

Supporting Information For:

Redox Non-Innocent Ligand Supported Vanadium Catalysts for the Chemoselective Reduction of C=X (X = O, N) Functionalities

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General Considerations. Unless specified otherwise, all reactions were carried out under a dry nitrogen atmosphere using standard glove-box and Schlenk techniques. Deuterated solvents were purchased from Cambridge Isotope Laboratories. Anhydrous grade solvents (stored over 4 Å molecular sieves) and alkyne substrates were purchased from Sigma-Aldrich, Fisher Scientific and TCI America. Pinacolborane was purchased from Acros or Alfa Aesar and redistilled under reduced pressure prior to use. FT-IR spectra were recorded on a Shimadzu 8400S instrument with solid samples under N₂ using a Golden Gate ATR accessory. ¹H NMR and ¹³C NMR spectra were obtained at room temperature on a Bruker AV 500 or 600 MHz NMR spectrometer, with chemical shifts (δ) referenced to the residual solvent signal. HR-MS data were obtained on an Agilent 6550 QToF coupled to an Agilent 1290 Infinity LC system. GC-MS analysis was obtained using a Shimadzu GCMS-QP2010S gas chromatograph mass spectrometer. 4'-Chloro-2,2';6',2''-terpyridine, aluminum chloride and trimethylsilylmethyl lithium were purchased from Sigma-Aldrich in the US and 4'-phenyl-2,2';6',2''-terpyridine was prepared according to literature procedures.¹ Note: vanadium alkyl complexes (**1/1H**, **1** and **2**) are sensitive to air and moisture and should be handled under inert atmosphere during the preparation, characterization, storage and catalytic reactions.

Synthesis of vanadium complex **1/1H.** In a glovebox under N₂, in a 20 mL scintillation vial, 2,2';6',2''-terpyridine (233 mg, 1.00 mmol) and vanadium(III) trichloride (156 mg, 1.00 mmol) were added to THF (10 mL). The solution was allowed to stir at room temperature for 24 h, during which time a light brown suspension had formed. The precipitate was filtered and washed with THF (3 × 2 mL), then dried in vacuo over P₂O₅ overnight to give a white solid. Yield: 366 mg (94%). FT-IR (solid, cm⁻¹): 3075w, 1599s, 1570m, 1473s, 1445s, 1399w, 1314m, 1239m, 1186w, 1157w, 1098m, 1051m, 1023s, 952m, 783s, 734m, 670w, 651s. The product is directly used for the next step. The above brown solid (130 mg, 0.33 mmol based on putative (terpy)VCl₃) was suspended in Et₂O (10 mL) in a 20 mL scintillation vial at room temperature, to which (trimethylsilyl)methyl lithium, LiCH₂Si(CH₃)₃ (94.0 mg, 1.00 mmol, 3.0 eq.), was added in small portions while stirring. The solution turned a dark brown color immediately after the addition of LiCH₂Si(CH₃)₃ and the solid was dissolved. The solution was allowed to stir at room temperature for an additional 2 h. The precipitate was carefully filtered off through celite and washed with Et₂O (1 mL). The resulting dark blue solution was allowed to slowly evaporate under N₂ over 6 h and the concentrated solution was cooled to -30 °C and kept at this temperature for 5 days. Dark brown plates of **1/1H** suitable for X-ray diffraction analysis were collected by decanting the solvent residue, and washed with cold pentane (2 × 0.5 mL) carefully. The crystals were recrystallized from Et₂O and dried under reduced pressure. Yield: 116.0 mg (64%). FT-IR (solid, cm⁻¹): 3055w, 2951m, 2892w, 1735w, 1604s, 1583s, 1566m, 1472s, 1404s, 1246s, 1147m, 834s, 793s, 693s. Anal. Calc. for C₂₇H₄₃N₃Si₃V, C 59.52, H 7.96, N 7.71%; Found C 59.07, H 7.91, N 7.25%. ¹H NMR (500 MHz, C₆D₆): No resonances observed. The synthesis is reproducible as confirmed by 3 independent experiments from which 3 randomly picked crystals were analyzed by X-ray crystallography.

Synthesis of vanadium complex **1.** A brown solid of putative (terpy)VCl₃ (130 mg, 0.33 mmol) was suspended in Et₂O (10 mL) in a 20 mL scintillation vial at room temperature, to which (trimethylsilyl)methyl lithium, LiCH₂Si(CH₃)₃ (108.60 mg, 1.16 mmol, 3.5 eq.) was added in small portions while stirring. The solution turned to a black color immediately after the addition of LiCH₂Si(CH₃)₃ and the solid was dissolved. The solution was allowed to stir at room

temperature for 48 h. The precipitate was carefully filtered off through celite and washed with Et₂O (1 mL). The resulting dark blue solution was allowed to slowly evaporate under N₂ over 6 h and the concentrated solution was cooled to -30 °C and kept at this temperature for 5 days. A small amount of dark brown crystals of **1** were picked manually under a microscope and subjected to single-crystal X-ray diffraction analysis. The synthesis is reproducible as confirmed by 3 independent experiments from which 3 randomly picked crystals were analyzed by X-ray crystallography. Even though efforts were made to isolate the bulk sample of **1**, a significant amount of impurity, tentatively assigned to V(CH₂Si(CH₃)₃)₄ (see the main text) was also observed according to EPR analysis at 123 K.

Synthesis of vanadium complex 2. In a glovebox under N₂, in a 20 mL scintillation vial, 4'-phenyl-2,2';6',2''-terpyridine (309 mg, 1.00 mmol) and vanadium(III) trichloride (156 mg, 1.00 mmol) were added to THF (10 mL). The solution was allowed to stir at room temperature for 24 h, during which time a brown suspension had formed. The precipitate was filtered and washed with THF (3 × 2 mL), dried in vacuo over P₂O₅ overnight to give a brown solid. Yield: 418 mg (90%). FT-IR (solid, cm⁻¹): 3058m, 1604s, 1548m, 1477s, 1450w, 1414s, 1305w, 1246m, 1160m, 1055w, 1026s, 893w, 793s, 767s, 731m, 689m, 657m. The product is directly used for the next step. The above brown solid (155 mg, 0.33 mmol based on (4'-Ph-terpy)VCl₃) was suspended in Et₂O (10 mL) in a 20 mL scintillation vial at room temperature, to which LiCH₂Si(CH₃)₃ (94.0 mg, 1.00 mmol, 3.0 eq.) was added in small portions while stirring. The solution turned a dark green color immediately after the addition of LiCH₂Si(CH₃)₃ and the solid was dissolved. The solution was allowed to stir at room temperature for additional 2 h. The precipitated LiCl was carefully filtered off through celite and washed with Et₂O (1 mL). The resulting dark green solution was allowed to slowly evaporate under N₂ over 6 h and the concentrated solution was cooled to -30 °C and kept at this temperature for 5 days. Brown plates of **2** suitable for X-ray diffraction analysis were collected by decanting the solvent residue, and washed with cold pentane (2 × 0.5 mL) carefully. The crystals were recrystallized from Et₂O and dried under reduced pressure. Yield: 80.1 mg (45%). Sample for elemental analysis was obtained by recrystallization of **2** from Et₂O twice. FT-IR (solid, cm⁻¹): 3057w, 2950m, 2892w, 739w, 1605s, 1473s, 1413m, 1291w, 1245s, 1158w, 1088w, 926s, 836s, 761s, 695s. Anal. Calc. for C₂₉H₃₇N₃Si₂V, C 65.14, H 6.97, N 7.86%; Found C 64.79, H 7.05, N 7.58%. ¹H NMR (500 MHz, C₆D₆): No resonances observed.

