Supporting information for article

Barium carbide – new opportunities in organic synthesis and sustainable acetylene chemistry

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Content

1. General Information

***Instrumentation*.** The synthesis of barium carbide was carried out in a tubular muffle furnace LOIP LF-20/250-1200. NMR spectra were recorded on a Bruker Avance 400 spectrometer (400 MHz for ^{1}H; 101 MHz for ^{13}C). Chemical shifts *δ* are given in ppm using residual protons of $CDCl_3$ (^{1}H, δ = 7.26 ppm; ^{13}C, δ = 77.00 ppm) as internal standards. High resolution mass spectra (HRMS) were recorded on a Q Exactive high-resolution liquid chromatograph/mass spectrometer with an UltiMate 3000 chromatograph (Termo Fisher Scientific) using electrospray ionization, ESI (Research Institute of Hygiene, Occupational Pathology, and Human Ecology, FMBA of Russia). X-ray diffraction patterns were recorded on a Bruker D2 Phaser powder diffractometer using CoK_{α} radiation, operating parameters of 30 kV, 10 mA, scanning range 10.00–80.00°, scanning step 0.02°. The $Ba(OH)_2 \cdot 8H_2O$ card for XRD analysis corresponds to that from the ICDD database (PDF-2 Release 2016 RDB), card number 01-076-0224, the $BaCO_3$ card for XRD analysis corresponds to that from the ICDD database (PDF-2 Release 2016 RDB), card number 01-083-3088. Quantitative phase analysis of the samples (wt.%) was carried out using full-profile analysis according to the Rietveld method. Quantitative elemental composition of the samples (with composition normalization to 100%) was carried out using an EDX-800HS Shimadzu X-ray fluorescence spectrometer (Rh radiation source). The measurements were carried out under vacuum conditions using two channels: C-Sc (15 kV) and Ti-U (50 kV). SEM analysis was performed using Zeiss EVO-40EP and Zeiss Merlin electron microscopes equipped with an Oxford INCA 350 energy-dispersive X-ray spectrometer with a detector area of 30 mm^2 at an accelerating voltage of 4–20 kV. Chromatographic analysis was performed using a Chromatec-Crystal 5000 chromatograph equipped with a flame ionization (FID) detector, sample injection temperature 100 °C, carrier gas flow rate 25 mL/min. Each sample was injected with a separate chromatographic syringe. Column chromatography was performed using Merck Silica gel 60 (60–200 mesh). Merck silica gel 60 uv-254 plates were used for thin-layer chromatography (TLC); a 5% aqueous solution of $KMnO_4$ and UV-light were used for visualization.

Chemicals. Barium rod (≥99% purity), 3-ethoxysalicylaldehyde (97% purity), tetrabutylammonium fluoride trihydrate (98% purity) were purchased from Sigma Aldrich, Cs_2CO_3 (99.5% purity), cyclohexanone (99.8% purity) were purchased from Acros Organics, acetophenone (99% purity), 4'-methylacetophenone (96% purity) were purchased from abcr, CuI (98% purity) was purchased from Alfa Aesar, salicylaldehyde was purchased from Reakhim (Russia). Graphite was purchased from a local company. $CDCl_3$ and benzene-d_6 were purchased from Solvex-D (Russia).

Organic solvents – hexane, diethyl ether, pentane, DMSO, DMF were purchased from Komponent Reactiv (Russia) and used without further purification.

Computational details. Quantum chemical, spin restricted calculations were performed using the ORCA 6.0.1 software package.[1] Geometry optimization and calculations of vibrational frequencies in gas phase were performed at the B3LYP(G)/6-31+G* level of theory. For Ba atom a LANL2DZ basis were selected for calculations with ECP to adjust for relativistic effects. To calculate the vibration

frequencies, the Hessian was calculated using an analytical method (the ANFREQ procedure): if each vibration frequency is valid, the optimized geometry corresponds to the true minimum PES. This control was performed for all geometries except for nDMSO systems (see table 1 in paper), because it was important to keep the exact geometry as in the complex with the base. A tight convergence criterion for the Kohn-Sham self-consistent field procedure (TightSCF) was selected. A integration grid (DefGRID3) with disabled the double integration grid procedure (NOFINALGRID) was used to calculate the energies.
A continuum model CPCM was used to simulate the reaction medium; the model solvent was DMSO. The cavity was built using the GEPOL approach[2] with electrostatic scale factor α = 1.1.[3] For the calculation, dielectric constant for DMSO ε = 46.8 was used. The calculations of the Gibbs free energy of solvation ΔG_{solv}^{A} were performed as a separate optimization of the geometry of the molecule, pre-optimized at the B3LYP/6-31+G* (or B3LYP/6-31+G*+LANL2DZ) theory level, and calculated as the difference of the Gibbs energy of the molecule in the solvent medium and in the gas phase. The standard Gibbs free energy of compound A in DMSO solution was calculated according to equation:

$$G^A = H^A - T \cdot S_{sol} + \Delta G_{solv}^{A},$$

where S_{sol} is entropy in the DMSO solution, according to the Wertz approach[4], which takes into account the change of state of the system from an ideal gas at 1 atm pressure and temperature 403.15 K to 1M DMSO solution at the same temperature as follows:

$$S_{sol} = 0.74 S_{harm} - 1.294\ cal \cdot mol^{-1} \cdot K^{-1}$$

2. Synthetic part

Barium carbide synthesis

Metallic barium (137 mg, 1 mmol) 0.5–1 cm size pieces and graphite powder (36 mg, 3 mmol) were placed in a sealed quartz tube pre-filled with argon and purged with argon for 10 minutes. Then the tube with the reaction mixture was placed in a muffle furnace and heated in an argon atmosphere at 600 °C for 30–60 minutes. The time was counted from the moment the temperature reached 600 °C. Upon completion of the reaction, the tube was cooled to room temperature, the carbide was removed from the tube, placed in a vial, blown with argon, covered with a lid and weighed.

Synthetic procedure for ketoximes 18, 19

Acetophenone (600 mg, 5 mmol) or 4'-methyl acetophenone (663 mg, 5 mmol), AcONa (820 mg, 10 mmol) dissolved in MeOH (20 mL), then $NH_2OH{\cdot}HCl$ (521 mg, 7.5 mmol) was added. The mixtures were refluxed, the reactions were monitored by TLC (eluent – $CHCl_3$, visualizer – UV light). After reactions complete the mixtures were extracted with EtOAc, washed with water and brine, dried over Na_2SO_4, the solvent was removed under reduced pressure.

Synthetic procedure for dodecyl vinyl thioether (1a)

KOH (62 mg, 1.1 mmol), thiol (1.0 mmol) and DMSO (2 mL) were placed in a test tube with a screw cap and stirred for 5 minutes at room temperature. Then BaC_2 (322 mg, 2 mmol) and H_2O (74 μL, 4 mmol) were added and the test tube was immediately stoppered and placed in a silicone oil bath preheated to 100 °C. The mixture was stirred for 3 h at 100 °C. After completion of the reaction, the mixture was cooled to room temperature, extracted with methyl *tert*-butyl ether (MTBE). The organic extract was washed with water and brine, dried over Na_2SO_4, the solvent was removed under reduced pressure. The residue was chromatographed on silica gel (eluent – pentane, visualizer – 5% $KMnO_4$).

General procedure for base-free vinylation of thiols

Thiol (1.0 mmol) and DMSO (2 mL) were placed in a test tube with a screw cap and stirred for 5 minutes at room temperature. Then BaC_2 (322 mg, 2 mmol) and H_2O (74 μL, 4 mmol) were added and the test tube was immediately stoppered and placed in a silicone oil bath preheated to 100 °C. The mixture was stirred for 3 h at 100 °C. After completion of the reaction, the mixture was cooled to room temperature, extracted with MTBE. The organic extract was washed with water and brine, dried over Na_2SO_4, the solvent was removed under reduced pressure. Thioethers were purified by column chromatography on silica gel (eluent – pentane, visualizer – 5% $KMnO_4$).

Synthetic procedure for vinyl ether 6a–9a

KOH (70 mg, 1.25 mmol), KF (116 mg, 2 mmol), alcohol (1.0 mmol), DMSO (2 mL) were placed in a test tube with a screw cap and stirred for 5 minutes at room temperature. Then BaC_2 (322 mg, 2 mmol), H_2O (74 μL, 4 mmol) were added and the test tube was immediately stoppered and placed in a silicone oil bath preheated to 130 °C. The mixture was stirred for 3 h at 130 °C. After completion of the reaction, the mixture was cooled to room temperature, extracted with MTBE. The organic extract was washed with water and

brine, dried over Na_2SO_4, the solvent was removed under reduced pressure. The residue was chromatographed on silica gel (eluent – pentane, visualizer – 5% $KMnO_4$).
Reaction of 2-naphthol with BaC_2 were carried out similarly using K_2CO_3 (69 mg, 0.5 mmol) and KF (232 mg, 4 mmol) as base.

Synthesis of *N*-vinyl ether 10a, 11a

KOH (62 mg, 1.1 mmol), KF (58 mg, 1 mmol), amine (1.0 mmol), DMSO (2 mL) were placed in a test tube with a screw cap and stirred for 5 minutes at room temperature. Then BaC_2 (322 mg, 2 mmol), H_2O (74 μL, 4 mmol) were added and the test tube was immediately stoppered and placed in a silicone oil bath preheated to 130 °C. The mixture was stirred for 4 h at 130 °C. After completion of the reaction, the mixture was cooled to room temperature, extracted with MTBE. The organic extract was washed with water and brine, dried over Na_2SO_4, the solvent was removed under reduced pressure. The residue was chromatographed on silica gel (eluent – pentane, visualizer – 5% $KMnO_4$).

Synthesis of *N*-vinylazepan-2-one (12a)

K_2CO_3 (138 mg, 1 mmol), KF (58 mg, 1 mmol), ε-caprolactam (113 mg, 1 mmol), DMSO (2 mL) were placed in a test tube with a screw cap and stirred for 5 minutes at room temperature. Then BaC_2 (322 mg, 2 mmol) and H_2O (74 μL, 4 mmol) were added and the test tube was immediately stoppered and placed in a silicone oil bath preheated to 110 °C. The mixture was stirred for 4 h at 110 °C. After completion of the reaction, the mixture was cooled to room temperature, extracted with MTBE. The organic extract was washed with water and brine, dried over Na_2SO_4, the solvent was removed under reduced pressure. The residue was chromatographed on silica gel (eluent – pentane, visualizer – 5% $KMnO_4$).

Synthetic procedures for ethynylalcohols 13a and 14a

Method 1. Cs_2CO_3 (163 mg, 0.5 mmol), BaC_2 (322 mg, 2 mmol), ketone (1 mmol), DMSO (3 mL), were placed in a test tube, water (74 μL, 4 mmol) was added, the test tube was immediately capped and heated at 80 °C for 6 h. After completion of the reaction, the mixture was cooled to room temperature, extracted with MTBE, washed with brine, and dried over Na_2SO_4.

Method 2. Ketone (0.5 mmol), TBAF·$3H_2O$ (8 mg, 0.025 mmol), DMSO (2 mL), BaC_2 (242 mg, 1.5 mmol), H_2O (56 μL, 3 mmol) were placed in a test tube. The test tube was immediately capped and stirred at room temperature for 24 h. After completion of the reaction, the mixture was cooled to room temperature, extracted with MTBE, washed with brine, and dried over Na_2SO_4, the solvent was removed under reduced pressure. The residue was chromatographed on silica gel (eluent – hexane:Et_2O 10:1, visualizers – UV-light и 5% $KMnO_4$).

Synthetic procedure for 1,2,3-triazoles 15a, 16a

2,4,6-Trimethylphenyl azide and 4-methylphenylazide were synthesized according to described procedure.[1] Mesityl azide or 4-methylphenyl azide (1 mmol), CuI (19 mg, 0.1 mmol), Et_3N (250 μL, 1.8 mmol), DMSO (2 mL), BaC_2 (322 mg, 2 mmol) and H_2O (74 μL, 4 mmol) were placed in a test tube with a screw cap and stirred for 6 h at 80 °C. After

[1] F. Shamsi, B. Aneja, P. Hasan, B. Zeya, M. Zafaryab, S. H. Mehdi, M. M. A. Rizvi, R. Patel, S. Rana, M. Abid, *ChemistrySelect* **2019**, *4*, 12176–12182.

completion of the reaction, the mixture was cooled to room temperature, extracted with EtOAc. The organic extract was washed with water and brine, dried over Na_2SO_4, the solvent was removed under reduced pressure. Triazoles were purified by flash chromatography (eluent – $CHCl_3$, visualizer – 5% $KMnO_4$).

Synthetic procedure for synthesis of arylpyrroles 20, 21

Ketoxime (0.5 mmol), NaOH (20 mg, 0.5 mmol), DMSO (2 mL), BaC_2 (242 mg, 1.5 mmol) and H_2O (56 μL, 3 mmol) were placed in a test tube with a screw cap and stirred for 6 h at 80 °C. After completion of the reaction, the mixture was cooled to room temperature, extracted with Et_2O. The organic extract was washed with water and brine, dried over Na_2SO_4, the solvent was removed under reduced pressure. The residue was chromatographed on silica gel (eluent – hexane:Et_2O 5:1, visualizer – 5% $KMnO_4$).

Synthetic procedure for the synthesis of benzofuran-2-ones 22a, 23a

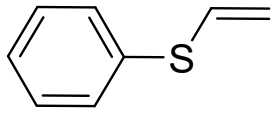
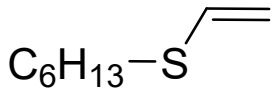
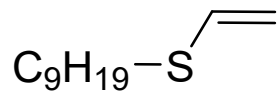
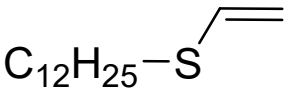
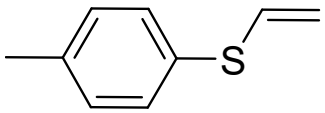
Salicylaldehyde (0.5 mmol), Cs_2CO_3 (326 mg, 1 mmol) and DMF (2 mL) were placed in a test tube with a screw cap and stirred for 5-10 minutes at room temperature. Then BaC_2 (232 mg, 2 mmol) and H_2O (74 μL, 4 mmol) were added and stirred for 15 h at 130 °C. After completion of the reaction, the mixture was cooled to room temperature, extracted with EtOAc. The organic extract was washed with water and brine, dried over Na_2SO_4, the solvent was removed under reduced pressure. Benzofuran-2-ones were purified by column chromatography (eluent – hexane:Et_2O 10:1, visualizer – 5% $KMnO_4$). Compound **23a** was additionally recrystallized from pentane.

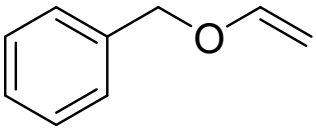
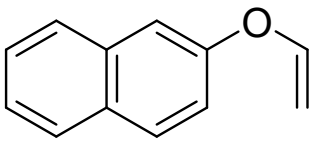
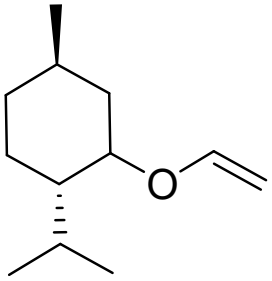
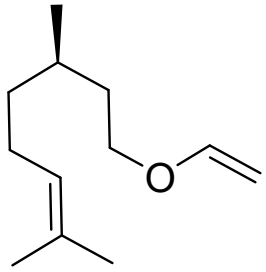
General procedures for Sonogashira cross-coupling

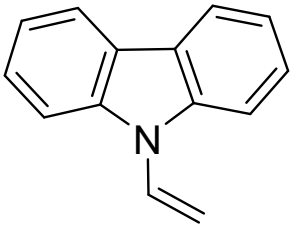
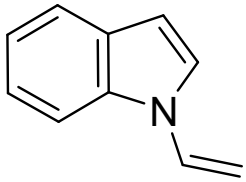
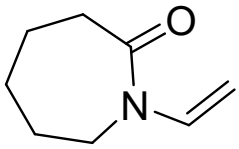
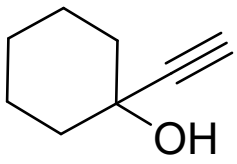
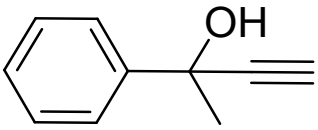
Method 1. CuI (10 mg, 0.05 mmol), $Pd(OAc)_2$ (6 mg, 0.025 mmol), PPh_3 (13 mg, 0.05 mmol) and MeCN (2 mL) were placed in a test tube with a screw cap, and the solution was purged with argon for 10 min. Then Et_3N (208 μL, 1.5 mmol), 4-anisyl iodide (117 mg, 0.5 mmol), BaC_2 (242 mg, 1.5 mmol) and water (565 μL, 3 mmol) were added to the reaction mixture, the test tube was capped and the mixture was stirred at room temperature for 24 h. After completion of the reaction, the mixture was extracted with MTBE, washed with water and brine, the organic extract was dried over Na_2SO_4, and the solvent was removed. The residue was chromatographed on silica gel, eluent – hexane:Et_2O 5:1, visualizer – UV light.

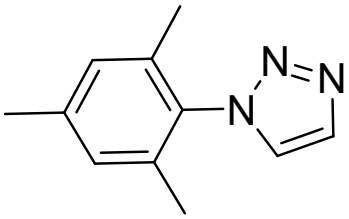
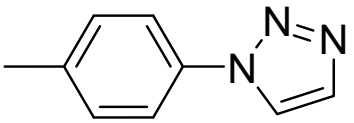
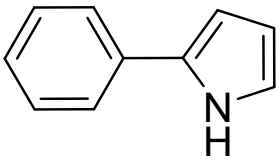
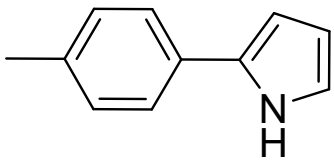
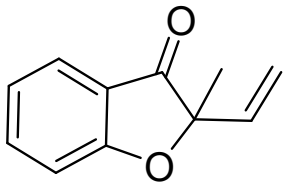
Method 2. $Cu(acac)_2$ (13 mg, 0.1 mmol), $Pd(OAc)_2$ (6 mg, 0.025 mmol), PPh_3 (26 mg, 0.1 mmol) and DMSO (2 mL) were placed in a test tube with a screw cap, and the solution was purged with argon for 5 min. Then TBAF·$3H_2O$ (16 mg, 0.5 mmol), 4-anisyl iodide (117 mg, 0.5 mmol), BaC_2 (242 mg, 1.5 mmol) and water (56 μL, 3 mmol) were added to the reaction mixture, the test tube was capped and the mixture was stirred at 65 °C for 24 h. Then the mixture was extracted with MTBE, washed with brine, dried over Na_2SO_4, and the solvent was removed. The residue was chromatographed on silica gel, eluent – hexane:Et_2O 10:1, then 5:1, visualizer – UV light.

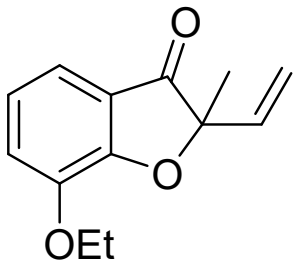
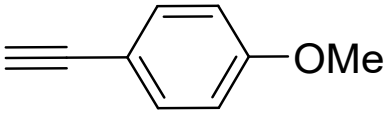
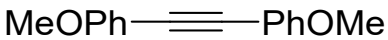
3. Spectral data of synthesized compounds

	**Phenyl vinyl thioether (1a)**. Colorless oil, yield 98%. ^{1}H NMR (400 MHz, C_6D_6) δ 7.33–7.22 (m, 2H), 7.01–6.85 (m, 3H), 6.32 (dd, *J* = 16.6, 9.6 Hz, 1H), 5.22 (d, *J* = 16.6 Hz, 1H), 5.04 (d, *J* = 9.6 Hz, 1H). ^{13}C NMR (101 MHz, C_6D_6) δ 134.8, 132.3, 130.8, 129.3, 127.2, 115.2. HRMS (ESI), *m/z*: 137.04180 $[M+H]^+$, (calc. for $C_8H_9S^+$, *m/z*: 137.04195). Spectral data correspond to those given in the references[5, 7].
	**1-Hexyl vinyl thioether (2a)**. Colorless oil, yield 59%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.36 (dd, *J* = 16.7, 10.2 Hz, 1H), 5.14 (dd, *J* = 32.1, 13.4 Hz, 2H), 2.81–2.62 (m, 2H), 1.78–1.55 (m, 2H), 1.47–1.32 (m, 2H), 1.34–1.21 (m, 4H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.6, 110.3, 31.9, 31.4, 29.2, 28.9, 22.7, 14.1. Spectral data correspond to those given in the reference[5].
	**1-Nonyl vinyl thioether (3a)**. Colorless oil, yield 68%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.36 (dd, *J* = 16.7, 10.2 Hz, 1H), 5.13 (dd, *J* = 32.2, 13.4 Hz, 2H), 2.68 (td, *J* = 7.4, 4.0 Hz, 2H), 1.72–1.60 (m, 2H), 1.46–1.35 (m, 2H), 1.34 – 1.21 (m, 9H), 0.88 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.6, 110.3, 31.8, 31.4, 29.4, 29.2, 29.2, 29.0, 28.9, 22.6, 14.1. HRMS (ESI), *m/z*: 293.04855 $[M+Ag]^+$, (calc. for $C_{11}H_{22}SAg^+$, *m/z*: 293.04877). Spectral data correspond to those given in the references[6].
	**Dodecyl vinyl thioether (1a)**. Colorless oil, yield 95%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.34 (dd, *J* = 16.7, 10.2 Hz, 1H), 5.12 (dd, *J* = 31.7, 13.4 Hz, 2H), 2.67 (dd, *J* = 12.8, 5.4 Hz, 2H), 1.62 (dt, *J* = 15.0, 7.3 Hz, 2H), 1.44–1.32 (m, 2H), 1.33–1.20 (m, 16H), 0.87 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.6, 110.3, 31.9, 31.4, 29.6, 29.6, 29.6, 29.5, 29.3, 29.2, 29.1, 28.9, 22.7, 14.1. HRMS (ESI), *m/z*: 335.09512 $[M+Ag]^+$, (calc. for $C_{14}H_{28}SAg^+$, *m/z*: 335.09572). Spectral data correspond to those given in the reference[5].
	**4-Methylphenyl vinyl thioether (5a)**. Colorless oil, yield 51%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 6.52 (dd, *J* = 16.6, 9.6 Hz, 1H), 5.28 (dd, *J* = 16.6, 13.2 Hz, 2H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.4, 132.7, 131.3, 130.2, 129.9, 114.2, 21.1. HRMS (ESI), *m/z*: 151.105710 $[M+H]^+$, (calc. for $C_9H_{11}S^+$, *m/z*: 151.05760). Spectral data correspond to those given in the reference[5].

	**Benzyl vinyl ether (6a)**. Colorless oil, yield 60%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44–7.30 (m, 5H), 6.60 (dd, *J* = 14.3, 6.8 Hz, 1H), 4.79 (s, 2H), 4.34 (dd, *J* = 14.3, 2.0 Hz, 1H), 4.12 (dd, *J* = 6.8, 1.9 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.6, 136.9, 128.5, 127.9, 127.5, 87.3, 70.1. HRMS (ESI), *m/z*: 240.97756 $[M+Ag]^+$, (calc. for $C_9H_{10}OAg^+$, *m/z*: 240.97771). Spectral data correspond to those given in the reference[8].
	**2-Vinyloxyphenantren (7a)**. Colorless oil, yield 60%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (dt, *J* = 8.9, 1.6 Hz, 2H), 7.51 (ddd, *J* = 39.0, 7.5, 1.4 Hz, 1H), 7.41–7.27 (m, 1H), 7.09 (t, *J* = 1.4 Hz, 1H), 6.60 (dd, *J* = 16.8, 10.1 Hz, 1H), 4.65 (dd, *J* = 16.9, 2.0 Hz, 1H), 4.42 (dd, *J* = 10.0, 2.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.6, 148.1, 134.2, 130.1, 129.8, 127.7, 127.1, 126.6, 124.6, 118.9, 111.6, 95.6. HRMS (ESI), *m/z*: 171.08029 $[M+H]^+$, (calc. for $C_{12}H_{11}O^+$, *m/z*: 171.08044). Spectral data correspond to those given in the reference[9].
	**Menthyl vinyl ether (8a)**. Yellow oil, yield 40%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.38–6.26 (m, 1H), 4.28 (dd, *J* = 14.1, 1.2 Hz, 1H), 3.94 (dd, *J* = 6.5, 1.2 Hz, 1H), 3.53 (td, *J* = 10.7, 4.3 Hz, 1H), 2.16–2.01 (m, 2H), 1.66 (ddt, *J* = 12.3, 6.2, 3.1 Hz, 2H), 1.48–1.20 (m, 4H), 1.03 (ddd, *J* = 12.7, 7.5, 3.6 Hz, 1H), 0.91 (t, *J* = 7.2 Hz, 6H), 0.78 (d, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.3, 87.5, 79.8, 47.8, 40.9, 34.4, 34.1, 31.48, 25.8, 23.5, 22.1, 20.7, 16.3. HRMS (ESI), *m/z*: 183.17418 $[M+H]^+$, (calc. for $C_{12}H_{22}O^+$, *m/z*: 183.17434). Spectral data correspond to those given in the references[8, 10].
	**Citronellyl vinyl ether (9a)**. Yellow oil, yield 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.46 (dd, *J* = 14.3, 6.8 Hz, 1H), 5.10 (t, *J* = 7.1 Hz, 1H), 4.17 (dd, *J* = 14.3, 1.7 Hz, 1H), 3.97 (dd, *J* = 6.8, 1.8 Hz, 1H), 3.78–3.63 (m, 2H), 2.09–1.93 (m, 2H), 1.77–1.66 (m, 1H), 1.68 (s, 3H), 1.60 (s,3H), 1.46 (dt, *J* = 20.8, 6.9 Hz, 1H), 1.18 (dddd, *J* = 13.6, 9.4, 7.7, 6.2 Hz, 1H), 0.91 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.0, 131.3, 124.7, 86.2, 66.4, 37.1, 35.9, 29.5, 25.7, 25.4, 19.5, 17.6. HRMS (ESI), *m/z*: 183.17422 $[M+H]^+$, (calc. for $C_{12}H_{23}O^+$, *m/z*: 183.17434). Spectral data correspond to those given in the references[10, 11].

	**N-vinyl carbazole (10a)**. White powder, yield 65%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.7 Hz, 2H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.52–7.44 (m, 1H), 7.44–7.37 (m, 1H), 7.35 (d, *J* = 2.2 Hz, 1H), 7.24 (dd, *J* = 9.0, 2.5 Hz, 1H), 6.80 (dd, *J* = 13.7, 6.1 Hz, 1H), 4.87 (dd, *J* = 13.7, 1.5 Hz, 1H), 4.53 (dd, *J* = 6.1, 1.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.3, 129.5, 126.2, 124.0, 120.6, 120.2, 110.4, 110.2, 102.0. HRMS (ESI), *m/z*: 194.1073 $[M+H]^+$, (calc. for $C_{14}H_{12}N^+$, *m/z*: 194.09637). Spectral data correspond to those given in the reference[12].
	**N-Vinyl indole (11a)**. Brown powder, yield – 60%.^{1}H NMR (400 MHz, DMSO-d_6) δ 7.81 (d, *J* = 3.4 Hz, 1H), 7.69 (d, *J* = 8.3 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.50 (dd, *J* = 15.6, 9.0 Hz, 1H), 7.21 (t, *J* = 7.5 Hz, 1H), 7.10 (t, *J* = 7.4 Hz, 1H), 6.65 (d, *J* = 3.3 Hz, 1H), 5.38 (dd, *J* = 15.7, 0.9 Hz, 1H), 4.75 (dd, *J* = 9.0, 0.9 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 135.1, 129.9, 128.6, 124.0, 122.4, 120.7, 120.5, 110.0, 104.7, 96.5. HRMS (ESI), *m/z*: 249.97807 $[M+Ag]^+$, (calc. for $C_{10}H_9NAg^+$, *m/z*: 249.97804). Spectral data correspond to those given in the reference[12].
	**1-Vinylazepan-2-one (12a)**. Yellow oil, yield 97%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (dd, *J* = 16.1, 9.4 Hz, 1H), 4.52–4.32 (m, 2H), 4.45 (d, *J* = 8.3 Hz, 1H), 4.42 (d, *J* = 15.8 Hz, 1H), 3.61–3.51 (m, 2H), 2.66–2.56 (m, 2H), 1.80–1.59 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.3, 132.1, 92.6, 44.1, 37.2, 29.4, 27.2, 23.4. HRMS (ESI), *m/z*: 140.10696 $[M+H]^+$, (calc. for $C_8H_{13}NO^+$, *m/z*: 140.10699). Spectral data correspond to those given in the reference[13].
	**1-Ethynylcyclohexan-1-ol (13a)**. Yellow oil, yield 96%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.46 (d, *J* = 0.9 Hz, 1H), 1.94–1.83 (m, 2H), 1.74–1.62 (m, 2H), 1.62–1.47 (m, 6H), 1.23 (br.s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 87.7, 72.0, 68.5, 39.7, 25.1, 23.1. HRMS (ESI), *m/z*: 125.109596 $[M+H]^+$, (calc. for $C_8H_{12}O^+$, *m/z*: 125.09609). Spectral data correspond to those given in the reference[14].
	**2-Phenylbut-3-yn-2-ol (14a)**. Yellow oil, yield 96%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71–7.63 (m, 2H), 7.41–7.34 (m, 2H), 7.34–7.26 (m, 1H), 2.68 (s, 1H), 2.49 (d, *J* = 3.6 Hz, 1H), 1.80 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.0, 128.3, 127.8, 124.8, 87.3, 73.0, 69.8, 33.1. HRMS (ESI), *m/z*: 252.97839 $[M+Ag]^+$, (calc. for $C_{10}H_{10}OAg^+$, *m/z*: 252.97771). Spectral data correspond to those given in the reference[14].

	**2,4,6-Trimethylphenyl-1H-1,2,3-triazole (15a)**. Brown powder, yield 87%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.62 (s, 1H), 6.99 (s, 2H), 2.35 (s, 3H), 1.93 (s, 5H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.0, 135.1, 133.6, 133.4, 129.0, 125.3, 21.1, 17.2. HRMS (ESI), *m/z*: 188.11803 $[M+H]^+$, (calc. for $C_{11}H_{13}N_3^+$, *m/z*: 188.11822). Spectral data correspond to those given in the reference[7].
	**4-Methylphenyl-1H-1,2,3-triazole (16a)**. Brown powder, yield 85%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.83 (s, 1H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.32 (d, *J* = 8.2 Hz, 1H), 2.43 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.9, 134.8, 134.3, 130.2, 121.7, 120.6, 21.1. HRMS (ESI), *m/z*: 160.08685 $[M+H]^+$, (calc. for $C_9H_9N_3^+$, *m/z*: 160.08692). Spectral data correspond to those given in the reference[7].
	**2-Phenyl-1*H*-pyrrole (20)**. Dark red powder, yield 95%, m. p. 131–132 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.50 (d, *J* = 7.9 Hz, 2H), 7.40 (t, *J* = 7.7 Hz, 2H), 7.26 (t, *J* = 14.5 Hz, 1H), 6.86 (s, 1H), 6.60 (d, *J* = 1.0 Hz, 1H), 6.40–6.33 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 132.7, 132.0, 128.8, 126.1, 123.8, 118.9, 110.0, 105.9. HRMS (ESI), *m/z*: 144.08078 $[M+H]^+$, (calc. for $C_{10}H_{19}N^+$, *m/z*: 144.08078). Spectral data correspond to those given in the reference[15].
	**2-(4-Methylphenyl)-1*H*-pyrrole (21)**. Dark red powder, yield 96%, m. p. 153–154 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (br.s, 1H), 7.38 (d, *J* = 8.1 Hz, 1H), 7.19 (d, *J* = 7.9 Hz, 1H), 6.89–6.78 (m, 1H), 6.50 (s, 1H), 6.31 (dd, *J* = 5.8, 2.7 Hz, 1H), 2.37 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.9, 132.3, 130.0, 129.5, 123.8, 118.4, 110.0, 105.4, 21.1. HRMS (ESI), *m/z*: 158.09641 $[M+H]^+$, (calc. for $C_{11}H_{12}N^+$, *m/z*: 158.09643). Spectral data correspond to those given in the reference[15].
	**2-Methyl-2-vinylbenzofuran-3(2*H*)-one (22a)**. Yellow oil, yield 59%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 16.3, 8.0 Hz, 2H), 7.13 (d, *J* = 8.4 Hz, 1H), 7.07 (t, *J* = 7.4 Hz, 1H), 5.93 (dd, *J* = 17.2, 10.7 Hz, 1H), 5.46 (d, *J* = 17.2 Hz, 1H), 5.21 (d, *J* = 10.7 Hz, 1H), 1.56 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.4, 171.1, 138.1, 134.9, 125.0, 121.9, 119.4, 115.7, 113.5, 89.6, 20.0. HRMS (ESI), *m/z*: 175.07536 $[M+H]^+$, (calc. for $C_{11}H_{10}O_2^+$, *m/z*: 175.07536). Spectral data correspond to those given in the reference[16].

	**7-Ethoxy-2-methyl-2-vinylbenzofuran-3(2*H*)-one (23a)**. White powder, yield 45%, m. p. 69–70 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (d, *J* = 7.7 Hz, 1H), 7.11 (d, *J* = 7.7 Hz, 1H), 6.98 (t, *J* = 7.8 Hz, 1H), 5.93 (dd, *J* = 17.2, 10.7 Hz, 1H), 5.49 (d, *J* = 17.2 Hz, 1H), 5.22 (d, *J* = 10.7 Hz, 1H), 4.21 (q, *J* = 7.0 Hz, 2H), 1.60 (s, 3H), 1.49 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 201.6, 161.5, 146.0, 134.7, 122.3, 120.7, 120.0, 116.0, 90.1, 64.9, 21.9, 14.7. HRMS (ESI), *m/z*: 219.10155 $[M+H]^+$, (calc. for $C_{13}H_{15}O_3^+$, *m/z*: 219.10157). Spectral data correspond to those given in the reference[16].
	**4-Anisylacetylene (25)**. Brown oil, yield 32-34%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.8 Hz, 2H), 6.84 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H), 3.00 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.9, 133.6, 114.2, 113.9, 83.6, 75.7, 55.3. Spectral data correspond to those given in the reference[17].
	**1,2-Bis(4-anisyl)acetylene (26)**. Brown oil, yield 32-45%. ^{1}H NMR (400 MHz, $CDCl_3$) δ (1 isomer) 7.45 (d, *J* = 8.8 Hz, 1H), 6.87 (d, *J* = 8.8 Hz, 1H), 3.82 (s, 1H); (2 isomer) 7.47 (d, *J* = 8.8 Hz, 1H), 6.85 (d, *J* = 8.8 Hz, 1H), 3.82 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ (1 isomer) 159.4, 133.0, 115.7, 113.9, 87.9, 55.3; (2 isomer) 160.2, 134.0, 133.0, 115.7, 114.1, 87.9, 55.3. HRMS (ESI), *m/z*: 241.12254 $[M+H]^+$, (calc. for $C_{16}H_6O_2^+$, *m/z*: 241.12231). Spectral data correspond to those given in the reference[18].

4. Barium carbide study

Figure S1. Barium carbide synthesized from elemental Ba and graphite at 600 °C.

Table S1. Optimization of conditions for the barium carbide synthesis.

Entry	Ba source	Ba/C molar ratio	T, °C	Time, h	Yield BaC_2, %
1	BaO	1:3	1100	1.0	0
2	BaO	1:3	1200	2.5	0
3	Ba metal	1:2	900	1.0	0
4	Ba metal	1:3	700	2.5	65
5	Ba metal	1:11	700	2.5	85
6	Ba metal	1:2.3	600	2.5	85
7	Ba metal	1:2.3	500	2.5	0
8	Ba metal	1:5	600	1.5	98
9	Ba metal	1:3	600	0.5	98

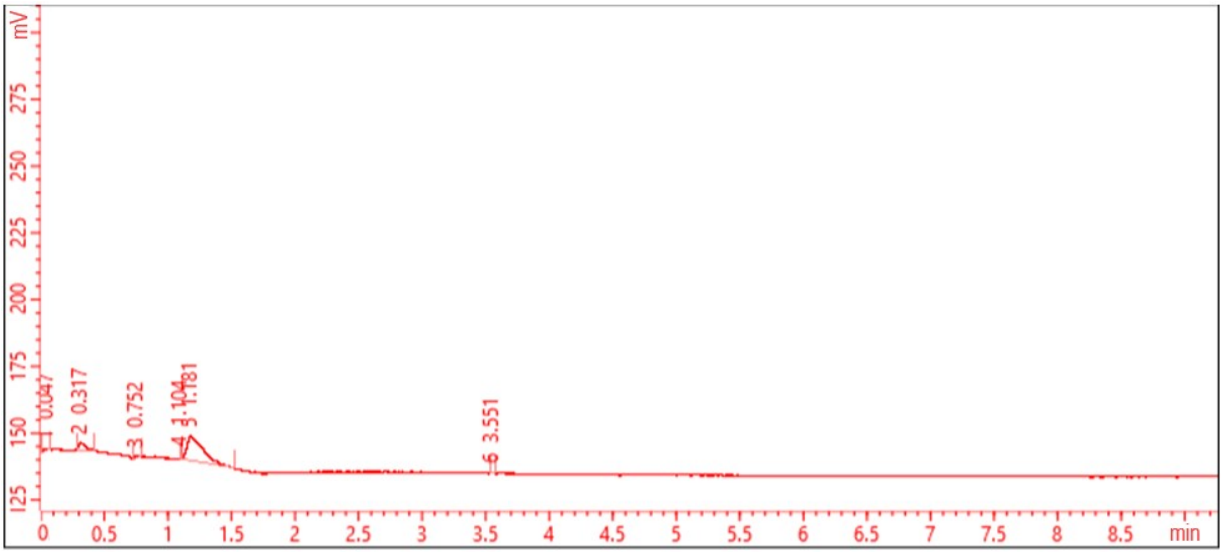


Figure S2. Chromatogram of air before acetylene analysis.

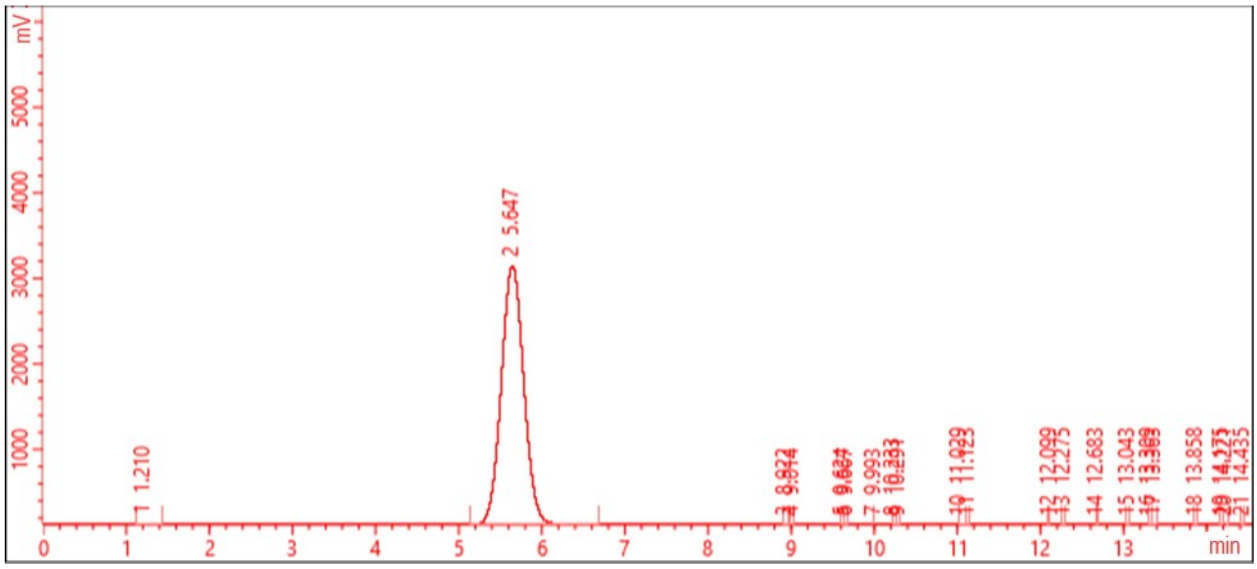


Figure S3. Chromatogram of acetylene from BaC_2. The peak at a retention time of 5.647 min belongs to acetylene.

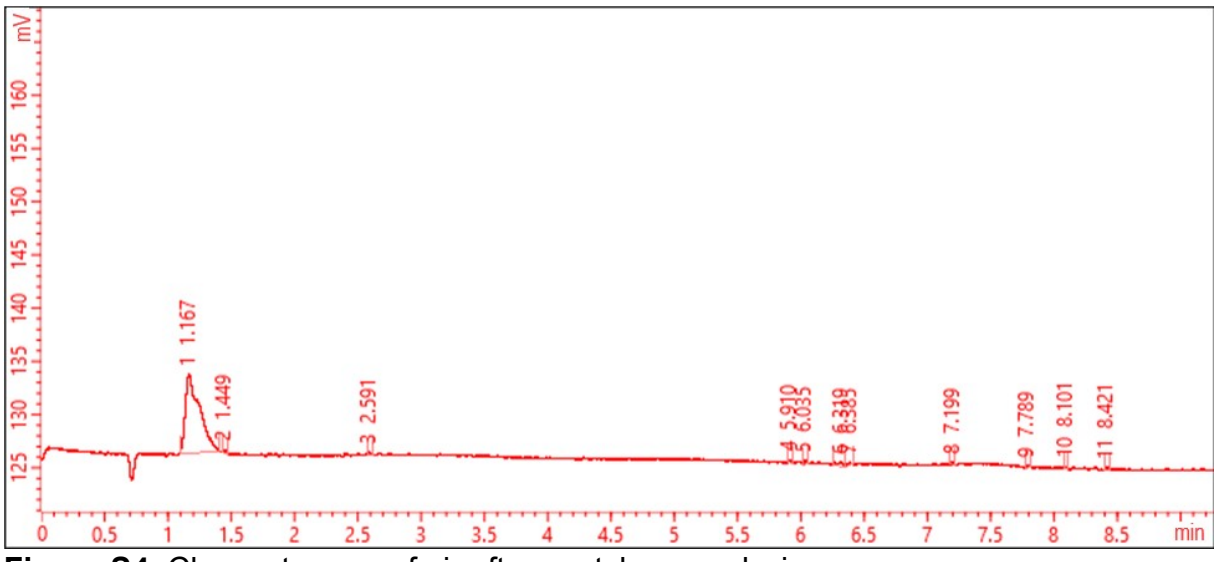


Figure S4. Chromatogram of air after acetylene analysis.

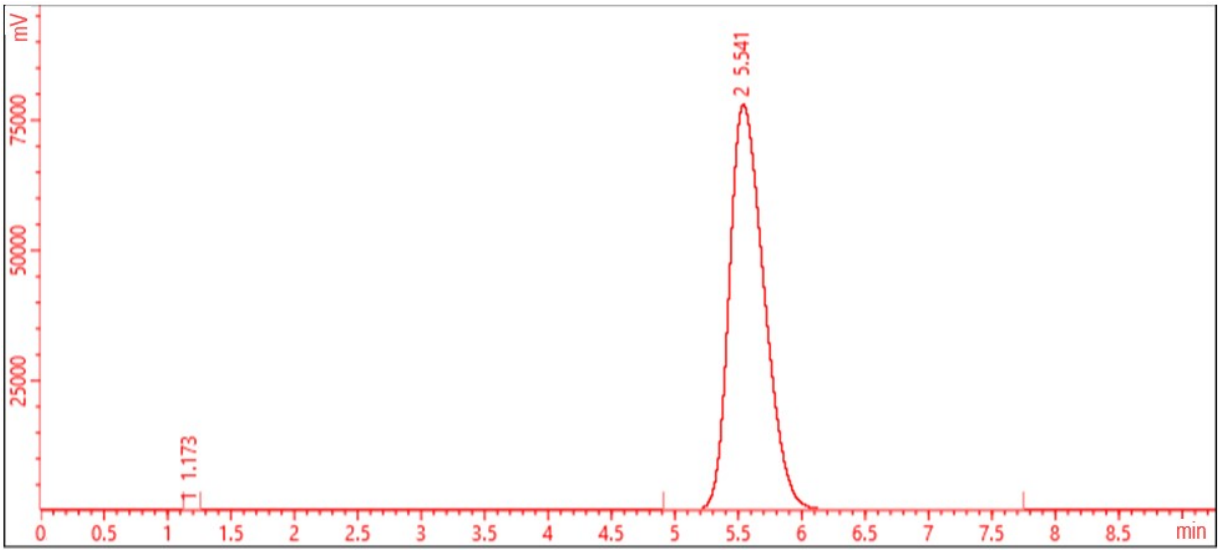


Figure S5. Chromatogram of acetylene from CaC_2. The peak at a retention time of 5.541 min belongs to acetylene.

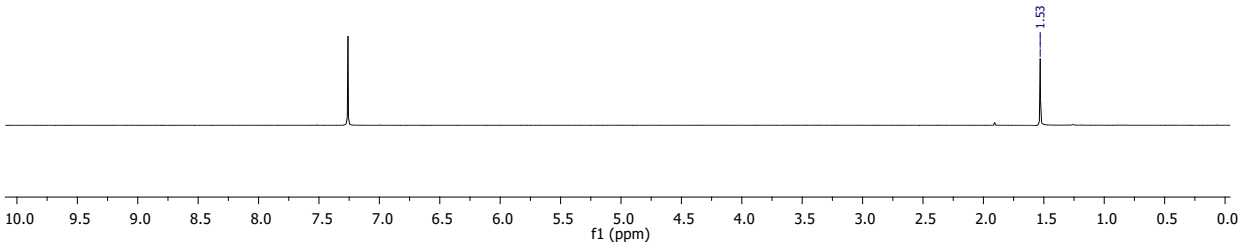


Figure S6. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of acetylene from BaC_2.

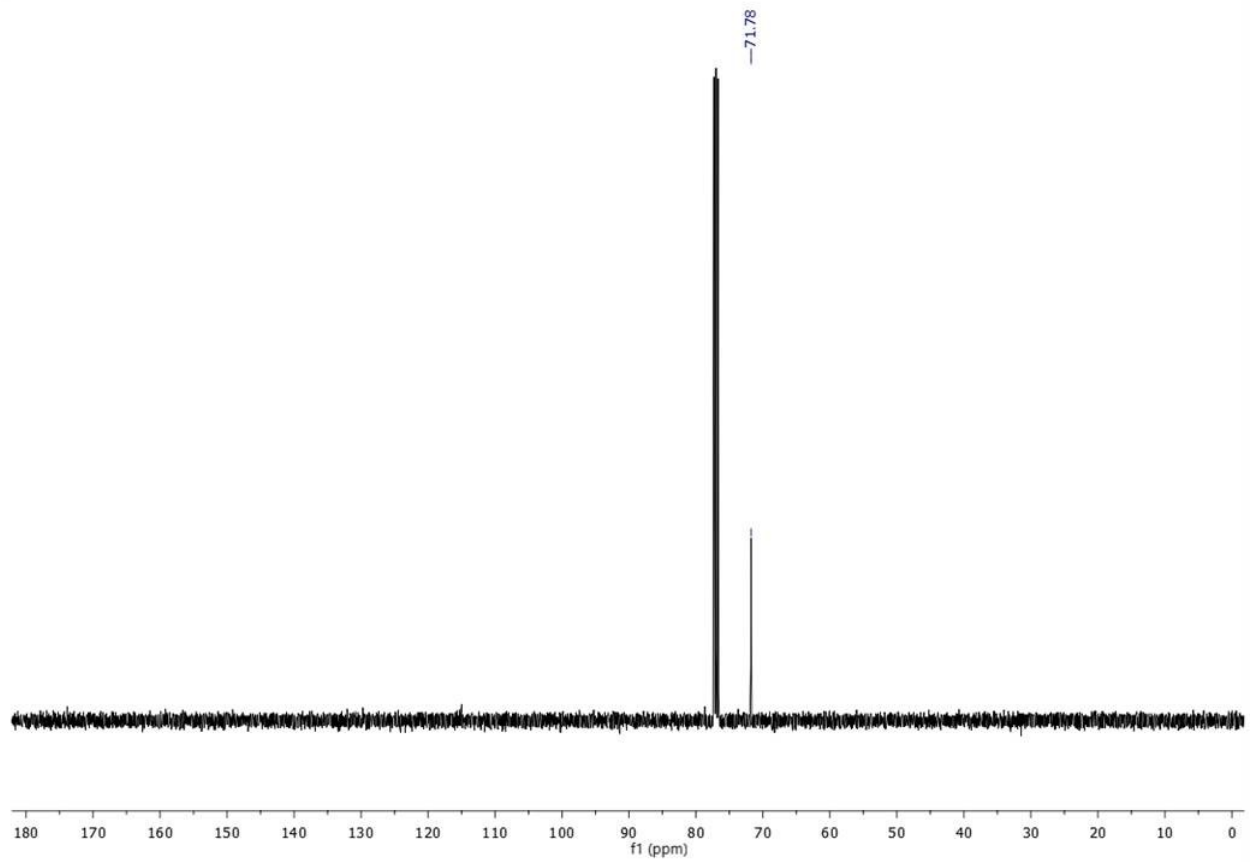


Figure S7. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of acetylene from BaC_2.

