

Supporting Information

Organocatalytic approach to vinylic nucleophilic substitution at electrophilic alkenes

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1. General information

Materials

Unless noted otherwise, all reagents were obtained from commercial suppliers and used without additional purification. purchased from.

Instrumentations

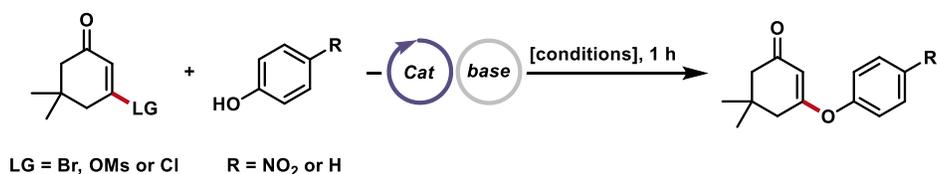
NMR spectroscopy: ^1H NMR and ^{13}C NMR spectra were recorded on Bruker AM-300 spectrometer (^1H : 300 MHz, ^{13}C : 75 MHz). Chemical shifts are reported in parts per million (ppm), using tetramethylsilane for CDCl_3 and residual solvent signal for DMSO-d_6 as internal standards. Multiplicities were given as: s (singlet), d (doublet), t (triplet), m (multiplets), dd (doublet of doublets), dt (doublet of triplets), and br (broad). Coupling constants (J) were recorded in Hertz (Hz). Product purity assessment and reaction monitoring were done with use of the internal standard (1,4-dibromobenzene).

High-resolution mass spectroscopy: HRMS spectra were obtained with a Bruker microTOF II instrument (ESI, positive or negative ion modes, capillary voltage 4500 V). All reagents and solvents are commercially available and used without additional purification.

Gas chromatography mass spectroscopy: GC-MS were recorded with a ThermoFisher Scientific system.

Liquid chromatography: TLC was performed on pre-coated plates Merck Silica Gel 60 GF254. Flash chromatography was performed on silica gel Machery-Nagel 60 40-60 mesh.

2. Reaction optimization



N ^o	LG	R	Catalyst	Base	Solvent	Additive	T, °C	Yield ^a , %	Conversion, %	Selectivity, %
1	Br	NO ₂	DMAP (0.25 eq.)	TEA (1 eq.)	DCE (0.4 M)	-	85	14	21	67
2	Br	NO ₂	DMAP (0.25 eq.)	TEA (1 eq.)	PhMe (0.4 M)	-	85	15	29	52
3	Br	NO ₂	DMAP (0.25 eq.)	TEA (1 eq.)	PhCF ₃ (0.4 M)	-	85	24	41	59
4	Br	NO ₂	DMAP (0.25 eq.)	TEA (1 eq.)	MeCN (0.4M)	-	85	8	25	32
5	Br	NO ₂	DMAP (0.25 eq.)	TEA (1 eq.)	DCM (0.4 M)	-	45	3	11	27
6	Br	NO ₂	DMAP (0.25 eq.)	TEA (1 eq.)	THF (0.4 M)	-	70	8	25	32
7 ^b	OMs	NO ₂	DMAP (0.25 eq.)	TEA (1 eq.)	PhCF ₃ (0.4 M)	-	85	-	-	-
8	Cl	NO ₂	DMAP (0.25 eq.)	TEA (1 eq.)	PhCF ₃ (0.4 M)	-	85	19	32	59
9	Br	NO ₂	DMAP (0.25 eq.)	K ₂ CO ₃ (1 eq.)	PhCF ₃ (0.4 M)	-	85	8	8	100
10	Br	NO ₂	DMAP (0.25 eq.)	DBU (1 eq.)	PhCF ₃ (0.4 M)	-	85	35	46	76
11	Br	NO ₂	DMAP (0.25 eq.)	DIPEA (1 eq.)	PhCF ₃ (0.4 M)	-	85	41	58	71
12	Br	NO ₂	DMAP (1.25 eq.)	-	PhCF ₃ (0.4 M)	-	85	43	53	81
13	Br	NO ₂	DMAP (0.25 eq.)	K ₂ CO ₃ (1 eq.)	EA (0.4 M)	-	85	17	17	100
14	Br	NO ₂	DMAP (0.25 eq.)	K ₂ CO ₃ (1 eq.)	PhCF ₃ (0.4 M)	Bu ₄ NBr (0.25 eq.)	85	25	30	83
15	Br	NO ₂	DMAP (0.25 eq.)	DIPEA (1.5 eq.)	PhCF ₃ (0.4 M)	-	105	57	64	89
16	Br	NO ₂	DMAP (0.25 eq.)	K ₂ CO ₃ (1 eq.)	PhCF ₃ (0.4 M)	CetylMe ₃ NBr (0.25 eq.)	85	<1%	-	-
17	Br	NO ₂	DMAP (0.25 eq.)	K ₃ PO ₄ (1 eq.)	PhCF ₃ (0.4 M)	Bu ₄ NBr (0.25 eq.)	85	22	33	67
18	Br	NO ₂	DMAP (0.25 eq.)	K ₂ CO ₃ (1 eq.)	PhCF ₃ (0.4 M)	Bu ₄ NI (0.25 eq.)	85	<1%	-	-
19	Br	NO ₂	DMAP (0.25 eq.)	KOH (1 eq.)	PhCF ₃ (0.4 M)	Bu ₄ NBr (0.25 eq.)	85	17	28	61
20	Br	NO ₂	DMAP (0.25 eq.)	K ₂ CO ₃ (1 eq.)	PhCF ₃ (0.4 M)	Bu ₄ NBr (0.25 eq.)	85	17	32	53
21	Br	H	DMAP (0.25 eq.)	DBU (1 eq.)	PhCF ₃ (0.4 M)	-	85	25	48	52
22	Br	H	DMAP (0.25 eq.)	DIPEA (1 eq.)	PhCF ₃ (0.4 M)	-	85	20	22	91
23	Br	H	DMAP (0.25 eq.)	K ₂ CO ₃ (1 eq.)	PhCF ₃ (0.4 M)	Bu ₄ NBr (0.25 eq.)	23	18	22	82
24	Br	H	DMAP (0.25 eq.)	DIPEA (3 eq.)	PhCF ₃ (0.4 M)	-	85	21	21	100
25	Br	H	DMAP (0.25 eq.)	DIPEA (1 eq.)	iPrOH (0.4 M)	-	85	13	42	31
26	Br	H	DMAP (0.25 eq.)	DIPEA (1 eq.)	Acetone (0.4 M)	-	55	<1%	-	-
27	Br	H	DMAP (0.25 eq.)	DIPEA (1.1 eq.)	PhCF ₃ (1 M)	-	105	35	35	100
28 ^b	Br	H	DMAP (0.25 eq.)	DIPEA (1.1 eq.)	PhCF ₃ (1 M)	HOBT (0.25 eq.)	105	22	51	43
29 ^b	Br	H	DMAPO (0.25 eq.)	DIPEA (1.1 eq.)	PhCF ₃ (1 M)	-	105	21	63	33
30	Cl	H	DMAP (0.25 eq.)	DIPEA (1.1 eq.)	PhCF ₃ (1 M)	-	105	39	48	81
31	Cl	H	-	DIPEA (1.1 eq.)	PhCF ₃ (1 M)	-	105	<1%	-	-
32	Cl	H	DMAP (0.25 eq.)	K ₂ CO ₃ (1 eq.)	PhCF ₃ (1 M)	Bu ₄ NBr (0.25 eq.)	105	43	52	83
33	Cl	H	DMAP (0.5 eq.)	DIPEA (1.1 eq.)	PhCF ₃ (1 M)	-	105	47	58	81
34	Cl	H	DMAP (0.25 eq.)	DIPEA (2.2 eq.)	PhCF ₃ (1 M)	-	105	47	58	81
35	Cl	H	DMAP (0.25 eq.)	DIPEA (3 eq.)	PhCF ₃ (1 M)	-	105	45	46	98
36	Cl	H	DMAP (0.25 eq.)	TEA (3 eq.)	PhCF₃ (1 M)	-	105	64	65	98
37	Cl	H	DMAP (0.25 eq.)	TEA (7 eq.)	PhCF ₃ (1 M)	-	105	21	21	100
38^c	Cl	H	DMAP (0.25 eq.)	TEA (3 eq.)	PhCF₃ (1 M)	-	105	94	100	94

Table SII. Optimization table for catalytic nucleophilic vinylic substitution reaction. ^a NMR yield ^b check text below. ^c 9 hours, isolated yield.

General consideration regarding reaction optimization

- The highest reaction rate is observed when relatively non-polar and high-boiling trifluorotoluene was used as a solvent, which is consistent with data on the influence of solvent polarity on the kinetics of organocatalyzed acylation reactions.
- When using the sulfonate derivative instead of the target substitution process, a process of DMAP-catalyzed transfer of the sulfonyl group to the nucleophile is observed (Table 1, No. 7). The more synthetically accessible chloride is practically not inferior in activity to bromide (Table 1, No. 8).
- Low polarity of the solvents used increases the effect of the solubility of the reagents on the reaction rate. For example, in the case of p-nitrophenol, the use of DIPEA as a base generates a more soluble phenolate, which significantly increases the reaction rate (Table 1, No. 3 and 11). When switching to unsubstituted phenol, this effect no longer occurs. The effect of the phase-transfer catalyst on the reaction rate in cases where inorganic bases are used is evident (Table 1, No. 9 and 14). Although not listed here, Et₄NBr was eventually used as a PTC instead of Bu₄NBr for reactions with K₂CO₃ as a cheaper alternative with effectively no drop in reaction rate.
- The addition of HOBT leads to a rapid generation of the product of its interaction with the electrophile, but the rate of formation of the final product does not change (Table 1, No. 28).
- Experiments involving the highly nucleophilic DMAPO led to disappointing results (Table 1, No. 29). It interacts with the initial electrophile noticeably faster than in the case of DMAP, but the concomitant deoxygenation to the corresponding pyridine proceeds extremely quickly in the reaction. Thus, the reaction is catalyzed and the coupling product is formed, but with the participation of DMAP, rather than the N-oxide itself. The cause of the catalyst degradation is probably the structure of the activated vinylative reagent, whose interaction with nucleophiles can proceed through their attack at the α -position of the enone fragment or pyridinium ring with the elimination of neutral pyridine. Similar results were obtained even with lower reaction temperature or exchange of DMAPO for PPYO.
- In the absence of a catalyst, the formation of the product in such a non-polar solvent and with a relatively weak base is not observed (Table 1, No. 31). Traditional conditions for these transformations are boiling the reaction mixture in acetone in the presence of K₂CO₃.
- In most experiments, the product of the interaction of DMAP with the electrophile is easily identified in using ¹H NMR spectroscopy, but its amount is quite sensitive to the reaction conditions and reagents chosen.
- Due to the high concentration of reagents, a further increase in the amount of organic base increases the polarity of the medium, which negatively affects the reaction rate (Table 1, No. 37).

3. General notes on the synthetic procedures

- As mentioned in the main text, some of the starting vinyl chlorides, specifically **1i-j**, **1m** and **1n**, are too unstable for prolonged storage (>1d in the fridge) and should be utilized as soon as possible.
- Although not explicitly stated in the experiment protocols, the purity of the electrophiles in substitution reactions, both neutral and ionic, was assessed and used in calculating the reaction stoichiometry.
- Set of reaction conditions, such as reaction temperature, time and base, for most substitution reactions was selected on the basis of one or several preliminary probe reactions, usually starting with Et₃N as a base at 70 °C for catalytic reactions or at 60 °C for reactions with vinylpyridinium salts. Since the transition to K₂CO₃/Et₄NBr combination may (not necessarily!) lead to a drop in selectivity, it was carried out only if the observed reaction rate was insufficient. That being said, immediate use of inorganic base can be recommended if no side reactions are expected.
- Generally, reactions with vinylpyridinium salts proceed cleaner and provide a broader substrate scope. The main disadvantage in this case is the limitation of the reaction temperature by the solvent (CHCl₃), sometimes leading to prolonged reaction times. PhCF₃ at the selected concentrations (0.25–0.5 M) is not able to dissolve all the pyridinium salt, which, in turn, negatively affected the reaction selectivity and yield. Notably, we did not perform a full separate screening and optimization of conditions for reactions with vinylpyridinium salts.
- Overall, substitution reactions were found to be robust, reproducible and insensitive to small changes in conditions, including reagent addition sequence.
- Stoichiometry of the coupling reagents was fixed at the 1:1 ratio to demonstrate efficiency of the protocol used. In our experience, no reaction suffered from increase in number of reagent or catalyst equivalents. Lesser amounts of DMAP in catalytic version of the reaction (< 0.25 eq.) were not tested.
- Transition to substitution reactions with vinylpyridinium salts as substrates provided a purification “workaround”, as demonstrated in the synthesis of **5d**. If separation of unreacted starting material and reaction product is challenging, the amount of vinylpyridinium salt used can be increased, ensuring complete conversion of the nucleophilic component. After this, filtration of the reaction mixture through a layer of silica gel provides a SM-free solution of the product.
- Extractive work-up is applicable, but has no advantages over the filtration procedure. Separation from DMAP was achieved during flash column chromatography – its R_f is too low in the common eluent.
- While reaction monitoring was performed with the use of an internal standard (p-dibromobenzene), in most cases DMAP and corresponding vinylpyridinium intermediates were equally suitable for determining the amounts of reactants in the reaction mixture. TLC analysis can be tricky since vinylpyridinium salts have negligible R_f in the common eluent.
- Specific substrates:
 - For dinucleophilic substrate such as TsNH₂ the use of a 1:1 ratio of electrophile/nucleophile leads to a sluggish reaction with moderate conversion, supposedly, due to the product’s reactivity as a nucleophile. Thus, an increase in electrophile amount was employed; a similar protocol has been described for gold-catalyzed sulfonamide addition to ynones.^[1]
 - In case of catalytic reactions with 4-pyridone and 4-nitrophenol as nucleophiles more solubilizing reagents (DIPEA or Bu₄NBr) were required. These were somewhat unique precedents, and, for instance, a reaction of 4-nitrophenol with vinylpyridinium salt in CHCl₃ did not suffer from this factor.
- Below is an infographic representation of the successful substitution reactions with respect to the pK_a and N values of the nucleophile components. Although these parameters do not determine the outcome of the reaction, they can still serve as a reasonable reference for the reaction development with similar substrates.

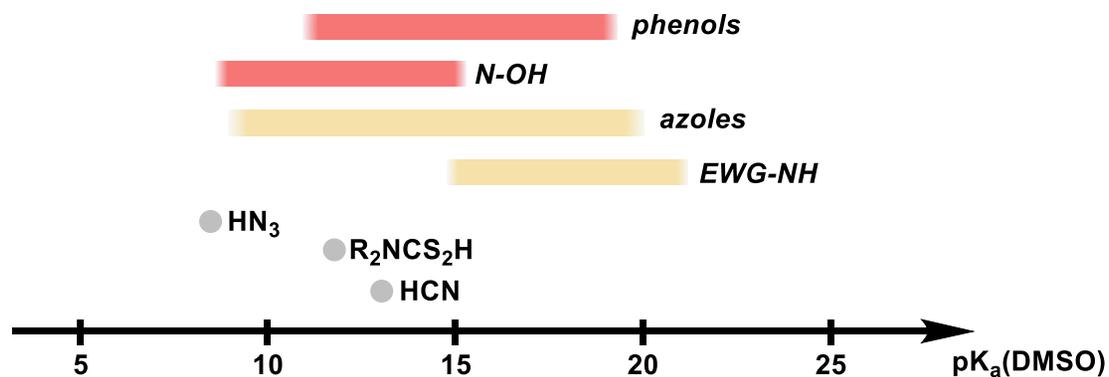


Figure S11. Range of the pK_a values for corresponding nucleophile classes with productive nucleophilic substitution reactions. $pK_a(\text{DMSO})$ values are taken from the reference^[2], for several compound types (oximes, phthalimide, NHPI and $\text{R}_2\text{NCS}_2\text{H}$) values were obtained using Luo and Chang pK_a prediction tool.^[3]

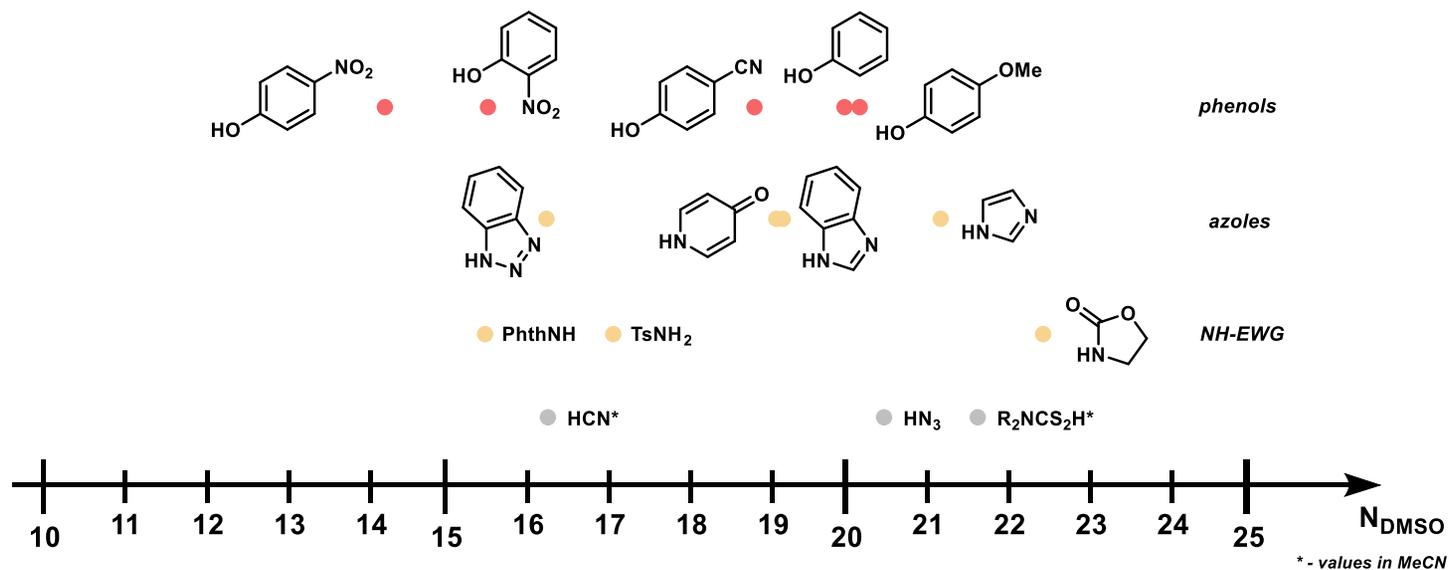


Figure S12. N_{DMSO} values for nucleophiles with productive vinylic substitution reactions. Nucleophilicity values are taken from Mayr's database,^[4] values for HCN and $\text{R}_2\text{NCS}_2\text{H}$ correspond to N_{MeCN} .

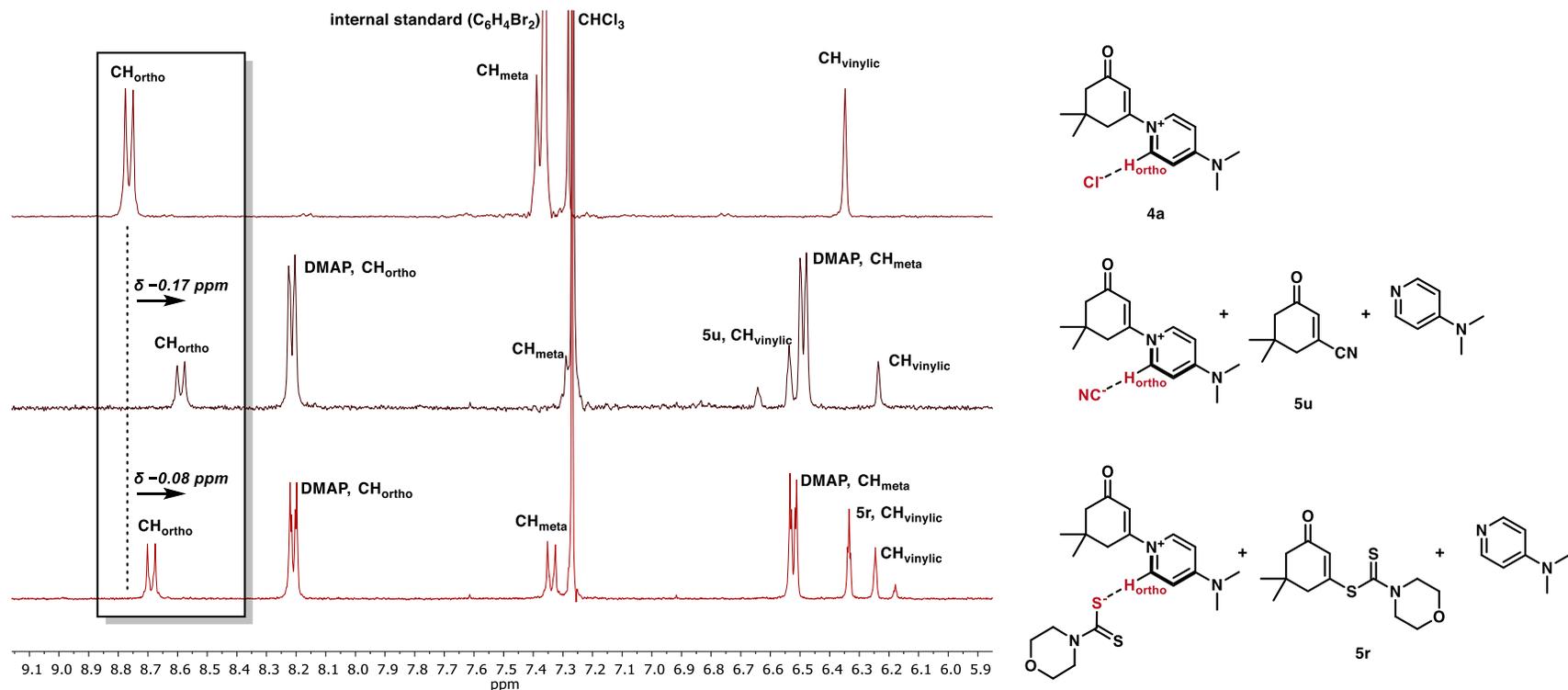


Figure S13. Fragments of ^1H NMR spectra for dimesone-derived pyridinium salts with chloride (**4a**), cyanide and dithiocarbamate anions in CDCl_3 . The last two represent reaction monitoring spectra (the corresponding substitution products are shown). The CH_{ortho} signals of pyridinium moiety (highlighted) show the largest shift upon counterion exchange.

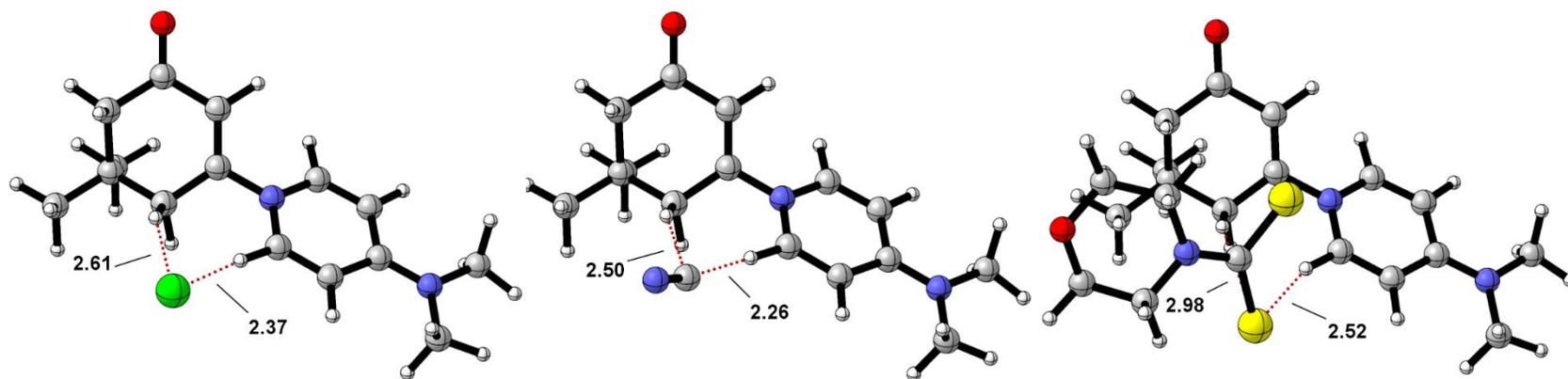
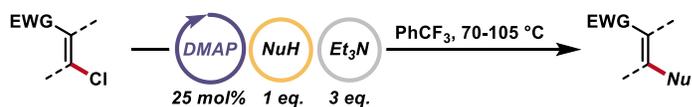


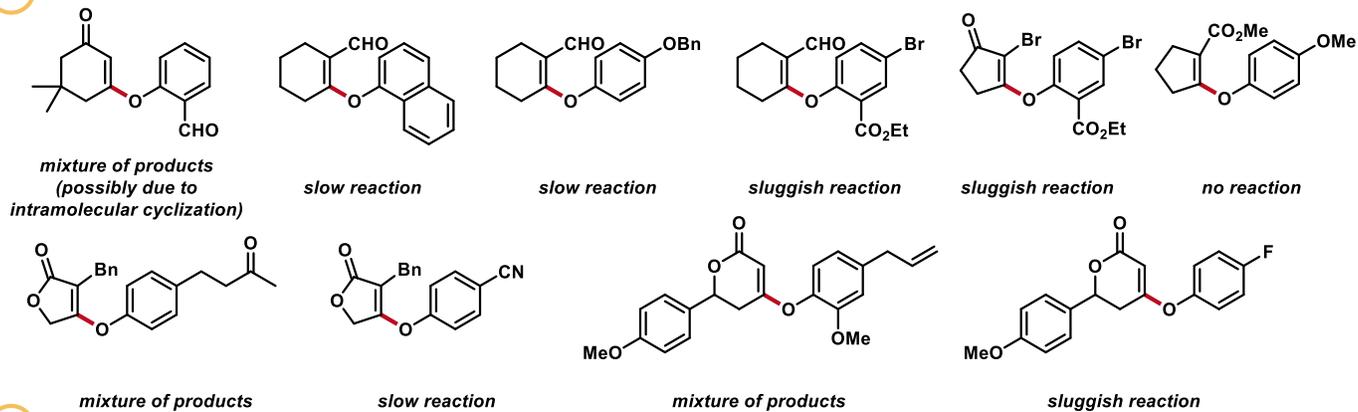
Figure S14. Optimized geometries of dimesone-derived pyridinium salts with chloride (**4a**), cyanide and dithiocarbamate anions with highlighted interactions between two ions (bond lengths in Å). For calculation details see section 9.

4. Attempted reactions

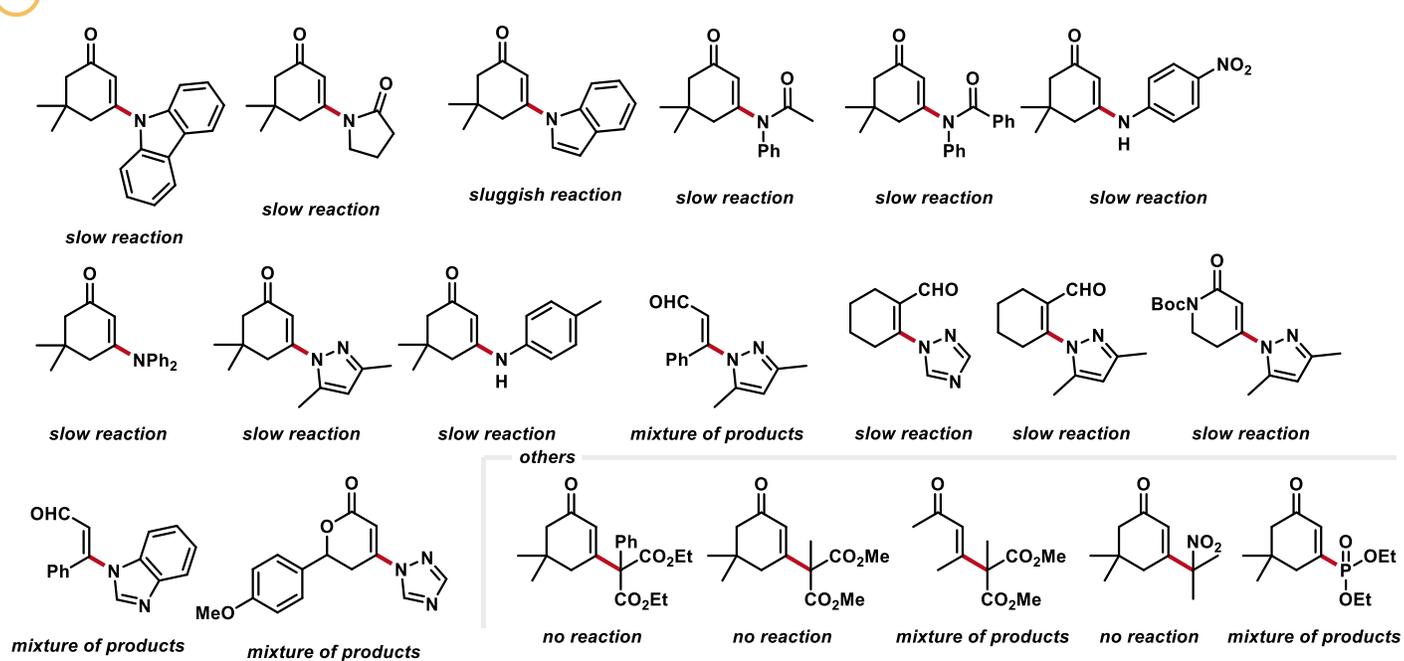


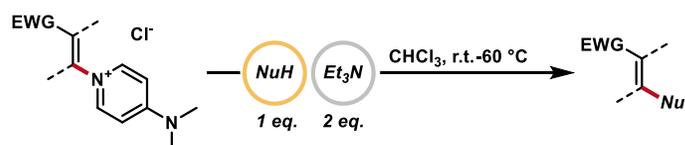
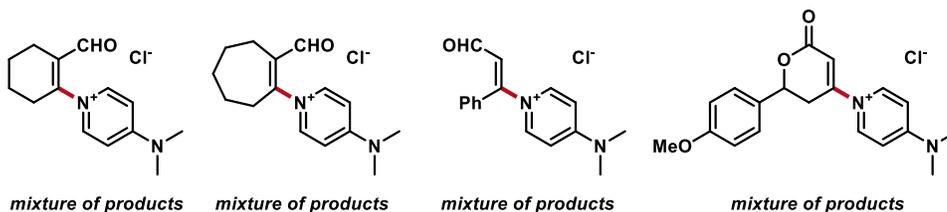
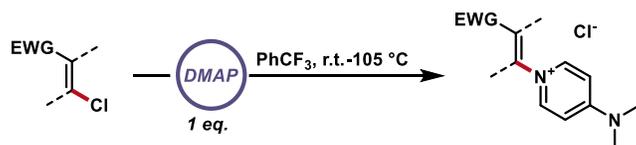
Most of reactions exhibiting low rates were also subjected to $\text{K}_2\text{CO}_3/\text{Et}_3\text{NBr}$ conditions

OH



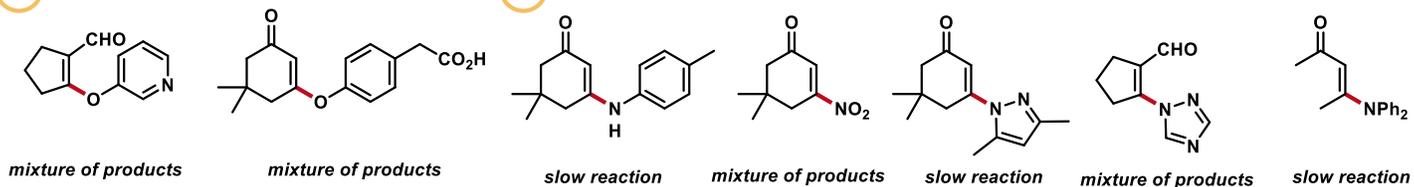
NH



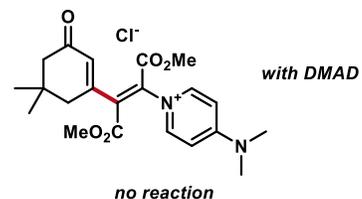
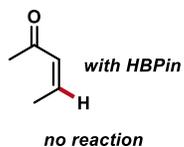
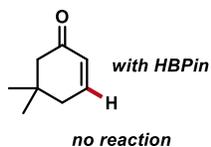
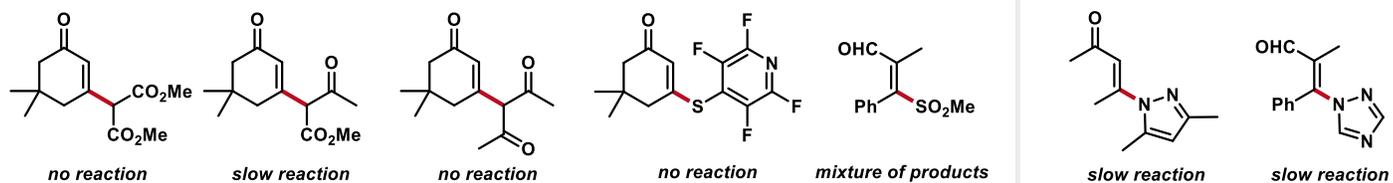


OH

NH

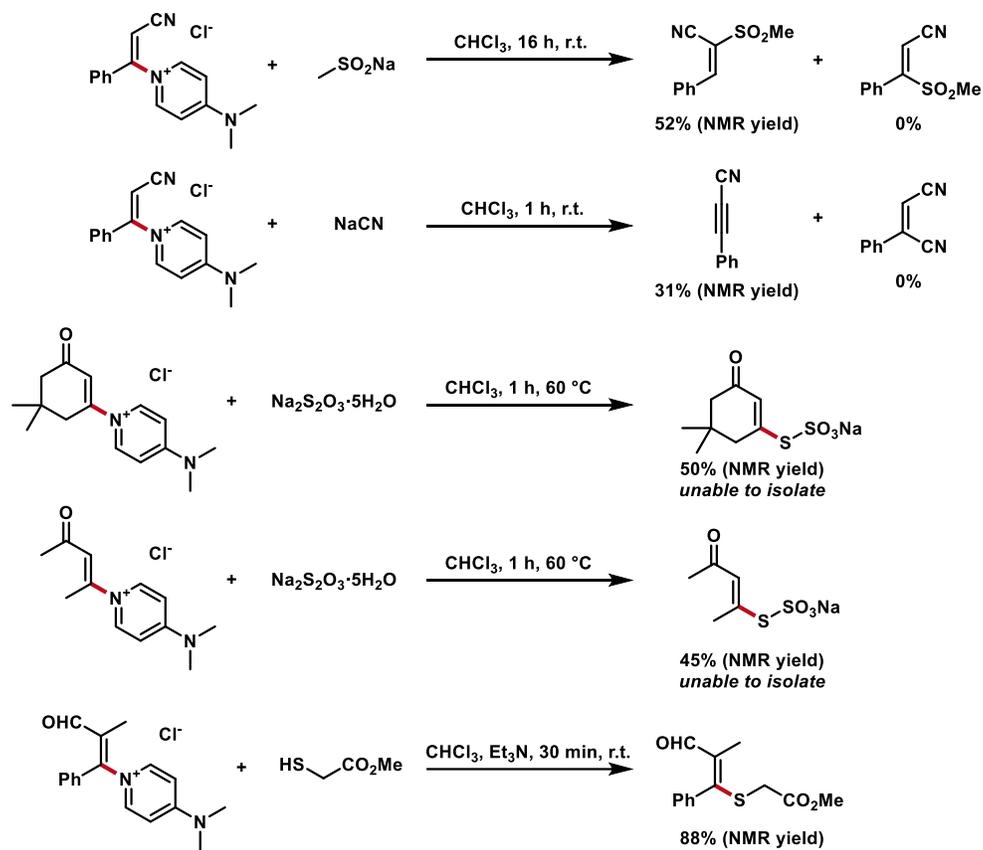


others



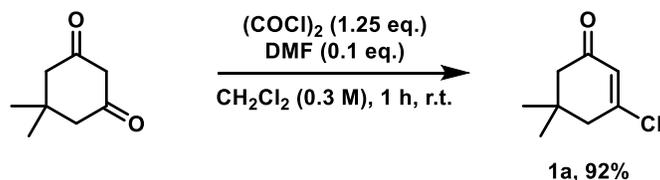
Other attempted reactions

with the exception of the last reaction, conversions were incomplete



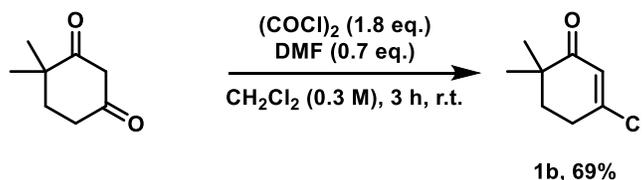
5. Precursor synthesis procedures

3-Chloro-5,5-dimethylcyclohex-2-en-1-one (1a)



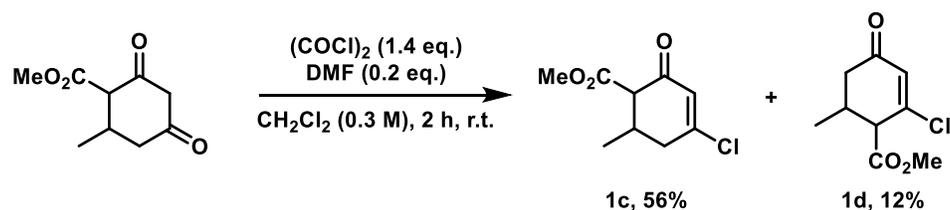
Literature protocol^[5]: dimedone (2.0 g, 14.3 mmol, 1 eq.) was weighed into a round-bottom flask, followed by addition of CH₂Cl₂ (45 ml), oxalyl chloride (1.5 ml, 17.8 mmol, 1.25 eq.) and DMF (0.11 ml, 1.4 mmol, 0.1 eq.). The reaction mixture was stirred for 1 hour at room temperature (monitored by TLC). Upon completion, the solvent was removed *in vacuo* at room temperature. The residue was passed through a silica gel plug, eluting with CH₂Cl₂, and the solvent was removed *in vacuo* at room temperature to afford the title product as a light yellow oil (2.3 g, 92% yield, 91 wt% purity by assay). NMR data matched the literature.^[6]

3-Chloro-6,6-dimethylcyclohex-2-en-1-one (1b)

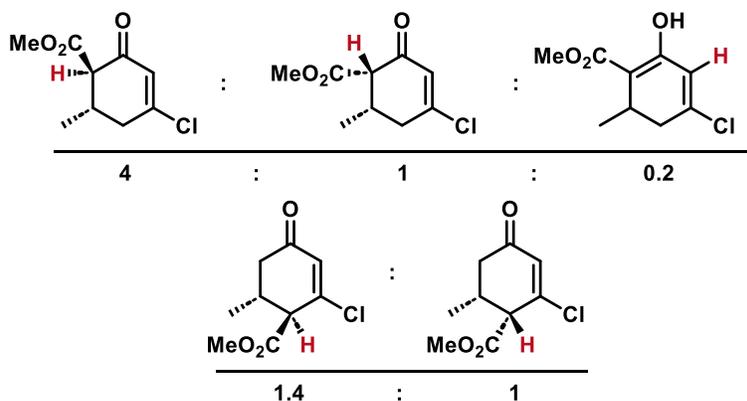


Literature protocol^[7]: 4,4-dimethylcyclohexane-1,3-dione (619 mg, 4.4 mmol, 1 eq.) was weighed into a round-bottom flask, followed by addition of CH₂Cl₂ (15 ml), oxalyl chloride (0.68 ml, 8.0 mmol, 1.8 eq.) and DMF (0.24 ml, 3.1 mmol, 0.7 eq.). The reaction mixture was stirred for 3 hours at room temperature (monitored by TLC). Upon completion, the solvent was removed *in vacuo* at room temperature. The residue was purified by flash column chromatography (PE:EA = 20:1) and the solvent was removed *in vacuo* at room temperature to afford the title product as a light yellow oil (567 mg, 69% yield, 85 wt% purity by assay). NMR data matched the literature.^[7]

Methyl 4-chloro-6-methyl-2-oxocyclohex-3-ene-1-carboxylate (1c) and methyl 2-chloro-6-methyl-4-oxocyclohex-2-ene-1-carboxylate (1d)



product composition (by integrals of H)



Literature protocol^[5]: methyl 2-methyl-4,6-dioxocyclohexane-1-carboxylate (499 mg, 2.7 mmol, 1 eq.) was weighed into a round-bottom flask, followed by addition of CH_2Cl_2 (10 ml), oxalyl chloride (0.33 ml, 3.8 mmol, 1.4 eq.) and DMF (0.04 ml, 0.5 mmol, 0.2 eq.). The reaction mixture was stirred for 2 hours at room temperature (monitored by TLC). Upon completion, the solvent was removed *in vacuo* at room temperature. The residue was purified by flash column chromatography (PE:EA = 10:1) and the solvent was removed *in vacuo* at room temperature to afford title products **1c** as a colorless oil (334 mg, 56% yield, 92 wt% purity by assay), and **1d** as a colorless oil (70 mg, 12% yield, 95 wt% purity by assay). *Note: a formation of inseparable mixture of tautomers for similar cyclohexenone system was described previously.*^[8]

Spectral data for **1c**^[9,10]:

¹H NMR (300 MHz, CDCl_3): δ 6.27 (m, 1H), 3.78 (s, 3H, *anti*), 3.72 (s, 3H, *syn*), 3.38 (d, $J = 4.8$ Hz, 1H, *syn*), 3.10 (d, $J = 11.0$ Hz, 1H, *anti*), 2.98 – 2.43 (m, 3H), 1.16 (d, $J = 6.7$ Hz, 3H, *syn*), 1.11 (d, $J = 6.5$ Hz, 3H, *anti*).

HRMS (ESI): m/z calc. for $[\text{C}_9\text{H}_{11}\text{ClO}_3+\text{H}^+]$ 203.0469, found 203.0471.

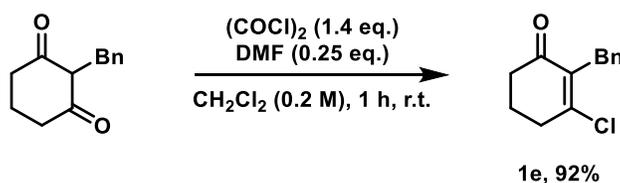
Spectral data for **1d**:

¹H NMR (300 MHz, CDCl_3): δ 6.33 (m, 1H), 3.81 (s, 3H, *anti*), 3.79 (s, 3H, *syn*), 3.56 (d, $J = 4.8$ Hz, 1H, *syn*), 3.39 (dd, $J = 6.6, 1.6$ Hz, 1H, *anti*), 2.77 – 2.47 (m, 2H), 2.44 – 2.11 (m, 1H), 1.15 (d, $J = 6.7$ Hz, 3H, *anti*), 1.11 (d, $J = 6.3$ Hz, 3H, *syn*).

¹³C{¹H} NMR (75 MHz, CDCl_3): δ 196.2, 195.2, 170.3, 168.8, 153.2, 152.3, 130.0, 129.8, 56.7, 55.0, 52.8, 52.6, 42.4, 40.5, 33.2, 32.3, 19.8, 18.5. *Note: data for both tautomers.*

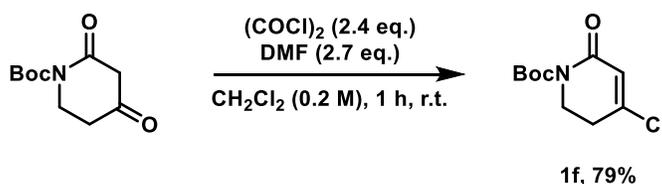
HRMS (ESI): m/z calc. for $[\text{C}_9\text{H}_{11}\text{ClO}_3+\text{H}^+]$ 203.0469, found 203.0474.

2-Benzyl-3-chlorocyclohex-2-en-1-one (1e)



Literature protocol^[5]: 2-benzylcyclohexane-1,3-dione (430 mg, 2.1 mmol, 1 eq.) was weighed into a round-bottom flask, followed by addition of CH_2Cl_2 (10 ml), oxalyl chloride (0.25 ml, 3.2 mmol, 1.4 eq.) and DMF (0.04 ml, 0.5 mmol, 0.25 eq.). The reaction mixture was stirred for 1 hour at room temperature (monitored by TLC). Upon completion, the solvent was removed *in vacuo* at room temperature. The residue was passed through a silica gel plug (PE:EA = 2:1) and the solvent was removed *in vacuo* at room temperature to afford the title product as a light yellow oil (452 mg, 92% yield, 95 wt% purity by assay). NMR data matched the literature.^[11]

Tert-butyl 4-chloro-6-oxo-3,6-dihydropyridine-1-carboxylate (1f)



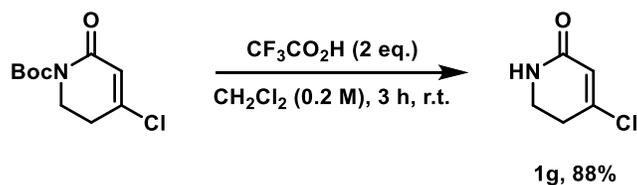
N-Boc-piperidine-2,4-dione (350 mg, 1.6 mmol, 1 eq.) was weighed into a round-bottom flask, followed by addition of CH_2Cl_2 (8 ml), oxalyl chloride (0.34 ml, 3.9 mmol, 2.4 eq.) and DMF (0.34 ml, 4.4 mmol, 2.7 eq.). The reaction mixture was stirred for 1 hour at room temperature (monitored by TLC). Upon completion, the solvent was removed *in vacuo* at room temperature. The residue was passed through a silica gel plug (PE:EA = 1:1) and the solvent was removed *in vacuo* at room temperature to afford the title product as a light yellow oil (315 mg, 79% yield, 96 wt% purity by assay).

^1H NMR (300 MHz, CDCl_3): δ 6.12 (t, $J = 1.4$ Hz, 1H), 3.93 (t, $J = 6.5$ Hz, 2H), 2.72 (td, $J = 6.5, 1.4$ Hz, 2H), 1.54 (s, 9H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 162.0, 152.2, 151.1, 123.7, 83.5, 43.2, 32.8, 28.1.

HRMS (ESI): m/z calc. for $[\text{C}_{10}\text{H}_{14}\text{ClNO}_3+\text{H}^+]$ 232.0735, found 232.0740.

4-Chloro-5,6-dihydropyridin-2-one (**1g**)



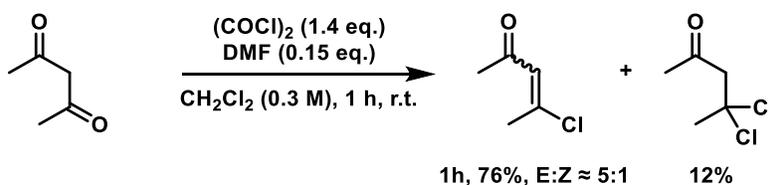
Tert-butyl 4-chloro-6-oxo-3,6-dihydropyridine-1-carboxylate (**1f**, 315 mg, 1.4 mmol, 1 eq.) was weighed into a round-bottom flask, followed by addition of CH₂Cl₂ (8 ml) and CF₃CO₂H (0.21 ml, 2.7 mmol, 2 eq.). The reaction mixture was stirred for 3 hours at room temperature (monitored by TLC). Upon completion, the reaction mixture was washed with saturated NaHCO₃, and the water layer was additionally extracted twice with CH₂Cl₂. Collected organic layers were washed with brine, dried over Na₂SO₄ and the solvent was removed *in vacuo* at room temperature. The residue was passed through a silica gel plug (CHCl₃:MeOH = 20:1) and the solvent was removed *in vacuo* at room temperature to afford the title product as a white solid (161 mg, 88% yield, 98 wt% purity by assay).

¹H NMR (300 MHz, CDCl₃): δ 6.07 (m, 1H), 6.00 (br s, 1H), 3.51 (td, *J* = 7.1, 2.6 Hz, 2H), 2.70 (td, *J* = 7.1, 1.4 Hz, 2H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 165.8, 148.5, 122.3, 39.2, 32.1.

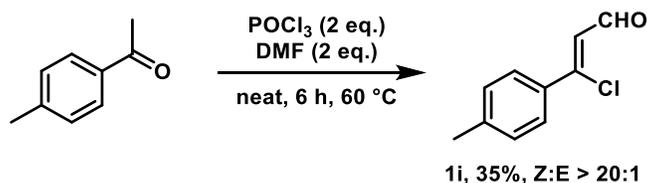
HRMS (ESI): *m/z* calc. for [C₅H₆ClNO+H⁺] 132.0211, found 132.0211.

4-Chloropent-3-en-2-one (**1h**)



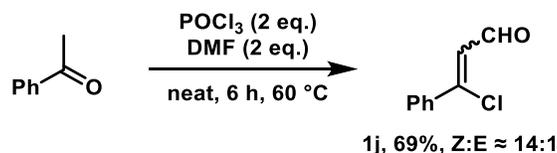
Literature protocol^[12]: acetylacetone (1.5 g, 15 mmol, 1 eq.) was weighed into a round-bottom flask, followed by addition of CH₂Cl₂ (50 ml), oxalyl chloride (1.8 ml, 21 mmol, 1.4 eq.) and DMF (0.17 ml, 2.3 mmol, 0.15 eq.). The reaction mixture was stirred for 1 hour at room temperature (monitored by TLC). Upon completion, the solvent was removed *in vacuo* until approx. 3 ml of solution remains. The residue was passed through a silica gel plug, eluting with CH₂Cl₂ and the solvent was removed *in vacuo* to afford a light yellow oil (1.67 g) consisting of the title product as a mixture of stereoisomers (76% yield, 81 wt% purity by assay, E:Z ≈ 5:1) and 4,4-dichloropent-2-one (12% yield, ¹H NMR (300 MHz, CDCl₃): δ 3.42 (s, 2H), 2.30 (s, 3H), 2.28 (s, 3H)). NMR data matched the literature.^[12]
Note: title compound was found to be volatile; solvent was evaporated at room temperature under the pressure above 250 mmHg. Title compound is relatively unstable and not suited for long-term storage upon isolation. Attempts to induce HCl elimination from the dichloride byproduct led to decomposition.

(Z)-3-Chloro-3-(p-tolyl)acrylaldehyde (1i)



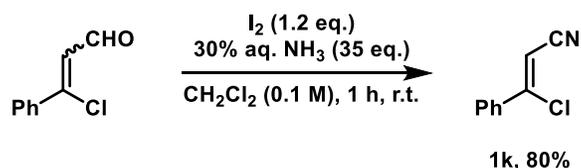
Literature protocol^[13]: DMF (1.2 ml, 14.9 mmol, 2 eq.) was weighed into a round-bottom flask, the flask was flushed with Ar and cooled to 0 °C. POCl₃ (1.4 ml, 14.9 mmol, 2 eq.) was slowly added dropwise, the reaction mixture was allowed to warm up to room temperature and stirred for 20 minutes. The reaction mixture was cooled back to 0 °C and 4-methylacetophenone (1.0 ml, 7.5 mmol, 1 eq.) was slowly added dropwise. The reaction mixture was heated for 6 hours in an oil bath at 60 °C (monitored by TLC). Upon completion, the reaction mixture was poured on ice and neutralized with aqueous NaOAc (25 ml, 2 M, checked with pH paper). The solution was extracted with PE:EA mixture (1:1), collected organic layers were washed with brine, dried over Na₂SO₄ and the solvent was removed *in vacuo* at room temperature. The residue was passed through a silica gel plug (PE:EA = 20:1) and the solvent was removed *in vacuo* at room temperature to afford the title product as a light-yellow oil (500 mg, 35% yield, 94 wt% purity by assay, Z:E > 20:1). NMR data matched the literature.^[14]

3-Chloro-3-phenylacrylaldehyde (1j)



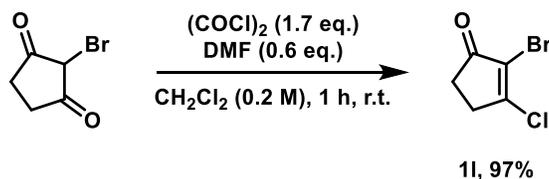
Literature protocol^[13]: DMF (1.93 ml, 25 mmol, 2 eq.) was weighed into a round-bottom flask, the flask was flushed with Ar and cooled to 0 °C. POCl₃ (2.3 ml, 25 mmol, 2 eq.) was slowly added dropwise, the reaction mixture was allowed to warm up to room temperature and stirred for 20 minutes. The reaction mixture was cooled back to 0 °C and acetophenone (1.5 ml, 12.5 mmol, 1 eq.) was slowly added dropwise. The reaction mixture was heated for 6 hours in an oil bath at 60 °C (monitored by TLC). Upon completion, the reaction mixture was poured on ice and neutralized with aqueous NaOAc (50 ml, 2 M, checked with pH paper). The solution was extracted with PE:EA mixture (1:1), collected organic layers were washed with brine, dried over anhydrous Na₂SO₄ and the solvent was removed *in vacuo* at room temperature. The residue was passed through a silica gel plug (PE:EA = 10:1) and the solvent was removed *in vacuo* at room temperature to afford the title product as a light-yellow oil (1.43 g, 69% yield, ~100 wt% purity by assay, Z:E ≈ 14:1). NMR data matched the literature.^[13]

(Z)-3-Chloro-3-phenylacrylonitrile (1k)



Literature protocol^[15]: 3-chloro-3-phenylacrylaldehyde (**1j**, 700 mg, 4.2 mmol, 1 eq.) was weighed into a round-bottom flask, followed by addition of CH₂Cl₂ (42 ml), I₂ (1.3 g, 5 mmol, 1.2 eq.) and 30% aqueous NH₃ (10 ml). The reaction mixture was stirred for 1 hour at room temperature (monitored by TLC). Upon completion, the reaction mixture was quenched with aqueous Na₂S₂O₃ and extracted with CH₂Cl₂. Collected organic layers were washed with brine, dried over Na₂SO₄ and the solvent was removed *in vacuo* at room temperature. The residue was purified by flash column chromatography (PE:EA = 15:1) and the solvent was removed *in vacuo* at room temperature to afford the title product as a yellow oil (556 mg, 80% yield, 98 wt% purity by assay). NMR data matched the literature.^[15]

2-Bromo-3-chlorocyclopent-2-en-1-one (1l)



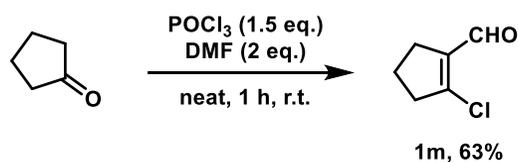
Literature protocol^[5]: 2-bromocyclopentane-1,3-dione (394 mg, 2.2 mmol, 1 eq.) was weighed into a round-bottom flask, followed by addition of CH₂Cl₂ (11 ml), oxalyl chloride (0.32 ml, 3.8 mmol, 1.7 eq.) and DMF (0.1 ml, 1.3 mmol, 0.6 eq.). The reaction mixture was stirred for 1 hour at room temperature (monitored by TLC). Upon completion, the solvent was removed *in vacuo* at room temperature. The residue was passed through a silica gel plug (PE:EA = 1:1) and the solvent was removed *in vacuo* at room temperature to afford the title product as a beige solid (410 mg, 97% yield, ~100 wt% purity by assay).

¹H NMR (300 MHz, CDCl₃): δ 2.98 – 2.88 (m, 2H), 2.77 – 2.67 (m, 2H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 197.7, 167.2, 124.2, 34.4, 33.7.

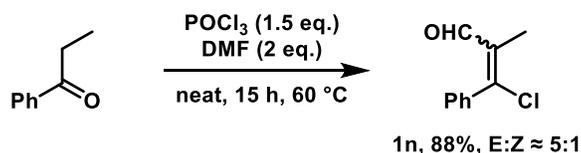
HRMS (ESI): m/z calc. for [C₅H₄BrClO+Na⁺] 216.9026, found 216.9031.

2-Chlorocyclopent-1-ene-1-carbaldehyde (1m)



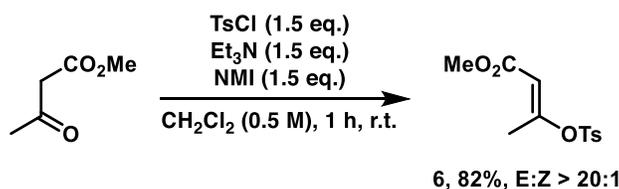
Literature protocol^[16]: DMF (3.2 ml, 41.6 mmol, 2 eq.) was weighed into a round-bottom flask, the flask was flushed with Ar and cooled to 0 °C. POCl₃ (2.9 ml, 31.2 mmol, 1.5 eq.) was slowly added dropwise, the reaction mixture was allowed to warm up to room temperature and stirred for 20 minutes. The reaction mixture was cooled back to 0 °C and cyclopentanone (1.8 ml, 20.8 mmol, 1 eq.) was slowly added dropwise. The reaction mixture was stirred for 2 hours at room temperature (monitored by TLC). Upon completion, the reaction mixture was poured on ice and neutralized with aqueous NaHCO₃ (75 ml, 1 M, checked with pH paper). The solution was extracted with PE, collected organic layers were washed with brine, dried over Na₂SO₄ and the solvent was removed *in vacuo* at room temperature to afford the title product as a dark yellow oil (1.85 g, 63% yield, 92 wt% purity by assay). NMR data matched the literature.^[16]

3-Chloro-2-methyl-3-phenylacrylaldehyde (1n)



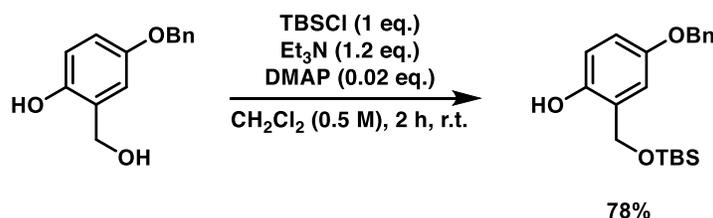
Literature protocol^[17]: DMF (1.7 ml, 22.4 mmol, 2 eq.) was weighed into a round-bottom flask, the flask was flushed with Ar and cooled to 0 °C. POCl₃ (1.6 ml, 16.8 mmol, 1.5 eq.) was slowly added dropwise, the reaction mixture was allowed to warm up to room temperature and stirred for 20 minutes. The reaction mixture was cooled back to 0 °C and propiophenone (1.5 ml, 11.2 mmol, 1 eq.) was slowly added dropwise. The reaction mixture was heated for 15 hours in an oil bath at 60 °C (monitored by TLC). Upon completion, the reaction mixture was poured on ice and neutralized with aqueous NaHCO₃ (40 ml, 1 M, checked with pH paper). The solution was extracted with Et₂O, collected organic layers were washed with brine, dried over Na₂SO₄ and the solvent was removed *in vacuo* at room temperature to afford the title product as an orange oil (2 g, 88% yield, 89 wt% purity by assay, E:Z ≈ 5:1). NMR data matched the literature.^[17]

Methyl (E)-3-(tosyloxy)but-2-enoate (6)



Literature protocol^[18]: methyl acetoacetate (500 mg, 4.3 mmol, 1 eq.) was weighed into a round-bottom flask, followed by addition of CH₂Cl₂ (8 ml), NMI (0.52 ml, 6.5 mmol, 1.5 eq.), Et₃N (0.9 ml, 6.5 mmol, 1.5 eq.) and TsCl (1.2 g, 6.5 mmol, 1.5 eq.). The reaction mixture was stirred for 1 hour at room temperature (monitored by TLC). Upon completion, the solvent was removed *in vacuo* at room temperature. The residue was passed through a silica gel plug (CHCl₃:EA = 4:1), and the solvent was removed *in vacuo* at room temperature to afford the title product as a light-yellow oil (1.1 g, 82% yield, 86 wt% purity by assay, E:Z > 20:1). NMR data matched the literature.^[18]

4-(Benzyloxy)-2-(((tert-butyldimethylsilyl)oxy)methyl)phenol



4-(Benzyloxy)-2-(hydroxymethyl)phenol (231 mg, 1 mmol, 1 eq.) and DMAP (3 mg, 6.5 mmol, 0.02 eq.) were weighed into a round-bottom flask, followed by addition of CH₂Cl₂ (2 ml), Et₃N (0.17 ml, 1.2 mmol, 1.2 eq.) and TBSCl (151 mg, 1 mmol, 1 eq.). The reaction mixture was stirred for 2 hours at room temperature (monitored by TLC). Upon completion, the reaction mixture was washed with water, and the water layer was additionally extracted twice with CH₂Cl₂. Collected organic layers were washed with brine, dried over Na₂SO₄ and the solvent was removed on the rotary evaporator. The residue was purified by flash column chromatography (PE:EA = 10:1) to afford the title product as a colorless oil (270 mg, 78%).

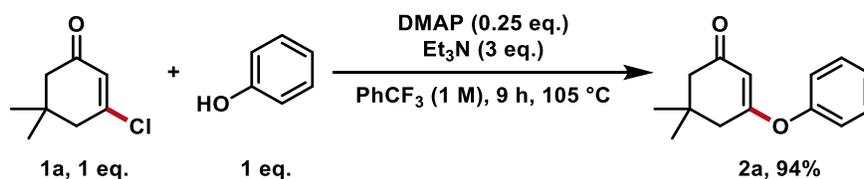
¹H NMR (300 MHz, CDCl₃): δ 7.60 (s, 1H), 7.45 – 7.25 (m, 5H), 6.85 – 6.76 (m, 2H), 6.64 – 6.57 (m, 1H), 4.98 (s, 2H), 4.84 (s, 2H), 0.92 (s, 9H), 0.12 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 152.1, 150.8, 137.5, 128.7, 128.0, 127.6, 125.0, 117.2, 115.1, 113.8, 70.9, 65.8, 25.9, 18.3, -5.4.

HRMS (ESI): m/z calc. for [C₂₀H₂₈O₃Si+Na⁺] 367.1700, found 367.1688.

6. Procedure for catalytic nucleophilic vinylic substitution reactions

5,5-Dimethyl-3-phenoxycyclohex-2-en-1-one (2a)



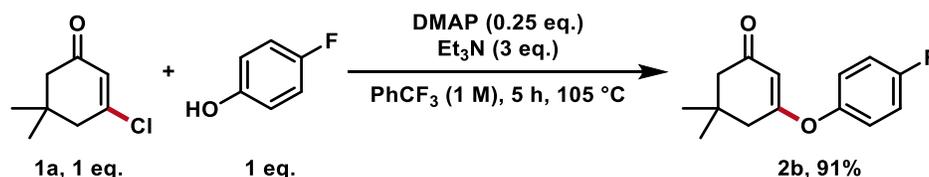
Phenol (48 mg, 0.5 mmol, 1 eq.) and DMAP (15 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**I**, 80 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial, followed by Et₃N (0.21 ml, 1.5 mmol, 3 eq.). The vial was sealed and the reaction mixture was heated for 9 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 3:1) to afford the title product as a white solid (102 mg, 94% yield).

¹H NMR (300 MHz, CDCl₃): δ 7.38 (dd, J = 8.5, 7.2 Hz, 2H), 7.31 – 7.17 (m, 1H), 7.07 – 6.96 (m, 2H), 5.11 (s, 1H), 2.51 (s, 2H), 2.23 (s, 2H), 1.14 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 199.3, 176.7, 152.88, 130.0, 126.1, 121.4, 105.0, 50.8, 42.4, 32.8, 28.4.

HRMS (ESI): m/z calc. for [C₁₄H₁₆O₂+H⁺] 217.1223, found 217.1224.

3-(4-Fluorophenoxy)-5,5-dimethylcyclohex-2-en-1-one (2b)



4-Fluorophenol (57 mg, 0.5 mmol, 1 eq.) and DMAP (15 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**I**, 80 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial, followed by Et₃N (0.21 ml, 1.5 mmol, 3 eq.). The vial was sealed and the reaction mixture was heated for 5 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 2:1) to afford the title product as an off-white solid (107 mg, 91% yield).

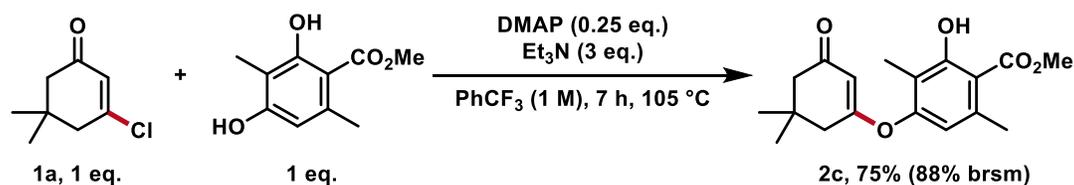
¹H NMR (300 MHz, CDCl₃): δ 7.08 (t, *J* = 8.6 Hz, 2H), 7.05 – 6.94 (m, 2H), 5.08 (s, 1H), 2.51 (s, 2H), 2.24 (s, 2H), 1.14 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 199.2, 176.7, 160.4 (d, *J* = 245.2 Hz), 148.7 (d, *J* = 2.7 Hz), 122.9 (d, *J* = 8.6 Hz), 116.7 (d, *J* = 23.6 Hz), 104.9, 50.8, 42.3, 32.8, 28.3.

¹⁹F NMR (282 MHz, CDCl₃): δ -116.97 (q, *J* = 6.3 Hz).

HRMS (ESI): *m/z* calc. for [C₁₄H₁₅FO₂+H⁺] 235.1129, found 235.1132.

Methyl 4-((5,5-dimethyl-3-oxocyclohex-1-en-1-yl)oxy)-2-hydroxy-3,6-dimethylbenzoate (2c)



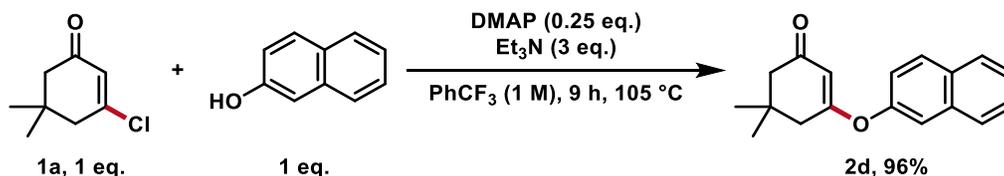
Methyl β -orsellinate (94 mg, 0.48 mmol, 1 eq.) and DMAP (15 mg, 0.12 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**I**, 76 mg, 0.48 mmol, 1 eq.) in PhCF₃ (0.48 ml) was added to the vial, followed by Et₃N (0.21 ml, 1.5 mmol, 3 eq.). The vial was sealed and the reaction mixture was heated for 7 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:Et₂O = 1:1) to afford the title product as a white solid (114 mg, 75% yield), along with recovered phenol (12 mg, 13%).

¹H NMR (300 MHz, CDCl₃): δ 11.89 (s, 1H), 6.36 (s, 1H), 5.03 (s, 1H), 3.97 (s, 3H), 2.52 (s, 2H), 2.48 (s, 3H), 2.24 (s, 2H), 2.00 (s, 3H), 1.15 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 199.2, 175.1, 172.2, 163.2, 154.8, 140.2, 116.5, 115.7, 109.8, 104.9, 52.3, 50.7, 42.1, 32.8, 28.3, 24.0, 8.8.

HRMS (ESI): m/z calc. for [C₁₈H₂₂O₅+H⁺] 319.1540, found 319.1539.

5,5-Dimethyl-3-(naphthalen-2-yloxy)cyclohex-2-en-1-one (2d)



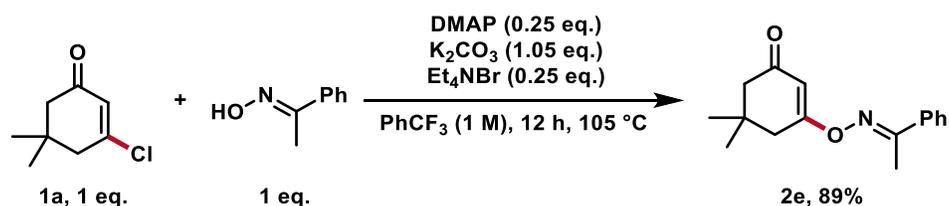
2-Naphthol (72 mg, 0.5 mmol, 1 eq.) and DMAP (15 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**I**, 79 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial, followed by Et₃N (0.21 ml, 1.5 mmol, 3 eq.). The vial was sealed and the reaction mixture was heated for 9 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (hexane:Et₂O = 1:1) to afford the title product as a light-yellow solid (128 mg, 96% yield).

¹H NMR (300 MHz, CDCl₃): δ 7.83 (dd, J = 9.0, 4.3 Hz, 2H), 7.80 – 7.71 (m, 1H), 7.54 – 7.39 (m, 3H), 7.15 (dd, J = 8.8, 2.4 Hz, 1H), 5.16 (s, 1H), 2.54 (s, 2H), 2.24 (s, 2H), 1.14 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 199.2, 176.6, 150.4, 133.9, 131.5, 130.2, 127.9, 127.5, 126.9, 126.0, 120.7, 118.4, 105.2, 50.8, 42.4, 32.7, 28.3.

HRMS (ESI): m/z calc. for [C₁₈H₁₈O₂+H⁺] 267.1380, found 267.1380

(E)-5,5-Dimethyl-3-(((1-phenylethylidene)amino)oxy)cyclohex-2-en-1-one (2e)



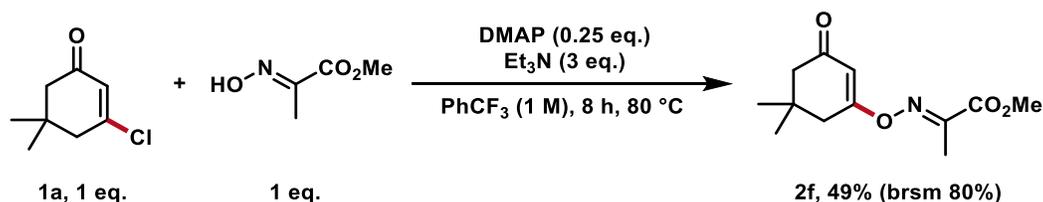
Acetophenone oxime (68 mg, 0.5 mmol, 1 eq.), DMAP (15 mg, 0.13 mmol, 0.25 eq.), freshly powdered K₂CO₃ (73 mg, 0.53 mmol, 1.05 eq.) and Et₄NBr (27 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**I**, 80 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial. The vial was sealed and the reaction mixture was heated for 12 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 2:1) to afford the title product as a white solid (116 mg, 89% yield).

¹H NMR (300 MHz, CDCl₃): δ 7.78 – 7.68 (m, 2H), 7.50 – 7.34 (m, 3H), 6.13 (d, J = 1.0 Hz, 1H), 2.43 (s, 2H), 2.39 (s, 3H), 2.27 (s, 2H), 1.14 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 199.6, 174.6, 160.9, 134.7, 130.6, 128.7, 126.7, 103.8, 51.0, 40.7, 32.8, 28.4, 13.7.

HRMS (ESI): m/z calc. for [C₁₆H₁₉NO₂+H⁺] 258.1489, found 258.1496.

Methyl (E)-2-(((5,5-dimethyl-3-oxocyclohex-1-en-1-yl)oxy)imino)propanoate (2f)



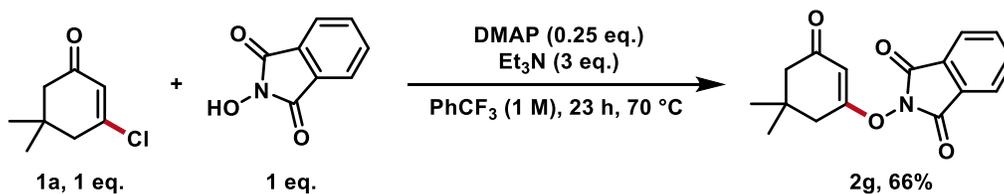
Methyl pyruvate oxime (59 mg, 0.5 mmol, 1 eq.) and DMAP (15 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**I**, 79 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial, followed by Et₃N (0.21 ml, 1.5 mmol, 3 eq.). The vial was sealed and the reaction mixture was heated for 8 hours in an oil bath at 80 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (CHCl₃:EA = 8:1) to afford the title product as a light yellow oil (59 mg, 49% yield), along with recovered vinyl chloride (29 mg, 37% yield) and oxime (18 mg, 31%). *Note: attempts to increase the conversion led to significant drop in product yield.*

¹H NMR (300 MHz, CDCl₃): δ 6.06 (d, J = 1.0 Hz, 1H), 3.88 (s, 3H), 2.44 (d, J = 1.1 Hz, 2H), 2.26 (s, 2H), 2.23 (s, 3H), 1.13 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 199.2, 173.6, 163.4, 154.4, 104.9, 53.1, 50.9, 40.3, 32.8, 28.3, 12.5.

HRMS (ESI): m/z calc. for [C₁₂H₁₇NO₄+H⁺] 240.1230, found 240.1239.

2-((5,5-Dimethyl-3-oxocyclohex-1-en-1-yl)oxy)isoindoline-1,3-dione (2g)



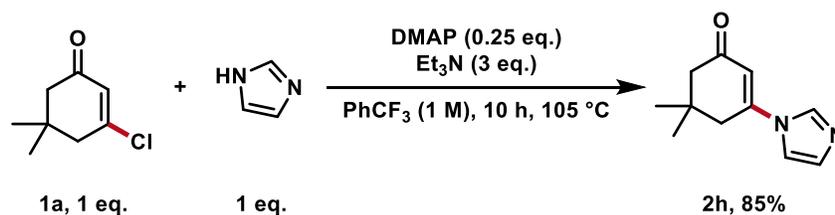
N-Hydroxyphthalimide (81 mg, 0.5 mmol, 1 eq.) and DMAP (15 mg, 0.12 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**I**, 79 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial, followed by Et₃N (0.21 ml, 1.5 mmol, 3 eq.). The vial was sealed and the reaction mixture was heated for 23 hours in an oil bath at 70 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 2:1) to afford the title product as a white solid (94 mg, 66% yield).

¹H NMR (300 MHz, CDCl₃): δ 7.96 – 7.87 (m, 2H), 7.87 – 7.81 (m, 2H), 5.50 (s, 1H), 2.59 (s, 2H), 2.28 (s, 2H), 1.17 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 198.5, 174.9, 161.5, 135.3, 128.6, 124.2, 103.1, 50.9, 39.2, 33.2, 28.2.

HRMS (ESI): m/z calc. for [C₁₆H₁₅NO₄+H⁺] 286.1074, found 286.1076.

3-(imidazol-1-yl)-5,5-dimethylcyclohex-2-en-1-one (2h)



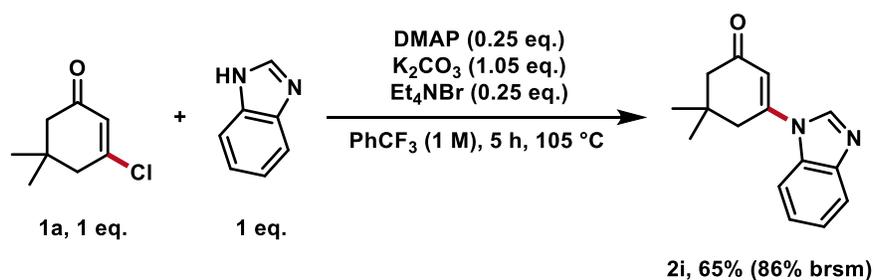
Imidazole (34 mg, 0.5 mmol, 1 eq.) and DMAP (15 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (I, 80 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial, followed by Et₃N (0.21 ml, 1.5 mmol, 3 eq.). The vial was sealed and the reaction mixture was heated for 10 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with acetone. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (acetone:MTBE = 4:1) to afford the title product as a light-yellow solid (82 mg, 85% yield).

¹H NMR (300 MHz, CDCl₃): δ 7.92 (t, *J* = 1.1 Hz, 1H), 7.27 (d, *J* = 1.6 Hz, 1H), 7.20 (dd, *J* = 1.6, 0.8 Hz, 1H), 6.18 (t, *J* = 1.3 Hz, 1H), 2.72 (d, *J* = 1.3 Hz, 2H), 2.37 (s, 2H), 1.19 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 199.2, 176.6, 150.4, 133.9, 131.5, 130.2, 127.9, 127.5, 126.9, 126.0, 120.7, 118.4, 105.2, 50.8, 42.4, 32.7, 28.3.

HRMS (ESI): *m/z* calc. for [C₁₁H₁₄N₂O+H⁺] 191.1179, found 191.1179.

3-(Benzoimidazol-1-yl)-5,5-dimethylcyclohex-2-en-1-one (2i)



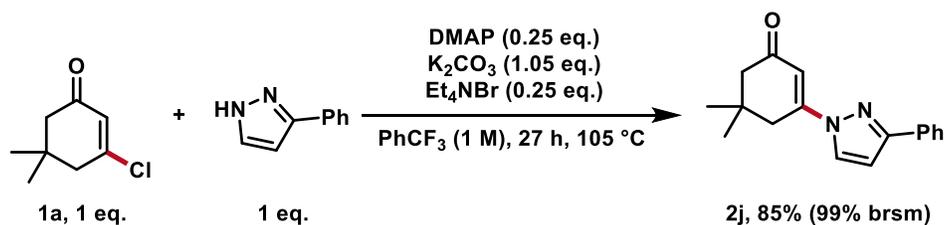
Benzimidazole (59 mg, 0.5 mmol, 1 eq.), DMAP (15 mg, 0.13 mmol, 0.25 eq.), freshly powdered K₂CO₃ (73 mg, 0.53 mmol, 1.05 eq.) and Et₄NBr (26 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**I**, 79 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial. The vial was sealed and the reaction mixture was heated for 5 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (EA) to afford the title product as a light beige solid (78 mg, 65% yield), along with recovered benzimidazole (12 mg, 21% yield).

¹H NMR (300 MHz, CDCl₃): δ 8.19 (s, 1H), 7.90 – 7.79 (m, 1H), 7.74 – 7.62 (m, 1H), 7.44 – 7.30 (m, 2H), 6.42 (d, J = 1.2 Hz, 1H), 2.87 (d, J = 1.3 Hz, 2H), 2.43 (s, 2H), 1.23 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 198.2, 151.5, 144.8, 140.5, 131.9, 124.6, 123.9, 121.1, 116.1, 112.6, 50.5, 42.2, 33.6, 28.3.

HRMS (ESI): m/z calc. for [C₁₅H₁₆N₂O+H⁺] 241.1335, found 241.1342

5,5-Dimethyl-3-(3-phenyl-pyrazol-1-yl)cyclohex-2-en-1-one (2j)



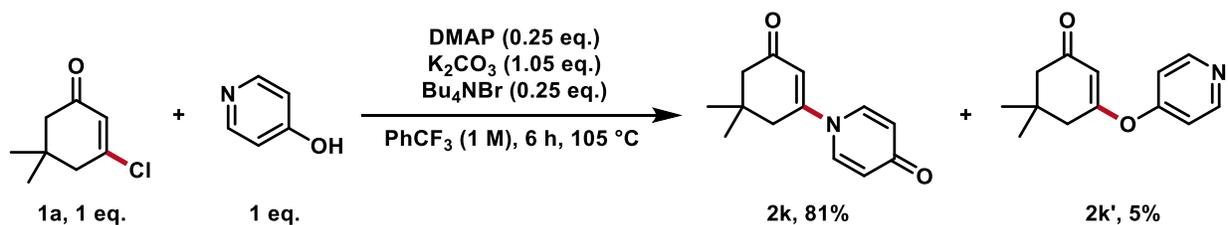
3-Phenylpyrazole (72 mg, 0.5 mmol, 1 eq.), DMAP (15 mg, 0.13 mmol, 0.25 eq.), freshly powdered K₂CO₃ (73 mg, 0.53 mmol, 1.05 eq.) and Et₄NBr (26 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (I, 79 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial. The vial was sealed and the reaction mixture was heated for 27 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator and the residue was purified by flash column chromatography (PE:EA = 2:1) to afford the title product as a light beige solid (113 mg, 85% yield), along with recovered pyrazole (10 mg, 14% yield).

¹H NMR (300 MHz, CDCl₃): δ 7.91 – 7.81 (m, 3H), 7.48 – 7.31 (m, 3H), 6.79 (d, J = 2.7 Hz, 1H), 6.47 (d, J = 1.3 Hz, 1H), 2.94 (d, J = 1.3 Hz, 2H), 2.34 (s, 2H), 1.18 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 199.0, 154.5, 153.9, 132.1, 128.9, 128.8, 128.8, 126.1, 110.9, 107.1, 50.8, 39.5, 33.0, 28.5.

HRMS (ESI): m/z calc. for [C₁₇H₁₈N₂O+H⁺] 267.1492, found 267.1497.

1-(5,5-Dimethyl-3-oxocyclohex-1-en-1-yl)pyridin-4-one (**2k**)



4-Pyridone (48 mg, 0.5 mmol, 1 eq.), DMAP (15 mg, 0.13 mmol, 0.25 eq.), freshly powdered K₂CO₃ (73 mg, 0.53 mmol, 1.05 eq.) and Bu₄NBr (41 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**I**, 80 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial. The vial was sealed and the reaction mixture was heated for 6 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Then, the reaction mixture was excessively washed through a plug of silica gel with acetone. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography first to afford pyridine **2k'** (acetone:PE = 1:1) as a yellow solid (6 mg, 5% yield), and then pyridone **2k** (CHCl₃:MeOH = 10:1) as a yellow solid (89 mg, 81% yield).

Spectral data for **2k**:

¹H NMR (300 MHz, CDCl₃): δ 7.72 – 7.62 (m, 2H), 6.48 – 6.37 (m, 2H), 6.09 (s, 1H), 2.68 (s, 2H), 2.37 (s, 2H), 1.19 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 197.7, 179.4, 155.7, 135.6, 119.3, 116.7, 50.2, 41.2, 33.8, 28.2.

HRMS (ESI): m/z calc. for [C₁₃H₁₅NO₂+H⁺] 218.1176, found 218.1175.

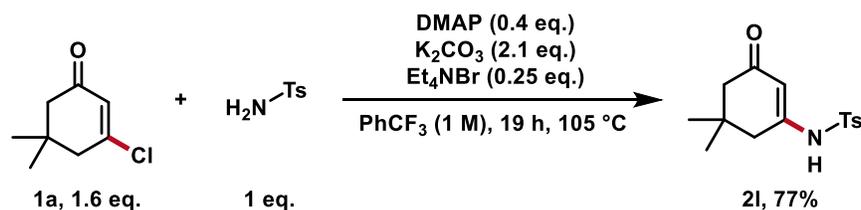
Spectral data for **2k'**:

¹H NMR (300 MHz, CDCl₃): δ 8.69 – 8.61 (m, 2H), 7.06 – 6.98 (m, 2H), 5.26 (s, 1H), 2.52 (s, 2H), 2.27 (s, 2H), 1.16 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 199.1, 174.2, 160.0, 152.2, 116.6, 106.6, 50.8, 42.3, 32.9, 28.4.

HRMS (ESI): m/z calc. for [C₁₃H₁₅NO₂+H⁺] 218.1176, found 218.1175.

N-(5,5-Dimethyl-3-oxocyclohex-1-en-1-yl)-4-methylbenzenesulfonamide (2l)



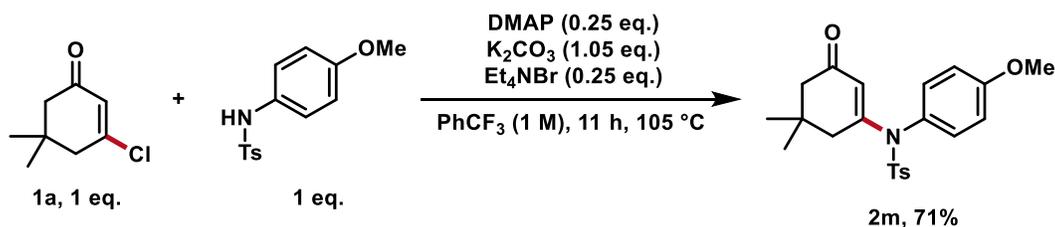
P-Toluenesulfonamide (86 mg, 0.5 mmol, 1 eq.), DMAP (15 mg, 0.13 mmol, 0.25 eq.), freshly powdered K₂CO₃ (146 mg, 1.06 mmol, 2.1 eq.) and Et₄NBr (27 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1**, 128 mg, 0.81 mmol, 1.6 eq.) in PhCF₃ (0.8 ml) was added to the vial. The vial was sealed, and the reaction mixture was heated for 10 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Afterwards, additional DMAP (9.2 mg, 0.08 mmol, 0.15 eq.) was added to the vial and the reaction mixture was further heated for 9 h. Then, CF₃CO₂H (0.17 ml, 2.12 mmol, 4.2 eq.) was added to the vial (*Note: acidification was made to ensure full protonation of the acidic product*) and after 5 minutes the reaction mixture was excessively washed through a plug of silica gel with EA. The solvent was removed on the rotary evaporator and the residue was purified by flash column chromatography (PE:EA = 1:2) to afford the title product as a yellow solid (114 mg, 77% yield).

¹H NMR (300 MHz, CDCl₃): δ 8.53 (s, 1H), 7.88 – 7.78 (m, 2H), 7.33 (d, J = 8.0 Hz, 2H), 5.93 (s, 1H), 2.42 (s, 3H), 2.22 (s, 2H), 2.15 (s, 2H), 0.97 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 199.3, 154.3, 145.0, 135.6, 130.1, 127.7, 107.5, 50.2, 41.7, 32.9, 28.1, 21.7.

HRMS (ESI): m/z calc. for [C₁₅H₁₉NO₃S+H⁺] 294.1158, found 294.1159.

N-(5,5-Dimethyl-3-oxocyclohex-1-en-1-yl)-N-(4-methoxyphenyl)-4-methylbenzenesulfonamide (2m)



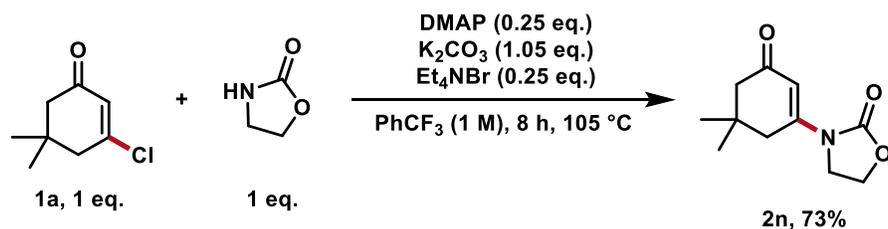
N-(4-Methoxyphenyl)-4-methylbenzenesulfonamide (140 mg, 0.5 mmol, 1 eq.), DMAP (15 mg, 0.13 mmol, 0.25 eq.), freshly powdered K₂CO₃ (73 mg, 0.53 mmol, 1.05 eq.) and Et₄NBr (27 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**I**, 80 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial. The vial was sealed, and the reaction mixture was heated for 11 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 1:1) to afford the title product as a yellow oil (143 mg, 71% yield), along with recovered sulfonamide (37 mg, 26% yield).

¹H NMR (300 MHz, CDCl₃): δ 7.69 – 7.59 (m, 2H), 7.30 (d, J = 8.5 Hz, 2H), 7.15 – 7.03 (m, 2H), 6.96 – 6.85 (m, 2H), 5.87 (d, J = 1.1 Hz, 1H), 3.83 (s, 3H), 2.43 (s, 3H), 2.24 (d, J = 1.1 Hz, 2H), 2.14 (s, 2H), 0.93 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 198.8, 160.1, 158.0, 144.7, 136.2, 131.5, 130.0, 129.8, 128.0, 114.8, 114.7, 55.5, 50.2, 42.7, 33.2, 28.0, 21.6.

HRMS (ESI): m/z calc. for [C₂₂H₂₅NO₄S+H⁺] 400.1577, found 400.1576.

3-(5,5-Dimethyl-3-oxocyclohex-1-en-1-yl)oxazolidin-2-one (2n)



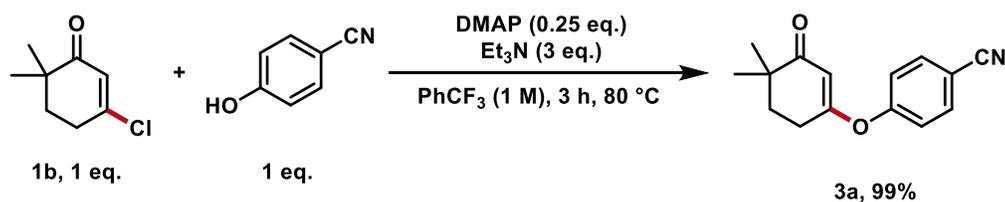
2-Oxazolidinone (44 mg, 0.5 mmol, 1 eq.), DMAP (15 mg, 0.13 mmol, 0.25 eq.), freshly powdered K₂CO₃ (73 mg, 0.53 mmol, 1.05 eq.) and Et₄NBr (27 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (I, 80 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial. The vial was sealed, and the reaction mixture was heated for 8 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with acetone. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:acetone = 1:1) to afford the title product as a white solid (77 mg, 73% yield).

¹H NMR (300 MHz, CDCl₃): δ 5.44 (s, 1H), 4.48 (t, J = 7.9 Hz, 2H), 3.88 (t, J = 8.0 Hz, 2H), 2.96 (s, 2H), 2.24 (s, 2H), 1.10 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 198.8, 155.9, 153.9, 109.2, 61.6, 50.3, 44.9, 39.4, 33.1, 28.4.

HRMS (ESI): m/z calc. for [C₁₁H₁₅NO₃+H⁺] 210.1125, found 210.1124.

4-((4,4-Dimethyl-3-oxocyclohex-1-en-1-yl)oxy)benzonitrile (**3a**)



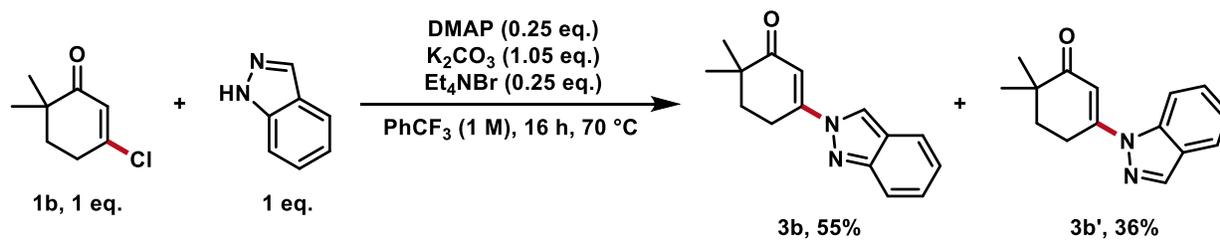
4-Cyanophenol (48 mg, 0.4 mmol, 1 eq.) and DMAP (12 mg, 0.1 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1b**, 64 mg, 0.4 mmol, 1 eq.) in PhCF₃ (0.4 ml) was added to the vial, followed by Et₃N (0.17 ml, 1.21 mmol, 3 eq.). The vial was sealed and the reaction mixture was heated for 3 hours in an oil bath at 80 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 3:1) to afford the title product as a white solid (96 mg, 99% yield).

¹H NMR (300 MHz, CDCl₃): δ 7.77 – 7.66 (m, 2H), 7.24 – 7.14 (m, 2H), 5.02 (s, 1H), 2.74 – 2.64 (m, 2H), 1.92 (t, *J* = 6.3 Hz, 2H), 1.14 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 203.6, 174.5, 156.2, 134.2, 122.4, 117.9, 109.7, 105.3, 40.2, 34.7, 25.6, 24.2.

HRMS (ESI): *m/z* calc. for [C₁₅H₁₅NO₂+H⁺] 242.1176, found 242.1182.

3-(Indazol-2-yl)-6,6-dimethylcyclohex-2-en-1-one (3b) and 3-(indazol-1-yl)-6,6-dimethylcyclohex-2-en-1-one (3b')



Indazole (47 mg, 0.4 mmol, 1 eq.), DMAP (12 mg, 0.1 mmol, 0.25 eq.), freshly powdered K₂CO₃ (58 mg, 0.42 mmol, 1.05 eq.) and Et₄NBr (21 mg, 0.1 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1b**, 63 mg, 0.4 mmol, 1 eq.) in PhCF₃ (0.4 ml) was added to the vial. The vial was sealed, and the reaction mixture was heated for 16 hours in an oil bath at 70 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 5:1) to afford the title products **3b'** as a white solid (35 mg, 36% yield) and **3b** as a white solid (53 mg, 55% yield).

Spectral data for 3b:

¹H NMR (300 MHz, CDCl₃): δ 8.34 – 8.28 (m, 1H), 7.72 – 7.64 (m, 1H), 7.64 – 7.58 (m, 1H), 7.35 – 7.24 (m, 1H), 7.08 (dd, *J* = 8.6, 6.5 Hz, 1H), 6.60 (t, *J* = 1.4 Hz, 1H), 3.26 – 3.15 (m, 2H), 2.05 (t, *J* = 6.2 Hz, 2H), 1.20 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 203.6, 154.3, 150.4, 128.2, 123.6, 122.9, 120.8, 120.60, 118.2, 114.3, 40.8, 35.2, 24.2, 23.7.

HRMS (ESI): *m/z* calc. for [C₁₅H₁₆N₂O+H⁺] 241.1335, found 241.1339.

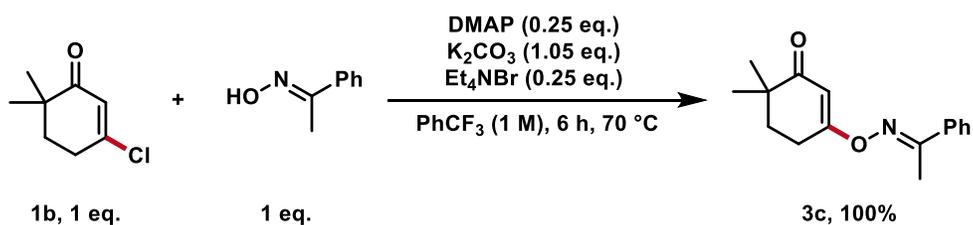
Spectral data for 3b':

¹H NMR (300 MHz, CDCl₃): δ 8.20 (d, *J* = 0.9 Hz, 1H), 7.88 (dd, *J* = 8.6, 1.0 Hz, 1H), 7.78 (dt, *J* = 8.1, 1.0 Hz, 1H), 7.50 (ddd, *J* = 8.5, 7.1, 1.2 Hz, 1H), 7.35 – 7.24 (m, 1H), 6.42 (t, *J* = 1.2 Hz, 1H), 3.25 (td, *J* = 6.2, 1.2 Hz, 2H), 2.04 (t, *J* = 6.2 Hz, 2H), 1.23 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 204.3, 156.0, 138.9, 138.0, 128.4, 126.9, 123.3, 121.8, 113.0, 111.7, 40.5, 35.4, 25.1, 24.4.

HRMS (ESI): *m/z* calc. for [C₁₅H₁₆N₂O+H⁺] 241.1335, found 241.1341.

(E)-6,6-dimethyl-3-(((1-phenylethylidene)amino)oxy)cyclohex-2-en-1-one (3c)



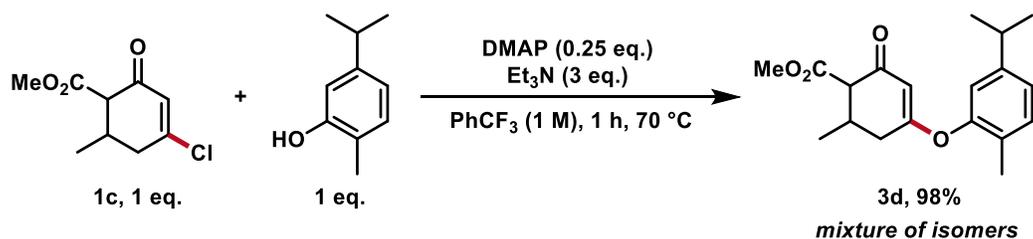
Acetophenone oxime (54 mg, 0.4 mmol, 1 eq.) and DMAP (12 mg, 0.1 mmol, 0.25 eq.), freshly powdered K₂CO₃ (58 mg, 0.42 mmol, 1.05 eq.) and Et₄NBr (21 mg, 0.1 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1b**, 63 mg, 0.4 mmol, 1 eq.) in PhCF₃ (0.4 ml) was added to the vial. The vial was sealed, and the reaction mixture was heated for 6 hours in an oil bath at 70 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 5:1) to afford the title product as a white solid (103 mg, 100%).

¹H NMR (300 MHz, CDCl₃): δ 7.77 – 7.67 (m, 2H), 7.48 – 7.32 (m, 3H), 6.02 (s, 1H), 2.59 (t, *J* = 6.3 Hz, 2H), 2.37 (s, 3H), 1.88 (t, *J* = 6.3 Hz, 2H), 1.15 (s, 6H).

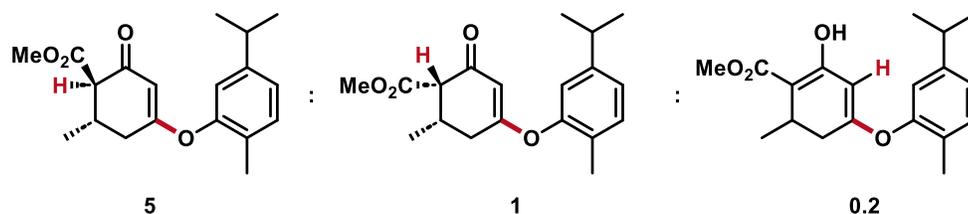
¹³C{¹H} NMR (75 MHz, CDCl₃): δ 204.4, 174.1, 160.6, 134.7, 130.5, 128.6, 126.6, 103.1, 40.4, 35.0, 24.5, 24.1, 13.5.

HRMS (ESI): *m/z* calc. for [C₁₅H₁₅NO₂+H⁺] 242.1176, found 242.1182.

Methyl 4-(5-isopropyl-2-methylphenoxy)-6-methyl-2-oxocyclohex-3-ene-1-carboxylate (3d)



product composition (by integrals of H)



Carvacrol (75 mg, 0.5 mmol, 1 eq.) and DMAP (15 mg, 0.1 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1c**, 101 mg, 0.5 mmol, 1 eq.) in PhCF_3 (0.5 ml) was added to the vial, followed by Et_3N (0.21 ml, 1.5 mmol, 3 eq.). The vial was sealed, and the reaction mixture was heated for 1 hour in an oil bath at 70 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 5:1) to afford the title product as a colorless oil (154 mg, 98% yield). *Note: formation of inseparable mixture of tautomers for similar cyclohexenone system was described previously.*^[8]

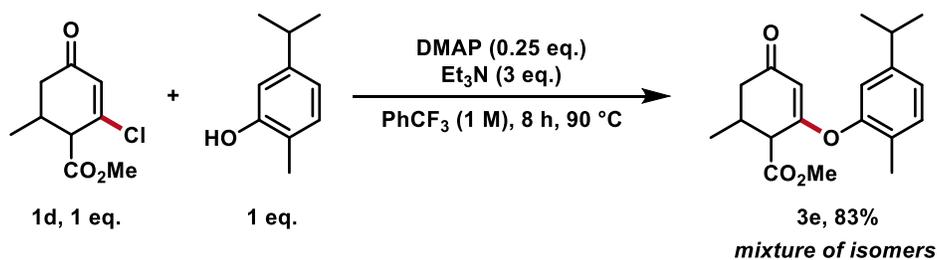
^1H NMR (300 MHz, CDCl_3): δ 7.19 – 7.09 (m, 1H), 7.06 – 6.97 (m, 1H), 6.87 – 6.75 (m, 1H), 5.12 – 4.67 (m, 1H), 3.79 – 3.67 (m, 3H), 3.41 – 3.05 (m, 1H), 3.00 – 2.38 (m, 4H), 2.15 – 2.03 (m, 3H), 1.26 – 1.08 (m, 9H).

Multiplet at 3.41 – 3.05 – composite of 3.36 (d, $J = 4.9$ Hz) for minor *syn* and 3.10 (d, $J = 10.9$ Hz) for major *trans* isomers.

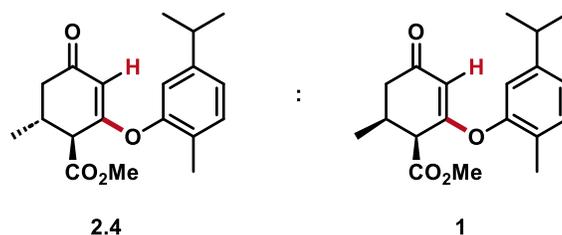
$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 193.9, 193.9, 178.3, 176.6, 170.5, 168.9, 150.8, 150.7, 148.8, 148.7, 131.4, 126.9, 126.7, 124.5, 124.4, 119.3, 119.1, 119.0, 104.1, 104.0, 60.4, 57.3, 52.0, 51.8, 35.1, 33.4, 33.18, 31.5, 30.6, 23.8, 19.6, 17.8, 15.2.

HRMS (ESI): m/z calc. for $[\text{C}_{19}\text{H}_{24}\text{O}_4 + \text{H}^+]$ 317.1747, found 317.1750.

Methyl 2-(5-isopropyl-2-methylphenoxy)-6-methyl-4-oxocyclohex-2-ene-1-carboxylate (3e)



product composition (by integrals of H) _____



Carvacrol (43 mg, 0.29 mmol, 1 eq.) and DMAP (9 mg, 0.07 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1d**, 58 mg, 0.29 mmol, 1 eq.) in PhCF₃ (0.29 ml) was added to the vial, followed by Et₃N (0.12 ml, 0.86 mmol, 3 eq.). The vial was sealed, and the reaction mixture was heated for 6 hours in an oil bath at 90 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 4:1) to afford the title product as a colorless oil (75 mg, 83% yield). *Note: the formation of an inseparable mixture of tautomers for similar cyclohexenone system was described previously.*^[8]

¹H NMR (300 MHz, CDCl₃): δ 7.18 – 7.09 (m, 1H), 7.06 – 6.97 (m, 1H), 6.82 – 6.74 (m, 1H), 5.13 – 5.04 (m, 1H), 3.87 – 3.78 (m, 3H), 3.68 – 3.42 (m, 1H), 2.85 (hept, *J* = 6.9 Hz, 1H), 2.75 – 2.01 (m, 6H), 1.29 – 1.11 (m, 9H).

Multiplet at 6.82 – 6.74 – composite of 5.10 (s) for minor *syn* and 5.07 (d, *J* = 1.3 Hz) for major *anti* isomers.

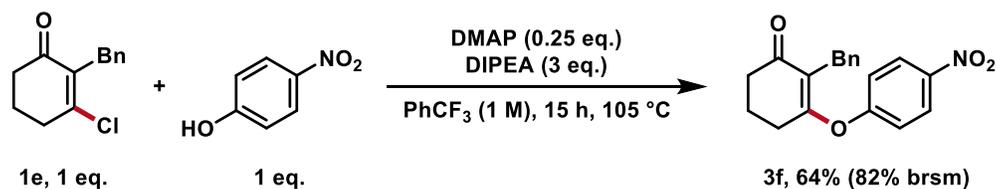
Multiplet at 3.87 – 3.78 – composite of 3.84 (s) for major *anti* and 3.82 (s) for minor *syn* isomers.

Multiplet at 3.68 – 3.42 – composite of 3.65 (d, *J* = 5.2 Hz) for minor *syn* and 3.46 (dd, *J* = 8.1, 1.3 Hz) for major *anti* isomers.

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 198.9, 197.8, 173.0, 173.3, 171.0, 169.7, 150.7, 149.0, 131.6, 127.2, 124.7, 124.6, 119.1, 106.5, 105.8, 52.9, 52.6, 52.3, 50.2, 43.1, 41.0, 33.6, 32.4, 31.1, 24.0, 24.0, 23.9, 19.7, 18.4, 15.2, 15.1.

HRMS (ESI): *m/z* calc. for [C₁₉H₂₄O₄+H⁺] 317.1747, found 317.1739.

2-Benzyl-3-(4-nitrophenoxy)cyclohex-2-en-1-one (3f)



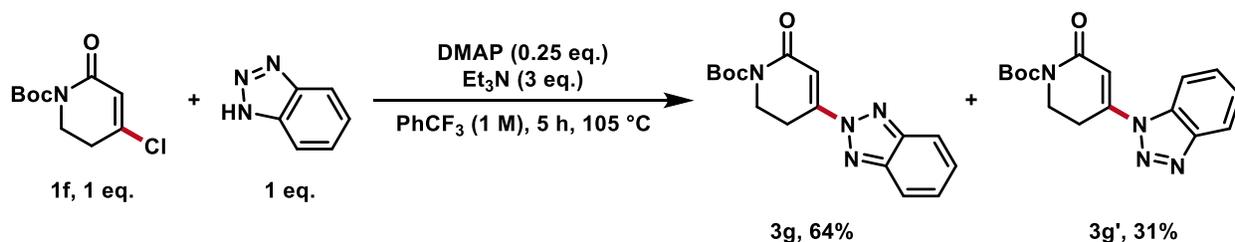
4-Nitrophenol (69 mg, 0.5 mmol, 1 eq.) and DMAP (15.2 mg, 0.12 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1e**, 110 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial, followed by DIPEA (0.26 ml, 1.5 mmol, 3 eq.). The vial was sealed, and the reaction mixture was heated for 15 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (MTBE:PE = 1:1) to afford the title product as a white solid (103 mg, 64% yield), along with recovered vinyl chloride (20 mg, 18% yield).

¹H NMR (300 MHz, CDCl₃): δ 8.20 (d, *J* = 8.7 Hz, 2H), 7.23 – 7.07 (m, 5H), 6.93 (d, *J* = 8.8 Hz, 2H), 3.67 (s, 2H), 2.50 (t, *J* = 6.6 Hz, 2H), 2.43 (t, *J* = 6.2 Hz, 2H), 2.10 – 1.96 (m, 2H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 198.3, 167.3, 159.4, 143.9, 140.1, 128.9, 128.3, 127.5, 126.0, 118.7, 37.2, 28.4, 27.3, 21.1. Note: two signals at 126.0 ppm overlap.

HRMS (ESI): *m/z* calc. for [C₁₉H₁₇NO₄+H⁺] 324.1230, found 324.1230.

Tert-butyl 4-(benzo[d][1,2,3]triazol-2-yl)-6-oxo-3,6-dihydropyridine-1-carboxylate (3g**) and tert-butyl 4-(benzo[d][1,2,3]triazol-1-yl)-6-oxo-3,6-dihydropyridine-1-carboxylate (**3g'**)**



Benzotriazole (59 mg, 0.5 mmol, 1 eq.) and DMAP (15.1 mg, 0.12 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1f**, 115 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial, followed by Et₃N (0.21 ml, 1.5 mmol, 3 eq.). The vial was sealed, and the reaction mixture was heated for 5 hours in an oil bath at 70 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 2:1) to afford the title products **3g** as a white solid (100 mg, 64% yield) and **3g'** as a white solid (48 mg, 31% yield).

Spectral data for **3g**:

¹H NMR (300 MHz, CDCl₃): δ 7.92 – 7.80 (m, 2H), 7.49 – 7.37 (m, 2H), 7.03 (t, *J* = 1.3 Hz, 1H), 4.12 (t, *J* = 6.5 Hz, 2H), 3.40 (td, *J* = 6.6, 1.3 Hz, 2H), 1.59 (s, 9H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 163.5, 152.4, 150.0, 145.7, 128.7, 118.7, 113.5, 83.5, 42.9, 28.2, 25.1.

HRMS (ESI): *m/z* calc. for [C₁₆H₁₈N₄O₃+Na⁺] 337.1271, found 337.1271.

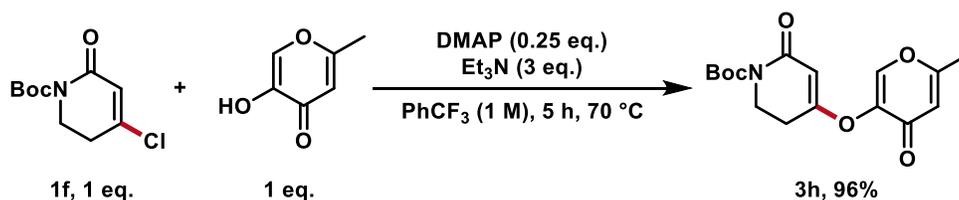
Spectral data for **3g'**:

¹H NMR (300 MHz, CDCl₃): δ 8.16 (dt, *J* = 8.2, 1.0 Hz, 1H), 7.87 (dt, *J* = 8.5, 0.9 Hz, 1H), 7.66 (ddd, *J* = 8.4, 7.0, 1.1 Hz, 1H), 7.51 (ddd, *J* = 8.2, 7.0, 1.0 Hz, 1H), 6.44 (d, *J* = 1.2 Hz, 1H), 4.16 (t, *J* = 6.5 Hz, 2H), 3.50 (td, *J* = 6.5, 1.2 Hz, 2H), 1.60 (s, 9H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 163.8, 152.1, 148.9, 147.2, 131.2, 129.8, 125.7, 121.1, 111.9, 110.2, 83.6, 42.7, 28.2, 26.6.

HRMS (ESI): *m/z* calc. for [C₁₆H₁₈N₄O₃+Na⁺] 337.1271, found 337.1270.

Tert-butyl 4-((6-methyl-4-oxo-pyran-3-yl)oxy)-6-oxo-3,6-dihydropyridine-1-carboxylate (**3h**)



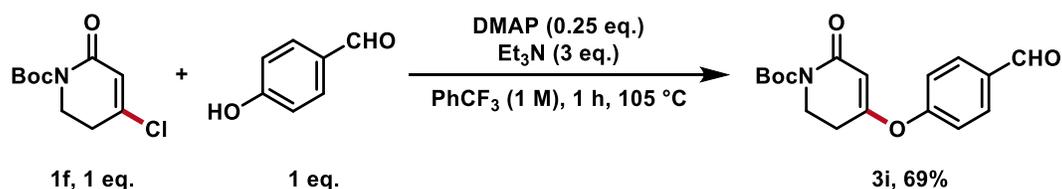
Allomaltol (37 mg, 0.29 mmol, 1 eq.) and DMAP (9 mg, 0.07 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1f**, 67 mg, 0.29 mmol, 1 eq.) in PhCF₃ (0.29 ml) was added to the vial, followed by Et₃N (0.12 ml, 0.87 mmol, 3 eq.). The vial was sealed, and the reaction mixture was heated for 5 hours in an oil bath at 70 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (hexane:acetone = 3:2) to afford the title product as a light-yellow solid (89 mg, 96% yield).

¹H NMR (300 MHz, CDCl₃): δ 7.91 (s, 1H), 6.28 (d, *J* = 0.9 Hz, 1H), 5.06 (s, 1H), 3.94 (t, *J* = 6.5 Hz, 2H), 2.72 (t, *J* = 6.5 Hz, 2H), 2.33 (d, *J* = 0.9 Hz, 3H), 1.52 (s, 9H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 172.1, 169.7, 166.4, 164.8, 152.1, 148.4, 142.2, 115.6, 100.2, 82.6, 42.4, 28.0, 27.1, 19.5.

HRMS (ESI): *m/z* calc. for [C₁₆H₁₉NO₆+H⁺] 322.1285, found 322.1286.

Tert-butyl 4-(4-formylphenoxy)-6-oxo-3,6-dihydropyridine-1-carboxylate (**3i**)



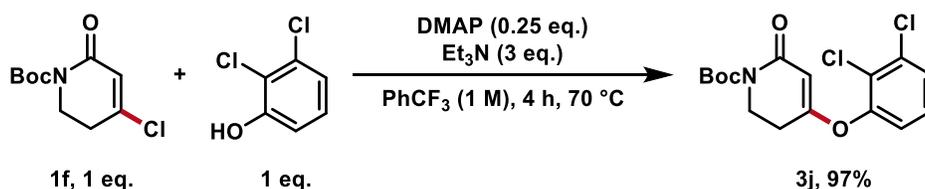
4-Hydroxybenzaldehyde (61 mg, 0.5 mmol, 1 eq.) and DMAP (15 mg, 0.12 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1f**, 115 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial, followed by Et₃N (0.21 ml, 1.5 mmol, 3 eq.). The vial was sealed, and the reaction mixture was heated for 1 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 1:1) to afford the title product as a white solid (109 mg, 69% yield).

¹H NMR (300 MHz, CDCl₃): δ 10.01 (s, 1H), 8.01 – 7.90 (m, 2H), 7.28 – 7.20 (m, 2H), 4.99 (s, 1H), 3.98 (t, *J* = 6.5 Hz, 2H), 2.75 (t, *J* = 6.5 Hz, 2H), 1.54 (s, 9H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 190.6, 170.5, 165.0, 157.4, 152.3, 134.3, 131.9, 121.9, 101.0, 83.0, 42.4, 28.1, 27.8.

HRMS (ESI): *m/z* calc. for [C₁₇H₁₉NO₅+H⁺] 318.1336, found 318.1336.

Tert-butyl 4-(2,3-dichlorophenoxy)-6-oxo-3,6-dihydropyridine-1-carboxylate (**3j**)



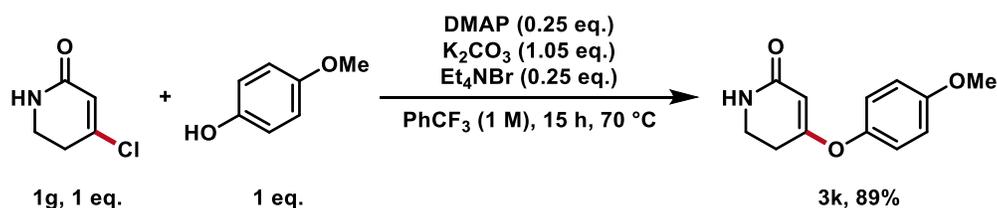
2,3-Dichlorophenol (48 mg, 0.29 mmol, 1 eq.) and DMAP (9 mg, 0.07 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1f**, 68 mg, 0.29 mmol, 1 eq.) in PhCF₃ (0.29 ml) was added to the vial, followed by Et₃N (0.12 ml, 0.9 mmol, 3 eq.). The vial was sealed, and the reaction mixture was heated for 4 hours in an oil bath at 70 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (hexane:EA = 3:1) to afford the title product as a colorless oil (102 mg, 97% yield).

¹H NMR (300 MHz, CDCl₃): δ 7.40 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.25 (t, *J* = 8.1 Hz, 1H), 7.07 (dd, *J* = 8.1, 1.5 Hz, 1H), 4.81 (s, 1H), 3.97 (t, *J* = 6.5 Hz, 2H), 2.76 (t, *J* = 6.5 Hz, 2H), 1.54 (s, 9H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 169.9, 164.9, 152.2, 149.9, 134.7, 128.3, 128.0, 126.2, 121.5, 100.3, 82.9, 42.5, 28.1, 27.4.

HRMS (ESI): *m/z* calc. for [C₁₆H₁₇Cl₂NO₄+H⁺] 358.0607, found 358.0602.

4-(4-Methoxyphenoxy)-5,6-dihydropyridin-2-one (3k)



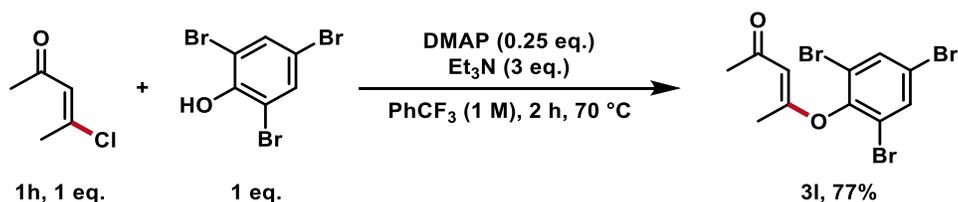
4-Methoxyphenol (50 mg, 0.4 mmol, 1 eq.), DMAP (12.3 mg, 0.1 mmol, 0.25 eq.), freshly powdered K₂CO₃ (58 mg, 0.42 mmol, 1.05 eq.) and Et₄NBr (21 mg, 0.1 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1g**, 53 mg, 0.4 mmol, 1 eq.) in PhCF₃ (0.4 ml) was added to the vial. The vial was sealed, and the reaction mixture was heated for 15 hours in an oil bath at 70 °C (monitored by NMR spectroscopy). Then, the reaction mixture was excessively washed through a plug of silica gel with acetone. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (CHCl₃:acetone = 3:1) to afford the title product as a bright-gray solid (78.5 mg, 89% yield).

¹H NMR (300 MHz, CDCl₃): δ 7.04 – 6.93 (m, 2H), 6.93 – 6.83 (m, 2H), 5.46 (s, 1H), 4.87 – 4.80 (m, 1H), 3.80 (s, 3H), 3.50 (td, *J* = 7.1, 2.5 Hz, 2H), 2.67 (t, *J* = 7.1 Hz, 2H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 170.4, 169.7, 157.4, 146.3, 122.2, 114.9, 97.5, 55.7, 38.6, 27.4.

HRMS (ESI): *m/z* calc. for [C₁₂H₁₃NO₃+H⁺] 220.0968, found 220.0963.

(E)-4-(2,4,6-Tribromophenoxy)pent-3-en-2-one (3l)



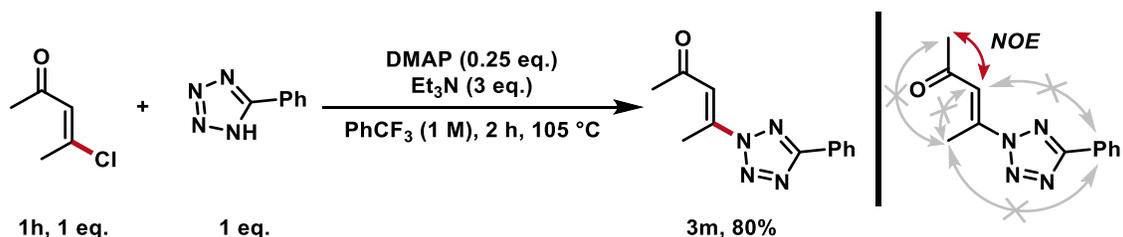
2,4,6-Tribromophenol (167 mg, 0.51 mmol, 1 eq.) and DMAP (16 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1h**, 60 mg, 0.51 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial, followed by Et₃N (0.21 ml, 1.5 mmol, 3 eq.). The vial was sealed, and the reaction mixture was heated for 2 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 10:1) to afford the title product as a white solid (161 mg, 77% yield).

¹H NMR (300 MHz, CDCl₃): δ 7.75 (d, *J* = 1.2 Hz, 2H), 5.12 (s, 1H), 2.50 (s, 3H), 2.08 (s, 3H). *Note: stereochemistry of the product was deduced on the basis of ¹H NMR spectral data for similar β-aryloxy-α,β-unsaturated ketones.*^[19]

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 196.9, 168.1, 147.3, 135.5, 119.8, 118.5, 103.6, 32.3, 18.1.

HRMS (ESI): *m/z* calc. for [C₁₁H₉Br₃O₂+H⁺] 410.8225, found 410.8225.

(E)-4-(5-Phenyl-tetrazol-2-yl)pent-3-en-2-one (3m)



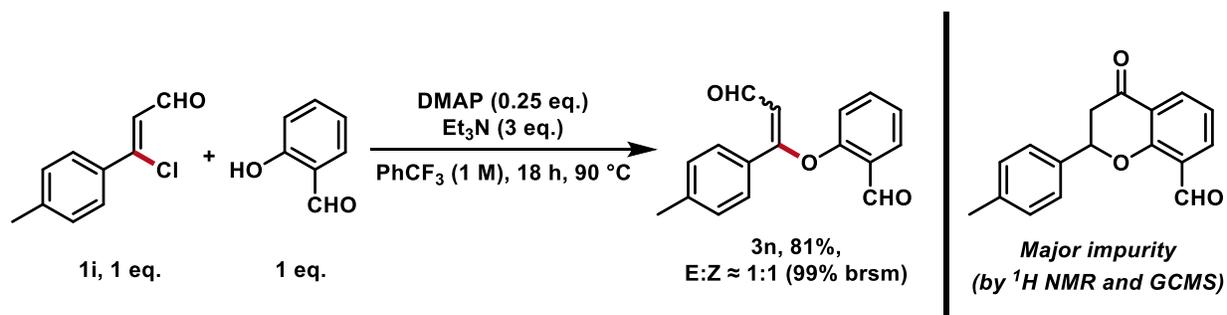
5-Phenyltetrazole 74 mg, 0.51 mmol, 1 eq.) and DMAP (16 mg, 0.13 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1h**, 60 mg, 0.51 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial, followed by Et₃N (0.21 ml, 1.5 mmol, 3 eq.). The vial was sealed, and the reaction mixture was heated for 2 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 3:1) to afford the title product as a white solid (92 mg, 80% yield).

¹H NMR (300 MHz, CDCl₃): δ 8.26 – 8.14 (m, 2H), 7.58 – 7.45 (m, 3H), 7.35 (d, *J* = 1.3 Hz, 1H), 2.91 (d, *J* = 1.2 Hz, 3H), 2.40 (s, 3H). *Note: the structure of the product was deduced on the basis of NOESY experiments.*

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 197.6, 165.1, 145.2, 131.0, 129.1, 127.3, 126.7, 116.5, 32.8, 29.8, 15.0.

HRMS (ESI): *m/z* calc. for [C₁₂H₁₂N₄O + H⁺] 229.1084, found 229.1083.

2-((3-Oxo-1-(p-tolyl)prop-1-en-1-yl)oxy)benzaldehyde (3n)



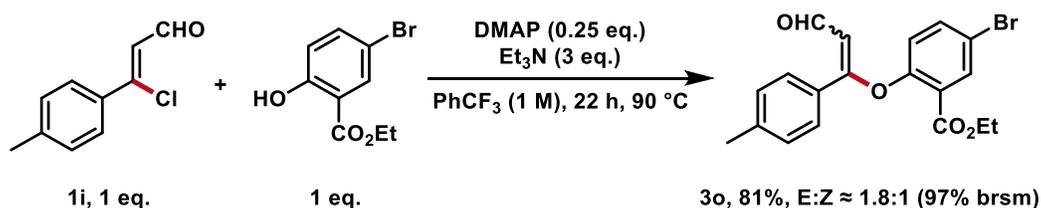
DMAP (12 mg, 0.1 mmol, 0.25 eq.) was weighed into a screw-cap vial. A solution of vinyl chloride (**1i**, 72 mg, 0.4 mmol, 1 eq.) and salicylaldehyde (49 mg, 0.4 mmol, 1 eq.) in PhCF₃ (0.4 ml) was added to the vial, followed by Et₃N (0.17 ml, 1.2 mmol, 3 eq.). The vial was sealed, and the reaction mixture was heated for 18 hours in an oil bath at 90 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator and the residue was purified by flash column chromatography (hexane:EA = 5:1) to afford the title product in several separate fractions containing single *E*-isomer (19 mg, 18% yield) as a bright-yellow solid, a mixture of *E*- and *Z*-isomers as a bright-yellow oil (59 mg, 55% yield, E:Z \approx 1.8:1) and single *Z*-isomer (7 mg, 7% yield), along with recovered salicylaldehyde (9 mg, 18% yield). *Note: according to $^1\text{H NMR}$ and GCMS analysis, the main impurity in the isolated product is isomeric dihydrobenzopyrone, which forms during the reaction and on silica gel during purification. Attempts to efficiently isolate individual isomers were unfruitful.*

$^1\text{H NMR}$ (300 MHz, CDCl₃): δ 10.75 (d, $J = 0.8$ Hz, 1H, *E*), 10.24 (d, $J = 0.6$ Hz, 1H, *Z*), 10.08 (d, $J = 7.7$ Hz, 1H, *E*), 9.56 (d, $J = 7.7$ Hz, 1H, *Z*), 8.01 – 6.77 (m, 8H), 6.35 (d, $J = 7.6$ Hz, 1H, *E*), 5.38 (d, $J = 7.6$ Hz, 1H, *Z*), 2.46 (s, 3H, *Z*), 2.36 (s, 3H, *E*). *Note: spectral data for individual isomers was deduced on the basis of $^1\text{H NMR}$ spectral data for similar β -aryloxy- α,β -unsaturated aldehydes.^[20] $^1\text{H NMR}$ data for individual *E*-isomer (300 MHz, CDCl₃):* δ 10.75 (s, 1H), 10.08 (d, $J = 7.7$ Hz, 1H), 7.93 (dd, $J = 7.7, 1.8$ Hz, 1H), 7.48 (d, $J = 8.2$ Hz, 2H), 7.40 (ddd, $J = 8.9, 7.4, 1.8$ Hz, 1H), 7.22 – 7.08 (m, 3H), 6.80 (d, $J = 8.3$ Hz, 1H), 6.35 (d, $J = 7.6$ Hz, 1H), 2.36 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl₃): δ 192.1, 189.9, 188.4, 188.0, 176.7, 166.2, 159.3, 155.0, 142.8, 142.4, 136.1, 136.0, 130.5, 130.1, 130.1, 129.5, 129.4, 127.3, 126.8, 123.5, 122.8, 116.5, 116.4, 110.2, 21.6, 21.6. *Note: some signals from individual isomers overlap.*

HRMS (ESI): m/z calc. for [C₁₇H₁₄O₃+H⁺] 267.1016, found 267.1016.

Ethyl 5-bromo-2-((3-oxo-1-(p-tolyl)prop-1-en-1-yl)oxy)benzoate (**3o**)



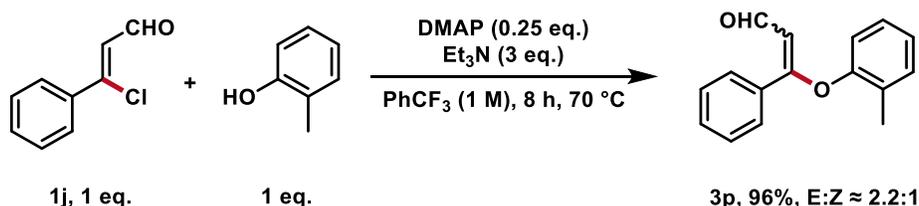
Ethyl 4-bromosalicylate (98 mg, 0.4 mmol, 1 eq.) and DMAP (12 mg, 0.1 mmol, 0.25 eq.) were weighed into a screw-cap vial. A solution of vinyl chloride (**1i**, 72 mg, 0.4 mmol, 1 eq.) in PhCF₃ (0.4 ml) was added to the vial, followed by Et₃N (0.17 ml, 1.2 mmol, 3 eq.). The vial was sealed, and the reaction mixture was heated for 22 hours in an oil bath at 90 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator and the residue was purified by flash column chromatography (hexane:EA = 5:1) to afford the title product as a mixture of E- and Z-isomers as an orange oil (126 mg, 81% yield, E:Z ≈ 1.8:1), along with recovered salicylate (18 mg, 18% yield). *Note: as judged by ¹H NMR and GCMS analysis, isolated product contained minute amounts of its analog with 2,4-dibrominated phenol fragment, originating from the impurity in the starting material. Attempts to efficiently isolate individual product isomers were unfruitful.*

¹H NMR (300 MHz, CDCl₃): δ 10.04 (d, *J* = 7.7 Hz, 1H, E), 9.54 (d, *J* = 7.7 Hz, 1H, Z), 8.16 (d, *J* = 2.5 Hz, 1H, Z), 7.98 (d, *J* = 2.5 Hz, 1H, E), 7.79 – 6.64 (m, 6H), 6.22 (d, *J* = 7.7 Hz, 1H, E), 5.25 (d, *J* = 7.7 Hz, 1H, Z), 4.46 (q, *J* = 7.1 Hz, 2H, E), 4.32 (q, *J* = 7.1 Hz, 2H, Z), 2.43 (d, *J* = 1.6 Hz, 3H, Z), 2.33 (s, 3H, E), 1.43 (t, *J* = 7.2 Hz, 3H, E), 1.28 (t, *J* = 7.1 Hz, 3H, Z). *Note: spectral data for individual isomers was deduced on the basis of ¹H NMR spectral data for similar β-aryloxy-α,β-unsaturated aldehydes.*

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 192.1, 190.3, 176.7, 166.7, 164.1, 162.9, 155.3, 151.6, 142.5, 142.1, 137.1, 136.1, 135.2, 134.5, 130.4, 130.3, 130.0, 129.4, 129.3, 127.5, 125.5, 125.4, 123.0, 119.3, 119.1, 116.0, 115.5, 108.8, 61.8, 21.6, 21.5, 14.3, 14.2. *Note: some signals from individual isomers overlap.*

HRMS (ESI): *m/z* calc. for [C₁₉H₁₇BrO₄+H⁺] 389.0383, found 389.0388.

3-Phenyl-3-(o-tolyloxy)acrylaldehyde (3p)



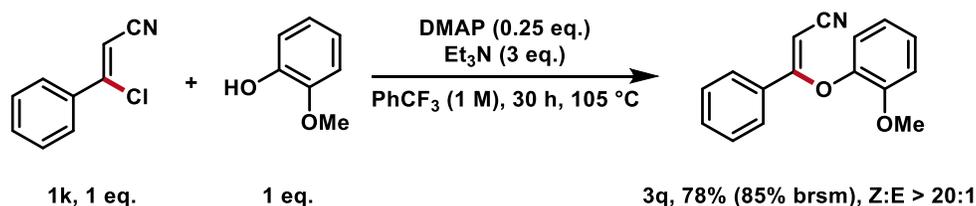
DMAP (15 mg, 0.13 mmol, 0.25 eq.) was weighed into a screw-cap vial. A solution of vinyl chloride (115 mg, 0.5 mmol, 1 eq.) and 2-methylphenol (54 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial, followed by Et₃N (0.21 ml, 1.49 mmol, 3 eq.). The vial was sealed, and the reaction mixture was heated for 8 hours in an oil bath at 70 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 5:1) to afford the title product as a mixture of E- and Z-isomers as an orange oil (114 mg, 96% yield, E:Z \approx 2.2:1). *Note: attempts to efficiently isolate individual product isomers were unfruitful.*

¹H NMR (300 MHz, CDCl₃): δ 10.02 (d, J = 7.8 Hz, 1H, E), 9.54 (d, J = 7.9 Hz, 1H, Z), 7.73 – 6.60 (m, 9H), 6.24 (d, J = 7.8 Hz, 1H, E), 5.32 (d, J = 7.9 Hz, 1H, Z), 2.47 (s, 3H, E), 2.25 (s, 3H, Z). NMR data matched the literature, confirming stereochemistry of the product.^[20]

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 192.4, 190.7, 176.2, 167.7, 155.5, 151.4, 133.0, 132.5, 131.9, 131.5, 131.4, 131.4, 130.1, 129.9, 129.0, 128.6, 127.8, 127.2, 127.2, 126.9, 126.5, 123.3, 121.5, 116.1, 115.7, 108.6, 16.2, 15.9.

HRMS (ESI): m/z calc. for [C₁₆H₁₄O₂+H⁺] 239.1067, found 239.1071.

(Z)-3-(2-Methoxyphenoxy)-3-phenylacrylonitrile (3q)



DMAP (15 mg, 0.13 mmol, 0.25 eq.) was weighed into a screw-cap vial. A solution of vinyl chloride (**1k**, 82 mg, 0.5 mmol, 1 eq.) and guaiacol (62 mg, 0.5 mmol, 1 eq.) in PhCF₃ (0.5 ml) was added to the vial, followed by Et₃N (0.21 ml, 1.5 mmol, 3 eq.). The vial was sealed, and the reaction mixture was heated for 30 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 7:1) to afford the title product as a light-yellow solid (98 mg, 78% yield, Z:E > 20:1), along with recovered guaiacol (4 mg, 7% yield).

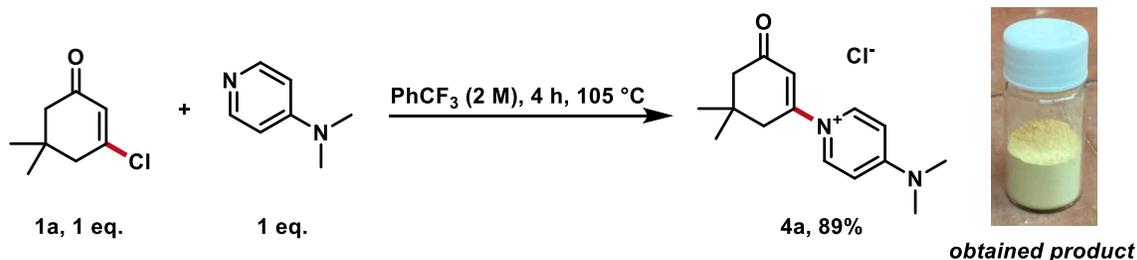
¹H NMR (300 MHz, CDCl₃): δ 7.68 – 7.57 (m, 2H), 7.50 – 7.32 (m, 3H), 7.17 (ddd, *J* = 8.1, 7.4, 1.6 Hz, 1H), 7.07 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.00 – 6.84 (m, 2H), 5.17 (s, 1H), 3.87 (s, 3H). NMR data matched the literature, confirming stereochemistry of the product.^[20]

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 169.2, 150.9, 143.9, 132.9, 131.3, 128.7, 126.9, 126.4, 121.0, 120.9, 115.0, 112.7, 76.9, 56.0.

HRMS (ESI): *m/z* calc. for [C₁₆H₁₃NO₂+H⁺] 266.1176, found 266.1180.

7. Pyridinium salt synthesis procedures

1-(5,5-Dimethyl-3-oxocyclohex-1-en-1-yl)-4-(dimethylamino)pyridin-1-ium chloride (4a)



DMAP (1.6 g, 13.1 mmol, 1 eq.) was weighed into a round-bottom flask equipped with a condenser, followed by addition of PhCF_3 (6 ml). After DMAP dissolution (*Note: heating may be applied to achieve dissolution*), a solution of vinyl chloride (**I**, 2.08 g, 13.1 mmol, 1 eq.) in PhCF_3 (0.6 ml) was added and the reaction mixture was refluxed for 4 hours (monitored by NMR spectroscopy). Upon completion, Et_2O (6.6 ml) was added to the reaction mixture. After a few minutes, precipitate was filtered, washed with Et_2O and dried to afford the title product as a light-yellow powder (3.71 g, 89% yield, 89 wt% purity by assay).

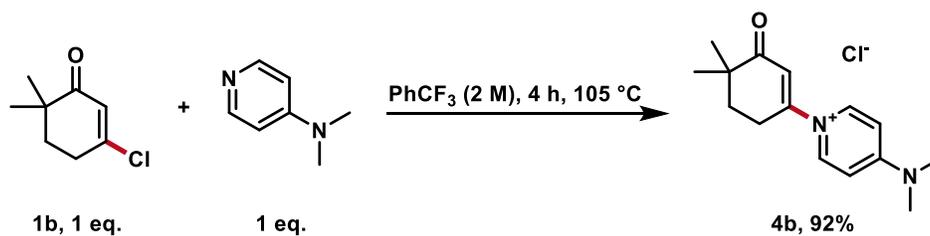
$^1\text{H NMR}$ (300 MHz, CDCl_3): δ 8.81 – 8.72 (m, 2H), 7.40 – 7.35 (m, 2H), 6.35 (br s, 1H), 3.41 (s, 6H), 2.98 (d, $J = 1.4$ Hz, 2H), 2.39 (s, 2H), 1.19 (s, 6H).

$^1\text{H NMR}$ (300 MHz, $\text{DMSO}-d_6$): δ 8.61 (d, $J = 7.5$ Hz, 2H), 7.16 (d, $J = 7.6$ Hz, 2H), 6.43 (s, 1H), 3.31 (s, 6H), 2.93 – 2.87 (m, 2H), 2.33 (s, 2H), 1.08 (s, 6H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, $\text{DMSO}-d_6$): δ 198.2, 156.6, 156.2, 139.0, 119.4, 107.9, 49.9, 40.4, 40.1, 33.3, 27.5.

HRMS (ESI): m/z calc. for $\text{C}_{15}\text{H}_{21}\text{N}_2\text{O}^+$ 245.1648, found 245.1648.

1-(4,4-Dimethyl-3-oxocyclohex-1-en-1-yl)-4-(dimethylamino)pyridin-1-ium chloride (4b)



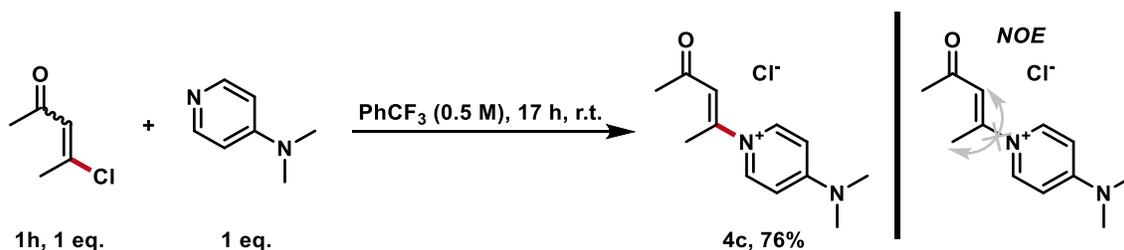
DMAP (139 mg, 1.1 mmol, 1 eq.) was weighed into a screw-cap vial, followed by addition of PhCF₃ (0.5 ml). After DMAP dissolution (*Note: heating may be applied to achieve dissolution*), a solution of vinyl chloride (**1b**, 181 mg, 1.1 mmol, 1 eq.) in PhCF₃ (0.1 ml) was added, the vial was sealed, and the reaction mixture was heated for 4 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, Et₂O (0.6 ml) was added to the reaction mixture. After a few minutes, precipitate was filtered, washed with Et₂O and dried to afford the title product as a light gray powder (323 mg, 92% yield, 91 wt% purity by assay).

¹H NMR (300 MHz, CDCl₃): δ 8.84 (d, *J* = 7.4 Hz, 2H), 7.33 (d, *J* = 7.3 Hz, 2H), 6.24 (s, 1H), 3.40 (s, 6H), 3.19 – 3.09 (m, 2H), 2.06 (t, *J* = 6.0 Hz, 2H), 1.17 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 202.8, 157.3, 156.2, 139.4, 119.6, 109.1, 41.1, 40.7, 35.3, 25.3, 23.9.

HRMS (ESI): *m/z* calc. for C₁₅H₂₁N₂O⁺ 245.1648, found 245.1647.

(E)-4-(Dimethylamino)-1-(4-oxopent-2-en-2-yl)pyridin-1-ium chloride (4c)



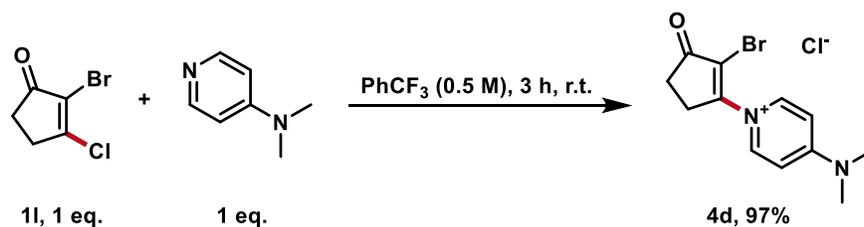
DMAP (1.21 g, 9.9 mmol, 1 eq.) was weighed into a round-bottom flask, followed by addition of PhCF₃ (11.5 ml). After DMAP dissolution, a solution of vinyl chloride (**1h**, 1.18 g, 9.9 mmol, 1 eq.) in PhCF₃ (1 ml) was added (*Note: some amount of dark residue may form immediately after mixing the reagents*) and the reaction mixture was stirred for 17 hours at room temperature (monitored by NMR spectroscopy). Upon completion, Et₂O (12.5 ml) was added to the reaction mixture. After a few minutes, precipitate was filtered, washed with Et₂O and dried to afford the title product as a white powder (2.3 g, 76% yield, 79 wt% purity by assay). *Note: attempts to convert 4,4-dichloropentanone, contained in the starting vinyl chloride, to the target product by increasing DMAP loading did not improve yield. The isolated product contained DMAPHCl as a by-product from HCl elimination from the dichloride. The target product was initially formed and isolated as a mixture of stereoisomers, however, storage at room temperature for several months resulted in complete conversion to a single stereoisomer, as confirmed by NMR spectroscopy.*

¹H NMR (300 MHz, CDCl₃): δ 8.85 – 8.75 (m, 2H), 7.36 – 7.27 (m, 2H), 6.86 (br s, 1H), 3.39 (s, 6H), 2.67 (d, *J* = 1.0 Hz, 3H), 2.41 (s, 3H). *Note: stereochemistry of the product was deduced on the basis of NOESY experiments.*

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 197.2, 156.6, 149.5, 139.6, 122.2, 108.4, 40.5, 32.3, 17.3.

HRMS (ESI): *m/z* calc. for C₁₂H₁₇N₂O⁺ 205.1335, found 205.1337.

1-(2-Bromo-3-oxocyclopent-1-en-1-yl)-4-(dimethylamino)pyridin-1-ium chloride (4d)



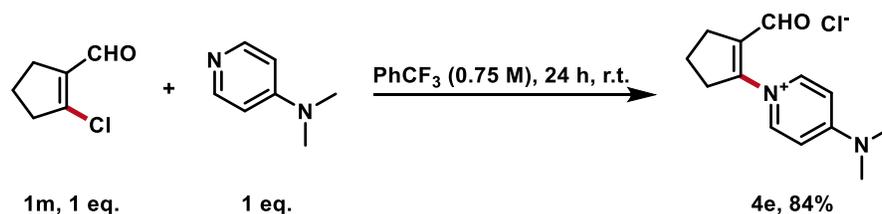
Vinyl chloride (**11**, 102 mg, 0.52 mmol, 1 eq.) and DMAP (64 mg, 0.52 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of PhCF₃ (1 ml). The vial was sealed, and the reaction mixture was stirred for 3 hours at room temperature (monitored by NMR spectroscopy). Upon completion, Et₂O (1 ml) was added to the reaction mixture. After a few minutes, precipitate was filtered, washed with Et₂O and dried to afford the title product as a white powder (179 mg, 97% yield, 90 wt% purity by assay).

¹H NMR (300 MHz, DMSO-*d*₆): δ 8.55 – 8.45 (m, 2H), 7.29 – 7.20 (m, 2H), 3.31 (s, 6H), 3.25 – 3.18 (m, 2H), 2.84 – 2.75 (m, 2H).

¹³C{¹H} NMR (75 MHz, DMSO-*d*₆): δ 199.2, 166.1, 156.6, 139.2, 116.5, 107.8, 40.5, 33.1, 29.3.

HRMS (ESI): *m/z* calc. for C₁₂H₁₄BrN₂O⁺ 281.0284, found 281.0276.

4-(Dimethylamino)-1-(2-formylcyclopent-1-en-1-yl)pyridin-1-ium chloride (**4e**)



DMAP (773 mg, 6.3 mmol, 1 eq.) was weighed into a screw-cap vial, followed by addition of PhCF₃ (7.5 ml). After DMAP dissolution, a solution of vinyl chloride (**1m**, 826 mg, 6.3 mmol, 1 eq.) in PhCF₃ (1 ml) was added and the reaction mixture was stirred for 24 hours at room temperature (monitored by NMR spectroscopy). Upon completion, Et₂O (8.5 ml) was added to the reaction mixture. After a few minutes, precipitate was filtered, washed with Et₂O and dried to afford the title product as a beige powder (1.44 g, 84% yield, 93 wt% purity by assay). *Note: the title compound was found to be poorly degradable upon storage (≈5% drop in purity after 5 months in the fridge).*

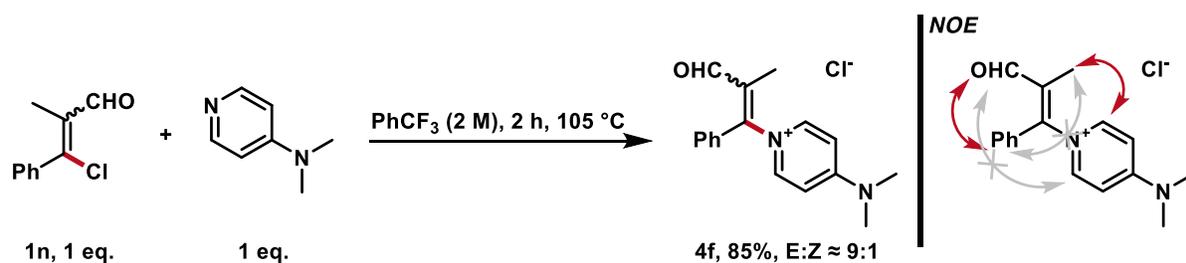
¹H NMR (300 MHz, DMSO-*d*₆): δ 9.63 (s, 1H), 8.60 – 8.50 (m, 2H), 7.19 – 7.10 (m, 2H), 3.29 (s, 6H), 3.12 (tt, *J* = 7.8, 2.4 Hz, 2H), 2.72 – 2.62 (m, 2H), 2.02 (p, *J* = 7.7 Hz, 2H).

¹H NMR (300 MHz, CDCl₃): δ 9.76 (s, 1H), 8.76 – 8.65 (m, 2H), 7.38 – 7.28 (m, 2H), 3.39 (s, 6H), 3.31 – 3.18 (m, 2H), 2.87 – 2.74 (m, 2H), 2.15 (p, *J* = 7.8 Hz, 2H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 185.9, 156.7, 153.3, 141.4, 135.1, 108.5, 40.8, 36.3, 29.5, 19.8.

HRMS (ESI): *m/z* calc. for C₁₃H₁₇N₂O⁺ 217.1335, found 217.1334.

4-(Dimethylamino)-1-(2-methyl-3-oxo-1-phenylprop-1-en-1-yl)pyridin-1-ium chloride (4f)



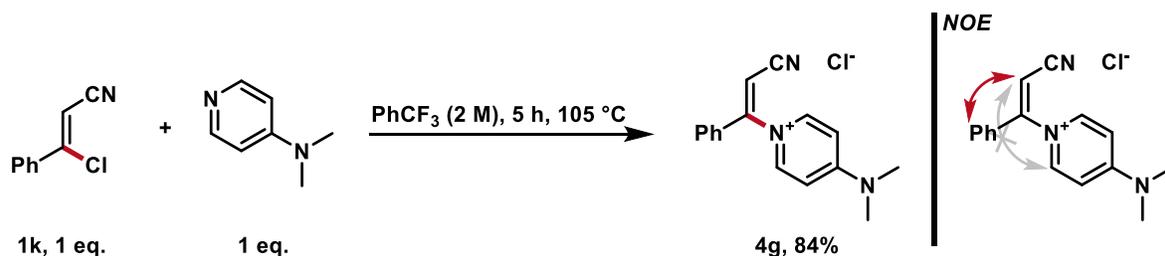
DMAP (482 mg, 3.9 mmol, 1 eq.) was weighed into a screw-cap vial, followed by addition of PhCF_3 (1.5 ml). After DMAP dissolution (*Note: heating may be applied to achieve dissolution*), a solution of vinyl chloride (**1n**, 712 mg, 3.9 mmol, 1 eq.) in PhCF_3 (0.5 ml) was added, the vial was sealed, and the reaction mixture was heated for 2 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, Et_2O (2 ml) was added to the reaction mixture. After a few minutes, precipitate was filtered, washed with Et_2O and dried to afford the title product as a white powder (1.06 g, 85% yield, E:Z \approx 9:1, 95 wt% purity by assay).

^1H NMR (300 MHz, CDCl_3): δ 9.53 (s, 1H), 8.31 – 8.21 (m, 2H), 7.62 – 7.43 (m, 5H), 7.34 – 7.24 (m, 2H), 3.42 (s, 6H), 1.97 (s, 3H). *Note: stereochemistry of the product was deduced on the basis of NOESY experiments.*

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 191.3, 156.8, 153.9, 141.7, 134.1, 132.0, 131.3, 130.9, 129.3, 108.9, 41.0, 12.8.

HRMS (ESI): m/z calc. for $\text{C}_{17}\text{H}_{19}\text{N}_2\text{O}^+$ 267.1492, found 267.1489.

