

Supporting Information

Photosensitized Diradical Rearrangement of Alkenyl Oxime Ethers towards Amino-Featured Oxiranes: Reaction, Mechanism, and Structural Prediction

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1 General information

All reagents were purchased from commercial suppliers and used without further purification. Flash chromatography was carried out with silica gel (200-300 mesh). Analytical TLC was performed with silica gel GF254 plates, and the products were visualized by UV detection. ^1H NMR, ^{13}C NMR, and ^{19}F NMR spectra were detected in CDCl_3 or D_2O on a Bruker AM 400 MHz spectrometer. Chemical shifts in ^1H NMR spectra were reported in parts per million (ppm) on the δ scale from an internal standard of residual TMS (0 ppm) or D_2O (4.79 ppm). Data for ^1H NMR were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, brs = broad single), coupling constant in Hertz (Hz) and integration. Data for ^{13}C NMR spectra were reported in terms of chemical shift in ppm from the central peak of CDCl_3 (77.0 ppm). Data for ^{19}F NMR were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant in Hertz (Hz) and integration. The high-resolution mass spectra (HRMS) were measured on a Bruker Daltonics APEX II 47e spectrometer by ESI. UV/Vis absorption spectra were recorded on a Lambda 950+Refle UV/Vis spectrometer. Photochemical reactions were carried with 30 W blue LED obtained from SuZhou Uking Photoelectric Technology Co., Ltd.

2 General setup for the reaction

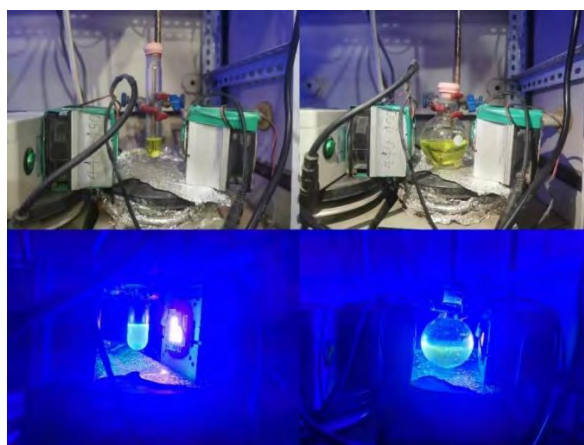
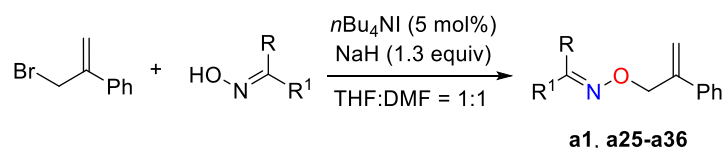


Figure S1. General setup for the reaction. A variable temperature photoreactor equipped with 30 W blue LEDs ($\lambda_{\text{max}} = 443 \text{ nm}$) was used for the reaction and the gram-scale reaction.

3 Synthesis of Starting Materials

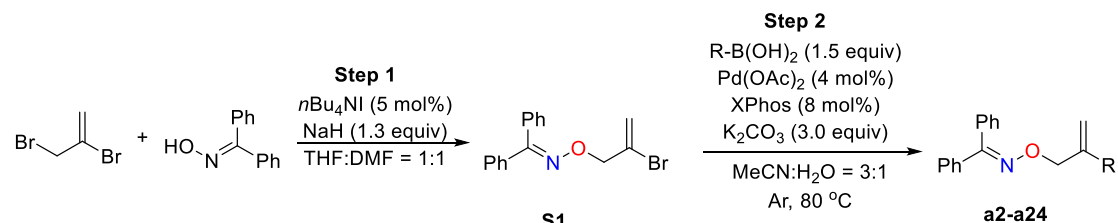
Method A



To a solution of (3-bromoprop-1-en-2-yl)benzene (1.3 equiv), oxime (1.0 equiv) and $n\text{Bu}_4\text{NI}$ (5 mol%) in $\text{THF/DMF} = 1/1$ (20 mL) was added NaH (1.3 equiv) at 0°C . The solution was

stirred at room temperature monitoring the conversion *via* TLC. The reaction was carefully quenched with saturated NH₄Cl aqueous at 0 °C. Then, the resulting mixture was extracted with ethyl acetate, and the combined organic extracts were washed with brine, dried over Na₂SO₄ and concentrated under in vacuo. The residue was purified by flash chromatography on silica gel to afford the desired ketoxime ethers **a1**, **a25-a36**.

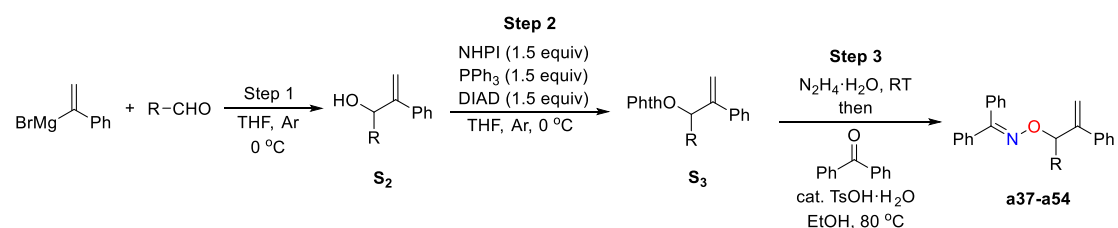
Method B



Step 1: To a solution of 2,3-dibromoprop-1-ene (1.3 equiv), benzophenone oxime (1.0 equiv) and *n*Bu₄NI (5 mol%) in THF/DMF = 1/1 (20 mL) was added NaH (1.3 equiv) at 0 °C. The solution was stirred at room temperature monitoring the conversion *via* TLC. The reaction was carefully quenched with saturated NH₄Cl aqueous at 0 °C. Then, the resulting mixture was extracted with ethyl acetate, and the combined organic extracts were washed with brine, dried over Na₂SO₄ and concentrated under in vacuo. The residue was purified by flash chromatography on silica gel to afford the desired **S1**.

Step 2: Charge a 15 mL Schlenk tube with **S1** (1.0 equiv), RB(OH)₂ (1.5 equiv), K₂CO₃ (3.0 equiv), Pd(OAc)₂ (4 mol%), XPhos (8 mol%) and MeCN/H₂O = 3/1 (10 mL). Then the reaction mixture was stirred at 80 °C oil bath for 12 hours under Ar. After completion, concentrate the reaction mixture. Purify the product by flash silica gel column chromatography to afford the product **a2-a24**.

Method C



Step 1: To a solution of the Grignard reagent (1.0 equiv, 1M in THF) was added aldehyde (1.5 equiv) in THF (1 M) dropwise over 5 minutes under argon and stirred at room temperature overnight. Upon completion, the solution was stirred at room temperature monitoring the conversion *via* TLC. The reaction was carefully quenched with saturated NH₄Cl aqueous at 0 °C. Then, the resulting mixture was extracted with ethyl acetate, and the combined organic extracts were washed with brine, dried over Na₂SO₄ and concentrated under in vacuo. The residue was purified by flash chromatography on silica gel to afford the desired **S2**.

Step 2: To a solution of the allylic alcohols (2.0 mmol) in THF (0.1 M) were added PPh₃ (1.5 equiv.) and NHPI (N-hydroxyphthalimide) (1.5 equiv.). The resulting mixture was cooled to 0 °C before DIAD (diisopropyl azodiformate) (1.5 equiv.) was added dropwise under argon. After stirring for 30 minutes at 0 °C, the reaction mixture was allowed to reach room temperature. The solution was stirred at room temperature monitoring the conversion *via* TLC. Then, the resulting mixture was concentrated under in vacuo. The residue was purified by flash chromatography on silica gel to afford the desired N-alkoxyphthalimides **S3**.

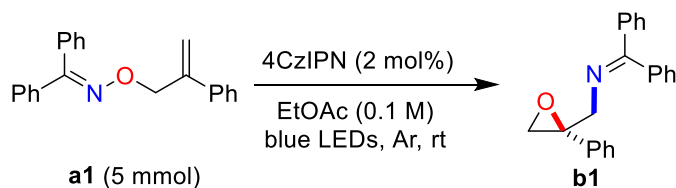
Step 3: To a solution of the previously synthesized N-alkoxyphthalimides (1.0 mmol) in THF (0.1 M) was slowly added hydrazine monohydrate (5.0 equiv.). After stirring for 1 h, the mixture was filtered through celite and concentrated in vacuo. To the hydroxylamine residue were added benzophenone (1.0 equiv.) in EtOH (0.1 M) and TsOH (0.2 equiv.), then the mixture was refluxed at 80 °C until the condensation was completed. The reaction was cooled to room temperature and then the solvent was removed under in vacuo. The residue was purified by flash chromatography on silica gel to afford the desired ketoxime ethers **a37-a54**.

4 General procedure for synthesis of products



In an oven dried 10 mL screw-caped tube equipped with a magnetic stirring bar, **a** (0.2 mmol, 1.0 equiv.) and 4CzIPN (2 mol%) was added. The tube was evacuated and back-filled with argon for 3 times. Subsequently, EtOAc (2 mL) was added under argon. The reaction mixture was allowed to stir at room temperature for 15 h under irradiation from 30 W blue LEDs ($\lambda_{\text{max}} = 443 \text{ nm}$). Then the solution was concentrated under in vacuo and the crude product was purified by flash column chromatography (gradient eluent of ethyl acetate and petroleum ether) to give the corresponding product **b**. The identity and purity of the product was confirmed by ¹H, ¹³C and ¹⁹F NMR spectroscopic analysis.

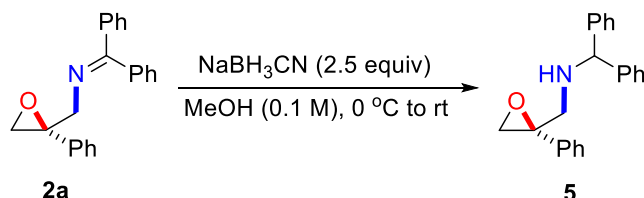
5 Gram-scale synthesis of b1



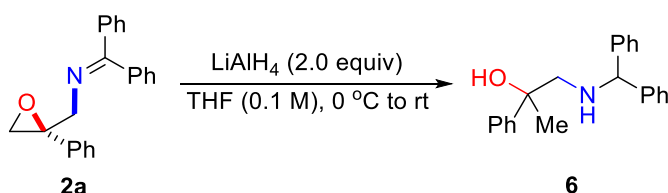
In an oven dried 100 mL round bottom flask equipped with a magnetic stirring bar, **a1** (1.57 g, 5 mmol, 1.0 equiv.) and 4CzIPN (78.9 mg, 2 mol%) was added. The flask was evacuated and back-filled with argon for 3 times. Subsequently, EtOAc (50 mL) was added under

argon. The reaction mixture was allowed to stir at room temperature for 30 h under irradiation from 30 W blue LEDs ($\lambda_{\text{max}} = 443 \text{ nm}$). Then the solution was concentrated under in vacuo and the crude product was purified by flash column chromatography (gradient eluent of petroleum ether/ethyl acetate: 20/1 to 10/1) to give the corresponding product **b1** in 80% yield.

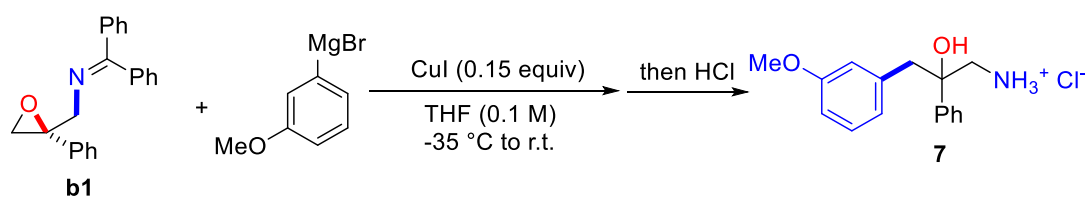
6 Follow-up transformations



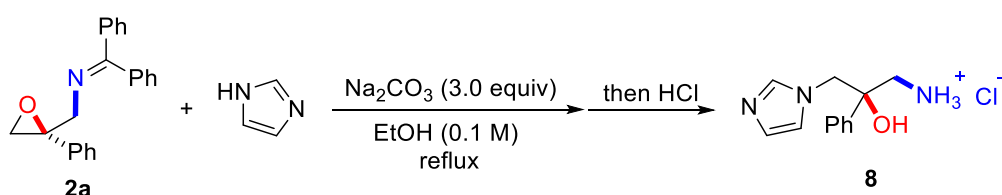
To a solution of the **2a** (62.7 mg, 0.2 mmol, 1.0 equiv.) in MeOH (2 mL) were added NaBH₃CN (31.4 mg, 0.5 mmol, 2.5 equiv.) at 0 °C. Then, the mixture allowed to warm to room temperature and was stirred for 12 h monitoring the conversion *via* TLC. After that, the reaction was quenched with saturated NaHCO₃ solution (2 mL). Then, the resulting mixture was extracted with ethyl acetate, and the combined organic extracts were washed with brine, dried over Na₂SO₄ and concentrated under in vacuo. The residue was purified by flash chromatography on silica gel (gradient eluent of petroleum ether/ethyl acetate) directly to give the desired product **5** in 62% yield.



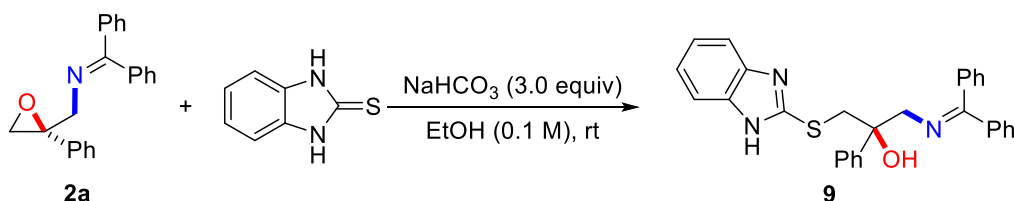
To a solution of the **2a** (62.7 mg, 0.2 mmol, 1.0 equiv.) in THF (2 mL) were added LiAlH₄ (15.2 mg, 0.4 mmol, 2.0 equiv.) at 0 °C. Then, the mixture allowed to warm to room temperature and was stirred for 12 h at room temperature monitoring the conversion *via* TLC. After that, the reaction was quenched with saturated NaHCO₃ solution (2 mL). Then, the resulting mixture was extracted with ethyl acetate, and the combined organic extracts were washed with brine, dried over Na₂SO₄ and concentrated under in vacuo. The residue was purified by flash chromatography on silica gel (gradient eluent of petroleum ether/ethyl acetate) directly to give the desired product **6** in 73% yield.



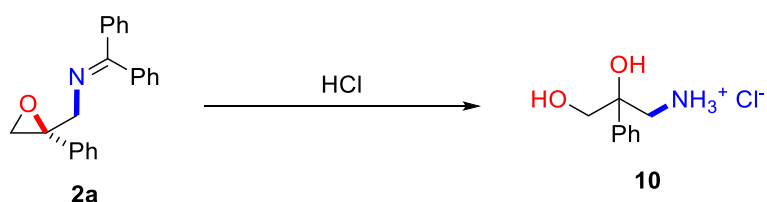
To a solution of the **2a** (62.7 mg, 0.2 mmol, 1.0 equiv.) in THF (2 mL) were added 3-anisylmagnesium bromide (0.4 mL (1.0 M in THF), 0.4 mmol, 2.0 equiv.) at -35 °C. The stirred for 3 h at -35 °C monitoring the conversion *via* TLC. After that, the reaction was quenched with saturated NH₄Cl solution (2 mL). Then, the resulting mixture was extracted with ethyl acetate, and the combined organic extracts were washed with brine, dried over Na₂SO₄ and concentrated under in vacuo. The residue was added to tube charged with MeOH (1.0 mL) and HCl (1 M, aq., 1 mL), then the mixture was stirred at room temperature for 1 h. The system was concentrated under in vacuo, and water (2.0 mL) was added, washed with ethyl acetate (2 mL×3), then combined aqueous phase was concentrated under in vacuo to give the desired product **7** in 64% yield.



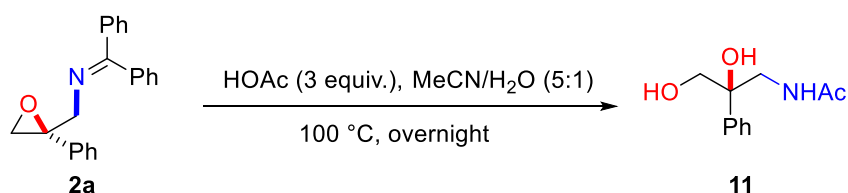
In an oven dried 10 mL screw-caped tube equipped with a magnetic stirring bar, **2a** (62.7 mg, 0.2 mmol, 1.0 equiv.), imidazole (20.4 mg, 0.3 mmol, 3 equiv.), Na₂CO₃ (63.6 mg, 0.6 mmol, 3.0 equiv.) and EtOH (2 mL) were added. The mixture was stirred for 20 h at 85 °C monitoring the conversion *via* TLC. After that, the solution was concentrated in vacuo. The residue was added to tube charged with MeOH (1.0 mL) and HCl (1 M, aq., 1 mL), then the mixture was stirred at room temperature for 1 h. The system was concentrated under in vacuo, and water (2.0 mL) was added, washed with ethyl acetate (2 mL×3), then combined aqueous phase was concentrated under in vacuo to give the desired product **8** in 60% yield.



In an oven dried 10 mL screw-caped tube equipped with a magnetic stirring bar, **2a** (62.7 mg, 0.2 mmol, 1.0 equiv.), 2-Mercaptobenzimidazole (90.1 mg, 0.6 mmol, 3 equiv.), NaHCO₃ (50.4 mg, 0.6 mmol, 3.0 equiv.) and EtOH (2 mL) were added. The mixture was stirred for 20 h at room temperature monitoring the conversion *via* TLC. After that, the solution was concentrated in vacuo. The residue was purified by flash chromatography on silica gel (gradient eluent of dichloromethane/methanol) directly to give the desired product **9** in 60% yield.



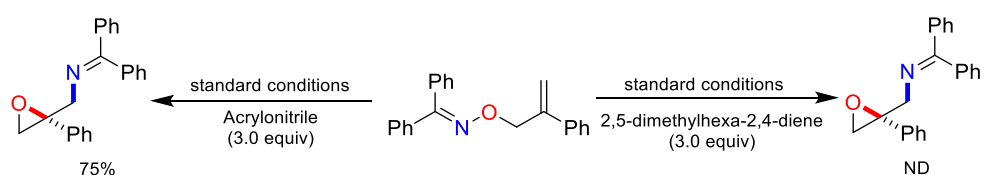
In an oven dried 10 mL screw-caped tube equipped with a magnetic stirring bar, **2a** (62.7 mg, 0.2 mmol, 1.0 equiv.), HCl (1 M, aq., 1 mL) and MeCN (2 mL) were added. The mixture was stirred for 1 h at room temperature. After that, the system was concentrated under in vacuo, and water (2.0 mL) was added, washed with ethyl acetate (2 mL×3), then combined aqueous phase was concentrated under in vacuo to give the desired product **10** in 62% yield.



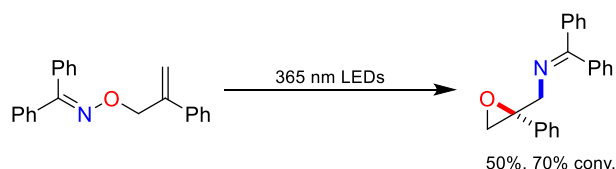
In an oven dried 10 mL screw-caped tube equipped with a magnetic stirring bar, **2a** (62.7 mg, 0.2 mmol, 1.0 equiv.), HOAc (20 μ L, 0.6 mmol, 3 equiv.) and MeCN/H₂O (2 mL, 5:1) were added. The mixture was stirred for overnight at 100°C. After that, the solution was concentrated in vacuo. The residue was purified by flash chromatography on silica gel (gradient eluent of dichloromethane/methanol) directly to give the desired product **11** in 83% yield.

7 Mechanistic investigations

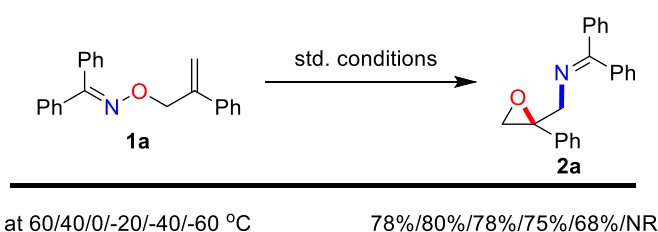
7.1 Control experiments



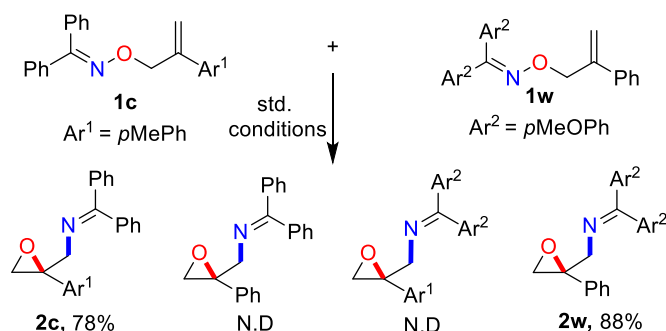
In an oven dried 10 mL screw-caped tube equipped with a magnetic stirring bar, **1a** (0.2 mmol, 1.0 equiv.), 4CzIPN (2 mol%), and acrylonitrile (or 2,5-dimethylhexa-2,4-diene) (3 equiv.) was added. The tube was evacuated and back-filled with argon for 3 times. Subsequently, EtOAc (2 mL) was added under argon. The reaction mixture was allowed to stir at room temperature for 15 h under irradiation from 30 W blue LEDs ($\lambda_{\text{max}} = 443$ nm). Then the solution was concentrated under in vacuo and the crude product was purified by flash column chromatography (gradient eluent of ethyl acetate and petroleum ether) to give the corresponding product.



In an oven dried 10 mL screw-caped tube equipped with a magnetic stirring bar, **1a** (0.2 mmol, 1.0 equiv.) was added. The tube was evacuated and back-filled with argon for 3 times. Subsequently, EtOAc (2 mL) was added under argon. The reaction mixture was allowed to stir at room temperature for 15 h under irradiation from 20 W blue LEDs ($\lambda_{\text{max}} = 365 \text{ nm}$). Then the solution was concentrated under in vacuo and the crude product was purified by flash column chromatography (gradient eluent of ethyl acetate and petroleum ether) to give the corresponding product.



In an oven dried 10 mL screw-caped tube equipped with a magnetic stirring bar, **1a** (0.2 mmol, 1.0 equiv.), and 4CzIPN (2 mol%) was added. The tube was evacuated and back-filled with argon for 3 times. Subsequently, EtOAc (2 mL) was added under argon. The reaction mixture was allowed to stir a series of temperature-variable experiments at 60, 40, 0, -20 -40, and -60 °C, respectively for 15 h under irradiation from 30 W blue LEDs ($\lambda_{\text{max}} = 443 \text{ nm}$). Then the solution was concentrated under in vacuo and the crude product was purified by flash column chromatography (gradient eluent of ethyl acetate and petroleum ether) to give the corresponding product.



In an oven dried 10 mL screw-caped tube equipped with a magnetic stirring bar, **1c** (0.2 mmol, 1.0 equiv.), **1w** (0.2 mmol, 1.0 equiv.), and 4CzIPN (2 mol%) was added. The tube was evacuated and back-filled with argon for 3 times. Subsequently, EtOAc (2 mL) was added under argon. The reaction mixture was allowed to stir at room temperature for 15 h under irradiation from 30 W blue LEDs ($\lambda_{\text{max}} = 443 \text{ nm}$). Then the solution was concentrated under in vacuo and the crude product was purified by flash column chromatography (gradient eluent of ethyl acetate and petroleum ether) to give the corresponding product.

7.2 UV/Vis absorption spectroscopy

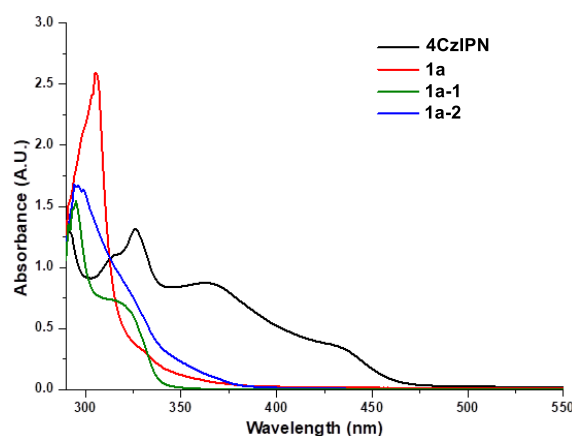


Figure S2: UV-Vis absorption spectra of photocatalyst 4CzIPN (0.05 mM), **1a** (25 mM), **1a-1** (25 mM), **1a-2** (25 mM) in deoxygenated EtOAc.

7.3 Cyclic voltammetry studies

Cyclic voltammetry (CV) experiments were conducted in a 10 mL glass vial fitted with a glassy carbon working electrode (3 mm in diameter), an Ag/AgNO₃ reference electrode, and a platinum wire counter electrode. The electrolyte of *n*Bu₄NBF₄ (0.1 M) in MeCN (10.0 mL) was sparged with argon for 3-5 minutes before data collection. The scan rate is 100 mV/s. The measured cyclic voltammogram of **1a**, **1a-1** and **1a-2** is shown in Figure S3. The measured reduction peak potentials of **1a** by cyclic voltammetry is -2.62 V and the peak oxidation potentials of it is +2.08 V, indicating that its reduction and oxidation are much more difficult than its photosensitization. Apparently, the energy transfer (EnT)-mediated process is more reasonable rather than a single electron transfer (SET) process.

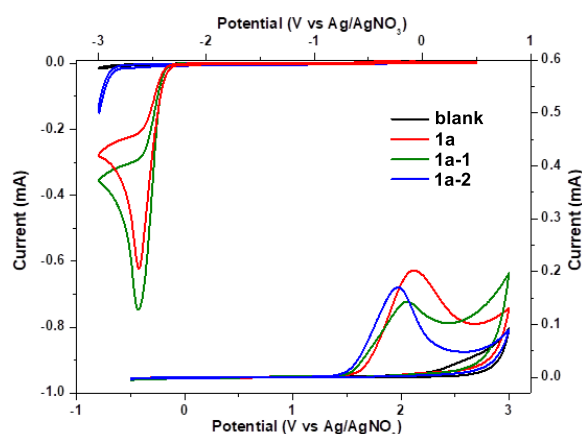


Figure S3. Cyclic voltammograms: **1a** (10.0 mM); **1a-1** (10.0 mM); **1a-2** (10.0 mM).

7.4 Stern-Volmer quenching Experiments

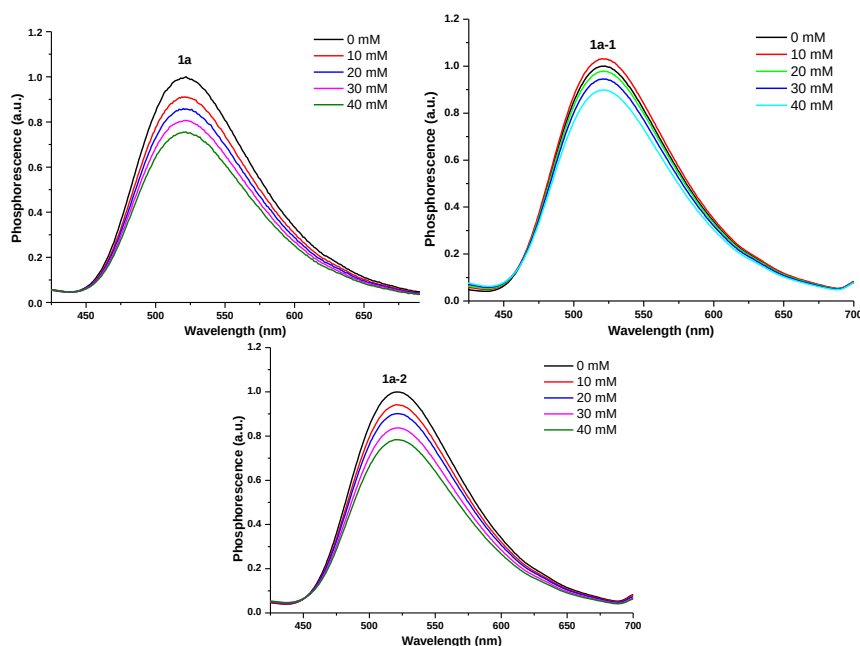


Figure S4. Fluorescence emission spectra of 4CzIPN (0.05 mM in EtOAc) with different concentration of **1a**, **1a-1**, and **1a-2**.

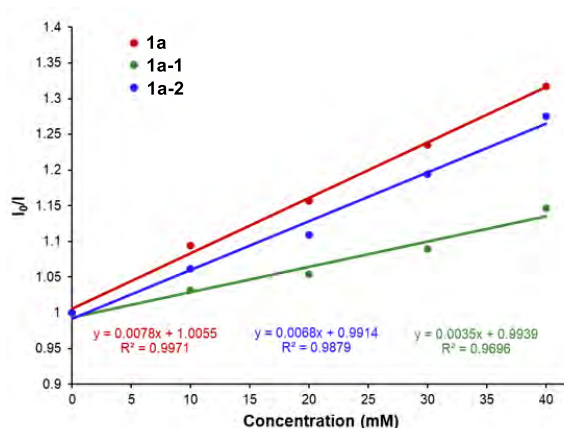


Figure S5. Stern-Volmer plot for the fluorescence quenching of 4CzIPN (0.05 mM in EtOAc) by **1a**, **1a-1**, and **1a-2**.

Stern-Volmer luminescence quenching analysis was conducted using a Jasco FP-8300 spectrofluorometer. The following parameters were employed: Excitation bandwidth = 3 nm, data interval = 1 nm, scan speed = 6000 nm/min. The solution of 4CzIPN (0.05 mM in EtOAc) were excited at $\lambda_{\text{ex}} = 400$ nm and the emission was collected at 520 nm. The substrates **1a**, **1a-1**, and **1a-2** were dissolved in EtOAc (500 mM), respectively. For each quenching experiment, 60 μL of the stock solution were titrated to a solution (3 mL) of 4CzIPN. The addition of 60 μL stock solution refers to an increase of the quencher concentration of 10 mM. I_0 is the luminescence intensity without the quencher, I is the intensity in the presence of the quencher.

7.5 Phosphorescence emission spectroscopy

The lifetime, and temperature dependent photoluminescence spectra were measured using an Edinburgh FLS 1000 fluorescence spectrophotometer equipped with a xenon lamp, laser device (330 nm), or a microsecond flash-lamp.

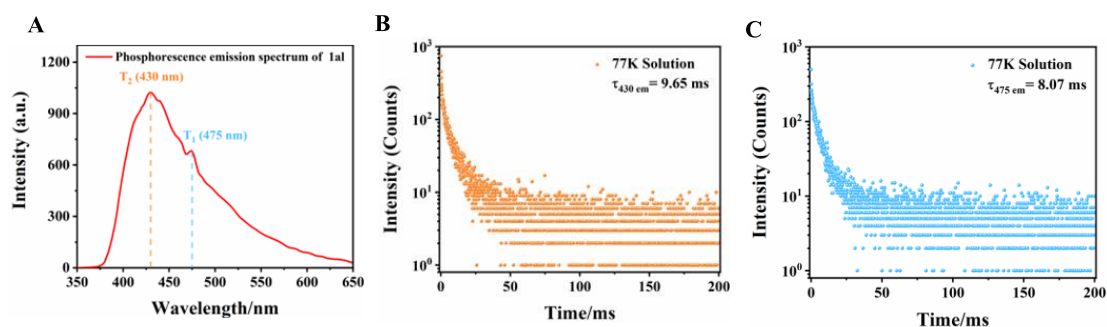


Figure S6 A) Phosphorescence emission spectra of **1al**. Phosphorescence spectra of **1al** (1×10^{-4} M) in methanol at 77 K. B) Phosphorescence lifetime decay curves of T₂ (excited at 300 nm, monitored at 430 nm). C) Phosphorescence lifetime decay curves of T₁ (excited at 300 nm, monitored at 475 nm).

7.6 DFT calculation

Computational details

All the Density functional theory (DFT) calculations and time-dependent (TD)-DFT calculations were performed with the GAUSSIAN 16 series of programs^[2]. DFT method B3LYP^[3] with a standard 6-31G(d, p)^[4] was used for geometry optimizations. The vibrational frequencies at the same level were computed to characterize all optimized structure as minima or a transition state and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K. IRC calculations were used to confirm that the transition states found from the optimization calculations connect the related reactants and products. The minimum energy crossing point (MECP) in this work was located with the code sobMECP at B3LYP/6-31G(d,p) level. All structural figures were generated with CYLview.^[5] To compare energetics, we also carried out single-point energy calculations for the lowest energy structures using B3LYP/Def2TZVP, SMD(ethylethanoate).^[6]

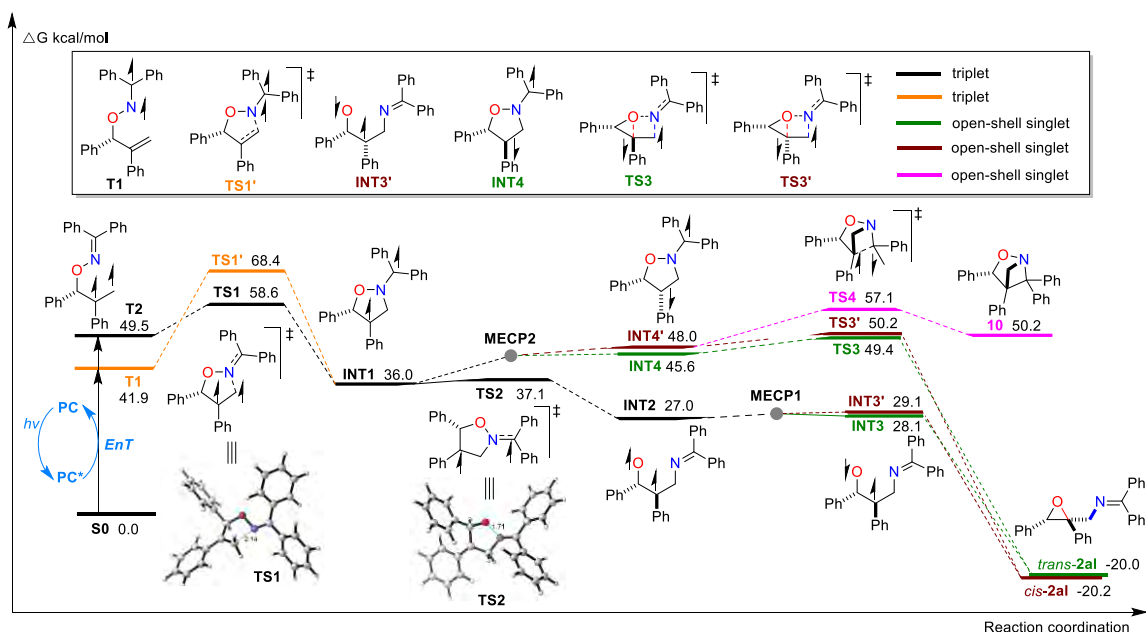


Figure S7. DFT Calculated energy profiles

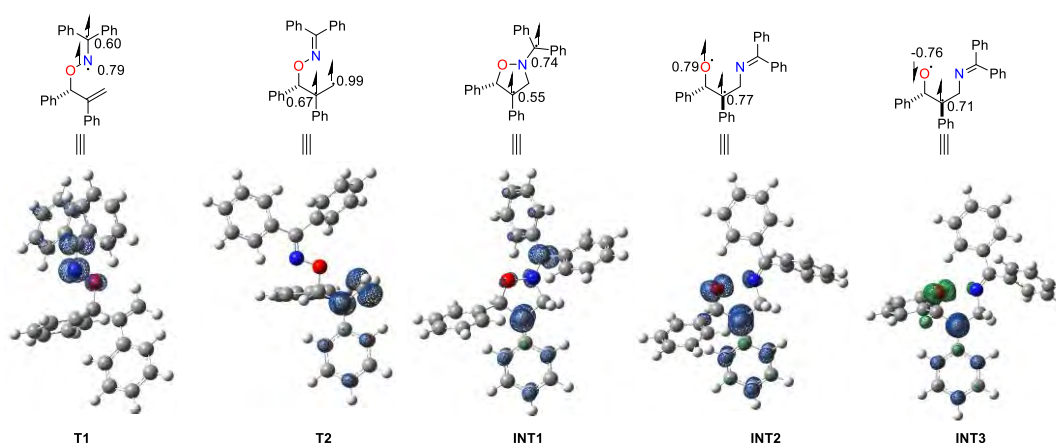


Figure S8 Atomic spin population analysis and spin density visualization. (Blue isosurfaces indicate regions of positive spin density, and green isosurfaces indicate regions of negative spin density, at an isovalue of 0.01 a.u.)

TD-DFT was indeed utilized to calculate the two excited states T1 and T2 of the substrate ketoxime **1a**. The TD-DFT optimization results indicate that the T1 state is associated with the iminyl C=N bond excitation, while the T2 state involves the olefinic C=C bond excitation. In fact, the structures optimized using TD-DFT are identical to those optimized using the UKS method

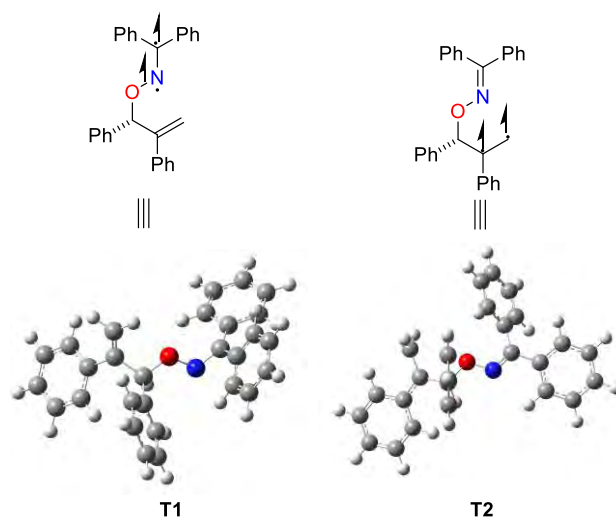


Figure S9 The TD-DFT Optimized T₁ and T₂ Structures of **1al**.

Table S1. Sum of electronic and thermal free energies (G, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal Energies (E, in a.u.), sum of electronic and zero-point energies (E_{zero}, in a.u.).

Table S1 Coordinates of all stationary points.

	E _{zero}	E	H	G	IF
S0	-1210.338517	-1210.338517	-1210.312731	-1210.397664	
T1	-1210.272084	-1210.247033	-1210.246089	-1210.332433	
T2	-1210.256084	-1210.230400	-1210.229456	-1210.304830	
TS1	-1210.246526	-1210.222056	-1210.221111	-1210.304830	-313.20
TS1'	-1210.233374	-1210.233374	-1210.208284	-1210.290892	-562.98
INT1	-1210.280084	-1210.255619	-1210.254675	-1210.338476	
TS2	-1210.277773	-1210.253402	-1210.252458	-1210.336432	-383.44
INT2	-1210.286019	-1210.260782	-1210.259838	-1210.346784	
INT4	-1210.281060	-1210.256660	-1210.255716	-1210.338090	
INT4'	-1210.281081	-1210.256618	-1210.255674	-1210.338684	
TS3'	-1210.279586	-1210.255426	-1210.254482	-1210.336442	-400.32
TS3	-1210.278579	-1210.254240	-1210.253296	-1210.336121	-372.69
TS4	-1210.257198	-1210.257198	-1210.233110	-1210.311331	-294.11
10	-1210.291002	-1210.268008	-1210.267064	-1210.267064	
INT3	-1210.291979	-1210.266905	-1210.265960	-1210.350876	
INT3'	-1210.287242	-1210.261982	-1210.261038	-1210.346913	

trans-2t	-1210.366965	-1210.342294	-1210.341350	-1210.426972	
cis-2t	-1210.367913	-1210.343403	-1210.342459	-1210.344811	

Table S2. Sum of electronic and thermal free energies (G, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal Energies (E, in a.u.), sum of electronic and zero-point energies (E_{zero} , in a.u.).

Table S2 Coordinates of all stationary points

	E_{zero}	E	H	G
1a-T1	-979.280082	-979.259048	-979.258104	-979.334902
1a-T2	-979.295396	-979.274815	-979.273870	-979.349986
1b-T1	-1093.788232	-1093.765036	-1093.764092	-1093.846308
1b-T2	-1093.774128	-1093.750524	-1093.749579	-1093.832224
1A-T1	-748.310142	-748.294150	-748.293206	-748.293206
1A-T2	-748.304481	-748.288069	-748.287124	-748.352377
1B-T1	-862.803261	-862.784666	-862.783722	-862.854992
1B-T2	-862.797778	-862.778746	-862.777802	-862.849156
1C-T1	-1085.341932	-1085.322322	-1085.321378	-1085.396580
1C-T2	-1085.335542	-1085.315493	-1085.314549	-1085.389531
1D-T1	-784.442855	-784.425344	-784.424400	-784.492433
1D-T2	-784.447122	-784.430035	-784.429090	-784.497014
1E-T1	-787.604043	-787.586254	-787.585309	-787.655194
1E-T2	-787.591322	-787.573404	-787.572459	-787.642322
1F-T1	-596.034408	-595.894045	-595.893101	-595.954369
1F-T2	-595.904166	-595.889442	-595.888497	-595.948741
1g-T1	-1071.538988	-1071.516717	-1071.515773	-1071.595552
1g-T2	-1071.525634	-1071.502712	-1071.501767	-1071.583266
1I-T1	-1132.892138	-1132.868928	-1132.867984	-1132.950617
1I-T2	-1132.876086	-1132.852593	-1132.851649	-1132.933798
1n-T1	-1300.082506	-1300.062238	-1300.061293	-1300.137499
1n-T2	-1300.067272	-1300.046579	-1300.045634	-1300.121890
1p-T1	-825.685898	-825.667658	-825.666714	-825.736823

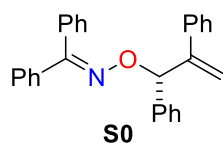
1p-T2	-825.671805	-825.653084	-825.652140	-825.722387
1w-T1	-1208.281659	-1208.255810	-1208.254866	-1208.343027
1w-T2	-1208.266610	-1208.240364	-1208.239420	-1208.328177
1y-T1	-1163.783251	-1163.758968	-1163.758024	-1163.843152
1y-T2	-1163.766304	-1163.741584	-1163.740640	-1163.826933
1aa-T1	-978.126136	-978.106719	-978.105775	-978.178845
1aa-T2	-978.111710	-978.092061	-978.091117	-978.163138
1ab-T1	-1620.877072	-1620.856976	-1620.856031	-1620.931494
1ab-T2	-1620.855556	-1620.835284	-1620.834340	-1620.909546
1af-T1	-1085.337228	-1085.317603	-1085.316659	-1085.391665
1af-T2	-1085.324148	-1085.304390	-1085.303446	-1085.376839
1ag-T1	-1015.442456	-1015.420754	-1015.419810	-1015.499749
1ag-T2	-1015.421278	-1015.399176	-1015.398232	-1015.478202

Table S3. The electronic and thermal energy gaps between the LOMO and HOMO (ΔE_{FO} , in eV), the electronic and thermal free energies gaps between the T1 and T2 triplet states (ΔG_T , in Kcal/mol).

Table S3 Coordinates of all stationary points

	1a	1b	1A	1B	1C	1D	1E	1F	1g	1I
ΔE_{FO}	3.70	3.38	3.71	3.89	3.35	5.37	3.86	4.84	3.97	3.54
ΔG_T	9.47	8.83	3.8	3.66	4.42	2.87	5.57	-3.53	8.96	10.56
	1n	1p	1w	1y	1aa	1ab	1af	1ag	1al	
ΔE_{FO}	3.71	3.99	3.86	2.93	3.24	3.42	3.72	3.48	3.47	
ΔG_T	9.79	9.06	9.32	10.18	9.86	13.77	9.3	13.5	9.14	

Artesian coordinates (xyz format) of all the structures involved in each reaction mechanism studied calculated at the B3LYP/6-31G(d, p) and single-point energies calculated at a larger basis set (B3LYP/def2-TZVP , SMD(ethylethanoate)).

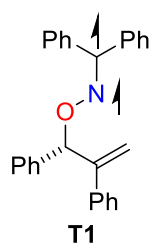


B3LYP /def2-TZVP E(scf) =-1211.199292 a.u.

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C	-5.52708300	-1.07510700	-1.06112100
C	-6.21378400	-0.27301000	-1.97187000
C	-5.64095100	0.92954200	-2.39058700
C	-4.39925100	1.32410300	-1.89944600
H	-3.77769900	-1.31177100	0.15359800
H	-5.95962000	-2.01420600	-0.72784900
H	-7.17977200	-0.58434900	-2.35840900
H	-6.15564800	1.55607800	-3.11355800
H	-3.94778700	2.24198000	-2.26196200
C	-2.37609100	0.98522600	-0.45359700
C	-2.07729700	2.28347000	-0.29714900
H	-1.09265900	2.60107600	0.02305900
H	-2.81124900	3.05778300	-0.49460500
C	-1.34887500	-0.09246500	-0.13144400
H	-1.38883400	-0.86944100	-0.90270700
O	-0.04051000	0.51961700	-0.20585700
N	0.91212200	-0.45889800	-0.48534300
C	2.12787600	-0.02688600	-0.40660400
C	-1.51930500	-0.75170100	1.23520100
C	-1.22399100	-2.11287500	1.38597900
C	-1.89396700	-0.01143300	2.36371400
C	-1.30583300	-2.72424000	2.63756200
H	-0.91676500	-2.68929900	0.51832100
C	-1.97194700	-0.62054600	3.61618300
H	-2.13573300	1.04111100	2.25381700
C	-1.67992000	-1.97873600	3.75645100
H	-1.07506900	-3.78086600	2.73834700
H	-2.26779100	-0.03549000	4.48240800

H	-1.74623700	-2.45332100	4.73123600
C	2.52707500	1.34208700	0.03565600
C	2.04559700	1.88715300	1.23668100
C	3.41180600	2.10014900	-0.74593900
C	2.44394100	3.15912500	1.64298400
H	1.35889800	1.31029500	1.84564900
C	3.79636100	3.37943800	-0.34489300
H	3.79430200	1.68503900	-1.67326000
C	3.31599200	3.91106000	0.85223300
H	2.07120600	3.56516600	2.57890400
H	4.47409100	3.95758700	-0.96617600
H	3.62017100	4.90443500	1.16905800
C	3.17358100	-1.00943600	-0.80342200
C	2.87748700	-2.04068200	-1.71220000
C	4.46641500	-0.94352900	-0.25888800
C	3.84462000	-2.97969800	-2.05824200
H	1.88316500	-2.08821300	-2.14157300
C	5.43306000	-1.88624400	-0.60787300
H	4.71122000	-0.15740400	0.44729600
C	5.12718800	-2.90683200	-1.50823700
H	3.60067500	-3.76607600	-2.76681500
H	6.42594600	-1.82286600	-0.17211300
H	5.88236000	-3.63715400	-1.78389700



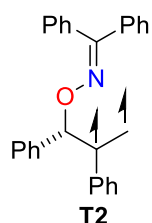
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0 3

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C	6.17097400	-1.73727800	-0.42741800
C	5.48870400	-2.52525200	0.50170300
C	4.21148000	-2.16552700	0.92344100
H	3.83170900	0.67851500	-0.89911100
H	6.07739200	0.03138100	-1.65501500

H	7.16501600	-2.01998600	-0.76100700
H	5.94634100	-3.43111700	0.88891200
H	3.67696800	-2.80614200	1.61750500
C	2.22128100	-0.63667800	0.91067900
C	1.79646100	-0.91798100	2.15180400
H	0.78535000	-0.69289100	2.46800600
H	2.45310000	-1.38354000	2.87907900
C	1.30394200	0.05807600	-0.08606000
H	1.42323800	-0.39943700	-1.07280700
O	-0.07171900	-0.20743800	0.33022700
N	-0.92005500	-0.17098800	-0.76201600
C	-2.24470000	-0.40309200	-0.32074400
C	1.49975600	1.56283400	-0.21187500
C	1.36602900	2.17027300	-1.46793000
C	1.75148100	2.36519700	0.90739100
C	1.48430200	3.55414000	-1.60340400
H	1.16075800	1.55401700	-2.33854000
C	1.86557600	3.74858200	0.77311800
H	1.86520400	1.90146900	1.88194600
C	1.73397000	4.34649000	-0.48172700
H	1.38225300	4.01141500	-2.58330000
H	2.06195800	4.36001300	1.64903600
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C	-4.21599100	0.67744800	0.80080000
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H	-1.70315300	2.14941300	-0.96989500
C	-4.93588200	1.81791900	1.13717000
H	-4.53893200	-0.28618300	1.17707700
C	-4.50975100	3.08000300	0.71301900
H	-2.99078100	4.16281100	-0.37152300
H	-5.82975900	1.72312200	1.74740000
H	-5.07657100	3.96778000	0.97693800
C	-2.70896700	-1.78169200	-0.35922000
C	-1.78868600	-2.84704800	-0.19907000
C	-4.05956200	-2.11756700	-0.62332100
C	-2.20674600	-4.17061500	-0.26445800

H	-0.74882000	-2.61924500	0.00355500
C	-4.46800700	-3.44507600	-0.68941100
H	-4.77780700	-1.32846200	-0.81377900
C	-3.54859600	-4.48144900	-0.50487800
H	-1.48164200	-4.96740400	-0.12444700
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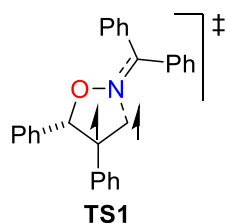


B3LYP /def2-TZVP E(scf) = -1211.112677 a.u.

0 3

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C	-6.25659300	-0.18144500	-1.91644500
C	-5.86992900	1.16174400	-1.82710200
C	-4.60628600	1.50128100	-1.36925700
H	-3.41645000	-1.64812800	-0.76814600
H	-5.64473800	-2.22453000	-1.59165700
H	-7.24718100	-0.44565100	-2.27379300
H	-6.56325000	1.94611200	-2.11794600
H	-4.31306400	2.54472100	-1.30392100
C	-1.32864000	-0.17531400	-0.17559100
H	-1.32222000	-0.95697500	-0.94496100
O	-0.03728100	0.47815300	-0.22986700
N	0.94766200	-0.47545500	-0.48629400
C	2.15009700	-0.01109500	-0.39052800
C	-1.52346100	-0.84216600	1.18247400
C	-1.26493500	-2.21030700	1.32788900
C	-1.91127700	-0.10475900	2.30894800
C	-1.39590000	-2.83222500	2.57044200
H	-0.94721900	-2.78607600	0.46313000
C	-2.03883100	-0.72275200	3.55212600
H	-2.12149700	0.95582200	2.21057300
C	-1.78332400	-2.08941400	3.68590200
H	-1.19320200	-3.89505400	2.66646300

H	-2.34342200	-0.13919300	4.41628300
H	-1.88761600	-2.57147200	4.65360900
C	2.50815600	1.37049200	0.04732400
C	1.98325700	1.91867500	1.22833400
C	3.39880900	2.13807600	-0.71854700
C	2.34723500	3.20139500	1.63223200
H	1.28992900	1.33554800	1.82329900
C	3.74781700	3.42853200	-0.32113300
H	3.81458400	1.72102900	-1.63055700
C	3.22589500	3.96220200	0.85761900
H	1.94155200	3.60965300	2.55339900
H	4.43083700	4.01348900	-0.93015300
H	3.50290600	4.96414200	1.17247700
C	3.22685700	-0.97038600	-0.76174700
C	2.97367000	-2.01144800	-1.67222700
C	4.50609900	-0.87296400	-0.19055900
C	3.96912100	-2.92911700	-1.99448000
H	1.98970200	-2.08363700	-2.12156500
C	5.50121400	-1.79442700	-0.51550700
H	4.71786400	-0.07909700	0.51763300
C	5.23786300	-2.82483900	-1.41813200
H	3.75814100	-3.72341000	-2.70481400
H	6.48296400	-1.70680900	-0.05919500
H	6.01521500	-3.53852400	-1.67507500
C	-2.36004300	0.88486000	-0.52768900
C	-1.96972500	2.29428300	-0.40879100
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H	-2.07522100	2.83888000	0.52808500

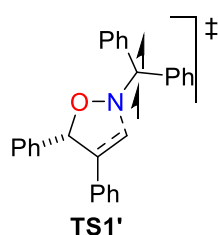


B3LYP /def2-TZVP E(scf) = -1211.101921 a.u.
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C	4.22856900	-3.38233700	-1.24687500
C	3.01480600	-2.71728200	-1.16788700

C	2.82181200	-1.62148700	-0.27608800
C	3.93455900	-1.24942300	0.53406800
C	1.55507000	-0.96514100	-0.20567900
C	1.29982200	0.22196100	0.72598700
O	-0.04309900	0.69849500	0.51720200
N	-0.89059000	-0.41123700	0.49206200
C	0.36155100	-1.47721400	-0.89114300
C	-2.14890200	-0.12603700	0.22483800
C	-3.05189900	-1.29788300	0.29663100
C	-2.66962900	1.21478900	-0.13507500
C	-1.98663200	2.07290300	-1.01736300
C	-2.51131100	3.32149500	-1.34118200
C	-3.71822700	3.74947500	-0.78405300
C	-4.40186800	2.91298200	0.09990200
C	-3.88630000	1.65839300	0.41708300
C	-4.21264200	-1.37356700	-0.49638500
C	-5.02938300	-2.50190300	-0.45968800
C	-4.70624100	-3.58098500	0.36479500
C	-3.55530300	-3.52093600	1.15477800
C	-2.73808800	-2.39483600	1.12373500
C	2.17936600	1.44570300	0.53180900
C	2.58744400	2.19266900	1.64183300
C	3.35085700	3.34947200	1.47841000
C	3.70730500	3.77369900	0.19802200
C	3.29795100	3.03712000	-0.91597600
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H	6.25247200	-3.52343300	-0.49588700
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H	3.84348200	-0.42113300	1.22654200
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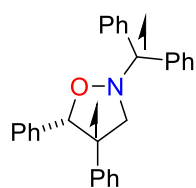
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H	-3.29902100	-4.35176100	1.80615200
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H	2.30253300	1.86663900	2.63897700
H	3.66388100	3.91845000	2.34895700
H	4.30267900	4.67270900	0.06773200
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H	2.23104000	1.30101000	-1.61488000



B3LYP /def2-TZVP E(scf) = -1211.087925 a.u.
0 3

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C	-5.31263300	-1.64217300	0.92869100
C	-4.90179400	-1.63123100	-0.40789800
C	-3.78194000	-0.90529600	-0.79280900
H	-2.89787000	0.33426100	2.25891100
H	-4.88863400	-0.91891100	2.91504300
H	-6.19349900	-2.20182600	1.22801100
H	-5.46771600	-2.17983300	-1.15534400
H	-3.50050000	-0.87446300	-1.84028500
C	-1.85035300	0.57409600	-0.29481000
C	-1.06490300	0.21709200	-1.40119200
H	-0.58063300	0.97950200	-1.99765900
H	-1.25500100	-0.71872300	-1.92073600
C	-1.04690600	1.46606900	0.63323300
H	-1.52075400	1.58653000	1.61055200
O	0.13755100	0.67659000	0.94075200
N	0.64721800	0.19669400	-0.30260900
C	1.54085800	-0.86165500	-0.12902100

C	-0.70669200	2.84884600	0.08901600
C	0.50781200	3.45788200	0.42770000
C	-1.63170700	3.56049100	-0.68421700
C	0.79448100	4.75105500	-0.00942300
H	1.22650300	2.90722200	1.02487800
C	-1.34622100	4.85668600	-1.11604300
H	-2.57621900	3.09563900	-0.95208200
C	-0.13130900	5.45543600	-0.78145800
H	1.74281900	5.20980500	0.25579800
H	-2.07260100	5.39543800	-1.71779400
H	0.09303500	6.46261200	-1.12037300
C	1.09793300	-2.23387000	-0.33985500
C	-0.20786800	-2.63535900	0.02691300
C	1.93559700	-3.19959100	-0.94852800
C	-0.64797100	-3.93558700	-0.19736200
H	-0.85917600	-1.92360400	0.51902300
C	1.48836100	-4.49748700	-1.16985600
H	2.93053300	-2.91106400	-1.27008200
C	0.19488700	-4.87595200	-0.79671300
H	-1.65261700	-4.21778400	0.10458400
H	2.14784000	-5.21614500	-1.64847400
H	-0.15135400	-5.89011900	-0.97239200
C	2.91823700	-0.47888900	0.15876000
C	3.81943400	-1.36803900	0.79263900
C	3.38613200	0.82335800	-0.14391500
C	5.12009100	-0.97665100	1.09163800
H	3.47985500	-2.35839200	1.07486900
C	4.68705300	1.20548400	0.16018800
H	2.71342800	1.51637500	-0.63651600
C	5.56642000	0.30983200	0.77682300
H	5.78726800	-1.67738700	1.58599400
H	5.02296200	2.20714800	-0.09394100
H	6.58297300	0.61104200	1.01139000



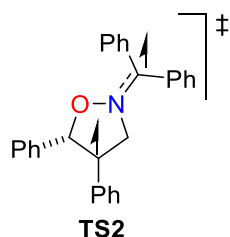
INT1

B3LYP /def2-TZVP E(scf) = -1211.140832 a.u.

0 3

C	5.03688000	1.29019400	-1.55581700
C	5.01561600	2.68175500	-1.71240500
C	3.82566900	3.38020700	-1.47292700
C	2.67713100	2.70540300	-1.08815700
C	2.67129100	1.28864100	-0.92204300
C	3.89714000	0.60277700	-1.16692000
C	1.48998900	0.60595200	-0.54117800
C	1.30873900	-0.88723600	-0.33634200
O	-0.02411000	-1.00530800	0.18945500
N	-0.76586700	0.10304500	-0.45502800
C	0.13923000	1.24692400	-0.38045900
C	-2.12085000	0.11125100	-0.20085100
C	-2.89331800	-1.01829100	-0.68782200
C	-2.73026400	1.25029900	0.50125000
C	-3.86853900	1.90395100	-0.01651800
C	-4.43299700	2.99156600	0.64426000
C	-3.87755100	3.45897000	1.83856500
C	-2.75602800	2.81849600	2.37172900
C	-2.19002100	1.72863900	1.71531800
C	-4.18335500	-1.30357000	-0.17940600
C	-4.91372600	-2.39095400	-0.64592500
C	-4.38352600	-3.23576100	-1.62502000
C	-3.10582900	-2.97524100	-2.13250700
C	-2.37098800	-1.88985300	-1.67474500
C	2.22813700	-1.58321400	0.64890300
C	2.81916500	-2.80563500	0.31534400
C	3.64405000	-3.46808400	1.22671900
C	3.87673600	-2.91441800	2.48522900
C	3.28148400	-1.69745600	2.82924900
C	2.46225700	-1.03687900	1.91711200
H	5.95513000	0.73926300	-1.73861500
H	5.91225900	3.21365400	-2.01498700
H	3.79813500	4.45995500	-1.58923900
H	1.76779000	3.26903000	-0.90502700
H	3.93959800	-0.47318400	-1.04368400
H	1.37069100	-1.40581800	-1.31039500
H	0.06728900	1.80954800	0.56457900

H	-0.11081000	1.93833700	-1.19298000
H	-4.29698000	1.55378800	-0.95045800
H	-5.30548700	3.48227800	0.22214100
H	-4.31764800	4.30893600	2.35143100
H	-2.33031700	3.15995200	3.31117800
H	-1.34871200	1.20635200	2.16071100
H	-4.59946400	-0.67237600	0.59822300
H	-5.90017000	-2.58733900	-0.23499100
H	-4.95533700	-4.08535000	-1.98613000
H	-2.68463100	-3.62180200	-2.89762700
H	-1.38909700	-1.68330900	-2.08455600
H	2.62945500	-3.24212400	-0.66205200
H	4.09861700	-4.41611200	0.95443700
H	4.51705600	-3.42756600	3.19672600
H	3.45796600	-1.26398600	3.80936000
H	1.99948100	-0.09158100	2.18370500

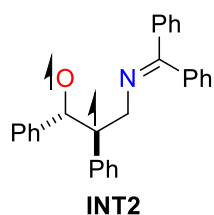


B3LYP /def2-TZVP E(scf) = -1211.13744 a.u.

0 3

C	5.03956200	1.20225400	-1.60304500
C	5.02106500	2.59297900	-1.76615200
C	3.82860800	3.29150900	-1.54206500
C	2.67554100	2.61794100	-1.16736900
C	2.66538400	1.20183800	-0.99576900
C	3.89523600	0.51698400	-1.22370200
C	1.48165900	0.51225600	-0.62396000
C	1.33798400	-0.98627000	-0.40946600
O	0.02090400	-1.20675900	0.04962700
N	-0.84262200	0.10034600	-0.68377100
C	0.13461400	1.16692400	-0.50114800
C	-2.12114000	0.16549700	-0.32557000
C	-2.63447200	1.27959600	0.51843000
C	-3.00629700	-0.92078200	-0.75629100
C	-4.29294800	-1.08236500	-0.20169700
C	-5.12281600	-2.12099400	-0.61590200

C	-4.68968800	-3.02563600	-1.58680300
C	-3.41253300	-2.88268500	-2.14002600
C	-2.58052500	-1.84797100	-1.73286900
C	-3.63668700	2.14545600	0.05097700
C	-4.09591200	3.19479200	0.84638200
C	-3.56529300	3.39322000	2.12263700
C	-2.57493700	2.53286500	2.60229600
C	-2.11162700	1.48520100	1.80802000
C	2.25222100	-1.61212600	0.63912900
C	2.87136300	-2.84009900	0.38581200
C	3.67288700	-3.44622900	1.35534200
C	3.85453600	-2.83082900	2.59363000
C	3.22987800	-1.60875500	2.85839700
C	2.43174600	-1.00620900	1.88899900
H	5.95945500	0.64980600	-1.77302900
H	5.92112200	3.12363900	-2.06085700
H	3.80209300	4.37104600	-1.66165900
H	1.76710700	3.18581200	-0.99378600
H	3.93777600	-0.55815900	-1.09515500
H	1.51700700	-1.50585000	-1.37146900
H	0.02312100	1.69713000	0.45726400
H	-0.03360500	1.90362100	-1.29655200
H	-4.63567700	-0.39607700	0.56468800
H	-6.10920200	-2.22750500	-0.17362200
H	-5.33812500	-3.83509600	-1.90901200
H	-3.06765300	-3.58226000	-2.89618500
H	-1.59164000	-1.73445700	-2.16011600
H	-4.05010700	1.99254600	-0.94154900
H	-4.86800900	3.85884100	0.46865000
H	-3.92432500	4.21010400	2.74161400
H	-2.16872900	2.67272700	3.59994900
H	-1.35889800	0.79993500	2.18722400
H	2.72239900	-3.32393500	-0.57629600
H	4.15071100	-4.39848800	1.14363400
H	4.47758100	-3.29946400	3.34987600
H	3.36694100	-1.12612700	3.82191900
H	1.94732600	-0.05631300	2.09453400

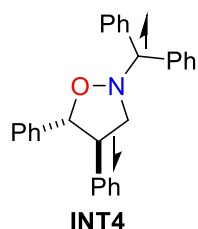


B3LYP /def2-TZVP E(scf) = -1211.152145 a.u

0 3

C	1.41302700	0.45103600	-0.51061100
C	1.55721000	-1.06676600	-0.45393100
C	0.02469600	0.97884300	-0.24339800
H	-0.12677300	1.90855800	-0.80305900
H	-0.10948700	1.23916200	0.82086600
N	-0.97122200	0.00350000	-0.66699900
O	0.41156400	-1.67521700	0.04021700
C	2.48648900	1.30861000	-0.90241700
C	3.73775100	0.79041100	-1.34980100
C	2.36487800	2.72953000	-0.86867200
C	4.77042900	1.62842700	-1.74382800
H	3.89011900	-0.28108300	-1.38872600
C	3.40762800	3.55803100	-1.25817900
H	1.44746800	3.18419100	-0.51111900
C	4.61956500	3.01925200	-1.70363200
H	5.70588400	1.19472300	-2.08620400
H	3.27763600	4.63579500	-1.21213300
H	5.43228200	3.67065200	-2.00985300
C	-2.19975800	0.06265400	-0.30164700
C	-3.11542600	-1.04145000	-0.69868200
C	-2.58843200	-2.27980600	-1.10875700
C	-4.50864300	-0.86536500	-0.68259800
C	-3.44113400	-3.30838400	-1.49668100
H	-1.51290200	-2.41720700	-1.09216900
C	-5.35775300	-1.89787800	-1.07981500
H	-4.92818400	0.08475300	-0.36915600
C	-4.82693300	-3.12171800	-1.48726800
H	-3.02486200	-4.26410100	-1.80209900
H	-6.43298100	-1.74474100	-1.07056400
H	-5.48809000	-3.92842800	-1.79094200
C	-2.75862000	1.19027200	0.52285600

C	-3.15206200	0.96294500	1.84982700
C	-2.87738400	2.48092900	-0.01140500
C	-3.63796700	2.01159900	2.63101300
H	-3.07263200	-0.03669500	2.26653100
C	-3.37739200	3.52527200	0.76696000
H	-2.59035100	2.66217100	-1.04337400
C	-3.75372400	3.29385000	2.09107700
H	-3.93131600	1.82522200	3.65997400
H	-3.47359100	4.51867200	0.33858600
H	-4.13890800	4.10784600	2.69802300
H	1.81372600	-1.43508800	-1.46758000
C	2.63578600	-1.58835300	0.51195800
C	3.40271100	-2.70279900	0.15578700
C	2.79417700	-1.02709300	1.78475500
C	4.34507300	-3.22567000	1.04230500
H	3.26257000	-3.15680800	-0.82180900
C	3.73411500	-1.54841400	2.67093600
H	2.18705600	-0.17394200	2.07085600
C	4.51355900	-2.64795800	2.30130800
H	4.94319600	-4.08440400	0.75133000
H	3.85893000	-1.09878000	3.65181900
H	5.24605600	-3.05328200	2.99330300



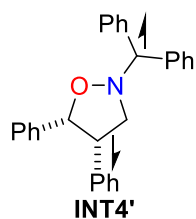
B3LYP /def2-TZVP E(scf) = -1211.126502 a.u

0 1

C	-4.90165100	-0.45571200	2.09127100
C	-4.52125400	-0.12712000	3.39880400
C	-3.16924800	0.09962100	3.68371600
C	-2.21152300	0.00070800	2.68527900
C	-2.57228900	-0.33275600	1.34725300
C	-3.95504100	-0.55765100	1.08341900
C	-1.59185800	-0.45056600	0.33167100
C	-1.82590400	-0.88296400	-1.09718100
O	-0.50351100	-1.11209200	-1.62077700

N	0.35388000	-0.16956700	-0.85339200
C	-0.11255700	-0.28979100	0.52598400
C	1.66519000	-0.10482500	-1.25954100
C	2.73677700	-0.43424000	-0.30571500
C	1.93837600	0.33398300	-2.61828100
C	3.19313700	0.08835100	-3.22601300
C	3.45351300	0.50370200	-4.52721900
C	2.47273600	1.16661300	-5.27006600
C	1.22280300	1.40697400	-4.68966500
C	0.95472600	0.99933200	-3.38931700
C	2.71943900	-1.64491600	0.42073100
C	3.72320100	-1.94333100	1.33985600
C	4.77209800	-1.04685200	1.55488100
C	4.81294300	0.15030700	0.83371100
C	3.81081700	0.45366600	-0.08308000
C	-2.63429600	0.06410100	-1.97620500
C	-3.41194700	-0.46426000	-3.01391300
C	-4.12554600	0.37472100	-3.86996300
C	-4.06757400	1.75847200	-3.69808600
C	-3.29636400	2.29568800	-2.66544200
C	-2.58759900	1.45418400	-1.80784400
H	-5.94851300	-0.63133300	1.86035900
H	-5.26739500	-0.04836100	4.18333200
H	-2.86392700	0.35405600	4.69474100
H	-1.16867200	0.17680600	2.92960300
H	-4.27198000	-0.80110500	0.07492800
H	-2.30042800	-1.87413400	-1.13182600
H	0.16305100	0.62577100	1.06193700
H	0.32823800	-1.13815300	1.07677900
H	3.95693200	-0.44631800	-2.67204400
H	4.42510400	0.29955400	-4.96865400
H	2.67751600	1.48821900	-6.28692800
H	0.45163400	1.92234700	-5.25560000
H	-0.01361500	1.19933100	-2.94806400
H	1.93606800	-2.36966500	0.22233200
H	3.69456000	-2.88637400	1.87851800
H	5.55376200	-1.28099600	2.27139700
H	5.62585100	0.85315400	0.99299400

H	3.84108200	1.39012000	-0.63134500
H	-3.45364900	-1.54170300	-3.15452100
H	-4.72531800	-0.05131400	-4.66905300
H	-4.62349100	2.41444100	-4.36163700
H	-3.25129200	3.37159900	-2.52317700
H	-1.99877800	1.87454600	-0.99884200



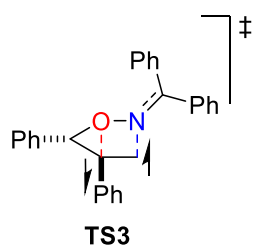
B3LYP /def2-TZVP E(scf) = -1211.123345 a.u

0 1

C	-4.89676900	1.21429400	1.85529000
C	-4.89320200	2.60731600	2.00038200
C	-3.75868600	3.33310900	1.61750700
C	-2.64615700	2.68422100	1.10317500
C	-2.62192100	1.26695200	0.94927000
C	-3.79223500	0.55274100	1.34060100
C	-1.48182000	0.60539400	0.43041000
C	-1.31198500	-0.88886400	0.23638800
O	0.01772100	-1.02860000	-0.29525500
N	0.73969000	0.13194400	0.24753600
C	-0.17331000	1.25709400	0.08084700
C	2.10236700	0.12161700	0.10136000
C	2.83311500	-0.98265300	0.70588200
C	2.76272900	1.23435300	-0.59032000
C	3.89042100	1.87579700	-0.03115300
C	4.50040100	2.94529000	-0.67850900
C	4.00436500	3.40912800	-1.90109600
C	2.89646400	2.78134800	-2.47497100
C	2.28427300	1.70781500	-1.83288700
C	4.13877100	-1.32015400	0.27942200
C	4.82756300	-2.38351700	0.85312300
C	4.23747600	-3.15031500	1.86152200
C	2.94334800	-2.83623800	2.28986900
C	2.25014900	-1.77394100	1.72420200
C	-2.24879300	-1.57590800	-0.74090100

C	-3.90216300	-0.46994100	1.31902800
C	-2.50143900	-0.24003200	1.45820100
C	-2.00523900	-0.04984500	2.78157900
C	-1.63532300	-0.21107500	0.33592300
C	-2.01106800	-0.50048100	-1.10136100
O	-0.82914400	-0.96976900	-1.71238900
N	0.31548200	0.01864600	-0.95016500
C	-0.14215900	-0.07672600	0.43160300
C	1.57198200	-0.18335500	-1.35963800
C	2.58682900	-0.79753900	-0.46712200
C	1.90288000	0.19383100	-2.73540200
C	3.06616500	-0.29090200	-3.37047200
C	3.36542200	0.06913900	-4.68148000
C	2.51199400	0.91477200	-5.39334700
C	1.35123300	1.39702900	-4.77922100
C	1.04701300	1.04397400	-3.47053500
C	2.34968500	-2.05475400	0.12038000
C	3.29199700	-2.63057700	0.97111000
C	4.48590900	-1.96296200	1.25229200
C	4.73652700	-0.71827700	0.66953500
C	3.79796300	-0.14142900	-0.18387200
C	-2.65565100	0.64937500	-1.88759500
C	-2.70693300	0.53810000	-3.28454800
C	-3.29780200	1.53650000	-4.05648800
C	-3.84785000	2.66525000	-3.44290800
C	-3.79705400	2.78594700	-2.05515400
C	-3.20330600	1.78442900	-1.28174600
H	-2.44347100	0.05911100	4.87545900
H	-4.88195700	-0.34716800	4.57723800
H	-5.79990300	-0.68345700	2.28660000
H	-4.32305100	-0.61061100	0.32886000
H	-0.94560100	0.12818100	2.93490800
H	-2.69748800	-1.36320400	-1.13036500
H	0.15911400	0.85029700	0.93900900
H	0.30520300	-0.91072600	0.99406200
H	3.72743100	-0.96311200	-2.83479600
H	4.26487100	-0.31815900	-5.15161000
H	2.74742200	1.19509200	-6.41591700

H	0.68193300	2.05697200	-5.32381800
H	0.15145600	1.42252900	-2.99331800
H	1.43504800	-2.58708500	-0.12344900
H	3.09772000	-3.60608300	1.40760600
H	5.21840400	-2.41168300	1.91670900
H	5.66422000	-0.19484600	0.88219000
H	3.99335800	0.82743700	-0.63357000
H	-2.26215100	-0.33127800	-3.75855900
H	-3.32880600	1.43508000	-5.13785700
H	-4.30912100	3.44406500	-4.04345100
H	-4.21497600	3.66291800	-1.56868500
H	-3.16500200	1.89317900	-0.20308500

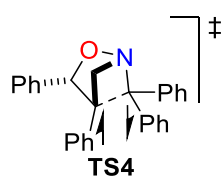


B3LYP /def2-TZVP E(scf) = -1211.119983 a.u

0 1

C	-2.80453600	0.46696500	-3.93185500
C	-4.19056600	0.54905400	-3.75306200
C	-4.73240100	0.30183000	-2.48564800
C	-3.91270800	-0.02004100	-1.41449700
C	-2.49731700	-0.10397100	-1.56613700
C	-1.97313300	0.14880700	-2.86813400
C	-1.64630300	-0.41707600	-0.47378900
C	-2.08424800	-0.72166900	0.94911100
O	-0.92094800	-1.05595600	1.67270900
N	0.27556200	-0.13031400	0.82313300
C	-0.14596000	-0.42483800	-0.54106100
C	1.51074000	-0.25921900	1.29004800
C	2.56897600	-0.94180600	0.49723100
C	1.79422500	0.27085600	2.62836000
C	2.97538100	-0.07136500	3.31801000
C	3.22865000	0.43210400	4.59151100
C	2.31009600	1.28259200	5.20905000
C	1.12993800	1.62431000	4.53981500
C	0.87213800	1.12684900	3.26895800

C	2.40257800	-2.28126800	0.10101100
C	3.38052200	-2.92315800	-0.65761600
C	4.53789100	-2.23911200	-1.03525200
C	4.71696100	-0.91084500	-0.64204900
C	3.74291300	-0.26778400	0.12009200
H	-2.37237700	0.65262400	-4.91121500
H	-4.83786900	0.79933000	-4.58788800
H	-5.80682700	0.36030700	-2.33577800
H	-4.35711900	-0.21717000	-0.44596400
H	-0.90299400	0.08566700	-3.03699100
H	0.24077400	0.37620300	-1.18239300
H	0.25693400	-1.37314100	-0.93096700
H	3.68907000	-0.74460900	2.85617800
H	4.14400500	0.15344000	5.10566900
H	2.50904900	1.67474100	6.20210700
H	0.41011800	2.28603400	5.01319200
H	-0.03934800	1.39158600	2.74679800
H	1.51449500	-2.81929900	0.41929000
H	3.24242700	-3.96091100	-0.94716000
H	5.29799800	-2.73942000	-1.62795000
H	5.61630900	-0.37442400	-0.93044700
H	3.88304400	0.76518900	0.42450800
H	-2.58222700	0.17087800	1.37439200
C	-3.02763700	-1.90914700	1.12305700
C	-2.78311300	-3.12497500	0.47175900
C	-4.12036800	-1.81294600	1.99016600
C	-3.62485500	-4.21605500	0.67278300
H	-1.93253900	-3.20984400	-0.19780800
C	-4.96669800	-2.90519500	2.19276200
H	-4.30719700	-0.87725100	2.51112100
C	-4.72113300	-4.10909300	1.53348100
H	-3.42814900	-5.15187500	0.15737700
H	-5.81354500	-2.81463600	2.86699400
H	-5.37788300	-4.96024400	1.68803500

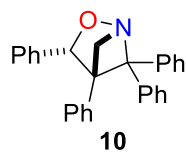


B3LYP /def2-TZVP E(scf) = -1211.113182 a.u

0 1

C	-3.55427000	1.11890100	2.08103100
C	-2.97446300	0.96034400	3.34310700
C	-1.83867500	0.15683500	3.47549400
C	-1.28804900	-0.47375900	2.36608300
C	-1.85481900	-0.32514400	1.07365900
C	-3.01154400	0.48917100	0.96720600
C	-1.25758200	-0.98595100	-0.06527300
C	-1.90784600	-1.15314800	-1.40978100
O	-0.92446100	-2.00528400	-2.13210200
N	0.24773200	-2.13654300	-1.28477200
C	-0.40185000	-2.24173400	0.03255300
C	0.87791700	-0.84306900	-1.21030200
C	1.86014200	-0.68883000	-0.08571400
C	1.20059200	-0.11971700	-2.44974700
C	1.83752400	1.14169800	-2.38506800
C	2.17584400	1.84111300	-3.53753200
C	1.91573100	1.29505100	-4.79652600
C	1.31011500	0.04011600	-4.88190300
C	0.94727200	-0.65674600	-3.73370300
C	2.91585700	-1.61091700	0.02627900
C	3.87299500	-1.47737500	1.03131400
C	3.79952200	-0.41641700	1.93601600
C	2.75680800	0.50492700	1.83319900
C	1.79129300	0.36739800	0.83443200
C	-2.33797500	0.04109700	-2.23662400
C	-3.35210300	-0.14197800	-3.18631400
C	-3.77474300	0.91143300	-3.99718100
C	-3.19124000	2.17135300	-3.86087400
C	-2.18599600	2.36756800	-2.91150600
C	-1.76061200	1.31056500	-2.10885400
H	-4.44329200	1.73253900	1.96539800
H	-3.40381000	1.45203100	4.21080300
H	-1.37940600	0.02086000	4.45060500
H	-0.40016800	-1.08278600	2.49393400
H	-3.48582700	0.61939500	0.00203800
H	-2.78105200	-1.82040000	-1.31372100

H	0.33893800	-2.24757000	0.82757100
H	-0.98647000	-3.17073000	0.08208400
H	2.07243200	1.57399800	-1.41946700
H	2.65639700	2.81156700	-3.45194400
H	2.18694300	1.83745300	-5.69747000
H	1.11361200	-0.40280900	-5.85415000
H	0.46739900	-1.62037300	-3.82218000
H	2.97901700	-2.43040200	-0.68297200
H	4.68077900	-2.20010600	1.10318200
H	4.54755300	-0.31056700	2.71618400
H	2.68537300	1.32885100	2.53739600
H	0.96534700	1.06814400	0.77664600
H	-3.81122600	-1.12202500	-3.29114400
H	-4.56032900	0.74908900	-4.72957100
H	-3.51892500	2.99588800	-4.48751600
H	-1.72913600	3.34636900	-2.79757400
H	-0.97905300	1.46489800	-1.37462400

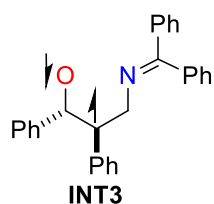


B3LYP /def2-TZVP E(scf) = -1211.146938 a.u

0 1

C	-2.42098900	1.77981400	1.73124400
C	-2.69865600	1.11614900	2.92786400
C	-2.38251100	-0.23652800	3.05016400
C	-1.78462200	-0.91555400	1.98777900
C	-1.49562800	-0.26230700	0.78030200
C	-1.83254800	1.09772600	0.66673300
C	-0.85690700	-1.02256200	-0.34604800
C	-1.69518100	-1.28978600	-1.64019200
O	-0.70535300	-2.05335600	-2.38546000
N	0.41884100	-2.24339000	-1.44921500
C	-0.36090600	-2.48758900	-0.18640600
C	0.62125600	-0.81433800	-0.94791900
C	1.75368300	-0.79773400	0.08634800
C	0.97733500	0.19372300	-2.02886400
C	0.84791300	1.57061000	-1.81357900
C	1.26298500	2.48543600	-2.78141900

C	1.83522200	2.03728000	-3.97199900
C	1.99270100	0.66641000	-4.18350800
C	1.56840900	-0.24867100	-3.22057300
C	2.87437000	-1.61935300	-0.10904800
C	3.95253600	-1.57320900	0.77356900
C	3.93466600	-0.69941200	1.86186200
C	2.82814300	0.12615400	2.05897600
C	1.74530400	0.07898100	1.17913300
C	-2.33411400	-0.19500800	-2.46971300
C	-3.53707800	0.37039800	-2.01714100
C	-4.19828700	1.34119700	-2.76754500
C	-3.68173600	1.74292700	-4.00087500
C	-2.50694500	1.15967900	-4.47498000
C	-1.83833000	0.19610700	-3.71824500
H	-2.66876500	2.83168500	1.62159900
H	-3.15831000	1.64851300	3.75526700
H	-2.59520300	-0.76562100	3.97457000
H	-1.53609000	-1.96623200	2.10276500
H	-1.64450400	1.62168900	-0.26305600
H	-2.51146500	-1.96465700	-1.34195700
H	0.31378000	-2.65644700	0.65073500
H	-1.08304400	-3.30133200	-0.28037500
H	0.43188300	1.93703900	-0.88128700
H	1.14418200	3.54971100	-2.59970500
H	2.16222300	2.74918600	-4.72420400
H	2.44555700	0.30556500	-5.10275400
H	1.67869000	-1.31320100	-3.39355700
H	2.88869800	-2.30051500	-0.95300500
H	4.80893900	-2.22075800	0.60812400
H	4.77544400	-0.66162400	2.54832700
H	2.80213700	0.81124900	2.90158200
H	0.89401600	0.72688600	1.35165100
H	-3.96081500	0.04519500	-1.07118200
H	-5.12355400	1.77194800	-2.39545400
H	-4.19912100	2.49294600	-4.59226100
H	-2.10578400	1.45128900	-5.44137300
H	-0.93425600	-0.26204100	-4.09558700

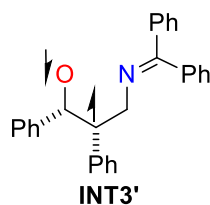


B3LYP /def2-TZVP E(scf) = -1211.154795 a.u

0 1

C	-5.01347500	2.09232400	-0.56403100
C	-3.62775300	2.21706600	-0.35835000
C	-3.04908000	3.49653400	-0.35606000
C	-3.83414300	4.62802200	-0.57474000
C	-5.20756400	4.49587400	-0.78261300
C	-5.79322100	3.22648400	-0.77165200
H	-5.45684100	1.10300000	-0.52881200
H	-1.98113900	3.60442500	-0.19634700
H	-3.37277300	5.61128200	-0.58234300
H	-5.82067600	5.37780100	-0.94549600
H	-6.86433700	3.12157200	-0.91840100
C	-2.79762800	0.99646000	-0.16032500
C	-1.51628700	1.13624500	0.61345700
C	-0.28040900	0.83445500	0.02360100
C	-1.54387600	1.57224400	1.94689000
C	0.90273000	0.96165500	0.75165600
H	-0.24629600	0.51452000	-1.01390000
C	-0.36224000	1.68196400	2.67904800
H	-2.49597100	1.81773500	2.40729800
C	0.86368500	1.38008500	2.08262400
H	1.85394000	0.73493100	0.27898700
H	-0.39855200	2.00873600	3.71411800
H	1.78413400	1.47422100	2.65121900
N	-3.22842700	-0.11036800	-0.64808500
C	-2.56121100	-1.37519800	-0.41597200
H	-2.03214100	-1.41106500	0.55229400
H	-1.78621200	-1.50219400	-1.18502800
C	-3.53672000	-2.52062400	-0.54378200
C	-5.00925600	-2.19453000	-0.33646600
O	-5.17616000	-1.08574100	0.44945400
C	-3.05792800	-3.86554600	-0.68977700
C	-3.94279500	-4.96995800	-0.84657500

C	-1.66462200	-4.15951600	-0.70195200
C	-3.46729300	-6.26177100	-1.01256500
H	-5.01333600	-4.80174300	-0.86001300
C	-1.19767300	-5.45762900	-0.86172100
H	-0.94283800	-3.36101000	-0.57297700
C	-2.09146200	-6.52062400	-1.01969000
H	-4.17314100	-7.07787000	-1.13759500
H	-0.12744600	-5.64386800	-0.86007400
H	-1.72373300	-7.53444000	-1.14433000
H	-5.38825000	-3.01755900	0.30637300
C	-5.85722200	-2.20192000	-1.61499400
C	-7.03372900	-2.95698700	-1.67289100
C	-5.50376000	-1.41494400	-2.71907500
C	-7.83953000	-2.94124700	-2.81324000
H	-7.32935100	-3.55786700	-0.81507800
C	-6.30903000	-1.39476100	-3.85696600
H	-4.60722200	-0.80598000	-2.66513800
C	-7.47657500	-2.16061900	-3.91032500
H	-8.74906300	-3.53478800	-2.84154300
H	-6.02538600	-0.77847200	-4.70569900
H	-8.09973100	-2.14557500	-4.79995700



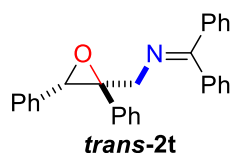
B3LYP /def2-TZVP E(scf) = -1211.149819 a.u

0 1

C	-5.11066600	2.00468300	0.54241300
C	-3.72768300	2.15149400	0.33282100
C	-3.16001200	3.43382100	0.40201500
C	-3.95243400	4.54432600	0.69173600
C	-5.32268500	4.38937500	0.90238300
C	-5.89785100	3.11735500	0.82240900
H	-5.54532900	1.01493500	0.45445700
H	-2.09451600	3.56043400	0.24046900
H	-3.49861500	5.52927100	0.75227800
H	-5.94158000	5.25502400	1.12101300
H	-6.96691000	2.99533400	0.97163300

C	-2.88934800	0.95285000	0.05305200
C	-1.57689300	1.15787400	-0.65360100
C	-0.36183800	0.89188000	-0.00660100
C	-1.55562100	1.61091000	-1.98103100
C	0.85011500	1.07114600	-0.67408200
H	-0.36749200	0.55786400	1.02710200
C	-0.34386800	1.77479900	-2.65207000
H	-2.49237300	1.82942000	-2.48490400
C	0.86137000	1.50768000	-1.99982600
H	1.78465900	0.87098100	-0.15808700
H	-0.34121800	2.11655000	-3.68299300
H	1.80459700	1.64300400	-2.52081200
N	-3.33107400	-0.19623200	0.41419900
C	-2.63276200	-1.43204300	0.09342600
H	-2.19727500	-1.40594300	-0.92093000
H	-1.78656100	-1.54661700	0.78088500
C	-3.57247400	-2.60072900	0.27116600
C	-5.03784000	-2.28907300	0.02461700
H	-5.57489300	-2.30115600	0.99362800
O	-5.22395300	-1.10412400	-0.66070500
C	-5.78164900	-3.25358200	-0.91982000
C	-7.11214900	-3.59331600	-0.65004600
C	-5.18308500	-3.71078700	-2.10083100
C	-7.82272400	-4.41427000	-1.52615100
H	-7.58759200	-3.21728200	0.25174100
C	-5.89385900	-4.52832000	-2.97645900
H	-4.15729300	-3.43466900	-2.32202500
C	-7.21451500	-4.88464200	-2.69081700
H	-8.85073700	-4.68256200	-1.30041900
H	-5.41757400	-4.88819700	-3.88386000
H	-7.76602500	-5.52415000	-3.37377400
C	-3.09824000	-3.88687800	0.68085200
C	-3.98750500	-4.93483100	1.05938300
C	-1.70478300	-4.18201600	0.74565800
C	-3.51483900	-6.16982400	1.47874900
H	-5.05680000	-4.76644700	1.02893000
C	-1.24304600	-5.42341400	1.16001000
H	-0.98076100	-3.43210400	0.44639600

C	-2.14076200	-6.42911300	1.53368300
H	-4.22369400	-6.94071100	1.76766300
H	-0.17354200	-5.61236000	1.18971300
H	-1.77628100	-7.39817900	1.86041400

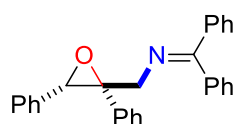


B3LYP /def2-TZVP E(scf) = -1211.231135 a.u

0 1

C	1.27719300	0.16630300	-0.77973900
C	1.47680200	-1.23900300	-0.32765700
O	1.52789900	-0.88344800	-1.72004500
H	0.55955900	-1.76331700	-0.05729100
C	2.71463900	-1.75495400	0.32392500
C	2.63571000	-2.24874000	1.63330400
C	3.94733800	-1.77915000	-0.33864700
C	3.77161600	-2.73660000	2.27753000
H	1.67783700	-2.25165800	2.14832400
C	5.08196700	-2.27372100	0.30409200
H	4.00123200	-1.41873800	-1.35941300
C	5.00002300	-2.74949000	1.61385300
H	3.69645000	-3.11328700	3.29367800
H	6.03264800	-2.29064800	-0.22135700
H	5.88516500	-3.13449700	2.11189000
C	2.35638900	1.20572500	-0.65210800
C	2.50009000	1.94220600	0.53103500
C	3.19579200	1.48787600	-1.73545900
C	3.46987300	2.93921500	0.63011800
H	1.85978300	1.72549700	1.38204500
C	4.16461900	2.48741100	-1.63738300
H	3.08520200	0.91154000	-2.64835000
C	4.30371800	3.21579800	-0.45526800
H	3.57749600	3.49706500	1.55589900
H	4.81111900	2.69672500	-2.48494400
H	5.05917700	3.99234200	-0.37797600
C	-0.13673200	0.75721100	-0.83490200
H	-0.24712200	1.49094500	-0.02500900
H	-0.19878200	1.32363100	-1.77583700

N	-1.15972400	-0.26697600	-0.83513000
C	-2.32504700	-0.05335600	-0.34507500
C	-2.75402900	1.26110200	0.25385400
C	-2.84586400	1.41549000	1.64457700
C	-3.04382000	2.35611000	-0.57174500
C	-3.21189200	2.64330300	2.19759600
H	-2.62884300	0.57093100	2.29250000
C	-3.41820500	3.58071700	-0.01802600
H	-2.98017100	2.24454100	-1.65045000
C	-3.50068200	3.72777400	1.36759800
H	-3.27387000	2.75117700	3.27658400
H	-3.64428600	4.41982700	-0.66942600
H	-3.78922500	4.68202400	1.79821100
C	-3.31858100	-1.16905200	-0.37799500
C	-4.62902300	-1.00169100	0.09551000
C	-2.94659900	-2.41915000	-0.90523700
C	-5.54050800	-2.05799900	0.05418900
H	-4.94062400	-0.04282700	0.49462800
C	-3.85644100	-3.46930700	-0.94542300
H	-1.93834500	-2.53788600	-1.28546000
C	-5.15801700	-3.29432400	-0.46345500
H	-6.55062600	-1.91053100	0.42513200
H	-3.55340800	-4.42847700	-1.35544800
H	-5.86747000	-4.11620500	-0.49604100



cis-2t

B3LYP /def2-TZVP E(scf) = -1210.859334 a.u

0 1

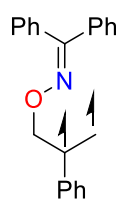
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O	2.72059600	1.72549300	0.94327800
H	3.48298900	1.23083500	-0.97466500
C	3.54035500	-0.55381900	0.28434200
C	3.78181400	-1.51125900	-0.71029400
C	3.83964000	-0.86266600	1.61615800
C	4.29588800	-2.76251500	-0.37587200

H	3.56256800	-1.27394900	-1.74831200
C	4.35821800	-2.11510700	1.94921800
H	3.67330400	-0.10846800	2.37814000
C	4.58468800	-3.06873300	0.95635500
H	4.47443000	-3.49833200	-1.15472100
H	4.59046800	-2.34305300	2.98564800
H	4.98880500	-4.04274200	1.21629700
C	1.01824500	2.28952400	-0.76516100
C	1.25564200	3.64935800	-0.53113400
C	0.22869800	1.91280000	-1.86232500
C	0.70417100	4.61824000	-1.37050800
H	1.88142000	3.93466200	0.30764600
C	-0.31996500	2.88446400	-2.70029400
H	0.05382100	0.86033600	-2.05828500
C	-0.08699800	4.23954300	-2.45573700
H	0.89487400	5.67003400	-1.17637000
H	-0.92523700	2.58065500	-3.54974900
H	-0.51432300	4.99365200	-3.11044500
C	0.62935700	0.39058100	0.94770100
H	1.22020800	-0.23328400	1.62740600
H	0.00214200	1.04876000	1.56246800
N	-0.11028100	-0.50222600	0.07349300
C	-1.37102100	-0.69862100	0.20679400
C	-2.24798100	0.00141600	1.21178000
C	-2.72130600	-0.68536900	2.33863400
C	-2.60041700	1.34726400	1.03572000
C	-3.52133800	-0.03521200	3.27841600
H	-2.45995800	-1.73059200	2.47754200
C	-3.40701700	1.99347900	1.97352800
H	-2.24018200	1.88462000	0.16325400
C	-3.86702200	1.30521700	3.09720200
H	-3.87662100	-0.57660400	4.15042000
H	-3.67418000	3.03569000	1.82529300
H	-4.49258300	1.81008400	3.82742700
C	-2.01652600	-1.69855500	-0.69762200
C	-1.21692800	-2.55904900	-1.47104400
C	-3.41224800	-1.79400400	-0.80878500
C	-1.79943200	-3.48460200	-2.32993100

1a-T1

C	3.93099000	-0.43139100	-0.25738800
C	4.01507700	-1.43561900	0.75079700
C	5.17891200	-1.62656600	1.48117900
C	6.31055400	-0.83593700	1.24739300
C	6.25586600	0.16049800	0.26488300
C	5.09780600	0.36111200	-0.46948500
H	3.15654200	-2.06040700	0.96826400
H	5.20710700	-2.39859000	2.24504400
H	7.21790000	-0.99218600	1.82264100
H	7.12568600	0.78310400	0.07474500
H	5.06400100	1.13671800	-1.22855100
C	1.51345200	-1.03124500	-0.94060500
H	1.59777400	-1.85387000	-0.22574900
O	0.43446300	-0.16138800	-0.53823900
N	-0.74632800	-0.90324500	-0.51814500
C	-1.78210000	-0.21353400	-0.16786400
C	-1.77891500	1.24927400	0.13137600
C	-1.21884000	2.17500700	-0.76285900
C	-2.35636000	1.72110700	1.32003500
C	-1.24103300	3.53792000	-0.47405800
H	-0.76584800	1.82010500	-1.68133400
C	-2.36271800	3.08410000	1.61493500
H	-2.79697200	1.01397300	2.01599000
C	-1.80828200	3.99663300	0.71678100
H	-0.81244200	4.24406000	-1.17943200

H	-2.80467600	3.43212200	2.54397700
H	-1.81898900	5.05911500	0.94198000
C	-3.05157200	-0.98601200	-0.06725500
C	-3.02783000	-2.36921800	0.18571600
C	-4.29427900	-0.35796500	-0.24968100
C	-4.21085600	-3.09895800	0.24881500
H	-2.07026300	-2.85576700	0.33245600
C	-5.47831300	-1.09247600	-0.18534600
H	-4.33228300	0.70696600	-0.45210700
C	-5.44227500	-2.46415800	0.06452100
H	-4.17390400	-4.16561200	0.45104800
H	-6.42972000	-0.59001400	-0.33415300
H	-6.36500100	-3.03441900	0.11963100
H	1.26185600	-1.46484700	-1.91919200
C	2.75946000	-0.19563400	-1.04368000
C	2.70162200	0.89439100	-2.02757200
H	2.97051000	0.73207900	-3.07027500
H	2.25512700	1.85332200	-1.77588700

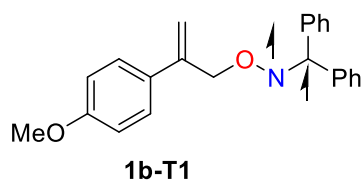


1a-T2

0 3

C	4.06379200	0.07580900	0.26297200
C	4.52031300	0.71559200	-0.90265900
C	5.86564600	0.66912600	-1.26757900
C	6.78506600	-0.02376200	-0.48041600
C	6.34568700	-0.67455800	0.67423000
C	5.00196000	-0.63009700	1.03703900
H	3.82829200	1.27545000	-1.52397100
H	6.19457900	1.17941700	-2.16823000
H	7.83182700	-0.06266100	-0.76674600
H	7.04930400	-1.23001300	1.28765100
H	4.66373600	-1.16625300	1.91805400
C	2.63359600	0.12655500	0.67101500
C	2.25087500	0.15809900	1.95428100
H	1.20422000	0.17024100	2.23155900

H	2.98149100	0.18880900	2.75553300
C	1.62904600	0.12769900	-0.45822300
H	1.80336900	-0.71684900	-1.13611500
O	0.29659900	0.03683500	0.07286100
H	1.69471900	1.04531400	-1.05573600
N	-0.62386200	0.06506400	-0.96099700
C	-1.92763000	-0.00399800	-0.41487200
C	-2.58596800	1.26255700	-0.15203900
C	-2.11136500	2.45162900	-0.76137600
C	-3.67086800	1.37929400	0.75220300
C	-2.70798200	3.67842000	-0.50143000
H	-1.28110800	2.38673200	-1.45593600
C	-4.25865000	2.61278100	1.00906300
H	-4.02076900	0.50085200	1.28194100
C	-3.78881000	3.77002800	0.38151900
H	-2.33151400	4.57111600	-0.99296300
H	-5.08152800	2.67415800	1.71571900
H	-4.25255200	4.73070600	0.58391900
C	-2.51462900	-1.32552000	-0.27639400
C	-3.91105100	-1.54704400	-0.37292600
C	-1.68272300	-2.45990700	-0.10345400
C	-4.44208600	-2.82743900	-0.26801100
H	-4.57147500	-0.70986100	-0.56734300
C	-2.22293900	-3.73551700	0.00174300
H	-0.61094500	-2.32014400	-0.02724800
C	-3.60548500	-3.93048600	-0.07416100
H	-5.51590600	-2.96830700	-0.35338100
H	-1.56206000	-4.58540600	0.14701600
H	-4.02419900	-4.92899200	0.00722500

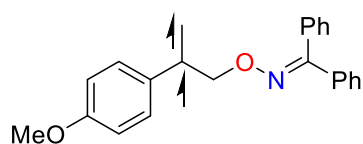


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C	-3.28875400	-0.16688000	0.36889800
C	-3.75536400	-0.83898500	-0.77818000
C	-5.09904200	-0.83500400	-1.12532000
C	-6.03095600	-0.14721500	-0.33595600

C	-5.59082800	0.53951400	0.80189000
C	-4.23674500	0.52679400	1.13503800
H	-3.06457100	-1.39550600	-1.40384300
H	-5.45363700	-1.36297700	-2.00429300
H	-6.28375100	1.09599200	1.42157500
H	-3.90554000	1.09002600	2.00183600
C	-1.85397900	-0.17485800	0.75675300
C	-1.44700500	-0.16428700	2.03337900
H	-0.39585600	-0.13708300	2.29159200
H	-2.16200800	-0.19794500	2.84858400
C	-0.86859900	-0.17514700	-0.38939500
H	-1.06615900	0.65896000	-1.07377800
O	0.47273400	-0.05992200	0.11529900
H	-0.93194100	-1.10041300	-0.97533400
N	1.37267100	-0.07457000	-0.93588500
C	2.68587700	0.01813600	-0.41653300
C	3.37156500	-1.23600100	-0.16473000
C	2.90251600	-2.43515800	-0.75848200
C	4.47969500	-1.33129200	0.71355700
C	3.52571200	-3.65081500	-0.50896200
H	2.05475700	-2.38660500	-1.43291700
C	5.09410500	-2.55383800	0.96021200
H	4.82752500	-0.44512100	1.23168000
C	4.62885800	-3.72110600	0.34795200
H	3.15249600	-4.55148700	-0.98829000
H	5.93465400	-2.59885800	1.64704300
H	5.11340900	-4.67315300	0.54228600
C	3.25298700	1.35005000	-0.29451200
C	4.64286200	1.59558000	-0.42226200
C	2.40532900	2.47032300	-0.10678700
C	5.15360900	2.88541700	-0.33328700
H	5.31322500	0.76916100	-0.62830500
C	2.92533900	3.75551300	-0.01761700
H	1.33812600	2.31198200	-0.00654300
C	4.30226500	3.97438500	-0.12468600
H	6.22267200	3.04468200	-0.44277000
H	2.25302200	4.59426900	0.13952400
H	4.70508500	4.98035800	-0.05580900

O	-7.32568200	-0.20037100	-0.76194400
C	-8.31269300	0.47639300	0.00124300
H	-8.12510400	1.55705700	0.03895700
H	-9.26145600	0.29519400	-0.50559600
H	-8.37058200	0.08668900	1.02548400



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0 3

C	-2.88122900	-1.12148400	0.56389900
C	-2.57908200	-0.69377900	-0.76405100
C	-3.53152200	-0.09490700	-1.56298400
C	-4.83814600	0.11803100	-1.08459200
C	-5.16581500	-0.27576700	0.22172500
C	-4.20390200	-0.87822100	1.02173100
H	-1.57134400	-0.81042000	-1.14533300
H	-3.29330900	0.23279400	-2.56972000
H	-6.16224700	-0.11820000	0.61763100
H	-4.46794900	-1.18245900	2.03013400
C	-0.55129000	-2.11424500	0.86798100
H	-0.60805700	-2.58737100	-0.12185500
O	0.23331800	-0.90143200	0.74894100
N	1.51421900	-1.24882000	0.31486000
C	2.29946500	-0.23571300	0.14548600
C	1.94788400	1.19052200	0.40989800
C	1.32632000	1.58543600	1.60513100
C	2.25059000	2.17036700	-0.54914600
C	1.02353700	2.92594400	1.83442600
H	1.07840100	0.83692800	2.34787300
C	1.93116000	3.50876300	-0.32480800
H	2.73409800	1.87769200	-1.47589600
C	1.32030600	3.89113900	0.87007500
H	0.54947600	3.21697400	2.76729700
H	2.16320500	4.25199000	-1.08205500
H	1.07662200	4.93436600	1.04911000
C	3.65812400	-0.57810800	-0.36367700
C	3.85794500	-1.72802600	-1.14752300

C	4.76967000	0.21862000	-0.04463200
C	5.13111000	-2.06981400	-1.59377600
H	3.00122900	-2.34337800	-1.39789200
C	6.04448000	-0.12716900	-0.49262700
H	4.63597000	1.10577900	0.56508200
C	6.23067600	-1.27072700	-1.26918100
H	5.26593600	-2.95862800	-2.20359500
H	6.89302200	0.49822700	-0.23050900
H	7.22282900	-1.53641300	-1.62236500
H	-0.03474700	-2.80285300	1.54377300
C	-1.91716500	-1.76636100	1.39763700
C	-2.20668400	-2.10707100	2.79583700
H	-2.59538400	-3.08393000	3.08019500
H	-1.94452700	-1.43277700	3.60985600
O	-5.69843000	0.71392800	-1.95849000
C	-7.02945000	0.96003900	-1.53178900
H	-7.05935000	1.63804600	-0.66941200
H	-7.53412200	1.43142800	-2.37622100
H	-7.55028100	0.02915100	-1.27397600

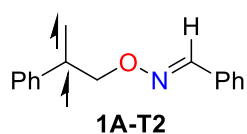


1A-T1

0 3

C	-3.26550900	0.05227500	0.25072100
C	-3.83979400	-0.79400800	-0.71389300
C	-5.13617500	-0.57626100	-1.17990000
C	-5.88650700	0.49620500	-0.69841000
C	-5.32650500	1.35281300	0.25155600
C	-4.03107200	1.13673700	0.71481000
H	-3.28363100	-1.64594300	-1.09221000
H	-5.56030800	-1.25002600	-1.91877300
H	-6.89456900	0.66753100	-1.06403000
H	-5.89540000	2.20005500	0.62366200
H	-3.59183000	1.82625100	1.42869000
C	-1.88813200	-0.17480200	0.76687400
C	-1.54204500	0.08560500	2.03431000
H	-0.52735000	-0.06069300	2.38283300
H	-2.27370600	0.43705200	2.75394700

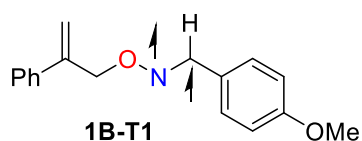
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H	-0.84434900	-0.05439100	-1.11894300
O	0.41369100	-0.77991700	0.36102000
N	1.29861100	-1.38336000	-0.51902600
C	2.55781200	-1.47214200	0.07721100
C	3.56941200	-0.48974600	-0.07626900
C	3.33612700	0.73335700	-0.76410200
C	4.86452400	-0.70992000	0.46889700
C	4.34467800	1.67666400	-0.88933300
H	2.35583900	0.91597200	-1.19121200
C	5.86257300	0.24343300	0.33871900
H	5.06236100	-1.63968900	0.99570000
C	5.61286300	1.44360700	-0.34036300
H	4.14769600	2.60482300	-1.41846000
H	6.84398400	0.05650000	0.76533700
H	6.39729100	2.18730600	-0.44140600
H	2.77743400	-2.40335800	0.60006200
H	-1.16317100	-1.70846700	-0.58582000



0 3

C	3.24982500	-0.24623900	0.07396200
C	2.76646500	0.99709900	0.57277400
C	3.58448700	2.11689800	0.61512000
C	4.90805200	2.05298000	0.16228000
C	5.40320700	0.84482800	-0.34406400
C	4.59476600	-0.28084000	-0.39098100
H	1.73543400	1.07821500	0.89724200
H	3.18871600	3.05338500	0.99809100
H	5.54248900	2.93337700	0.19839900
H	6.42722400	0.78609800	-0.70222800
H	4.98477100	-1.21541100	-0.78309500
C	1.03644900	-1.40620500	0.60450700
H	1.00397500	-0.92238300	1.58981200
O	0.18189800	-0.67101900	-0.30097300
N	-1.11924200	-0.65641200	0.21074900
C	-1.91192800	-0.02802600	-0.57808700

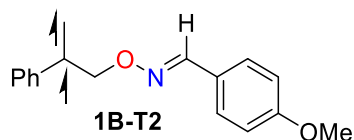
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C	-3.91413000	-0.39126900	0.89984100
C	-4.15058700	0.83121000	-1.17577800
C	-5.27018700	-0.21588000	1.15104300
H	-3.28506800	-0.93188000	1.59878600
C	-5.51025400	1.00513500	-0.92064200
H	-3.71208800	1.23868700	-2.08311200
C	-6.07405200	0.48239000	0.24316800
H	-5.70629600	-0.62426700	2.05815900
H	-6.12754100	1.54824300	-1.63014500
H	-7.13282900	0.61657600	0.44415500
C	2.43371100	-1.42158500	0.03929700
C	2.90286500	-2.67476200	-0.56260100
H	2.68975200	-2.91513900	-1.60279300
H	3.37941300	-3.45237500	0.03200100
H	-1.53256300	0.40579800	-1.50702500
H	0.64973900	-2.42474500	0.71198100



0 3

C	4.16313800	0.00002400	0.24566000
C	4.60968700	-0.21682700	-1.06975100
C	5.84291000	-0.81803800	-1.32074700
C	6.65642700	-1.22327200	-0.26306900
C	6.22244000	-1.02608300	1.04958100
C	4.98981800	-0.42858300	1.29971100
H	4.00247200	0.10304500	-1.91074900
H	6.16809000	-0.96622200	-2.34646900
H	7.61507900	-1.69457800	-0.45831400
H	6.83999700	-1.35133200	1.88194200
H	4.64690900	-0.31141200	2.32277700
C	2.85408400	0.65048900	0.52240500
C	2.64071800	1.41917700	1.59834400
H	1.66926200	1.85766600	1.78964200
H	3.43658100	1.63590900	2.30267300
C	1.76113500	0.38817000	-0.49042400
H	1.65871200	-0.69032700	-0.67139500

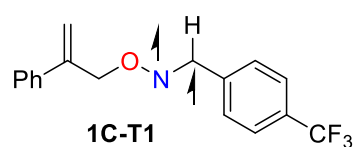
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N	-0.32194200	1.20967400	-1.09156400
C	-1.54232600	1.68647800	-0.60632400
C	-2.67370600	0.86121000	-0.39425500
C	-2.62495000	-0.55452500	-0.55558400
C	-3.91681500	1.42623600	-0.00696200
C	-3.74046100	-1.33633500	-0.33922900
H	-1.69076000	-1.01594600	-0.85704200
C	-5.04022700	0.64078600	0.21478400
H	-3.98777700	2.50287500	0.12234300
C	-4.96130600	-0.75114100	0.04994100
H	-3.70448800	-2.41391400	-0.46264900
H	-5.96854500	1.11379900	0.51271500
H	-1.62414000	2.76693900	-0.48585200
H	1.97742400	0.86468500	-1.45320500
O	-5.99741300	-1.61739900	0.23858400
C	-7.25505900	-1.08886900	0.63031300
H	-7.92565000	-1.94430700	0.72215600
H	-7.19368500	-0.57310100	1.59700000
H	-7.65470700	-0.39610500	-0.12114300



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C	4.13097600	0.21192700	-0.14706800
C	3.58375700	-1.02787100	-0.58515600
C	4.36647700	-2.17158800	-0.64943700
C	5.71652000	-2.13600600	-0.27907600
C	6.27466500	-0.93170800	0.16743500
C	5.50198200	0.21780500	0.23558200
H	2.53274700	-1.08556500	-0.84361700
H	3.92231100	-3.10466600	-0.98478500
H	6.32306400	-3.03503900	-0.33209700
H	7.31982900	-0.89469800	0.46185100
H	5.94083500	1.14941900	0.58025300
C	1.92465700	1.42358500	-0.58426500
H	1.82974800	0.92864600	-1.56039900
O	1.10203100	0.72294400	0.37297900

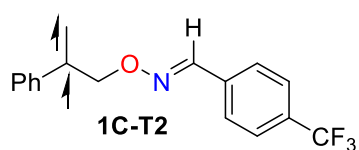
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C	-0.99152200	0.12736900	0.75560200
C	-2.42790300	-0.02007200	0.52005200
C	-3.05752200	0.47704300	-0.63171600
C	-3.21915600	-0.68409500	1.47469300
C	-4.42560600	0.32046800	-0.83080100
H	-2.45855400	0.99159700	-1.37556100
C	-4.58408900	-0.84715100	1.28874600
H	-2.75293200	-1.07717200	2.37446500
C	-5.19886400	-0.34569200	0.13253000
H	-4.87941500	0.71648400	-1.73130100
H	-5.19756600	-1.35897600	2.02249100
C	3.35108900	1.41107100	-0.09542400
C	3.88993100	2.66455100	0.44406200
H	3.74348000	2.93857900	1.48746400
H	4.35260700	3.41228200	-0.19802300
H	-0.57665200	-0.28854400	1.67780500
H	1.55945300	2.45084600	-0.68759000
O	-6.54243000	-0.55427700	0.03753400
C	-7.22142200	-0.07059700	-1.11201100
H	-8.26895200	-0.34398400	-0.97897100
H	-7.14148100	1.02017100	-1.20018000
H	-6.84139500	-0.53395900	-2.03117100



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C	4.71173100	-0.21140700	0.25123200
C	5.35488800	0.30685700	-0.88644100
C	6.56979800	-0.21808800	-1.32647300
C	7.16702400	-1.27748700	-0.64407100
C	6.53540400	-1.81115500	0.48119700
C	5.32094100	-1.28882000	0.91876800
H	4.92070900	1.14265200	-1.42619900
H	7.05076800	0.20595600	-2.20312400
H	8.11119300	-1.68842100	-0.98875900
H	6.98310400	-2.64604400	1.01253600
H	4.82120700	-1.73202600	1.77421800

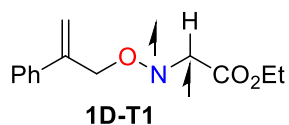
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H	2.14443300	0.78649300	2.36751300
H	3.79695900	0.06992100	2.80047200
C	2.47893100	0.84619300	-0.33299600
H	2.29875300	0.06892600	-1.08625100
O	1.22279800	1.22485900	0.25761500
N	0.41784100	1.82127700	-0.69402300
C	-0.79260700	2.20112000	-0.11389900
C	-1.95297600	1.38795300	-0.12549000
C	-1.93848900	0.05942700	-0.63438000
C	-3.18284300	1.89264300	0.38089800
C	-3.08566300	-0.71459800	-0.62518700
H	-1.01420600	-0.33963100	-1.03715100
C	-4.32451500	1.11110800	0.38860700
H	-3.21861300	2.90767800	0.76602400
C	-4.28599400	-0.19835700	-0.11402900
H	-3.06396300	-1.72389700	-1.02184900
H	-5.25636400	1.51027600	0.77433200
H	-0.84669700	3.22153600	0.26627600
H	2.88451400	1.72076800	-0.85483100
C	-5.50990800	-1.06486000	-0.04516900
F	-6.64767500	-0.33953500	-0.14092500
F	-5.53203000	-1.98865200	-1.03260300
F	-5.58079100	-1.74517200	1.12538400



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C	4.87713800	0.18548200	-0.12688300
C	4.34372700	-1.05479600	-0.58011600
C	5.12754400	-2.19888800	-0.61837500
C	6.46534600	-2.16270300	-0.20624600
C	7.00993400	-0.95774700	0.25496800
C	6.23588800	0.19194600	0.29734600
H	3.30188200	-1.11408100	-0.87350300
H	4.69400700	-3.13226700	-0.96628700
H	7.07295700	-3.06188900	-0.23902900

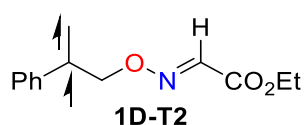
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H	6.66417800	1.12388500	0.65402300
C	2.68411300	1.39791700	-0.62001600
H	2.60331100	0.88299100	-1.58607500
O	1.83268000	0.71877500	0.33642900
N	0.51700100	0.75017000	-0.11734500
C	-0.26853400	0.15886600	0.70694400
C	-1.70816500	0.06173600	0.44926600
C	-2.30242200	0.61936900	-0.69782300
C	-2.52085600	-0.61272800	1.37324300
C	-3.66930100	0.50348800	-0.90801900
H	-1.67636500	1.13811400	-1.41508400
C	-3.89222800	-0.72998600	1.16378800
H	-2.07284800	-1.05113300	2.26057100
C	-4.46951800	-0.17194400	0.02222400
H	-4.12182600	0.92844200	-1.79746200
H	-4.51179500	-1.25909200	1.87925400
C	4.09676100	1.38509900	-0.09702900
C	4.61941800	2.63791400	0.46023700
H	4.44723100	2.90796900	1.50066600
H	5.10379800	3.38483200	-0.16638800
H	0.12586100	-0.28765100	1.62299800
H	2.32451600	2.42365700	-0.74659100
C	-5.95783700	-0.24242200	-0.18243300
F	-6.58475500	0.84579900	0.32469700
F	-6.49986000	-1.32342200	0.42154800
F	-6.28281500	-0.30330200	-1.49345000



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C	-3.06361600	-0.21855800	0.19159600
C	-2.56621800	1.10649900	0.34868000
C	-3.40023400	2.20555500	0.20260800
C	-4.75545200	2.03756300	-0.10703600
C	-5.26672200	0.74491000	-0.27663900
C	-4.44204900	-0.36061500	-0.13412500
H	-1.51424100	1.26367000	0.55811400

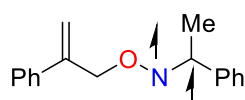
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H	-5.40249700	2.90203700	-0.21996700
H	-6.31582000	0.60450700	-0.52115900
H	-4.84466700	-1.36043200	-0.26593800
C	-0.79435800	-1.22983400	0.78044900
H	-0.38572400	-2.19015700	1.10724900
O	-0.01689000	-0.76052500	-0.35802700
N	1.30511800	-0.62082600	0.01604000
C	2.02489600	-0.22103400	-0.96546000
H	1.61674500	-0.02522600	-1.95636600
C	3.48408600	0.00721200	-0.80445800
C	5.35490300	-0.05677400	0.65282100
H	5.59832200	-0.73213600	1.47601700
H	5.90054200	-0.36277000	-0.24284300
C	5.65357700	1.39053900	1.01146900
H	5.42092900	2.05069400	0.17253500
H	5.07097200	1.70359500	1.88259800
H	6.71653800	1.50111800	1.25024000
O	3.93798300	-0.26335100	0.43195900
O	4.16962300	0.39864300	-1.73007300
H	-0.67688300	-0.50706200	1.59649400
C	-2.23007800	-1.37130200	0.35276800
C	-2.71987800	-2.72786200	0.08129800
H	-3.13751100	-3.35397200	0.86781800
H	-2.58844600	-3.18925600	-0.89583800



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C	2.99416200	0.02157500	0.22505400
C	3.26299700	0.73350500	-0.95693500
C	4.57160400	1.04397400	-1.32623600
C	5.64216900	0.64434300	-0.52679500
C	5.39258300	-0.07349600	0.64459000
C	4.08615100	-0.38592200	1.01183600
H	2.44712800	1.07207100	-1.58793100
H	4.75221300	1.60295900	-2.23978600
H	6.66108400	0.88322700	-0.81640200

H	6.21876200	-0.40321100	1.26789400
H	3.90400000	-0.97279900	1.90648600
C	0.64219200	-0.61263100	-0.48609400
H	1.02686300	-1.42024200	-1.12071000
O	-0.62995700	-1.01335600	0.05699100
N	-1.51705200	-1.25637700	-0.96417900
C	-2.76088600	-1.62262300	-0.50389700
H	-3.00253200	-2.67878100	-0.40629500
C	-3.85175700	-0.67193300	-0.31288600
C	-4.48091400	1.62070300	-0.33152100
H	-4.13802300	2.46012800	-0.94113000
H	-5.42554800	1.24421500	-0.73187900
C	-4.62559600	2.01682800	1.13014700
H	-4.98943800	1.17340900	1.72155500
H	-3.66773800	2.35103900	1.53922500
H	-5.34489900	2.83738000	1.22303200
O	-3.46080000	0.61109600	-0.50903600
O	-4.98321200	-1.01326100	-0.00196500
H	0.47430100	0.26098100	-1.12636900
C	1.60270900	-0.30566300	0.63898300
C	1.22032100	-0.34134800	1.92213700
H	0.20920500	-0.60670200	2.20427600
H	1.91131700	-0.08874500	2.71907800

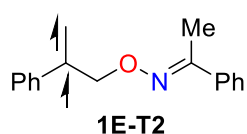


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C	3.42078900	0.00056100	0.24294800
C	3.92707300	0.29183600	-1.03587700
C	5.22021200	-0.08344400	-1.39948500
C	6.03563600	-0.76476600	-0.49628700
C	5.54375900	-1.07218200	0.77394800
C	4.25155100	-0.69997200	1.13566100
H	3.31909800	0.83559900	-1.75208900
H	5.59054700	0.16143400	-2.39077700
H	7.04120200	-1.05994500	-0.78076100
H	6.16361100	-1.61585200	1.48114300
H	3.86626700	-0.97315900	2.11285100

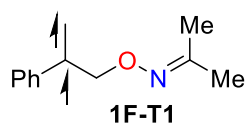
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C	1.73967500	0.75856200	1.90263400
H	0.72699400	1.02239700	2.18045900
H	2.49933300	0.80276600	2.67564400
C	1.00649500	0.38581800	-0.44862200
H	0.98916100	-0.59324500	-0.94521400
O	-0.29259400	0.65760300	0.09941000
N	-1.19317100	0.91876300	-0.92587800
C	-2.45178400	1.19757600	-0.36490200
C	-3.40798400	0.14868700	-0.20297900
C	-3.09005000	-1.19565200	-0.54363500
C	-4.71135000	0.40592700	0.30360100
C	-4.01967200	-2.21163800	-0.38389200
H	-2.10459200	-1.41612300	-0.93896700
C	-5.63204200	-0.62133400	0.46090800
H	-4.99018300	1.41763300	0.57863700
C	-5.29780200	-1.93676400	0.11977300
H	-3.75156600	-3.22946500	-0.65321500
H	-6.62021200	-0.39799900	0.85346200
H	-6.02201700	-2.73601900	0.24387100
H	1.21456300	1.13838500	-1.21823000
C	-2.72426300	2.63938500	-0.03295400
H	-3.65188800	2.99935300	-0.49436400
H	-2.81930800	2.79292100	1.05118200
H	-1.90376500	3.26665900	-0.38796000



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C	-3.09600700	-0.07838600	-0.18760100
C	-3.58481500	0.95468800	0.66461000
C	-4.81575900	0.84572600	1.29521300
C	-5.61886900	-0.28616300	1.11122600
C	-5.16458200	-1.31665100	0.27873600
C	-3.93655800	-1.21856900	-0.35597500
H	-2.99218200	1.84625200	0.83382800
H	-5.15631800	1.65138000	1.93965500
H	-6.58096700	-0.36373000	1.60815300

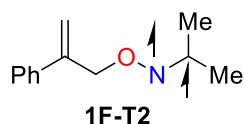
H	-5.77678800	-2.20133900	0.12721900
H	-3.59258100	-2.02296400	-0.99907300
C	-0.92258700	1.17522600	-0.79029000
H	-1.21773300	1.89980000	-0.02677400
O	0.40377800	0.69831500	-0.49654800
N	1.26757400	1.79965500	-0.48629900
C	2.48810700	1.51711500	-0.17860500
C	3.07609300	0.17985000	0.10691600
C	2.64091500	-0.98887400	-0.54525400
C	4.14395700	0.07339800	1.01600900
C	3.25245200	-2.21411800	-0.28931700
H	1.82718300	-0.92849400	-1.25507000
C	4.74124800	-1.15683300	1.28365700
H	4.50666500	0.95714600	1.52997700
C	4.29899300	-2.30678300	0.62969800
H	2.90754200	-3.10245800	-0.81078000
H	5.55573700	-1.21441600	1.99986200
H	4.76719000	-3.26571500	0.83187700
H	-0.89582200	1.70352800	-1.75614300
C	3.38846200	2.73104400	-0.12470400
H	3.73830800	2.92663500	0.89531300
H	4.27481800	2.59185400	-0.75260400
H	2.83625000	3.60745900	-0.46678100
C	-1.83741400	-0.01712000	-0.86479600
C	-1.38560300	-1.10778400	-1.73957800
H	-1.59199600	-1.09762500	-2.80882200
H	-0.72073800	-1.88601000	-1.37303300



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C	1.73622500	0.37496400	-0.11717000
C	1.42540400	-0.93197700	-0.59043700
C	2.36079700	-1.95496000	-0.53124800
C	3.63577200	-1.72841800	0.00199100
C	3.96158000	-0.45492500	0.48490300
C	3.03478200	0.57530600	0.43043800
H	0.43369500	-1.13679500	-0.97675500

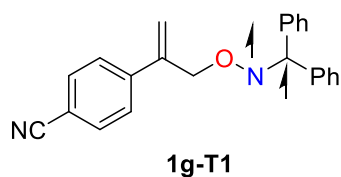
H	2.09617800	-2.94288400	-0.89798400
H	4.36281600	-2.53374100	0.04495300
H	4.94664500	-0.26979900	0.90422300
H	3.29408800	1.56150800	0.80391300
C	-0.54904500	1.25960400	-0.84253700
H	-0.45582300	0.75188100	-1.81229600
O	-1.37250400	0.45691500	0.02660900
N	-2.61978600	0.25064400	-0.60372300
C	-3.41007200	-0.42262700	0.15064800
H	-1.03784900	2.22479200	-1.01378500
C	0.79701300	1.45271400	-0.18930500
C	1.08694500	2.77316800	0.38051600
H	1.51304800	3.57525100	-0.21993400
H	0.77658400	3.03140900	1.39161800
C	-4.77411400	-0.72007000	-0.40715700
H	-5.55576500	-0.30359900	0.24011500
H	-4.88010900	-0.29837900	-1.40826500
H	-4.94439100	-1.80268200	-0.45638100
C	-3.04370400	-0.91573800	1.52639000
H	-2.19009300	-1.59969700	1.47207600
H	-2.72776900	-0.07964400	2.15824900
H	-3.88221400	-1.42968900	2.00125200



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C	0.57535200	1.83134200	0.60854000
H	0.63393400	1.54410900	1.66369000
O	1.42877300	0.93730800	-0.13366400
H	0.97685200	2.84501500	0.50687800
C	-0.83949900	1.77909300	0.08147100
C	-1.54472600	0.46980100	0.07203600
C	-2.57480500	0.21592100	-0.85101600
C	-1.21198400	-0.54748500	0.98357500
C	-3.26826300	-0.99162600	-0.84242800
H	-2.81663500	0.96529300	-1.59808300
C	-1.90692000	-1.75658800	0.99252100
H	-0.40154500	-0.40093800	1.68897500

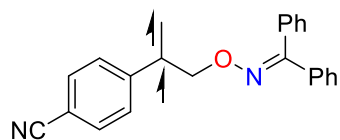
C	-2.94090300	-1.98357100	0.08398700
H	-4.05775400	-1.16305800	-1.56861800
H	-1.63673400	-2.52350600	1.71285800
H	-3.47820000	-2.92737900	0.08916900
C	-1.42355200	2.91919200	-0.31877100
H	-2.46367000	2.96094800	-0.62401000
H	-0.87651500	3.85686900	-0.33057100
N	2.14302800	0.08947000	0.73552400
C	2.96785800	-0.74616900	-0.01320900
C	4.30690300	-0.22693400	-0.44165000
H	5.03145500	-1.04130600	-0.55410100
H	4.24563600	0.28996100	-1.41384900
H	4.69797200	0.49296500	0.28352000
C	2.37317700	-1.98179300	-0.61806700
H	3.11951100	-2.77945300	-0.70778100
H	1.53450200	-2.34693200	-0.01874900
H	1.98398200	-1.78443700	-1.63060300



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C	-3.35370600	-0.06712600	0.26312100
C	-3.82059400	0.79726200	-0.74401200
C	-5.18110200	0.99733400	-0.94923100
C	-6.11855500	0.33846900	-0.13862600
C	-5.66857100	-0.51960600	0.87916500
C	-4.30730300	-0.70931500	1.07515200
H	-3.11850000	1.30487600	-1.39667700
H	-5.52447000	1.65829100	-1.73776600
H	-6.38977400	-1.02001300	1.51643900
H	-3.96905200	-1.34887500	1.88344900
C	-1.90147500	-0.29747100	0.48170400
C	-1.41540000	-1.49092200	0.84500200
H	-0.35716900	-1.63589900	1.02258100
H	-2.06332000	-2.35459200	0.95016300
C	-1.00012800	0.90899600	0.29978500
H	-1.29731500	1.70586800	0.99183400

O	0.37496200	0.62159900	0.58950500
H	-1.05119400	1.30324500	-0.71984900
N	1.09706700	0.46132700	-0.59139500
C	2.43203600	0.12118900	-0.27118400
C	2.74503600	-1.29810400	-0.24397800
C	1.90213900	-2.22607400	-0.90639100
C	3.84943400	-1.81474600	0.47721000
C	2.16735600	-3.58950400	-0.86743600
H	1.05010700	-1.85331800	-1.46406400
C	4.10418100	-3.18126800	0.51261300
H	4.48155800	-1.13875800	1.04153700
C	3.27162000	-4.07842100	-0.16251300
H	1.51240600	-4.27675200	-1.39547700
H	4.95164900	-3.55082400	1.08298100
H	3.47624000	-5.14431200	-0.13349400
C	3.37787900	1.21167600	-0.11682500
C	4.75704700	1.06074200	-0.40767300
C	2.92844600	2.49854700	0.27232300
C	5.63666400	2.12936000	-0.28113900
H	5.12470500	0.10728200	-0.76868500
C	3.81558900	3.56023800	0.39681200
H	1.87883800	2.64432500	0.49766500
C	5.17644400	3.38461100	0.12741600
H	6.68719000	1.98656300	-0.51788200
H	3.44530100	4.53258800	0.70903400
H	5.86691400	4.21683300	0.22483300
C	-7.52217900	0.54457400	-0.34255400
N	-8.66177500	0.71124900	-0.50790700

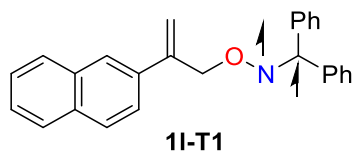


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C	-3.44516000	0.04558600	0.44059900
C	-3.80341700	-1.24333500	-0.06041000
C	-5.09394900	-1.52894100	-0.46098700
C	-6.10337900	-0.54569300	-0.38589800
C	-5.77713300	0.73658600	0.10664100
C	-4.48831800	1.01983400	0.50901400

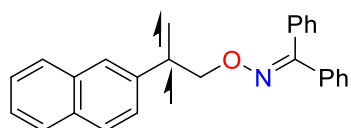
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H	-5.34104200	-2.51587600	-0.83772400
H	-6.54921000	1.49643500	0.16642200
H	-4.24750500	2.00810700	0.88714200
C	-0.99670500	-0.61120300	0.85761900
H	-1.15987400	-1.43753200	0.15868000
O	0.19175900	0.09647100	0.48042500
N	1.25932900	-0.80648600	0.48302300
C	2.38241600	-0.26864000	0.13615500
C	2.58030400	1.17761900	-0.17723100
C	2.15606000	2.17985300	0.70907900
C	3.21323000	1.55309900	-1.37198400
C	2.36450100	3.52402000	0.40641900
H	1.66264400	1.89955400	1.63254100
C	3.40523100	2.89941100	-1.68075100
H	3.55037300	0.78570100	-2.06184400
C	2.98480900	3.88830900	-0.79069000
H	2.04106300	4.28914400	1.10624600
H	3.88740400	3.17428500	-2.61419300
H	3.14114100	4.93683700	-1.02665800
C	3.53523500	-1.20707200	0.05238300
C	3.32651600	-2.57569400	-0.19401200
C	4.84943500	-0.74995500	0.24170900
C	4.40116900	-3.45807200	-0.24432700
H	2.31360000	-2.93017500	-0.34747400
C	5.92413000	-1.63745100	0.19106800
H	5.02886500	0.30156400	0.43814900
C	5.70521000	-2.99312100	-0.05280600
H	4.22289100	-4.51109500	-0.44220100
H	6.93335400	-1.26692500	0.34511900
H	6.54307900	-3.68264400	-0.09790600
H	-0.85101100	-1.04764800	1.85915700
C	-2.13073200	0.38159700	0.87107000
C	-1.81915200	1.70349500	1.43059400
H	-1.86406700	1.87793800	2.50444400
H	-1.33949000	2.46730600	0.82470300
C	-7.43623400	-0.84471000	-0.80122000
N	-8.52398600	-1.08826200	-1.14015600



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C	-1.76738300	-0.63481800	-0.40557800
C	-1.45079200	-0.85473100	-1.68538100
H	-0.43619200	-0.72911100	-2.04544500
H	-2.20534600	-1.17031400	-2.39850600
C	-0.75515200	-0.20207200	0.62760700
H	-0.70415300	-0.91449900	1.45868200
O	0.55053600	-0.08979500	0.03756600
H	-1.03731300	0.77205600	1.05059300
N	1.52360900	-0.13754500	1.02255900
C	2.79294900	0.03597600	0.42180500
C	3.29889100	1.39523500	0.36359000
C	2.73660100	2.39880000	1.19264300
C	4.31133100	1.79002900	-0.54591100
C	3.18308900	3.71242700	1.13239900
H	1.95914500	2.12019800	1.89554900
C	4.74843700	3.10872400	-0.60157100
H	4.72172600	1.06271900	-1.23678000
C	4.19516500	4.07860400	0.23923800
H	2.74269600	4.45753300	1.78899000
H	5.51786700	3.38524500	-1.31695700
H	4.54150100	5.10664600	0.19324800
C	3.50369500	-1.16800500	0.02777200
C	4.91887300	-1.24362100	0.02243800
C	2.78448000	-2.34400400	-0.30313000
C	5.57213900	-2.41957600	-0.32798700
H	5.49980100	-0.38251200	0.33175400
C	3.44657700	-3.51388800	-0.65388200
H	1.70122300	-2.31721900	-0.30362900
C	4.84393600	-3.56128100	-0.67489500
H	6.65800500	-2.45067100	-0.31569800
H	2.86960500	-4.39640900	-0.91556000
H	5.35803400	-4.47782800	-0.94804500
C	-3.15334200	-0.80149000	0.13392800
C	-4.22744500	0.06659200	-0.26114300

C	-3.39900500	-1.80634800	1.05419000
C	-4.05608900	1.15008300	-1.16754600
C	-5.53339800	-0.15124900	0.29549300
C	-4.68632900	-2.01690100	1.59662300
H	-2.58818300	-2.46649200	1.34977800
C	-5.11283200	1.96167700	-1.51400600
H	-3.07293800	1.33033100	-1.58684400
C	-6.60267900	0.70175400	-0.09067600
C	-5.73249500	-1.20772800	1.22253600
H	-4.84209700	-2.82456800	2.30552000
C	-6.40162200	1.73460500	-0.97593900
H	-4.95669000	2.78449900	-2.20554000
H	-7.58741600	0.52244300	0.33304800
H	-6.72683400	-1.36319100	1.63270400
H	-7.22758900	2.37955400	-1.26099700

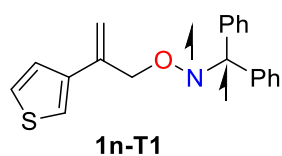


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C	0.46722400	-1.91717600	-0.35442000
H	0.43188600	-2.35895900	0.64992200
O	-0.40728200	-0.76627900	-0.39202300
N	-1.72161900	-1.20780300	-0.21107800
C	-2.58924500	-0.25040500	-0.16411200
C	-2.28935200	1.20352600	-0.31644500
C	-1.48197500	1.68407700	-1.35954900
C	-2.82954400	2.12260600	0.59756900
C	-1.22865400	3.04835200	-1.48542300
H	-1.05192100	0.98378800	-2.06524400
C	-2.56108000	3.48548300	0.47926000
H	-3.45795400	1.76356200	1.40658200
C	-1.76285800	3.95281100	-0.56551200
H	-0.60770700	3.40565600	-2.30170800
H	-2.97877700	4.18126600	1.20108200
H	-1.55774900	5.01495400	-0.66279200
C	-3.99267100	-0.69301400	0.07460200
C	-4.25609400	-1.88073800	0.77919000
C	-5.07696600	0.04750000	-0.42324400

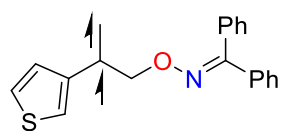
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H	-3.42104100	-2.45241300	1.16801600
C	-6.38666700	-0.38956300	-0.22551900
H	-4.89291100	0.96305900	-0.97516100
C	-6.63594900	-1.56970900	0.47493600
H	-5.74932800	-3.23029900	1.52812300
H	-7.21231200	0.19348800	-0.62317700
H	-7.65633300	-1.90643100	0.63329600
H	0.09279600	-2.66180500	-1.06317400
C	1.87113700	-1.49012600	-0.73260300
C	2.24496100	-1.84975600	-2.10538100
H	2.57995500	-2.85586000	-2.35425200
H	1.96741400	-1.21057700	-2.94242700
C	2.67991400	-0.78818800	0.20324300
C	4.09260200	-0.44679700	-0.00466000
C	2.09588600	-0.38090000	1.43274000
C	4.81878700	-0.77229400	-1.17427000
C	4.80333900	0.24793500	1.03214700
C	2.81043600	0.29674900	2.42292000
H	1.04143000	-0.56044700	1.59630500
C	6.15213900	-0.43923400	-1.32916000
H	4.31065900	-1.29568200	-1.97675100
C	6.17156800	0.57606900	0.84904100
C	4.14351100	0.60690100	2.23987100
H	2.30300900	0.58557100	3.33873200
C	6.84067600	0.24228300	-0.30787700
H	6.66862000	-0.70752700	-2.24617000
H	6.68561400	1.10194600	1.64944300
H	4.70422400	1.13284400	3.00741100
H	7.88794800	0.50153100	-0.43237300



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C	2.56118900	0.16415500	0.74532500
C	2.15376200	0.55339700	1.96180200
H	1.10096400	0.61348400	2.20523500
H	2.85731400	0.82132500	2.74161600

C	1.57097000	-0.19329400	-0.33837600
H	1.72525700	-1.22564700	-0.67886800
O	0.22768500	-0.06964600	0.15405600
H	1.68339300	0.46459400	-1.20818600
N	-0.66523000	-0.10141000	-0.90430500
C	-1.98337900	-0.03287100	-0.39393300
C	-2.57433900	1.28875100	-0.27574600
C	-3.96831200	1.50853700	-0.40678000
C	-1.74753200	2.42514500	-0.09019400
C	-4.50267700	2.78903900	-0.32236700
H	-4.62328700	0.66976600	-0.61224000
C	-2.29130600	3.70075800	-0.00547600
H	-0.67744000	2.28777300	0.01048000
C	-3.67184300	3.89402200	-0.11527400
H	-5.57423800	2.92836600	-0.43440200
H	-1.63464900	4.55214600	0.14976900
H	-4.09312700	4.89262400	-0.05006100
C	-2.64763100	-1.29991800	-0.14846100
C	-3.75748900	-1.41743400	0.72475000
C	-2.15441200	-2.48866400	-0.74344100
C	-4.35085000	-2.65154800	0.96538200
H	-4.12336200	-0.53923800	1.24400400
C	-2.75665700	-3.71608200	-0.49994400
H	-1.30485100	-2.42309900	-1.41421500
C	-3.86204000	-3.80847600	0.35193800
H	-5.19339100	-2.71362700	1.64839400
H	-2.36532600	-4.60854400	-0.98014000
H	-4.33026200	-4.76958800	0.54153800
S	6.14721900	-0.29966600	-1.02508800
C	4.42117500	-0.24375000	-0.91122900
C	3.98226100	0.05032500	0.36170200
C	5.09340300	0.22774600	1.26148000
C	6.30699900	0.07260900	0.66334900
H	3.83150800	-0.42529600	-1.79814600
H	4.98600500	0.45315900	2.31515500
H	7.28736900	0.14883000	1.11212500

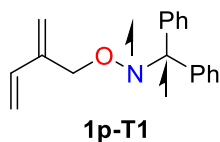


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C	-1.39090000	-1.53402300	1.31235900
H	-1.38424300	-2.34399400	0.57196700
O	-0.49716400	-0.49093900	0.85822500
H	-1.02055700	-1.93542800	2.26213000
S	-4.38663700	-0.43920200	-2.13801300
C	-3.15834500	-0.87317300	-1.00111300
C	-3.55630800	-0.66563200	0.32532800
C	-4.90359000	-0.12957600	0.37124500
C	-5.46692200	0.03876600	-0.85149900
H	-2.20372200	-1.23533200	-1.35293700
H	-5.40663700	0.10533000	1.30181800
H	-6.45427400	0.40997000	-1.08860700
N	0.72715100	-1.07106800	0.51887000
C	1.64259100	-0.21070400	0.21174300
C	1.47134300	1.27153700	0.18129300
C	0.36661200	1.87687800	-0.43928400
C	2.43948900	2.09160900	0.78396200
C	0.24122300	3.26456300	-0.46018700
H	-0.39467200	1.25804100	-0.89806900
C	2.30277500	3.47884100	0.77647900
H	3.29924800	1.63600200	1.26497200
C	1.20473900	4.06988400	0.15007100
H	-0.61539000	3.71742300	-0.95081300
H	3.05604800	4.09670600	1.25654700
H	1.10017100	5.15095100	0.13728500
C	2.96778400	-0.80686500	-0.12240700
C	3.83645500	-0.17360900	-1.02593200
C	3.35921400	-2.03512700	0.43843900
C	5.05948400	-0.75404600	-1.36172500
H	3.54818200	0.77137500	-1.47386900
C	4.58074400	-2.61117800	0.10221000
H	2.69201900	-2.52455200	1.13889700
C	5.43720300	-1.97318400	-0.79902300
H	5.71561800	-0.25225000	-2.06704100

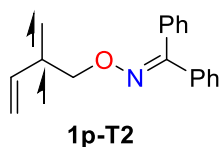
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H	6.39214000	-2.42187400	-1.05677100
C	-2.76606100	-0.94395600	1.47603200
C	-3.23280000	-0.61583400	2.82716900
H	-2.97799000	0.33264700	3.29709000
H	-3.75083000	-1.34628700	3.44647300