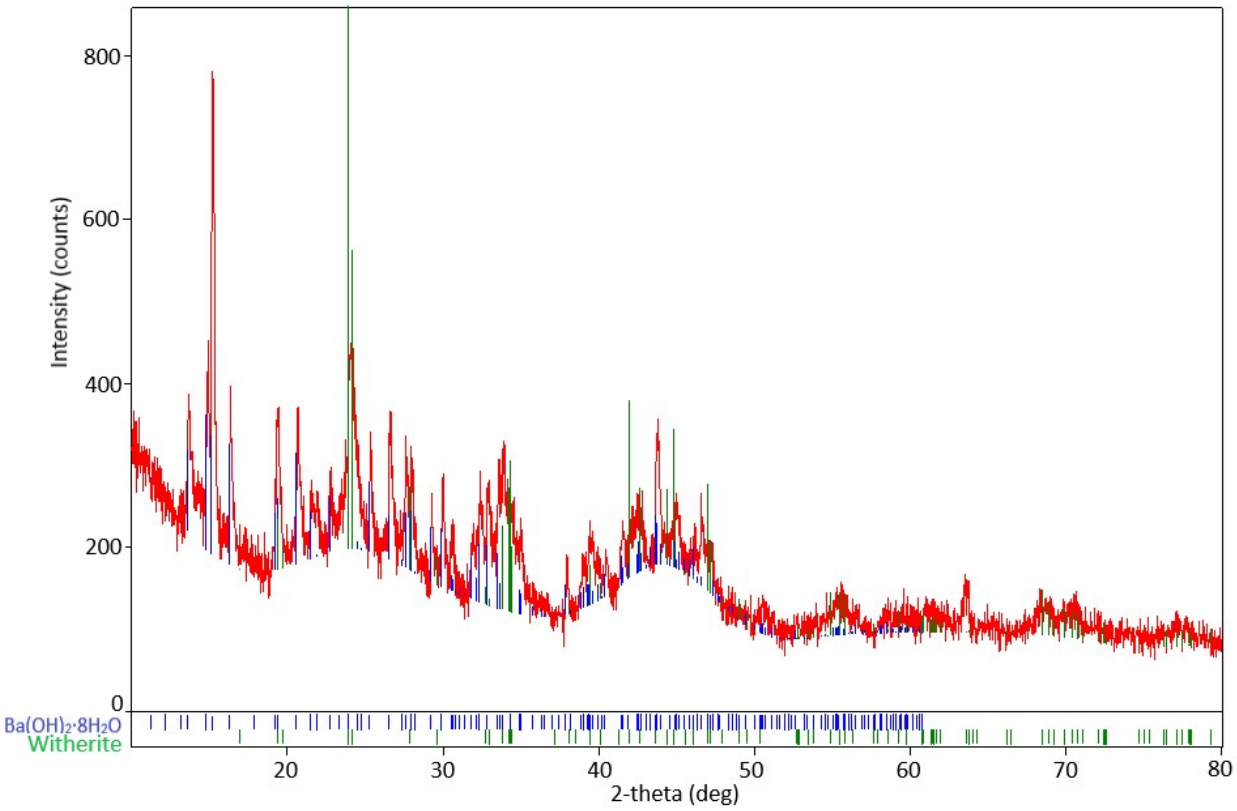


Figure S8. X-Ray diffractogram of the barium carbide residue after BaC_2 hydrolysis.

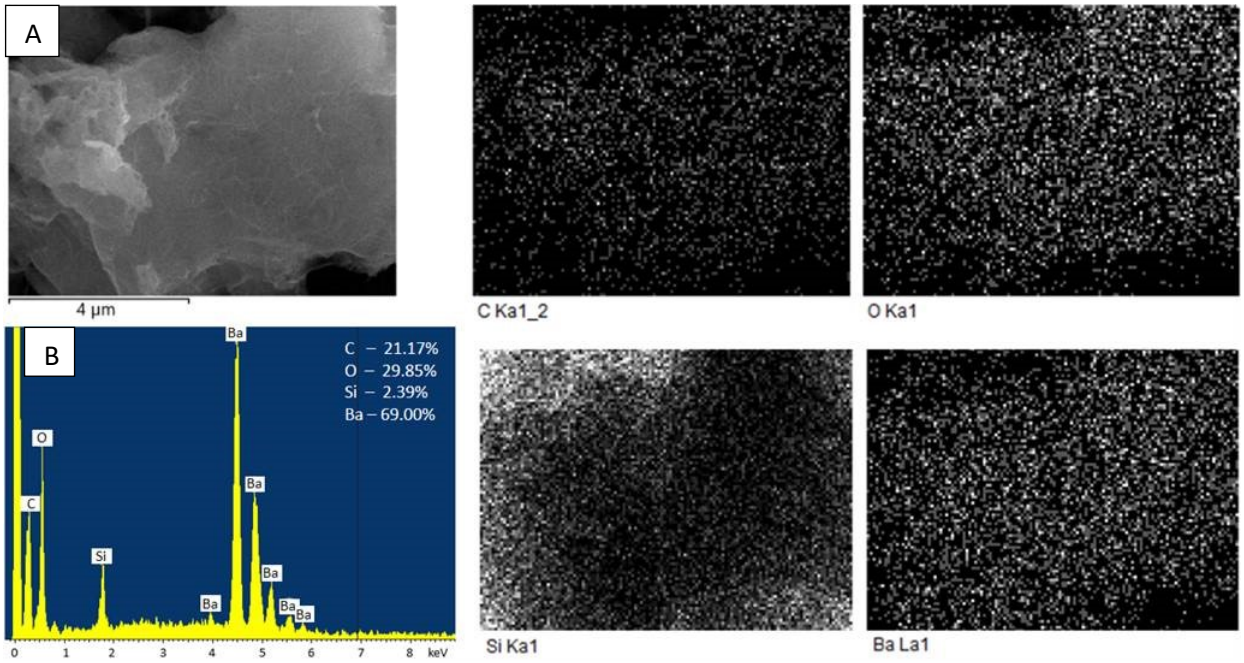


Figure S9. SEM image (A) and EDX spectrum (B) of the barium carbide residue after BaC_2 hydrolysis.

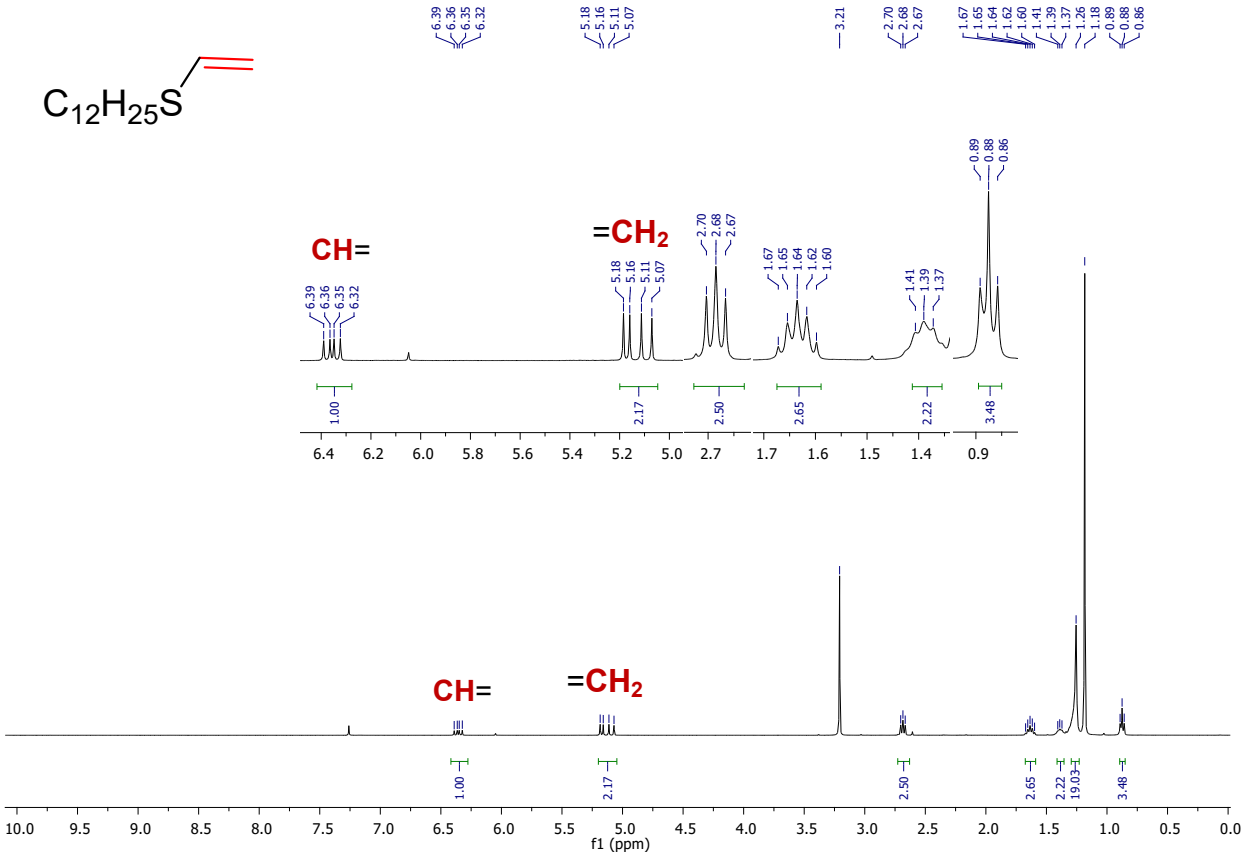


Figure S10. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of reaction mixture after dodecane thiol vinylation with BaC_2.

5. NMR spectra of synthesized compounds

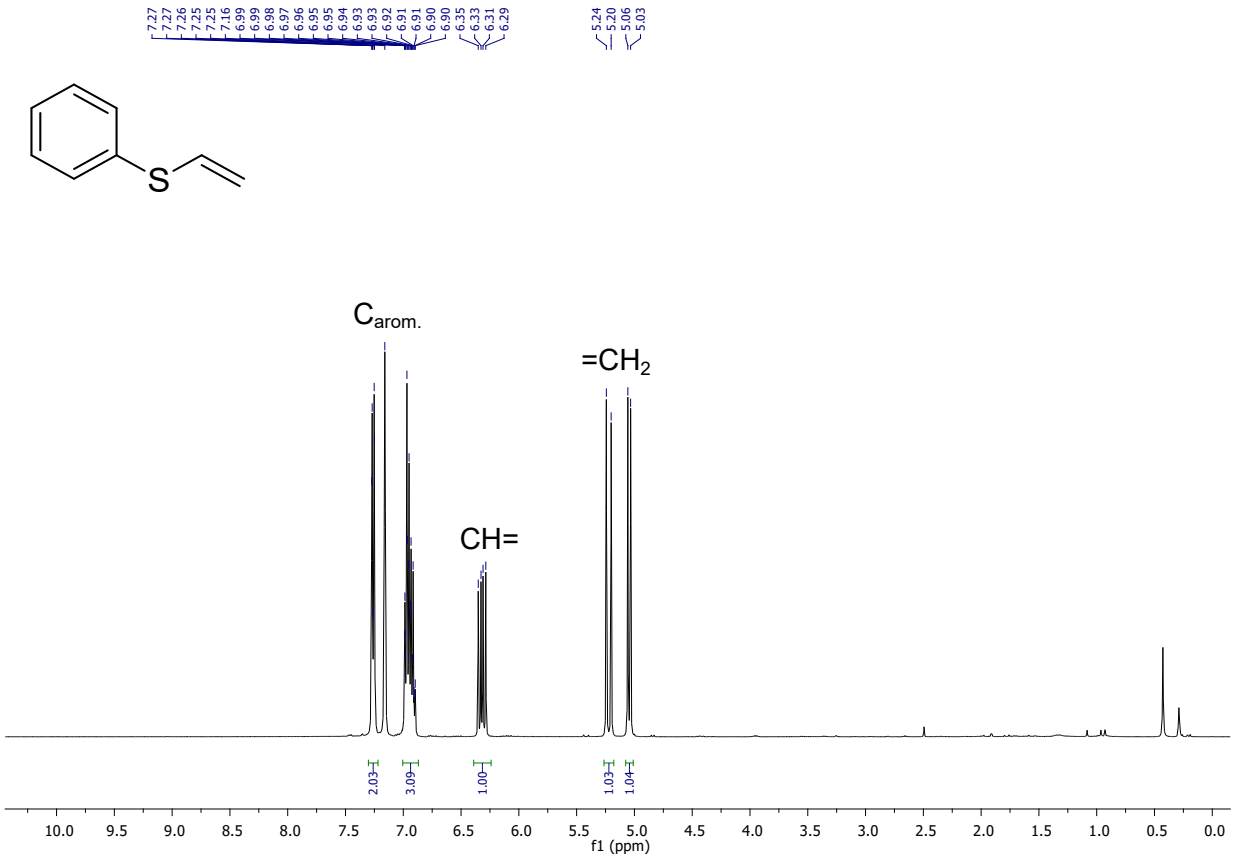


Figure S11. ^{1}H NMR spectrum (400 MHz, C_6D_6) of phenyl vinyl thioether (**1a**).

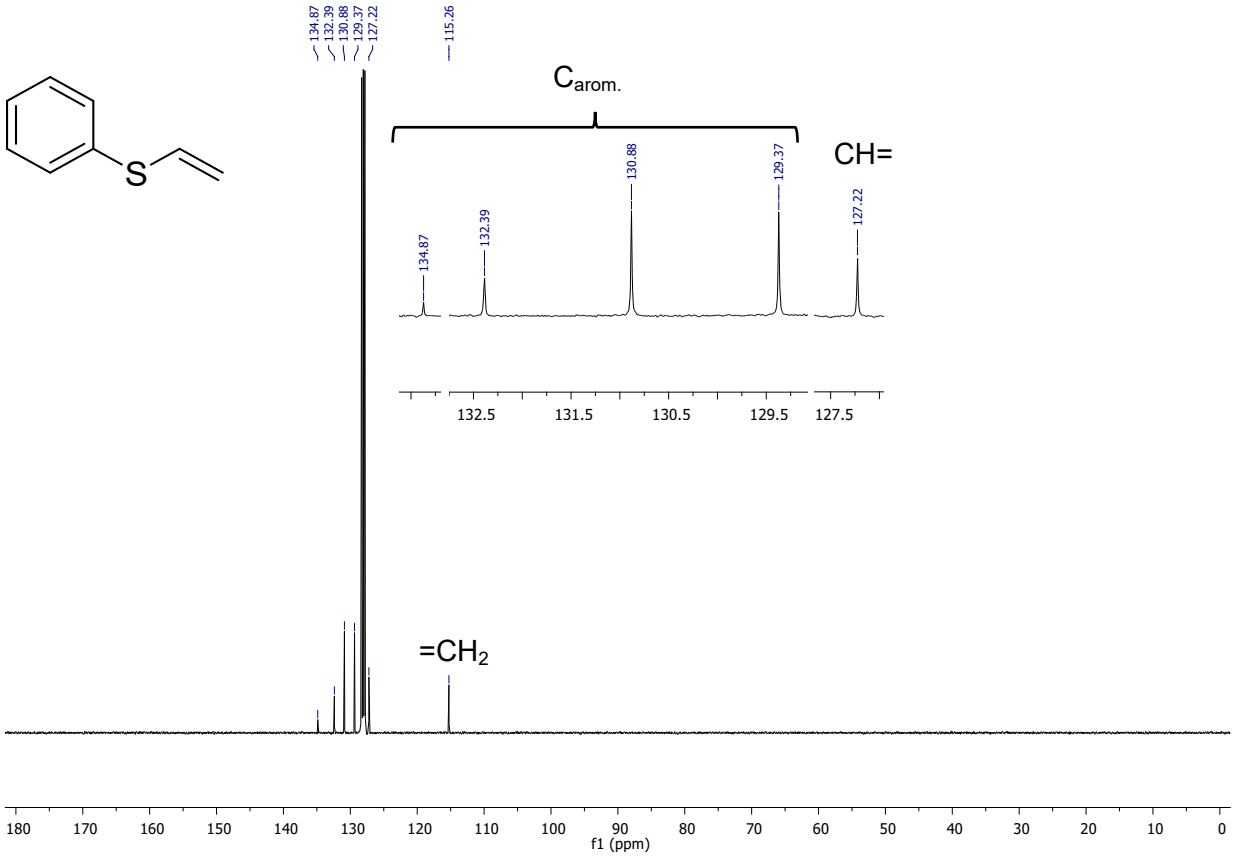


Figure S12. ^{13}C NMR spectrum (101 MHz, C_6D_6) of phenyl vinyl thioether (**1a**).

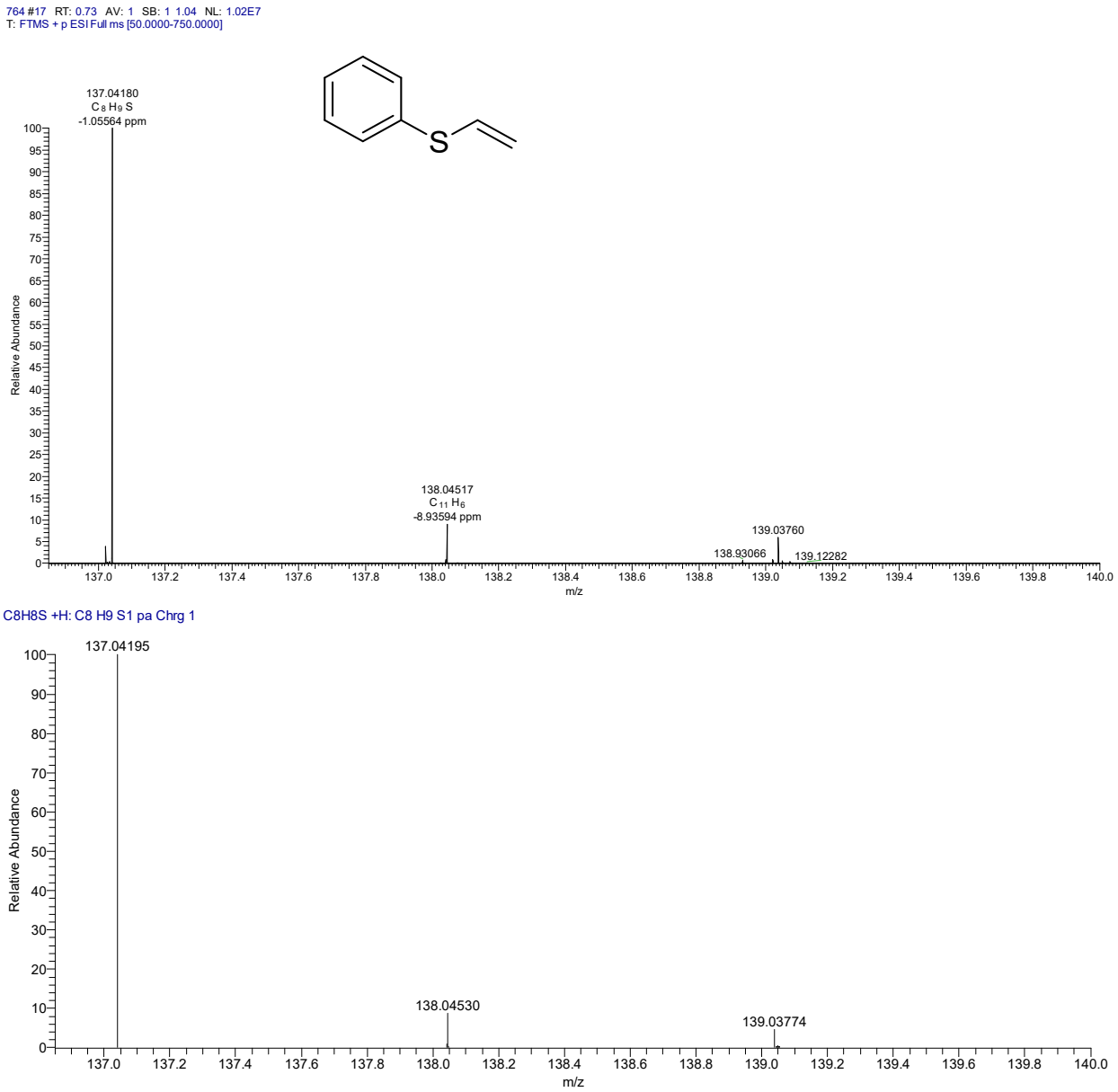


Figure S13. HRMS spectrum of phenyl vinyl thioether (**1a**).

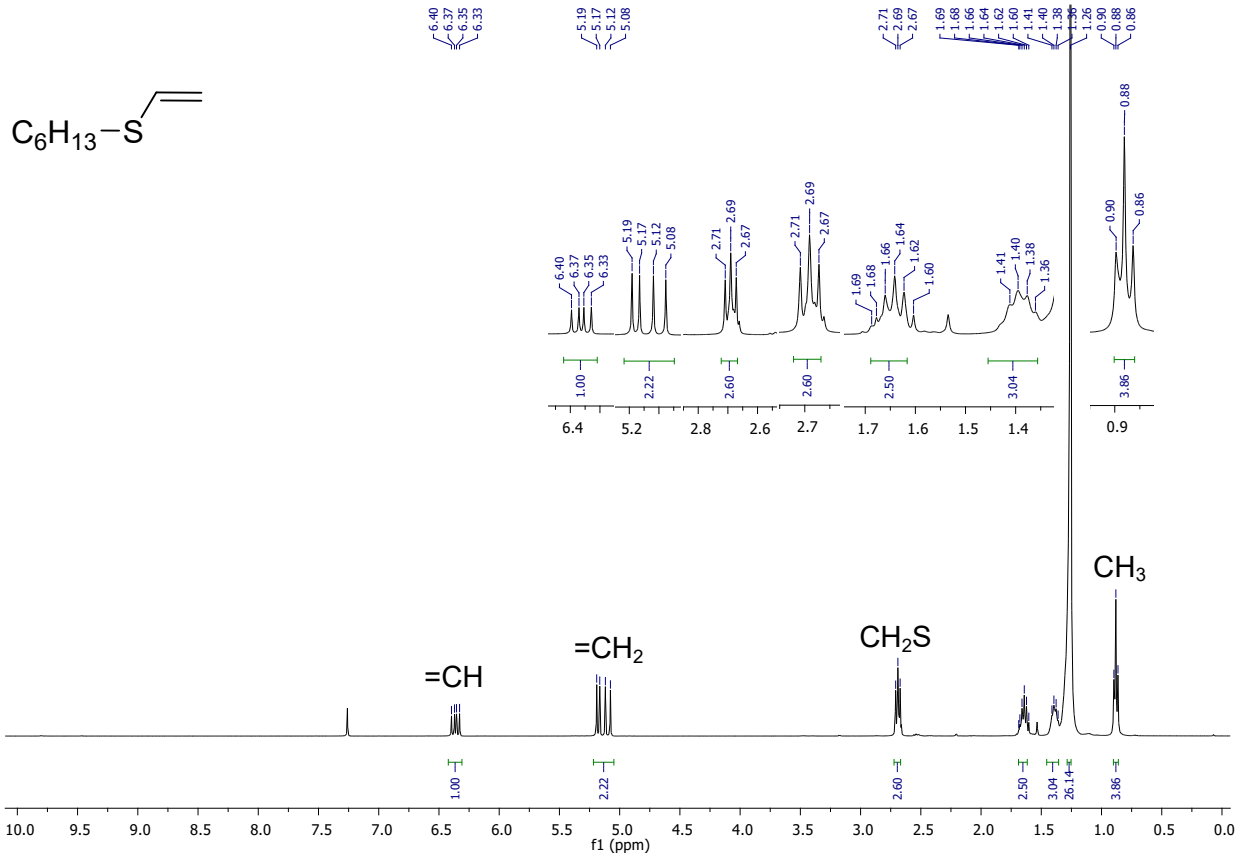


Figure S14. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1-hexyl vinyl ether (**2a**) (pentane as stabilizer).

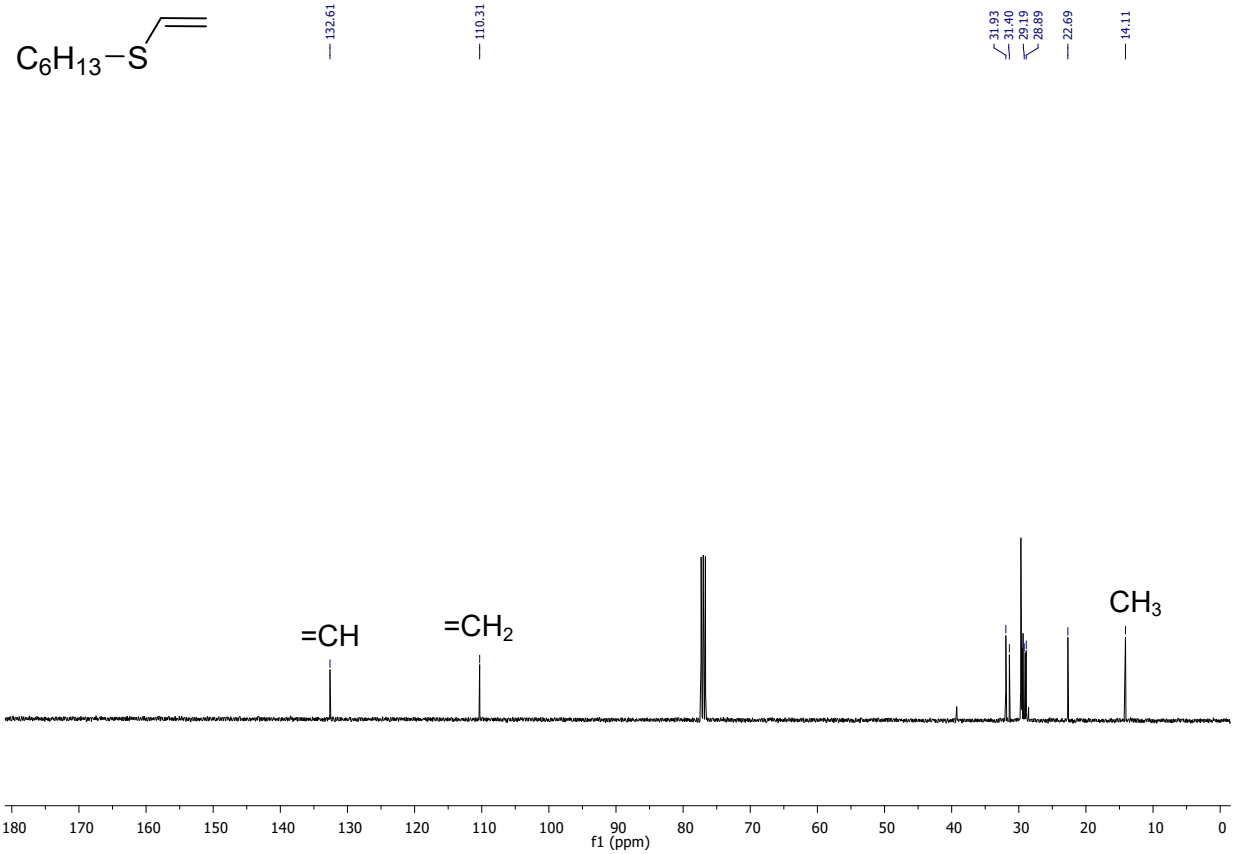


Figure S15. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 1-hexyl vinyl ether (**2a**).

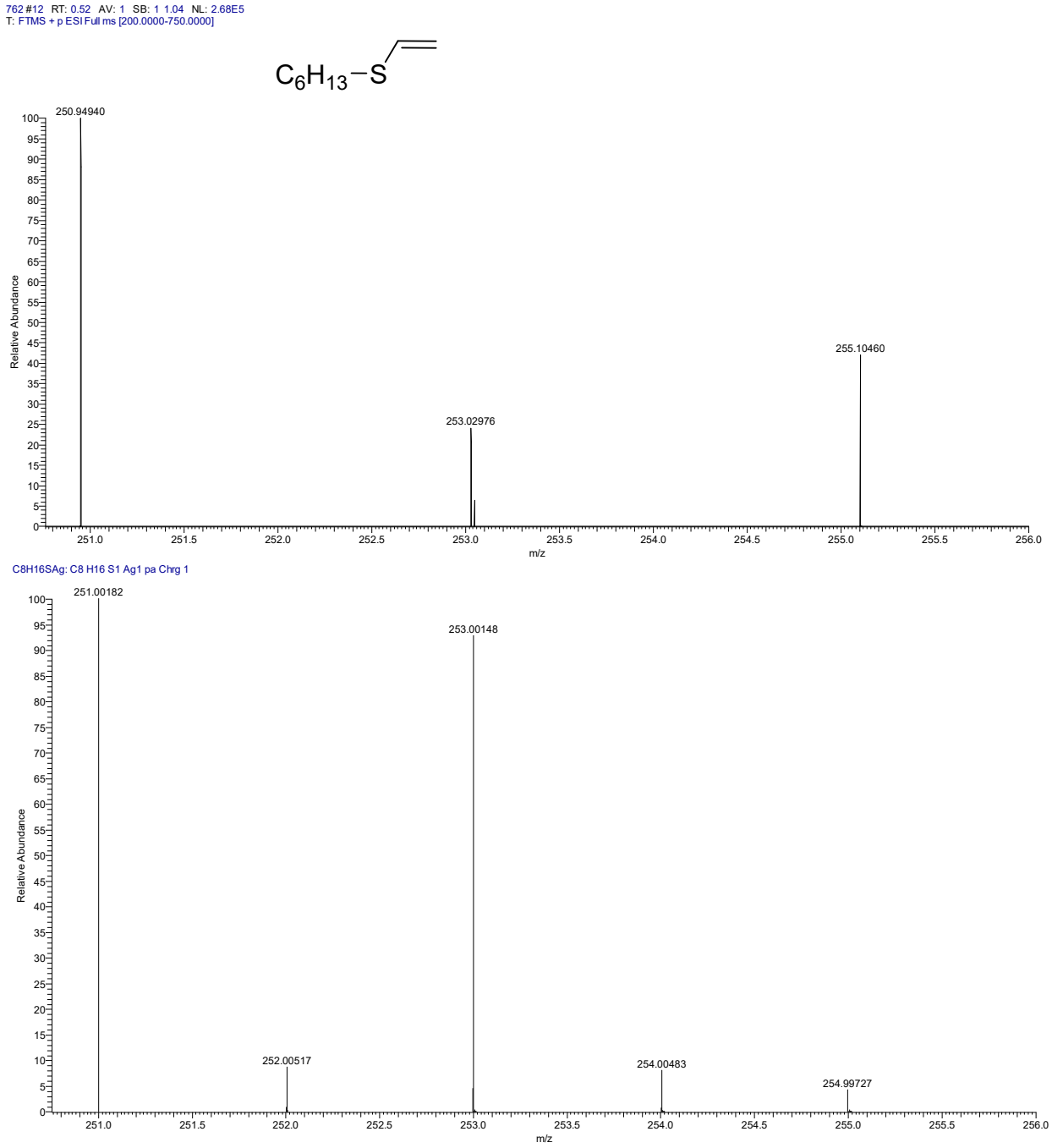


Figure S16. HRMS spectrum of 1-hexyl vinyl ether (**2a**).

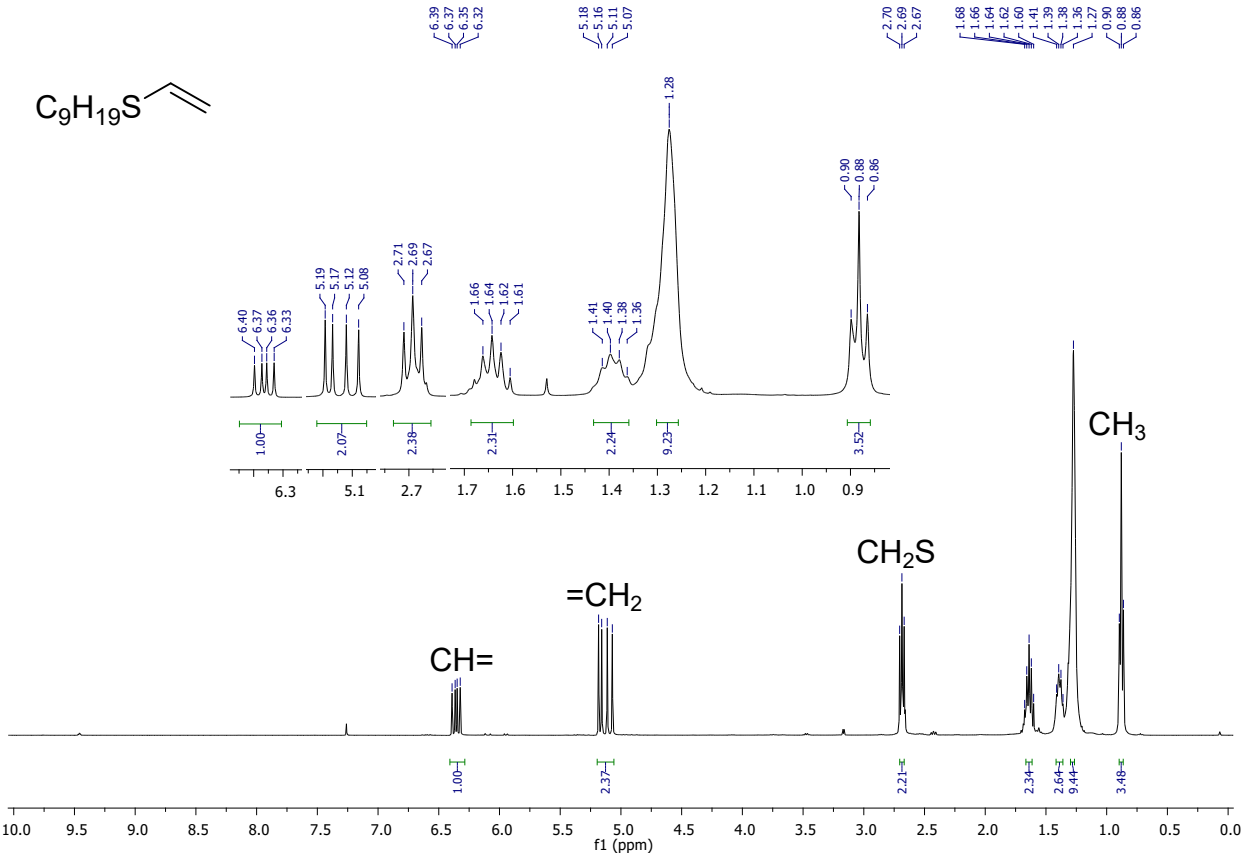


Figure S17. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1-nonyl vinyl thioether (**3a**).

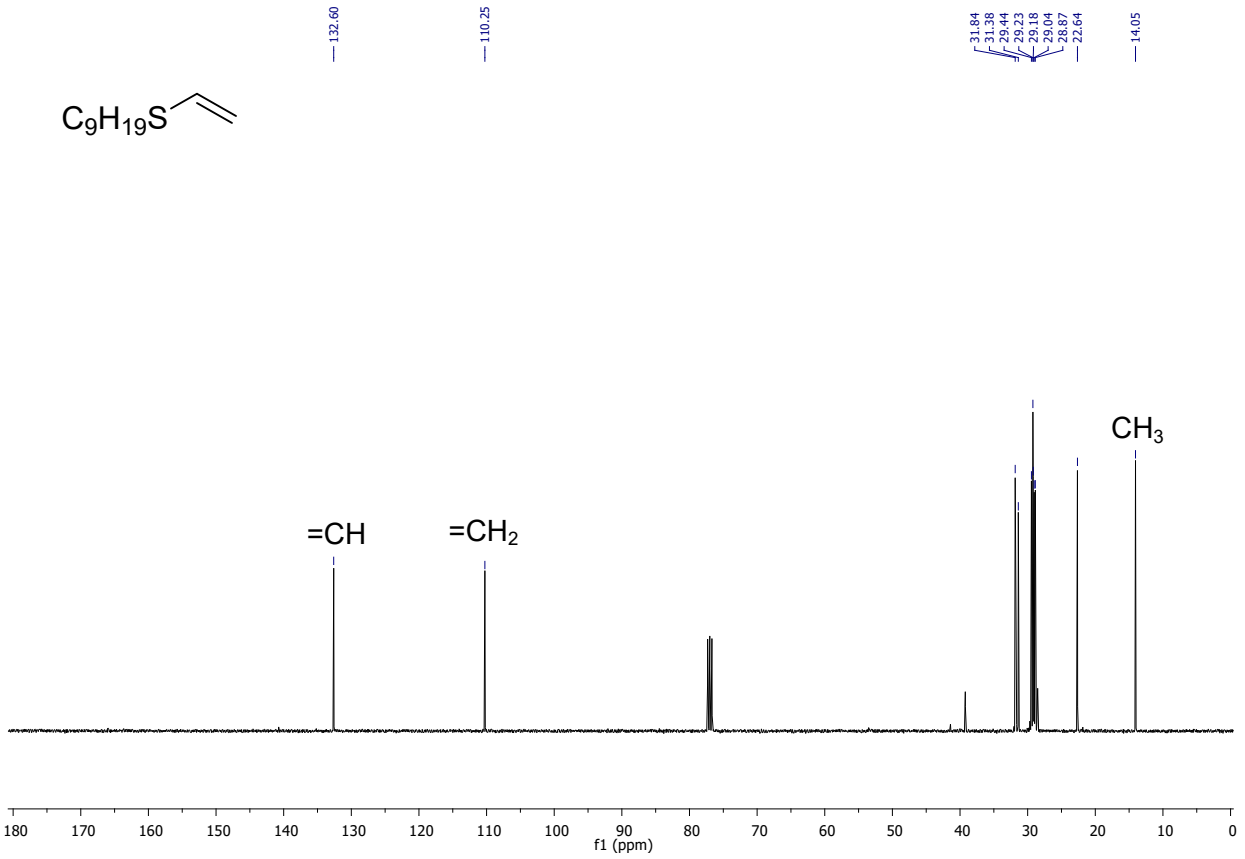


Figure S18. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 1-nonyl vinyl thioether (**3a**).

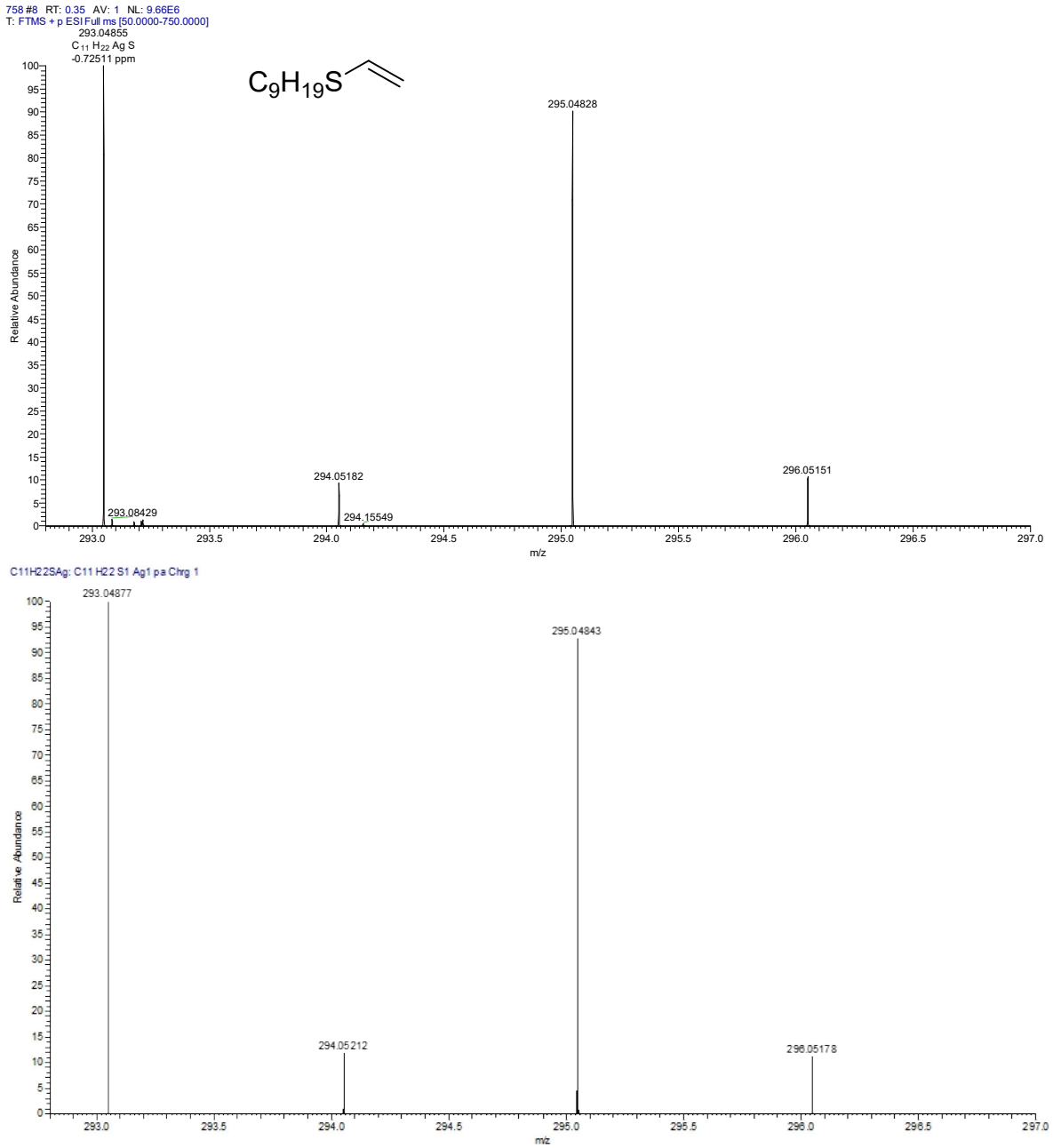


Figure S19. HRMS spectrum of 1-nonyl vinyl thioether (**3a**).

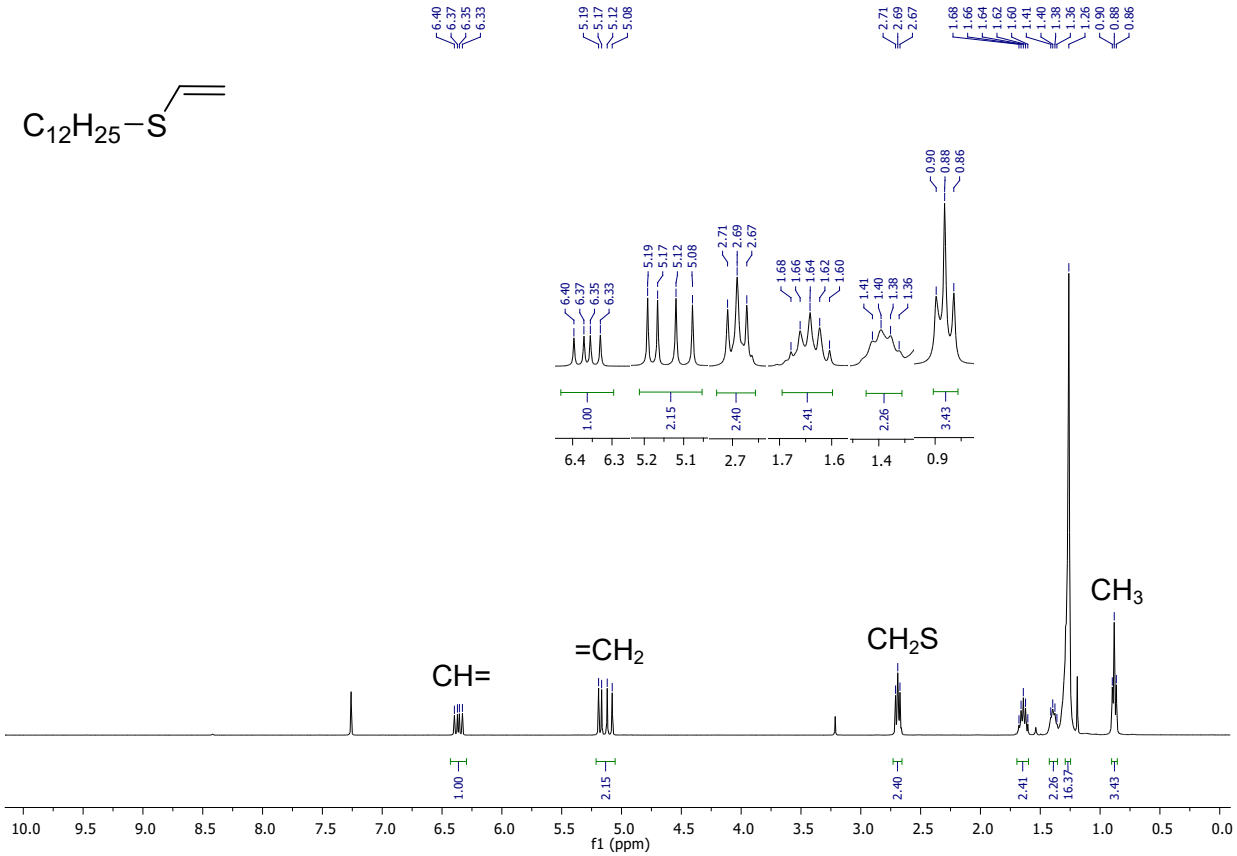


Figure S20. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of dodecyl vinyl thioether (**4a**).