(Z)-1-(2-Cyano-1-phenylvinyl)-4-(dimethylamino)pyridin-1-ium chloride (4g)



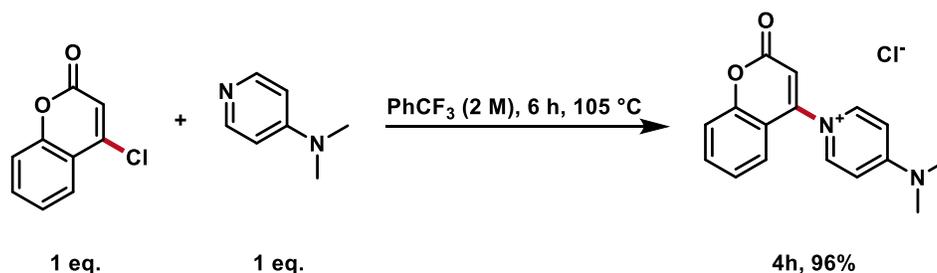
DMAP (187 mg, 1.5 mmol, 1 eq.) was weighed into a screw-cap vial, followed by addition of PhCF₃ (0.5 ml). After DMAP dissolution (*Note: heating may be applied to achieve dissolution*), a solution of vinyl chloride (**1k**, 250 mg, 1.5 mmol, 1 eq.) in PhCF₃ (0.25 ml) was added, the vial was sealed, and the reaction mixture was heated for 5 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, Et₂O (0.75 ml) was added to the reaction mixture. After a few minutes, precipitate was filtered, washed with Et₂O and dried to afford the title product as a white powder (389 mg, 84% yield, 94 wt% purity by assay).

¹H NMR (300 MHz, DMSO-*d*₆): δ 8.51 – 8.40 (m, 2H), 7.71 – 7.60 (m, 1H), 7.60 – 7.51 (m, 2H), 7.51 – 7.41 (m, 2H), 7.34 – 7.23 (m, 2H), 7.17 (s, 1H), 3.33 (s, 6H).

¹³C{¹H} NMR (75 MHz, DMSO-*d*₆): δ 156.6, 156.0, 141.4, 132.8, 131.8, 129.5, 127.4, 115.0, 108.2, 97.0, 40.4.

HRMS (ESI): m/z calc. for C₁₆H₁₆N₃⁺ 250.1339, found 250.1340.

4-(Dimethylamino)-1-(2-oxo-chromen-4-yl)pyridin-1-ium chloride (4h)



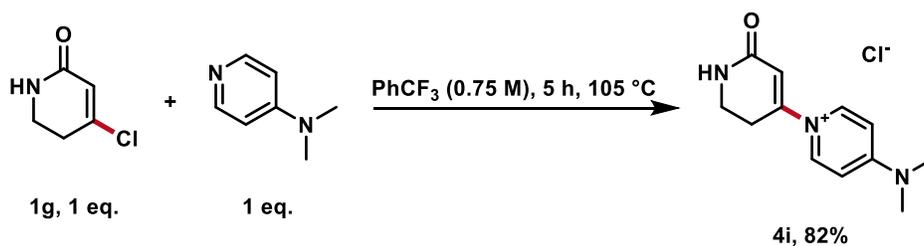
DMAP (108 mg, 0.9 mmol, 1 eq.) was weighed into a screw-cap vial, followed by addition of PhCF₃ (0.4 ml). After DMAP dissolution (*Note: heating may be applied to achieve dissolution*), a solution of 4-chloro-chromen-2-one (159 mg, 0.9 mmol, 1 eq.) in PhCF₃ (0.05 ml) was added, the vial was sealed and the reaction mixture was heated for 6 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, Et₂O (0.45 ml) was added to the reaction mixture. After a few minutes, precipitate was filtered, washed with Et₂O and dried to afford the title product as a white powder (260 mg, 96% yield, 99 wt% purity by assay).

¹H NMR (300 MHz, DMSO-*d*₆): δ 8.51 (d, *J* = 7.4 Hz, 2H), 7.80 (t, *J* = 8.1 Hz, 1H), 7.63 (d, *J* = 8.3 Hz, 1H), 7.44 (t, *J* = 7.7 Hz, 1H), 7.33 (d, *J* = 7.4 Hz, 2H), 7.28 (d, *J* = 7.9 Hz, 1H), 7.13 (s, 1H), 3.34 (s, 6H).

¹³C{¹H} NMR (75 MHz, DMSO-*d*₆): δ 159.4, 156.7, 153.3, 151.3, 141.2, 133.8, 125.3, 123.7, 117.2, 115.8, 114.6, 107.9, 40.3.

HRMS (ESI): *m/z* calc. for C₁₆H₁₅N₂O₂⁺ 267.1128, found 267.1139.

4-(Dimethylamino)-6'-oxo-1',2',3',6'-tetrahydro-[1,4'-bipyridin]-1-ium chloride (**4i**)



DMAP (35 mg, 0.3 mmol, 1 eq.) was weighed into a screw-cap vial, followed by addition of PhCF₃ (0.3 ml). After DMAP dissolution, a solution of vinyl chloride (**1g**, 38 mg, 0.3 mmol, 1 eq.) in PhCF₃ (0.1 ml) was added, the vial was sealed and the reaction mixture was heated for 5 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Upon completion, Et₂O (0.4 ml) was added to the reaction mixture. After a few minutes, precipitate was filtered, washed with Et₂O and dried to afford the title product as a white powder (63 mg, 82% yield, 95 wt% purity by assay).

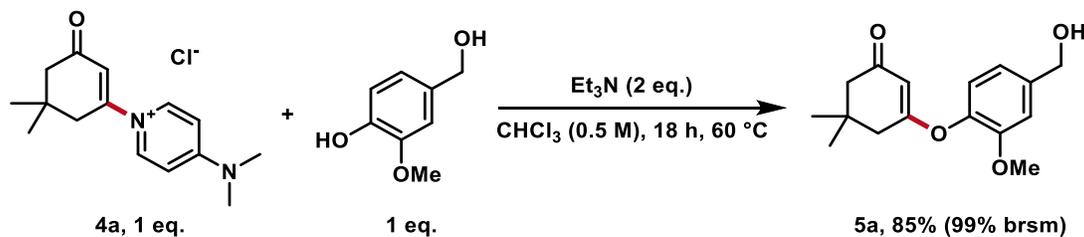
¹H NMR (500 MHz, DMSO-*d*₆): δ 8.52 – 8.46 (m, 2H), 7.81 (br s, 1H), 7.15 – 7.08 (m, 2H), 6.21 (m, 1H), 3.43 (td, *J* = 7.1, 2.7 Hz, 2H), 3.28 (s, 6H), 2.88 (td, *J* = 7.0, 1.3 Hz, 2H).

¹³C{¹H} NMR (126 MHz, DMSO-*d*₆): δ 164.5, 156.5, 150.4, 138.9, 115.7, 107.7, 40.3, 38.0, 25.6.

HRMS (ESI): *m/z* calc. for C₁₂H₁₆N₃O⁺ 218.1288, found 218.1296.

8. Procedures for stoichiometric nucleophilic vinylic substitution reactions

3-(4-(Hydroxymethyl)-2-methoxyphenoxy)-5,5-dimethylcyclohex-2-en-1-one (5a)



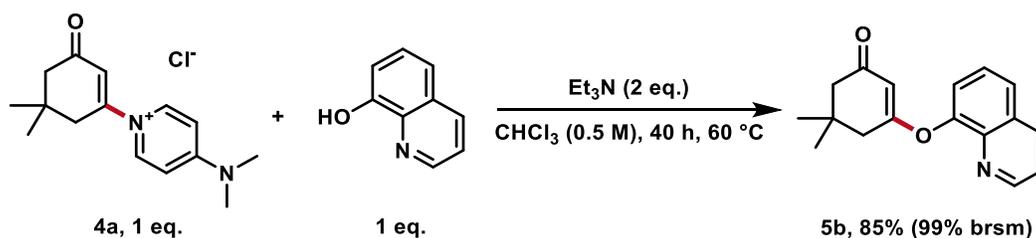
Pyridinium salt (**4a**, 141 mg, 0.5 mmol, 1 eq.) and vanilyl alcohol (77 mg, 0.5 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl_3 (1 ml) and Et_3N (0.14 ml, 1 mmol, 2 eq.). The vial was sealed, and the reaction mixture was heated for 18 hours in an oil bath at 60 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with acetone. The solvent was removed on the rotary evaporator and the residue was purified by flash column chromatography ($\text{Et}_2\text{O}:\text{EA} = 3:1$) to afford the title product as a light gray solid (118 mg, 85%), along with recovered phenol (8 mg, 10%).

$^1\text{H NMR}$ (300 MHz, CDCl_3): δ 7.05 – 6.95 (m, 2H), 6.91 (dd, $J = 8.1, 1.8$ Hz, 1H), 5.04 (s, 1H), 4.68 (d, $J = 5.0$ Hz, 2H), 3.81 (s, 3H), 2.53 (s, 2H), 2.23 (s, 2H), 1.87 (t, $J = 5.6$ Hz, 1H), 1.14 (s, 6H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 200.0, 177.0, 150.9, 140.6, 140.5, 122.4, 119.1, 111.3, 104.2, 64.5, 55.8, 50.7, 42.0, 32.9, 28.3.

HRMS (ESI): m/z calc. for $[\text{C}_{16}\text{H}_{20}\text{O}_4+\text{H}^+]$ 277.1434, found 277.1434.

5,5-Dimethyl-3-(quinolin-8-yloxy)cyclohex-2-en-1-one (5b)



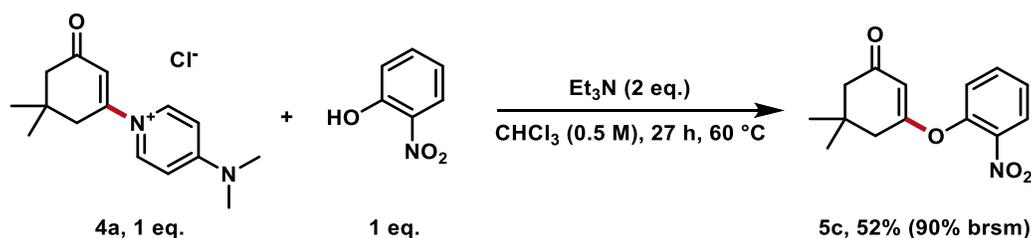
Pyridinium salt (**4a**, 141 mg, 0.5 mmol, 1 eq.) and 8-hydroxyquinoline (73 mg, 0.5 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl₃ (1 ml) and Et₃N (0.14 ml, 1 mmol, 2 eq.). The vial was sealed, and the reaction mixture was heated for 40 hours in an oil bath at 60 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (EA:hexane = 5:2) to afford the title product as a light-yellow oil (114 mg, 85%), along with recovered phenol (10 mg, 14%).

¹H NMR (300 MHz, CDCl₃): 8.89 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.19 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.73 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.53 (t, *J* = 7.9 Hz, 1H), 7.48 – 7.38 (m, 2H), 4.89 (t, *J* = 0.9 Hz, 1H), 2.76 (br s, 2H), 2.25 (s, 2H), 1.20 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 199.5, 177.6, 150.7, 149.0, 140.8, 136.0, 129.8, 126.3, 126.1, 121.9, 121.4, 105.4, 50.7, 42.0, 32.9, 28.3.

HRMS (ESI): *m/z* calc. for [C₁₇H₁₇NO₂+H⁺] 268.1332, found 268.1334.

5,5-Dimethyl-3-(2-nitrophenoxy)cyclohex-2-en-1-one (5c)



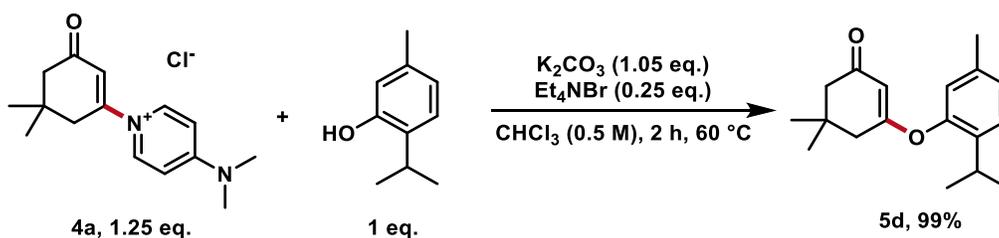
Pyridinium salt (**4a**, 141 mg, 0.5 mmol, 1 eq.) and 2-nitrophenol (70 mg, 0.5 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl₃ (1 ml) and Et₃N (0.14 ml, 1 mmol, 2 eq.). The vial was sealed, and the reaction mixture was heated for 27 hours in an oil bath at 60°C (monitored by NMR spectroscopy). Then, the reaction mixture was excessively washed through a plug of silica gel with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (hexane:EA = 3:2) to afford the title product as a light orange oil (68 mg, 52%), along with recovered phenol (26 mg, 38%).

¹H NMR (300 MHz, CDCl₃): δ 8.10 (dd, *J* = 8.2, 1.6 Hz, 1H), 7.74 – 7.62 (m, 1H), 7.43 (ddd, *J* = 8.7, 7.5, 1.4 Hz, 1H), 7.24 (dd, *J* = 8.1, 1.3 Hz, 1H), 5.03 (d, *J* = 0.9 Hz, 1H), 2.60 (d, *J* = 1.0 Hz, 2H), 2.26 (s, 2H), 1.17 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 199.0, 176.1, 146.0, 141.7, 135.1, 127.0, 126.4, 125.1, 105.0, 50.7, 42.0, 32.9, 28.3.

HRMS (ESI): *m/z* calc. for [C₁₄H₁₅NO₄+H⁺] 262.1074, found 262.1080.

3-(2-Isopropyl-5-methylphenoxy)-5,5-dimethylcyclohex-2-en-1-one (5d)



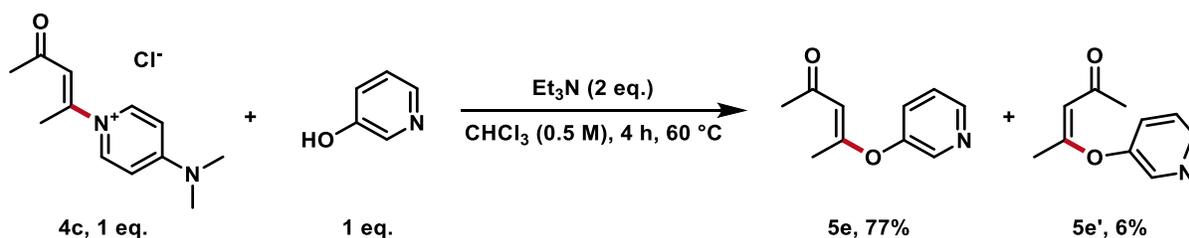
Pyridinium salt (**4a**, 117 mg, 0.42 mmol, 1.25 eq.), thymol (50 mg, 0.33 mmol, 1 eq.), freshly powdered K_2CO_3 (48 mg, 0.35 mmol, 1.05 eq.) and Et_4NBr (18 mg, 0.08 mmol, 0.25 eq.) were weighed into a screw-cap vial, followed by addition of $CHCl_3$ (0.66 ml). The vial was sealed, and the reaction mixture was heated for 2 hours in an oil bath at 60 °C (monitored by NMR spectroscopy). Then, the reaction mixture was excessively washed through a plug of silica gel with EA. The solvent was removed on the rotary evaporator, and the residue was again passed through a plug of silica gel (hexane:Et₂O = 3:2) to afford the title product as a colorless oil (90 mg, 99%).

¹H NMR (300 MHz, CDCl₃): δ 7.19 (d, $J = 7.9$ Hz, 1H), 7.01 (dd, $J = 8.0, 1.8$ Hz, 1H), 6.72 (d, $J = 1.6$, 1H), 5.06 (t, $J = 0.9$ Hz, 1H), 2.92 (hept, $J = 6.9$ Hz, 1H), 2.53 (br s, 2H), 2.29 (s, 3H), 2.24 (s, 2H), 1.17 (d, $J = 6.9$ Hz, 6H), 1.14 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 199.3, 176.9, 149.8, 137.1, 137.1, 127.3, 127.1, 122.1, 104.5, 50.7, 42.4, 32.8, 28.3, 26.9, 23.2, 20.8.

HRMS (ESI): m/z calc. for $[C_{18}H_{24}O_2+H^+]$ 273.1849, found 273.1840.

(E)-4-(Pyridin-3-yloxy)pent-3-en-2-one (5e)



Pyridinium salt (**4c**, 120 mg, 0.5 mmol, 1 eq.) and 3-hydroxypyridine (48 mg, 0.5 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl_3 (1 ml) and Et_3N (0.14 ml, 1 mmol, 2 eq.). The vial was sealed, and the reaction mixture was heated for 4 hours in an oil bath at 60 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with acetone. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:acetone = 2:1) to afford the *E*-isomer **5e** as a light red oil (68 mg, 77%) and the *Z*-isomer **5e'** as a bright-red oil (5 mg, 6%).

Spectral data for **5e**:

^1H NMR (300 MHz, CDCl_3): δ 8.53 (dd, $J = 3.6, 2.6$ Hz, 1H), 8.40 (dd, $J = 2.1, 1.3$ Hz, 1H), 7.44 – 7.32 (m, 2H), 5.27 (br s, 1H), 2.49 (d, $J = 0.6$ Hz, 3H), 2.05 (s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 197.0, 171.4, 149.9, 147.0, 143.8, 129.1, 124.4, 104.7, 32.0, 18.8.

HRMS (ESI): m/z calc. for $[\text{C}_{10}\text{H}_{11}\text{NO}_2 + \text{H}^+]$ 178.0863, found 178.0864.

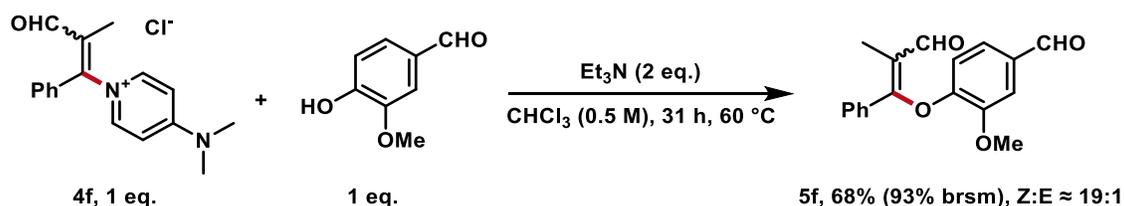
Spectral data for **5e'**:

^1H NMR (300 MHz, CDCl_3): δ 8.49 – 8.39 (m, 2H), 7.41 – 7.30 (m, 2H), 5.59 (s, 1H), 2.36 (s, 3H), 1.93 (br s, 3H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 197.2, 161.5, 151.0, 146.0, 141.8, 126.6, 124.4, 115.7, 31.2, 20.0.

HRMS (ESI): m/z calc. for $[\text{C}_{10}\text{H}_{11}\text{NO}_2 + \text{H}^+]$ 178.0863, found 178.0866.

3-Methoxy-4-((2-methyl-3-oxo-1-phenylprop-1-en-1-yl)oxy)benzaldehyde (5f)



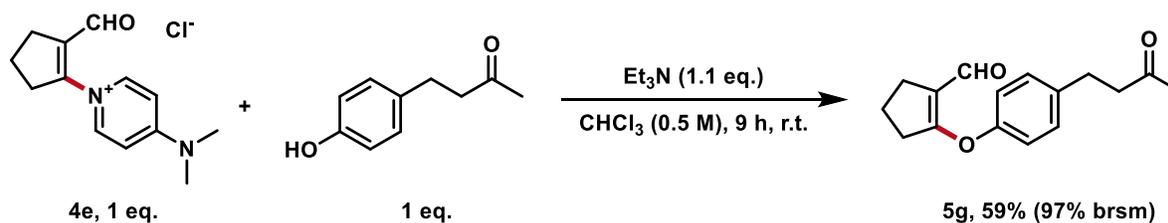
Pyridinium salt (**4f**, 151 mg, 0.5 mmol, 1 eq.) and vanillin (76 mg, 0.5 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl_3 (0.5 ml) and Et_3N (0.14 ml, 1 mmol, 2 eq.). The vial was sealed, and the reaction mixture was heated for 31 hours in an oil bath at $60 \text{ }^\circ\text{C}$ (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (CHCl_3 :EA = 5:1) to afford the title product as a light-yellow solid (101 mg, 68%, Z:E \approx 19:1), along with recovered phenol (19 mg, 25%). *Note: despite R_f of the title compound of approx. 0.7, only the given eluent provides clean separation from the starting material ($R_f \approx 0.4$).*

^1H NMR (300 MHz, CDCl_3): δ 10.31 (s, 1H, E), 9.79 (s, 1H), 9.55 (s, 1H, Z), 7.54 – 7.23 (m, 7H), 6.99 (m, 1H), 3.97 (s, 3H, E), 3.89 (s, 3H, Z), 2.01 (s, 3H, Z), 1.94 (s, 3H, E). *Note: stereochemistry of the product was deduced on the basis of NOESY experiments and on the basis of ^1H NMR spectral data for similar β -aryloxy- α,β -unsaturated aldehydes.^[20]*

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 193.3, 190.7, 169.6, 151.0, 150.6, 149.3, 133.2, 131.0, 130.7, 130.6, 129.2, 128.5, 128.2, 125.0, 123.8, 120.4, 118.5, 110.7, 55.9, 11.2, 9.1. *Note: some signals from individual isomers overlap.*

HRMS (ESI): m/z calc. for $[\text{C}_{18}\text{H}_{16}\text{O}_4+\text{H}^+]$ 297.1121, found 297.1117.

2-(4-(3-Oxobutyl)phenoxy)cyclopent-1-ene-1-carbaldehyde (5g)



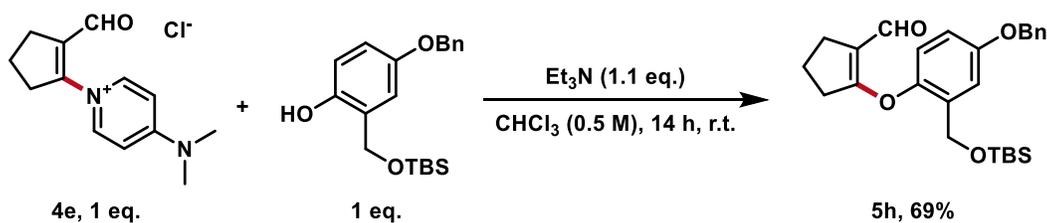
Pyridinium salt (**4e**, 126 mg, 0.5 mmol, 1 eq.) and raspberry ketone (82 mg, 0.5 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl_3 (1 ml) and Et_3N (0.08 ml, 0.55 mmol, 1.1 eq.). The vial was sealed, and the reaction mixture was stirred for 9 hours at room temperature (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with acetone. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (CHCl_3 :EA = 15:1) to afford the title product as a colorless oil (76 mg, 59%), along with recovered phenol (31 mg, 38%). *Note: title compound is relatively unstable and not suited for long-term storage upon isolation.*

^1H NMR (300 MHz, CDCl_3): δ 9.98 (s, 1H), 7.24 – 7.13 (m, 2H), 7.04 – 6.93 (m, 2H), 2.95 – 2.83 (m, 2H), 2.82 – 2.70 (m, 2H), 2.64 – 2.52 (m, 2H), 2.52 – 2.40 (m, 2H), 2.15 (s, 3H), 1.98 – 1.82 (m, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 207.7, 186.8, 173.4, 153.4, 138.4, 129.7, 120.7, 120.1, 45.0, 32.3, 30.1, 28.9, 26.1, 19.6.

HRMS (ESI): m/z calc. for $[\text{C}_{16}\text{H}_{18}\text{O}_3+\text{H}^+]$ 259.1329, found 259.1333.

2-(4-(Benzyloxy)-2-(((tert-butyldimethylsilyl)oxy)methyl)phenoxy)cyclopent-1-ene-1-carbaldehyde (5h)



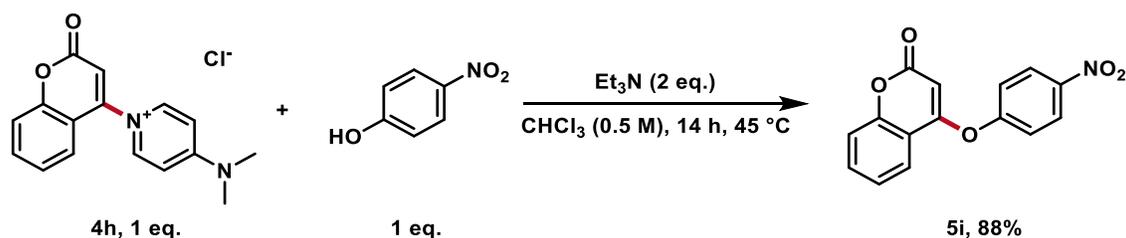
Pyridinium salt (**4e**, 126 mg, 0.5 mmol, 1 eq.) and 4-(benzyloxy)-2-(((tert-butyldimethylsilyl)oxy)methyl)phenol (172 mg, 0.5 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl₃ (1 ml) and Et₃N (0.08 ml, 0.55 mmol, 1.1 eq.). The vial was sealed, and the reaction mixture was stirred for 14 hours at room temperature (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:Et₂O = 2:1) to afford the title product as a white solid (151 mg, 69%). *Note: title compound is relatively unstable and not suited for long-term storage upon isolation.*

¹H NMR (300 MHz, CDCl₃): δ 9.99 (s, 1H), 7.46 – 7.27 (m, 5H), 7.14 (d, *J* = 2.9 Hz, 1H), 6.95 – 6.76 (m, 2H), 5.05 (s, 2H), 4.70 (s, 2H), 2.63 – 2.51 (m, 2H), 2.47 – 2.35 (m, 2H), 1.86 (p, *J* = 7.7 Hz, 2H), 0.93 (s, 9H), 0.09 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 186.4, 173.8, 156.6, 145.8, 136.8, 134.3, 128.6, 128.1, 127.5, 121.1, 119.6, 114.3, 114.2, 70.4, 60.0, 32.5, 26.3, 25.9, 19.4, 18.4, -5.3.

HRMS (ESI): *m/z* calc. for [C₂₆H₃₄O₄Si+H⁺] 439.2299, found 439.2290.

4-(4-Nitrophenoxy)-chromen-2-one (5i)



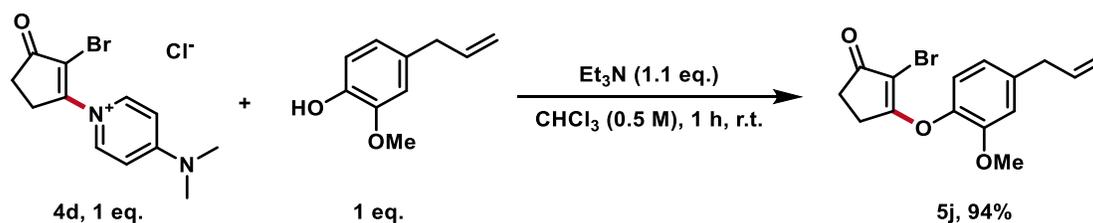
Pyridinium salt (**4h**, 76 mg, 0.25 mmol, 1 eq.) and 4-nitrophenol (35 mg, 0.25 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl₃ (0.5 ml) and Et₃N (0.07 ml, 0.5 mmol, 2 eq.). The vial was sealed, and the reaction mixture was heated for 14 hours in an oil bath at 45 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 1:1) to afford the title product as a white solid (62 mg, 88%).

¹H NMR (300 MHz, CDCl₃): δ 8.39 (d, *J* = 8.6 Hz, 2H), 7.99 (d, *J* = 7.9 Hz, 1H), 7.66 (t, *J* = 7.8 Hz, 1H), 7.46 – 7.34 (m, 4H), 5.47 (s, 1H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 165.1, 161.8, 157.3, 153.7, 145.9, 133.4, 126.3, 124.5, 123.0, 122.2, 117.0, 114.9, 94.8.

HRMS (ESI): *m/z* calc. for [C₁₅H₉NO₅+H⁺] 284.0553, found 284.0560.

3-(4-Allyl-2-methoxyphenoxy)-2-bromocyclopent-2-en-1-one (5j)



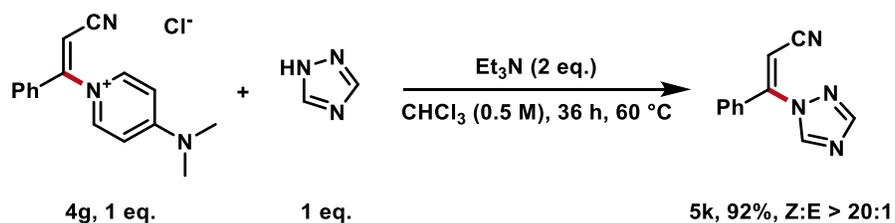
Pyridinium salt (**4d**, 63 mg, 0.2 mmol, 1 eq.) was weighed into a screw-cap vial, followed by addition of CHCl₃ (0.5 ml), eugenol (0.03 ml, 0.2 mmol, 1 eq.) and Et₃N (0.03 ml, 0.22 mmol, 1.1 eq.). The vial was sealed, and the reaction mixture was stirred for 1 hour at room temperature (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 1:1) to afford the title product as a white solid (61 mg, 94%).

¹H NMR (300 MHz, CDCl₃): δ 7.08 (d, *J* = 8.0 Hz, 1H), 6.86 – 6.75 (m, 2H), 6.06 – 5.87 (m, 1H), 5.16 – 5.12 (m, 1H), 5.12 – 5.07 (m, 1H), 3.85 (s, 3H), 3.44 – 3.37 (m, 2H), 2.61 – 2.52 (m, 2H), 2.52 – 2.44 (m, 2H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 198.2, 184.1, 150.7, 140.3, 140.2, 136.7, 122.1, 121.1, 116.6, 113.2, 99.9, 56.1, 40.0, 32.8, 26.5.

HRMS (ESI): *m/z* calc. for [C₁₅H₁₅BrO₃+H⁺] 323.0277, found 323.0277.

(Z)-3-Phenyl-3-(1,2,4-triazol-1-yl)acrylonitrile (5k)



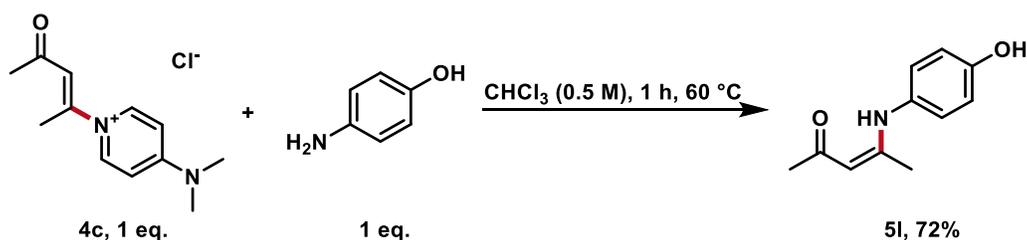
Pyridinium salt (**4g**, 94 mg, 0.33 mmol, 1 eq.) and 1,2,4-triazole (23 mg, 0.33 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl_3 (0.66 ml) and Et_3N (0.09 ml, 0.66 mmol, 2 eq.). The vial was sealed, and the reaction mixture was heated for 36 hours in an oil bath at 60 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (EA:PE = 2:1) to afford the title product as a light orange oil (59 mg, 92%, Z:E > 20:1).

^1H NMR (300 MHz, CDCl_3): δ 8.41 (s, 1H), 8.20 (s, 1H), 7.65 – 7.54 (m, 1H), 7.54 – 7.44 (m, 2H), 7.42 – 7.32 (m, 2H), 5.62 (s, 1H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 153.2, 151.3, 145.1, 132.5, 132.4, 129.4, 128.3, 114.9, 89.5.

HRMS (ESI): m/z calc. for $[\text{C}_{11}\text{H}_8\text{N}_4+\text{H}^+]$ 197.0822, found 197.0828.

(Z)-4-((4-Hydroxyphenyl)amino)pent-3-en-2-one (5I)



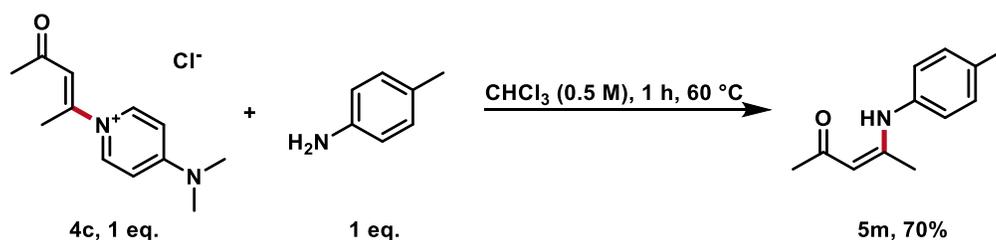
Pyridinium salt (**4c**, 96 mg, 0.4 mmol, 1 eq.) and 4-aminophenol (44 mg, 0.4 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl₃ (0.8 ml). The vial was sealed, and the reaction mixture was heated for 1 hour in an oil bath at 60 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (hexane:EA = 1:1) to afford the title product as a bright-yellow solid (41 mg, 72%). *Note: addition of Et₃N to the reaction resulted in slightly poorer chemoselectivity (N vs. O), although with a higher yield of the target product (93%).*

¹H NMR (300 MHz, CDCl₃): δ 12.24 (s, 1H), 8.90 (br s, 1H), 6.95 – 6.82 (m, 4H), 5.17 (s, 1H), 2.11 (s, 3H), 1.92 (s, 3H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 195.7, 163.5, 155.8, 130.0, 126.9, 116.2, 96.8, 28.6, 19.8.

HRMS (ESI): m/z calc. for [C₁₁H₁₃NO₂+H⁺] 192.1019, found 192.1025.

(Z)-4-(p-Tolylamino)pent-3-en-2-one (5m)



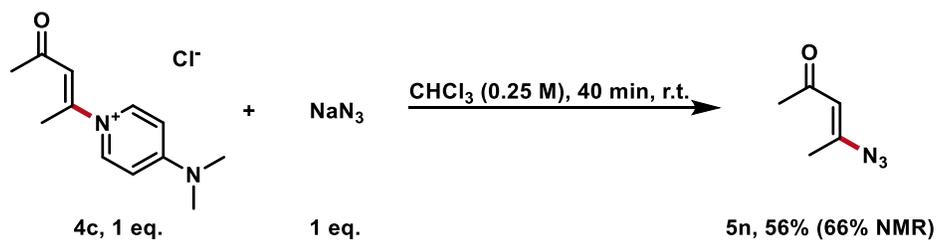
Pyridinium salt (**4c**, 72 mg, 0.3 mmol, 1 eq.) and 4-methylaniline (32 mg, 0.3 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl₃ (0.6 ml). The vial was sealed, and the reaction mixture was heated for 1 hour in an oil bath at 60 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (hexane:EA = 4:1) to afford the title product as a bright-yellow solid (40 mg, 70%).

¹H NMR (300 MHz, CDCl₃): δ 12.40 (s, 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 6.99 (d, *J* = 8.3 Hz, 2H), 5.16 (s, 1H), 2.33 (s, 3H), 2.09 (s, 3H), 1.95 (s, 3H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 197.0, 160.7, 136.2, 135.6, 129.8, 125.0, 97.3, 29.2, 21.0, 19.8.

HRMS (ESI): *m/z* calc. for [C₁₂H₁₅NO+H⁺] 190.1226, found 190.1227.

(E)-4-Azidopent-3-en-2-one (5n)



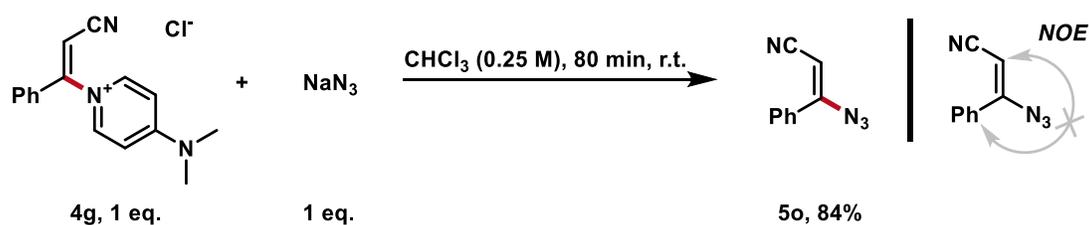
Pyridinium salt (**4c**, 120 mg, 0.5 mmol, 1 eq.) and NaN₃ (33 mg, 0.5 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl₃ (2 ml). The vial was sealed, and the reaction mixture was stirred for 40 minutes at room temperature (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (hexane:Et₂O = 5:1) to afford the title product as a colorless oil (35 mg, 56%). *Note: title compound was found to be volatile; remaining solvent before and after chromatography was evaporated at room temperature under the pressure above 50 mmHg. Title compound is relatively unstable and not suited for long-term storage upon isolation.*

¹H NMR (300 MHz, CDCl₃): δ 5.92 (br s, 1H), 2.32 (br s, 3H), 2.19 (s, 3H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 196.8, 153.9, 112.4, 32.0, 16.7.

HRMS (ESI): m/z calc. for [C₅H₇N₃O+H⁺] 126.0662, found 126.0657.

(E)-3-Azido-3-phenylacrylonitrile (5o)



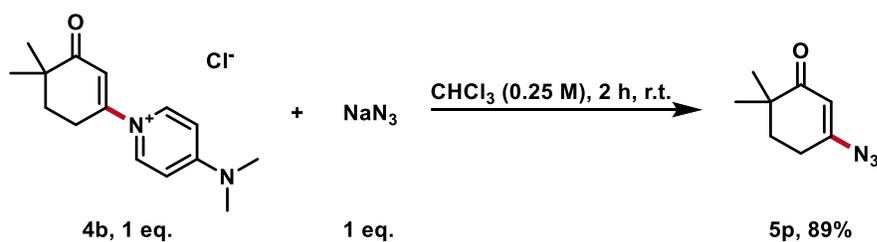
Pyridinium salt (**4g**, 114 mg, 0.4 mmol, 1 eq.) and NaN_3 (26 mg, 0.4 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl_3 (1.6 ml). The vial was sealed, and the reaction mixture was stirred for 80 minutes at room temperature (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 8:1) to afford the title product as an orange solid (57 mg, 84%). *Note: title compound is relatively unstable and not suited for long-term storage upon isolation.*

^1H NMR (300 MHz, CDCl_3): δ 7.57 – 7.43 (m, 5H), 5.05 (s, 1H). *Note: the structure of the product was deduced on the basis of NOESY experiments.*

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 157.1, 132.0, 131.7, 129.3, 126.8, 115.2, 83.8.

HRMS (ESI): m/z calc. for $[\text{C}_9\text{H}_6\text{N}_4+\text{Na}^+]$ 193.0485, found 193.0484.

3-Azido-6,6-dimethylcyclohex-2-en-1-one (5p)



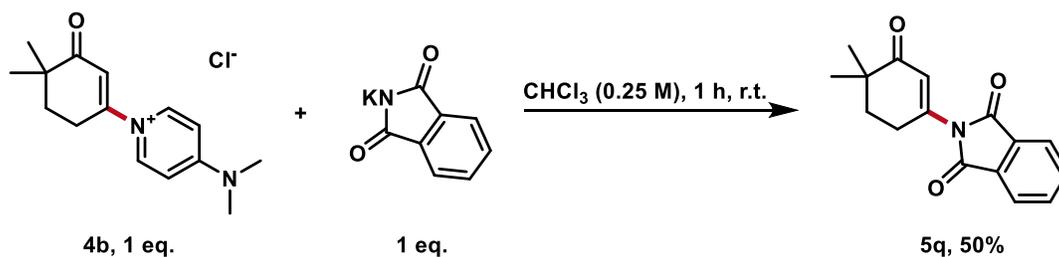
Pyridinium salt (**4b**, 84 mg, 0.3 mmol, 1 eq.) and NaN_3 (20 mg, 0.3 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl_3 (1.2 ml). The vial was sealed, and the reaction mixture was stirred for 2 hours at room temperature (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 5:1) to afford the title product as a bright-yellow oil (44 mg, 89%).

^1H NMR (300 MHz, CDCl_3): δ 5.67 (t, J = 1.2 Hz, 1H), 2.42 (td, J = 6.2, 1.2 Hz, 2H), 1.87 (t, J = 6.2 Hz, 2H), 1.12 (s, 6H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 202.6, 159.1, 113.0, 40.4, 35.2, 24.9, 24.2.

HRMS (ESI): m/z calc. for $[\text{C}_8\text{H}_{11}\text{N}_3\text{O}+\text{Na}^+]$ 188.0794, found 188.0793.

2-(4,4-Dimethyl-3-oxocyclohex-1-en-1-yl)isoindoline-1,3-dione (5q)



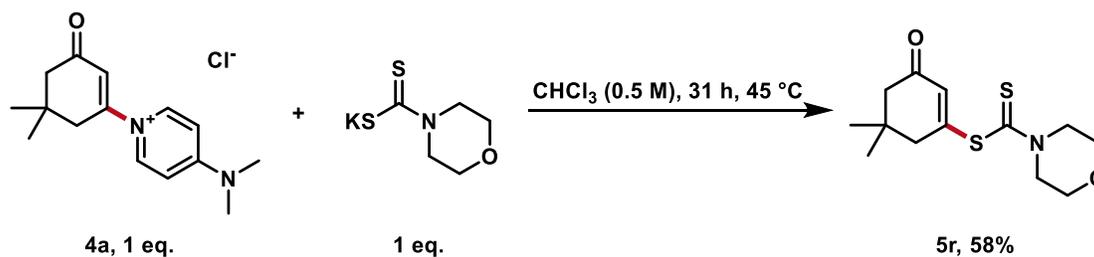
Pyridinium salt (**4b**, 56 mg, 0.2 mmol, 1 eq.) and potassium phthalimide (37 mg, 0.2 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl₃ (0.8 ml). The vial was sealed, and the reaction mixture was stirred for 1 hour at room temperature (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (CHCl₃:EA = 20:1) to afford the title product as a white solid (27 mg, 50%).

¹H NMR (300 MHz, CDCl₃): δ 7.93 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.80 (dd, *J* = 5.5, 3.1 Hz, 2H), 6.22 (t, *J* = 1.5 Hz, 1H), 2.89 (td, *J* = 6.1, 1.5 Hz, 2H), 1.97 (t, *J* = 6.1 Hz, 2H), 1.20 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 203.7, 166.1, 149.3, 134.9, 131.6, 124.1, 123.4, 40.8, 35.7, 25.3, 24.2.

HRMS (ESI): *m/z* calc. for [C₁₆H₁₅NO₃+H⁺] 270.1125, found 270.1121.

5,5-Dimethyl-3-oxocyclohex-1-en-1-yl morpholine-4-carbodithioate (5r)



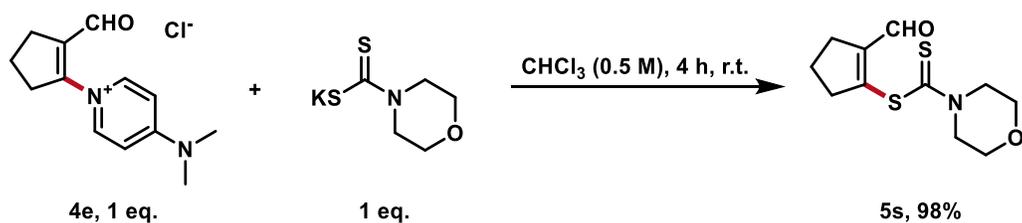
Pyridinium salt (**4a**, 141 mg, 0.5 mmol, 1 eq.) and potassium morpholine dithiocarbamate (101 mg, 0.5 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl₃ (1 ml). The vial was sealed, and the reaction mixture was heated for 31 hours in an oil bath at 45 °C (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with CHCl₃. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 1:1) to afford the title product as a light-yellow solid (83 mg, 58%).

¹H NMR (300 MHz, CDCl₃): δ 6.33 (t, *J* = 1.6 Hz, 1H), 4.51 – 3.87 (m, 4H), 3.79 (t, *J* = 4.9 Hz, 4H), 2.65 (d, *J* = 1.7 Hz, 2H), 2.30 (s, 2H), 1.13 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 198.1, 191.3, 153.2, 135.0, 66.3, 51.4 (Note: signal from NCH₂ carbon is registered as a broad and unresolved “doublet” due to rotational dynamics of dithiocarbamate fragment), 51.2, 45.5, 34.3, 28.2.

HRMS (ESI): *m/z* calc. for [C₁₃H₁₉NO₂S₂+H⁺] 284.0773, found 284.0770.

2-Formylcyclopent-1-en-1-yl morpholine-4-carbodithioate (5s)



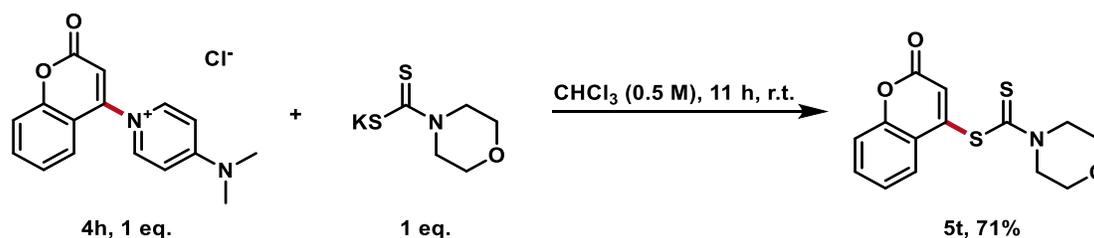
Pyridinium salt (**4e**, 127 mg, 0.5 mmol, 1 eq.) and potassium morpholine dithiocarbamate (101 mg, 0.5 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl_3 (1 ml). The vial was sealed, and the reaction mixture was stirred for 4 hours at room temperature (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 3:2) to afford the title product as a light yellow solid (126 mg, 98%). *Note: title compound darkens upon storage in the fridge for several days, but, according to an ^1H NMR spectrum, no degradation occurs.*

^1H NMR (300 MHz, CDCl_3): δ 9.97 (s, 1H), 4.49 – 3.89 (m, 4H), 3.85 – 3.76 (m, 4H), 2.94 (tt, $J = 7.6, 2.2$ Hz, 2H), 2.71 (tt, $J = 7.6, 2.3$ Hz, 2H), 2.04 (p, $J = 7.6$ Hz, 2H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 192.0, 188.9, 150.7, 150.0, 66.2, 51.2, 40.1, 30.6, 21.9.

HRMS (ESI): m/z calc. for $[\text{C}_{11}\text{H}_{15}\text{NO}_2\text{S}_2+\text{H}^+]$ 258.0617, found 258.0612.

2-Oxo-chromen-4-yl morpholine-4-carbodithioate (5t)



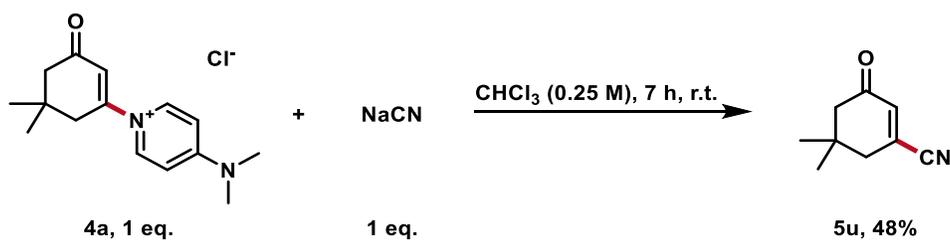
Pyridinium salt (**4h**, 92 mg, 0.3 mmol, 1 eq.) and potassium morpholine dithiocarbamate (61 mg, 0.3 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl₃ (0.6 ml). The vial was sealed, and the reaction mixture was stirred for 11 hours at room temperature (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 3:2) to afford the title product as a bright-yellow solid (66 mg, 71%).

¹H NMR (300 MHz, CDCl₃): δ 7.75 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.54 (ddd, *J* = 8.6, 7.3, 1.6 Hz, 1H), 7.35 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.32 – 7.24 (m, 1H), 6.72 (s, 1H), 4.43 – 3.96 (m, 4H), 3.89 – 3.80 (m, 4H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 190.0, 159.4, 153.4, 147.5, 132.4, 126.6, 124.9, 124.5, 119.5, 117.3, 66.3, 51.6.

HRMS (ESI): *m/z* calc. for [C₁₄H₁₃NO₃S₂+H⁺] 308.0410, found 308.0406.

5,5-Dimethyl-3-oxocyclohex-1-ene-1-carbonitrile (5u)



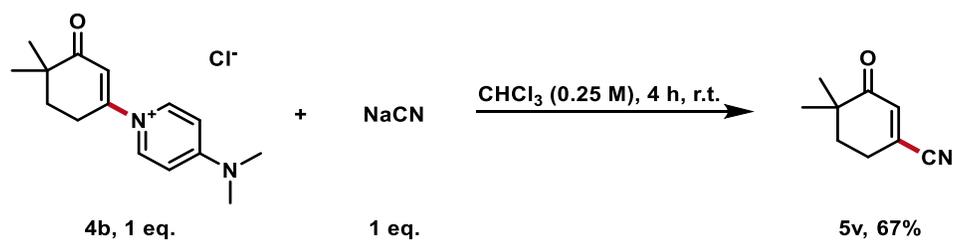
Pyridinium salt (**4a**, 113 mg, 0.4 mmol, 1 eq.) and NaCN (20 mg, 0.4 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl_3 (1.6 ml). The vial was sealed, and the reaction mixture was stirred for 7 hours at room temperature. Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 2:1) to afford the title product as a white solid (29 mg, 48%).

$^1\text{H NMR}$ (300 MHz, CDCl_3): δ 6.54 (t, $J = 2.0$ Hz, 1H), 2.43 (d, $J = 2.0$ Hz, 2H), 2.35 (s, 2H), 1.10 (s, 6H).

$^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3): δ 196.9, 138.0, 129.1, 117.3, 51.1, 41.4, 34.1, 28.0.

HRMS (ESI): m/z calc. for $[\text{C}_9\text{H}_{11}\text{NO}+\text{Na}^+]$ 172.0733, found 172.0737.

4,4-Dimethyl-3-oxocyclohex-1-ene-1-carbonitrile (5v)



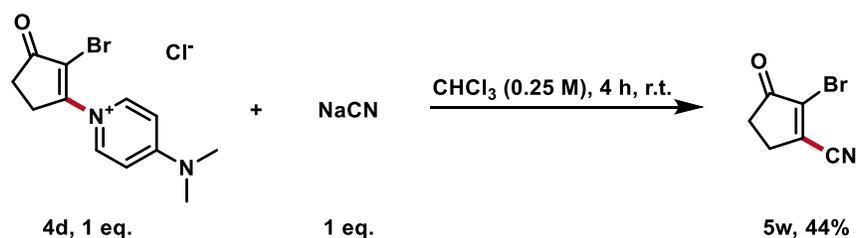
Pyridinium salt (**4b**, 84 mg, 0.3 mmol, 1 eq.) and NaCN (15 mg, 0.3 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl₃ (1.2 ml). The vial was sealed, and the reaction mixture was stirred for 4 hours at room temperature (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 2:1) to afford the title product as a bright-yellow oil (30 mg, 67%).

¹H NMR (300 MHz, CDCl₃): δ 6.43 (t, *J* = 2.0 Hz, 1H), 2.57 (td, *J* = 6.1, 2.0 Hz, 2H), 1.93 (t, *J* = 6.1 Hz, 2H), 1.14 (s, 6H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 201.5, 137.5, 129.4, 117.0, 41.4, 35.4, 25.3, 23.7.

HRMS (ESI): *m/z* calc. for [C₉H₁₁NO+Na⁺] 172.0733, found 172.0735.

2-Bromo-3-oxocyclopent-1-ene-1-carbonitrile (5w)



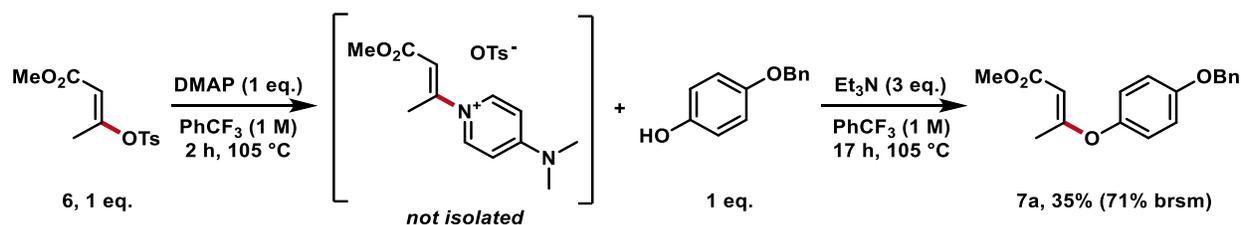
Pyridinium salt (**4d**, 64 mg, 0.2 mmol, 1 eq.) and NaCN (10 mg, 0.2 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of CHCl₃ (0.8 ml). The vial was sealed, and the reaction mixture was stirred for 4 hours at room temperature (monitored by NMR spectroscopy). Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:Et₂O = 3:2) to afford the title product as a bright-yellow oil (16 mg, 44%).

¹H NMR (300 MHz, CDCl₃): δ 2.94 – 2.85 (m, 2H), 2.76 – 2.65 (m, 2H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 198.7, 140.6, 137.9, 114.2, 32.4, 29.5.

MS (EI): m/z calc. for C₆H₄BrNO⁺ 185.0, found 185.0. *Note: no molecular ions were observed under ESI conditions.*

Methyl (E)-3-(4-(benzyloxy)phenoxy)but-2-enoate (7a)



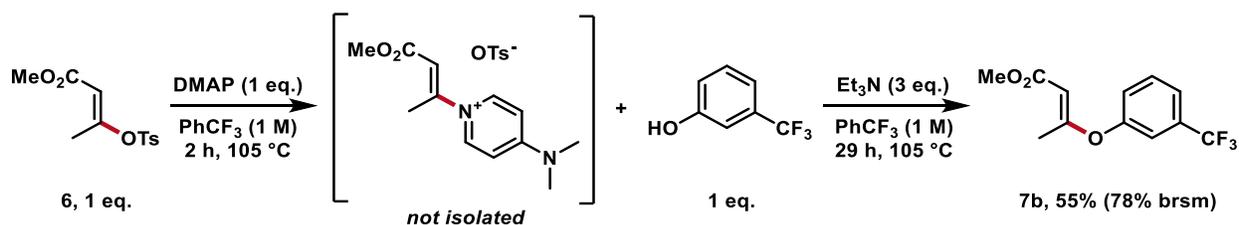
DMAP (37 mg, 0.3 mmol, 1 eq.) was weighed into a screw-cap vial. A solution of vinyltosylate (**6**, 81 mg, 0.3 mmol, 1 eq.) in PhCF₃ (0.3 ml) was added to the vial. The vial was sealed, and the reaction mixture was heated for 2 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Once all the starting material has converted to the pyridinium salt, 4-benzyloxyphenol (60 mg, 0.3 mmol, 1 eq.) and Et₃N (0.08 ml, 0.6 mmol, 2 eq.) were added to the vial, and the reaction mixture was further heated at 105 °C for 17 h. Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 10:1) to afford the title product as a light beige solid (31 mg, 35% yield), along with recovered phenol (21 mg, 36% yield).

¹H NMR (300 MHz, CDCl₃): δ 7.47 – 7.29 (m, 5H), 7.01 – 6.86 (m, 4H), 5.04 (s, 2H), 4.86 (s, 1H), 3.61 (s, 3H), 2.47 (s, 3H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 173.6, 168.2, 156.6, 147.0, 136.9, 128.8, 128.2, 127.6, 122.5, 116.1, 95.4, 70.6, 50.9, 18.6.

HRMS (ESI): m/z calc. for [C₁₂H₁₁F₃O₃+H⁺] 261.0733, found 261.0731.

Methyl (E)-3-(3-(trifluoromethyl)phenoxy)but-2-enoate (7b)



DMAP (37 mg, 0.3 mmol, 1 eq.) was weighed into a screw-cap vial. A solution of vinyltosylate (**6**, 81 mg, 0.3 mmol, 1 eq.) in 0.3 ml PhCF₃ was added to the vial. The vial was sealed, and the reaction mixture was heated for 2 hours in an oil bath at 105 °C (monitored by NMR spectroscopy). Once all the starting material has converted to the pyridinium salt, 3-trifluoromethylphenol (48.6 mg, 0.3 mmol, 1 eq.) and Et₃N (0.08 ml, 0.6 mmol, 2 eq.) were added to the vial, and the reaction mixture was further heated at 105 °C for 29 h. Upon completion, the crude mixture was passed through a silica gel plug, eluting with EA. The solvent was removed on the rotary evaporator, and the residue was purified by flash column chromatography (PE:EA = 15:1) to afford the title product as a light beige solid (43 mg, 55% yield), along with recovered phenol (11 mg, 23% yield).

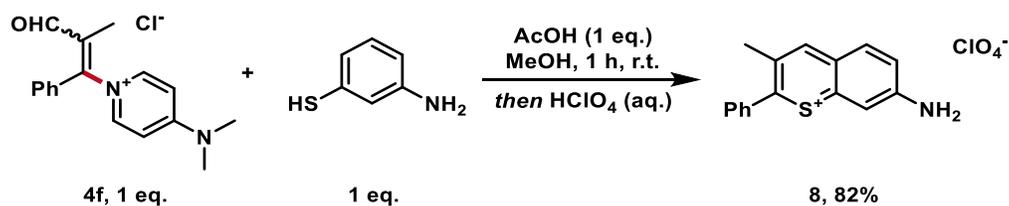
¹H NMR (300 MHz, CDCl₃): δ 7.58 – 7.45 (m, 2H), 7.32 – 7.28 (m, 1H), 7.27 – 7.17 (m, 1H), 4.87 (s, 1H), 3.64 (s, 3H), 2.50 (s, 3H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 172.3, 167.7, 153.7, 132.8 (q, *J* = 33.0 Hz), 130.8, 125.2 (q, *J* = 1.3 Hz), 123.6 (q, *J* = 272.4 Hz), 122.6 (q, *J* = 3.8 Hz), 118.9 (q, *J* = 3.8 Hz), 97.1, 51.1, 18.4.

¹⁹F NMR (282 MHz, CDCl₃): δ -63.58 (s, 3F).

HRMS (ESI): *m/z* calc. for [C₁₂H₁₁F₃O₃+H⁺] 261.0733, found 261.0731.

7-Amino-3-methyl-2-phenylthiochromenylium perchlorate (8)



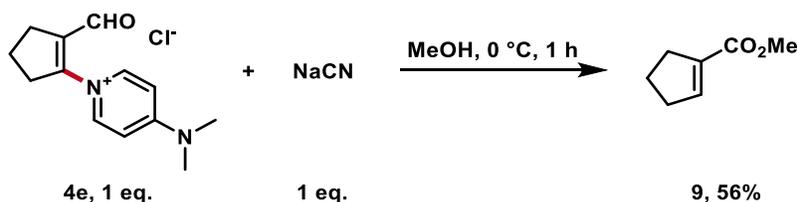
Pyridinium salt (**4f**, 48 mg, 0.16 mmol, 1 eq.) was weighed into a screw-cap vial, followed by addition of MeOH (0.9 ml), 3-aminothiophenol (17 μ l, 0.16 mmol, 1 eq.) and AcOH (9 μ l, 0.16 mmol, 1 eq.). The vial was sealed, and the reaction mixture was stirred for 1 hour at room temperature (monitored by NMR spectroscopy). Upon completion, aqueous HClO₄ (10%, 3.5 ml) was added to the reaction mixture. After a few minutes, precipitate was filtered, washed with water and dried to afford the title product as a dark red solid (46 mg, 82%). *Note: attempts to purify the product by column chromatography resulted in its decomposition.*

¹H NMR (300 MHz, DMSO-*d*₆): 8.76 (s, 1H), 8.49 (br s, 2H), 8.22 (d, *J* = 9.1 Hz, 1H), 7.71 – 7.61 (m, 5H), 7.47 – 7.35 (m, 2H), 2.43 (s, 3H).

¹³C{¹H} NMR (75 MHz, DMSO-*d*₆): δ 158.1, 156.4, 151.6, 148.0, 137.6, 134.1, 132.0, 131.1, 129.4, 129.3, 124.5, 123.5, 105.2, 20.5.

HRMS (ESI): *m/z* calc. for C₁₆H₁₄NS⁺ 252.0841, found 252.0838.

Methyl cyclopent-1-ene-1-carboxylate (9)



Pyridinium salt (**4e**, 76 mg, 0.3 mmol, 1 eq.) and NaCN (15 mg, 0.3 mmol, 1 eq.) were weighed into a screw-cap vial, followed by addition of MeOH (1.5 ml). The vial was sealed, and the reaction mixture was stirred for 1 hour at 0 °C (monitored by NMR spectroscopy). Upon completion, the reaction mixture was washed with water, and the water layer was additionally extracted twice with CHCl₃. Collected organic layers were washed with brine, dried over Na₂SO₄ and the solvent was removed on the rotary evaporator. The residue was purified by flash column chromatography (PE) to afford the title product as a light-yellow oil (21 mg, 56% yield). *Note: reaction can be conducted with catalytic cyanide loading albeit in slightly lower yield. Title compound was found to be relatively volatile; remaining solvent before and after chromatography was evaporated at 40 °C under the pressure above 100 mmHg.*

¹H NMR (300 MHz, CDCl₃): δ 6.77 (dt, *J* = 4.3, 2.2 Hz, 1H), 3.73 (s, 3H), 2.64 – 2.43 (m, 4H), 1.96 (p, *J* = 7.6 Hz, 2H).

¹³C{¹H} NMR (75 MHz, CDCl₃): δ 166.0, 144.0, 136.5, 51.5, 33.5, 31.5, 23.3.

HRMS (ESI): *m/z* calc. for [C₇H₁₀O₂+H⁺] 127.0754, found 127.0751.

9. Computational data

Quantum chemical calculations were performed using ORCA 5.0.4.^[21] The CREST package identified the most stable conformers, for conformationally flexible species (primarily ion pairs) several conformers were checked.^[22] Geometries were optimized and frequencies were calculated at the PBE0/def2-TZVP/D3BJ/CPCM(CH₂Cl₂) level, while single-point energies were obtained at the DLPNO-CCSD(T)/def2-TZVPP/CPCM(CH₂Cl₂) level.^[23,24] All optimized structures were confirmed as minima (no imaginary frequencies) or transition states (one imaginary frequency). LED (local energy decomposition) method was applied to obtain ΔE_{NCI} components at the DLPNO-CCSD(T)/def2-TZVPP/CPCM(CH₂Cl₂) level.^[25] $\Delta\Delta E_{\text{NCI}}(\text{SN})$ denotes the change of sum of ΔE_{NCI} upon transition from VONu to TS_{SN} geometry. Nucleophilicities were taken from the Mayr's database.^[4] Fukui functions f^+ and electrophilicities ω and ω_{CB} were calculated using the formulas given in the reference.^[26] NCI analysis was performed with Multiwfn 3.8 program package.^[27] Visualization was performed with Chemcraft and CYLview20 program packages.^[28] The charges of the nucleophilic components in the nucleophile variation segment are equal to the sum of the NBO charges of the nucleophile atoms in the molecular complexes; in other cases, Mulliken atomic charges are provided.

In all cases where energetic parameters were considered, the following expression for Gibbs free energy of formation was used:

$$\Delta G_f(X) = \Delta G_f(\text{PBE0/def2-TZVP/D3BJ/CPCM}(\text{CH}_2\text{Cl}_2)) - E_{\text{SPE}}(\text{PBE0/def2-TZVP/D3BJ/CPCM}(\text{CH}_2\text{Cl}_2)) + E_{\text{SPE}}(\text{DLPNO-CCSD(T)/def2-TZVPP/CPCM}(\text{CH}_2\text{Cl}_2)).$$

Calculated data concerns five separate reaction stages, presented below, with variation of the nucleophile, catalyst and electrophile components. Other intermediates, mostly ion pairs and intermolecular complexes, were also identified, but the values of their associated reaction energies ΔG_r and ΔG^\ddagger render them irrelevant to the discussion of the reaction pathways and their potential energy surfaces.

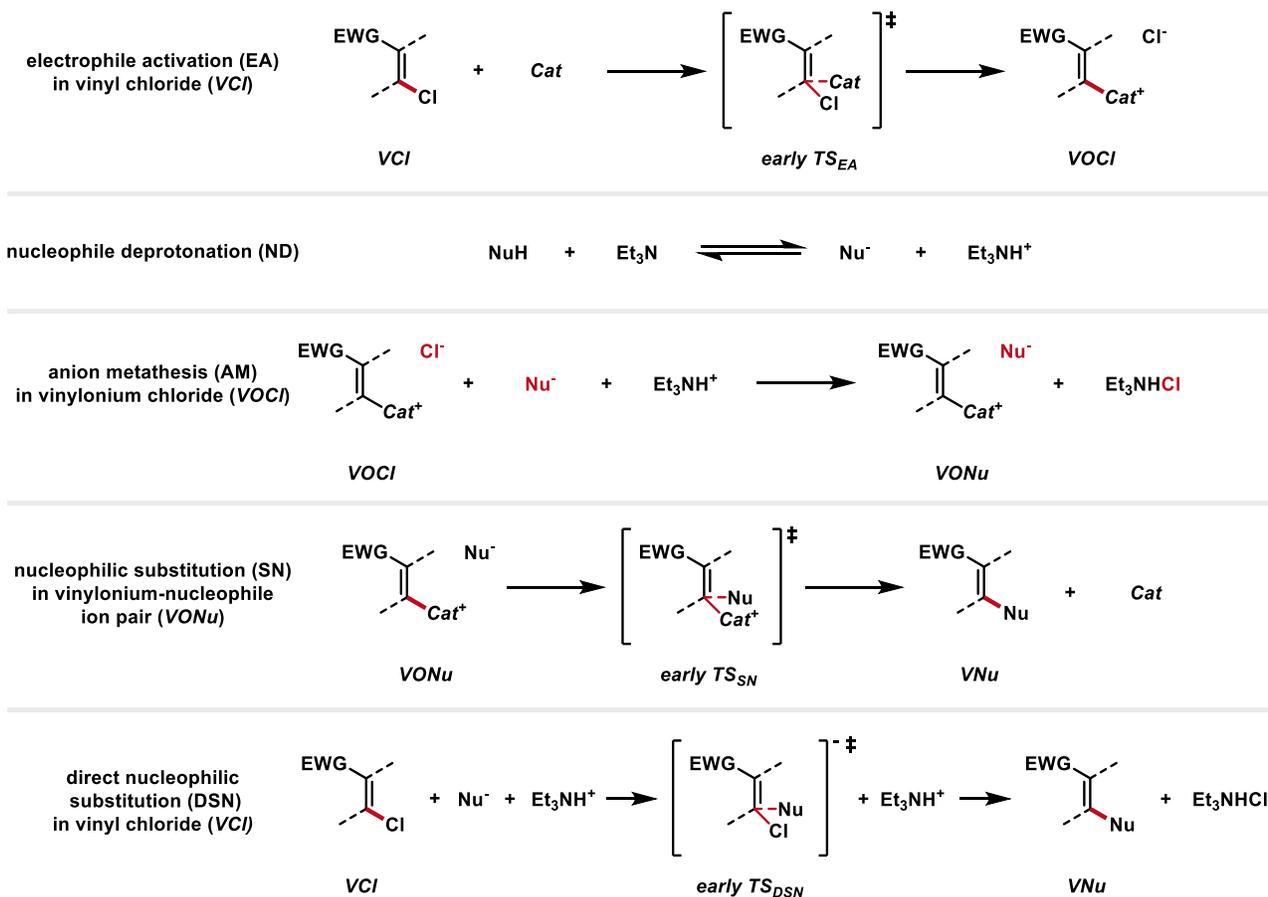


Figure SI5. Five calculated nucleophilic substitution reaction stages.

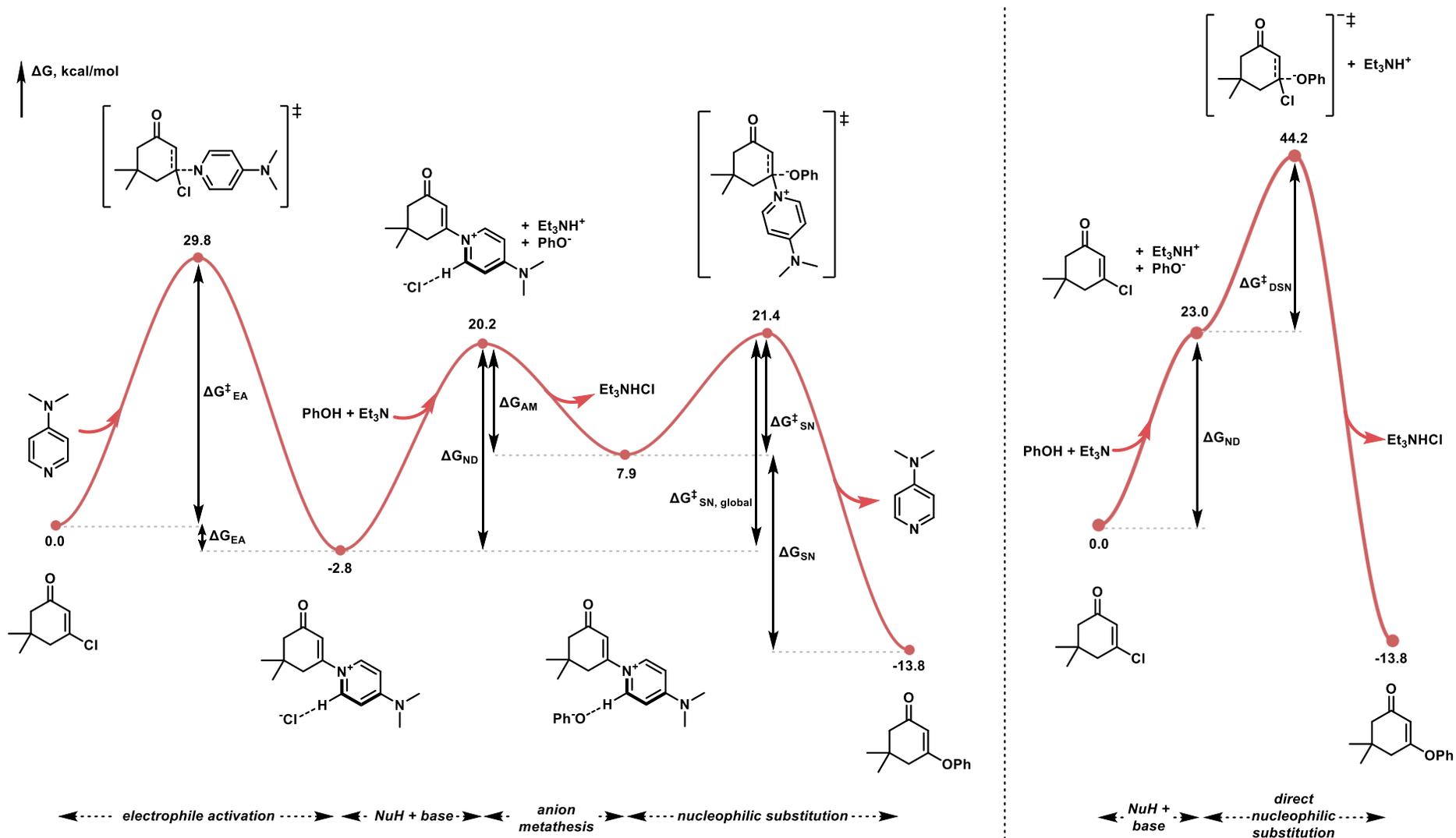
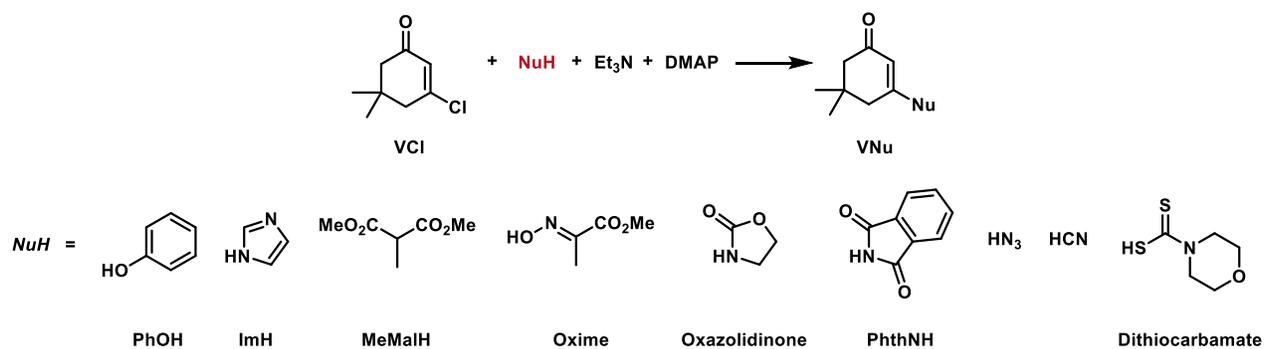
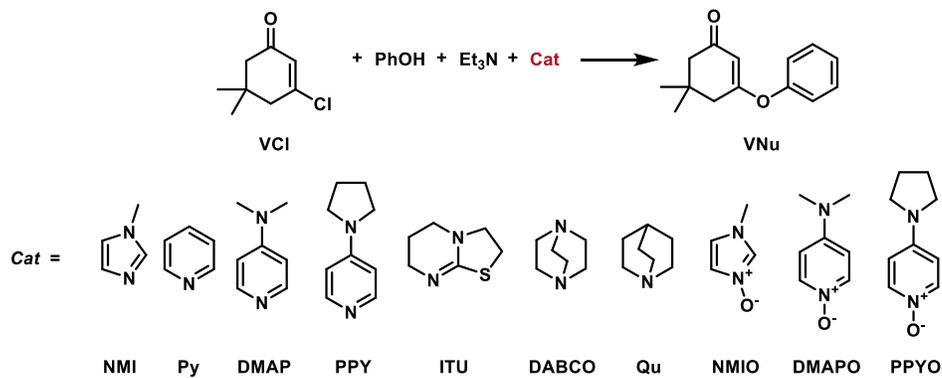


Figure SI6. Example of the PES structures for the DMAP-catalyzed (left) and direct (right) nucleophilic substitution reactions between dimedone-derived vinyl chloride **1a** and phenol with use of Et₃N as a base, at a PBE0/def2-TZVP/D3BJ/CPCM(CH₂Cl₂)/DLPNO-CCSD(T)/def2-TZVP/CPCM(CH₂Cl₂) level of theory.

Nucleophile variation



Catalyst variation



Electrophile (VCl) variation

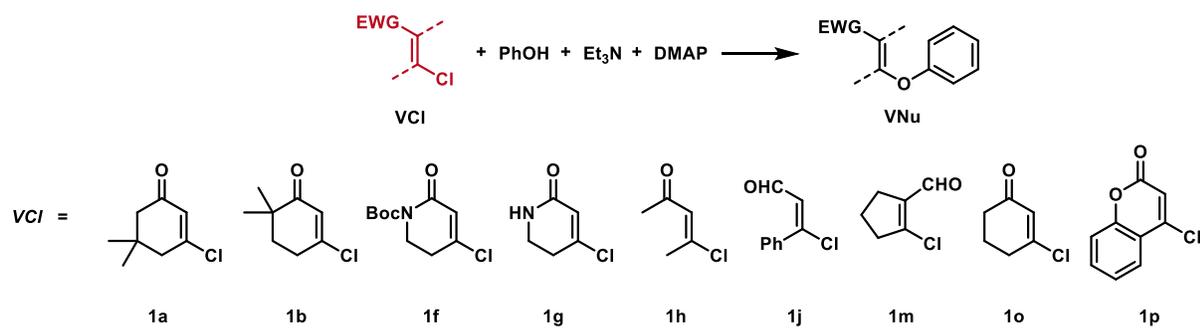


Figure SI7. Three sets of variable components of nucleophilic substitution reactions in the performed quantum chemical calculations.

ΔG_f / NuH	PhOH	ImH	MeMalH	Oxime	Oxazolidinone	PhthNH	HCN	HN ₃	Dithiocarbamate
VCl	-845.6228								
Cat	-381.4548								
TS _{EA}	-1227.0301								
VOCl	-1227.0820								
NuH	-306.8715	-225.8018	-534.6520	-436.2861	-322.0091	-512.1751	-93.2872	-164.5476	-1120.7365
Et ₃ N	-291.7180								
Nu ⁻	-306.3863	-225.3181	-534.1579	-435.8023	-321.5173	-511.7006	-92.8172	-164.0783	-1120.2785
Et ₃ NH ⁺	-292.1666								
VONu	-1073.5682	-992.4951	-1301.3400	-1202.9817	-1088.6954	-1278.8804	-859.9915	-931.2606	-1887.4568
Et ₃ NHCl	-752.0864								
TS _{SN}	-1073.5467	-992.4683	-1301.3126	-1202.9639	-1088.6775	-1278.8426	-859.9581	-931.2341	-1887.4227
VNu	-692.1480	-611.0834	-919.9355	-821.5640	-707.2951	-897.4528	-478.5814	-549.8315	-1506.0152
TS _{DSN}	-1151.9753	-1070.8984	-1379.7467	-1281.3896	-1167.1024	-1357.2699	-938.3929	-1009.6650	-1965.8501
VO ⁺	-767.1735								
Cl ⁻	-459.8999								
ΔG_{EA}^\ddagger	29.8								
ΔG_{EA}	-2.8								
ΔG_{ND}	23.0	22.1	28.6	22.1	27.1	16.3	13.5	13.1	5.9
ΔG_{AM}	-12.4	-9.3	-12.5	-10.8	-10.0	-11.0	-7.6	-12.6	-10.1
ΔG_{SN}^\ddagger	13.5	16.8	17.2	11.2	11.2	23.7	20.9	16.6	21.4
ΔG_{SN}	-21.7	-27.0	-31.5	-23.3	-34.2	-17.0	-28.0	-16.1	-8.3
ΔG_{DSN}^\ddagger	21.2	26.7	21.3	22.3	23.6	33.6	29.5	22.7	32.1
$\Delta G_{EA, rel}^\ddagger$	29.8								
$\Delta G_{EA, rel}$	-2.8								
$\Delta G_{ND, rel}$	20.2	19.3	25.8	19.4	24.4	13.5	10.7	10.3	3.2
$\Delta G_{AM, rel}$	7.9	10.0	13.3	8.5	14.4	2.5	3.1	-2.4	-7.0
$\Delta G_{SN, rel}^\ddagger$	21.4	26.8	30.5	19.7	25.6	26.2	24.0	14.3	14.4
$\Delta G_{SN, rel}$	-13.8	-17.0	-18.2	-14.8	-19.8	-14.6	-24.9	-18.4	-15.2
$\Delta G_{DSN, rel}^\ddagger$	44.2	48.8	49.9	44.4	50.8	49.9	43.0	35.7	38.0

Table SI2. Calculated ΔG values for modeled reaction species with varying nucleophiles. ΔG_{rel} correspond to the values with respect to the reaction starting materials (VCl, Cat and Et₃N).

ΔE_{NCI}	PhOH		ImH		MeMalH		Oxime		Oxazolidinone		PhthNH		HCN		HN ₃		Dithiocarbamate	
	VONu	TS _{SN}	VONu	TS _{SN}	VONu	TS _{SN}	VONu	TS _{SN}	VONu	TS _{SN}	VONu	TS _{SN}						
Elst	-131.88	-559.11	-112.24	-374.57	-136.95	-646.07	-114.83	-507.40	-127.07	-413.17	-104.63	-510.32	-102.03	-359.51	-105.57	-624.48	-123.68	-708.24
Exch	-13.15	-72.16	-10.71	-54.77	-12.40	-95.21	-10.60	-64.24	-9.68	-61.89	-9.63	-65.20	-6.19	-54.00	-7.78	-80.17	-11.83	-92.93
Disp	-13.60	-20.40	-10.98	-18.94	-13.62	-27.15	-13.99	-15.98	-9.19	-19.93	-15.99	-20.92	-3.71	-11.42	-6.64	-16.72	-11.41	-23.17
Geo-prep	0.62	18.48	0.39	13.96	0.60	33.04	0.89	15.69	0.20	14.53	1.04	20.19	0.34	14.45	0.47	22.35	0.45	26.52
Non-disp	-0.46	5.97	-0.08	3.50	-0.01	1.95	-0.86	3.04	0.01	2.73	-1.00	6.11	-0.19	1.14	-0.26	6.96	-1.28	1.63
C-T	-1.08	-1.37	-0.79	-1.99	-0.92	-2.57	-0.94	-1.59	-0.65	-2.32	-1.01	-1.29	-0.43	-1.70	-0.56	-1.11	-1.08	-2.56
El. Prep.	179.90	656.28	164.63	474.40	179.91	769.43	164.94	602.35	171.21	509.46	159.37	612.90	151.59	463.01	152.30	731.76	169.08	832.56
$\Sigma \Delta E_{\text{NCI}}$	20.35	27.70	30.23	41.59	16.60	33.43	24.61	31.87	24.83	29.40	28.17	41.48	39.38	51.97	31.96	38.59	20.25	33.82

Table SI3. Calculated ΔE_{NCI} values between modeled reaction reactants with varying nucleophiles. ΔE_{NCI} values are given in kcal/mol.

Parameter	NuH								
	PhOH	ImH	MeMalH	Oxime	Oxazolidinone	PhthNH	HCN	HN ₃	Dithiocarbamate
$\Delta G^{\ddagger}_{\text{SN}}$, kcal/mol	13.5	16.8	17.2	11.2	11.2	23.7	20.9	16.6	21.4
$\Delta G^{\ddagger}_{\text{SN, global}}$, kcal/mol	24.1	29.6	33.3	22.5	28.3	28.9	26.8	17.0	18.4
$\Delta G^{\ddagger}_{\text{SN, ionic}}$, kcal/mol	8.3	14.7	11.8	7.5	8.3	19.8	20.4	11.1	17.2
$Q_{\text{Nu}}(\text{VONu})$	-0.8672	-0.9418	-0.9431	-0.9475	-0.9467	-0.9812	-0.9465	-0.9526	-0.9346
$Q_{\text{Nu}}(\text{TS}_{\text{SN}})$	-0.5502	-0.6428	-0.3897	-0.5592	-0.6053	-0.5688	-0.5768	-0.4728	-0.3060
$N_{\text{DMSO}}(\text{Nu}^-)$	19.86	21.09	21.13	-	22.4	15.52	16.27*	20.5	21.72*
$\text{p}K_{\text{a}}(\text{DMSO})$	18	18.6	18	-	20.8	-	12.9	7.9	-
$\Delta E_{\text{NCI}}(\text{TS}_{\text{SN}})$, kcal/mol	27.7	41.6	33.4	31.9	29.4	41.5	52.0	38.6	33.8
$\Delta \Delta E_{\text{NCI}}(\text{SN})$, kcal/mol	7.3	11.4	16.8	7.3	4.6	13.3	12.6	6.6	13.6
$\Delta E_{\text{strain}}(\text{TS}_{\text{SN}})$, kcal/mol	18.5	14.0	33.0	15.7	14.5	20.2	14.5	22.4	26.5
$\Delta \Delta E_{\text{strain}}(\text{SN})$, kcal/mol	17.9	13.6	32.4	14.8	14.3	19.1	14.1	21.9	26.1

Table SI4. Calculated parameters for nucleophilic substitution reactions with varying nucleophiles. $\Delta G^{\ddagger}_{\text{SN, global}}$ was calculated relative to the VOCl, $\Delta G^{\ddagger}_{\text{SN, ionic}}$ was calculated relative to the individual ions, VO⁺ and Nu⁻. * values in MeCN.

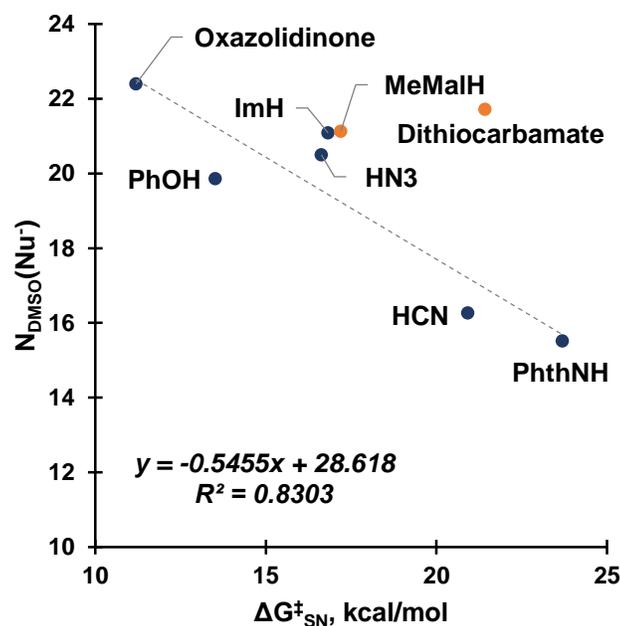


Figure SI8. Correlation graph for calculated $N_{DMSO}(Nu^-)$ and ΔG^{\ddagger}_{SN} in nucleophilic substitution reactions with varying nucleophiles. MeMalH and dithiocarbamate data points are not included in the linear regression formula. HCN and dithiocarbamate data points correspond to values in MeCN.

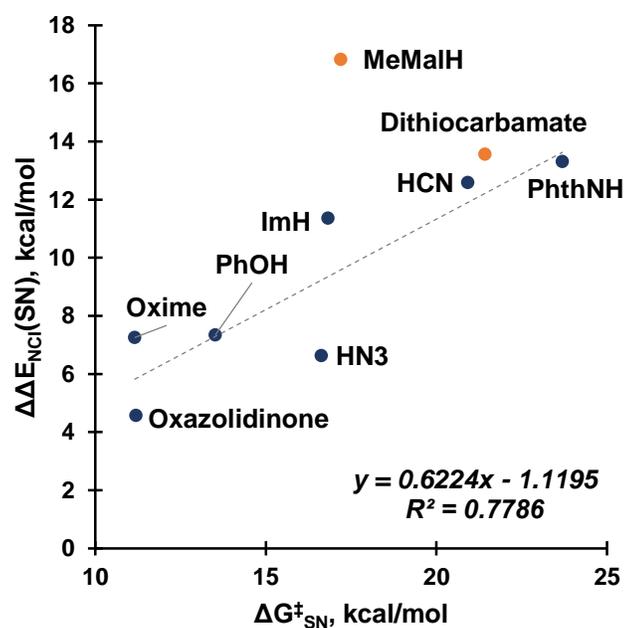


Figure SI9. Correlation graph for calculated $\Delta\Delta E_{NCl}(SN)$ and ΔG^{\ddagger}_{SN} in nucleophilic substitution reactions with varying nucleophiles. MeMalH and dithiocarbamate data points are not included in the linear regression formula.

ΔG_f / Cat	NMI	Py	DMAP	PPY	ITU	DABCO	Qu	NMIO	DMAPO	PPYO
VCl	-845.6228									
Cat	-265.0090	-247.7776	-381.4548	-458.7026	-741.1668	-344.5815	-328.5588	-340.0661	-456.5198	-533.7687
TS _{EA}	-1110.5789	-1093.3486	-1227.0301	-1304.2786	-1586.7394	-1190.1516	-1174.1293	-1185.6487	-1302.1031	-1379.3516
VOCl	-1110.6361	-1093.3932	-1227.0820	-1304.3311	-1586.8070	-1190.2047	-1174.1845	-1185.6936	-1302.1480	-1379.3970
NuH	-306.8715									
Et ₃ N	-291.7180									
Nu ⁻	-306.3863									
Et ₃ NH ⁺	-292.1666									
VONu	-957.1223	-939.8801	-1073.5682	-1150.8171	-1433.2904	-1036.6914	-1020.6718	-1032.1819	-1148.6298	-1225.8789
Et ₃ NHCl	-752.0864									
TS _{SN}	-957.0947	-939.8600	-1073.5467	-1150.7954	-1433.2624	-1036.6722	-1020.6515	-1032.1567	-1148.6112	-1225.8602
VNu	-692.1480									
TS _{DSN}	-1151.9753									
VO ⁺	-650.7223	-633.4816	-767.1735	-844.4227	-1126.8946	-730.2936	-714.2736	-725.7811	-842.2385	-919.4881
Cl ⁻	-459.8999									
ΔG_{EA}^\ddagger	33.2	32.5	29.8	29.4	31.5	33.1	32.9	25.3	24.8	25.1
ΔG_{EA}	-2.7	4.5	-2.8	-3.6	-10.9	-0.2	-1.8	-2.9	-3.4	-3.4
ΔG_{ND}	23.0									
ΔG_{AM}	-12.4	-12.8	-12.4	-12.2	-10.6	-12.7	-13.0	-13.7	-9.6	-9.7
ΔG_{SN}^\ddagger	17.3	12.6	13.5	13.6	17.6	12.1	12.7	15.8	11.7	11.7
ΔG_{SN}	-21.8	-28.6	-21.7	-21.0	-15.3	-24.0	-22.0	-20.2	-23.8	-23.7
ΔG_{DSN}^\ddagger	21.2									
$\Delta G_{EA, rel}^\ddagger$	33.2	32.5	29.8	29.4	31.5	33.1	32.9	25.3	24.8	25.1
$\Delta G_{EA, rel}$	-2.7	4.5	-2.8	-3.6	-10.9	-0.2	-1.8	-2.9	-3.4	-3.4
$\Delta G_{ND, rel}$	20.3	27.5	20.2	19.4	12.1	22.8	21.2	20.1	19.6	19.6
$\Delta G_{AM, rel}$	8.0	14.7	7.9	7.2	1.5	10.1	8.2	6.4	10.0	9.9
$\Delta G_{SN, rel}^\ddagger$	25.3	27.3	21.4	20.8	19.1	22.2	20.9	22.2	21.7	21.6
$\Delta G_{SN, rel}$	-13.8									
$\Delta G_{DSN, rel}^\ddagger$	44.2									

Table SI5. Calculated ΔG values for modeled reaction species with varying catalysts. ΔG_{rel} correspond to the values with respect to the reaction starting materials (VCl, Cat and Et₃N).

ΔE_{NCI}	NMI			Py			DMAP			PPY			ITU			DABCO			Qu			NMIO			DMAPO			PPYO		
	VONu	TS _{EA}	TS _{SN}																											
Elst	-167.46	-383.74	-574.34	-149.86	-451.27	-587.66	-131.88	-372.28	-559.11	-132.03	-370.63	-562.12	-131.21	-452.51	-548.68	-152.16	-479.81	-598.41	-145.95	-445.26	-606.58	-198.03	-562.05	-522.04	-114.25	-550.21	-488.49	-112.75	-533.17	-485.82
Exch	-15.85	-62.00	-72.66	-15.78	-70.55	-74.71	-13.15	-63.94	-72.16	-13.08	-63.82	-72.82	-11.28	-73.08	-71.73	-16.44	-76.58	-75.78	-15.98	-74.42	-76.25	-19.07	-73.68	-65.52	-10.73	-76.14	-63.37	-10.62	-75.29	-63.25
Disp	-13.96	-18.12	-20.24	-15.27	-20.08	-21.08	-13.60	-19.21	-20.40	-13.32	-19.15	-20.89	-13.81	-22.93	-21.81	-15.48	-23.02	-23.38	-15.37	-22.72	-23.41	-13.94	-18.98	-20.03	-11.55	-20.03	-19.54	-11.77	-19.77	-19.49
Geo-prep	1.27	16.91	19.85	0.58	19.72	18.64	0.62	16.48	18.48	0.59	16.36	18.24	0.32	20.05	19.37	0.46	28.13	18.03	0.05	26.63	18.01	3.25	20.36	18.67	0.27	19.60	18.23	0.24	18.90	18.15
Non-disp	-0.09	5.87	5.57	-0.79	6.14	5.05	-0.46	4.97	5.97	-0.32	4.87	5.99	-1.02	6.24	5.24	-1.02	5.73	4.59	-1.00	4.93	4.74	0.16	9.08	5.86	-0.55	9.01	5.61	-0.70	8.48	5.54
C-T	-1.06	-1.46	-1.38	-1.41	-1.73	-1.55	-1.08	-1.97	-1.37	-1.07	-1.97	-1.40	-1.06	-1.94	-1.51	-1.23	-2.16	-1.87	-1.25	-2.34	-1.82	-0.92	-0.65	-1.12	-0.79	-0.94	-1.14	-0.83	-1.07	-1.16
El. Prep.	208.27	485.55	675.28	197.06	556.82	682.09	179.90	470.95	656.28	179.08	468.81	660.47	167.85	562.89	649.39	201.09	587.35	697.11	193.63	548.75	704.29	238.07	665.86	611.76	164.79	654.06	578.81	162.65	636.24	575.85
$\Sigma \Delta E_{\text{NCI}}$	11.11	43.02	32.08	14.52	39.05	20.77	20.35	35.01	27.70	19.85	34.47	27.49	9.79	38.71	30.29	15.22	39.62	20.30	14.13	35.58	18.97	9.51	39.94	27.59	27.20	35.35	30.10	26.22	34.32	29.82

Table SI6. Calculated ΔE_{NCI} values between modeled reaction reactants with varying catalysts. ΔE_{NCI} values are given in kcal/mol.

Parameter	NMI	Py	DMAP	PPY	ITU	DABCO	Qu	NMIO	DMAPO	PPYO
$\Delta G_{\text{EA}}^{\ddagger}$, kcal/mol	33.2	32.5	29.8	29.4	31.5	33.1	32.9	25.3	24.8	25.1
$\Delta G_{\text{SN}}^{\ddagger}$, kcal/mol	17.3	12.6	13.5	13.6	17.6	12.1	12.7	15.8	11.7	11.7
$\Delta G_{\text{SN, global}}^{\ddagger}$, kcal/mol	28.0	22.8	24.1	24.4	30.0	22.4	22.7	25.1	25.1	25.1
$\Delta G_{\text{SN, ionic}}^{\ddagger}$, kcal/mol	8.8	5.0	8.3	8.6	11.7	4.9	5.3	6.7	8.6	9.0
$N_{\text{MeCN}}(\text{Cat})$	11.9	13.6	15.51	14.99	14.45*	18.8	20.54	-	-	-
$Q_{\text{Cp}}(\text{VO}^+)$	0.1004	0.1322	0.1574	0.1558	0.0438	0.1025	0.0978	0.1963	0.1990	0.1994
$f_{\text{Cp}}^+(\text{VO}^+)$	0.0501	0.0020	0.0295	0.0299	0.0638	0.0833	0.0978	0.1231	0.0096	0.0103
HOMO (VO ⁺), eV	-7.8233	-7.9553	-7.3224	-7.2500	-7.7044	-7.4364	-7.9123	-7.7063	-7.4459	-7.3656
LUMO (VO ⁺), eV	-2.5710	-3.3029	-2.6945	-2.6569	-2.2956	-2.3508	-2.3176	-1.7843	-2.0852	-2.0322
ω	2.5712	3.4055	2.7101	2.6711	2.3110	2.3544	2.3382	1.9012	2.1183	2.0699
ω_{Cp}	0.1289	0.0067	0.0798	0.0799	0.1475	0.1961	0.2287	0.2339	0.0203	0.0214
$\Delta E_{\text{NCI}}(\text{TS}_{\text{EA}})$, kcal/mol	43.0	39.1	35.0	34.5	38.7	39.6	35.6	39.9	35.3	34.3
$\Delta E_{\text{strain}}(\text{TS}_{\text{EA}})$, kcal/mol	16.9	19.7	16.5	16.4	20.0	28.1	26.6	20.4	19.6	18.9
$\Delta E_{\text{NCI}}(\text{TS}_{\text{SN}})$, kcal/mol	32.1	20.8	27.7	27.5	30.3	20.3	19.0	27.6	30.1	29.8
$\Delta \Delta E_{\text{NCI}}(\text{SN})$, kcal/mol	21.0	6.2	7.3	7.6	20.5	5.1	4.8	18.1	2.9	3.6
$\Delta E_{\text{strain}}(\text{TS}_{\text{SN}})$, kcal/mol	19.8	18.6	18.5	18.2	19.4	18.0	18.0	18.7	18.2	18.1
$\Delta \Delta E_{\text{strain}}(\text{SN})$, kcal/mol	18.6	18.1	17.9	17.6	19.1	17.6	18.0	15.4	18.0	17.9

Table SI7. Calculated parameters for nucleophilic substitution reactions with varying catalysts. $\Delta G_{\text{SN, global}}^{\ddagger}$ was calculated relative to the VOCl, $\Delta G_{\text{SN, ionic}}^{\ddagger}$ was calculated relative to the individual ions, VO⁺ and Nu⁻. * value in CH₂Cl₂.

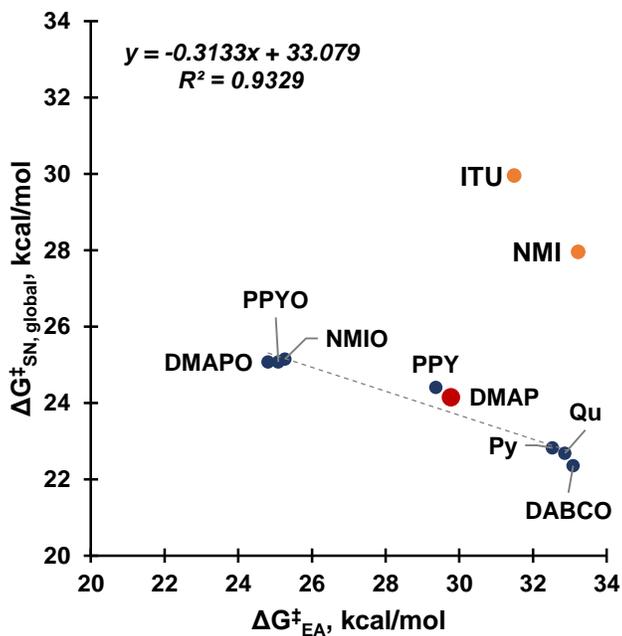


Figure SI10. Correlation graph for calculated $\Delta G_{SN, global}^\ddagger$ and ΔG_{EA}^\ddagger in nucleophilic substitution reactions with varying catalysts. ITU and NMI data points are not included in the linear regression formula.

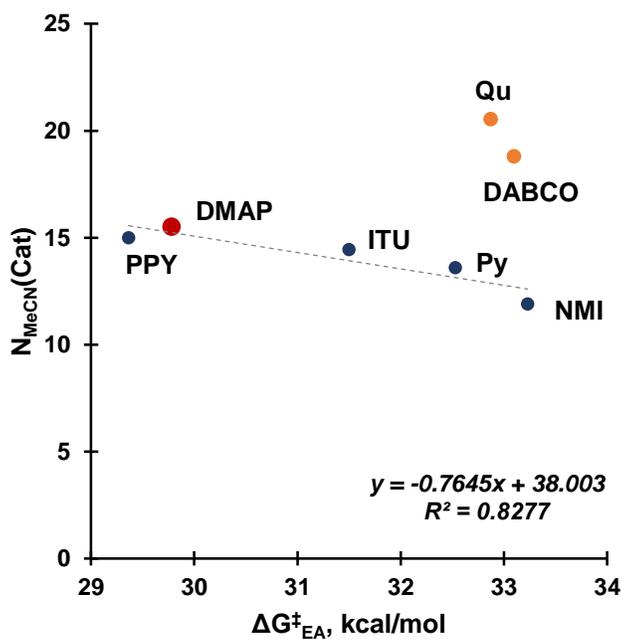


Figure SI11. Correlation graph for $N_{MeCN}(Cat)$ and calculated ΔG_{EA}^\ddagger in nucleophilic substitution reactions with varying catalysts. Qu and DABCO data points are not included in the linear regression formula. N(ITU) data point corresponds to value in CH_2Cl_2 .

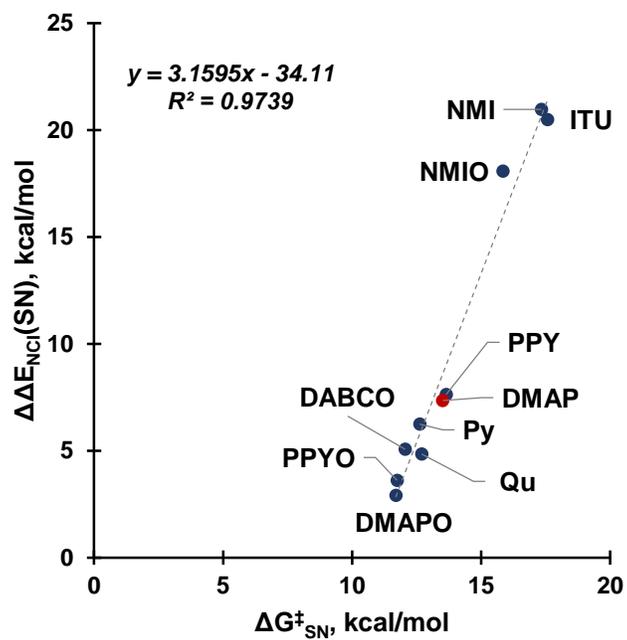


Figure SI12. Correlation graph for calculated $\Delta \Delta E_{NCI}(SN)$ and ΔG_{SN}^{\ddagger} in nucleophilic substitution reactions with varying catalysts.

ΔG_f \ VCI	1a	1b	1f	1g	1h	1j	1m	1o	1p
VCI	-845.6228	-845.6215	-1128.4057	-783.2463	-729.1529	-881.2555	-767.1744	-767.1883	-955.2324
Cat	-381.4548								
TS_{EA}	-1227.0301	-1227.0313	-1509.8154	-1164.6521	-1110.5616	-1262.6664	-1148.5850	-1148.5986	-1336.6421
VOCI	-1227.0820	-1227.0805	-1509.8635	-1164.7055	-1110.6125	-1262.7159	-1148.6323	-1148.6472	-1336.6897
NuH	-306.8715								
Et₃N	-291.7180								
Nu⁻	-306.3863								
Et₃NH⁺	-292.1666								
VONu	-1073.5682	-1073.5649	-1356.3519	-1011.1914	-957.0993	-1109.2023	-995.1198	-995.1332	-1183.1783
Et₃NHCl	-752.0864								
TS_{SN}	-1073.5467	-1073.5482	-1356.3316	-1011.1656	-957.0799	-1109.1837	-995.0991	-995.1121	-1183.1632
VNu	-692.1480	-692.1467	-974.9314	-629.7714	-575.6782	-727.7814	-613.6942	-613.7140	-801.7598
TS_{DSN}	-1151.9753	-1151.97691	-1434.7618	-1089.5938	-1035.5055	-1187.6132	-1073.5328	-1073.5408	-1261.5953
VO⁺	-767.1735	-767.1721	-1049.9558	-704.7974	-650.7064	-802.8094	-688.7242	-688.7390	-876.7817
Cl⁻	-459.8999								
ΔG_{EA}^\ddagger	29.8	28.2	28.3	30.7	28.9	27.5	27.7	27.9	28.3
ΔG_{EA}	-2.8	-2.7	-1.9	-2.8	-3.0	-3.5	-2.0	-2.6	-1.6
ΔG_{ND}	23.0								
ΔG_{AM}	-12.4	-11.2	-13.7	-12.2	-12.7	-12.5	-13.1	-12.2	-13.9
ΔG_{SN}^\ddagger	13.5	10.5	12.7	16.2	12.2	11.7	13.0	13.3	9.5
ΔG_{SN}	-21.7	-23.0	-21.5	-21.8	-21.1	-21.3	-18.3	-22.3	-22.8
ΔG_{DSN}^\ddagger	21.2	19.4	19.0	24.4	21.2	17.9	17.5	21.2	14.7
$\Delta G_{EA,rel}^\ddagger$	29.8	28.2	28.3	30.7	28.9	27.5	27.7	27.9	28.3
$\Delta G_{EA,rel}$	-2.8	-2.7	-1.9	-2.8	-3.0	-3.5	-2.0	-2.6	-1.6
$\Delta G_{ND,rel}$	20.2	20.3	21.0	20.2	20.0	19.4	21.0	20.4	21.4
$\Delta G_{AM,rel}$	7.9	9.1	7.3	8.1	7.2	6.9	7.9	8.2	7.5
$\Delta G_{SN,rel}^\ddagger$	21.4	19.6	20.1	24.3	19.4	18.6	20.9	21.5	17.0
$\Delta G_{SN,rel}$	-13.8	-13.9	-14.2	-13.8	-13.9	-14.3	-10.4	-14.1	-15.2
$\Delta G_{DSN,rel}^\ddagger$	44.2	42.4	41.9	47.4	44.2	40.9	40.5	44.2	37.7

Table SI8. Calculated ΔG values for modeled reaction species with varying electrophiles. ΔG_{rel} correspond to the values with respect to the reaction starting materials (VCI, Cat and Et₃N).

ΔE_{NCI}	VCI			1a			1b			1f			1g			1h			1j			1m			1o			1p		
	VONu	TSE _A	TS _{SN}	VONu	TSE _A	TS _{SN}																								
Elst	-131.88	-372.28	-559.11	-134.51	-385.78	-528.50	-137.47	-397.08	-549.75	-129.24	-451.77	-594.97	-133.36	-324.92	-446.33	-116.06	-381.92	-617.68	-139.61	-370.75	-526.65	-132.23	-378.27	-559.52	-136.00	-465.63	-585.86			
Exch	-13.15	-63.94	-72.16	-11.86	-64.48	-68.08	-14.21	-65.40	-72.69	-12.42	-69.53	-73.58	-14.30	-58.58	-64.22	-13.54	-65.64	-78.82	-15.64	-63.35	-71.48	-13.01	-63.68	-71.97	-15.76	-72.28	-77.73			
Disp	-13.60	-19.21	-20.40	-10.74	-18.20	-20.26	-15.53	-18.04	-23.02	-12.56	-18.37	-19.67	-13.53	-16.32	-20.02	-16.44	-18.58	-22.39	-15.38	-17.42	-21.56	-13.04	-17.85	-20.02	-16.14	-19.23	-22.95			
Geo-prep	0.62	16.48	18.48	0.51	15.33	15.59	1.03	14.91	18.32	0.65	16.20	20.65	0.84	16.13	14.69	0.84	14.61	18.52	0.93	12.94	15.84	0.64	14.98	18.39	0.68	17.84	17.62			
Non-disp	-0.46	4.97	5.97	0.02	5.21	5.37	-0.47	5.62	5.42	-0.45	6.69	7.14	-0.63	4.44	4.00	-0.64	4.57	6.31	-0.53	4.61	5.34	-0.43	5.15	5.78	-0.59	5.89	5.39			
C-T	-1.08	-1.97	-1.37	-0.83	-1.83	-1.48	-1.12	-1.64	-1.59	-0.92	-1.34	-1.00	-1.22	-1.84	-1.93	-1.38	-2.02	-1.58	-1.35	-1.83	-1.81	-1.07	-1.80	-1.43	-1.30	-1.36	-1.49			
El-prep	179.90	470.95	656.28	177.97	482.71	622.66	191.29	497.81	651.70	180.74	558.70	694.73	177.75	414.02	534.38	169.04	481.83	723.77	189.35	467.78	625.60	179.74	474.90	656.21	192.63	570.10	688.96			
$\Sigma \Delta E_{\text{NCI}}$	20.35	35.01	27.70	20.55	32.96	25.30	23.53	36.19	28.39	25.80	40.58	33.30	15.55	32.93	20.57	21.81	32.85	28.13	17.77	31.97	25.28	20.59	33.43	27.44	23.51	35.33	23.94			

Table SI9. Calculated ΔE_{NCI} values between modeled reaction reactants with varying electrophiles. ΔE_{NCI} values are given in kcal/mol.

ΔE_{NCI}	1a	1b	1f	1g	1h	1j	1m	1o	1p
$\Delta G_{\text{EA}}^{\ddagger}$, kcal/mol	29.8	28.2	28.3	30.7	28.9	27.5	27.7	27.9	28.3
$\Delta G_{\text{SN}}^{\ddagger}$, kcal/mol	13.5	10.5	12.7	16.2	13.2	11.7	13	13.3	9.5
$\Delta G_{\text{SN, global}}^{\ddagger}$, kcal/mol	24.1	22.3	22	27	23.5	22.2	22.8	24.1	18.6
$\Delta G_{\text{SN, ionic}}^{\ddagger}$, kcal/mol	8.3	6.4	6.6	11.4	9.1	7.6	7.2	8.4	3.1
$Q_{\text{CB}}(\text{VO}^+)$	0.1574	0.0993	0.1171	0.0996	0.1139	0.2189	0.0995	0.1156	0.2004
$f_{\text{CB}}^+(\text{VO}^+)$	0.0295	0.0299	0.0241	0.011	0.0688	0.0415	0.0682	0.0272	0.0302
HOMO(VO^+), eV	-7.3224	-7.3134	-7.3477	-7.2821	-7.2712	-7.364	-7.2699	-7.3286	-7.4435
LUMO(VO^+), eV	-2.6945	-2.6689	-2.7179	-2.5386	-2.4534	-2.9157	-2.7037	-2.7018	-2.7723
ω	2.7101	2.6819	2.7354	2.5415	2.4536	2.9695	2.7231	2.7181	2.7927
ω_{CB}	0.0798	0.0803	0.066	0.028	0.1688	0.1233	0.1856	0.074	0.0844
$\Delta E_{\text{NCI}}(\text{TS}_{\text{EA}})$, kcal/mol	35	33	36.2	40.6	32.9	32.9	32	33.4	35.3
$\Delta E_{\text{strain}}(\text{TS}_{\text{EA}})$, kcal/mol	16.5	15.3	14.9	16.2	16.1	14.6	12.9	15	17.8
$\Delta E_{\text{NCI}}(\text{TS}_{\text{SN}})$, kcal/mol	27.7	25.3	28.4	33.3	20.6	28.1	25.3	27.4	23.9
$\Delta \Delta E_{\text{NCI}}(\text{SN})$, kcal/mol	7.3	4.7	4.9	7.5	5	6.3	7.5	6.9	0.4
$\Delta E_{\text{strain}}(\text{TS}_{\text{SN}})$, kcal/mol	18.5	15.6	18.3	20.6	14.7	18.5	15.8	18.4	17.6
$\Delta \Delta E_{\text{strain}}(\text{SN})$, kcal/mol	17.9	15.1	17.3	20	13.9	17.7	14.9	17.7	16.9

Table SI10. Calculated parameters for nucleophilic substitution reactions with varying electrophiles. $\Delta G_{\text{SN, global}}^{\ddagger}$ was calculated relative to the VOCl , $\Delta G_{\text{SN, ionic}}^{\ddagger}$ was calculated relative to the individual ions, VO^+ and Nu^- .

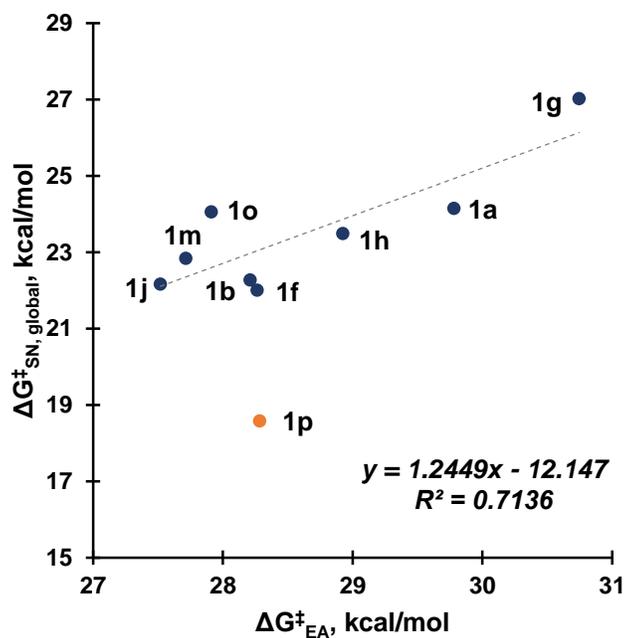


Figure SI13. Correlation graph for calculated $\Delta G^{\ddagger}_{\text{SN, global}}$ and $\Delta G^{\ddagger}_{\text{EA}}$ in nucleophilic substitution reactions with varying electrophiles. **1p** data point is not included in the linear regression formula.

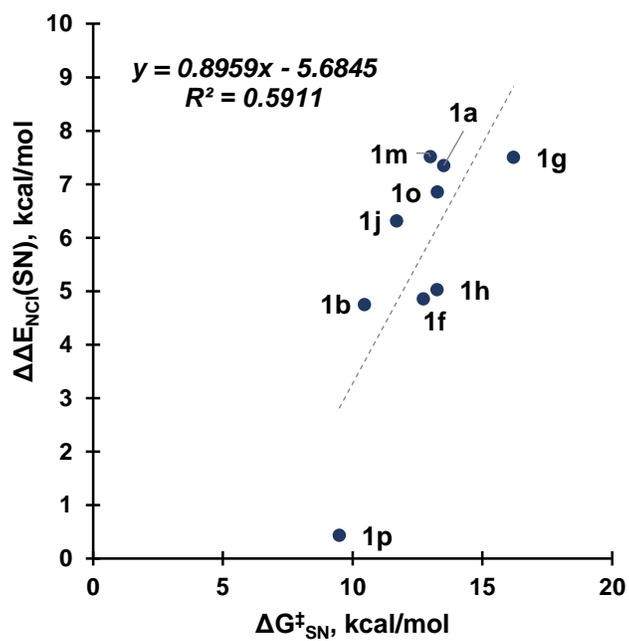


Figure SI14. Correlation graph for calculated $\Delta\Delta E_{\text{NCl(SN)}}$ and $\Delta G^{\ddagger}_{\text{SN}}$ in nucleophilic substitution reactions with varying electrophiles.

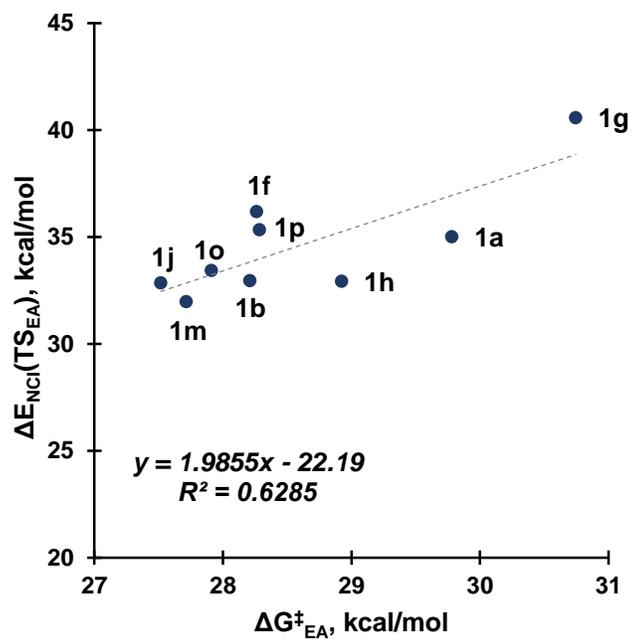


Figure SI15. Correlation graph for calculated $\Delta E_{\text{NCI}}(\text{TS}_{\text{EA}})$ and $\Delta G^{\ddagger}_{\text{EA}}$ in nucleophilic substitution reactions with varying electrophiles.

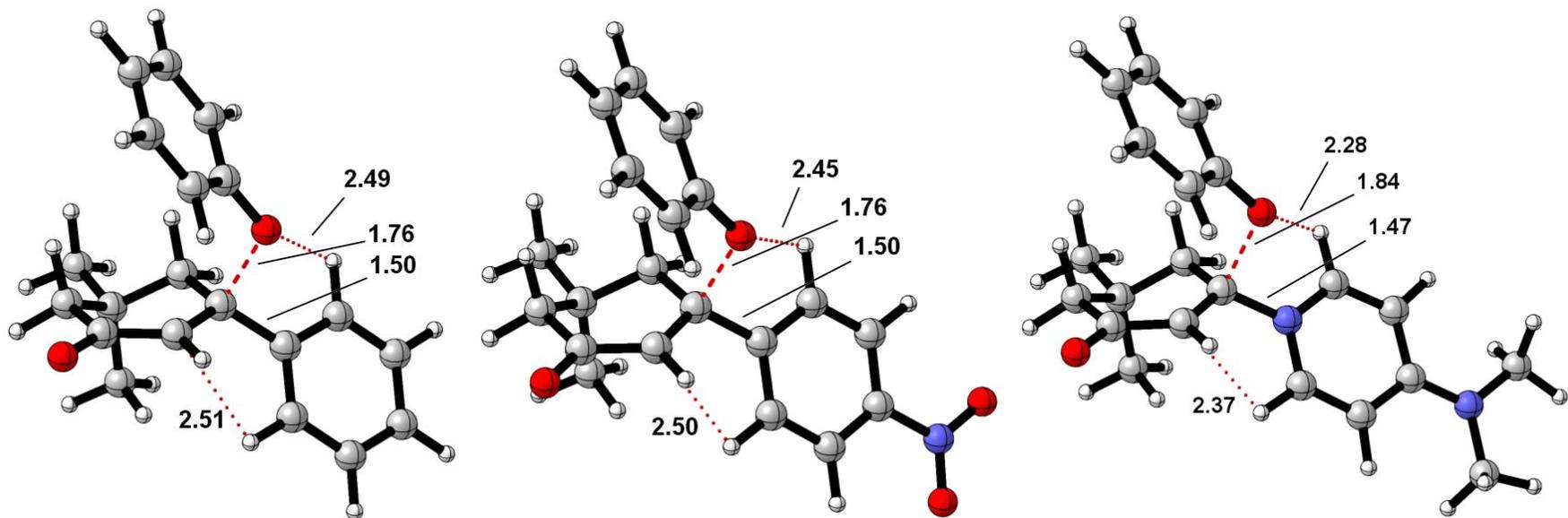


Figure SII16. Calculated geometries for TSs of phenolate addition to β -phenyl- (TS_{Ph} , left), β -(4-nitrophenyl)- ($\text{TS}_{4\text{NO}_2\text{Ph}}$, center) and β -(4-dimethylaminopyridinium)-substituted (right) dimedone-derived Michael acceptors, with corresponding interatomic distances given in Å.

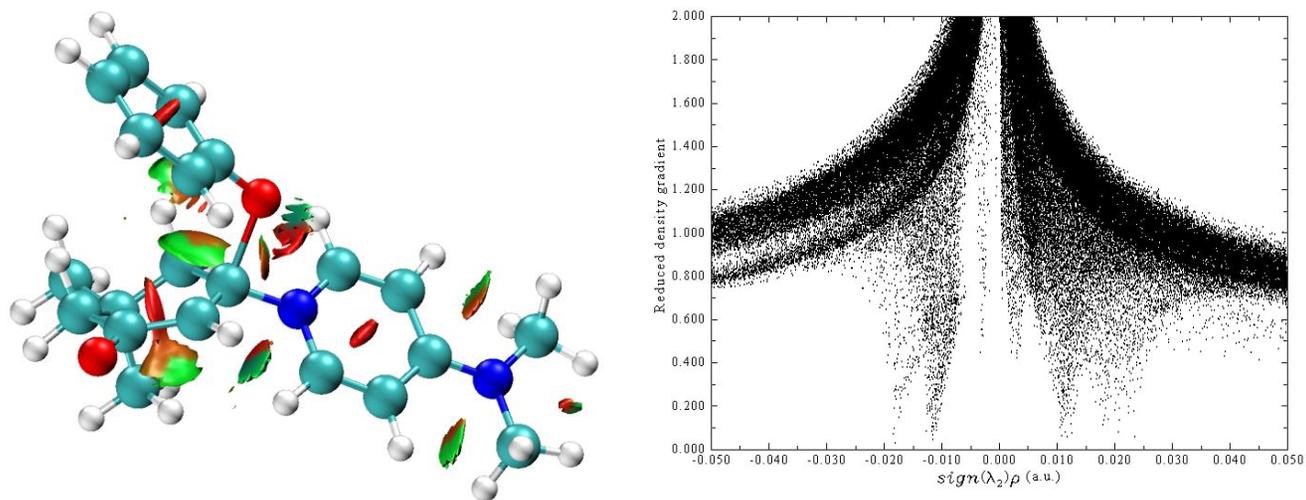


Figure SII17. Left – NCI analysis for the calculated TS_{SN} geometry for the dimedone-derived vinylpyridinium and phenolate (see above). Green areas represent weak, dispersive interactions in the transition state complex. Right – Quantitative NCI analysis for the same TS_{SN} geometry. Absence of points with $\text{RDG} = 0.5$ and $\text{sign}(\lambda_2)\rho < -0.02$ indicates lack of strong NCI (like H-bonding) in the molecular complex.

10. XYZ coordinates

10.1. Common structures

VCl (1a)

C	0.246292000	-1.195863000	-2.606945000
C	-0.850127000	-1.839092000	-3.017244000
C	-2.020247000	-1.085232000	-3.468607000
C	0.391032000	0.282166000	-2.536928000
H	-0.908062000	-2.920510000	-3.034635000
O	-3.052839000	-1.655347000	-3.778102000
C	-1.866018000	0.406131000	-3.576986000
C	-0.957660000	1.008958000	-2.504466000
C	-0.733675000	2.486405000	-2.796550000
H	-1.681947000	3.028626000	-2.764211000
H	-0.065009000	2.928823000	-2.053150000
H	-0.290352000	2.629402000	-3.785419000
C	-1.603352000	0.858650000	-1.128304000
H	-2.574847000	1.358463000	-1.112014000
H	-1.759125000	-0.189025000	-0.860104000
H	-0.972940000	1.314038000	-0.360571000
H	-2.857780000	0.862681000	-3.559175000
H	0.986829000	0.546916000	-1.659164000
H	0.972340000	0.602002000	-3.411730000
H	-1.434352000	0.600840000	-4.568181000
Cl	1.638771000	-2.097488000	-2.130168000

PhOH

C	2.753402000	-4.003651000	-6.703482000
C	2.753402000	-2.780706000	-6.043390000
C	2.753402000	-5.175414000	-5.959561000
H	2.753402000	-1.857296000	-6.611922000
H	2.753402000	-6.137594000	-6.459521000
C	2.753402000	-2.723565000	-4.658684000
C	2.753402000	-5.132146000	-4.572701000
H	2.753402000	-1.773412000	-4.136909000
H	2.753402000	-6.049343000	-3.991709000
C	2.753402000	-3.903265000	-3.920570000
H	2.753402000	-4.042060000	-7.786228000
O	2.753402000	-3.800441000	-2.568374000
H	2.753402000	-4.680413000	-2.175081000

Et₃N

N	0.501351000	-2.825002000	-5.857094000
C	1.792978000	-2.262262000	-5.486578000
H	1.659355000	-1.392726000	-4.817622000
H	2.334070000	-3.013010000	-4.907135000

C	-0.427273000	-1.783453000	-6.275165000
H	-0.839007000	-1.255453000	-5.395975000
H	0.133962000	-1.038628000	-6.842931000
C	-0.055113000	-3.621505000	-4.771031000
H	-1.121857000	-3.755447000	-4.961568000
H	0.021108000	-3.075813000	-3.813035000
C	2.642466000	-1.874409000	-6.681280000
H	3.604455000	-1.478763000	-6.346261000
H	2.829223000	-2.745030000	-7.314190000
H	2.166364000	-1.105945000	-7.294046000
C	0.584857000	-4.990390000	-4.642882000
H	1.654175000	-4.927985000	-4.429360000
H	0.118831000	-5.549433000	-3.827717000
H	0.457143000	-5.558503000	-5.567271000
C	-1.553782000	-2.301727000	-7.147593000
H	-1.152155000	-2.763173000	-8.052693000
H	-2.166164000	-3.045294000	-6.632880000
H	-2.211751000	-1.480554000	-7.442357000

PhO⁻

C	10.230100000	1.375759000	-8.517678000
C	10.230100000	2.596746000	-7.844414000
C	10.230100000	0.209849000	-7.753067000
H	10.230100000	3.522324000	-8.415130000
H	10.230100000	-0.756666000	-8.251269000
C	10.230100000	2.658231000	-6.462232000
C	10.230100000	0.254178000	-6.370105000
H	10.230100000	3.621817000	-5.958856000
H	10.230100000	-0.668500000	-5.795143000
C	10.230100000	1.485834000	-5.642250000
H	10.230100000	1.334424000	-9.600884000
O	10.230100000	1.535081000	-4.367044000

Et₃NH⁺

N	0.490440000	-2.816380000	-5.862335000
C	1.826549000	-2.247746000	-5.490721000
H	1.621532000	-1.391925000	-4.845990000
H	2.340559000	-3.003890000	-4.900274000
C	-0.465400000	-1.738999000	-6.277150000
H	-0.822024000	-1.280539000	-5.353840000
H	0.113115000	-0.996780000	-6.824543000
C	-0.076769000	-3.652685000	-4.756248000
H	-1.139577000	-3.769827000	-4.960377000
H	0.031975000	-3.060605000	-3.846315000
C	2.647572000	-1.876083000	-6.700589000
H	3.609495000	-1.489061000	-6.362322000
H	2.837763000	-2.750876000	-7.326700000
H	2.173899000	-1.104104000	-7.308123000

C	0.590359000	-5.002000000	-4.650650000
H	1.649208000	-4.930944000	-4.399438000
H	0.099671000	-5.569086000	-3.858562000
H	0.485019000	-5.563957000	-5.581411000
C	-1.591438000	-2.263383000	-7.133584000
H	-1.206410000	-2.723858000	-8.046326000
H	-2.217113000	-2.988041000	-6.611411000
H	-2.226517000	-1.425225000	-7.422919000
H	0.632656000	-3.427429000	-6.670453000

Et₃NHCl

N	0.512227000	-2.903894000	-5.975440000
C	1.857920000	-2.430164000	-5.545484000
H	1.709021000	-1.817873000	-4.652870000
H	2.416491000	-3.318969000	-5.259351000
C	-0.350008000	-1.776503000	-6.428438000
H	-0.458369000	-1.097679000	-5.579241000
H	0.206205000	-1.260122000	-7.208001000
C	-0.152905000	-3.709083000	-4.912309000
H	-1.108613000	-4.026425000	-5.323933000
H	-0.347738000	-3.032505000	-4.076779000
C	2.611408000	-1.685045000	-6.623629000
H	3.641365000	-1.551603000	-6.289084000
H	2.629313000	-2.258411000	-7.552861000
H	2.198066000	-0.696703000	-6.823062000
C	0.639608000	-4.923214000	-4.483622000
H	1.520727000	-4.668549000	-3.894906000
H	-0.004238000	-5.547151000	-3.861837000
H	0.947710000	-5.512776000	-5.349490000
C	-1.689106000	-2.217596000	-6.973955000
H	-1.564515000	-2.995091000	-7.730551000
H	-2.364833000	-2.579700000	-6.199548000
H	-2.162314000	-1.356983000	-7.449264000
H	0.658056000	-3.544140000	-6.811401000
Cl	0.960292000	-4.741111000	-8.353685000

VNu

C	9.468012000	0.020612000	-5.694924000
C	10.586881000	-0.069042000	-4.948917000
C	11.628935000	0.928365000	-5.066341000
C	9.215348000	1.100921000	-6.685005000
H	10.741498000	-0.879127000	-4.247491000
O	12.672525000	0.846520000	-4.429051000
C	11.364651000	2.104078000	-5.972362000
C	10.495467000	1.772008000	-7.184694000
C	10.134736000	3.053648000	-7.923302000
H	11.036353000	3.551555000	-8.289193000
H	9.494842000	2.837946000	-8.783422000

H	9.603336000	3.748109000	-7.267217000
C	11.247696000	0.839008000	-8.131673000
H	12.170514000	1.313292000	-8.474706000
H	11.512351000	-0.104415000	-7.648615000
H	10.636299000	0.610545000	-9.008374000
H	12.324276000	2.528021000	-6.276584000
H	8.643385000	0.684023000	-7.518835000
H	8.567996000	1.845518000	-6.203607000
H	10.854870000	2.860201000	-5.360285000
O	8.443802000	-0.846759000	-5.636614000
C	8.455729000	-1.850321000	-4.679160000
C	8.101655000	-1.554602000	-3.374026000
C	8.756609000	-3.139535000	-5.077804000
C	8.054712000	-2.582607000	-2.444170000
C	8.702221000	-4.160958000	-4.138887000
C	8.354491000	-3.884752000	-2.823994000
H	7.869213000	-0.532964000	-3.097417000
H	9.024871000	-3.332896000	-6.109574000
H	7.779030000	-2.363905000	-1.419127000
H	8.932591000	-5.176253000	-4.439986000
H	8.313168000	-4.685013000	-2.094553000

TS_{Ph}

C	0.524240000	0.025024000	-0.121939000
C	0.011012000	0.478749000	-1.368947000
C	-0.891184000	1.527748000	-1.526968000
C	0.072118000	0.807653000	1.099531000
H	0.335318000	-0.028138000	-2.273505000
O	-1.381145000	1.887059000	-2.630838000
C	-1.277093000	2.320906000	-0.291708000
C	-0.242187000	2.278828000	0.830130000
C	1.011290000	3.059419000	0.442796000
H	1.454831000	2.668644000	-0.474669000
H	0.770697000	4.114892000	0.285106000
H	1.761541000	2.999225000	1.237010000
C	-0.831038000	2.889711000	2.096707000
H	-0.108557000	2.858914000	2.918210000
H	-1.107887000	3.934944000	1.929746000
H	-1.727207000	2.346834000	2.410591000
H	-2.228124000	1.920509000	0.084774000
H	-0.849103000	0.354618000	1.477324000
H	0.816682000	0.721816000	1.895182000
H	-1.470455000	3.352043000	-0.605030000
C	4.700059000	-1.040864000	0.002912000
C	3.844147000	-1.436362000	1.024791000
C	2.499386000	-1.107163000	0.976677000

C	1.972623000	-0.382338000	-0.094248000
C	2.842148000	0.013261000	-1.106030000
C	4.192211000	-0.313936000	-1.062643000
H	4.228413000	-2.005108000	1.864794000
H	1.838134000	-1.428067000	1.771539000
H	2.453417000	0.600027000	-1.929604000
H	4.847965000	0.008444000	-1.864292000
C	-4.253255000	-1.793320000	0.172424000
C	-3.535267000	-1.738760000	-1.016348000
C	-3.565714000	-1.789456000	1.380848000
H	-4.061340000	-1.754182000	-1.965490000
H	-4.112350000	-1.845782000	2.316697000
C	-2.149667000	-1.670097000	-1.005607000
C	-2.181915000	-1.706072000	1.399544000
H	-1.590979000	-1.645208000	-1.931922000
H	-1.642072000	-1.699769000	2.340842000
C	-1.441782000	-1.648885000	0.207032000
H	-5.335787000	-1.851627000	0.157381000
O	-0.119142000	-1.576995000	0.239749000
H	5.753372000	-1.295857000	0.041255000

TS_{4NO2Ph}

C	0.531262000	0.011533000	-0.086563000
C	0.026878000	0.471471000	-1.333004000
C	-0.884556000	1.515434000	-1.486975000
C	0.104219000	0.805263000	1.138971000
H	0.351503000	-0.033737000	-2.238181000
O	-1.373772000	1.874373000	-2.588754000
C	-1.275455000	2.297642000	-0.247180000
C	-0.228963000	2.271323000	0.864485000
C	1.012806000	3.063462000	0.462834000
H	1.453658000	2.673486000	-0.456336000
H	0.759635000	4.115205000	0.301224000
H	1.769313000	3.015818000	1.251834000
C	-0.812755000	2.881192000	2.133976000
H	-0.083963000	2.858499000	2.950014000
H	-1.098481000	3.923613000	1.965392000
H	-1.702526000	2.332724000	2.455970000
H	-2.214833000	1.878631000	0.137630000
H	-0.801638000	0.344906000	1.543515000
H	0.868137000	0.734167000	1.917883000
H	-1.490070000	3.325677000	-0.555910000
C	4.656701000	-1.106566000	0.006238000
C	3.819916000	-1.530966000	1.029299000
C	2.487825000	-1.173773000	0.988229000

C	1.973608000	-0.412428000	-0.065833000
C	2.845794000	0.003281000	-1.069761000
C	4.186447000	-0.337768000	-1.044412000
H	4.215169000	-2.128195000	1.839510000
H	1.823971000	-1.503248000	1.775680000
H	2.463272000	0.614951000	-1.876588000
H	4.861082000	-0.015137000	-1.825412000
C	-4.246044000	-1.762891000	0.080222000
C	-3.486857000	-1.746794000	-1.083684000
C	-3.602412000	-1.733234000	1.312117000
H	-3.979369000	-1.784242000	-2.049905000
H	-4.182551000	-1.761242000	2.228744000
C	-2.102079000	-1.689070000	-1.025143000
C	-2.219350000	-1.660919000	1.378115000
H	-1.510433000	-1.697063000	-1.931016000
H	-1.713116000	-1.637136000	2.337529000
C	-1.439354000	-1.640758000	0.211008000
H	-5.327878000	-1.811913000	0.028146000
O	-0.116188000	-1.577047000	0.287136000
N	6.060710000	-1.478089000	0.037484000
O	6.440061000	-2.222562000	0.922215000
O	6.794210000	-1.030945000	-0.824390000

10.2. Nucleophile variation

ImH

NuH

N	3.53800667997689	0.65875305528726	-0.98930384976816
C	2.25100890251069	0.69552380311056	-0.72827454132238
C	3.65012433756262	-0.03326531903711	-2.16872447165133
C	2.41525185455245	-0.41281557255926	-2.61424272904972
N	1.53630905040845	0.06189689744344	-1.68166300360381
H	1.78812604897066	1.16260069012845	0.12826505409314
H	0.53491908498253	-0.04391858245000	-1.70057146290906
H	2.09143605590249	-0.96025183562052	-3.48389046194414
H	4.60808586913322	-0.21989321730281	-2.62999419884454

Nu⁻

H	-0.90054541929888	-0.40272345976744	-4.30892941279668
C	-0.89353416864978	-0.40431642153952	-3.22344909707717
N	-1.17992956146070	-1.50352014312823	-2.51113365187477
C	-1.05755049106125	-1.07486989212703	-1.21952146564460
N	-0.59772703099417	0.69265382834448	-2.51156322112362
C	-0.70367530819652	0.26027264756624	-1.21973475603538
H	-0.52281460106723	0.91956601645749	-0.37955304747274
H	-1.22726725927147	-1.73644424980600	-0.37876186097503

VONu

C	-0.14795711802225	-0.69381845817637	0.32912413590045
C	0.40579041234179	0.08731477038388	1.25801394488165
C	1.85693747344644	0.29461086938047	1.29132314928555
C	0.61379755613425	-1.38008362756845	-0.75087510189060
H	-0.18429024357141	0.55819575431809	2.03499201418103
O	2.38040492090847	0.87947794585346	2.22355888403374
C	2.64099377860965	-0.24758055287597	0.13327704059397
C	2.09431087894135	-1.56849289641446	-0.41214644042604
C	2.84635954799235	-1.93703747068689	-1.68373138772925
H	2.74994979286936	-1.14844748662070	-2.43447363646524
H	3.90876942607114	-2.08089320320046	-1.47193302228340
H	2.45621660635448	-2.86620538442318	-2.10844846981002
C	2.26120768497090	-2.68032877830309	0.62074099661453
H	1.89949453366206	-3.63092367051270	0.22039129749121
H	3.31584724801625	-2.79969809846909	0.88059845089816
H	1.71069933864061	-2.46893279614158	1.54095663512609
H	3.68750682517766	-0.34163261931409	0.42997423297255
H	0.16403549371149	-2.34638422113665	-0.99335517547575
H	0.51202696491480	-0.75917641892570	-1.64997887332972

H	2.57458363667196	0.51323486784363	-0.65429597466394
C	-4.33835883596647	-1.21355999703724	0.38463556934155
C	-3.44586384750739	-2.31569244488460	0.30795963817261
C	-2.10540682341225	-2.11055100266463	0.27639630149975
N	-1.56906817588828	-0.86664657316981	0.32297022697459
C	-2.38903730605735	0.21049568178861	0.40628388682416
C	-3.74068412085510	0.07092299048188	0.43879300882481
H	-3.80425331822957	-3.33367527111209	0.28352286959234
H	-1.40829104532475	-2.93533230199209	0.24280617116091
H	-1.90438128085100	1.18496723503246	0.37065223775818
H	-4.33780574208006	0.96975137761149	0.47996025850597
H	-1.12329409618272	1.63289700711584	-2.34902622357872
C	-0.46498887495040	2.15442731423920	-1.66159631221473
N	0.86471522720857	2.17605160165224	-1.82100385234976
C	1.29524195016461	2.91821044222451	-0.75891210391123
N	-0.93110247275436	2.82026497637947	-0.59282493200879
C	0.20271155977843	3.30833781321536	-0.00936612493080
H	0.17174708025414	3.89719377304716	0.89854612189254
H	2.34522547295930	3.12130147189954	-0.59002395748948
N	-5.65820331854682	-1.37955853448050	0.39660038467602
C	-6.53922500468385	-0.23072071217460	0.49507925049214
H	-6.41309251101085	0.43510597024078	-0.36267796220455
H	-7.56808162231923	-0.57834771459178	0.51507775973829
H	-6.34540146933201	0.33432917519134	1.41014563459094
C	-6.23338116280772	-2.70883398779764	0.30834110047881
H	-7.31520263487488	-2.62080917576499	0.26826707980634
H	-5.89466770333794	-3.22145395276638	-0.59515117312750
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C	8.54256793649798	-1.09835994475627	-6.73201709630921
H	9.19619545013015	-2.05496828031761	-3.44220555144511
O	11.60954563127490	-2.35196241519605	-4.26110043772326
C	10.97436344376888	-1.49322269894755	-6.39270417133905
C	9.79748289035821	-1.73438753069121	-7.33568418504659
C	10.07722338694105	-1.08365224472260	-8.68339380101468
H	10.96861123280180	-1.51948575523021	-9.14156404411343
H	9.23743817168536	-1.23513900718501	-9.36712881886100
H	10.23966075712957	-0.00821515166569	-8.57372409873978
C	9.58412047546295	-3.23373941126194	-7.53430116769724
H	10.48521906179112	-3.69156501065218	-7.94954964057258
H	9.35006019266336	-3.74179177092442	-6.59580533449551
H	8.76033578728327	-3.41255735313776	-8.22970529832453
H	11.88112896964692	-1.98302838691778	-6.75394942580779
H	7.67019761265121	-1.42229493978678	-7.30511137270458
H	8.59768207872785	-0.00685437513773	-6.83359676066475

H	11.18391399995599	-0.41630951646841	-6.34097149376985
N	7.04574309591737	-1.28562348589318	-4.79317733077034
C	6.00479149979108	-0.64960962100394	-5.41910755892332
C	6.56305833052730	-1.70085464671358	-3.56591562956992
H	6.10396484275140	-0.20306957115225	-6.39547888520486
C	5.26676134769259	-1.30067442881104	-3.52474937768188
H	4.55270845306094	-1.45634629888419	-2.73058019082807
H	7.16423985284086	-2.25222495252680	-2.86464253864070
N	4.92861716076624	-0.63859686089206	-4.68491500487276

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C	8.69042154440840	-0.91889935754814	-6.63491842976723
H	9.50412925168371	-1.76924893844829	-3.35472640473401
O	11.90550201872190	-1.97976764688808	-4.25873973273567
C	11.13324519975068	-1.25830996122861	-6.39037807483189
C	9.93268389108747	-1.52412282696857	-7.29264136797492
C	10.13618041261531	-0.83702427954910	-8.63828494720498
H	11.03536802848925	-1.21926216604073	-9.12837195133886
H	9.28570027814635	-1.02250108136463	-9.30065169009018
H	10.24640116504761	0.24411671853926	-8.51691863348191
C	9.79365456945016	-3.02686321999926	-7.52171911542431
H	10.68419174535989	-3.39821184250262	-8.03616593226144
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H	8.78208691523698	0.17520031894818	-6.65733089946420
H	11.35995825948403	-0.18399230654633	-6.38448998634701
N	7.47806384568131	-3.04498978562662	-5.40086117831144
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C	7.82627938599868	-4.07326117650076	-4.58457173261344
H	6.20276377603607	-3.00176703133767	-7.11307497564168
C	7.16471670145673	-5.19473345710550	-5.03096326030864
H	7.19016907487554	-6.19867759173449	-4.62969036024645
H	8.52515299567992	-3.94232197110289	-3.77109892357960
N	6.40870013486825	-4.87466647060095	-6.12622383811534
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C	5.32633786179176	0.86090753638510	-3.34758658260249
C	6.62641368227832	0.80661228171077	-2.78795506915744
C	6.17800346809989	-0.54294958508608	-5.11130453264482
H	4.19782876171963	0.13674235705171	-5.07440191258045
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H	6.04872834541461	-1.10108570595837	-6.02309778320160
C	7.61286572369168	0.10134686779805	-3.40367199040247
H	8.61991732996646	0.07769895858163	-3.01668072209840
H	6.87493184908814	1.33412876836473	-1.87938535876813

H	3.09382959447435	2.02314545711968	-4.40763286621087
C	3.02836104693879	1.60149517443331	-3.40148324531068
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H	2.38191764754587	2.23743573278994	-2.80349858989001
N	4.33610185248794	1.54288629217544	-2.77587312059125
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C	-0.01454820901428	-1.58642693336552	-2.73619489063942
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C	-2.20930316677378	-0.87043809876591	-3.52481760193101
C	0.43035073741727	-0.16923443255007	-2.46082794275174
H	-1.65443365691504	-2.90929330020191	-3.09598804218062
O	-3.36223392289473	-1.10743233838385	-3.91527003389667
C	-1.70517992998735	0.55347068772055	-3.49115210315173
C	-0.73202495834491	0.82332038266867	-2.34531046548291
C	-0.17507661032703	2.23658089326974	-2.46672607986608
H	-0.98010272556017	2.97312437088681	-2.39377217577660
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H	0.33086823297840	2.37681350870345	-3.42570966836068
C	-1.44079041295274	0.68329236162063	-0.99998828073024
H	-2.27006388041518	1.39277903124710	-0.92970109809621
H	-1.84055718089897	-0.32275403673417	-0.85901729649204
H	-0.74645734948267	0.89117054068061	-0.18125935637531
H	-2.56971940792515	1.22030011062404	-3.43734005049078
H	1.02187968484492	-0.15279910385997	-1.54267799719175
H	1.08922851413199	0.15129320725694	-3.26817479337960
H	-1.20100238500461	0.74961064902296	-4.44671411050297
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N	1.14259146307255	-1.95041552427032	-4.39623489679011
C	0.56027665757523	-2.09000586651962	-5.58867220571223
C	2.48281265092086	-1.95307643856105	-4.64029685602588
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N	1.42281578860267	-2.19242163044546	-6.60368293217295
H	-0.51670083856945	-2.11342446560997	-5.70092527884828
H	3.56799388413600	-2.15714398085579	-6.56866016293112
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MeMalH

NuH

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C	-1.16681918766350	-0.18854458397708	2.09027456157357

C	1.24582689784809	0.01571161372145	2.66618831869760
O	2.35305627397657	-0.12096415519399	2.21237029543510
O	0.89913920877626	-0.32961129468835	3.90181319755621
C	1.93107105757222	-0.89259290636867	4.71599502351135
H	1.46782761729562	-1.09860296739673	5.67727937831353
H	2.30544380809347	-1.81295745362854	4.26747281937089
H	2.75002492002329	-0.18233355249650	4.83117383784071
O	-0.95587465692441	-1.43405916418243	1.67462603301610
C	-2.06183913256959	-2.33286889833801	1.79334306222187
H	-2.90413733816579	-1.97617777100053	1.20040298895269
H	-1.70702313862735	-3.28807430766301	1.41549997569108
H	-2.36295373398477	-2.42331723755304	2.83738614400804
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H	-0.39954153696451	2.11313502007838	3.45003270516982
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H	-0.92066277333216	2.54971026755677	1.81738160321548
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Nu⁻

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C	-0.00883434121982	1.02319866462268	-0.28792152693256
C	1.45142403215301	-0.50844834509141	0.95064392918121
O	0.61209485116780	-1.20819401887117	1.51764989974072
O	2.79006869480879	-0.79779677932605	1.14991022536235
C	3.05548608970593	-1.89039448466957	2.00432393917627
H	2.66308900520770	-1.72017213099410	3.01003223058600
H	2.62293977300391	-2.81699237544459	1.61884783442452
H	4.14081392003116	-1.98362984607266	2.04626762903223
O	0.01682960238383	2.08508384043971	-1.17646513661151
C	-1.24623734729113	2.59493215099651	-1.54769289851021
H	-1.85288314661705	1.84140469871656	-2.05581480980308
H	-1.80477144510768	2.95715724574380	-0.68072563662519
H	-1.04856796298373	3.42393283671801	-2.22744998309550
C	2.51906851552688	1.28089912766775	-0.46607715877335
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H	3.05552779554021	0.66952984607606	-1.20351328769290
H	2.25447241382967	2.21703406958168	-0.95411236481280

VONu

C	1.51862704624136	-0.83903178269566	3.18301914034433
C	1.89136848675577	-1.71983276945557	4.11926848098826
C	0.95672584424969	-2.72749552870874	4.61317823481859
C	0.17148092984678	-0.81425920937404	2.55745252113477
H	2.87067446828219	-1.69514696946373	4.58171023325872
O	1.31051159716711	-3.55825435361494	5.43399939890952
C	-0.45655507968348	-2.64289803924244	4.11422579567915
C	-0.56560247951888	-2.15213661664932	2.67030441998812

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H	-0.48010167064996	-4.13801062535134	1.81718182179153
H	-0.06123503837173	-2.84542947123799	0.68286332171653
C	-2.03078430365230	-1.93288147755570	2.31787711811779
H	-2.48598208936736	-1.19859799877538	2.98693949891173
H	-2.12948863146170	-1.56818036560128	1.29170201639407
H	-2.58716654597291	-2.86996325447478	2.40004015686566
H	-0.97217708605819	-1.93309607232175	4.77586944789369
H	-0.42758107732537	-0.03945679610936	3.05301447573902
H	0.26092829103303	-0.52068591033403	1.50723140649396
H	-0.93415765018030	-3.61653771184825	4.24291978621263
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C	2.89123210679504	2.35413109548034	2.01938901835784
C	2.02163031691155	1.39277154895652	2.42614158570783
N	2.44785085830180	0.13774064207695	2.72460677830779
C	3.76471814069226	-0.16589487354436	2.59670274487419
C	4.67845821219042	0.75158163955501	2.19649282427364
H	2.49092101650189	3.33669069916550	1.81882952803795
H	0.96820467154646	1.61228319816238	2.58377122400305
H	4.03994322903425	-1.19052908417475	2.80028608127064
H	5.70547754313491	0.43437225291587	2.09621963185217
C	-1.87096102177021	1.35944860793965	4.51301797966822
O	-0.84870261900464	2.47027898969997	2.65369184572735
C	-1.82956460096822	2.04596414937962	3.27644620121920
C	-0.67364008379284	1.17205848611394	5.24932784415660
O	0.47795058415694	1.51909451293869	4.98452880310191
O	-0.90412098830644	0.47847743298321	6.41534975172392
C	0.24133650488500	0.20270819622012	7.19787140680457
H	-0.11233841618673	-0.36156364300959	8.06006373599578
H	0.96983763370363	-0.39238942966779	6.64206914935301
H	0.72862432885604	1.12130152845427	7.53244841490704
O	-3.07573319932550	2.22172360620215	2.72370636773590
C	-3.10336949051879	2.84004404863019	1.45232003852795
H	-4.15296102463640	2.88178616780166	1.16306665645885
H	-2.69178158269580	3.85111736948680	1.48921253249725
H	-2.54106380704213	2.26249098438401	0.71486851990401
C	-3.16455663767560	0.83840923262505	5.07875660656562
H	-3.96482207055271	0.91644155981870	4.34553098637677
H	-3.08005357130210	-0.21289095503386	5.37065606783061
H	-3.48493790442101	1.38295257397507	5.97513162285208
N	5.15023764545947	3.00687369964265	1.51247986268548
C	4.70112023194369	4.34895090595572	1.19082304404906
H	5.54803588336750	4.92563335089659	0.83026876508220
H	3.93896218318606	4.32665606546371	0.40877980393590
H	4.28656964203249	4.84735031257946	2.07156085770377
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H	7.10824068958225	3.59725156097611	1.16538757570204