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C	5.18732800	0.11993300	0.26107700
C	5.66854500	0.45891100	-0.94281200
H	5.03016800	0.68033700	-1.79280400
C	3.77403100	-0.00825900	0.63375600
C	3.42137300	-0.36260500	1.87949300
H	2.38416800	-0.45754300	2.17471700
H	4.17829300	-0.56207800	2.63204700
C	2.75569900	0.27671000	-0.44154500
H	2.87856700	-0.40418200	-1.29178800
O	1.42793500	0.12161500	0.08558700
H	2.86615400	1.30164500	-0.81877900
N	0.50767000	0.11275400	-0.94887100
C	-0.79368800	0.01230900	-0.40172800
C	-1.48773800	1.26355300	-0.15510100
C	-1.05166800	2.45520400	-0.78746800
C	-2.56941600	1.36398600	0.75462200
C	-1.68218500	3.66846200	-0.54414400
H	-0.22397500	2.40258100	-1.48615400
C	-3.19130200	2.58413500	0.99482400
H	-2.88975600	0.48497200	1.30183000
C	-2.75956800	3.74357300	0.34449300
H	-1.33505100	4.56321900	-1.05320600
H	-4.01092700	2.63364100	1.70616800
H	-3.24989400	4.69366100	0.53382700
C	-1.34188600	-1.32341400	-0.24675000
C	-2.73285100	-1.58455100	-0.32492100
C	-0.47669800	-2.43347800	-0.07647600
C	-3.22672600	-2.87828100	-0.20441700

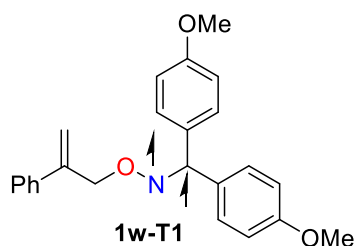
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C	-0.98012700	-3.72257500	0.04430300
H	0.59186600	-2.26447400	-0.01634000
C	-2.35761800	-3.95635200	-0.01294100
H	-4.29716100	-3.04942500	-0.27581800
H	-0.29414200	-4.55284000	0.18669300
H	-2.74745600	-4.96543100	0.08050900
H	5.89038800	-0.08843100	1.06604000
H	6.73710100	0.52615500	-1.11762500



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C	4.94338900	-1.07083300	0.41857100
C	4.99064400	-2.06280500	1.37869000
H	4.13906800	-2.68714600	1.62502400
C	2.53437800	-1.41032900	-0.34974100
H	2.46873500	-2.13102400	0.47117600
O	1.50980800	-0.41214200	-0.19356100
N	0.26608200	-1.03933200	-0.25372800
C	-0.72739500	-0.22742500	-0.09515000
C	-0.60848600	1.25065700	0.07936600
C	0.14379400	2.03259700	-0.81107300
C	-1.26651900	1.88326900	1.14524700
C	0.22983400	3.41274900	-0.63931300
H	0.66169200	1.55290400	-1.63346600
C	-1.16550400	3.26247500	1.32489500
H	-1.85458300	1.28857200	1.83739300
C	-0.42020400	4.03162500	0.43063700
H	0.80778300	4.00672400	-1.34148900
H	-1.67273900	3.73530100	2.16079500
H	-0.34678500	5.10689800	0.56518300
C	-2.07238100	-0.86704500	-0.08905400
C	-2.21974400	-2.21676800	0.27752200
C	-3.21516200	-0.14681200	-0.47293000
C	-3.47110000	-2.82469400	0.25558600
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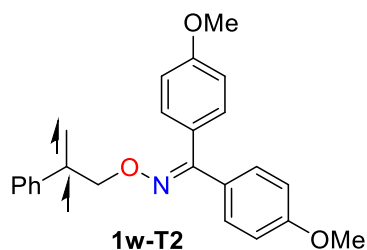
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H	-5.33972700	-0.18724100	-0.79813900
H	-5.57857300	-2.57386000	-0.14009300
H	2.35508500	-1.95293800	-1.28968800
C	3.86103700	-0.69922700	-0.39208900
C	3.99230900	0.39502200	-1.36599600
H	4.27508700	0.19895300	-2.39885300
H	3.65727600	1.40086800	-1.12650200
H	5.85822000	-0.50123900	0.25949700
H	5.90334100	-2.24252900	1.93549400



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C	-4.85220800	-0.10838900	0.30330900
C	-5.33963800	-0.76000600	-0.84310300
C	-6.69519100	-0.72241100	-1.16916900
C	-7.59467000	-0.02678800	-0.36162500
C	-7.12484200	0.63575200	0.77418500
C	-5.77092600	0.60009600	1.09812500
H	-4.66329300	-1.32227700	-1.47925700
H	-7.04769800	-1.24191100	-2.05556700
H	-8.64947200	0.00518100	-0.61782100
H	-7.81283900	1.19353500	1.40307700
H	-5.40961500	1.14508500	1.96445400
C	-3.41071400	-0.14986100	0.67090400
C	-2.99301800	-0.17447000	1.94344400
H	-1.93885300	-0.18070400	2.19073000
H	-3.70105000	-0.20615900	2.76476500
C	-2.43677800	-0.14870700	-0.48501000
H	-2.62557000	0.70115200	-1.15246900
O	-1.09109400	-0.06990000	0.00958300
H	-2.52640500	-1.06167800	-1.08694100
N	-0.19939700	-0.04806300	-1.05409900

C	1.11924300	0.00268900	-0.53820000
C	1.79316200	-1.26897500	-0.36907600
C	1.30818200	-2.43334900	-1.02420200
C	2.90797800	-1.43814600	0.48385200
C	1.91350000	-3.66429900	-0.85807000
H	0.45194000	-2.34258200	-1.68339600
C	3.52130600	-2.67622700	0.65791000
H	3.27602500	-0.59305900	1.05414400
C	3.03207300	-3.80108800	-0.01811100
H	1.54385300	-4.54512800	-1.37306000
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C	3.08320400	1.56917300	-0.44382200
C	0.86183200	2.44005100	-0.08316500
C	3.61689900	2.84432200	-0.27806100
H	3.75318600	0.75620000	-0.69913100
C	1.38470800	3.70897100	0.08176500
H	-0.20763300	2.29131600	0.00615400
C	2.76994100	3.92683600	-0.00721000
H	4.68645100	2.98523600	-0.38072300
H	0.74077300	4.55791800	0.28744700
O	3.18272300	5.21431300	0.17606400
O	3.55598400	-5.05755000	0.07526500
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H	5.14386600	4.94109800	0.84422300
H	4.96994300	5.25694000	-0.90633900
C	4.68239000	-5.25445400	0.91532600
H	4.45436000	-5.01393200	1.96160600
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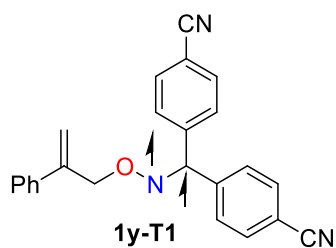


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C	-6.96419600	-0.90051800	-0.33810800
C	-5.83414400	-0.55545300	0.38606300
H	-3.63014000	-2.75444100	-1.03016100
H	-5.63246300	-3.34631500	-2.29084300
H	-7.79206000	-2.17859500	-1.87534600
H	-7.90042200	-0.38253700	-0.14926500
H	-5.88791100	0.22812700	1.13578200
C	-2.09874700	-1.48819500	0.82827500
H	-2.04983700	-2.22814100	0.02454900
O	-1.12075100	-0.46064500	0.58543400
N	0.14413700	-1.05828400	0.54657800
C	1.10128100	-0.21842300	0.31397700
C	0.94356900	1.25643200	0.17594800
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C	1.56476900	1.93584300	-0.87907500
C	0.06506000	3.38579800	0.95628100
H	-0.30800600	1.50981800	1.91465000
C	1.43620300	3.31672000	-1.03872300
H	2.15652300	1.37725000	-1.59752100
C	0.68447300	4.04995900	-0.11413600
H	-0.50788400	3.97287200	1.66647700
H	1.92397300	3.80209000	-1.87528600
C	2.45035200	-0.83002500	0.17708300
C	2.59758000	-2.15246100	-0.26621800
C	3.61565000	-0.11837900	0.51855500
C	3.85027100	-2.75400800	-0.36550500
H	1.70927400	-2.71214700	-0.53687200
C	4.86969400	-0.70509400	0.42436700
H	3.53474400	0.90365400	0.87278800
C	4.99812400	-2.02887900	-0.01891200
H	3.92131100	-3.77525000	-0.72041100
H	5.76757000	-0.15902400	0.69414800
H	-1.84047500	-2.00118000	1.76738900
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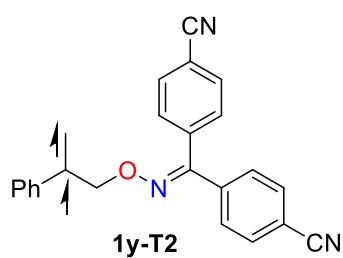
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C	1.09495100	6.12548300	-1.22434300
H	0.72105300	5.79390900	-2.20127400
H	0.81778300	7.16909700	-1.06946100
H	2.18869700	6.03685000	-1.21028900
C	6.46089100	-3.85286200	-0.51220900
H	6.10303900	-4.00431000	-1.53862200
H	7.53661900	-4.03091800	-0.47804200
H	5.95570200	-4.56580300	0.15163000



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C	-4.63092700	-0.13941900	0.28370000
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C	-6.45490800	-0.76412800	-1.20666000
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C	-6.90686300	0.61292000	0.71900700
C	-5.55746400	0.57792100	1.06100400
H	-4.42157000	-1.37245400	-1.48487600
H	-6.79736500	-1.29143400	-2.09219500
H	-8.41400100	-0.02766400	-0.68682400
H	-7.60198000	1.17719500	1.33381700
H	-5.20670900	1.12996000	1.92717900
C	-3.19447700	-0.17893400	0.67027500
C	-2.21172100	-0.18578200	-0.47744400
H	-2.39588800	0.65332400	-1.15834400
O	-0.86603800	-0.08520300	0.03126200
H	-2.28014800	-1.10878500	-1.06543900
N	0.03169100	-0.05365200	-1.01187900
C	1.34470600	0.01514500	-0.48907300
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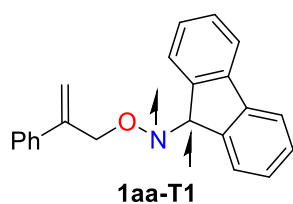
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C	3.73247700	-2.60825600	0.81059200
H	3.47863500	-0.51891300	1.15488000
C	3.25856400	-3.75743200	0.15014800
H	1.78220000	-4.53228400	-1.22255100
H	4.56701000	-2.69337000	1.49833400
C	1.91745200	1.33506200	-0.32191500
C	3.31163500	1.57753100	-0.42369100
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C	3.83012000	2.85458800	-0.28902700
H	3.98352700	0.75832600	-0.64981500
C	1.58499400	3.73016600	0.02522700
H	0.00037000	2.29870500	-0.03660300
H	4.89797900	3.02205500	-0.37994900
H	0.92232600	4.57089100	0.20027200
C	2.97416700	3.94736600	-0.05443500
C	-2.78933300	-0.19378300	1.94686900
C	3.50913200	5.26611100	0.08962600
C	3.88831400	-5.02402900	0.36263100
N	3.94433700	6.33941500	0.20793000
N	4.40123400	-6.05487300	0.53482900
H	-1.73895500	-0.19727000	2.20997600
H	-3.50675200	-0.21909200	2.75985100



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C	-3.92467800	-1.55455400	0.06861400
C	-3.43144600	-1.38767300	-1.25684400
C	-4.27810300	-1.02424100	-2.29397700
C	-5.64175200	-0.80803800	-2.06012600
C	-6.14922600	-0.95492600	-0.76321400
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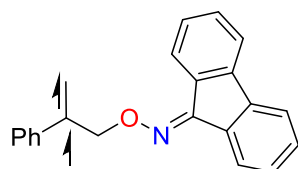
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H	-5.71110600	-1.43201400	1.28428400
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H	-1.49230400	-2.91909900	0.03856900
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C	1.06245400	1.92387500	-0.82679200
C	-0.54919500	2.95189600	1.20720900
H	-0.40212100	1.00949400	2.10261900
C	0.61668700	3.23847900	-0.90471000
H	1.69038100	1.52581100	-1.61717200
C	-0.19116300	3.76252300	0.11695100
H	-1.17157800	3.35954500	1.99630500
H	0.89022400	3.86296300	-1.74815400
C	2.63010200	-0.60432400	0.08367300
C	3.03109400	-1.86601900	-0.39335000
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C	4.37336300	-2.16414400	-0.57621600
H	2.27214600	-2.60583200	-0.61830400
C	4.96673300	0.06201300	0.18994200
H	3.33300800	1.32728000	0.74842400
C	5.35511900	-1.19938500	-0.28688800
H	4.67292400	-3.13727400	-0.95014600
H	5.72222600	0.80532400	0.42022200
H	-1.19888100	-2.79105200	1.78612400
C	-3.07792300	-1.94675000	1.15430900
C	-3.57109400	-2.02405400	2.53461100
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H	-3.48789800	-1.17783100	3.21436400
C	-0.64704100	5.12042000	0.04898100
C	6.74265800	-1.50123700	-0.48197700
N	-1.01527100	6.22257100	-0.00539400
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C	4.30161000	0.08670800	0.25202500
C	4.78201900	0.25296600	-1.05873100
C	6.13560600	0.09184300	-1.35393900
C	7.03994100	-0.24597000	-0.34759400
C	6.57705600	-0.42654100	0.95747300
C	5.22514800	-0.26856500	1.25137400
H	4.10217300	0.53146800	-1.85789900
H	6.48250700	0.23438000	-2.37328000
H	8.09325600	-0.37467500	-0.57809400
H	7.26897700	-0.70486600	1.74718100
H	4.87002200	-0.44447500	2.26174600
C	2.86178300	0.26781400	0.58048500
C	1.88764800	-0.12768300	-0.50576100
H	2.08807000	-1.14917100	-0.85359400
O	0.54108200	-0.06308400	-0.00576600
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C	-2.11357400	2.48606100	-0.43880500
C	-3.74792100	0.72393200	0.08052900
C	-3.09333100	3.43492300	-0.14440900
H	-1.11880200	2.78934700	-0.75013800
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H	-2.86026100	4.49229900	-0.22694800
H	-5.70987100	1.39127000	0.68439600
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C	-3.77645500	-0.74325700	0.09763700
C	-2.21314000	-2.57976800	-0.37959900
C	-4.77612500	-1.65519400	0.41022400
C	-3.22952100	-3.48216400	-0.06416900
H	-1.23164900	-2.92951500	-0.68428900

H	-5.76336400	-1.31827300	0.71427800
H	-3.03828700	-4.54952000	-0.12214100
C	-4.49621000	-3.02698100	0.32697900
C	2.44236400	0.74219100	1.76089400
H	-5.27278500	-3.74658200	0.56865900
H	-5.12396000	3.79411500	0.48221300
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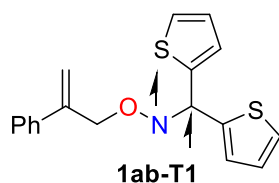


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C	-5.83327900	0.72991200	-0.35947600
C	-5.06837700	-0.09080600	0.45534800
H	-2.34517700	-0.45018500	-1.58070500
H	-3.72302900	0.98243900	-3.01797800
H	-5.96059500	1.76158300	-2.25555000
H	-6.80603400	1.07111000	-0.01657500
H	-5.44173000	-0.39048600	1.43004800
C	-1.70789300	-1.99331800	0.41450500
H	-1.77613400	-2.39018900	-0.60686400
O	-0.71636800	-0.93644900	0.43105200
N	0.52730700	-1.47580500	0.12305900
C	1.46175200	-0.58703700	0.10160800
C	1.46390500	0.87546800	0.32767800
C	0.43859400	1.76936700	0.63545400
C	2.79784700	1.33377700	0.17477800
C	0.75457200	3.12417700	0.79024900
H	-0.57888800	1.41991200	0.74974100
C	3.10103800	2.68254900	0.33130700
C	2.06870200	3.57506000	0.64075300
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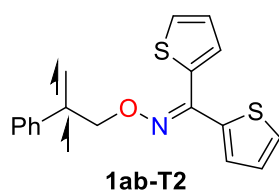
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C	4.78547500	-2.29995200	-0.71789000
H	2.78075300	-3.10236000	-0.50910800
C	5.03205300	0.09889800	-0.38776400
C	5.58651400	-1.15326700	-0.67317700
H	5.23691500	-3.26201400	-0.94121000
H	5.66263800	0.98282500	-0.35498300
H	-1.37024200	-2.79829600	1.07348900
C	-3.02226700	-1.42678300	0.88405000
C	-3.45954900	-1.77899700	2.23980200
H	-4.03633200	-2.68076000	2.43816400
H	-3.12450400	-1.21140800	3.10619900
H	2.29237100	4.63068000	0.76543000
H	6.65278800	-1.23637500	-0.86235900



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C	-4.07264300	-0.08789300	-0.25064600
C	-4.52856800	1.17913800	0.15296500
C	-5.87209500	1.39391300	0.45927300
C	-6.78954600	0.34664700	0.37625400
C	-6.35080500	-0.92007000	-0.01388200
C	-5.00857000	-1.13516500	-0.31744200
H	-3.83920000	2.01587300	0.20606200
H	-6.20148800	2.38446500	0.75929100
H	-7.83478200	0.51387200	0.61855200
H	-7.05330300	-1.74662700	-0.07009000
H	-4.66922600	-2.12940300	-0.59054000
C	-2.64578100	-0.33427100	-0.59610800
C	-1.62949700	0.37023300	0.27263500
H	-1.72329700	0.06268100	1.32018500
O	-0.29689800	0.06795300	-0.17777100
H	-1.75569000	1.45922100	0.23684700
N	0.60731600	0.26547400	0.84211200

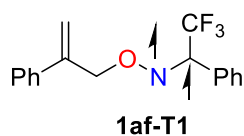
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H	-1.23539900	-1.33196500	-1.81927400
C	1.91513700	0.03446900	0.31870100
C	2.34121400	-1.32173400	0.26694500
C	1.53216000	-2.44475000	0.47542600
S	4.00876200	-1.84460800	-0.00755300
C	2.22887700	-3.67119900	0.40446600
H	0.46994600	-2.35979200	0.66045500
C	3.56820800	-3.51760800	0.14582900
H	1.75741100	-4.63831200	0.53656500
H	4.32309700	-4.28289700	0.03157500
C	2.66745700	1.20341900	0.01894400
C	3.92666800	1.37239100	-0.56219500
S	1.96953200	2.78643000	0.40029700
C	4.30944500	2.72781200	-0.69255000
H	4.53345300	0.55019100	-0.91650500
C	3.36395600	3.60618100	-0.22446800
H	5.25174600	3.04335200	-1.12597300
H	3.40651200	4.68631800	-0.20918200



0 3

C	-3.52051500	-0.72115600	0.20827300
C	-3.04431800	-0.88153200	-1.12417200
C	-3.87371100	-0.65019600	-2.21203800
C	-5.20221300	-0.24879100	-2.02539800
C	-5.69090100	-0.07328800	-0.72481400
C	-4.87069500	-0.30046600	0.36993200
H	-2.01043300	-1.15972200	-1.29357200
H	-3.48290300	-0.77620900	-3.21777600
H	-5.84567800	-0.06984400	-2.88146200
H	-6.71892800	0.24203300	-0.56971300
H	-5.25553700	-0.16442900	1.37621900
C	-1.29648500	-1.51277500	1.18372800

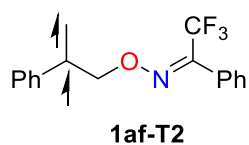
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C	1.71314300	-0.04492800	0.19525000
H	-0.90477000	-1.88140300	2.13654800
C	-2.69250500	-0.97307200	1.34869200
C	-3.15226600	-0.70433000	2.71622600
H	-3.61988700	-1.47621900	3.32516600
H	-2.93900000	0.24419200	3.20586200
C	1.46535200	1.38867900	0.00636800
C	2.26375700	2.27237700	-0.69769900
S	0.08113000	2.23915900	0.67642700
C	1.79100300	3.60965800	-0.68185000
H	3.15536800	1.95730300	-1.22321700
C	0.63306800	3.74497700	0.03824500
H	2.28677500	4.43035000	-1.18688600
H	0.05571800	4.64413400	0.20701000
C	3.07249700	-0.57282200	-0.02728500
C	4.29411800	0.01624100	0.21128800
S	3.28343300	-2.21316700	-0.60001300
C	5.39739700	-0.83925100	-0.07117100
H	4.39592100	1.02036400	0.60300800
C	5.00717300	-2.07099700	-0.52203100
H	6.43336800	-0.54899300	0.06078400
H	5.63162400	-2.90603900	-0.80848500



0 3

C	-3.87918900	0.16404200	0.24068800
C	-4.40653100	-0.72519200	-0.71191200
C	-5.74111700	-0.64336300	-1.10858200
C	-6.57767200	0.33279200	-0.56790800
C	-6.06631700	1.23042700	0.37147800
C	-4.73297200	1.15056300	0.76540700
H	-3.78232100	-1.50638400	-1.13424200
H	-6.12705100	-1.34825100	-1.83920600
H	-7.61581500	0.39813200	-0.87954600

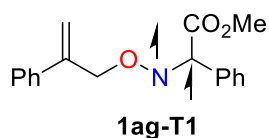
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C	-2.08176500	0.35155100	1.94060800
H	-1.04169300	0.31229500	2.23917400
H	-2.81183200	0.59997600	2.70333600
C	-1.46435300	-0.30493400	-0.38256700
H	-1.51589400	0.37994500	-1.23744400
O	-0.13016500	-0.27306600	0.15896800
N	0.78571800	-0.52486100	-0.83883100
C	2.07391000	-0.56953300	-0.28932200
C	2.90776800	0.58991800	-0.24746100
C	2.37752400	1.85421900	-0.62426200
C	4.26941000	0.53465400	0.16028500
C	3.16433400	2.99492000	-0.58846400
H	1.34365300	1.91515200	-0.94429300
C	5.04281600	1.68567500	0.19165000
H	4.70778100	-0.41118200	0.45191300
C	4.50156600	2.92196600	-0.18004800
H	2.73727600	3.94960600	-0.88105200
H	6.07979200	1.62153800	0.50771800
H	5.11494300	3.81729500	-0.15351100
H	-1.64788400	-1.31753300	-0.76022400
C	2.57246100	-1.94067700	0.08591700
F	3.07063200	-1.96694800	1.34889900
F	3.57703100	-2.36359300	-0.72369100
F	1.59073600	-2.85718900	0.02223100



0 3

C	3.32343700	-0.41908400	0.25172100
C	2.95912900	-0.37480700	-1.12472400
C	3.76365500	0.26340700	-2.05802600
C	4.95653300	0.88384000	-1.66721500
C	5.33365800	0.86015700	-0.31870000
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H	2.03142100	-0.83154600	-1.45056300

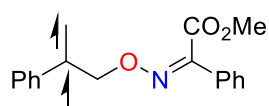
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H	5.58154500	1.38099900	-2.40264800
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H	4.83527800	0.21016400	1.66647700
C	1.25571300	-1.79529000	0.84078300
H	0.90574900	-2.44800100	1.64573000
O	0.22967400	-0.79653900	0.57610500
N	-0.90430600	-1.43510800	0.11451600
C	-1.91304500	-0.65690500	-0.06888500
C	-2.02627800	0.81079100	0.11929400
C	-0.94209300	1.66542100	-0.15158400
C	-3.24045000	1.37736400	0.54938300
C	-1.07437800	3.04319800	0.00391600
H	-0.00068000	1.25044700	-0.48513500
C	-3.36105400	2.75485700	0.71361700
H	-4.08877400	0.73958100	0.76449100
C	-2.28005700	3.59363600	0.44056800
H	-0.22882200	3.68790100	-0.21653800
H	-4.30392900	3.17208400	1.05420400
H	-2.37684500	4.66808100	0.56583700
H	1.38526000	-2.40050500	-0.06373300
C	-3.14253400	-1.41875800	-0.54961800
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F	-3.74007900	-0.76721900	-1.57053600
F	-4.06700000	-1.52860400	0.44218300
C	2.51925700	-1.07959900	1.23515200
C	2.85908800	-1.05083800	2.66251200
H	3.44299800	-1.84352800	3.12680700
H	2.44615600	-0.29224500	3.32504900



0 3

C	3.85511300	-0.27247800	0.24805400
C	4.36148900	0.53452600	-0.78573600
C	5.70756700	0.47857500	-1.14649300
C	6.57765200	-0.38965000	-0.48757100
C	6.08813800	-1.20575600	0.53421800

C	4.74343100	-1.15190700	0.89239000
H	3.70976700	1.23198300	-1.30243700
H	6.07598800	1.11910900	-1.94255200
H	7.62487000	-0.43534600	-0.77116600
H	6.75266400	-1.89637200	1.04541000
H	4.36456300	-1.81309100	1.66527800
C	1.43391500	0.00441800	-0.46512000
H	1.53421800	-0.76954000	-1.23601600
O	0.09393100	-0.02307600	0.05447100
N	-0.80832500	0.06128600	-0.98220900
C	-2.11158700	0.14497800	-0.46231800
C	-2.63682800	1.50921900	-0.25557000
C	-2.07164400	3.82074400	-0.33275800
H	-1.39148100	4.37565700	-0.98346900
H	-3.09716100	3.94818000	-0.68766300
C	-1.93523900	4.25991100	1.11752900
H	-2.63538800	3.71151800	1.75186700
H	-0.91796500	4.08890900	1.48140900
H	-2.15712700	5.32884200	1.20414100
O	-1.68169000	2.43980700	-0.50698200
O	-3.77029200	1.79735500	0.10041500
H	1.58419700	0.97481200	-0.95282900
C	2.42427200	-0.21658600	0.65413100
C	2.03008900	-0.36887200	1.92512200
H	0.98231900	-0.35132400	2.19767600
H	2.75308700	-0.49790600	2.72340200
C	-2.86796100	-1.06374400	-0.26790800
C	-2.23809500	-2.31560900	-0.51020900
C	-4.22328000	-1.07496100	0.16080600
C	-2.92180900	-3.50744300	-0.32658800
H	-1.20849800	-2.32931700	-0.84818300
C	-4.89339100	-2.27756800	0.34080500
H	-4.71996600	-0.13292200	0.34696000
C	-4.25459500	-3.49897200	0.10126600
H	-2.41807500	-4.45015800	-0.51915200
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H	-4.78891400	-4.43359300	0.24360700



1ag-T2

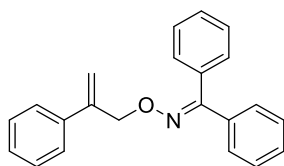
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C	-3.41767200	-0.87949800	-0.04372000
C	-2.93347500	-0.56221400	1.25725100
C	-3.77016200	-0.00944400	2.21597200
C	-5.11428900	0.25384700	1.92482700
C	-5.61153400	-0.03829900	0.64865300
C	-4.78417200	-0.59003000	-0.31764400
H	-1.88819700	-0.72450200	1.49389200
H	-3.37314500	0.22736500	3.19896600
H	-5.76341100	0.68654500	2.67996800
H	-6.65171300	0.16700600	0.41186700
H	-5.17556700	-0.81622900	-1.30497000
C	-1.16492500	-1.86869100	-0.72900000
H	-0.75323900	-2.51192800	-1.51115500
O	-0.34596600	-0.66802200	-0.64296300
N	0.97074500	-1.04277700	-0.46184600
C	1.78076800	-0.04899200	-0.29899100
C	3.22187500	-0.45122000	-0.09087900
C	4.75627300	-2.24686700	0.12331300
H	4.75825700	-3.24369100	-0.32349300
H	5.42928700	-1.59485900	-0.43833600
C	5.13963500	-2.29590400	1.59428300
H	5.15399700	-1.29068300	2.02191900
H	4.43501500	-2.91291000	2.15925200
H	6.13968800	-2.72881400	1.70232500
O	3.39563200	-1.78414200	-0.05281200
O	4.12488700	0.35519100	0.02363300
H	-1.09391900	-2.39976100	0.22828100
C	1.44924400	1.40030800	-0.30756000
C	0.58037400	1.93589100	-1.27273500
C	2.00634700	2.26103900	0.65264300
C	0.28000600	3.29599400	-1.27678600
H	0.14195200	1.28355400	-2.01752700
C	1.68996200	3.61777600	0.65480800
H	2.69290500	1.86680300	1.39164200

C	0.82893600	4.14065400	-0.31077000
H	-0.38785100	3.69534200	-2.03437200
H	2.12386200	4.26812000	1.40856500
H	0.58839500	5.19988000	-0.31174400
C	-2.58117200	-1.46847200	-1.04509800
C	-3.05358900	-1.69503600	-2.41600900
H	-2.88926200	-0.95777600	-3.19992300
H	-3.49327300	-2.64328800	-2.72044600

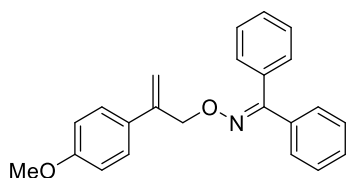
8 Analytical data for substrates

diphenylmethanone O-(2-phenylallyl) oxime (1a)



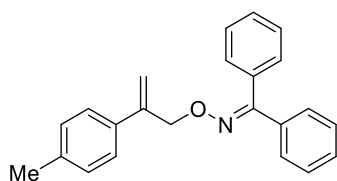
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.48–7.41 (m, 4H), 7.36–7.28 (m, 9H), 7.22–7.18 (m, 2H), 5.50 (s, 1H), 5.31 (d, J = 1.2 Hz, 1H), 5.09 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.2, 144.2, 138.8, 136.4, 133.3, 130.0, 129.3, 129.2, 128.7, 128.3, 128.2, 127.9, 127.6, 126.3, 114.6, 76.3.

diphenylmethanone O-(2-(4-methoxyphenyl)allyl) oxime (1b)



Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.48–7.46 (m, 2H), 7.38–7.29 (m, 8H), 7.23–7.21 (m, 2H), 6.88–6.84 (m, 2H), 5.43 (s, 1H), 5.23 (d, J = 1.2 Hz, 1H), 5.06 (s, 2H), 3.82 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 159.2, 157.1, 143.4, 136.4, 133.3, 131.2, 129.3, 129.2, 128.7, 128.2, 127.9, 127.4, 113.6, 113.0, 76.4, 55.3.

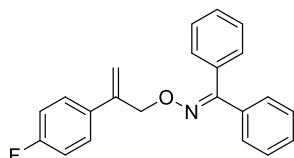
diphenylmethanone O-(2-(p-tolyl)allyl) oxime (1c)



Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.48–7.46 (m, 2H), 7.36–7.20 (m, 8H), 7.13–7.11 (d, J = 8.0 Hz, 2H), 6.88–6.84 (m, 2H), 5.46 (s, 1H), 5.26 (d, J = 1.2 Hz, 1H), 5.07 (s,

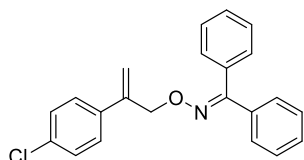
2H), 2.34 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.1, 143.9, 137.4, 136.4, 135.9, 133.3, 129.2, 129.18, 128.9, 128.6, 128.2, 127.9, 126.1, 113.7, 76.4, 21.1.

diphenylmethanone O-(2-(4-fluorophenyl)allyl) oxime (1d)



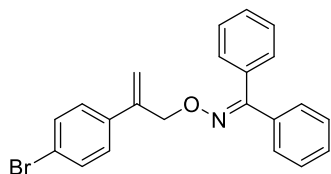
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.47–7.45 (m, 2H), 7.40–7.29 (m, 8H), 7.19–7.17 (m, 2H), 7.01–6.97 (m, 2H), 5.45 (s, 1H), 5.30 (s, 1H), 5.05 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 162.4 (d, $^1J_{\text{C-F}} = 245$ Hz), 157.4, 143.2, 136.3, 134.8 (d, $^4J_{\text{C-F}} = 3$ Hz), 133.2, 129.3, 129.1, 128.7, 128.2, 128.0 (d, $^3J_{\text{C-F}} = 8$ Hz), 127.94, 127.88, 115.0 (d, $^2J_{\text{C-F}} = 21$ Hz), 114.8, 76.4; ^{19}F NMR (376 MHz, CDCl_3): δ -114.72 (s, 1F).

diphenylmethanone O-(2-(4-chlorophenyl)allyl) oxime (1e)



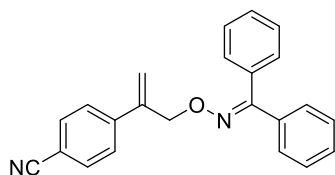
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.47–7.42 (m, 2H), 7.37–7.24 (m, 10H), 7.18–7.16 (m, 2H), 5.50 (s, 1H), 5.34 (d, $J = 1.2$ Hz, 1H), 5.05 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.4, 143.1, 137.2, 136.2, 133.4, 133.2, 129.4, 129.1, 128.7, 128.4, 128.2, 128.0, 127.9, 127.6, 115.5, 76.2.

diphenylmethanone O-(2-(4-bromophenyl)allyl) oxime (1f)



Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.46–7.41 (m, 4H), 7.37–7.27 (m, 8H), 7.18–7.15 (m, 2H), 5.50 (s, 1H), 5.34 (m, 1H), 5.04 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.5, 143.2, 137.7, 136.2, 133.2, 131.3, 129.3, 129.0, 128.7, 128.2, 128.0, 127.9, 121.6, 115.5, 76.1.

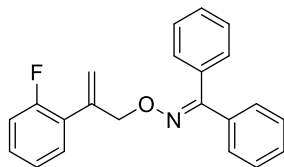
4-(3-(((diphenylmethylene)amino)oxy)prop-1-en-2-yl)benzonitrile (1g)



Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.60–7.58 (m, 2H), 7.52–7.50 (m, 2H), 7.45–

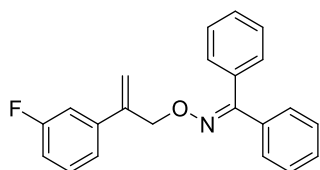
7.43 (m, 2H), 7.39–7.30 (m, 6H), 7.15–7.13 (m, 2H), 5.62 (s, 1H), 5.49 (s, 1H), 5.07 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.8, 143.3, 142.9, 136.0, 133.1, 132.0, 129.5, 128.9, 128.8, 128.2, 128.0, 127.8, 127.0, 118.9, 118.1, 111.1, 75.8.

diphenylmethanone O-(2-(2-fluorophenyl)allyl) oxime (1h)



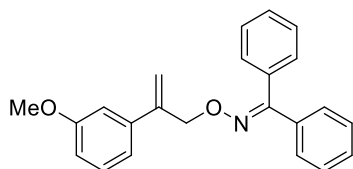
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.44 (d, J = 6.8 Hz, 2H), 7.33–7.13 (m, 8H), 7.09–7.00 (m, 4H), 5.46 (s, 1H), 5.40 (s, 1H), 5.05 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 160.1 (d, $^1J_{\text{C-F}}$ = 246 Hz), 157.1, 141.3, 136.4, 133.2, 130.3 (d, $^4J_{\text{C-F}}$ = 4.0 Hz), 129.2, 129.04, 129.03 (d, $^3J_{\text{C-F}}$ = 8.0 Hz), 128.6, 128.1, 127.89, 127.86, 127.3 ($^2J_{\text{C-F}}$ = 14.0 Hz), 123.9 (d, $^4J_{\text{C-F}}$ = 3.0 Hz), 117.7, 115.6 (d, $^2J_{\text{C-F}}$ = 23 Hz), 76.6; ^{19}F NMR (376 MHz, CDCl_3): δ -113.37 (s, 1F).

diphenylmethanone O-(2-(3-fluorophenyl)allyl) oxime (1i)



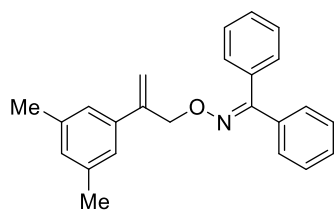
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.47–7.46 (m, 2H), 7.36–7.18 (m, 10H), 7.12 (d, J = 10.4 Hz, 1H), 6.99–6.94 (m, 1H), 5.52 (s, 1H), 5.36 (s, 1H), 5.04 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 162.8 (d, $^1J_{\text{C-F}}$ = 244 Hz), 157.4, 143.1 (d, $^4J_{\text{C-F}}$ = 2.0 Hz), 141.0 (d, $^3J_{\text{C-F}}$ = 8.0 Hz), 136.2, 133.2, 129.6 (d, $^3J_{\text{C-F}}$ = 9 Hz), 129.3, 129.0, 128.7, 128.2, 128.0, 127.9, 121.9 (d, $^4J_{\text{C-F}}$ = 3.0 Hz), 116.0, 114.4 (d, $^2J_{\text{C-F}}$ = 21 Hz), 113.3 (d, $^2J_{\text{C-F}}$ = 22 Hz), 76.1; ^{19}F NMR (376 MHz, CDCl_3): δ -113.41 (s, 1F).

diphenylmethanone O-(2-(3-methoxyphenyl)allyl) oxime (1j)



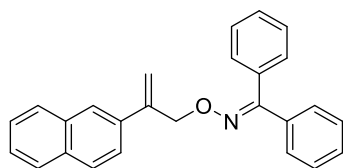
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.48–7.45 (m, 2H), 7.35–7.26 (m, 6H), 7.23–7.18 (m, 3H), 7.03–7.01 (m, 1H), 6.97–6.96 (m, 1H), 6.83 (dd, J = 8.0, 2.4 Hz, 1H), 5.50 (s, 1H), 5.31 (d, J = 1.2 Hz, 1H), 5.07 (s, 2H), 3.73 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 159.5, 157.1, 144.0, 140.3, 136.3, 133.2, 129.22, 129.17, 129.1, 128.7, 128.1, 127.89, 127.87, 118.7, 114.9, 113.3, 111.7, 76.3, 55.1.

diphenylmethanone O-(2-(3,5-dimethylphenyl)allyl) oxime (1k)



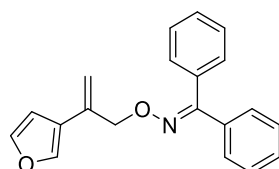
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.48–7.46 (m, 2H), 7.37–7.30 (m, 6H), 7.24–7.21 (m, 2H), 7.05 (s, 2H), 6.93 (s, 1H), 5.47 (s, 1H), 5.27 (d, $J=1.2$ Hz, 1H), 5.06 (s, 2H), 2.30 (s, 6H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.1, 144.3, 138.8, 137.6, 136.4, 133.3, 129.3, 129.2, 128.7, 128.2, 127.92, 127.90, 124.1, 114.3, 76.5, 21.3.

diphenylmethanone O-(2-(naphthalen-2-yl)allyl) oxime (1l)



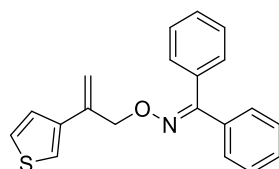
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.86 (s, 1H), 7.83–7.77 (m, 3H), 7.61 (dd, $J = 8.8, 1.6$ Hz, 1H), 7.48–7.46 (m, 4H), 7.35–7.23 (m, 6H), 6.17 (d, $J = 7.2$ Hz, 2H), 5.68 (s, 1H), 5.43 (d, $J = 0.8$ Hz, 1H), 5.21 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.3, 143.9, 136.3, 135.9, 133.3, 133.2, 132.9, 129.3, 129.1, 128.7, 128.3, 128.2, 127.9, 127.8, 127.5, 126.1, 125.9, 125.1, 124.5, 115.4, 76.5;

diphenylmethanone O-(2-(furan-3-yl)allyl) oxime (1m)



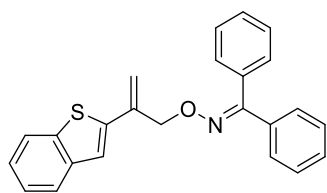
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.48 (d, $J = 7.6$ Hz, 2H), 7.40 (s, 4H), 7.35–7.29 (m, 6H), 6.53 (s, 1H), 5.39 (s, 1H), 5.21 (s, 1H), 4.92 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.2, 142.9, 139.5, 136.3, 136.0, 133.3, 129.3, 129.1, 128.8, 128.2, 128.0, 127.9, 124.1, 112.8, 108.1, 76.4;

diphenylmethanone O-(2-(thiophen-3-yl)allyl) oxime (1n)



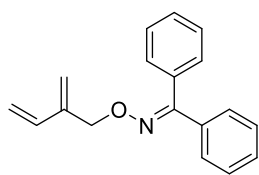
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.48 (d, $J = 6.4$ Hz, 2H), 7.39–7.22 (m, 11H), 5.52 (s, 1H), 5.27 (s, 1H), 5.02 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.2, 139.8, 138.9, 136.3, 133.2, 129.3, 129.1, 128.7, 128.2, 128.0, 127.9, 125.7, 125.2, 121.1, 113.6, 76.5.

diphenylmethanone O-(2-(benzo[b]thiophen-2-yl)allyl) oxime (1o)



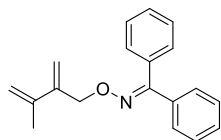
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.95–7.93 (m, 1H), 7.87–7.85 (m, 1H), 7.46–7.45 (d, J = 6.4 Hz, 2H), 7.36–7.30 (m, 8H), 7.27 (s, 1H), 7.23–7.20 (m, 2H), 5.58 (d, J = 1.2 Hz, 1H), 5.51 (s, 1H), 5.04 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.3, 140.2, 139.6, 138.0, 136.2, 135.4, 133.2, 129.3, 129.1, 128.7, 128.2, 128.0, 127.9, 124.3, 124.2, 123.5, 123.2, 122.7, 116.8, 77.3.

diphenylmethanone O-(2-methylenebut-3-en-1-yl) oxime (1p)



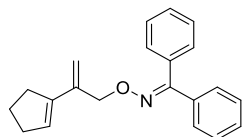
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.50–7.47 (m, 2H), 7.42–7.39 (m, 4H), 7.37–7.31 (m, 4H), 6.38 (dd, J = 17.6, 10.8 Hz, 1H), 5.28 (s, 1H), 5.20 (t, J = 12.8 Hz, 2H), 5.10 (d, J = 11.2 Hz, 1H), 4.89 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.0, 142.2, 136.6, 136.5, 133.3, 129.3, 129.2, 128.8, 128.2, 128.0, 127.9, 117.5, 114.3, 74.1.

diphenylmethanone O-(3-methyl-2-methylenebut-3-en-1-yl) oxime (1q)



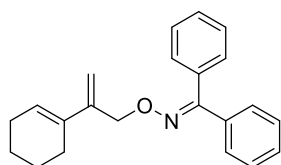
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.50–7.46 (m, 2H), 7.42–7.28 (m, 8H), 5.24 (s, 1H), 5.20 (s, 1H), 5.07 (s, 1H), 5.00 (s, 1H), 4.92 (s, 2H), 1.92 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 156.8, 143.6, 140.8, 136.5, 133.4, 129.3, 129.2, 128.7, 128.2, 128.0, 127.9, 114.2, 113.0, 75.4, 21.0.

diphenylmethanone O-(2-(cyclopent-1-en-1-yl)allyl) oxime (1r)



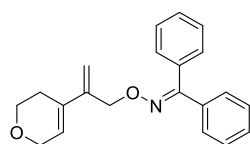
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.49–7.45 (m, 2H), 7.42–7.17 (m, 8H), 5.78 (m, 1H), 5.12 (s, 1H), 5.04 (s, 1H), 4.91 (s, 2H), 2.51–2.40 (m, 4H), 1.91–1.82 (m, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 156.8, 141.0, 140.3, 136.4, 133.4, 129.2, 129.1, 128.7, 128.1, 127.9, 127.9, 127.4, 112.9, 75.5, 33.5, 32.6, 22.6.

diphenylmethanone O-(2-(cyclohex-1-en-1-yl)allyl) oxime (1s)



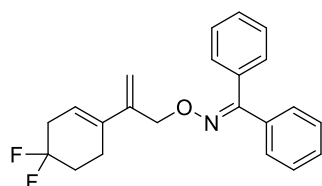
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.52–7.45 (m, 2H), 7.44–7.22 (m, 8H), 5.93–5.82 (m, 1H), 5.12 (s, 1H), 5.05 (s, 1H), 4.90 (s, 2H), 2.14 (d, J = 22.9 Hz, 4H), 1.76–1.63 (m, 2H), 1.61–1.49 (m, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 156.8, 144.1, 136.5, 134.1, 133.4, 129.3, 129.1, 128.7, 128.1, 127.9, 125.2, 111.0, 75.7, 25.8, 25.7, 22.8, 22.2.

diphenylmethanone O-(2-(3,6-dihydro-2H-pyran-4-yl)allyl) oxime (1t)



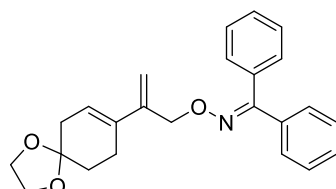
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.50–7.45 (m, 2H), 7.43–7.38 (m, 3H), 7.36–7.27 (m, 5H), 5.82–5.80 (m, 1H), 5.17–5.15 (m, 2H), 4.89 (s, 2H), 4.23–4.19 (m, 2H), 3.83 (t, J = 5.6 Hz, 2H), 2.30–2.26 (m, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.1, 142.5, 136.3, 133.3, 131.8, 129.3, 129.2, 128.7, 128.2, 127.9, 127.9, 123.2, 112.6, 75.3, 65.6, 64.3, 25.7.

diphenylmethanone O-(2-(4,4-difluorocyclohex-1-en-1-yl)allyl) oxime (1u)



Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.50–7.45 (m, 2H), 7.44–7.38 (m, 3H), 7.37–7.28 (m, 5H), 5.74–5.63 (m, 1H), 5.18 (d, J = 6.2 Hz, 2H), 4.87 (s, 2H), 2.60 (t, J = 14.1 Hz, 2H), 2.47 (t, J = 6.0 Hz, 2H), 2.17–1.92 (m, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.2, 142.8, 136.3, 133.6, 133.4, 129.3, 129.2, 128.7, 128.2, 128.0, 127.9, 122.7 (t, $J_{\text{C-F}}$ = 239.5 Hz), 119.5 (t, $J_{\text{C-F}}$ = 5.2 Hz), 113.7, 75.7, 34.8 (t, $J_{\text{C-F}}$ = 26.7 Hz), 30.2 (t, $J_{\text{C-F}}$ = 24.3 Hz), 24.3 (t, $J_{\text{C-F}}$ = 5.3 Hz); ^{19}F NMR (376 MHz, CDCl_3): δ -96.97.

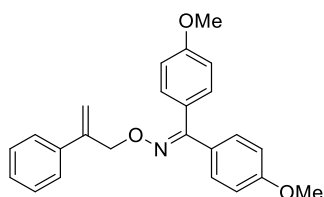
diphenylmethanone O-(2-(1,4-dioxaspiro[4.5]dec-7-en-8-yl)allyl) oxime (1v)



^1H NMR (400 MHz, CDCl_3) δ 7.51–7.45 (m, 2H), 7.44–7.37 (m, 3H), 7.37–7.28 (m, 5H), 5.75 (t, J = 3.9 Hz, 1H), 5.17 (s, 1H), 5.11 (s, 1H), 4.89 (s, 2H), 3.99 (s, 4H), 2.48–2.42 (m, 2H), 2.38 (s, 2H), 1.82 (t, J = 6.6 Hz, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 156.9, 143.1, 136.5, 133.6,

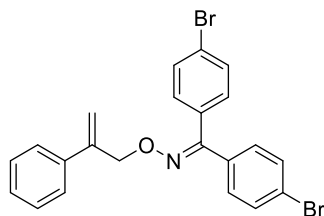
133.4, 129.3, 129.2, 128.7, 128.2, 127.9, 127.9, 122.0, 112.5, 107.7, 75.7, 64.4, 36.0, 31.0, 25.1.

bis(4-methoxyphenyl)methanone O-(2-phenylallyl) oxime (1w)



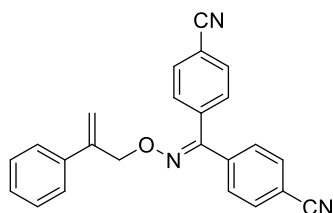
Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.46–7.39 (m, 4H), 7.36–7.27 (m, 3H), 7.25–7.15 (m, 2H), 6.87–6.81 (m, 4H), 5.50 (s, 1H), 5.32 (d, J = 1.2 Hz, 1H), 5.07 (s, 2H), 3.82 (s, 3H), 3.80 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 160.5, 159.7, 156.6, 144.3, 138.9, 131.0, 129.5, 129.4, 128.3, 127.6, 126.3, 125.5, 114.5, 113.5, 113.2, 76.1, 55.3, 55.2.

bis(4-bromophenyl)methanone O-(2-phenylallyl) oxime(1x)



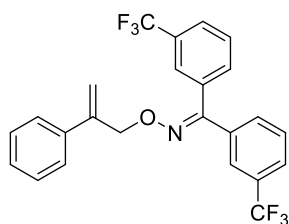
Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.48 – 7.38 (m, 6H), 7.36 – 7.27 (m, 5H), 7.00 (d, J = 8.2 Hz, 2H), 5.51 (s, 1H), 5.29 (d, J = 1.3 Hz, 1H), 5.08 (s, 2H). ^{13}C NMR (100.6 MHz, CDCl_3) δ 155.2, 144.0, 138.6, 134.8, 131.5, 131.4, 131.3, 130.8, 129.3, 128.3, 127.8, 126.3, 123.9, 123.2, 115.1, 76.7;

4,4'-((((2-phenylallyl)oxy)imino)methylene)dibenzonitrile (1y)



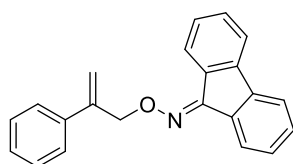
Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.65–7.59 (m, 4H), 7.53–7.49 (m, 2H), 7.40–7.31 (m, 5H), 7.18–7.14 (m, 2H), 5.53 (s, 1H), 5.30 (d, J = 0.9 Hz, 1H), 5.13 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 154.0, 143.7, 139.3, 138.3, 136.6, 132.2, 132.1, 129.7, 128.4, 128.0, 127.9, 126.3, 118.4, 118.2, 115.7, 113.2, 113.0, 77.3.

bis(3-(trifluoromethyl)phenyl)methanone O-(2-phenylallyl) oxime (1z)



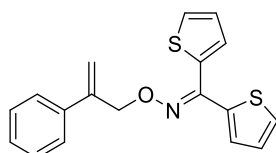
Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 7.78 (s, 1H), 7.66–7.60 (m, 2H), 7.54–7.40 (m, 6H), 7.36–7.28 (m, 4H), 5.53 (s, 1H), 5.32 (s, 1H), 5.13 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 154.4, 143.8, 138.4, 136.5, 133.1, 132.5, 131.0, 130.9 (q, $J_{\text{C-F}} = 32.5$ Hz), 130.7 (q, $J_{\text{C-F}} = 32.5$ Hz), 128.9, 128.8, 128.4, 127.9, 126.2, 126.0 (q, $J_{\text{C-F}} = 3.8$ Hz), 125.9 (q, $J_{\text{C-F}} = 3.8$ Hz), 124.3 (q, $J_{\text{C-F}} = 3.8$ Hz), 123.8 (q, $J_{\text{C-F}} = 270.7$ Hz), 115.4, 71.9; ^{19}F NMR (377 MHz, CDCl_3) δ -62.63 (s, 3F), -62.71 (s, 3F);

9H-fluoren-9-one O-(2-phenylallyl) oxime (1aa)



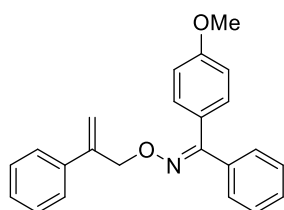
Colorless oil; ^1H NMR (400 MHz, CDCl_3) δ 8.16 (d, $J = 7.6$ Hz, 1H), 7.78 (d, $J = 7.5$ Hz, 1H), 7.66–7.52 (m, 4H), 7.42–7.33 (m, 3H), 7.33–7.27 (m, 2H), 7.26–7.18 (m, 2H), 5.64 (s, 1H), 5.50 (s, 1H), 5.31 (s, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 152.6, 143.6, 141.3, 140.2, 138.6, 135.5, 130.9, 130.5, 129.8, 129.3, 128.40, 128.2, 127.9, 127.8, 126.1, 121.7, 119.8, 119.7, 115.4, 77.7.

di(thiophen-2-yl)methanone O-(2-phenylallyl) oxime(1ab)



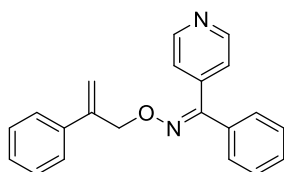
^1H NMR (400 MHz, Chloroform-d) δ 7.55 – 7.49 (m, 3H), 7.46 (dd, $J = 3.9, 1.2$ Hz, 1H), 7.36 – 7.27 (m, 5H), 7.05 (ddd, $J = 11.2, 5.1, 3.7$ Hz, 2H), 5.61 (d, $J = 1.1$ Hz, 1H), 5.49 (q, $J = 1.3$ Hz, 1H), 5.22 (d, $J = 1.2$ Hz, 2H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 145.8, 143.4, 138.6, 138.0, 132.1, 131.7, 130.5, 128.8, 128.3, 127.8, 126.9, 126.2, 125.6, 115.5, 71.9

(Z)-(4-methoxyphenyl)(phenyl)methanone O-(2-phenylallyl) oxime (1ac)



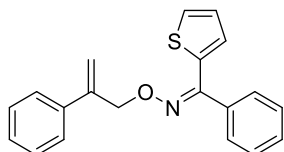
Colorless oil; (Z/E=1.9:1); ^1H NMR (400 MHz, CDCl_3) δ 7.47–7.38 (m, 6.32H), 7.35–7.28 (m, 9.06H), 7.25–7.18 (m, 3.04H), 6.86–6.81 (m, 3.04H), 5.51 (s, 1H), 5.48 (s, 0.53H), 5.33 (d, J = 1.2 Hz, 1H), 5.29 (d, J = 1.2 Hz, 0.54H), 5.10 (s, 2.01H), 5.06 (s, 1.03H), 3.82 (s, 2.99H), 3.80 (s, 1.54H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 160.5, 159.8, 156.9, 156.8, 144.3, 144.2, 138.9, 136.9, 133.5, 131.1, 129.2, 129.1, 129.1, 128.9, 128.5, 128.3, 128.2, 128.1, 127.9, 127.6, 127.6, 126.3, 125.3, 114.6, 114.5, 113.6, 113.2, 76.3, 76.1, 55.3, 55.2.

(Z)-phenyl(pyridin-2-yl)methanone O-(2-phenylallyl) oxime (1ad)



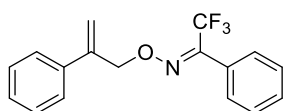
Colorless oil; (Z/E=2.3:1); ^1H NMR (400 MHz, CDCl_3) δ 8.55 – 8.52 (m, 4.6H), 8.51 – 8.48 (m, 2H), 7.40 – 7.22 (m, 33H), 7.12 – 7.06 (m, 2H), 6.98 – 6.93 (m, 4.6H), 5.46 (d, J = 1.1 Hz, 1H), 5.45 (d, J = 1.1 Hz, 2.3H), 5.25 (q, J = 1.4 Hz, 1H), 5.24 (q, J = 1.3 Hz, 2.3H), 5.06 (s, 2H), 5.04 (s, 4.6H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 155.0, 154.8, 149.8, 149.6, 143.9, 143.8, 143.5, 141.0, 138.4, 134.6, 131.6, 129.6, 129.1, 128.9, 128.3, 128.2, 128.1, 127.7, 127.4, 126.1, 123.4, 121.7, 115.03, 114.96, 76.8, 76.6;

(Z)-phenyl(thiophen-2-yl)methanone O-(2-phenylallyl) oxime (1ae)



Colorless oil; (Z:E = 2.2:1); ^1H NMR (400 MHz, CDCl_3): δ 7.56–7.49 (m, 5.1H), 7.43–7.39 (m, 4H), 7.37–7.32 (m, 3.5H), 7.31–7.28 (m, 2.6H), 7.25–7.22 (m, 1H), 7.13 (dd, J = 4.0, 1.2 Hz, 1H), 6.99 (dd, J = 5.2, 4.0 Hz, 1H), 6.93 (dd, J = 5.2, 3.6Hz, 0.46H), 6.80 (dd, J = 3.6, 1.2 Hz, 0.43H), 5.62 (s, 1H), 5.52 (d, J = 1.2Hz, 1H), 5.49 (s, 0.45H), 5.29 (d, J = 1.2Hz, 0.45H), 5.26 (s, 2H), 5.05 (s, 0.9H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 153.1, 151.4, 144.0, 143.6, 140.2, 138.7, 138.7, 136.2, 132.6, 132.6, 132.5, 130.9, 129.4, 129.2, 129.1, 128.9, 128.7, 128.3, 128.3, 128.2, 128.0, 127.8, 127.6, 127.3, 126.9, 126.2, 126.2, 125.5, 115.3, 114.8, 77.0, 76.4.

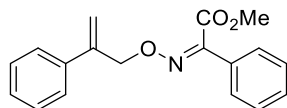
(Z)-2,2,2-trifluoro-1-phenylethan-1-one O-(2-phenylallyl) oxime (1af)



Colorless oil; (Z:E = 2:1); ^1H NMR (400 MHz, CDCl_3): δ 7.49–7.22 (m, 30H), 5.60 (s, 1H), 5.53 (s, 2H), 5.41 (d, J = 0.8Hz, 1H), 5.29 (d, J = 1.2Hz, 2H), 5.18 (s, 2H), 5.11 (s, 4H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 146.7 (q, $^2J_{\text{C-F}}$ = 32.2 Hz), 146.6 (q, $^2J_{\text{C-F}}$ = 32.2 Hz), 143.1,

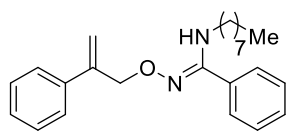
143.0, 138.3, 138.2, 130.2, 130.1, 128.5, 128.4, 128.4, 128.3, 127.9, 127.0, 126.8, 126.2, 126.1, 120.5 (q, $^1J_{C-F} = 274.6$ Hz), 118.3 (q, $^1J_{C-F} = 274.6$ Hz), 115.8, 115.6, 78.1, 77.8; ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.24 (s, 1F), -66.1 (s, 2F).

methyl (Z)-2-phenyl-2-(((2-phenylallyl)oxy)imino)acetate (1ag)



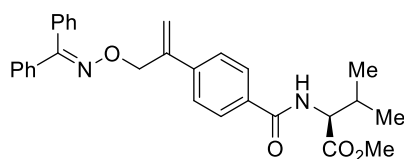
Colorless oil; 1H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.07 (m, 10H), 5.52 (s, 1H), 5.33–5.26 (m, 1H), 5.17 (s, 2H), 3.87 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ 163.9, 149.6, 143.1, 138.2, 129.5, 129.3, 129.0, 128.4, 127.9, 127.8, 126.2, 115.3, 77.7, 52.9.

N-octyl-N'-((2-phenylallyl)oxy)benzimidamide (1ah)



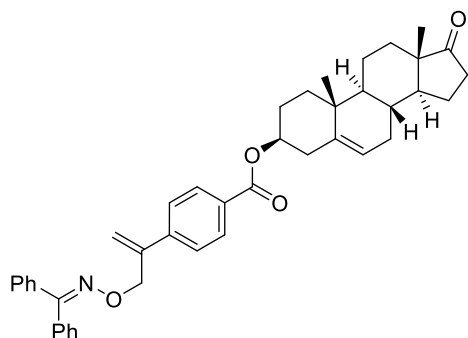
Colorless oil; (Z:E = 2:1); 1H NMR (400 MHz, $CDCl_3$): δ 7.64–7.61 (m, 2H), 7.48–7.45 (m, 2H), 7.43–7.40 (m, 1H), 7.38–7.28 (m, 10H), 5.56–5.50 (m, 2.4H), 5.40 (s, 1H), 5.31 (s, 0.5H), 5.13 (s, 2H), 5.07 (s, 1H), 3.32 (q, $J = 6.8$ Hz, 1H), 3.23 (q, $J = 6.8$ Hz, 2H), 1.38–1.24 (m, 21H), 0.89 (t, $J = 5.6$ Hz, 4.6H); ^{13}C NMR (100.6 MHz, $CDCl_3$): 162.7, 162.6, 153.3, 150.9, 143.7, 143.6, 138.5, 138.4, 131.4, 130.0, 129.6, 129.4, 128.6, 128.5, 128.4, 128.4, 127.9, 127.9, 127.6, 126.9, 126.2, 126.2, 115.9, 115.5, 77.2, 76.9, 39.6, 39.3, 31.8, 29.5, 29.3, 29.2, 29.2, 29.1, 26.9, 26.8, 22.6, 14.1.

methyl (4-(3-(((diphenylmethylene)amino)oxy)prop-1-en-2-yl)benzoyl)-L-valinate (1ai)



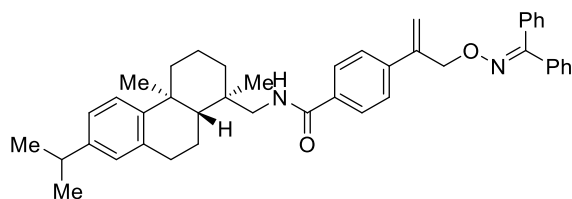
Colorless oil; 1H NMR (400 MHz, $CDCl_3$): δ 7.76–7.75 (m, 2H), 7.53–7.44 (m, 6H), 7.37–7.31 (m, 4H), 7.19–7.17 (m, 2H), 5.60 (s, 1H), 5.42 (m, 1H), 5.08 (s, 2H), 4.81 (dd, $J = 8.8$, 4.8 Hz, 1H), 3.79 (s, 3H), 2.32–2.26 (m, 1H), 1.03–0.99 (m, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.6, 167.4, 157.6, 143.3, 142.4, 136.2, 129.4, 133.1, 130.2, 129.1, 128.8, 128.2, 128.0, 127.9, 127.1, 126.5, 116.7, 76.1, 57.5, 52.3, 31.7, 19.0, 18.0.

(3S,8R,9S,10R,13S,14S)-10,13-dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 4-(3-(((diphenylmethylene)amino)oxy)prop-1-en-2-yl)benzoate (1aj)



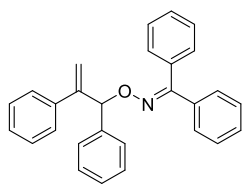
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.99–7.97 (m, 2H), 7.47–7.47 (m, 4H), 7.38–7.31 (m, 6H), 7.19–7.17 (m, 2H), 5.60 (m, 1H), 5.46 (d, J = 4.8 Hz, 1H), 5.42 (d, J = 1.3 Hz, 1H), 5.09 (s, 2H), 4.89–4.86 (m, 1H), 2.50–2.43 (m, 3H), 2.15–2.04 (m, 2H), 2.01–1.85 (m, 4H), 1.75–1.67 (m, 4H), 1.59–1.50 (m, 2H), 1.35–1.25 (m, 4H), 1.08 (s, 3H), 0.90 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 221.1, 165.8, 157.5, 143.5, 143.2, 139.9, 136.2, 133.2, 129.8, 129.5, 129.4, 129.1, 128.7, 128.2, 128.0, 127.9, 126.2, 122.0, 116.8, 76.1, 74.3, 51.7, 50.1, 47.5, 38.2, 37.0, 36.8, 35.8, 31.5, 31.4, 30.8, 27.8, 21.9, 20.3, 19.4, 13.5.

4-(3-(((diphenylmethylene)amino)oxy)prop-1-en-2-yl)-N-(((1R,4aS,10aR)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthren-1-yl)methyl)benzamide (1ak)



Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.68–7.66 (m, 2H), 7.46–7.43 (m, 4H), 7.34–7.29 (m, 6H), 7.18–7.15 (m, 3H), 7.00–6.97 (m, 1H), 6.13 (t, J = 6.0 Hz, 1H), 5.55 (m, 1H), 5.38 (m, 1H), 5.06 (s, 2H), 3.43 (dd, J_1 = 14.0 Hz, J_2 = 6.0 Hz, 1H), 3.34 (dd, J_1 = 14.0 Hz, J_2 = 6.0 Hz, 1H), 2.96–2.90 (m, 1H), 2.87–2.77 (m, 2H), 2.32–2.29 (m, 1H), 2.01–1.96 (m, 1H), 1.82–1.66 (m, 3H), 1.54–1.48 (m, 2H), 1.42–1.33 (m, 2H), 1.24 (s, 3H), 1.21 (s, 3H), 1.19 (s, 3H), 1.01 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 167.2, 157.5, 147.0, 145.6, 143.4, 141.9, 136.2, 134.7, 133.8, 133.2, 129.3, 129.0, 128.7, 128.2, 127.93, 127.88, 126.9, 126.8, 126.5, 124.2, 123.9, 116.3, 76.1, 50.3, 45.9, 38.4, 37.7, 37.6, 36.4, 33.4, 30.5, 25.4, 23.9, 19.1, 18.8, 18.6.

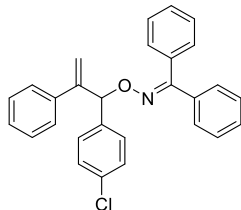
diphenylmethanone O-(1,2-diphenylallyl) oxime (1al)



Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.44–7.42 (m, 2H), 7.37–7.35 (m, 3H), 7.30–

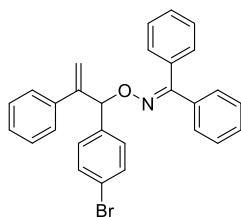
7.20 (m, 15H), 6.27 (s, 1H), 5.46 (s, 1H), 5.22 (s, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.3, 148.1, 139.8, 139.5, 136.4, 133.4, 129.3, 129.2, 129.1, 128.6, 128.1, 128.02, 127.99, 127.9, 127.4, 127.3, 127.2, 115.9, 87.2.

diphenylmethanone O-(1-(4-chlorophenyl)-2-phenylallyl) oxime (1am)



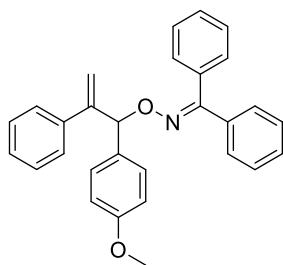
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.43–7.22 (m, 19H), 6.22 (s, 1H), 5.45 (m, 1H), 5.22 (m, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.7, 147.7, 139.2, 138.5, 136.2, 133.3, 133.2, 129.4, 129.2, 128.8, 128.7, 128.3, 128.2, 128.1, 128.0, 127.9, 127.5, 127.2, 116.0, 86.5.

diphenylmethanone O-(1-(4-bromophenyl)-2-phenylallyl) oxime (1an)



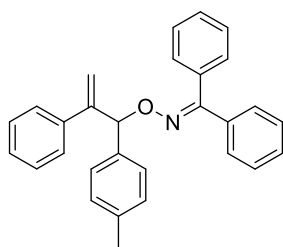
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.43–7.36 (m, 7H), 7.32–7.21 (m, 10H), 7.16–7.14 (m, 2H), 6.20 (s, 1H), 5.44 (s, 1H), 5.21 (s, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.7, 147.6, 139.2, 139.0, 136.2, 133.2, 131.2, 129.4, 129.2, 128.7, 128.2, 128.1, 128.0, 127.9, 127.5, 127.1, 121.4, 116.1, 86.5.

diphenylmethanone O-(1-(4-methoxyphenyl)-2-phenylallyl) oxime (1ao)



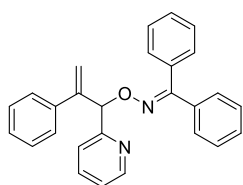
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.44–7.43 (m, 2H), 7.36–7.34 (m, 3H), 7.30–7.19 (m, 12H), 6.79–6.77 (s, 2H), 6.22 (s, 1H), 5.45 (s, 1H), 5.22 (s, 1H), 3.72 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 158.9, 157.1, 148.1, 139.6, 136.5, 133.4, 131.9, 129.3, 129.2, 128.8, 128.6, 128.1, 127.99, 127.98, 127.8, 127.3, 127.1, 115.3, 113.4, 86.8, 55.1.

diphenylmethanone O-(2-phenyl-1-(p-tolyl)allyl) oxime (1ap)



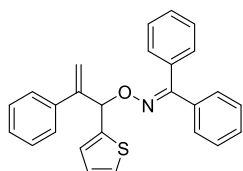
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.45–7.42 (m, 2H), 7.38–7.25 (m, 10H), 7.23–7.18 (m, 5H), 7.07–7.05 (m, 2H), 6.23 (s, 1H), 5.46 (m, 1H), 5.22 (m, 1H), 2.29 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.1, 148.1, 139.6, 137.0, 136.8, 136.5, 133.4, 129.3, 129.2, 128.8, 128.6, 128.1, 128.0, 127.8, 127.4, 127.3, 127.2, 115.6, 87.1, 21.2.

diphenylmethanone O-(2-phenyl-1-(pyridin-2-yl)allyl) oxime (1aq)



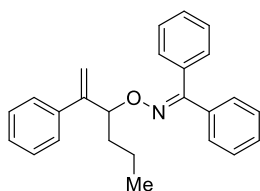
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 8.55 (d, J = 4.2 Hz, 1H), 7.58–7.53 (m, 1H), 7.44–7.37 (m, 5H), 7.32–7.19 (m, 11H), 7.12–7.08 (m, 1H), 6.38 (s, 1H), 5.48 (s, 1H), 5.23 (s, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 159.8, 157.7, 148.9, 147.0, 139.3, 136.2, 136.1, 133.3, 129.3, 129.2, 128.7, 128.1, 128.0, 127.9, 127.3, 127.2, 122.2, 121.7, 117.1, 88.4.

diphenylmethanone O-(2-phenyl-1-(thiophen-2-yl)allyl) oxime (1ar)



Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.50–7.47 (m, 2H), 7.39–7.27 (m, 10H), 7.25–7.20 (m, 4H), 6.95–6.94 (m, 1H), 6.90–6.87 (m, 1H), 6.44 (s, 1H), 5.53 (s, 1H), 5.37 (s, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 157.6, 147.5, 143.3, 139.1, 136.4, 133.2, 129.3, 128.7, 128.2, 128.10, 128.07, 127.9, 127.5, 127.1, 126.4, 126.2, 125.6, 115.8, 82.9.

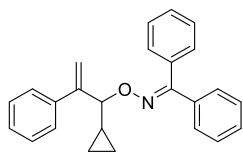
diphenylmethanone O-(2-phenylhex-1-en-3-yl) oxime (1as)



Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.50–7.48 (m, 2H), 7.43–7.40 (m, 3H), 7.36–7.25 (m, 10H), 5.32 (s, 1H), 5.21 (s, 1H), 5.18 (t, J = 6.4 Hz, 1H), 1.70–1.53 (m, 2H), 1.43–1.30 (m, 1H), 0.84 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 156.5, 149.0, 140.1,

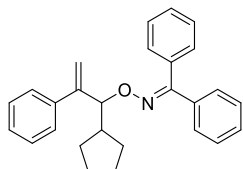
136.7, 133.7, 129.3, 129.1, 128.5, 128.14, 12.07, 127.89, 127.87, 127.3, 127.1, 114.8, 86.0, 35.4, 18.8, 14.0.

diphenylmethanone O-(1-cyclopropyl-2-phenylallyl) oxime (1at)



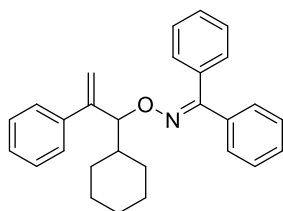
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.47–7.44 (m, 2H), 7.37–7.35 (m, 5H), 7.33–7.27 (m, 3H), 7.26–7.22 (m, 5H), 5.33 (m, 1H), 5.30 (m, 1H), 4.56 (d, J = 8.0 Hz 1H), 1.10 (m, 1H), 0.60–0.50 (m, 2H), 0.42–0.46 (m, 1H), 0.26–0.20 (m, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 156.4, 148.6, 140.4, 136.8, 133.6, 129.4, 129.1, 128.5, 128.1, 128.0, 127.9, 127.8, 127.3, 127.2, 115.0, 89.6, 14.3, 4.0, 2.8.

diphenylmethanone O-(1-cyclopentyl-2-phenylallyl) oxime (1au)



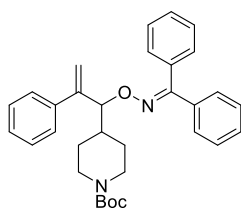
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.50–7.48 (m, 2H), 7.43–7.42 (m, 3H), 7.37–7.30 (m, 7H), 7.24–7.22 (m, 3H), 5.33 (m, 1H), 5.24 (s, 1H), 4.92 (d, J = 8.0 Hz, 1H), 2.04–1.98 (m, 1H), 1.64–1.61 (m, 1H), 1.54–1.37 (m, 6H), 1.28–1.24 (m, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 156.4, 149.0, 140.5, 136.6, 133.7, 129.3, 129.1, 128.5, 128.1, 128.0, 127.8, 127.3, 127.2, 115.9, 90.9, 42.3, 29.3, 29.1, 25.50, 25.45.

diphenylmethanone O-(1-cyclohexyl-2-phenylallyl) oxime (1av)



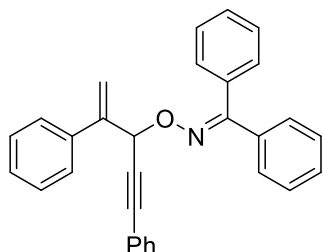
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.50–7.48 (m, 2H), 7.45–7.40 (m, 3H), 7.37–7.34 (m, 4H), 7.32–7.27 (m, 3H), 7.26–7.22 (m, 3H), 5.35 (m, 1H), 5.16 (m, 1H), 4.91 (d, J = 7.2 Hz, 1H), 1.81–1.78 (m, 1H), 1.62–1.45 (m, 5H), 1.05–0.90 (m, 5H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 156.4, 147.9, 140.5, 136.7, 133.8, 129.3, 129.0, 128.5, 128.1, 128.0, 127.9, 127.8, 127.19, 127.17, 116.0, 91.3, 40.0, 29.7, 28.4, 26.5, 26.0, 25.9.

tert-butyl 4-(1-(((diphenylmethylene)amino)oxy)-2-phenylallyl)piperidine-1-carboxylate (1aw)



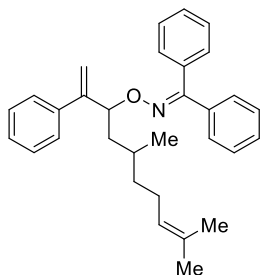
Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.49–7.47 (m, 2H), 7.43–7.39 (m, 3H), 7.35–7.32 (m, 4H), 7.30–7.22 (m, 6H), 5.39 (m, 1H), 5.20 (s, 1H), 4.95 (d, J = 4.8 Hz 1H), 4.01 (m, 2H), 2.48 (m, 2H), 1.73–1.70 (m, 1H), 1.67–1.61 (m, 1H), 1.49–1.47 (m, 1H), 1.43 (s, 9H), 1.27–1.14 (m, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 156.8, 154.6, 147.2, 139.9, 136.2, 133.5, 129.1, 128.9, 128.5, 128.1, 128.0, 127.9, 127.7, 127.3, 127.0, 116.5, 90.2, 78.9, 43.5, 38.5, 28.6, 28.3, 27.6.

diphenylmethanone O-(2,5-diphenylpent-1-en-4-yn-3-yl) oxime (1ax)



Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.50–7.48 (m, 4H), 7.44–7.41 (m, 2H), 7.36–7.28 (m, 12H), 7.16–7.14 (m, 2H), 6.12 (s, 1H), 5.73 (s, 1H), 5.57 (s, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 158.0, 144.7, 138.6, 136.4, 133.0, 131.8, 129.43, 129.39, 128.7, 128.4, 128.21, 128.17, 128.11, 127.8, 127.7, 127.1, 126.6, 122.8, 117.2, 87.7, 86.7, 76.5.

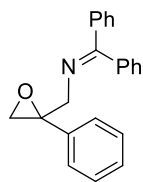
diphenylmethanone O-(5,9-dimethyl-2-phenyldeca-1,8-dien-3-yl) oxime (1ay)



Colorless oil; ^1H NMR (400 MHz, CDCl_3): δ 7.50–7.47 (m, 2H), 7.42–7.20 (m, 13H), 5.33–5.32 (m, 1H), 5.32–5.22 (m, 2H), 5.21–5.00 (m, 1H), 1.89–1.85 (m, 2H), 1.70–1.63 (m, 4H), 1.54–1.53 (m, 4H), 1.34–1.24 (m, 2H), 1.13–1.10 (m, 1H), 0.90–0.84 (m, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 156.49, 156.47, 149.7, 149.4, 140.2, 140.1, 136.7, 133.8, 133.7, 130.98, 130.96, 129.2, 129.1, 128.5, 128.1, 128.04, 127.90, 127.87, 127.84, 127.28, 127.26, 127.2, 127.1, 124.8, 115.1, 114.3, 85.2, 84.4, 41.0, 40.5, 37.4, 36.7, 29.4, 29.2, 25.70, 25.69, 25.4, 25.3, 20.0, 19.5, 17.6.

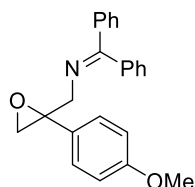
9 Analytical data for product

1,1-diphenyl-N-((2-phenyloxiran-2-yl)methyl)methanimine (2a)



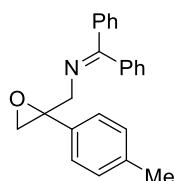
Colorless oil; (0.050 g, 80%); R_f = 0.23 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.60–7.58 (m, 2H), 7.45–7.35 (m, 5H), 7.33–7.27 (m, 6H), 7.12–7.10 (m, 2H), 3.96 (d, J = 14.8 Hz, 1H), 3.85 (d, J = 14.8 Hz, 1H), 3.35 (d, J = 5.6 Hz, 1H), 2.83 (d, J = 6.0 Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 170.0, 139.6, 139.5, 136.4, 130.1, 128.51, 128.48, 128.46, 128.15, 127.97, 127.7, 127.5, 126.4, 60.4, 57.2, 53.2; ESI-HRMS: Calcd for $\text{C}_{22}\text{H}_{20}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 314.1539, found 314.1538,

N-((2-(4-methoxyphenyl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2b)



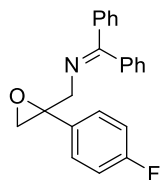
Colorless oil; (0.048 g, 70%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.59 (d, J = 7.2 Hz, 2H), 7.44–7.26 (m, 8H), 7.13–7.11 (m, 2H), 6.85 (d, J = 8.8 Hz, 2H), 3.93 (d, J = 14.8 Hz, 1H), 3.83–3.79 (m, 4H), 3.33 (d, J = 5.6 Hz, 1H), 2.83 (d, J = 5.6 Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 169.9, 159.0, 139.5, 136.4, 131.7, 130.1, 128.53, 128.49, 128.47, 128.0, 127.74, 127.65, 113.5, 60.1, 57.4, 55.3, 53.3; ESI-HRMS: Calcd for $\text{C}_{23}\text{H}_{22}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 344.1645, found 344.1643.

1,1-diphenyl-N-((2-(p-tolyl)oxiran-2-yl)methyl)methanimine (2c)



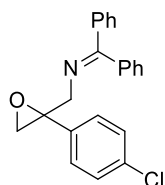
Colorless oil; (0.060 g, 92%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.60–7.58 (m, 2H), 7.44–7.35 (m, 4H), 7.33–7.28 (m, 4H), 7.13–7.11 (m, 4H), 3.94 (d, J = 10.0 Hz, 1H), 3.83 (d, J = 10.0 Hz, 1H), 3.34 (d, J = 3.6 Hz, 1H), 2.81 (d, J = 3.6 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 169.9, 139.6, 137.2, 136.6, 136.5, 130.1, 128.8, 128.51, 128.49, 128.4, 128.0, 127.8, 126.3, 60.3, 57.2, 53.2, 21.1; ESI-HRMS: Calcd for $\text{C}_{23}\text{H}_{22}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 344.1696, found 344.1697.

N-((2-(4-fluorophenyl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2d)



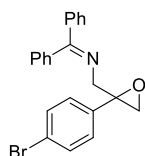
Colorless oil; (0.056 g, 84%); R_f = 0.30 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.59–7.57 (m, 2H), 7.46–7.36 (m, 6H), 7.33–7.29 (m, 2H), 7.12–7.10 (m, 2H), 7.02–6.98 (m, 2H), 3.90 (d, J = 14.8 Hz, 1H), 3.82 (d, J = 14.8 Hz, 1H), 3.30 (d, J = 6.4 Hz, 1H), 2.81 (d, J = 6.4 Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 170.1, 162.2 (d, $^1J_{\text{C-F}}$ = 246.5 Hz), 139.4, 136.3, 135.3 (d, $^4J_{\text{C-F}}$ = 3.0 Hz), 130.2, 128.6, 128.5, 128.2 (d, $^3J_{\text{C-F}}$ = 8.1 Hz), 128.0, 127.7, 114.1 (d, $^2J_{\text{C-F}}$ = 21.1 Hz), 60.0, 57.5, 53.4; ^{19}F NMR (376 MHz, CDCl_3): δ -114.67 (s, 1F); ESI-HRMS: Calcd for $\text{C}_{22}\text{H}_{19}\text{FNO}^+$ $[\text{M}+\text{H}]^+$ 332.1445, found 332.1446.

N-((2-(4-chlorophenyl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2e)



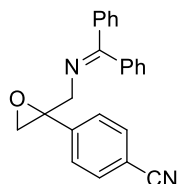
Colorless oil; (0.052 g, 75%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.82–7.80 (m, 2H), 7.58–7.25 (m, 10H), 7.12–7.10 (m, 2H), 3.89 (d, J = 14.8 Hz, 1H), 3.82 (d, J = 14.8 Hz, 1H), 3.29 (d, J = 6.4 Hz, 1H), 2.79 (d, J = 6.4 Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 170.2, 139.3, 138.1, 136.3, 133.4, 130.2, 130.0, 128.6, 128.5, 128.3, 128.0, 127.8, 127.7, 59.9, 57.3, 53.5; ESI-HRMS: Calcd for $\text{C}_{22}\text{H}_{19}\text{ClNO}^+$ $[\text{M}+\text{H}]^+$ 348.1150, found 348.1138.

N-((2-(4-bromophenyl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2f)



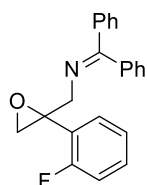
Colorless oil; (0.065 g, 84%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.59–7.56 (m, 2H), 7.46–7.29 (m, 10H), 7.12–7.10 (m, 2H), 3.89 (d, J = 14.8 Hz, 1H), 3.82 (d, J = 14.8 Hz, 1H), 3.28 (d, J = 5.6 Hz, 1H), 2.79 (d, J = 5.6 Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 170.2, 139.3, 138.6, 136.3, 131.3, 130.2, 130.0, 128.6, 128.5, 128.2, 128.0, 127.7, 121.5, 60.0, 57.3, 53.5; ESI-HRMS: Calcd for $\text{C}_{22}\text{H}_{19}\text{BrNO}^+$ $[\text{M}+\text{H}]^+$ 392.0645, found 392.0647.

4-((2-(((diphenylmethylene)amino)methyl)oxiran-2-yl)benzonitrile (2g)



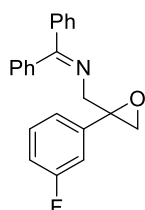
Colorless oil; (0.054 g, 81%); R_f = 0.28 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.63 (d, J = 8.4 Hz, 2H), 7.57–7.55 (m, 4H), 7.47–7.37 (m, 4H), 7.33–7.30 (m, 2H), 7.14–7.12 (m, 2H), 3.88 (s, 2H), 3.29 (d, J = 5.6 Hz, 1H), 2.80 (d, J = 5.6 Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 170.4, 145.0, 139.1, 136.1, 132.0, 130.4, 128.7, 128.6, 128.5, 128.05, 127.6, 127.1, 118.7, 111.3, 59.9, 57.1, 53.9; ESI-HRMS: Calcd for $\text{C}_{23}\text{H}_{19}\text{N}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 339.1492, found 339.1498.

N-((2-(2-fluorophenyl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2h)



Colorless oil; (0.046 g, 70%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.57–7.56 (m, 2H), 7.49–7.26 (m, 8H), 7.14–7.08 (m, 3H), 7.03–6.98 (m, 1H), 3.90 (d, J = 2.8 Hz, 1H), 3.76 (d, J = 2.8 Hz, 1H), 3.38 (d, J = 4.8 Hz, 1H), 2.88 (d, J = 5.2 Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 170.0, 160.4 (d, $^1J_{\text{C-F}}$ = 246.5 Hz), 139.5, 136.4, 132.4, 130.1 (d, $^3J_{\text{C-F}}$ = 5.2 Hz), 129.5 (d, $^3J_{\text{C-F}}$ = 7.9 Hz), 129.4, 128.5, 128.4, 128.2, 127.8 (d, $^2J_{\text{C-F}}$ = 25.0 Hz), 126.8, 123.9 (d, $^4J_{\text{C-F}}$ = 3.4 Hz), 115.1 (d, $^2J_{\text{C-F}}$ = 21.0 Hz), 58.3, 57.0, 51.5; ^{19}F NMR (376 MHz, CDCl_3): δ -116.23 (s, 1F); ESI-HRMS: Calcd for $\text{C}_{22}\text{H}_{19}\text{NFO}^+$ $[\text{M}+\text{H}]^+$ 332.1445, found 332.1450.

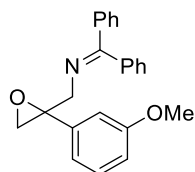
N-((2-(3-fluorophenyl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2i)



Colorless oil; (0.046 g, 70%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (600 MHz, CDCl_3): δ 7.59–7.58 (m, 2H), 7.46–7.41 (m, 3H), 7.38–7.36 (m, 1H), 7.32–7.24 (m, 3H), 7.21–7.20 (m, 1H), 7.15–7.12 (m, 3H), 6.97–6.94 (m, 1H), 3.92 (d, J = 9.8 Hz, 1H), 3.84 (d, J = 10.0 Hz, 1H), 3.31 (d, J = 3.6 Hz, 1H), 2.80 (d, J = 3.6 Hz, 1H); ^{13}C NMR (150.6 MHz, CDCl_3): δ 170.2, 162.7 (d, $^1J_{\text{C-F}}$ = 244.0 Hz), 142.2 (d, $^3J_{\text{C-F}}$ = 7.5 Hz), 139.4, 136.3, 130.2, 129.7 (d, $^3J_{\text{C-F}}$ = 9.0 Hz), 128.58, 128.57, 128.5, 128.0, 127.7, 122.0 (d, $^4J_{\text{C-F}}$ = 1.5 Hz), 114.4 (d, $^2J_{\text{C-F}}$ = 21.1 Hz), 113.4 (d, $^2J_{\text{C-F}}$ = 22.6 Hz), 59.9 (d, $^4J_{\text{C-F}}$ = 1.5 Hz), 57.1, 53.6;

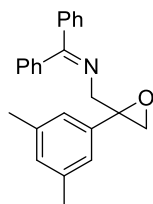
^{19}F NMR (376 MHz, CDCl_3): δ -112.99 (m, 1F); ESI-HRMS: Calcd for $\text{C}_{22}\text{H}_{19}\text{NFO}^+$ $[\text{M}+\text{H}]^+$ 332.1445, found 332.1445.

N-((2-(3-methoxyphenyl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2j)



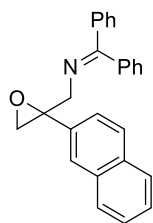
Colorless oil; (0.056 g, 82%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.61–7.59 (m, 2H), 7.46–7.29 (m, 6H), 7.25–7.21 (m, 1H), 7.13–7.10 (m, 2H), 7.00–6.97 (m, 2H), 6.81 (ddd, J = 8.0, 2.4, 0.8 Hz, 1H), 3.95 (d, J = 14.8 Hz, 1H), 3.84 (d, J = 14.8 Hz, 1H), 3.77 (s, 3H), 3.36 (d, J = 6.0 Hz, 1H), 2.83 (d, J = 5.6 Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 170.0, 159.5, 141.2, 139.5, 136.4, 130.1, 129.2, 128.51, 128.48, 128.0, 127.7, 118.7, 113.3, 111.6, 60.4, 57.1, 55.2, 53.3; ESI-HRMS: Calcd for $\text{C}_{23}\text{H}_{12}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 344.1645, found 344.1646.

N-((2-(3,5-dimethylphenyl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2k)



Colorless oil; (0.063 g, 92%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.60–7.58 (m, 2H), 7.44–7.29 (m, 6H), 7.13–7.11 (m, 2H), 7.01 (m, 2H), 6.90 (s, 1H), 3.95 (d, J = 14.8 Hz, 1H), 3.90 (d, J = 14.8 Hz, 1H), 3.31 (d, J = 6.0 Hz, 1H), 2.87 (d, J = 6.0 Hz, 1H), 2.28 (s, 6H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 169.9, 139.6, 139.4, 137.7, 136.5, 130.0, 129.2, 128.49, 128.47, 128.4, 128.0, 127.8, 124.1, 60.5, 57.0, 53.0, 21.3; ESI-HRMS: Calcd for $\text{C}_{24}\text{H}_{24}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 342.1852, found 342.1855.

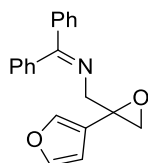
N-((2-(naphthalen-2-yl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2l)



Colorless oil; (0.055 g, 76%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.88 (d, J = 0.8 Hz, 1H), 7.80–7.78 (m, 3H), 7.60–7.58 (m, 2H), 7.54–7.51 (m, 1H), 7.49–7.37 (m, 5H), 7.35 (m, 1H), 7.32–7.26 (m, 2H), 7.17–7.10 (m, 2H), 4.05 (d, J = 14.8 Hz, 1H), 3.96 (d, J = 14.8 Hz, 1H), 3.42 (d, J = 5.6 Hz, 1H), 2.92 (d, J = 5.6 Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 170.1, 139.5, 137.0, 136.4, 133.0, 132.7, 130.1,

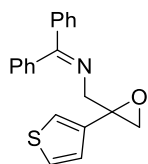
128.54, 128.51, 127.99, 127.94, 127.85, 127.76, 127.6, 126.1, 126.0, 125.4, 124.3, 60.6, 57.3, 53.5; ESI-HRMS: Calcd for $C_{26}H_{22}NO^+$ $[M+H]^+$ 364.1696, found 364.1696.

N-((2-(furan-3-yl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2m)



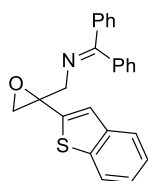
Colorless oil; (0.039 g, 64%); R_f = 0.35 (10:1 petroleum ether / ethyl acetate); 1H NMR (400 MHz, $CDCl_3$): δ 7.63–7.61 (m, 2H), 7.52–7.26 (m, 8H), 7.18–7.16 (m, 2H), 6.34 (s, 1H), 3.90 (d, J = 14.8 Hz, 1H), 3.72 (d, J = 14.8 Hz, 1H), 3.24 (d, J = 5.2 Hz, 1H), 2.96 (d, J = 5.2 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ 170.1, 142.90, 140.9, 139.4, 136.3, 130.2, 128.61, 128.59, 128.5, 128.0, 127.7, 124.9, 108.8, 57.3, 55.3, 53.7; ESI-HRMS: Calcd for $C_{20}H_{18}NO_2^+$ $[M+H]^+$ 304.1332, found 304.1335.

1,1-diphenyl-N-((2-(thiophen-3-yl)oxiran-2-yl)methyl)methanimine (2n)



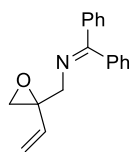
Colorless oil; (0.035 g, 55%); R_f = 0.28 (10:1 petroleum ether / ethyl acetate); 1H NMR (400 MHz, $CDCl_3$): δ 7.62–7.60 (m, 2H), 7.52–7.31 (m, 8H), 7.18–7.16 (m, 2H), 3.90 (d, J = 15.0 Hz, 1H), 3.72 (d, J = 15.0 Hz, 1H), 3.24 (d, J = 6.0 Hz, 1H), 2.95 (d, J = 6.0 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ 170.0, 141.2, 139.5, 136.4, 130.2, 128.59, 128.55, 128.5, 128.0, 127.7, 126.1, 125.6, 122.3, 57.9, 57.2, 54.0; ESI-HRMS: Calcd for $C_{20}H_{18}NOS^+$ $[M+H]^+$ 320.1104, found 320.1107.

N-((2-(benzo[b]thiophen-2-yl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2o)



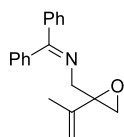
Colorless oil; (0.044g, 60%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); 1H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.80 (m, 2H), 7.58 – 7.56 (m, 2H), 7.45 (s, 1H), 7.37 – 7.24 (m, 8H), 7.00 – 6.98 (m, 2H) 3.99 (d, J = 14.8 Hz, 1H), 3.91 (d, J = 14.4 Hz, 1H), 3.44 (d, J = 5.6 Hz, 1H), 2.99 (d, J = 5.6 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.3, 140.2, 139.4, 137.7, 136.3, 134.7, 130.2, 128.5, 128.44, 128.41, 128.0, 127.6, 124.8, 124.3, 124.1, 122.7, 122.6, 58.5, 57.1, 51.1; ESI-HRMS: Calcd for $C_{24}H_{20}NOS^+$ $[M+H]^+$ 370.1260, found 370.1263.

1,1-diphenyl-N-((2-vinyloxiran-2-yl)methyl)methanimine (2p)



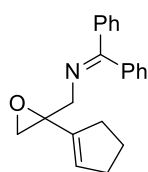
Colorless oil; (0.026 g, 50%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3) δ 7.62–7.61 (m, 2H), 7.48–7.42 (m, 3H), 7.40–7.37 (m, 1H), 7.34–7.26 (m, 2H), 7.18–7.17 (m, 2H), 5.95 (dd, J = 7.2, 4.4 Hz, 1H), 5.37 (d, J = 11.6 Hz, 1H), 5.24 (d, J = 7.2 Hz, 1H), 3.76 (d, J = 10.0 Hz, 1H), 3.61 (d, J = 9.6 Hz, 1H), 3.13 (d, J = 3.6 Hz, 1H), 2.75 (d, J = 4.0 Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 169.9, 139.5, 136.7, 136.4, 130.1, 128.6, 128.53, 128.48, 128.0, 127.7, 116.8, 58.7, 55.8, 53.7; ESI-HRMS: Calcd for $\text{C}_{18}\text{H}_{18}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 264.1383, found 264.1391.

1,1-diphenyl-N-((2-(prop-1-en-2-yl)oxiran-2-yl)methyl)methanimine (2q)



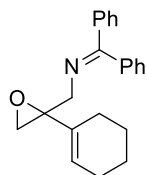
Colorless oil; (0.028 g, 50%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.61–7.59 (m, 2H), 7.48–7.42 (m, 3H), 7.38–7.30 (m, 3H), 7.19–7.16 (m, 2H), 5.09–5.08 (m, 1H), 4.98–4.97 (m, 1H), 3.72 (d, J = 16 Hz, 1H), 3.66 (d, J = 16 Hz, 1H), 3.08 (d, J = 6.4 Hz, 1H), 2.75 (d, J = 6.4 Hz, 1H), 1.78–1.77 (m, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 169.7, 143.0, 139.7, 136.5, 130.1, 128.5, 128.0, 127.9, 113.3, 61.4, 55.9, 51.8, 19.4; ESI-HRMS: Calcd for $\text{C}_{19}\text{H}_{20}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 278.1539, found 278.1540.

N-((2-(cyclopent-1-en-1-yl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2r)



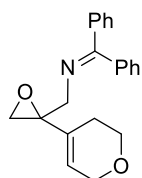
Colorless oil; (0.041 g, 67%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3) δ 7.61–7.59 (m, 2H), 7.46–7.26 (m, 6H), 7.19–7.16 (m, 2H), 5.75 (dd, J = 2.0, 2.0 Hz, 1H), 3.84 (d, J = 14.8 Hz, 1H), 3.51 (d, J = 14.8 Hz, 1H), 3.16 (d, J = 5.6 Hz, 1H), 2.89 (d, J = 5.6 Hz, 1H), 2.37–2.25 (m, 4H), 1.89–1.82 (m, 2H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 169.6, 142.3, 139.7, 136.5, 130.0, 129.2, 128.52, 128.48, 128.0, 127.8, 58.0, 56.0, 51.4, 32.9, 31.8, 23.0; ESI-HRMS: Calcd for $\text{C}_{21}\text{H}_{22}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 304.1696, found 304.1670.

N-((2-(cyclohex-1-en-1-yl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2s)



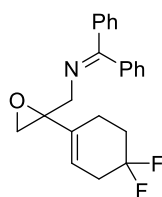
Colorless oil; (0.048 g, 75%); $R_f = 0.25$ (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3) δ 7.60–7.58 (m, 2H), 7.48–7.30 (m, 6H), 7.26–7.16 (m, 2H), 5.80 (m, 1H), 3.73 (d, $J = 14.8$ Hz, 1H), 3.61 (d, $J = 14.8$ Hz, 1H), 3.09 (d, $J = 5.6$ Hz, 1H), 2.76 (d, $J = 5.6$ Hz, 1H), 2.01–1.98 (m, 4H), 1.64–1.55 (m, 4H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 169.5, 139.7, 136.5, 135.4, 130.0, 128.48, 128.45, 128.0, 127.9, 124.9, 61.7, 55.8, 51.4, 25.0, 24.9, 22.5, 22.2; ESI-HRMS: Calcd for $\text{C}_{22}\text{H}_{24}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 318.1852, found 318.1854.

N-((2-(3,6-dihydro-2H-pyran-4-yl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2t)



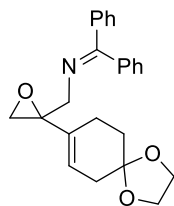
Colorless oil; (0.046 g, 72%); $R_f = 0.25$ (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3) δ 7.61–7.59 (m, 2H), 7.48–7.36 (m, 6H), 7.34–7.16 (m, 2H), 5.83–5.82 (m, 1H), 4.15 (m, 2H), 3.82–3.63 (m, 4H), 3.09 (d, $J = 5.6$ Hz, 1H), 2.78 (d, $J = 5.6$ Hz, 1H), 2.14–2.12 (m, 2H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 169.8, 139.5, 136.4, 133.6, 130.1, 128.6, 128.5, 128.0, 127.8, 123.4, 65.2, 64.1, 60.3, 55.6, 51.3, 25.0; ESI-HRMS: Calcd for $\text{C}_{21}\text{H}_{22}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 320.1645, found 320.1643.

N-((2-(4,4-difluorocyclohex-1-en-1-yl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2u)



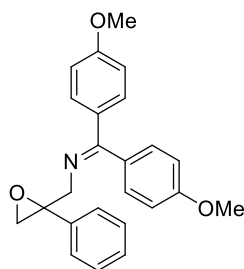
Colorless oil; (0.058 g, 82%); $R_f = 0.40$ (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3) δ 7.60–7.56 (m, 2H), 7.49–7.26 (m, 6H), 7.17–7.14 (m, 2H), 5.69 (m, 1H), 3.70–3.61 (m, 2H), 3.05 (d, $J = 5.2$ Hz, 1H), 2.74 (d, $J = 5.2$ Hz, 1H), 2.57–2.50 (m, 2H), 2.34–2.27 (m, 2H), 2.07–1.95 (m, 2H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 169.9, 139.5, 136.32, 135.28, 132.4, 130.2, 128.6, 128.5, 128.0, 127.8, 122.7 (t, $J = 239.4$ Hz), 119.5 (t, $J = 5.0$ Hz), 60.8, 56.1, 51.8, 34.4 (t, $J = 26.2$ Hz), 30.1 (t, $J = 24.1$ Hz), 23.6 (t, $J = 5.0$ Hz); ^{19}F NMR (376 MHz, CDCl_3) δ -96.74 (d, $J = 235.0$ Hz, 1F), -96.06 (d, $J = 235.0$ Hz, 1F); ESI-HRMS: Calcd for $\text{C}_{22}\text{H}_{22}\text{F}_2\text{NO}^+$ $[\text{M}+\text{H}]^+$ 354.1664, found 354.1667.

N-((2-(1,4-dioxaspiro[4.5]dec-7-en-8-yl)oxiran-2-yl)methyl)-1,1-diphenylmethanimine (2v)



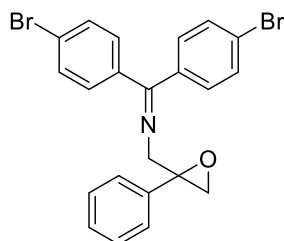
Colorless oil; (0.062 g, 82%); R_f = 0.35 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3) δ 7.60–7.58 (m, 2H), 7.47–7.26 (m, 6H), 7.18–7.16 (m, 2H), 5.73–5.71 (m, 1H), 3.96 (m, 4H), 3.75 (d, J = 14.8 Hz, 1H), 3.65 (d, J = 14.8 Hz, 1H), 3.13 (d, J = 5.6 Hz, 1H), 2.77 (d, J = 5.6 Hz, 1H), 2.29–2.23 (m, 4H), 1.76–1.73 (m, 2H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 169.7, 139.7, 136.5, 135.2, 130.0, 128.50, 128.46, 128.0, 127.8, 121.9, 107.8, 64.3, 61.0, 55.5, 51.3, 35.5, 30.9, 24.2; ESI-HRMS: Calcd for $\text{C}_{24}\text{H}_{26}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$ 376.1907, found 376.1908.

1,1-bis(4-methoxyphenyl)-N-((2-phenyloxiran-2-yl)methyl)methanimine (2w)



Colorless oil; (0.049 g, 65%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3) δ 7.55 – 7.53 (m, 2H), 7.42 – 7.40 (m, 1H), 7.33 – 7.24 (m, 3H), 7.06 – 7.03 (m, 2H), 6.95 – 6.93 (m, 2H), 6.83 – 6.80 (m, 2H), 3.98 – 3.94 (m, 1H), 3.87 (d, J = 3.4 Hz, 1H), 3.84 (s, 3H), 3.79 (s, 3H), 3.35 (d, J = 5.7 Hz, 1H), 2.82 (d, J = 5.7 Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 169.3, 161.2, 159.6, 139.8, 133.0, 132.3, 130.2, 129.4, 128.8, 128.2, 127.6, 126.5, 113.8, 113.3, 60.6, 57.1, 55.3, 53.3; ESI-HRMS: Calcd for $\text{C}_{24}\text{H}_{24}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$ 374.1751, found 374.1755.

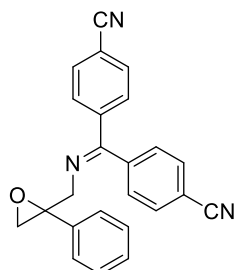
1,1-bis(4-bromophenyl)-N-((2-phenyloxiran-2-yl)methyl)methanimine (2x)



Colorless oil; (0.060 g, 83%); R_f = 0.34 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3) δ 7.61 – 7.56 (m, 2H), 7.46 – 7.36 (m, 6H), 7.35 – 7.27 (m, 3H), 7.01 – 6.95

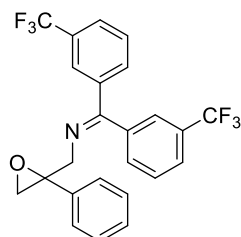
(m, 2H), 3.90 (d, $J = 14.7$ Hz, 1H), 3.84 (d, $J = 14.7$ Hz, 1H), 3.32 (d, $J = 5.6$ Hz, 1H), 2.83 (d, $J = 5.6$ Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 167.9, 139.2, 138.0, 134.5, 132.0, 131.3, 129.9, 129.5, 128.3, 127.7, 126.3, 125.1, 123.1, 60.3, 57.3, 53.1; ESI-HRMS: Calcd for $\text{C}_{22}\text{H}_{18}\text{Br}_2\text{NO}^+$ $[\text{M}+\text{H}]^+$ 469.9750, found 469.9757.

4,4'-((((2-phenyloxiran-2-yl)methyl)imino)methylene)dibenzonitrile (2y)



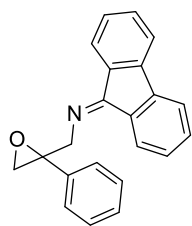
Colorless oil; (0.052 g, 71%); $R_f = 0.40$ (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3) δ 7.79 – 7.77 (m, 2H), 7.63 (s, 4H), 7.38 – 7.30 (m, 5H), 7.25 – 7.23 (m, 2H), 3.90 (s, 1H), 3.29 (d, $J = 5.5$ Hz, 1H), 2.85 (d, $J = 5.5$ Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 166.5, 142.0, 139.7, 138.7, 132.7, 132.0, 128.7, 128.6, 128.3, 127.9, 126.2, 118.3, 117.9, 114.0, 113.2, 60.1, 57.5, 53.0; ESI-HRMS: Calcd for $\text{C}_{24}\text{H}_{18}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 364.1444, found 364.1445.

N-((2-phenyloxiran-2-yl)methyl)-1,1-bis(3-(trifluoromethyl)phenyl)methanimine (2z)



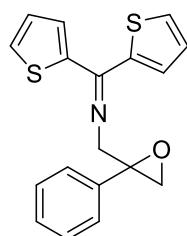
Colorless oil; (0.067 g, 75%); $R_f = 0.25$ (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.92 (m, 1H), 7.73–7.71 (m, 1H), 7.66–7.59 (m, 3H), 7.46–7.38 (m, 4H), 7.36–7.24 (m, 4H), 3.95 (d, $J = 14.4$ Hz, 1H), 3.86 (d, $J = 14.4$ Hz, 1H), 3.33 (d, $J = 5.6$ Hz, 1H), 2.86 (d, $J = 5.6$ Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 167.1, 139.6, 139.0, 136.2, 131.8, 131.4 (q, $^2J_{\text{C-F}} = 32$ Hz), 131.2, 130.8 (q, $^2J_{\text{C-F}} = 32$ Hz), 129.5, 128.8, 128.3, 127.8, 127.0 (q, $^3J_{\text{C-F}} = 4$ Hz), 126.4, 125.9 (q, $^3J_{\text{C-F}} = 4$ Hz), 124.9 (q, $^3J_{\text{C-F}} = 4$ Hz), 124.6 (q, $^3J_{\text{C-F}} = 4$ Hz), 123.9 (q, $^1J_{\text{C-F}} = 270$ Hz), 123.7 (q, $^1J_{\text{C-F}} = 270$ Hz), 60.3, 57.5, 53.0; ^{19}F NMR (376 MHz, CDCl_3): δ -62.66 (s, 3F), -62.69 (s, 3F); ESI-HRMS: Calcd for $\text{C}_{24}\text{H}_{18}\text{F}_6\text{NO}^+$ $[\text{M}+\text{H}]^+$ 450.1287, found 450.1287.

N-((2-phenyloxiran-2-yl)methyl)-9H-fluoren-9-imine (2aa)



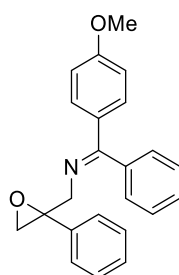
Colorless oil; (0.039 g, 63%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.82–7.78 (m, 2H), 7.66–7.63 (m, 1H), 7.61–7.54 (m, 3H), 7.44–7.37 (m, 4H), 7.35–7.24 (m, 3H), 4.74 (d, J = 16.8 Hz, 1H), 4.56 (d, J = 16.8 Hz, 1H), 3.55 (d, J = 5.6 Hz, 1H), 2.95 (d, J = 5.6 Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 163.9, 143.6, 141.0, 139.6, 138.3, 131.9, 131.4, 130.9, 128.34, 128.28, 127.9, 127.8, 127.5, 126.4, 122.7, 120.4, 119.3, 60.3, 56.6, 53.5; ESI-HRMS: Calcd for $\text{C}_{22}\text{H}_{18}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 312.1383, found 312.1385.

N-((2-phenyloxiran-2-yl)methyl)-1,1-di(thiophen-2-yl)methanimine(2ab)



Colorless oil; (0.039 g, 61%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.49 – 7.43 (m, 3H), 7.40 (dd, J = 5.1, 1.1 Hz, 1H), 7.36 – 7.26 (m, 3H), 7.12 (t, J = 3.1 Hz, 2H), 7.05 (d, J = 3.6 Hz, 1H), 6.98 (dd, J = 5.0, 3.8 Hz, 1H), 4.14 (d, J = 14.8 Hz, 1H), 3.97 (d, J = 14.7 Hz, 1H), 3.36 (d, J = 5.6 Hz, 1H), 2.82 (d, J = 5.6 Hz, 1H). ^{13}C NMR (100.6 MHz, CDCl_3): δ 158.0, 147.1, 139.5, 133.6, 130.7, 129.8, 129.1, 128.2, 127.7, 127.3, 127.2, 126.8, 126.4, 60.3, 56.7, 52.9; ESI-HRMS: Calcd for $\text{C}_{18}\text{H}_{16}\text{NOS}_2^+$ $[\text{M}+\text{H}]^+$ 326.0668, found 326.0668.

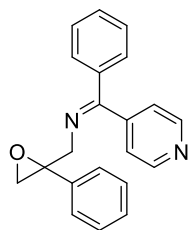
1-(4-methoxyphenyl)-1-phenyl-N-((2-phenyloxiran-2-yl)methyl)methanimine (2ac)



Colorless oil; (0.044 g, 64%, Z:E = 2:1); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.55–7.52 (m, 2H), 7.45–7.38 (m, 4H), 7.36–7.23 (m, 4H), 7.11–7.05 (m, 2H), 6.96–6.80 (m, 2H), 4.04–3.78 (m, 5H), 3.37–3.33 (m, 1H), 2.83–2.81 (m, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 170.1, 169.7, 161.3, 159.6, 140.0, 139.5, 136.5, 132.5, 132.2, 130.2, 130.0, 129.7, 129.4, 128.6, 128.44, 128.39, 128.36, 128.12, 128.10, 127.9,

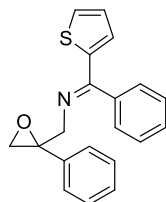
127.7, 127.5, 126.4, 126.3, 113.8, 113.3, 60.4, 57.1, 56.7, 55.23, 55.20, 53.19, 53.16; ESI-HRMS: Calcd for $C_{23}H_{22}NO_2^+$ $[M+H]^+$ 344.1645, found 344.1647.

(Z)-1-phenyl-N-((2-phenyloxiran-2-yl)methyl)-1-(pyridin-4-yl)methanimine (2ad)



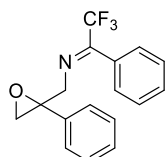
Colorless oil; (0.045 g, 72%); R_f = 0.2 (5:1 petroleum ether / ethyl acetate); 1H NMR (400 MHz, $CDCl_3$) δ 8.74 – 8.69 (m, 2H), 8.60 – 8.59 (m, 3H), 7.58 – 7.52 (m, 2H), 7.49 – 7.24 (m, 23H), 7.13 – 7.09 (m, 3H), 7.08 – 7.02 (m, 2H), 4.01 – 3.92 (m, 3H), 3.91 (d, J = 14.5 Hz, 1H), 3.80 (d, J = 14.5 Hz, 1H), 3.33 (t, J = 5.7 Hz, 2.5H), 2.84 (t, J = 5.5 Hz, 2.5H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ 168.3, 167.3, 150.1, 149.7, 146.4, 144.5, 139.13, 139.07, 137.9, 134.8, 130.7, 129.1, 128.8, 128.24, 128.19, 127.74, 127.70, 127.6, 126.31, 126.28, 122.6, 122.4, 60.24, 60.21, 57.5, 57.2, 53.2, 52.9; ESI-HRMS: Calcd for $C_{21}H_{19}N_2O^+$ $[M+H]^+$ 315.1492, found 315.1495.

(E)-1-phenyl-N-((2-phenyloxiran-2-yl)methyl)-1-(thiophen-2-yl)methanimine (2ae)



Colorless oil; (0.045 g, 74%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); 1H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.38 (m, 6H), 7.33 – 7.24 (m, 3H), 7.21 – 7.18 (m, 2H), 6.94 – 6.92 (m, 1H), 6.76 – 6.47 (m, 1H), 3.98 (d, J = 14.5 Hz, 1H), 3.77 (d, J = 14.5 Hz, 1H), 3.36 (d, J = 5.7 Hz, 1H), 2.80 (d, J = 5.7 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ 165.0, 147.0, 139.5, 135.4, 130.6, 129.4, 128.8, 128.4, 128.1, 127.7, 127.6, 127.2, 126.4, 60.4, 56.2, 52.8; ESI-HRMS: Calcd for $C_{20}H_{18}NOS^+$ $[M+H]^+$ 320.1104, found 320.1101.

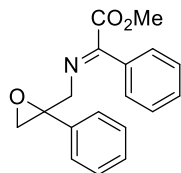
(E)-2,2,2-trifluoro-1-phenyl-N-((2-phenyloxiran-2-yl)methyl)ethan-1-imine (2af)



Colorless oil; (0.049 g, 80%, E only); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); 1H NMR (400 MHz, $CDCl_3$): δ 7.48–7.41 (m, 3H), 7.37–7.25 (m, 5H), 7.20–7.18 (m, 2H), 4.00 (dd, J_1 = 14.4 Hz, J_2 = 1.6 Hz, 1H), 3.85 (dd, J_1 = 14.4 Hz, J_2 = 1.2 Hz, 1H), 3.30 (d, J = 5.6 Hz, 1H), 2.82 (d, J = 5.6 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ 160.6 (q, $^2J_{C-F}$ = 34 Hz),

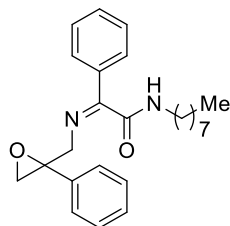
138.5, 130.2, 129.9, 128.8, 128.4, 128.0, 127.8, 126.3, 119.5 (q, $^1J_{\text{C-F}} = 277$ Hz), 59.5, 56.3, 52.8; ^{19}F NMR (376 MHz, CDCl_3): δ -71.07 (s, 3F); E ESI-HRMS: Calcd for $\text{C}_{17}\text{H}_{15}\text{F}_3\text{NO}^+$ $[\text{M}+\text{H}]^+$ 306.1100, found 306.1104.

methyl-2-phenyl-2-(((2-phenyloxiran-2-yl)methyl)imino)acetate (2ag)



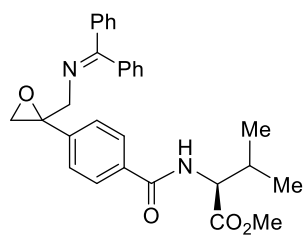
Colorless oil; (0.043 g, 72%, Z:E = 7:1); $R_f = 0.25$ (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.95–7.92 (m, 0.15H), 7.62–7.59 (m, 2H), 7.42–7.22 (m, 9H), 7.16–7.11 (m, 0.3H), 6.66 (m, 1.07H), 4.09–4.03 (m, 1.15H), 3.92–3.88 (m, 1.16H), 3.83 (s, 3H), 3.76 (s, 0.31H), 3.27 (d, $J = 5.2$ Hz, 0.15H), 3.23 (d, $J = 5.6$ Hz, 1H), 2.78 (d, $J = 5.6$ Hz, 1H), 2.73 (d, $J = 5.2$ Hz, 0.15H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 165.3, 164.9, 163.7, 161.5, 139.0, 138.8, 134.9, 134.0, 131.2, 130.0, 128.5, 128.4, 128.30, 128.27, 127.84, 127.75, 127.7, 127.3, 126.3, 126.2, 59.8, 59.7, 58.0, 56.9, 53.5, 52.9, 52.8, 51.9; ESI-HRMS: Calcd for $\text{C}_{18}\text{H}_{18}\text{NO}_3^+$ $[\text{M}+\text{H}]^+$ 296.1281, found 296.1282.

N-octyl-2-phenyl-2-(((2-phenyloxiran-2-yl)methyl)imino)acetamide (2ah)



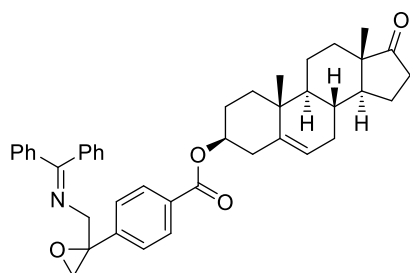
Colorless oil; (0.053 g, 67%, Z:E = 1.4:1); $R_f = 0.25$ (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.82–7.79 (m, 2H), 7.46–7.29 (m, 20.89H), 7.18–7.16 (m, 3H), 4.41 (d, $J = 13.2$ Hz, 1H), 4.15 (d, $J = 13.2$ Hz, 1H), 4.06 (d, $J = 15.2$ Hz, 1.41H), 3.84 (d, $J = 15.2$ Hz, 1.40H), 3.44–3.25 (m, 5.83H), 3.14 (d, $J = 5.6$ Hz, 1.41H), 2.84–2.81 (m, 2.42H), 1.57–1.50 (m, 4.82H), 1.29–1.24 (m, 24.45H), 0.91–0.86 (m, 7.29H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 167.0, 165.4, 165.1, 163.3, 138.6, 134.7, 134.3, 132.2, 131.2, 131.0, 129.3, 128.5, 128.4, 128.3, 128.10, 128.06, 127.8, 127.7, 126.2, 125.9, 60.5, 59.9, 57.1, 55.9, 53.5, 52.7, 39.4, 39.2, 31.78, 31.75, 29.5, 29.4, 29.22, 29.17, 29.15, 29.1, 27.0, 26.9, 22.62, 22.60, 14.1; ESI-HRMS: Calcd for $\text{C}_{25}\text{H}_{33}\text{N}_2\text{O}_2^+$ $[\text{M}+\text{H}]^+$ 393.2537, found 393.2536.

methyl (4-(2-(((diphenylmethylene)amino)methyl)oxiran-2-yl)benzoyl)-L-valinate (2ai)



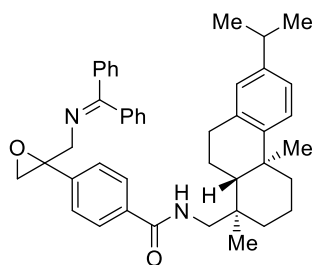
Colorless oil; (0.047 g, 49%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.79–7.77 (m, 2H), 7.59–7.57 (m, 2H), 7.53–7.51 (m, 2H), 7.46–7.37 (m, 4H), 7.34–7.26 (m, 2H), 7.15–7.12 (m, 2H), 6.62 (m, J = 8.4 Hz, 1H), 4.78 (q, J = 8.8 Hz, 1H), 3.91 (dd, J = 4.8 Hz, 2H), 3.77 (s, 3H), 3.32 (d, 1H), 2.81 (d, 1H), 2.31–2.23 (m, 1H), 1.01–0.97 (m, 6H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 172.6, 166.9, 143.4, 136.2, 133.3, 130.3, 130.0, 128.61, 128.56, 128.2, 128.1, 127.7, 127.0, 126.6, 60.1, 57.4, 53.7, 52.2, 31.6, 19.0, 17.9; ESI-HRMS: Calcd for $\text{C}_{29}\text{H}_{31}\text{N}_2\text{O}_4^+$ $[\text{M}+\text{H}]^+$ 471.2278, found 471.2280.

(3S,8R,9S,10R,13S,14S)-10,13-dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-te-tradecahydro-1H-cyclopenta[a]phenanthren-3-yl 4-(2-(((diphenylmethylene)amino)methyl)oxiran-2-yl)benzoate (2aj)



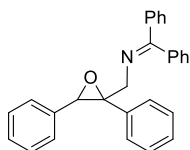
Colorless oil; (0.085 g, 68%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 8.01–7.99 (m, 2H), 7.58–7.56 (m, 2H), 7.51–7.42 (m, 5H), 7.40–7.26 (m, 3H), 7.13–7.11 (m, 2H), 5.46–5.44 (m, 1H), 4.88–4.82 (m, 1H), 3.90–3.86 (m, 2H), 3.26–3.13 (m, 1H), 2.82–2.81 (m, 1H), 2.50–2.43 (m, 3H), 2.15–1.85 (m, 6H), 1.76–1.67 (m, 4H), 1.58–1.49 (m, 2H), 1.35–1.19 (m, 4H), 1.09 (s, 3H), 0.90 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 221.0, 170.2, 165.7, 144.6, 139.9, 139.3, 136.3, 130.2, 129.9, 129.4, 128.6, 128.5, 128.0, 127.7, 126.3, 122.0, 74.3, 60.2, 57.3, 53.7, 51.7, 50.1, 47.5, 38.1, 36.9, 36.8, 35.8, 31.4, 31.4, 30.8, 27.8, 21.9, 20.3, 19.4, 13.5; ESI-HRMS: Calcd for $\text{C}_{42}\text{H}_{46}\text{NO}_4^+$ $[\text{M}+\text{H}]^+$ 628.3421, found 628.3420.

4-(2-(((diphenylmethylene)amino)methyl)oxiran-2-yl)-N-(((1R,4aS,10aR)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthren-1-yl)methyl)benzamide (2ak)



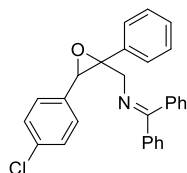
Colorless oil; (0.059 g, 47%); R_f = 0.3 (2:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.70–7.68 (m, 2H), 7.58–7.56 (m, 2H), 7.48–7.40 (m, 5H), 7.37–7.35 (m, 1H), 7.31–7.25 (m, 2H), 7.17–7.10 (m, 3H), 7.00–6.97 (m, 1H), 6.88 (s, 1H), 6.11–6.07 (t, 1H), 3.92–3.89 (m, 1H), 3.87–3.83 (m, 1H), 3.44–3.39 (m, 1H), 3.35–3.30 (m, 2H), 2.94–2.89 (m, 1H), 2.85–2.78 (m, 3H), 2.31–2.28 (m, 1H), 1.99–1.94 (m, 1H), 1.81–1.65 (m, 3H), 1.52–1.46 (m, 2H), 1.38–1.37 (m, 2H), 1.34–1.33 (m, 3H), 1.23–1.22 (m, 3H), 1.20 (s, 3H), 1.00 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 170.2, 167.2, 147.0, 145.6, 143.1, 139.4, 136.3, 134.7, 134.0, 130.2, 128.6, 128.5, 128.0, 127.7, 126.9, 126.7, 126.6, 124.2, 123.9, 60.1, 57.3, 53.6, 50.3, 45.8, 38.3, 37.7, 37.6, 36.4, 33.4, 30.4, 25.4, 24.0, 23.9, 19.1, 18.8, 18.6; ESI-HRMS: Calcd for $\text{C}_{43}\text{H}_{49}\text{N}_2\text{O}_2^+$ $[\text{M}+\text{H}]^+$ 625.3789, found 625.3788.

N-((2,3-diphenyloxiran-2-yl)methyl)-1,1-diphenylmethanimine (2al)



Colorless oil; (0.051 g, 65%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, J = 8.0 Hz, 2H), 7.47–7.45 (m, 2H), 7.41–7.30 (m, 7H), 7.26–7.23 (m, 7H), 6.75 (d, J = 8.0 Hz, 2H), 4.08 (s, 1H), 3.73–3.65 (m, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 169.4, 140.4, 139.5, 136.2, 135.3, 129.9, 128.4, 128.3, 128.2, 128.1, 128.0, 127.8, 127.7, 127.5, 126.5, 126.4, 66.4, 65.8, 55.2; ESI-HRMS: Calcd for $\text{C}_{28}\text{H}_{24}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 390.1852, found 390.1850.

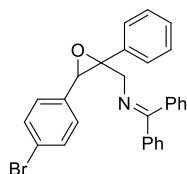
N-((3-(4-chlorophenyl)-2-phenyloxiran-2-yl)methyl)-1,1-diphenylmethanimine (2am)



Colorless oil; (0.061 g, 72%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.62–7.60 (m, 2H), 7.47–7.45 (m, 2H), 7.41–7.31 (m, 7H), 7.27–7.23 (m, 2H), 7.20–7.14 (m, 4H), 6.77–6.75 (m, 2H), 4.03 (s, 1H), 3.71 (d, J = 14.4 Hz, 1H), 3.65 (d, J = 14.4 Hz, 1H); ^{13}C NMR (150.6 MHz, CDCl_3): δ 169.4, 140.1, 139.5, 136.0, 133.9, 133.3,

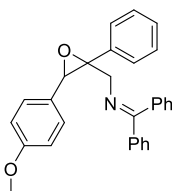
130.0, 128.5, 128.4, 128.3, 128.24, 128.19, 127.9, 127.8, 127.7, 127.6, 126.5, 66.3, 65.2, 55.2; ESI-HRMS: Calcd for $C_{28}H_{23}ClNO^+$ $[M+H]^+$ 424.1463, found 424.1469.

N-((3-(4-bromophenyl)-2-phenyloxiran-2-yl)methyl)-1,1-diphenylmethanimine (2an)



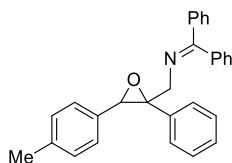
White Solid; (0.080 g, 85%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); 1H NMR (400 MHz, $CDCl_3$): δ 7.63–7.61 (m, 2H), 7.48–7.45 (m, 2H), 7.41–7.31 (m, 9H), 7.28–7.25 (m, 2H), 7.10–7.08 (m, 2H), 6.77–6.75 (m, 2H), 4.02 (s, 1H), 3.71 (d, J = 14.4 Hz, 1H), 3.65 (d, J = 14.4 Hz, 1H); ^{13}C NMR (150.6 MHz, $CDCl_3$): δ 169.4, 140.1, 139.5, 136.0, 134.4, 131.2, 130.0, 128.5, 128.4, 128.3, 128.2, 127.9, 127.7, 127.6, 126.5, 121.5, 66.3, 65.2, 55.2; ESI-HRMS: Calcd for $C_{28}H_{23}BrNO^+$ $[M+H]^+$ 468.0958, found 468.0953.

N-((3-(4-methoxyphenyl)-2-phenyloxiran-2-yl)methyl)-1,1-diphenylmethanimine (2ao)



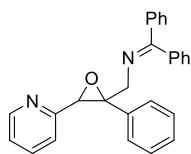
Colorless oil (0.063 g, 75%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); 1H NMR (400 MHz, $CDCl_3$): δ 7.60–7.58 (m, 2H), 7.47–7.45 (m, 2H), 7.40–7.31 (m, 7H), 7.27–7.23 (m, 2H), 7.16–7.14 (m, 2H), 6.80–6.76 (m, 4H), 4.02 (s, 1H), 3.79 (s, 3H), 3.74 (d, J = 14.4 Hz, 1H), 3.67 (d, J = 14.4 Hz, 1H); ^{13}C NMR (150.6 MHz, $CDCl_3$): δ 169.3, 159.0, 140.5, 139.6, 136.3, 129.9, 128.5, 128.3, 128.2, 128.1, 127.9, 127.8, 127.6, 127.42, 127.38, 126.5, 113.5, 66.4, 65.7, 55.2, 55.1; ESI-HRMS: Calcd for $C_{29}H_{26}NO_2^+$ $[M+H]^+$ 420.1958, found 420.1955.

1,1-diphenyl-N-((2-phenyl-3-(p-tolyl)oxiran-2-yl)methyl)methanimine (2ap)



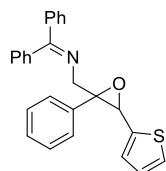
Colorless oil; (0.068 g, 84%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); 1H NMR (400 MHz, $CDCl_3$): δ 7.60–7.58 (m, 2H), 7.47–7.45 (m, 2H), 7.40–7.31 (m, 7H), 7.27–7.24 (m, 1H), 7.12 (d, J = 8 Hz, 2H), 7.05 (d, J = 8 Hz, 2H), 6.77–6.75 (m, 2H), 4.04 (s, 1H), 3.73 (d, J = 14.4 Hz, 1H), 3.68 (d, J = 14.4 Hz, 1H), 2.33 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ 169.4, 140.5, 139.6, 137.1, 136.3, 132.3, 130.1, 129.9, 128.8, 128.5, 128.2, 128.1, 127.9, 127.8, 127.4, 126.6, 126.4, 66.4, 65.8, 55.1, 21.2; ESI-HRMS: Calcd for $C_{29}H_{26}NO^+$ $[M+H]^+$ 404.2009, found 404.2010.

1,1-diphenyl-N-((2-phenyl-3-(pyridin-2-yl)oxiran-2-yl)methyl)methanimine (2aq)



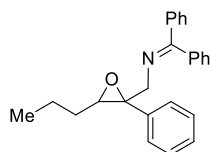
Colorless oil (0.056 g, 72%); R_f = 0.2 (5:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 8.53–8.52 (m, 2H), 7.60–7.58 (m, 2H), 7.52–7.50 (m, 1H), 7.46–7.44 (m, 2H), 7.39–7.31 (m, 7H), 7.26–7.23 (m, 2H), 7.17–7.14 (m, 2H), 6.84–6.82 (m, 2H), 4.17 (s, 1H), 3.89 (d, J = 14.4 Hz, 1H), 3.84 (d, J = 14.4 Hz, 1H); ^{13}C NMR (150.6 MHz, CDCl_3): δ 169.6, 155.4, 149.1, 139.8, 139.5, 136.2, 136.1, 129.9, 128.5, 128.3, 128.1, 127.83, 127.78, 127.6, 126.7, 122.5, 121.0, 67.0, 65.8, 55.1; ESI-HRMS: Calcd for $\text{C}_{27}\text{H}_{23}\text{N}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 391.1805, found 391.1810.

1,1-diphenyl-N-((2-phenyl-3-(thiophen-2-yl)oxiran-2-yl)methyl)methanimine (2ar)



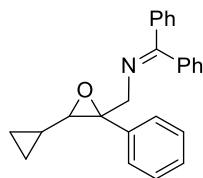
Colorless oil (0.050 g, 63%); R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.59–7.57 (m, 2H), 7.51–7.49 (m, 2H), 7.40–7.31 (m, 7H), 7.29–7.24 (m, 2H), 7.21–7.19 (m, 1H), 6.94–6.92 (m, 2H), 6.84–6.82 (m, 2H), 4.20 (s, 1H), 3.89 (d, J = 15 Hz, 1H), 3.84 (d, J = 15 Hz, 1H); ^{13}C NMR (150.6 MHz, CDCl_3): δ 169.5, 139.9, 139.5, 138.7, 136.3, 129.9, 128.5, 128.3, 128.2, 127.9, 127.7, 127.6, 126.9, 126.5, 125.7, 125.0, 67.0, 62.7, 55.7; ESI-HRMS: Calcd for $\text{C}_{26}\text{H}_{22}\text{NOS}^+$ $[\text{M}+\text{H}]^+$ 396.1417, found 396.1422.

1,1-diphenyl-N-((2-phenyl-3-propyloxiran-2-yl)methyl)methanimine (2as)



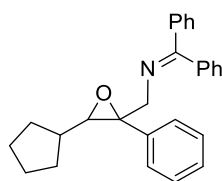
Colorless oil (0.050 g, 70%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.60–7.57 (m, 2H), 7.48–7.24 (m, 11H), 7.01–6.99 (m, 2H), 3.93 (d, J = 14.8 Hz, 1H), 3.79 (d, J = 14.8 Hz, 1H), 2.97 (t, J = 6.0 Hz, 1H), 1.69–1.52 (m, 4H), 0.96 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 169.1, 141.5, 139.5, 136.4, 130.0, 128.5, 128.0, 128.0, 127.6, 127.2, 126.4, 65.8, 63.8, 56.8, 30.8, 19.9, 14.0; ESI-HRMS: Calcd for $\text{C}_{25}\text{H}_{26}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 356.2009, found 356.2015.

N-((3-cyclopropyl-2-phenyloxiran-2-yl)methyl)-1,1-diphenylmethanimine (2at)



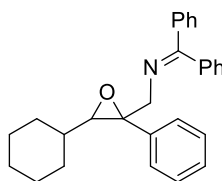
Colorless oil (0.037 g, 52%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate) ^1H NMR (400 MHz, CDCl_3): δ 7.58–7.57 (m, 2H), 7.46–7.41 (m, 5H), 7.37–7.35 (m, 1H), 7.32–7.28 (m, 4H), 7.26–7.23 (m, 1H), 7.04–7.03 (m, 2H), 4.05–4.01 (m, 2H), 2.47 (d, J = 4.8 Hz, 1H), 0.88–0.85 (m, 1H), 0.61–0.58 (m, 2H), 0.48–0.39 (m, 2H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 169.3, 141.0, 139.5, 136.4, 130.0, 128.6, 128.5, 128.3, 127.99, 127.96, 127.8, 127.2, 126.3, 69.1, 64.5, 9.0, 3.8, 2.8; ESI-HRMS: Calcd for $\text{C}_{25}\text{H}_{24}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 354.1852, found 354.1859.

N-((3-cyclopentyl-2-phenyloxiran-2-yl)methyl)-1,1-diphenylmethanimine (2au)



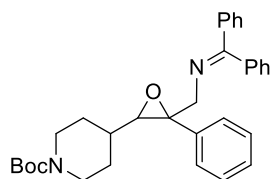
Colorless oil; (0.034 g, 45%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.61–7.59 (m, 2H), 7.49–7.47 (m, 2H), 7.41–7.36 (m, 4H), 7.33–7.26 (m, 4H), 6.99–6.97 (m, 2H), 3.96 (d, J = 14.4 Hz, 1H), 3.78 (d, J = 14.4 Hz, 1H), 2.79 (d, J = 8.8 Hz, 1H), 1.89–1.77 (m, 3H), 1.65–1.43 (m, 6H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 168.9, 141.6, 139.5, 136.3, 132.4, 130.05, 130.02, 128.51, 128.47, 128.00, 127.6, 127.2, 126.4, 70.2, 64.5, 57.2, 38.9, 31.1, 29.3, 25.54, 25.47; ESI-HRMS: Calcd for $\text{C}_{27}\text{H}_{28}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 382.2165, found 382.2166.

N-((3-cyclohexyl-2-phenyloxiran-2-yl)methyl)-1,1-diphenylmethanimine (2av)



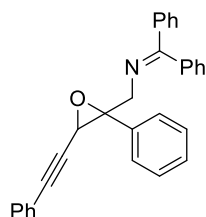
Colorless oil; (0.040 g, 50%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.81–7.78 (m, 2H), 7.60–7.56 (m, 2H), 7.49–7.39 (m, 5H), 7.35–7.23 (m, 5H), 6.97–6.95 (m, 1H), 3.92 (d, J = 14.4 Hz, 1H), 3.76 (d, J = 14.4 Hz, 1H), 2.69 (d, J = 9.2 Hz, 1H), 1.94–1.86 (m, 1H), 1.75–1.59 (m, 3H), 1.29–1.11 (m, 7H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 169.0, 141.5, 139.5, 137.6, 136.4, 132.4, 130.0, 128.48, 128.44, 128.3, 128.0, 127.7, 126.6, 70.2, 64.4, 57.0, 37.3, 30.4, 29.1, 26.2, 25.5, 25.4; ESI-HRMS: Calcd for $\text{C}_{28}\text{H}_{30}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 396.2322, found 396.2324.

tert-butyl 4-(3-(((diphenylmethylene)amino)methyl)-3-phenyloxiran-2-yl)piperidine-1-carboxylate (2aw)



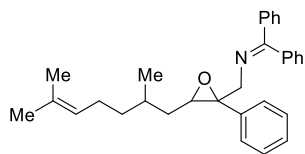
Colorless oil; (0.072 g, 72%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.60–7.58 (m, 2H), 7.44–7.36 (m, 6H), 7.33–7.25 (m, 5H), 6.97–6.95 (m, 2H), 4.13–4.11 (m, 2H), 4.02–3.97 (m, 1H), 3.78–3.74 (d, J = 14.4 Hz, 1H), 2.74 (d, J = 8.8 Hz, 1H), 2.66 (m, 2H), 1.94–1.87 (t, J = 12.8 Hz, 2H), 1.45 (s, 9H), 1.41–1.29 (m, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 169.2, 154.8, 141.0, 139.3, 136.2, 130.2, 128.6, 128.5, 128.4, 128.0, 127.6, 127.4, 126.4, 79.4, 69.1, 64.4, 57.1, 35.9, 29.4, 28.4, 28.1; ESI-HRMS: Calcd for $\text{C}_{32}\text{H}_{37}\text{N}_2\text{O}_3^+$ $[\text{M}+\text{H}]^+$ 497.2799, found 497.2803.

1,1-diphenyl-N-((2-phenyl-3-(phenylethynyl)oxiran-2-yl)methyl)methanimine (2ax)



Colorless oil; (0.045 g, 55%); R_f = 0.25 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.59–7.46 (m, 5H), 7.37–7.25 (m, 13H), 7.04–7.02 (m, 2H), 4.17 (d, J = 14.8 Hz, 1H), 4.06 (d, J = 15.2 Hz, 1H), 3.65 (s, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 169.8, 139.5, 138.7, 136.5, 132.4, 131.9, 130.0, 128.7, 128.56, 128.45, 128.21, 128.15, 127.9, 127.8, 127.7, 126.7, 122.0, 86.0, 84.2, 66.1, 57.5, 52.9; ESI-HRMS: Calcd for $\text{C}_{30}\text{H}_{24}\text{NO}^+$ $[\text{M}+\text{H}]^+$ 414.1852, found 414.1855.

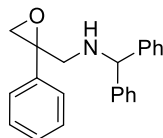
N-((3-(2,6-dimethylhept-5-en-1-yl)-2-phenyloxiran-2-yl)methyl)-1,1-diphenylmethanimine (2ay)



Colorless oil (0.046 g, 53%, dr = 1:1); R_f = 0.25 (10:1 petroleum ether / ethyl acetate) ^1H NMR (400 MHz, CDCl_3): δ 7.59–7.56 (m, 2H), 7.48–7.36 (m, 2H), 7.35–7.31 (m, 3H), 7.30–7.25 (m, 6H), 7.01–6.98 (m, 2H), 5.09–5.06 (m, 1H), 3.92–3.77 (m, 2H), 3.01–2.98 (t, J = 5.6 Hz, 1H), 2.00–1.93 (m, 2H), 1.79–1.72 (m, 1H), 1.67–1.66 (m, 3H), 1.59–1.56 (m, 4H), 1.44–1.37 (m, 2H), 1.24–1.19 (m, 1H), 1.00–0.96 (m, 3H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 169.2, 141.5, 139.5, 136.4, 132.4, 131.29, 131.28, 130.03, 130.01, 128.51, 128.45, 128.2,

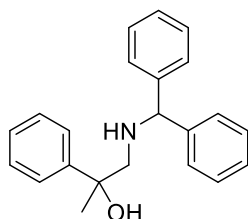
128.0, 127.9, 127.6, 127.2, 126.41, 126.39, 124.6, 124.5, 64.9, 64.8, 63.8, 63.4, 56.8, 37.1, 35.8, 35.7, 31.5, 31.0, 25.69, 25.67, 25.5, 25.4, 19.8, 19.7, 17.7, 17.6; ESI-HRMS: Calcd for $C_{31}H_{36}NO^+$ $[M+H]^+$ 438.2791, found 438.2798.

1,1-diphenyl-N-((2-phenyloxiran-2-yl)methyl)methanamine (3)



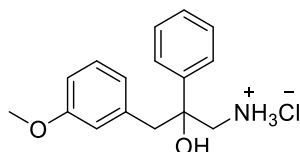
Colorless oil; R_f = 0.20 (10:1 petroleum ether / ethyl acetate); 1H NMR (400 MHz, $CDCl_3$): δ 7.38–7.31 (m, 8H), 7.30–7.24 (m, 5H), 7.21–7.16 (m, 2H), 4.84 (s, 1H), 3.28 (d, J = 8.0 Hz, 1H), 3.27 (d, J = 14 Hz, 1H), 3.02 (d, J = 14 Hz, 1H), 2.75 (d, J = 8 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ 143.9, 143.7, 139.1, 128.5, 128.4, 128.3, 127.7, 127.3, 127.2, 127.1, 127.0, 126.0, 67.1, 59.9, 53.7, 50.8; ESI-HRMS: Calcd for $C_{22}H_{22}NO^+$ $[M+H]^+$ 316.1696, found 316.1698.

1-(benzhydrylamino)-2-phenylpropan-2-ol (4)



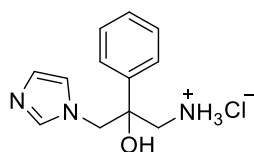
Colorless oil; R_f = 0.20 (10:1 petroleum ether / ethyl acetate); 1H NMR (400 MHz, $CDCl_3$): δ 7.44–7.42 (m, 2H), 7.34–7.18 (m, 13H), 4.74 (s, 1H), 3.01 (d, J = 15.6 Hz, 1H), 3.72 (d, J = 15.6 Hz, 1H), 1.44 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ 146.7, 143.5, 143.1, 128.6, 128.49, 128.45, 128.3, 127.3, 127.1, 127.0, 126.7, 124.9, 73.1, 66.9, 58.5, 28.4; ESI-HRMS: Calcd for $C_{22}H_{24}NO^+$ $[M+H]^+$ 318.1852, found 318.1850.

2-hydroxy-3-(3-methoxyphenyl)-2-phenylpropan-1-aminium chloride (5)



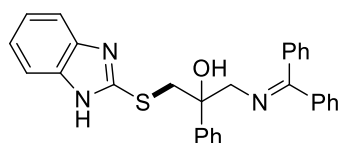
White solid; 1H NMR (400 MHz, CD_3OD): δ 7.48–7.46 (m, 2H), 7.47–7.31 (m, 2H), 7.34–7.30 (m, 1H), 7.08 (t, J = 8.0 Hz, 1H), 6.73 (dd, J_1 = 7.6 Hz, J_2 = 2.0 Hz, 1H), 6.62 (d, J = 7.6 Hz, 1H), 6.51 (t, J = 2.0 Hz, 1H), 3.64 (s, 3H), 3.46 (d, J = 12.8 Hz, 1H), 3.36 (s, 1H), 3.21 (d, J = 12.8 Hz, 1H), 3.14 (m, 2H); ^{13}C NMR (100.6 MHz, CD_3OD): δ 160.6, 142.9, 138.1, 129.8, 129.6, 128.8, 127.2, 124.2, 117.2, 113.4, 75.4, 55.4; ESI-HRMS: Calcd for $C_{16}H_{20}NO_2^+$ $[M+H]^+$ 258.1489, found 258.1489.

