	0.06318	-697.99270	-697.98886	
D_ket_conf_14	-698.28424	-698.09778	0.33946	-697.92594	0.06630	0.06298	-697.99225	-697.98893	
D_ket_conf_15	-698.28343	-698.09687	0.33929	-697.92517	0.06734	0.06339	-697.99251	-697.98856	
D_ket_conf_16	-698.28424	-698.09778	0.33946	-697.92595	0.06633	0.06299	-697.99228	-697.98894	
D_ket_conf_17	-698.28435	-698.09781	0.33959	-697.92596	0.06617	0.06294	-697.99212	-697.98890	
D_ket_conf_18	-698.28698	-698.10119	0.33950	-697.92865	0.06635	0.06303	-697.99499	-697.99168	
D_ket_conf_19	-698.28375	-698.09715	0.33977	-697.92528	0.06546	0.06255	-697.99074	-697.98783	
D_ket_conf_2	-698.28739	-698.10164	0.33944	-697.92907	0.06666	0.06307	-697.99573	-697.99214	
D_ket_conf_20	-698.28765	-698.10166	0.33918	-697.92940	0.06768	0.06371	-697.99708	-697.99311	
D_ket_conf_21	-698.28384	-698.09730	0.33956	-697.92550	0.06610	0.06291	-697.99160	-697.98840	
D_ket_conf_22	-698.28500	-698.09855	0.33961	-697.92667	0.06571	0.06264	-697.99238	-697.98931	
D_ket_conf_23	-698.28909	-698.10352	0.33968	-697.93065	0.06643	0.06299	-697.99708	-697.99363	
D_ket_conf_25	-698.28876	-698.10316	0.33963	-697.93034	0.06615	0.06288	-697.99649	-697.99322	
D_ket_conf_26	-698.28631	-698.10040	0.33903	-697.92828	0.06700	0.06355	-697.99528	-697.99182	
D_ket_conf_27	-698.28410	-698.09767	0.33955	-697.92574	0.06629	0.06290	-697.99203	-697.98864	

D_ket_conf_28	-698.28618	-698.10011	0.33890	-697.92819	0.06721	0.06371	-697.99540	-697.99190	
D_ket_conf_29	-698.28695	-698.10091	0.33955	-697.92854	0.06674	0.06317	-697.99528	-697.99171	
D_ket_conf_3	-698.28772	-698.10207	0.33934	-697.92952	0.06643	0.06302	-697.99595	-697.99254	
D_ket_conf_30	-698.28299	-698.09636	0.33897	-697.92501	0.06737	0.06366	-697.99238	-697.98867	
D_ket_conf_31	-698.28500	-698.09942	0.33954	-697.92676	0.06461	0.06215	-697.99136	-697.98891	
D_ket_conf_32	-698.27846	-698.09288	0.33983	-697.91985	0.06635	0.06293	-697.98620	-697.98278	
D_ket_conf_33	-698.28169	-698.09690	0.34014	-697.92300	0.06475	0.06208	-697.98775	-697.98508	
D_ket_conf_4	-698.28733	-698.10142	0.33930	-697.92909	0.06675	0.06318	-697.99584	-697.99227	
D_ket_conf_6	-698.28759	-698.10181	0.33930	-697.92939	0.06675	0.06318	-697.99614	-697.99257	
D_ket_conf_7	-698.28417	-698.09771	0.33966	-697.92574	0.06616	0.06275	-697.99190	-697.98849	
D_ket_conf_8	-698.28699	-698.10096	0.33972	-697.92855	0.06558	0.06260	-697.99413	-697.99115	
D_sty	-310.34178	-310.26817	0.14152	-310.19177	0.04022	0.04000	-310.23198	-310.23176	
E_ket_anti_conf_1	-698.28401	-698.10038	0.33938	-697.92619	0.06380	0.06153	-697.98999	-697.98772	
E_ket_anti_conf_10	-698.29200	-698.10750	0.34250	-697.93173	0.06262	0.06042	-697.99435	-697.99216	
E_ket_anti_conf_12	-698.28459	-698.10080	0.33940	-697.92665	0.06478	0.06195	-697.99143	-697.98860	
E_ket_anti_conf_11	-698.27940	-698.09453	0.34004	-697.92105	0.06343	0.06128	-697.98447	-697.98233	
E_ket_anti_conf_15	-698.29145	-698.10702	0.34253	-697.93109	0.06337	0.06067	-697.99445	-697.99176	
E_ket_anti_conf_16	-698.29113	-698.10713	0.34285	-697.93048	0.06363	0.06085	-697.99411	-697.99133	
E_ket_anti_conf_17	-698.29136	-698.10691	0.34258	-697.93093	0.06346	0.06079	-697.99438	-697.99172	
E_ket_anti_conf_4	-698.28283	-698.09862	0.34006	-697.92426	0.06561	0.06227	-697.98987	-697.98653	
E_ket_anti_conf_5	-698.28311	-698.09870	0.33955	-697.92491	0.06561	0.06230	-697.99051	-697.98721	
E_ket_anti_conf_7	-698.28445	-698.10056	0.33957	-697.92639	0.06472	0.06184	-697.99110	-697.98823	
E_ket_anti_conf_8	-698.28468	-698.10067	0.33932	-697.92678	0.06518	0.06208	-697.99196	-697.98886	
E_ket_syn_conf_10	-698.28710	-698.10422	0.34242	-697.92694	0.06264	0.06040	-697.98958	-697.98734	
E_ket_syn_conf_11	-698.28714	-698.10352	0.34306	-697.92651	0.06146	0.05985	-697.98798	-697.98637	
E_ket_syn_conf_12	-698.27774	-698.09527	0.33939	-697.92013	0.06324	0.06108	-697.98337	-697.98122	

E_ket_syn_conf_16	-698.28761	-698.10365	0.34279	-697.92718	0.06175	0.05998	-697.98893	-697.98716	
E_ket_syn_conf_15	-698.28291	-698.10074	0.33946	-697.92542	0.06257	0.06067	-697.98799	-697.98609	
E_ket_syn_conf_16	-698.27732	-698.09395	0.33975	-697.91957	0.06249	0.06067	-697.98206	-697.98024	
E_ket_syn_conf_2	-698.28632	-698.10381	0.34253	-697.92615	0.06237	0.06005	-697.98851	-697.98620	
E_ket_syn_conf_20	-698.28533	-698.10062	0.34233	-697.92534	0.06142	0.05996	-697.98676	-697.98530	
E_ket_syn_conf_21	-698.28641	-698.10324	0.34252	-697.92618	0.06293	0.06054	-697.98911	-697.98672	
E_ket_syn_conf_22	-698.28648	-698.10211	0.34263	-697.92611	0.06250	0.06038	-697.98861	-697.98649	
E_ket_syn_conf_4	-698.28772	-698.10469	0.34242	-697.92742	0.06291	0.06065	-697.99033	-697.98808	
E_ket_syn_conf_6	-698.28503	-698.10229	0.34276	-697.92458	0.06273	0.06033	-697.98731	-697.98491	
E_ket_syn_conf_15	-698.28272	-698.10009	0.34017	-697.92465	0.06236	0.06048	-697.98701	-697.98513	
E_ket_syn_conf_7	-698.28605	-698.10355	0.34262	-697.92572	0.06268	0.06038	-697.98840	-697.98611	
E_ket_syn_conf_13	-698.28150	-698.09871	0.33978	-697.92358	0.06244	0.06073	-697.98602	-697.98431	
E_ket_syn_conf_8	-698.28575	-698.10251	0.34277	-697.92534	0.06283	0.06024	-697.98817	-697.98558	
E_ket_syn_conf_17	-698.28115	-698.09839	0.33984	-697.92328	0.06189	0.06049	-697.98517	-697.98378	
E_ket_syn_conf_9	-698.28504	-698.10229	0.34274	-697.92459	0.06305	0.06048	-697.98764	-697.98507	
E_sty	-310.89171	-310.80768	0.15768	-310.72581	0.04070	0.03973	-310.76651	-310.76554	
F_ket_anti_conf_1	-698.25189	-698.06469	0.34585	-697.88825	0.06418	0.06066	-697.95243	-697.94890	
F_ket_anti_conf_11	-698.24803	-698.05958	0.34637	-697.88399	0.06293	0.05996	-697.94692	-697.94395	
F_ket_anti_conf_2	-698.25208	-698.06417	0.34581	-697.88936	0.06005	0.05812	-697.94941	-697.94749	-11.04
F_ket_anti_conf_3	-698.25252	-698.06481	0.34562	-697.88905	0.06391	0.06045	-697.95296	-697.94950	
F_ket_anti_conf_4	-698.25079	-698.06287	0.34606	-697.88690	0.06408	0.06054	-697.95098	-697.94745	
F_ket_anti_conf_8	-698.25252	-698.06481	0.34561	-697.88905	0.06391	0.06045	-697.95296	-697.94951	
F_ket_anti_conf_9	-698.25141	-698.06419	0.34640	-697.88749	0.06145	0.05931	-697.94894	-697.94680	
F_ket_syn_conf_10	-698.24202	-698.05518	0.34623	-697.87821	0.06225	0.05959	-697.94046	-697.93779	
F_ket_syn_conf_11	-698.24398	-698.05706	0.34653	-697.88008	0.06028	0.05873	-697.94036	-697.93881	
F_ket_syn_conf_5	-698.25085	-698.06457	0.34601	-697.88733	0.06092	0.05918	-697.94825	-697.94651	

F_ket_syn_conf_6	-698.24874	-698.06217	0.34587	-697.88515	0.06258	0.05991	-697.94773	-697.94506	
F_ket_syn_conf_7	-698.24902	-698.06255	0.34618	-697.88541	0.06075	0.05894	-697.94616	-697.94435	
F_ket_syn_conf_8	-698.24877	-698.06172	0.34645	-697.88497	0.06044	0.05877	-697.94541	-697.94374	
F_ket_syn_conf_9	-698.24551	-698.05895	0.34642	-697.88166	0.06125	0.05900	-697.94291	-697.94066	
TSIII_ket_anti_conf_1	-698.27405	-698.09256	0.33953	-697.91644	0.06404	0.06130	-697.98047	-697.97774	-266.14
TSIII_ket_anti_conf_11	-698.27084	-698.08847	0.34031	-697.91286	0.06252	0.06031	-697.97538	-697.97317	-263
TSIII_ket_anti_conf_2	-698.27401	-698.09249	0.33969	-697.91644	0.06286	0.06074	-697.97929	-697.97717	-249.74
TSIII_ket_anti_conf_3	-698.27451	-698.09264	0.33998	-697.91671	0.06261	0.06063	-697.97932	-697.97734	-241.89
TSIII_ket_anti_conf_4	-698.27500	-698.09342	0.33999	-697.91718	0.06310	0.06077	-697.98028	-697.97794	-281.94
TSIII_ket_anti_conf_8	-698.27249	-698.09065	0.33918	-697.91526	0.06350	0.06108	-697.97877	-697.97635	-161.05
TSIII_ket_anti_conf_9	-698.27424	-698.09302	0.33974	-697.91668	0.06262	0.06056	-697.97930	-697.97724	-270.38
TSIII_ket_syn_conf_10	-698.26843	-698.08721	0.34024	-697.91055	0.06207	0.06011	-697.97262	-697.97066	-294.63
TSIII_ket_syn_conf_11	-698.26885	-698.08780	0.34016	-697.91115	0.06114	0.05973	-697.97228	-697.97087	-324.28
TSIII_ket_syn_conf_5	-698.27420	-698.09246	0.33953	-697.91674	0.06316	0.06089	-697.97990	-697.97763	-335.09
TSIII_ket_syn_conf_6	-698.27364	-698.09222	0.33939	-697.91626	0.06352	0.06100	-697.97978	-697.97726	-343.52
TSIII_ket_syn_conf_7	-698.27348	-698.09202	0.33979	-697.91602	0.06182	0.06009	-697.97783	-697.97611	-361.19
TSIII_ket_syn_conf_8	-698.27069	-698.08952	0.33986	-697.91323	0.06141	0.05985	-697.97464	-697.97308	-216.19
TSIII_ket_syn_conf_9	-698.27034	-698.08968	0.33983	-697.91280	0.06194	0.06014	-697.97474	-697.97294	-265.42
TSII_ket_conf_1	-698.23766	-698.05136	0.33550	-697.88242	0.06956	0.06540	-697.95198	-697.94782	-272.4
TSII_ket_conf_10	-698.23442	-698.04742	0.33558	-697.87918	0.06940	0.06533	-697.94858	-697.94451	-291.11
TSII_ket_conf_11	-698.23698	-698.05061	0.33481	-697.88227	0.07037	0.06583	-697.95264	-697.94810	-310.47
TSII_ket_conf_12	-698.23685	-698.05044	0.33514	-697.88196	0.06928	0.06534	-697.95124	-697.94730	-309.15
TSII_ket_conf_15	-698.23673	-698.05043	0.33518	-697.88184	0.06911	0.06517	-697.95095	-697.94701	-327.76
TSII_ket_conf_2	-698.23732	-698.05110	0.33550	-697.88206	0.07027	0.06565	-697.95232	-697.94771	-269.31
TSII_ket_conf_4	-698.23723	-698.05087	0.33536	-697.88208	0.06986	0.06565	-697.95195	-697.94773	-289.41
TSII_ket_conf_6	-698.23717	-698.05103	0.33560	-697.88190	0.06909	0.06518	-697.95099	-697.94707	-286.83

TSII_ket_conf_7	-698.23756	-698.05132	0.33537	-697.88246	0.06932	0.06532	-697.95178	-697.94778	-267.86
TSII_ket_conf_8	-698.23714	-698.05090	0.33553	-697.88190	0.06915	0.06530	-697.95105	-697.94719	-286.76
TSII_ket_conf_9	-698.23398	-698.04721	0.33563	-697.87870	0.06953	0.06524	-697.94823	-697.94394	-286.41
TSII_sty	-386.79433	-386.68824	0.16216	-386.62144	0.04625	0.04518	-386.66769	-386.66662	-1385.38
TSI_ket_conf_1	-388.55602	-388.44146	0.19885	-388.34526	0.04885	0.04802	-388.39411	-388.39328	-545.65
TSI_ket_conf_10	-388.55553	-388.44106	0.19876	-388.34481	0.04894	0.04819	-388.39375	-388.39300	-548.95
TSI_ket_conf_11	-388.55202	-388.43654	0.19904	-388.34118	0.04835	0.04775	-388.38953	-388.38893	-525.37
TSI_ket_conf_4	-388.55251	-388.43718	0.19893	-388.34165	0.04917	0.04814	-388.39082	-388.38979	-530.73
TSI_ket_conf_8	-388.55475	-388.44003	0.19901	-388.34392	0.04848	0.04783	-388.39239	-388.39174	-545.33
TSI_sty_conf_conf_1	-386.15665	-386.05199	0.14958	-385.99679	0.04582	0.04486	-386.04260	-386.04165	-1223.15
h2o	-76.44851	-76.41641	0.02154	-76.42319	0.02208	0.02208	-76.44527	-76.44527	
oh_anion	-75.92183	-75.89559	0.00863	-75.90989	0.01956	0.01956	-75.92945	-75.92945	
perylene_S0	-769.41346	-769.27782	0.25540	-769.14423	0.05152	0.05078	-769.19575	-769.19501	
perylene_radical_anion	-769.50391	-769.37424	0.25143	-769.23830	0.05336	0.05222	-769.29167	-769.29052	
pyrene_S0	-615.77838	-615.66753	0.20832	-615.55904	0.04637	0.04621	-615.60541	-615.60525	
pyrene_radical_anion	-615.85444	-615.74814	0.20365	-615.63941	0.04760	0.04745	-615.68701	-615.68686	
Aket_reorg	-388.44859								
Asty_reorg	-309.60645								
Bket_reorg	-388.50539								
Bsty_reorg	-309.66906								
Cket_reorg	-388.50539								
perylene_S0_reorg	-769.37638								
perylene_radical_anion_reorg	-769.46843								
pyrene_S0_reorg	-615.73778								
pyrene_radical_anion_reorg	-615.81573								

Table S3.3: Thermochemistry computed at the ωB97X-D /def2-TZVPD(SMD=acetonitrile)//M06-2X-D3/6-311+G(d) (SMD=acetonitrile) level of theory

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Cartesian coordinates

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A_ket Eopt -388.414598
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H 3.755333 1.437915 0.414058
H 3.669803 -0.076767 -0.500247
H 2.834000 1.358556 -1.097148
23
B_ket_conf_9 Eopt -388.455077
C 1.000812 -1.342744 -0.529628
C 0.367310 -0.450166 0.514385

C 1.663570 -0.042509 -0.150019
H 1.472526 -2.270075 -0.218374
H 0.505954 -1.385015 -1.496252
H 0.519160 -0.798370 1.545543
C 1.674847 1.082984 -1.159498
H 1.795409 2.052626 -0.663863
H 2.508972 0.964705 -1.860323
H 0.747889 1.115725 -1.735111
C 2.928470 -0.127806 0.676319
H 3.085212 0.793296 1.248821
H 2.885184 -0.958669 1.385796
H 3.809072 -0.275542 0.041003
C -0.948322 0.245791 0.285317
O -1.140479 1.376242 0.900393
C -2.141366 -0.689519 0.145860
H -1.863892 -1.579286 -0.431153
H -2.436012 -1.057384 1.151289
C -3.361319 -0.022916 -0.486143
H -3.145028 0.282437 -1.515994
H -4.230176 -0.688257 -0.506820
H -3.634452 0.875179 0.072734
16
B_sty Eopt -309.647511
C -1.792426 -1.034816 -0.000006
C -0.440113 -1.297555 -0.000005
C 0.543530 -0.253626 0.000004
C 0.024738 1.091525 0.000003
C -1.339201 1.336565 0.000004
C -2.279543 0.295713 0.000001
H -2.494260 -1.864750 -0.000014
H -0.096448 -2.330096 -0.000009
H 0.711859 1.932080 0.000001
H -1.686139 2.367381 0.000003
H -3.343769 0.501952 0.000001
C 1.931898 -0.549913 0.000013
H 2.180288 -1.612245 0.000043
C 2.993748 0.345002 -0.000012
H 2.854967 1.421820 -0.000035
H 4.017714 -0.013503 -0.000001
23
C_ket_conf1 Eopt -388.465169
C -1.238993 -0.380721 1.106062
C 0.074900 -0.865052 0.521953
C -2.188599 0.131920 0.056041
H -1.731418 -1.189865 1.663804

H -1.016546 0.420704 1.819365
H 0.080091 -1.824475 0.009902
C -1.938477 1.492179 -0.512955
H -1.070073 1.490232 -1.193179
H -2.792361 1.851776 -1.095762
H -1.721165 2.226437 0.268601
C -2.846814 -0.870627 -0.838413
H -3.733426 -0.457668 -1.330407
H -2.169608 -1.199639 -1.644243
H -3.146163 -1.769687 -0.290654
C 1.233277 -0.114893 0.562329
O 1.375896 1.035485 1.105339
C 2.481536 -0.700420 -0.106359
H 3.265349 -0.795054 0.655750
H 2.281625 -1.704693 -0.493085
C 2.990030 0.201082 -1.231173
H 3.204943 1.201657 -0.850406
H 3.903033 -0.192777 -1.686691
H 2.237392 0.298367 -2.020622
23
C_ket_conf10 Eopt -388.464129
C 1.066421 -0.252134 -1.113619
C -0.284990 0.237775 -0.626493
C 2.169321 0.007633 -0.121959
H 0.987590 -1.327728 -1.304300
H 1.329857 0.230178 -2.065968
H -0.439580 1.312078 -0.592713
C 2.645825 1.416973 0.036930
H 2.705823 1.936810 -0.924335
H 1.964612 2.004739 0.674782
H 3.630291 1.463049 0.513817
C 2.263137 -0.880869 1.077801
H 2.153181 -1.936631 0.812091
H 3.215468 -0.755495 1.602494
H 1.468265 -0.655263 1.808271
C -1.272673 -0.615473 -0.182340
O -1.210777 -1.896284 -0.153968
C -2.600502 -0.032812 0.325387
H -3.393445 -0.476072 -0.289328
H -2.754041 -0.441277 1.331597
C -2.772056 1.482804 0.361597
H -2.682144 1.925142 -0.633926
H -3.759177 1.748556 0.750369
H -2.027386 1.958800 1.005072
23

C_ket_conf11 Eopt -388.465037
C -1.108404 -0.185084 1.102471
C 0.112879 -0.661454 0.338650
C -2.292551 0.064128 0.206736
H -1.393411 -0.919024 1.869425
H -0.840145 0.741737 1.621770
H 0.110582 -1.683145 -0.034398
C -3.020595 -1.125373 -0.335052
H -3.122946 -1.915684 0.415142
H -4.020778 -0.861926 -0.694142
H -2.489486 -1.568519 -1.193980
C -2.288284 1.300869 -0.634570
H -1.583032 1.211500 -1.477534
H -3.273037 1.498626 -1.069651
H -1.982067 2.181757 -0.062420
C 1.181444 0.162002 0.043692
O 1.316381 1.387028 0.390436
C 2.337043 -0.438676 -0.764894
H 2.123519 -1.477924 -1.034069
H 2.425053 0.126718 -1.701432
C 3.663634 -0.355298 -0.010951
H 3.618869 -0.930665 0.919501
H 4.493371 -0.747016 -0.606213
H 3.891464 0.680657 0.248022
23
C_ket_conf12 Eopt -388.464498
C -1.200287 -1.005239 0.112543
C 0.197918 -0.951671 -0.452599
C -2.095776 0.151856 -0.249350
H -1.705800 -1.934064 -0.184416
H -1.116376 -1.046212 1.213485
H 0.339583 -1.253902 -1.487759
C -3.573514 -0.077081 -0.272250
H -3.835154 -1.016527 -0.768434
H -3.982274 -0.135862 0.751310
H -4.107298 0.736171 -0.773943
C -1.630201 1.530466 0.090793
H -2.116332 2.293826 -0.526039
H -1.870051 1.776649 1.139530
H -0.547343 1.624196 -0.020342
C 1.280349 -0.503929 0.275732
O 1.257355 -0.096516 1.489735
C 2.644579 -0.469596 -0.419859
H 3.338725 -1.093998 0.156472
H 2.579649 -0.898091 -1.425022

C 3.201384 0.952202 -0.494481
H 3.282589 1.384125 0.505152
H 4.192648 0.976995 -0.956068
H 2.541885 1.596773 -1.084988
23
C_ket_conf13 Eopt -388.464338
C -1.089405 -0.845726 0.407611
C 0.229286 -0.757147 -0.320859
C -2.228394 -0.071872 -0.205187
H -1.407017 -1.891841 0.514682
H -0.931170 -0.472917 1.435250
H 0.352269 -1.356940 -1.219953
C -2.044167 1.395970 -0.415624
H -1.018108 1.632733 -0.706723
H -2.725865 1.792493 -1.175473
H -2.253443 1.953508 0.513607
C -3.623166 -0.549218 0.046290
H -3.711045 -1.634263 -0.063690
H -3.946004 -0.308651 1.073968
H -4.346448 -0.076403 -0.625480
C 1.251770 0.078919 0.077553
O 1.238919 0.858783 1.093287
C 2.535639 0.083605 -0.758907
H 2.440224 -0.586921 -1.618854
H 2.680229 1.097592 -1.153175
C 3.759207 -0.302635 0.071427
H 3.657529 -1.319763 0.463711
H 4.678789 -0.263177 -0.519381
H 3.874080 0.372913 0.921388
23
C_ket_conf14 Eopt -388.464498
C 1.199840 -1.004186 0.115689
C -0.197474 -0.949962 -0.452078
C 2.095821 0.152403 -0.246842
H 1.113341 -1.043832 1.216372
H 1.705390 -1.933586 -0.179416
H -0.335919 -1.245747 -1.489558
C 1.633688 1.530626 0.099697
H 2.118253 2.295453 -0.516534
H 0.550542 1.626043 -0.006731
H 1.877811 1.773061 1.148336
C 3.573057 -0.078235 -0.279818
H 4.104551 0.736064 -0.782259
H 3.988514 -0.140955 0.740820
H 3.830302 -1.016324 -0.780833

C -1.281958 -0.505212 0.275010
O -1.262813 -0.103620 1.491021
C -2.644209 -0.467553 -0.424538
H -2.576570 -0.892895 -1.430851
H -3.340767 -1.093077 0.147660
C -3.199344 0.955078 -0.496404
H -2.538137 1.600353 -1.084189
H -4.189844 0.982229 -0.959517
H -3.281491 1.384420 0.504235
23
C_ket_conf3 Eopt -388.461012
C 0.940198 0.091064 -1.139395
C -0.039140 1.019993 -0.433205
C 2.068827 -0.362155 -0.249282
H 0.427538 -0.785813 -1.548999
H 1.367213 0.621196 -2.001389
H 0.264568 2.066799 -0.375002
C 3.090439 0.653322 0.154540
H 3.329391 1.337115 -0.665944
H 2.735839 1.273996 0.993722
H 4.019804 0.182180 0.490716
C 1.805965 -1.483749 0.704591
H 1.295481 -2.321516 0.219046
H 2.731438 -1.859545 1.151680
H 1.160456 -1.161800 1.539220
C -1.207366 0.691713 0.225793
O -1.965680 1.526307 0.839291
C -1.701074 -0.759674 0.239588
H -0.985003 -1.446249 -0.215866
H -1.803097 -1.059559 1.289844
C -3.058276 -0.896557 -0.451988
H -3.440451 -1.919680 -0.393745
H -3.791927 -0.232804 0.009445
H -2.983250 -0.628520 -1.510923
23
C_ket_conf5 Eopt -388.461120
C -1.058385 -0.585010 1.047334
C 0.022748 -1.244974 0.202061
C -1.993944 0.279424 0.242541
H -1.649246 -1.367338 1.542914
H -0.617191 0.013925 1.850626
H -0.293487 -2.129435 -0.354331
C -2.994566 -0.399048 -0.638282
H -2.535569 -0.743754 -1.579659
H -3.429701 -1.280326 -0.156825

H -3.809577 0.274993 -0.921537
C -1.516596 1.628197 -0.193458
H -2.352934 2.288548 -0.446085
H -0.913050 2.118977 0.576365
H -0.890662 1.562748 -1.098398
C 1.320789 -0.827783 -0.018683
O 2.161597 -1.422896 -0.784754
C 1.862944 0.424508 0.681526
H 1.128900 0.878233 1.350286
H 2.712626 0.113623 1.302239
C 2.347792 1.467325 -0.326699
H 3.115766 1.043031 -0.975993
H 1.526051 1.810649 -0.962914
H 2.770611 2.343457 0.173302
23
C_ket_conf6 Eopt -388.465147
C -1.228781 -0.546319 1.018947
C 0.074389 -0.921113 0.339026
C -2.196717 0.132043 0.086623
H -1.713341 -1.437149 1.443603
H -0.990107 0.123799 1.852435
H 0.060552 -1.753170 -0.361352
C -2.896709 -0.714900 -0.928791
H -3.201099 -1.680232 -0.512494
H -3.786181 -0.218602 -1.330257
H -2.245810 -0.931703 -1.792373
C -1.936211 1.558432 -0.279674
H -1.677576 2.162893 0.594865
H -1.091375 1.644951 -0.983513
H -2.800840 2.015897 -0.770732
C 1.248651 -0.222436 0.534306
O 1.415157 0.783666 1.308473
C 2.482844 -0.677149 -0.251447
H 3.272473 -0.929181 0.467431
H 2.266498 -1.582241 -0.827789
C 2.991633 0.423139 -1.182978
H 2.230713 0.684004 -1.926003
H 3.227814 1.326090 -0.616152
H 3.892437 0.115134 -1.721520
23
C_ket_conf7 Eopt -388.465036
C 1.108458 -0.184390 1.102594
C -0.112768 -0.661186 0.338936
C 2.292567 0.064190 0.206670
H 0.840078 0.742827 1.621093

H 1.393405 -0.917717 1.870170
H -0.110017 -1.682709 -0.034565
C 3.020416 -1.125626 -0.334637
H 3.122476 -1.915748 0.415799
H 2.489371 -1.568909 -1.193538
H 4.020713 -0.862504 -0.693651
C 2.288223 1.300532 -0.635235
H 1.582135 1.211131 -1.477505
H 1.982979 2.181867 -0.063244
H 3.272672 1.497566 -1.071303
C -1.181451 0.162079 0.043847
O -1.316681 1.387087 0.390574
C -2.336799 -0.438772 -0.764917
H -2.424808 0.126638 -1.701447
H -2.123117 -1.477993 -1.034081
C -3.663493 -0.355637 -0.011106
H -4.493001 -0.747963 -0.606287
H -3.618547 -0.930629 0.919574
H -3.891807 0.680303 0.247467
23
C_ket_conf8 Eopt -388.461012
C 0.940517 -0.091571 1.139375
C -0.038935 -1.020075 0.432908
C 2.069051 0.362091 0.249322
H 0.428041 0.785173 1.549503
H 1.367689 -0.622159 2.001011
H 0.264574 -2.066921 0.374394
C 1.805879 1.484065 -0.704019
H 2.731181 1.859944 -1.151384
H 1.159935 1.162459 -1.538442
H 1.295711 2.321686 -0.217904
C 3.090608 -0.653162 -0.155119
H 2.735616 -1.273851 -0.994136
H 4.019695 -0.181847 -0.491816
H 3.330156 -1.336959 0.665182
C -1.207365 -0.691627 -0.225573
O -1.965853 -1.526171 -0.839034
C -1.701068 0.759712 -0.239124
H -0.985327 1.446086 0.217186
H -1.802292 1.060107 -1.289316
C -3.058788 0.896421 0.451438
H -2.984614 0.628106 1.510359
H -3.440820 1.919594 0.393149
H -3.792110 0.232834 -0.010757
17

C_sty Eopt -310.160943
C 1.887882 -0.981675 0.000056
C 0.543788 -1.310060 -0.000021
C -0.458226 -0.304383 -0.000063
C -0.028410 1.047609 -0.000087
C 1.321412 1.365069 -0.000024
C 2.289774 0.358558 0.000063
H 2.633610 -1.769818 0.000124
H 0.238088 -2.352066 -0.000028
H -0.764969 1.844093 -0.000149
H 1.625987 2.406473 -0.000037
H 3.343602 0.613324 0.000127
C -1.831816 -0.657845 -0.000150
H -2.077686 -1.714635 -0.000052
C -2.940085 0.338749 0.000114
H -2.896084 0.995878 -0.876968
H -3.912078 -0.154304 -0.000284
H -2.896386 0.994926 0.877944
39
D_ket_conf_1 Eopt -698.101468
C 1.675222 -1.433562 -0.328122
C 2.719191 -0.515839 -0.900438
C 0.491977 -0.783416 0.439033
H 1.230033 -2.051895 -1.122001
H 2.164544 -2.125717 0.368935
H 2.513774 -0.029748 -1.851288
C 1.006926 -0.029615 1.665661
H 0.184703 0.408941 2.239684
H 1.551236 -0.708248 2.328506
H 1.691444 0.773334 1.377942
C -0.461062 -1.891711 0.891379
H 0.059083 -2.598348 1.546577
H -1.316222 -1.492860 1.446013
H -0.848558 -2.454681 0.035863
C 3.930521 -0.270565 -0.283744
O 4.335056 -0.768209 0.823842
C 4.892077 0.705075 -0.970724
H 5.842030 0.185753 -1.148576
H 4.502845 1.015231 -1.945663
C 5.154030 1.935514 -0.101583
H 5.558969 1.640809 0.868750
H 5.864897 2.621717 -0.570833
H 4.225393 2.487637 0.077511
C -0.246203 0.188802 -0.522159
H -0.559963 -0.379180 -1.404574

H 0.491541 0.923647 -0.864036
C -1.395168 0.922937 0.079692
H -1.164067 1.783198 0.701985
C -2.770455 0.611109 -0.075674
C -3.238119 -0.497382 -0.830770
C -3.751960 1.428508 0.549093
C -4.594216 -0.758964 -0.949306
H -2.528088 -1.154416 -1.319526
C -5.102839 1.157957 0.424000
H -3.421604 2.281843 1.134065
C -5.539051 0.061302 -0.327330
H -4.922894 -1.613466 -1.531868
H -5.826908 1.801753 0.912558
H -6.597855 -0.150542 -0.424805
39
D_ket_conf_10 Eopt -698.101549
C -1.745842 1.043421 -1.035222
C -3.098386 0.821034 -0.418681
C -0.523527 1.037054 -0.078001
H -1.574444 0.263933 -1.788035
H -1.720452 2.005569 -1.568472
H -3.584034 1.658875 0.076084
C -0.389038 -0.328100 0.596089
H -0.223731 -1.117753 -0.142882
H 0.445905 -0.344881 1.304132
H -1.304289 -0.573173 1.141635
C -0.683340 2.123581 0.986614
H 0.165902 2.139389 1.676278
H -0.765195 3.115974 0.528928
H -1.586190 1.952032 1.578993
C -3.754037 -0.393874 -0.456651
O -3.326064 -1.472342 -0.997686
C -5.125162 -0.483256 0.222059
H -5.441924 0.497279 0.591446
H -5.859946 -0.802248 -0.527811
C -5.117001 -1.493146 1.369879
H -6.101252 -1.585792 1.837873
H -4.819248 -2.480026 1.009760
H -4.405190 -1.191899 2.145716
C 0.735922 1.328945 -0.943624
H 0.569113 2.291622 -1.443228
H 0.788427 0.570397 -1.731081
C 2.020358 1.405925 -0.191058
H 2.233983 2.330580 0.337966
C 2.995759 0.380679 -0.083178

C 2.858960 -0.894247 -0.694205
C 4.176934 0.611988 0.673518
C 3.840490 -1.862723 -0.552090
H 1.974015 -1.121133 -1.277201
C 5.149925 -0.362188 0.809054
H 4.306732 1.578242 1.152049
C 4.992490 -1.610378 0.197202
H 3.708396 -2.828437 -1.029028
H 6.039947 -0.154385 1.393929
H 5.754953 -2.373707 0.304215
39
D_ket_conf_11 Eopt -698.102324
C -1.257224 0.390795 -1.077352
C -2.206062 -0.629976 -0.513856
C -0.492599 1.276251 -0.059532
H -0.498673 -0.089001 -1.713878
H -1.824240 1.065035 -1.730221
H -1.787412 -1.515842 -0.040489
C -1.467015 2.174313 0.702531
H -0.941852 2.779690 1.449222
H -1.981792 2.857036 0.019165
H -2.226626 1.581718 1.220156
C 0.505822 2.152545 -0.818655
H -0.013850 2.772208 -1.556983
H 1.045952 2.823208 -0.142104
H 1.244922 1.548470 -1.354102
C -3.579465 -0.497667 -0.564890
O -4.234592 0.471557 -1.087191
C -4.422332 -1.603771 0.078911
H -5.101536 -2.007290 -0.682377
H -3.788682 -2.428526 0.420293
C -5.249145 -1.067008 1.247824
H -5.896740 -0.252258 0.917274
H -5.880146 -1.842995 1.690594
H -4.596742 -0.676541 2.036001
C 0.261794 0.399890 0.979427
H -0.496217 -0.102653 1.591647
H 0.818571 1.064408 1.647786
C 1.152330 -0.639726 0.389400
H 0.679083 -1.547738 0.024974
C 2.561359 -0.562340 0.244526
C 3.324876 0.568906 0.638367
C 3.270108 -1.654303 -0.327289
C 4.700515 0.594840 0.470494
H 2.828319 1.429335 1.072006

C 4.643353 -1.617374 -0.490262
H 2.710102 -2.531075 -0.638944
C 5.373878 -0.492353 -0.092812
H 5.258466 1.473025 0.778834
H 5.154726 -2.467185 -0.930390
H 6.449946 -0.463611 -0.221932
39
D_ket_conf_12 Eopt -698.101982
C 2.100926 -1.735023 -0.297796
C 2.648845 -0.433169 -0.813501
C 0.619094 -1.744382 0.166380
H 2.196793 -2.521348 -1.061192
H 2.704574 -2.057422 0.560059
H 2.452684 -0.166253 -1.849326
C 0.443454 -0.815666 1.367702
H 1.024683 -1.183985 2.218711
H 0.798823 0.192638 1.139635
H -0.604117 -0.755544 1.679474
C 0.239834 -3.171119 0.569648
H 0.927640 -3.547853 1.333696
H -0.772328 -3.222314 0.982648
H 0.287544 -3.851370 -0.287636
C 3.374925 0.445061 -0.033067
O 3.694526 0.284618 1.195446
C 3.832466 1.756972 -0.679418
H 4.923141 1.827548 -0.584124
H 3.596642 1.768769 -1.748298
C 3.194515 2.965921 0.005935
H 3.537250 3.909085 -0.429218
H 2.103560 2.932328 -0.086876
H 3.438470 2.976250 1.070325
C -0.271808 -1.278734 -1.018831
H -0.049108 -1.937674 -1.868229
H 0.047507 -0.273914 -1.306642
C -1.739743 -1.314488 -0.761930
H -2.246853 -2.270051 -0.864593
C -2.546274 -0.208419 -0.387453
C -2.026363 1.098110 -0.184823
C -3.942684 -0.387347 -0.190971
C -2.854567 2.145680 0.185947
H -0.965555 1.282033 -0.313516
C -4.760017 0.665853 0.179202
H -4.365485 -1.376972 -0.337282
C -4.224936 1.944143 0.371145
H -2.429961 3.133004 0.335991

H -5.822373 0.496879 0.321698
H -4.865736 2.768865 0.662105
39
D_ket_conf_13 Eopt -698.097528
C -1.886281 -0.816306 0.892196
C -3.169883 -0.945923 0.111620
C -0.556385 -1.065915 0.125803
H -1.807836 0.169855 1.365126
H -1.897902 -1.535201 1.724738
H -3.528475 -1.962659 -0.058165
C -0.345598 0.007263 -0.942024
H -0.275052 1.003506 -0.493907
H 0.572098 -0.170547 -1.511500
H -1.181354 0.016216 -1.647750
C -0.579760 -2.446695 -0.530675
H -1.401124 -2.517402 -1.248496
H 0.349685 -2.649919 -1.070695
H -0.716900 -3.236880 0.216239
C -3.956370 0.056999 -0.418142
O -5.054894 -0.126109 -1.058296
C -3.555379 1.525954 -0.237594
H -2.530700 1.637660 0.121408
H -3.600502 1.998080 -1.225913
C -4.513062 2.252068 0.709389
H -5.544033 2.154042 0.362529
H -4.457197 1.828956 1.717596
H -4.280964 3.318440 0.782825
C 0.590306 -0.998373 1.175191
H 0.364290 -1.741632 1.949961
H 0.549940 -0.016773 1.658681
C 1.955370 -1.275132 0.643774
H 2.231574 -2.315873 0.498816
C 2.934770 -0.309980 0.293323
C 4.198398 -0.738249 -0.197486
C 2.722970 1.090442 0.399181
C 5.178876 0.169486 -0.556086
H 4.386449 -1.803942 -0.289263
C 3.712589 1.990964 0.037101
H 1.773522 1.465628 0.763017
C 4.946608 1.544372 -0.442744
H 6.133009 -0.189479 -0.927751
H 3.522721 3.055602 0.126815
H 5.714892 2.255356 -0.724910
39
D_ket_conf_14 Eopt -698.097781

C -1.727327 -0.771552 0.956455
C -2.885546 -1.301168 0.149200
C -0.568219 -0.086243 0.178082
H -2.063933 -0.061483 1.720491
H -1.270176 -1.601891 1.514863
H -2.730275 -2.270933 -0.327573
C -1.059853 1.199513 -0.486022
H -0.273805 1.665558 -1.087910
H -1.902821 0.986357 -1.148149
H -1.392592 1.930731 0.259462
C -0.016218 -1.033248 -0.887590
H 0.302490 -1.983679 -0.445611
H -0.778869 -1.253412 -1.639484
H 0.843419 -0.595986 -1.404620
C -4.113270 -0.716663 -0.092949
O -5.045746 -1.236307 -0.806678
C -4.457914 0.645226 0.524859
H -5.292768 0.488374 1.219983
H -3.630907 1.054797 1.108071
C -4.888636 1.660854 -0.533493
H -5.739993 1.282222 -1.101666
H -5.177621 2.613646 -0.080544
H -4.078768 1.861310 -1.241843
C 0.540949 0.245643 1.217229
H 0.868299 -0.692004 1.677846
H 0.071582 0.840327 2.011132
C 1.702371 1.011731 0.681686
H 1.578910 2.084932 0.565135
C 2.957990 0.476779 0.293574
C 3.268978 -0.907697 0.357366
C 3.971763 1.346122 -0.194092
C 4.510905 -1.378882 -0.038577
H 2.525567 -1.611087 0.714433
C 5.207740 0.864713 -0.587068
H 3.759181 2.409368 -0.255463
C 5.491059 -0.503249 -0.513091
H 4.720762 -2.441955 0.019523
H 5.960244 1.554098 -0.955638
H 6.459413 -0.880110 -0.822442
39
D_ket_conf_15 Eopt -698.096874
C 1.384587 0.518193 0.007901
C 2.482016 0.423791 -1.023914
C 0.539913 -0.761543 0.256335
H 1.775016 0.843553 0.979951

H 0.680985 1.303833 -0.299078
H 2.165910 0.512548 -2.064976
C 1.412738 -1.881923 0.822622
H 1.844142 -1.597641 1.787888
H 0.826251 -2.794295 0.973846
H 2.235917 -2.119273 0.143481
C -0.106088 -1.235662 -1.046103
H 0.658873 -1.516323 -1.775043
H -0.739997 -2.111586 -0.875341
H -0.725664 -0.453343 -1.496503
C 3.829694 0.198055 -0.831630
O 4.705475 0.114648 -1.768402
C 4.391011 0.045914 0.586781
H 3.605043 0.007158 1.343056
H 4.918402 -0.915036 0.627868
C 5.373240 1.169655 0.922106
H 6.176505 1.209010 0.183640
H 4.867556 2.140750 0.919316
H 5.824806 1.032561 1.908837
C -0.559702 -0.454442 1.315897
H -0.043148 -0.155920 2.236849
H -1.085963 -1.388076 1.539896
C -1.528188 0.619253 0.950211
H -1.215331 1.648744 1.097306
C -2.835973 0.429217 0.431705
C -3.396024 -0.850070 0.173701
C -3.646445 1.560688 0.142211
C -4.678246 -0.977935 -0.337261
H -2.815860 -1.743034 0.375104
C -4.924670 1.421460 -0.368303
H -3.242260 2.551125 0.329346
C -5.454583 0.150268 -0.613817
H -5.080505 -1.968107 -0.525227
H -5.517890 2.305111 -0.579519
H -6.456265 0.041550 -1.014136
39
D_ket_conf_16 Eopt -698.097781
C 1.727275 -0.771267 0.956001
C 2.885403 -1.301017 0.148639
C 0.568309 -0.085598 0.177704
H 1.269937 -1.601617 1.514219
H 2.064048 -0.061370 1.720098
H 2.730013 -2.270760 -0.328130
C 0.016215 -1.032312 -0.888196
H -0.843179 -0.594712 -1.405354

H 0.778981 -1.252654 -1.639911
H -0.302898 -1.982645 -0.446310
C 1.060222 1.200215 -0.486154
H 1.393258 1.931087 0.259534
H 1.903046 0.986962 -1.148420
H 0.274169 1.666594 -1.087743
C 4.113555 -0.717045 -0.092558
O 5.046277 -1.237008 -0.805798
C 4.458183 0.644816 0.525238
H 3.631333 1.054107 1.108860
H 5.293492 0.488155 1.219844
C 4.888076 1.660608 -0.533348
H 5.739172 1.282063 -1.102003
H 4.077745 1.860886 -1.241211
H 5.177173 2.613417 -0.080527
C -0.540914 0.246190 1.216817
H -0.071686 0.841006 2.010708
H -0.868102 -0.691490 1.677470
C -1.702474 1.011964 0.681164
H -1.579132 2.085122 0.564095
C -2.958099 0.476720 0.293427
C -3.268833 -0.907798 0.357501
C -3.972107 1.345814 -0.194185
C -4.510781 -1.379258 -0.038032
H -2.525182 -1.611012 0.714427
C -5.208116 0.864130 -0.586751
H -3.759722 2.409081 -0.255858
C -5.491219 -0.503861 -0.512429
H -4.720445 -2.442356 0.020286
H -5.960813 1.553328 -0.955274
H -6.459598 -0.880930 -0.821445
39
D_ket_conf_17 Eopt -698.097805
C 1.914697 -1.086425 0.916908
C 3.245928 -0.975840 0.217677
C 0.635944 -1.119218 0.033274
H 1.897253 -2.012818 1.509998
H 1.779816 -0.277182 1.643661
H 3.648169 -1.902893 -0.195163
C 0.704887 -2.289281 -0.948547
H 0.780709 -3.245427 -0.418464
H -0.180417 -2.328369 -1.590218
H 1.579337 -2.194950 -1.597984
C 0.485953 0.190302 -0.739620
H 1.335149 0.336635 -1.412181

H -0.425007 0.193886 -1.346341
H 0.443774 1.049783 -0.061746
C 4.041865 0.139153 0.041203
O 5.182566 0.141293 -0.548645
C 3.590640 1.507306 0.568295
H 2.632673 1.456522 1.089377
H 4.337124 1.840852 1.300173
C 3.507047 2.543970 -0.552809
H 3.235321 3.531261 -0.168235
H 4.467348 2.630686 -1.064227
H 2.757505 2.259411 -1.297808
C -0.570605 -1.306184 0.997324
H -0.568788 -0.472593 1.707084
H -0.380804 -2.216629 1.579584
C -1.899969 -1.440881 0.336574
H -2.156448 -2.413895 -0.073196
C -2.870164 -0.417059 0.181118
C -2.677359 0.914956 0.634836
C -4.103177 -0.709426 -0.463375
C -3.656498 1.879171 0.453394
H -1.750728 1.188419 1.126073
C -5.073511 0.260930 -0.639071
H -4.275353 -1.720197 -0.821359
C -4.860678 1.566076 -0.182566
H -3.481829 2.889462 0.808840
H -6.004281 0.006026 -1.135166
H -5.621060 2.326361 -0.321231
39
D_ket_conf_18 Eopt -698.101188
C 0.750819 -0.069678 -0.071746
C 2.024752 -0.520658 -0.732792
C 0.609190 1.448296 0.208511
H -0.115373 -0.364626 -0.680755
H 0.649620 -0.592784 0.887647
H 2.111946 -0.403404 -1.810723
C 0.757062 2.249767 -1.086783
H 0.529064 3.308593 -0.922095
H 1.780007 2.184316 -1.466993
H 0.087860 1.879020 -1.869767
C 1.671520 1.905267 1.208578
H 2.672611 1.645151 0.854485
H 1.629349 2.989668 1.357745
H 1.527604 1.424726 2.181377
C 3.080081 -1.080584 -0.041494
O 3.139006 -1.286467 1.221300

C 4.317538 -1.494157 -0.845662
H 4.483638 -2.567900 -0.691876
H 4.155222 -1.340724 -1.917296
C 5.562523 -0.730744 -0.393599
H 6.455192 -1.046055 -0.941393
H 5.435977 0.345521 -0.552005
H 5.744035 -0.891716 0.671083
C -0.783689 1.726291 0.845059
H -0.796603 2.780909 1.149994
H -0.861715 1.133510 1.761849
C -1.953803 1.489933 -0.048631
H -2.166259 2.249182 -0.796392
C -2.829931 0.373846 -0.019078
C -2.668410 -0.720049 0.872190
C -3.926995 0.317426 -0.921180
C -3.550326 -1.789143 0.856872
H -1.838933 -0.728335 1.569807
C -4.801254 -0.755025 -0.927957
H -4.071715 1.139557 -1.616008
C -4.623249 -1.819415 -0.037867
H -3.401176 -2.612677 1.547557
H -5.629447 -0.768388 -1.628934
H -5.307924 -2.660052 -0.044219
39
D_ket_conf_19 Eopt -698.097151
C -1.317335 -0.672186 -0.329775
C -2.437776 -1.118436 0.577258
C -0.588577 0.649357 0.036485
H -0.548115 -1.456382 -0.348912
H -1.657592 -0.575820 -1.367704
H -2.132498 -1.620207 1.497549
C 0.024081 0.550548 1.433818
H 0.725108 -0.287193 1.508090
H 0.563970 1.466709 1.694201
H -0.756460 0.399984 2.184608
C -1.558778 1.829701 -0.005074
H -2.360641 1.701713 0.726068
H -1.041928 2.767840 0.223030
H -2.018411 1.931109 -0.994296
C -3.800828 -0.986120 0.404028
O -4.691238 -1.410433 1.227347
C -4.362381 -0.298425 -0.847072
H -3.575714 0.030263 -1.529119
H -4.965719 -1.039379 -1.386830
C -5.254599 0.889615 -0.485460

H -5.698093 1.345278 -1.375522
H -6.064269 0.570814 0.173555
H -4.685573 1.664934 0.037052
C 0.525226 0.928447 -1.016052
H 0.987882 1.891076 -0.774788
H 0.026510 1.053468 -1.985370
C 1.563722 -0.133280 -1.155852
H 1.322617 -0.990953 -1.776884
C 2.851634 -0.132675 -0.559094
C 3.319135 0.907121 0.287823
C 3.737069 -1.218583 -0.799774
C 4.585625 0.855395 0.848898
H 2.678683 1.753946 0.505453
C 4.998867 -1.260267 -0.233933
H 3.404072 -2.028064 -1.442673
C 5.437098 -0.223392 0.596644
H 4.916514 1.663614 1.492992
H 5.650683 -2.103680 -0.436731
H 6.425791 -0.256529 1.040256
39
D_ket_conf_2 Eopt -698.101643
C 1.654130 0.412865 -1.195208
C 2.894505 0.905895 -0.504342
C 0.499920 -0.092050 -0.288562
H 1.229199 1.202056 -1.833603
H 1.931892 -0.412945 -1.861746
H 2.888485 1.910364 -0.087393
C 0.056008 1.018002 0.665034
H -0.228868 1.921926 0.115353
H -0.800909 0.707411 1.270873
H 0.866853 1.284114 1.348815
C 0.958100 -1.308373 0.516450
H 1.160123 -2.161293 -0.139760
H 1.881114 -1.077676 1.054816
H 0.202840 -1.614424 1.247271
C 4.036610 0.140961 -0.370797
O 4.206315 -1.052934 -0.800535
C 5.224722 0.760603 0.373120
H 6.086422 0.776810 -0.306059
H 5.011701 1.797416 0.652246
C 5.589644 -0.049157 1.617462
H 4.754581 -0.068782 2.325773
H 5.821968 -1.081416 1.347536
H 6.457002 0.369781 2.135673
C -0.678796 -0.486892 -1.223493

H -0.282395 -1.201715 -1.955622
H -0.983204 0.402753 -1.784072
C -1.846076 -1.113807 -0.540470
H -1.764584 -2.166185 -0.282580
C -3.058384 -0.469776 -0.182043
C -3.308821 0.907974 -0.420162
C -4.089175 -1.214847 0.453363
C -4.510834 1.489182 -0.047979
H -2.549905 1.519520 -0.894539
C -5.285119 -0.624222 0.820522
H -3.922541 -2.270079 0.648854
C -5.509223 0.734406 0.573418
H -4.674777 2.544370 -0.240975
H -6.052487 -1.220213 1.303558
H -6.446290 1.197096 0.861989
39
D_ket_conf_20 Eopt -698.101659
C -1.277625 1.063858 -1.024257
C -1.296969 -0.415478 -0.757219
C -1.110688 1.993897 0.205179
H -0.469653 1.315235 -1.727043
H -2.215930 1.346582 -1.517202
H -0.346029 -0.915952 -0.590073
C -2.328636 1.878342 1.122033
H -2.489764 0.840515 1.426688
H -2.201421 2.486598 2.024253
H -3.233979 2.219502 0.610661
C -0.988942 3.441287 -0.277871
H -1.887485 3.735167 -0.830076
H -0.873003 4.134287 0.562258
H -0.135664 3.578935 -0.948328
C -2.453465 -1.168065 -0.724060
O -3.647054 -0.741346 -0.908152
C -2.315736 -2.663481 -0.417612
H -2.760135 -3.228339 -1.246678
H -1.261477 -2.952329 -0.354577
C -3.034362 -3.036596 0.879297
H -4.091090 -2.767142 0.822589
H -2.968503 -4.108224 1.088227
H -2.598354 -2.502865 1.730533
C 0.140331 1.596179 1.031162
H -0.061150 0.640699 1.519706
H 0.249729 2.339730 1.835171
C 1.408047 1.536513 0.249699
H 1.692037 2.426372 -0.305840

C 2.304057 0.439352 0.166390
C 2.113003 -0.790293 0.853002
C 3.465832 0.549386 -0.646948
C 3.022003 -1.828639 0.724393
H 1.245369 -0.927450 1.487795
C 4.365897 -0.494017 -0.768476
H 3.637887 1.478144 -1.182929
C 4.153464 -1.695734 -0.084670
H 2.848676 -2.756275 1.260191
H 5.240781 -0.377564 -1.399708
H 4.858312 -2.513929 -0.180653
39
D_ket_conf_21 Eopt -698.097297
C -0.803878 -0.030917 -0.333199
C -1.985599 -0.408753 -1.193165
C -0.713621 1.442278 0.147335
H -0.741488 -0.665319 0.558648
H 0.119220 -0.232082 -0.894579
H -1.905565 -0.151769 -2.251365
C -1.865527 1.768230 1.097529
H -2.829616 1.614513 0.606353
H -1.836862 1.132176 1.989092
H -1.818218 2.811372 1.427267
C -0.756347 2.400353 -1.044561
H -0.570898 3.431942 -0.725974
H -0.005907 2.140082 -1.797783
H -1.735653 2.371750 -1.529577
C -3.152599 -1.049982 -0.829338
O -4.102996 -1.362002 -1.635591
C -3.388982 -1.457690 0.631132
H -3.460093 -2.552462 0.661966
H -2.557554 -1.173787 1.279201
C -4.688043 -0.867406 1.180700
H -5.535014 -1.165729 0.560328
H -4.879965 -1.201729 2.204358
H -4.651345 0.226470 1.189114
C 0.612508 1.638913 0.938031
H 0.609380 0.944354 1.784092
H 0.590093 2.651075 1.362290
C 1.862957 1.502194 0.136945
H 2.139020 2.340785 -0.496518
C 2.740994 0.387228 0.122815
C 2.505301 -0.799859 0.865854
C 3.916833 0.428883 -0.674786
C 3.391060 -1.864388 0.810096

H 1.616232 -0.883147 1.480128
C 4.794319 -0.639813 -0.723095
H 4.119968 1.324092 -1.255201
C 4.541107 -1.798080 0.019224
H 3.184025 -2.760360 1.386189
H 5.683152 -0.577464 -1.342329
H 5.228157 -2.635881 -0.020061
39
D_ket_conf_22 Eopt -698.098550
C -1.323959 -0.072128 -1.006814
C -2.144315 -1.104873 -0.274836
C -0.601903 1.005760 -0.152654
H -0.543004 -0.579760 -1.591291
H -1.926439 0.466476 -1.746863
H -1.584470 -1.930115 0.170653
C -1.619345 1.923773 0.523483
H -1.117622 2.687989 1.126424
H -2.238554 2.437158 -0.219937
H -2.283847 1.358298 1.182407
C 0.291089 1.841549 -1.071550
H -0.306837 2.318418 -1.855449
H 0.806081 2.633707 -0.518301
H 1.050893 1.225653 -1.562594
C -3.510908 -1.151384 -0.081858
O -4.131899 -2.078751 0.553743
C -4.413843 -0.049870 -0.652446
H -3.846992 0.716724 -1.184424
H -5.083538 -0.519148 -1.384459
C -5.263239 0.606672 0.436211
H -5.859215 -0.143431 0.958876
H -4.634215 1.108193 1.178306
H -5.944408 1.353663 0.018494
C 0.255241 0.343159 0.960762
H -0.438396 -0.155605 1.647668
H 0.749557 1.136645 1.530238
C 1.241359 -0.664328 0.476420
H 0.863049 -1.656047 0.243131
C 2.631962 -0.458664 0.284394
C 3.445928 -1.534137 -0.165223
C 3.275037 0.787019 0.513483
C 4.805261 -1.375105 -0.367156
H 2.978732 -2.496933 -0.350258
C 4.637811 0.934897 0.307959
H 2.695131 1.639100 0.848821
C 5.416427 -0.138832 -0.131881

H 5.399193 -2.215800 -0.710491
H 5.102784 1.898355 0.490146
H 6.481685 -0.014580 -0.290808
39
D_ket_conf_23 Eopt -698.103522
C 1.623164 1.306696 -1.051645
C 2.739558 0.493782 -0.456027
C 0.662719 2.015313 -0.060272
H 2.013457 2.099335 -1.708987
H 1.027642 0.645399 -1.691054
H 3.529544 1.015904 0.079257
C -0.468590 2.671364 -0.855198
H -1.153992 3.217670 -0.198460
H -0.066153 3.384110 -1.582681
H -1.051924 1.927442 -1.407033
C 1.414968 3.093925 0.720975
H 1.834986 3.844613 0.043195
H 0.749425 3.610651 1.420589
H 2.238122 2.664771 1.299542
C 2.810062 -0.881557 -0.548724
O 1.977421 -1.652719 -1.148015
C 3.981021 -1.581145 0.147549
H 4.523929 -2.172122 -0.600562
H 4.684196 -0.850010 0.558728
C 3.491451 -2.512246 1.257187
H 2.804000 -3.259307 0.855121
H 4.318738 -3.038713 1.741640
H 2.957074 -1.947447 2.028543
C 0.063191 1.012467 0.961076
H -0.644592 1.553037 1.596934
H 0.881605 0.677739 1.609490
C -0.557258 -0.190896 0.337353
H 0.129189 -0.912616 -0.102529
C -1.946014 -0.453613 0.219613
C -2.379600 -1.661823 -0.394305
C -2.956682 0.436404 0.673921
C -3.723021 -1.958907 -0.536764
H -1.628179 -2.358414 -0.754683
C -4.300178 0.128585 0.525367
H -2.678892 1.375457 1.138989
C -4.699144 -1.067349 -0.077430
H -4.019887 -2.889643 -1.009262
H -5.049538 0.828467 0.880958
H -5.751995 -1.300579 -0.189671
39

D_ket_conf_25 Eopt -698.103161
C 1.530509 1.220283 0.960076
C 2.648894 0.588475 0.177966
C 0.458884 2.000473 0.154691
H 1.024868 0.430470 1.526824
H 1.921139 1.930536 1.705427
H 3.376216 1.240705 -0.300409
C 1.090752 3.221626 -0.515288
H 1.878993 2.928120 -1.214521
H 0.344235 3.794895 -1.075176
H 1.533944 3.889556 0.230940
C -0.635113 2.469284 1.116768
H -0.211314 3.103380 1.902567
H -1.402321 3.052711 0.596689
H -1.128678 1.622428 1.604075
C 2.807042 -0.776744 0.046442
O 2.053746 -1.685411 0.549444
C 4.000697 -1.279120 -0.772196
H 3.611538 -1.867061 -1.613185
H 4.562346 -0.440603 -1.196020
C 4.930050 -2.162411 0.059675
H 4.381607 -3.010414 0.474585
H 5.759015 -2.553792 -0.536973
H 5.357228 -1.598816 0.895493
C -0.168012 1.114159 -0.954141
H 0.619146 0.907376 -1.688831
H -0.937323 1.699289 -1.467485
C -0.699321 -0.189559 -0.463866
H 0.042911 -0.935556 -0.184544
C -2.065838 -0.524622 -0.285295
C -3.135136 0.379998 -0.526525
C -2.413423 -1.826423 0.171713
C -4.452896 -0.000975 -0.326396
H -2.922434 1.387754 -0.864924
C -3.732012 -2.196321 0.366194
H -1.615465 -2.536899 0.367255
C -4.767325 -1.287695 0.118865
H -5.248528 0.712307 -0.516216
H -3.962971 -3.197960 0.714097
H -5.800631 -1.577696 0.272677
39
D_ket_conf_26 Eopt -698.100404
C 1.662915 0.893382 0.659531
C 3.107825 0.531478 0.862471
C 0.668903 -0.269148 0.388649

H 1.277598 1.435075 1.536490
H 1.595290 1.585103 -0.189601
H 3.412435 0.150176 1.834428
C 0.721463 -1.276130 1.539933
H 1.715161 -1.725619 1.616474
H 0.498353 -0.789431 2.496059
H 0.002455 -2.089346 1.402703
C 1.028845 -0.961447 -0.927324
H 0.411334 -1.847359 -1.104874
H 0.894821 -0.281590 -1.775045
H 2.075491 -1.277060 -0.915986
C 4.066251 0.676678 -0.120567
O 3.875155 1.111476 -1.309546
C 5.503614 0.269295 0.220638
H 6.151677 1.143066 0.077126
H 5.585672 -0.027653 1.271040
C 5.993867 -0.864281 -0.680481
H 7.029601 -1.139372 -0.461517
H 5.375563 -1.758649 -0.549429
H 5.936483 -0.570263 -1.730539
C -0.739826 0.345057 0.296398
H -0.729358 1.128227 -0.477748
H -0.952002 0.879071 1.235473
C -1.849107 -0.614214 0.014601
H -1.619578 -1.665640 -0.126484
C -3.213758 -0.234942 -0.077833
C -3.638717 1.109810 0.080177
C -4.214086 -1.209808 -0.333429
C -4.980542 1.448084 -0.012048
H -2.904818 1.884392 0.274659
C -5.550149 -0.861247 -0.422267
H -3.912928 -2.245796 -0.458186
C -5.946868 0.471117 -0.262109
H -5.280361 2.483564 0.112087
H -6.293637 -1.627196 -0.616780
H -6.994272 0.742390 -0.332026
39
D_ket_conf_27 Eopt -698.097671
C 1.674983 1.048085 0.841854
C 2.739222 0.556020 -0.104891
C 0.593338 1.986051 0.243542
H 1.157683 0.206988 1.313255
H 2.120925 1.614151 1.675791
H 3.335391 1.326710 -0.597554
C 1.224840 3.302189 -0.215341