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C	0.27944111861889	-0.31061117034468	-0.43222840275138
C	0.55544926098084	-1.33573901066346	0.38311126671001
C	1.92324878561668	-1.79179513041118	0.62360219334651
C	1.36413057189925	0.43073169747677	-1.14961911563209
H	-0.21516201025091	-1.87694099658054	0.92124796919991
O	2.15232313386358	-2.70337539241889	1.40246439295034
C	3.01900393978640	-1.11778610016869	-0.15269720635509
C	2.73005055981023	0.34971081715614	-0.46586127573052
C	2.73519523995949	1.17217998446977	0.82087709414517
H	1.98031796389478	0.82717222163015	1.53024679511430
H	3.71299321076337	1.10624756345483	1.30470667044266
H	2.53210071452195	2.22341347619190	0.60105929161593
C	3.79356686109779	0.89237088173025	-1.41069271600992
H	3.82334132155538	0.31735933230231	-2.34005858029306
H	3.58844928692527	1.93709538386910	-1.66049956640313
H	4.78168777191271	0.84360162228969	-0.94574774543599
H	3.11896821340699	-1.67608617837834	-1.09378643445542
H	1.44531379075141	0.01510236136875	-2.16270653906606
H	1.07963228009063	1.47994379731002	-1.28088690877329
H	3.95730797280191	-1.23465528194430	0.39439217579843
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O	-2.77326803625681	-0.37343070587025	1.00208564296646
C	-2.16806430053963	-0.69883268307178	0.01217097486082
C	-1.30246095705212	1.58837027642954	-0.11156047966198
O	-1.97390162628035	2.44691321786178	-0.62017270972216
O	-0.61999251935490	1.73933750211337	1.00987729641332
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H	-1.76223140483907	3.19172187740143	1.95265502266493
H	-0.08280308760356	2.95798958322068	2.52308395722590
H	-0.40085655523445	3.80330345790949	0.97815516573874
O	-2.32483026502008	-1.85700586816283	-0.60702702757884
C	-3.25292059197192	-2.77074455283695	-0.01262389583153
H	-2.94206423747406	-3.01373645380439	1.00355510286922
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C	1.35334520775080	0.43675834709947	-1.92799052786136
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O	3.99813767432559	3.10257557835496	-0.25202810150060
C	2.79511157482919	2.41444582211538	-2.18251558699299

C	2.34827205971410	1.12807189598650	-2.86777675820616
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H	0.74039220788437	2.07731990431308	-3.97375366987961
C	3.54201539376893	0.23009618076712	-3.17942512904013
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H	3.20992948126576	-0.71289820501839	-3.62328020441086
H	4.20751472160976	0.72334623468655	-3.89272363473970
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H	0.97564880892761	-0.46176091229467	-2.41521662472011
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H	1.96084641291576	3.12737998131891	-2.17295216403846
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C	-0.76579985858434	-0.63565877889480	0.28286387813718
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O	-3.51850698314199	-1.42947389659123	-3.26603091496132
C	-2.34517860189898	0.64235419141545	-3.28953843820384
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H	-0.13454942821964	3.18562691972436	-2.51923341672374
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H	-0.23373798594870	1.47761727047491	-0.67117413972356
H	-3.25433368727439	1.02140423485409	-2.81322091226116
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H	0.17290854917661	0.86724947947561	-4.31702929670751
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O	3.27090083765712	-1.45656334506977	-4.77363240804094
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H	5.25092503138347	-1.44581286089511	-4.42396607750419
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Oxime

NuH

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C	-2.01494689846261	0.93852196320408	-3.59913015225787
O	-2.60360659315267	1.90304538158760	-3.16951978050495
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H	-1.08447842272085	2.92022936919319	-5.06583186984297
H	-1.04277030215998	1.86827326564729	-6.51126692334607
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O	-1.12865882432268	-2.36920398100505	-2.57723306060675
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VONu

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H	-3.65845638964884	-0.96254092156752	-2.28345519560879
H	-3.85272956285293	-2.62392042664208	-1.70903487581723
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H	-1.92966137721374	-2.23465264941135	-0.20515019127769

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H	-4.07953928697785	0.53182769510834	1.18944377179117
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C	1.89260636591049	-1.43309512157615	-0.19170553962612
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H	4.42602373558063	-2.65343996778847	-0.42913878062302
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H	4.52555879749029	-1.24632291340024	0.65411932983083
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H	5.67832353234808	-0.27837864015637	-2.28257610535554
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H	2.84831515854595	-0.10647189720675	3.42383391448423
H	1.41199122392025	-0.45486623362382	4.41803888553509
C	0.99436984259630	0.44838386318825	2.52582077271072
C	1.65781114866345	1.45601637125785	1.71900646716763
O	2.86587947767864	1.64745990931809	1.71793517919061
O	0.84181977931503	2.17338284746061	0.92061396693192
C	1.47728483404671	3.15471011066402	0.11499481532707
H	0.68336136779191	3.61542777276331	-0.47025773080109
H	1.97215971477463	3.90791707931130	0.73080134027856
H	2.21374035439433	2.69986909204808	-0.54968723770733
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C	-1.59654074619415	0.75840355497589	6.03881223431504
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H	-3.87614899653752	-2.09762676858897	3.77339318218574
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H	-4.62503059525964	-2.25922655088559	2.16418138414226
C	-2.75088930208336	-1.26344947123562	2.17412696001295
C	-2.48562968722742	-1.74979709846851	0.77874548471836
O	-3.14256918889809	-2.62717681804938	0.27470367644373
O	-1.48387323771623	-1.12635721001787	0.18528790752383
C	-1.17686497444076	-1.56996179149172	-1.14029334710596
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H	-2.04032752113306	-1.43384392598744	-1.79181343087812
H	-0.34790759749423	-0.95007390341273	-1.47052681786341
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C	-1.77834731824859	0.49497724903207	6.20952307659925
H	0.50573461347369	0.18877373504157	3.59220469970954
O	2.17943862488050	1.22331941087018	5.27853656453581
C	0.40172218577886	1.45268407680102	6.83992228406674
C	-1.10169820729297	1.71827248048913	6.83288012919661
C	-1.60541240242206	1.87002741832051	8.26266804010283
H	-1.39675975292722	0.97013646000740	8.84762063600585
H	-1.11729503516823	2.71643451360069	8.75351620215684
H	-2.68500950197260	2.04584936457275	8.27965367161077
C	-1.42603763763649	2.98876525832003	6.05126083220323
H	-1.05838873878589	2.93495837100853	5.02447830016268
H	-2.50653774879311	3.15518087825669	6.02026584578606
H	-0.96343409847630	3.85604310957764	6.52969730952969
H	0.95447777496355	2.33576950771448	7.17258297269699
H	-2.85774575438195	0.65554869889394	6.15518811806557
H	-1.60365981636329	-0.35668332052468	6.87223327710372
H	0.62259498453747	0.65071703218423	7.55569450630973
C	-4.02448299433611	0.43721887481959	1.65427086240284
C	-4.30888140209690	-0.29249782113031	2.83585905309074
C	-3.38999755655306	-0.37009289576456	3.83419052777905
N	-2.18603407072077	0.24126461880860	3.75498134205103
C	-1.89959109338179	0.97145648646350	2.65686491653315

C	-2.76571059567670	1.08625422725002	1.61441258917105
H	-5.24768515811589	-0.80849556237633	2.96939434201897
H	-3.57397311437309	-0.93908136998115	4.73176104686938
H	-0.94426904971399	1.47513886372775	2.66981339641076
H	-2.46924268624299	1.69475679124165	0.77341076898631
N	-4.89295427721170	0.51496993718180	0.64637976283890
C	-6.18195976708557	-0.14304031084008	0.73748908650358
H	-6.73072144428537	0.03197061061906	-0.18350289096349
H	-6.06449133964458	-1.22162210122975	0.87105141371926
H	-6.76768327830546	0.25269343607431	1.57153892792658
C	-4.55840934132990	1.26214865307623	-0.55067301694764
H	-5.37302907707077	1.16727833313325	-1.26309968138132
H	-4.41371898598804	2.32278063642436	-0.32729864421907
H	-3.64717777504079	0.87325115249147	-1.01218871579469
C	-1.22880621803758	-4.39818699829596	5.03880530589338
H	-2.29398111272691	-4.30683962835883	5.27150543985730
H	-1.11656240334542	-4.17295176943750	3.97488191155729
H	-0.91100374546351	-5.42088583172389	5.22923413221368
C	-0.43059175077493	-3.43956909118336	5.85271439555725
C	0.54220020676006	-3.95854549360276	6.83152225296966
O	0.72803653962649	-5.14445247333535	7.01458811279287
O	1.20441294223701	-3.01442212924173	7.50220940852604
C	2.15962030347694	-3.48581685293314	8.44917200014811
H	1.67500590655766	-4.08807866727689	9.21887485942665
H	2.92820753351489	-4.08290561583707	7.95658547176641
H	2.60035752184468	-2.59457040954187	8.88971457680489
N	-0.53480928854112	-2.15812925751980	5.75405972713577
O	-1.40188607680105	-1.72186273472179	4.89510489559613

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C	-0.10020874998771	-1.35014354443533	-3.20720186135748
C	-1.43998745148544	-1.69705850642657	-3.19708233623437
C	-2.46169697761060	-0.71985467589117	-3.19322842358061
C	0.34333194756415	0.06906849668807	-2.97906425888317
H	-1.72749039010915	-2.74163661864925	-3.22183400557156
O	-3.67415273763648	-0.99282194923106	-3.25558919810567
C	-2.03738295902826	0.72923740947767	-3.08539488024024
C	-0.73254197988382	0.93652935227007	-2.31957941479194
C	-0.30335393389334	2.39545026789690	-2.41592512953869
H	-1.05318810562231	3.04705414033377	-1.95847281958989
H	0.64619040504587	2.55711210195820	-1.89718423166857
H	-0.17771310004872	2.69877898965331	-3.45888655436826
C	-0.90774932902938	0.56642820286043	-0.84876883556244
H	-1.67859081915433	1.19063390907022	-0.38830264092889
H	-1.20017274437407	-0.47870969415896	-0.73096678785344
H	0.02659898026466	0.72279208236639	-0.30253221335225
H	-2.85682763607743	1.28615025558494	-2.62247988266401
H	1.25438428268340	0.08231303338913	-2.37854230262483
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H	-1.91976430872531	1.11796440145680	-4.10554902720827
Cl	1.00302559775154	-2.56695942100793	-2.52951019657192
C	1.29166618128598	-1.97755460263274	-7.55886532855771
H	0.92168863234049	-2.96711153948417	-7.27610221103157
H	0.41096458059633	-1.35820722094501	-7.75420636445708
H	1.87986797192272	-2.05929765471566	-8.47041516147392
C	2.10688255600731	-1.39169015458634	-6.45737862581531
C	3.48834477259011	-0.97334569546550	-6.72354279118645
O	4.04319880371499	-1.13338422861266	-7.79412934647029
O	4.10077416240906	-0.39112079229482	-5.68549146694974
C	5.44812879261673	0.00748099994843	-5.91182729127298
H	6.07178345361225	-0.85359126881942	-6.15720528393806
H	5.50650847828147	0.73407775737268	-6.72367034095993
H	5.78217015096106	0.45841330797225	-4.97992620548975
N	1.66561772194525	-1.23220891323039	-5.25037986686635
O	0.44621524706672	-1.60515751372243	-5.03292714775566

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NuH

C	-1.54230323540145	-1.70365001661609	1.34511232590806
H	-0.99940947729379	-0.95309932618640	1.92350068181456
H	-1.15565367165676	-1.70512846441413	0.32390088285408
C	-1.46013075307443	-3.09622265971507	1.99210193786799
H	-1.05271231719393	-3.84700415487409	1.31560721162274
H	-0.88673334659778	-3.09318946118488	2.91854620518634
O	-2.81126955641559	-3.46201272602696	2.30433046348618
N	-2.96353455359100	-1.47538766399113	1.37704380108990
C	-3.66348182442594	-2.48571421479538	1.91889104828388
O	-4.86046212550470	-2.57774174936109	2.07358318075780
H	-3.42017703484463	-0.65695293183477	1.01513945712847

Nu⁻

C	-1.58316098273496	-1.71807808218750	1.35629216175607
H	-1.02128759063257	-0.96847915397354	1.93036580299818
H	-1.15830082457580	-1.71054242356252	0.34357269314313
C	-1.46084609363086	-3.11394945039733	1.99931011597592
H	-1.03755138443039	-3.85773508646799	1.31672350415292
H	-0.86126498743023	-3.10761873859608	2.91484766448824
O	-2.79321375012660	-3.47377490346180	2.31548209440978
N	-2.99933500076981	-1.42722163486009	1.34286462676910
C	-3.63956358104377	-2.42696365474085	1.88970404239327
O	-4.85036269162498	-2.59828226675229	2.09022317891338

VONu

C	-2.13786927813815	3.49268112348289	2.63794597547252
C	-1.78540229386656	4.66294282554194	2.09015067112074
C	-0.77461649481735	5.51433089568573	2.71557675193899
C	-1.53797668020801	2.95950105278747	3.89213848442519
H	-2.20468055150737	5.02395361661527	1.15899862919940
O	-0.50531473691048	6.60685416560285	2.24447738182548
C	-0.05932969267354	4.95997653773667	3.91311402998061
C	-0.93036932554370	4.05035515863138	4.77844842872890
C	-0.07141574796703	3.38937244023087	5.84787906662249
H	0.73887072287317	2.81235020339914	5.39442252270518
H	0.36959523520783	4.14410638701256	6.50395830093733
H	-0.66993916587623	2.70941976950353	6.45889689379236
C	-2.03718254806365	4.86354795082019	5.44531272653612
H	-2.69052905871023	5.34409367315582	4.71262600069073
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H	-1.60395345948921	5.64621635384550	6.07277614274852
H	0.35039390110633	5.78993992708111	4.49250465595965
H	-2.29722339808106	2.40336765980520	4.45006741070652
H	-0.76362255891141	2.22933240995376	3.62695408576145
H	0.78982232490171	4.38237232119226	3.52299613643995
C	-5.01545379440687	1.06832729124794	0.72817267198422
C	-3.97951448996047	0.52467882661593	1.52616546917445
C	-3.08138991652453	1.32882190886148	2.14997023337550
N	-3.13104334052991	2.68216351481756	2.02110887339418
C	-4.13257765794582	3.23879239829953	1.28793247423286
C	-5.06112221045461	2.48737919890818	0.65026341602654
H	-3.87512348066154	-0.54013407401277	1.67199363312067
H	-2.28874221127428	0.89089202320670	2.76003564068142
H	-4.16979353625119	4.31771035880549	1.26854276272643
H	-5.84168460010550	2.99924624438875	0.10766086985196
N	-5.90331343748964	0.30178242512924	0.10338393029700
C	-5.84921684846198	-1.14232634427823	0.24440691241466
H	-6.65275011655757	-1.58243825063994	-0.33882687390223
H	-4.89716192511155	-1.53423642591579	-0.12142105128700
H	-5.97316064768573	-1.43802044919312	1.28928323328572
C	-6.95752120249608	0.89654575484602	-0.69750850319219
H	-7.52948563768205	0.10255275135157	-1.16877969239037
H	-7.63310458739052	1.49389872613135	-0.07926920117241
H	-6.53967920524931	1.53293158596067	-1.48081243907121
C	0.07404815685080	-0.50373744884312	4.50487960788125
H	0.64780224570692	0.38368505609816	4.19419559839640
H	0.60717952531131	-1.37610672633837	4.11365273593232
C	-0.06062682624749	-0.56403717068343	6.02907882644088
H	0.01642651045953	-1.59110943650532	6.40438407768680
H	0.65750010630233	0.06164883109440	6.56258535621960
O	-1.37424234520317	-0.08007056295951	6.26936968076519
N	-1.29232145102919	-0.43605320728109	4.02830865511336
C	-2.06182740489663	-0.13749383357872	5.04729532081872
O	-3.27235742642292	0.12362258703515	5.08208899919870

VNu

C	0.25195351675315	2.73314335382818	3.28331876901411
C	0.61861769417309	3.99272418181175	2.94765380596812
C	0.38387035108857	5.11881827633707	3.82389279062761
C	-0.46780439256060	2.43367530807742	4.55990870445447
H	1.12642109536597	4.21225875244597	2.01752575428191
O	0.72334240474661	6.25343606487501	3.50747276347455
C	-0.24327147778876	4.83653347980407	5.16089091215547
C	-1.19727407813764	3.64630357252477	5.14448514909211
C	-1.62788573626340	3.31561635684570	6.56751294052932
H	-0.76241472936943	3.09067024952455	7.19630521220528
H	-2.16262489658743	4.15933128639966	7.01134007766929
H	-2.29393281214229	2.44845503307827	6.57878501477875
C	-2.43522744265937	3.97463703464700	4.31163188793932
H	-2.18089923892889	4.20460310429514	3.27443756658819
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H	-2.95318158816522	4.84010249811694	4.73226935774644
H	-0.74082027045733	5.74332178496063	5.51284478213070
H	-1.17654400808350	1.62091595617745	4.39968374175166
H	0.26176599831402	2.05667991340487	5.28575747801057
H	0.58358427323161	4.63103012619333	5.85410426802081
C	1.10063740068291	1.90977060818167	1.10237320657412
H	2.13790889028124	2.24445838489329	1.19204654884209
H	0.53323521653973	2.65131820839188	0.54102034858396
C	0.98590937832780	0.52078843867189	0.49897057787734
H	0.09130702472482	0.41206679713023	-0.11621673091809
H	1.86482163721660	0.22170041365019	-0.06700714006984
O	0.85938537265650	-0.34997290517896	1.63083688118442
N	0.51953932307984	1.69590290394558	2.41619911666443
C	0.50374892913606	0.34608306399141	2.71964693426949
O	0.24916343941804	-0.18407239259952	3.76748296816267

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C	-1.25702860437046	2.42626272840377	2.87436647068332
C	-0.89394317604884	3.61216624033537	2.26551045026964
C	-0.26839123903428	4.68000213825032	2.96423838488291
C	-1.04089889605618	2.26746946834538	4.35839545032532
H	-1.05179554955226	3.75007697935412	1.20121895680172
O	0.11516685125298	5.71556978264205	2.40172330001358
C	-0.11206729491299	4.54979410068856	4.46345778204869
C	-1.10855200404271	3.59664604263793	5.11763644304228
C	-0.70473881892303	3.34557892979858	6.56519851730964
H	0.29993910796573	2.91801466649738	6.62275911909722
H	-0.70964440951506	4.28111110905419	7.13084771008675
H	-1.39975257347540	2.65366020339608	7.04959190664314
C	-2.51811153995420	4.18184458909982	5.08818085300387
H	-2.84326360041936	4.40735611169487	4.07033015832982
H	-3.23311357591277	3.48082263383257	5.52768162307711
H	-2.55374805476681	5.10884037437973	5.66633815959303

H	-0.18317977760294	5.55171735275912	4.89530081967285
H	-1.77308090621149	1.57240591228614	4.77472091162201
H	-0.05697080577542	1.82988063423060	4.53180055608156
H	0.90740982525100	4.19228033554454	4.65683051350376
C	-4.68225379153426	0.40630267757705	1.37616367182086
C	-3.74413721034134	-0.23034493381209	2.22720592186561
C	-2.65279122969129	0.44394590565154	2.67081588131791
N	-2.42964712597357	1.74049289167131	2.36086393512345
C	-3.32698827418343	2.38545999187841	1.58739917021810
C	-4.42944115716979	1.76870447729819	1.08466317213473
H	-3.85238589439842	-1.26576227550441	2.51308164617641
H	-1.88760197200217	-0.03216998204289	3.26321042629772
H	-3.12743938727002	3.43111049847083	1.40773505787778
H	-5.10399369186547	2.35219604744474	0.47666624425616
N	-5.73998200099800	-0.23679271695741	0.88255381103756
C	-5.97481412593251	-1.62773711426399	1.21821709818074
H	-6.88860482297926	-1.95616084543867	0.73142326055752
H	-5.15146856220787	-2.26023291498364	0.87527761723027
H	-6.09110719431526	-1.75770701126792	2.29717801771156
C	-6.65512270128863	0.44226108516398	-0.01403334973301
H	-7.40498248192849	-0.26660606183078	-0.35368767102395
H	-7.16164814687026	1.27039862029011	0.48963844965516
H	-6.12768773963620	0.83370381970373	-0.88759544280744
C	1.40843065249747	1.47181258813219	2.53076392735476
H	1.81753510353353	1.00694477582813	3.42996764369858
H	1.38939194722132	2.56360005144428	2.68417487141659
C	2.22109828101711	1.11922690888423	1.28934857139926
H	2.92599827015198	1.89387167762174	0.98713868855114
H	2.75324147080731	0.17039508727714	1.40549466958105
O	1.23345896948935	0.97060440411785	0.27318170202354
N	0.08172088091663	0.99585558587667	2.21984584860828
C	0.01053570304720	0.82960807641854	0.88926374805001
O	-0.96620872199099	0.58692644211980	0.19526928733116

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C	-1.30977597719796	-8.02366587091849	-6.97908168306660
C	-1.50338488519972	-7.87600827141259	-8.34967737731007
C	-1.80553564577951	-6.60029554353775	-8.88052161042205
C	-2.07823723714722	-7.17993825292738	-6.00106670569577
H	-1.27995171810817	-8.68981710264343	-9.02853196837268
O	-1.95000403277083	-6.36162048758677	-10.09297220936408
C	-1.90457548553519	-5.48515058041166	-7.86579443258171
C	-2.67437104258180	-5.89270108062526	-6.60837291325343
C	-2.59253516906174	-4.77182540843809	-5.57862963294896
H	-3.04159544789259	-3.85403752159803	-5.96912369949460
H	-3.12447678429035	-5.04646045537614	-4.66287749453716
H	-1.55255322712202	-4.56313604610444	-5.31547978593786
C	-4.13769988309451	-6.12906479324884	-6.97990725237800
H	-4.57160334650770	-5.23188148504249	-7.43069526161814

H	-4.23583496088360	-6.95132510981714	-7.69299883942910
H	-4.72157730622971	-6.38093283637147	-6.09034858536398
H	-2.37576425753310	-4.61890009007142	-8.33691707611851
H	-2.89642459144555	-7.80280036622155	-5.62730188500172
H	-1.44426283476997	-6.95199429448050	-5.14437886926338
H	-0.88276938015030	-5.19441779732885	-7.59012171874624
Cl	-1.19222202350152	-9.71257522260309	-6.44296902469907
C	1.37135714717026	-7.29701543840677	-7.75102185088293
H	0.74652411923667	-7.19376702794493	-8.64488774010290
H	2.04537759758910	-8.14552218911192	-7.91866361279269
C	2.14296166595600	-6.01513168270936	-7.43695401394820
H	3.21018436055345	-6.09091896136831	-7.64747909214588
H	1.73719564871032	-5.14367776697176	-7.95978723638157
O	1.96061903624086	-5.83092897101682	-6.03415991733235
N	0.55723956621608	-7.50425524433777	-6.58234682262714
C	0.94291608878896	-6.67190957331304	-5.61996169402847
O	0.54785141734142	-6.57051770205370	-4.46271203915444

PhthNH

NuH

C	0.55550543008168	-1.31830814364662	0.06483934737955
C	-0.66980409613617	-1.53008219251986	0.66019213089168
C	1.63937341415723	-1.07413943651343	0.90487467487107
H	2.61961730568801	-0.90286533340106	0.47602566111119
C	-0.82288941404587	-1.50081113796397	2.04032779313950
C	1.48623025814367	-1.04631913374506	2.28822028368642
H	2.34961417936422	-0.85434416969016	2.91424469669351
C	0.24383996371078	-1.26082635942263	2.88013917350064
H	0.11985331257107	-1.24016375217506	3.95622097698937
H	0.67028263987958	-1.34115445797763	-1.01220737107480
C	-1.99666497170263	-1.81433537245040	0.05481577183546
O	-2.29337668230097	-1.92575390180723	-1.10969526287607
C	-2.25190194417300	-1.76195800920788	2.35158004813391
O	-2.79778986842950	-1.81846159820622	3.42640490394545
N	-2.86903474121422	-1.93529826333802	1.12387329519742
H	-3.85399927459386	-2.12964522693475	1.01855924757571

Nu⁻

C	0.56064421943049	-1.31725699413710	0.06861215100563
C	-0.66546479324045	-1.52840603467959	0.66301106220826
C	1.64983696801591	-1.07262466698948	0.90644348974177
H	2.63103012682771	-0.90257257925658	0.47713488559439
C	-0.81792182128102	-1.49912190561833	2.03769697192472
C	1.49643124743529	-1.04380939730691	2.28904211738506
H	2.36012908059247	-0.85186159700608	2.91608029466581
C	0.24906979419525	-1.25851646860865	2.87710616889137

H	0.12574773556541	-1.23697739915986	3.95438343107379
H	0.67714001683220	-1.34061973103477	-1.00939841663839
C	-2.03364217534092	-1.81924226036755	0.10252063161243
O	-2.27652783647538	-1.92009987222339	-1.09756880316631
C	-2.27666075819991	-1.77013343664667	2.29722270160531
O	-2.77683735841991	-1.81812772375982	3.41838006151864
N	-2.92806940593716	-1.94892958020520	1.11794411757750

VONu

C	-1.67821160900241	-0.14838616642662	-0.28245730290177
C	-2.04912868571306	0.18208689481996	-1.52526204535336
C	-3.07866632885542	1.19392349379241	-1.76170852387052
C	-2.30849073115148	0.40976054604734	0.94397086512085
H	-1.59987067998080	-0.27173167192619	-2.40051623064281
O	-3.47685286437754	1.42585139805875	-2.89028220936316
C	-3.56480549847897	1.94727225560696	-0.55885387279962
C	-3.66495169930248	1.06972411351492	0.68884494056626
C	-4.02202447602818	1.93107404283295	1.89248673634375
H	-4.99156566757469	2.41293217194465	1.74403872305748
H	-4.08139165203355	1.32057275946850	2.79755475398243
H	-3.27175712964779	2.70920984739283	2.05428390772007
C	-4.74024878644538	0.00307591482243	0.48963139308107
H	-4.50108249653612	-0.66856103781830	-0.33851444956929
H	-4.84690178901725	-0.60087233416536	1.39404013789952
H	-5.70402622861308	0.47180785137472	0.27658149517809
H	-4.52312085649647	2.41347325036286	-0.79562022730380
H	-2.43156188818246	-0.36213572894681	1.70758071942645
H	-1.59726194300460	1.12723623440812	1.37568712911197
H	-2.83962352664977	2.75257287367752	-0.37985120350377
C	1.68486791268903	-2.65133492309966	0.26337322326839
C	0.54149839327190	-2.74257305778225	1.10182164618784
C	-0.52606101795704	-1.93360553489307	0.90198659380175
N	-0.56007223264611	-1.01372548562536	-0.09873588412445
C	0.51323289321977	-0.91813810175246	-0.92935916146465
C	1.60678680038972	-1.70320327774061	-0.78992054679192
H	0.49454274050918	-3.44759939501139	1.91779442437721
H	-1.40361913519743	-2.00393250441064	1.52527697981474
H	0.46437195782489	-0.14242947931879	-1.67903037552471
H	2.43360409045228	-1.53990247753567	-1.46380846570902
N	2.76603923393709	-3.39227312933677	0.46075118903803
C	2.83486401836555	-4.30733197682876	1.58604943990971
H	2.73842597036185	-3.76772968129667	2.53146226196957
H	2.04666589324330	-5.06143923737551	1.52503997618460
H	3.79697877614314	-4.81037233061798	1.56947041763413
C	3.92137734499751	-3.25031878796916	-0.40953782108700
H	4.68516785633934	-3.95378944348308	-0.09155038045925
H	3.65464946759159	-3.47096005245327	-1.44566343435321
H	4.32434637069545	-2.23678896468998	-0.34533541713574
C	3.03051300635709	1.68827376425846	-1.15782602605236

C	2.59220835934649	1.36945153348131	0.10899997759107
C	2.21585075799113	2.51706551299401	-1.93167442111680
H	2.52235332416555	2.78530345068317	-2.93650528352810
C	1.39609013787773	1.85670266217812	0.60596027703491
C	1.01050832070143	3.00271447416886	-1.43468159973848
H	0.39514033071355	3.63955807929097	-2.06013922885231
C	0.58370157943602	2.67912037396927	-0.14573530798737
H	-0.35606156321542	3.05626258647474	0.24239379930005
H	3.96559154296345	1.30136780354315	-1.54760847147226
C	3.14463105816243	0.46451407847937	1.17841865194367
O	4.19011106906955	-0.17109179562937	1.06769944124216
C	1.24600835140941	1.25689100889644	1.97912804829908
O	0.28857139030569	1.47125101037676	2.71942765992765
N	2.30357195957638	0.44680199921413	2.24632454469320

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C	-6.70133401159543	-2.26064043247770	4.75045650673323
C	-6.67968704838339	-3.51583354662287	4.27914627875641
C	-5.88975036314938	-3.86708445662929	3.10368166860941
C	-5.92662563054642	-1.14395901904400	4.12874598285232
H	-7.24461714101714	-4.31062622562367	4.74736781162763
O	-5.86103820529755	-5.01460383293575	2.68798897717788
C	-5.16102095718242	-2.75382945074217	2.40578620647565
C	-4.70724460368026	-1.63518518202025	3.34255825864337
C	-3.62667552290714	-2.14890892341267	4.29115042956597
H	-3.98544890944045	-2.96904381794294	4.91749791704952
H	-2.76723262983690	-2.51149681300498	3.72190465808956
H	-3.28512400157868	-1.34558651506220	4.94860156447399
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H	-4.89905493942631	-0.09466702245701	1.82718454769228
H	-3.83366357505614	0.33939028482142	3.17490565732618
H	-3.28089920035648	-0.80594661946762	1.94473112297915
H	-5.86282255570773	-2.34396491849212	1.66635326701319
H	-6.59085298958679	-0.58476623259533	3.46132007760095
H	-5.61555179680000	-0.44300749984020	4.90790566206798
H	-4.32104759186975	-3.17971315404518	1.85245963364756
C	-9.62727317636827	-0.00098736976896	8.09123559855869
C	-8.78988162410948	-0.87604988837087	7.43100992446204
C	-10.03138950774608	-0.35502150596974	9.37555634252124
H	-10.68917595433184	0.30457930882724	9.92891425229285
C	-8.36799952331359	-2.05921337589257	8.01633043509680
C	-9.60656604031287	-1.54396859196966	9.96363995984214
H	-9.94236011154849	-1.79072871570673	10.96386453485443
C	-8.76120539700023	-2.41979311632456	9.28832801764916
H	-8.42890929057159	-3.34687371674905	9.73942051760521
H	-9.95579355921005	0.92190128638083	7.62901636793989
C	-8.20899497305268	-0.79214093918616	6.07427274024981
O	-8.35916457931356	0.06544092830248	5.24306239768007
C	-7.49641150533668	-2.77252972080287	7.06018653369544

O	-6.91576153104024	-3.81409427015814	7.20795691248251
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C	0.40599980325748	-2.02292640446016	-1.01788729900803
H	0.36479462427424	-0.78020598219749	2.24275670481605
O	1.78534093205966	-2.87495186834491	2.78149491130691
C	1.53004159087640	-3.57882578302463	0.52324547814690
C	0.48178471805866	-3.48860812735631	-0.58248695147559
C	0.92385076521074	-4.31593987939828	-1.78389702757435
H	1.88288517187068	-3.96222268179498	-2.17172420567591
H	1.03487469885668	-5.36718373110649	-1.50446876069086
H	0.18644708637848	-4.25650848714384	-2.58971577855920
C	-0.86843781362226	-4.00702243102449	-0.09371859268430
H	-1.21054731112183	-3.46934281839250	0.79246829492487
H	-1.62654833373888	-3.89989163043290	-0.87474447307801
H	-0.79556546928824	-5.06714817766005	0.16330120554570
H	1.56660742325948	-4.58529470735208	0.94958882708179
H	-0.35700618970063	-1.90691973490296	-1.79114943088345
H	1.35931851633182	-1.74934880923520	-1.46606982627244
H	2.52147011271582	-3.37852078472474	0.09700983962416
C	-3.75882779494700	0.66468165063756	-0.10262171686086
C	-2.82684720747141	0.76176414359809	-1.16776535569972
C	-1.59586895616023	0.19972363073953	-1.05451191950042
N	-1.20759035462628	-0.46702072550732	0.05311124739951
C	-2.07806784047971	-0.59765709740639	1.07225115149708
C	-3.32660035593928	-0.05911547081636	1.03468947926415
H	-3.06437674939962	1.28795266413798	-2.07993033579128
H	-0.85834835322561	0.28730648236364	-1.83784376609877
H	-1.72324176426778	-1.16946904169809	1.91680273095662
H	-3.96967406699357	-0.20826177705997	1.88881256173615
N	-4.96890603045330	1.21830065798746	-0.17176387866717
C	-5.37353590506419	1.94911804717844	-1.35743166252665
H	-6.39380338297503	2.29722625852951	-1.22389955008776
H	-4.72916496624679	2.81665788221449	-1.52415089271578
H	-5.33846933758901	1.31010749176627	-2.24336612825955
C	-5.88421922229334	1.11466184099189	0.94814863003758
H	-6.80046606997553	1.64431175836217	0.70314616463695
H	-6.13170835099747	0.07082165752392	1.15922024945024
H	-5.45492893197949	1.56205547071893	1.84862294039498
C	4.17266353846878	2.40731155875010	-0.97110470371205
C	2.96665546188296	1.85349656062336	-0.59680937728133
C	4.52013272646090	3.62819053903565	-0.39426615133599
H	5.46057346205224	4.09773576621205	-0.65907476473495
C	2.13118345601895	2.47717847944258	0.31108541700776
C	3.67894209848282	4.25615279808015	0.52043862260306

H	3.97847455681022	5.20408703106177	0.95258305609407
C	2.46132108250247	3.68540242777118	0.88808012996153
H	1.80423509757507	4.17091160028818	1.60024714524698
H	4.82458995451006	1.91419046226359	-1.68270656623235
C	2.29449947130851	0.58622382477945	-1.01514351506112
O	2.75607340438310	-0.22093282903844	-1.80233257205969
C	0.93510561081823	1.59998001435431	0.47084086299498
O	-0.00525834250114	1.80850576966601	1.21484645829945
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C	-1.15174158222042	-6.63026912807228	-6.34968504932429
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C	-0.79582421893586	-9.02154990943693	-6.17925712578803
C	-1.88217805827150	-6.73009593071466	-7.66865709482653
H	-0.85732899953529	-7.68843947168498	-4.49341581449229
O	-0.55350162509872	-10.08197821738108	-5.56731414883367
C	-0.82139319575039	-9.01628821261941	-7.69162979269046
C	-1.95205490665032	-8.15682109894458	-8.25598357415917
C	-1.83535320422060	-8.08338883234245	-9.77428754447834
H	-1.90085456735270	-9.08316684163854	-10.21364207530051
H	-2.64213226692141	-7.47654112001543	-10.19641812764583
H	-0.88446697594209	-7.63507568611716	-10.07001250190730
C	-3.29077416976517	-8.79855958462084	-7.89195618644821
H	-3.35169814919518	-9.81557445577674	-8.29025570873443
H	-3.42240489787031	-8.84630398028923	-6.80853356830940
H	-4.11859935892087	-8.21873253472075	-8.30961353744667
H	-0.91460106547266	-10.04704812410231	-8.04343100144402
H	-2.90010085059098	-6.38252968704960	-7.47429319128825
H	-1.44108750487696	-6.03925103415345	-8.38327975056672
H	0.14474059003596	-8.63535200752869	-8.04756964017681
Cl	-1.68939450107184	-5.18750004478838	-5.44611189032411
C	3.60486670167801	-5.83419412289992	-8.86770000709311
C	2.59631792864605	-5.92523529598778	-7.93192584628924
C	4.91495402789527	-5.96617291955057	-8.40891066021074
H	5.73785704599982	-5.90729820004934	-9.11217341861579
C	2.86484240279743	-6.13221244589471	-6.59238770900844
C	5.18560521940268	-6.17246214006629	-7.05899901708979
H	6.21495349074360	-6.27016349622110	-6.73317734982755
C	4.15557779309963	-6.25471945398131	-6.12305528358027
H	4.36177047693528	-6.41235841898019	-5.07071761953214
H	3.38895859185079	-5.67048278439689	-9.91716402475186
C	1.11040684856618	-5.82443726331022	-8.07269601859508
O	0.52841305563774	-5.58633718655547	-9.11674594194709
C	1.54808902360373	-6.16611927291951	-5.88674298071526
O	1.39413623490421	-6.28513656862152	-4.68817308086272
N	0.55039198484469	-6.01644191980039	-6.82956468125886

HCN

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H	-0.86012430334273	7.17086594592114	1.54363620717563
C	-0.86012430327681	7.17086602791631	2.61689523917094
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C	-0.03324439613747	0.91555974691921	4.40335384215601
C	0.93972763235857	1.07469906665065	5.48519152114219
C	-1.93302236283505	1.21353845389050	5.99564962802094
H	0.36430892774381	0.71665565972305	3.41528328319771
O	2.13551951415723	1.08561862308310	5.24921839406290
C	0.39204182365605	1.15895086728164	6.88042929433518
C	-0.95332590375042	1.88042308724255	6.96575252523533
C	-1.50755641854736	1.76454740523591	8.37934226188626
H	-1.63664782140803	0.71773913829400	8.66517791251107
H	-0.83002663581946	2.23729351063149	9.09487090879452
H	-2.47886992791513	2.26084643079732	8.45269701928372
C	-0.77809073281590	3.35520667896366	6.60943892780664
H	-0.40945322988159	3.49002994547105	5.58937223403115
H	-1.73139104054446	3.88195107575649	6.69660280951963
H	-0.06437607165809	3.82611419788363	7.28984348179562
H	1.13808365696748	1.63039917939120	7.52348103826964
H	-2.83074609033081	1.83119688598802	5.89064965047149
H	-2.27560638775219	0.25281245830429	6.40491897490341
H	0.26949001911686	0.12286856092126	7.22455859369454
C	-4.09745418374171	0.43975256359124	1.49486165250038
C	-4.33544011720153	-0.06199041793712	2.80045203518637
C	-3.43662573426378	0.13917389805900	3.79739825095648
N	-2.27638397236173	0.81308325729345	3.58138517737233
C	-2.01557759138081	1.30715112951884	2.34421988311436
C	-2.87708462899395	1.14403390917335	1.31048431353590
H	-5.22665581395209	-0.62444632911320	3.03657055524517
H	-3.59463562484814	-0.28137672702081	4.79176613432325
H	-1.09664504681613	1.86499633178775	2.23673017136844
H	-2.61304234844419	1.58081323529539	0.35914048586008
N	-4.96663501141156	0.26922151882798	0.50432471231841
C	-6.21273230282421	-0.43885177731607	0.73754102817897
H	-6.79131237867780	-0.44320799460972	-0.18146913352300
H	-6.02561584222632	-1.47317689351694	1.03693718313102
H	-6.80008595586124	0.05287696964735	1.51670044643794

C	-4.68425154809473	0.78921075391255	-0.82105820135788
H	-5.50826164290106	0.53359591636818	-1.48051436000924
H	-4.57940278733812	1.87700214638531	-0.80129720095194
H	-3.76769100937578	0.35281661939824	-1.22570356837263
C	-3.90298083718097	-1.63347727521564	6.58133930085049
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C	-1.13879490892926	0.35755777291681	4.66208369585655
C	0.10902644605873	0.55829548648072	4.21417512897884
C	1.12177994105018	1.19536515027139	5.07177553538448
C	-1.61038651952724	0.76043712910385	6.02636894115152
H	0.41366400633601	0.26433364137800	3.21650724450405
O	2.22890479407129	1.44425077528554	4.63428832226073
C	0.72541173612125	1.46851151187829	6.49287377977570
C	-0.74688894398876	1.85744317273296	6.65343954788849
C	-1.08504562932584	1.96999776622237	8.13346415430843
H	-0.89518117621545	1.02741332371258	8.65331729433791
H	-0.48178616786985	2.74981979504713	8.60475924385005
H	-2.13865746090323	2.22904503265217	8.26737776407355
C	-1.01320892796713	3.19717505833689	5.97015512692320
H	-0.81327827206289	3.16050158833523	4.89652476866221
H	-2.05595837930536	3.49273970024403	6.10846866281624
H	-0.37804432026952	3.97363523161406	6.40312849175899
H	1.38835141830495	2.23383226916807	6.90160839810235
H	-2.65416108143912	1.08191319386446	5.97115522942676
H	-1.59833192713969	-0.13512822771871	6.66110601049204
H	0.91531472238361	0.53932821408791	7.04803109327154
C	-2.08960267230800	-0.28247436322857	3.81186868496136
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T_{SN}

C	9.08431032068885	1.15632494669399	-4.32251681357050
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C	11.30865389695396	1.49572306279447	-5.31651669437831
C	8.49776536565864	2.16310682064618	-5.28843791699586
H	10.86534811362066	0.11679702723691	-3.73816211755437
O	12.52524228533326	1.26932115282787	-5.33529172598054
C	10.71419703630445	2.46132027879414	-6.31494157239452
C	9.24006997856923	2.21195881559095	-6.62638294727458
C	8.67996906956009	3.37395115114521	-7.43813585025177
H	9.21876559182561	3.47247441756869	-8.38424218006926
H	7.62224685016575	3.21456198536550	-7.66607324110651
H	8.77430569800453	4.31634158812700	-6.89222255885407
C	9.06186683664212	0.92111143036057	-7.42157625276463
H	9.56176273181380	1.00382338521135	-8.39015202329813
H	9.48197767038793	0.05881215611519	-6.89975815784937
H	8.00144375819628	0.72699693705243	-7.60467391251390

H	11.32331755659201	2.42243785483797	-7.22184869100552
H	7.43938780109065	1.94968000044883	-5.45543140799260
H	8.55426232547542	3.15326227242964	-4.83396293459874
H	10.82693286340680	3.47013924147665	-5.89666843455247
C	6.42293838286166	-2.05189260932598	-3.42502524711597
C	6.04512841858902	-0.69306975694067	-3.26410008452873
C	6.92848169783489	0.30161319223774	-3.53482580708590
N	8.18349844992982	0.05467187595174	-3.97219656242676
C	8.56449502423115	-1.22674426879650	-4.15903670626824
C	7.74113060064750	-2.27592596989901	-3.89327036107773
H	5.06125375660750	-0.41790450057361	-2.91480324160981
H	6.67709352909943	1.34181515796608	-3.38861955323748
H	9.56002274400219	-1.36744569108885	-4.55294573952678
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N	5.58735927402202	-3.05325523837956	-3.15885245621751
C	6.01582449016662	-4.42818389539391	-3.33361141054945
H	5.19426512638728	-5.08820590431663	-3.07094999148181
H	6.29919888594077	-4.62199446240232	-4.37150539853180
H	6.86745251236776	-4.65828332945027	-2.68810338696061
C	4.23921019680497	-2.78284225041520	-2.69588978602448
H	3.73109281035632	-3.72760787539967	-2.52518519325710
H	4.25090805591210	-2.22196722856184	-1.75790824343576
H	3.67455253905726	-2.21386731650285	-3.43917932705143
C	8.80452330070967	2.19538827095596	-2.55682206041230
N	9.10829716648793	2.81287446791402	-1.61967125890945

TS_{DSN}

C	-0.24537017673978	-1.21205931371313	-3.09890400994296
C	-1.57827461172073	-1.54170458886082	-3.19098925048415
C	-2.60780446722822	-0.59325654883272	-2.93397953622822
C	0.17772902782951	0.21365705707116	-2.93042520363837
H	-1.87403149696481	-2.54912946844484	-3.45826269957784
O	-3.81135486301714	-0.88652580923721	-2.97720445049431
C	-2.20788579035424	0.84944666903557	-2.71551682248077
C	-0.81723513258707	1.04841627330144	-2.11864698447106
C	-0.41269020291102	2.51391245279407	-2.22924068753162
H	-1.12533375634763	3.14830669704714	-1.69490128843904
H	0.57776919666110	2.67734855518047	-1.79479025384403
H	-0.38473890094691	2.83590854271861	-3.27390251666245
C	-0.84069530434204	0.64906645335183	-0.64700467291345
H	-1.52234321182980	1.30828667944923	-0.10165864106785
H	-1.18012332831449	-0.37859156462933	-0.51158121340515
H	0.15205711413909	0.73514856935263	-0.19901632988849
H	-2.96962110916864	1.32575895588803	-2.09215063730534
H	1.17615466721271	0.25926293039266	-2.49361353334195
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H	-2.25568757260776	1.33279481317123	-3.70022004874918
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C	0.58517499324929	-2.04349911140938	-1.32912052280248
N	0.79022908925380	-2.68467117472290	-0.37962612850806

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NuH

N	7.21902094770278	5.31322729808465	-8.46643368578882
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N	7.90800296058312	7.52134263376367	-8.09915398095236
H	8.75808967932419	7.60239798747181	-7.54171015167638

Nu⁻

N	7.18529200504614	5.27731967969777	-8.48530170452392
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N	7.97176982077627	7.44187595948337	-8.05589885273233

VONu

C	8.93113029442689	0.71115838128735	-4.88010428012529
C	10.23952820364676	0.62325940693124	-4.62725767330265
C	11.16812128040693	1.63687281609382	-5.13522877253812
C	8.30085481767512	1.77997394599002	-5.70199550326277
H	10.65856586412491	-0.16813725423905	-4.01671762251994
O	12.37012971025751	1.51085479550992	-4.98141086930561
C	10.55203283979524	2.84169996470667	-5.77906766137352
C	9.30257993781108	2.51475232018627	-6.59888694433754
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H	9.35437940145622	4.34907002915585	-7.74223694931758
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H	8.40663922204059	4.45681336226528	-6.24810689558552
C	9.67549493521995	1.64608253101153	-7.79792060185805
H	10.41136868239771	2.15953869195035	-8.42148687914778
H	10.10331168179532	0.68723910483668	-7.49374477095061
H	8.79265539655932	1.44348483108231	-8.40926783829570
H	11.30643930436312	3.34579736072801	-6.38625082210673
H	7.50830942909499	1.33341651900306	-6.31182298557245
H	7.80301131321000	2.49541885259518	-5.03570089439372
H	10.27338349800952	3.51506580702204	-4.95550083097531
C	6.32672378325320	-2.19457040035356	-3.27391031603460
C	6.00564604080166	-0.81243620847110	-3.27741807575280
C	6.85919483988148	0.09630736447981	-3.81412259567371
N	8.04689637531977	-0.27922963727583	-4.35470774564714
C	8.38461690337150	-1.59224788773665	-4.37295160325214
C	7.57168195005912	-2.54862673301200	-3.85883497127617
H	5.08794065887591	-0.44524719236381	-2.84296046003389
H	6.65383693156466	1.16491430826314	-3.77933245878946
H	9.32664447282698	-1.83388329338231	-4.84408163350356

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N	5.50905447047897	-3.10580854995394	-2.75632150735365
C	5.87425370115743	-4.51052475650831	-2.76427380388078
H	5.08132558582686	-5.08138125015603	-2.28998657836274
H	6.00255005609108	-4.87598045891098	-3.78627909782134
H	6.80163114838414	-4.67673835732764	-2.21048750798367
C	4.24227897514801	-2.70542824273693	-2.17072546283691
H	3.72541791742895	-3.59189424378992	-1.81532618336708
H	4.39818541552856	-2.03011684473566	-1.32561453684448
H	3.61070308605969	-2.20562364953457	-2.90917492429204
N	6.59927727804903	3.23397709603902	-3.08978681286442
N	7.70604634732758	3.55543913459442	-2.86377381361572
N	8.81080749591086	3.86777032147170	-2.65429132744807

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C	-1.43933589679136	0.32982284144843	4.73675194094938
C	-0.22298186510595	0.46188185095559	4.17099577474849
C	0.88354092305128	1.04388383019855	4.90705933930346
C	-1.75043005470411	0.77451971825878	6.12419947072208
H	-0.02427590166283	0.14317786250875	3.15300053401388
O	1.97828663434577	1.21039645699154	4.38611130754227
C	0.64012903342305	1.39161830814486	6.35207052929043
C	-0.78993307881023	1.84393376914985	6.64682317049220
C	-0.98279269387365	1.99471553282548	8.14951477051612
H	-0.78503656702587	1.05268066116399	8.66783895031226
H	-0.30629126827397	2.75456225075100	8.54908892964366
H	-2.00765397418604	2.30138288305151	8.37613770059527
C	-1.06590834461300	3.18389630275120	5.96724215856926
H	-0.95945947646832	3.12136370733220	4.88171907278676
H	-2.08139516734932	3.52132684107693	6.18950932214754
H	-0.36807603400895	3.94223548710202	6.33089922265585
H	1.36652802165808	2.14984212374278	6.65282272557184
H	-2.78319571212833	1.13259880986419	6.15806115622327
H	-1.70853966035244	-0.10959290957572	6.77387160121231
H	0.85943329502198	0.48405738631911	6.93081722914942
N	-2.54248661179867	-0.24428765637278	4.10325729749722
N	-2.38392545851816	-0.70050579660974	2.97030572051798
N	-2.36291846982896	-1.14547310707853	1.94453730653898

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C	8.75435868510501	1.80083939158030	-3.99586517948638
C	10.09978184828196	1.46329061675640	-4.18863661699021
C	10.90079310280620	2.01657307344994	-5.21119823240531
C	8.14368986896563	2.81239813317059	-4.94191252469750
H	10.57188177515141	0.74657800062806	-3.52437385270570
O	12.10781649639179	1.74866851208936	-5.35180263086452
C	10.24079421491022	2.94116360330340	-6.21493479434414
C	8.73254817907354	2.75164525088843	-6.35300709009710

C	8.13804696889777	3.89346300111790	-7.16871596547585
H	8.57312367722718	3.91361770874022	-8.17151902939016
H	7.05532849469410	3.77638182948780	-7.27237280727712
H	8.33373860777634	4.85828683584587	-6.69305072393116
C	8.40981580180188	1.42835504092198	-7.04245162338089
H	8.77289066490047	1.44438821827118	-8.07333866735435
H	8.87798747300022	0.58103643726726	-6.53772880821516
H	7.32954564268235	1.25929513352735	-7.06699248844780
H	10.74453811822487	2.80083878964410	-7.17527630196198
H	7.05918633116588	2.68775173408889	-4.98172898430372
H	8.33356639739715	3.81324313304344	-4.54736517482641
H	10.44443480152529	3.97143648515154	-5.89704007010444
C	6.10380826216621	-1.43814997203132	-3.13890558417935
C	5.73988290403573	-0.08705781997645	-2.90821197429307
C	6.61625695910471	0.91656029893307	-3.17539690498642
N	7.85251814840451	0.68273046556277	-3.66894391248448
C	8.22281103366520	-0.59067395698969	-3.91200315684052
C	7.40449956833417	-1.64768308641140	-3.65877624113965
H	4.77168683898441	0.17665327376553	-2.50973115444052
H	6.37021962369271	1.94950593594869	-2.98459372032270
H	9.20688175296979	-0.71456421802270	-4.33962985515001
H	7.77224227388083	-2.63751273325639	-3.88327009523201
N	5.27039878216920	-2.44731731975430	-2.88860981531452
C	5.69389682192543	-3.81637607559283	-3.11085710100291
H	4.88140171945324	-4.48398148267522	-2.83889715979668
H	5.94441420334435	-3.98470478413648	-4.16165455705648
H	6.56567194100445	-4.06237904654508	-2.49872823263967
C	3.94202463577855	-2.19074065403270	-2.36589088022538
H	3.40777978390311	-3.13335821885807	-2.28730570596464
H	3.98830439524480	-1.73265546687172	-1.37387966162285
H	3.38010441086021	-1.53069456929659	-3.03114440068649
N	8.52470849543917	2.65421823273613	-2.36146839588911
N	9.46583382295512	3.37794237956161	-2.24379199512311
N	10.40162025670394	4.03313271796907	-2.20554837134906

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C	8.66855668073612	1.44921099092001	-3.98257910871463
C	9.97924188143886	1.02285666339339	-4.20218280951285
C	10.84058457035316	1.64782290017840	-5.12991825059334
C	8.12704817966487	2.60139609368823	-4.79410119482157
H	10.34747368437395	0.14397471791829	-3.68441454833578
O	12.01881584977946	1.28990354927734	-5.32268111346163
C	10.27775446366492	2.77586140843953	-5.97296249747402
C	8.76564801475560	2.71256134956097	-6.17990232123073
C	8.27938330639751	4.00143323805440	-6.83153697498769
H	8.75405569385758	4.14201371294079	-7.80679250808910
H	7.19628128304902	3.97639904639039	-6.98336923668523
H	8.51725221066169	4.86865688293618	-6.20930302106779
C	8.38927810492300	1.53060228917400	-7.06900077667332

H	8.82839516386598	1.65087000355818	-8.06324598900001
H	8.74292948358109	0.58590225155526	-6.65204377477833
H	7.30354766108356	1.46709223981457	-7.18372002684162
H	10.80350178051922	2.76494685231546	-6.93192015644830
H	7.04083512144481	2.52654130266931	-4.86897237268247
H	8.34507853921605	3.52683340793069	-4.25417033355719
H	10.53372640223735	3.72275400853774	-5.48027428524590
N	8.44381794836739	2.13557104006831	-2.25131049378615
N	9.49493029624268	2.61873503159639	-1.96537496714387
N	10.54353378148354	3.04003118097608	-1.77146790035238
Cl	7.48118408730207	0.11243611310597	-3.76997463051581

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NuH

C	-1.59702012358979	2.70702030581467	-1.85293381266709
C	-2.25896342526689	2.66604229796311	-0.48797245541998
N	-1.31252269211149	2.17911033770344	0.50421874044291
C	-0.06441511324295	2.92815784265206	0.49519999279082
C	0.50402148615264	2.95861163282160	-0.90813533514619
O	-0.42384614461775	3.48770533316175	-1.83295270288391
H	-2.27760182416258	3.15986759083817	-2.57473189534851
H	-1.36327727532105	1.68329235835223	-2.17720051263317
H	-3.13710927395856	2.02422673644711	-0.53461240441593
H	-2.58076150540424	3.67136619329628	-0.19639514242053
H	0.63171924206915	2.45721617063804	1.18562483870146
H	-0.27486758776106	3.94700500256905	0.83782205308693
H	1.38591015370224	3.59959447841992	-0.93214763716278
H	0.79498250107206	1.94313121887707	-1.21084557857346
C	-1.55455432493339	1.20270301870469	1.37277759576824
S	-0.48135873739679	0.66256589226859	2.53453276352791
S	-3.15484066563262	0.46475066456860	1.23914352922467
H	-2.92568533559693	-0.39236308609642	2.24370578112860

Nu⁻

C	-1.56459491678095	2.80499469594808	-1.86811769450455
C	-2.20559267927128	2.83685096338571	-0.49674881392934
N	-1.29808085904353	2.28855859303582	0.49167042182478
C	-0.00681628550423	2.94688066068588	0.45842690552011
C	0.56096451806247	2.90967308125960	-0.94450884988531
O	-0.32295831212320	3.48156379269734	-1.88852244356534
H	-2.21080005103250	3.30255427662836	-2.59334528999140
H	-1.42088625903945	1.76011522913720	-2.17994383182823
H	-3.12320324699069	2.25202121542336	-0.49016954684824
H	-2.44393600503518	3.87347165764478	-0.22485790219552
H	0.66043586151813	2.44195187539947	1.15421492974166
H	-0.12973040307036	3.98956101602991	0.77961704218353

H	1.48800849318015	3.48403646780080	-0.98712618121915
H	0.77600662596034	1.86793654345408	-1.22363487096090
C	-1.64123986340758	1.33934412294542	1.39292455887421
S	-0.48870020950076	0.81703951993041	2.54864874109670
S	-3.22125940792135	0.67511428859377	1.36339482568699

VONu

C	8.71410362061466	0.64842800335832	-4.79473772727329
C	9.96856987576953	0.31619114515857	-4.47106854577660
C	11.09832209224465	1.12420177228744	-4.92768974830504
C	8.35690340675841	1.81552196092081	-5.64477828530540
H	10.19996804406290	-0.52220371562443	-3.82521990751829
O	12.24464464119541	0.78863188523904	-4.68252165185311
C	10.76902358216446	2.40189907569469	-5.64306221290931
C	9.51851352412117	2.30008669558365	-6.51599980328047
C	9.16955724124333	3.67238308969002	-7.07414132059036
H	9.98535365613331	4.05466639842862	-7.69268424087623
H	8.26919789973675	3.61945169464070	-7.69203732726963
H	8.98722156467133	4.38506723167809	-6.26692119975837
C	9.76360121791404	1.33179893865340	-7.67132840699047
H	10.60189547718404	1.67661980405402	-8.28178887801088
H	9.99709803248707	0.32345691279235	-7.32050836356294
H	8.87930957836817	1.27105307140211	-8.31038132878219
H	11.63861255633483	2.71589877416216	-6.22403321518334
H	7.49913804619497	1.55826028739305	-6.27366787468578
H	8.03024161235908	2.62826917637917	-4.98311715006435
H	10.60297296319648	3.15600160036227	-4.86104917016932
C	5.50694821254956	-1.61359086931402	-3.25316371157340
C	5.41793010374526	-0.21353883807488	-3.45219358736140
C	6.46341250865384	0.48235902679691	-3.96708515518256
N	7.62574250890290	-0.12996095923790	-4.31143841589864
C	7.74037565998971	-1.47294709796773	-4.14687613532915
C	6.73280397686949	-2.22228867872495	-3.63736101009971
H	4.53404770606611	0.34420881088349	-3.18010645999094
H	6.40898266499304	1.56235737579942	-4.07202850348821
H	8.66965878128226	-1.91541013500220	-4.47477851083854
H	6.88467026944220	-3.28799012539612	-3.55589820102109
N	4.50202176389794	-2.31949260233530	-2.74456581502010
C	4.64504496960574	-3.74544206497413	-2.51622432654740
H	3.74455291168053	-4.11505607169334	-2.03446613335524
H	4.78294231652823	-4.28325290784349	-3.45808907611376
H	5.49662128710040	-3.95223150299823	-1.86388998286428
C	3.25120544257993	-1.66918121247009	-2.39944668234976
H	2.53828966479208	-2.42611422670169	-2.08546331415763
H	3.39011289680470	-0.95688029955305	-1.58168451820071
H	2.83761696906537	-1.14001445502083	-3.26082446957782
C	8.08499132011299	7.20198976323373	-4.78047878551402
C	7.17489070430129	6.58916188588615	-3.73683596900812
N	7.81809834011997	5.44552715064310	-3.11800646605481

C	9.12391802091899	5.78892578923401	-2.58778750728599
C	9.97112558210552	6.41850582829674	-3.67433481026421
O	9.34530369470131	7.55061262655803	-4.24361433472326
H	7.63934114474904	8.11917705531261	-5.16906323661285
H	8.21822783975557	6.49602015813428	-5.61199875472383
H	6.23985755668113	6.26522963882535	-4.18851984202594
H	6.95649648578980	7.33165246874460	-2.95893809156683
H	9.59755212726174	4.88609903864825	-2.20885205264859
H	8.99698017489223	6.49796242309395	-1.76006938685582
H	10.92125888051529	6.75547801920500	-3.25660142149297
H	10.17390619209922	5.67297643228122	-4.45679650124067
C	7.24421738386042	4.23052799372463	-2.98861850646732
S	8.06697196144675	2.98340196669490	-2.15158372615742
S	5.70011447338362	3.94485567805721	-3.68393225722086

VNu

C	9.95212484317757	1.25074594111989	-4.84226260734454
C	10.30558084016096	0.69068418881538	-6.00818107375355
C	10.87001254486849	1.49305888622569	-7.09827845173472
C	10.09829216130835	2.71316654981152	-4.56368528260941
H	10.17262731494336	-0.36885720981947	-6.19612577489785
O	11.14254595444759	0.98342116601066	-8.17173682769896
C	11.12421985764869	2.94485774267995	-6.81184885077630
C	10.11708871636805	3.56294208161081	-5.84008009798742
C	10.55849891632843	4.97559347918093	-5.48343044304432
H	10.58413133156135	5.60703501233424	-6.37545486083735
H	9.86533962166537	5.42686682045233	-4.76834426720532
H	11.55642012160672	4.97193909323122	-5.03740073506787
C	8.73063454574266	3.61176684339681	-6.47647525860140
H	8.75683278895424	4.19924120139732	-7.39777196567878
H	8.35758892260658	2.61505854656386	-6.72417700417832
H	8.01597582296027	4.07955037431985	-5.79473667513107
H	11.15521653409003	3.48827058876137	-7.75877340163345
H	9.29318702924344	3.04205695538278	-3.90144374721190
H	11.03277043105738	2.86298262327202	-4.01536317070599
H	12.12837950049915	2.99940910682101	-6.36940878564174
C	9.50957312334513	-1.37700114612274	0.79238322130612
C	9.74171502032323	0.00841048378615	0.22143312548358
N	9.18107695751686	0.08026785043448	-1.11983584389989
C	7.77453019278132	-0.29780217990329	-1.13021770281876
C	7.61523642242613	-1.67676321654294	-0.51859722051248
O	8.13901704835471	-1.71836377892712	0.79015186108060
H	9.847763711101042	-1.40837861962100	1.82876126366535
H	10.08006767448375	-2.11365283494873	0.21009965902118
H	10.80405380676960	0.23608163106497	0.17411009227227
H	9.23912267244567	0.76014909470226	0.83857082244940
H	7.37306847323128	-0.28735506325166	-2.14105393092595
H	7.22446706813055	0.43747671684660	-0.53397621815981
H	6.55607530628966	-1.92812024308413	-0.45164122481404

H	8.11971268554353	-2.41999818475583	-1.15163512345257
C	9.91392031801175	0.39589762862813	-2.18600879215685
S	9.04818677990660	0.22875369212514	-3.73071829917136
S	11.52261051819091	0.82476554700148	-2.14833753062644

TS_{SN}

C	8.15230675287039	2.67130288368467	-4.79772492253794
C	9.48512609604571	2.41558405142804	-4.41156953849352
C	10.57521977814359	2.48123759336471	-5.29116143965434
C	7.91200302786651	2.99872426137000	-6.26117431252949
H	9.70400933981058	2.21240372445282	-3.36843995073123
O	11.76410770228953	2.35385694276629	-4.92345201122709
C	10.29687538932914	2.68119403258595	-6.76575432689638
C	8.88870579428794	2.29049801609432	-7.20330212621827
C	8.62999578808951	2.78889266143082	-8.62012939448170
H	9.34475891183368	2.34267336444531	-9.31691637447872
H	7.62251419053276	2.52105652018879	-8.95171495291275
H	8.73208245780863	3.87601573784684	-8.67855047624446
C	8.70909453029351	0.77492313405938	-7.16851910246174
H	9.35978814300678	0.30381446618401	-7.91001779462269
H	8.96207612024853	0.36091433363080	-6.19090629559246
H	7.67646713054852	0.50040635931093	-7.40183165652373
H	11.05075258326641	2.12014997217520	-7.32554680808901
H	6.88414140852929	2.75992576942230	-6.54349177903605
H	8.03782993903974	4.07552213121567	-6.39987854715275
H	10.46109257930164	3.74299957854203	-6.99144363594232
C	5.28923798383772	-0.13437013178716	-3.29056093701050
C	4.89697685039704	1.07002566523623	-3.92869924861689
C	5.83274222129883	1.94705845117542	-4.37452439095644
N	7.15792123454891	1.71585206646562	-4.25690961860912
C	7.55986126270509	0.57280378026032	-3.66853682056301
C	6.68297444859795	-0.34932744327718	-3.18460128375334
H	3.85657328731006	1.32590281157352	-4.06147495629386
H	5.55088825965400	2.88590025834298	-4.82573236453240
H	8.62872238807742	0.42393777585838	-3.62794569485835
H	7.08612537625793	-1.24038814221107	-2.72763698216503
N	4.39833428408447	-1.00923816047670	-2.82321080244961
C	4.84318741655674	-2.23374419233500	-2.18689186083368
H	3.97276950198348	-2.80879270459105	-1.88405919946053
H	5.43817521314711	-2.84103895183285	-2.87446289349287
H	5.44465734325364	-2.01970916051992	-1.29927845153902
C	2.97755407041033	-0.75561871327058	-2.96296123769256
H	2.42849022487624	-1.56000012186551	-2.48170490651250
H	2.69867275769636	0.18674270837686	-2.48497071697435
H	2.68447152436065	-0.71568894729332	-4.01581823643692
C	11.42653365182640	5.21370891300031	-2.79694378241821
C	10.00019231513846	5.72713453914003	-2.75367419444953
N	9.18745500966217	4.85080976955602	-1.92121324707679
C	9.76505493173773	4.70255914649675	-0.59513965392637

C	11.19305710140839	4.20883239261133	-0.71883069174139
O	11.97659701950215	5.08519487846575	-1.49997489526346
H	12.05154948478957	5.92450336290411	-3.33984761008395
H	11.45394771720438	4.24597950348201	-3.31436103683686
H	9.58372867556263	5.76494187615383	-3.75608569919417
H	9.97601426875992	6.73088908146629	-2.31511860136606
H	9.16089702526867	4.00355017649927	-0.02186081587517
H	9.75279215480765	5.68229107299477	-0.10504805157086
H	11.65269342389539	4.15848707676257	0.26929698026750
H	11.19474956781189	3.20417758532923	-1.16462373466170
C	8.06097200593273	4.23430766611532	-2.29300723038002
S	7.21731765649147	3.17654897755937	-1.29043129733774
S	7.48579056200229	4.51978201743464	-3.92109053550673

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C	8.18853599815241	2.61768071159197	-4.75562284977008
C	9.51032656407494	2.38150401949534	-4.35703368214246
C	10.60058593748835	2.48379502255906	-5.23912259321623
C	7.91511897954599	2.96381906780821	-6.20380747436231
H	9.70742584185802	2.04817769189825	-3.34464785676027
O	11.78748700714245	2.29689790558359	-4.89074263798222
C	10.31526165878566	2.79264618321891	-6.69400452657807
C	8.93281882756766	2.35138038681687	-7.16810614688118
C	8.66483967249114	2.90484773335734	-8.56259225037660
H	9.39867162669786	2.51753653340268	-9.27496577953066
H	7.66916799283911	2.61646570044703	-8.91221288085494
H	8.72682349948698	3.99667026608917	-8.57022315931752
C	8.83260947257527	0.82907025340514	-7.20797478936059
H	9.54143657534371	0.42400854598834	-7.93563518325193
H	9.05162618188482	0.38617434378105	-6.23501670636091
H	7.82709506607070	0.51778955203102	-7.50429640479309
H	11.10229291193453	2.32527825721029	-7.29266075383262
H	6.89836768629597	2.67108545185556	-6.47127725494798
H	7.97703566575715	4.05069210083285	-6.31048556476810
H	10.41171280543294	3.87789320304185	-6.83252972078885
C	11.44125071579298	5.06631563173806	-2.89322962578986
C	9.97578283557080	5.43026658261196	-2.96663827780989
N	9.18866331198287	4.65528176908385	-2.01323189729782
C	9.76580454955634	4.64709632361591	-0.67893798560427
C	11.24136023801354	4.31546099019306	-0.72909593761653
O	11.94879232428687	5.19125694899807	-1.57793178043741
H	12.01010925910655	5.75043090580106	-3.52511595063668
H	11.59230766586051	4.04251103413594	-3.25562097903195
H	9.59780981305171	5.24780925908121	-3.96834935230163
H	9.84646175443793	6.49461930348656	-2.72867081269005
H	9.23195199522550	3.91586570975460	-0.07522098869686
H	9.61981917219497	5.63535387427423	-0.22373859244544
H	11.66650826027827	4.41315063037951	0.27102873237016
H	11.37640007571299	3.27909867855150	-1.07004136535554

C	7.91797313959731	4.27560497622257	-2.22352029447815
S	6.93118598270857	3.69157404720381	-0.98979171060296
S	7.29299898702184	4.39608957619936	-3.84784417920725
CI	7.03372065017389	1.37162713025388	-4.12268117849070

10.3. Catalyst variation

NMI

Cat

C	8.31154787161648	-1.16001972808716	-2.66565856577220
N	7.99794999005733	-1.31295290296778	-3.93353491592610
C	7.82178227539104	-2.66184478024879	-4.09761886203988
H	8.52391074026181	-0.22396734425177	-2.16916856556979
C	8.03439067618574	-3.31295989120450	-2.91429527502175
H	7.99279342764011	-4.35455064848708	-2.63921426021342
H	7.55356838881813	-3.08981330762509	-5.05189910786195
N	8.34721213402223	-2.33821902197442	-2.00693062723663
C	8.65393355137834	-2.53012286216953	-0.60825100389079
H	7.80572478604219	-2.98103324356311	-0.09175037322919
H	9.52689738803483	-3.17422380013768	-0.49616543152916
H	8.86755577055170	-1.56046646928309	-0.16170901170914

VOCI

C	1.3736969999428	-0.51816758243080	-7.22683736880161
C	0.57109943430116	-0.80017118821659	-8.25903582095988
C	0.71521695257387	-0.09649362580561	-9.53386629176206
C	2.43137987128590	0.52825949267049	-7.26012637007380
H	-0.21393038674552	-1.54382659384704	-8.19885161625498
O	-0.04619416811052	-0.32549064912393	-10.45768417525289
C	1.85630117587064	0.87191998826620	-9.65468714385955
C	2.19424646834396	1.58152994455534	-8.34425153937421
C	3.46613267445812	2.40059795908074	-8.51509940223912
H	3.32355707508814	3.17540257940818	-9.27246628927040
H	3.73479773815981	2.88925734003957	-7.57477155623565
H	4.30208558867839	1.76766175402906	-8.82423374493314
C	1.05071307275742	2.50705884572447	-7.93162843957645
H	0.87870039181090	3.26090779113370	-8.70366569206293
H	0.11534332270737	1.96308393668248	-7.77850671534477
H	1.29618027618556	3.02081265301203	-6.99914224414124
H	1.62657095604056	1.58479251081514	-10.44926655174720
H	2.52288074968295	1.02724719205120	-6.28971538586760
H	3.38933357479185	0.01794460479355	-7.43031686473250
H	2.72509556430526	0.28527926904892	-9.98364047578426
N	1.26333252079082	-1.26702160623244	-6.03088293206955
C	1.65183119541047	-0.84446211569293	-4.81789764658649
C	0.73000961311176	-2.53708192169681	-5.90530832879433
H	2.07845659807904	0.13184482760919	-4.56017722009161
C	0.80507961269964	-2.86554660011333	-4.59788977540218
H	0.51438076482028	-3.76318935424212	-4.07871891266597
H	0.37565976853086	-3.10050537084998	-6.75006626326502
N	1.37764633020967	-1.79712508250337	-3.94560393549153

C	1.64405473290924	-1.71557361240850	-2.52028149678834
H	0.70627957888669	-1.80349438603937	-1.97366332429628
H	2.31751200548617	-2.52208852127826	-2.23402237318519
H	2.10640389611673	-0.75362019331848	-2.31118113514155
Cl	2.78529253376845	2.09932037887929	-3.89064997794746

VONu

C	1.15306186306157	-0.21688182952895	-7.34741708148469
C	0.44148978091467	-0.44752070387236	-8.45354285725305
C	0.71322583607181	0.30813185133197	-9.67821017126446
C	2.20766865953611	0.82232801158093	-7.21359887033647
H	-0.31475914296713	-1.22195311059757	-8.50162816689600
O	0.03278856075466	0.14515085385954	-10.67598605302417
C	1.90393520566703	1.22116063787610	-9.65284655920970
C	2.12578974876897	1.89903734643692	-8.30004013724975
C	3.43706272718988	2.67241915714715	-8.32626027398806
H	3.40578858397699	3.45221388182637	-9.09132797406684
H	3.62101906428891	3.15070698638919	-7.36047067332116
H	4.27696178469882	2.00819421768362	-8.54484738759142
C	0.97443750260358	2.85790304363139	-8.00541245707335
H	0.89879752284495	3.61188778443725	-8.79280387350710
H	0.01477901690294	2.33815284512423	-7.94478750182230
H	1.14009111736876	3.37259144666100	-7.05568453395442
H	1.80488760558761	1.95536662642922	-10.45482327882096
H	2.11998732746108	1.28528763281768	-6.22517578396683
H	3.18583089570603	0.32432542135274	-7.23243543598245
H	2.77089402330899	0.58817879139649	-9.88302599949933
N	0.91294497778759	-0.99729229387517	-6.18880510144334
C	1.88028449044083	-1.43004175430628	-5.37015292278197
C	-0.30177720358231	-1.48877433947487	-5.75641443511772
H	2.96671478516031	-1.29942595416131	-5.53943134807973
C	-0.04879108289157	-2.22307235523714	-4.65010962932194
H	-0.71114642913084	-2.76064849563441	-3.99305302683155
H	-1.22583836985100	-1.24692166556017	-6.25213705320760
N	1.31079744783867	-2.17454815617726	-4.43641300796564
C	2.02486785878567	-2.86400521589613	-3.37812264757727
H	1.69546691059237	-2.48711825328154	-2.41067810919119
H	1.82553332628207	-3.93258025858064	-3.44608398911715
H	3.08917573141456	-2.68041726581836	-3.50360127327514
C	3.06366878338562	-3.36306593102251	-9.80279688760723
C	2.86241712710704	-3.90853754791350	-8.53886368262597
C	3.81156334432634	-2.19223687438968	-9.90350460825064
H	2.29696214621600	-4.83039861283672	-8.43475670289165
H	3.99128363206399	-1.75235949036583	-10.88062105824782
C	3.37352402526305	-3.29767088522153	-7.40508496868805
C	4.32440961590599	-1.57013629934191	-8.77904771553785
H	3.21814798768421	-3.74926179814247	-6.42895105834247
H	4.89792791375707	-0.65231936280989	-8.87565822045941
C	4.11208106380327	-2.08389639811847	-7.47071986819455

H	2.66005315087837	-3.84263641364967	-10.68678106423067
O	4.52496316401629	-1.46897731616736	-6.41243854070016

VO⁺

C	1.57575581692772	-1.00627091492047	-3.22241033688992
C	0.45259181202572	-1.08220085053599	-3.94075269372183
C	0.17426471036731	-0.10931805187575	-5.00315177279920
C	2.60396253536296	0.05722791898602	-3.39080555935655
H	-0.29539048026232	-1.84669053859476	-3.76991893216148
O	-0.89140470695420	-0.12642335449777	-5.59004358450445
C	1.27298173735981	0.85623145659109	-5.33727353217768
C	2.07141508487118	1.29974216649439	-4.11099617582010
C	3.25011722551687	2.15720425100699	-4.55042681495850
H	2.89601545052652	3.05603241431104	-5.06058126398690
H	3.84253772621051	2.46977134884742	-3.68630049767715
H	3.90242524572762	1.60869065606831	-5.23472123469425
C	1.17885325355568	2.10855519796628	-3.17121463946604
H	0.78894967414524	2.98782064477288	-3.68893883114674
H	0.32756357230977	1.52687514248327	-2.80909893867893
H	1.74939351335852	2.44930253517489	-2.30390570071294
H	0.84352681954959	1.71137020169667	-5.86238253418873
H	3.00988003151940	0.35910029330685	-2.42229139333184
H	3.44172177849270	-0.37828355488936	-3.95127405409363
H	1.94118757379855	0.33953910635727	-6.03947483597718
N	1.85429545237360	-2.01614607051155	-2.26443566669918
C	2.60247380119481	-1.87062088041632	-1.16304661622837
C	1.39295238548103	-3.31746304726264	-2.30526513370944
H	3.09212015253044	-0.97011250259196	-0.83387466497303
C	1.87613326520449	-3.94205990725231	-1.20918007674338
H	1.76817870354536	-4.95889701036282	-0.87105702145153
H	0.79376443712186	-3.68853160465405	-3.11780491034423
N	2.62221246898944	-3.02018481471459	-0.51355296444264
C	3.32476789383078	-3.27198719229666	0.73333326718867
H	2.60516976649660	-3.56668475024753	1.49546383028830
H	4.05014703810649	-4.06921884861214	0.57864813734071
H	3.83527435971587	-2.36162938582669	1.03778288311822

TS_{EA}

C	-0.36800079377375	-0.90620132135599	0.00332104282957
C	-0.07063441740767	-1.02976695140522	-1.34667698863352
C	-0.59722622688790	-0.14408176662859	-2.31810673656879
C	-1.05862633887405	0.32750029598112	0.50326538912095
H	0.58104872149305	-1.82661521627526	-1.68549247559274
O	-0.38041851614526	-0.27115090064169	-3.53481232937568
C	-1.37053151355407	1.06926472831127	-1.84235144068932
C	-2.06216942672120	0.92207134781500	-0.48980642475358
C	-2.47668517535461	2.29487531198679	0.02987281134810
H	-3.16467941230409	2.77570202227333	-0.67052904816539

H	-2.98299602805960	2.20875932658423	0.99581569470881
H	-1.60710006231184	2.94536488436615	0.15570034560555
C	-3.31452549509858	0.06154818021395	-0.64244074965259
H	-4.04506387355859	0.59034139350110	-1.26031651750053
H	-3.10111103244617	-0.89278646830824	-1.12424782363332
H	-3.77344084341115	-0.14119124154840	0.32882353913590
H	-2.09415633259884	1.33688926198199	-2.61696215247563
H	-1.53388421780335	0.13804103716113	1.46817440428842
H	-0.27045511537718	1.06678903465990	0.68347089362690
H	-0.64400050381422	1.89077787786100	-1.79384451067867
Cl	0.92961395118116	-1.42931753225059	1.12190039874261
N	-1.58946839010590	-2.27158947898423	0.47962983566169
C	-2.22646814720312	-2.52451429075521	1.60419172326278
C	-1.96763519389505	-3.20297811546982	-0.43500412086036
H	-2.14466438009730	-1.97112807080293	2.52645497047133
C	-2.86250246525405	-4.04288891023385	0.15807142221453
H	-3.39557759141177	-4.90240600600314	-0.21332452706456
H	-1.58010350745545	-3.18896714796034	-1.44191727910276
N	-3.01407416299786	-3.59824032837340	1.44606371190109
C	-3.88997002467098	-4.16997512046249	2.44794249543825
H	-4.92845712640730	-4.07873302372457	2.12975853464943
H	-3.64509820680797	-5.22134756619962	2.59573611095517
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TS_{SN}

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C	3.06677692047069	0.15016478714168	-1.54330163264320
C	3.74400153923669	0.90679130087346	-2.52126185554437
C	3.62992122708543	-1.99898876354620	-2.70484167868730
H	2.64791252101349	0.67302719879466	-0.68984765522744
O	3.86664308646492	2.14479421030975	-2.47243872595013
C	4.37578224044742	0.14614477340382	-3.66706414012906
C	4.83782070423656	-1.25871517524161	-3.28412936388707
C	5.30340603962665	-2.00440469439515	-4.52908596868867
H	6.15363052028378	-1.49298774403220	-4.98840269145245
H	5.61617077865657	-3.02285003595622	-4.28006584591022
H	4.50158230474522	-2.06495330149812	-5.27001761448606
C	5.99088073538475	-1.19297403325944	-2.28628723308974
H	6.84175367830286	-0.66373274980393	-2.72356672006129
H	5.70493887601581	-0.67103804503739	-1.37057220097712
H	6.32416631196795	-2.20024279231249	-2.01901311106624
H	5.20984900673512	0.74146725527790	-4.04792924554348
H	3.92814795910128	-2.97240115389555	-2.30744896015449
H	2.94618879022098	-2.20612023495300	-3.53128360539218
H	3.63310601645797	0.07367886583833	-4.47214216614785
N	2.71633423930991	-1.91195756880189	-0.38406163056109
C	1.65290852902663	-1.86123202114464	0.40879768942473
C	3.72279291668907	-2.57883984991144	0.27152434729442
H	0.71301058910275	-1.40363676920904	0.15842877049115

C	3.23551877796513	-2.94129172146166	1.48320170996700
H	3.69063074841942	-3.48166940209977	2.29572490439623
H	4.69500391726436	-2.72697090860002	-0.16416881495015
N	1.94424442855980	-2.48097019547327	1.54720100446412
C	1.03328810060540	-2.66205687562817	2.66089899728397
H	0.82550316767809	-3.72280407048980	2.79614825416419
H	1.48377614031259	-2.25611813834545	3.56550672384619
H	0.10871524646656	-2.13259551962140	2.44392239498889
C	0.12099372310586	0.43431176794688	-5.58034474549329
C	0.37169220464515	-0.93309493367829	-5.62150851547895
C	0.19011140506610	1.10185433694581	-4.36416879946322
H	0.30398357906938	-1.46888779641188	-6.56254177636961
H	-0.01861236859116	2.16565702268593	-4.31932562653094
C	0.71540276742665	-1.61761873074608	-4.46701194141497
C	0.51862958341331	0.42100900310250	-3.20077188157144
H	0.91276234374511	-2.68429007107108	-4.49530530240762
H	0.55311539563408	0.93952716464032	-2.25141608262447
C	0.79848658903223	-0.95408418047198	-3.23199425023340
H	-0.14092736789148	0.97013110374223	-6.48557351712442
O	1.15448356109233	-1.61143136320690	-2.13817925082709

Py

Cat

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H	4.408288000000	-1.521342000000	-2.046999000000
C	3.637042000000	1.084043000000	0.604563000000
C	2.930445000000	0.971046000000	-0.583768000000
H	3.371570000000	1.848852000000	1.324345000000
H	2.108787000000	1.649364000000	-0.796190000000
H	5.254141000000	0.256340000000	1.758715000000

VOCI

C	-0.00749390266509	0.52490124586309	-0.08436522811825
C	0.57628034889401	1.21313547177546	-1.06367402150976
C	2.03699208740491	1.16102286486513	-1.22741841268079
C	0.69333643227991	-0.31783254978608	0.91444843849853
H	0.01083640203172	1.80534312375965	-1.77399829877969
O	2.58954126123544	1.85899734044614	-2.05578660952416
C	2.76941961943796	0.17407633986902	-0.36730848072964
C	2.17938842993541	0.03429724891857	1.03882217930644
C	2.88984575598594	-1.09191911982668	1.77720441618238
H	2.79202554047361	-2.03666181054841	1.23696919065221

H	3.95301548778633	-0.86465998662376	1.88822662193348
H	2.46480486181816	-1.22350690373837	2.77586549855372
C	2.35493138294515	1.33917680189971	1.81211051370770
H	1.83384247765404	2.17428352033809	1.33642427160726
H	1.96640696700993	1.23376606622738	2.82792453146324
H	3.41425781043662	1.59916187971753	1.87788024606728
H	3.82464102628713	0.45135883354519	-0.33175116089295
H	0.19438877275570	-0.21720583086436	1.88386940074416
H	0.57596240904406	-1.36984729526000	0.60674855617141
H	2.69700647030442	-0.79320207407363	-0.88327125109733
C	-4.16168498566821	0.67403211247324	0.27095518531748
C	-3.50646020043645	-0.54492364325822	0.19456435179960
C	-2.13636657179873	-0.57557803095008	0.07874597130439
N	-1.44447620330632	0.57930240446170	0.03478993201253
C	-2.05720730020069	1.77581861645841	0.10907618669806
C	-3.42316674168353	1.84792310603447	0.22599078041543
H	-4.04651642154275	-1.48198301007010	0.21548975449191
H	-1.56969148027030	-1.50455536981547	-0.02844695596897
H	-1.41473054969968	2.64469205325119	0.08857662375659
H	-3.89500523315883	2.81889335968456	0.28938585293604
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Cl	-0.28403847369706	-3.39762512519041	-0.50910057347809

VONu

C	-0.26102685351379	0.84990653249316	-0.30538180959439
C	0.33336392636457	0.49475211788812	-1.44370318645768
C	1.78049175102038	0.67573876706537	-1.61128537852709
C	0.43281936427943	1.42297039964088	0.87729019947988
H	-0.21070529513673	0.05438714683878	-2.27040780591763
O	2.31411258530258	0.41776322859588	-2.67466666721560
C	2.54820403834862	1.15150944572167	-0.41405577679710
C	1.76020234604403	2.09121470154946	0.50054933393047
C	2.55748877094264	2.34758861076284	1.77205856730846
H	2.76795759497062	1.41250430001598	2.29716795885988
H	3.50876596625132	2.83109582355261	1.53622348284489
H	2.00235525763973	3.00332856961750	2.44825969795621
C	1.49902425879656	3.41686755411523	-0.21134264496313
H	0.90552725015661	3.28382704025011	-1.11944096741857
H	0.96061117673071	4.10337381744050	0.44674609954611
H	2.44402660129426	3.88675391588156	-0.49434148234447
H	3.47638405205101	1.61473458156907	-0.75491560540958
H	-0.22441636001938	2.14917598058518	1.36581775993049
H	0.60296148270238	0.61463200435847	1.60194617176113
H	2.81445627416831	0.24587450140018	0.14505116921378
C	-4.39520262835119	0.40263496036864	0.03165162307383
C	-3.55785861111695	-0.01131203029572	1.05351854732680
C	-2.19530751782261	0.14120490137925	0.92773341955290
N	-1.68850890568264	0.69603449741531	-0.19018070841413
C	-2.48335385062979	1.11069488801572	-1.19708781853866

C	-3.84464821022604	0.96865498121576	-1.11075206520297
H	-3.94643530844278	-0.47027481153507	1.95270419891101
H	-1.48245025543468	-0.21890016826595	1.68077050643372
H	-1.98696451479934	1.56735049969970	-2.04114944725835
H	-4.46182304367094	1.31267819889394	-1.92940410731006
C	1.03297049083900	-3.08412561813259	-1.02002311800518
C	-0.30643399886978	-3.12342684888293	-0.64580101350524
C	1.94837377699371	-2.52223422715211	-0.13219045658892
H	-1.03739633104801	-3.57644077584182	-1.31000061708882
H	3.00208718955940	-2.49310070294818	-0.39608273348543
C	-0.72873902256199	-2.59264052322363	0.56167173189318
C	1.53977065257543	-1.98637941004666	1.07513519050726
H	-1.77733963640266	-2.64733623429759	0.84025910891306
H	2.26593595007472	-1.54234537925493	1.75062973091059
C	0.17270008725461	-1.96502847055114	1.46855413001050
H	1.35900948399219	-3.49359856149707	-1.96891817119921
O	-0.22474380911895	-1.38523845192824	2.54762381874274
H	-5.46861677250460	0.28831734252268	0.12094720713533

VO⁺

C	8.808955000000	0.421313000000	-5.524062000000
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H	10.440999000000	-0.552042000000	-4.576495000000
O	12.225512000000	1.210718000000	-5.157868000000
C	10.524936000000	2.602640000000	-6.098012000000
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H	10.196906000000	0.555832000000	-7.963930000000
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C	6.142753000000	-2.674491000000	-4.645976000000
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C	8.274430000000	-1.927925000000	-5.403456000000
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H	4.775316000000	-1.083371000000	-4.128037000000
H	6.414753000000	0.696965000000	-4.674580000000
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TS_{EA}

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H	-0.007928000000	-0.753382000000	-1.868402000000
O	-1.006660000000	1.609583000000	-2.281323000000
C	-1.165528000000	1.914470000000	0.067626000000
C	-1.477737000000	1.119195000000	1.330680000000
C	-1.415216000000	2.033369000000	2.549771000000
H	-2.135378000000	2.849582000000	2.449651000000
H	-1.654035000000	1.480914000000	3.463234000000
H	-0.419019000000	2.468854000000	2.663759000000
C	-2.882699000000	0.528122000000	1.235434000000
H	-3.620318000000	1.333989000000	1.266275000000
H	-3.035376000000	-0.018097000000	0.304180000000
H	-3.084946000000	-0.149600000000	2.069223000000
H	-1.987226000000	2.593869000000	-0.174387000000
H	-0.608618000000	-0.574919000000	2.370498000000
H	0.557342000000	0.538241000000	1.688423000000
H	-0.279974000000	2.539779000000	0.240072000000
C	-3.201763000000	-3.367938000000	-0.514652000000
C	-3.277277000000	-4.177122000000	0.607182000000
C	-2.402720000000	-3.956184000000	1.662256000000
C	-2.256416000000	-2.359582000000	-0.540516000000
H	-3.863214000000	-3.507058000000	-1.359745000000
N	-1.430593000000	-2.166784000000	0.472912000000
H	-2.137520000000	-1.668968000000	-1.371857000000
C	-1.478421000000	-2.936535000000	1.555468000000
H	-0.757025000000	-2.732859000000	2.337218000000
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C	9.126851000000	0.399384000000	-4.829154000000
H	9.739282000000	-2.906299000000	-3.882187000000
O	12.159729000000	-2.424454000000	-4.622492000000
C	11.538471000000	-0.162747000000	-5.037055000000
C	10.372184000000	0.558418000000	-5.705057000000
C	10.685256000000	2.046017000000	-5.821147000000
H	11.576815000000	2.200123000000	-6.434585000000

H	9.85562000000	2.58279400000	-6.29035800000
H	10.86722600000	2.48821700000	-4.83781000000
C	10.14845200000	-0.01104600000	-7.10295200000
H	11.04175600000	0.14636600000	-7.71330000000
H	9.93133700000	-1.07777800000	-7.07001200000
H	9.30654800000	0.48489600000	-7.59260100000
H	12.41827300000	-0.15692500000	-5.68529000000
H	8.25930800000	0.78535100000	-5.36821800000
H	9.24791000000	1.01355600000	-3.92769700000
H	11.81535100000	0.36473100000	-4.11490600000
C	5.83245400000	-1.21456500000	-1.44250700000
C	5.64254200000	-0.48183100000	-2.60560800000
C	6.63813900000	-0.44324600000	-3.55015500000
N	7.80344300000	-1.08640000000	-3.35244100000
C	8.01229200000	-1.77624300000	-2.22183300000
C	7.03577000000	-1.87137200000	-1.25580100000
H	4.72081900000	0.05134100000	-2.79517400000
H	6.53110200000	0.06996900000	-4.49057900000
H	8.98829100000	-2.22503500000	-2.11806400000
H	7.23853400000	-2.44689900000	-0.36287100000
C	7.36585300000	-5.68811000000	-5.76342000000
C	6.40245300000	-4.90753600000	-5.13282500000
C	8.43359400000	-5.06498200000	-6.39707500000
H	5.56025400000	-5.38176700000	-4.63933900000
H	9.19077700000	-5.66284400000	-6.89393200000
C	6.50755100000	-3.52627100000	-5.12952300000
C	8.54518100000	-3.68247500000	-6.40047600000
H	5.75005100000	-2.91962500000	-4.64379200000
H	9.37770000000	-3.20119600000	-6.89899000000
C	7.57902800000	-2.87805800000	-5.77164300000
H	7.28055700000	-6.76870600000	-5.76602000000
O	7.68951400000	-1.56330700000	-5.75339600000
H	5.05323400000	-1.26743500000	-0.69208900000

DMAP

Cat

N	3.18458400000	0.05937400000	-1.54312600000
C	4.96149400000	-0.75675100000	-0.13723400000
C	4.19613700000	-0.77315500000	-1.28447400000
C	4.68924100000	0.19707200000	0.86357300000
H	5.75924900000	-1.47792400000	-0.02541600000
H	4.41582100000	-1.51321500000	-2.05012900000
C	3.62371700000	1.07906800000	0.59373700000
C	2.93051200000	0.96240600000	-0.59273100000
H	3.33705600000	1.84711700000	1.29854800000
H	2.10994800000	1.64782200000	-0.79013100000
N	5.40391100000	0.26199300000	2.00959300000

C	5.083748000000	1.256498000000	3.006367000000
C	6.484408000000	-0.667321000000	2.241914000000
H	5.763963000000	1.146095000000	3.847428000000
H	5.189575000000	2.272306000000	2.610845000000
H	4.059384000000	1.140924000000	3.376404000000
H	6.129292000000	-1.703417000000	2.256012000000
H	7.259284000000	-0.584346000000	1.472513000000
H	6.938134000000	-0.450156000000	3.206056000000

VOCI

C	-0.09580714631426	1.51180162064732	-0.24847911296313
C	0.35690092817505	2.06313121421016	-1.37958478403303
C	1.79124998372515	2.25423244816744	-1.59682040855435
C	0.77815291641616	1.05291233692852	0.86312055846217
H	-0.30374206657854	2.36171057151598	-2.18480238344965
O	2.19767720641340	2.81743105347790	-2.59864165066411
C	2.71686590853342	1.67553092119408	-0.56581097885723
C	2.15507944999674	1.72363999621869	0.85563853490451
C	3.07673640344591	0.95894891328244	1.79590548923005
H	3.17849810855486	-0.08300760179742	1.48238408468635
H	4.07029866389346	1.41398771452828	1.81198626850162
H	2.68106482057941	0.97125627774622	2.81498725424561
C	2.04278562128333	3.17308280860629	1.32355508343078
H	1.36515975080181	3.75625683210681	0.69480493955439
H	1.67054247729855	3.21322525663648	2.35010760512218
H	3.02327749721288	3.65481019642189	1.29716350745121
H	3.67931840756326	2.18707686896568	-0.63138317276140
H	0.27480359632780	1.24347000174946	1.81637904221324
H	0.89053701860337	-0.03970896283316	0.79852245406711
H	2.88138550189553	0.62833508854894	-0.85424153438346
C	-4.24249442841265	0.92961892579787	0.26072720570636
C	-3.28494865022239	-0.01168423714589	0.71873401059457
C	-1.95669572306621	0.21352238631601	0.55551954977528
N	-1.49708549231701	1.33476014099582	-0.05904871029388
C	-2.38454584455676	2.26308882023002	-0.49834239974016
C	-3.72265580297539	2.09943612881904	-0.35568585191862
H	-3.58106003452520	-0.93371932096956	1.19664882662780
H	-1.21791452922060	-0.52481686623731	0.86862114439299
H	-1.96328228786025	3.15391312468705	-0.94146940815860
H	-4.37032769243253	2.88705571565464	-0.71016024219047
Cl	0.06820204914299	-2.47676981398212	1.26818942585569
N	-5.54888801284788	0.73358993074262	0.40446967017594
C	-6.49821229276062	1.72033732957930	-0.07759974230159
H	-6.40016485939376	1.86338698719166	-1.15671599304407
H	-7.50424363242439	1.37113036062406	0.13552550623902
H	-6.35149340172186	2.68163605231035	0.42119695362522
C	-6.04361173928246	-0.47530508136417	1.03835617536316
H	-7.12926273765581	-0.44745010745236	1.04543540291148

H	-5.72141465203695	-1.36389447717486	0.48994748196129
H	-5.68946684625749	-0.54962558894432	2.06960940121569

VONu

C	-1.92925648612115	3.35502004623533	2.62782947194092
C	-1.28564796692782	4.29065459991427	1.92286001958963
C	-0.27937977285339	5.14176182538509	2.55702081239348
C	-1.71308916497189	3.09668323570776	4.07635844086244
H	-1.45516953966514	4.43347137395337	0.86217749598846
O	0.27243859003363	6.02979665969798	1.92890727382791
C	0.07095850977333	4.83119824231015	3.98232229303302
C	-1.10219040714770	4.29769332437142	4.80540879671181
C	-0.60252464449654	3.84253692097028	6.16906023285958
H	0.15756894021917	3.06386020657329	6.06636557025165
H	-0.16571686756394	4.68151232167075	6.71668008395043
H	-1.42593540931441	3.44058627094088	6.76572415601986
C	-2.15181134113844	5.39147137771630	4.98853562440828
H	-2.55230984648247	5.73627988711521	4.03187445457382
H	-2.98518276502751	5.02136606522503	5.59088288035903
H	-1.71656917423855	6.25306442727146	5.50093140428058
H	0.50626402988774	5.72279459162703	4.43871787787185
H	-2.67169303084557	2.83443838091349	4.53577289141826
H	-1.06968943335047	2.21163985713372	4.18060673173439
H	0.85485019236623	4.06442888303648	3.93602995774641
C	-4.85900452173870	0.95409780414400	0.77603663002852
C	-3.91887326745734	0.42297406030193	1.69472624657836
C	-2.98401966395827	1.21995939622761	2.27468623420820
N	-2.91814939248793	2.54655125542389	1.99312998439047
C	-3.79750070436087	3.08888953112081	1.11518646816659
C	-4.75317365715821	2.34443173831535	0.50551858941039
H	-3.90644083250988	-0.62760196858763	1.94395331940203
H	-2.21388402355440	0.81614455007119	2.93727250216174
H	-3.71099457924011	4.15339901226374	0.95133442246337
H	-5.43114560391885	2.84322215326847	-0.17031526674986
C	1.67752168965918	2.02892564831672	0.49876711729518
C	0.65329075575800	1.13386273093874	0.20245458506542
C	2.00795414417149	2.22964143763200	1.83749525845144
H	0.38596345886593	0.94724472383588	-0.83427750700271
H	2.81033134578956	2.91585692311696	2.09488401651953
C	-0.03685558016462	0.47478545138988	1.20610977199383
C	1.32839768036246	1.57623714976663	2.84948635159470
H	-0.82996970132294	-0.22274938735335	0.95242973495703
H	1.59886151785300	1.74584441312032	3.88812609968869
C	0.25335912429463	0.68079744090305	2.58573423764462
H	2.21162676565502	2.54594490783058	-0.28983730094866
O	-0.42544697758214	0.12417296399250	3.52654247905664
N	-5.79009680266361	0.19739885483505	0.20134829752317
C	-5.86983275355151	-1.22011322967834	0.50228995601333
H	-6.69184325937244	-1.65237470693680	-0.06074055986415

H	-4.94679728129516	-1.73280352759536	0.22012460728453
H	-6.05233420331306	-1.38468165705994	1.56727806410929
C	-6.73679342016574	0.77852445067135	-0.73243611919871
H	-7.41050401286848	-0.00010874775554	-1.07780629758800
H	-7.32835737469068	1.56261235853014	-0.25279325200607
H	-6.22360570316932	1.20417455718074	-1.59851532747088

VO⁺

C	8.826702	0.399635	-5.530925
C	10.113053	0.273773	-5.187863
C	11.086691	1.321525	-5.506661
C	8.274933	1.601968	-6.220346
H	10.493174	-0.590076	-4.656221
O	12.265088	1.169133	-5.240597
C	10.557056	2.584075	-6.122557
C	9.339266	2.363211	-7.019297
C	8.763426	3.707108	-7.443476
H	9.499795	4.272606	-8.019338
H	7.879405	3.565076	-8.070822
H	8.475958	4.303724	-6.573959
C	9.735895	1.569549	-8.262410
H	10.503313	2.108830	-8.822442
H	10.134309	0.582899	-8.013841
H	8.871427	1.430979	-8.916097
H	11.367366	3.074728	-6.665502
H	7.460293	1.303130	-6.886358
H	7.841552	2.275813	-5.470142
H	10.279658	3.242022	-5.287564
C	6.108002	-2.706428	-4.626889
C	5.716651	-1.340768	-4.643481
C	6.612631	-0.371665	-4.951978
N	7.908587	-0.652315	-5.249721
C	8.307627	-1.951690	-5.263448
C	7.462994	-2.968029	-4.966986
H	4.707132	-1.039272	-4.408081
H	6.334052	0.671725	-4.950291
H	9.331115	-2.132951	-5.556110
H	7.847676	-3.975381	-5.019065
N	5.259185	-3.679844	-4.325917
C	5.699177	-5.064591	-4.325549
H	4.865607	-5.696489	-4.034556
H	6.036353	-5.367874	-5.319947
H	6.514447	-5.213081	-3.613786
C	3.874036	-3.377602	-4.008476
H	3.357488	-4.304410	-3.777295
H	3.807690	-2.717880	-3.140126
H	3.374151	-2.901468	-4.855802

TS_{EA}

C	-0.138840000000	-0.756648000000	0.269732000000
C	-0.304213000000	-0.194418000000	-0.986298000000
C	-0.875548000000	1.091337000000	-1.169426000000
C	-0.372422000000	0.071288000000	1.496925000000
H	0.038491000000	-0.725413000000	-1.866840000000
O	-1.056051000000	1.594735000000	-2.289382000000
C	-1.176859000000	1.923036000000	0.060155000000
C	-1.466606000000	1.129600000000	1.330354000000
C	-1.412042000000	2.053608000000	2.542492000000
H	-2.152606000000	2.851984000000	2.446648000000
H	-1.627052000000	1.501155000000	3.461899000000
H	-0.425137000000	2.513025000000	2.642801000000
C	-2.863060000000	0.517484000000	1.246098000000
H	-3.611560000000	1.313859000000	1.268933000000
H	-3.008636000000	-0.045772000000	0.324369000000
H	-3.052339000000	-0.152619000000	2.088821000000
H	-2.008098000000	2.592828000000	-0.175836000000
H	-0.581816000000	-0.564404000000	2.359608000000
H	0.574193000000	0.580760000000	1.709934000000
H	-0.295379000000	2.557741000000	0.219491000000
C	-3.210190000000	-3.373094000000	-0.524611000000
C	-3.329419000000	-4.222675000000	0.598361000000
C	-2.427613000000	-3.984758000000	1.662148000000
C	-2.261621000000	-2.382064000000	-0.523094000000
H	-3.852634000000	-3.482155000000	-1.386190000000
N	-1.433761000000	-2.178348000000	0.491113000000
H	-2.144649000000	-1.697900000000	-1.361081000000
C	-1.510912000000	-2.970315000000	1.559286000000
H	-0.802267000000	-2.784623000000	2.359090000000
H	-2.437723000000	-4.589565000000	2.557207000000
Cl	1.290259000000	-1.817686000000	0.452905000000
N	-4.247088000000	-5.203214000000	0.653775000000
C	-4.333817000000	-6.054356000000	1.820005000000
H	-4.528720000000	-5.470751000000	2.724562000000
H	-3.411321000000	-6.624517000000	1.969727000000
H	-5.152053000000	-6.756993000000	1.684791000000
H	-5.783921000000	-6.271127000000	-0.234367000000
C	-5.135670000000	-5.429820000000	-0.464749000000
H	-5.762734000000	-4.554371000000	-0.659878000000
H	-4.578055000000	-5.664267000000	-1.376763000000

TS_{SN}

C	1.70117808705046	-4.09301078892022	-2.62476181424815
C	1.74937158179606	-4.10982883296055	-4.01701053422870
C	0.60087063738146	-4.01079066825504	-4.82920763733980
C	0.37658399599851	-3.84514939512259	-1.95129289971230
H	2.69728466292507	-4.27132779317757	-4.51843977151628
O	0.62842360881688	-4.11537000661366	-6.06936420407180

C	-0.72290561156450	-3.73164765154036	-4.15004623787133
C	-0.59960264535179	-3.02815930482480	-2.80067087211077
C	-0.11680366791356	-1.59090774899334	-2.97850943693301
H	0.83785739629856	-1.54934636366919	-3.50679277757755
H	-0.84615020993402	-1.01497902808398	-3.55434670394618
H	0.00753156826465	-1.10453587319282	-2.00675035277993
C	-1.95235784802499	-3.01598871228778	-2.09946437212072
H	-1.88157220899512	-2.52775187339786	-1.12298506118803
H	-2.68917836291978	-2.47206981355591	-2.69676173620148
H	-2.32208451934303	-4.03375675939989	-1.94673217689616
H	-1.22797071203488	-4.69599964969871	-4.00794153135909
H	-0.08996439063752	-4.81370154947450	-1.75289074440785
H	0.52851587280020	-3.35940361676453	-0.98432486270055
H	-1.33791507612132	-3.14964850868499	-4.84211928963358
C	4.97540135802860	-2.21291108169022	-0.63937771591717
C	4.09265448389217	-3.09419558172801	0.03340485481675
C	3.06766631512676	-3.68649668219170	-0.63521726109156
N	2.84092101140638	-3.46371727737888	-1.94914859356311
C	3.64979659411936	-2.61228056785144	-2.61135653834874
C	4.70095932752042	-1.99063772361991	-2.01054887204488
H	4.21387278354512	-3.32173826414138	1.08177348023784
H	2.39629237878685	-4.38054086375046	-0.15574482855744
H	3.39714994926881	-2.44014465940536	-3.64716375446758
H	5.30034718040199	-1.31843575166152	-2.60572781848027
C	-0.22131628301505	-8.70985480335744	-3.64161706734168
C	0.83573616425133	-8.15956106692685	-4.35624331244752
C	-0.46934114987400	-8.26767243337923	-2.34651584561635
H	1.04514572632243	-8.50587458807799	-5.36307736654183
H	-1.28302728622773	-8.69928697396593	-1.77289800307318
C	1.63243031053559	-7.17308607532008	-3.79438675069613
C	0.31385513865203	-7.27331782221822	-1.78266172153611
H	2.46863589602017	-6.76037471027962	-4.34431658965716
H	0.12418375379725	-6.92773990434622	-0.77156059781819
C	1.38684909240191	-6.70637662961453	-2.49221575905973
H	-0.83721277421305	-9.48476336319932	-4.08354380159073
O	2.12662442249384	-5.75498837946217	-1.95079930627859
N	5.99466224576574	-1.62076385131424	-0.01588291655203
C	6.23255307117068	-1.86605795842979	1.39325328700347
H	7.09787068261382	-1.29012570995142	1.70880962131615
H	5.37400353163448	-1.55992289041935	1.99684518638386
H	6.43322623943511	-2.92439601918065	1.58074026934124
C	6.87654767536111	-0.72888199361621	-0.74303066259412
H	7.64415383684611	-0.36404653169249	-0.06632944562214
H	7.36400084791914	-1.24787037409966	-1.57270121681674
H	6.32869155752113	0.12975965488895	-1.14083996954288

PPY

Cat

C	7.24874373898497	-5.79607680956671	-6.31356638644138
C	7.40641065191472	-6.08510875321107	-7.68375652871619
C	8.63049972624641	-5.87379398717616	-8.28153477051909
N	9.71617269027307	-5.40518015015168	-7.65959235095125
C	9.56129748714089	-5.13476690563858	-6.36034578894710
C	8.39117817829741	-5.30394265802107	-5.65144782004040
H	6.58629898899211	-6.47726899519094	-8.27026464579301
H	8.74527371418298	-6.10104037567230	-9.33862204631294
H	10.43756549754558	-4.75077405937686	-5.84366046809831
H	8.36179872370233	-5.04848330992802	-4.60057644917783
N	6.07830729850172	-5.97947719760458	-5.67593200436652
C	5.89075404701835	-5.75339397642575	-4.25284627658981
H	6.67946068252440	-6.23970446392764	-3.67272792020139
H	5.91788427027757	-4.68048722359574	-4.02121324589701
C	4.85344028565994	-6.39228202786144	-6.34096690798627
H	4.69327731850756	-5.81581014071218	-7.25593591688124
H	4.89854618464512	-7.45363431103570	-6.61754844038775
C	4.51686816619196	-6.34778666077467	-3.97947962060027
H	4.61119722012326	-7.41727968287508	-3.77288358690465
H	4.02551307124977	-5.87881835612835	-3.12687515392380
C	3.77850431295924	-6.13351622798002	-5.29516333202741
H	3.43450702575464	-5.09819328594906	-5.36766939691320
H	2.91540671930596	-6.78786544119640	-5.41848194232313

VOCI

C	-0.16015681578019	1.53031716959763	-0.29953894268904
C	0.28247278225892	2.27308377213817	-1.32057978609818
C	1.71502615409448	2.50378890644202	-1.51300005377911
C	0.72680045728206	0.89020884016421	0.70898985506179
H	-0.38372005865814	2.71259332384936	-2.05335509903850
O	2.11294008449964	3.25836718694532	-2.38391374561348
C	2.64811002053006	1.73001733923321	-0.62789358756349
C	2.11041919396809	1.54111703863366	0.79092109036217
C	3.03816732877305	0.62109230442947	1.57235683624202
H	3.12842696268437	-0.35146790996819	1.08226170927055
H	4.03506634221250	1.06158022914361	1.65325351532613
H	2.65491369366179	0.45846779533539	2.58328330836462
C	2.02169057227594	2.89275201699555	1.49602135929087
H	1.34079757876238	3.57765820631736	0.98424466236081
H	1.66495107296915	2.76491025358012	2.52092609617647
H	3.00687531444214	3.36406149375331	1.53359730306843
H	3.62143344135732	2.22464420573862	-0.62288723985351
H	0.23940407888048	0.93121852813865	1.68851789168463
H	0.82706942557770	-0.17919542919076	0.47057375634075
H	2.77896021903268	0.74630101555052	-1.09879298159935

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C	-3.32882528219231	-0.12386779710842	0.50876625775003
C	-2.00583695149068	0.12395458156697	0.34360359249435
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C	-2.45714317060601	2.29646904524157	-0.41541014290386
C	-3.79106195219616	2.11250113872794	-0.26441208054670
H	-3.61795091069199	-1.09883725355781	0.87370399071992
H	-1.26221011646079	-0.64870769576050	0.53725268571161
H	-2.04675337186376	3.2385222456872	-0.74854163475165
H	-4.45130219034787	2.93283934417601	-0.50499808402760
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N	-5.59001232041797	0.65897563939350	0.37401855556893
C	-6.15757932941689	-0.61582550140414	0.81205320649770
H	-5.72183038177995	-1.44238411414569	0.24842482539386
H	-5.94199174829318	-0.77066209519550	1.87467437308536
C	-7.64686611326021	-0.44682423846956	0.55839939188471
H	-7.88145005930182	-0.72763187185864	-0.47139577608271
H	-8.24593642268785	-1.06509601231324	1.22603799447028
H	-7.90613407086402	1.28193444321682	1.82645219182525
C	-7.86661255222816	1.04680442303336	0.75980650305570
H	-8.78005847860456	1.41563559388356	0.29454441499395
C	-6.62371293722028	1.66659726691763	0.14188548428833
H	-6.74551060737233	1.83127532479780	-0.93412195426336
H	-6.34703022631512	2.61418256202795	0.60705216821637

VONu

C	-2.04371634010714	3.35016524183436	2.66014239387173
C	-1.12881794982182	3.96384542951964	1.90266891045140
C	-0.10836188826404	4.81889897774921	2.50620623906343
C	-2.12922565462431	3.47595047784032	4.14021094833231
H	-1.08614454877432	3.83038593042277	0.82820341268298
O	0.68560411474384	5.42853978342046	1.80928018380388
C	-0.06021610773126	4.85858170178128	4.00488525092914
C	-1.43255459153461	4.73520157484008	4.66738117940526
C	-1.25872433657643	4.60699320116049	6.17438488019568
H	-0.65251556893072	3.73290113798627	6.42507080858363
H	-0.76629371140599	5.49479947793078	6.57932819304233
H	-2.22928479019102	4.50341712992199	6.66712406148204
C	-2.27271167417185	5.97244609671081	4.35740883923262
H	-2.44633082393234	6.09144276256007	3.28478230582588
H	-3.24504627995315	5.90725200645141	4.85201284404570
H	-1.76743675379420	6.87231582379522	4.71704384045908
H	0.45151529484687	5.77131223562085	4.31713701223994
H	-3.18410410471466	3.48669590084953	4.43373385102238
H	-1.69303158722576	2.57620741000276	4.59577628823111
H	0.56251159844052	4.00619438440686	4.30584632733932
C	-4.92332376057503	0.89891838817884	0.80271927769958
C	-4.31016841773165	0.54171371014009	2.03036096136886
C	-3.39277293626378	1.35622240667352	2.61197159778118

N	-3.03524617097924	2.53567360874016	2.04005063861771
C	-3.61077588087441	2.91552577705138	0.87067083979572
C	-4.53467454297053	2.14668734308390	0.24472008410942
H	-4.54619590306860	-0.39013985919225	2.52328720652127
H	-2.86134836638116	1.06584819425312	3.52274700757115
H	-3.30586906208976	3.87650755158187	0.48206031057492
H	-4.96370417422475	2.50801372696218	-0.67831883560921
C	1.65888543904149	0.99288220986858	1.95163366335757
C	0.55907630247254	0.22043698165918	1.58796531788355
C	1.71505267555973	1.48481710799854	3.25408025651686
H	0.49811945393907	-0.18650058890666	0.58213453803554
H	2.56728362589716	2.08288050482035	3.56555429327475
C	-0.46337914951623	-0.04038697450134	2.48480780056446
C	0.70017093806027	1.23326582920246	4.15980765816217
H	-1.31001102666380	-0.64957981842638	2.18164840608094
H	0.75888544233332	1.62865208878112	5.17024734956386
C	-0.45242210115544	0.47171747378565	3.81411148429852
H	2.45589179476947	1.19480665768524	1.24562095477003
O	-1.42753535668376	0.28835742166198	4.63339852833821
N	-5.80944597583526	0.11688464583983	0.20739021974487
C	-6.18865025126104	-1.20819789661681	0.69505703341729
H	-5.30272547597305	-1.77870547079017	0.97843280734068
H	-6.83327933862593	-1.10945956968313	1.57513328772032
C	-6.93255605488696	-1.81564935945489	-0.48300895215488
H	-6.22148357302336	-2.28646398649735	-1.16667435520411
H	-7.65233176750331	-2.56978714094002	-0.16649152624517
H	-7.86346241393281	-0.78338538489544	-2.18311582084369
C	-7.57833989438461	-0.60619564630788	-1.14662590124755
H	-8.47036038709592	-0.30311971564475	-0.59258454476910
H	-6.92311287468798	1.47434614008171	-0.96013124938005
C	-6.50804841641848	0.46715002391103	-1.02802194568483
H	-5.80859925054363	0.43728863709106	-1.87050672121085

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C	8.53508840031356	0.53134041574357	-5.61810015912739
C	9.39485685321043	1.03287874677568	-4.72434411656336
C	10.28770302257672	2.14058659863310	-5.07243311651149
C	8.39197161323254	1.06384409500277	-7.00464835428631
H	9.46243853856921	0.66128723869894	-3.70905340377811
O	11.09326103937853	2.56187855939316	-4.26154339101894
C	10.12648393544153	2.75076728378868	-6.43472851796621
C	9.66391833712450	1.76029769286299	-7.50225817470665
C	9.34132994186593	2.50696807099236	-8.78900243983484
H	10.23198156347554	3.01376753226003	-9.16816959812417
H	8.99255291772419	1.81409790736380	-9.55938901828229
H	8.56425291375797	3.25777745402971	-8.62419285027253
C	10.75847849661152	0.73077568468268	-7.77454206628966
H	11.66574527660771	1.23092358819972	-8.12109797415754
H	11.01320635286219	0.15501301433109	-6.88159026851042

H	10.43865106982988	0.03017093636366	-8.54974322268395
H	11.06627319203068	3.22987749373976	-6.71658000945686
H	8.12860954262145	0.25053640061503	-7.68675749978413
H	7.56061183341994	1.78010743745042	-7.02709308442688
H	9.37590138474264	3.54579657523528	-6.32637206938885
C	6.03885993459709	-2.70810925887245	-4.56696561557081
C	5.62267106910657	-1.69838818830250	-5.47661156232626
C	6.45594924043260	-0.68102651422185	-5.79993876716010
N	7.70372257299019	-0.57005574633563	-5.26964248792802
C	8.13186158521400	-1.52520412563705	-4.40032688030809
C	7.35224856434909	-2.57152054341236	-4.03956569598766
H	4.64384187944557	-1.72243497822703	-5.93237861789301
H	6.15301090284252	0.09995694351316	-6.48136502546646
H	9.14331937639182	-1.41955672232460	-4.03697365317845
H	7.75962986784403	-3.30022984087396	-3.35436444476758
N	5.25700736852268	-3.71980506769469	-4.24232040957795
C	3.88620804747220	-3.88366915458098	-4.72897388848424
H	3.33231306512273	-2.94903818204762	-4.62966304832137
H	3.90464878215779	-4.16563477334497	-5.78697863997703
H	2.92428641092361	-4.58266325239664	-2.93440276374941
C	3.33189264184406	-4.99968886396998	-3.85861380513660
H	2.53949682598920	-5.55150834697854	-4.36297538133905
C	4.55977721101545	-5.84916213790772	-3.55740432404222
H	4.79869202952445	-6.48528181846033	-4.41320276046202
H	4.43946185504502	-6.48548459121158	-2.68143305419476
H	5.69988861724641	-4.45977677054861	-2.32617713966897
C	5.65810993573735	-4.81700387407186	-3.36042065310193
H	6.64535148278885	-5.18861800625460	-3.63910715718732

T_{SEA}

C	-0.22485749316579	-0.75995392777516	0.35232778411667
C	-0.71524173176552	0.13941664973198	-0.58121295992205
C	-1.23678617364075	1.40556778443733	-0.20854914223268
C	-0.02909225534527	-0.33118052510872	1.77494972012090
H	-0.68398013932757	-0.10366008685064	-1.63695012104912
O	-1.71150920990958	2.20604096857243	-1.02960954862295
C	-1.10517275288194	1.83644433872341	1.23780069199704
C	-1.05188248455888	0.70200515728825	2.25669362708248
C	-0.57851486514001	1.23686400981533	3.60400925816137
H	-1.25449626115067	2.01751511928817	3.96304188705095
H	-0.55626418597654	0.43890627104805	4.35196597064765
H	0.42554197532489	1.66255045685544	3.52789395400961
C	-2.44654028248463	0.10547764217101	2.43319174917432
H	-3.09758389213731	0.84038658304506	2.91409092910781
H	-2.90113418466450	-0.16426871357813	1.48008036546847
H	-2.41794016224222	-0.78787600357441	3.06258118907988
H	-1.92523407760167	2.52201029094085	1.46752783853851
H	-0.01176779605054	-1.19533370210813	2.44240497330230
H	0.96881024502569	0.11912690687839	1.82507363481955

H	-0.17840014638282	2.42220013311190	1.29512715932289
C	-3.57249259771327	-3.08783367920184	-0.19047304606712
C	-3.41082873484861	-4.23831227599232	0.61448100556468
C	-2.22420614955711	-4.30666653389409	1.38229330799847
C	-2.59962969794830	-2.12146939293505	-0.18589530086223
H	-4.44503532190248	-2.95835938260883	-0.81523019259253
N	-1.49559435842885	-2.21194351399889	0.54224707288732
H	-2.68621359997251	-1.21661366757304	-0.78422731238340
C	-1.31010461829566	-3.28808188930768	1.30619405407421
H	-0.38822478470771	-3.33092781920004	1.87608767174031
H	-2.02400019788885	-5.14834219183315	2.03036362156884
Cl	1.11793066272694	-1.79736526866793	-0.21363469369334
N	-4.32732059025982	-5.21119655418983	0.64811047203749
H	-6.07938586136779	-4.19520361779984	0.06100450543658
C	-5.58857308735152	-5.16119638050308	-0.07870016495731
H	-5.41699199271448	-5.30136579147466	-1.15293524743609
C	-6.38447588237183	-6.31277506992709	0.51636724006930
H	-7.12026202526586	-6.70919761415353	-0.18316035168770
H	-6.91189795240963	-5.97296797090423	1.41155126066071
H	-4.97252315961404	-7.86443444617478	0.00740943815766
C	-5.30598616940632	-7.32023095367461	0.89487546629753
H	-5.63456596663024	-8.04757586395412	1.63704954278094
H	-3.19246533076831	-6.88400602982234	1.24984631697835
C	-4.17781476080703	-6.44140201740142	1.41381547059838
H	-4.28421953242099	-6.23988786771993	2.48670965265528

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C	-0.22107713806749	-3.03542740663209	-4.04647304027943
C	0.87430846602605	-4.66066958619257	-1.91565572754032
H	1.77959085077127	-2.37216930869200	-4.38791823069693
O	-0.74383851705098	-2.39910522047951	-4.98095322211346
C	-1.10691684484661	-3.87691574535387	-3.15271652180772
C	-0.54481796467735	-4.11079486508923	-1.75323381674970
C	-0.55324361307524	-2.81945974446482	-0.93876243523668
H	0.04162623811870	-2.03674873416242	-1.41369636215686
H	-1.57543914245625	-2.44693677451182	-0.83017230269678
H	-0.15013586130956	-2.99661207995671	0.06243710389903
C	-1.38448714246404	-5.15642288732963	-1.02971265422892
H	-0.98017034881217	-5.36023113282803	-0.03380976790522
H	-2.41370681682529	-4.80659729379116	-0.91128817830089
H	-1.40635582611180	-6.09561173881333	-1.58925237211655
H	-1.24910666788882	-4.84489238665076	-3.65078927678166
H	0.79117622880035	-5.65372734489301	-2.36514958309661
H	1.33610552122572	-4.79289099290095	-0.93412046929157
H	-2.08853784731758	-3.39712846941278	-3.10541260530383
C	5.09669622005785	-2.17742554490423	-0.71843326241724
C	4.82747688433763	-3.56923210892377	-0.73149515133831

C	3.76135155972736	-4.05535323765812	-1.41922419420143
N	2.91865297860939	-3.25014637821727	-2.10603523181772
C	3.13573872173842	-1.91877778874189	-2.09229358283413
C	4.18865643296796	-1.36059875810269	-1.43588666274269
H	5.46721158771621	-4.26911733534922	-0.21404255922986
H	3.54671807464996	-5.11051600240478	-1.47315653408008
H	2.40415074864256	-1.32302201023483	-2.61822554005591
H	4.29533259579263	-0.28588033908386	-1.45570954269678
C	0.48338633401460	-7.36858578763817	-6.20631584472116
C	0.88285328104948	-6.08808090464350	-6.56848757741573
C	0.88563916073712	-7.88526056733620	-4.97939611666318
H	0.58397820286956	-5.68050047923998	-7.52871524897573
H	0.59114960231810	-8.88892953966227	-4.69085647108250
C	1.66715436066868	-5.32336297737765	-5.71733282945413
C	1.65566226861714	-7.12219445325005	-4.11678850229629
H	1.99311335661746	-4.33329068491682	-6.00929371833666
H	1.96862534378361	-7.52054487540606	-3.15702928172842
C	2.06561522511670	-5.82384904619421	-4.46677834270333
H	-0.12431602295199	-7.96335080081157	-6.87858870784736
O	2.78282128803141	-5.09605939145247	-3.62853719201319
N	6.13258707074343	-1.66947218344520	-0.06360055633699
C	7.04757216645443	-2.45925047145611	0.75597967741419
H	7.69533214279160	-3.06720719486275	0.11452910993328
H	6.49271700377506	-3.12867016288213	1.41606552677290
C	7.83853684545050	-1.40588199210338	1.51527094604121
H	8.82686274840448	-1.76422863470403	1.80158086916412
H	7.30026516858405	-1.12263698011196	2.42357772581638
H	8.09872219470601	0.71838810204398	1.02157050171080
C	7.87834774609850	-0.23475916432422	0.54187446505743
H	8.63113300220818	-0.41260451568494	-0.23028432302953
H	5.77309185486378	0.32044896001583	0.51871532573206
C	6.49020043479219	-0.25399340444909	-0.07852943038983
H	6.47583530856299	0.13442838994410	-1.09860700761889

ITU

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C	1.23979706138494	2.03035517181438	1.31463842352249
C	1.20248976436834	0.51412793428001	1.31614517751486
S	0.75973499577321	2.49761033939140	-0.36733181146607
N	0.10838683029308	0.13764276123939	0.45046458470623
C	-0.14901449123526	0.99324487693953	-0.57813418601562
C	-0.27993062142286	-1.26029955643063	0.34255319732045
C	-1.53544769840995	-0.49499077932433	-1.66311057243675
N	-0.91242354240419	0.81770942606061	-1.58370715953984
C	-0.65088043669865	-1.58993958209232	-1.09012816229328
H	0.52234239358363	2.44745980052672	2.02203221402663
H	2.23297781007376	2.41804246763298	1.53315504858431

H	2.14958385110796	0.09766196409976	0.94609181543099
H	1.03061258552215	0.13025048320706	2.32463580545071
H	0.56164597572810	-1.87535629681570	0.67392127737113
H	-1.11941457578274	-1.46104036329393	1.01678556811896
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H	-2.49427260049037	-0.47763605875404	-1.12659748104945
H	0.25727511859356	-1.66519338231082	-1.69624516533006
H	-1.15512118386786	-2.55764922259273	-1.12592990047847

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N	4.98348250312340	4.42527767853213	-2.33284750234467
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C	5.82255235657040	4.53667824997812	-1.15471961894714
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H	5.67905607943472	6.15098004078065	-3.26804738047975
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H	3.89177802410741	2.26678997577240	0.53766196787941
H	3.64131271498908	4.03205066206378	0.43631471703735
H	6.01842479295054	2.45342813576560	-0.66607677293076
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C	0.85477859058480	0.60268099337302	-2.61659623163590
C	1.22050416258561	2.49092105288423	-0.42546615012342
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C	-0.27657089859859	0.98008890472481	-1.70348177706701
C	0.18531745879898	1.37279238117647	-0.29934689331835
C	-1.00156769563186	1.88370886452981	0.50511269034494
H	-1.75735490852225	1.10163964758048	0.61310572227046
H	-0.68410148529356	2.18935127262953	1.50576528879115
H	-1.46609645684683	2.74425338115263	0.01669828364523
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H	0.06394506549150	-0.63958242136740	0.48807592526274
H	1.67020435464079	-0.22079567223563	-0.11919257573852
H	1.11000688126538	0.44087538630397	1.42172141074822
H	-0.99350737875767	0.15700721992778	-1.67399289996027
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H	0.73575711886584	3.43345735569132	-0.71592818884634

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C	3.13696447831035	3.10398447904548	-2.75861042007054
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C	3.23421905216178	3.49576396706988	-0.37280887926341
N	2.80705151444478	2.69874556254319	-1.53634090310652
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H	2.20277020548112	4.42160935497561	-5.27680393798448
H	3.41668164618641	3.44307959795919	-6.15606070543531
H	5.16746723586603	4.04753077479294	-4.62007798935867
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H	5.47253855731190	5.26734795449374	-2.26955933543056
H	3.85877309607217	5.83583339887196	-1.76521953922285
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H	5.34131465258765	3.34901341740136	-0.77521303470441
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C	1.96982465371891	1.58317228197151	-1.32335701464705
C	2.27225247062539	0.39521035114686	-1.86287269835880
C	1.37329188203830	-0.74974180952328	-1.71679718615713
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O	1.68332707449000	-1.84616464887327	-2.15094714201616
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C	0.13854000023053	0.55318931147998	0.07332693180936
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H	-1.71772294359695	-0.03484011401143	1.01649472064005
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H	-0.63201578330577	-0.14408900282303	-1.81557990796059
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VO⁺

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C	1.38264945556385	0.02381193541855	-1.16370757699445
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C	1.97516170358486	-1.12466106405174	-1.94717794184785
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H	1.89728538974278	-0.14276030340106	-5.81472857312571
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H	3.03445044898208	-1.38727851922022	-3.81211029836134
H	3.73861766559572	-0.15718784435117	-2.75349081972051
H	0.71805584390207	-0.34206335140564	-0.38305704556145
H	2.16519518591728	0.63279987611632	-0.70375088879490
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H	2.60630581367823	-1.72292096490882	-1.29022082224453
C	-0.56346005215133	1.52719877518136	-1.56171589452992
C	-1.72718194581985	1.45032802654322	-2.21797538156158
C	-2.89131999767859	2.22553483685463	-1.78215176118843
C	-0.36873371428153	2.31961779993575	-0.31531039493120
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C	-2.68063464161891	3.16884054182170	-0.63336700349687
C	-1.67890737372242	2.65166482499340	0.40112992326820
C	-1.41787766589157	3.73357008825022	1.43999164833686
H	-2.33969016855785	3.98182804235636	1.97146415712460
H	-0.68409340083513	3.39247872540514	2.17516874793626
H	-1.03620926516485	4.64427646362231	0.97122718404119
C	-2.22926963682044	1.40644688810801	1.09369602883918
H	-3.18059076437965	1.63363478124074	1.58042676906578
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H	-1.53098864397686	1.05684025331897	1.85820048587875
H	-3.64838651452139	3.38921287798285	-0.17852962534287
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H	-2.30025337165270	4.10428028142887	-1.06589043444268

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C	1.34606883726024	1.43560464219593	-3.11531897282906
C	1.36945123235522	-0.83627096334887	-4.02119999236711
C	-0.58963168711118	0.13734084085865	-2.88599451618641
N	0.11873354767466	1.38628191087376	-2.71399970862923
C	-0.11863608662218	-0.58714644358355	-4.12958698213366
H	4.26187862356734	1.65651049672171	-2.42117636733917
H	4.53511669024860	2.51030480124384	-3.96200721771062
H	3.28081764396873	0.88825644063110	-5.21426896441279
H	4.02010234557697	-0.15313841095889	-3.97746080422830
H	1.79050581160234	-1.13224756960374	-4.98521031514974
H	1.58377224590173	-1.63409262385574	-3.30384691806121
H	-1.65545321331845	0.36888883092199	-2.92620466959394
H	-0.43707283271076	-0.50322779375584	-2.01010637387317
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H	-0.64644728437300	-1.53567496165421	-4.23588485919983
C	-0.94485223128436	2.79283692922982	-2.02319684971287
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C	-2.79511503368616	2.07838753808290	-0.56310889202329
C	-0.18079036431065	3.29233693032716	-0.83171959722799
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C	-1.99804264180313	2.48819750960944	0.65859377623018
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C	0.14970294301195	3.33014859797528	1.61304947323187
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H	-0.22651382780176	4.35626200664839	1.64271981774586
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H	-0.43457539617023	0.48530045782030	-0.23410310862481
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H	-2.25875637416209	1.81407197855703	1.47922815503288
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H	-0.46549540248045	4.34291700604305	-0.70671008580882
H	-2.36980818276419	3.48230927107236	0.93945000611920
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N	-3.26934785521992	-0.80235607759596	0.27815022182865
C	-2.16146306669750	-0.15066851758507	-0.03968895438347
C	-3.41425981304425	-1.68394042644574	1.42654215018914

C	-1.30276971909893	-0.62309272610627	2.12918848989556
N	-1.10610962712064	-0.12446064811128	0.76405034699188
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H	-5.28923445403802	-0.76606771615733	-0.23478337144082
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H	-3.85706825860565	-2.61756795666321	1.07079796536950
H	-1.84758921805158	0.13086789463439	2.70644829724493
H	-0.31390415011223	-0.76449034749595	2.54961558681335
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C	0.38519154152254	0.68505187852009	-0.93989267470266
C	0.99513249575940	1.82375594354156	-1.52360268136033
C	0.34410130423655	1.78192923544630	1.30629398819538
H	0.21721792380456	-0.17197961444932	-1.57932917903290
O	1.29377203122902	1.88403549792339	-2.72625302391484
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H	-0.59561423079151	2.34970815630630	1.34762328686421
H	0.55286227658673	1.44052077952054	2.32215501513004
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C	3.21689237528549	-3.37839118059901	-1.14971130743520
C	3.94562537094908	-2.52200013971793	-0.33091110535455
C	1.83095061644607	-3.27799921598439	-1.15657490723037
H	5.02912384577941	-2.58478680403286	-0.31105708521231
H	1.24495347745672	-3.93937585989494	-1.78710999229626
C	3.30525142518944	-1.57864055152977	0.45530137327911
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H	3.87723184487304	-0.91019341719131	1.08962473700666
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DABCO

Cat

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H	0.88355094106983	-1.88142260600212	1.17035347405688
H	-0.88355314025489	-1.88142119020023	1.17035213928070
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H	2.07082800546143	0.17630375286459	1.17003758721302
C	-1.18834387869395	0.68641723410105	-0.77460263298498
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H	1.1856007784088	1.70575803933159	-1.17006906694425
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VOCI

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H	0.46235230105408	2.58431323201731	-0.86072902713824
H	-1.02425226469596	2.19991148774372	-1.74659782875386
C	0.47686916466732	0.40132835463359	0.78831947716133
H	-0.12736046405914	0.80396226420704	1.60466271020603
H	0.69045798699380	-0.64629421118758	1.01385189531036
H	1.42610357245802	0.94241994468830	0.76875784982637
H	-2.22857075069698	0.18973551283533	0.31622552988058
H	1.58089698182695	0.42174789860192	-1.64203118973433
H	0.14755417349406	0.31662886396833	-2.64426535053253
H	-2.13605316716057	0.01888417401419	-1.44161133830097
N	1.76822945792412	-2.11547111561964	-2.40192870902384
C	2.99942911130199	-2.00797765108354	-1.53792544948127
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C	2.01414281576873	-1.39083147495836	-3.70763486106702
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H	0.71562246178537	-3.60747587348112	-3.40896383895773
C	4.21942182527090	-2.43169626291910	-2.37786956540643
H	3.07569033439173	-0.98082431006008	-1.18787474169373
H	2.82346718185959	-2.66252243766374	-0.68496592037102
C	3.14324422479328	-2.10359890167024	-4.46512331513543
H	1.06476866751684	-1.41267491546316	-4.24740679935200
H	2.28825375840636	-0.37095347391091	-3.45440608762698
H	4.82853823606153	-1.56149167753712	-2.62612514482965
H	4.83150052987702	-3.12122345192651	-1.79498558631084
H	3.33241066732677	-4.82533318867891	-2.60516388622404
H	2.63769788135953	-4.68708569373568	-4.22409426810648
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N	3.81143451360567	-3.07633853155186	-3.61573908273549
H	2.74223691788738	-2.62479141608787	-5.33571498399647
Cl	-1.06330424405686	-2.40749461216730	-4.96718551118696

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C	0.63735465417506	-1.69310084799221	-1.79049649065948
C	-0.16005804863896	-2.61385670906782	-1.25376661677772
C	-1.38490105263178	-2.23527467270835	-0.53139665504010
C	0.33782734773661	-0.23511517330010	-1.73894015489174
H	0.02652335625216	-3.67607699702713	-1.30088582318245
O	-2.02269054254362	-3.08282810605619	0.06778888724051
C	-1.79276655878629	-0.80035311413455	-0.58950864147197
C	-0.60069344763581	0.15382824482628	-0.59243568834728
C	-1.09137805650993	1.57476206422658	-0.83403701056693
H	-1.76055423394506	1.88873246252556	-0.02918525531682
H	-0.25114184173412	2.27371244656337	-0.86966441443447
H	-1.63620483108584	1.64151649220934	-1.77921063684326
C	0.13612382401368	0.08818375797443	0.74296225495530
H	-0.54120054916387	0.35108345423494	1.55910118797955
H	0.53175022185004	-0.91046704180585	0.94511019125144
H	0.97241260468907	0.79200253773335	0.75482536843944
H	-2.47194657173550	-0.58832774400391	0.23877130705210
H	1.25076832838050	0.35976313178042	-1.65794770193170
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H	-2.35911396259632	-0.68266246759793	-1.52415381602616
N	1.88654289547262	-2.07836793933899	-2.48956357468992
C	3.06035603828510	-1.82557794475207	-1.58001641938293
C	1.91549140117810	-3.52720950460067	-2.88329692356996
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H	1.74044036535547	-4.11532358874429	-1.98734275750947
H	1.08982684565566	-3.65150078382351	-3.58602632387047
C	4.35643833426616	-2.03063575267029	-2.38751332714251
H	2.97242012601838	-0.81300988219164	-1.19234386307190

H	2.95773935173893	-2.53105184251885	-0.75624136412940
C	3.30816810971553	-1.73220520971383	-4.49250240387332
H	1.12834721985213	-1.42708703306178	-4.32144320203928
H	2.13424807265243	-0.22139636026781	-3.44796645488043
H	4.84926780528747	-1.07299134253132	-2.56100567155527
H	5.03723650173557	-2.66506314720455	-1.81824792574186
H	3.84941822605819	-4.51536573097724	-2.79920752802886
H	3.17849041859994	-4.36599141367177	-4.42641074737502
H	3.92345434638030	-0.86981432075410	-4.75362063024990
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H	3.03388700823072	-2.24520908879693	-5.41565972188048
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C	-3.77676023122330	-2.26266033553241	-3.16167737406897
C	-3.15895884684293	-0.14122825545658	-4.07517395605107
H	-4.47923383446364	-2.89125340163528	-2.62148410874017
H	-3.37530854422257	0.90709685705841	-4.26231112875017
C	-2.58236964191906	-2.80761143739045	-3.59761085306148
C	-1.96250026857177	-0.67353182667538	-4.52221876489151
H	-2.35803979624647	-3.85339747732991	-3.40808700738508
H	-1.25674047623704	-0.05043831553776	-5.06528140043214
C	-1.61606517808167	-2.04179921638927	-4.31289313177630
H	-5.02037735918494	-0.50024163522951	-3.03844933734116
O	-0.51176369896333	-2.54196164420429	-4.72933128790689

VO⁺

C	0.67480377620086	-1.58060307849122	-1.75348888662464
C	-0.23013948172952	-2.34484829977843	-1.14773284234631
C	-1.38097452045303	-1.74811396395653	-0.44266571311825
C	0.58358268991212	-0.09079130829078	-1.79294008288083
H	-0.18581183856636	-3.42340549218793	-1.11325284331557
O	-2.14590652505082	-2.46503264542527	0.17046815343783
C	-1.55799522656799	-0.26560047727168	-0.55026277086648
C	-0.23062089913261	0.48741438432167	-0.62941585305655
C	-0.49421818763792	1.96039815463658	-0.90863029585978
H	-1.07349206833549	2.40306257641869	-0.09505088052461
H	0.44638751009397	2.51098263380140	-0.99319505229543
H	-1.05415945712050	2.08988635997732	-1.83823720512736
C	0.53862197753112	0.34997910583752	0.68196578717932
H	-0.05058395750516	0.75869452549887	1.50591540400365
H	0.77064776385498	-0.69086397598782	0.92035922704217
H	1.47994304820771	0.90260098770352	0.63082006076080
H	-2.16987286672192	0.07893674272762	0.28543129447348
H	1.57240774891266	0.37260168430890	-1.79327676411410
H	0.10901528467616	0.19953424066968	-2.73857578695762
H	-2.12908211006951	-0.08755546345775	-1.47183602344225
N	1.83661295613002	-2.19312898201246	-2.44172207363676
C	3.09392354905997	-1.89068911257637	-1.65958345508303
C	1.73202669559003	-3.68674837914267	-2.55966556578331
C	1.96140083280684	-1.62051644162908	-3.83304412427507

C	2.97288084325742	-4.22169540280277	-3.30335232419489
H	1.67723065369367	-4.08287638189212	-1.54842622419716
H	0.80427502065591	-3.90145769469155	-3.08733192003429
C	4.30333372889002	-2.47398700137162	-2.41938416277545
H	3.16390359012249	-0.81174052506496	-1.55311974710923
H	2.95172509841771	-2.33782586364433	-0.67676943049079
C	3.21391850112938	-2.20799613061133	-4.50983069362073
H	1.03639532453167	-1.87463589620896	-4.34962274493212
H	2.03196266016336	-0.54129707140171	-3.73456336576459
H	4.99487468047055	-1.67269907993836	-2.68098672140001
H	4.82883543501241	-3.18550850606168	-1.78185780444915
H	3.48935263219564	-4.94855677985225	-2.67592442762399
H	2.66556456977530	-4.72038150846685	-4.22292917474761
H	3.90592755139622	-1.40522969787476	-4.76632134517492
N	3.89005210643347	-3.14927465583551	-3.63647119776001
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TS_{EA}

C	-0.27698306574157	-0.80757016324273	0.30619407225450
C	0.30511233000748	-1.24019391467273	-0.87986690455356
C	0.41650861293128	-0.41774200937971	-2.02659196355458
C	-0.94467918486636	0.54475620035703	0.36473258135317
H	0.84617635635480	-2.17905637520625	-0.90043839706246
O	0.94429401287992	-0.79982154906914	-3.08482808725405
C	-0.00248927211634	1.02921306158652	-1.89613873239848
C	-1.19464296300995	1.25903287940249	-0.97741146518042
C	-1.33121950656702	2.74854819287571	-0.66798354741541
H	-1.48881402877312	3.31566724898148	-1.58900232481996
H	-2.18479950172036	2.93140017676946	-0.00849567197462
H	-0.43295228594910	3.13271626184799	-0.17795645208976
C	-2.46679384774079	0.81178412940635	-1.69269056322466
H	-2.64587764800089	1.46792309689138	-2.54826133499710
H	-2.39169784634035	-0.20705656072496	-2.07135718071979
H	-3.33657125227181	0.87585171909491	-1.03355562995076
H	-0.20603659021313	1.42434445020507	-2.89445703940244
H	-1.87720328641107	0.49783613885239	0.93176692482376
H	-0.28092911288609	1.18243971699244	0.95337024245315
H	0.87118231624553	1.56915252093243	-1.50890597508690
N	-1.59486767964745	-2.10778889022637	0.83504743758869
C	-3.58213428496740	-3.31808786728324	0.04872283187379
C	-2.66562242398622	-2.09464353738872	-0.16976185661756
H	-3.21799246153146	-1.16469617958080	-0.05154016505091
H	-2.19071685721797	-2.10794993598726	-1.15110494259663
C	-1.98533417526105	-4.48111304762334	1.33460033987307
C	-0.96884447343630	-3.44300070624470	0.81206147686723
H	-0.68329971244134	-3.64612342859308	-0.21946421263607
H	-0.07103318249283	-3.41652768577652	1.42684534269608
C	-3.36752729094122	-2.86128425378679	2.35716722976457
C	-2.18358693522140	-1.88276861626091	2.16693013584078

H	-1.40389574411688	-2.05105944736028	2.90656916662058
H	-2.51294431367703	-0.84662663514093	2.23972928486458
H	-1.97280912646776	-5.36647836656512	0.69617045502252
H	-1.73085167697618	-4.79294329340956	2.34962074465568
N	-3.32786581654677	-3.91580036371624	1.35253160441196
H	-4.62783984590925	-3.01104006674108	-0.01217359929508
H	-3.40671577466323	-4.07648750710319	-0.71681656523340
H	-4.32022752022576	-2.33602735533894	2.26517970566543
H	-3.32027005172472	-3.30688473465116	3.35251557156955
Cl	0.77379638064121	-1.02451223412186	1.79515719191550

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C	-4.13427338841480	-1.04067319950892	-5.15532379967935
C	-4.57844835692691	-1.12668988708733	-3.81436722114654
C	-6.08910265595624	0.36542166172837	-5.80897682435609
H	-3.19600134242385	-1.53749915941258	-5.36266891335821
O	-3.91581641876510	-1.67171094840453	-2.91510386850510
C	-5.92105137475824	-0.52098830272642	-3.48901711093662
C	-6.20771524770194	0.72299507295808	-4.32082000606007
C	-7.63182986712875	1.20149843409427	-4.06582250404455
H	-7.76342656462357	1.46710546753104	-3.01361472507402
H	-7.86181839892552	2.08538466436096	-4.66853831329338
H	-8.35560479444279	0.42077500303458	-4.31479767300734
C	-5.23687497195262	1.83881742303928	-3.93929799972702
H	-5.37041194654956	2.11191861786174	-2.88924820065561
H	-4.19727676854405	1.53518243827344	-4.07774852802966
H	-5.41777003176592	2.73123820424880	-4.54555980405178
H	-5.94779874384419	-0.29133021494956	-2.42089238030761
H	-6.05793339255882	1.30027045173829	-6.37008879460181
H	-7.00662106570037	-0.13836411869383	-6.11766089051357
H	-6.68689122111914	-1.28129424847476	-3.68475360313739
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C	-3.27667446807597	1.09337712154019	-7.02100586074660
C	-3.26708335384639	-1.13675965283723	-7.98508359211499
C	-5.04280501001504	0.41401476041302	-8.53033773855793
C	-2.28772877851855	-0.49331790107613	-8.97728017525752
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H	-3.88560589410814	1.79580508239136	-6.45623791217660
H	-2.51103358294279	0.69108039100333	-6.36137113614818
C	-4.18154701212584	0.65012810231652	-9.77961323135364
H	-5.81222361279584	-0.33716723069259	-8.67358980539999
H	-5.49812210046809	1.34347599679931	-8.20061003751606
H	-3.22678311972762	2.64160109482470	-8.55324280440992
H	-1.64676267963485	1.98609607620749	-8.11388869783393
H	-1.30480127506982	-0.35515026348655	-8.52316433523525
H	-2.17156924785538	-1.15323978082836	-9.83876258952480

H	-4.53351980295188	1.54916339771563	-10.28831828184108
N	-2.77844230093695	0.80498592514881	-9.41838357378122
H	-4.26601455652313	-0.18648844095751	-10.47521954644537
C	-7.78945349337986	-4.31725355610521	-4.47577583648037
C	-8.48647943638105	-3.40889723917734	-5.26558944638678
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H	-9.56610983551088	-3.33686526557224	-5.18507038182620
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C	-7.80952279652626	-2.58735124308138	-6.15156372782314
C	-5.72630507350305	-3.60717426717850	-5.50454174557057
H	-8.35001370295407	-1.87512055180297	-6.76644615533890
H	-4.65361260727741	-3.69658366907966	-5.61917905092414
C	-6.41331134617665	-2.66438921710266	-6.28510301886317
H	-8.31922878784886	-4.95366543852056	-3.77622031596500
O	-5.77180507903422	-1.85147250480121	-7.10836356082551

Qu

Cat

N	0.00000005499063	-0.00071522775979	1.25630892458787
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C	-0.00000032693624	-1.37624685067427	0.76541655704761
C	-1.19113377756556	0.68777336874097	0.76501496711239
C	0.00000043391890	-1.43456925113899	-0.78022958140981
H	0.88082106607662	-1.87813479884186	1.17485318471202
H	-0.88082284599477	-1.87813375205869	1.17485205542121
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H	1.18491325615623	1.70155004461451	1.17429669479091
H	2.06671832853157	0.17639439621389	1.17372484464401
C	-1.24107549730749	0.71709998724167	-0.78093017005850
H	-2.06671819294248	0.17639535934234	1.17372568788599
H	-1.18491227176302	1.70155059834120	1.17429669145477
H	1.25992832011838	1.74629771294211	-1.15056675571027
H	2.14356661231387	0.22249204726001	-1.15110887064929
H	0.88064746800475	-1.96723615645218	-1.15051618139031
H	-0.88064550252658	-1.96723722278876	-1.15051715070851
H	-1.25992928870525	1.74629712925536	-1.15056690790027
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H	-2.14356665085432	0.22249101217865	-1.15110799384905
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VOCI

Cl	-1.09017901405741	-2.51900530715717	-4.99424541274825
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C	-0.34504410348541	-2.24209268173983	-1.18139508478270
C	-1.49385431773216	-1.62410809448540	-0.49863417528587
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O	-2.32988285432632	-2.32669806390093	0.03674479123340
C	-1.59339857342373	-0.13058681816646	-0.53188580138996
C	-0.23007564620613	0.55657301829671	-0.52492298016497
C	-0.41019046157134	2.05340500036485	-0.73564127225839
H	-1.00677308717590	2.48241521648001	0.07309059348100
H	0.55891753171164	2.55925620959629	-0.74705092783741
H	-0.91687437271313	2.25909357857700	-1.68195291474344
C	0.48203314716279	0.31476427053896	0.80390659352625
H	-0.11489321771907	0.71307401250732	1.62769490746413
H	0.65176444932918	-0.74740178950578	0.99506351546843
H	1.45176417634634	0.81857506649146	0.81203795289093
H	-2.21961511303719	0.20060267693135	0.29888728309155
H	1.60357042502295	0.41243357664880	-1.63739212088576
H	0.16523677032699	0.34319972453828	-2.63340524556296
H	-2.12050984447205	0.11990091455427	-1.46288631756066
N	1.77227570656772	-2.11651710436261	-2.40670236451343
C	3.00745971459596	-1.97368918962497	-1.54506295944151
C	1.58552426275757	-3.58369794918589	-2.69226534418494
C	1.99417664162546	-1.40962724119452	-3.73139892210932
C	2.89788758536772	-4.18741693228447	-3.19722760877813
H	1.28422849512702	-4.05936881632156	-1.76406681849743
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C	4.25058782528781	-2.28794058915802	-2.37658232735007
H	3.02289309578521	-0.96231535673489	-1.14682494886047
H	2.86437191418809	-2.66935372015778	-0.71848253202183
C	3.06006686874082	-2.13900831870602	-4.54275852004741
H	1.02357599500021	-1.40584037094493	-4.23086367070665
H	2.30085556366095	-0.39593801064437	-3.48817609578416
H	4.75901880825289	-1.36512676461122	-2.66343917362454
H	4.94070000765435	-2.87133338669678	-1.76516969114926
H	3.36076940908080	-4.79264619900531	-2.41500008039946
H	2.67940417129793	-4.84417891644190	-4.04041462486948
H	3.72036420072574	-1.40033371284831	-4.99983519714895
C	3.83591636116502	-3.06740297556256	-3.61988396531373
H	2.59319343120313	-2.71334074900972	-5.34586065456305
H	4.71314930734912	-3.46989278347229	-4.12704128770191