General Procedure for Vanadium-Catalyzed Reduction of Ketones and Aldehydes by Hydroboration Using **1/1H.** In a glovebox under N₂ atmosphere, catalyst **1/1H** (1.0 µmol, 10 µL from a stock solution of **1/1H**, 0.1 M in Et₂O, 0.1 mol%) was dissolved in Et₂O (1 mL) in a 3.8 mL glass vial equipped with a stir bar. Ketones or aldehydes (1.0 mmol) and pinacolborane (1.1 mmol, 1.1 eq.) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. The crude reaction mixture was analyzed by GC-MS and then purified through column chromatography (SiO₂) using ethyl acetate/hexane (1 : 9, v/v) as an eluent. The isolated alcohol products were characterized by ¹H and ¹³C NMR spectroscopies.

General Procedure for Vanadium-Catalyzed Reduction of Ketones and Aldehydes by Hydrosilylation Using **1/1H.** In a glovebox under N₂ atmosphere, catalyst **1/1H** (1.0 µmol, 10 µL from a stock solution of **1/1H**, 0.1 M in Et₂O, 0.1 mol%) was dissolved in Et₂O (1 mL) in a 3.8 mL glass vial equipped with a stir bar. Ketones or aldehydes (1.0 mmol) and phenylsilane (1.1 mmol, 1.1 eq.) were then added. The reaction mixture was allowed to stir at room temperature for

2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The crude product was redissolved in methanol and 1 N NaOH (2 mL) was added. The solution was stirred for 30 min at room temperature and then extracted with CH₂Cl₂ for three times. The combined organic phase was dried over anhydrous Na₂SO₄ and filtered. The solvent was removed under reduced pressure and the crude product was passed over a SiO₂ column using ethyl acetate/hexane (1:9, v/v) as an eluent. The isolated alcohol products were characterized by ¹H and ¹³C NMR spectroscopies.

General Procedure for Vanadium-Catalyzed Reduction of Imines by Hydroboration Using 1/1H. In a glovebox under N₂ atmosphere, catalyst **1/1H** (1.0 µmol, 10 µL from a stock solution of **1/1H**, 0.1 M in THF, 0.1 mol%) was dissolved in THF (1 mL) in a schlenk tube equipped with a stir bar. Imines (1.0 mmol) and pinacolborane (1.1 mmol, 1.1 eq.) were then added. The reaction tube was sealed and allowed to heat at 50 °C for 16 h. The resulting product was subject to a column chromatography (SiO₂) using ethyl acetate/hexane (1 : 6, v/v) as an eluent. The isolated amine product was characterized by ¹H and ¹³C NMR spectroscopies.

General Procedure for Vanadium-Catalyzed Reduction of Esters by Hydroboration Using 1/1H. In a glovebox under N₂ atmosphere, catalyst **1/1H** (1.0 µmol, 10 µL from a stock solution of **1/1H**, 0.1 M in THF, 0.1 mol%) was dissolved in THF (1 mL) in a schlenk tube equipped with a stir bar. Esters (1.0 mmol) and pinacolborane (2.0 mmol, 2.0 eq.) were then added. The reaction tube was sealed and brought out of the glovebox. The reaction mixture was allowed to heat at 50 °C for 16 h. The crude reaction mixture was analyzed by GC-MS and then subject to purification by a column chromatography (SiO₂) using ethyl acetate/hexane (1 : 9, v/v) as an eluent. The isolated alcohol product was characterized by ¹H and ¹³C NMR spectroscopies.

Procedure for Vanadium-Catalyzed Reduction of Methyl Benzoate by Hydrosilylation Using 1/1H. In a glovebox under N₂ atmosphere, catalyst **1/1H** (1.0 µmol, 10 µL from a stock solution of **1/1H**, 0.1 M in THF, 0.1 mol%) was dissolved in THF (1 mL) in a schlenk tube equipped with a stir bar. Methyl Benzoate (136 mg, 1.0 mmol) and phenylsilane (118.8 mg, 2.0 mmol, 2.0 eq.) were then added. The reaction tube was sealed and allowed to heat at 50 °C for 16 h. The reaction mixture was then exposed to the air and to which 1 N NaOH (2 mL) was added. The solution was stirred for 30 min at room temperature and then extracted with CH₂Cl₂ for three times. The combined organic phase was dried over anhydrous Na₂SO₄ and filtered. The solvent was removed under reduced pressure and the crude product was passed over a SiO₂ column using ethyl acetate/hexane (1:9, v/v) as an eluent. The isolated alcohol product was characterized by ¹H and ¹³C NMR spectroscopies.

General Procedure for Vanadium-Catalyzed Reduction of Amides by Hydroboration Using 1/1H. In a glovebox under N₂ atmosphere, catalyst **1/1H** (5.0 µmol, 0.5 mol%) was dissolved in THF (1 mL) in a schlenk tube equipped with a stir bar. Amides (1.0 mmol) and pinacolborane (2.0 mmol, 2.0 eq.) were then added. The reaction tube was sealed and allowed to heat at 60 °C for 16 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The reduced product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:6, v/v) as eluent. The isolated product was characterized by ¹H and ¹³C NMR spectroscopies.

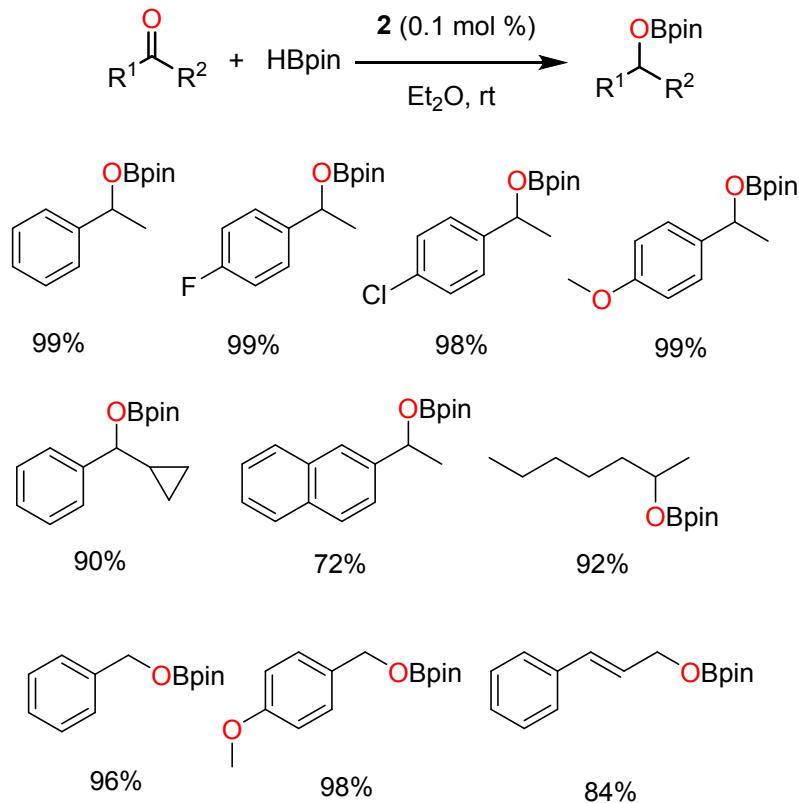
General Procedure for Vanadium-Catalyzed Reduction of Ketones and Aldehydes by Hydroboration Using **2.** In a glovebox under N₂ atmosphere, catalyst **2** (1.0 µmol, 10 µL from a stock solution of **2**, 0.1 M in Et₂O, 0.1 mol%) was dissolved in Et₂O (1 mL) in a 3.8 mL glass vial equipped with a stir bar. Ketones or aldehydes (0.5 mmol) and pinacolborane (1.1 mmol, 1.1 eq.) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. The crude reaction mixture was analyzed by GC-MS to determine the yields using hexamethylbenzene as an internal standard.