H 1.965778 3.139841 -1.002726
H 0.464695 3.984634 -0.609824
H 1.724177 3.805131 0.619418
C -0.439338 2.288401 1.331719
H 0.044564 2.746502 2.200725
H -1.206169 2.983132 0.973916
H -0.941298 1.377994 1.673397
C 3.084311 -0.740521 -0.430392
O 4.018398 -1.063903 -1.252924
C 2.373907 -1.935175 0.218902
H 1.494995 -1.645770 0.798398
H 2.022808 -2.586265 -0.590908
C 3.331234 -2.725565 1.113171
H 4.208649 -3.044799 0.547234
H 3.677368 -2.110545 1.950175
H 2.852927 -3.616433 1.530191
C -0.104703 1.340871 -0.985571
H 0.637655 1.286682 -1.789270
H -0.893822 2.021208 -1.322873
C -0.637182 -0.031536 -0.755330
H 0.070668 -0.850982 -0.837669
C -1.974935 -0.380408 -0.438783
C -3.016709 0.573966 -0.292394
C -2.316467 -1.747265 -0.247028
C -4.307040 0.178399 0.023099
H -2.802074 1.628274 -0.424647
C -3.607618 -2.130589 0.068869
H -1.537059 -2.496716 -0.351713
C -4.617175 -1.171751 0.207289
H -5.083755 0.928750 0.129677
H -3.836541 -3.181759 0.210446
H -5.628754 -1.472542 0.455660
39
D_ket_conf_28 Eopt -698.100109
C 1.696324 -0.381255 -0.673502
C 3.117260 0.108753 -0.680423
C 0.597998 0.613965 -0.210394
H 1.400548 -0.721845 -1.677855
H 1.642722 -1.260160 -0.019686
H 3.422133 0.799136 -1.463526
C 0.614730 1.856805 -1.103413
H 1.571755 2.379272 -1.022385
H 0.468082 1.585040 -2.154753
H -0.170631 2.567451 -0.828951
C 0.836396 1.016183 1.245995

H 1.835732 1.443077 1.366286
H 0.112277 1.762724 1.586220
H 0.760602 0.147516 1.908442
C 4.061285 -0.303972 0.239046
O 3.874979 -1.116349 1.211890
C 5.484664 0.244863 0.090743
H 5.541413 0.960661 -0.735518
H 5.736972 0.789533 1.009496
C 6.505490 -0.873714 -0.116271
H 6.464846 -1.585563 0.710646
H 6.298261 -1.422734 -1.040627
H 7.526163 -0.485750 -0.180067
C -0.754530 -0.110090 -0.342228
H -0.706389 -1.045412 0.236277
H -0.879284 -0.431650 -1.388145
C -1.956100 0.669127 0.080400
H -1.834975 1.693175 0.418914
C -3.276508 0.148588 0.064473
C -3.565082 -1.173472 -0.363216
C -4.369376 0.951922 0.484660
C -4.866399 -1.653004 -0.365151
H -2.757796 -1.818298 -0.693308
C -5.663809 0.463182 0.478558
H -4.173118 1.967510 0.815731
C -5.925277 -0.844232 0.053809
H -5.061354 -2.667850 -0.696247
H -6.480079 1.098833 0.805609
H -6.940121 -1.225772 0.049822
39
D_ket_conf_29 Eopt -698.100908
C 0.802059 0.375493 -0.781135
C 2.191449 -0.159062 -0.996744
C 0.681037 1.724060 -0.026786
H 0.286346 0.508306 -1.744381
H 0.229184 -0.374394 -0.222982
H 2.795063 0.275848 -1.790167
C 1.413740 2.824854 -0.795637
H 1.310752 3.792056 -0.292643
H 2.481200 2.602413 -0.875876
H 1.014882 2.930056 -1.810579
C 1.269116 1.614183 1.380522
H 2.338699 1.392629 1.333253
H 1.141472 2.552362 1.932269
H 0.792964 0.814585 1.953662
C 2.730407 -1.181924 -0.242482

O 2.157538 -1.802347 0.720560
C 4.161623 -1.625259 -0.565548
H 4.141430 -2.692176 -0.821308
H 4.548052 -1.089033 -1.438174
C 5.095791 -1.419349 0.627104
H 6.111576 -1.763759 0.412666
H 5.152117 -0.359369 0.896647
H 4.730059 -1.965878 1.498896
C -0.818210 2.133609 0.057369
H -1.201885 2.229941 -0.963209
H -0.857774 3.135588 0.504174
C -1.680222 1.228564 0.870859
H -1.609324 1.317250 1.951472
C -2.590907 0.257136 0.379973
C -2.785466 -0.004758 -1.002246
C -3.354777 -0.513908 1.298117
C -3.685166 -0.970318 -1.425921
H -2.219945 0.550831 -1.741203
C -4.249830 -1.475376 0.864209
H -3.223165 -0.336190 2.361368
C -4.425256 -1.713813 -0.502996
H -3.811729 -1.150833 -2.488439
H -4.817045 -2.047745 1.590899
H -5.125561 -2.468505 -0.842781
39
D_ket_conf_3 Eopt -698.102071
C 1.896721 1.659126 0.518824
C 3.070729 0.879418 -0.003472
C 0.542241 1.468093 -0.213891
H 1.738764 1.393371 1.571685
H 2.110693 2.738013 0.496021
H 3.594062 1.259209 -0.878050
C 0.697068 1.802922 -1.698966
H -0.268677 1.804711 -2.213383
H 1.139647 2.797346 -1.821967
H 1.346676 1.083059 -2.205259
C -0.490971 2.409253 0.408343
H -1.477981 2.288848 -0.049471
H -0.593902 2.226528 1.483204
H -0.189399 3.453635 0.275206
C 3.508802 -0.296935 0.571747
O 3.001914 -0.874667 1.595294
C 4.703599 -1.004783 -0.075615
H 5.112108 -0.407531 -0.896996
H 5.494298 -1.106779 0.678271

C 4.319797 -2.394944 -0.583253
H 3.542385 -2.325878 -1.351498
H 5.174617 -2.919731 -1.019402
H 3.928431 -3.005249 0.233283
C 0.090719 -0.006378 -0.030915
H -0.060507 -0.181941 1.038276
H 0.935670 -0.635916 -0.332890
C -1.113760 -0.395581 -0.817179
H -0.970331 -0.616151 -1.871793
C -2.441592 -0.501764 -0.329190
C -2.802986 -0.214730 1.014584
C -3.484540 -0.907972 -1.206424
C -4.116526 -0.331868 1.441123
H -2.044032 0.106050 1.718834
C -4.792244 -1.021502 -0.769632
H -3.236454 -1.132254 -2.239720
C -5.122870 -0.735292 0.559414
H -4.363516 -0.105229 2.473232
H -5.565041 -1.334787 -1.463958
H -6.147942 -0.824363 0.901043
39
D_ket_conf_30 Eopt -698.096358
C -1.504399 -0.497892 -0.766622
C -3.010658 -0.543705 -0.849637
C -0.818353 -1.456941 0.246484
H -1.078922 -0.744026 -1.751447
H -1.161949 0.520216 -0.555734
H -3.438862 -1.365893 -1.425958
C -1.252846 -2.898172 -0.029289
H -1.041592 -3.181854 -1.066185
H -0.723231 -3.598002 0.625491
H -2.324619 -3.026611 0.141740
C -1.186696 -1.095748 1.687039
H -0.860870 -0.086689 1.955016
H -2.269713 -1.141737 1.833062
H -0.722723 -1.794369 2.391732
C -3.918921 0.333096 -0.292720
O -5.195434 0.261077 -0.422789
C -3.423622 1.522998 0.538956
H -4.009349 1.535404 1.465266
H -2.375271 1.423688 0.827490
C -3.628801 2.845775 -0.202274
H -3.353372 3.705542 0.415362
H -3.020051 2.880148 -1.111544
H -4.674461 2.962944 -0.495893

C 0.709539 -1.386962 0.059986
H 0.953706 -1.734569 -0.955194
H 1.181991 -2.121661 0.731001
C 1.328521 -0.046563 0.286334
H 0.708674 0.774313 0.632595
C 2.707286 0.227726 0.090919
C 3.218426 1.531357 0.326580
C 3.625388 -0.765206 -0.339150
C 4.558541 1.821395 0.141193
H 2.534755 2.307715 0.657333
C 4.966764 -0.463434 -0.521313
H 3.274666 -1.774356 -0.526872
C 5.446152 0.827023 -0.285022
H 4.921687 2.826780 0.327323
H 5.649142 -1.240133 -0.850887
H 6.495923 1.056043 -0.430173
39
D_ket_conf_31 Eopt -698.099417
C 2.112096 -0.718419 0.472867
C 1.368452 -1.519337 -0.566069
C 2.615701 0.684991 0.041814
H 1.497598 -0.586990 1.368634
H 3.010239 -1.256857 0.817505
H 1.914808 -1.735989 -1.486237
C 3.664509 0.555917 -1.065642
H 3.246901 0.090667 -1.962580
H 4.053899 1.538661 -1.351827
H 4.510175 -0.054036 -0.731407
C 3.267399 1.362503 1.250643
H 4.116075 0.770978 1.608929
H 3.641904 2.358888 0.993732
H 2.569034 1.469296 2.085673
C 0.098015 -2.056356 -0.502234
O -0.448141 -2.753954 -1.434990
C -0.769594 -1.885219 0.750337
H -0.386621 -1.122754 1.431473
H -1.757021 -1.543404 0.416248
C -0.922260 -3.210772 1.499317
H -1.602612 -3.119669 2.350971
H -1.314682 -3.983138 0.834103
H 0.044248 -3.556017 1.880635
C 1.460486 1.559105 -0.505802
H 1.144049 1.147837 -1.465583
H 1.880305 2.554684 -0.717136
C 0.297674 1.704957 0.414281

H 0.500743 2.038299 1.428626
C -1.064173 1.461890 0.097453
C -2.049047 1.596532 1.113902
C -1.514179 1.053212 -1.186185
C -3.382993 1.321661 0.870464
H -1.732905 1.908223 2.105259
C -2.853492 0.782332 -1.419773
H -0.805729 0.934292 -1.997447
C -3.799727 0.907638 -0.399241
H -4.107702 1.424687 1.671564
H -3.166647 0.462994 -2.408549
H -4.844129 0.687179 -0.589448
39
D_ket_conf_32 Eopt -698.092882
C 1.284637 0.705468 1.378493
C 2.480280 -0.198265 1.117240
C 0.564019 1.452882 0.241940
H 0.514780 0.139479 1.926614
H 1.601143 1.481395 2.092126
H 2.939014 -0.531713 2.047260
C 1.545327 2.354418 -0.508769
H 2.317063 1.752305 -0.992443
H 1.027085 2.941151 -1.275915
H 2.022926 3.060005 0.180443
C -0.528393 2.325804 0.872000
H -0.095142 3.050060 1.569564
H -1.071663 2.887149 0.104852
H -1.256945 1.724548 1.425381
C 3.073268 -0.688019 -0.030443
O 2.765993 -0.481236 -1.259454
C 4.298806 -1.593428 0.175887
H 4.475078 -1.794915 1.236618
H 4.090121 -2.556209 -0.307315
C 5.554108 -0.988171 -0.452017
H 6.417695 -1.652796 -0.356560
H 5.392588 -0.792223 -1.513963
H 5.809340 -0.038209 0.029075
C -0.092283 0.476727 -0.775390
H 0.735726 -0.023402 -1.288230
H -0.639045 1.075933 -1.511564
C -0.973694 -0.558478 -0.167715
H -0.483275 -1.404706 0.308093
C -2.392276 -0.566102 -0.154450
C -3.181688 0.484166 -0.695752
C -3.087436 -1.662003 0.427436

C -4.566128 0.430776 -0.655927
H -2.697861 1.345224 -1.142190
C -4.469686 -1.705191 0.460873
H -2.508960 -2.478273 0.850104
C -5.224996 -0.659403 -0.081192
H -5.143086 1.248408 -1.075899
H -4.969403 -2.556806 0.910913
H -6.308323 -0.693607 -0.054620
39
D_ket_conf_33 Eopt -698.096900
C -1.169736 -0.954257 1.222154
C -1.852330 0.398045 1.088479
C -1.234953 -2.009577 0.090945
H -0.105763 -0.841129 1.484933
H -1.614553 -1.433239 2.104807
H -2.230202 0.784325 2.033271
C -2.630625 -2.056415 -0.529225
H -2.710376 -2.883984 -1.242948
H -3.393857 -2.206954 0.242022
H -2.846478 -1.121966 -1.052150
C -0.916070 -3.377170 0.708959
H -1.708238 -3.684901 1.398845
H -0.824354 -4.149010 -0.062880
H 0.022384 -3.354629 1.272257
C -2.009834 1.229165 -0.000722
O -1.650852 1.019586 -1.215564
C -2.682601 2.585209 0.251144
H -3.550267 2.663326 -0.415673
H -3.052777 2.662354 1.277835
C -1.724972 3.740114 -0.043283
H -1.350335 3.675094 -1.067230
H -2.209407 4.713024 0.079981
H -0.862943 3.708863 0.631354
C -0.208927 -1.720206 -1.044523
H -0.477973 -0.755744 -1.478046
H -0.359186 -2.493478 -1.809699
C 1.222206 -1.749842 -0.624033
H 1.707453 -2.718278 -0.530240
C 2.017541 -0.612696 -0.323615
C 1.507844 0.713792 -0.376684
C 3.377937 -0.776398 0.054925
C 2.321392 1.794734 -0.070540
H 0.471269 0.879145 -0.662547
C 4.176996 0.312426 0.357560
H 3.788864 -1.780779 0.103347

C 3.657064 1.610189 0.298149
H 1.911769 2.799056 -0.118539
H 5.212665 0.156734 0.641983
H 4.283537 2.462813 0.535680
39
D_ket_conf_4 Eopt -698.101417
C -1.662445 0.203626 0.893233
C -2.861613 0.693378 0.130658
C -0.425582 -0.229519 0.061748
H -1.310569 0.975692 1.594576
H -1.966830 -0.655044 1.503762
H -2.826496 1.694108 -0.293825
C 0.045729 0.926495 -0.821769
H -0.719590 1.184803 -1.558876
H 0.251682 1.821994 -0.225106
H 0.958251 0.668024 -1.367873
C -0.770959 -1.435996 -0.811341
H -1.644970 -1.218186 -1.430772
H 0.056803 -1.701127 -1.476491
H -1.006050 -2.312145 -0.197660
C -4.009037 -0.055569 -0.042458
O -4.219712 -1.241109 0.393900
C -5.163850 0.587447 -0.819031
H -4.875792 1.573328 -1.197644
H -5.381061 -0.043365 -1.690332
C -6.427585 0.706490 0.032755
H -6.251388 1.350119 0.900815
H -7.260337 1.132144 -0.534466
H -6.736295 -0.273715 0.401501
C 0.693345 -0.611559 1.072777
H 0.274696 -1.372666 1.743191
H 0.910056 0.266635 1.689292
C 1.940360 -1.155784 0.463601
H 1.933935 -2.200129 0.163996
C 3.141012 -0.438576 0.223715
C 3.300064 0.938776 0.532364
C 4.253747 -1.103916 -0.359562
C 4.493279 1.594761 0.273702
H 2.477187 1.490847 0.971522
C 5.440021 -0.438983 -0.613787
H 4.158461 -2.157066 -0.607086
C 5.572870 0.917773 -0.299612
H 4.586267 2.647813 0.518645
H 6.271102 -0.974801 -1.060494
H 6.502491 1.438535 -0.499836

39
D_ket_conf_6 Eopt -698.101810
C -1.823672 1.220581 0.892120
C -2.951965 0.739976 0.023219
C -0.429567 1.368192 0.227457
H -2.062418 2.204535 1.323203
H -1.713132 0.528833 1.736373
H -3.409627 1.448126 -0.663894
C 0.542819 1.950617 1.255033
H 0.598125 1.318795 2.147774
H 1.554317 2.048496 0.848514
H 0.215519 2.946527 1.571808
C -0.517251 2.311905 -0.973938
H 0.473114 2.537916 -1.380560
H -1.120480 1.879944 -1.777755
H -0.979473 3.260833 -0.681206
C -3.440430 -0.551311 0.063628
O -3.018398 -1.500588 0.811652
C -4.610543 -0.897557 -0.864020
H -4.876290 -0.040062 -1.490414
H -4.285197 -1.701459 -1.536613
C -5.835643 -1.372946 -0.083486
H -6.657089 -1.652905 -0.749216
H -5.586177 -2.241497 0.529268
H -6.200581 -0.585882 0.584438
C 0.053510 -0.037920 -0.220165
H -0.745869 -0.465161 -0.836375
H 0.131411 -0.667657 0.671038
C 1.324379 -0.045028 -0.998223
H 1.266048 0.222242 -2.050036
C 2.616011 -0.353075 -0.498486
C 2.865612 -0.691173 0.858766
C 3.736487 -0.322900 -1.373517
C 4.148077 -0.978328 1.298868
H 2.044674 -0.721495 1.565785
C 5.012448 -0.610853 -0.923095
H 3.574584 -0.066840 -2.416488
C 5.232593 -0.941962 0.418343
H 4.308917 -1.232141 2.341630
H 5.846703 -0.578904 -1.616282
H 6.232918 -1.166857 0.770780
39
D_ket_conf_7 Eopt -698.097709
C 1.759317 0.390232 0.824640
C 2.870716 1.135093 0.129627

C 0.526899 -0.012972 -0.033640
H 2.132718 -0.522115 1.304672
H 1.369344 1.009168 1.646307
H 2.709817 2.203150 -0.028157
C 0.922330 -1.053084 -1.082257
H 0.091767 -1.273797 -1.759721
H 1.757919 -0.689584 -1.687435
H 1.230663 -1.992954 -0.611410
C -0.057455 1.218107 -0.726731
H -0.299762 2.002760 -0.001462
H 0.657752 1.633547 -1.441674
H -0.971395 0.971447 -1.275768
C 4.070424 0.638643 -0.338774
O 4.986135 1.335214 -0.910023
C 4.408496 -0.846962 -0.163535
H 3.536566 -1.444513 0.108861
H 4.757925 -1.217060 -1.134327
C 5.513034 -1.045945 0.876659
H 5.175753 -0.724485 1.867346
H 5.816380 -2.094141 0.952216
H 6.395756 -0.457235 0.617050
C -0.523738 -0.619681 0.939898
H -0.788632 0.146110 1.675747
H -0.024495 -1.427466 1.490069
C -1.742393 -1.178430 0.288346
H -1.660210 -2.166755 -0.155498
C -3.005425 -0.541593 0.178591
C -3.267842 0.761094 0.680572
C -4.078369 -1.215179 -0.466663
C -4.520150 1.339101 0.543979
H -2.479159 1.317688 1.173630
C -5.324226 -0.628293 -0.597696
H -3.904033 -2.211755 -0.861560
C -5.558913 0.655347 -0.093267
H -4.692179 2.336300 0.935834
H -6.122660 -1.168260 -1.095970
H -6.535141 1.115372 -0.197054
39
D_ket_conf_8 Eopt -698.100964
C -1.270340 -0.645279 0.411859
C -2.489237 -0.770313 -0.460475
C -0.502592 0.700934 0.358432
H -1.570822 -0.813829 1.453741
H -0.545743 -1.433626 0.163141
H -2.343093 -0.924122 -1.527304

C -1.404638 1.853057 0.801568
H -0.867333 2.806751 0.763097
H -2.281958 1.933355 0.154433
H -1.756666 1.705461 1.827236
C 0.001216 0.972235 -1.059976
H 0.644979 0.163259 -1.420534
H -0.838210 1.066183 -1.754612
H 0.574373 1.904019 -1.104292
C -3.779537 -0.723314 0.027485
O -4.128184 -0.563024 1.249951
C -4.925397 -0.868124 -0.979783
H -4.538057 -1.057533 -1.985939
H -5.526654 -1.740104 -0.692712
C -5.822605 0.369467 -0.992004
H -6.232192 0.555395 0.002946
H -5.255050 1.257123 -1.290832
H -6.659259 0.258570 -1.687786
C 0.699887 0.648952 1.347289
H 0.282393 0.511321 2.352486
H 1.188083 1.629244 1.341042
C 1.694450 -0.434957 1.100189
H 1.459528 -1.425906 1.477400
C 2.935270 -0.299027 0.424522
C 3.387821 0.923733 -0.138446
C 3.786717 -1.429110 0.286698
C 4.609129 1.000884 -0.789536
H 2.771202 1.811775 -0.063822
C 5.003599 -1.340847 -0.365556
H 3.463914 -2.377210 0.706586
C 5.428547 -0.124387 -0.910222
H 4.929681 1.948257 -1.210574
H 5.630646 -2.221977 -0.453837
H 6.381976 -0.055637 -1.421747
17
D_sty Eopt -310.268170
C -1.900041 -0.965878 -0.000135
C -0.568129 -1.317002 0.000245
C 0.499394 -0.335345 0.000174
C 0.034089 1.037368 0.000361
C -1.314816 1.359461 0.000053
C -2.318373 0.381904 -0.000308
H -2.647595 -1.756512 -0.000240
H -0.295029 -2.370549 0.000407
H 0.764304 1.841610 0.000504
H -1.596171 2.410795 0.000135

H -3.369274 0.647206 -0.000602
C 1.841888 -0.676639 0.000075
H 2.117863 -1.728358 -0.000363
C 2.938686 0.354628 -0.000274
H 2.912795 1.023000 0.875335
H 3.923585 -0.120290 0.000245
H 2.913332 1.022114 -0.876573
39
E_ket_anti_conf_1 Eopt -698.100379
C -2.140540 -0.051722 -1.039701
C -0.806569 0.583808 -0.614120
C -2.492005 -1.088179 0.044593
H -2.930326 0.691511 -1.171663
H -2.004498 -0.569643 -1.994628
H -0.106191 0.601937 -1.456129
C -3.398395 -2.193263 -0.487149
H -3.605321 -2.939092 0.287282
H -4.358977 -1.787644 -0.821945
H -2.936044 -2.707407 -1.335169
C -3.165327 -0.410500 1.242429
H -3.330333 -1.130519 2.050584
H -2.567383 0.412235 1.641860
H -4.137708 0.001911 0.955372
C -0.911280 2.001514 -0.100662
O -1.974357 2.586541 0.001754
C 0.381059 2.681629 0.309233
H 0.129002 3.694154 0.630947
H 0.782275 2.144645 1.176457
C 1.442378 2.708931 -0.793496
H 1.797965 1.705375 -1.036591
H 1.052245 3.164554 -1.707854
H 2.302967 3.297198 -0.468106
C -1.099967 -1.608025 0.427295
H -0.742100 -2.282829 -0.358830
H -1.096526 -2.163717 1.370826
C -0.184797 -0.368347 0.491914
H -0.319450 0.101886 1.471957
C 1.281787 -0.647466 0.309130
C 2.200661 -0.298819 1.278814
C 1.759708 -1.221685 -0.935860
C 3.599357 -0.488315 1.118920
H 1.832510 0.155043 2.199118
C 3.152349 -1.474988 -1.070984
H 1.060404 -1.563408 -1.692797
C 4.056743 -1.126321 -0.089559

H 4.289233 -0.234383 1.916277
H 3.516570 -1.949464 -1.980649
H 5.115582 -1.324186 -0.235129
39
E_ket_anti_conf_10 Eopt -698.107499
C 2.365682 0.851744 0.241067
C 0.831365 0.839834 0.419362
C 2.843739 -0.614579 0.051495
H 2.586697 1.442330 -0.653993
H 2.863930 1.340516 1.084811
H 0.596731 0.599267 1.466205
C 3.687148 -1.091447 1.233625
H 3.919804 -2.158463 1.146534
H 4.634508 -0.545216 1.290000
H 3.155807 -0.941087 2.178928
C 3.652929 -0.756375 -1.239605
H 3.048769 -0.489522 -2.112793
H 4.527640 -0.097670 -1.227413
H 4.006632 -1.784059 -1.374996
C 0.160055 2.144394 0.031062
O 0.223473 2.522401 -1.215483
C -0.986195 2.672033 0.879162
H -0.866500 2.356396 1.923536
H -0.944028 3.771641 0.880969
C -2.398735 2.283116 0.396591
H -2.500781 2.497306 -0.671322
H -2.597982 1.218139 0.545253
H -3.175101 2.845901 0.927578
C 1.527435 -1.426171 -0.047311
H 1.280763 -1.853251 0.931560
H 1.608260 -2.260214 -0.753320
C 0.449669 -0.408949 -0.437426
H 0.589824 -0.116127 -1.484342
C -0.967067 -0.882354 -0.265454
C -1.868377 -0.850507 -1.333260
C -1.439640 -1.318193 0.979799
C -3.198244 -1.235364 -1.169654
H -1.524063 -0.507855 -2.305141
C -2.765773 -1.703946 1.149849
H -0.765488 -1.346314 1.830973
C -3.653450 -1.662851 0.074603
H -3.878399 -1.198156 -2.014454
H -3.110068 -2.034256 2.124596
H -4.687988 -1.960829 0.207280
39

E_ket_anti_conf_11 Eopt -698.100801
C 2.071647 -0.482620 -1.043965
C 0.802448 0.337198 -0.757434
C 2.261721 -1.431622 0.155014
H 1.917721 -1.078984 -1.949013
H 2.945329 0.152982 -1.207362
H 0.132511 0.331653 -1.623925
C 2.980017 -0.715600 1.303098
H 4.003644 -0.456123 1.015104
H 2.477169 0.211210 1.589486
H 3.031905 -1.359396 2.187166
C 3.038870 -2.688073 -0.223615
H 3.132267 -3.365891 0.631130
H 2.539198 -3.231229 -1.031425
H 4.050398 -2.438285 -0.560837
C 1.040701 1.787893 -0.408467
O 2.150647 2.258161 -0.243094
C -0.206214 2.633573 -0.264016
H -0.778668 2.535092 -1.194684
H -0.835930 2.162541 0.500465
C 0.068784 4.090871 0.067752
H -0.867130 4.646406 0.155804
H 0.608361 4.185218 1.012379
H 0.673279 4.566378 -0.707496
C 0.806664 -1.737468 0.533819
H 0.709445 -2.179821 1.530645
H 0.389342 -2.447725 -0.189500
C 0.047819 -0.399619 0.425799
H 0.217246 0.164787 1.349689
C -1.439218 -0.534455 0.231784
C -1.959431 -1.127779 -0.982730
C -2.325427 -0.055710 1.174618
C -3.363136 -1.370814 -1.062092
H -1.285143 -1.593447 -1.695618
C -3.738056 -0.149423 1.016427
H -1.923872 0.426012 2.066073
C -4.233740 -0.901998 -0.102484
H -3.757721 -1.923288 -1.912788
H -4.404541 0.183720 1.804668
H -5.300685 -1.083218 -0.206254
39
E_ket_anti_conf_11_a Eopt -698.094527
C 2.245225 -0.228570 -0.425536
C 0.857361 0.349915 -0.698306
C 1.972796 -1.635701 0.135679

H 2.887373 -0.249066 -1.312069
H 2.755589 0.365000 0.340760
H 0.410098 -0.132063 -1.573069
C 3.152148 -2.150245 0.957379
H 3.381042 -1.470996 1.784040
H 2.935840 -3.136014 1.381703
H 4.050711 -2.244333 0.338526
C 1.691929 -2.619500 -1.004943
H 1.437284 -3.606652 -0.606705
H 0.858622 -2.293865 -1.633099
H 2.572134 -2.731654 -1.646203
C 0.756608 1.834822 -0.940944
O -0.201722 2.289549 -1.540139
C 1.818657 2.771432 -0.398276
H 2.811740 2.400745 -0.667230
H 1.673222 3.736319 -0.887644
C 1.723933 2.943905 1.123566
H 2.421530 3.716600 1.453213
H 0.717501 3.250780 1.419978
H 1.968635 2.024143 1.657707
C 0.704800 -1.423746 1.000110
H 0.972060 -1.361497 2.059098
H 0.015692 -2.266196 0.892345
C 0.021974 -0.092081 0.561351
H 0.195853 0.650567 1.345284
C -1.461791 -0.186221 0.336894
C -1.991500 -1.095620 -0.660027
C -2.338291 0.591604 1.065859
C -3.405618 -1.260138 -0.734749
H -1.331811 -1.779703 -1.184768
C -3.750834 0.523455 0.896170
H -1.926215 1.289901 1.794666
C -4.267895 -0.483367 0.009464
H -3.816259 -2.009399 -1.409307
H -4.412283 1.114858 1.520021
H -5.341595 -0.623513 -0.088286
39
E_ket_anti_conf_15 Eopt -698.107022
C -2.306910 -0.140922 0.541508
C -0.800221 -0.407554 0.744518
C -2.462326 1.264928 -0.109522
H -2.730187 -0.907001 -0.116428
H -2.847584 -0.211517 1.490595
H -0.489827 0.038252 1.698924
C -3.244803 2.224840 0.785172

H -3.257597 3.235194 0.362006
H -4.283110 1.897950 0.903279
H -2.795532 2.284215 1.781504
C -3.162223 1.151648 -1.466512
H -4.158382 0.711030 -1.356003
H -3.278179 2.134878 -1.934341
H -2.593157 0.516296 -2.152933
C -0.367962 -1.866654 0.783590
O 0.632829 -2.192654 1.551118
C -0.501194 -2.624688 -0.529834
H -1.351376 -2.254750 -1.115300
H 0.399028 -2.430411 -1.147657
C -0.626436 -4.136185 -0.347343
H -0.617238 -4.669154 -1.303618
H 0.201089 -4.512818 0.258458
H -1.557783 -4.388430 0.171427
C -1.006258 1.749625 -0.301918
H -0.692550 2.332716 0.571256
H -0.895557 2.392845 -1.181986
C -0.164577 0.470644 -0.379282
H -0.365860 -0.019546 -1.339847
C 1.322373 0.676503 -0.265448
C 2.188962 0.180435 -1.244148
C 1.884050 1.357825 0.822701
C 3.569068 0.349503 -1.142965
H 1.774832 -0.348960 -2.097737
C 3.260387 1.529572 0.929291
H 1.238977 1.750747 1.602870
C 4.111684 1.024205 -0.053386
H 4.218721 -0.047352 -1.916309
H 3.672095 2.057240 1.783540
H 5.184866 1.157471 0.030816
39
E_ket_anti_conf_16 Eopt -698.107134
C -2.274840 0.042745 0.227540
C -0.803933 0.411177 0.510113
C -2.256484 -1.442110 -0.175234
H -2.934011 0.238426 1.080169
H -2.637477 0.643254 -0.617075
H -0.505800 -0.073784 1.447815
C -3.455962 -1.817813 -1.042581
H -3.494807 -1.201815 -1.946133
H -3.406887 -2.867052 -1.353281
H -4.395039 -1.675947 -0.497234
C -2.244546 -2.331322 1.072647

H -1.399074 -2.101403 1.727262
H -3.163851 -2.201961 1.653070
H -2.168440 -3.387543 0.794429
C -0.521388 1.896899 0.696929
O -0.631650 2.373591 1.904843
C -0.947635 2.813564 -0.441261
H -0.875368 2.304753 -1.409366
H -2.017773 3.073643 -0.313627
C -0.153708 4.118312 -0.495818
H 0.901041 3.921260 -0.716752
H -0.537893 4.802073 -1.259771
H -0.199234 4.629599 0.468790
C -0.914595 -1.582903 -0.947393
H -1.093948 -1.672028 -2.022945
H -0.390953 -2.493334 -0.642583
C -0.071993 -0.311243 -0.654448
H -0.128047 0.343252 -1.529367
C 1.387786 -0.565592 -0.371915
C 2.386062 0.138391 -1.051410
C 1.782223 -1.480892 0.611186
C 3.735920 -0.065517 -0.766180
H 2.099422 0.857074 -1.814269
C 3.127191 -1.685814 0.904674
H 1.025228 -2.036915 1.158115
C 4.111710 -0.978759 0.214597
H 4.491998 0.492670 -1.308614
H 3.408935 -2.398596 1.672830
H 5.160327 -1.139101 0.441128
39
E_ket_anti_conf_17 Eopt -698.106911
C 2.234316 -0.185160 -0.743969
C 0.768830 0.316649 -0.805762
C 2.270978 -1.488813 0.103136
H 2.613730 -0.361494 -1.755467
H 2.883545 0.575127 -0.299172
H 0.316523 -0.042318 -1.738790
C 2.931532 -1.222591 1.460001
H 2.417384 -0.429252 2.010827
H 2.926789 -2.123103 2.082975
H 3.972286 -0.909730 1.328387
C 3.016252 -2.619919 -0.601766
H 2.581836 -2.822395 -1.585493
H 4.071862 -2.367228 -0.746187
H 2.972043 -3.545201 -0.017024
C 0.572794 1.825490 -0.779357

O -0.458905 2.325128 -1.396647
C 1.006627 2.519113 0.504313
H 0.169788 2.480124 1.230911
H 1.839869 1.987037 0.978801
C 1.384588 3.985835 0.303131
H 0.572665 4.518350 -0.198038
H 1.588933 4.493732 1.251262
H 2.276416 4.073298 -0.326984
C 0.781058 -1.831673 0.298482
H 0.606656 -2.446522 1.188810
H 0.418757 -2.396084 -0.568851
C 0.069123 -0.475159 0.349352
H 0.320602 0.013987 1.297240
C -1.431774 -0.541640 0.252075
C -2.237540 0.049897 1.230066
C -2.067171 -1.188195 -0.816911
C -3.628179 0.007986 1.145715
H -1.766070 0.555023 2.068583
C -3.454709 -1.232081 -0.907174
H -1.470311 -1.655240 -1.594653
C -4.244007 -0.632350 0.074076
H -4.229193 0.477595 1.917658
H -3.923360 -1.734965 -1.746913
H -5.325830 -0.666102 0.002873
39
E_ket_anti_conf_4_a Eopt -698.098624
C 2.354887 0.495542 -0.122420
C 0.859217 0.717879 0.064172
C 2.553863 -1.017223 0.103450
H 2.622901 0.760107 -1.150730
H 2.970431 1.101681 0.549851
H 0.578051 0.628095 1.117467
C 2.707667 -1.308107 1.600036
H 1.851857 -0.938475 2.173246
H 2.782425 -2.385431 1.778311
H 3.610840 -0.836054 1.999922
C 3.783444 -1.535651 -0.638477
H 3.913901 -2.611289 -0.481803
H 3.694666 -1.360376 -1.714782
H 4.692499 -1.035009 -0.288706
C 0.318965 2.019890 -0.479890
O 0.840415 2.583424 -1.422647
C -0.909240 2.589936 0.191060
H -1.380620 3.300273 -0.491144
H -1.612481 1.778239 0.402084

C -0.521374 3.284065 1.503016
H 0.188510 4.095310 1.324007
H -1.406543 3.709024 1.979791
H -0.068102 2.582059 2.207225
C 1.234967 -1.642909 -0.430354
H 0.815933 -2.336162 0.304010
H 1.407540 -2.214621 -1.346652
C 0.237126 -0.487483 -0.712933
H 0.304106 -0.232363 -1.777195
C -1.204946 -0.772834 -0.380449
C -2.189814 -0.624053 -1.332964
C -1.574543 -1.123178 0.971754
C -3.575125 -0.821153 -1.034971
H -1.899558 -0.323291 -2.339281
C -2.929079 -1.518553 1.213289
H -0.805247 -1.333233 1.709520
C -3.901812 -1.369972 0.249895
H -4.320465 -0.764013 -1.821104
H -3.200983 -1.917323 2.188594
H -4.928207 -1.651714 0.473260
39
E_ket_anti_conf_5 Eopt -698.098701
C 2.310529 0.643464 -0.068561
C 0.797050 0.730731 0.124814
C 2.688114 -0.851595 0.151876
H 2.549039 0.947828 -1.091733
H 2.855585 1.308677 0.607332
H 0.538450 0.761769 1.188463
C 3.439889 -1.039159 1.469703
H 2.871946 -0.621264 2.307039
H 3.608221 -2.101237 1.676064
H 4.415236 -0.542574 1.442041
C 3.550390 -1.358828 -1.005201
H 3.850544 -2.399421 -0.846095
H 3.005312 -1.305144 -1.952984
H 4.459610 -0.757451 -1.108197
C 0.106650 1.870229 -0.590331
O 0.496115 2.277974 -1.667021
C -1.100192 2.471112 0.090221
H -1.708753 2.982303 -0.658324
H -1.689659 1.668284 0.544132
C -0.644800 3.455757 1.175290
H -1.509859 3.885853 1.683236
H -0.025923 2.961482 1.928346
H -0.065237 4.274421 0.742152

C 1.324665 -1.589685 0.187468
H 1.032241 -1.785692 1.224018
H 1.359488 -2.553264 -0.330444
C 0.304916 -0.631423 -0.446918
H 0.486088 -0.596171 -1.529294
C -1.151752 -0.943006 -0.213131
C -1.650340 -1.108030 1.128813
C -2.020540 -1.033326 -1.279055
C -3.071869 -1.174422 1.312107
H -0.994940 -0.963419 1.982176
C -3.422022 -1.292107 -1.102345
H -1.623308 -0.915179 -2.286591
C -3.928708 -1.262816 0.237844
H -3.479556 -1.171778 2.320946
H -4.094825 -1.292242 -1.953111
H -5.000495 -1.330956 0.411441
39
E_ket_anti_conf_7 Eopt -698.100564
C -2.327067 0.863418 0.263297
C -0.817497 0.737545 0.481107
C -2.855334 -0.579295 -0.002282
H -2.829272 1.332275 1.114057
H -2.502189 1.496945 -0.610789
H -0.587794 0.458045 1.514821
C -3.655108 -0.619509 -1.306129
H -3.027925 -0.345354 -2.160393
H -4.058023 -1.620587 -1.489819
H -4.495661 0.081222 -1.270925
C -3.733342 -1.068212 1.149251
H -3.205807 -0.987583 2.104922
H -4.654288 -0.480516 1.221355
H -4.013846 -2.117306 1.008562
C 0.003897 1.948718 0.096039
O -0.285299 2.633585 -0.864723
C 1.230479 2.222860 0.932546
H 0.869804 2.524169 1.924869
H 1.739774 1.264611 1.092993
C 2.163782 3.263923 0.339517
H 1.658852 4.223026 0.209589
H 3.027691 3.419659 0.988719
H 2.530009 2.944693 -0.639401
C -1.573072 -1.440545 -0.122286
H -1.667516 -2.223203 -0.881778
H -1.366105 -1.933905 0.832650
C -0.437777 -0.459469 -0.440847

H -0.566729 -0.103324 -1.471353
C 0.976020 -0.960672 -0.283199
C 1.389477 -1.609970 0.934937
C 1.908207 -0.706089 -1.266753
C 2.721045 -2.139857 0.995578
H 0.663018 -1.875108 1.695732
C 3.288646 -1.069579 -1.124342
H 1.584858 -0.187273 -2.168766
C 3.640238 -1.881920 0.004246
H 3.016449 -2.738665 1.854691
H 3.982908 -0.927789 -1.945708
H 4.648619 -2.280809 0.089681
39
E_ket_anti_conf_8_a Eopt -698.100672
C 2.305083 0.921179 -0.202043
C 0.805680 0.743202 -0.438284
C 2.884428 -0.513658 -0.022832
H 2.796070 1.462911 -1.015356
H 2.445553 1.503606 0.713168
H 0.600533 0.459569 -1.476229
C 3.760321 -0.581579 1.229197
H 4.576751 0.146060 1.174982
H 3.176201 -0.361718 2.128492
H 4.202200 -1.576045 1.347624
C 3.705560 -0.928813 -1.243733
H 4.606155 -0.313992 -1.341723
H 4.018617 -1.975235 -1.166650
H 3.121589 -0.821239 -2.163383
C -0.067414 1.918445 -0.061738
O 0.191116 2.625080 0.891898
C -1.305002 2.129847 -0.901890
H -0.956538 2.462752 -1.888696
H -1.758482 1.146492 -1.072485
C -2.297112 3.111883 -0.302651
H -1.847193 4.096636 -0.162843
H -3.167092 3.224409 -0.952626
H -2.646538 2.763738 0.672649
C 1.632352 -1.417447 0.129211
H 1.769831 -2.194021 0.888126
H 1.417996 -1.921165 -0.818622
C 0.469386 -0.475283 0.472029
H 0.595548 -0.128115 1.506018
C -0.927191 -1.022524 0.317381
C -1.326436 -1.647286 -0.916151
C -1.846219 -0.864498 1.332564

C -2.724860 -1.911130 -1.112680
H -0.637914 -1.702506 -1.753585
C -3.208343 -1.305510 1.203367
H -1.523027 -0.394630 2.260779
C -3.633151 -1.745816 -0.091095
H -3.070146 -2.262109 -2.082918
H -3.928509 -1.111285 1.990844
H -4.683035 -1.970816 -0.266665
39
E_ket_syn_conf_10_a Eopt -698.104224
C 2.309931 0.608855 -0.884211
C 0.760345 0.618529 -0.942174
C 2.765470 -0.553076 0.048412
H 2.731786 0.470923 -1.885681
H 2.668358 1.569925 -0.507868
H 0.405627 0.746524 -1.971353
C 3.678534 -0.058202 1.168323
H 3.928818 -0.870052 1.860399
H 4.617826 0.338966 0.768317
H 3.185512 0.736135 1.734906
C 3.497672 -1.634475 -0.753643
H 4.398395 -1.226959 -1.224456
H 3.803532 -2.464201 -0.107533
H 2.867099 -2.043568 -1.549176
C 0.155695 1.719983 -0.080846
O 0.567850 1.854803 1.144516
C -1.267676 2.150641 -0.397377
H -1.494949 1.974661 -1.456162
H -1.990566 1.535496 0.176503
C -1.539347 3.615222 -0.047692
H -0.925285 4.283551 -0.661246
H -2.589856 3.885285 -0.198403
H -1.288179 3.803657 0.999186
C 1.443209 -1.108871 0.615349
H 1.169834 -0.526475 1.497808
H 1.523119 -2.165135 0.898643
C 0.420025 -0.853305 -0.487267
H 0.660869 -1.504033 -1.339185
C -1.032840 -1.078417 -0.159688
C -1.514874 -1.179678 1.147769
C -1.961087 -1.144147 -1.207248
C -2.879965 -1.314524 1.402086
H -0.824841 -1.143265 1.983534
C -3.323529 -1.272031 -0.960789
H -1.604814 -1.079218 -2.232274

C -3.791503 -1.351893 0.351089
H -3.230070 -1.386597 2.426807
H -4.021960 -1.310514 -1.790533
H -4.853409 -1.451180 0.549089
39
E_ket_syn_conf_11 Eopt -698.103520
C 1.673472 0.567460 0.732683
C 0.852999 1.037920 -0.482980
C 2.608212 -0.529447 0.187682
H 2.226686 1.386260 1.206237
H 1.002830 0.144642 1.491064
H 1.550249 1.535123 -1.167152
C 3.001191 -1.542364 1.262582
H 3.551850 -1.053652 2.073322
H 2.124748 -2.026569 1.702253
H 3.644855 -2.326442 0.849547
C 3.888966 0.098488 -0.374479
H 3.670150 0.851972 -1.136287
H 4.468767 0.580012 0.419587
H 4.523261 -0.664510 -0.837385
C -0.225881 2.082986 -0.218397
O 0.088594 3.324693 -0.470658
C -1.134141 1.847450 0.980994
H -1.327533 0.780660 1.128526
H -0.612577 2.190707 1.897653
C -2.463412 2.595179 0.889872
H -2.291068 3.662548 0.733286
H -3.058030 2.228613 0.045569
H -3.062368 2.478243 1.798957
C 1.777503 -1.177403 -0.965124
H 1.530142 -2.217621 -0.736636
H 2.370022 -1.196078 -1.884244
C 0.502642 -0.323078 -1.184992
H 0.352550 -0.124137 -2.249703
C -0.772435 -0.955971 -0.674983
C -0.814264 -1.778877 0.455443
C -1.985578 -0.666630 -1.313614
C -2.022511 -2.264703 0.952538
H 0.104098 -2.038556 0.970056
C -3.196809 -1.149022 -0.823352
H -1.976996 -0.047679 -2.205881
C -3.221742 -1.945497 0.319575
H -2.025117 -2.893940 1.836677
H -4.121453 -0.903973 -1.336078
H -4.163099 -2.322111 0.705223

39
E_ket_syn_conf_11_a Eopt -698.095272
C -2.379364 0.502187 -0.918668
C -0.859983 0.512275 -1.112221
C -2.702664 -0.491511 0.218649
H -2.783899 1.498060 -0.719084
H -2.838261 0.137005 -1.844126
H -0.609634 0.680307 -2.165789
C -4.072125 -1.135957 0.000793
H -4.296021 -1.860873 0.790097
H -4.866211 -0.381445 0.006943
H -4.113318 -1.660075 -0.958835
C -2.696971 0.194910 1.588060
H -3.453051 0.985805 1.634183
H -2.920911 -0.533165 2.374913
H -1.729913 0.650219 1.804621
C -0.135599 1.624343 -0.366013
O -0.686875 2.328200 0.470696
C 1.243475 1.976436 -0.889681
H 1.785589 1.055721 -1.124800
H 1.085137 2.480288 -1.854927
C 2.038142 2.875508 0.044206
H 3.027003 3.087387 -0.369372
H 1.527624 3.826769 0.205919
H 2.173216 2.401228 1.019793
C -1.556162 -1.529429 0.141683
H -1.919143 -2.478765 -0.263356
H -1.165754 -1.742729 1.140749
C -0.432449 -0.977744 -0.779606
H -0.486100 -1.515412 -1.730811
C 0.956689 -1.135040 -0.233989
C 1.271102 -0.557347 1.046912
C 1.959327 -1.719917 -0.980529
C 2.635118 -0.530391 1.458057
H 0.489839 -0.146107 1.677061
C 3.309288 -1.772000 -0.532246
H 1.706172 -2.134017 -1.956046
C 3.628888 -1.108492 0.694153
H 2.900839 -0.044895 2.395119
H 4.081918 -2.224644 -1.143803
H 4.659608 -1.073254 1.038622
39
E_ket_syn_conf_12 Eopt -698.103645
C 1.707616 0.704653 0.677964
C 0.819316 1.036332 -0.524962

C 2.670769 -0.394753 0.189289
H 2.243272 1.582877 1.055412
H 1.102762 0.316270 1.504205
H 1.455058 1.524646 -1.275504
C 3.161935 -1.273881 1.338155
H 3.825260 -2.065866 0.974374
H 3.720973 -0.682876 2.071411
H 2.326558 -1.750264 1.860012
C 3.886672 0.231567 -0.503089
H 4.471851 0.831337 0.201503
H 4.543473 -0.544804 -0.908687
H 3.591222 0.879585 -1.333063
C -0.362825 1.969556 -0.327996
O -0.915780 2.449958 -1.406084
C -1.251167 1.818550 0.895016
H -2.092318 1.133730 0.666145
H -0.706987 1.362182 1.728777
C -1.855573 3.147209 1.356911
H -2.568020 3.009641 2.177297
H -1.073224 3.833740 1.698793
H -2.381410 3.630517 0.529718
C 1.820446 -1.198327 -0.839925
H 1.580183 -2.192096 -0.451028
H 2.392829 -1.356951 -1.758555
C 0.530731 -0.392405 -1.140095
H 0.386296 -0.278236 -2.216794
C -0.733171 -1.008045 -0.588266
C -0.786325 -1.627787 0.665515
C -1.922379 -0.915951 -1.320151
C -1.988910 -2.105714 1.182761
H 0.118785 -1.737049 1.254236
C -3.125527 -1.400785 -0.814781
H -1.902742 -0.444243 -2.297821
C -3.166388 -1.990205 0.447346
H -2.004257 -2.572407 2.162447
H -4.032422 -1.314893 -1.404675
H -4.102224 -2.364582 0.848322
39
E_ket_syn_conf_15 Eopt -698.100738
C -2.128381 0.957082 0.322493
C -0.862708 0.854418 -0.537896
C -2.889526 -0.359952 0.119714
H -1.833400 1.046961 1.373207
H -2.734371 1.836380 0.080632
H -1.085777 1.215258 -1.553145

C -3.611958 -0.374834 -1.231075
H -4.097852 -1.341145 -1.400499
H -4.385765 0.398885 -1.265423
H -2.927599 -0.196631 -2.065315
C -3.893453 -0.627240 1.236112
H -3.402899 -0.624533 2.214313
H -4.677886 0.136891 1.251116
H -4.380885 -1.599227 1.106111
C 0.283794 1.713231 -0.023047
O 0.115219 2.527020 0.919700
C 1.441212 1.882131 -0.986473
H 1.685451 0.913735 -1.438070
H 1.097832 2.516423 -1.823823
C 2.672984 2.511806 -0.349947
H 3.487215 2.609994 -1.073052
H 2.445092 3.505263 0.041216
H 3.032676 1.902953 0.483977
C -1.729367 -1.365084 0.124061
H -2.012070 -2.342154 -0.281290
H -1.399739 -1.518303 1.158242
C -0.585643 -0.709093 -0.684809
H -0.691172 -0.991192 -1.736427
C 0.783827 -1.096810 -0.217574
C 1.227719 -0.560827 1.023577
C 1.665486 -1.812309 -1.008773
C 2.557450 -0.826995 1.446893
H 0.516550 -0.122198 1.715274
C 2.994072 -2.064670 -0.596342
H 1.329328 -2.165505 -1.981858
C 3.424592 -1.550496 0.642632
H 2.903936 -0.448066 2.404792
H 3.666196 -2.641493 -1.222277
H 4.442799 -1.730617 0.977421
39
E_ket_syn_conf_16 Eopt -698.093950
C 1.971700 0.448969 0.805310
C 0.865237 0.966877 -0.111503
C 2.728830 -0.586010 -0.046624
H 2.627972 1.239230 1.184558
H 1.519415 -0.046092 1.671076
H 1.271156 1.750704 -0.767813
C 3.561963 -1.535706 0.808562
H 2.939925 -2.037572 1.556281
H 4.037713 -2.307194 0.193942
H 4.355530 -0.997112 1.337372

C 3.638243 0.112043 -1.063532
H 4.384331 0.735679 -0.560272
H 4.172361 -0.625144 -1.671443
H 3.071148 0.752120 -1.745557
C -0.389036 1.502080 0.573250
O -0.516680 1.523079 1.813183
C -1.347594 2.275849 -0.303125
H -1.209920 1.997860 -1.352657
H -2.377003 2.007774 -0.031840
C -1.150905 3.788240 -0.137439
H -1.306723 4.084667 0.902482
H -0.138078 4.088026 -0.423825
H -1.853449 4.351510 -0.758414
C 1.576213 -1.311807 -0.773553
H 1.227312 -2.144962 -0.156246
H 1.904213 -1.736782 -1.727329
C 0.431931 -0.270870 -0.946333
H 0.330012 0.007990 -1.999356
C -0.937383 -0.725144 -0.452987
C -1.103239 -1.436144 0.774745
C -2.062960 -0.719355 -1.333272
C -2.322691 -1.966490 1.147014
H -0.262671 -1.525932 1.458226
C -3.283769 -1.256660 -0.959766
H -1.962777 -0.255733 -2.312486
C -3.453056 -1.876685 0.295580
H -2.411474 -2.468240 2.107449
H -4.119868 -1.207017 -1.653334
H -4.406575 -2.303524 0.585761
39
E_ket_syn_conf_2 Eopt -698.103810
C -2.326667 0.071729 -1.056845
C -0.820728 0.371559 -1.034678
C -2.649086 -0.761205 0.218609
H -2.908173 0.994250 -1.093326
H -2.565858 -0.520786 -1.946979
H -0.431988 0.436342 -2.068855
C -3.489211 -1.988758 -0.139856
H -4.420790 -1.693880 -0.634766
H -2.946283 -2.652448 -0.821029
H -3.751527 -2.564808 0.753866
C -3.394129 0.082217 1.254028
H -3.508055 -0.463592 2.197337
H -2.847983 1.009529 1.445589
H -4.395943 0.347193 0.898016

C -0.477953 1.673859 -0.293873
O -1.414859 2.554880 -0.101608
C 0.906464 2.222516 -0.617052
H 1.618017 1.412271 -0.804922
H 0.837103 2.792095 -1.567140
C 1.465850 3.152757 0.457184
H 1.652345 2.602789 1.386546
H 2.406346 3.620756 0.148528
H 0.749481 3.946452 0.682167
C -1.259580 -1.186956 0.761303
H -1.249447 -2.224856 1.111132
H -0.991264 -0.551815 1.609444
C -0.286950 -0.955207 -0.398015
H -0.476565 -1.735758 -1.147554
C 1.187510 -1.010010 -0.086018
C 1.720321 -0.685278 1.166082
C 2.081802 -1.349722 -1.108855
C 3.099253 -0.672398 1.377223
H 1.061286 -0.428359 1.987716
C 3.458190 -1.335674 -0.905637
H 1.686891 -1.614912 -2.086235
C 3.974670 -0.990232 0.342740
H 3.488582 -0.411083 2.355993
H 4.127556 -1.595841 -1.719114
H 5.046620 -0.977768 0.508412
39
E_ket_syn_conf_20 Eopt -698.100621
C 1.701284 0.586983 0.752079
C 0.891432 1.120878 -0.432594
C 2.618397 -0.503201 0.162650
H 2.271634 1.369115 1.265121
H 1.026631 0.139258 1.492461
H 1.606517 1.595289 -1.126750
C 2.993496 -1.558703 1.202544
H 3.546611 -1.106139 2.032507
H 2.109323 -2.047235 1.621222
H 3.629359 -2.335368 0.764519
C 3.912716 0.121039 -0.373453
H 4.534501 -0.636928 -0.860967
H 3.710770 0.904837 -1.108689
H 4.498934 0.562859 0.438892
C -0.203839 2.119657 -0.176163
O -0.789271 2.667143 -1.210135
C -0.749701 2.399715 1.205076
H -0.046390 2.078093 1.982244

H -0.857745 3.491816 1.323041
C -2.131322 1.787220 1.514198
H -2.844070 2.046285 0.725636
H -2.079398 0.695064 1.571199
H -2.534767 2.155009 2.465499
C 1.777798 -1.095579 -1.011952
H 1.518376 -2.140899 -0.822000
H 2.370052 -1.088802 -1.931590
C 0.514418 -0.219104 -1.194147
H 0.357321 0.023686 -2.247456
C -0.768860 -0.830136 -0.686195
C -0.822160 -1.709405 0.400573
C -1.981373 -0.465908 -1.286809
C -2.037949 -2.205316 0.871857
H 0.093620 -2.020747 0.890839
C -3.197098 -0.960948 -0.825768
H -1.961426 0.233219 -2.116892
C -3.232104 -1.834765 0.260377
H -2.048128 -2.885045 1.717935
H -4.120248 -0.662798 -1.312722
H -4.178105 -2.222268 0.623403
39
E_ket_syn_conf_21 Eopt -698.103243
C -1.694147 0.424992 0.636796
C -0.808223 0.856350 -0.535411
C -2.493360 -0.788539 0.117214
H -1.065862 0.132613 1.488494
H -2.359723 1.221056 0.985226
H -1.483688 1.276767 -1.308330
C -3.777542 -0.315958 -0.575876
H -4.446414 0.178881 0.135738
H -3.563507 0.388831 -1.384216
H -4.317464 -1.163778 -1.010011
C -2.881126 -1.744604 1.244908
H -2.002373 -2.123249 1.774379
H -3.519500 -1.241000 1.978577
H -3.435553 -2.606205 0.858193
C 0.272858 1.894609 -0.289792
O 0.997418 2.220667 -1.315102
C -0.084386 2.998897 0.695684
H -0.810483 3.692458 0.218339
H -0.592865 2.589764 1.574438
C 1.125294 3.815113 1.143216
H 1.646201 4.233767 0.279714
H 0.840487 4.640124 1.803531

H 1.837856 3.180555 1.682188
C -1.537464 -1.448974 -0.922604
H -2.063536 -1.599462 -1.869660
H -1.215026 -2.439000 -0.588257
C -0.324768 -0.504591 -1.134319
H -0.123051 -0.368731 -2.198673
C 0.961420 -1.001477 -0.505930
C 0.995522 -1.673540 0.720641
C 2.180646 -0.766745 -1.151518
C 2.201507 -2.076828 1.292374
H 0.071056 -1.892350 1.243733
C 3.388751 -1.168446 -0.588610
H 2.176234 -0.237105 -2.097903
C 3.406015 -1.822198 0.642261
H 2.197101 -2.591501 2.247784
H 4.319171 -0.970224 -1.111200
H 4.345615 -2.135914 1.084519
39
E_ket_syn_conf_22 Eopt -698.102105
C -1.720007 0.564461 0.855164
C -0.693083 1.129398 -0.124745
C -2.679103 -0.293603 0.010635
H -1.197288 -0.051533 1.594166
H -2.246967 1.353467 1.403850
H -1.209161 1.835625 -0.788547
C -3.793414 0.580997 -0.576679
H -4.437172 -0.004611 -1.241158
H -4.421838 0.998697 0.216573
H -3.388482 1.413651 -1.159068
C -3.322536 -1.413259 0.827767
H -3.986655 -2.024782 0.207458
H -2.569845 -2.075686 1.264661
H -3.920122 -1.002049 1.648347
C 0.475180 1.860734 0.512633
O 1.045610 1.369578 1.570872
C 1.331921 2.676797 -0.442904
H 2.114333 2.031758 -0.890345
H 0.724130 3.042424 -1.280323
C 2.041007 3.851721 0.231024
H 2.625440 3.498353 1.083990
H 2.719616 4.371132 -0.453481
H 1.314609 4.580733 0.606579
C -1.771778 -0.843054 -1.132964
H -2.239238 -0.655245 -2.104026
H -1.653601 -1.927521 -1.052323

C -0.400157 -0.122562 -1.055980
H -0.108309 0.249998 -2.041970
C 0.730212 -0.999526 -0.570424
C 0.567066 -1.963936 0.431732
C 2.005722 -0.856362 -1.129238
C 1.643007 -2.722242 0.885753
H -0.410519 -2.123909 0.873469
C 3.086102 -1.613423 -0.683311
H 2.153803 -0.135045 -1.927820
C 2.911571 -2.546489 0.336116
H 1.489448 -3.454842 1.671653
H 4.063329 -1.476842 -1.135273
H 3.749345 -3.138288 0.689143
39
E_ket_syn_conf_4 Eopt -698.104692
C 2.273355 0.976615 -0.066473
C 0.840638 0.852911 -0.640379
C 2.866586 -0.437241 0.057142
H 2.907115 1.636669 -0.669152
H 2.183833 1.414590 0.932296
H 0.835343 1.094375 -1.709127
C 3.925613 -0.532869 1.151271
H 4.778829 0.117762 0.932042
H 3.516253 -0.234331 2.121214
H 4.305684 -1.555928 1.246269
C 3.476805 -0.888229 -1.274249
H 3.766656 -1.943775 -1.238829
H 2.785455 -0.757777 -2.111248
H 4.374267 -0.303126 -1.499208
C -0.125094 1.803381 0.060762
O -0.125164 1.861557 1.359512
C -1.428285 2.104670 -0.660460
H -1.296775 1.997339 -1.744674
H -2.199705 1.363690 -0.369717
C -1.986942 3.493887 -0.345751
H -1.311511 4.277255 -0.706679
H -2.968924 3.655285 -0.802716
H -2.092220 3.620703 0.734667
C 1.612542 -1.257426 0.398532
H 1.341816 -1.064367 1.442459
H 1.766534 -2.337075 0.287112
C 0.528463 -0.710855 -0.537855
H 0.711810 -1.130481 -1.531729
C -0.890844 -1.076191 -0.183531
C -1.394328 -0.943890 1.116165

C -1.762588 -1.528079 -1.179728
C -2.722599 -1.243829 1.403287
H -0.752328 -0.557036 1.898139
C -3.096099 -1.823279 -0.900347
H -1.392162 -1.641217 -2.195200
C -3.583074 -1.680258 0.395766
H -3.092636 -1.126784 2.417013
H -3.751344 -2.165850 -1.694722
H -4.619569 -1.908296 0.620793
39
E_ket_syn_conf_6 Eopt -698.102288
C -2.257574 0.184742 -0.761860
C -0.762996 0.620754 -0.703264
C -2.397719 -1.159536 0.013991
H -2.905099 0.957455 -0.335546
H -2.569221 0.042939 -1.802838
H -0.466391 1.062719 -1.660476
C -2.956784 -2.247666 -0.908341
H -3.068807 -3.197966 -0.375652
H -3.939885 -1.963477 -1.298440
H -2.297087 -2.418713 -1.765521
C -3.304132 -1.016671 1.235774
H -2.933729 -0.212948 1.877243
H -4.333278 -0.782922 0.941138
H -3.327671 -1.944792 1.818045
C -0.514454 1.639183 0.402307
O -0.860373 1.324383 1.617757
C -0.701301 3.091768 -0.023145
H -1.731710 3.252375 -0.403557
H -0.627899 3.698882 0.885446
C 0.281223 3.630184 -1.065564
H 0.080348 4.680603 -1.301423
H 1.311030 3.558990 -0.700774
H 0.228850 3.072417 -2.004532
C -0.953044 -1.510963 0.438767
H -0.773786 -2.592147 0.429526
H -0.763743 -1.130791 1.443963
C -0.055936 -0.762239 -0.555150
H -0.154776 -1.262984 -1.527458
C 1.411119 -0.746793 -0.213575
C 1.869873 -0.270695 1.024576
C 2.357778 -1.203602 -1.134240
C 3.228893 -0.273496 1.328337
H 1.143879 0.105492 1.738334
C 3.721704 -1.197868 -0.837509