2-hydroxy-3-(1H-imidazol-1-yl)-2-phenylpropan-1-aminium chloride (6)



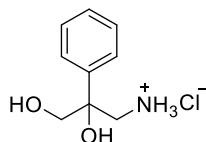
White solid; ^1H NMR (400 MHz, D_2O): δ 8.42 (d, J = 6.8 Hz, 1H), 7.47 (m, 5H), 7.29 (d, J = 4.0 Hz, 1H), 7.12 (d, J = 6.0 Hz, 1H), 4.73–4.67 (m, 2H), 3.74 (dd, J_1 = 13.2 Hz, J_2 = 8.0 Hz, 1H), 3.51 (dd, J_1 = 13.2 Hz, J_2 = 8.0 Hz, 1H); ^{13}C NMR (100.6 MHz, D_2O): δ 136.2, 135.4, 129.5, 129.3, 125.6, 123.1, 119.0, 74.3, 56.9, 46.6; ESI-HRMS: Calcd for $\text{C}_{12}\text{H}_{16}\text{N}_3\text{O}^+$ $[\text{M}+\text{H}]^+$ 218.1288, found 218.1286.

1-((1H-benzo[d]imidazol-2-yl)thio)-3-((diphenylmethylene)amino)-2-phenylpropan-2-ol (7)



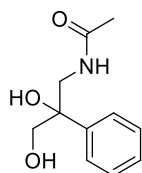
Colorless oil; R_f = 0.23 (10:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, CDCl_3): δ 7.69–7.64 (m, 1H), 7.56–7.54 (m, 2H), 7.43–7.39 (m, 6H), 7.35–7.22 (m, 4H), 7.17–7.14 (m, 4H), 6.94–6.91 (m, 2H), 5.68 (s, 1H), 3.95 (d, J = 14.0 Hz, 1H), 3.84 (d, J = 14.8 Hz, 1H), 3.67 (d, J = 14.8 Hz, 1H), 1.65 (s, 1H); ^{13}C NMR (100.6 MHz, CDCl_3): δ 170.4, 151.4, 143.9, 139.0, 136.2, 130.5, 128.8, 128.6, 128.5, 128.4, 128.2, 127.5, 127.3, 125.9, 125.8, 125.7, 62.0, 43.3; ESI-HRMS: Calcd for $\text{C}_{29}\text{H}_{26}\text{N}_3\text{OS}^+$ $[\text{M}+\text{H}]^+$ 464.1791, found 464.1790.

2,3-dihydroxy-2-phenylpropan-1-aminium chloride (8)



White solid; ^1H NMR (400 MHz, D_2O): 7.66–7.51 (m, 5H), 4.06 (d, J = 9.6 Hz, 1H), 4.02 (m, 2H), 3.87 (d, J = 9.2 Hz, 1H); ^{13}C NMR (100.6 MHz, D_2O): δ 139.8, 128.9, 128.6, 124.7, 86.7, 66.7, 48.9; ESI-HRMS: Calcd for $\text{C}_9\text{H}_{14}\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 168.1019, found 168.1020.

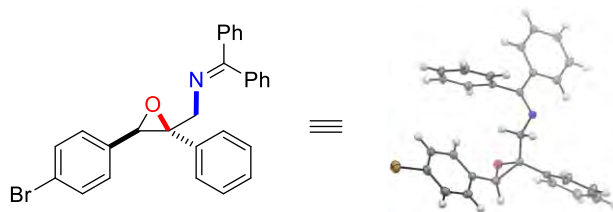
N-(2,3-dihydroxy-2-phenylpropyl)acetamide (9)



Colorless oil; R_f = 0.20 (10:1 DCM / MeOH); ^1H NMR (400 MHz, CDCl_3): δ 7.46–7.38 (m, 2H), 7.36–7.31 (m, 2H), 7.29–7.27 (m, 1H), 6.05 (s, 1H), 3.79 – 3.68 (m, 2H), 3.62 (d, J = 11.6 Hz, 1H), 3.51 (dd, J = 14.3, 6.2 Hz, 1H), 1.94 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3):

δ 172.5, 142.0, 128.5, 127.6, 125.3, 67.6, 47.2, 23.0; ESI-HRMS: Calcd for $C_{11}H_{16}NO_3^+$ $[M+H]^+$ 210.1125, found 210.1125.

10 X-Ray single-crystal diffraction study for **b39**



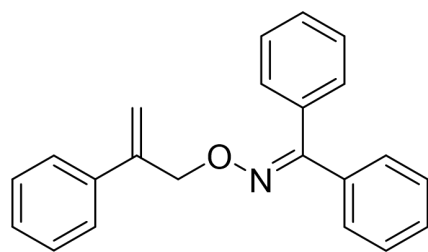
X-ray ORTEP of **b39**

Table S4. The crystal data and refinement results of compound **b39**.

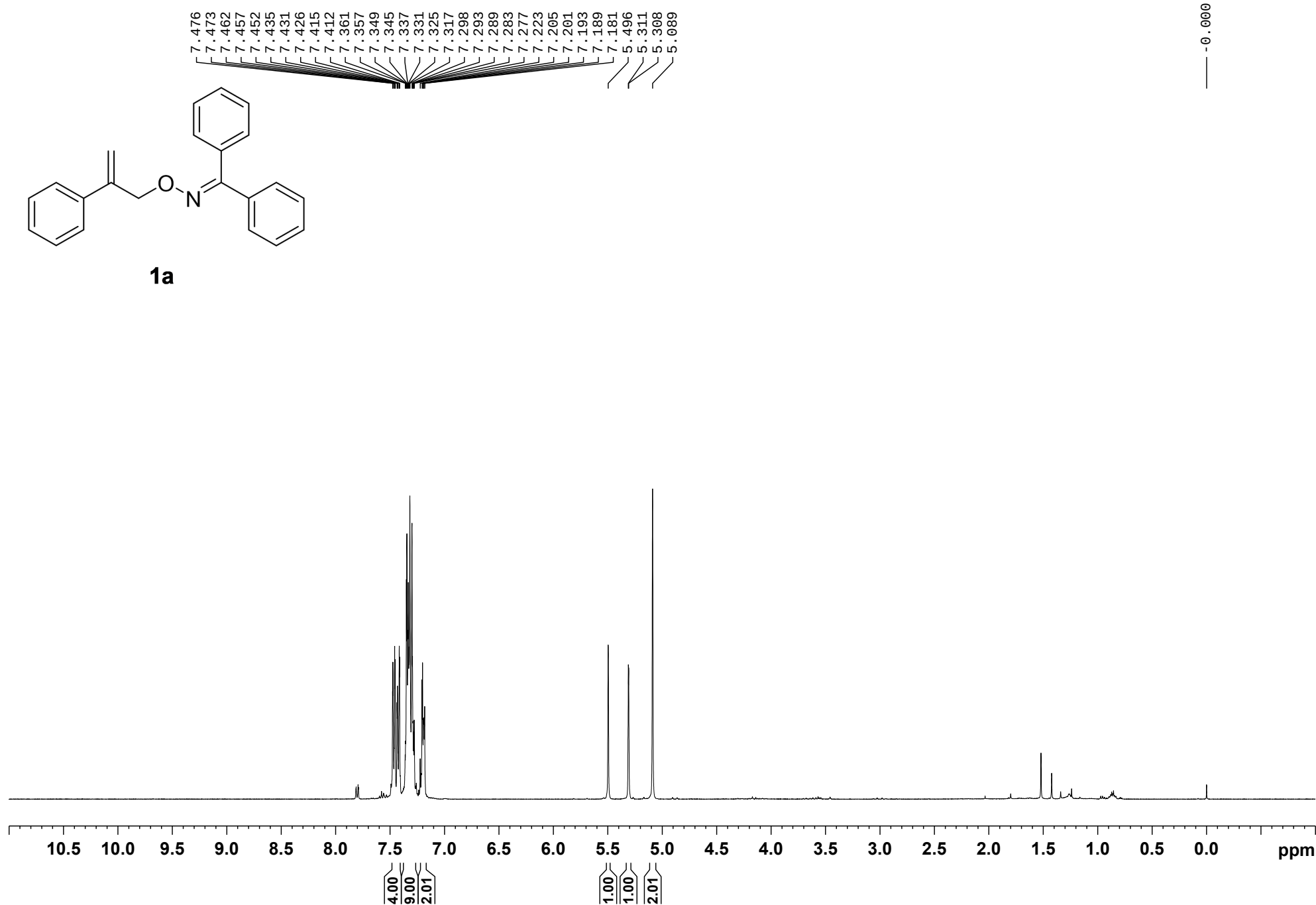
Empirical formula	$C_{28}H_{22}BrNO$
Formula weight	468.37
Temperature/K	149.97(10)
Crystal system	triclinic
Space group	P-1
a/Å	5.8212(2)
b/Å	14.1940(4)
c/Å	14.7214(5)
$\alpha/^\circ$	69.915(3)
$\beta/^\circ$	81.048(2)
$\gamma/^\circ$	86.989(2)
Volume/Å ³	1128.48(7)
Z	2
$\rho_{\text{calc}}/\text{cm}^3$	1.378
μ/mm^{-1}	2.625
F(000)	480.0
Crystal size/mm ³	0.11 × 0.07 × 0.06
Radiation	Cu K α (λ = 1.54184)
2 θ range for data collection/ $^\circ$	6.462 to 133.192
Index ranges	-6 ≤ h ≤ 6, -15 ≤ k ≤ 16, -15 ≤ l ≤ 17
Reflections collected	11567
Independent reflections	3928 [R_{int} = 0.0341, R_{sigma} = 0.0376]
Data/restraints/parameters	3928/0/280
Goodness-of-fit on F^2	1.029
Final R indexes [$ I \geq 2\sigma(I)$]	R_1 = 0.0433, wR_2 = 0.1222
Final R indexes [all data]	R_1 = 0.0492, wR_2 = 0.1255
CCDC number	2439472

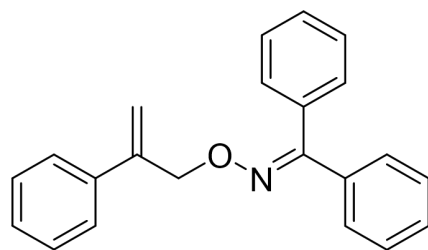
11 Reference

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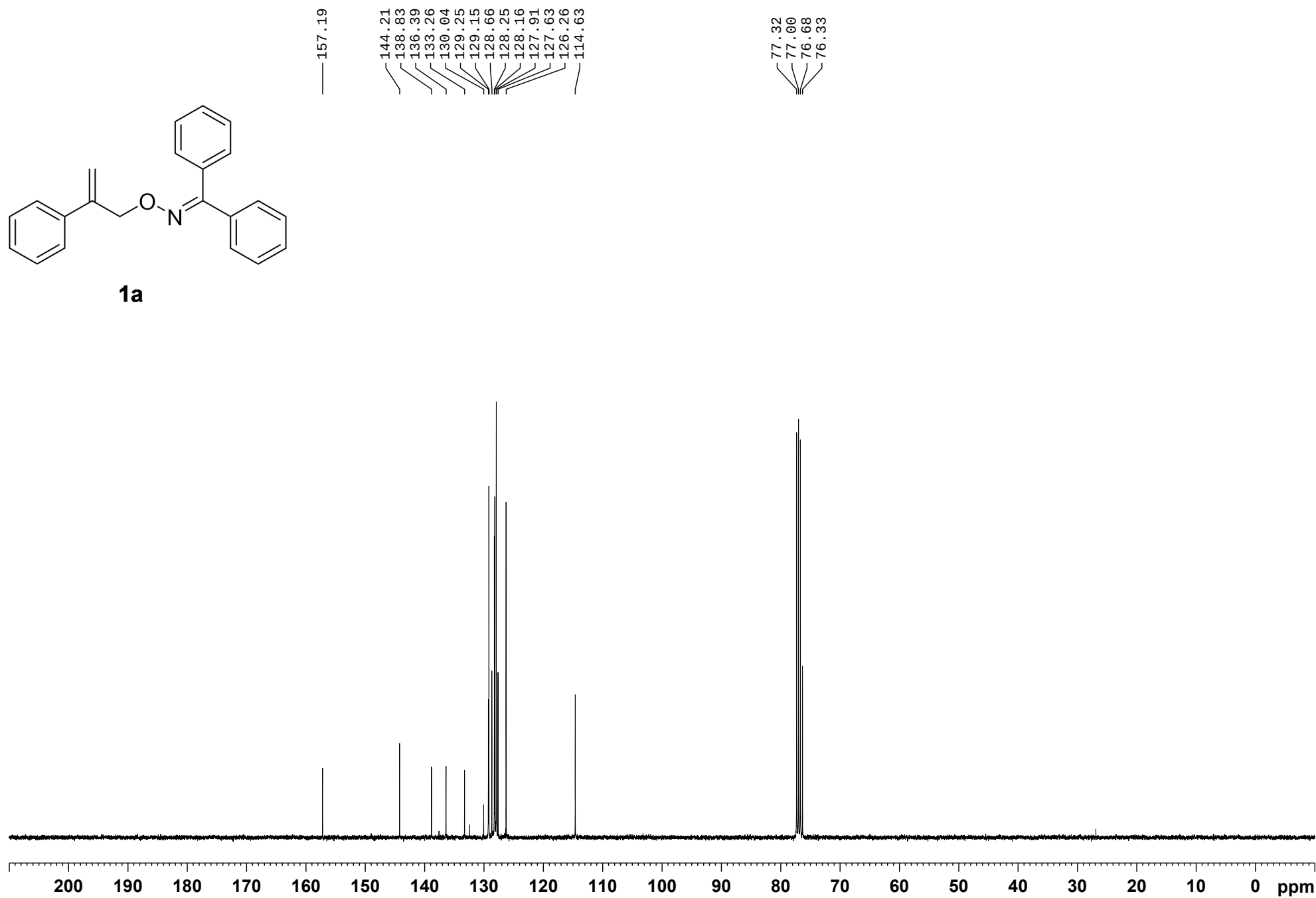


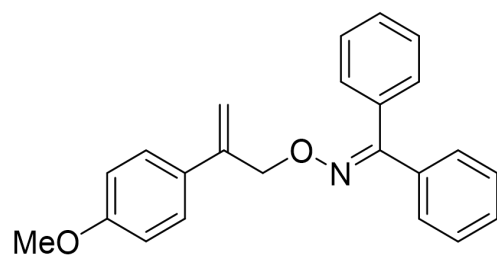
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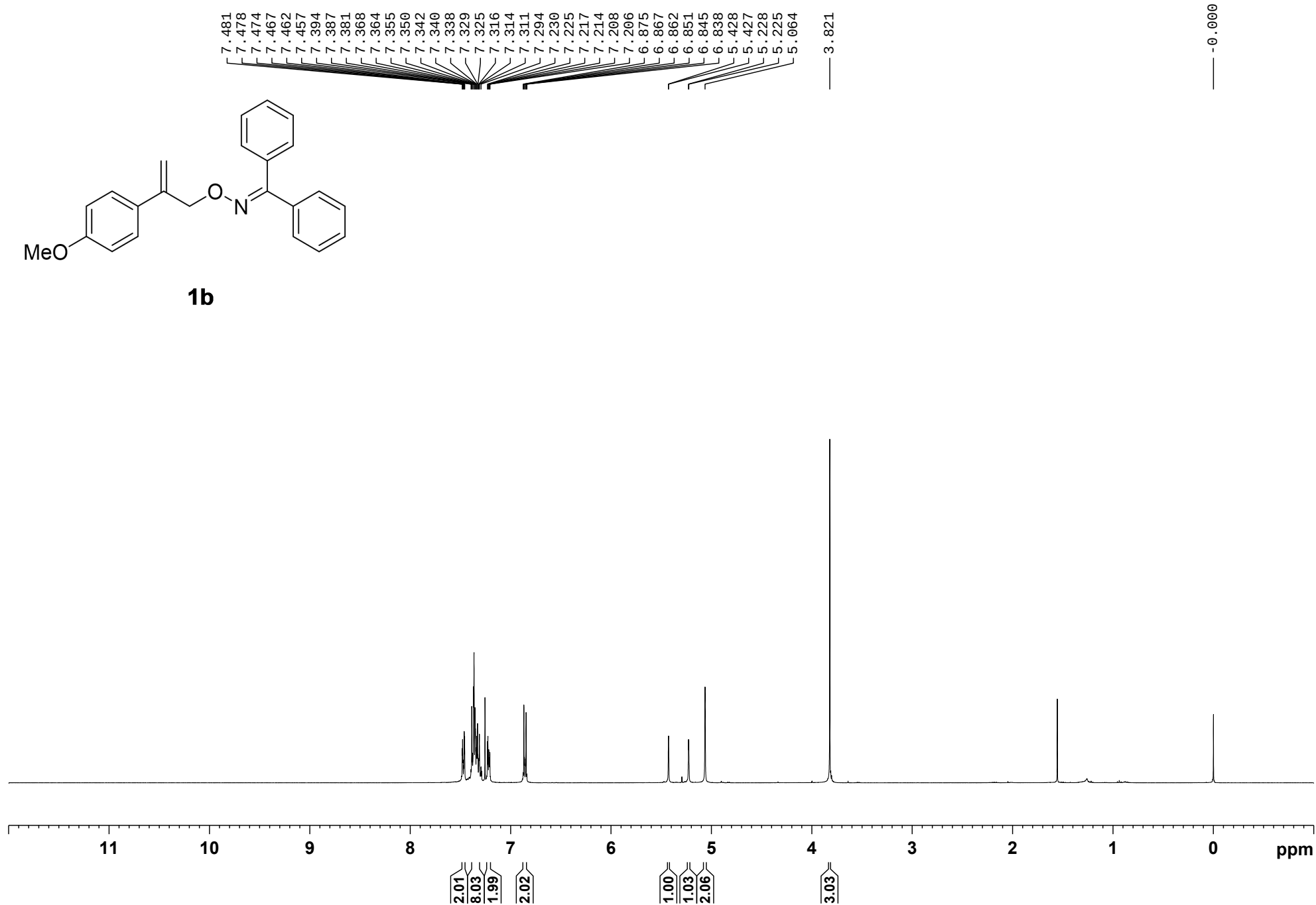


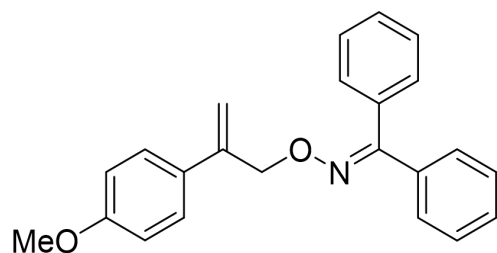
1a



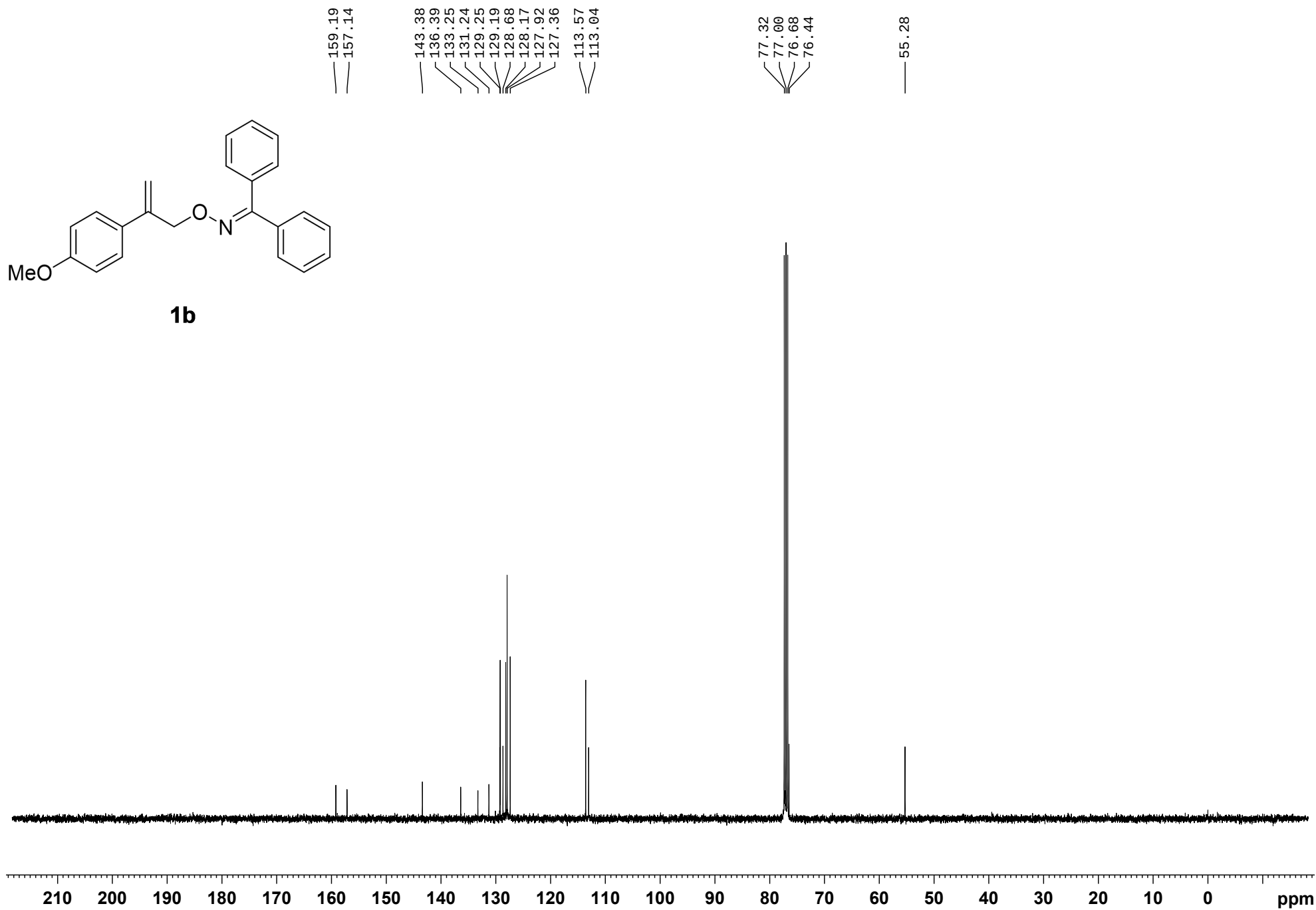


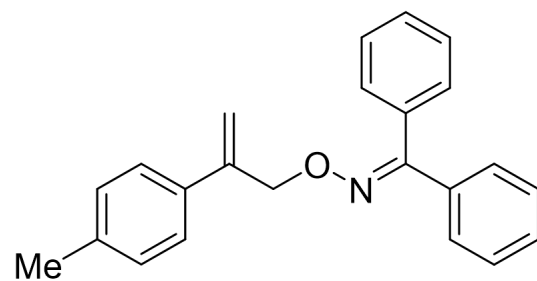
1b



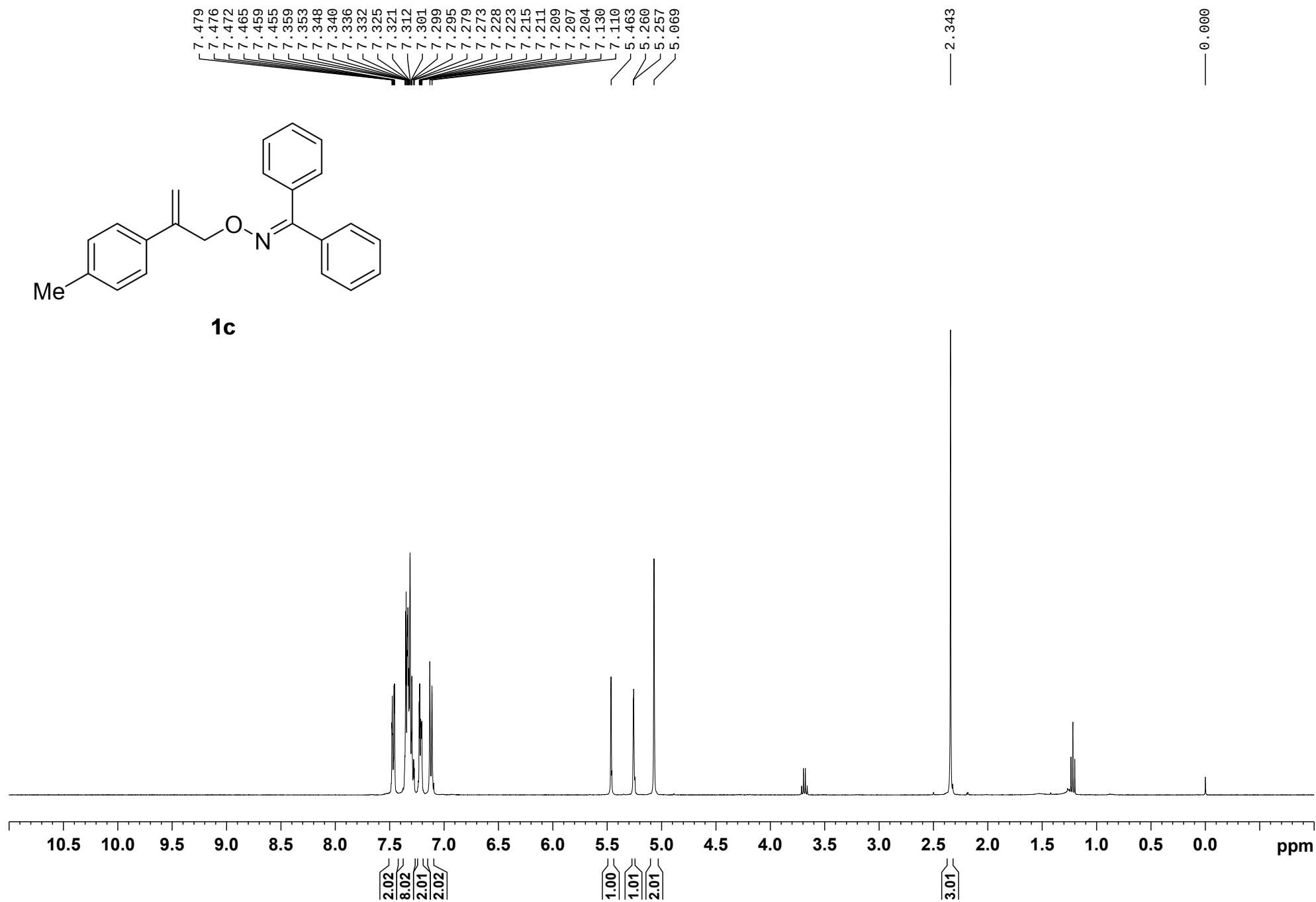


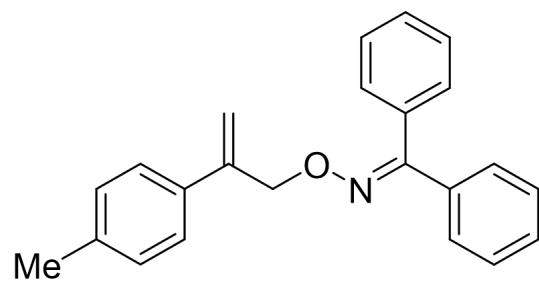
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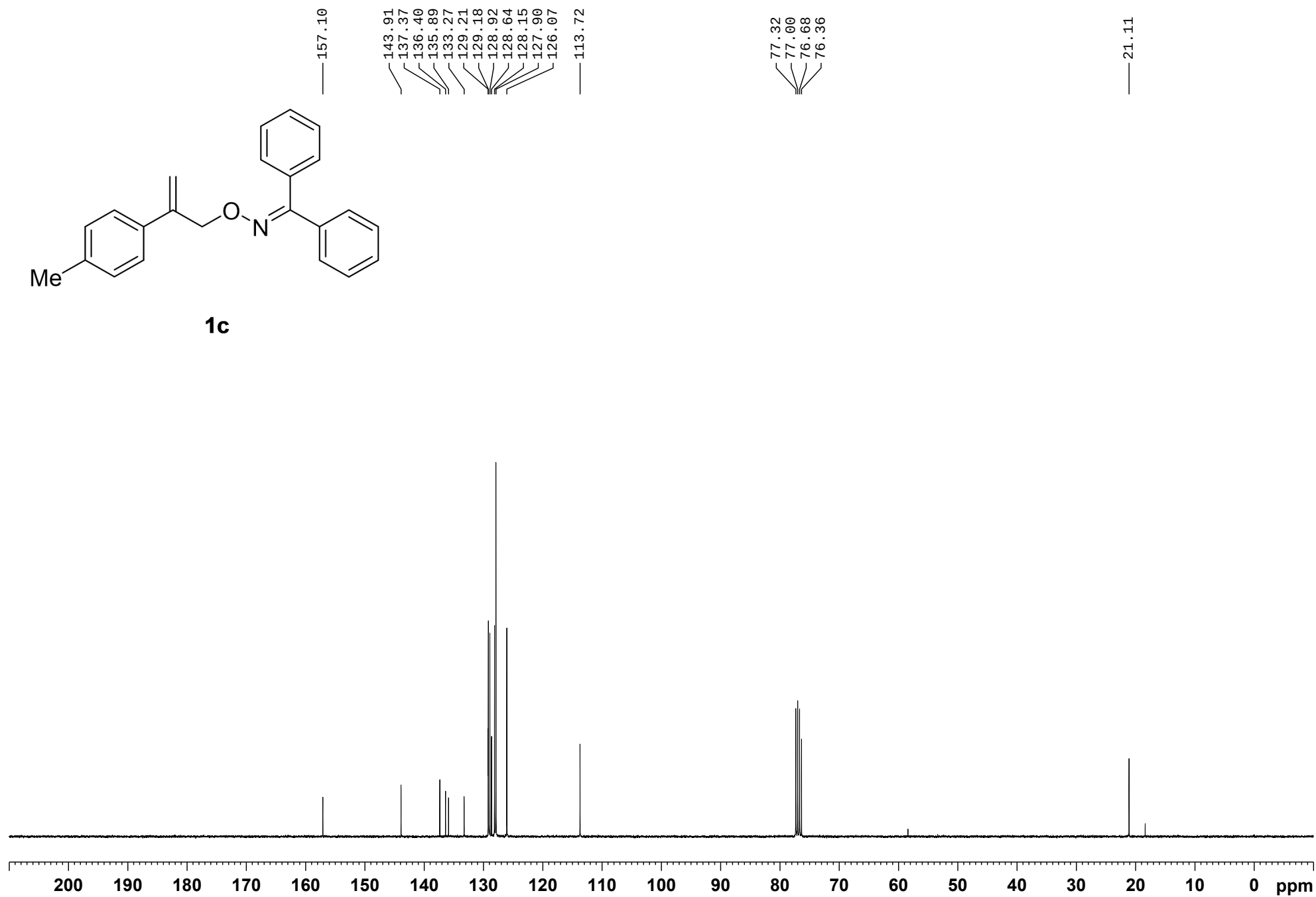


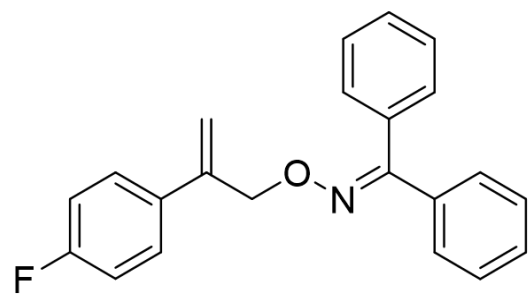
1c





1c



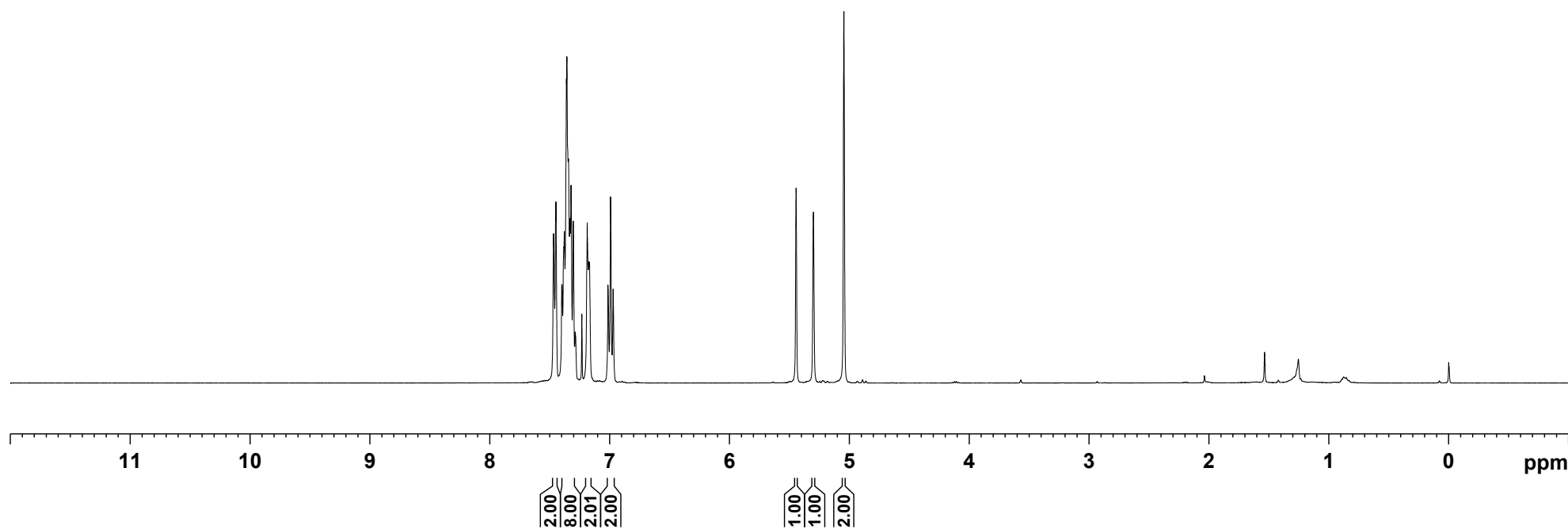


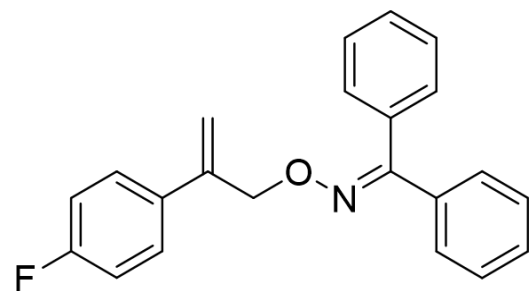
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7.382
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7.173
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6.970

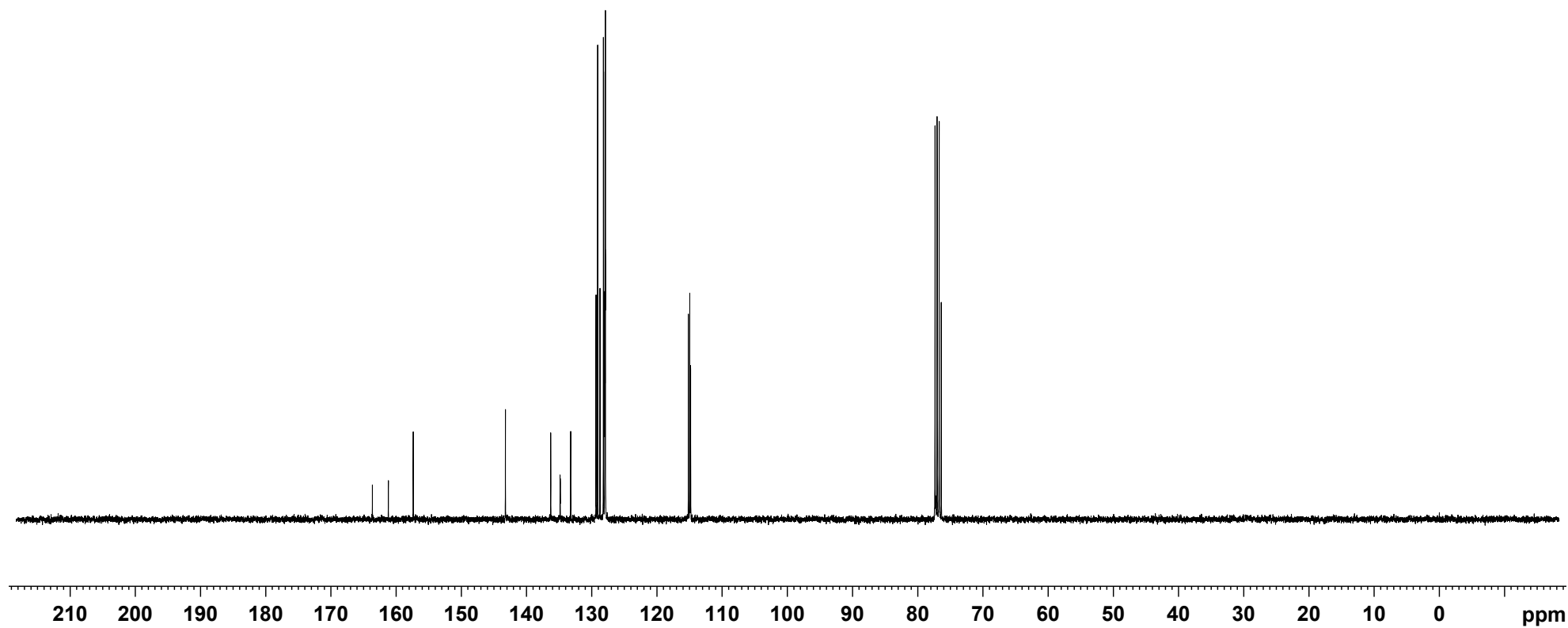
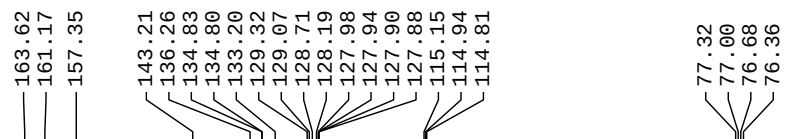
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5.046

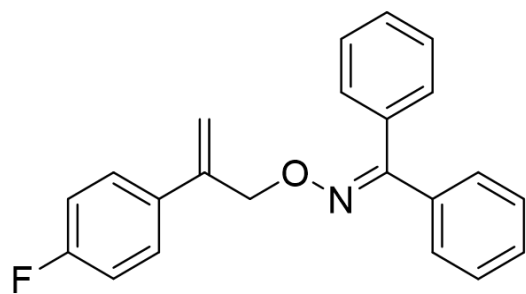
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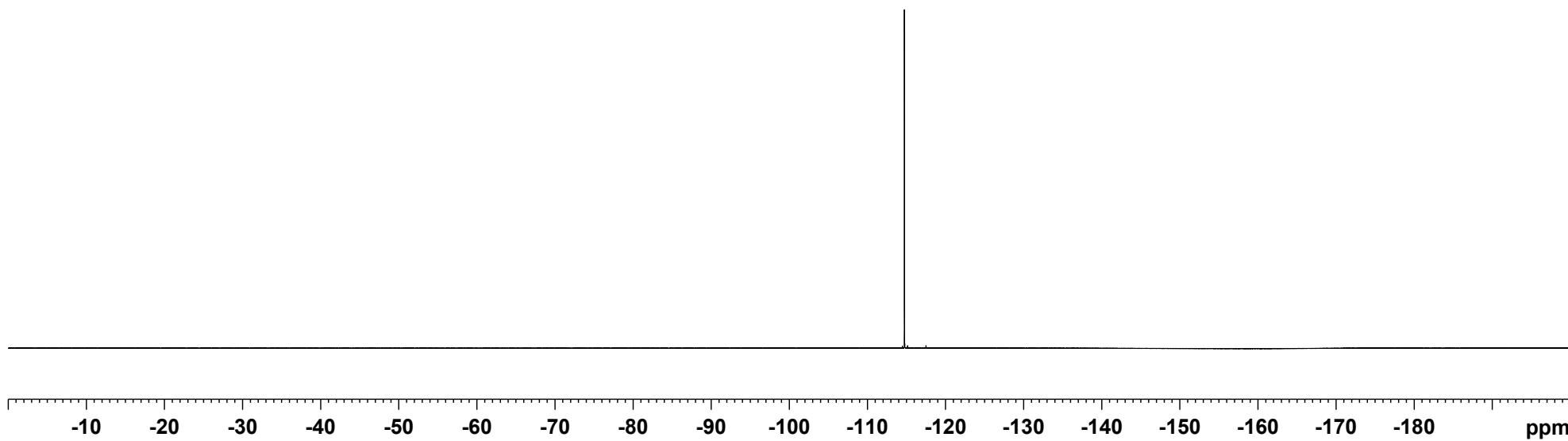
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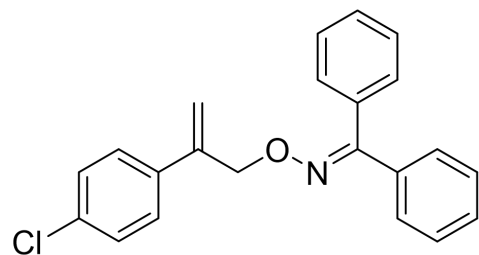




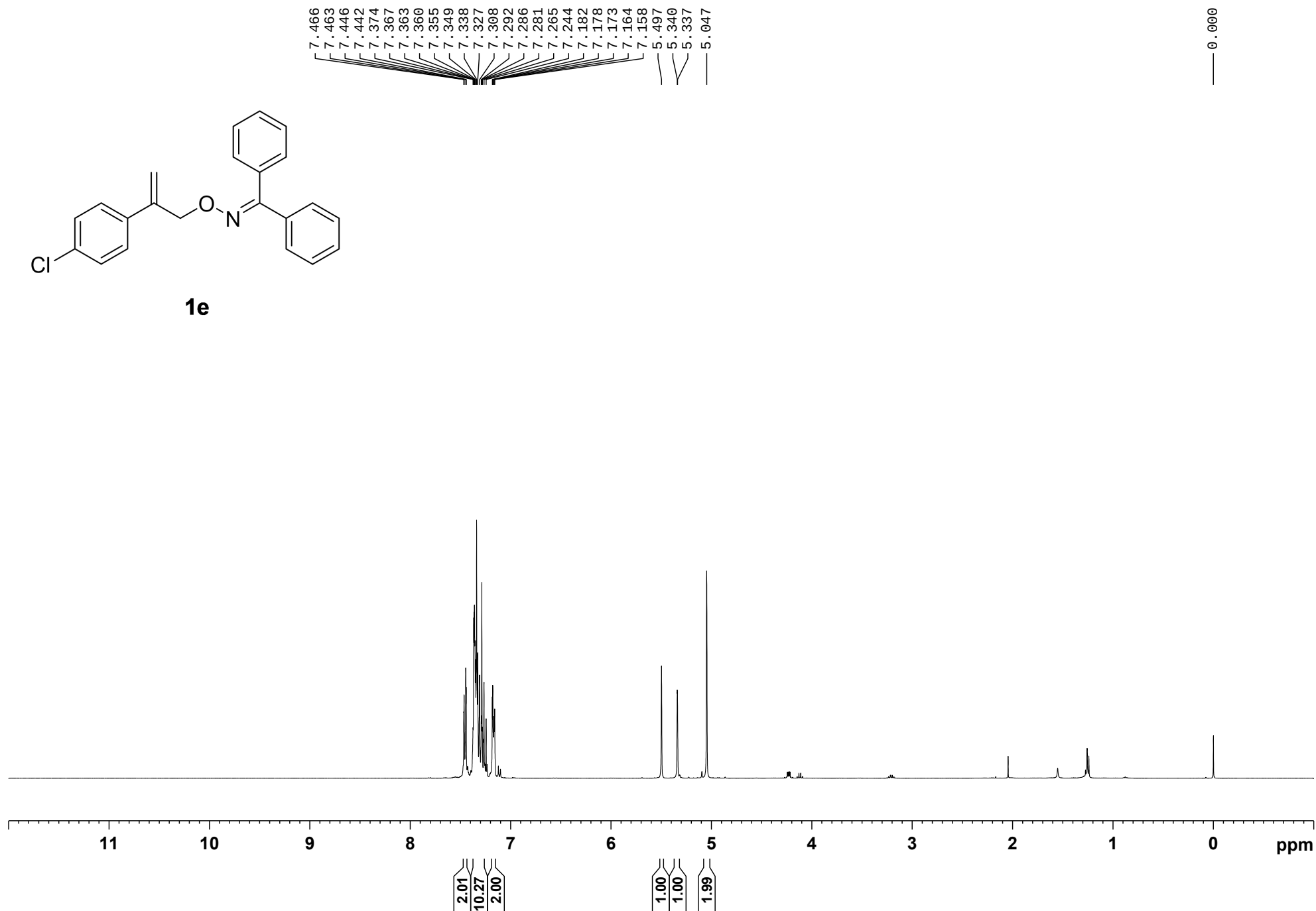
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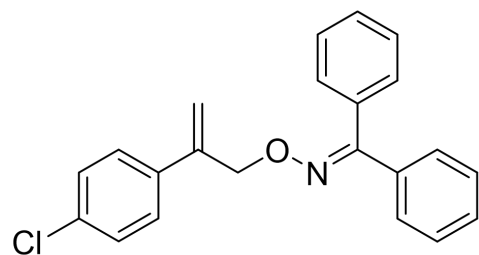
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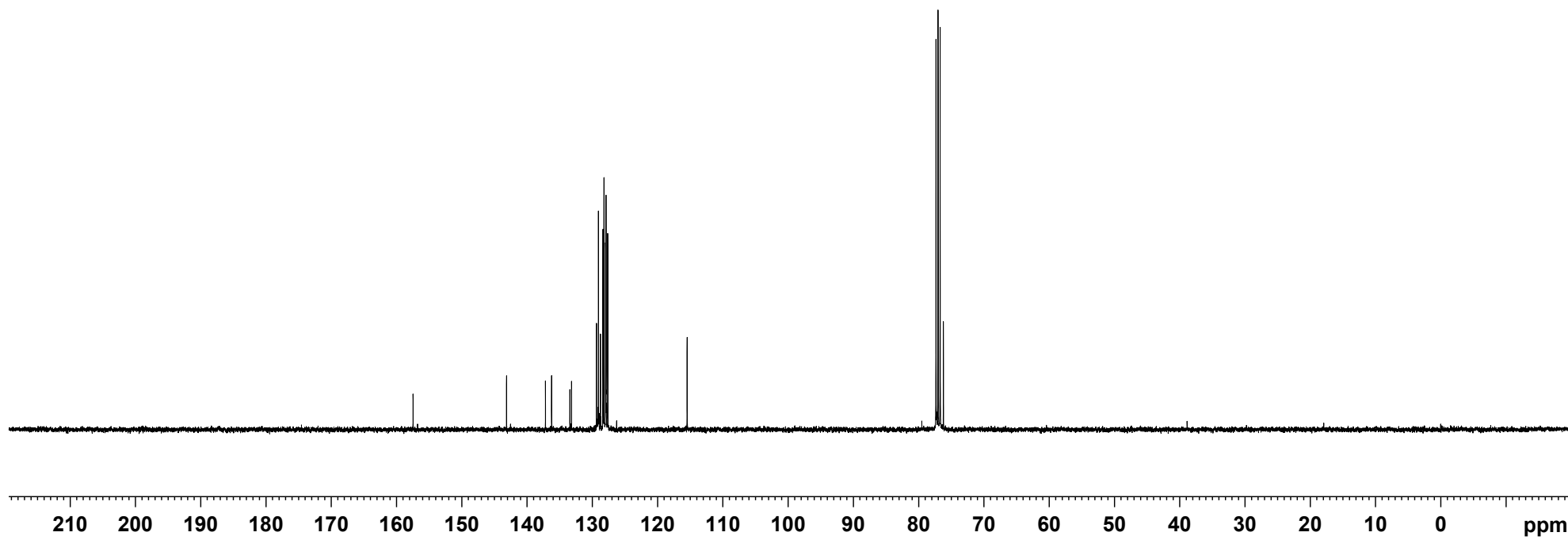
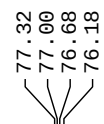
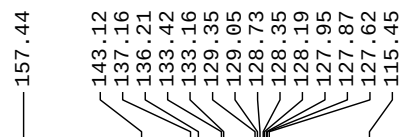


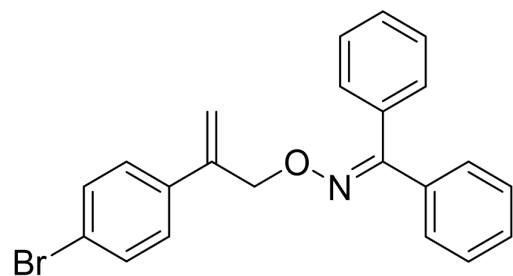
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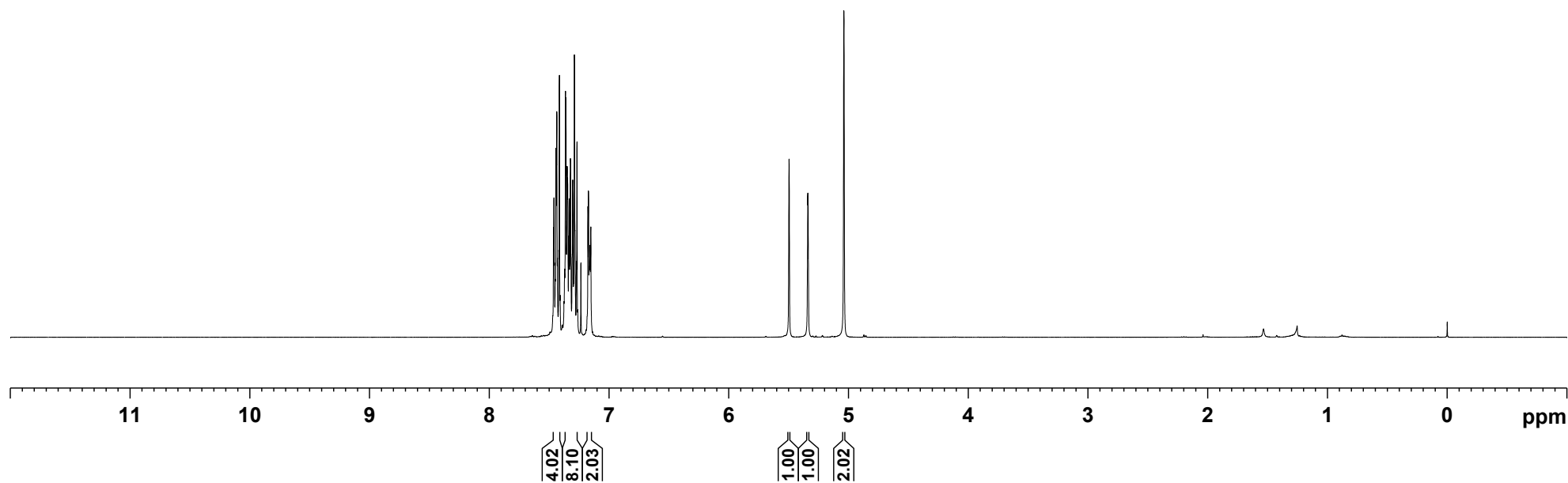


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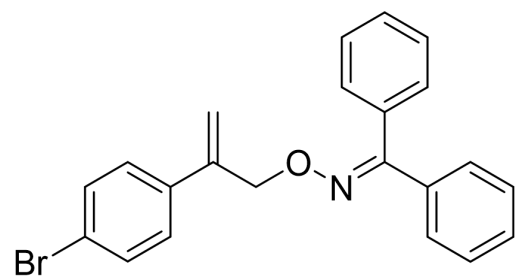


1f



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7.295
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5.039

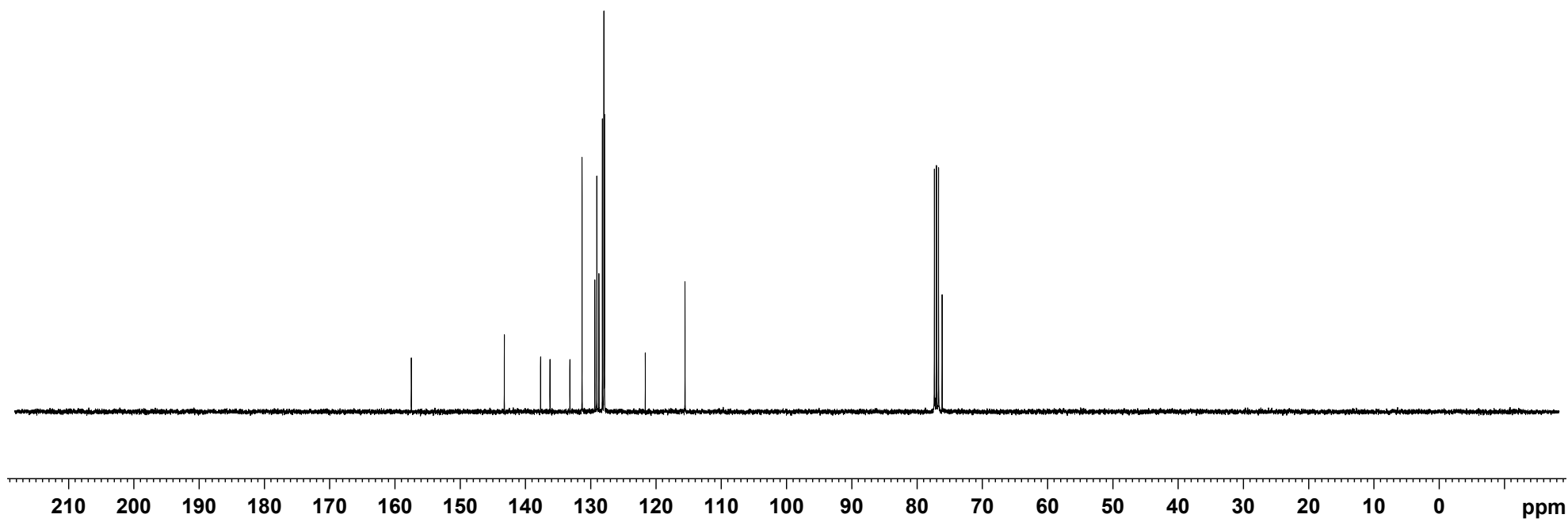
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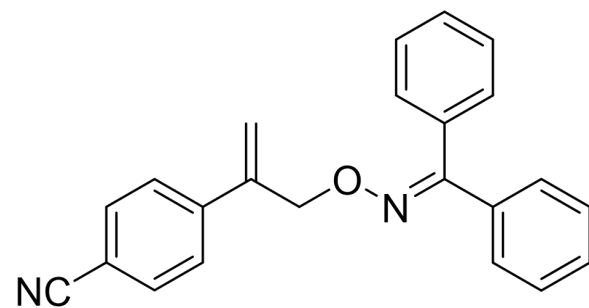


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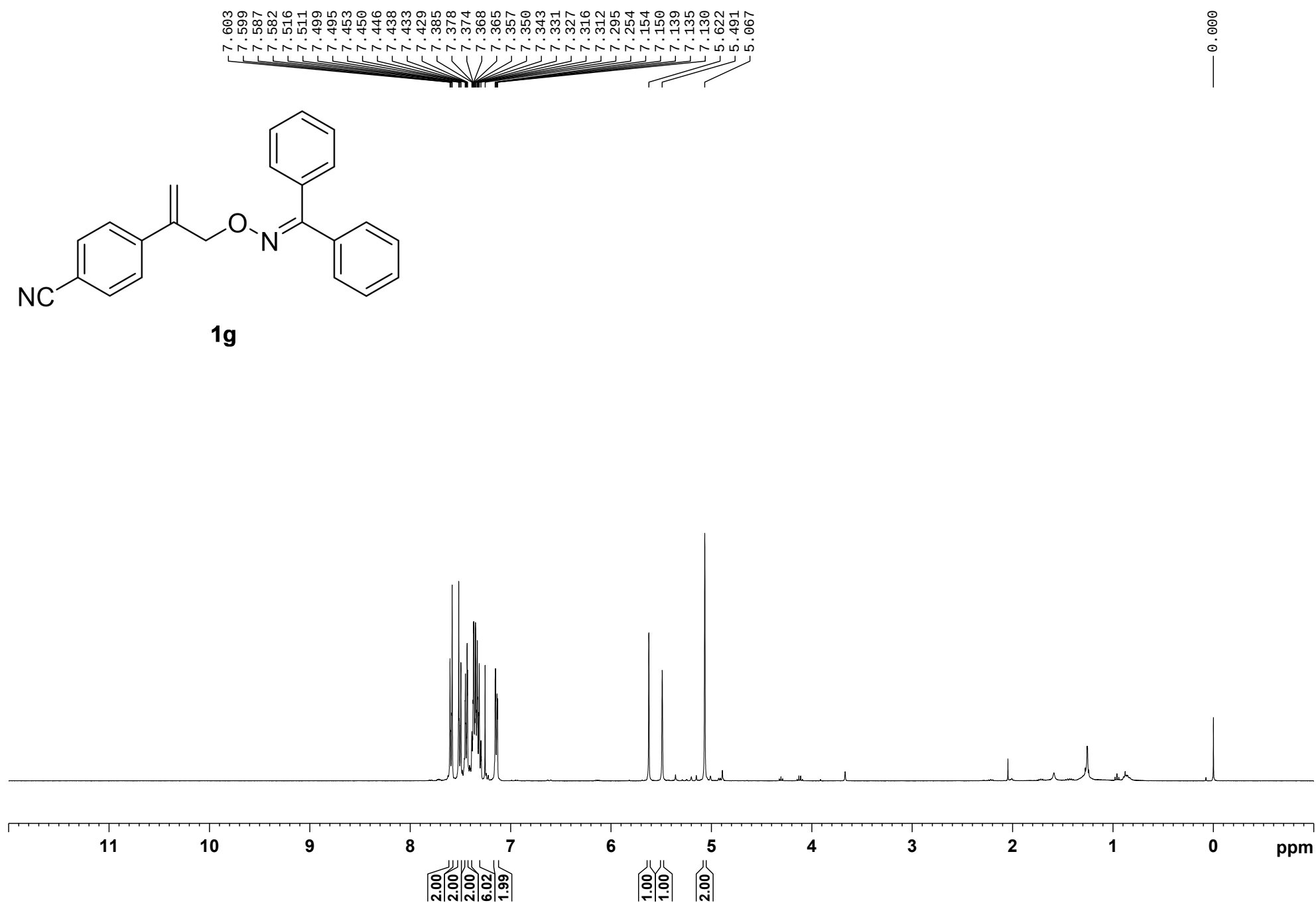
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115.53

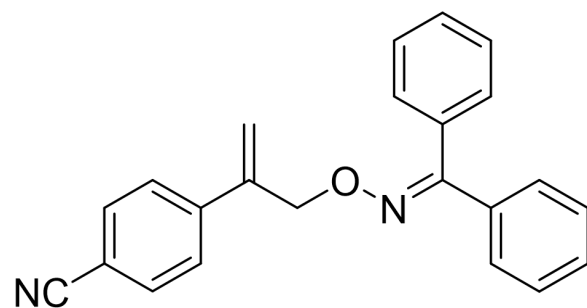
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77.00
76.68
76.13



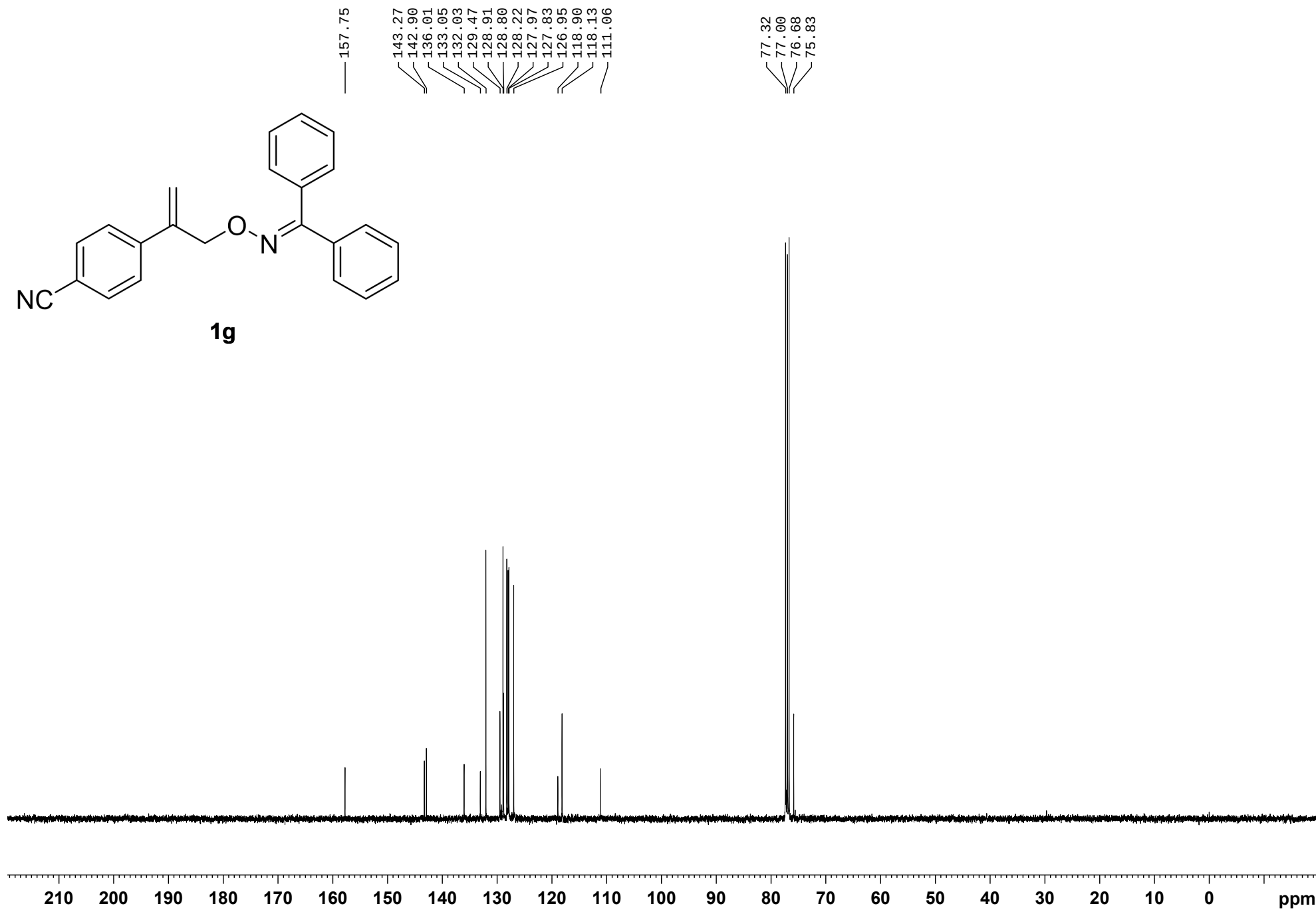


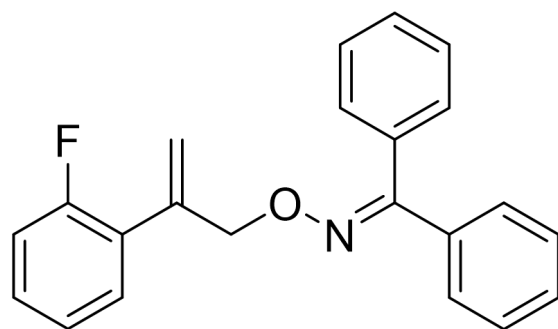
1g





1g



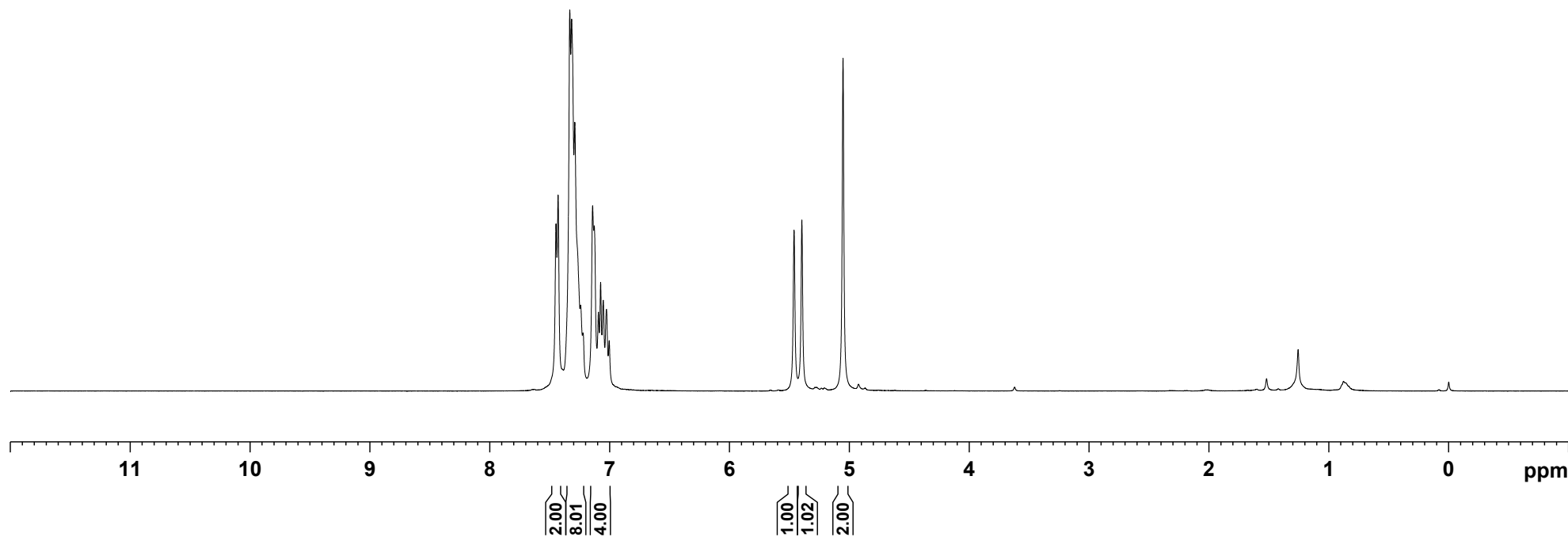


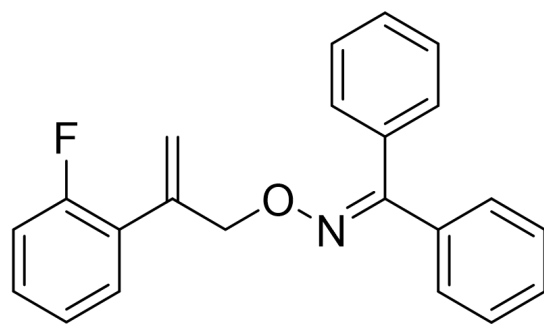
1h

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7.316
7.290
7.242
7.221
7.141
7.128
7.093
7.074
7.053
7.026
7.003

5.461
5.396
5.052

0.000

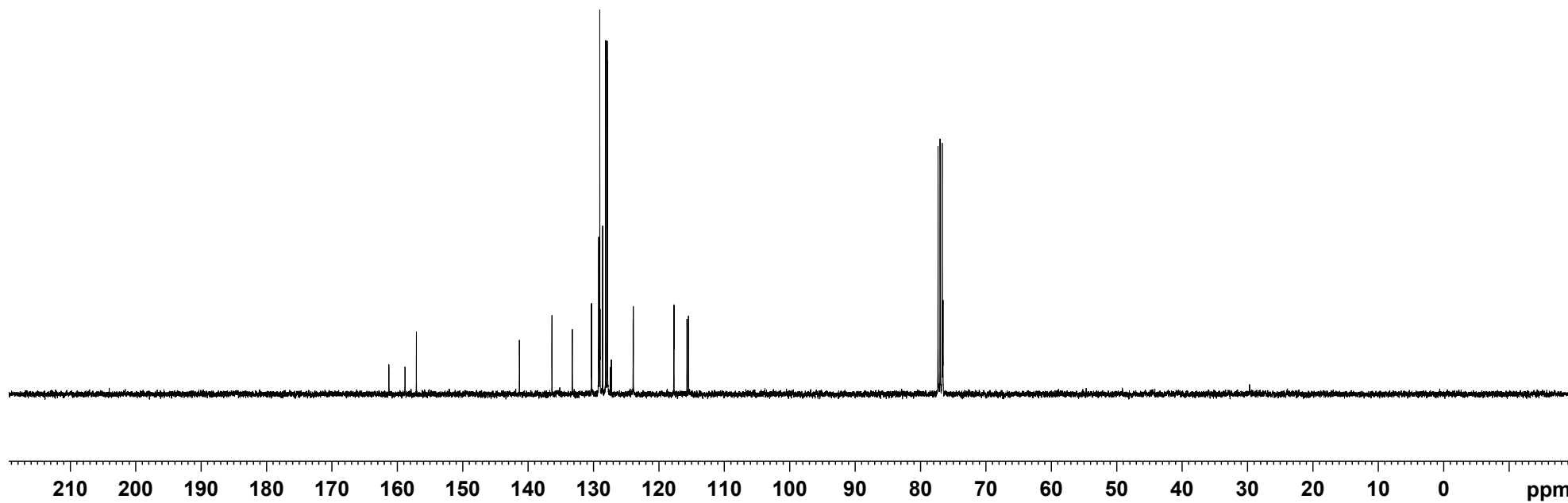


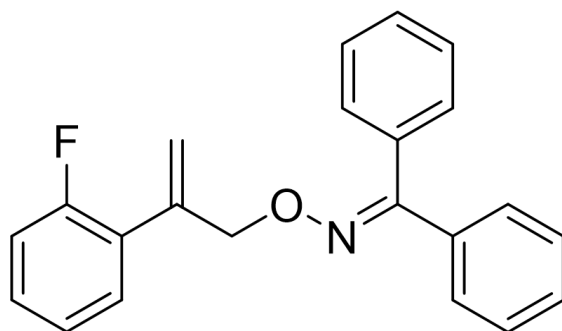


1h

161.28
158.82
157.09
141.33
136.35
133.24
130.32
130.28
129.21
129.07
129.04
128.99
128.60
128.13
127.89
127.86
127.41
127.27
123.94
123.91
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115.71
115.48

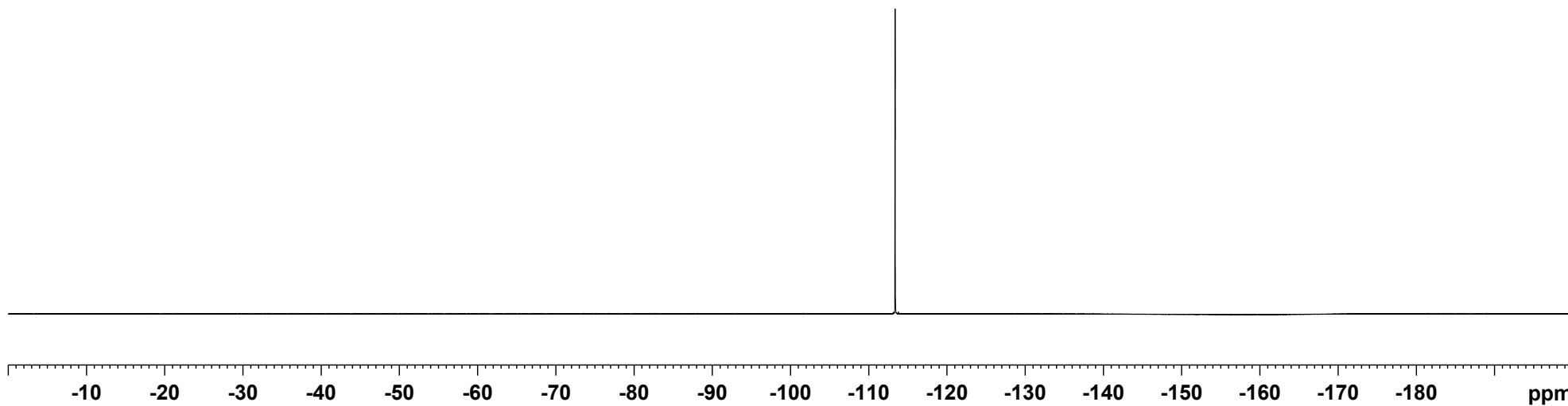
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76.59
76.55

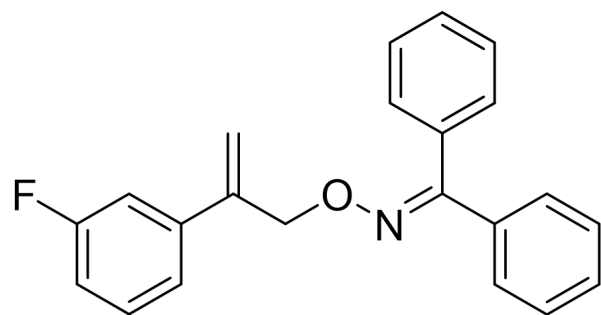




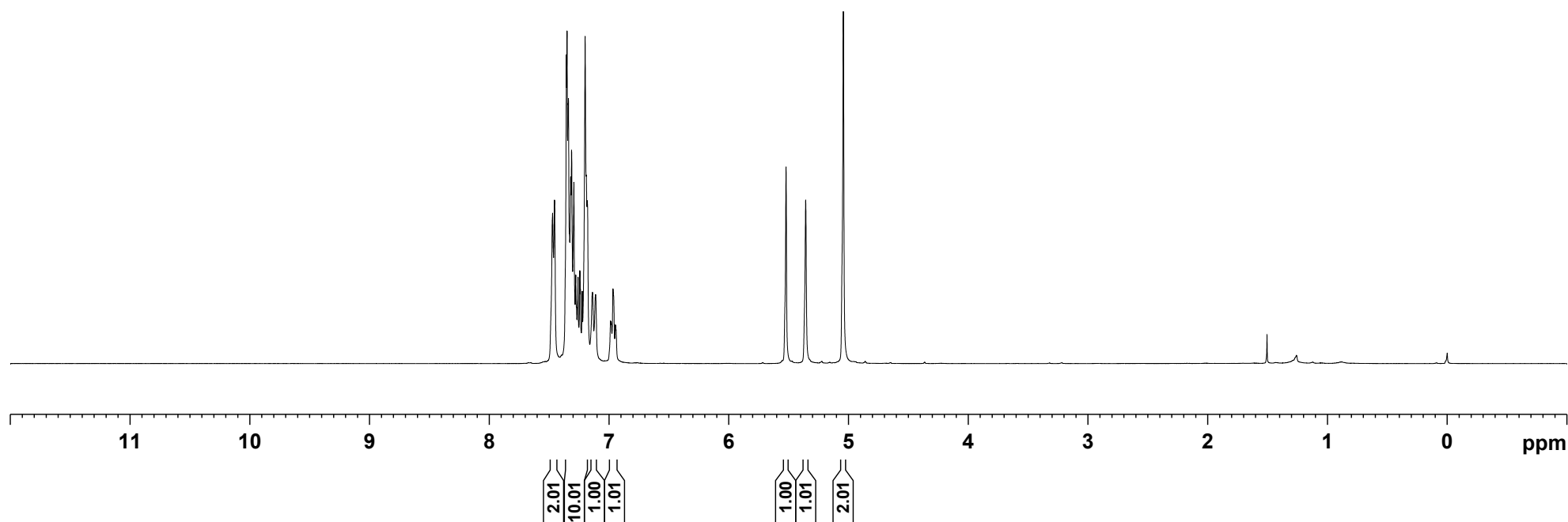
1h

— -113.368

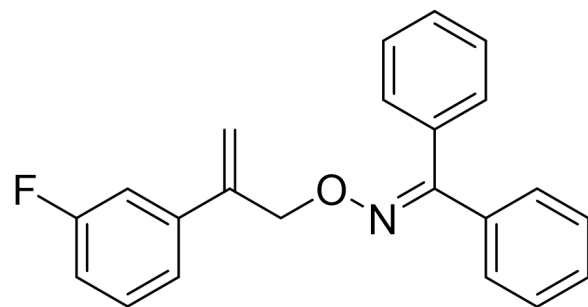




1i



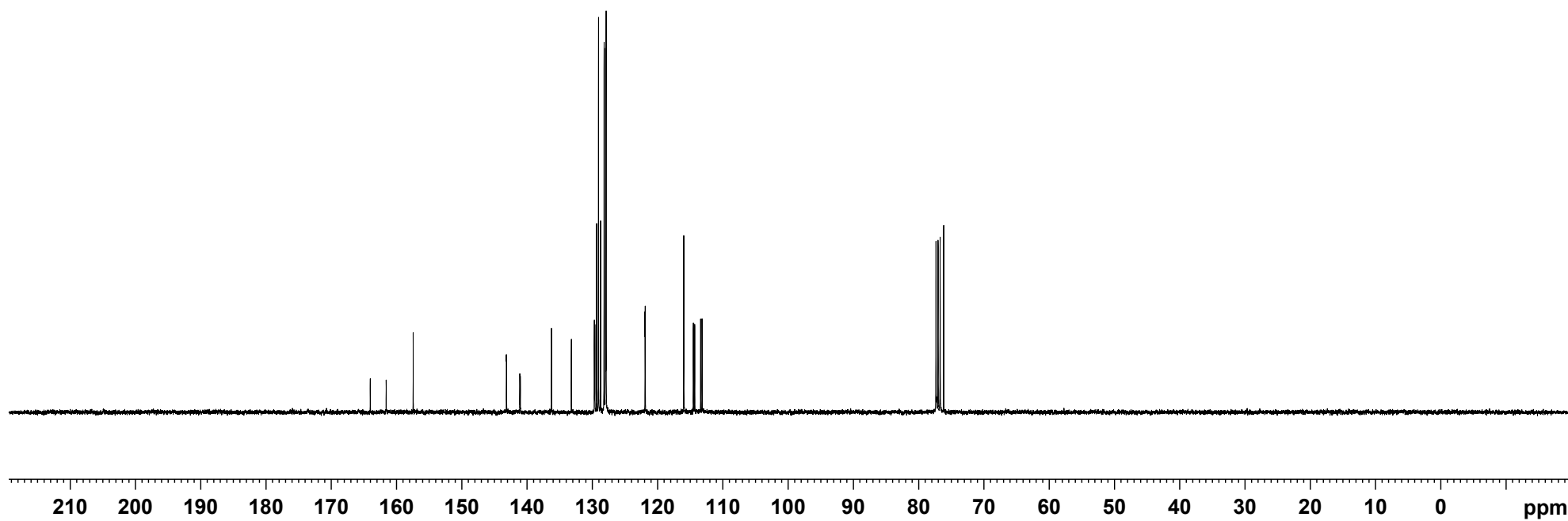
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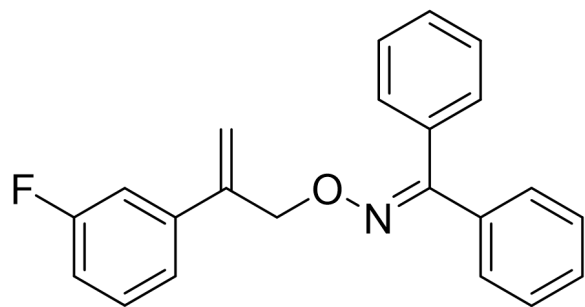


1i

164.00
161.57
157.43
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143.13
141.08
141.01
136.23
133.19
129.67
129.58
129.32
129.03
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127.90
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114.29
113.38
113.16

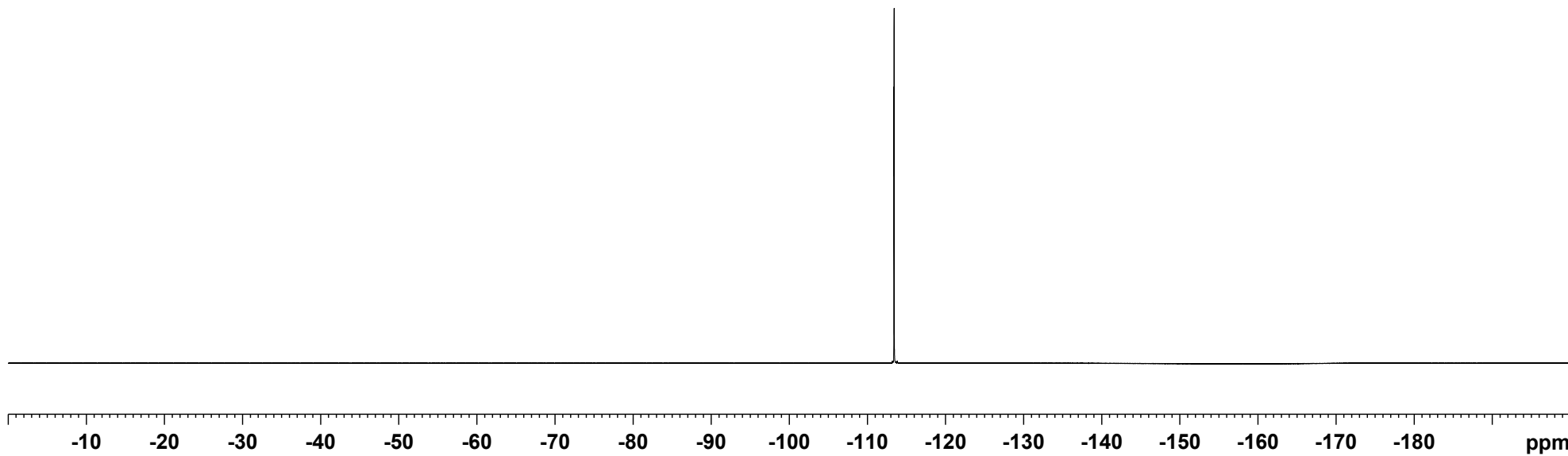
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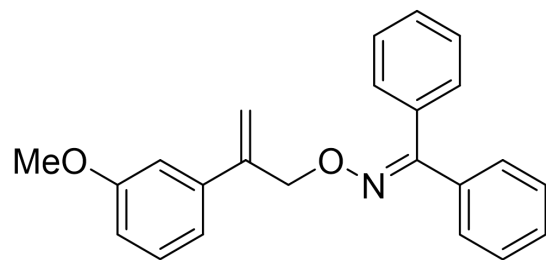




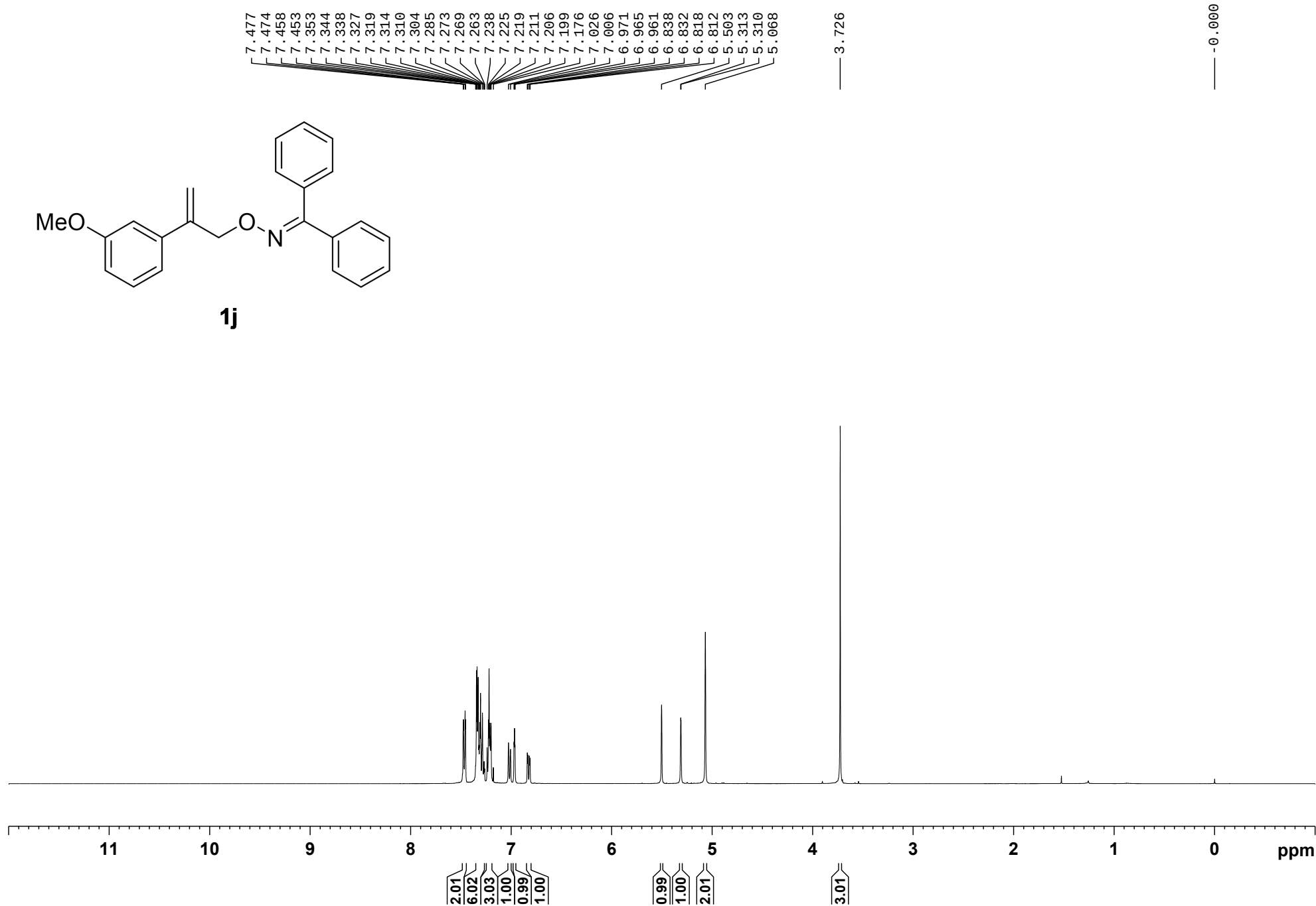
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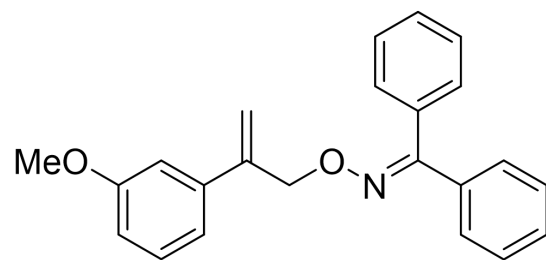
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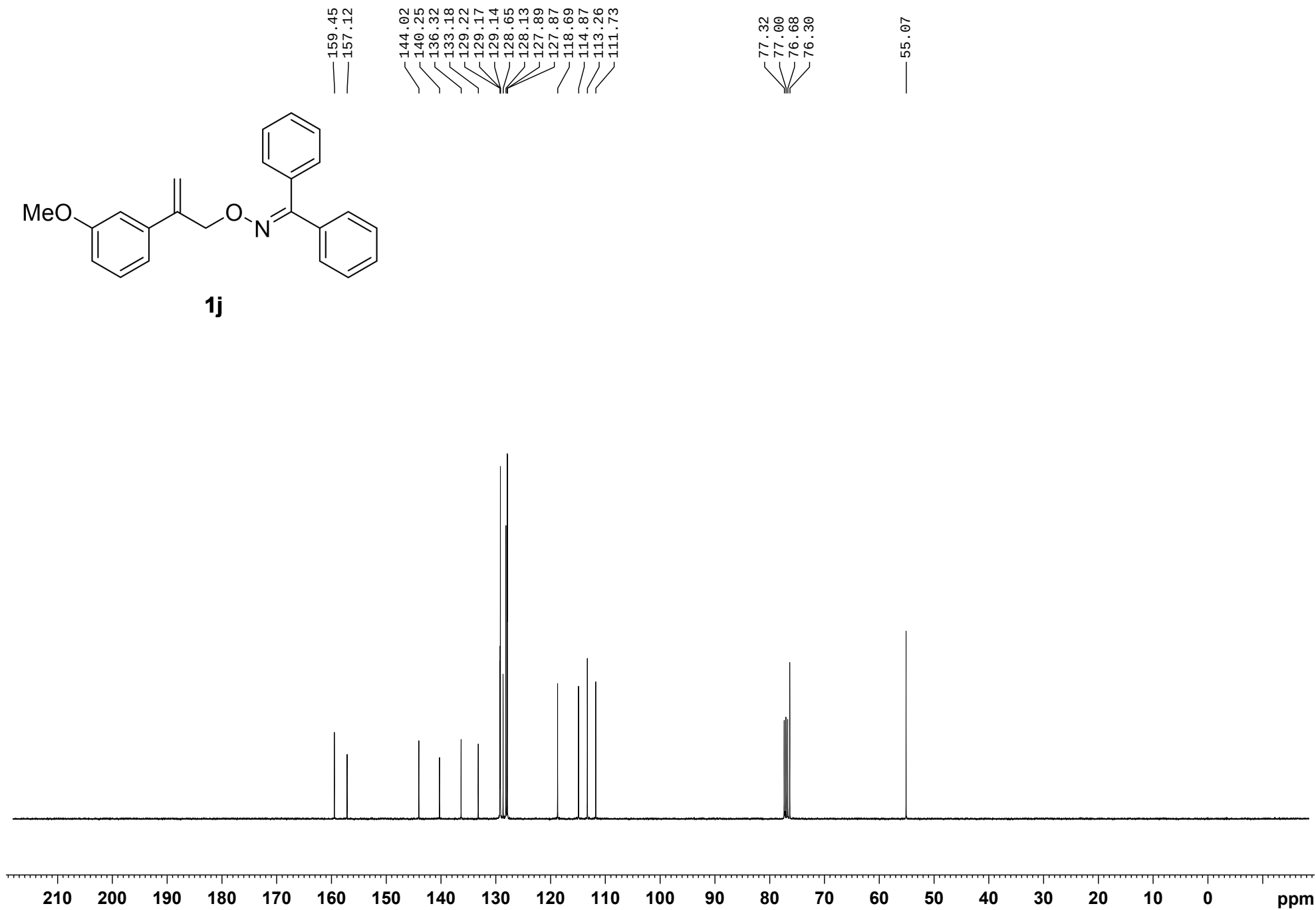


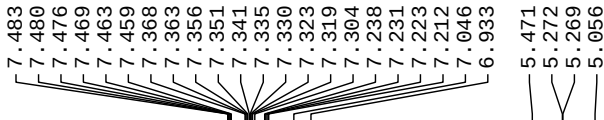
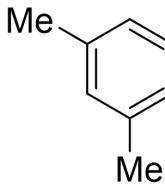
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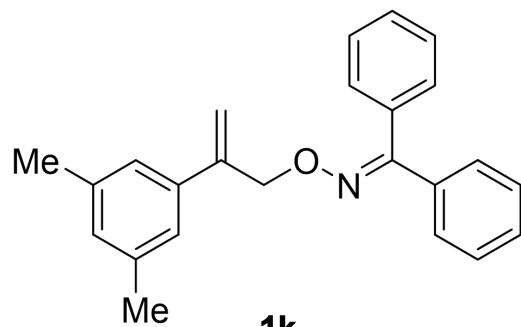




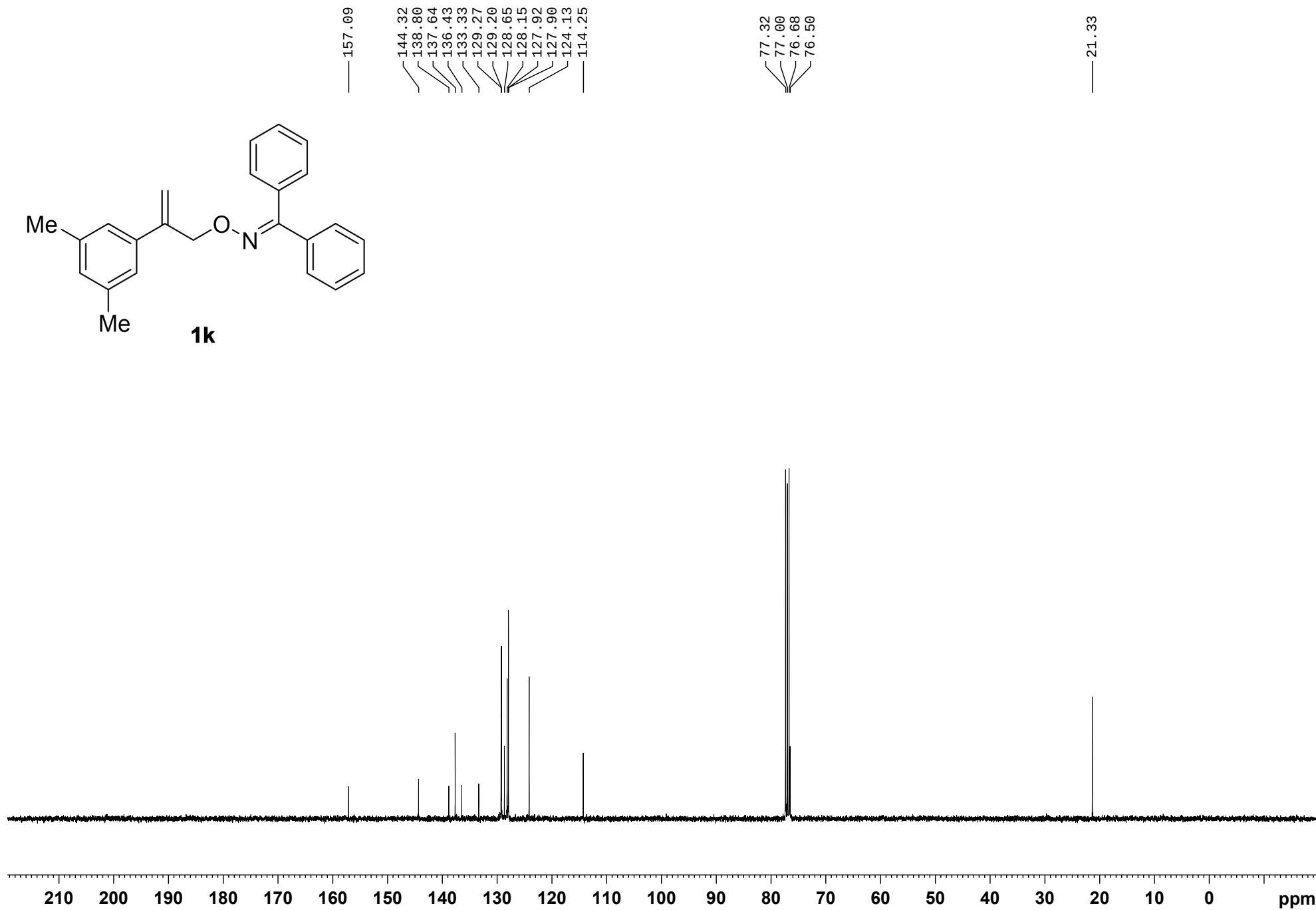
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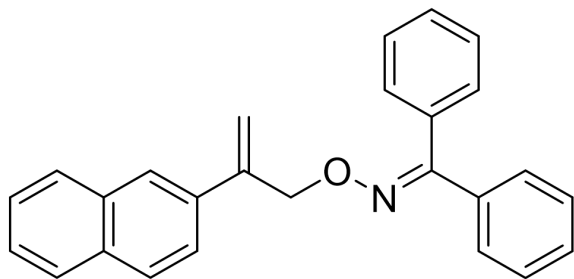






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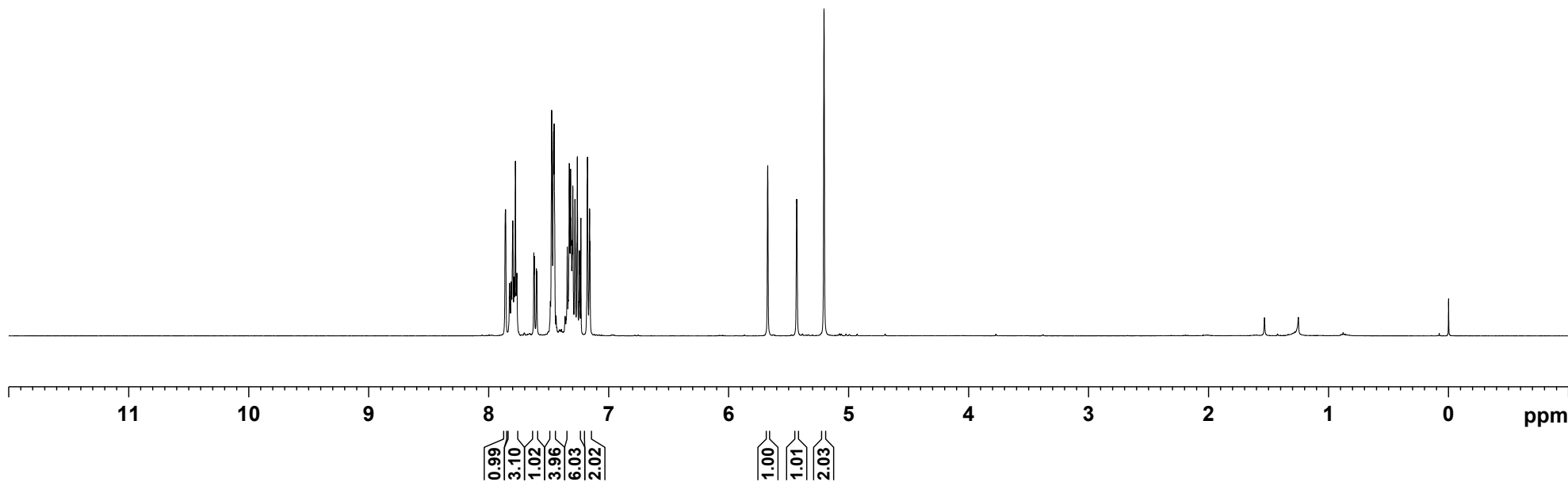


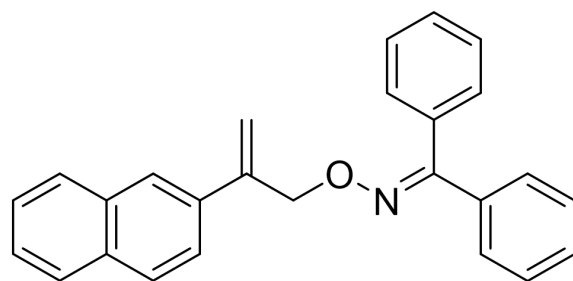


11

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7.825
7.812
7.798
7.788
7.777
7.765
7.624
7.620
7.603
7.598
7.475
7.459
7.455
7.345
7.328
7.324
7.317
7.314
7.311
7.304
7.299
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7.244
7.232
7.177
7.159
7.156
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5.432
5.205

0.000

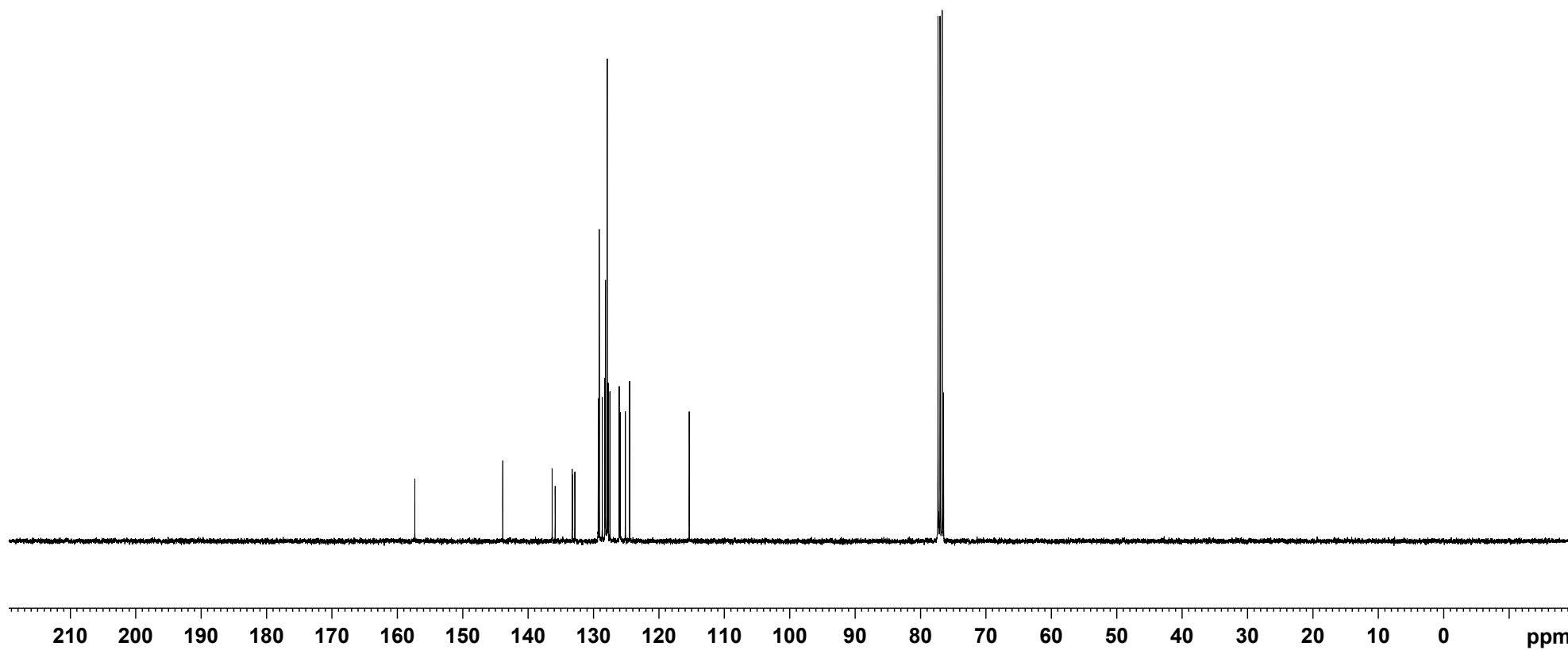


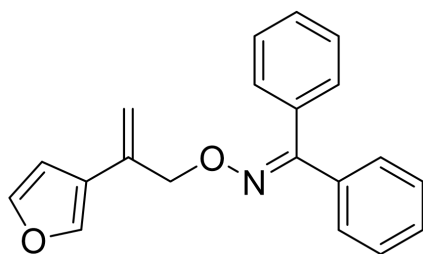


11

157.32
143.87
136.32
135.86
133.27
133.22
132.85
129.27
129.11
128.65
128.26
128.17
127.90
127.75
127.49
126.07
125.92
125.13
124.47
115.36

77.31
77.00
76.68
76.47





1m

7.487
7.468
7.399
7.347
7.322
7.302
7.288

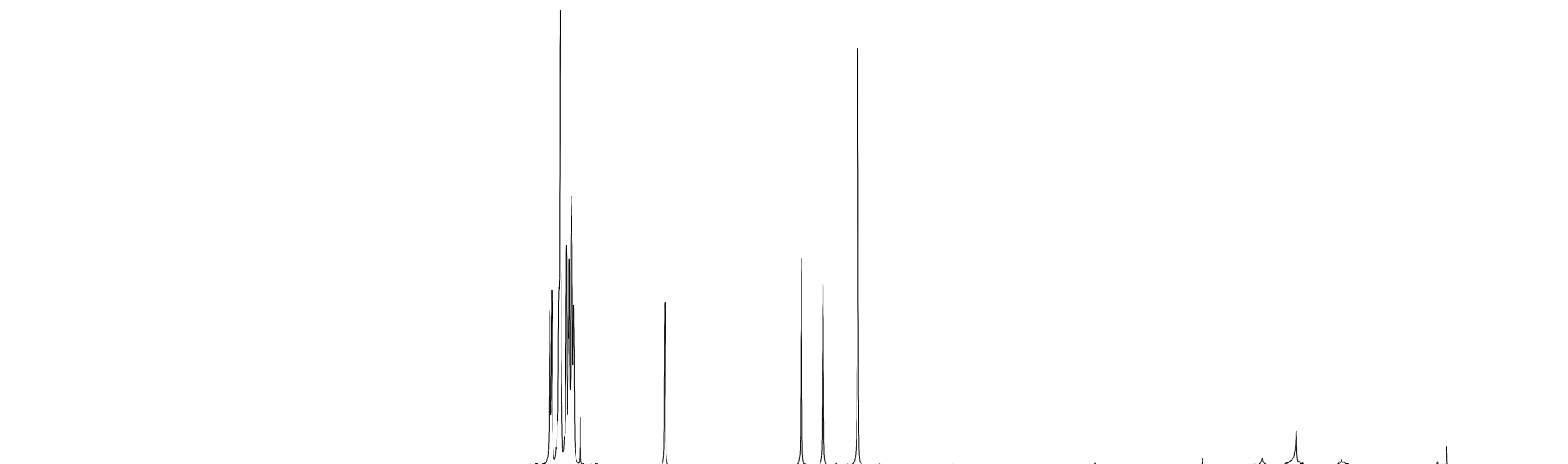
6.525

5.387

5.205

4.916

0.000



11

10

9

8

7

6

5

4

3

2

1

0

ppm

2.01

4.02

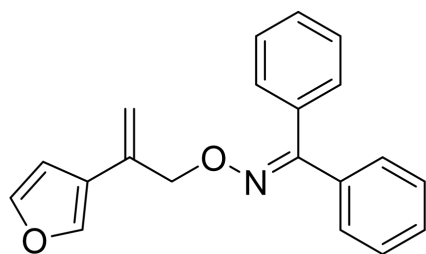
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0.96

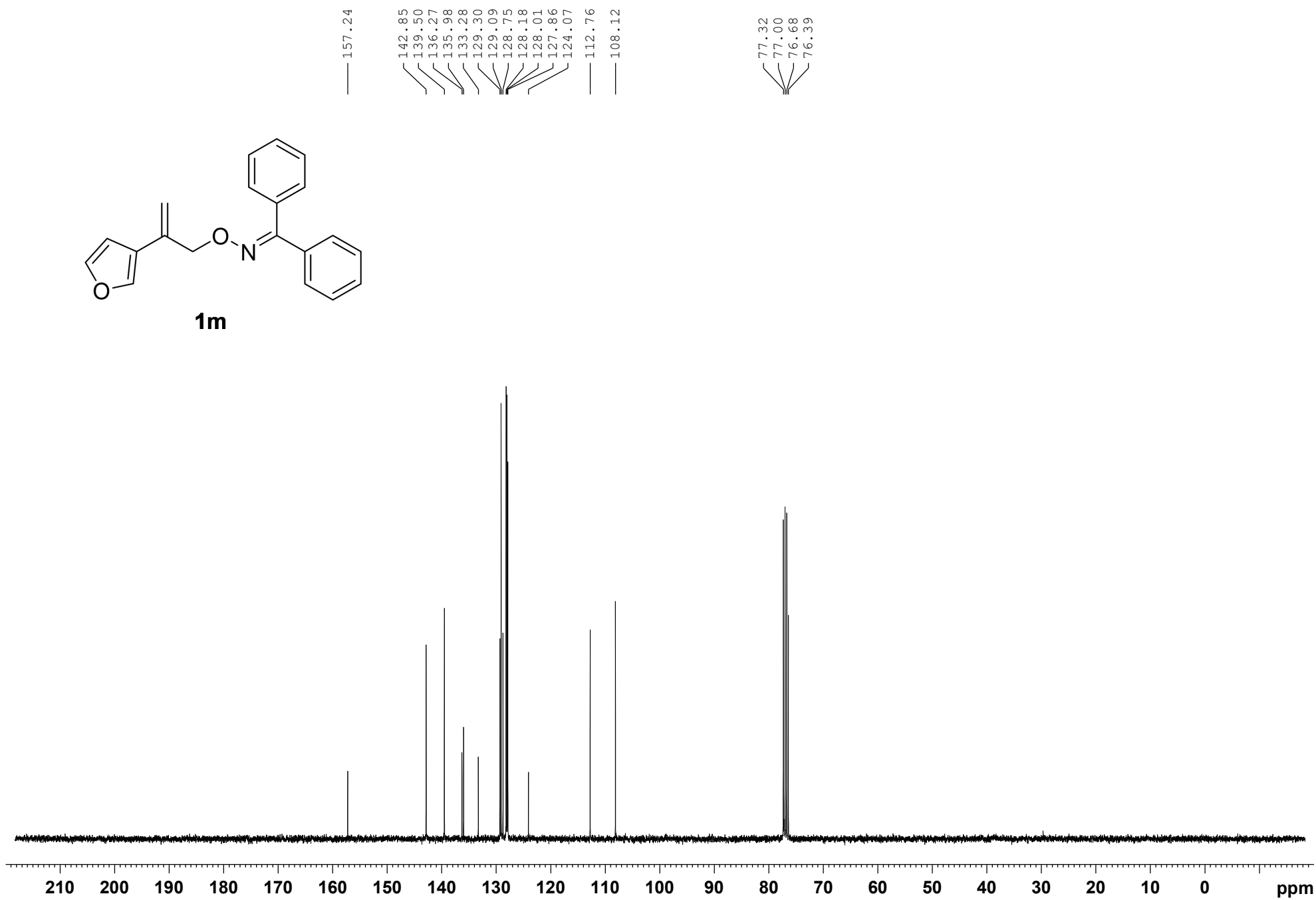
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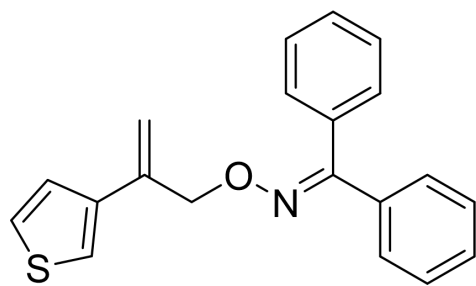
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2.00

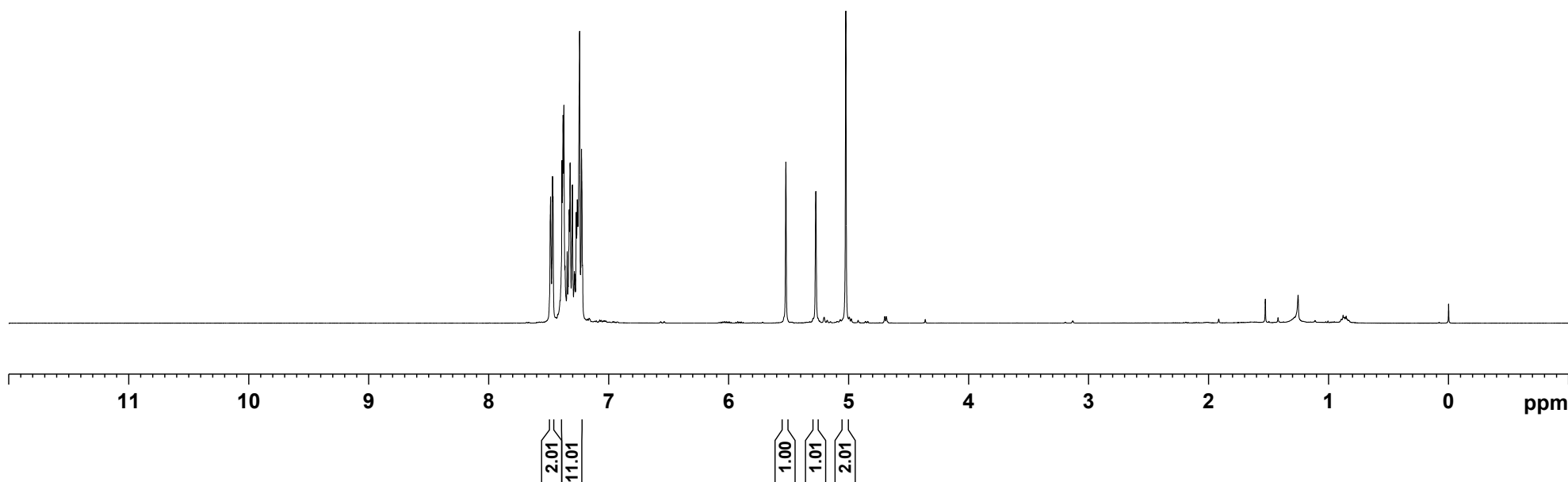
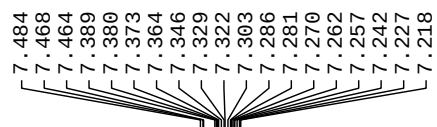


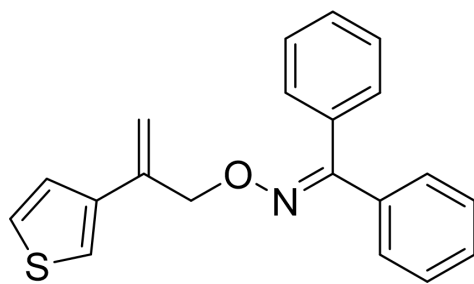
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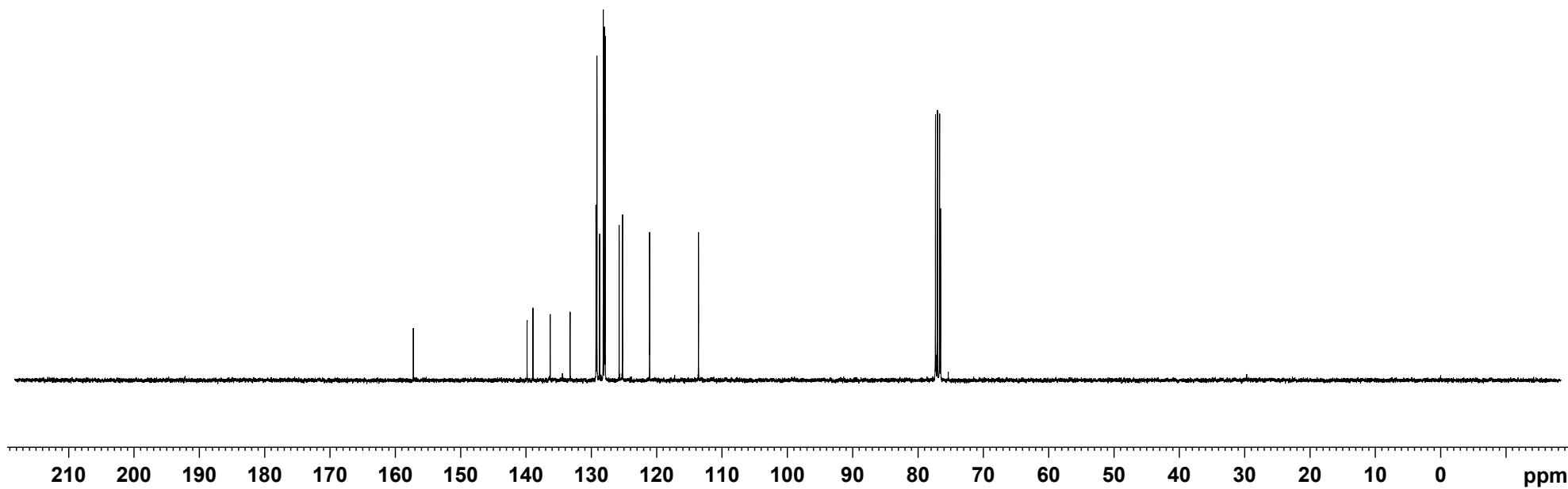
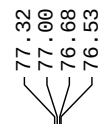
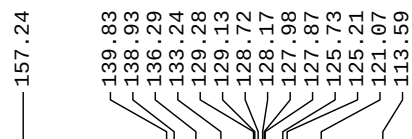


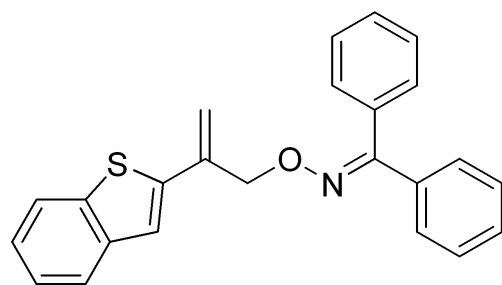
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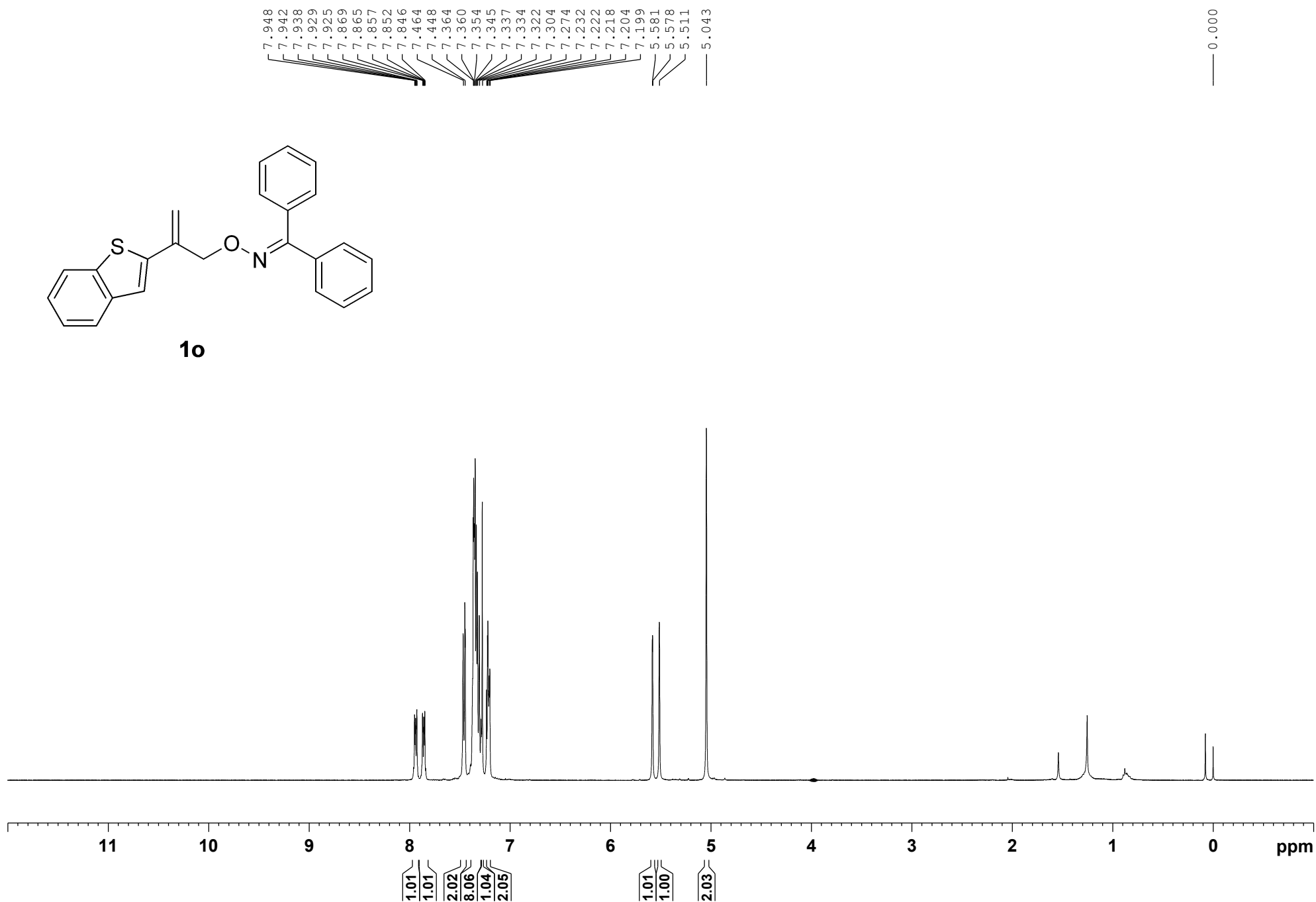


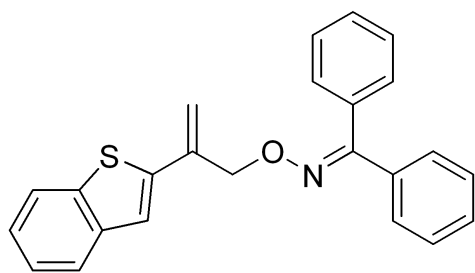
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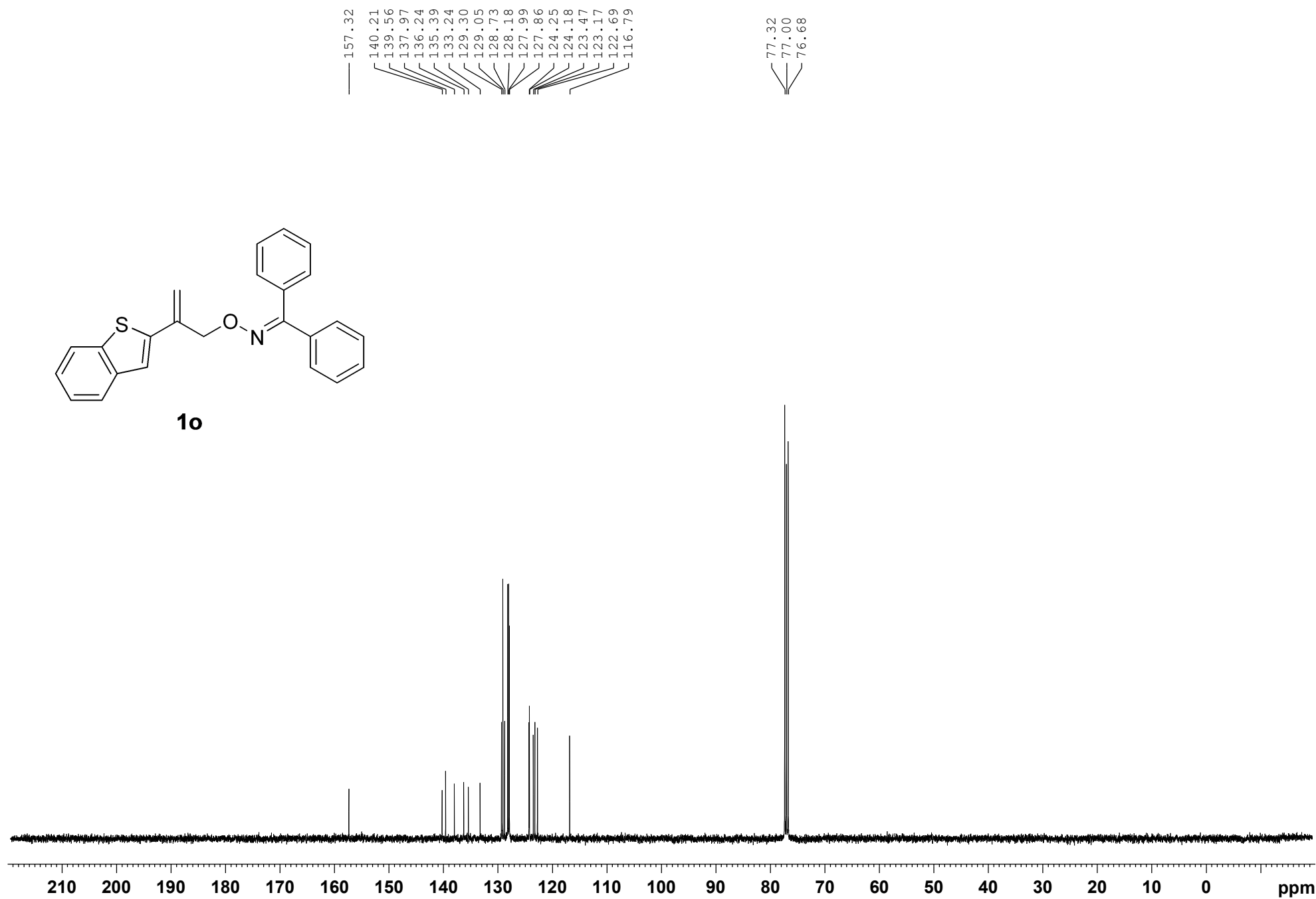


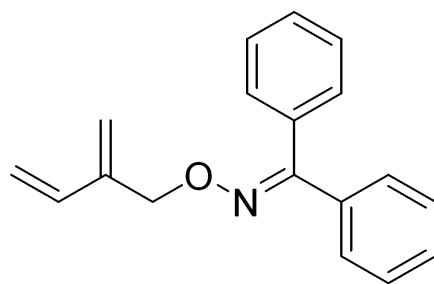
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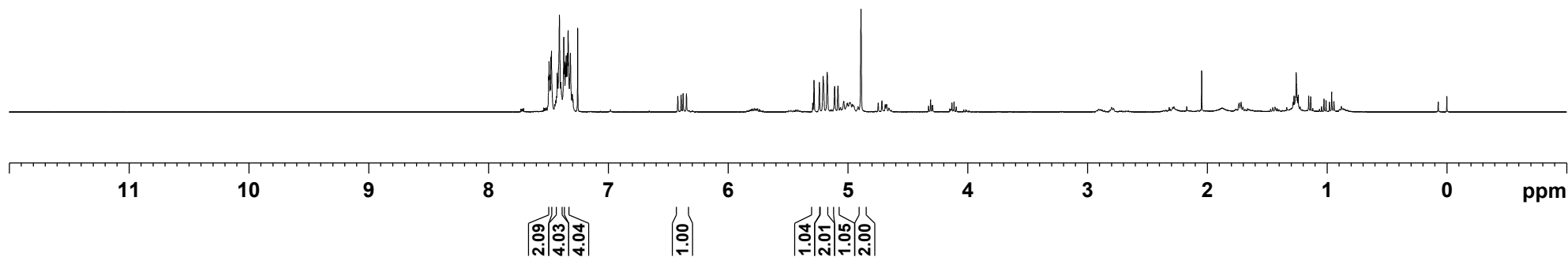


1o



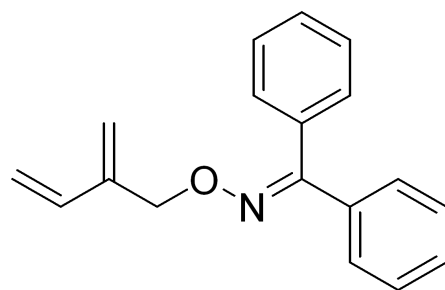


1p

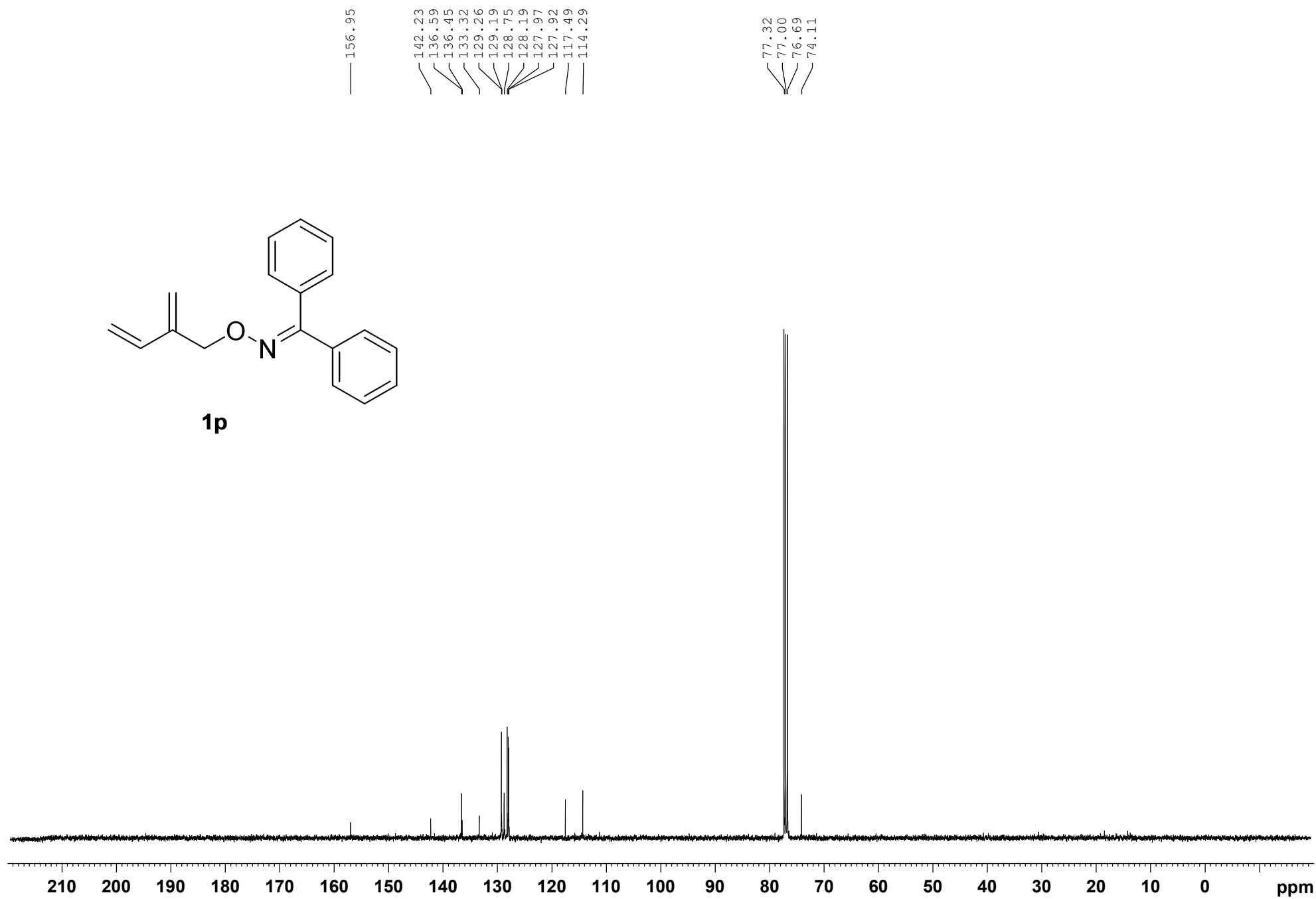


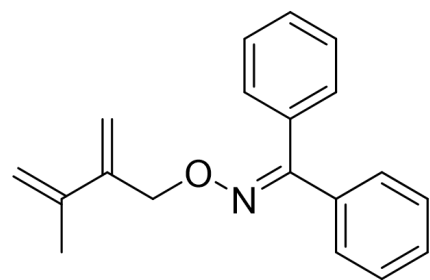
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7.477
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7.422
7.413
7.406
7.402
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7.369
7.363
7.356
7.349
7.345
7.339
7.332
7.314
7.253
6.417
6.390
6.373
6.345
5.280
5.236
5.204
5.170
5.109
5.081
4.888

— 0.000



1p





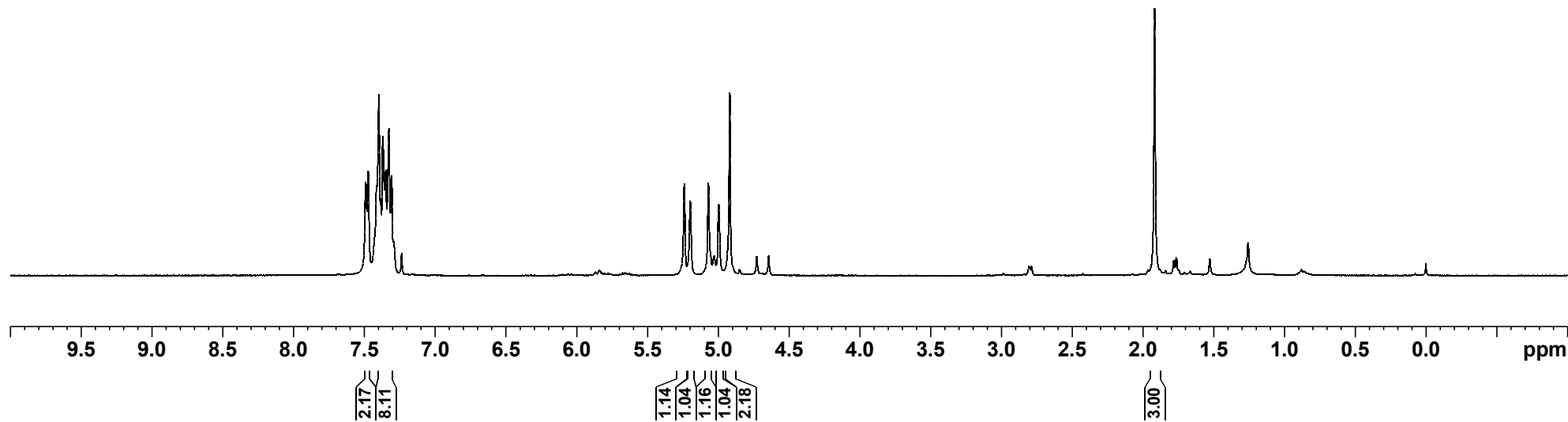
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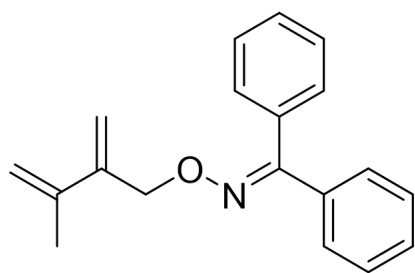
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7.472
7.413
7.398
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7.326
7.307
7.292

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5.198
5.069
4.995
4.918

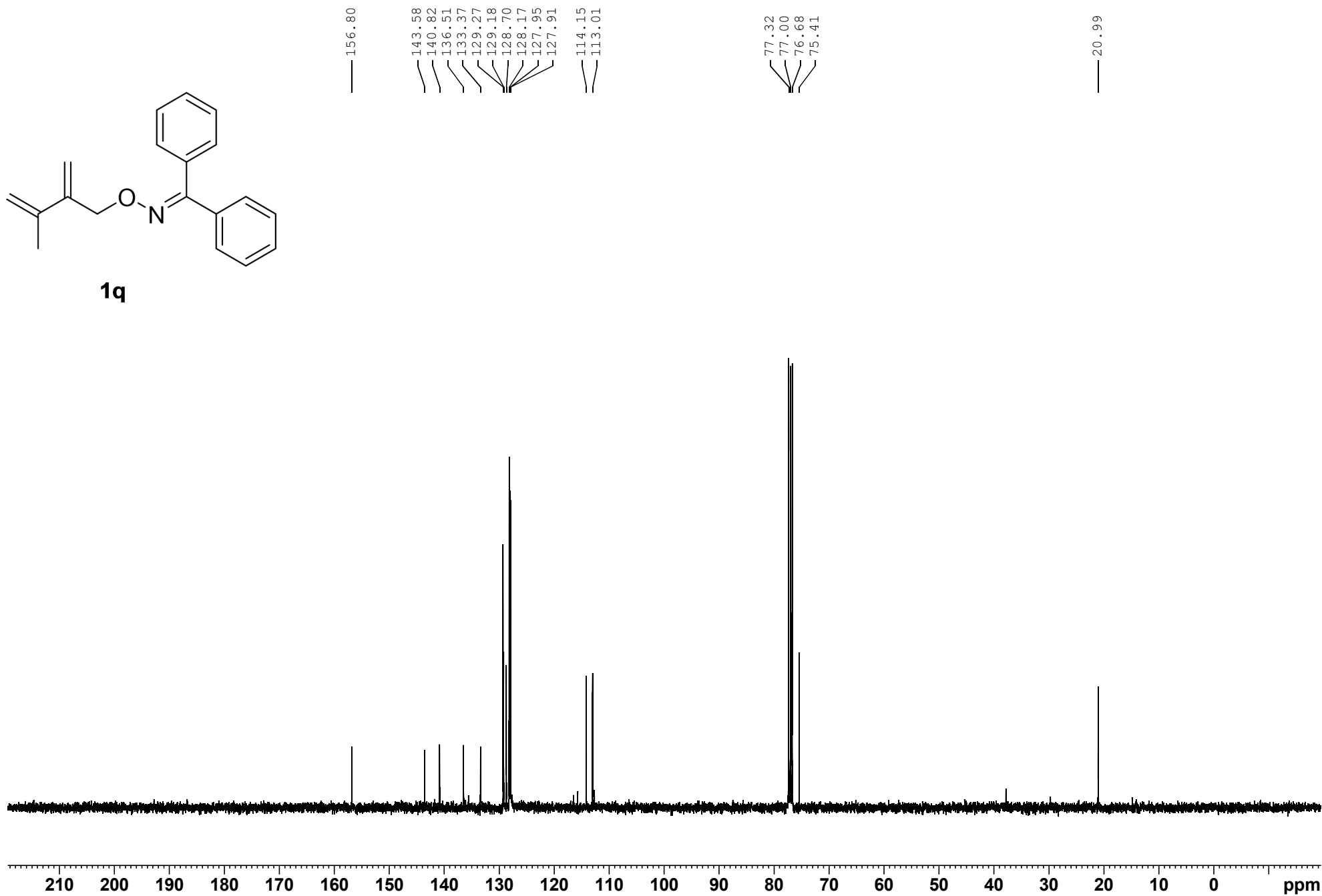
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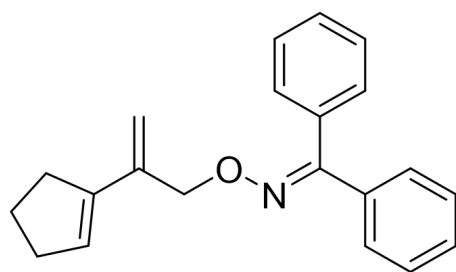
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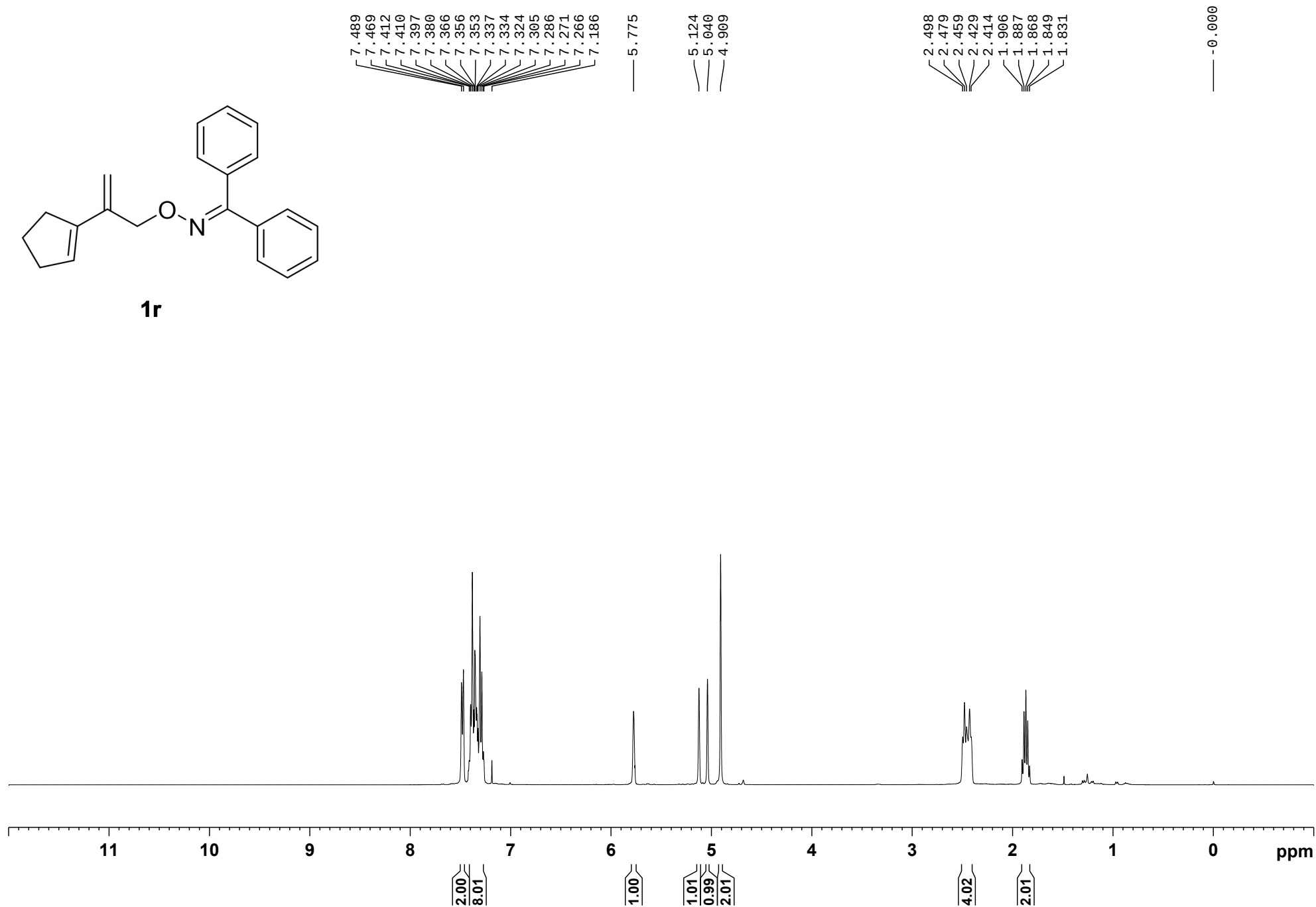