VONu

C	0.64424874369059	-1.72036850861319	-1.80479122444037
C	-0.15711533128556	-2.63814466608865	-1.26727624860990
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C	0.34044189756631	-0.26240483747116	-1.75669996708691
H	0.02589217549361	-3.70110256209787	-1.30914418759011
O	-2.02916280984071	-3.10603808557767	0.04006718643384
C	-1.78433595783166	-0.81969624053598	-0.59501624350618
C	-0.58938381388261	0.13040610652636	-0.60483891715517
C	-1.07687863212568	1.55289622120769	-0.84413127591704
H	-1.74337240168083	1.86820329126061	-0.03750531967914

H	-0.23491595452526	2.24970009964740	-0.88136473747444
H	-1.62382334033779	1.62156831302447	-1.78793044544545
C	0.15435953670802	0.06312922988265	0.72656109605100
H	-0.51718241930974	0.33094776731977	1.54593142410088
H	0.54568355624784	-0.93728492816945	0.92827390786928
H	0.99434865448037	0.76265994508080	0.73291673688641
H	-2.45376993471230	-0.61037806317997	0.24200077341021
H	1.25218603282045	0.33553734100677	-1.68796810999187
H	-0.14257861192992	0.00181143387119	-2.70758191164067
H	-2.36165351819112	-0.69302407003022	-1.52170375445192
N	1.89868411742799	-2.09925126323255	-2.49423082840116
C	3.06401908989339	-1.84119597358071	-1.56815061642753
C	1.94311560184443	-3.54987022207939	-2.89186150350266
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C	3.34684530104955	-3.91638295042302	-3.38058493003195
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C	4.37194311775396	-1.90913200386984	-2.35589583909701
H	2.90992202515911	-0.86997544416074	-1.10316638322755
H	2.99658353010917	-2.60909050747683	-0.79785083180954
C	3.25774012358867	-1.76957150789678	-4.56128501913009
H	1.11550096196684	-1.38038965655730	-4.29183678360705
H	2.20652875441431	-0.24331307404850	-3.43165081910928
H	4.74923177078818	-0.90353651651445	-2.55337900587895
H	5.11668599029307	-2.43066424236765	-1.75260002470818
H	3.86410787736321	-4.51539359625745	-2.62805960329743
H	3.25782859375489	-4.52306894542841	-4.28295941781713
H	3.81767534512124	-0.90895182378795	-4.93082838429976
C	4.12705252122544	-2.64346529659467	-3.66992512017573
H	2.91710676529493	-2.34237523210673	-5.42673075961004
H	5.07408938954140	-2.87498619778351	-4.15848601672656
C	-4.10427122276748	-0.88595602493546	-3.37429235956136
C	-3.79404473230677	-2.22910286062616	-3.16996646681577
C	-3.18142286023294	-0.09397652393302	-4.05507831190322
H	-4.49439070799811	-2.86596541627683	-2.63668587828245
H	-3.39979451230576	0.95661290803519	-4.22670504410940
C	-2.60069674380133	-2.76654831189301	-3.61730020719467
C	-1.98630133067512	-0.61865607716125	-4.51425088075526
H	-2.37419298239721	-3.81463960806254	-3.44366083260168
H	-1.28345551874252	0.01276875710611	-5.05160153135392
C	-1.63667125844723	-1.98952489765318	-4.32455688493635
H	-5.03851013028721	-0.46963730825825	-3.01617051587647
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VO⁺

C	0.67947622615939	-1.58636042798119	-1.76419136038258
C	-0.22517042579922	-2.34887380808448	-1.15419730964558
C	-1.37407924663524	-1.75274443854434	-0.44734183761313
C	0.58269056308672	-0.09614083523576	-1.80451600233204

H	-0.18114705775576	-3.42708118721256	-1.11625098829575
O	-2.13949454365275	-2.47008423048003	0.16581812231799
C	-1.55052297997660	-0.26989659558186	-0.54960212607148
C	-0.22322239239957	0.48189611784742	-0.63552102099286
C	-0.48717159404192	1.95538842449160	-0.91149905662651
H	-1.06157390283419	2.39771428170925	-0.09423659340078
H	0.45341744048043	2.50530028152399	-1.00080504102339
H	-1.05217250472545	2.08628092538129	-1.83785744881095
C	0.55413768969447	0.34255786731889	0.67087828455083
H	-0.02899213660643	0.75166389467434	1.49897830942733
H	0.78621536714746	-0.69878940784565	0.90690264853282
H	1.49602369654170	0.89368676259246	0.61383135508260
H	-2.15690644029533	0.07284226603055	0.29090281096700
H	1.56965750268044	0.37076047331899	-1.81370786197910
H	0.09901413456815	0.19164172310881	-2.74623623393302
H	-2.12743821086112	-0.08885588230707	-1.46696090532699
N	1.84339480793054	-2.19702072341676	-2.44939718437738
C	3.09382240937535	-1.88660696923896	-1.65346608998437
C	1.73377753505539	-3.69348466878133	-2.56254890523709
C	1.96415805777703	-1.61818779365912	-3.84162126429681
C	2.94621104090633	-4.27341498101392	-3.29772652771024
H	1.67207190220664	-4.07539490766423	-1.54639612658450
H	0.79798402600711	-3.89726070340988	-3.08012327700115
C	4.33119037370025	-2.44625285192966	-2.36230724832468
H	3.14445006136086	-0.80682945139018	-1.54568208425651
H	2.93075302034047	-2.32885150716023	-0.6716060098788
C	3.20242449399104	-2.16803366726920	-4.55312633275189
H	1.03358521960072	-1.87402395538737	-4.34739988431787
H	2.01886003250488	-0.53945441280879	-3.73108260244674
H	5.01875976446994	-1.63101718711343	-2.59168566191202
H	4.84698085094755	-3.14042847913138	-1.69748521732907
H	3.43171147515424	-5.01489123755457	-2.66200488657931
H	2.61508909992303	-4.77913489079545	-4.20574740524112
H	3.86854535926681	-1.34450907578748	-4.81449338197035
C	3.91539295489412	-3.15585939124460	-3.64337936025212
H	2.90161454076685	-2.66016845159914	-5.47893797016953
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T_{SEA}

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C	0.31664282928953	-1.23809498443490	-0.87371942177091
C	0.40365174347553	-0.42601675851635	-2.03171948981934
C	-0.93783377379128	0.54509771050694	0.36904987570576
H	0.86366131563307	-2.17357920952994	-0.89134563201112
O	0.91575339279339	-0.81625189365982	-3.09376289272163
C	-0.01443900644560	1.02150567294344	-1.90459879884097
C	-1.19518778743147	1.25857708205238	-0.97270824209849
C	-1.32015921074804	2.74945560202975	-0.66428110480551

H	-1.48726819248954	3.31592843968074	-1.58403653085561
H	-2.16397851804788	2.93753141884444	0.00622497376555
H	-0.41358378879536	3.12980245051824	-0.18674422177141
C	-2.47773422722441	0.81854179766186	-1.67416365763798
H	-2.66492010888408	1.47859217387560	-2.52499701263976
H	-2.41170759496719	-0.19899393598209	-2.05763463601038
H	-3.33878937143553	0.88264633159203	-1.00379306670958
H	-0.22961001178316	1.41156128698854	-2.90245752528838
H	-1.86930945856169	0.49167085945807	0.93701636084140
H	-0.27669987615895	1.18617838283616	0.95741140493259
H	0.86471960958797	1.56210394894544	-1.53101741615505
N	-1.60909268303079	-2.12592264696746	0.84218943285139
C	-3.58258912425964	-3.32956408452506	-0.02988588491339
C	-2.67455924044378	-2.09726241275199	-0.16817932578568
H	-3.23793258610363	-1.17753560964645	-0.02076952752598
H	-2.18660957041781	-2.05863182653068	-1.14248461682070
C	-1.94013692004712	-4.51457353864583	1.37209013498310
C	-0.97713065648150	-3.45879165586876	0.80647737515222
H	-0.73088775174778	-3.66290483809815	-0.23530360833331
H	-0.05074510784816	-3.41495078662788	1.37662540940160
C	-3.41569271797498	-2.80697389769888	2.37824988639504
C	-2.18821448924559	-1.90032724892951	2.17939026074988
H	-1.41241731937908	-2.12138365044634	2.90959440911678
H	-2.45246975156179	-0.84735043601243	2.27528210070107
H	-1.88281408817957	-5.42219369364137	0.76790926447602
H	-1.65949938746835	-4.78051692371914	2.39455648986254
C	-3.34921145063575	-3.93299739233130	1.35045875043202
H	-4.62494491900286	-3.03007766520468	-0.15569954225807
H	-3.35379281683522	-4.06556313443753	-0.80469457348184
H	-4.33959698442473	-2.23749432915369	2.24853964721439
H	-3.41237986278600	-3.20465778842056	3.39511326476337
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TS_{SN}

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C	-4.57844016316991	-1.12135724548090	-3.82540865831620
C	-6.08369219729929	0.37965182408199	-5.81833933779725
H	-3.19542222731821	-1.53050620236426	-5.37236273739721
O	-3.91677446959246	-1.66625930494943	-2.92404289151510
C	-5.92236777553361	-0.51735987851156	-3.50102715491776
C	-6.20740559560410	0.72956812912246	-4.32879509206043
C	-7.63274966965546	1.20610335119779	-4.07611544820084
H	-7.76642324748515	1.47314099628143	-3.02448935317513
H	-7.86371171457962	2.08859289791246	-4.68055601497762
H	-8.35471521125464	0.42363815475970	-4.32492507524247
C	-5.23888748676284	1.84433089082709	-3.93840671035865
H	-5.37256130878377	2.10828236390724	-2.88599227477570
H	-4.19872724552721	1.54365080648874	-4.07927327425714

H	-5.42189181680138	2.74143124832497	-4.53709982131923
H	-5.95158518581609	-0.29118470845394	-2.43214669768084
H	-6.04070261385122	1.31732708838387	-6.37390915782259
H	-7.00403396827320	-0.11370470316909	-6.13503451764937
H	-6.68773092143655	-1.27690427777003	-3.70106410581301
N	-4.15142420124115	-0.05803771972995	-7.42386123031395
C	-3.25383702448119	1.07947794821396	-7.01515634643169
C	-3.29203154899998	-1.15123523859550	-8.01043419845465
C	-5.04559487075982	0.44575129205938	-8.52961913039463
C	-2.25434820725464	-0.54753318357620	-8.95401277406447
H	-2.83009445654148	-1.69324778025746	-7.19344687394259
H	-3.97661294437589	-1.82150422171305	-8.51885635745928
C	-2.68673333064777	1.77177480501104	-8.25434325183331
H	-3.84522354539876	1.75434699251699	-6.40052091392069
H	-2.47820292560497	0.64281566452087	-6.39002277505485
C	-4.23205451240535	0.63530372862081	-9.80866152358812
H	-5.85292318106185	-0.27124191130775	-8.63443513742282
H	-5.45046051521591	1.39700205193207	-8.19527135483073
H	-3.24289874220638	2.68580754052512	-8.47541172106020
H	-1.65250559620302	2.05516783078394	-8.05187290916361
H	-1.28942901450912	-0.43476599432309	-8.45386573104894
H	-2.11393348107257	-1.23046240544235	-9.79370178492891
H	-4.60925782879688	1.51657364221208	-10.33029845269969
C	-2.76537069948012	0.80540722877936	-9.43022953534997
H	-4.35223250404690	-0.22107026578714	-10.47623004971198
H	-2.18158888749829	1.17166629184758	-10.27519914651226
C	-7.76906125521138	-4.32735809195141	-4.47831546126265
C	-8.47426332548665	-3.41407084855709	-5.25517971976315
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H	-5.83346655330213	-5.14114728274106	-4.03235535880760
C	-7.80592239154081	-2.58308351636748	-6.13886511964454
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H	-4.64326208214095	-3.68725219143348	-5.63800692012838
C	-6.41068607065739	-2.65511887302347	-6.28333624687103
H	-8.29187875239976	-4.97150955546314	-3.78061441967736
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NMIO

Cat

C	7.76833171645042	-1.22446717784613	-2.53595616594376
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C	8.14209054715270	-2.63320023172514	-4.17768754824333
H	7.46177438773239	-0.34971482529925	-1.98967715897822
C	8.58285863817031	-3.20795242815050	-3.02191378552313
H	9.04075243533429	-4.16629006233182	-2.84194532028532

H	8.13869382602050	-2.98315836739848	-5.19510339970985
N	8.34699311214055	-2.32580813800781	-2.01453597852065
C	8.65442293894029	-2.52080042774582	-0.61449284116643
H	7.74340049213728	-2.46863556032319	-0.01778212289571
H	9.10526260212036	-3.50367840190188	-0.49655384045669
H	9.35634993209364	-1.75977955743807	-0.27221924247335
O	7.12626809400382	-0.54518892315829	-4.68535950427456

VOCI

C	5.04189873948424	-2.88809546155751	-0.73915313676408
C	5.01370218261123	-2.63363409670820	-2.04921898339060
C	4.24703735724617	-1.49420958214703	-2.54087878963959
C	4.33698443176224	-2.12025488208646	0.31160562058110
H	5.54174575991248	-3.23139737598699	-2.78109497585955
O	4.13351725030400	-1.28232246052335	-3.73707428903936
C	3.65152102193234	-0.57710795236130	-1.50815880858751
C	3.17257142334208	-1.29696058149722	-0.24564085964455
C	2.74746448255765	-0.27198697467025	0.79657186054885
H	1.90945513296486	0.32364841451200	0.42632571691227
H	2.42985947899754	-0.76792316776487	1.71768526354340
H	3.57004814524066	0.40572516399143	1.03854295977551
C	1.99178547538025	-2.20729867886862	-0.57587122738346
H	1.17259034537140	-1.62248580643102	-1.00082312355763
H	2.26277922865388	-2.98218179846449	-1.29701165236351
H	1.62601314470267	-2.69962208485391	0.32857381981451
H	2.84222607852913	-0.00936610305081	-1.97130833797099
H	3.99122068666794	-2.80790490139147	1.08936962213241
H	5.08022113803984	-1.46257054613450	0.78097318325842
H	4.44220021014560	0.13542515791174	-1.23744943444605
O	5.76588775228988	-3.91069310198697	-0.16148066849261
N	6.65075908826227	-4.51512708139918	-0.99023006695027
C	7.85215379596473	-4.01116415431715	-1.25941075111924
C	6.46507016396186	-5.72855535435357	-1.59515031326244
H	5.55429918561290	-6.29268668579558	-1.49021631705820
H	8.21341719702830	-3.03281651387131	-0.90786056747454
N	8.45216810776294	-4.89184239354197	-2.04662666406985
C	7.61910044423298	-5.96362535764906	-2.26745028430500
H	7.91571762879338	-6.79893375247759	-2.87886186573650
H	10.42968130471637	-5.53519950023786	-2.19579578360671
C	9.79415444090472	-4.74146946721654	-2.58553028105785
H	9.75093549913534	-4.79762884479557	-3.67194684804135
H	10.18150719500124	-3.77263569580152	-2.28008293955983
Cl	8.39494457248665	-0.98573795147323	-0.20213277618517

VONu

C	-0.71938786741270	-1.74528093096727	0.67802798188073
C	0.48859290762486	-2.12645702322156	0.25803987062782
C	0.60487904440166	-3.00518669678670	-0.89844905806606

C	-2.01027568796506	-2.13986859658058	0.07406446692025
H	1.40747120577692	-1.80070364731217	0.72833093122828
O	1.69351261147955	-3.42163003237346	-1.26322937200081
C	-0.65924671035315	-3.32686394518071	-1.64084647339073
C	-1.90378778098241	-3.42120232894243	-0.75677774051184
C	-3.14042883071462	-3.53914475380754	-1.63810477269987
H	-4.04681773271044	-3.58516729369576	-1.02825617500671
H	-3.22054555674551	-2.68143268529478	-2.31070953283640
H	-3.09229165619831	-4.44736290307659	-2.24402692466161
C	-1.81259793372365	-4.63881072240875	0.15948732568496
H	-1.71904393034917	-5.55127822475918	-0.43441164396526
H	-0.95107010355201	-4.58357179208500	0.82975851858445
H	-2.71338736075393	-4.72307020619060	0.77270731224154
H	-0.50583409583671	-4.24999690690357	-2.20387213174191
H	-2.76500912800070	-2.24397721199440	0.85950899778545
H	-2.32647257781346	-1.30333624873548	-0.56400737636823
H	-0.78911973750434	-2.51596326464092	-2.37140231677299
O	-0.92849266302303	-0.87608259879315	1.73023920890075
C	-0.22096028853501	-0.74641426597701	-4.24144450965601
C	-1.50526468781917	-0.34630795329903	-3.88229893968609
C	0.83942643781721	-0.37142721609445	-3.42083619815988
H	-2.35043339248723	-0.63076515165557	-4.50274467120530
H	1.85023565155822	-0.67638772245328	-3.67599427554752
C	-1.72853413069318	0.40317681470188	-2.73987358861849
C	0.63099282333609	0.38447969002685	-2.28018291722889
H	-2.73579810752654	0.70702880764835	-2.46946709677933
H	1.47438715985246	0.67024851407062	-1.65796178207516
C	-0.66646161341041	0.80978520211323	-1.88975932509402
H	-0.05115376990082	-1.33589094489091	-5.13479091496445
O	-0.87579085345125	1.52028674690971	-0.82915859185040
N	0.17053515084270	-0.16160336697572	2.07941456508564
H	0.06974303524132	1.25975347543870	0.43057407330682
C	0.57518761499569	0.90206455207256	1.38856543053793
C	0.96592035510399	-0.40836137816753	3.16552336207133
H	0.78924428632278	-1.22785980227159	3.84072132305999
C	1.90829295235761	0.56590816331982	3.12994510571620
H	2.73403275912758	0.76508855521006	3.79192167654130
N	1.64707521281088	1.35172755762857	2.03041686148425
C	2.42431891601483	2.50942104463773	1.62293514613970
H	2.40574055969948	3.25616250856953	2.41549857853027
H	3.45091451595775	2.20440568387519	1.42508480959861
H	1.98151834114128	2.92013189431309	0.71879137796175

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C	6.23962337316794	-2.85256405809389	0.73799516904177
C	7.45694673235741	-2.35593241572123	0.51180423153554
C	7.87589048391705	-1.13826459627384	1.20301842119942
C	5.22394116795565	-2.27992438838356	1.65158794376870
H	8.16614156604678	-2.80220285138016	-0.17349264602915

O	8.95662964959787	-0.62802204283118	0.96449889165415
C	6.93777034466722	-0.58026499276180	2.23808516447950
C	5.45767175352381	-0.78747859312996	1.91119040778364
C	4.60600913059918	-0.35443496327455	3.09649550730358
H	4.75476357639487	0.70788083932315	3.30423072341453
H	3.54499643293927	-0.51347763148226	2.88657474438046
H	4.86704640328810	-0.91946374009434	3.99501049328617
C	5.07068023099611	0.03084263499032	0.68124105067907
H	5.25220998603794	1.09236089167914	0.86470765036287
H	5.64344107475890	-0.25983351215266	-0.20277867715323
H	4.00954595301257	-0.09900191528201	0.45519842658080
H	7.16741109708910	0.47756524583919	2.37969325719514
H	4.22771223902863	-2.44882374186243	1.23271724100572
H	5.26822296062311	-2.83777952513698	2.59533332869613
H	7.17574759862075	-1.09421028600021	3.17930172712237
O	5.74323741708755	-3.99774436040675	0.14322389941953
N	6.61917508640444	-4.64463563980538	-0.65886111862106
C	6.65529224586972	-4.49092082727837	-1.97921292254725
C	7.52177137352241	-5.58699411853322	-0.24633141737186
H	7.64046949391862	-5.85526066990480	0.78972512569935
H	6.04194273016395	-3.81577937474369	-2.55367944660664
N	7.57862774537980	-5.32384309592243	-2.43338408244620
C	8.13080929095988	-6.01259885999733	-1.38059454072536
H	8.90419717419141	-6.74776744816952	-1.52727075725801
H	9.00282498973612	-5.20950557779023	-3.94826369229958
C	7.95503171750528	-5.48057125922239	-3.82993380417544
H	7.80110729695215	-6.51710015413136	-4.12479947931811
H	7.33248178068629	-4.82641138006523	-4.43476547505653

T_{SEA}

C	0.00668250617294	-2.67073811137431	0.09925062618201
C	1.04180501179698	-2.55774222980236	-0.83649205446920
C	2.04534205285569	-3.53631260400482	-0.97030097625025
C	-0.18447928813538	-3.95709936284487	0.84466759157778
H	1.07140504343001	-1.70371811263786	-1.50341814105860
O	2.99637525575346	-3.43752214487280	-1.77127848779081
C	1.90928322029203	-4.81823536011458	-0.17113778377052
C	1.12105823245064	-4.70591090250935	1.13107526683470
C	0.76255359444446	-6.09875713838601	1.63917694714839
H	0.14909130773883	-6.63667122432266	0.91135892912063
H	1.66874685356222	-6.68320041916011	1.82018681350913
H	0.20545290199859	-6.03936184321454	2.57881446442789
C	1.96741831553762	-4.00619097747917	2.19072468432325
H	2.83889533475351	-4.62133252644715	2.43108201709455
H	2.32244311513802	-3.03458038570688	1.84949141189755
H	1.39419162937486	-3.85250306650173	3.10859561370495
H	2.91322612963966	-5.20626717488592	0.02218499057426
H	-0.73321754897012	-3.76501083047339	1.77041513526868
H	-0.82093469386685	-4.59405284223562	0.22275365634113

H	1.41616868963966	-5.54086505433377	-0.83444870232558
O	0.19385318009185	-1.59414850848182	1.43001220430365
Cl	-1.58412642820131	-2.03222390842628	-0.49736960909424
N	0.70674712165878	-0.44589074141087	1.02913318154920
C	-0.00617249869249	0.62223374149540	0.67222400420650
C	2.04219618121089	-0.19448757277616	0.83761757194652
H	2.79648377003812	-0.92816696437891	1.05569979012463
H	2.98007287679880	1.67645817645361	0.10130518834542
C	2.12627565773215	1.07986183042691	0.37384678632253
N	0.84758494279680	1.56307439263010	0.27686209814433
H	-1.07810094726811	0.70409783258667	0.71830149004399
H	0.70246366742490	3.61148264667777	0.66605713100072
C	0.48357938552444	2.90567534606075	-0.13488054596211
H	-0.57926768419834	2.92754102762134	-0.36414134635396
H	1.05299034747661	3.16967992482954	-1.02430510091715

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C	8.41358510354187	0.55372689268741	-3.33470777997959
C	8.33646206018400	0.38915944324167	-1.95859043449973
C	7.91267219297819	1.43053429435296	-1.10664646979725
C	8.22670090517412	1.90134567760665	-3.95607959397965
H	8.53061992084113	-0.57564811162375	-1.50533657025360
O	7.75601586986625	1.29067179008582	0.12000353825490
C	7.66193431454228	2.78918374405354	-1.72777197563713
C	8.47938356500211	3.06123426009652	-2.98933419133886
C	7.99887970621715	4.34990803116458	-3.64480018537436
H	8.13279603607547	5.19783425006654	-2.96760230811211
H	8.56077143685679	4.55650256414004	-4.56053290185830
H	6.93822011744218	4.28452432275302	-3.90258844550132
C	9.96279589384306	3.19345560225096	-2.65536421865956
H	10.12527255509991	4.03559308271562	-1.97734369658061
H	10.34782246480769	2.29164187861972	-2.17500659487750
H	10.54507605296892	3.37301491293496	-3.56349721125359
H	7.85701813261793	3.54763879072152	-0.96475098528530
H	8.86753732475247	1.98070048568465	-4.83844490395158
H	7.19293533644940	1.96935735506111	-4.30372862898238
H	6.59328910070729	2.84765420379259	-1.97213887205677
O	9.42263897855254	-0.14048183818497	-4.06567188920776
C	3.35002167620710	0.42756763072742	-2.57043577467239
C	3.72154806586467	0.95000240913451	-3.80459764823254
C	4.23596896811506	-0.40070406072991	-1.89181602256059
H	3.03504916513981	1.58886320035108	-4.35072901118549
H	3.95390073328397	-0.82275292148250	-0.93255345456577
C	4.96679961723116	0.66613965812183	-4.34270987591218
C	5.47989859335390	-0.69798779720908	-2.42836888631491
H	5.25732844315730	1.07271855075018	-5.30613199564760
H	6.16292193917916	-1.35377048024250	-1.90246022804275
C	5.87690880118548	-0.16688963703166	-3.66803043006246
H	2.37777714005138	0.65473323797795	-2.14826088410448

O	7.06811645663145	-0.41693322380621	-4.17861037012191
N	9.71554203766242	-1.34914301419622	-3.55098619334976
C	10.81003347043020	-1.61541620923872	-2.77563211929902
H	11.51316782231620	-0.84941060490551	-2.49847321941274
C	10.74910572811323	-2.94358845633343	-2.50578679035877
H	11.40587289328739	-3.57433365426485	-1.93141901469552
N	9.62278039777509	-3.43556091493891	-3.11978046979359
C	9.18158671400991	-4.81892502964430	-3.08635862747561
H	9.93880399897207	-5.45083029850691	-3.54820735812319
H	9.02568796933191	-5.12140354714481	-2.05202614697743
H	8.24806557619457	-4.90018037753429	-3.63769528393055
C	9.00040967693069	-2.45110148105463	-3.75521625683743
H	8.07938542005476	-2.49394492301972	-4.31068578639113

DMAPO

Cat

C	7.21844544272333	-5.80524820506778	-6.29475398758399
C	7.37371070494564	-6.06838043882173	-7.66906432170015
C	8.57829596244997	-5.86693142718310	-8.29163998159104
N	9.66765325539052	-5.41211614990058	-7.63452622762502
C	9.54547609325759	-5.15333069457309	-6.31407967700696
C	8.36897011957244	-5.33435130642494	-5.63388577955055
H	6.55333828277829	-6.43246454295952	-8.27075585094300
H	8.73512062969577	-6.05613132506469	-9.34423579000503
H	10.44785145755769	-4.79261003358841	-5.84065864095721
H	8.35916189531751	-5.10299032056978	-4.57832273980085
N	6.04197850972883	-5.99250261797634	-5.65217105118126
C	5.92757399679701	-5.66838372927042	-4.25080442400268
H	6.60646294739815	-6.27345403383744	-3.64025511497911
H	6.14922261052672	-4.61220022263804	-4.06147937567004
C	4.89051561184857	-6.46524165228709	-6.38223963658655
H	4.60044180960442	-5.76848130831038	-7.17694498099417
H	5.07798393862832	-7.44298880926245	-6.83856208212659
O	10.79461105484296	-5.22841317016141	-8.25326036630257
H	4.05308261256375	-6.56672595994193	-5.69628338340613
H	4.90951118437242	-5.86563021916083	-3.92386995098707

VOCI

C	-1.64398981557981	-1.23817312799291	0.40335354782932
C	-1.32444392506462	-1.29639402177797	-0.89368328569981
C	-2.38394108579806	-1.33725086305654	-1.89257307114185
C	-3.01675160918019	-1.23576879451272	0.95647438116424
H	-0.30315292658330	-1.29918175899356	-1.25178917536805
O	-2.12728154337619	-1.45880477040223	-3.08031605653055
C	-3.79501685702520	-1.17172889168863	-1.39684517089133
C	-4.04507745801374	-1.80169925172742	-0.02564247018397

C	-5.44173756202582	-1.43723912255636	0.45848675342772
H	-5.62884248188833	-1.86310102879310	1.44804414318798
H	-5.56276565849267	-0.35300884532065	0.52341753974408
H	-6.19785973130394	-1.82740564242576	-0.22736962560608
C	-3.91964101087707	-3.32125335920634	-0.11191504632087
H	-4.63878912940263	-3.71902031107631	-0.83213361512498
H	-2.92044851389859	-3.63289585692661	-0.42591999864471
H	-4.12580184359819	-3.77534967573346	0.86051246433629
H	-4.47824222587631	-1.57216031194924	-2.14845060396398
H	-3.02726774996014	-1.79392370655924	1.89746009484540
H	-3.25066282854793	-0.19118819706058	1.20078563346332
H	-3.97205045868441	-0.08964434672600	-1.33216584866897
C	0.94420117849916	0.32341102627913	0.75173519272129
N	0.56110364055111	-0.93853065844945	1.01553851345867
C	1.39753517320837	-1.98924457325148	0.97351285413146
O	-0.72997668133212	-1.15138148819134	1.42338390078134
C	2.23753349246095	0.56626626578281	0.41047535050653
C	3.17960518340290	-0.49470245432672	0.33576212863186
H	2.51825554021455	1.58772430920404	0.20254688098779
H	0.15836848340858	1.08307957898573	0.81834567846323
C	2.70086668408928	-1.79874671866626	0.64005737056747
H	3.34819660787185	-2.66191671619981	0.61543608914541
H	0.96826565546262	-2.95143173297661	1.21686544149676
H	4.80189911762917	1.72090969326287	0.56160306210164
H	4.34635432363119	1.48644537455694	-1.14035781263900
C	4.90837553204448	1.06256398611756	-0.30464552589395
C	5.39140785588160	-1.38181730992475	-0.05464984531119
H	5.07491486607126	-2.13099744434511	-0.78493945252903
H	5.49234471630982	-1.86215956194184	0.92210980236178
N	4.44908754052161	-0.27987204950438	0.00068185366432
Cl	-1.74773863141261	2.38393561286800	0.75345453224560
H	5.95799968190436	1.01916782826920	-0.58027323626411
H	6.36230667575904	-0.99746829106287	-0.35293100748108

VONu

C	-1.67892675330576	-1.17234004411363	0.35574299692042
C	-1.32057828562201	-1.29995479241992	-0.92707218196618
C	-2.35085489398869	-1.43258843937901	-1.94685142044768
C	-3.06273660156337	-1.16763451778692	0.87143562842274
H	-0.29140978399805	-1.28453500886374	-1.26091976043549
O	-2.05765073987993	-1.59083224200793	-3.12255502396322
C	-3.78161154906758	-1.31064127685992	-1.49735077106373
C	-4.04222984380114	-1.84710284843752	-0.08869222942596
C	-5.46322217110229	-1.50041625573927	0.33464936557898
H	-5.66103229251565	-1.86419381336125	1.34659409150912
H	-5.62115581301865	-0.41928035420388	0.32198661039733
H	-6.18794526504838	-1.96339889706330	-0.34000519200344
C	-3.86038703711238	-3.36286826014859	-0.05906496845843
H	-4.54838213752119	-3.84075480973978	-0.76107473711832

H	-2.84367085461496	-3.65919280644466	-0.32913838855996
H	-4.07125963592052	-3.75033660072402	0.94085618214618
H	-4.41973538811402	-1.80233289463734	-2.23468361049392
H	-3.08377105499084	-1.64580456185132	1.85532733695706
H	-3.33112809824106	-0.10608633389015	1.00731564167086
H	-4.01839876939755	-0.23840248177841	-1.52176296450785
C	0.92262048150926	0.41849812606594	0.67367297672416
N	0.50910550496016	-0.81906515365115	0.99913601680644
C	1.32694170106172	-1.88606746328272	1.01524734455351
O	-0.79195614213432	-0.99046242560127	1.39043112972663
C	2.22185334773824	0.62027559861681	0.33037928428314
C	3.14183581554998	-0.46149770286944	0.31303361121457
H	2.51722318096228	1.62632775892856	0.07552465044161
H	0.17623037063905	1.20440433434989	0.70575967192970
C	2.63563229872571	-1.73820900275370	0.68243713016038
H	3.26595403977001	-2.61398193363539	0.70588381523013
H	0.87710936787425	-2.82644627489606	1.30256548312581
H	4.81522501297913	1.73181019196640	0.42036294136683
H	4.33657554171792	1.41513484888840	-1.26202276669570
C	4.89885754064016	1.02561106545491	-0.41007184332489
C	5.33715401437532	-1.40968462414805	-0.02093170116020
H	5.01391077454081	-2.18755265765985	-0.71744708887518
H	5.41928718432059	-1.84300669234307	0.97919665342269
N	4.41556895033953	-0.28892220215779	-0.02899497727789
C	0.34160229208726	3.65305837389403	-0.12390983815255
C	-0.44549920176462	3.03805808543314	-1.09730763749816
C	-0.13523121323375	3.67161381116737	1.18548812961419
H	-0.09247521868223	2.99683820793782	-2.12428951936715
H	0.46242755913520	4.13317169251273	1.96709252633892
C	-1.66764089509714	2.47044744409107	-0.78295553232775
C	-1.35507077724930	3.10466786908636	1.51606605919780
H	-2.26086775413601	1.99362882444719	-1.55845572752980
H	-1.70590805241647	3.12934136795854	2.54407390872095
C	-2.20201224315384	2.49048292475384	0.54248811110664
H	1.29624943375060	4.09947639788424	-0.37706592787013
O	-3.34215438154904	1.99305381110911	0.83646808571392
H	6.31839463902862	-1.05869798575250	-0.32656878954420
H	5.94435450453494	0.94608113665522	-0.69325844021296

VO⁺

C	6.36035841190905	-2.56174951194217	0.58984749246916
C	7.58859275379111	-2.03525030985967	0.59486419788941
C	7.91254131581949	-0.97336211144687	1.54173067227839
C	5.24430238961865	-2.15469294291187	1.47661760850414
H	8.37739601995488	-2.35314041660499	-0.07476342102778
O	9.01636741861752	-0.45419334842416	1.54291329568796
C	6.85134065773748	-0.58576440457596	2.53588018614044
C	5.42014144403889	-0.73078396401597	2.01539846477936
C	4.43588920493717	-0.50825842293260	3.15543545133411

H	4.53968242147255	0.50308738363494	3.55571774587473
H	3.40715622795510	-0.62968346367493	2.80594498534902
H	4.60825626602247	-1.21821678632870	3.96844080894344
C	5.15269457042233	0.28886394633031	0.91022153881818
H	5.28891409667968	1.30280239849490	1.29323292798096
H	5.82481170609765	0.15753590320158	0.05894327865790
H	4.12550282767692	0.19694180557448	0.54896313640563
H	7.04882799542602	0.43406646515196	2.87223993059635
H	4.30104213644550	-2.24781661907455	0.93077201549677
H	5.19911659807912	-2.86908962365275	2.30824105707662
H	6.98843580320471	-1.24539071941771	3.40331084681087
C	7.68955574020246	-5.09590595348197	-0.60925628494150
N	6.93390615313499	-4.07675007826139	-1.05840784223758
C	7.05156555154045	-3.57464287983914	-2.30099674923300
O	5.95302922132373	-3.57758259821528	-0.24347207683079
C	8.62994427839037	-5.64701042780226	-1.41836554659878
C	8.81840225509507	-5.15858733367543	-2.74162166755530
H	9.21891327534233	-6.46181603902852	-1.02604387679256
H	7.49621557024975	-5.42250935210130	0.40342832790872
C	7.97459441268290	-4.08964581297135	-3.15356413576678
H	8.03867043535988	-3.66474675527029	-4.14367551608558
H	6.37959434202093	-2.76574291225346	-2.55310995313787
H	10.14737139750044	-4.10266188198652	-4.88564068033156
H	8.98253480255662	-5.30553998247680	-5.48643500413998
C	9.89514536229290	-5.16559539088095	-4.90135647991419
C	10.57011053225384	-6.77874557061725	-3.10788770840127
H	9.96521046233367	-7.65058658365770	-2.84696306251990
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H	11.24303571744346	-7.05286298045650	-3.91467948998751
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TS_{EA}

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C	-2.59869438239336	-1.32228789393126	-1.14887840544328
C	-2.10763291100913	-2.95579302007305	1.21003307923508
H	-2.01223222918858	0.34068962216759	0.07075374345623
O	-2.86620012649225	-0.66590846849234	-2.17351804232553
C	-2.92662569062038	-2.80239592950593	-1.13436669514298
C	-2.12522853906716	-3.65496428261876	-0.15394740438089
C	-2.80560366072933	-5.00909194274419	0.02238350470040
H	-3.82647848965929	-4.89047205601739	0.39528491508844
H	-2.85037179841733	-5.54082230796407	-0.93198368354887
H	-2.25296727421020	-5.63293098001983	0.73100655403829
C	-0.71962567761297	-3.89168720844251	-0.69805522024359
H	-0.77739445206047	-4.45932002081238	-1.63069318291055
H	-0.19696605215259	-2.95871057546866	-0.90211797066567
H	-0.11797158496837	-4.46306298119471	0.01352869006049

H	-2.81623477325033	-3.18471780033481	-2.15289791421709
H	-1.43442015610680	-3.47265283686277	1.89910966116872
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H	-3.99452980080218	-2.87119950478194	-0.88858210913019
C	0.89055316327122	0.40871021367382	1.94513624710605
N	0.57130755533613	-0.48986653641903	0.99129867947256
C	0.75580188187497	-0.19559478829539	-0.31109917124547
C	1.41824840371325	1.62218622925653	1.62329111717829
C	1.62438082756558	1.97972019047524	0.26702232163114
H	1.66927622840846	2.29501917748811	2.42949191062952
H	0.70700106984592	0.08828130613380	2.95969895051337
C	1.28471790198628	1.00434905013825	-0.69606649054662
H	1.42815466446842	1.17624593804319	-1.75210503978982
O	-0.01030105114257	-1.63428601092137	1.33134690866146
H	0.49611258951437	-0.97435917439958	-1.00942295187848
N	2.12347455234367	3.17397079561133	-0.07884328704795
C	2.47382938813444	4.14240833599714	0.93868987656546
H	1.60193582864500	4.42355631943800	1.53666145239248
H	3.24488132694159	3.75288702257983	1.60986152941607
C	2.31174175097159	3.50431052150577	-1.47589217605413
H	3.03493858129992	2.83346792595124	-1.94952360444981
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Cl	-2.09017920693388	-0.68679474366310	2.72479838115768
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C	8.95876941234437	2.20177363206443	-4.05920587923832
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O	10.84091539389546	2.06174939872219	-0.37731878857163
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C	10.09329362223789	3.19091634647052	-3.77946726105612
C	9.74534610317666	4.52613560189984	-4.42477709202229
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H	9.67051888552890	4.42562959874012	-5.51152094773134
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H	12.21318253029991	3.41689601634759	-4.15403290213082
H	11.71047939783513	1.73871843234068	-3.90485745631329
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H	11.02884495897037	3.98370399779904	-1.98379874363753
H	8.87865754908624	1.98732649217568	-5.12826701882637
H	8.01961756087015	2.66592193500623	-3.74897007085937
H	9.27479918907195	3.86333910536123	-1.90496681258660
C	8.69974373550313	-2.14107526121002	-3.18322229949922
N	9.63416400167898	-1.31637155083081	-3.68584609932089

C	10.94286793732305	-1.61847373459309	-3.67757086797959
C	9.06763585727608	-3.33825860495184	-2.65086530024152
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C	12.22701804394078	-5.24810133031287	-2.07832503402960
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H	12.64010552486989	-5.29930596349243	-3.08931541868308
H	9.31083543427800	-5.36891223219797	-0.71558073269069
C	9.84257909828596	-5.81281158514774	-1.56165885666647
H	9.11354181061918	-6.10362765211575	-2.32232303893226
C	5.71170178940602	2.71952266878795	0.084192220227068
C	5.41340007542483	3.03030944226316	-1.23794198794083
C	6.53529038979049	1.63277336715546	0.35403890420910
H	4.76254231099005	3.86912376467593	-1.46304724147383
H	6.76871693984103	1.37464843304132	1.38209923783977
C	5.94525577427963	2.27992707990439	-2.27493067377775
C	7.06384629162756	0.87137121568595	-0.67732081118768
H	5.71069119464920	2.52110132727853	-3.30683736663165
H	7.69660896886187	0.01897050479818	-0.46188118106874
C	6.78386320956772	1.17876407954604	-2.02128474529707
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H	12.33196099339587	-6.22421112291775	-1.61357212347232
H	10.35560999142554	-6.70588675190626	-1.21691974838217

PPYO

Cat

C	7.24723579870510	-5.79911501255273	-6.31077424682763
C	7.40755478775785	-6.08890035163929	-7.67903319701891
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C	9.56525348735287	-5.12210553118661	-6.33436231048425
C	8.38942501287192	-5.30410018765716	-5.65347668175841
H	6.59198176998946	-6.48524133361793	-8.26780826887420
H	8.77539126260088	-6.09602898408146	-9.34932644904587
H	10.46175663351465	-4.73925850081297	-5.86725389570294
H	8.36560829801586	-5.04702409268865	-4.60348631342376
N	6.07598444259955	-5.98366645583737	-5.67245779086271
C	5.88977760483196	-5.75795758599697	-4.24996271700750
H	6.67654423385575	-6.24843299504154	-3.67007866810005
H	5.92123099829607	-4.68508846479527	-4.01757580818441

C	4.85202984631033	-6.39190860652844	-6.34030212124466
H	4.69493231455719	-5.81251646184227	-7.25436821460717
H	4.89502825754985	-7.45296909040939	-6.61909588278891
C	4.51348355486103	-6.34776622003271	-3.97855244782416
H	4.60428877636974	-7.41738481643757	-3.77151037767019
H	4.02262337187255	-5.87672368723288	-3.12690044581385
C	3.77699561677148	-6.13130728548925	-5.29517305409552
H	3.43547258397600	-5.09526774988977	-5.36797258657277
H	2.91281487203148	-6.78389621040517	-5.41957535376321
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VOCI

C	-1.660457000000	-1.233351000000	0.403341000000
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H	5.283603000000	-1.980259000000	-0.885712000000
H	5.410710000000	-1.940826000000	0.883212000000
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VONu

C	-1.70682699579852	-1.16840450130769	0.38644709909407
C	-1.37053196053988	-1.24601523255823	-0.90576022315154
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C	-3.08239898952219	-1.19851018740777	0.92579232504352
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O	-2.14296126360728	-1.47168569953476	-3.09662927064602
C	-3.84094780580297	-1.26863195321358	-1.43325124214653
C	-4.06898507435000	-1.85871150119234	-0.04049085756797
C	-5.48716603915816	-1.54953353139266	0.41981524511080
H	-5.66269478884609	-1.95352204480451	1.42068510664117
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H	-6.21679760510821	-1.99798114534659	-0.25940000456607
C	-3.86474830507736	-3.37185690499216	-0.06871689860045
H	-4.56247051439414	-3.83448930365726	-0.77130299462486
H	-2.85077222821183	-3.64256412840434	-0.37341337765375
H	-4.04596867298061	-3.79869671554494	0.92097934682413
H	-4.48652884495229	-1.74233994378261	-2.17592077220453
H	-3.08173019889201	-1.70799648827663	1.89391964071840
H	-3.36006300306012	-0.14540660862088	1.09219985498913
H	-4.09012803141145	-0.19928287767114	-1.41282723942219
C	0.91702805788526	0.41879938611635	0.75923262201623
N	0.49188701398043	-0.83357229983409	1.00805234123056
C	1.29651140637498	-1.91024837316041	0.94513419657312
O	-0.80455185559031	-1.01418358373277	1.41171075458987
C	2.21586839393199	0.62710646168945	0.42045543879117
C	3.12208163652197	-0.46285011526832	0.32897590758476
H	2.52894442050017	1.64302012537523	0.23297298083291
H	0.18062508007235	1.20958816368185	0.85501051891187
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H	3.22521793477377	-2.63848830651206	0.55637635140263
H	0.83507364935026	-2.86208403844697	1.16942887062405
H	7.04232149386036	1.47788811831732	-0.78788420093072
C	6.32777629396603	0.66556135407395	-0.91625130452743
C	6.70459727514947	-0.59597082838254	-0.14946246392819
H	7.05939899464651	-0.33801201783530	0.85154446950265
H	7.47512113260987	-1.18713196032995	-0.64320763312681
H	6.24570214605990	0.44721647004923	-1.98395326764927
H	5.03863738959383	1.64563721545659	0.54001301410439
H	4.32212824403483	1.52981997494393	-1.07807337219194

C	4.95980573065495	1.01862861734377	-0.35475660191882
C	5.38745145088379	-1.34804967346606	-0.05070363174142
H	5.21281878935369	-1.97685670880991	-0.93056519154187
H	5.32372234949934	-1.97565166571054	0.83983401547151
N	4.39088180964646	-0.28056426067489	0.00038758538262
C	0.38483646354490	3.64519294004239	-0.15852852399937
C	-0.34041190191019	2.99885295655101	-1.15948530780048
C	-0.16427948846859	3.68793462817166	1.12125896792059
H	0.06863716320420	2.93968568506183	-2.16460704597145
H	0.38318489093332	4.17525331784709	1.92378681013524
C	-1.57100975605035	2.42330289331282	-0.90046621374596
C	-1.39419074017479	3.11238086160872	1.39709689066868
H	-2.11383009297811	1.92135439600573	-1.69661985545270
H	-1.80121776189417	3.15571138502539	2.40360896141806
C	-2.17711072075843	2.46312030865970	0.39336077715586
H	1.34698069073486	4.09779289298022	-0.36873105926516
O	-3.32387200975065	1.95382666013593	0.63526006874985

VO⁺

C	6.34196445533705	-2.56340924383594	0.59682457189675
C	7.57573529266020	-2.04975614573676	0.60497864169602
C	7.90979305647953	-0.99332600571399	1.55429068299894
C	5.22839099248868	-2.14416636724056	1.48100716878106
H	8.36189429076752	-2.37546942937871	-0.06401292811029
O	9.01878414450182	-0.48522420797941	1.55789335376732
C	6.85078304654448	-0.59682238338550	2.54741723840400
C	5.41986233683269	-0.72314992492133	2.02185194957220
C	4.43464071510802	-0.48952684662462	3.15885164984009
H	4.55017070523940	0.51988685554904	3.56092884499916
H	3.40561081464312	-0.59707499068347	2.80563002722674
H	4.59496467673574	-1.20277532106762	3.97146589197464
C	5.16907218299403	0.30145433758663	0.91744823559337
H	5.31729143475999	1.31292923348917	1.30271285047516
H	5.84216735038637	0.16311782219358	0.06801579199448
H	4.14190030078063	0.22363412066666	0.55284433285908
H	7.05945609412695	0.41954198772742	2.88764427114641
H	4.28571527465213	-2.22562120321104	0.93224405984379
H	5.17211856846423	-2.85871672787704	2.31181061407653
H	6.97737164294028	-1.26091887750187	3.41301229458624
C	7.66002124056034	-5.09805847208519	-0.60226971947968
N	6.90361252050819	-4.07890008305341	-1.05360837608650
C	7.02098776708023	-3.57682650248544	-2.29740962976552
O	5.92620619226910	-3.57450954170274	-0.23766366547258
C	8.60328709521495	-5.64661453176544	-1.40853763524787
C	8.79116318332472	-5.15616841753391	-2.73170757071382
H	9.18929471310296	-6.46841170458927	-1.02467386236384
H	7.46098217112190	-5.42707066976456	0.40856816403111
C	7.94384567840807	-4.09154059641064	-3.14900176696818
H	8.02127866257636	-3.66437016142172	-4.13777995399276

H	6.35161832920397	-2.76503416412813	-2.54718896701473
H	11.42250449334586	-5.93508187156414	-6.31624405326918
C	10.82977995002142	-6.31526704554657	-5.48513188912902
C	11.66798548032853	-6.70937499608643	-4.27569174412890
H	12.44031420340282	-5.95882066538117	-4.08987266922215
H	12.15265291674999	-7.67892736155418	-4.38414655556531
H	10.25221499630804	-7.17257782745854	-5.83973666588466
H	10.34126140860362	-4.25900900032499	-4.96024889239546
H	8.93269561307940	-5.22306250209226	-5.44641902142307
C	9.89201412888146	-5.25729815078771	-4.92743053239727
C	10.65932821535555	-6.70420884063669	-3.13872163814198
H	10.14464374763199	-7.66673503838332	-3.04949848342023
H	11.10702153729663	-6.45957514178836	-2.17403641128601
N	9.70537537918096	-5.66821739550979	-3.53565200428404

T_{SEA}

C	2.85462801866618	-4.20401022682122	2.44100833245216
C	3.39584053603423	-3.11739387372373	1.88275346704453
C	3.86992303313725	-3.16053296102934	0.50031127939733
C	2.72818476057347	-5.52642540048936	1.77459426727774
H	3.48337845171345	-2.18063425447975	2.41848368261876
O	4.42458088376713	-2.19842039385778	-0.00532549335903
C	3.59091929451161	-4.42108939032847	-0.27061976968893
C	3.69200899716427	-5.67919581502033	0.59345695210782
C	3.27176857986752	-6.89336672629581	-0.22477770127357
H	3.94043616577543	-7.02463685011997	-1.07913268334489
H	3.31955081227148	-7.80015767328167	0.38427075126370
H	2.25057102677029	-6.78400547478401	-0.59955576761519
C	5.14071383522998	-5.85478694712937	1.09875962109687
H	5.78259008020490	-5.02872553745001	0.78616779651436
H	5.19339758282171	-5.90951352474008	2.18842593001984
H	5.57985223806351	-6.77077841922318	0.69910568276797
H	4.27270307121788	-4.46944964984096	-1.12206001246229
H	2.89732435249853	-6.31953403280805	2.50759474440853
H	1.68909344629201	-5.63213541080086	1.43547315141428
H	2.57125313995552	-4.32747596535653	-0.66824531323376
C	5.39977161627424	-2.91003543383281	4.89574293086111
N	6.05855880167600	-3.88904674119467	4.23962365978821
C	6.84795017568160	-3.53740903232650	3.20108334227162
C	5.48352530456040	-1.59315551046849	4.52548457261574
C	6.26929064832037	-1.20461700626814	3.42415140257831
H	4.92577254134553	-0.86753364748946	5.10094765821780
H	4.79986185478379	-3.25041752750571	5.72713992669690
C	6.97106221733878	-2.24005171756827	2.77839383405290
H	7.60657141623110	-2.04134994308742	1.92674826868501
O	5.93421296727209	-5.13506594450802	4.59480043323776
H	7.36297059295947	-4.36106765678819	2.72851337624873
N	6.34344790903620	0.07511728776862	3.01328095055378
C	5.55346317856650	1.15094426423331	3.58612550212531

H	4.50958414009038	0.84747552619068	3.70462915427889
H	5.93581197404705	1.43203275437785	4.57621332928735
H	5.60537118167370	3.26328267751304	3.04090886921076
C	5.71849613347739	2.28143715537112	2.58104163079367
H	4.96762346728026	2.18542197001095	1.79212327876177
H	7.87002575328482	2.40726919082378	2.70528361920964
C	7.11080989337723	2.03842167789564	2.01042403539222
H	7.27159855397824	2.51845338172915	1.04508718514983
C	7.18957172282926	0.52125830919402	1.91980337947623
H	8.21096794530742	0.14917922687106	2.03969761624829
H	6.80839939607091	0.15310267744694	0.95838553357292
Cl	2.21034930800011	-4.11748041080762	4.03836559327866

TS_{SN}

C	9.10244498363335	0.90853295674096	-3.30393052720309
C	9.80063982156534	0.85784510537474	-2.10430598047422
C	10.29309386557177	2.02356077164068	-1.47917377089746
C	8.96253865968056	2.19930250662188	-4.04494778683371
H	9.92754954754323	-0.07827481096490	-1.57412637182840
O	10.83394099768533	2.02282425098515	-0.35824645609996
C	10.18143670510649	3.33230191344436	-2.23536052387234
C	10.10146897539982	3.18013664760040	-3.75349421012722
C	9.76417672339516	4.52184202040133	-4.39101732907523
H	10.53917985319713	5.25946617373278	-4.16538589411008
H	9.69294668135817	4.42918127517605	-5.47868659001221
H	8.81050717544790	4.90503729333150	-4.01730683929050
C	11.42643728758906	2.67783650754188	-4.32114404461700
H	12.22475398268267	3.39567665418541	-4.11461405239943
H	11.71002382472405	1.71878732407557	-3.88340030055279
H	11.35522021836192	2.55338261798421	-5.40526151502055
H	11.03159905144969	3.95713074401354	-1.94792941986058
H	8.88614601836146	1.99175995655473	-5.11561246674893
H	8.02507583384044	2.66814972756433	-3.73627982292782
H	9.27675918747114	3.84116333625621	-1.87758737758365
C	8.69252128508832	-2.15152917478891	-3.19157565124597
N	9.62447166585603	-1.32272316093772	-3.69453229596342
C	10.93441151336888	-1.62340991936115	-3.69556215570173
C	9.06448292912081	-3.34943776279013	-2.66518864101739
C	10.43278587996316	-3.72988886044836	-2.63983503202930
H	8.29377205604943	-4.00006625030981	-2.27925198762230
H	7.67944981373383	-1.77638109695811	-3.22773385977725
C	11.36425621083342	-2.80938918163147	-3.18861345929226
H	12.42317633843891	-3.02018804568553	-3.20241238624533
H	11.58772019804933	-0.87478903292555	-4.12022430649330
O	9.24063672180716	-0.14039284027358	-4.24670487612054
N	10.82422384265784	-4.88953106108203	-2.13013131927947
C	12.20853102558552	-5.35579608116215	-2.13639724521567
H	12.80172308463072	-4.77364550047916	-1.42244672852521
H	12.64977253926264	-5.23588980744662	-3.12769643962259

C	12.09350757994647	-6.81230620906532	-1.71582240682059
H	11.90814188190136	-7.43778155032191	-2.59275023270175
H	13.00015923689298	-7.16861785784232	-1.22785127665665
H	10.43089693566883	-7.80100868134447	-0.67552921819211
C	10.87530764488671	-6.81422300368860	-0.80124951171533
H	11.14535632935120	-6.43128988731768	0.18620905752914
H	9.26309926177293	-5.33451160526458	-0.78485389603953
C	9.92566427285819	-5.84456158367504	-1.48649580141446
H	9.30969596278483	-6.34589386838464	-2.24149420919534
C	5.69487749812507	2.77793982658865	0.04349866343737
C	5.39844694370026	3.06313124678998	-1.28486991671362
C	6.51883253907071	1.69712332109263	0.33512637378587
H	4.74760897336914	3.89714942752741	-1.52720981848581
H	6.75087395951078	1.45889399707382	1.36830219102026
C	5.93275624498440	2.29344718303103	-2.30625493221498
C	7.04911077892263	0.91582113844673	-0.68045634530991
H	5.70050729780295	2.51519842327030	-3.34305708565896
H	7.68193491178725	0.06826475452493	-0.44708362320102
C	6.77149577310189	1.19745168625292	-2.03063978656427
H	5.28066845413100	3.38394725829816	0.84118250555570
O	7.29348298991876	0.48362068402752	-3.00772352375684

10.4. Electrophile variation

1b

VCI

C	0.27098044030322	-1.17773874370758	-2.57984895556610
C	-0.81049888763286	-1.81952529867837	-3.02943085790561
C	-1.98032679652442	-1.08956263813272	-3.52843109280029
C	0.39463975113762	0.29806833791526	-2.48337908216725
H	-0.85558516851275	-2.90154541485205	-3.06441337551516
O	-2.98303930214763	-1.69731910957999	-3.85920892508461
C	-1.85847095206171	0.42029092597252	-3.67915040559128
C	-0.96849149000300	0.96554200446795	-2.56087389070530
H	0.89888049905440	0.55637991625734	-1.54898304615993
H	1.05814233373961	0.63771790039711	-3.28798590134484
Cl	1.65948498754096	-2.07682680489910	-2.08580752140180
H	-0.84118900232983	2.04231902665335	-2.69974026110971
H	-1.48432463966427	0.82371756915098	-1.60537643093323
C	-3.23032625277563	1.07232863602374	-3.61142138167665
H	-3.88691429602088	0.68498531402893	-4.39091494485477
H	-3.70462893070592	0.89159051555643	-2.64366734725286
H	-3.12987219470430	2.15178571086311	-3.74793818026096
C	-1.23131048964218	0.67963435515113	-5.05547803282230
H	-0.25806415546384	0.19673887388239	-5.16554925338459
H	-1.88539298267925	0.30759652650070	-5.84673575068397
H	-1.09782207490735	1.75533555402884	-5.19529722677875

VOCI

C	0.16468239119961	-1.38706336093012	-2.67819911319777
C	-0.77266019589140	-1.86592926130889	-3.50308300148088
C	-1.88602591925835	-1.03620618458862	-3.97550095032943
C	0.16845512114212	0.00152801950216	-2.15109477113666
H	-0.73608128640617	-2.87843859143095	-3.88793690277043
O	-2.77975006452846	-1.53821854915751	-4.63293592910148
C	-1.82816258774634	0.45099353722343	-3.67187674879768
C	-1.20041906970067	0.64486564356102	-2.29054277363686
H	0.47646921116926	-0.01974597075189	-1.10148100581053
H	0.93788501950385	0.58480488225425	-2.67876318305118
H	-1.12121489007057	1.71503121894176	-2.08364382730846
H	-1.87401959970831	0.22023028916651	-1.53828548781800
C	-3.22290552624376	1.05425093975730	-3.69926565942779
H	-3.69113381058620	0.91681537032648	-4.67448716069381
H	-3.86491282859605	0.59406866192504	-2.94416539423554
H	-3.16199310669390	2.12528777173867	-3.49235027896785
C	-0.96012345678932	1.09347294233807	-4.76285130470565
H	0.04585956628422	0.67066017230660	-4.79527539838893
H	-1.42048656797317	0.95788121194869	-5.74366785692160

H	-0.87019699414990	2.16484534564247	-4.56741049389422
N	1.23275698924782	-2.23081169758081	-2.25467755338566
C	2.48362694002347	-1.71962660343788	-2.11799531727807
H	2.62274380935900	-0.67207926318333	-2.38118507524496
C	3.53204398413230	-2.49838049080622	-1.74790757104039
H	4.50316624523210	-2.03096916765696	-1.68052972485389
C	3.35209169315055	-3.87993778969727	-1.48274884703615
C	2.02716587435175	-4.37460232563794	-1.62121000326503
H	1.78432920761764	-5.40619882188848	-1.41618973361615
C	1.02207310311745	-3.54701082456873	-1.99841937495076
H	0.00151639952760	-3.89078826826515	-2.08452594443610
N	4.36069360665512	-4.66594563512288	-1.12117736502368
C	5.69840280360027	-4.11989045411434	-0.97725824927158
H	6.05419864230034	-3.70230931653187	-1.92254436134396
H	5.71995826965702	-3.33627527528316	-0.21594802832448
H	6.37132800542445	-4.91676468709874	-0.67473510302782
C	4.13932174903264	-6.07748717567042	-0.86525189904525
H	3.43896783656614	-6.22167618106037	-0.03842098184073
H	3.74604390910063	-6.57870028225129	-1.75315564610598
H	5.08647313081410	-6.53755838420321	-0.59933546160743
Cl	3.21258691513310	1.26415724959464	-3.64453860162713

VONu

C	0.55484550170251	-1.51150288612084	-2.80241380034867
C	-0.32764050615858	-2.03257006593029	-3.66236704458156
C	-1.35531218095636	-1.21744097755064	-4.31600087138170
C	0.57793636389889	-0.07428706753138	-2.42427712823673
H	-0.30322411829319	-3.07815222008046	-3.94673968923135
O	-2.17077581040368	-1.74836991587410	-5.04941697987829
C	-1.31274871243645	0.28551195284431	-4.10298385155012
C	-0.76167824438730	0.58320898870201	-2.70790098500488
H	0.82703979095074	0.01287153187426	-1.36315184137461
H	1.39002672840962	0.42603016153675	-2.96423649844587
H	-0.66669107366056	1.66533276648822	-2.58745578148224
H	-1.48946628372942	0.23994790212760	-1.96481489927744
C	-2.70657690638025	0.87744693299935	-4.24593818626482
H	-3.11843574850580	0.66977056150624	-5.23388386370467
H	-3.38827045245906	0.46622221562455	-3.49725232429395
H	-2.65859952480492	1.96043242437025	-4.10977486482849
C	-0.39292546058685	0.85454761052587	-5.19130553664132
H	0.62091806092201	0.45066410282575	-5.14492707747462
H	-0.80069769752452	0.63751218561228	-6.18081608874552
H	-0.32805342228159	1.93934025210326	-5.07660483827870
N	1.52949580192000	-2.35168090950268	-2.19191585405716
C	2.78338109207898	-1.88032061407218	-1.96165903760257
H	3.02565506518638	-0.85737885356984	-2.28547798131764
C	3.74311597138613	-2.67404804667335	-1.41785491609542
H	4.72507123190260	-2.24523398217215	-1.28223150176729
C	3.46608086740076	-4.01738186932895	-1.06099399993472

C	2.13763372031209	-4.46308558837143	-1.29574025772650
H	1.81909390174056	-5.45938592807783	-1.02885374526800
C	1.22317607798684	-3.62911833991104	-1.84785740524277
H	0.20048039637849	-3.93534276350106	-2.01240850343930
N	4.38951283726663	-4.81373066624213	-0.53058126007914
C	5.73240478643941	-4.31754537915349	-0.29100407224372
H	6.19674606993176	-3.98173327108327	-1.22130480855816
H	5.72209219715867	-3.48510018513239	0.41734309501582
H	6.33347029086022	-5.12032642569417	0.12563197517826
C	4.06229054311561	-6.18073353205294	-0.16941659012806
H	3.28041714767950	-6.20797460297945	0.59400893245478
H	3.72348503066948	-6.74525524241028	-1.04151333009145
H	4.95134341033054	-6.66119430425519	0.22865948056401
O	3.82102076935175	0.68498946395478	-2.98860607422402
C	3.55743196228243	0.77511676693377	-4.24527306680295
C	3.44633729941361	-0.36708486747183	-5.08974343934938
H	3.61827668028780	-1.34724032277009	-4.65379396482389
C	3.14116455755597	-0.25855070465880	-6.43675021847951
H	3.06619163819439	-1.16216050141370	-7.03587312689359
C	2.93360590951873	0.98126484763852	-7.03306035878028
H	2.69753894421944	1.06024654805072	-8.08782756941306
C	3.04047624188497	2.11917557630922	-6.23592557003319
H	2.88264835728246	3.09965780963006	-6.67717635734655
C	3.33874719993187	2.02643586483226	-4.88830892306544
H	3.41181187601648	2.92402693809606	-4.28038132842322

VNu

C	9.19036130652341	-2.27443251404464	-5.66133682983001
C	10.29983882476036	-2.87684446270651	-5.19104476834394
C	11.54509508592128	-2.15556880374717	-5.01605112039136
C	9.14768466305209	-0.85506545231085	-6.09267355416942
H	10.29341089298889	-3.91949921976554	-4.89785988790783
O	12.54980692683020	-2.73102681643067	-4.61864668038270
C	11.54949442580006	-0.65050045704967	-5.27314780557920
C	10.53824867780947	-0.31508144389630	-6.36991422388326
H	8.51150557028483	-0.77908366212093	-6.97819310489231
H	8.64477323828828	-0.28042685842192	-5.30572098733413
C	7.42238617315934	-6.74515978506754	-4.42344563299253
C	7.31754090797245	-5.67621606178286	-3.54289218291456
C	7.73597574393332	-6.51773738781468	-5.75642356354277
H	7.06909383831028	-5.84997129774186	-2.50239069594332
H	7.81614383958804	-7.34932448680144	-6.44680624345584
C	7.52725362294163	-4.37958772520546	-3.98937202394099
C	7.94859674097937	-5.22444119497900	-6.21459161755946
H	7.44975564470454	-3.53195172885766	-3.31872906111085
H	8.19523341787292	-5.02533702768427	-7.25071508985641
C	7.84225820560266	-4.17407242812439	-5.32133929805911
H	7.25648677717442	-7.75616970837797	-4.07040749943005
O	7.99562859396524	-2.87647190311195	-5.78806694842415

H	10.89973704700117	-0.73481441809419	-7.31456423285569
H	10.49501177732737	0.76979871732084	-6.49822085793922
C	12.93595844550339	-0.19225254326194	-5.69925042772560
H	13.67749726004201	-0.42629840601531	-4.93514248900250
H	13.24020617515026	-0.67689466262310	-6.63017827761753
H	12.93211316735194	0.88869895623305	-5.86020493034621
C	11.17182927431524	0.02747987268229	-3.95023882468983
H	10.18647727130698	-0.28031823607498	-3.59364338821800
H	11.90247477718796	-0.21828864965447	-3.17675612849079
H	11.16481166935039	1.11249836653115	-4.08351318317034

VO⁺

C	0.21374096484288	-1.37114147583799	-2.72687836848292
C	-0.76443715909100	-1.86400132033754	-3.49376102282515
C	-1.88476558742705	-1.03837403203407	-3.96102979757135
C	0.26526096519435	0.05090102432230	-2.28597938482890
H	-0.76880272974165	-2.89319640672454	-3.83203817317365
O	-2.79137479580143	-1.55542605278617	-4.58630800067156
C	-1.82548423636333	0.45501057426401	-3.69143146674659
C	-1.11101099926605	0.69157420888988	-2.36077041811119
H	0.65112481360868	0.10159917219282	-1.26424805659091
H	0.97578766517844	0.60091099403818	-2.91450516813532
H	-1.01948002396616	1.76700264005177	-2.19084799401859
H	-1.73076809781338	0.28862095584403	-1.55316991291506
C	-3.22802640083350	1.03999461039314	-3.63727360855879
H	-3.75783184303554	0.87199899773405	-4.57517172584457
H	-3.80984279389237	0.58967611382484	-2.82956691432727
H	-3.16915688762024	2.11640900778283	-3.46050792459573
C	-1.04692043786762	1.08239469671777	-4.85611618624598
H	-0.04588405231613	0.65943709834182	-4.96603245461083
H	-1.58283035637555	0.92808156593252	-5.79451724759654
H	-0.94753575622482	2.15739761439472	-4.68743505070915
N	1.26855862837926	-2.22147576422885	-2.28602777811128
C	2.52240046655022	-1.72657540122943	-2.11537254569790
H	2.65714375050543	-0.67588460062049	-2.32391418351104
C	3.56080542502285	-2.50936442826569	-1.73296444965381
H	4.53137194365188	-2.04795019193007	-1.63083080326902
C	3.36754663656642	-3.89528626535721	-1.48857561338289
C	2.04028840159224	-4.37646384615795	-1.65215370871683
H	1.78485686598092	-5.40627530443867	-1.45343073219383
C	1.04772172308624	-3.53965008885316	-2.03852862796507
H	0.02670635710196	-3.87756971961831	-2.13553485354744
N	4.36251806846017	-4.68994128065210	-1.11819008907526
C	5.69983372547444	-4.15396673656511	-0.93074437399594
H	6.08641134124081	-3.73438900313308	-1.86288089547131
H	5.70306457091341	-3.37627636051453	-0.16341757971522
H	6.35734628484208	-4.95745408952433	-0.61292414196205
C	4.12780231770177	-6.10409436146055	-0.88259570391418
H	3.43235547488531	-6.25276650346395	-0.05256622751367

H	3.72266970348540	-6.58476594364424	-1.77590454272767
H	5.07229335337065	-6.57813850834659	-0.63316435901549

TS_{EA}

C	0.07577831550557	-0.82266775611370	0.29700760230660
C	-0.04968236845631	-0.24568076216902	-0.96090093018773
C	-0.69599680386276	0.99662377179335	-1.18366884452685
C	-0.19787309657495	0.00919954334863	1.51035828235558
H	0.35676807882635	-0.75663000120720	-1.82619557297360
O	-0.79596914059414	1.49378580916088	-2.31628390271101
C	-1.22128244019864	1.79516324299357	0.01868147608076
C	-1.39298089502009	0.90477951384997	1.24908234012796
H	-0.36044534102515	-0.62121176451492	2.38562281169784
H	0.70002631881666	0.60170485429833	1.71061809588600
C	-3.21149297106931	-3.14726977248180	-0.44549270607577
C	-3.31047373649650	-4.06936822473542	0.62086557714890
C	-2.32024031545096	-3.97182579214913	1.62719220158921
C	-2.19128852231438	-2.23002345418841	-0.45265268288333
H	-3.92339411372077	-3.14529759016356	-1.25798246922137
N	-1.27474268039399	-2.16575284436724	0.50252426870836
H	-2.07582539507065	-1.50105214881984	-1.25194502732949
C	-1.33837677519865	-3.02168568260645	1.52239517697098
H	-0.56272467138746	-2.94169185813816	2.27614496147841
H	-2.31243376675301	-4.63818108079906	2.47744102424362
Cl	1.48084919858918	-1.89677959282805	0.50306565207838
N	-4.28730886985393	-4.99003422479988	0.67667580237221
C	-4.35791772835723	-5.91260376415216	1.78871956349273
H	-4.43454448296364	-5.37983209672010	2.74086864160354
H	-3.47926867709326	-6.56462695151265	1.82756659708121
H	-5.24210707915088	-6.53434466019432	1.67491673550835
H	-5.93439365813038	-5.90891702014645	-0.18072936836234
C	-5.25446726388013	-5.08853106656383	-0.39469212988175
H	-5.84131589944294	-4.16970012422811	-0.48993579560983
H	-4.76659338487356	-5.28647436741015	-1.35405505684584
H	-2.28149643659539	0.27847548474196	1.11680391108810
H	-1.57784964793011	1.53369873864436	2.12525476623092
C	-2.56630946687383	2.41934575528082	-0.33241773810370
H	-2.47342824507771	3.08440036218559	-1.19122599118967
H	-3.30368088185666	1.64867848455347	-0.57321029742905
H	-2.94206137933965	2.99661914440665	0.51716607516250
C	-0.20405785415946	2.90707525566858	0.29273860310820
H	-0.55301205249068	3.54263490655305	1.11169660591042
H	0.77424951937350	2.50438187636627	0.56564197594215
H	-0.07761685445401	3.52768186016418	-0.59642440284160

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C	8.69101482438691	-1.61980557863269	-4.20123360960140
C	9.80853719014720	-2.36126652711769	-3.83213085192815

C	11.09719552717224	-2.17080625984165	-4.38329279232890
C	8.89211562632322	-0.36295486900603	-4.99127790358327
H	9.69617476516664	-3.20446207071908	-3.15987873938692
O	12.06410944453413	-2.88422226865920	-4.06754757218376
C	11.32795400588291	-0.99757493925369	-5.34555799174271
C	10.01481054238272	-0.55474549880002	-5.98819357672830
H	7.96998989390265	-0.09080358711204	-5.50705170673292
H	9.12124180962677	0.44690176547466	-4.28915349439693
C	5.61291681823587	-1.28327335110900	-1.26665848626441
C	5.37938415696068	-1.01445765762537	-2.63902909086479
C	6.38257831842912	-1.13993206869735	-3.54710947010293
N	7.63340227208031	-1.51331631241369	-3.19293640038246
C	7.89567935720840	-1.73772248278107	-1.88820524991087
C	6.93900536641358	-1.64198700754256	-0.92484948784231
H	4.40560872648672	-0.71667635684777	-2.99788088530081
H	6.22172566575846	-0.97822318914808	-4.59988933003855
H	8.92011647528560	-1.98479759007858	-1.65378652833964
H	7.22812130887271	-1.83746115301320	0.09676830618025
C	8.14407769753995	-6.61648086997765	-5.09278873193184
C	7.07511236539002	-5.97680611597753	-4.47306619278439
C	9.04792811554530	-5.86377585232127	-5.83228808486839
H	6.36202020292025	-6.55440459759646	-3.89363775559719
H	9.88793069985088	-6.35099544250721	-6.31677762872732
C	6.91298027735885	-4.60543095475223	-4.58822381436889
C	8.89035582817587	-4.49117356919725	-5.95387651144401
H	6.08030897376664	-4.10442698542768	-4.10471443743835
H	9.59458001501385	-3.90165833027340	-6.52984307666375
C	7.81087838592558	-3.83283851366540	-5.34405875552135
H	8.26866061504034	-7.68941339376406	-5.00155799257284
O	7.66403517418242	-2.52484337690589	-5.45111822499556
N	4.64480799579068	-1.19579828926411	-0.35449134382027
C	4.92777417166548	-1.47441775494716	1.04004178978814
H	4.01290062790496	-1.35830393727354	1.61424318705879
H	5.29224889698620	-2.49690941474167	1.17017194347529
H	5.67633434349765	-0.78281256708534	1.43600165740387
C	3.30124983480810	-0.81687147167246	-0.74679613854149
H	2.89764504636467	-1.51371721470113	-1.48586429633546
H	2.66057130051909	-0.83652764794096	0.13020813936699
H	3.28246388099590	0.19171332245634	-1.16872785363357
H	9.70089445207820	-1.31352071352759	-6.71060667326535
H	10.17978089682647	0.37356511054642	-6.54424214439524
C	12.29877868602924	-1.41600103914786	-6.44217319820158
H	13.25226536888639	-1.73275050942812	-6.01897276916606
H	11.89273474546915	-2.24448361790890	-7.02885105020010
H	12.47935275559694	-0.57602607526929	-7.11926307074489
C	11.94850693148947	0.14116796811041	-4.53071145932079
H	11.28965105475566	0.47253985416776	-3.72438336668707
H	12.89018357297220	-0.18380486247024	-4.08318835891549
H	12.15294626239629	0.99855927038767	-5.17862496847187

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C	8.72166104019961	-1.58716145120279	-4.12917917223183
C	9.83697361593947	-2.32008185570279	-3.74547113707701
C	11.11354821648009	-2.14157925795260	-4.32546779636739
C	8.89106178879354	-0.35128382269985	-4.94733946080198
H	9.73821908389236	-3.09182486329431	-2.99101138648994
O	12.10243742881965	-2.81740389616408	-3.98614054917305
C	11.31604172831597	-1.01537261108496	-5.35214962304330
C	9.98867157628837	-0.57526868618738	-5.96893112986309
H	7.94796064967847	-0.10202066393952	-5.43501928072165
H	9.14198632443151	0.47571310660839	-4.27451748164056
C	8.16846303499588	-6.61056092931174	-5.14776678352979
C	7.04491133205550	-6.00573381591817	-4.59222211346408
C	9.11809389013904	-5.81723535721887	-5.78021067104849
H	6.29364359599845	-6.61308976487455	-4.09697206339610
H	9.99943989438505	-6.27534749483500	-6.21820505514369
C	6.87622691230276	-4.63227334349358	-4.66148571778278
C	8.95324753490455	-4.44215310778931	-5.85877377133284
H	6.00278803361688	-4.15950301498587	-4.22450037624063
H	9.69204949298395	-3.82769273465805	-6.35999438258311
C	7.82096237886412	-3.81379269871801	-5.30810630357219
H	8.29870568609085	-7.68539520502243	-5.09149260526052
O	7.65776216596792	-2.51097502492315	-5.37626073574454
H	9.64915654011118	-1.34511775783276	-6.66713925382387
H	10.14831844875852	0.34001003329865	-6.54880696525009
C	12.24071964054283	-1.49949500121344	-6.46203457737208
H	13.20053300572039	-1.82075750190632	-6.05641521112894
H	11.79603801402821	-2.34282912669905	-6.99775474500609
H	12.41646427672362	-0.69415363064112	-7.18143046423812
C	11.98039974884886	0.15066613225987	-4.61336208209044
H	11.33594170729334	0.55033364630219	-3.82679429586573
H	12.91462958292712	-0.17552713409995	-4.15142772010966
H	12.20553295708620	0.95934034481979	-5.31503187960440
Cl	7.46604143681538	-1.43359263691915	-2.87912919700182

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VCI

C	0.14389790737598	-1.26355281455310	-2.42344755009249
C	-1.01707096549023	-1.78357417185690	-2.81697258802193
C	-1.98413948733628	-1.01570062571627	-3.61778089641123
C	0.48183221361957	0.16421758045487	-2.64786471436521
O	-2.94398544341511	-1.57388643632218	-4.10862077938284
N	-1.70101548498912	0.34135357406597	-3.76652924286080
C	-0.79607713644653	0.95959028257382	-2.79639006402921
H	1.05179351251516	0.55556017725821	-1.80322724219276
H	1.11843667629417	0.24956323612409	-3.53626971954920
H	-1.29921853993163	1.03310830252005	-1.82738554523213

H	-0.58310474033910	1.96715376011195	-3.14091422552921
Cl	1.33530127356784	-2.23978431931152	-1.65937134654421
H	-1.27181673956533	-2.82289655667447	-2.65975743703609
C	-2.39555916875591	1.21656707370191	-4.60845137513782
O	-2.40095055763552	2.40924534884558	-4.40561811535540
O	-2.95401631723618	0.59166660714972	-5.61985269915516
C	-3.82771492790334	1.29326123259233	-6.56802113892570
C	-4.99983461463716	1.91649743886536	-5.83334550346246
H	-5.70739673645929	2.30481512358440	-6.56832236435830
H	-5.51159149591192	1.16342935980881	-5.23030023286088
H	-4.68360473198532	2.73550139481770	-5.18994269626855
C	-3.02565130712221	2.30916140816120	-7.35930011016143
H	-2.68465685535598	3.12934757021059	-6.73016750979487
H	-2.16119862844876	1.83010688867586	-7.82413548965831
H	-3.65764717606485	2.71470643095703	-8.15200187558583
C	-4.30139702472874	0.16871459943920	-7.46911650283791
H	-3.45318761434674	-0.31275116190991	-7.95916671247503
H	-4.84657067713025	-0.58072290302554	-6.89280895096411
H	-4.96443870213723	0.57150141645124	-8.23624611675084

VOCI

C	8.21680945812113	7.62352499369430	4.33499831719708
C	8.07516892118580	6.64752948981260	3.43723622047150
C	7.32865756598458	5.41330133502711	3.72890933735240
C	7.73518994001478	7.46675368227863	5.73221986134504
H	8.38368676936161	6.74742358918037	2.40496949621716
O	7.07521976181043	4.63208277823445	2.83450804449007
N	6.93820857421768	5.24863476011575	5.05189097192965
C	7.67021259369421	5.99606819845686	6.07494750971897
H	8.42440995374880	7.96087699369203	6.42132815949872
H	6.76146619778005	7.95952209834656	5.85721154212576
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H	5.32496613587064	1.62623697700324	6.18148705121918
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C	9.80743725574436	11.36555101870528	3.35543953525935
C	8.80742882365197	11.20372260227446	4.34731032468537
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C	10.23355549683389	10.18112279388364	2.69659373046127
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C	4.73524821725219	9.13110546122119	2.47538786638366
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C	5.20158518270814	9.71641449833734	3.64083950349436
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C	4.12101117574275	2.96661078372942	4.97916016072432
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C	3.23825715238933	3.57585169265165	6.05257530215194
H	3.75462823865415	3.63890575657959	7.00861165720052
H	2.91490032555351	4.57542778057028	5.75344297275214
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C	3.36776471728946	2.85985758135706	3.66671187489074
H	2.99649467924257	3.83794309828100	3.35565345320644
H	4.01693816162902	2.46458846288566	2.88333111647146
H	2.51748842490551	2.18743510618168	3.79003412928230

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O	-0.84671558859819	-6.45571854910262	-5.52297904829931
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H	0.05722407772076	-4.01614634720337	-1.15889329615783
C	3.49871564966147	-9.59962573936042	-1.89865367436766
C	4.02100802746293	-8.33015814299160	-2.10589394651801
C	2.17955349906307	-9.74999013472810	-1.49079671323097
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H	1.77005491852476	-10.73948104257918	-1.32469476683483

C	3.22838093886198	-7.20719451265073	-1.91217786892664
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C	1.91700030785320	-7.37960539070939	-1.50877053142351
H	4.12118735556172	-10.47301580673310	-2.05316456355140
O	1.13623886653806	-6.25626952659418	-1.26601626193337
H	-0.01705162001472	-3.34146395654834	-3.47475292858289
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C	-2.54427878547117	-4.24488536018550	-4.81019230478686
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C	-4.26468840167552	-4.87694372163092	-6.40401756239133
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C	-3.77122531346233	-3.92507876739002	-7.47794809863490
H	-2.87742672664720	-4.32966922536740	-7.95754786463731
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C	-5.46050572670529	-4.33415496679209	-5.64378266550328
H	-6.30535133800847	-4.24642662929589	-6.33002592050466
H	-5.74177386374362	-5.02063295635056	-4.84230038714571
H	-5.25166329489747	-3.35459228054260	-5.21814143040505

VO⁺

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C	11.66961763039988	-0.32699221320791	-4.68665022174518
C	12.28513067788912	0.98119367784255	-4.97017604833530
C	9.64452995797632	0.29337804805493	-5.92969055890725
H	12.26132858078757	-0.95929120737306	-4.03866715227597
O	13.33543566583049	1.28101646886521	-4.44156355457907
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C	10.59170547393684	1.17070735484361	-6.71729204458743
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H	8.98273345771832	0.90393293323786	-5.30463488474558
C	8.63974654452626	-4.26152425593685	-3.86484996544470
C	7.87972700964354	-3.08995247517492	-4.12647229240498
C	8.48945593506559	-1.95132242792907	-4.53531172817769
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C	10.58825654180662	-2.98470649653691	-4.48718218026359
C	10.04111697325539	-4.15457332818461	-4.08056268013507
H	6.80757078918570	-3.07250959782845	-4.00232563799125
H	7.92612888202980	-1.04787836080989	-4.71745676474566
H	11.64602683087006	-2.89216755267609	-4.68415416537909
H	10.69890193674392	-4.99986488613076	-3.94550435122437
N	8.07505133964397	-5.38878689759450	-3.45563814991819
C	8.88451852381043	-6.56829642156898	-3.20105494703269

H	8.23592163351881	-7.37251677881805	-2.86718982136737
H	9.40009911311546	-6.89067890239426	-4.10882106908025
H	9.62483573033123	-6.37097322160432	-2.42225865843914
C	6.63785350858718	-5.45934306588981	-3.25355768147073
H	6.38141130879840	-6.45532221099378	-2.90569227527935
H	6.31521615506778	-4.73420092946615	-2.50279607934260
H	6.10286528515051	-5.26662069888417	-4.18663493586037
H	11.10555723894388	0.57452080165052	-7.47724261363754
H	10.04656089012174	1.96230099849207	-7.22213765735787
C	11.88283121674482	3.14337505957762	-6.10304091964549
O	11.54610353187586	3.66616949336121	-7.13935808515377
O	12.48975158524235	3.71335456241534	-5.08940226580379
C	12.95447510892668	5.10659079798124	-5.15090904944168
C	11.76391708113249	6.03912813458279	-5.26853019640711
H	11.26198353581859	5.92968759563649	-6.22822051416449
H	11.04997825389310	5.84387561921047	-4.46550811957839
H	12.11251355550162	7.06931394720077	-5.17281983412572
C	13.94744066986597	5.27570456937158	-6.28480465660286
H	14.74867925224092	4.53877677213423	-6.19826883744216
H	13.47053050294006	5.17520025529636	-7.25801828693922
H	14.38961384259152	6.27131899913462	-6.21488150399936
C	13.64088776219400	5.28107496492326	-3.80998097369010
H	12.93640888474071	5.11308761731592	-2.99320894225341
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H	14.02972340440624	6.29738283002242	-3.73098201342497

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C	-1.68399797602624	-0.90311134543650	-0.57364256399112
C	-2.31307907562863	0.36178495796413	-0.76251210555140
C	0.35901553486228	0.16007432623367	0.28556152518191
H	-2.23478250568117	-1.75748959589854	-0.94294874829294
O	-3.40765993740404	0.48134485630690	-1.30704936992196
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H	0.86464445877256	0.42028621389446	-0.64932482277279
C	-2.34185216717496	-1.93071130644689	3.56537074064707
C	-1.34410552974422	-2.33753016589568	4.47988037949270
C	-0.01765916773785	-2.36862874303022	3.98641350513038
C	-1.98689854107183	-1.59532649054328	2.28413740368982
H	-3.38227683883960	-1.87672812597543	3.85080853077996
N	-0.73513522004217	-1.63506961180339	1.84958697401519
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H	1.23978470245514	-2.04015416220767	2.28786822640690
H	0.81040964266502	-2.66665436585868	4.61292315192955
Cl	0.50371628326930	-2.46531248238630	-0.48381714710983
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H	-0.06820904070602	-3.98251722025482	6.27117974061909
H	-1.03179606976242	-3.34807209162782	7.61043207845295
H	-3.03226356899789	-2.91266826410783	7.26032043700090
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C	-1.93348503145491	2.81717607479098	-0.52542633545496
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O	-2.60885239830493	2.97315730810659	-1.64904509418493
C	-3.13119358189977	4.27655621895851	-2.05478755061945
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H	-4.84212397781121	4.08853323512209	-0.75872485424850
H	-3.54097973716585	5.09694186298733	-0.08791453714711
H	-4.56459775363211	5.71654754999040	-1.39444029725572
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H	-1.43452005847470	5.48781969373719	-1.46333523542265
H	-1.30323365499309	4.77065782609475	-3.08336642378356
H	-2.39203402110130	6.13791743003003	-2.80717404268427
C	-3.89830811924715	3.94222718406446	-3.32091537836269
H	-3.23438494138827	3.49736807335442	-4.06473012739373
H	-4.70468124618635	3.23881835523572	-3.10564586508569
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C	0.36117814607981	-3.68237129028421	-1.97754425701887
H	2.64555692169344	-4.47412106722812	-4.47302932172895
O	0.57533989622309	-4.65922795766764	-5.97605309583881
N	-0.66276175571385	-3.95901015163383	-4.15340355727937
C	-0.51885331595294	-3.04616261353176	-3.03078391198435
H	-0.14782284839438	-4.56026465186420	-1.57470999495539
H	0.52358937767077	-2.98548035218109	-1.15368616961871
C	5.06397089691468	-2.29970138917044	-0.74192529558775
C	4.10006170936981	-3.03148616378519	-0.00391535212740
C	3.03861987364330	-3.60177017440868	-0.63253183424284
N	2.85058079914682	-3.49612985163438	-1.96766351334396
C	3.73514683798449	-2.78162893304823	-2.69373562561332
C	4.82588233475430	-2.19194776503808	-2.13393112216159
H	4.18554327598971	-3.16087469070100	1.06449990900913
H	2.30340313601876	-4.18477166378942	-0.10136043124323
H	3.51090384632280	-2.68809052449935	-3.74567679869670
H	5.48502744261256	-1.63036245185668	-2.77845918752151
C	-0.54341251372053	-8.67708896350402	-3.18312345526402

C	0.56789464682477	-8.28156598822838	-3.91632994950646
C	-0.80156315821258	-8.07042306710456	-1.95876867405106
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H	2.29167558095630	-6.99853259921332	-4.00252930831766
H	-0.16215684826894	-6.60604544610269	-0.52003334028284
C	1.16712336255291	-6.66737915592208	-2.20489437645501
H	-1.20080765936344	-9.45244854698063	-3.55951251125998
O	1.96424705935982	-5.72364607465068	-1.73883139585414
N	6.12278431416783	-1.73698615657627	-0.15976589714702
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H	7.22082683953988	-1.31042922600168	1.54652894107198
H	5.47696172638928	-1.41612267741822	1.81996649553870
H	6.43247450447697	-2.89421224275825	1.57416938649590
C	7.09047015336681	-1.00605778816174	-0.95475372387558
H	7.89412287834154	-0.66819001223129	-0.30663835304475
H	7.51756189633469	-1.64282448609419	-1.73365726169025
H	6.63433417580061	-0.13199839415098	-1.42804467637822
H	-0.08081613365923	-2.10892305515662	-3.38600648764595
H	-1.50963257618954	-2.83785128670288	-2.63581667197156
C	-1.91191829062214	-4.47286079528102	-4.41197072500537
O	-2.91887484878636	-4.02347058068740	-3.89773092102042
O	-1.87090591845882	-5.51002889753638	-5.23310549162077
C	-3.08512386056545	-6.20759773512223	-5.64626178862387
C	-2.54278440370795	-7.28791585080014	-6.56472802889826
H	-1.85790757239078	-7.94114587318318	-6.02071028695720
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H	-3.05601220044375	-7.42539639257513	-3.87142460601790
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C	0.42745027922727	-3.72161741873844	-1.93677176713142
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O	0.51400042969138	-4.64981200638879	-5.96665403642327
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C	0.51993040473056	-8.30431013689355	-3.91132146187943
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H	2.25306309097585	-7.03683901770036	-4.02608826715246
H	-0.10260596831068	-6.67272108957625	-0.47320777813570
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H	-1.49398403939027	-2.93974760276162	-2.52906093608519
C	-1.91993954103813	-4.54887703908250	-4.32900980996827
O	-2.93037166182757	-4.08907497860158	-3.82837935306129
O	-1.87990434042752	-5.60406859739760	-5.13097516600905
C	-3.09341354564679	-6.22056779094375	-5.65129441882815
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C	-3.89092863105278	-5.21139227028374	-6.45837131002328
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H	-4.70511889624822	-5.72850390921921	-6.97064641048335
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O	-2.87616669055679	-1.54598149179221	-4.25680933720088
N	-1.68232497667616	0.30839256021326	-3.74530145628022
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H	1.05231871761881	0.55139409788138	-1.79106738982636
H	1.14407614133734	0.20819667824472	-3.51539145400979
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C	7.71015967021262	7.48666844509824	5.71880107484884
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N	8.77612221822101	8.87066774456251	3.94971679299870
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H	11.21350509757014	10.04426925981076	2.00869205819097
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H	8.94972512038736	13.88172522156893	3.27671766607955
H	10.13036874127645	13.69119633630069	4.59121856133571
C	11.57494602323978	12.52467264708922	1.95784111264720
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H	12.44550615024460	11.98434355502197	2.33927125691358
H	11.28249739661605	12.09121131513437	0.99854396871322
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H	7.11880053056921	5.89101570418760	7.02393630950852
Cl	5.39269115605171	10.24651224309428	6.26298951324465
H	6.63776506064098	4.34313907281876	5.31464548127739

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C	8.18877222467122	7.56951183672496	4.35639100010054
C	7.89920754354021	6.67951717094922	3.40863464834782
C	7.25812936565625	5.39518006538353	3.74674615872937
C	7.94378986223846	7.30424344204738	5.80256962578832
H	8.01368081821664	6.88911424381416	2.35319860537876
O	6.78431487617459	4.67444449684381	2.87183434629044
N	7.18996352474387	5.09957252619913	5.05764037447953
C	7.95584162150384	5.80990810061462	6.06169061931334
H	8.72590008254553	7.77692775046435	6.40165646322168

H	6.99260967059967	7.76627220782469	6.09673665326304
C	9.78177416585535	11.33986543225573	3.35184180903058
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C	9.67887928267349	8.95253987885556	3.04898462361875
C	10.20659301118729	10.15216405302371	2.69906951245767
H	8.38388895758623	12.03108738197955	4.88136673711742
H	7.47585930635829	9.82119682155538	5.36864224071026
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H	10.96924205028310	10.16800687770832	1.93524254923344
C	4.19561386587385	7.99608067299034	2.40948621787087
C	4.75596729470298	9.26896489700985	2.46583143519793
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H	4.45310490528070	7.20709721443285	5.70825993533941
C	5.13783457082232	9.07866497242676	4.88669207666706
H	3.84530712052702	7.58201263467601	1.47121594906212
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C	9.86908008427487	13.71562596836473	3.76768108168675
H	10.43364780380952	14.56855127329074	3.40210581110003
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C	11.28418222411650	12.65722207037008	1.99424993658590
H	11.50571765365101	13.71029069556191	1.84696467931619
H	12.20939791362422	12.14000533365794	2.26362795117641
H	10.91281768101355	12.24741526978577	1.05220286667182
H	8.99071886111711	5.44545306759995	6.07347422226755
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C	0.33645487368083	-5.82047630759458	-2.26200016682641
C	0.22602793506390	-6.36779976915420	-3.48191146004320
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C	-0.50212214346140	-4.66496294882204	-1.84013080362716
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C	-0.92644191935822	-3.86158485690481	-3.05251126885144
H	-1.37402897088127	-5.04898474880903	-1.29741012944647
H	0.06141663417118	-4.03602771670314	-1.14867259077022
C	3.52073439720103	-9.59882055441259	-1.88663922083879
C	4.04126360354121	-8.32999877462443	-2.10185165036830

C	2.19949704959888	-9.74802355372484	-1.48484162635022
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H	1.79117721925695	-10.73699882969929	-1.31220358433885
C	3.24483110433541	-7.20740055482326	-1.92180804201823
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H	3.63099327613356	-6.20816866392202	-2.08497460857265
H	0.36185307573593	-8.72802699355524	-0.98612736492339
C	1.93145413520493	-7.37705254505543	-1.52247873620212
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O	1.15459795211679	-6.25280411246903	-1.28470023148176
H	-0.07031361910483	-3.28230996887822	-3.42241492212614
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VO⁺

C	10.42434223642995	-0.61878321138364	-5.03748998316269
C	11.64124943593767	-0.28782196829661	-4.60597346911612
C	12.25151346179113	1.01110423329949	-4.95497243871351
C	9.63035737936939	0.30089858160144	-5.90766730582744
H	12.21087640868251	-0.89948493797075	-3.91912921902501
O	13.26019510426989	1.40633155508962	-4.37911260033679
N	11.61081156634185	1.72591454752574	-5.89881670024472
C	10.57223225853573	1.15702672533517	-6.73232115671542
H	8.98397304812146	-0.26618182507138	-6.58018965639971
H	8.98635765214083	0.93288213464107	-5.28487615104607
C	8.64070372316103	-4.25661289773384	-3.85076780980990
C	7.87642818159556	-3.08277423317699	-4.08669488293031
C	8.48166296144060	-1.93586915942515	-4.48120163071906
N	9.82541725509252	-1.85316576831955	-4.66041889072318
C	10.58286087677240	-2.96212393326168	-4.45409394618521
C	10.04131613411826	-4.14013708170275	-4.06123555398598
H	6.80482343016663	-3.07074680357576	-3.95717718538958
H	7.91697367738211	-1.03033982196965	-4.64905314138673
H	11.64000579094431	-2.85981231438903	-4.65051493688377
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H	8.24530652288737	-7.40069829526744	-2.95743580794476
H	9.42000940730652	-6.86419628349344	-4.16599641833052
H	9.62393426804155	-6.41065688921742	-2.45806039195942
C	6.64242111983471	-5.47770208307205	-3.27406073041118
H	6.38917495737694	-6.48214526548096	-2.94881379821323
H	6.31350791609541	-4.77091532726402	-2.50865096428259
H	6.10910669196674	-5.26665437502335	-4.20434134414676
H	11.01339087044508	0.54937914801006	-7.53175021594296
H	10.01754299460240	1.97103681390067	-7.19726018515043
H	12.06617958859011	2.57280055663027	-6.20372328026069

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C	0.36895398881162	0.13376226957420	0.29652039690155
H	-2.22181193029517	-1.76166958229991	-0.99056539209114
O	-3.31806172551018	0.57264989978884	-1.39806689262683
N	-1.56556150020038	1.46106968358693	-0.28671607313241
C	-0.51589226868543	1.29841278196273	0.69157089424578
H	1.13735251726803	-0.03443557989674	1.05097826728518
H	0.87315043332847	0.35085078583311	-0.64996743371206
C	-2.35524702791603	-1.93011117221088	3.55785220253353
C	-1.35266726353665	-2.32446894844368	4.47294808004561
C	-0.02692500389354	-2.34961338128620	3.97649653814486
C	-2.00618595588512	-1.59701315934501	2.27447271007609
H	-3.39555391900390	-1.88399015475269	3.84535170469371
N	-0.75444891515404	-1.63149457103992	1.83883082351722
H	-2.73816807508806	-1.28615832064866	1.53150232997100
C	0.21736557527877	-2.00197726270877	2.67503840978514
H	1.22390312695360	-2.02532023189039	2.27324474366363
H	0.80408317398324	-2.64225229507732	4.60154941453546
Cl	0.48940474941913	-2.49970132324806	-0.44458836806699
N	-1.63804260983755	-2.65871703546283	5.74151605580675
C	-0.58352705770143	-3.07344261896150	6.64180757046041
H	0.16413132184451	-2.28497602202006	6.76964997390776
H	-0.07810048072255	-3.97326215453140	6.27777152905389
H	-1.01650504056239	-3.29387675928692	7.61404864531956
H	-3.02660027723968	-2.91693568586328	7.25828505609939
C	-3.00708033834021	-2.63356556960789	6.20926633672811
H	-3.44104142658434	-1.63370614287606	6.11564609938479
H	-3.63366946048087	-3.33573947548866	5.65034297805738
H	-0.92136986997146	1.12917280251835	1.69865638750566
H	0.08027006961438	2.21175018787410	0.72789670153112
H	-2.10212564414462	2.31372191743645	-0.25908228402922

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C	5.04390161196523	-2.30672689255596	-0.74955013498568
C	4.09762969813352	-3.05236974099601	-0.00314306815426
C	3.04148957665445	-3.64284312484622	-0.62407913325574

N	2.84201500745560	-3.54271371664740	-1.95660189828604
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H	2.32036654866826	-4.23621133296430	-0.08510080787184
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H	5.44339969801388	-1.64176661403394	-2.79138215419650
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H	0.65170818815838	-8.77295700893233	-4.88466141669790
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C	1.37172121283203	-7.33865892869797	-3.46797355719412

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H	2.18808190354837	-7.00524415638738	-4.09593048849486
H	0.03870745012101	-6.77851588514407	-0.40614895379130
C	1.21378333199093	-6.74994907440395	-2.20078508070595
H	-1.18849073322725	-9.57037301590631	-3.42890913152157
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H	-0.22644053684815	-1.32436630638825	-2.91598568504677
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H	3.43217541557081	-0.92610865513544	-3.00493522546210
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H	3.66692853484201	1.07950905474018	-9.41331679246563
H	1.91854307658175	1.27376242142099	-9.67229307034893
C	2.90597142322033	3.81968957925863	-7.91891386318662
H	1.99438186145025	4.30836333222965	-7.56538327923088
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C	-0.15450412458310	-1.24326952157785	-4.18256537663088
C	3.29345518279346	-2.03719076823720	-2.67265053138978
H	0.71152282497601	-2.25794855192352	-2.49676873738168
O	-0.07972813316083	-0.43667066297308	-5.11984647807275
H	2.94149102574748	-2.03849487268610	-1.64011999023945
H	3.41954137393431	-3.07080977576860	-3.00379146341451
H	4.26203814400226	-1.54184711932362	-2.72269434643649
C	-1.51558055275688	-1.79888123283035	-3.82116481409949
H	-1.48092137359498	-2.52777910884304	-3.01119901122186
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H	-1.95126162198004	-2.26782991970063	-4.70706345071276
N	2.54354068887887	0.49015965416823	-2.92866592082272
C	1.52489520746345	1.02572491873476	-2.27324771446304
C	3.63732574355624	1.22206317657966	-3.13309196892840
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H	0.67125704958167	2.68341020567052	-1.26586139430723
H	4.67185245040561	3.05246024408376	-2.88781306786249
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C	3.93297510506501	5.17705978195886	-1.78051201728153
H	4.82394099539588	4.73791733860392	-1.32079077577467

H	4.11727092182337	5.28632739206927	-2.85375407146135
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O	-0.84850798853856	-0.59777789096877	-1.87333169016641
H	-0.13143592949013	-1.53343138684335	3.09308145079098
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VCl

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C	-3.78091756310004	-15.08392826077470	-2.44006311518957
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H	-5.36444842761216	-10.16612373485037	-4.53122466161662
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C	-8.20574805269852	-3.92785108189405	-0.49515773226588
H	-8.66834699900391	-4.63787257639703	0.19730487672671
H	-8.64049370672199	-4.08187246714335	-1.48762596610707
C	-6.21785338549037	-5.25303461149713	-0.86991089151695
C	-7.00710585988848	-6.36109211426650	-1.25235660818144
C	-4.81547946208414	-5.44749397187515	-0.87673461030274
H	-4.13544612858821	-4.65569405410077	-0.59822154796179
H	-8.08541292203605	-6.30413443628970	-1.28000662838356
C	-6.39284188603510	-7.53708699361611	-1.60378246807068
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H	-3.23117898645983	-6.83920484746439	-1.25360776134386
N	-5.07759202412337	-7.68789455385491	-1.59542536833455
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C	-1.61049074953674	4.07332584682414	-0.14675303244654
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H	-4.73929508274624	2.87187091405864	-0.60926688689820
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H	-3.48841708080687	5.01295421724159	-0.59252200405234
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C	-1.49360618515448	-0.35358427684776	1.48241707262165
H	-2.45462991878085	-0.03864093553019	1.87028083266412
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O	-1.40699503626574	-2.21251969258916	2.93260408691489
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H	6.28215455416545	0.93460730730429	-1.25335383837074
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H	6.47061527872359	0.66873014194361	0.79693205558183
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C	1.05988904656781	0.65012295147631	-0.93811442731138
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C	-1.28599475922487	-4.57478955487437	-0.82908433812767
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C	-0.18743141196572	-2.51953821675907	-1.44569272123687
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C	-2.30806453384625	-7.59612345693312	-3.77822657421508
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H	-4.27017400672202	-8.45743629998375	-3.82697250357931
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H	-2.53651887280263	-6.86492219074544	-4.54550751734191
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C	-4.11081946451758	-10.37570941539761	-1.95976773567669
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H	0.74065215534671	-2.35792345783872	-6.06630652245227
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H	2.13633719096019	-0.81250162112900	-3.49909172850147
H	1.44329763561455	-2.41427164987544	-5.95276769402144
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C	-0.88041798028462	0.47957465944332	-0.88344856968864
C	-2.80376368364501	0.31713835204354	-2.32375328362970
C	-2.28883883382618	0.55880845415054	-1.02253964603043
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H	-0.39837207724008	0.64678214100813	0.06821017169378
H	-3.86493725123155	0.31523741533612	-2.52175376808417
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H	-1.99415175173647	0.15954784382670	1.68028762210595
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H	-4.78412330203096	1.66688247642167	-0.91462499323274
H	-4.93063765311782	-0.05401733502810	-0.49246051918936
C	1.87627245834374	3.55615095133923	-5.03453408921179
C	1.24973859096973	3.60643005341042	-3.79267049177745
C	2.88725267620616	2.61622204210532	-5.22424875423743
H	0.47176227210469	4.34361773592099	-3.61293161802480
H	3.40154447282946	2.56807223662230	-6.18028717114338
C	1.59965328286641	2.73242606881546	-2.77801603823403
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H	1.10535414994925	2.79527330033950	-1.81313592557154
H	4.01479872704393	0.98911508697511	-4.39888313323497
C	2.59190137225971	1.72533843150490	-2.95561003611408
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H	1.50484793063341	-3.31976027401583	-5.52921195924764
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C	1.68848938845062	4.08935822871725	-4.58310093132958
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H	2.45132228170131	4.67591820452578	-5.08159881208751
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H	-1.00825131946626	1.97634593782140	-2.79079928674019
H	2.79748568851434	2.24024089926820	-4.71444355983283
C	0.90410880292078	1.99949212158445	-3.74652348501965
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C	-0.13155787165838	-0.13182815617341	-4.36010526173164
C	1.07898844828033	-1.00508568425112	-4.27924911174048
H	2.36967102362044	-1.48632768942724	-5.98603439028475
H	0.18938165291118	-0.58552636307963	-7.48192326250385
H	1.36599726778197	0.54612055266763	-6.83567072049043
H	0.92213969751882	-1.87069380634641	-3.63138678830982
H	1.92061185496032	-0.43647976478380	-3.86423106639770
H	0.81053692705296	-2.30898046868762	-5.97100410448729
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O	-1.43015688329784	1.74964408873615	-7.13246563984428
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C	-0.98651116206505	0.68829849156028	-0.90177720377013
C	-3.02094991428729	0.41223659208673	-2.16604937876331
C	-2.40741683695017	0.72626381081218	-0.92353129985653

H	0.79181671637189	0.38174857945967	-2.03783499899313
H	-2.70427118924667	-0.16092458128301	-4.19803038367576
H	-0.43026995446532	0.89411747289085	0.00029306255228
H	-4.09451954853854	0.36274160319382	-2.26945988684050
N	-3.11747901475506	1.01891260631760	0.15764697760720
C	-2.45462980303814	1.28635964364463	1.42233899946295
H	-1.81025956960807	2.16566327126965	1.34686928300823
H	-3.20969922566848	1.47284323103722	2.18003614027857
H	-1.85204185817462	0.43031803907536	1.73470928024220
C	-4.56805790059010	1.06543102986947	0.09512579493478
H	-4.94938798099906	1.39452237333881	1.05724285406745
H	-4.90014067738541	1.77096758656364	-0.66953853213134
H	-4.98289107595441	0.07888345120339	-0.12748555905319

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C	0.28381089810893	1.73305690283880	-1.79074280870179
C	0.67081514276174	0.38843043164728	-2.34573205349440
H	2.68914021475624	-0.44768367689046	-2.43754953932636
H	3.43773339493120	2.09488015007205	-1.59831221586853
H	2.91321549079333	0.88509885747621	-0.43961034800911
H	0.16160713999715	0.13100634215749	-3.27454943035523
H	0.39876169996497	-0.36220182636123	-1.59591483451226
H	2.42952181186266	0.98337628837109	-3.43197237902179
C	1.24772500449975	3.27008286360654	-0.08180008146809
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Cl	-1.38279135930742	1.90696398663177	-1.26111272469121
C	0.16317631114451	4.29321715375179	-5.75057031418969
C	1.02588907444295	4.56690081875665	-4.66559602381247
C	0.97764141179212	3.77300570119379	-3.54757944934966
N	0.14451678301304	2.74954002691541	-3.42571045860417
C	-0.69034898932411	2.46991090323871	-4.42704853791540
C	-0.71762734498062	3.19710266749894	-5.58908714014721
H	1.73021324166871	5.38538164989540	-4.69556016831398
H	1.62849392716426	3.94494364058447	-2.69304704930133
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H	-1.42016414760093	2.91920597038211	-6.36137707009843
N	0.17787187094365	5.03090903152331	-6.87383805596850
C	1.09514648724633	6.14253054682669	-6.99859792826011
H	0.95323782229158	6.61066455190531	-7.96917954394496
H	0.91725653497320	6.89497232387446	-6.22428808386132
H	2.13578194742188	5.81152768349563	-6.92481554633442
C	-0.71086544554823	4.70940811142915	-7.96918781494532
H	-0.53479189735690	5.40832729495376	-8.78285007967594
H	-0.53357935646860	3.69584396444549	-8.34162987765218
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C	0.56896736991117	-0.39503935809934	-4.12186920263798
C	1.21489159419158	-1.75927802885636	-3.97755267849700
H	1.95271704571901	-3.01931151002253	-5.61065167016457
H	0.43654611304929	-1.39072380677910	-7.22931232267850
H	1.98974955056208	-0.81956049265049	-6.63474677741255
H	0.71324907231166	-2.35995993459457	-3.21529098054278
H	2.25381046370996	-1.63235937216135	-3.66940797414474
H	0.19661093482748	-2.96623338293633	-5.45026236286871
C	-0.30958528309459	1.01770694104613	-6.00453776424704
O	-0.45874497234073	1.26026095924818	-7.21285623937492
H	-0.69834722347379	1.74800824000206	-5.26774120473386
N	-0.36870902278650	-0.01899216396624	-3.07825549311364
C	0.02927302465537	-0.03316057857862	-1.78382441866378
C	-1.66662437411419	0.23653529266894	-3.35040332482231
C	-0.81646149699931	0.25878137493742	-0.76186870660801
C	-2.56468269428740	0.55723281186792	-2.37977026112230
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H	1.06855630462675	-0.26725074329223	-1.62081127808078
H	-1.95630535406230	0.14230404718016	-4.38517908807245
H	-0.42567233019746	0.22346597561265	0.24392293200041
H	-3.58460225674830	0.74617029714046	-2.67887898618957
N	-3.01177473558771	0.93726016012061	-0.04595187256965
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H	-1.71063595968606	1.56289348445017	1.48486956711979
H	-3.38737450308160	1.27897674869941	1.96462175852794
H	-2.31780297889641	-0.09818351561428	1.65664859765575
C	-4.39455043321897	1.25085643379822	-0.35011275002097
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H	-4.45920524176436	2.06837979494720	-1.07206374265224
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C	1.62940844079280	4.54573168756310	-4.82520702156831
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C	2.21552316290615	3.57872703544596	-5.63115517778787
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H	2.57075646916312	3.84277415378970	-6.62184322647022
C	1.30034362538782	2.88786721104733	-3.10464533477989
C	2.34168204707308	2.27139168917019	-5.18495848404014
H	0.94976106477017	2.61566063714073	-2.11462914670357
H	2.79794454204901	1.51386943491950	-5.81239441827262
C	1.89364386555003	1.89663111095184	-3.90759827723876
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C	0.16144941587101	-0.09377457639959	-5.48596732856181
C	0.39912997530334	-0.35084264140421	-4.13421206700858
C	0.95794913768884	-1.73367180807543	-3.97071625286438
H	2.69427898656726	-1.53756597908934	-5.21839392216830
H	0.15787844957337	-1.75297891782438	-6.86005657080137
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H	1.76508402835635	-2.99638965146305	-5.56911804470717
C	-0.60302158067576	0.95646651450507	-6.00542908900435
O	-0.81696367265630	1.17719982645853	-7.21284568994379
H	-1.05841068891183	1.62643787574912	-5.25005407045559
C	1.89653921904462	4.49257513225696	-4.82031773052885
C	1.54178462739177	4.18490063255476	-3.50975089419546
C	2.26334840812951	3.46505822059039	-5.68033989528563
H	1.25626785017964	4.97901067724594	-2.82686129713268
H	2.54214433909264	3.69131019958022	-6.70470216444934
C	1.54410462163072	2.87209275555104	-3.06888510499052
C	2.27282797373908	2.14781588200792	-5.24491084884141
H	1.26234083577982	2.62832677240628	-2.05001667208551
H	2.56849500100126	1.34888338868334	-5.91526406227423
C	1.92231927392388	1.81821834887547	-3.92236079598218
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O	1.91814890700563	0.57220018977206	-3.50619588328994
Cl	-0.73745647428323	0.19612174258189	-2.91319817222775

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VCI

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C	0.40972922070909	0.28634105156244	-2.53752474189864
O	-3.03483399767879	-1.66944904431049	-3.79877661070670
C	-1.86891728284083	0.40436545990037	-3.58510917262417
C	-0.94560701618429	0.97596646749447	-2.52236330696398
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H	-0.31025944011929	2.38775528898097	-2.14969911198577
O	2.18304172099899	2.75131334232175	-2.63983540568299
C	2.73026758933144	1.66302064400409	-0.58358884542670
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H	3.68545604832178	2.18450798968809	-0.65840752196616
H	0.29685514936875	1.24841293699260	1.83612732340416
H	0.88364968862532	-0.04620104737398	0.81295510368578
H	2.90576808306797	0.61798775274124	-0.87242439239809
C	-4.24240548583195	0.93294818421020	0.26845085500973
C	-3.28575377705467	-0.00797568618545	0.72839191383367
C	-1.95683115844029	0.21998931879107	0.57415158939355
N	-1.49502821341375	1.34460979384250	-0.03264191191156
C	-2.38196179573087	2.27590932886688	-0.46763355267611
C	-3.72044836753591	2.10978561903583	-0.33283102599008
H	-3.58186897087377	-0.93286055343686	1.20080602944444
H	-1.22151593797089	-0.52026303325885	0.89075467321045
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H	-4.36686051651253	2.90056135908805	-0.68258415445187
Cl	0.04280706155013	-2.48262077329160	1.28591574118212
N	-5.54930549896429	0.73065432814325	0.39702579046213
C	-6.49753662130777	1.71810032879740	-0.08558232352983
H	-6.38364620036800	1.87706775064180	-1.16085199633322
H	-7.50439426764480	1.35936567806479	0.10673925482191
H	-6.36483800980164	2.67317014529019	0.42896596359675
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H	-5.71163149323706	-1.36796240186094	0.46187042949996
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H	2.04634080976145	2.76583839465230	1.12626622802607
H	2.82395640123850	1.24019275269712	1.52753351205320

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C	-1.94767301854988	3.36086703403628	2.65216355619094
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C	-1.70885379771448	3.09431738329874	4.09665801545956
H	-1.49819132364591	4.44764047307578	0.88645827215336
O	0.31331824858110	5.97496694241798	1.88726712159853
C	0.09559909848682	4.83870952837410	3.97549015724821
C	-1.07911232291215	4.30057683866165	4.77446190171059
H	0.52039663600058	5.74084117686268	4.41785348802600
H	-2.66136521507588	2.83875329100071	4.56945863924561
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C	-4.86335819231574	0.95445617572037	0.78382283412049
C	-3.92561932082163	0.42463968688980	1.70555057920907
C	-2.99773442658939	1.22344536674297	2.29421829614401
N	-2.93802239576817	2.55210098043415	2.02020636018737
C	-3.81882768529791	3.09433403334751	1.14312141858676
C	-4.76694345079736	2.34762119494519	0.52490859121293
H	-3.90741729857198	-0.62731148978021	1.94861886264188
H	-2.22672498526612	0.81768094661202	2.95515646398217
H	-3.73895243340688	4.16040531688585	0.98644322938708
H	-5.44601433127150	2.84629932025222	-0.14994452433106
C	1.67488839389116	2.02533383461024	0.50151823409491
C	0.64242471509171	1.14133748644681	0.20084174776201
C	2.00766635681428	2.21584954749602	1.84112761649894
H	0.37266123989309	0.96323355925782	-0.83675073806873
H	2.81577093129637	2.89401533698713	2.10189662846832
C	-0.05276853601479	0.48240124017545	1.20120750325936
C	1.32262857785403	1.56304268366088	2.84995738024850
H	-0.85251456344417	-0.20621587243528	0.94411153591984
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C	0.24038670415134	0.67784727918040	2.58162055626605
H	2.21291739282377	2.54226515002110	-0.28446603421200
O	-0.44275055578513	0.12173172250777	3.51987998641882
N	-5.78281477319976	0.19424239551108	0.19550723478938
C	-5.85073037846643	-1.22688400509438	0.48241091014232
H	-6.66439688717611	-1.66162132723057	-0.09074136482776
H	-4.92058387423336	-1.72771184444847	0.20221816383626
H	-6.03948454369098	-1.40338909839979	1.54434232457574
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H	-7.38841517082688	-0.00811120831278	-1.10182985428805
H	-7.32746423955497	1.54972290061592	-0.26607837642647
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H	-1.83433194004282	5.08582669529488	4.88209102428421
H	-0.75393009807297	4.02520891685775	5.77922572935525

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C	0.33722893997569	-4.69374152480415	-2.80622463448616
C	0.02370377139738	-4.84735499856243	-4.10942294826359
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C	0.25048776017548	-3.39722624486647	-2.08214669084186
H	0.10935791969318	-5.80727357193775	-4.60323271732100
O	-0.78757027774459	-3.87716271536725	-6.07253205712633
C	-0.68464266275955	-2.42225932472185	-4.18656090951299
C	0.29558861252114	-2.22301494507435	-3.04389933151845
H	-1.71300312460645	-2.42185748334746	-3.80128167087068
H	-0.68531060037023	-3.39344767571041	-1.50879832955313
H	1.06329809787680	-3.35238161173377	-1.35344418972158
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C	1.01864391285265	-9.57070495169853	-3.42357855022077
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H	-1.04304567229402	-9.75626225225600	-2.84826347267807
C	2.03444508705693	-7.42392187896757	-3.02939452574131
C	-0.28082904588095	-7.79714241154461	-2.44242693176319
H	2.88387793639277	-6.75238232609712	-3.06937020720691
H	-1.20665208088376	-7.41197387359788	-2.03176962399685
C	0.83073165077291	-6.97651868687340	-2.51576675154694
H	1.09253611215038	-10.59151465536645	-3.77957753383656
O	0.75544847597211	-5.68767121231012	-2.00567605380350
H	1.30877497284053	-2.13071494262825	-3.44753378680298
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C	10.11013254801118	0.26806611645437	-5.22525267218646
C	11.08373641158330	1.33275157180431	-5.48976311928584
C	8.26362094927747	1.60830595574244	-6.23089906522624
H	10.48990066758916	-0.60394083007264	-4.70644857630717
O	12.25242805904377	1.18703508711608	-5.18111779102191
C	10.56265232743211	2.60176924829376	-6.10192369664260
C	9.35268171965595	2.35479784832483	-6.98542490006704
H	11.37710001191628	3.08758807608642	-6.64079746777783
H	7.46216966051190	1.31095779877628	-6.91159832784833
H	7.81336237494487	2.26696668811218	-5.47722554377672
H	10.28901642641426	3.26029997077178	-5.26650314543437
C	6.10643902732153	-2.70691934177680	-4.63322425933702
C	5.71482628824612	-1.34142030825957	-4.65102160133090
C	6.60872358780297	-0.37314923134710	-4.96788364327517
N	7.90281364681750	-0.65464571170655	-5.27344319148518
C	8.30101457347905	-1.95440190741659	-5.28945058953342
C	7.45814192474379	-2.96980429389947	-4.98530888907664
H	4.70714069305178	-1.03926878101686	-4.40878412277550
H	6.33002639751237	0.67009918838249	-4.96626541737279
H	9.32199974676372	-2.13713560827248	-5.58975974477265
H	7.84159357310176	-3.97747067755627	-5.04029408839853
N	5.26069524697715	-3.67912053822336	-4.32022387481346
C	5.70186973722798	-5.06343903678840	-4.31433036461549
H	4.87499711282440	-5.69265439884683	-3.99939856009647
H	6.01915833210266	-5.37734860775605	-5.31206618212472
H	6.53146374599755	-5.20335759583137	-3.61771090958306
C	3.87811474016256	-3.37584702783446	-3.99306901519986
H	3.36190187126852	-4.30259070229289	-3.76085757356532
H	3.81820247466523	-2.71779888935836	-3.12289524793504
H	3.37349845061634	-2.89728071009059	-4.83611330102755
H	9.65057669547474	1.76336011961652	-7.85646048981015
H	8.95463522667928	3.30023465709972	-7.35661119893249

TS_{EA}

C	-0.01373159089651	-0.77073440445204	0.32261994059899
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C	-0.82534572574536	0.98570704256682	-1.19727056609534
C	-0.36607059355339	0.05912304244122	1.52037214430484
H	0.32236693237163	-0.73127701217806	-1.79530734284713
O	-0.93212186546429	1.48424593211238	-2.32954169194178
C	-1.40652588121614	1.73600783559322	-0.01438089595552
C	-1.60501117257672	0.88611331490628	1.22804593548488
H	-2.34259596729012	2.19596143229658	-0.33905990972120
H	-0.50262775995338	-0.57286304635843	2.39892189548115
H	0.48823086806604	0.71367135001121	1.72571721335657
H	-0.71293669179938	2.55941055321393	0.19882958400222
C	-3.19652526956573	-3.23294683318919	-0.46101147877535
C	-3.29163716466438	-4.14138350610797	0.61727491164878
C	-2.32208913256836	-4.00378097300852	1.63889199143818
C	-2.20383428897720	-2.28608844310116	-0.46094828559962
H	-3.89059371636923	-3.26387425812549	-1.28819795711670
N	-1.30924832444896	-2.17990594225366	0.51149857070850
H	-2.09548741186043	-1.56530332765274	-1.26855456545952
C	-1.36699774391286	-3.02571374724842	1.54028935829893
H	-0.60880742903030	-2.91355735151022	2.30764846906676
H	-2.31113083334031	-4.65844204821612	2.49819193944123
Cl	1.43275986305534	-1.77221959319339	0.59047397227874
N	-4.24730336358043	-5.08426224282302	0.67041184475300
C	-4.30945310398146	-5.99746041979213	1.79057966649484
H	-4.42948620123661	-5.45919504419465	2.73536590232351
H	-3.40720398486834	-6.61379213033183	1.85689396930111
H	-5.16504560793912	-6.65532757055956	1.66218955523543
H	-5.88179523607466	-6.02912229065163	-0.18251133746408
C	-5.20363497982065	-5.21030169262263	-0.40770649236217
H	-5.79386796029004	-4.29647188265156	-0.52623705355920
H	-4.70692964517621	-5.42516205426278	-1.35900186449381
H	-2.45920413313356	0.21601566440744	1.08984098597774
H	-1.83348197262901	1.51720614192686	2.09020198471891

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C	0.57215781295500	-4.05456111478406	-4.84356442591111
C	0.34579787717539	-3.79487457547787	-1.95826893798073
H	2.67696032524758	-4.19425702913450	-4.52205568098130
O	0.60987855285482	-4.22570710205129	-6.07527013213541
C	-0.76277049135064	-3.79829464900295	-4.17580906171913
C	-0.61303487608262	-3.04484168243203	-2.86777280504947
H	-1.23778071758522	-4.77081237174559	-3.99298508788757
H	-0.09679877734786	-4.76501504981320	-1.71727894129338
H	0.49156129117177	-3.26431170956782	-1.01567348181614
H	-1.39407087994977	-3.26353555769426	-4.88896514507155

C	4.94941971219459	-2.14104225966775	-0.65618187163195
C	4.06482379308606	-3.01687092174558	0.02114770176145
C	3.03729079908896	-3.60858979005868	-0.64404581985319
N	2.80830877274808	-3.38857650465404	-1.95811506097806
C	3.61543657150297	-2.53763254168162	-2.62330115881684
C	4.66948610820915	-1.91734907418164	-2.02601813998727
H	4.18858774871335	-3.24351331301969	1.06941342138949
H	2.36654716928428	-4.30103146121262	-0.16139814565622
H	3.35965670887595	-2.36500364846402	-3.65813864828551
H	5.26691445261201	-1.24490037469322	-2.62288181990808
C	-0.18678953519098	-8.67859485710874	-3.62970617357372
C	0.85387200809577	-8.10880716699329	-4.35311624114864
C	-0.42917178681069	-8.24372783053209	-2.33108435005668
H	1.05928100030259	-8.44905342772316	-5.36282907243031
H	-1.22948034910854	-8.69052053018341	-1.75028843863628
C	1.63919944732763	-7.11040572692781	-3.79669952448340
C	0.34195610831023	-7.23676239947636	-1.77297415564980
H	2.46209447695546	-6.68187705884912	-4.35453957449894
H	0.15587852181436	-6.89637304467495	-0.75939889438125
C	1.39754548210356	-6.64941039824713	-2.49181149900741
H	-0.79386637290229	-9.46277722759464	-4.06744469897490
O	2.12507254949892	-5.68528989204098	-1.95610771568302
N	5.97582041870880	-1.55540385267895	-0.03820766933506
C	6.21326837188323	-1.79299225072883	1.37231761253254
H	7.07170609855369	-1.20665412707753	1.68764995696572
H	5.35042976249634	-1.49271718977147	1.97245405167434
H	6.42374457196424	-2.84866749819153	1.56491698477586
C	6.86535712659897	-0.67710682340323	-0.77255181756086
H	7.65621203410339	-0.34152181065281	-0.10760023211571
H	7.32224716834147	-1.19908014191211	-1.61727140842062
H	6.33264199234399	0.20032348952328	-1.14992071973939
H	-0.23526361039551	-2.03582402439649	-3.06247939225783
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C	-1.82237292270370	-1.02453058529440	-3.80978485938525
C	0.54309844862931	0.13410640500680	-2.54474418405031
H	-1.18296816098978	-2.87590567229369	-2.93745376410418
O	-2.83902026297830	-1.46706050577750	-4.37951478148436
C	-1.51756250425857	0.45777468789997	-3.89364037708282
C	-0.73817374031350	0.93967817107021	-2.68390789020986
H	-2.46646132495138	0.98664586396093	-4.00892772140935
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H	1.19434096646487	0.37067039584415	-3.39038929077938
H	-0.93551928759557	0.63365225793130	-4.80749169085184
Cl	0.86523702759977	-2.19625735708771	-1.10126150727069
C	1.04321401451616	-0.96608420141328	-7.56683933310580

C	0.34562748990390	-2.01506531786832	-6.97953921128709
C	1.98119596092327	-0.26967690390369	-6.81182649185372
H	-0.37943949421992	-2.57413280083591	-7.56239645180691
H	2.54459778550942	0.54147405153878	-7.26205055000114
C	0.56756775228816	-2.35993800613950	-5.65497016491555
C	2.19807850419275	-0.59865868269091	-5.48320149852271
H	0.03346539205449	-3.18728367539949	-5.20530180792660
H	2.92873891846556	-0.05475853054418	-4.89293456220239
C	1.49544337384947	-1.65230039639870	-4.86897217584298
H	0.86919401037253	-0.70344405819762	-8.60419734370914
O	1.68812440081201	-1.94479174413591	-3.59822715193080
H	-1.35170870658522	0.82611295226147	-1.78416133160295
H	-0.48865123722073	2.00049761841982	-2.77735413155018

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VCI

C	0.38805672121746	-1.08219752170208	-2.73927423852489
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C	-1.97766542397187	-0.98187402338649	-3.26618362673457
C	0.41495650566136	0.33753937525130	-2.51709668939717
H	-0.78336510670823	-2.78055497565525	-3.26701622165911
O	-3.03960936908854	-1.46028835776231	-3.58259521334123
O	-1.93386372587645	0.36597644603744	-3.04687214955339
C	-0.79744915097226	1.01366708465247	-2.69001098576826
Cl	1.83610251339322	-1.97993952565840	-2.54378070595624
C	1.54575400383323	1.07287577471040	-2.14834033917780
C	-0.88984594205553	2.38430815429341	-2.50161576675617
C	1.45999495437529	2.43545290315908	-1.96008707737335
C	0.24111662358501	3.08925732373571	-2.13769428068608
H	2.48777728092383	0.55700617914369	-2.01278785563140
H	2.34043669267706	2.99730924271270	-1.67432532001413
H	0.17484289692402	4.16048193086884	-1.98937579928142
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VOCI

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C	1.28516740835079	-2.00364760647381	-3.90334864572174
C	0.11441258318673	-1.31076076065585	-4.39219129234515
C	1.36390875547075	-0.55105301815160	-1.96262571961943
H	1.64492282508344	-2.83519689750549	-4.49373033535279
O	-0.47026686394423	-1.56482985039990	-5.41530935437715
O	-0.37025252240897	-0.30217774384657	-3.61335917219232
C	0.21623007705356	0.08174151199542	-2.45157157392234
C	1.94635730307710	-0.06775979502696	-0.78552460846378
C	-0.36476652670066	1.14270112724339	-1.77588790101741
C	1.37636689765705	0.99032207918997	-0.11262029669392

C	0.21648116070114	1.58825816504981	-0.60465338601618
H	2.84763539759801	-0.52923542687372	-0.40235511240927
H	1.82966278521212	1.35517614337993	0.80043522697288
H	-0.23311689357385	2.41615285589814	-0.06952535249382
H	-1.25761596945691	1.60234984157753	-2.18094452048956
N	3.00843816897027	-2.36305690119009	-2.29055229091188
C	4.11954424803440	-2.42747655590063	-3.06458382514740
H	4.08649404228559	-1.87050630308744	-3.99101314159260
C	5.20986434413746	-3.13710232424294	-2.68159474676036
H	6.06935962266303	-3.13946754961189	-3.33456355771812
C	5.20810348609230	-3.84557381332026	-1.44932391110789
C	4.02215415643267	-3.75632239915282	-0.67408585430525
H	3.92346711693982	-4.27084031995193	0.27015096760063
C	2.96349101406061	-3.02539409023914	-1.10638790523539
H	2.02701563734773	-2.96857333008769	-0.54404338988456
N	6.25865650863462	-4.55330234398097	-1.04821470833455
C	7.45822991877943	-4.61349497670799	-1.86355024792428
H	7.24112320296999	-5.03654603515715	-2.84731922789195
H	7.89349130281496	-3.61944705276371	-1.99443327847786
H	8.18719167429292	-5.24799673385877	-1.36821596009610
C	6.22717658757064	-5.25742730784597	0.22137260660202
H	6.10210043882166	-4.55966400080501	1.05331554535710
H	5.41103649360728	-5.98336733402226	0.24421255095488
H	7.16571318092425	-5.78846916381892	0.35025988854434
Cl	0.08333052269459	-3.19380306339282	0.67299154096055

VONu

C	1.37463215009929	-1.46537199300794	-2.45594982152690
C	0.30765588092225	-2.06349931342904	-3.01219137982117
C	-0.93154099986992	-1.34703877195500	-3.20043939440935
C	1.32504682845108	-0.09386214160425	-2.03135583316233
H	0.33410408082668	-3.08813718930532	-3.35490914163488
O	-1.95106085651717	-1.81590079492342	-3.64286949598611
O	-0.94228766956013	-0.03359656863878	-2.83568627565973
C	0.12530619788925	0.58357920166275	-2.27309357624711
C	2.35910220505744	0.59166338911575	-1.38533997455591
C	-0.03273834025218	1.91598751295149	-1.92762363718628
C	2.20633620459689	1.91590863293255	-1.03425571199015
C	1.01362048309377	2.57963548257344	-1.31582548285872
H	3.28576841511063	0.08101184772617	-1.15790612959009
H	3.01606141174582	2.43887295965985	-0.54095949259525
H	0.89780600206053	3.62269482173845	-1.04620279522037
H	-0.97324415172916	2.40827396927376	-2.14150973311926
N	2.56287176900096	-2.22379651077539	-2.24379906984138
C	3.74621959574876	-1.81211981391658	-2.76863467552556
H	3.74555851103853	-0.88244223085547	-3.35096850082336
C	4.87413279857259	-2.55226341761301	-2.60615228330602
H	5.78236296273672	-2.18254252184144	-3.05832655219478
C	4.84913598554634	-3.77577286150422	-1.89016700974546

C	3.58899326989471	-4.17023739965923	-1.36566363075461
H	3.47043871814745	-5.08168198591227	-0.79966877958898
C	2.49546945539553	-3.39241499737601	-1.55808207542210
H	1.52347948396739	-3.65570429336504	-1.16443025398654
N	5.94116041172130	-4.51484838518793	-1.71871091506795
C	7.21340410500819	-4.07948013676883	-2.26548633526219
H	7.16729810874318	-4.00629260873649	-3.35510612039509
H	7.50105727994034	-3.10661406395968	-1.85934704833855
H	7.97585108550753	-4.80535264935015	-1.99839621208775
C	5.87525746039336	-5.76877252634424	-0.99060504334926
H	5.55461954696333	-5.60678006706252	0.04179226781084
H	5.18279364774107	-6.46498930640064	-1.47035460527515
H	6.86366636699008	-6.21863397307606	-0.97895248442495
O	3.66685240972147	0.45318411499181	-4.71263747177315
C	2.65828453428076	-0.11068358403555	-5.27689223223561
C	1.39829868253680	0.53800735048786	-5.41689179146328
H	1.31438963500668	1.55923361601199	-5.05594217227814
C	0.30173076093647	-0.10084398787247	-5.96360002831499
H	-0.64295147164374	0.43164806105896	-6.03191257675735
C	0.38028670082027	-1.41945551983355	-6.41095202874051
H	-0.48821752552557	-1.91697219475002	-6.82631126806657
C	1.60289857184211	-2.07489832931811	-6.31357076259830
H	1.69234925899644	-3.09952851906429	-6.66455593876682
C	2.71110156820235	-1.44613621401184	-5.77107807264096
H	3.65893133684211	-1.97329313072905	-5.70762410922249

VNu

C	2.67863185784748	-1.37256851904422	-4.51143380848264
C	2.53171302731496	-2.65029578857436	-4.93756140066496
C	1.86224792133388	-3.62620884265012	-4.12923788354486
C	2.16408848780004	-0.96807288811132	-3.22847805974024
H	2.90698358153246	-2.98818587194456	-5.89254590136881
O	1.68569135021073	-4.78751964417259	-4.42021142635709
O	1.37329713923096	-3.21488844436693	-2.91397509899405
C	1.51486222643028	-1.94292233778985	-2.47068645577576
C	2.27906724290039	0.32711132181064	-2.71550882942105
C	0.98525309265296	-1.64285890944646	-1.22363310066271
C	1.75556803452539	0.63067883224138	-1.47626980493986
C	1.10835177386295	-0.35676733412512	-0.73340027955944
H	2.78354460425394	1.08226102966727	-3.30467656372156
H	1.84631156605851	1.63496419643801	-1.08117499996046
H	0.69596681276623	-0.11763508656243	0.23982252055466
H	0.48649372459891	-2.42163994029582	-0.66003702407285
O	3.28953978579972	-0.40288879573063	-5.19924459665835
C	3.78096269842997	-0.68599913088415	-6.46813821667854
C	5.12081435437589	-0.99625176034992	-6.60804288245806
H	5.75256005835752	-1.06021549419406	-5.73013269406487
C	5.62456579482154	-1.21698671606151	-7.88266375963662
H	6.67340730719422	-1.45883010072595	-8.00832019658600

C	4.79141606589344	-1.12733821216076	-8.98943852623033
H	5.18949479097818	-1.30025996482334	-9.98233779479208
C	3.44877204278268	-0.81230757047374	-8.82528043773305
H	2.79699456865374	-0.73734429320022	-9.68782017511096
C	2.93325951632636	-0.58786273544891	-7.55674889742406
H	1.88930131406663	-0.33945118302028	-7.40631066791534

VO⁺

C	1.67472056402608	-1.75558094744687	-2.72175051584103
C	0.64049321792644	-2.36566261488698	-3.32417133470890
C	-0.58621981535360	-1.64934707989552	-3.59547428564260
C	1.59547821981005	-0.38644066718936	-2.29634462800711
H	0.69004132810715	-3.39291360334347	-3.65886706077181
O	-1.55725823448857	-2.11287474361817	-4.13620710634731
O	-0.62359479868564	-0.33605800994402	-3.22778609238234
C	0.40267126529430	0.28312303911820	-2.59319020872640
C	2.59142311915258	0.29823074873472	-1.58954810159008
C	0.21320948285089	1.60828871444110	-2.23437896029445
C	2.40604045404601	1.61439642595098	-1.22697048026441
C	1.21971392458258	2.26946184250367	-1.55729947413315
H	3.50661869967592	-0.21151908385880	-1.31562387427402
H	3.18079109734011	2.13751517538714	-0.68073259469464
H	1.07760468550893	3.30514173954042	-1.27265496849283
H	-0.72103303712491	2.09497261183271	-2.48526630785236
N	2.87448729872479	-2.49003370241607	-2.49261432269581
C	4.04313581022085	-2.07424442306452	-3.04487940538075
H	3.99758030004086	-1.16728272205689	-3.63168297205134
C	5.19161708526734	-2.77582241688817	-2.88862397282495
H	6.08406178677547	-2.39921487158139	-3.36487923542507
C	5.20413544886134	-3.97780658708853	-2.12864157626854
C	3.95999796199629	-4.38276204361057	-1.57301087808328
H	3.87201386714168	-5.27934807758309	-0.97847803568041
C	2.84415239232731	-3.63932379273282	-1.77234839480815
H	1.88361919525205	-3.91435156763300	-1.35874764047013
N	6.31376369312293	-4.68192469100184	-1.95113863047827
C	7.56846666758765	-4.23830905028372	-2.53399638370192
H	7.50829145441320	-4.22264613612953	-3.62516659738641
H	7.83142727658913	-3.23947649974628	-2.17857036611794
H	8.35373079477236	-4.92796476251039	-2.23956714927437
C	6.28935049296401	-5.91309576513650	-1.18006857611863
H	5.98215343990148	-5.72149094502471	-0.14901789352318
H	5.60530494720765	-6.63921986852471	-1.62561933549825
H	7.28808335716525	-6.33893875631296	-1.17114877718911

TS_{EA}

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C	-0.78573897542983	-1.63739670556389	-2.83590520817538
C	-2.01512657633151	-1.04115005516656	-3.16493856179869

C	0.21340824639528	0.54633476607352	-2.43831123922989
H	-0.72093100615467	-2.71100418137503	-2.94155934256941
O	-3.03430071526261	-1.59879869293613	-3.54228414732603
O	-2.10761036604845	0.34109971254120	-3.06087764786396
C	-1.01952372000081	1.09693651895826	-2.78814749774102
Cl	1.88785759041303	-1.62102068169548	-2.62464822553400
C	1.28727291228438	1.40697562380766	-2.21065438795441
C	-1.18164421610736	2.47536615677666	-2.88059282437194
C	1.13405942416745	2.77601415304657	-2.30562419724296
C	-0.10920427902693	3.31005661331715	-2.63488157719665
H	2.25552057706639	0.98844998803343	-1.96586873806925
H	1.97976852057275	3.42868678994962	-2.12655509138673
H	-0.23844901066645	4.38340670317276	-2.71126406373429
H	-2.15398263875594	2.86692565801929	-3.15468278417423
N	0.29222861856840	-1.12318968928886	-0.44270359408824
C	1.30533407750615	-0.79425221244787	0.36202853791352
H	2.22814808115867	-0.48619396088043	-0.11354164481210
C	1.20622882453301	-0.84927009015853	1.72649470656711
H	2.06462605610290	-0.57105193940843	2.32028371028927
C	-0.00549793238382	-1.26621937468811	2.32804188815925
C	-1.05472635585030	-1.60878978632955	1.44508942502416
H	-2.01490241497467	-1.94273712856242	1.80997851655506
C	-0.85730630431018	-1.51581245911936	0.09230674034905
H	-1.63944004707487	-1.76883678600172	-0.61870186486999
N	-0.14855137214468	-1.33181753127801	3.66059360541531
C	0.95345868953631	-0.98173995003036	4.53083482656438
H	1.82617317778183	-1.61322122153980	4.34019226510112
H	1.24801429150796	0.06427837985769	4.40151415523555
H	0.64721132105267	-1.12672739554771	5.56340873418899
C	-1.41102667030209	-1.74407286073520	4.23588097750639
H	-2.22420681402434	-1.08232663890566	3.92332649914442
H	-1.66715153091535	-2.76756813201076	3.94534224832740
H	-1.33484766890879	-1.70418865767072	5.31927320463078

TS_{SN}

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C	1.28775523274385	-1.54307362051831	-3.71640369028083
C	0.02288267683299	-0.93325180864508	-3.76611377778251
C	2.07266000230703	0.10033428304997	-2.11384406481977
H	1.42648964468331	-2.41844856114954	-4.33634352083786
O	-0.95457509989165	-1.29459169395424	-4.40435144607531
O	-0.17022286493258	0.20199632961072	-2.99101137814877
C	0.79507797302471	0.65854846966359	-2.16214644136504
C	2.98397126468968	0.61290336482989	-1.18851324424582
C	0.44632383823708	1.71882098946765	-1.33137606064490
C	2.64147326661948	1.65734426480476	-0.35383769244180
C	1.36850999368827	2.21815870110227	-0.43413321852886
H	3.97980954771076	0.19196398399474	-1.12707379287734
H	3.36382412738498	2.04053683682712	0.35666370810881

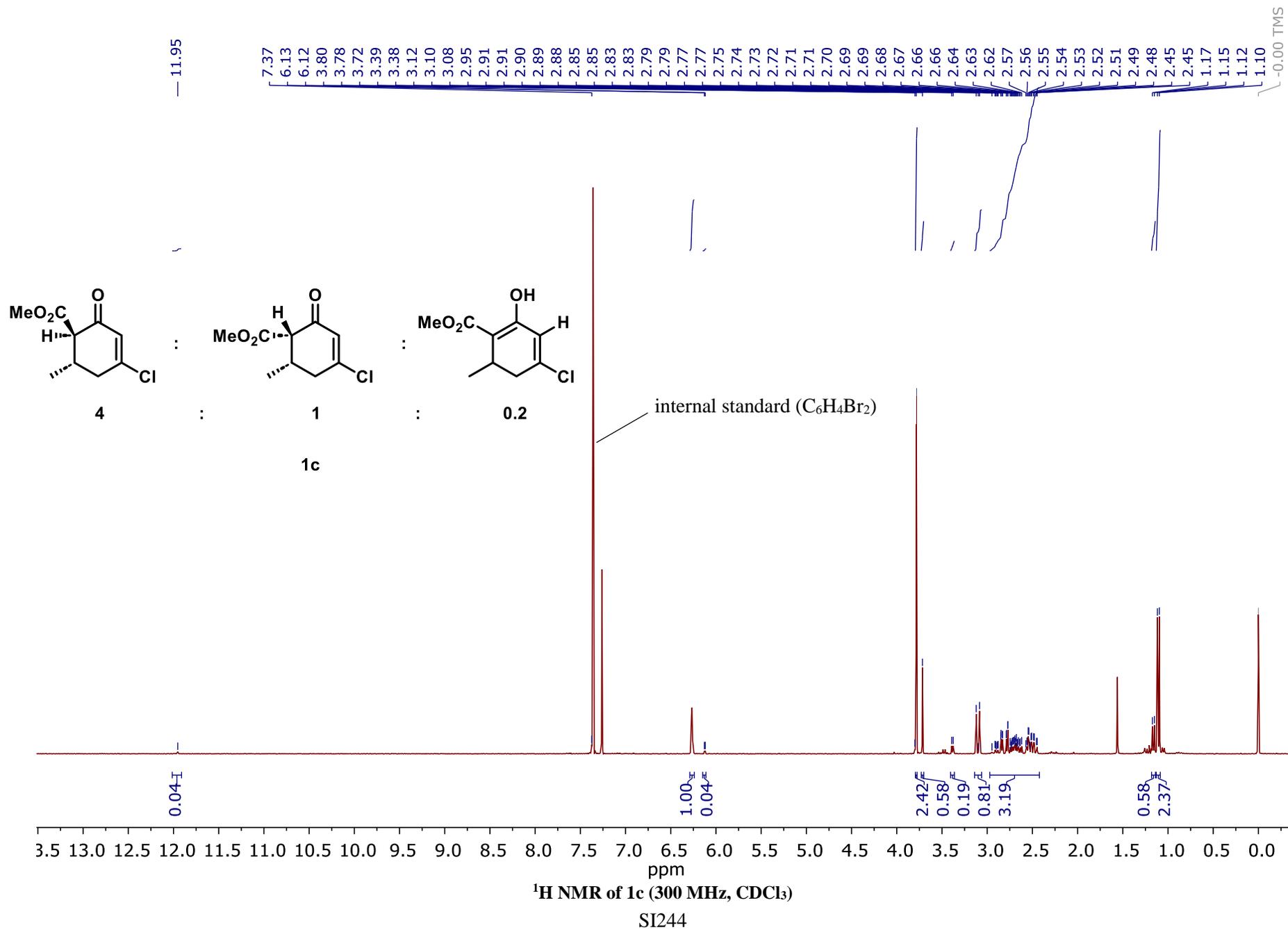
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H	-0.55354519966543	2.12961022003776	-1.40450043204196
N	3.42648592903205	-1.90593283998825	-2.66126197358268
C	4.74561646751654	-1.60839944574288	-2.70021778031654
H	4.99203376661797	-0.65198628078954	-3.13078982370064
C	5.69195363758318	-2.47417033580163	-2.24639427273633
H	6.72563318083819	-2.16978801737223	-2.31346099623203
C	5.32503735002843	-3.73134907152285	-1.70685953287454
C	3.93526117699175	-4.00728322997900	-1.67401333359239
H	3.55047082161725	-4.93420977233416	-1.27613117822027
C	3.04299410907795	-3.09468251328020	-2.14058997013222
H	1.97691874561870	-3.26786603330553	-2.11367771579555
N	6.22902747804054	-4.59811868816320	-1.25267904665157
C	7.64245083928137	-4.27680448683016	-1.30731832644214
H	7.96238452665549	-4.08699741290558	-2.33502816820234
H	7.86984262758208	-3.39618862376709	-0.70046467710669
H	8.20911812010470	-5.11893293663971	-0.92034699907777
C	5.80904970799067	-5.86894289684305	-0.69347262669663
H	5.14233206412027	-5.72105543182951	0.16003073004017
H	5.29282659151585	-6.47738894345720	-1.44092765794718
H	6.68751000595460	-6.41017219999303	-0.35399713215384
O	3.42437787391182	-0.06505357256754	-4.30058205688968
C	2.67499669416379	0.81304985402416	-4.94806882908806
C	2.60334409636858	2.15003002348763	-4.52449953669803
H	3.19845827068327	2.45405761719644	-3.67026449209308
C	1.78970013078838	3.05861717112790	-5.17980133480395
H	1.75236330414986	4.08798487688015	-4.83872118357122
C	1.01417153952685	2.65749385413879	-6.26327415023781
H	0.37278998713445	3.36949461856866	-6.77006815631804
C	1.07773837574490	1.33922498702726	-6.69564561796095
H	0.48074576343104	1.01820010936378	-7.54281671102788
C	1.89628505517494	0.42466317624492	-6.04882574230765
H	1.95339972720895	-0.60347011201713	-6.38598132068566