H 2.022873 -1.570696 -2.100706
C 4.161485 -0.735577 0.399021
H 3.565020 0.094357 2.292744
H 4.435485 -1.559606 -1.570531
H 5.219773 -0.733404 0.638208
39
E_ket_syn_conf_6_a Eopt -698.100094
C 2.091359 0.736791 0.504817
C 0.784932 0.835053 -0.294875
C 2.793462 -0.542612 0.029111
H 2.720648 1.626645 0.398060
H 1.844891 0.642743 1.567485
H 0.972001 1.387091 -1.227397
C 3.825378 -1.047085 1.032319
H 4.271205 -1.990873 0.700831
H 4.637960 -0.323832 1.158901
H 3.369939 -1.215991 2.012933
C 3.466453 -0.325297 -1.329803
H 4.274411 0.408964 -1.248152
H 3.899805 -1.258751 -1.703272
H 2.762616 0.039645 -2.083113
C -0.318766 1.573841 0.454783
O -0.088395 2.164619 1.548502
C -1.527960 1.978239 -0.359141
H -1.733871 1.231536 -1.133737
H -2.402372 2.013980 0.304678
C -1.341106 3.354409 -1.012837
H -0.495294 3.352391 -1.707245
H -2.230563 3.656735 -1.574320
H -1.148418 4.116588 -0.253364
C 1.596861 -1.495099 -0.104912
H 1.294881 -1.825016 0.895994
H 1.829886 -2.389641 -0.691920
C 0.458047 -0.664383 -0.736717
H 0.528381 -0.739765 -1.825719
C -0.917375 -1.077920 -0.312171
C -1.861773 -1.555028 -1.203841
C -1.300915 -0.771660 1.021074
C -3.201383 -1.775673 -0.810455
H -1.569012 -1.731359 -2.236990
C -2.646754 -0.977037 1.413818
H -0.549379 -0.533249 1.765632
C -3.580553 -1.456893 0.502401
H -3.926279 -2.163325 -1.518044
H -2.952745 -0.758128 2.433045

H -4.610958 -1.601224 0.816276
39
E_ket_syn_conf_7 Eopt -698.103548
C 2.235845 -0.175388 -0.897951
C 0.767065 0.341235 -0.953910
C 2.310326 -1.297093 0.181410
H 2.528685 -0.581589 -1.872653
H 2.927482 0.642030 -0.669650
H 0.487810 0.570559 -1.988807
C 3.217360 -0.902344 1.346154
H 3.195050 -1.662097 2.135620
H 4.257407 -0.792632 1.019311
H 2.881630 0.048137 1.768488
C 2.821745 -2.599629 -0.442093
H 2.157384 -2.943966 -1.241668
H 3.818204 -2.462162 -0.875201
H 2.887928 -3.396365 0.306363
C 0.576717 1.599671 -0.118690
O 0.884593 1.564495 1.142158
C 0.847161 2.898090 -0.865973
H 1.944434 3.058810 -0.940307
H 0.479992 2.835317 -1.896854
C 0.245551 4.120996 -0.176949
H -0.848187 4.056724 -0.161205
H 0.587147 4.175125 0.859083
H 0.522678 5.054026 -0.677735
C 0.848875 -1.471233 0.657471
H 0.675796 -0.861576 1.546008
H 0.616719 -2.515510 0.895441
C -0.009399 -0.931957 -0.494204
H 0.066074 -1.649407 -1.322152
C -1.474662 -0.770010 -0.183423
C -1.912515 0.008788 0.898966
C -2.440378 -1.396310 -0.975951
C -3.270593 0.136716 1.180180
H -1.171290 0.515403 1.508800
C -3.802507 -1.262871 -0.702765
H -2.121890 -1.999883 -1.821663
C -4.222092 -0.497446 0.381035
H -3.590177 0.740542 2.023757
H -4.531294 -1.761174 -1.333823
H -5.279302 -0.393566 0.601746
39
E_ket_syn_conf_7_a Eopt -698.098714
C 2.135344 0.547020 0.711158

C 0.886530 0.933070 -0.084909
C 2.736273 -0.644324 -0.048101
H 2.838284 1.377827 0.826180
H 1.840353 0.224657 1.715709
H 1.183933 1.592933 -0.909512
C 3.712686 -1.441280 0.810163
H 3.237233 -1.776882 1.736762
H 4.074045 -2.326553 0.276775
H 4.585362 -0.836598 1.078480
C 3.439205 -0.183073 -1.328687
H 4.277999 0.480778 -1.096031
H 3.834935 -1.041854 -1.879897
H 2.763516 0.355363 -1.999421
C -0.107275 1.761093 0.708171
O 0.145135 2.137512 1.841487
C -1.374130 2.230712 0.016154
H -2.111818 1.424627 0.101643
H -1.754032 3.079006 0.590359
C -1.203600 2.604270 -1.455837
H -0.461131 3.396520 -1.585401
H -0.893053 1.746740 -2.057017
H -2.151039 2.965729 -1.862157
C 1.468143 -1.441305 -0.384080
H 1.153019 -1.994790 0.506713
H 1.625803 -2.168864 -1.186667
C 0.371148 -0.409530 -0.756352
H 0.374096 -0.267004 -1.840646
C -1.009794 -0.849680 -0.346476
C -1.306530 -1.001350 1.051738
C -2.000005 -1.050360 -1.282237
C -2.675446 -1.172544 1.433915
H -0.540013 -0.817072 1.797905
C -3.336028 -1.414764 -0.905570
H -1.758907 -0.916529 -2.336209
C -3.658809 -1.369156 0.486200
H -2.943928 -1.162196 2.488175
H -4.113480 -1.515062 -1.655184
H -4.688529 -1.513670 0.806057
39
E_ket_syn_conf_8 Eopt -698.102512
C 2.333735 0.617953 -0.795212
C 0.790531 0.787490 -0.775620
C 2.706331 -0.663885 0.008140
H 2.690398 0.523969 -1.826990
H 2.811755 1.500257 -0.363315

H 0.428380 1.075478 -1.767169
C 3.643767 -0.351181 1.172862
H 3.198147 0.413546 1.814067
H 3.831838 -1.245165 1.778131
H 4.611483 0.018035 0.815791
C 3.367078 -1.699905 -0.907312
H 2.704843 -1.987444 -1.730274
H 4.286910 -1.301089 -1.347852
H 3.627377 -2.607590 -0.352485
C 0.350239 1.829834 0.239978
O 0.832890 1.775142 1.450016
C -0.981842 2.549713 0.068165
H -1.749409 2.087764 0.715843
H -0.865768 3.568258 0.465514
C -1.547655 2.635582 -1.349138
H -0.825257 3.080761 -2.041803
H -1.812816 1.648150 -1.739348
H -2.451996 3.250647 -1.375252
C 1.349027 -1.190412 0.517082
H 1.126525 -0.734162 1.484169
H 1.343978 -2.280570 0.633851
C 0.328968 -0.698559 -0.512636
H 0.495898 -1.250058 -1.447676
C -1.116225 -0.883144 -0.136813
C -2.024831 -1.431629 -1.048123
C -1.598157 -0.494648 1.119558
C -3.372189 -1.585404 -0.724505
H -1.670840 -1.740164 -2.028199
C -2.941625 -0.648818 1.449132
H -0.914363 -0.032601 1.825327
C -3.836321 -1.194475 0.528607
H -4.056752 -2.012263 -1.450340
H -3.295085 -0.334804 2.426262
H -4.883351 -1.313160 0.786637
39
E_ket_syn_conf_8_a Eopt -698.098390
C 1.615762 0.679346 0.805986
C 0.801959 1.128629 -0.409498
C 2.684199 -0.266425 0.219961
H 2.059726 1.514270 1.357655
H 0.974228 0.125578 1.498767
H 1.421554 1.777087 -1.036924
C 3.130601 -1.308215 1.244401
H 3.576336 -0.825564 2.120585
H 2.288512 -1.914475 1.589259

H 3.880643 -1.982817 0.818852
C 3.909828 0.536789 -0.229764
H 3.640321 1.321158 -0.943115
H 4.401495 1.012086 0.625003
H 4.640593 -0.115977 -0.717751
C -0.463450 1.914290 -0.138090
O -0.792783 2.824454 -0.886991
C -1.234263 1.617195 1.129228
H -1.297266 0.531243 1.256991
H -0.618589 1.974847 1.966906
C -2.609966 2.262403 1.165905
H -2.539990 3.350107 1.105206
H -3.221601 1.922682 0.326157
H -3.131506 2.006178 2.090917
C 1.976618 -0.906884 -1.013955
H 1.864915 -1.986457 -0.893825
H 2.589736 -0.756771 -1.907267
C 0.607222 -0.215078 -1.207193
H 0.456521 0.048907 -2.260697
C -0.614563 -0.979310 -0.756918
C -0.586910 -2.028121 0.137349
C -1.888128 -0.479939 -1.213429
C -1.781149 -2.630715 0.637803
H 0.368962 -2.405455 0.491711
C -3.077190 -0.987830 -0.613020
H -1.928044 0.335012 -1.928763
C -3.030918 -2.025505 0.294851
H -1.729808 -3.439936 1.357988
H -4.039065 -0.552377 -0.877075
H -3.953330 -2.398732 0.733649
39
E_ket_syn_conf_9_a Eopt -698.102292
C -2.255938 0.178718 -0.762011
C -0.762775 0.619800 -0.701689
C -2.392574 -1.166138 0.013537
H -2.907101 0.949174 -0.337071
H -2.565078 0.035547 -1.803572
H -0.466951 1.063491 -1.658308
C -2.950034 -2.255157 -0.908630
H -3.060146 -3.205690 -0.375931
H -3.933762 -1.972793 -1.298447
H -2.290192 -2.425022 -1.765954
C -3.298252 -1.025555 1.236215
H -2.929246 -0.220638 1.876941
H -4.328403 -0.794979 0.942611

H -3.318358 -1.953696 1.818597
C -0.517747 1.637182 0.405335
O -0.861425 1.318038 1.620276
C -0.713429 3.090000 -0.014916
H -1.749882 3.248258 -0.379805
H -0.629092 3.695802 0.893514
C 0.251560 3.634012 -1.070655
H 0.048018 4.686368 -1.295111
H 1.287612 3.559172 -0.724678
H 0.181612 3.083840 -2.012857
C -0.946762 -1.514497 0.437202
H -0.764538 -2.595192 0.425694
H -0.758175 -1.136089 1.443191
C -0.052065 -0.761655 -0.555614
H -0.149933 -1.260947 -1.528754
C 1.415034 -0.743107 -0.214486
C 1.872569 -0.268137 1.024509
C 2.362874 -1.195043 -1.136337
C 3.231670 -0.267138 1.327843
H 1.145503 0.104443 1.738961
C 3.726719 -1.185698 -0.839881
H 2.028735 -1.561137 -2.103439
C 4.165539 -0.724441 0.397402
H 3.567000 0.099800 2.292871
H 4.441565 -1.543533 -1.573820
H 5.223888 -0.719348 0.636214
18
E_sty Eopt -310.807677
C 1.923279 -0.976412 -0.000015
C 0.570358 -1.293559 -0.000003
C -0.410694 -0.293276 0.000014
C 0.008044 1.037984 0.000018
C 1.366336 1.362059 0.000011
C 2.328409 0.358893 -0.000012
H 2.663606 -1.769637 -0.000030
H 0.261936 -2.335649 -0.000009
H -0.722525 1.839516 0.000030
H 1.667843 2.404315 0.000014
H 3.383371 0.610669 -0.000024
C -1.870837 -0.697230 0.000033
H -2.049133 -1.335580 -0.871861
C -2.872347 0.450690 -0.000037
H -2.759758 1.083909 -0.883758
H -3.891650 0.059092 -0.000068
H -2.759833 1.083957 0.883658

H -2.049140 -1.335479 0.871999
39
F_ket_anti_conf_1 Eopt -698.064686
C -2.089650 -0.455237 -1.035168
C -0.807199 0.349651 -0.754792
C -2.258233 -1.432308 0.144152
H -2.960367 0.191517 -1.162194
H -1.959386 -1.027289 -1.958634
H -0.165910 0.368043 -1.641000
C -3.048257 -2.676889 -0.245765
H -4.065730 -2.414519 -0.552827
H -2.569567 -3.202416 -1.077376
H -3.124238 -3.373071 0.595549
C -2.946186 -0.740126 1.325010
H -2.440625 0.183916 1.616765
H -3.977484 -0.480068 1.067811
H -2.972550 -1.399925 2.198025
C -1.030564 1.806075 -0.378969
O -2.136480 2.289159 -0.266266
C 0.221448 2.629606 -0.153528
H 0.754533 2.192957 0.698832
H 0.880881 2.473175 -1.014378
C -0.050582 4.106741 0.079928
H -0.672847 4.258548 0.963739
H 0.886336 4.647207 0.228120
H -0.568271 4.552452 -0.771970
C -0.795903 -1.757729 0.478690
H -0.397901 -2.439010 -0.282256
H -0.671810 -2.234875 1.455606
C -0.054411 -0.410760 0.395499
H -0.214811 0.125106 1.335939
C 1.437604 -0.552530 0.204010
C 2.324879 -0.165237 1.210297
C 1.964728 -1.099968 -0.971264
C 3.701997 -0.315039 1.050822
H 1.932262 0.261232 2.129081
C 3.337589 -1.250817 -1.136006
H 1.293879 -1.412154 -1.767161
C 4.213118 -0.857144 -0.124212
H 4.373059 -0.005245 1.844950
H 3.726343 -1.675828 -2.055368
H 5.283770 -0.972771 -0.253352
39
F_ket_anti_conf_11 Eopt -698.059584
C -2.256858 0.037728 -0.428798

C -0.808078 -0.371876 -0.689470
C -2.151203 1.472492 0.122884
H -2.886794 -0.022180 -1.321210
H -2.697560 -0.609416 0.336760
H -0.416719 0.168624 -1.556113
C -3.372747 1.841621 0.960475
H -3.501500 1.145407 1.794439
H -3.274476 2.850124 1.374369
H -4.284253 1.816991 0.354592
C -2.007404 2.475359 -1.026619
H -1.880419 3.489746 -0.636305
H -1.141250 2.255147 -1.657049
H -2.897883 2.467611 -1.662868
C -0.517904 -1.837742 -0.948724
O 0.479392 -2.149919 -1.569700
C -1.451255 -2.904616 -0.415944
H -2.478694 -2.661207 -0.701935
H -1.175871 -3.841144 -0.904035
C -1.362814 -3.066537 1.107264
H -1.956298 -3.928051 1.419350
H -0.330838 -3.237423 1.423886
H -1.742621 -2.192068 1.637956
C -0.851364 1.434919 0.970784
H -1.082918 1.407952 2.038647
H -0.252395 2.332532 0.798062
C -0.066021 0.151587 0.578963
H -0.201820 -0.587061 1.372567
C 1.418357 0.339821 0.378558
C 1.906973 1.297796 -0.517453
C 2.337231 -0.448681 1.072496
C 3.273828 1.459441 -0.714228
H 1.208614 1.922973 -1.067750
C 3.709603 -0.290096 0.879988
H 1.974539 -1.197424 1.771019
C 4.182246 0.664427 -0.014506
H 3.633274 2.206843 -1.413712
H 4.406615 -0.913446 1.430120
H 5.248589 0.790962 -0.167218
39
F_ket_anti_conf_2 Eopt -698.064174
C -2.290440 0.277215 -0.849596
C -0.779629 0.557374 -0.684966
C -2.636402 -0.939576 0.045359
H -2.891185 1.148390 -0.578459
H -2.500215 0.045647 -1.896977

H -0.253788 0.361854 -1.623001
C -3.658506 -1.862643 -0.611788
H -3.870189 -2.728595 0.023603
H -4.603916 -1.339037 -0.785933
H -3.294219 -2.230753 -1.575396
C -3.179672 -0.467395 1.398060
H -2.508322 0.244295 1.885446
H -4.144187 0.032593 1.266642
H -3.328585 -1.314286 2.075243
C -0.429205 1.957983 -0.222115
O -1.146046 2.575457 0.537089
C 0.881548 2.518088 -0.723539
H 1.646254 1.742291 -0.596942
H 0.772490 2.633909 -1.809335
C 1.291208 3.823814 -0.064867
H 0.542005 4.600552 -0.228667
H 1.410416 3.698974 1.013712
H 2.240614 4.176936 -0.471942
C -1.273013 -1.627683 0.218196
H -1.032862 -2.196015 -0.688004
H -1.248298 -2.318763 1.066262
C -0.271831 -0.475553 0.375514
H -0.403895 -0.038301 1.369415
C 1.181060 -0.859143 0.233288
C 1.663271 -1.453402 -0.938680
C 2.082837 -0.610383 1.270227
C 3.007386 -1.787594 -1.067952
H 0.982687 -1.651824 -1.761653
C 3.431002 -0.943251 1.145389
H 1.725167 -0.145274 2.184425
C 3.897945 -1.532711 -0.025219
H 3.362385 -2.246481 -1.984672
H 4.114378 -0.739177 1.962847
H 4.946272 -1.791439 -0.127196
39
F_ket_anti_conf_3 Eopt -698.064812
C -2.287221 0.896928 0.195328
C -0.782180 0.734983 0.419945
C -2.856862 -0.542364 0.024465
H -2.771374 1.437240 1.012881
H -2.440034 1.475025 -0.720280
H -0.566823 0.465703 1.459985
C -3.734245 -0.620978 -1.225765
H -4.556795 0.099212 -1.170042
H -3.154288 -0.397165 -2.126693

H -4.166820 -1.619748 -1.340391
C -3.670577 -0.960558 1.249011
H -4.575196 -0.352230 1.346627
H -3.975781 -2.009333 1.174850
H -3.085034 -0.845689 2.166655
C 0.065568 1.927924 0.023443
O -0.169570 2.559203 -0.985711
C 1.238832 2.249385 0.917378
H 0.821753 2.529058 1.893220
H 1.778494 1.311367 1.098034
C 2.156710 3.328631 0.370927
H 1.619668 4.267731 0.224750
H 2.983183 3.513721 1.059665
H 2.577975 3.032704 -0.592555
C -1.600262 -1.440768 -0.127412
H -1.732686 -2.218036 -0.885302
H -1.384394 -1.941215 0.821502
C -0.450325 -0.488392 -0.474656
H -0.565515 -0.159250 -1.514026
C 0.951814 -1.015000 -0.294940
C 1.903830 -0.834548 -1.301264
C 1.354377 -1.622385 0.900115
C 3.223252 -1.248480 -1.124445
H 1.608417 -0.359227 -2.232324
C 2.669677 -2.038913 1.080018
H 0.638354 -1.761473 1.704480
C 3.610627 -1.852309 0.067939
H 3.946465 -1.097861 -1.918911
H 2.962732 -2.507460 2.013626
H 4.636177 -2.175624 0.209425
39
F_ket_anti_conf_4 Eopt -698.062870
C 2.238144 0.097592 -0.228154
C 0.791576 0.542768 0.044466
C 2.264247 -1.426967 0.076436
H 2.460575 0.274408 -1.285560
H 2.971331 0.651641 0.363584
H 0.632540 0.636733 1.124121
C 2.918699 -1.692896 1.432660
H 2.438262 -1.105298 2.221605
H 2.835282 -2.749936 1.704695
H 3.981230 -1.431235 1.414692
C 3.024450 -2.175250 -1.018404
H 3.082800 -3.245037 -0.795048
H 2.530406 -2.057648 -1.987919

H 4.046293 -1.794132 -1.113954
C 0.443261 1.853007 -0.635336
O 0.303521 1.910648 -1.839893
C 0.303214 3.071131 0.243599
H 0.014873 3.919334 -0.379654
H -0.506935 2.874024 0.955526
C 1.597061 3.365912 1.009945
H 2.430595 3.530474 0.322784
H 1.477463 4.265905 1.615596
H 1.865331 2.546363 1.680073
C 0.766893 -1.842088 0.105722
H 0.444679 -2.005149 1.139156
H 0.580606 -2.769170 -0.443315
C -0.013413 -0.657297 -0.485429
H 0.098350 -0.663126 -1.574645
C -1.485907 -0.617604 -0.156662
C -2.442146 -0.613211 -1.174508
C -1.928636 -0.565310 1.170752
C -3.804111 -0.561056 -0.880656
H -2.115407 -0.649703 -2.209601
C -3.286439 -0.511222 1.468761
H -1.204952 -0.565727 1.980955
C -4.230777 -0.509392 0.442629
H -4.529389 -0.559021 -1.687528
H -3.609428 -0.470118 2.503646
H -5.289373 -0.467466 0.675018
39
F_ket_anti_conf_8 Eopt -698.064812
C 2.287330 0.896826 -0.194946
C 0.782288 0.735193 -0.419847
C 2.856747 -0.542637 -0.024524
H 2.771690 1.437435 -1.012174
H 2.440032 1.474537 0.720932
H 0.567060 0.466342 -1.460037
C 3.733366 -0.621985 1.226177
H 4.555974 0.098207 1.171359
H 3.152865 -0.398642 2.126870
H 4.165828 -1.620838 1.340511
C 3.671181 -0.960267 -1.248793
H 4.575943 -0.352003 -1.345507
H 3.976199 -2.009125 -1.175021
H 3.086213 -0.844800 -2.166726
C -0.065320 1.928069 -0.023026
O 0.169408 2.558571 0.986711
C -1.237900 2.250604 -0.917454

H -0.819931 2.531203 -1.892674
H -1.777615 1.312922 -1.099569
C -2.155915 3.329569 -0.370691
H -1.618765 4.268426 -0.223377
H -2.981900 3.515401 -1.059815
H -2.577897 3.032950 0.592266
C 1.600038 -1.441099 0.126116
H 1.732255 -2.219306 0.883084
H 1.384171 -1.940335 -0.823430
C 0.450255 -0.488920 0.474284
H 0.565751 -0.160350 1.513801
C -0.951995 -1.015312 0.294625
C -1.354945 -1.622054 -0.900624
C -1.903728 -0.835238 1.301266
C -2.670345 -2.038304 -1.080389
H -0.639162 -1.760847 -1.705254
C -3.223266 -1.248893 1.124593
H -1.608020 -0.360446 2.232501
C -3.611023 -1.852085 -0.067973
H -2.963715 -2.506359 -2.014144
H -3.946221 -1.098521 1.919339
H -4.636637 -2.175223 -0.209388
39
F_ket_anti_conf_9 Eopt -698.064186
C 2.169126 -0.004772 -1.018905
C 0.814012 0.603595 -0.612767
C 2.493765 -1.082845 0.032697
H 2.069663 -0.479985 -1.999322
H 2.953640 0.751263 -1.090917
H 0.144457 0.643406 -1.476947
C 3.138744 -0.452978 1.271345
H 3.275914 -1.201303 2.058340
H 4.121600 -0.041119 1.023006
H 2.539033 0.362240 1.684081
C 3.409732 -2.169723 -0.519232
H 4.377721 -1.753009 -0.815337
H 3.596878 -2.943797 0.231816
H 2.966377 -2.650041 -1.396538
C 0.883643 2.021086 -0.066458
O 1.932376 2.621179 0.042537
C -0.424382 2.666633 0.350115
H -0.828320 2.105833 1.200198
H -0.190909 3.673066 0.702005
C -1.468164 2.715341 -0.769588
H -1.064693 3.195783 -1.664756

H -1.819015 1.719244 -1.046189
H -2.334684 3.292955 -0.441746
C 1.092761 -1.619325 0.359605
H 1.062875 -2.216429 1.276062
H 0.751054 -2.252972 -0.466773
C 0.196727 -0.371433 0.455197
H 0.326374 0.065577 1.449622
C -1.276423 -0.650336 0.271917
C -1.764008 -1.168521 -0.933628
C -2.186727 -0.386133 1.296348
C -3.122333 -1.406682 -1.111033
H -1.073557 -1.377618 -1.746450
C -3.550556 -0.622143 1.123634
H -1.824813 0.014991 2.238803
C -4.023058 -1.130865 -0.081827
H -3.481283 -1.804740 -2.054275
H -4.241276 -0.405570 1.931665
H -5.083198 -1.312592 -0.221175
39
F_ket_syn_conf_10 Eopt -698.055182
C 2.349784 0.750208 -0.659010
C 0.838334 0.831091 -0.900813
C 2.630369 -0.579790 0.063594
H 2.850083 0.734577 -1.632967
H 2.728967 1.611858 -0.104118
H 0.629319 1.338285 -1.848523
C 2.461053 -0.441100 1.579373
H 2.602935 -1.410659 2.067592
H 3.202365 0.254250 1.985822
H 1.477794 -0.059342 1.852644
C 4.045730 -1.079310 -0.223613
H 4.793368 -0.378315 0.161337
H 4.223141 -2.048955 0.252607
H 4.212823 -1.195804 -1.298360
C 0.064728 1.650252 0.124442
O 0.566411 2.053333 1.152001
C -1.363180 2.041263 -0.227706
H -1.597669 1.730154 -1.246873
H -2.030748 1.484366 0.438973
C -1.583489 3.542909 -0.050138
H -0.930773 4.117591 -0.712390
H -2.616999 3.806148 -0.283024
H -1.376586 3.847038 0.976854
C 1.565190 -1.526609 -0.530993
H 1.243315 -2.273683 0.198855

H 1.994740 -2.073907 -1.374600
C 0.376309 -0.672966 -1.055236
H 0.283748 -0.847612 -2.128181
C -0.972469 -1.005707 -0.451269
C -1.140253 -1.212477 0.921708
C -2.102237 -1.074158 -1.270885
C -2.401073 -1.454538 1.460631
H -0.280511 -1.183087 1.582560
C -3.366023 -1.316931 -0.738324
H -1.990182 -0.922187 -2.340805
C -3.521162 -1.501973 0.633150
H -2.508046 -1.607263 2.529432
H -4.228494 -1.361322 -1.395020
H -4.503547 -1.689766 1.052710
39
F_ket_syn_conf_11 Eopt -698.057063
C -2.424150 0.900414 -0.551382
C -0.936772 0.973728 -0.925762
C -2.678652 -0.469200 0.104809
H -2.728086 1.728164 0.094926
H -3.011922 0.967724 -1.472391
H -0.812896 1.476022 -1.889298
C -4.113695 -0.940580 -0.130403
H -4.276441 -1.932036 0.304586
H -4.830990 -0.253938 0.330356
H -4.340259 -0.999623 -1.198906
C -2.427628 -0.415582 1.614703
H -3.178096 0.217246 2.099560
H -2.497444 -1.416575 2.052490
H -1.452263 0.005371 1.855534
C -0.056616 1.752645 0.036408
O -0.372602 1.990202 1.182410
C 1.238826 2.290459 -0.541915
H 1.509539 1.724895 -1.435000
H 0.996936 3.304763 -0.887983
C 2.380728 2.326552 0.464089
H 3.279128 2.751220 0.011567
H 2.119698 2.932330 1.333217
H 2.620893 1.319062 0.814575
C -1.666471 -1.387719 -0.612393
H -2.149565 -1.834978 -1.485759
H -1.345547 -2.213164 0.028045
C -0.470185 -0.531000 -1.108636
H -0.363739 -0.686096 -2.183080
C 0.876698 -0.885999 -0.502518

C 1.033616 -1.205974 0.849788
C 2.016354 -0.898944 -1.314299
C 2.286183 -1.518366 1.374155
H 0.170444 -1.227063 1.505018
C 3.271751 -1.205179 -0.795770
H 1.915858 -0.664183 -2.370402
C 3.411840 -1.516368 0.554718
H 2.379653 -1.765763 2.426377
H 4.138144 -1.208014 -1.448829
H 4.386797 -1.760296 0.962579
39
F_ket_syn_conf_5 Eopt -698.064570
C 2.156992 0.829902 0.571148
C 0.957433 1.013477 -0.355306
C 2.867842 -0.425327 0.042351
H 2.807446 1.709050 0.597547
H 1.803183 0.644849 1.591123
H 1.261258 1.544212 -1.264209
C 3.824918 -1.021178 1.068695
H 4.260637 -1.956500 0.703251
H 4.648464 -0.332315 1.282221
H 3.309457 -1.233552 2.010081
C 3.627487 -0.123391 -1.253108
H 2.968848 0.251585 -2.041813
H 4.405739 0.626855 -1.082223
H 4.111590 -1.028678 -1.631858
C -0.188451 1.821494 0.213243
O -0.236482 2.160395 1.376347
C -1.265111 2.229701 -0.773645
H -0.972818 3.225455 -1.132554
H -1.231487 1.571355 -1.645087
C -2.658388 2.270297 -0.160163
H -3.393205 2.604141 -0.895449
H -2.956824 1.278948 0.192371
H -2.692951 2.954368 0.689151
C 1.669904 -1.347109 -0.236800
H 1.346772 -1.799128 0.705812
H 1.915414 -2.162061 -0.923826
C 0.538222 -0.448167 -0.797390
H 0.549797 -0.483494 -1.888272
C -0.838099 -0.888934 -0.344028
C -1.830278 -1.201277 -1.276232
C -1.155398 -0.980590 1.016726
C -3.102562 -1.598006 -0.867209
H -1.603401 -1.130304 -2.336225

C -2.424437 -1.373414 1.430626
H -0.402910 -0.736124 1.761092
C -3.404028 -1.685132 0.488862
H -3.856536 -1.838026 -1.609439
H -2.649847 -1.435211 2.490075
H -4.393053 -1.992667 0.810831
39
F_ket_syn_conf_6 Eopt -698.062167
C 2.104040 0.625641 0.640636
C 0.877649 0.908222 -0.224856
C 2.768718 -0.596323 -0.011215
H 2.774199 1.486917 0.715168
H 1.781079 0.366168 1.654667
H 1.160614 1.521616 -1.088649
C 3.741367 -1.295853 0.931503
H 4.145449 -2.205170 0.475322
H 4.585851 -0.644030 1.177075
H 3.248476 -1.577203 1.866861
C 3.495722 -0.203965 -1.301026
H 4.301579 0.506431 -1.092162
H 3.939706 -1.085570 -1.773328
H 2.824259 0.257477 -2.030857
C -0.221801 1.695929 0.453620
O -0.170475 2.010820 1.623880
C -1.379754 2.148793 -0.416501
H -1.299621 1.706403 -1.411729
H -2.305539 1.783054 0.038989
C -1.405474 3.676546 -0.508328
H -0.485880 4.058607 -0.959487
H -2.245001 4.008451 -1.121834
H -1.509211 4.121790 0.482680
C 1.540386 -1.464588 -0.325679
H 1.224876 -1.972398 0.591121
H 1.746044 -2.235084 -1.074363
C 0.424045 -0.496727 -0.792966
H 0.429133 -0.435869 -1.882754
C -0.956610 -0.948071 -0.368902
C -1.951248 -1.190208 -1.318198
C -1.276038 -1.112217 0.984316
C -3.232685 -1.580430 -0.932545
H -1.721232 -1.063077 -2.372147
C -2.555039 -1.495424 1.375239
H -0.518126 -0.929561 1.741267
C -3.540060 -1.730237 0.416624
H -3.990592 -1.762415 -1.687147

H -2.784197 -1.610441 2.429397
H -4.537370 -2.029177 0.720540
39
F_ket_syn_conf_7 Eopt -698.062552
C 2.150803 0.503667 0.749148
C 0.910834 0.970166 -0.015421
C 2.726906 -0.640900 -0.096893
H 2.867536 1.312433 0.918705
H 1.850355 0.114957 1.727707
H 1.208033 1.683740 -0.790949
C 3.694082 -1.512903 0.696019
H 3.220229 -1.901853 1.602201
H 4.033997 -2.365477 0.099524
H 4.579536 -0.943147 0.995482
C 3.427462 -0.103672 -1.348531
H 4.278757 0.527728 -1.075882
H 3.804212 -0.928832 -1.960574
H 2.757453 0.492051 -1.975197
C -0.100871 1.714645 0.838451
O 0.050065 1.835618 2.036739
C -1.313782 2.336694 0.166335
H -2.137484 1.625779 0.304233
H -1.575494 3.222242 0.750640
C -1.165740 2.683476 -1.311397
H -0.369021 3.414159 -1.470956
H -0.945111 1.804717 -1.920730
H -2.094851 3.117761 -1.686263
C 1.443530 -1.394931 -0.475358
H 1.129650 -2.005257 0.377243
H 1.579717 -2.065928 -1.328489
C 0.370963 -0.315370 -0.764877
H 0.361159 -0.098968 -1.834881
C -1.021632 -0.757395 -0.376907
C -1.323169 -1.100122 0.946842
C -2.045245 -0.807152 -1.324584
C -2.614806 -1.462386 1.313933
H -0.541165 -1.070168 1.700893
C -3.340379 -1.176251 -0.963281
H -1.827517 -0.546340 -2.356262
C -3.630629 -1.499277 0.358874
H -2.830593 -1.715543 2.346560
H -4.121619 -1.207568 -1.715444
H -4.638269 -1.781177 0.644401
39
F_ket_syn_conf_8 Eopt -698.061720

C 1.660488 0.681693 0.784555
C 0.828205 1.119815 -0.419112
C 2.689213 -0.301344 0.186509
H 2.138777 1.519825 1.299572
H 1.030518 0.160366 1.512712
H 1.437352 1.747939 -1.075241
C 3.180904 -1.305148 1.227281
H 3.682561 -0.791942 2.053981
H 2.355323 -1.887029 1.646353
H 3.897038 -2.006112 0.787027
C 3.895992 0.468676 -0.362005
H 3.600396 1.214788 -1.105071
H 4.426379 0.985423 0.443757
H 4.600516 -0.215704 -0.844439
C -0.449206 1.899928 -0.171548
O -0.891794 2.618416 -1.045312
C -1.148676 1.755015 1.160120
H -1.223538 0.687812 1.394399
H -0.473487 2.168874 1.920056
C -2.509869 2.428673 1.205540
H -2.429389 3.500383 1.015222
H -3.180047 2.006875 0.452726
H -2.970814 2.290435 2.185502
C 1.913488 -0.984719 -0.981256
H 1.732136 -2.041730 -0.773855
H 2.505608 -0.943522 -1.898731
C 0.581636 -0.222643 -1.189299
H 0.419905 0.007858 -2.244096
C -0.659319 -0.936914 -0.687414
C -0.643447 -1.815052 0.400050
C -1.893958 -0.645632 -1.279939
C -1.824377 -2.367169 0.893094
H 0.294567 -2.069545 0.880765
C -3.076325 -1.193476 -0.790918
H -1.926499 0.026933 -2.132257
C -3.046461 -2.054122 0.304391
H -1.787035 -3.042253 1.741594
H -4.020249 -0.949971 -1.267205
H -3.965385 -2.482528 0.689442
39
F_ket_syn_conf_9 Eopt -698.058947
C -2.334986 0.561876 -0.870130
C -0.802865 0.728091 -0.834616
C -2.708269 -0.662120 0.023110
H -2.837169 1.470290 -0.531522

H -2.646695 0.381757 -1.902311
H -0.395104 1.012557 -1.805205
C -3.356184 -1.757222 -0.829939
H -3.629922 -2.620401 -0.215379
H -4.265195 -1.385374 -1.313116
H -2.679736 -2.103737 -1.617466
C -3.661073 -0.273424 1.151910
H -3.236920 0.535306 1.751772
H -4.624127 0.063316 0.754485
H -3.852391 -1.126950 1.810718
C -0.362571 1.741350 0.208398
O -1.022677 1.920715 1.212957
C 0.914487 2.548592 0.021793
H 0.618975 3.595066 0.151706
H 1.547730 2.313367 0.883652
C 1.695563 2.376489 -1.274366
H 2.588408 3.005184 -1.250932
H 2.021348 1.344719 -1.421106
H 1.106917 2.674605 -2.144840
C -1.354095 -1.151753 0.579949
H -1.336015 -2.233608 0.741834
H -1.153042 -0.668250 1.539961
C -0.320438 -0.713710 -0.461092
H -0.482132 -1.306101 -1.367598
C 1.133494 -0.867345 -0.080525
C 1.620699 -0.491156 1.175631
C 2.040849 -1.376544 -1.015167
C 2.976036 -0.600800 1.477781
H 0.944121 -0.100126 1.929210
C 3.395715 -1.491926 -0.716786
H 1.678202 -1.679209 -1.993456
C 3.869689 -1.098351 0.532269
H 3.333313 -0.297653 2.456300
H 4.080082 -1.888403 -1.459307
H 4.924477 -1.184361 0.769637
39
TSIII_ket_anti_conf_1 Eopt -698.092560
C -2.127391 -0.107319 -0.991028
C -0.813336 0.596061 -0.683203
C -2.396787 -1.265414 -0.007151
H -2.958153 0.606121 -0.960406
H -2.084991 -0.519806 -2.005886
H -0.036797 0.463052 -1.434981
C -3.342240 -2.301820 -0.608683
H -4.306492 -1.850999 -0.866646

H -2.922197 -2.739116 -1.520067
H -3.536632 -3.116945 0.096777
C -3.003540 -0.724774 1.291019
H -2.430275 0.117326 1.681932
H -4.022488 -0.364549 1.113569
H -3.053432 -1.508085 2.055597
C -0.834508 1.890483 -0.080981
O -1.815610 2.350710 0.575004
C 0.445112 2.717528 -0.114730
H 0.823337 2.808329 0.913049
H 1.220305 2.205262 -0.693262
C 0.206825 4.120831 -0.675405
H -0.565674 4.634729 -0.099507
H 1.116152 4.727110 -0.641674
H -0.127226 4.073025 -1.716543
C -1.010505 -1.868592 0.252776
H -0.684606 -2.381969 -0.658406
H -1.069744 -2.632338 1.041757
C -0.037816 -0.768808 0.611559
H -0.265905 -0.282507 1.559301
C 1.374953 -0.900232 0.381528
C 2.300469 -0.136566 1.149502
C 1.931051 -1.651840 -0.693382
C 3.658657 -0.140248 0.883037
H 1.919577 0.461780 1.973797
C 3.295384 -1.650941 -0.951669
H 1.282775 -2.243901 -1.331094
C 4.183627 -0.902308 -0.171962
H 4.324176 0.453530 1.503350
H 3.675706 -2.244170 -1.778750
H 5.247757 -0.907794 -0.379298
39
TSIII_ket_anti_conf_11 Eopt -698.088473
C -2.063344 0.668498 -0.633972
C -1.015727 -0.408967 -0.843242
C -1.421627 1.923471 -0.030692
H -2.576885 0.925142 -1.571209
H -2.831809 0.311896 0.059814
H -0.257876 -0.165302 -1.587950
C -2.481781 2.895000 0.483567
H -3.128683 2.416531 1.225525
H -2.019467 3.768863 0.955533
H -3.115659 3.256718 -0.332804
C -0.571598 2.640823 -1.083543
H -0.046251 3.496873 -0.647227

H 0.176435 1.984246 -1.531737
H -1.208572 3.017682 -1.890911
C -1.374478 -1.791906 -0.880257
O -0.611587 -2.683298 -1.373951
C -2.643466 -2.268085 -0.176091
H -3.512978 -1.667381 -0.463840
H -2.832259 -3.287414 -0.523037
C -2.522893 -2.270001 1.353263
H -3.407968 -2.714516 1.818045
H -1.651311 -2.847664 1.675229
H -2.414914 -1.256404 1.749091
C -0.561804 1.384733 1.134750
H -1.231707 1.221298 1.987142
H 0.161353 2.147324 1.451270
C 0.109099 0.063122 0.788943
H -0.212205 -0.763405 1.415929
C 1.523227 0.000967 0.506633
C 2.295748 1.109630 0.061653
C 2.217046 -1.239310 0.600648
C 3.643200 0.980689 -0.253673
H 1.835534 2.088168 -0.016064
C 3.557265 -1.360906 0.278129
H 1.668656 -2.113886 0.941686
C 4.297102 -0.250571 -0.157227
H 4.194747 1.858755 -0.578441
H 4.041144 -2.329138 0.370741
H 5.347559 -0.345123 -0.408510
39
TSIII_ket_anti_conf_2 Eopt -698.092489
C -2.177182 -0.172605 -1.073812
C -0.830063 0.512973 -0.908107
C -2.496763 -1.068447 0.140655
H -2.970850 0.570535 -1.207835
H -2.156399 -0.801775 -1.971491
H -0.061641 0.183394 -1.606704
C -3.509303 -2.154212 -0.211976
H -3.737501 -2.780470 0.657286
H -4.450738 -1.715267 -0.559265
H -3.130350 -2.805942 -1.005649
C -3.047387 -0.218082 1.289150
H -2.419466 0.653920 1.480664
H -4.047229 0.154325 1.042048
H -3.127151 -0.807159 2.209597
C -0.791450 1.911485 -0.616360
O -1.764144 2.565509 -0.138710

C 0.537184 2.635304 -0.806788
H 1.314600 1.924680 -1.105031
H 0.429954 3.353468 -1.631888
C 0.970855 3.395671 0.447111
H 0.232923 4.156019 0.710040
H 1.069786 2.721155 1.302352
H 1.933679 3.892639 0.298437
C -1.141368 -1.677188 0.521890
H -0.855075 -2.396537 -0.253313
H -1.228775 -2.242398 1.460800
C -0.101373 -0.582981 0.631422
H -0.269721 0.082752 1.477770
C 1.294672 -0.842829 0.404468
C 1.765683 -1.743074 -0.595778
C 2.292605 -0.072033 1.067463
C 3.118374 -1.870022 -0.879972
H 1.056601 -2.343903 -1.156625
C 3.639550 -0.203746 0.774714
H 1.980347 0.628544 1.837373
C 4.079297 -1.110580 -0.202206
H 3.432761 -2.571882 -1.647628
H 4.363219 0.399240 1.316100
H 5.134187 -1.217219 -0.428613
39
TSIII_ket_anti_conf_3 Eopt -698.092635
C -2.297832 0.742689 0.311426
C -0.821463 0.984264 0.526248
C -2.574068 -0.740543 0.042816
H -2.891605 1.084530 1.171526
H -2.621158 1.333944 -0.552583
H -0.382610 0.479075 1.384424
C -4.017880 -0.963917 -0.400724
H -4.722143 -0.695454 0.393730
H -4.257349 -0.359775 -1.281340
H -4.193124 -2.014495 -0.657165
C -2.311496 -1.571787 1.302476
H -2.976897 -1.261083 2.115253
H -2.493154 -2.634515 1.110105
H -1.283624 -1.472328 1.657199
C -0.263959 2.264364 0.247953
O -0.757770 3.077529 -0.587764
C 1.022788 2.663492 0.970734
H 0.751005 3.332249 1.800703
H 1.485562 1.782534 1.426276
C 2.024028 3.391633 0.077328

H 1.573535 4.287397 -0.353631
H 2.910056 3.694363 0.642199
H 2.354761 2.757897 -0.750160
C -1.584154 -1.124433 -1.082901
H -2.050813 -0.869369 -2.041366
H -1.433948 -2.210800 -1.090506
C -0.273833 -0.367597 -0.967311
H -0.148442 0.406521 -1.721828
C 0.955808 -1.003126 -0.593757
C 2.195164 -0.347366 -0.849002
C 1.034088 -2.220186 0.139964
C 3.402529 -0.857614 -0.399764
H 2.183160 0.574726 -1.423826
C 2.249459 -2.728538 0.575852
H 0.126233 -2.770982 0.363980
C 3.452578 -2.057949 0.320723
H 4.321544 -0.321035 -0.619244
H 2.262980 -3.664783 1.126966
H 4.397662 -2.459168 0.669032
39
TSIII_ket_anti_conf_4 Eopt -698.093421
C 2.313610 -0.226429 0.255335
C 1.075582 0.637276 0.345781
C 1.940798 -1.708054 0.132468
H 2.879623 0.080129 -0.631197
H 2.970901 -0.076573 1.123468
H 0.467331 0.500161 1.237496
C 1.325849 -2.212547 1.441353
H 0.441676 -1.640001 1.729234
H 1.026496 -3.262252 1.352068
H 2.051037 -2.140593 2.259124
C 3.160677 -2.563059 -0.201113
H 2.878174 -3.610948 -0.350624
H 3.648304 -2.213781 -1.116577
H 3.899060 -2.531666 0.606927
C 1.105689 1.969393 -0.156851
O 1.890765 2.353275 -1.075774
C 0.066614 2.966194 0.341789
H -0.535525 3.298853 -0.514369
H -0.617272 2.491236 1.051853
C 0.721959 4.191570 0.984146
H 1.407790 4.669415 0.280998
H -0.022263 4.932648 1.288803
H 1.295648 3.906687 1.871567
C 0.905399 -1.750794 -1.015200

H 0.341294 -2.690732 -0.972917
H 1.457306 -1.762146 -1.962095
C 0.000160 -0.533605 -0.995643
H 0.164547 0.148708 -1.827309
C -1.374028 -0.603728 -0.581884
C -2.253109 0.480893 -0.865813
C -1.919799 -1.658869 0.200062
C -3.560177 0.506954 -0.407078
H -1.880097 1.306221 -1.467454
C -3.233479 -1.628142 0.647511
H -1.304045 -2.516862 0.448548
C -4.074753 -0.547315 0.358449
H -4.192797 1.355911 -0.650788
H -3.611088 -2.461289 1.233737
H -5.098165 -0.527741 0.715822
39
TSIII_ket_anti_conf_8 Eopt -698.090647
C 2.333809 0.916846 -0.081043
C 0.908254 0.985707 -0.563895
C 2.844762 -0.546729 0.002630
H 3.014780 1.505249 -0.712389
H 2.364905 1.381828 0.909302
H 0.681867 0.486652 -1.506230
C 3.670000 -0.736791 1.277704
H 4.482917 -0.004547 1.328236
H 3.050528 -0.607553 2.171030
H 4.115813 -1.736314 1.316903
C 3.714782 -0.887751 -1.208991
H 4.648683 -0.316210 -1.199640
H 3.972895 -1.952351 -1.219025
H 3.190953 -0.661911 -2.143565
C 0.078890 2.081139 -0.227692
O 0.331808 2.906857 0.696455
C -1.226452 2.234210 -1.014167
H -1.022556 2.839309 -1.908613
H -1.547582 1.253104 -1.381958
C -2.346023 2.893979 -0.216848
H -2.054254 3.893390 0.110420
H -3.254830 2.984342 -0.818222
H -2.590733 2.313814 0.677021
C 1.601672 -1.467926 0.021245
H 1.841623 -2.402188 0.550370
H 1.361124 -1.756348 -1.007849
C 0.425135 -0.747828 0.619979
H 0.618545 -0.244145 1.566974

C -0.925545 -1.149884 0.418145
C -1.342184 -2.038328 -0.617214
C -1.969267 -0.552215 1.186634
C -2.685375 -2.284513 -0.862877
H -0.599168 -2.538677 -1.229529
C -3.305120 -0.804689 0.929930
H -1.695905 0.128553 1.989476
C -3.689695 -1.672091 -0.103303
H -2.958777 -2.968575 -1.661546
H -4.064364 -0.320732 1.538245
H -4.736783 -1.870366 -0.302477
39
TSIII_ket_anti_conf_9 Eopt -698.093015
C 2.213017 0.231757 -0.988735
C 0.829075 0.782058 -0.672648
C 2.594590 -0.922385 -0.036976
H 2.221550 -0.150039 -2.016443
H 2.962939 1.027405 -0.926288
H 0.076749 0.550600 -1.423260
C 3.169916 -0.358065 1.265581
H 3.284021 -1.145586 2.018887
H 4.158054 0.078968 1.086232
H 2.538530 0.433615 1.672657
C 3.617377 -1.859970 -0.672630
H 4.533435 -1.320855 -0.936812
H 3.895027 -2.667025 0.014015
H 3.222048 -2.316428 -1.585651
C 0.709690 2.069844 -0.070178
O 1.636705 2.618563 0.598862
C -0.651482 2.763083 -0.054580
H -1.094487 2.594615 0.937866
H -0.456554 3.840051 -0.105011
C -1.661578 2.374580 -1.132318
H -1.251248 2.531270 -2.134459
H -1.964211 1.327056 -1.056773
H -2.566122 2.983319 -1.046763
C 1.268820 -1.647532 0.225855
H 1.404316 -2.425321 0.991312
H 0.967395 -2.160090 -0.694612
C 0.216280 -0.641397 0.633230
H 0.431531 -0.156713 1.585232
C -1.186564 -0.893900 0.448332
C -1.710389 -1.612065 -0.664980
C -2.147558 -0.283934 1.304875
C -3.077331 -1.694940 -0.896641

H -1.033245 -2.096249 -1.361481
C -3.507165 -0.372974 1.066861
H -1.791689 0.272766 2.168668
C -3.998913 -1.077879 -0.044248
H -3.433248 -2.248445 -1.761340
H -4.200736 0.108684 1.750453
H -5.064400 -1.147783 -0.232132
39
TSIII_ket_syn_conf_10 Eopt -698.087207
C 2.290009 0.788064 -0.162438
C 0.888153 1.189726 -0.617499
C 2.436682 -0.728621 0.057292
H 3.007845 1.093279 -0.933467
H 2.558317 1.318361 0.758581
H 0.874814 1.678781 -1.589229
C 1.884422 -1.110343 1.432733
H 1.878794 -2.197502 1.567690
H 2.512802 -0.679503 2.220212
H 0.875543 -0.722089 1.577000
C 3.899582 -1.161343 -0.023899
H 4.500497 -0.664757 0.745439
H 3.999891 -2.242087 0.125706
H 4.333349 -0.916163 -0.998506
C -0.010213 1.806446 0.313797
O 0.012531 1.586684 1.563788
C -1.071812 2.763674 -0.216230
H -1.139307 2.707733 -1.307437
H -2.048320 2.466323 0.185808
C -0.786638 4.208320 0.209334
H 0.157964 4.561696 -0.215812
H -1.578054 4.890114 -0.116225
H -0.710148 4.276004 1.297397
C 1.615546 -1.369550 -1.081310
H 1.474692 -2.440907 -0.885818
H 2.210040 -1.298274 -1.999711
C 0.309776 -0.629069 -1.291617
H 0.158287 -0.288329 -2.313415
C -0.929197 -1.081318 -0.694779
C -1.040407 -2.124364 0.257587
C -2.132213 -0.394568 -1.014666
C -2.256067 -2.450110 0.843665
H -0.160367 -2.694565 0.533199
C -3.342439 -0.716126 -0.417453
H -2.094068 0.405299 -1.749601
C -3.423666 -1.744914 0.525862

H -2.297197 -3.265782 1.559931
H -4.235589 -0.159603 -0.687652
H -4.369135 -1.996924 0.993319
39
TSIII_ket_syn_conf_11 Eopt -698.087798
C -2.430660 0.749441 -0.671996
C -0.955951 1.031329 -0.943070
C -2.608919 -0.566270 0.107219
H -2.893165 1.577974 -0.123655
H -2.957431 0.650233 -1.629167
H -0.736998 1.272154 -1.983146
C -4.044393 -1.079929 0.005848
H -4.156747 -2.037818 0.525783
H -4.749214 -0.374223 0.458324
H -4.340608 -1.229090 -1.037206
C -2.257788 -0.380298 1.585255
H -2.977652 0.288671 2.069208
H -2.286723 -1.342244 2.109618
H -1.274635 0.072357 1.710388
C -0.263447 1.928776 -0.047063
O -0.676417 2.247063 1.115403
C 1.048789 2.541614 -0.524274
H 1.336328 2.123199 -1.494317
H 0.895316 3.621180 -0.678653
C 2.187629 2.362302 0.480683
H 3.109598 2.837962 0.131946
H 1.919123 2.808310 1.440806
H 2.397705 1.302680 0.653688
C -1.625119 -1.546707 -0.567285
H -2.139376 -2.018801 -1.412306
H -1.364106 -2.355051 0.126338
C -0.389176 -0.825728 -1.098435
H -0.339413 -0.862371 -2.185671
C 0.918569 -1.077257 -0.523295
C 1.120593 -1.371703 0.847602
C 2.087036 -0.889311 -1.304823
C 2.398987 -1.514638 1.378870
H 0.263433 -1.514001 1.497442
C 3.358526 -1.023509 -0.769712
H 1.974506 -0.646997 -2.359061
C 3.533298 -1.347529 0.582850
H 2.511053 -1.756063 2.432074
H 4.225355 -0.881328 -1.408579
H 4.527148 -1.456745 1.002680
39

TSIII_ket_syn_conf_5 Eopt -698.092464
C 2.333649 0.952407 0.103528
C 0.963637 1.062256 -0.550672
C 2.869893 -0.485093 0.040664
H 3.049850 1.647814 -0.354217
H 2.222974 1.247513 1.151330
H 0.984968 1.167961 -1.635379
C 3.961997 -0.723211 1.079644
H 4.332205 -1.753327 1.036266
H 4.816045 -0.057947 0.913552
H 3.587848 -0.542622 2.092212
C 3.432571 -0.788649 -1.352006
H 2.727028 -0.538062 -2.148162
H 4.344028 -0.208518 -1.529253
H 3.688194 -1.849015 -1.451235
C 0.026024 1.958219 0.075500
O 0.097978 2.330004 1.293313
C -1.144584 2.467668 -0.757352
H -0.986874 3.537098 -0.967241
H -1.167033 1.959957 -1.727396
C -2.493860 2.315094 -0.054607
H -3.307032 2.733075 -0.655915
H -2.721963 1.262620 0.137710
H -2.481616 2.833253 0.906535
C 1.626723 -1.337175 0.333231
H 1.366803 -1.207271 1.389774
H 1.843486 -2.404897 0.186180
C 0.496245 -0.855632 -0.550975
H 0.684090 -1.068345 -1.603131
C -0.885040 -1.124787 -0.213097
C -1.864788 -1.198279 -1.238171
C -1.370261 -1.184477 1.118594
C -3.212086 -1.364434 -0.959192
H -1.538538 -1.136968 -2.273850
C -2.722213 -1.357294 1.393486
H -0.676387 -1.102385 1.948918
C -3.662059 -1.457920 0.364944
H -3.923011 -1.428185 -1.777983
H -3.048947 -1.410480 2.428159
H -4.715035 -1.593459 0.585506
39
TSIII_ket_syn_conf_6 Eopt -698.092215
C 2.247820 0.970273 0.034499
C 0.838536 0.990507 -0.537948
C 2.848319 -0.446351 0.015748

H 2.907403 1.665957 -0.500456
H 2.183454 1.316695 1.070333
H 0.770348 1.108632 -1.618833
C 3.968907 -0.592364 1.041622
H 4.395137 -1.601310 1.021935
H 4.781576 0.113792 0.840467
H 3.601911 -0.401811 2.054974
C 3.402802 -0.773349 -1.375301
H 4.295102 -0.172665 -1.579232
H 3.687298 -1.828489 -1.449567
H 2.681681 -0.563180 -2.169194
C -0.144909 1.749501 0.186222
O -0.026530 2.093166 1.407716
C -1.464439 2.053494 -0.508521
H -1.429775 1.729180 -1.553817
H -2.258397 1.463868 -0.024313
C -1.839246 3.534667 -0.429603
H -1.104711 4.152304 -0.956269
H -2.820351 3.726864 -0.873224
H -1.866341 3.863991 0.611208
C 1.656207 -1.350354 0.362586
H 1.392867 -1.181561 1.412988
H 1.935370 -2.409825 0.269132
C 0.499270 -0.981266 -0.536950
H 0.704529 -1.198377 -1.584939
C -0.870884 -1.281507 -0.197369
C -1.839184 -1.445404 -1.223065
C -1.363709 -1.256702 1.132697
C -3.192455 -1.546659 -0.946180
H -1.501717 -1.477096 -2.256395
C -2.721880 -1.360203 1.405367
H -0.672880 -1.127390 1.959172
C -3.657692 -1.492118 0.375459
H -3.898446 -1.664421 -1.763213
H -3.059608 -1.325239 2.437340
H -4.716982 -1.568230 0.594593
39
TSIII_ket_syn_conf_7 Eopt -698.092019
C 2.283529 0.843431 0.372699
C 0.893511 1.120125 -0.177628
C 2.796381 -0.531860 -0.081798
H 2.993433 1.627878 0.078650
H 2.217799 0.858853 1.464538
H 0.877155 1.505417 -1.194334
C 3.924956 -1.033213 0.814753

H 3.592419 -1.121266 1.853814
H 4.281472 -2.017044 0.490743
H 4.779493 -0.348452 0.792767
C 3.299769 -0.464821 -1.527592
H 4.210375 0.140239 -1.586477
H 3.538237 -1.463504 -1.908916
H 2.565181 -0.015591 -2.200723
C -0.040500 1.753038 0.712272
O 0.087142 1.761092 1.982521
C -1.348856 2.300132 0.151931
H -2.149053 1.590782 0.417855
H -1.582684 3.218475 0.703837
C -1.410810 2.577135 -1.348248
H -0.660588 3.313983 -1.650672
H -1.243066 1.671710 -1.936679
H -2.392220 2.970646 -1.627777
C 1.556118 -1.430264 0.027711
H 1.330898 -1.575542 1.090187
H 1.762337 -2.425036 -0.392960
C 0.395543 -0.750470 -0.667635
H 0.527485 -0.714293 -1.749771
C -0.975003 -1.048393 -0.315554
C -1.397769 -1.246523 1.024278
C -1.999845 -0.989828 -1.295585
C -2.743803 -1.339001 1.353661
H -0.660081 -1.289253 1.818344
C -3.341431 -1.079909 -0.962419
H -1.716790 -0.855785 -2.336858
C -3.735718 -1.239401 0.373753
H -3.027570 -1.474371 2.393589
H -4.092450 -1.021796 -1.745016
H -4.785350 -1.305853 0.638098
39
TSIII_ket_syn_conf_8 Eopt -698.089515
C 1.592579 0.670769 0.809789
C 0.827831 1.352052 -0.297912
C 2.664814 -0.253399 0.209512
H 2.068835 1.383815 1.498367
H 0.903955 0.068884 1.414937
H 1.445190 1.825918 -1.059992
C 3.191550 -1.221605 1.268869
H 3.656178 -0.680226 2.100011
H 2.385560 -1.837549 1.679166
H 3.946383 -1.894194 0.847947
C 3.844552 0.573566 -0.315783

H 3.539144 1.271237 -1.100005
H 4.307692 1.152594 0.490186
H 4.612502 -0.080684 -0.741041
C -0.410069 2.023540 -0.103503
O -0.862021 2.878208 -0.924750
C -1.243716 1.651122 1.124711
H -1.285805 0.559097 1.211229
H -0.722829 1.993372 2.030419
C -2.655253 2.220635 1.101638
H -2.643105 3.311668 1.061286
H -3.207105 1.869180 0.226112
H -3.210921 1.919814 1.994297
C 1.981244 -1.020777 -0.971606
H 1.910743 -2.083679 -0.713846
H 2.631336 -0.969145 -1.850788
C 0.613351 -0.470935 -1.323848
H 0.509160 -0.034474 -2.314368
C -0.577105 -1.084388 -0.821390
C -0.594826 -1.988797 0.278844
C -1.850637 -0.677694 -1.318270
C -1.784286 -2.417538 0.848166
H 0.341970 -2.338711 0.700682
C -3.032311 -1.104892 -0.736653
H -1.884801 0.001624 -2.166206
C -3.022317 -1.969179 0.366634
H -1.751469 -3.103205 1.690426
H -3.979912 -0.757126 -1.139275
H -3.948945 -2.298744 0.823271
39
TSIII_ket_syn_conf_9 Eopt -698.089675
C -2.317113 0.456249 -0.979676
C -0.856776 0.872350 -0.903118
C -2.675779 -0.691315 0.018781
H -2.962411 1.318957 -0.779841
H -2.534942 0.123767 -1.999941
H -0.315640 0.916313 -1.844018
C -3.303033 -1.868554 -0.736854
H -3.593318 -2.669224 -0.048239
H -4.202120 -1.549211 -1.274566
H -2.612591 -2.291740 -1.472984
C -3.659867 -0.214069 1.086852
H -3.261604 0.669172 1.591228
H -4.628074 0.045874 0.644683
H -3.836494 -0.996626 1.833629
C -0.505965 1.843953 0.075274

O -1.242627 2.102213 1.077441
C 0.811603 2.614789 -0.009953
H 0.552233 3.681732 -0.027478
H 1.339663 2.464550 0.939435
C 1.751728 2.305293 -1.170591
H 2.656220 2.916333 -1.103250
H 2.059942 1.256485 -1.172671
H 1.285763 2.517906 -2.136724
C -1.351226 -1.121348 0.673833
H -1.449554 -2.131952 1.097238
H -1.137947 -0.441812 1.504529
C -0.249130 -1.027764 -0.347480
H -0.479266 -1.520996 -1.293144
C 1.140317 -1.076028 -0.008208
C 1.645820 -0.606082 1.237137
C 2.110951 -1.461123 -0.975393
C 3.011853 -0.508586 1.471910
H 0.954643 -0.301879 2.016789
C 3.469053 -1.367952 -0.729063
H 1.765533 -1.830313 -1.938284
C 3.944366 -0.880275 0.499463
H 3.358115 -0.134377 2.431536
H 4.173436 -1.673608 -1.497457
H 5.008611 -0.804278 0.692515
39
TSII_ket_conf_1 Eopt -698.051361
C 1.693867 0.051940 -1.167912
C 2.962369 0.753231 -0.731045
C 0.721145 -0.121659 -0.031452
H 1.197571 0.611378 -1.973100
H 1.961919 -0.933138 -1.567169
H 2.927451 1.831548 -0.595801
C 0.009775 1.097844 0.463169
H -0.286729 1.757699 -0.358141
H -0.885547 0.831326 1.034887
H 0.651612 1.685271 1.137473
C 1.032935 -1.160466 0.998015
H 1.353126 -2.101313 0.541957
H 1.848290 -0.828119 1.658052
H 0.164577 -1.359137 1.635217
C 4.121719 0.068945 -0.422498
O 4.298479 -1.195521 -0.501427
C 5.318312 0.888561 0.071106
H 6.163131 0.704753 -0.604174
H 5.098326 1.960065 0.033060