Procedure for Vanadium-Catalyzed Reduction of Methyl Benzoate and N, N-Dimethylbenzamide by Hydroboration Using **2.** In a glovebox under N₂ atmosphere, catalyst **2** (1.0 µmol, 50 µL from a stock solution of **2**, 0.1 M in THF, 0.5 mol%) was dissolved in THF (1 mL) in a schlenk tube equipped with a stir bar. Methyl benzoate or N, N-dimethylbenzamide (1.0 mmol) and pinacolborane (2.0 mmol, 2.0 eq.) were then added. The reaction tube was sealed and brought out of the glovebox. The reaction mixture was allowed to heat at 50 or 60 °C for 16 h. The crude reaction mixture was analyzed by GC-MS to determine the yields using hexamethylbenzene as an internal standard.

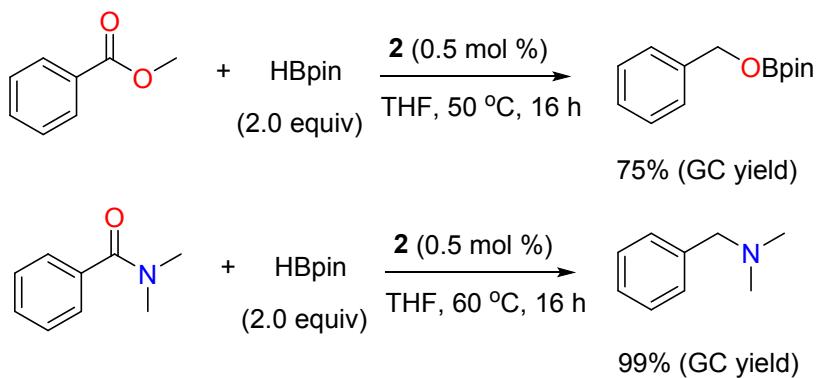
Stoichiometric Reaction of **1/H with HBpin.** In a glovebox under N₂ atmosphere, complex **1/H** (54.0 mg, 0.1 mmol) was dissolved in Et₂O (5 mL) in a 20 mL disposable vial equipped with a stir bar. Pinacolborane (28.5 mg, 0.22 mmol, 2.2 eq.) was then added. The reaction mixture was allowed to stir at room temperature for 1 h. The reaction mixture was then passed through a silica plug under N₂ and washed with pentane (5 mL), the colorless filtrate was concentrated to dryness under reduced pressure. The resultant colorless oil (28 mg, ~65%) was characterized by NMR spectroscopies and GC-MS. ¹H NMR (600 MHz, CDCl₃) δ 1.24 (s, 12H), 0.10 (s, 2H), 0.05 (s, 9H) ppm; ¹³C{¹H} NMR (151 MHz, CDCl₃) δ 82.85, 25.08, 0.51 ppm. GC-MS: 214 (calc. 214). In a separate experiment, the reaction of **1/H** with HBpin was conducted under the same conditions with hexamethylbenzene as an internal standard, and the yield of pinBCH₂Si(CH₃)₃ was determined to be 75% using GC-MS analysis.

Stoichiometric Reaction of **2 with HBpin.** In a glovebox under N₂ atmosphere, complex **1/H** (42.5 mg, 0.080 mmol) was dissolved in Et₂O (3 mL) in a 3.8 mL disposable vial equipped with a stir bar. Pinacolborane (22.5 mg, 0.176 mmol, 2.2 eq.) were added. Hexamethylbenzene (5.0 mg) was then added as an internal standard. The reaction mixture was allowed to stir at room temperature for 1 h. The reaction mixture was then passed through a silica plug under N₂ and washed with pentane (5 mL), the colorless filtrate was concentrated to dryness under reduced pressure. The yield of pinBCH₂Si(CH₃)₃ was determined to be 73% using GC-MS analysis.

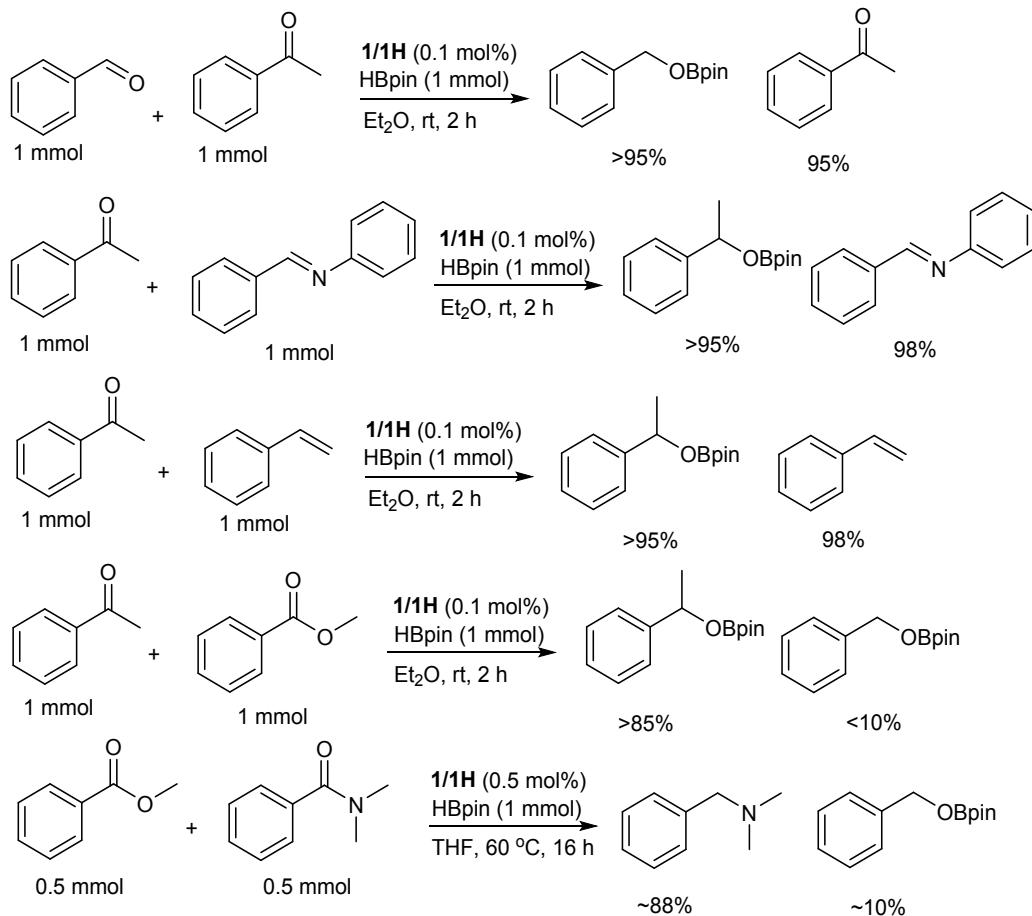
Stoichiometric Reaction of **1/H with PhSiH₃.** In a glovebox under N₂ atmosphere, complex **2** (35.0 mg, 0.065 mmol) was dissolved in Et₂O (5 mL) in a 20 mL disposable vial equipped with a stir bar. Phenylsilane (15.5 mg, 0.144 mmol, 2.2 eq.) were then added. Hexamethylbenzene (4.8 mg) was then added as an internal standard. The reaction mixture was allowed to stir at room temperature for 1 h. The reaction mixture was then passed through a silica plug under N₂ and washed with pentane (5 mL), the colorless filtrate was concentrated to dryness under reduced pressure. The yield of PhSiH₂CH₂Si(CH₃)₃ was determined to be 44% using GC-MS analysis. GC-MS: 194 (calc. 194).