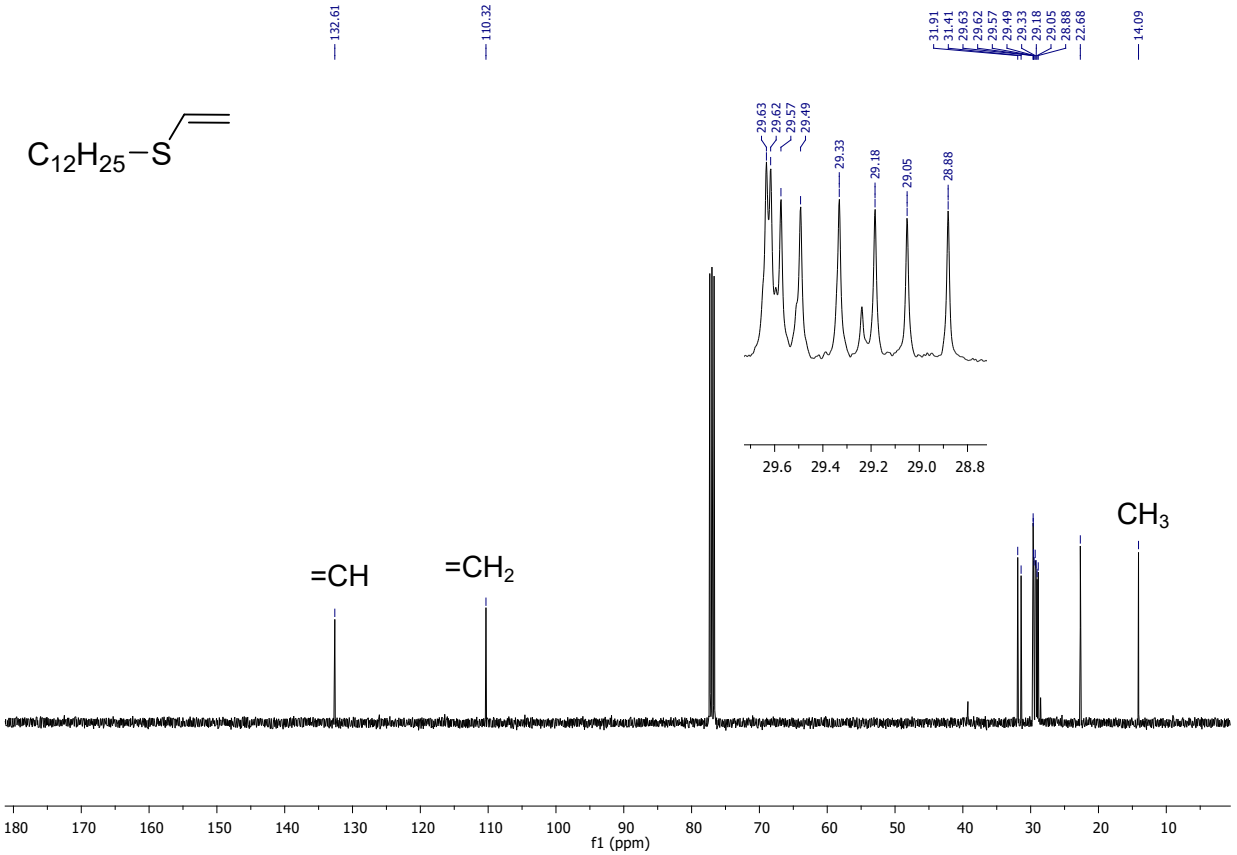


Figure S21. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of dodecyl vinyl thioether (**4a**).

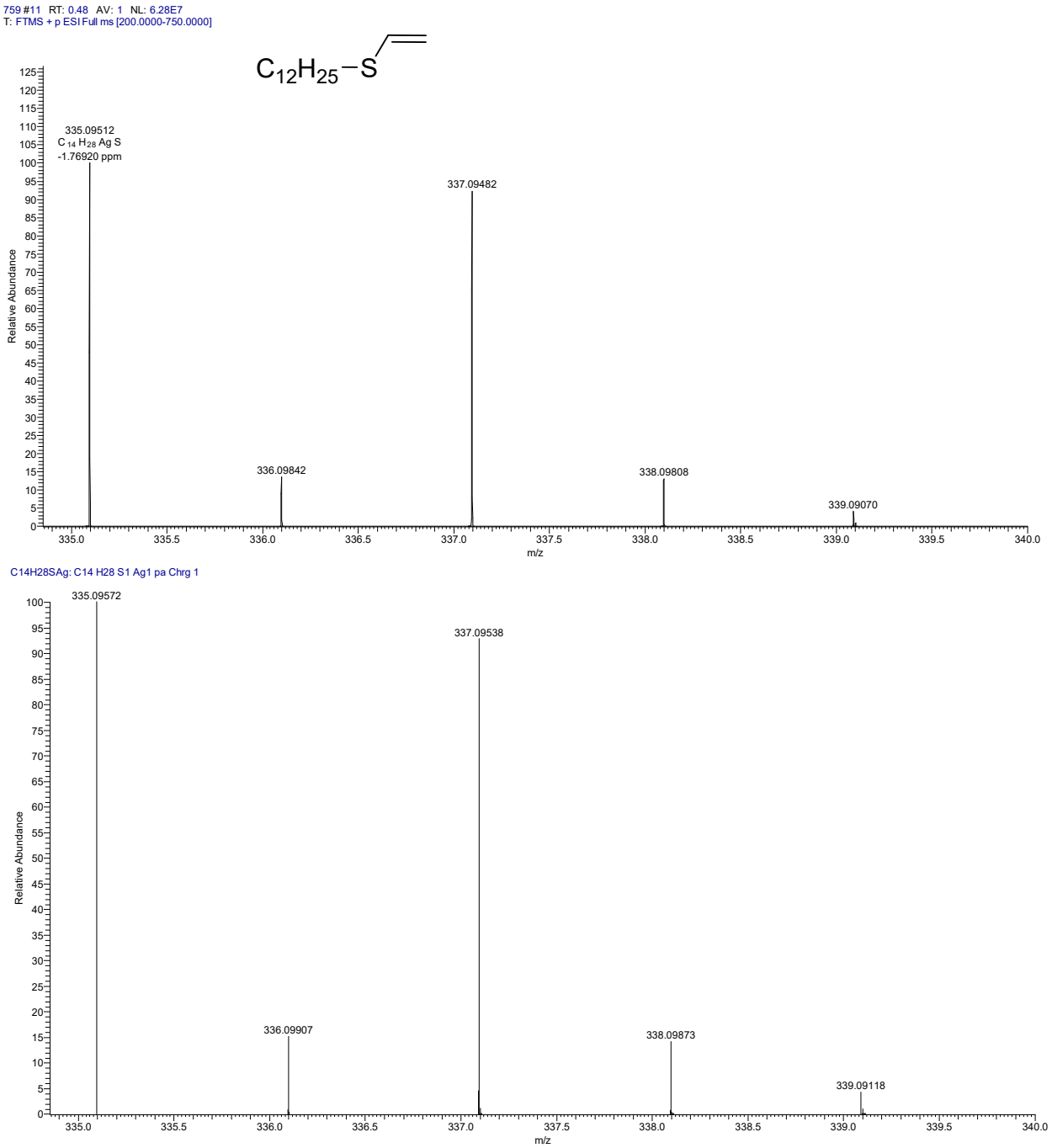


Figure S22. HRMS spectrum of dodecyl vinyl thioether (**4a**).

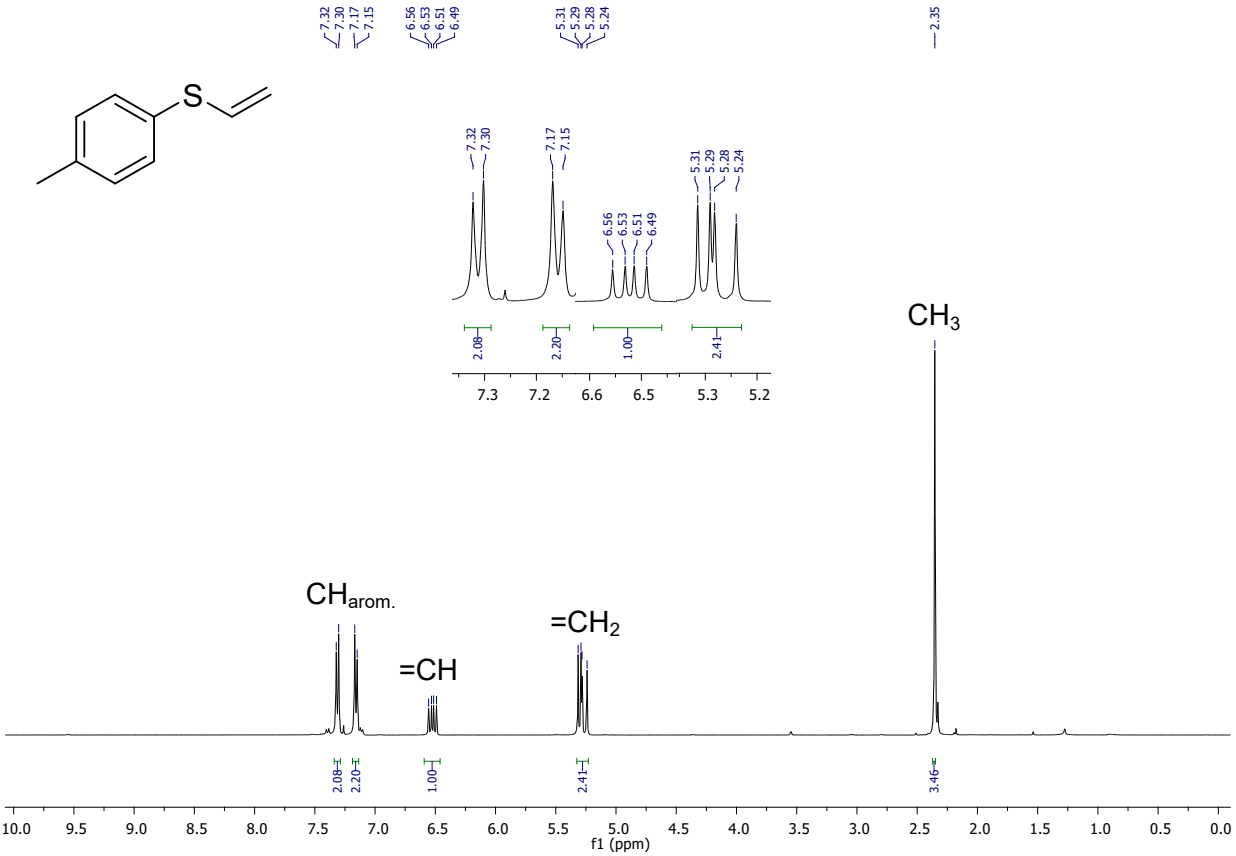


Figure S23. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of tolyl vinyl thioether (**5a**).

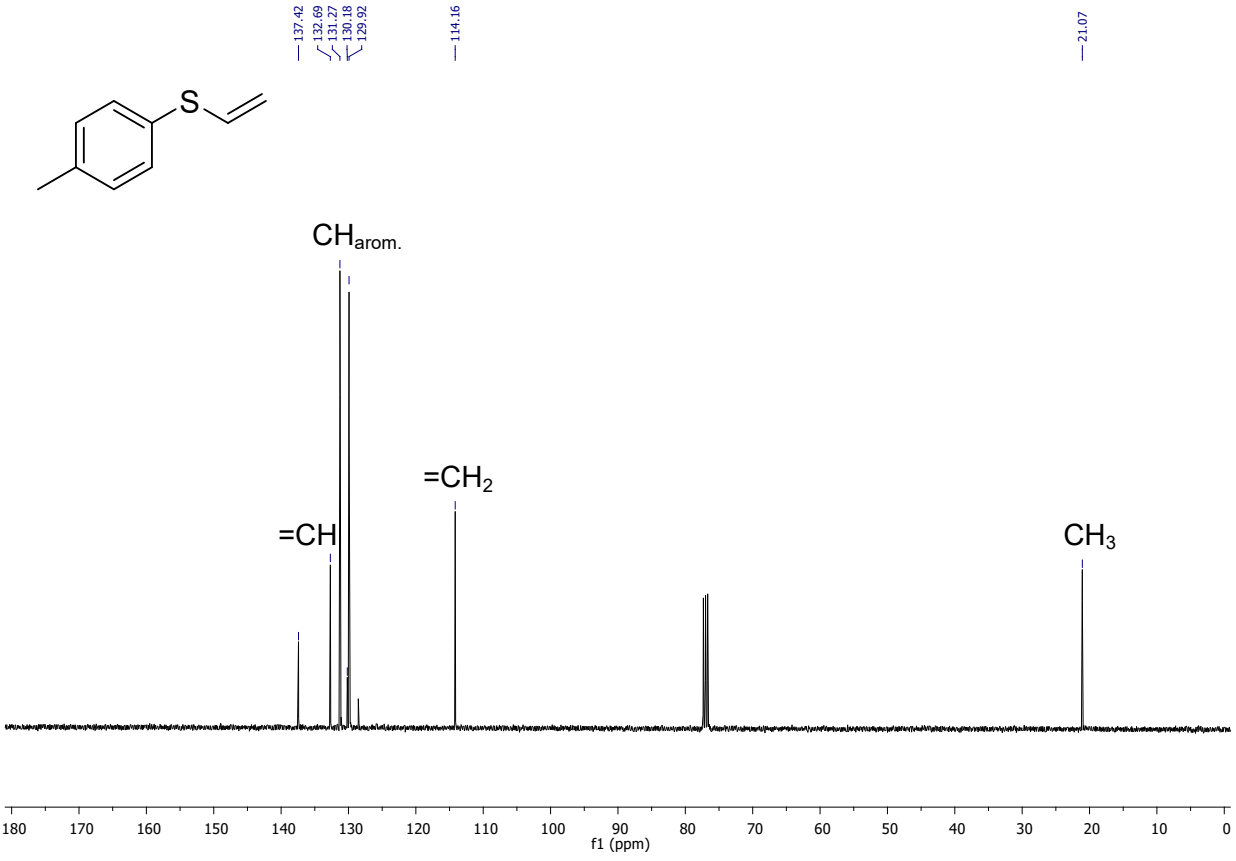


Figure S24. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of tolyl vinyl thioether (**5a**).

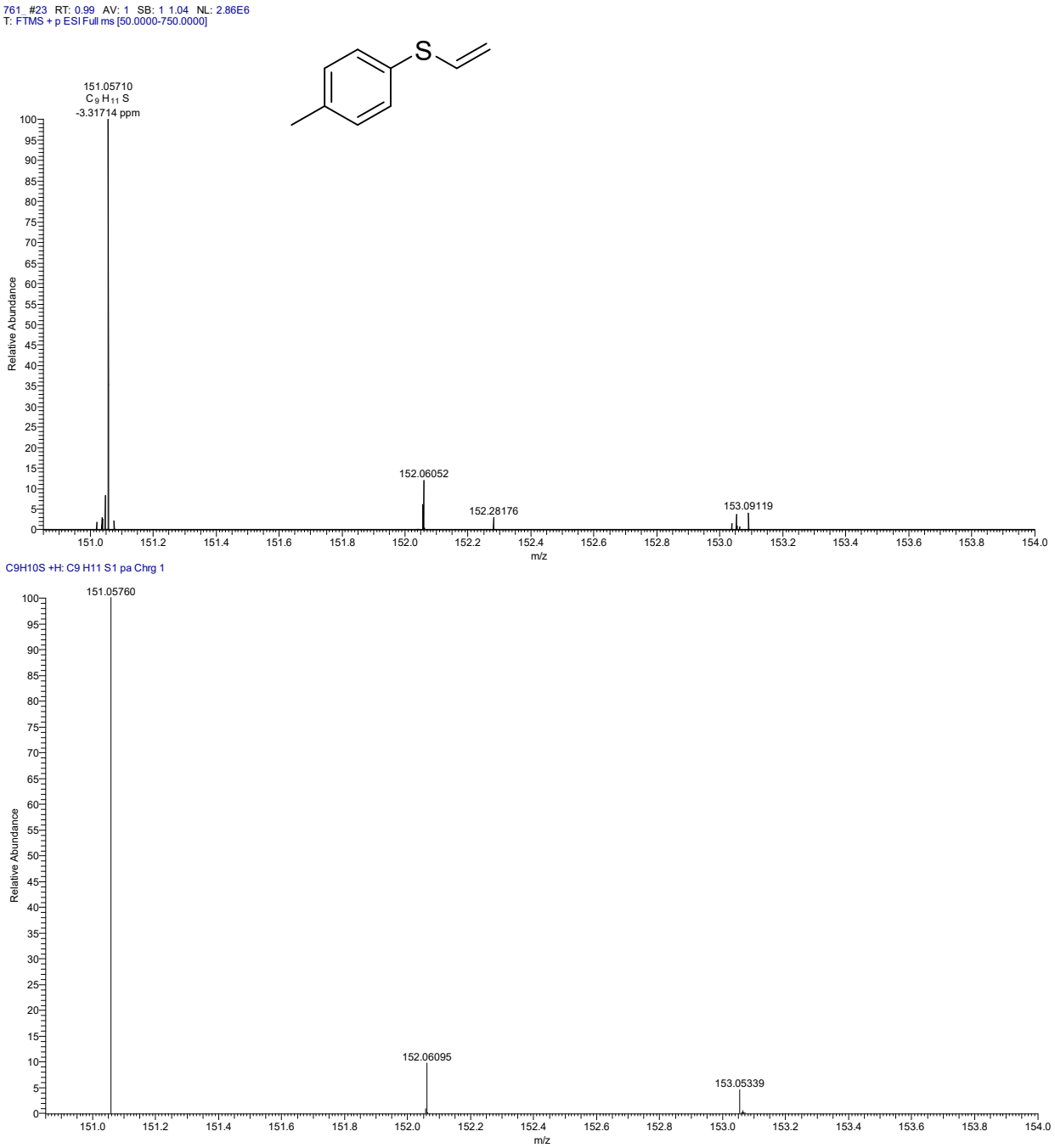


Figure S25. HRMS spectrum of tolyl vinyl thioether (**5a**).

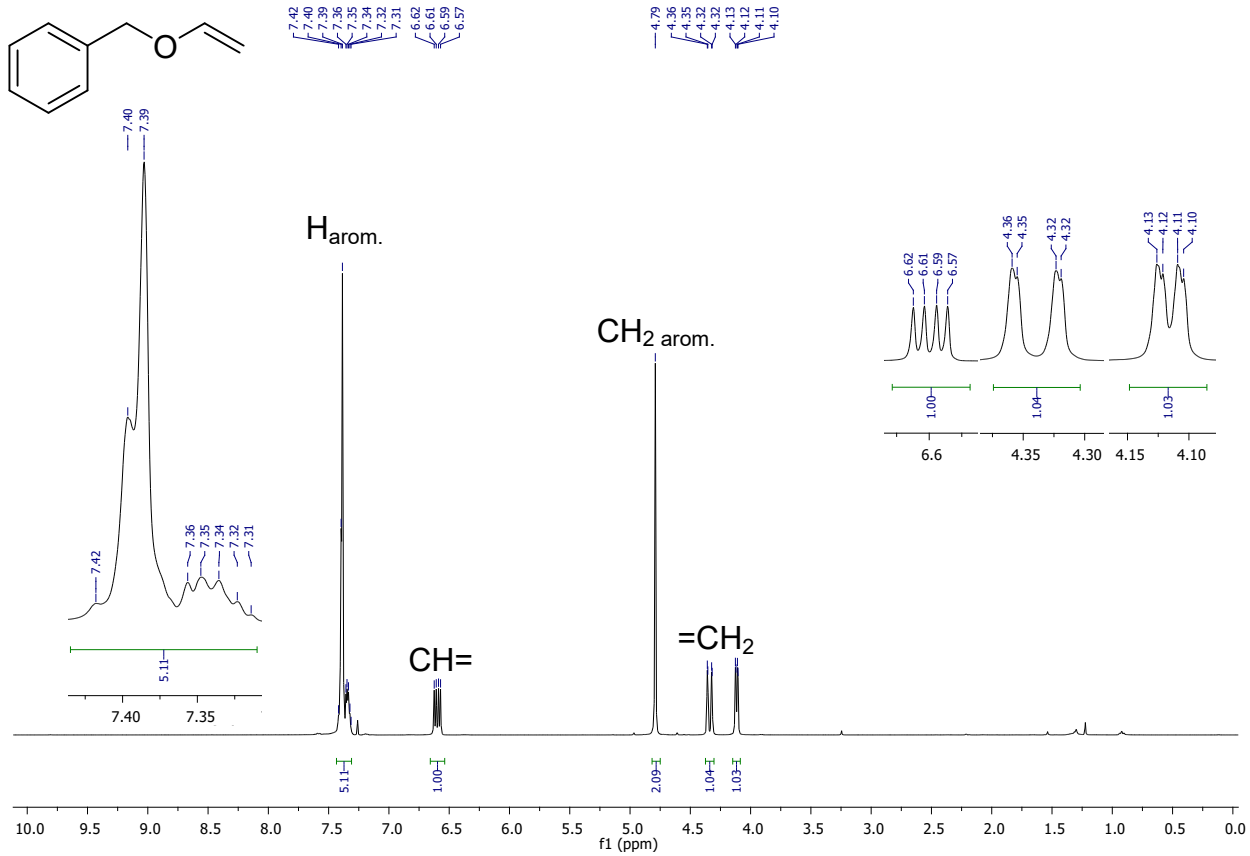


Figure S26. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of benzyl vinyl ether (**6a**).

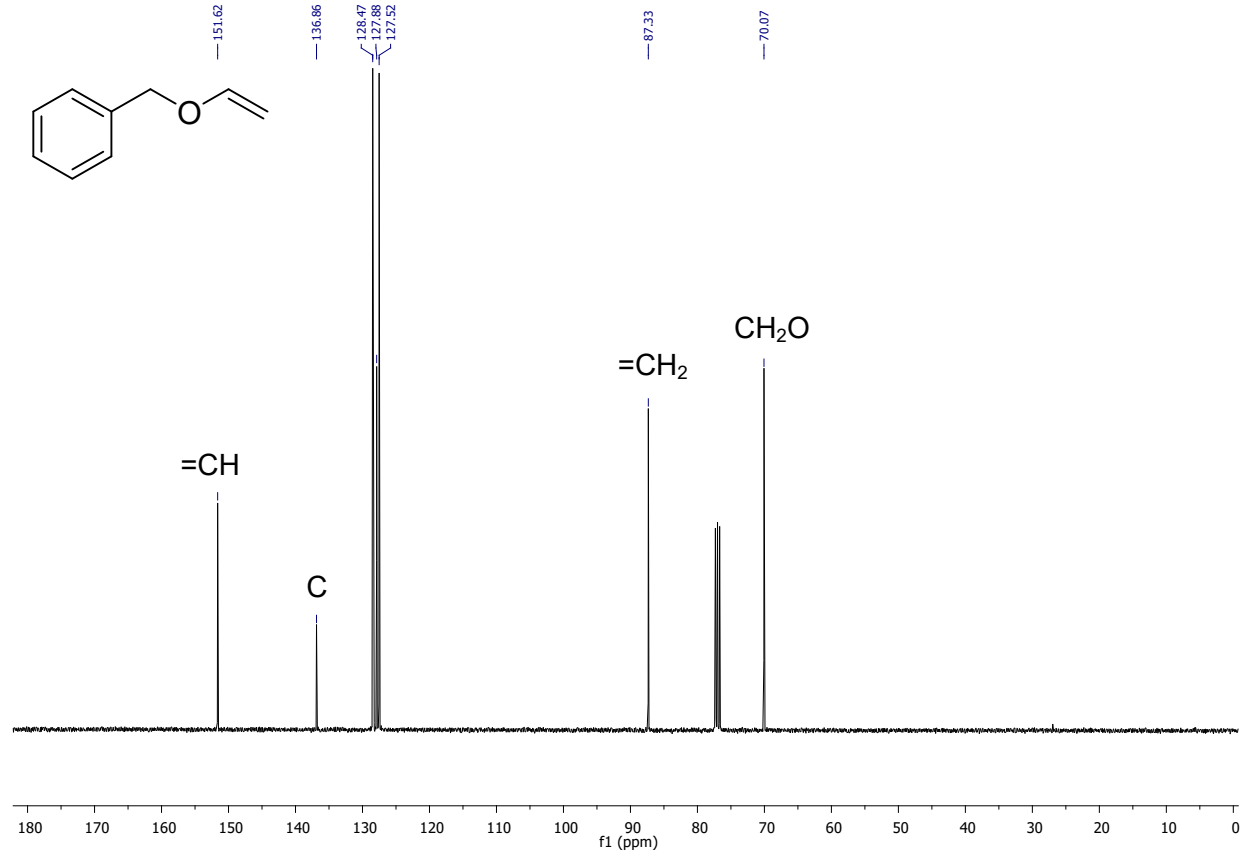


Figure S27. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of benzyl vinyl ether (**6a**).

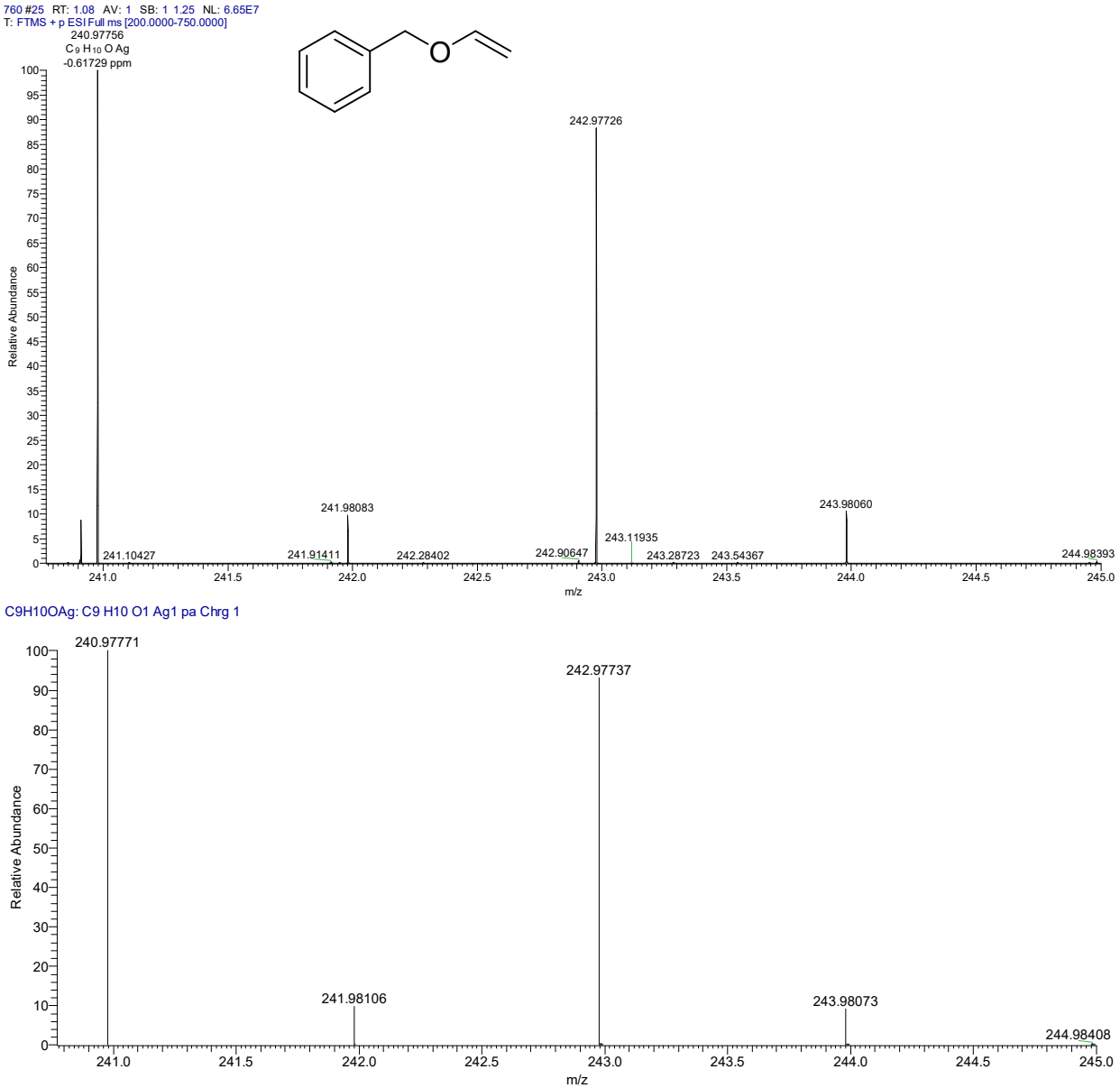


Figure S28. HRMS spectrum of benzyl vinyl ether (**6a**).

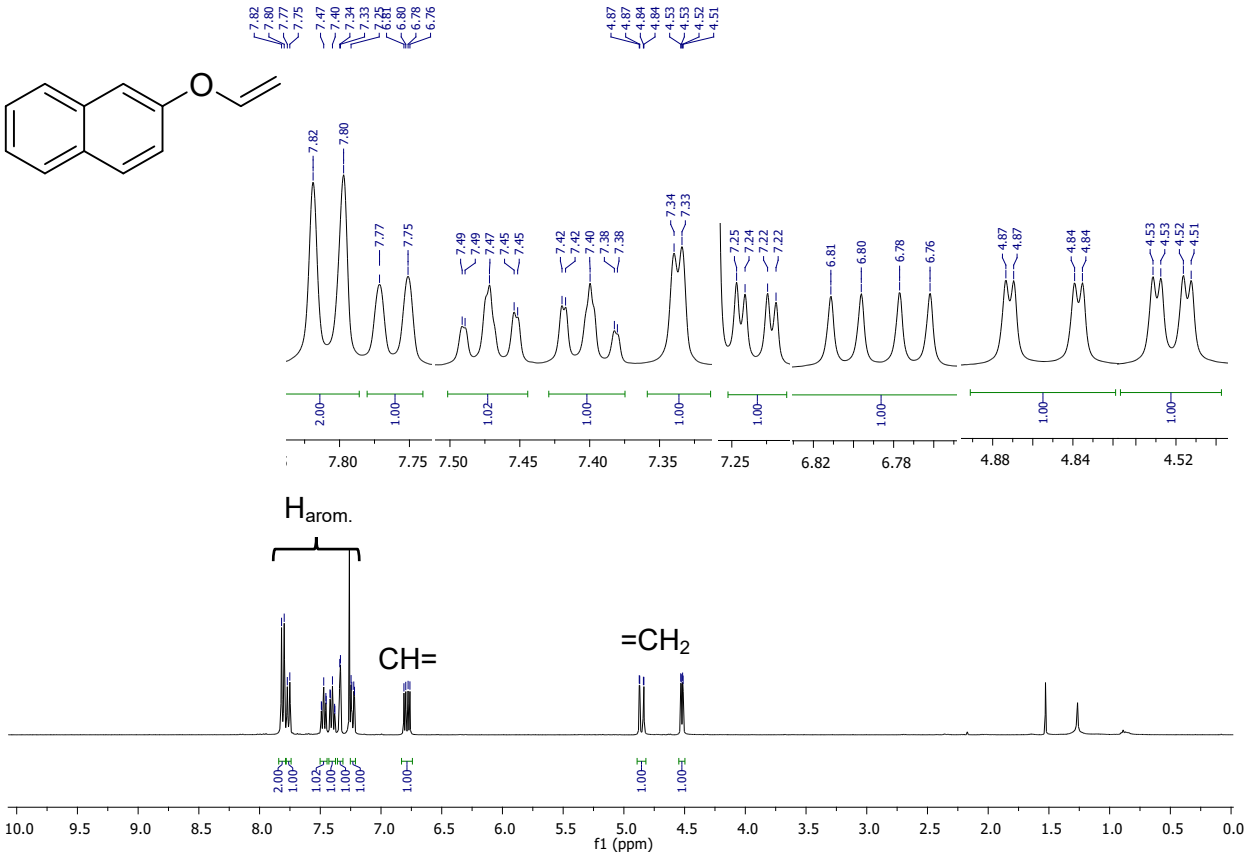


Figure S29. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 2-vinyloxyphenantren (**7a**).

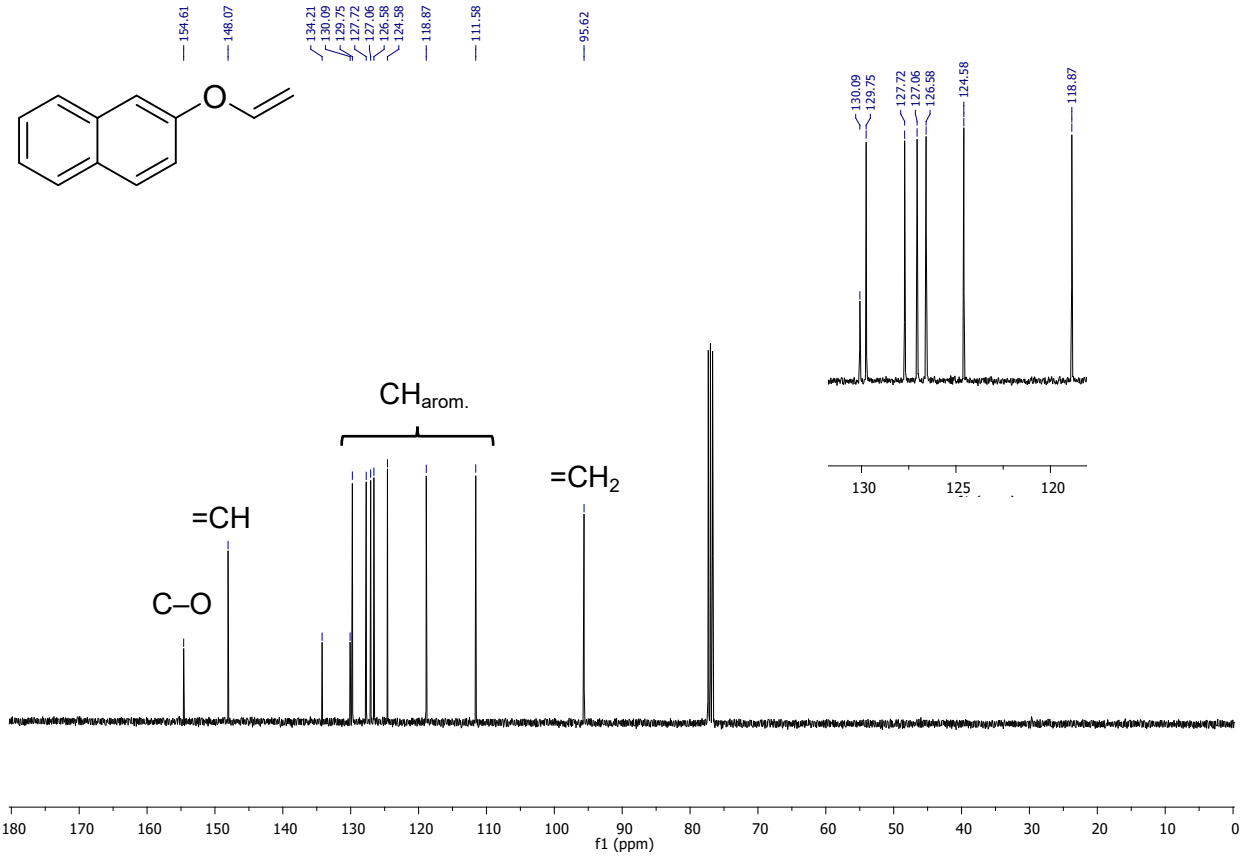


Figure S30. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 2-vinyloxyphenantren (**7a**).

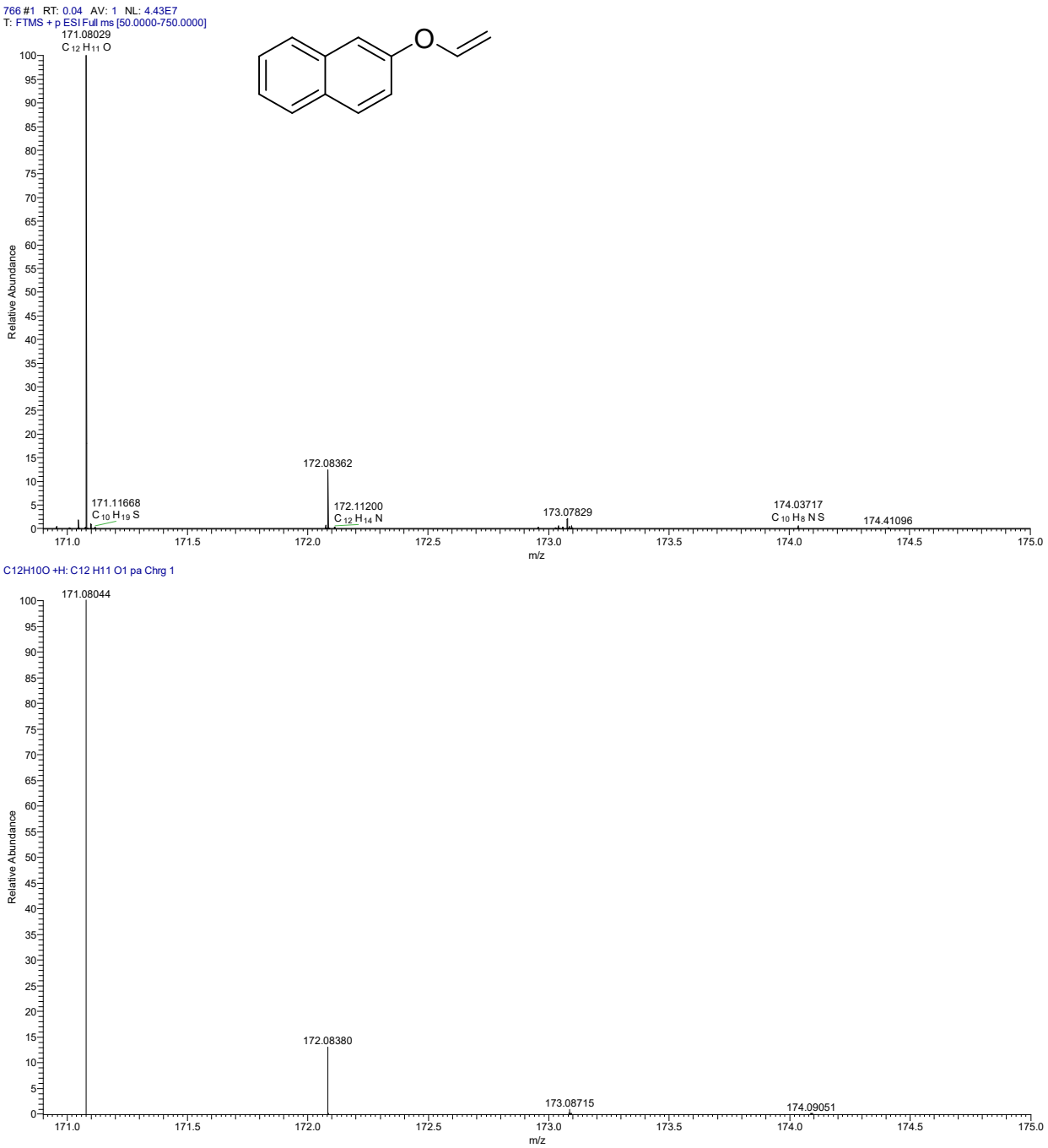


Figure S31. HRMS spectrum of 2-vinyloxyphenantren (**7a**).

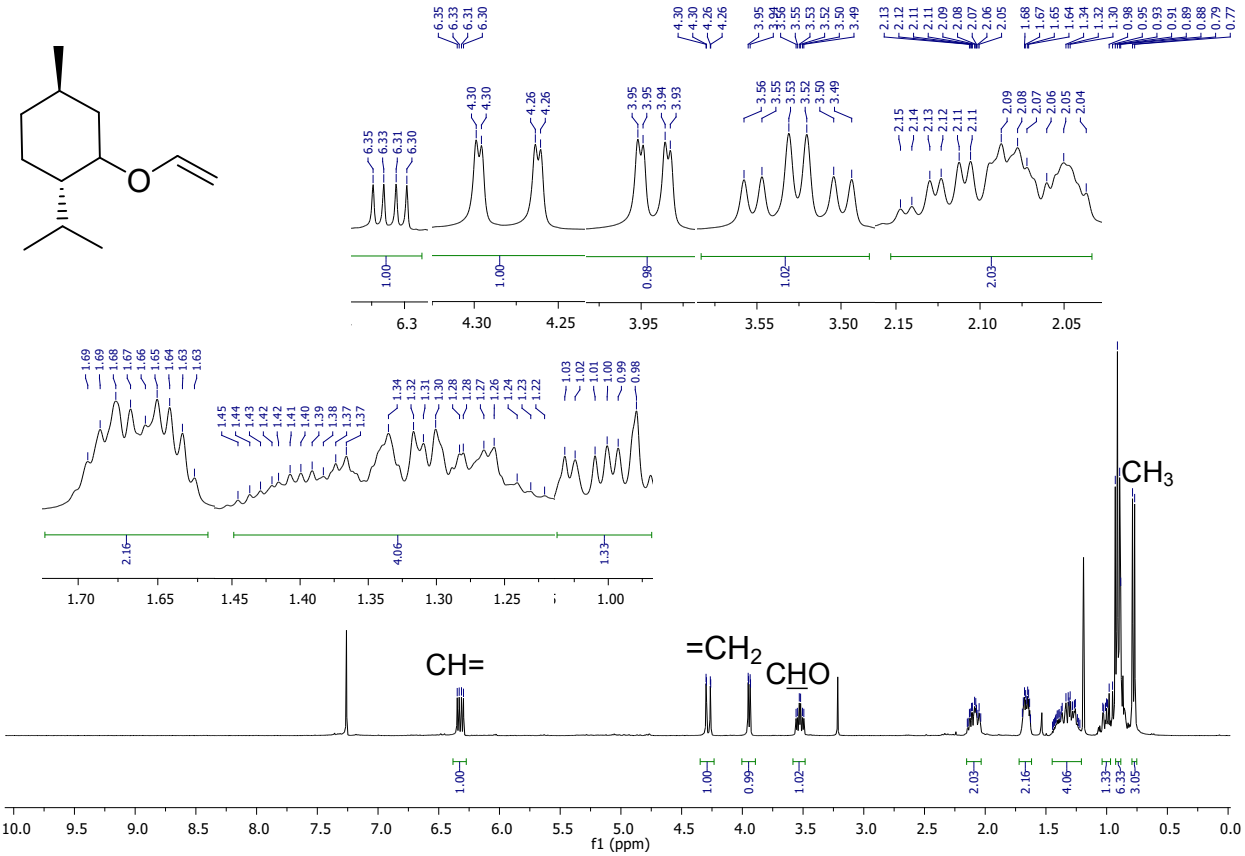


Figure S32. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of menthyl vinyl ether (**8a**).

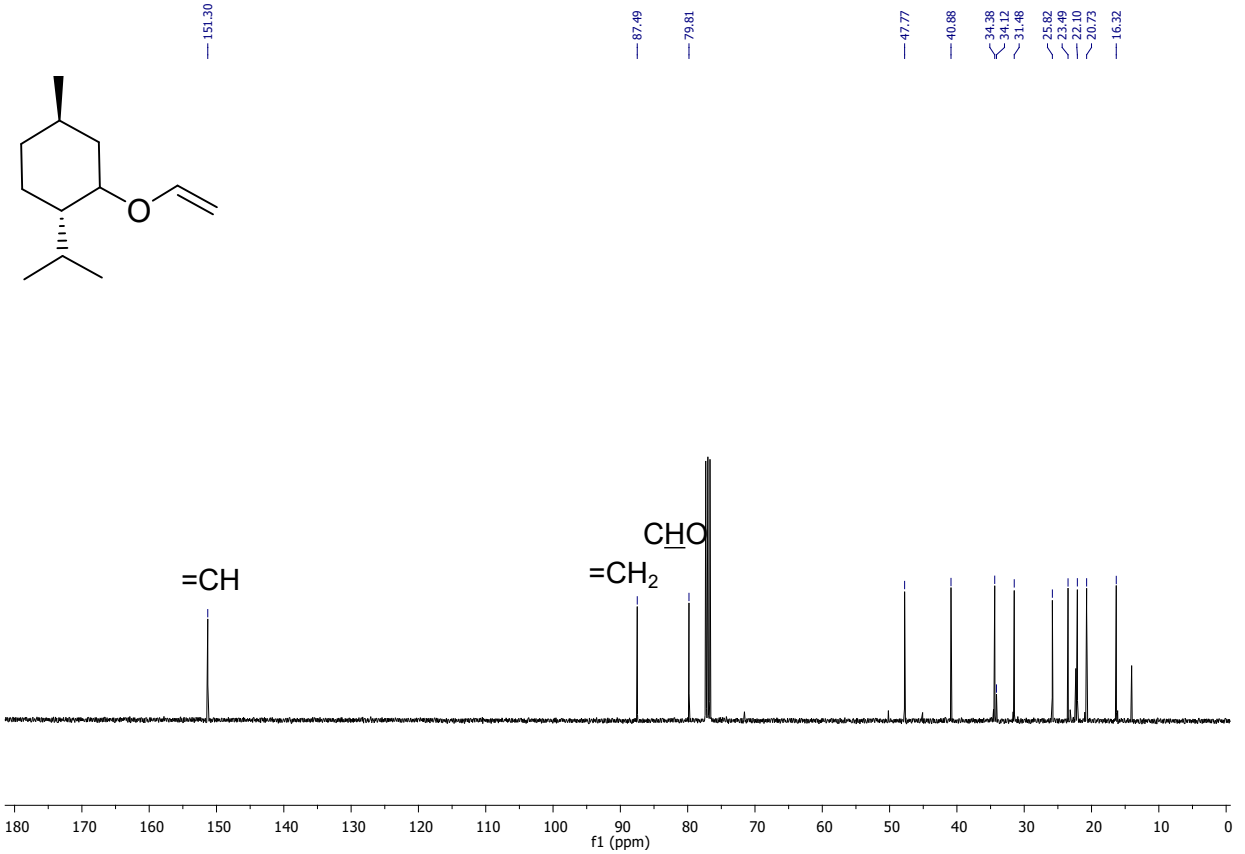


Figure S33. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of menthyl vinyl ether (**8a**).

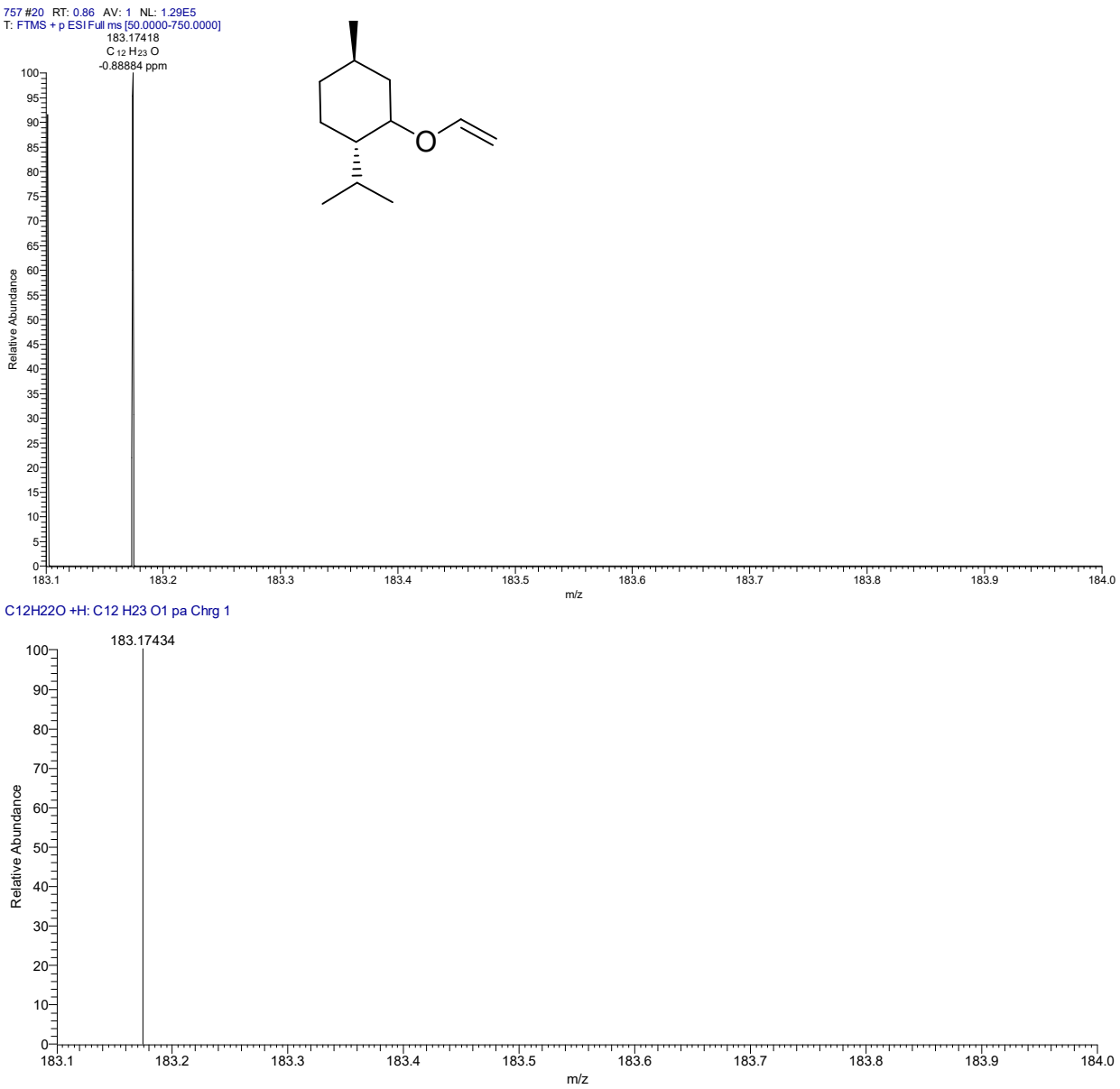


Figure S34. HRMS spectrum of menthyl vinyl ether (**8a**).