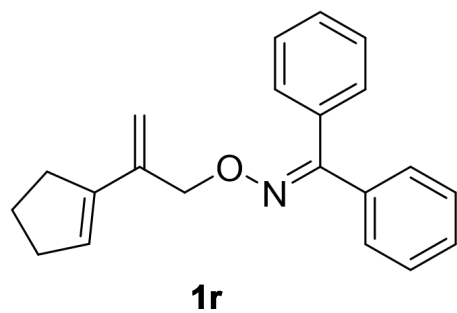
1q





1r



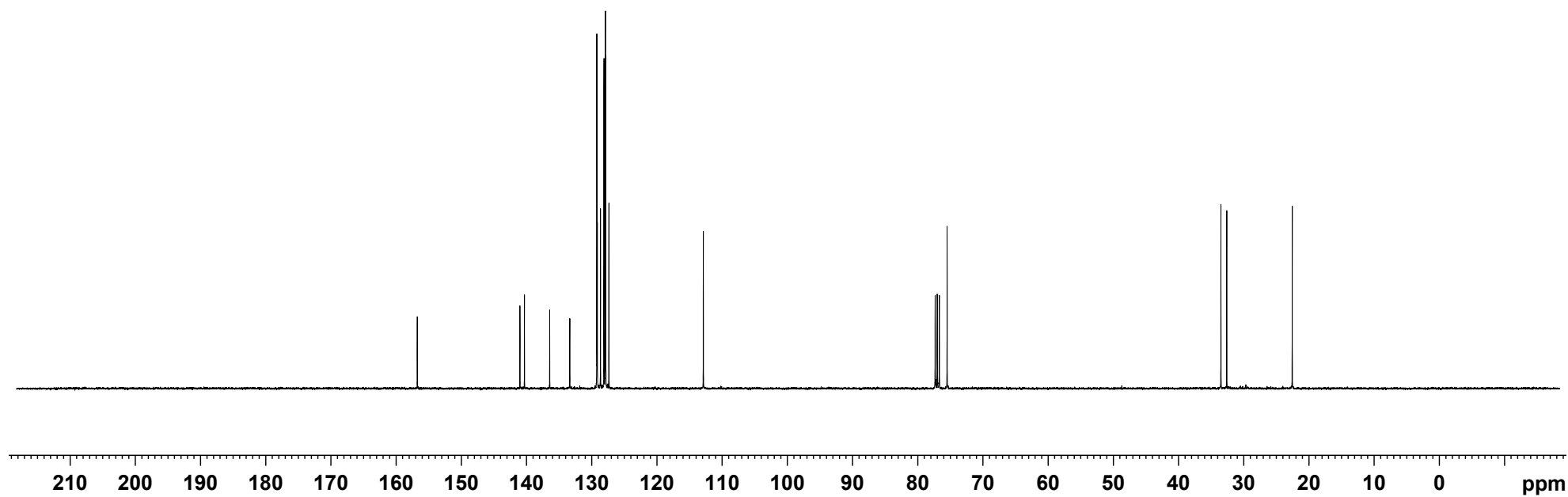


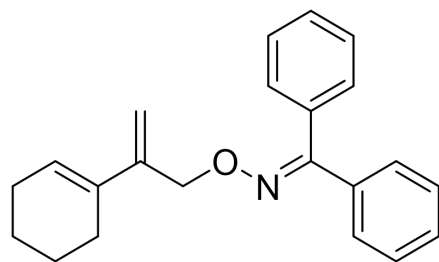
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 141.01
 140.31
 136.44
 133.36
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 128.65
 128.12
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 127.86
 127.36
 112.88

77.32
 77.00
 76.68
 75.49

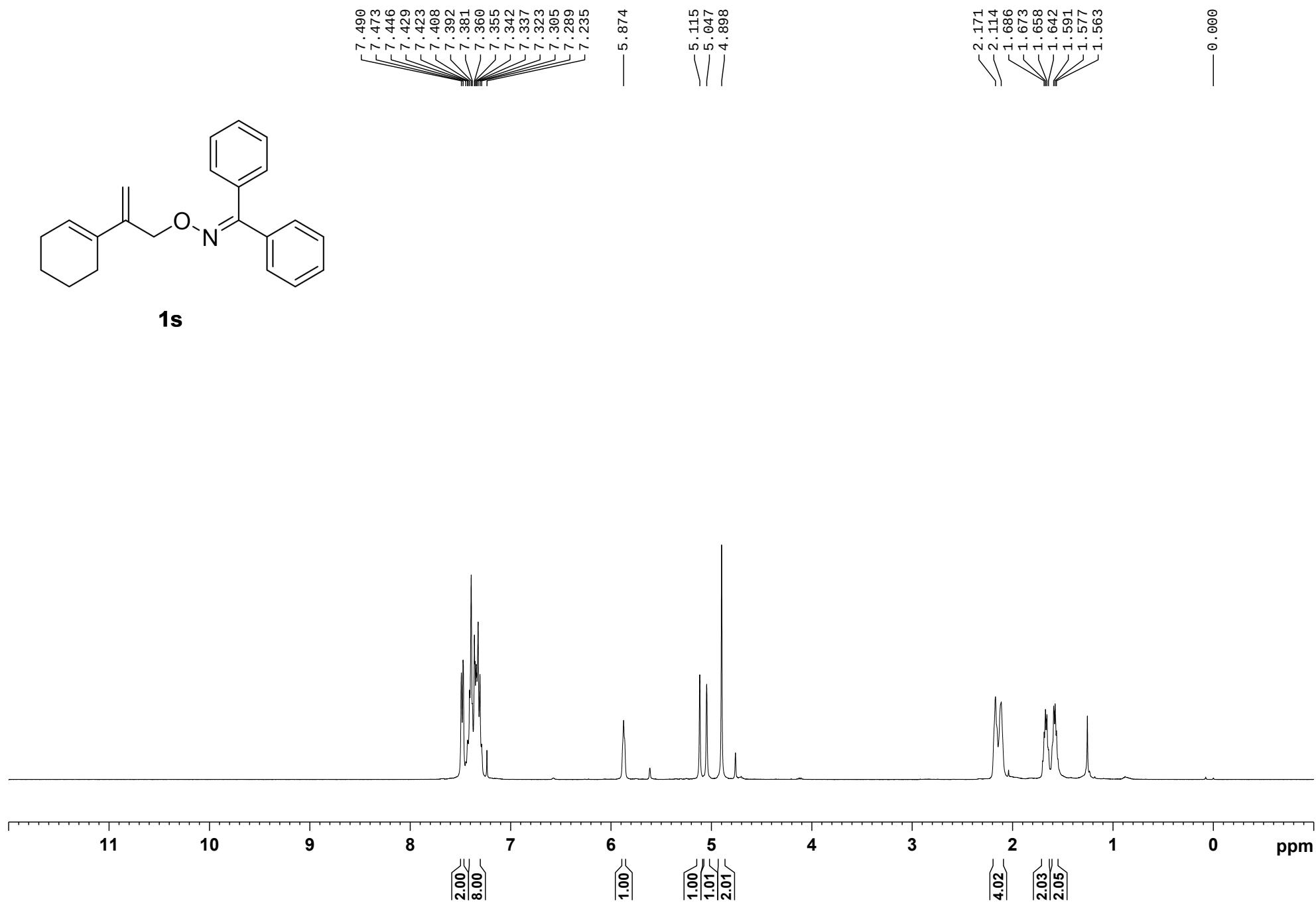
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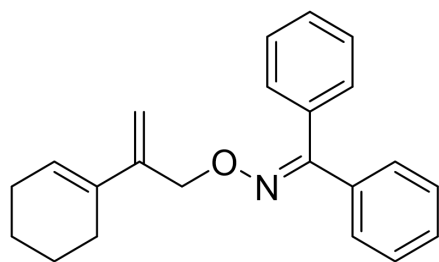
22.55





1s



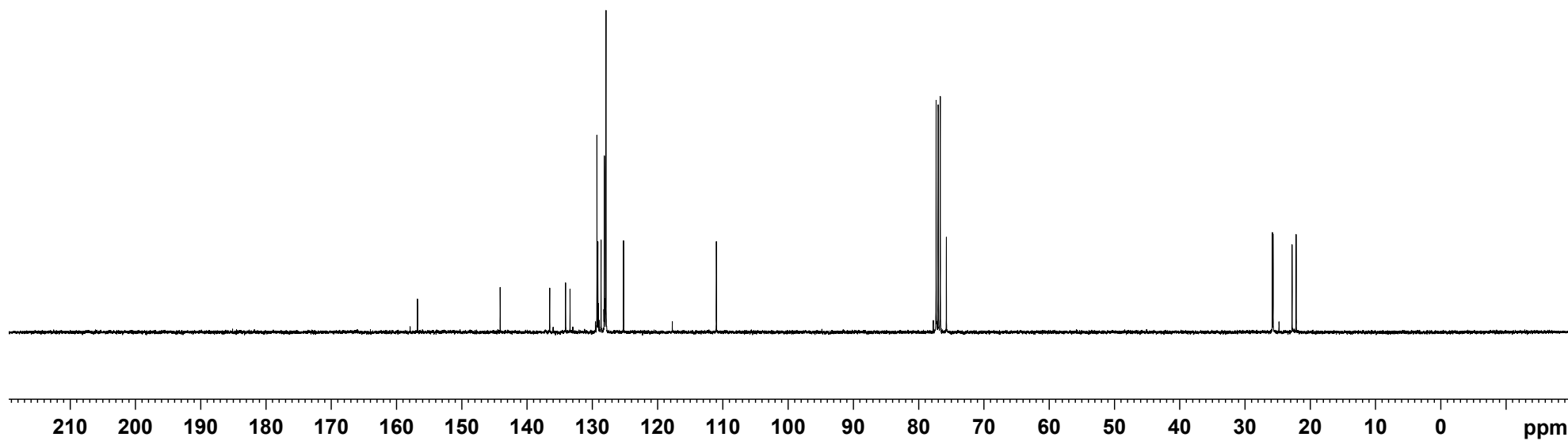


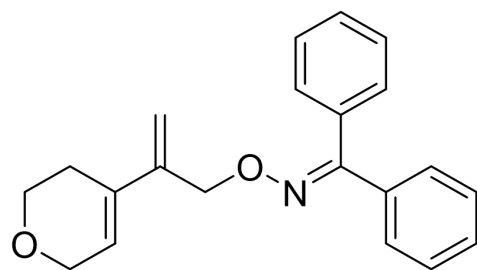
1s

— 156.76
 — 144.11
 — 136.53
 — 134.09
 — 133.41
 — 129.29
 — 129.14
 — 128.65
 — 128.14
 — 127.90
 — 125.21
 — 110.99

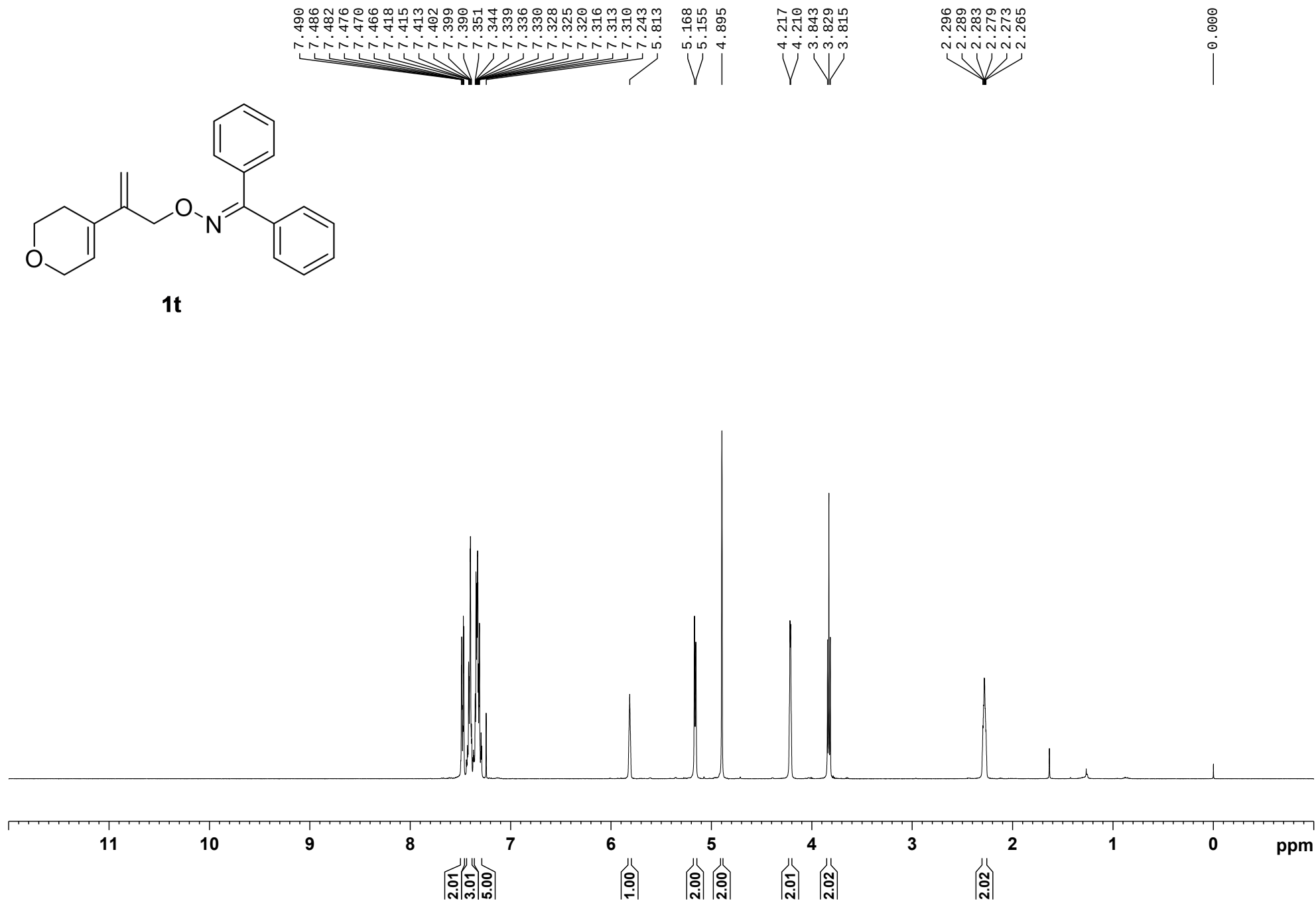
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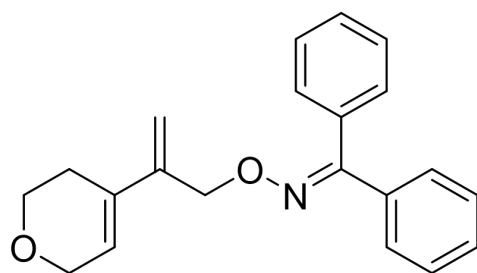
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 25.68
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 22.15





1t



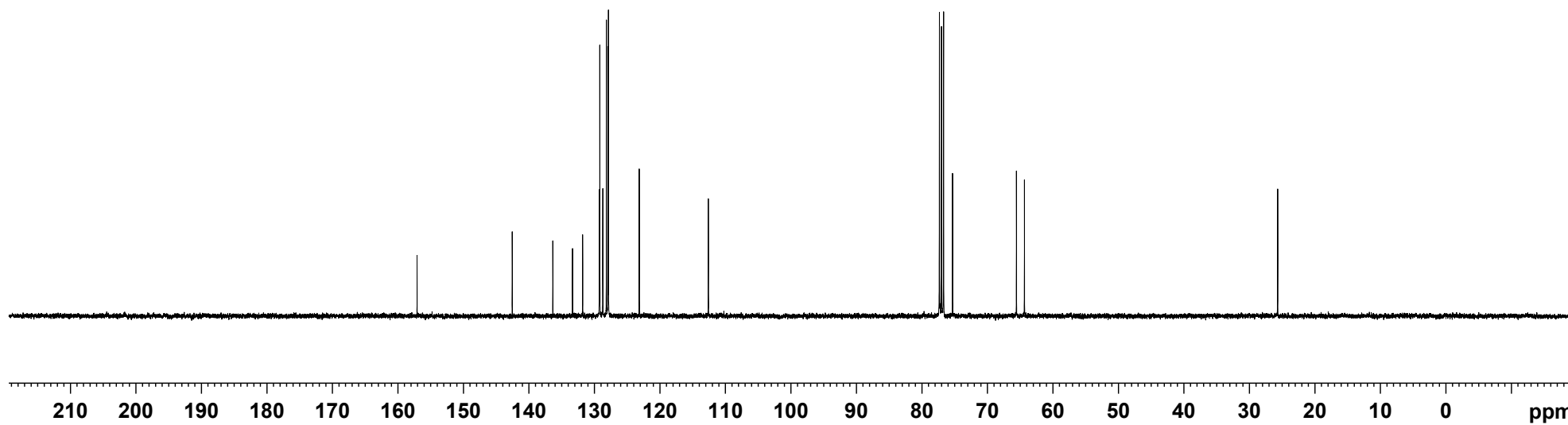


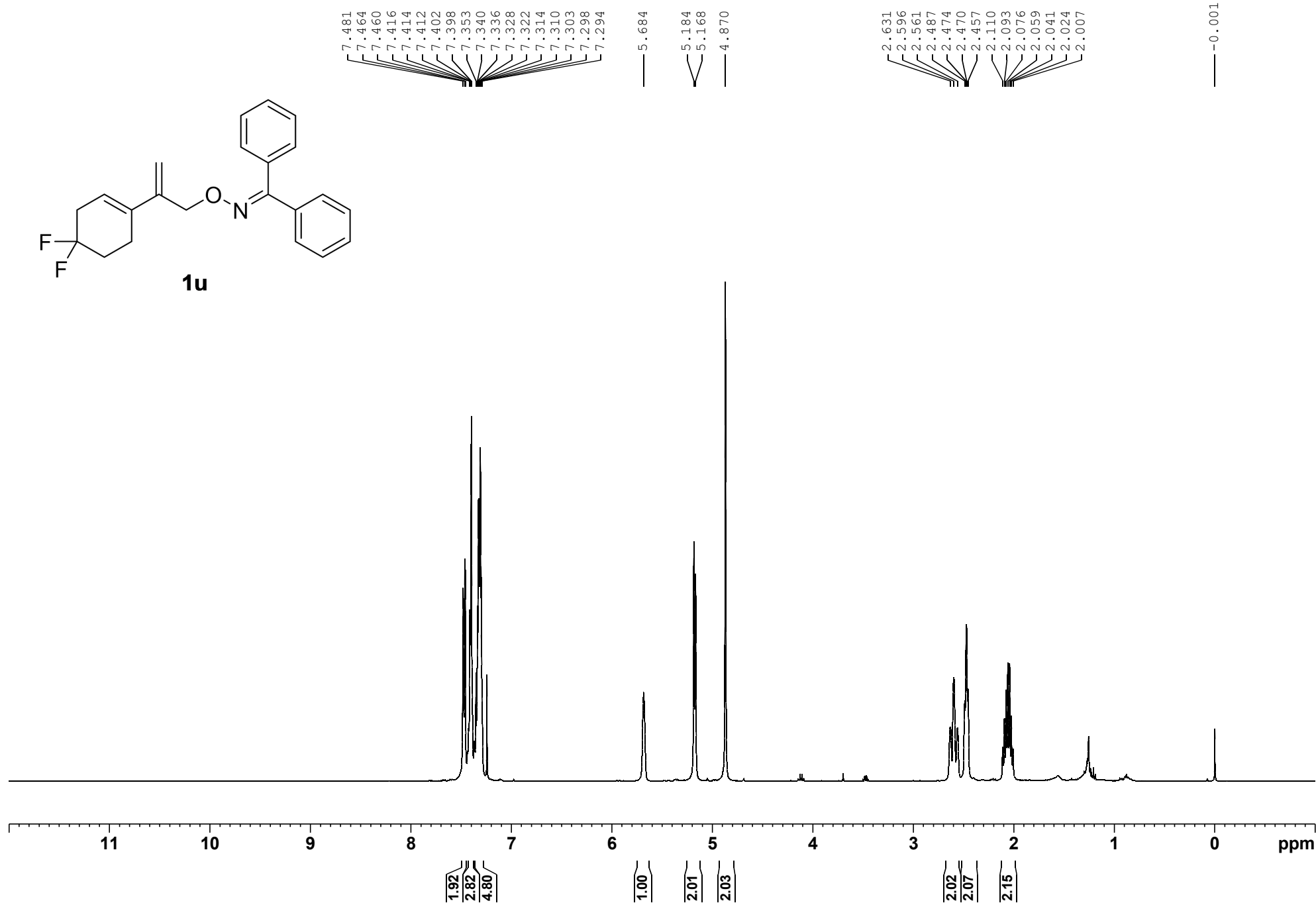
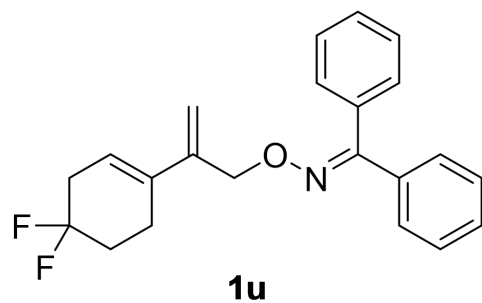
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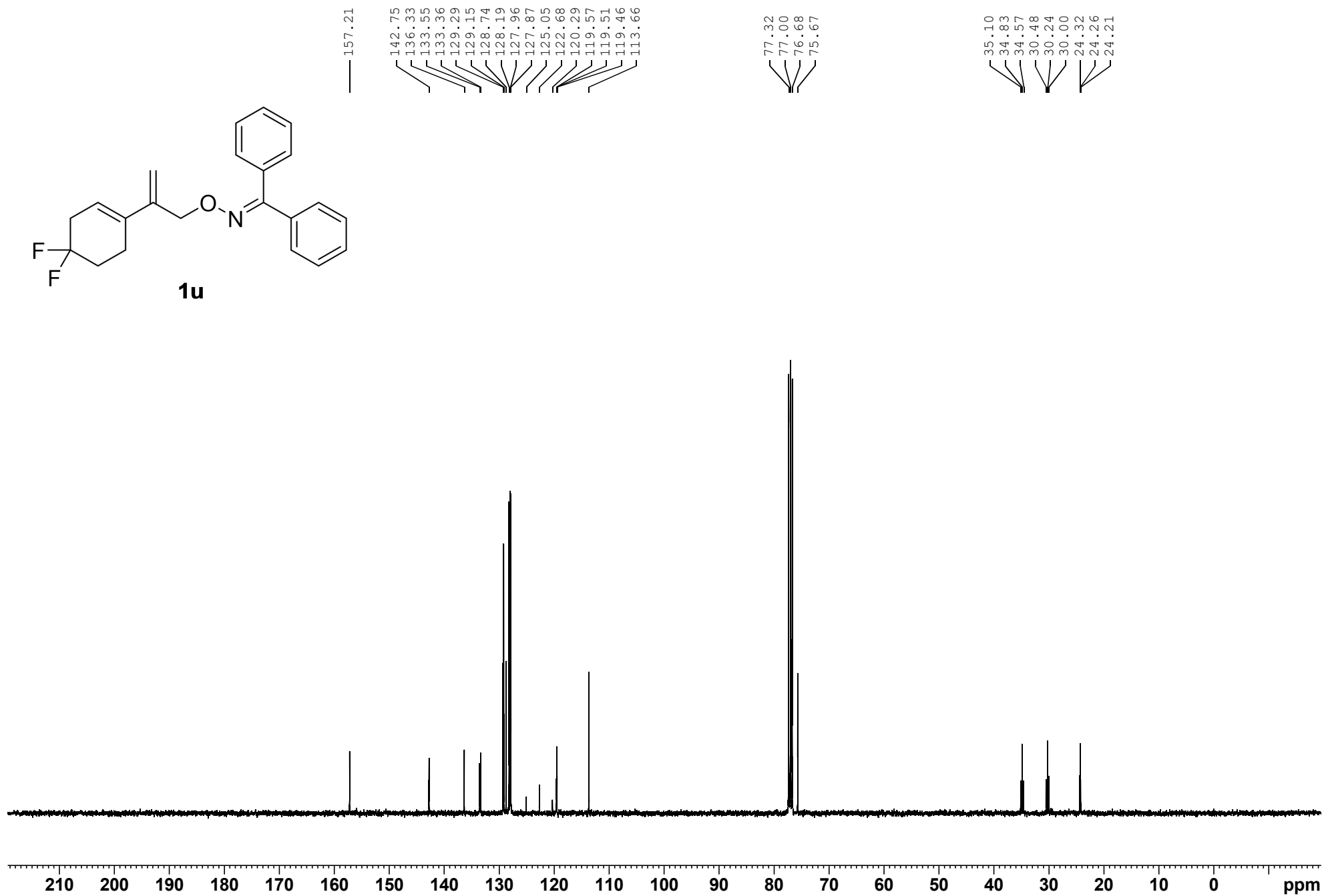
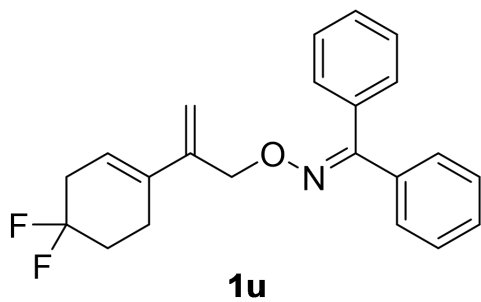
— 157.07
 142.54
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 129.17
 128.71
 128.17
 127.94
 127.86
 123.15
 — 112.60

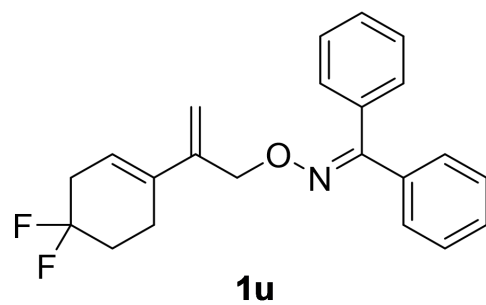
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 76.68
 75.31
 65.56
 64.34

— 25.67

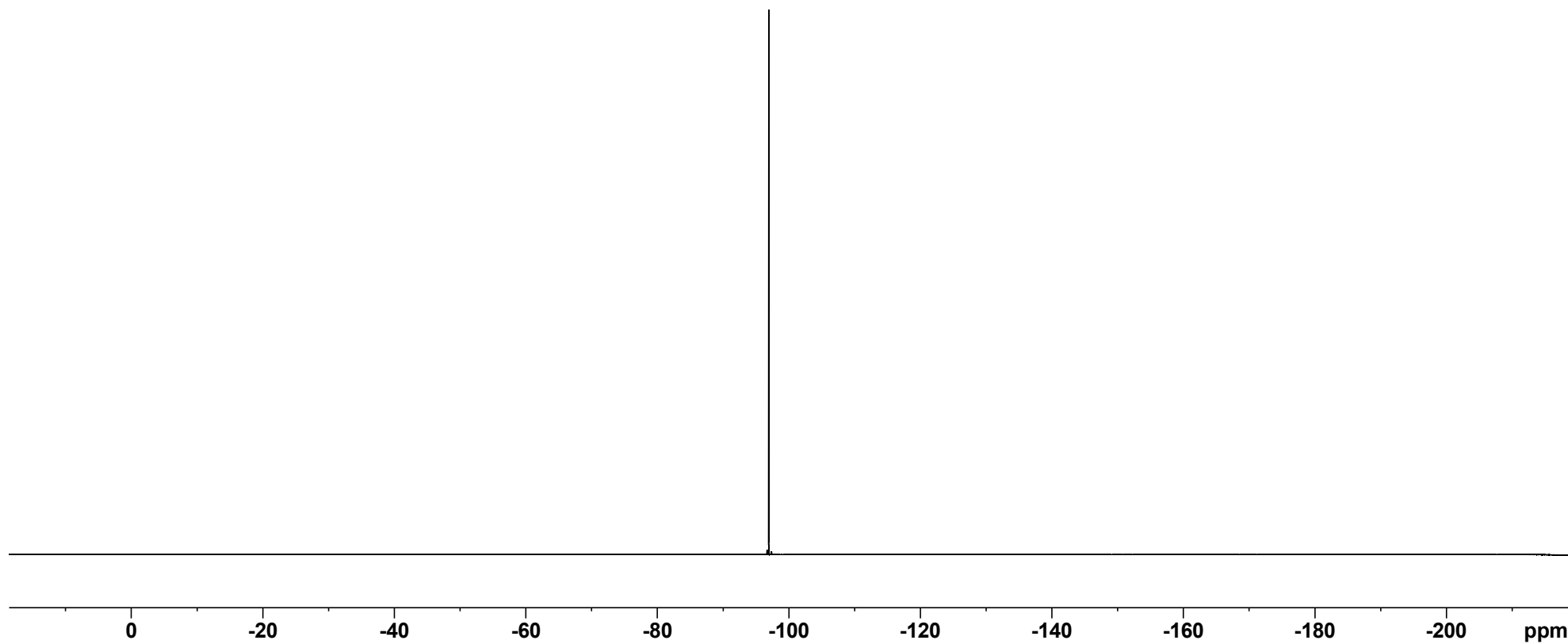


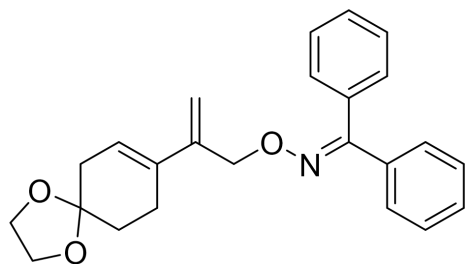




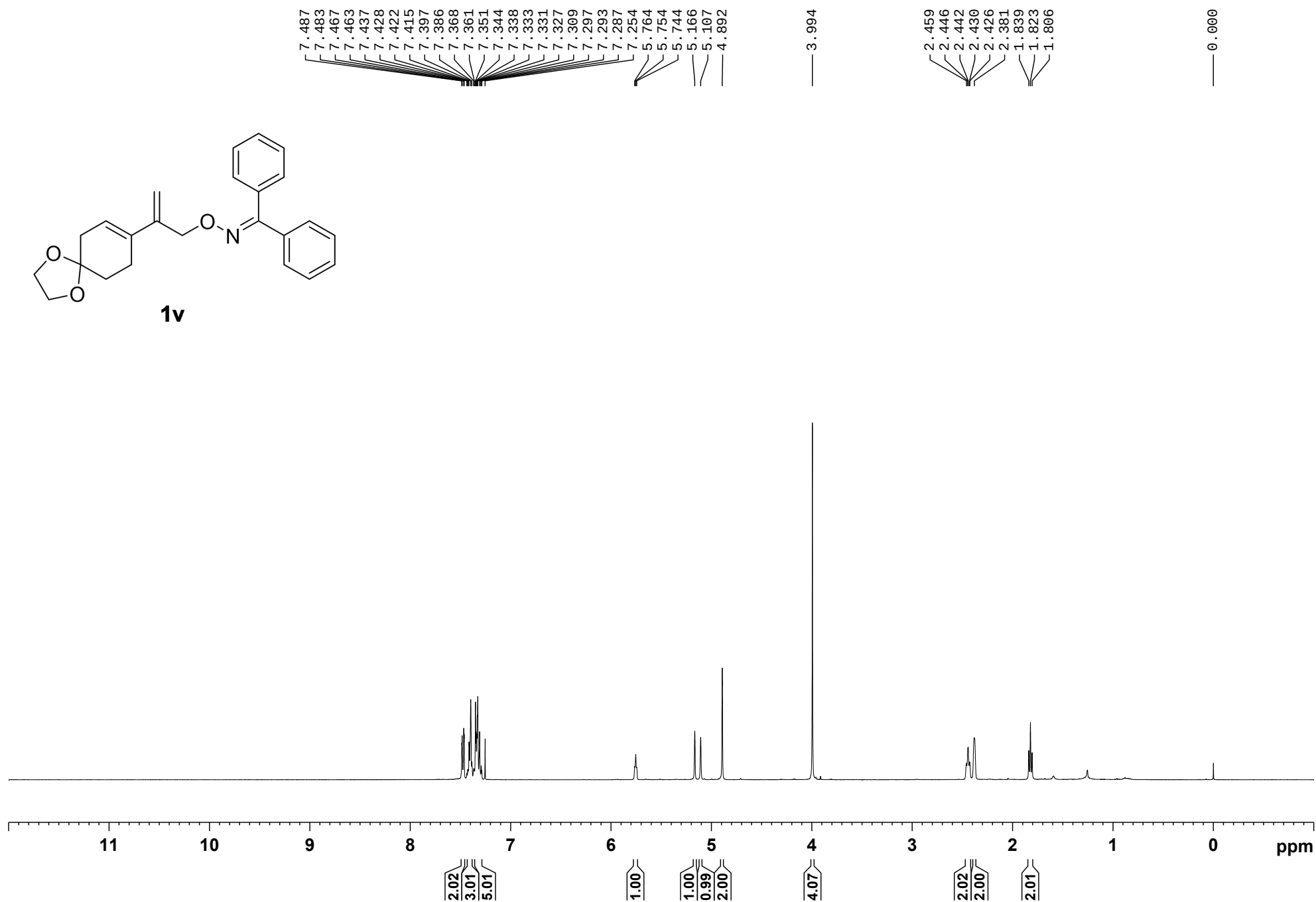


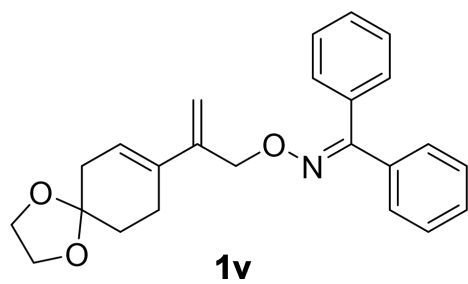
— -96.97





1v

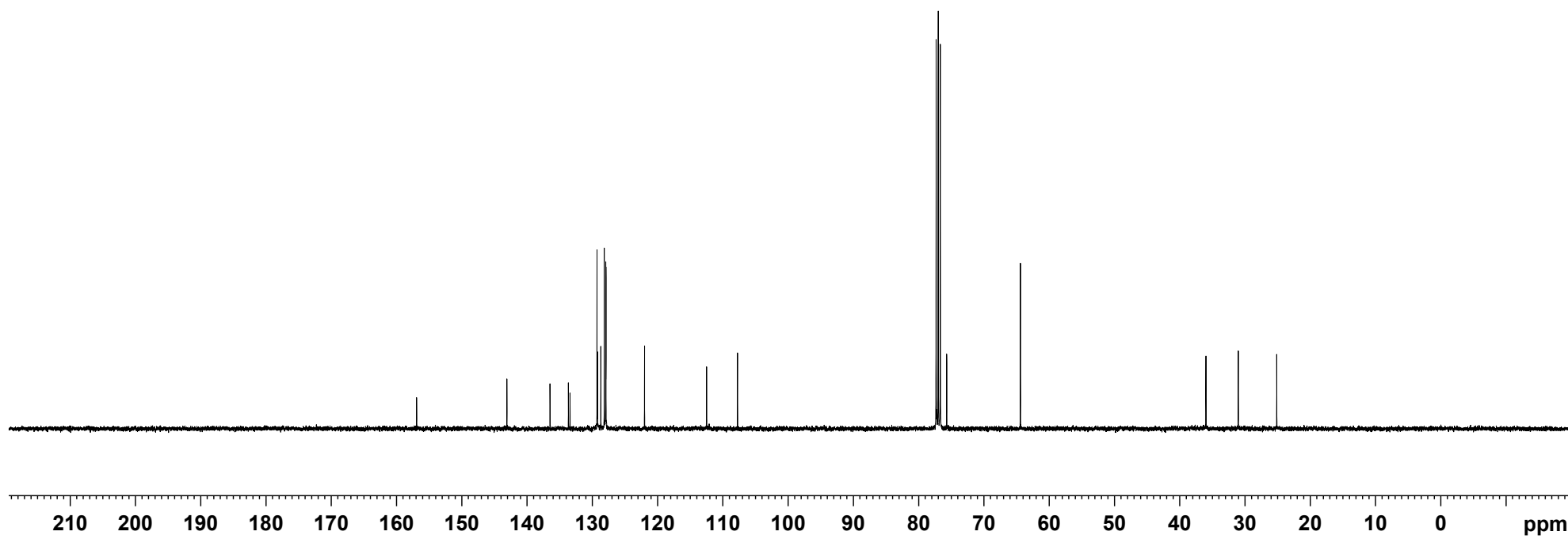


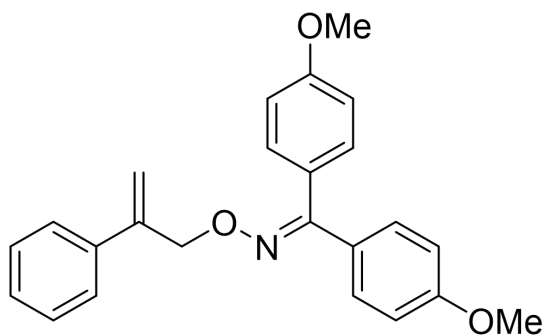


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 128.67
 128.15
 127.92
 127.89
 121.98
 112.47
 107.73

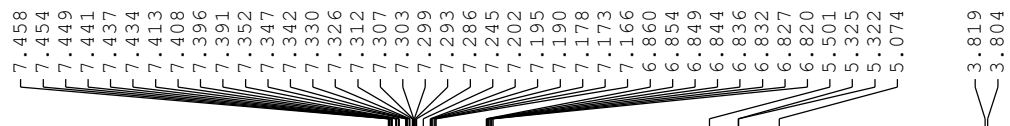
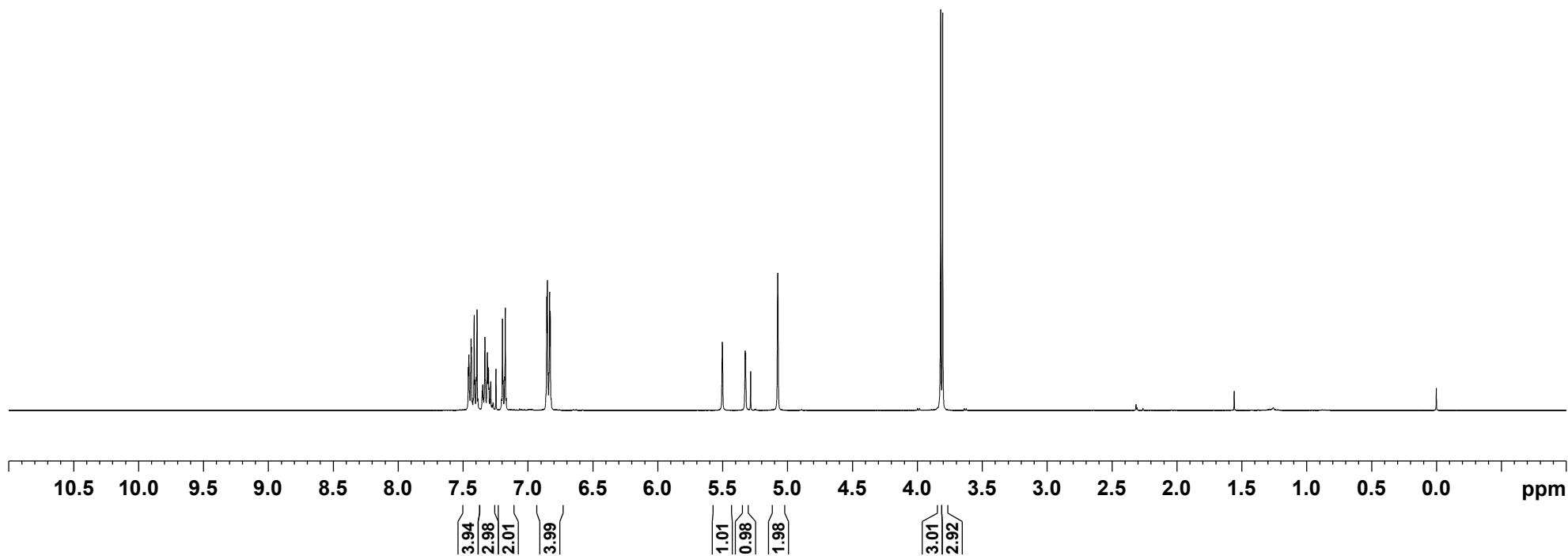
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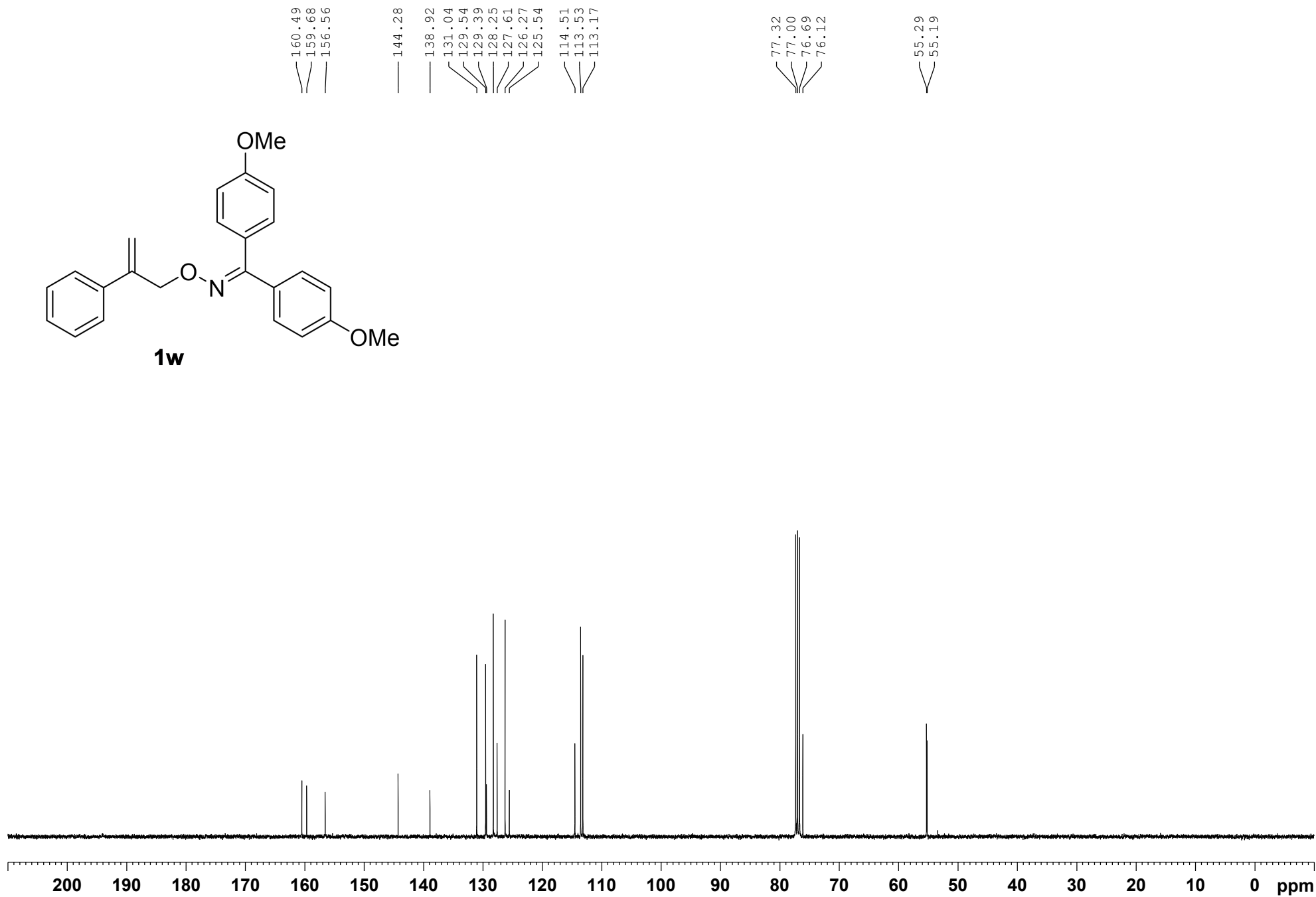
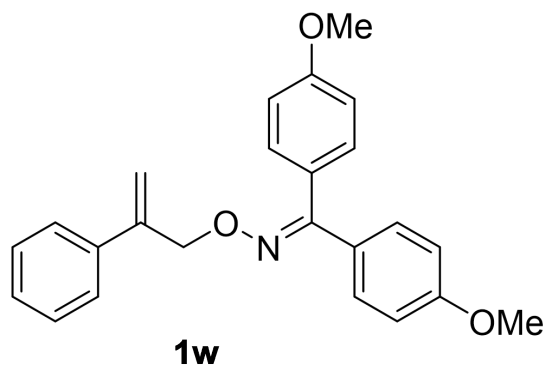
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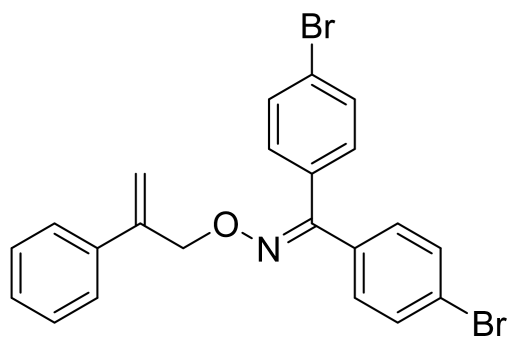




1w





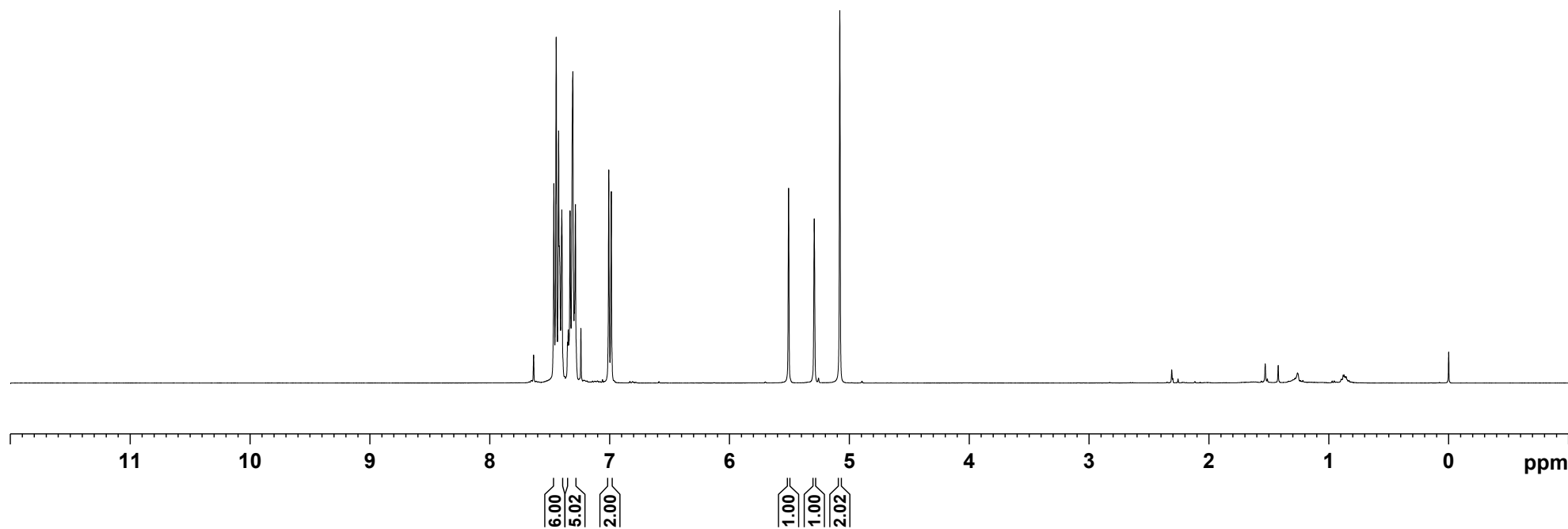


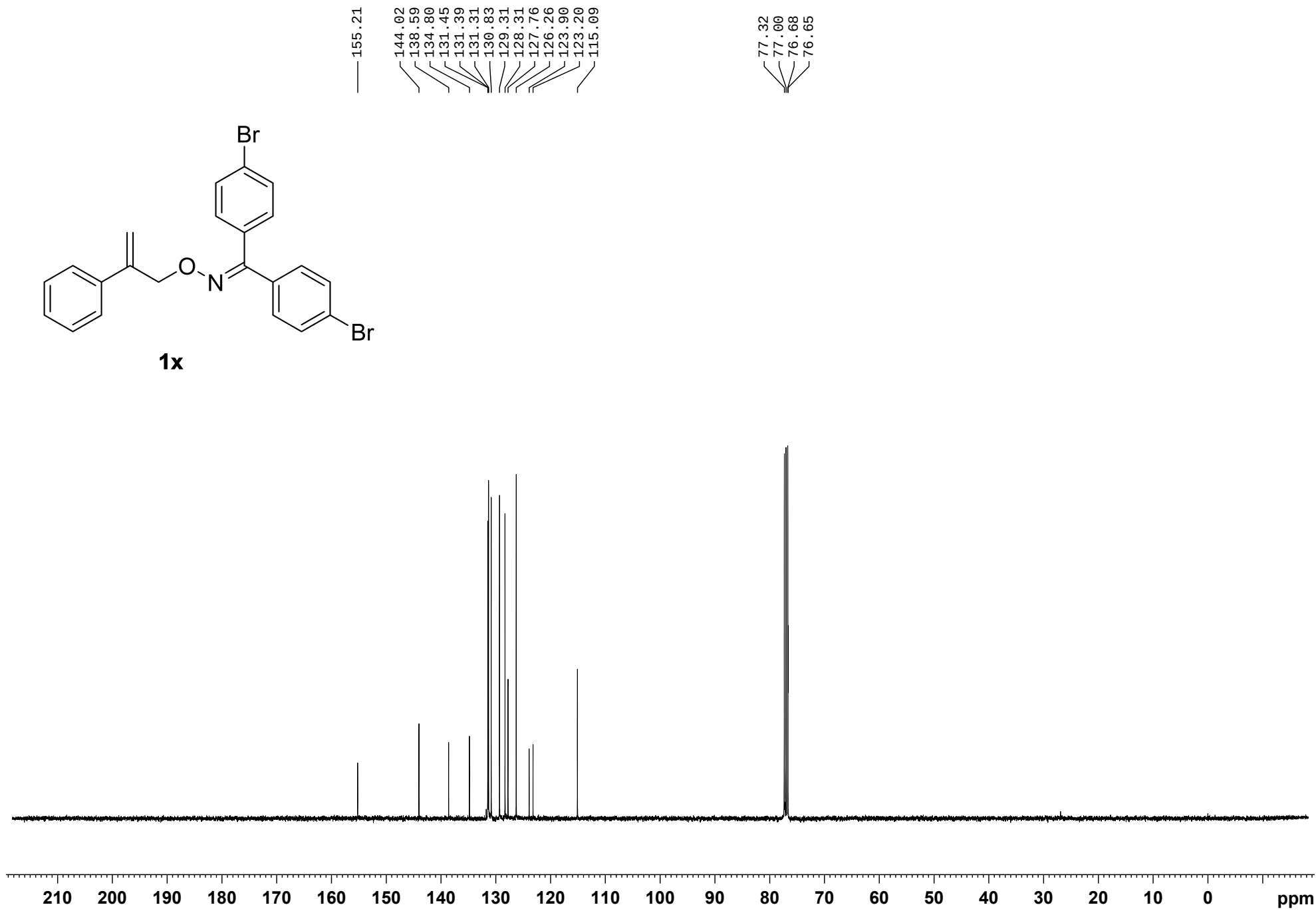
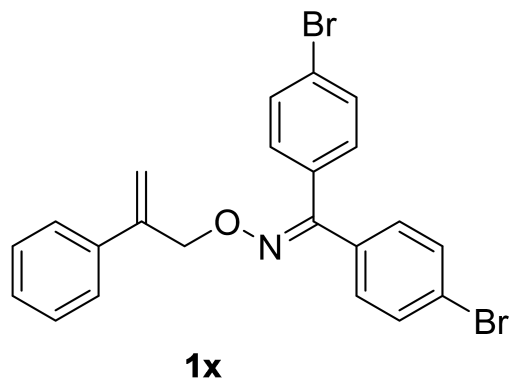
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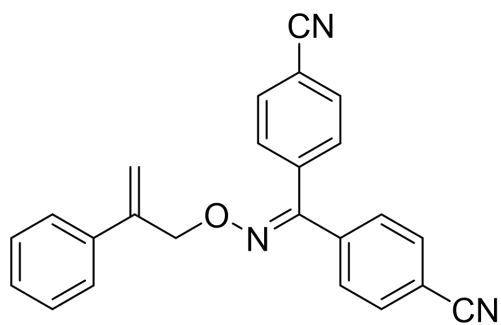
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6.986

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5.292
5.079

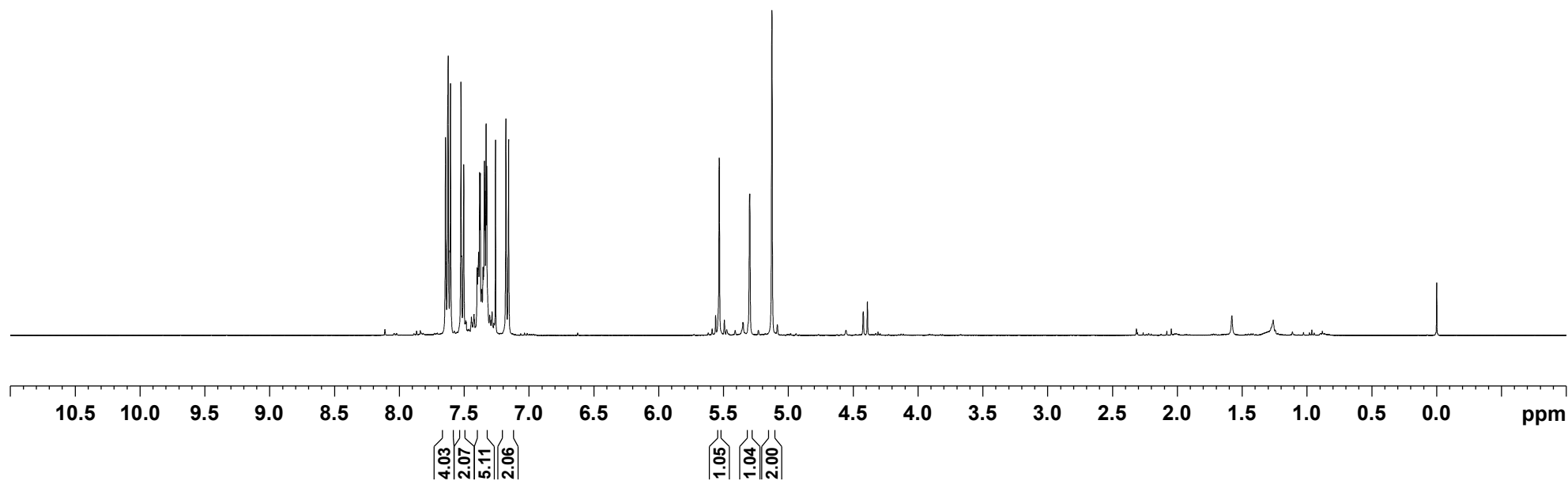
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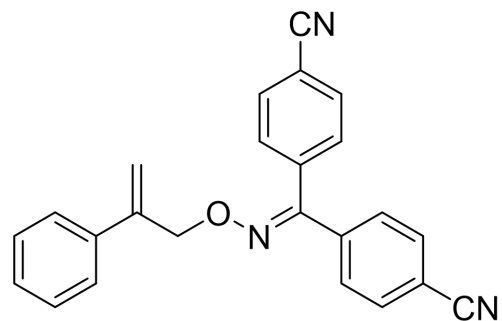




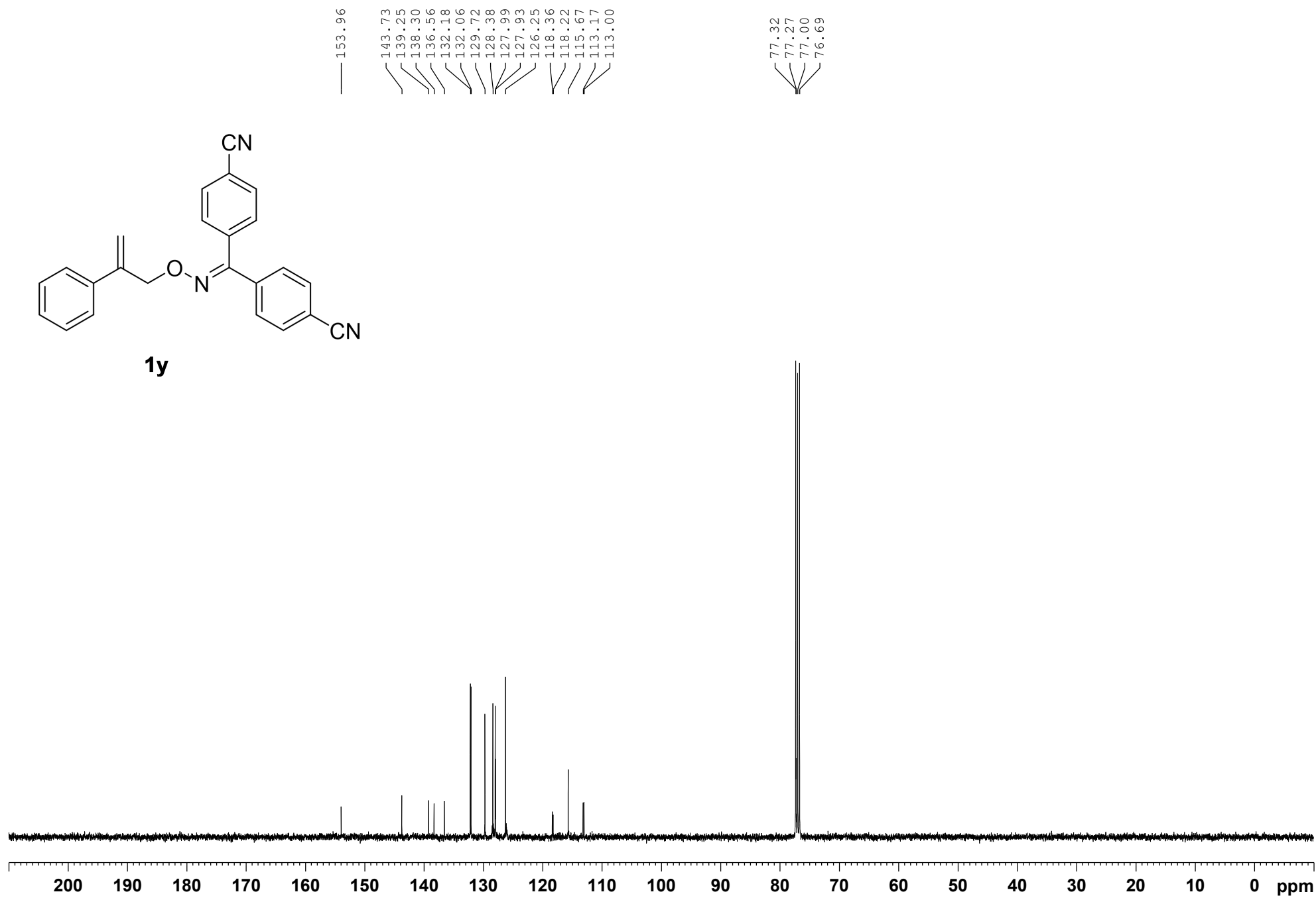


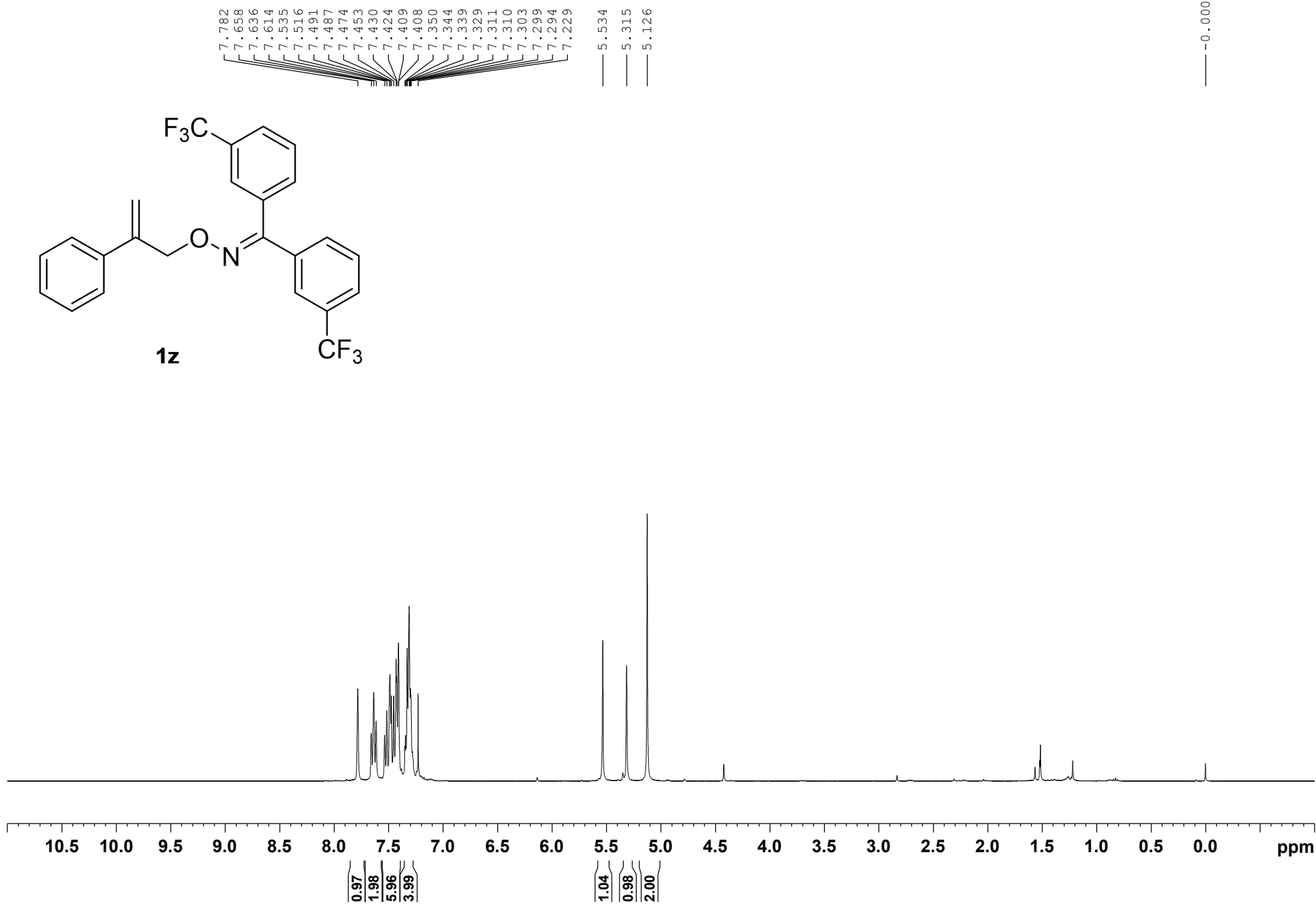
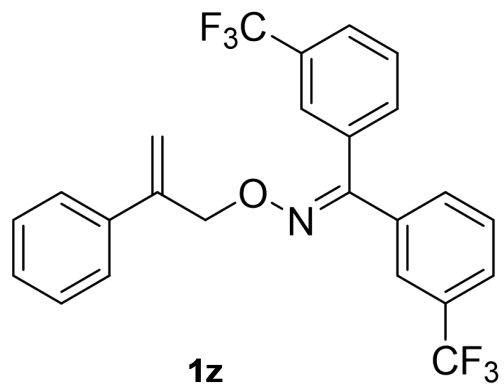
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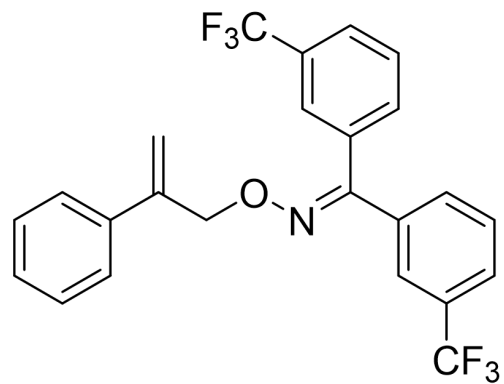




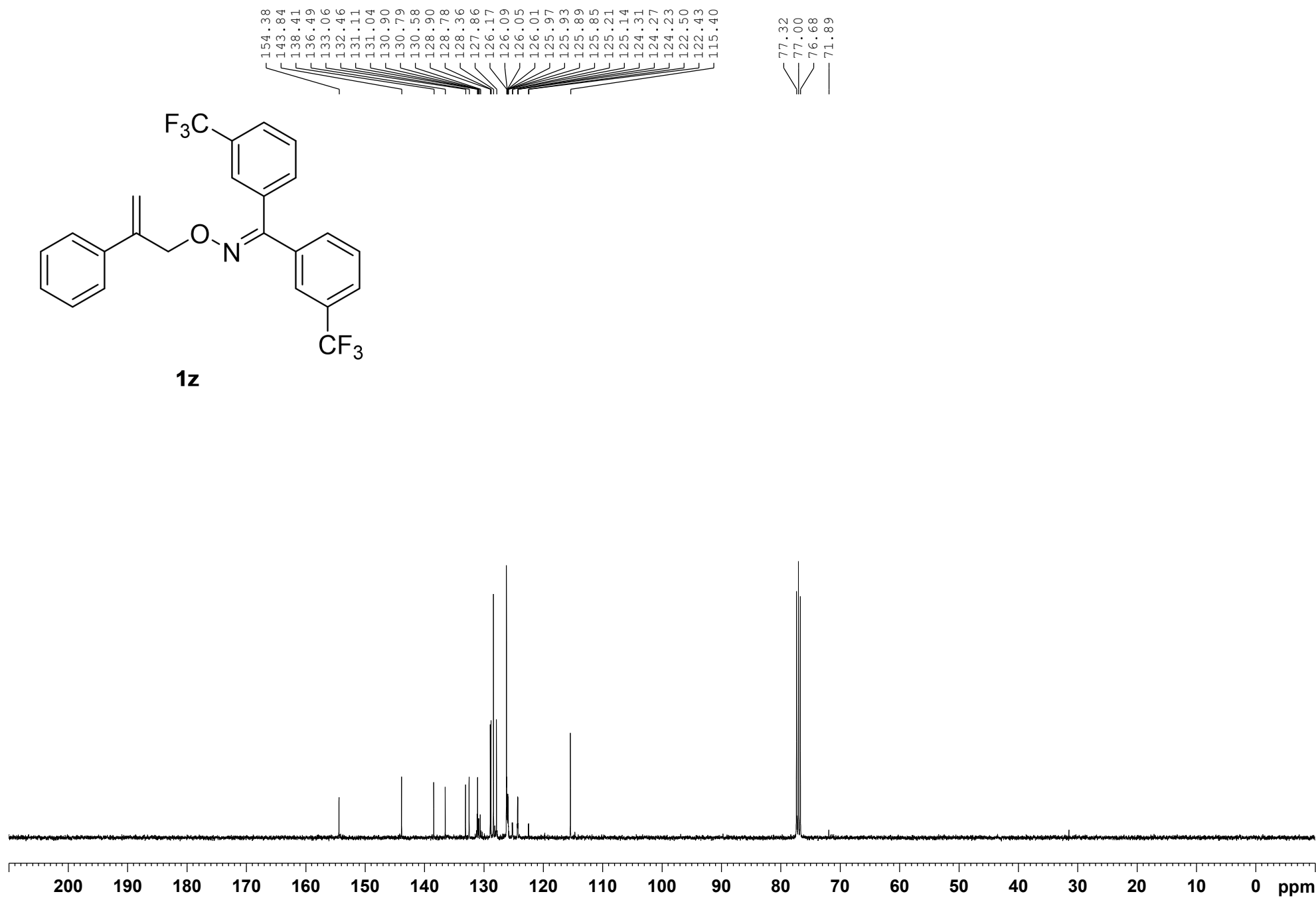
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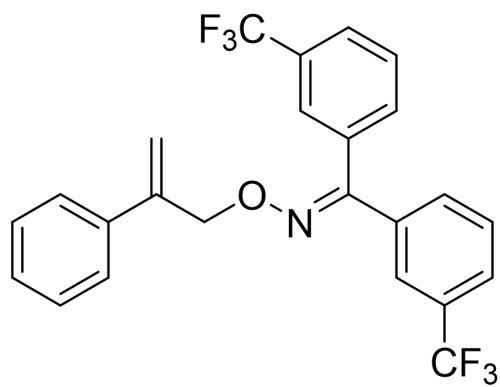




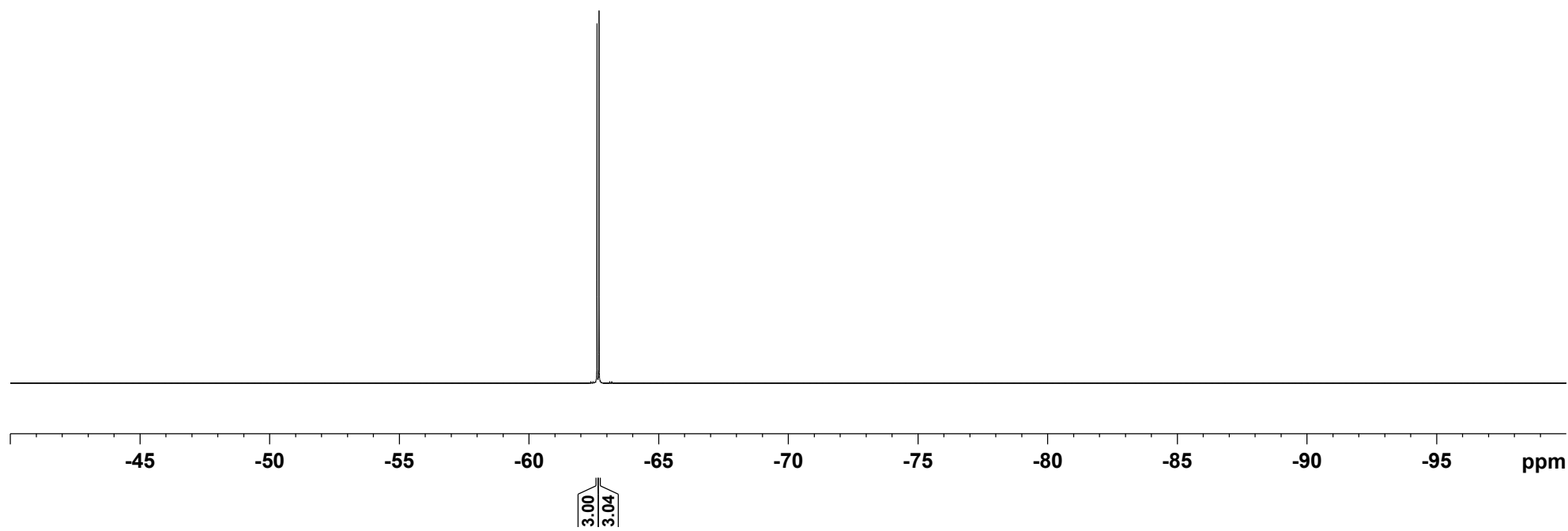


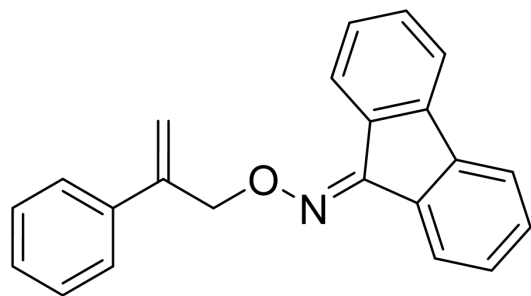
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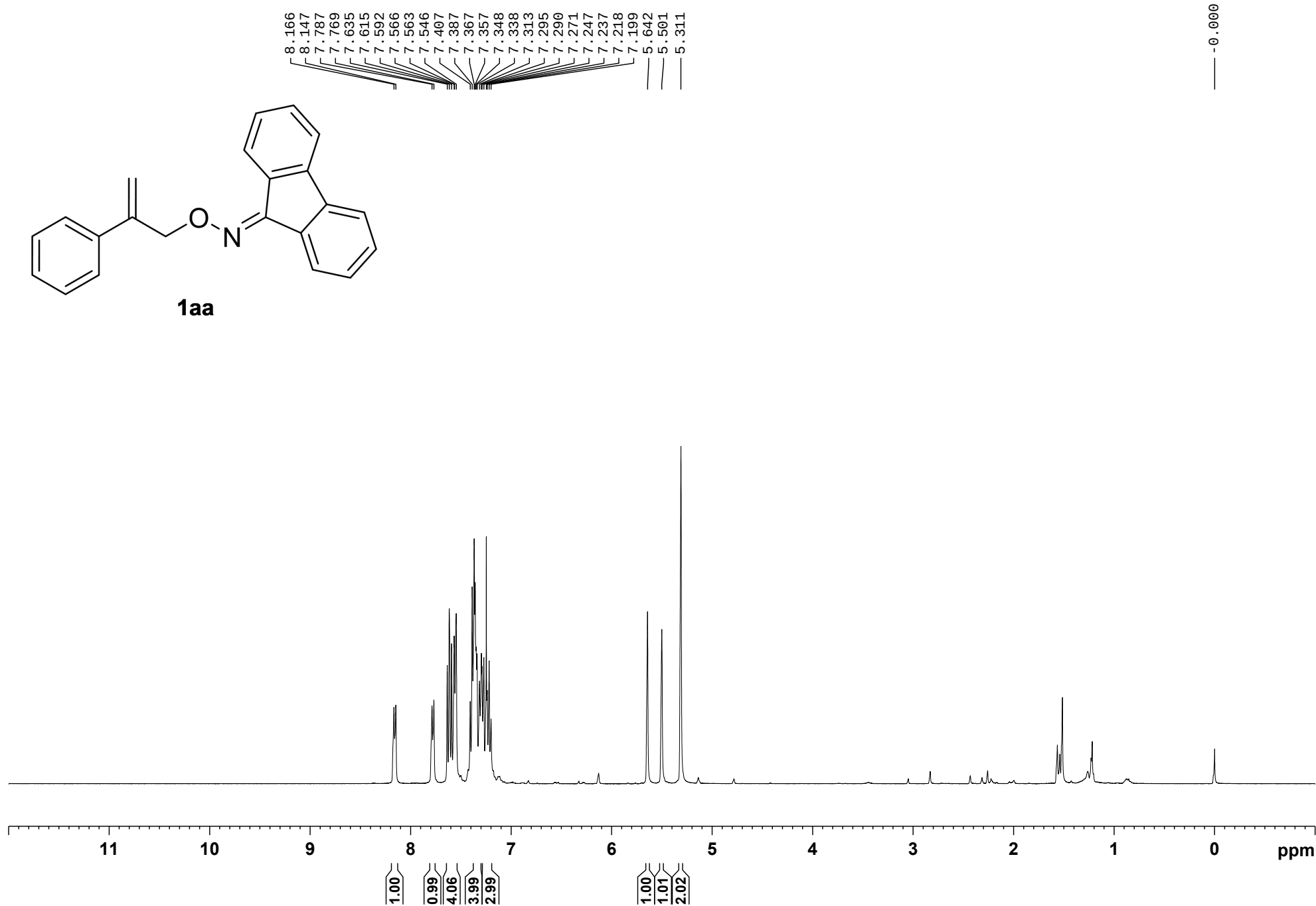


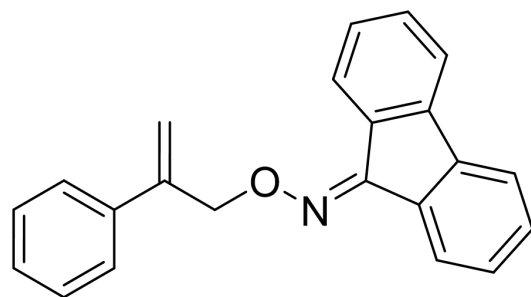
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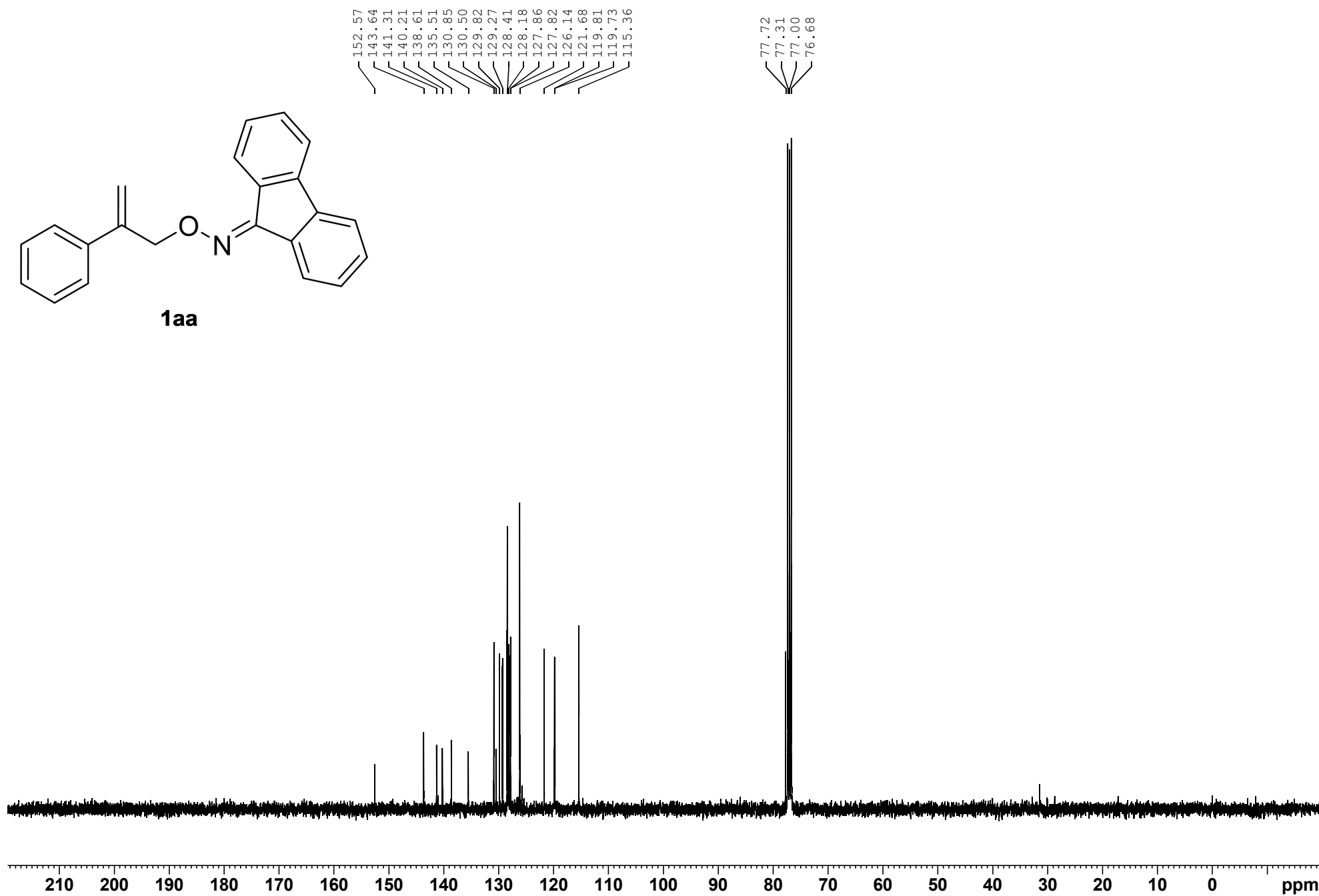


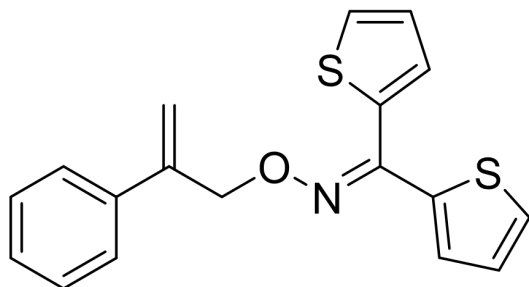
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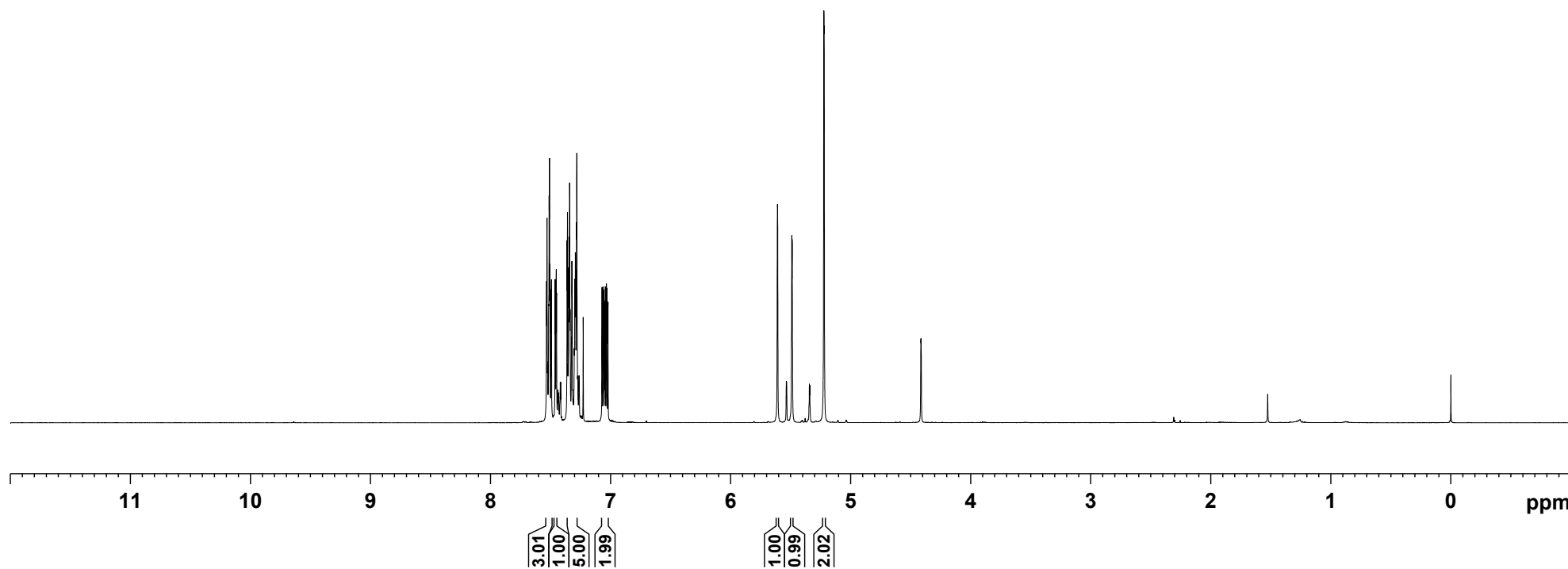


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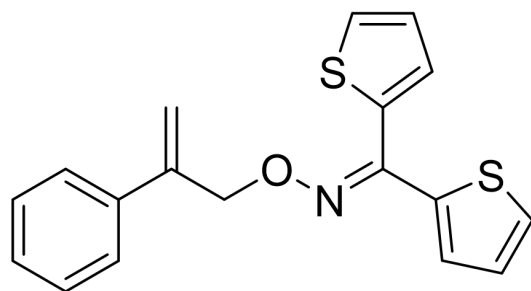




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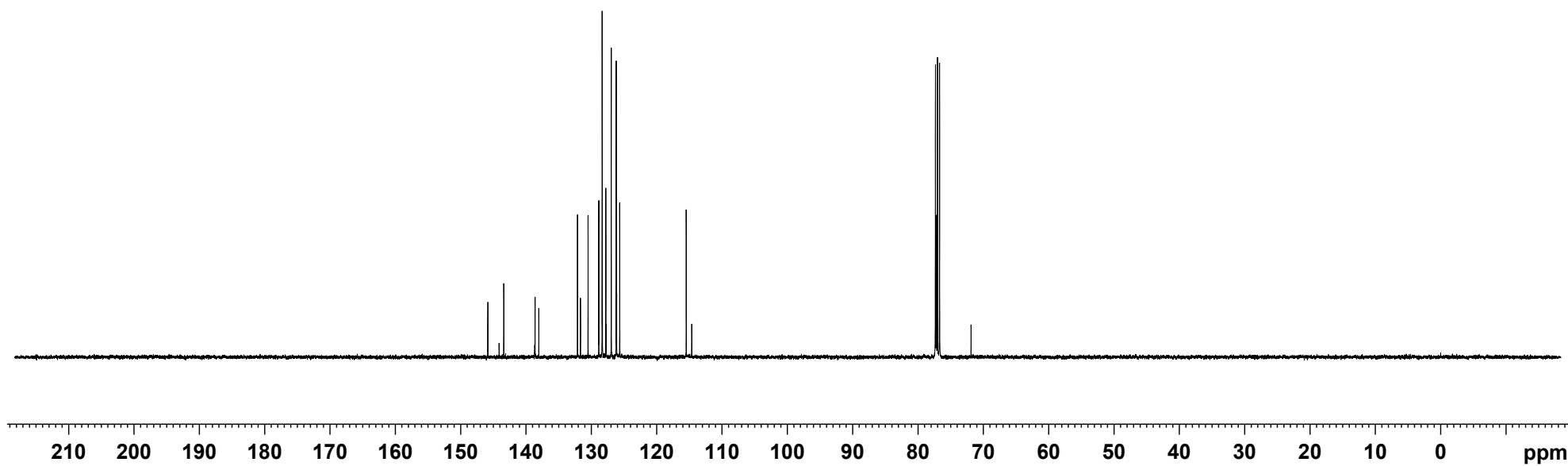
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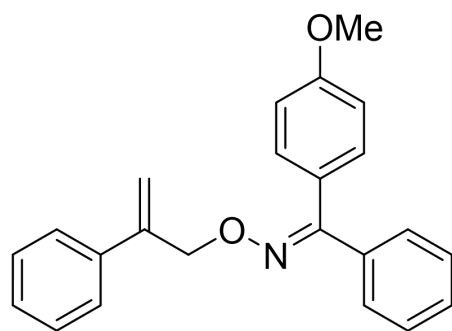


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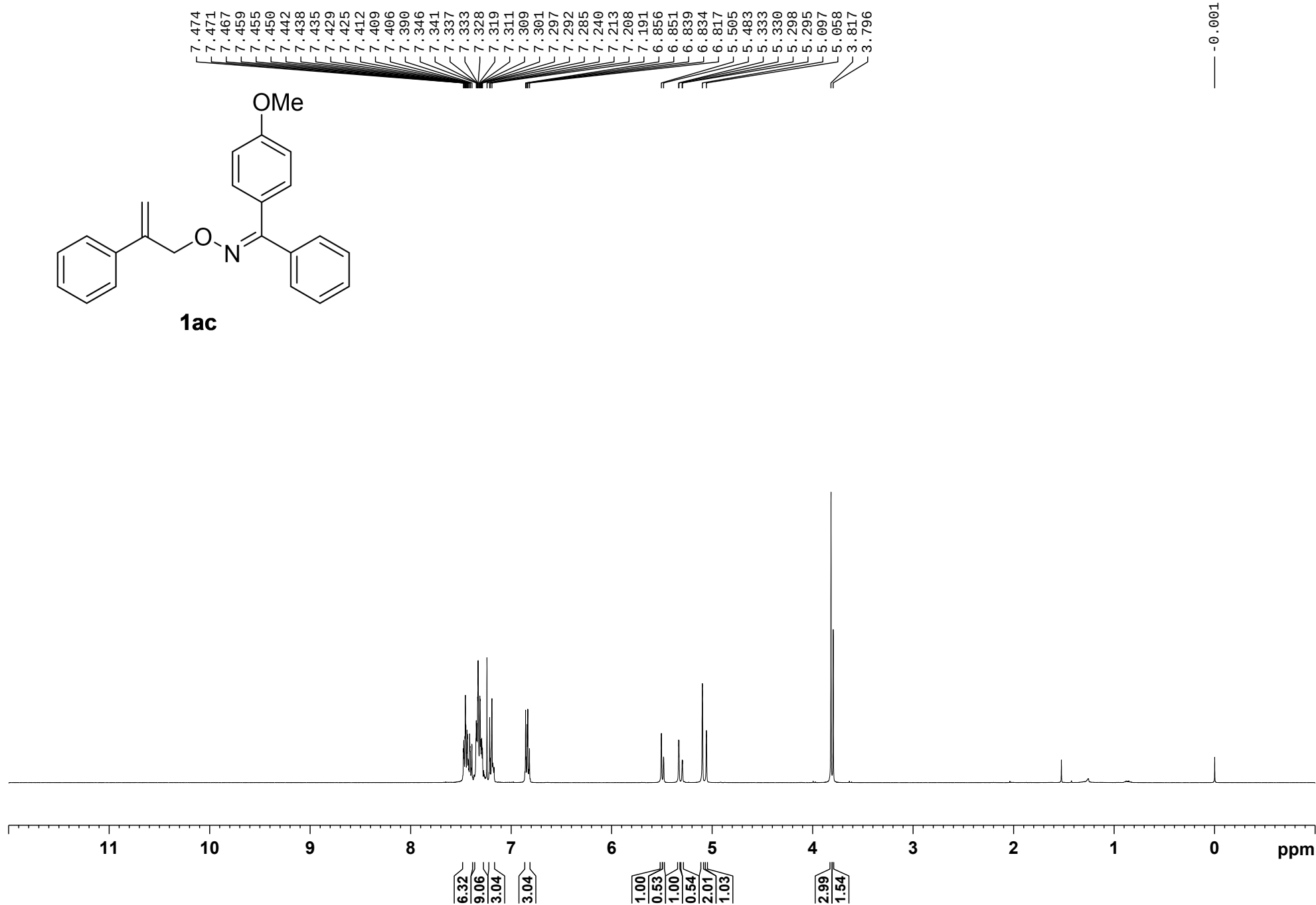
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127.77
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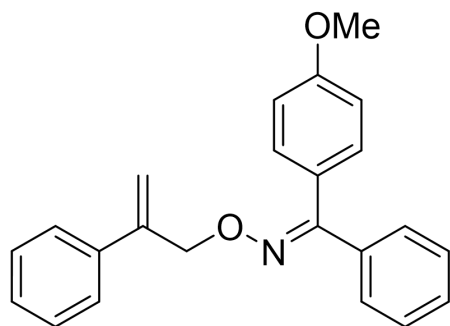
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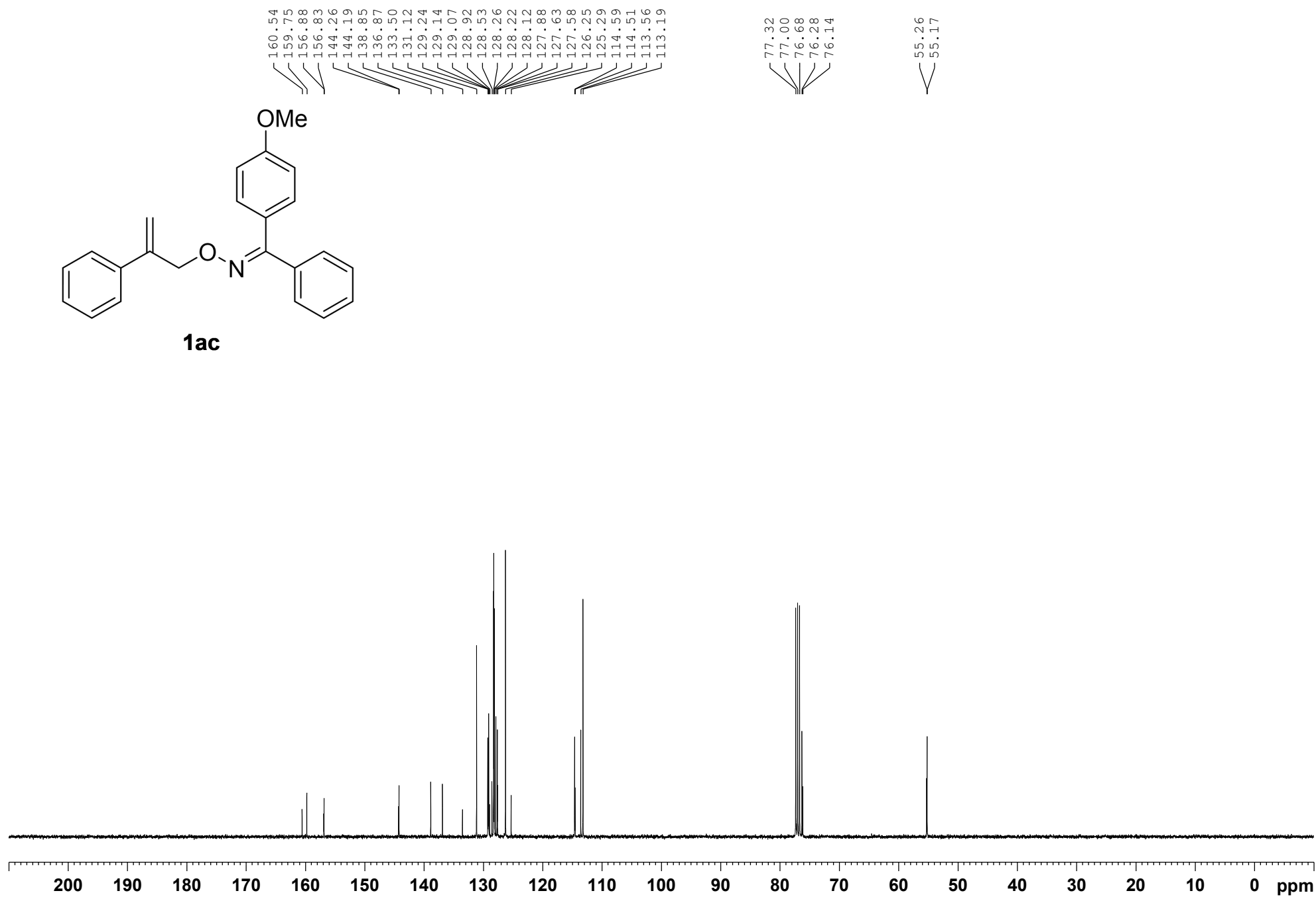


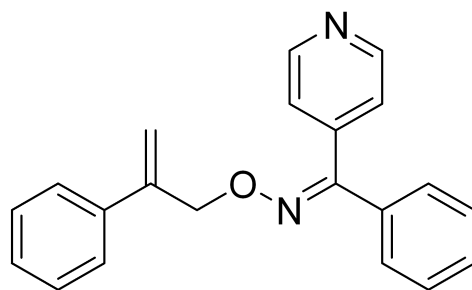
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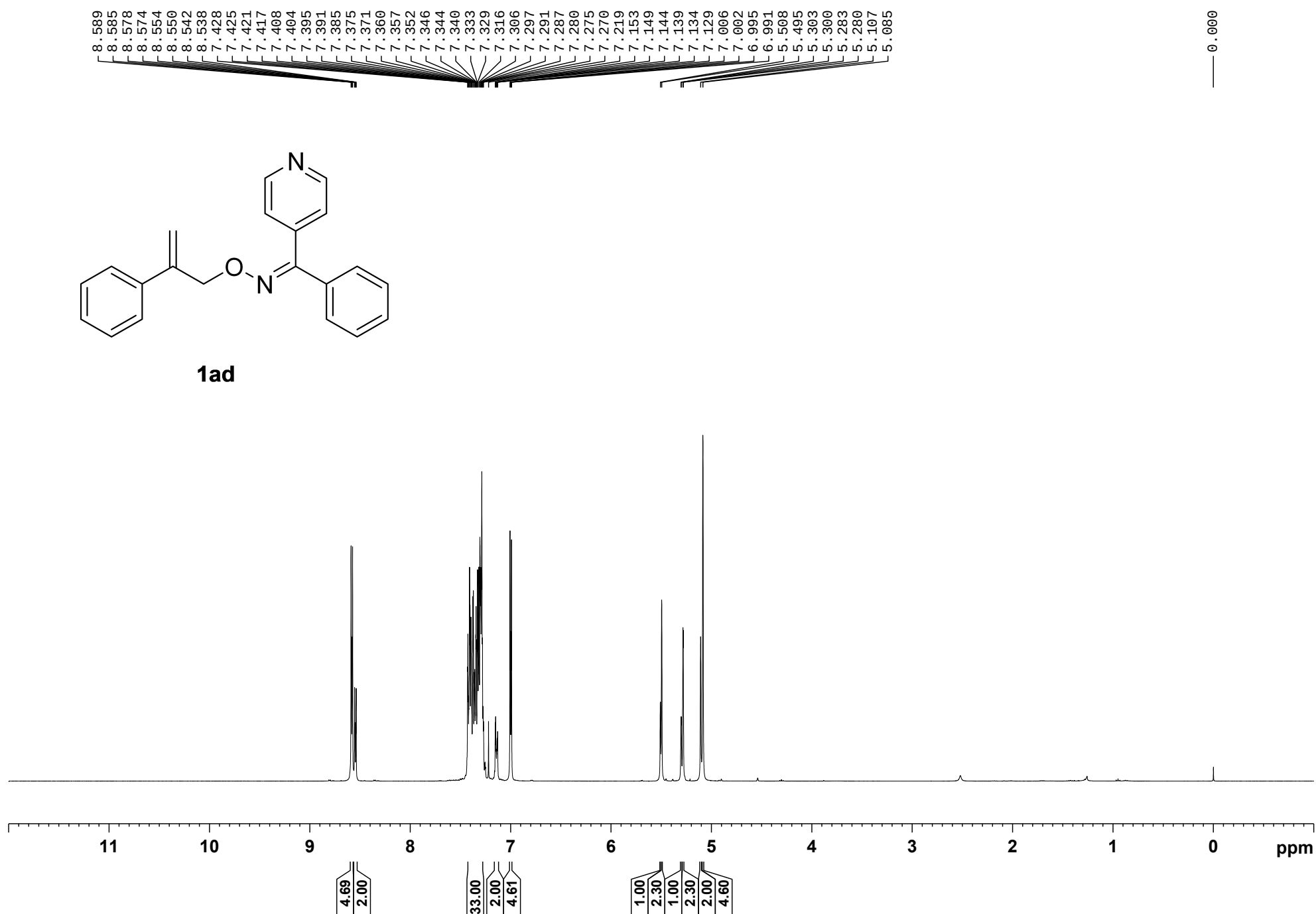


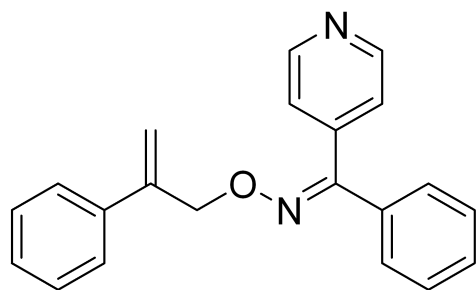
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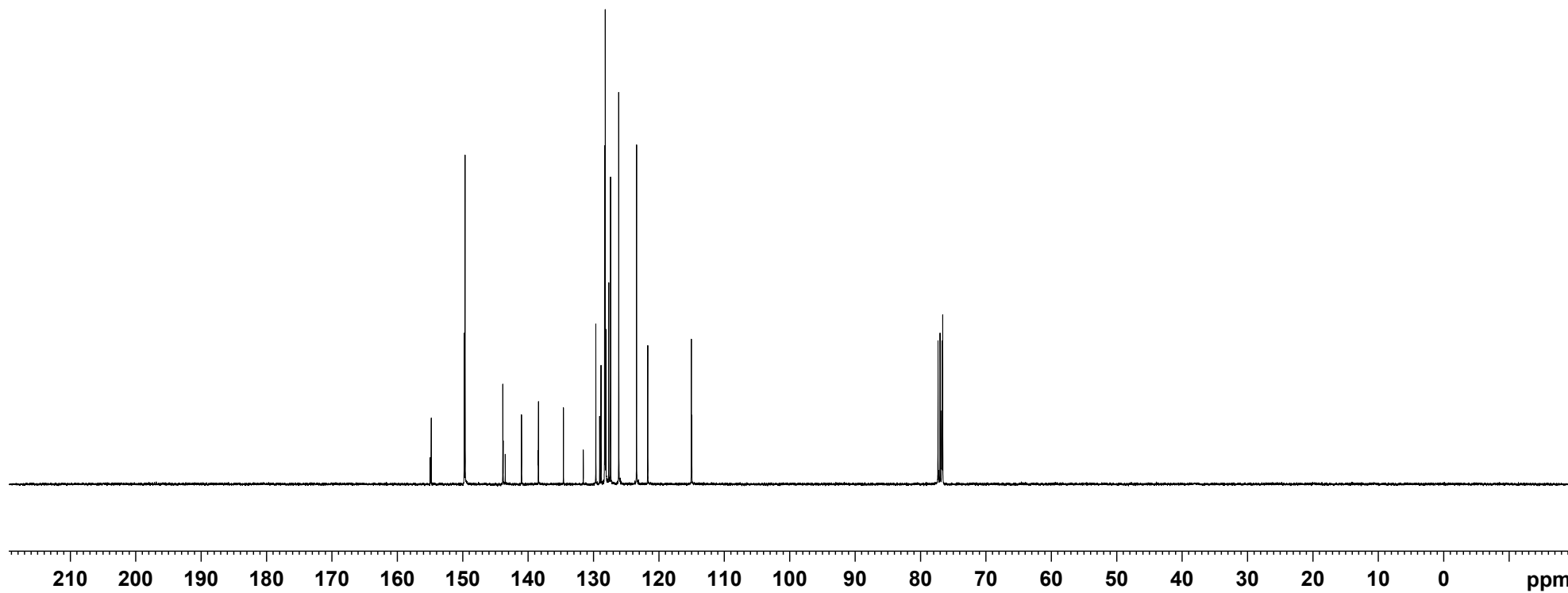


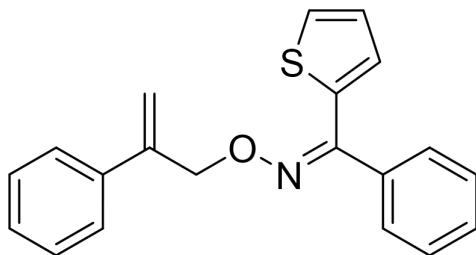


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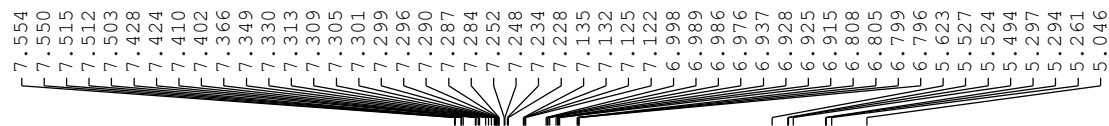
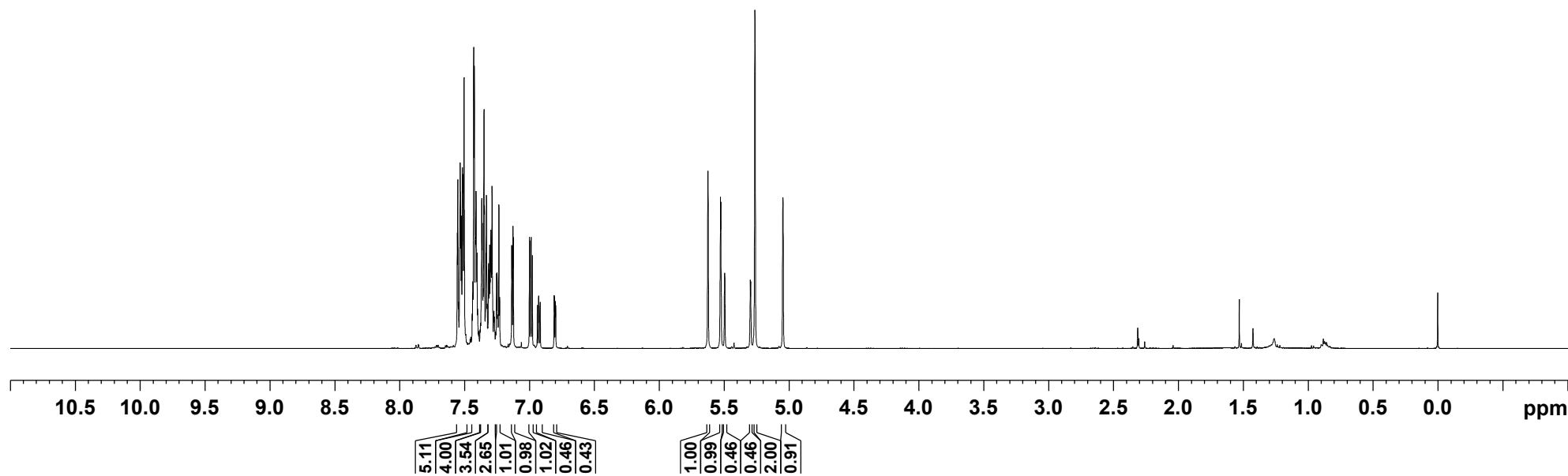
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76.68
76.59

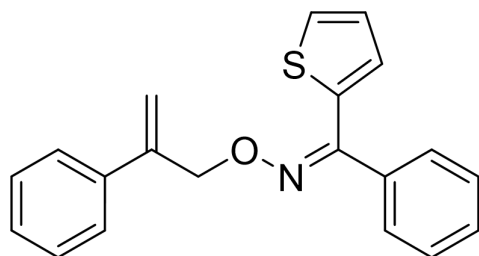




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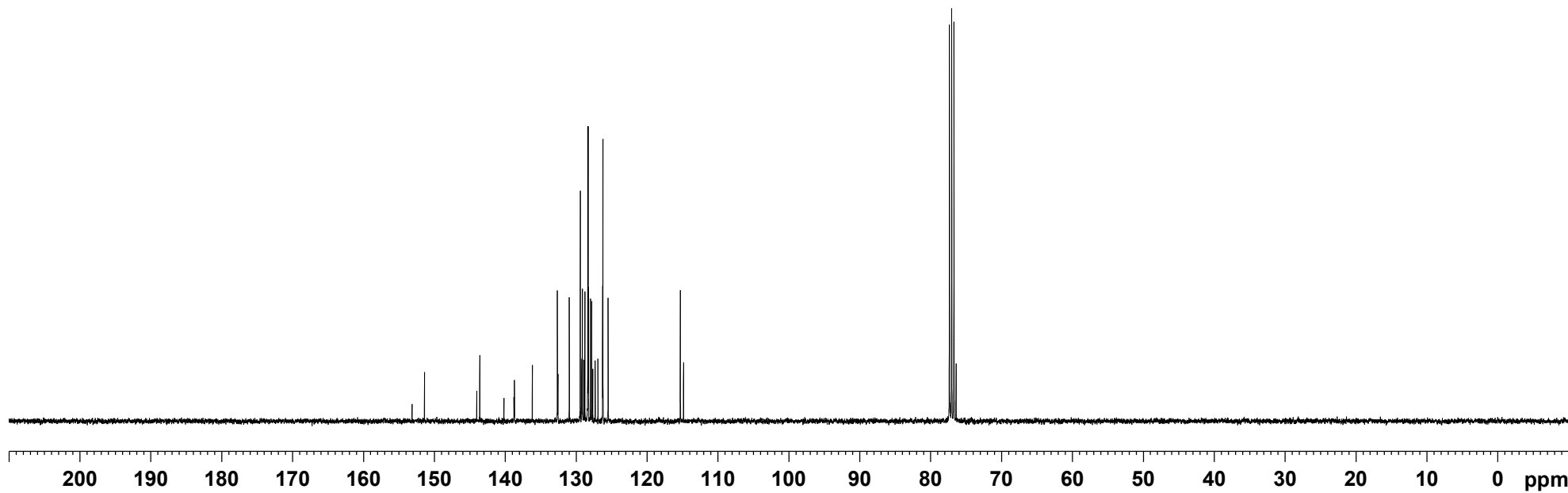
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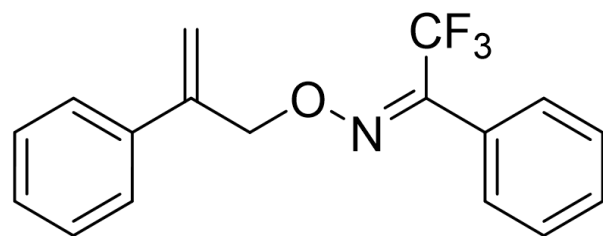


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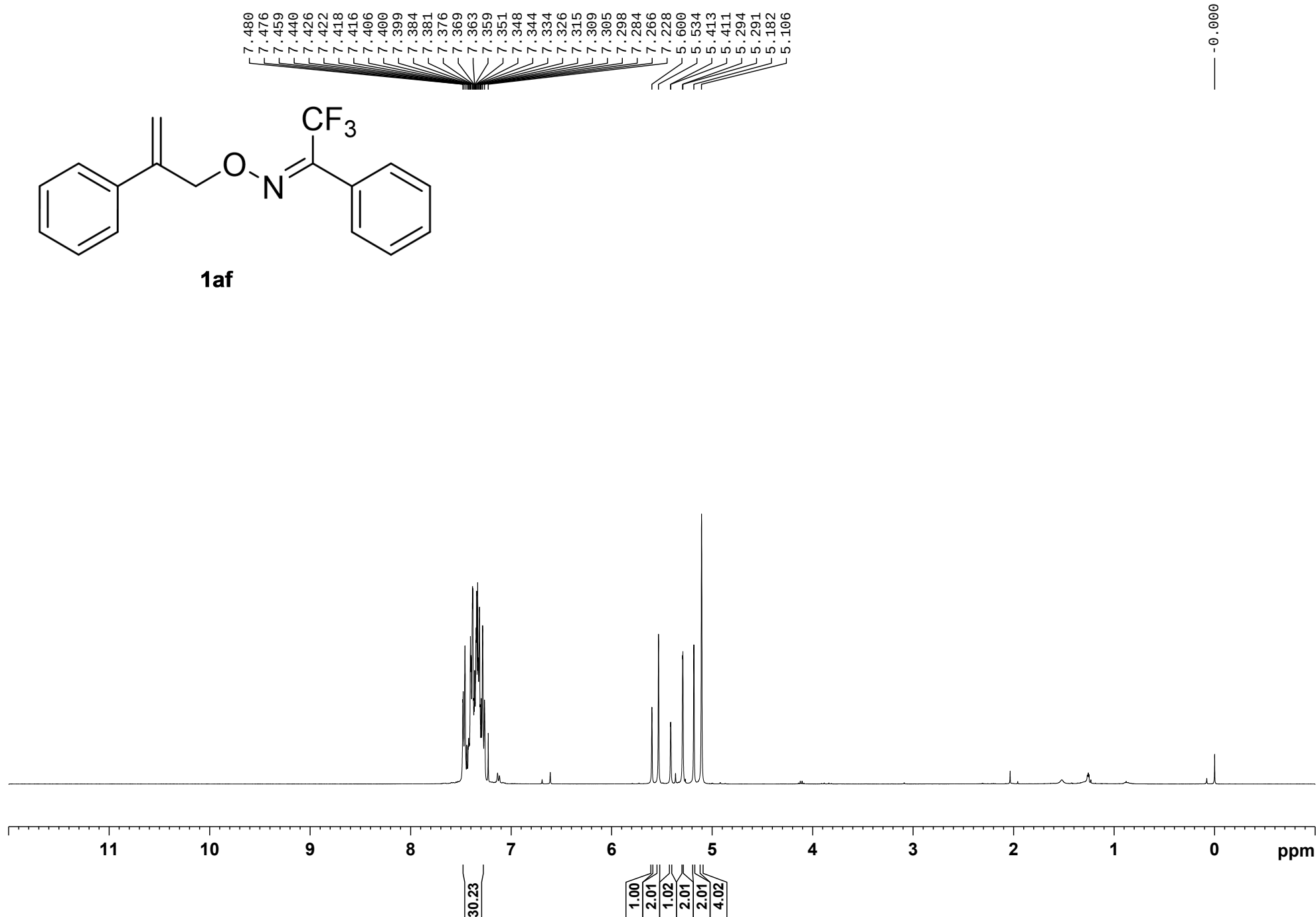
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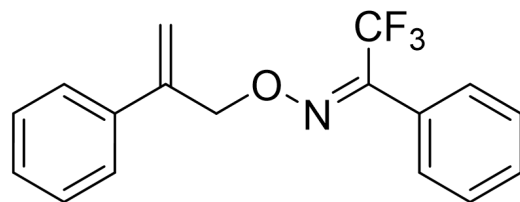
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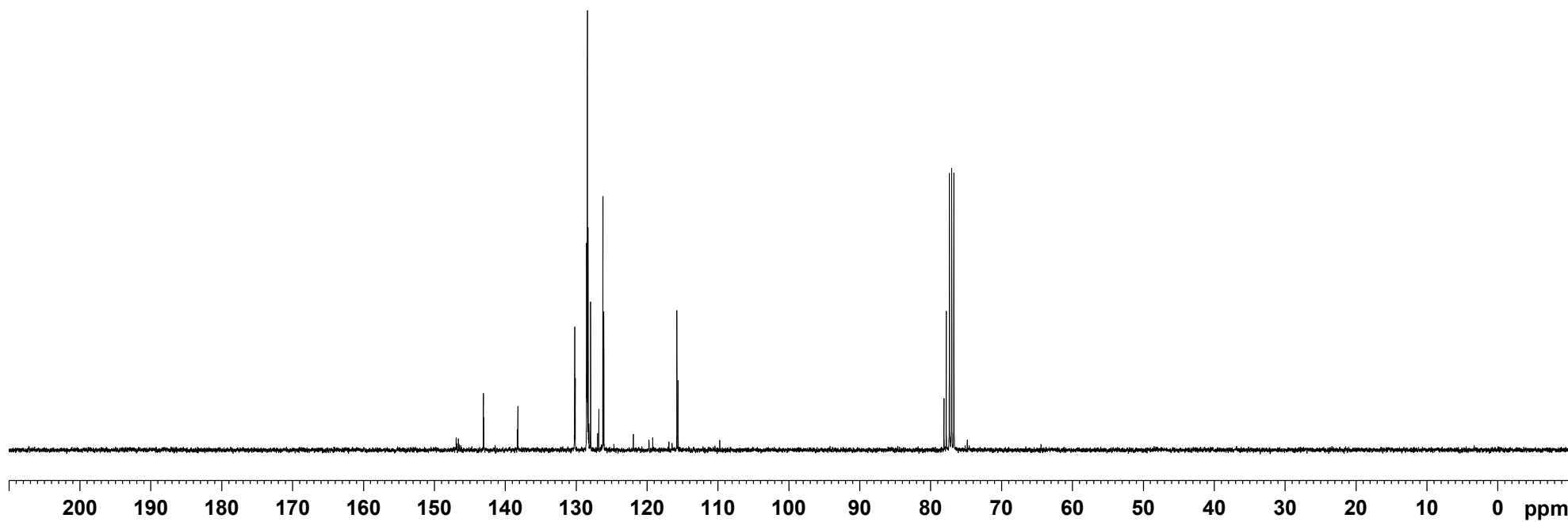


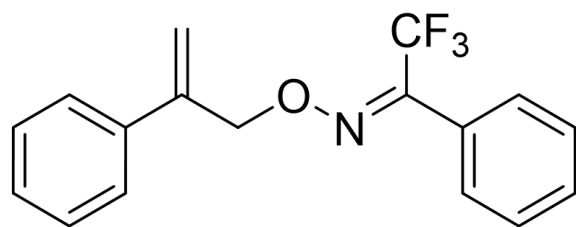


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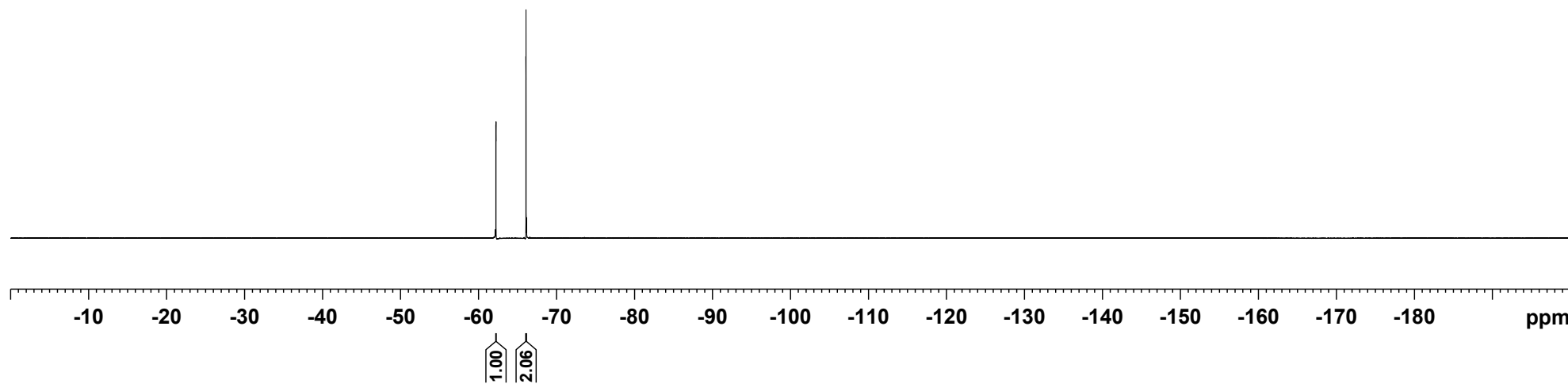
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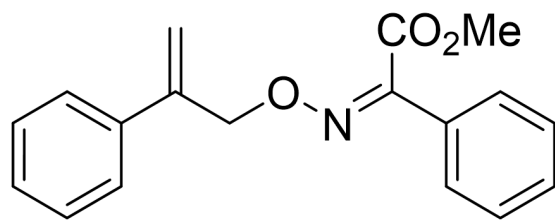




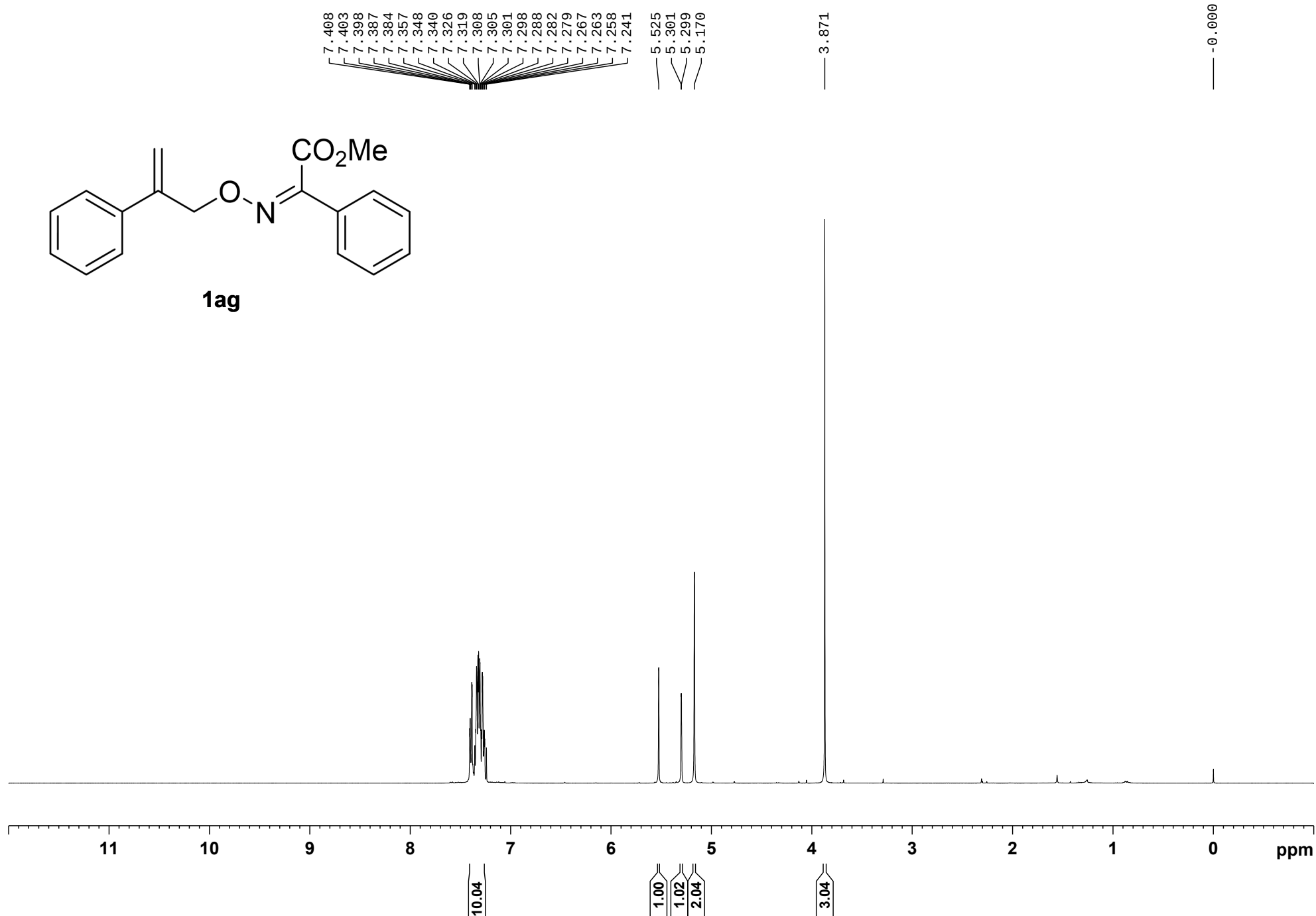
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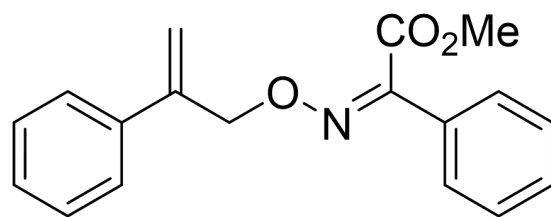
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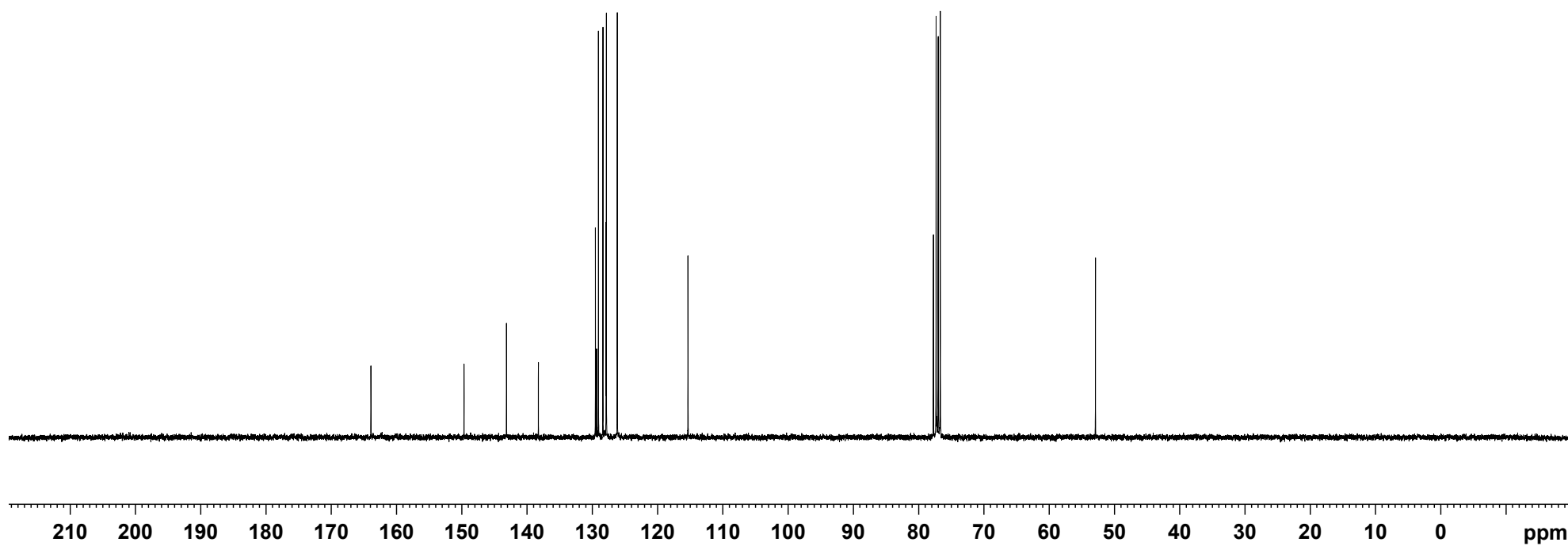
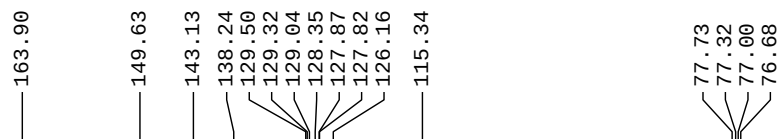


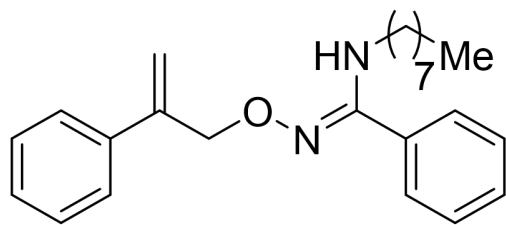
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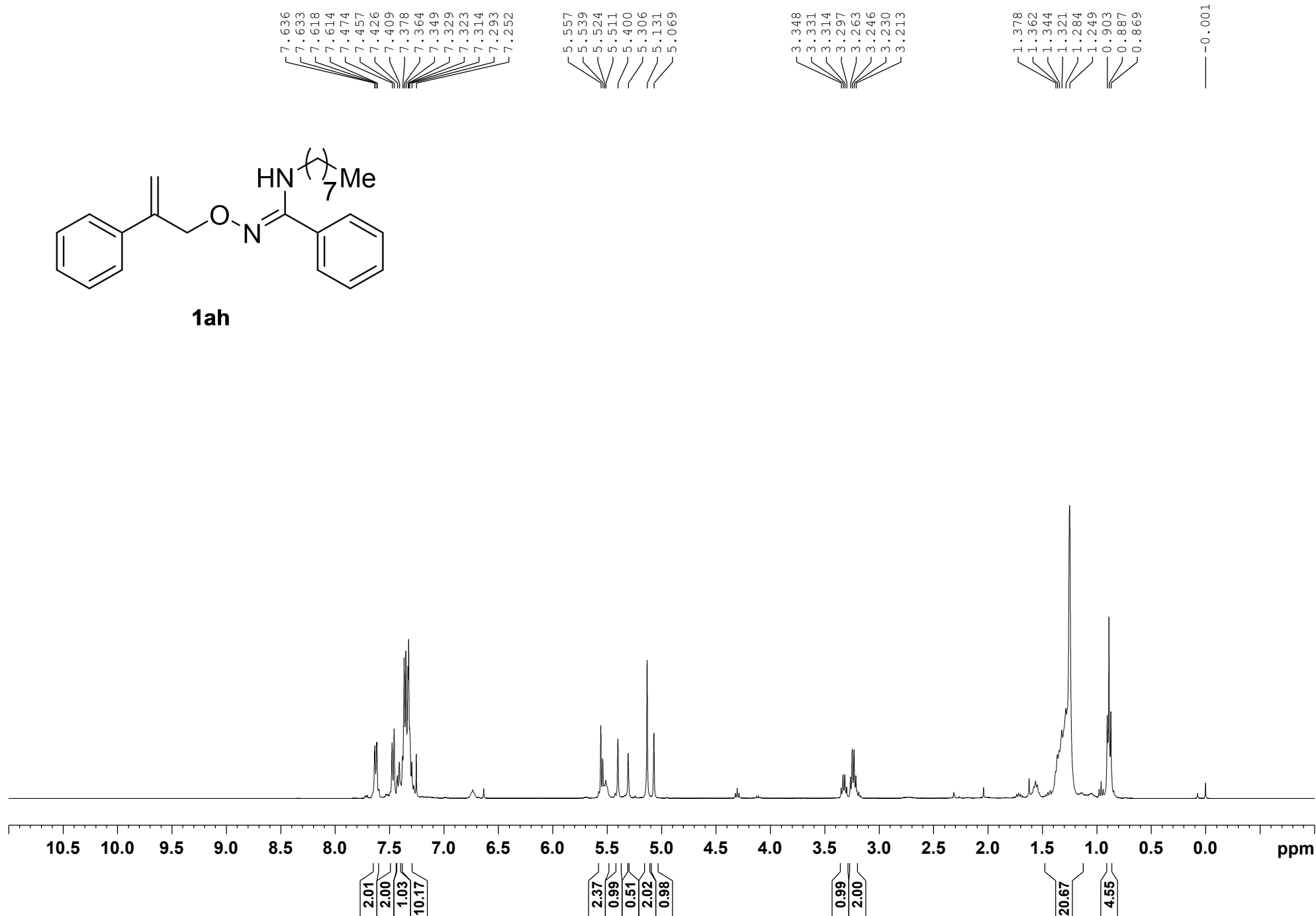


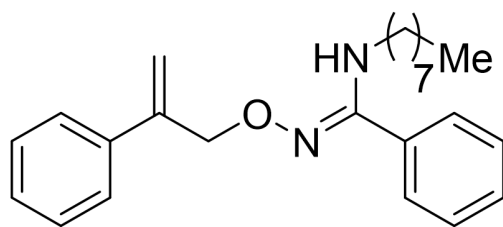
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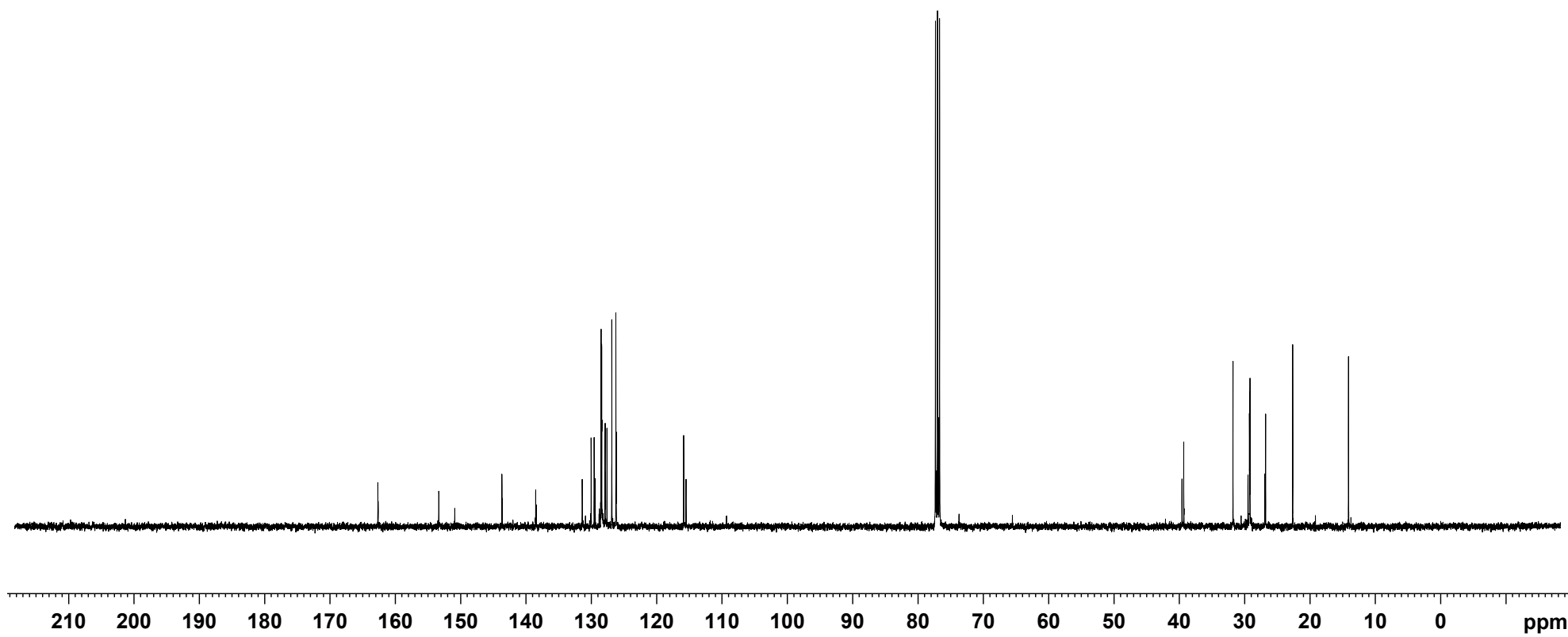


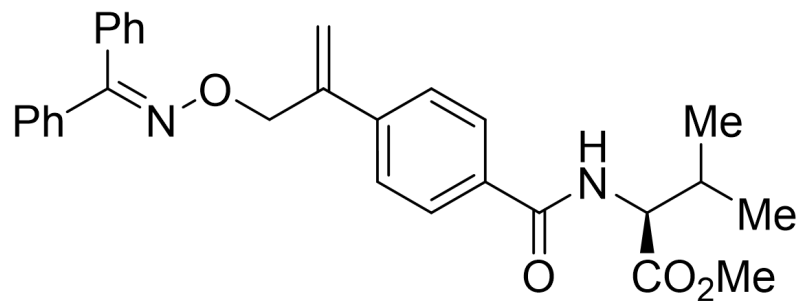
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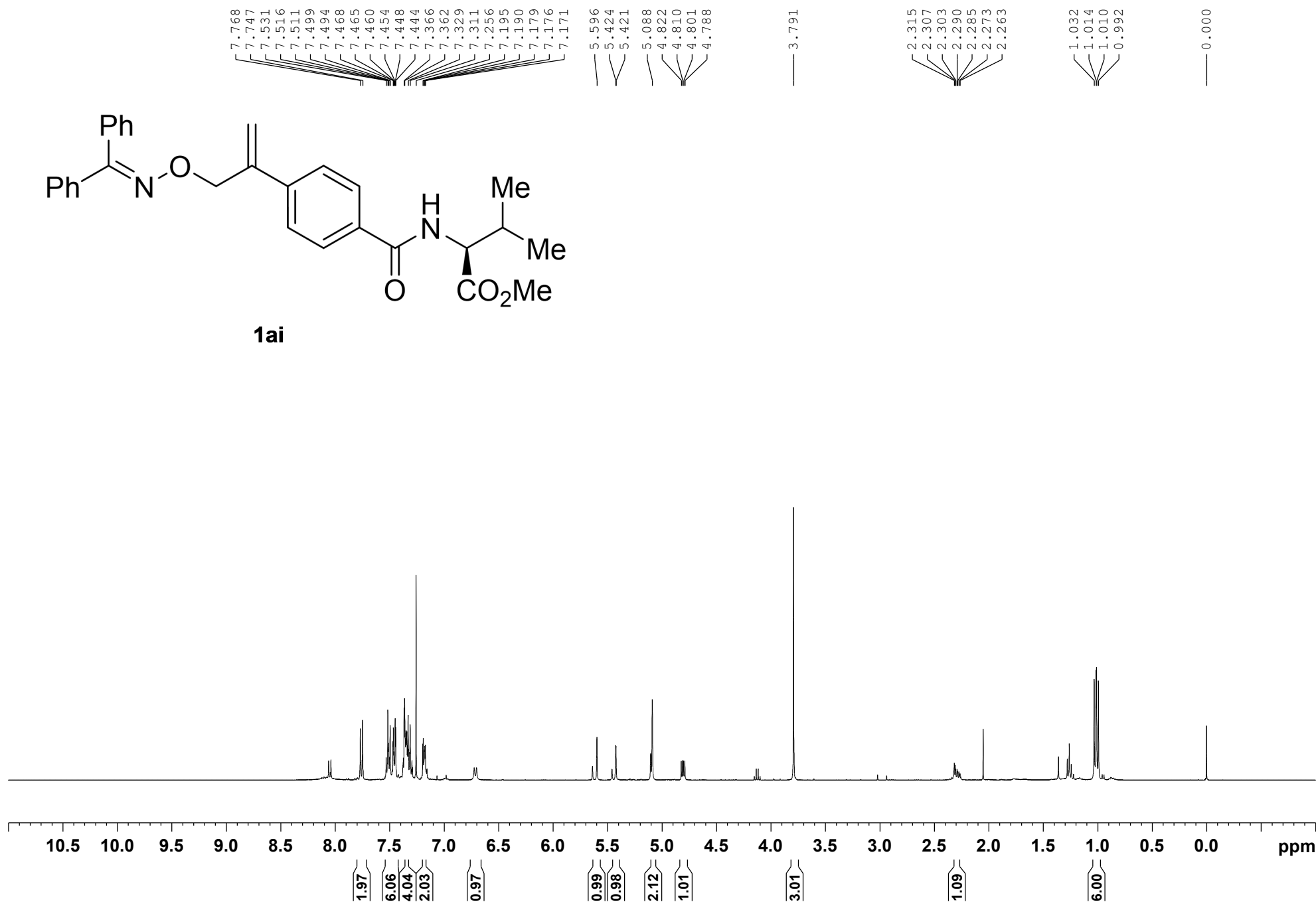
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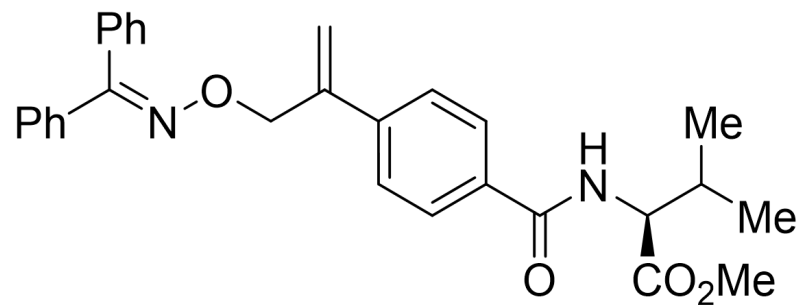
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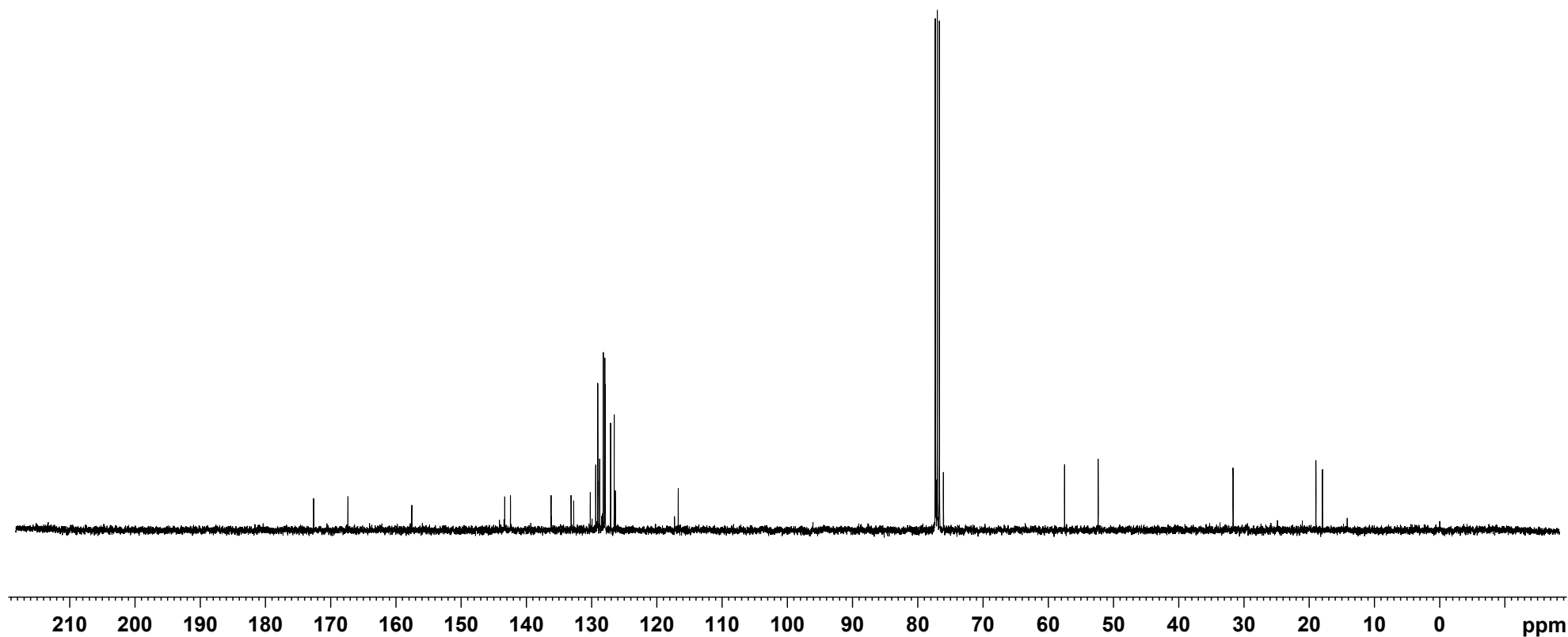