Scheme S1. Selected examples for hydroboration of ketones and aldehydes catalyzed using **2**.^a

^a Conditions: **2** (0.1 mol%), ketone or aldehyde (1.0 mmol), HBpin (1.1 mmol) and Et_2O (1 mL), 25 °C, 2 h, N_2 . Yields were determined by GC using hexamethylbenzene as an internal standard.

Scheme S2. Hydroboration of ester and carboxamide catalyzed using **2**.^a

Scheme S3. Competition experiments for hydroboration reactions using **1/1H**.



Electron Paramagnetic Resonance Spectroscopy

Instrumentation. Studies were performed at the EPR Facility of Arizona State University. Continuous wave EPR spectra were recorded at 118 and 123 K using a Bruker ELEXSYS E580 continuous wave X-band spectrometer (Bruker, Rheinstetten, Germany) equipped with a liquid nitrogen temperature control system (ER 4131VT). The magnetic field modulation frequency was 100 kHz with a field modulation amplitude of 0.5 mT peak-to-peak. The microwave power was 1 mW, the microwave frequency was 9.40 GHz and the sweep time was 671 seconds.

Spin Hamiltonian. The EPR spectra of **1/1H** and **2** were interpreted using a spin Hamiltonian, H , containing the electron Zeeman interaction with the applied magnetic field \mathbf{B}_0 , the zero-field interaction, and the hyperfine coupling (hfc) interaction with the ^{51}V ($I = 7/2$) nucleus:²

$$H = \beta_e \mathbf{S} \cdot \mathbf{g} \cdot \mathbf{B}_0 + h \mathbf{S} \cdot \mathbf{D} \cdot \mathbf{S} + h \mathbf{S} \cdot \mathbf{A} \cdot \mathbf{I} \quad (1)$$

where \mathbf{S} is the electron spin operator, \mathbf{I} is the nuclear spin operator of ^{51}V , \mathbf{D} and \mathbf{A} are the zero-field interaction and the hfc tensors, respectively, both in frequency units, \mathbf{g} is the electronic g -tensor, β_e is the electron magneton, and h is Planck's constant. The so-called zero-field interaction occurs in the absence of an applied magnetic field due to electron–electron repulsion. For a quartet state ($S = 3/2$) system, the zero-field interaction partially breaks the degeneracy of the Kramer's doublets causing the energy of these levels to shift by the term Dm_S^2 , where D is the axial zero-field splitting (ZFS) parameter and m_S is the magnetic quantum number of the quartet ($\pm 1/2, \pm 3/2$). Additional shifting of the energy of the Kramer's doublets is induced by the rhombic zero-field splitting term, which is characterized by the parameter E . The electron Zeeman interaction contributes to the Hamiltonian when an external magnetic field is applied. This interaction is anisotropic and depends on the relative orientation between the magnetic field and the molecular axes of the vanadium complex. The Zeeman interaction breaks the remaining degeneracy of the Kramer's doublets causing an additional shift given by the term $g\beta_eB_0m_S/h$ in the energy of these levels, where g is the g -value. A further energetic consideration is the contribution of the hfc interaction, which represents the interaction between the magnetic moment of the unpaired electron system and the magnetic moment of the ^{51}V nucleus. The hyperfine interaction is described as first order by the expression $A m_S m_I$, where A is the hfc interaction along an arbitrary magnetic field direction and m_I is the magnetic quantum number of the nucleus.

Fitting of EPR spectra. To quantitatively compare experimental and simulated spectra, we divided the spectra into N intervals, i.e. we treated the spectrum as an N -dimensional vector \mathbf{R} . Each component R_j has the amplitude of the EPR signal at a magnetic field B_j , with j varying from 1 to N . The amplitudes of the experimental and simulated spectra were normalized so that the span between the maximum and minimum values of R_j is 1. We compared the calculated amplitudes R_j^{calc} of the signal with the observed values R_j defining a root-mean-square deviation σ by:

$$\sigma(p_1, p_2, \dots, p_n) = [\sum_j (R_j^{\text{calc}}(p_1, p_2, \dots, p_n) - R_j^{\text{exp}})^2/N]^{1/2} \quad (2)$$

where the sums are over the N values of j , and p 's are the fitting parameters that produced the calculated spectrum. For our simulations, N was set equal to 2048. The EPR spectra were simulated using EasySpin (v 5.2.11), a computational package developed by Stoll and Schweiger³ and based on Matlab (The MathWorks, Natick, MA, USA). EasySpin calculates EPR resonance fields using the energies of the states of the spin system obtained by direct diagonalization of the spin Hamiltonian (see Eq. 1). The EPR fitting procedure used a Monte Carlo type iteration to minimize the root-mean-square deviation, σ (see Eq. 2) between measured and simulated spectra. We searched for the optimum values of the following parameters: the principal components of \mathbf{g} (i.e. g_x , g_y , and g_z), the ZFS parameters, D and E , the principal components of the hfc tensor \mathbf{A} (i.e. A_x , A_y , and A_z) and the peak-to-peak linewidths (ΔB_x , ΔB_y , and ΔB_z).⁴

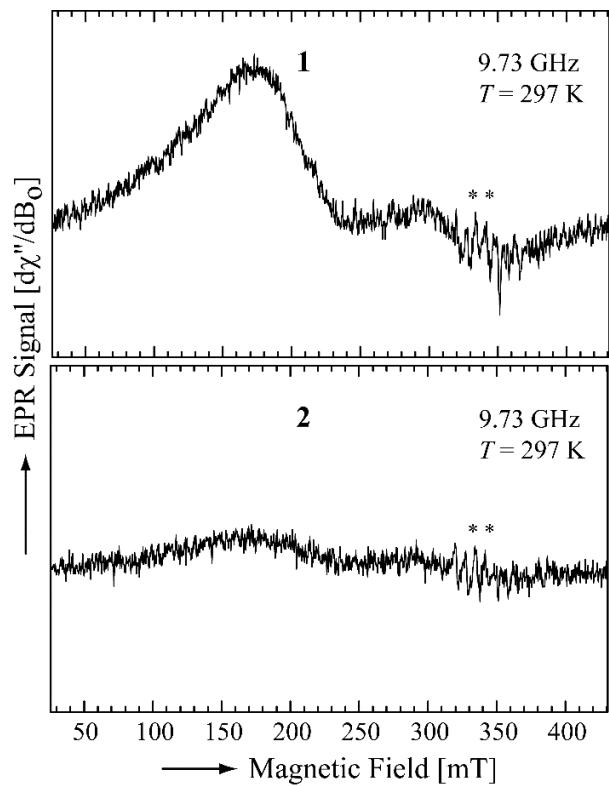


Figure S1. Ambient temperature EPR spectra of **1/1H** (top) and **2** (bottom). The small lines around 320 mT (marked with asterisks) belong to the minor impurity assigned to $\text{V}(\text{CH}_2\text{Si}(\text{CH}_3)_3)_4$.