C 5.721344 0.490195 1.491194
H 5.962502 -0.573863 1.536853
H 6.594107 1.050684 1.838104
H 4.902457 0.678051 2.193500
C -1.028646 -1.203925 -1.207869
H -0.303691 -1.984513 -1.412000
H -1.009416 -0.351323 -1.879505
C -2.087190 -1.460538 -0.399196
H -2.097480 -2.393314 0.160827
C -3.215588 -0.565573 -0.141379
C -3.370599 0.679454 -0.779547
C -4.202350 -0.951399 0.782346
C -4.459661 1.494846 -0.501166
H -2.631494 1.015924 -1.498744
C -5.292762 -0.134050 1.060573
H -4.103949 -1.908074 1.287178
C -5.428905 1.096262 0.421213
H -4.554615 2.450310 -1.006659
H -6.037590 -0.458824 1.779635
H -6.276992 1.736757 0.636659
39
TSII_ket_conf_10 Eopt -698.047416
C 1.992073 -1.169354 0.774435
C 3.358908 -0.989943 0.138008
C 0.865212 -1.119396 -0.226174
H 1.954409 -2.142431 1.283202
H 1.812678 -0.415736 1.548316
H 3.769089 -1.875548 -0.350357
C 0.705574 -2.284066 -1.150413
H 0.856101 -3.236945 -0.633243
H -0.289152 -2.291844 -1.608786
H 1.433800 -2.240416 -1.973775
C 0.484010 0.213587 -0.787159
H 1.169704 0.514055 -1.593385
H -0.520087 0.183964 -1.223606
H 0.509513 1.001287 -0.027649
C 4.125740 0.156172 0.049739
O 5.271576 0.226729 -0.522901
C 3.631004 1.471507 0.663218
H 2.680745 1.356304 1.188286
H 4.372739 1.787702 1.407043
C 3.499060 2.567437 -0.395580
H 4.451429 2.720653 -0.906663
H 2.755301 2.296700 -1.151299
H 3.192667 3.519516 0.047135

C -0.929092 -1.502568 1.262595
H -0.416182 -2.420353 1.529658
H -0.600820 -0.607015 1.780952
C -2.114862 -1.560762 0.605812
H -2.443108 -2.520721 0.212685
C -2.994251 -0.431108 0.305354
C -4.164045 -0.651528 -0.441776
C -2.730170 0.883723 0.732601
C -5.031465 0.390241 -0.752449
H -4.387927 -1.658521 -0.781844
C -3.596776 1.923285 0.421853
H -1.836873 1.096938 1.310068
C -4.753332 1.686083 -0.323258
H -5.926390 0.189116 -1.332085
H -3.369358 2.928234 0.762123
H -5.426402 2.501384 -0.564401
39
TSII_ket_conf_11 Eopt -698.050608
C -1.205349 0.319283 -1.125707
C -2.194003 -0.674215 -0.578117
C -0.682168 1.377332 -0.184193
H -0.331768 -0.193088 -1.553737
H -1.678714 0.852208 -1.969763
H -1.809064 -1.563672 -0.084706
C -1.643728 2.078780 0.717820
H -1.131253 2.550601 1.563454
H -2.166776 2.881932 0.175383
H -2.406677 1.396019 1.097713
C 0.457704 2.196624 -0.703446
H 0.112864 2.873100 -1.501968
H 0.905339 2.822723 0.074450
H 1.241270 1.566742 -1.136300
C -3.557167 -0.476211 -0.643963
O -4.146700 0.532403 -1.168079
C -4.465858 -1.541253 -0.021975
H -5.139259 -1.918300 -0.801817
H -3.877821 -2.391389 0.338325
C -5.302742 -0.965466 1.120659
H -5.901036 -0.122231 0.769173
H -5.982445 -1.711080 1.543008
H -4.658934 -0.604662 1.929689
C 0.448871 0.069786 1.429011
H -0.534719 -0.228846 1.774371
H 0.830754 1.004588 1.827729
C 1.254653 -0.837169 0.821950

H 0.832159 -1.801000 0.544749
C 2.645761 -0.628050 0.421077
C 3.358302 0.552034 0.705677
C 3.319394 -1.643118 -0.279955
C 4.678259 0.704883 0.302678
H 2.874244 1.359610 1.244517
C 4.641663 -1.489349 -0.682911
H 2.789156 -2.562696 -0.510424
C 5.330696 -0.313189 -0.395267
H 5.204390 1.625373 0.533828
H 5.134865 -2.290115 -1.224023
H 6.361291 -0.189255 -0.709032
39
TSII_ket_conf_12 Eopt -698.050435
C -1.264000 0.365719 -0.926510
C -2.240735 -0.479095 -0.153427
C -0.597991 1.509378 -0.200251
H -0.463541 -0.255529 -1.353730
H -1.792919 0.802306 -1.792452
H -1.847725 -1.298830 0.443439
C -1.436479 2.402337 0.654116
H -1.960008 3.148272 0.035513
H -2.199688 1.837617 1.193981
H -0.827629 2.959990 1.374142
C 0.539069 2.160932 -0.923113
H 1.245569 1.420803 -1.311958
H 0.167671 2.734470 -1.787580
H 1.086329 2.862242 -0.285823
C -3.598816 -0.239564 -0.157414
O -4.197058 0.699099 -0.790486
C -4.493049 -1.179758 0.657159
H -3.890782 -1.917268 1.197214
H -5.022643 -0.580281 1.408479
C -5.521074 -1.889643 -0.223565
H -5.024902 -2.521581 -0.967326
H -6.188809 -2.526225 0.363875
H -6.132459 -1.160880 -0.759770
C 0.588994 0.374538 1.501716
H -0.378723 0.198502 1.958041
H 1.056382 1.328050 1.727755
C 1.288516 -0.664743 0.981232
H 0.789230 -1.626762 0.882554
C 2.654266 -0.614545 0.459462
C 3.452303 0.544134 0.504318
C 3.214093 -1.769449 -0.113635

C 4.745021 0.541898 -0.002820
H 3.057848 1.457061 0.937817
C 4.509197 -1.770989 -0.620774
H 2.616713 -2.675425 -0.158776
C 5.284082 -0.614336 -0.570015
H 5.338687 1.449023 0.043263
H 4.913729 -2.677844 -1.058102
H 6.293755 -0.611385 -0.965540
39
TSII_ket_conf_15 Eopt -698.050431
C 1.986890 1.810282 -0.216871
C 3.095658 0.915427 0.265289
C 0.632028 1.665032 0.436611
H 2.268009 2.875714 -0.098230
H 1.864062 1.664376 -1.297293
H 3.509607 1.094023 1.254588
C -0.455996 2.530009 -0.120036
H -0.446149 2.544897 -1.214365
H -1.444958 2.201647 0.214181
H -0.333775 3.571691 0.217898
C 0.567715 1.414831 1.907599
H 0.872360 2.312427 2.469377
H -0.451053 1.168451 2.222718
H 1.230807 0.601698 2.213530
C 3.603358 -0.119062 -0.494175
O 3.225948 -0.453219 -1.671527
C 4.707080 -0.980544 0.126723
H 5.581615 -0.950942 -0.535024
H 5.017779 -0.577351 1.095798
C 4.254656 -2.432173 0.288046
H 3.959036 -2.850869 -0.676148
H 5.047275 -3.061731 0.702400
H 3.391741 -2.496637 0.959347
C 0.000263 -0.435211 -0.420164
H 1.025203 -0.734632 -0.228259
H -0.165394 0.069616 -1.367327
C -1.024906 -0.957774 0.299566
H -0.789930 -1.550931 1.181289
C -2.451304 -0.742939 0.055880
C -2.941648 -0.003731 -1.037347
C -3.392156 -1.295529 0.942170
C -4.305943 0.171596 -1.227795
H -2.249529 0.440624 -1.744795
C -4.758435 -1.119249 0.750859
H -3.037316 -1.870895 1.792434

C -5.225585 -0.382911 -0.335711
H -4.656893 0.746221 -2.078779
H -5.460095 -1.557540 1.452956
H -6.290039 -0.242424 -0.487951
39
TSII_ket_conf_2 Eopt -698.051099
C 1.710322 -0.161011 0.882315
C 2.948523 -0.763112 0.252279
C 0.654023 0.169289 -0.138736
H 1.281460 -0.850575 1.622387
H 1.996662 0.754809 1.412688
H 2.927642 -1.819935 -0.002320
C -0.075924 -0.971187 -0.775005
H -0.300344 -1.764041 -0.054578
H -1.015623 -0.637886 -1.228182
H 0.520833 -1.423535 -1.581678
C 0.875311 1.369836 -1.001990
H 1.650601 1.173195 -1.757281
H -0.038379 1.644033 -1.540211
H 1.209885 2.231918 -0.418602
C 4.058609 -0.008841 -0.074704
O 4.207270 1.244985 0.128063
C 5.243546 -0.733740 -0.721981
H 5.002998 -1.785715 -0.905092
H 5.433011 -0.269577 -1.698051
C 6.507823 -0.628503 0.130565
H 7.365171 -1.103228 -0.354973
H 6.759662 0.418058 0.314294
H 6.363008 -1.113176 1.101484
C -1.023848 1.004818 1.315413
H -0.294301 1.755530 1.599600
H -0.952156 0.053636 1.833539
C -2.134542 1.368719 0.627049
H -2.190368 2.380334 0.230333
C -3.268833 0.505803 0.296707
C -3.370784 -0.829245 0.730893
C -4.316794 1.017662 -0.487821
C -4.468269 -1.609398 0.391507
H -2.583539 -1.263241 1.338072
C -5.415522 0.235469 -0.827386
H -4.260031 2.045637 -0.834038
C -5.498793 -1.084896 -0.390814
H -4.521730 -2.636107 0.738565
H -6.208310 0.658165 -1.435788
H -6.353398 -1.698158 -0.654421

39
TSII_ket_conf_4 Eopt -698.050868
C -1.398620 -0.145137 0.516226
C -2.599565 -0.664216 -0.244685
C -0.654596 0.923160 -0.241104
H -1.742210 0.264305 1.473252
H -0.696971 -0.961213 0.739875
H -2.423890 -1.373279 -1.049993
C -1.264683 2.287987 -0.289250
H -1.576884 2.624430 0.703990
H -0.570104 3.025342 -0.704162
H -2.162448 2.297202 -0.925106
C 0.117660 0.482830 -1.444550
H -0.556890 0.222279 -2.274215
H 0.783198 1.270214 -1.810920
H 0.719027 -0.406776 -1.228693
C -3.885455 -0.221054 -0.004638
O -4.240891 0.629854 0.882248
C -5.009572 -0.811794 -0.862636
H -5.494540 0.012310 -1.401071
H -4.604212 -1.495297 -1.615312
C -6.056743 -1.532058 -0.013719
H -6.875612 -1.921664 -0.625148
H -5.609222 -2.375342 0.522272
H -6.482236 -0.852925 0.727820
C 1.114794 1.388910 1.257331
H 0.341542 1.630900 1.978575
H 1.394871 2.185250 0.574786
C 1.900945 0.300166 1.451992
H 1.629222 -0.401584 2.237676
C 3.066985 -0.079121 0.654427
C 3.567598 0.707471 -0.400109
C 3.732007 -1.283647 0.941659
C 4.677007 0.301325 -1.130061
H 3.084046 1.644996 -0.653474
C 4.843021 -1.689463 0.210291
H 3.363396 -1.906430 1.751633
C 5.322953 -0.900049 -0.832654
H 5.042100 0.925746 -1.938975
H 5.334484 -2.625508 0.454510
H 6.188043 -1.213631 -1.406426
39
TSII_ket_conf_6 Eopt -698.051031
C -0.792130 -0.065395 0.055581
C -2.028538 -0.684095 0.672974

C -0.846444 1.440269 0.059051
H 0.110952 -0.383571 0.593501
H -0.701889 -0.418482 -0.978684
H -2.072969 -0.771215 1.755707
C -0.676901 2.120414 1.380642
H 0.147481 1.679888 1.951247
H -0.481029 3.190870 1.262537
H -1.583933 2.026773 1.996095
C -1.761262 2.092356 -0.928396
H -1.646954 3.180785 -0.928490
H -1.586464 1.721720 -1.943248
H -2.812048 1.869185 -0.691468
C -3.121699 -1.056789 -0.084188
O -3.219535 -0.976505 -1.356826
C -4.342465 -1.616396 0.652922
H -4.541781 -2.625125 0.270196
H -4.141708 -1.708950 1.724930
C -5.579044 -0.746076 0.427640
H -5.800376 -0.663056 -0.638453
H -6.461527 -1.157176 0.926132
H -5.417052 0.265255 0.815193
C 1.217228 1.982473 -0.958967
H 0.850003 3.002580 -0.997433
H 0.904761 1.334507 -1.771984
C 2.268038 1.678279 -0.155461
H 2.606691 2.426943 0.557854
C 2.972859 0.398040 -0.094875
C 2.662752 -0.691863 -0.930003
C 4.013264 0.230849 0.835270
C 3.361802 -1.887755 -0.833253
H 1.863063 -0.606324 -1.657976
C 4.712780 -0.967397 0.931595
H 4.270013 1.058074 1.490738
C 4.391016 -2.036479 0.098282
H 3.101079 -2.713132 -1.487610
H 5.509923 -1.067008 1.660985
H 4.932504 -2.973104 0.171954
39
TSII_ket_conf_7 Eopt -698.051323
C -1.795523 1.129333 -0.921863
C -3.191561 0.844950 -0.409256
C -0.766490 1.069227 0.175814
H -1.547073 0.385868 -1.687978
H -1.749510 2.120255 -1.394825
H -3.719619 1.646125 0.102081

C -0.362119 -0.280065 0.676427
H -1.144352 -0.709179 1.321476
H -0.199684 -0.985785 -0.142382
H 0.552800 -0.222918 1.276004
C -0.771199 2.169460 1.189792
H -0.959173 3.145130 0.730738
H -1.553328 2.009016 1.946820
H 0.182046 2.217434 1.727266
C -3.773524 -0.405083 -0.491279
O -3.259933 -1.445355 -1.029429
C -5.167047 -0.581319 0.120538
H -5.546042 0.370076 0.506802
H -5.851643 -0.907149 -0.672491
C -5.159357 -1.630809 1.232218
H -4.495985 -1.326141 2.048517
H -6.157278 -1.785173 1.652369
H -4.800114 -2.588648 0.850312
C 1.155260 1.677125 -1.073980
H 0.668809 2.636877 -1.211558
H 0.866446 0.894826 -1.768928
C 2.279363 1.592357 -0.319590
H 2.578358 2.459014 0.266374
C 3.122831 0.408113 -0.156337
C 4.227131 0.464491 0.711347
C 2.885907 -0.802663 -0.833664
C 5.058810 -0.634713 0.896589
H 4.428920 1.388643 1.245305
C 3.717313 -1.899478 -0.648613
H 2.042337 -0.888839 -1.510266
C 4.809178 -1.825661 0.218107
H 5.903234 -0.561465 1.574061
H 3.511897 -2.821413 -1.182774
H 5.454571 -2.685309 0.361007
39
TSII_ket_conf_8 Eopt -698.050896
C -0.842297 0.226391 0.085743
C -2.135884 -0.260026 0.705211
C -0.728151 1.728513 0.102531
H 0.022864 -0.194484 0.615698
H -0.796769 -0.126169 -0.951494
H -2.193089 -0.316340 1.789393
C -0.491647 2.374151 1.431057
H -0.179791 3.417959 1.324286
H -1.406174 2.373684 2.042471
H 0.277160 1.840903 2.000262

C -1.552420 2.489631 -0.886629
H -2.624155 2.393915 -0.658890
H -1.310518 3.556894 -0.879123
H -1.413628 2.107981 -1.903082
C -3.255984 -0.551898 -0.048272
O -3.344796 -0.495271 -1.323036
C -4.515322 -1.006302 0.697646
H -4.353796 -0.984490 1.780019
H -5.317389 -0.291167 0.475062
C -4.963328 -2.401909 0.264909
H -5.146161 -2.429499 -0.811172
H -4.192702 -3.145466 0.492780
H -5.882711 -2.707613 0.772336
C 1.386508 2.045230 -0.904758
H 1.142411 3.102189 -0.916287
H 0.998626 1.458646 -1.731719
C 2.394930 1.598118 -0.114295
H 2.821552 2.281398 0.617276
C 2.941460 0.241536 -0.093815
C 2.505719 -0.774636 -0.964754
C 3.950536 -0.079792 0.830173
C 3.055087 -2.048621 -0.907288
H 1.725343 -0.569405 -1.689662
C 4.500294 -1.356133 0.886893
H 4.302447 0.688848 1.512189
C 4.055326 -2.350665 0.018742
H 2.699353 -2.814821 -1.588282
H 5.277083 -1.574550 1.612282
H 4.479443 -3.347772 0.061389
39
TSII_ket_conf_9 Eopt -698.047212
C 1.903626 -0.929703 0.865881
C 3.280569 -0.902251 0.222839
C 0.807050 -1.245494 -0.120869
H 1.890537 -1.696936 1.652213
H 1.674134 0.018155 1.364558
H 3.759989 -1.873770 0.091530
C 0.795449 -2.614924 -0.724889
H 1.070675 -3.383282 0.004302
H -0.192489 -2.859140 -1.130196
H 1.507073 -2.688072 -1.560220
C 0.314126 -0.141021 -1.000600
H 0.150741 0.784581 -0.441233
H 1.038386 0.083061 -1.799078
H -0.625297 -0.416935 -1.490951

C	3.943274	0.179498	-0.324792
O	5.082906	0.122427	-0.910754
C	3.335526	1.583276	-0.224559
H	3.268505	1.984175	-1.243195
H	2.320704	1.568366	0.176180
C	4.206836	2.512504	0.622383
H	5.221401	2.560916	0.222247
H	3.804357	3.529077	0.649904
H	4.270346	2.151218	1.653959
C	-0.998186	-1.444007	1.391134
H	-0.524438	-2.359165	1.729934
H	-0.634093	-0.526187	1.842034
C	-2.183081	-1.499921	0.732462
H	-2.551755	-2.470203	0.406050
C	-3.005177	-0.355432	0.339575
C	-2.694878	0.971045	0.693677
C	-4.162661	-0.571456	-0.427882
C	-3.504456	2.025693	0.292670
H	-1.811983	1.181527	1.287852
C	-4.972885	0.485354	-0.829023
H	-4.422342	-1.587158	-0.712037
C	-4.648453	1.792592	-0.472685
H	-3.242038	3.039133	0.578228
H	-5.859088	0.287229	-1.422920
H	-5.276643	2.619468	-0.785057

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TSII_sty Eopt -386.688238

C	2.121114	-0.996995	-0.515620
C	0.779733	-0.940289	-0.862671
C	-0.079728	0.083438	-0.390082
C	0.517150	1.052014	0.450336
C	1.865418	0.991140	0.799534
C	2.684657	-0.030854	0.325526
H	2.739572	-1.800527	-0.905359
H	0.366023	-1.703804	-1.517477
H	-0.085028	1.869061	0.835417
H	2.279902	1.757953	1.448006
H	3.733918	-0.074194	0.596024
C	-1.505710	0.067297	-0.694591
H	-1.697761	-0.408245	-1.662301
C	-2.255880	1.381419	-0.536580
H	-1.800172	2.230376	-1.070324
H	-3.280873	1.282915	-0.906757
H	-2.063424	-0.806261	0.272358
O	-2.576827	-1.519612	1.129775

H -2.000013 -1.515774 1.902335
H -2.338050 1.682367 0.514761
23
TSI_ket_conf_1 Eopt -388.441464
C -1.366307 -1.280074 -0.226494
C -0.141876 -0.648914 -0.803505
C -1.626757 0.152225 0.093800
H -2.055542 -1.754532 -0.927764
H -1.154322 -1.926642 0.625494
H -0.218710 -0.253109 -1.812041
C -1.335195 0.641524 1.478673
H -1.221509 1.731721 1.508050
H -2.132392 0.387149 2.198937
H -0.408196 0.195725 1.853444
C -2.618117 0.900448 -0.745055
H -3.662606 0.705549 -0.442785
H -2.471099 1.984906 -0.685799
H -2.545018 0.615624 -1.801148
C 1.133157 -0.724194 -0.189356
O 1.365529 -1.344888 0.920090
C 2.236365 0.161081 -0.749106
H 3.177872 -0.403236 -0.762714
H 2.015780 0.448794 -1.783471
C 2.436176 1.427406 0.094906
H 3.260219 2.044391 -0.277944
H 1.530026 2.042039 0.091297
H 2.656592 1.163711 1.132538
23
TSI_ket_conf_10 Eopt -388.441064
C -1.257309 0.095225 1.296802
C -0.116669 -0.548274 0.578942
C -1.835742 -0.026452 -0.071455
H -1.738316 -0.490460 2.082802
H -1.037002 1.109487 1.630856
H -0.133383 -1.630744 0.497436
C -1.856299 1.188388 -0.947324
H -0.928011 1.756127 -0.833850
H -1.964592 0.925026 -2.005872
H -2.688428 1.872573 -0.704204
C -2.841737 -1.109934 -0.319474
H -2.570367 -2.035831 0.200568
H -3.851042 -0.837133 0.037602
H -2.938112 -1.346506 -1.385046
C 1.059646 0.150283 0.205306
O 1.246572 1.410021 0.415751

C 2.075498 -0.578703 -0.663094
H 1.813677 -1.638903 -0.750347
H 2.036295 -0.161951 -1.683128
C 3.507572 -0.438295 -0.145023
H 4.232064 -0.906907 -0.817954
H 3.772702 0.616368 -0.043132
H 3.612187 -0.904749 0.840178
23
TSI_ket_conf_11 Eopt -388.436544
C 1.128733 -0.276923 1.266470
C 0.271123 -1.012656 0.285667
C 1.677446 0.252390 -0.014185
H 0.615349 0.446912 1.899736
H 1.801982 -0.893290 1.866564
H 0.718374 -1.917336 -0.122028
C 2.991130 -0.284892 -0.496411
H 3.851101 0.163578 0.032227
H 3.062106 -1.367474 -0.338044
H 3.144303 -0.097468 -1.565010
C 1.269751 1.628373 -0.439816
H 1.419718 1.786263 -1.514101
H 0.210337 1.808405 -0.226952
H 1.836553 2.419197 0.080628
C -1.100394 -0.825623 -0.024858
O -1.682933 -1.491773 -0.968193
C -1.954241 0.199463 0.712847
H -2.711511 -0.337818 1.304223
H -1.364107 0.779487 1.427431
C -2.694844 1.149279 -0.233087
H -3.312472 0.581710 -0.931684
H -3.345394 1.836594 0.316387
H -1.995105 1.748960 -0.823597
23
TSI_ket_conf_4 Eopt -388.437182
C -0.955415 -0.275655 -1.250090
C -0.174713 0.746136 -0.484843
C -1.788049 -0.188488 -0.017521
H -1.420951 0.076192 -2.173395
H -0.453028 -1.227944 -1.421884
H -0.542570 1.766576 -0.570239
C -1.657836 -1.275285 1.005412
H -2.207601 -2.190419 0.725544
H -0.610960 -1.566021 1.143816
H -2.042510 -0.961610 1.982379
C -3.078689 0.570971 -0.090354

H -3.886515 -0.015171 -0.563709
H -3.440225 0.864295 0.901367
H -2.971045 1.484959 -0.685973
C 1.068553 0.598118 0.181851
O 1.565255 1.535571 0.920009
C 1.840259 -0.714166 0.147260
H 1.943392 -1.084371 1.178156
H 1.310119 -1.489790 -0.411520
C 3.244717 -0.540201 -0.440180
H 3.825076 -1.466615 -0.386135
H 3.191535 -0.237643 -1.491015
H 3.790273 0.234415 0.103320
23
TSI_ket_conf_8 Eopt -388.440028
C -1.201785 -0.423574 -1.233732
C 0.082555 0.157846 -0.739256
C -1.641543 0.133836 0.077521
H -1.636675 0.031545 -2.125889
H -1.184270 -1.511187 -1.306006
H 0.245122 1.210518 -0.941256
C -1.800135 -0.808543 1.231329
H -1.783031 -0.281967 2.192607
H -2.751032 -1.369068 1.193680
H -0.991575 -1.545591 1.235131
C -2.433312 1.407114 0.074192
H -3.497822 1.240839 -0.170519
H -2.408814 1.909875 1.047539
H -2.052116 2.114231 -0.671622
C 1.145861 -0.636082 -0.242622
O 1.092157 -1.924515 -0.150796
C 2.337788 0.039885 0.427299
H 2.268718 -0.143189 1.512038
H 3.242968 -0.491627 0.107277
C 2.523962 1.537626 0.193638
H 3.435612 1.895878 0.679867
H 2.605705 1.768960 -0.872650
H 1.689614 2.118251 0.595957
19
TSI_sty_conf_conf_1 Eopt -386.051985
C -2.474048 0.613373 0.548013
C -1.242764 1.228561 0.420327
C -0.125987 0.555087 -0.154553
C -0.342019 -0.787421 -0.580963
C -1.582542 -1.392992 -0.446253
C -2.663521 -0.707184 0.115067

H -3.301671 1.160179 0.989425
H -1.112916 2.252463 0.760475
H 0.479229 -1.350321 -1.011869
H -1.711559 -2.418362 -0.779799
H -3.629692 -1.188284 0.217282
C 1.126272 1.206284 -0.289438
H 1.197305 2.201485 0.145683
C 2.327903 0.598815 -0.821277
H 2.164397 -0.084792 -1.661059
H 3.101389 1.327619 -1.075537
H 2.841685 -0.167668 0.080492
O 3.394252 -1.007742 1.027572
H 2.678059 -1.557524 1.368784
3
h2o Eopt -76.416406
H 0.771478 -0.461636 0.000000
O 0.000000 0.115425 -0.000000
H -0.771478 -0.461762 -0.000000
2
oh_anion Eopt -75.895588
H 0.000000 0.000000 -0.857920
O 0.000000 0.000000 0.107240
32
perylene_S0 Eopt -769.277821
C -0.017390 1.248227 -0.739484
C 0.017390 1.248227 0.739484
C 0.064016 2.420397 1.471831
C 0.076566 2.414590 2.880119
C 0.039596 1.230410 3.567176
C 0.000000 0.000000 2.863964
C 0.000000 0.000000 1.438488
C -0.017390 -1.248227 0.739484
C -0.064016 -2.420397 1.471831
C -0.076566 -2.414590 2.880119
C -0.039596 -1.230410 3.567176
C 0.000000 0.000000 -1.438488
C 0.017390 -1.248227 -0.739484
C 0.064016 -2.420397 -1.471831
C 0.076566 -2.414590 -2.880119
C 0.039596 -1.230410 -3.567176
C 0.000000 0.000000 -2.863964
C -0.039596 1.230410 -3.567176
C -0.076566 2.414590 -2.880119
C -0.064016 2.420397 -1.471831
H 0.093665 3.380490 0.972954

H 0.113262 3.358172 3.413003
H 0.042291 1.212689 4.652316
H -0.093665 -3.380490 0.972954
H -0.113262 -3.358172 3.413003
H -0.042291 -1.212689 4.652316
H 0.093665 -3.380490 -0.972954
H 0.113262 -3.358172 -3.413003
H 0.042291 -1.212689 -4.652316
H -0.042291 1.212689 -4.652316
H -0.113262 3.358172 -3.413003
H -0.093665 3.380490 -0.972954
32
perylene_radical_anion Eopt -769.374238
C 0.000055 1.247934 -0.726434
C -0.000055 1.247934 0.726434
C -0.000208 2.444988 1.473346
C -0.000235 2.428864 2.865751
C -0.000114 1.233632 3.564118
C 0.000000 0.000000 2.868052
C 0.000000 0.000000 1.428495
C 0.000055 -1.247934 0.726434
C 0.000208 -2.444988 1.473346
C 0.000235 -2.428864 2.865751
C 0.000114 -1.233632 3.564118
C 0.000000 0.000000 -1.428495
C -0.000055 -1.247934 -0.726434
C -0.000208 -2.444988 -1.473346
C -0.000235 -2.428864 -2.865751
C -0.000114 -1.233632 -3.564118
C 0.000000 0.000000 -2.868052
C 0.000114 1.233632 -3.564118
C 0.000235 2.428864 -2.865751
C 0.000208 2.444988 -1.473346
H -0.000333 3.404350 0.972971
H -0.000355 3.370240 3.406972
H -0.000105 1.223176 4.649685
H 0.000333 -3.404350 0.972971
H 0.000355 -3.370240 3.406972
H 0.000105 -1.223176 4.649685
H -0.000333 -3.404350 -0.972971
H -0.000355 -3.370240 -3.406972
H -0.000105 -1.223176 -4.649685
H 0.000105 1.223176 -4.649685
H 0.000355 3.370240 -3.406972
H 0.000333 3.404350 -0.972971

26
pyrene_S0 Eopt -615.667532
C 1.424889 1.230610 0.000000
C 0.677045 2.463030 0.000001
C -0.677045 2.463030 0.000000
C -1.424889 1.230610 0.000000
C -2.824099 1.208563 0.000000
C -3.513255 0.000000 -0.000001
C -2.824099 -1.208563 0.000000
C 0.713870 0.000000 0.000000
C -0.713870 0.000000 0.000000
C -1.424889 -1.230610 0.000000
C -0.677045 -2.463030 0.000001
C 0.677045 -2.463030 0.000000
C 1.424889 -1.230610 0.000000
C 2.824099 -1.208563 0.000000
C 3.513255 0.000000 -0.000001
C 2.824099 1.208563 0.000000
H 1.229270 3.397691 0.000001
H -1.229270 3.397691 0.000001
H -3.367383 2.148270 0.000000
H -4.597759 0.000000 -0.000001
H -3.367383 -2.148270 0.000000
H -1.229270 -3.397691 0.000001
H 1.229270 -3.397691 0.000001
H 3.367383 -2.148270 0.000000
H 4.597759 0.000000 -0.000001
H 3.367383 2.148270 0.000000
26
pyrene_radical_anion Eopt -615.748138
C 1.432468 1.241058 0.000000
C 0.690789 2.446739 0.000000
C -0.690789 2.446739 0.000000
C -1.432468 1.241058 0.000000
C -2.857963 1.214035 -0.000001
C -3.535087 0.000000 0.000000
C -2.857963 -1.214035 0.000000
C 0.715805 0.000000 0.000000
C -0.715805 0.000000 0.000000
C -1.432468 -1.241058 0.000000
C -0.690789 -2.446739 0.000000
C 0.690789 -2.446739 0.000000
C 1.432468 -1.241058 0.000000
C 2.857963 -1.214035 -0.000001
C 3.535087 0.000000 0.000000

C	2.857963	1.214035	0.000001
H	1.232530	3.388788	0.000001
H	-1.232530	3.388788	0.000000
H	-3.403478	2.152541	-0.000001
H	-4.621954	0.000000	0.000000
H	-3.403478	-2.152541	0.000001
H	-1.232530	-3.388788	0.000001
H	1.232530	-3.388788	0.000000
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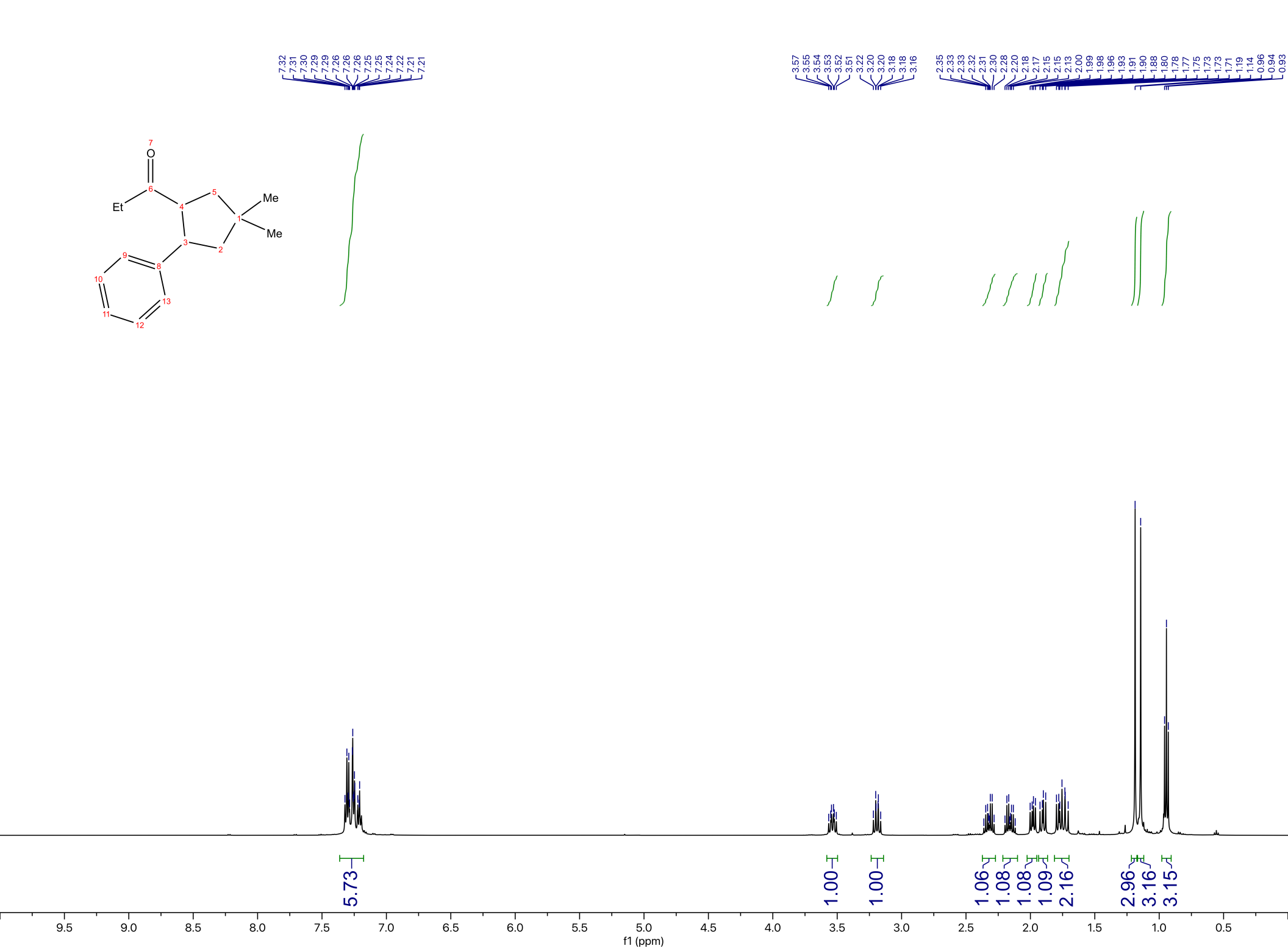
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7.29
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7.26
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7.25
7.24
7.22
7.21
7.21
3.57
3.55
3.54
3.53
3.52
3.51
3.22
3.20
3.20
3.18
3.18
3.16
2.35
2.33
2.33
2.32
2.31
2.30
2.28
2.20
2.18
2.17
2.15
2.15
2.13
2.00
1.99
1.98
1.96
1.93
1.91
1.90
1.88
1.80
1.78
1.77
1.75
1.73
1.73
1.71
1.19
1.14
0.96
0.94
0.93
O
Et
Me
Me
5.73
1.00
1.00
1.06
1.08
1.08
1.09
2.16
2.96
3.16
3.15
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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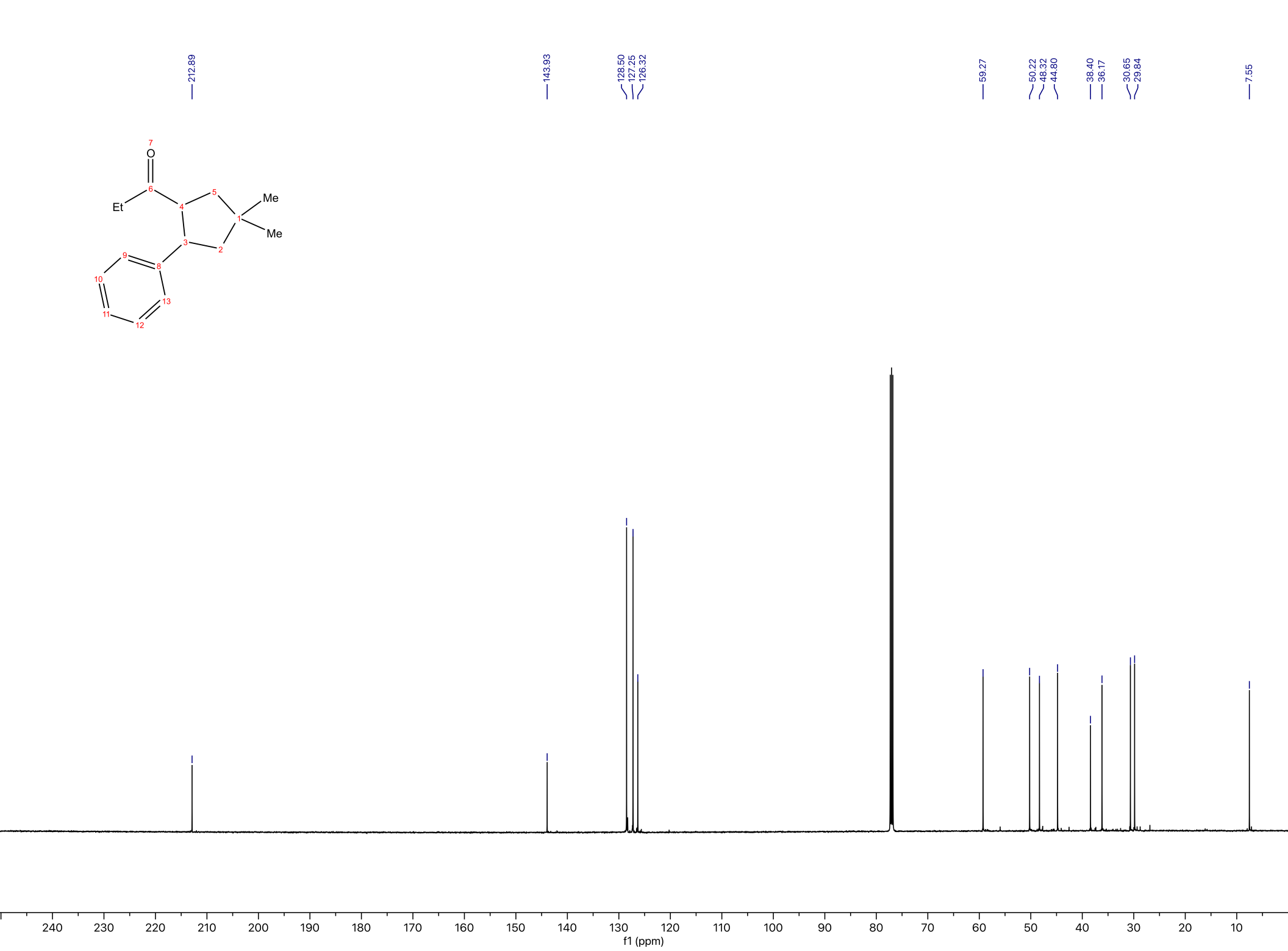
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


212.89
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128.50
127.25
126.32
59.27
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44.80
38.40
36.17
30.65
29.84
7.55
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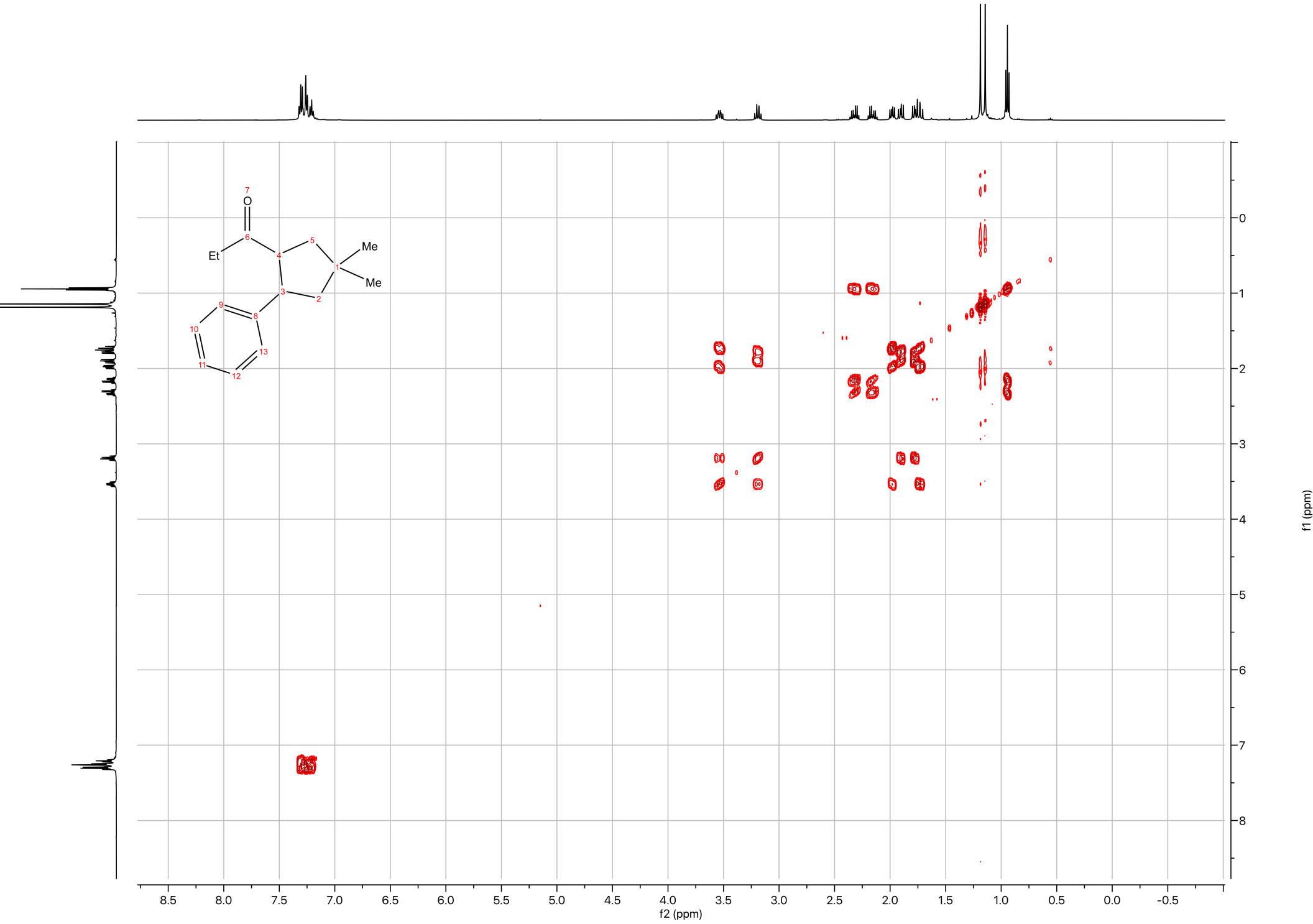
Et
Me
Me
f1 (ppm)


7
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6
Et
4
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Me
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Me
3
2
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8
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11
12
8.5
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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
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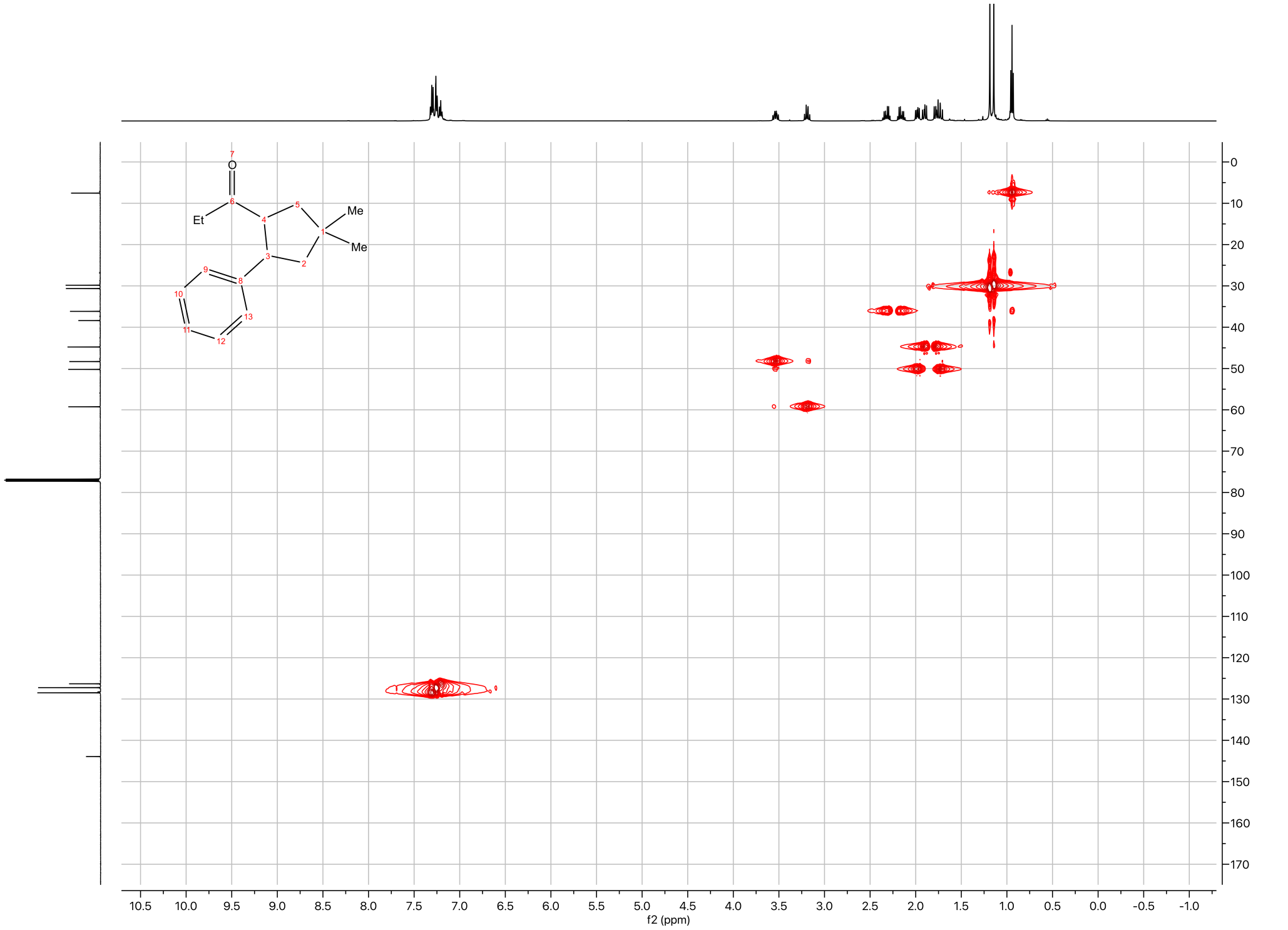
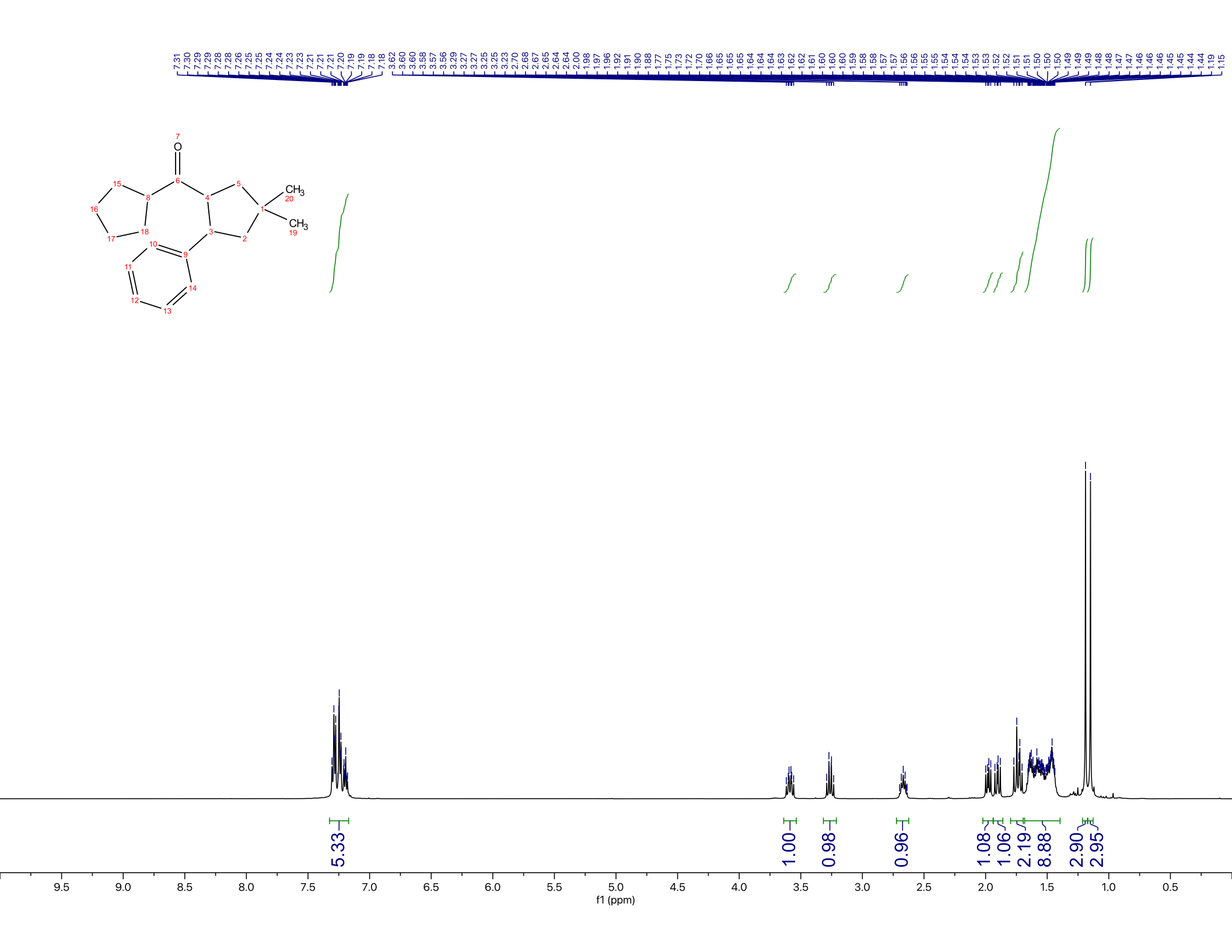
-0.5
f2 (ppm)
0
1
2
3
4
5
6
7
8
f1 (ppm)


O
Et
Me
Me
f2 (ppm)
f1 (ppm)


7.31 7.30 7.29 7.29 7.28 7.28 7.26 7.25 7.25 7.24 7.24 7.23 7.23 7.21 7.21 7.21 7.20 7.19 7.19 7.18 7.18
3.62 3.60 3.60 3.58 3.57 3.56 3.29 3.27 3.27 3.25 3.25 3.23 2.70 2.68 2.67 2.65 2.64 2.64 2.00 1.98 1.97 1.96 1.92 1.91 1.90 1.88 1.77 1.75 1.73 1.72 1.70 1.66 1.65 1.65 1.64 1.64 1.64 1.63 1.62 1.62 1.61 1.60 1.60 1.60 1.59 1.58 1.58 1.57 1.57 1.56 1.56 1.55 1.55 1.54 1.54 1.54 1.53 1.53 1.52 1.52 1.51 1.51 1.50 1.50 1.50 1.49 1.49 1.49 1.48 1.48 1.47 1.47 1.46 1.46 1.46 1.45 1.45 1.44 1.44 1.19 1.15
O
CH3
CH3
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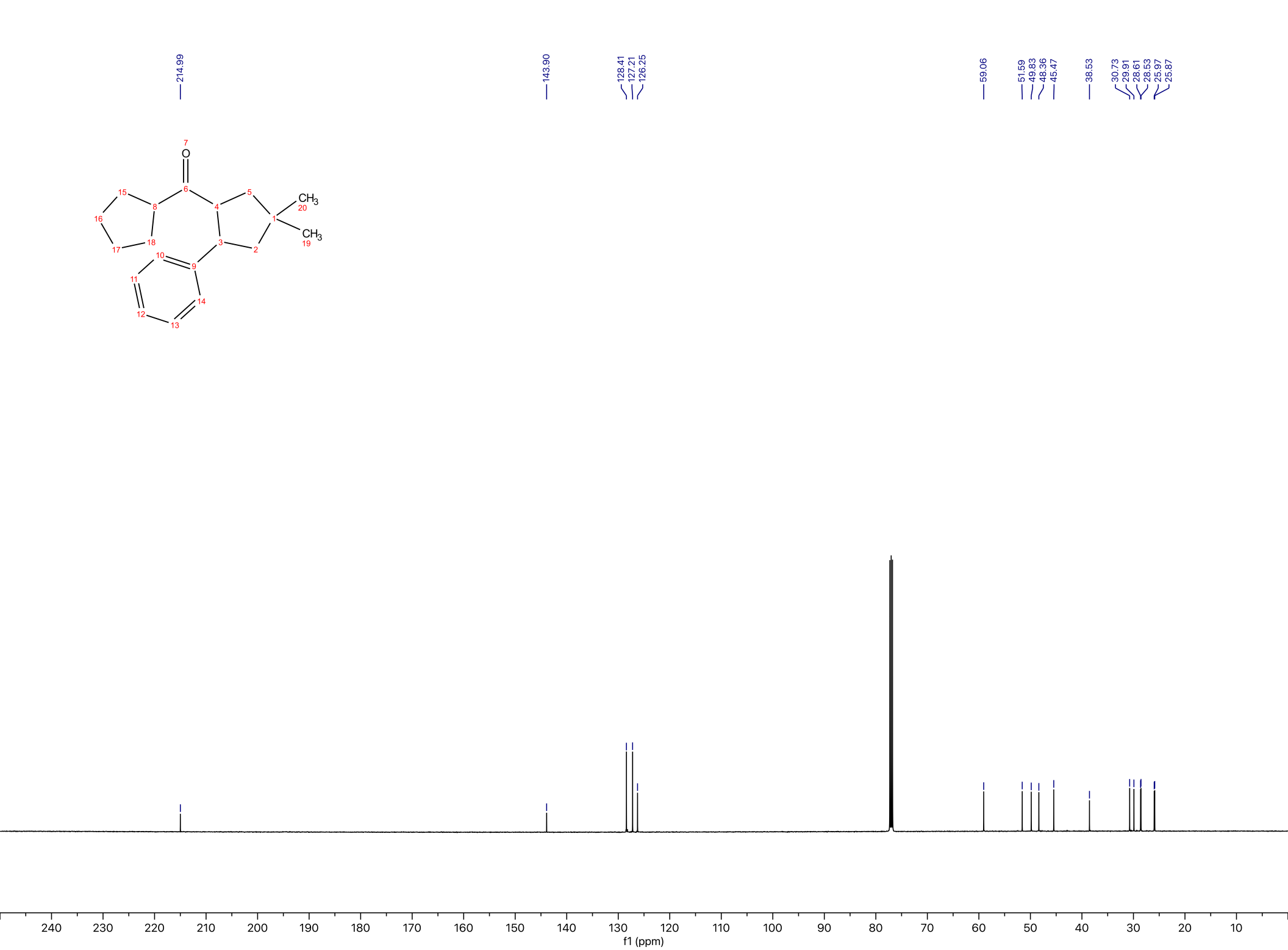
0.96
1.08
1.06
2.19
8.88
2.90
2.95
f1 (ppm)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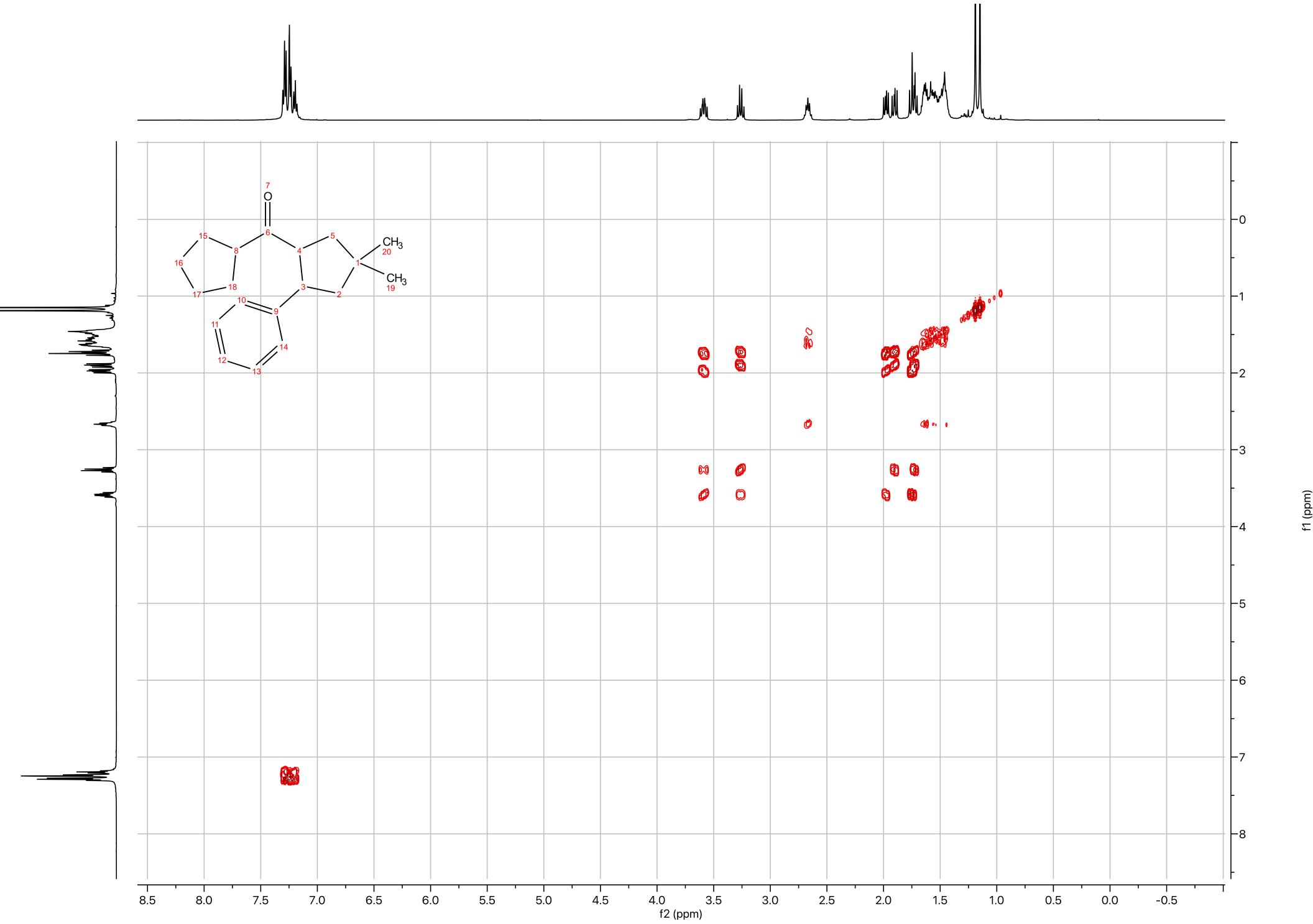
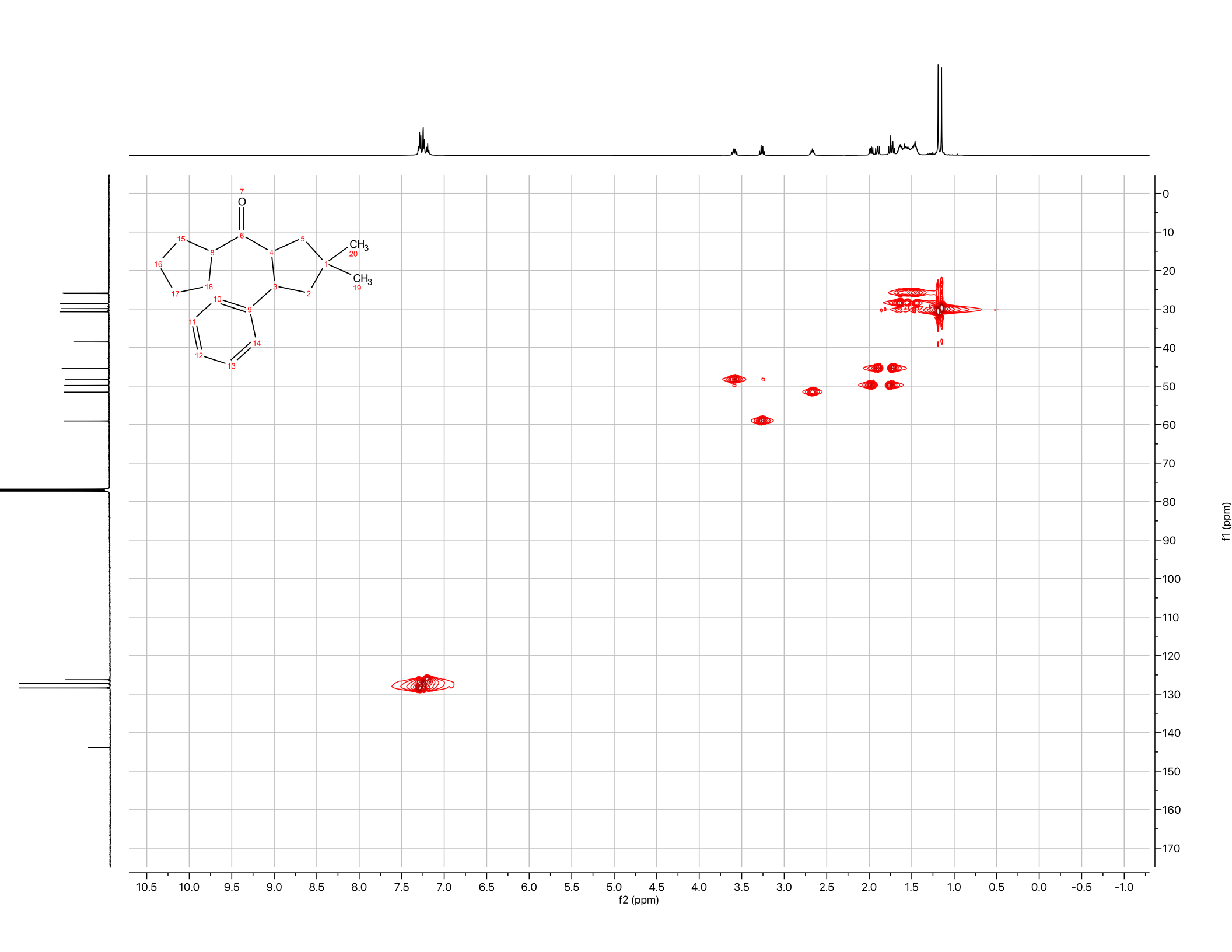
59.06
51.59
49.83
48.36
45.47
38.53
30.73
29.91
28.61
28.53
25.97
25.87
O
CH3
CH3
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