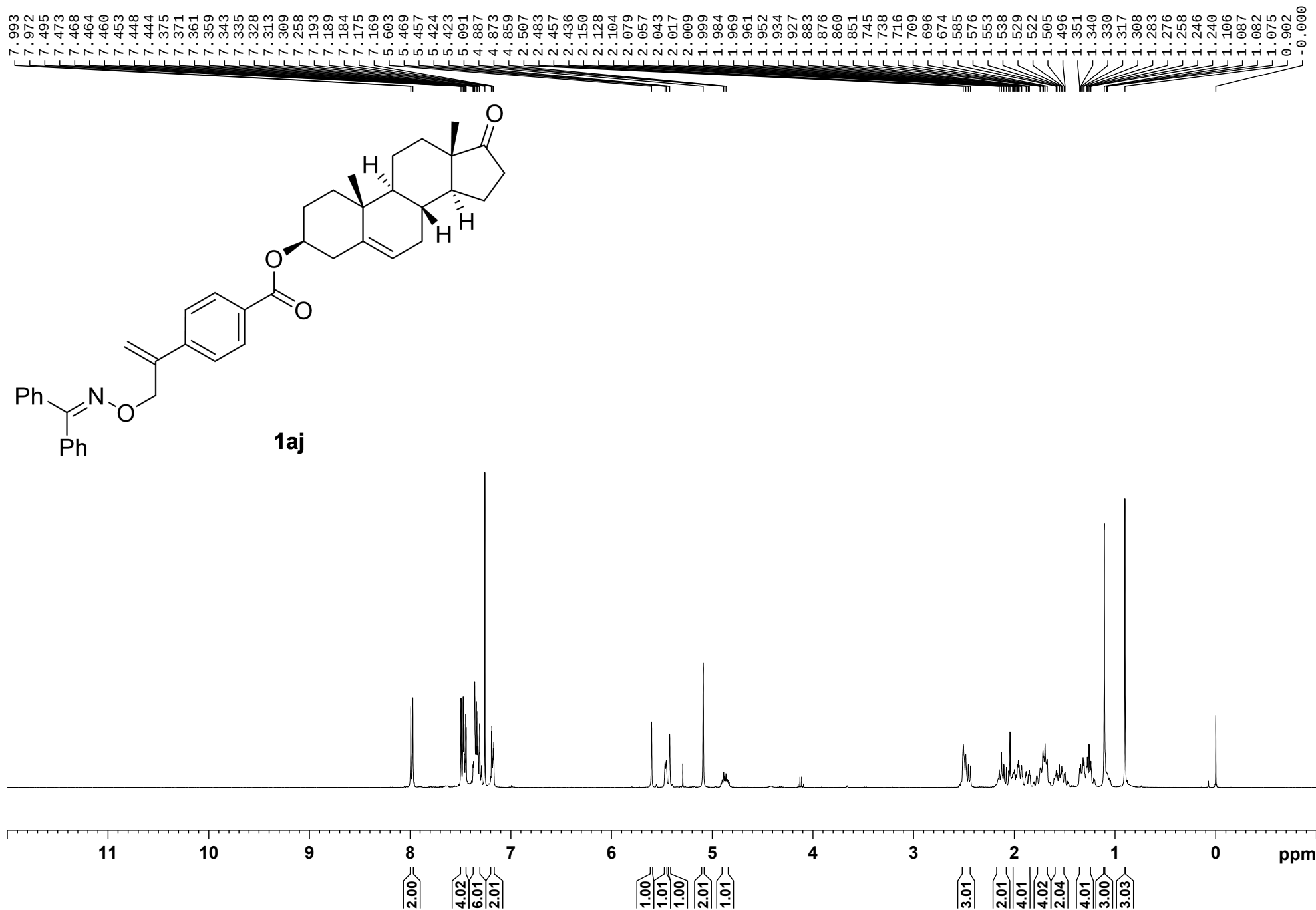
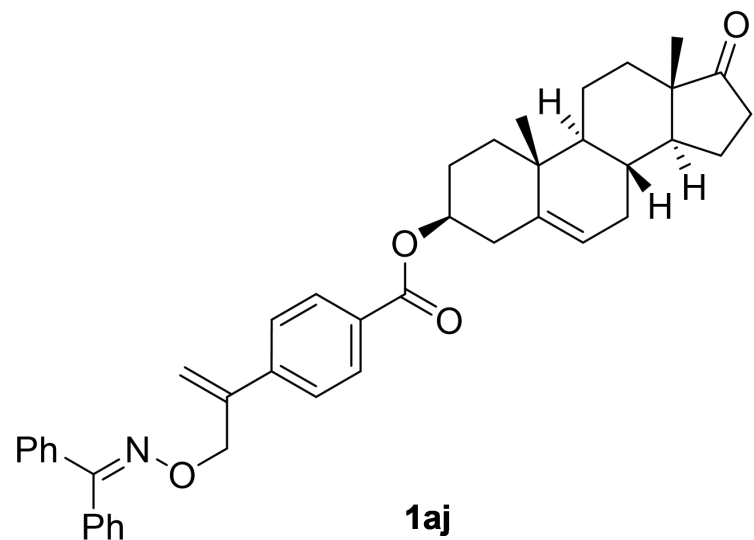
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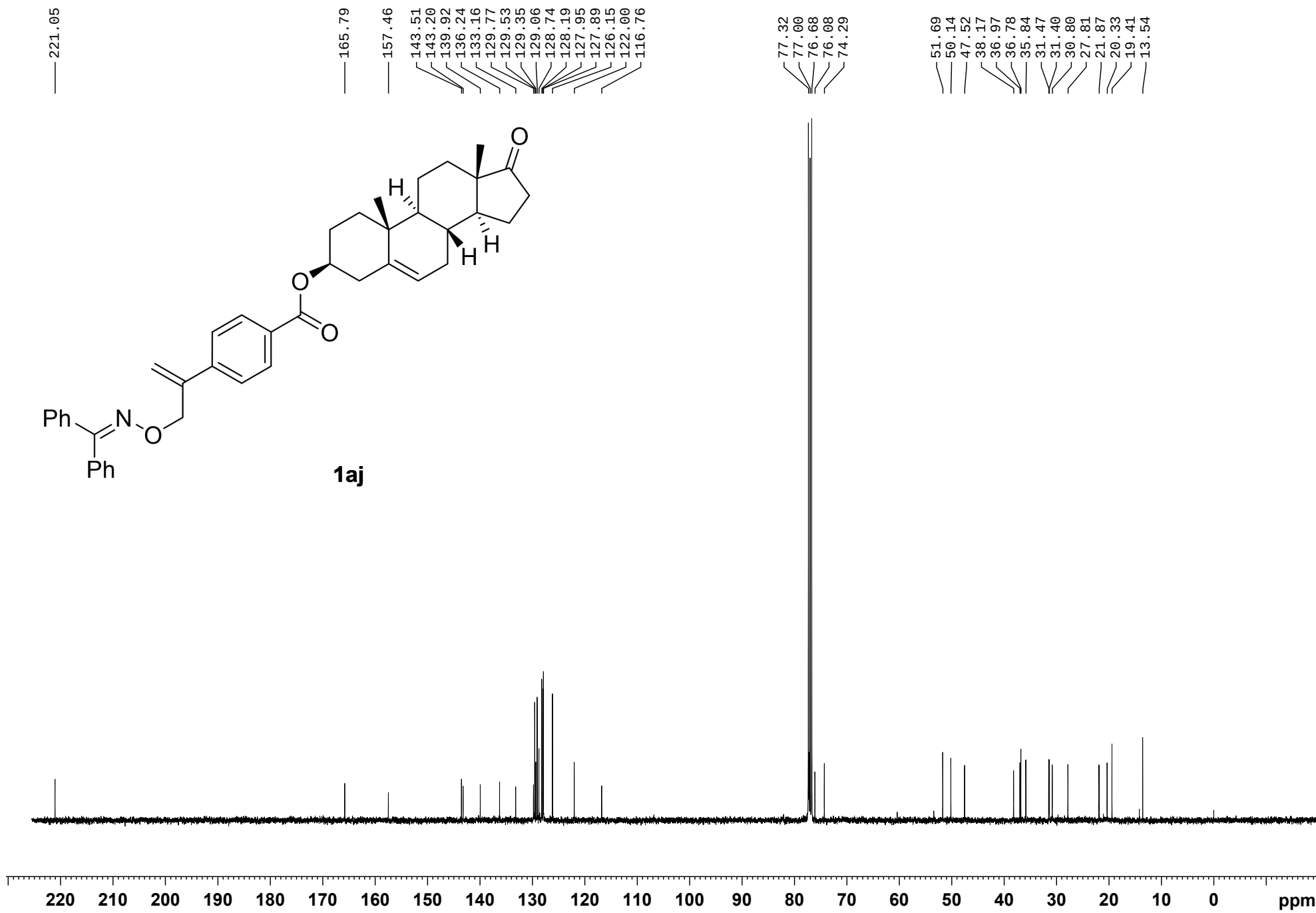
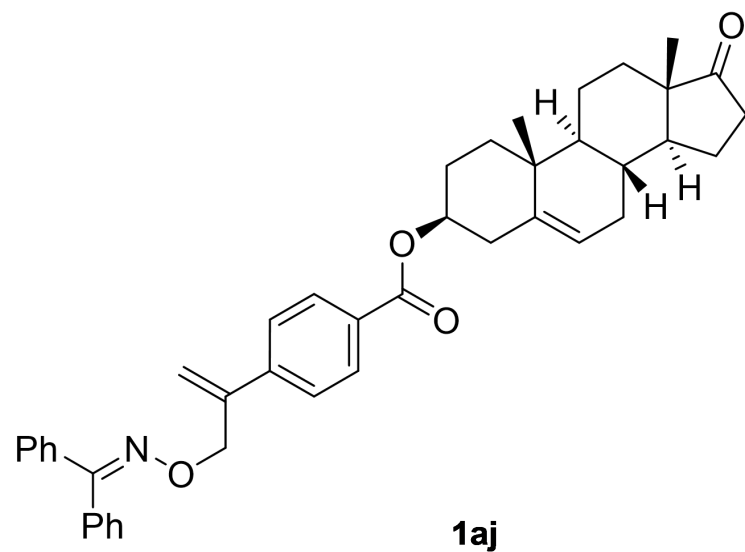


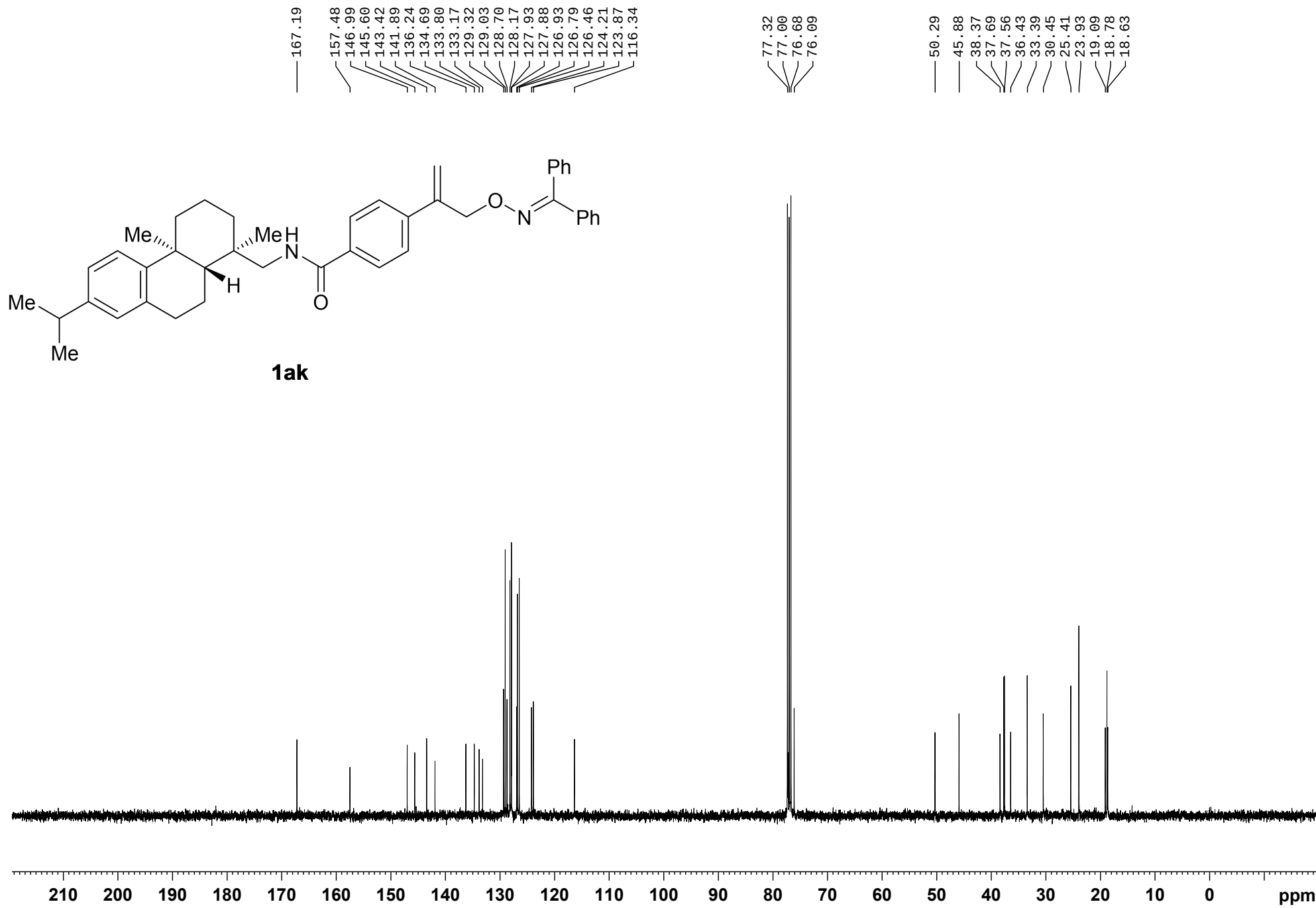


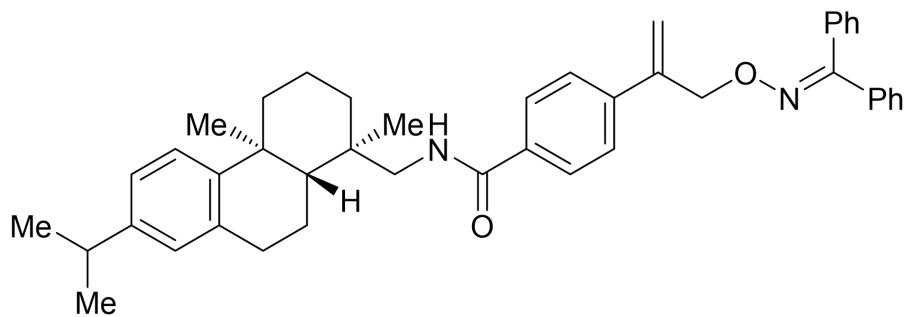
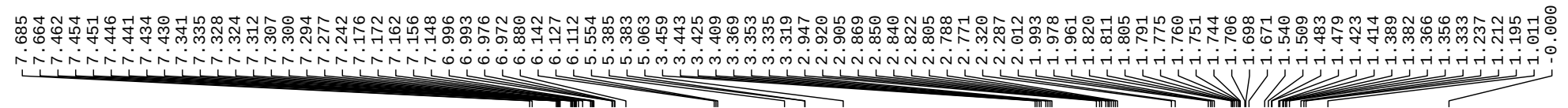
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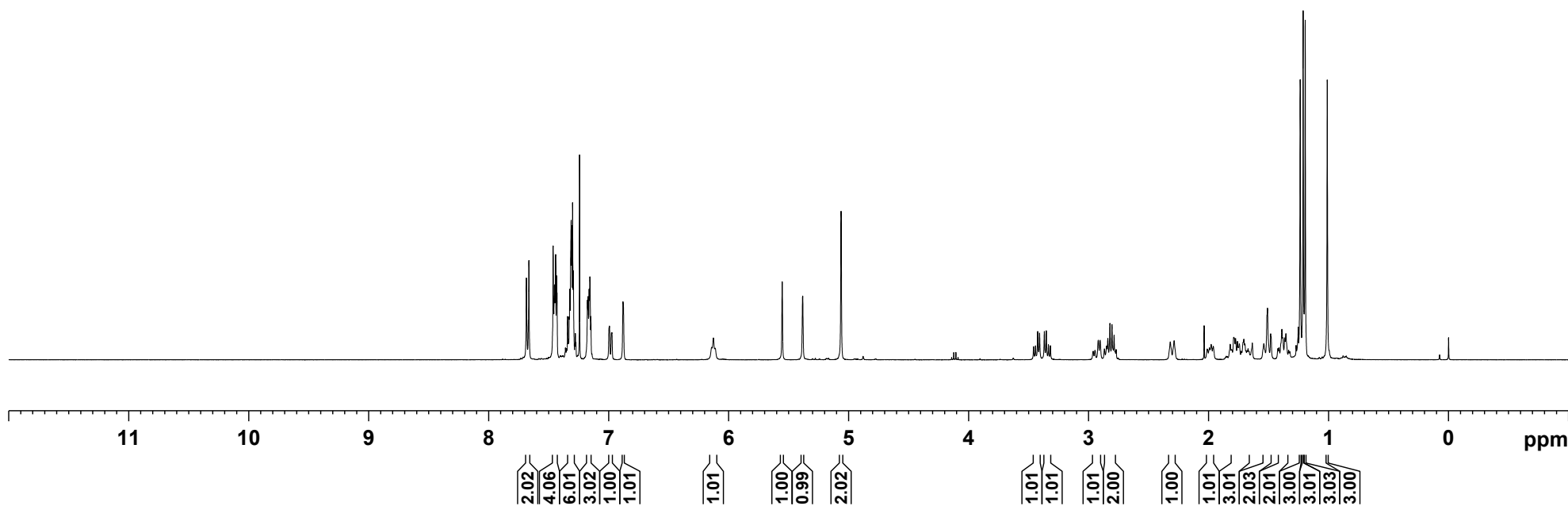


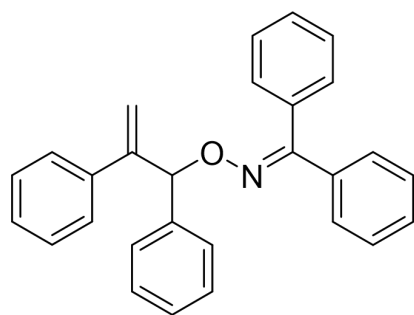




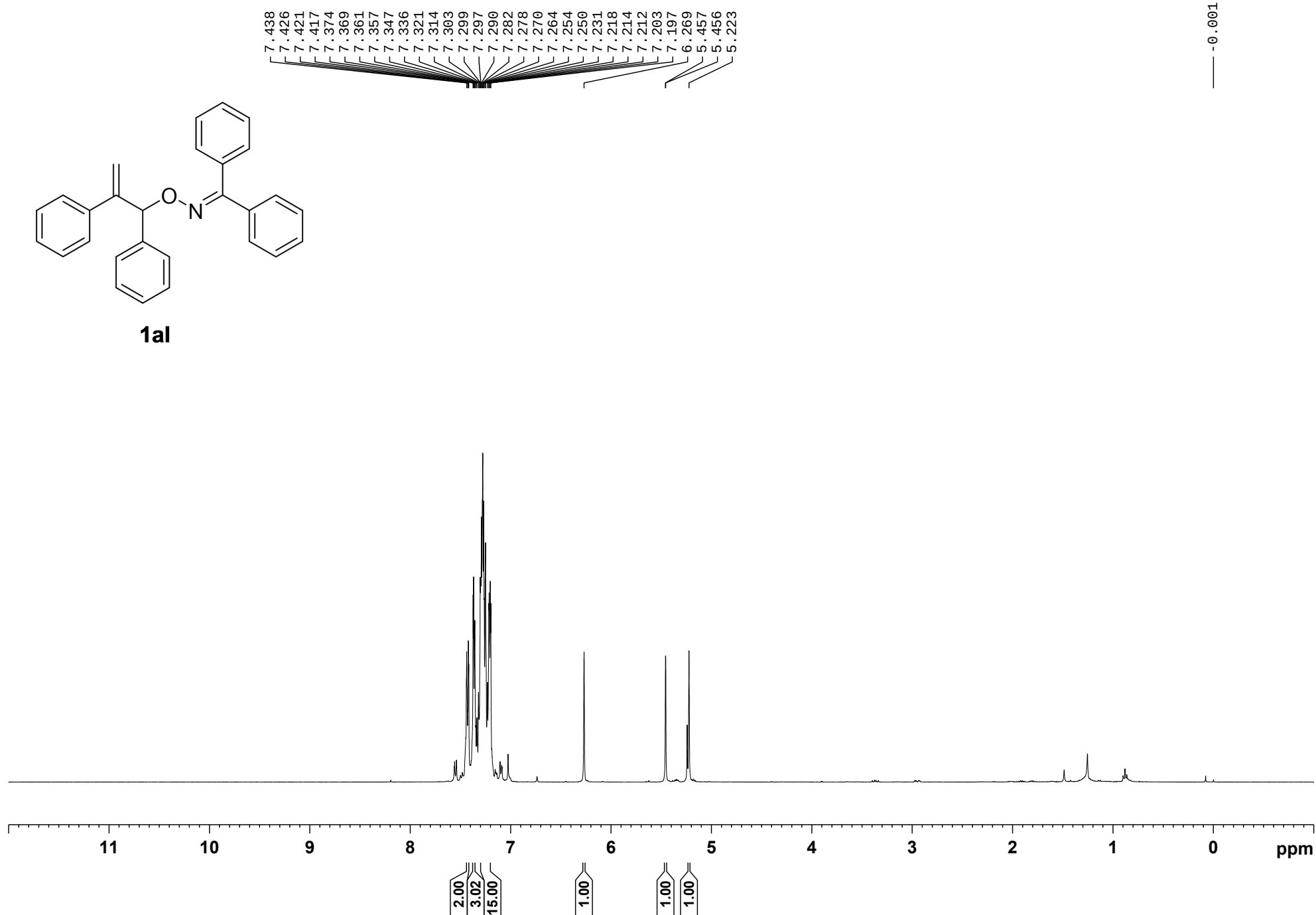


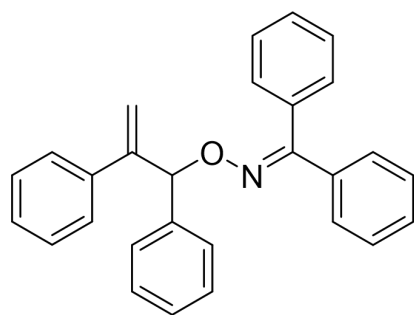
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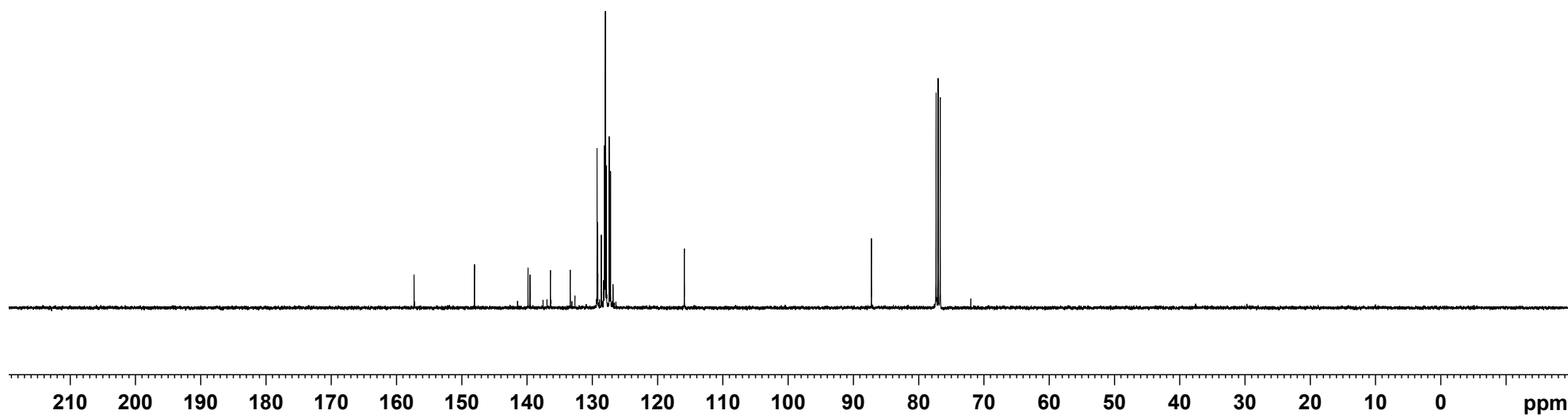
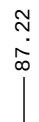
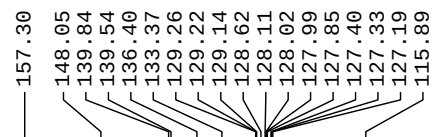


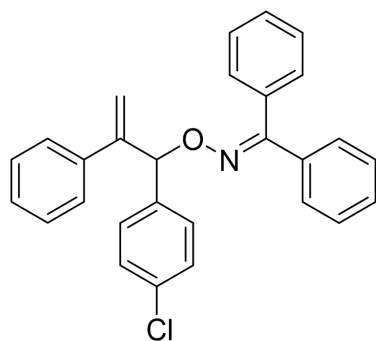
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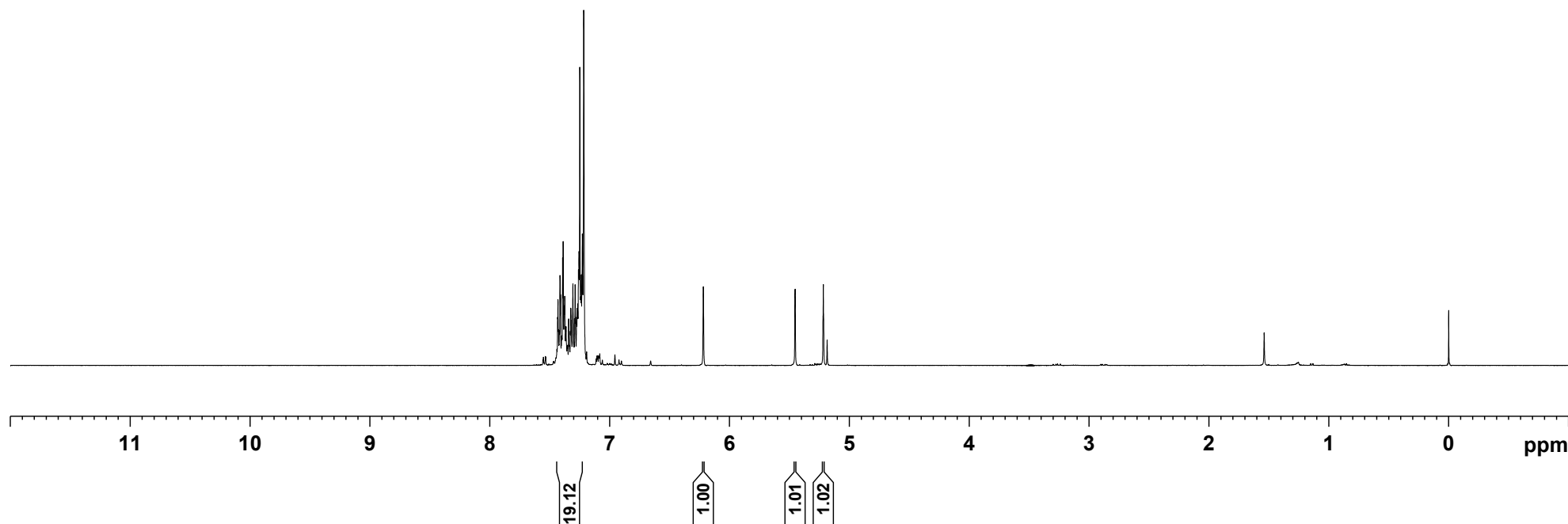
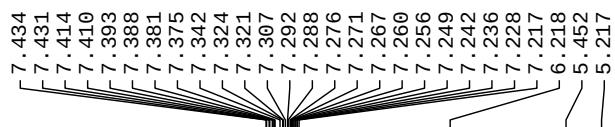


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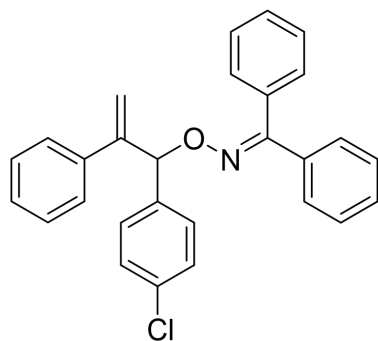




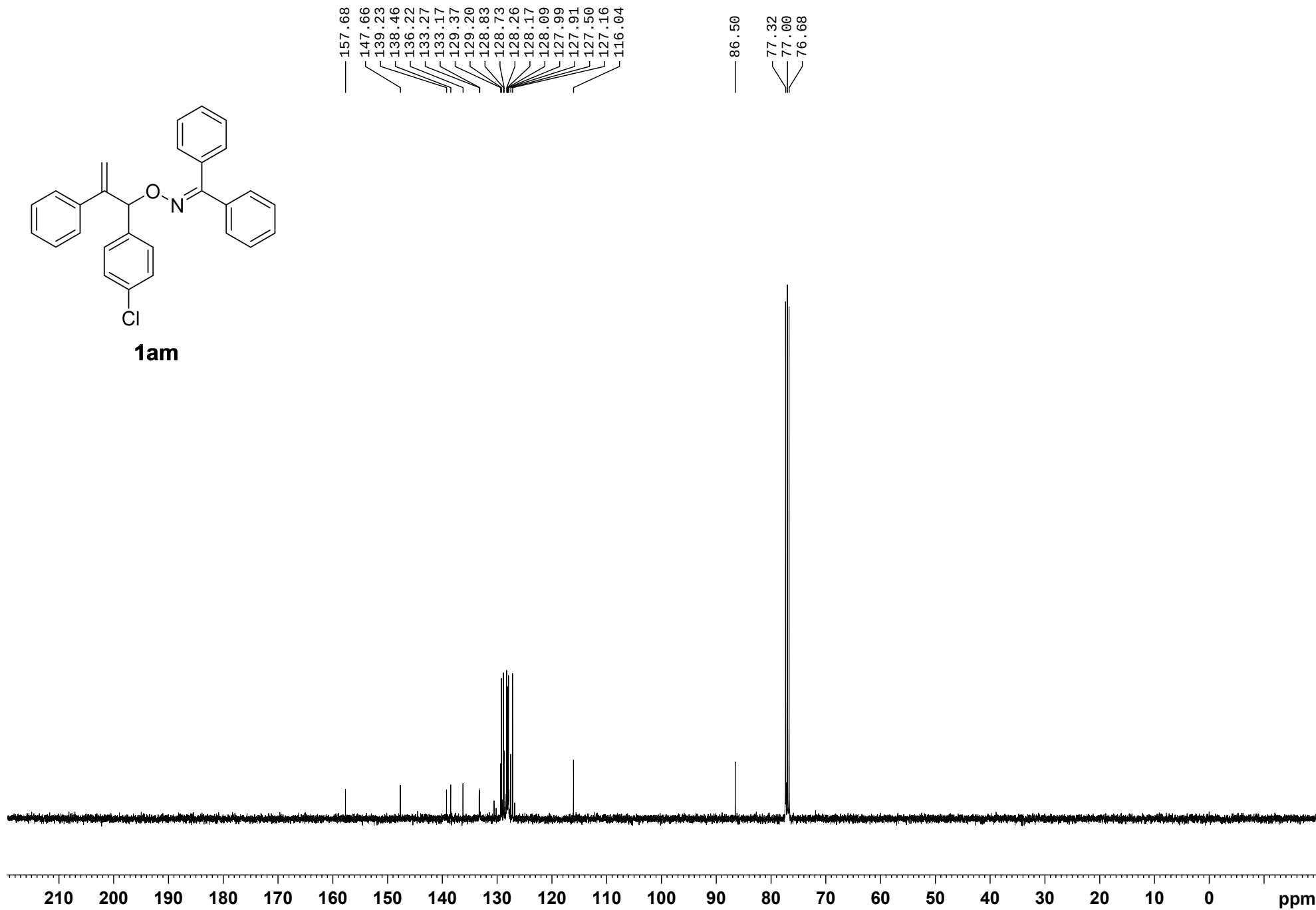
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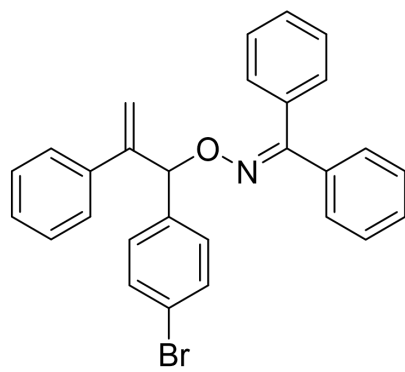


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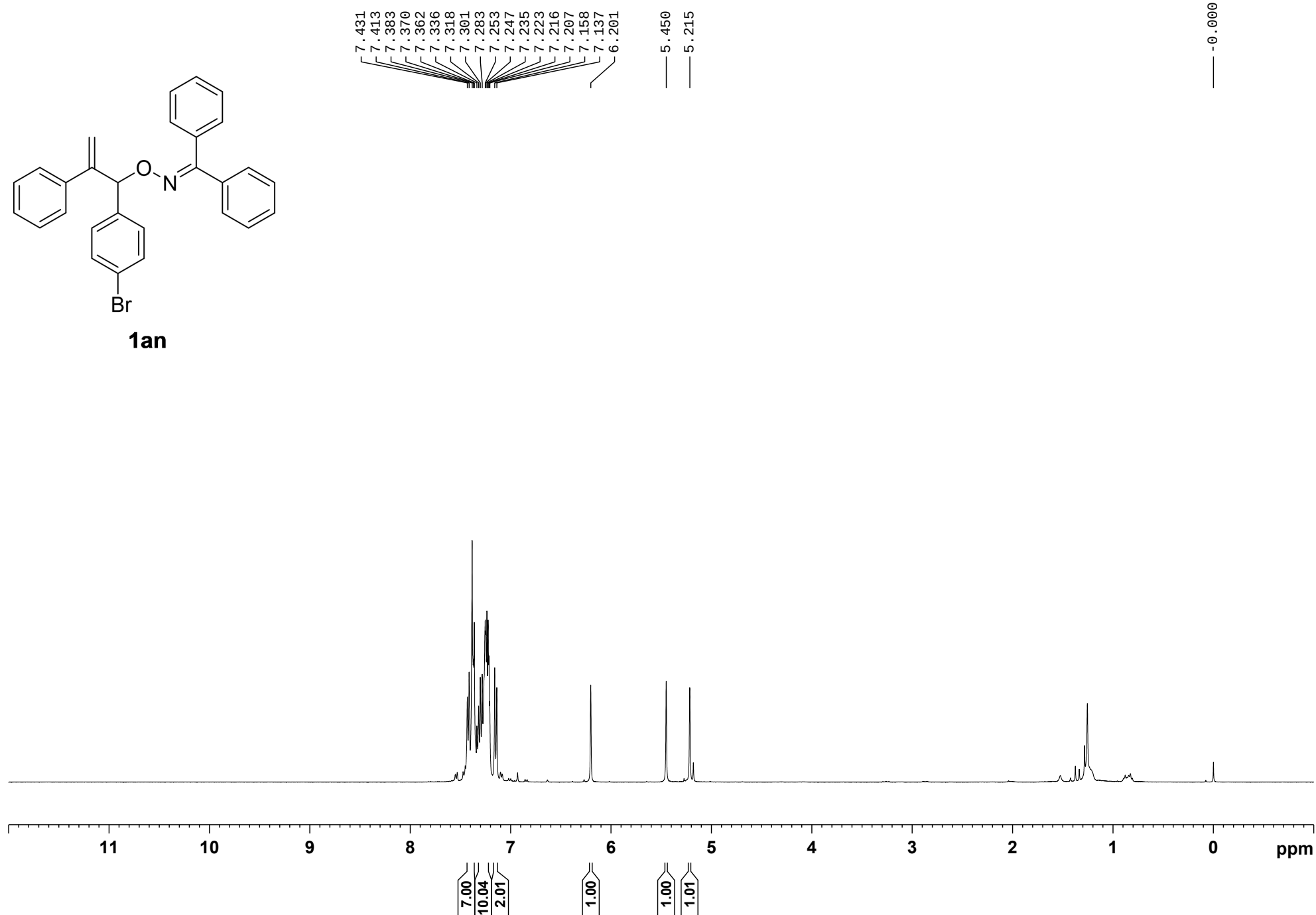


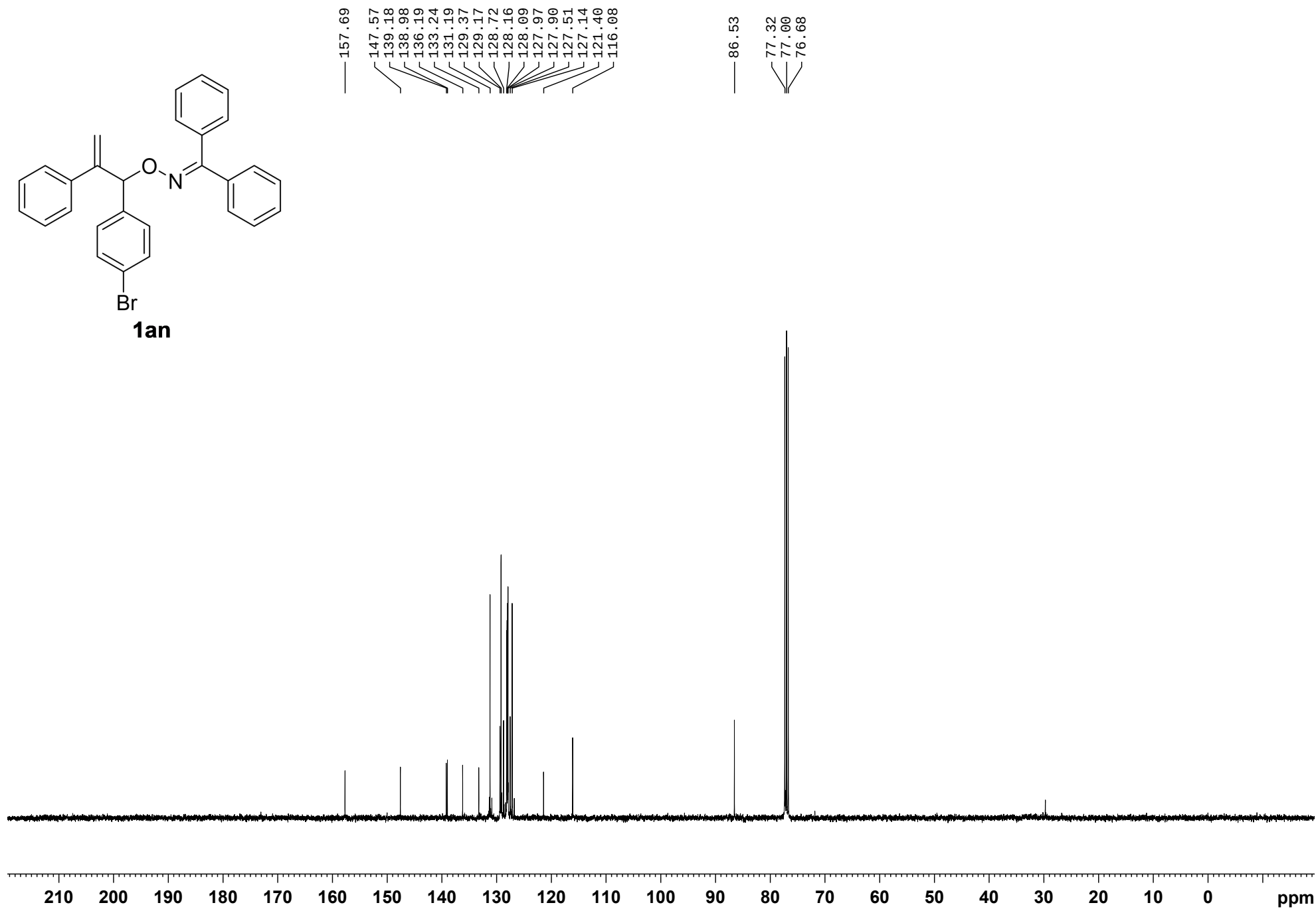
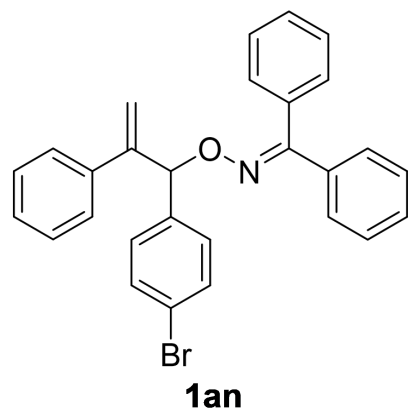
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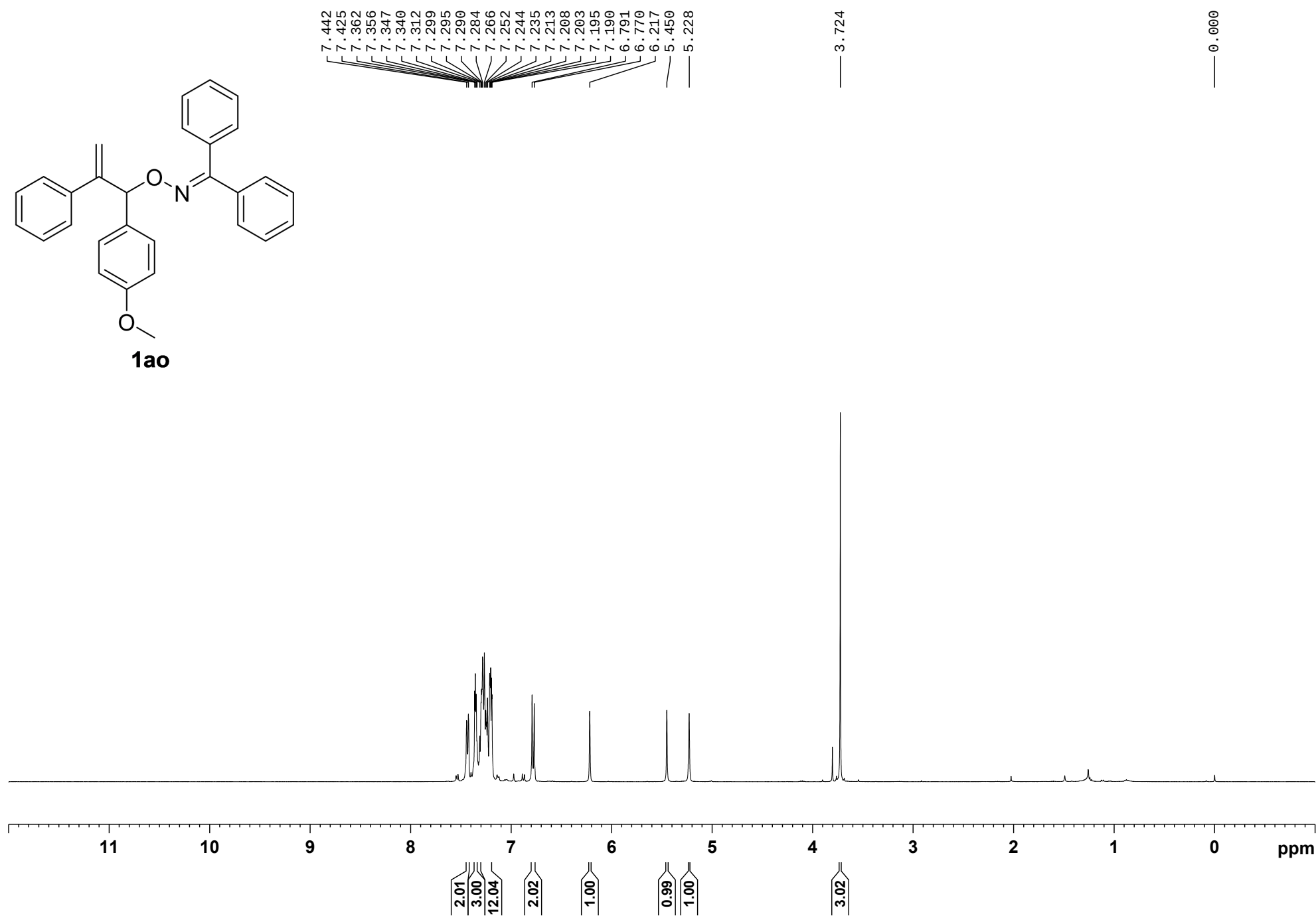
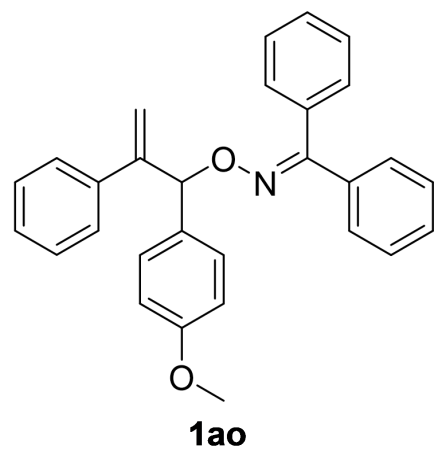


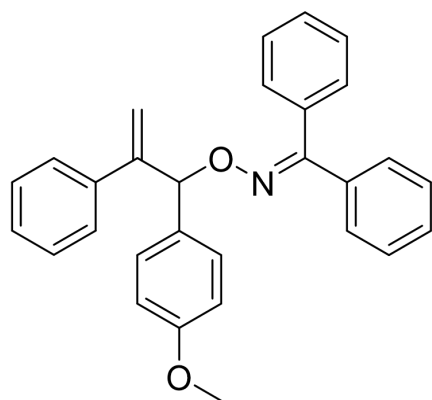


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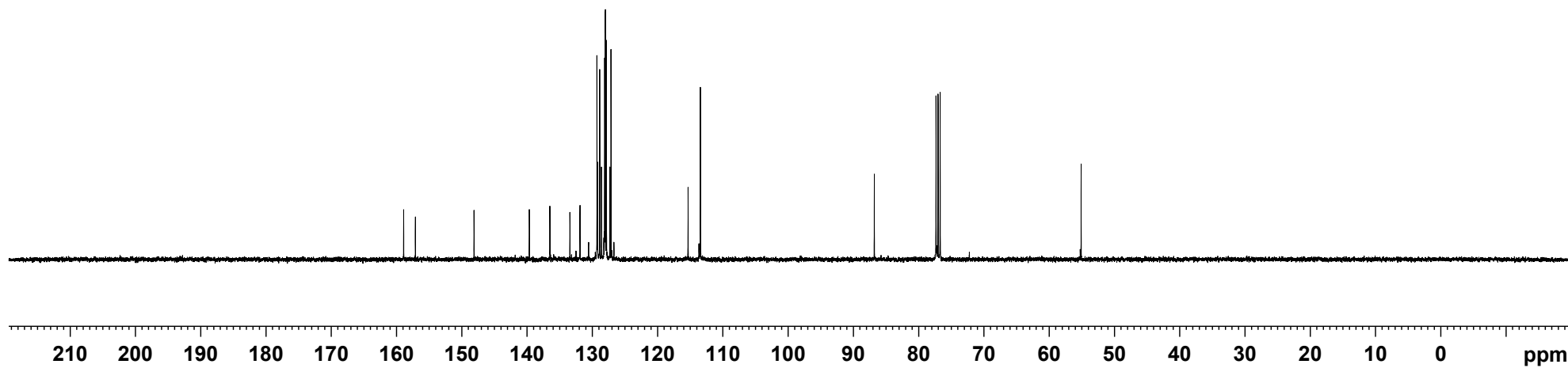
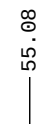
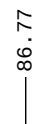
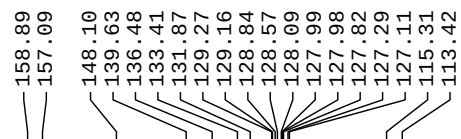


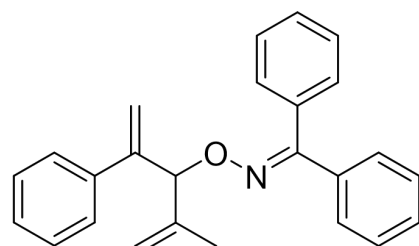




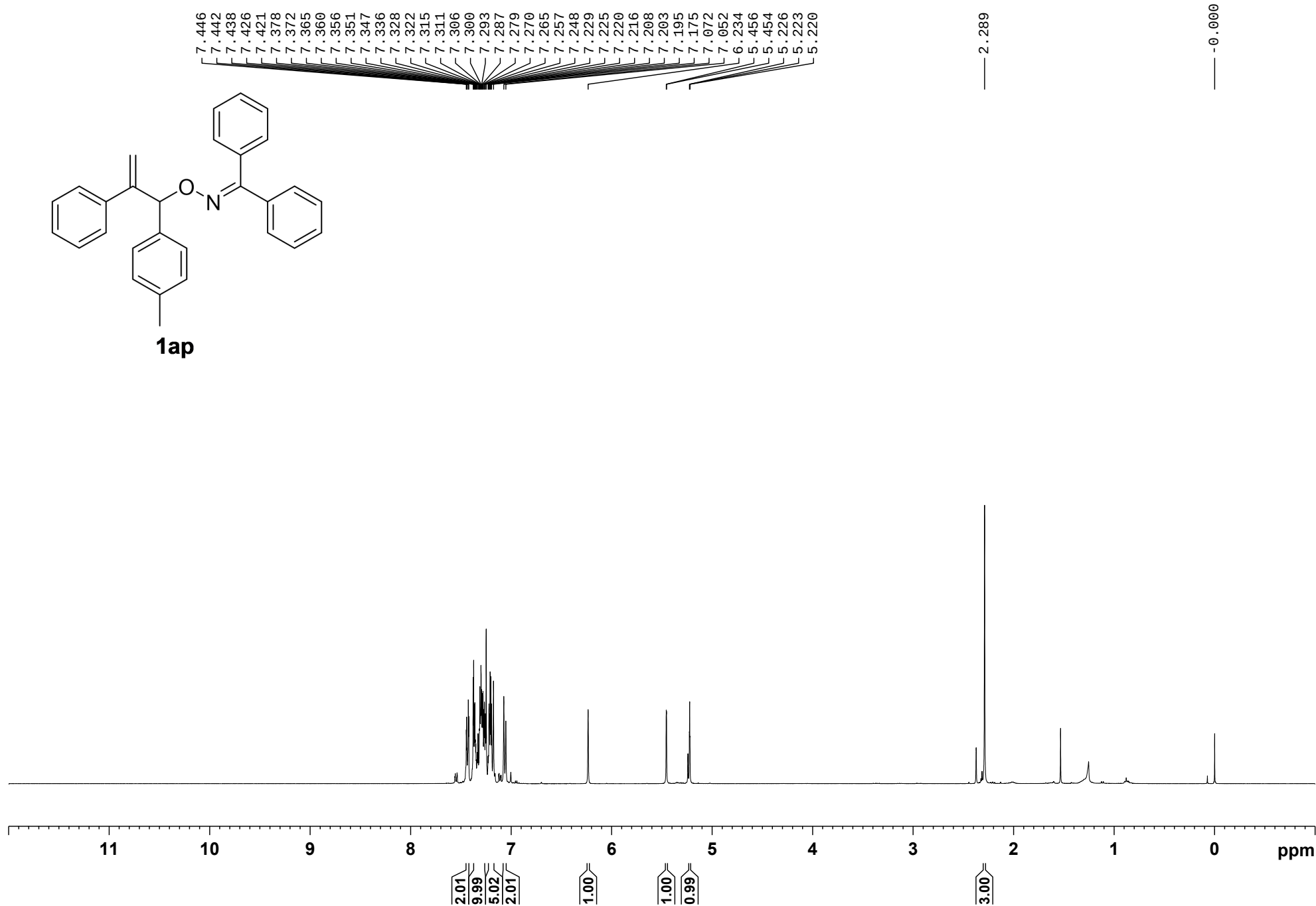


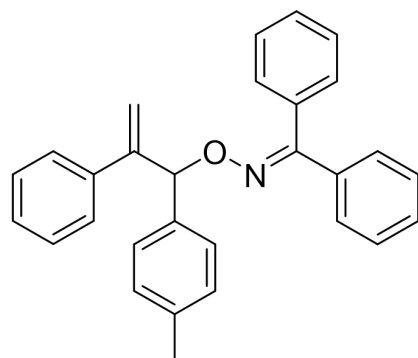
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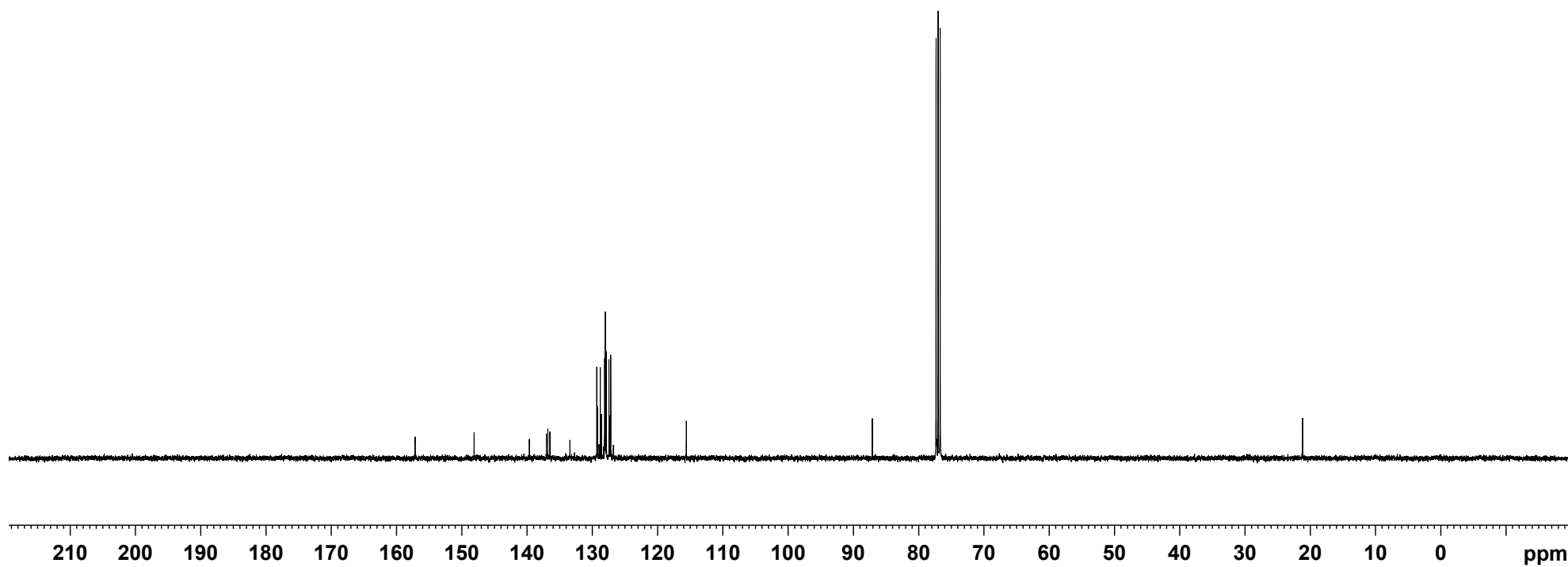
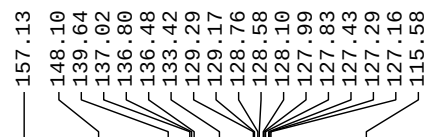


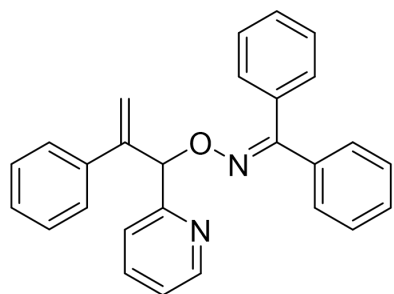
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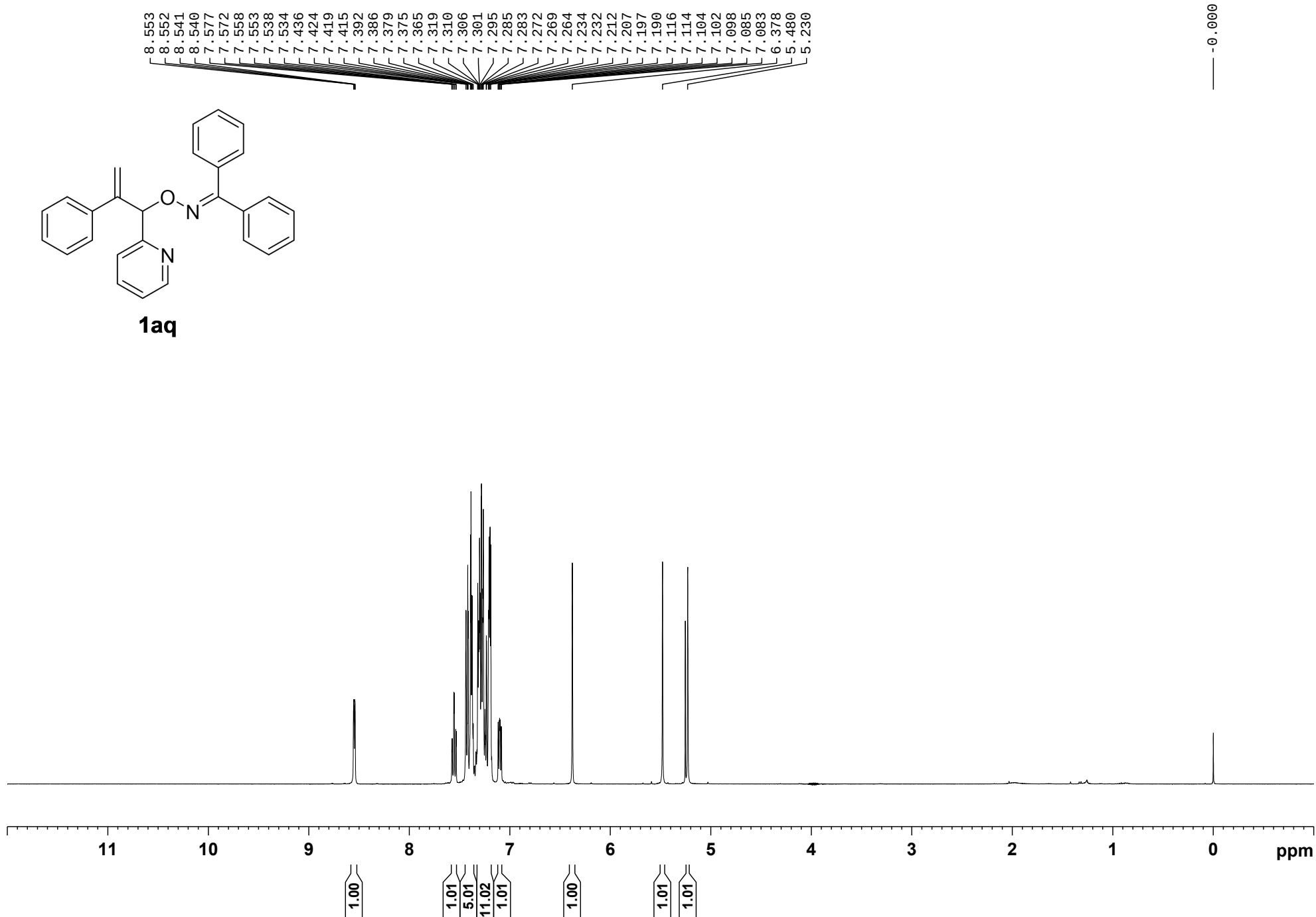


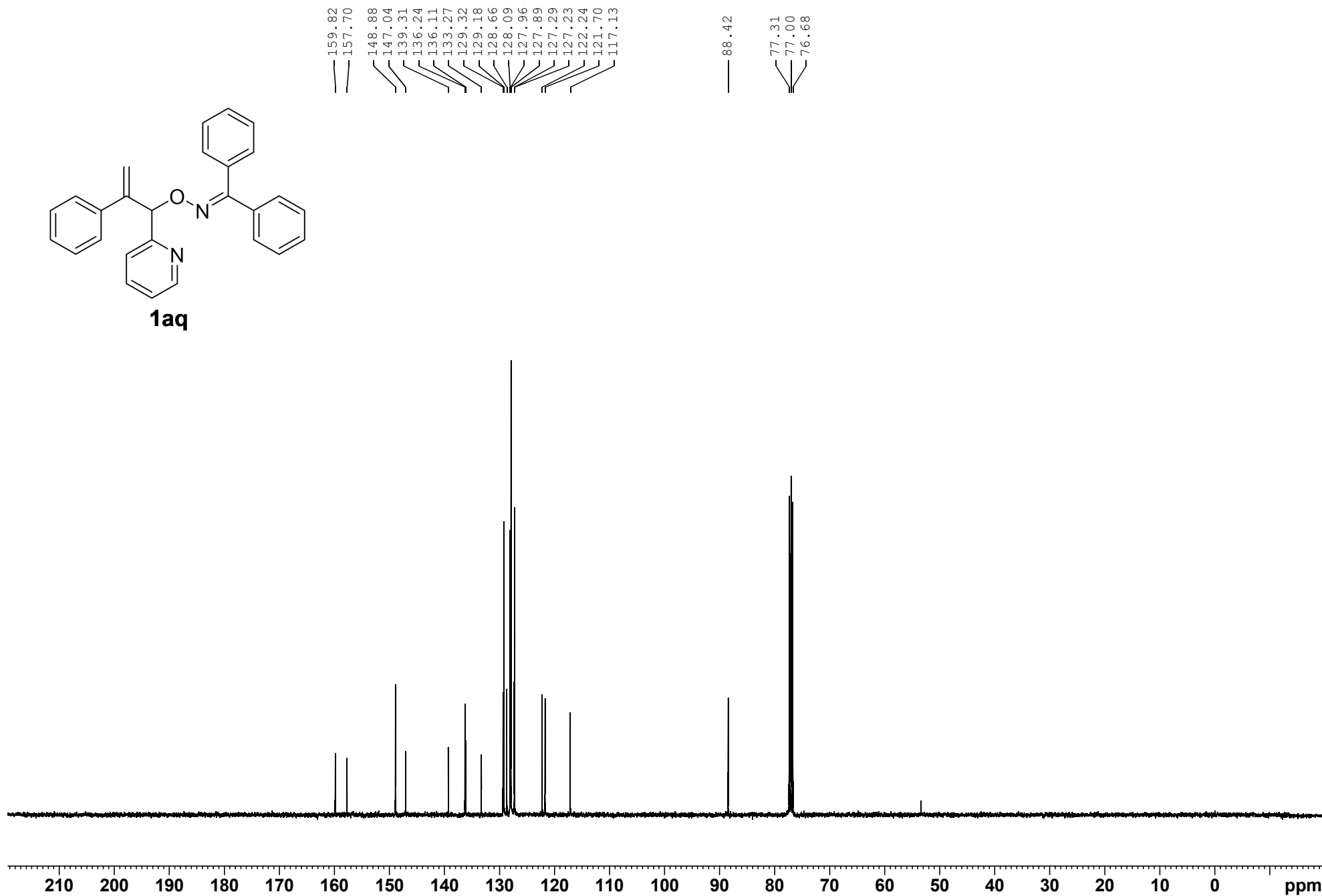
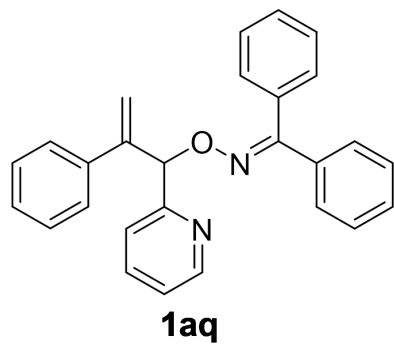
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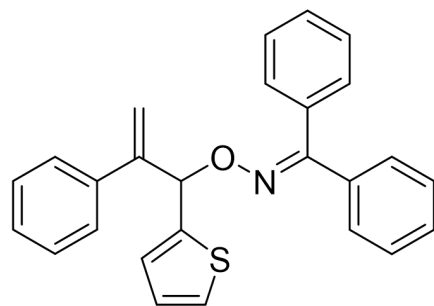




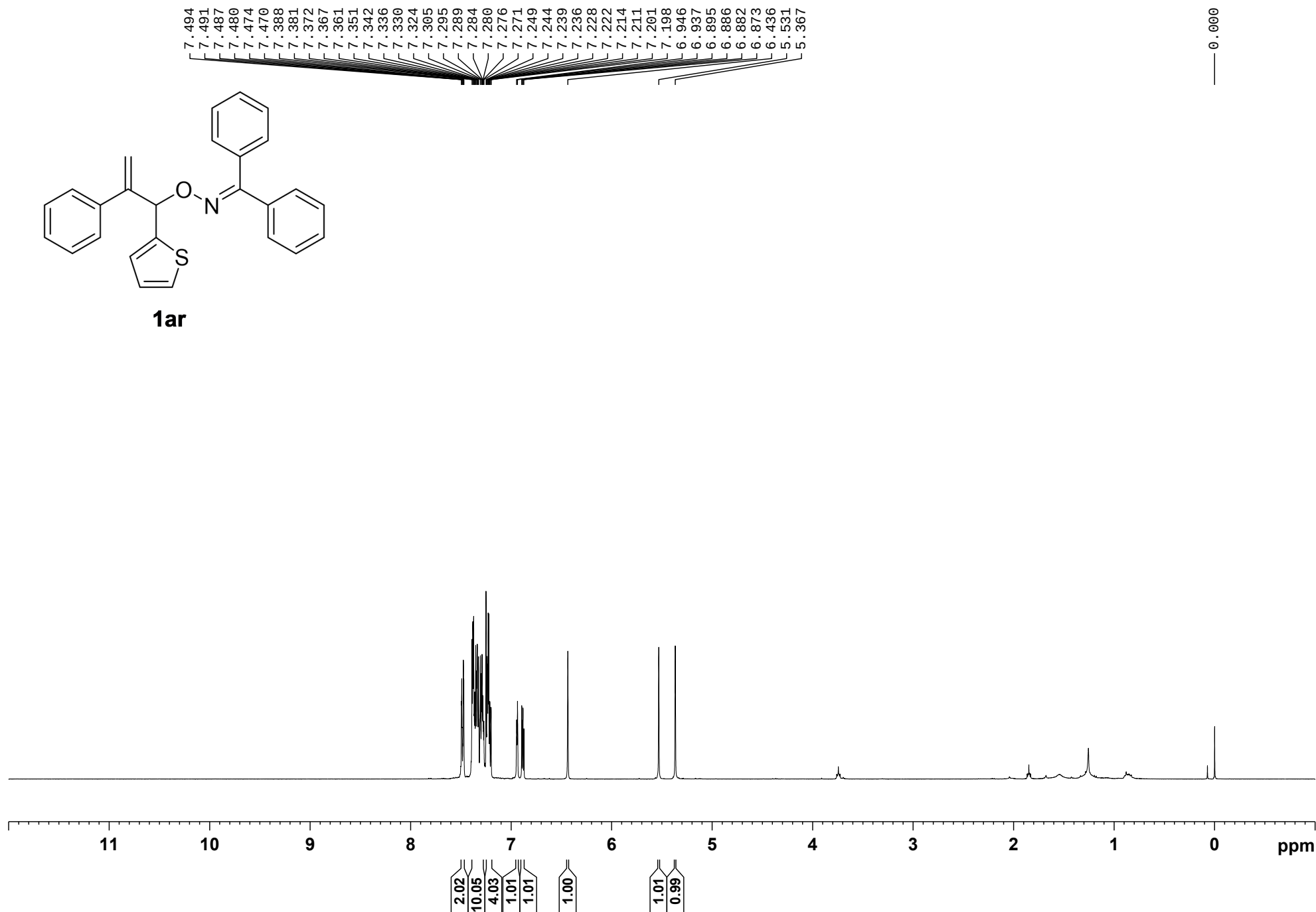
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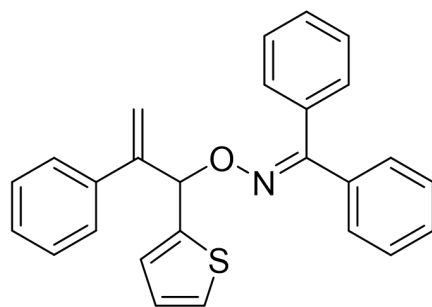




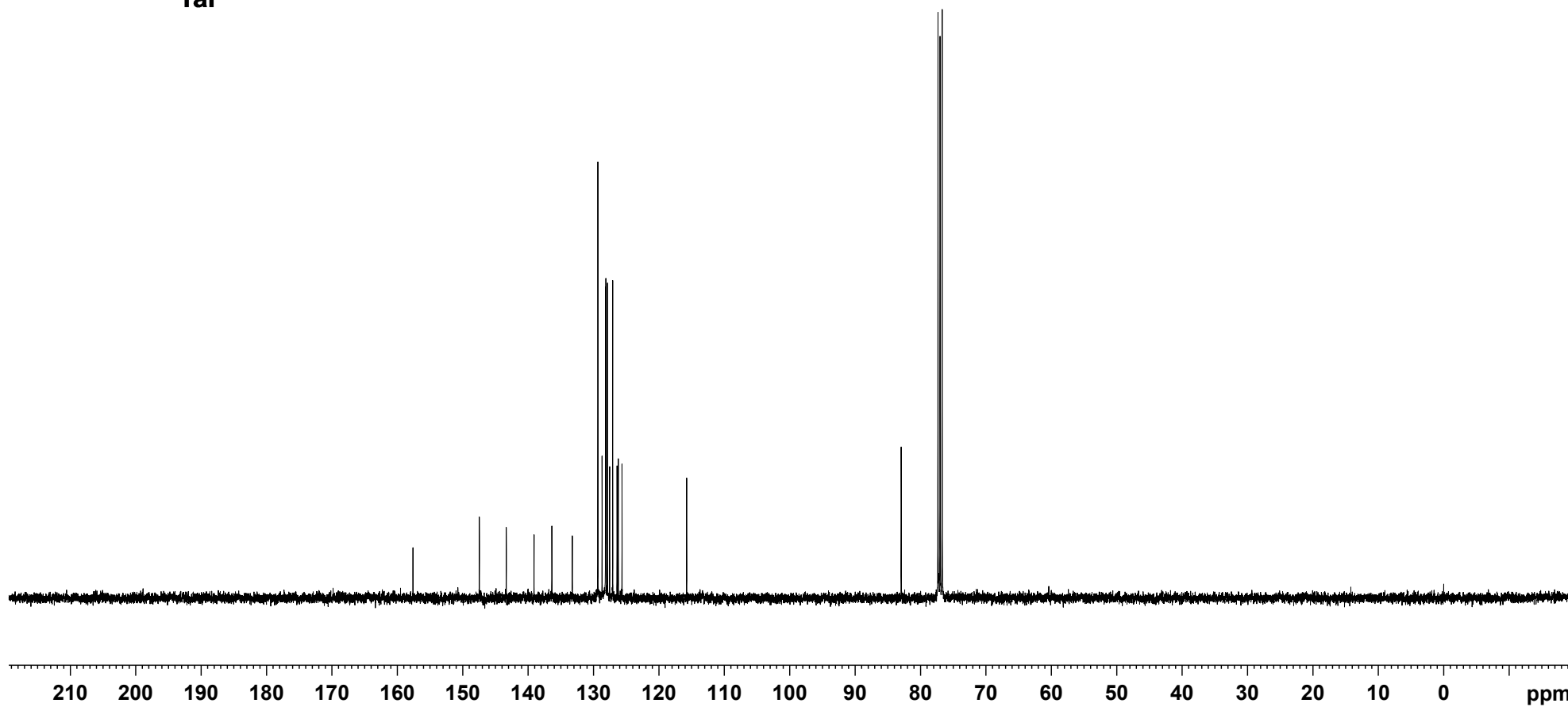
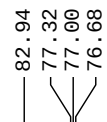
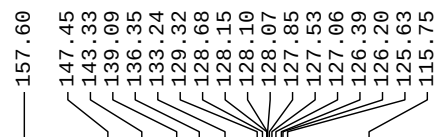


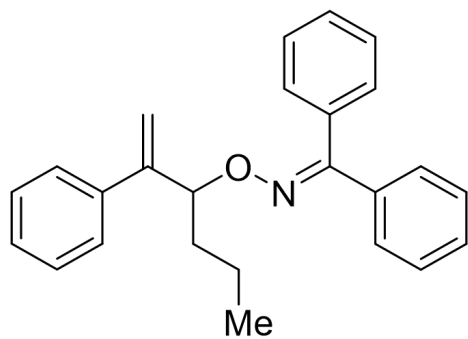
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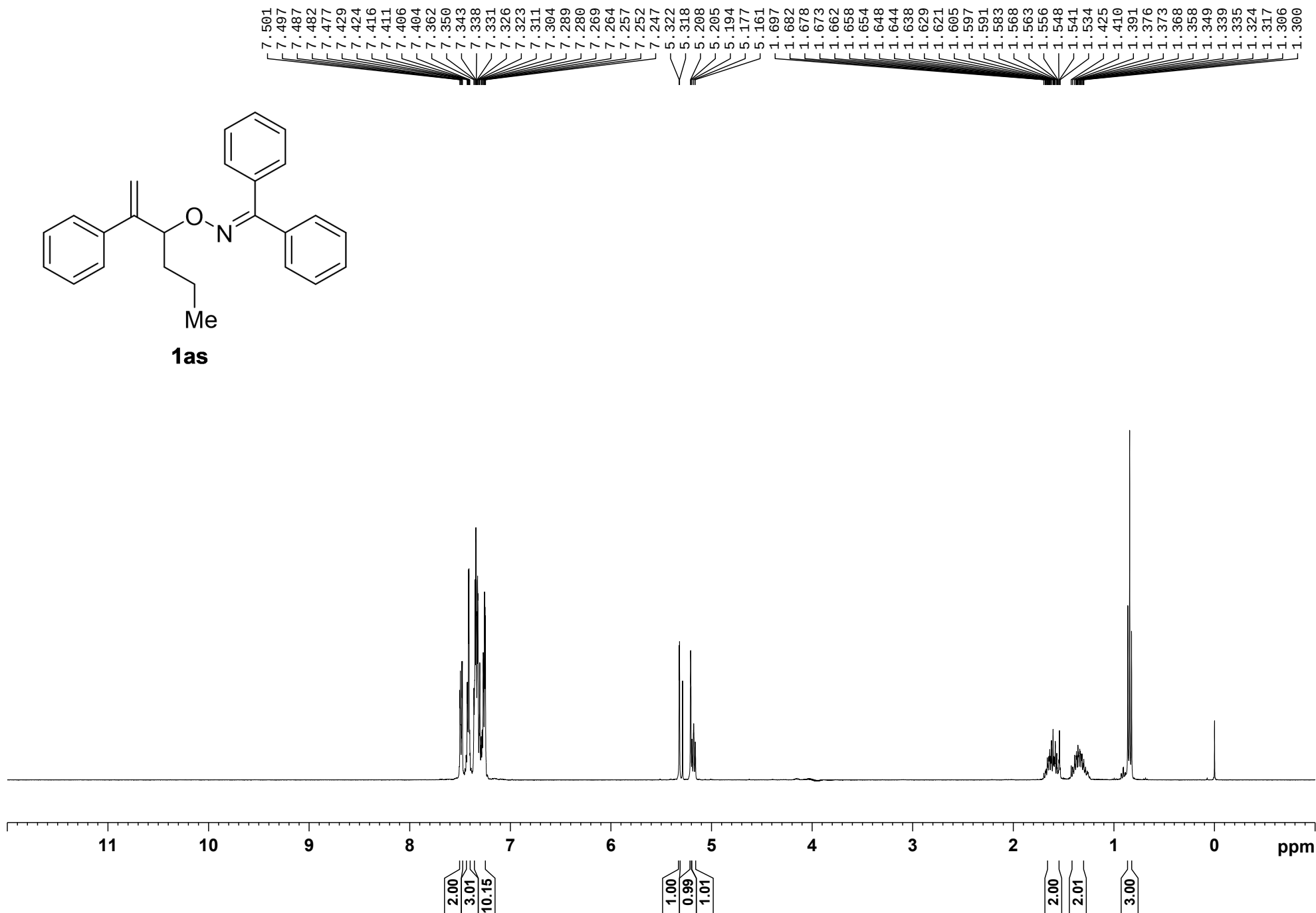


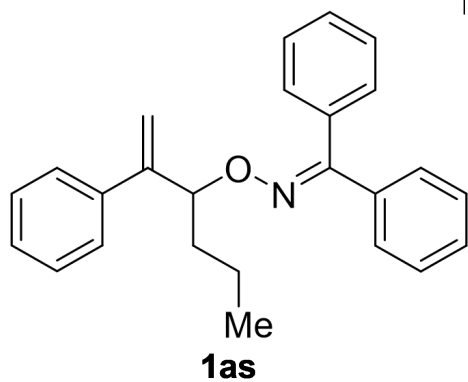
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1as





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127.14
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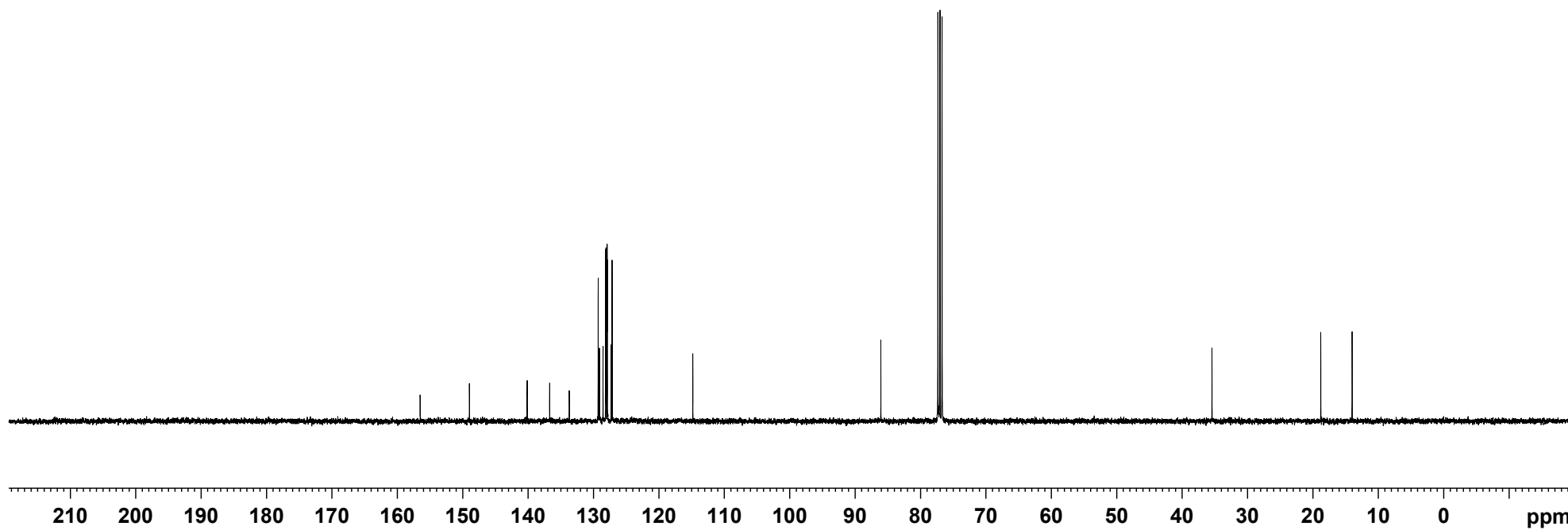
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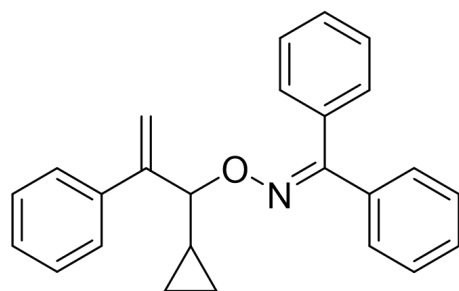
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13.97

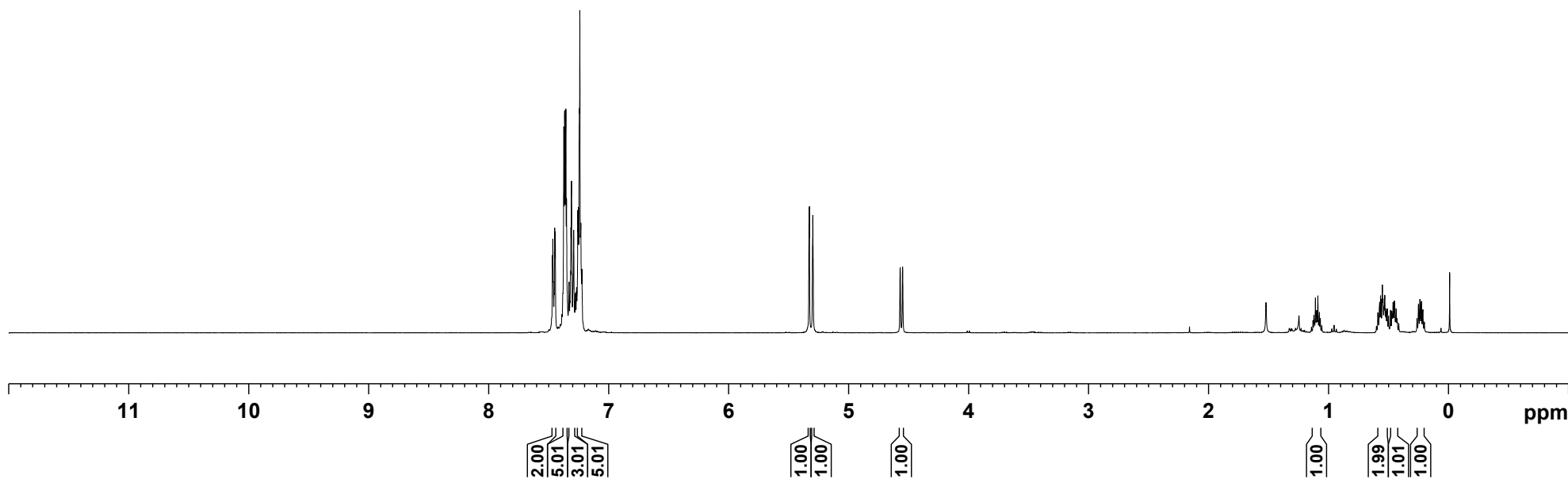


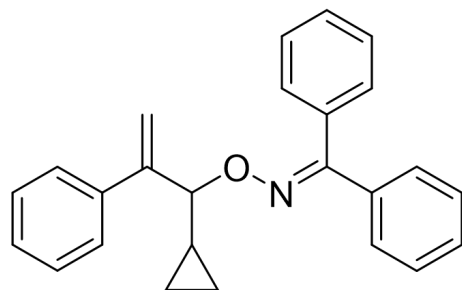


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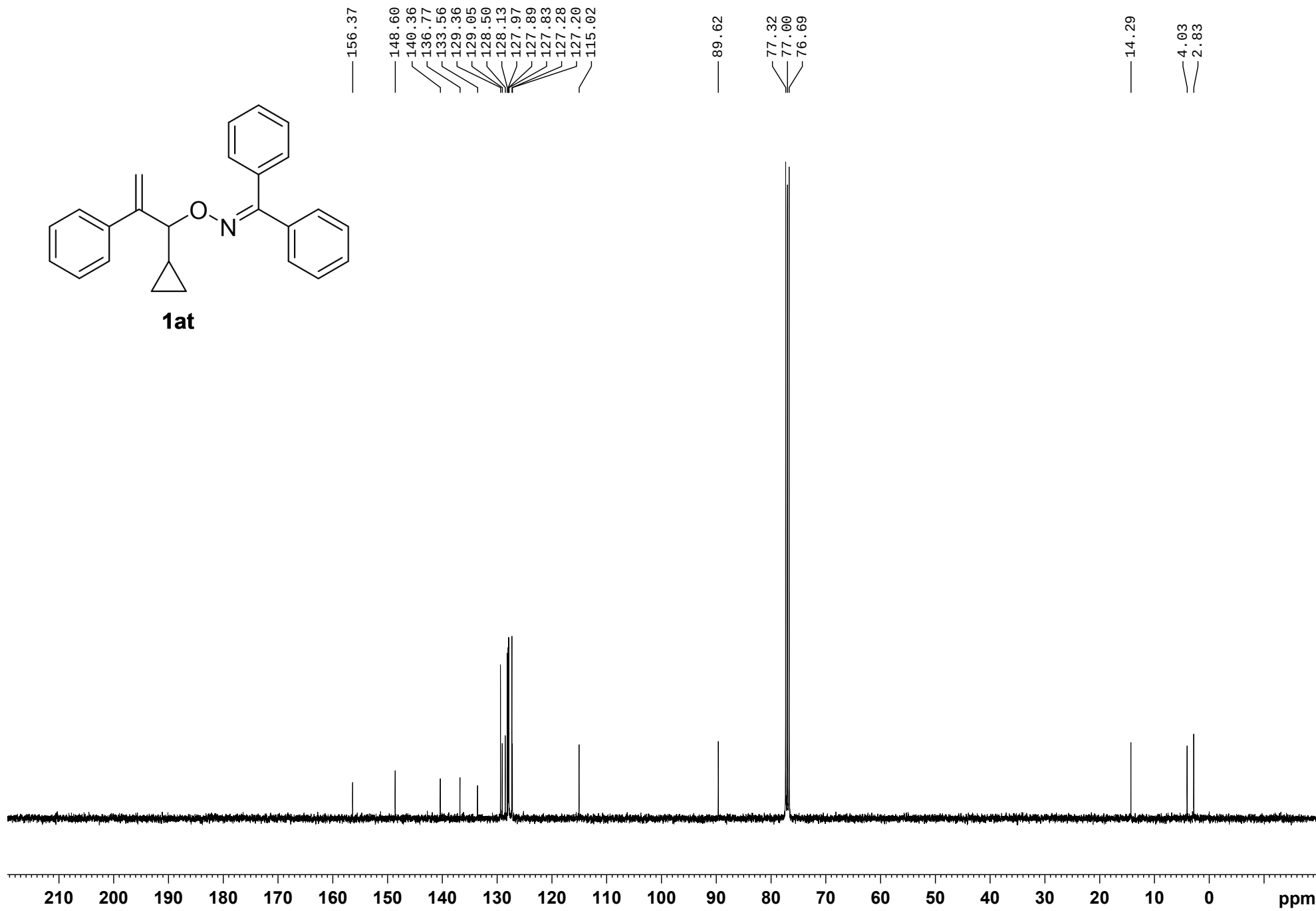
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4.550

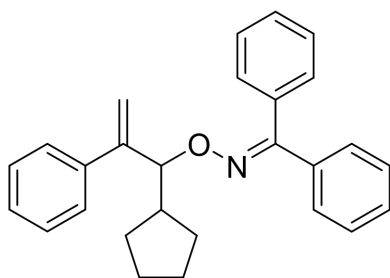
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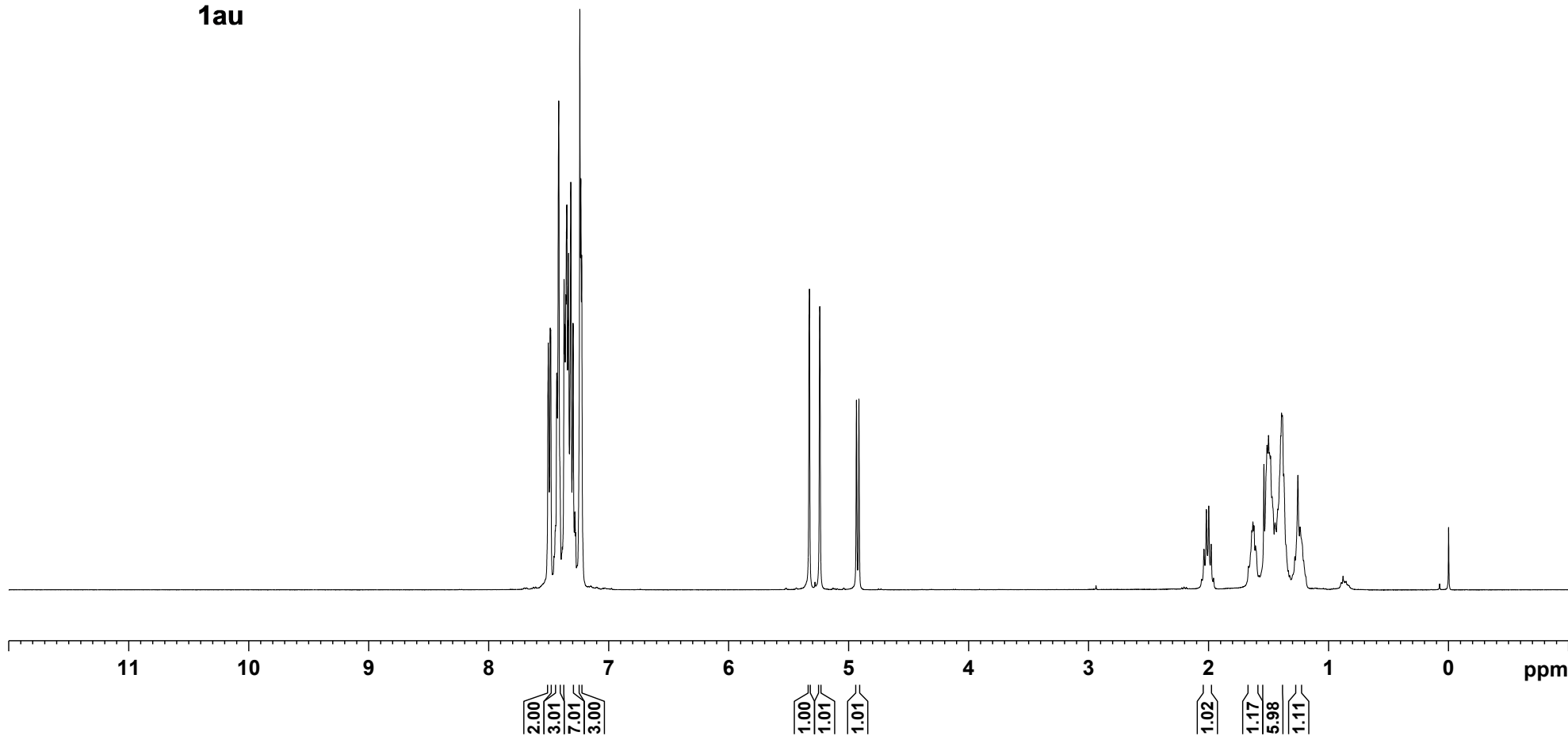
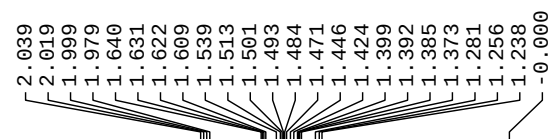
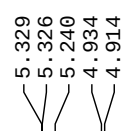
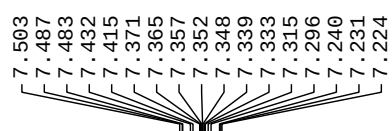


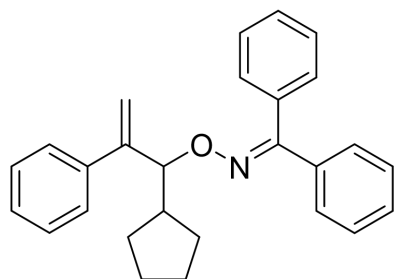
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1au

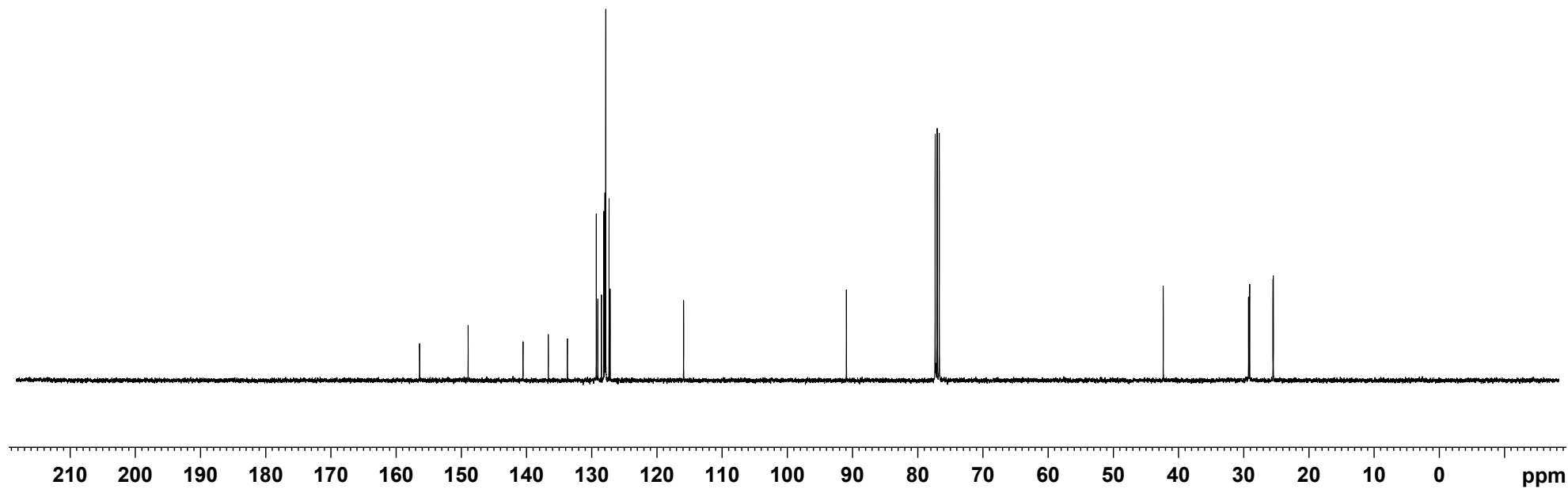
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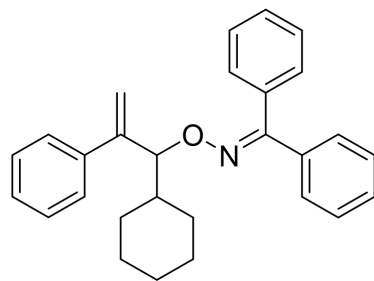
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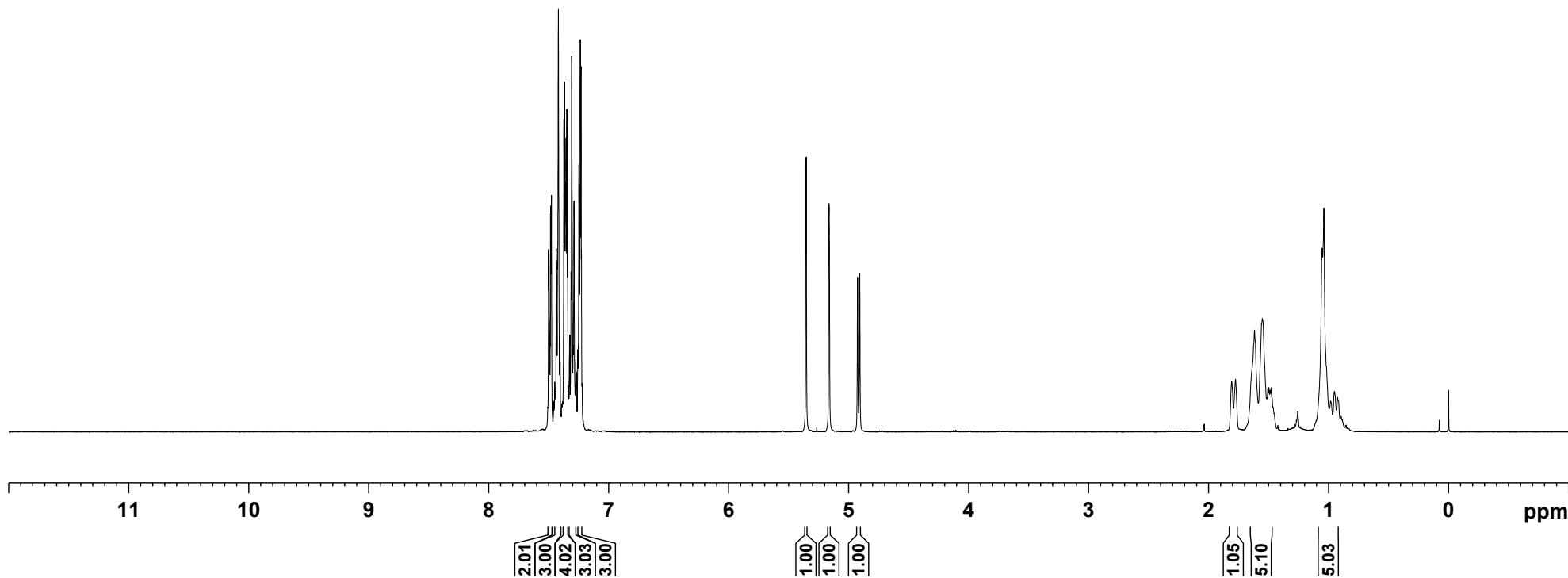


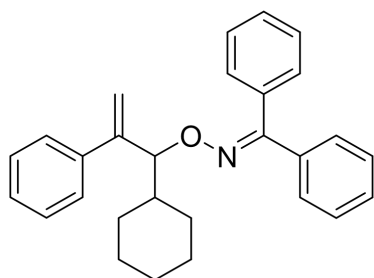


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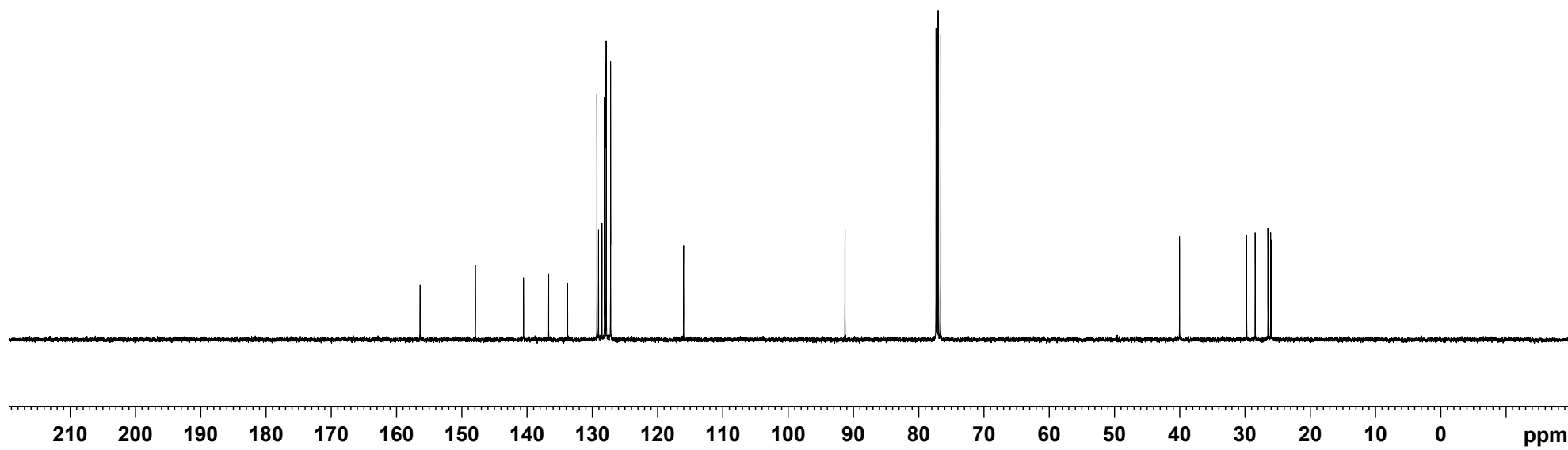
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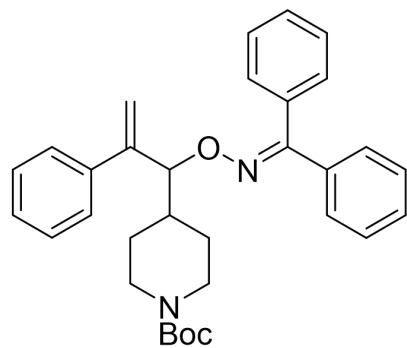
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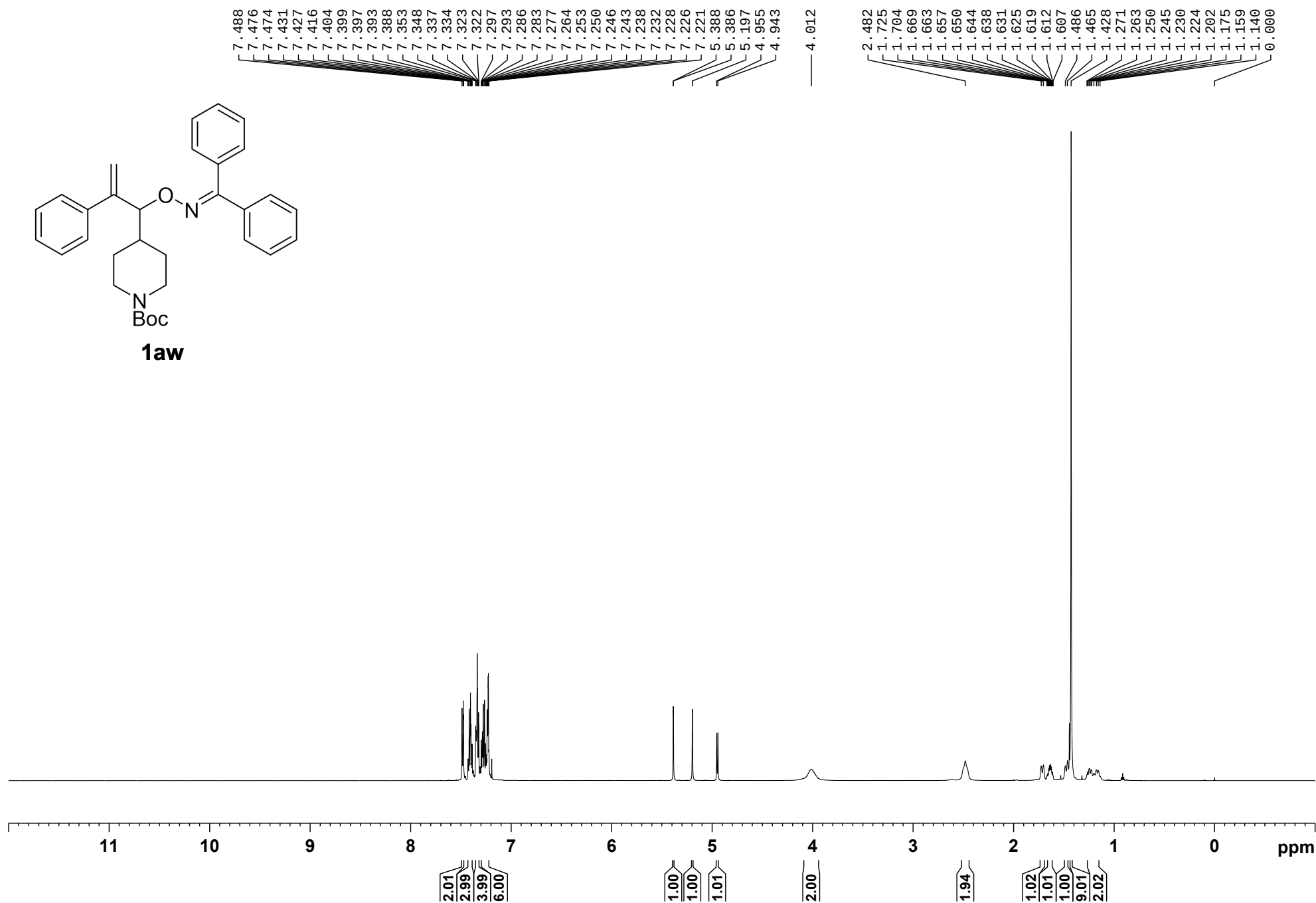
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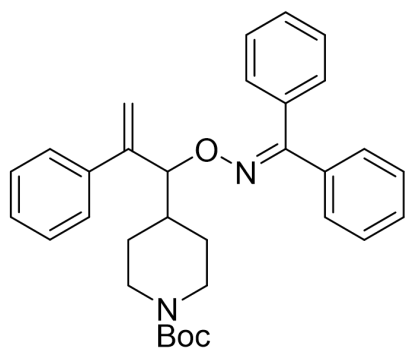
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1aw





1aw

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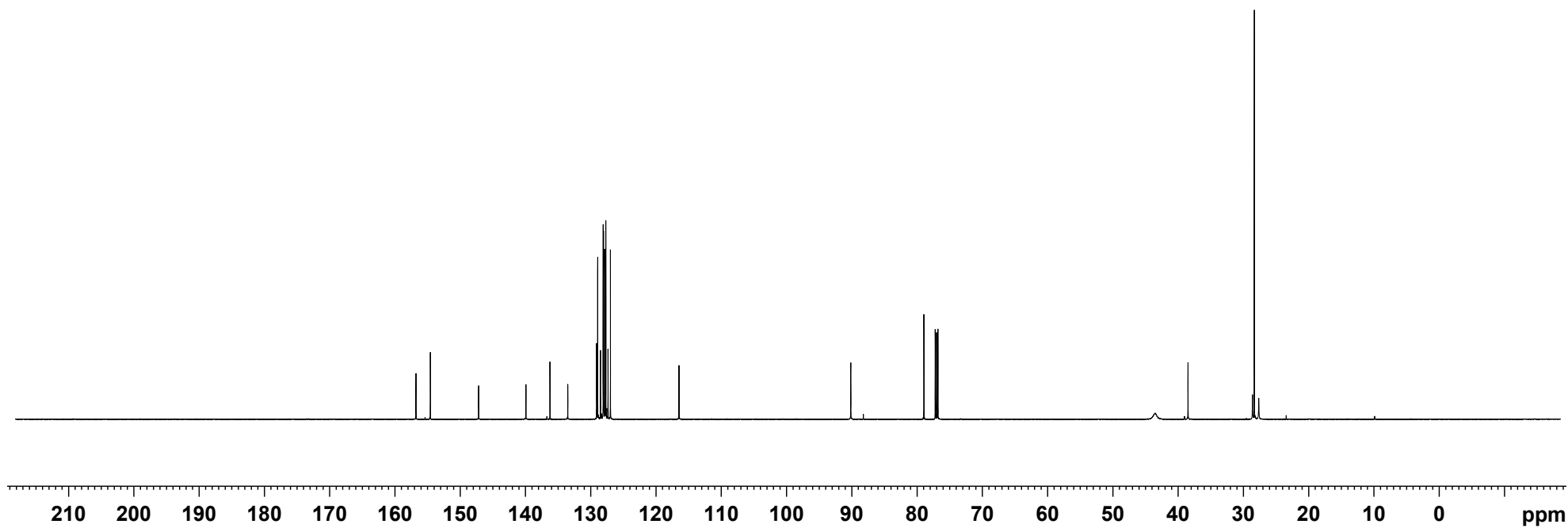
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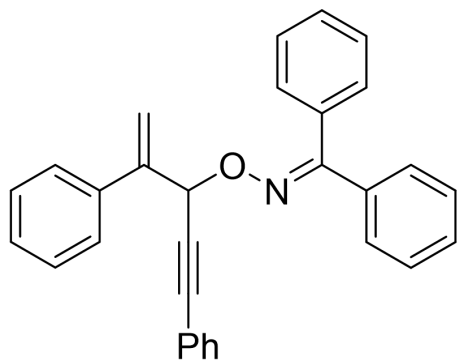
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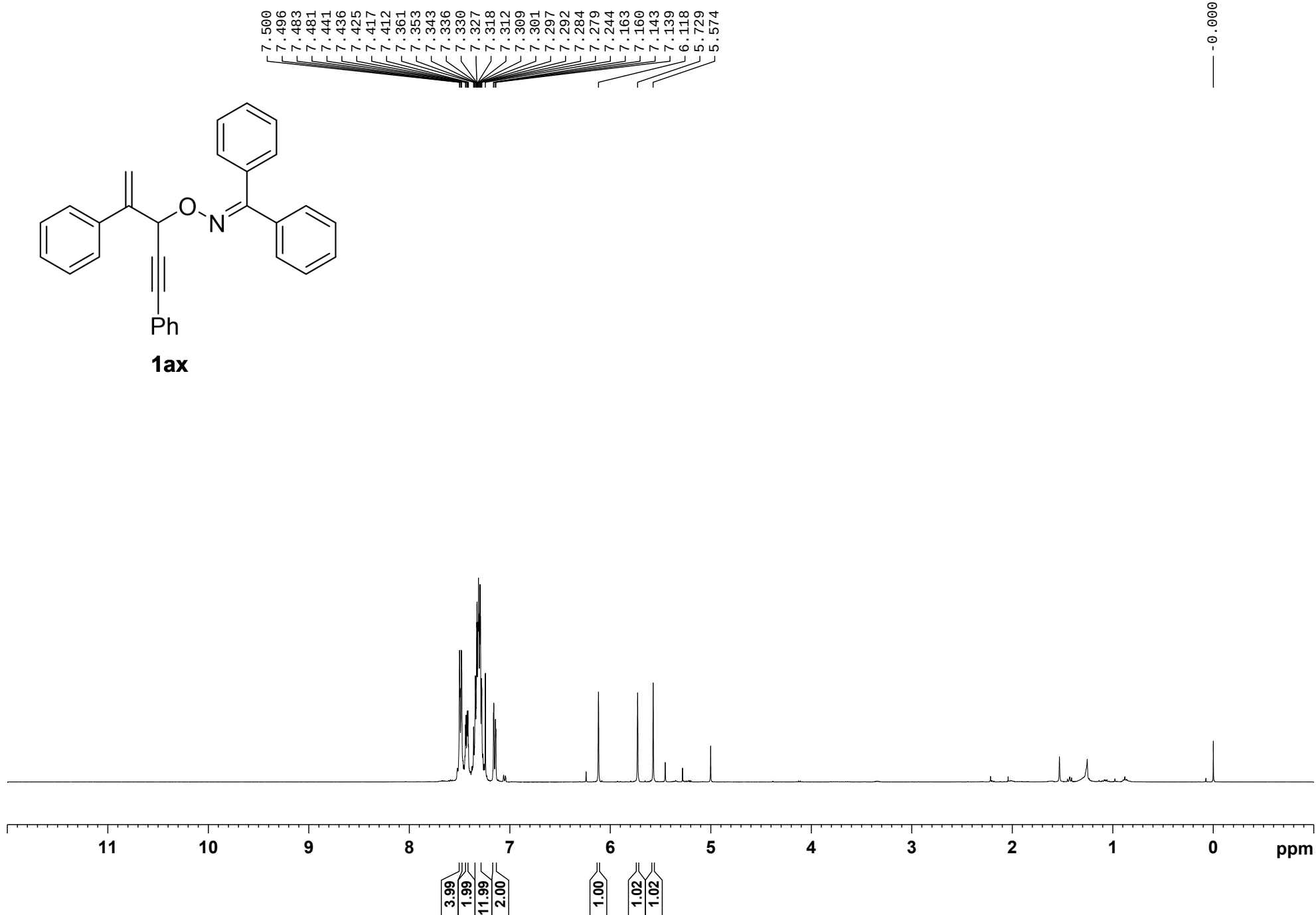
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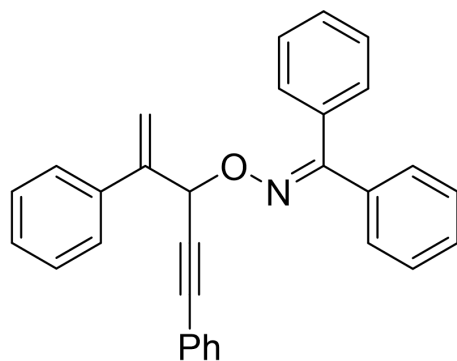
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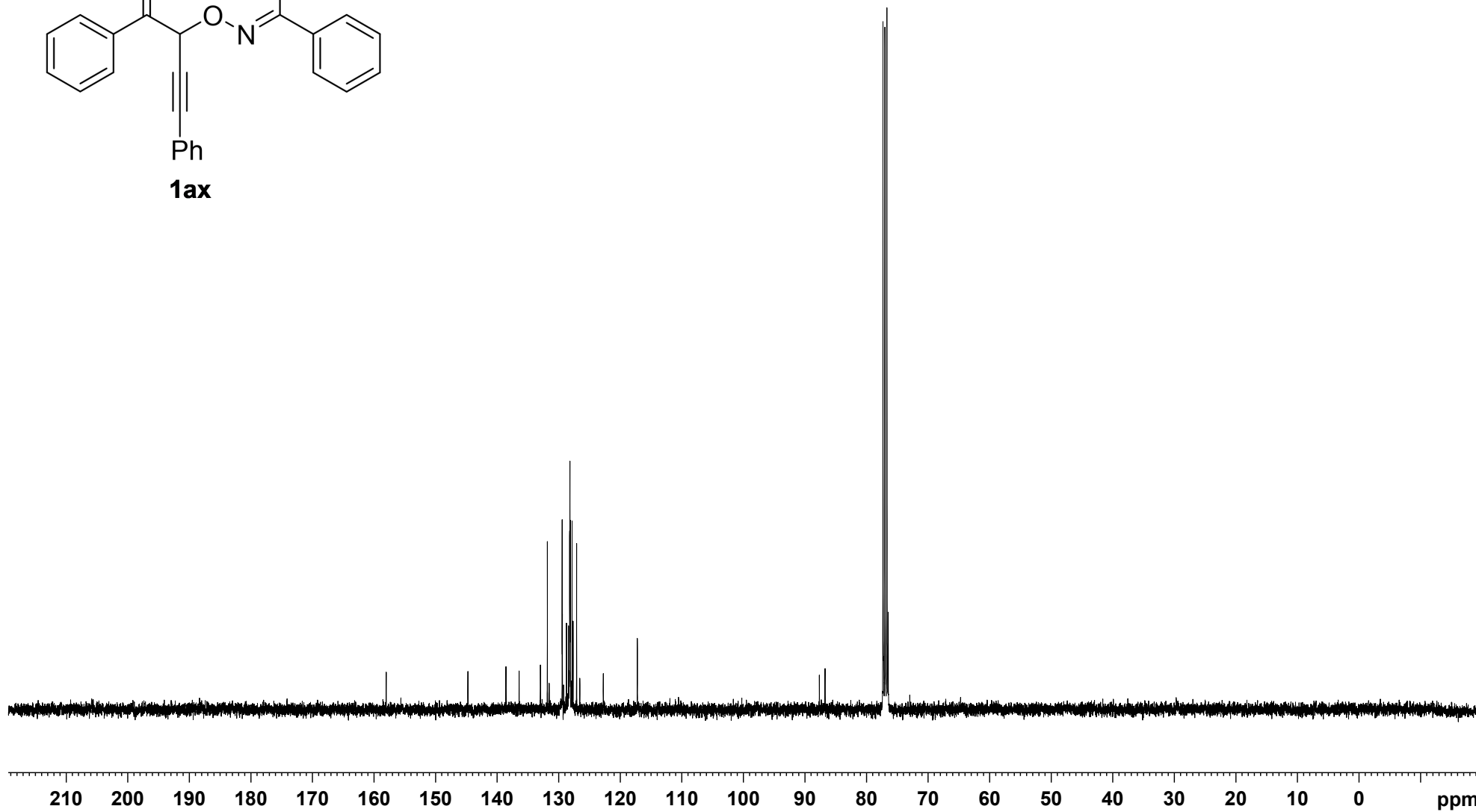
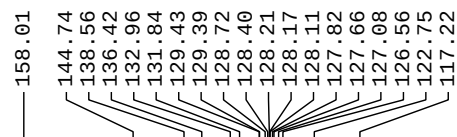


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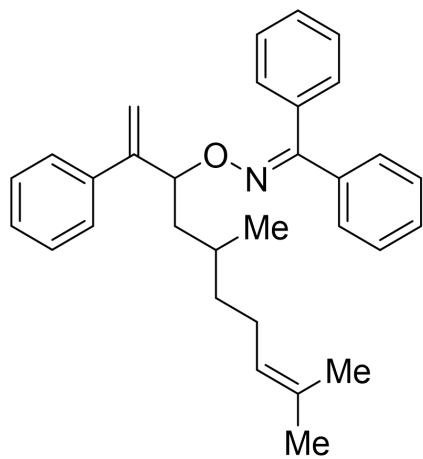




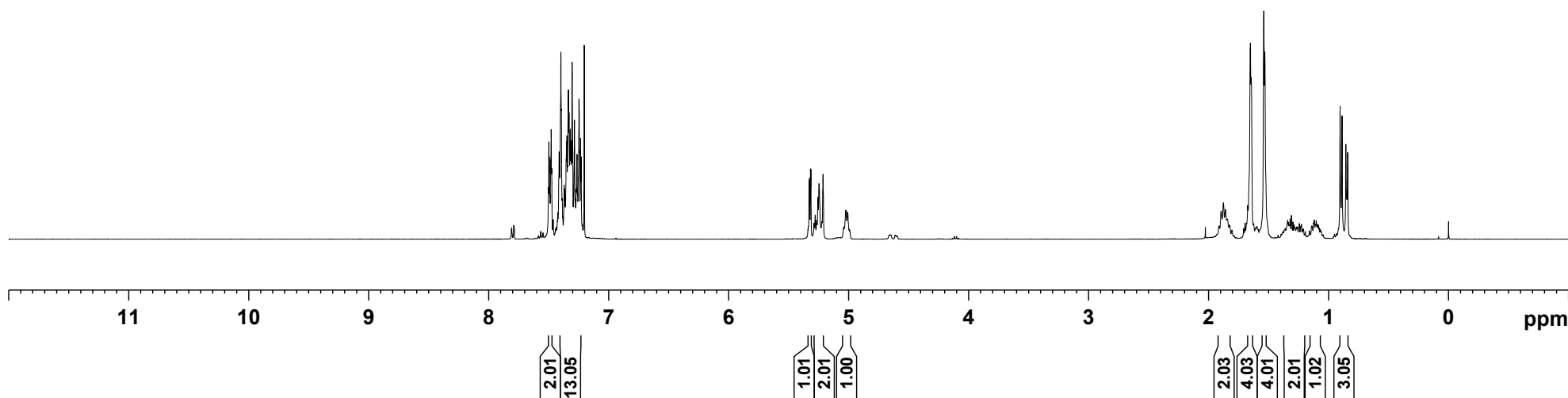
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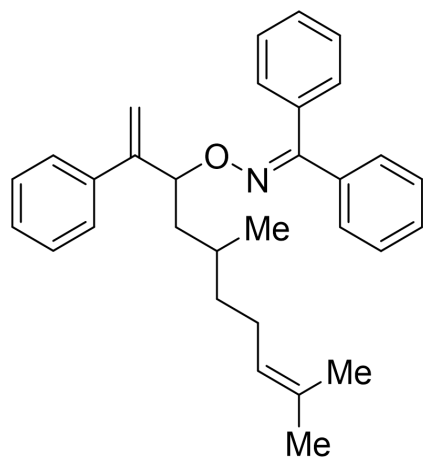


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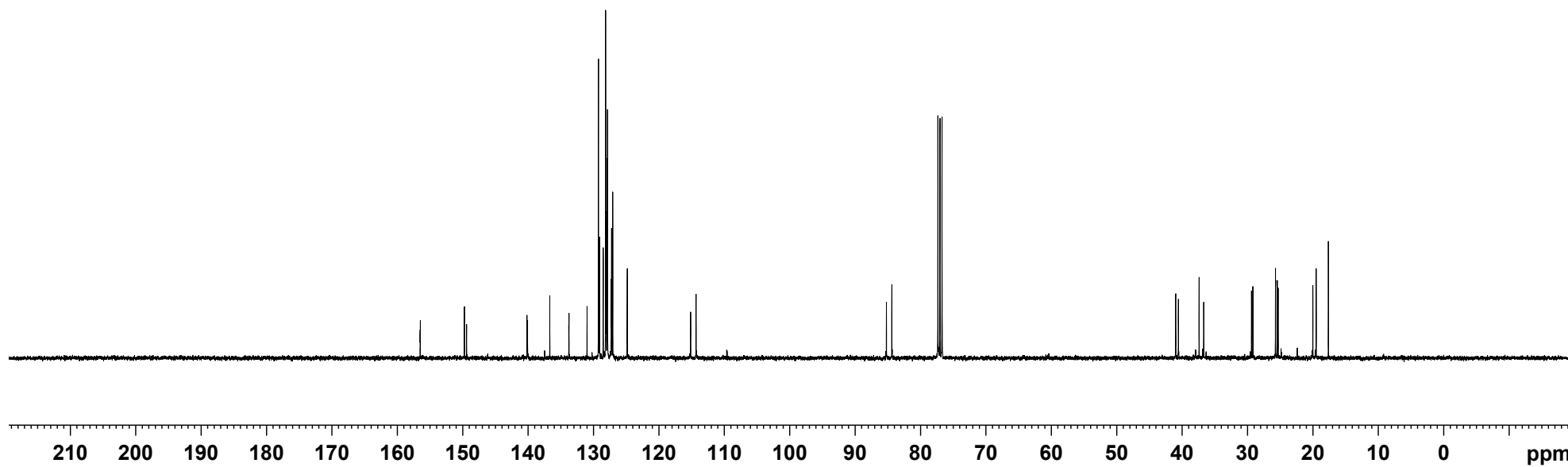


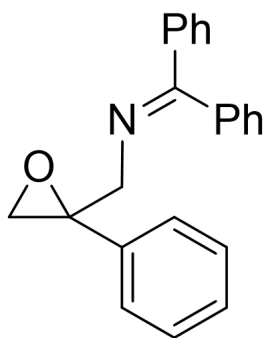
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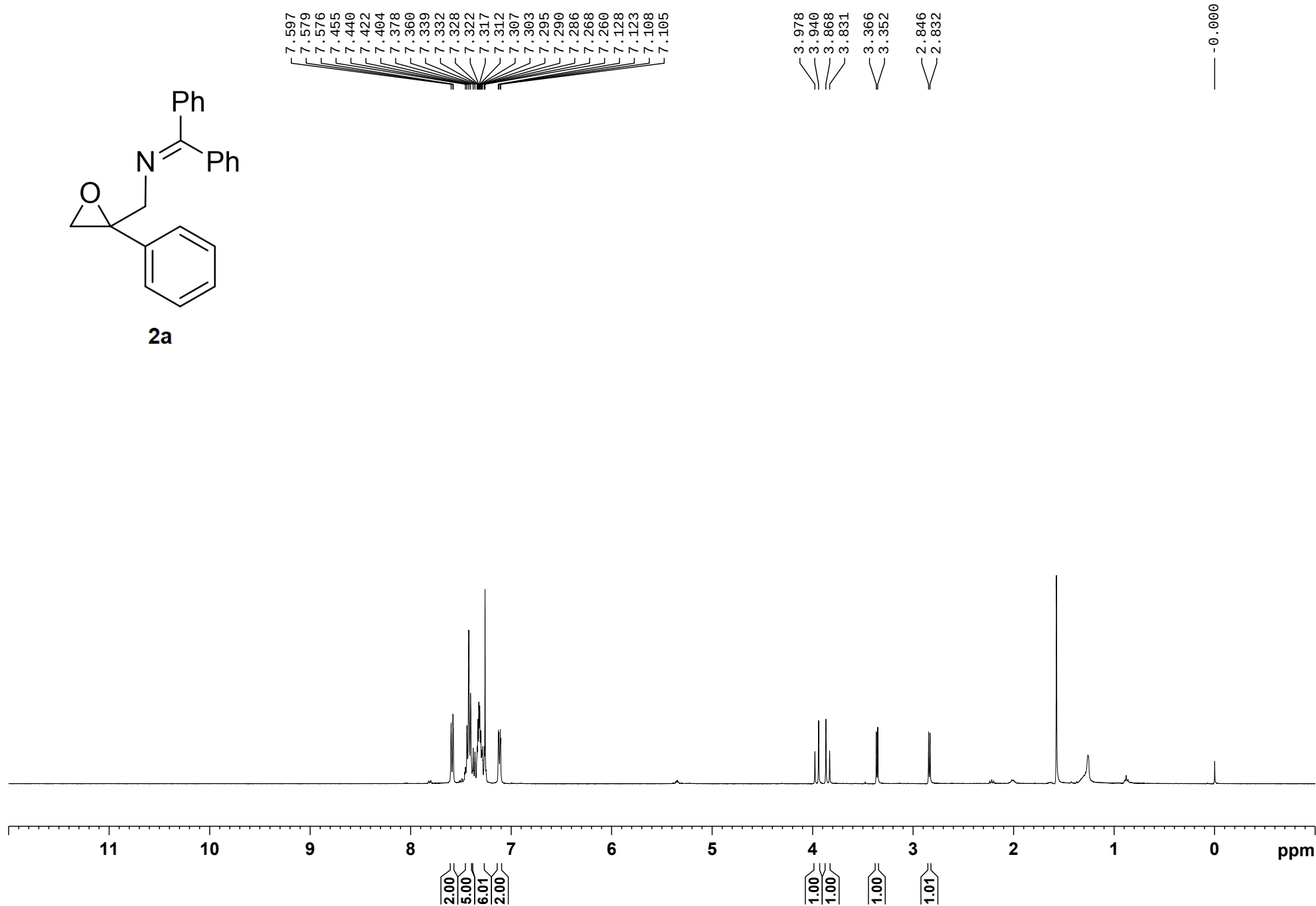
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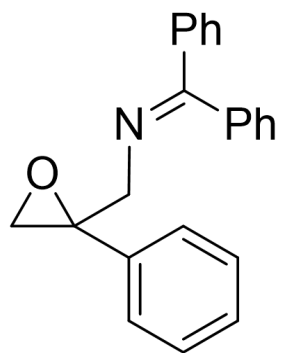
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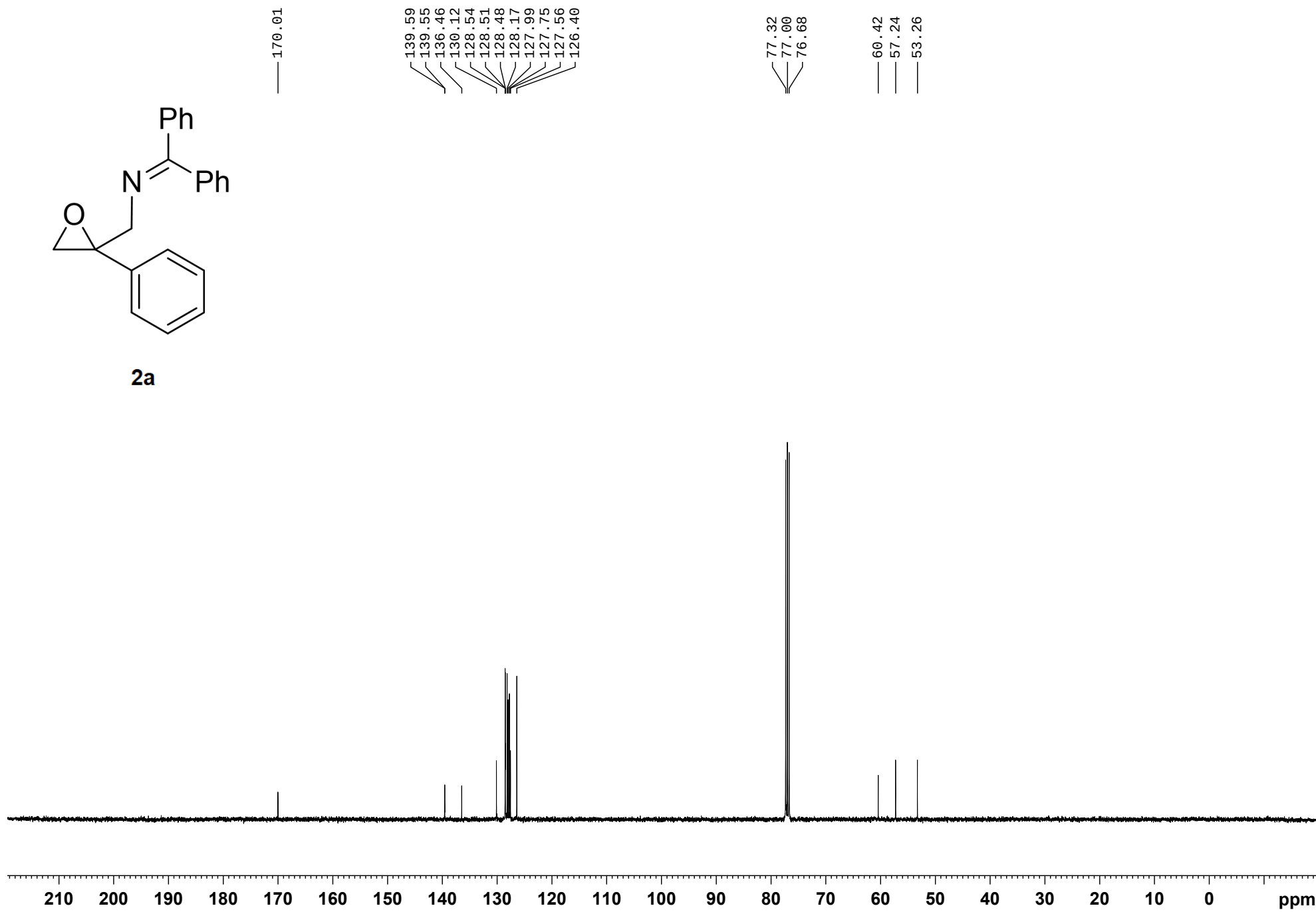


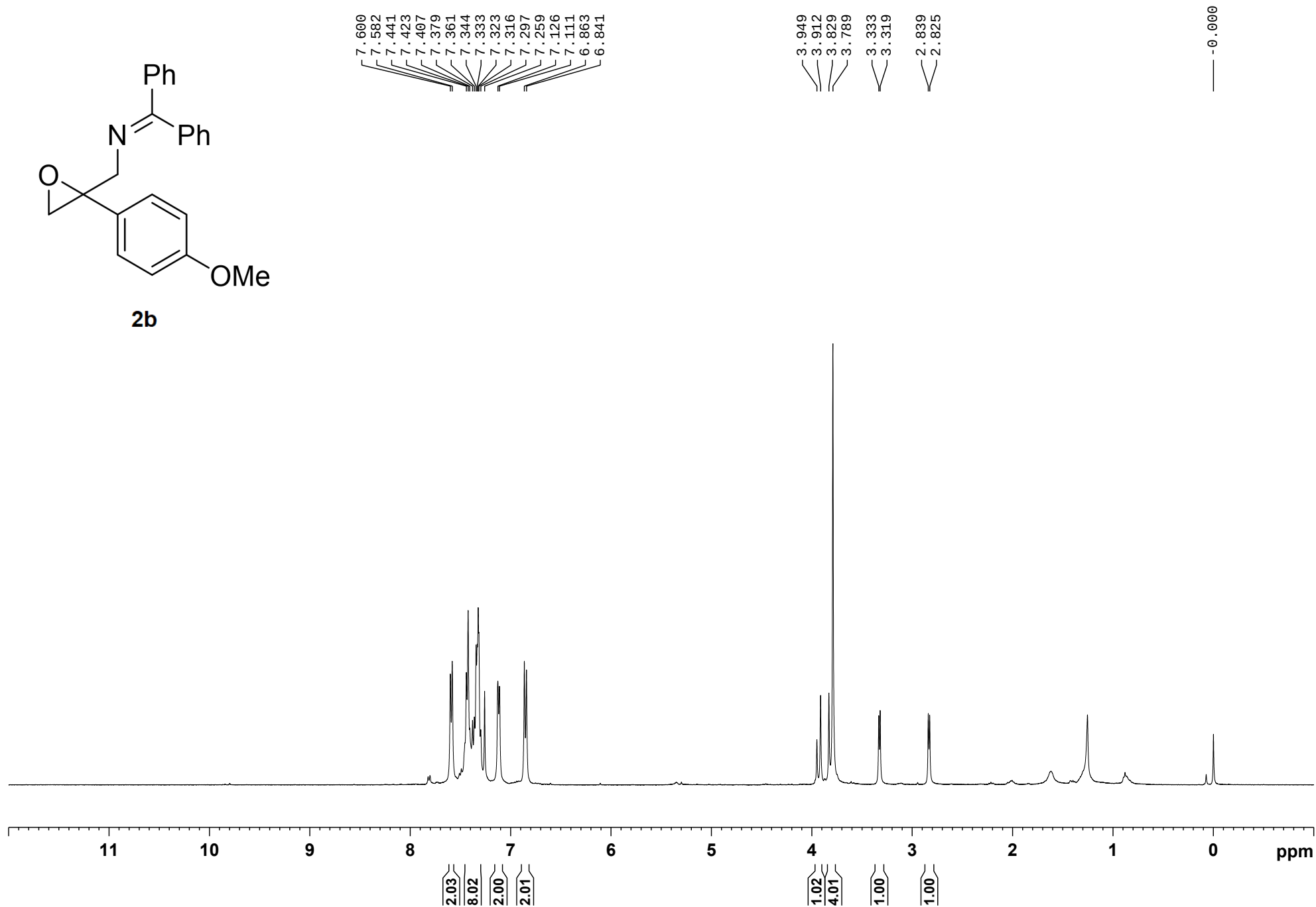
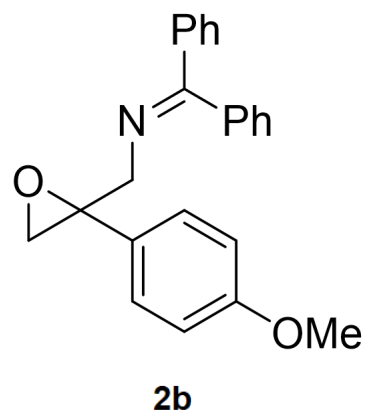
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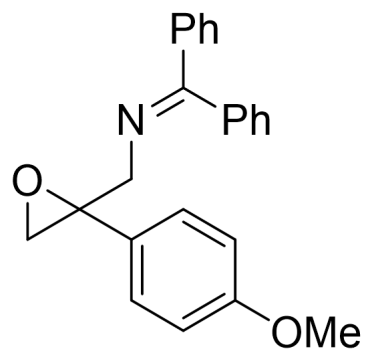




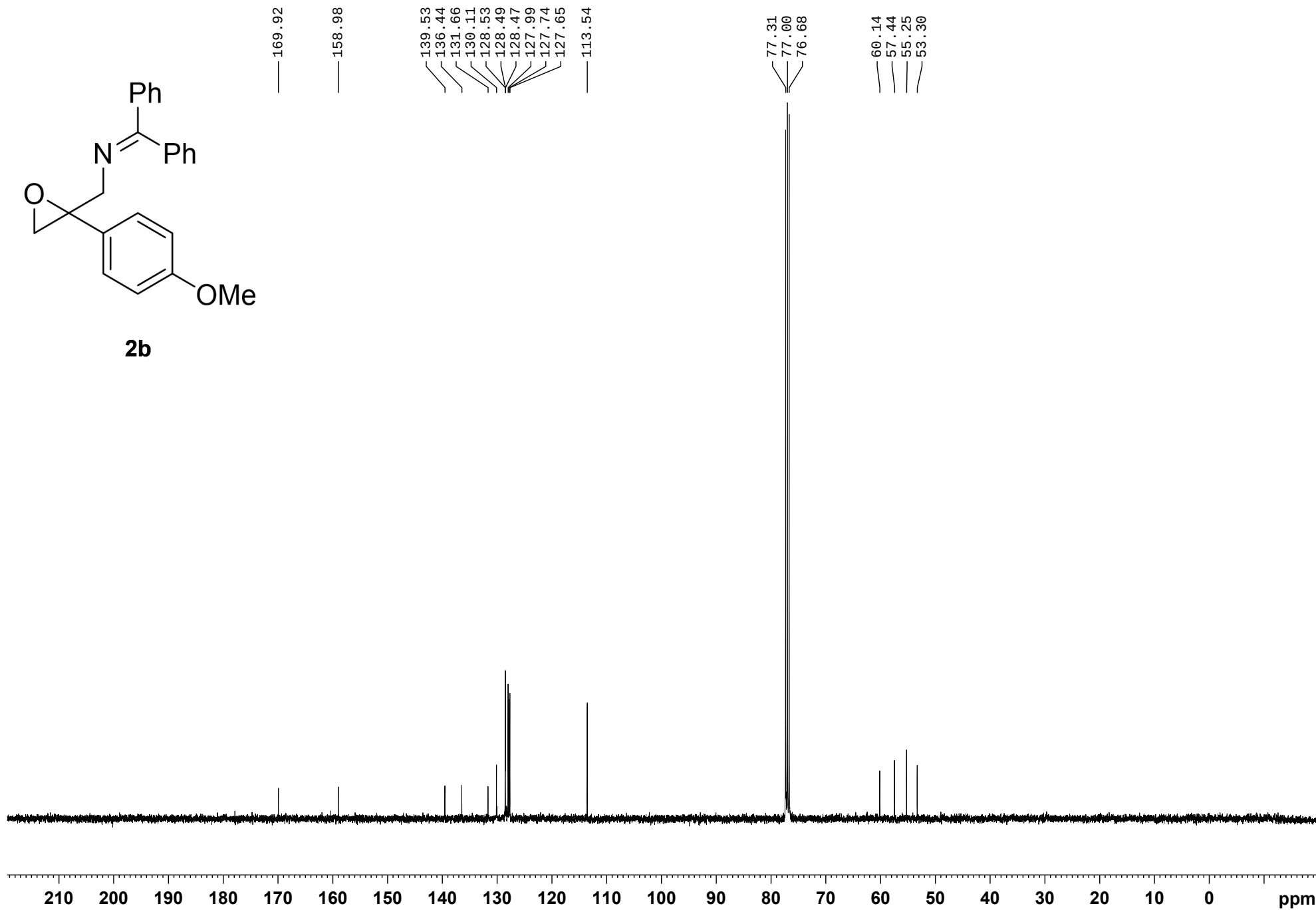
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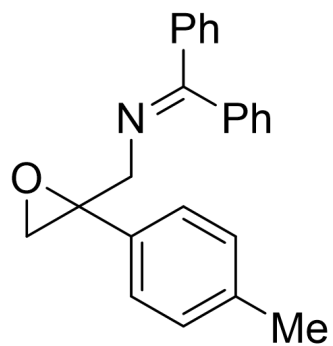