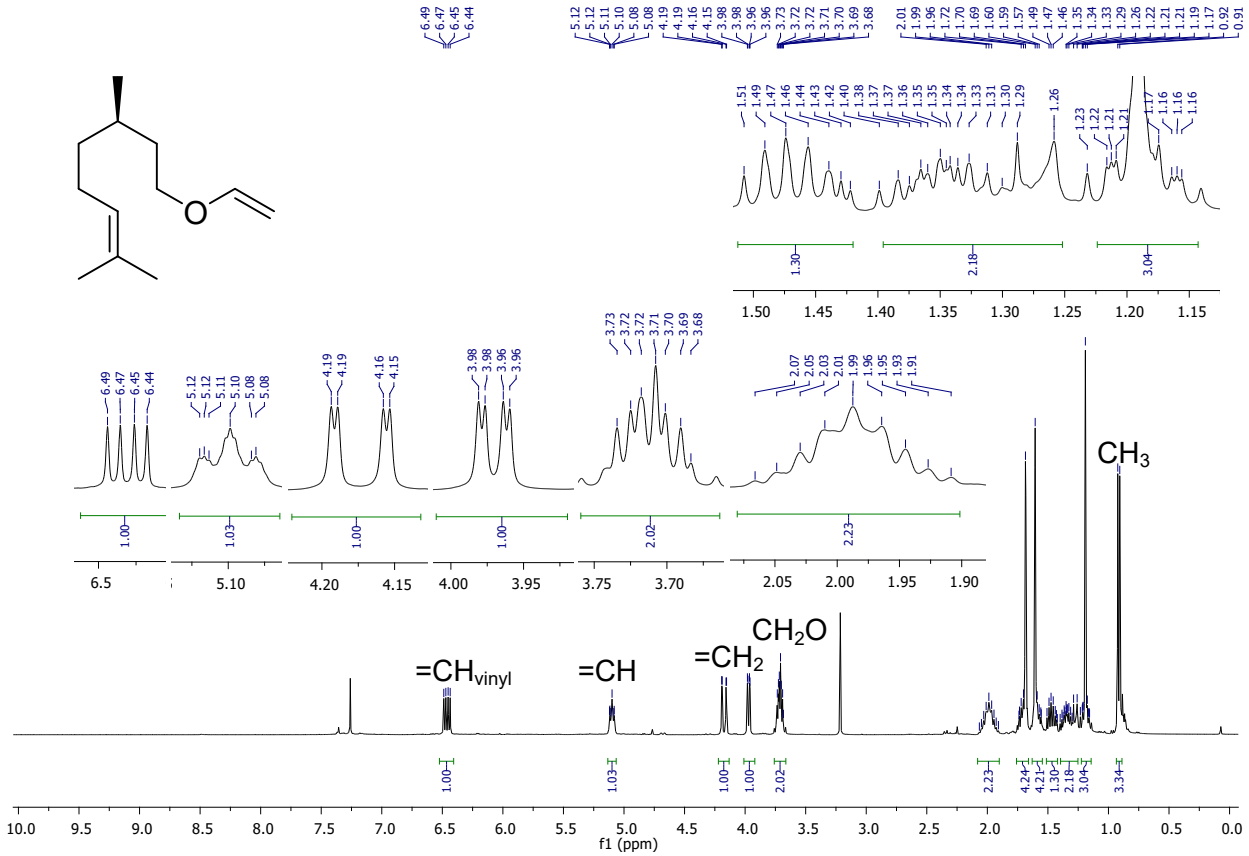


Figure S35. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of citronellyl vinyl ether (**9a**).

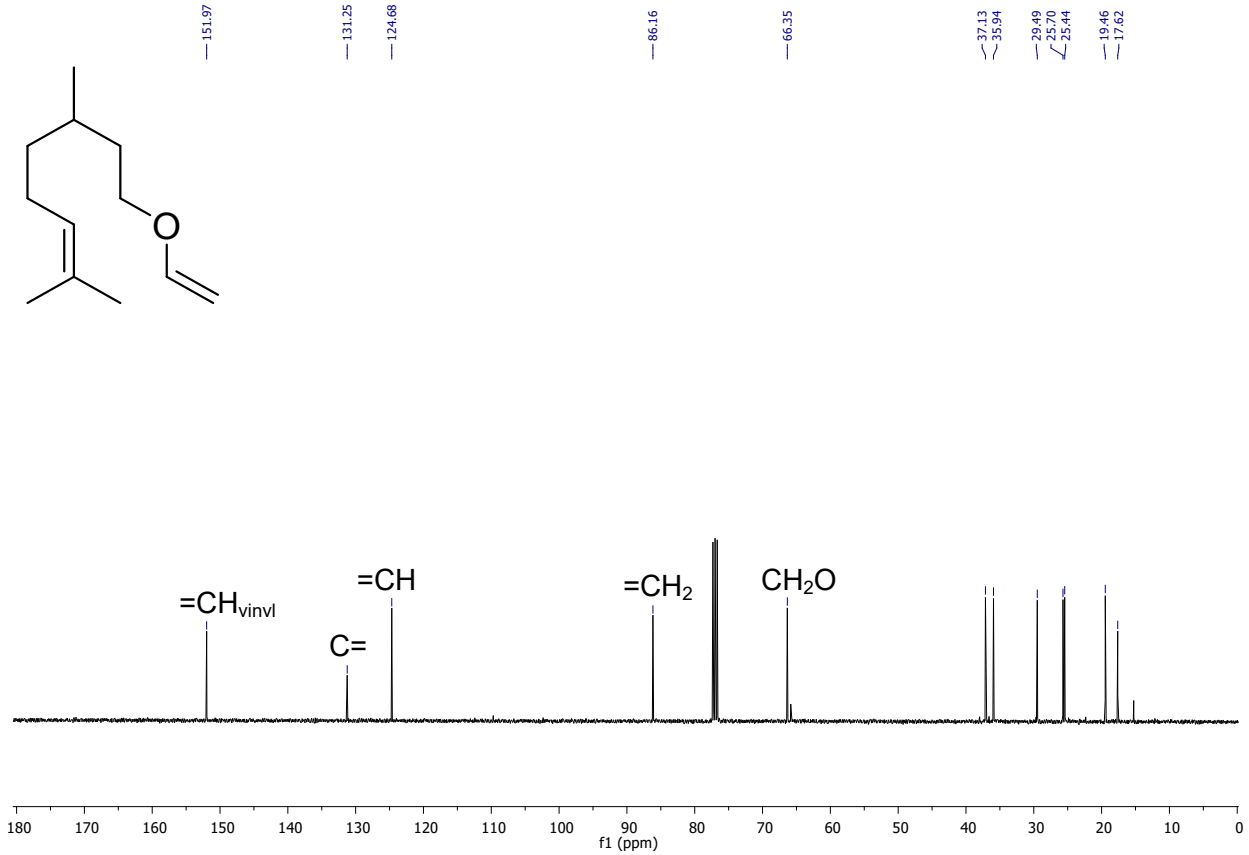


Figure S36. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of citronellyl vinyl ether (**9a**).

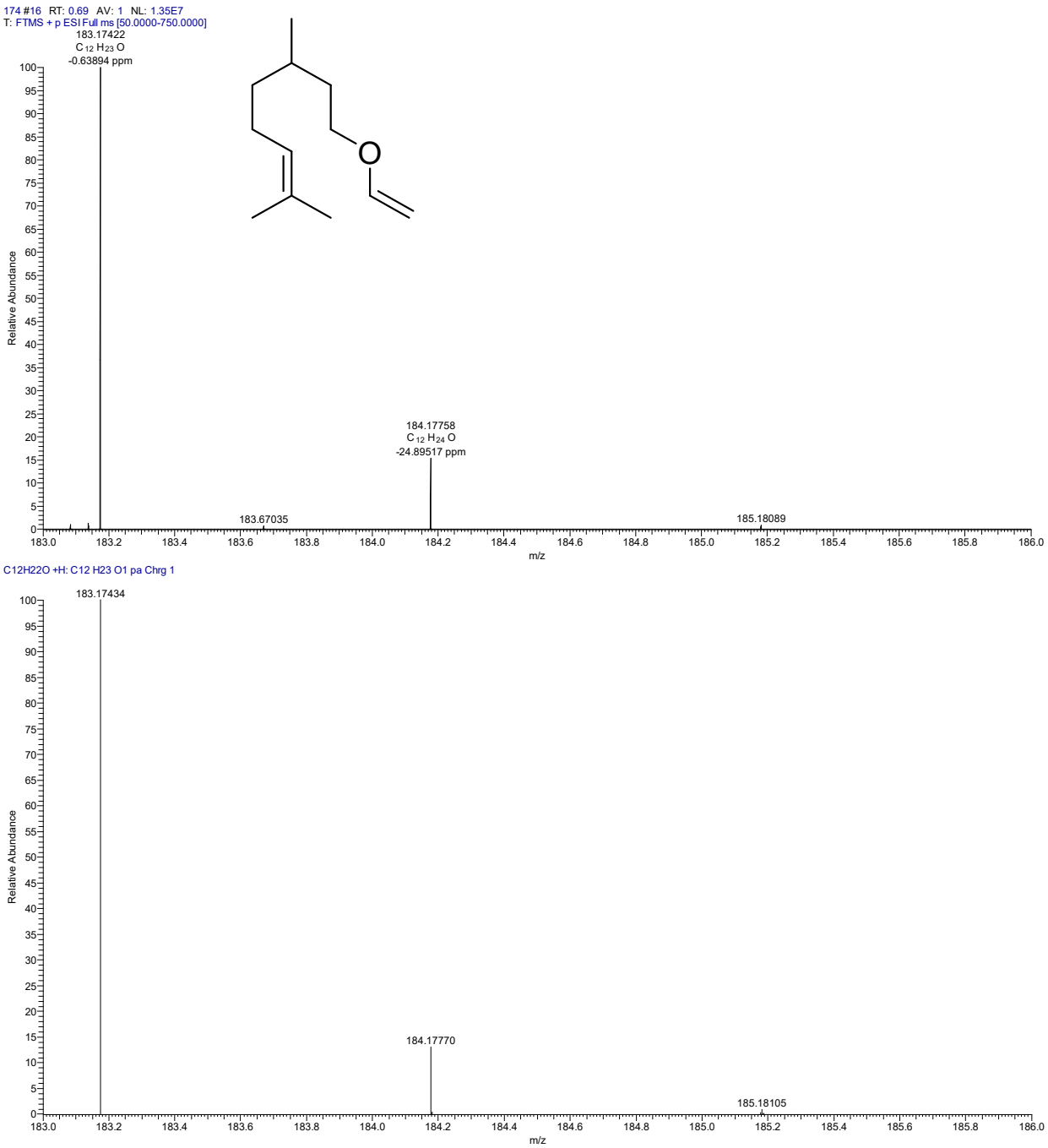


Figure S37. HRMS spectrum of citronellyl vinyl ether (**9a**).

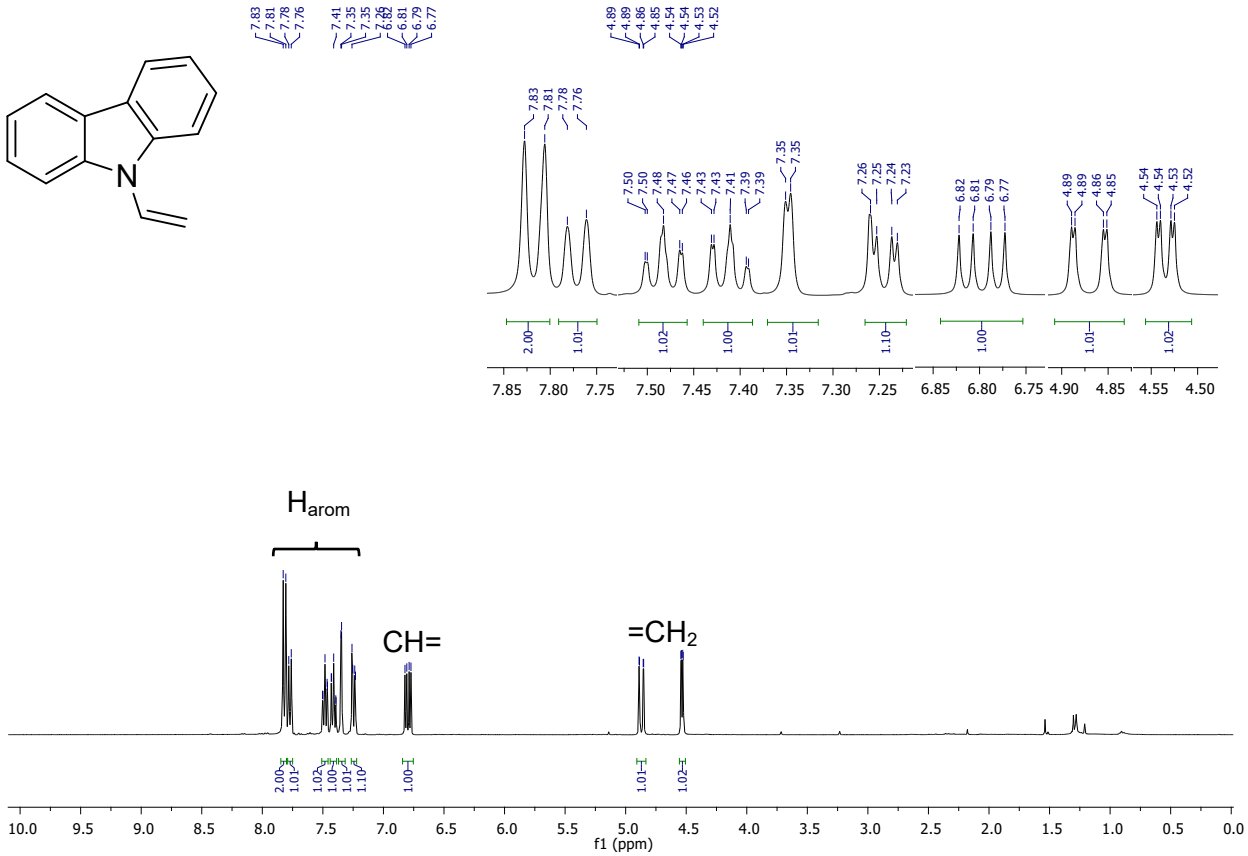


Figure S38. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of *N*-vinyl carbazole (**10a**).

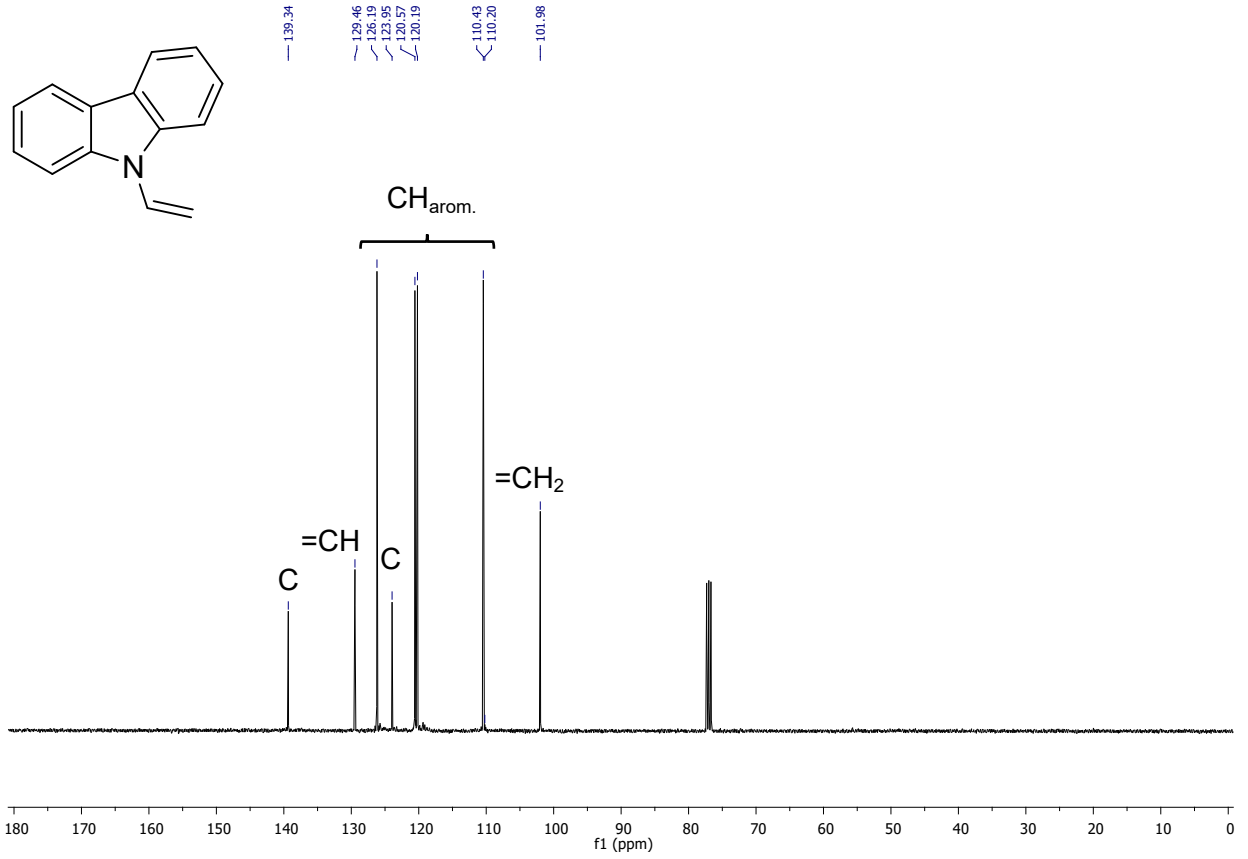


Figure S39. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of *N*-vinyl carbazole (**10a**).

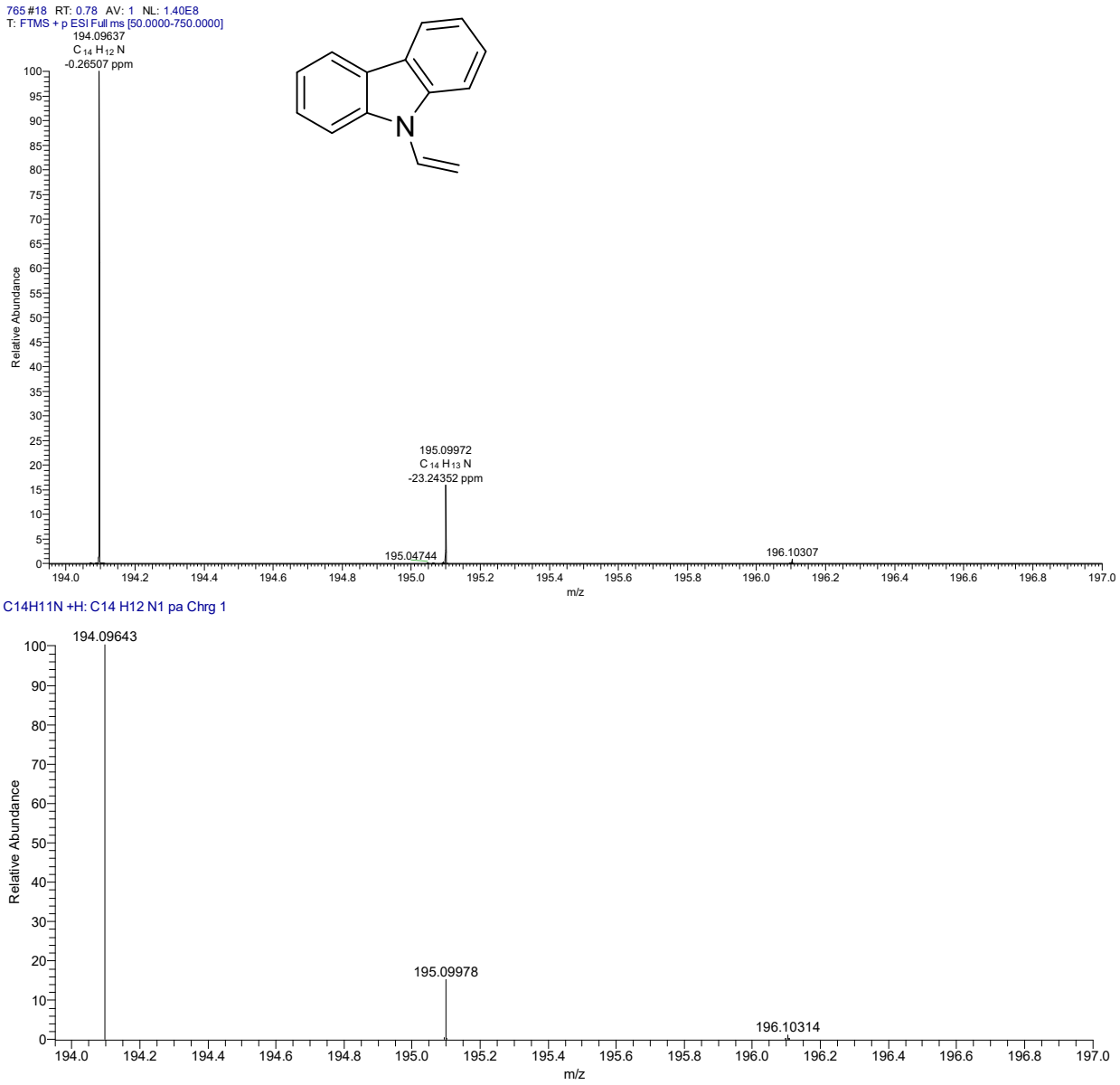


Figure S40. HRMS spectrum of *N*-vinyl carbazole (**10a**).

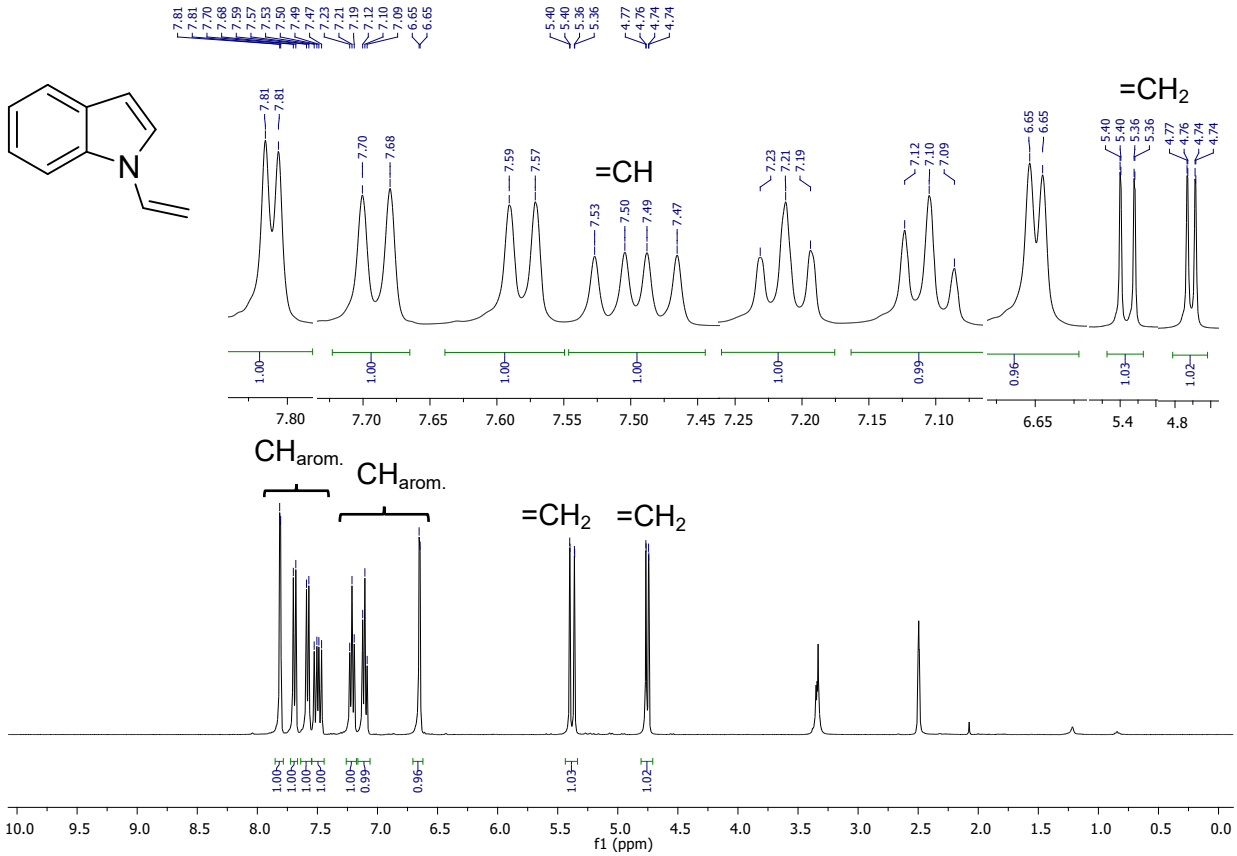


Figure S41. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of *N*-vinyl indole (**11a**).

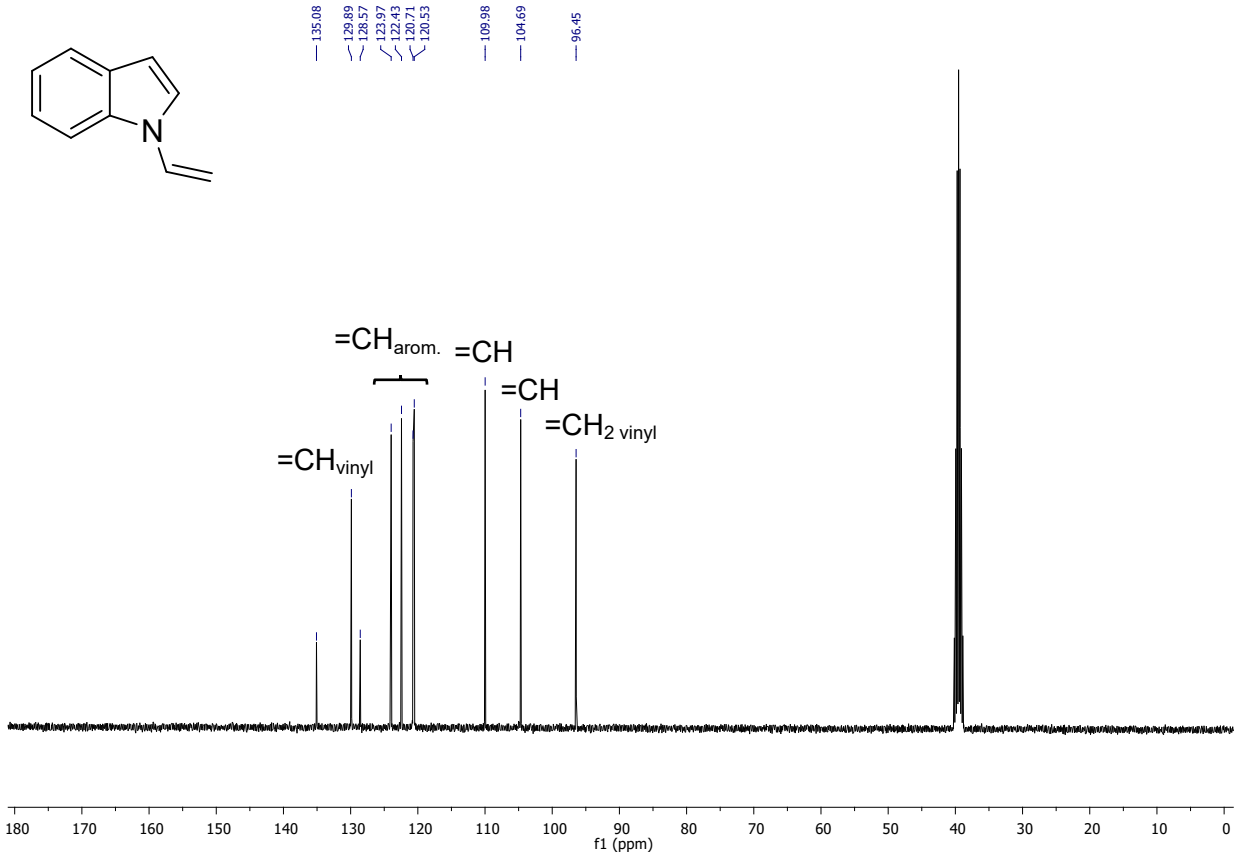


Figure S42. ^{13}C NMR spectrum (101 MHz, DMSO-d_6) of *N*-vinyl indole (**11a**).

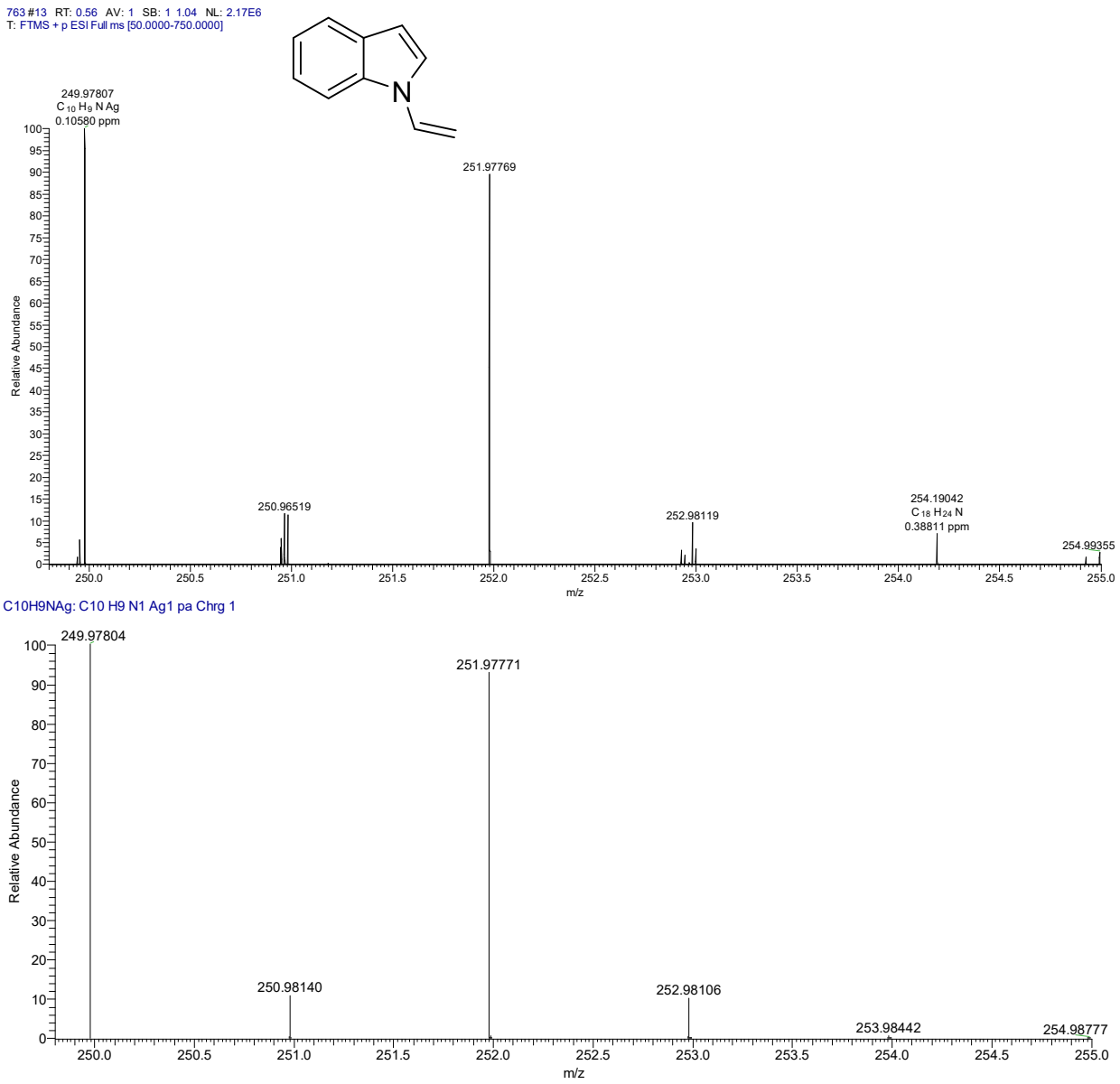


Figure S43. NMR spectrum of *N*-vinyl indole (**11a**).

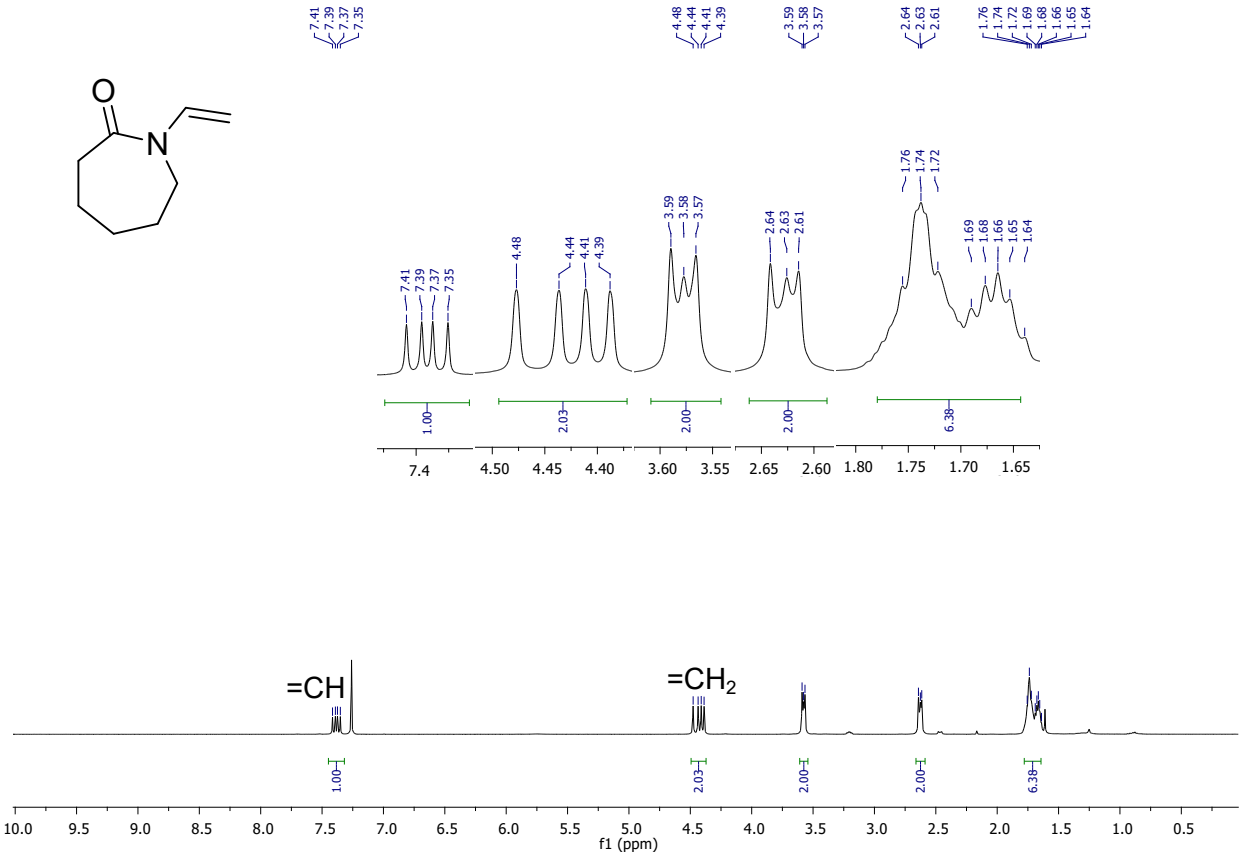


Figure S44. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1-vinylazepan-2-one (**12a**).

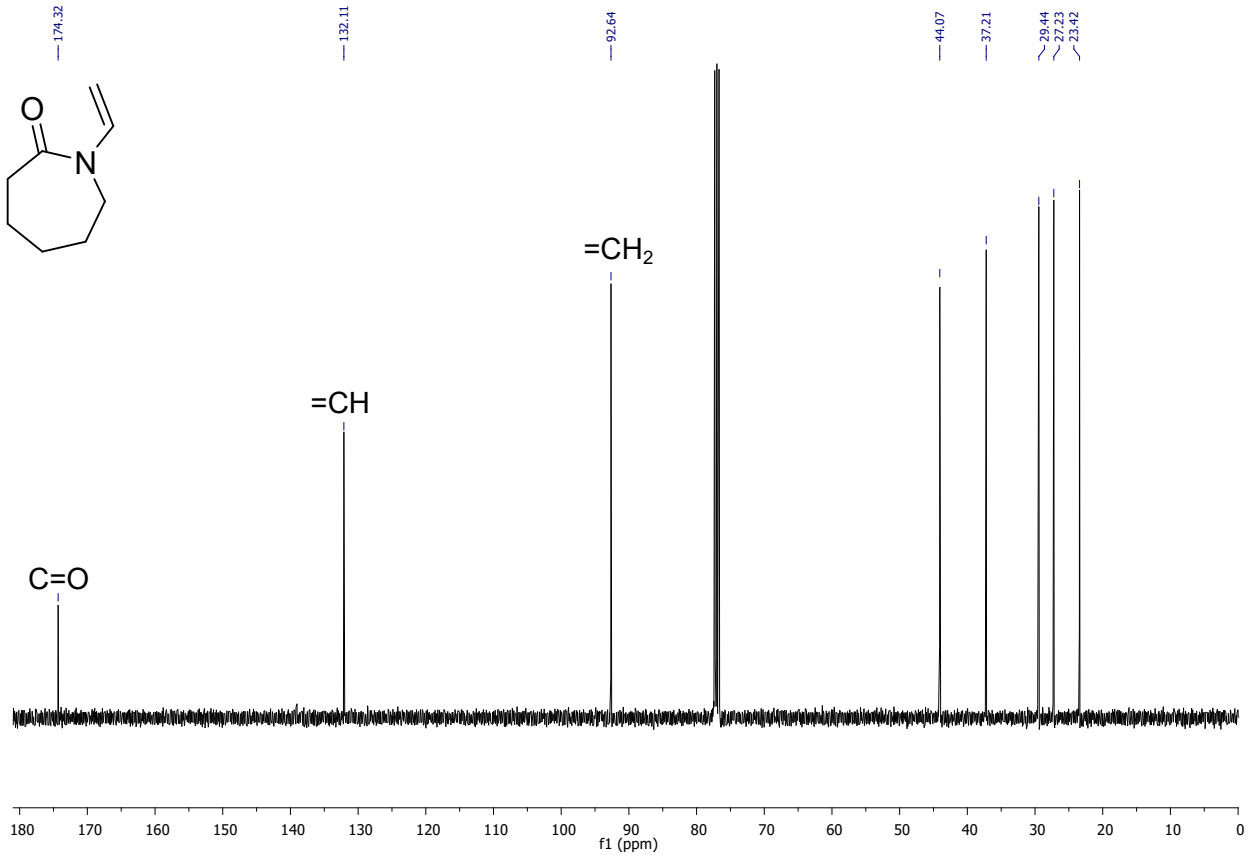


Figure S45. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 1-vinylazepan-2-one (**12a**).

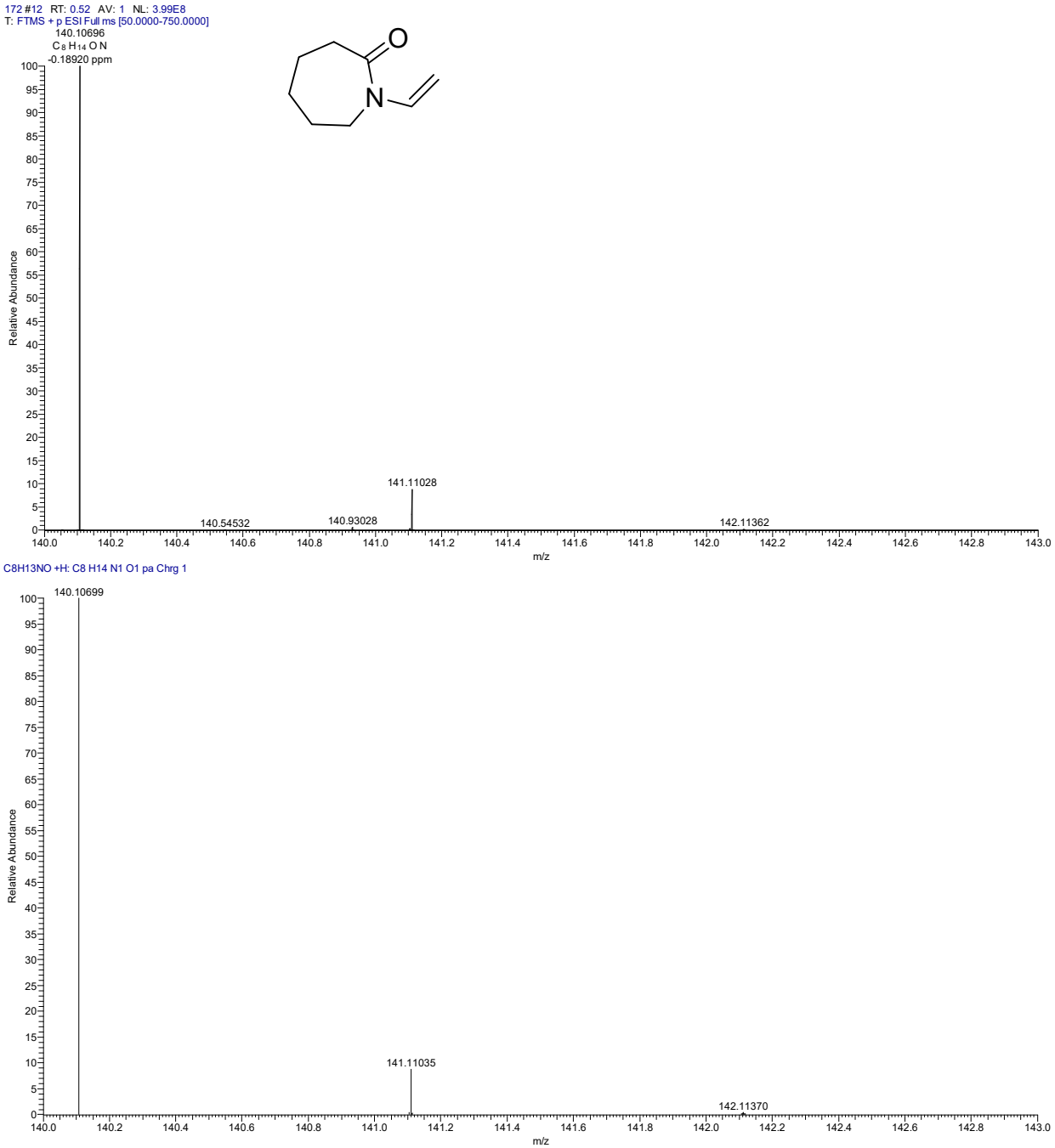


Figure S46. HRMS spectrum of 1-vinylazepan-2-one (**12a**).

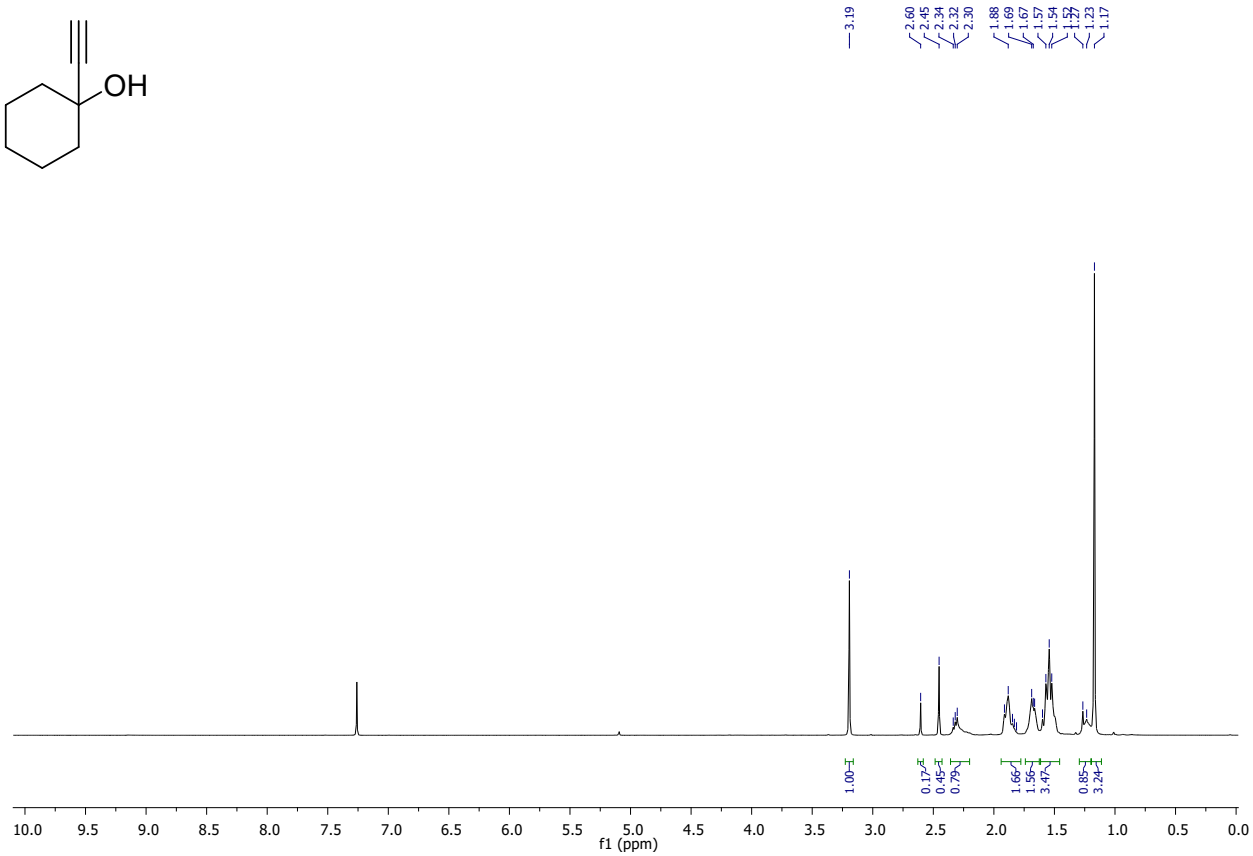


Figure S47. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of reaction mixture after cyclohexanone (**13**) vinylation with BaC_2.