O
CH3
20
CH3
19
f2 (ppm)
f1 (ppm)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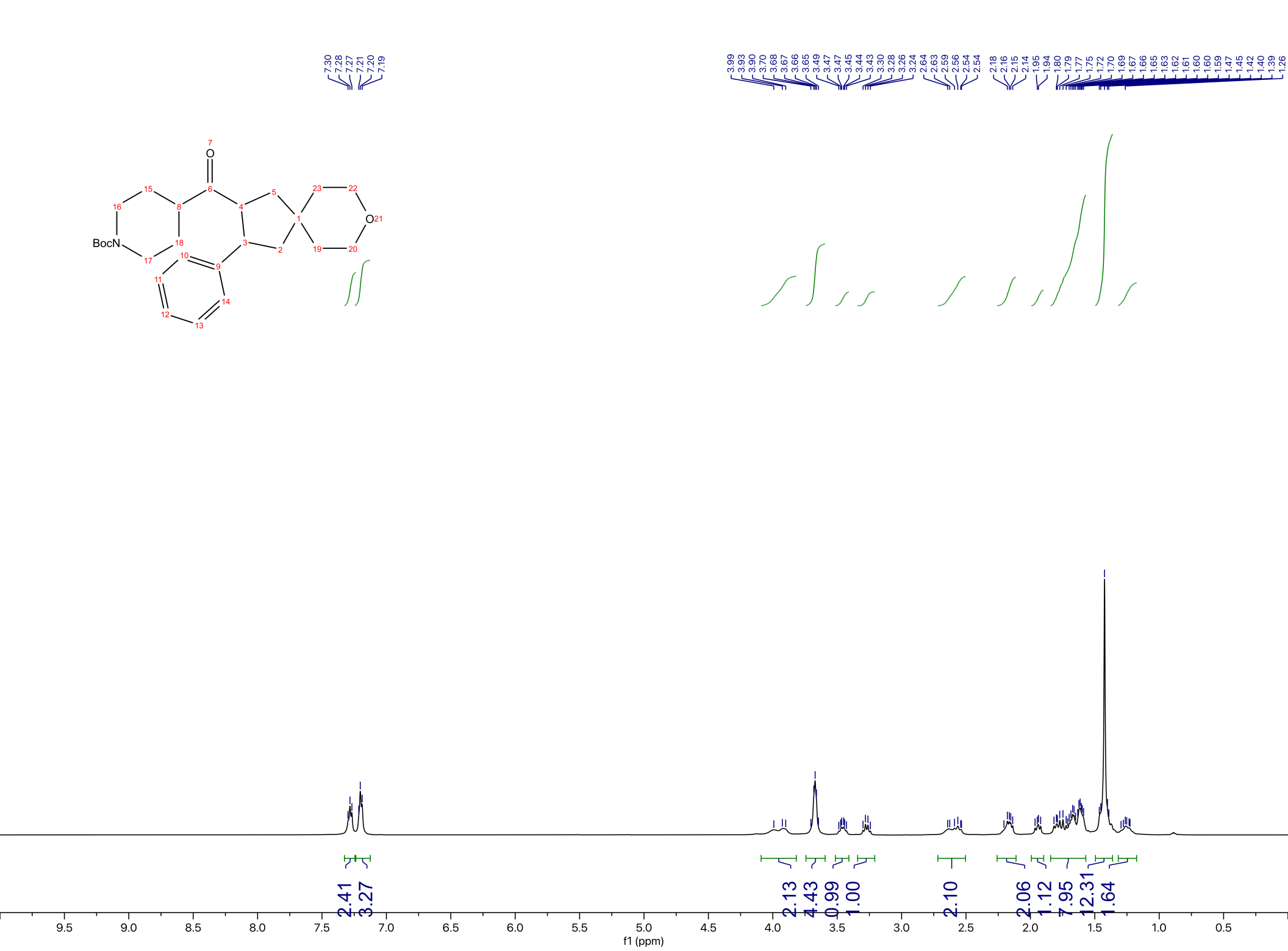
CH3
20
CH3
19
f2 (ppm)
f1 (ppm)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3.66
3.65
3.49
3.47
3.45
3.44
3.43
3.30
3.28
3.26
3.24
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2.63
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2.56
2.54
2.54
2.18
2.16
2.15
2.14
1.95
1.94
1.80
1.79
1.77
1.75
1.72
1.70
1.69
1.67
1.66
1.65
1.63
1.62
1.61
1.60
1.60
1.59
1.47
1.45
1.42
1.40
1.39
1.26
BocN
O
O
2.41
3.27
2.13
4.43
0.99
1.00
2.10
2.06
1.12
7.95
12.31
1.64
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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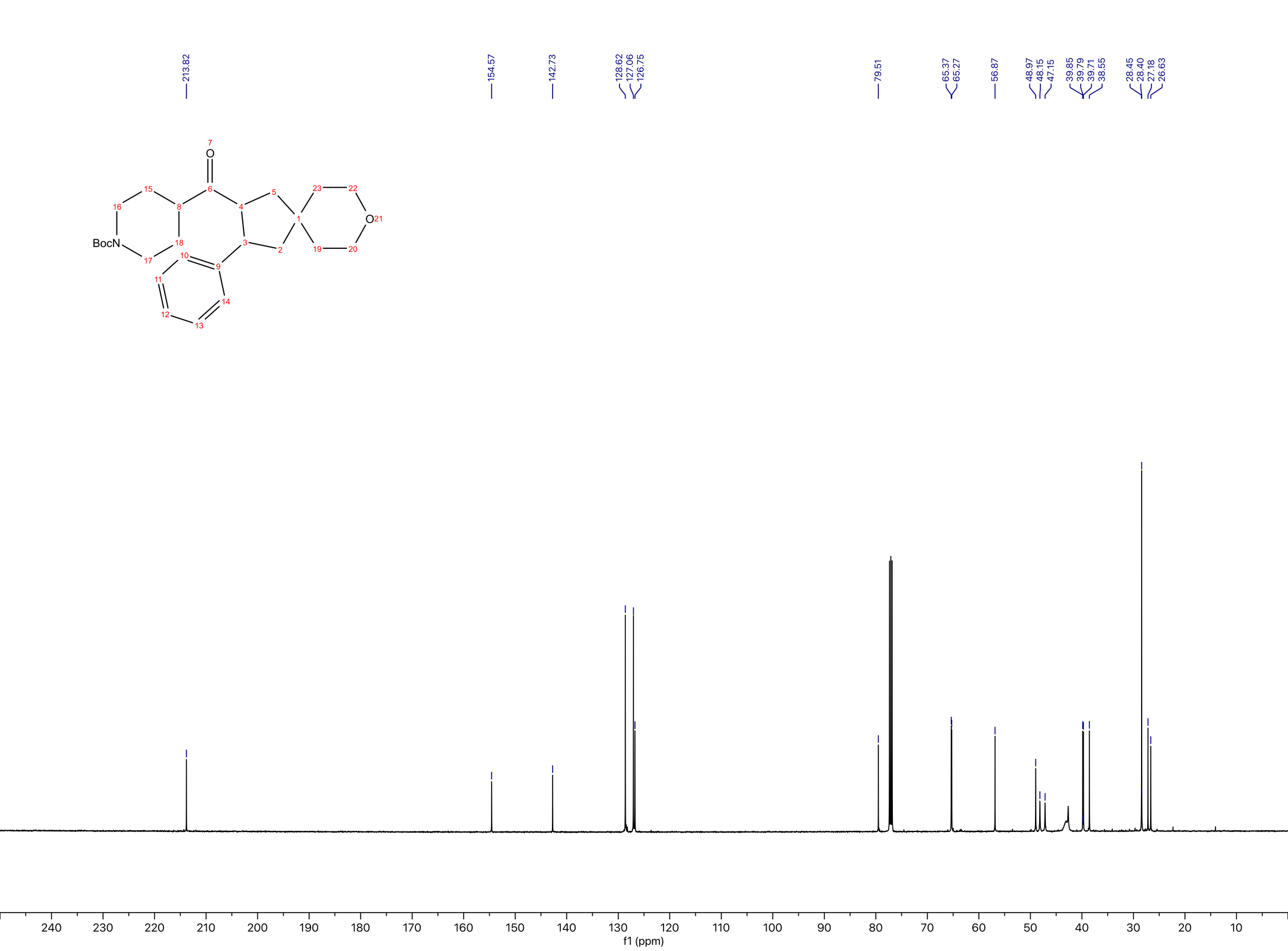
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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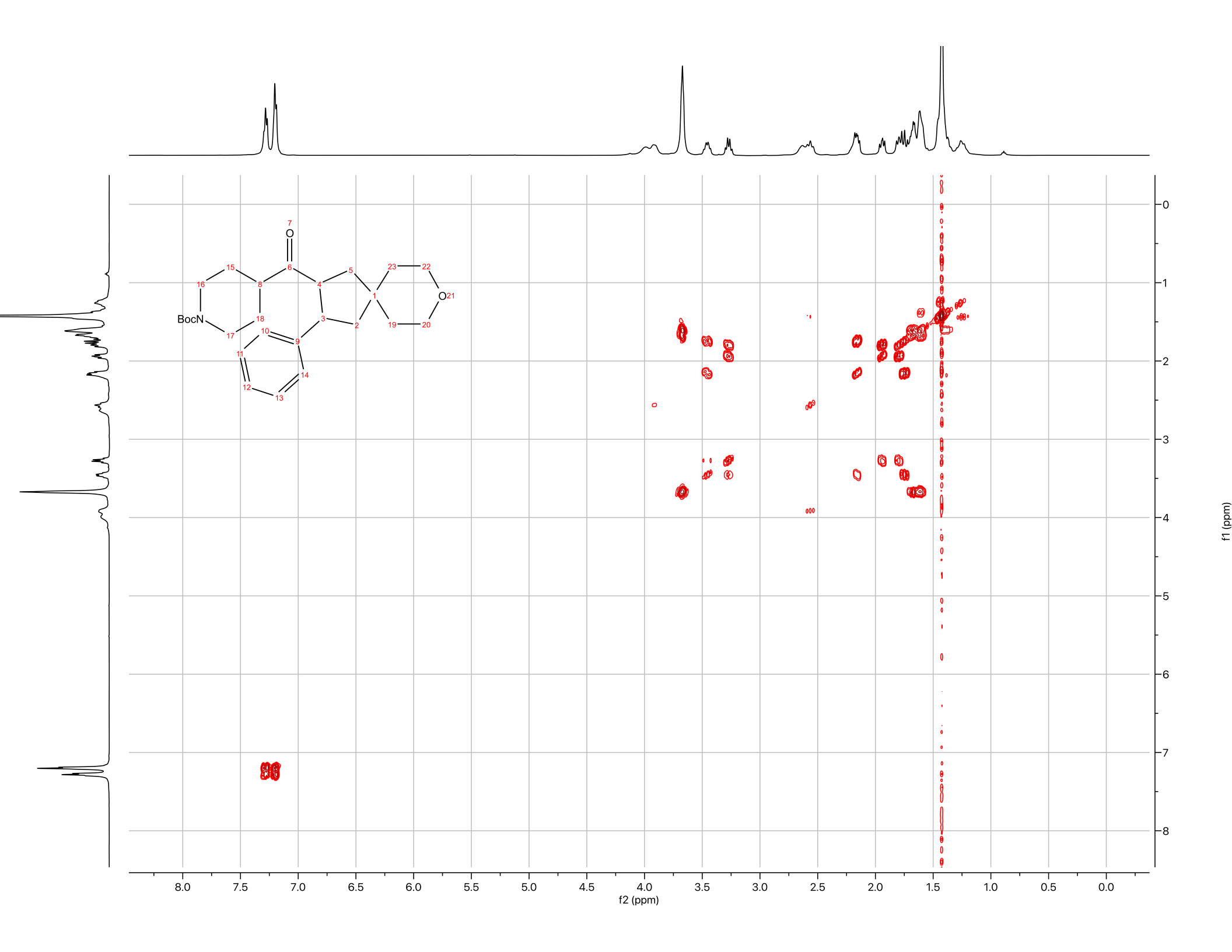
79.51
65.37
65.27
56.87
48.97
48.15
47.15
39.85
39.79
39.71
38.55
28.45
28.40
27.18
26.63
BocN
O
O
f1 (ppm)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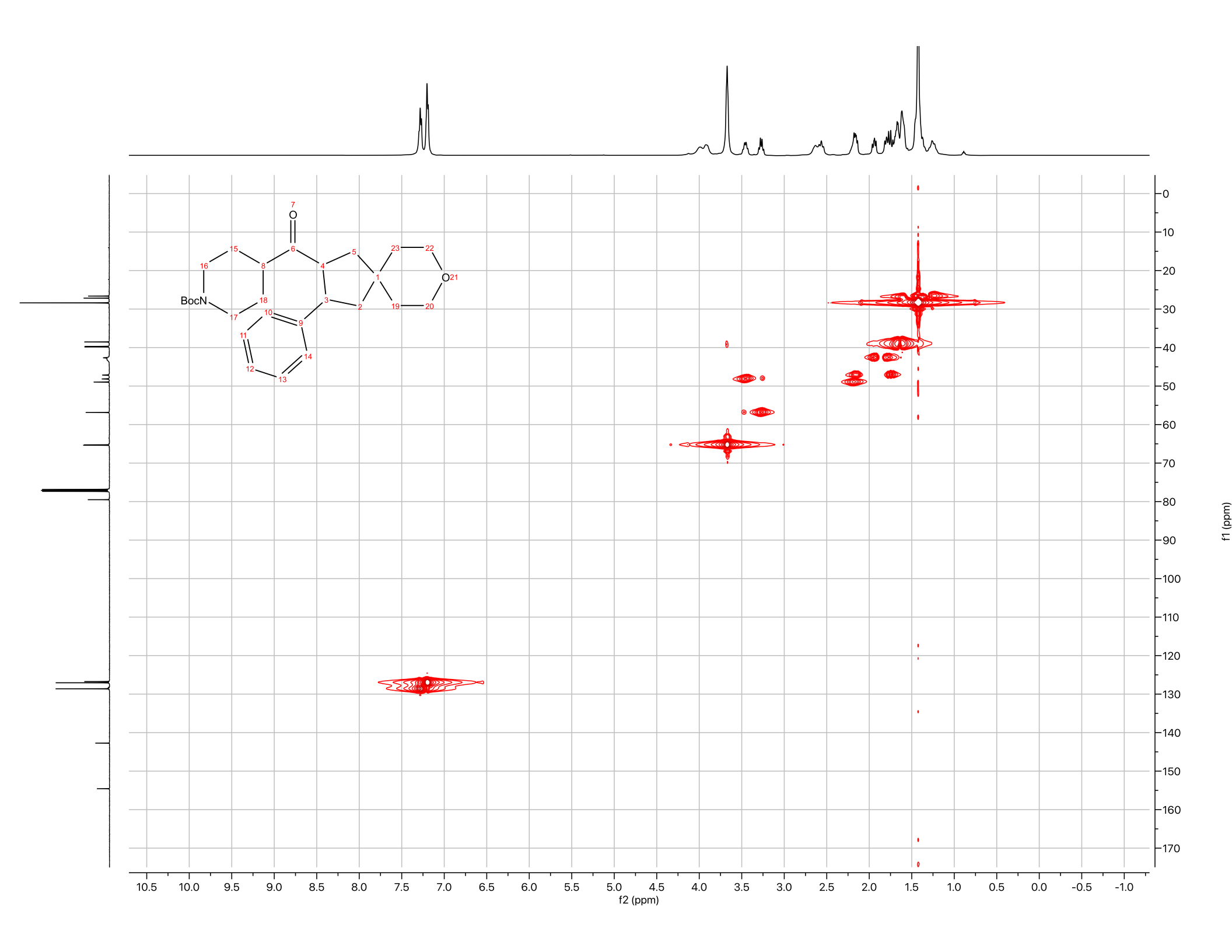
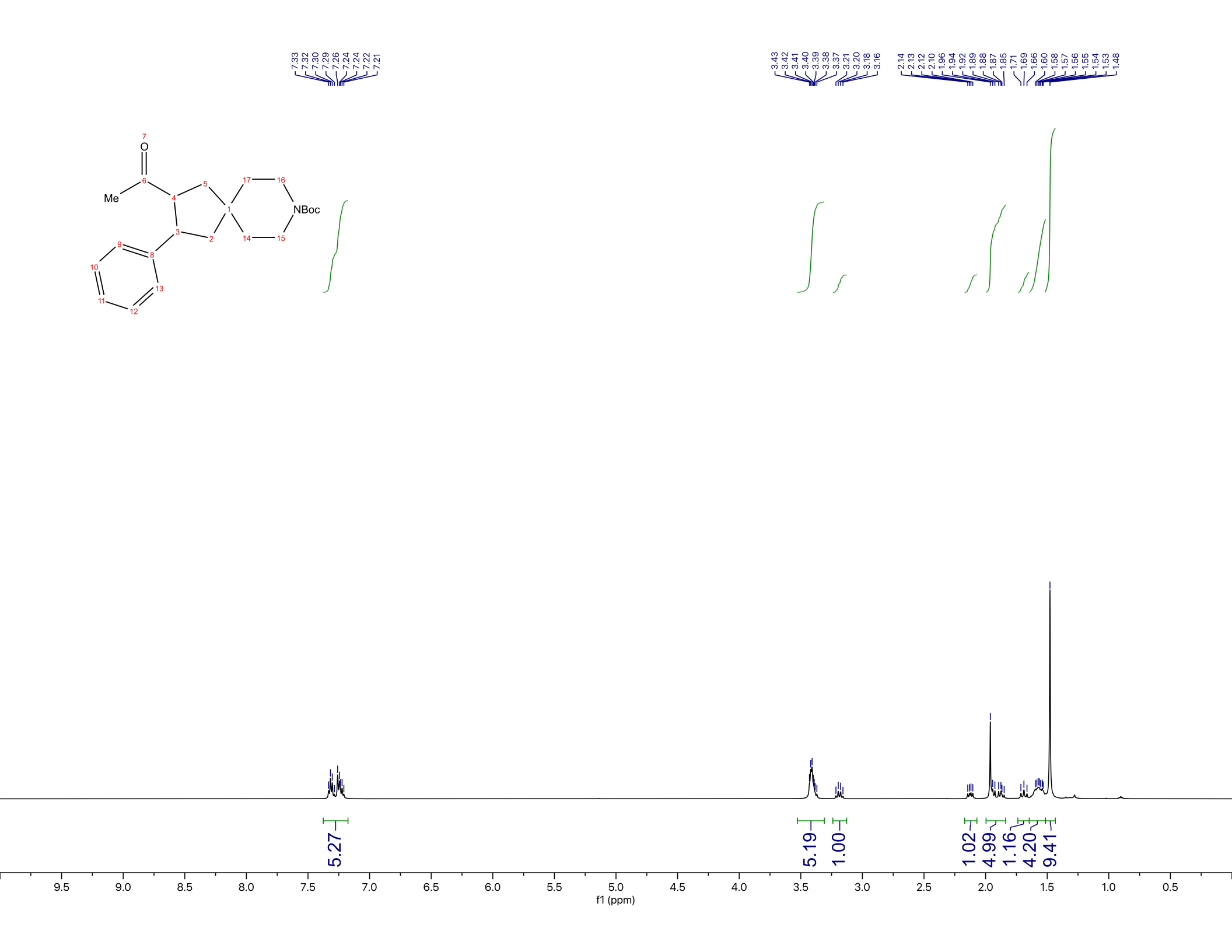
O
O21
f2 (ppm)
f1 (ppm)


BocN
O
O
f2 (ppm)
f1 (ppm)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3.42
3.41
3.40
3.39
3.38
3.37
3.21
3.20
3.18
3.16
2.14
2.13
2.12
2.10
1.96
1.94
1.92
1.89
1.88
1.87
1.85
1.71
1.69
1.66
1.60
1.58
1.57
1.56
1.55
1.54
1.53
1.48
O
Me
NBoc
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5.19
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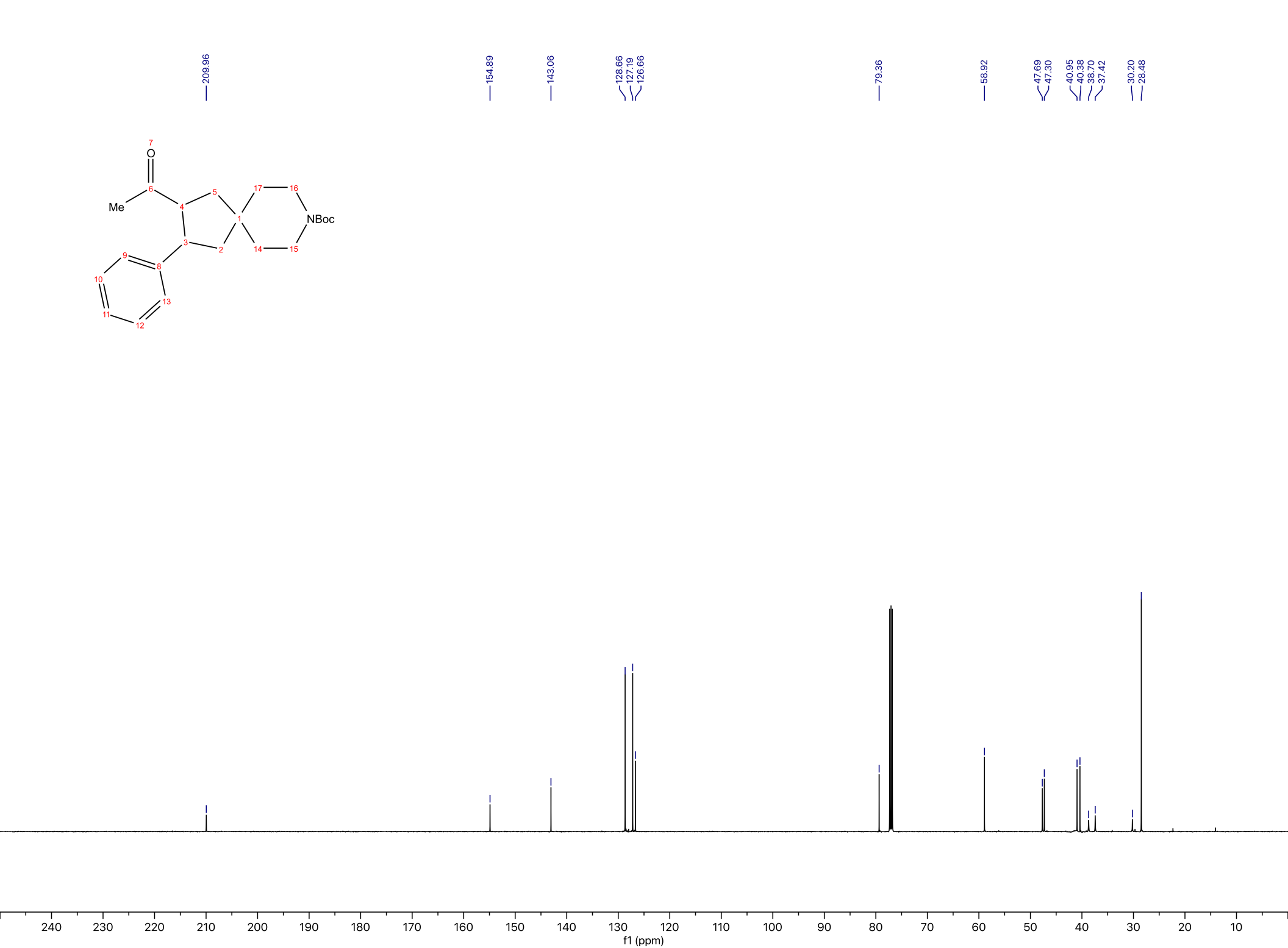
1.02
4.99
1.16
4.20
9.41
f1 (ppm)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126.66
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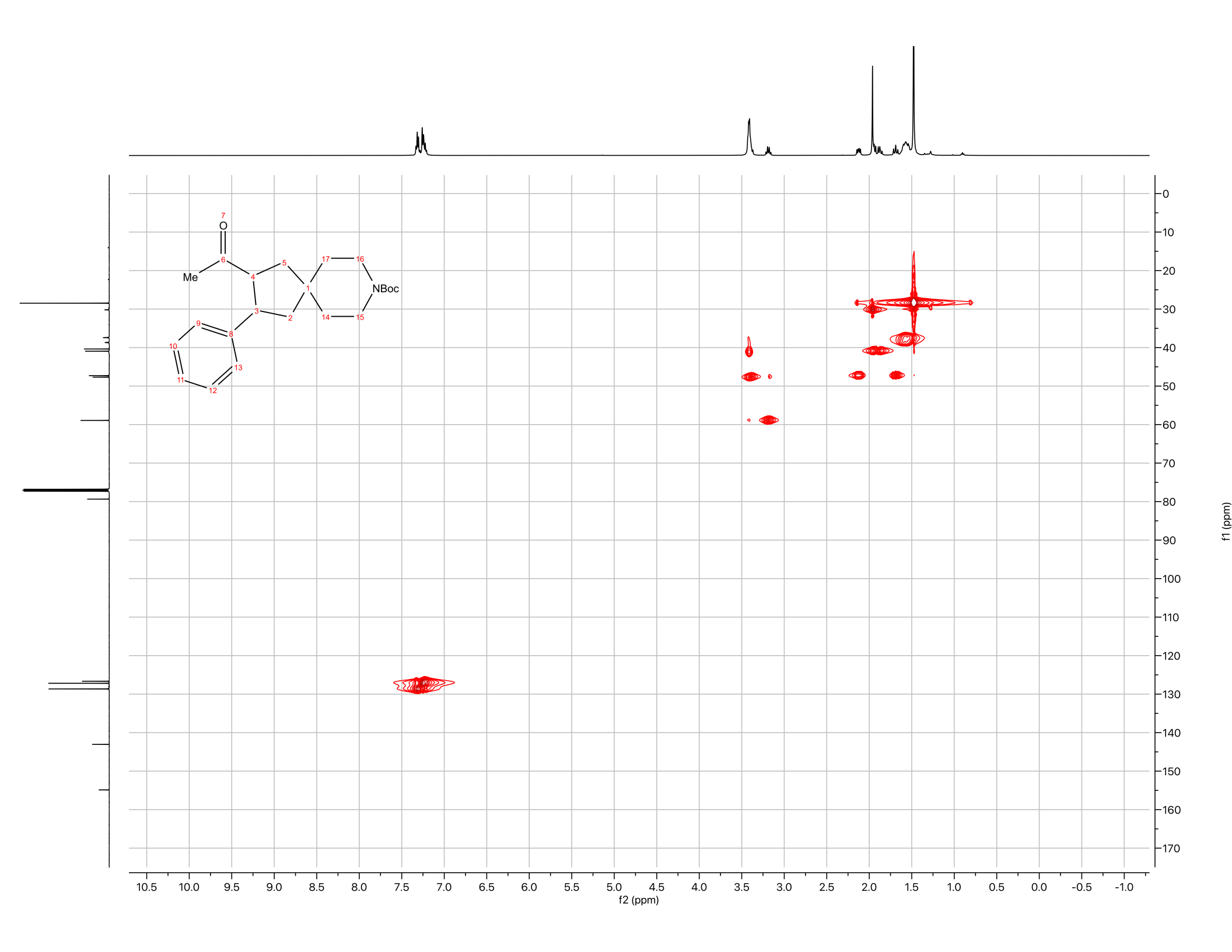
40.95
40.38
38.70
37.42
30.20
28.48
O
Me
NBoc
f1 (ppm)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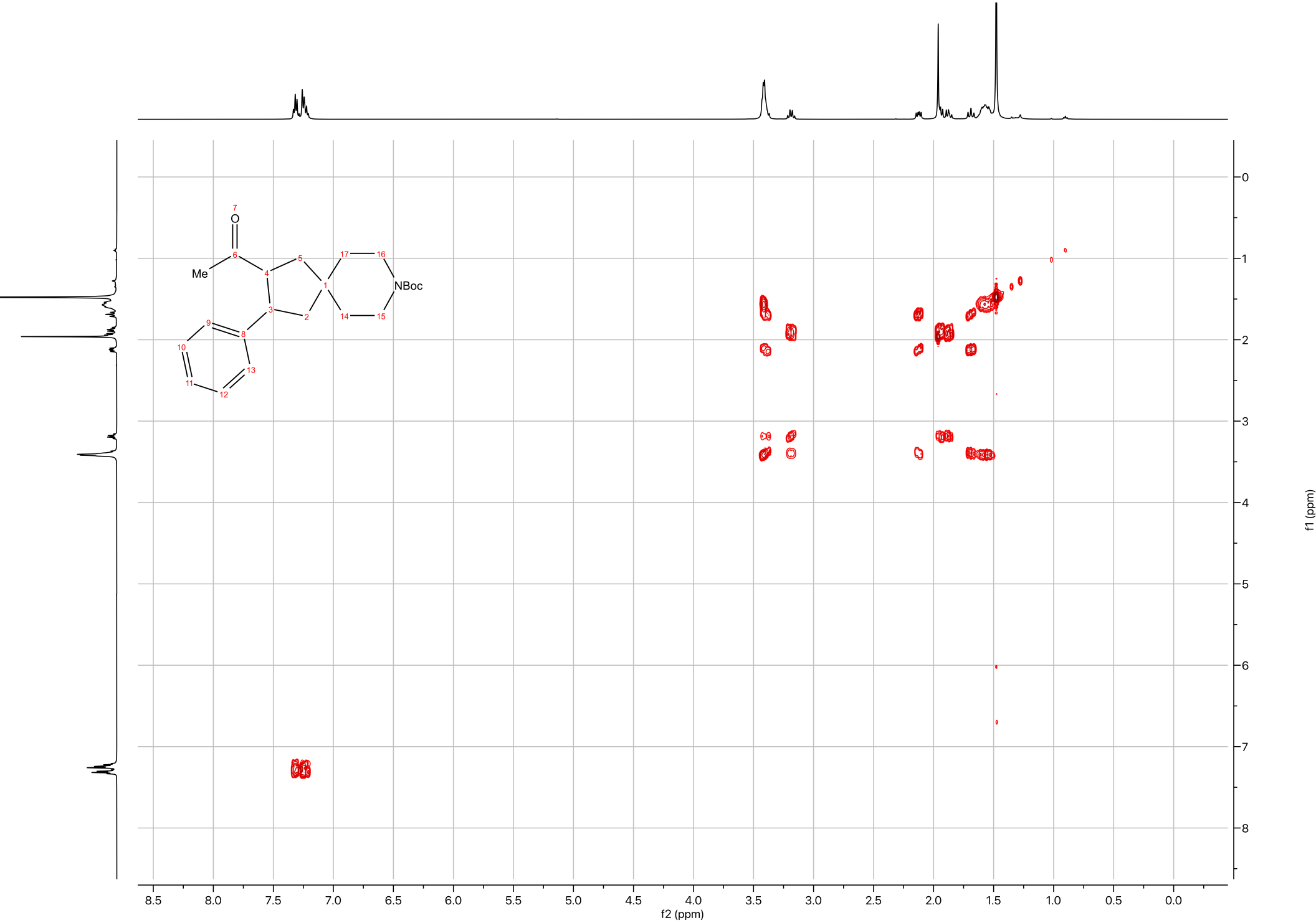
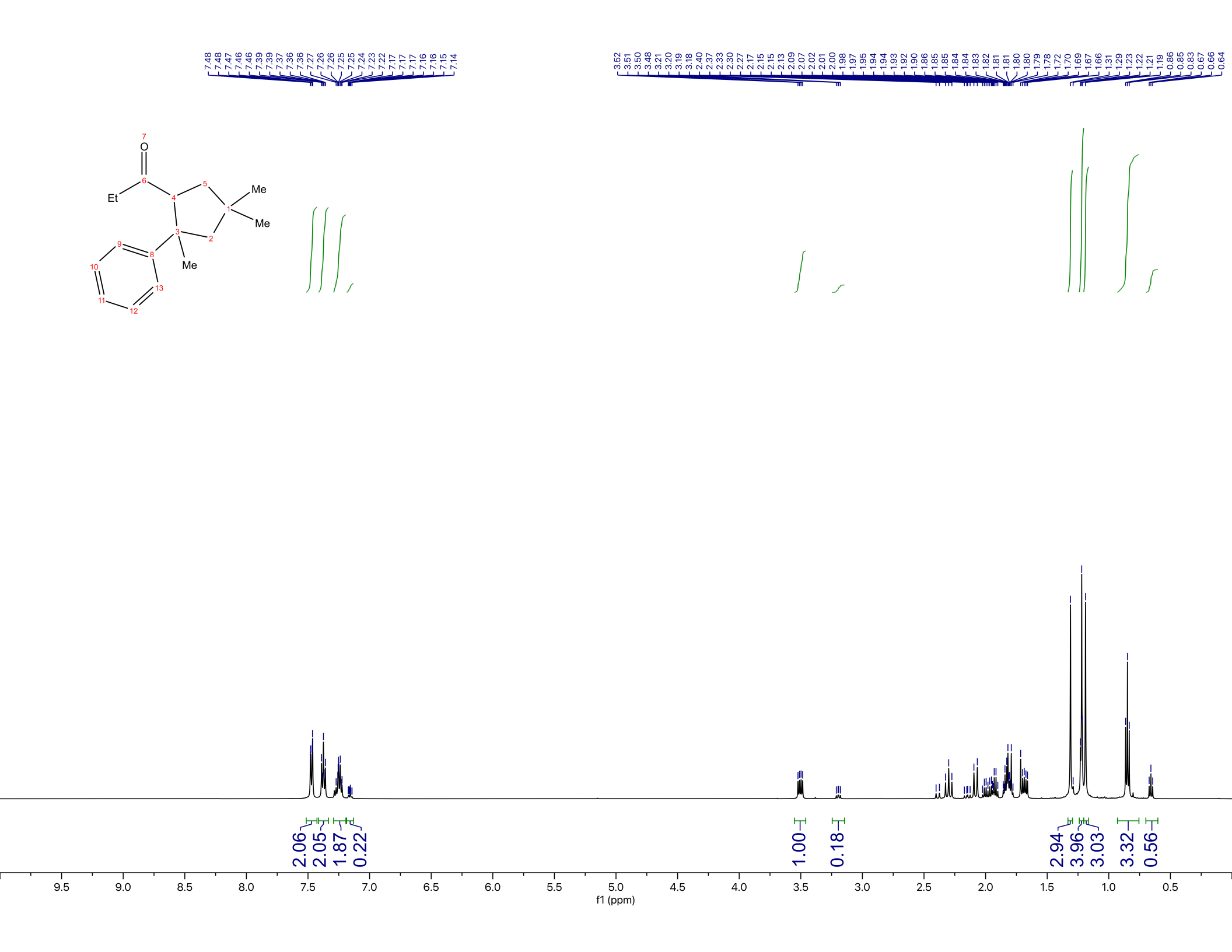
Me
NBoc
f2 (ppm)
f1 (ppm)


Me
NBoc
f2 (ppm)
f1 (ppm)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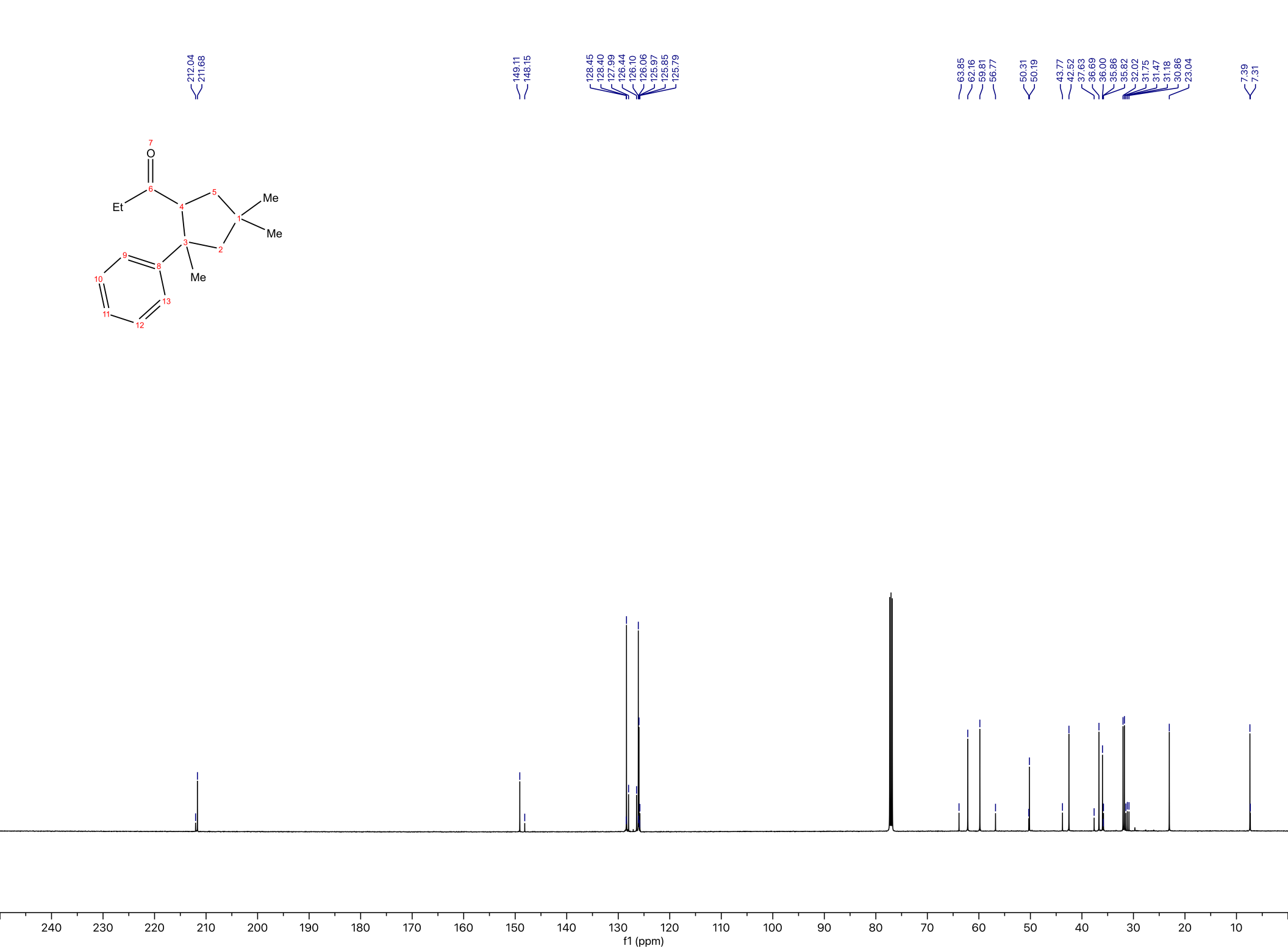
3.52 3.51 3.50 3.48 3.21 3.20 3.19 3.18 2.40 2.37 2.33 2.30 2.27 2.17 2.15 2.15 2.13 2.09 2.07 2.02 2.01 2.00 1.98 1.97 1.95 1.94 1.94 1.93 1.92 1.90 1.86 1.85 1.85 1.84 1.84 1.83 1.82 1.81 1.81 1.80 1.80 1.79 1.78 1.72 1.70 1.69 1.67 1.66 1.31 1.29 1.23 1.22 1.21 1.19 0.86 0.85 0.83 0.67 0.66 0.64
O
Et
Me
Me
Me
2.06
2.05
1.87
0.22
1.00
0.18
2.94
3.96
3.03
3.32
0.56
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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62.16
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56.77
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50.19
43.77
42.52
37.63
36.69
36.00
35.86
35.82
32.02
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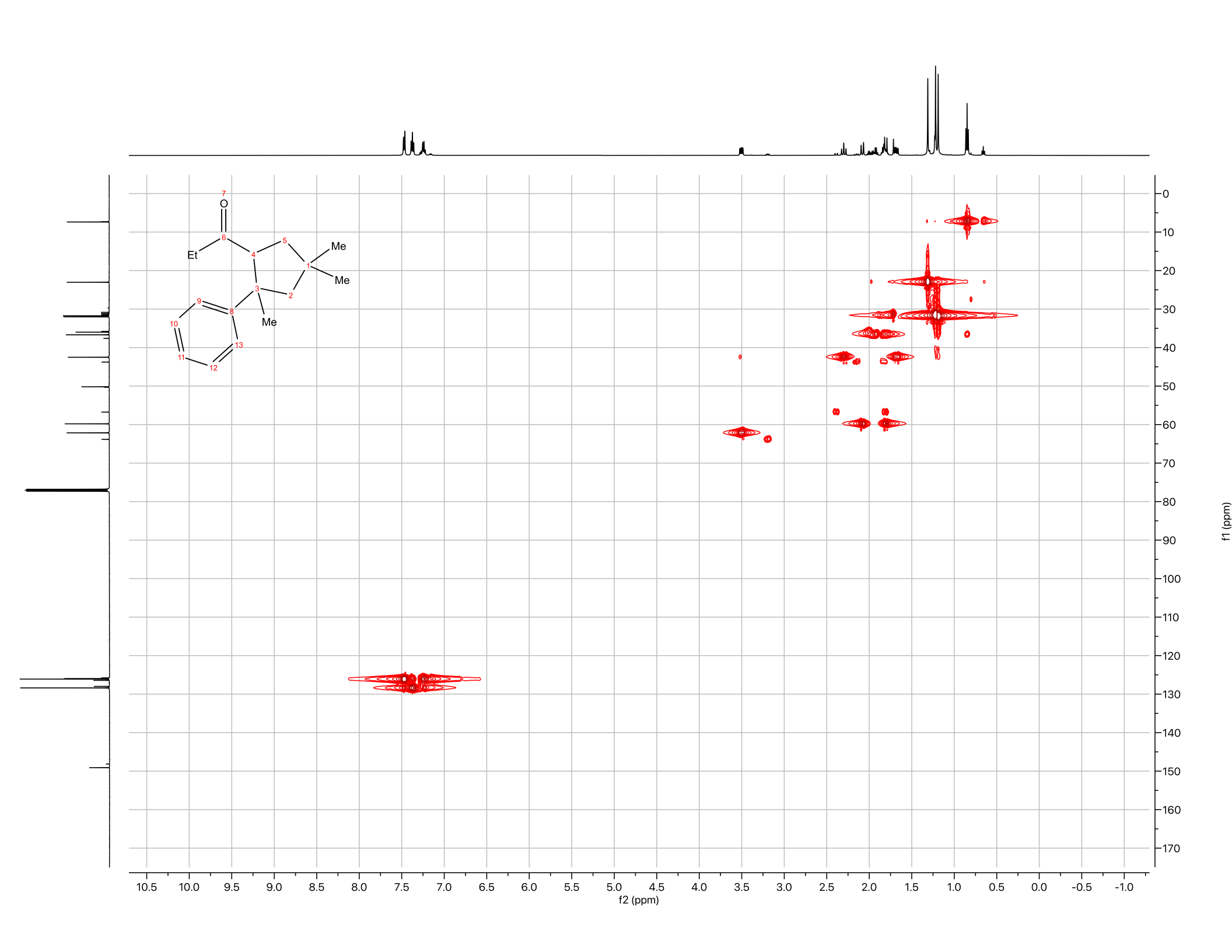
31.18
30.86
23.04
7.39
7.31
O
Et
Me
Me
Me
f1 (ppm)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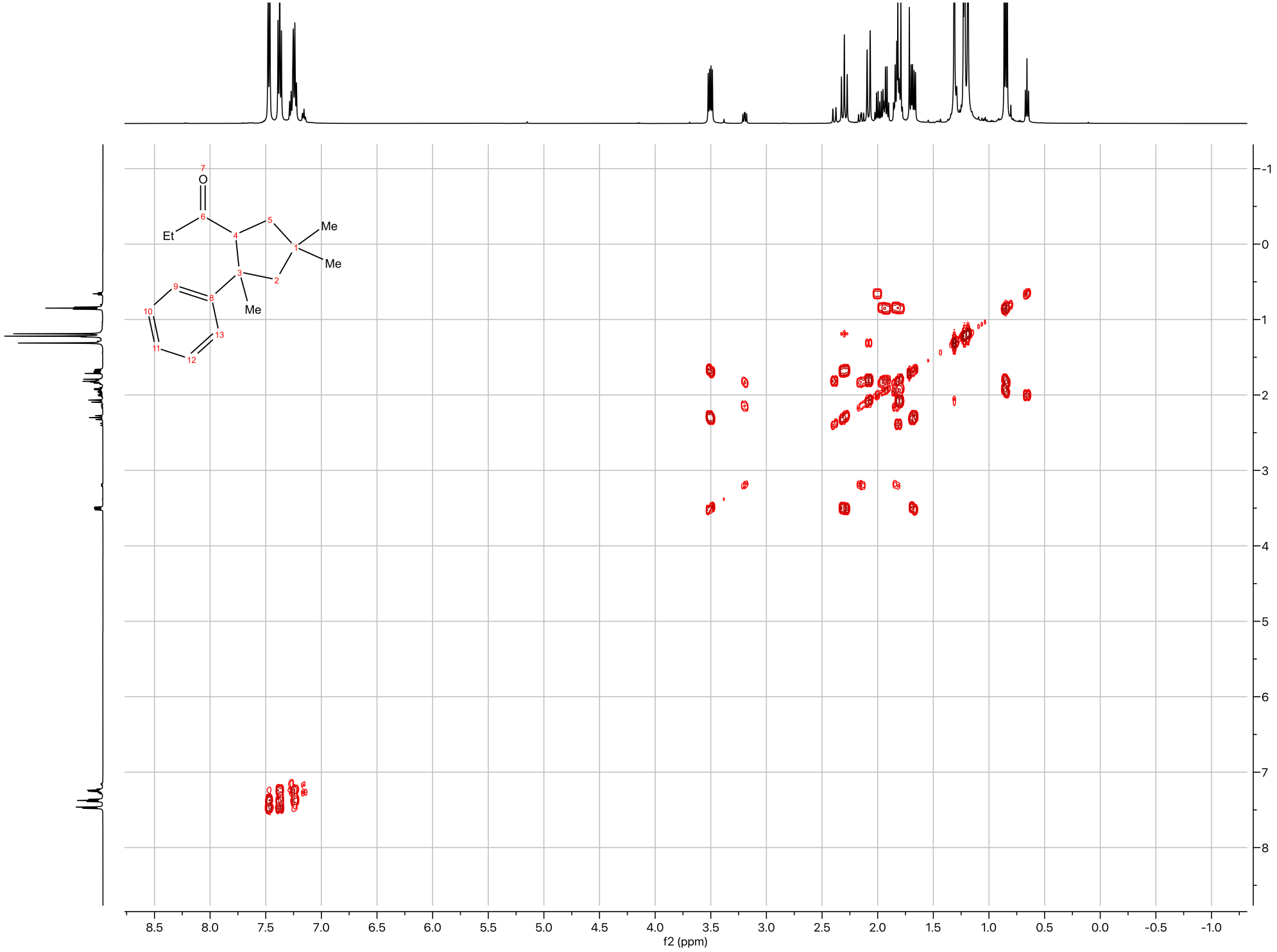
Et
Me
Me
Me
f2 (ppm)
f1 (ppm)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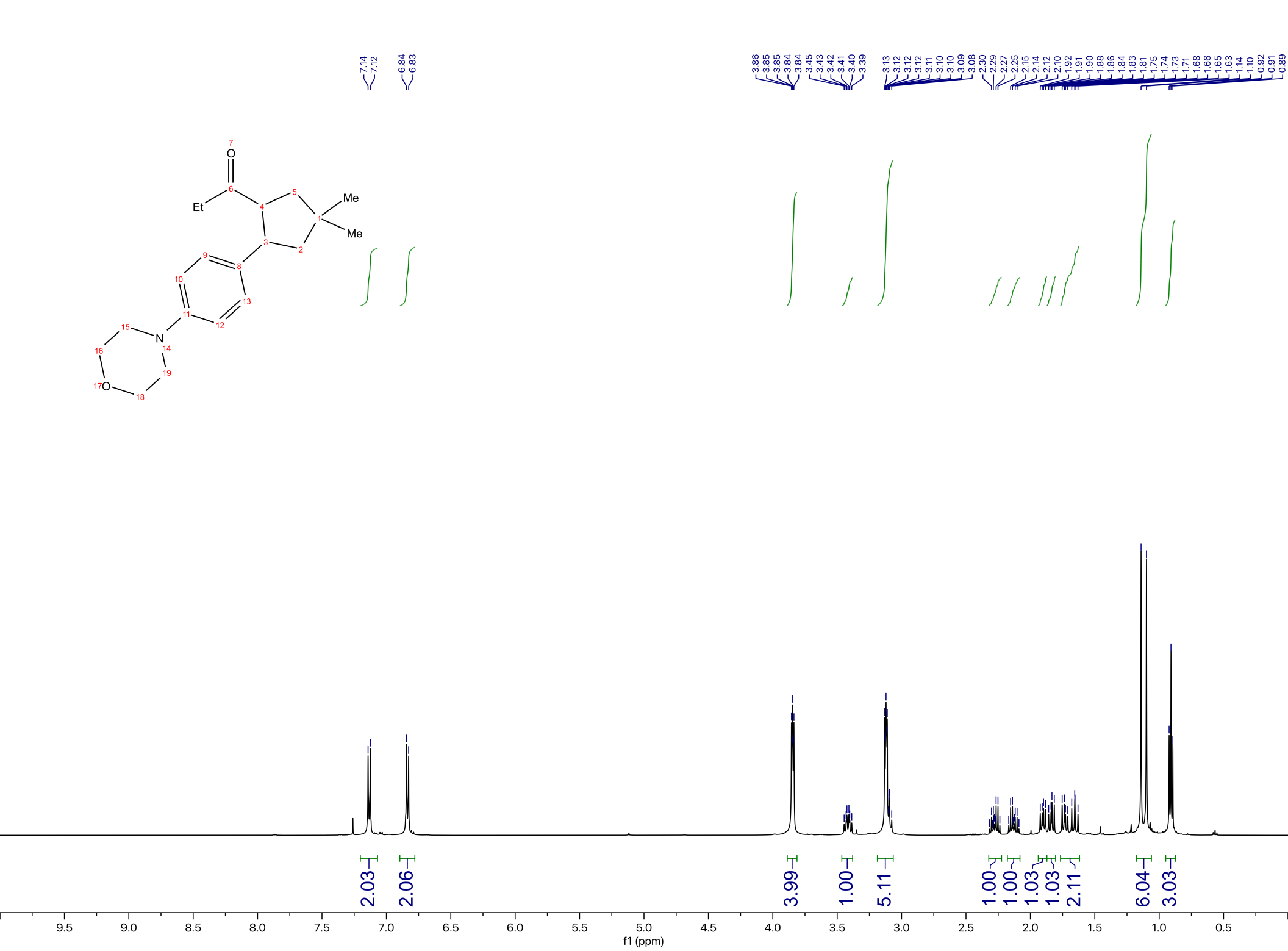
Et
Me
Me
Me
f2 (ppm)
f1 (ppm)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6.83
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3.84
3.84
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3.43
3.42
3.41
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3.39
3.13
3.12
3.12
3.12
3.11
3.10
3.10
3.09
3.08
2.30
2.29
2.27
2.25
2.15
2.14
2.12
2.10
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1.91
1.90
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1.86
1.84
1.83
1.81
1.75
1.74
1.73
1.71
1.68
1.66
1.65
1.63
1.14
1.10
0.92
0.91
0.89
O
Et
Me
Me
N
O
2.03
2.06
3.99
1.00
5.11
1.00
1.00
1.03
1.03
2.11
6.04
3.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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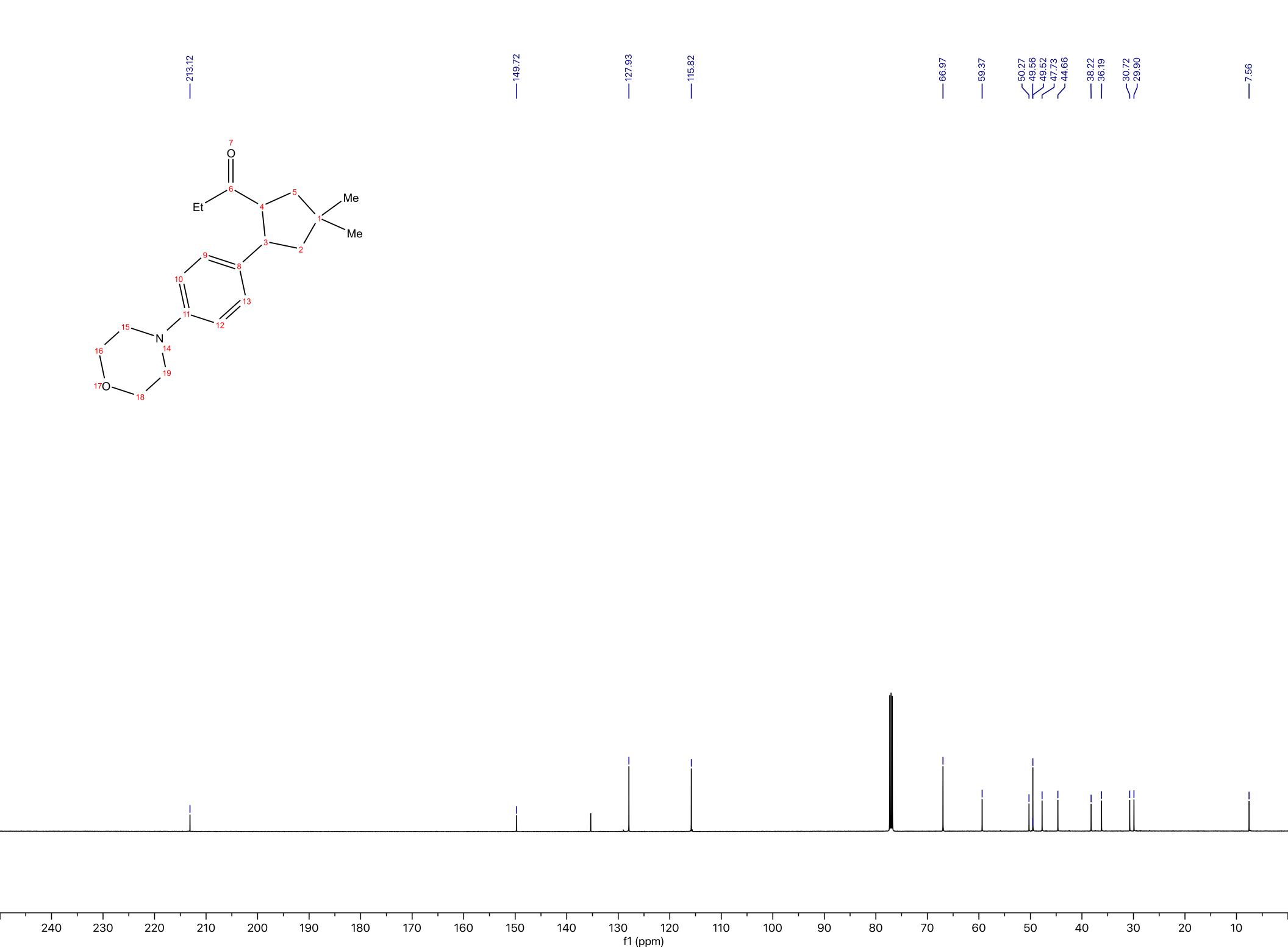
0.5
f1 (ppm)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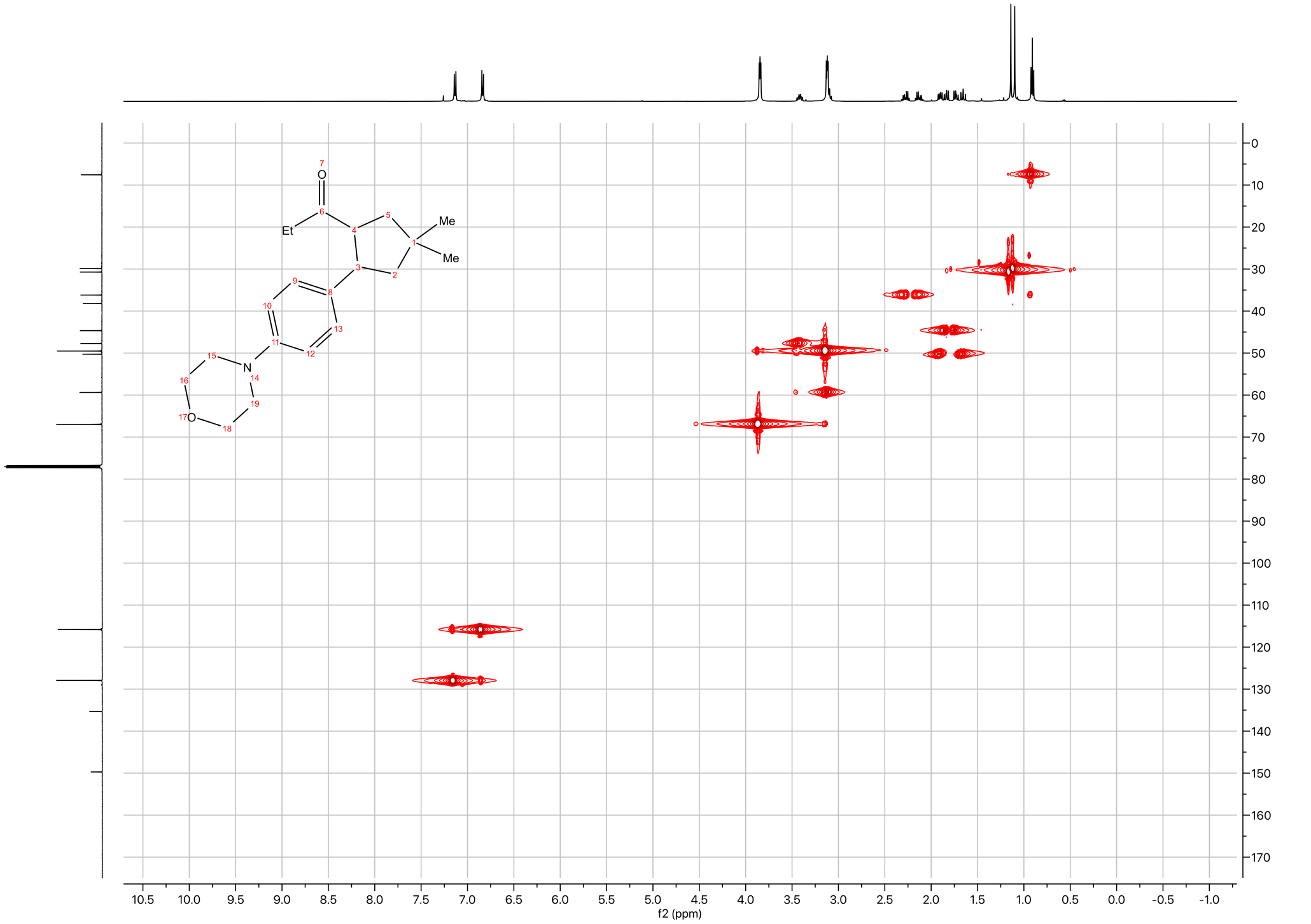
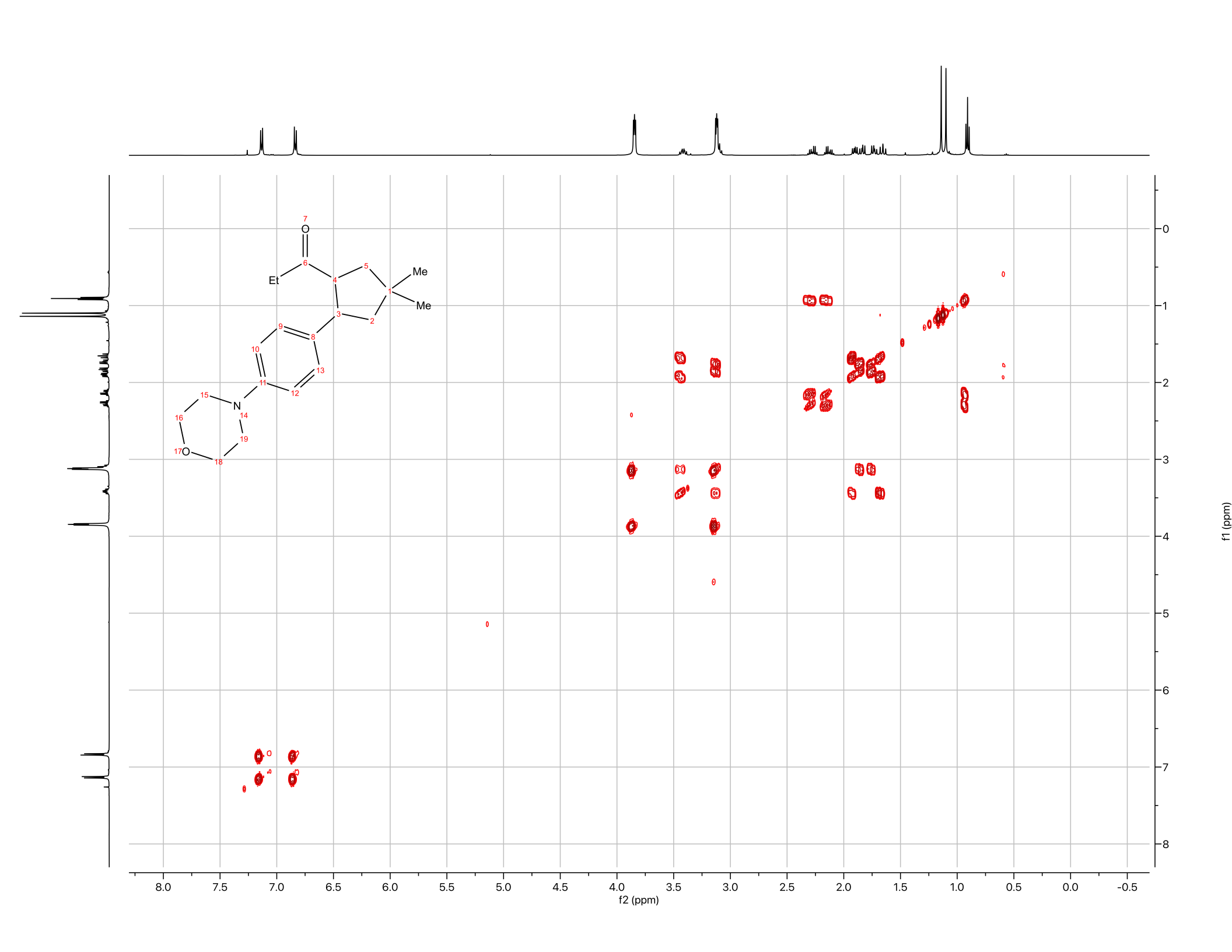
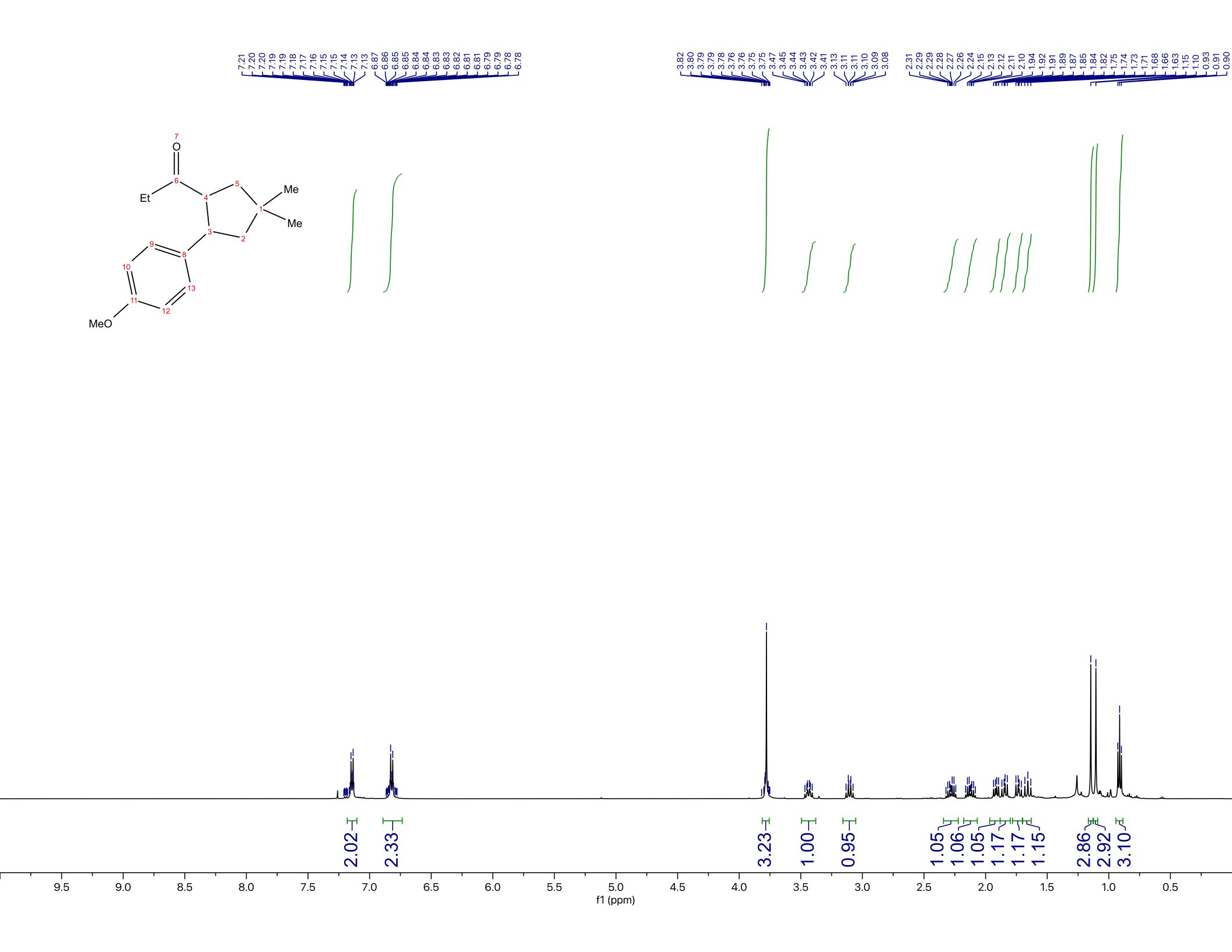
115.82
66.97
59.37
50.27
49.56
49.52
47.73
44.66
38.22
36.19
30.72
29.90
7.56
O
Et
Me
Me
N
O
f1 (ppm)