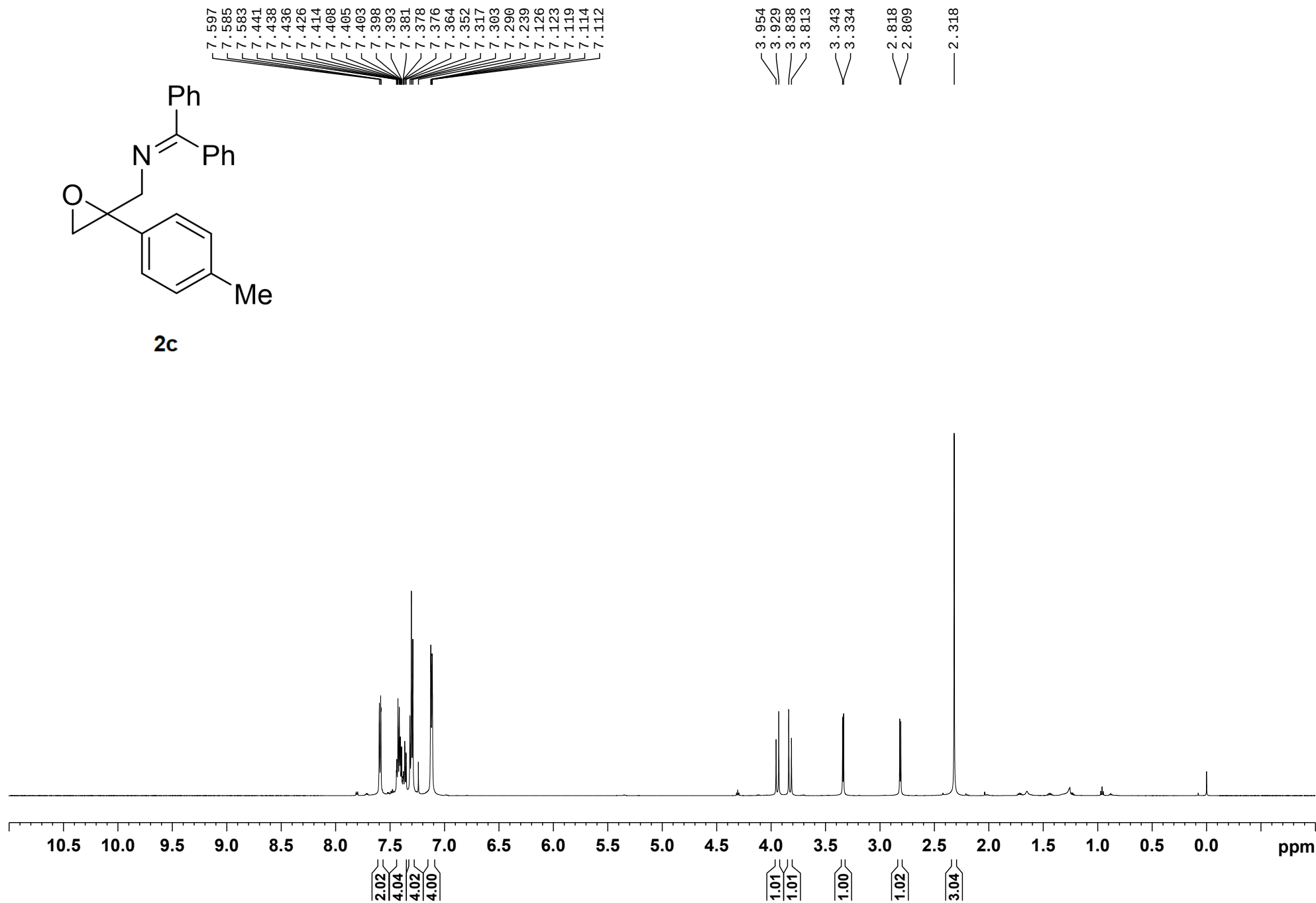


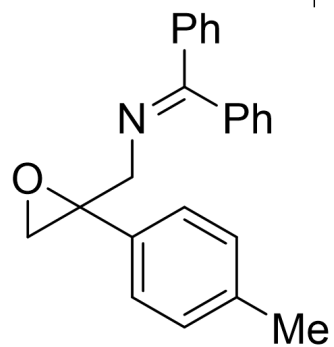
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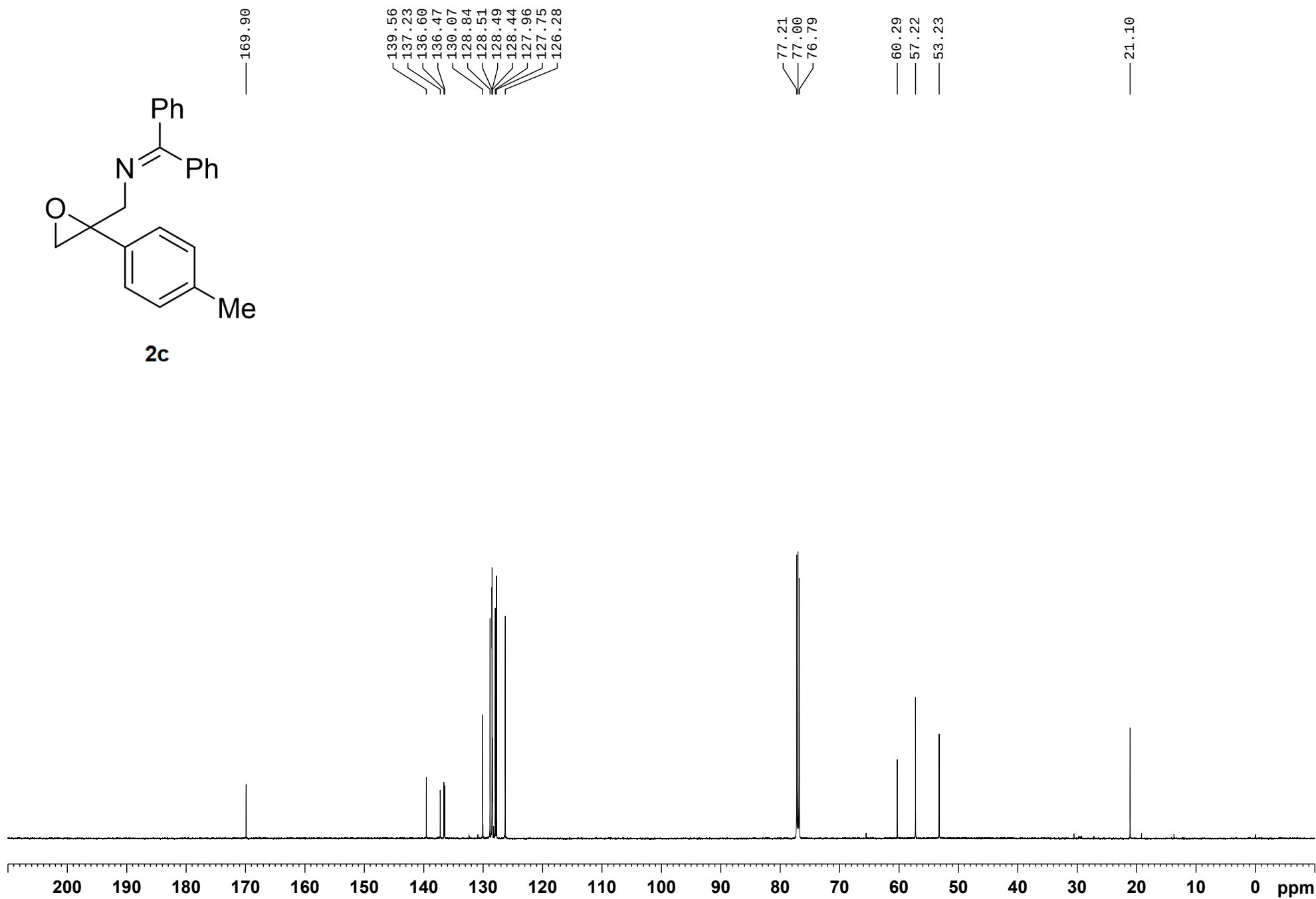


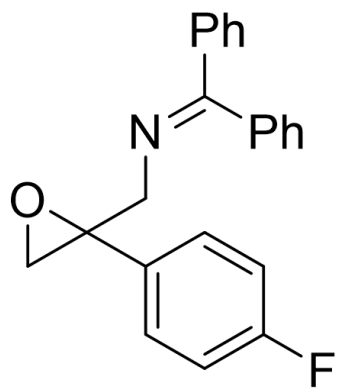
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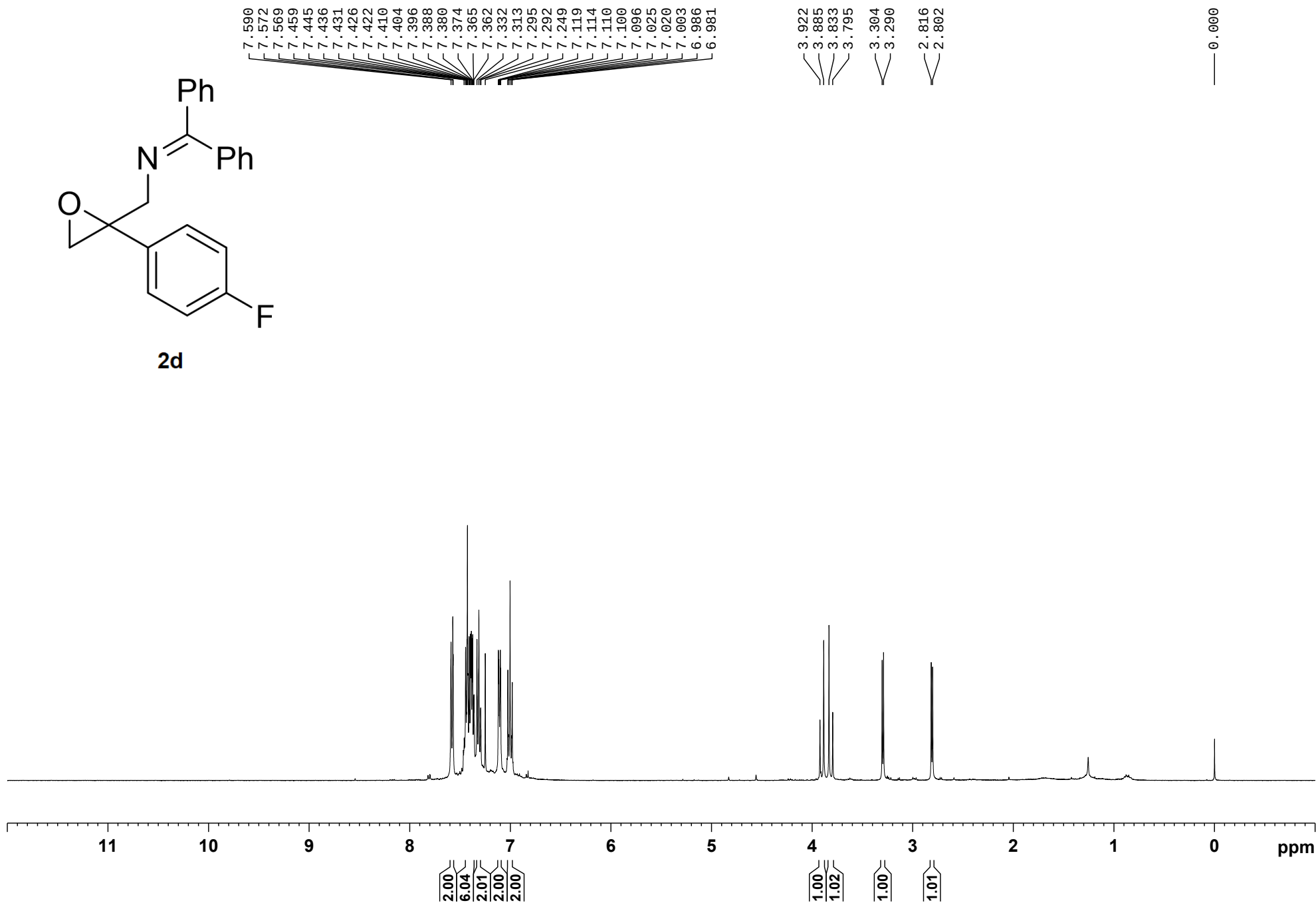


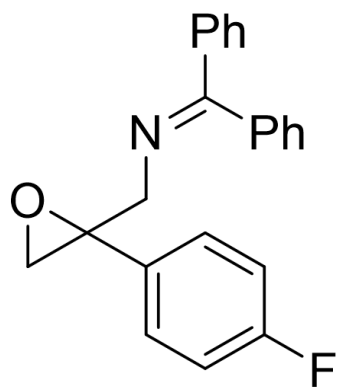
2c





2d





2d

— 170.11

— 163.39

— 160.94

139.39

136.32

135.34

135.31

130.21

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128.23

128.15

128.02

127.68

115.13

114.92

77.32

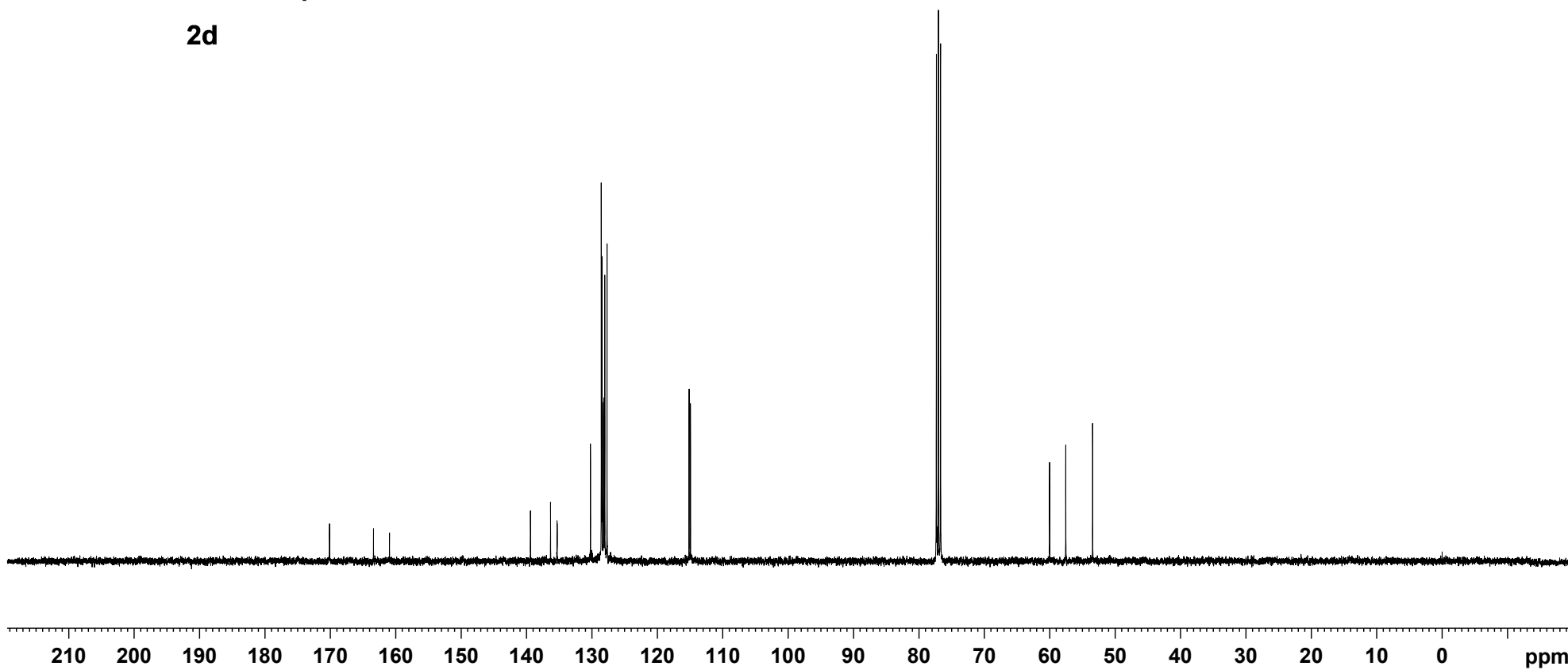
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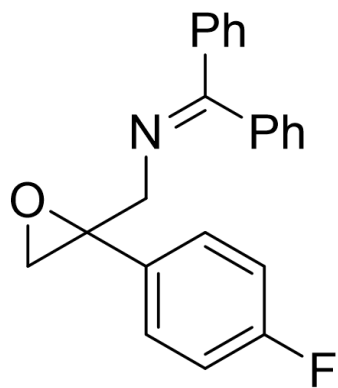
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60.01

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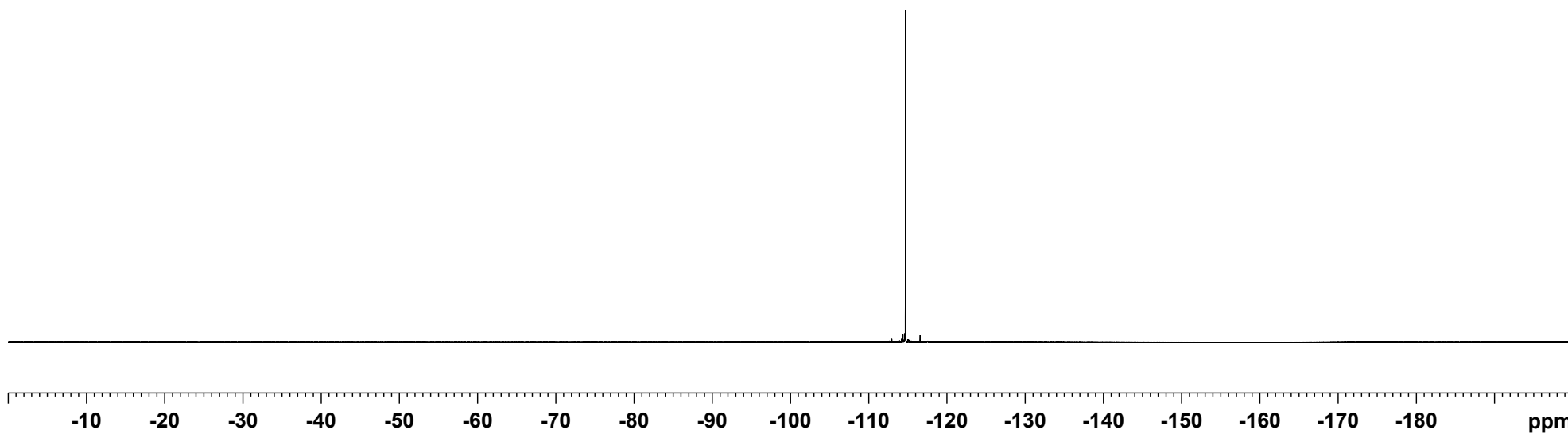
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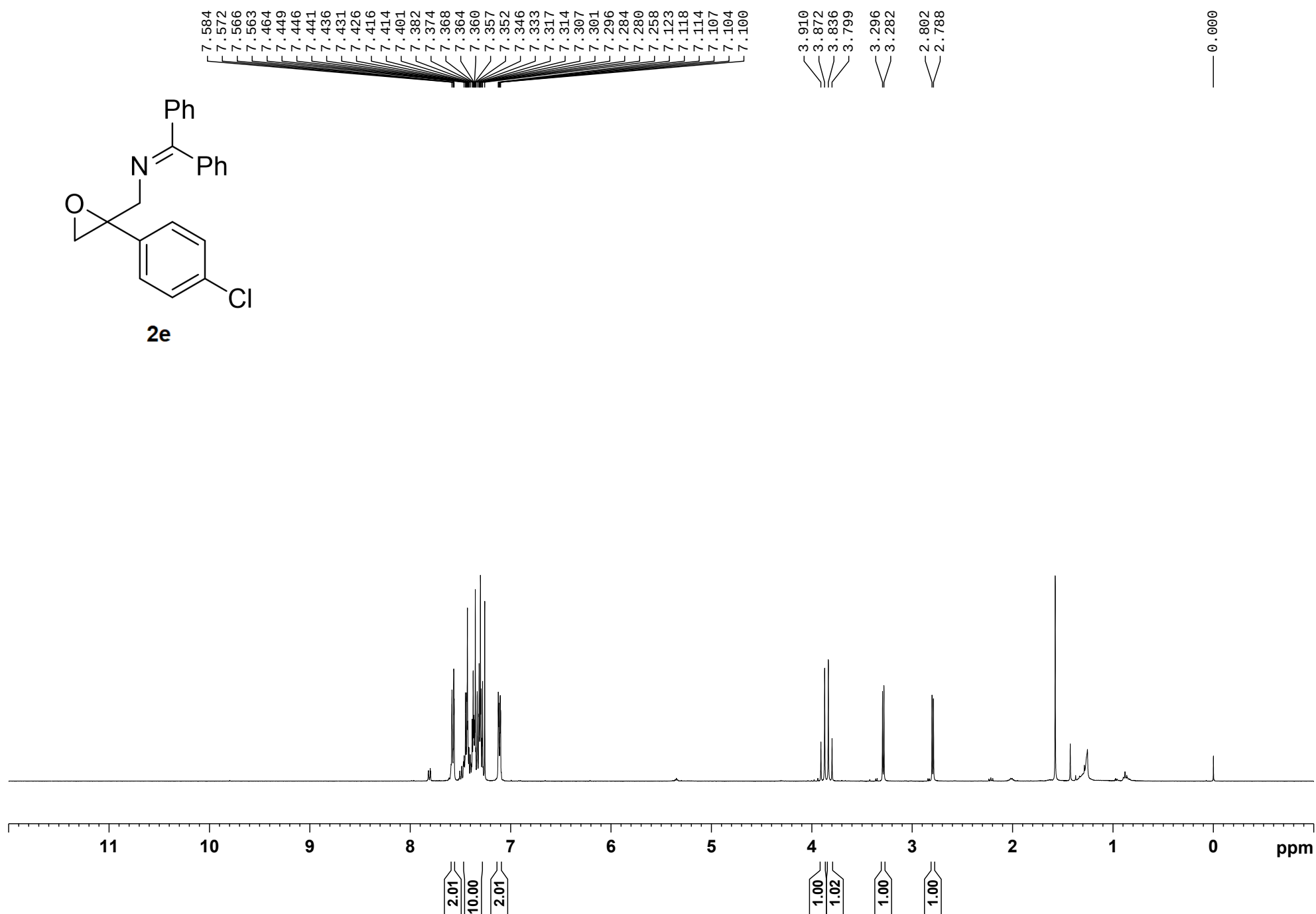


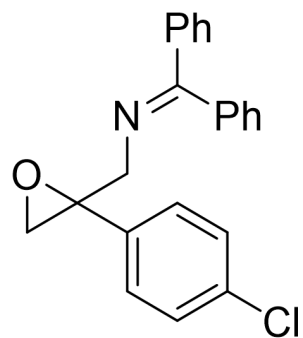


2d

— -114.668







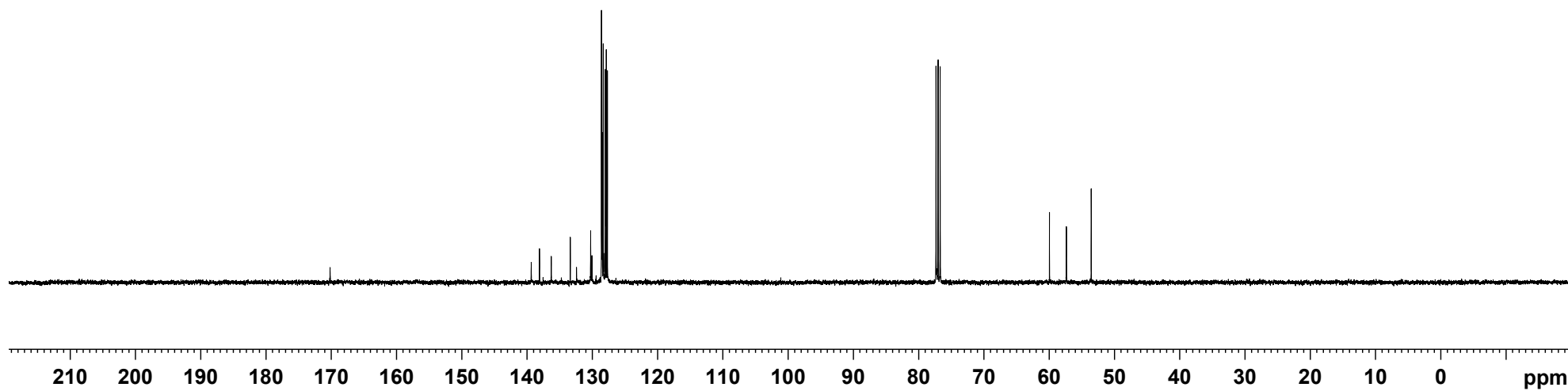
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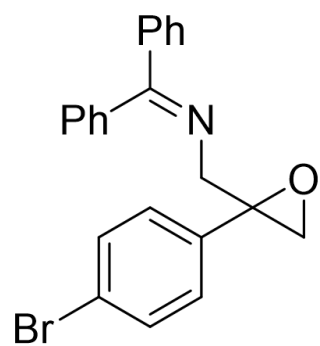
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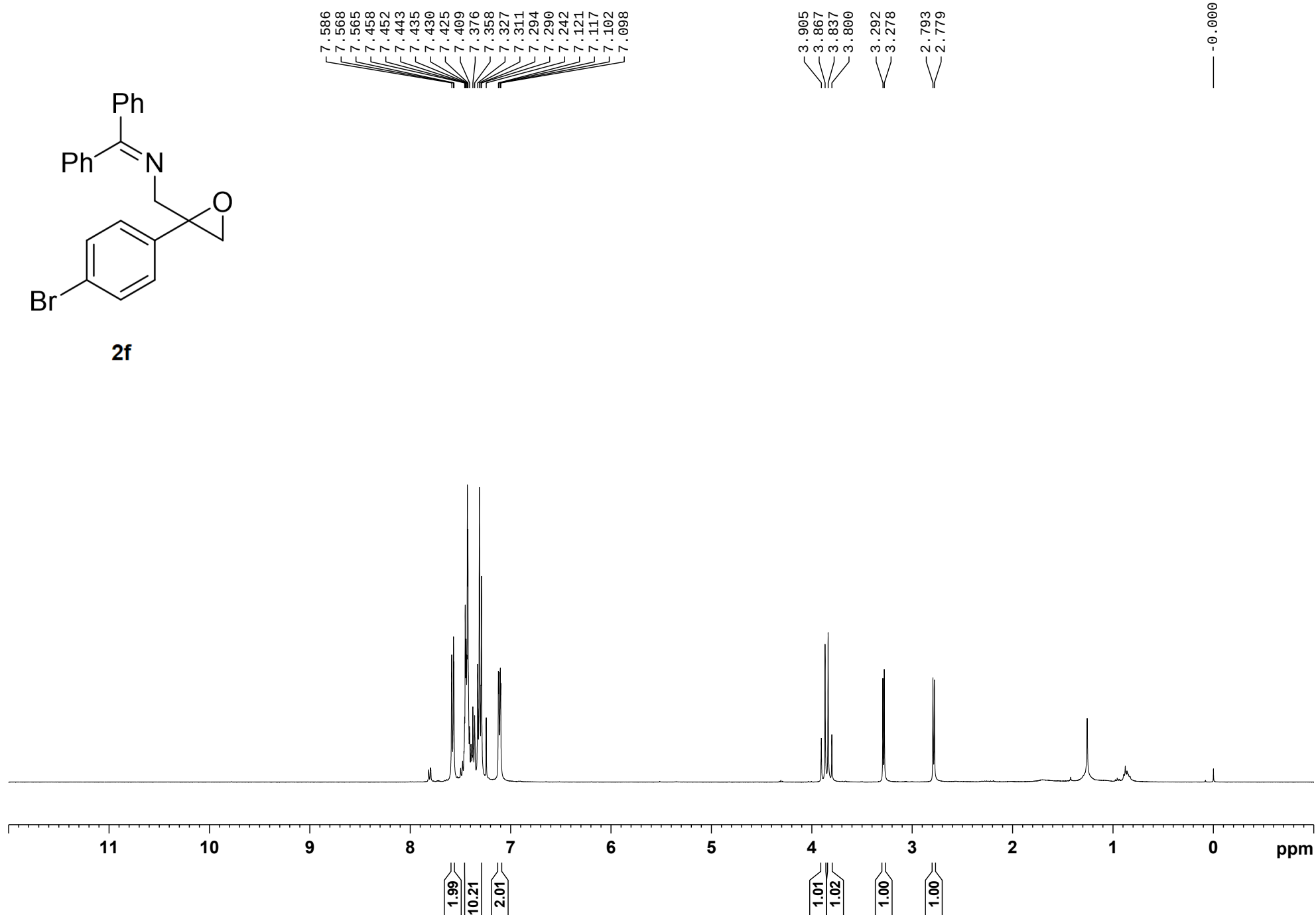
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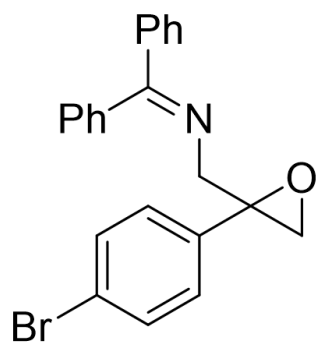
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2f





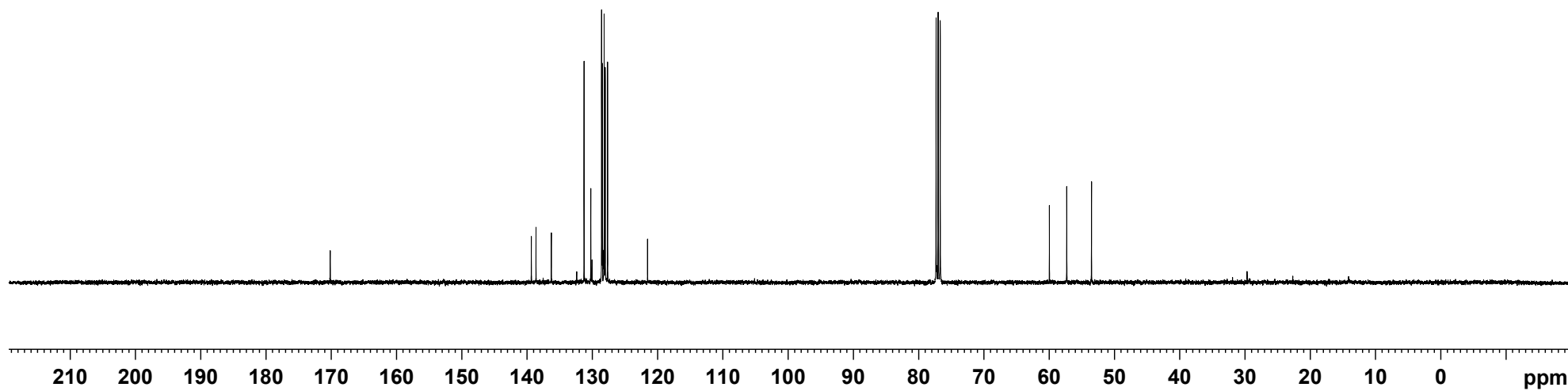
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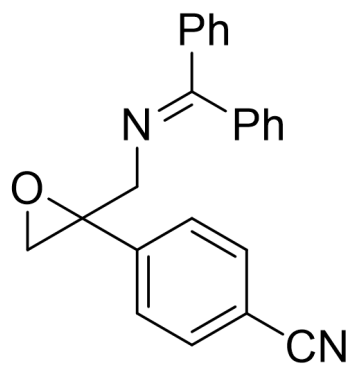
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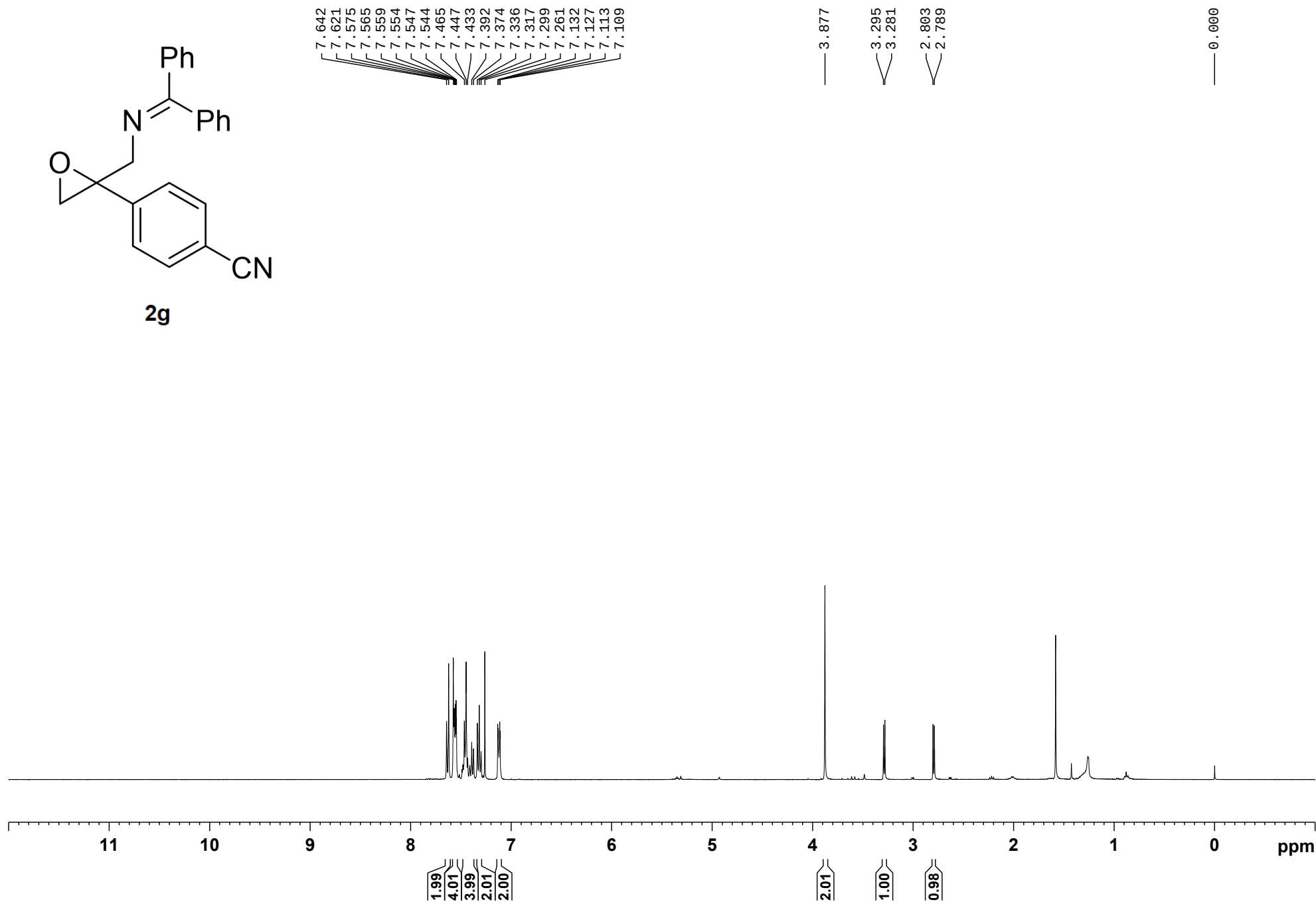
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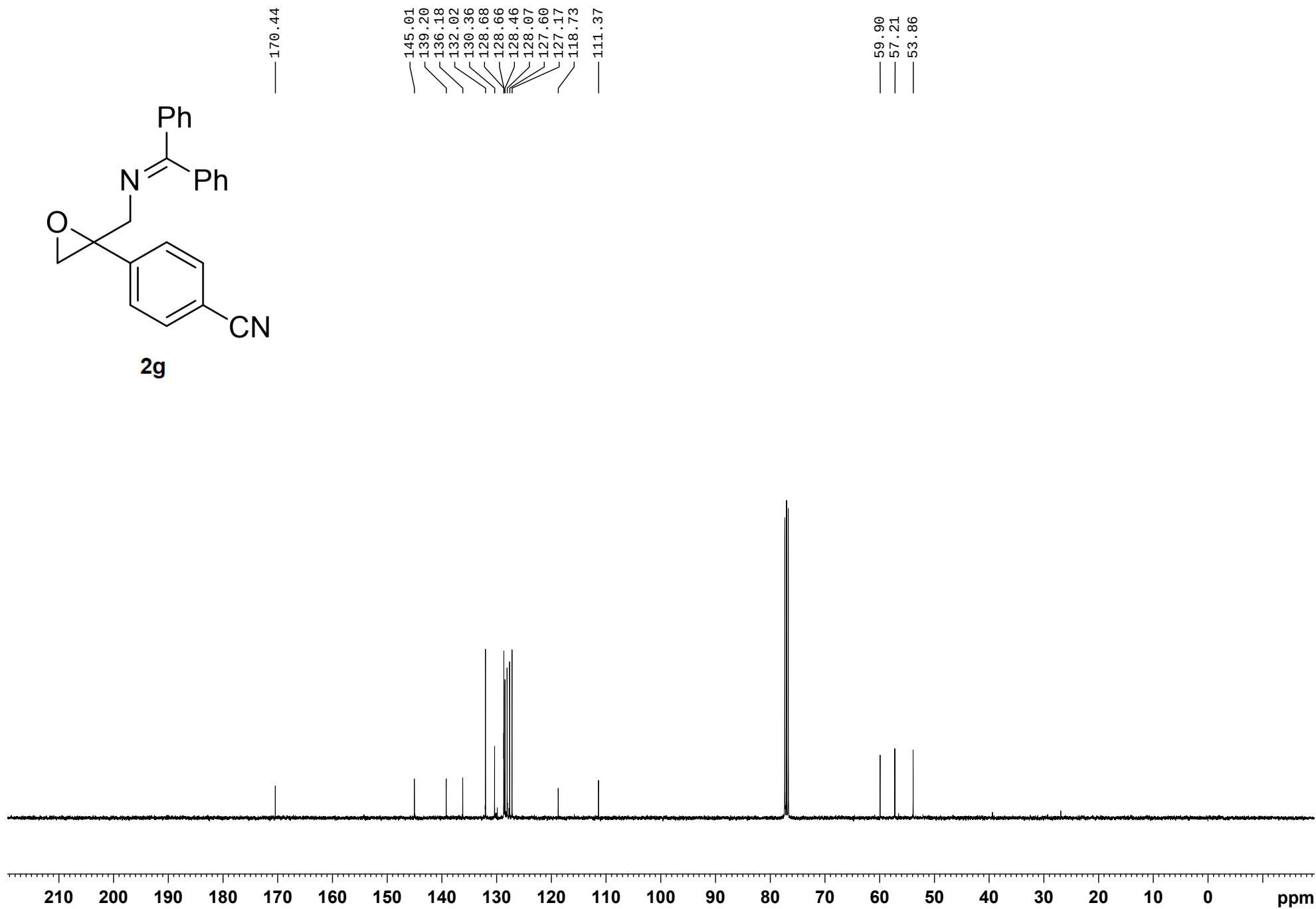
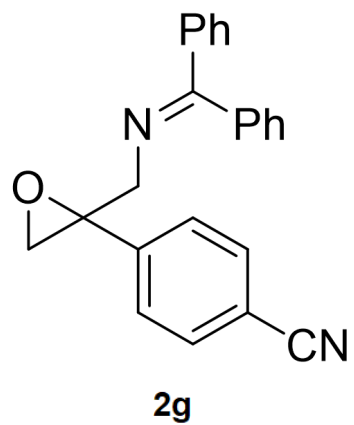
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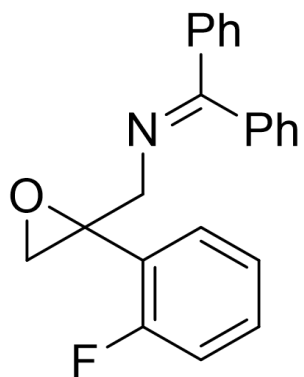




2g





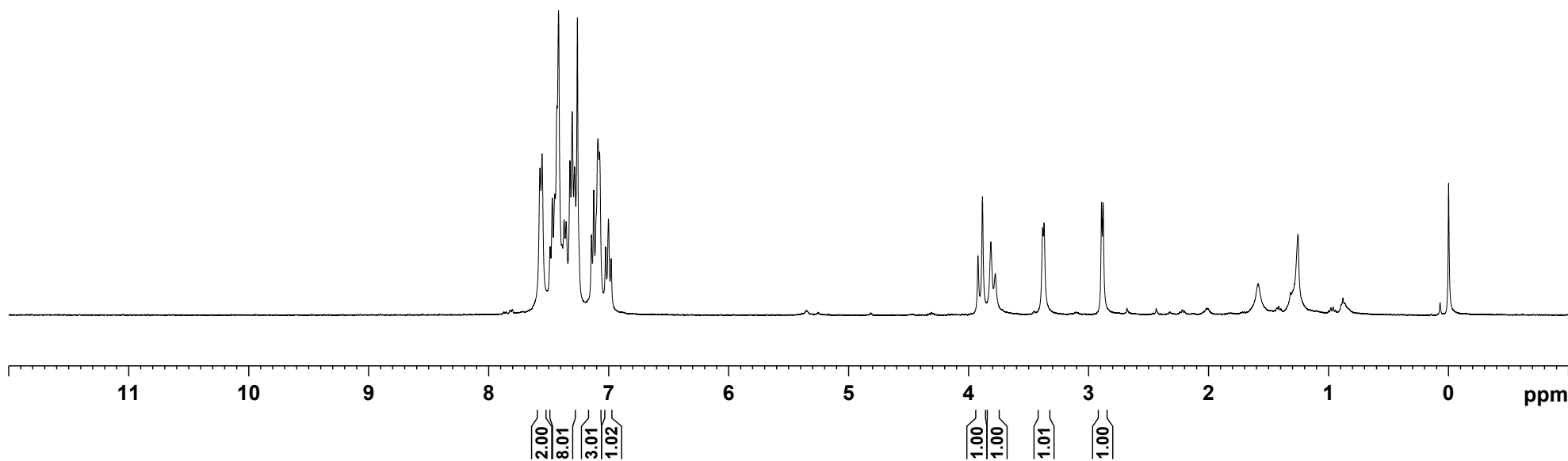


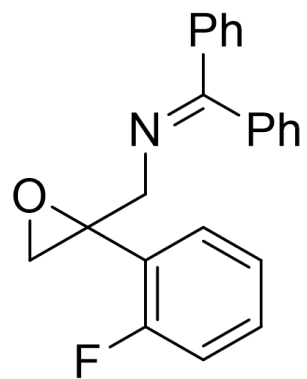
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6.979

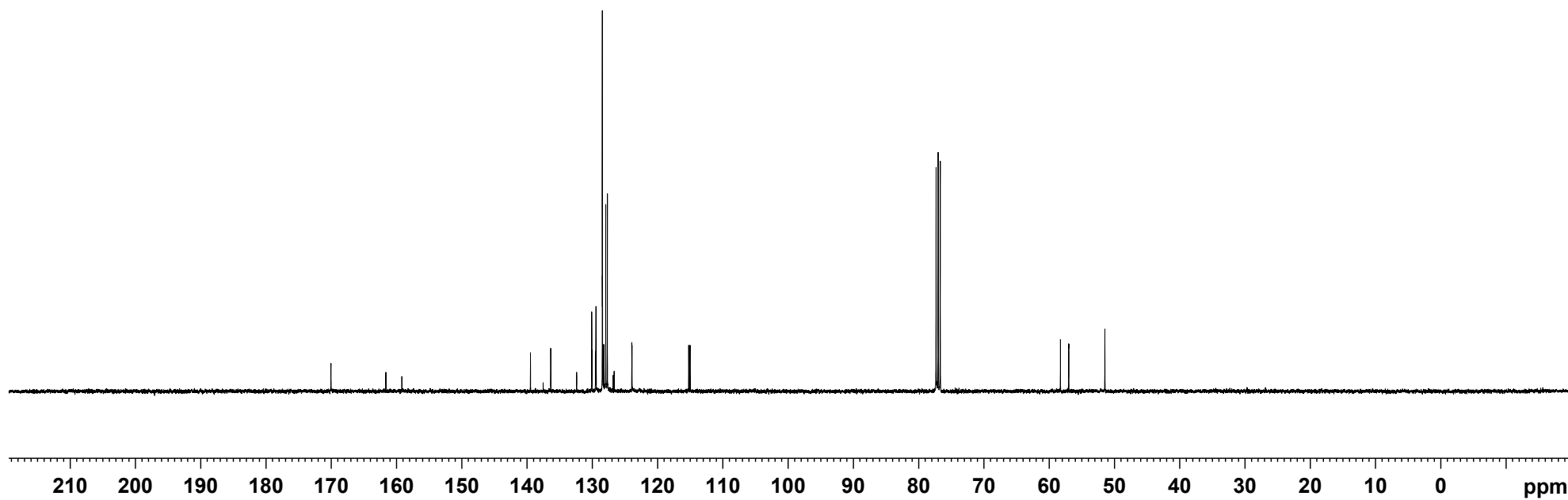
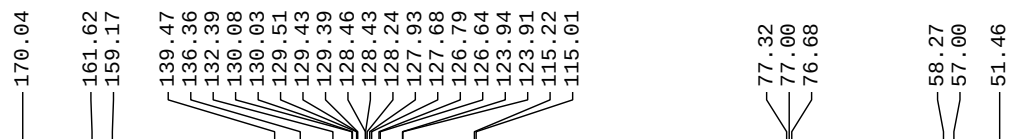
3.921
3.884
3.814
3.777
3.382
3.370
2.891
2.878

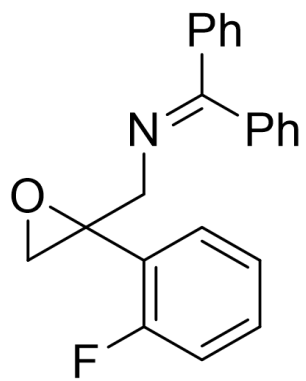
— 0.000





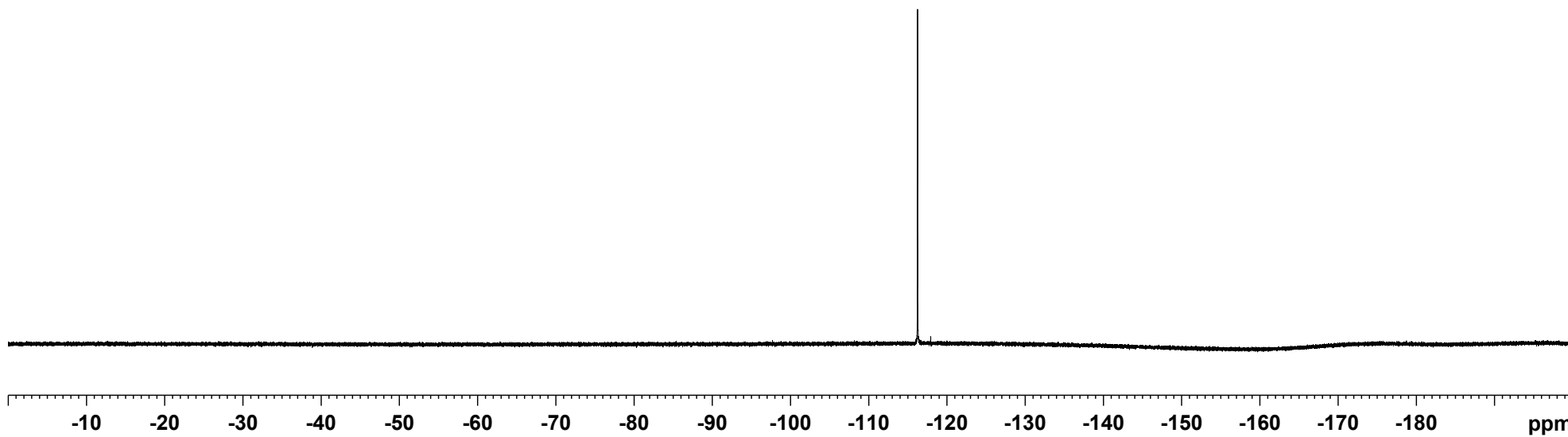
2h

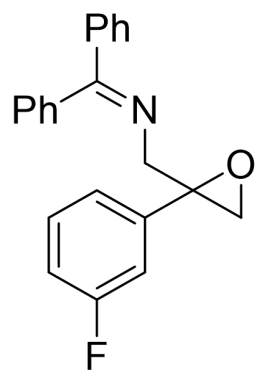




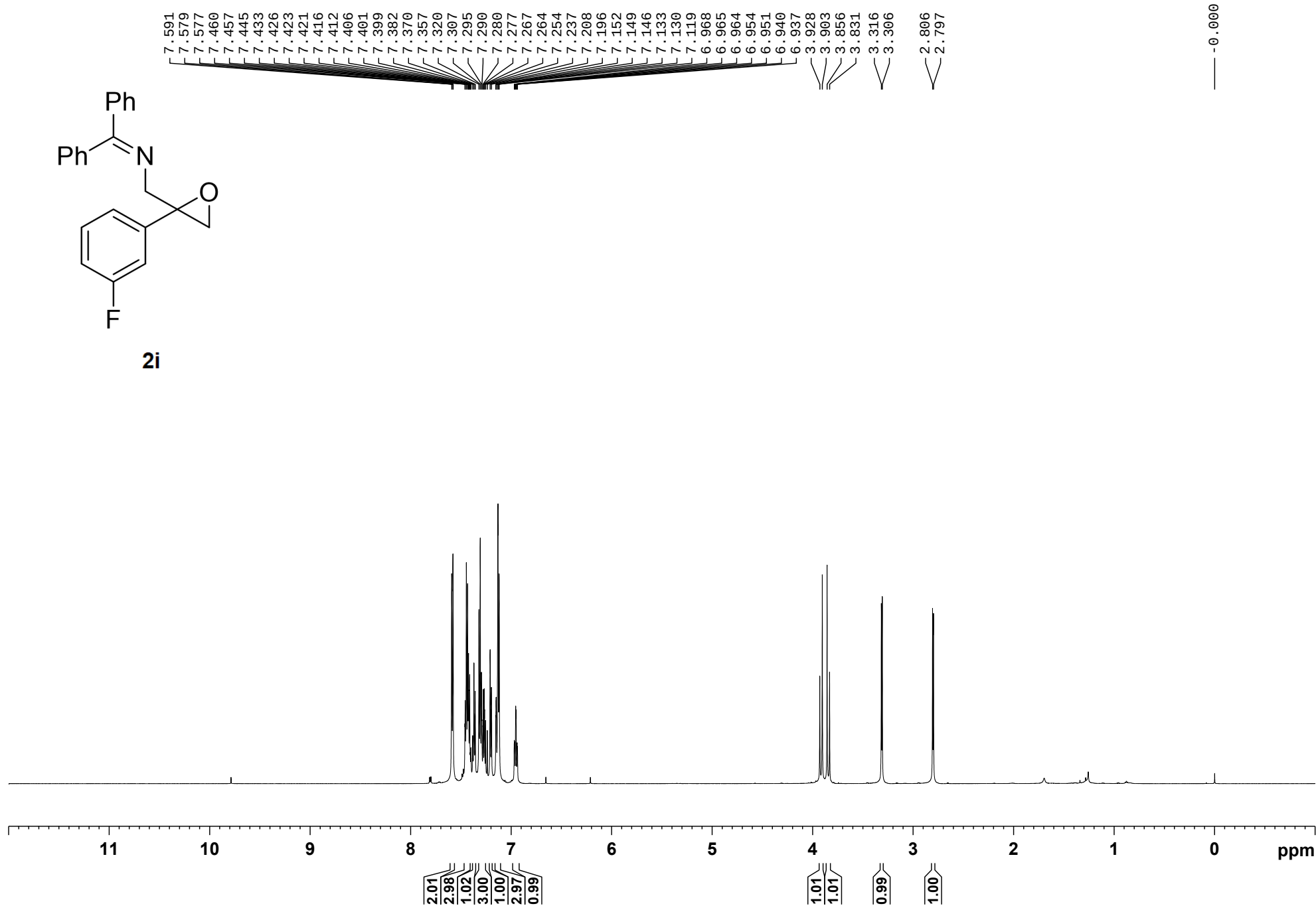
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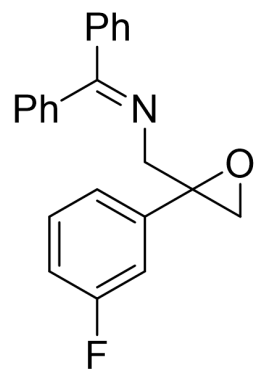
— -116.231



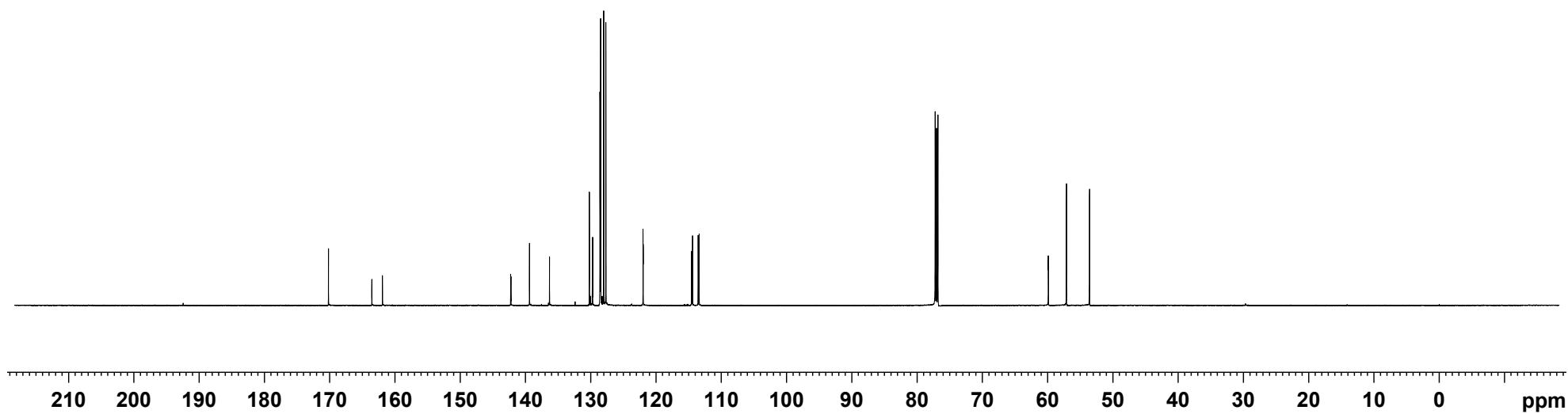
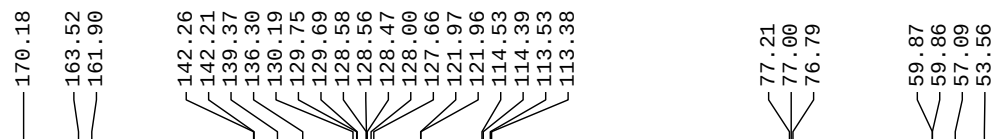


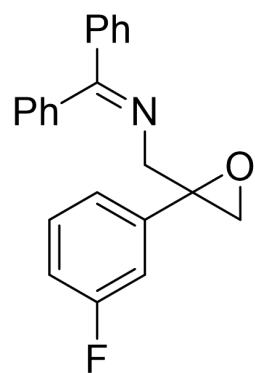
2i





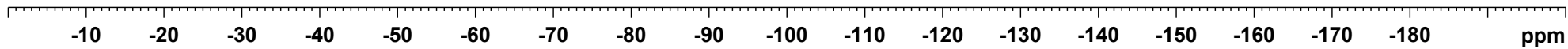
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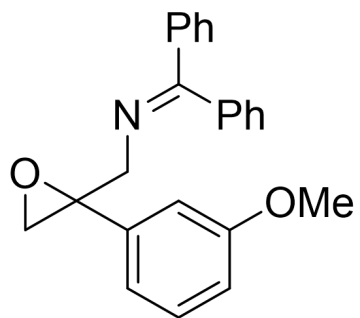




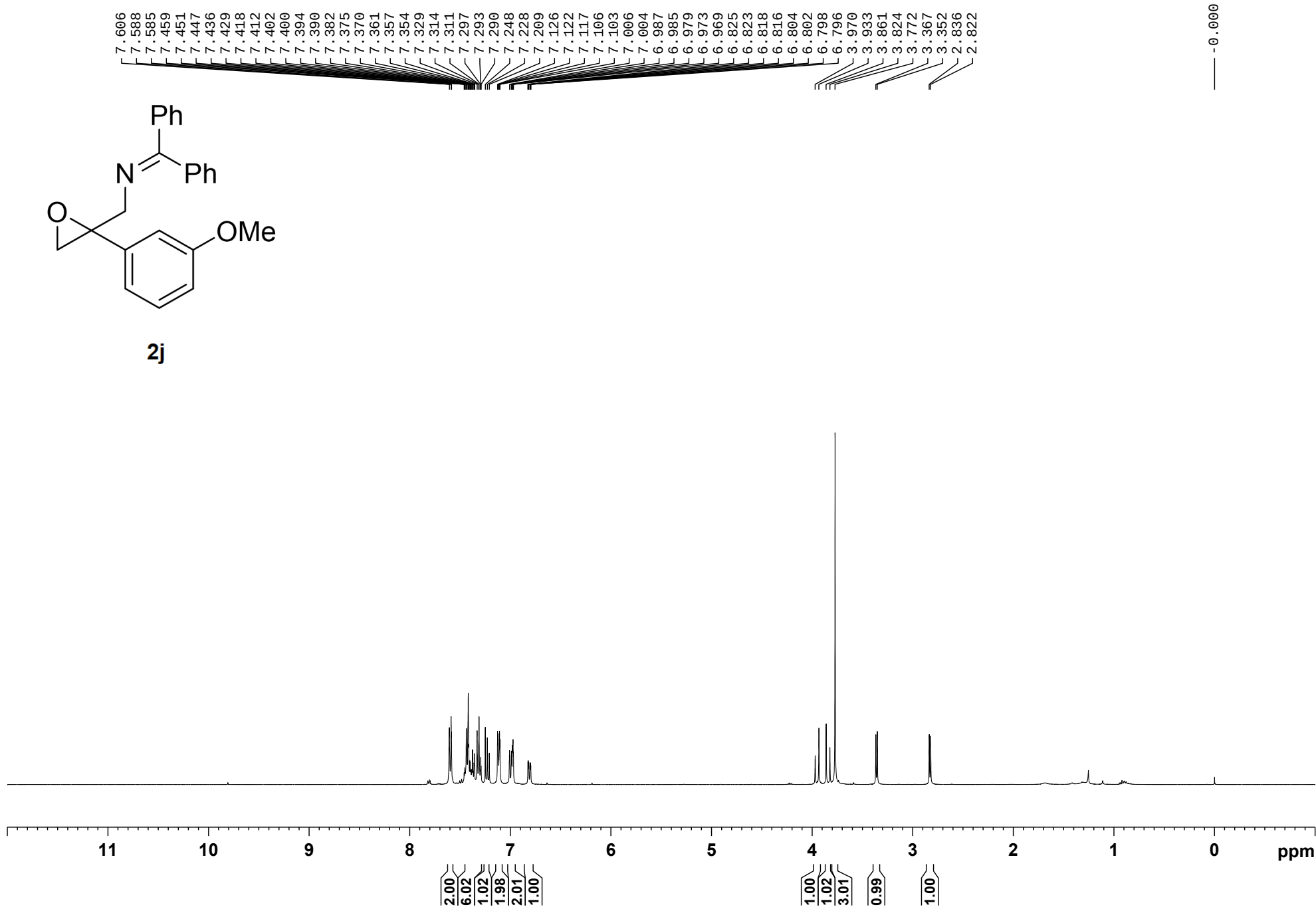
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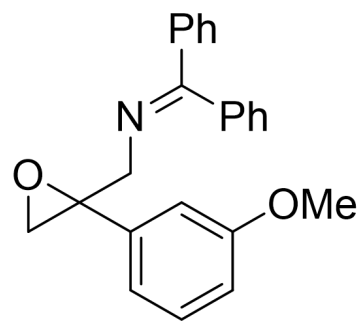
-112.976
-112.991
-113.002
-113.018





2j





2j

— 170.02

— 159.47

141.16

139.48

136.37

130.13

129.21

128.51

128.48

127.97

127.72

118.71

113.32

111.64

77.32

77.00

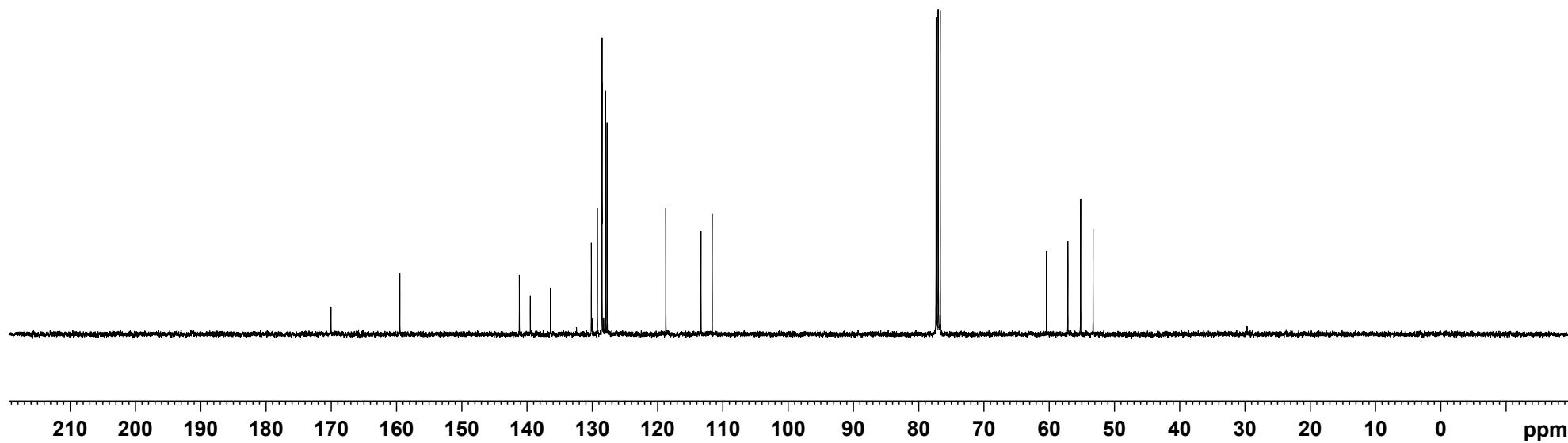
76.68

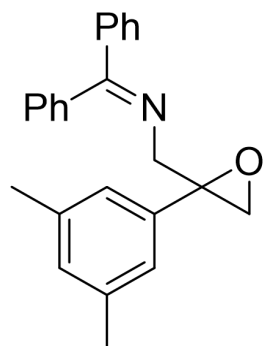
60.39

57.12

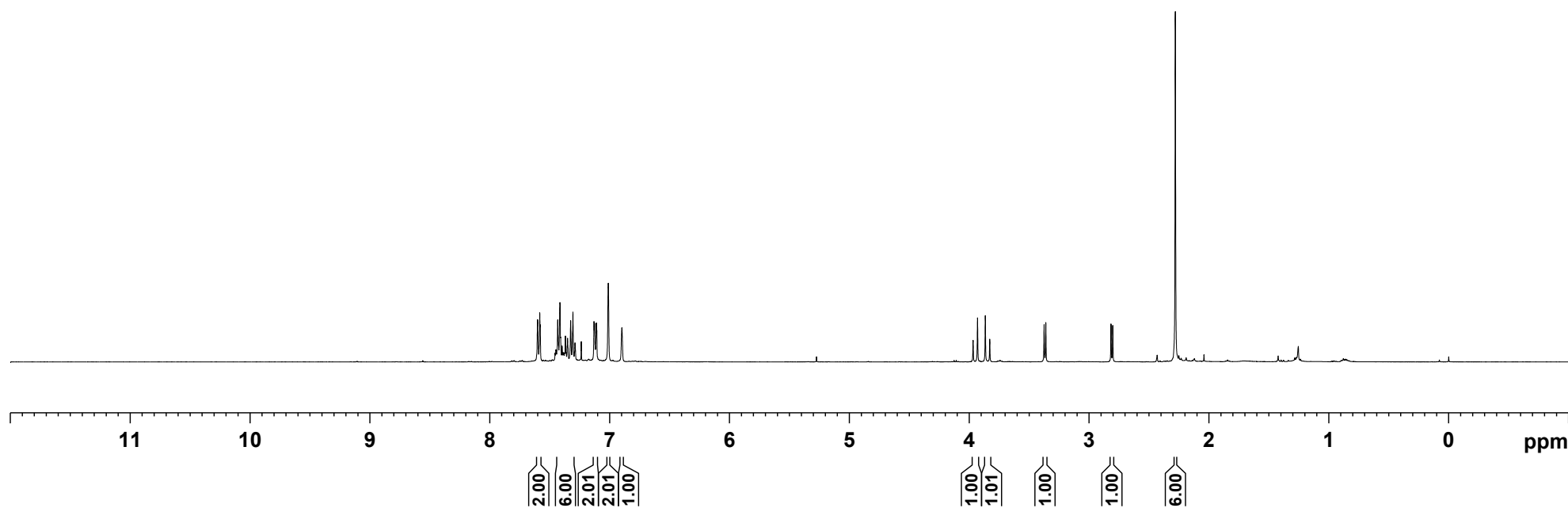
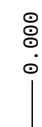
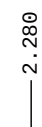
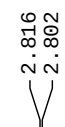
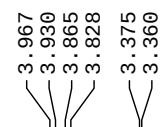
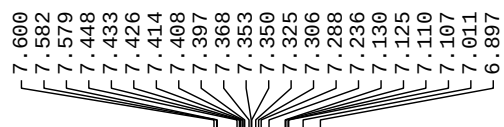
55.17

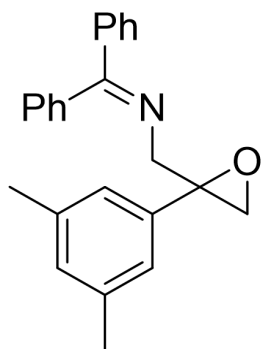
53.26





2k





2k

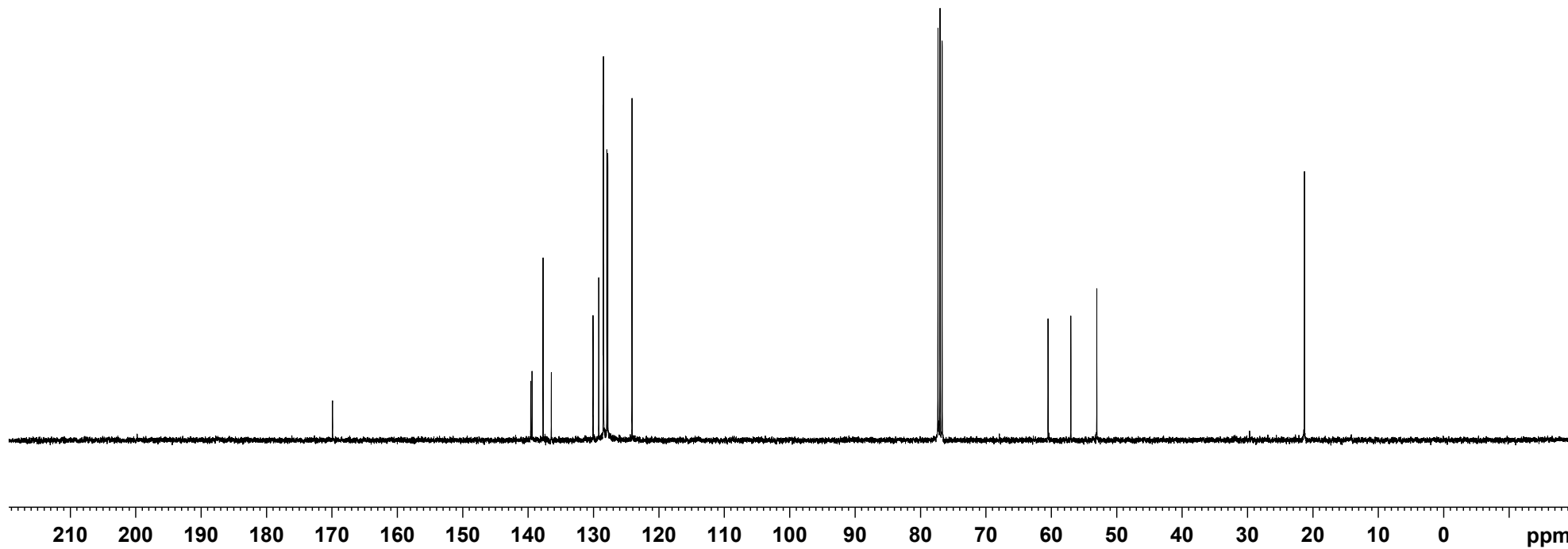
— 169.90

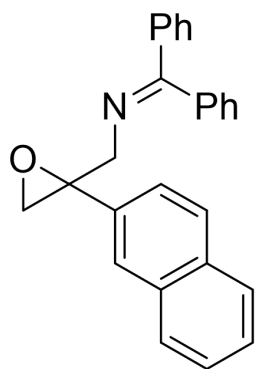
139.59
139.39
137.70
136.45
130.06
129.19
128.49
128.47
128.43
127.95
127.80
124.10

77.32
77.00
76.68

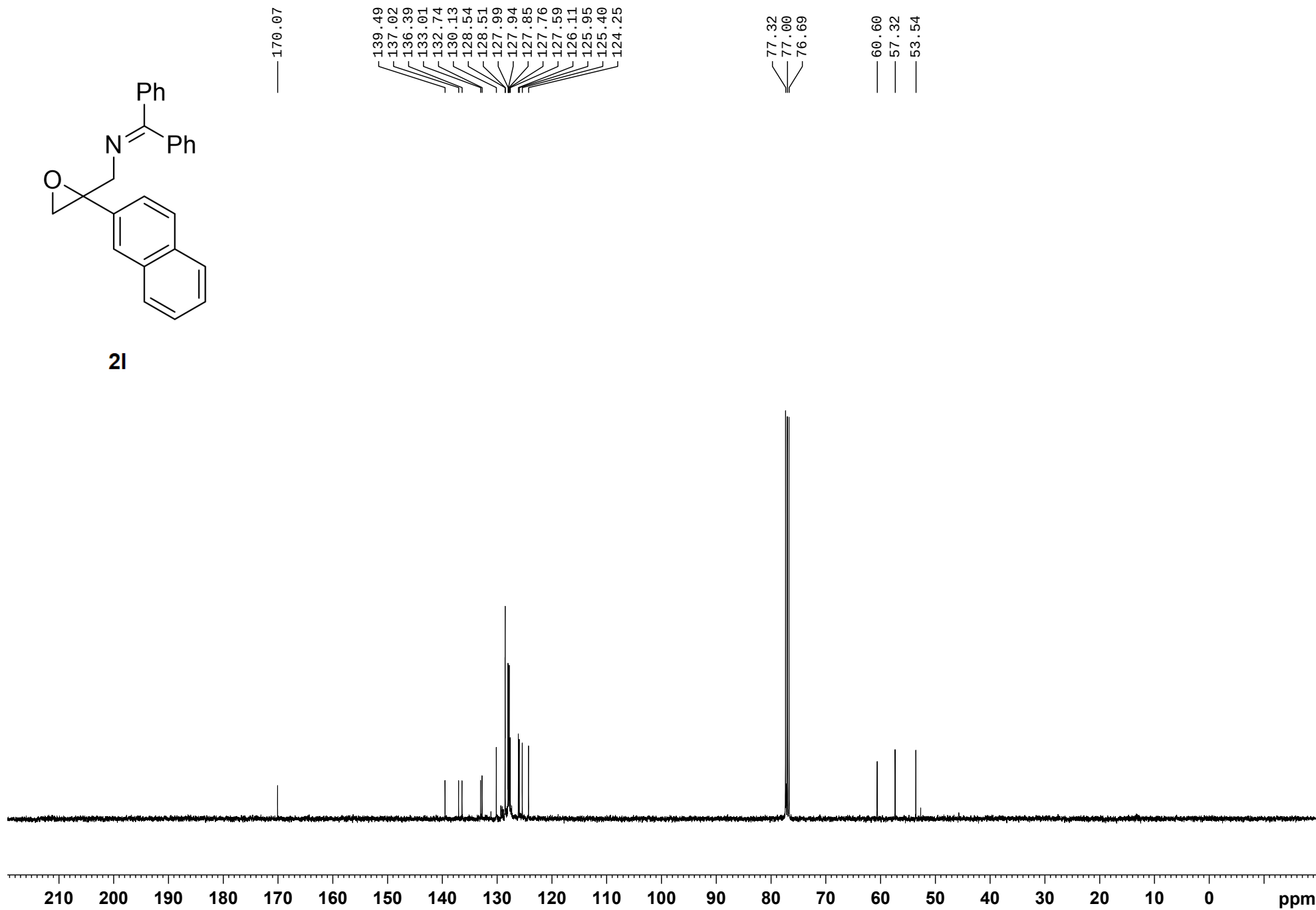
60.49
57.00
53.03

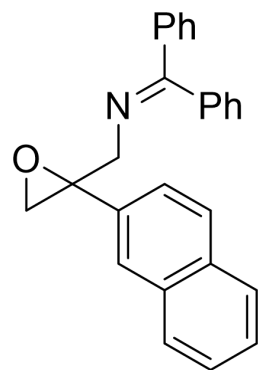
— 21.27



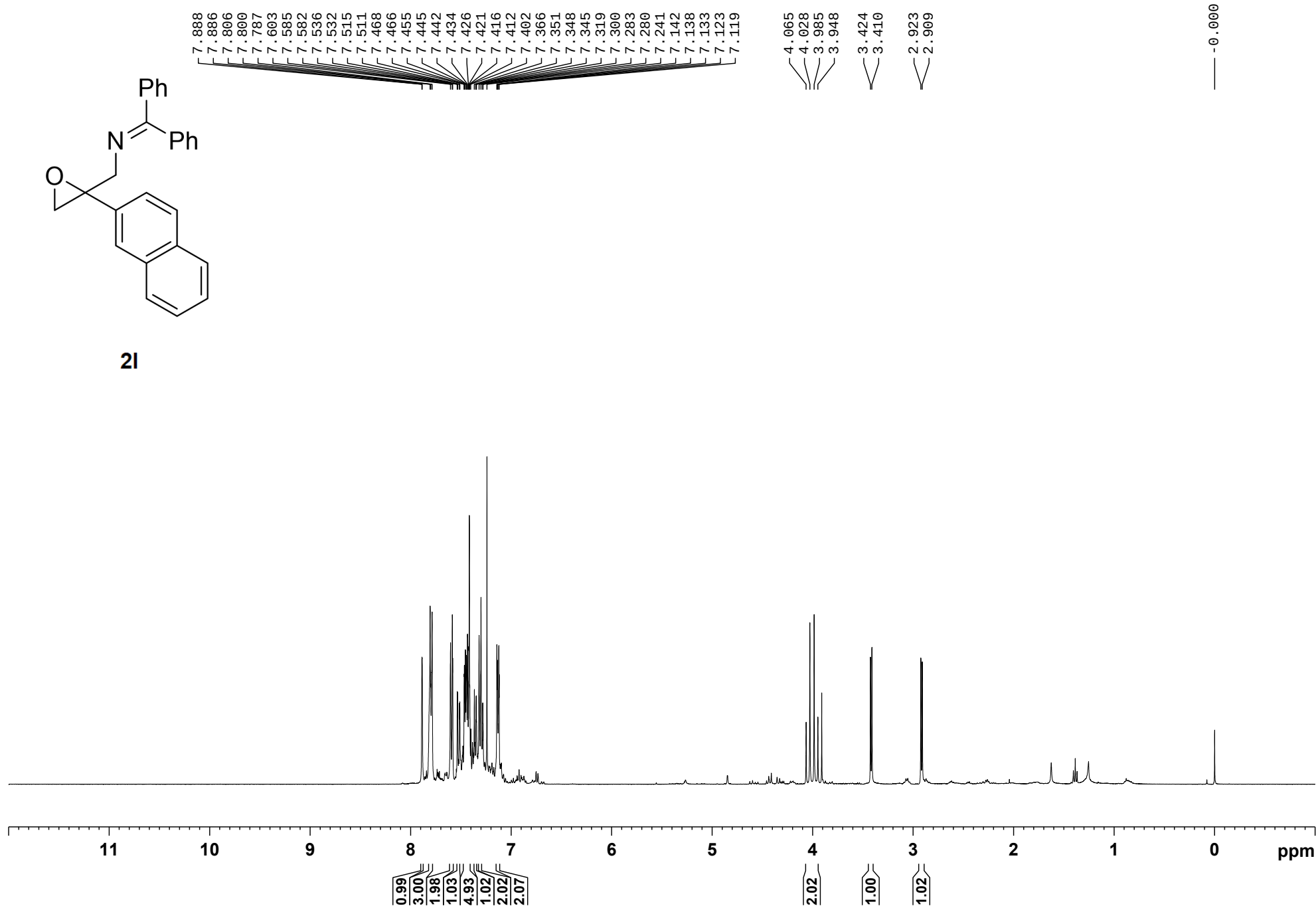


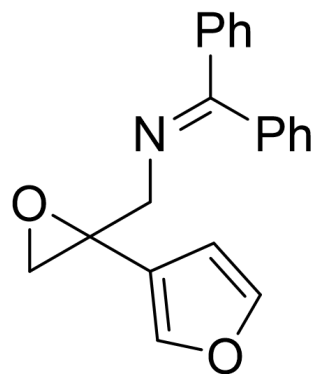
2l





2l



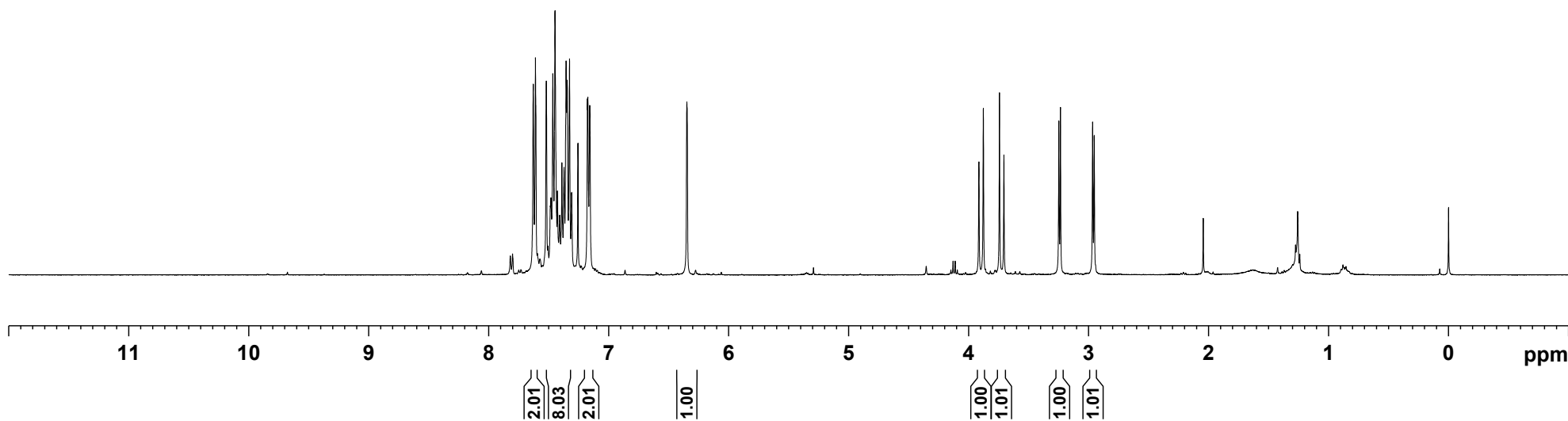


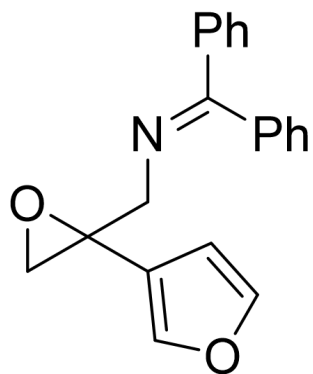
2m

7.628
7.610
7.519
7.486
7.481
7.465
7.447
7.426
7.407
7.389
7.371
7.354
7.350
7.345
7.326
7.308
7.255
7.176
7.173
7.157
6.348

3.914
3.877
3.742
3.705
3.248
3.235
2.967
2.953

0.000





2m

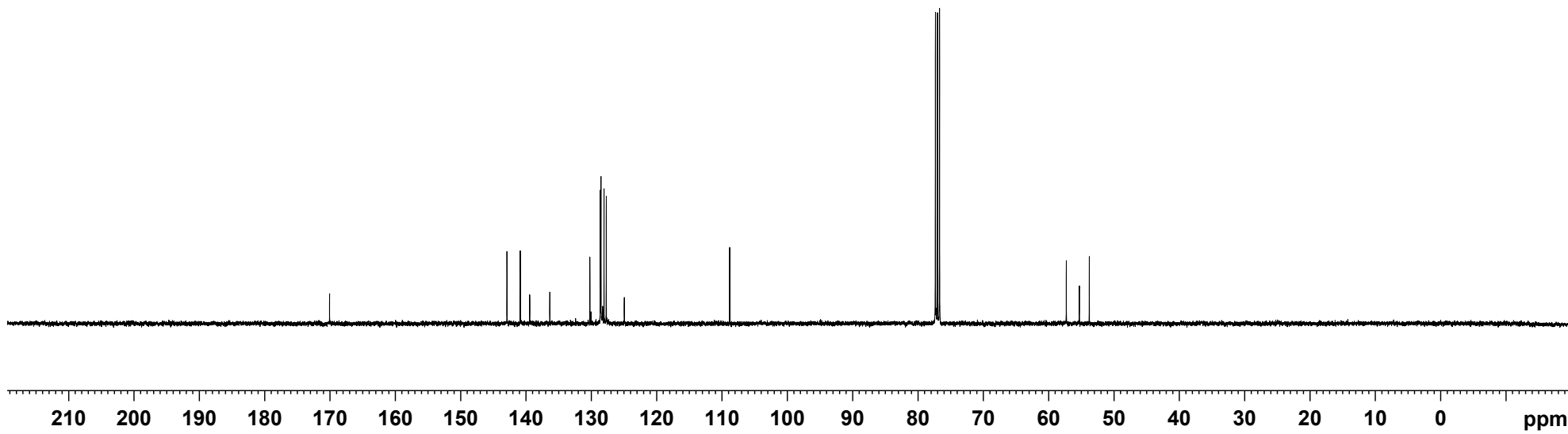
— 170.05

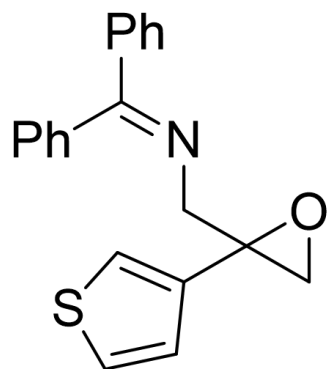
142.90
140.86
139.42
136.34
130.20
128.61
128.59
128.51
128.04
127.70
124.93

— 108.80

77.31
77.00
76.68

57.28
55.28
53.76



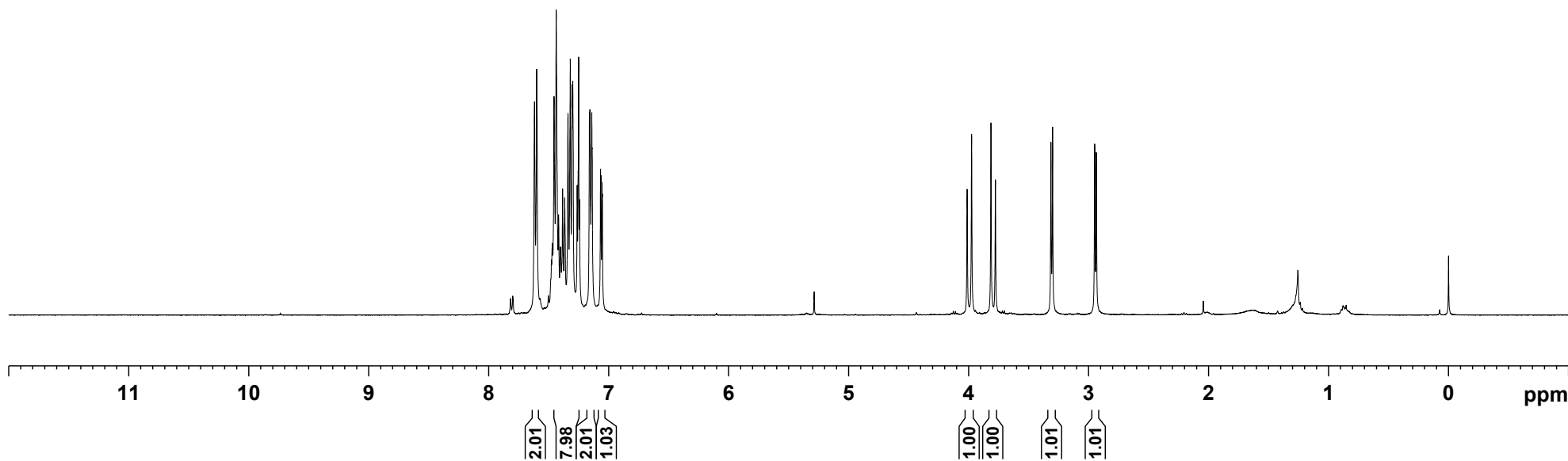


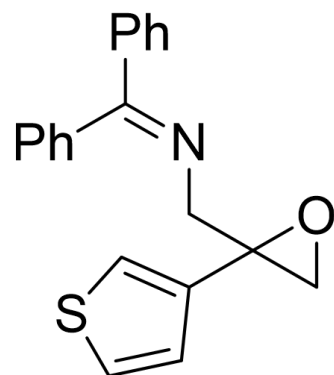
2n

7.618
7.601
7.597
7.477
7.471
7.467
7.455
7.437
7.418
7.402
7.384
7.366
7.339
7.320
7.306
7.303
7.299
7.263
7.254
7.250
7.243
7.160
7.156
7.141
7.068
7.065
7.056
7.053

4.012
3.975
3.814
3.777
3.314
3.300
2.949
2.936

— 0.000





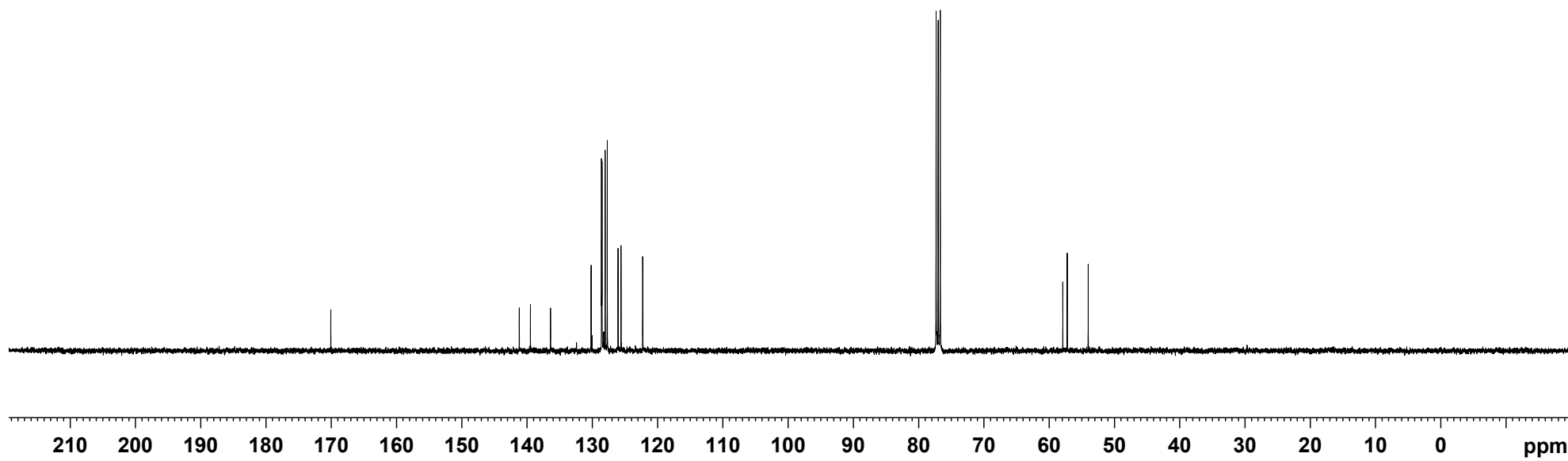
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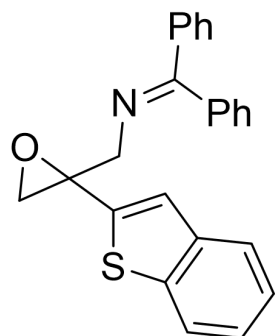
— 170.04

141.17
139.46
136.38
130.18
128.59
128.55
128.51
128.02
127.71
126.05
125.59
122.28

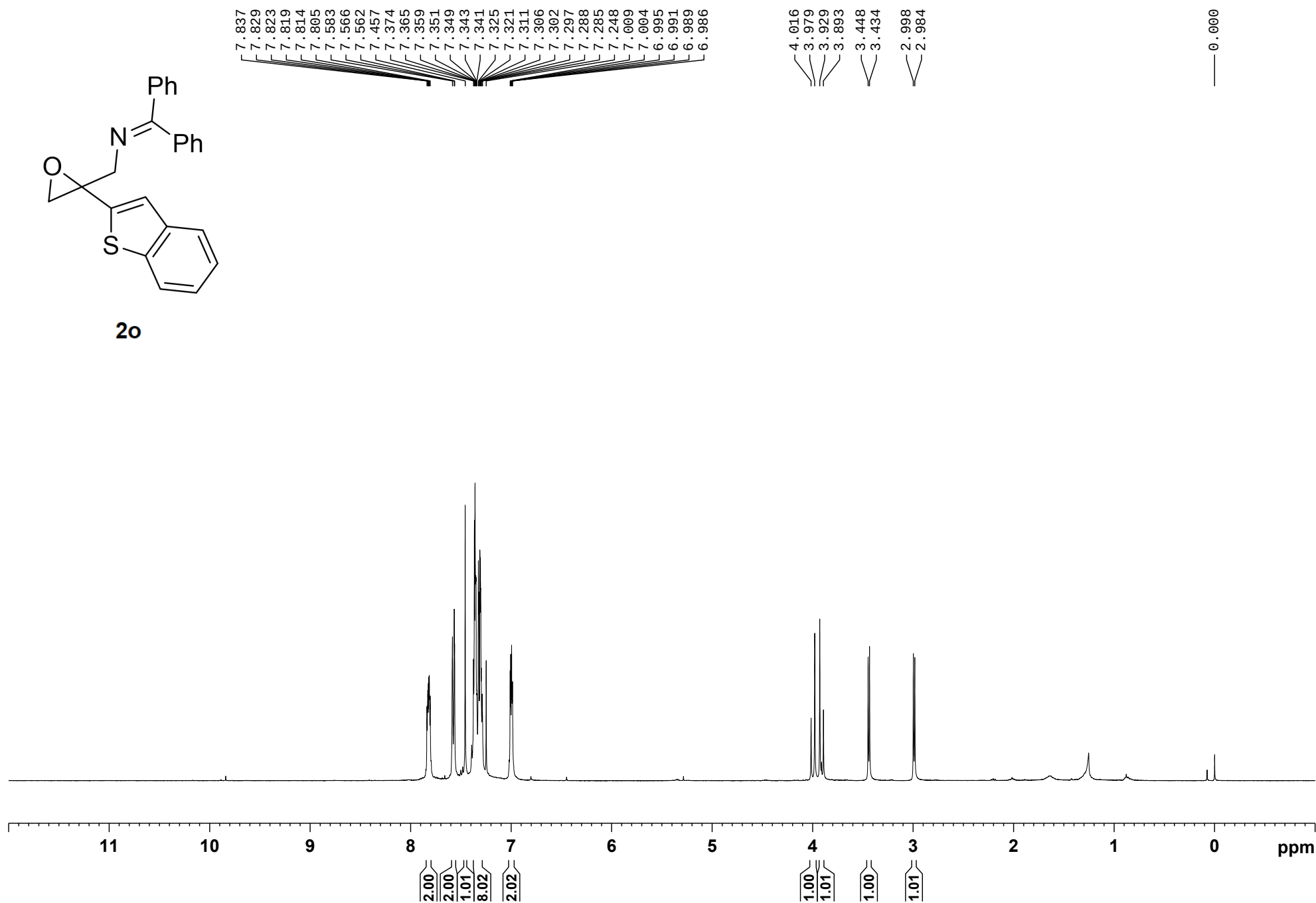
77.32
77.00
76.68

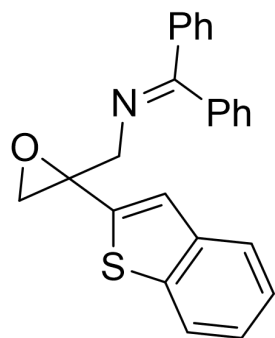
57.91
57.23
54.01



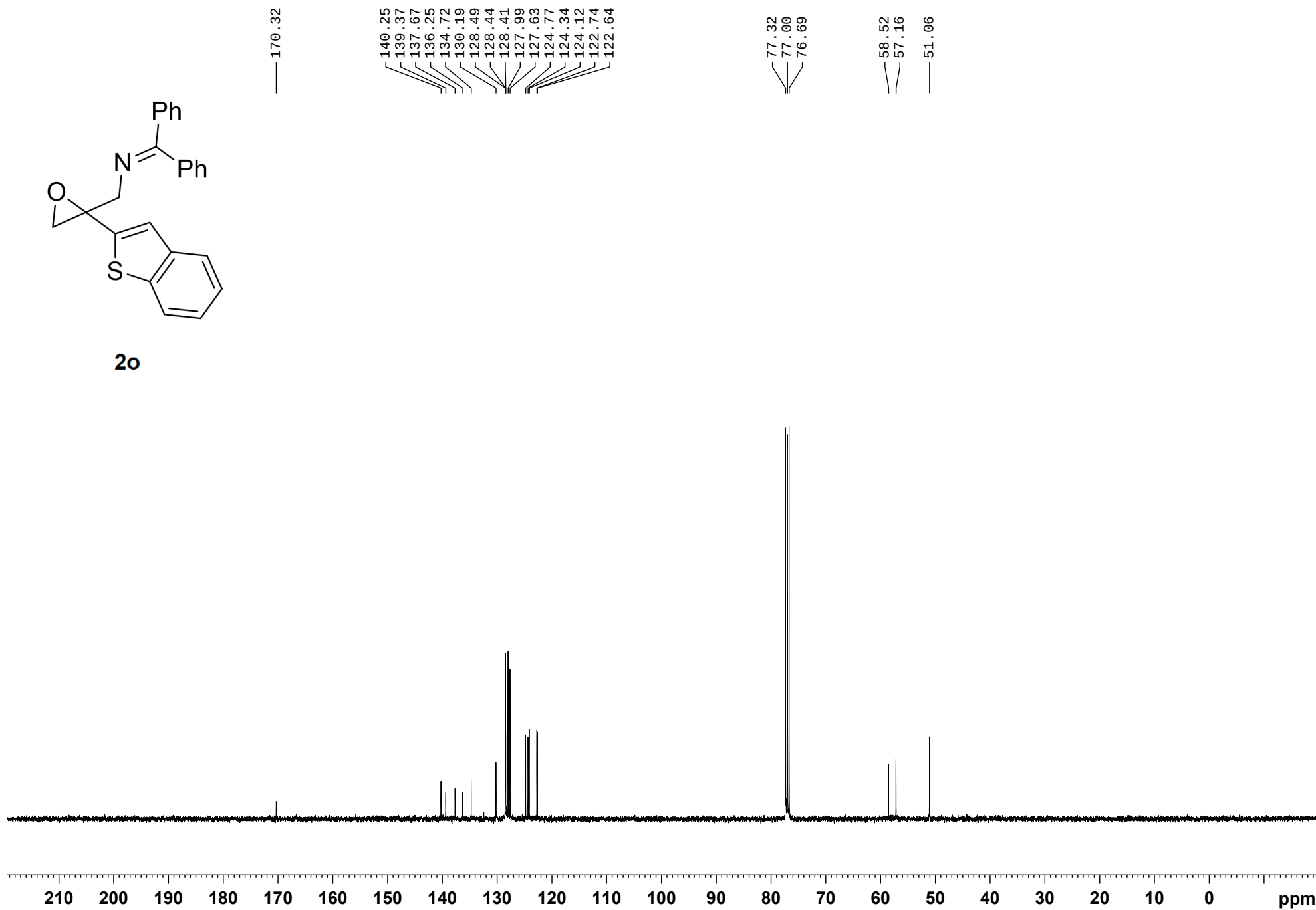


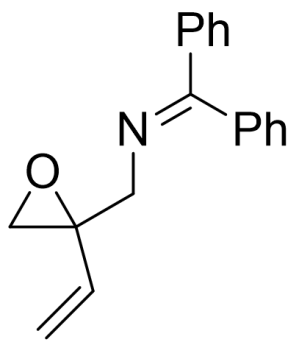
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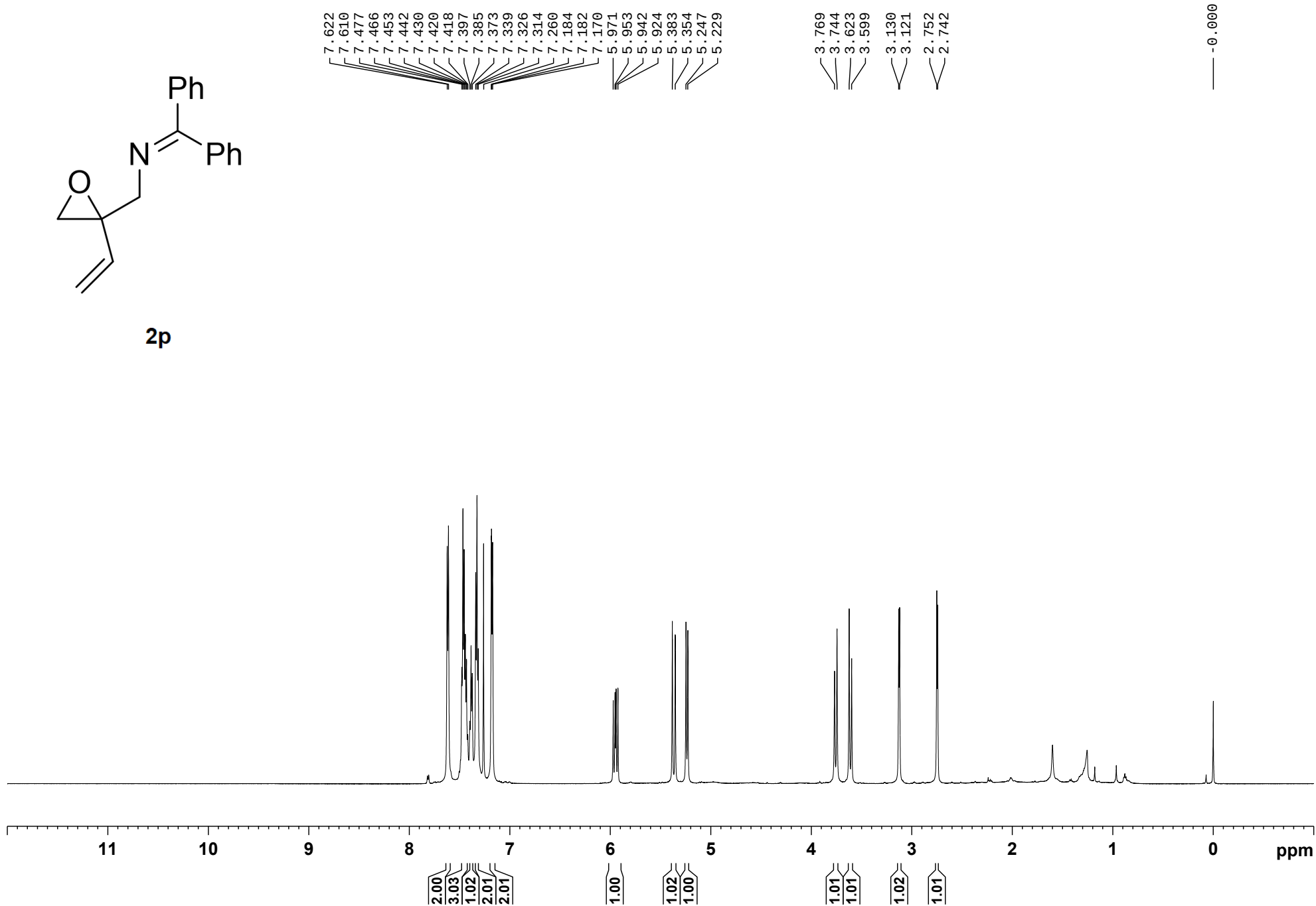


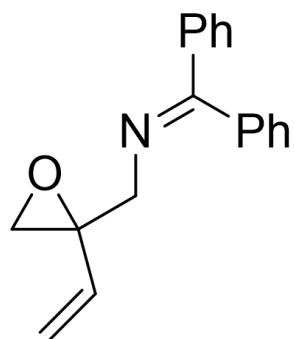
2o





2p





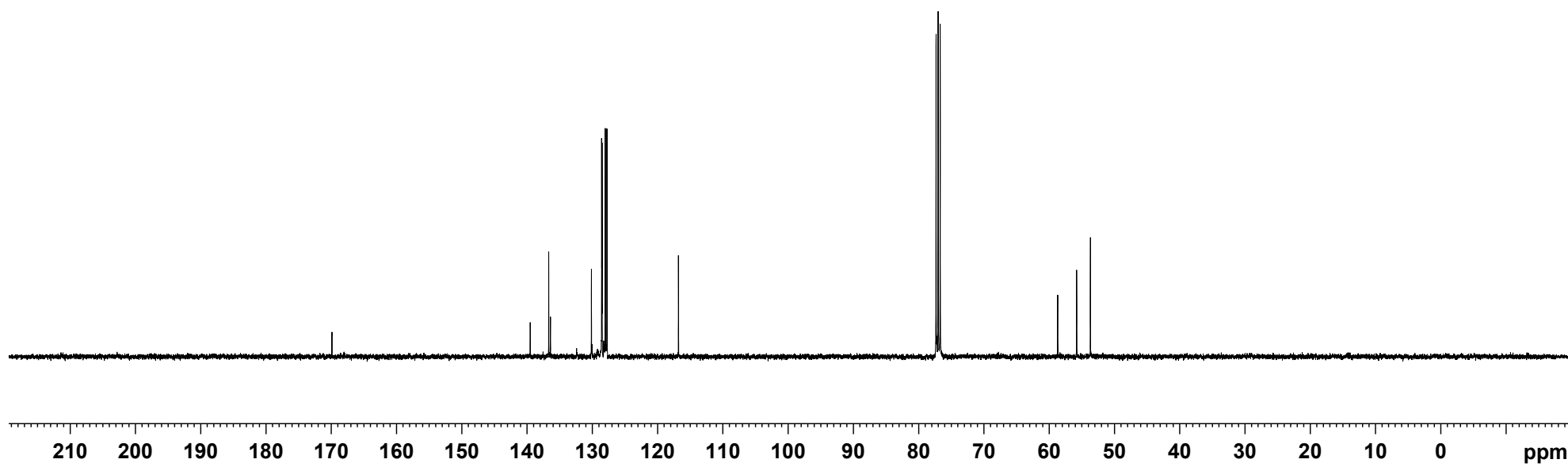
2p

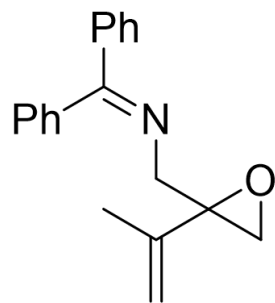
— 169.88

139.50
136.66
136.40
130.12
128.56
128.53
128.48
128.00
127.74
— 116.78

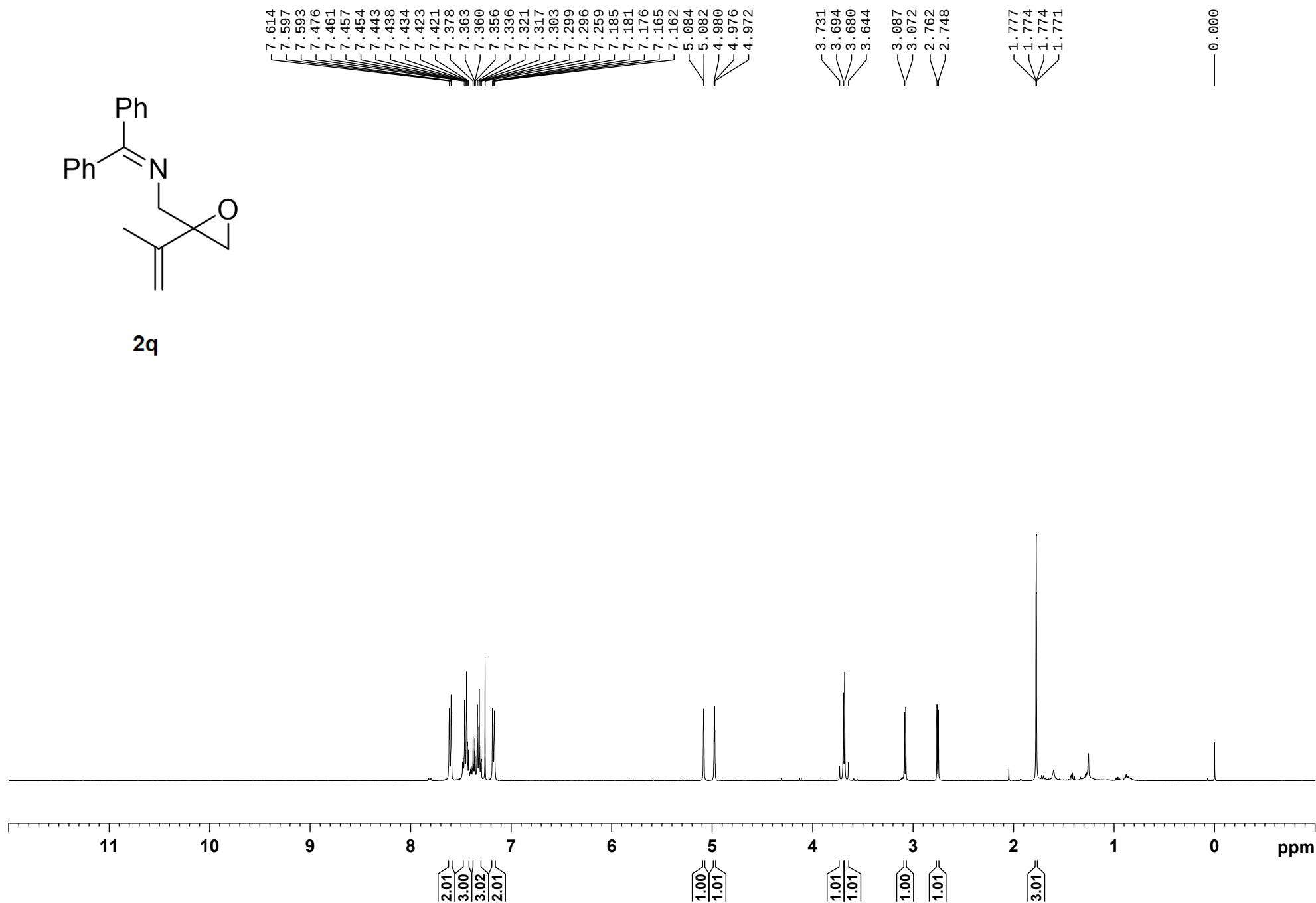
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77.00
76.68

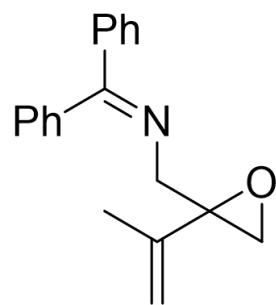
58.67
55.77
53.67



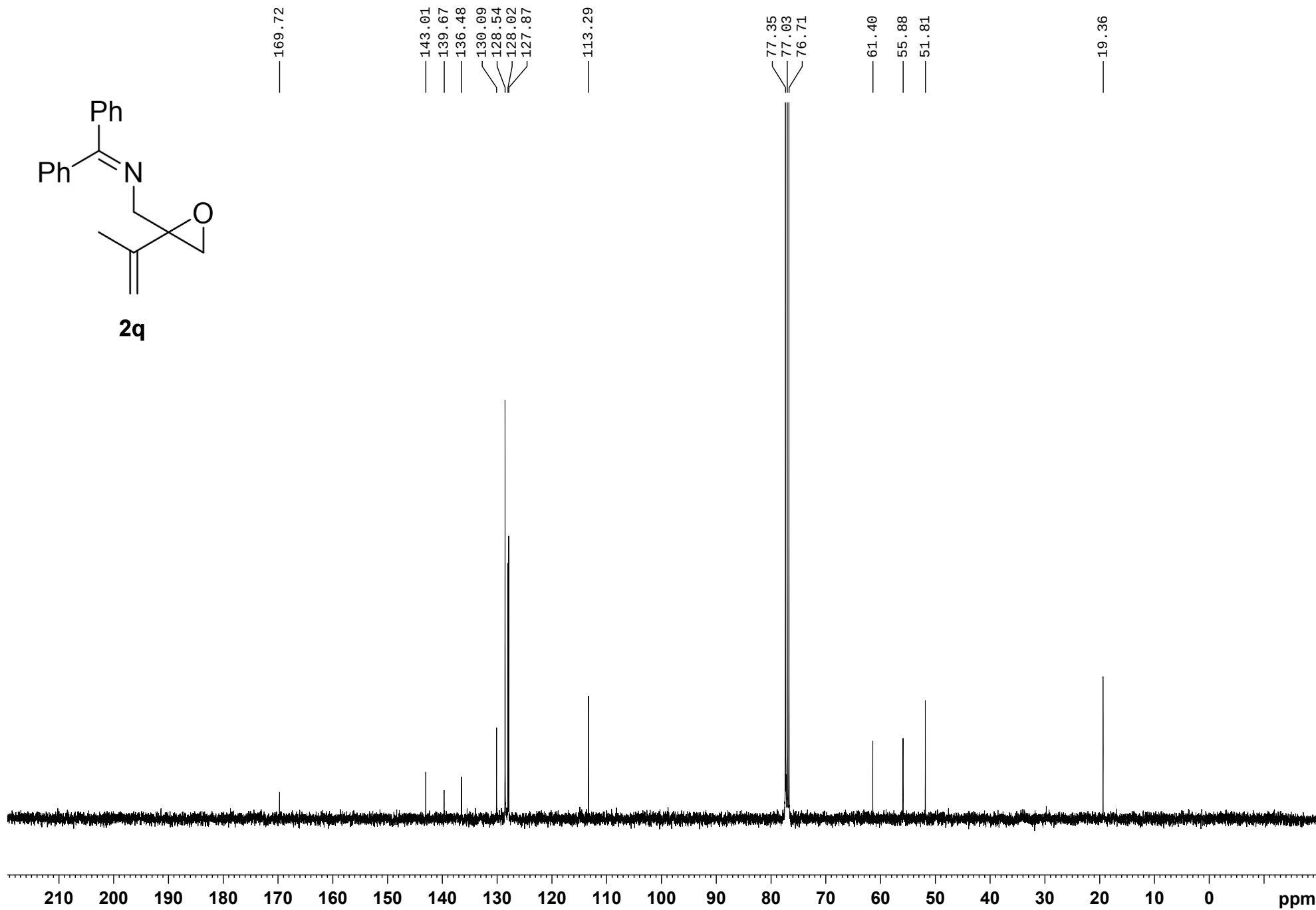


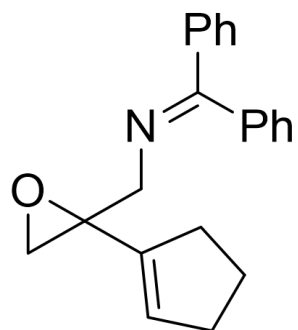
2q



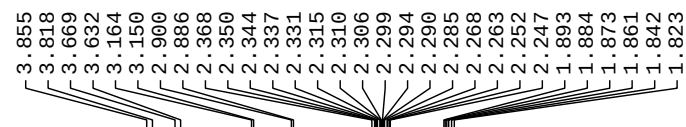
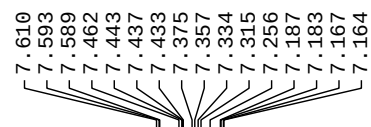


2q

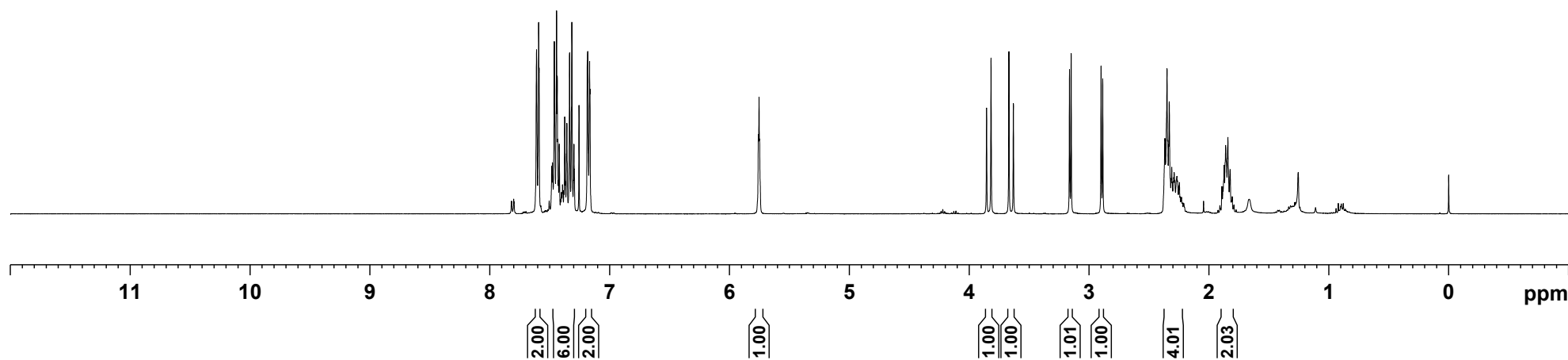


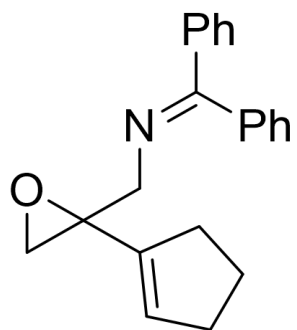


2r



— 0.000





2r

— 169.56

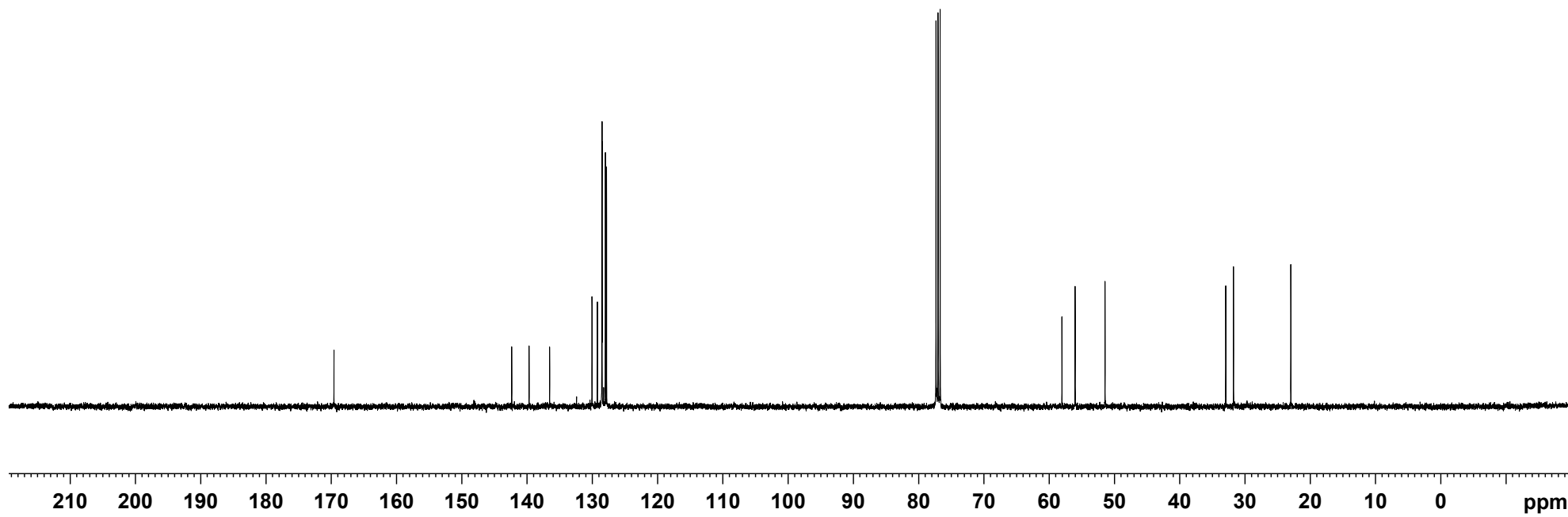
142.32
139.66
136.52
130.02
129.20
128.52
128.48
127.97
127.79

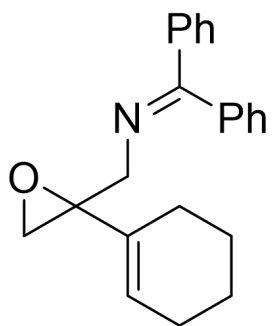
77.32
77.00
76.68

58.04
56.01
51.43

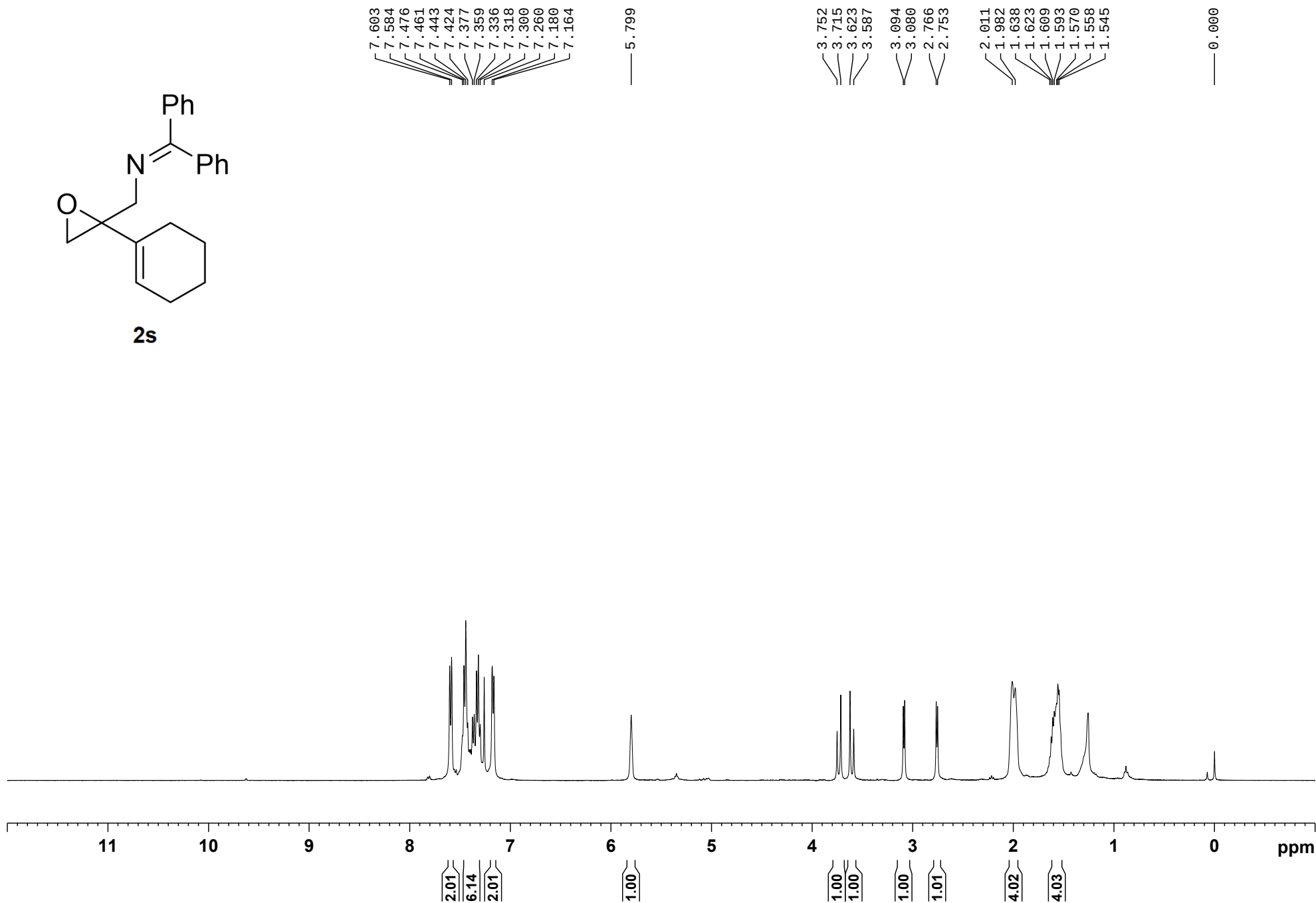
32.94
31.75

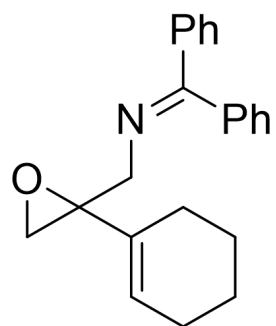
— 22.96



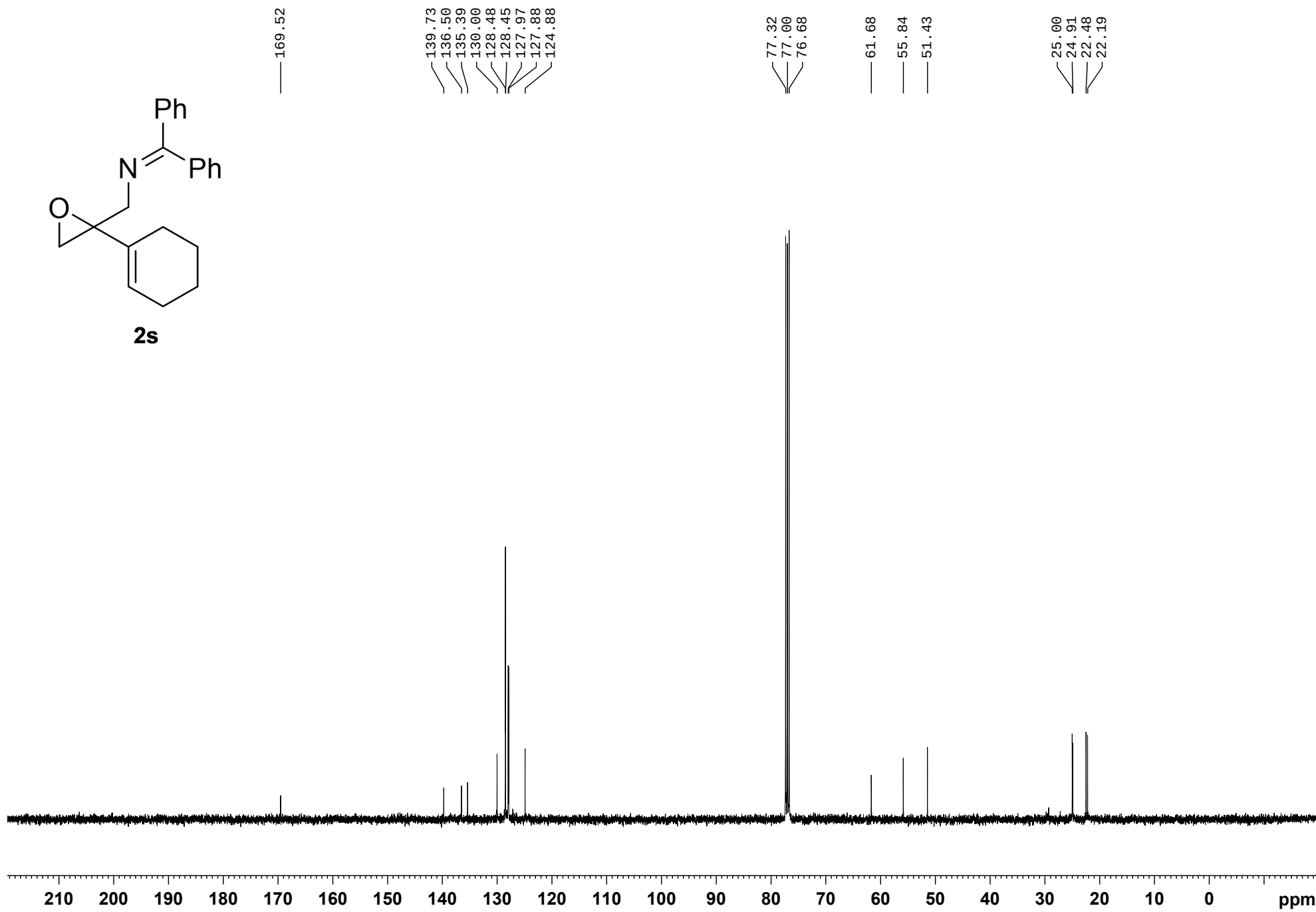


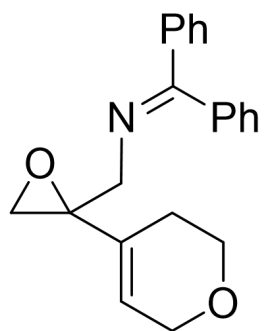
2s



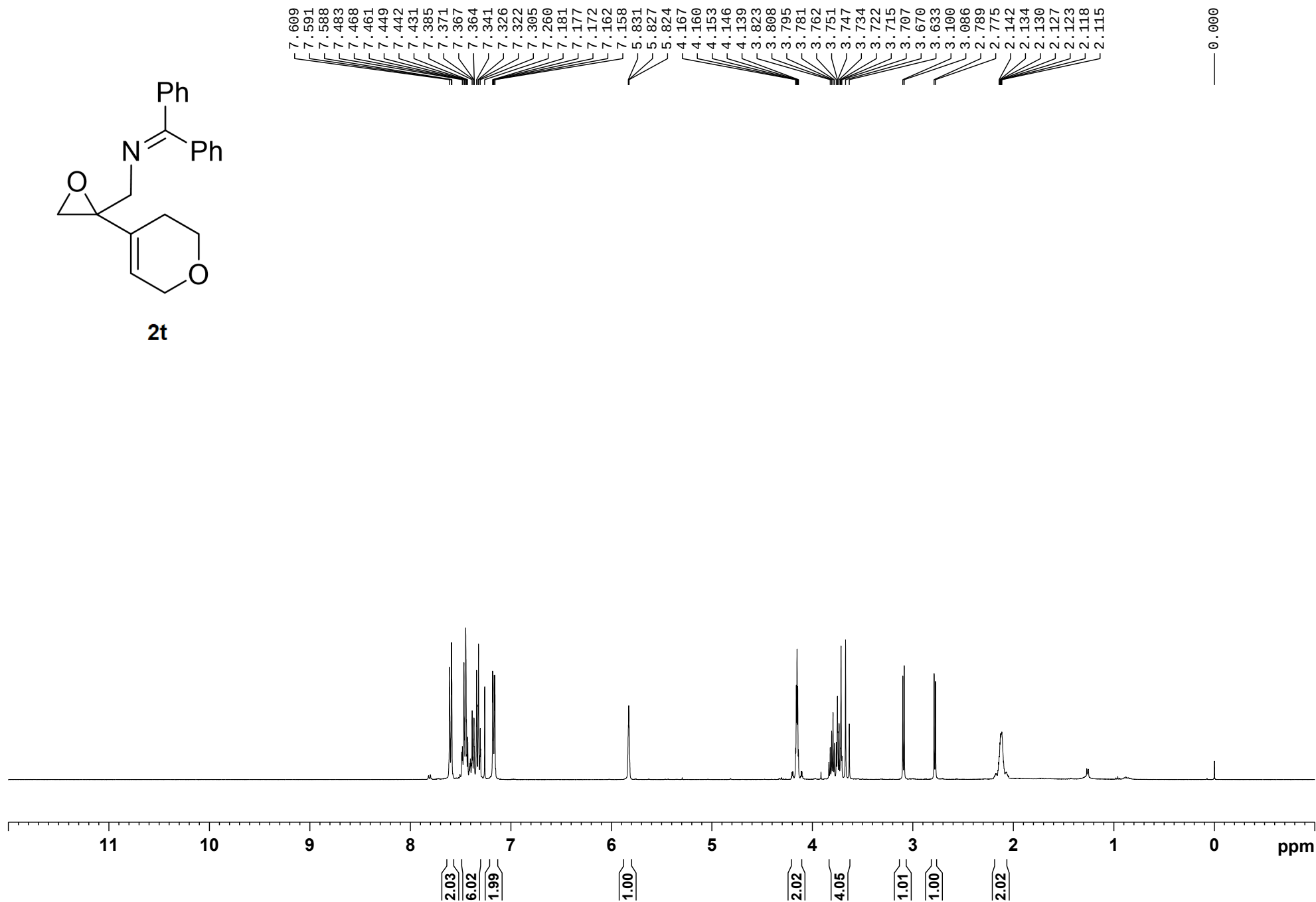


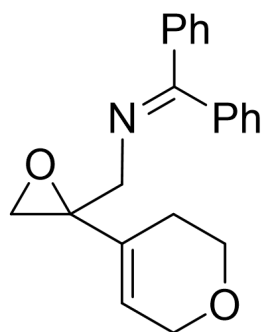
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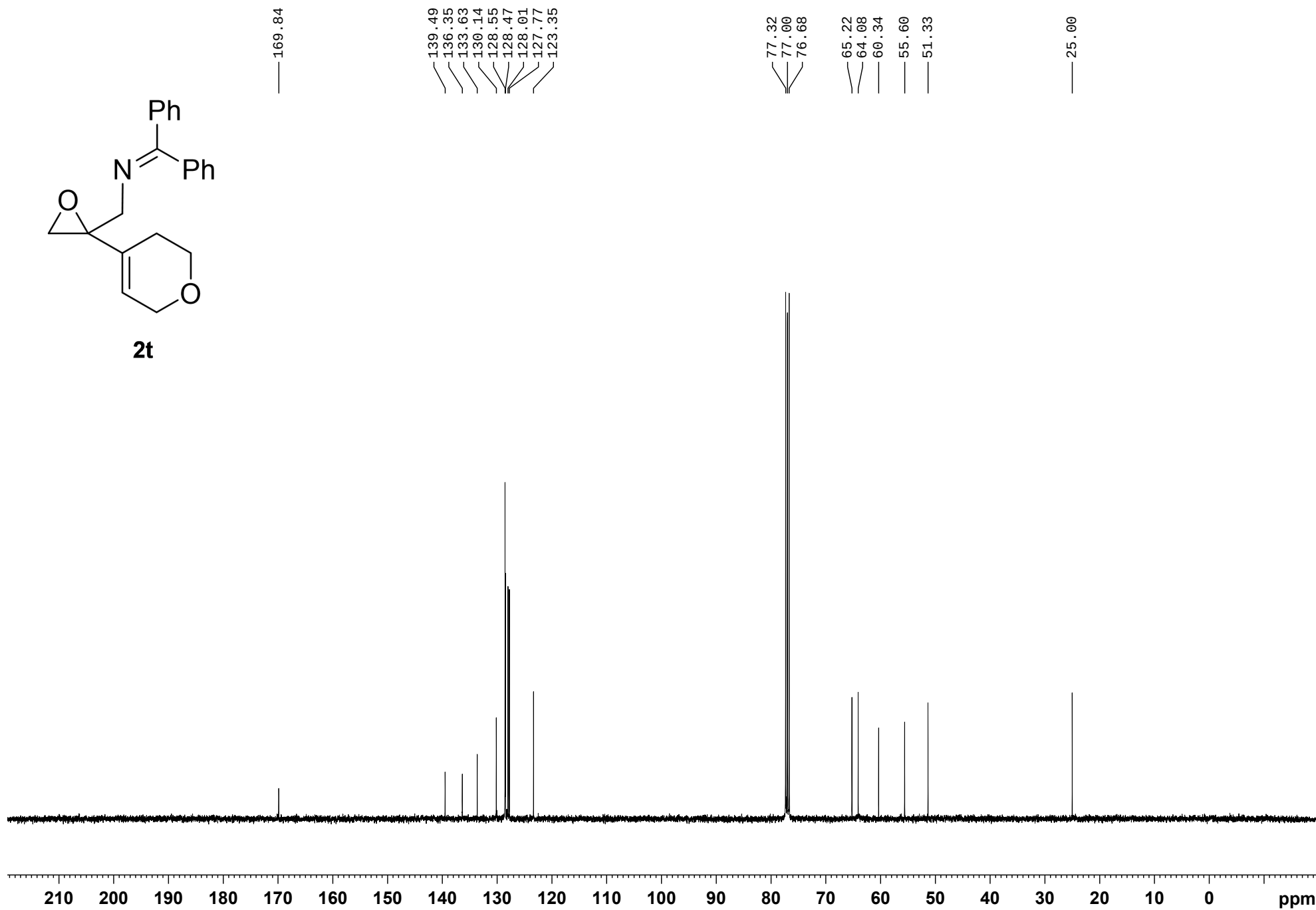


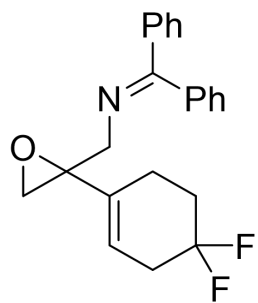
2t



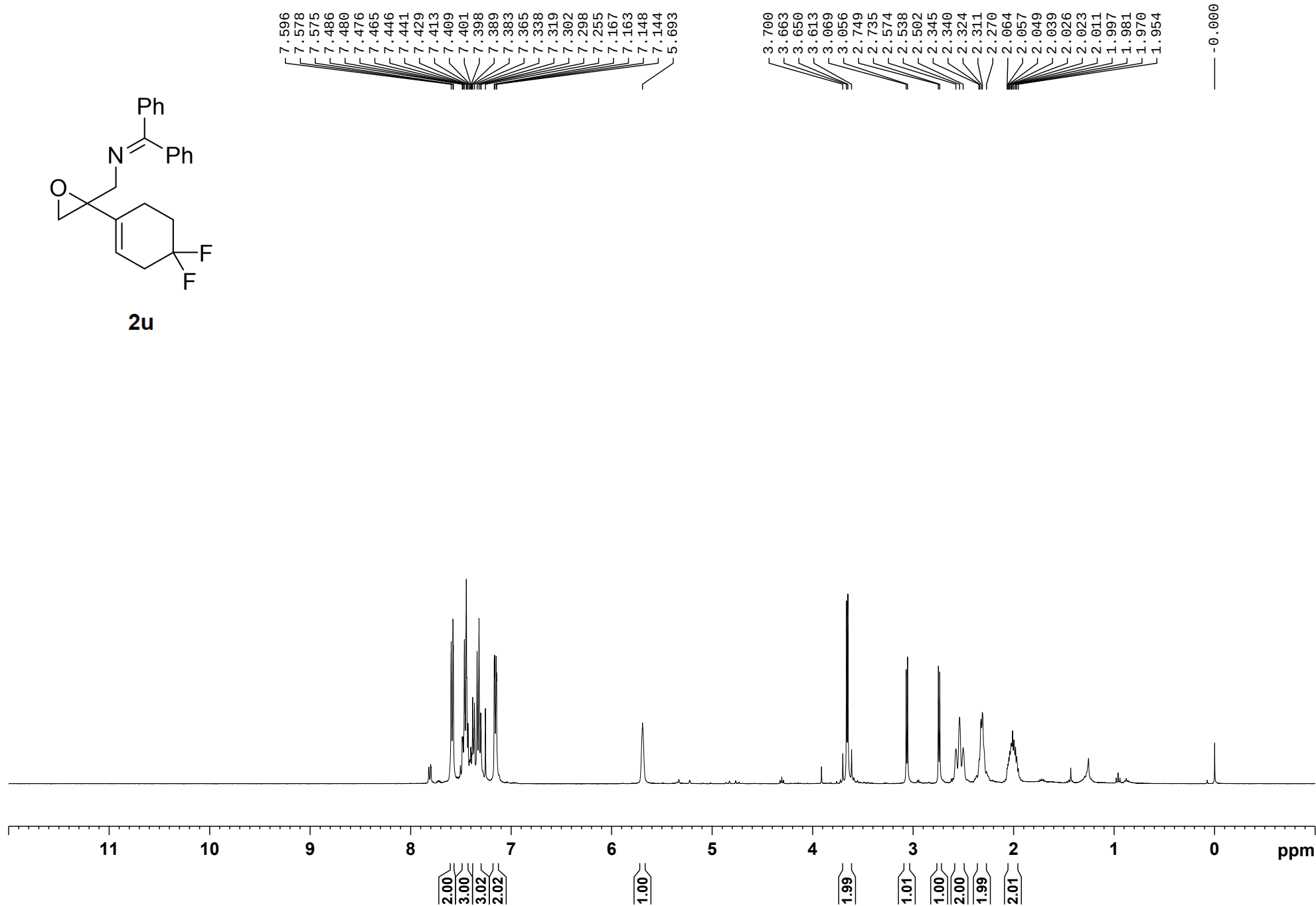


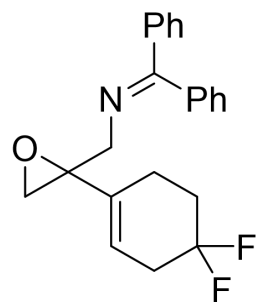
2t



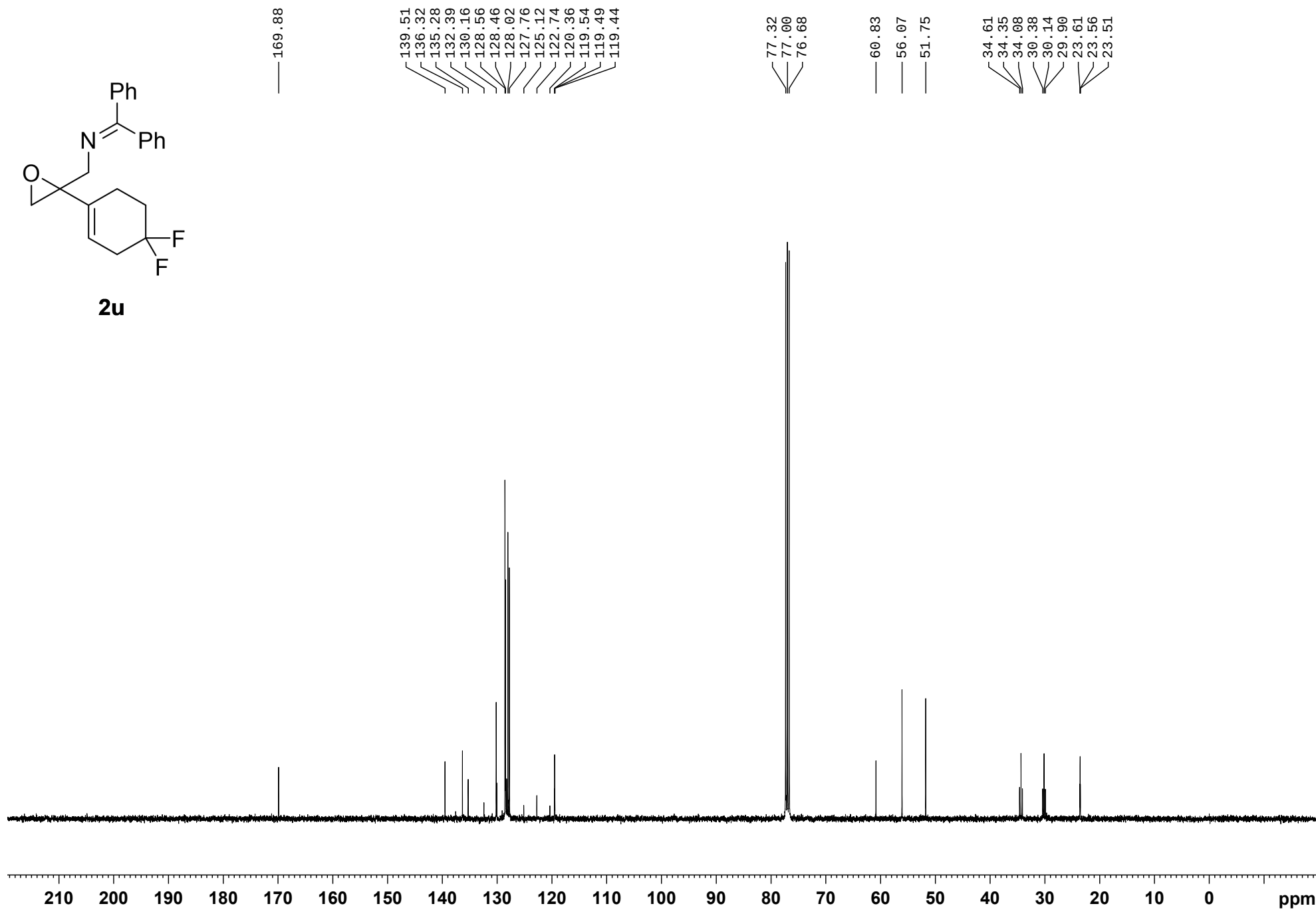


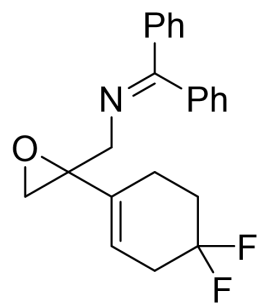
2u





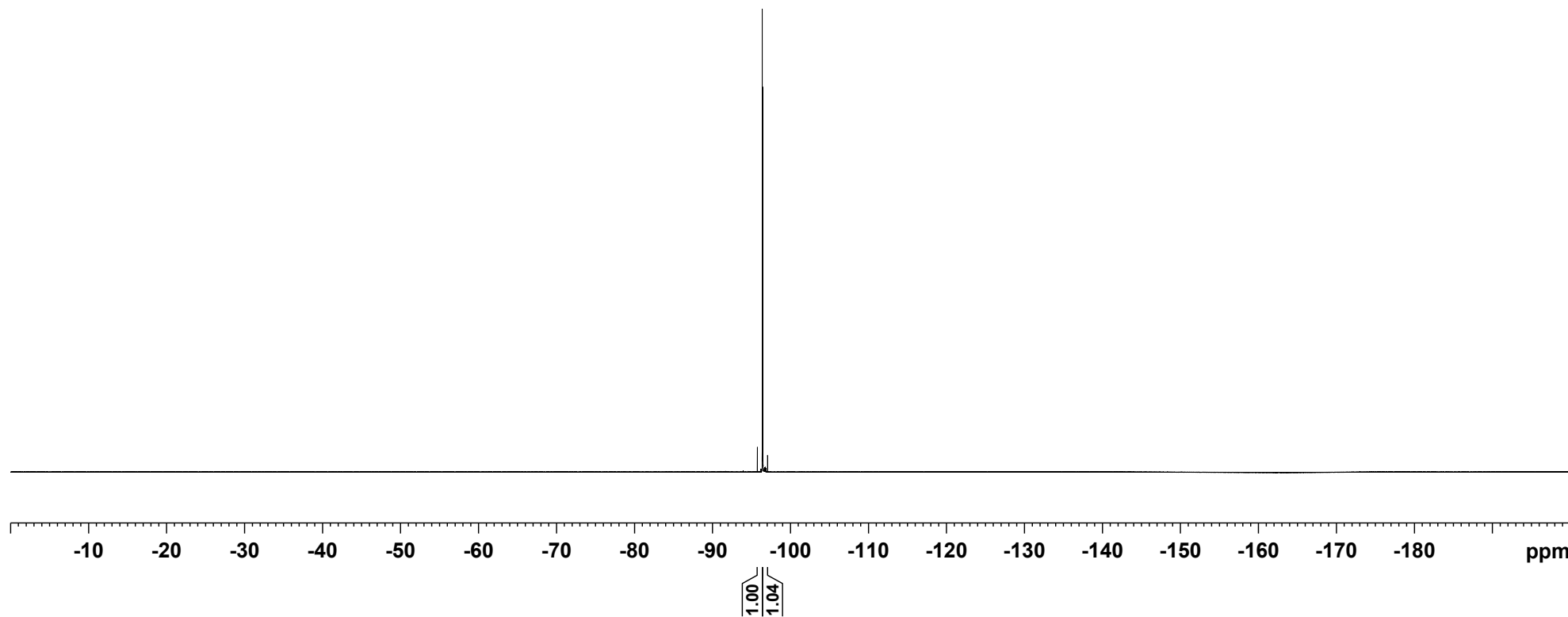
2u

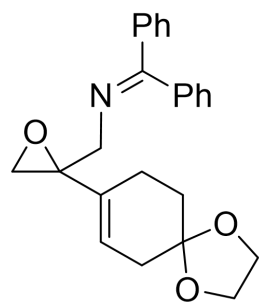




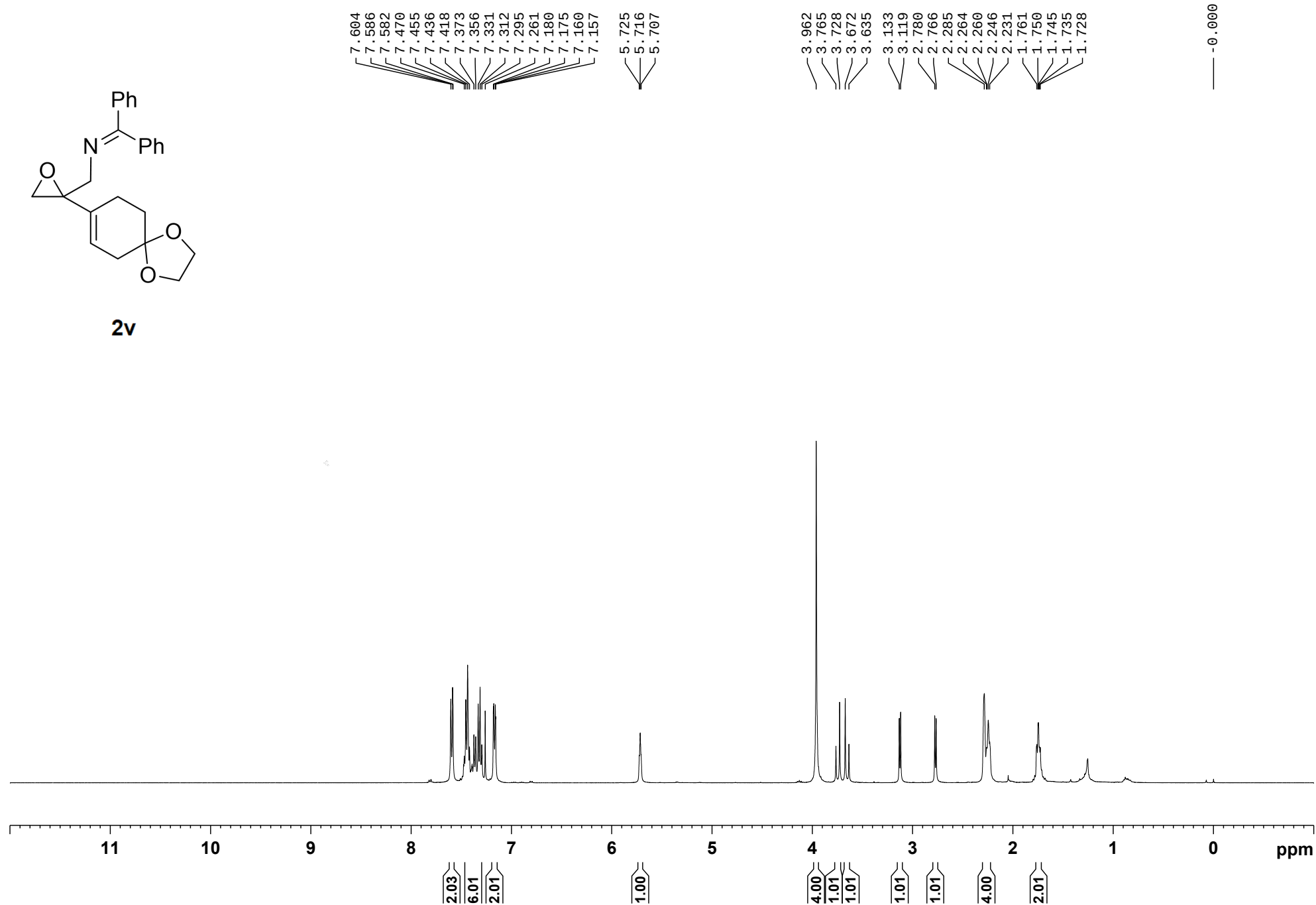
2u

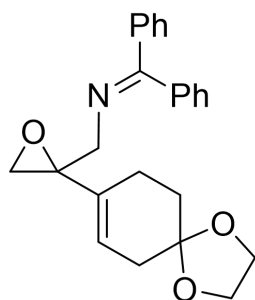
-95.743
-96.368
-96.429
-97.054





2v





2v

— 169.67

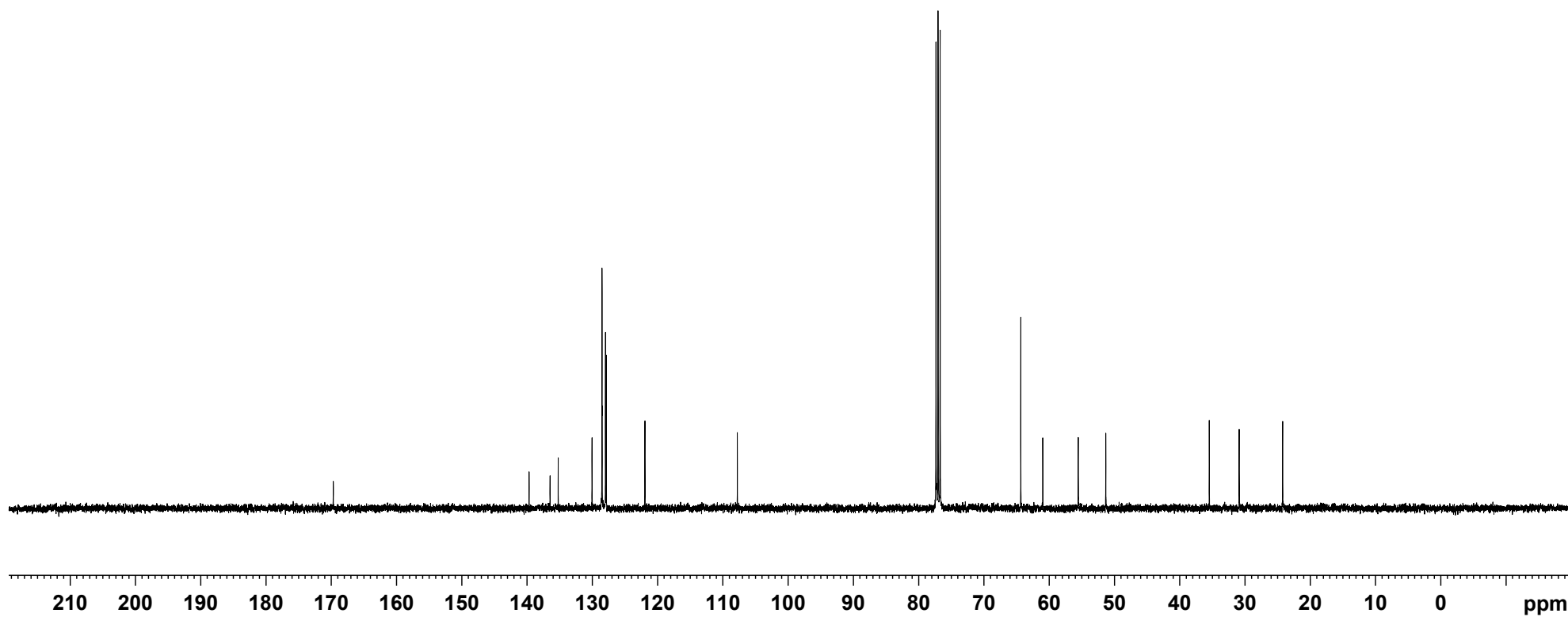
139.67
136.45
135.21
130.01
128.50
128.46
127.95
127.83
121.91