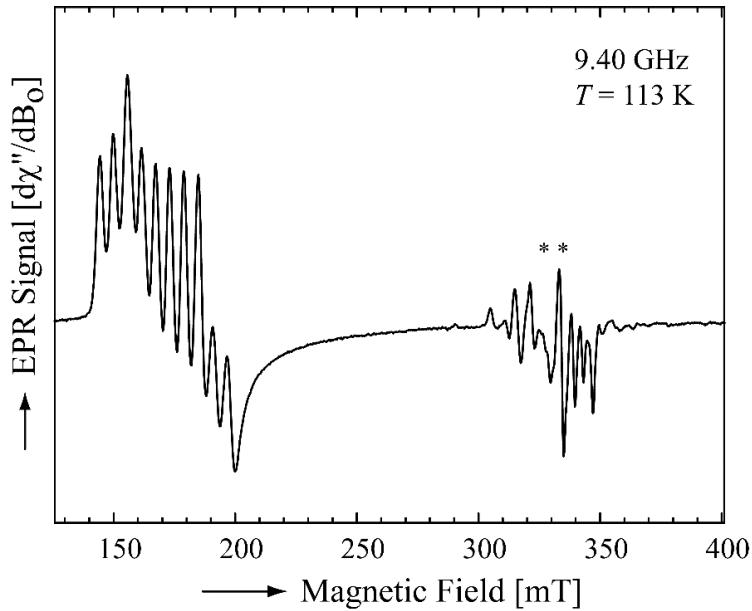


Figure S2. EPR spectrum of sample of **1** prepared using 3.5-4.0 equiv. of $\text{LiCH}_2\text{Si}(\text{CH}_3)_3$. The signal marked with asterisks has been attributed to increased formation of $\text{V}(\text{CH}_2\text{Si}(\text{CH}_3)_3)_4$.

X-ray Crystallography. X-ray diffraction data of **1/1H**, **1**, **2**, and **6c·HCl** were collected on a Bruker X8 Kappa Apex II diffractometer using Mo K α radiation. Crystal data, data collection and refinement parameters are summarized in Table S3. Data for **1/1H**, **1** and **2** were collected at 130 K, while **6c·HCl** was collected at a higher temperature of 240 K due to the crystal cracking at 130 K. The structures were solved using direct methods and standard difference map techniques, and were refined by full-matrix least-squares procedures on F^2 with SHELXTL (Version 2014/7, (a) Sheldrick, G. M. SHELXTL, An Integrated System for Solving, Refining, and Displaying Crystal Structures from Diffraction Data; University of Göttingen, Göttingen, Federal Republic of Germany, 1981. (b) Sheldrick, G. M. *Acta Cryst.* **2015**, *A71*, 3–8). All hydrogen atoms bound to carbon were placed in calculated positions and refined with a riding model [$U_{\text{iso}}(\text{H}) = 1.2 - 1.5U_{\text{eq}}(\text{C})$], while hydrogen atoms bound to nitrogen in **6c** were located on the difference map and freely refined. In the crystal of **1/1H**, complexes **1** and **1H** are clearly observed and structures are well solved in a ratio of approximately 55:45. Bond lengths and angles for vanadium complexes are given in Tables S2-S4. CCDC Nos. 1590117 (**1/1H**), 1937659 (**1**), 1590118 (**2**) and 1946740 (**6c·HCl**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/conts/retrieving.html>, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk.

Scheme S4. The bond length comparison for vanadium complexes **1H**, **1** (pure) and **2**.

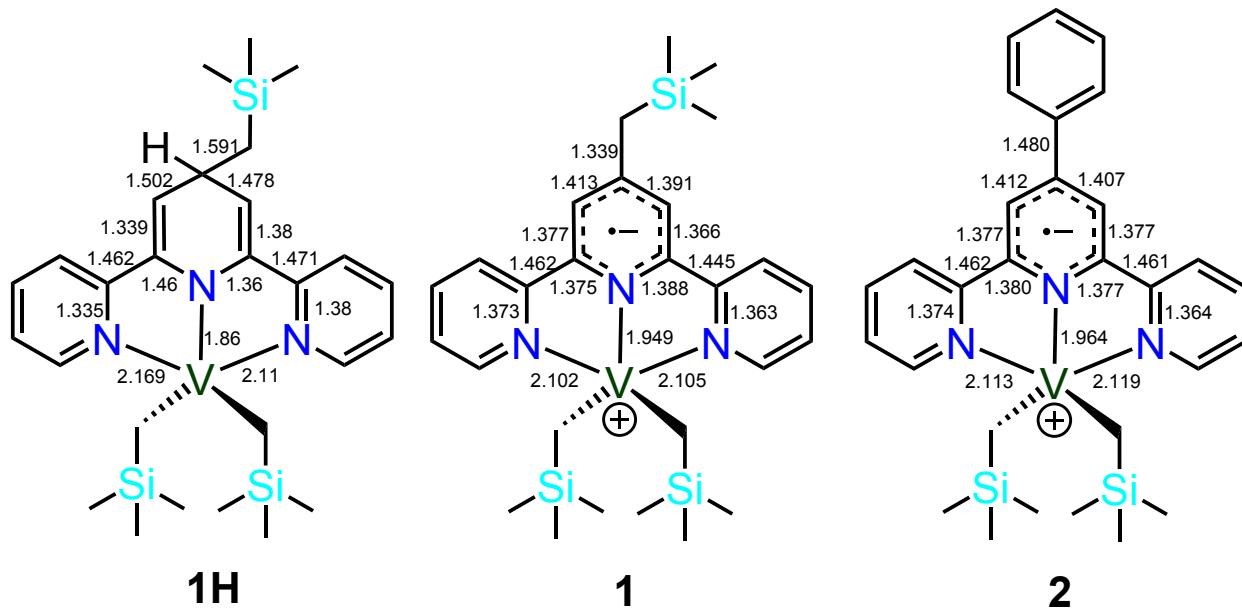


Table S1. X-ray crystallographic refinements for **1/1H**, **1**, **2**, and **6c·HCl**.