O
Et
Me
Me
N
O
f2 (ppm)
f1 (ppm)


Et
Me
Me
N
O
O
f2 (ppm)
f1 (ppm)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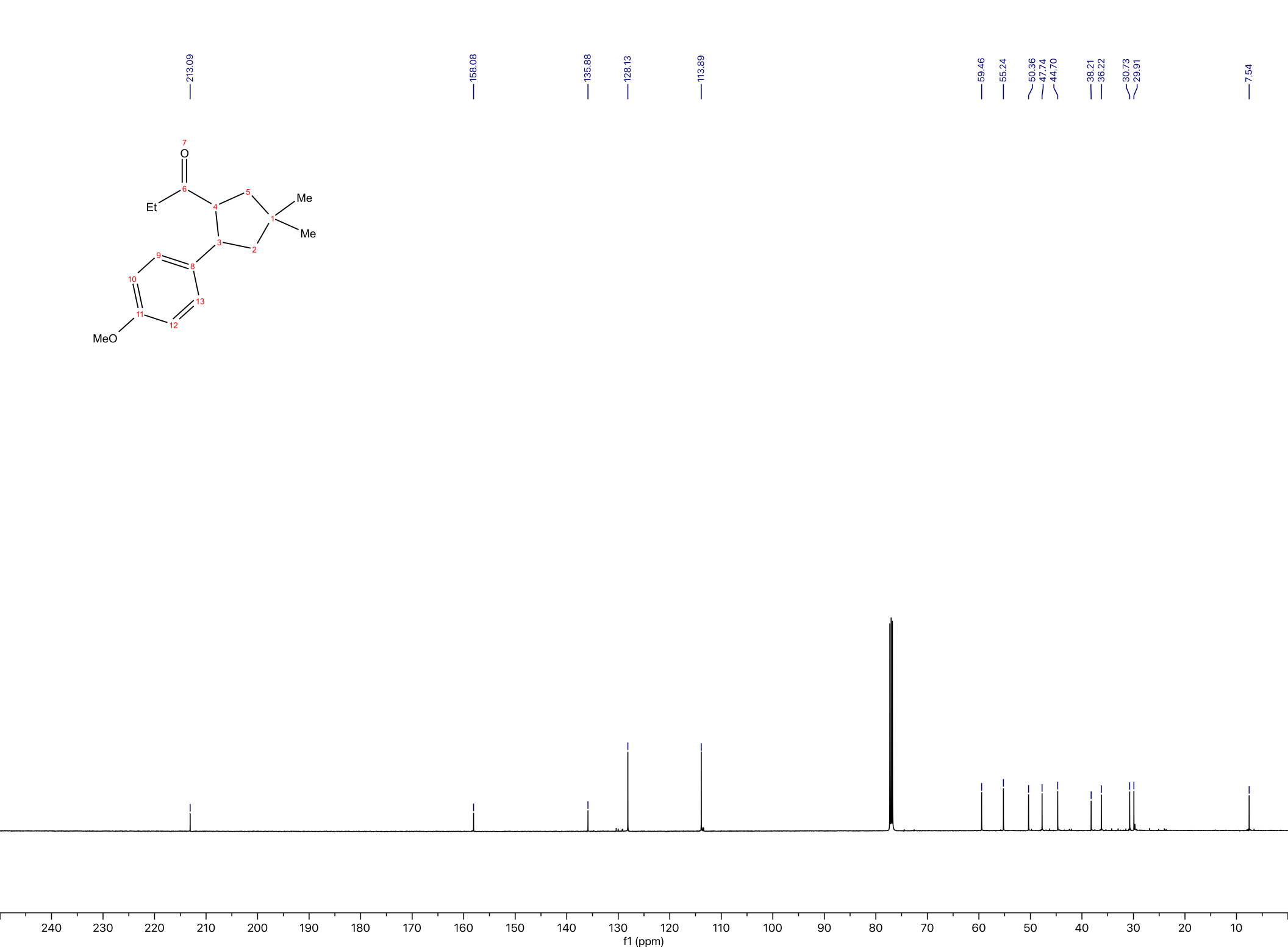
3.82 3.80 3.79 3.79 3.78 3.76 3.76 3.75 3.75 3.47 3.45 3.44 3.43 3.42 3.41 3.13 3.11 3.11 3.10 3.09 3.08
2.31 2.29 2.29 2.28 2.27 2.26 2.24 2.15 2.13 2.12 2.11 2.10 1.94 1.92 1.91 1.89 1.87 1.85 1.84 1.82 1.75 1.74 1.73 1.71 1.68 1.66 1.63 1.15 1.10 0.93 0.91 0.90
O
Et
Me
Me
MeO
2.02
2.33
3.23
1.00
0.95
1.05
1.06
1.05
1.17
1.17
1.15
2.86
2.92
3.10
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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128.13
113.89
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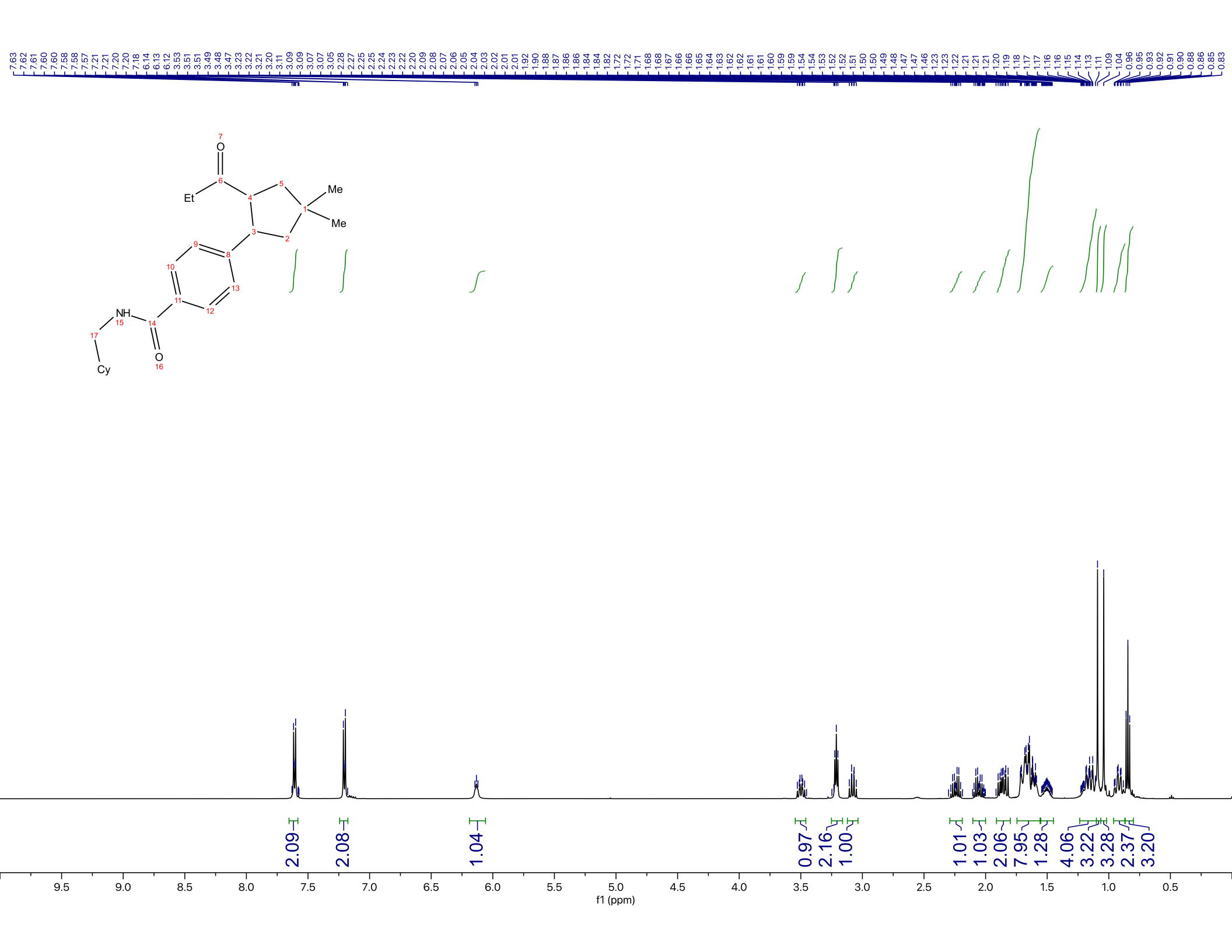
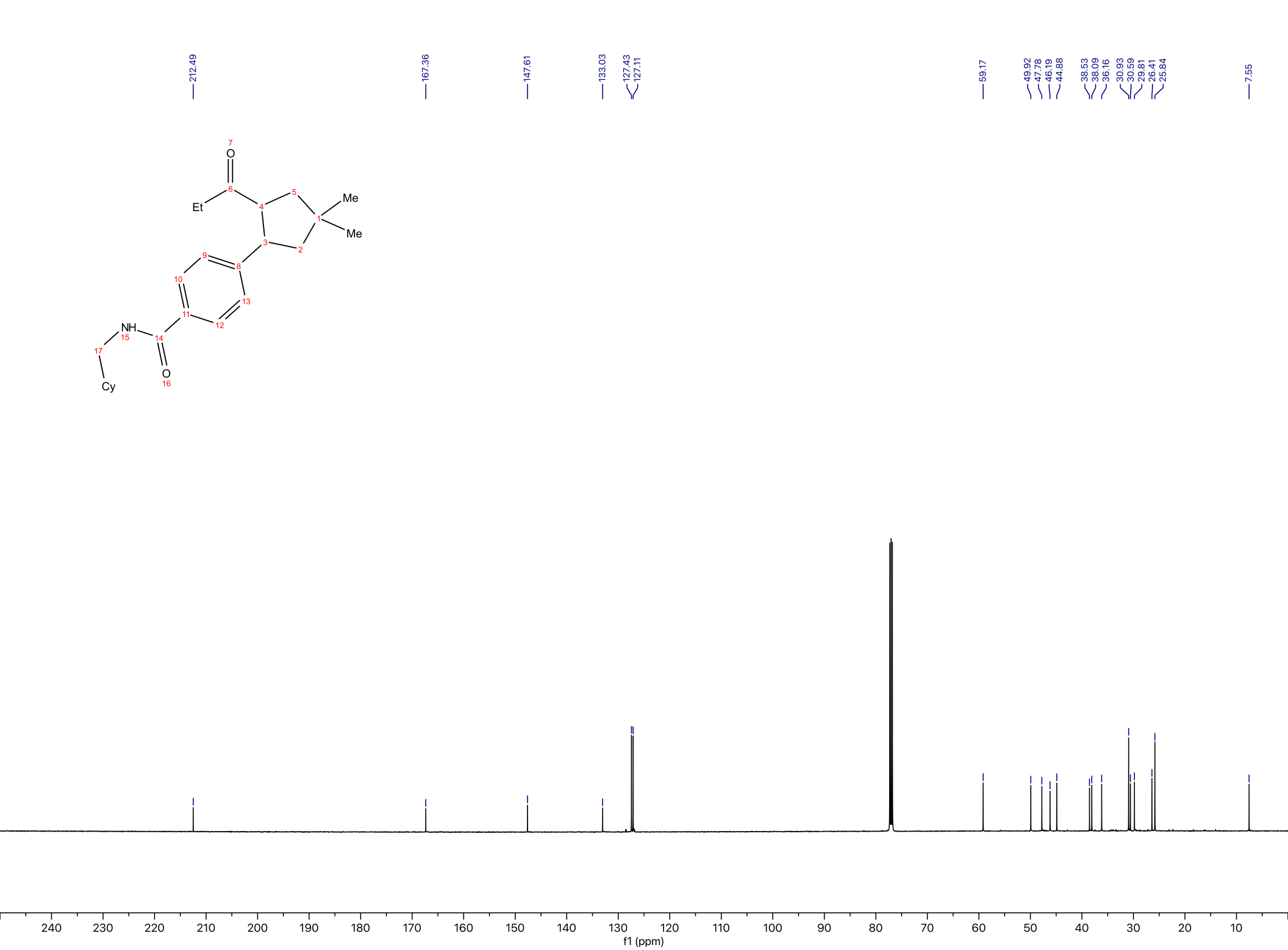
38.21
36.22
30.73
29.91
7.54
O
Et
Me
Me
MeO
f1 (ppm)


7.63 7.62 7.61 7.60 7.60 7.58 7.58 7.57 7.21 7.21 7.20 7.20 7.18 6.14 6.13 6.12 3.53 3.51 3.51 3.49 3.48 3.47 3.23 3.22 3.21 3.20 3.11 3.09 3.09 3.07 3.07 3.05 2.28 2.27 2.25 2.25 2.24 2.23 2.22 2.20 2.09 2.08 2.07 2.06 2.05 2.04 2.03 2.02 2.01 2.01 1.92 1.90 1.88 1.87 1.86 1.86 1.84 1.84 1.82 1.72 1.71 1.68 1.68 1.67 1.66 1.66 1.65 1.64 1.63 1.62 1.62 1.61 1.61 1.60 1.59 1.59 1.54 1.54 1.53 1.52 1.52 1.51 1.50 1.50 1.49 1.48 1.47 1.47 1.46 1.23 1.23 1.22 1.21 1.21 1.21 1.20 1.19 1.18 1.17 1.17 1.16 1.16 1.15 1.14 1.13 1.11 1.09 1.04 0.96 0.95 0.93 0.92 0.91 0.90 0.88 0.86 0.85 0.83
O
Et
Me
Me
NH
Cy
O
2.09
2.08
1.04
0.97
2.16
1.00
1.01
1.03
2.06
7.95
1.28
4.06
3.22
3.28
2.37
3.20
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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133.03
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127.11
59.17
49.92
47.78
46.19
44.88
38.53
38.09
36.16
30.93
30.59
29.81
26.41
25.84
7.55
O
7
6
Et
4
5
1
Me
Me
3
2
9
8
10
13
11
12
NH
15
14
17
O
16
Cy
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220
210
200
190
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100
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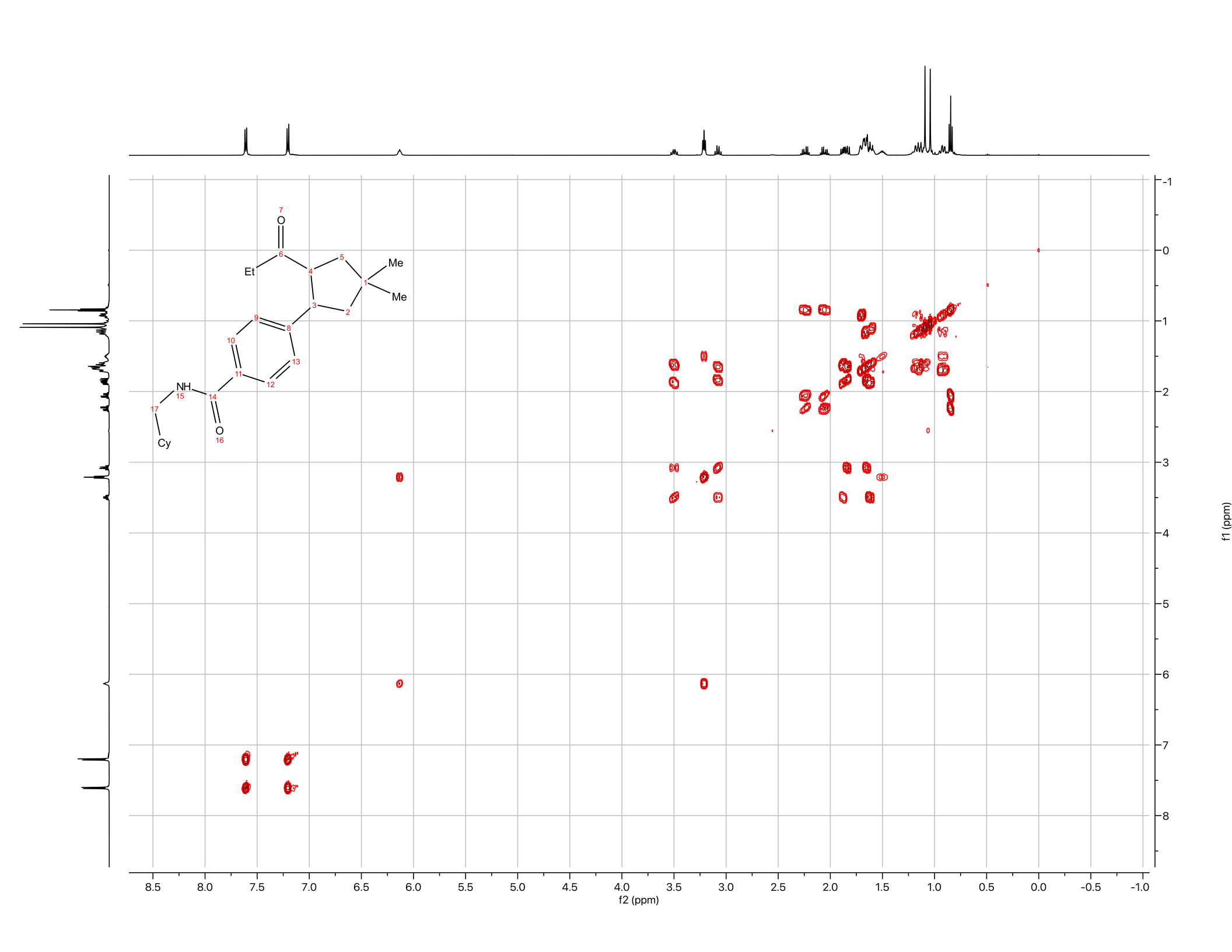
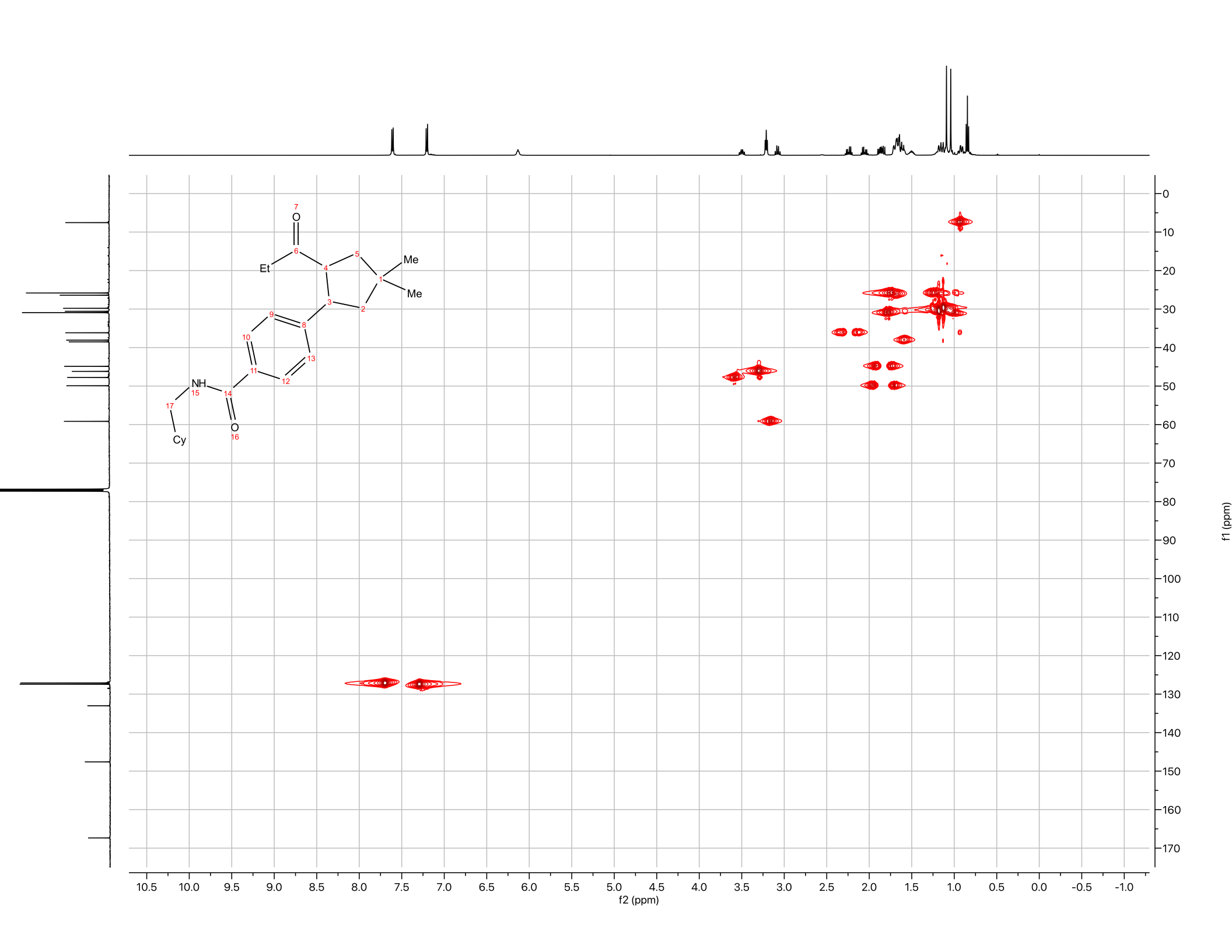
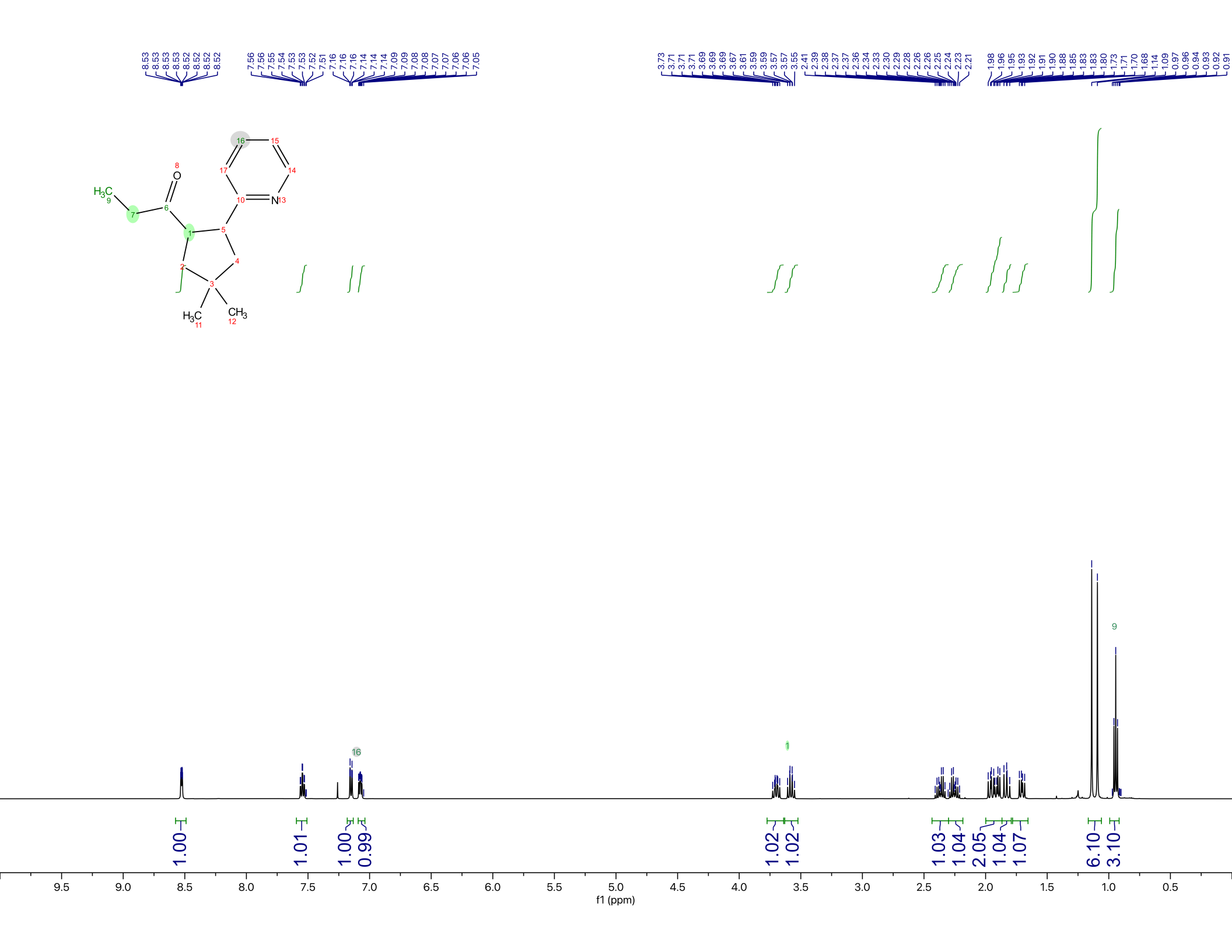
60
50
40
30
20
10
f1 (ppm)


O
Et
Me
Me
NH
Cy
O
f2 (ppm)
f1 (ppm)


O
Et
Me
Me
NH
Cy
O
f2 (ppm)
f1 (ppm)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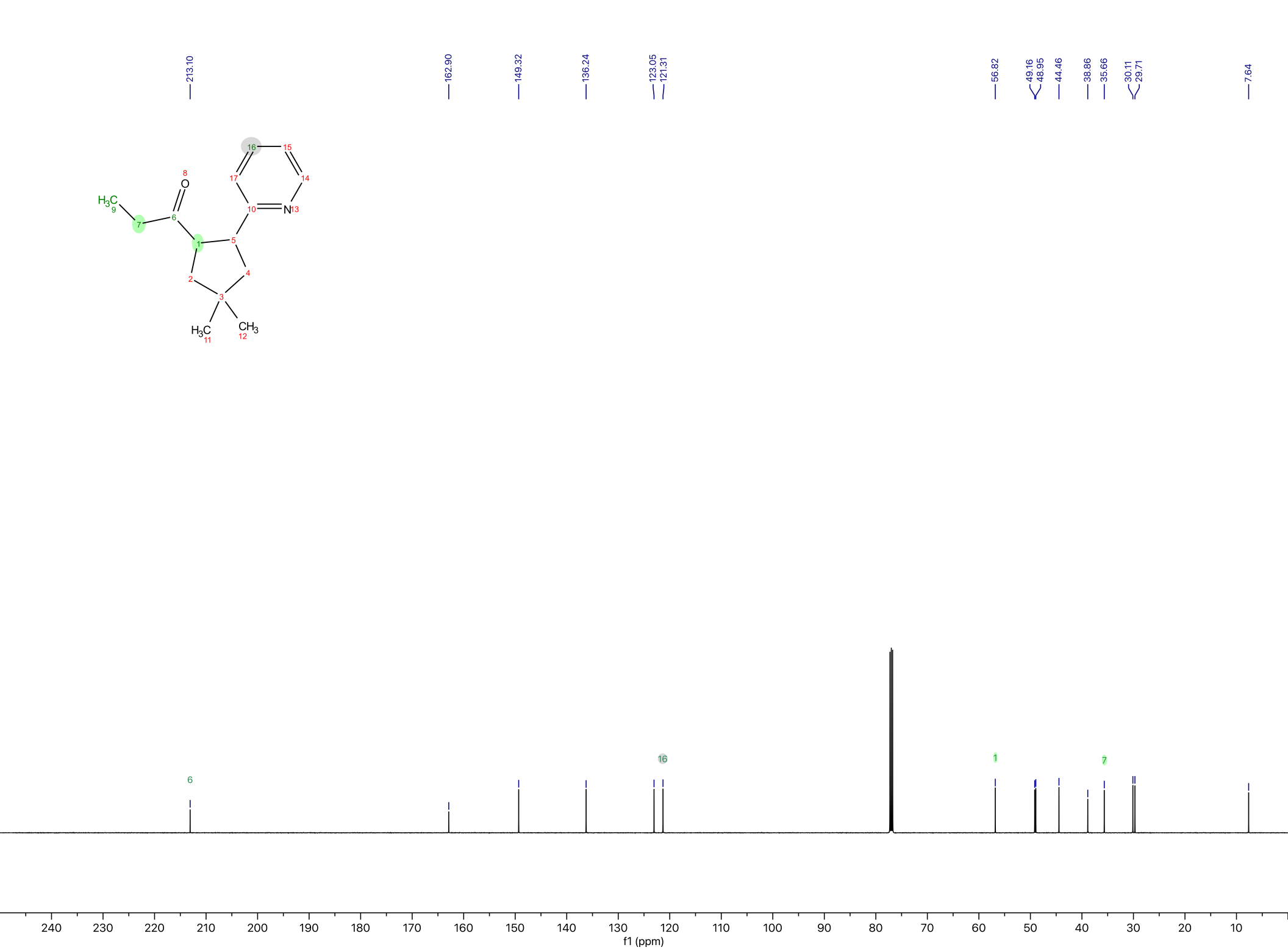
7.56 7.56 7.55 7.54 7.53 7.53 7.52 7.51 7.16 7.16 7.16 7.14 7.14 7.14 7.09 7.09 7.08 7.08 7.07 7.07 7.06 7.06 7.05
3.73 3.71 3.71 3.71 3.69 3.69 3.69 3.67 3.61 3.59 3.59 3.57 3.57 3.55 2.41 2.39 2.38 2.37 2.37 2.36 2.34 2.33 2.30 2.29 2.28 2.26 2.26 2.25 2.24 2.23 2.21
1.98 1.96 1.95 1.93 1.92 1.91 1.90 1.88 1.85 1.83 1.83 1.80 1.73 1.71 1.70 1.68 1.14 1.09 0.97 0.96 0.94 0.93 0.92 0.91
H3C 9
O 8
6
7
1
5
2
4
3
H3C 11
CH3 12
10
N 13
14
15
16
17
16
1
9
1.00
1.01
1.00
0.99
1.02
1.02
1.03
1.04
2.05
1.04
1.07
6.10
3.10
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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136.24
123.05
121.31
56.82
49.16
48.95
44.46
38.86
35.66
30.11
29.71
7.64
H3C
9
O
8
6
7
1
5
2
4
3
H3C
11
CH3
12
16
15
17
14
10
N
13
6
16
1
7
240
230
220
210
200
190
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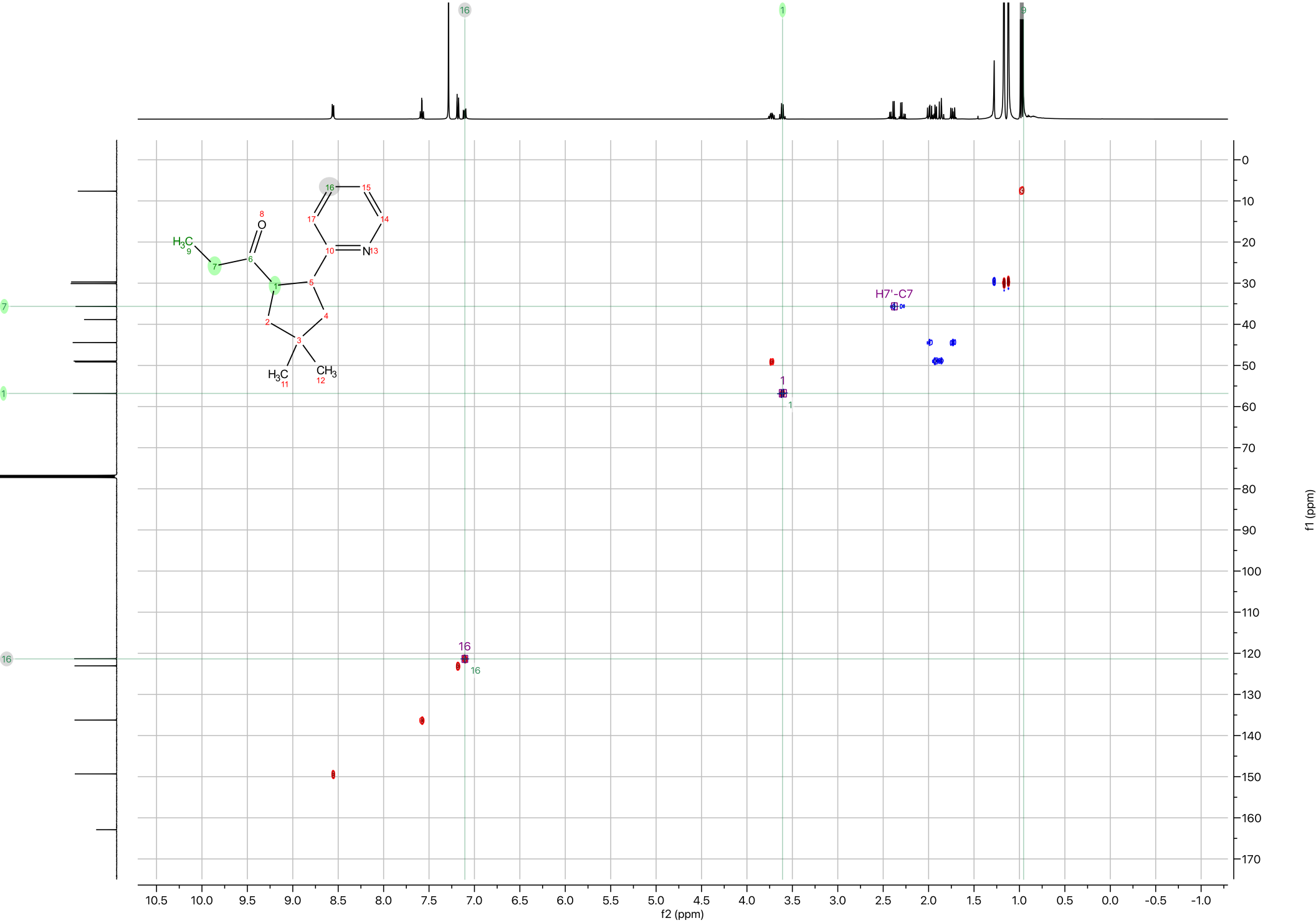
20
10
f1 (ppm)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9
H7'-C7
16
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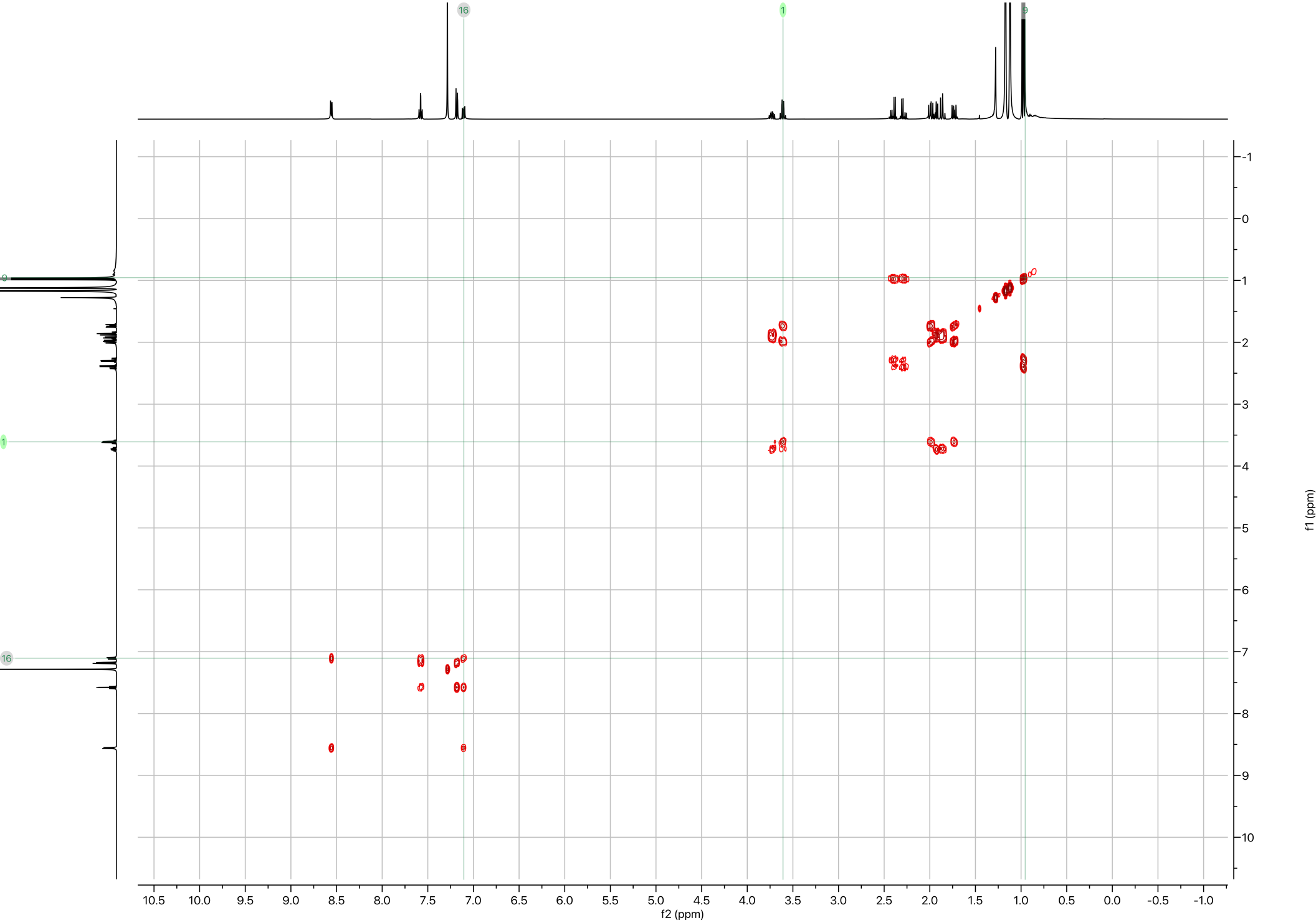
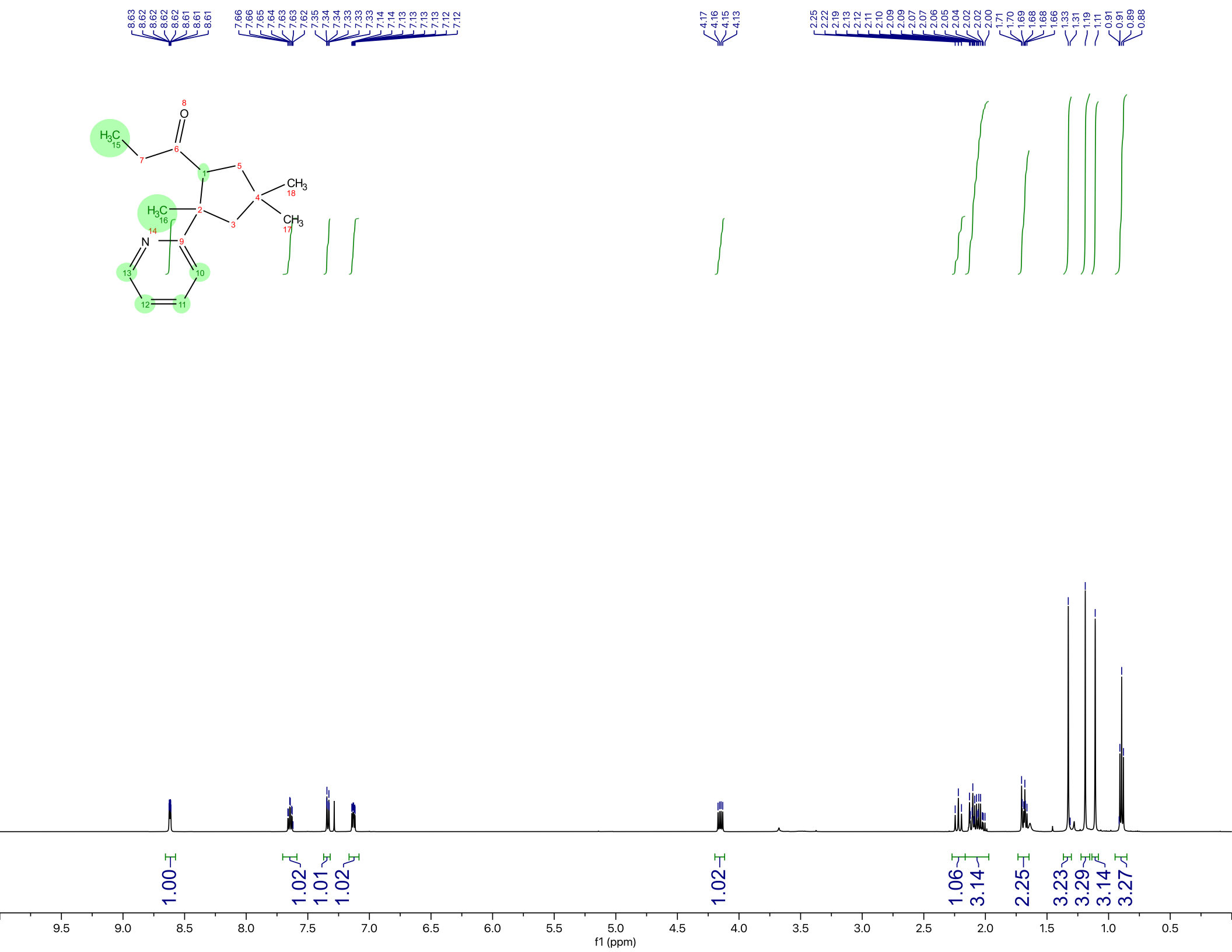
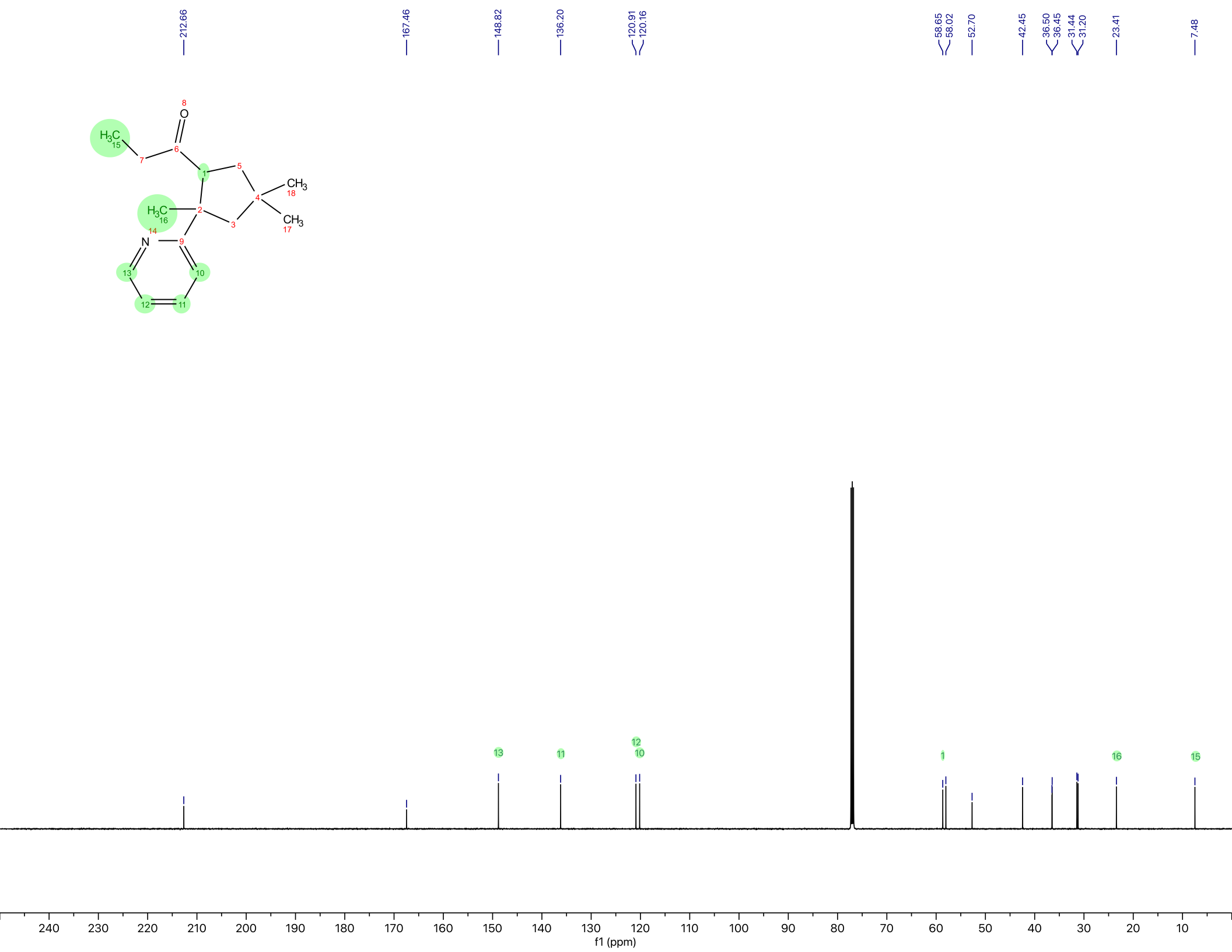
f1 (ppm)


16
1
9
f2 (ppm)
f1 (ppm)


8.63 8.62 8.62 8.62 8.62 8.61 8.61 8.61
7.66 7.66 7.65 7.64 7.63 7.63 7.62 7.35 7.34 7.34 7.33 7.33 7.14 7.14 7.13 7.13 7.13 7.12 7.12
4.17 4.16 4.15 4.13
2.25 2.22 2.19 2.13 2.12 2.11 2.10 2.09 2.09 2.07 2.07 2.06 2.05 2.04 2.02 2.02 2.00 1.71 1.70 1.69 1.68 1.68 1.66 1.33 1.31 1.19 1.11 0.91 0.91 0.89 0.88
O
H3C
CH3
CH3
N
1.00
1.02
1.01
1.02
1.02
1.06
3.14
2.25
3.23
3.29
3.14
3.27
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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148.82
136.20
120.91
120.16
58.65
58.02
52.70
42.45
36.50
36.45
31.44
31.20
23.41
7.48
O
8
H3C
15
6
7
1
5
4
CH3
18
H3C
16
2
3
CH3
17
14
N
9
13
10
12
11
13
11
12
10
1
16
15
240
230
220
210
200
190
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100
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80
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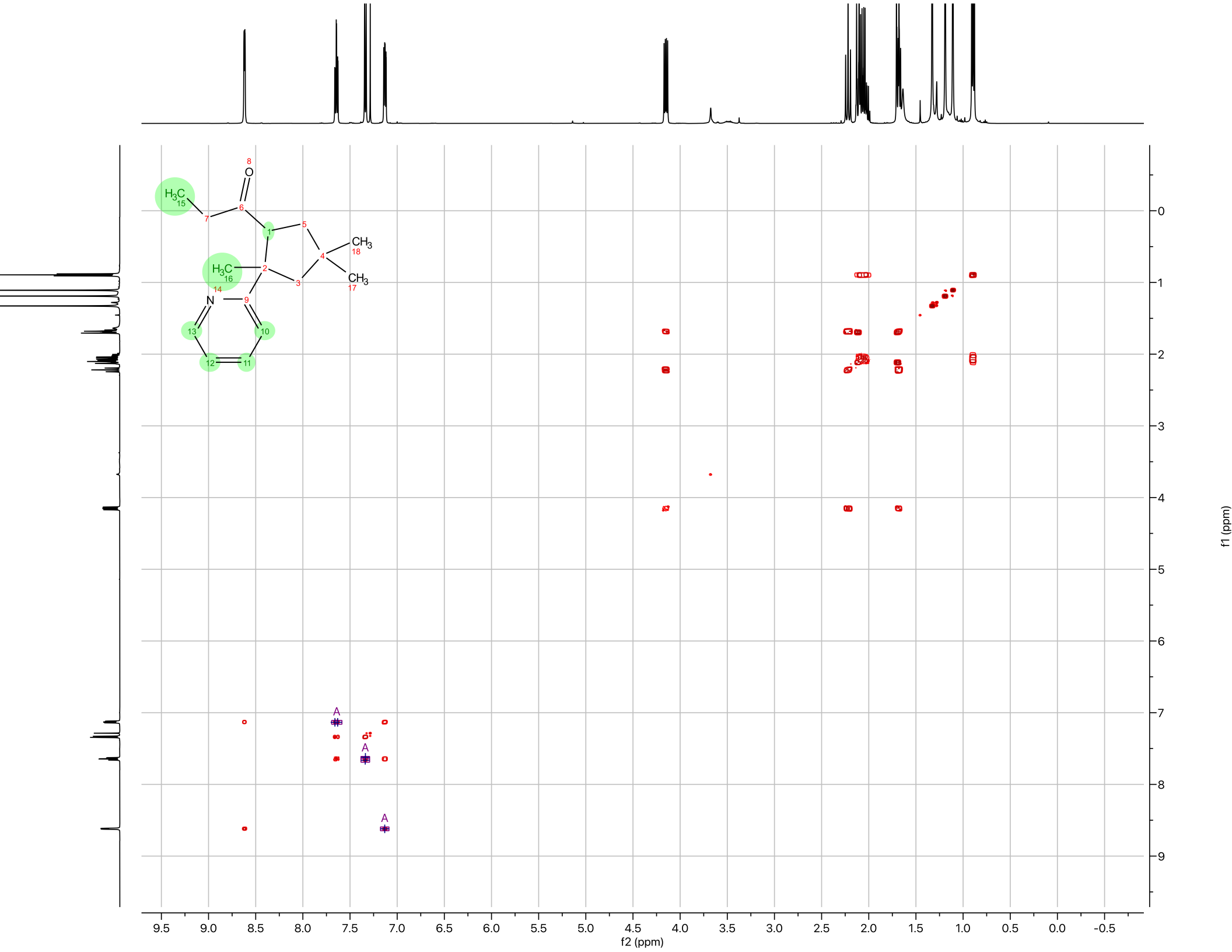
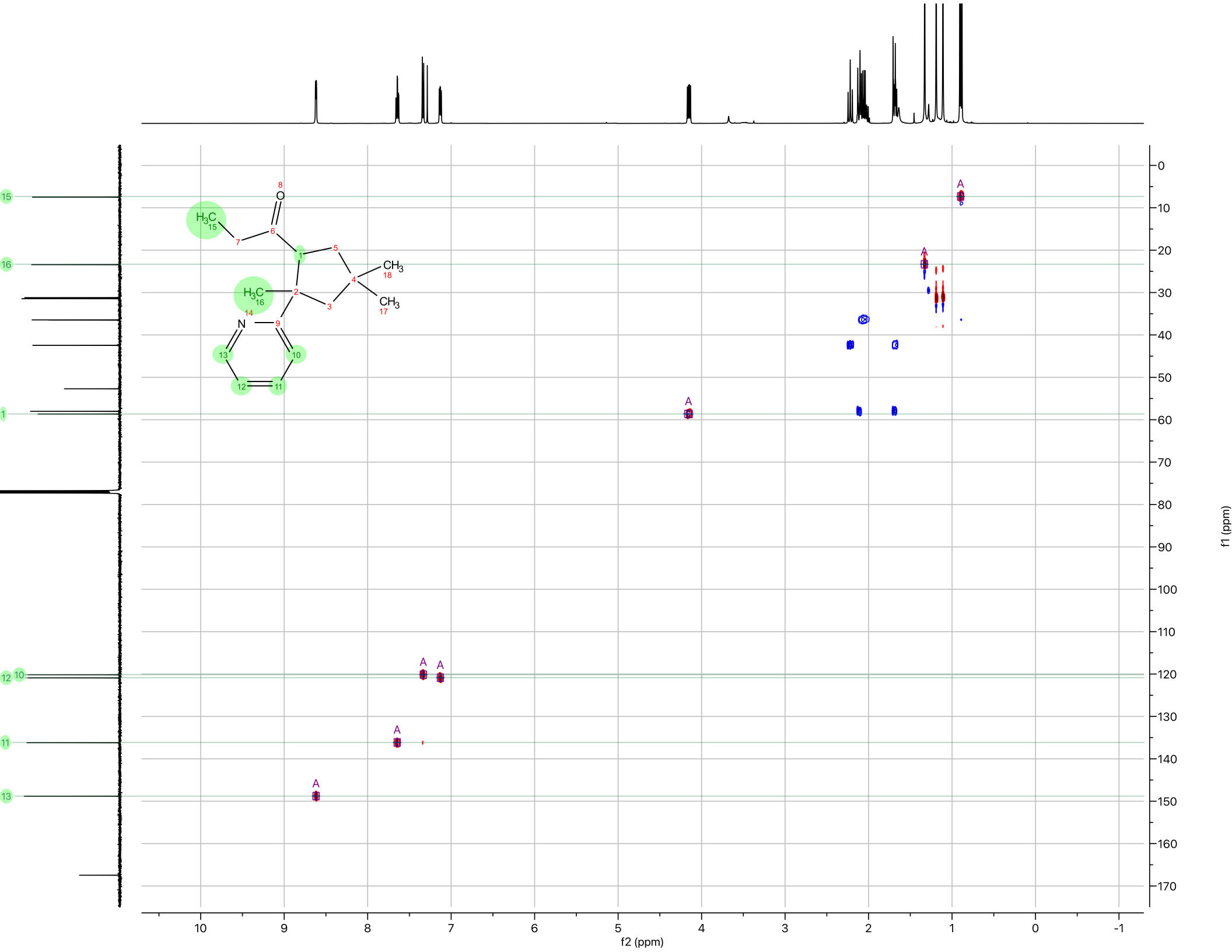
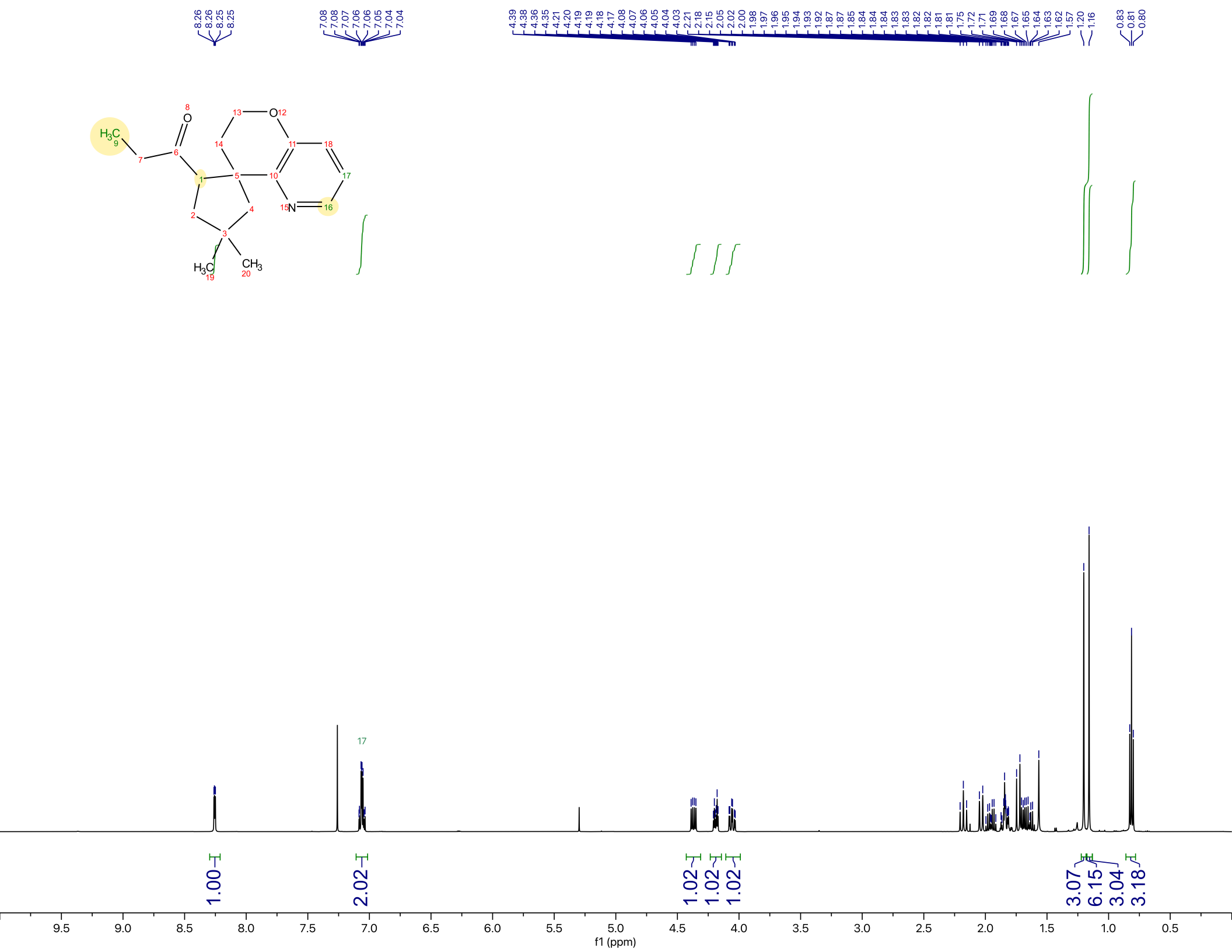
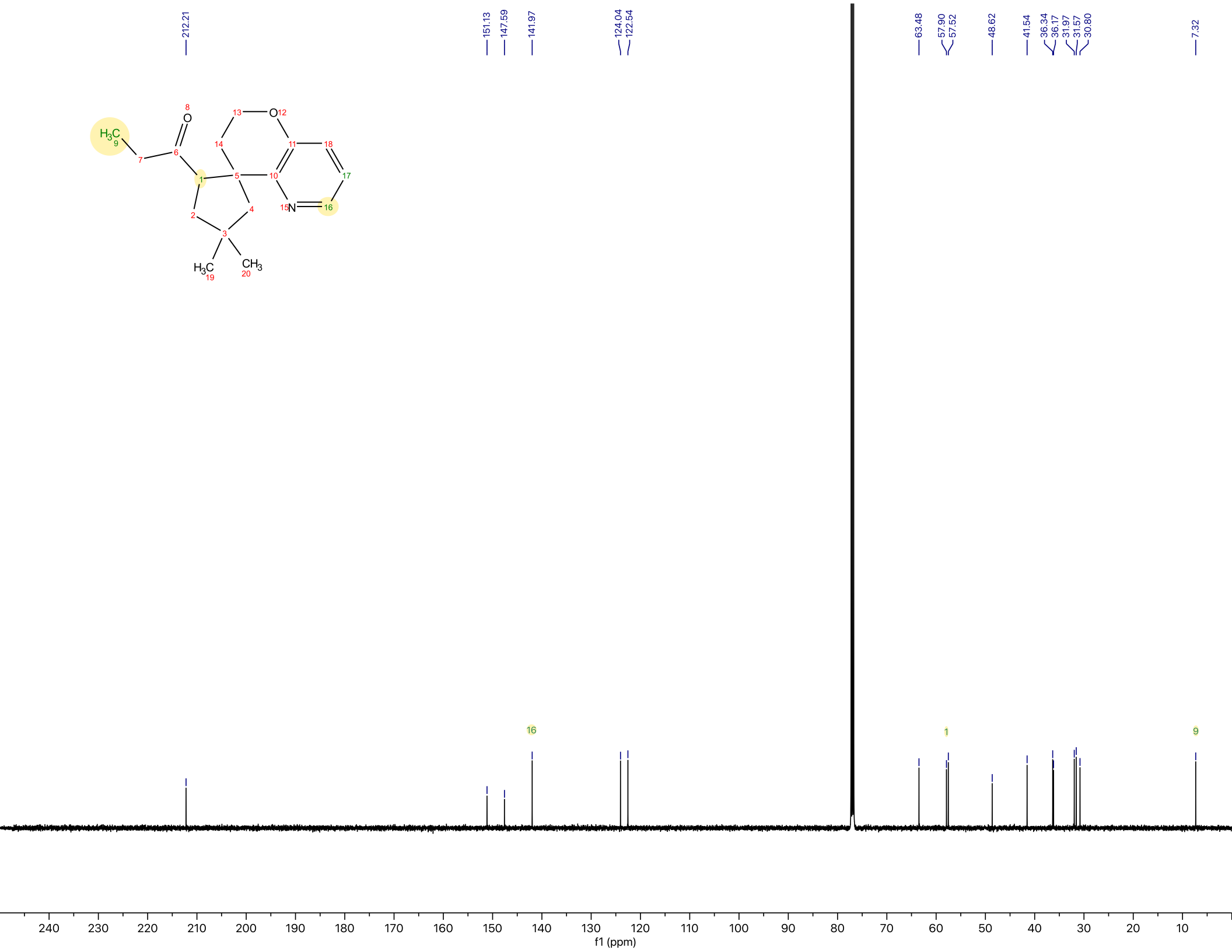
60
50
40
30
20
10
f1 (ppm)


f2 (ppm)
f1 (ppm)
A
A
A


f2 (ppm)
f1 (ppm)