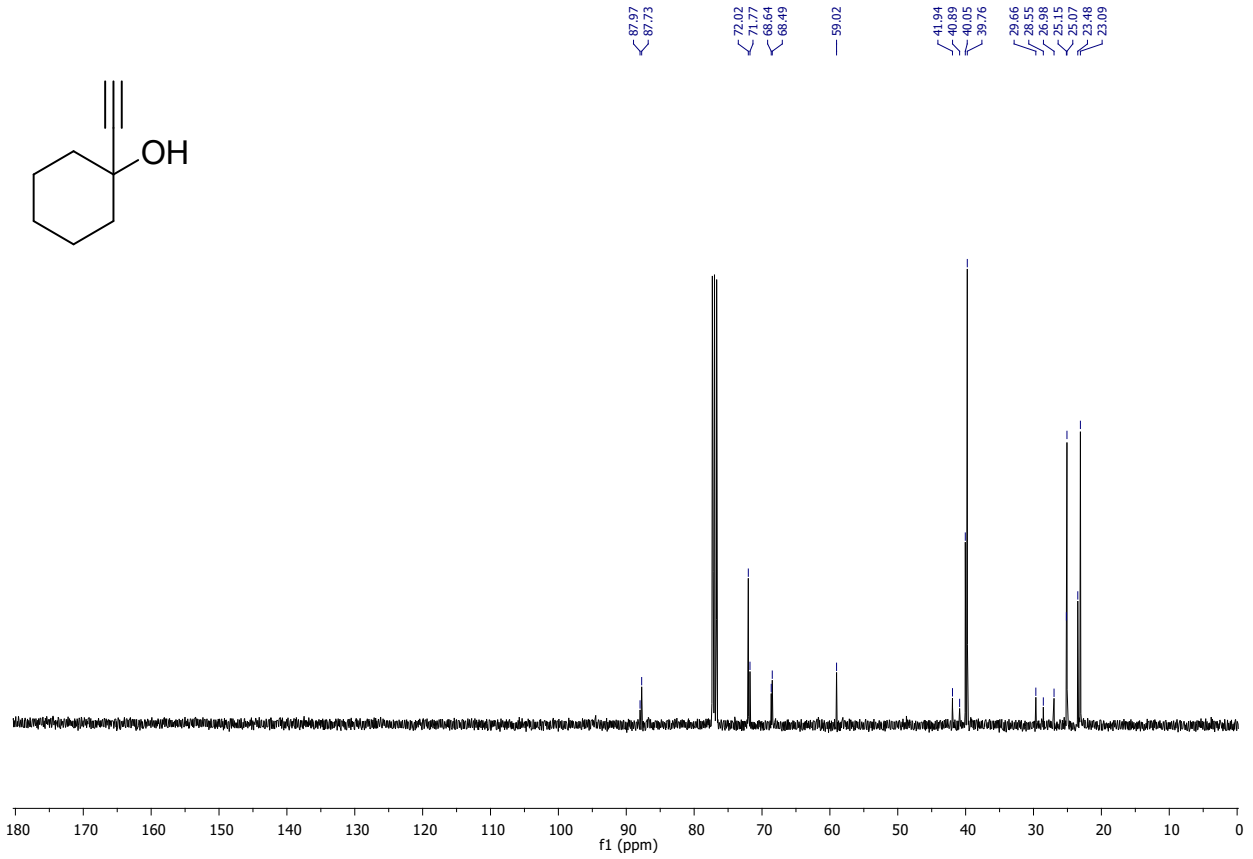


Figure S48. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of reaction mixture after cyclohexanone (**13**) vinylation with BaC_2.

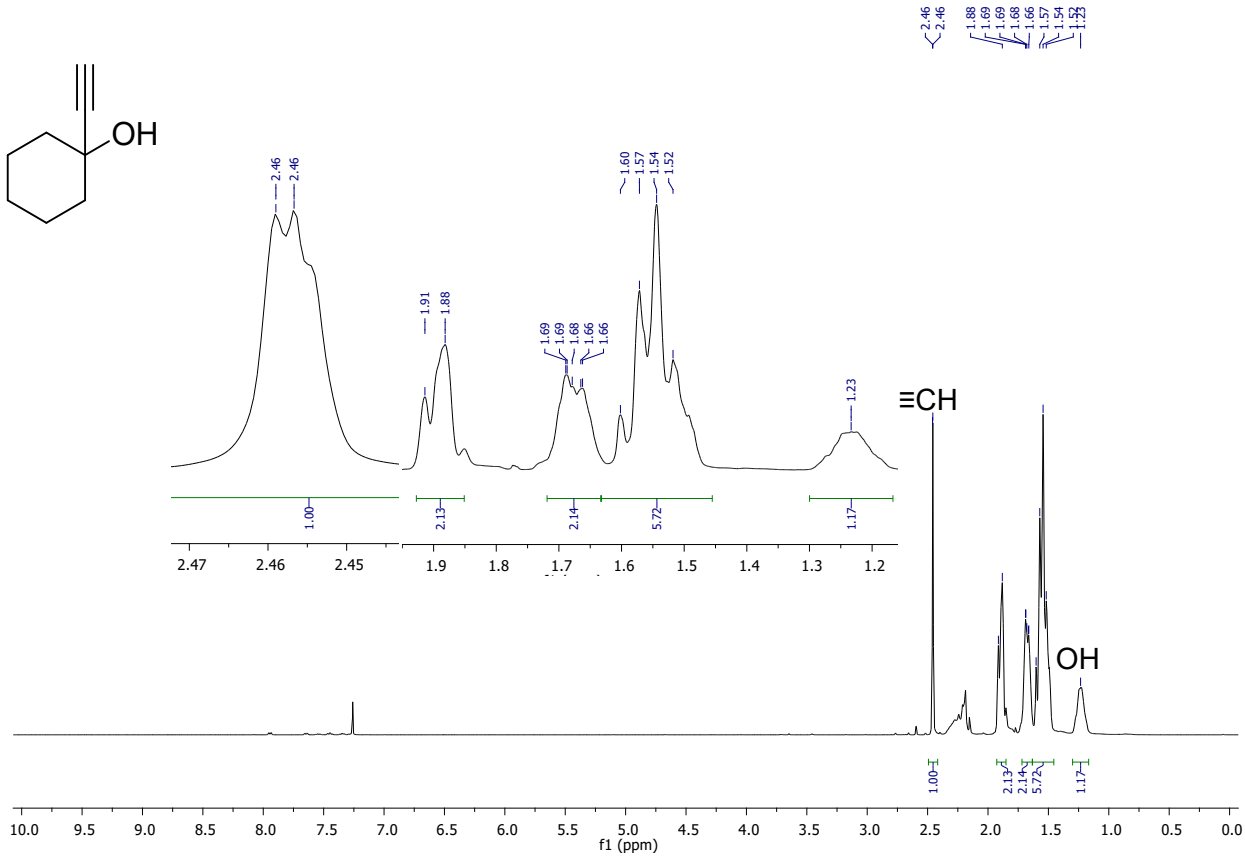


Figure S49. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1-ethynylcyclohexan-1-ol (**13a**).

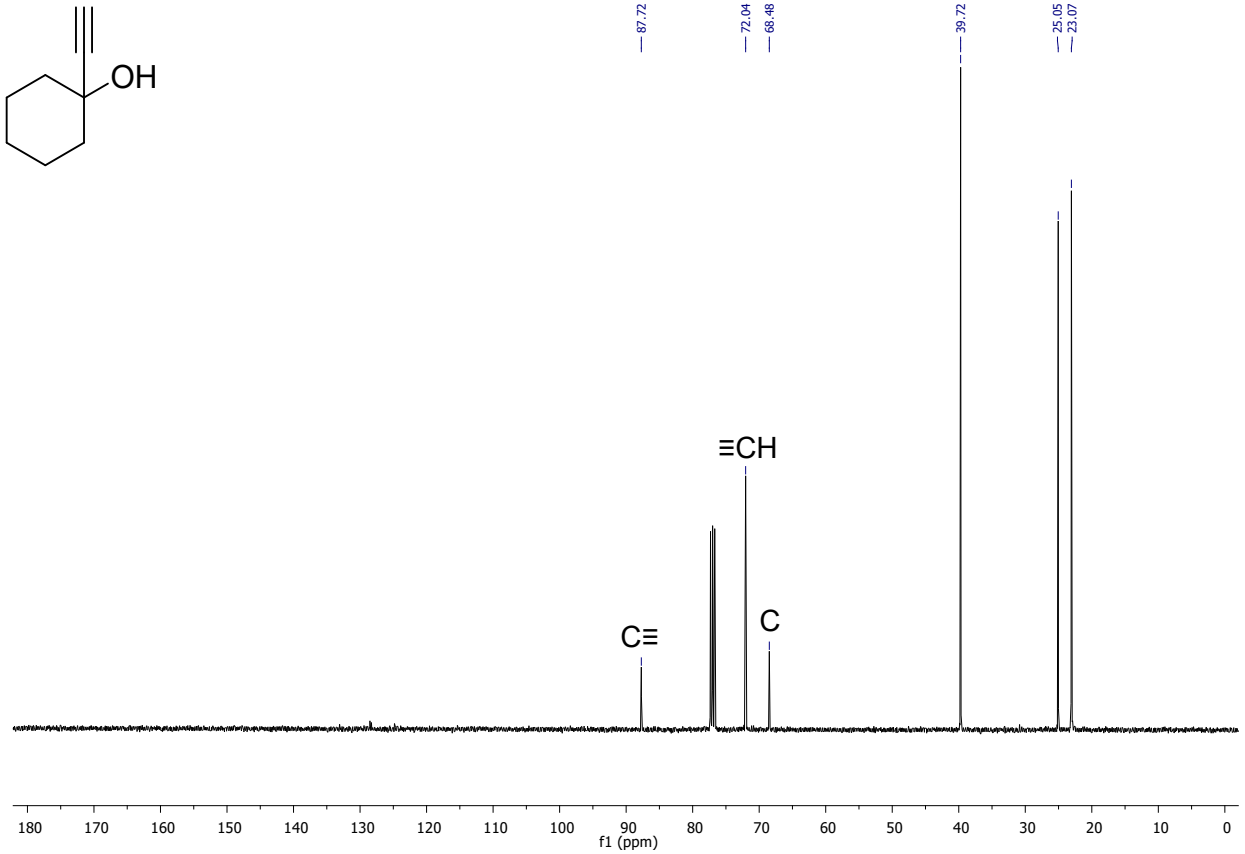


Figure S50. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 1-ethynylcyclohexan-1-ol (**13a**).

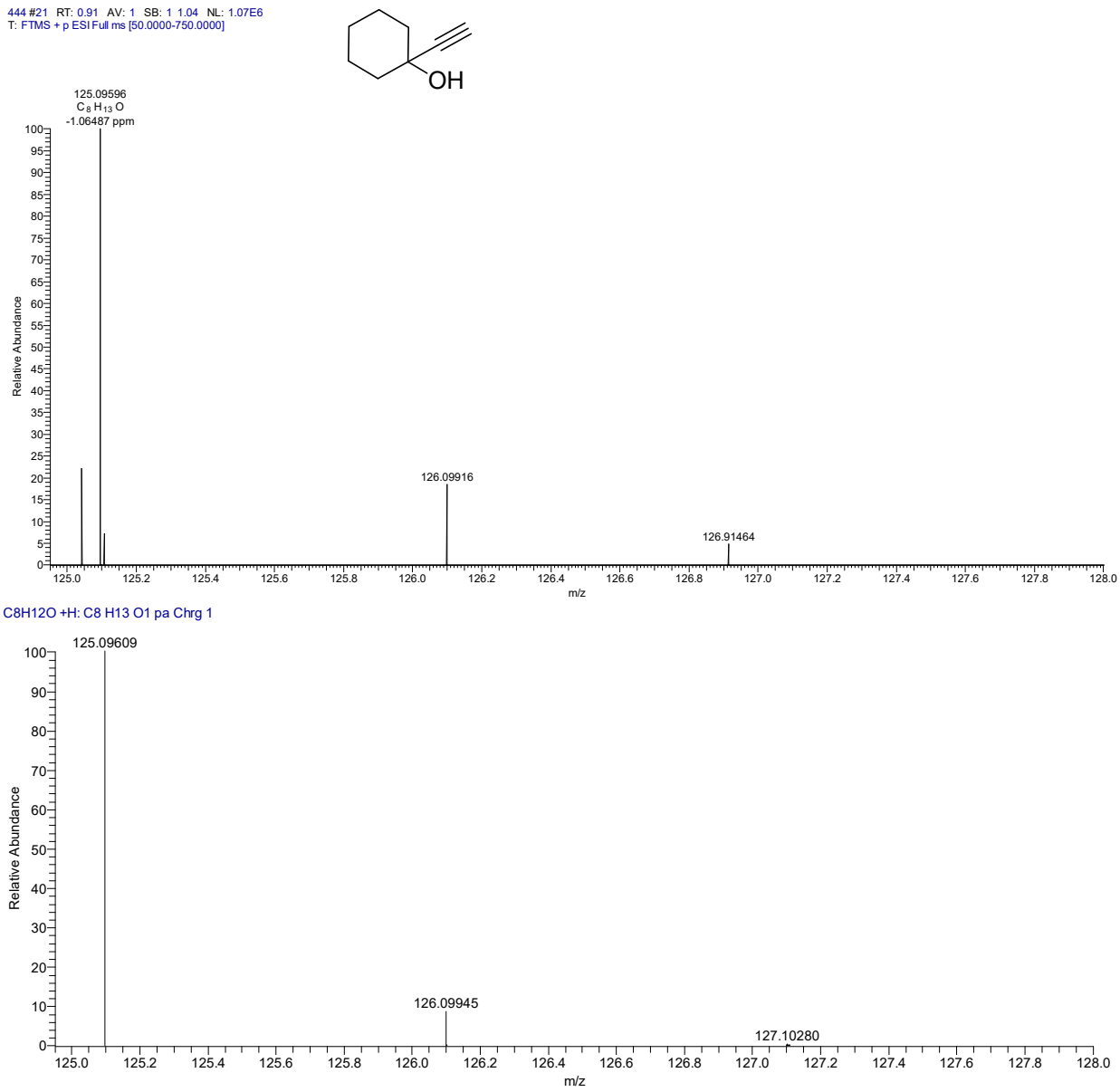


Figure S51. HRMS spectrum of 1-ethynylcyclohexan-1-ol (**13a**).

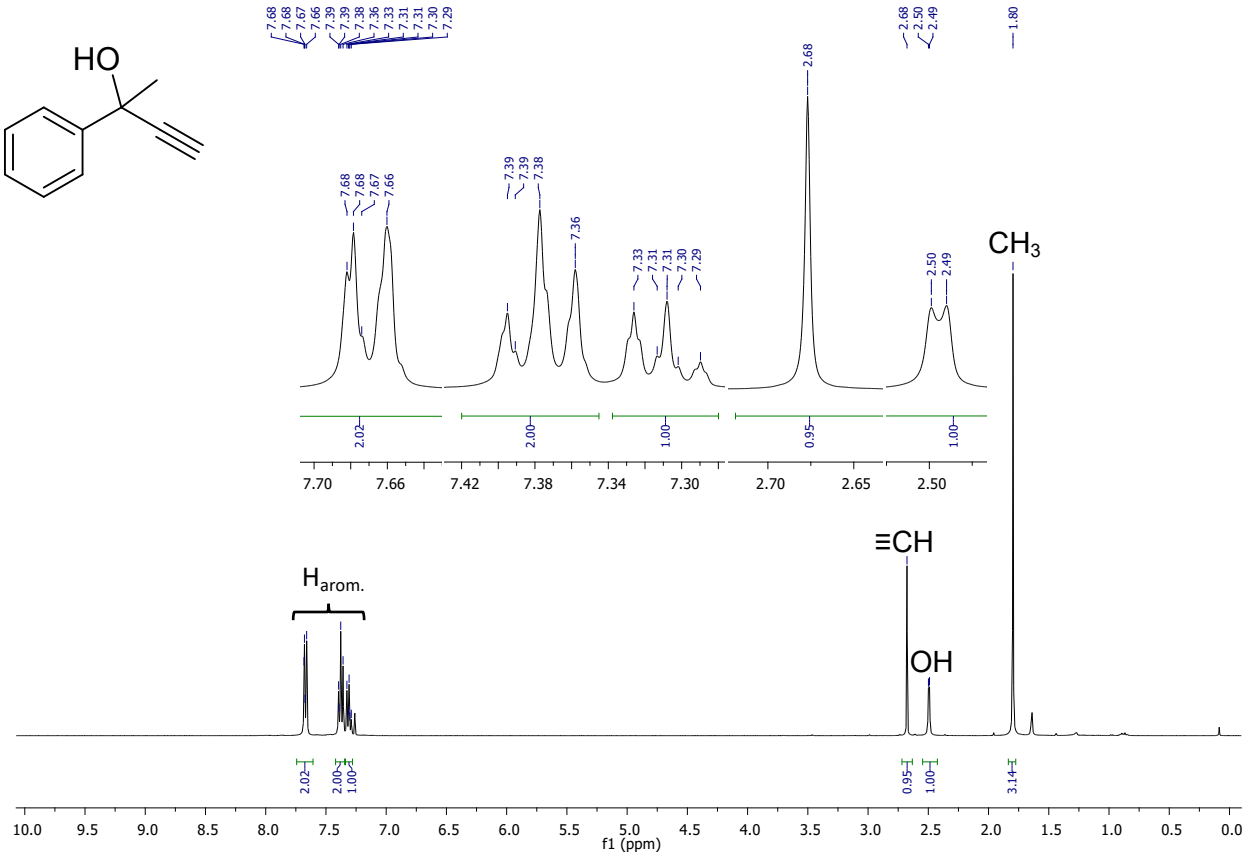


Figure S52. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 2-phenylbut-3-yn-2-ol (**14a**).

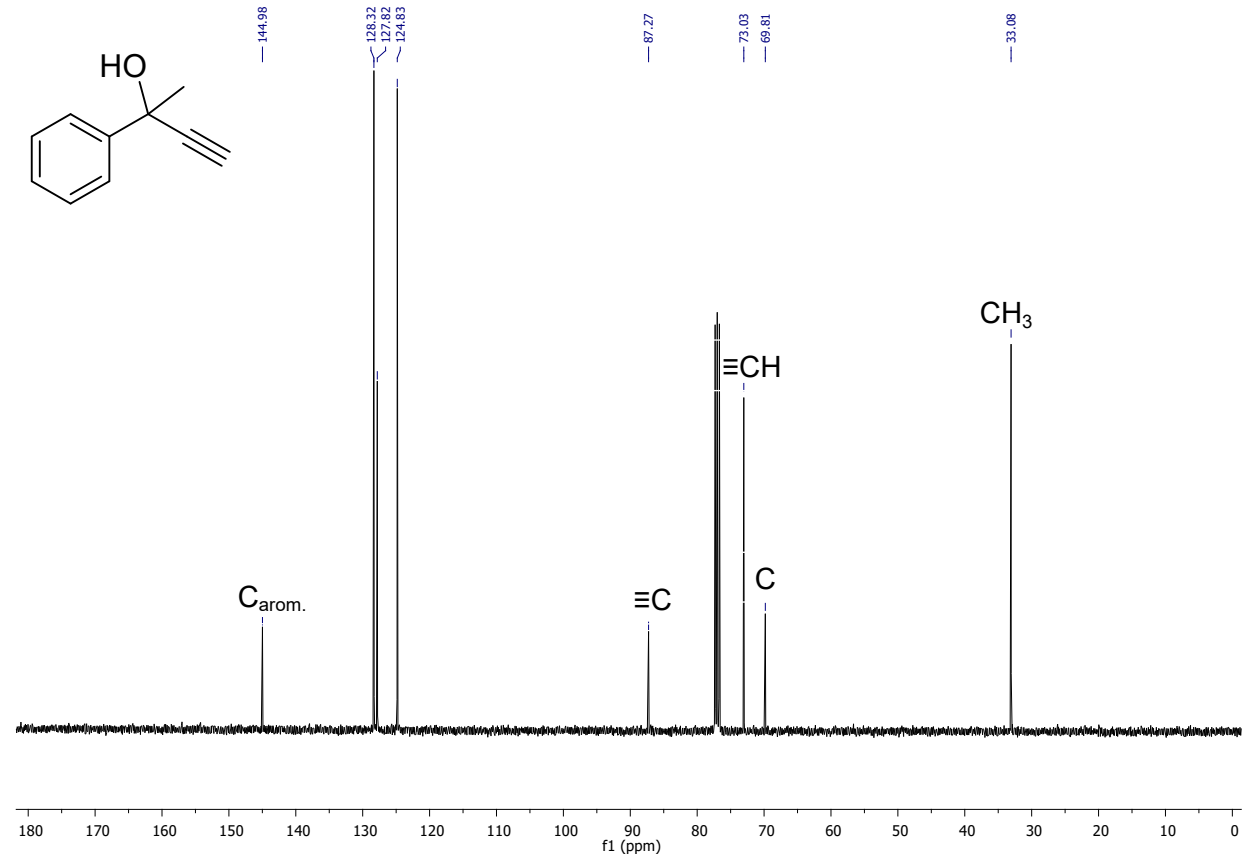


Figure S53. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 2-phenylbut-3-yn-2-ol (**14a**).

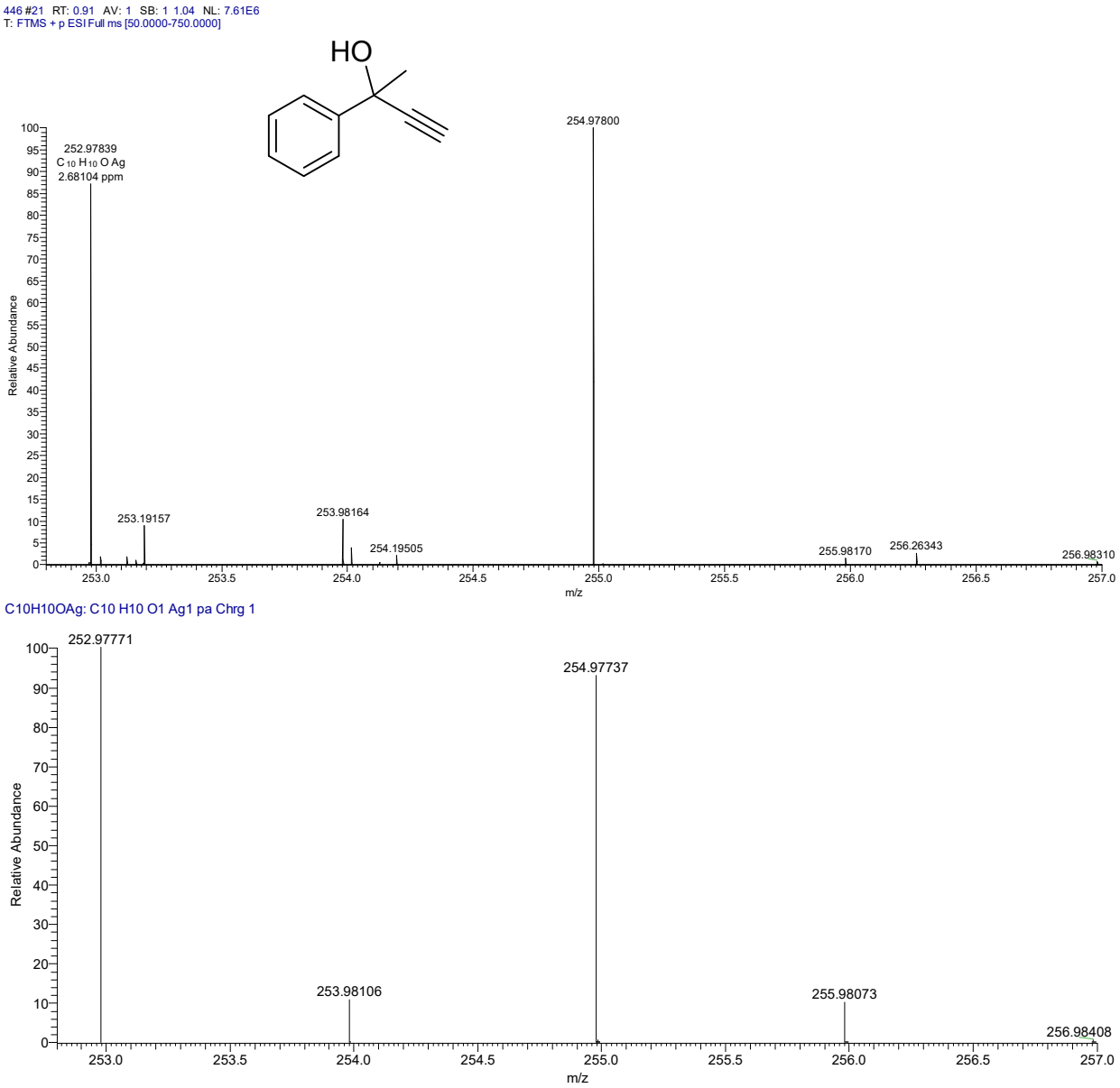


Figure S54. HRMS spectrum of 2-phenylbut-3-yn-2-ol (**14a**).

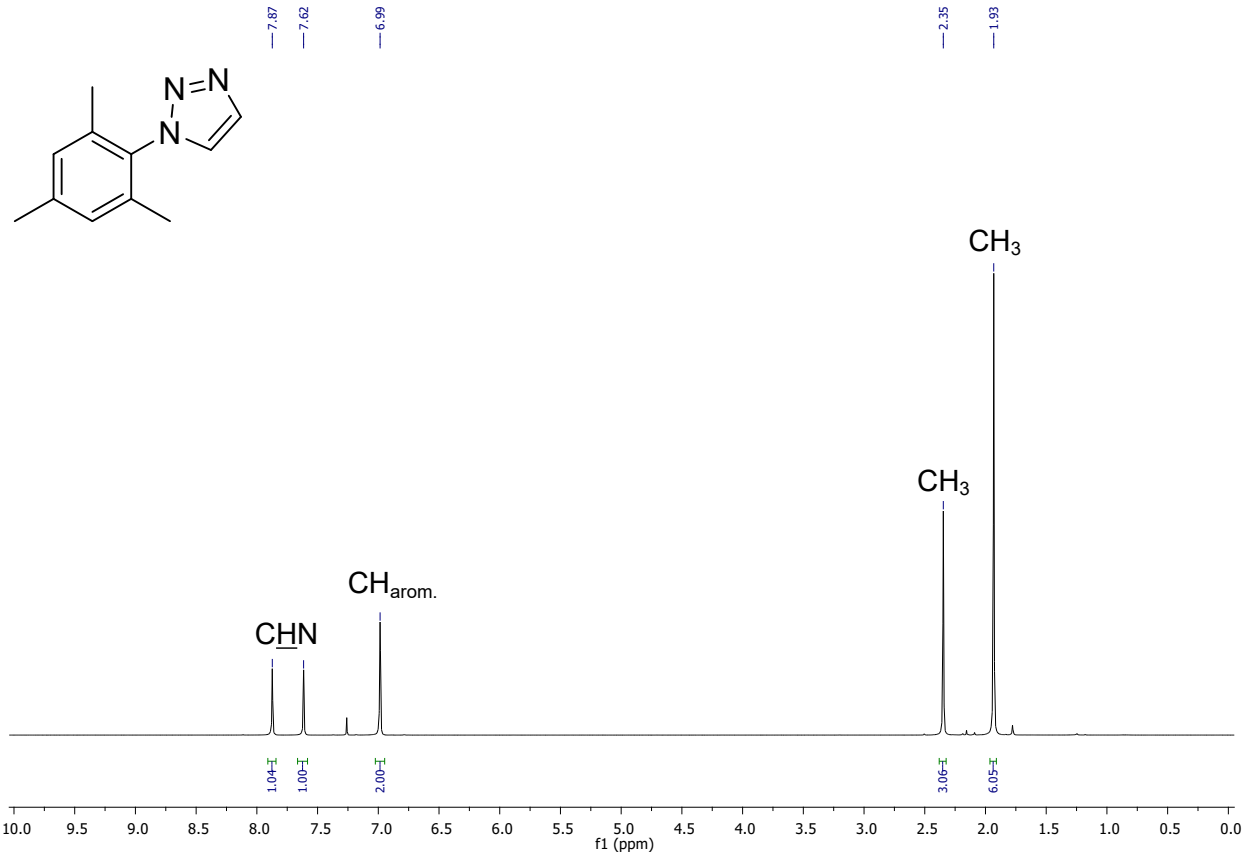


Figure S55. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 2,4,6-trimethylphenyl-1*H*-1,2,3-triazole (**15a**).

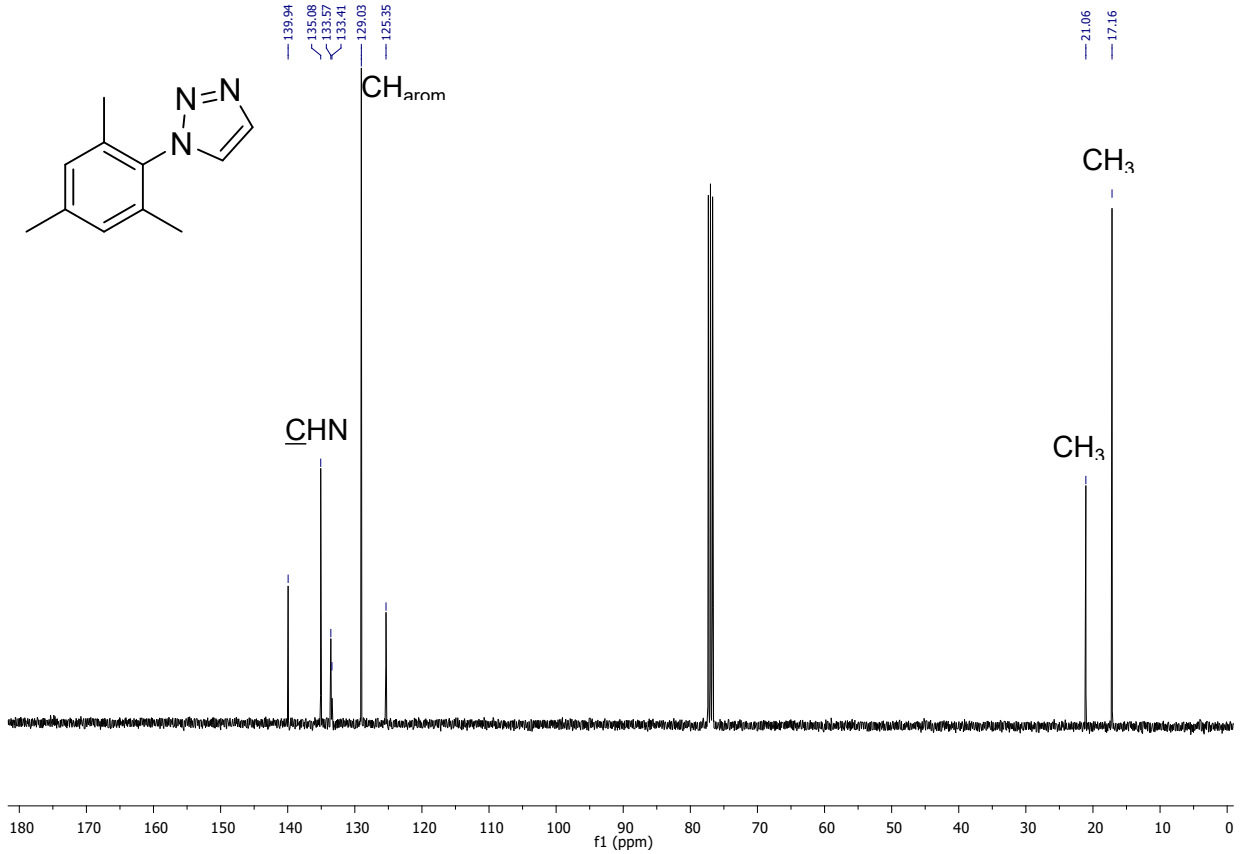


Figure S56. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 2,4,6-trimethylphenyl-1*H*-1,2,3-triazole (**15a**).

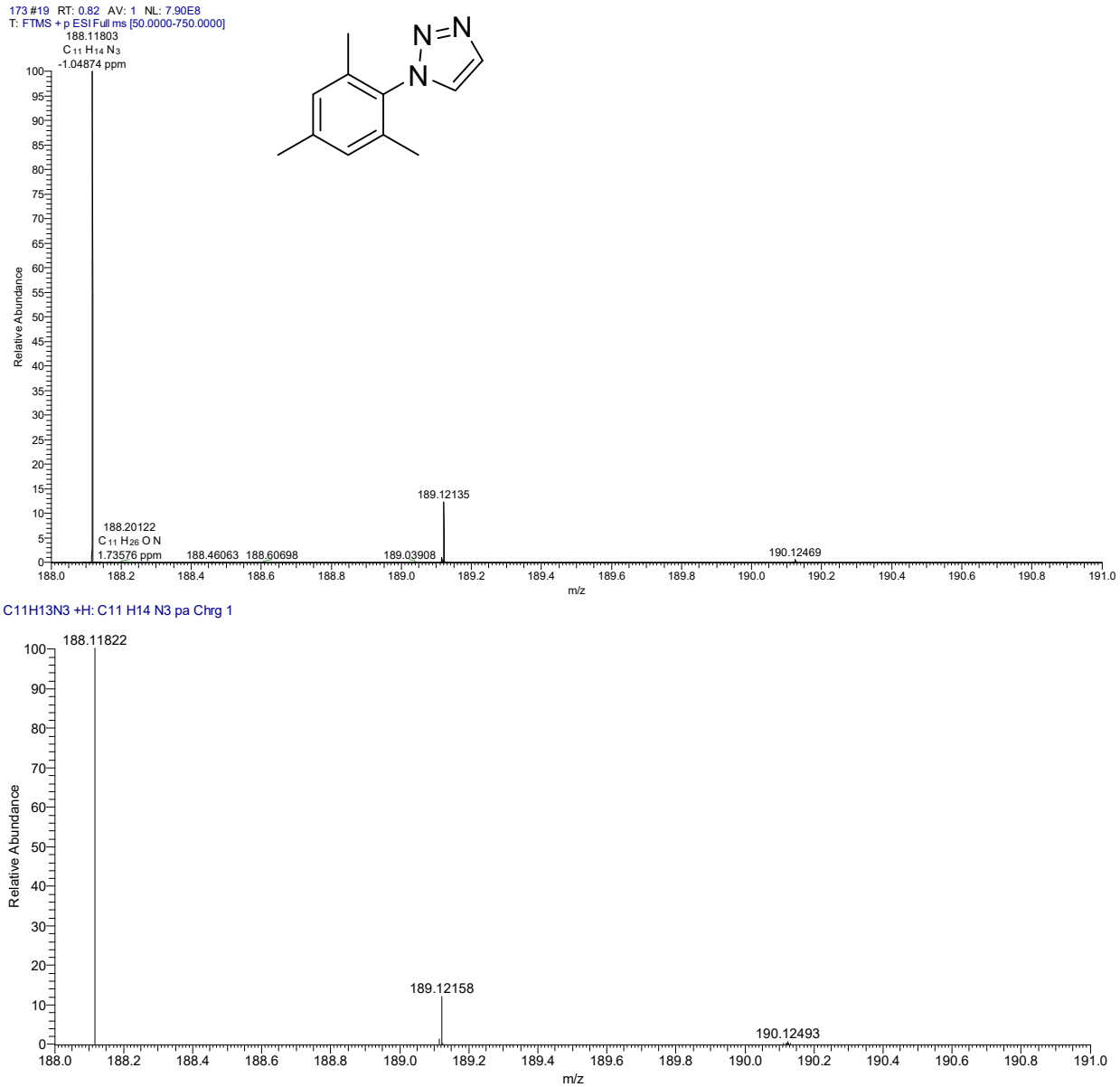


Figure S57. HRMS spectrum of 2,4,6-trimethylphenyl-1*H*-1,2,3-triazole (**15a**).

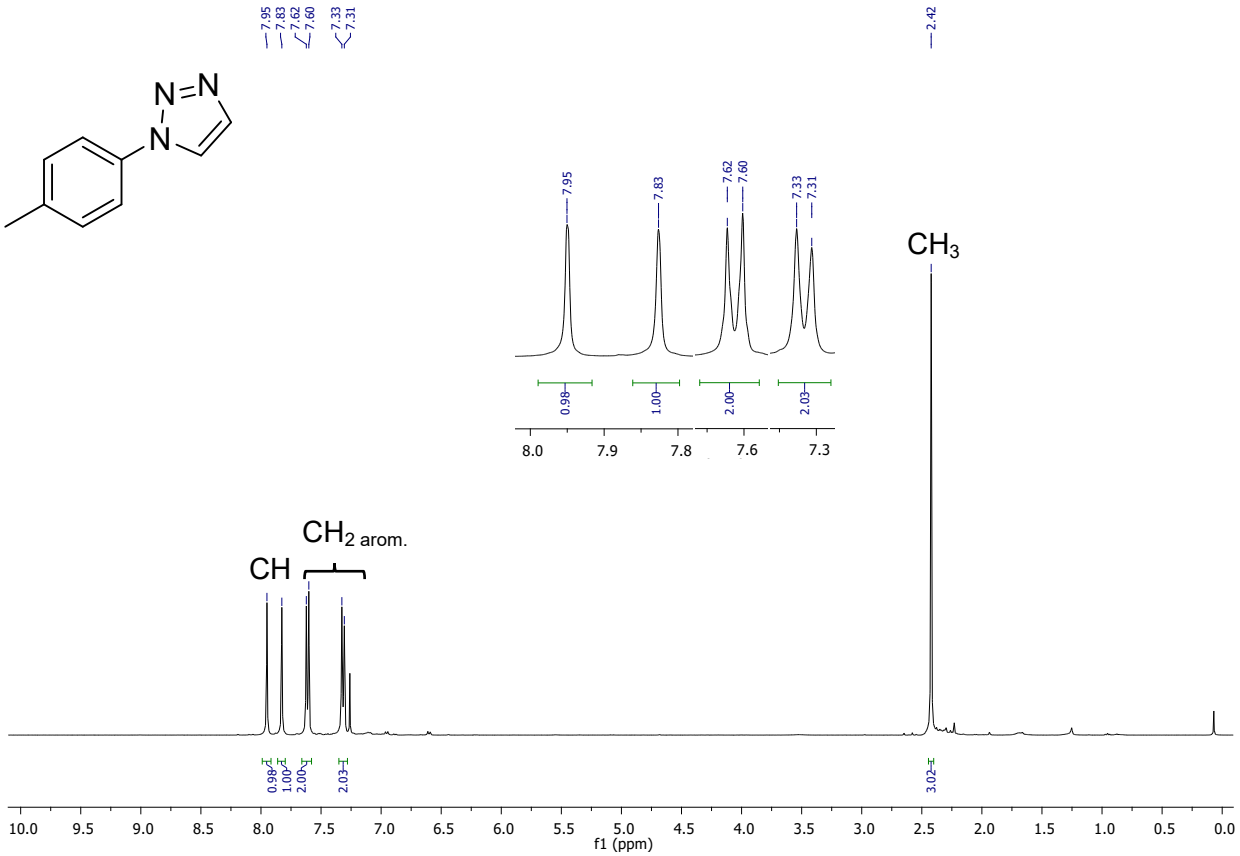


Figure S58. ^{1}H NMR spectrum (400 MHz, DCl_3) of 4-methylphenyl-1*H*-1,2,3-triazole (**16a**).

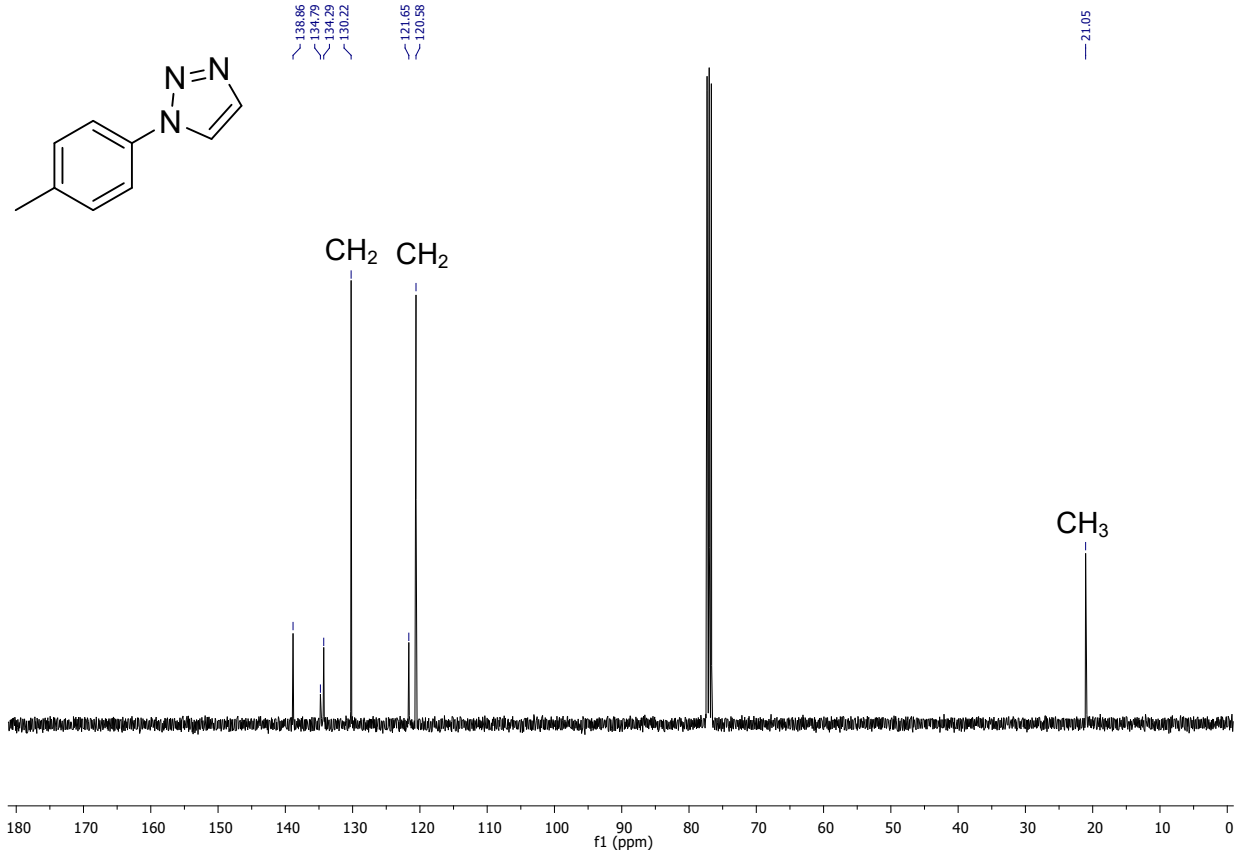


Figure S59. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 4-methylphenyl-1*H*-1,2,3-triazole (**16a**).

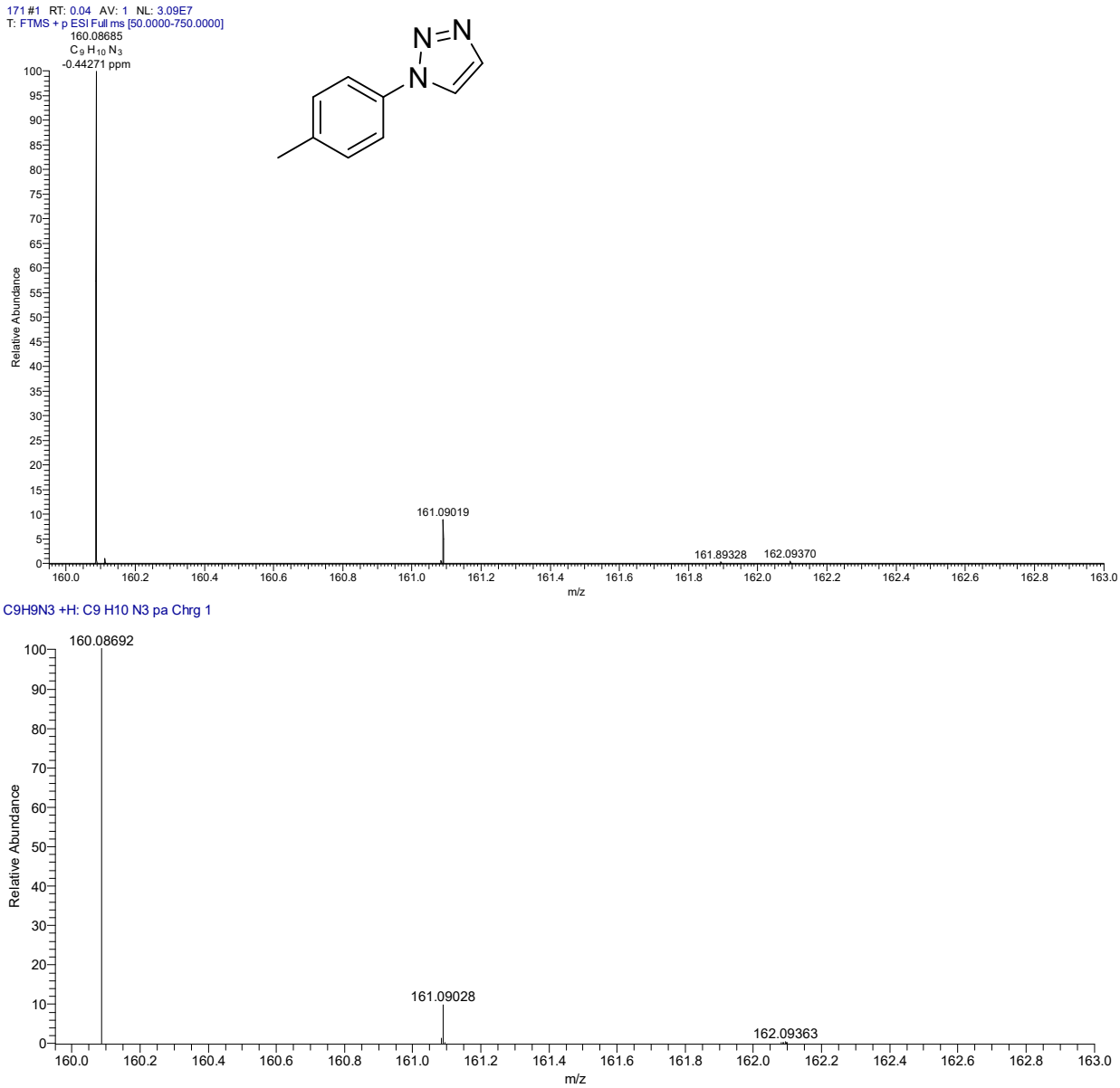


Figure S60. HRMS spectrum of 4-methylphenyl-1*H*-1,2,3-triazole (**16a**).

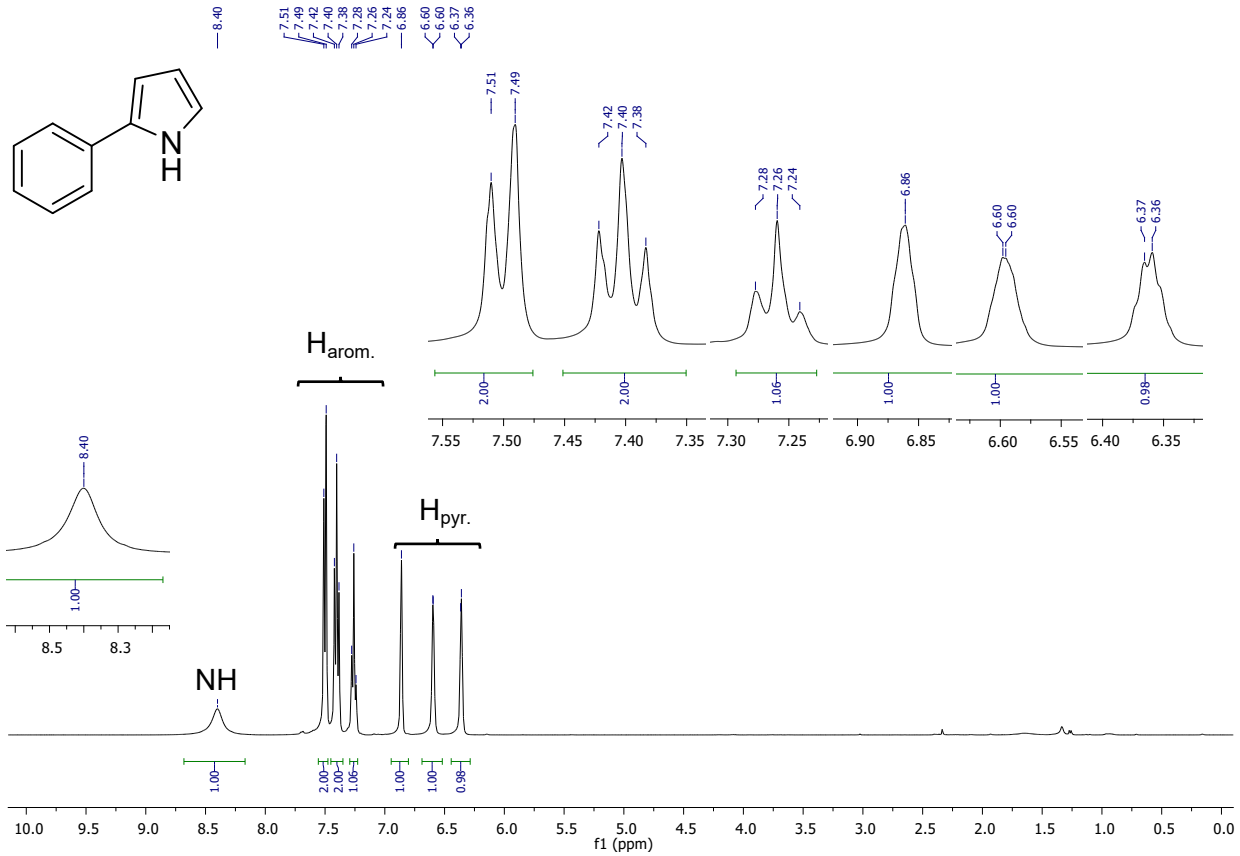


Figure S61. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 2-phenyl-1*H*-pyrrole (**20**).