	1/1H	1	2	6c·HCl
lattice	Triclinic	Triclinic	Monoclinic	Orthorhombic
formula	C ₂₇ H _{43.44} N ₃ Si ₃ V	C ₂₇ H ₄₃ N ₃ Si ₃ V	C ₂₉ H ₃₇ N ₃ Si ₂ V	C ₈ H ₁₂ ClN
formula weight	545.30	544.85	534.73	157.64
space group	<i>P</i> - <i>I</i>	<i>P</i> - <i>I</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> ca2 ₁
<i>a</i> /Å	10.8649(9)	10.8676(7)	15.9192(11)	17.5887(18)
<i>b</i> /Å	12.4225(10)	12.3856(8)	9.2597(5)	5.0205(5)
<i>c</i> /Å	13.0617(11)	12.9182(8)	19.7266(12)	10.2381(11)
α/°	115.202(4)	115.3120(10)	90	90
β/°	96.239(4)	95.6150(10)	91.164(3)	90
γ/°	96.088(4)	97.3690(10)	90	90
<i>V</i> /Å ³	1562.8(2)	1536.12(17)	2907.2(3)	904.07(16)
<i>Z</i>	2	2	4	4
temperature (K)	130(2)	130(2)	130(2)	240(2)
radiation (λ , Å)	0.71073	0.71073	0.71073	0.71073
ρ (calcd.) g cm ⁻³	1.159	1.178	1.222	1.158
μ (Mo K α), mm ⁻¹	0.451	0.459	0.445	0.353
θ max, deg.	25.025	27.103	30.290	31.803
no. of data collected	53879	37951	66883	25822
no. of data	5523	6778	8044	3068
no. of parameters	485	316	322	100
R_I [$I > 2\sigma(I)$]	0.0590	0.0499	0.0440	0.0377
wR_2 [$I > 2\sigma(I)$]	0.1173	0.1080	0.0976	0.0735
R_I [all data]	0.1150	0.0973	0.0842	0.0765
wR_2 [all data]	0.1524	0.1293	0.1146	0.0862
GOF	1.062	1.012	1.042	1.019
R_{int}	0.0628	0.0772	0.0667	0.0548

Table S2. Bond lengths [\AA] and angles [$^\circ$] for **1/H**.

V(1)-N(2A)	1.86(2)	C(44)-H(44A)	0.9500
V(1)-N(2)	2.004(16)	C(45)-C(51)	1.459(15)
V(1)-N(3)	2.079(12)	N(3)-C(61)	1.355(17)
V(1)-C(11)	2.085(4)	N(3)-C(65)	1.392(14)
V(1)-C(21)	2.087(4)	C(61)-C(62)	1.38(2)
V(1)-N(1A)	2.11(3)	C(61)-H(61A)	0.9500
V(1)-N(1)	2.13(2)	C(62)-C(63)	1.385(19)
V(1)-N(3A)	2.169(14)	C(62)-H(62A)	0.9500
Si(1)-C(12)	1.847(6)	C(63)-C(64)	1.352(17)
Si(1)-C(14)	1.848(5)	C(63)-H(63A)	0.9500
Si(1)-C(11)	1.864(4)	C(64)-C(65)	1.382(15)
Si(1)-C(13)	1.888(5)	C(64)-H(64A)	0.9500
C(11)-H(11A)	0.9900	C(65)-C(55)	1.460(14)
C(11)-H(11B)	0.9900	N(2)-C(55)	1.344(19)
C(12)-H(12A)	0.9800	N(2)-C(51)	1.387(15)
C(12)-H(12B)	0.9800	C(51)-C(52)	1.338(18)
C(12)-H(12C)	0.9800	C(52)-C(53)	1.420(18)
C(13)-H(13A)	0.9800	C(52)-H(52A)	0.9500
C(13)-H(13B)	0.9800	C(53)-C(54)	1.401(16)
C(13)-H(13C)	0.9800	C(53)-C(31)	1.498(16)
C(14)-H(14A)	0.9800	C(54)-C(55)	1.403(16)
C(14)-H(14B)	0.9800	C(54)-H(54A)	0.9500
C(14)-H(14C)	0.9800	Si(3)-C(33)	1.74(2)
Si(2)-C(22)	1.847(8)	Si(3)-C(32)	1.759(18)
Si(2)-C(23)	1.851(6)	Si(3)-C(31)	1.891(12)
Si(2)-C(21)	1.855(5)	Si(3)-C(34)	2.01(2)
Si(2)-C(24)	1.880(5)	C(31)-H(31A)	0.9900
C(21)-H(21A)	0.9900	C(31)-H(31B)	0.9900
C(21)-H(21B)	0.9900	C(32)-H(32D)	0.9800
C(22)-H(22A)	0.9800	C(32)-H(32E)	0.9800
C(22)-H(22B)	0.9800	C(32)-H(32F)	0.9800
C(22)-H(22C)	0.9800	C(33)-H(33D)	0.9800
C(23)-H(23A)	0.9800	C(33)-H(33F)	0.9800
C(23)-H(23B)	0.9800	C(33)-H(33G)	0.9800
C(23)-H(23C)	0.9800	C(34)-H(34F)	0.9800
C(24)-H(24A)	0.9800	C(34)-H(34G)	0.9800
C(24)-H(24B)	0.9800	C(34)-H(34D)	0.9800
C(24)-H(24C)	0.9800	N(1A)-C(45A)	1.38(2)
N(1)-C(41)	1.33(2)	N(1A)-C(41A)	1.39(3)
N(1)-C(45)	1.35(2)	C(41A)-C(42A)	1.35(2)
C(41)-C(42)	1.39(2)	C(41A)-H(41B)	0.9500
C(41)-H(41A)	0.9500	C(42A)-C(43A)	1.395(19)
C(42)-C(43)	1.380(18)	C(42A)-H(42B)	0.9500
C(42)-H(42A)	0.9500	C(43A)-C(44A)	1.390(18)
C(43)-C(44)	1.361(18)	C(43A)-H(43B)	0.9500
C(43)-H(43A)	0.9500	C(44A)-C(45A)	1.36(2)
C(44)-C(45)	1.41(2)	C(44A)-H(44B)	0.9500