8.26 8.26 8.25 8.25
7.08 7.08 7.07 7.06 7.06 7.05 7.04 7.04
4.39 4.38 4.36 4.35 4.21 4.20 4.19 4.19 4.18 4.17 4.08 4.07 4.06 4.05 4.04 4.03 2.21 2.18 2.15 2.05 2.02 2.00 1.98 1.97 1.96 1.95 1.94 1.93 1.92 1.87 1.87 1.85 1.84 1.84 1.84 1.83 1.83 1.82 1.82 1.81 1.81 1.75 1.72 1.71 1.69 1.68 1.67 1.65 1.64 1.63 1.62 1.57 1.20 1.16
0.83 0.81 0.80
H3C
O
O
N
CH3
H3C
1.00
2.02
1.02
1.02
1.02
3.07
6.15
3.04
3.18
f1 (ppm)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151.13
147.59
141.97
124.04
122.54
63.48
57.90
57.52
48.62
41.54
36.34
36.17
31.97
31.57
30.80
7.32
16
1
9
240
230
220
210
200
190
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140
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120
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100
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80
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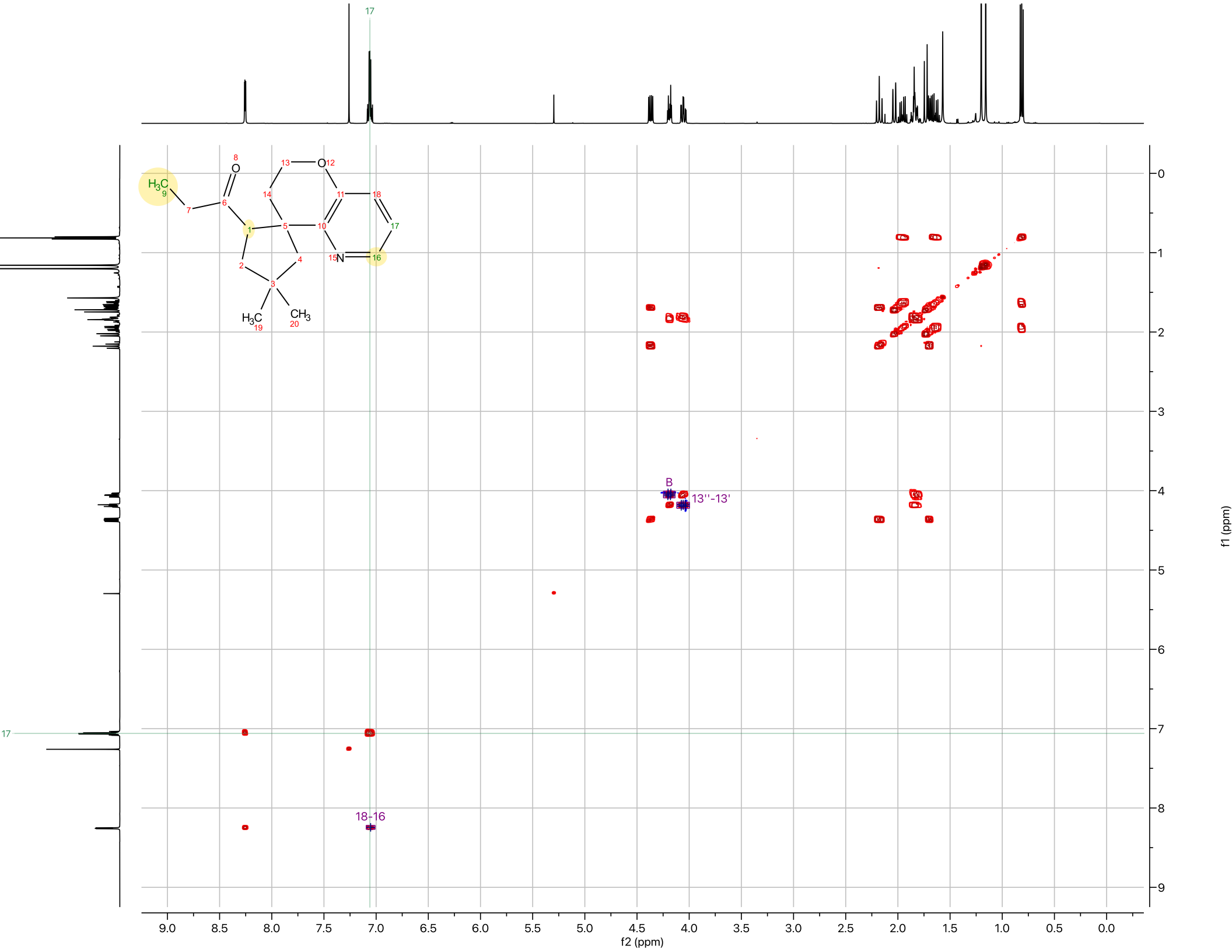
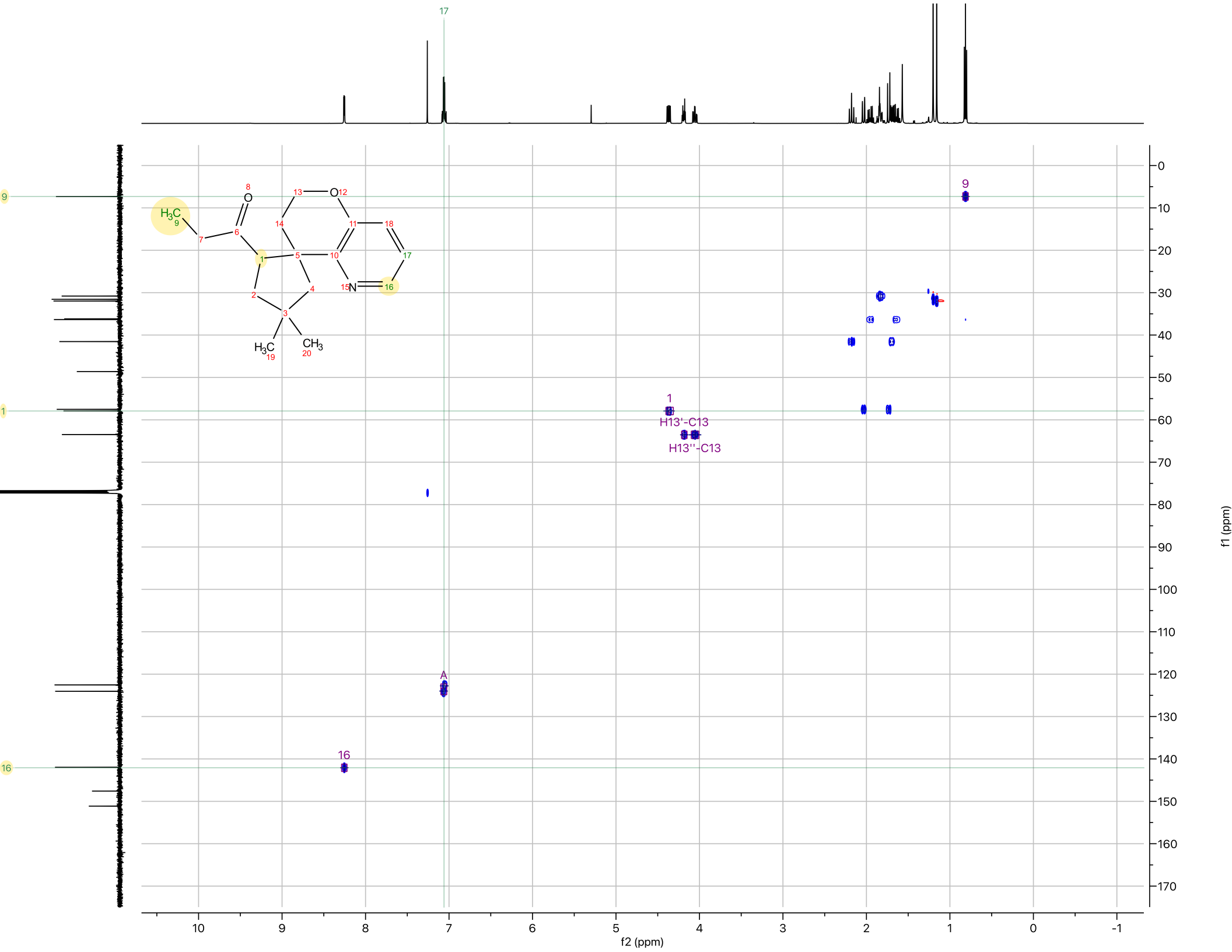
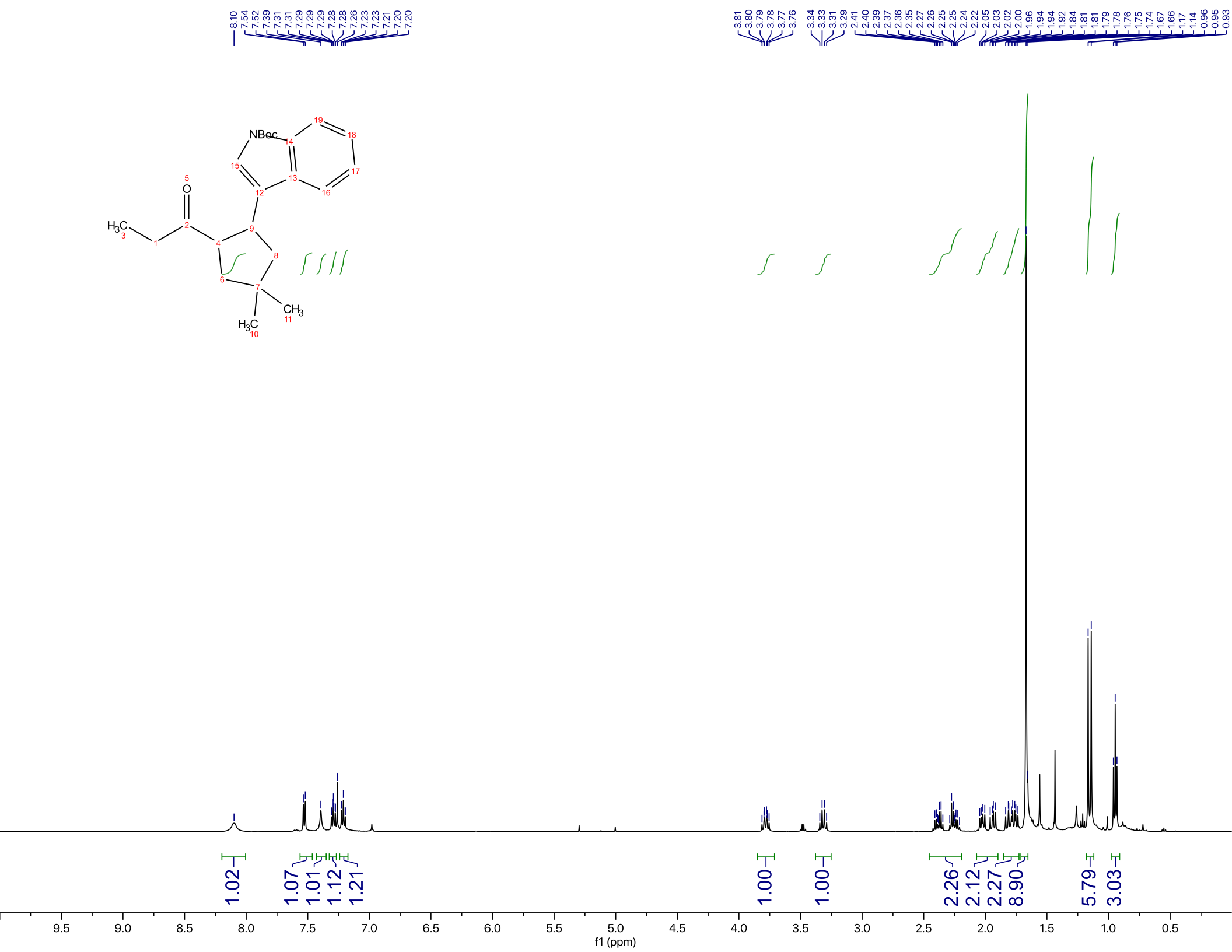
60
50
40
30
20
10
f1 (ppm)


17
B
13''-13'
18-16
f2 (ppm)
f1 (ppm)


17
9
1
16
A
H13'-C13
H13''-C13
f2 (ppm)
f1 (ppm)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7.29
7.29
7.28
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7.26
7.23
7.23
7.21
7.20
7.20
3.81
3.80
3.79
3.78
3.77
3.76
3.34
3.33
3.31
3.29
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2.26
2.25
2.25
2.24
2.22
2.05
2.03
2.02
2.00
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1.94
1.94
1.92
1.84
1.81
1.81
1.79
1.78
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1.75
1.74
1.67
1.66
1.17
1.14
0.96
0.95
0.93
NBoc
O
H3C
CH3
H3C
1.02
1.07
1.01
1.12
1.21
1.00
1.00
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2.12
2.27
8.90
5.79
3.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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5.0
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3.5
3.0
2.5
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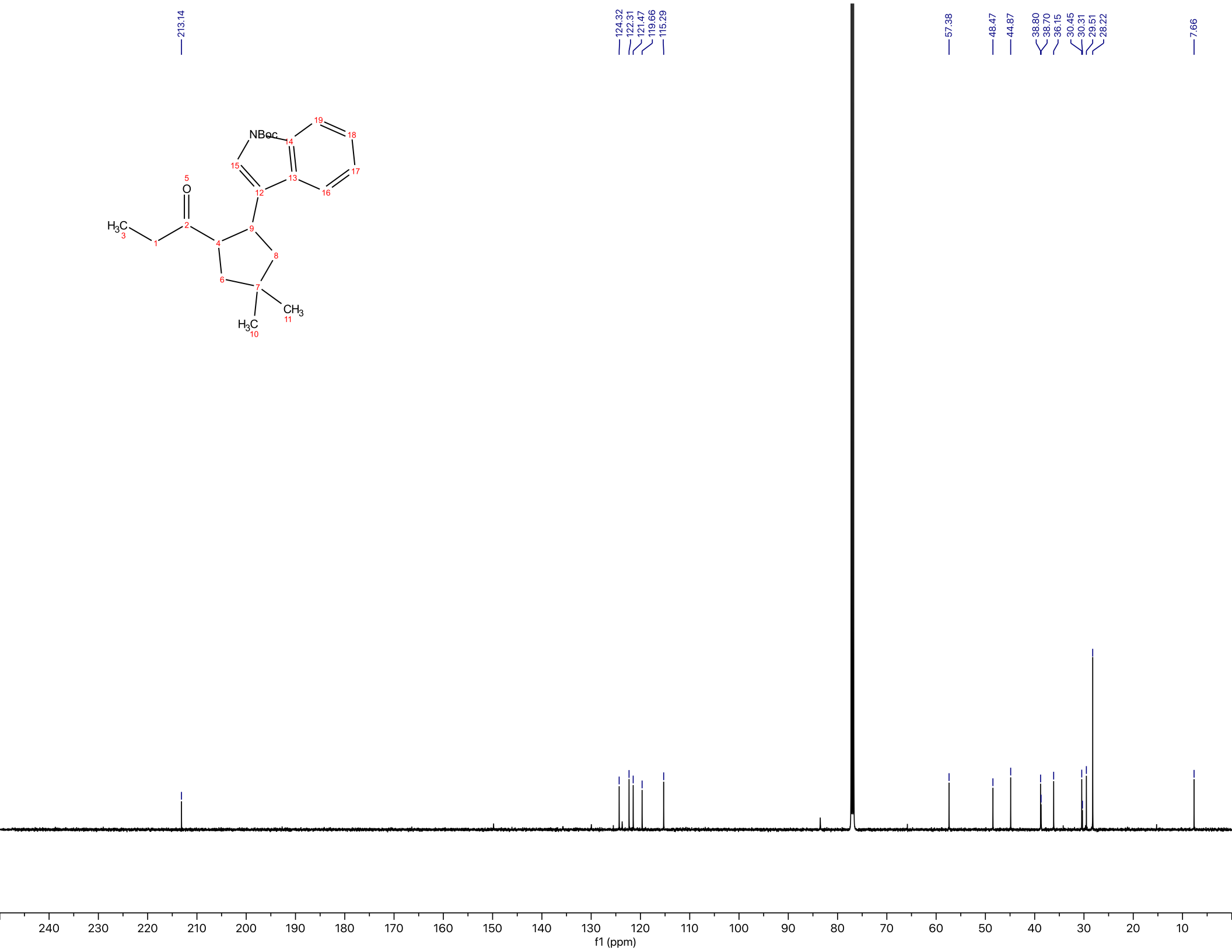
1.5
1.0
0.5
f1 (ppm)


213.14
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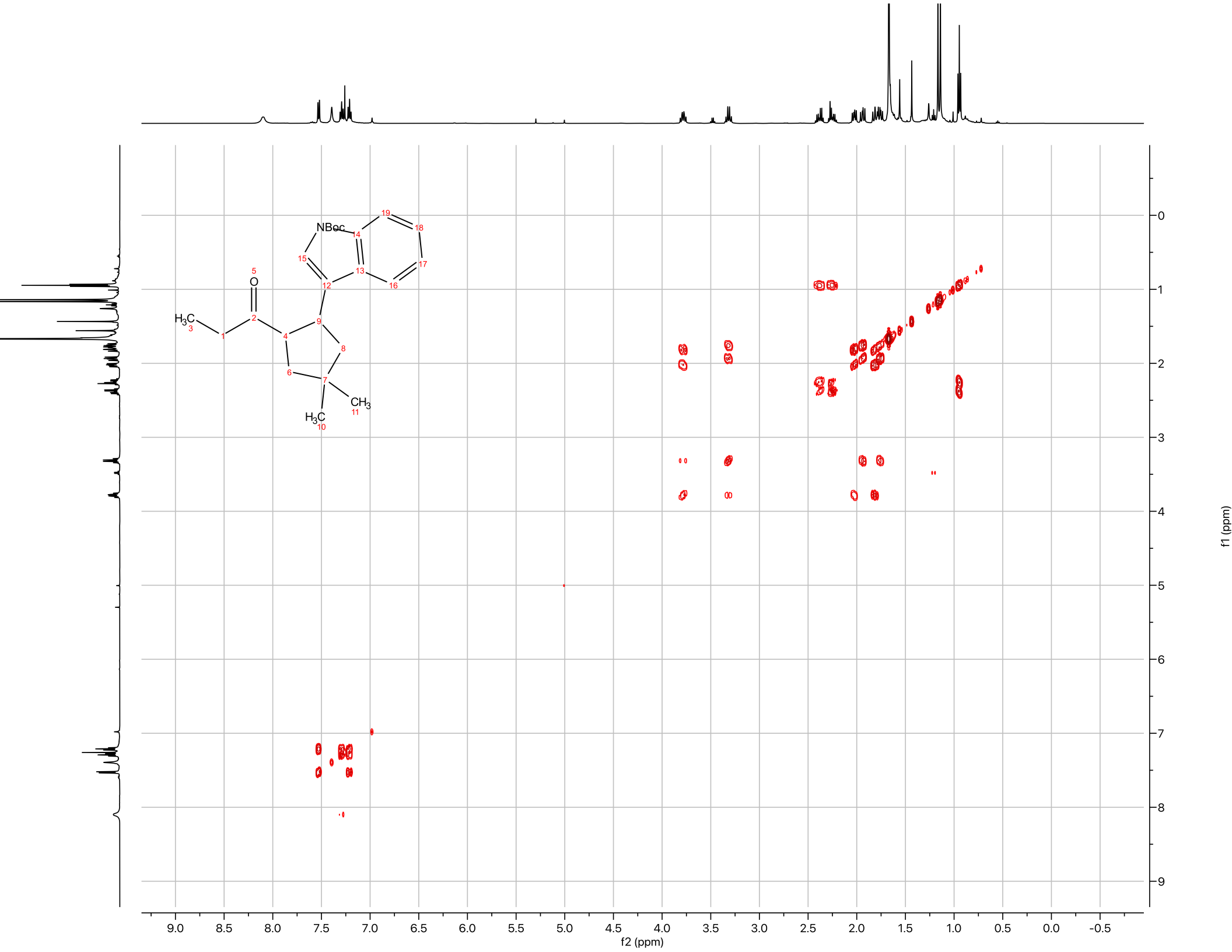
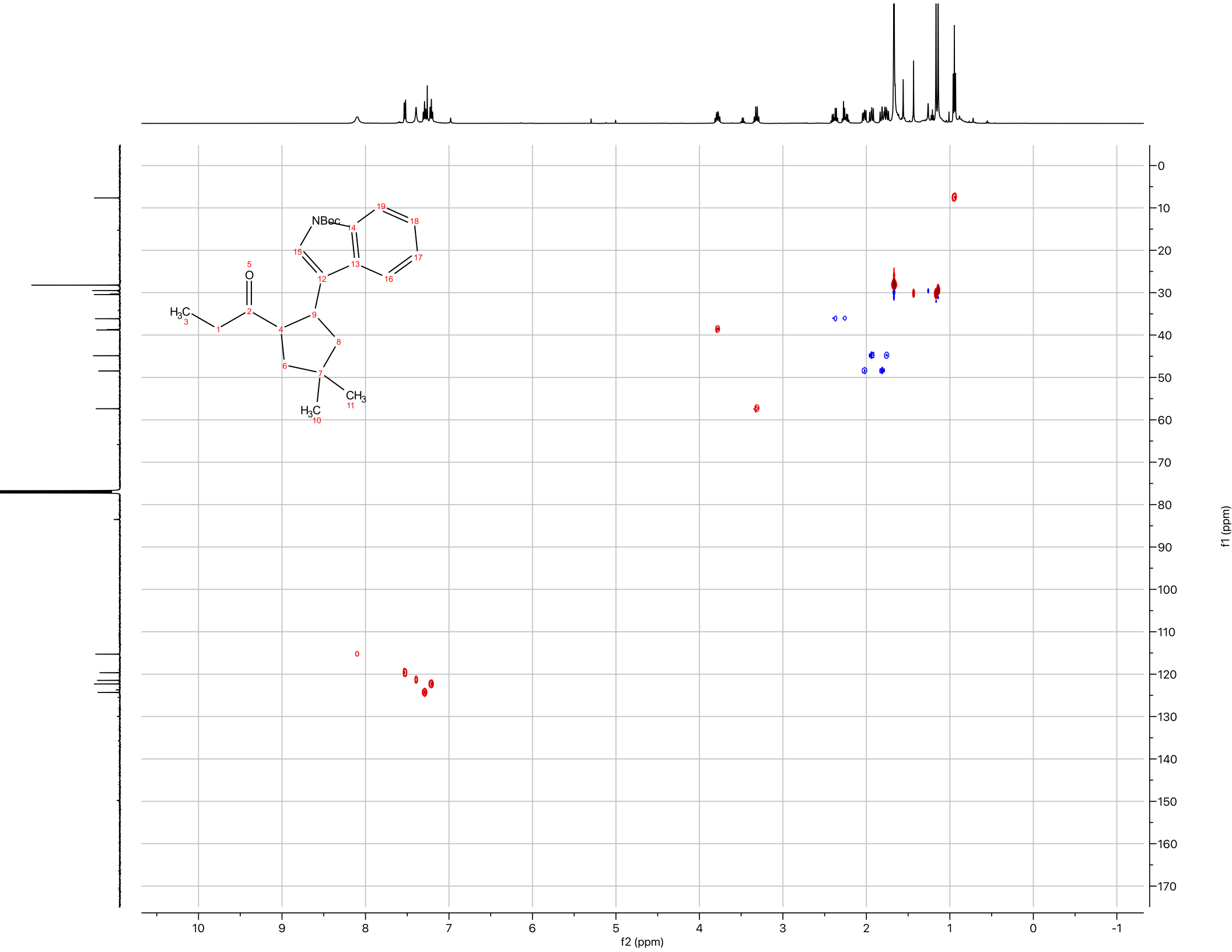
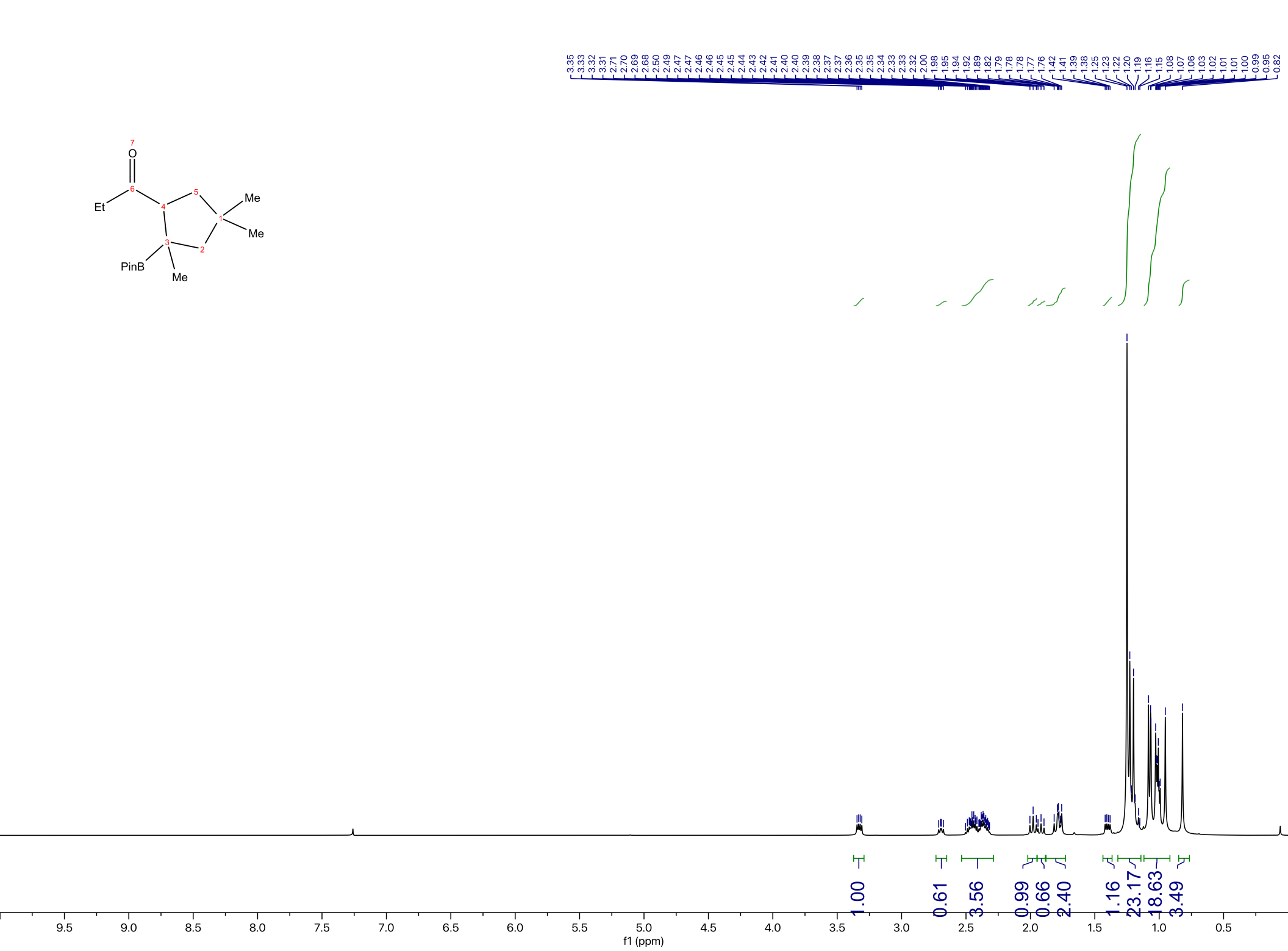
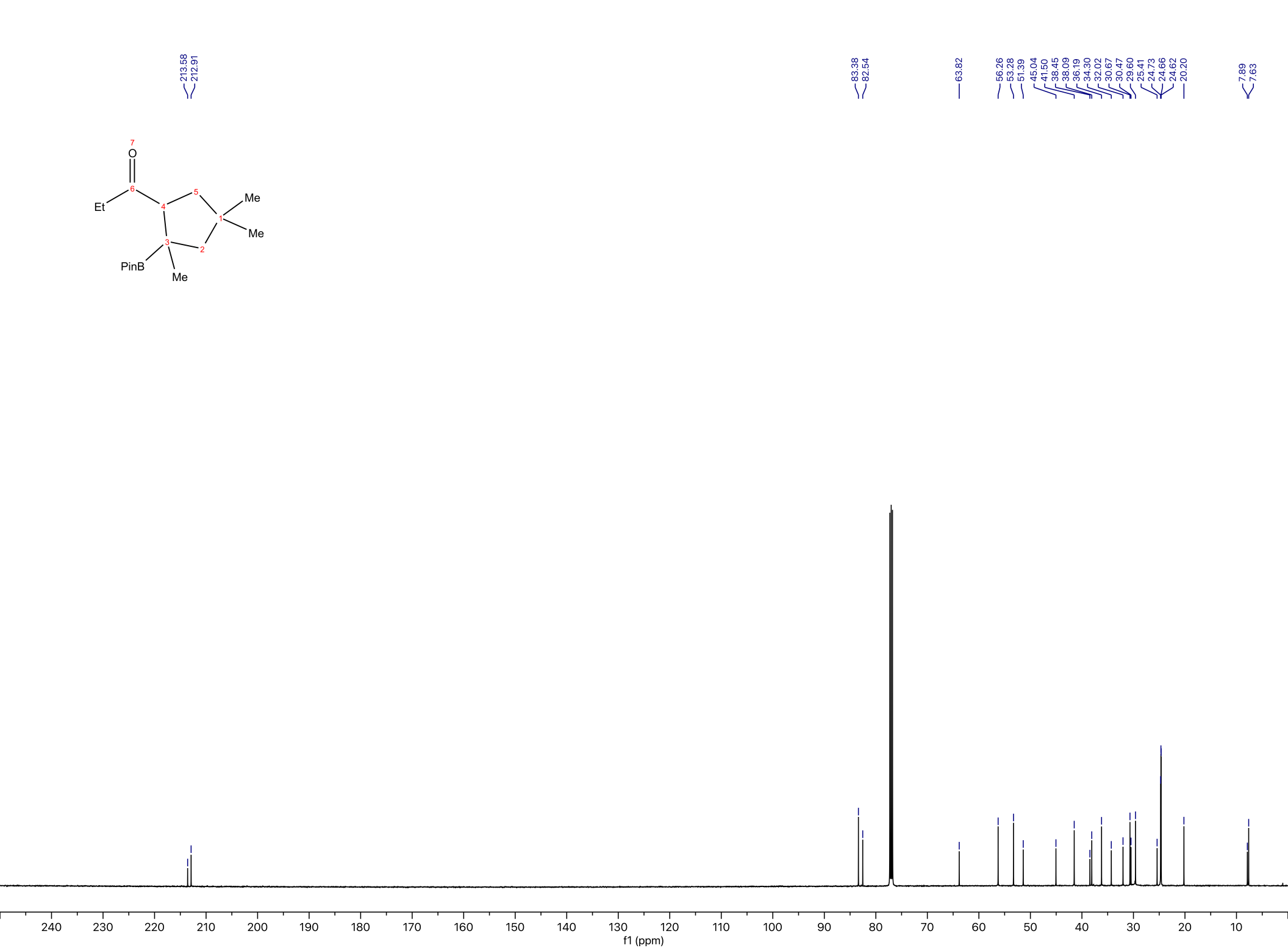
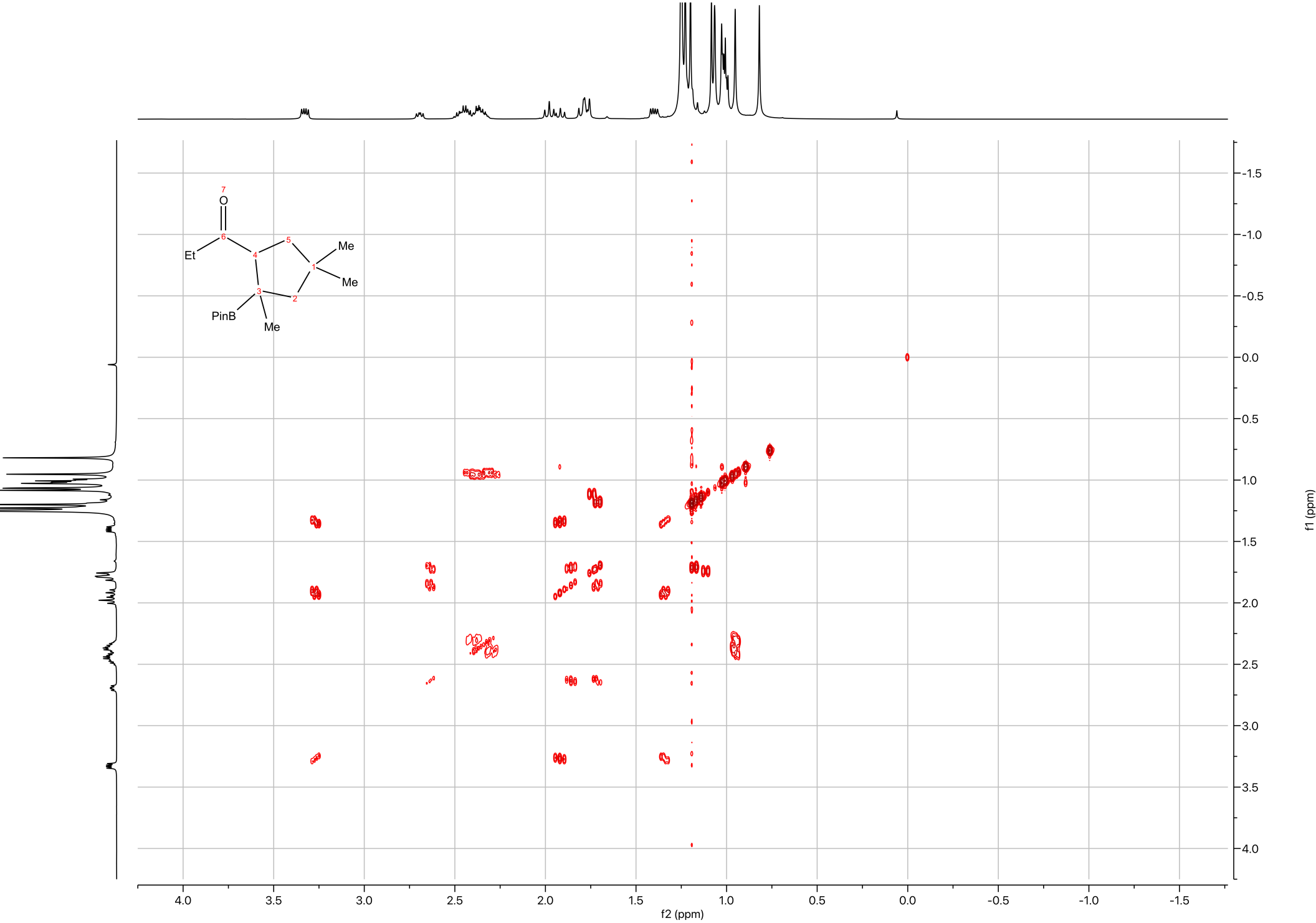
38.80
38.70
36.15
30.45
30.31
29.51
28.22
7.66
NBoc
O
H_3C
CH_3
H_3C
f1 (ppm)

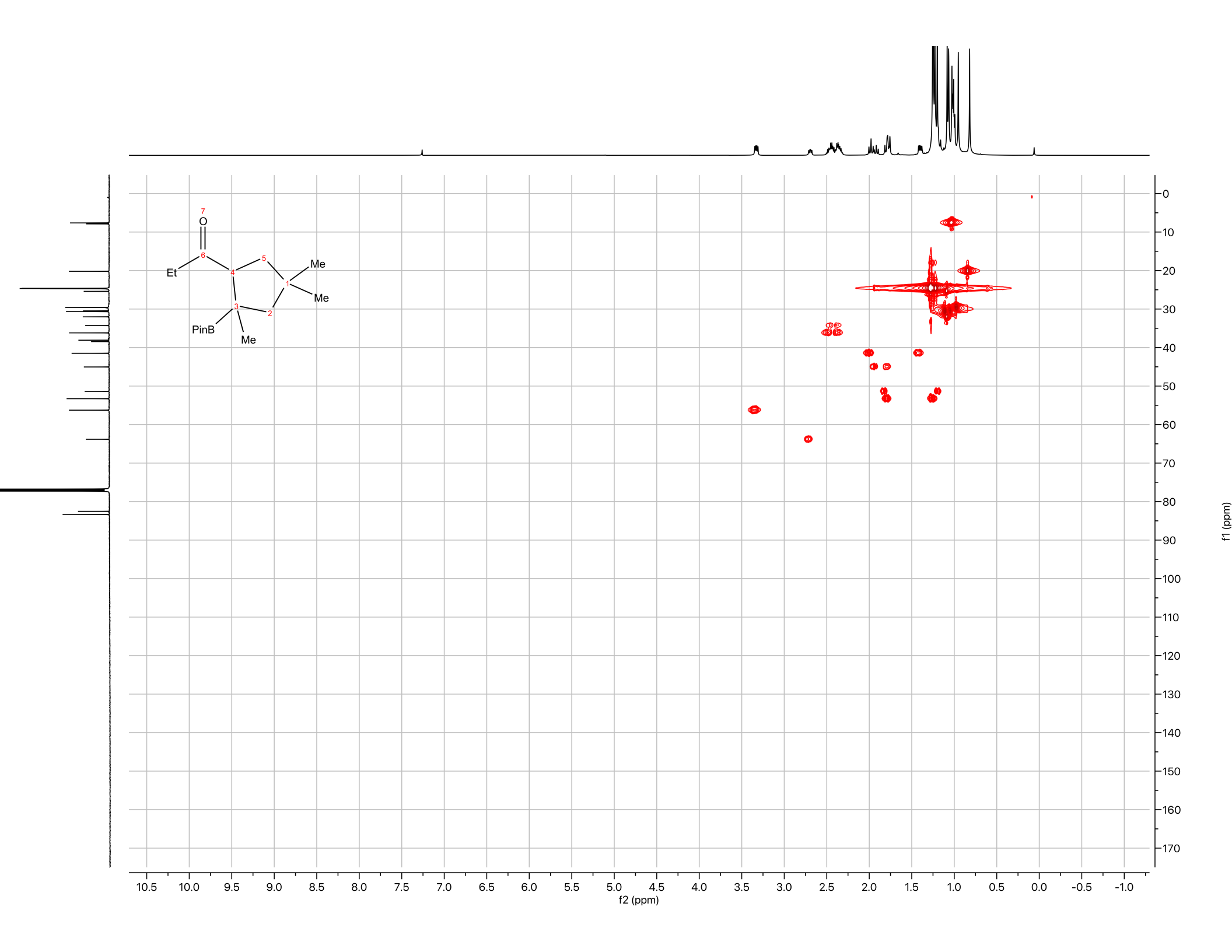

NBoc
O
H_3C
CH_3
H_3C
f2 (ppm)
f1 (ppm)

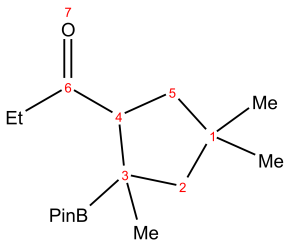

NBoc
O
H_3C
CH_3
H_3C
f2 (ppm)
f1 (ppm)


3.35 3.33 3.32 3.31 2.71 2.70 2.69 2.68 2.50 2.49 2.47 2.47 2.46 2.46 2.45 2.45 2.44 2.43 2.42 2.41 2.40 2.40 2.39 2.38 2.37 2.36 2.35 2.35 2.34 2.33 2.33 2.32 2.00 1.98 1.95 1.94 1.92 1.89 1.82 1.79 1.78 1.78 1.77 1.76 1.42 1.41 1.39 1.38 1.25 1.23 1.22 1.20 1.19 1.16 1.15 1.08 1.07 1.06 1.03 1.02 1.01 1.01 1.00 0.99 0.95 0.82
O
Et
Me
Me
PinB
Me
1.00 0.61 3.56 0.99 0.66 2.40 1.16 23.17 18.63 3.49
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)


213.58
212.91
83.38
82.54
63.82
56.26
53.28
51.39
45.04
41.50
38.45
38.09
36.19
34.30
32.02
30.67
30.47
29.60
25.41
24.73
24.66
24.62
20.20
7.89
7.63
O
Et
Me
Me
PinB
Me
f1 (ppm)


7
O
6
Et
4
5
Me
1
Me
3
2
PinB
Me
f2 (ppm)
f1 (ppm)


O
Et
Me
Me
PinB
Me
f2 (ppm)
f1 (ppm)

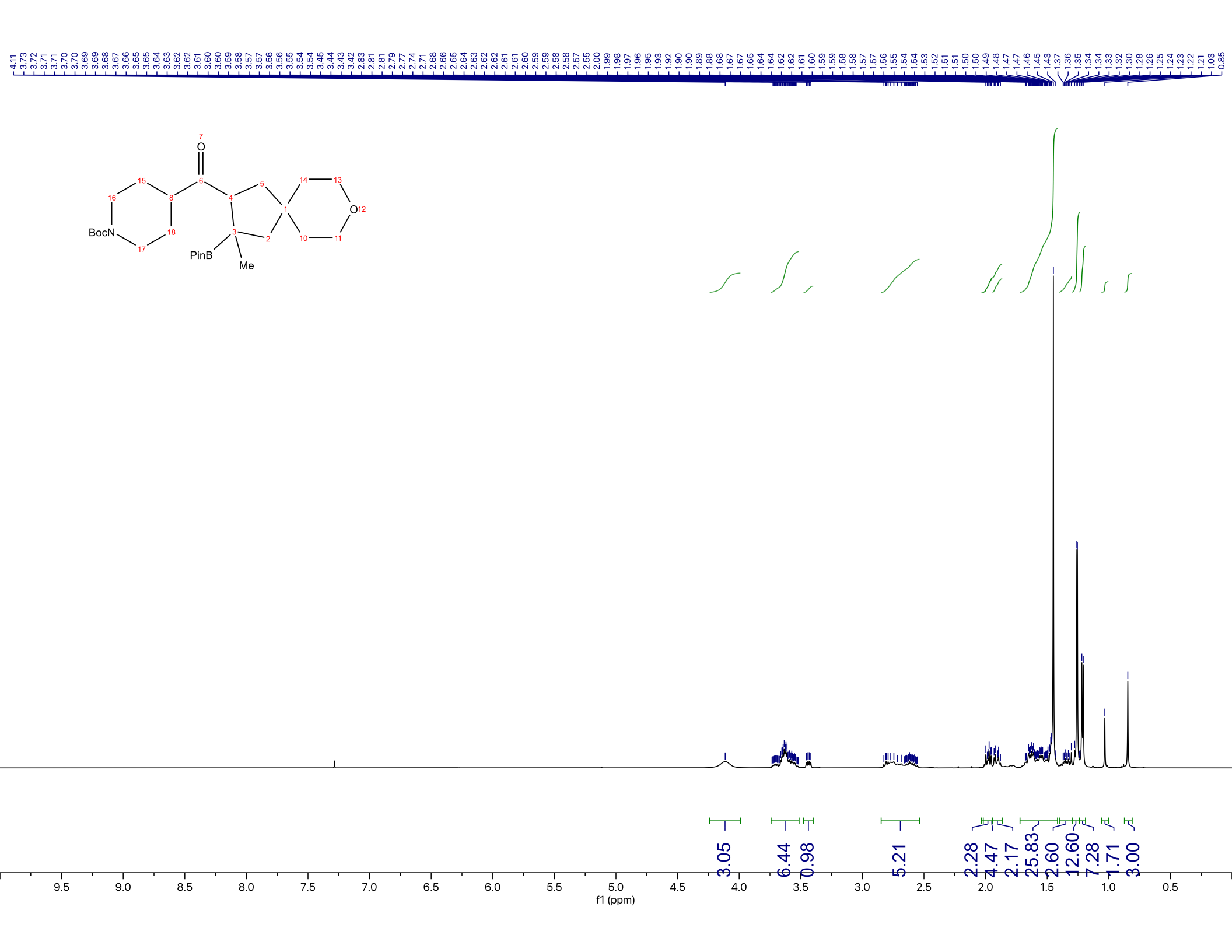


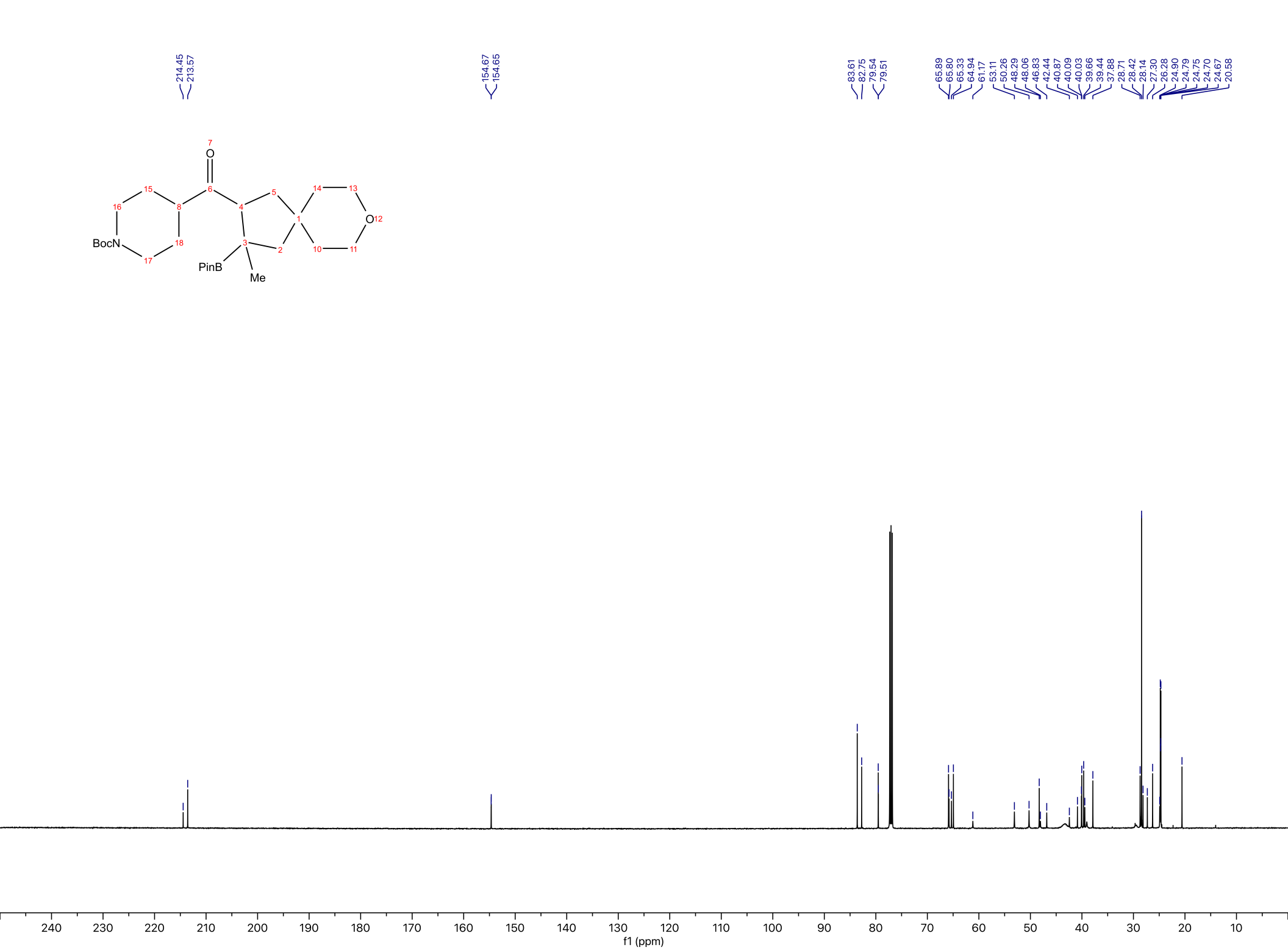
34.49

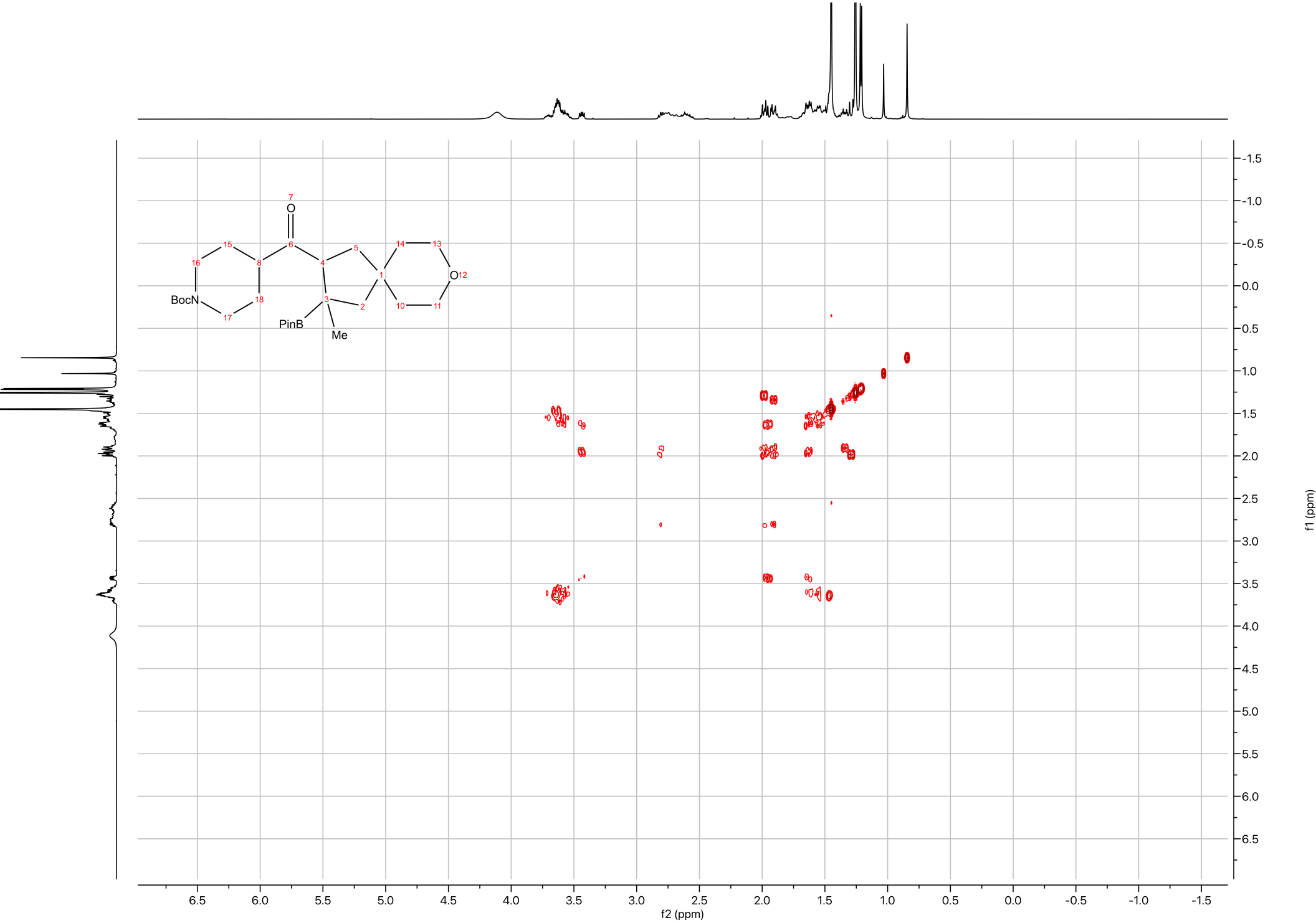
A (s)
34.49

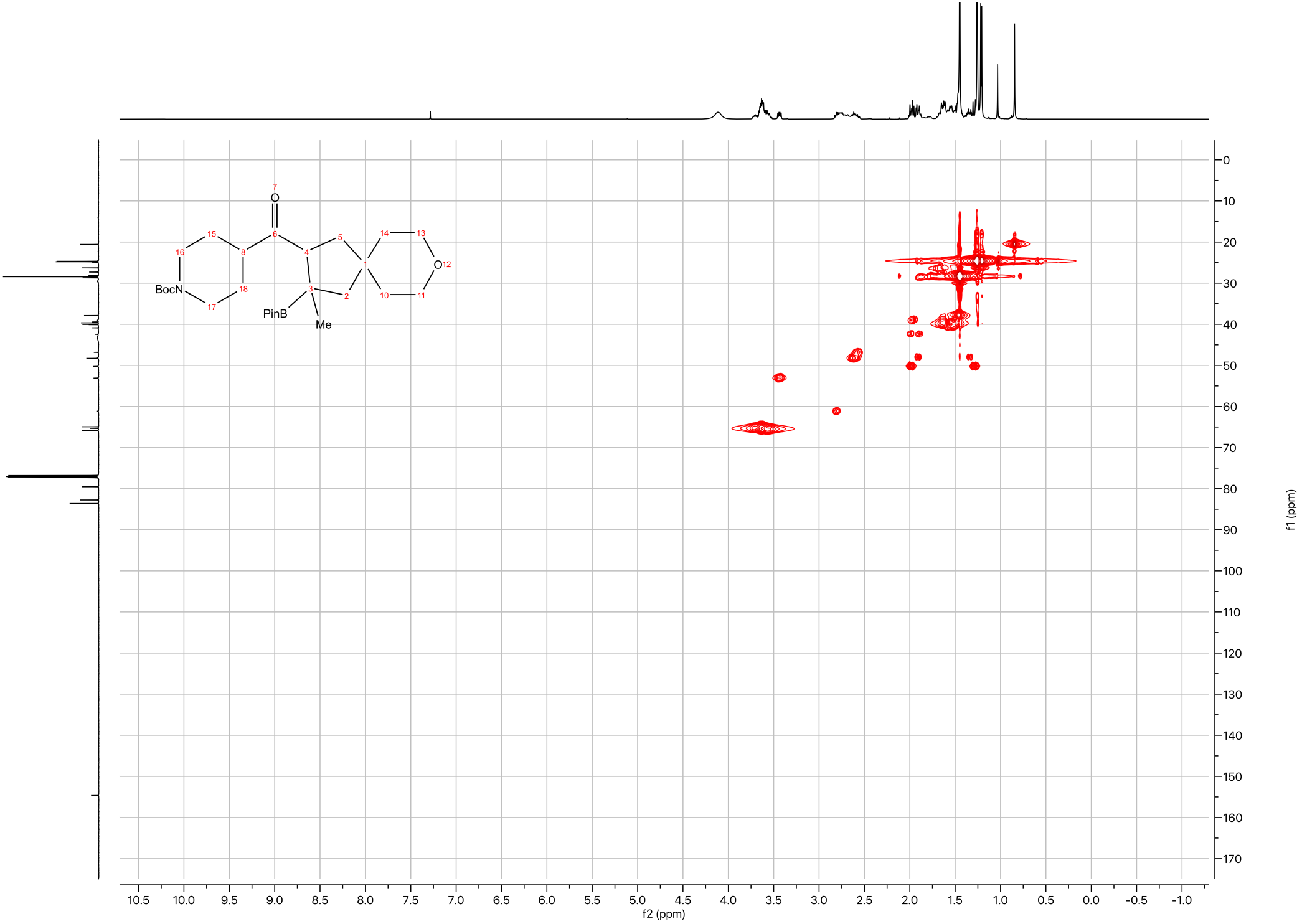
1.00

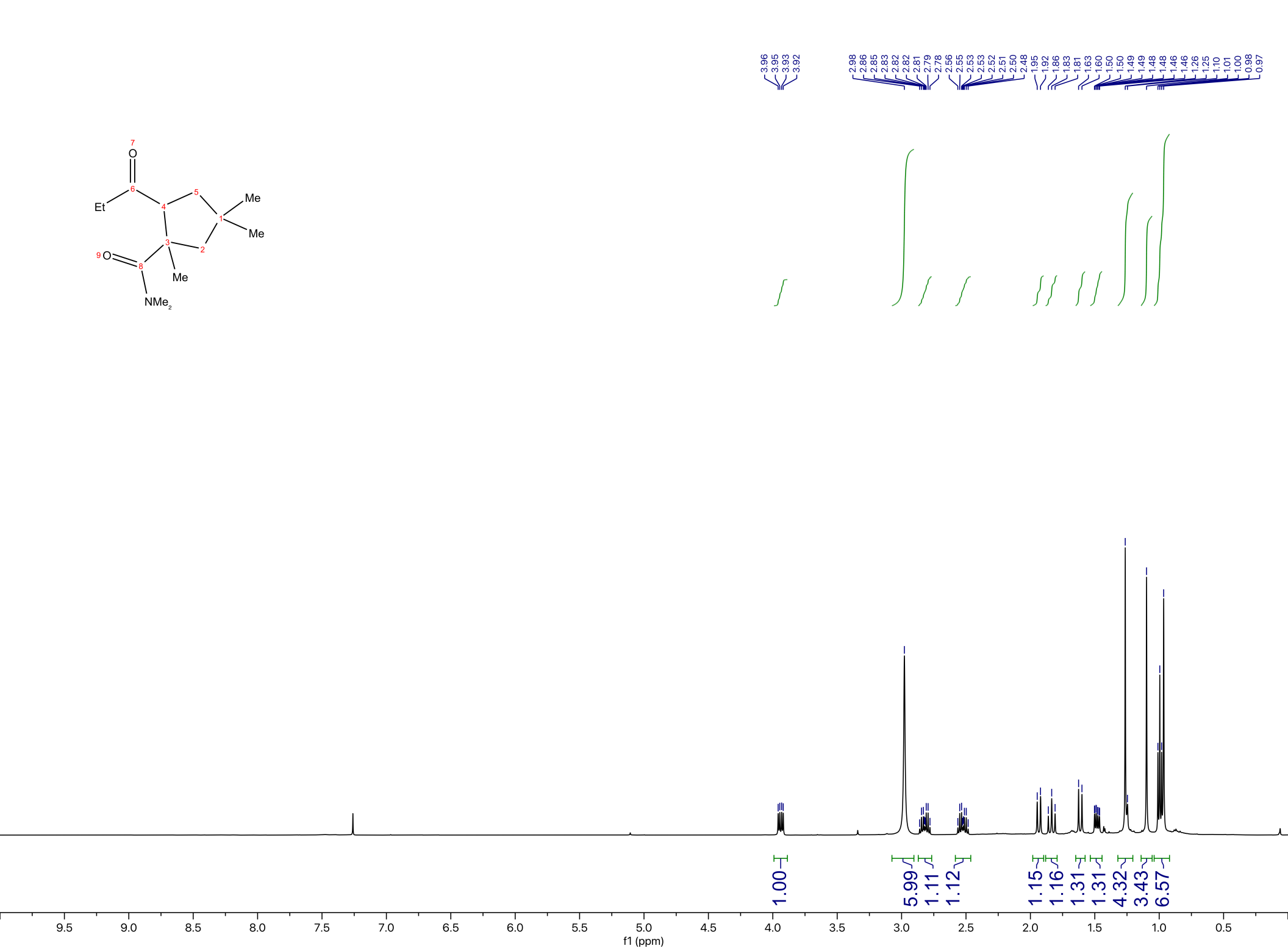
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