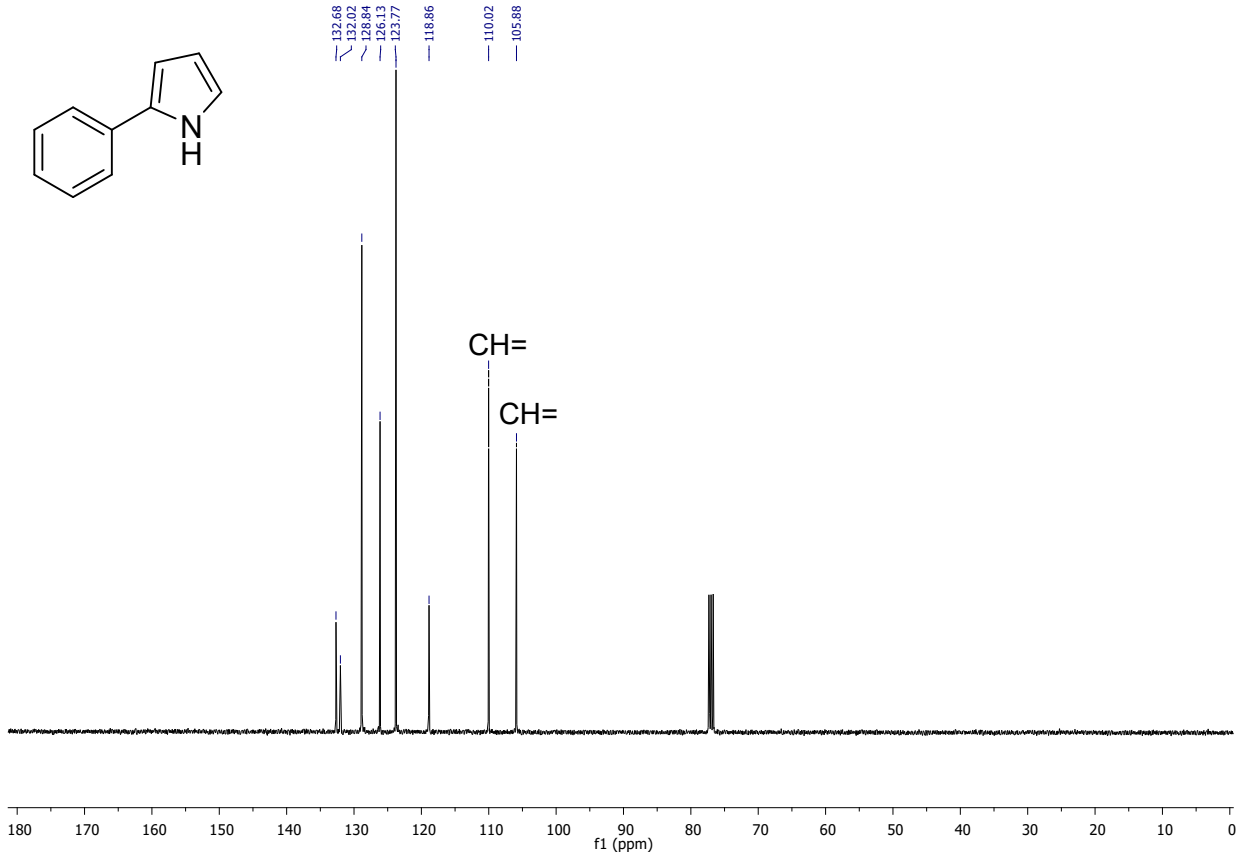


Figure S62. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 2-phenyl-1*H*-pyrrole (**20**).

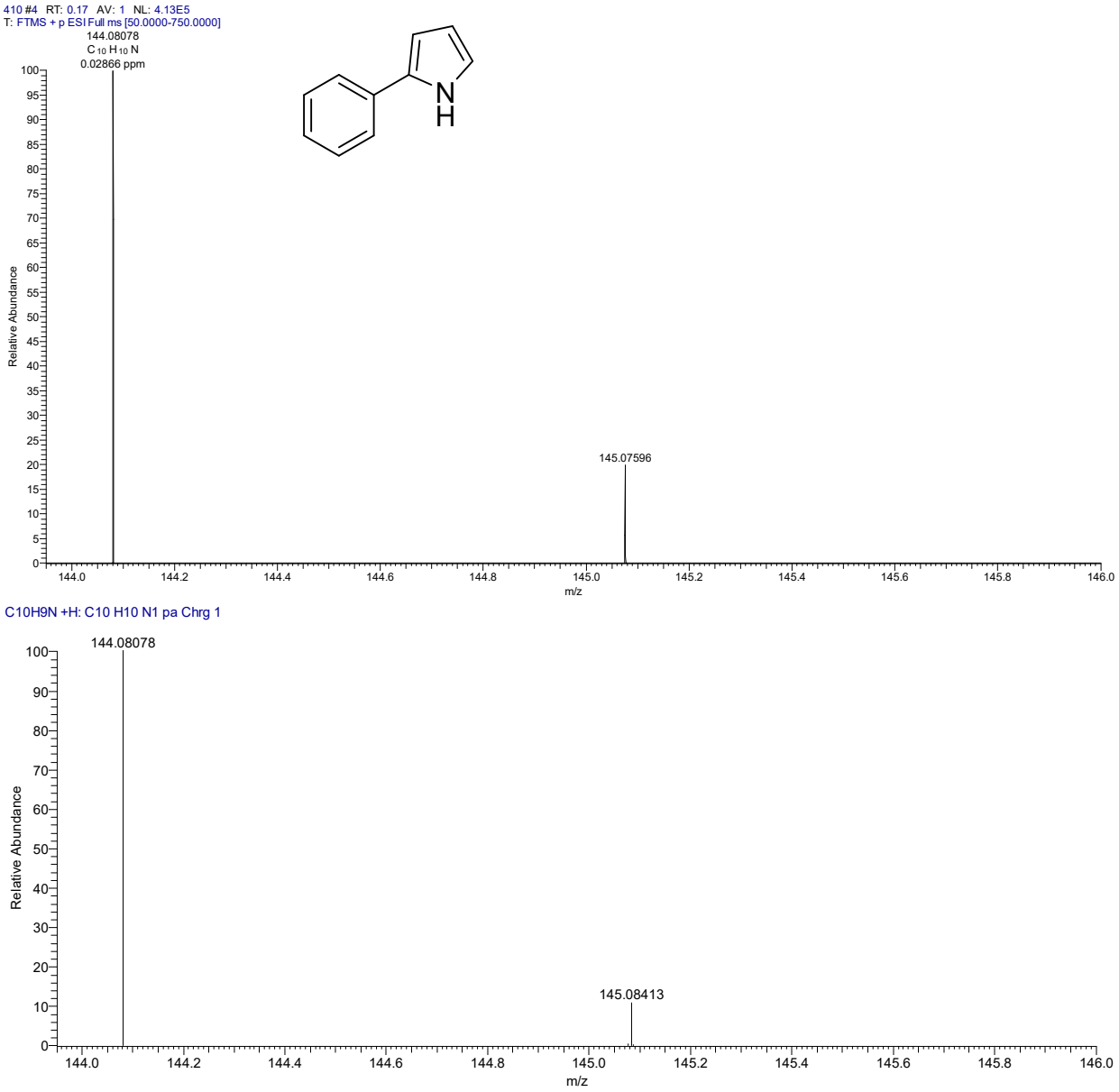


Figure S63. HRMS spectrum of 2-phenyl-1*H*-pyrrole (**20**).

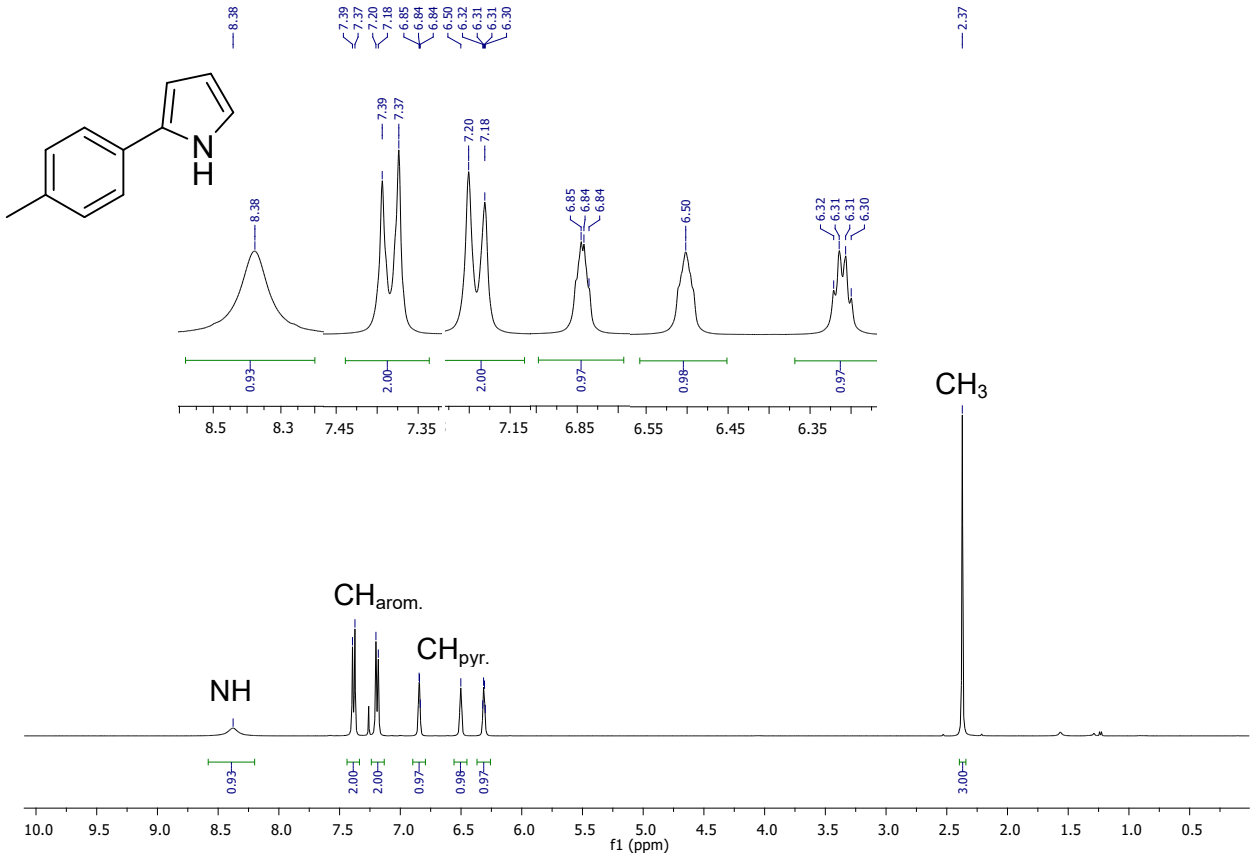


Figure S64. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 2-(4-methylphenyl)-1*H*-pyrrole (**21**).

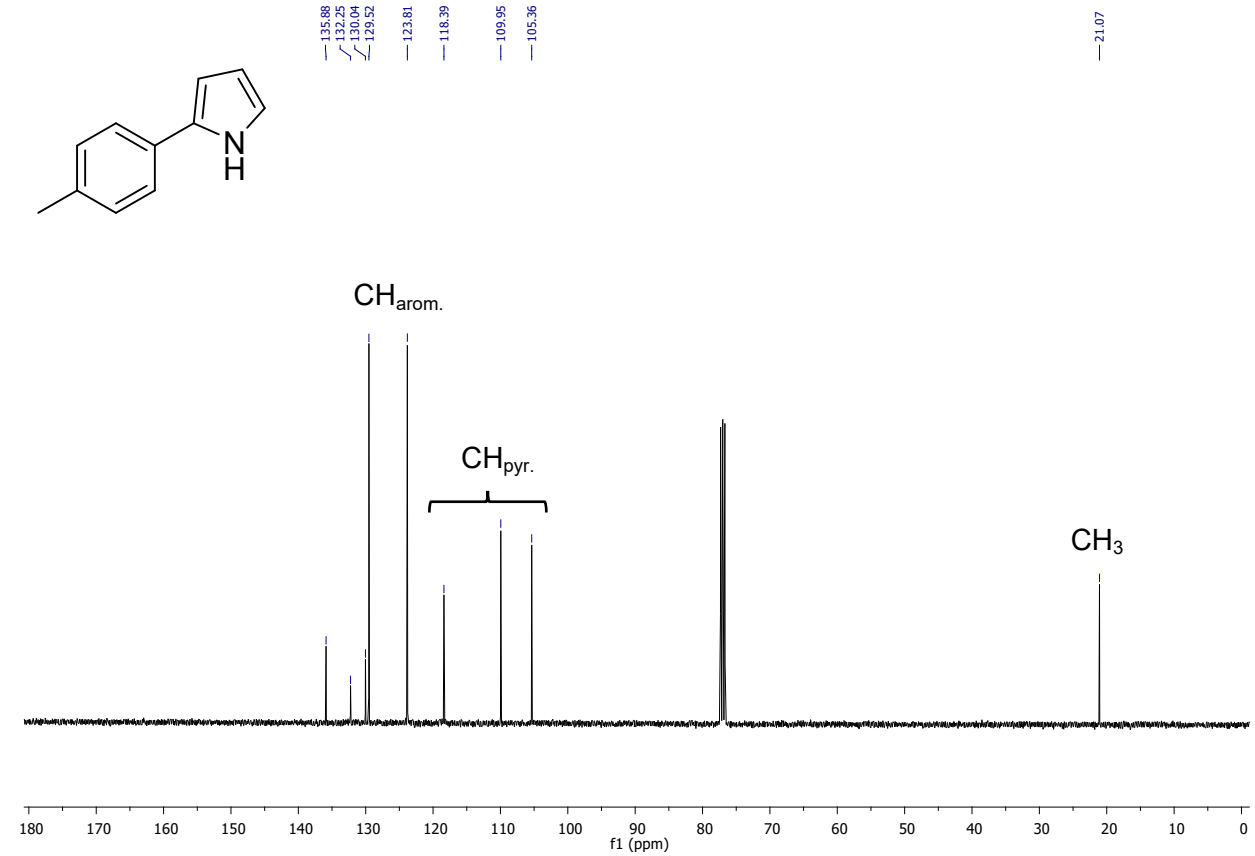


Figure S65. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 2-(4-methylphenyl)-1*H*-pyrrole (**21**).

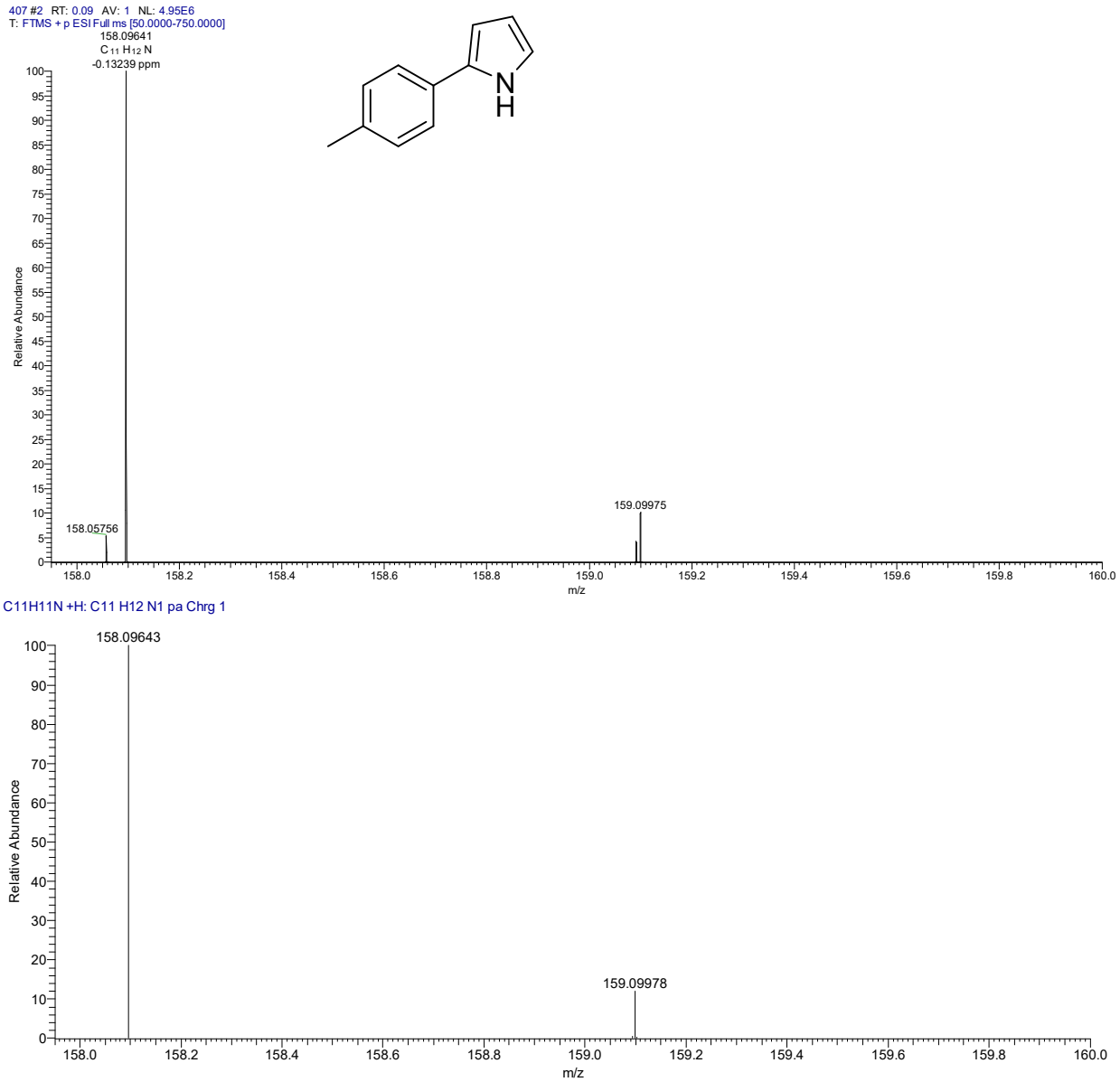


Figure S66. HRMS spectrum of 2-(4-methylphenyl)-1*H*-pyrrole (**21**).

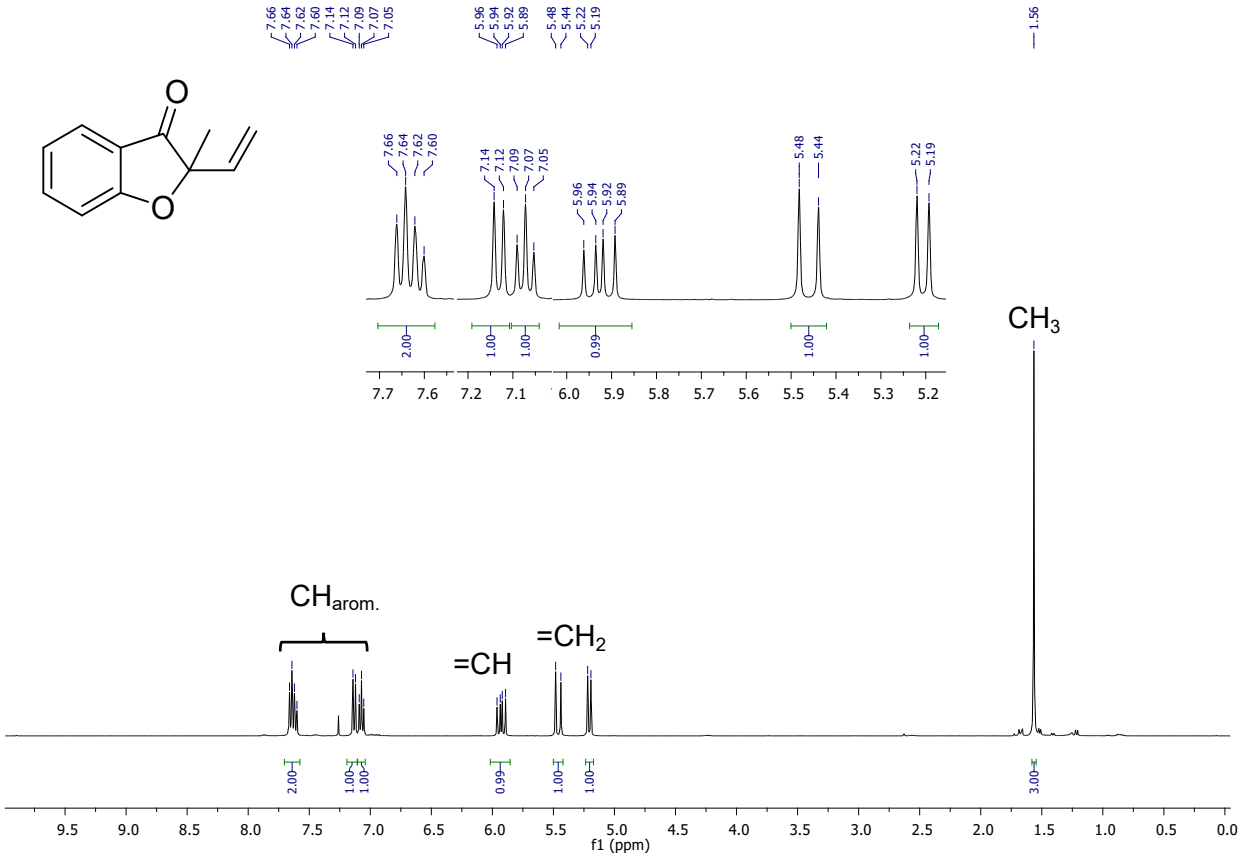


Figure S67. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 2-methyl-2-vinylbenzofuran-3(2*H*)-one (**22a**).

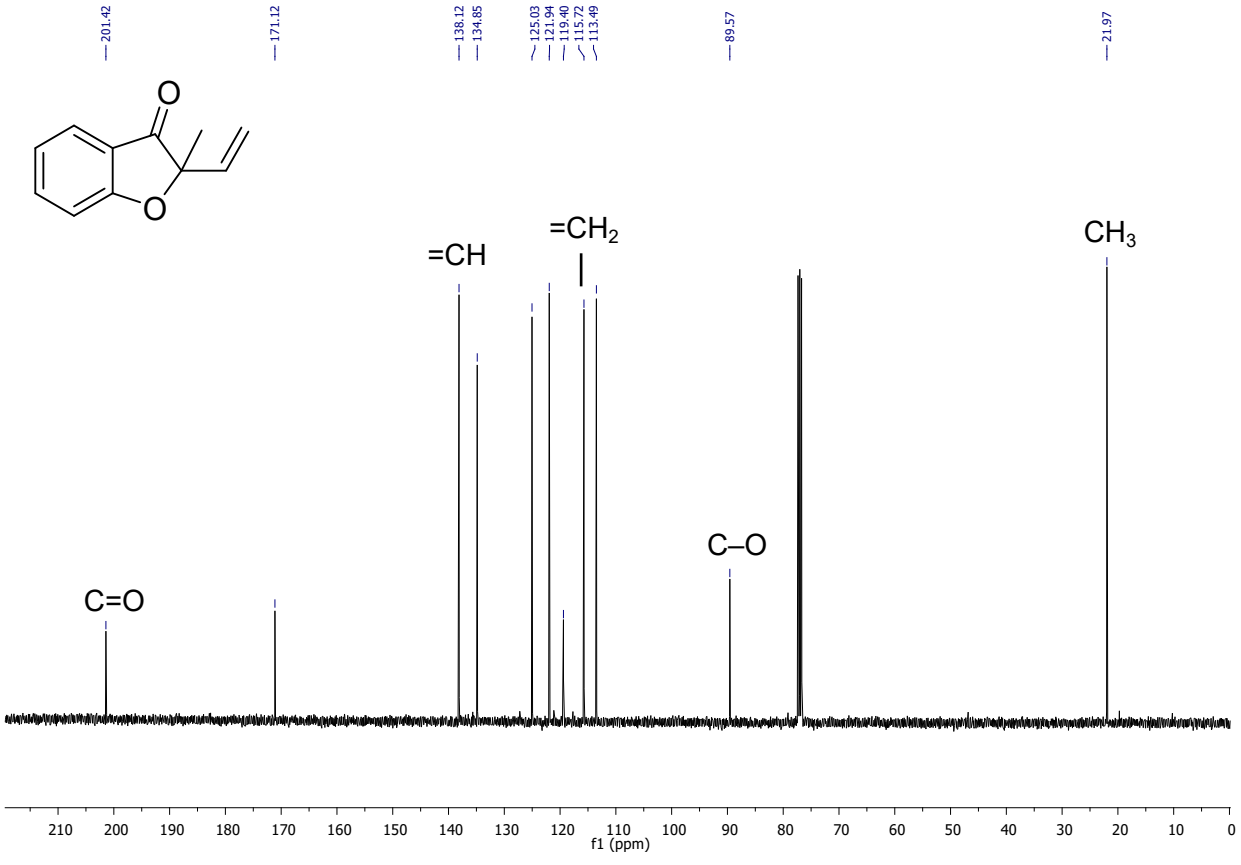


Figure S68. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 2-methyl-2-vinylbenzofuran-3(2*H*)-one (**22a**).

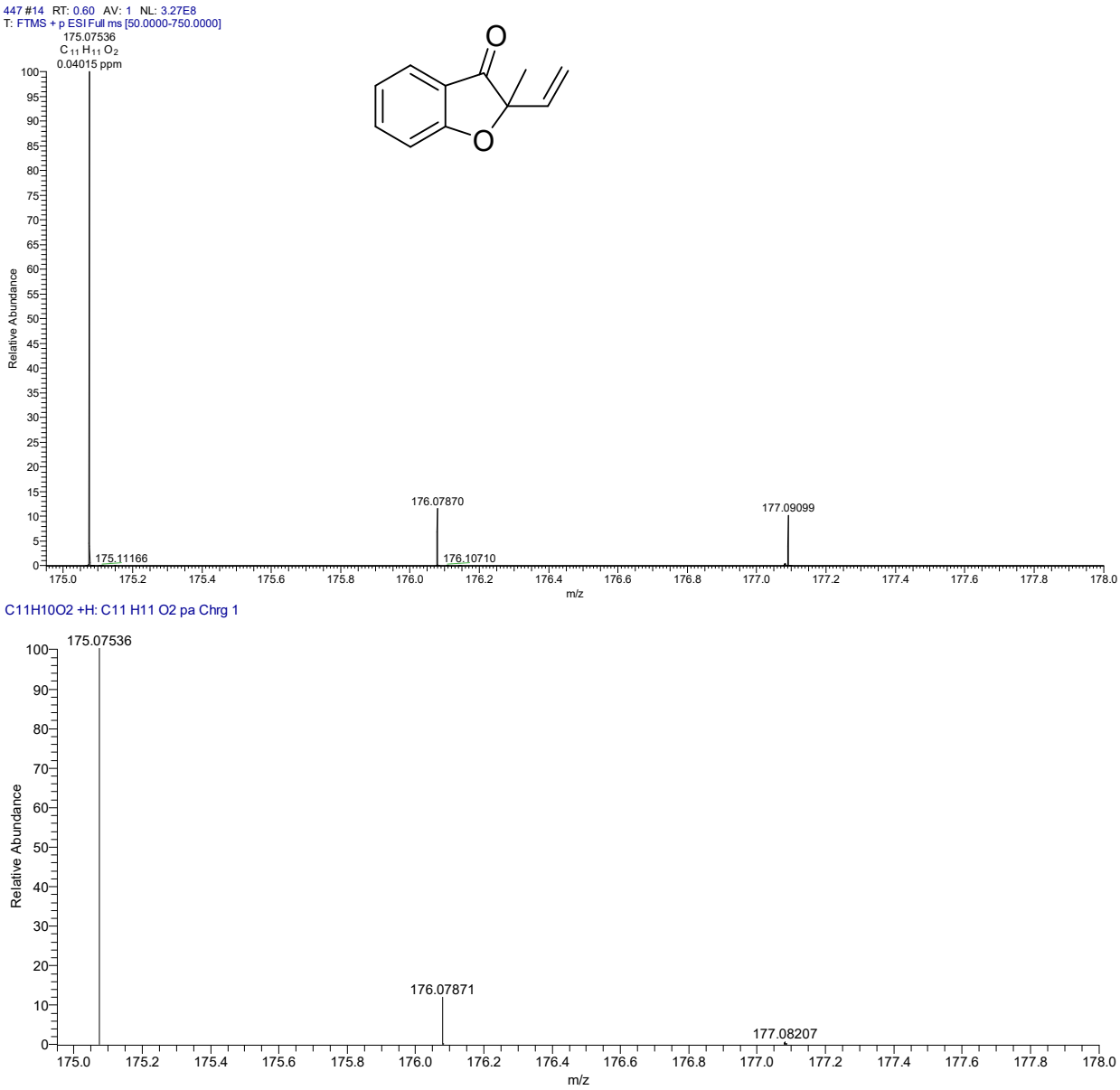


Figure S69. HRMS spectrum of 2-methyl-2-vinylbenzofuran-3(2*H*)-one (**22a**).

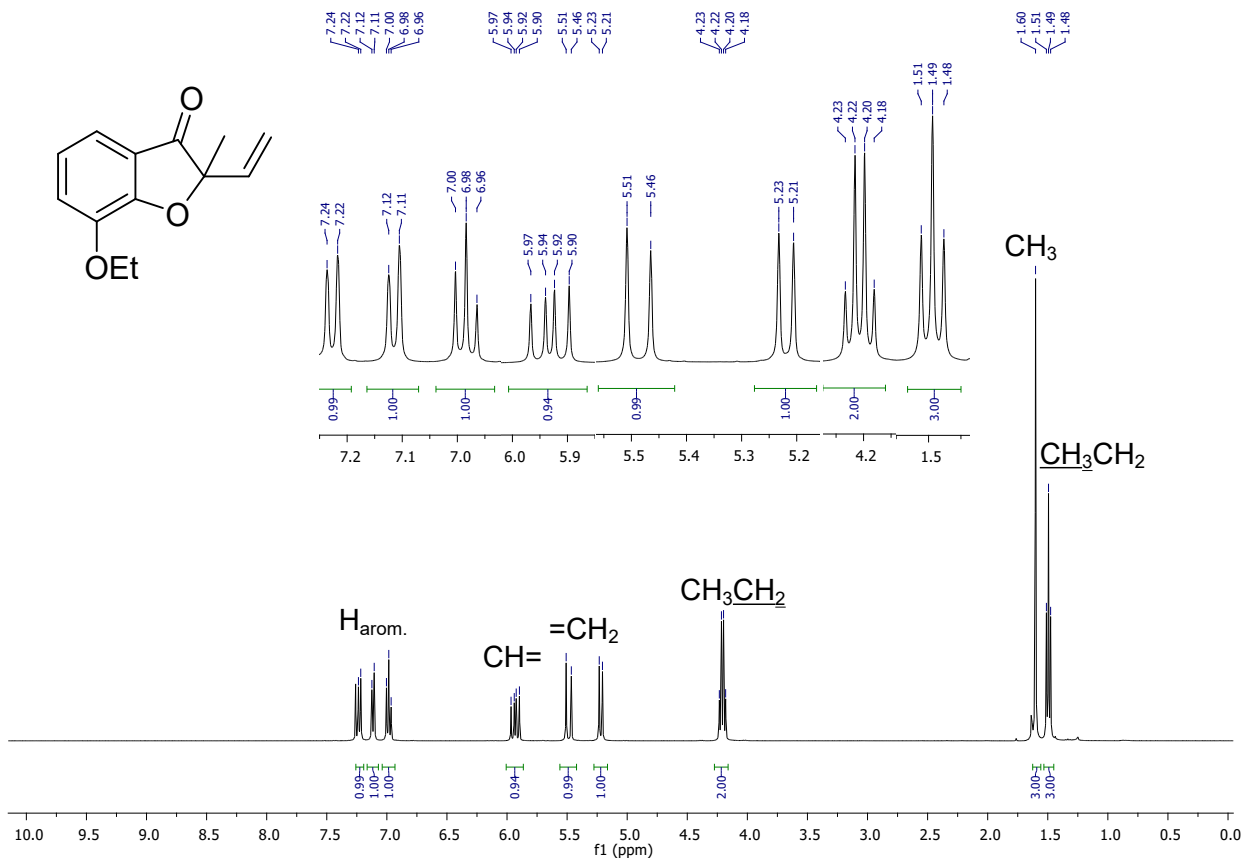


Figure S70. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 7-ethoxy-2-methyl-2-vinylbenzofuran-3(2*H*)-one (**23a**).

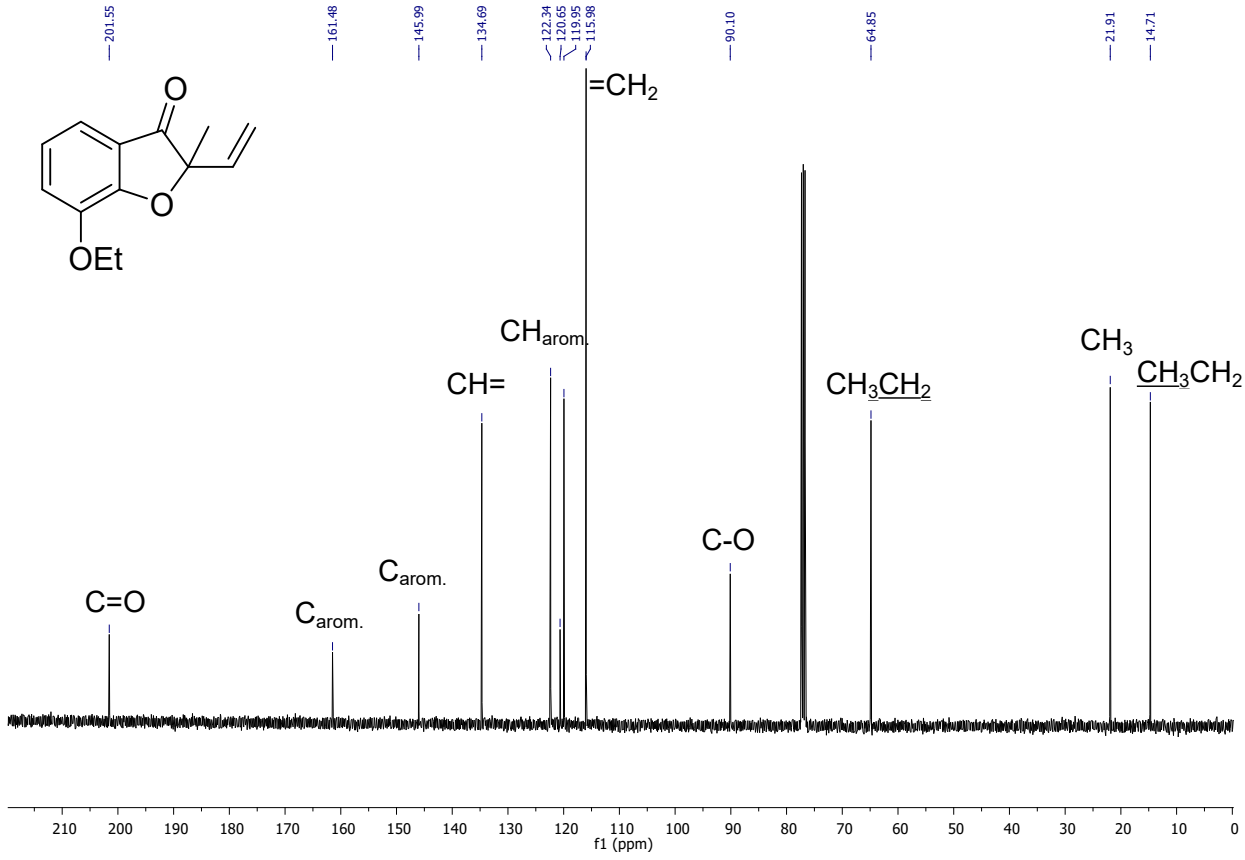


Figure S71. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 7-ethoxy-2-methyl-2-vinylbenzofuran-3(2*H*)-one (**23a**).

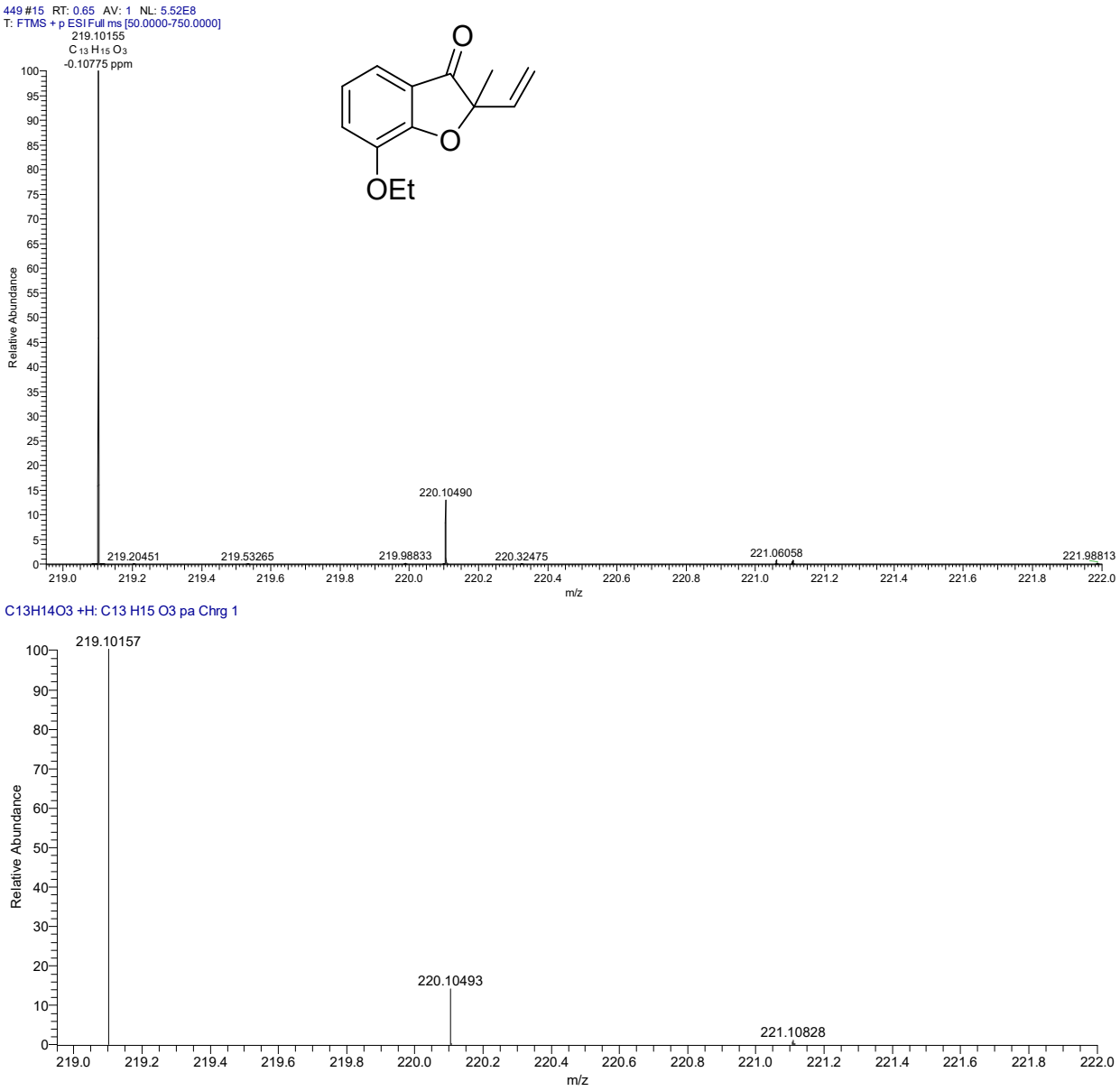


Figure S72. HRMS spectrum of 7-ethoxy-2-methyl-2-vinylbenzofuran-3(2*H*)-one (**23a**).

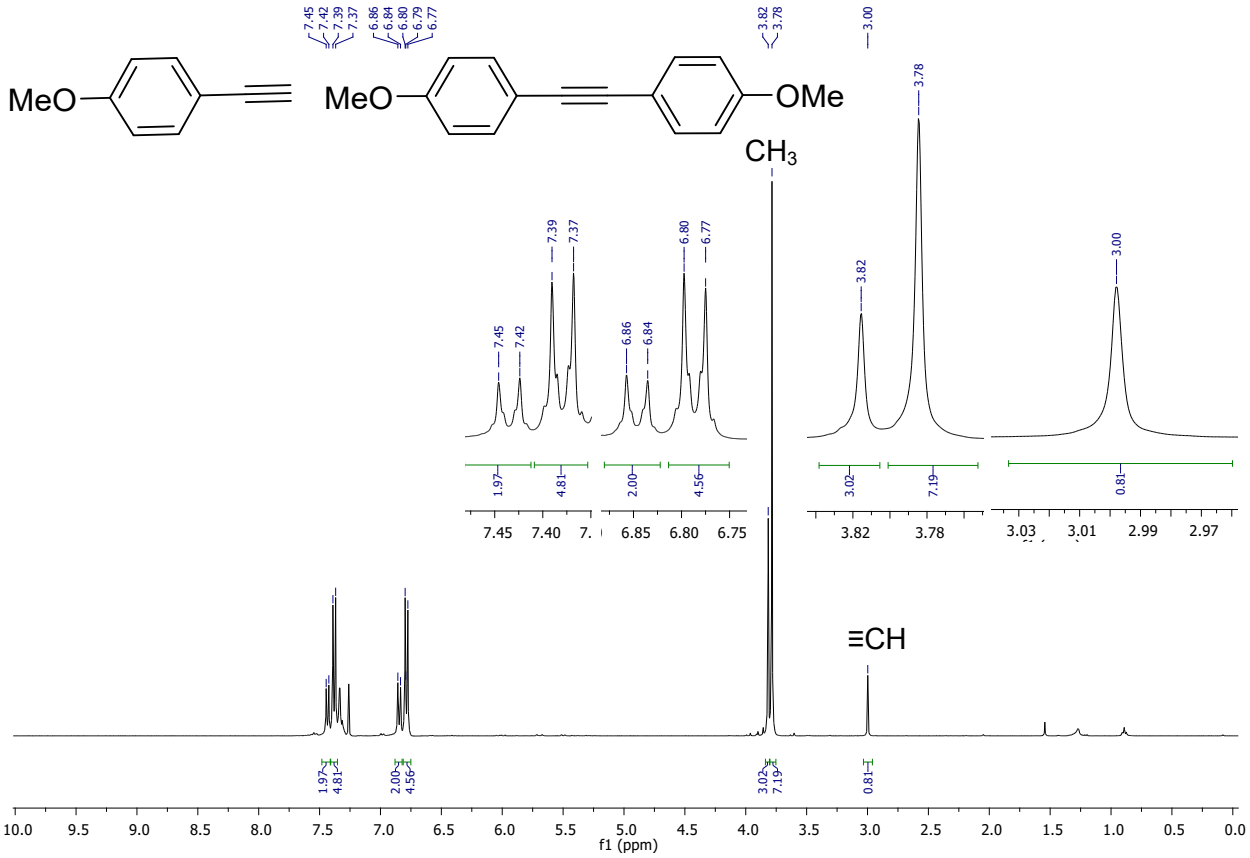


Figure S73. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of reaction mixture for 4-anisyl iodine with acetylene.

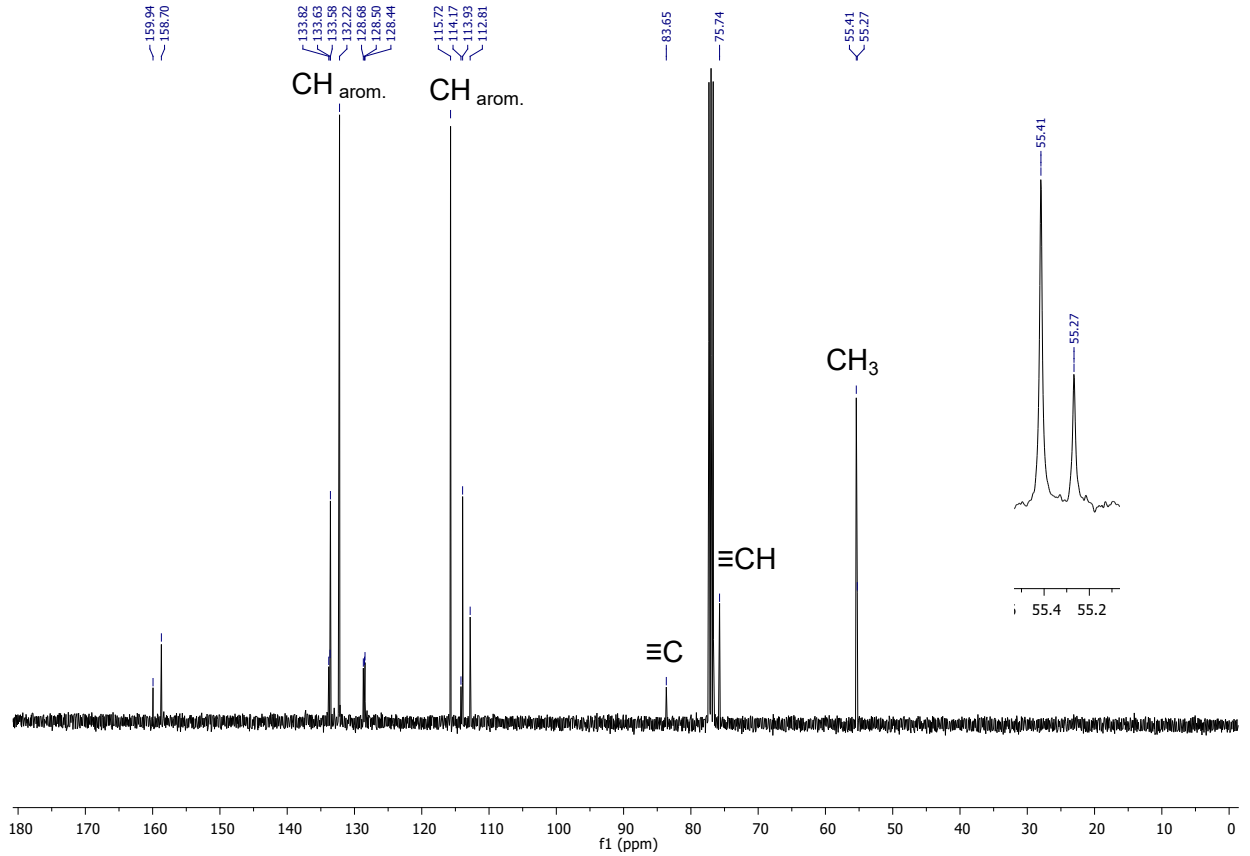


Figure S74. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of reaction mixture for 4-anisyl iodine with acetylene from BaC_2.