C(45A)-C(51A)	1.471(18)	C(11)-V(1)-N(1)	92.8(5)
N(3A)-C(65A)	1.335(19)	C(21)-V(1)-N(1)	95.9(4)
N(3A)-C(61A)	1.338(19)	N(2A)-V(1)-N(3A)	79.2(5)
C(61A)-C(62A)	1.36(2)	C(11)-V(1)-N(3A)	92.1(3)
C(61A)-H(61B)	0.9500	C(21)-V(1)-N(3A)	96.0(4)
C(62A)-C(63A)	1.37(2)	N(1A)-V(1)-N(3A)	157.2(4)
C(62A)-H(62B)	0.9500	C(12)-Si(1)-C(14)	109.7(3)
C(63A)-C(64A)	1.366(19)	C(12)-Si(1)-C(11)	109.3(2)
C(63A)-H(63B)	0.9500	C(14)-Si(1)-C(11)	110.7(2)
C(64A)-C(65A)	1.44(2)	C(12)-Si(1)-C(13)	106.5(3)
C(64A)-H(64B)	0.9500	C(14)-Si(1)-C(13)	106.9(3)
C(65A)-C(55A)	1.462(16)	C(11)-Si(1)-C(13)	113.5(2)
N(2A)-C(51A)	1.36(2)	Si(1)-C(11)-V(1)	115.9(2)
N(2A)-C(55A)	1.46(2)	Si(1)-C(11)-H(11A)	108.3
C(51A)-C(52A)	1.38(2)	V(1)-C(11)-H(11A)	108.3
C(52A)-C(53A)	1.478(19)	Si(1)-C(11)-H(11B)	108.3
C(52A)-H(52B)	0.9500	V(1)-C(11)-H(11B)	108.3
C(53A)-C(54A)	1.502(17)	H(11A)-C(11)-H(11B)	107.4
C(53A)-C(31A)	1.591(18)	Si(1)-C(12)-H(12A)	109.5
C(53A)-H(53A)	1.0000	Si(1)-C(12)-H(12B)	109.5
C(54A)-C(55A)	1.339(18)	H(12A)-C(12)-H(12B)	109.5
C(54A)-H(54B)	0.9500	Si(1)-C(12)-H(12C)	109.5
Si(3A)-C(32A)	1.809(15)	H(12A)-C(12)-H(12C)	109.5
Si(3A)-C(34A)	1.831(13)	H(12B)-C(12)-H(12C)	109.5
Si(3A)-C(31A)	1.895(13)	Si(1)-C(13)-H(13A)	109.5
Si(3A)-C(33A)	1.922(18)	Si(1)-C(13)-H(13B)	109.5
C(31A)-H(31C)	0.9900	H(13A)-C(13)-H(13B)	109.5
C(31A)-H(31D)	0.9900	Si(1)-C(13)-H(13C)	109.5
C(32A)-H(32A)	0.9800	H(13A)-C(13)-H(13C)	109.5
C(32A)-H(32B)	0.9800	H(13B)-C(13)-H(13C)	109.5
C(32A)-H(32C)	0.9800	Si(1)-C(14)-H(14A)	109.5
C(33A)-H(33A)	0.9800	Si(1)-C(14)-H(14B)	109.5
C(33A)-H(33B)	0.9800	H(14A)-C(14)-H(14B)	109.5
C(33A)-H(33C)	0.9800	Si(1)-C(14)-H(14C)	109.5
C(34A)-H(34A)	0.9800	H(14A)-C(14)-H(14C)	109.5
C(34A)-H(34B)	0.9800	H(14B)-C(14)-H(14C)	109.5
C(34A)-H(34C)	0.9800	C(22)-Si(2)-C(23)	108.2(5)
N(2)-V(1)-N(3)	76.9(4)	C(22)-Si(2)-C(21)	112.2(3)
N(2A)-V(1)-C(11)	122.5(5)	C(23)-Si(2)-C(21)	109.3(3)
N(2)-V(1)-C(11)	123.8(4)	C(22)-Si(2)-C(24)	106.2(4)
N(3)-V(1)-C(11)	99.4(3)	C(23)-Si(2)-C(24)	106.4(3)
N(2A)-V(1)-C(21)	120.3(5)	C(21)-Si(2)-C(24)	114.3(3)
N(2)-V(1)-C(21)	118.8(4)	Si(2)-C(21)-V(1)	116.6(2)
N(3)-V(1)-C(21)	98.8(3)	Si(2)-C(21)-H(21A)	108.1
C(11)-V(1)-C(21)	117.13(17)	V(1)-C(21)-H(21A)	108.1
N(2A)-V(1)-N(1A)	78.5(5)	Si(2)-C(21)-H(21B)	108.1
C(11)-V(1)-N(1A)	96.4(6)	V(1)-C(21)-H(21B)	108.1
C(21)-V(1)-N(1A)	98.7(5)	H(21A)-C(21)-H(21B)	107.3
N(2)-V(1)-N(1)	77.2(5)	Si(2)-C(22)-H(22A)	109.5
N(3)-V(1)-N(1)	154.0(3)	Si(2)-C(22)-H(22B)	109.5
		H(22A)-C(22)-H(22B)	109.5

Si(2)-C(22)-H(22C)	109.5	C(55)-N(2)-C(51)	118.9(13)
H(22A)-C(22)-H(22C)	109.5	C(55)-N(2)-V(1)	121.2(7)
H(22B)-C(22)-H(22C)	109.5	C(51)-N(2)-V(1)	119.8(10)
Si(2)-C(23)-H(23A)	109.5	C(52)-C(51)-N(2)	121.0(12)
Si(2)-C(23)-H(23B)	109.5	C(52)-C(51)-C(45)	126.9(12)
H(23A)-C(23)-H(23B)	109.5	N(2)-C(51)-C(45)	112.1(14)
Si(2)-C(23)-H(23C)	109.5	C(51)-C(52)-C(53)	122.0(11)
H(23A)-C(23)-H(23C)	109.5	C(51)-C(52)-H(52A)	119.0
H(23B)-C(23)-H(23C)	109.5	C(53)-C(52)-H(52A)	119.0
Si(2)-C(24)-H(24A)	109.5	C(54)-C(53)-C(52)	116.5(11)
Si(2)-C(24)-H(24B)	109.5	C(54)-C(53)-C(31)	119.9(13)
H(24A)-C(24)-H(24B)	109.5	C(52)-C(53)-C(31)	120.9(11)
Si(2)-C(24)-H(24C)	109.5	C(53)-C(54)-C(55)	119.6(11)
H(24A)-C(24)-H(24C)	109.5	C(53)-C(54)-H(54A)	120.2
H(24B)-C(24)-H(24C)	109.5	C(55)-C(54)-H(54A)	120.2
C(41)-N(1)-C(45)	121.0(18)	N(2)-C(55)-C(54)	121.9(10)
C(41)-N(1)-V(1)	124.3(14)	N(2)-C(55)-C(65)	112.0(11)
C(45)-N(1)-V(1)	114.6(9)	C(54)-C(55)-C(65)	126.2(12)
N(1)-C(41)-C(42)	120.9(16)	C(33)-Si(3)-C(32)	122.7(12)
N(1)-C(41)-H(41A)	119.6	C(33)-Si(3)-C(31)	109.7(8)
C(42)-C(41)-H(41A)	119.6	C(32)-Si(3)-C(31)	107.8(7)
C(43)-C(42)-C(41)	118.7(16)	C(33)-Si(3)-C(34)	105.4(11)
C(43)-C(42)-H(42A)	120.7	C(32)-Si(3)-C(34)	105.7(10)
C(41)-C(42)-H(42A)	120.7	C(31)-Si(3)-C(34)	104.0(10)
C(44)-C(43)-C(42)	121.3(14)	C(53)-C(31)-Si(3)	109.5(8)
C(44)-C(43)-H(43A)	119.3	C(53)-C(31)-H(31A)	109.8
C(42)-C(43)-H(43A)	119.3	Si(3)-C(31)-H(31A)	109.8
C(43)-C(44)-C(45)	117.5(13)	C(53)-C(31)-H(31B)	109.8
C(43)-C(44)-H(44A)	121.2	Si(3)-C(31)-H(31B)	109.8
C(45)-C(44)-H(44A)	121.2	H(31A)-C(31)-H(31B)	108.2
N(1)-C(45)-C(44)	120.6(12)	Si(3)-C(32)-H(32D)	109.5
N(1)-C(45)-C(51)	116.2(14)	Si(3)-C(32)-H(32E)	109.5
C(44)-C(45)-C(51)	123.2(13)	H(32D)-C(32)-H(32E)	109.5
C(61)-N(3)-C(65)	118.1(12)	Si(3)-C(32)-H(32F)	109.5
C(61)-N(3)-V(1)	126.5(10)	H(32D)-C(32)-H(32F)	109.5
C(65)-N(3)-V(1)	115.2(7)	H(32E)-C(32)-H(32F)	109.5
N(3)-C(61)-C(62)	122.4(13)	Si(3)-C(33)-H(33D)	109.5
N(3)-C(61)-H(61A)	118.8	Si(3)-C(33)-H(33F)	109.5
C(62)-C(61)-H(61A)	118.8	H(33D)-C(33)-H(33F)	109.5
C(61)-C(62)-C(63)	119.2(13)	Si(3)-C(33)-H(33G)	109.5
C(61)-C(62)-H(62A)	120.4	H(33D)-C(33)-H(33G)	109.5
C(63)-C(62)-H(62A)	120.4	H(33F)-C(33)-H(33G)	109.5
C(64)-C(63)-C(62)	118.8(13)	Si(3)-C(34)-H(34F)	109.5
C(64)-C(63)-H(63A)	120.6	Si(3)-C(34)-H(34G)	109.5
C(62)-C(63)-H(63A)	120.6	H(34F)-C(34)-H(34G)	109.5
C(63)-C(64)-C(65)	121.9(13)	Si(3)-C(34)-H(34D)	109.5
C(63)-C(64)-H(64A)	119.0	H(34F)-C(34)-H(34D)	109.5
C(65)-C(64)-H(64A)	119.0	H(34G)-C(34)-H(34D)	109.5
C(64)-C(65)-N(3)	119.5(12)	C(45A)-N(1A)-C(41A)	117(2)
C(64)-C(65)-C(55)	126.1(11)	C(45A)-N(1A)-V(1)	113.0(12)
N(3)-C(65)-C(55)	114.4(11)	C(41A)-N(1A)-V(1)	130.3(14)