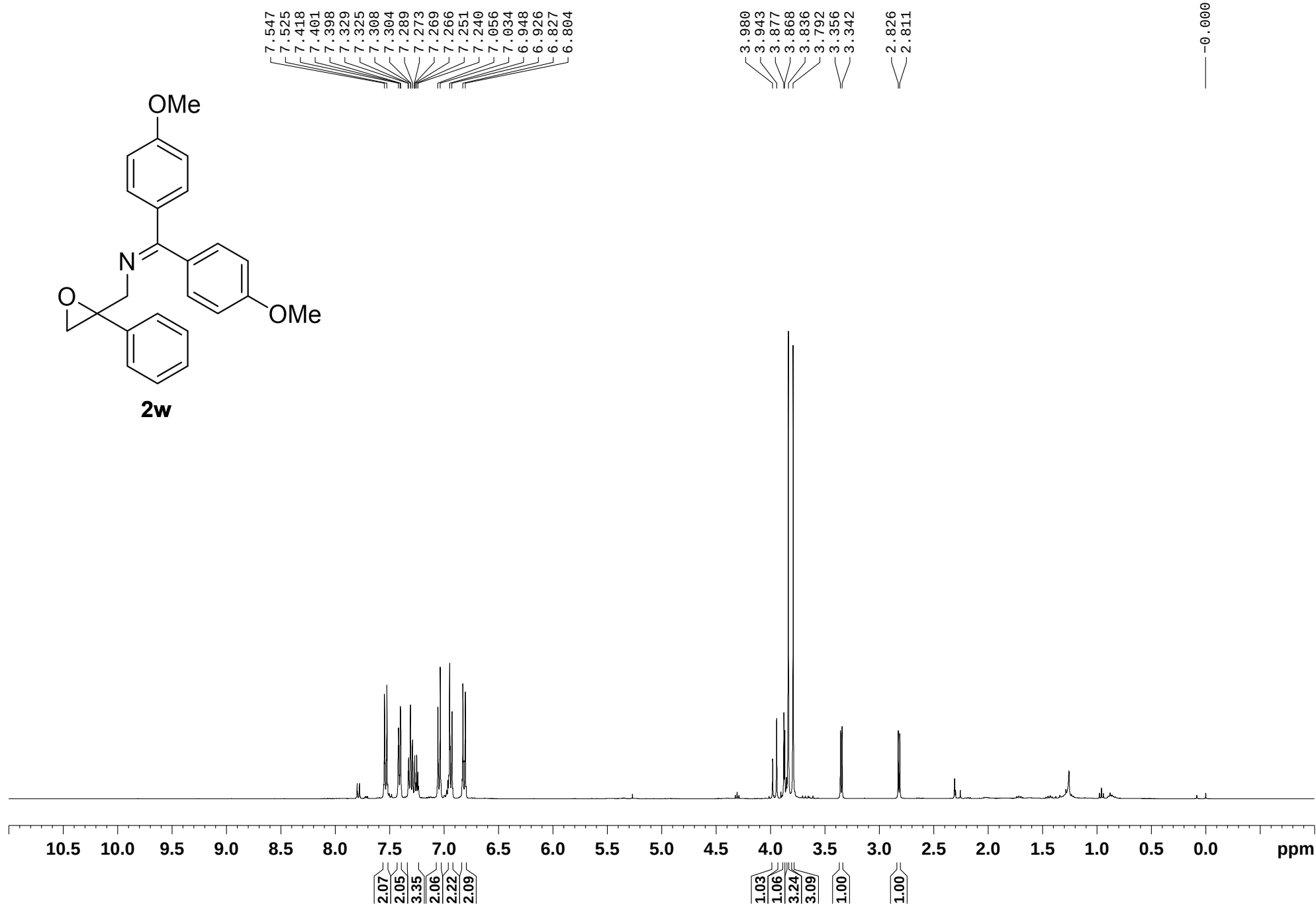
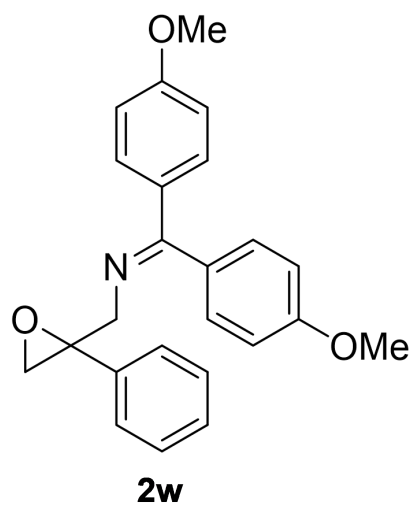
— 107.75

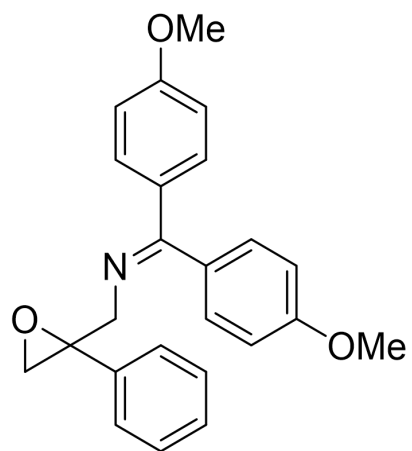
77.32
77.00
76.68

64.34
60.97
55.54
51.32

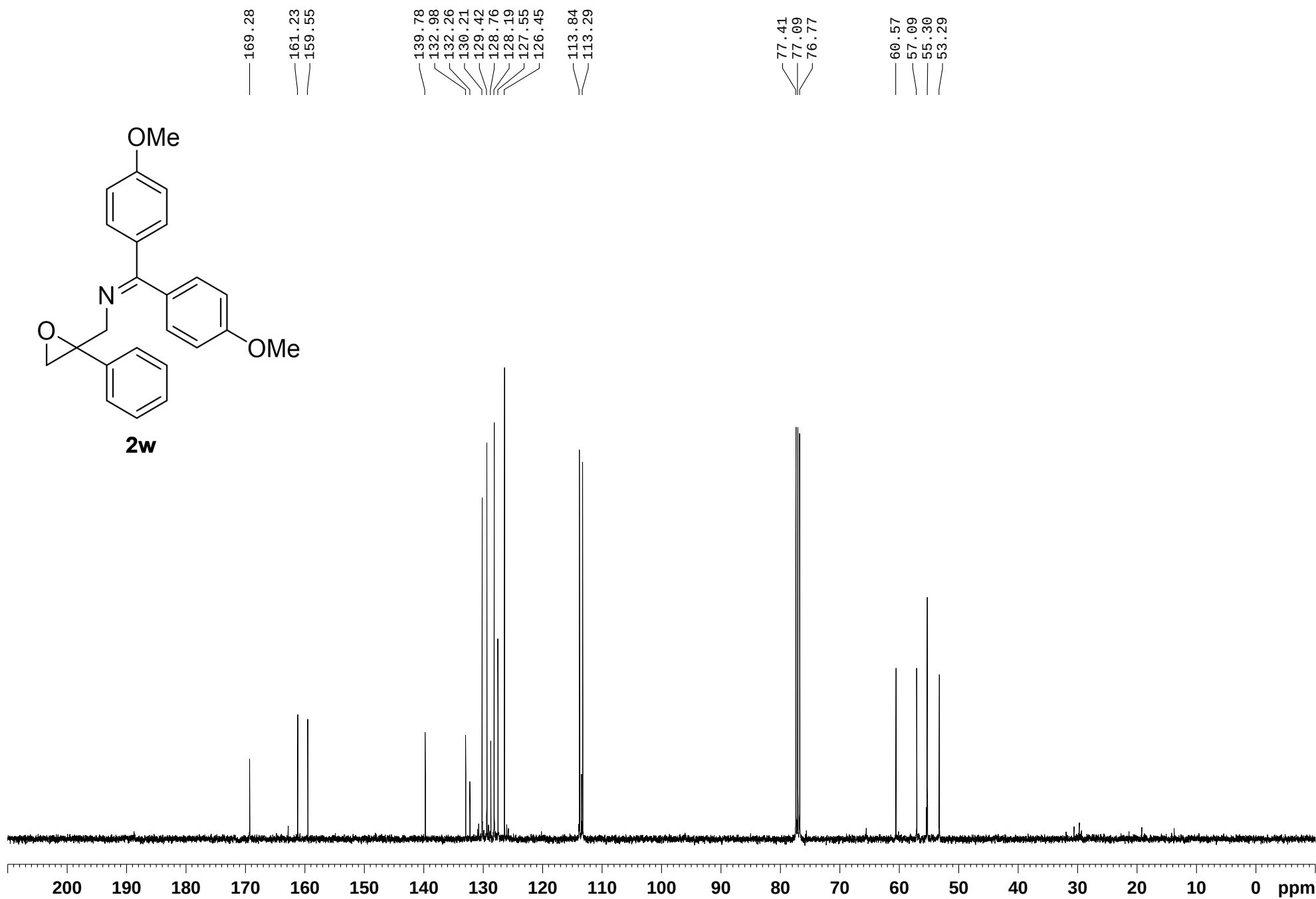
35.46
30.88
24.22

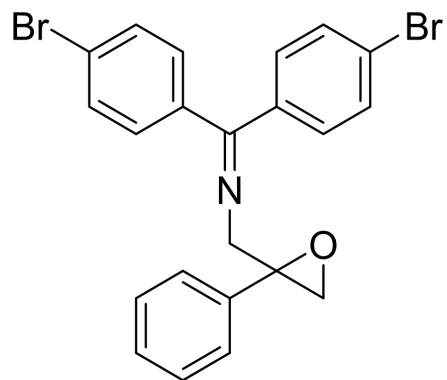




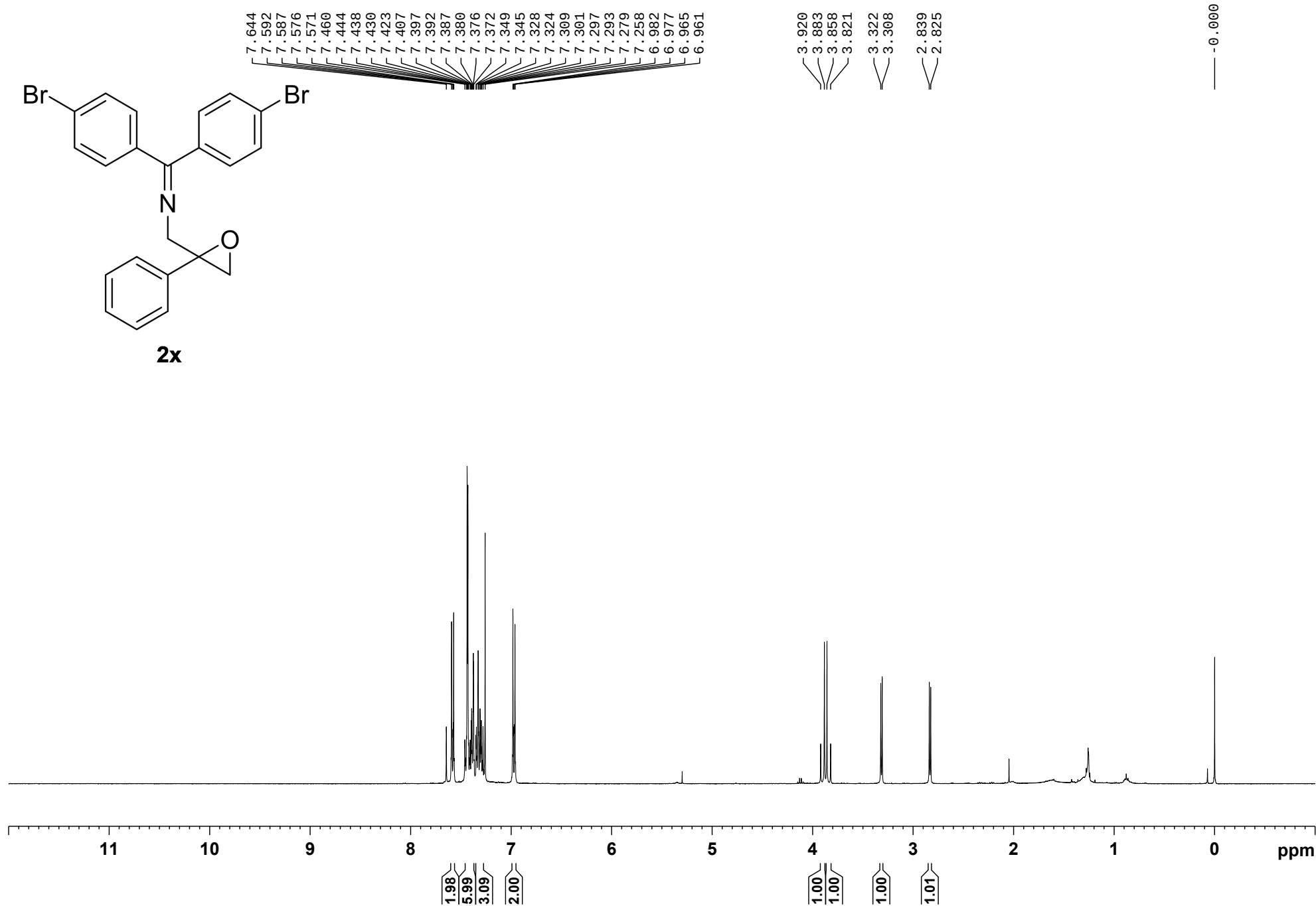


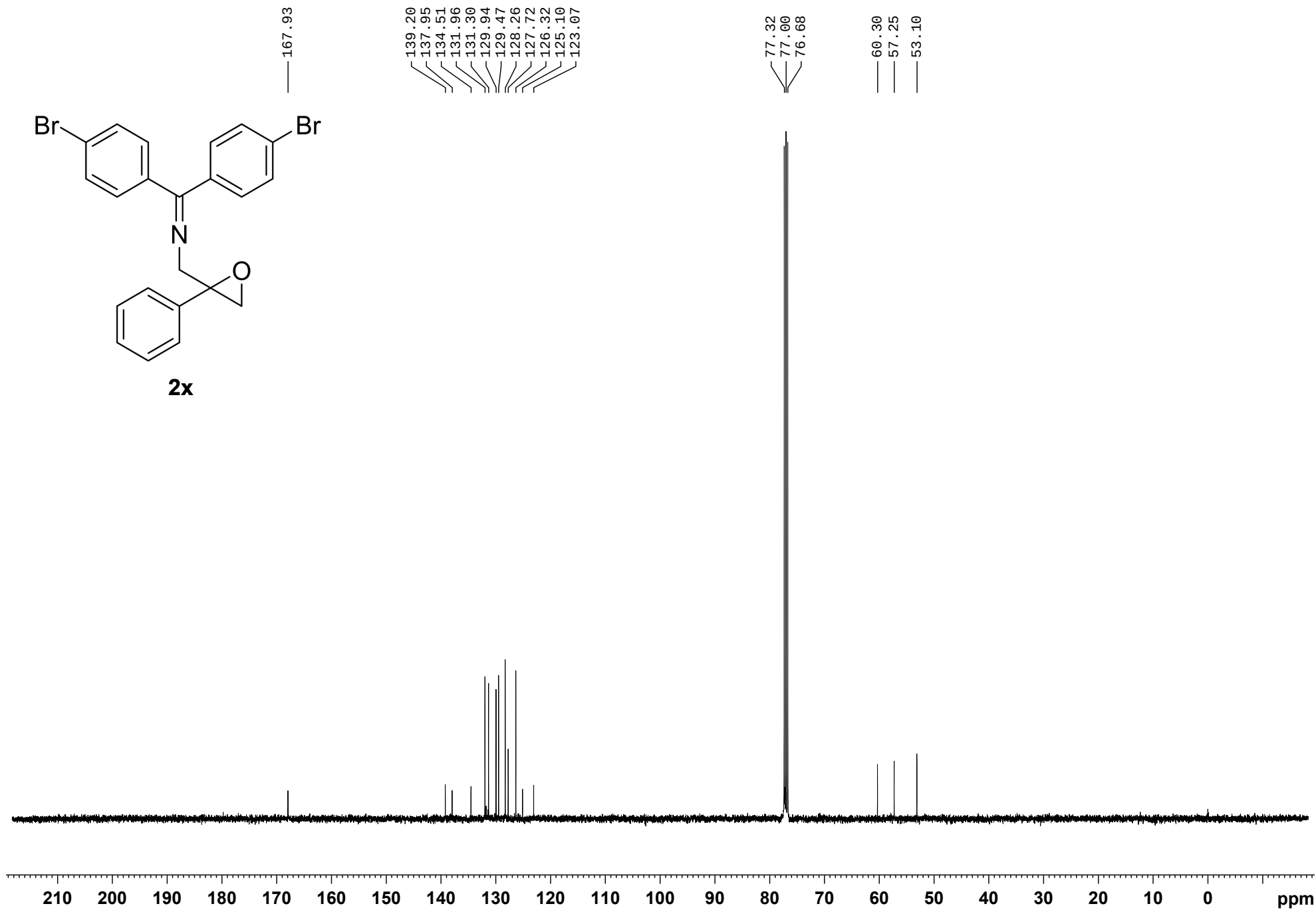
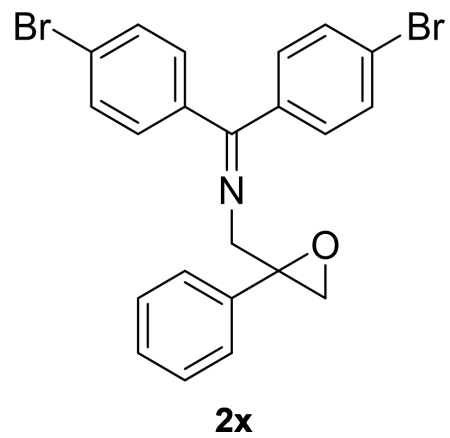
2w

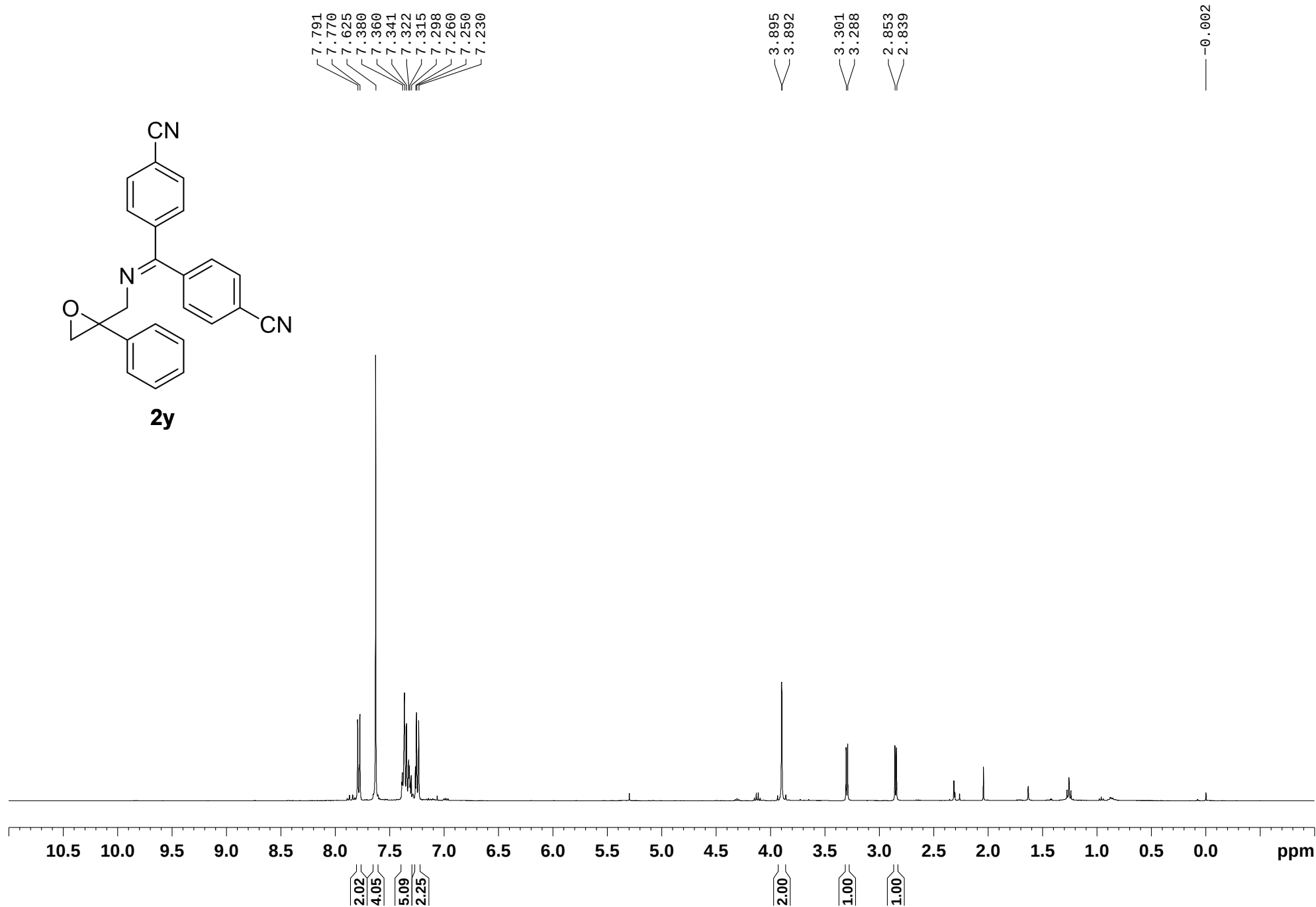
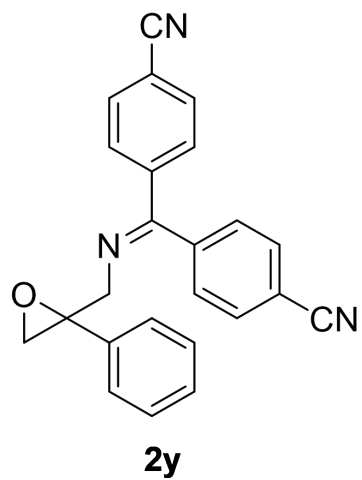


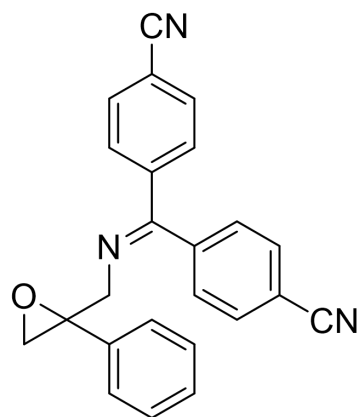


2x

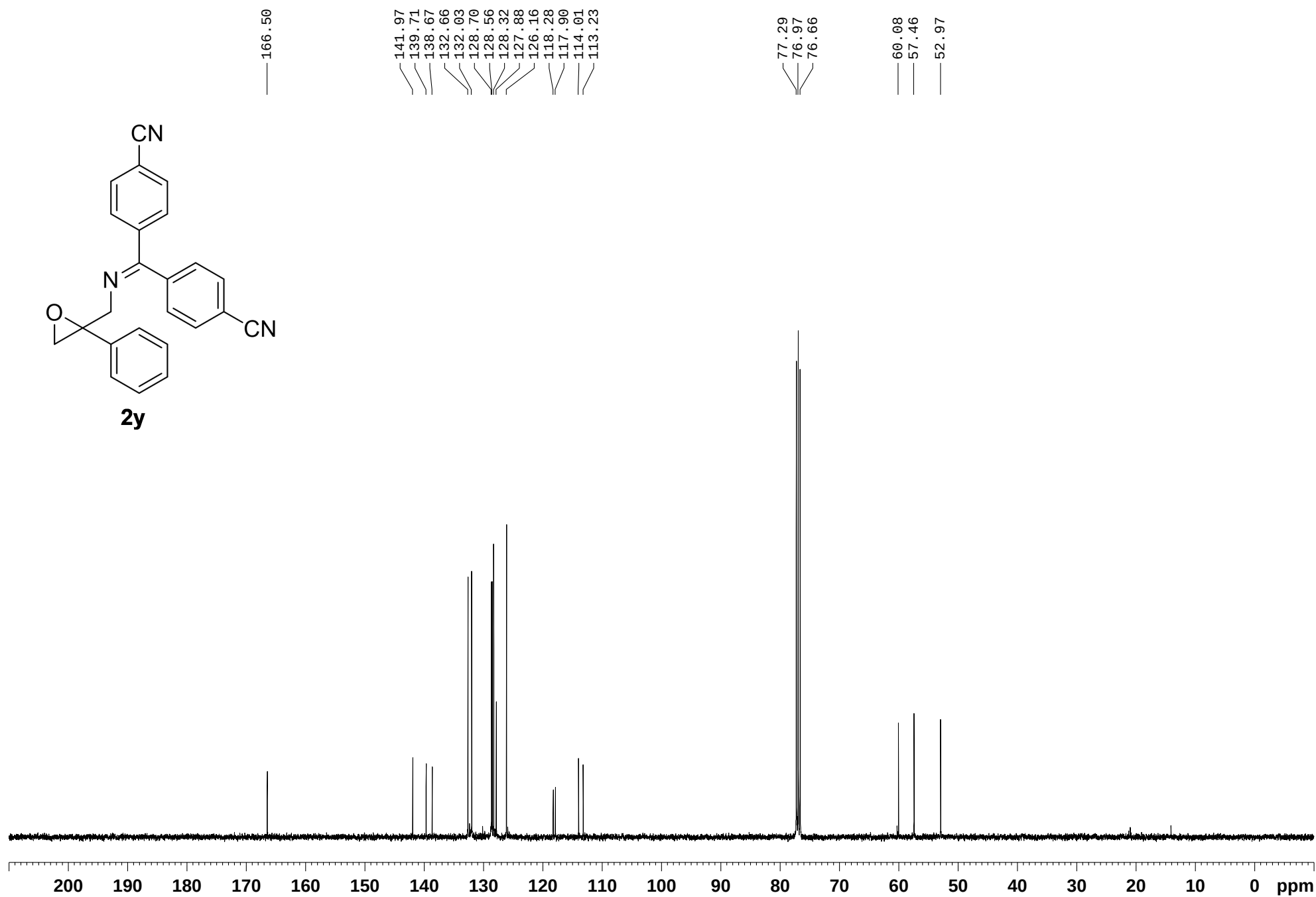


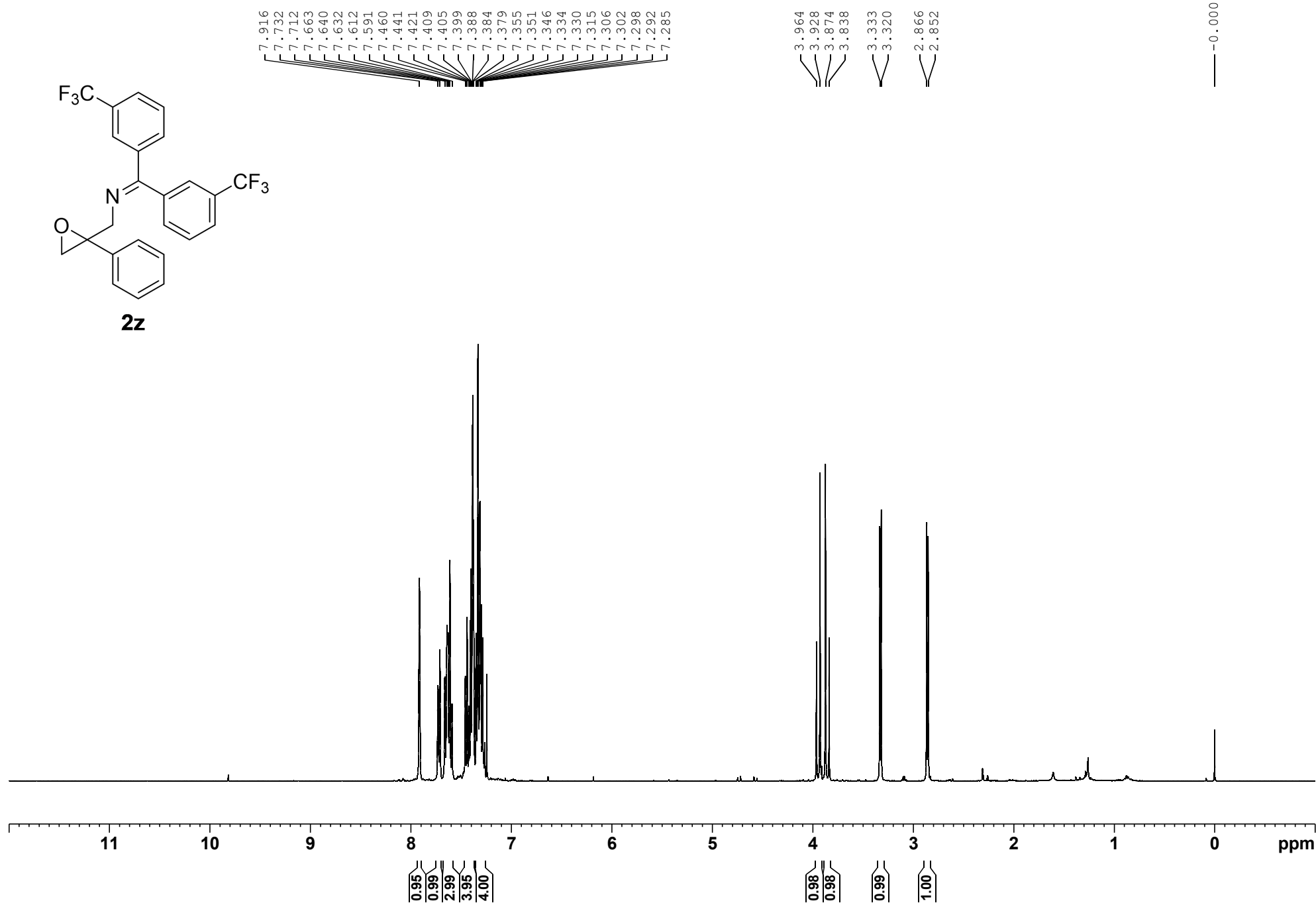
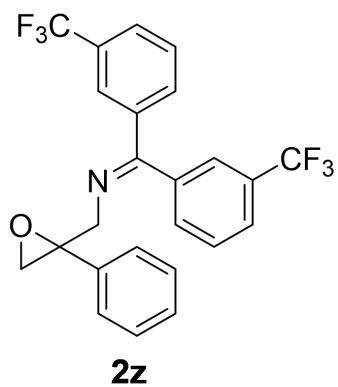


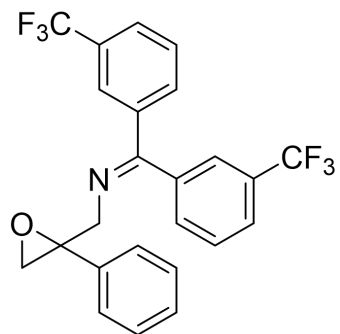




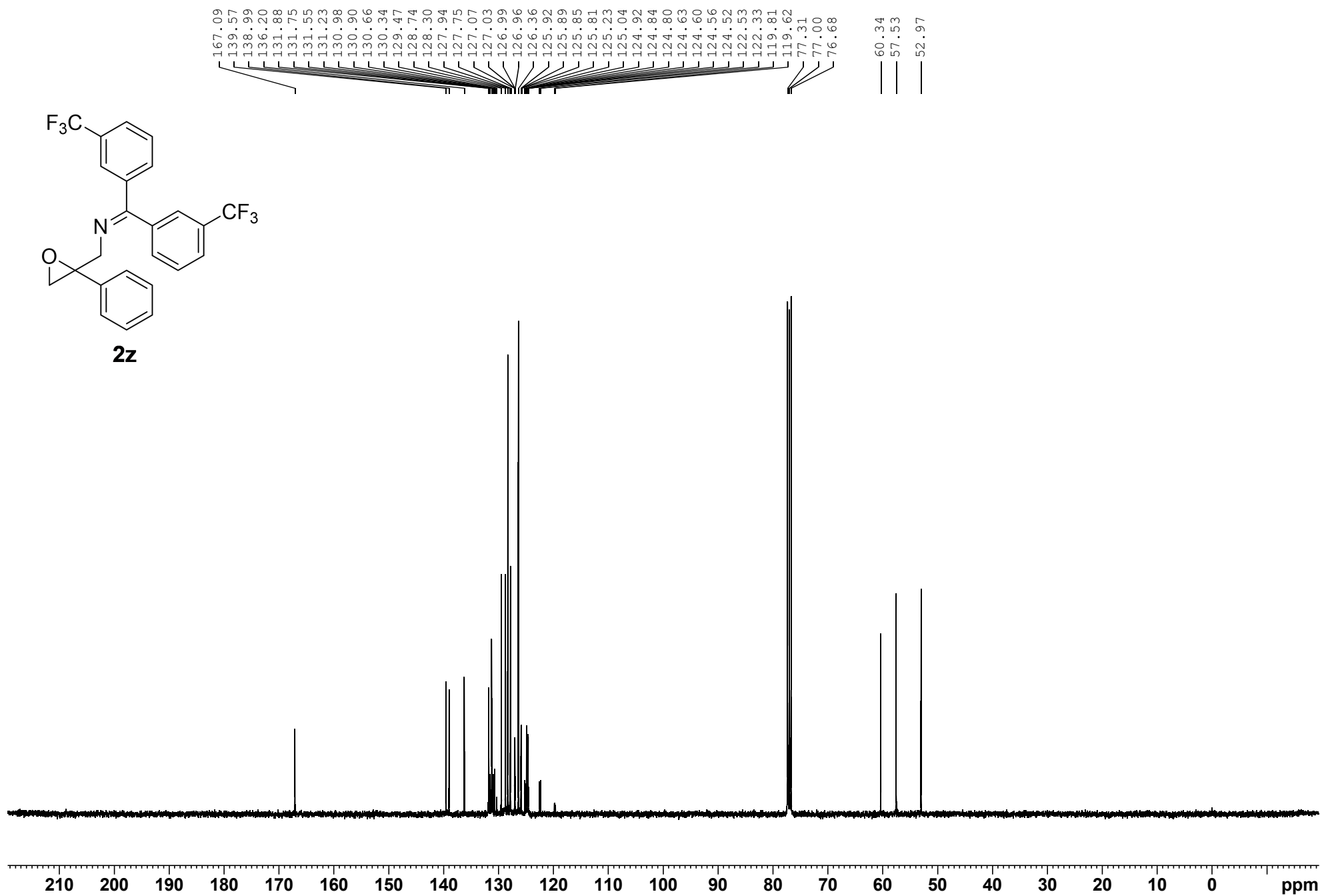
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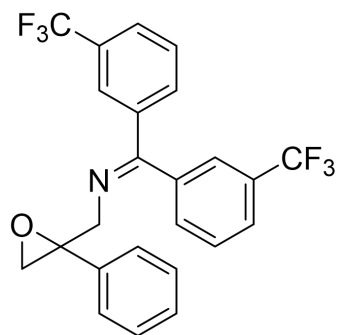






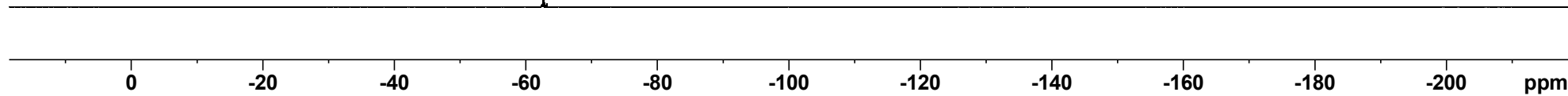
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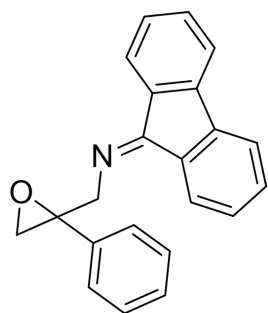




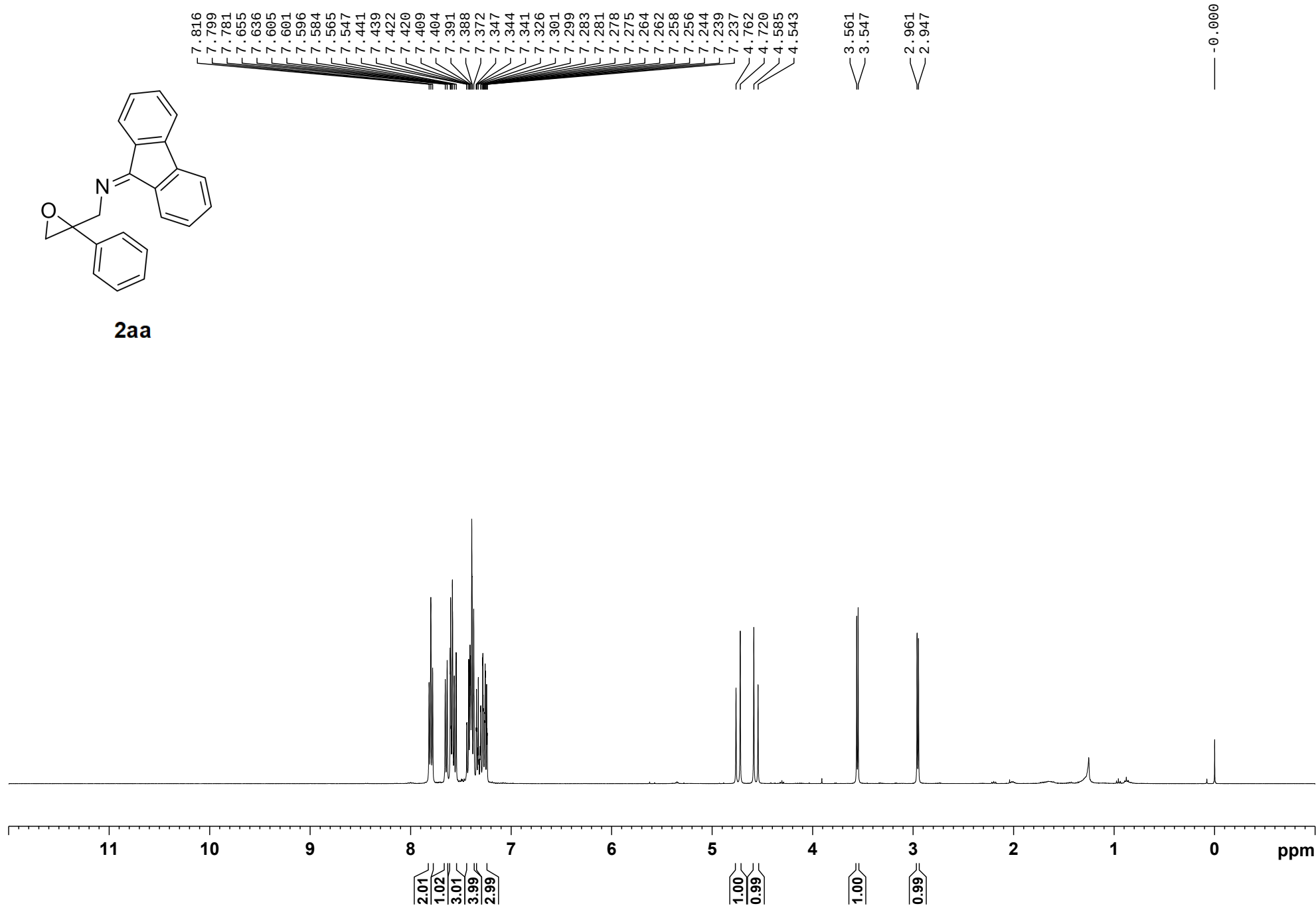
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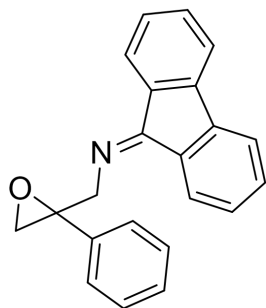
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-62.69





2aa





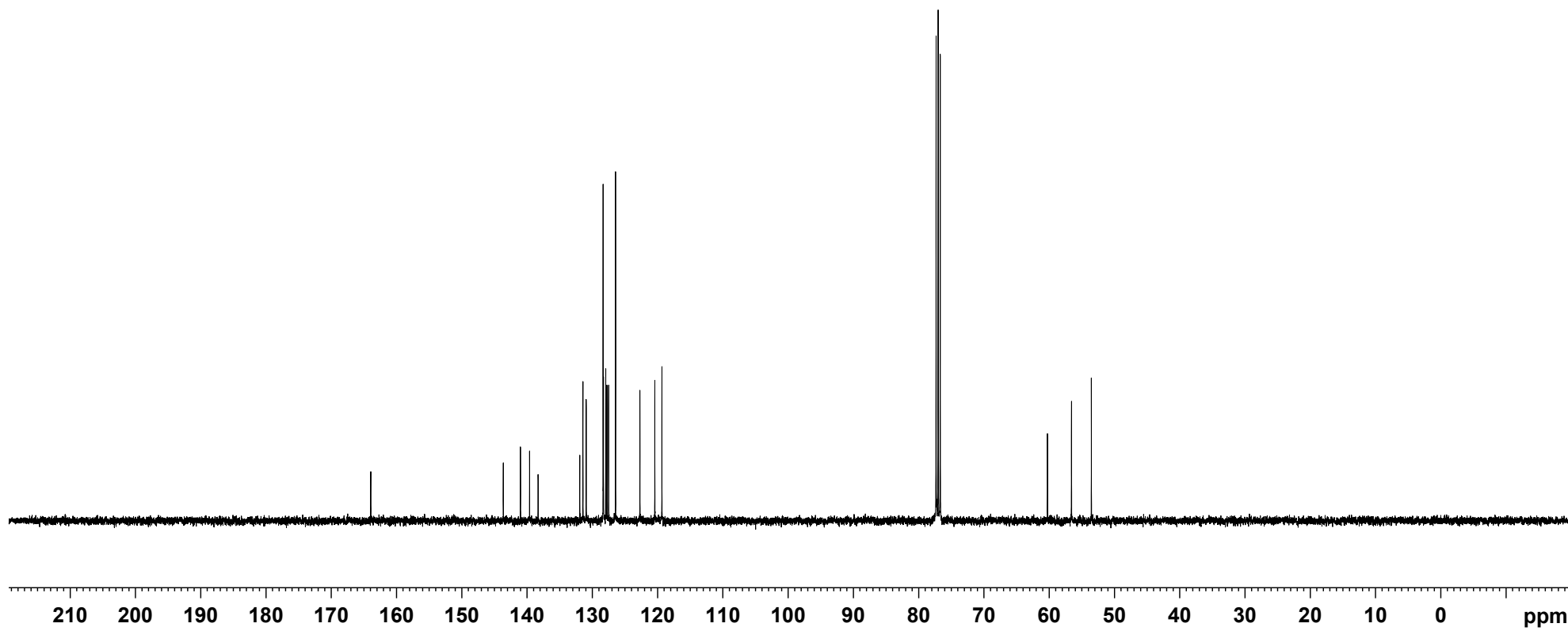
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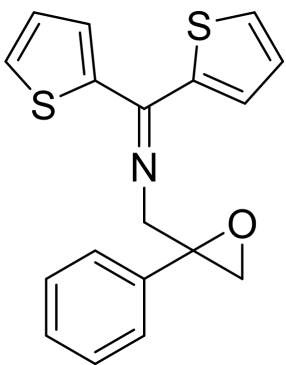
— 163.94

143.63
141.00
139.60
138.30
131.91
131.43
130.93
128.34
128.28
127.94
127.75
127.49
126.43
122.70
120.41
119.33

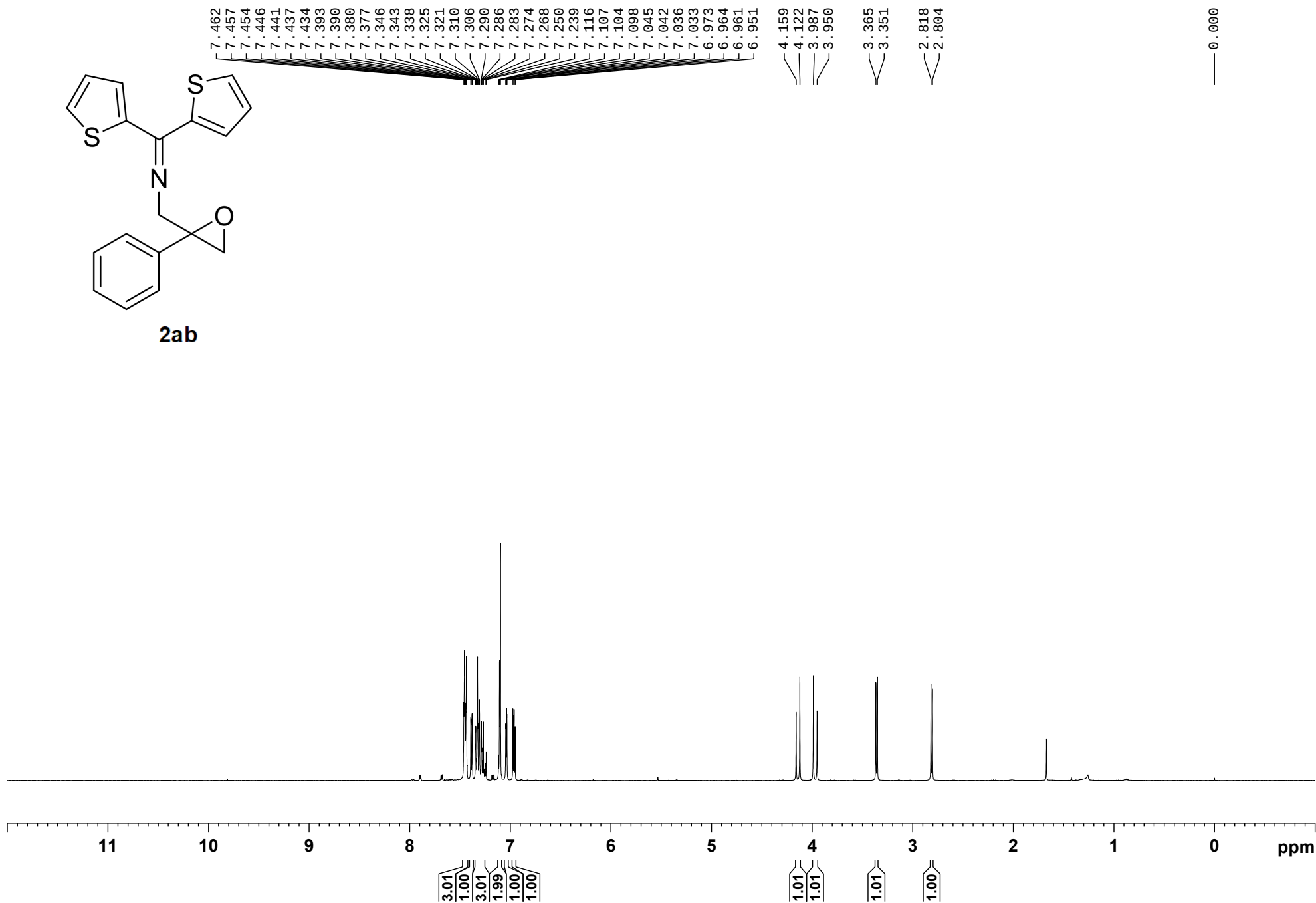
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77.00
76.68

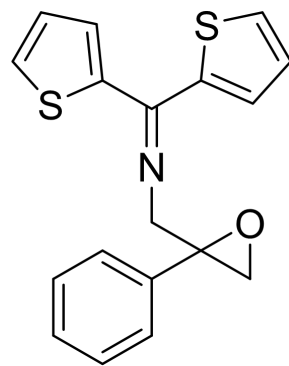
60.25
56.57
53.52





2ab



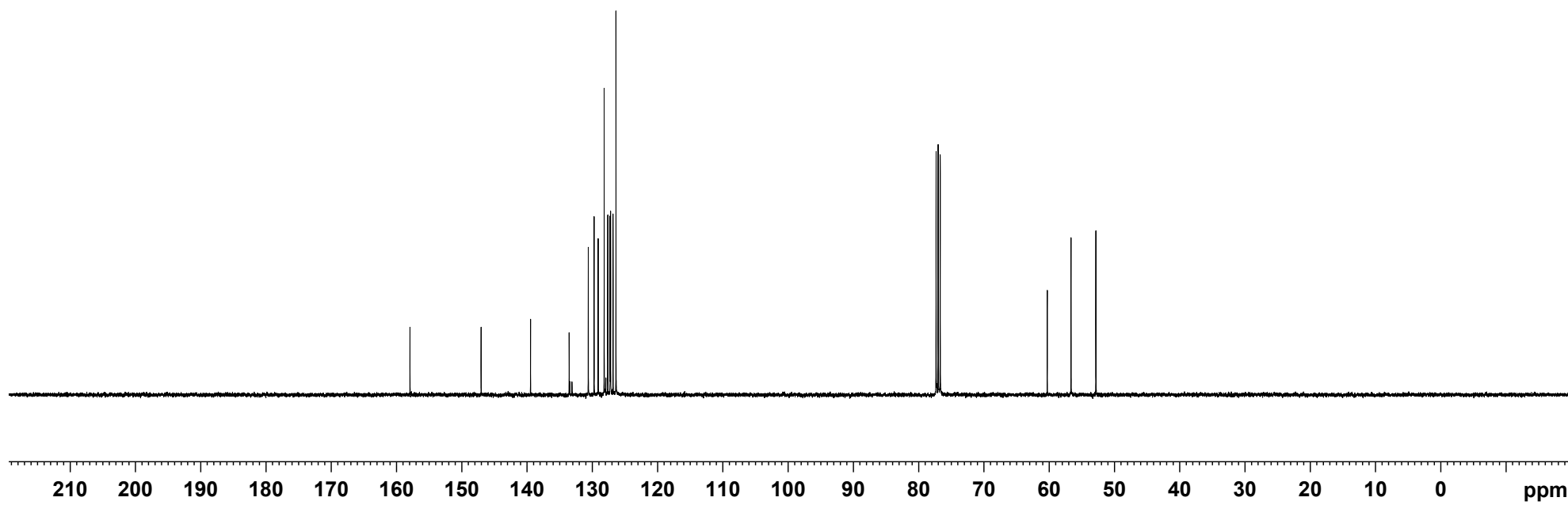


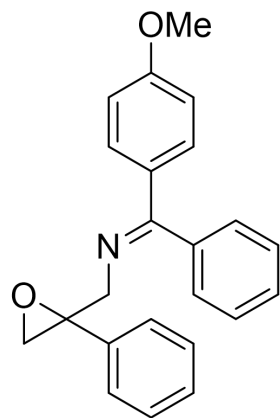
2ab

— 157.93
— 147.03
— 139.46
— 133.54
— 130.61
— 129.72
— 129.09
— 128.17
— 127.62
— 127.27
— 127.19
— 126.81
— 126.37

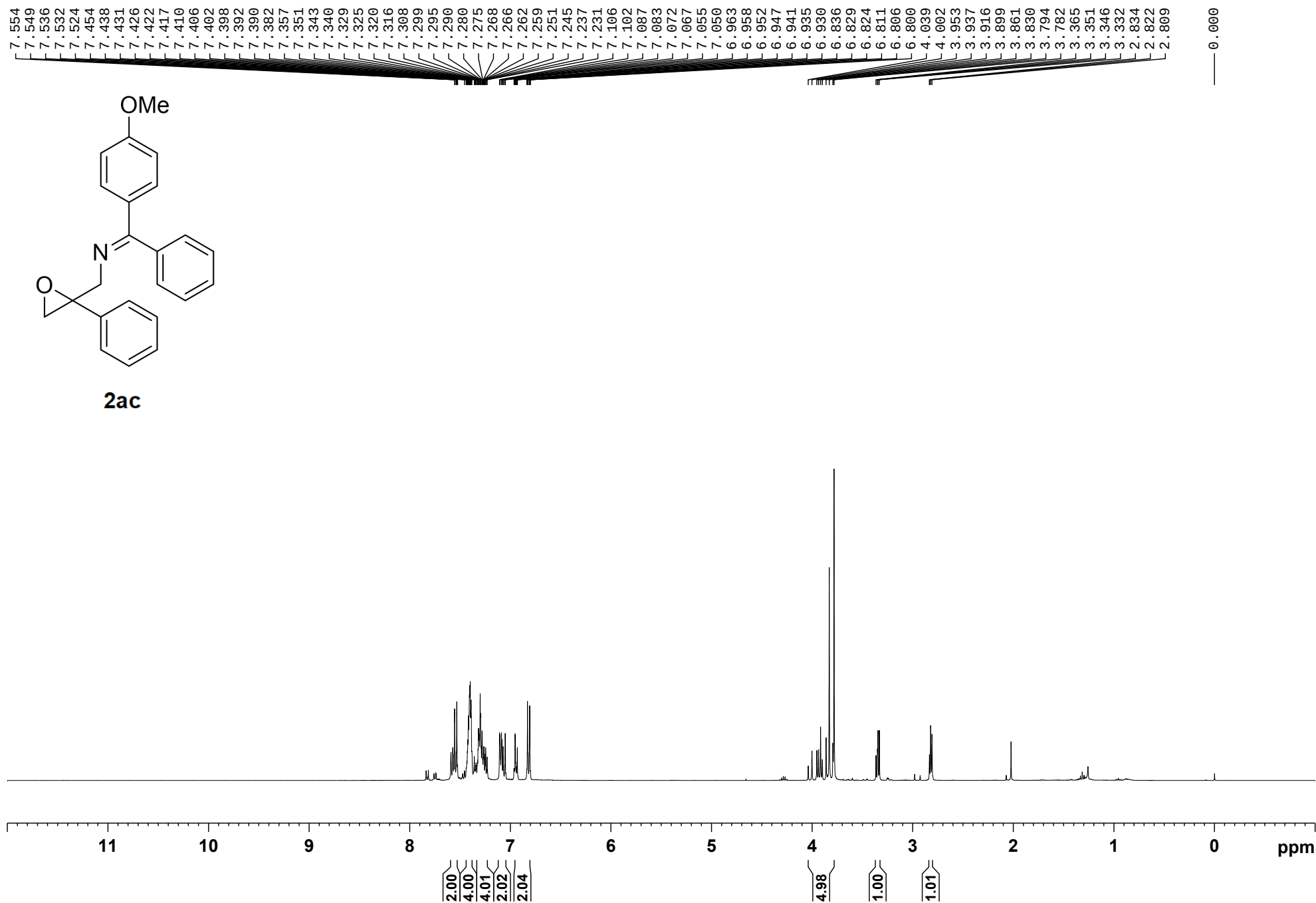
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77.00
76.68

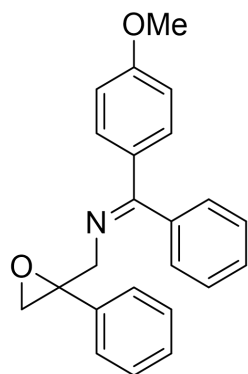
— 60.28
— 56.64
— 52.83



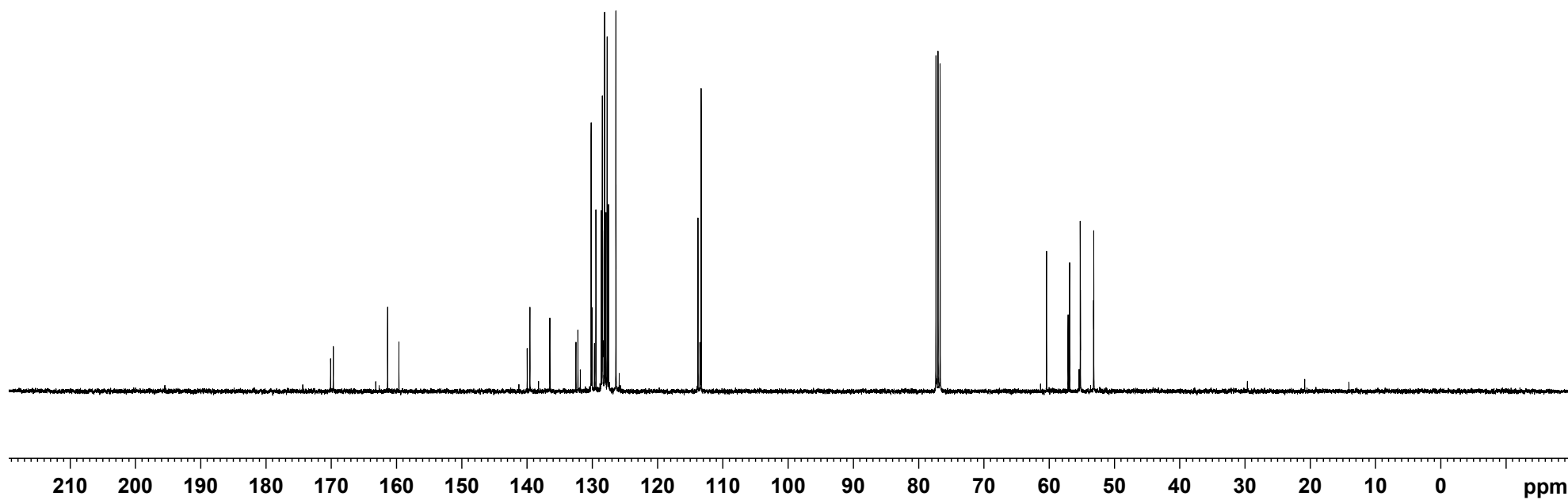
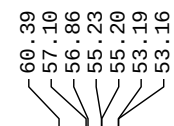
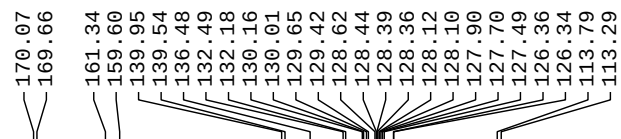


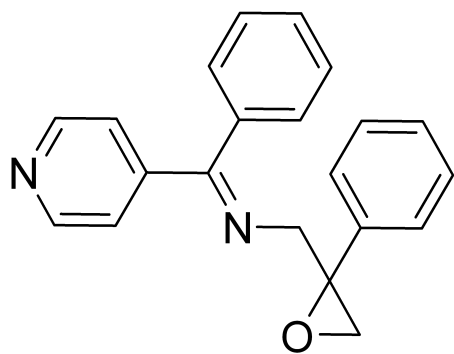
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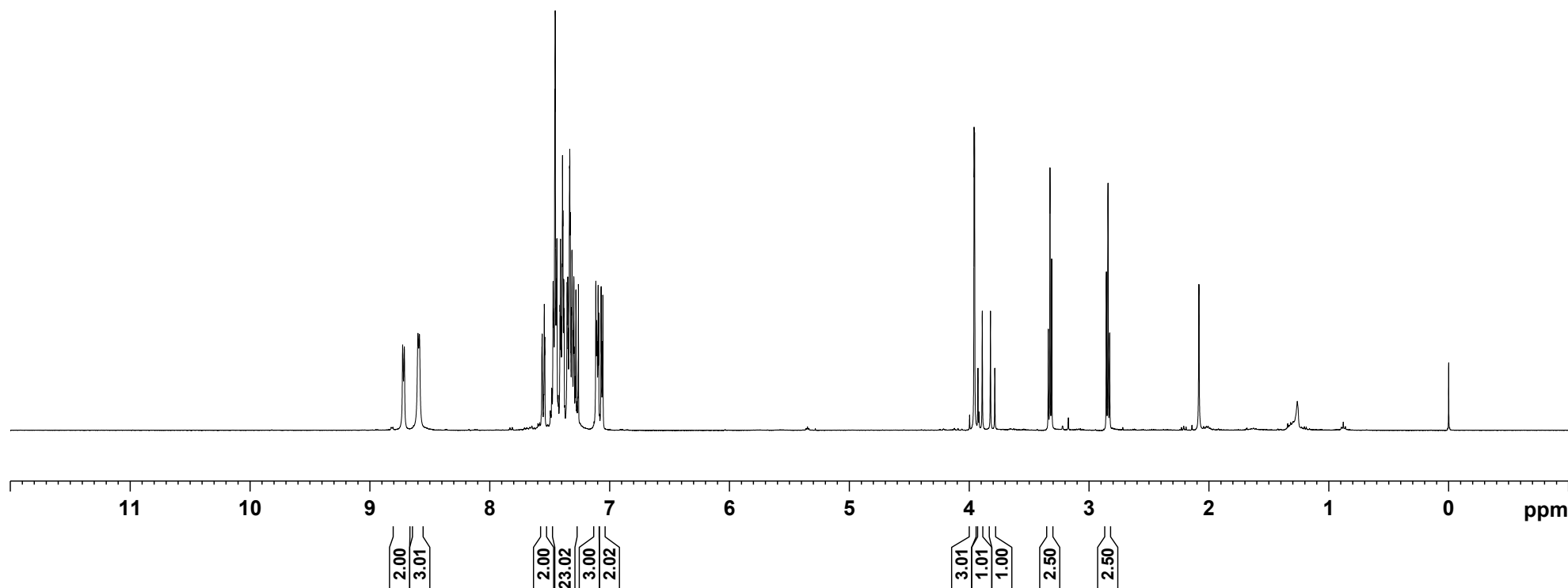


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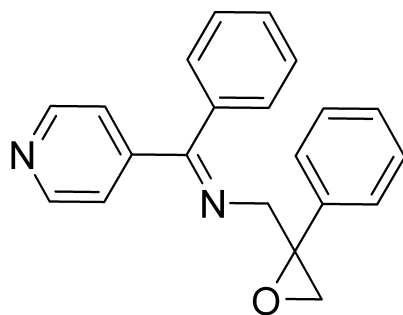


2ad



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8.586
7.562
7.549
7.544
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7.483
7.479
7.471
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7.464
7.457
7.453
7.443
7.439
7.429
7.413
7.410
7.404
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7.383
7.379
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7.313
7.302
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7.294
7.287
7.281
7.273
7.266
7.260
7.115
7.108
7.103
7.095
7.091
7.070
7.066
7.059
7.056
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3.956
3.928
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2.829

0.000

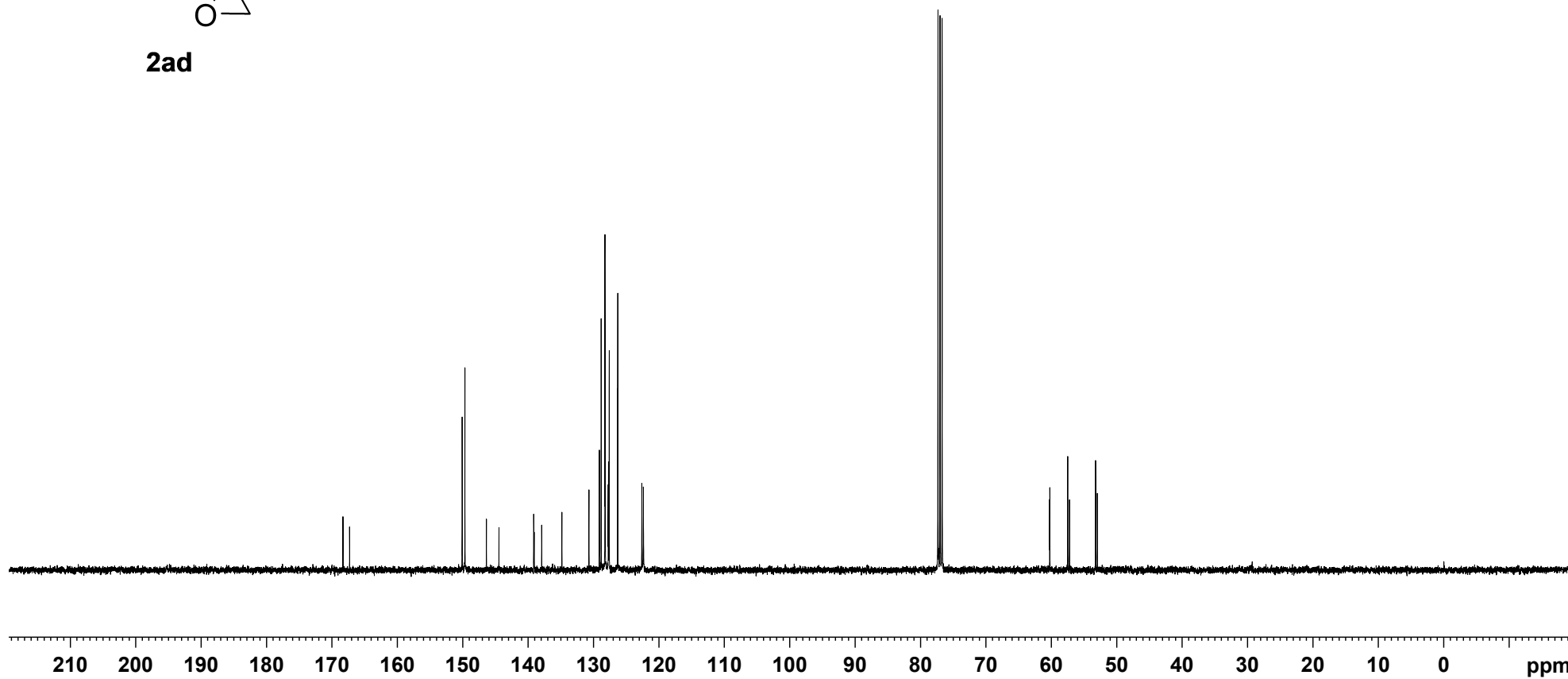


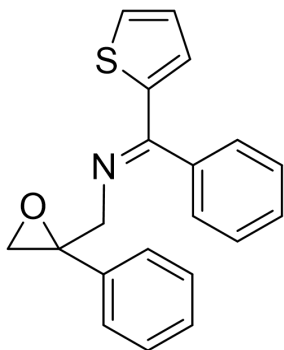
2ad

168.30
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146.37
144.45
139.13
139.07
137.91
134.83
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129.10
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128.24
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127.74
127.70
127.59
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122.60
122.36

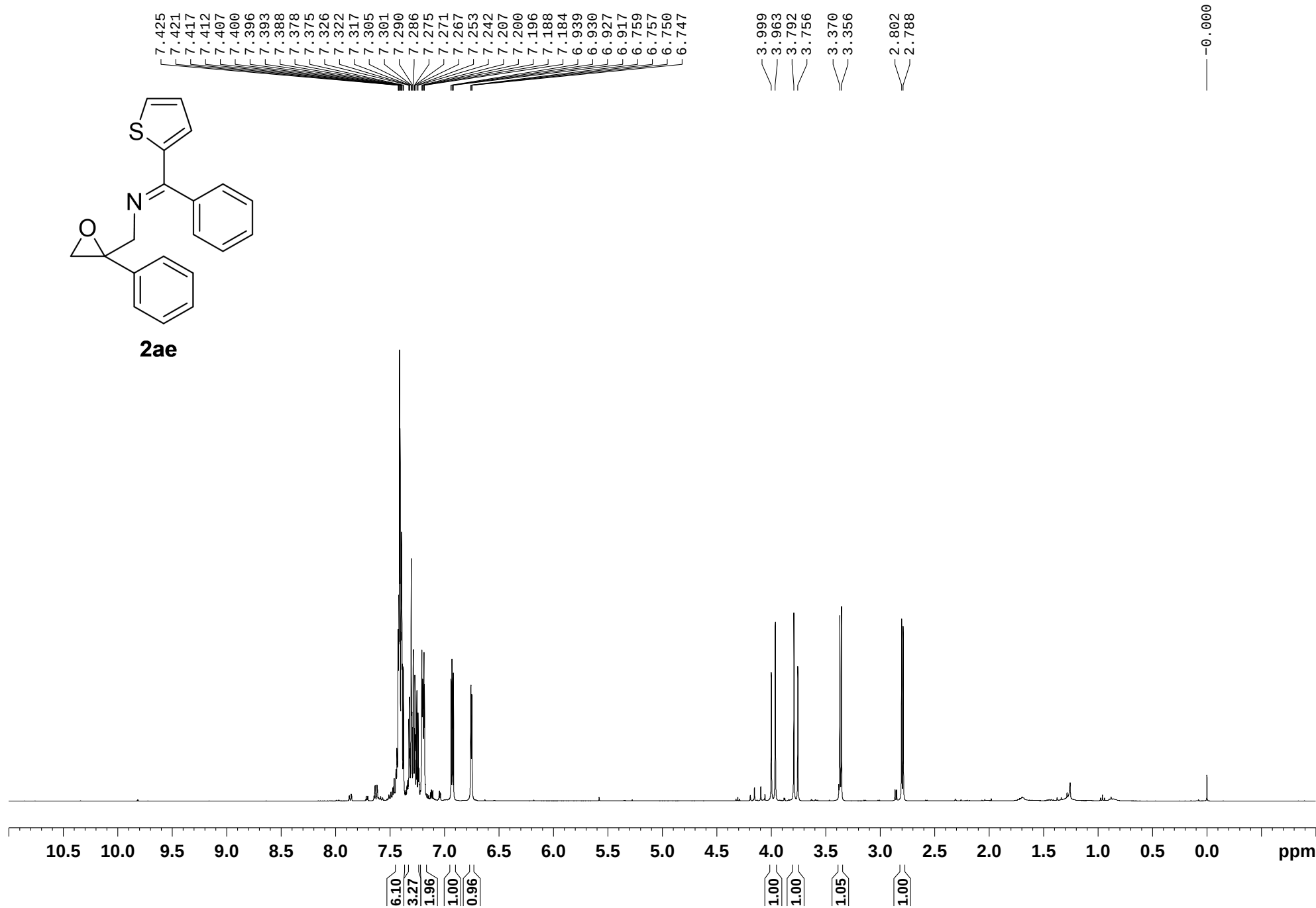
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77.00
76.69

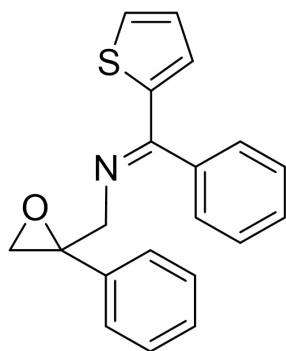
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57.47
57.20
53.21
52.94



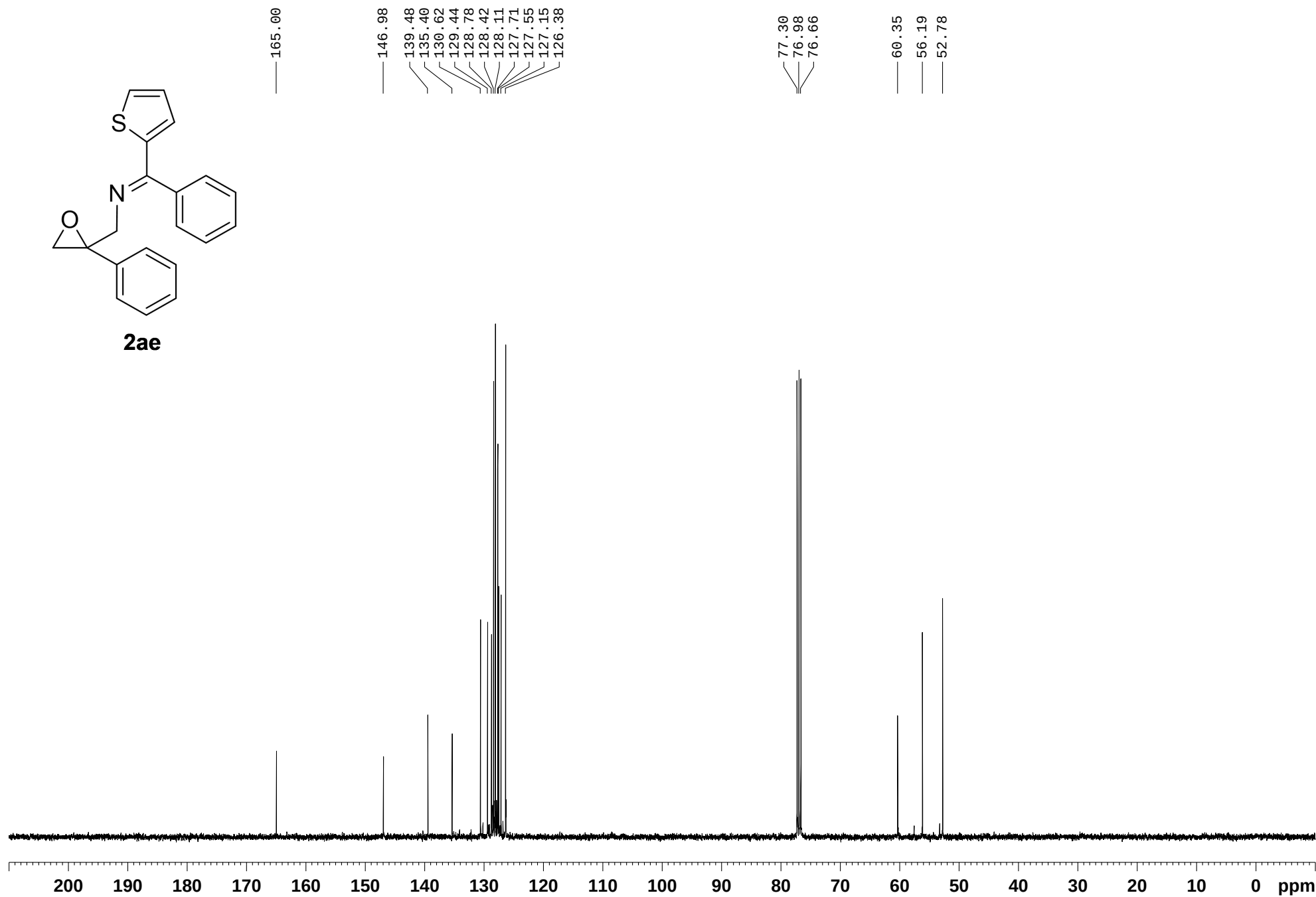


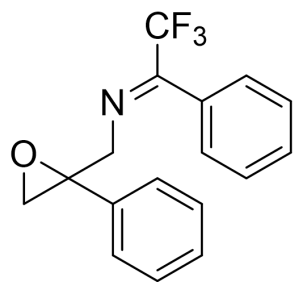
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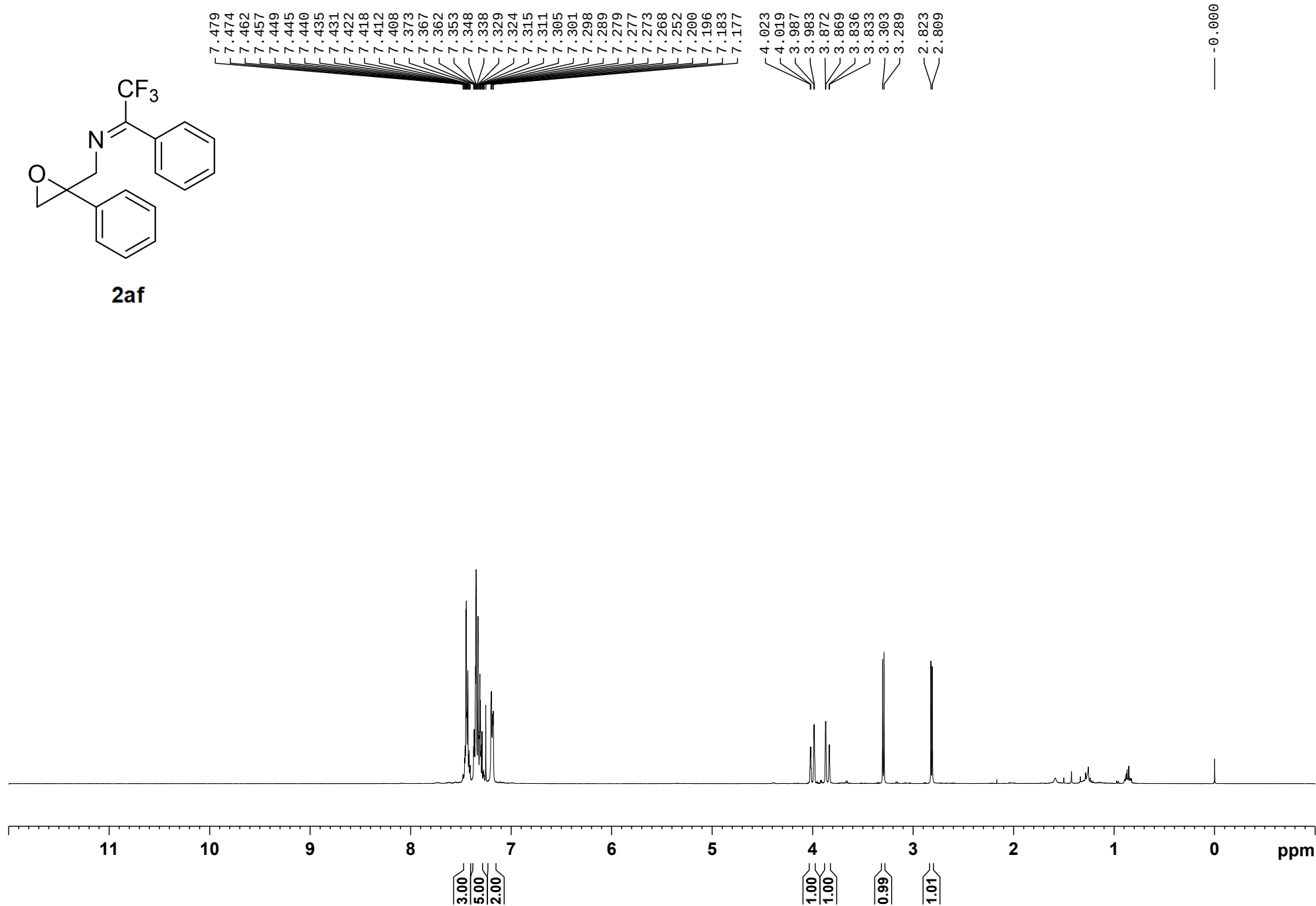


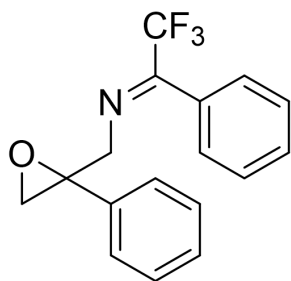
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2af





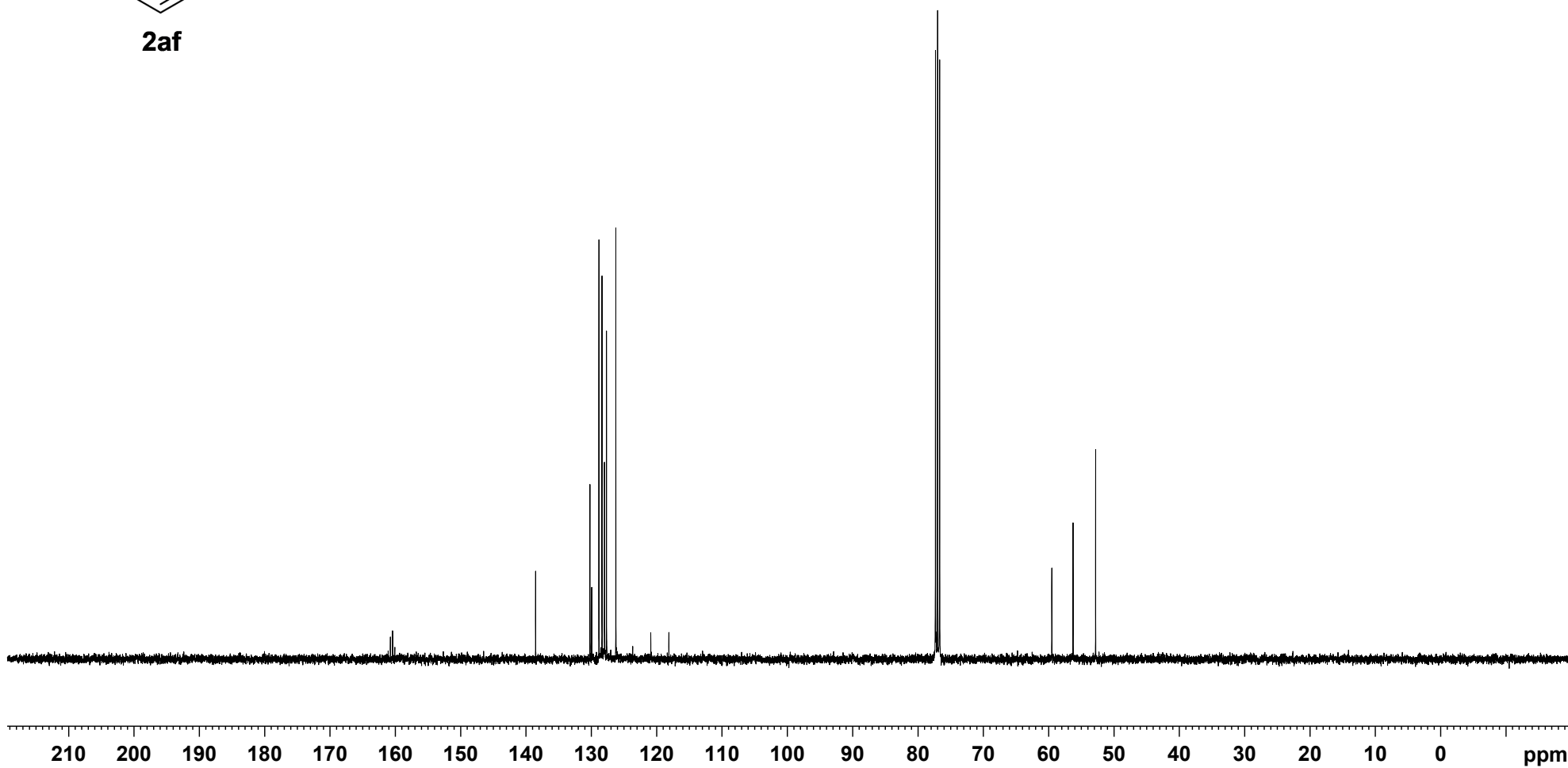
2af

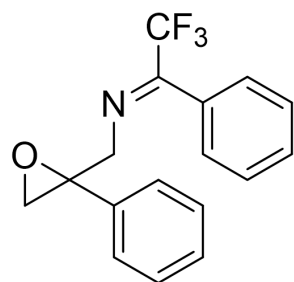
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160.74
160.40
160.06

138.51
130.21
129.94
128.84
128.36
127.98
127.68
126.26
123.67
120.89
118.12
115.35

77.32
77.00
76.69

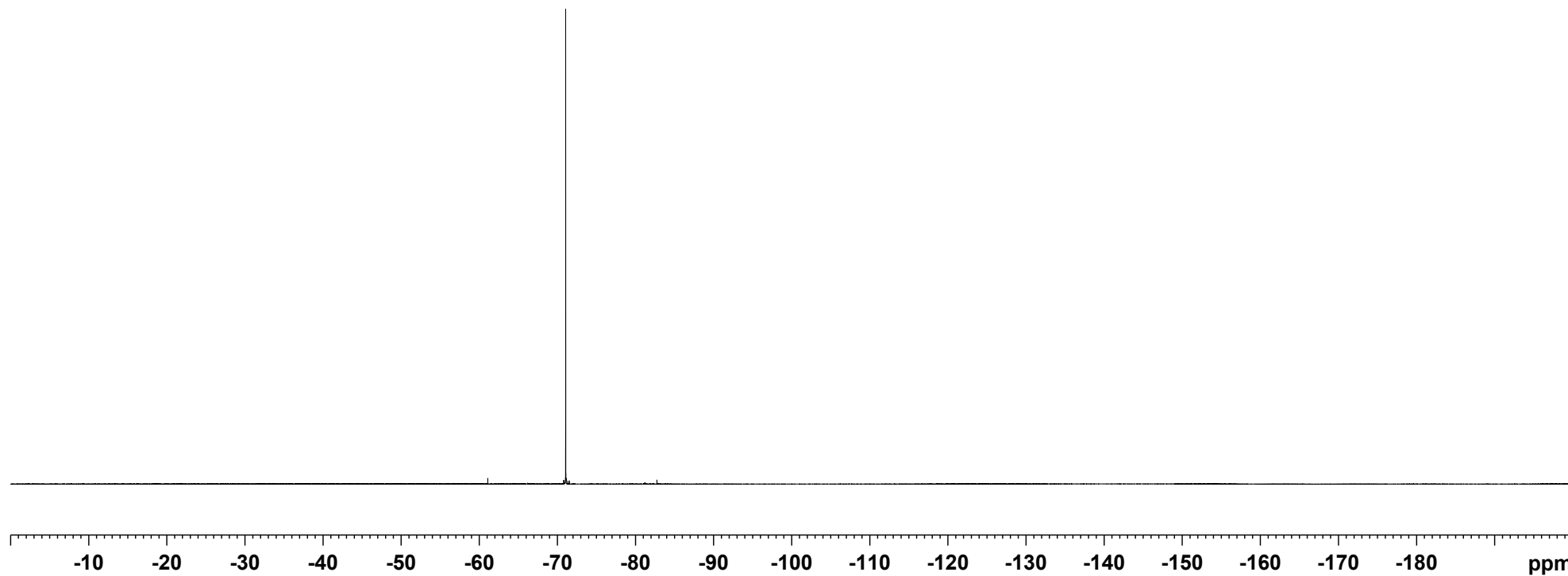
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56.28
52.82

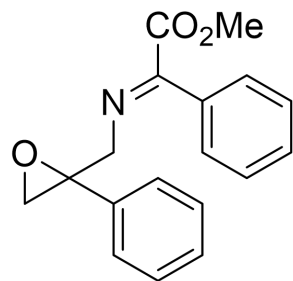




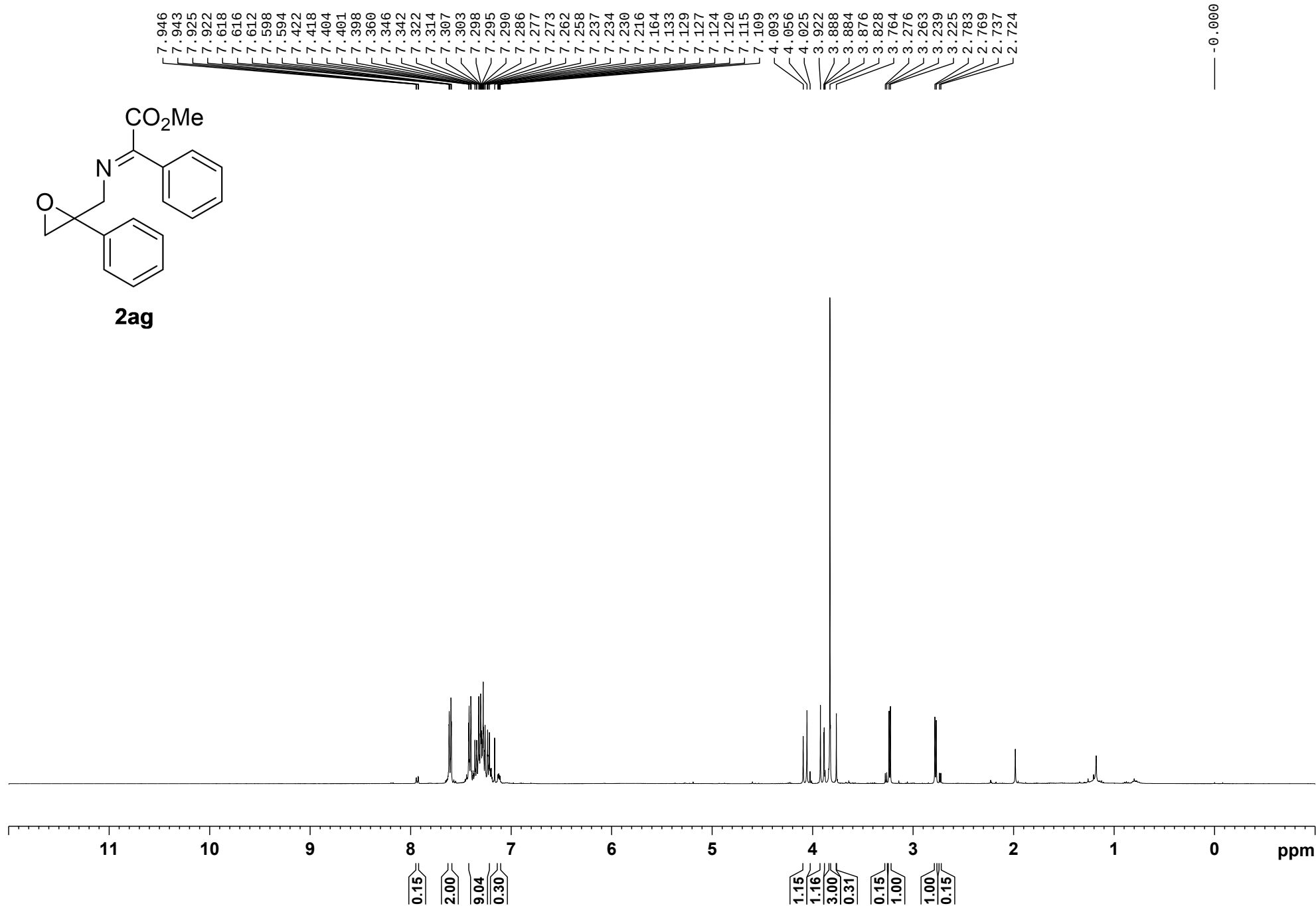
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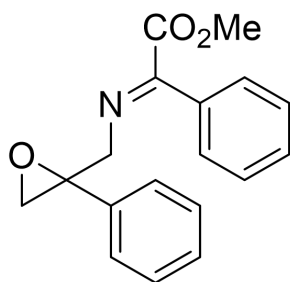
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2ag





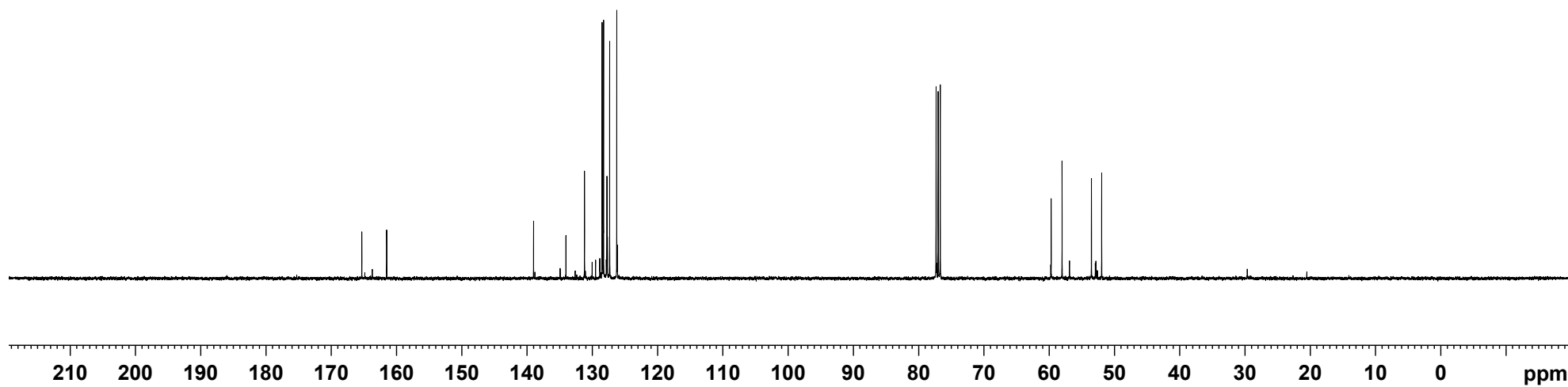
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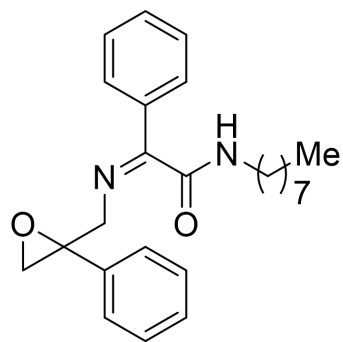
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163.70
161.50

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134.03
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127.68
127.34
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126.16

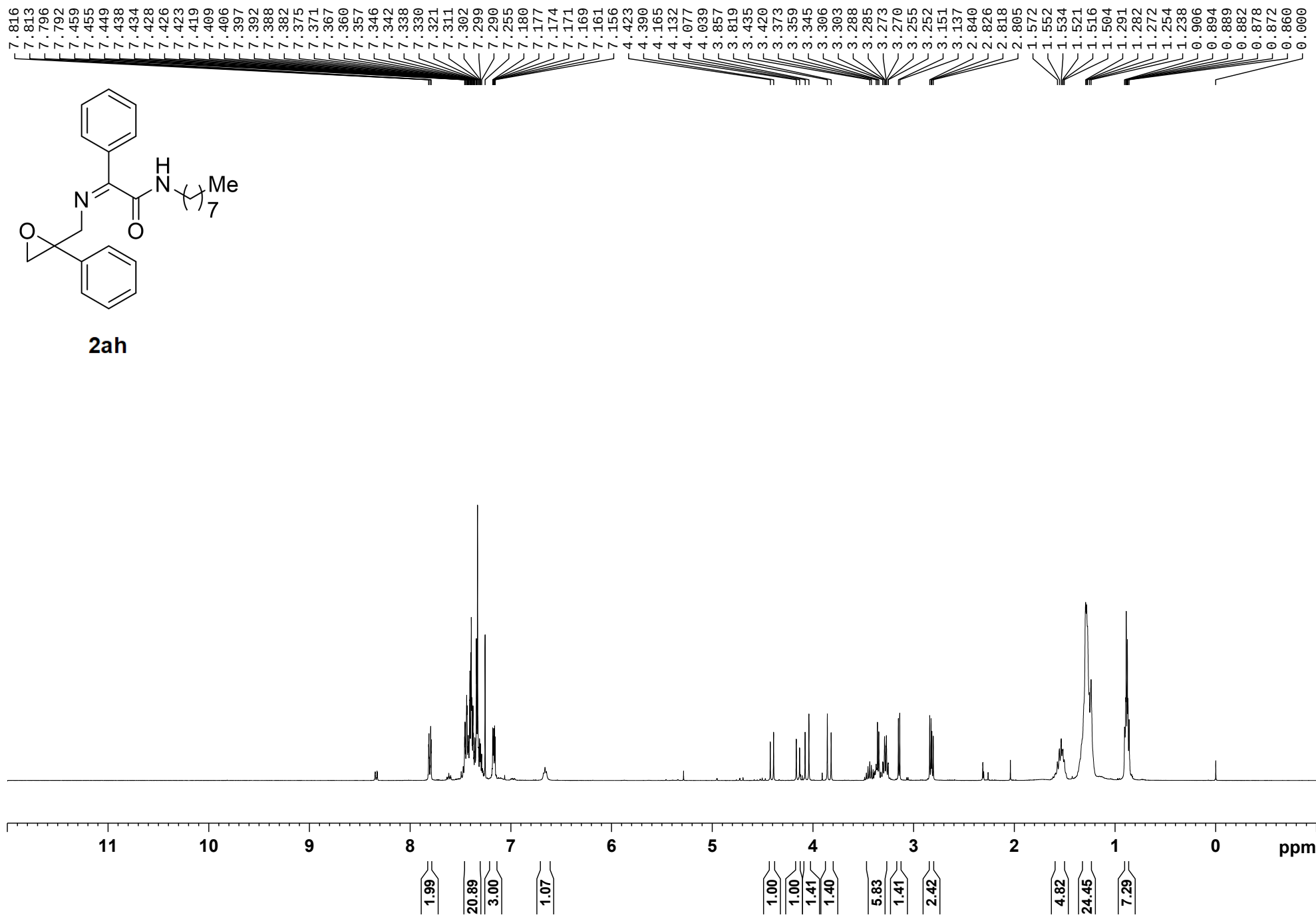
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77.00
76.68

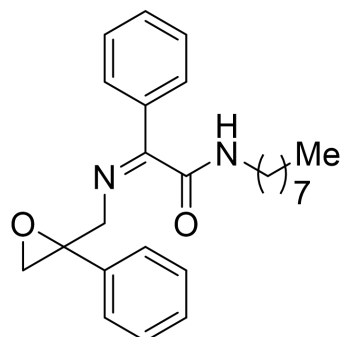
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58.02
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53.51
52.92
52.83
51.94





2ah





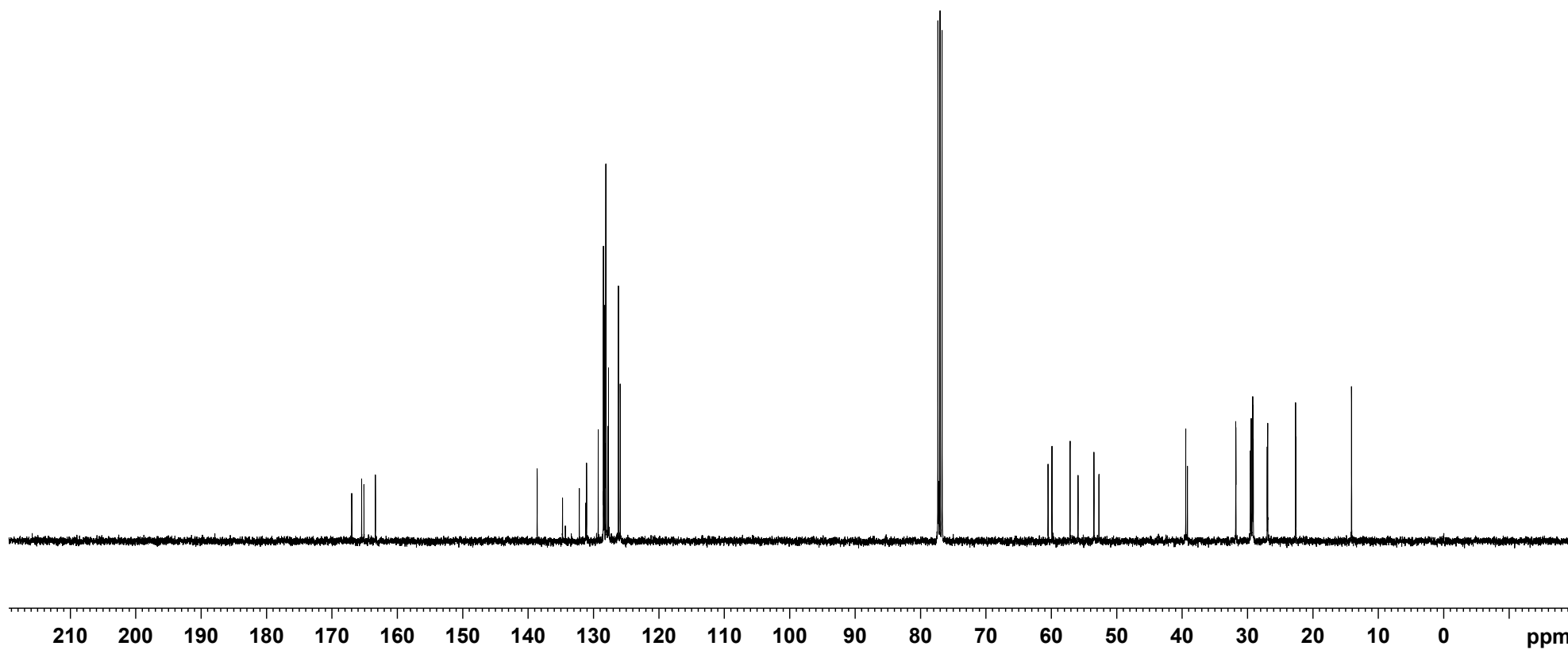
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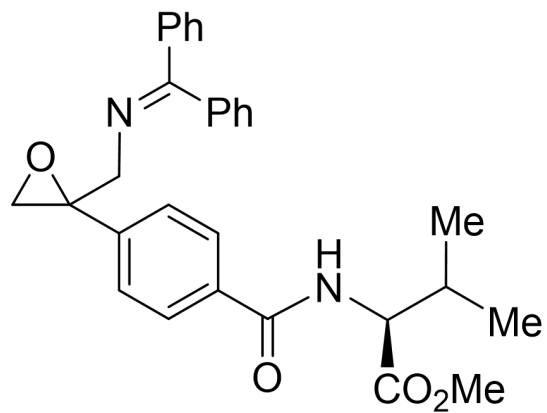
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165.09
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132.16
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128.30
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128.06
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127.69
126.18
125.89

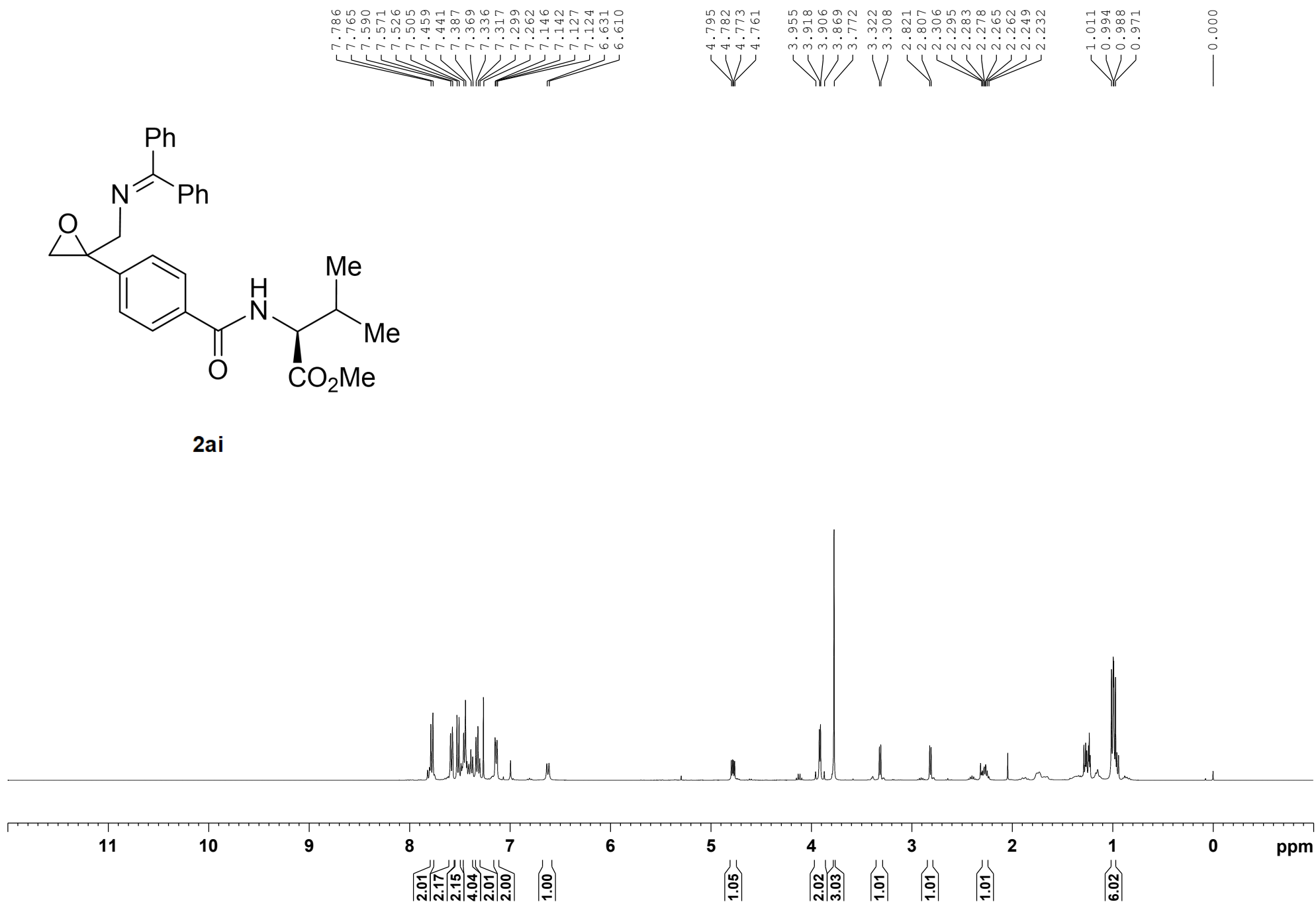
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77.00
76.68

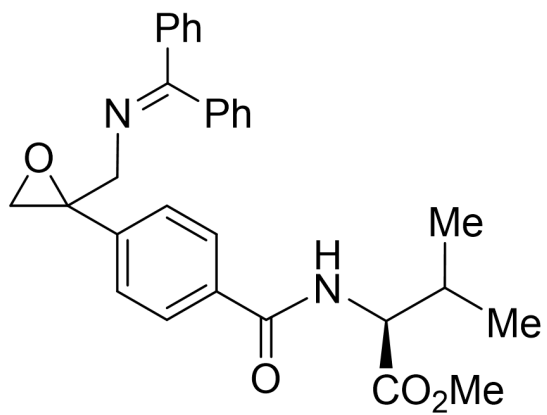
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22.62
22.60
14.07



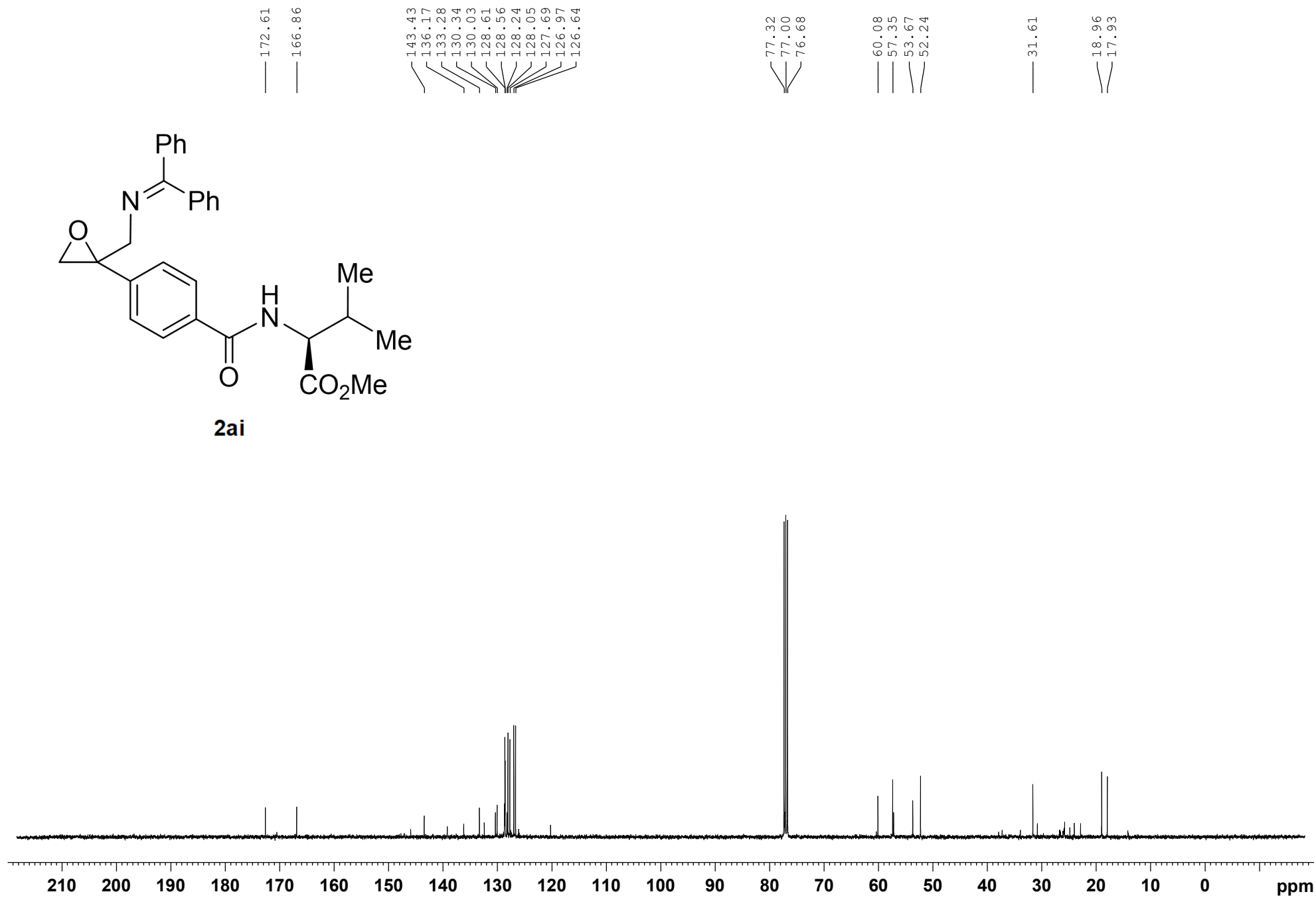


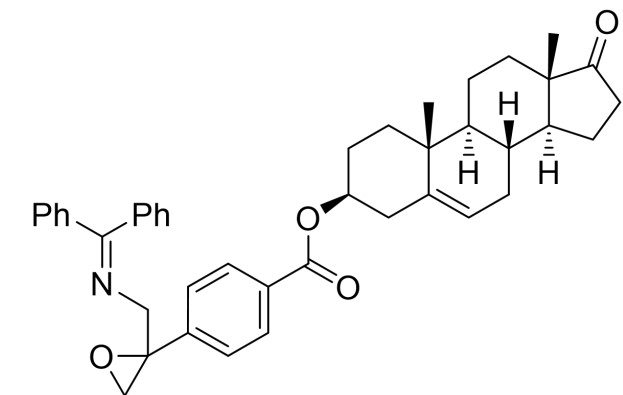
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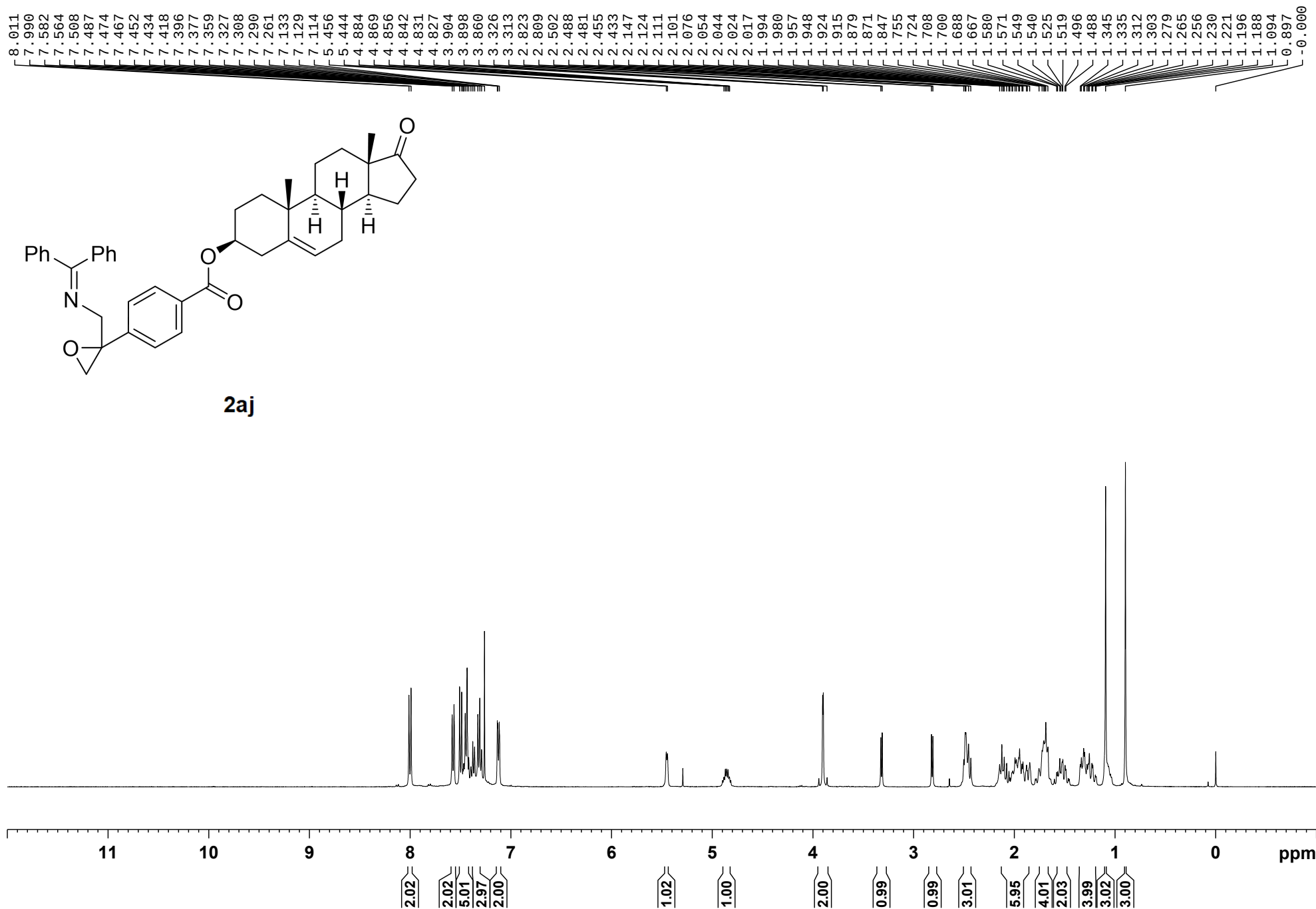


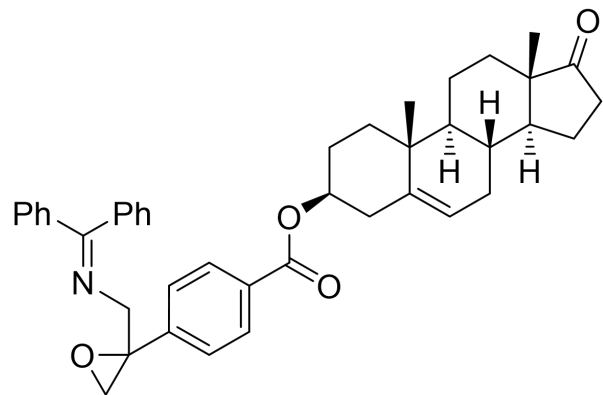
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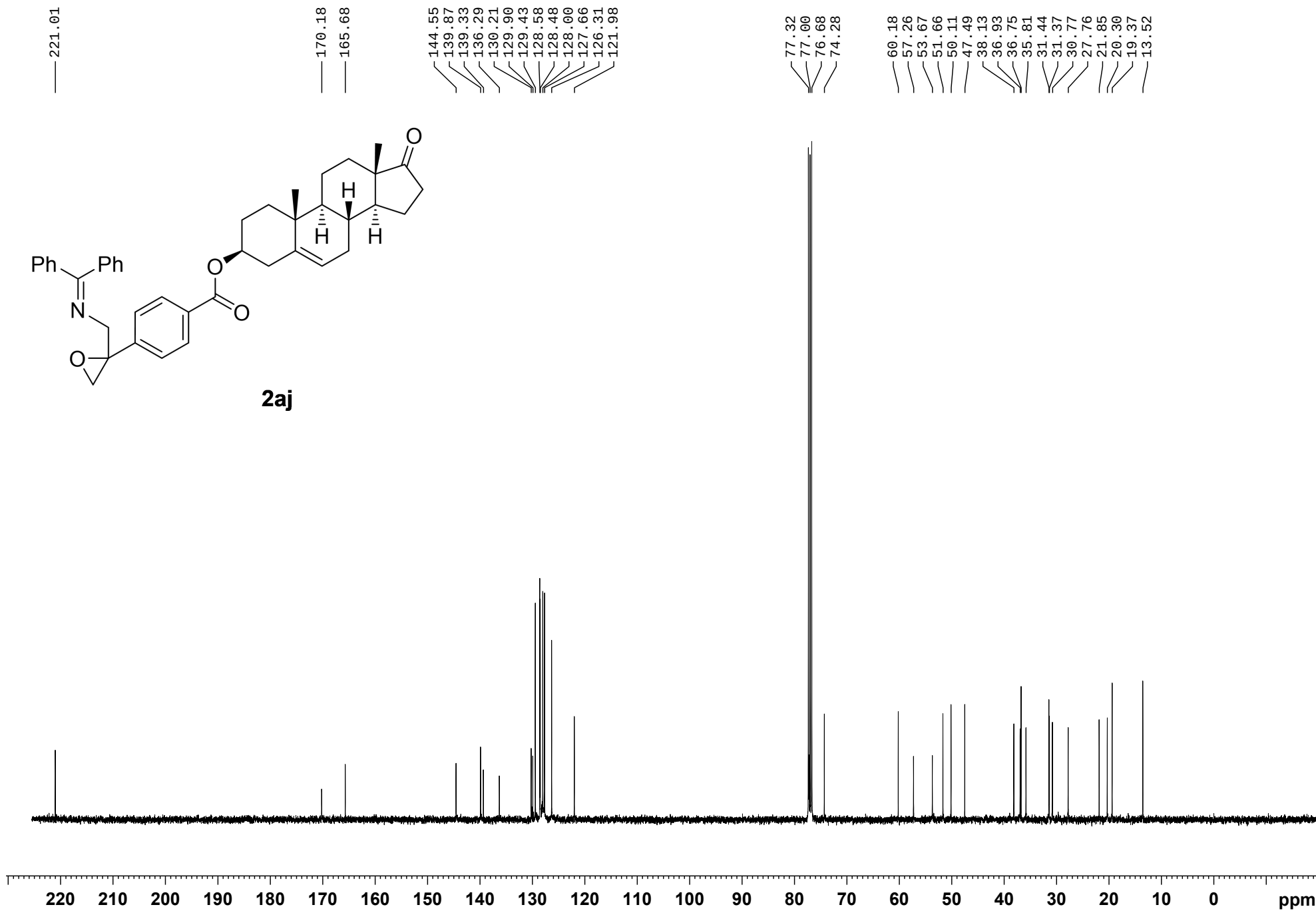


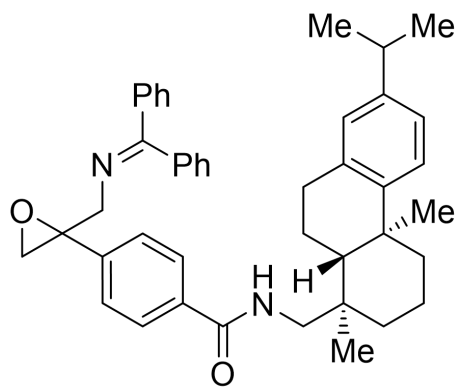
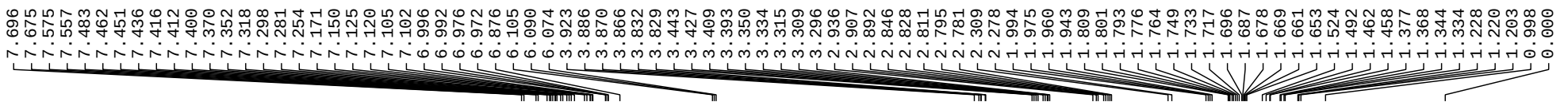
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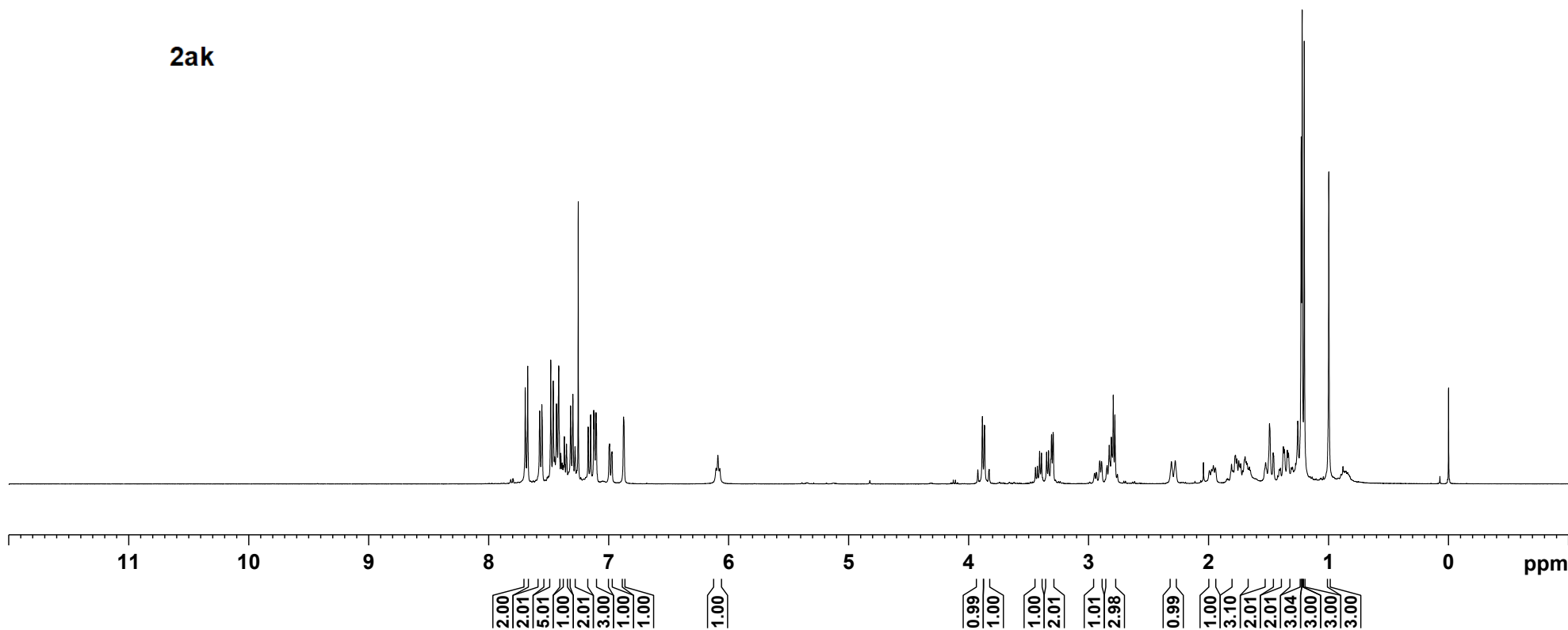


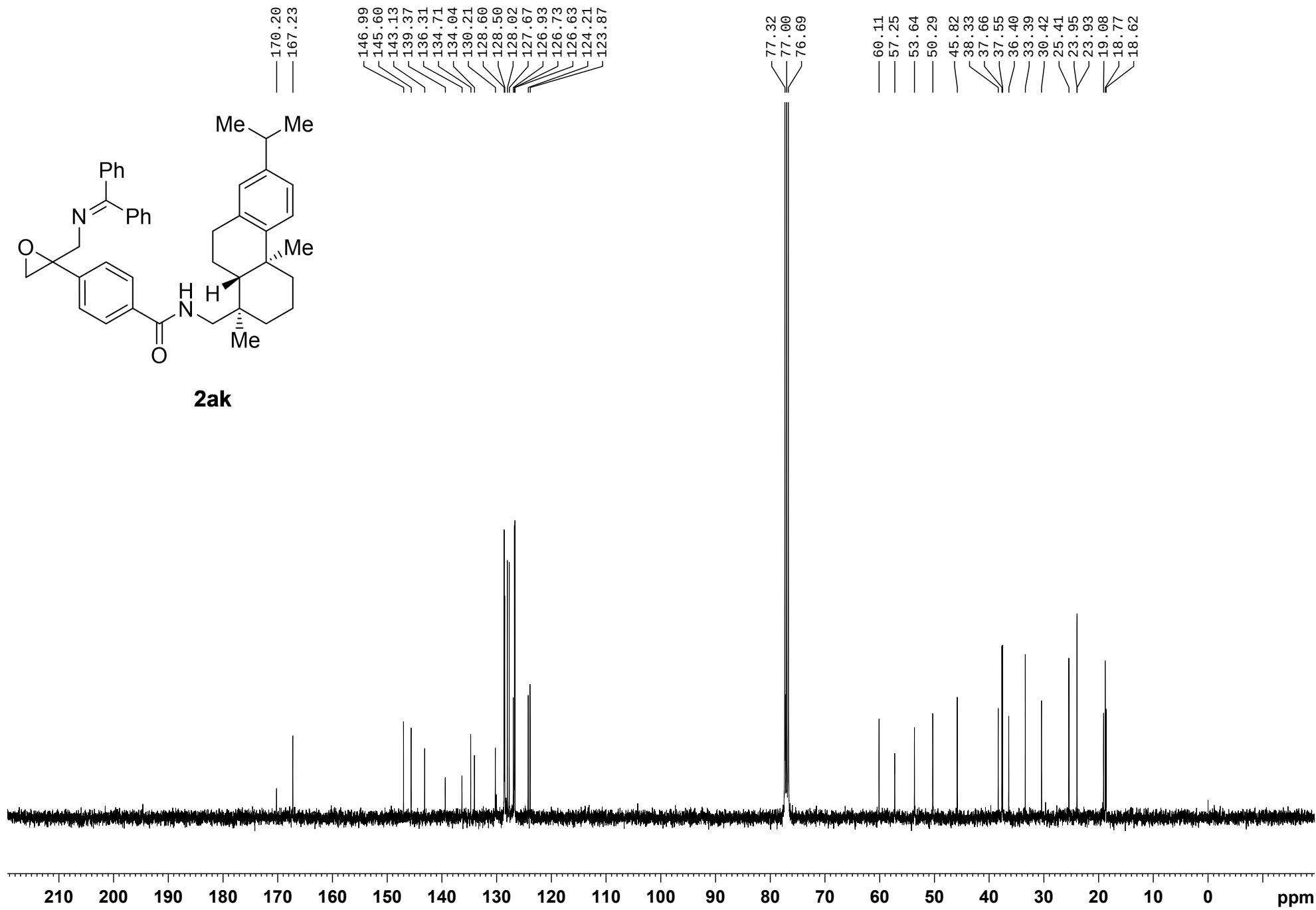
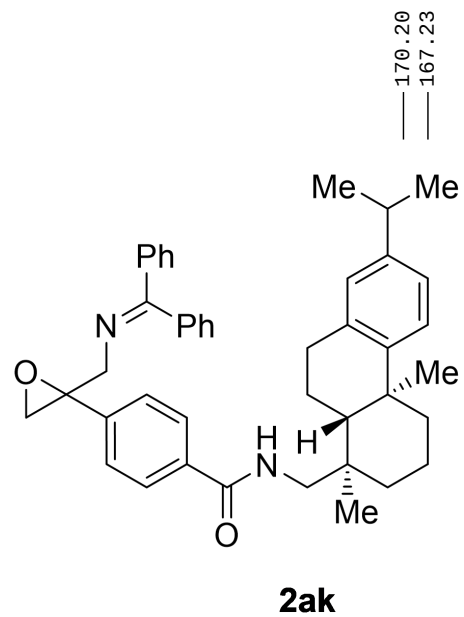
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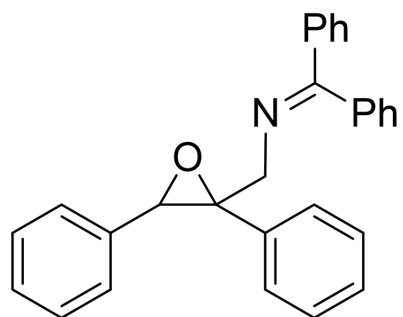




2ak





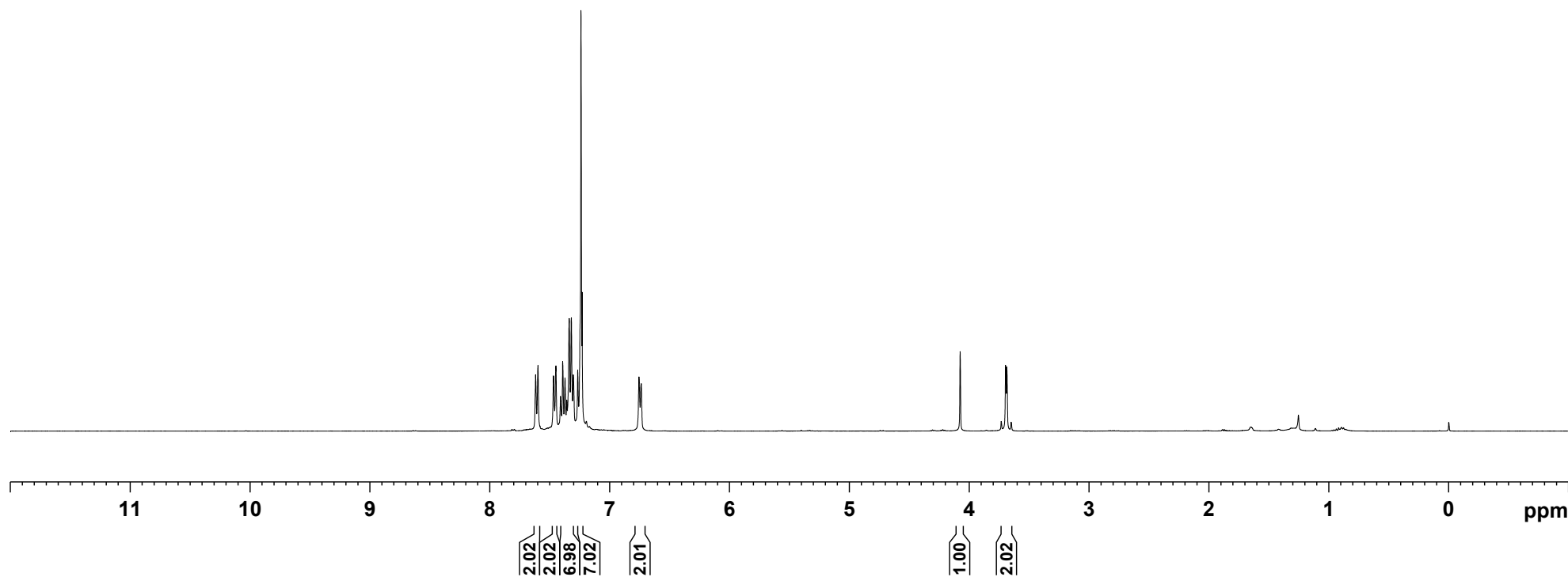


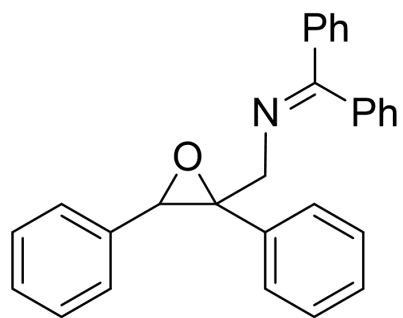
2aI

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7.449
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7.392
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7.358
7.337
7.320
7.304
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7.230
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6.736

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3.687
3.651

0.000





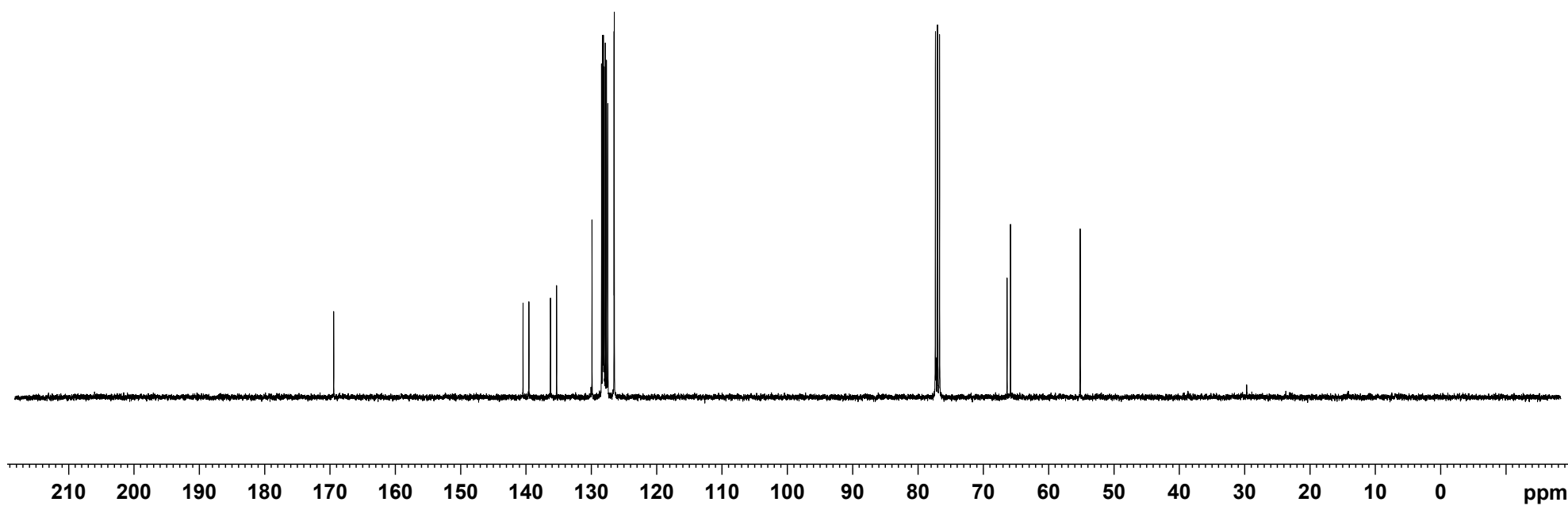
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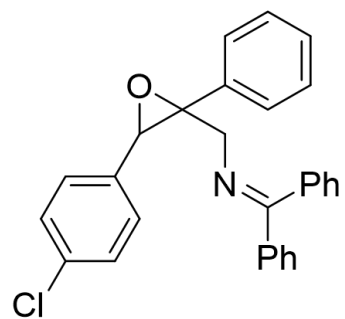
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128.04
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127.67
127.46
126.51
126.47