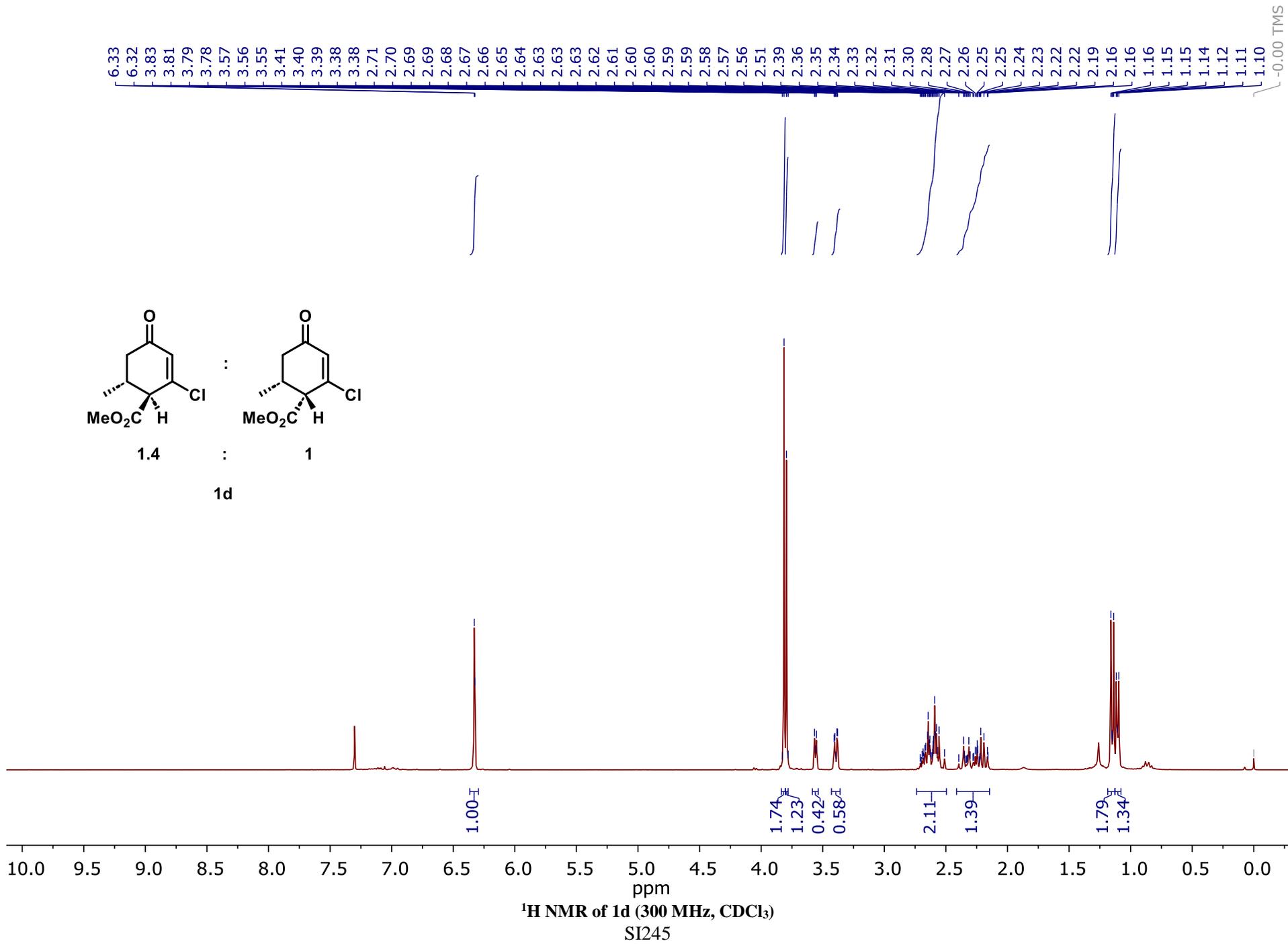
TS_{DSN}

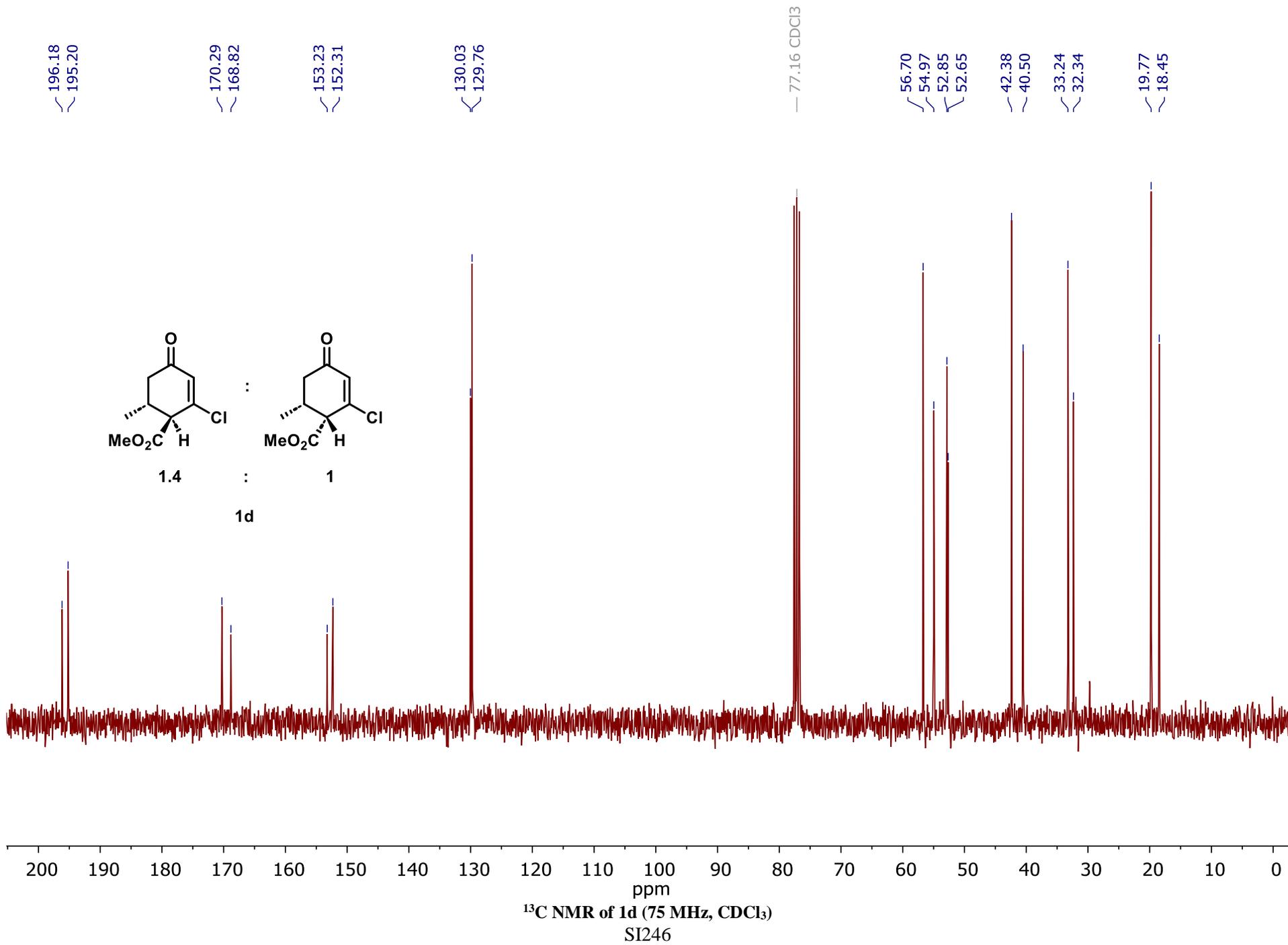
C	2.35046657312431	-0.92875123054457	-3.04483517745490
C	1.24472224703773	-1.51715150704432	-3.65860168214902
C	-0.02149461712508	-0.91407198863476	-3.67240548579273
C	2.07452601569332	0.15626535410570	-2.10498286857608
H	1.36195218754228	-2.41539683887019	-4.24796037571212
O	-1.02539533819638	-1.28957885765338	-4.26636561376329
O	-0.19604910463197	0.23659652886826	-2.91043494390004
C	0.79664456878651	0.71372170881600	-2.12634818693408
C	3.02561901684744	0.70722353211566	-1.24571653998028
C	0.47995588776225	1.80286683085883	-1.31868661338187
C	2.71695074453574	1.78147825634830	-0.43616901657450
C	1.43794125421806	2.33472765581180	-0.47929584740136
H	4.02075927895847	0.27996080767504	-1.23350737397342
H	3.46878323057563	2.19573607853655	0.22492241335663

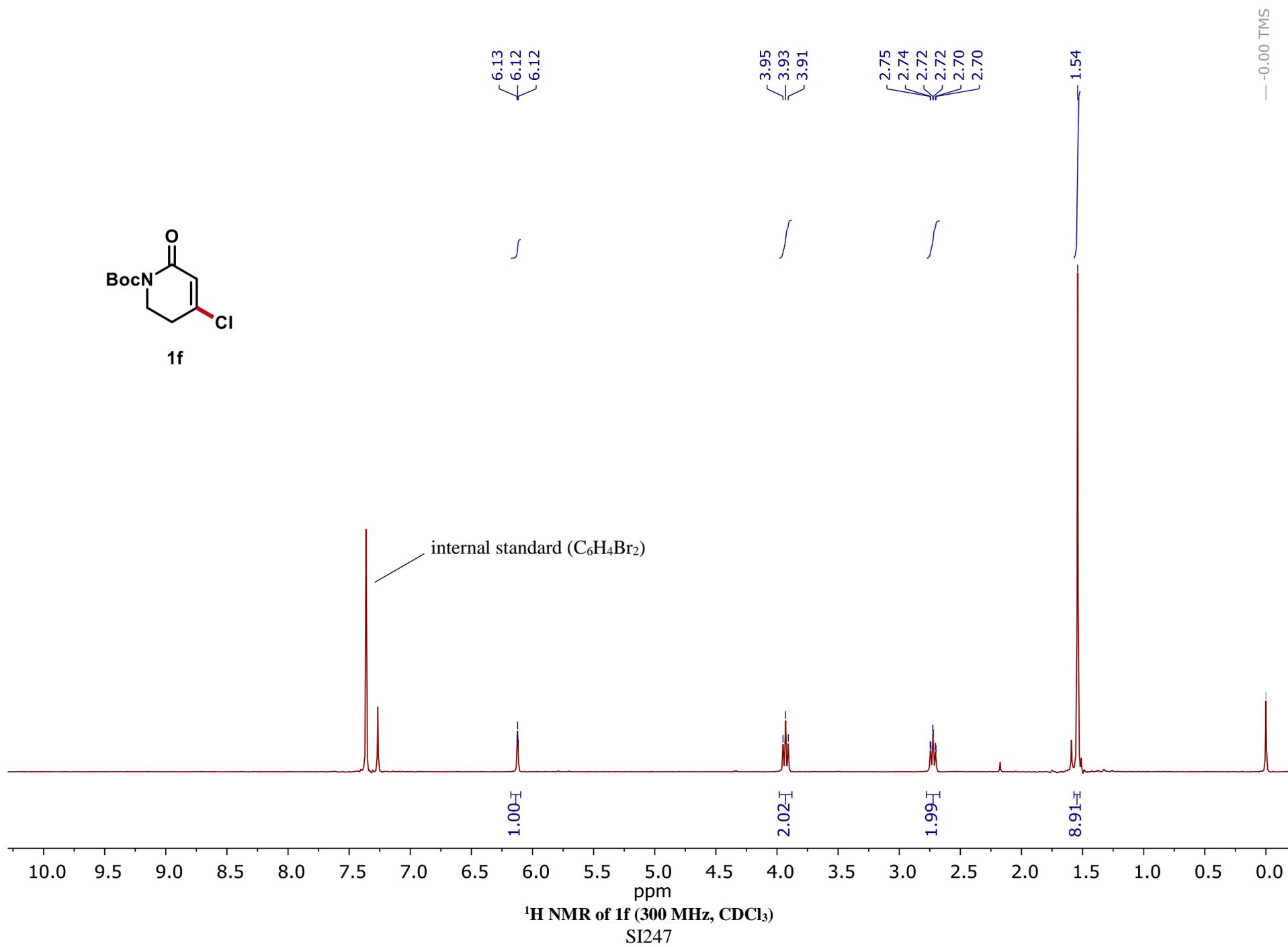
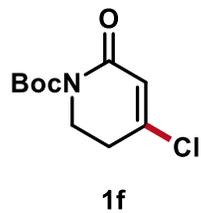
H	1.18892506483525	3.18197094567655	0.14931033232117
H	-0.52238849513758	2.21174815626924	-1.36673772184954
O	3.39703611656096	-0.04870563390430	-4.27349810508819
C	2.66214314251763	0.81377049731292	-4.95466761839414
C	2.61336706994405	2.17000094483993	-4.58971470185357
H	3.21413784500593	2.49829320993071	-3.74835976999532
C	1.81745498794498	3.06593402999215	-5.28374749310928
H	1.80060916872144	4.10959543331887	-4.98648836631987
C	1.03294741817303	2.63544895439611	-6.34945248963446
H	0.40599760940441	3.33792763407813	-6.88691449840196
C	1.06962319879950	1.29790480865007	-6.72326614492737
H	0.46524671542144	0.95221417429687	-7.55572625887415
C	1.87155304263566	0.39660632305052	-6.03857727586991
H	1.90813211286926	-0.64576496204682	-6.33217783223534
Cl	3.63673355117567	-2.05022375624990	-2.56750865953088

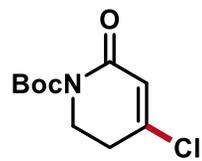
11. Spectral data



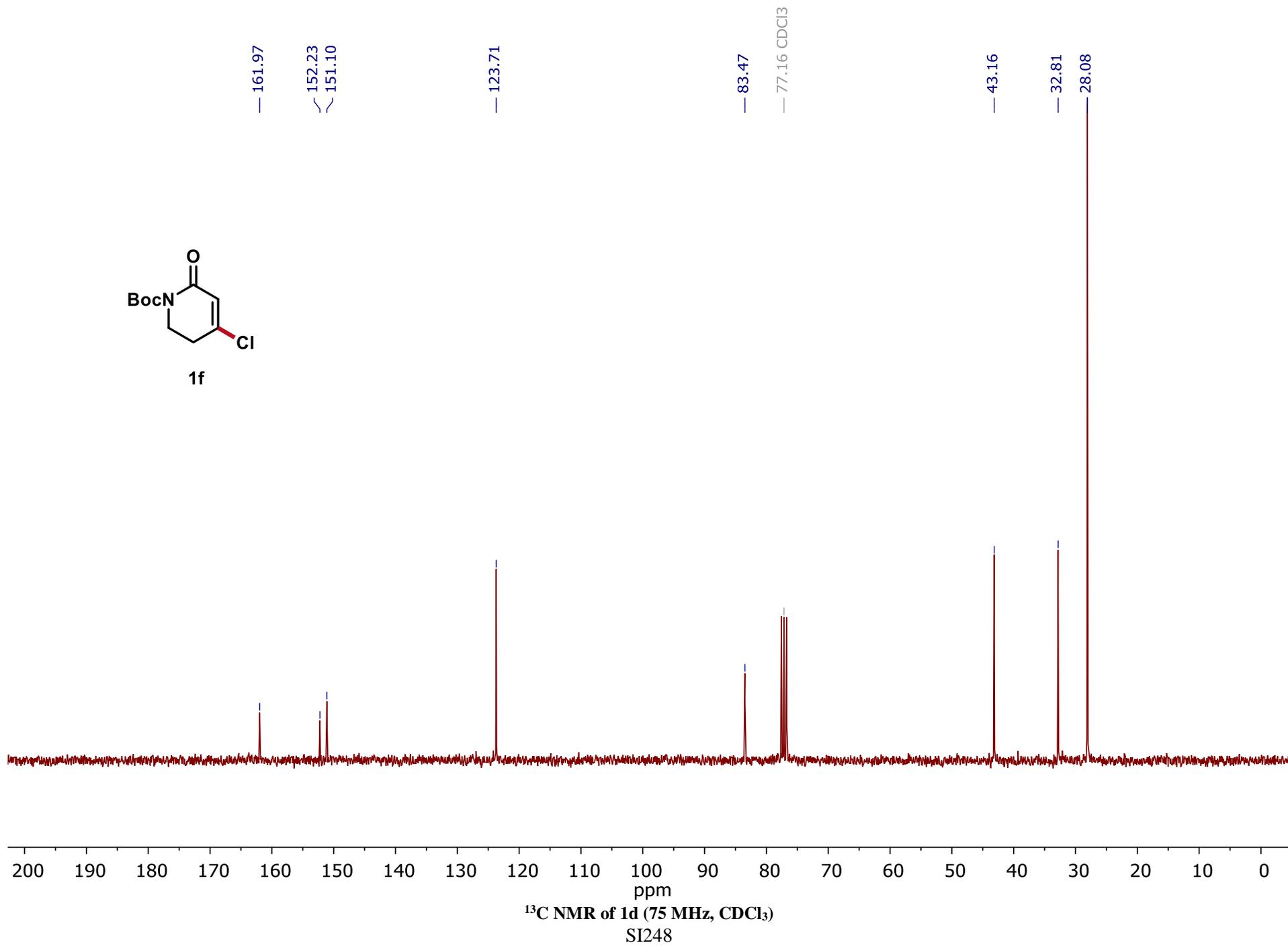


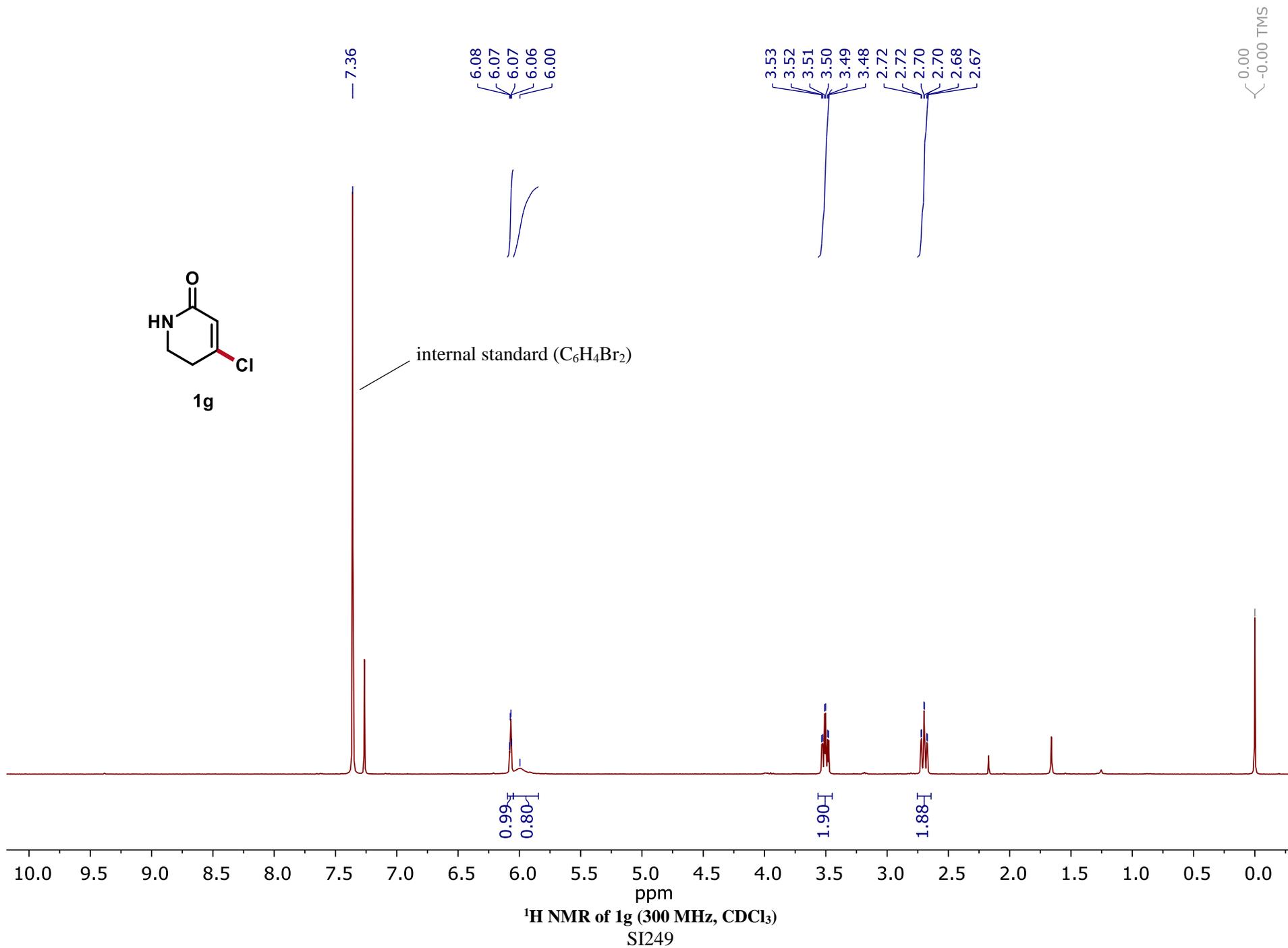
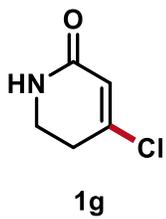


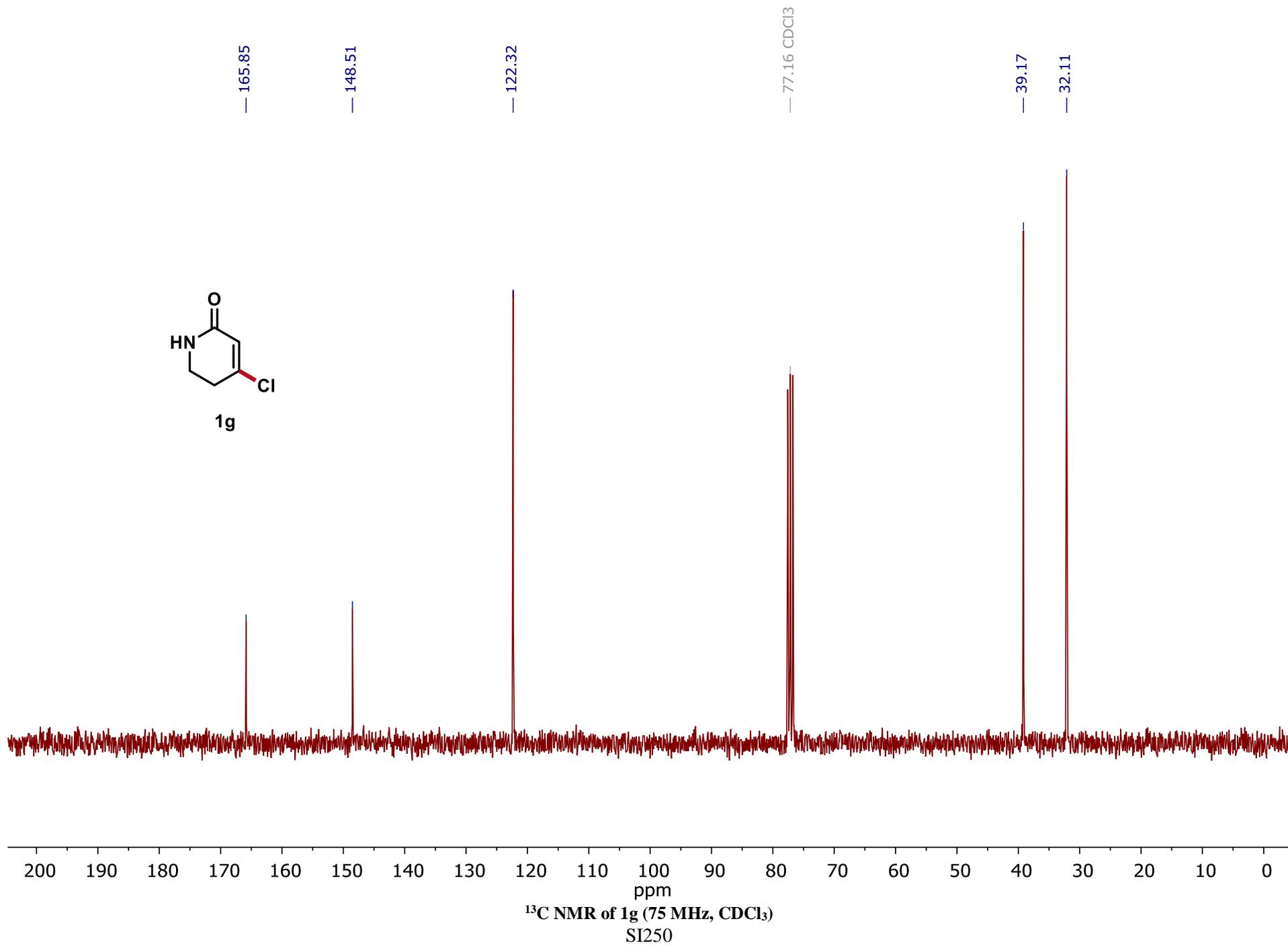
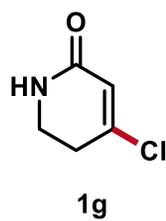




1f

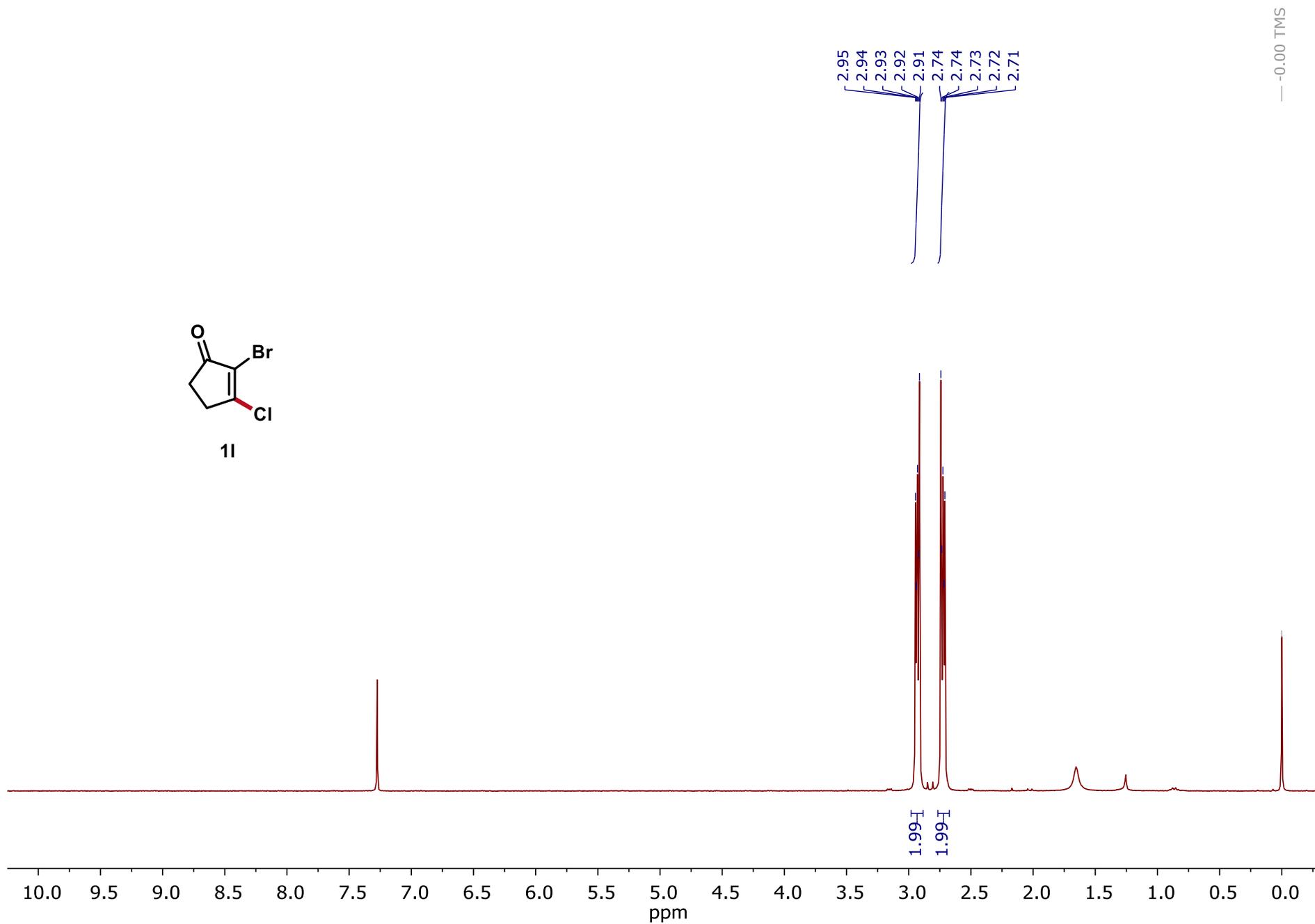








11



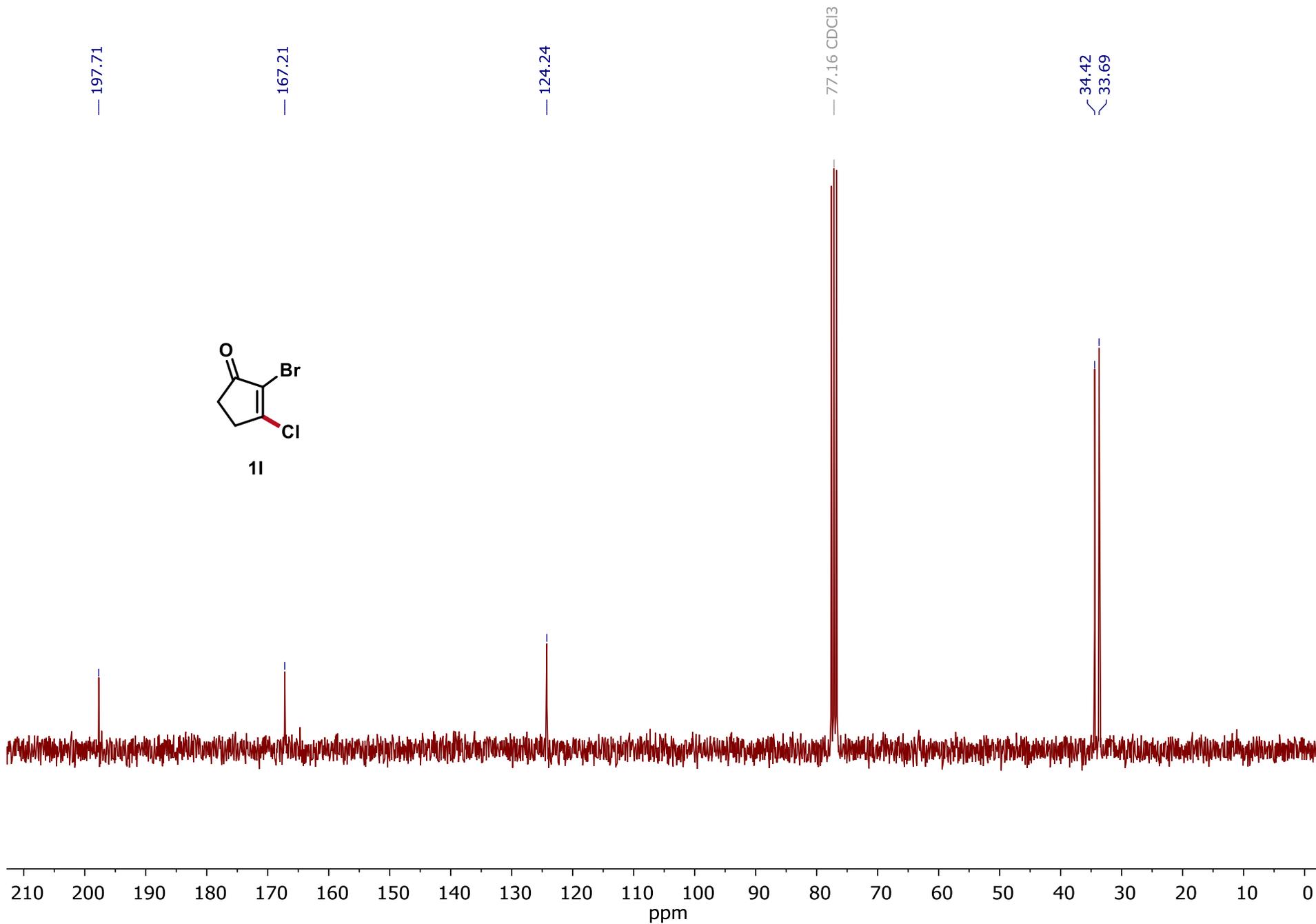
¹H NMR of 11 (300 MHz, CDCl₃)

SI251

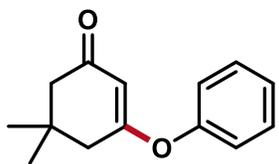
— -0.00 TMS



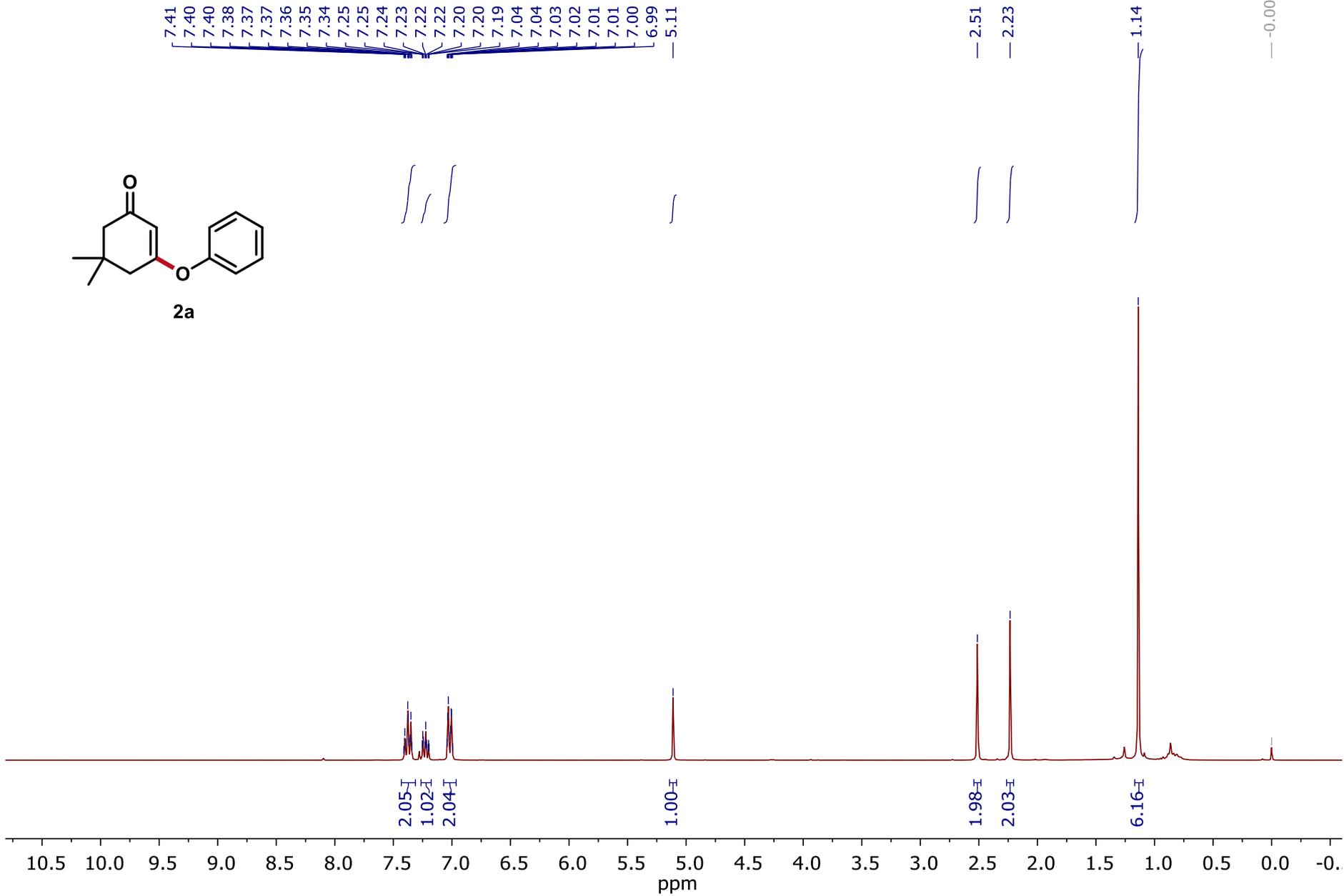
11



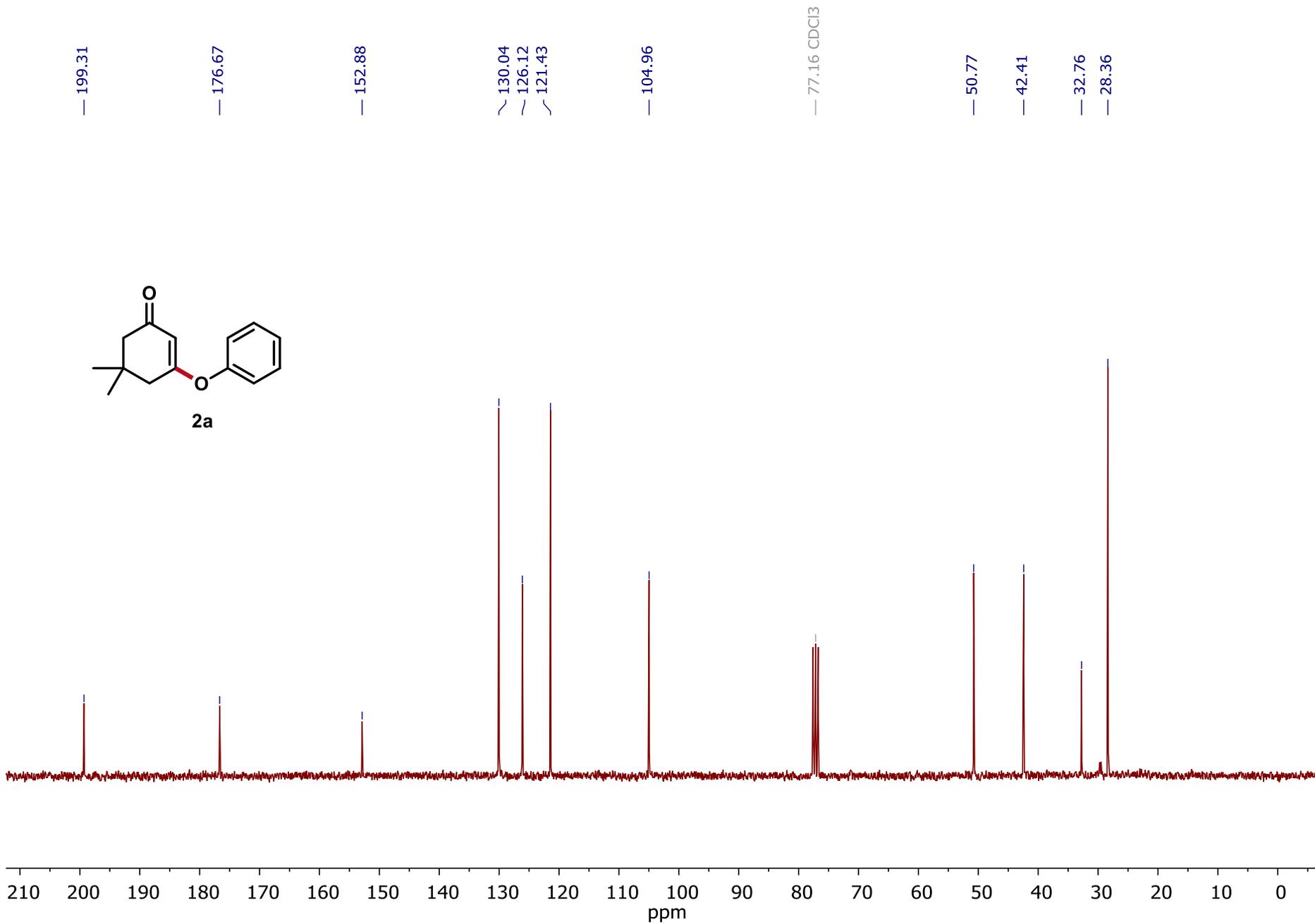
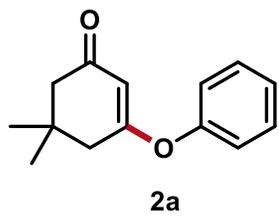
¹³C NMR of 11 (75 MHz, CDCl₃)
SI252



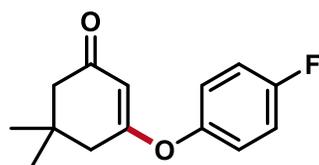
2a



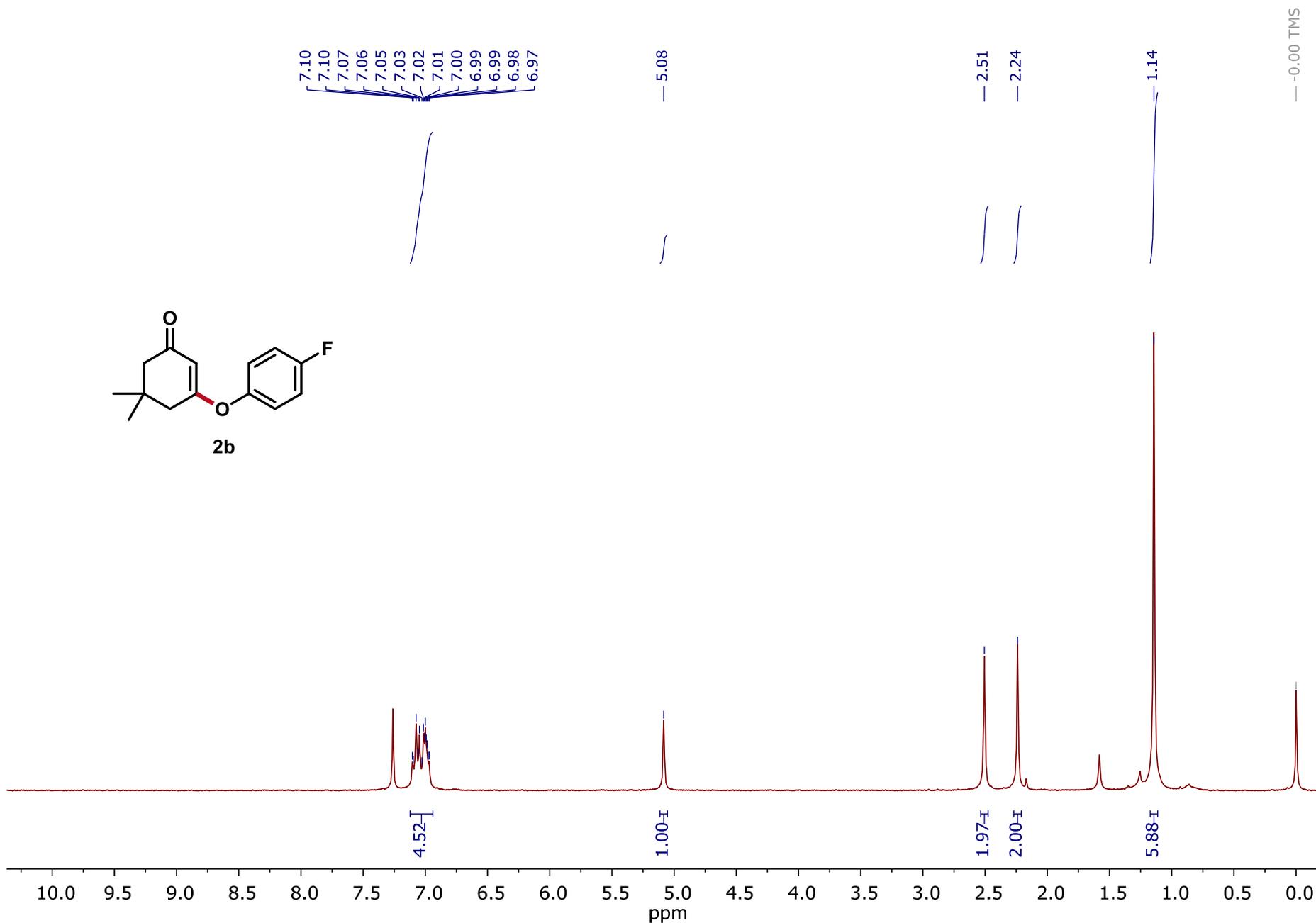
¹H NMR of 2a (300 MHz, CDCl₃)
SI253



^{13}C NMR of **2a** (75 MHz, CDCl_3)
SI254

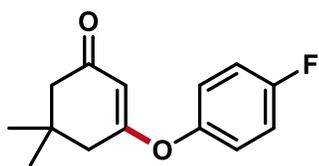


2b

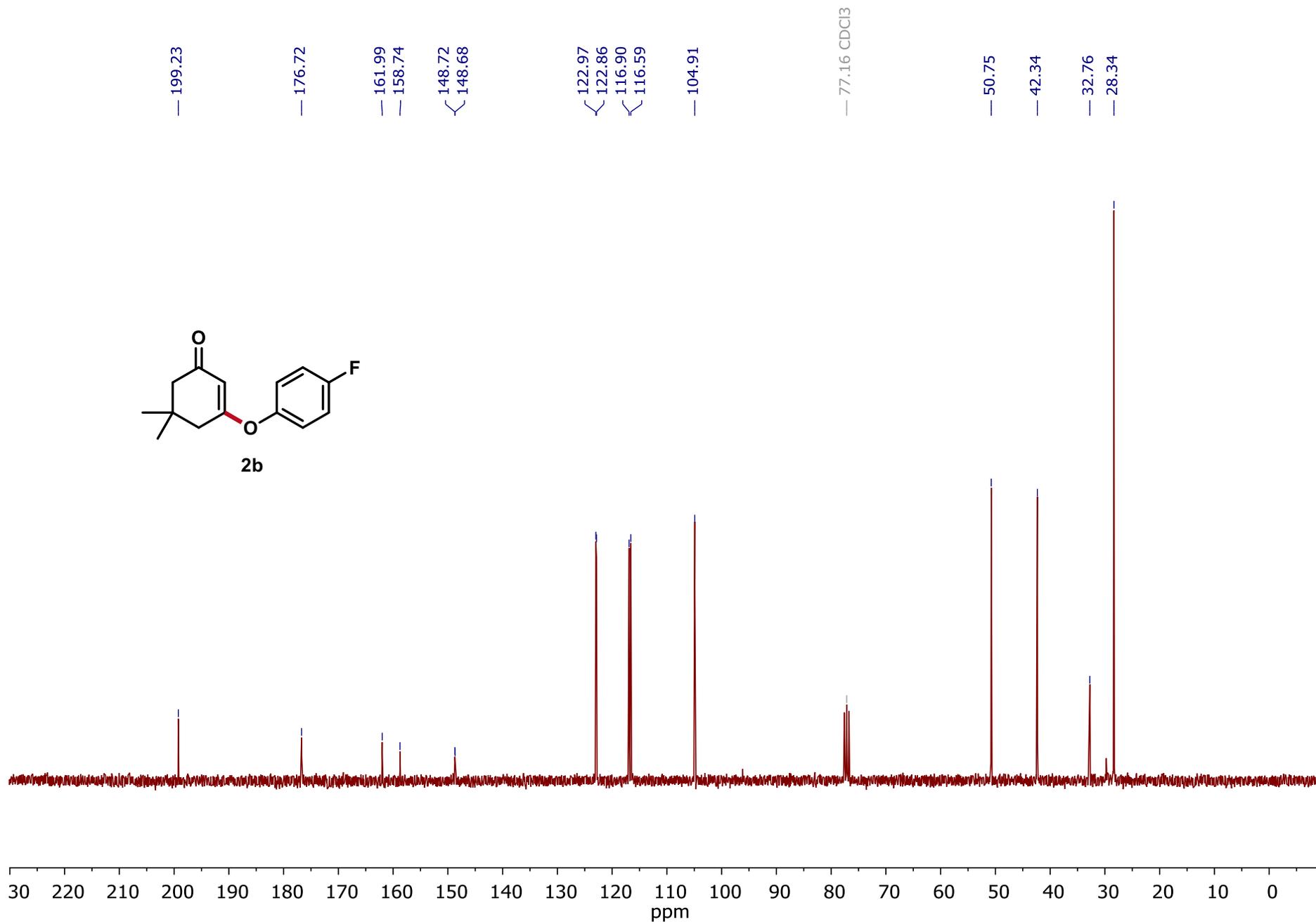


¹H NMR of 2b (300 MHz, CDCl₃)

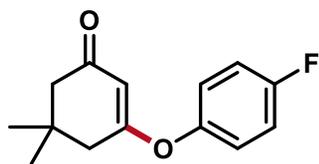
SI255



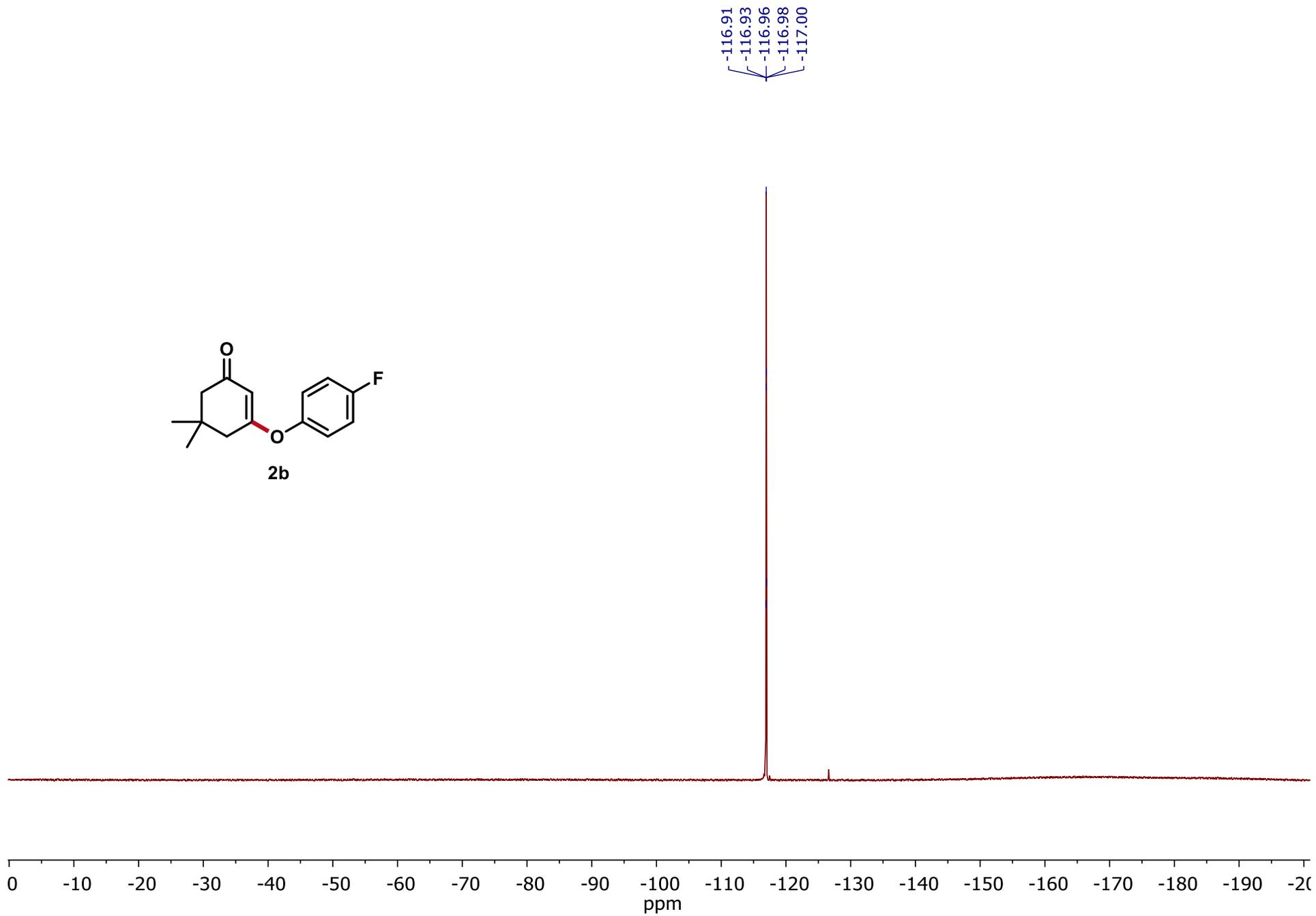
2b



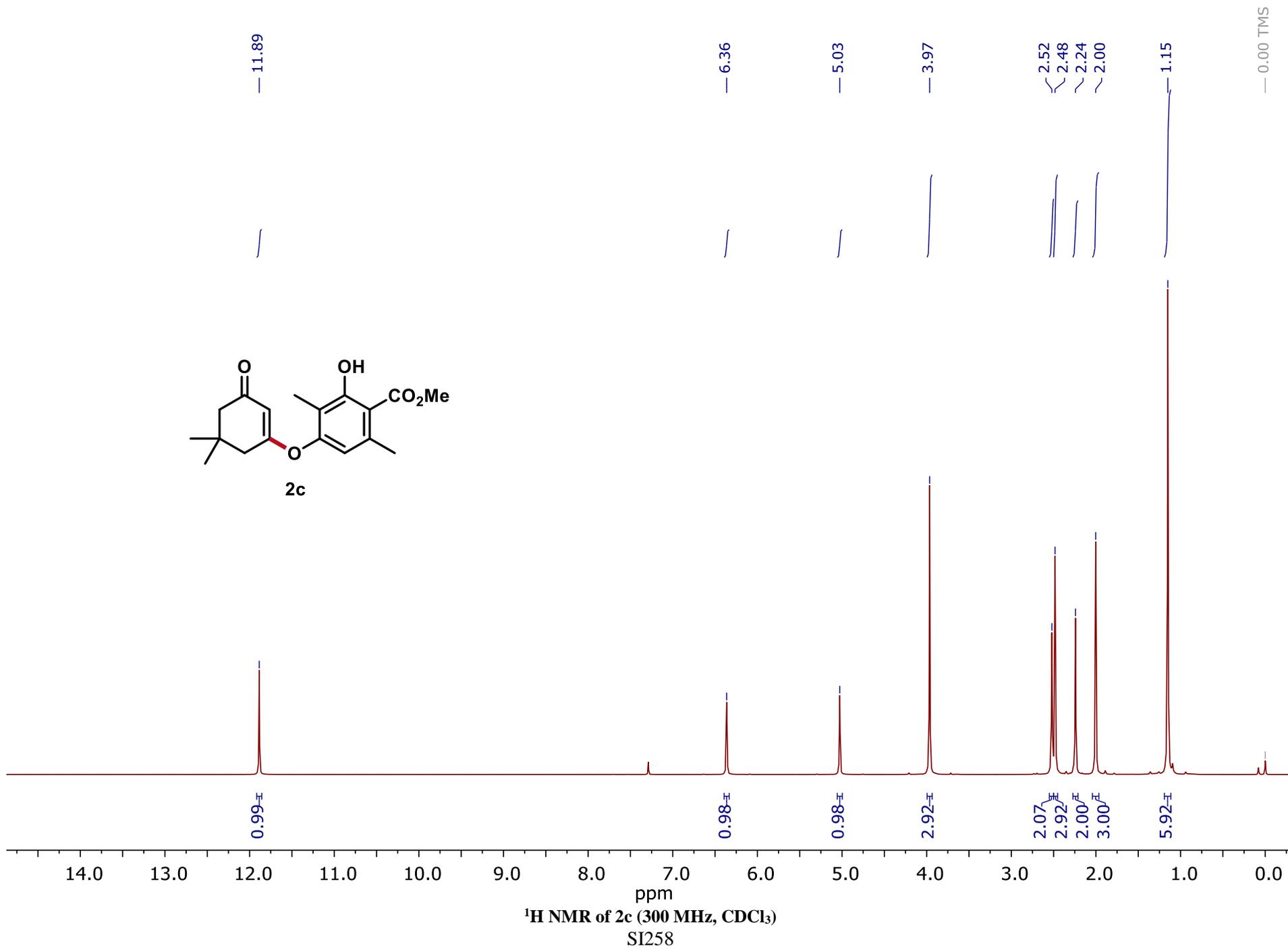
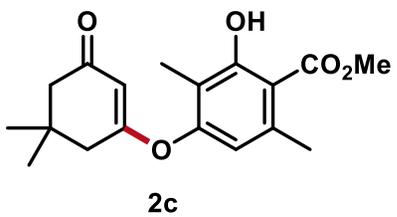
^{13}C NMR of 2b (75 MHz, CDCl_3)
SI256

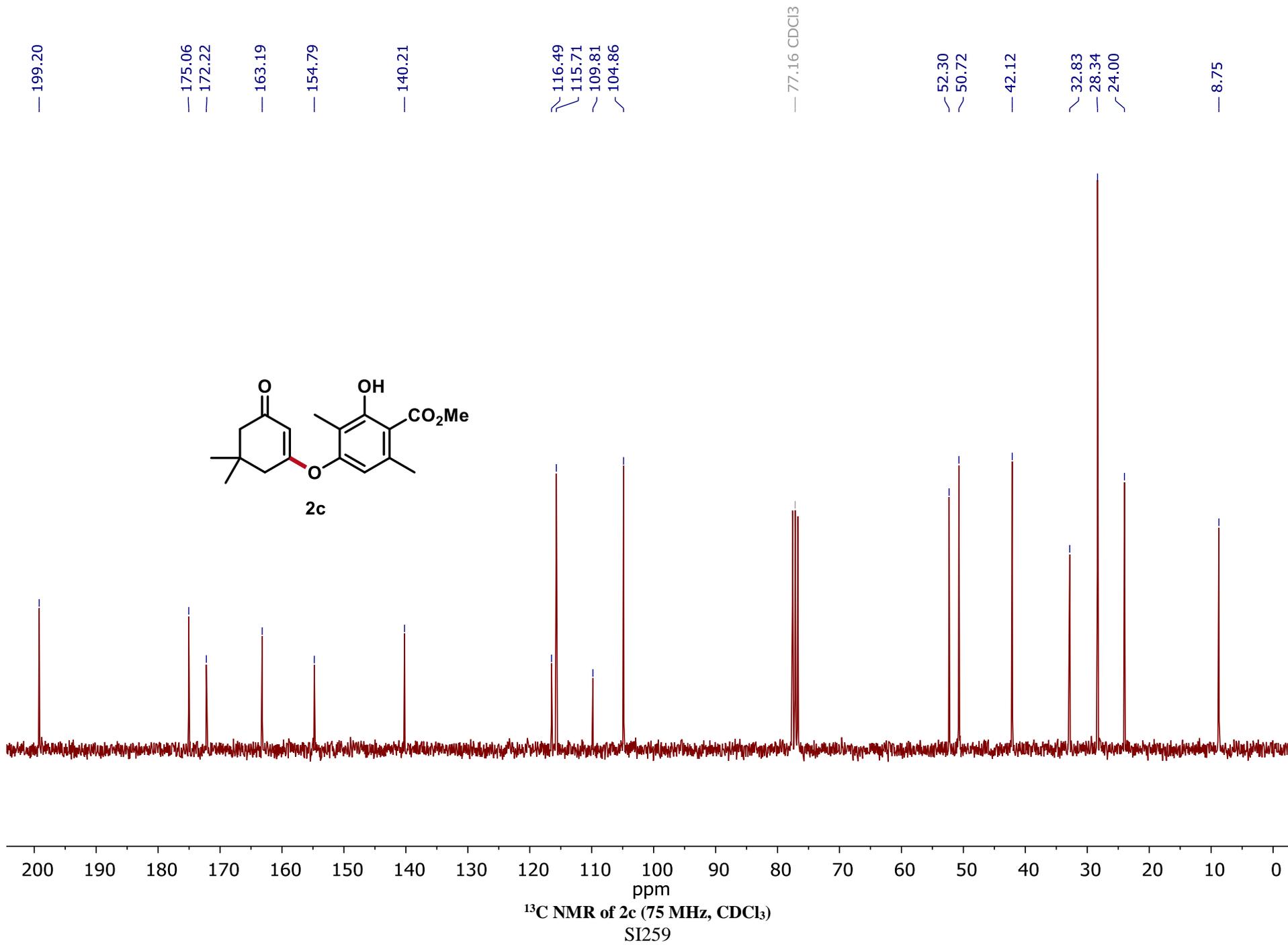


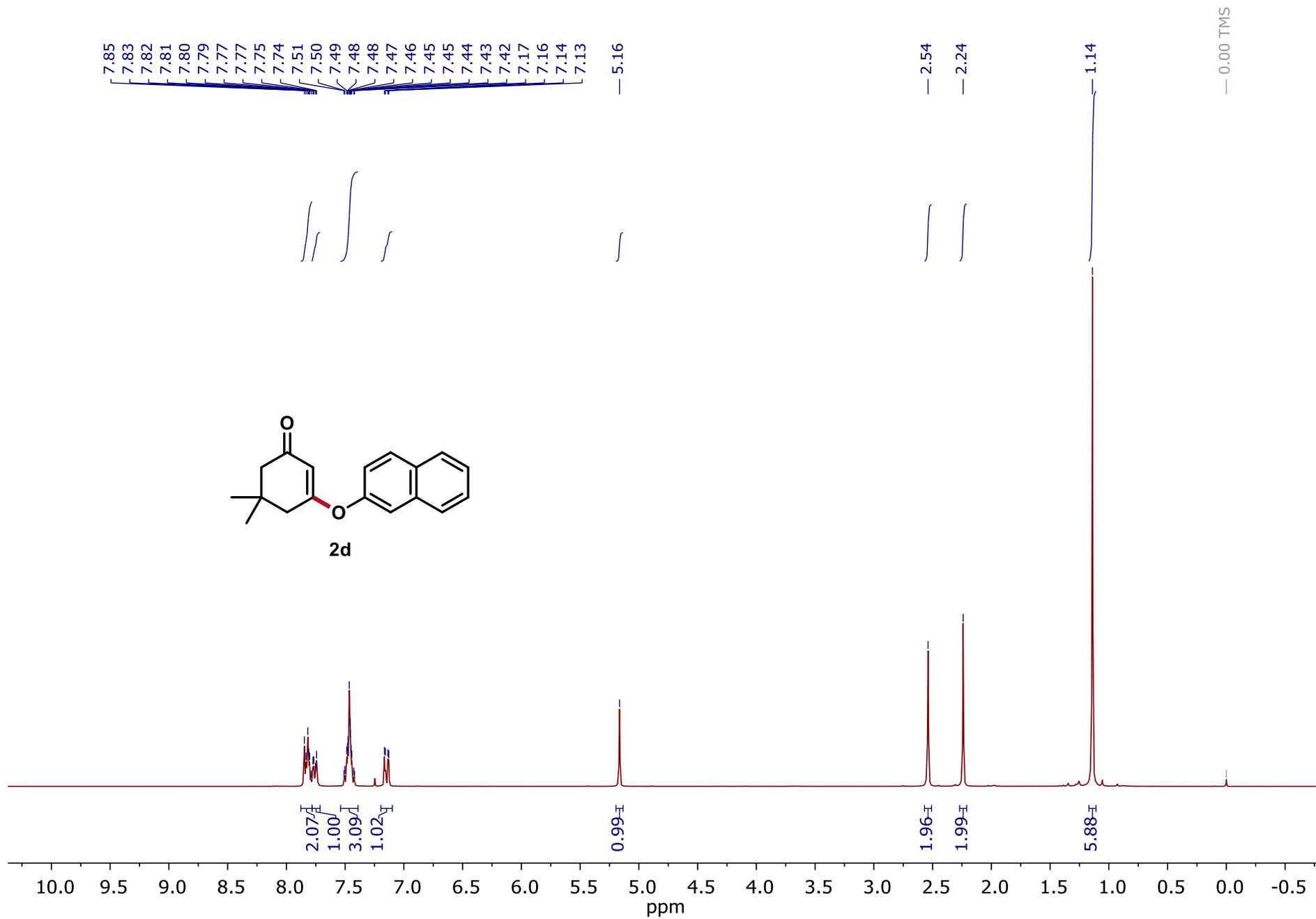
2b



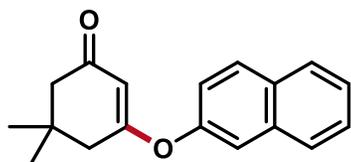
^{19}F NMR of 2b (282 MHz, CDCl_3)
SI257



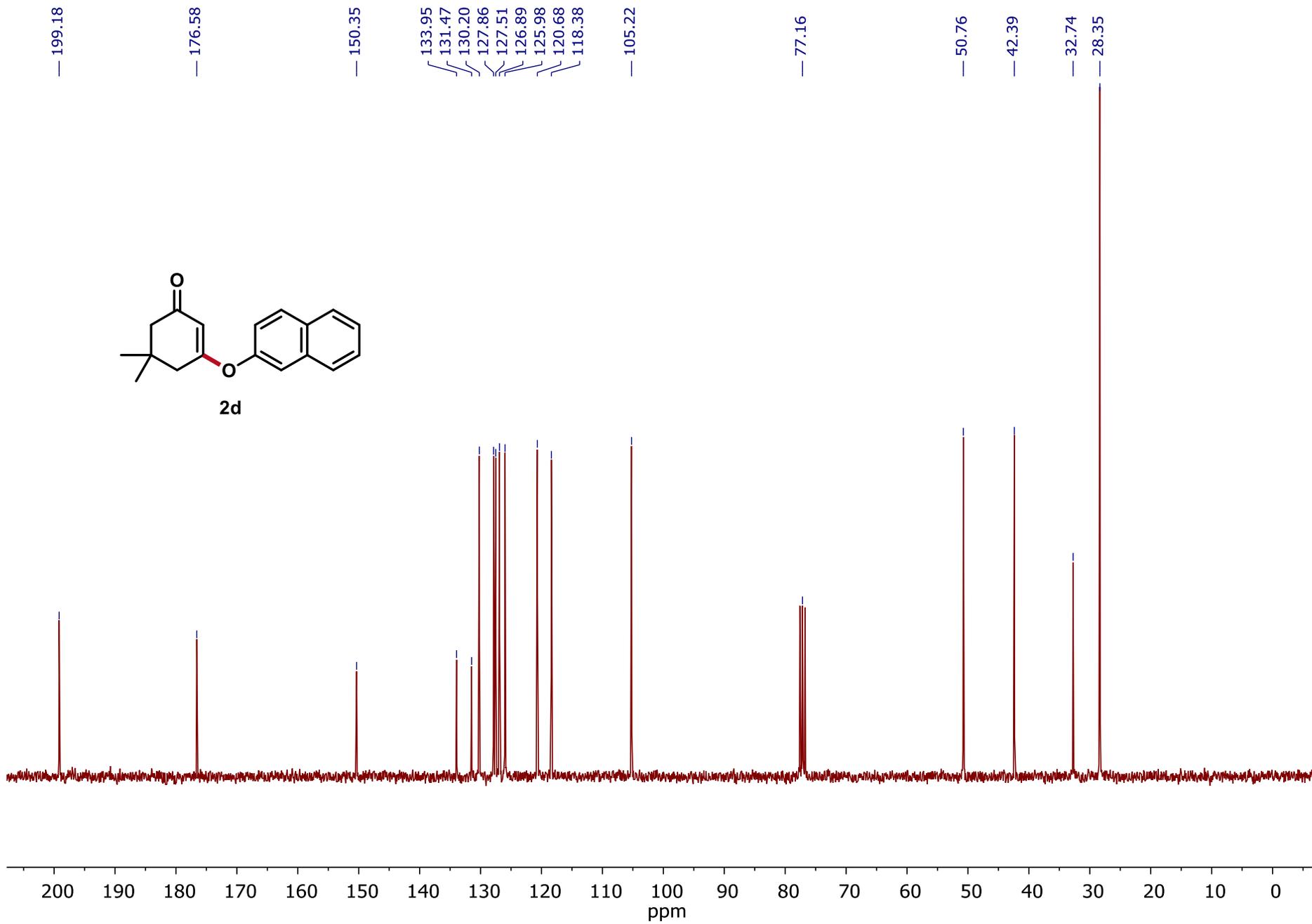




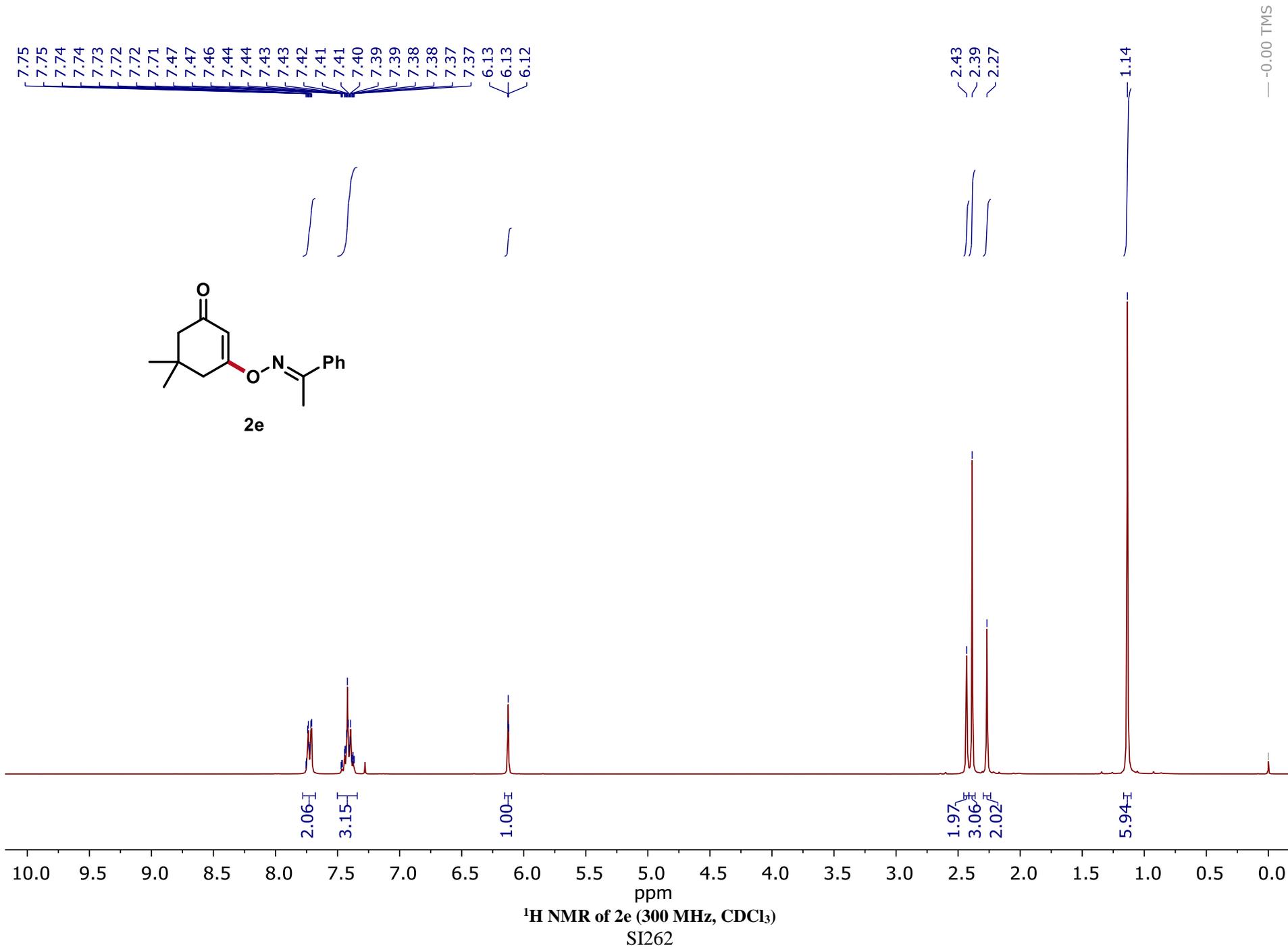
¹H NMR of 2d (300 MHz, CDCl₃)
SI260

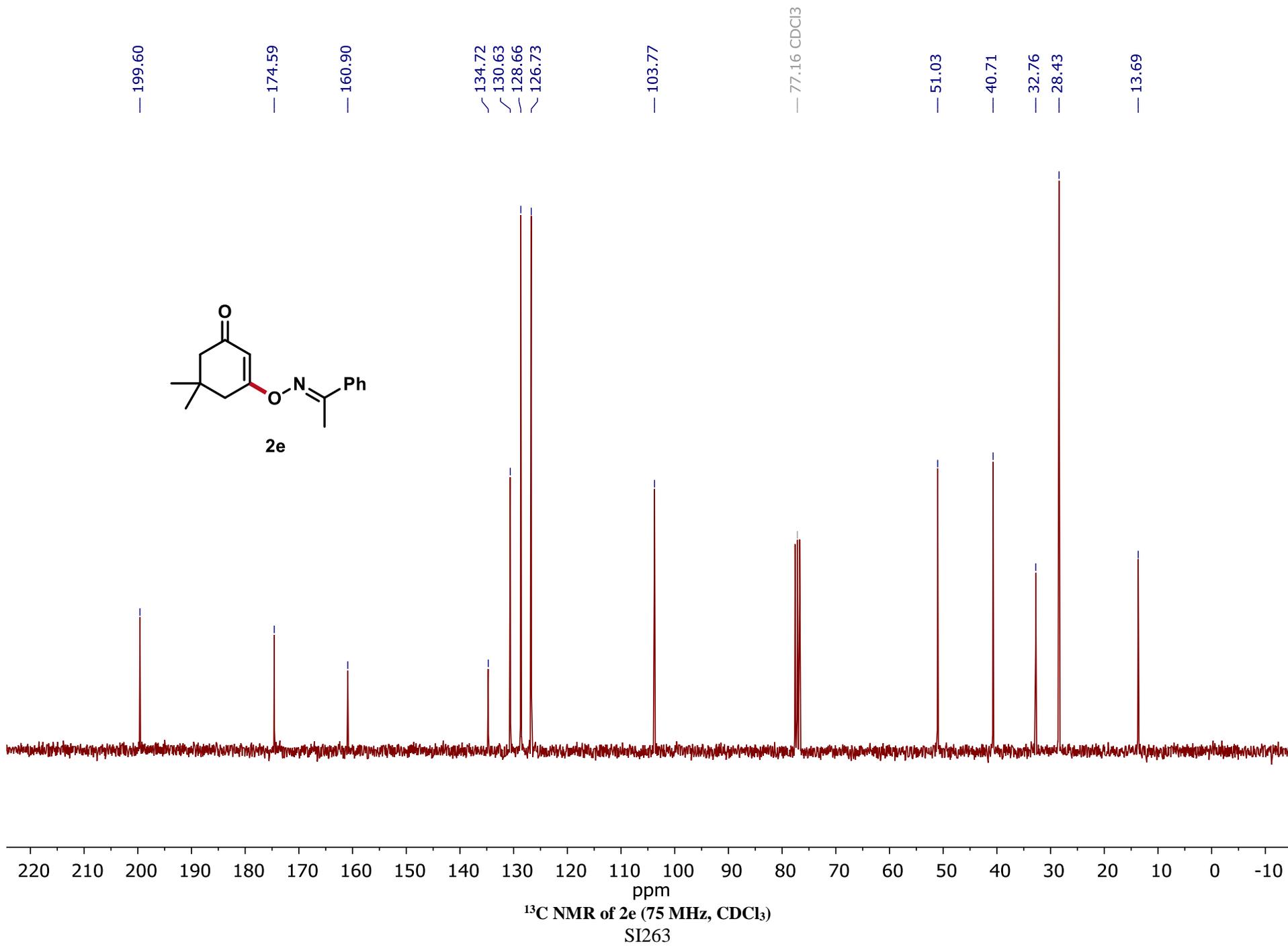
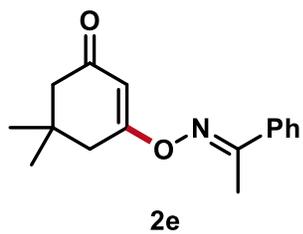


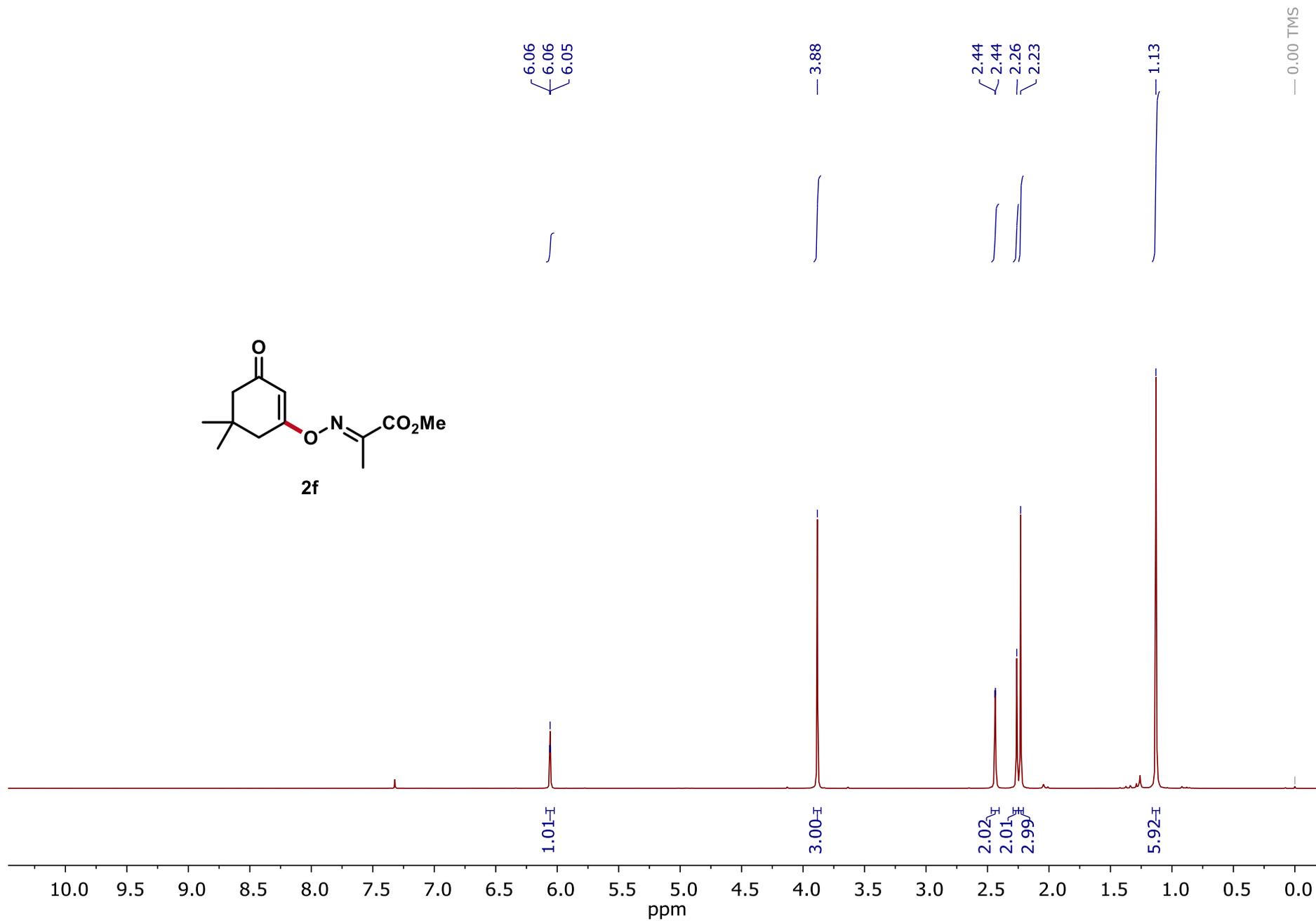
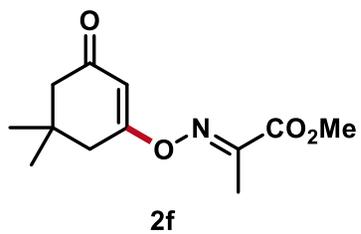
2d



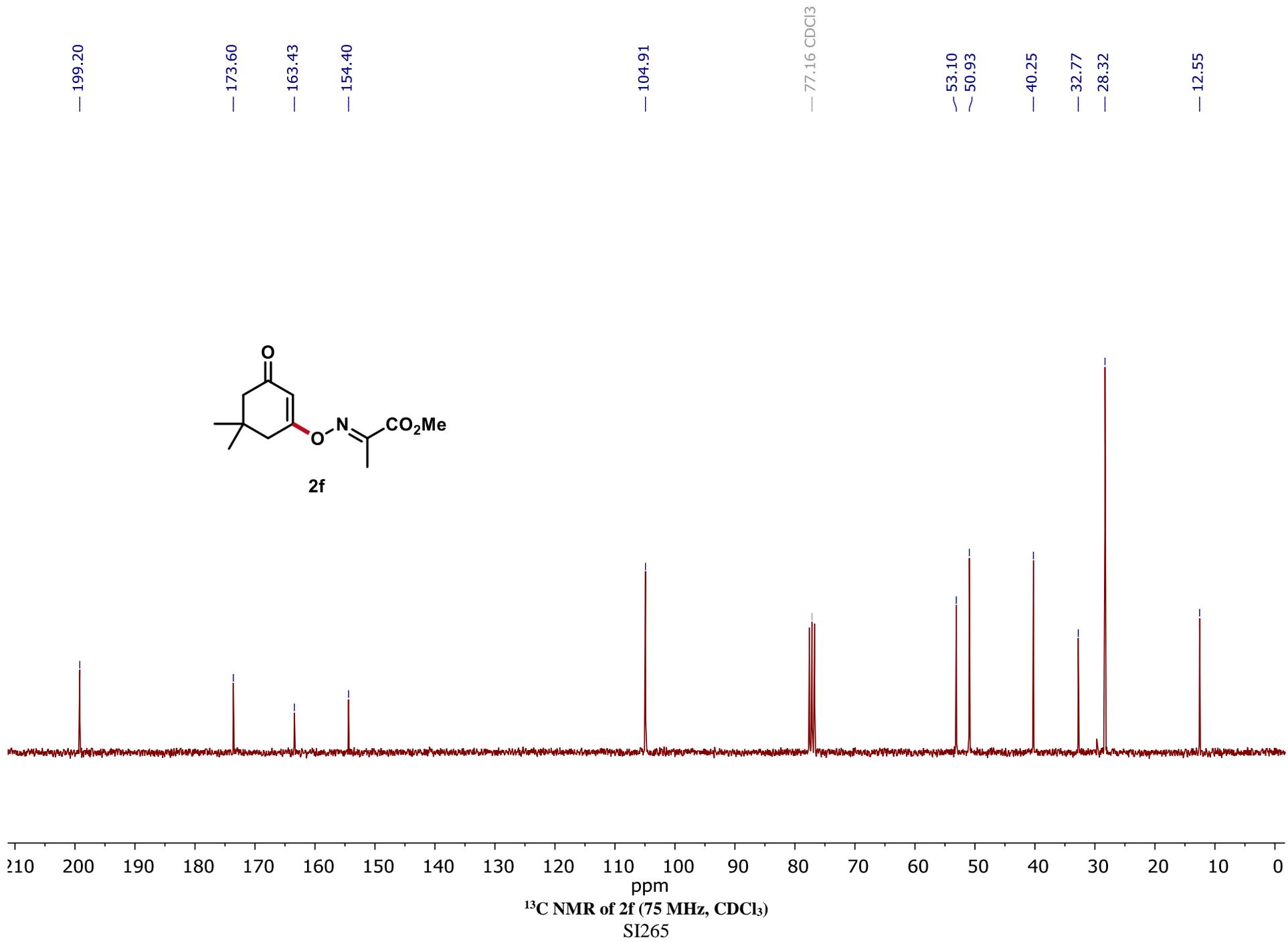
^{13}C NMR of 2d (75 MHz, CDCl_3)
SI261

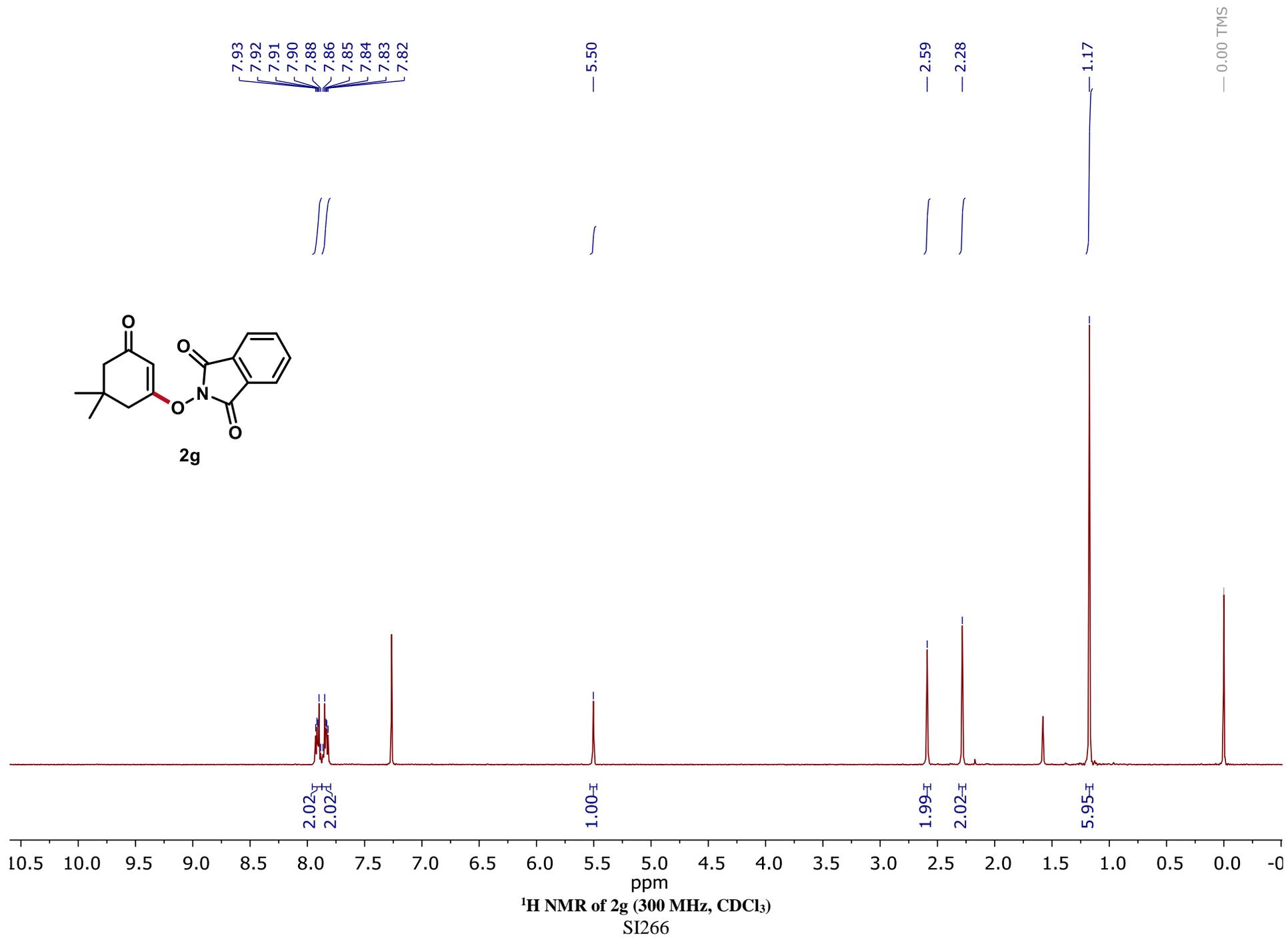
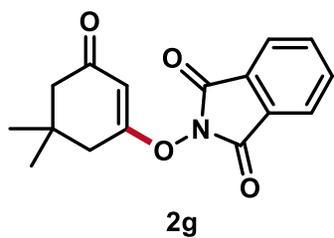


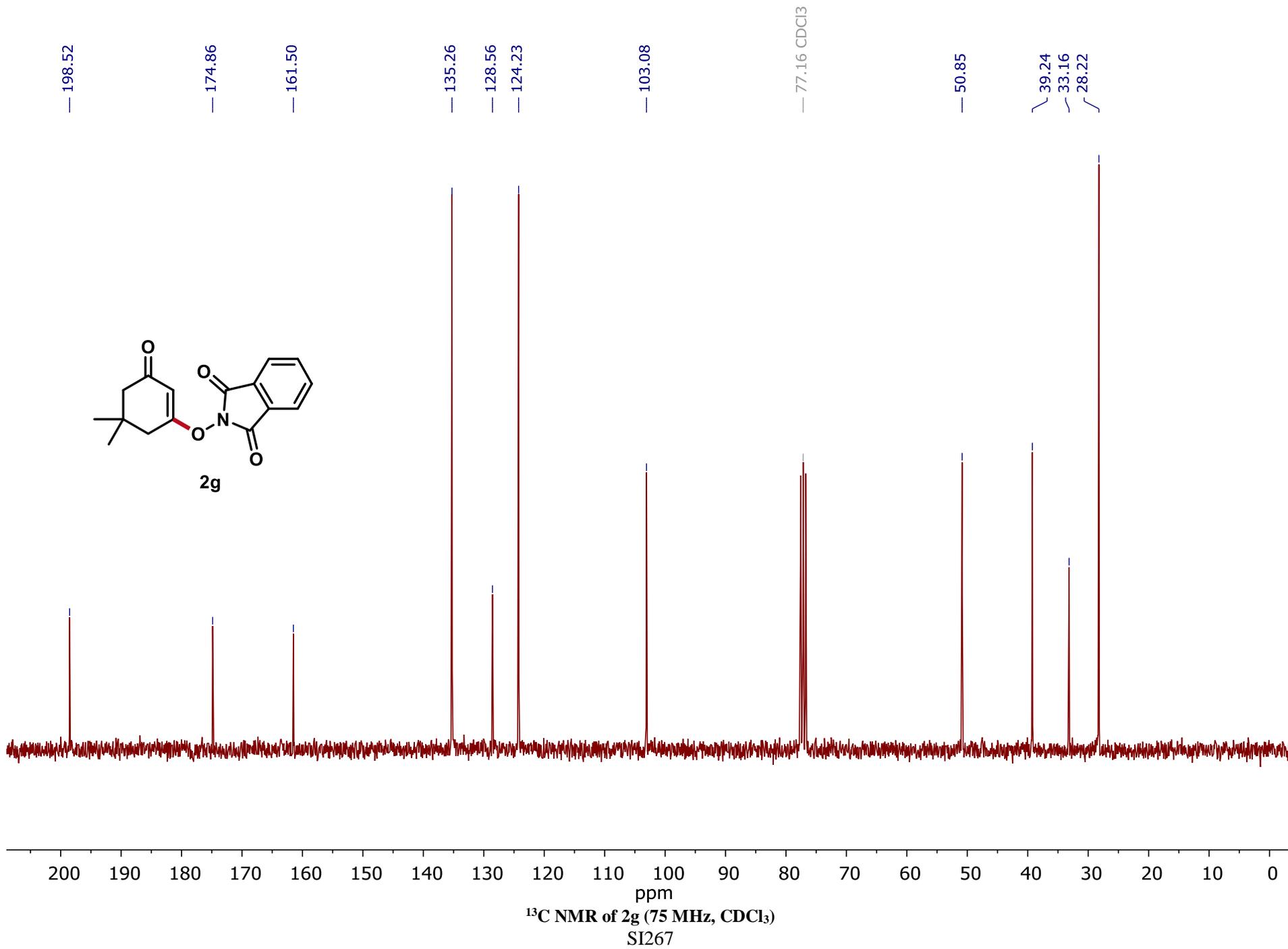


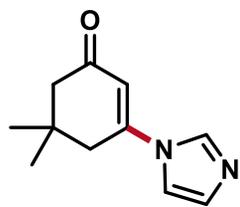


^1H NMR of **2f** (300 MHz, CDCl_3)
SI264

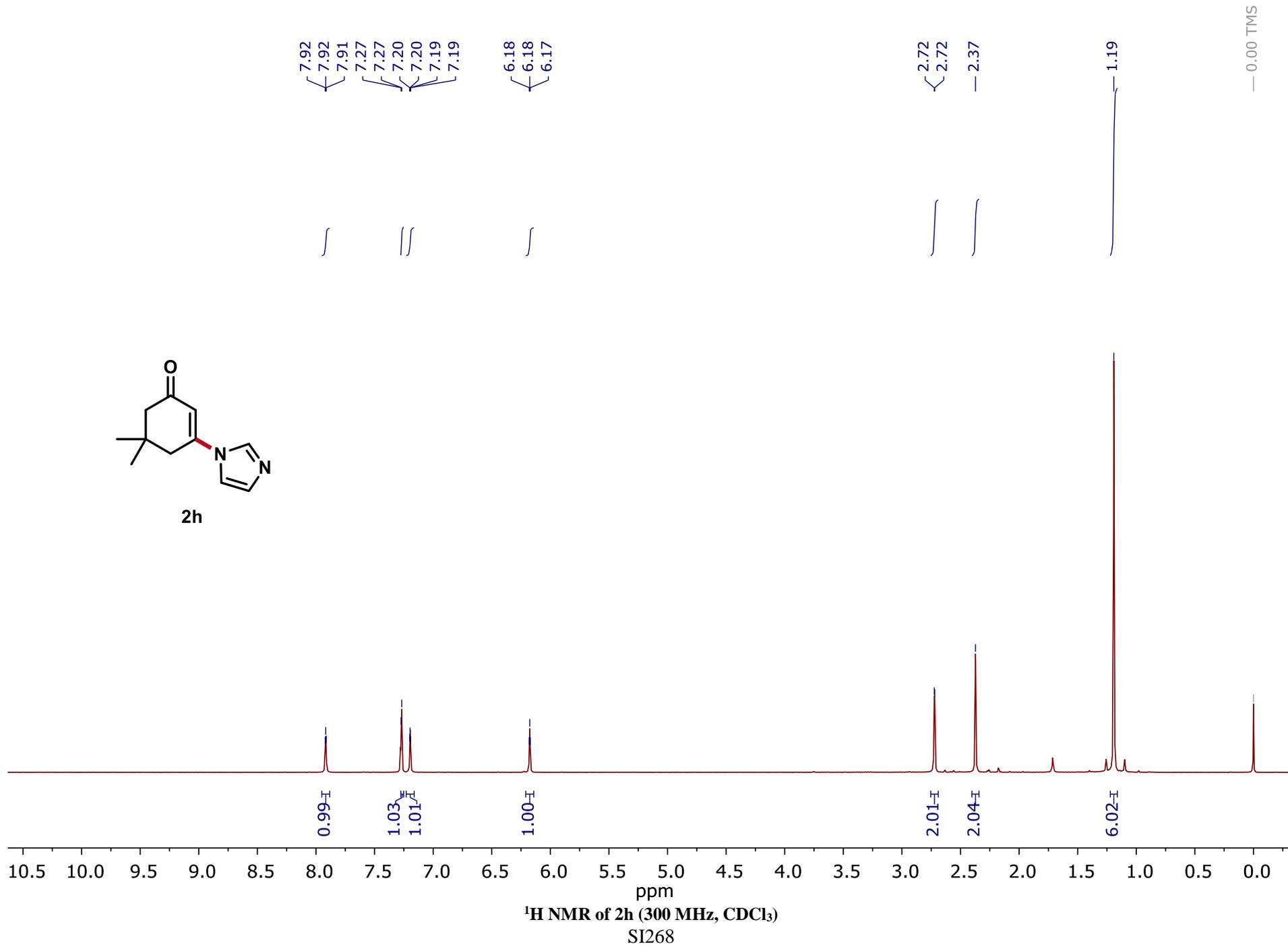


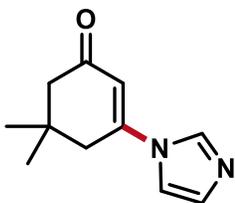




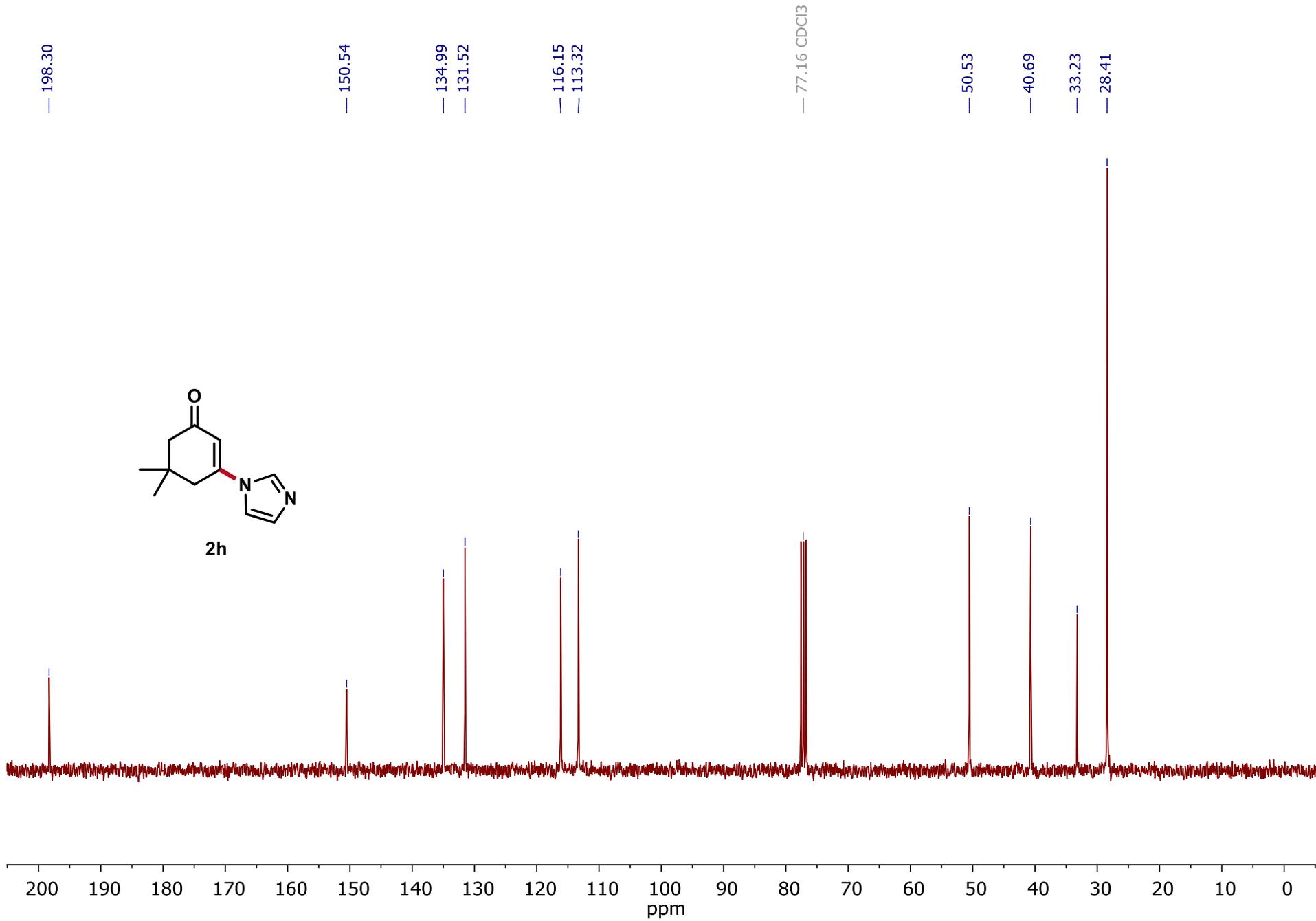


2h

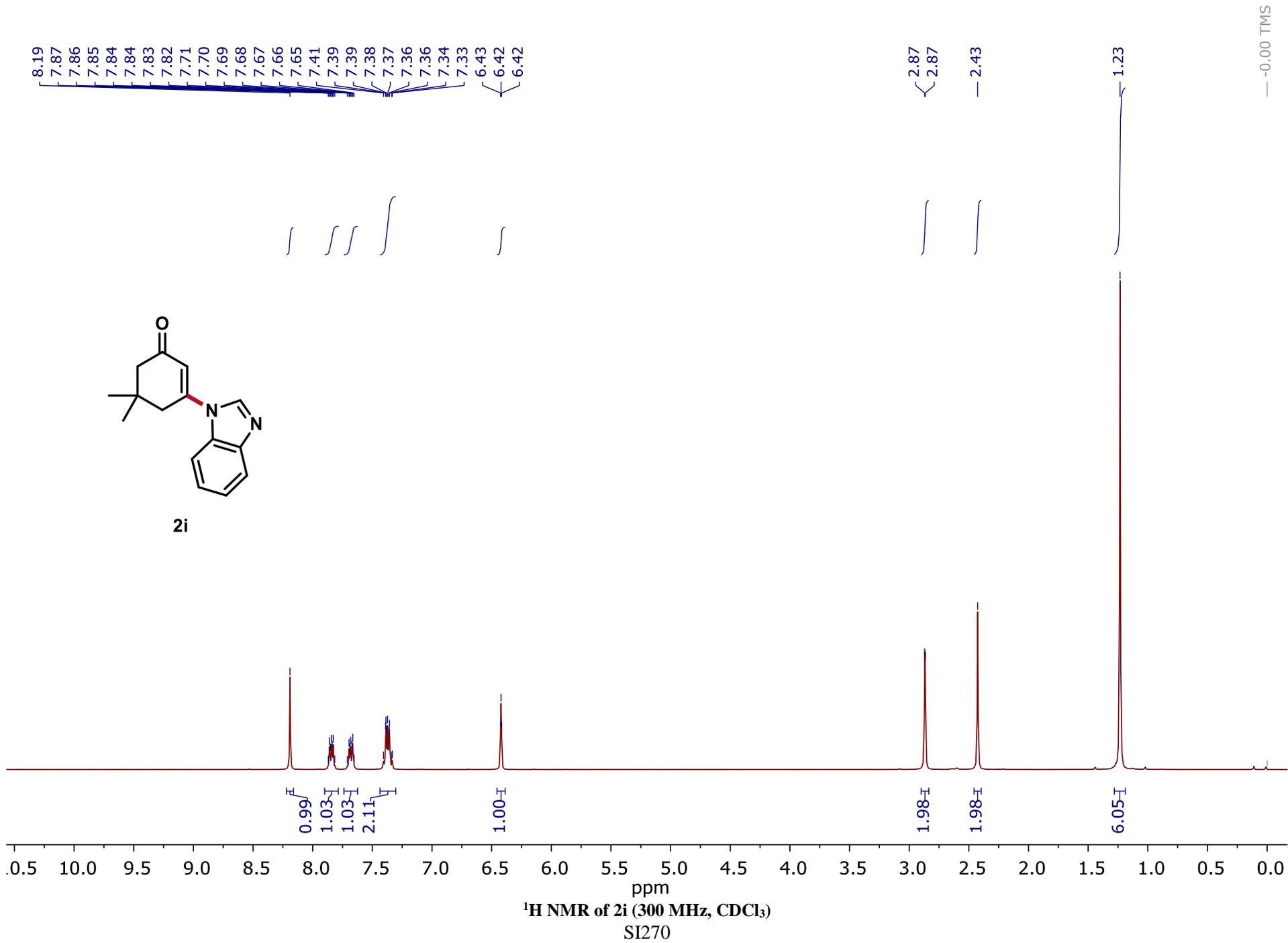


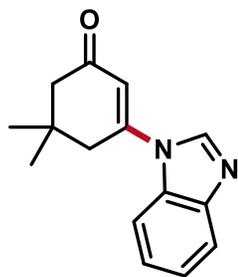


2h

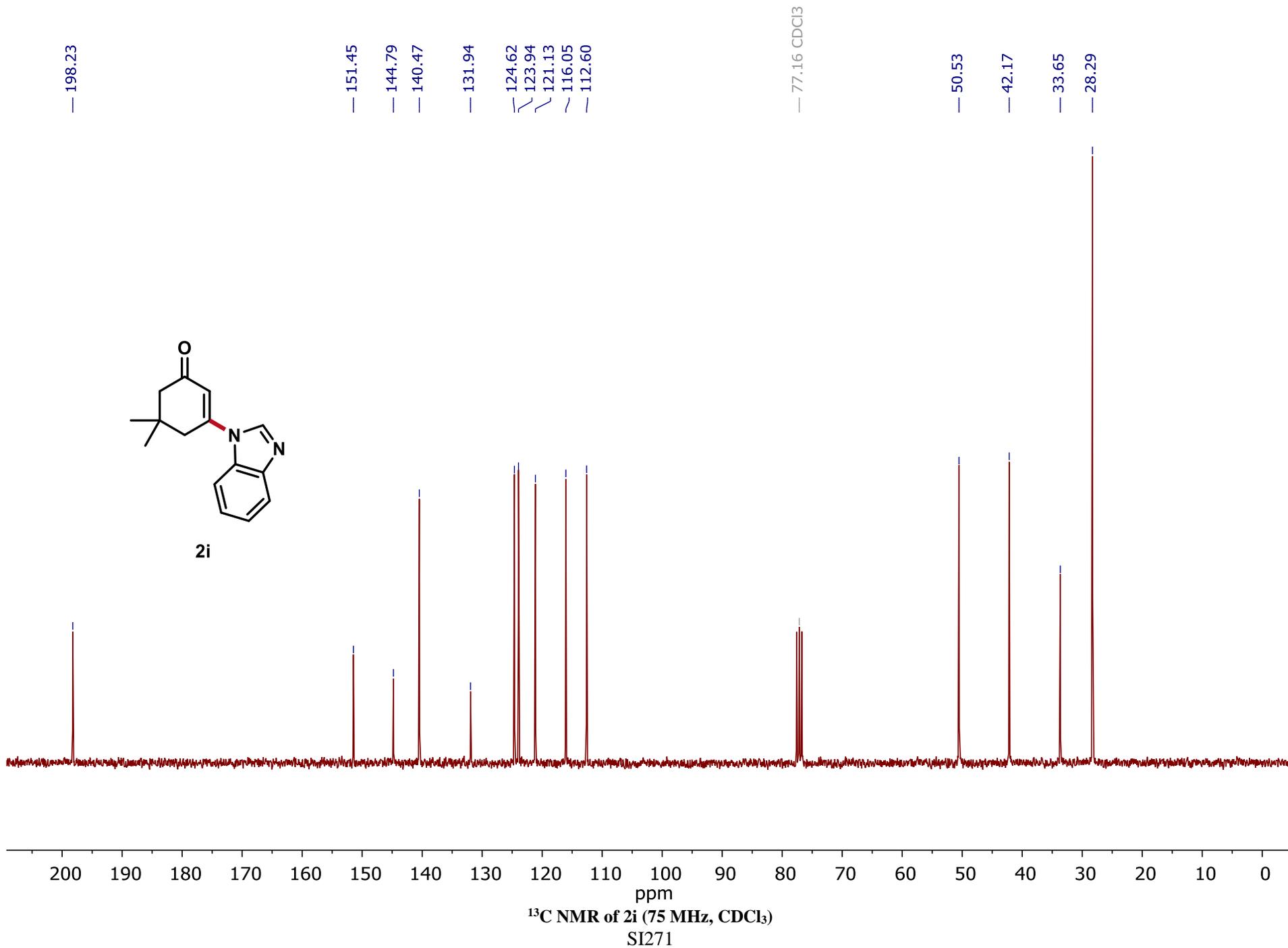


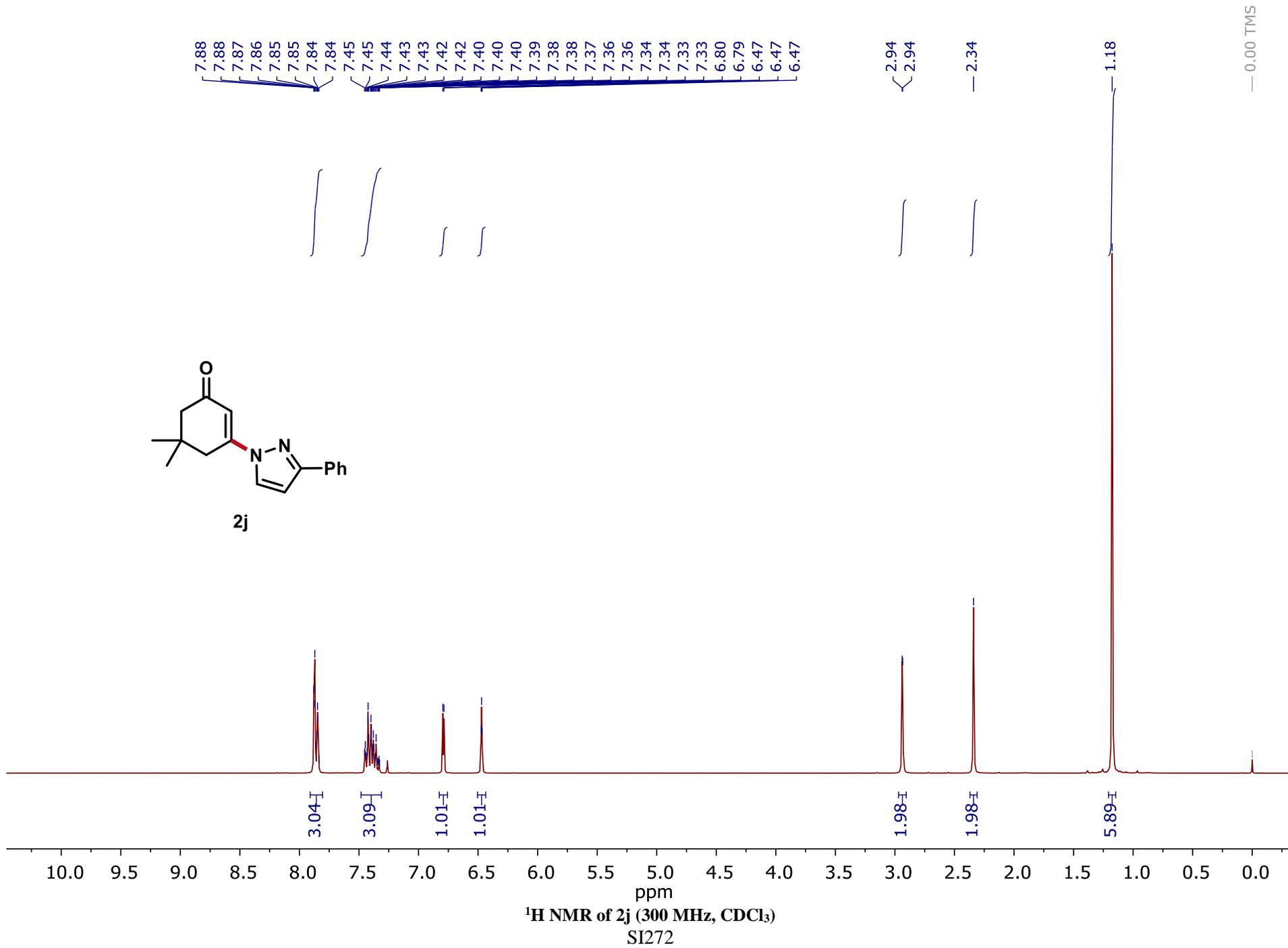
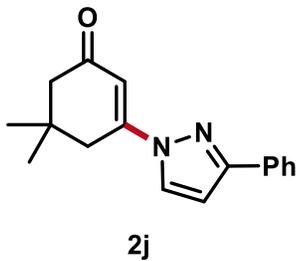
^{13}C NMR of 2h (75 MHz, CDCl_3)
SI269

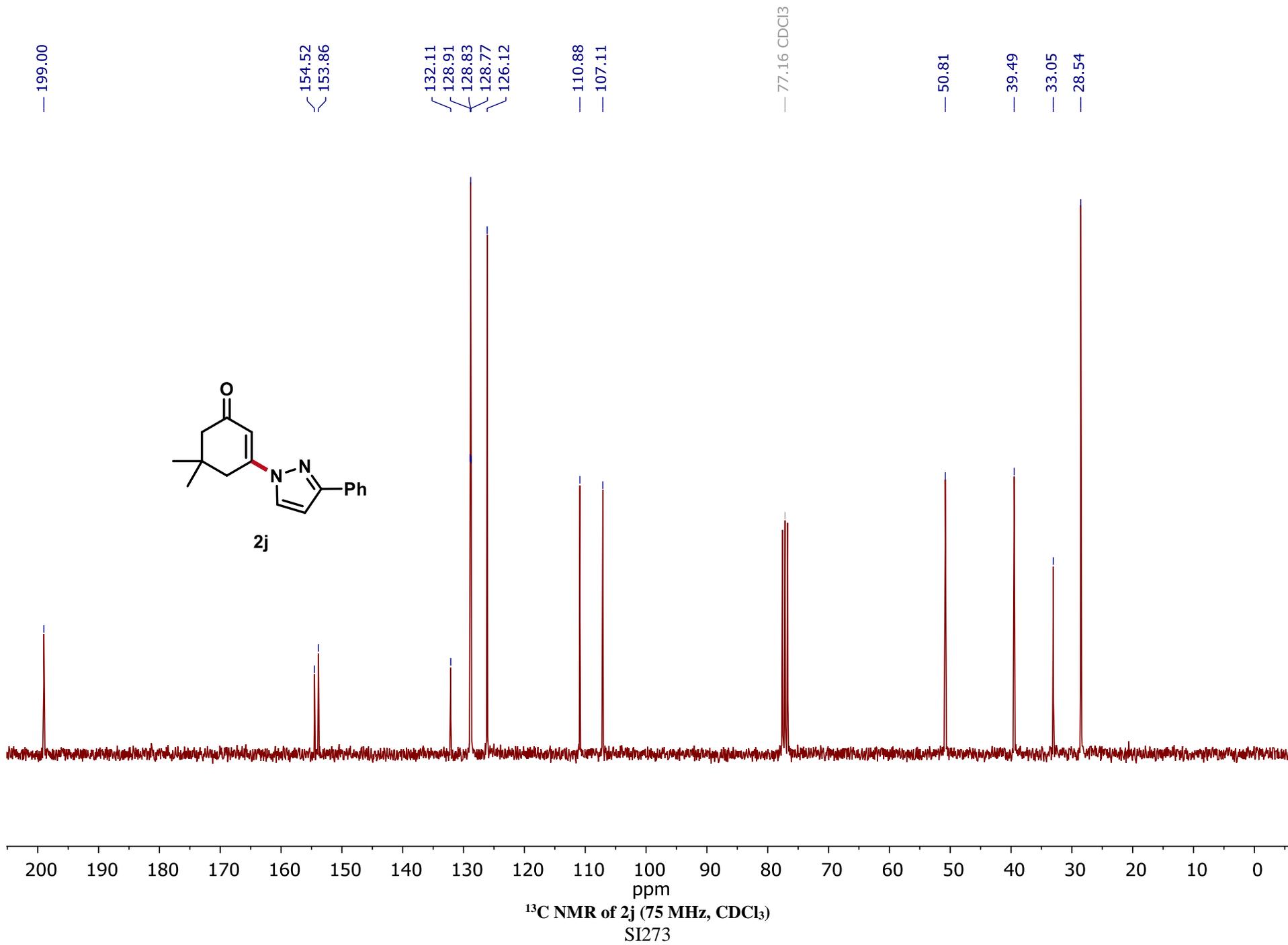


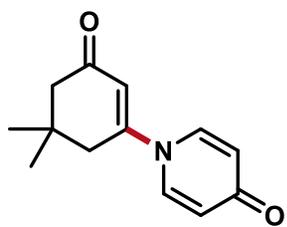


2i

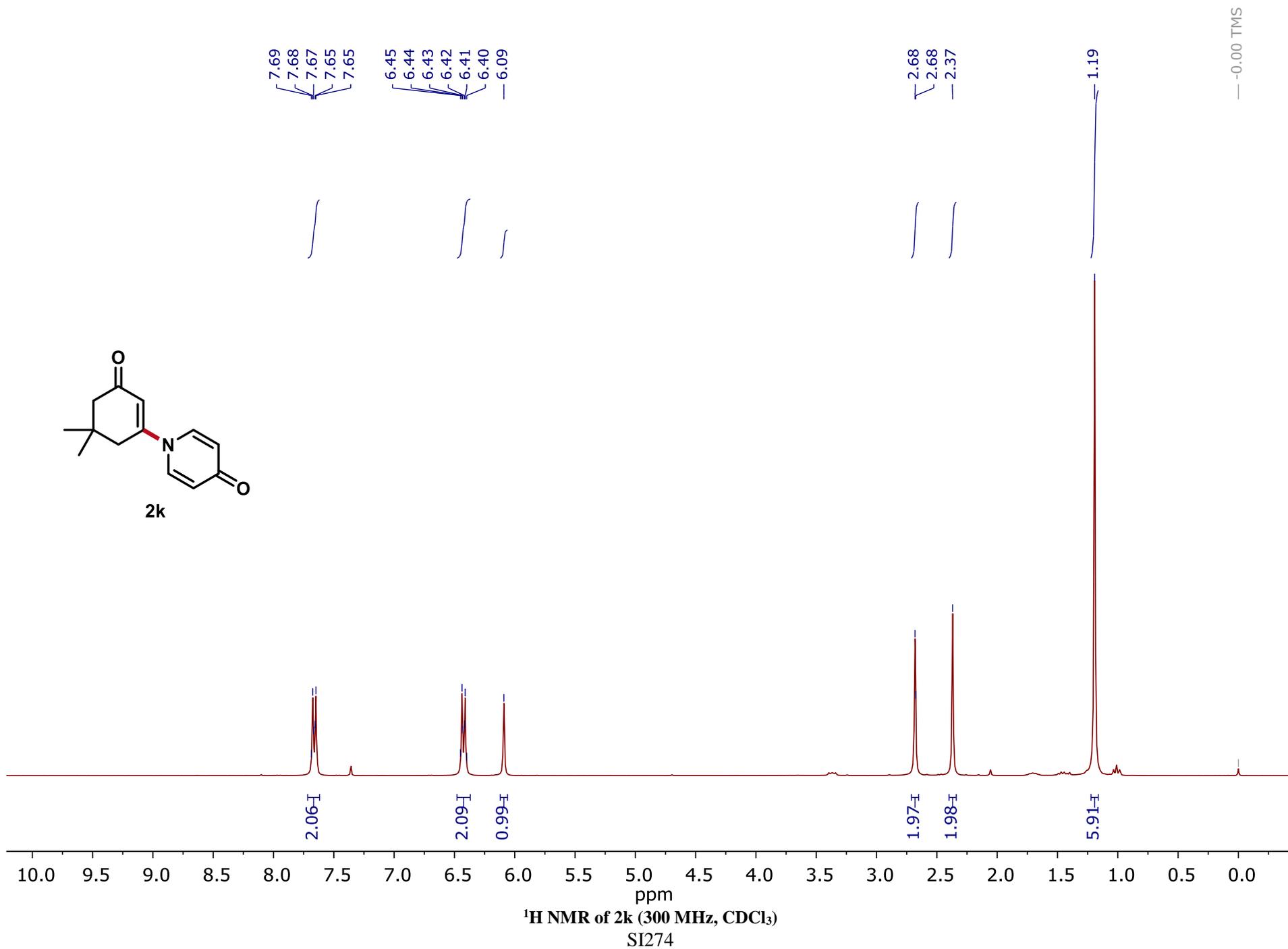


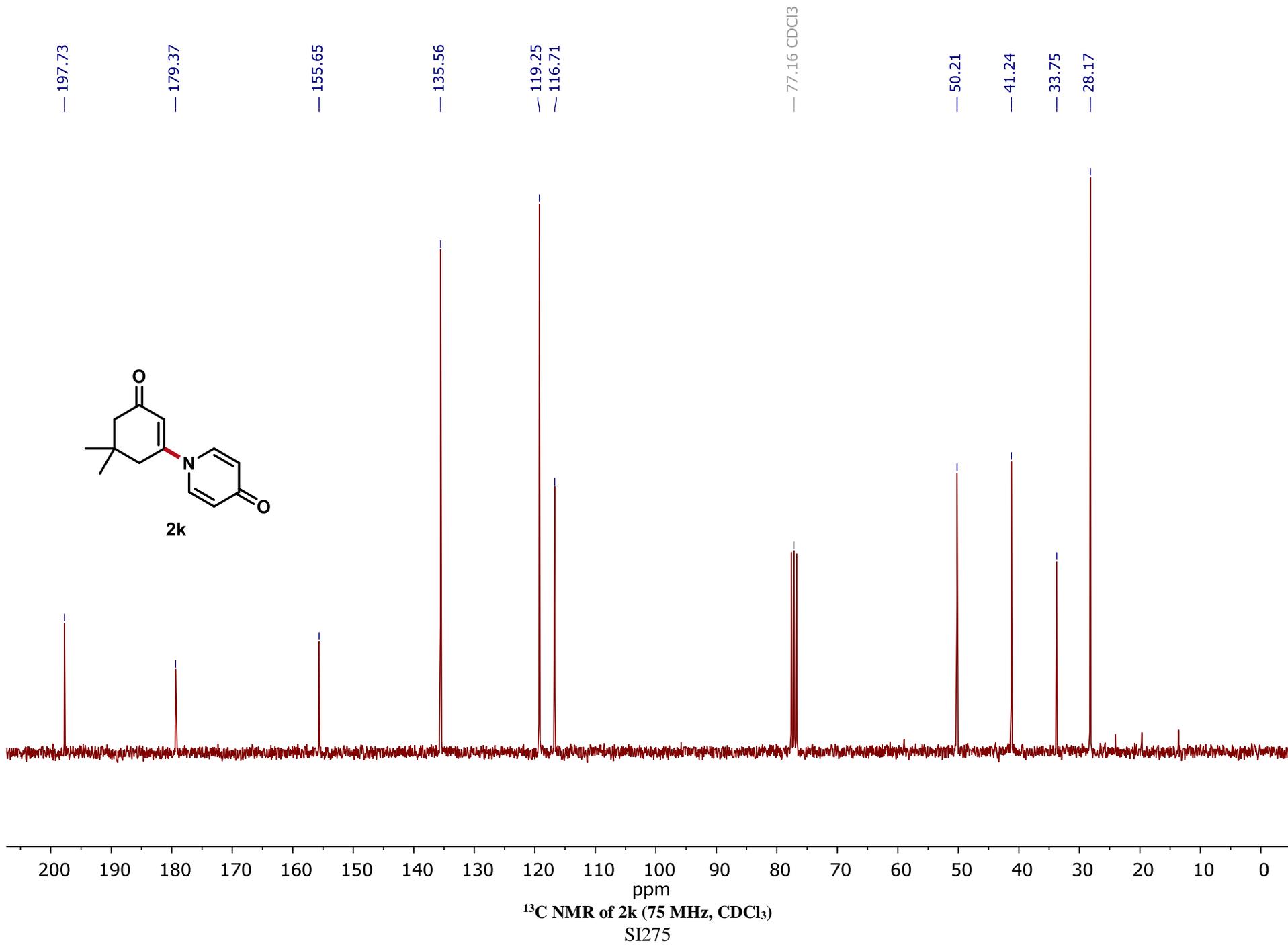


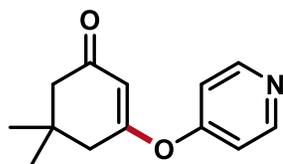




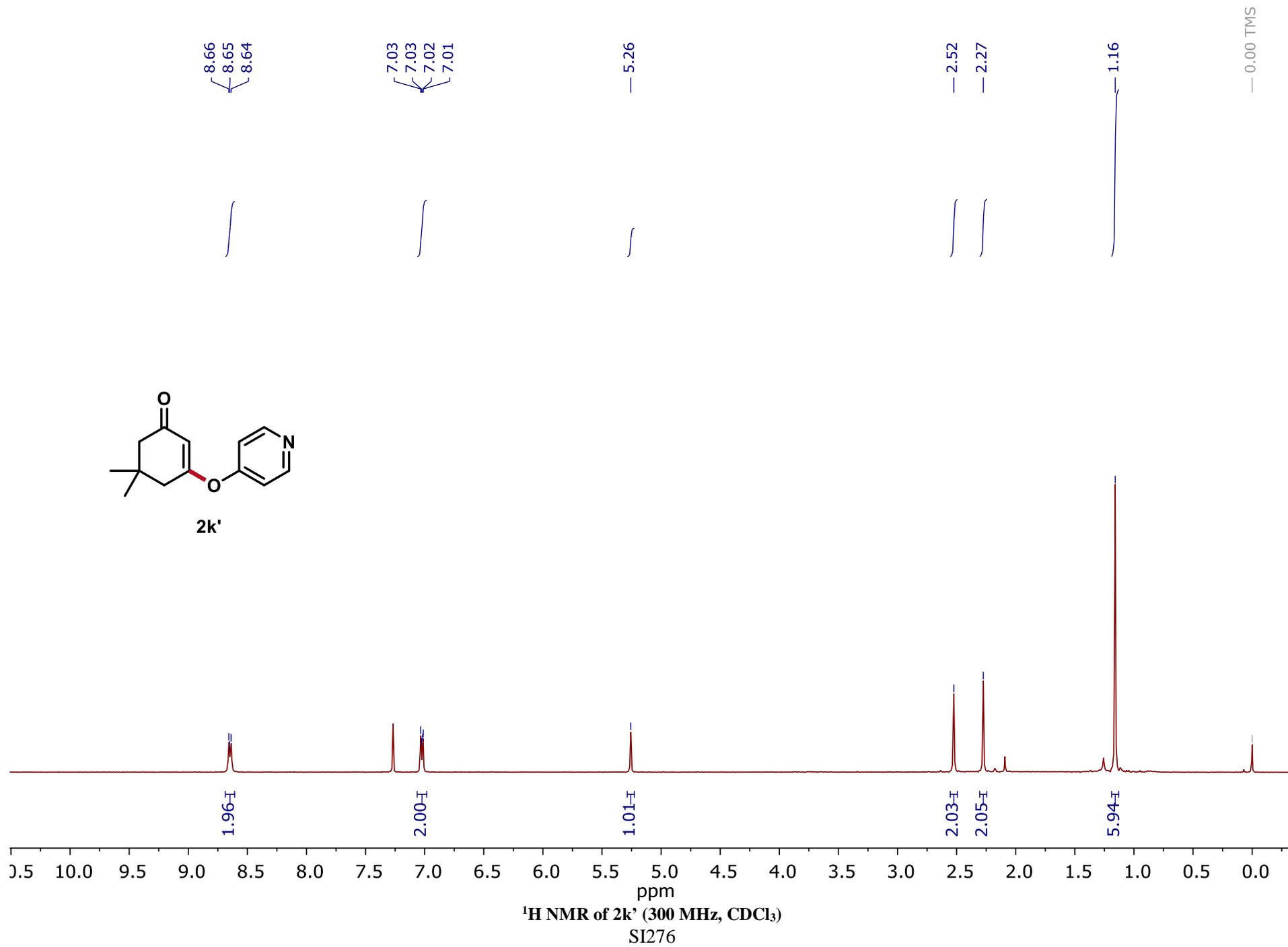
2k

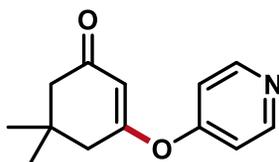




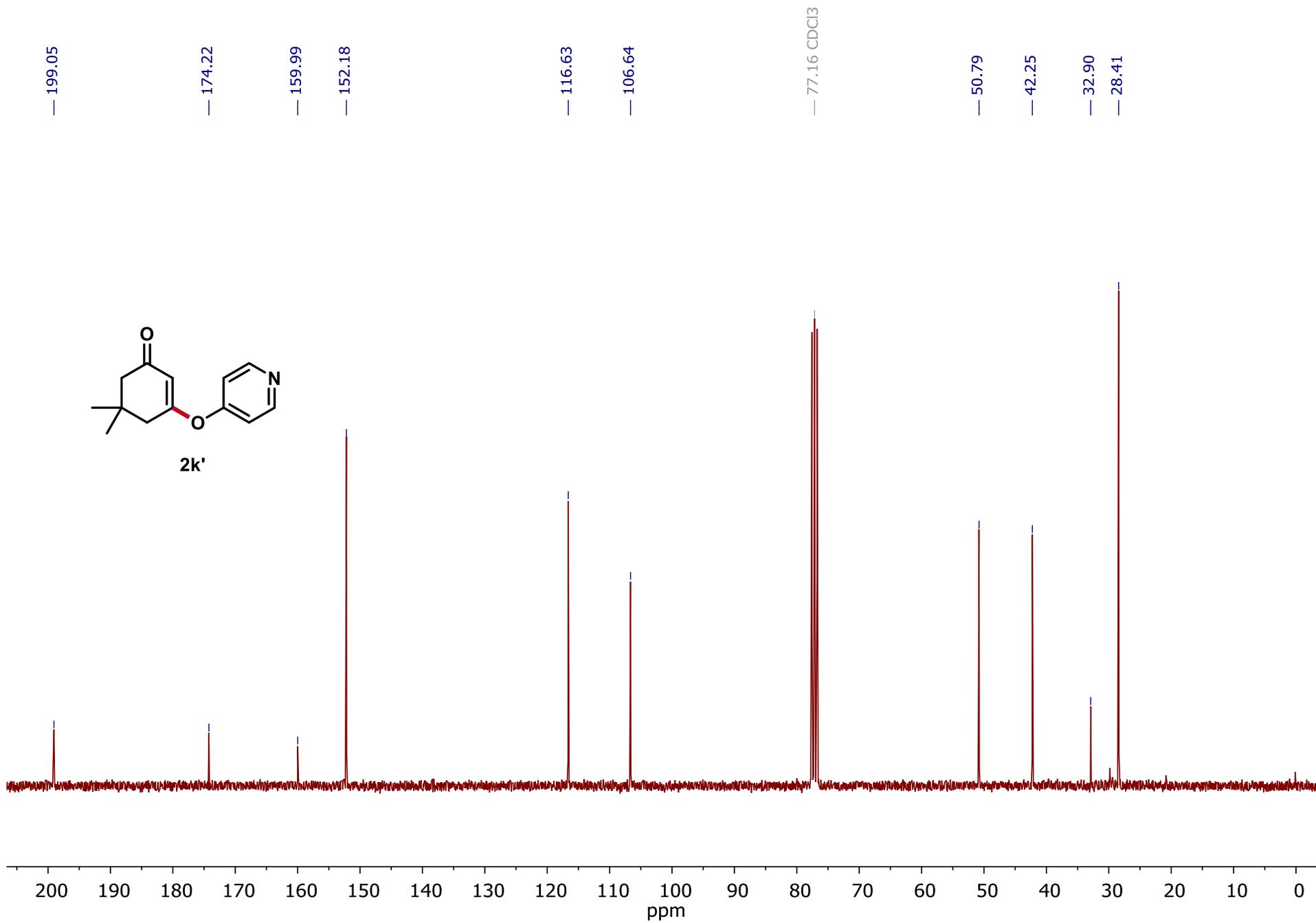


2k'

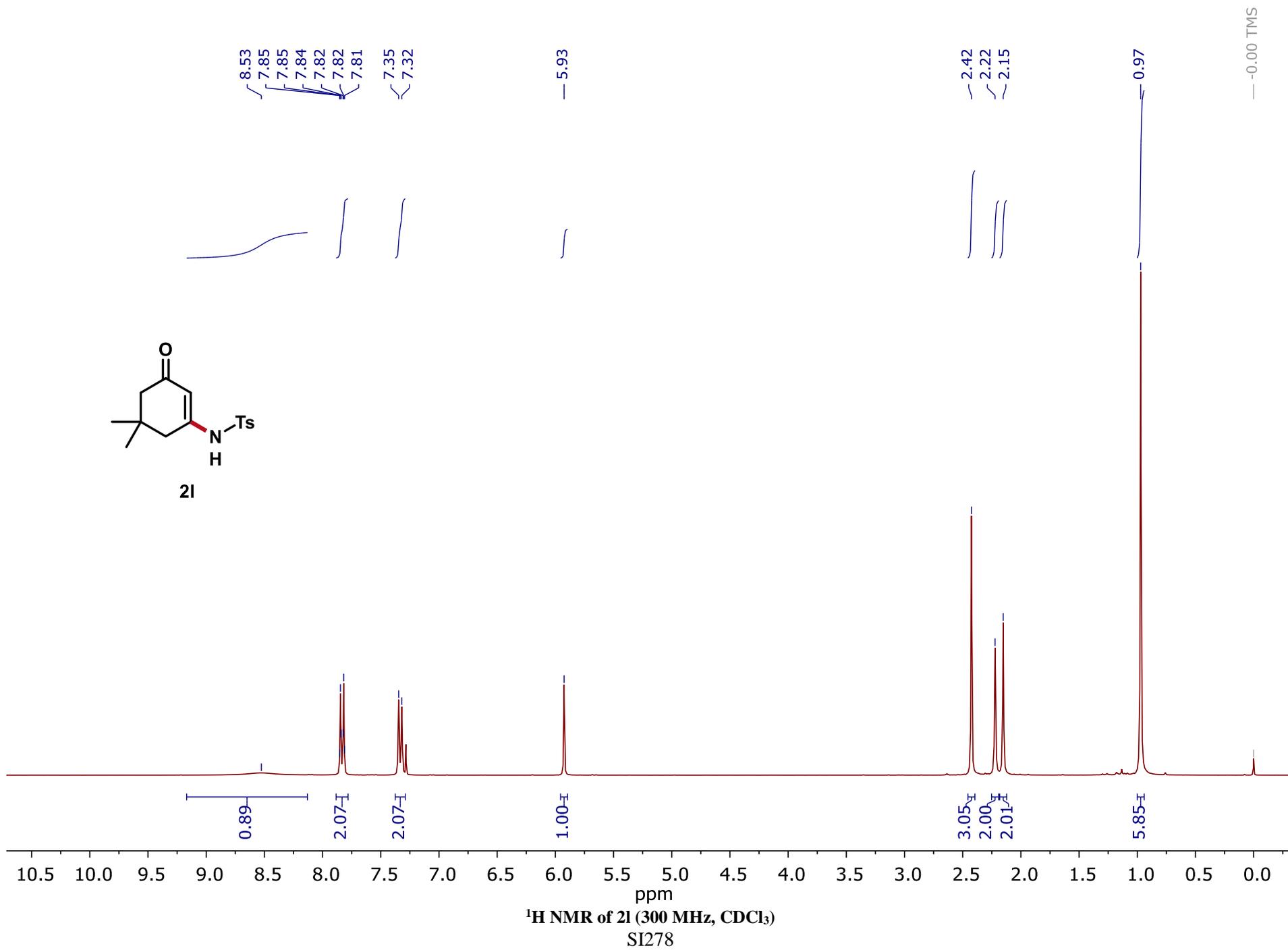
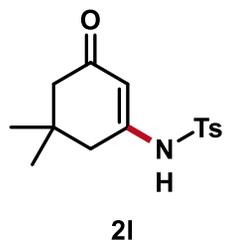


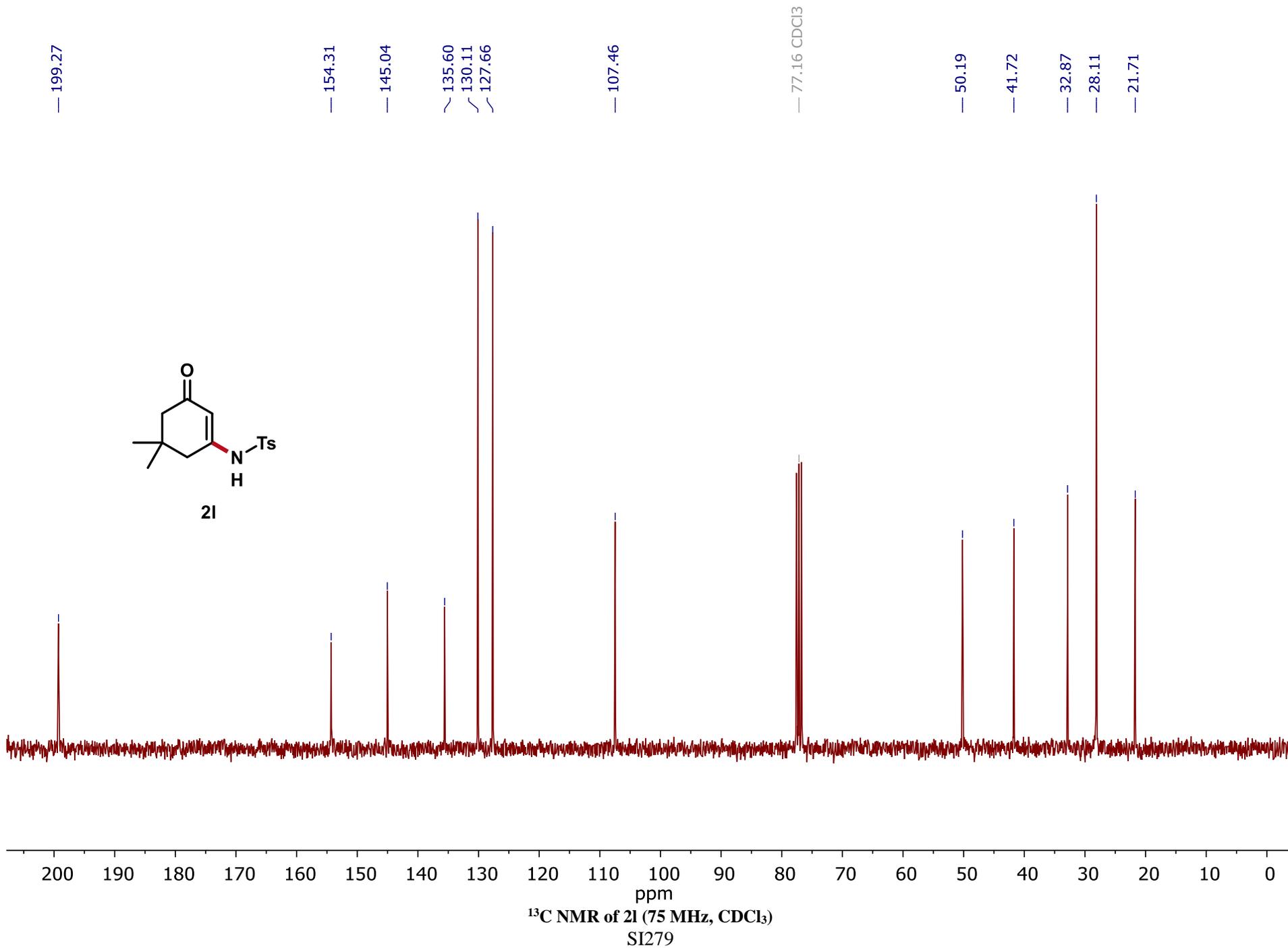


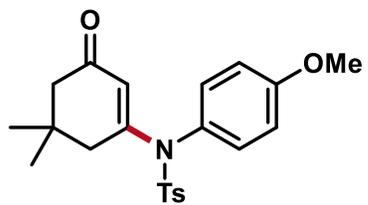
2k'