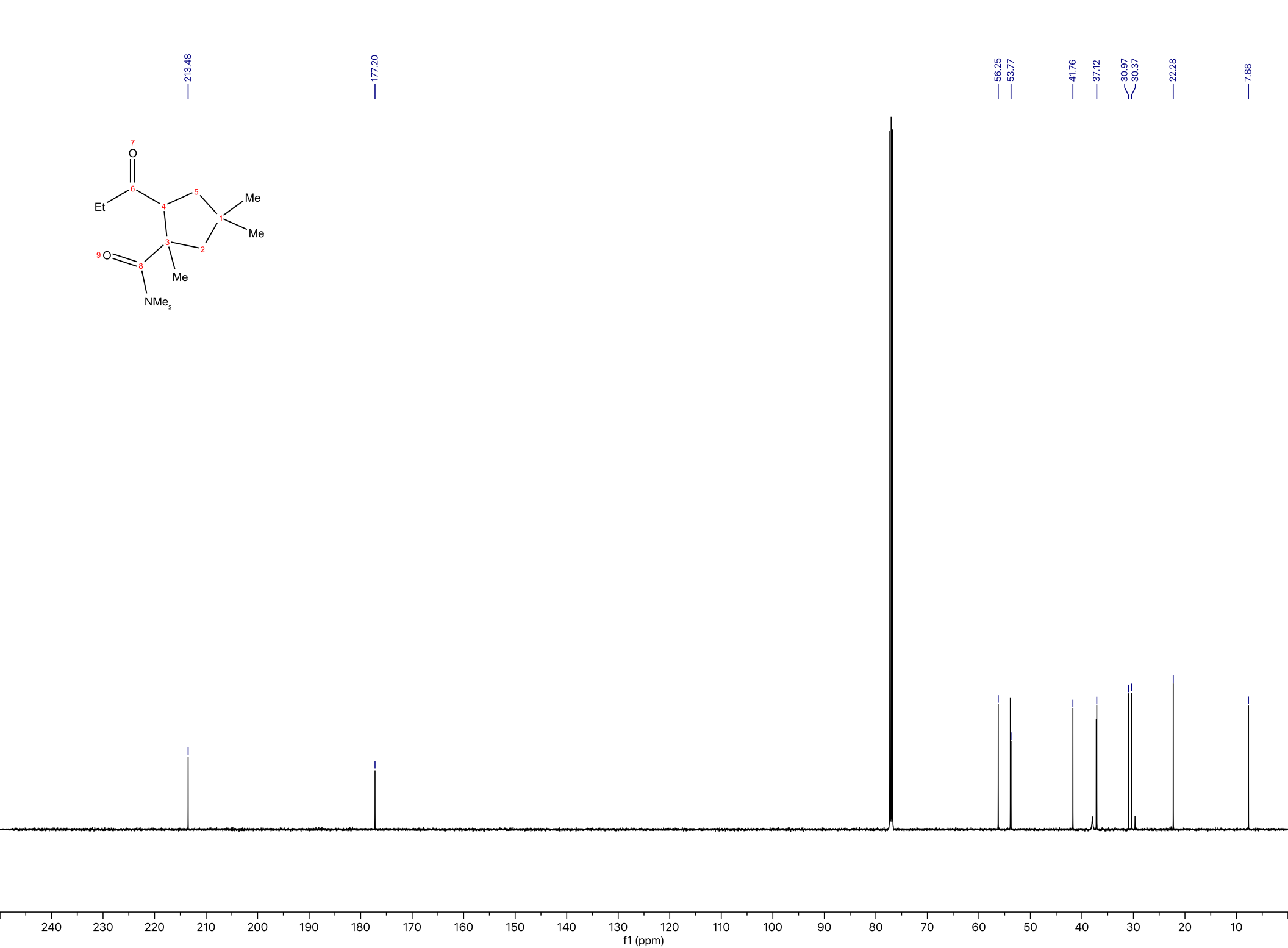

4.11 3.73 3.72 3.71 3.71 3.70 3.70 3.69 3.69 3.68 3.67 3.66 3.65 3.65 3.64 3.63 3.62 3.62 3.61 3.60 3.60 3.59 3.58 3.57 3.57 3.56 3.56 3.55 3.54 3.54 3.45 3.44 3.43 3.42 2.83 2.81 2.81 2.79 2.77 2.74 2.71 2.68 2.66 2.65 2.64 2.63 2.62 2.62 2.61 2.61 2.60 2.59 2.59 2.58 2.58 2.57 2.55 2.00 1.99 1.98 1.97 1.96 1.95 1.93 1.92 1.90 1.90 1.89 1.88 1.68 1.67 1.67 1.65 1.64 1.64 1.62 1.62 1.61 1.60 1.59 1.59 1.58 1.58 1.57 1.57 1.56 1.55 1.54 1.54 1.53 1.52 1.51 1.51 1.50 1.50 1.49 1.48 1.47 1.47 1.46 1.45 1.43 1.37 1.36 1.35 1.34 1.34 1.33 1.32 1.30 1.28 1.26 1.25 1.24 1.23 1.22 1.21 1.03 0.85
O
BocN
PinB
Me
3.05
6.44
0.98
5.21
2.28
4.47
2.17
25.83
2.60
12.60
7.28
1.71
3.00
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)

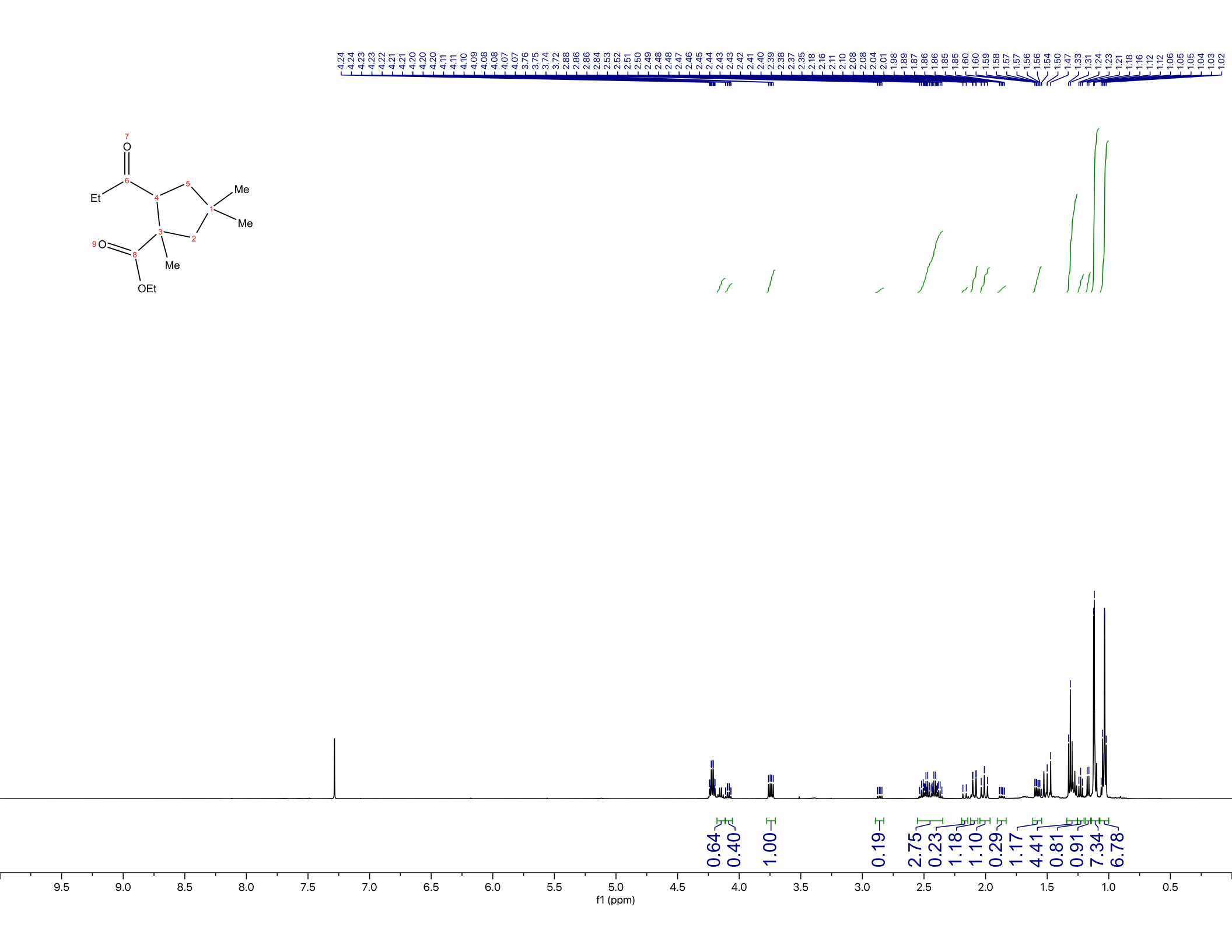

214.45
213.57
154.67
154.65
83.61
82.75
79.54
79.51
65.89
65.80
65.33
64.94
61.17
53.11
50.26
48.29
48.06
46.83
42.44
40.87
40.09
40.03
39.66
39.44
37.88
28.71
28.42
28.14
27.30
26.28
24.90
24.79
24.75
24.70
24.67
20.58
O
BocN
PinB
Me
f1 (ppm)

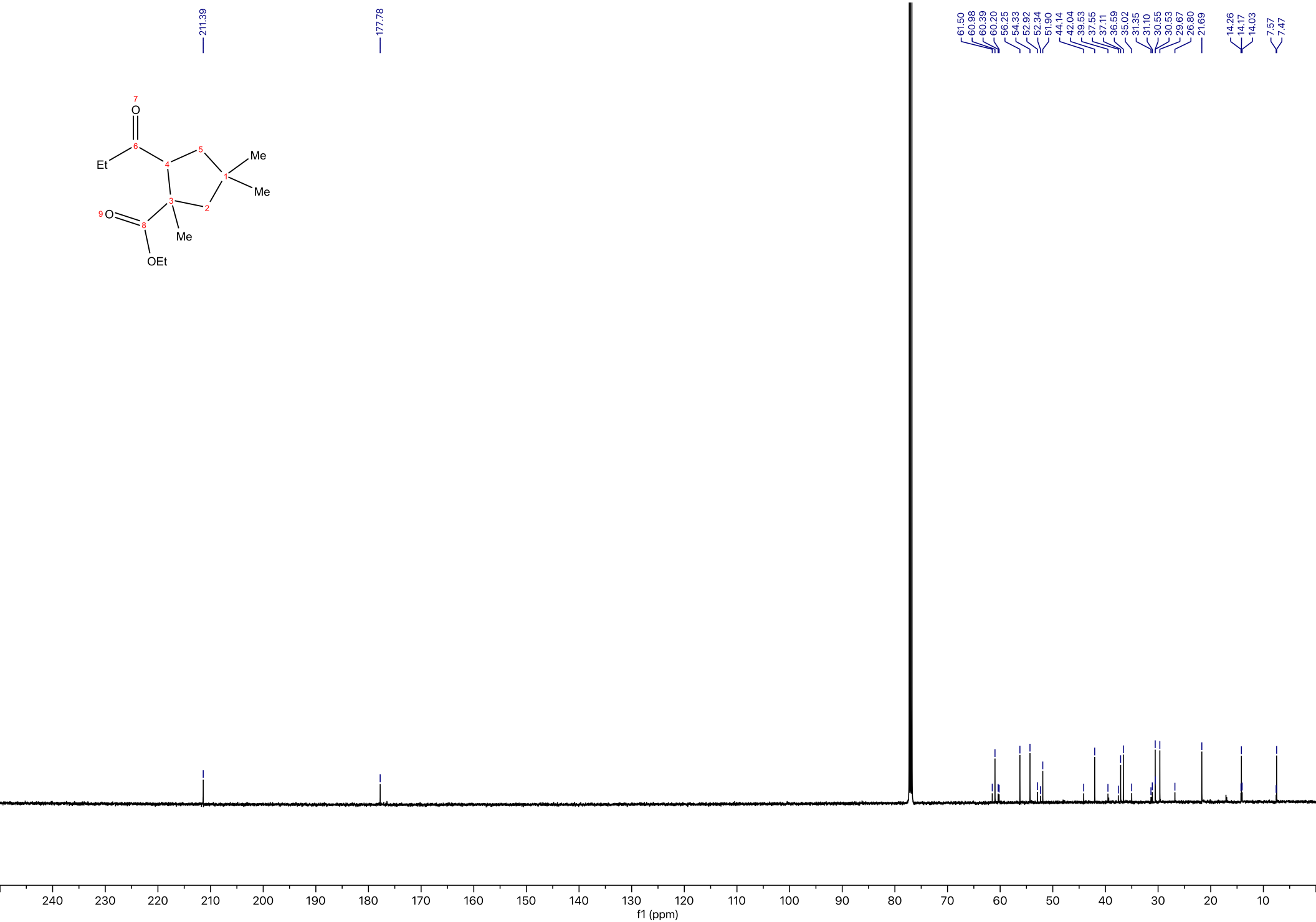

O
BocN
PinB
Me
f2 (ppm)
f1 (ppm)

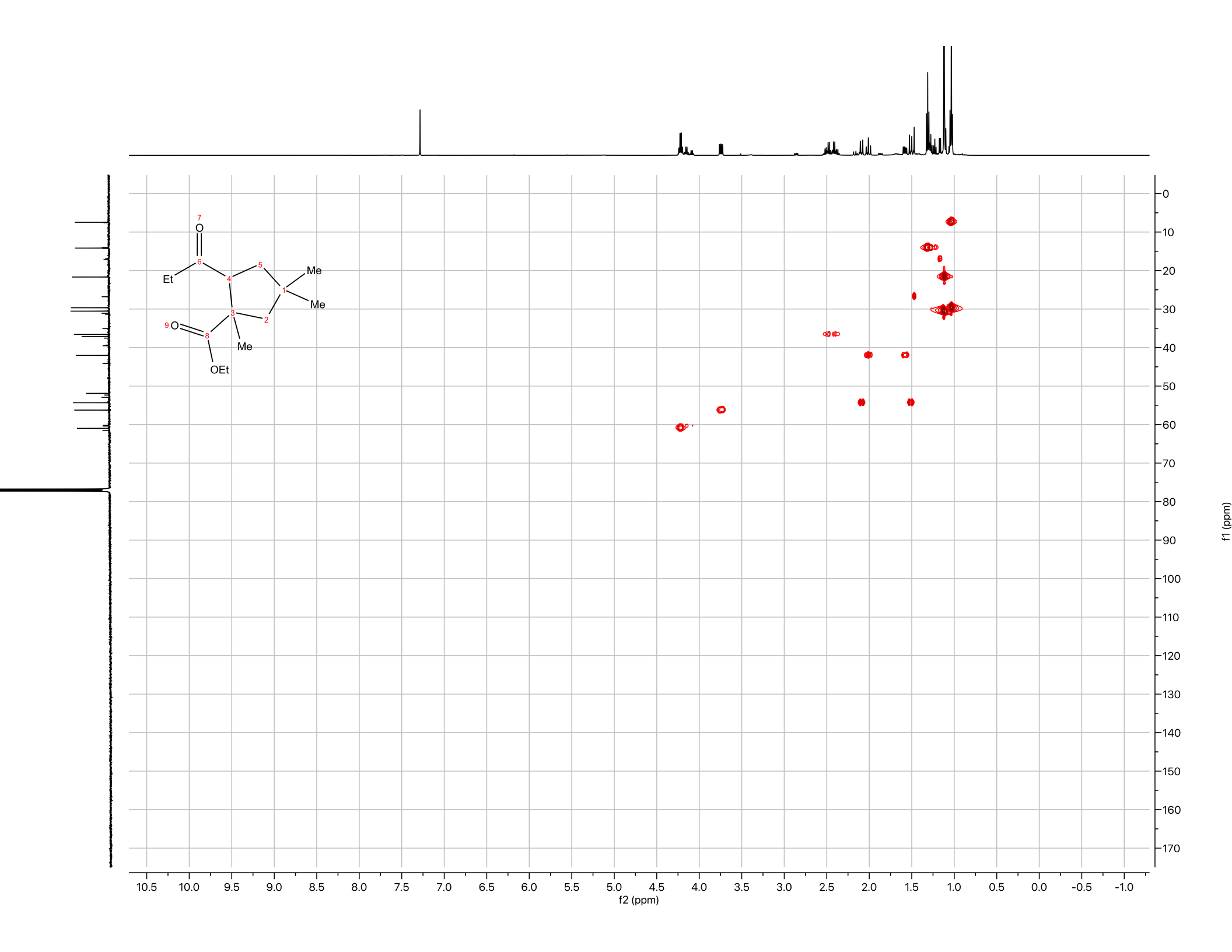

O
BocN
PinB
Me
O
f2 (ppm)
f1 (ppm)

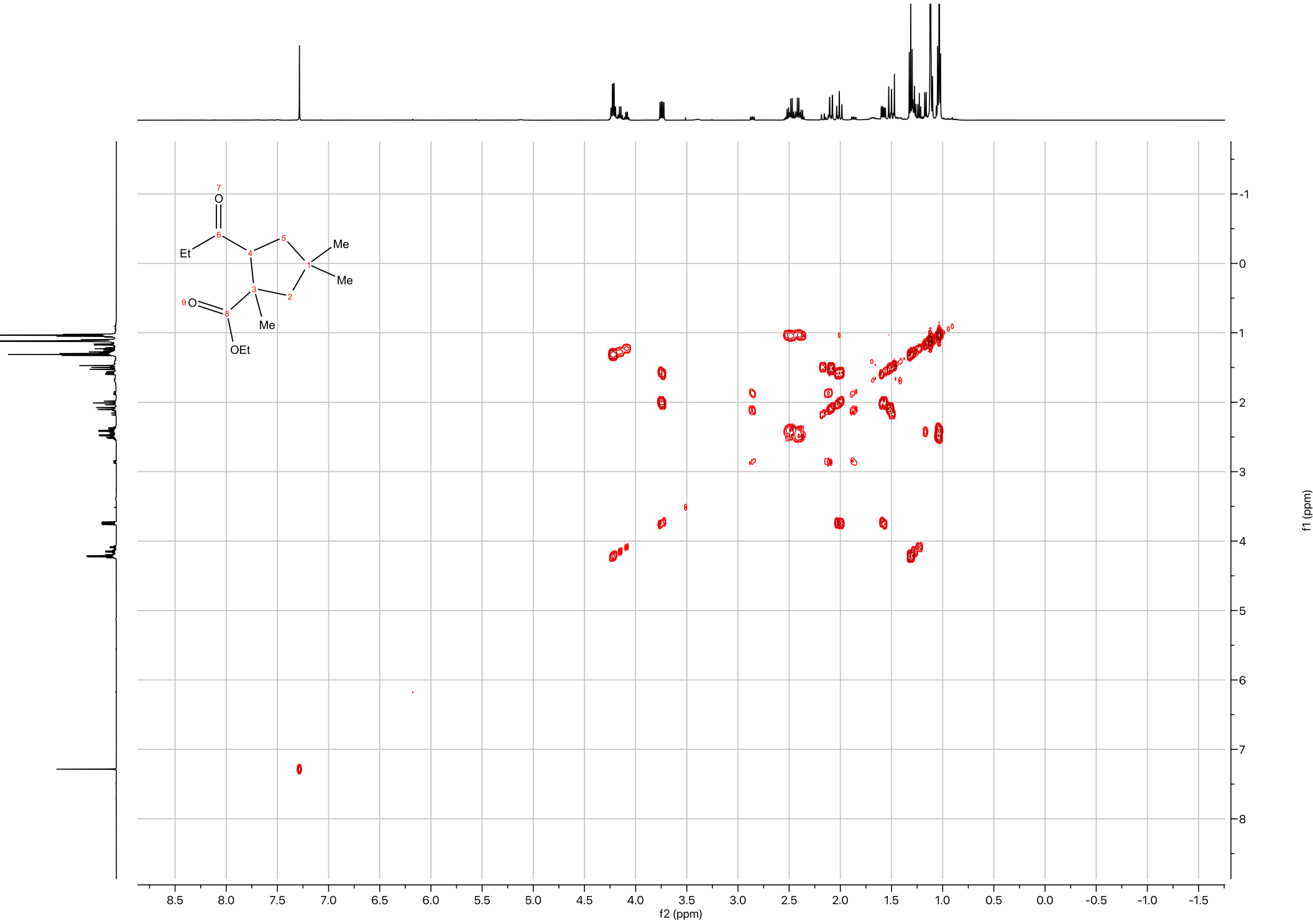

3.96
3.95
3.93
3.92
2.98
2.86
2.85
2.83
2.82
2.82
2.81
2.79
2.78
2.56
2.55
2.53
2.53
2.52
2.51
2.50
2.48
1.95
1.92
1.86
1.83
1.81
1.63
1.60
1.50
1.50
1.49
1.49
1.48
1.48
1.46
1.46
1.26
1.25
1.10
1.01
1.00
0.98
0.97
O
Et
Me
Me
O
Me
NMe2
1.00
5.99
1.11
1.12
1.15
1.16
1.31
1.31
4.32
3.43
6.57
9.5
9.0
8.5
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)

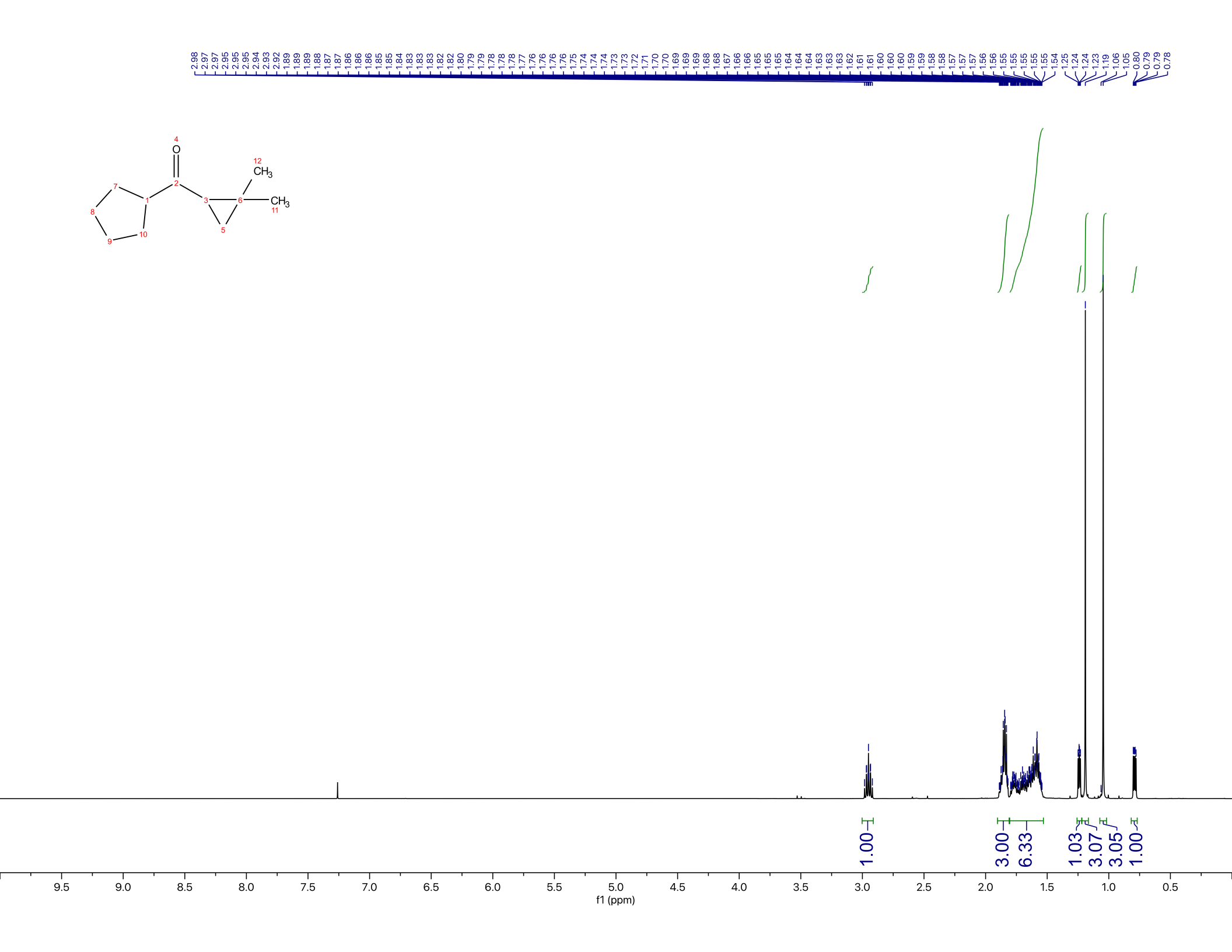

213.48
177.20
56.25
53.77
41.76
37.12
30.97
30.37
22.28
7.68
O
Et
Me
Me
O
Me
NMe2
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

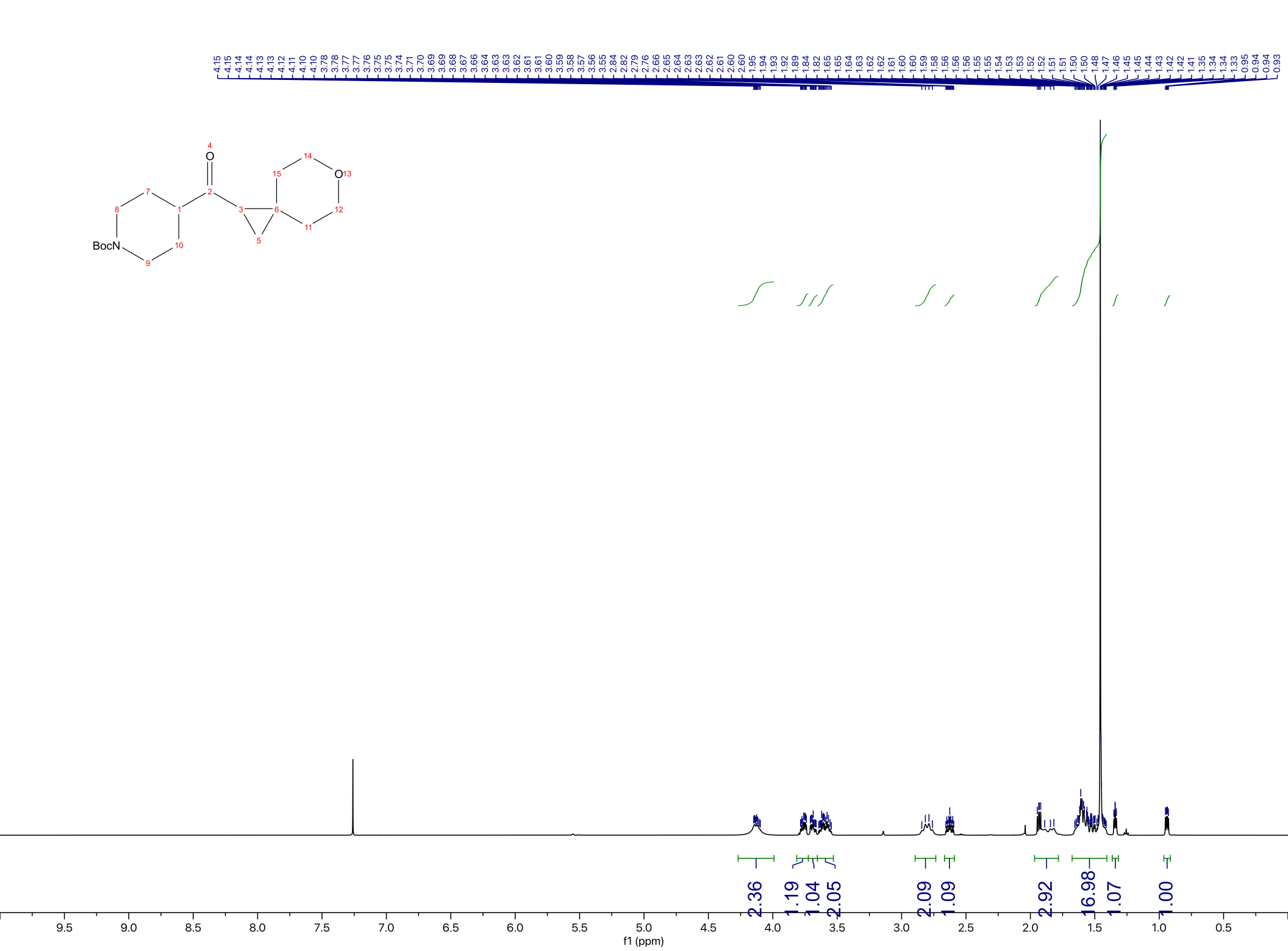

4.24 4.24 4.23 4.22 4.21 4.21 4.20 4.20 4.20 4.11 4.11 4.10 4.09 4.08 4.08 4.07 4.07 3.76 3.75 3.74 3.72 2.88 2.86 2.86 2.84 2.53 2.52 2.51 2.50 2.49 2.48 2.48 2.47 2.46 2.45 2.44 2.43 2.43 2.42 2.41 2.40 2.39 2.38 2.37 2.35 2.18 2.16 2.11 2.10 2.08 2.08 2.04 2.01 1.98 1.89 1.87 1.86 1.86 1.85 1.85 1.60 1.60 1.59 1.58 1.57 1.57 1.56 1.56 1.54 1.50 1.47 1.33 1.31 1.24 1.23 1.21 1.18 1.16 1.12 1.12 1.06 1.05 1.05 1.04 1.03 1.02
O
Et
Me
Me
O
Me
OEt
0.64 0.40 1.00 0.19 2.75 0.23 1.18 1.10 0.29 1.17 4.41 0.81 0.91 7.34 6.78
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)

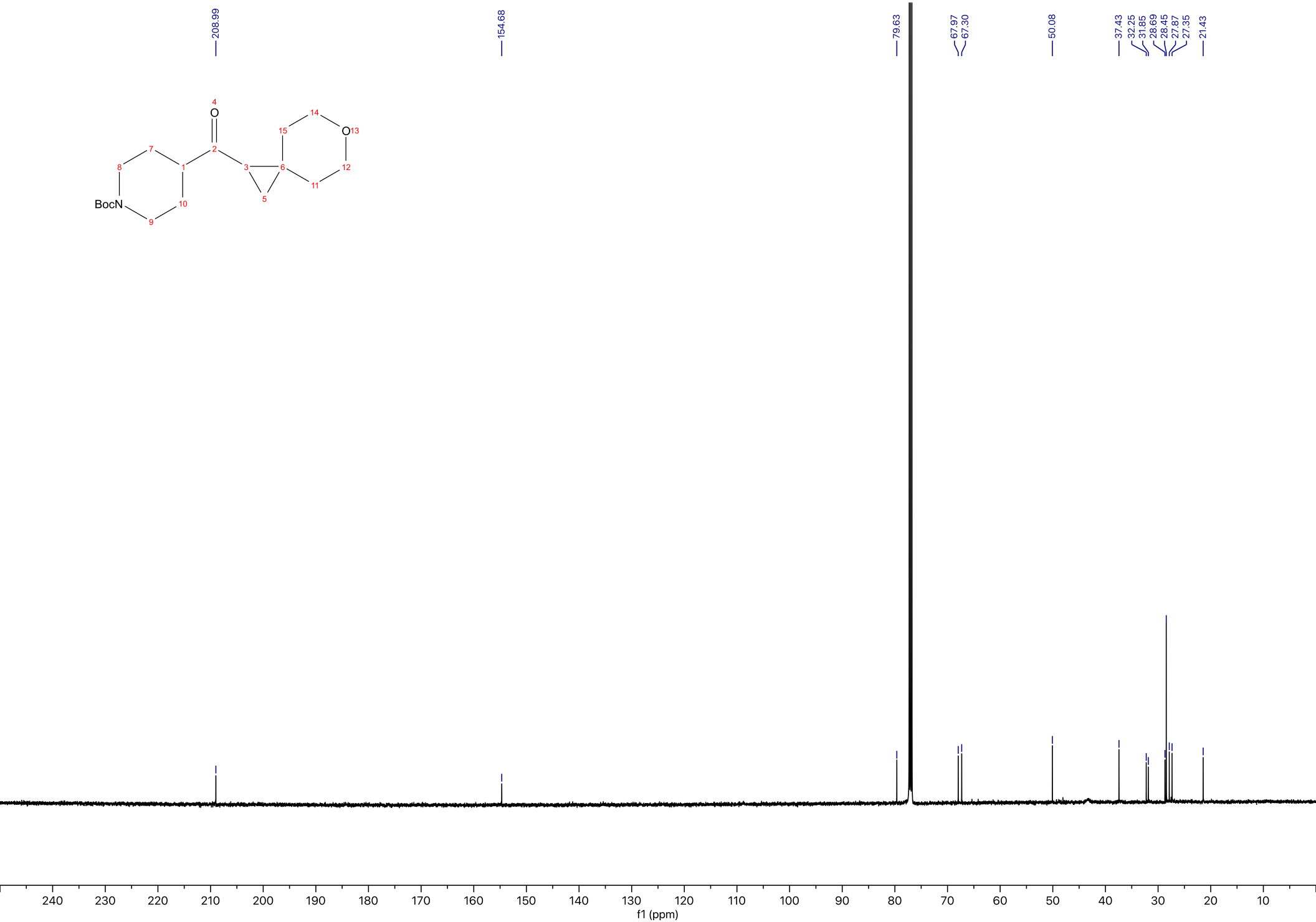

211.39
177.78
61.50
60.98
60.39
60.20
56.25
54.33
52.92
52.34
51.90
44.14
42.04
39.53
37.55
37.11
36.59
35.02
31.35
31.10
30.55
30.53
29.67
26.80
21.69
14.26
14.17
14.03
7.57
7.47
O
Et
Me
Me
O
Me
OEt
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

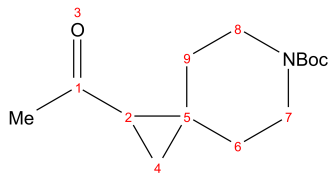

7
O
6
Et
4
5
1
Me
Me
9
O
8
3
2
Me
OEt
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f2 (ppm)
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
f1 (ppm)


O
Et
Me
Me
O
Me
OEt
f2 (ppm)
f1 (ppm)


2.98 2.97 2.97 2.95 2.95 2.95 2.94 2.93 2.92 1.89 1.89 1.89 1.88 1.87 1.87 1.86 1.86 1.86 1.85 1.85 1.84 1.83 1.83 1.83 1.82 1.82 1.80 1.79 1.79 1.78 1.78 1.78 1.77 1.76 1.76 1.76 1.76 1.75 1.74 1.74 1.73 1.73 1.72 1.71 1.70 1.70 1.69 1.69 1.69 1.68 1.68 1.67 1.66 1.66 1.65 1.65 1.65 1.64 1.64 1.64 1.63 1.63 1.63 1.62 1.61 1.61 1.60 1.60 1.60 1.59 1.59 1.58 1.58 1.57 1.57 1.57 1.56 1.56 1.55 1.55 1.55 1.55 1.55 1.54 1.25 1.24 1.24 1.23 1.19 1.06 1.05 0.80 0.79 0.79 0.78
O
CH3
CH3
1.00
3.00
6.33
1.03
3.07
3.05
1.00
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)


4.15 4.15 4.14 4.14 4.13 4.13 4.12 4.11 4.10 4.10 3.78 3.78 3.77 3.77 3.76 3.75 3.75 3.74 3.71 3.70 3.69 3.69 3.68 3.67 3.66 3.64 3.63 3.63 3.62 3.61 3.61 3.60 3.59 3.58 3.57 3.56 3.55 2.84 2.82 2.79 2.76 2.66 2.65 2.64 2.63 2.63 2.62 2.61 2.60 2.60 1.95 1.94 1.93 1.92 1.89 1.84 1.82 1.65 1.64 1.63 1.62 1.62 1.61 1.60 1.60 1.59 1.58 1.56 1.56 1.56 1.55 1.55 1.54 1.53 1.53 1.52 1.52 1.51 1.51 1.50 1.50 1.48 1.47 1.46 1.45 1.45 1.44 1.43 1.42 1.42 1.41 1.35 1.34 1.34 1.33 0.95 0.94 0.94 0.93
O
BocN
2.36
1.19
1.04
2.05
2.09
1.09
2.92
16.98
1.07
1.00
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)


208.99
154.68
79.63
67.97
67.30
50.08
37.43
32.25
31.85
28.69
28.45
27.87
27.35
21.43
BocN
O
O
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

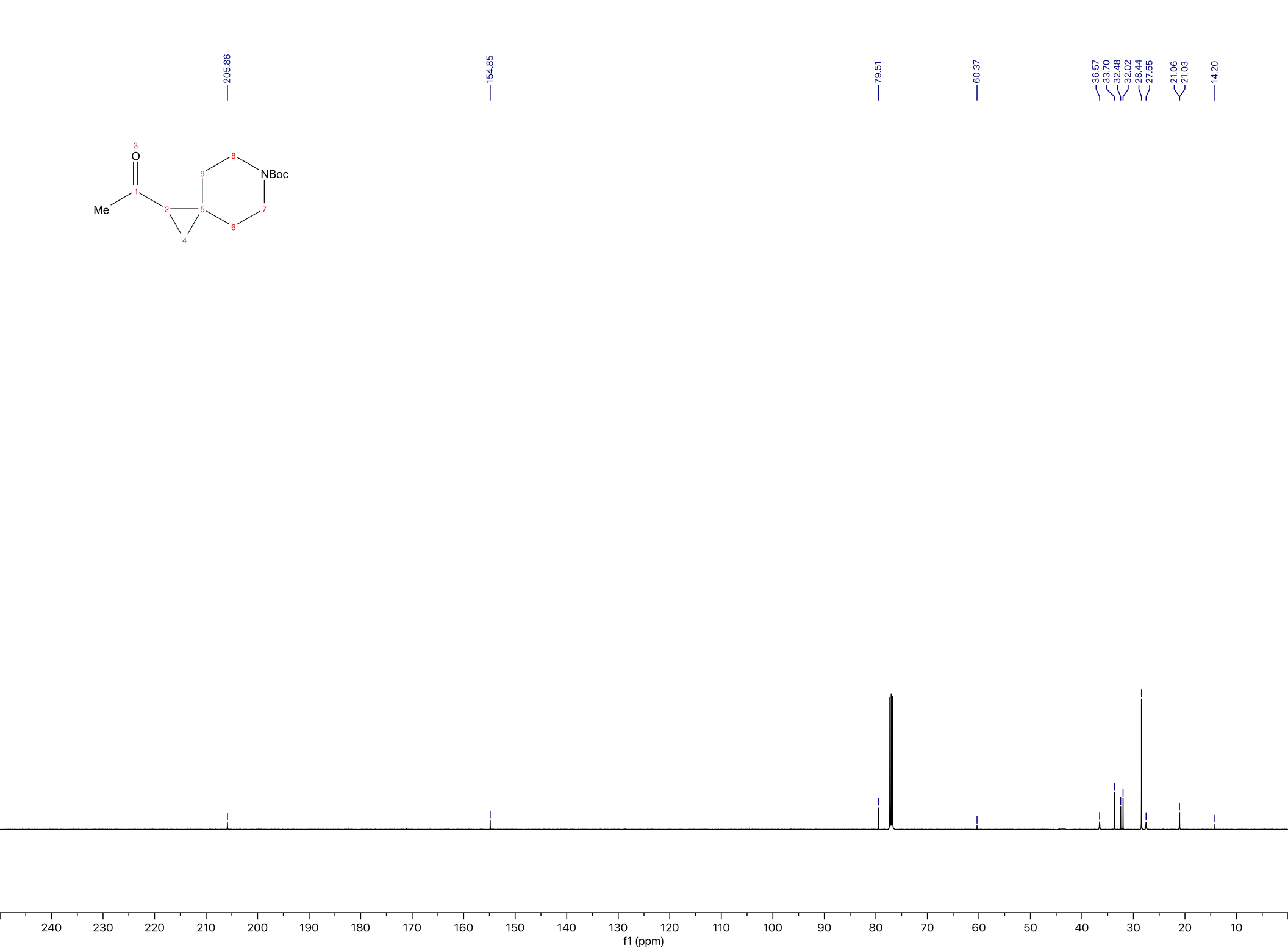


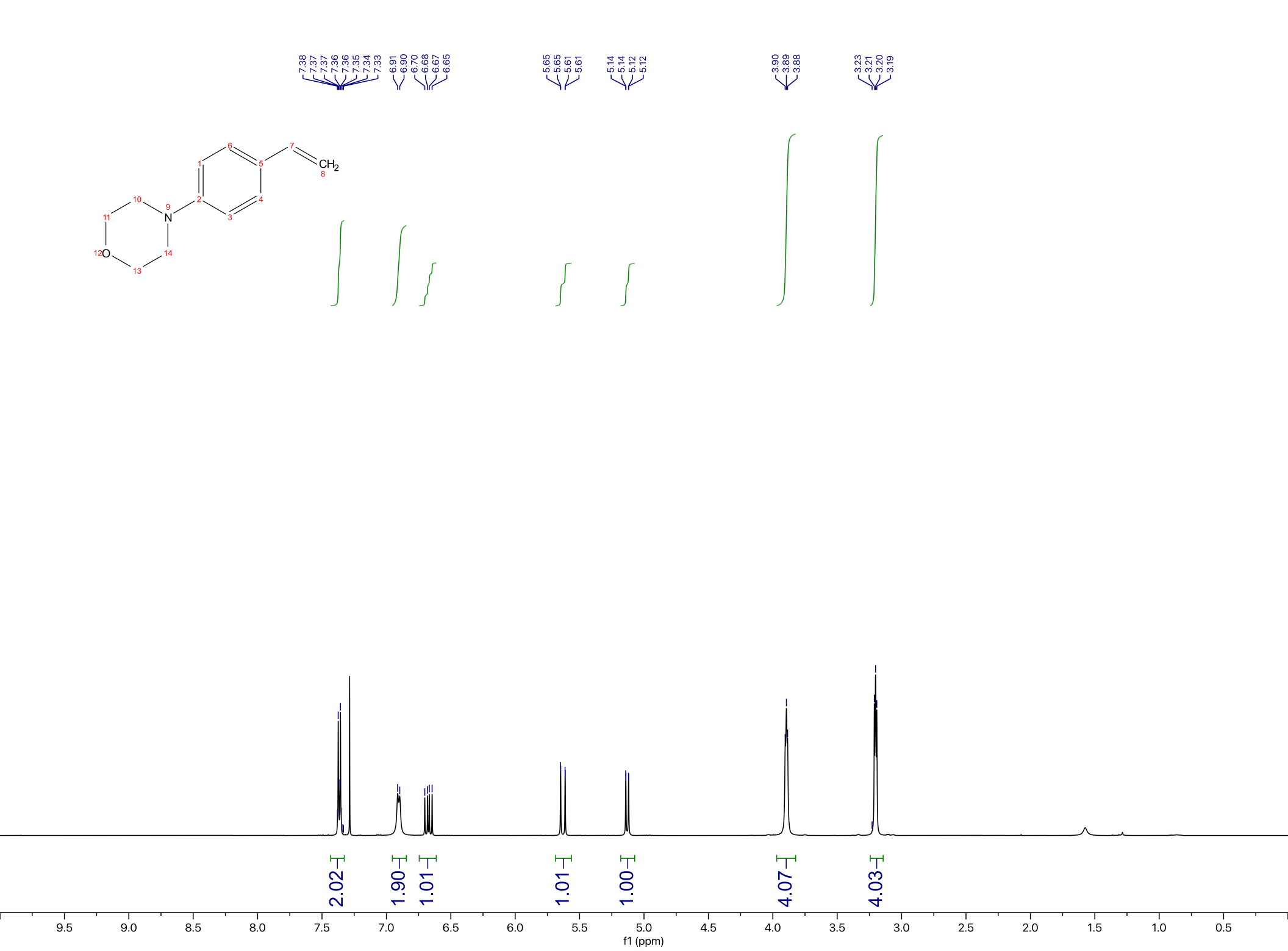
3.55 3.54 3.53 3.52 3.52 3.51 3.51 3.44 3.44 3.43 3.43 3.42 3.41 3.19 3.18 3.18 3.17 2.31 2.30 2.30 1.95 1.93 1.93 1.92 1.63 1.62 1.61 1.61 1.59 1.58 1.58 1.56 1.52 1.51 1.51 1.50 1.48 1.47 1.46 1.44 1.43 1.35 1.34 1.33 1.33 0.93 0.92 0.92 0.91

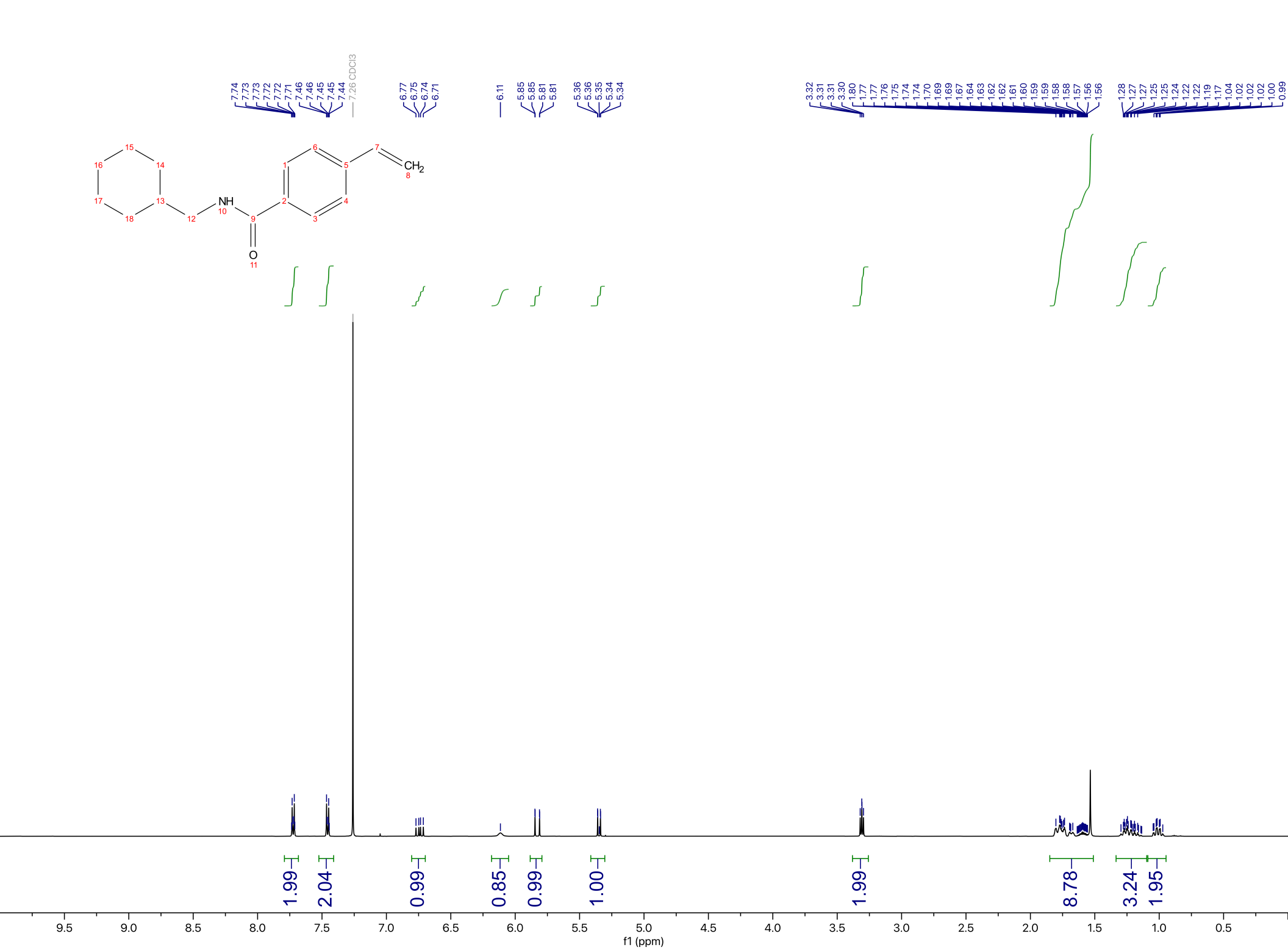
1.06 2.07 1.04 3.02 1.02 14.70 1.18 1.00

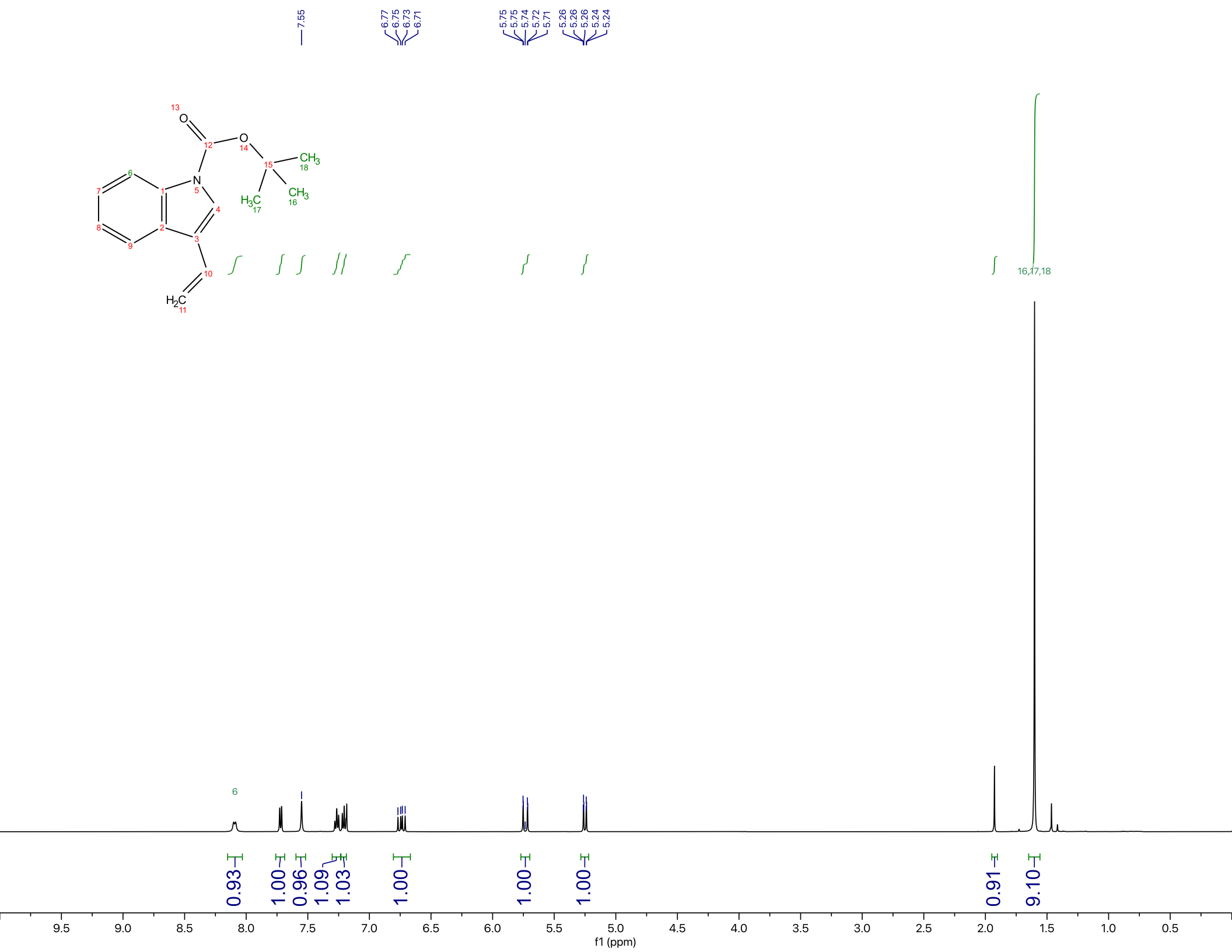
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5

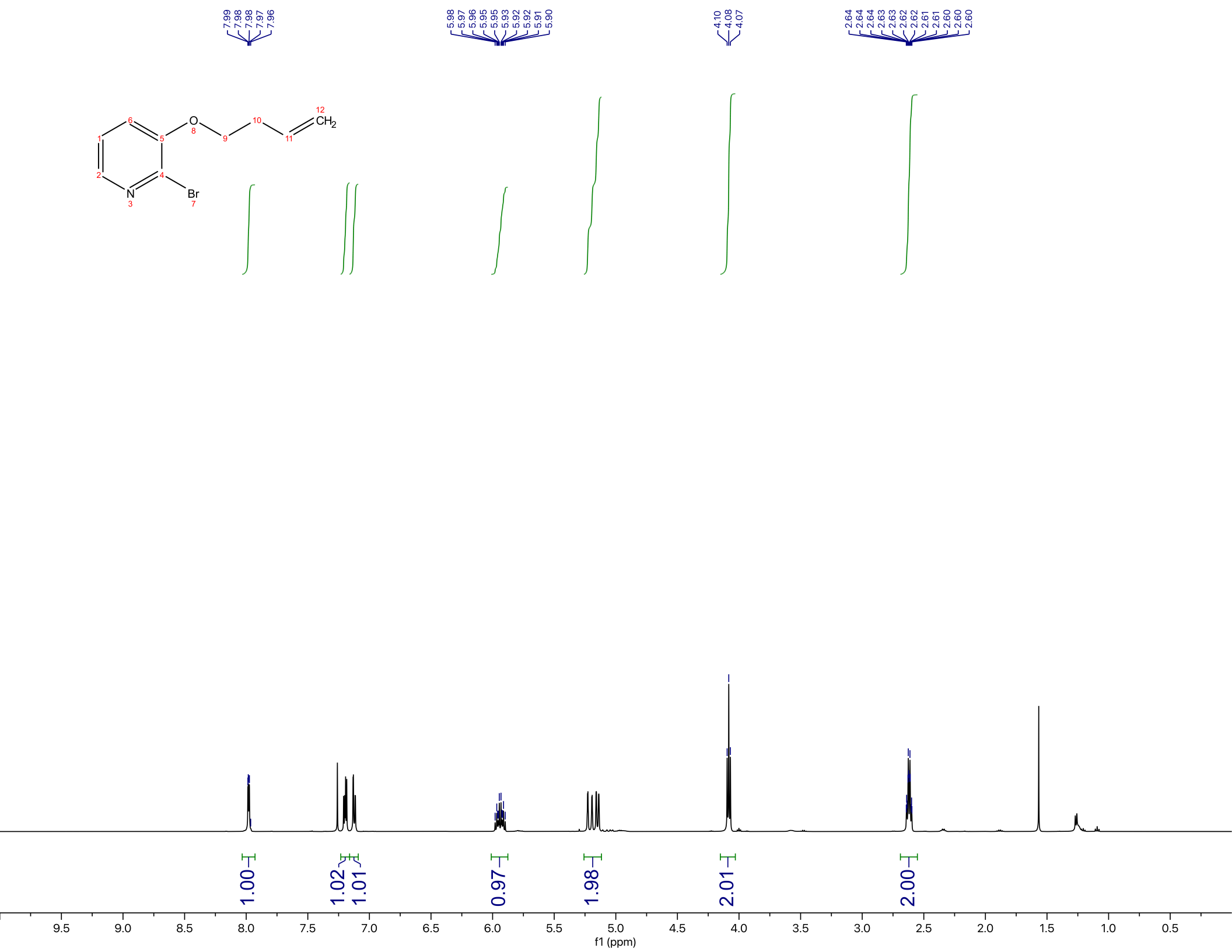
f1 (ppm)


205.86
154.85
79.51
60.37
36.57
33.70
32.48
32.02
28.44
27.55
21.06
21.03
14.20
O
NBoc
Me
f1 (ppm)


7.38
7.37
7.37
7.36
7.36
7.35
7.34
7.33
6.91
6.90
6.70
6.68
6.67
6.65
5.65
5.65
5.61
5.61
5.14
5.14
5.12
5.12
3.90
3.89
3.88
3.23
3.21
3.20
3.19
CH2
N
O
2.02
1.90
1.01
1.01
1.00
4.07
4.03
f1 (ppm)


7.74 7.73 7.73 7.72 7.72 7.71 7.46 7.46 7.45 7.45 7.44 7.26 CDCl3
6.77 6.75 6.74 6.71
6.11
5.85 5.85 5.81 5.81
5.36 5.36 5.35 5.34 5.34
3.32 3.31 3.31 3.30 1.80 1.77 1.77 1.76 1.75 1.74 1.74 1.70 1.69 1.69 1.67 1.64 1.63 1.62 1.62 1.61 1.60 1.59 1.59 1.58 1.58 1.57 1.56 1.56
1.28 1.27 1.27 1.25 1.25 1.24 1.22 1.22 1.19 1.17 1.04 1.02 1.02 1.02 1.00 0.99
NH
O
CH2
1.99
2.04
0.99
0.85
0.99
1.00
1.99
8.78
3.24
1.95
f1 (ppm)


7.55
6.77
6.75
6.73
6.71
5.75
5.75
5.74
5.72
5.71
5.26
5.26
5.26
5.24
5.24
16,17,18
6
0.93
1.00
0.96
1.09
1.03
1.00
1.00
1.00
0.91
9.10
f1 (ppm)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7.98
7.97
7.96
5.98
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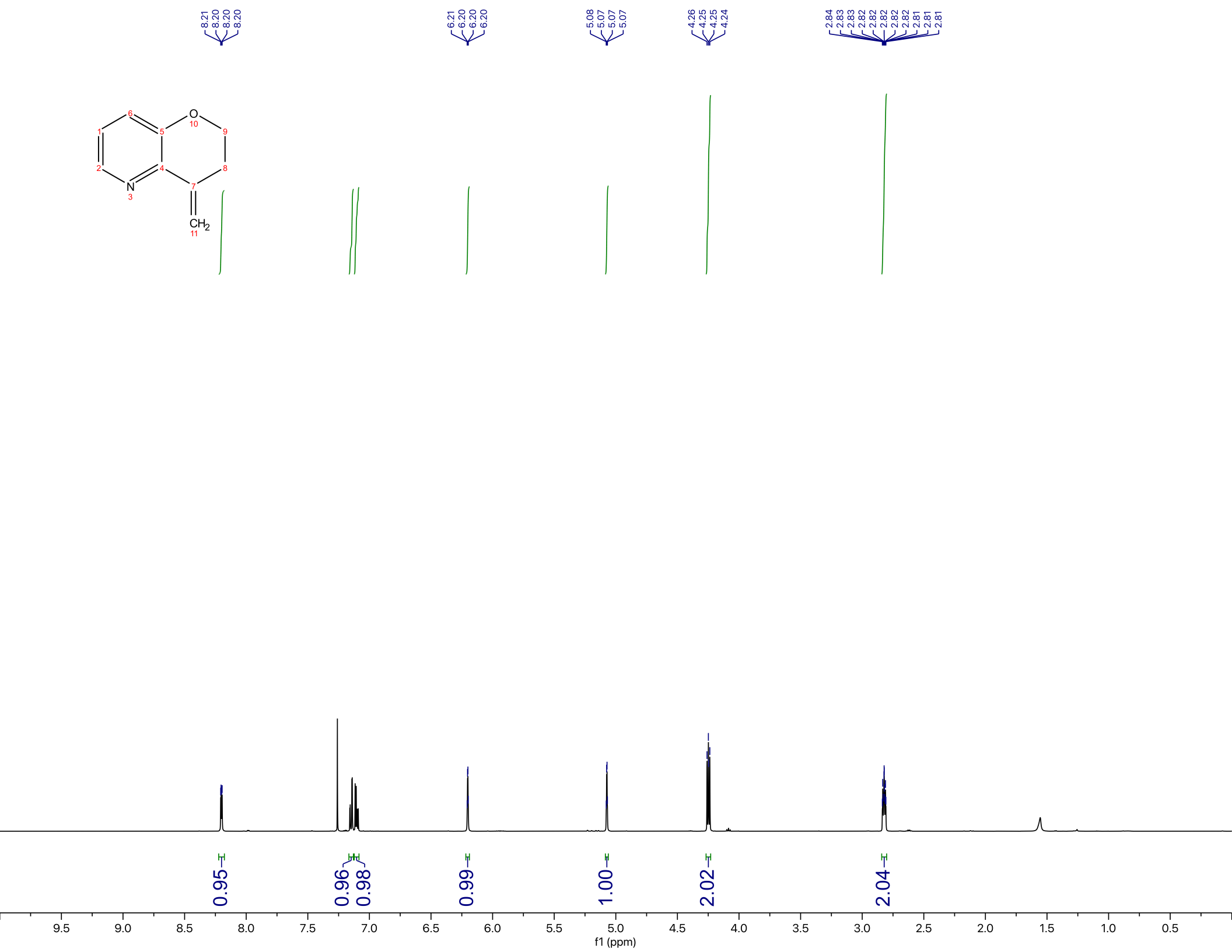
5.96
5.95
5.95
5.93
5.92
5.92
5.91
5.90
4.10
4.08
4.07
2.64
2.64
2.64
2.63
2.63
2.62
2.62
2.61
2.61
2.60
2.60
2.60
1
2
3
4
5
6
7
8
9
10
11
12
O
N
Br
CH2
1.00
1.02
1.01
0.97
1.98
2.01
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


8.21
8.20
8.20
8.20
6.21
6.20
6.20
6.20
5.08
5.07
5.07
5.07
4.26
4.25
4.25
4.24
2.84
2.83
2.83
2.82
2.82
2.82
2.82
2.82
2.81
2.81
2.81
O
10
N
3
CH2
11
0.95
0.96
0.98
0.99
1.00
2.02
2.04
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)