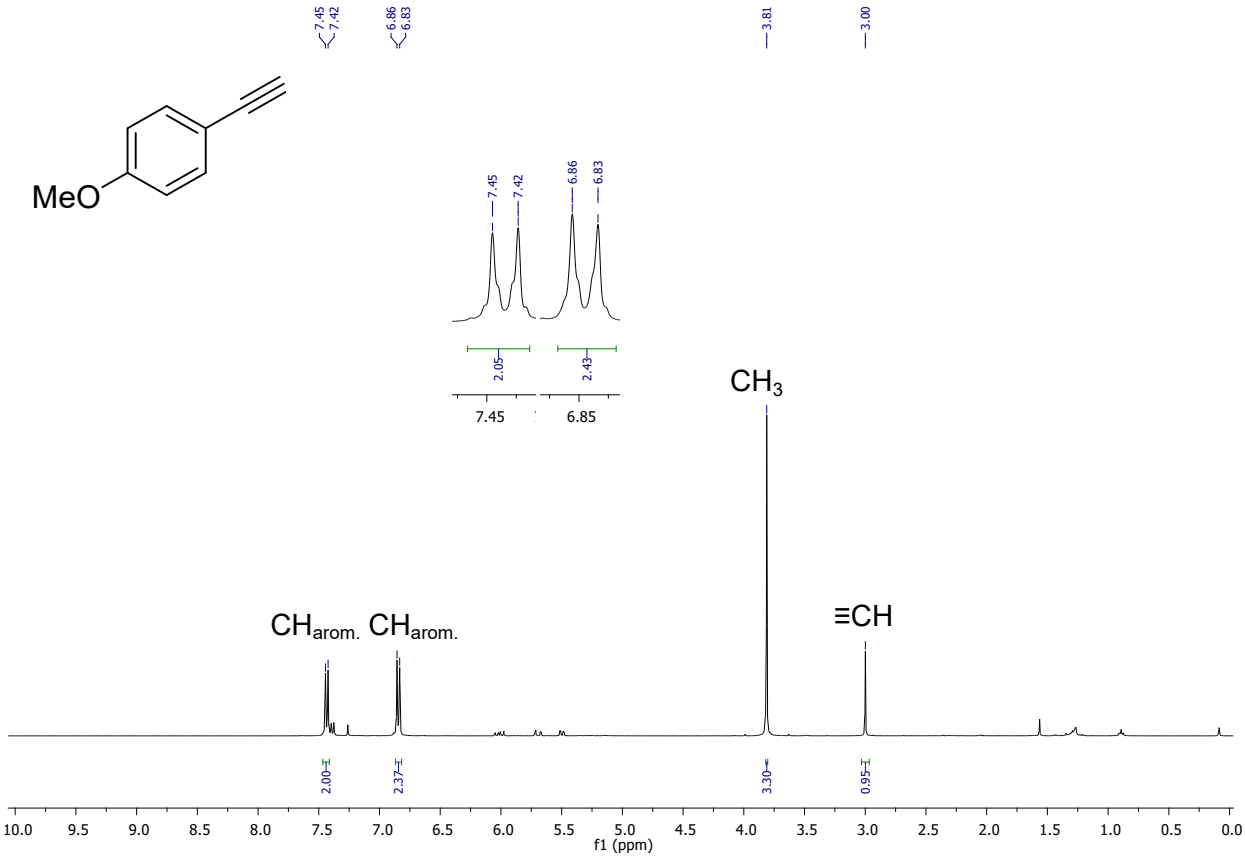


Figure S75. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4-anisylacetylene (**25**).

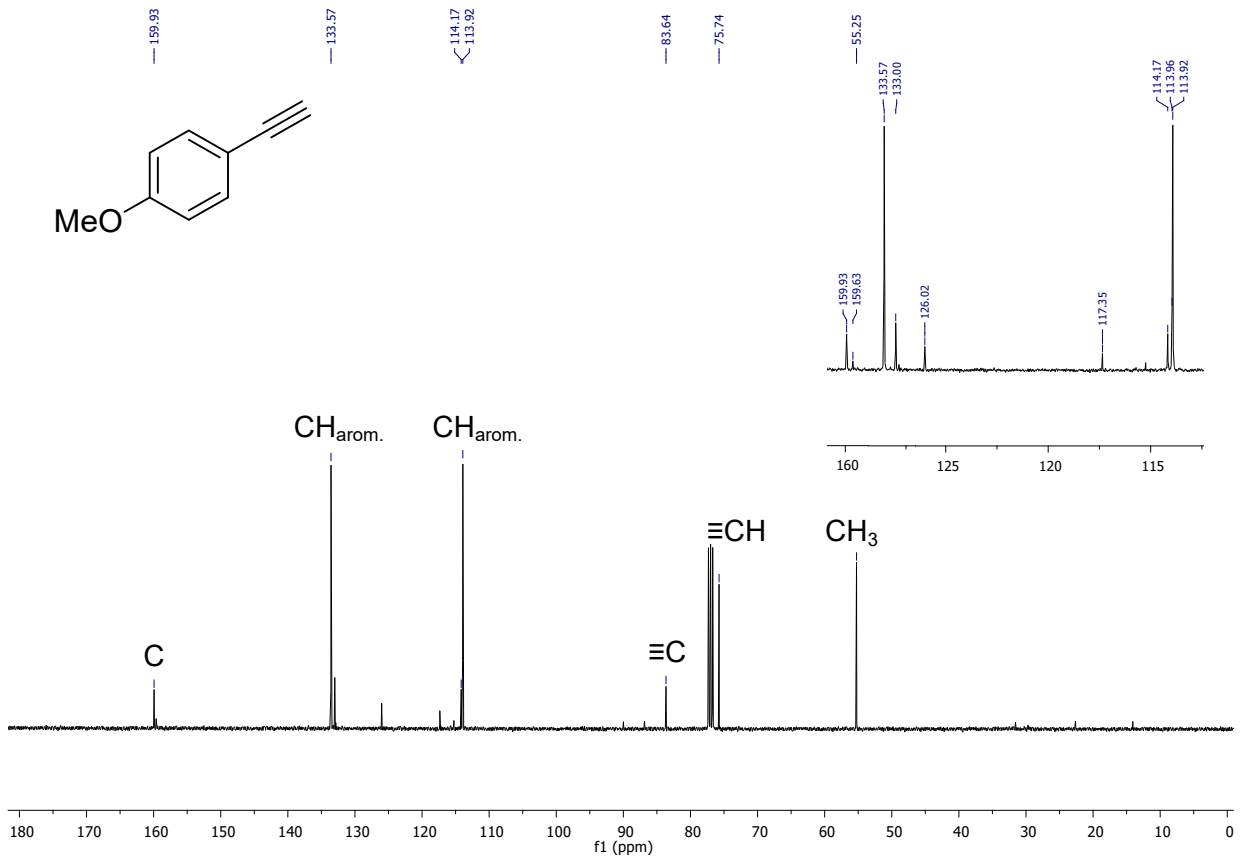


Figure S76. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 4-anisylacetylene (**25**).

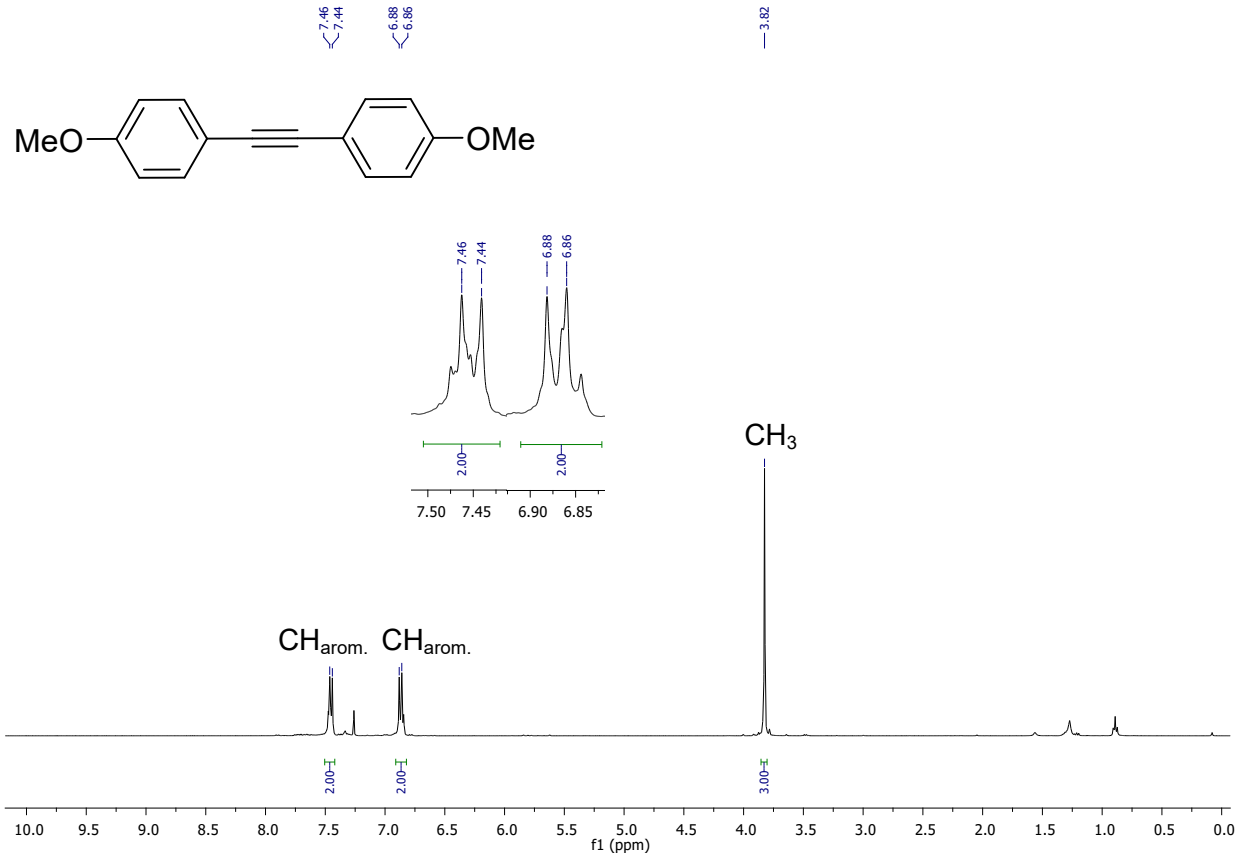


Figure S77. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1,2-bis(4-anisyl)acetylene (**26**).

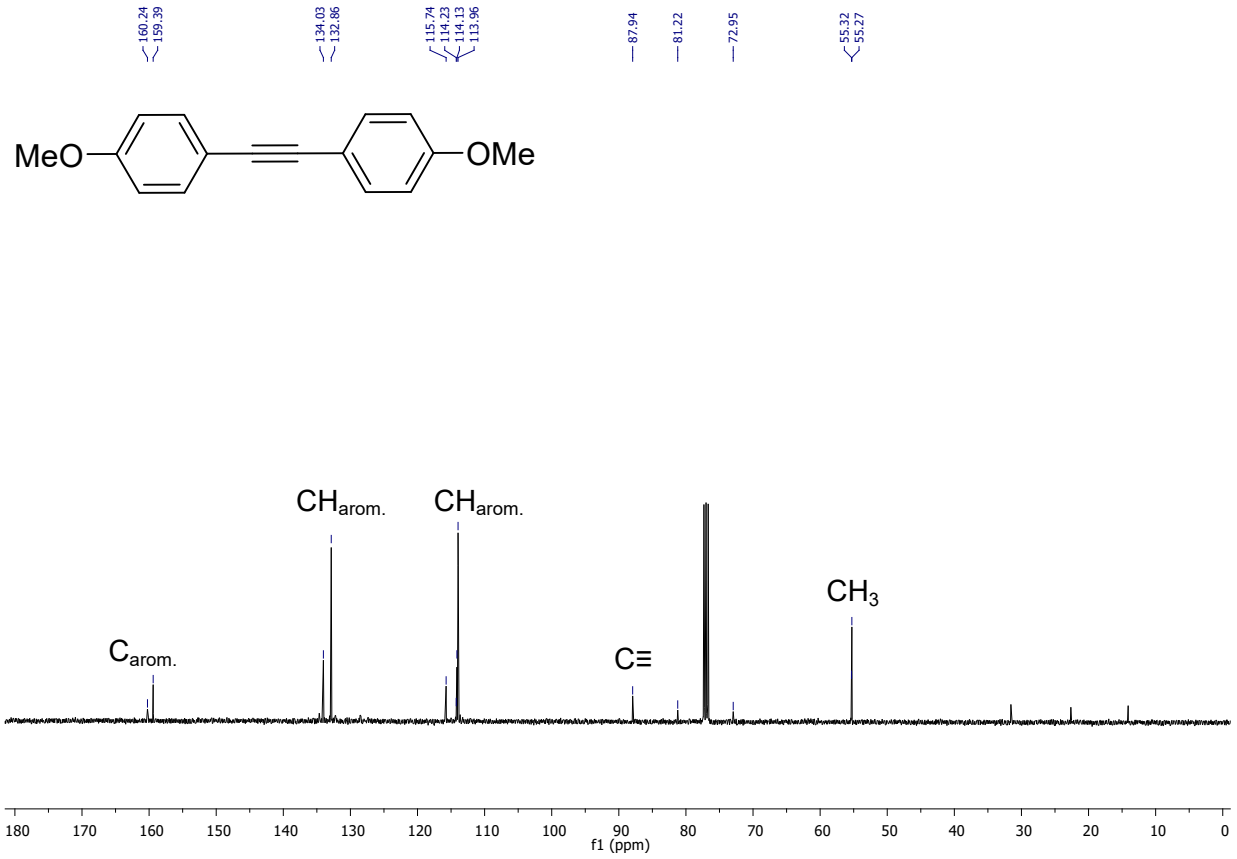


Figure S78. ^{1}H NMR spectrum (101 MHz, $CDCl_3$) of 1,2-bis(4-anisyl)acetylene (**26**).

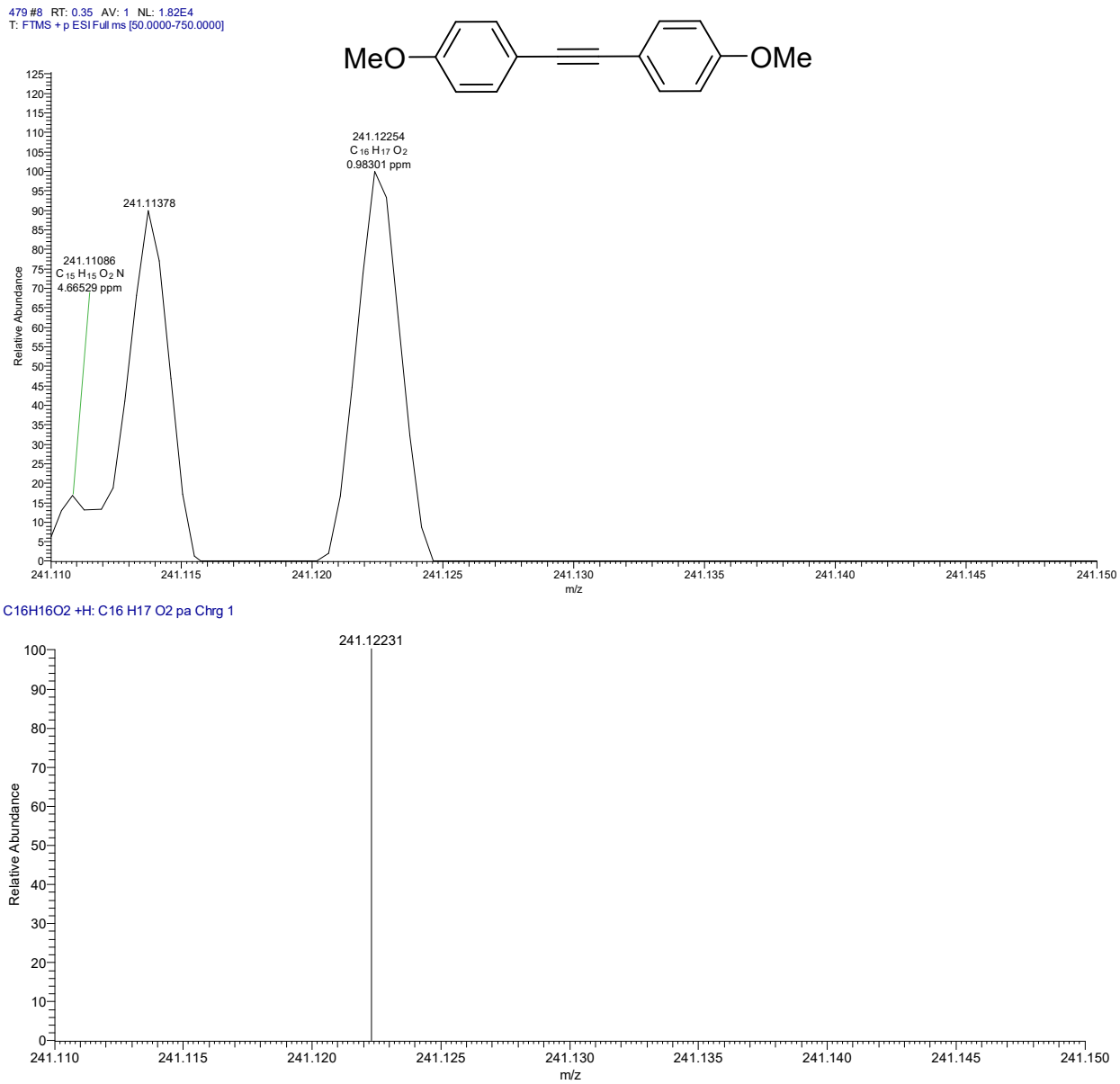


Figure S79. HRMS spectrum of 1,2-bis(4-anisyl)acetylene (**26**).

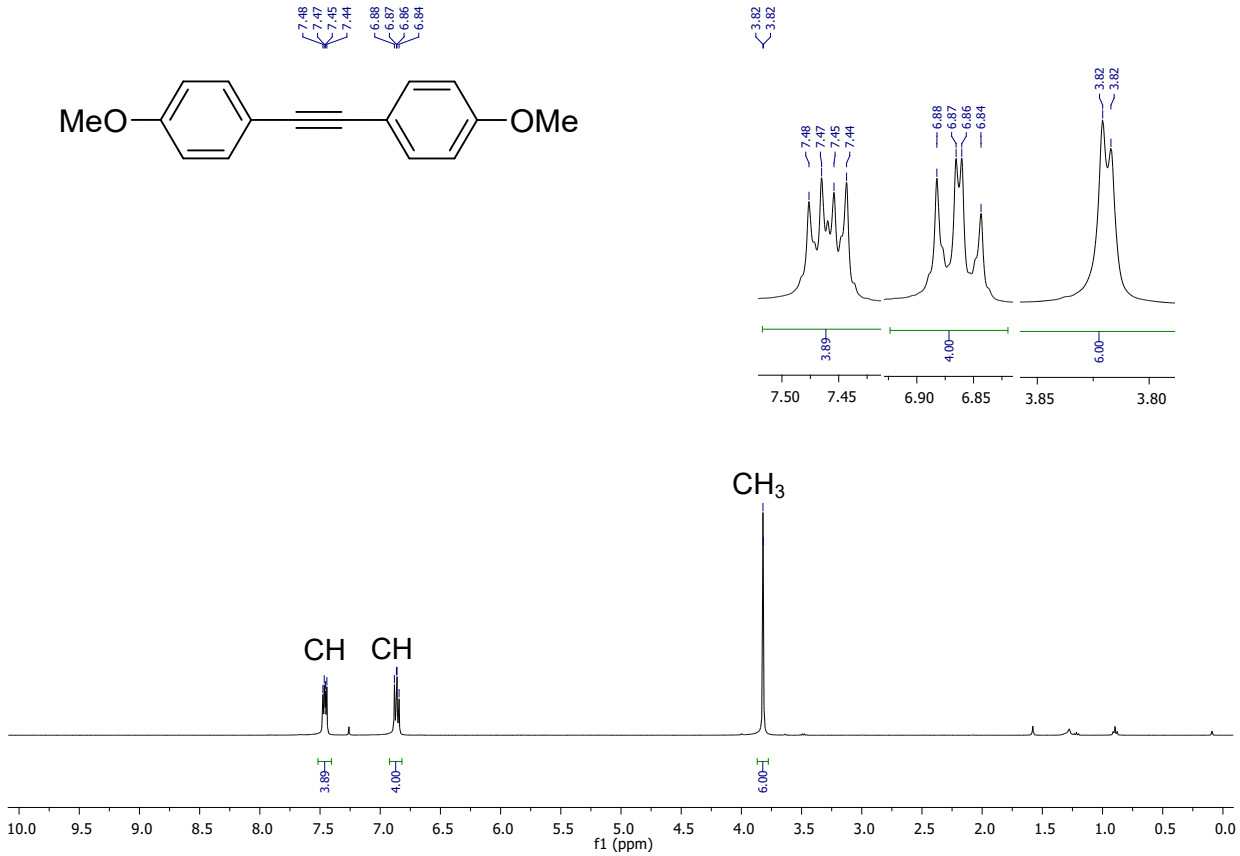


Figure S80. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1,2-bis(4-anisyl)acetylene (**26**) obtained in the presence of $Pd(OAc)_2$/CuI in acetonitrile.

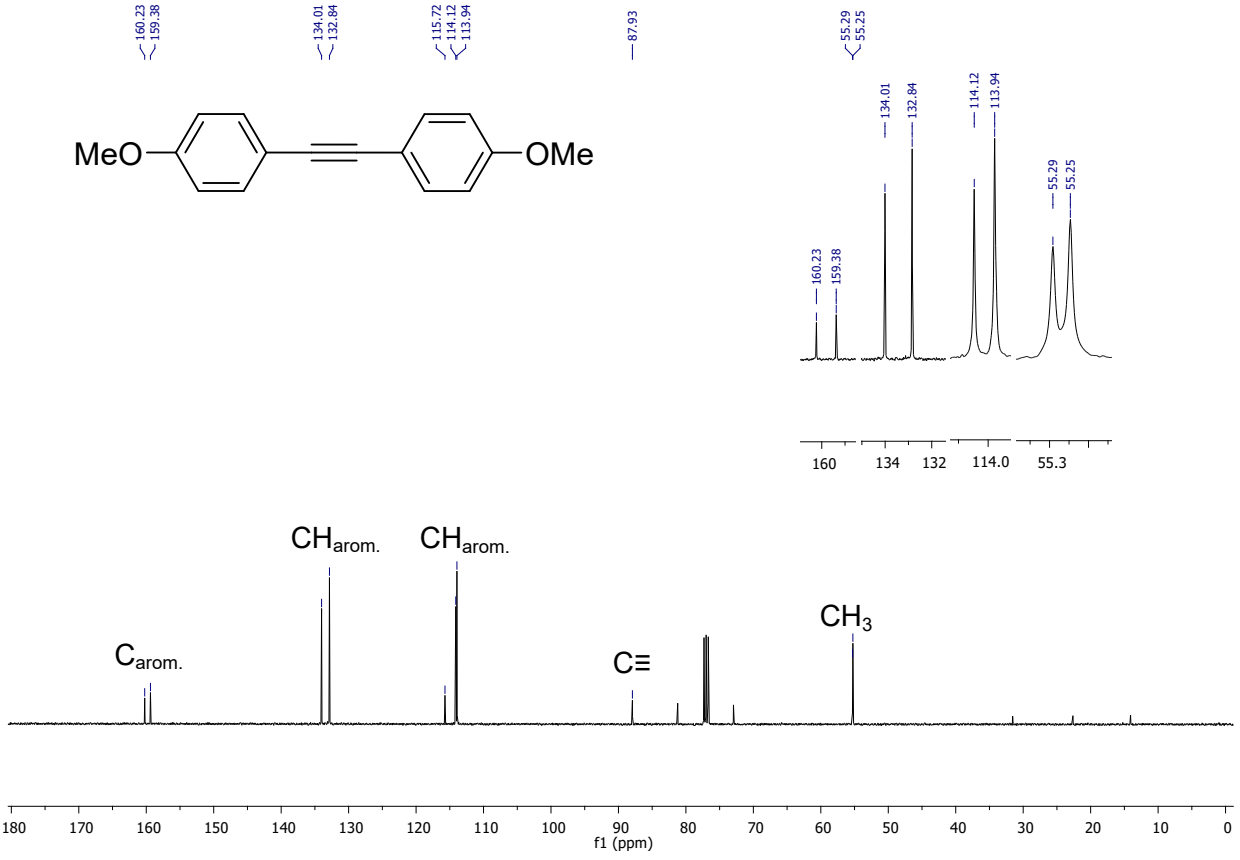
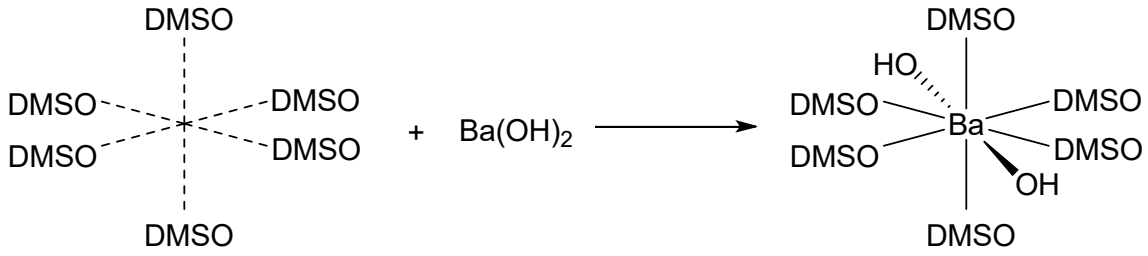


Figure S81. ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of 1,2-bis(4-anisyl)acetylene (**26**) obtained in the presence of $Pd(OAc)_2$/CuI in acetonitrile.

6. Optimized structures and structures for single point energy calculations (in nDMSO cases)

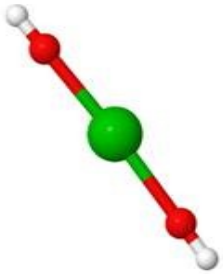
Table S2. Structures of Species from calculation.



Cartesian coordinates | Structure

5

Ba	1.19019704532155	-0.32963824248365	0.27572589004719
O	2.47168342786807	-1.79380159001923	1.75726283017338
O	-0.20975316726140	1.08227235181630	-1.14799521377864
H	2.97381012632182	-2.37162363508677	2.34187090437497
H	-0.76517475936779	1.63673241743689	-1.70645549593646



$Ba(OH)_2$

65

C	-3.65888648855225	2.54563843048598	2.61797886337007
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C	-1.80771979235599	3.62071836450202	0.88493195401081
O	-1.22250499883139	1.44427715957150	2.39432485798641
O	1.57978331682558	-2.00985912383028	-1.11713637044963
S	1.22935092313349	-3.16250669999268	-2.07028908369274
C	-0.14829925482831	-4.08071726922353	-1.32283930971899
C	2.55384808091608	-4.40355606840791	-1.81383457159369
O	2.30572008252779	0.26112686376587	1.43414489684686
S	3.34228261208089	1.32716910849602	1.04868403737500
C	2.71173151856648	2.92076548957654	1.66006336489654
C	4.70624538901588	1.10809672744170	2.25711777184724
O	-3.09322562503746	0.98832335359130	-0.50575460067508
S	-4.10682973578388	-0.02806542159864	-1.07854438156325
C	-5.51274584462437	1.06811192214952	-1.56493285980717
C	-3.58325129183429	-0.42713031476119	-2.78003814844231
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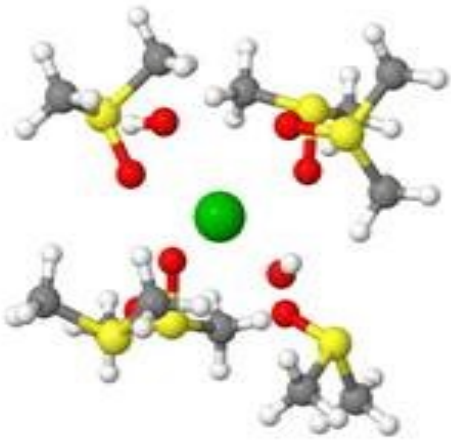
H	-0.77844820860324	3.49309509803319	0.51227860978297
H	-2.49287228873721	3.10003920156005	0.20939049570834
H	-4.18434167630902	3.50612518428031	2.57990429838044
H	-3.92930874913485	1.90789062476544	1.77117234872122
H	-3.86801303758484	2.04218382368622	3.56565095499976
H	3.49163490717952	3.68149832228165	1.53920073560880
H	1.85554015740972	3.11714086397656	0.99275008721184
H	2.41665152432639	2.81384445091615	2.70895369746850
H	5.45007357591413	1.89924526691982	2.11435479412259
H	4.30088747018123	1.13787833723944	3.27330619864797
H	5.16235915573413	0.13331932479105	2.06385360950443
H	-6.27615155291584	0.48064057318925	-2.08719874247834
H	-5.93635252953415	1.48166505725032	-0.64536199526090
H	-5.14751903070451	1.88085151337833	-2.20081245846654
H	-4.41475796360299	-0.93226485580149	-3.28489530007773
H	-3.30677894604140	0.49723088483042	-3.29553770031684
H	-2.73363278071498	-1.09992957235234	-2.66497569967361
H	-0.44644133632800	-4.87812539786271	-2.01381143098044



$Ba(OH)_2 \cdot 6DMSO$

bicapped octahedron

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H	3.48729692582104	-3.97725211720871	-2.19139758489161
H	2.64369698430850	-4.60583102174850	-0.74204597427156
S	0.56418670422826	-1.09301750032915	3.67377551898111
C	-0.35722414906851	-1.88395590456946	5.04729434848524
H	-0.45737376776932	-2.95530092102808	4.84778046359475
H	0.16231245433921	-1.70496671653803	5.99491451379815
H	-1.34504598186848	-1.41706682170357	5.07100103171437
C	2.08019211314016	-2.11098078152200	3.79454096683402
H	1.81439031502122	-3.16937405173255	3.71096948506946
H	2.59246047027605	-1.90615330924753	4.74119279206206
H	2.69956900757837	-1.80336005784092	2.94922602326881
O	-0.13850202648009	-1.57523707416553	2.40537316683948
S	0.74519808870793	0.93804324436353	-3.78579646544688
C	2.33735663678286	0.93985316751469	-2.89282712996024
H	2.60024058993172	-0.08867548786250	-2.62600184841895
H	3.09972145867612	1.40697361215220	-3.52676164220741
H	2.14838468763361	1.53641600186374	-1.98601845274924
C	1.23422356250773	-0.15057020092578	-5.17783840149947
H	1.56861728662807	-1.11205633221666	-4.77696641628635
H	2.02599601323209	0.33133698886793	-5.76114993023303
H	0.34835116883185	-0.29711740201005	-5.80144297573140
O	-0.23710833126981	0.10565490615225	-2.95594636305191
Ba	-0.34148566845539	-0.01071798354939	0.00118552032994
O	-2.14567128787722	-1.93378356295619	-0.67290085275508
O	0.79618245698730	2.43781897012556	-0.57550835320779
H	-2.63314714167652	-2.42512742865927	0.00593532975191
H	0.58947168396107	3.09348969936593	-1.25928259187340

60

C	-3.65888648855225	2.54563843048598	2.61797886337007
S	-1.85274404752678	2.83663736425162	2.53408586666201
C	-1.80771979235599	3.62071836450202	0.88493195401081
O	-1.22250499883139	1.44427715957150	2.39432485798641
O	1.57978331682558	-2.00985912383028	-1.11713637044963
S	1.22935092313349	-3.16250669999268	-2.07028908369274
C	-0.14829925482831	-4.08071726922353	-1.32283930971899
C	2.55384808091608	-4.40355606840791	-1.81383457159369
O	2.30572008252779	0.26112686376587	1.43414489684686
S	3.34228261208089	1.32716910849602	1.04868403737500
C	2.71173151856648	2.92076548957654	1.66006336489654
C	4.70624538901588	1.10809672744170	2.25711777184724
O	-3.09322562503746	0.98832335359130	-0.50575460067508
S	-4.10682973578388	-0.02806542159864	-1.07854438156325
C	-5.51274584462437	1.06811192214952	-1.56493285980717
C	-3.58325129183429	-0.42713031476119	-2.78003814844231
H	-2.06994798321736	4.67883285920788	0.99828636341747
H	-0.77844820860324	3.49309509803319	0.51227860978297
H	-2.49287228873721	3.10003920156005	0.20939049570834
H	-4.18434167630902	3.50612518428031	2.57990429838044
H	-3.92930874913485	1.90789062476544	1.77117234872122
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H	3.49163490717952	3.68149832228165	1.53920073560880
H	1.85554015740972	3.11714086397656	0.99275008721184
H	2.41665152432639	2.81384445091615	2.70895369746850
H	5.45007357591413	1.89924526691982	2.11435479412259
H	4.30088747018123	1.13787833723944	3.27330619864797
H	5.16235915573413	0.13331932479105	2.06385360950443
H	-6.27615155291584	0.48064057318925	-2.08719874247834
H	-5.93635252953415	1.48166505725032	-0.64536199526090
H	-5.14751903070451	1.88085151337833	-2.20081245846654
H	-4.41475796360299	-0.93226485580149	-3.28489530007773
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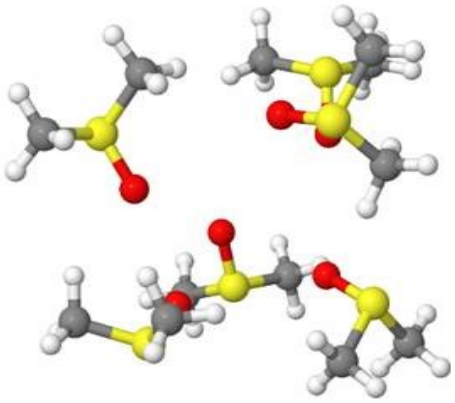

6DMSO

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H	-0.97317047314957	-3.34190941035901	-1.17046826859554
H	2.30932118999218	-5.31801293809353	-2.36449916291235
H	3.48729692582104	-3.97725211720871	-2.19139758489161
H	2.64369698430850	-4.60583102174850	-0.74204597427156
S	0.56418670422826	-1.09301750032915	3.67377551898111
C	-0.35722414906851	-1.88395590456946	5.04729434848524
H	-0.45737376776932	-2.95530092102808	4.84778046359475
H	0.16231245433921	-1.70496671653803	5.99491451379815
H	-1.34504598186848	-1.41706682170357	5.07100103171437
C	2.08019211314016	-2.11098078152200	3.79454096683402
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H	2.59246047027605	-1.90615330924753	4.74119279206206
H	2.69956900757837	-1.80336005784092	2.94922602326881
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S	0.74519808870793	0.93804324436353	-3.78579646544688
C	2.33735663678286	0.93985316751469	-2.89282712996024
H	2.60024058993172	-0.08867548786250	-2.62600184841895
H	3.09972145867612	1.40697361215220	-3.52676164220741
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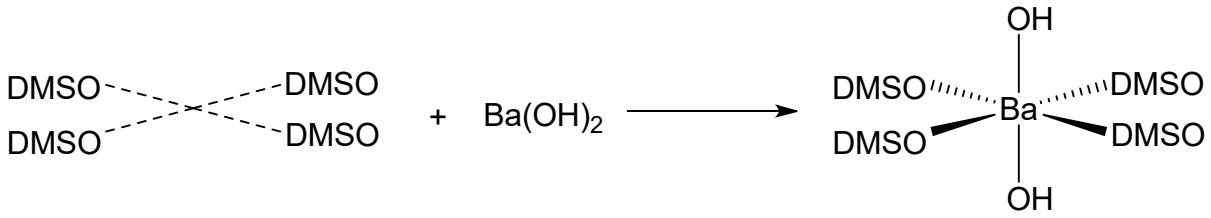
C	1.23422356250773	-0.15057020092578	-5.17783840149947
H	1.56861728662807	-1.11205633221666	-4.77696641628635
H	2.02599601323209	0.33133698886793	-5.76114993023303
H	0.34835116883185	-0.29711740201005	-5.80144297573140
O	-0.23710833126981	0.10565490615225	-2.95594636305191



45

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S	-1.68630352087821	3.18066516613017	0.20924079377873
C	-2.22703913262738	3.32782107497001	-1.51596458511331
O	-1.83813557700729	1.68802241676736	0.59014300815221
O	1.33220900653439	-2.42593715646483	-1.76723479778082
S	1.34597252961822	-3.93994114774846	-1.50542841032015
C	-0.35918620657710	-4.38718593098331	-1.01776411909941
C	2.10045455948802	-4.14218675549844	0.14817016762085
O	1.82847297201322	0.75390498902389	1.31456744923217
S	1.98872153186184	0.60360092804638	2.83428154419289
C	0.29703641003769	0.43597613817881	3.51152782992970
C	2.49634342974154	-1.13190190142967	3.10600591263981
O	-2.51680317408670	-1.49251272061352	-1.24973811872780
S	-3.68955693046527	-1.94645805072741	-0.37044646745651
C	-3.42309236857793	-1.19891543736310	1.27265348445312
C	-5.11202479078162	-0.92303929365788	-0.89600626039974
H	-2.17311973354474	4.38303284007916	-1.80782148725597
H	-1.47670815393929	2.71658911883310	-2.07437302750224
H	-3.24765087179949	2.94200562867240	-1.61373624607810
H	-3.13561543104792	5.05188294169650	0.72511723393839
H	-4.02703198000257	3.48741972044567	0.75671188139153
H	-2.94210591738789	3.93520003412982	2.11159504127835
H	0.36243399540936	0.27945974795321	4.59412231111087
H	-0.22640839874665	1.37158429295397	3.29844960103976
H	-0.18694394933551	-0.40898170755783	3.00122620371639
H	2.53259829432712	-1.33538628852777	4.18190000146186
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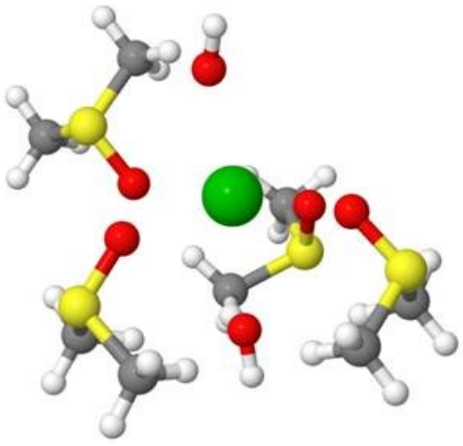

$Ba(OH)_2 \cdot 4DMSO$
octahedron

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H	-5.95984920524923	-1.10630090070394	-0.22775689864578
H	-4.81372712483679	0.12896042776093	-0.87578956774068
H	-5.36766689751727	-1.22075915010656	-1.91599474246629
H	-0.38592461310993	-5.45280445736993	-0.76406403205454
H	-0.64445513890550	-3.75433286736461	-0.16678069217985
H	-1.00087001947989	-4.19002723924272	-1.88023285535406
H	2.05147645348749	-5.19613061288157	0.44305645078015
H	3.14455627773706	-3.82919690581597	0.06288441791941
H	1.54230138489178	-3.49741308320834	0.84024790104024
Ba	-0.03136016252304	-0.28319733643875	-0.54841619479621
O	-0.25907831516996	-2.10047006658341	1.46689542182911
O	0.03748709178601	1.62665841219479	-2.29527871194457
H	-0.48109935310519	-2.76868101046067	2.13234511823463
H	0.54184161100132	1.98787107523285	-3.03621408893176

40

C	-3.10088247323544	4.00139589600923	1.03190366576481
S	-1.68630352087821	3.18066516613017	0.20924079377873
C	-2.22703913262738	3.32782107497001	-1.51596458511331
O	-1.83813557700729	1.68802241676736	0.59014300815221
O	1.33220900653439	-2.42593715646483	-1.76723479778082
S	1.34597252961822	-3.93994114774846	-1.50542841032015
C	-0.35918620657710	-4.38718593098331	-1.01776411909941
C	2.10045455948802	-4.14218675549844	0.14817016762085
O	1.82847297201322	0.75390498902389	1.31456744923217
S	1.98872153186184	0.60360092804638	2.83428154419289
C	0.29703641003769	0.43597613817881	3.51152782992970
C	2.49634342974154	-1.13190190142967	3.10600591263981
O	-2.51680317408670	-1.49251272061352	-1.24973811872780
S	-3.68955693046527	-1.94645805072741	-0.37044646745651
C	-3.42309236857793	-1.19891543736310	1.27265348445312
C	-5.11202479078162	-0.92303929365788	-0.89600626039974
H	-2.17311973354474	4.38303284007916	-1.80782148725597
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H	-3.24765087179949	2.94200562867240	-1.61373624607810
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H	-4.02703198000257	3.48741972044567	0.75671188139153
H	-2.94210591738789	3.93520003412982	2.11159504127835
H	0.36243399540936	0.27945974795321	4.59412231111087
H	-0.22640839874665	1.37158429295397	3.29844960103976
H	-0.18694394933551	-0.40898170755783	3.00122620371639
H	2.53259829432712	-1.33538628852777	4.18190000146186
H	1.75910233354931	-1.76389628369183	2.59290442178068
H	3.49406819215371	-1.24447488632850	2.67319021878663
H	-4.23258178695176	-1.51092088859576	1.94193638255511
H	-2.45016801433741	-1.58433984498172	1.61240670812358
H	-3.36963683241087	-0.10907892473163	1.17862813309667
H	-5.95984920524923	-1.10630090070394	-0.22775689864578
H	-4.81372712483679	0.12896042776093	-0.87578956774068
H	-5.36766689751727	-1.22075915010656	-1.91599474246629
H	-0.38592461310993	-5.45280445736993	-0.76406403205454
H	-0.64445513890550	-3.75433286736461	-0.16678069217985
H	-1.00087001947989	-4.19002723924272	-1.88023285535406
H	2.05147645348749	-5.19613061288157	0.44305645078015
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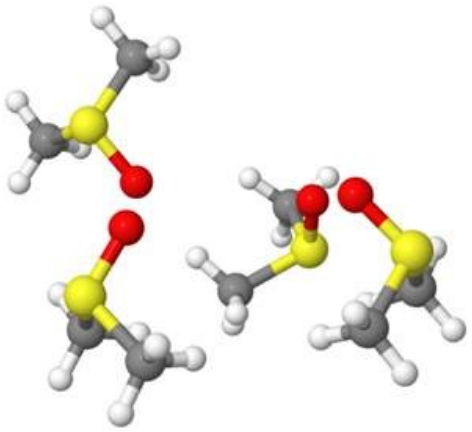

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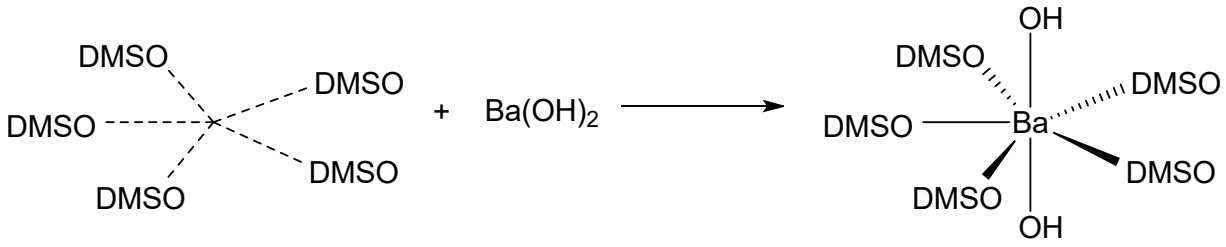

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S	-1.40276168592923	3.00507020436774	0.05688629763118
C	-1.41502041321936	3.42144163164050	-1.71202829815230
O	-2.02350570626851	1.59613553402894	0.16667376137804
O	0.10711699928162	-3.05306813201551	-2.18669814798841
S	-0.00162375961139	-4.53393492013203	-1.80093188020819
C	-1.54236352237846	-4.70192345907110	-0.82941726735861
C	1.16007966118751	-4.77461475254661	-0.40720190738159
O	0.99976985839688	0.85554727491367	1.47669600441617
S	1.69773858329150	0.37093983754006	2.75500377037377
C	0.35738844041250	-0.24862319572644	3.83679478008566
C	2.43413580206645	-1.25804161811262	2.36820140677587
O	-2.95059903096985	-1.48381658677021	-1.03097523475795
S	-4.11674361448613	-1.50723344846511	-0.03468718621008
C	-3.42996685571584	-1.02444758063867	1.59029051657446
C	-5.07203465936746	0.01778881033351	-0.36721935520273
H	-0.99128321431402	4.42463622285741	-1.83754227077553
H	-0.77051701405435	2.64778448330169	-2.18890141293527
H	-2.44082408578197	3.37531223981232	-2.09344581074191
H	-2.39010037870987	5.17863566631518	0.46590732178726
H	-3.63939064698972	3.94243083311295	0.07347023207146
H	-2.86970145281150	3.96719214501170	1.69392075708193
H	0.79394270423588	-0.71463267327031	4.72719281901516
H	-0.24703030180216	0.61507982070893	4.12697697424129
H	-0.22598064090036	-0.96665933567104	3.24559847383361
H	2.95491589485377	-1.62638584451163	3.25954218280000
H	1.62375738146821	-1.93163489693449	2.05291386675433
H	3.13633027794688	-1.09820751322245	1.54581127681306
H	-4.19805501026016	-1.17816200445715	2.35649654834666
H	-2.56016760076206	-1.67891862201111	1.75543083922258
H	-3.10081519699834	0.01857777451574	1.55302093372703
H	-5.84388450789544	0.13850454509874	0.40059544033849
H	-4.36882740169242	0.85615961565954	-0.36779070265472
H	-5.53717309943588	-0.09866037094062	-1.34968637065262
H	-1.63417788763688	-5.74009156797132	-0.49018482903631
H	-1.48980011823251	-3.99626096748254	0.01061658334793
H	-2.36794796271144	-4.44679258212433	-1.49820370947103
H	1.08241747921619	-5.80763208575289	-0.04967612975159
H	2.16451082860505	-4.58864594217535	-0.79641419222695
H	0.89870532414958	-4.05083710456246	0.37694786924514
Ba	-0.21598674595060	-0.68899831519962	-0.63377141754728
O	-0.45532940766628	-2.45670989737133	1.40590524796472
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H	-0.57048830037986	-3.10036515896491	2.12055398462981
H	0.16492815445887	0.98412714604865	-3.53644867616329
S	3.37388830845636	-0.43988384316975	-2.21619339651598
C	5.16499211309735	-0.62768055221857	-1.87856558715577
H	5.36814333095780	-1.69698375929721	-1.77694861860493
H	5.41373120837359	-0.10946682248877	-0.94731792137792
H	5.73813298247776	-0.21821400721341	-2.71699279968729
O	2.68682186988028	-0.91441046772795	-0.92220242203391
C	3.28811623279989	1.37796026867829	-2.21086806581094
H	3.66749290648510	1.75508809284541	-1.25547323144022

$Ba(OH)_2 \cdot 5DMSO$

pentagonal bipyramidal

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H	2.21062007933343	1.59186459610191	-2.34761735690431