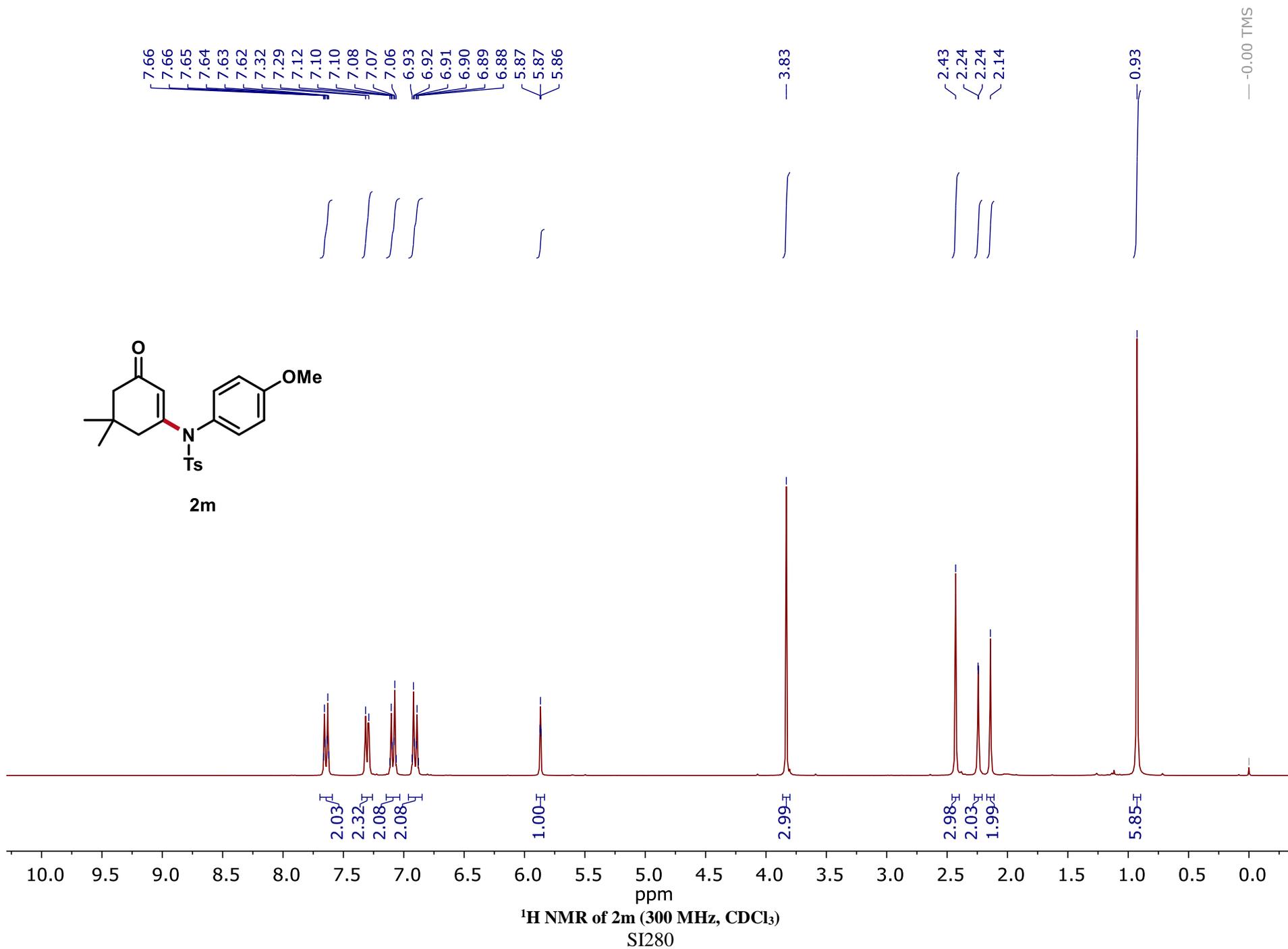
¹³C NMR of 2k' (75 MHz, CDCl₃)
SI277

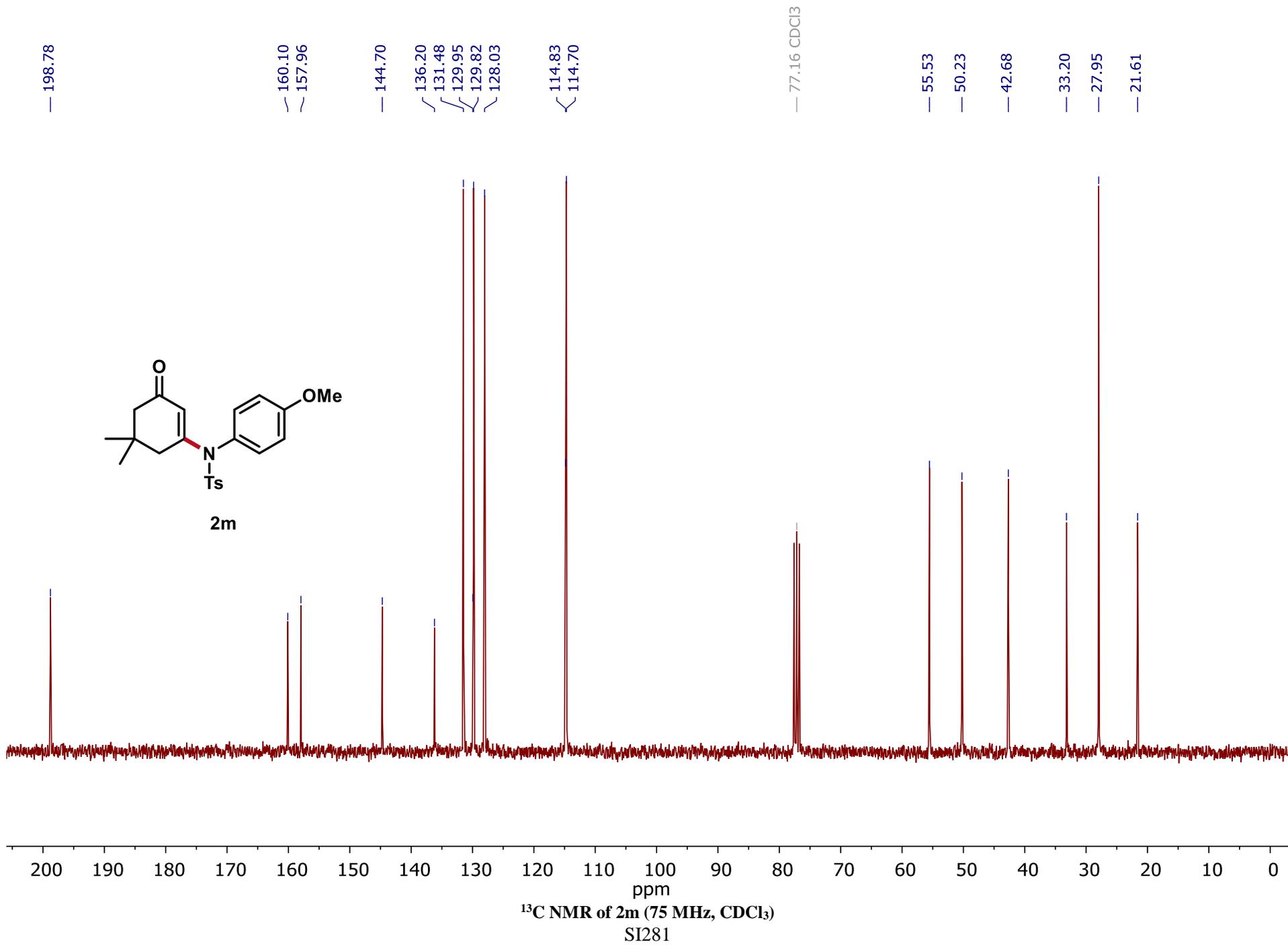


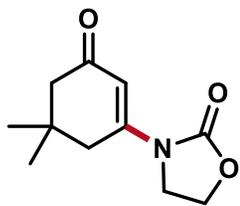




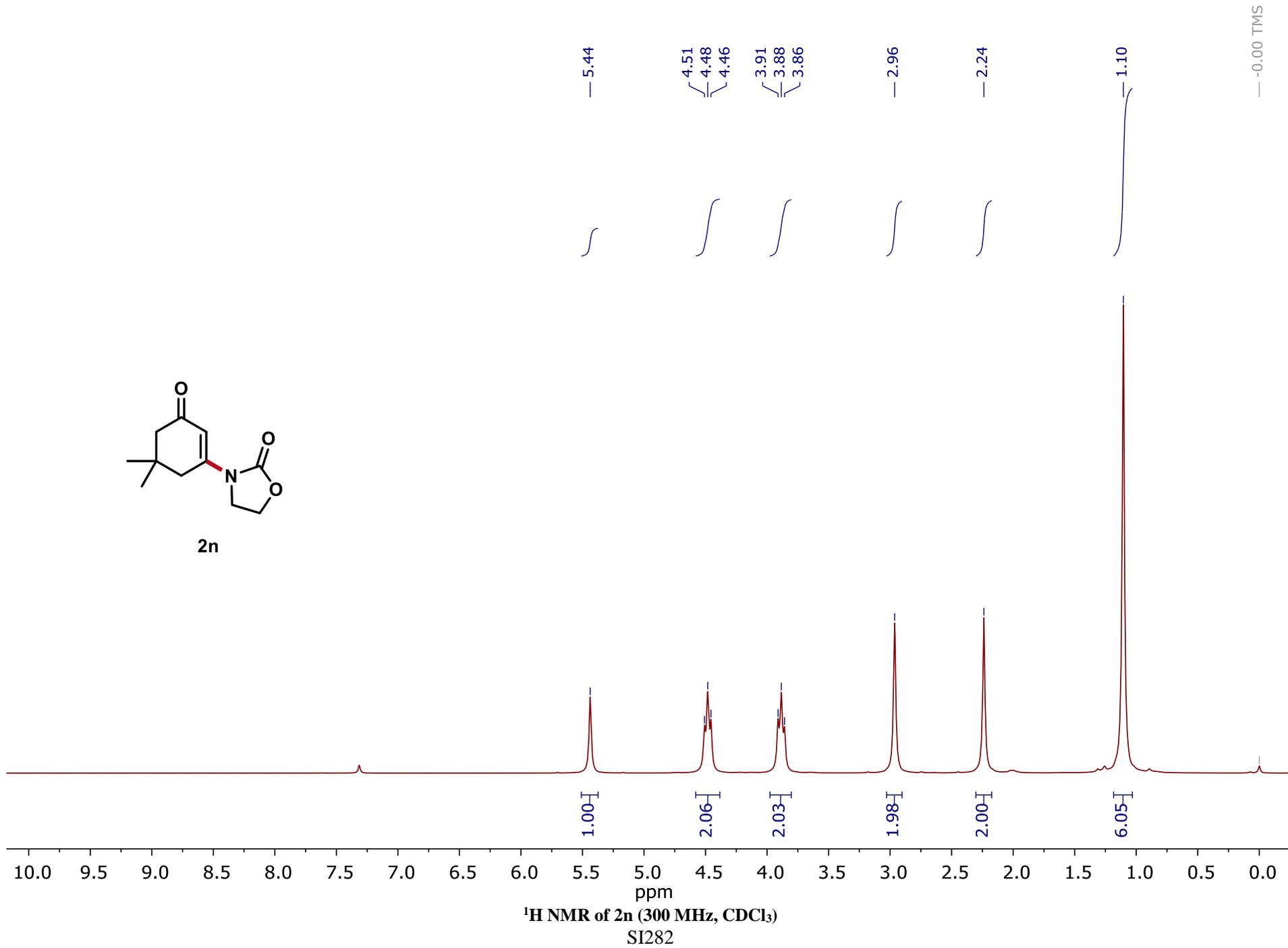
2m

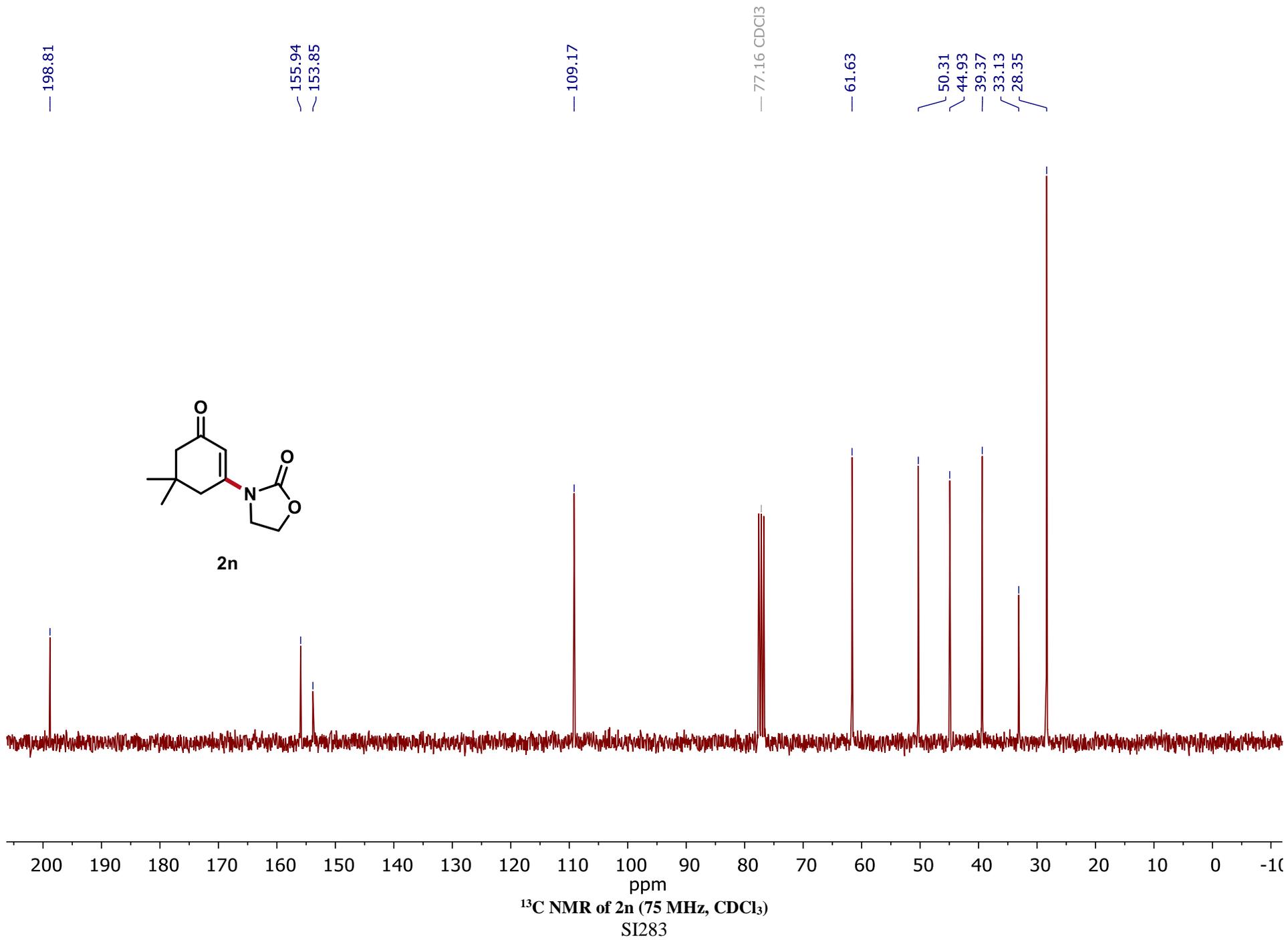


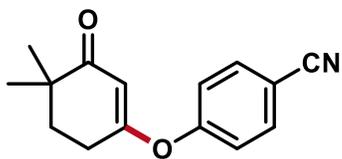




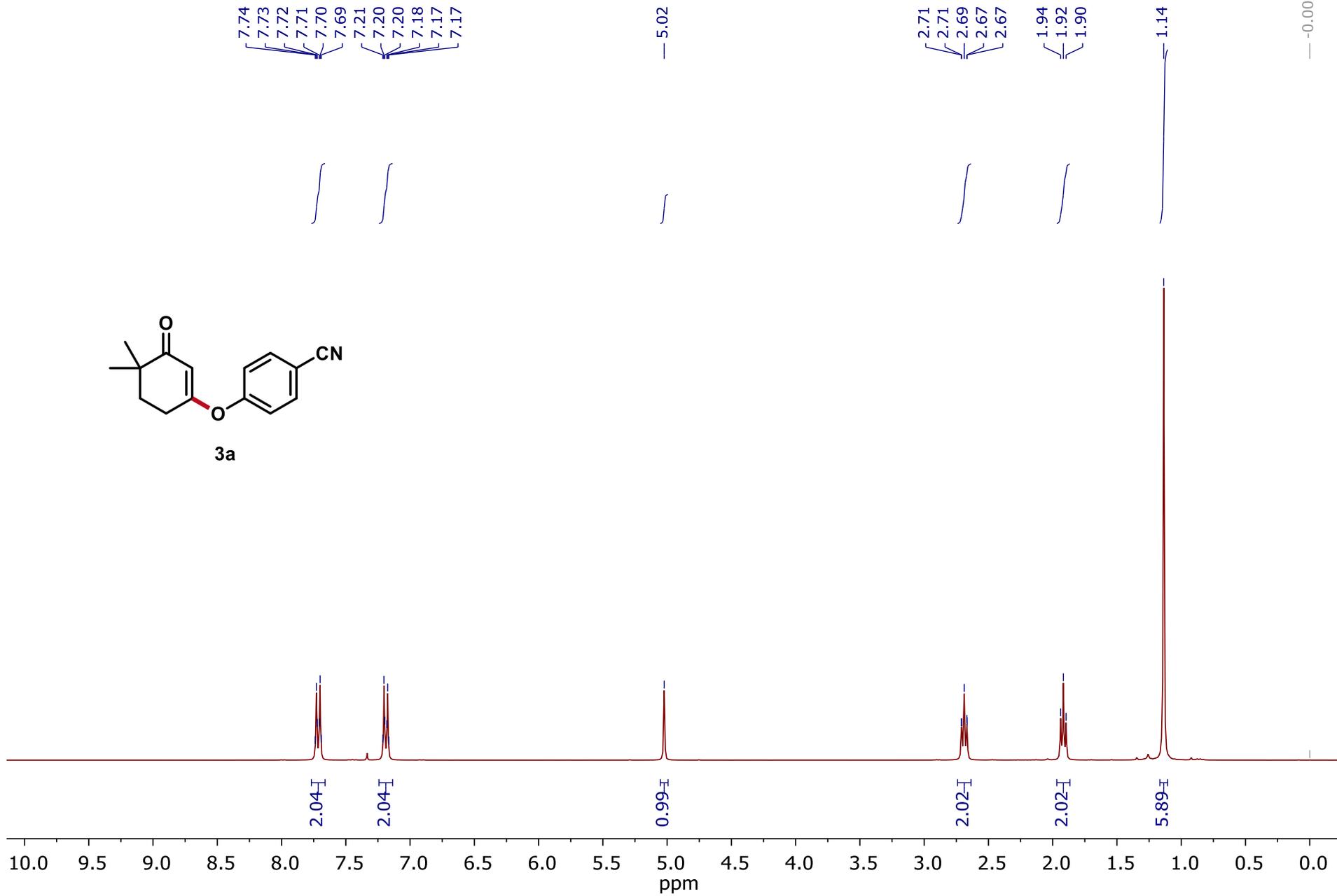
2n





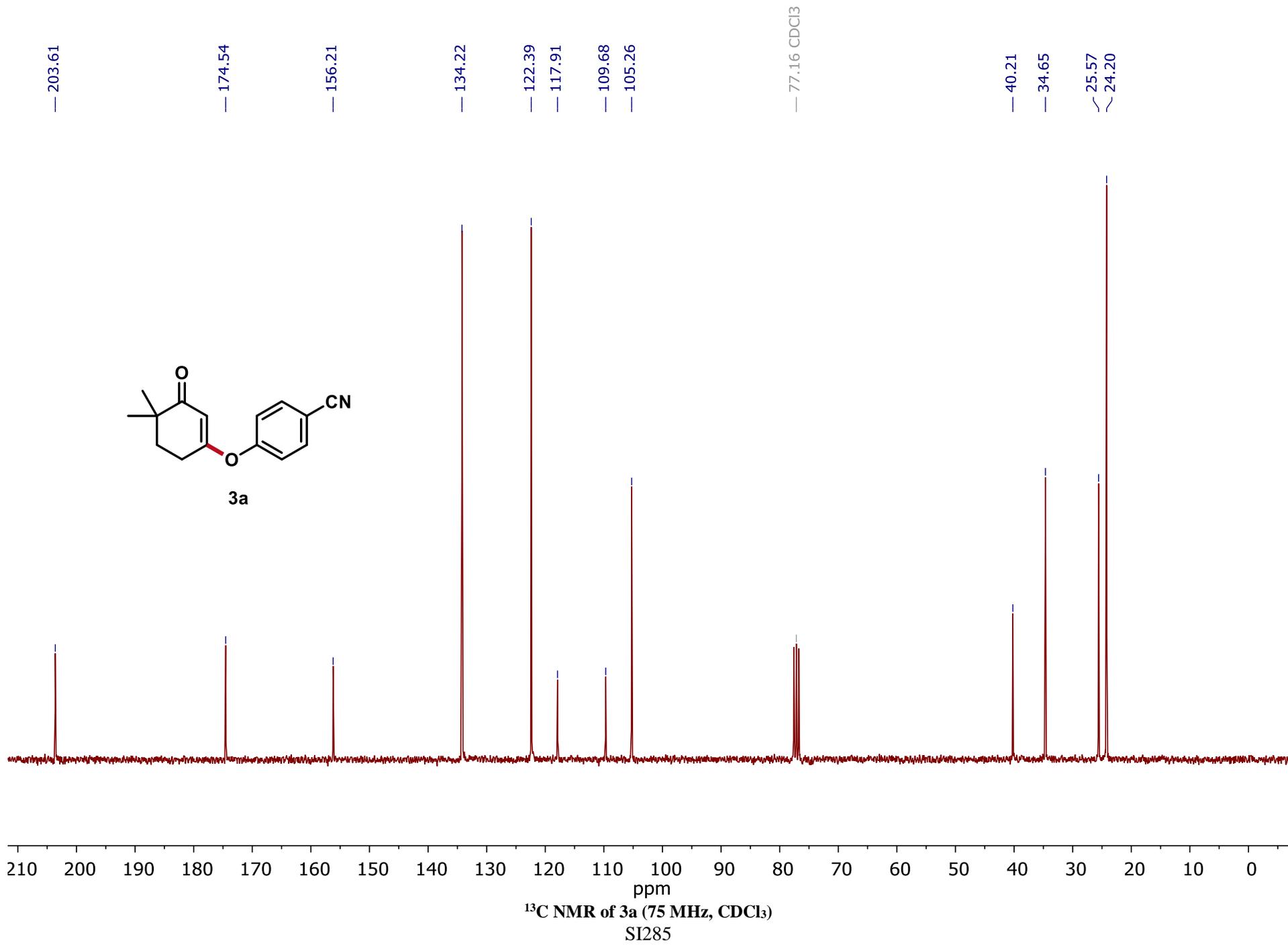


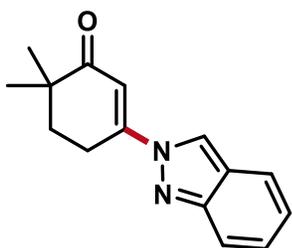
3a



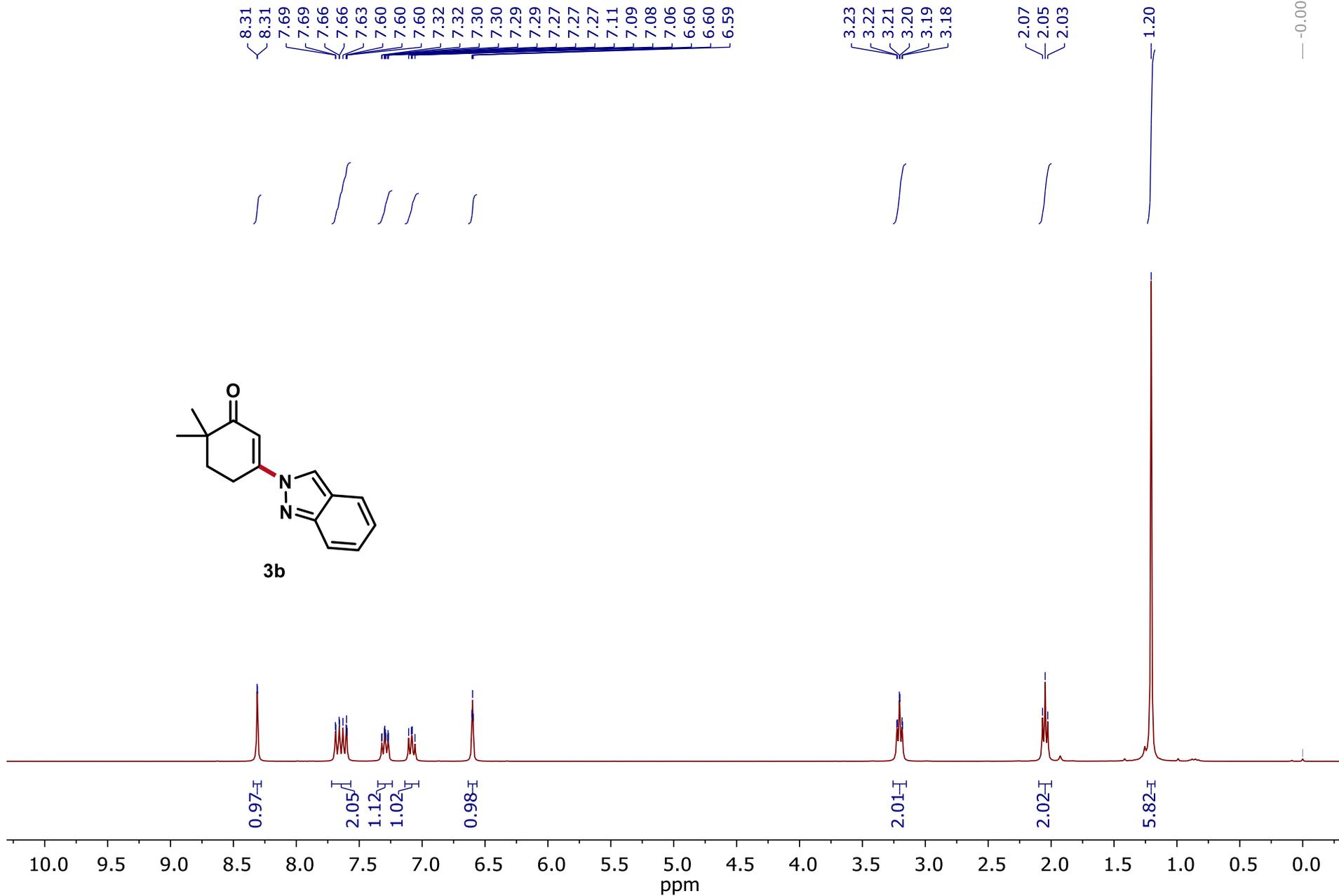
¹H NMR of 3a (300 MHz, CDCl₃)
SI284

— -0.00 TMS





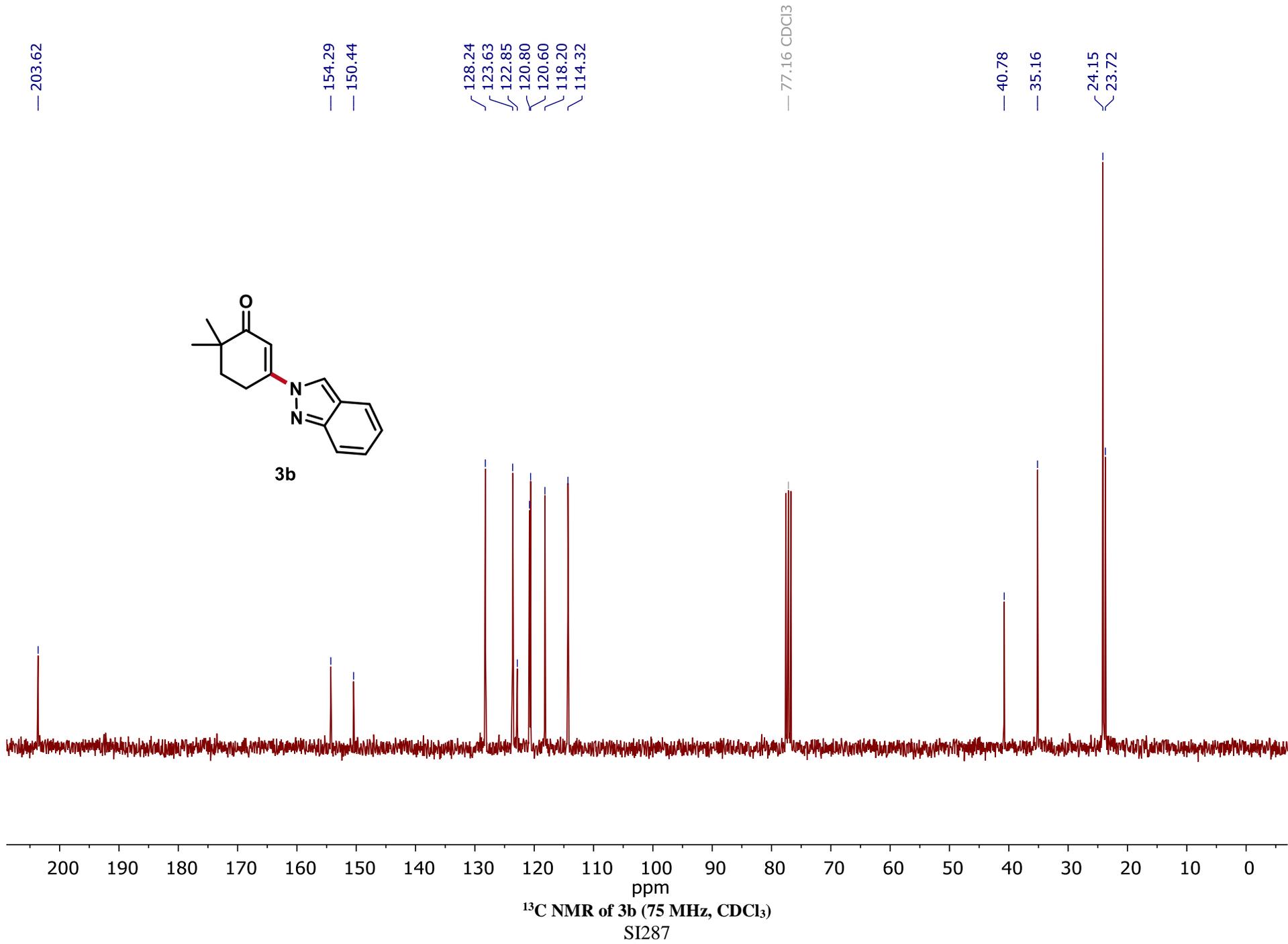
3b

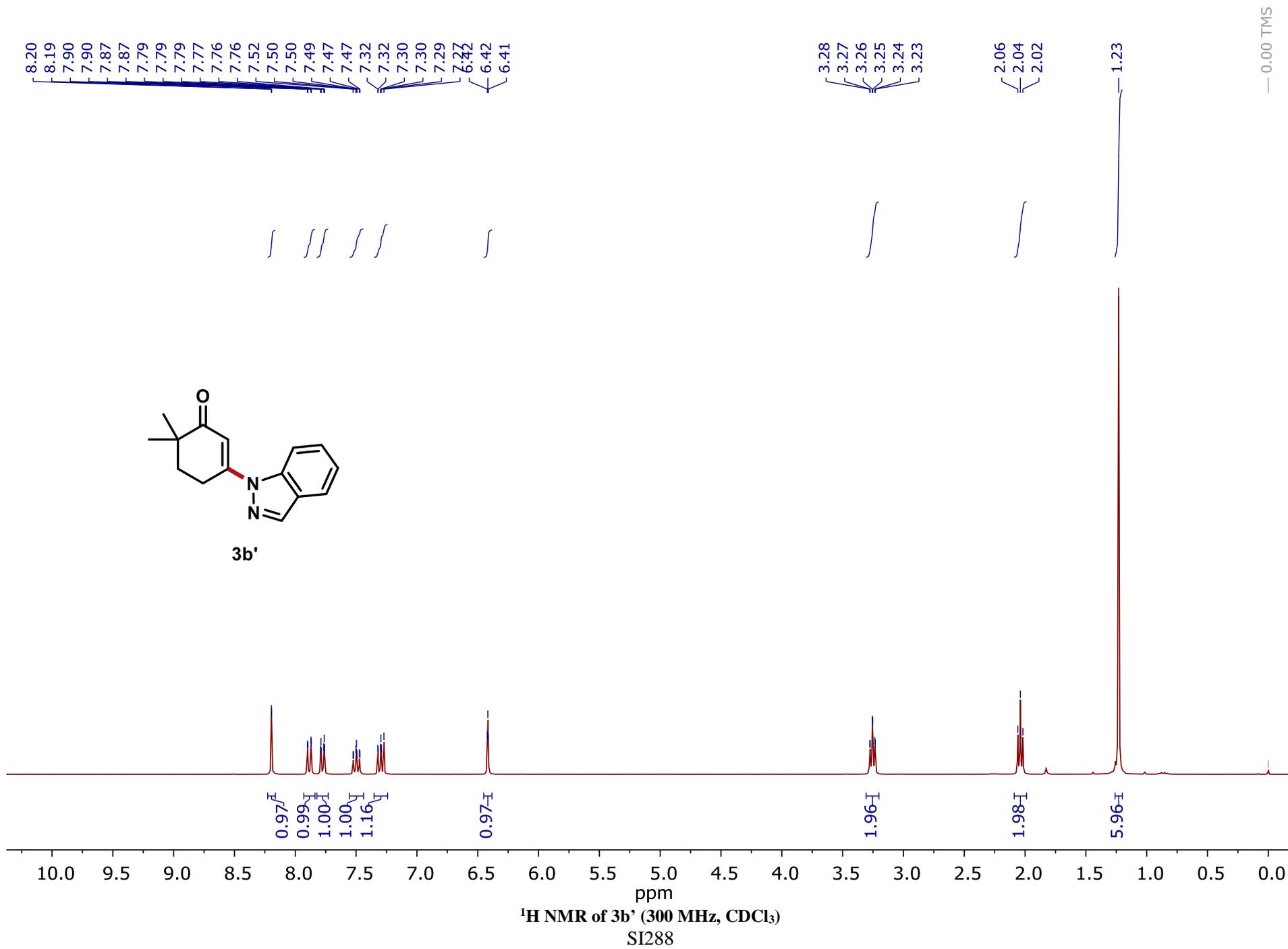


¹H NMR of 3b (300 MHz, CDCl₃)

S1286

— -0.00 TMS





— 204.27

— 155.99

— 138.90
— 138.00

— 128.41
— 126.88
— 123.25
— 121.82

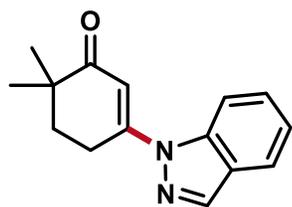
— 113.02
— 111.74

— 77.16 CDCl₃

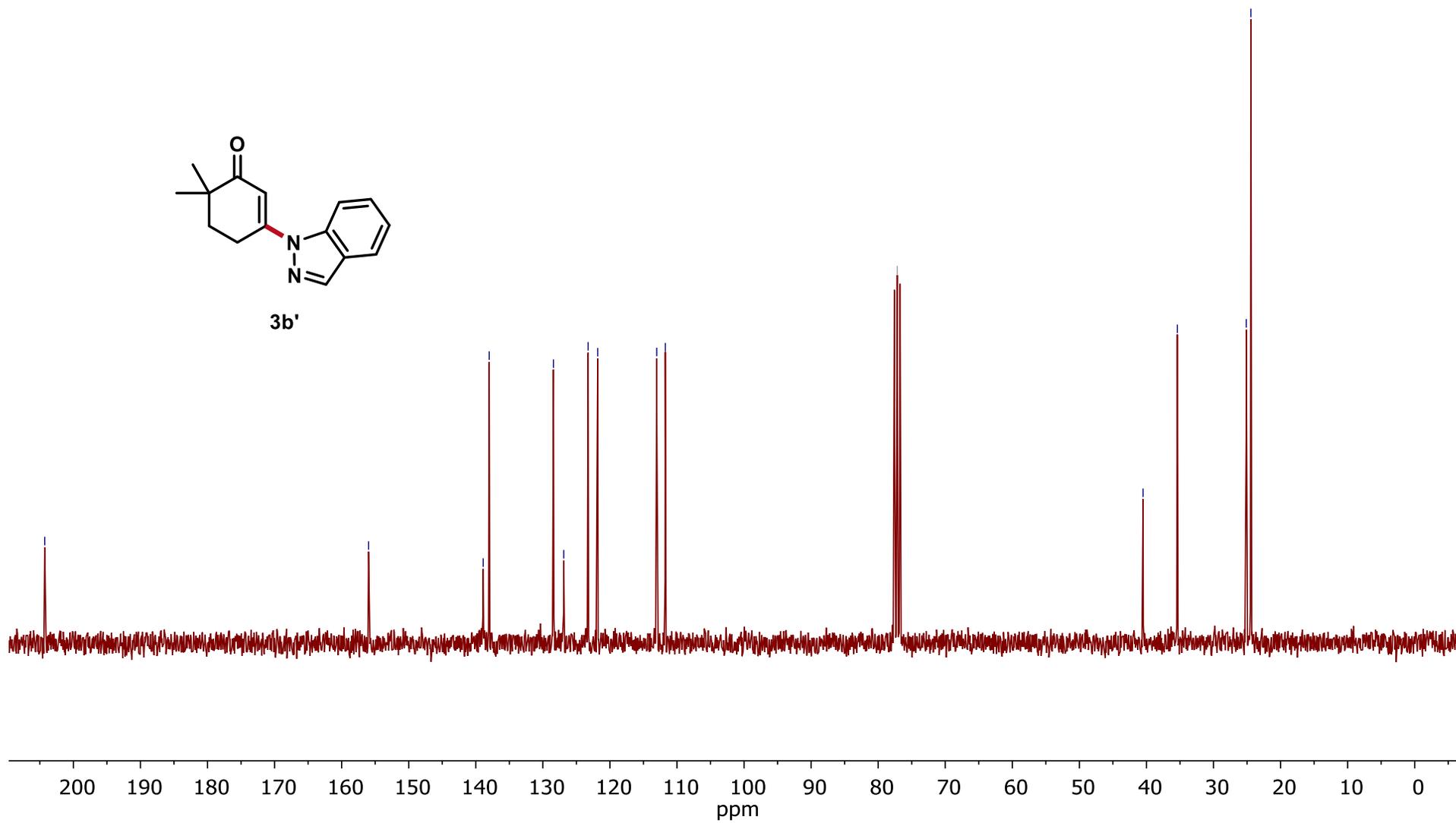
— 40.51

— 35.39

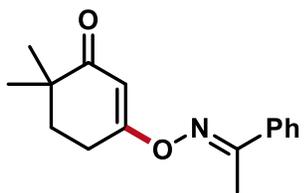
— 25.11
— 24.42



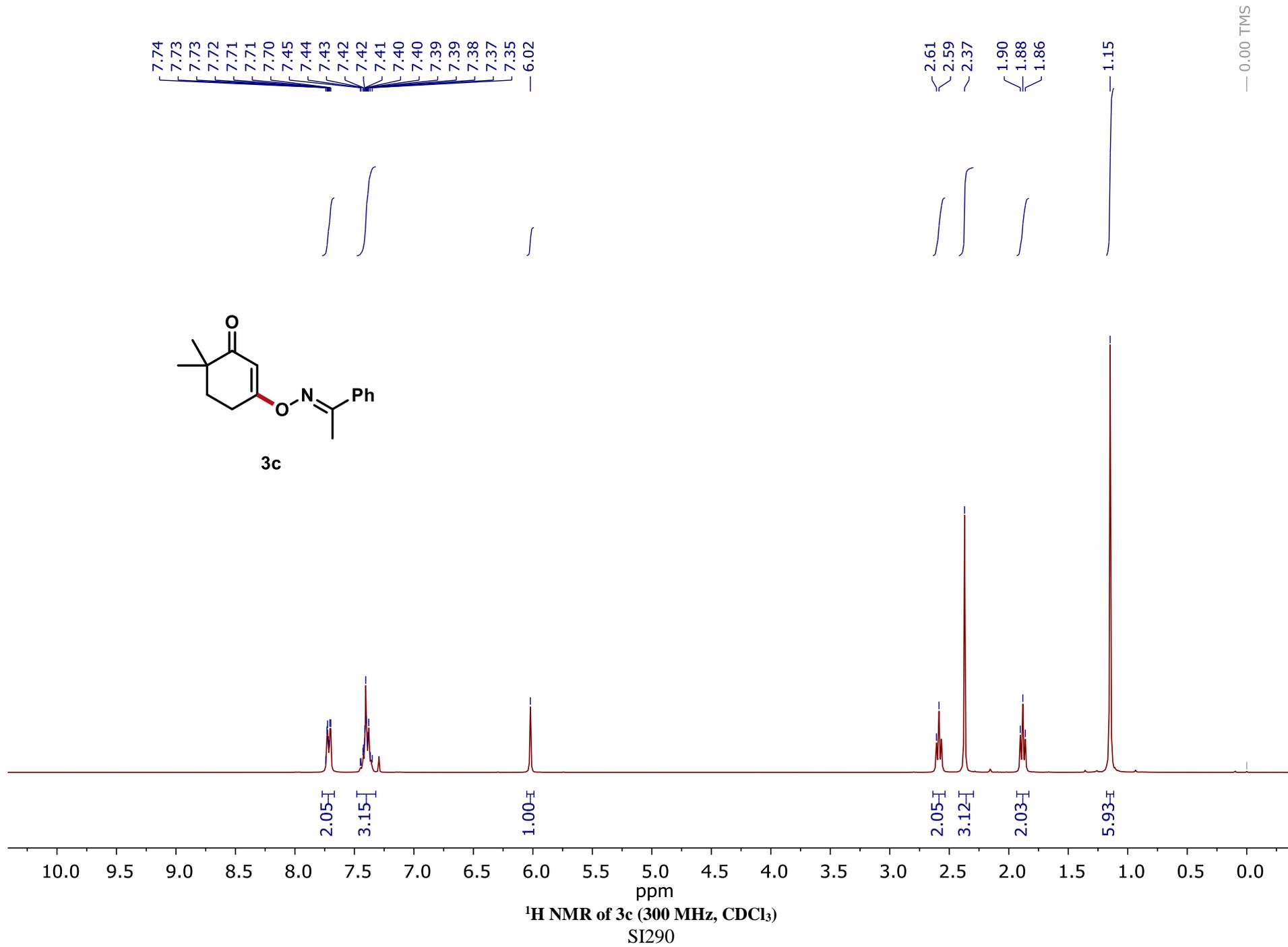
3b'

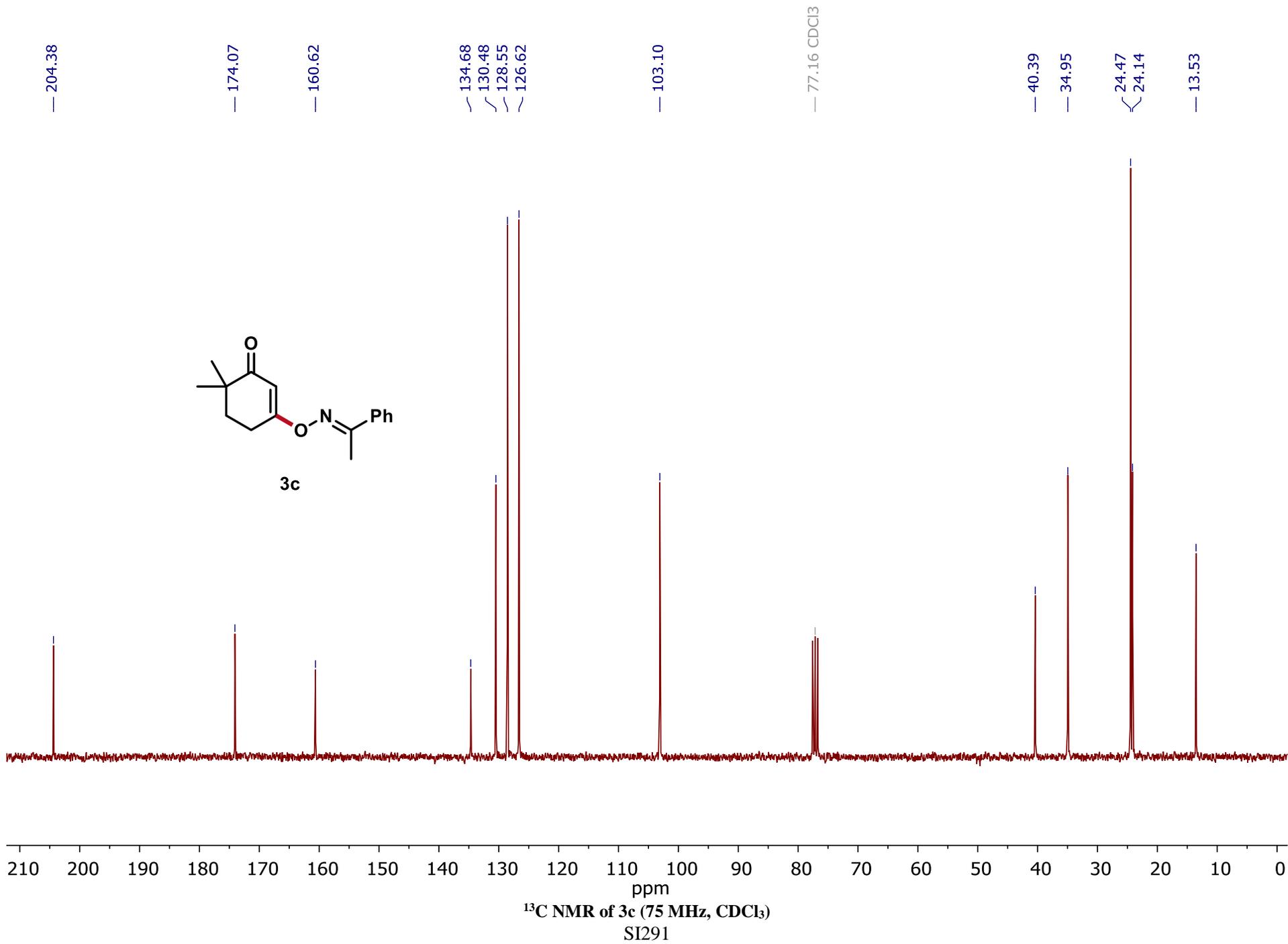


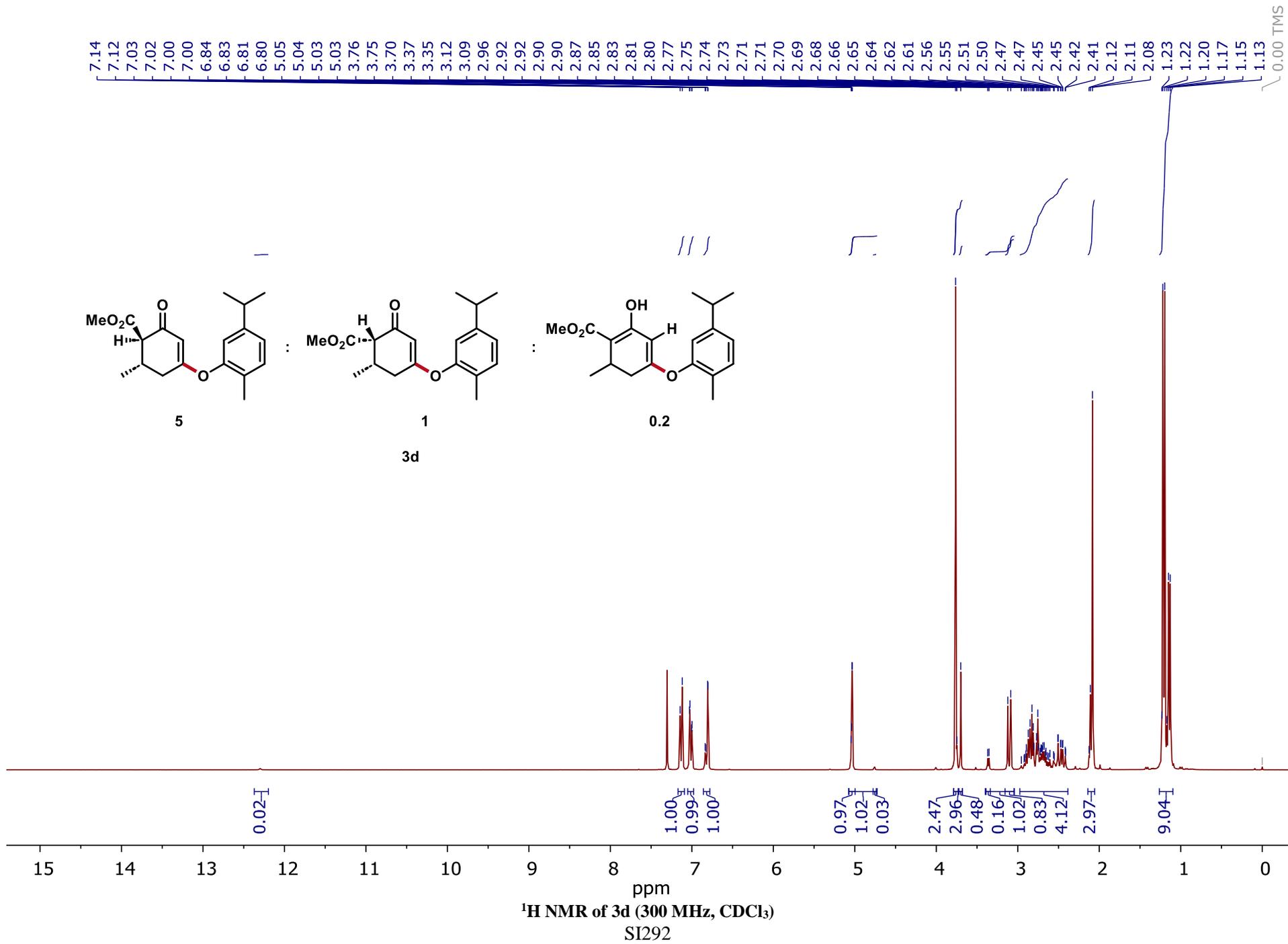
¹³C NMR of 3b' (75 MHz, CDCl₃)
SI289

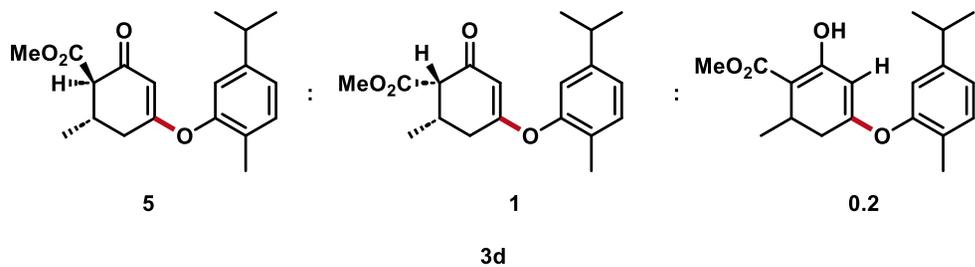


3c









193.93
 193.88
 178.29
 176.58
 170.51
 168.91

150.83
 150.68
 148.80
 148.72

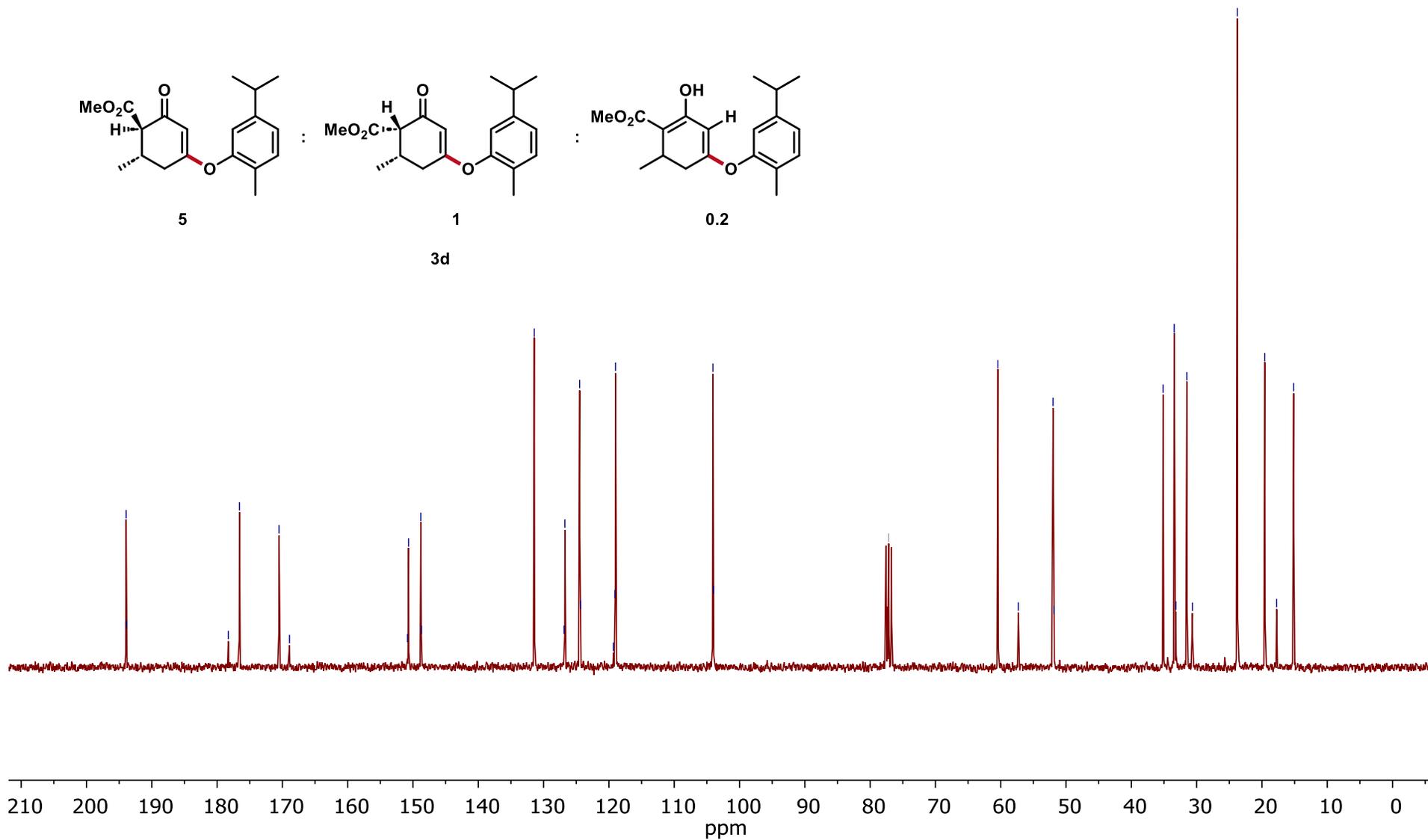
131.43
 126.86
 126.74
 124.48
 124.36
 119.32
 119.07
 118.99

104.07
 103.99

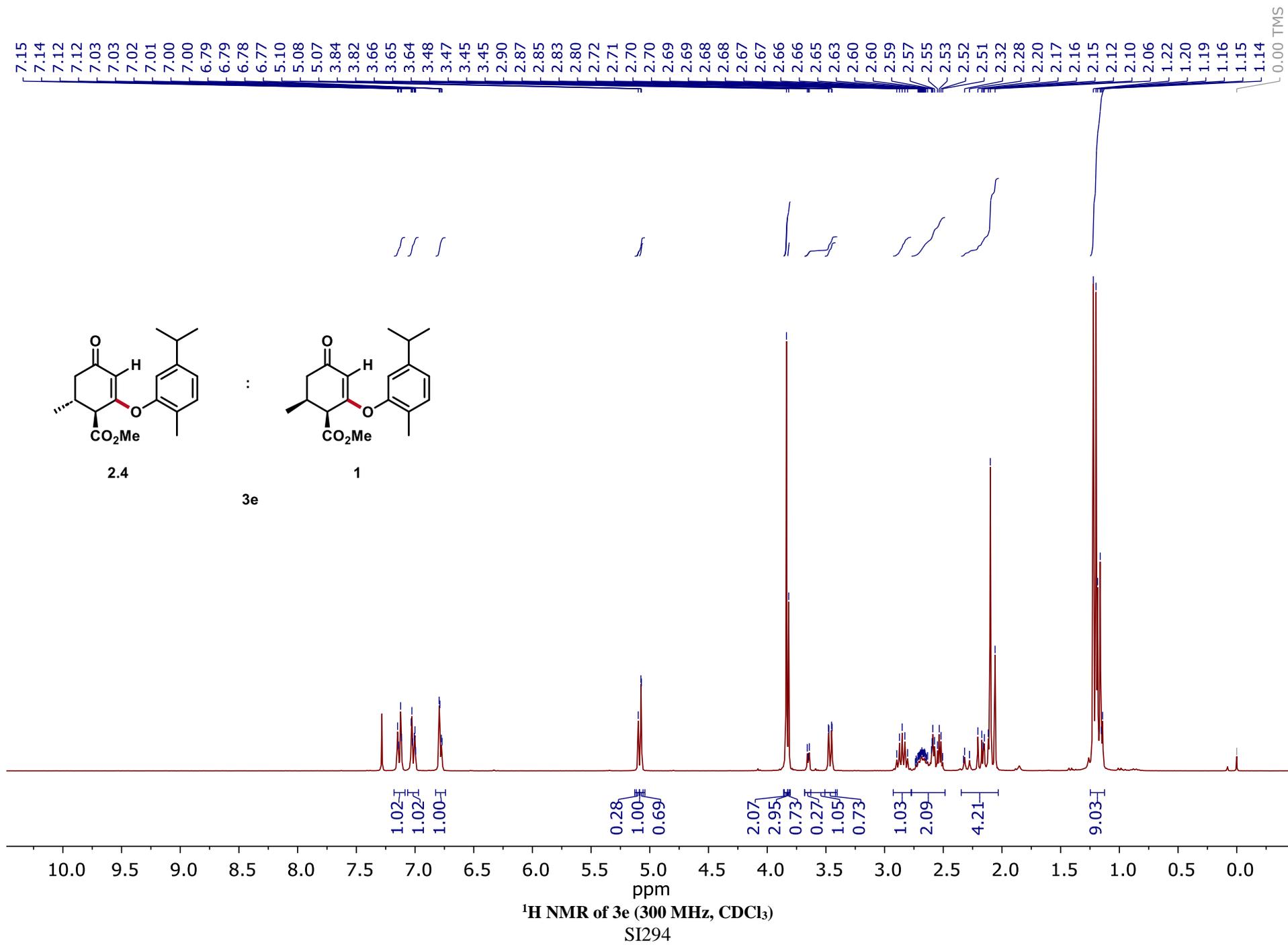
— 77.16 CDCl₃

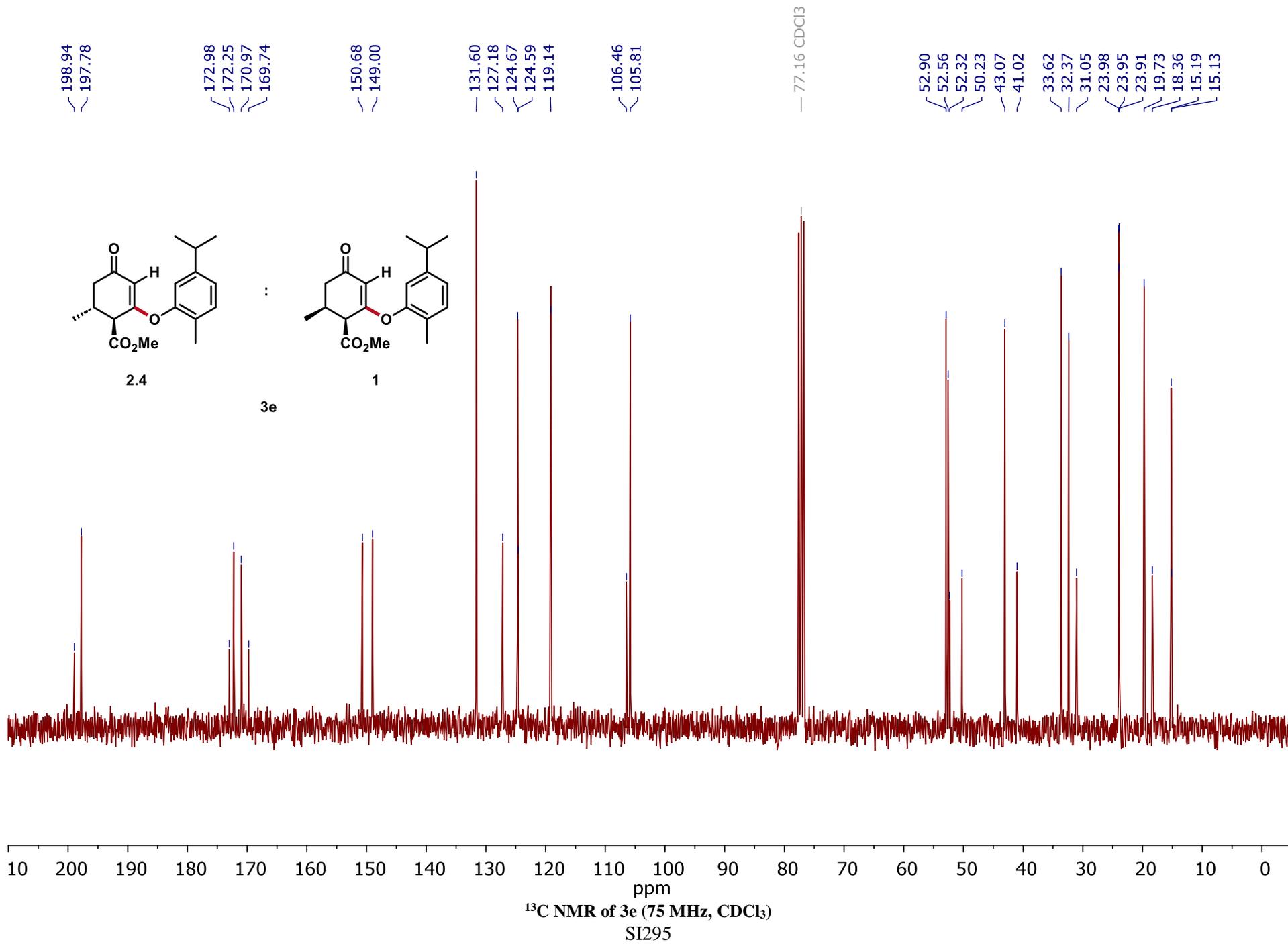
60.44
 57.31
 51.99
 51.83

35.14
 33.44
 33.18
 31.50
 30.64
 23.78
 19.57
 17.75
 15.15

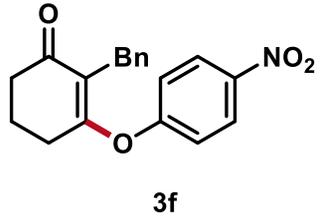
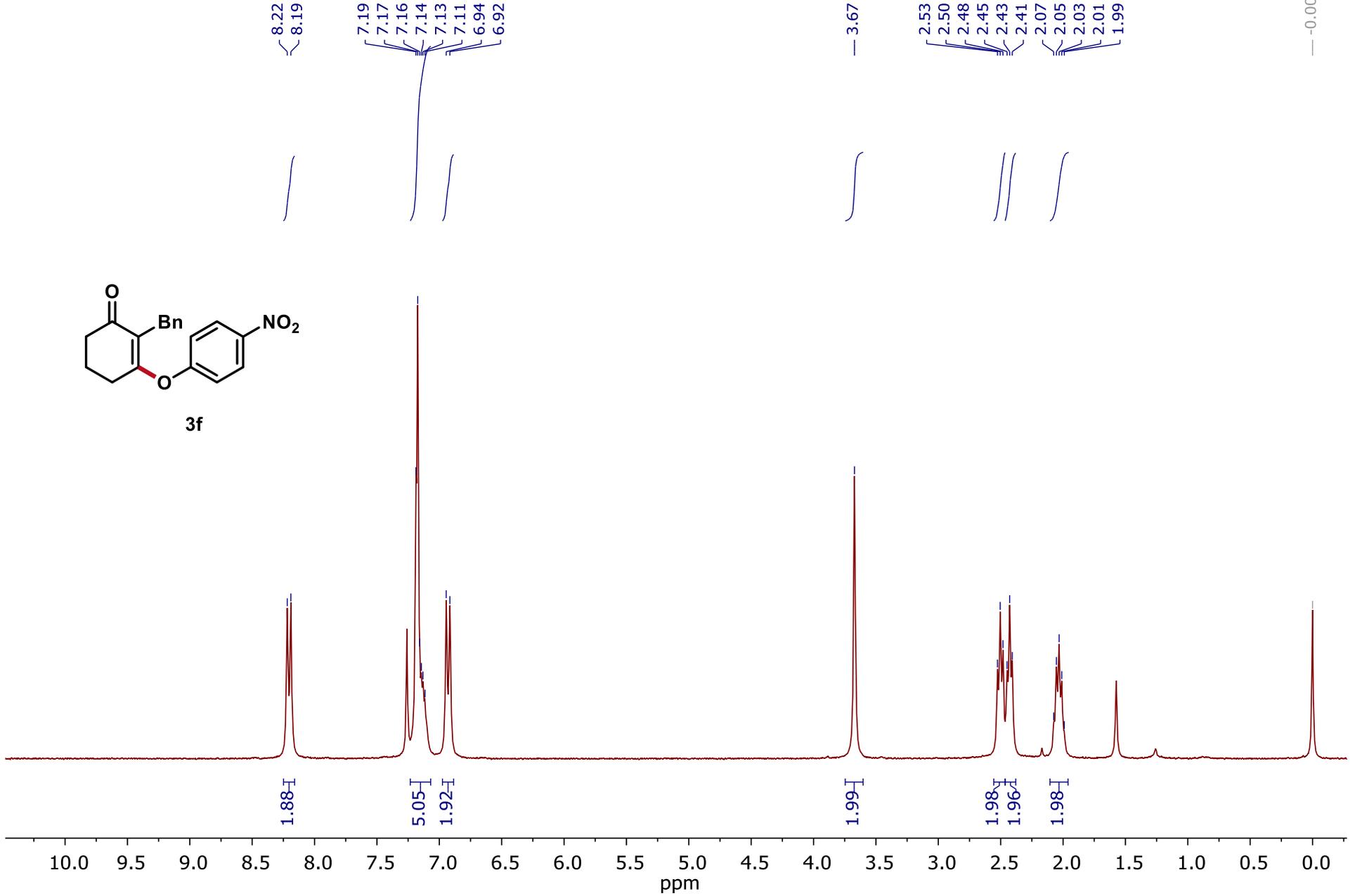


¹³C NMR of 3d (75 MHz, CDCl₃)
 S1293

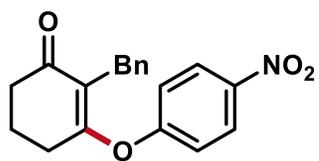




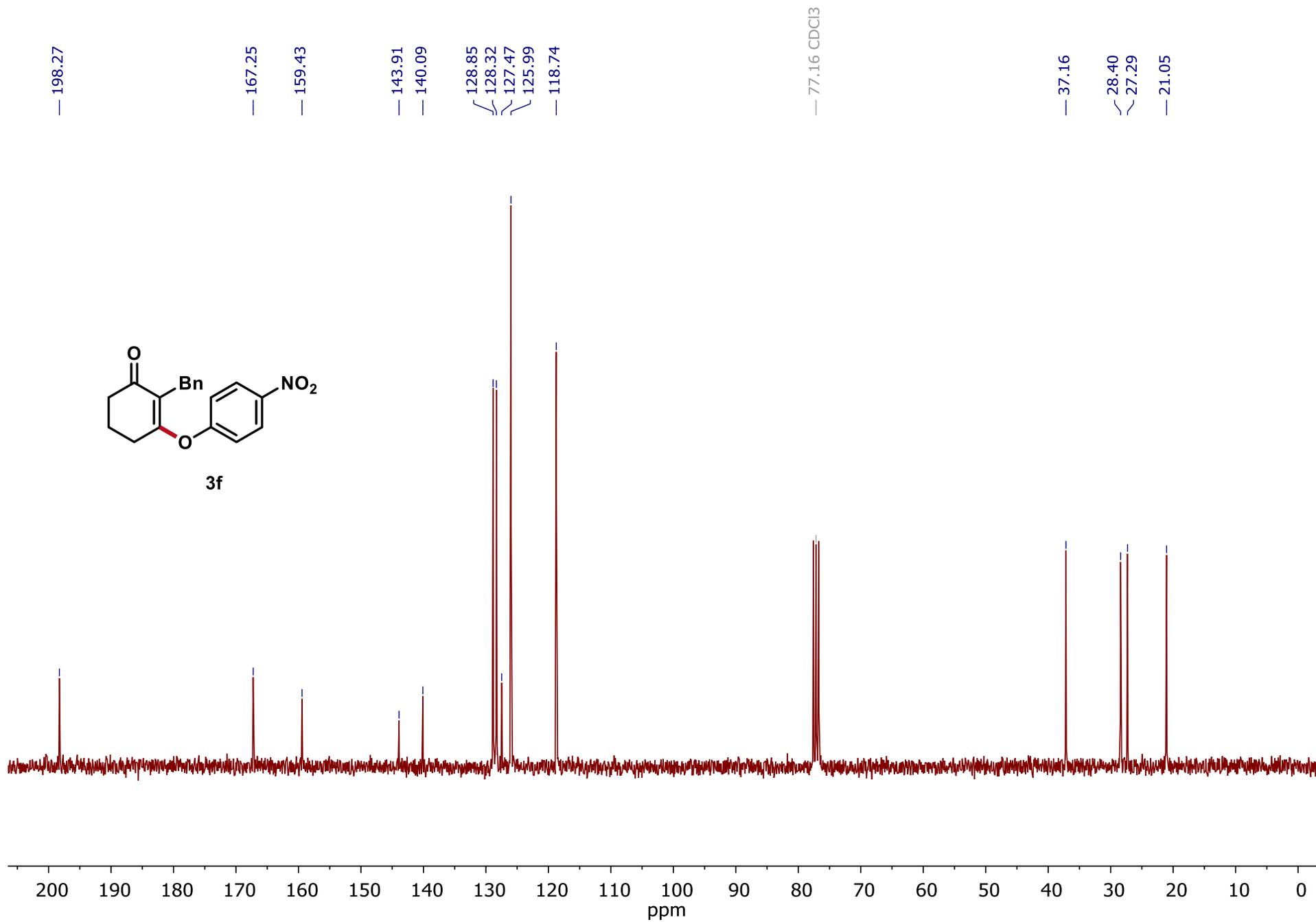
— -0.00 TMS



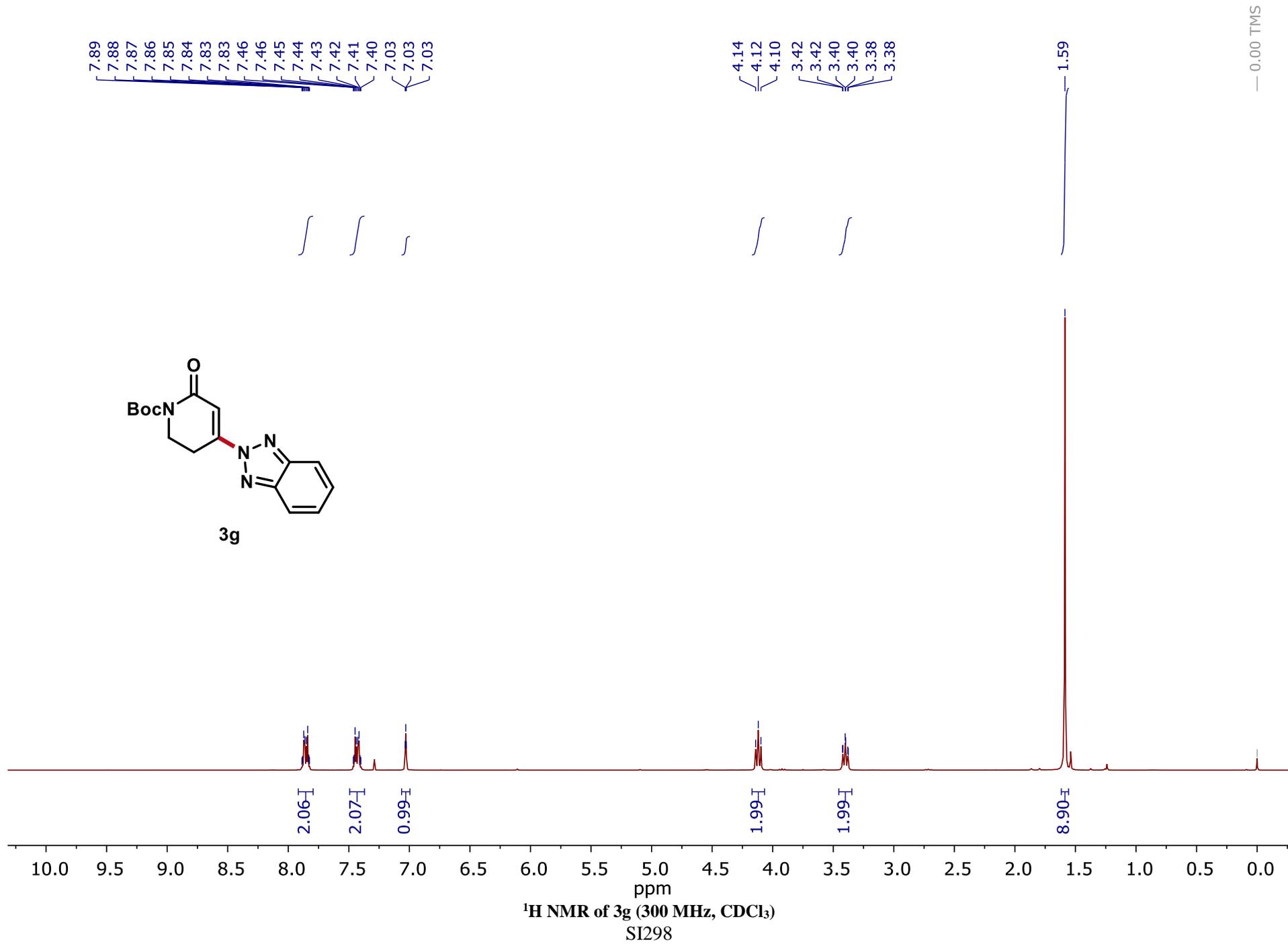
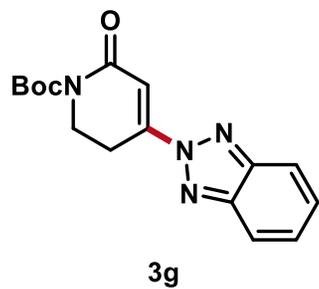
¹H NMR of 3f (300 MHz, CDCl₃)
SI296

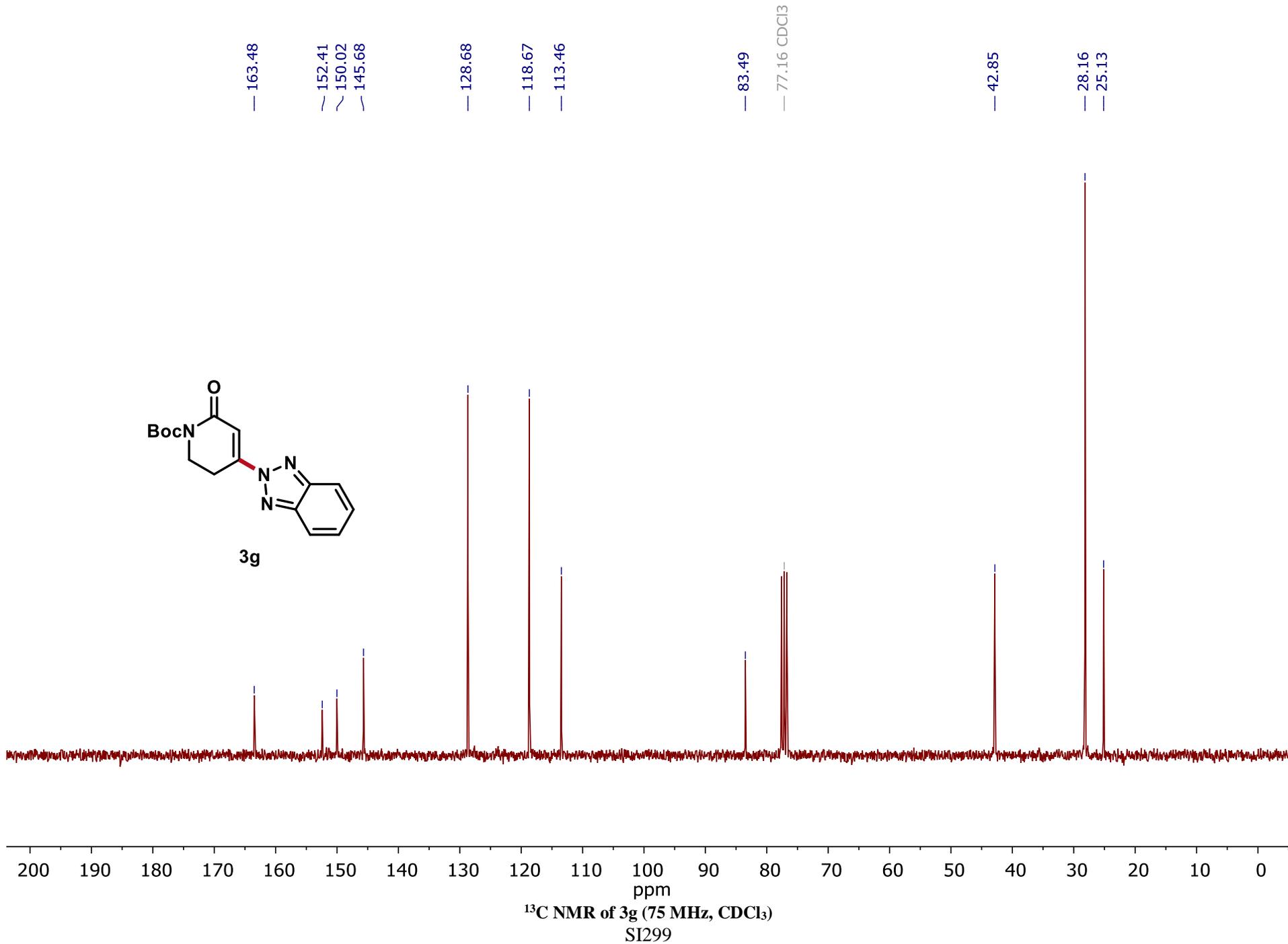
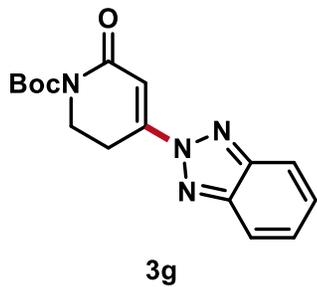


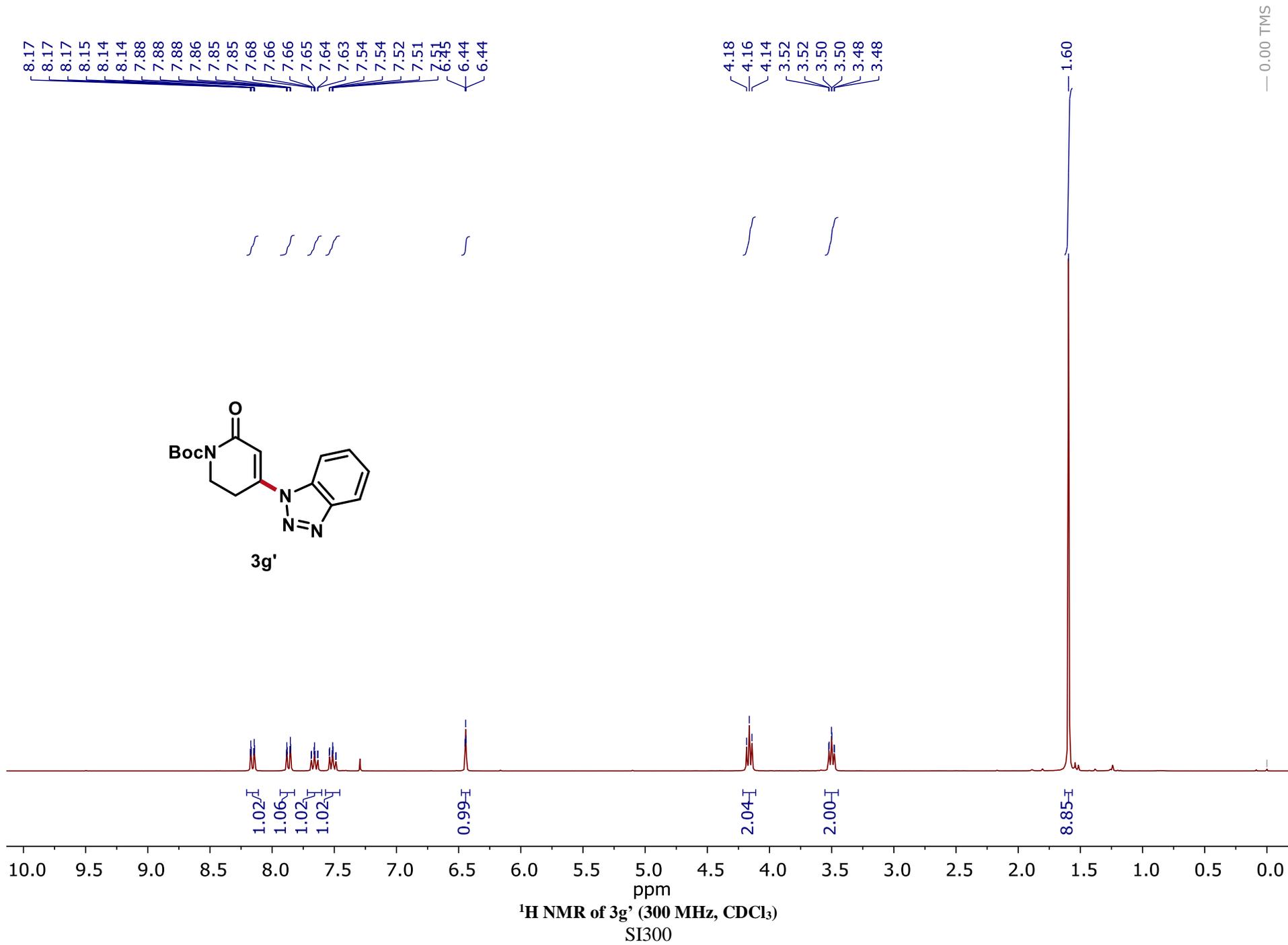
3f

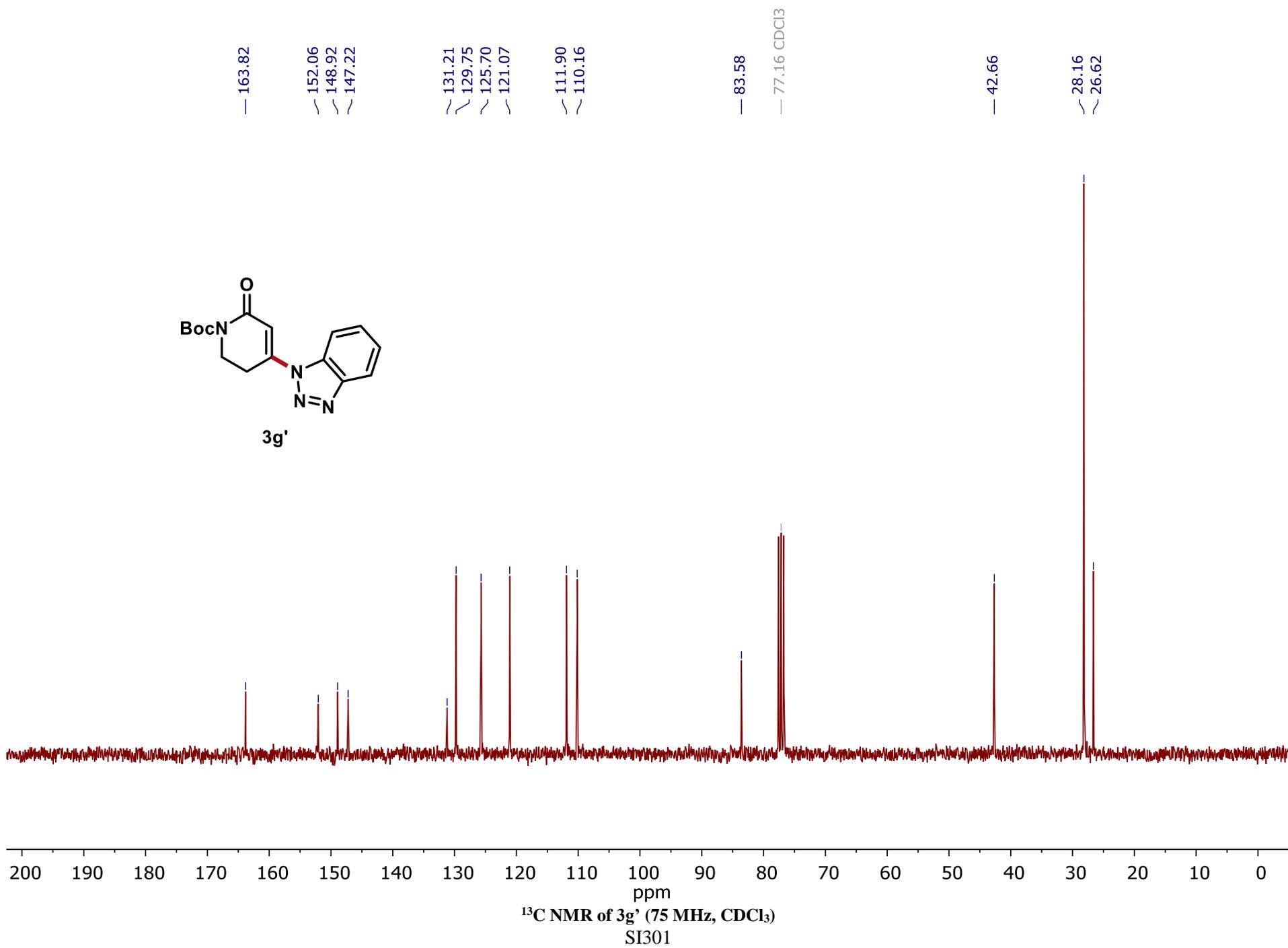
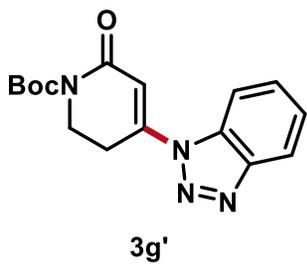


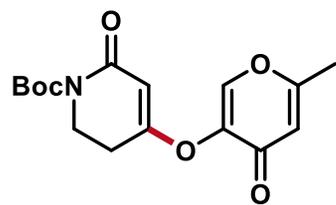
^{13}C NMR of 3f (75 MHz, CDCl_3)
SI297



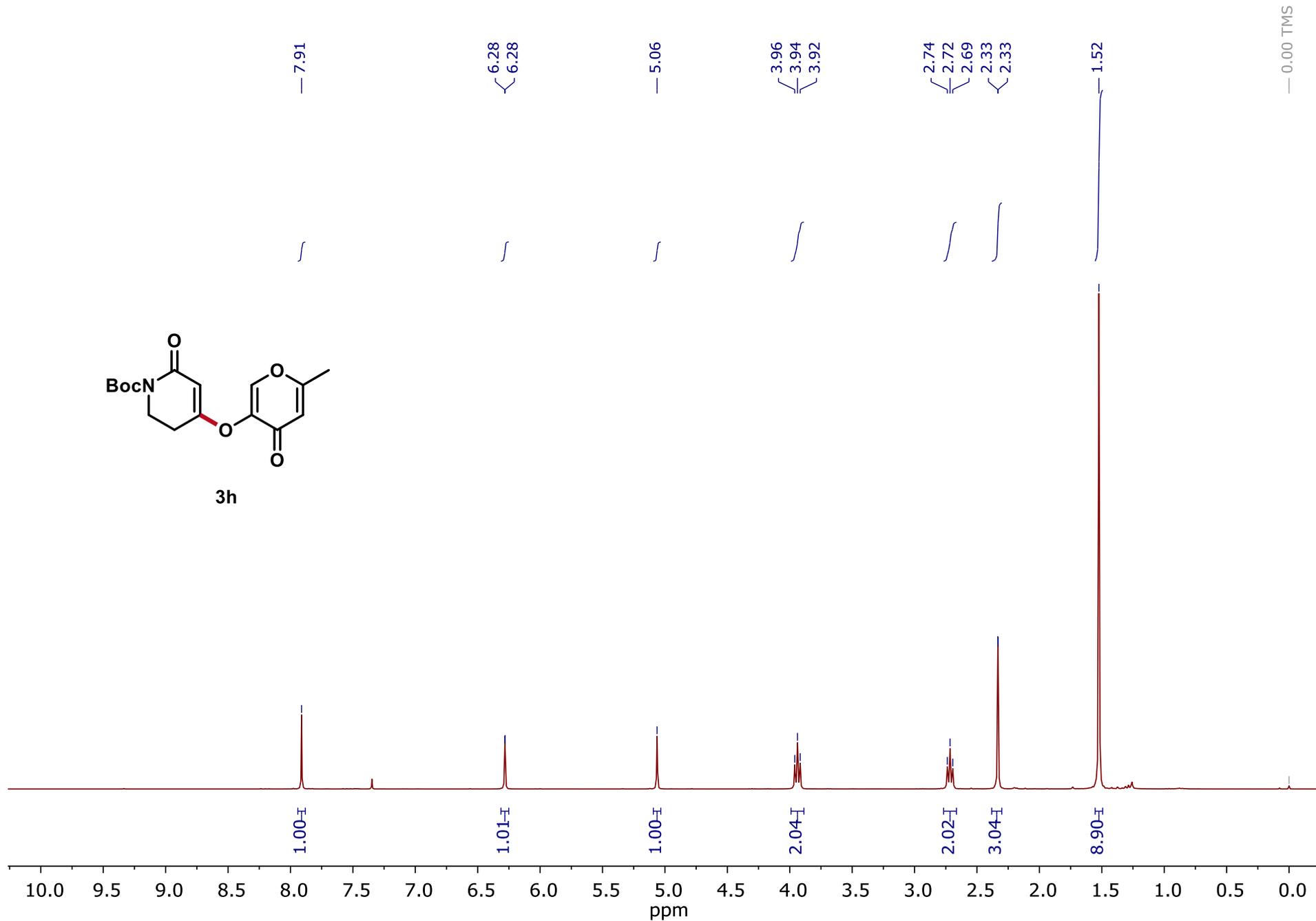






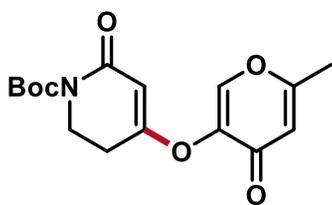


3h

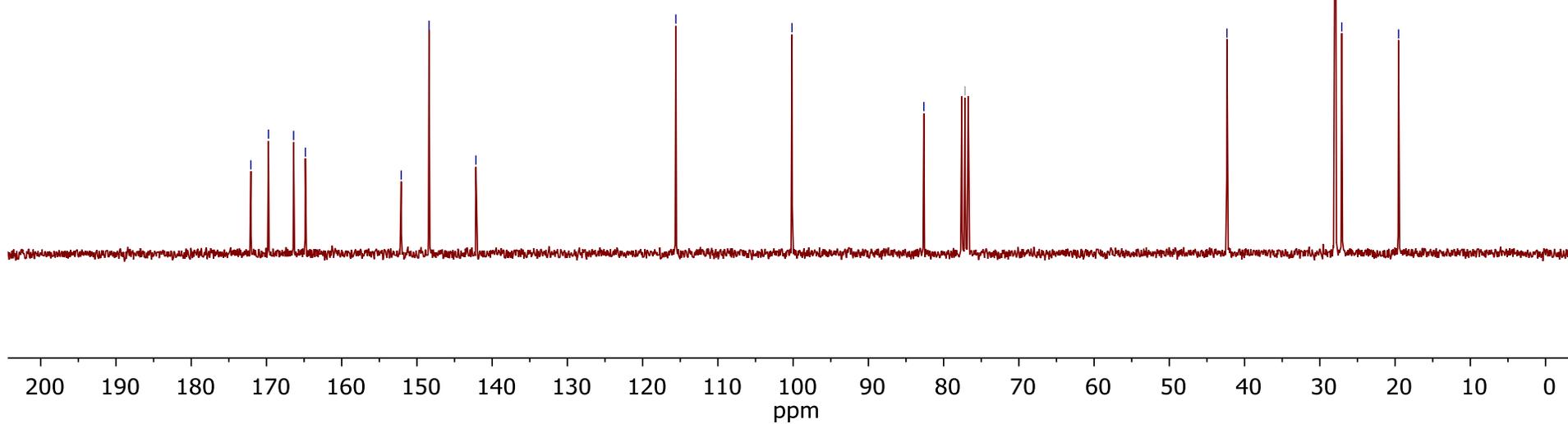


¹H NMR of 3h (300 MHz, CDCl₃)

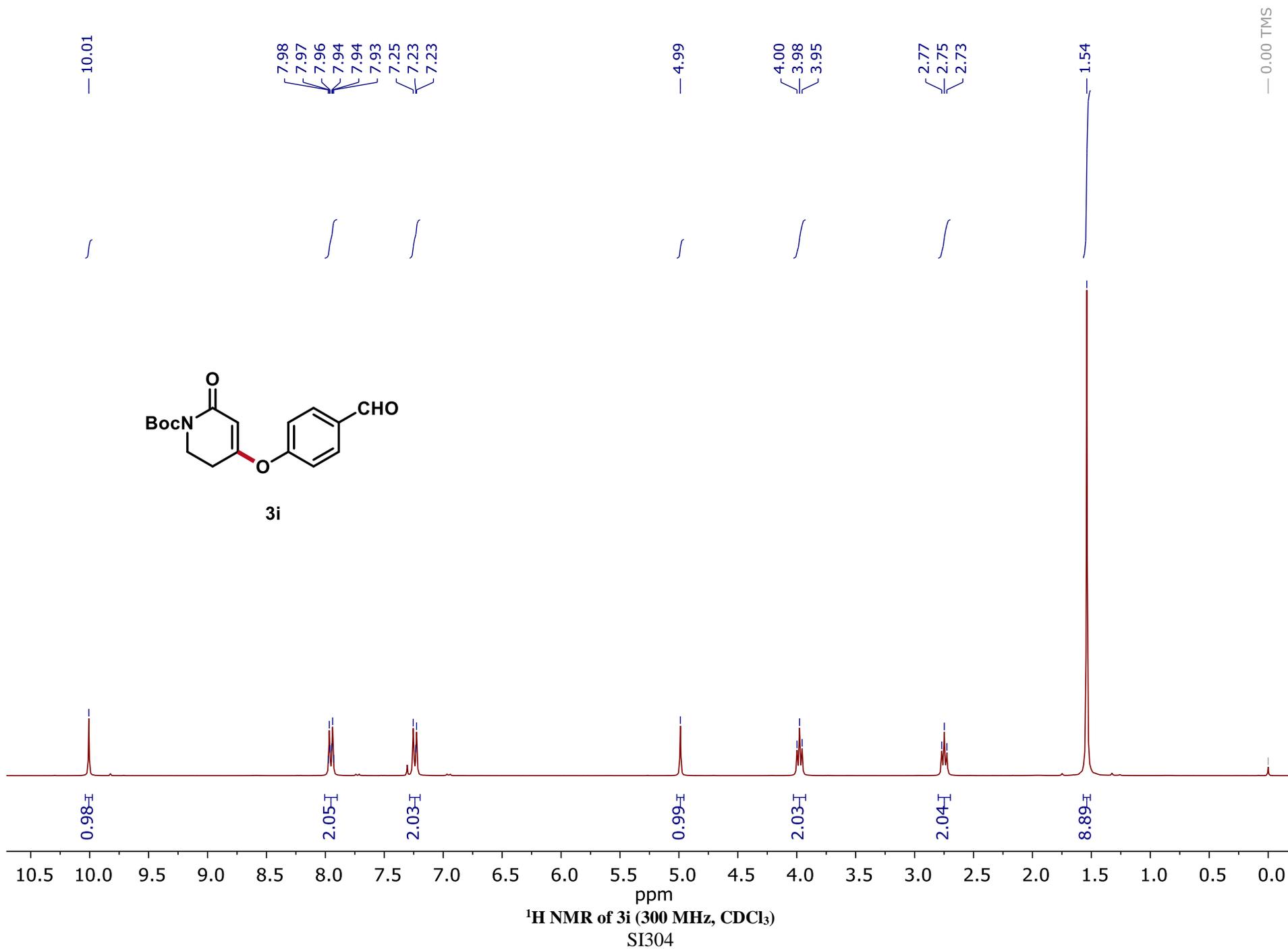
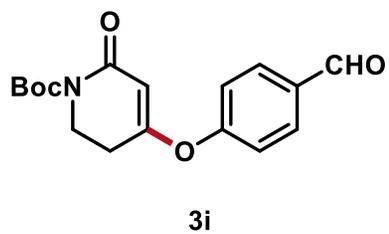
SI302

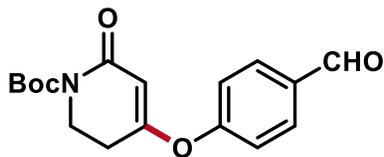


3h

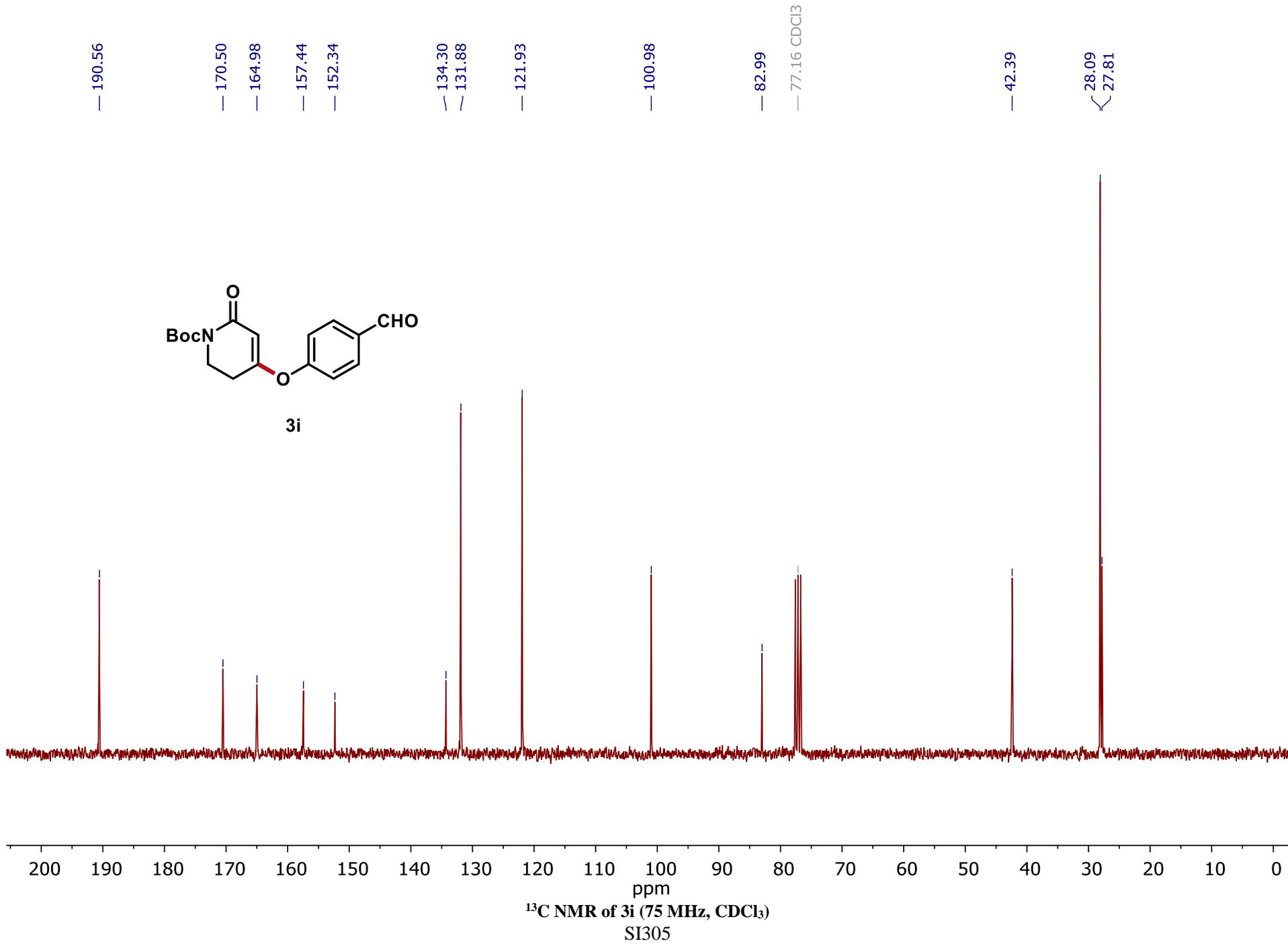


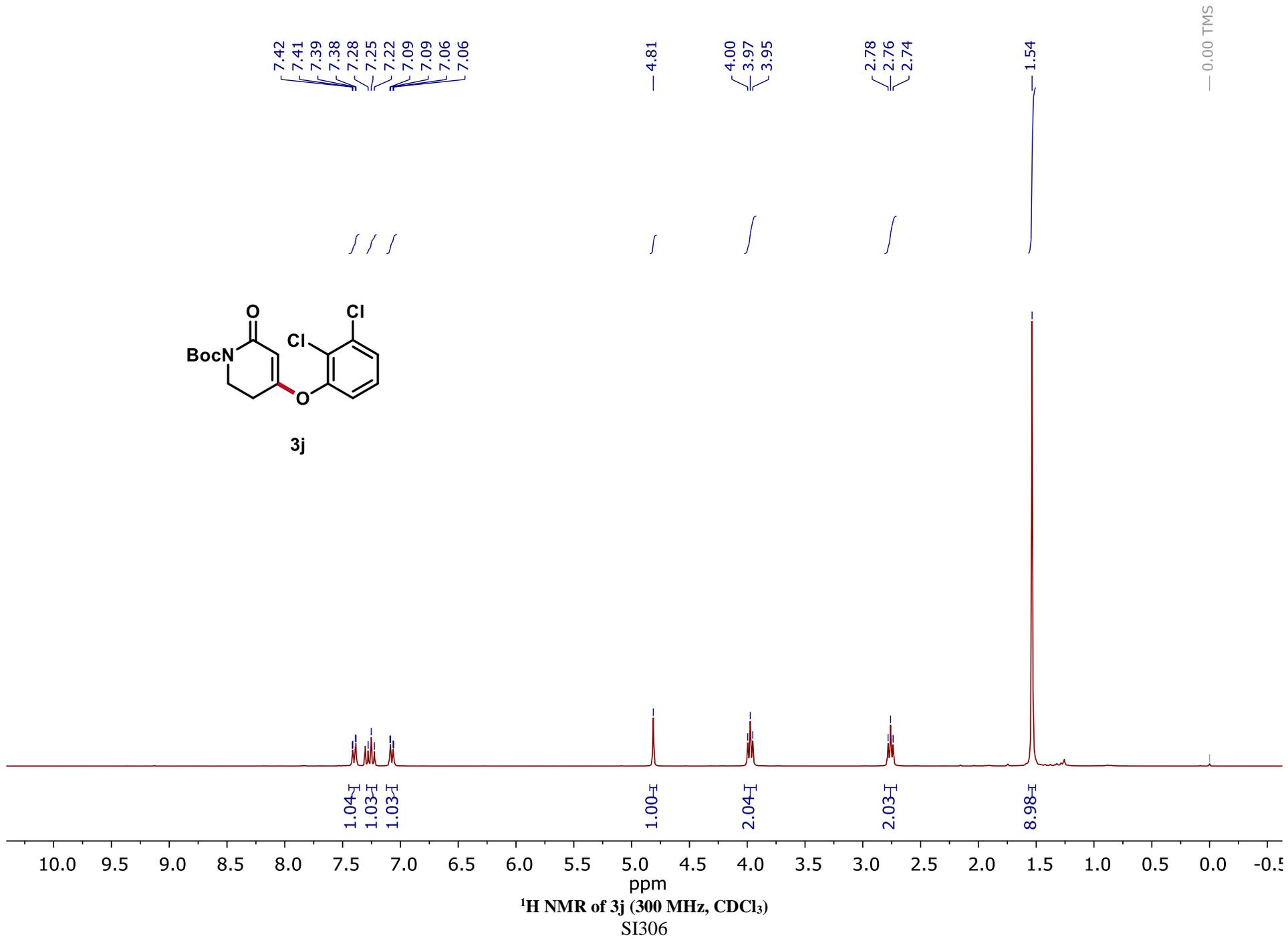
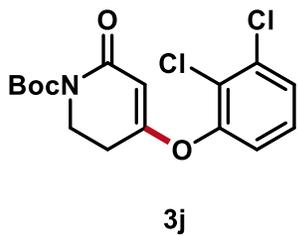
^{13}C NMR of 3h (75 MHz, CDCl_3)
SI303

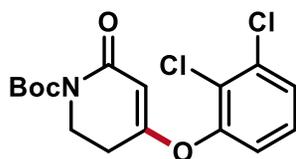




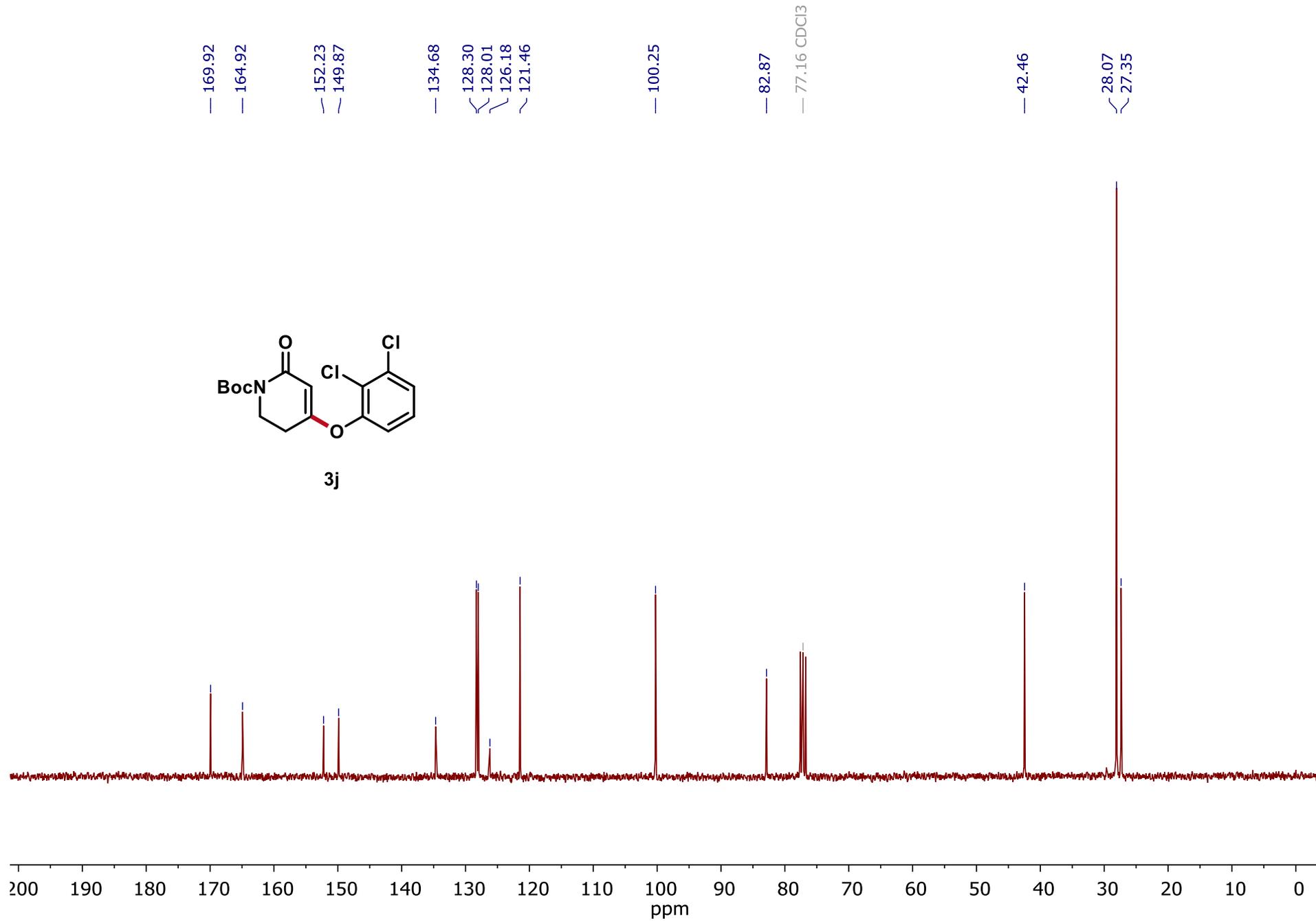
3i



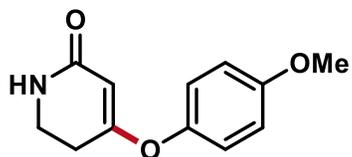




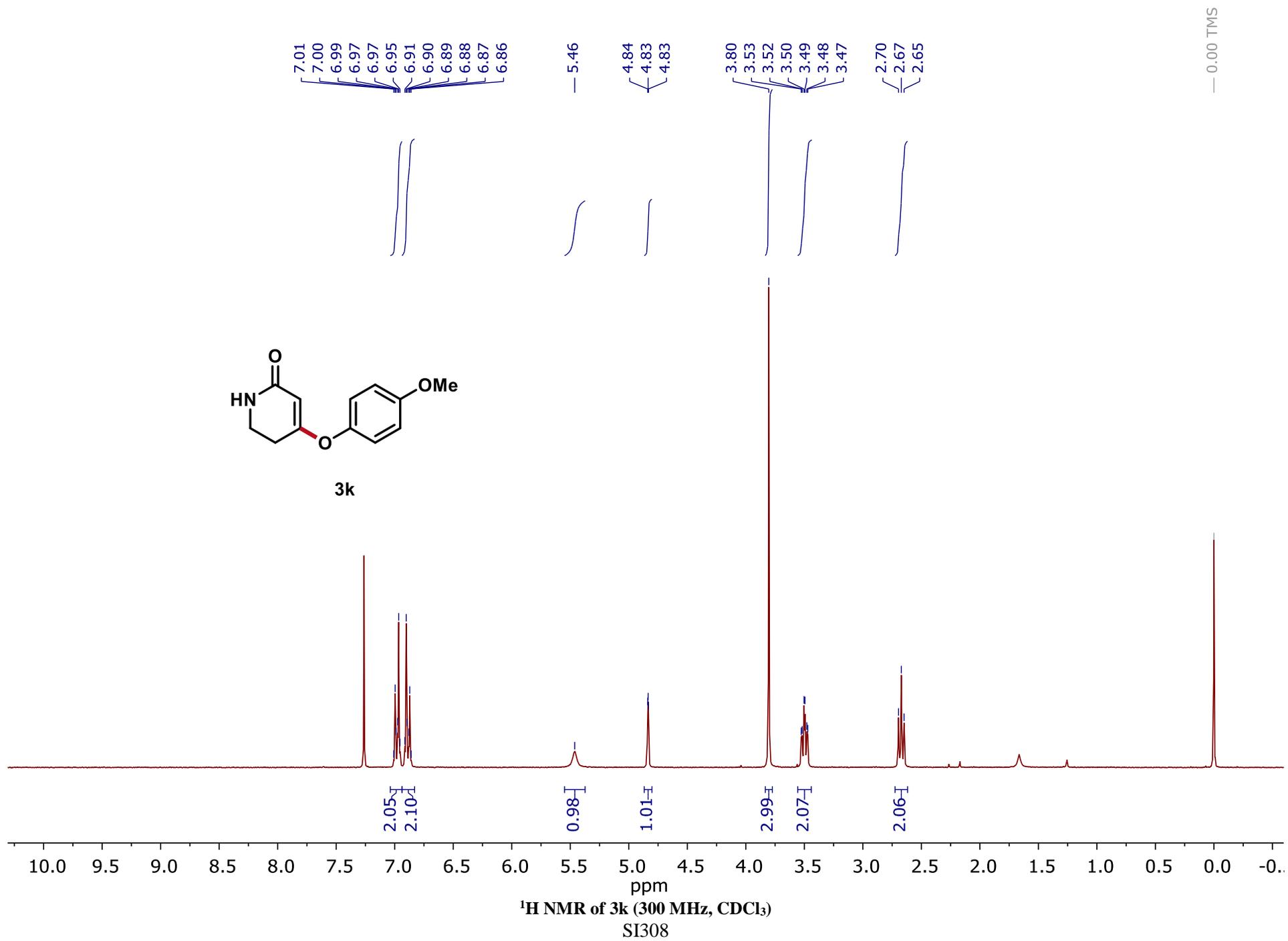
3j

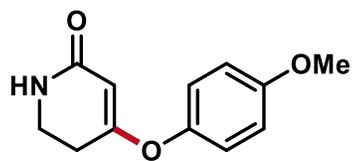


^{13}C NMR of 3j (75 MHz, CDCl_3)
SI307

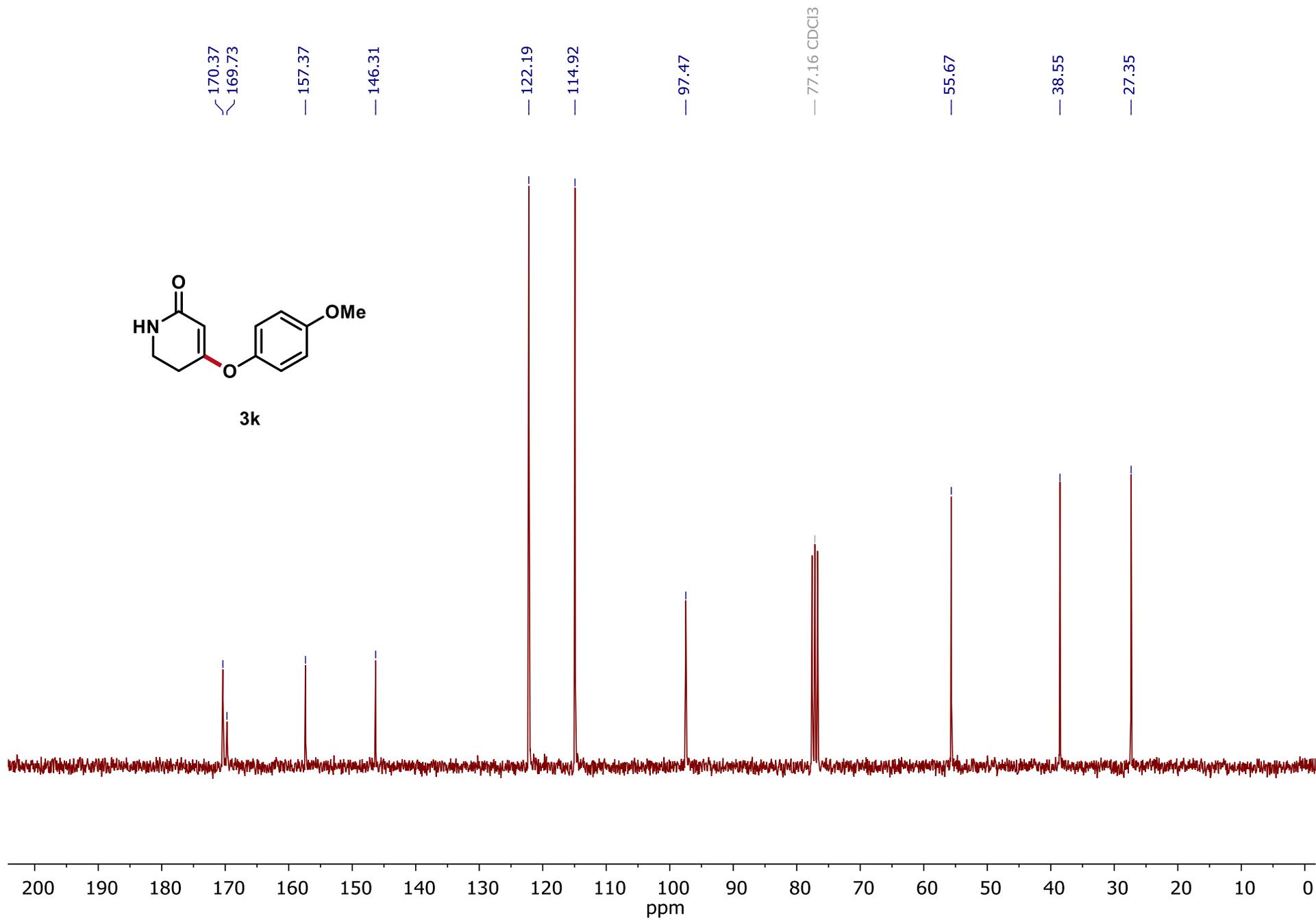


3k

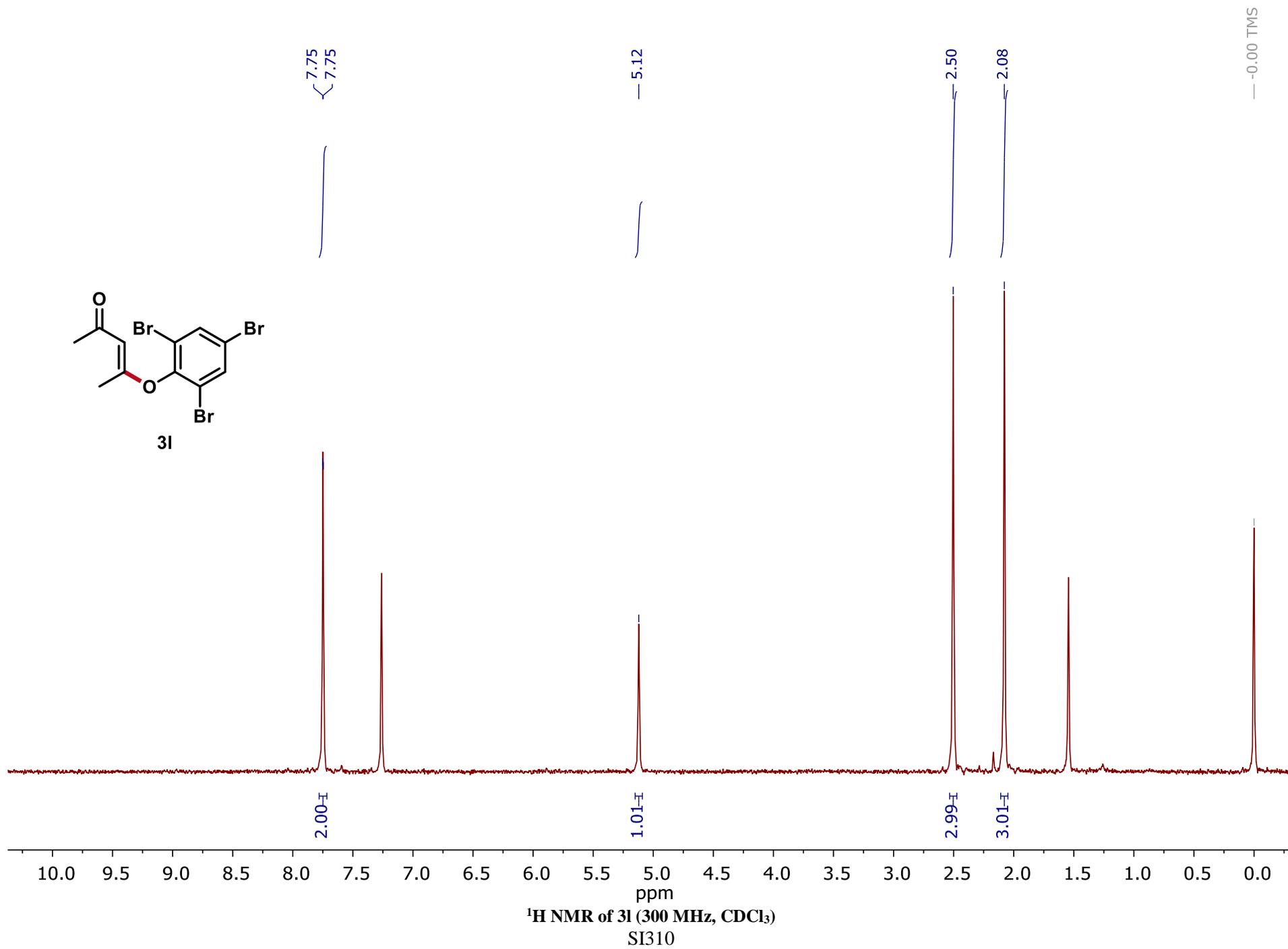
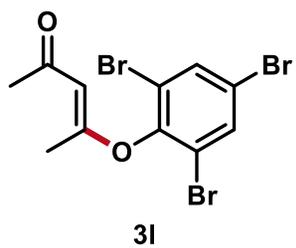


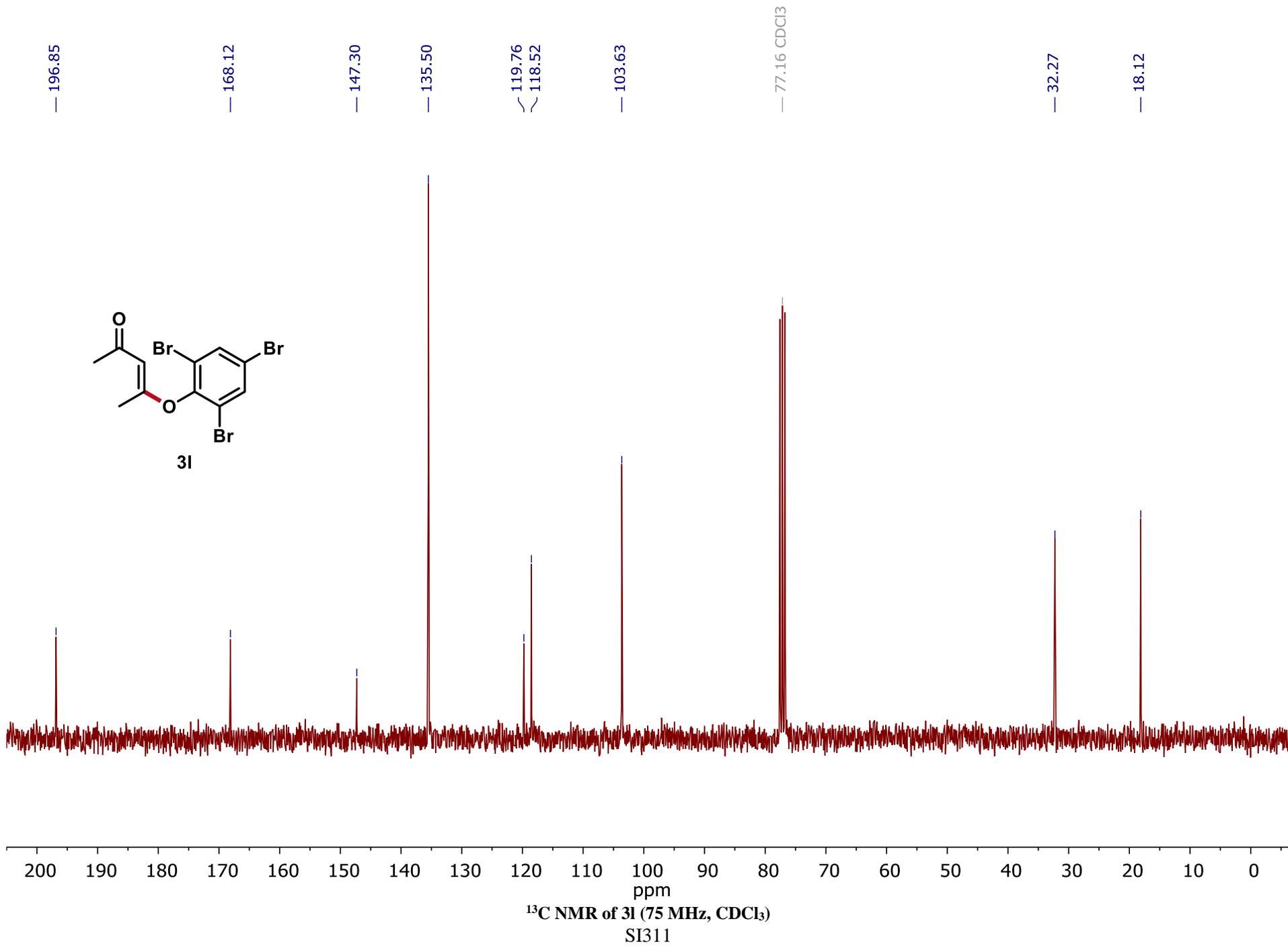
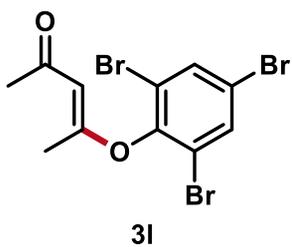


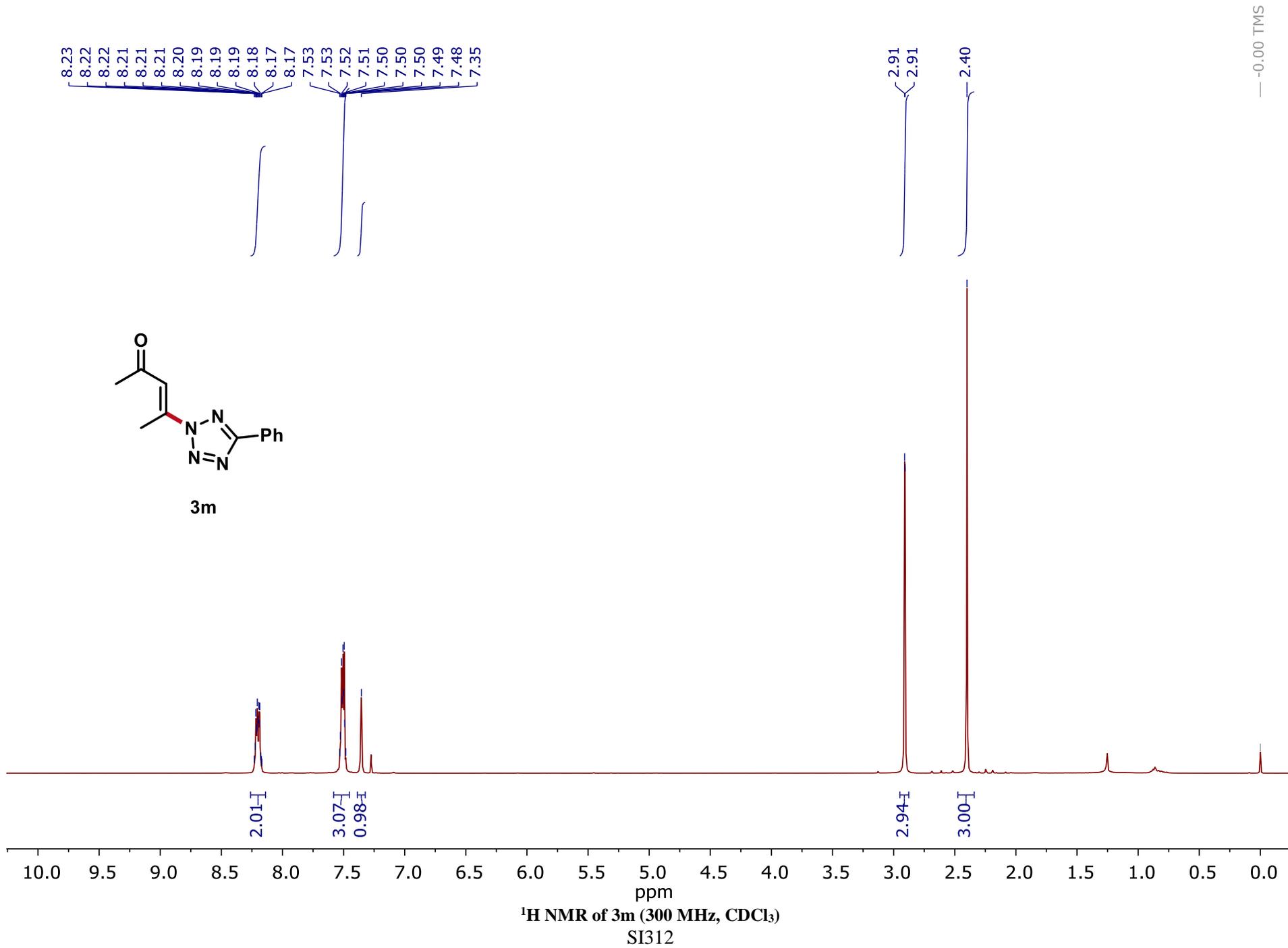
3k

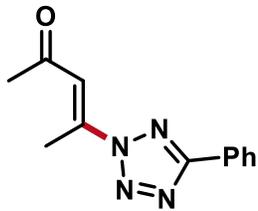


^{13}C NMR of 3k (75 MHz, CDCl_3)
SI309

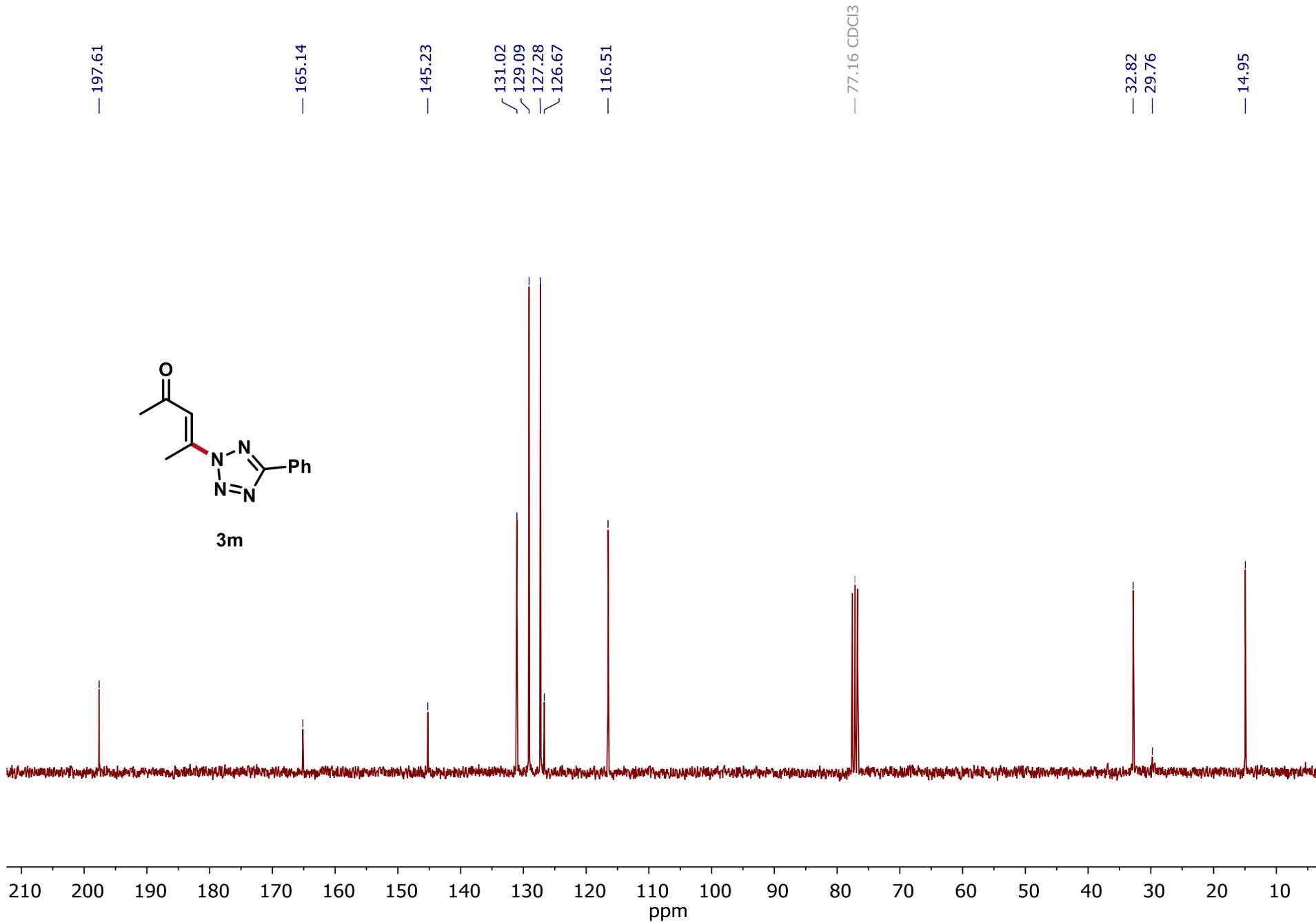




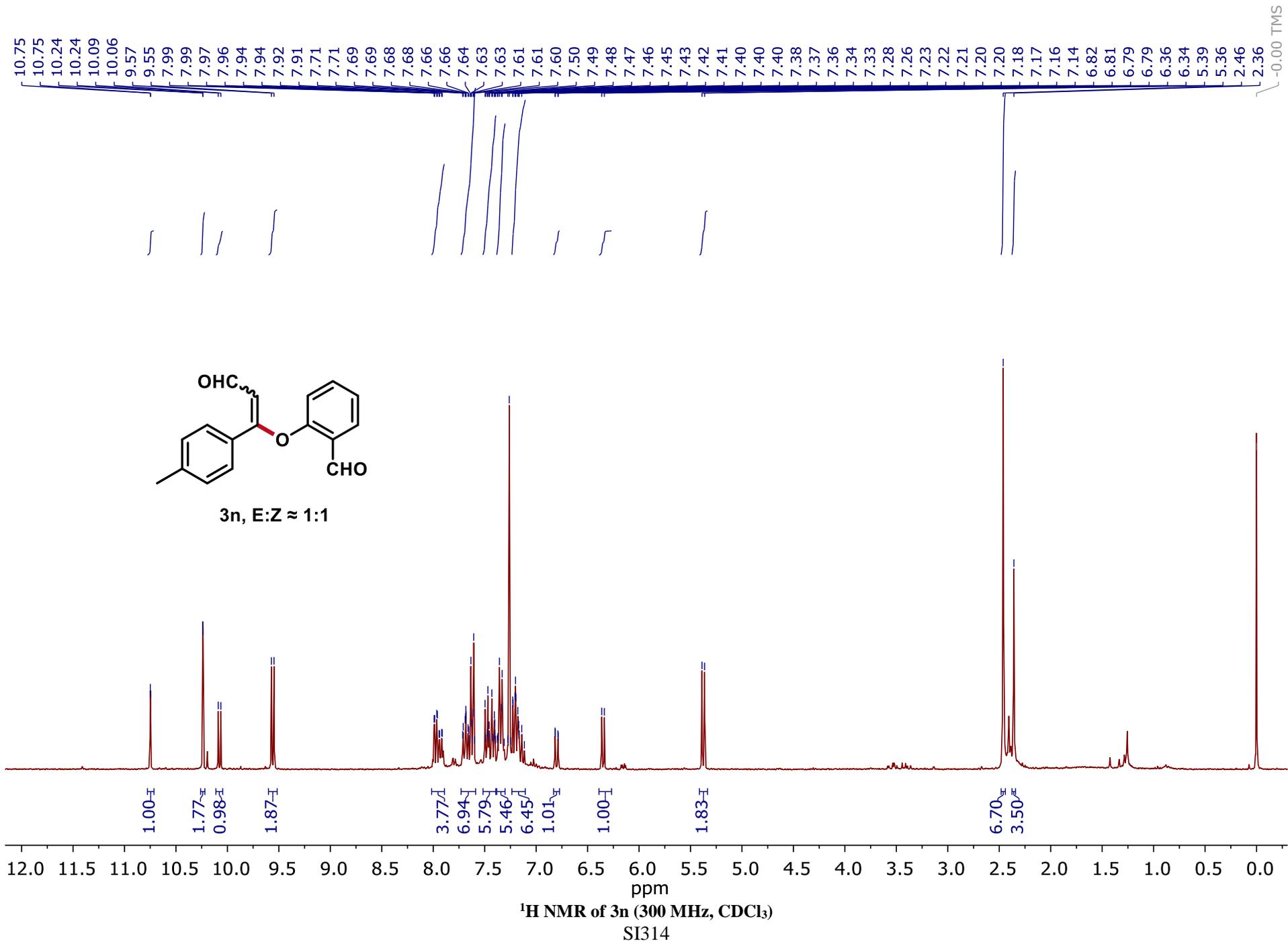




3m



^{13}C NMR of 3m (75 MHz, CDCl_3)
SI313



192.05
189.93
188.43
188.00

176.70

166.22

159.31

154.96

142.77

142.43

136.09

135.98

130.48

130.08

130.05

129.50

129.44

127.28

126.78

123.50

122.77

116.53

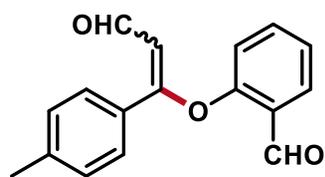
116.37

110.21

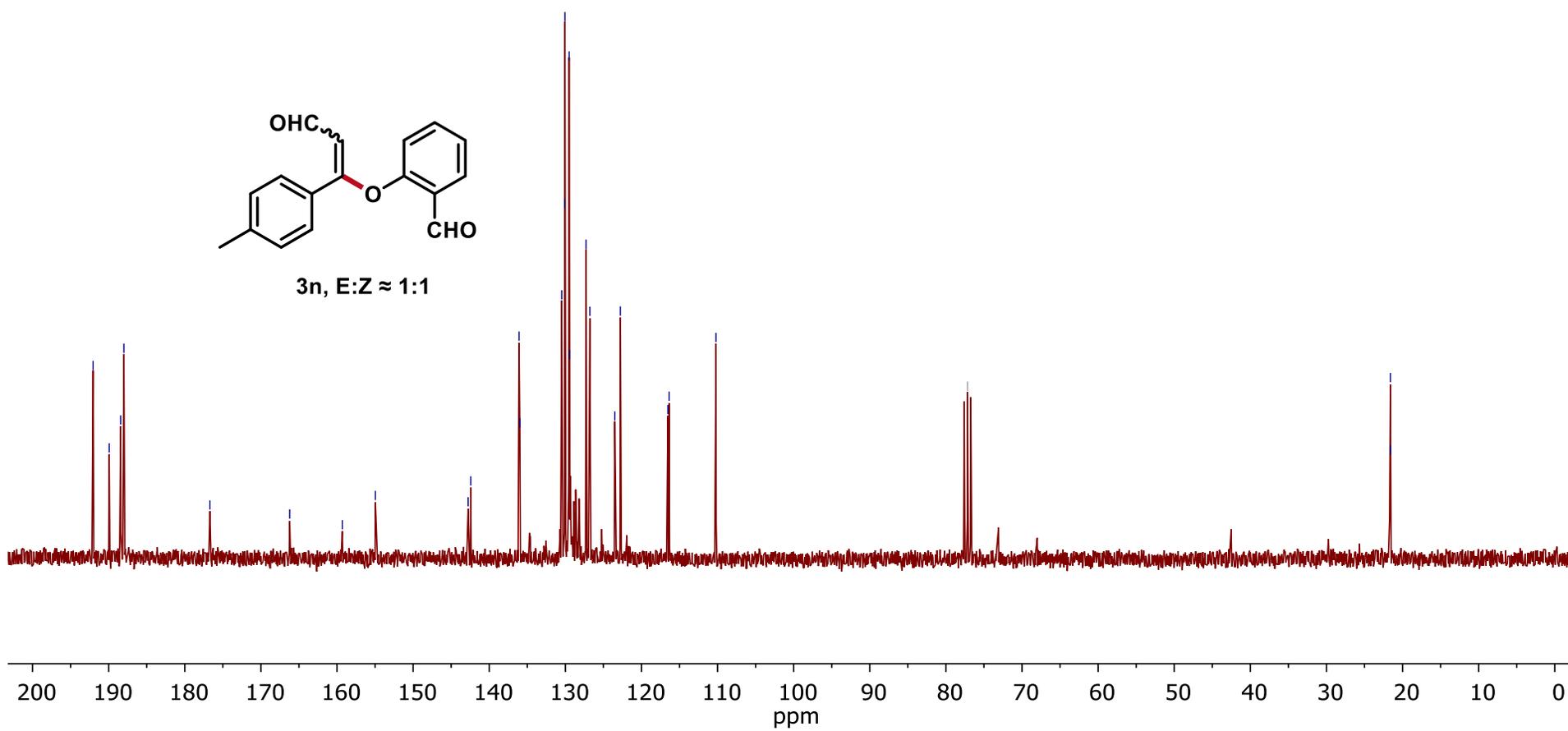
77.16 CDCl₃

21.60

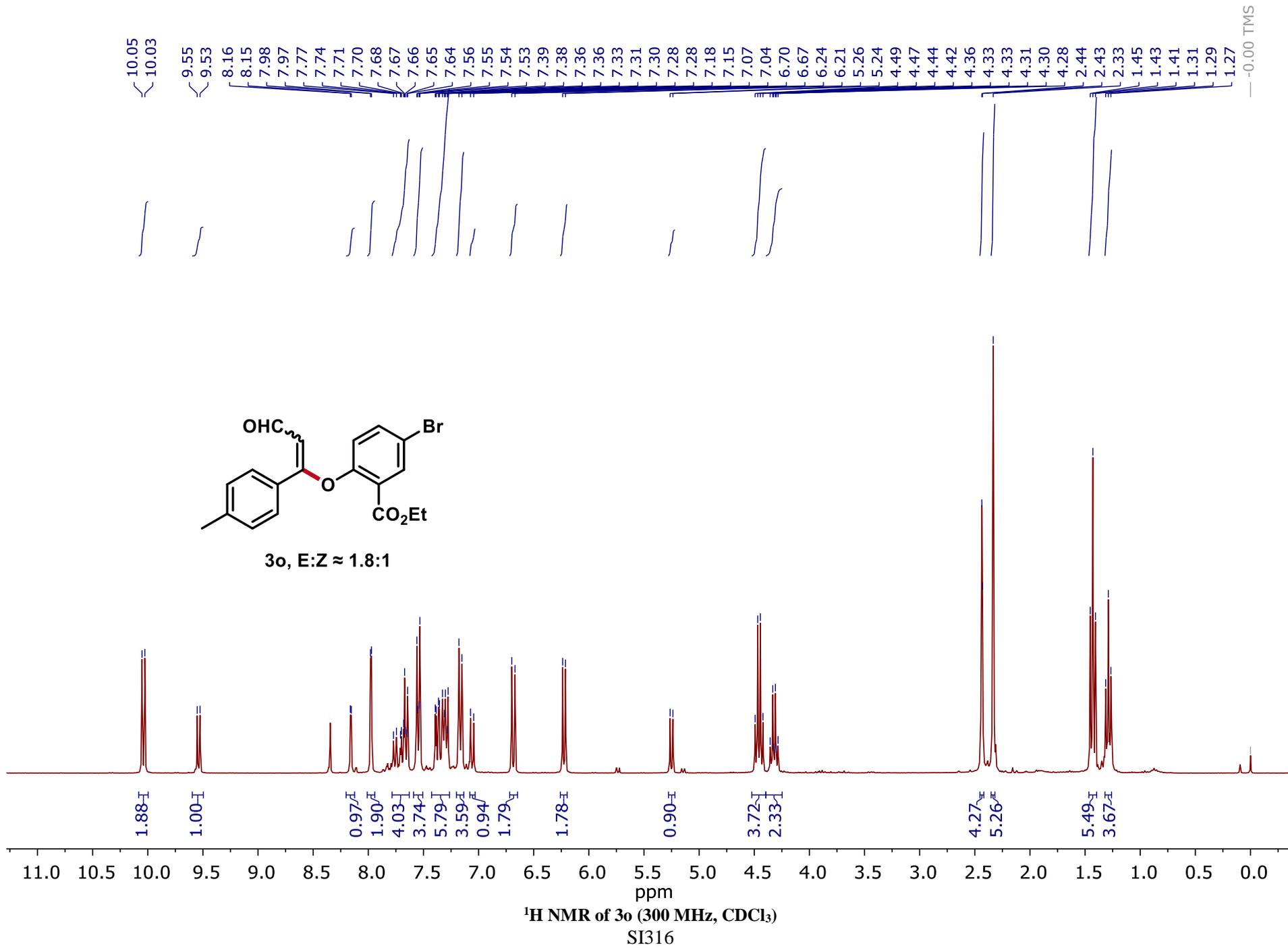
21.56



3n, E:Z ≈ 1:1



¹³C NMR of 3n (75 MHz, CDCl₃)
SI315



192.13
190.32

176.72

166.74
164.11
162.88

155.28
151.60

142.51
142.10

137.05
136.10

135.17
134.49

130.36
130.25

129.95
129.37

129.29
127.50

125.52
125.40

122.95
119.33

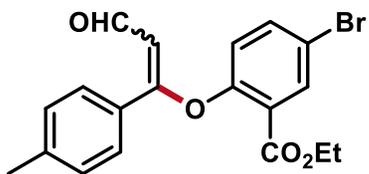
119.06
116.03
115.48
108.80

77.16 CDCl₃

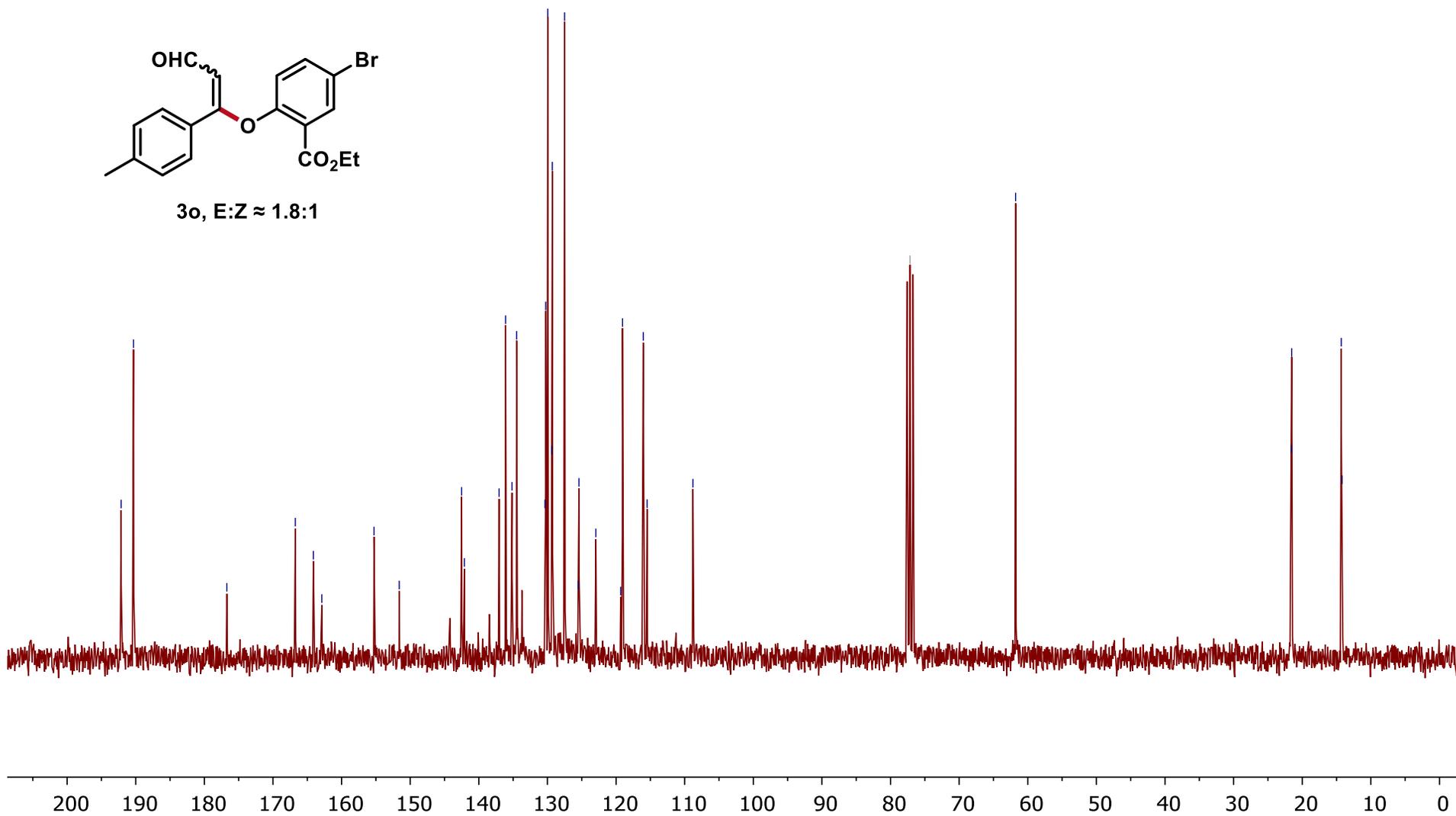
61.77

21.57
21.54

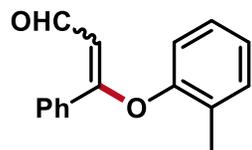
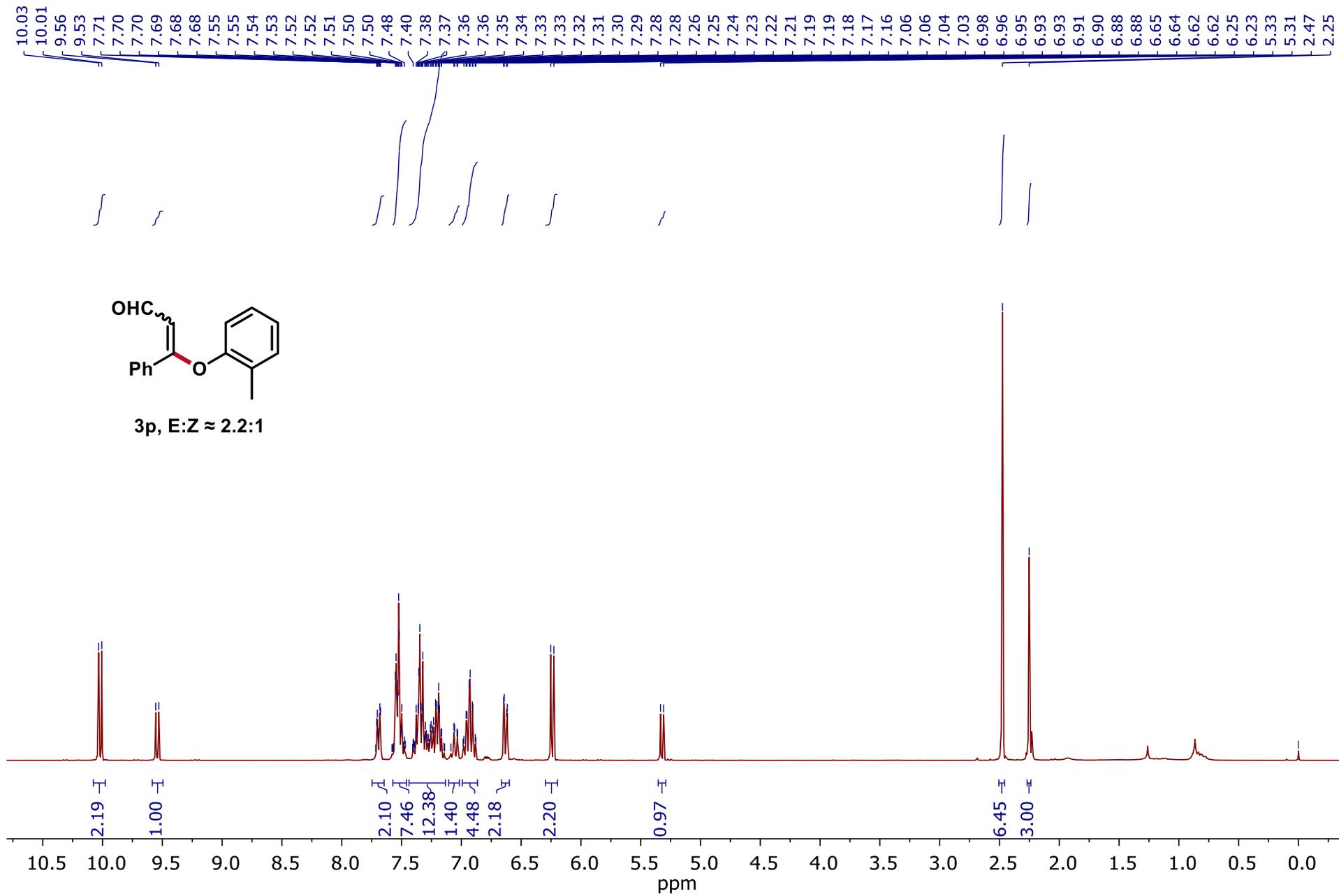
14.31
14.20