66.35
65.83

— 55.16



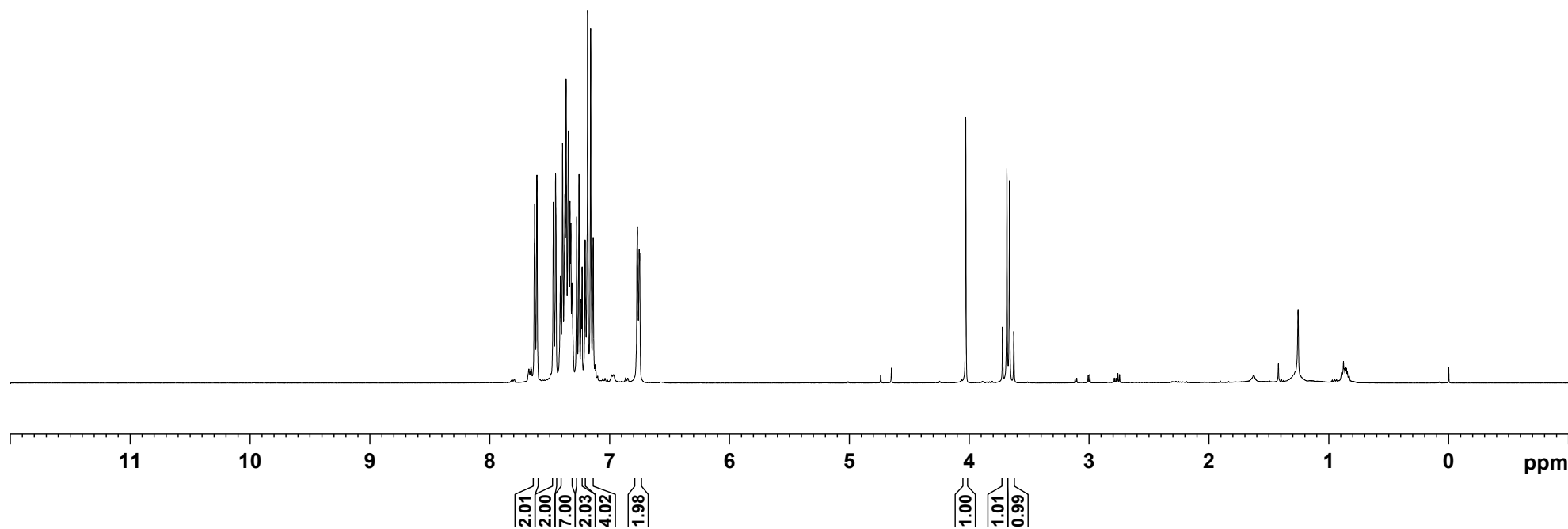


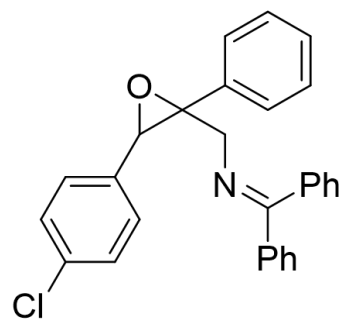
2am

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7.344
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7.313
7.274
7.255
7.237
7.229
7.204
7.183
7.158
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6.753
6.748

4.029
3.722
3.686
3.664
3.628

— 0.000





2am

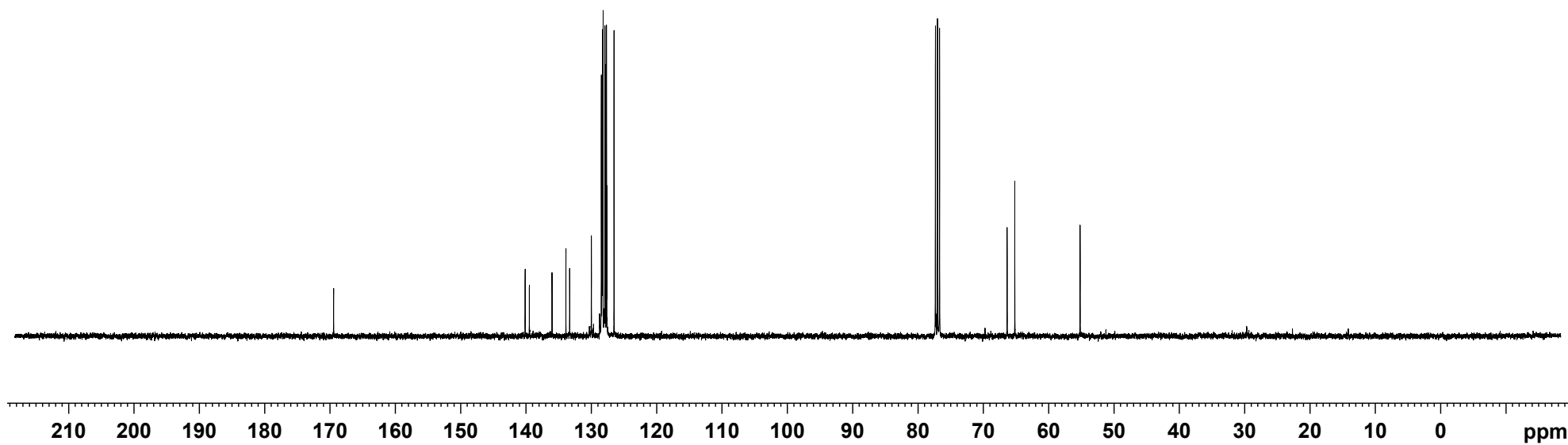
— 169.43

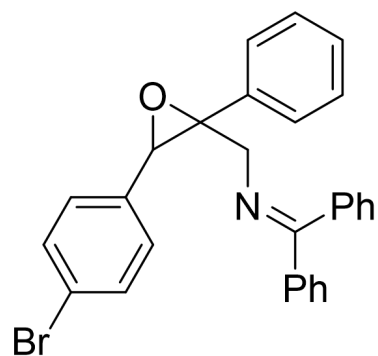
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128.36
128.29
128.24
128.19
127.90
127.84
127.67
127.61
126.51

77.32
77.00
76.68

66.34
65.16

— 55.17



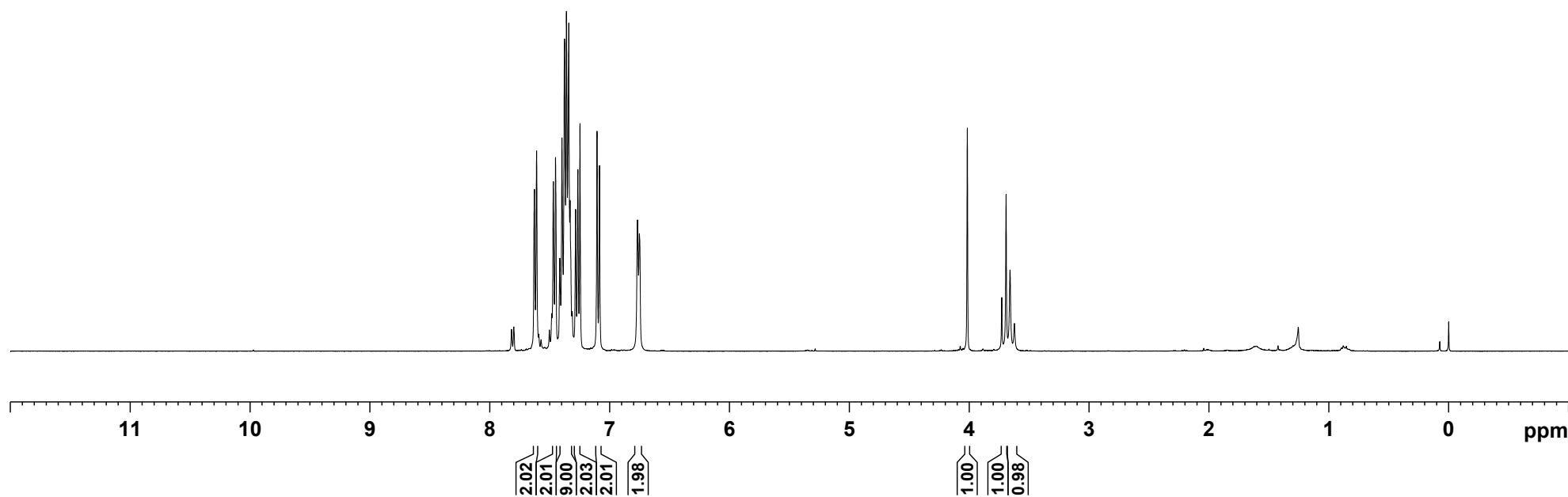


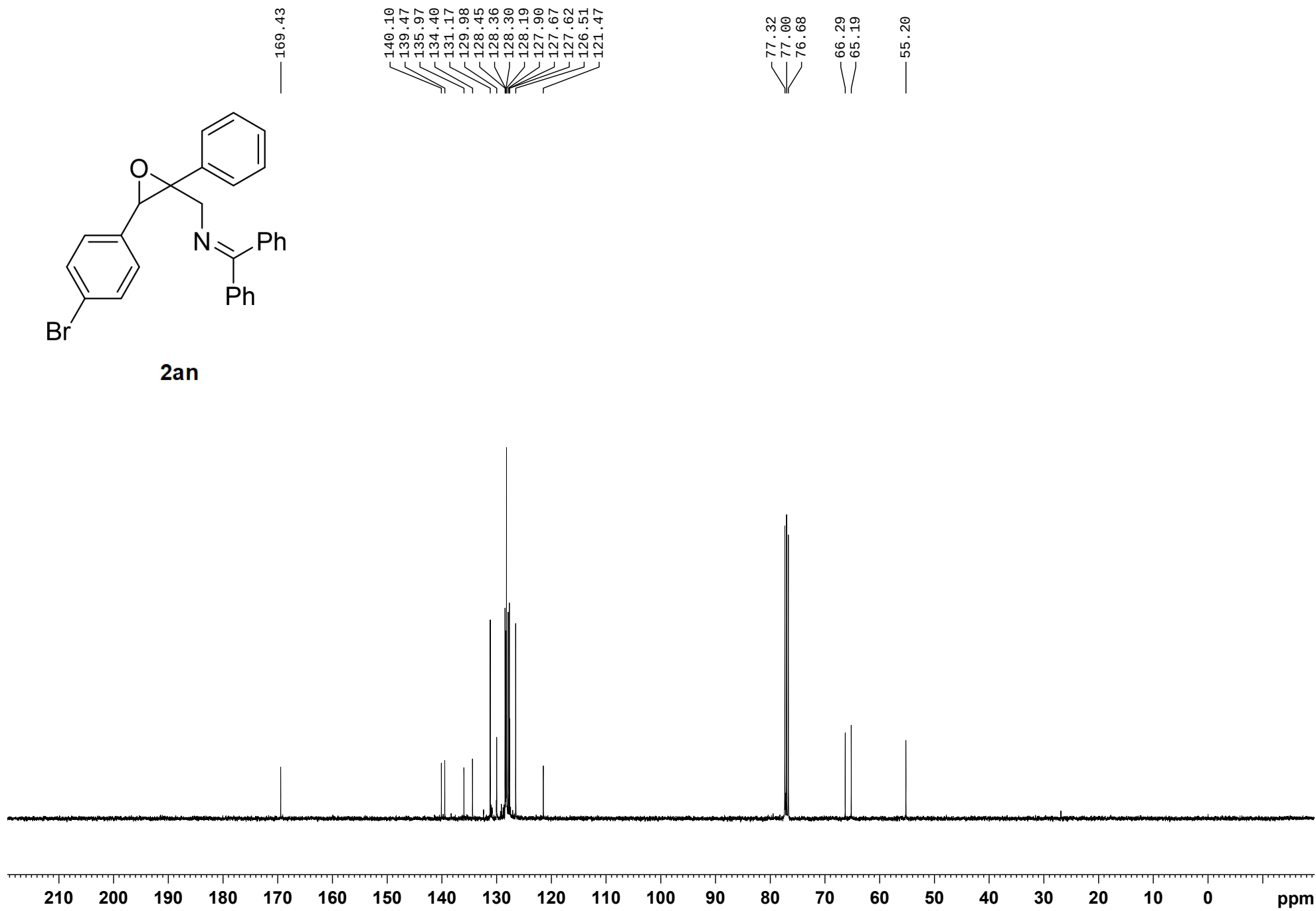
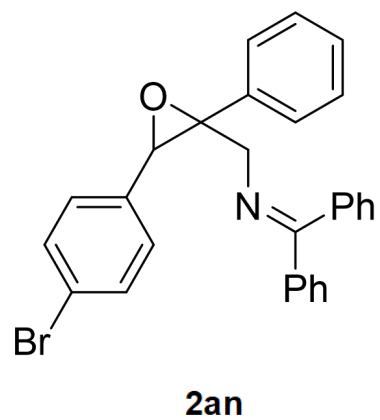
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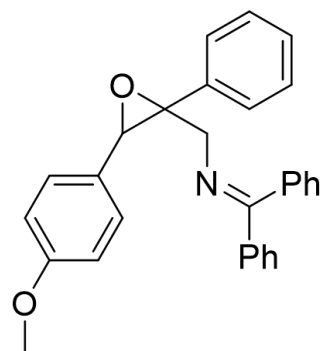
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7.283
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4.016
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3.660
3.624

— 0.000





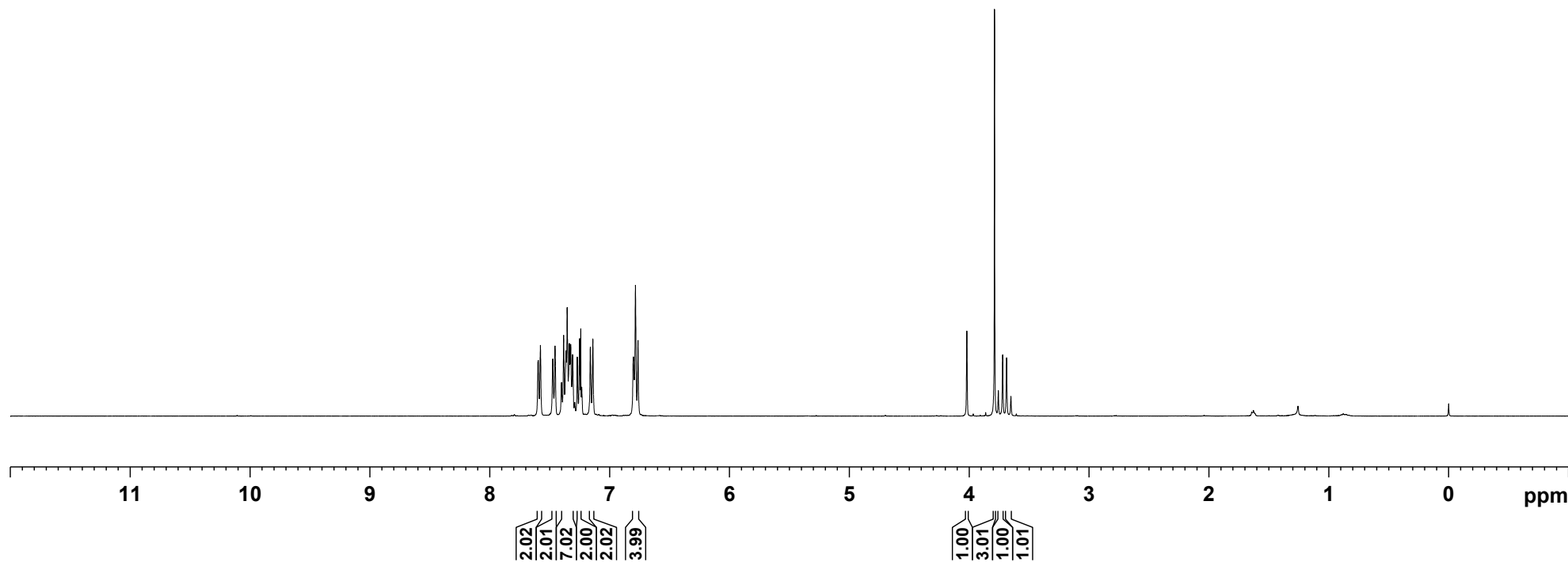


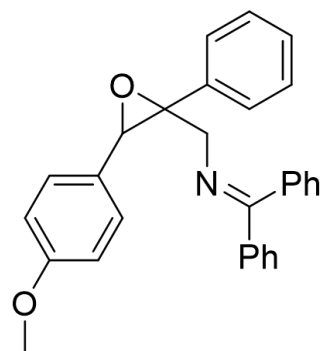
2ao

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7.232
7.160
7.139
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0.000





2ao

— 169.33

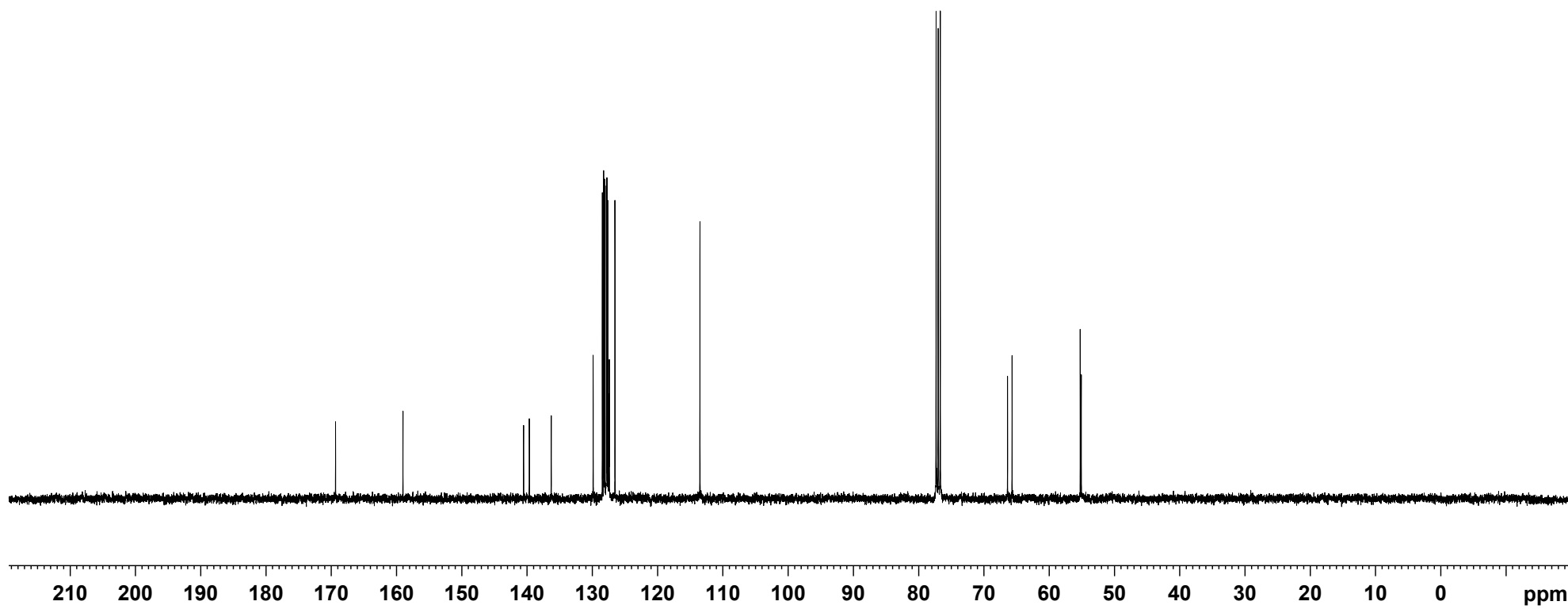
— 159.01

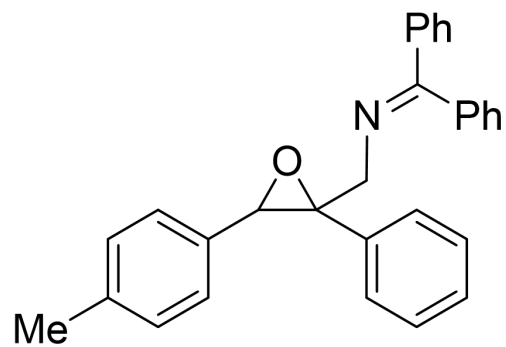
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126.52
113.51

77.32
77.00
76.68

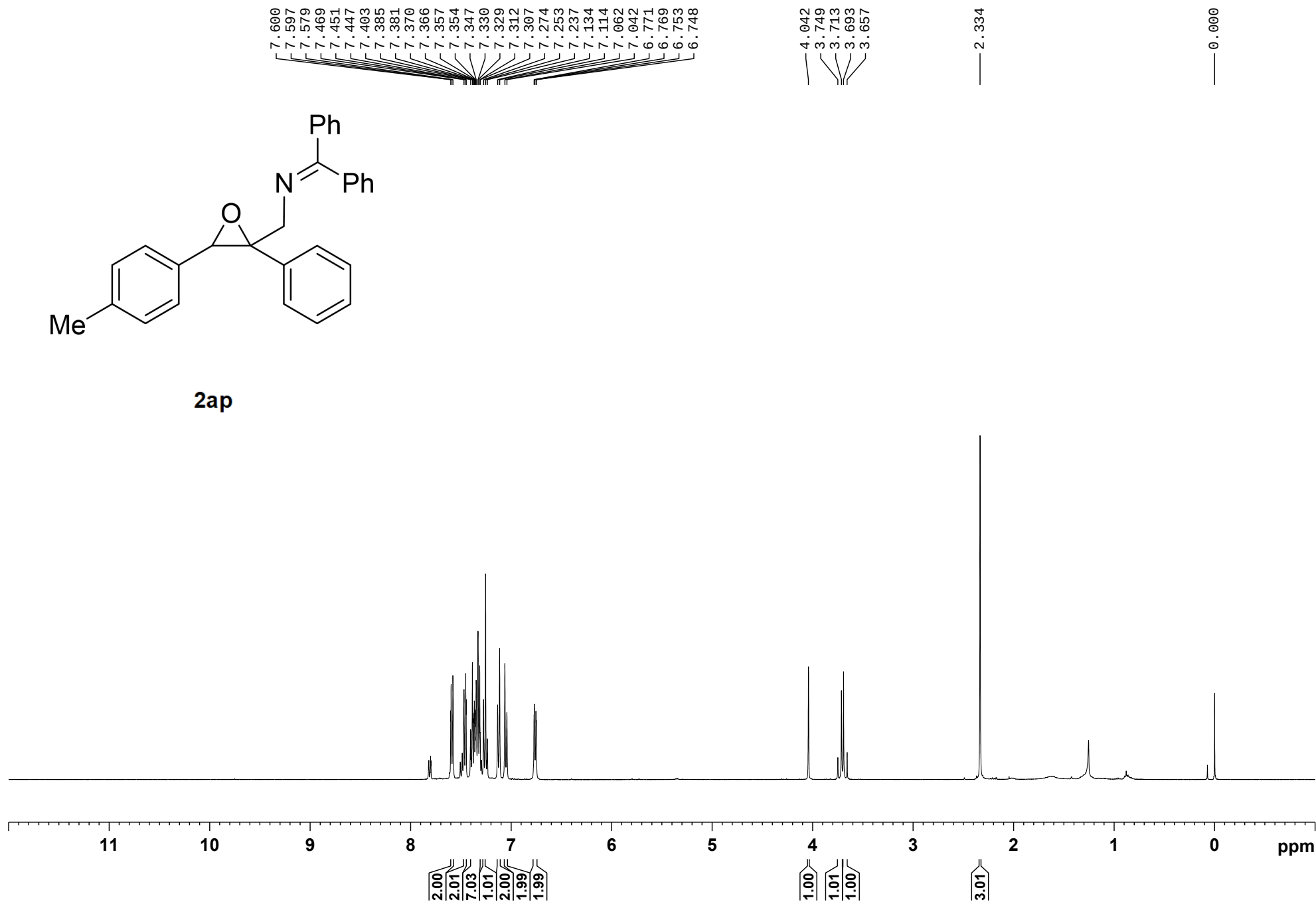
66.37
65.68

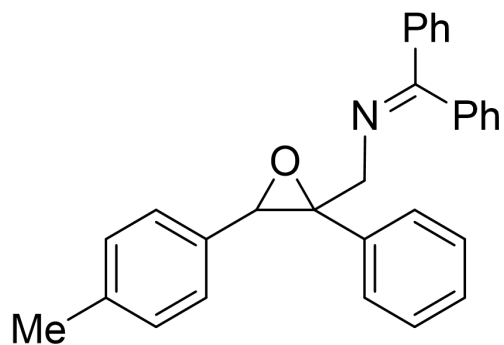
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55.08



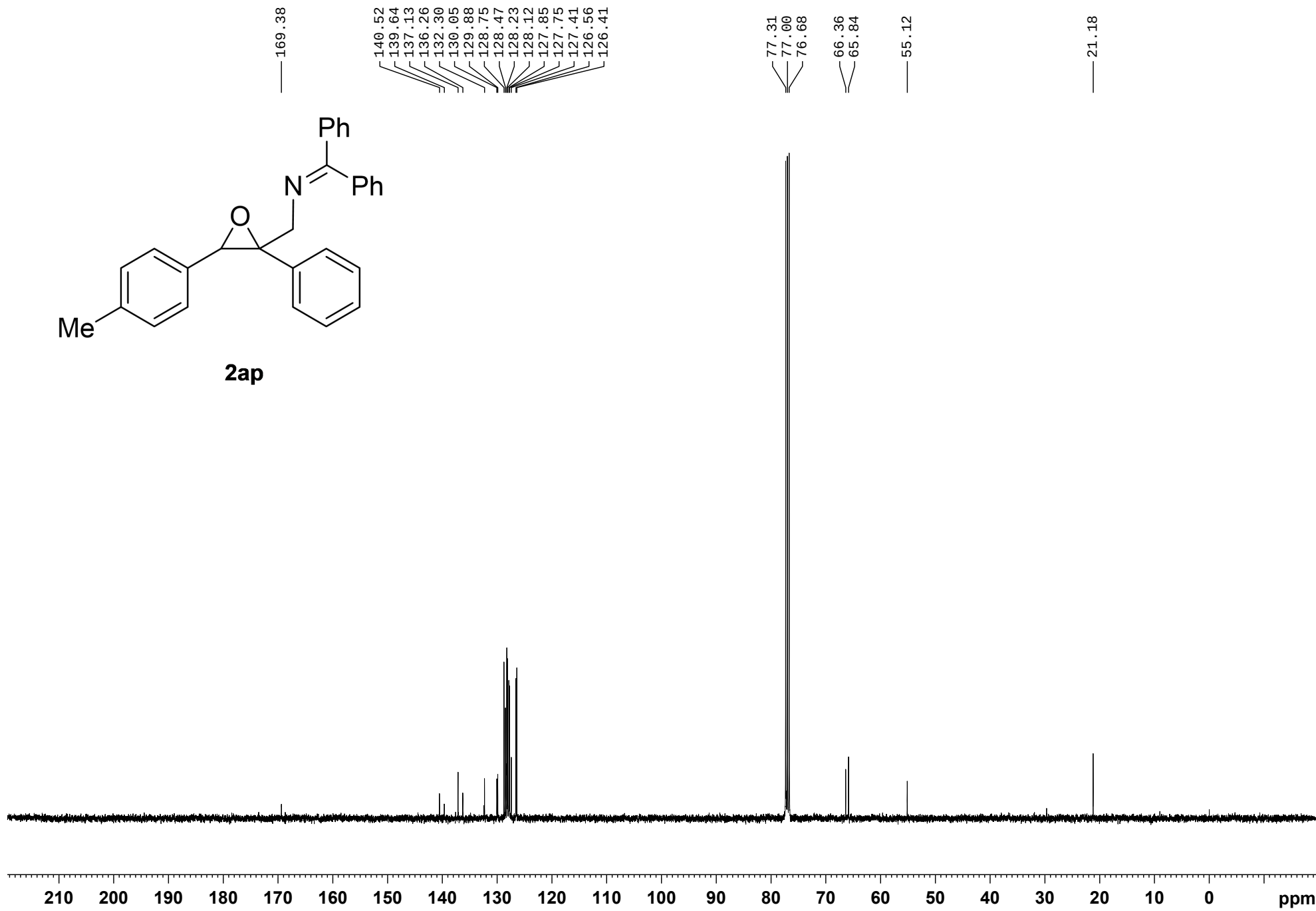


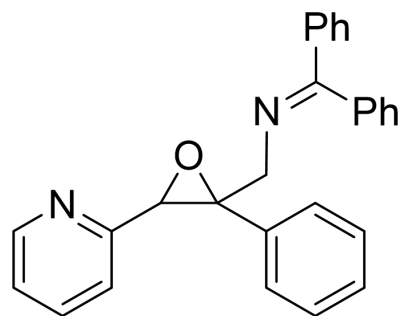
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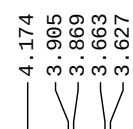
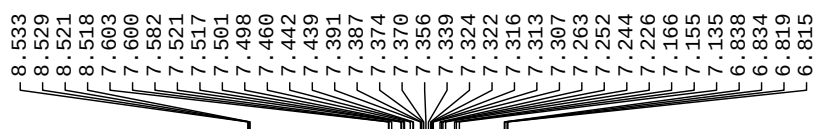
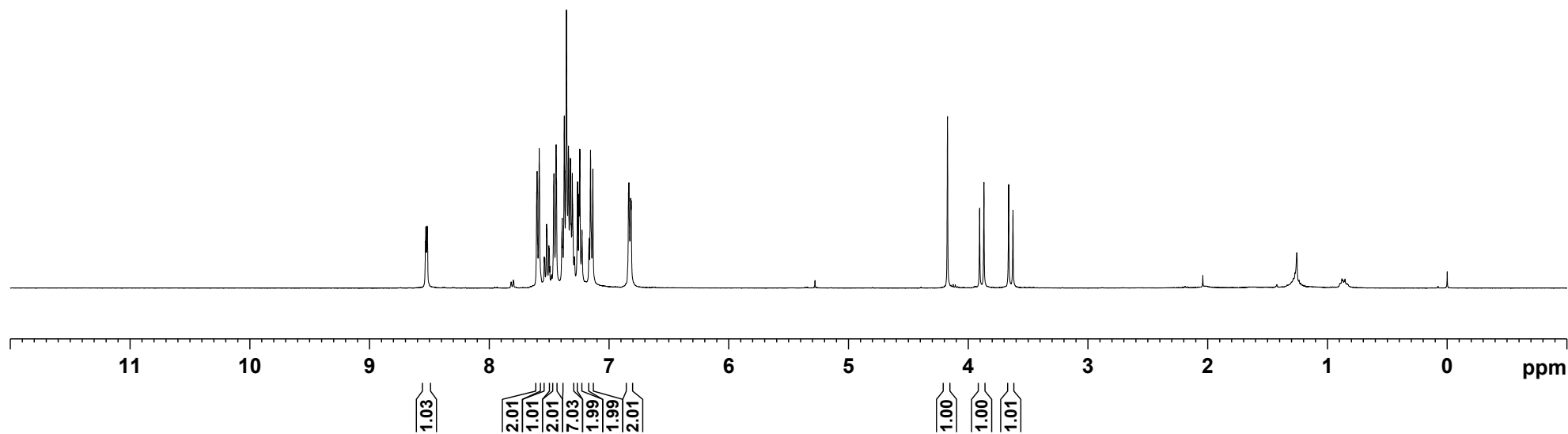


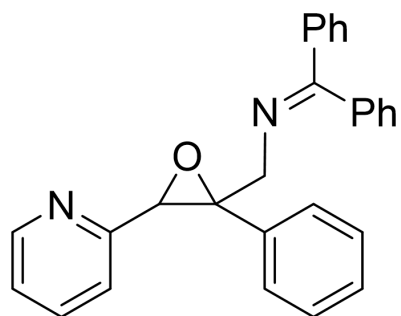
2ap





2aq





2aq

— 169.59

— 155.44

— 149.14

— 139.77

— 139.48

— 136.23

— 136.12

— 129.94

— 128.51

— 128.28

— 128.06

— 127.83

— 127.78

— 127.57

— 126.68

— 122.47

— 121.00

77.32

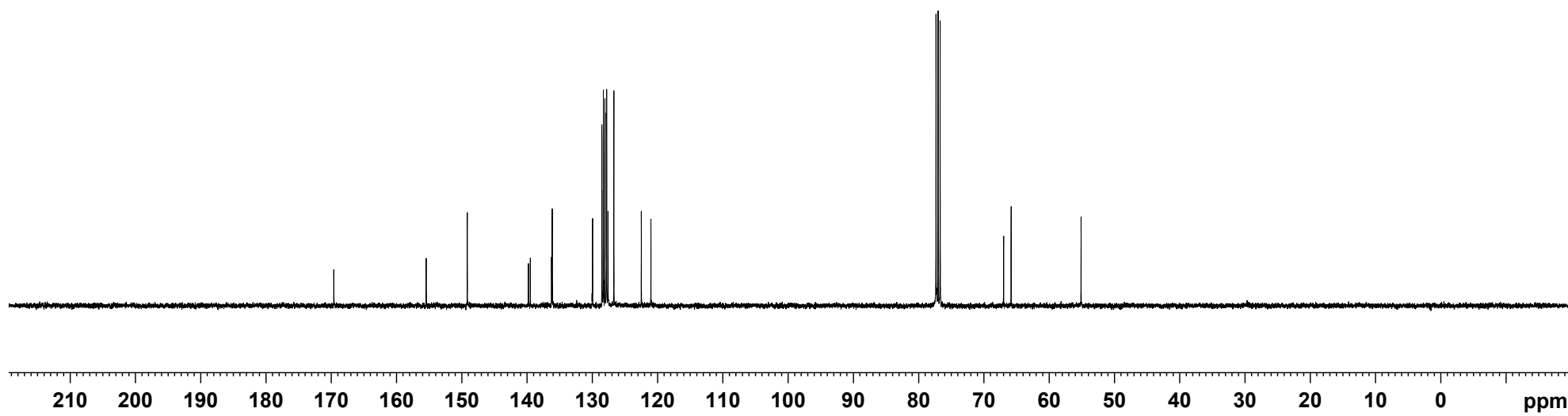
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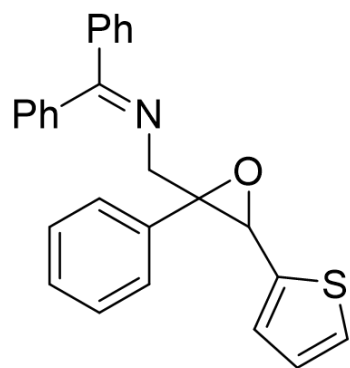
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66.95

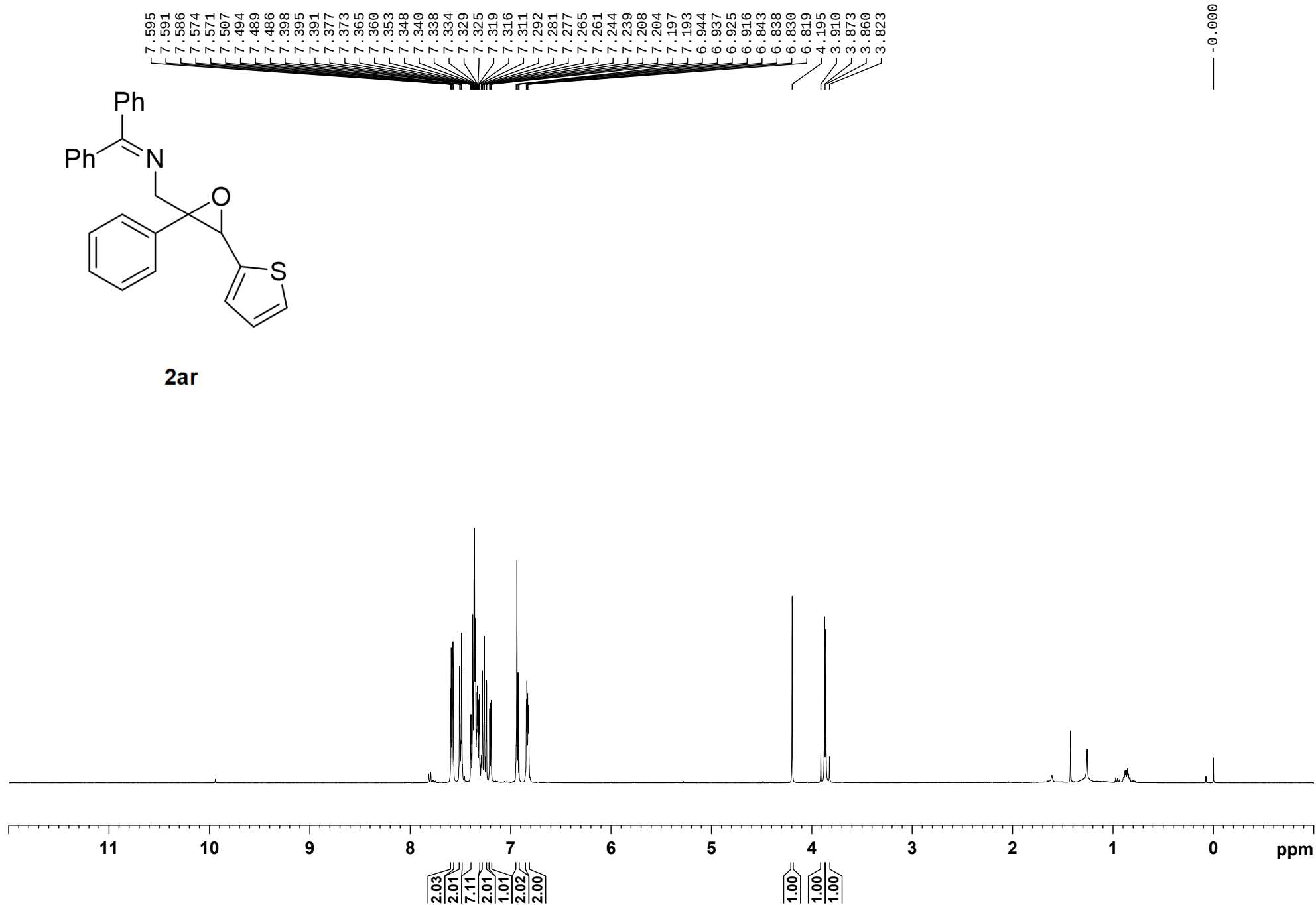
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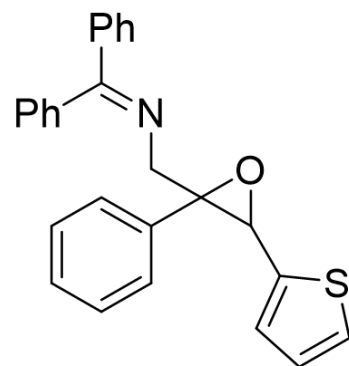
— 55.09





2ar



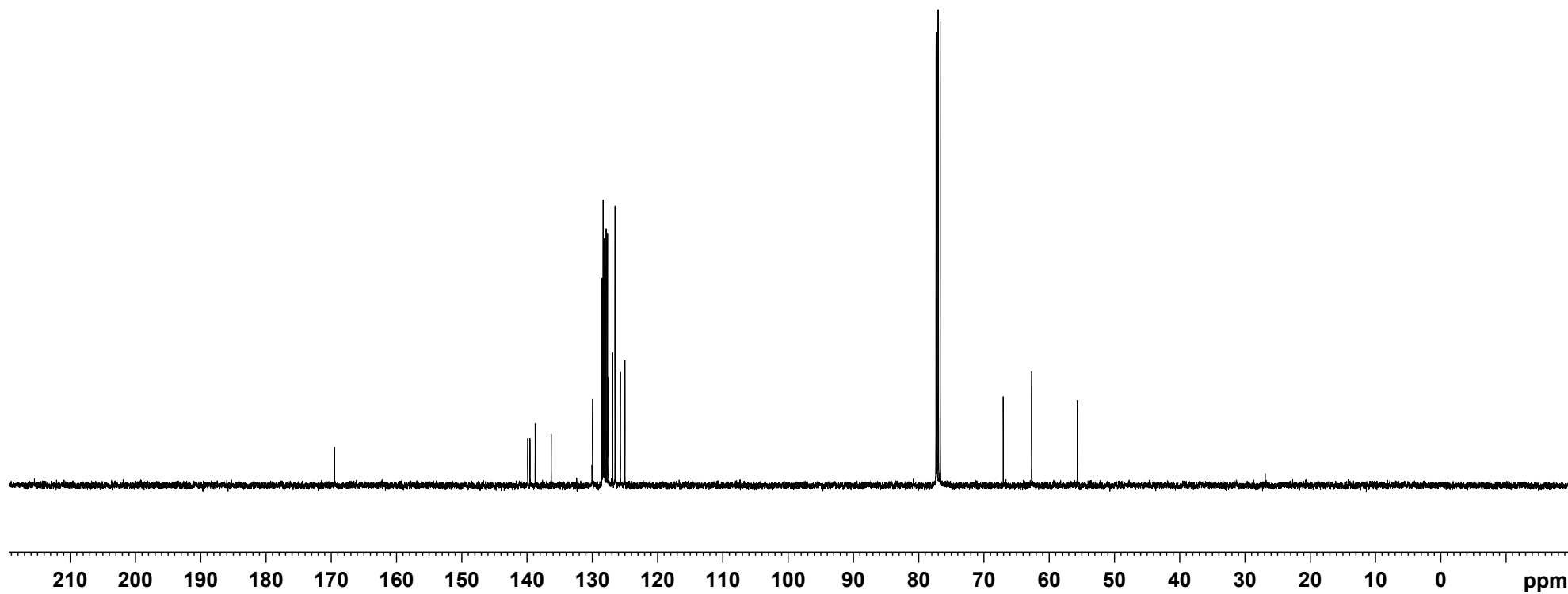


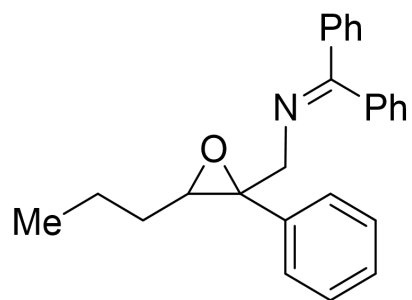
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169.49

139.88
139.54
138.74
136.28
129.93
128.48
128.33
128.16
127.87
127.66
127.60
126.87
126.51
125.69
124.99

77.32
77.00
76.68
67.02
62.66
55.65

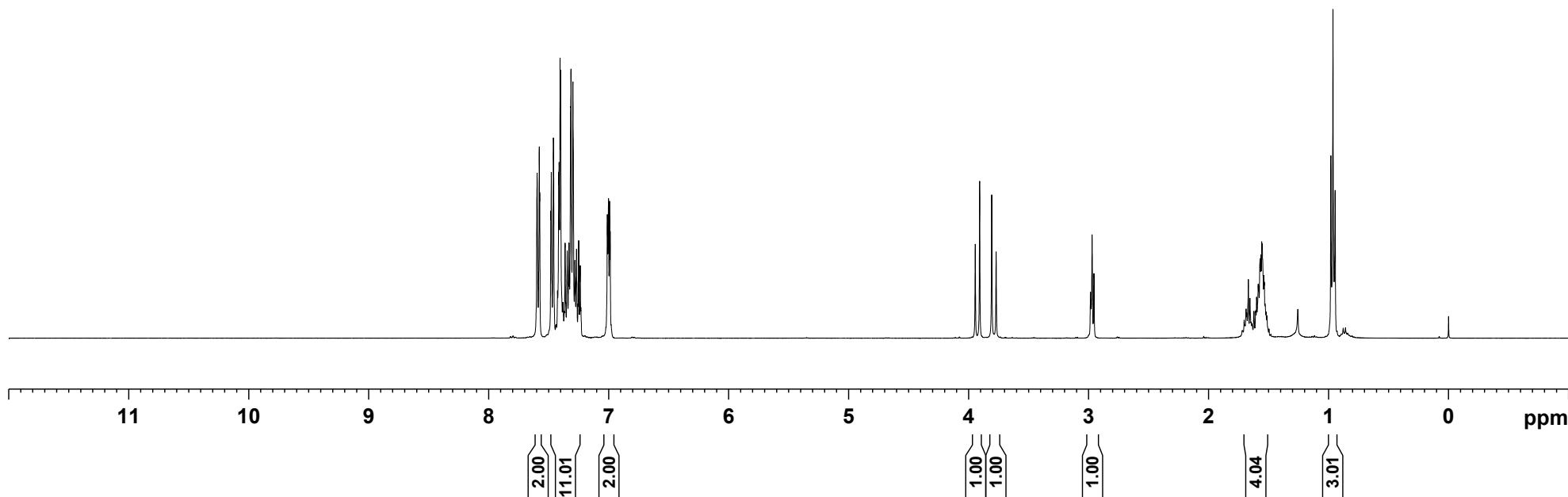


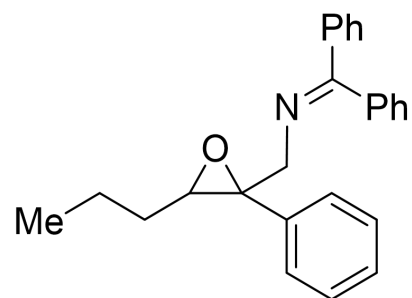


2as

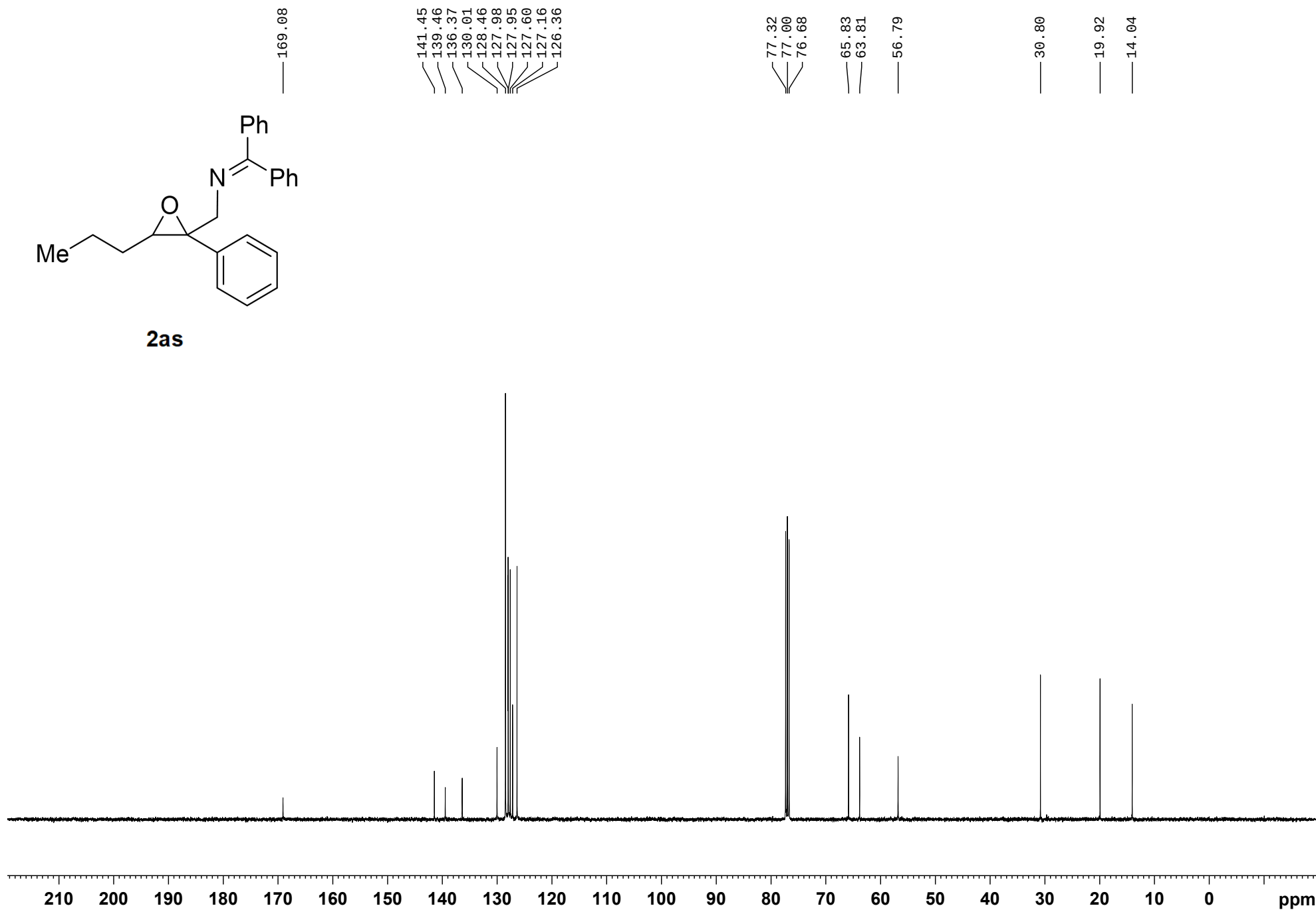
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7.578
7.574
7.481
7.478
7.460
7.425
7.416
7.412
7.404
7.399
7.363
7.345
7.330
7.326
7.316
7.313
7.298
7.280
7.277
7.270
7.267
7.249
7.236
7.011
7.000
6.992
6.987

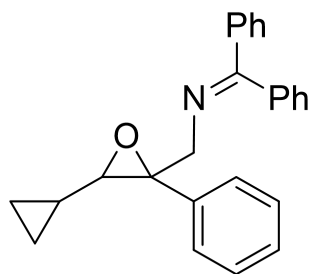
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3.908
3.771
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2.971
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1.683
1.669
1.656
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1.608
1.600
1.587
1.582
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1.540
1.536
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0.981
0.964
0.945
0.000



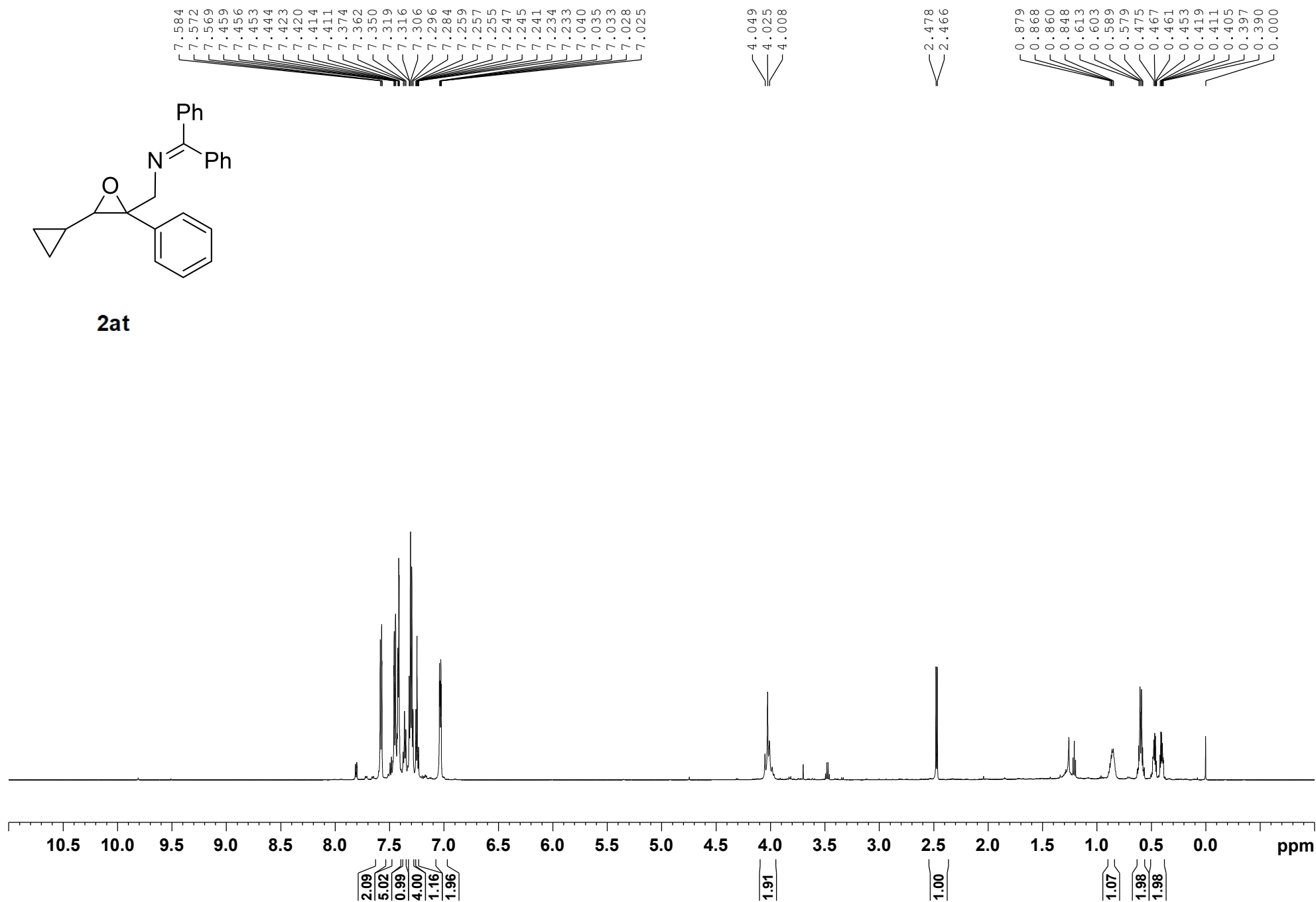


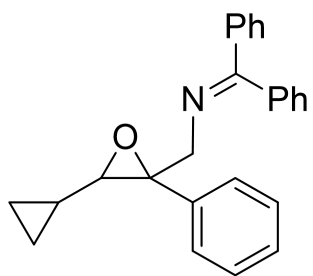
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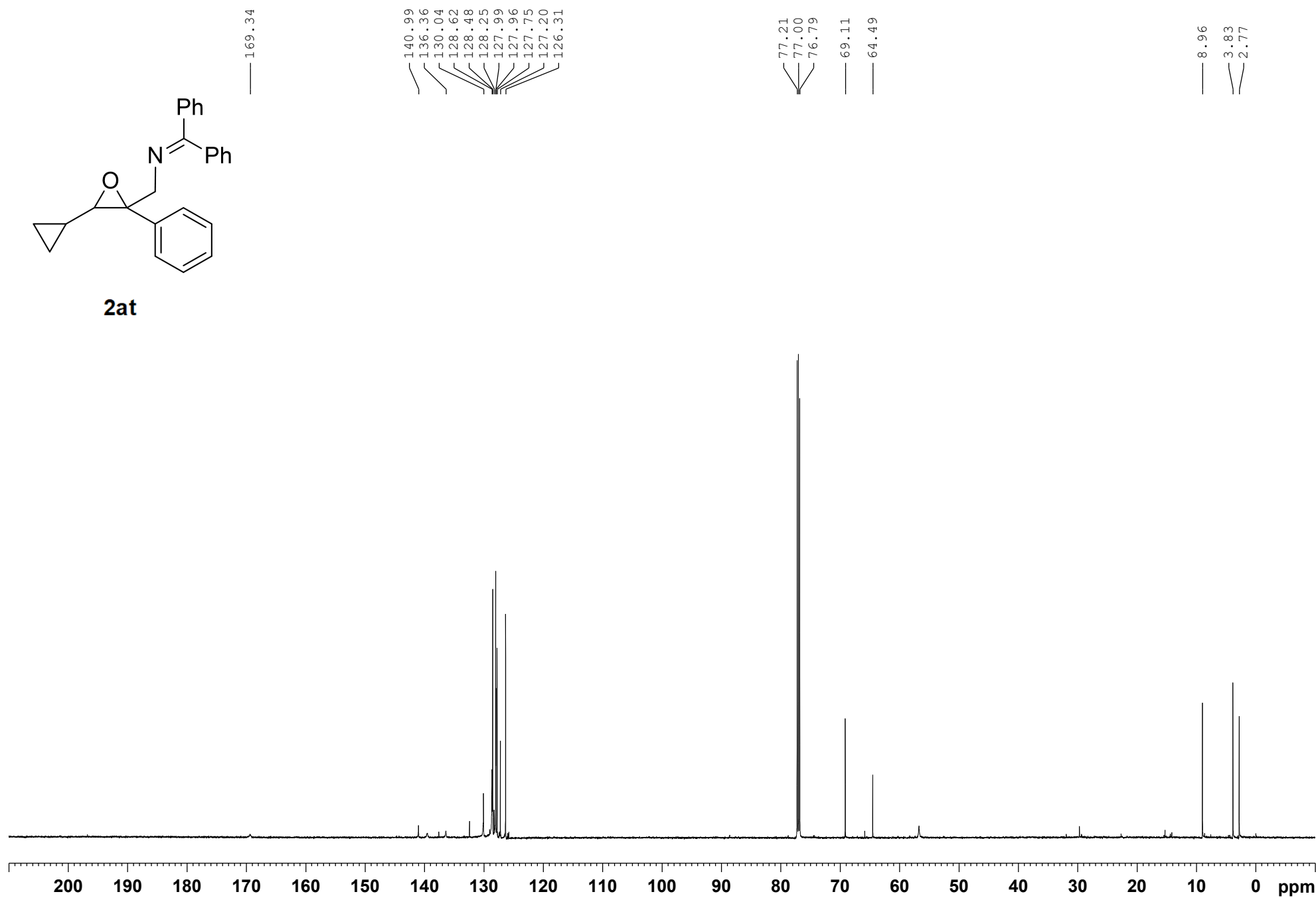


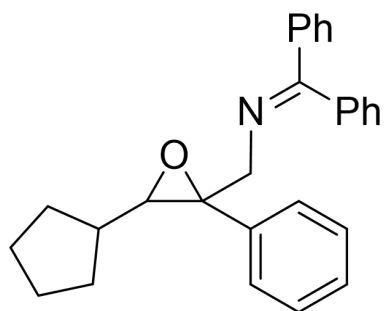
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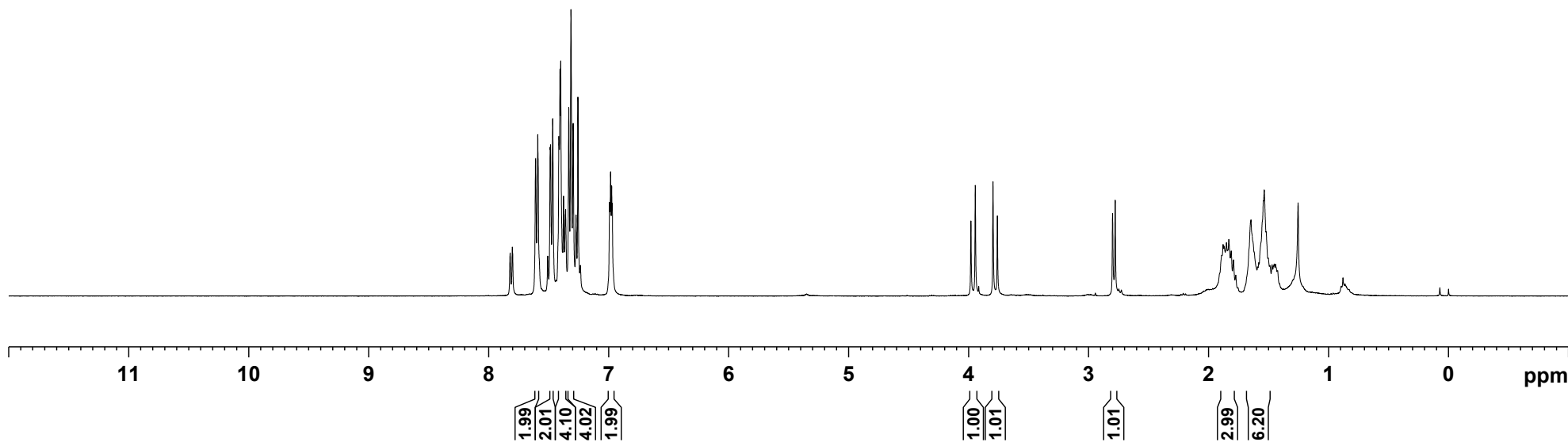
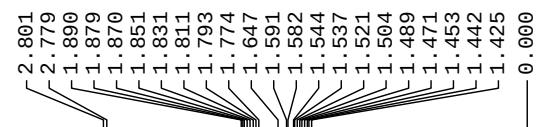
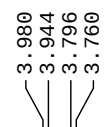
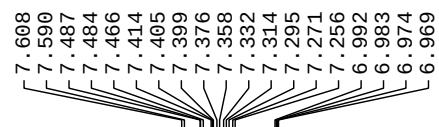


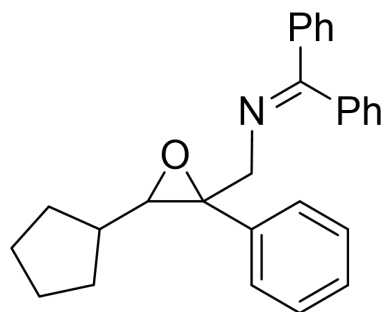
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2au





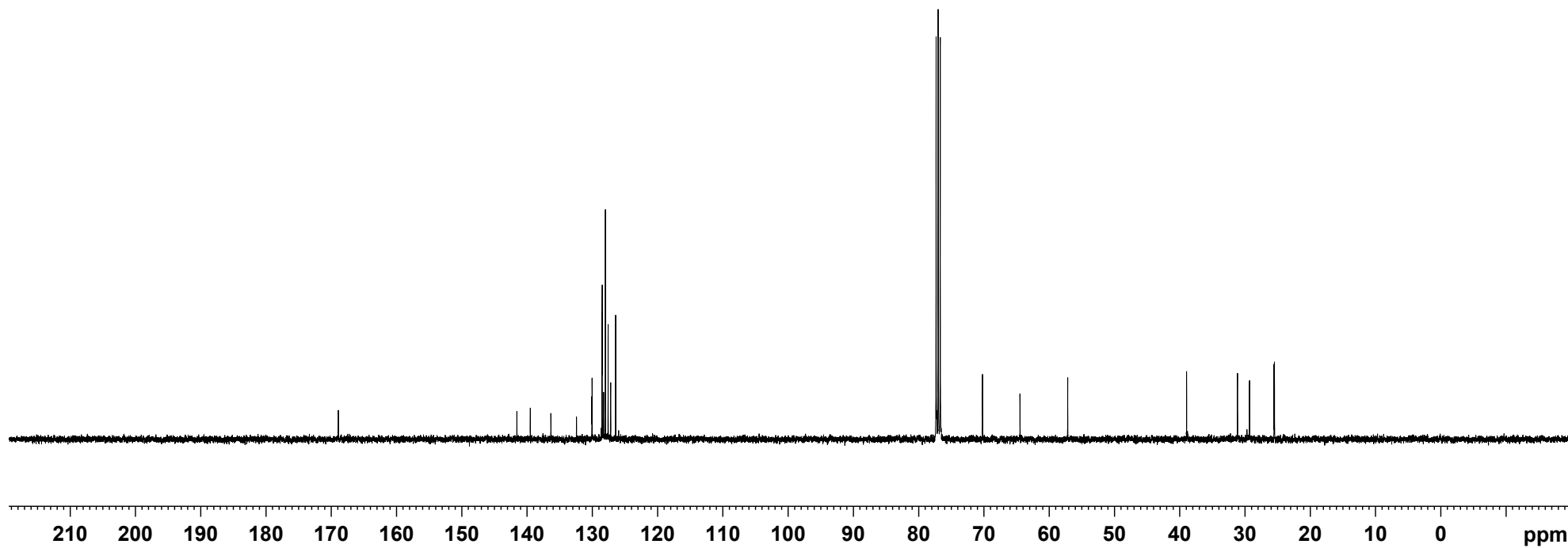
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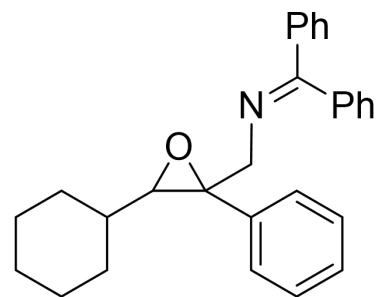
— 168.90

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130.02
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128.47
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127.57
127.17
126.41

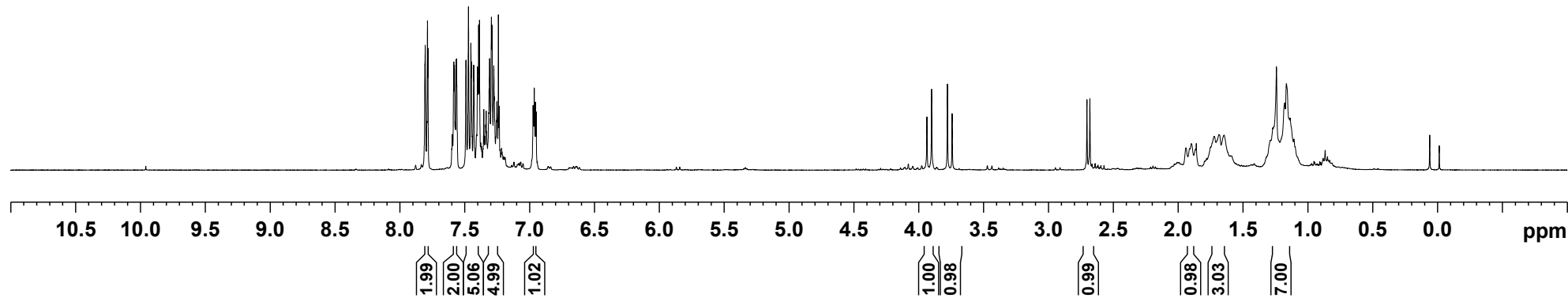
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70.20
64.46
57.15

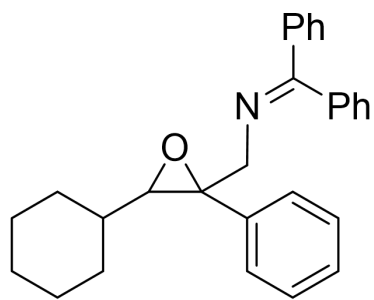
38.93
31.13
29.29
25.54
25.47



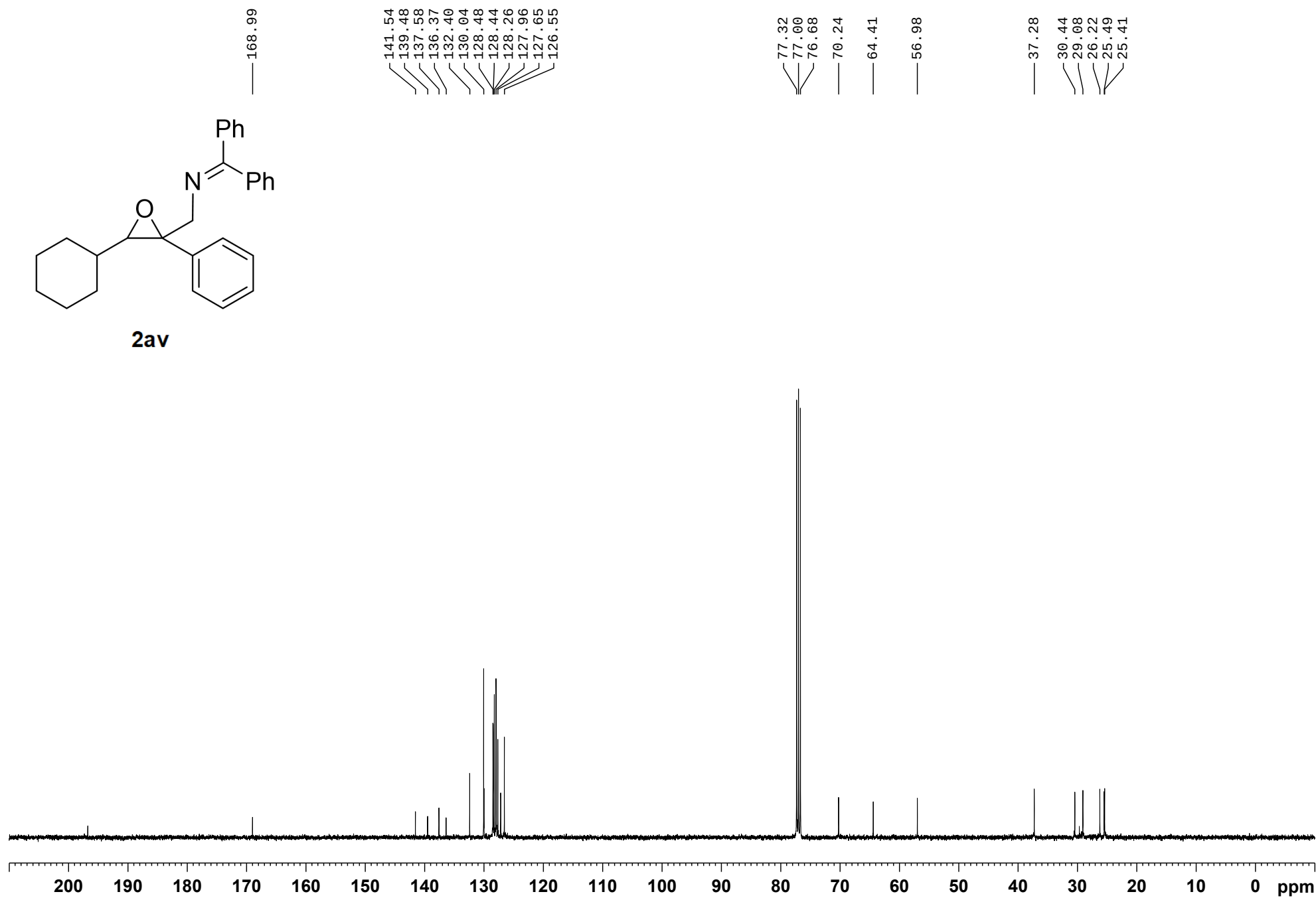


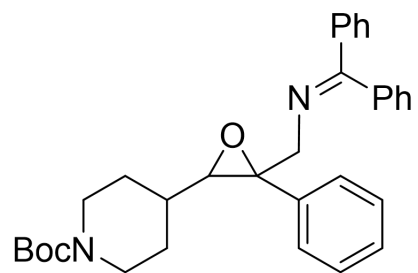
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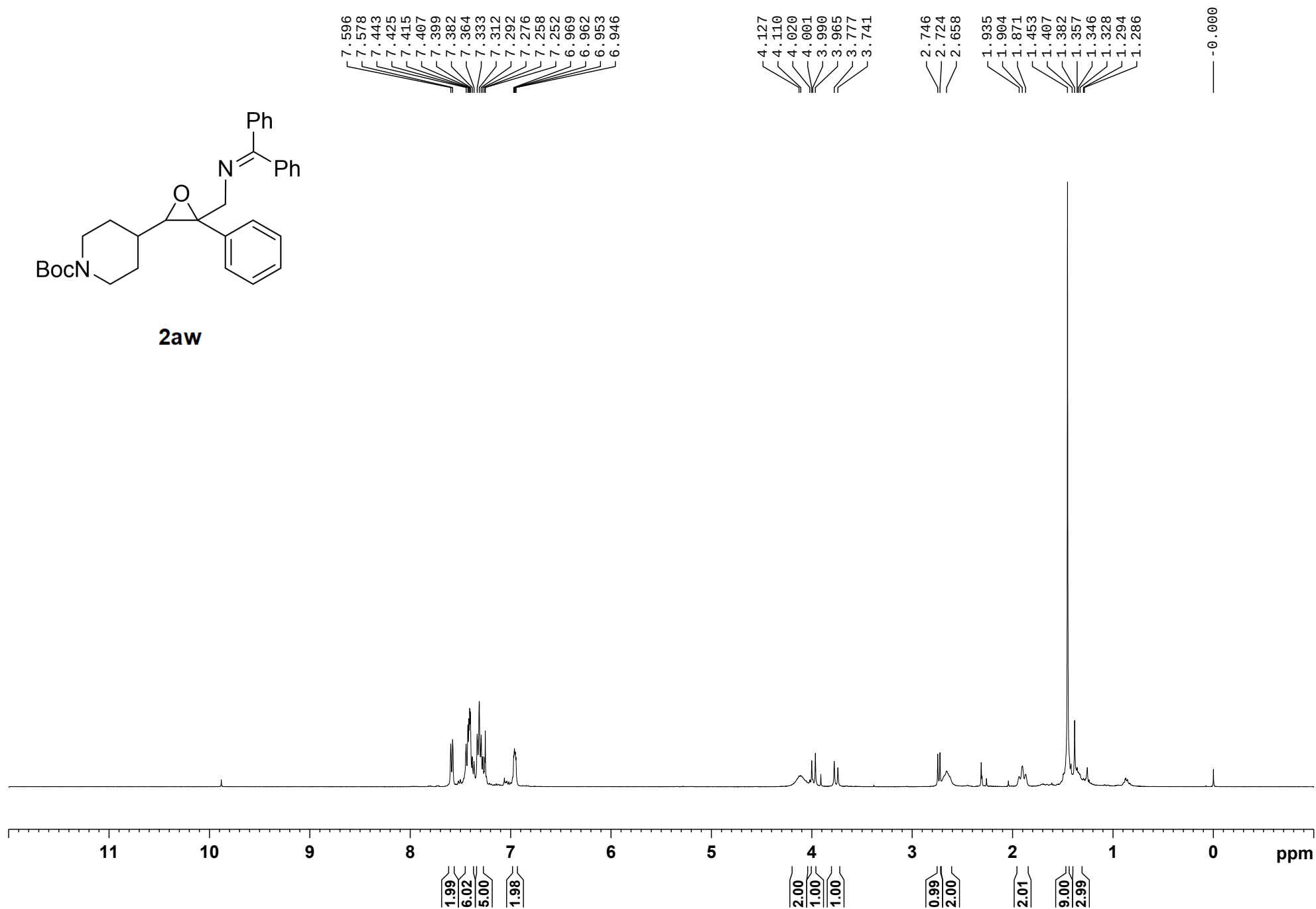


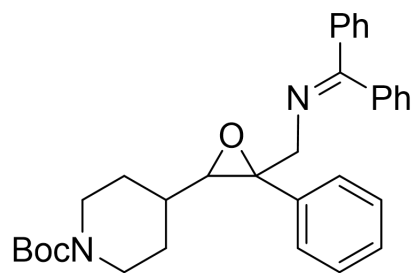
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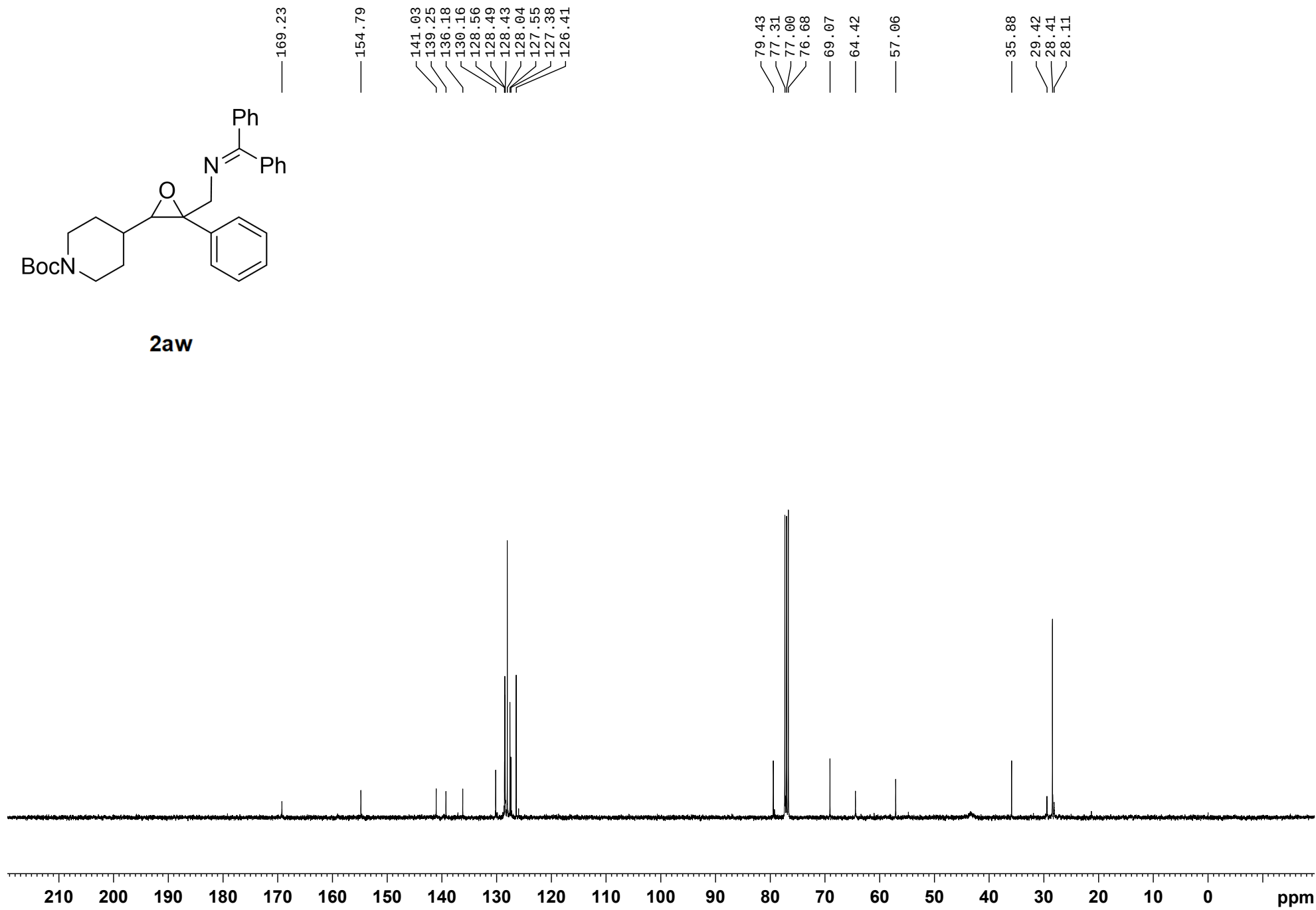


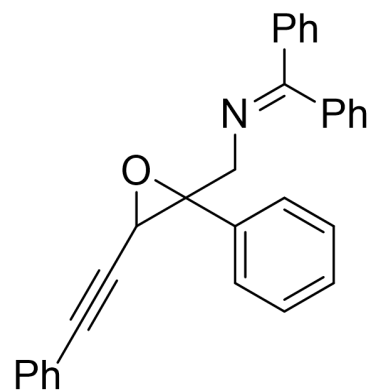
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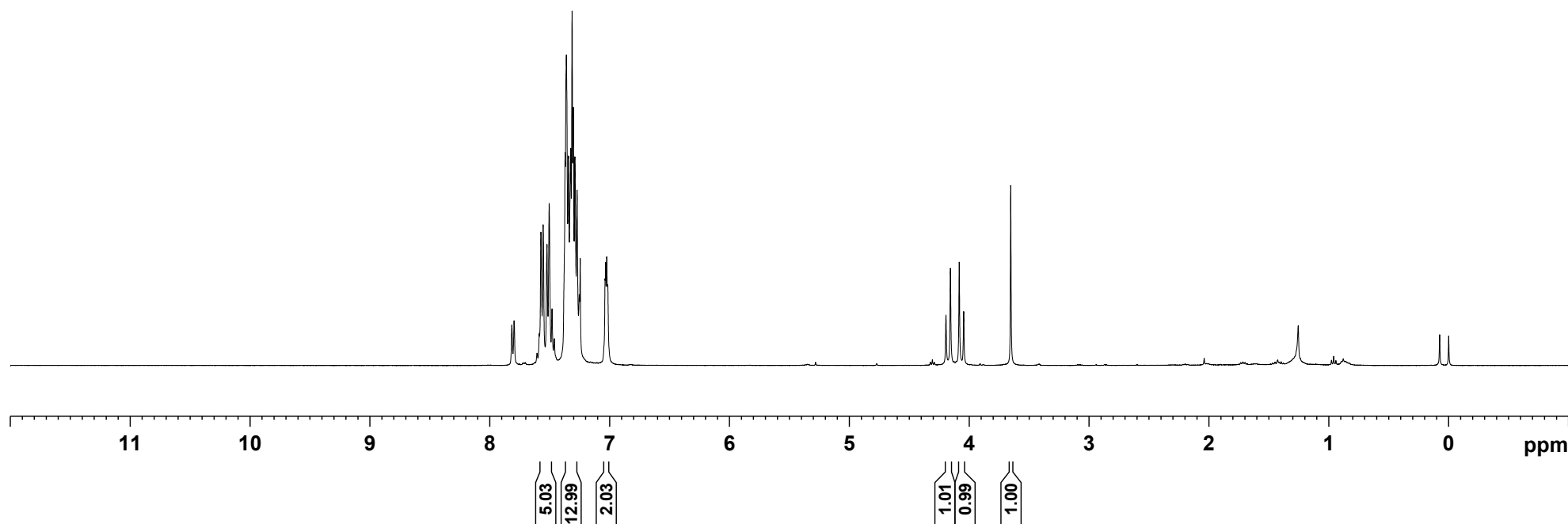
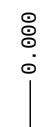
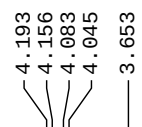
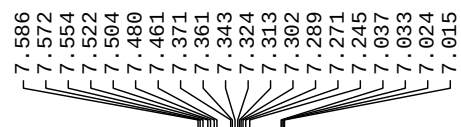


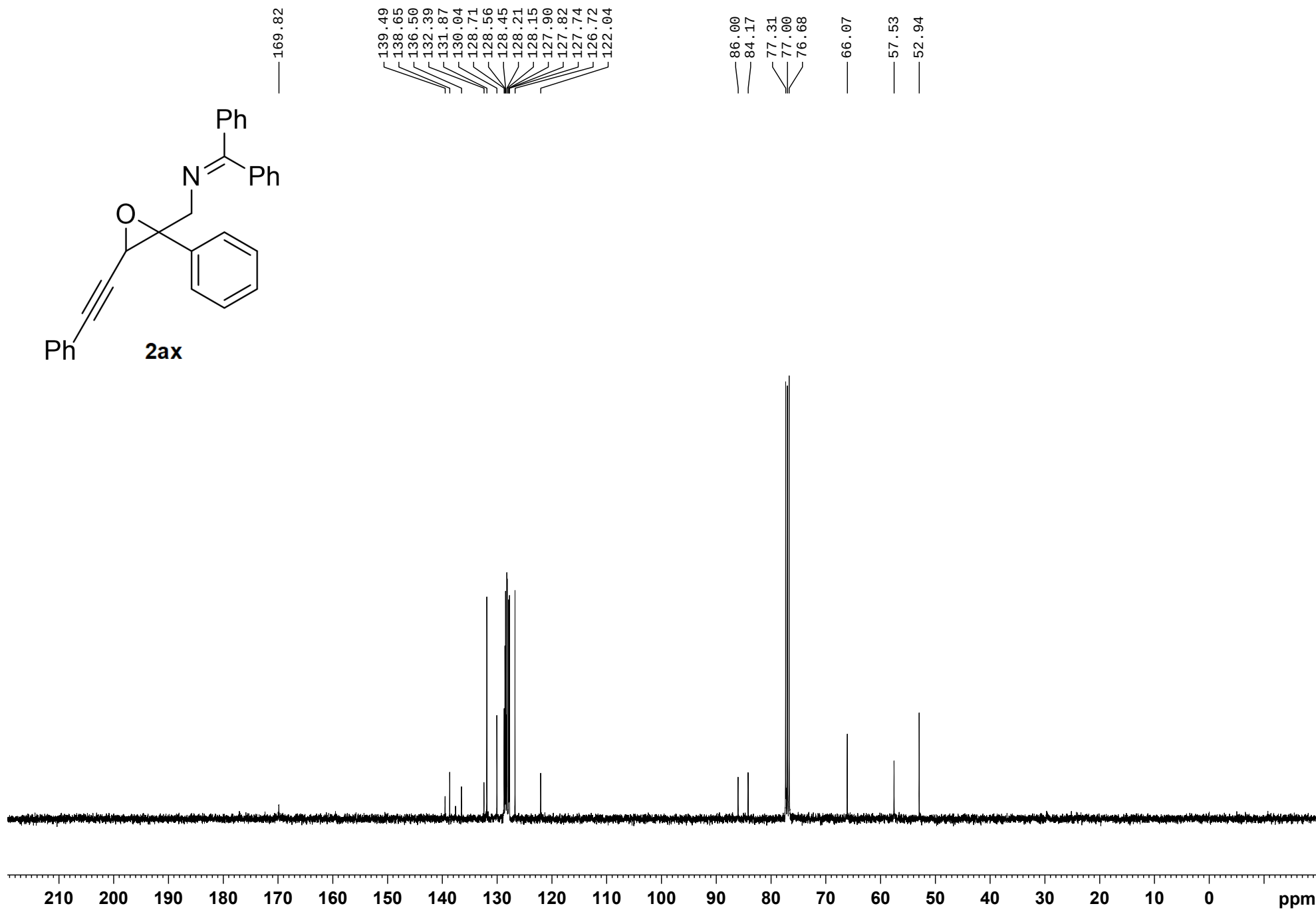
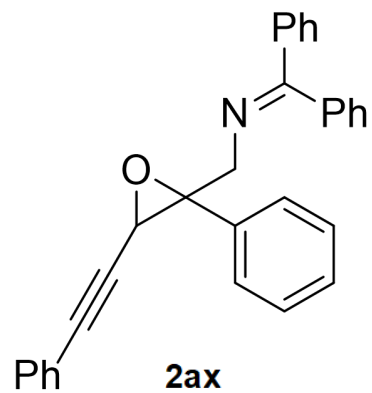
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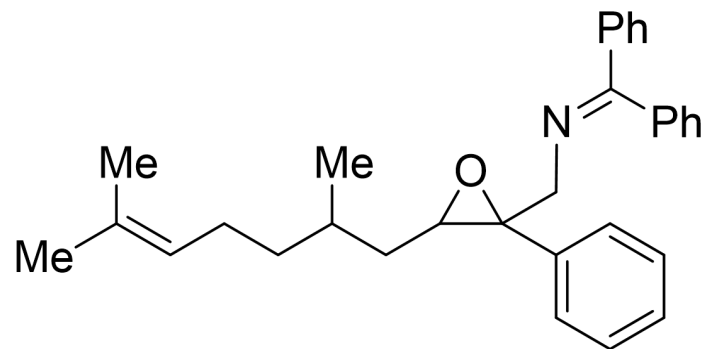




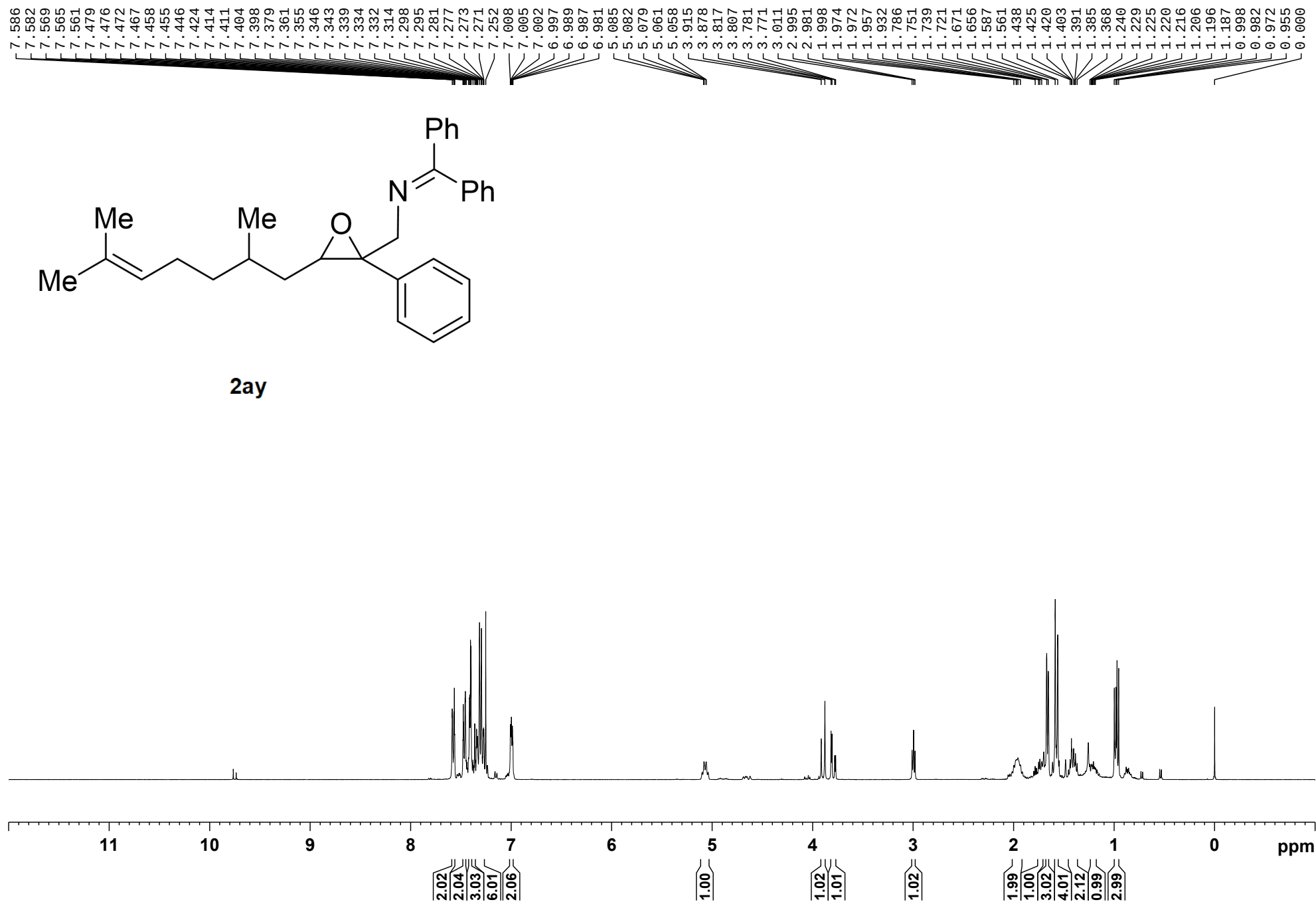
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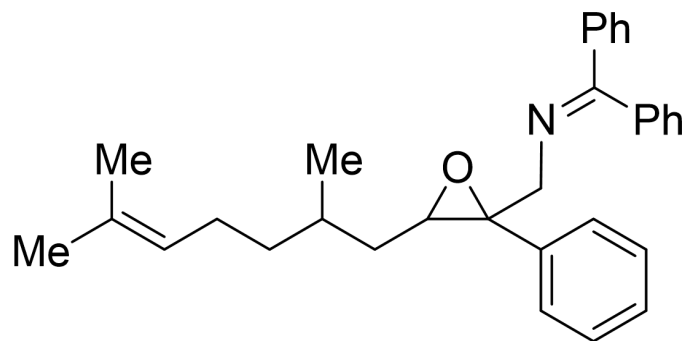




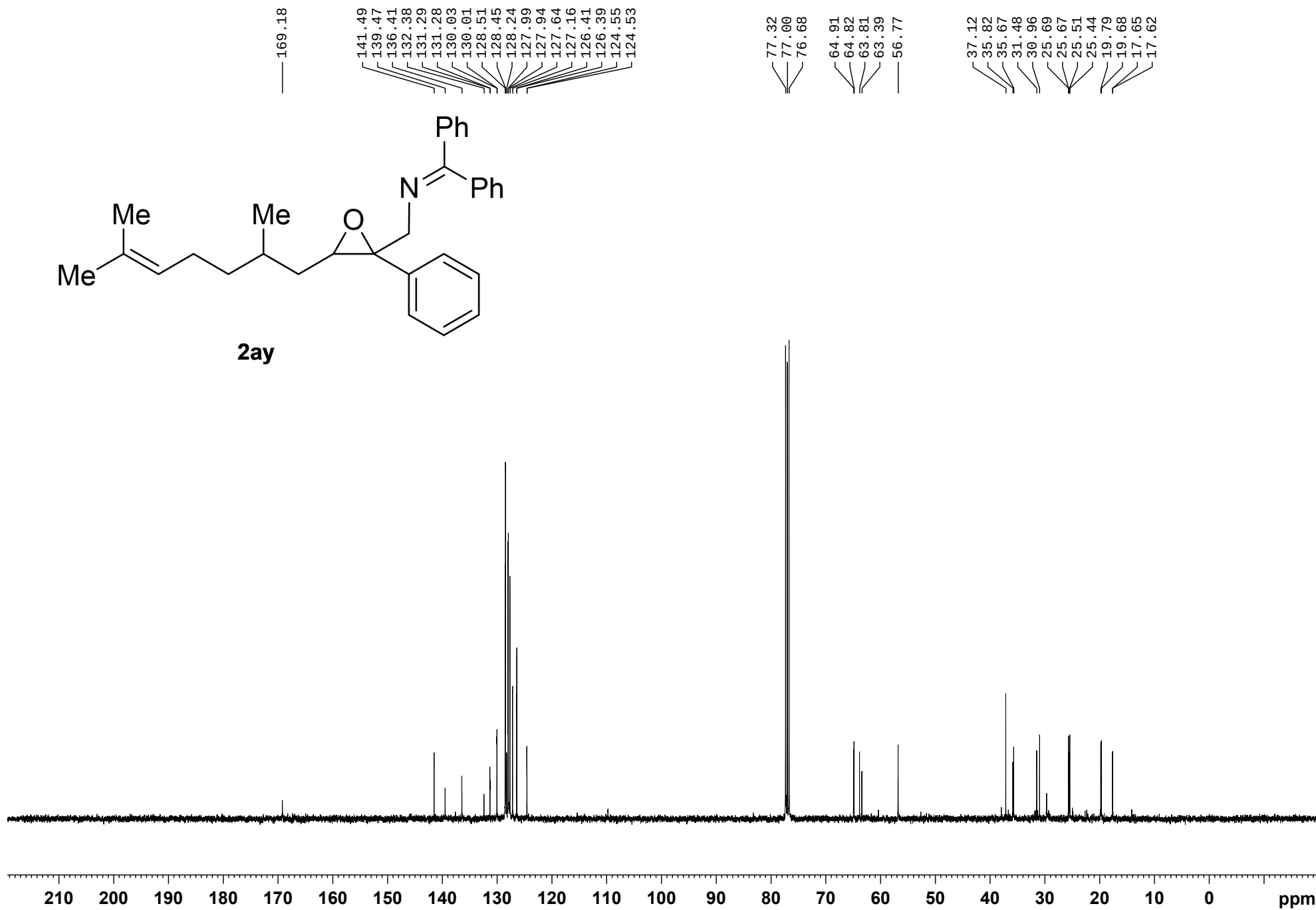


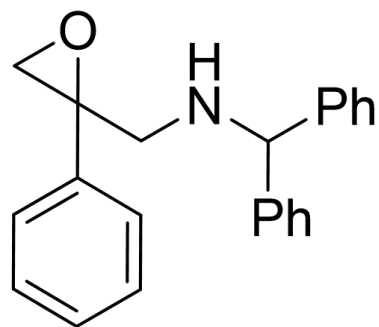
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2ay





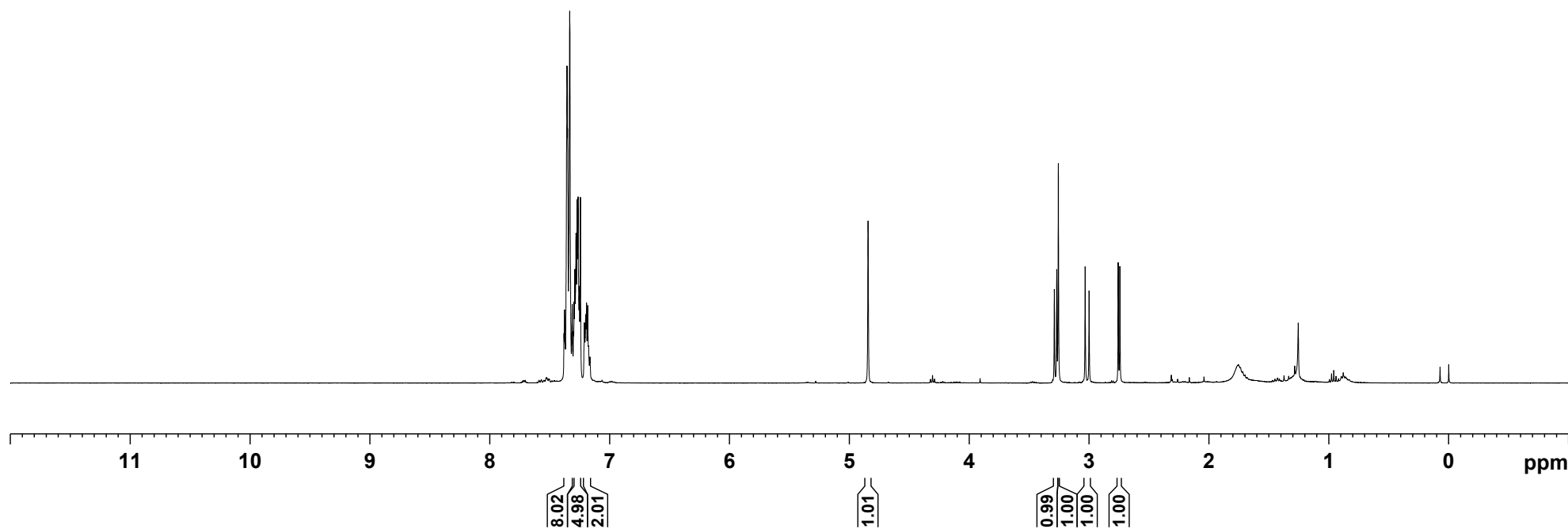
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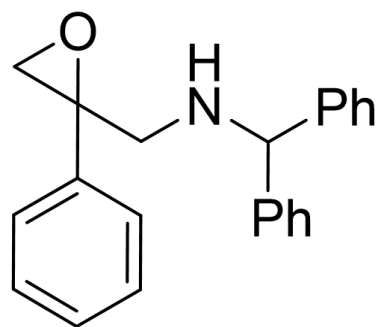
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7.333
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7.301
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7.280
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7.267
7.263
7.252
7.243
7.210
7.207
7.200
7.192
7.187
7.182
7.176
7.164

4.843

3.289
3.269
3.256
3.032
2.999
2.757
2.742

0.000

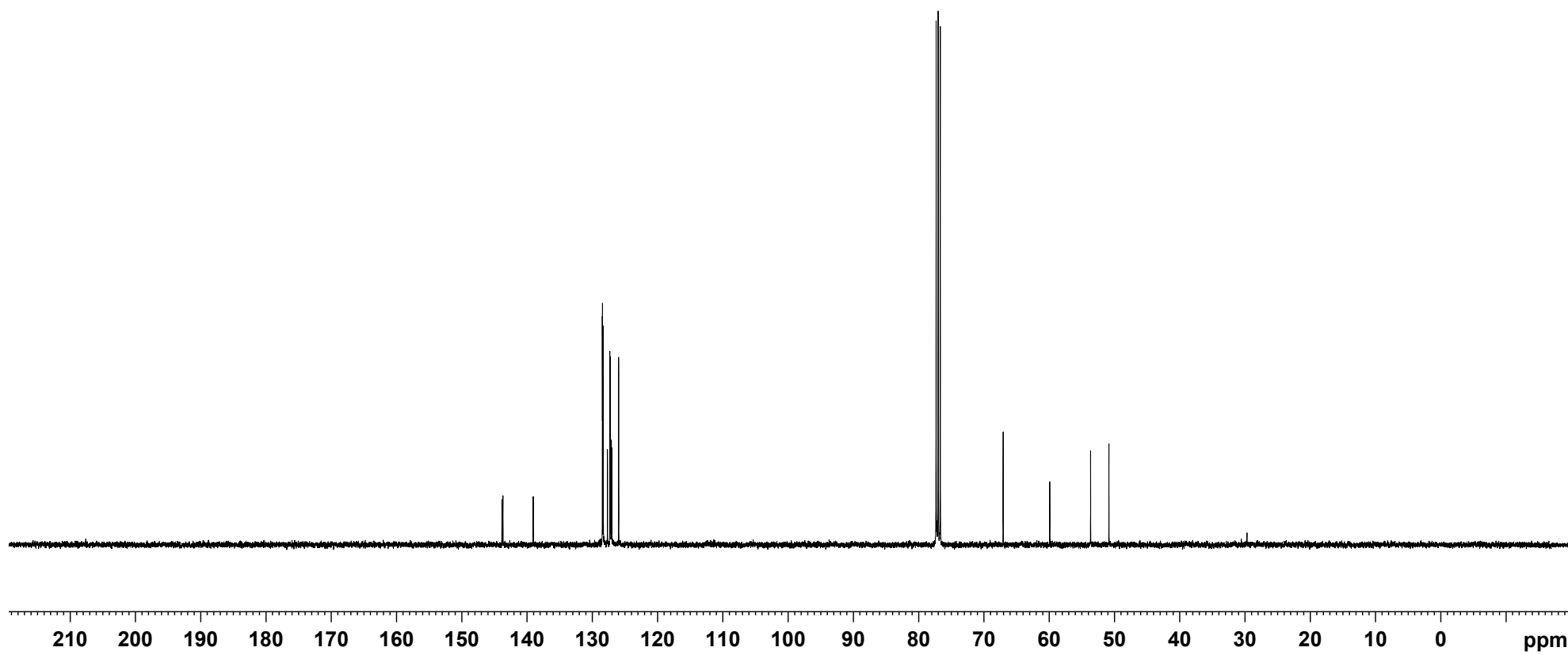


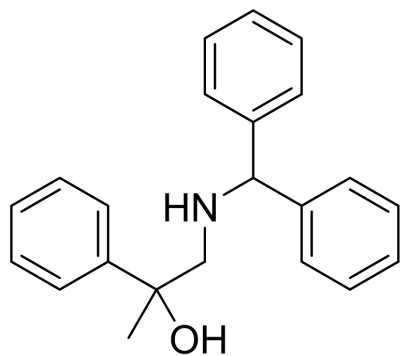


3

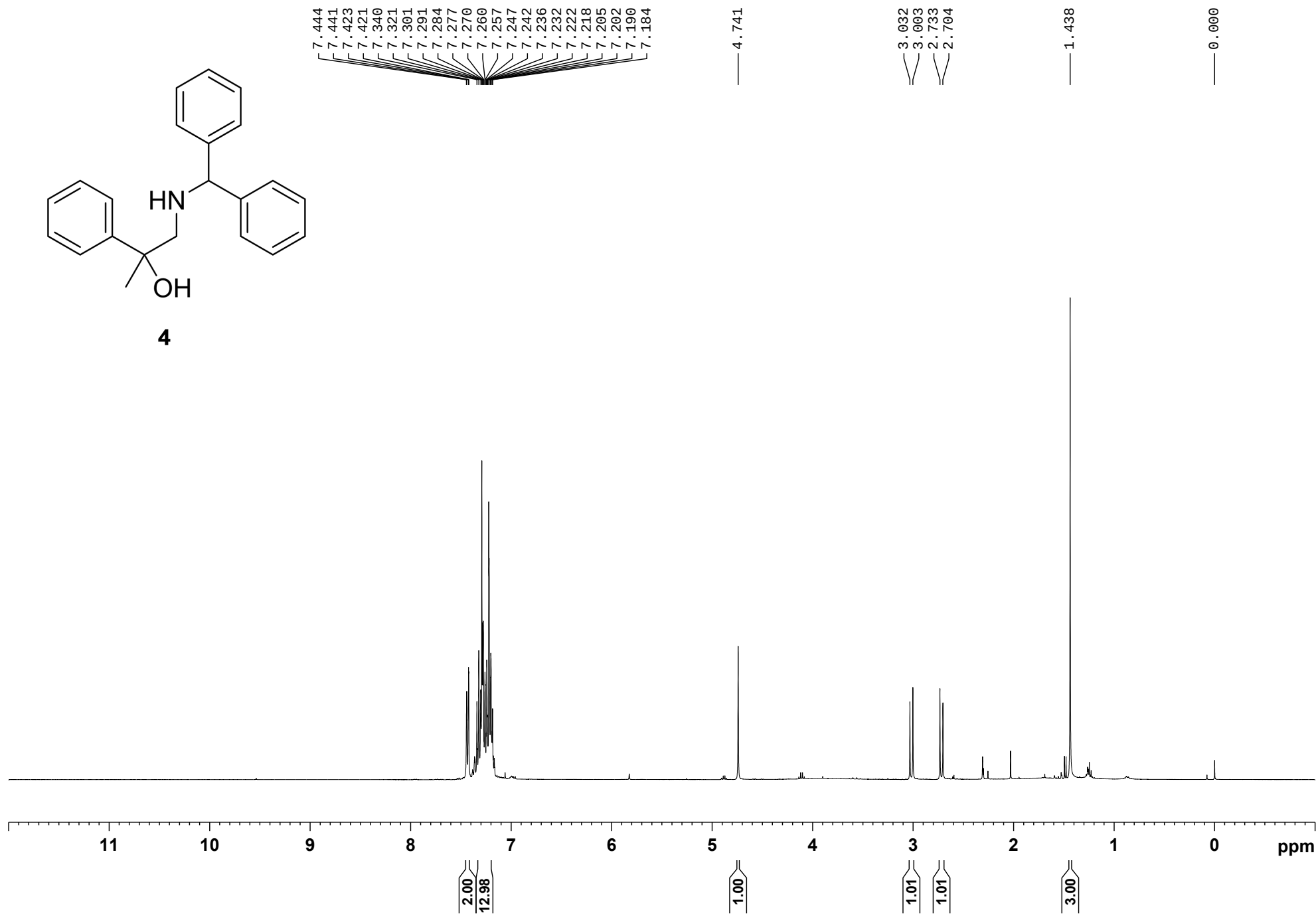
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143.69
139.05
128.45
128.43
128.32
127.67
127.30
127.22
127.07
127.01
125.96

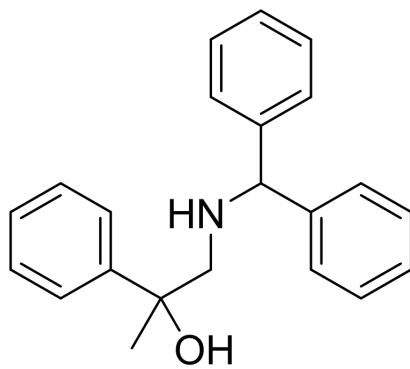
77.32
77.00
76.68
67.05
59.91
53.65
50.84





4



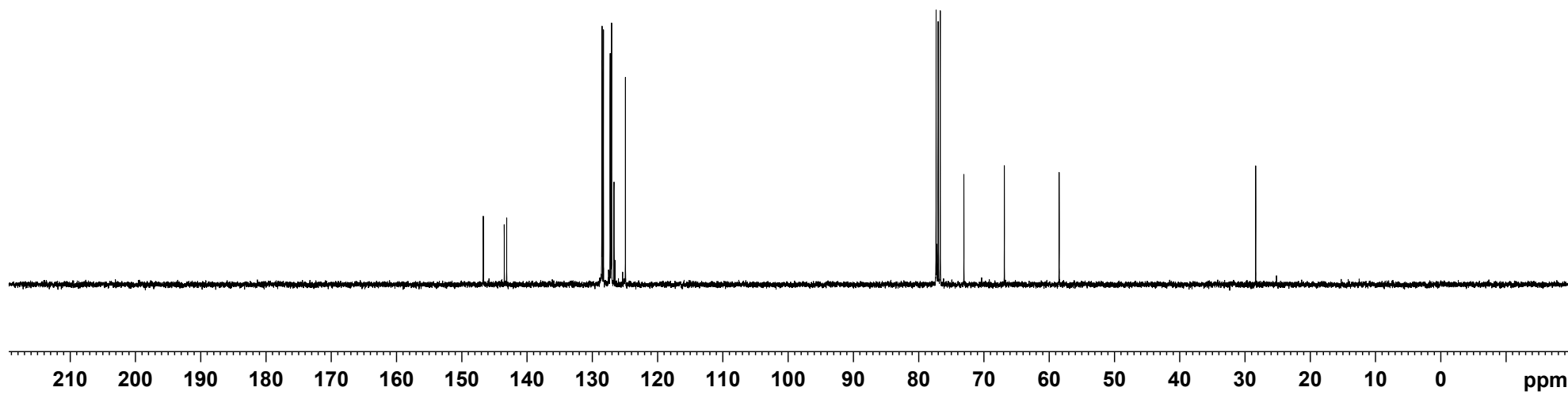


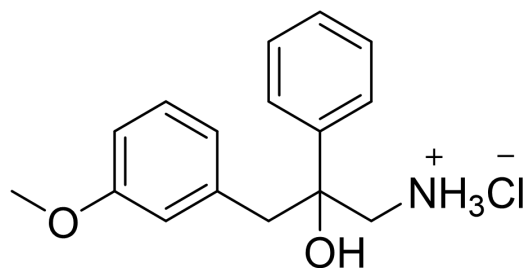
4

146.70
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128.55
128.49
128.45
128.29
127.26
127.13
127.04
126.68
124.92

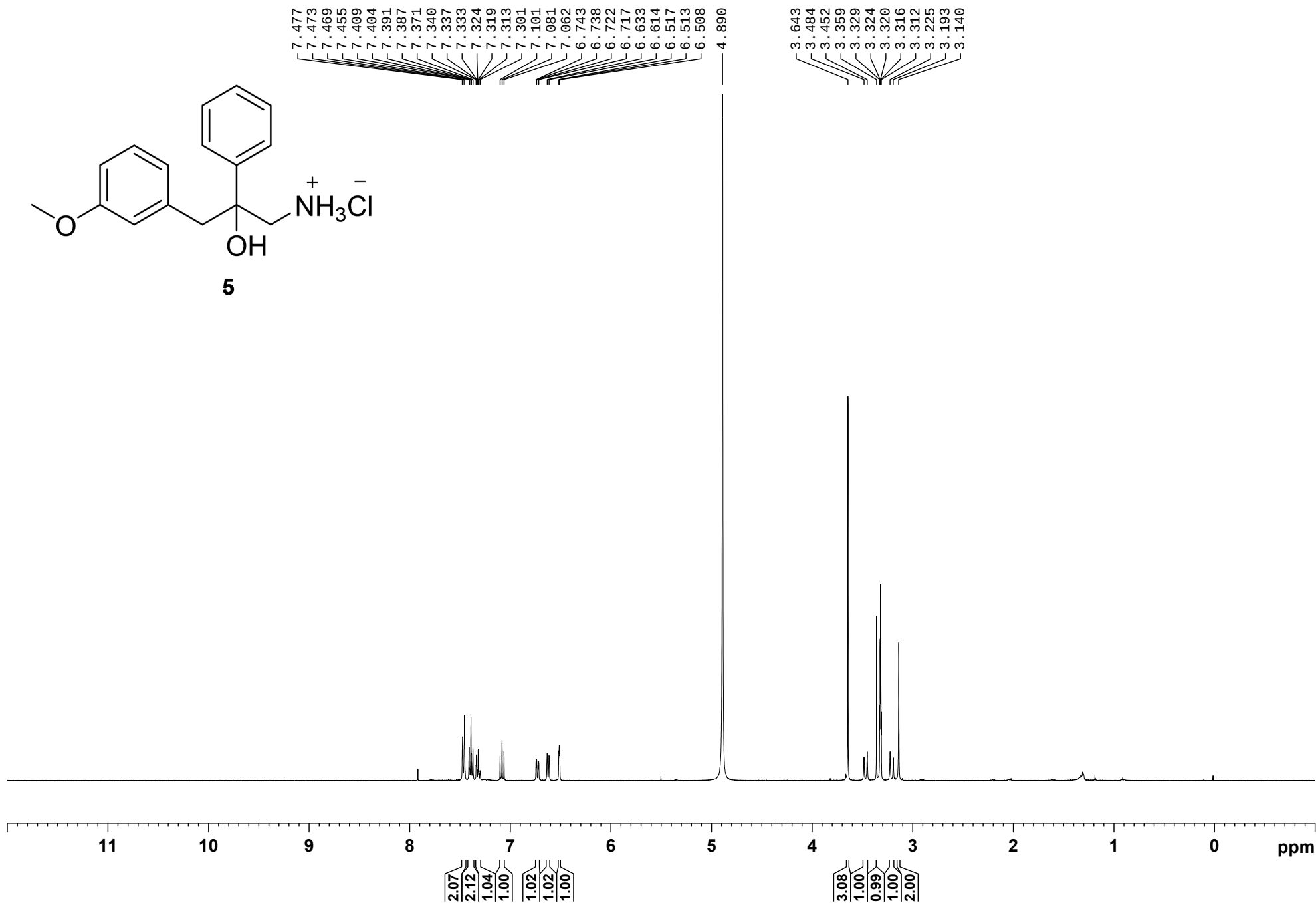
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73.06
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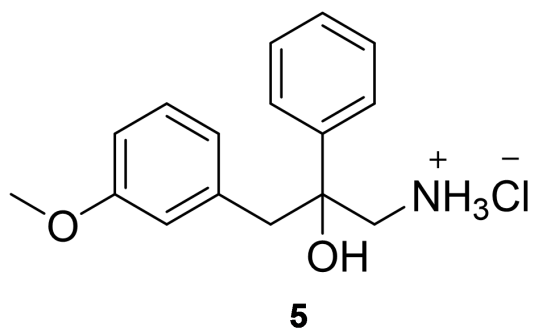
28.35



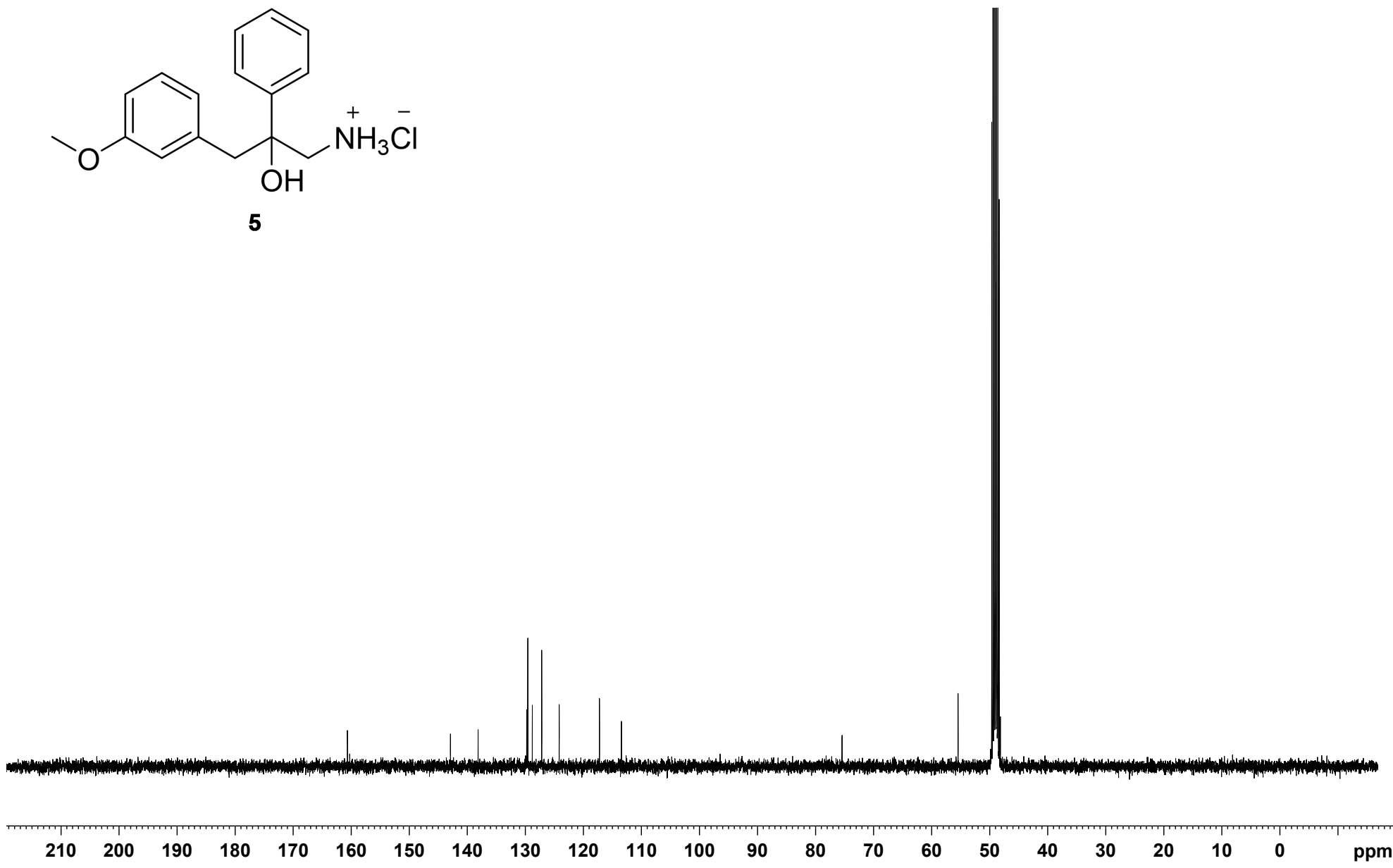


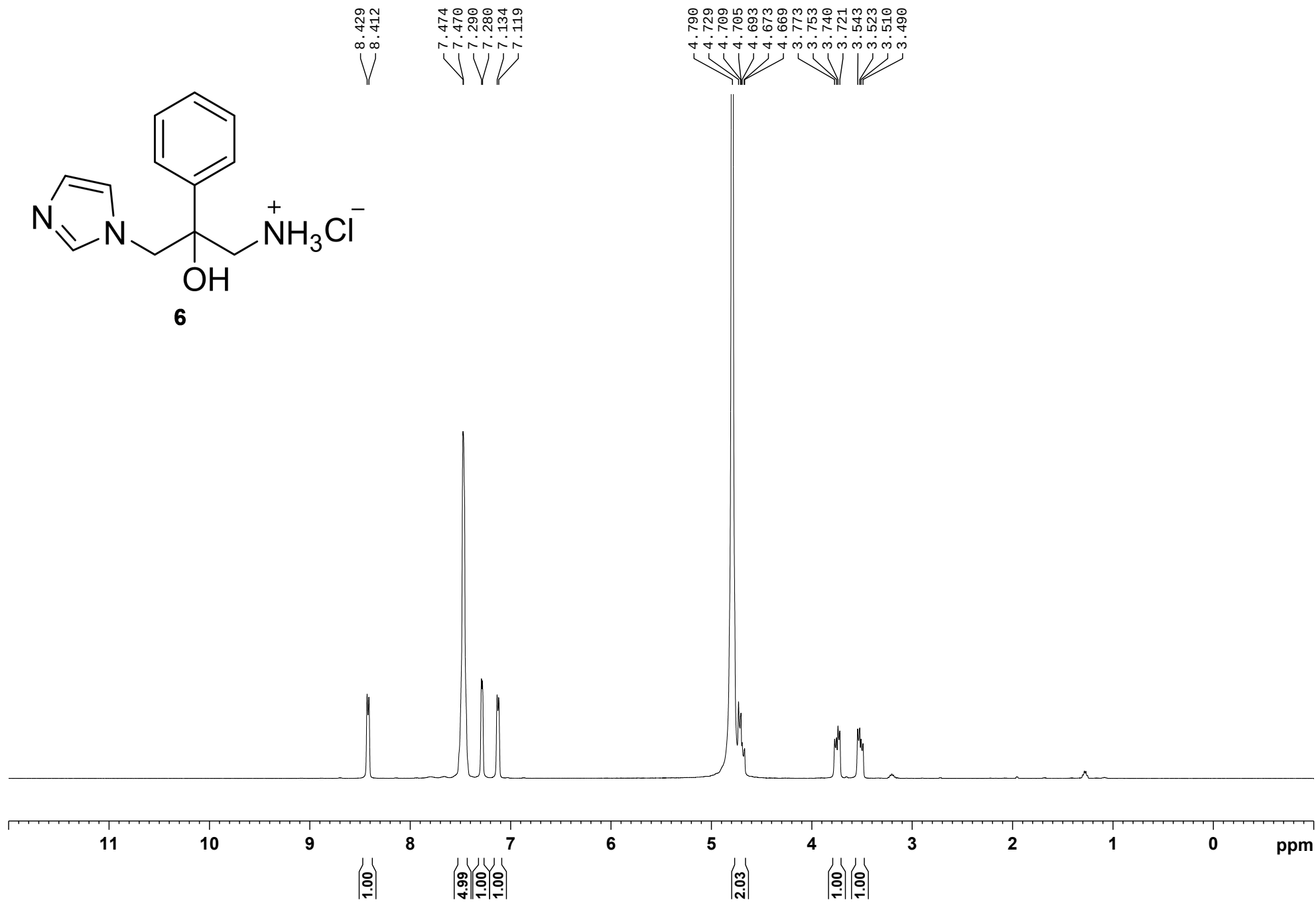
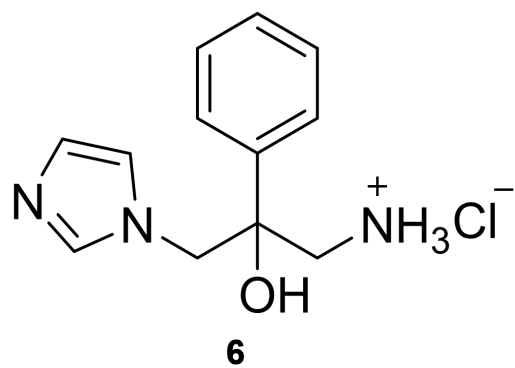
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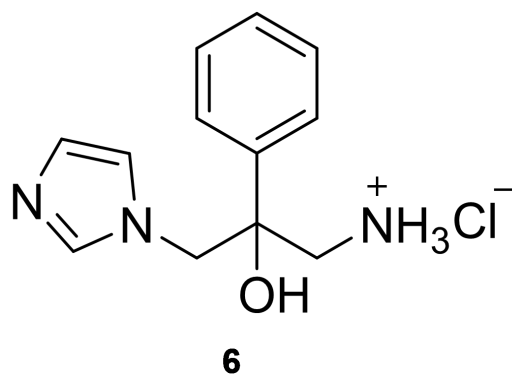




- 160.63
- 142.88
- 138.12
- 129.75
- 129.56
- 128.80
- 127.17
- 124.16
- 117.22
- 113.44
- 75.43
- 55.43
- 49.64
- 49.43
- 49.21
- 49.00
- 48.78
- 48.57
- 48.36
- 48.14





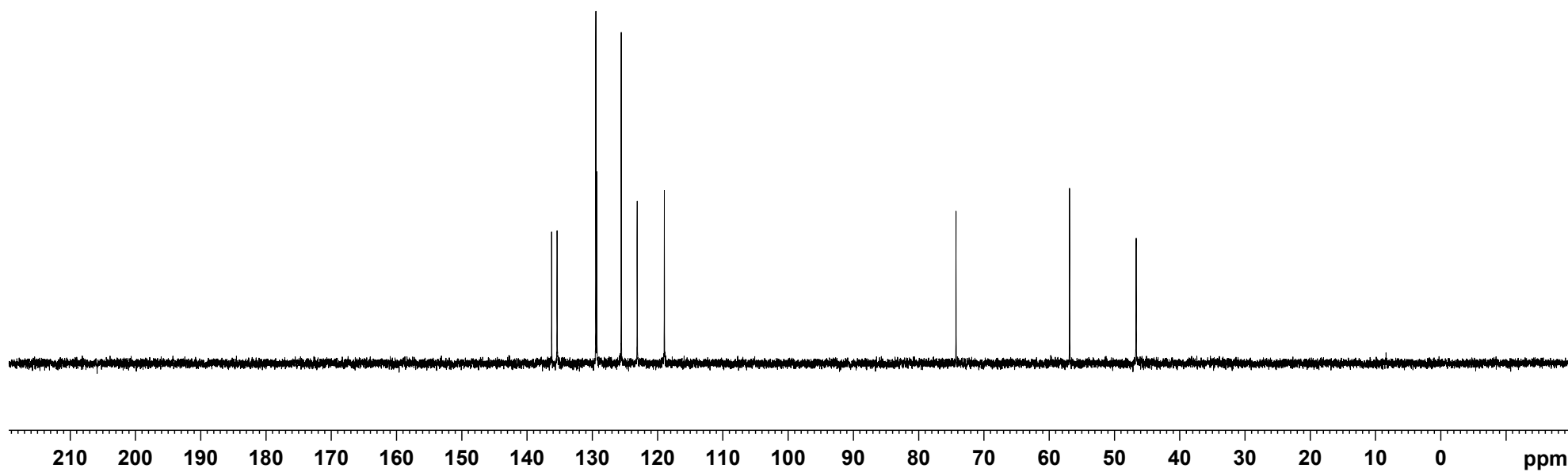


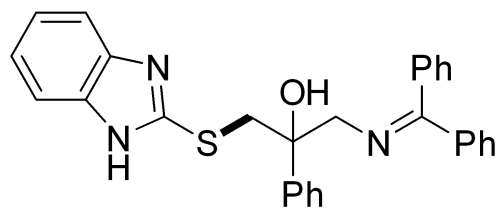
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129.30
125.56
123.11
118.95

74.26

56.86

46.65





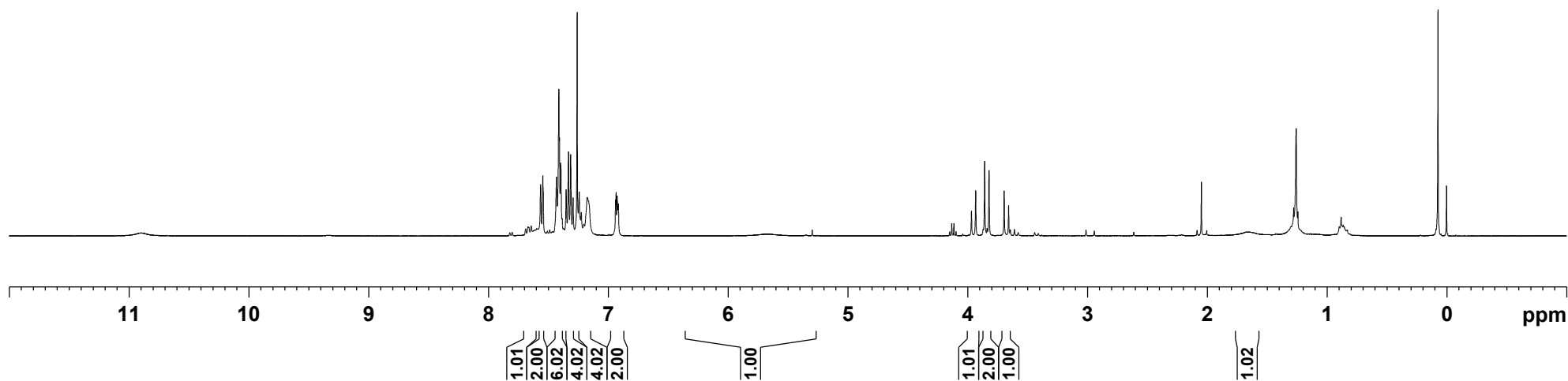
7

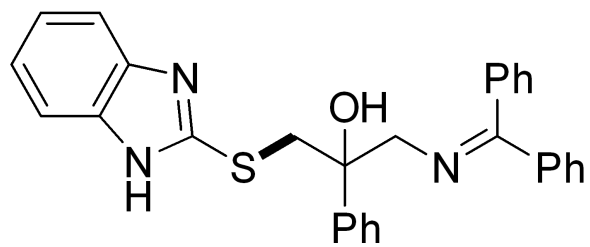
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7.430
7.410
7.405
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7.394
7.349
7.330
7.311
7.292
7.257
7.240
7.223
7.174
7.170
6.937
6.932
6.923
6.913
5.678

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3.856
3.819
3.693
3.656

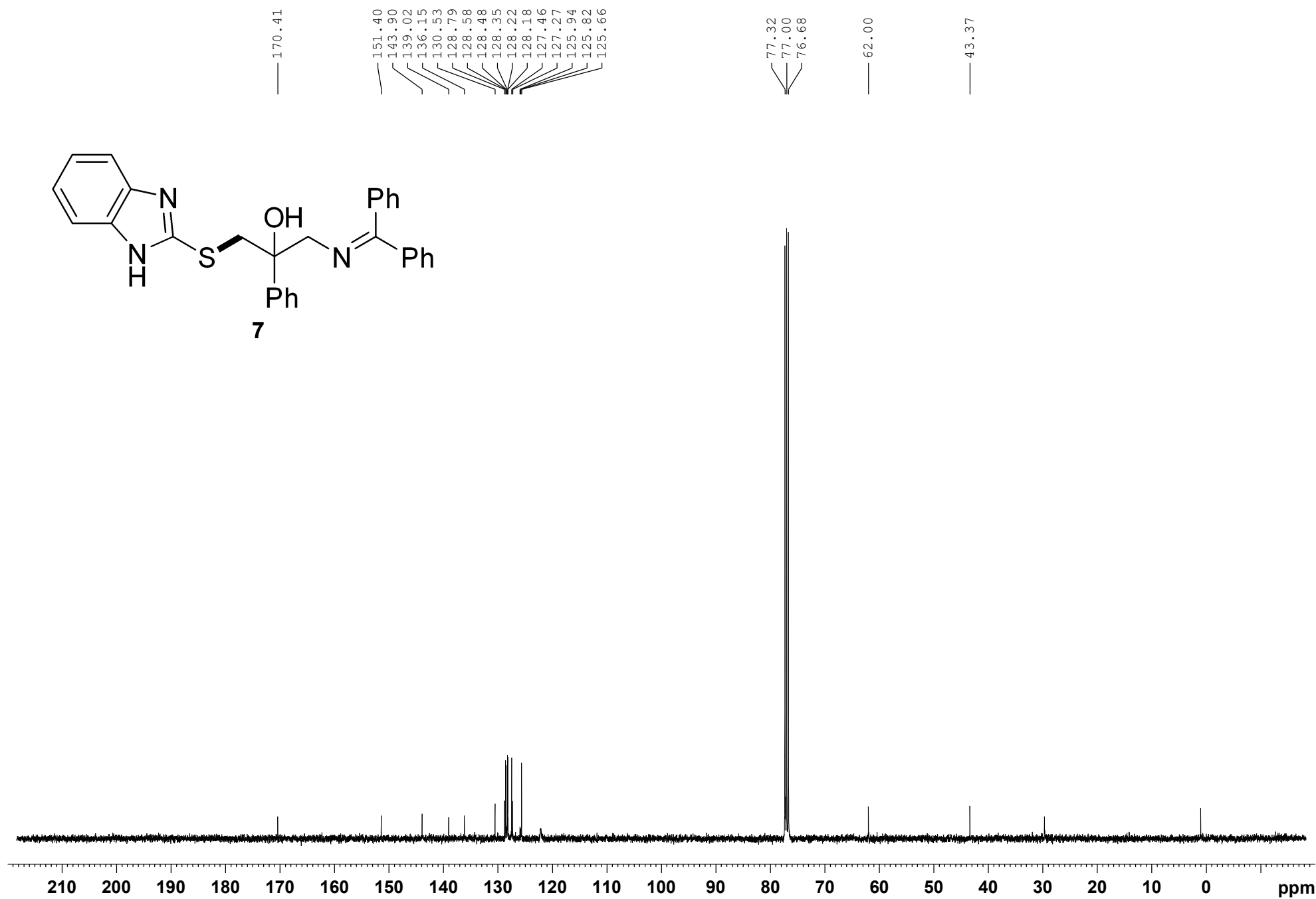
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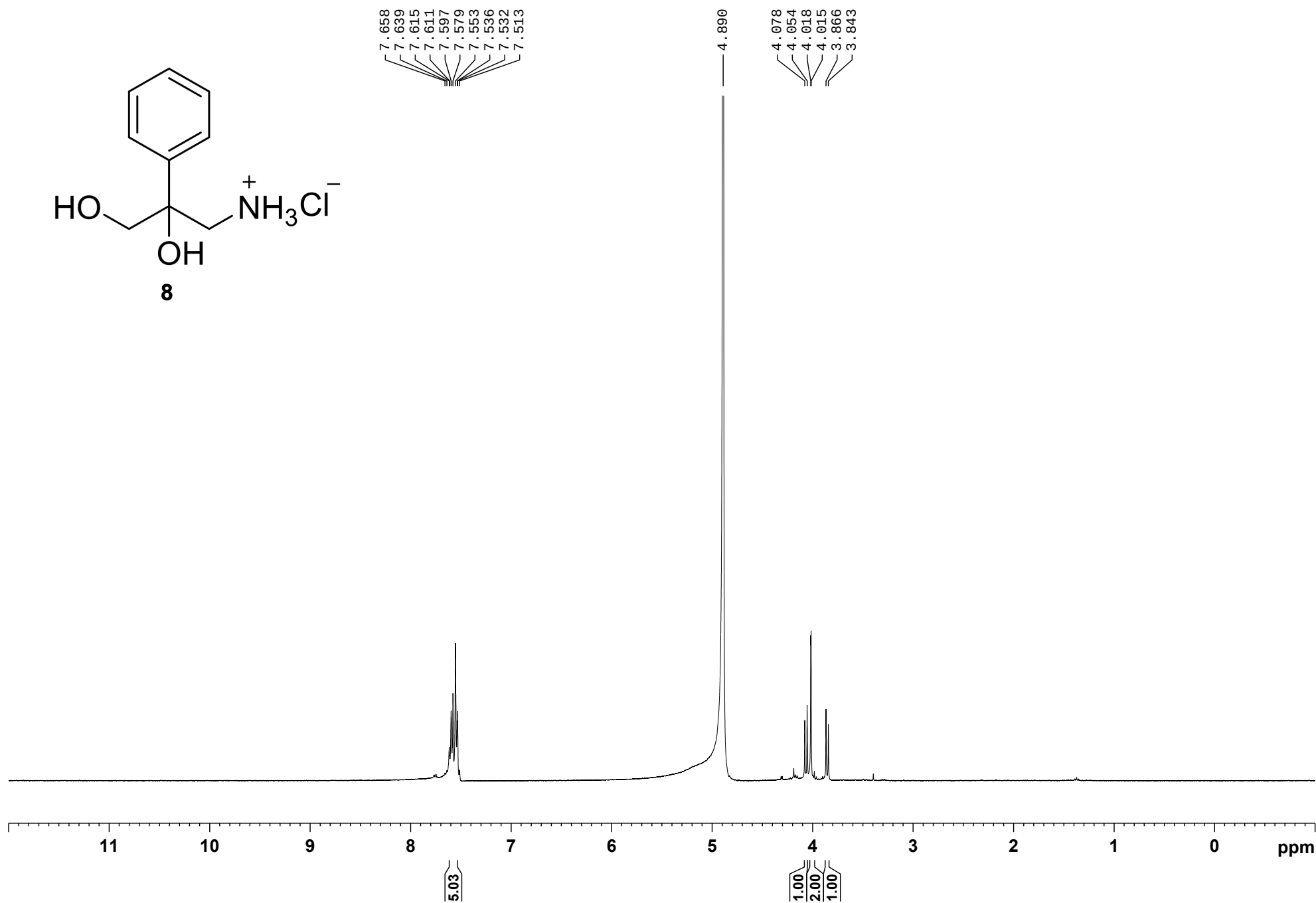
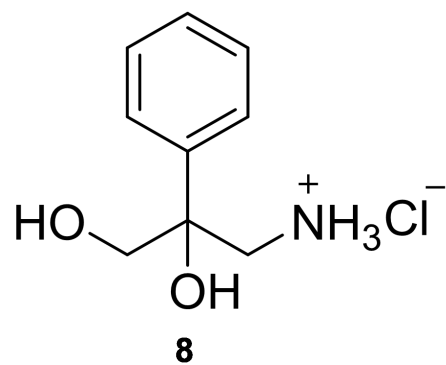
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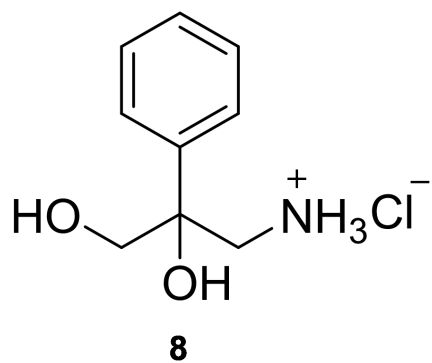




7







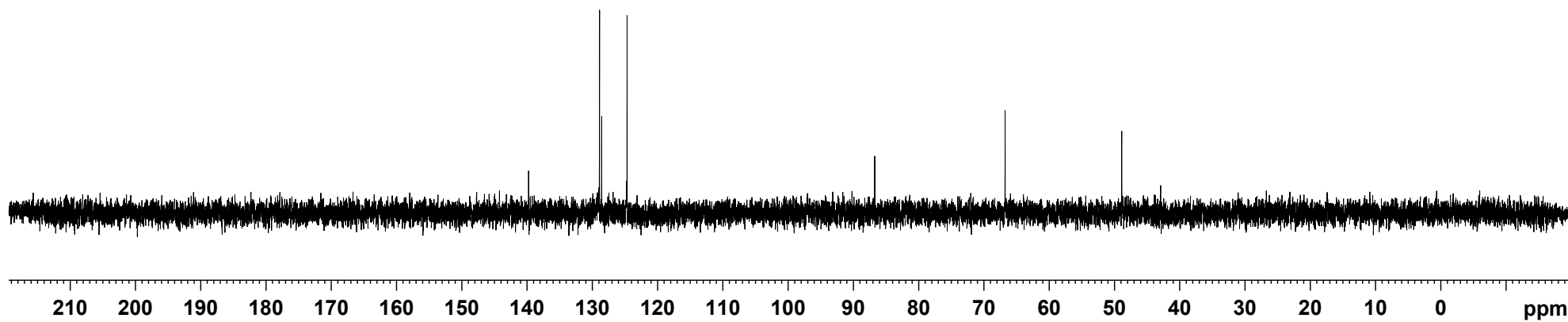
— 139.75

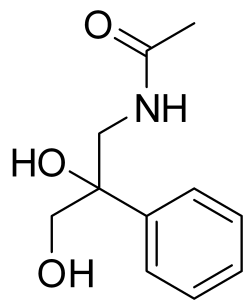
128.89
128.55
— 124.66

— 86.71

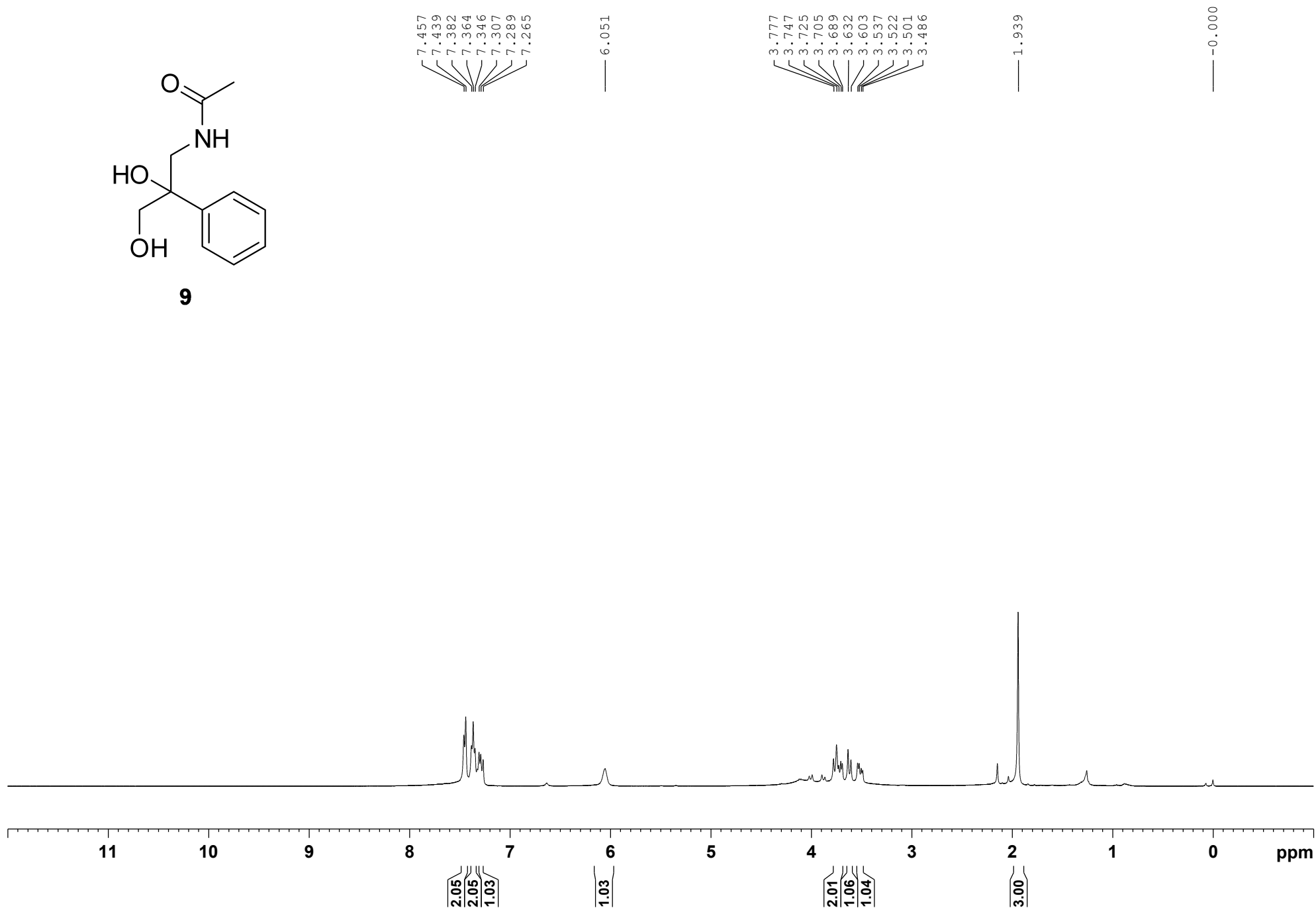
— 66.74

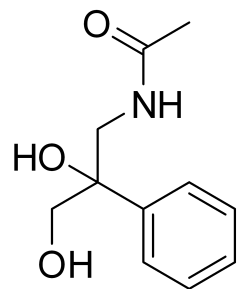
— 48.87





9





9