50

C	-2.71702300393308	4.14594638248311	0.62616326873903
S	-1.40276168592923	3.00507020436774	0.05688629763118
C	-1.41502041321936	3.42144163164050	-1.71202829815230
O	-2.02350570626851	1.59613553402894	0.16667376137804
O	0.10711699928162	-3.05306813201551	-2.18669814798841
S	-0.00162375961139	-4.53393492013203	-1.80093188020819
C	-1.54236352237846	-4.70192345907110	-0.82941726735861
C	1.16007966118751	-4.77461475254661	-0.40720190738159
O	0.99976985839688	0.85554727491367	1.47669600441617
S	1.69773858329150	0.37093983754006	2.75500377037377
C	0.35738844041250	-0.24862319572644	3.83679478008566
C	2.43413580206645	-1.25804161811262	2.36820140677587
O	-2.95059903096985	-1.48381658677021	-1.03097523475795
S	-4.11674361448613	-1.50723344846511	-0.03468718621008
C	-3.42996685571584	-1.02444758063867	1.59029051657446
C	-5.07203465936746	0.01778881033351	-0.36721935520273
H	-0.99128321431402	4.42463622285741	-1.83754227077553
H	-0.77051701405435	2.64778448330169	-2.18890141293527
H	-2.44082408578197	3.37531223981232	-2.09344581074191
H	-2.39010037870987	5.17863566631518	0.46590732178726
H	-3.63939064698972	3.94243083311295	0.07347023207146
H	-2.86970145281150	3.96719214501170	1.69392075708193
H	0.79394270423588	-0.71463267327031	4.72719281901516
H	-0.24703030180216	0.61507982070893	4.12697697424129
H	-0.22598064090036	-0.96665933567104	3.24559847383361
H	2.95491589485377	-1.62638584451163	3.25954218280000
H	1.62375738146821	-1.93163489693449	2.05291386675433
H	3.13633027794688	-1.09820751322245	1.54581127681306
H	-4.19805501026016	-1.17816200445715	2.35649654834666
H	-2.56016760076206	-1.67891862201111	1.75543083922258
H	-3.10081519699834	0.01857777451574	1.55302093372703
H	-5.84388450789544	0.13850454509874	0.40059544033849
H	-4.36882740169242	0.85615961565954	-0.36779070265472
H	-5.53717309943588	-0.09866037094062	-1.34968637065262
H	-1.63417788763688	-5.74009156797132	-0.49018482903631
H	-1.48980011823251	-3.99626096748254	0.01061658334793
H	-2.36794796271144	-4.44679258212433	-1.49820370947103
H	1.08241747921619	-5.80763208575289	-0.04967612975159
H	2.16451082860505	-4.58864594217535	-0.79641419222695
H	0.89870532414958	-4.05083710456246	0.37694786924514
S	3.37388830845636	-0.43988384316975	-2.21619339651598
C	5.16499211309735	-0.62768055221857	-1.87856558715577
H	5.36814333095780	-1.69698375929721	-1.77694861860493
H	5.41373120837359	-0.10946682248877	-0.94731792137792
H	5.73813298247776	-0.21821400721341	-2.71699279968729
O	2.68682186988028	-0.91441046772795	-0.92220242203391
C	3.28811623279989	1.37796026867829	-2.21086806581094
H	3.66749290648510	1.75508809284541	-1.25547323144022
H	3.87782008748208	1.76074421639838	-3.05206459231190
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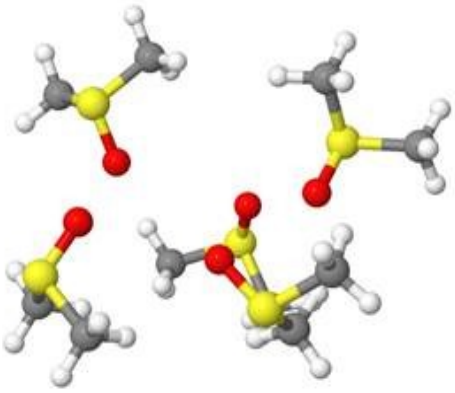

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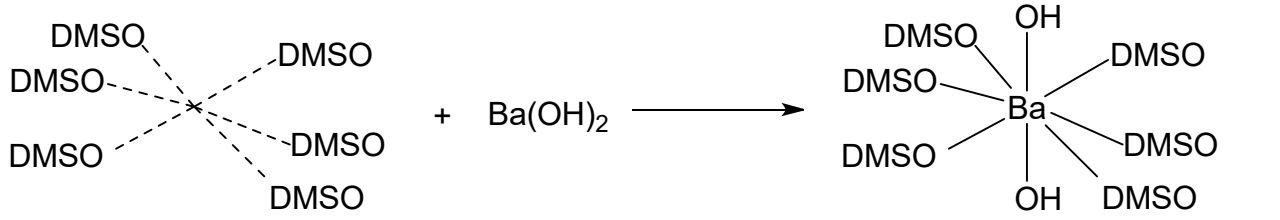

65

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H	-0.86427219255072	2.37441856119666	-1.52877166782084	
C	2.55133220938152	1.65266968057086	-2.35019002838711	
S	2.55658199902096	-0.09158856645283	-2.88877449445135	
C	4.35420848962762	-0.39181830367846	-2.85784796743725	
H	4.49368416057620	-1.45856571993043	-3.06321764258738	
H	4.73255799514155	-0.12577590050627	-1.86665485034701	
H	4.82624172724017	0.21827519222566	-3.63569869385496	
O	1.97524528036954	-0.90280840630193	-1.71080705861629	
H	3.18293149964663	1.76002822626090	-1.46257676726695	
H	2.90876613114276	2.27437048169251	-3.17849686630557	
H	1.50910407912824	1.89120349807530	-2.09489292447214	
O	-1.17890837378475	-1.88729340777429	-0.45679397277631	
S	-2.31460985767505	-1.58779572060641	-1.44950750654001	
C	-1.54047556816292	-0.74367273518259	-2.87563924851686	
C	-3.20160198913562	-0.12930497323409	-0.79139330097284	
O	0.82118270008667	2.26489253182000	2.48623644168972	
S	-0.00288723125844	3.56307374198065	2.42283563000597	
C	0.53178723001335	4.40736655646836	0.89109647235574	
C	-1.67226822703129	3.08969424361195	1.84774725921997	
H	-0.08867191568162	5.29684345114177	0.73551127549566	
H	1.57508124621639	4.70099173273802	1.03356719880214	
H	0.42582921789460	3.68853064298415	0.06762027991458	
H	-2.29639575360248	3.98992192604941	1.81331119880347	
H	-1.57087312611015	2.61944248143878	0.85924699928115	
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H	-0.99031669759451	0.12633315073866	-2.49273281040455	
H	-0.86741352893208	-1.46248890114971	-3.34908384350870	
H	-4.01498157716417	0.12539755456827	-1.48014046757664	
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O	4.07627357977182	-3.64690968394342	-3.24510639170763	
S	3.21733362937045	-4.57736502316925	-2.38662740015941	
C	1.46953497070997	-4.11235276681005	-2.68445987393547	
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H	1.34241177769190	-3.04814007746850	-2.46336364915497	
H	1.26604849056756	-4.32494187301059	-3.73774578578426	
C	3.31222668116691	-3.94956442275470	-0.66785038233276	
H	4.34050712029719	-4.10457146068029	-0.32979446387743	
H	2.62402406761848	-4.51722687679348	-0.03344054766522	
H	3.05653624555365	-2.88669943957669	-0.66032132267061	
H	2.97283428328154	1.68733072952554	3.47533586680585	
C	3.56576817662768	0.77014315233519	3.42690535886131	
H	2.90979929259905	-0.11413450679954	3.39912859390732	
H	4.28242958520319	0.72618144627988	4.25509570554822	
S	4.50929240189684	0.82947412610725	1.86342113531046	
C	5.02395397074265	-0.92534007466878	1.85291979138367	
H	5.57665809724056	-1.10023235047568	0.92605352870444	
H	4.10725919884922	-1.52662725138213	1.89738111972458	
H	5.67359968105665	-1.11506033849077	2.71441752471911	
O	3.47966882080555	0.95716601661163	0.72258268409392	
S	-1.78534744728531	-1.31270034488609	3.60752898145114	
C	-1.27230703590274	-2.91894883233538	2.89843522350070	
H	-0.22119503792162	-2.83265804141649	2.59171367121643	
H	-1.91279801976636	-3.10758414568112	2.03382196275558	
H	-1.41363706709813	-3.69606098098506	3.65796917892078	
C	-0.38698323043310	-1.12539996070821	4.76995394638646	
H	-0.47331989209539	-0.13020609171262	5.21433522232839	
H	0.54480646293189	-1.23491559790730	4.19191747146899	
H	-0.47402875175331	-1.89012279144096	5.55033839194730	
O	-1.56474710650525	-0.25958688581656	2.50500373610309	

60

C	2.55133220938152	1.65266968057086	-2.35019002838711
S	2.55658199902096	-0.09158856645283	-2.88877449445135
C	4.35420848962762	-0.39181830367846	-2.85784796743725
H	4.49368416057620	-1.45856571993043	-3.06321764258738
H	4.73255799514155	-0.12577590050627	-1.86665485034701
H	4.82624172724017	0.21827519222566	-3.63569869385496
O	1.97524528036954	-0.90280840630193	-1.71080705861629
H	3.18293149964663	1.76002822626090	-1.46257676726695
H	2.90876613114276	2.27437048169251	-3.17849686630557
H	1.50910407912824	1.89120349807530	-2.09489292447214
O	-1.17890837378475	-1.88729340777429	-0.45679397277631
S	-2.31460985767505	-1.58779572060641	-1.44950750654001
C	-1.54047556816292	-0.74367273518259	-2.87563924851686
C	-3.20160198913562	-0.12930497323409	-0.79139330097284
O	0.82118270008667	2.26489253182000	2.48623644168972
S	-0.00288723125844	3.56307374198065	2.42283563000597
C	0.53178723001335	4.40736655646836	0.89109647235574
C	-1.67226822703129	3.08969424361195	1.84774725921997
H	-0.08867191568162	5.29684345114177	0.73551127549566
H	1.57508124621639	4.70099173273802	1.03356719880214
H	0.42582921789460	3.68853064298415	0.06762027991458
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H	-1.57087312611015	2.61944248143878	0.85924699928115
H	-2.06715094341317	2.37433582829315	2.57354042052533
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H	-0.99031669759451	0.12633315073866	-2.49273281040455
H	-0.86741352893208	-1.46248890114971	-3.34908384350870
H	-4.01498157716417	0.12539755456827	-1.48014046757664
H	-3.60558979498225	-0.41427901769008	0.18303753531212
H	-2.47755404956373	0.69154491913722	-0.69102772267712
O	4.07627357977182	-3.64690968394342	-3.24510639170763
S	3.21733362937045	-4.57736502316925	-2.38662740015941
C	1.46953497070997	-4.11235276681005	-2.68445987393547
H	0.81978028980323	-4.72286455826002	-2.04862478853591
H	1.34241177769190	-3.04814007746850	-2.46336364915497
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H	3.05653624555365	-2.88669943957669	-0.66032132267061
H	2.97283428328154	1.68733072952554	3.47533586680585
C	3.56576817662768	0.77014315233519	3.42690535886131
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H	4.28242958520319	0.72618144627988	4.25509570554822
S	4.50929240189684	0.82947412610725	1.86342113531046
C	5.02395397074265	-0.92534007466878	1.85291979138367
H	5.57665809724056	-1.10023235047568	0.92605352870444
H	4.10725919884922	-1.52662725138213	1.89738111972458
H	5.67359968105665	-1.11506033849077	2.71441752471911
O	3.47966882080555	0.95716601661163	0.72258268409392
S	-1.78534744728531	-1.31270034488609	3.60752898145114
C	-1.27230703590274	-2.91894883233538	2.89843522350070
H	-0.22119503792162	-2.83265804141649	2.59171367121643
H	-1.91279801976636	-3.10758414568112	2.03382196275558
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C	-0.38698323043310	-1.12539996070821	4.76995394638646
H	-0.47331989209539	-0.13020609171262	5.21433522232839
H	0.54480646293189	-1.23491559790730	4.19191747146899
H	-0.47402875175331	-1.89012279144096	5.55033839194730
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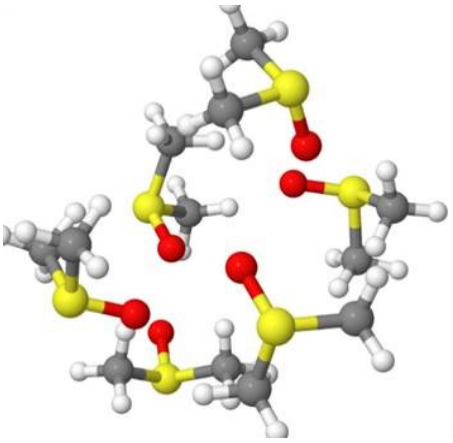

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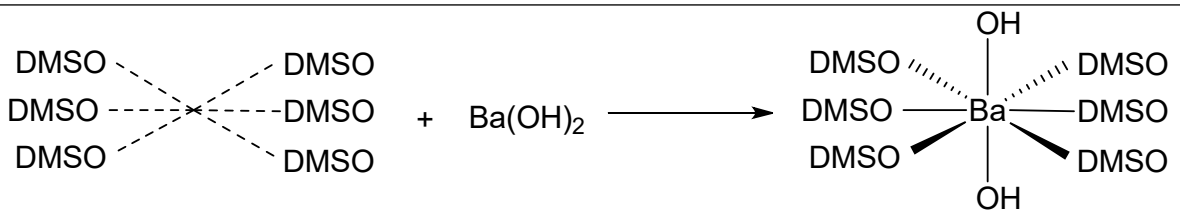

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C	-1.25182974313465	4.46222943666024	1.00173823067085
S	-0.64066815940572	3.20253932747292	-0.17717698591730
C	-0.89263888195169	4.12375651759258	-1.72714335608396
O	-1.71800945291461	2.10277305071004	-0.17172938710378
O	1.45745118850664	-2.55585010844330	-1.69118073352331
S	1.29420806224320	-4.08087980309413	-1.73240836088282
C	-0.48627179618482	-4.41633181138699	-1.98507870890672
C	1.37572013755134	-4.63536794598729	0.00945775079958
O	0.07195262299865	0.62228993384546	1.90613594450947
S	0.86946377613088	-0.02139467343465	3.05167178320599
C	-0.28422493423631	-1.17547904483431	3.88022952714267
C	1.92864981196871	-1.31110008266579	2.30565554340372
O	-3.45372576021282	-0.60350939716145	-0.92008930490411
S	-4.34586216461989	-0.43423814703568	0.32249484794732
C	-3.22318526885706	-0.30726145842873	1.75289208307330
C	-4.91024424605863	1.30738996761603	0.28917785294323
H	-0.23868214163153	5.00332012248113	-1.73585868010347
H	-0.59110593931685	3.39918313443403	-2.49845744601187
H	-1.94516610402079	4.41331582493547	-1.81356594823381
H	-0.59702235680267	5.33953896057265	0.96936829071085
H	-2.28017260446606	4.73664480466144	0.74675669989756
H	-1.21567322442521	4.00895510187374	1.99565458385305
H	0.26455358576423	-1.73868933928802	4.64351598169980
H	-1.06468611438382	-0.57454014465868	4.35551427211666
H	-0.68967356240272	-1.83220141492275	3.09479121952915
H	2.53532595979418	-1.76204880472015	3.09921661003466
H	1.27504957069124	-2.05019104185358	1.82892847726149
H	2.56058769875442	-0.81394623496831	1.56489774106397
H	-3.82545470630475	-0.31427969006524	2.66851701004646
H	-2.56120534672323	-1.18588004587818	1.70418426735398
H	-2.61881050510045	0.60153485841461	1.67658679809882
H	-5.40860239512707	1.54470140120508	1.23535745133221
H	-4.02989981105362	1.93749315628814	0.12523750631638
H	-5.61965776443934	1.40642486869353	-0.53734987454098
H	-0.63543215863052	-5.49992020246015	-2.04865296201688
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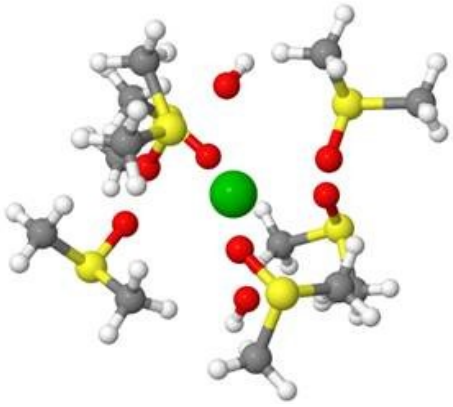
H	1.12096806993694	-5.70014300257428	0.06111075241344
H	2.40594443721986	-4.48710926136907	0.34566278176315
H	0.67006283326429	-4.01115783512955	0.58235180153026
Ba	-0.40521402782588	-0.49858384444742	-0.82187452339708
O	-0.89781653712233	-2.52355647201724	0.99843748948828
O	0.25781450346174	1.45018904446590	-2.69290999373424
H	-1.53322890542770	-3.24734960247069	1.10820794769399
H	0.68489343587265	1.19489440340179	-3.52595591313583
S	3.13443930526924	0.55596928214869	-1.76763585509168
C	4.90821281098424	0.28571648828470	-1.38862612911552
H	5.03546126446908	-0.78520744501723	-1.21131744709988
H	5.18039620303475	0.84921482317889	-0.49066844137968
H	5.51834629125396	0.59466370623361	-2.24413252957580
O	2.41404845508109	0.25144188450515	-0.44682607607567
C	3.18217257976724	2.37471762246975	-1.90098155445066
H	3.53635271204810	2.79655146190997	-0.95482173671909
H	3.83346394536575	2.66340360900582	-2.73376906964917
H	2.13999937430502	2.64133159722925	-2.10874787471543
C	-2.60463556209925	0.76019369134607	-3.81696080285216



$Ba(OH)_2 \cdot 6DMSO$
hexagonal bipyramidal

H	-1.60961549132445	1.17975923301835	-3.57521530185039
H	-3.22151958662181	0.74483400609519	-2.91402781293613
H	-3.08887903442025	1.31174649566318	-4.63109073420930
S	-2.31085278717801	-0.95107266607088	-4.38002175712999
O	-1.44463379154897	-1.63679098797641	-3.31133882309738
C	-4.00206078408371	-1.60130409182275	-4.11462353197342
H	-4.22941880673465	-1.50278209038264	-3.04854641236767
H	-4.70948284117127	-1.03867290116698	-4.73352877767165
H	-4.00091016282757	-2.65265604270892	-4.41536922310062

60

C	-1.25182974313465	4.46222943666024	1.00173823067085
S	-0.64066815940572	3.20253932747292	-0.17717698591730
C	-0.89263888195169	4.12375651759258	-1.72714335608396
O	-1.71800945291461	2.10277305071004	-0.17172938710378
O	1.45745118850664	-2.55585010844330	-1.69118073352331
S	1.29420806224320	-4.08087980309413	-1.73240836088282
C	-0.48627179618482	-4.41633181138699	-1.98507870890672
C	1.37572013755134	-4.63536794598729	0.00945775079958
O	0.07195262299865	0.62228993384546	1.90613594450947
S	0.86946377613088	-0.02139467343465	3.05167178320599
C	-0.28422493423631	-1.17547904483431	3.88022952714267
C	1.92864981196871	-1.31110008266579	2.30565554340372
O	-3.45372576021282	-0.60350939716145	-0.92008930490411
S	-4.34586216461989	-0.43423814703568	0.32249484794732
C	-3.22318526885706	-0.30726145842873	1.75289208307330
C	-4.91024424605863	1.30738996761603	0.28917785294323
H	-0.23868214163153	5.00332012248113	-1.73585868010347
H	-0.59110593931685	3.39918313443403	-2.49845744601187
H	-1.94516610402079	4.41331582493547	-1.81356594823381
H	-0.59702235680267	5.33953896057265	0.96936829071085
H	-2.28017260446606	4.73664480466144	0.74675669989756
H	-1.21567322442521	4.00895510187374	1.99565458385305
H	0.26455358576423	-1.73868933928802	4.64351598169980
H	-1.06468611438382	-0.57454014465868	4.35551427211666
H	-0.68967356240272	-1.83220141492275	3.09479121952915
H	2.53532595979418	-1.76204880472015	3.09921661003466
H	1.27504957069124	-2.05019104185358	1.82892847726149
H	2.56058769875442	-0.81394623496831	1.56489774106397
H	-3.82545470630475	-0.31427969006524	2.66851701004646
H	-2.56120534672323	-1.18588004587818	1.70418426735398
H	-2.61881050510045	0.60153485841461	1.67658679809882
H	-5.40860239512707	1.54470140120508	1.23535745133221
H	-4.02989981105362	1.93749315628814	0.12523750631638
H	-5.61965776443934	1.40642486869353	-0.53734987454098
H	-0.63543215863052	-5.49992020246015	-2.04865296201688
H	-1.04621476405403	-3.97989954742191	-1.15165127001443
H	-0.77115041089253	-3.92459263454999	-2.91841790632807
H	1.12096806993694	-5.70014300257428	0.06111075241344
H	2.40594443721986	-4.48710926136907	0.34566278176315
H	0.67006283326429	-4.01115783512955	0.58235180153026
S	3.13443930526924	0.55596928214869	-1.76763585509168
C	4.90821281098424	0.28571648828470	-1.38862612911552
H	5.03546126446908	-0.78520744501723	-1.21131744709988
H	5.18039620303475	0.84921482317889	-0.49066844137968
H	5.51834629125396	0.59466370623361	-2.24413252957580
O	2.41404845508109	0.25144188450515	-0.44682607607567
C	3.18217257976724	2.37471762246975	-1.90098155445066
H	3.53635271204810	2.79655146190997	-0.95482173671909
H	3.83346394536575	2.66340360900582	-2.73376906964917
H	2.13999937430502	2.64133159722925	-2.10874787471543
C	-2.60463556209925	0.76019369134607	-3.81696080285216
H	-1.60961549132445	1.17975923301835	-3.57521530185039
H	-3.22151958662181	0.74483400609519	-2.91402781293613
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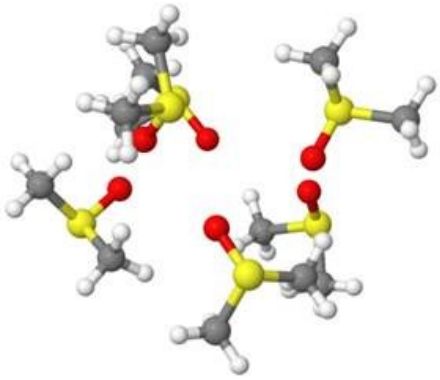

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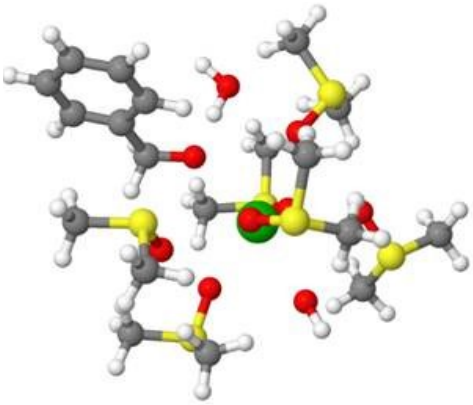
S	-2.31085278717801	-0.95107266607088	-4.38002175712999
O	-1.44463379154897	-1.63679098797641	-3.31133882309738
C	-4.00206078408371	-1.60130409182275	-4.11462353197342
H	-4.22941880673465	-1.50278209038264	-3.04854641236767
H	-4.70948284117127	-1.03867290116698	-4.73352877767165
H	-4.00091016282757	-2.65265604270892	-4.41536922310062

Table S3. Structures of species from vinylation study calculations.

Cartesian coordinates				Structure
				
16				
C	0.17170224350962	0.44242956038206	-0.80125906454672	
C	1.46029454950925	-0.08197376471841	-0.68970463390298	
C	1.91004710714696	-0.58980989661139	0.53553302455250	
C	1.06458110072004	-0.56537870880034	1.64691109753500	
C	-0.22518121446681	-0.03390272050666	1.53259023187991	
C	-0.68660025325098	0.47156564391604	0.31021870195715	
H	-0.17605830134190	0.84059167288593	-1.75144595799704	
H	2.11425048077561	-0.09918117406473	-1.55816727189873	
H	2.91324176013200	-0.99978500259344	0.62095158214666	
H	1.40695774719089	-0.95452173163891	2.60260305218110	
H	-0.87916630672276	-0.01389152661927	2.40252566168928	
C	-2.08495048573417	1.04048953759207	0.18242540600838	**BnOH**
O	-2.10990506815660	2.37309196808802	-0.33955388721746	
H	-2.59737631946128	0.99446830384610	1.15489814837783	
H	-2.67823617400953	0.45829362411311	-0.53079520561999	
H	-1.53730086584032	2.92968421472978	0.21287911485514	
81				
C	-2.95098002398806	3.26020420139900	2.73440539839144	
S	-1.13230962037830	3.45637333920003	2.66154934289116	
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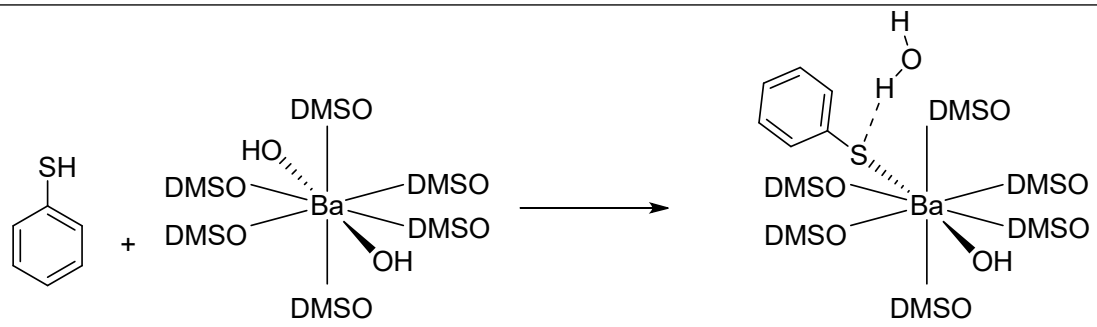
O	1.43978287214567	-1.41397845396208	-1.70307181599575	
S	2.49006894209516	-2.54035419540827	-1.68755275644965	
C	1.54121554327016	-4.10015810353628	-1.78530396157526	
C	3.06866219697446	-2.72357265214689	0.03334862368997	
O	3.47643947172860	0.48761166911585	-0.13494692001579	
S	4.34102141842463	1.71276589919786	0.21005563396133	
C	3.85983572437650	2.27420312060816	1.87938130618584	
C	5.95992096637164	0.97962842071886	0.67991343483650	
O	-2.41304768864990	1.55479684246871	-0.33591615487244	
S	-3.08848637682421	1.13855205473254	-1.65220693840644	
C	-4.86412484089585	0.95783605911400	-1.24733962726535	**Ba(OH)BnO^{-} · H_2O · 6DMSO**
C	-3.23202308084693	2.67195966665948	-2.63841062600935	
H	-1.21897491238965	5.31836546669131	1.14050959123023	
H	-0.00085606803802	4.04822833057301	0.65496077488511	
H	-1.74270114868178	3.77441769425684	0.34405068388359	
H	-3.42446582448663	4.24695032067705	2.68758235001401	
H	-3.25153636017455	2.63110954631452	1.89117875585620	
H	-3.19470973416584	2.77495094574274	3.68329947137222	
H	4.63665269521572	2.94461806074489	2.26415950617101	
H	2.91427245302210	2.80311974400528	1.72462370246281	
H	3.71912150536616	1.39556382699172	2.51576327658606	

H	6.63844257210398	1.77133138307880	1.01542920078920
H	5.80955621818446	0.23755034810706	1.46983060241033
H	6.36835999334972	0.49682066401358	-0.21200397023351
H	-5.43239377494871	0.81763306687806	-2.17294836497503
H	-4.95992492340685	0.06590824094741	-0.62385610325960
H	-5.20912439824394	1.84506696923315	-0.70713809626984
H	-3.79265238544623	2.46340495074540	-3.55594510582662
H	-3.72891062308792	3.44709001740919	-2.04646643127534
H	-2.20773984446184	2.96182196593484	-2.87835969815991
H	2.24230183584018	-4.94099591361922	-1.73619881688270
H	0.83259561620119	-4.12905460986463	-0.94996806047332
H	1.02523886924375	-4.10382297345582	-2.74914012200514
H	3.85523791483498	-3.48708087739231	0.04499040627694
H	3.46866919941147	-1.74887740261270	0.32514222688657
H	2.22795269415176	-3.01716934047668	0.66687481185292
S	1.53053885186269	-0.86772327056920	3.95690522836931
C	-0.29007757731140	-0.81555784874831	4.02635139652908
H	-0.67696005866047	-1.29090126638163	3.11744113198346
H	-0.62418207658047	-1.31758275297646	4.94061638747515
H	-0.57270703166102	0.24000776040772	4.02964201026260
C	1.72083221291260	-2.68668406141777	3.92296350841766
H	1.15627462541973	-3.10614713855081	3.08072655169436
H	1.36976104888813	-3.09189609801510	4.87870886141160
H	2.78953692695184	-2.89155928555988	3.81183748963981
O	1.93368547534374	-0.36977694680250	2.55794193434220
S	0.69010132316592	1.68482436408266	-3.73804603230758
C	2.35278517346198	1.82010674806454	-3.00635076631033
H	2.68639460994558	0.84223315830193	-2.64869006054520
H	3.03464015556487	2.22951545797152	-3.76011761770801
H	2.24352912570816	2.49518450688221	-2.14182699632501
C	0.92839101490683	0.12454869276831	-4.66241895273735
H	1.14790626577563	-0.65716502620465	-3.92822945593014
H	1.74442423619452	0.24937729817554	-5.38234947777994
H	-0.00483961794825	-0.09122220899310	-5.18974080879382
O	-0.26723792289867	1.33315506525513	-2.58587587512624
Ba	0.49599090672518	0.64571197591839	0.18841299696843
O	0.09805222821656	-3.76888364715604	1.20957585445742
O	1.65355850015038	3.07343014891183	-0.10954887766957
H	-0.59649846098439	-4.43972438674546	1.28766290070875
H	2.00275845379916	3.94690203797249	-0.33857239016713
C	-3.28654012575342	-2.30980749229591	0.11377199055940
C	-2.43777000098383	-1.65167491462124	1.20885726554655
H	-2.90489772342781	-0.66808916458144	1.42832496579692
H	-2.60394371600028	-2.25677186261365	2.13254090101452
O	-1.09948855996615	-1.51219105755650	0.91113012905796
C	-2.76061940094572	-2.54606669207779	-1.16216213238989
H	-1.72709590880901	-2.26741124170147	-1.34786772484989
C	-3.54813851736182	-3.12922756976259	-2.16328889746965
H	-3.12291507357456	-3.30571567982026	-3.14967812908399
C	-4.87429976541234	-3.48779364050665	-1.90342759741094
C	-5.40853055247973	-3.26190484721901	-0.62785101912128
H	-6.43598036697294	-3.54670936363617	-0.40918470300862
H	-5.48374767185097	-3.94532197191513	-2.67973802365922
C	-4.61807268033366	-2.68054035932805	0.36713575730890
H	-5.03698676628239	-2.51661771269222	1.36044971563556
H	-0.40280137989538	-2.86818434534220	1.05863166128319



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C	-1.74474629438470	-0.14813638162798	0.06447846802636
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C	0.28636737152615	1.17698912486253	-0.04206814448351
C	1.05810683685049	0.00650489573727	-0.08006772961241
C	0.41862298840205	-1.24232272337888	-0.04532528892351
C	-0.97387127480866	-1.31417963054021	0.02647640791051
S	2.84269123716674	0.02389985991352	-0.17198518333538
H	-2.82813118864401	-0.20751499903710	0.12038096823341
H	-1.69245698515566	2.01025102682375	0.05865319294429
H	0.76631740421042	2.15212406531509	-0.06817036208425
H	1.00722652842723	-2.15593007109261	-0.07434499909622
H	-1.45602754509588	-2.28818047018291	0.05270405133988
H	2.99057147365486	1.36456534114905	-0.18234364064252

PhSH

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C	-2.42731384134805	2.95920412701649	3.48550272905061
S	-0.75587223342239	2.93983296204660	2.73860638189865
C	-1.17177495382941	3.75763351540747	1.16676409864409
O	-0.47632335511985	1.45896562364007	2.42164329538540
O	1.62304560698130	-1.76961398318079	-1.62552883429626
S	2.29692321153412	-3.11942323244419	-1.33041569323564
C	1.04489051009432	-4.16527320070627	-0.51510575352399
C	3.37696949597044	-2.84803353874357	0.12086320345333
O	2.70436815283034	0.49843754580344	0.70598317614439
S	3.74482527586214	1.49795377178635	0.18190924484785
C	3.17995230964002	3.16054561737335	0.65685636358692
C	5.15047041565414	1.35598717357912	1.34997537402932
O	-2.83408594648885	1.17832848882195	0.08035312673018
S	-4.11428495653813	0.49948030687598	-0.46125973917840
C	-5.42214896673700	1.77377816612291	-0.28412004286550
C	-4.00371373796727	0.55354500102153	-2.28015722951817
H	-1.28778162735732	4.82997584694889	1.36172294553845
H	-0.33309066312309	3.55651175248359	0.47381771600035
H	-2.08075348445720	3.30988736786087	0.75399071972522
H	-2.76070128744302	3.99585158548379	3.60008774598794
H	-3.09765173880914	2.39823359509500	2.82807260762318
H	-2.36195352402078	2.48048481251726	4.46626436980617
H	3.93804520687206	3.89024261578372	0.34970481416035
H	2.24042948577204	3.28669722802629	0.08611550252043
H	3.01538737437688	3.19272114028993	1.73918955011437
H	5.89271820666823	2.12901821218295	1.12461656340672
H	4.77448833152110	1.46142186747088	2.37225601288265
H	5.59428408714802	0.36571302665720	1.21788482553890
H	-6.33058153015659	1.41672086523444	-0.78006476572725
H	-5.61373030554976	1.90514759498592	0.78425519019056
H	-5.08171413328224	2.71579165958999	-0.72533616048975
H	-4.86200285715130	0.01031076061807	-2.68547291157594
H	-3.97009772340236	1.59615292752946	-2.61108490488992
H	-3.07585246977136	0.04770707765830	-2.55604471111021
H	1.48910427754484	-5.14851565122803	-0.32270829795273
H	0.70832539037377	-3.67960659961210	0.40459617269878
H	0.19885910876816	-4.24541259766418	-1.20264075521197
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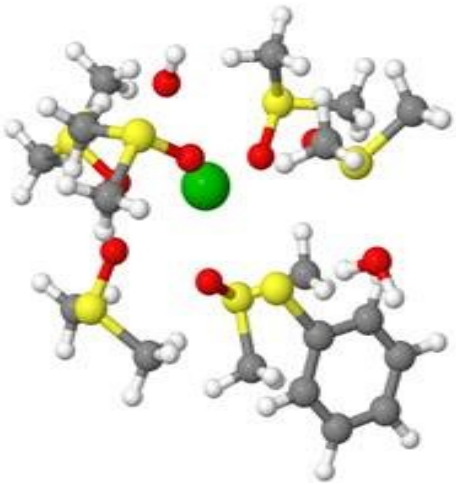

Ba(OH)PhS^{-} · H_2O · 6DMSO

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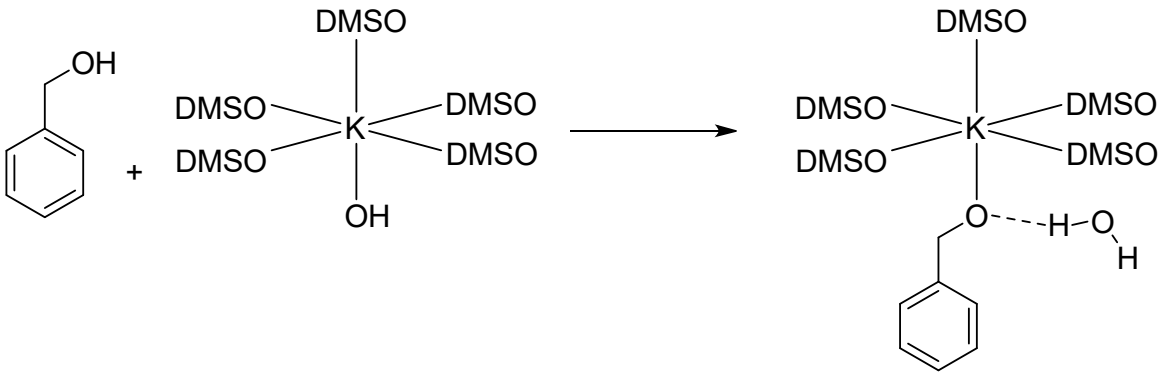
H	2.80059738624423	-2.33850880835862	0.89824428996314
S	0.36368936655029	-2.00205195565988	3.42732457062165
C	-1.30225408241458	-1.36289943656108	3.80133249827399
H	-2.04287073201554	-1.89914115993841	3.19986901714109
H	-1.49456423240627	-1.49661378645354	4.87168131853890
H	-1.28037451983977	-0.30071296989713	3.54171213455547
C	0.01242861183609	-3.77246606435973	3.72636915005867
H	-0.80053550973879	-4.10002939477238	3.07119911015613
H	-0.25509253475280	-3.90942257470640	4.77930031765759
H	0.92802558534193	-4.32746840888211	3.50513798819906
O	0.55076916568216	-1.87290061418748	1.90618658322358
S	0.03299408879641	0.46734600558222	-4.15053820226853
C	1.73160991586008	0.85658725234437	-3.59781895547095
H	2.17304874143806	-0.02964259004058	-3.13269124258876
H	2.31033184573501	1.18849703040013	-4.46716039387332
H	1.63333123357848	1.65824585569833	-2.84960260548524
C	0.37278655108115	-1.17041899136449	-4.89048849426108
H	0.78454296302444	-1.81251824765676	-4.10711736472231
H	1.07169584666703	-1.05389198967953	-5.72569397143607
H	-0.57942301296614	-1.56891365229115	-5.24961155858478
O	-0.79181490962310	0.17561132291475	-2.88891380210046
Ba	-0.06879588950339	0.12353244271302	-0.13181058537616
O	-5.33574427955992	-2.28851242105949	-2.12788748739624
O	0.77065354687225	2.57396417954397	-0.98062331034383
H	-5.76078997786839	-3.15124693417234	-2.01424746845122
H	0.29000771566626	3.10031243785177	-1.63773728620953
C	-3.95844620198552	-5.04650893627618	2.81150985744569
C	-4.36750779294839	-3.72360246169524	2.60139795220326
C	-3.87440476727492	-2.98452811322745	1.52248305570856
C	-2.95298593768765	-3.53747033478567	0.59979028306757
C	-2.56078041131833	-4.87938205285600	0.82784992003425
C	-3.05135514354718	-5.61650821798502	1.90901121013500
S	-2.34880946716232	-2.62742707621989	-0.79290652323015
H	-4.34915870020099	-5.62365086663270	3.64612827865362
H	-5.08583432299469	-3.26373566990256	3.27896528652055
H	-4.21646256944962	-1.96513793834933	1.36548789843543
H	-1.87594060574925	-5.34581453385188	0.12401598376489
H	-2.73167882682292	-6.64940840510563	2.03979040005584
H	-4.41958619899473	-2.41695074281878	-1.77148279431159



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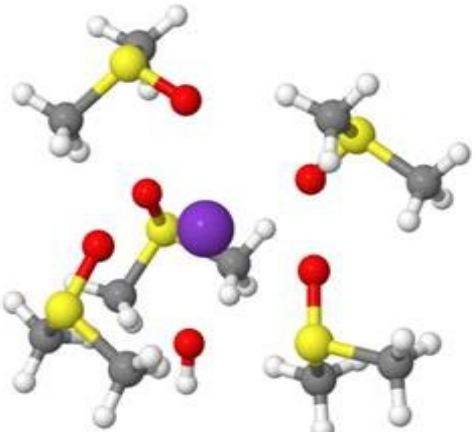
C	-3.37761629522665	3.32067845667621	0.43781550694686
S	-1.58414816449805	3.51102544342363	0.10856866249549
C	-1.62436074282984	2.95443889201619	-1.63348118745984
O	-0.89195180975069	2.41783660529853	0.92600088243905
K	0.07931805677965	-0.06297705596272	-0.14183110317253
O	1.12608970643935	-2.04845954441648	-1.88546723617031
S	1.06989966170673	-3.55915315412945	-1.61729618413811
C	-0.63577684827670	-3.91857706642052	-1.06032597206285
C	1.86453427064247	-3.81626150397713	0.01110581934287



O	-0.35277196246328	-2.03204584334309	1.59972936217423
O	1.32654345993968	1.74014708819298	-1.95258686199673
S	2.83002505603088	1.81798010568860	-2.24320250031875
C	3.55779598350410	2.80019673520794	-0.87953753230721
C	3.54732913493141	0.20372101866383	-1.76754965523981
O	2.45594772253995	0.57049478739087	1.37351350252062
S	2.33110516136047	0.48686939505086	2.90556057226860
C	0.55187200743502	0.63026304270647	3.30146222005200
C	2.49699570921973	-1.28747299518669	3.31906855818696
O	-2.86310054505494	-0.04634753009946	-0.81240216951790
S	-3.59280992792025	-1.33054495401995	-0.39645965096265
C	-3.43070984373469	-1.44993542344879	1.41249885737680
C	-5.38173415902197	-0.94109076529268	-0.48397296138692
H	-0.53488027920368	-2.67960264227530	2.29984356222289
H	-2.12965867785967	3.72335554054920	-2.22896631322565
H	-0.58536260993855	2.84000612856022	-1.95703772404311
H	-2.14805647798647	1.99582068429115	-1.69691709939498
H	-3.94230435707021	4.01213528325584	-0.19679163956197
H	-3.64935171551879	2.28091883547729	0.23324647133797
H	-3.54141933579660	3.56399112455797	1.49100890595922
H	0.44572604768483	0.63650749610931	4.39274558352228
H	0.20389695222850	1.57785473155597	2.87995148766172
H	0.02154061048104	-0.22283289193266	2.84867130210584
H	2.35067428331889	-1.41926464861784	4.39699162239382
H	1.73588903702534	-1.82927500092110	2.74229888559208
H	3.51002914132676	-1.59184452327183	3.04214135366177
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H	-2.34927607239460	-1.60449890325535	1.60261388762001
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H	-5.62597299797000	-0.76231409996809	-1.53445667171677
H	4.60835490265938	0.20271294801571	-2.04164367324975
H	3.41344806718180	0.04760939545414	-0.69304929497007
H	3.00188400526457	-0.56295782331182	-2.32496042441462
H	4.64902855065899	2.79664038304134	-0.97776523674488
H	3.18059904396902	3.82126944928791	-0.98218617705743
H	3.24153614865937	2.35902229515068	0.07165650492414
H	-0.71799789744238	-4.98976258373606	-0.84201753517350
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H	-1.30146955794151	-3.65795448388807	-1.88764652063518
H	1.80456882192716	-4.87892561560144	0.27327115423252
H	2.91197448652237	-3.52023195085301	-0.09423854878438
H	1.32887509230622	-3.18781661516415	0.74006762956782

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C	-3.39323484406394	2.90746102416862	1.35030377590707
S	-1.70314984775680	3.41302237743236	0.85725784810479
C	-1.85135510741824	2.99585840771892	-0.91801770734701
O	-0.75515023535313	2.38556987462120	1.48570614780796
K	-0.09936237399633	-0.14952038968335	0.48887446074789
O	0.70738229230219	-2.54211928247217	-0.73508908211452
S	0.93550706384408	-3.98938007219900	-0.28075603814528
C	-0.48328864282716	-4.42989405114062	0.78667713925328
C	2.21471567970648	-3.94823188997697	1.02771028504791
O	1.16602556408866	-2.23083677729054	3.67269243754532
O	0.74295713189886	1.24304731117860	-1.85481319403974
S	2.11970272503080	1.17305593937170	-2.52337741991939
C	3.19256969109355	2.33188553039597	-1.59488994573351
C	2.91701911558445	-0.37049648028807	-1.94934097323206
O	2.58443756041002	0.53658127060796	1.25991398441111
S	3.02402212357891	1.11741589335023	2.61506914510235
C	1.52499060469382	1.23280299291504	3.65187770672909
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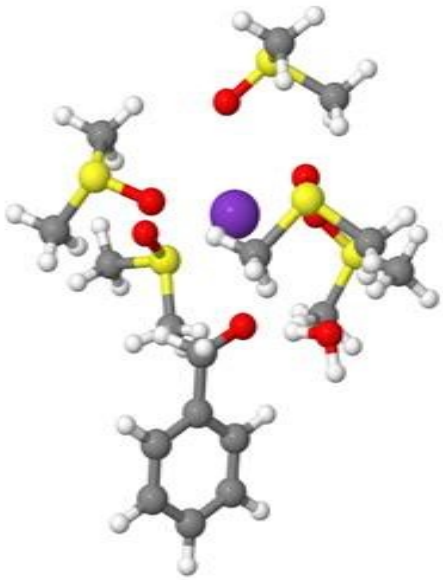

BnO·K · H_2O · 5DMSO

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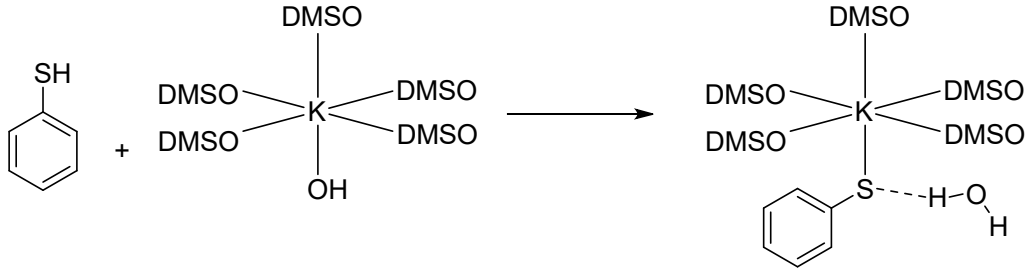

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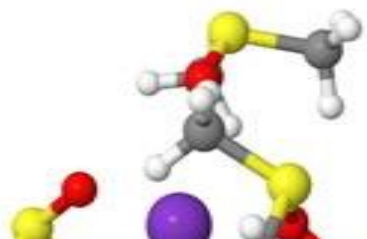

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References

1. F. Neese, *WIREs Comput. Mol. Sci.*, 2022, **12**, e1606.
2. J. L. Pascual-ahuir, E. Silla and I. Tuñon, *J. Comput. Chem.*, 1994, **15**, 1127-1138.
3. A. Bondi, *J. Phys. Chem.*, 1964, **68**, 441-451.
4. D. H. Wertz, *J. Am. Chem. Soc.*, 1980, **102**, 5316-5322.
5. K. S. Rodygin and V. P. Ananikov, *Green Chem.*, 2016, **18**, 482-486.
6. L. A. Oparina, S. I. Shaikhudinova, L. N. Parshina, O. V. Vysotskaya, T. Preiss, J. Henkelmann and B. A. Trofimov, *Russ. J. Org. Chem.*, 2005, **41**, 656-660.
7. Y. V. Gyrdymova, D. E. Samoylenko and K. S. Rodygin, *Chem. Asian J.*, 2023, **18**, e202201063.
8. G. Werner, K. S. Rodygin, A. A. Kostin, E. G. Gordeev, A. S. Kashin and V. P. Ananikov, *Green Chem.*, 2017, **19**, 3032-3041.
9. S. P. Teong, A. Y. H. Chua, S. Deng, X. Li and Y. Zhang, *Green Chem.*, 2017, **19**, 1659-1662.
10. S. A. Metlyaeva, K. S. Rodygin, K. A. Lotsman, D. E. Samoylenko and V. P. Ananikov, *Green Chem.*, 2021, **23**, 2487-2495.
11. Y. V. Gyrdymova, E. R. Saybulina, R. M. Mironenko and K. S. Rodygin, *Asian J. Org. Chem.*, 2024, **13**, e202400147.
12. K. S. Rodygin, A. S. Bogachenkov and V. P. Ananikov, *Molecules*, 2018, **23**, 648.
13. Y. V. Gyrdymova, S. M. Zarubina and K. S. Rodygin, *Mendeleev Commun.*, 2024, **34**, 732-733.
14. E. Y. Schmidt, N. A. Cherimichkina, I. A. Bidusenko, N. I. Protzuk and B. A. Trofimov, *Eur. J. Org. Chem.*, 2014, **2014**, 4663-4670.
15. N. Kaewchangwat, R. Sukato, V. Vchirawongkwin, T. Vilaivan, M. Sukwattanasinitt and S. Wacharasindhu, *Green Chem.*, 2015, **17**, 460-465.
16. R. Fu, Y. Lu, G. Yue, D. Wu, L. Xu, H. Song, C. Cao, X. Yu and Y. Zong, *Org. Lett.*, 2021, **23**, 3141-3145.
17. T. H. Jepsen and J. L. Kristensen, *J. Org. Chem.*, 2014, **79**, 9423-9426.
18. W. Guo, R. Pleixats, A. Shafir and T. Parella, *Adv. Synth. Catal* . 2015, **357**, 89-99.