3o, E:Z ≈ 1.8:1



¹³C NMR of 3o (75 MHz, CDCl₃)
SI317



3p, E:Z ≈ 2.2:1

¹H NMR of 3p (300 MHz, CDCl₃)
SI318

192.43
190.68

176.23

167.70

155.51

151.40

132.95

132.49

131.94

131.52

131.42

131.36

130.11

129.88

128.99

128.62

127.77

127.21

127.16

126.86

126.53

123.25

121.50

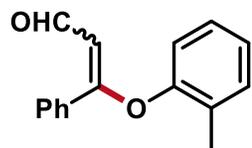
116.10

115.65

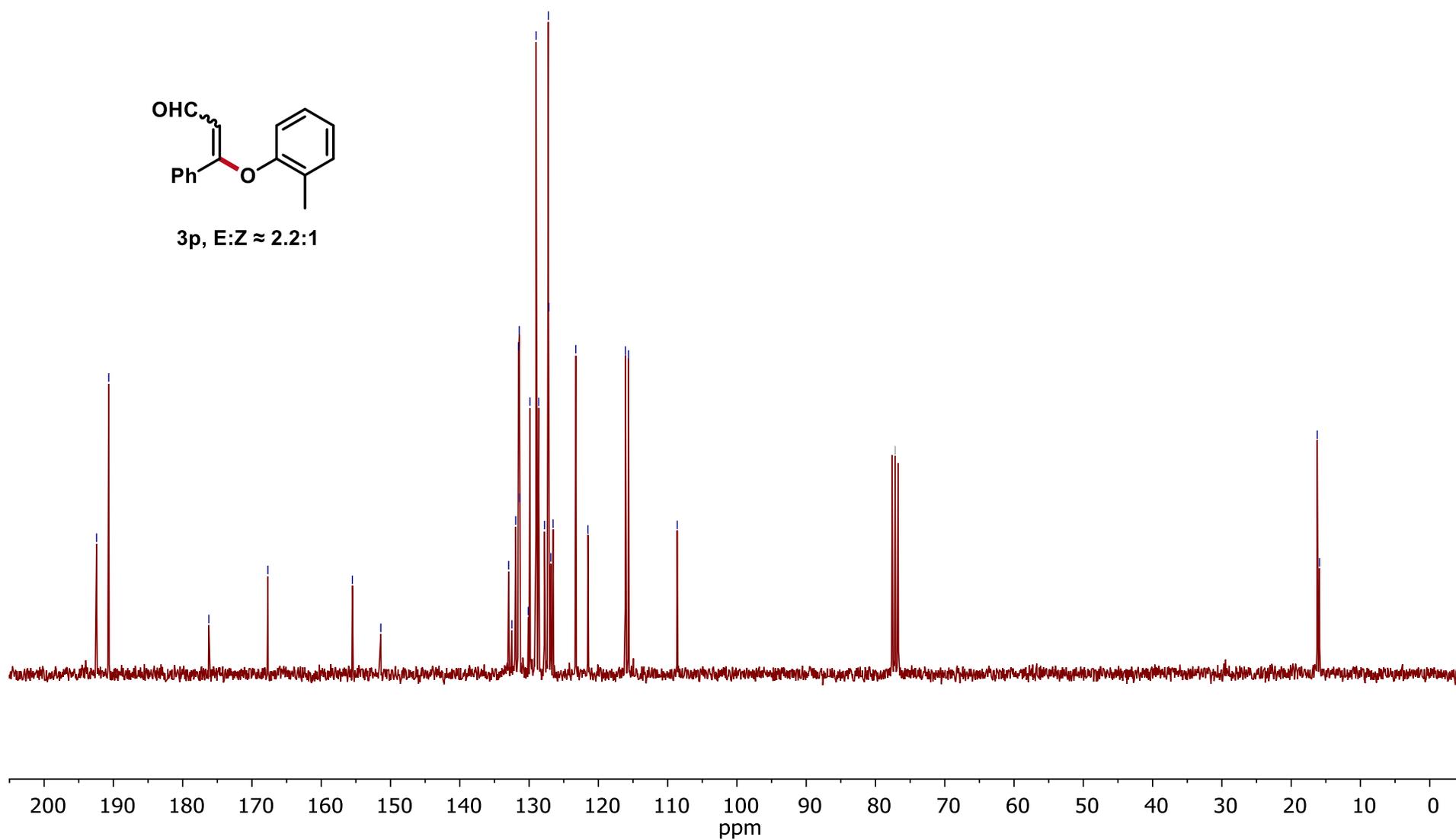
108.62

77.16 CDCl₃

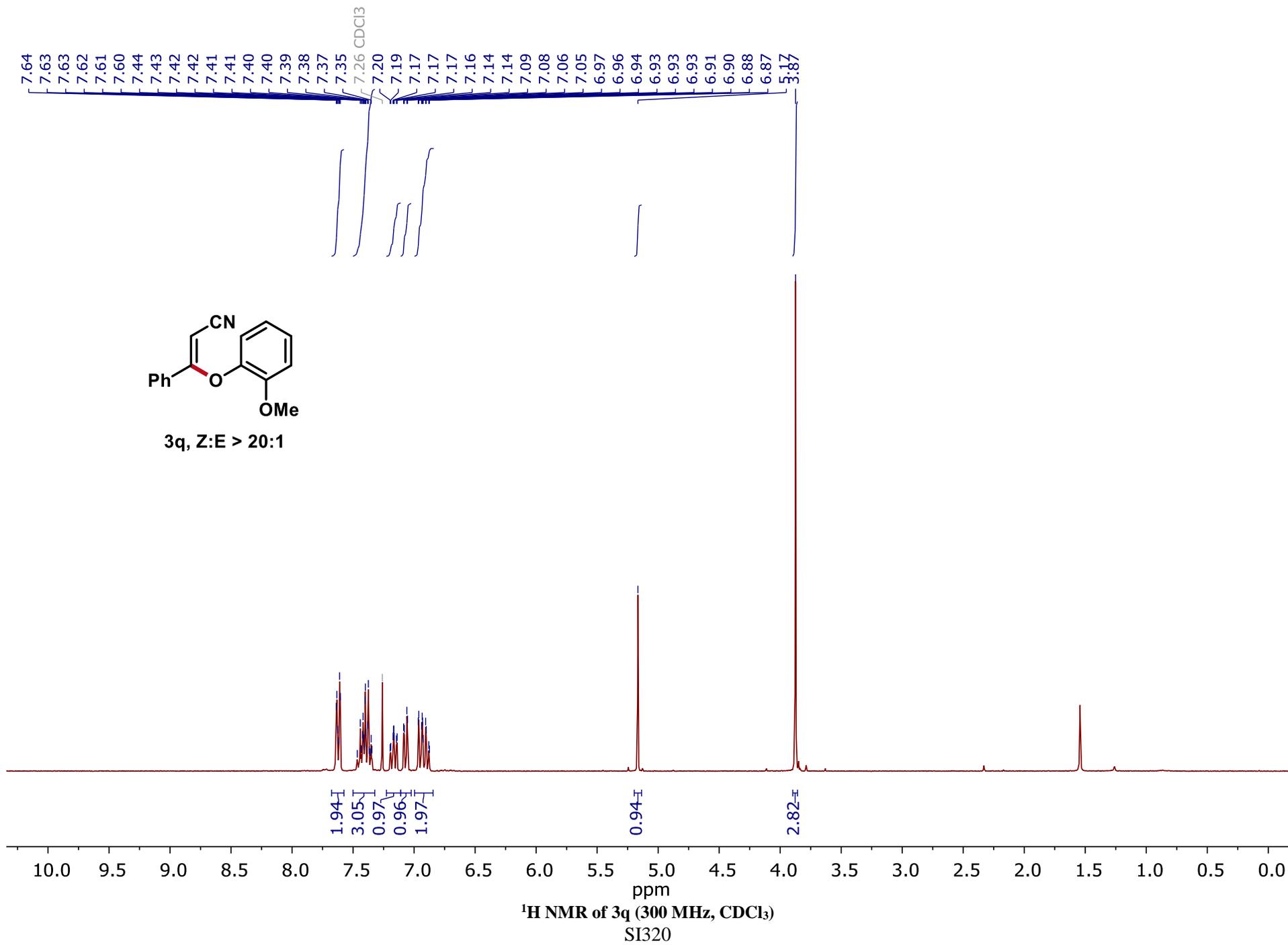
16.24
15.91

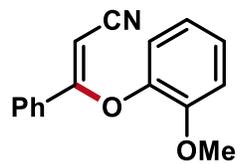


3p, E:Z ≈ 2.2:1

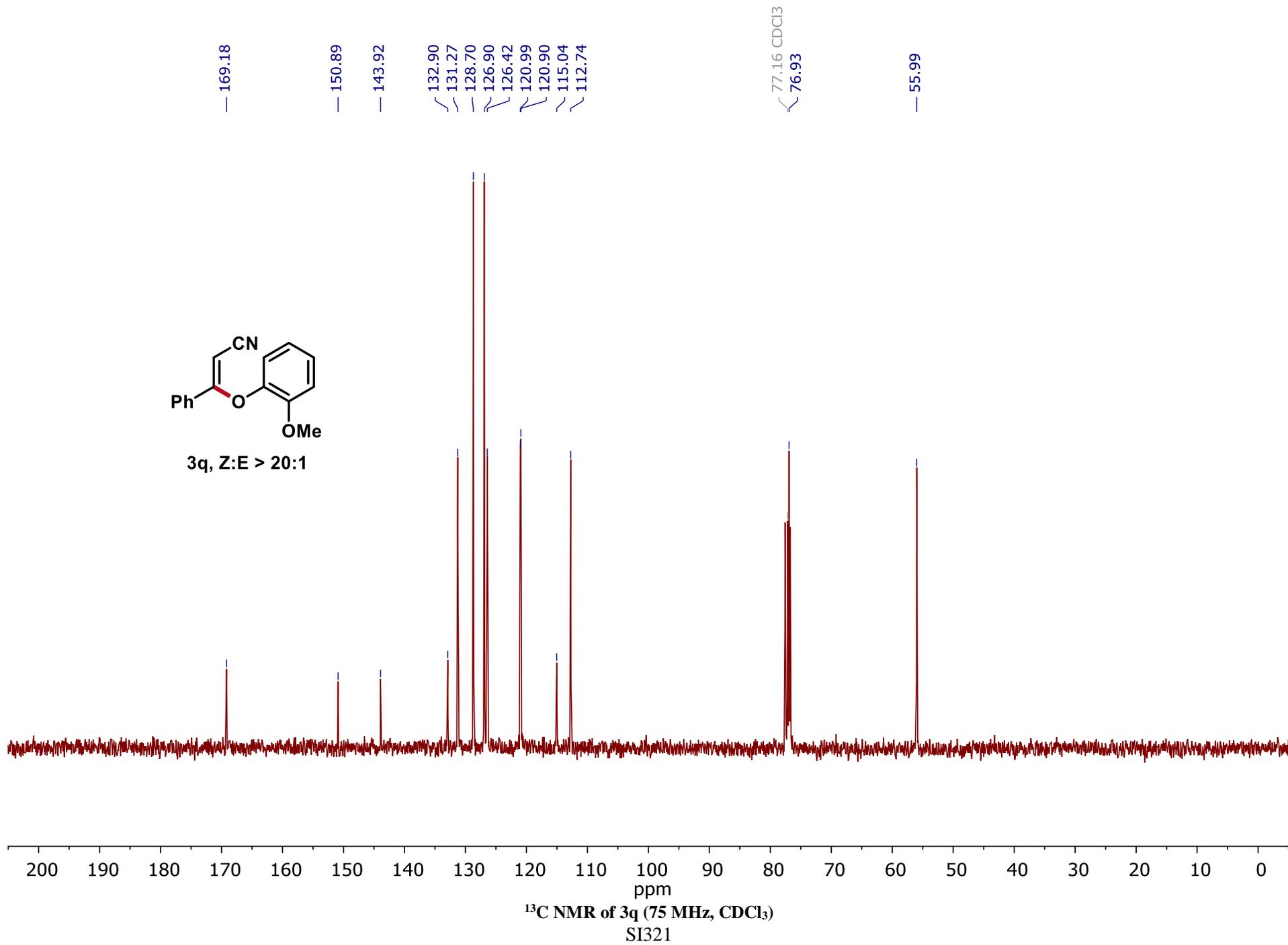


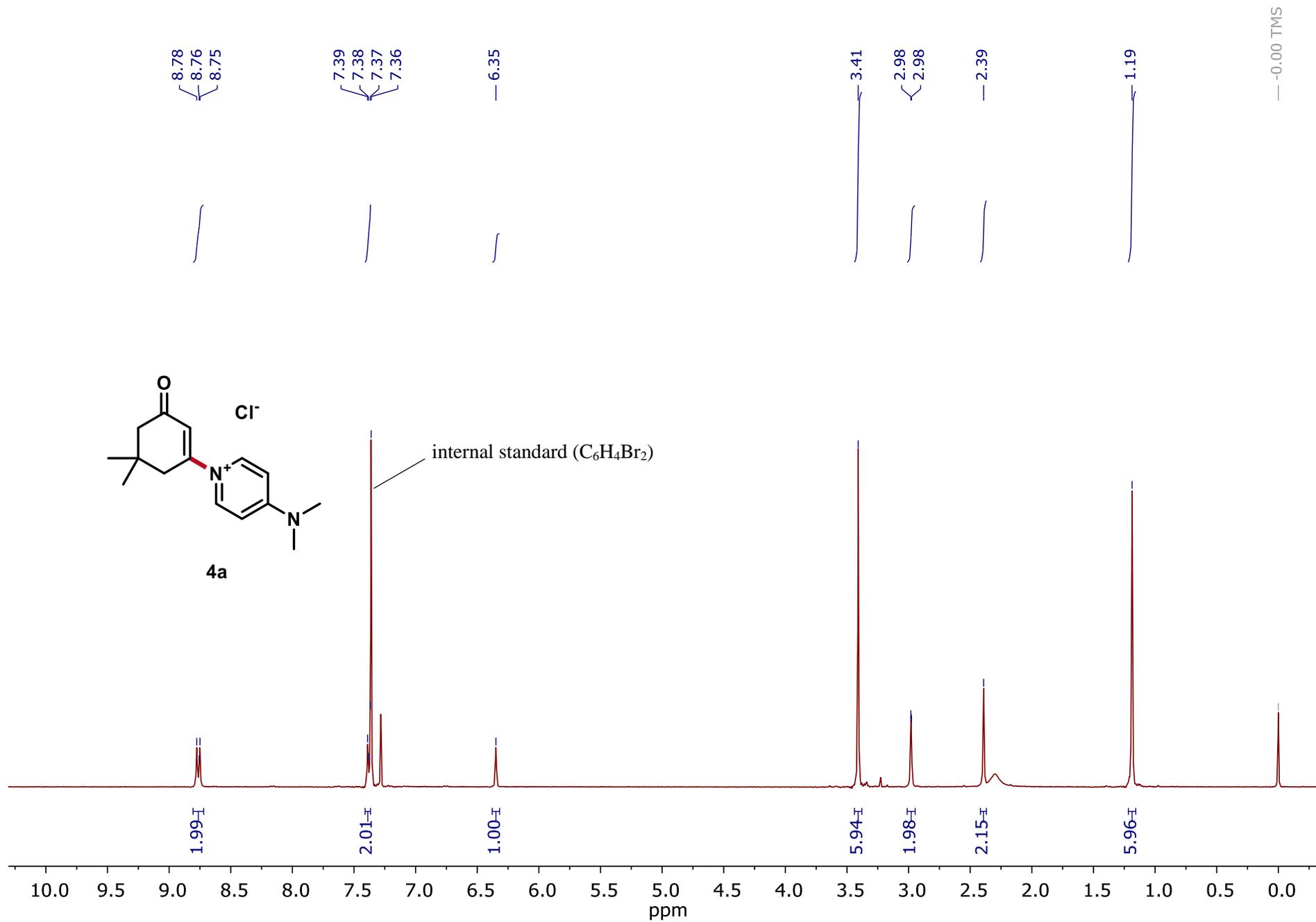
¹³C NMR of 3p (75 MHz, CDCl₃)
SI319





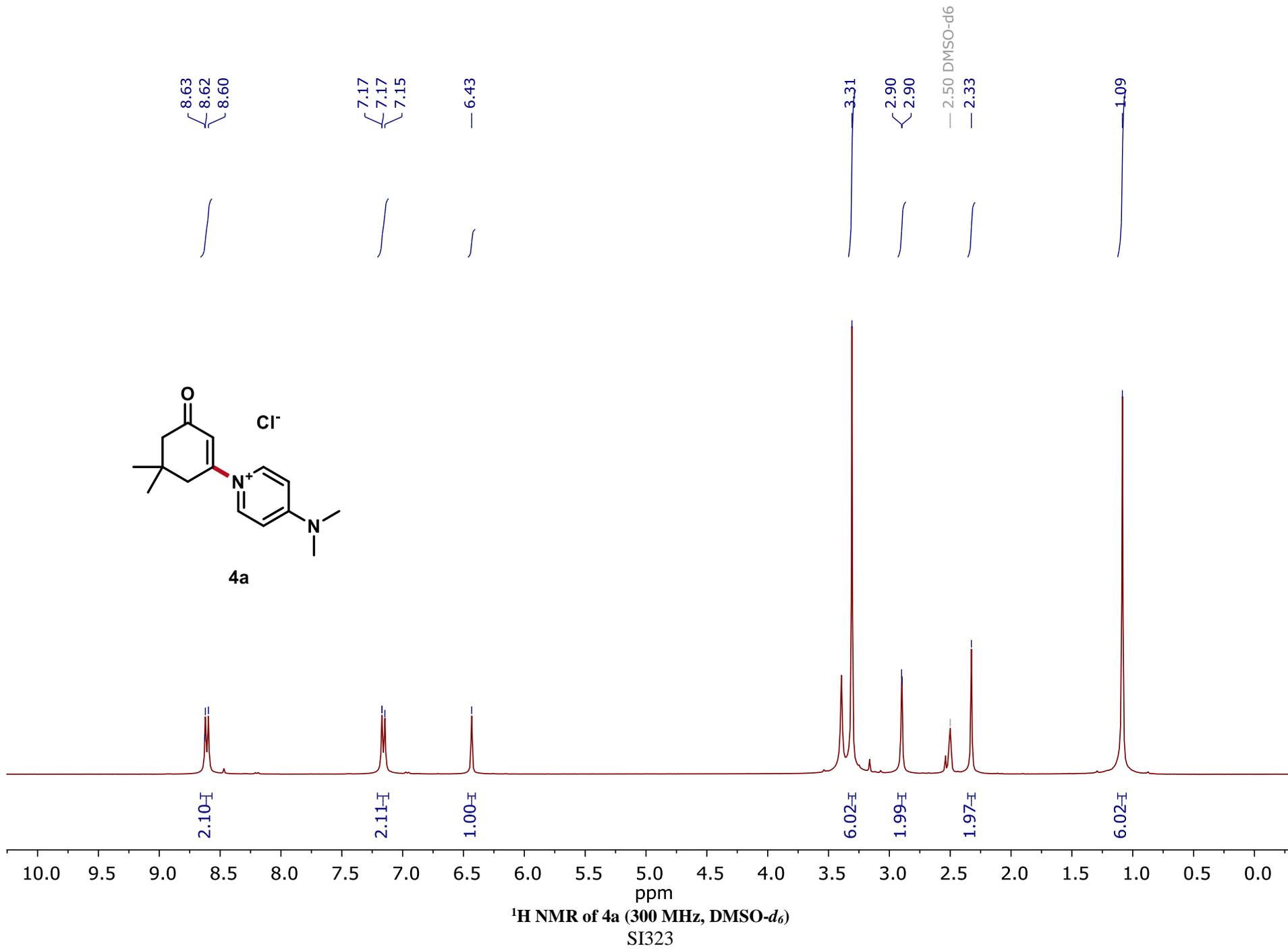
3q, Z:E > 20:1

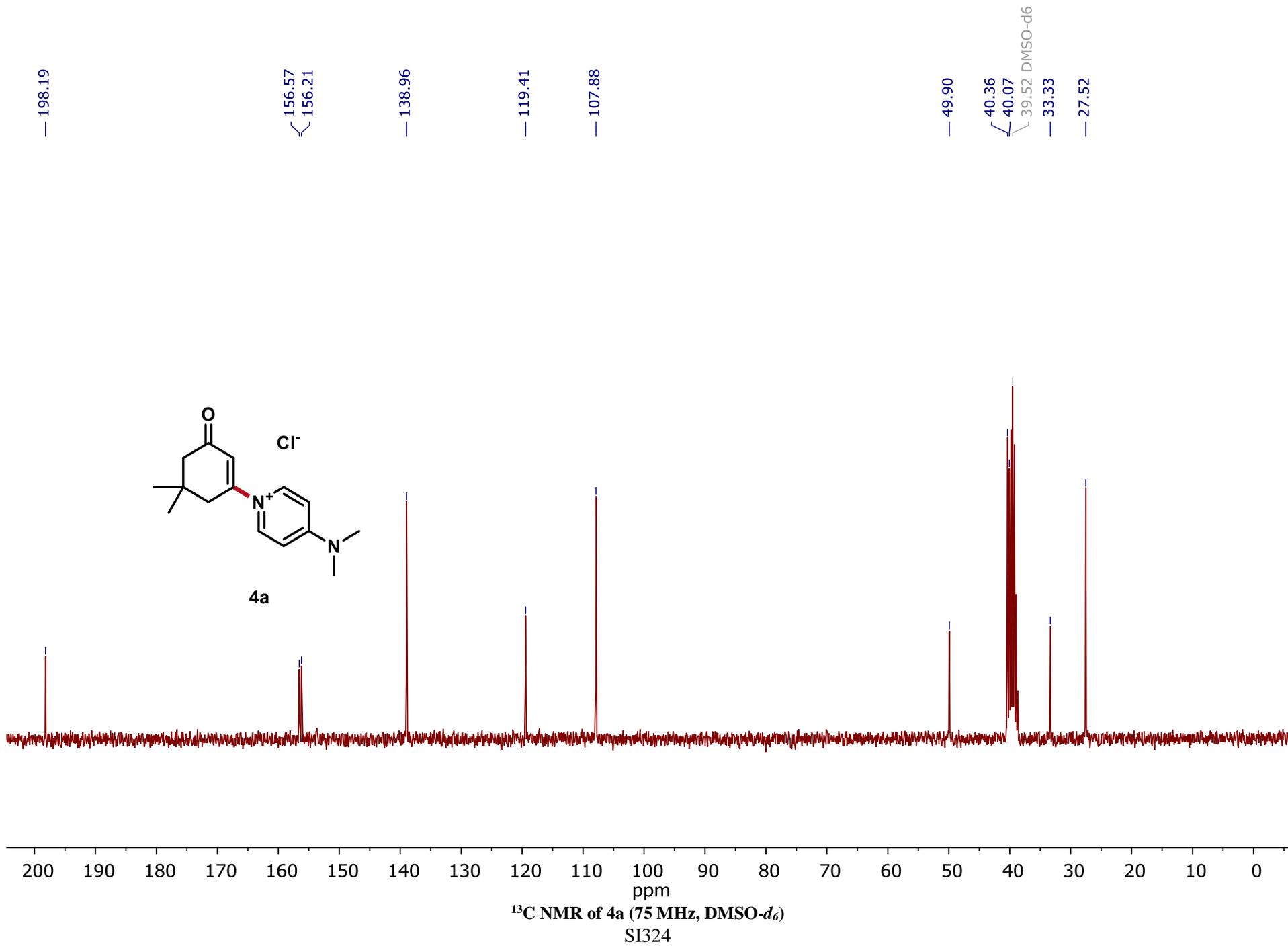


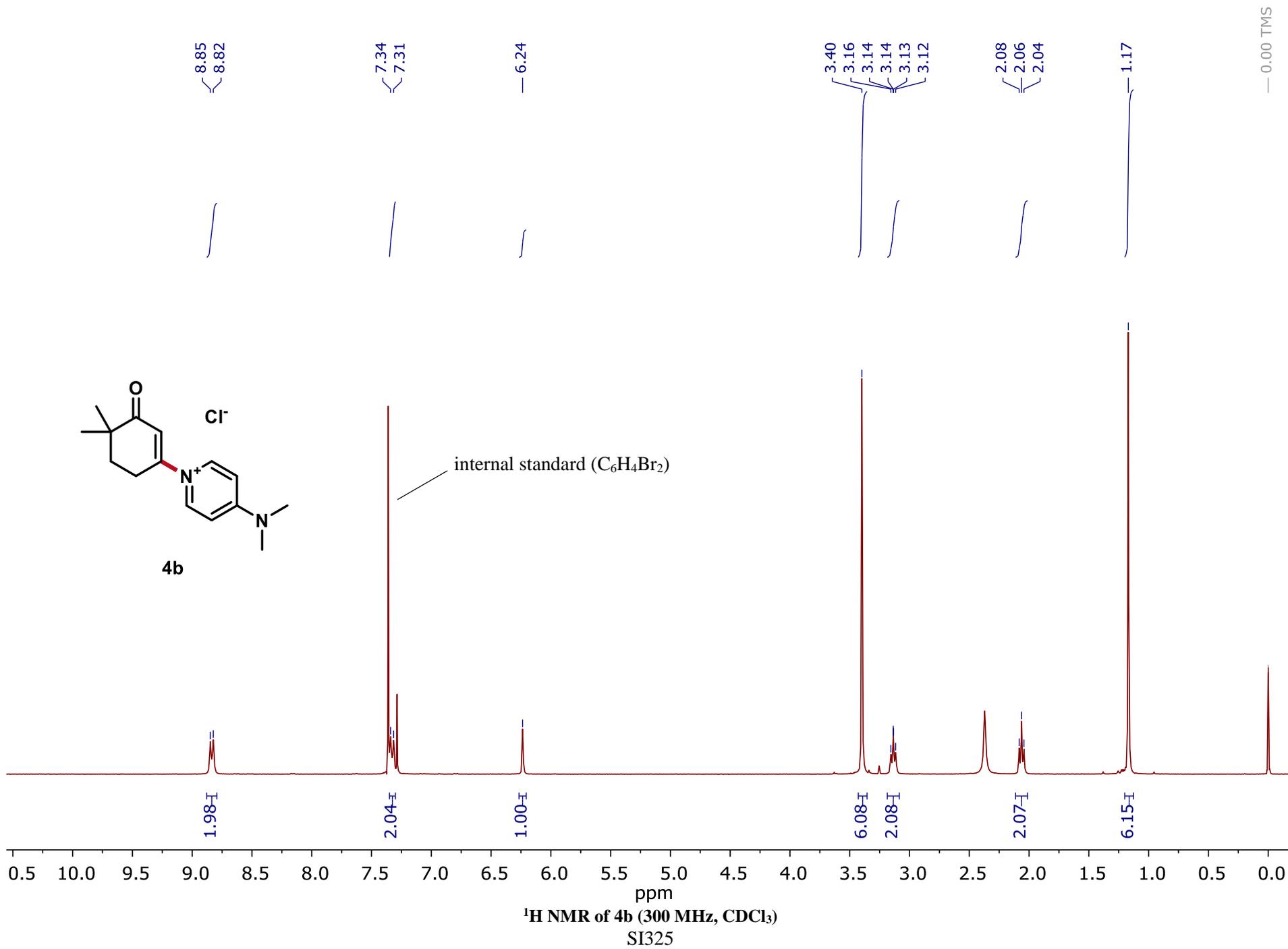


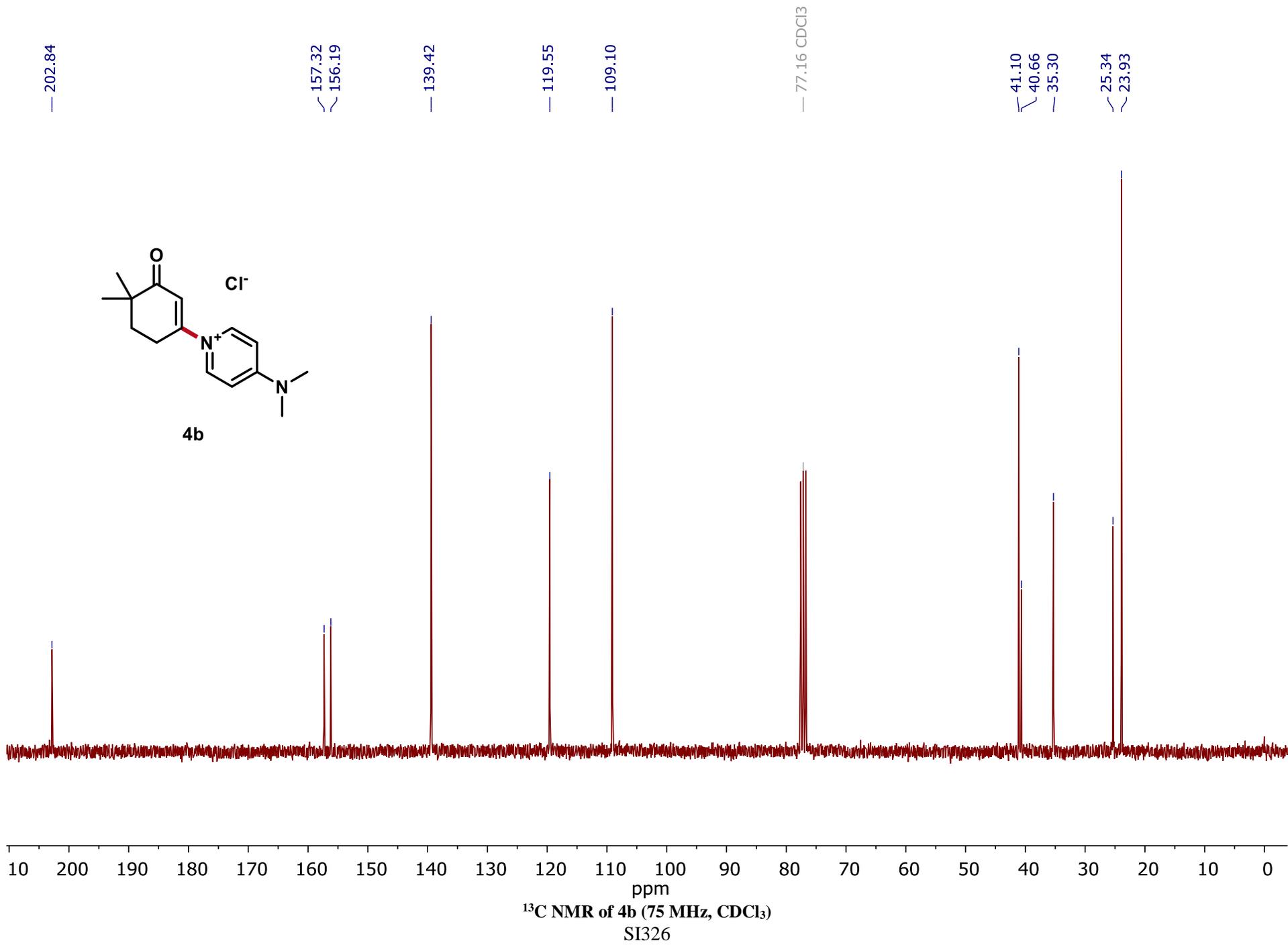
¹H NMR of 4a (300 MHz, CDCl₃)

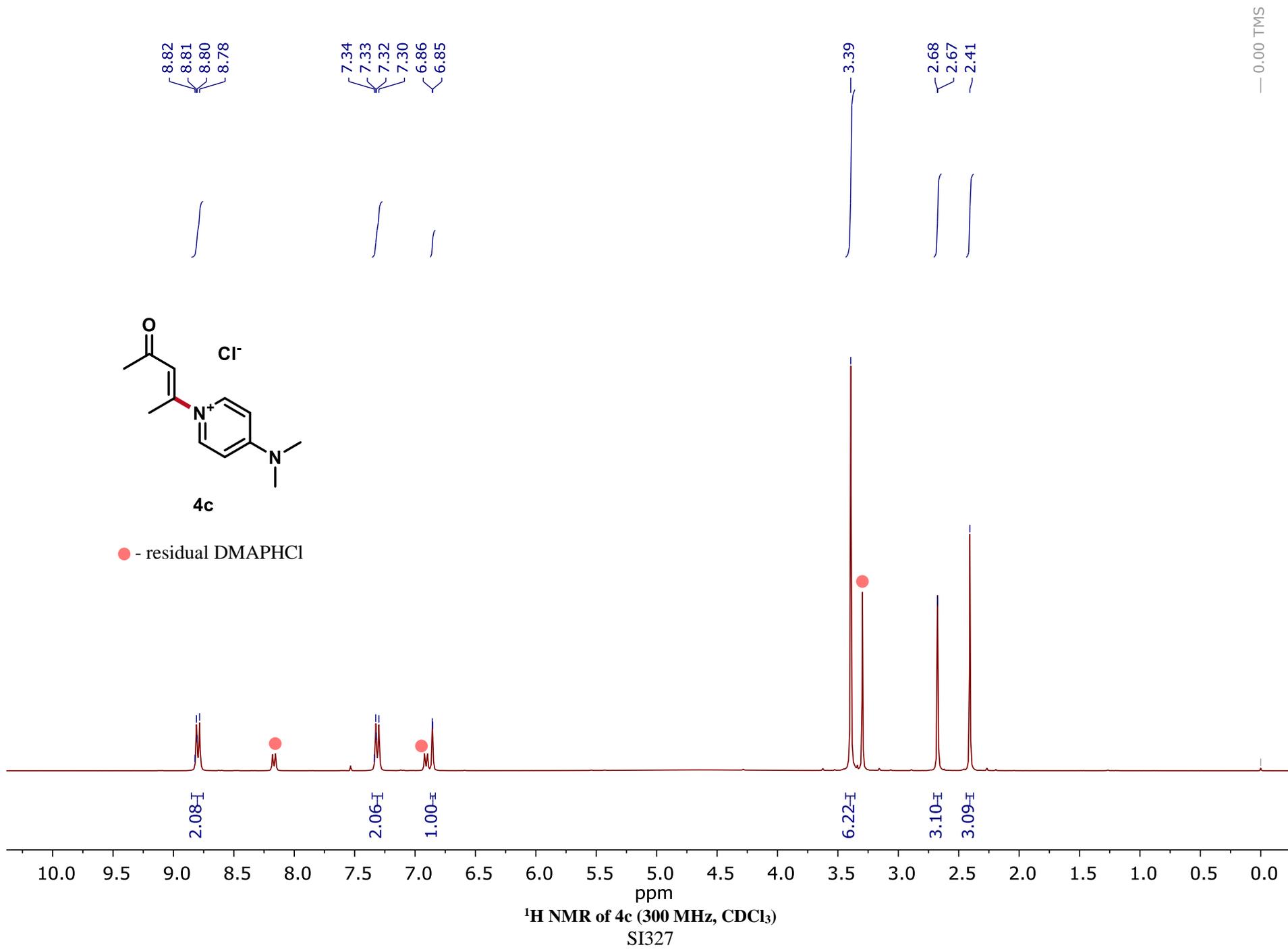
SI322

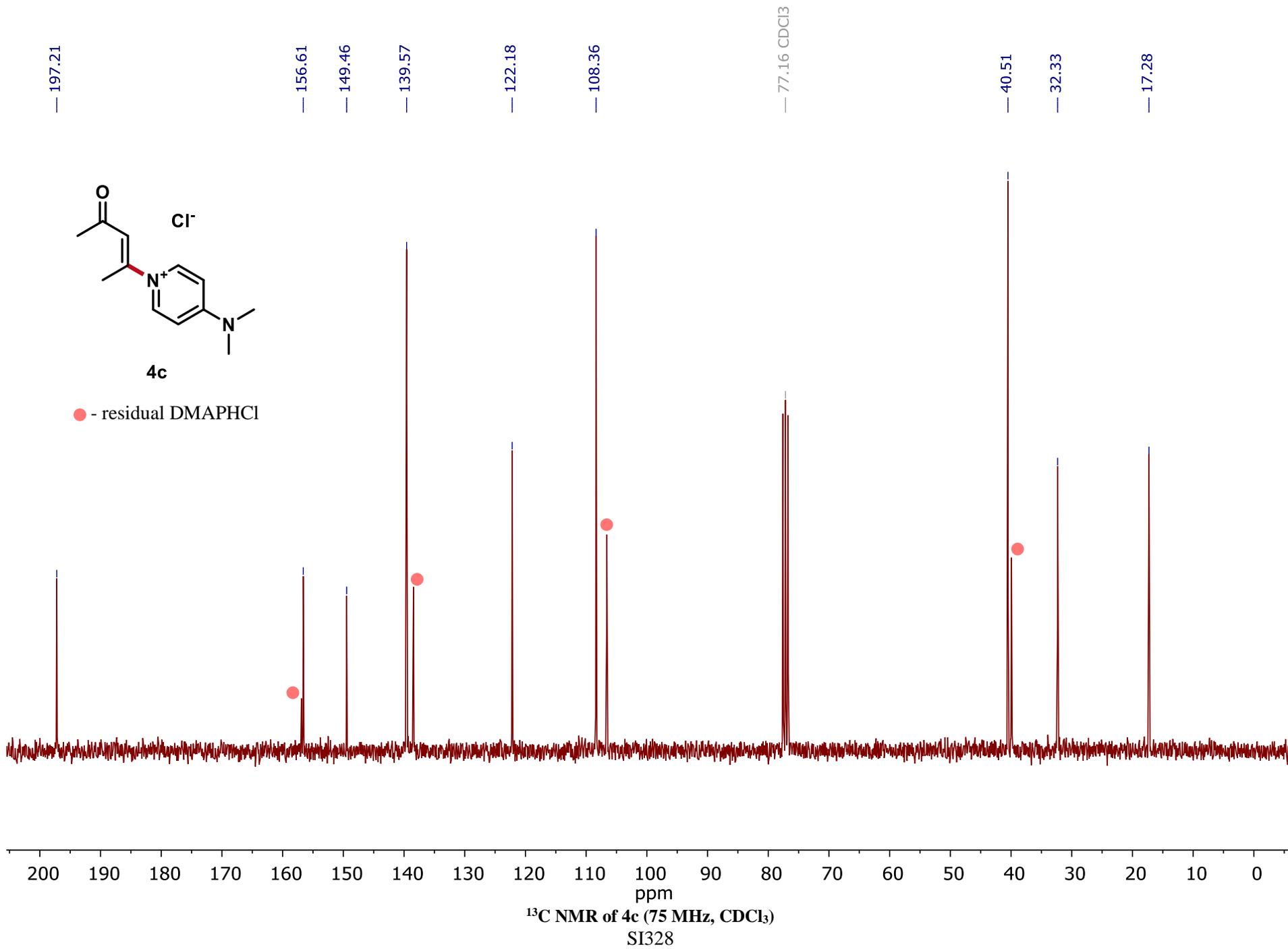


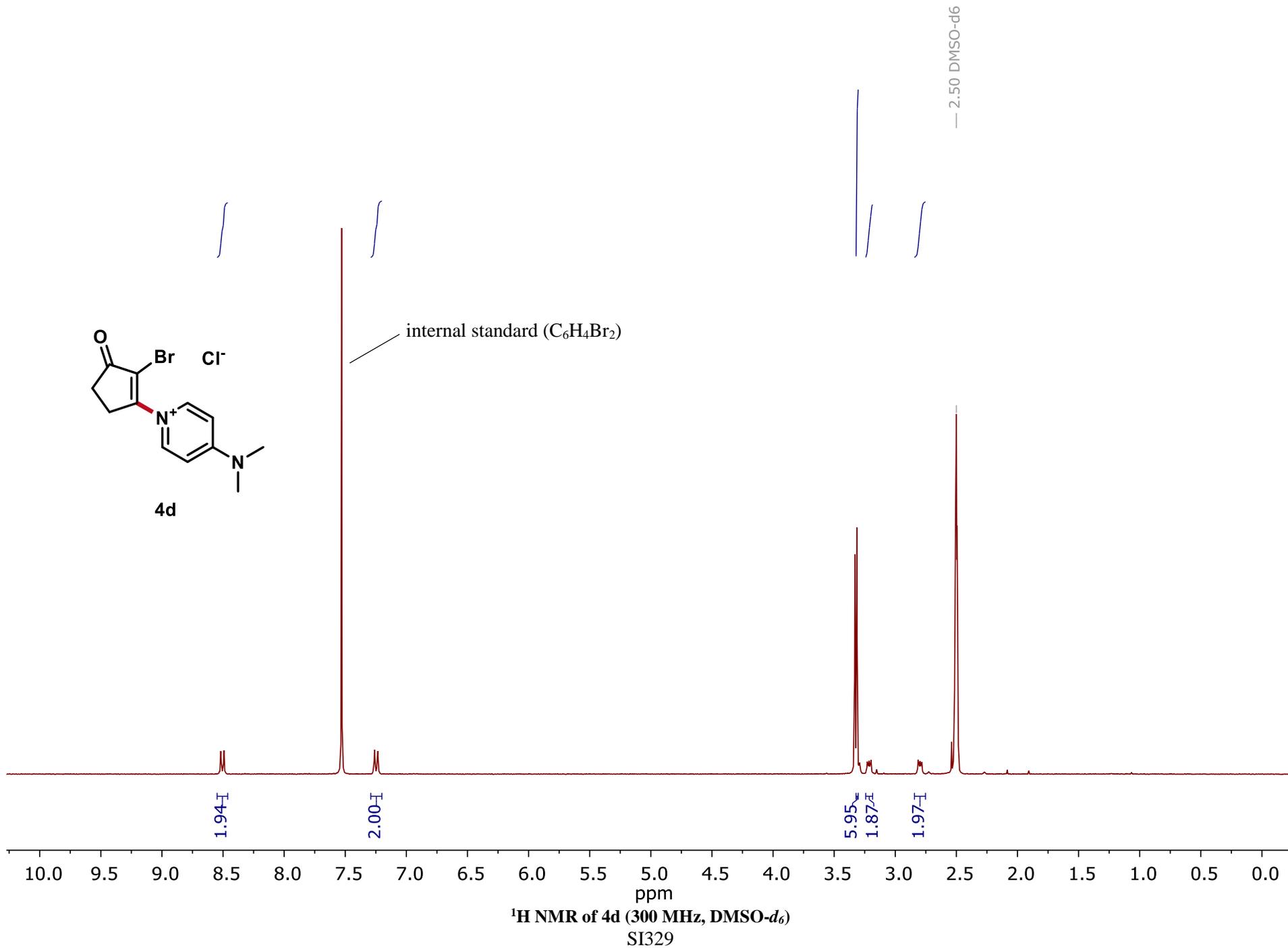


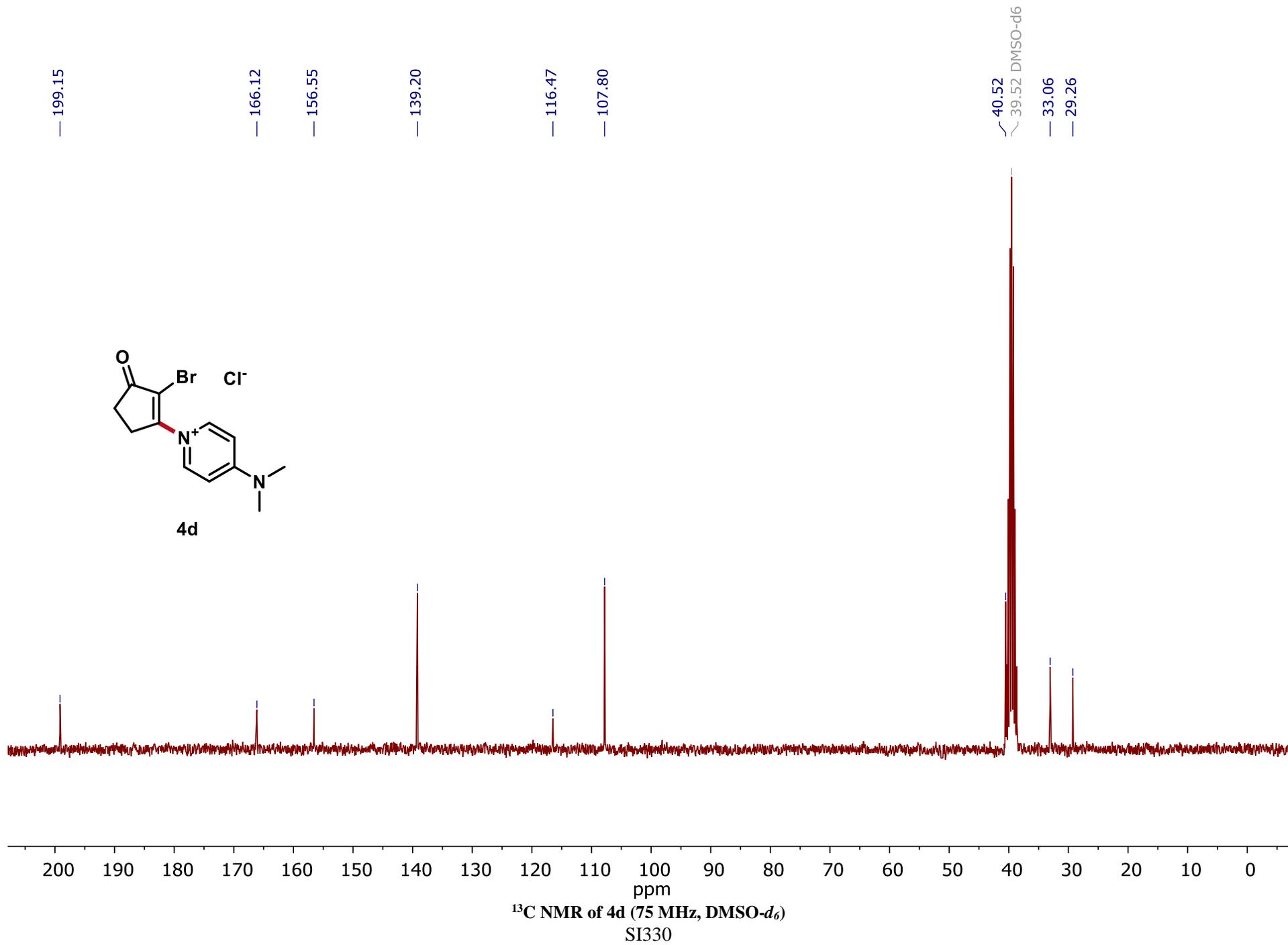


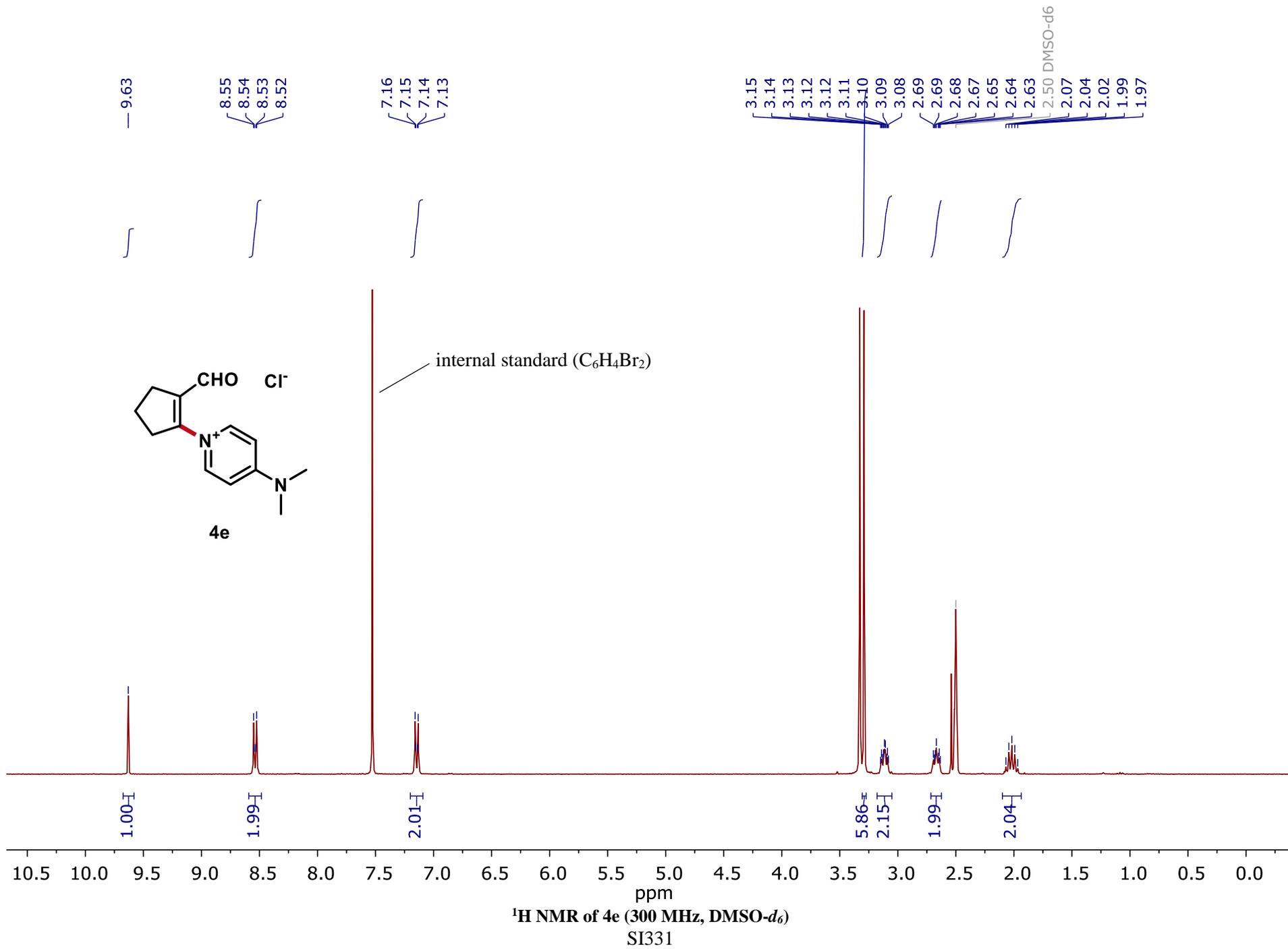


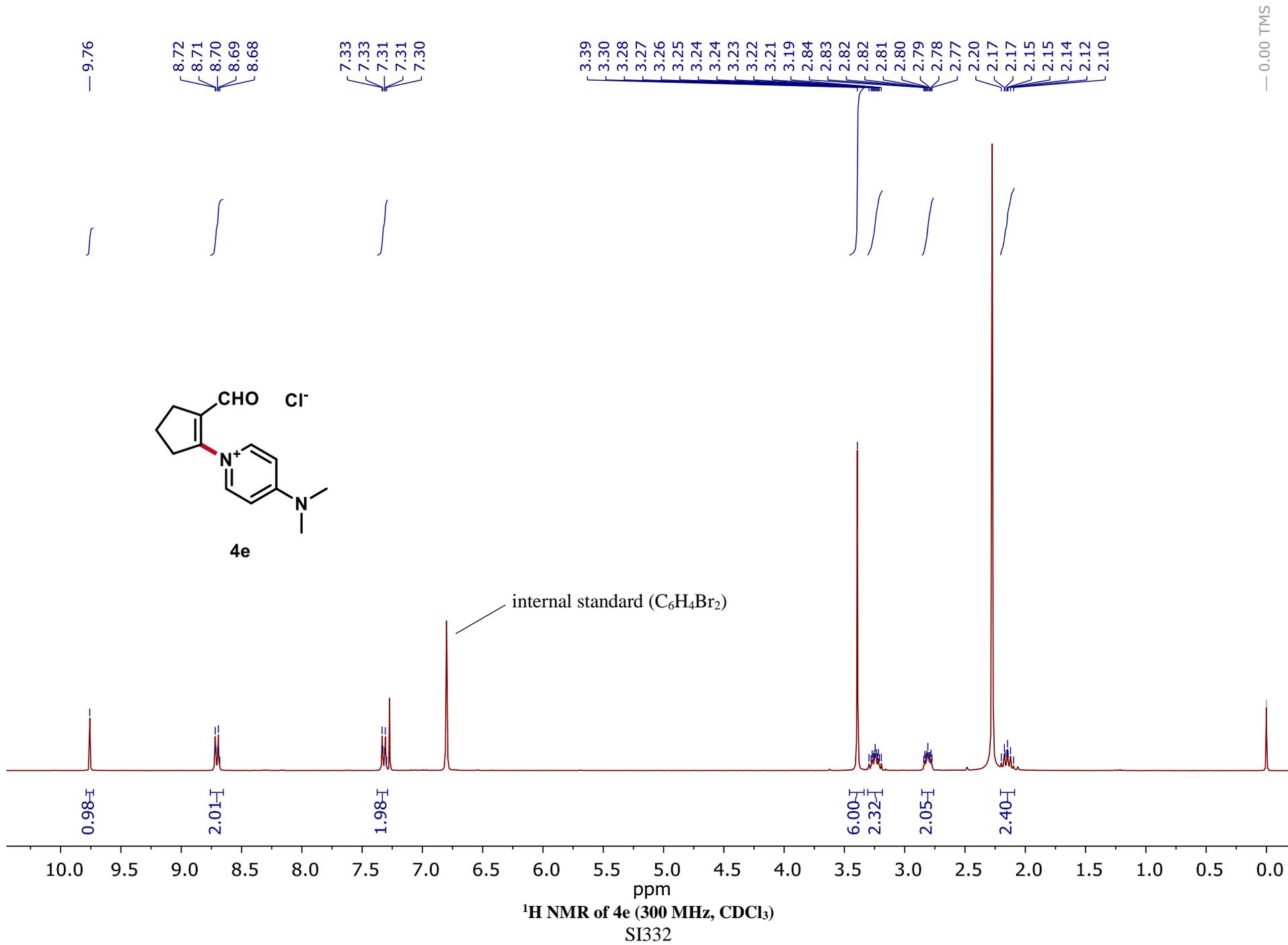


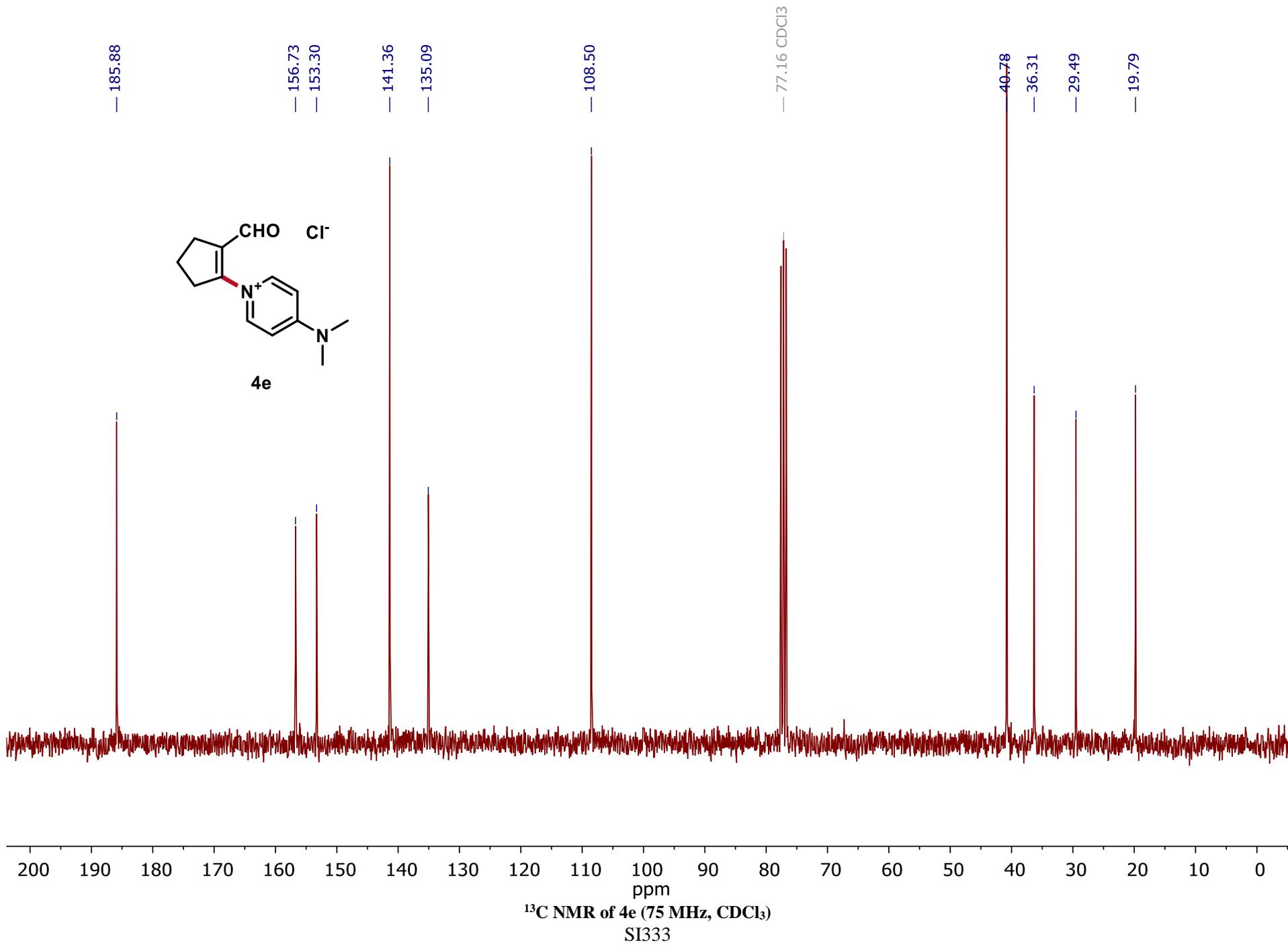


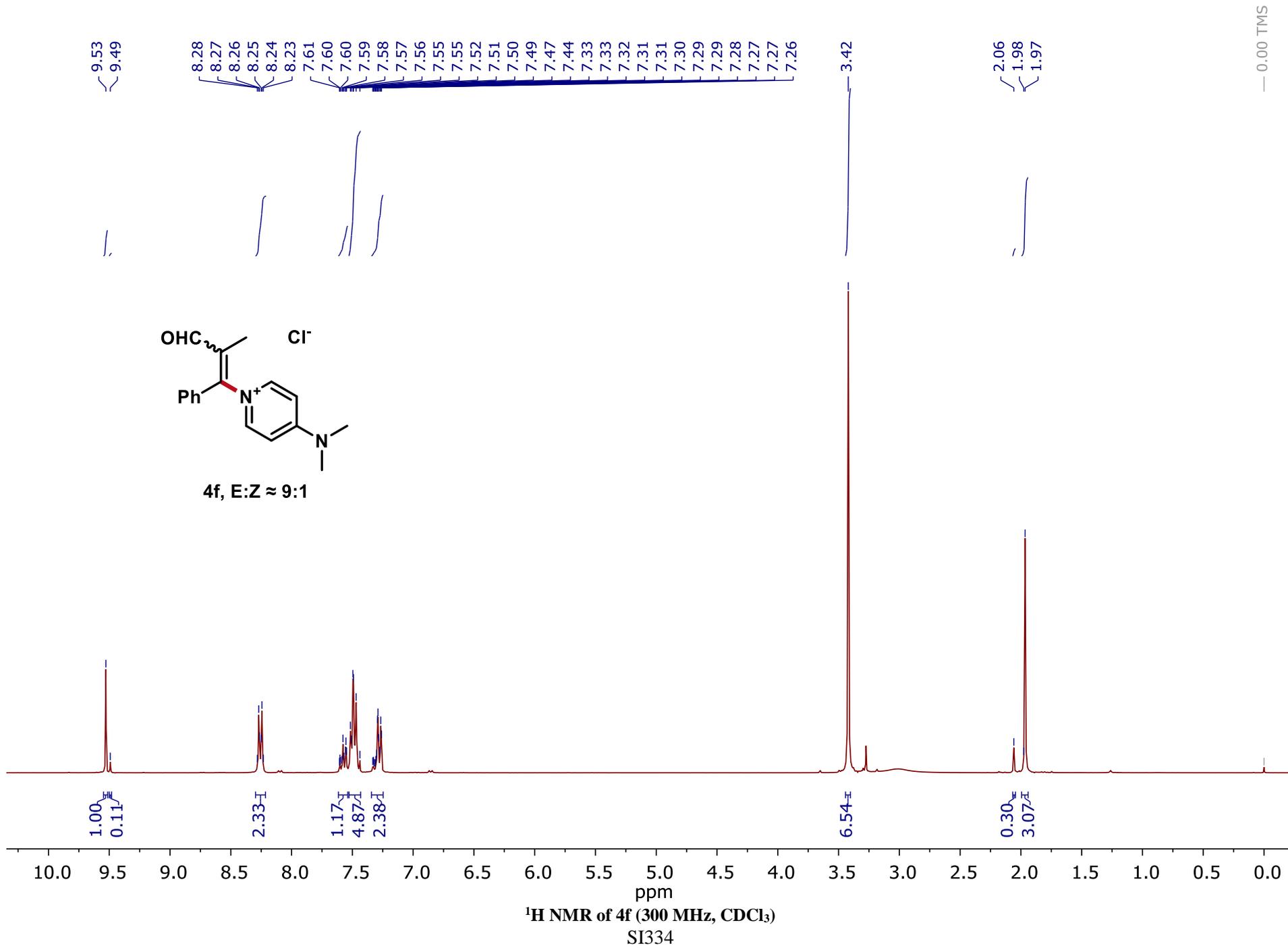




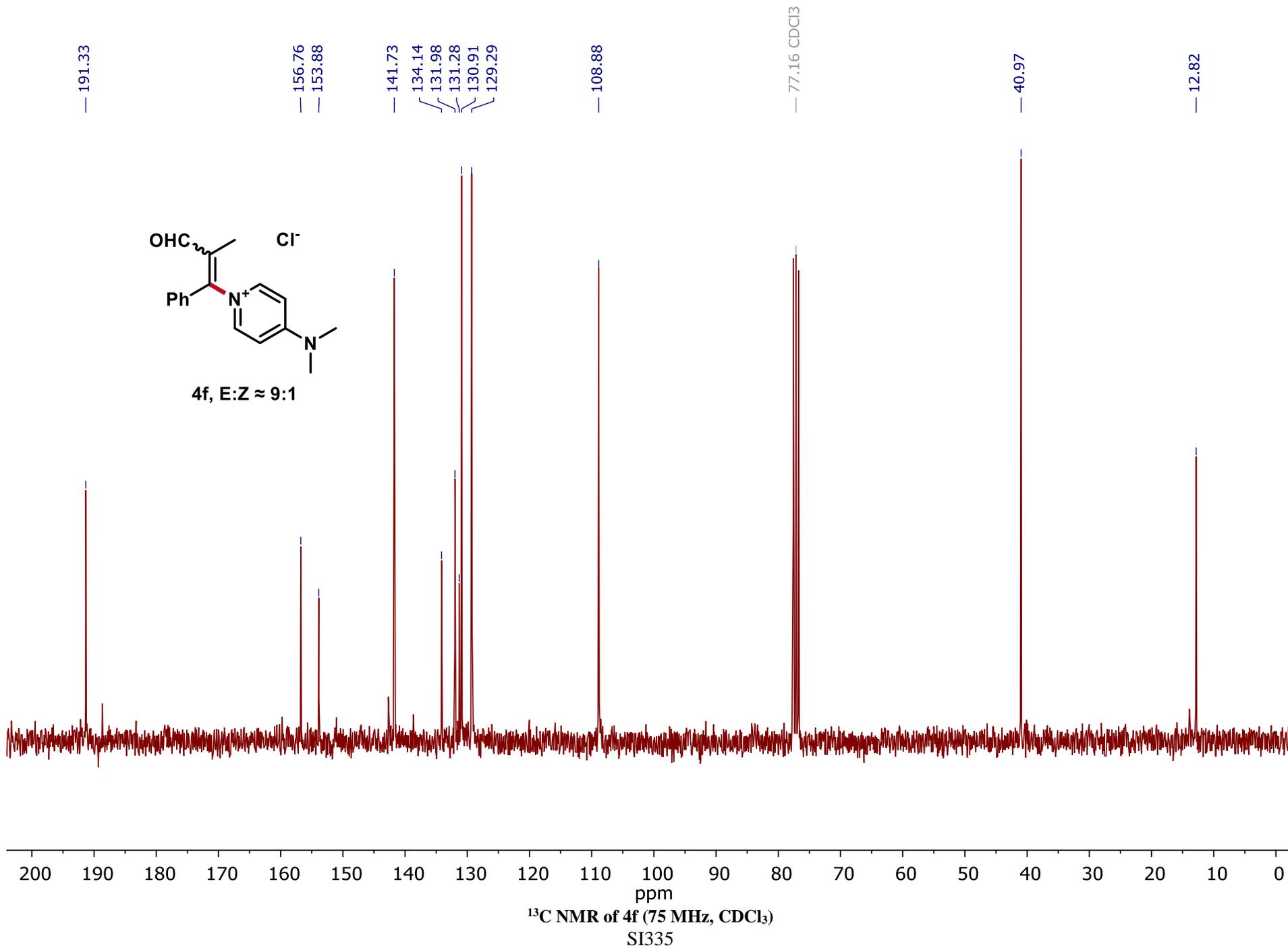


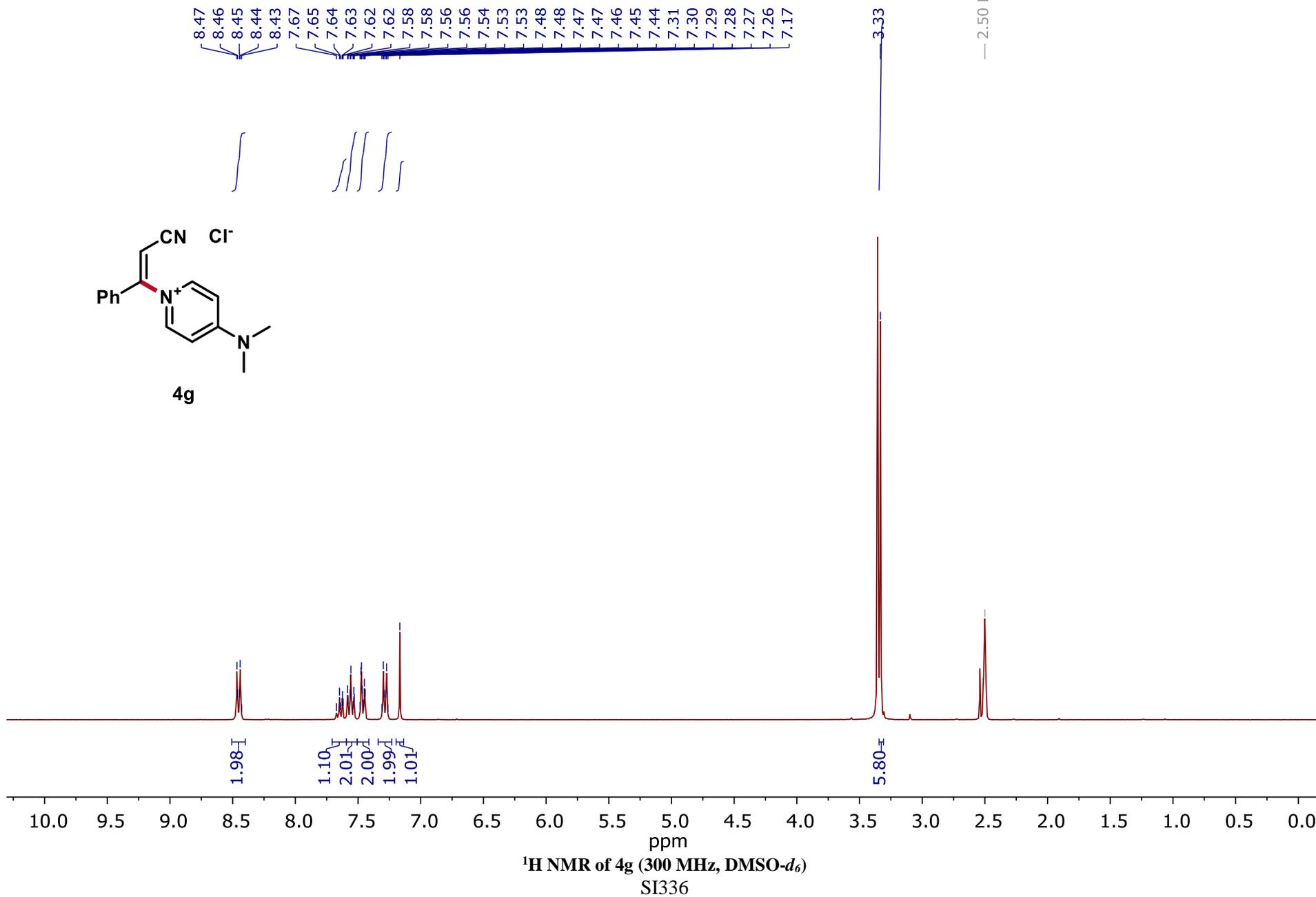
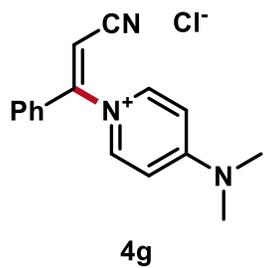


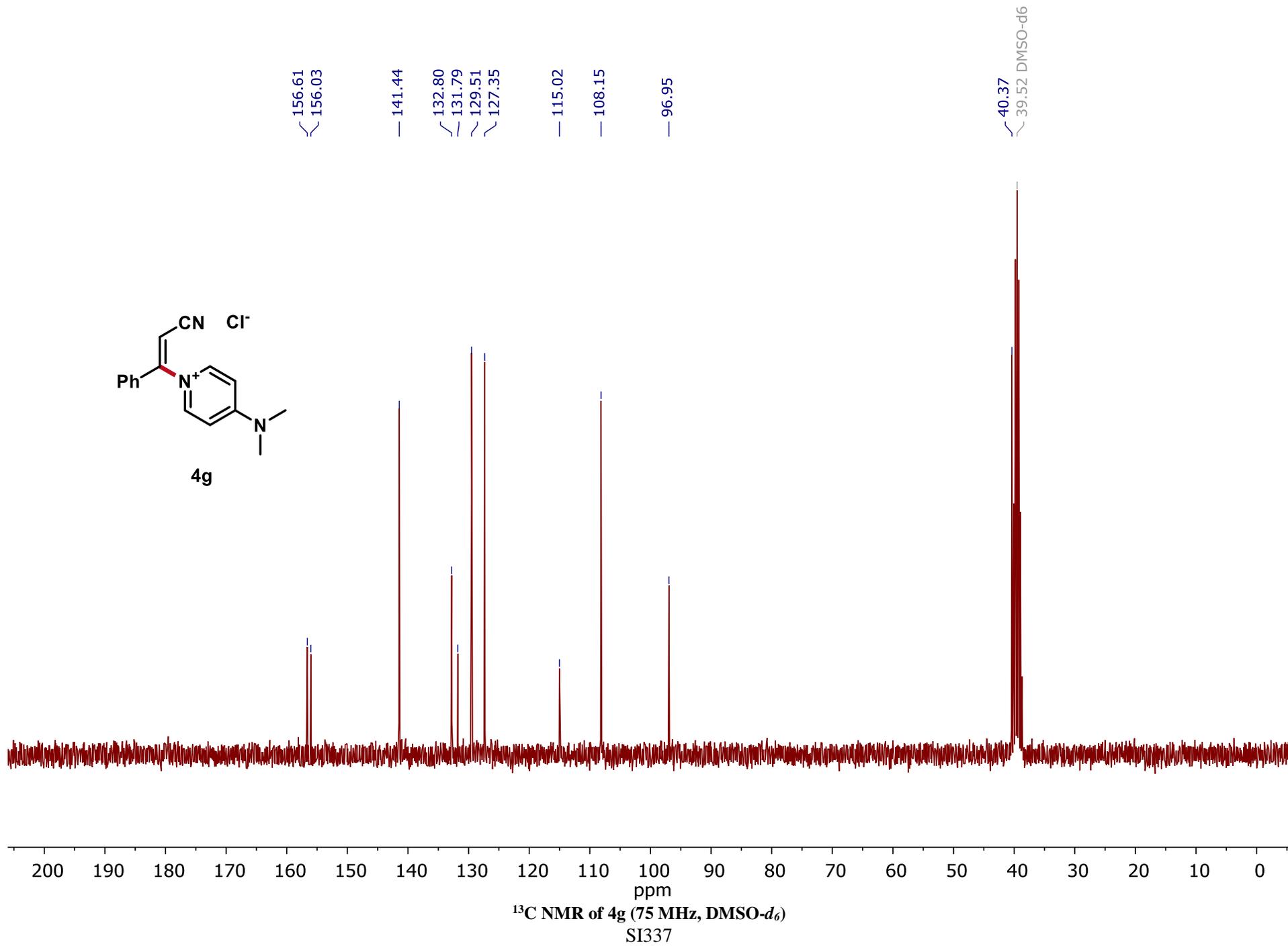
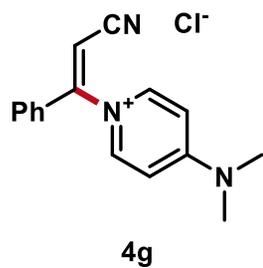


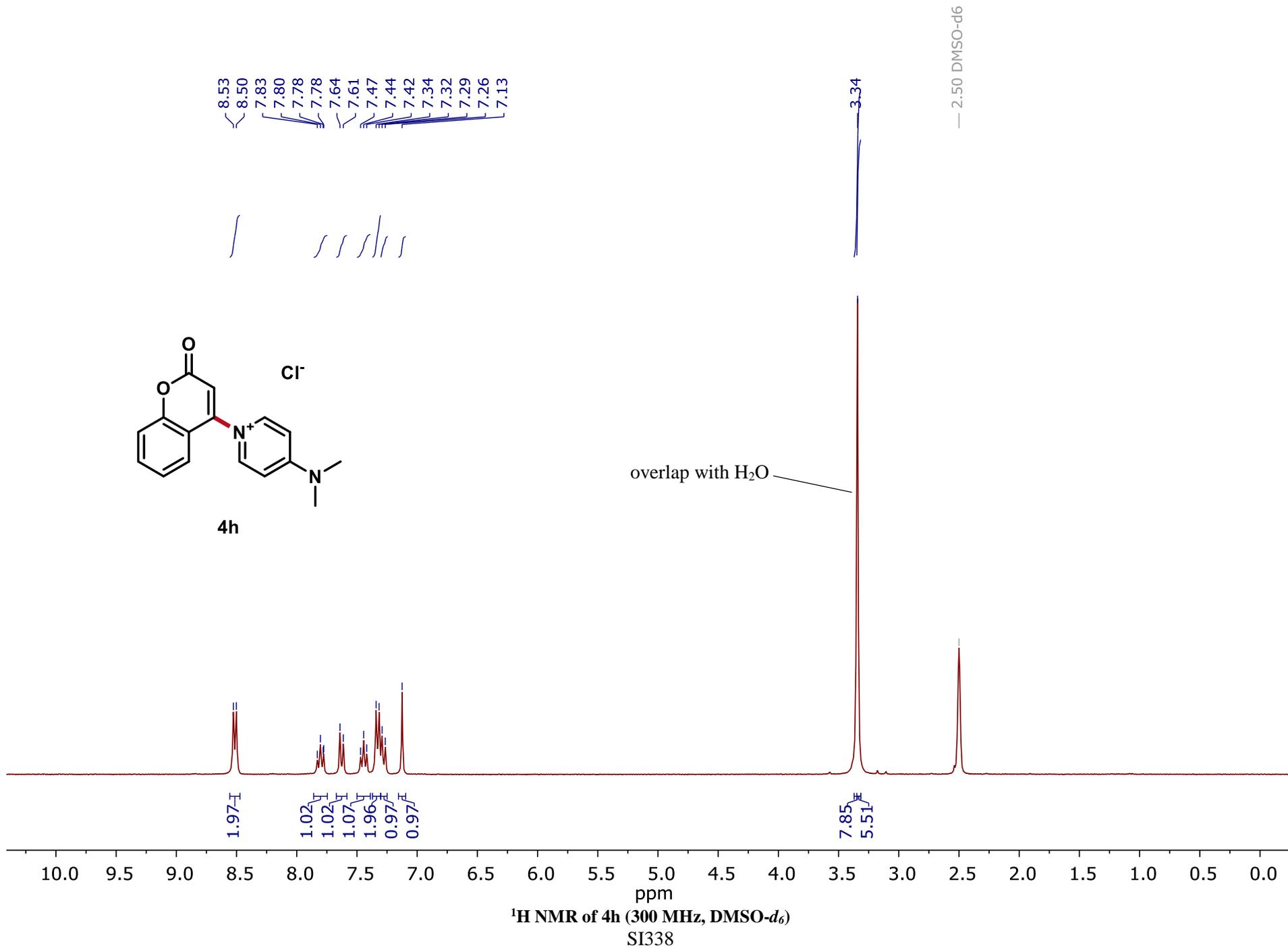


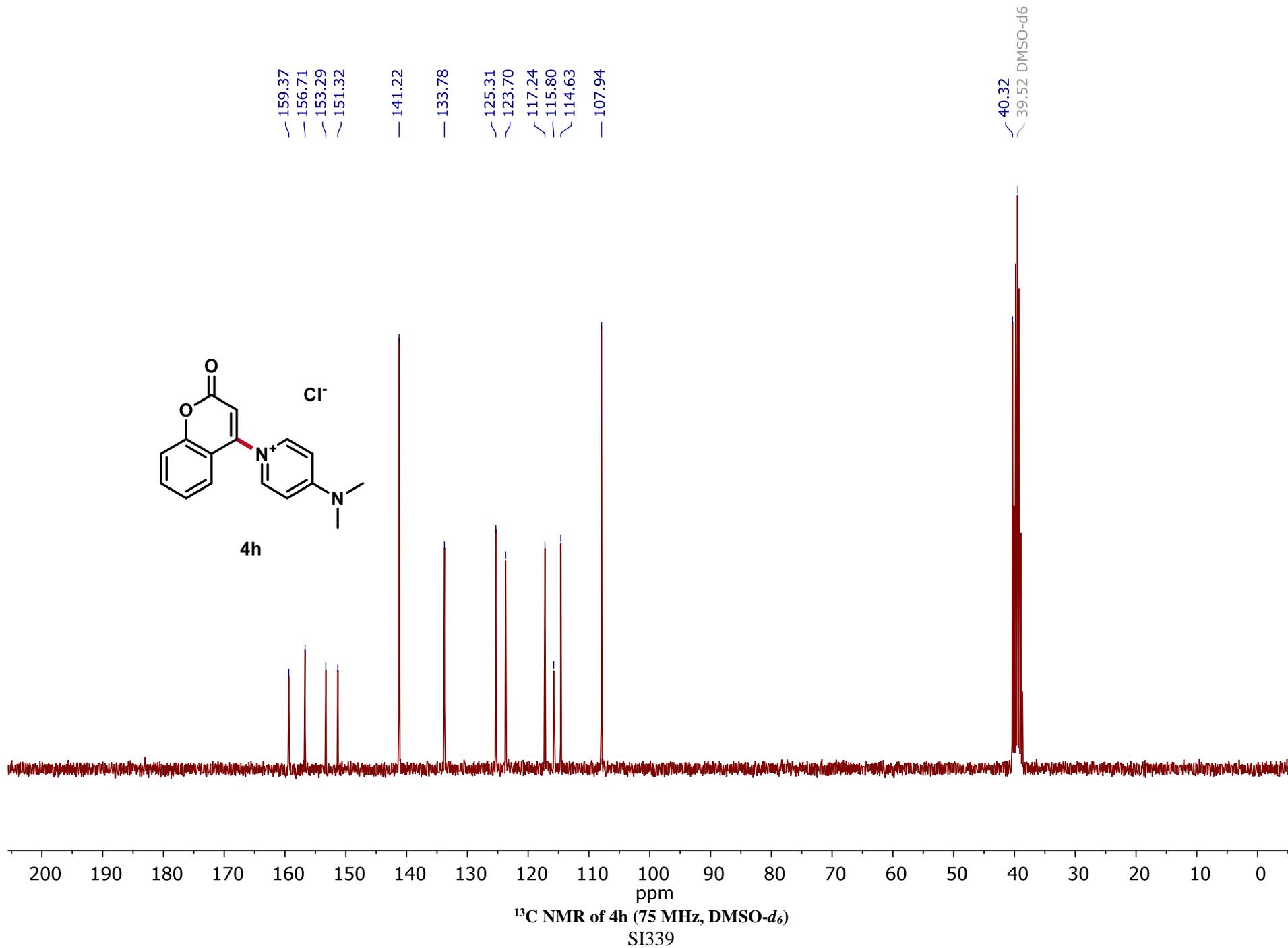
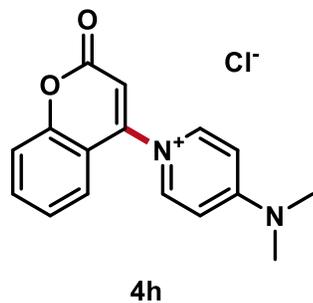
— 0.00 TMS

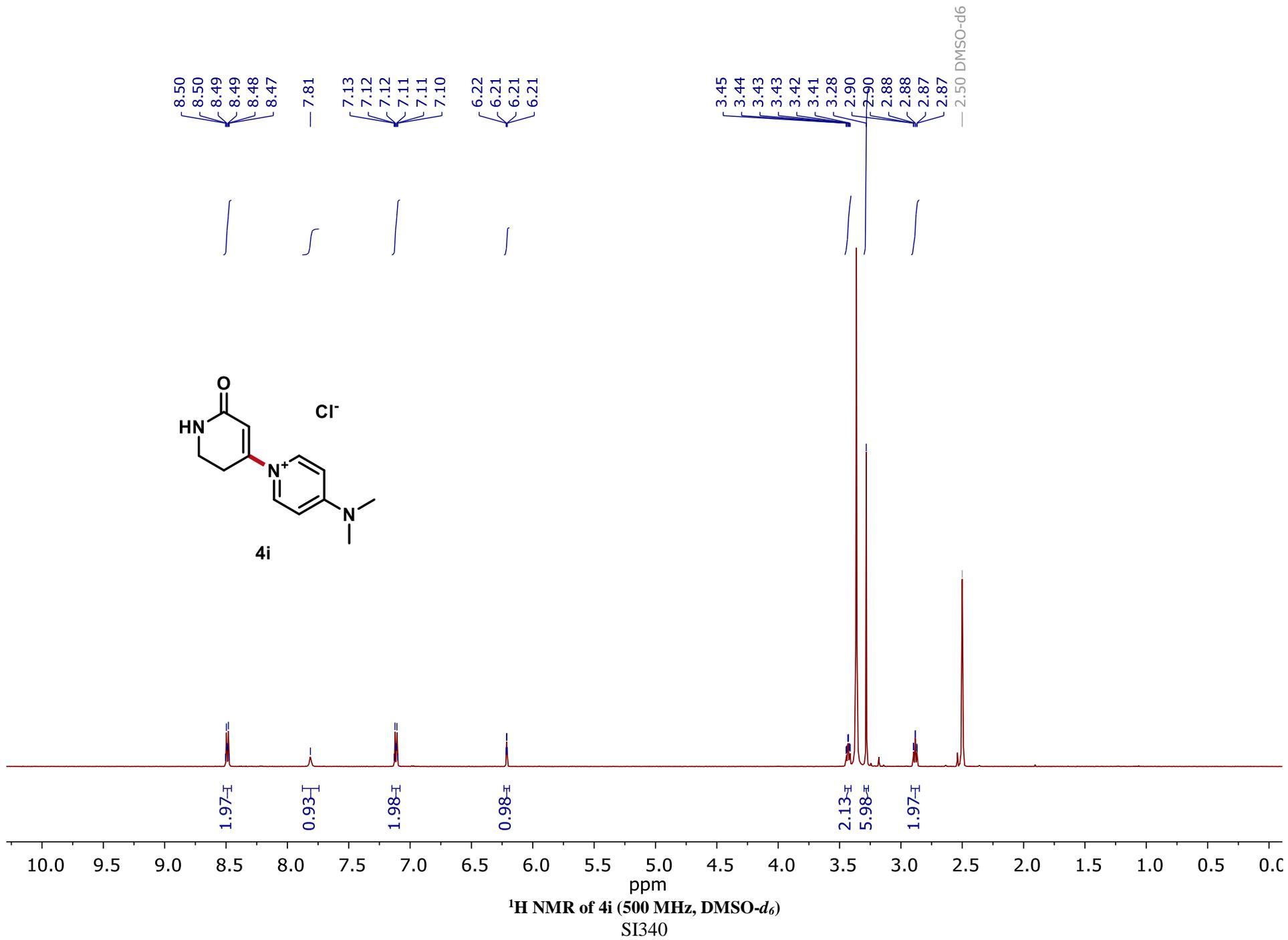


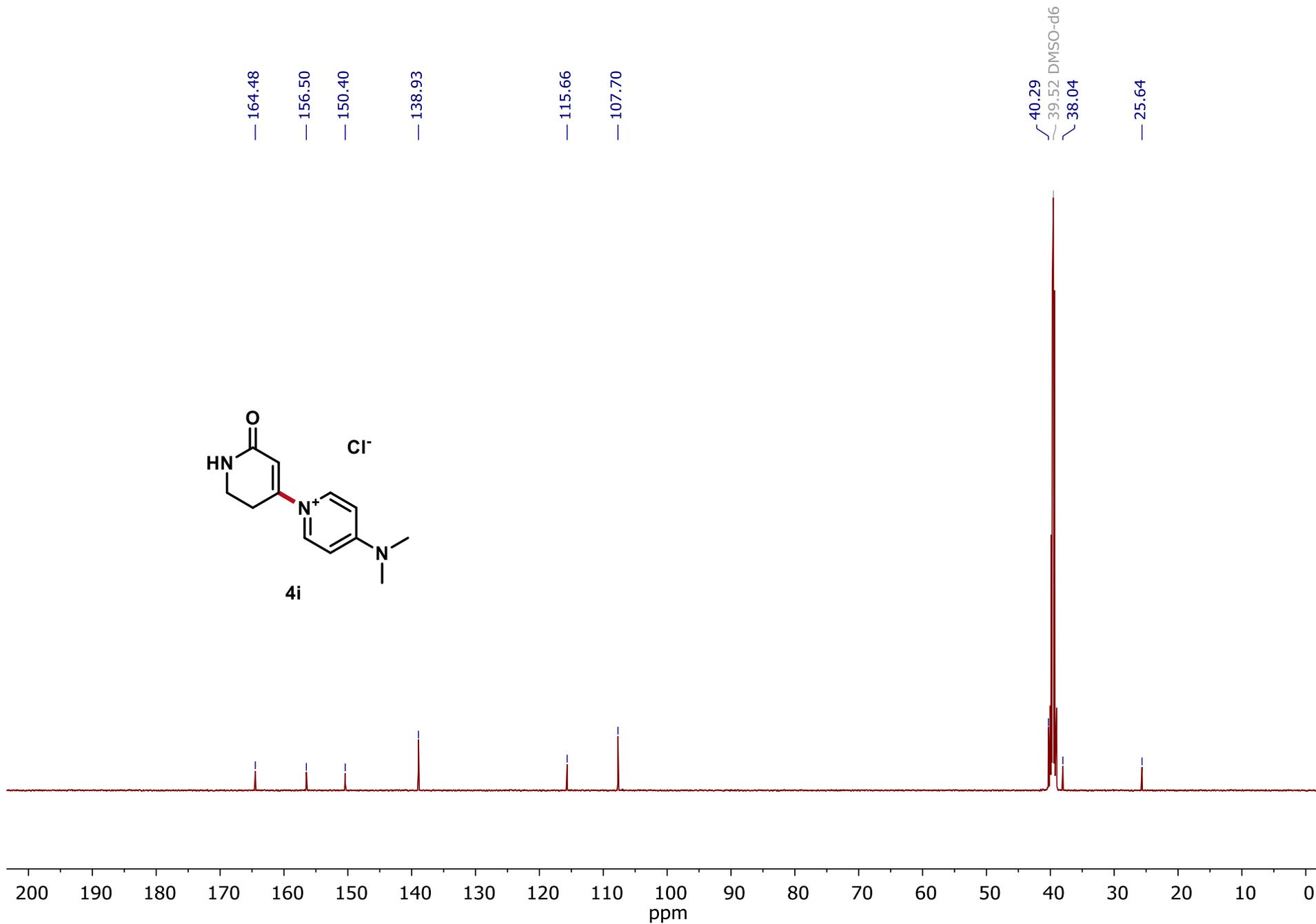
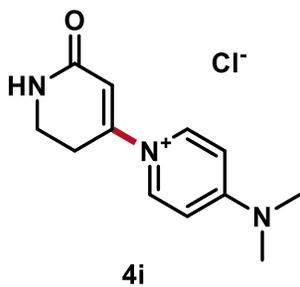




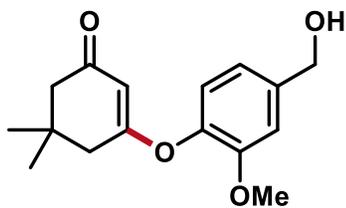




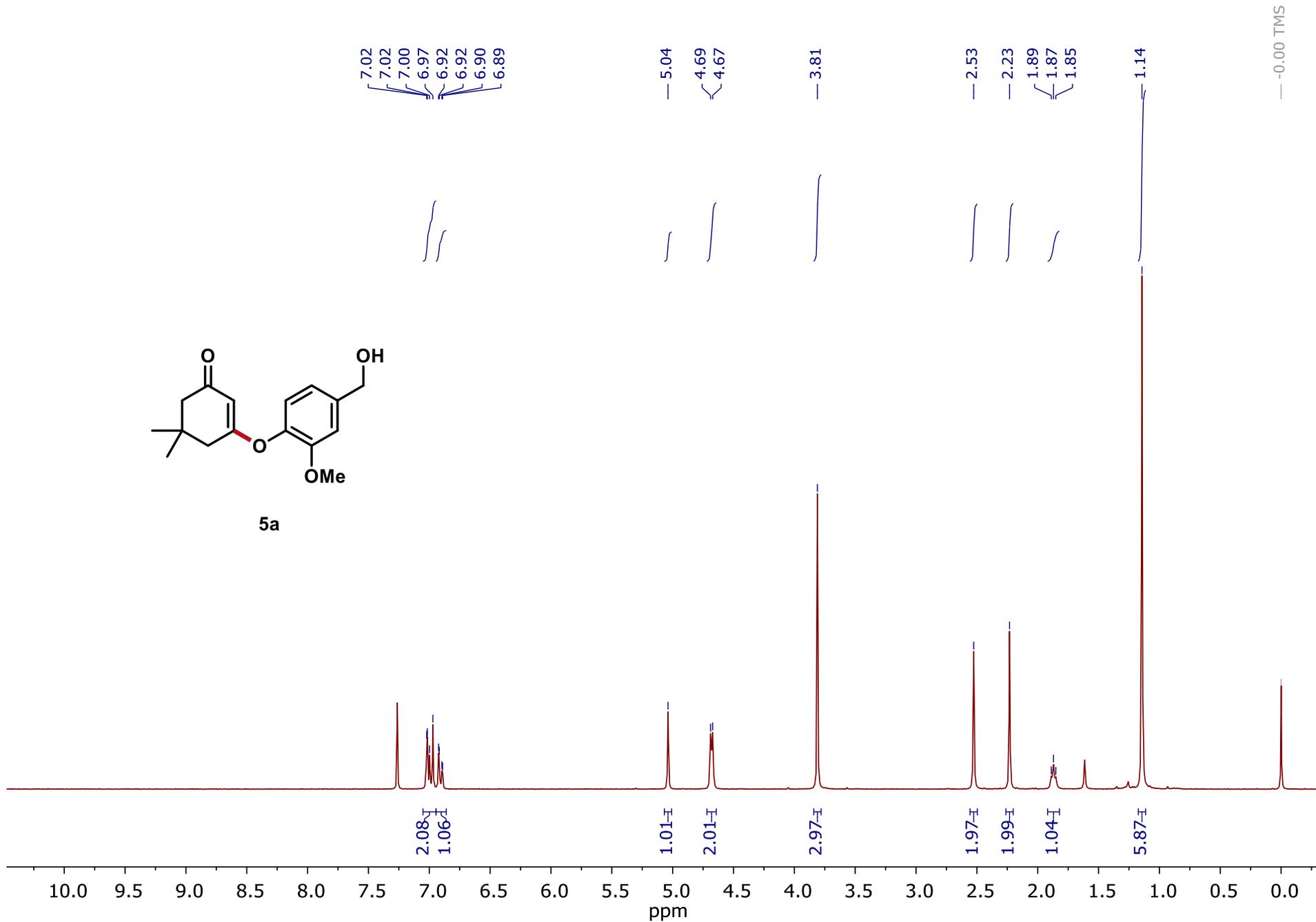




¹³C NMR of 4i (126 MHz, DMSO-*d*₆)
SI341

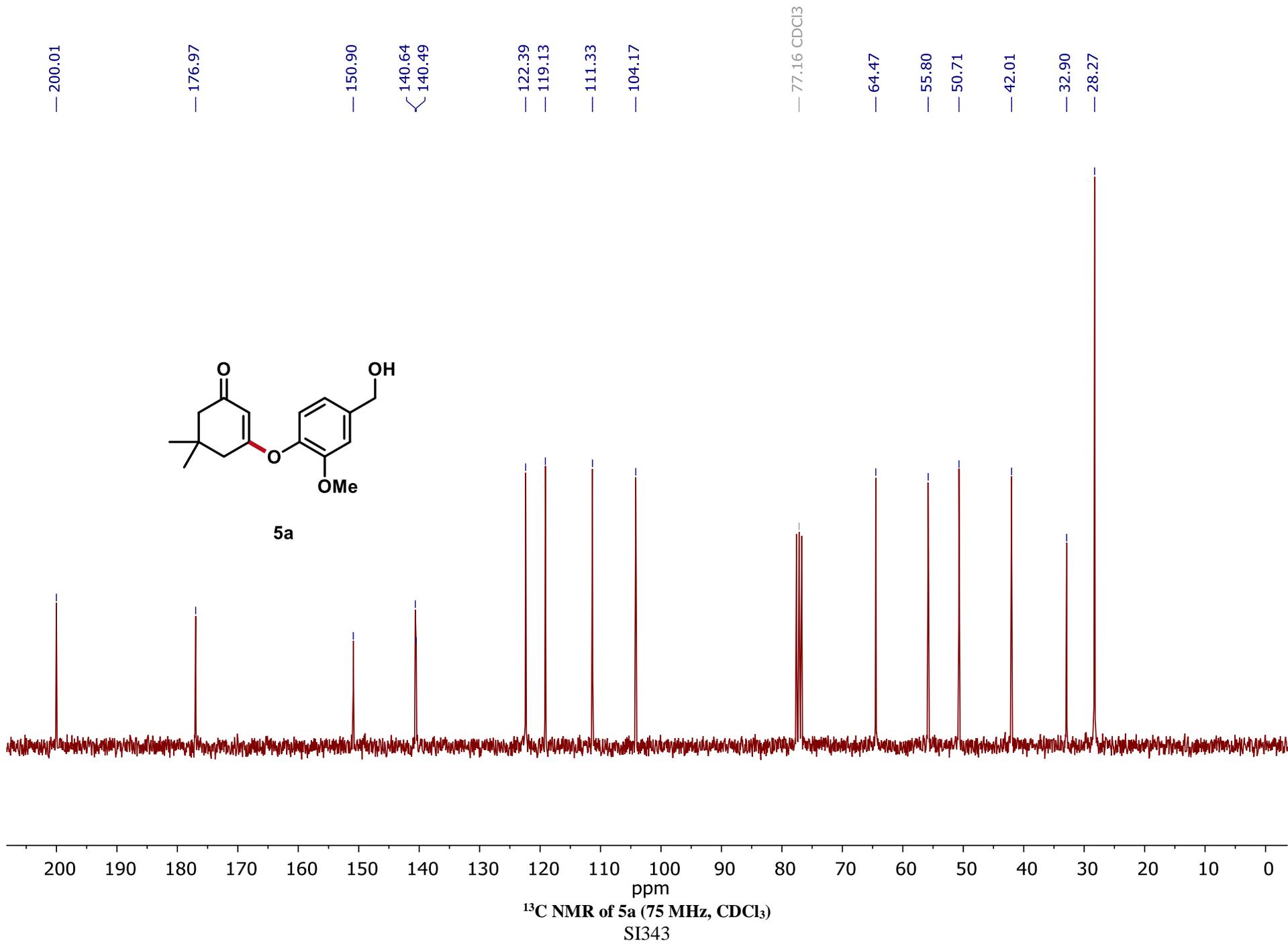


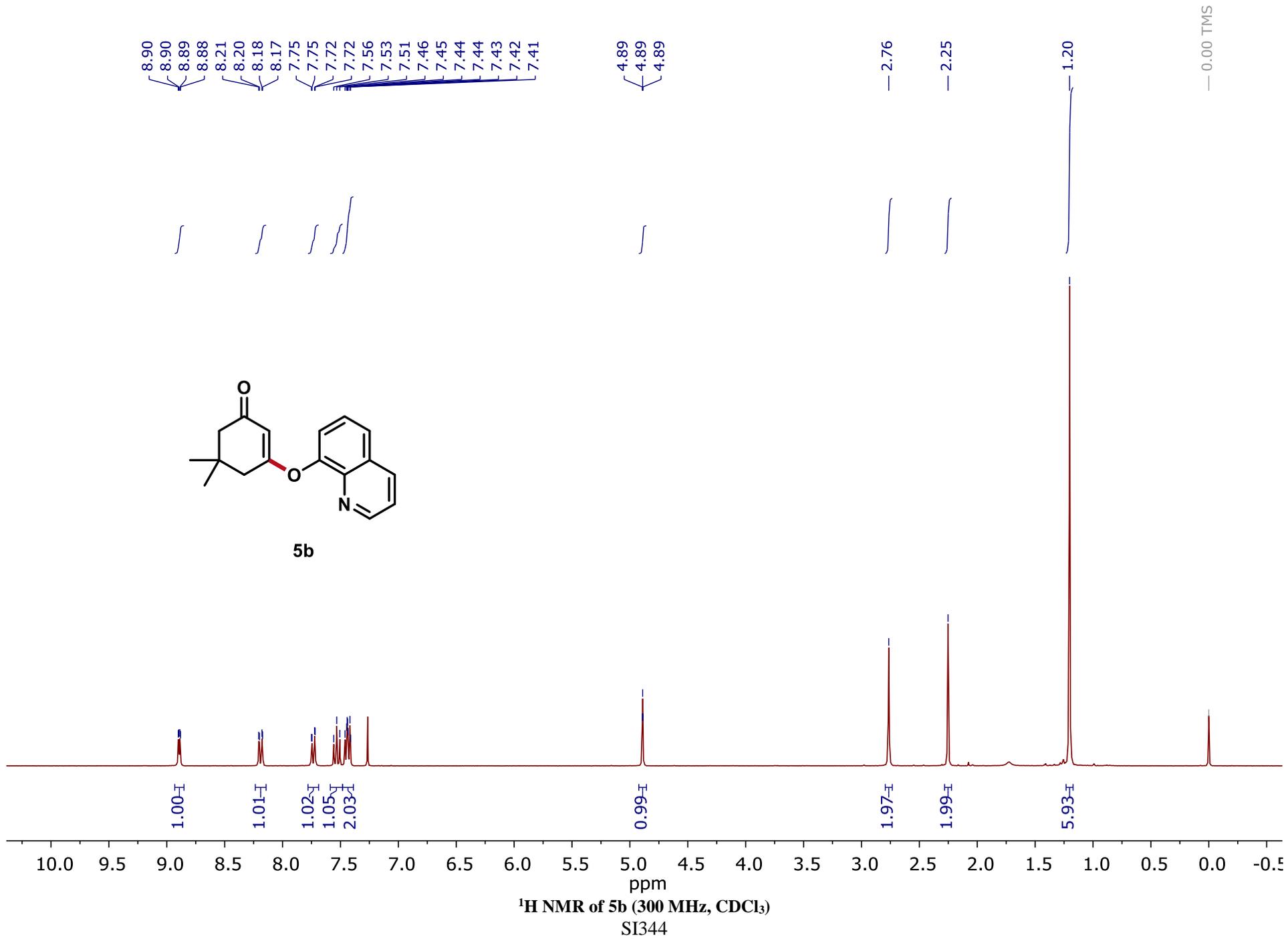
5a

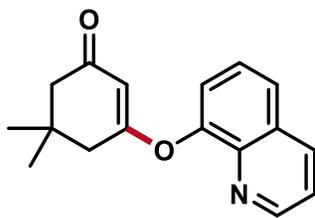


¹H NMR of 5a (300 MHz, CDCl₃)

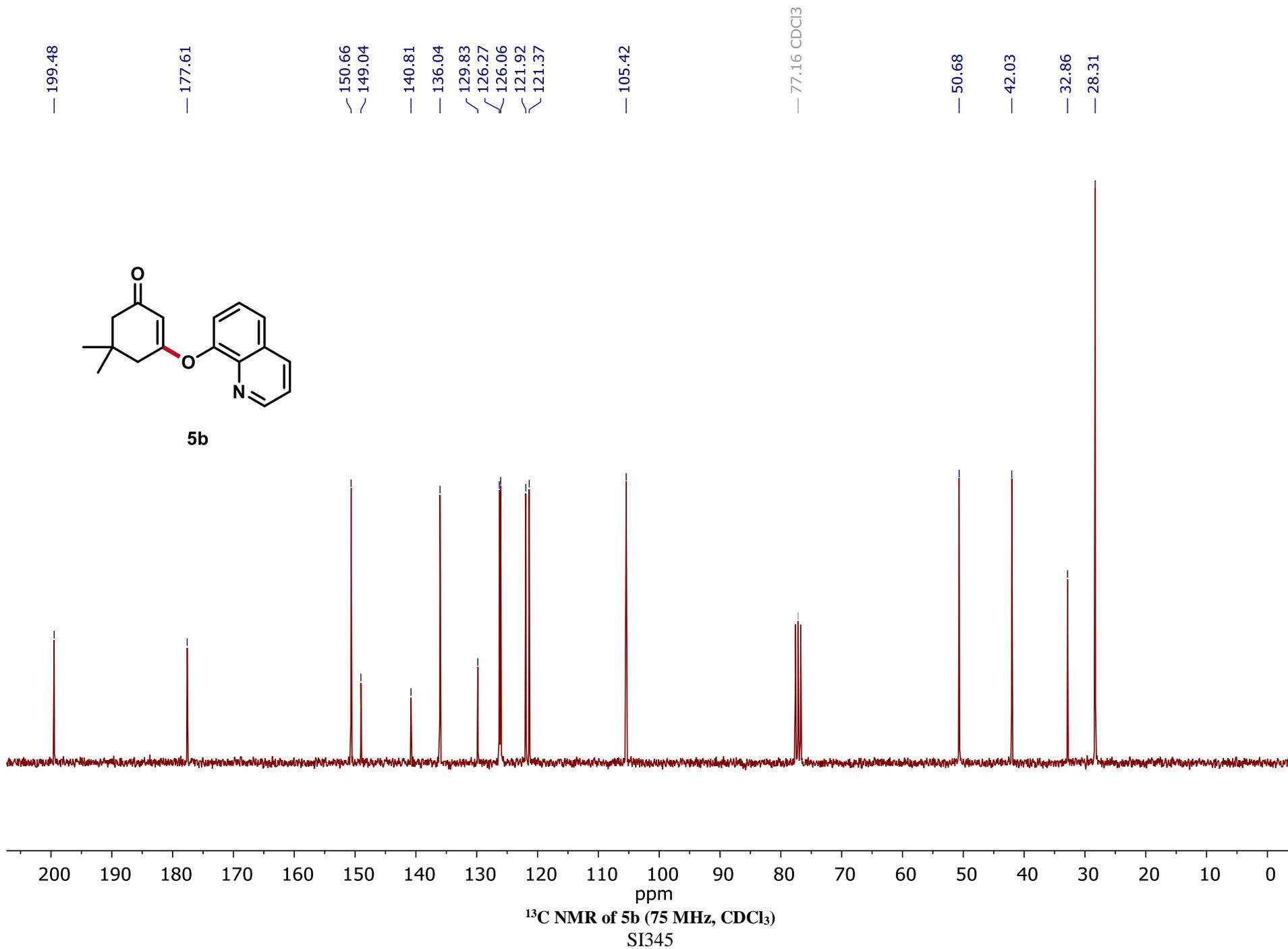
SI342

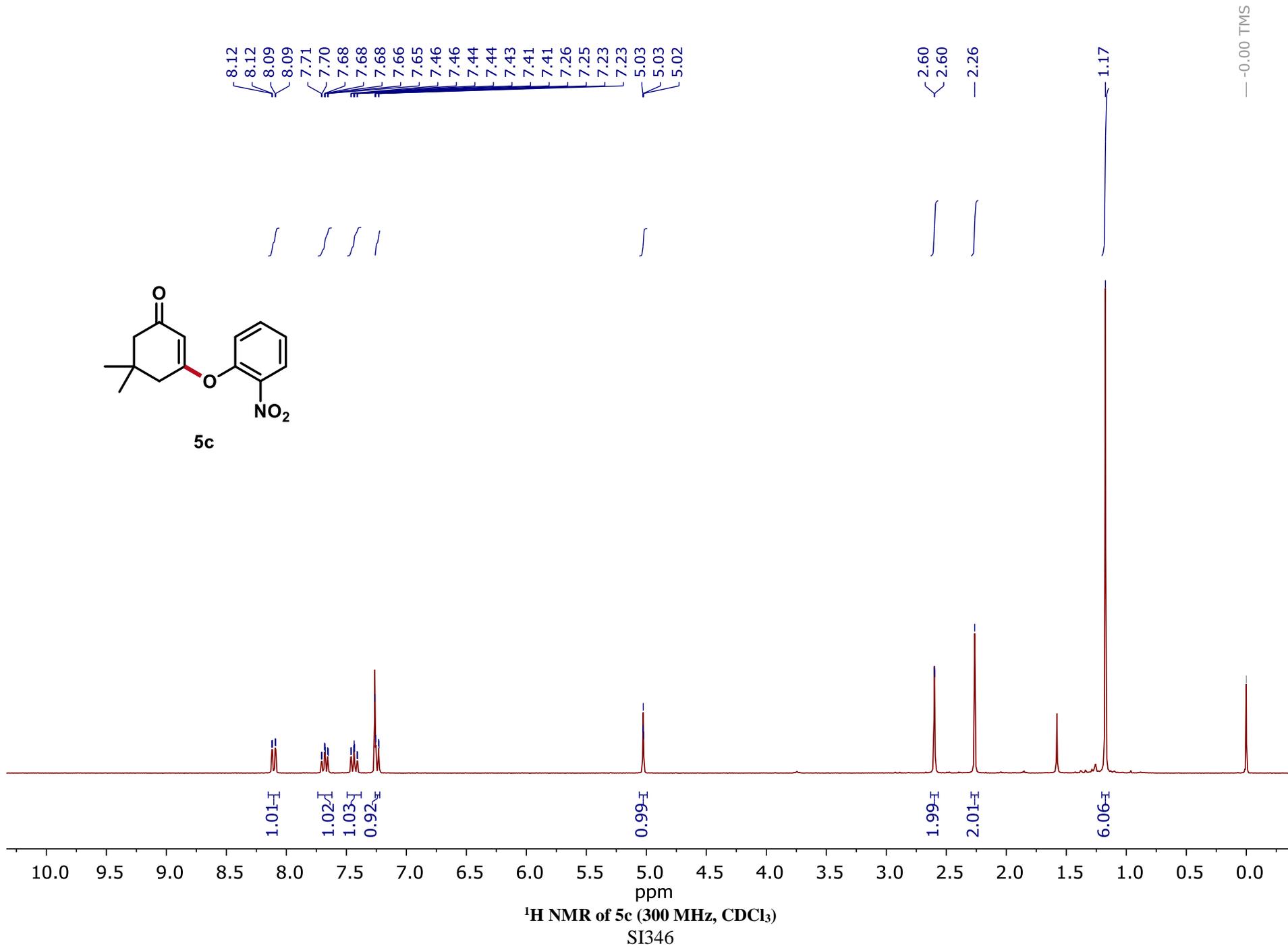
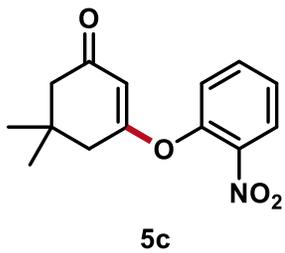


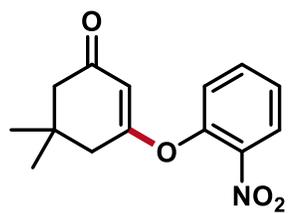




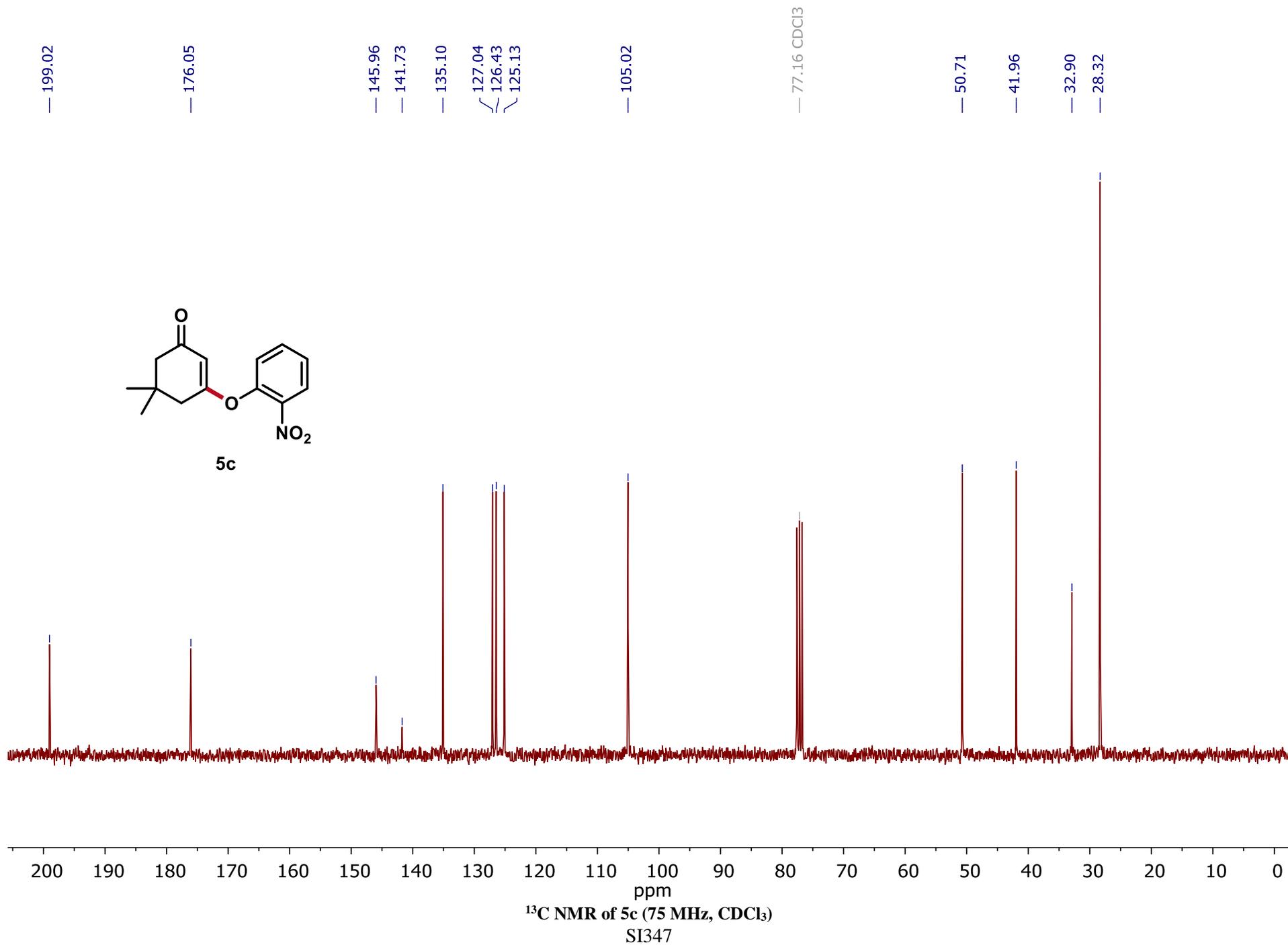
5b

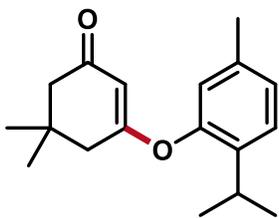




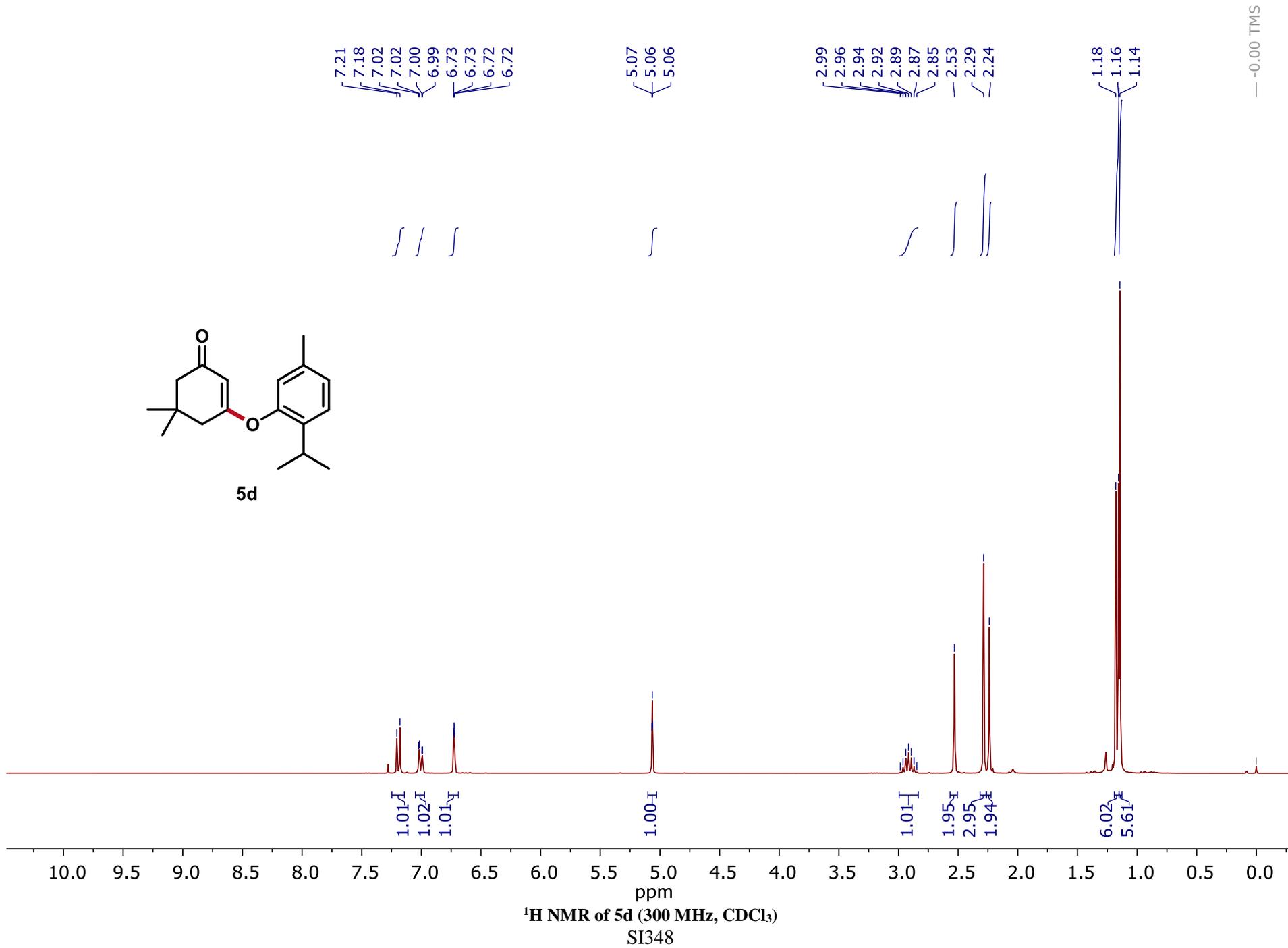


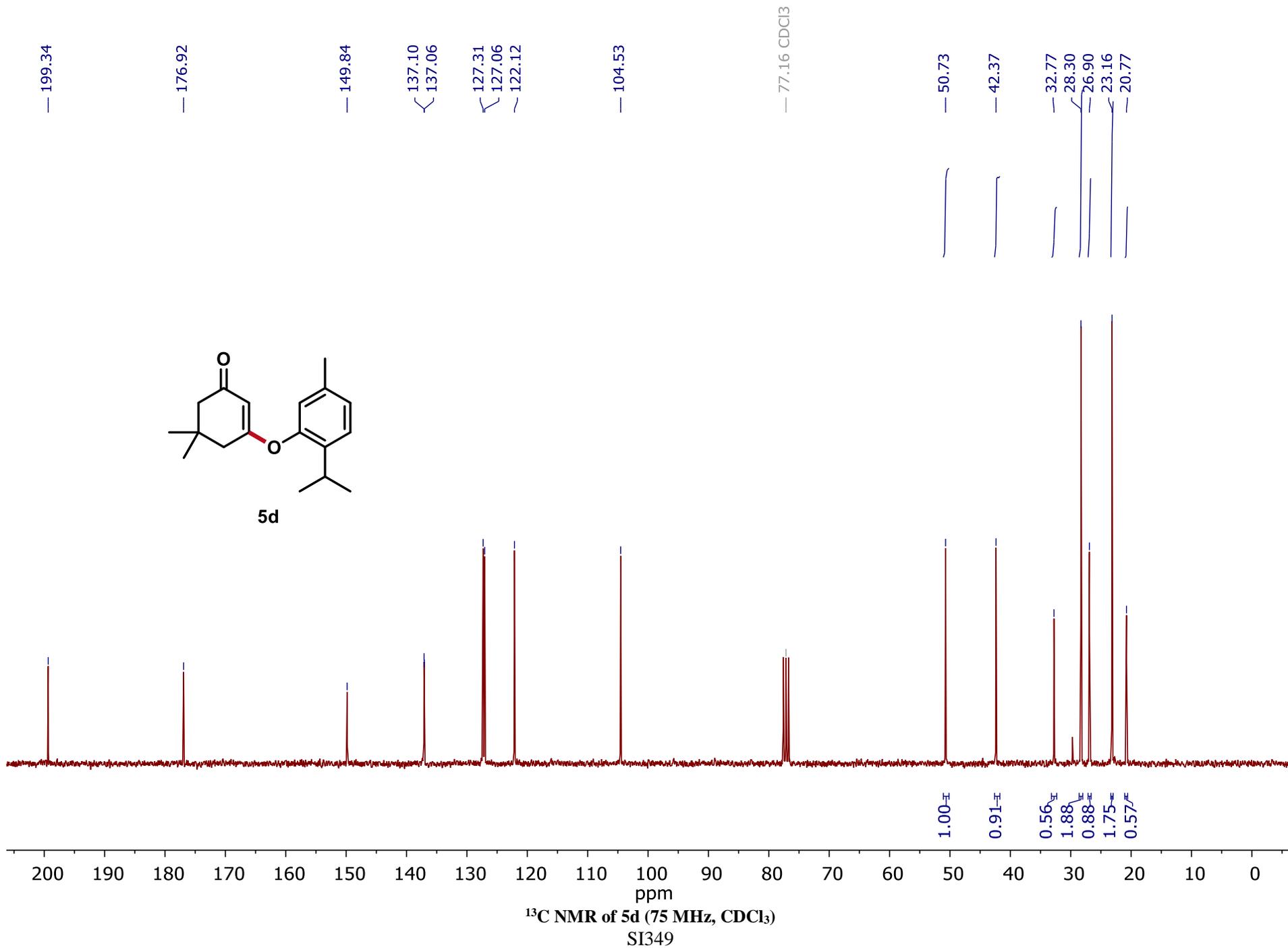
5c

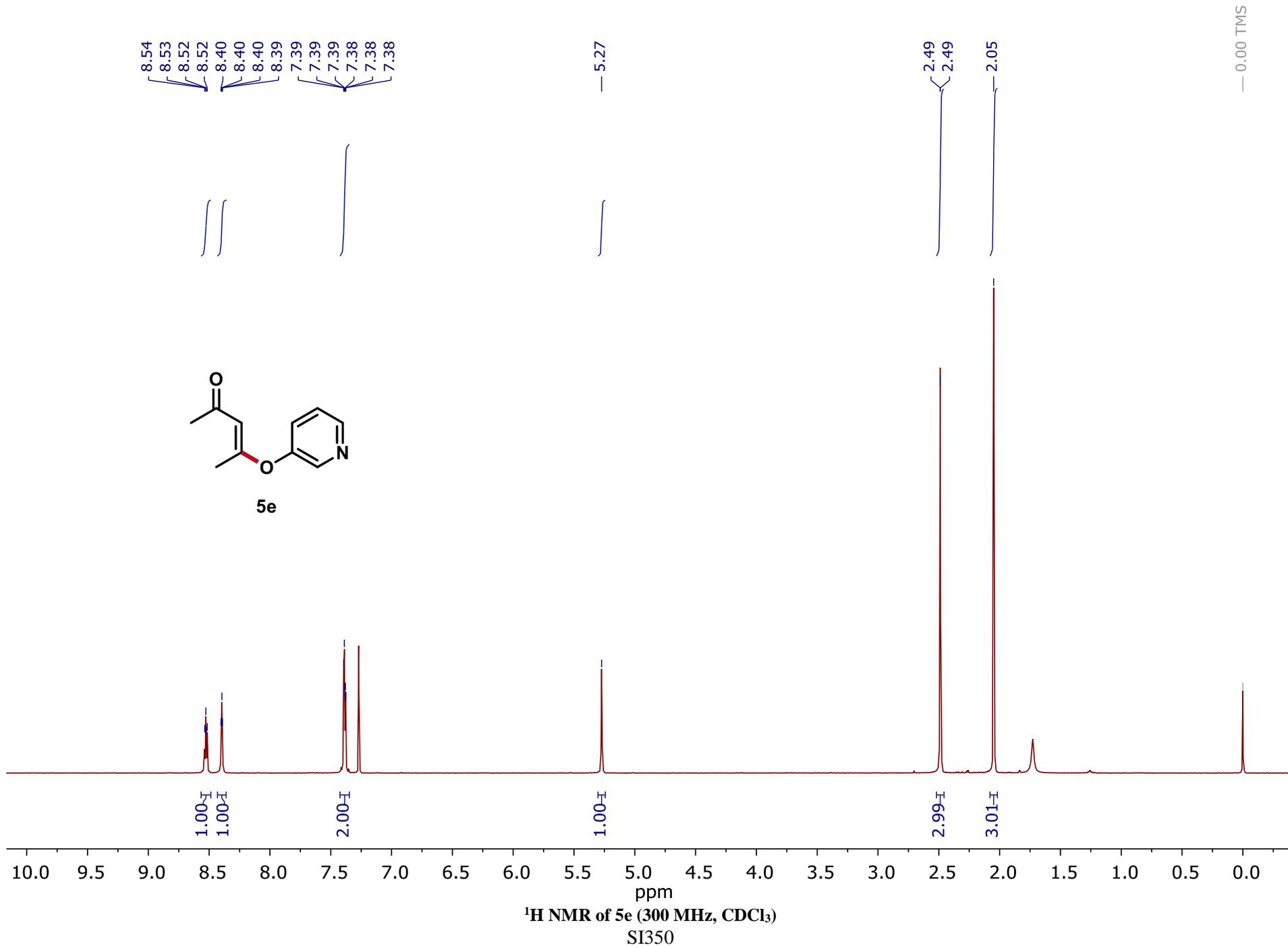


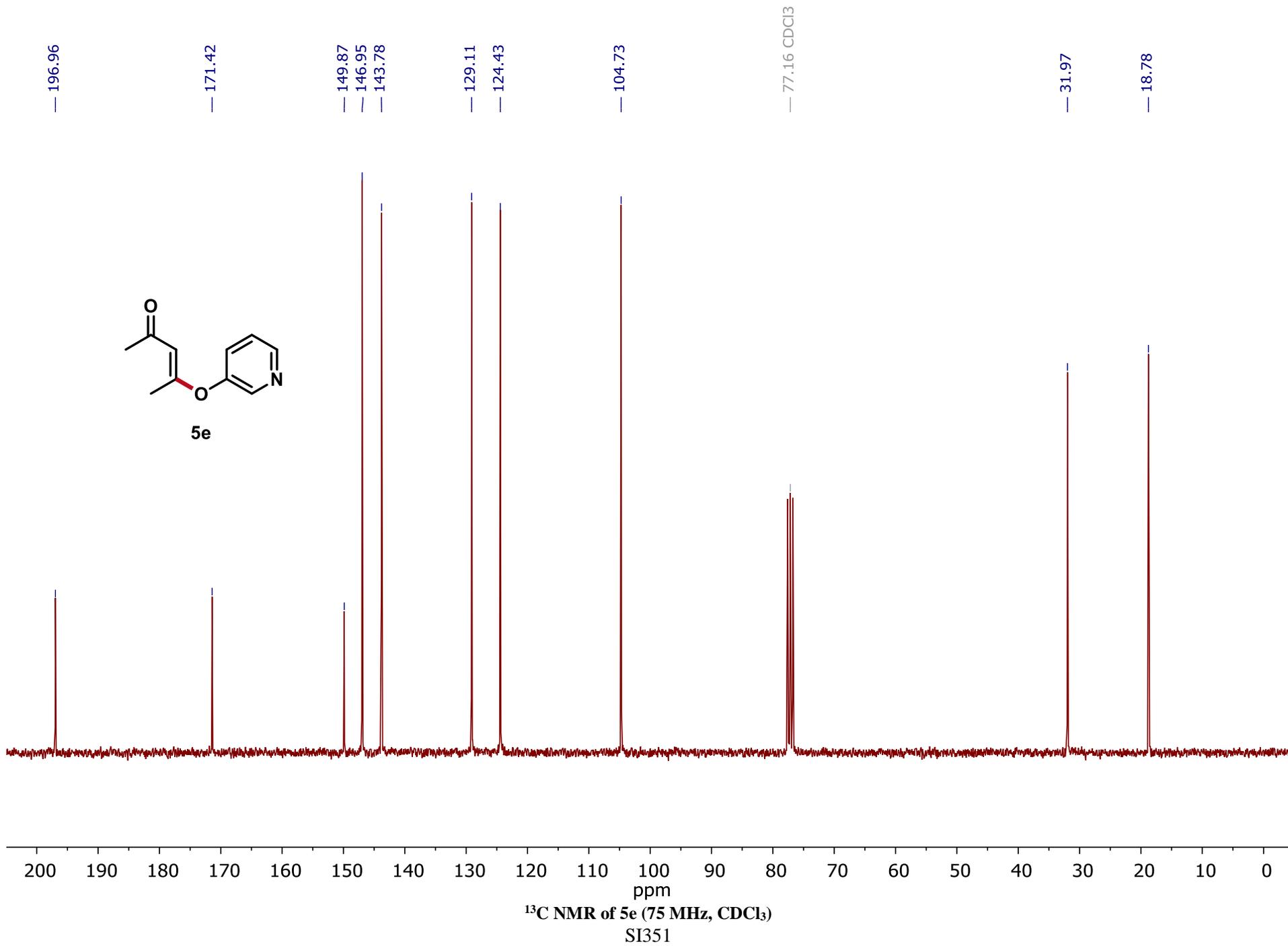
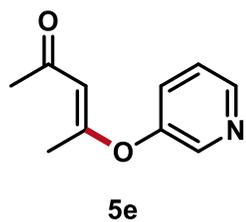


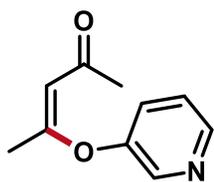
5d



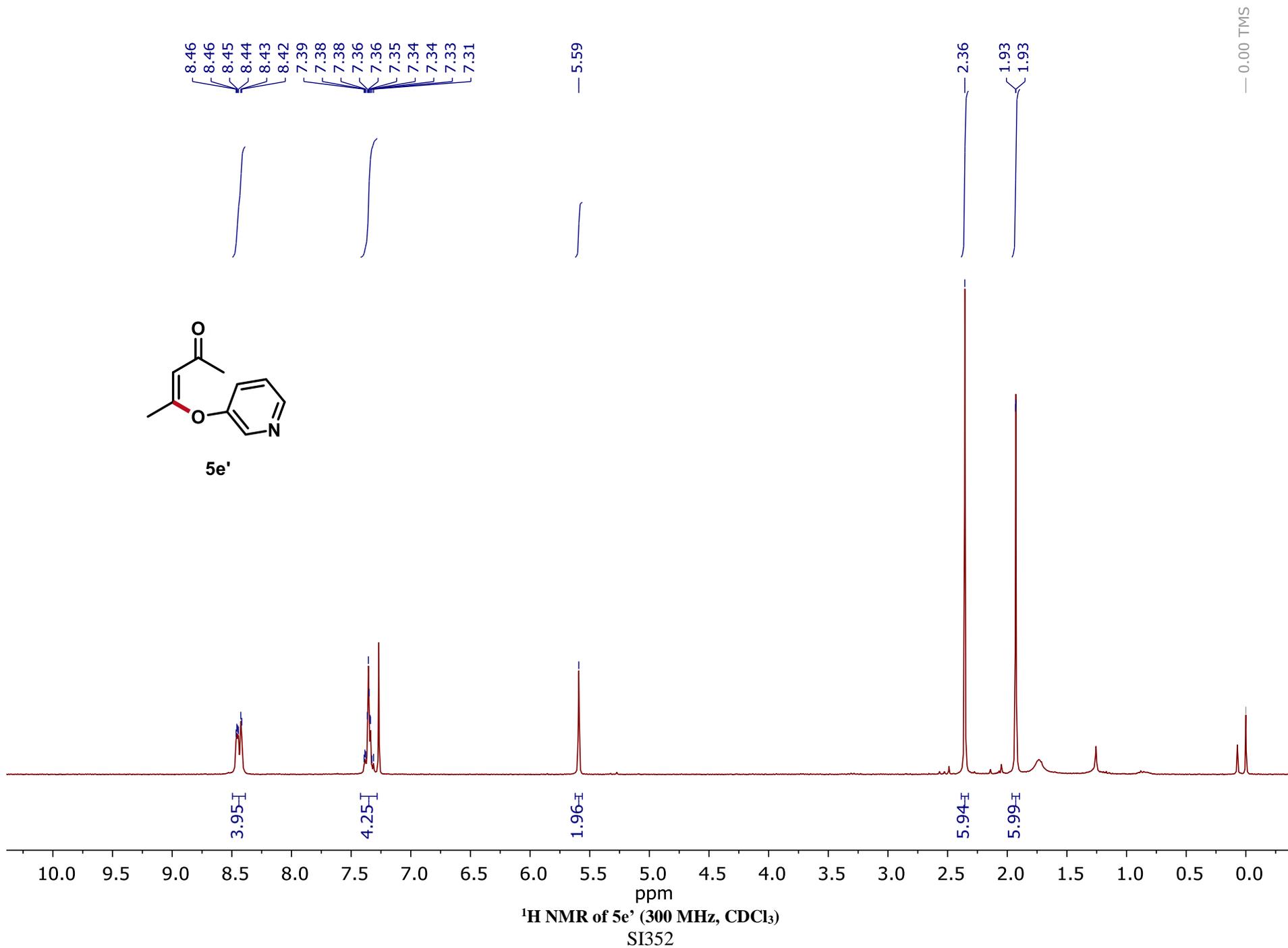


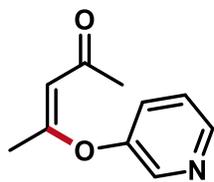




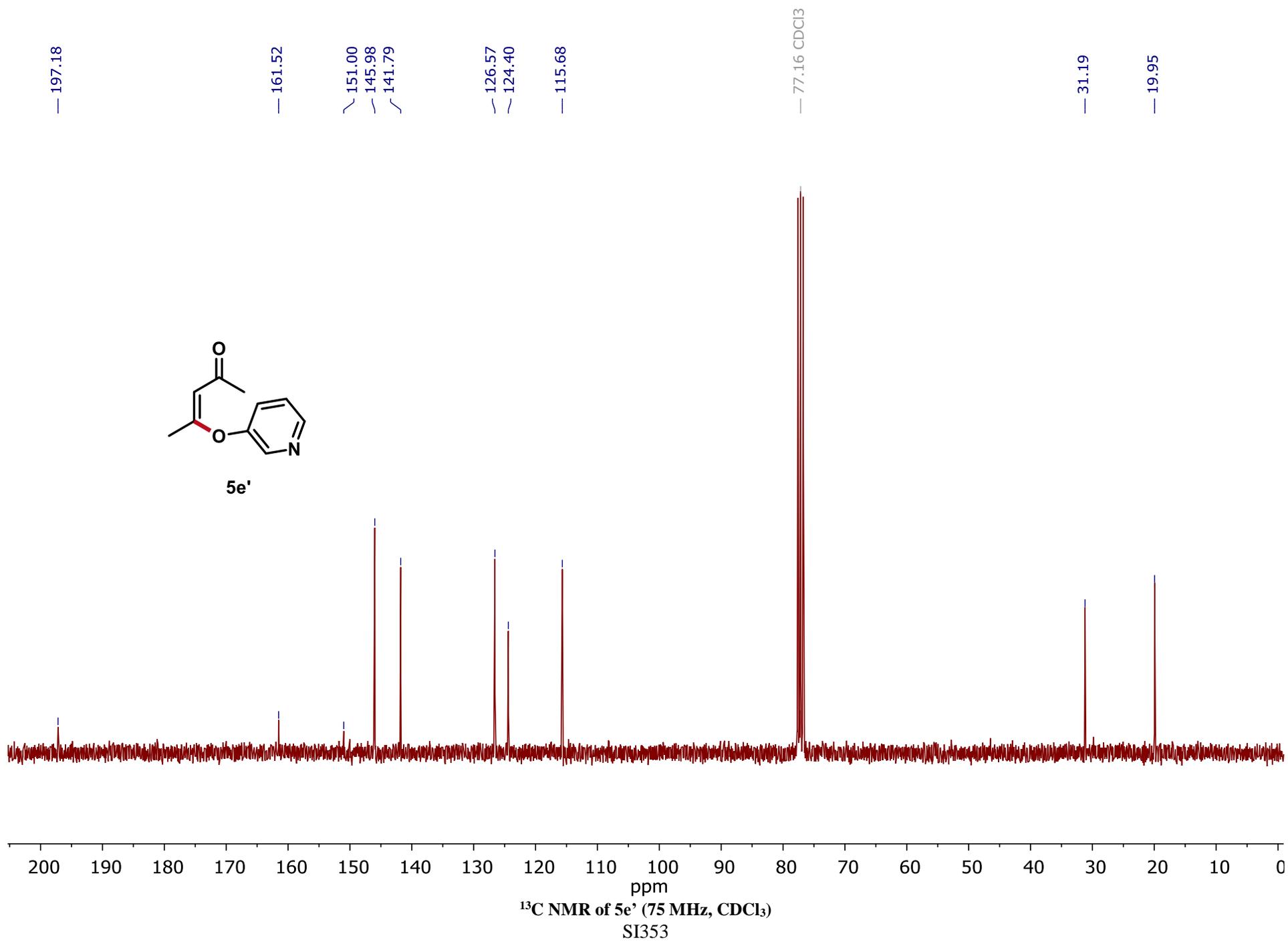


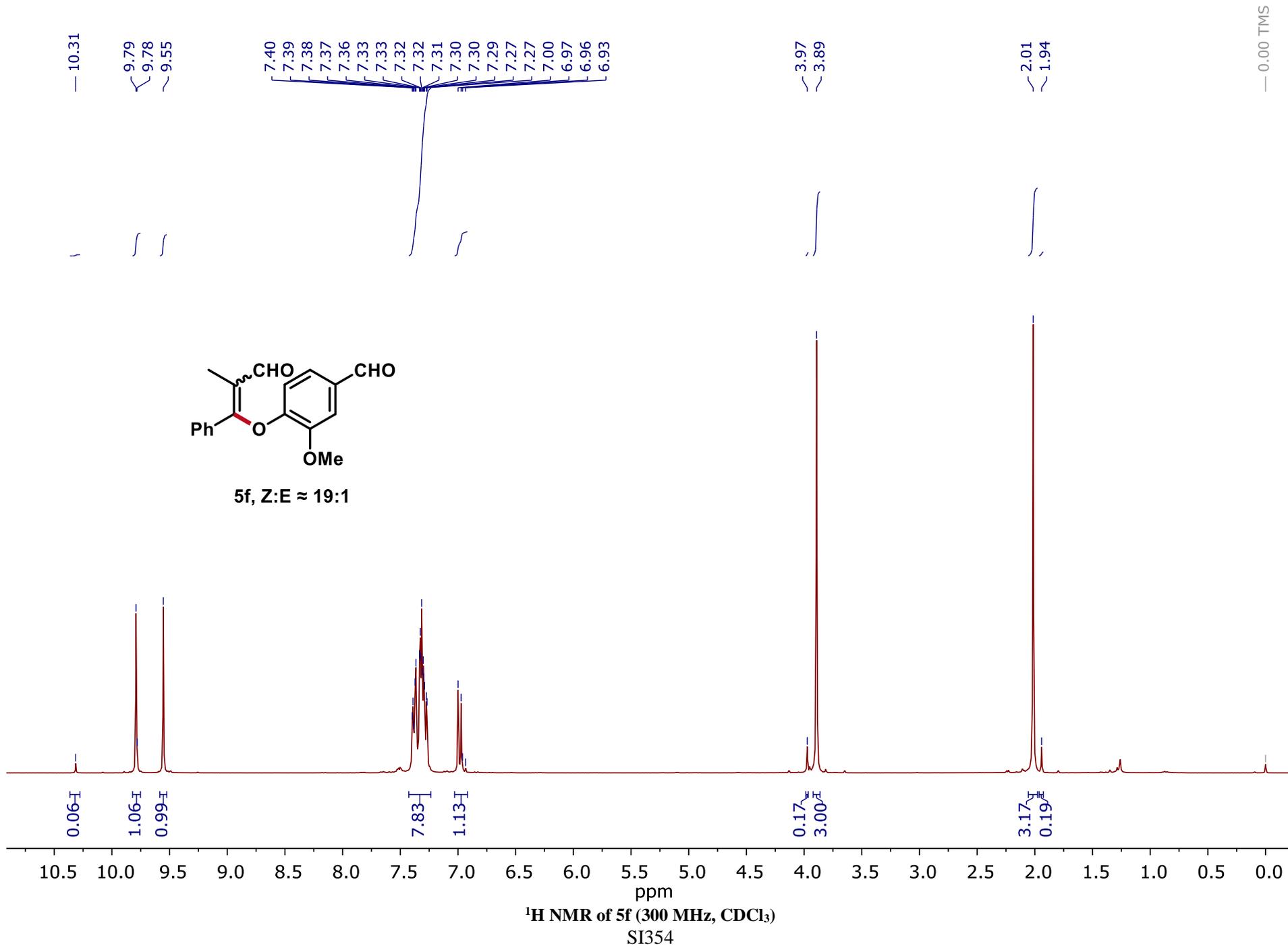
5e'

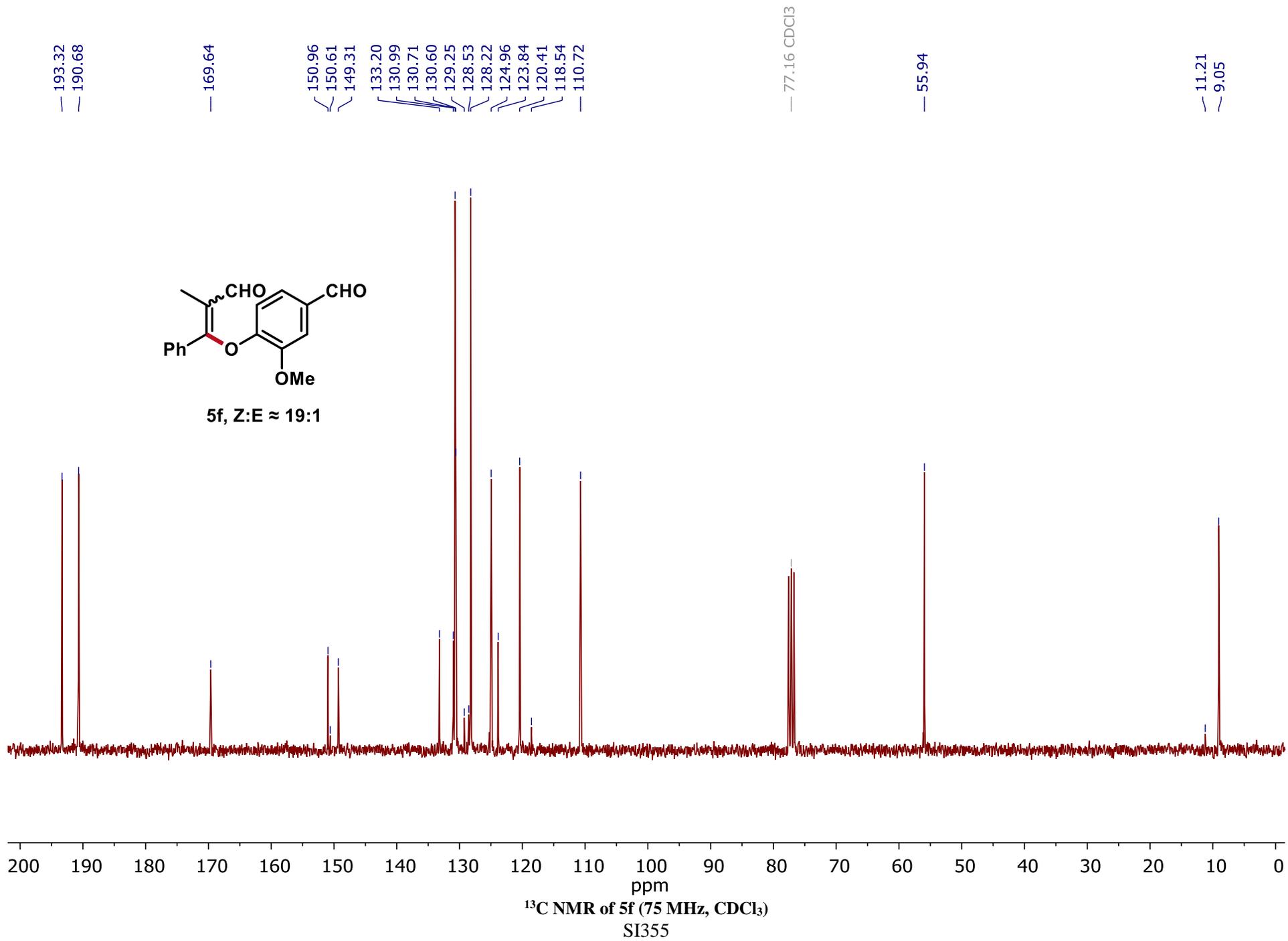


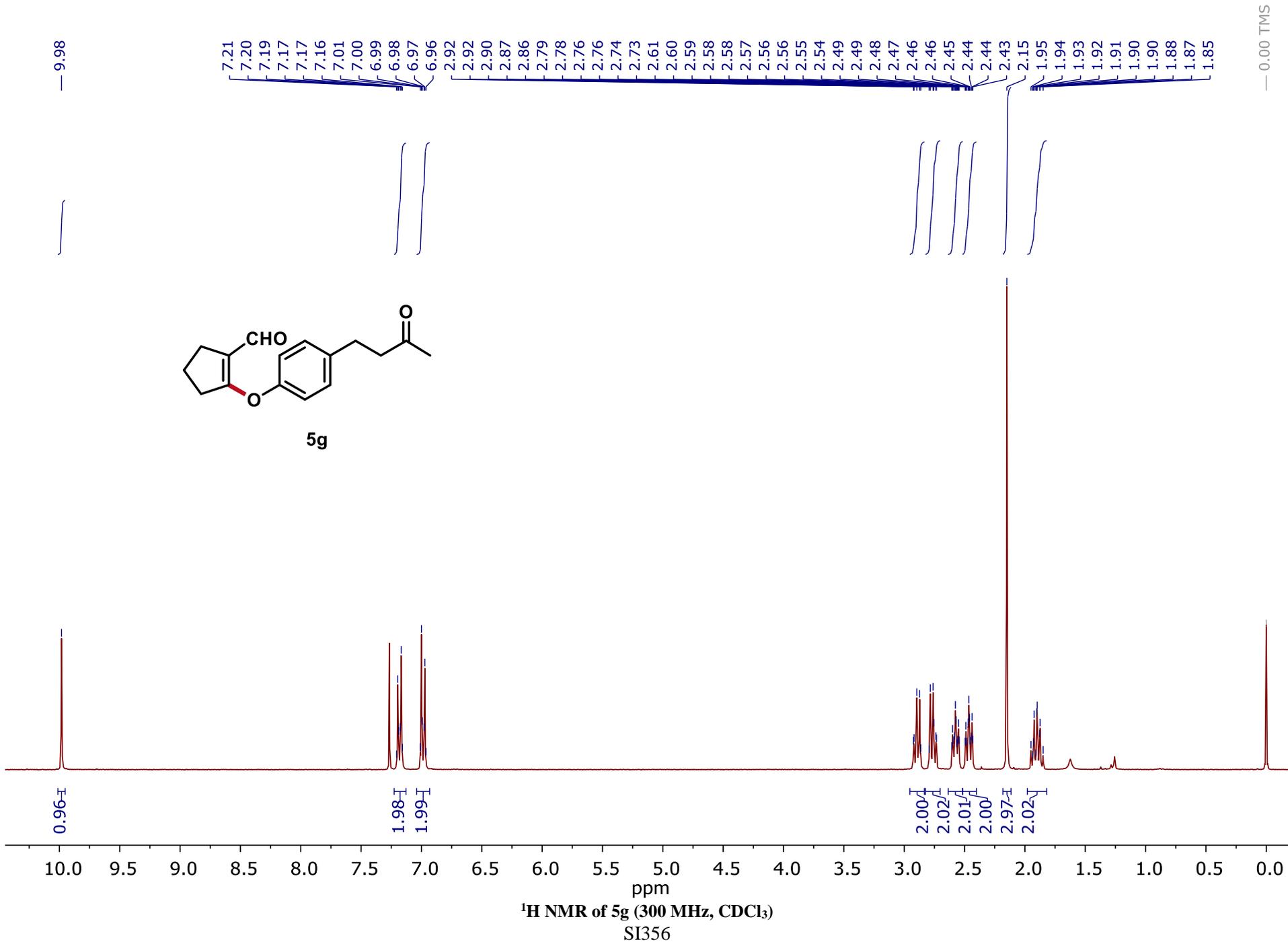


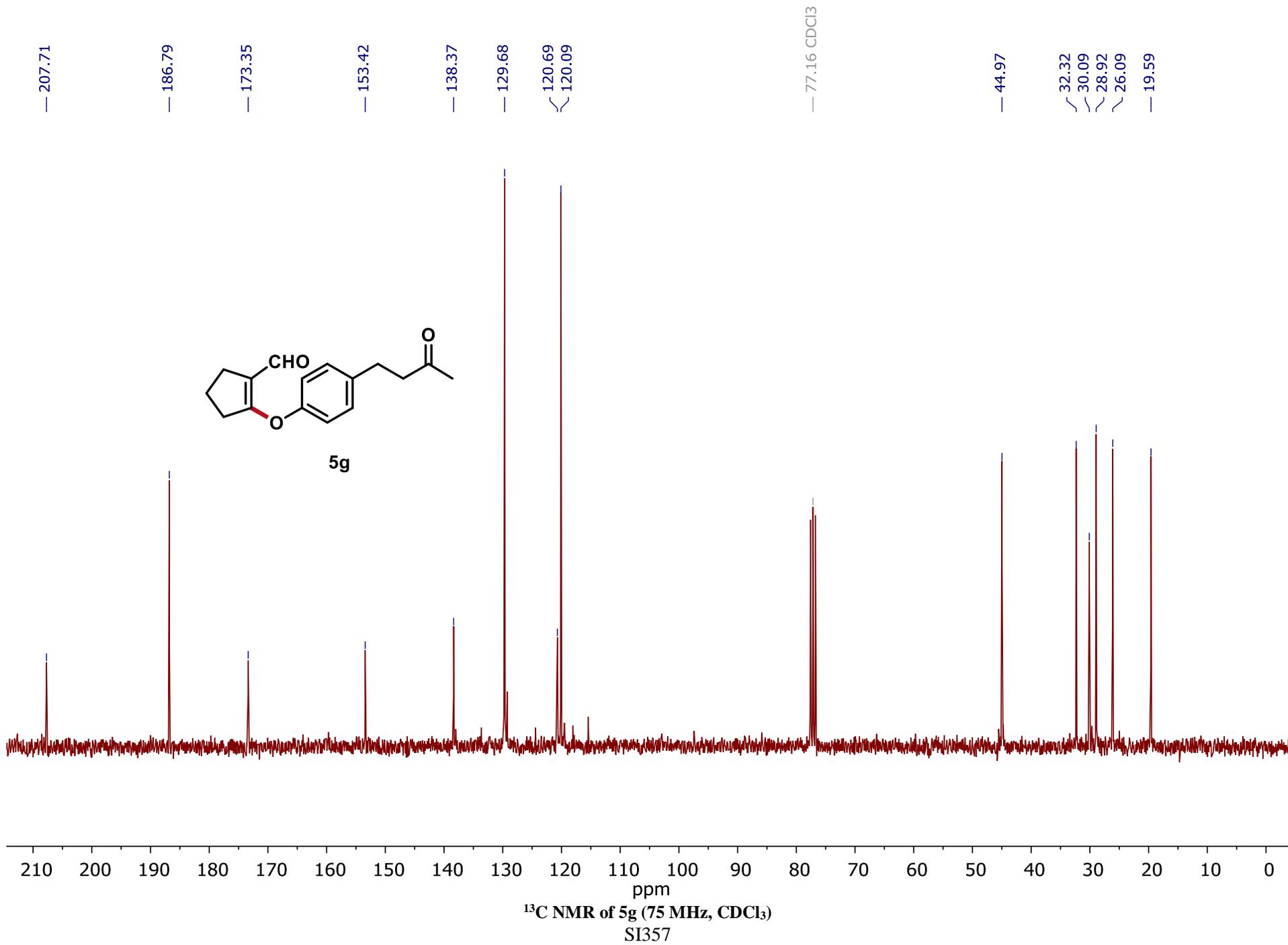
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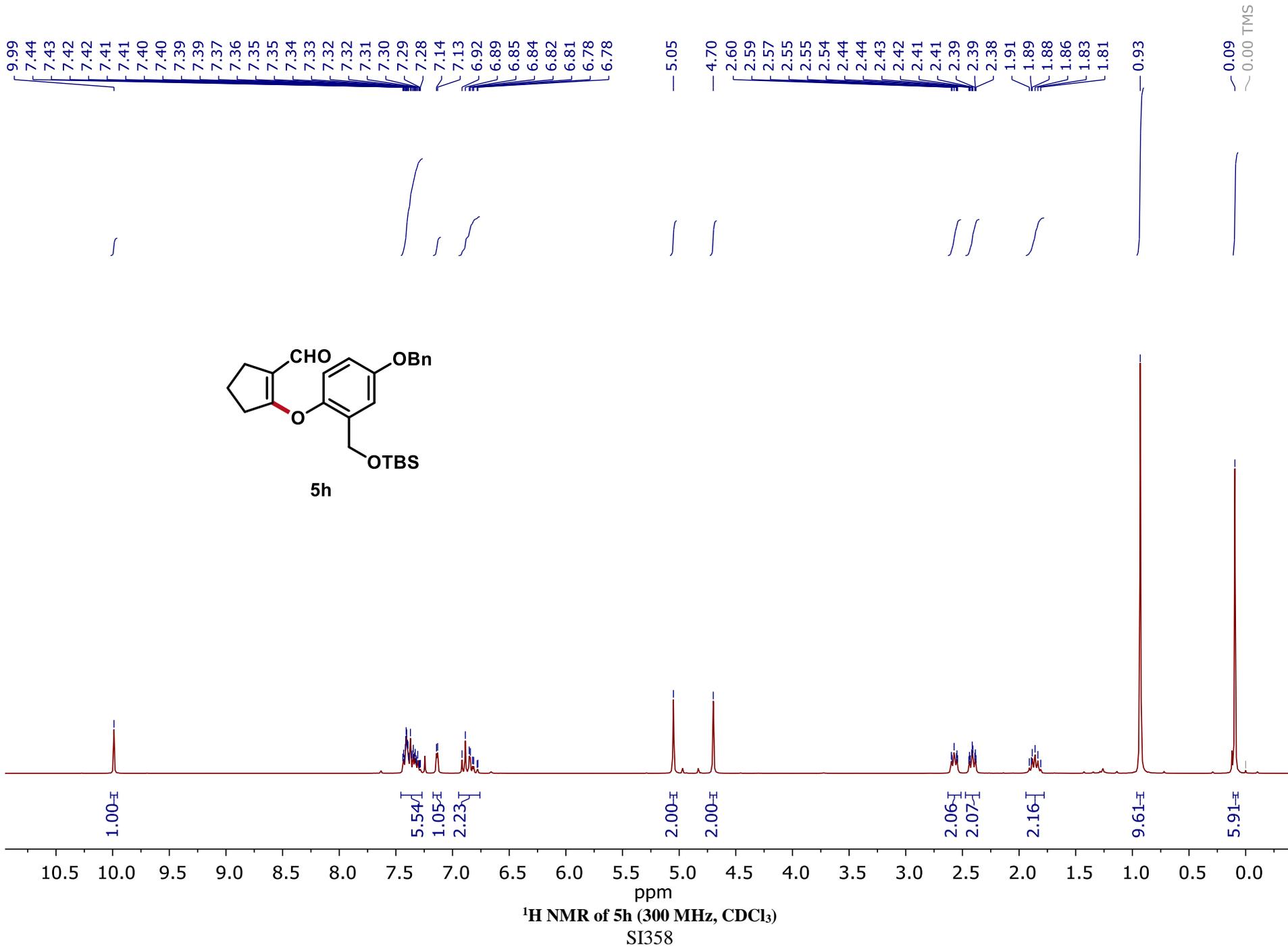


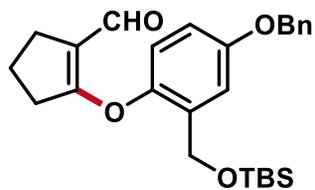




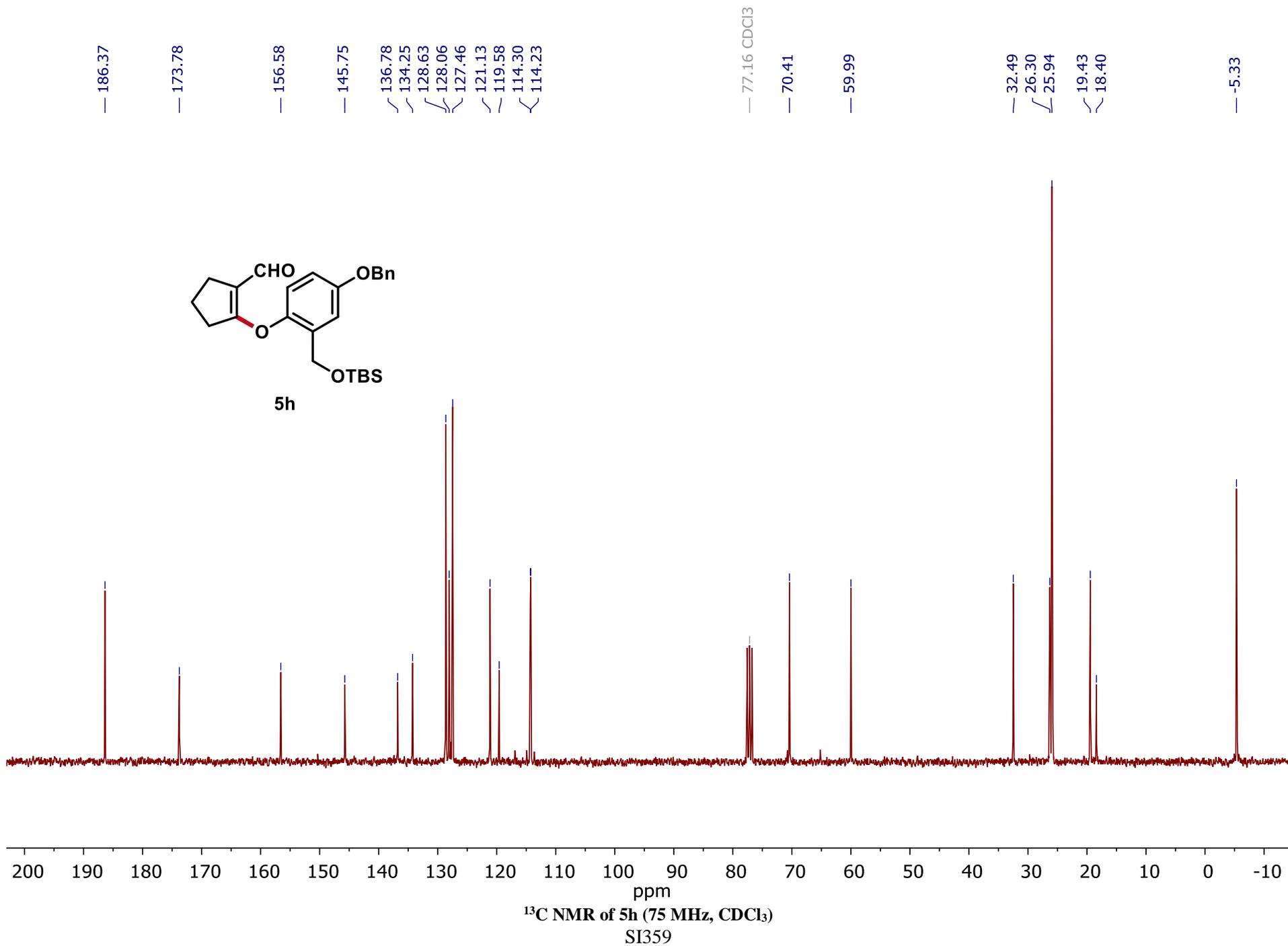


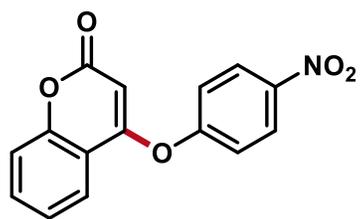




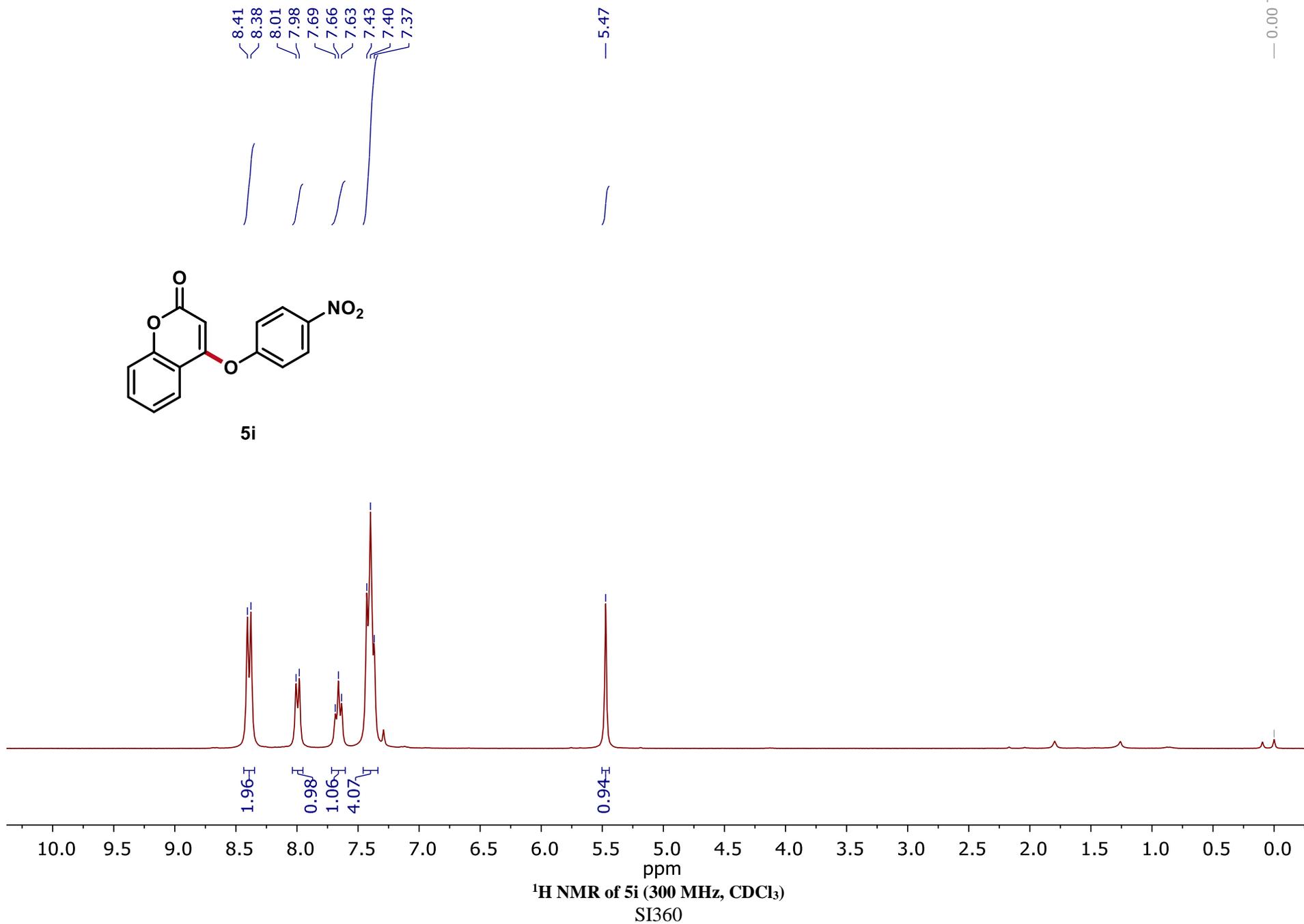


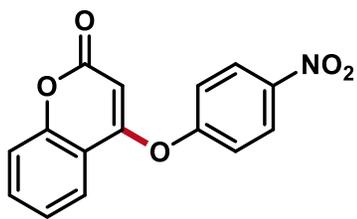
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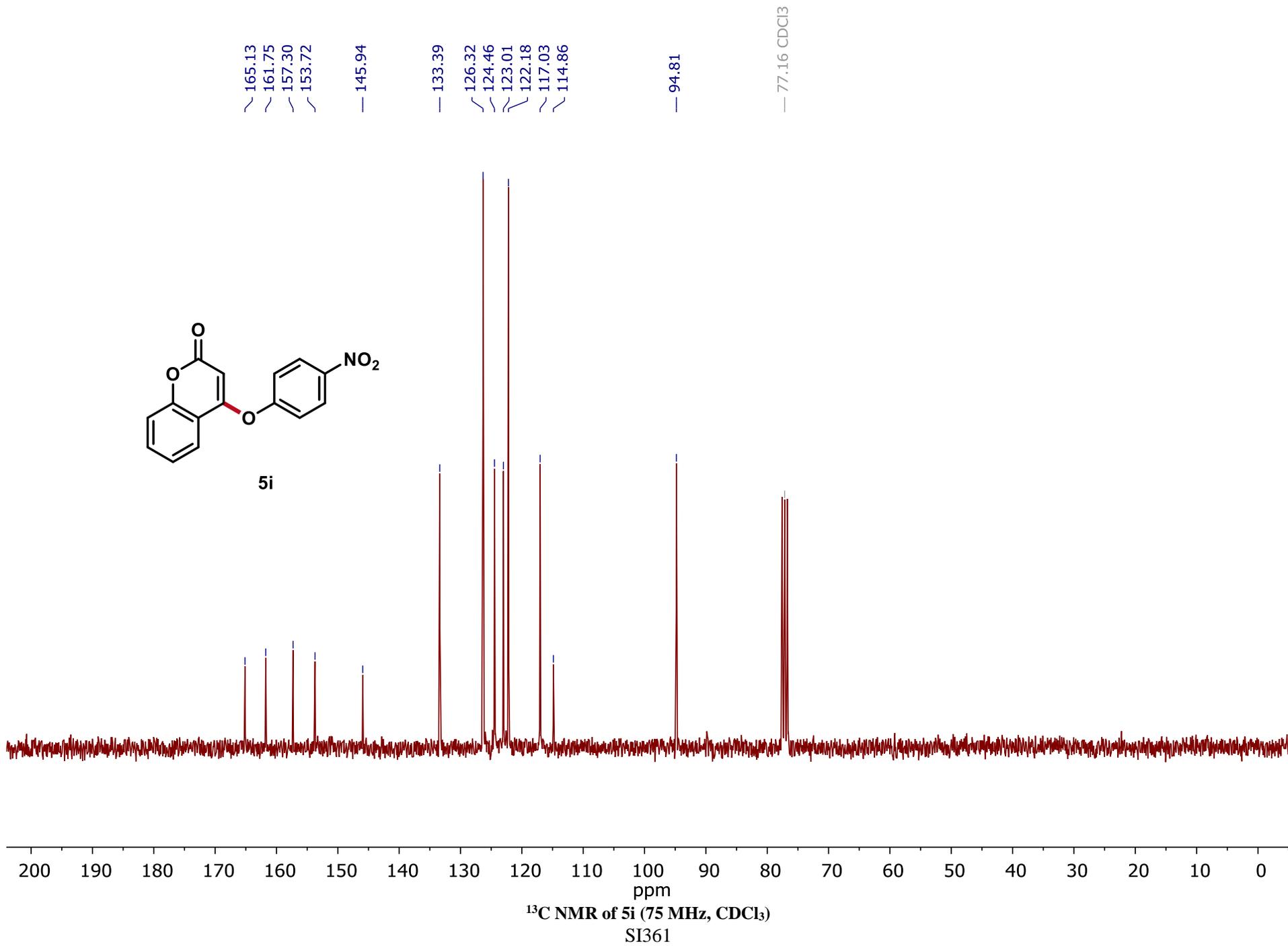


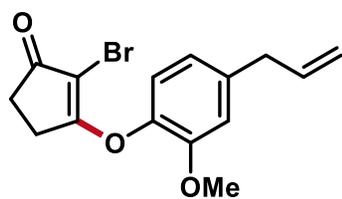
5i



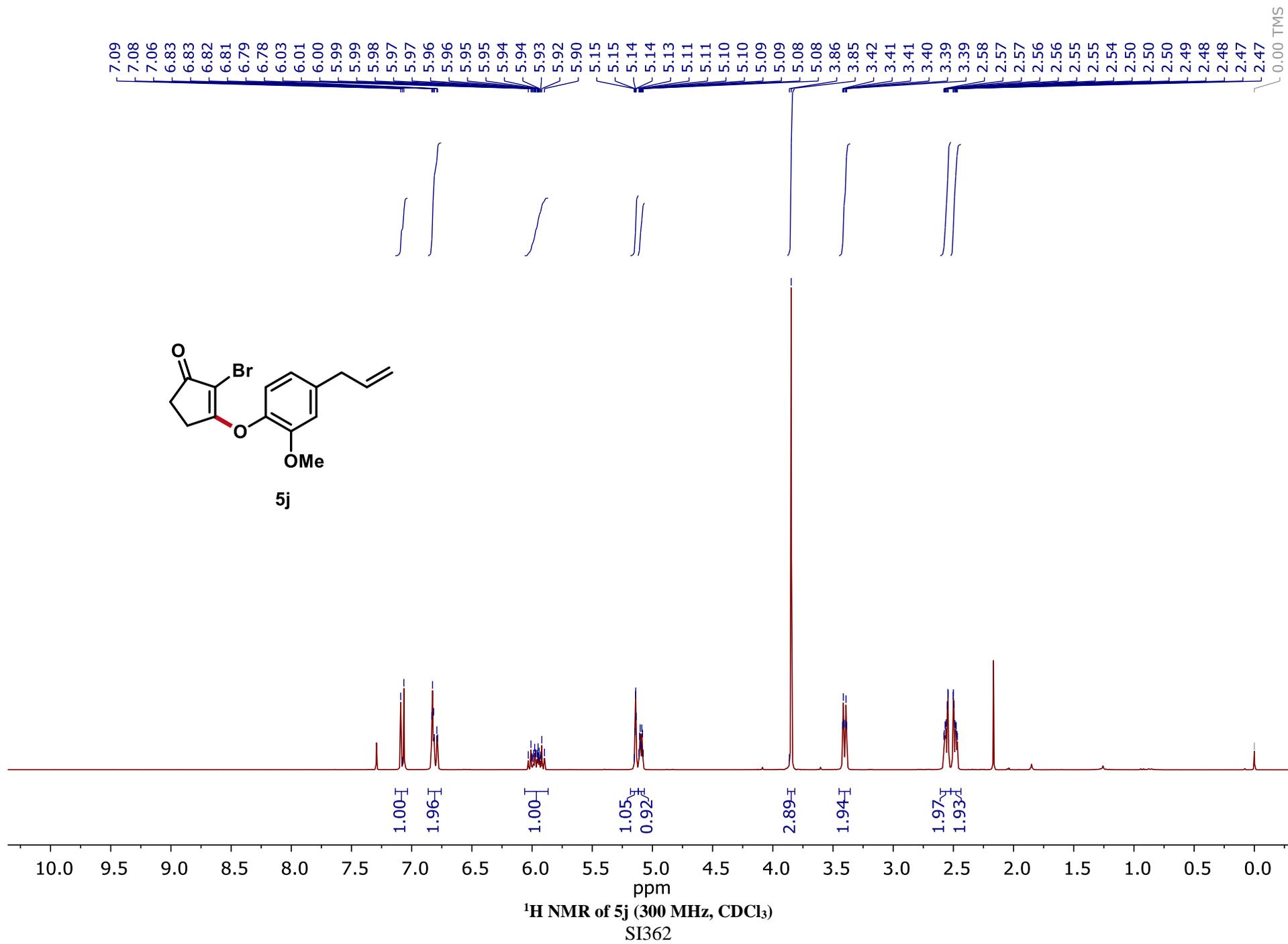


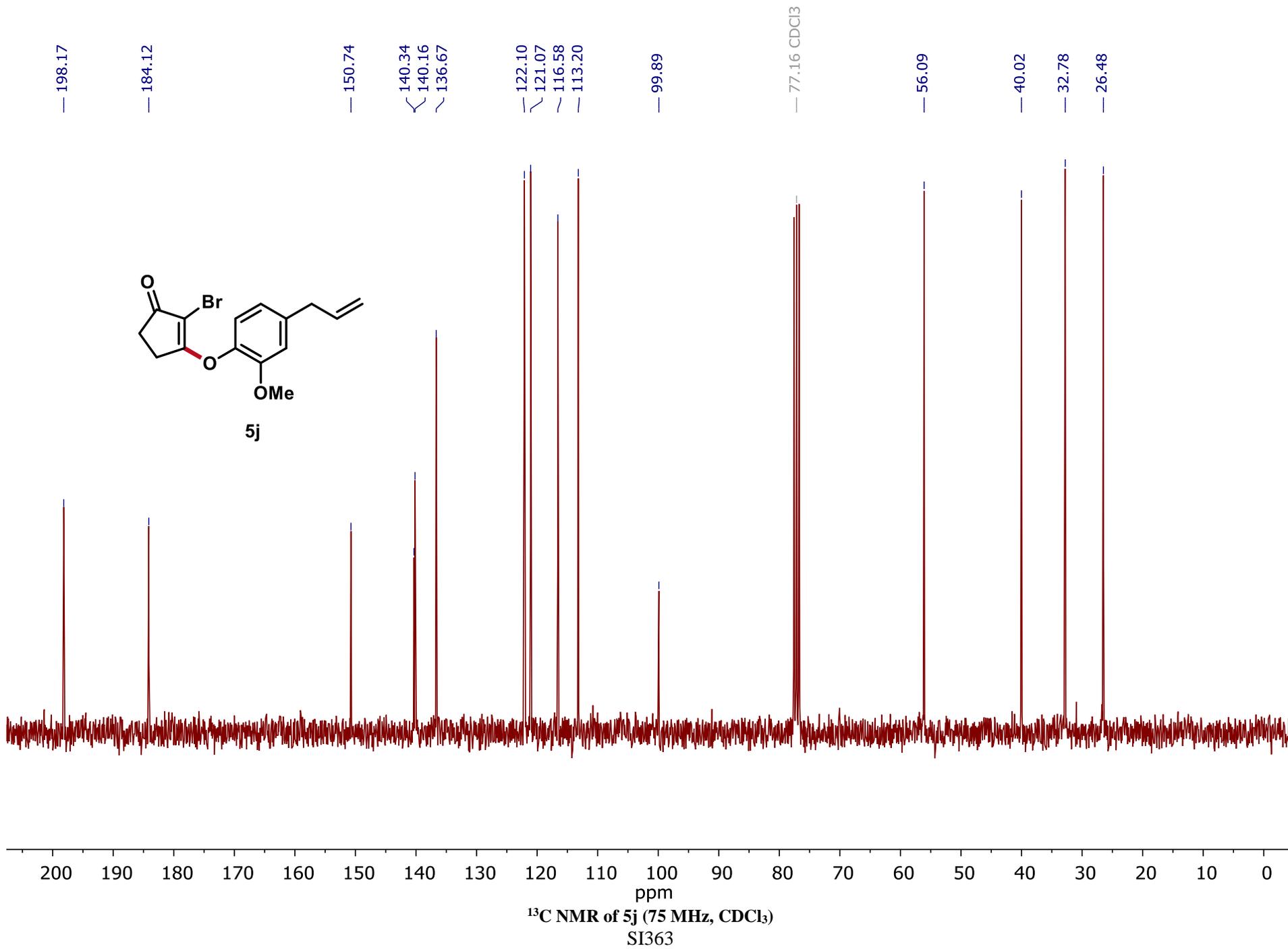
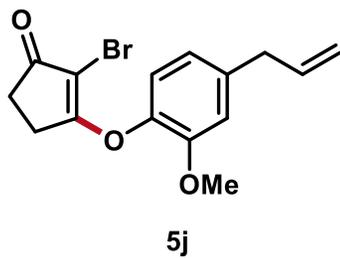
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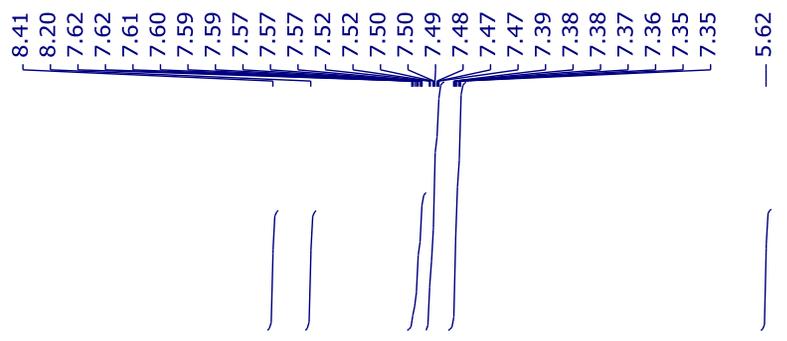


5j

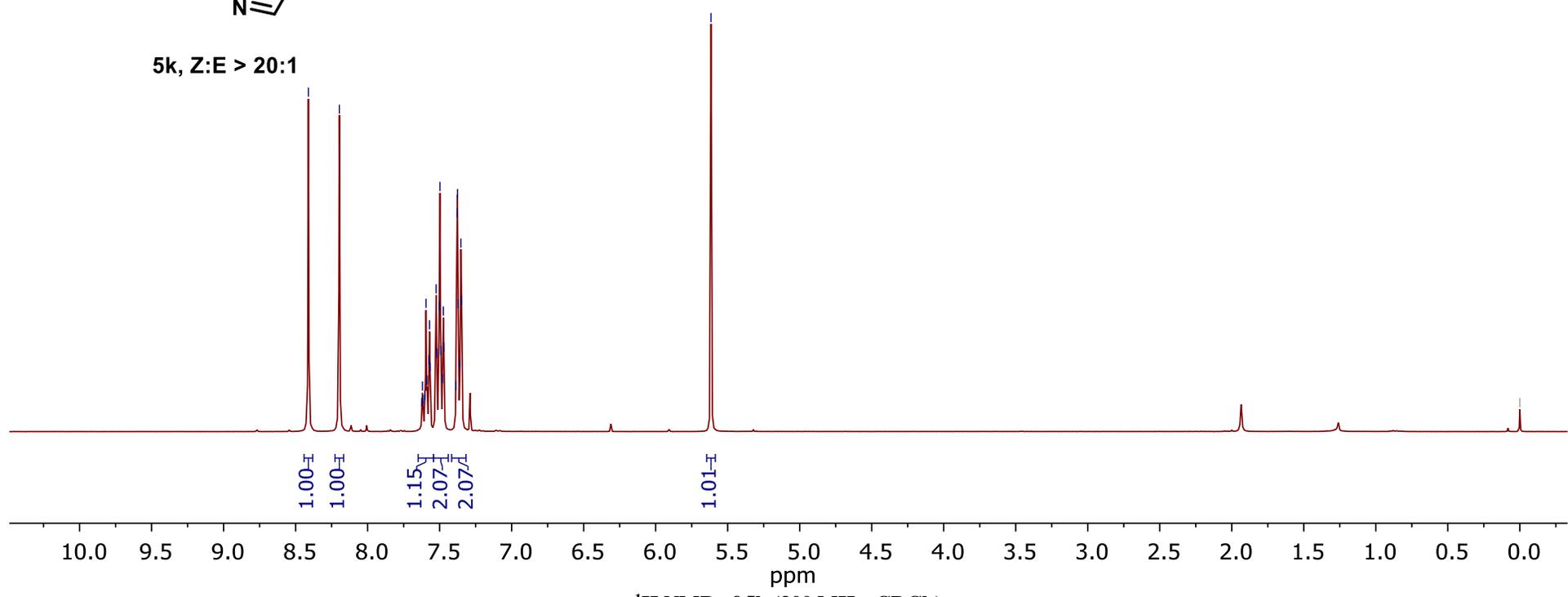




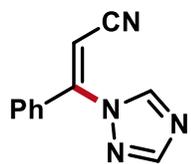
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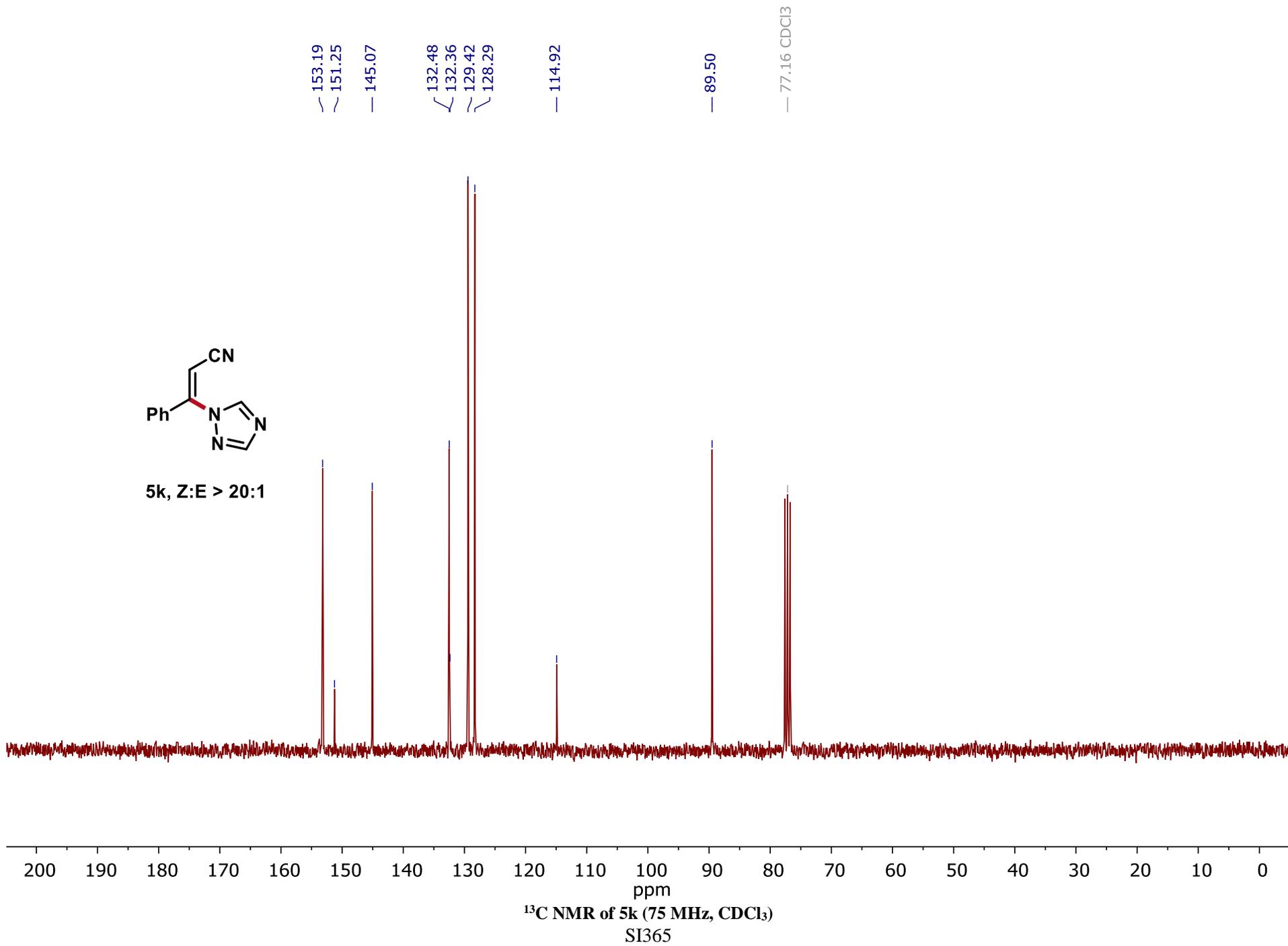
5k, Z:E > 20:1

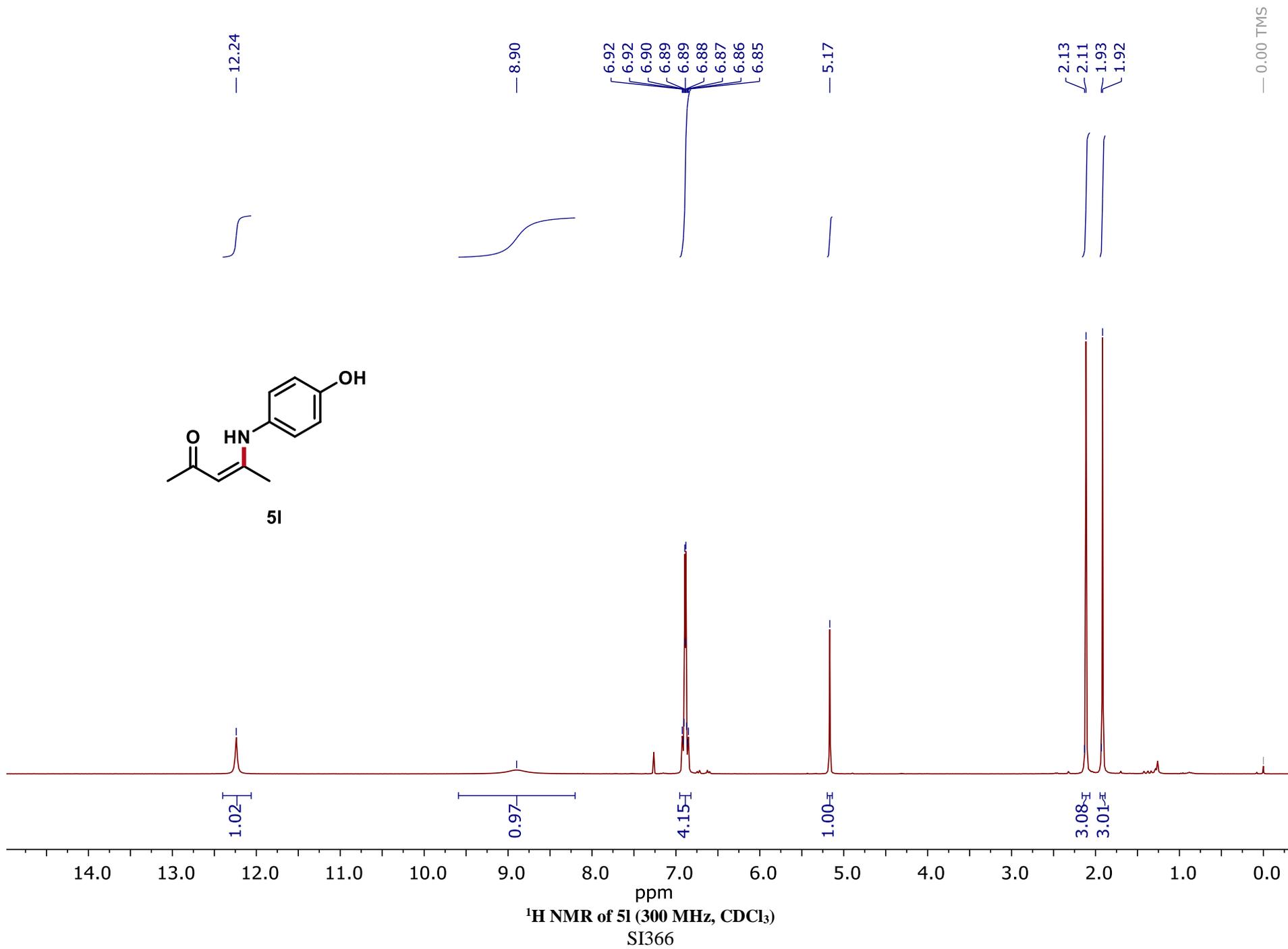
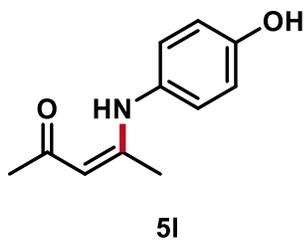


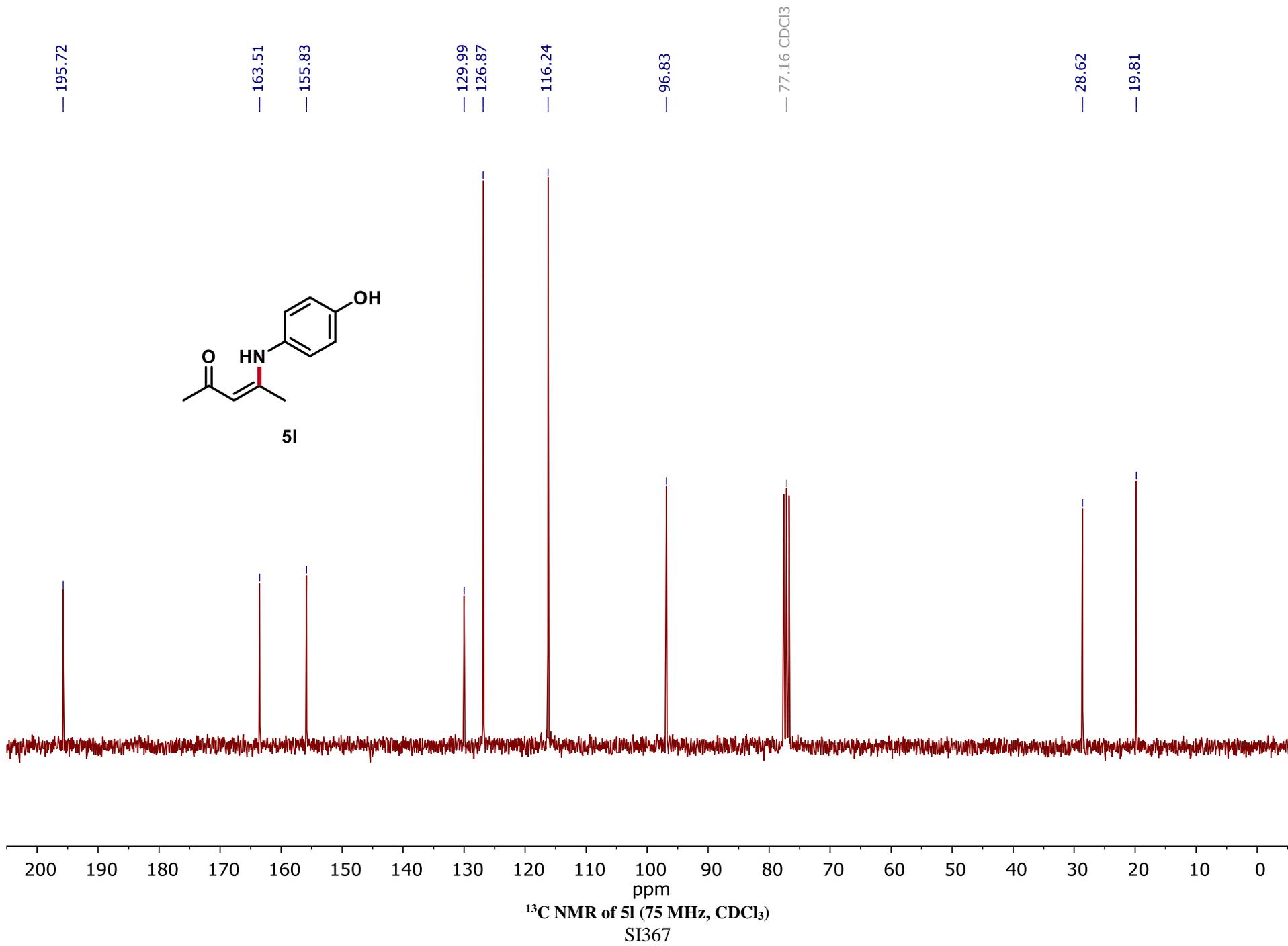
¹H NMR of 5k (300 MHz, CDCl₃)
SI364

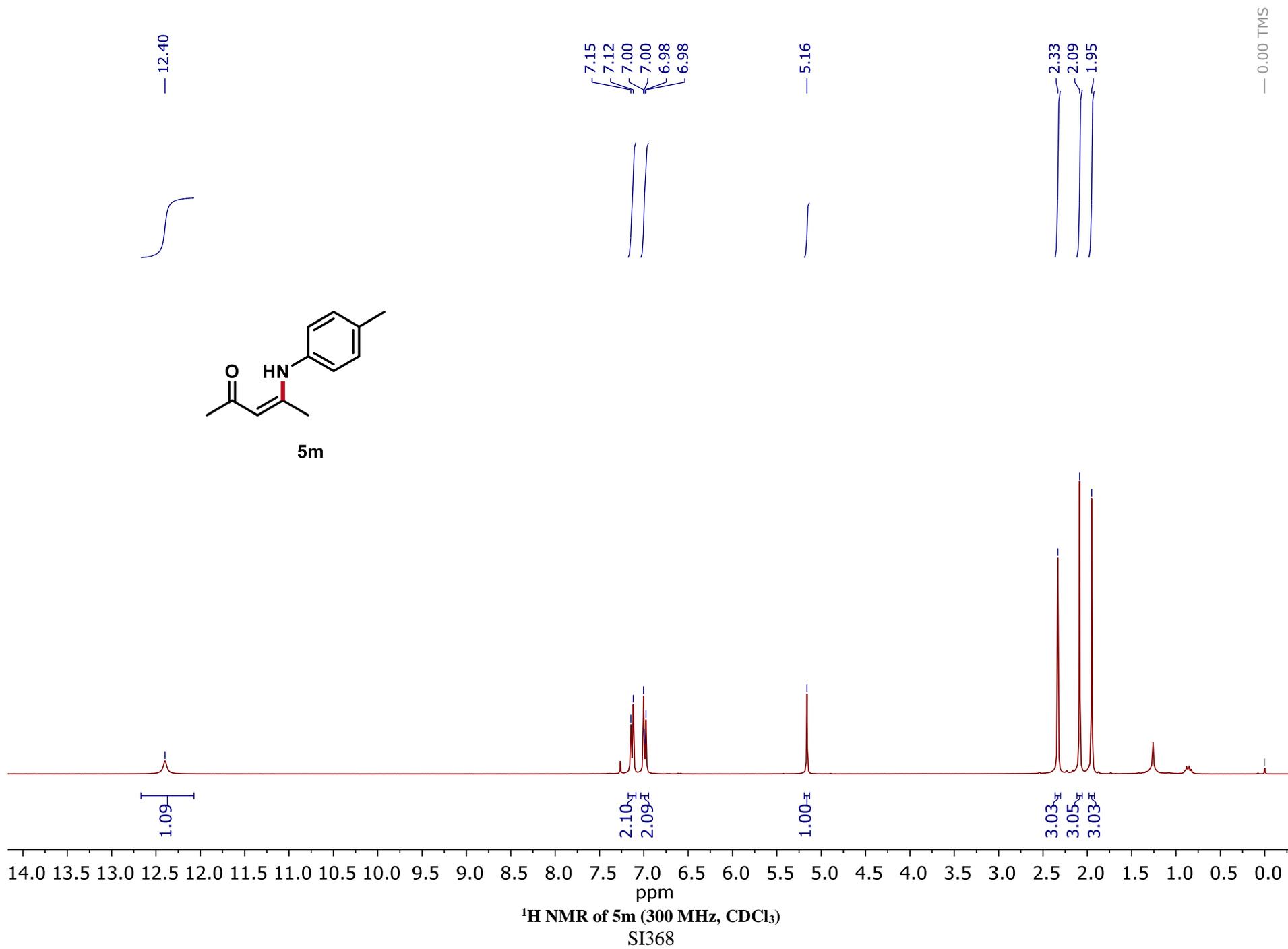
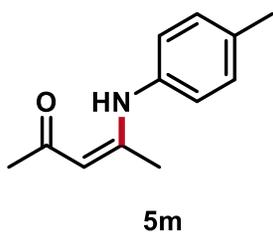


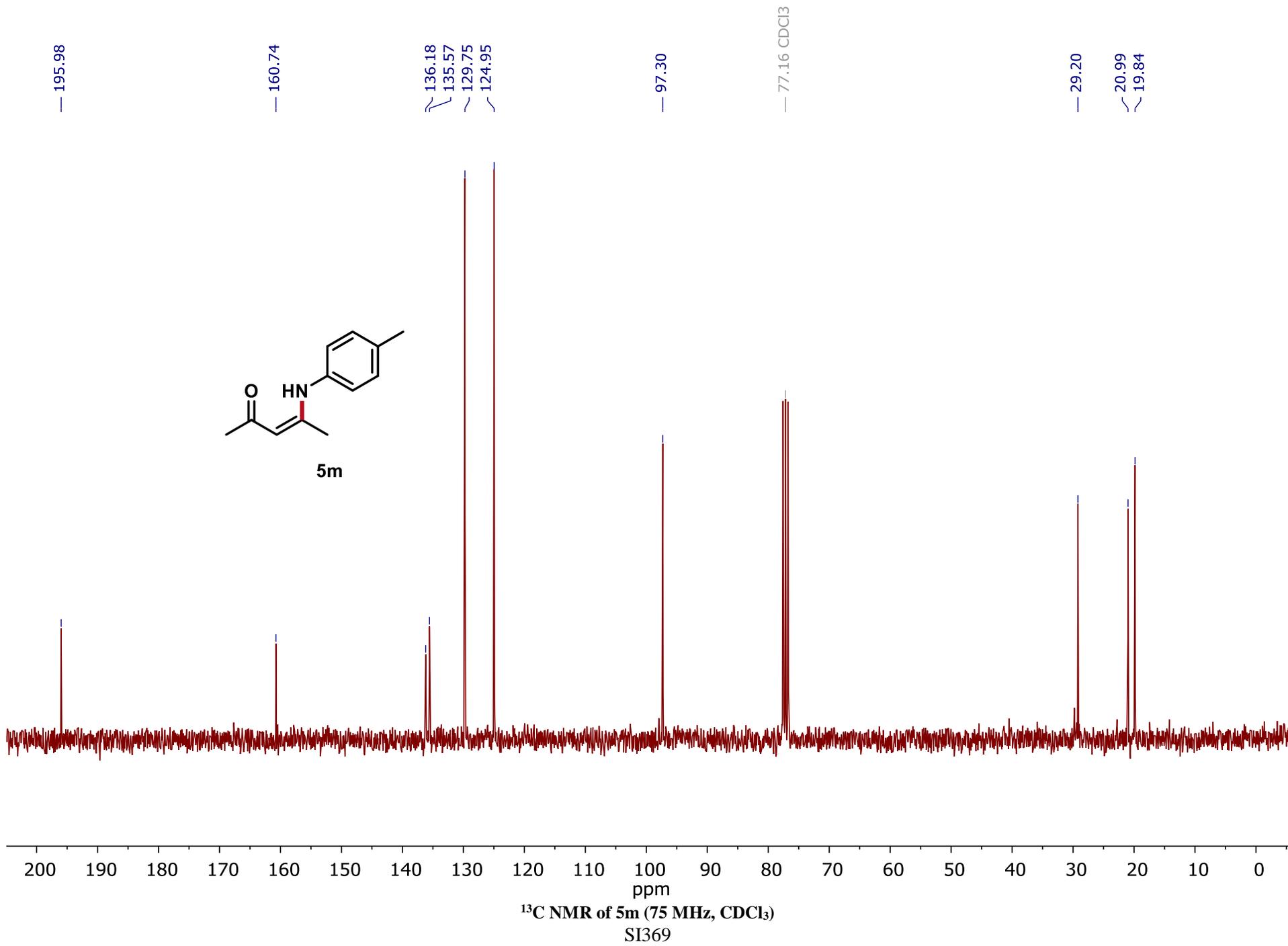
5k, Z:E > 20:1

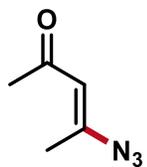






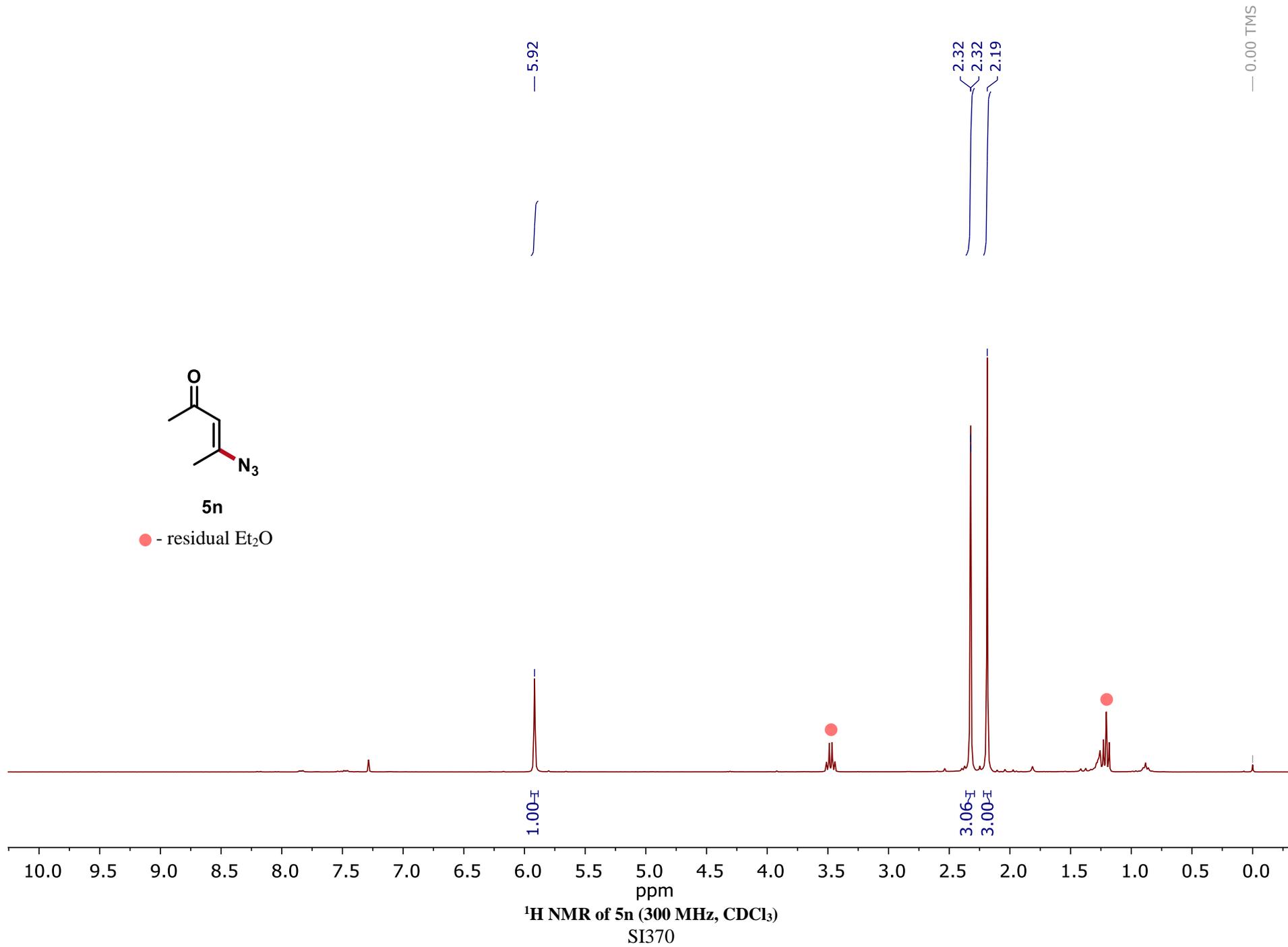


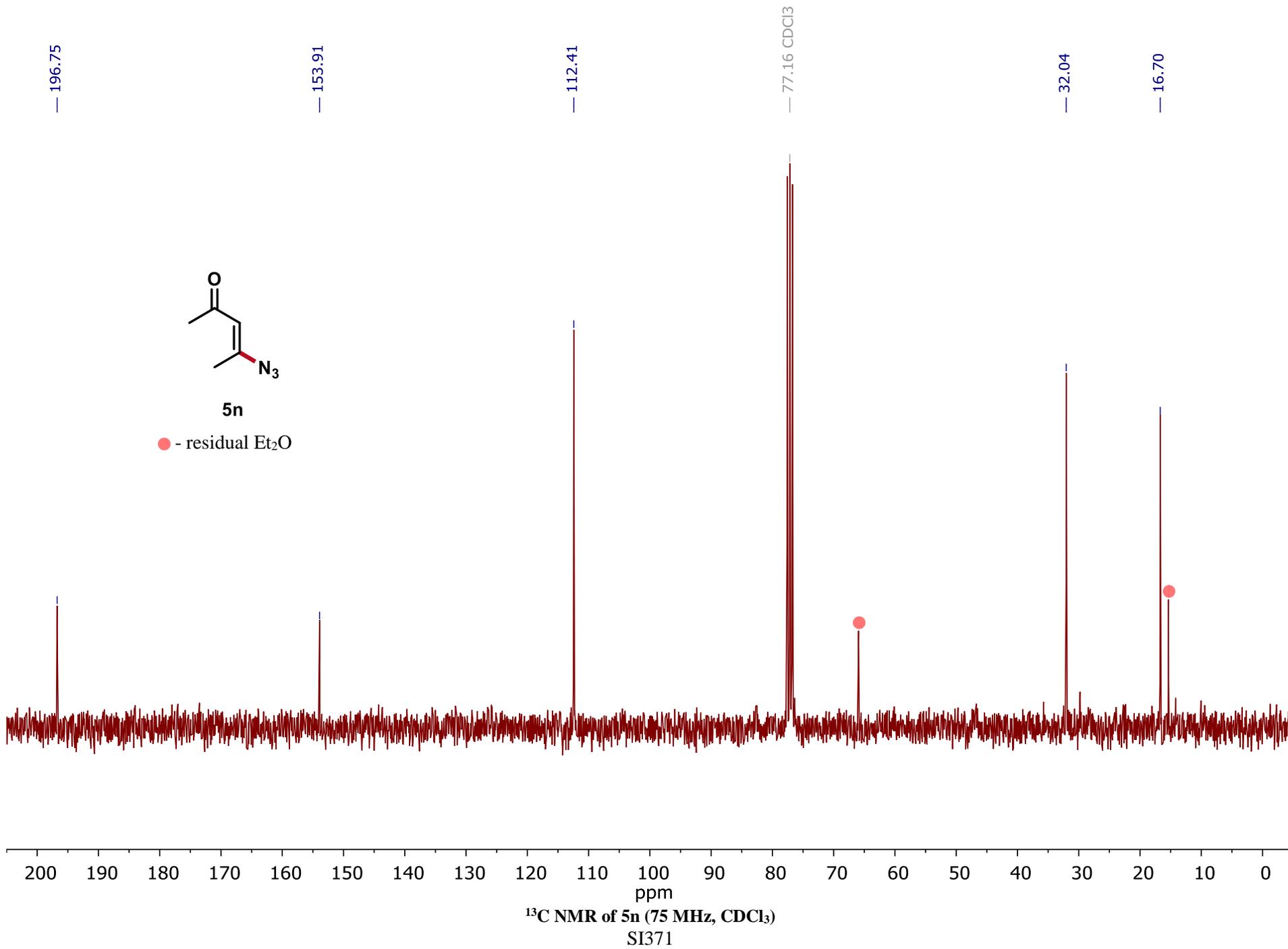


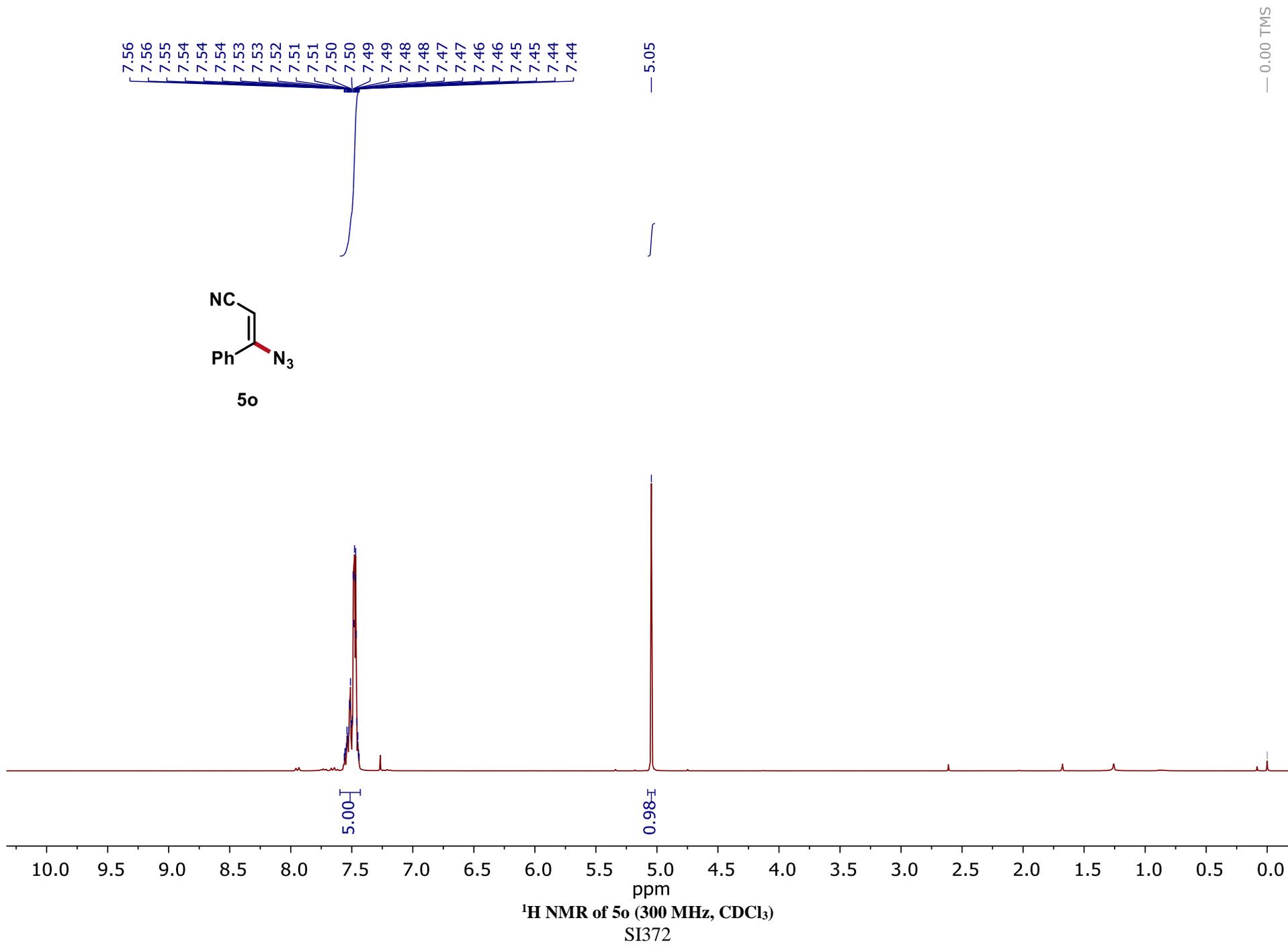
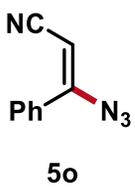


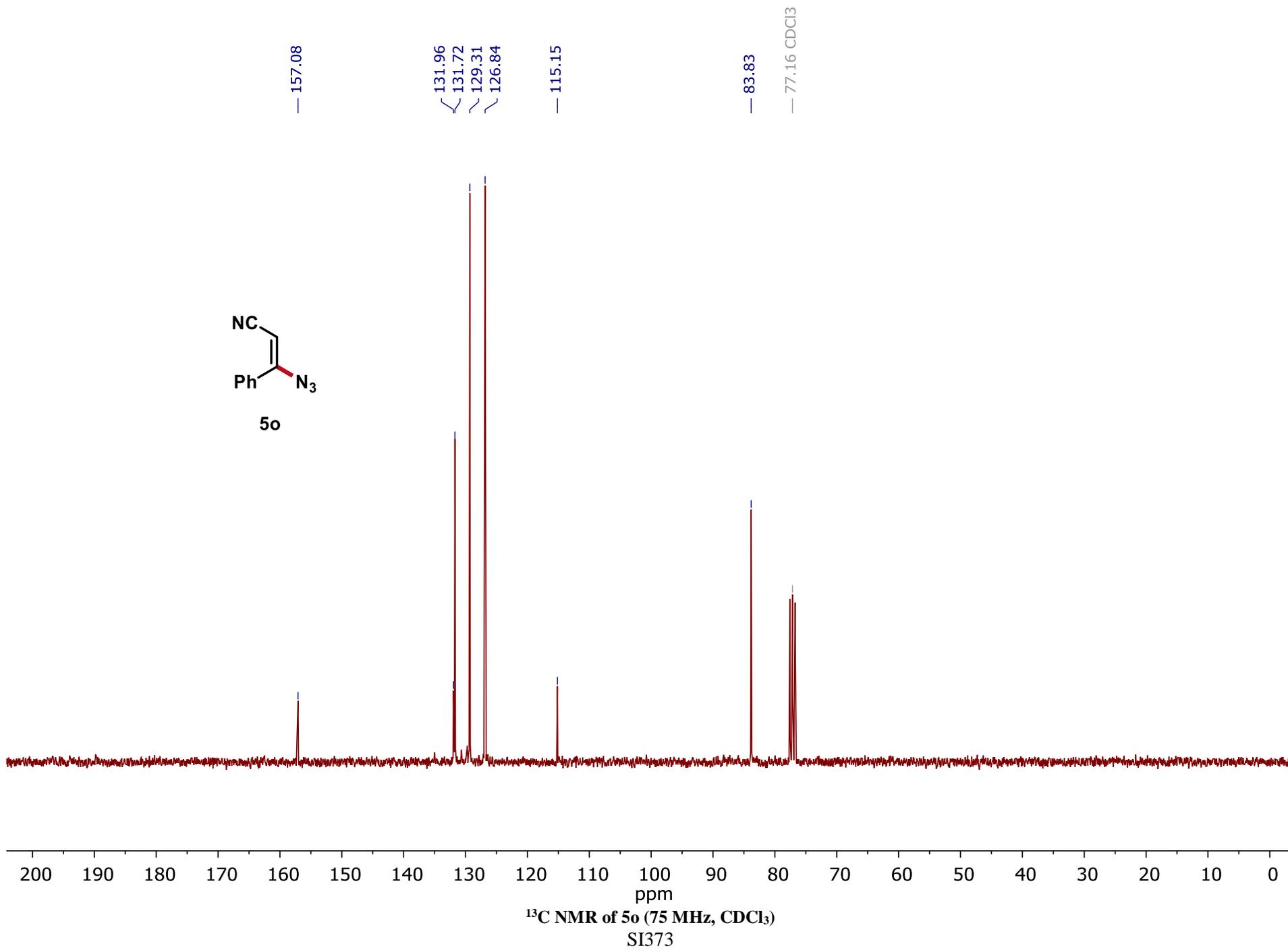
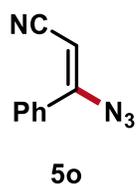
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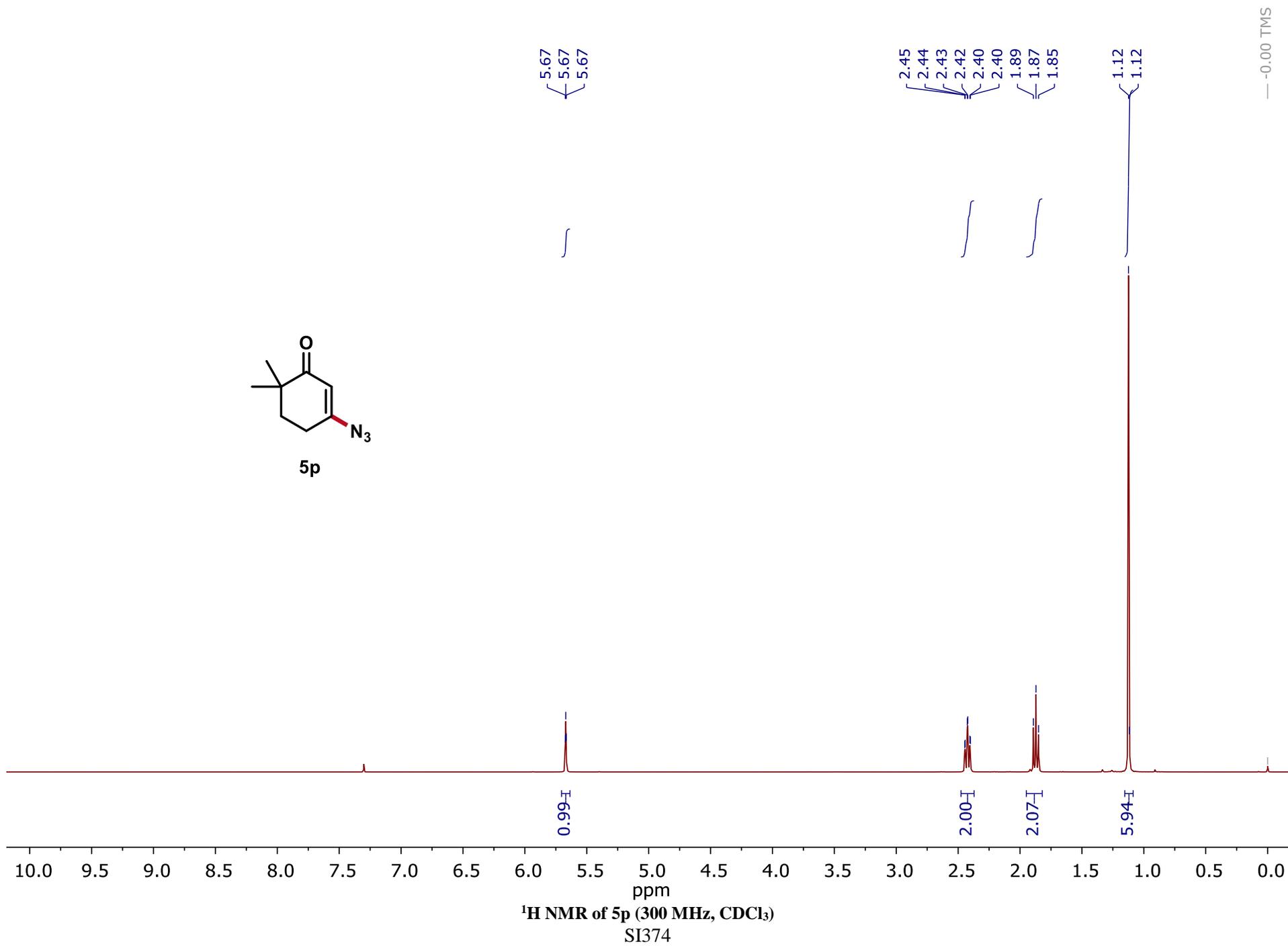
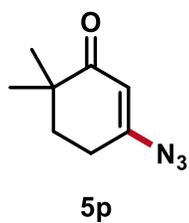
● - residual Et₂O

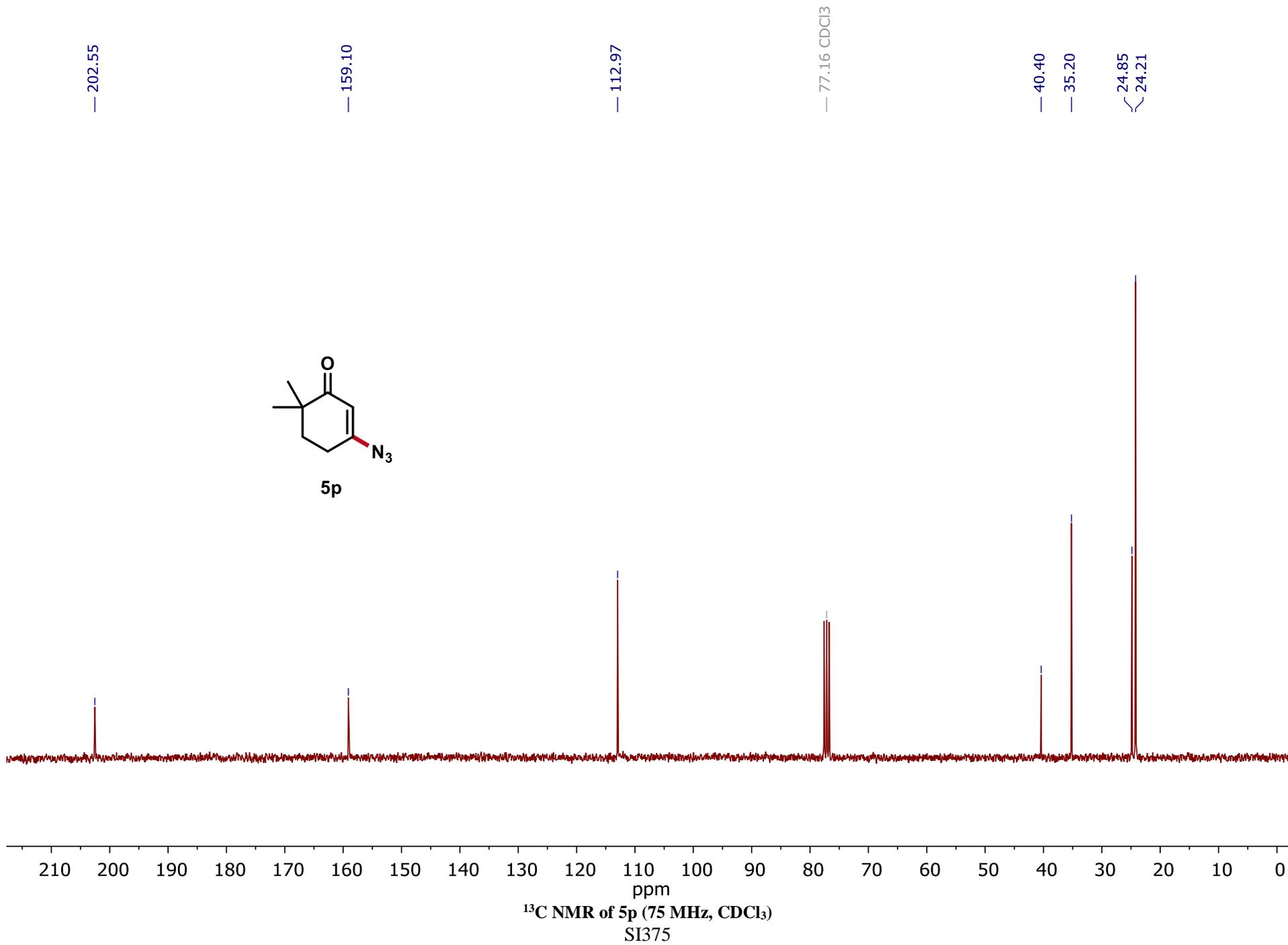
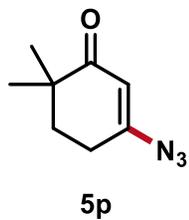


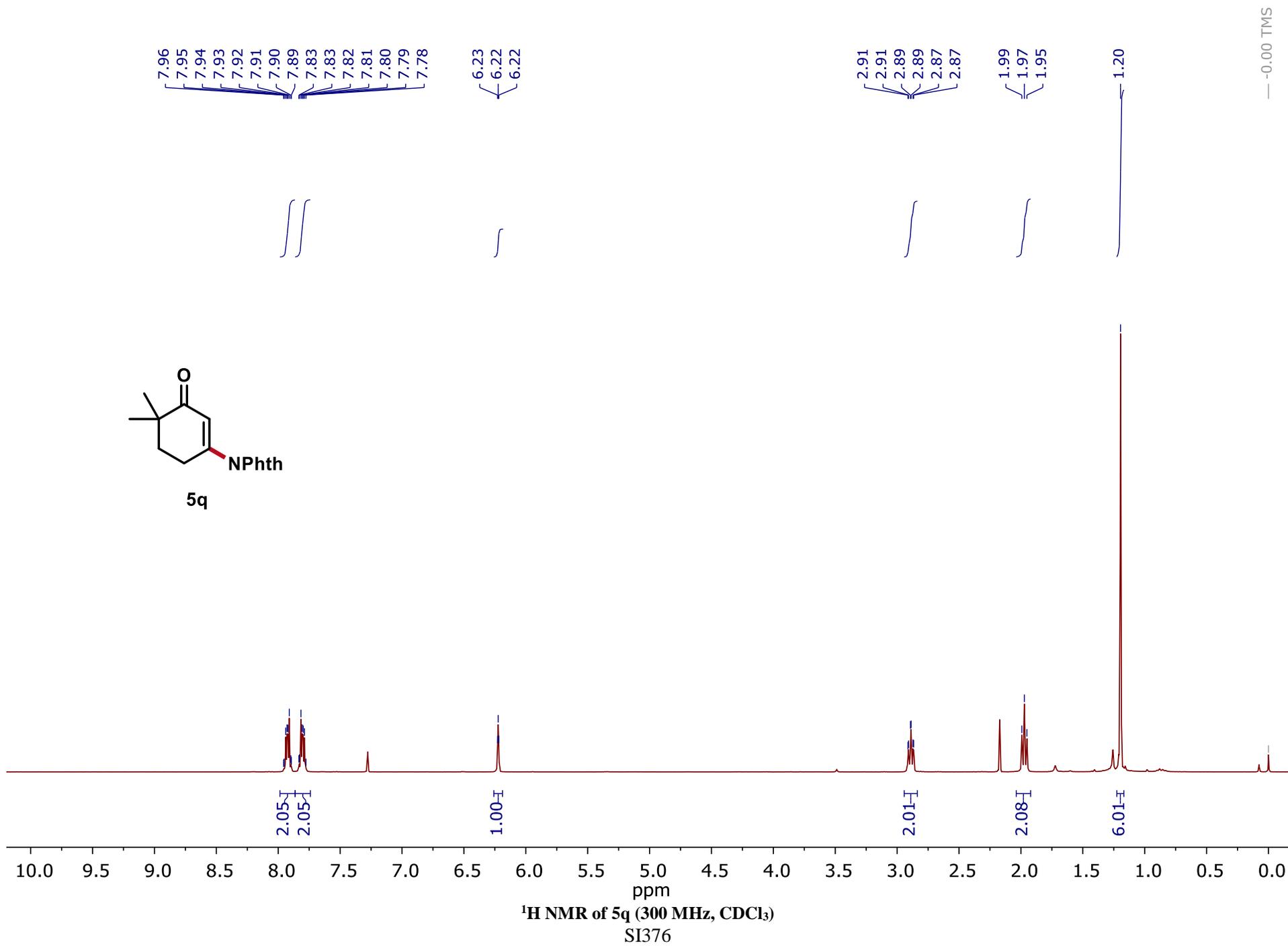
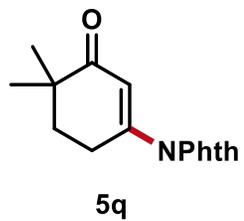


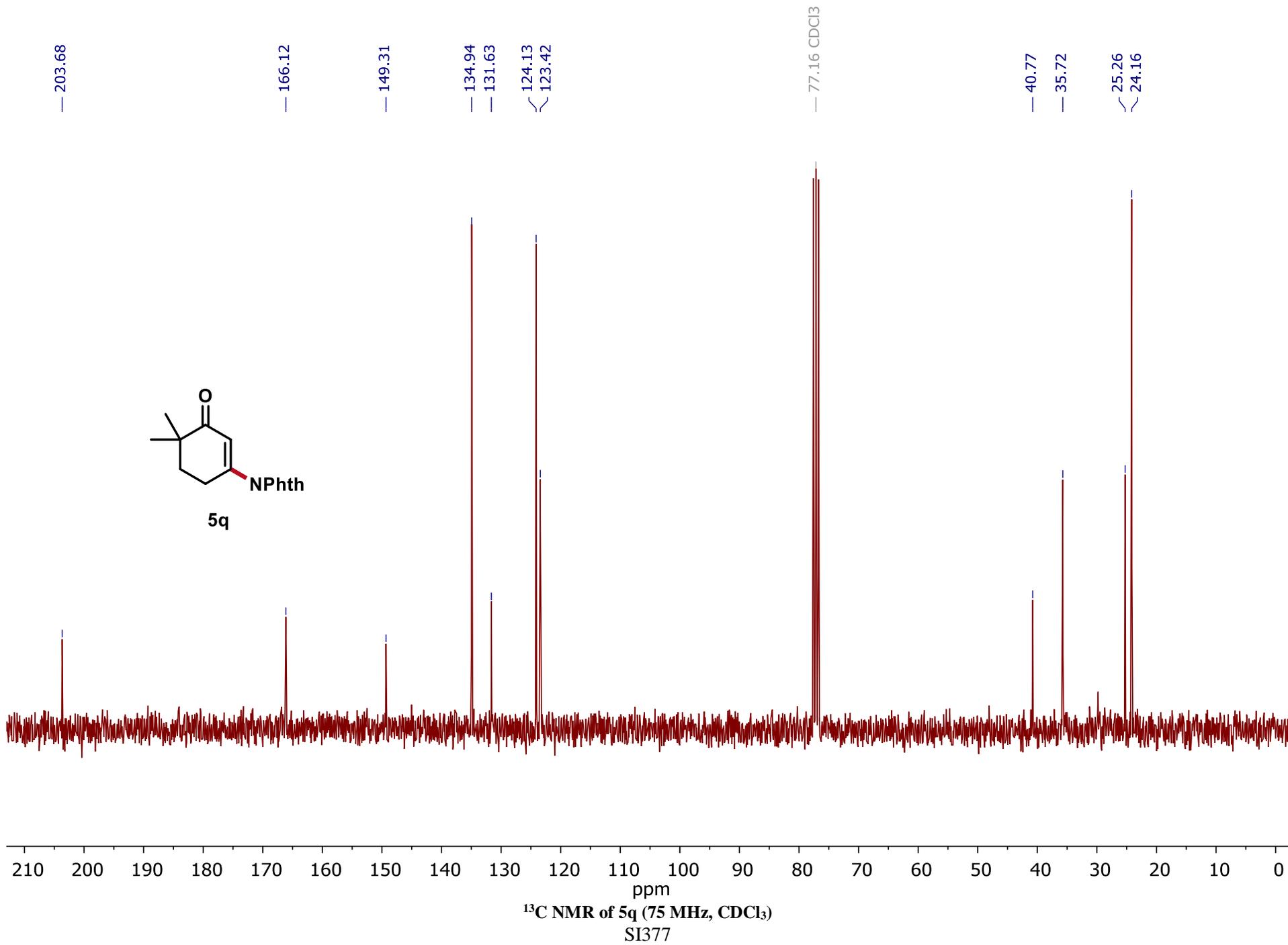


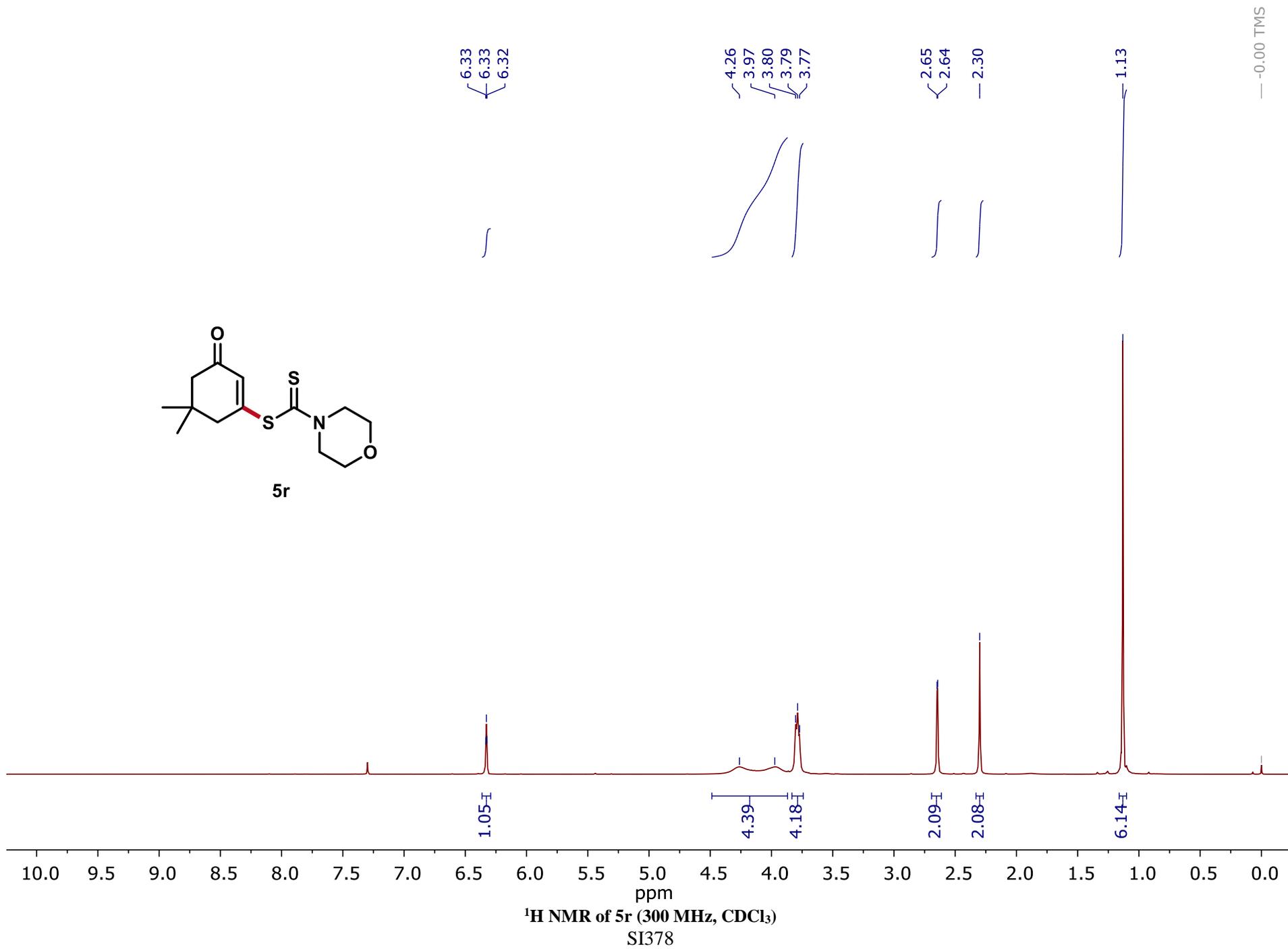
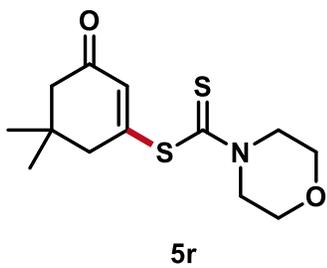


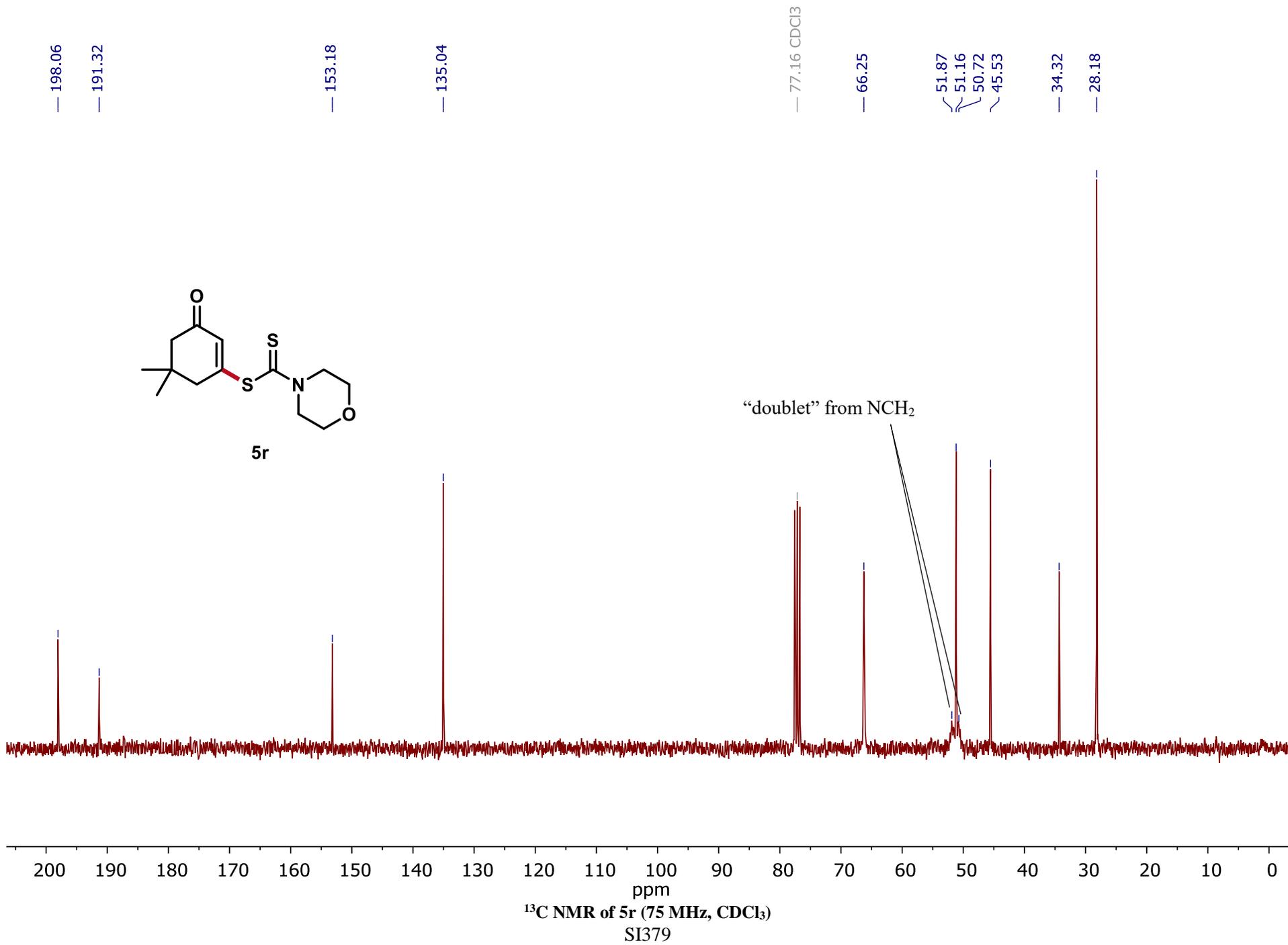


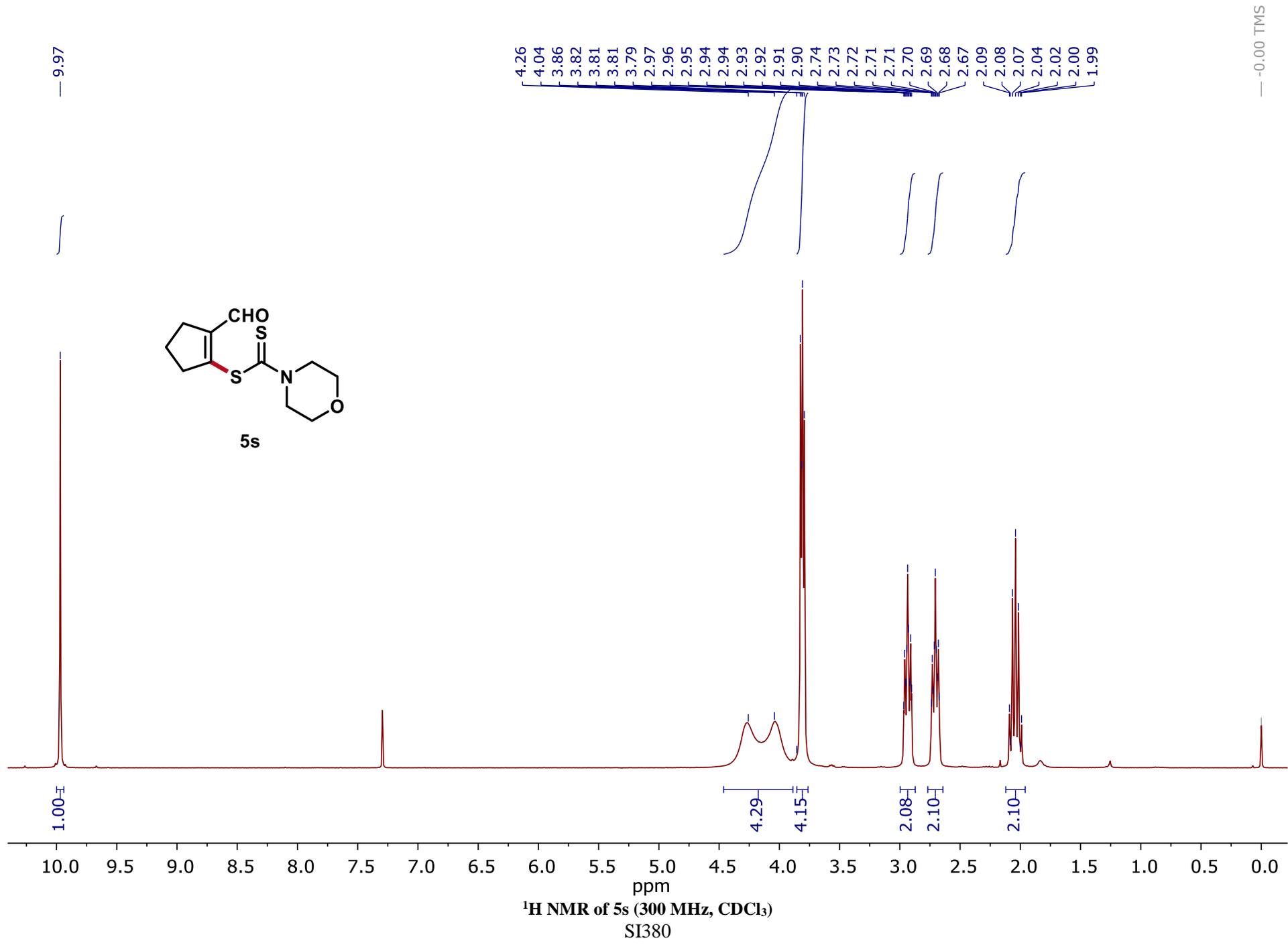


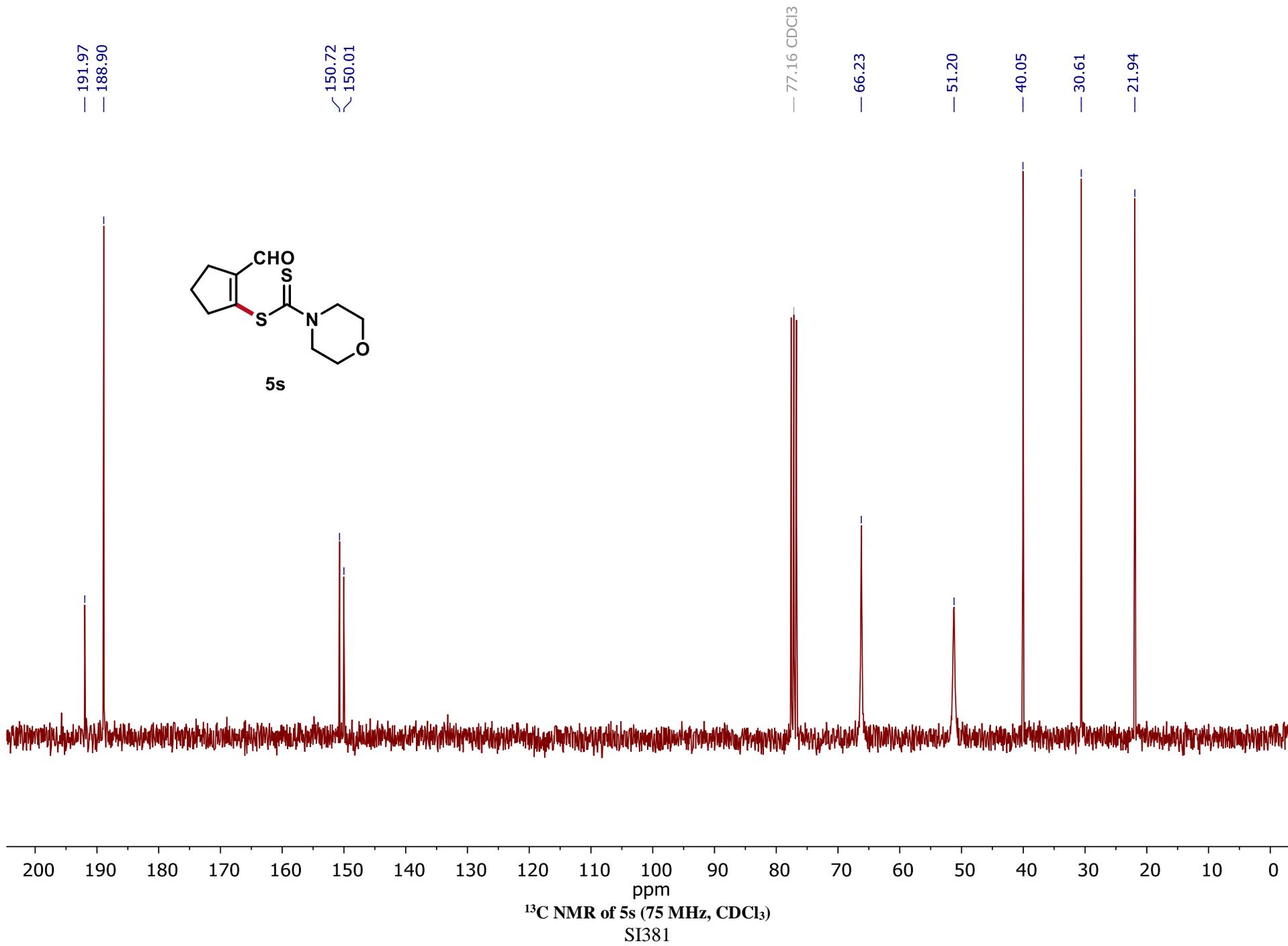








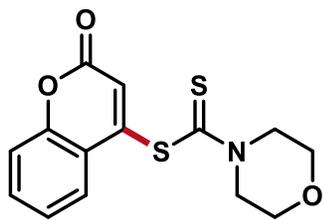




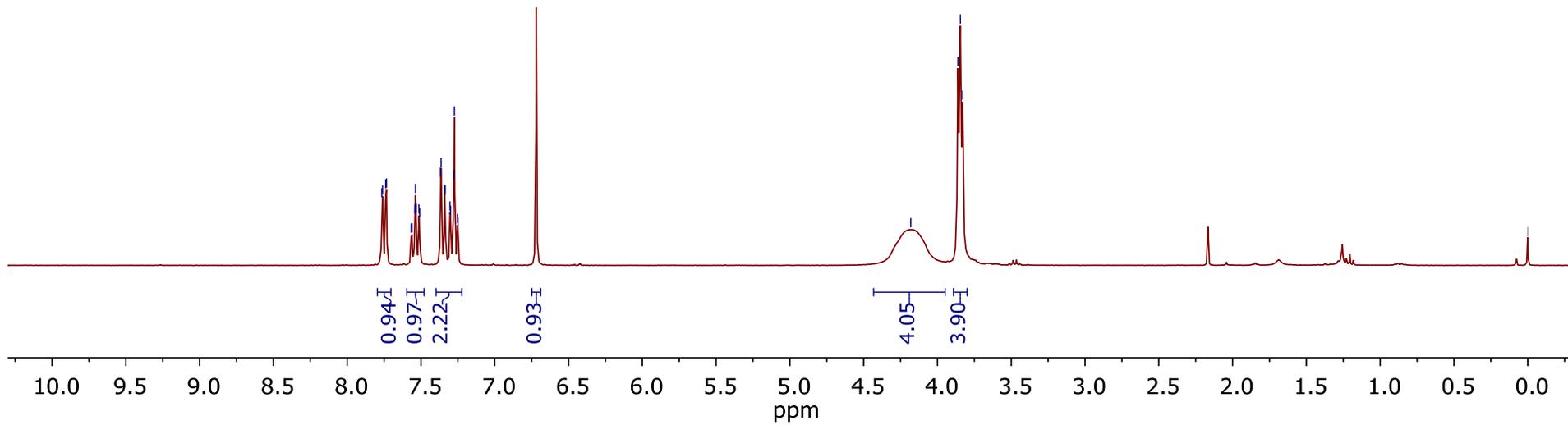
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7.25

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3.84
3.83

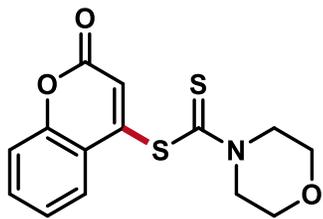
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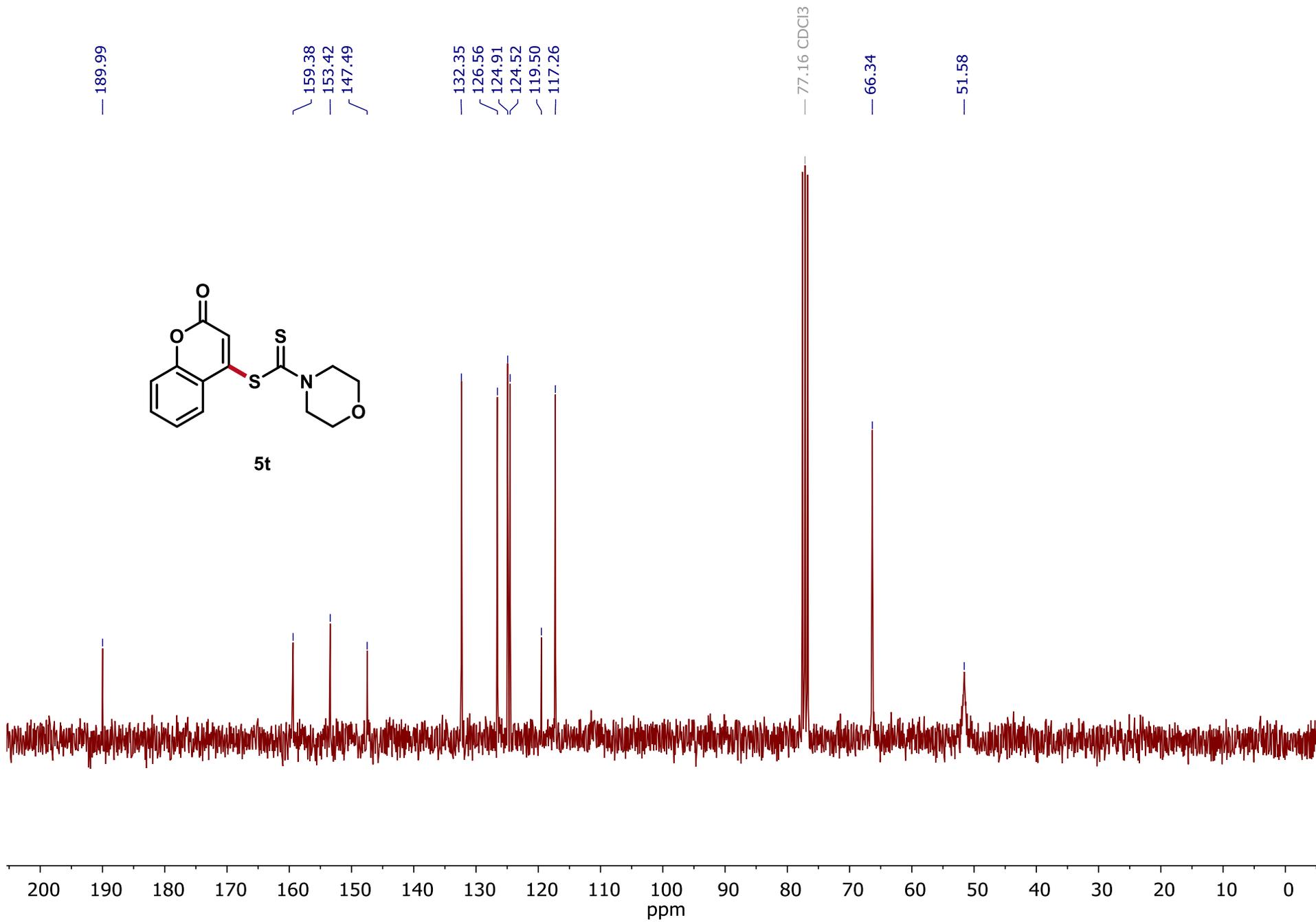
5t



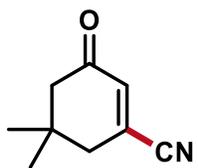
¹H NMR of 5t (300 MHz, CDCl₃)
SI382



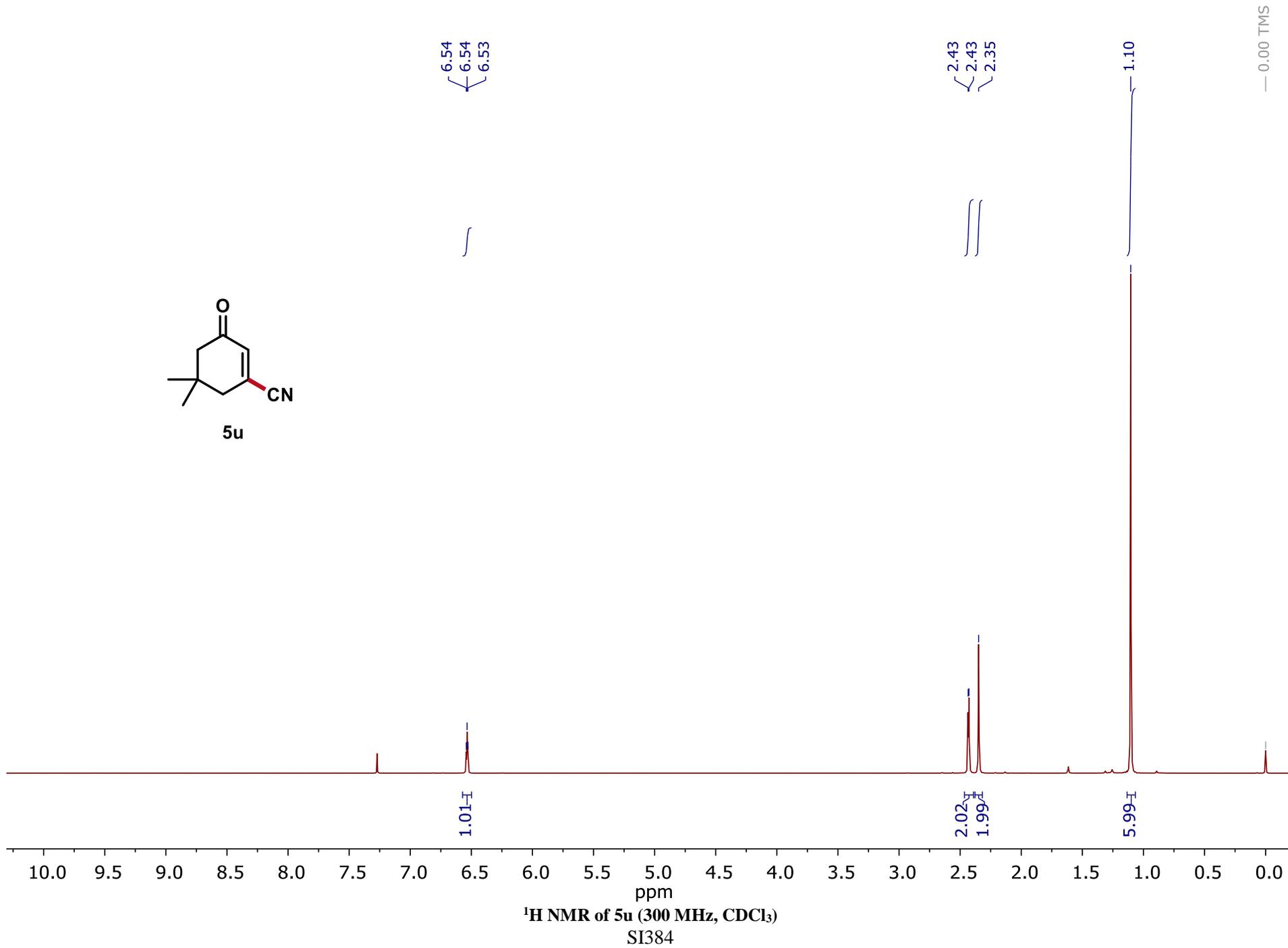
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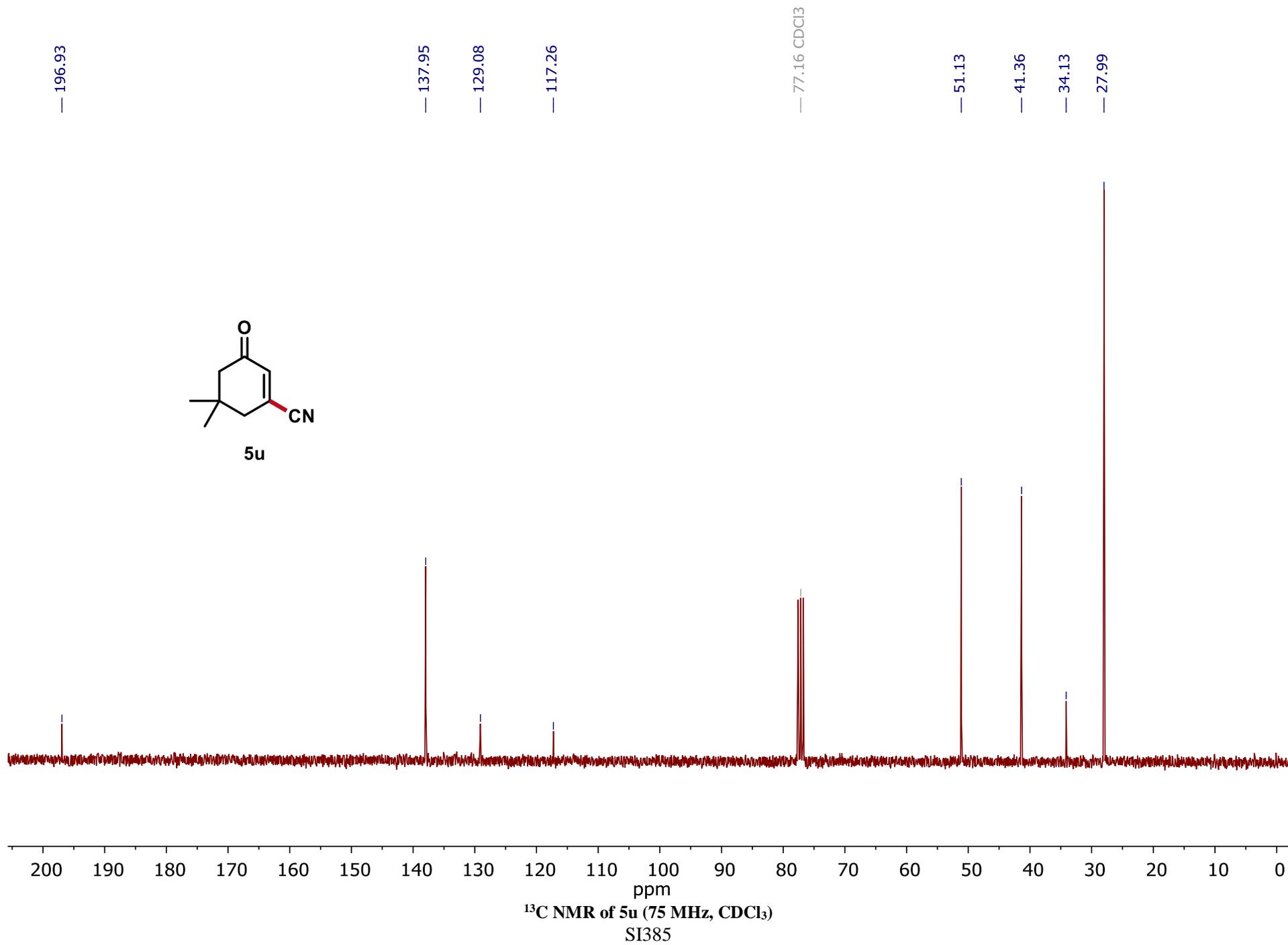
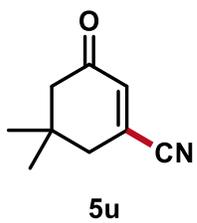


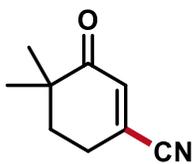
¹³C NMR of 5t (75 MHz, CDCl₃)
SI383



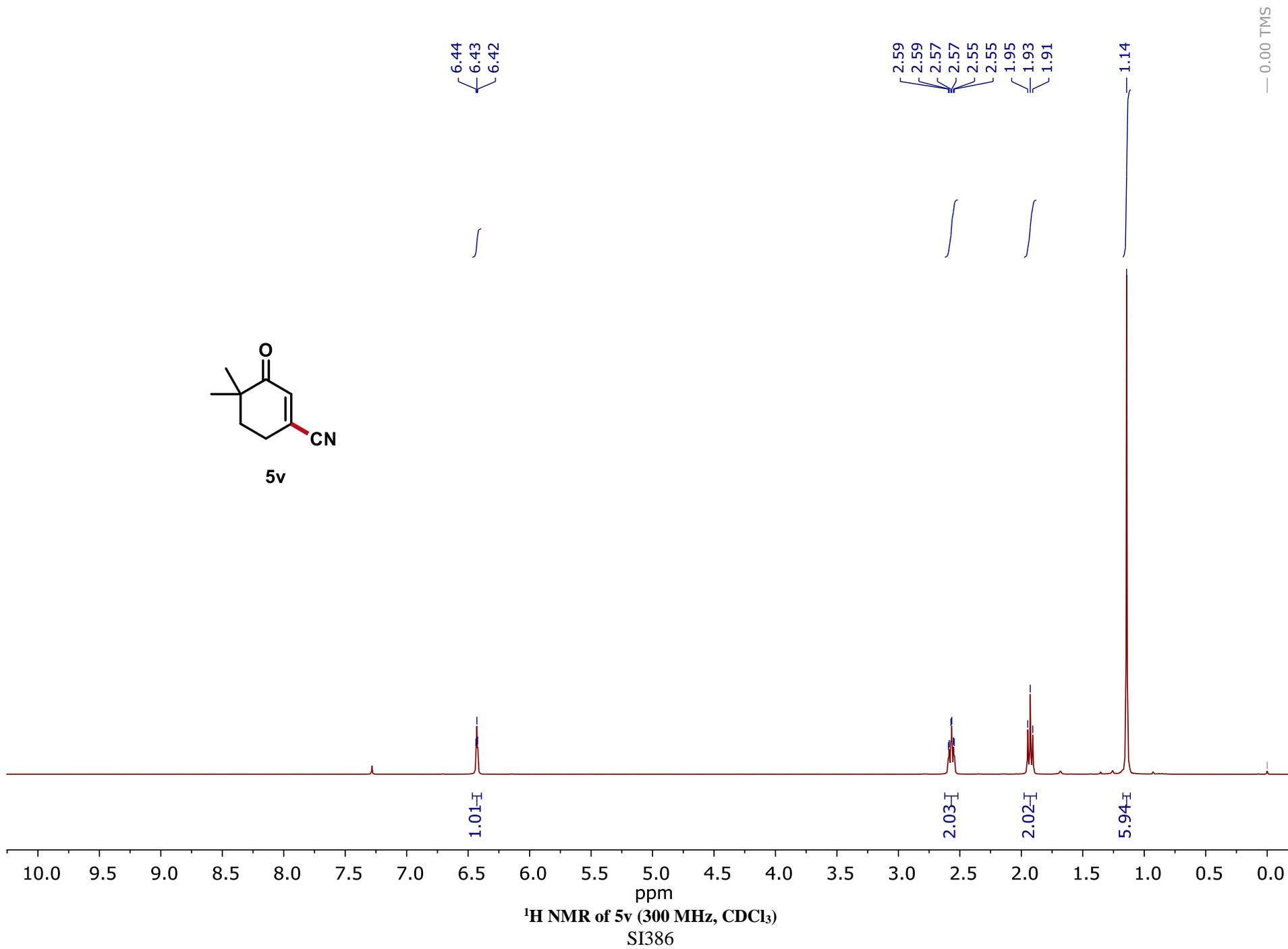
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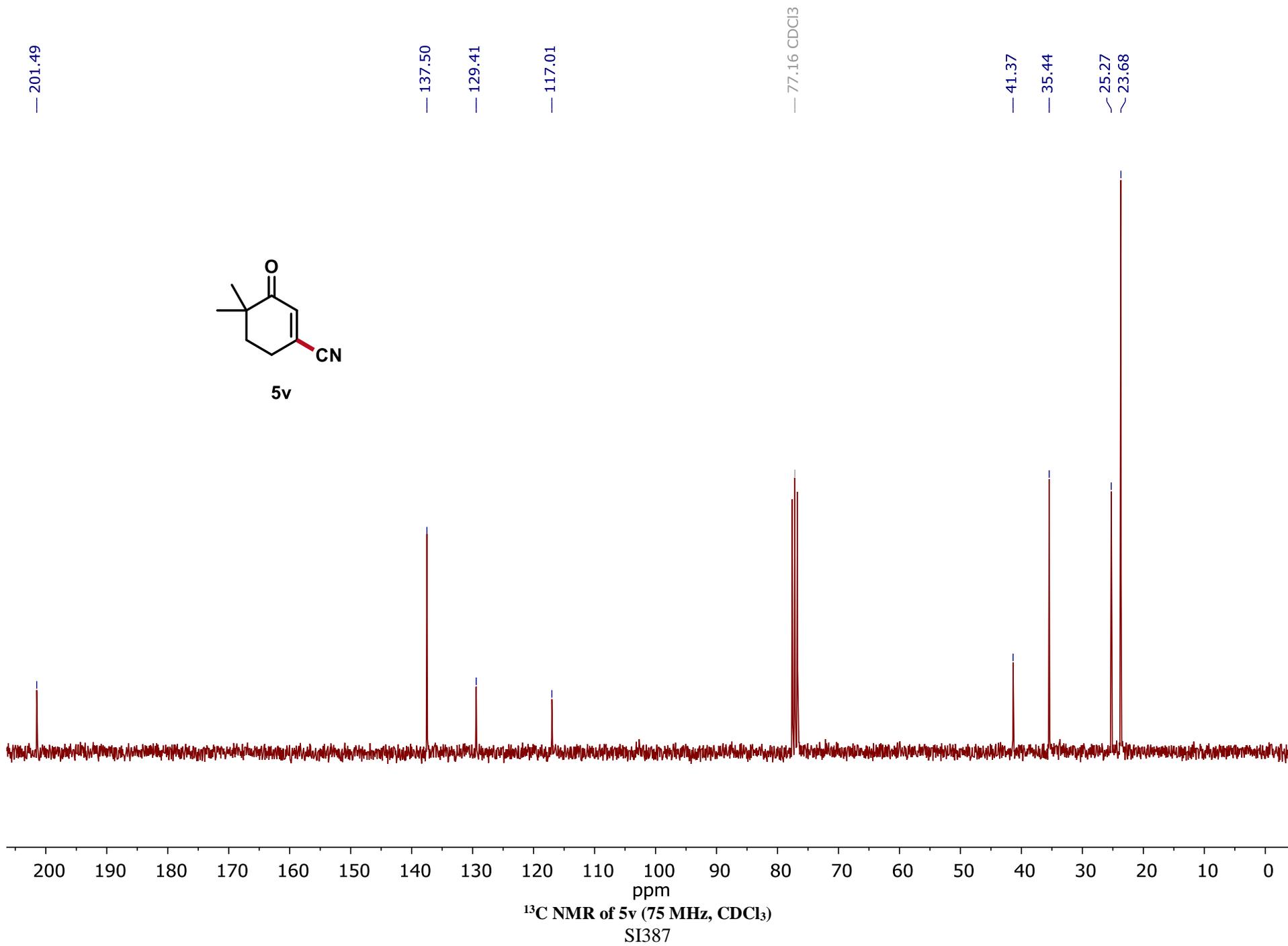
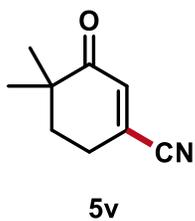






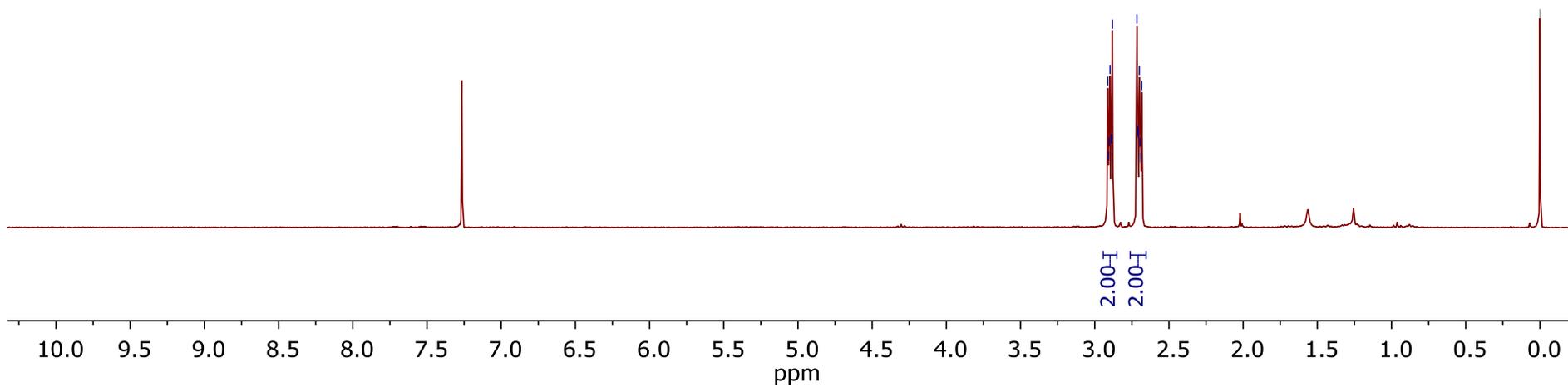
5v







5w

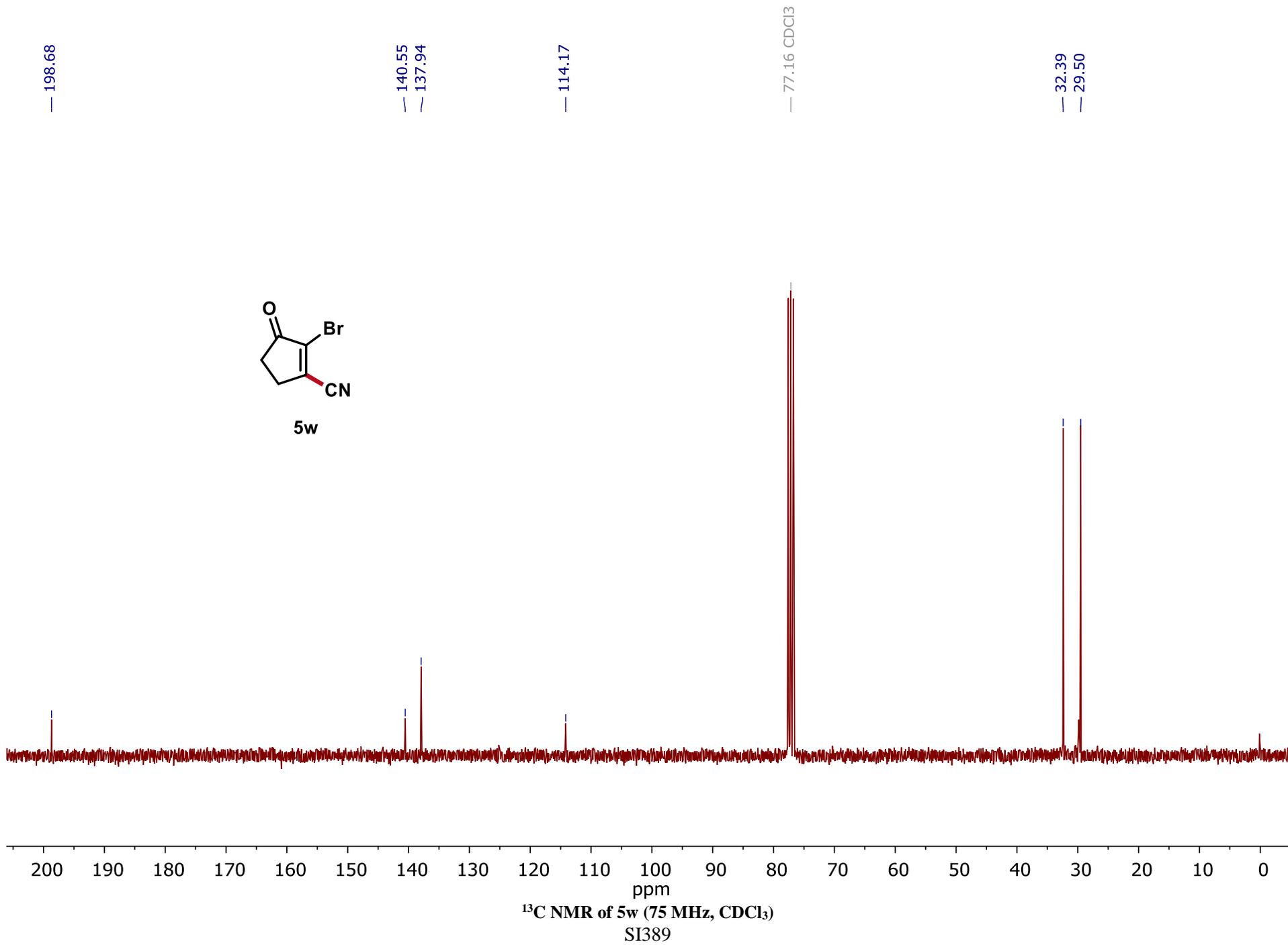


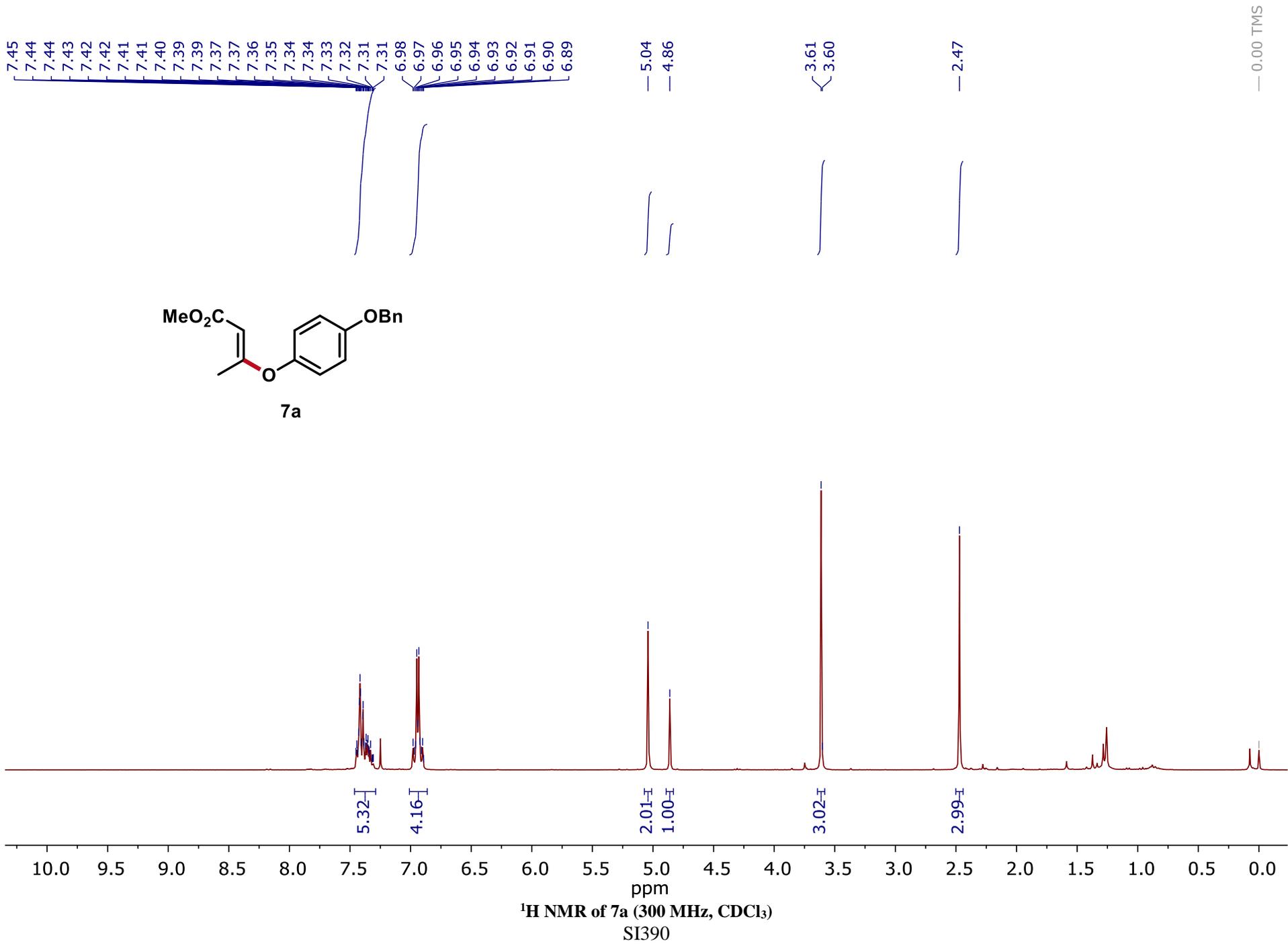
¹H NMR of 5w (300 MHz, CDCl₃)

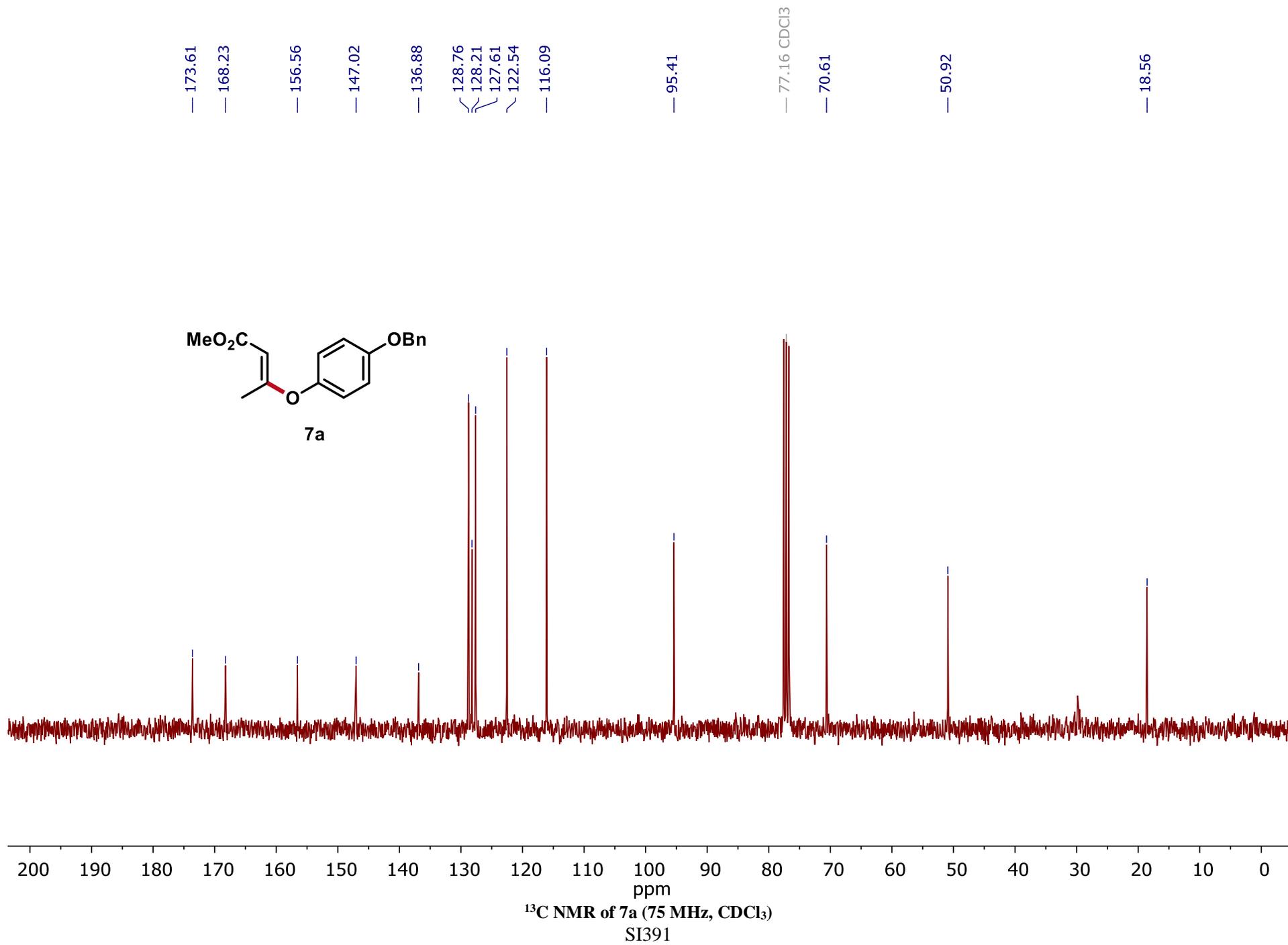
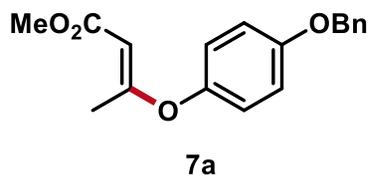
SI388

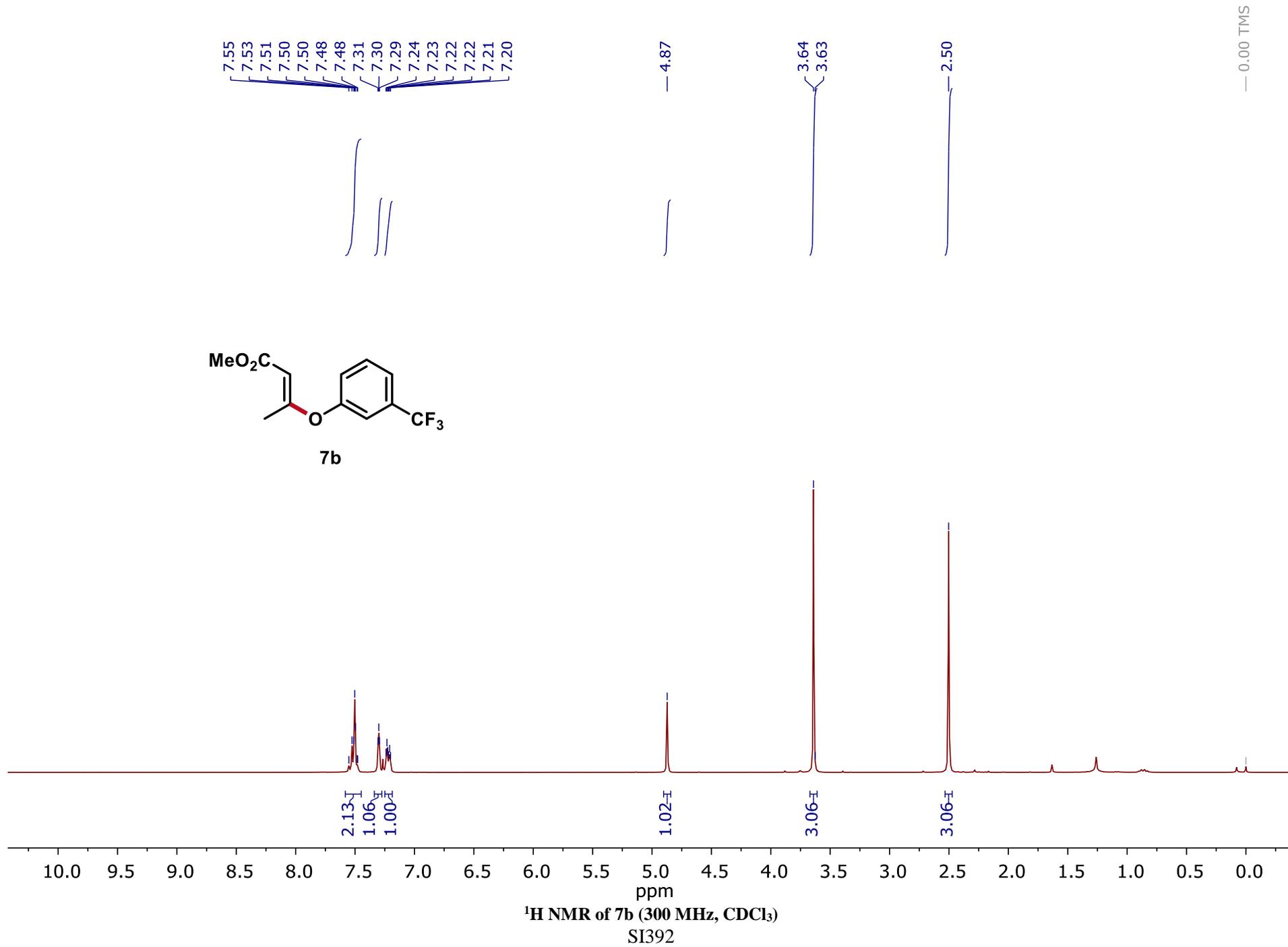
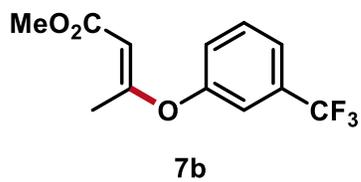
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2.69
2.68

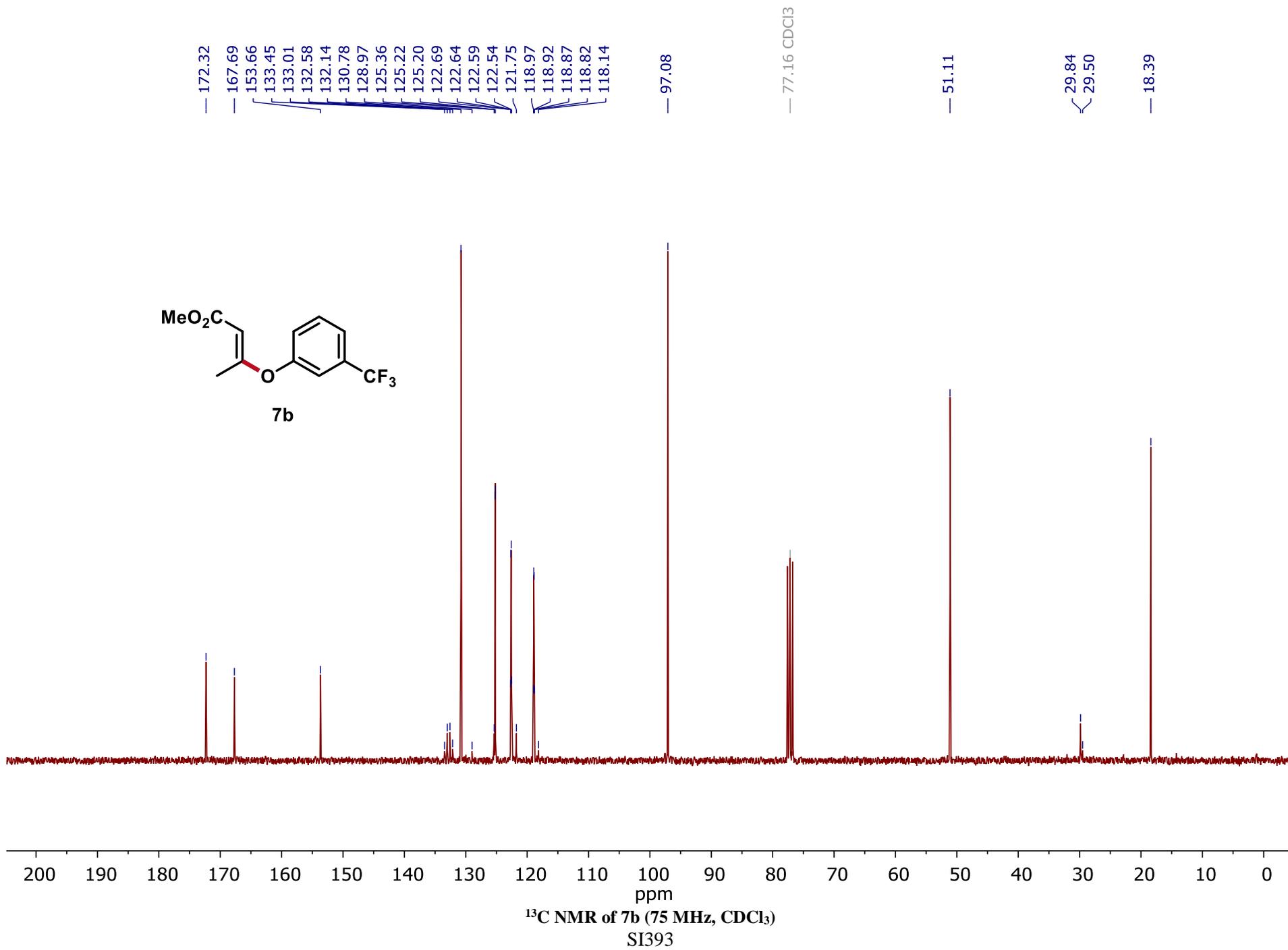
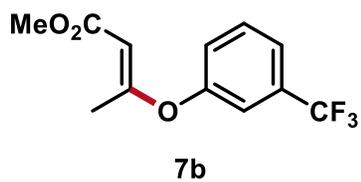
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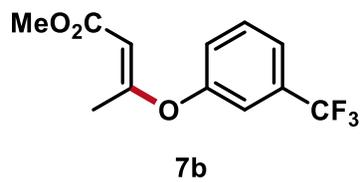




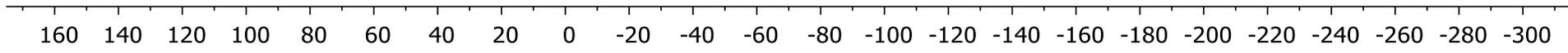




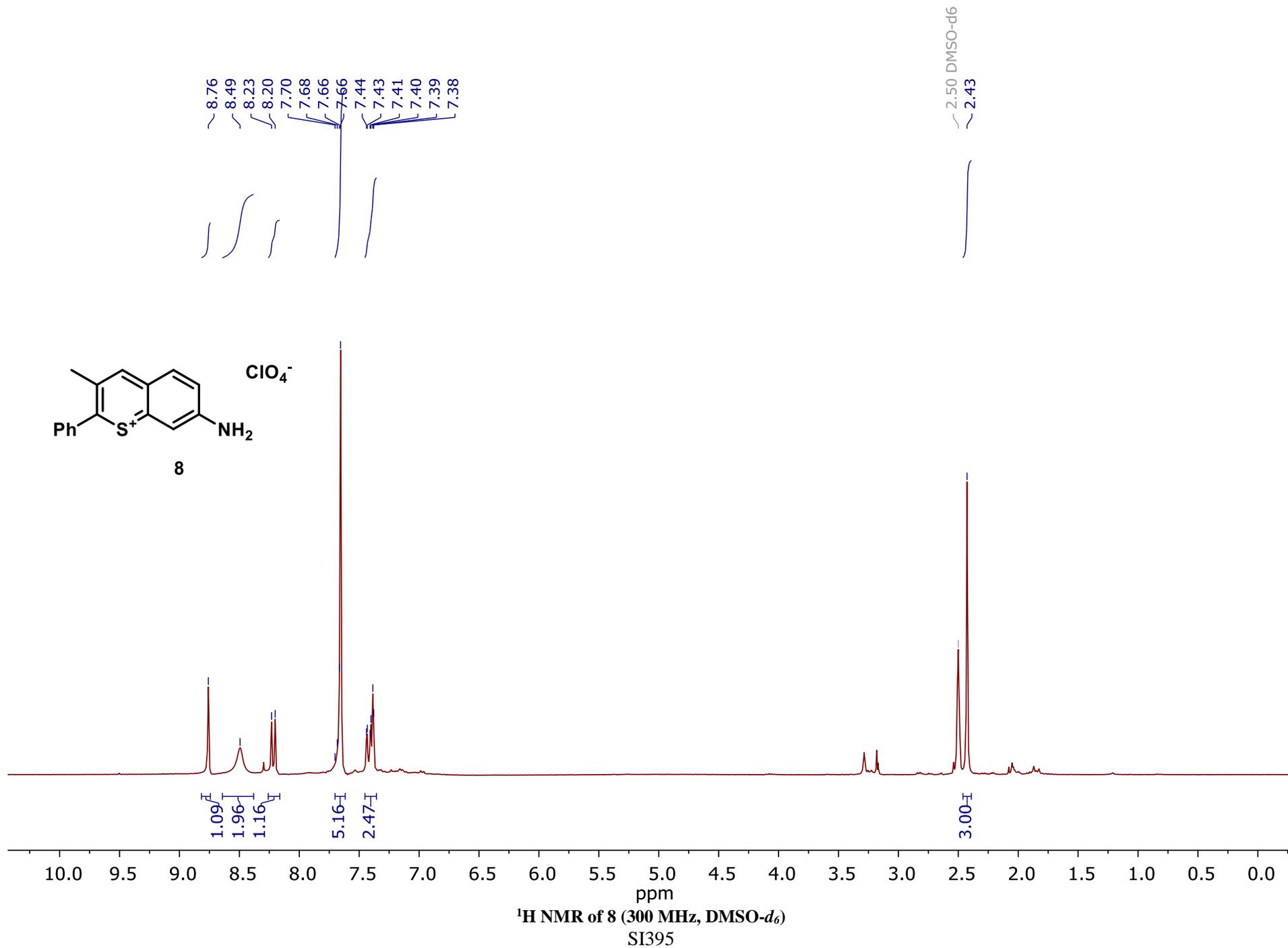
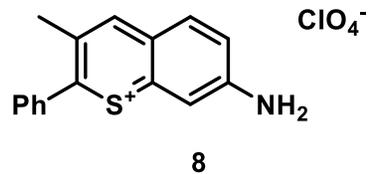


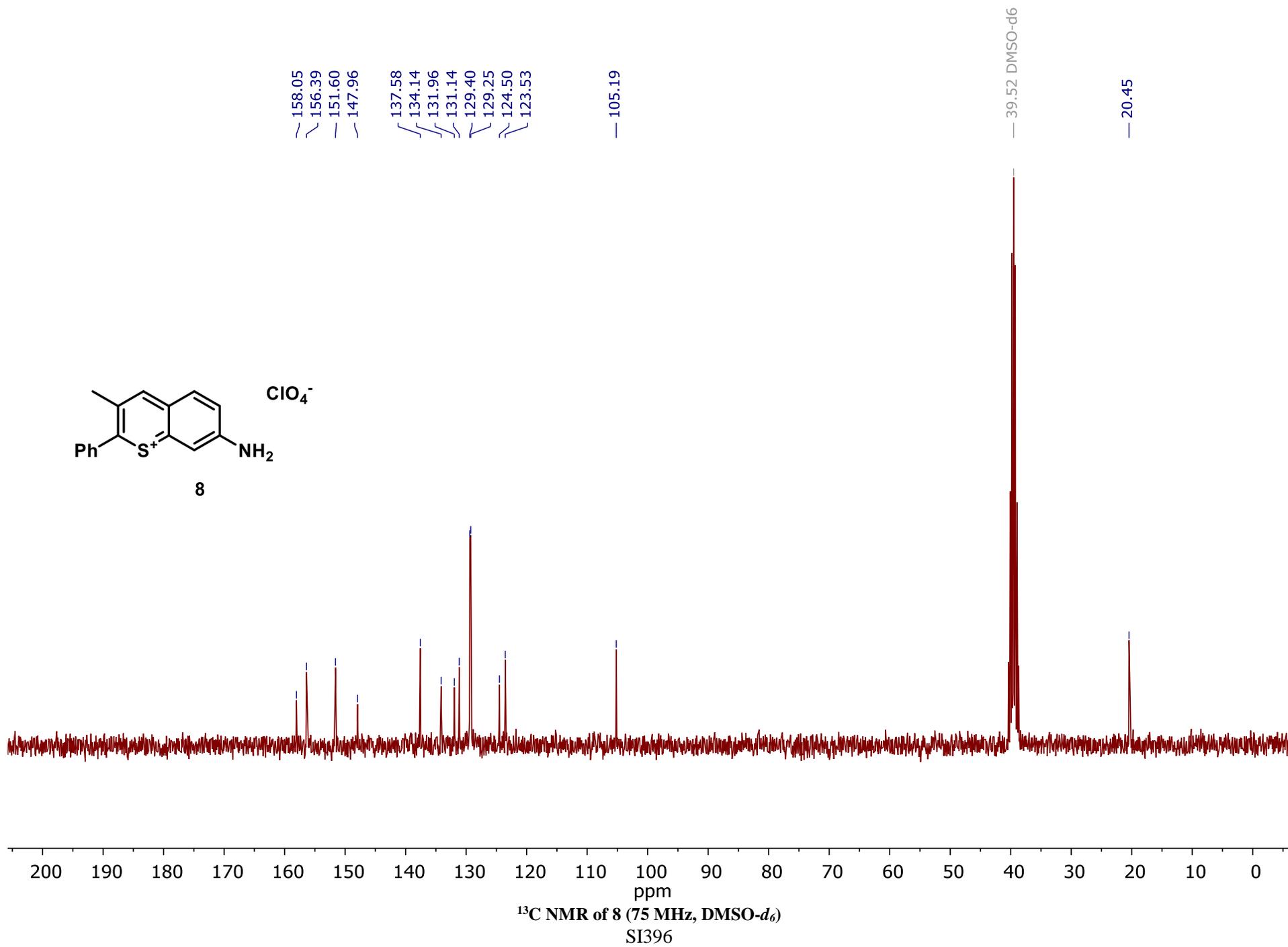
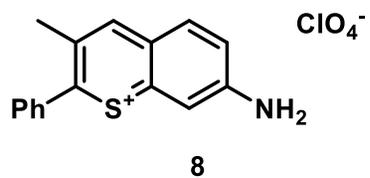


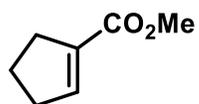
-63.58



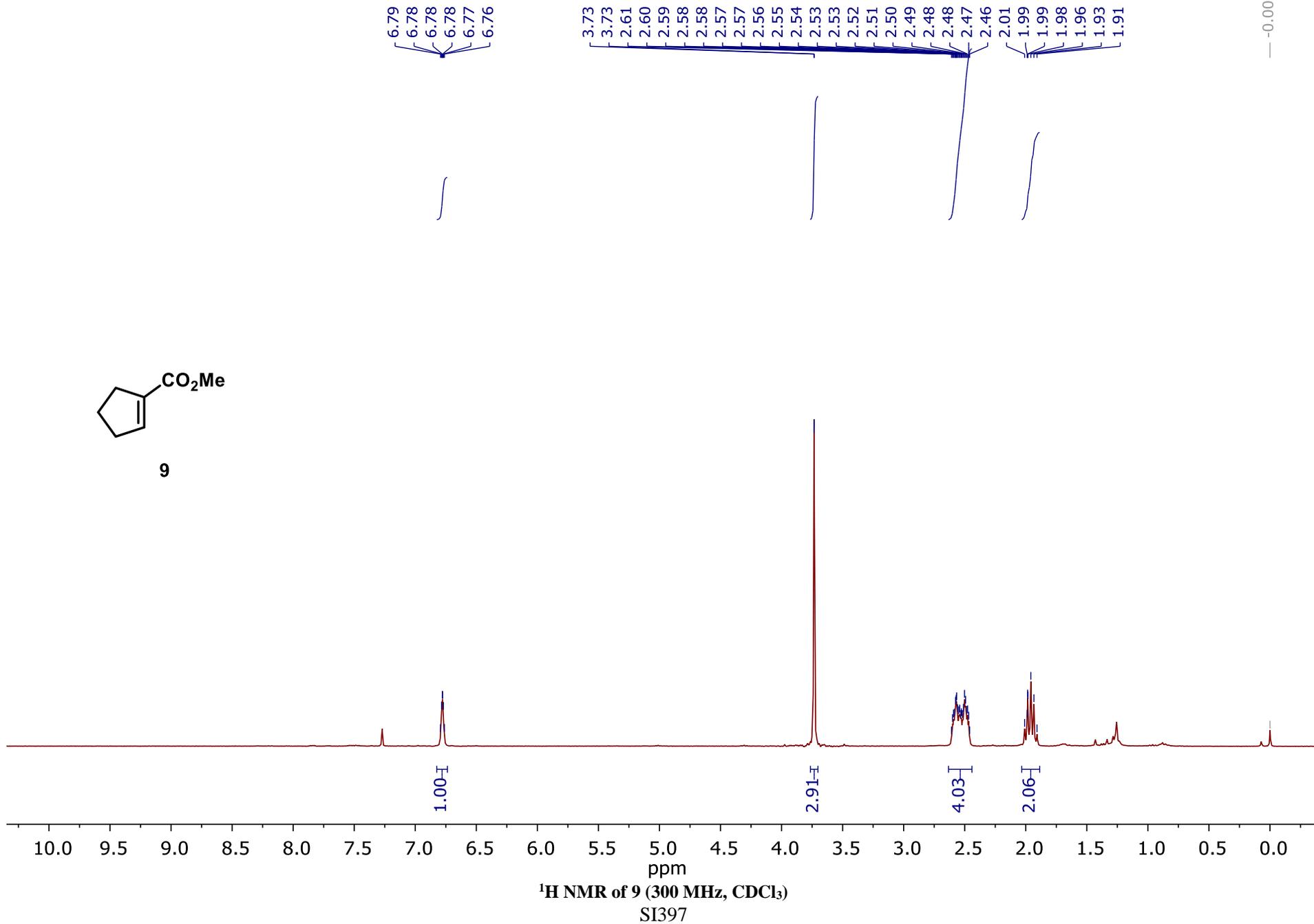
^{19}F NMR of 7b (282 MHz, CDCl_3)
SI394

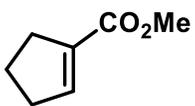




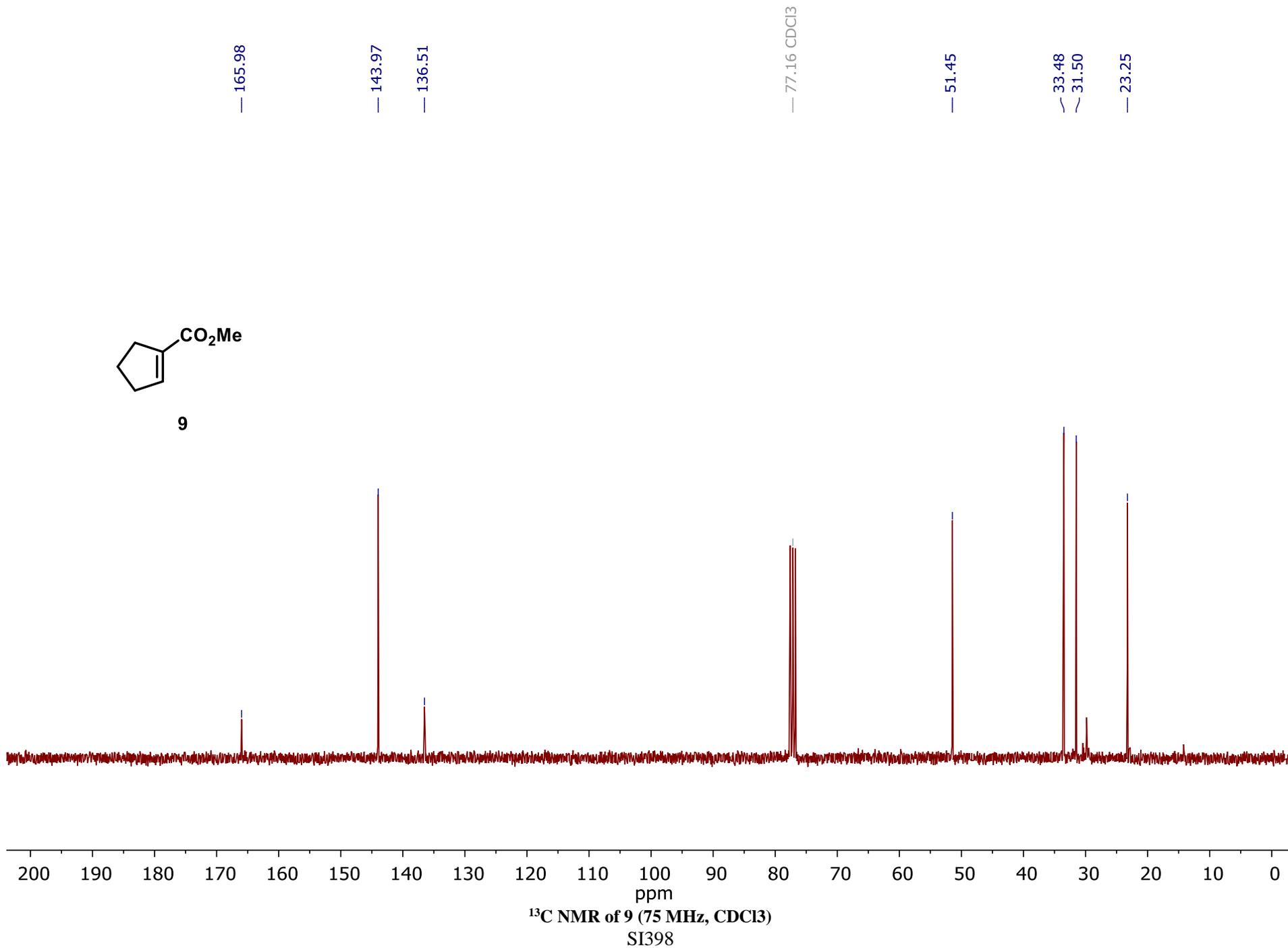


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12. List of references

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