C(42A)-C(41A)-N(1A)	125.8(17)	C(52A)-C(53A)-C(54A)	112.9(12)
C(42A)-C(41A)-H(41B)	117.1	C(52A)-C(53A)-C(31A)	109.6(12)
N(1A)-C(41A)-H(41B)	117.1	C(54A)-C(53A)-C(31A)	107.5(13)
C(41A)-C(42A)-C(43A)	116.0(16)	C(52A)-C(53A)-H(53A)	108.9
C(41A)-C(42A)-H(42B)	122.0	C(54A)-C(53A)-H(53A)	108.9
C(43A)-C(42A)-H(42B)	122.0	C(31A)-C(53A)-H(53A)	108.9
C(44A)-C(43A)-C(42A)	120.1(16)	C(55A)-C(54A)-C(53A)	123.1(12)
C(44A)-C(43A)-H(43B)	119.9	C(55A)-C(54A)-H(54B)	118.4
C(42A)-C(43A)-H(43B)	119.9	C(53A)-C(54A)-H(54B)	118.4
C(45A)-C(44A)-C(43A)	121.7(17)	C(54A)-C(55A)-N(2A)	121.6(14)
C(45A)-C(44A)-H(44B)	119.2	C(54A)-C(55A)-C(65A)	127.6(13)
C(43A)-C(44A)-H(44B)	119.2	N(2A)-C(55A)-C(65A)	110.8(13)
C(44A)-C(45A)-N(1A)	119.8(16)	C(32A)-Si(3A)-C(34A)	115.2(6)
C(44A)-C(45A)-C(51A)	127.0(16)	C(32A)-Si(3A)-C(31A)	107.0(7)
N(1A)-C(45A)-C(51A)	113.2(18)	C(34A)-Si(3A)-C(31A)	107.8(6)
C(65A)-N(3A)-C(61A)	118.9(14)	C(32A)-Si(3A)-C(33A)	107.4(9)
C(65A)-N(3A)-V(1)	112.5(8)	C(34A)-Si(3A)-C(33A)	107.7(7)
C(61A)-N(3A)-V(1)	128.5(12)	C(31A)-Si(3A)-C(33A)	111.9(8)
N(3A)-C(61A)-C(62A)	122.6(15)	C(53A)-C(31A)-Si(3A)	118.3(9)
N(3A)-C(61A)-H(61B)	118.7	C(53A)-C(31A)-H(31C)	107.7
C(62A)-C(61A)-H(61B)	118.7	Si(3A)-C(31A)-H(31C)	107.7
C(61A)-C(62A)-C(63A)	119.7(14)	C(53A)-C(31A)-H(31D)	107.7
C(61A)-C(62A)-H(62B)	120.2	Si(3A)-C(31A)-H(31D)	107.7
C(63A)-C(62A)-H(62B)	120.2	H(31C)-C(31A)-H(31D)	107.1
C(64A)-C(63A)-C(62A)	120.2(14)	Si(3A)-C(32A)-H(32A)	109.5
C(64A)-C(63A)-H(63B)	119.9	Si(3A)-C(32A)-H(32B)	109.5
C(62A)-C(63A)-H(63B)	119.9	H(32A)-C(32A)-H(32B)	109.5
C(63A)-C(64A)-C(65A)	117.3(14)	Si(3A)-C(32A)-H(32C)	109.5
C(63A)-C(64A)-H(64B)	121.4	H(32A)-C(32A)-H(32C)	109.5
C(65A)-C(64A)-H(64B)	121.4	H(32B)-C(32A)-H(32C)	109.5
N(3A)-C(65A)-C(64A)	121.3(12)	Si(3A)-C(33A)-H(33A)	109.5
N(3A)-C(65A)-C(55A)	116.4(13)	Si(3A)-C(33A)-H(33B)	109.5
C(64A)-C(65A)-C(55A)	122.2(13)	H(33A)-C(33A)-H(33B)	109.5
C(51A)-N(2A)-C(55A)	115.4(16)	Si(3A)-C(33A)-H(33C)	109.5
C(51A)-N(2A)-V(1)	123.6(13)	H(33A)-C(33A)-H(33C)	109.5
C(55A)-N(2A)-V(1)	121.0(9)	H(33B)-C(33A)-H(33C)	109.5
N(2A)-C(51A)-C(52A)	126.9(15)	Si(3A)-C(34A)-H(34A)	109.5
N(2A)-C(51A)-C(45A)	111.6(17)	Si(3A)-C(34A)-H(34B)	109.5
C(52A)-C(51A)-C(45A)	121.4(15)	H(34A)-C(34A)-H(34B)	109.5
C(51A)-C(52A)-C(53A)	118.9(14)	Si(3A)-C(34A)-H(34C)	109.5
C(51A)-C(52A)-H(52B)	120.6	H(34A)-C(34A)-H(34C)	109.5
C(53A)-C(52A)-H(52B)	120.6	H(34B)-C(34A)-H(34C)	109.5

Table S3. Bond lengths [\AA] and angles [$^\circ$] for **1**.

V(1)-N(2)	1.949(2)	N(1)-C(41)	1.350(4)
V(1)-C(21)	2.096(3)	N(1)-C(45)	1.363(3)
V(1)-C(11)	2.097(3)	N(2)-C(55)	1.375(4)
V(1)-N(3)	2.102(2)	N(2)-C(51)	1.388(3)
V(1)-N(1)	2.105(2)	N(3)-C(61)	1.346(3)

N(3)-C(65)	1.373(4)	C(31)-H(31A)	0.9900
Si(1)-C(11)	1.847(3)	C(31)-H(31B)	0.9900
Si(1)-C(12)	1.851(4)	C(32)-H(32A)	0.9800
Si(1)-C(14)	1.863(3)	C(32)-H(32B)	0.9800
Si(1)-C(13)	1.870(3)	C(32)-H(32C)	0.9800
Si(2)-C(21)	1.843(3)	C(33)-H(33A)	0.9800
Si(2)-C(22)	1.864(4)	C(33)-H(33B)	0.9800
Si(2)-C(24)	1.875(3)	C(33)-H(33C)	0.9800
Si(2)-C(23)	1.881(3)	C(34)-H(34A)	0.9800
Si(3)-C(32)	1.856(4)	C(34)-H(34B)	0.9800
Si(3)-C(34)	1.862(4)	C(34)-H(34C)	0.9800
Si(3)-C(33)	1.872(5)	C(41)-C(42)	1.369(4)
Si(3)-C(31)	1.874(3)	C(41)-H(41A)	0.9500
C(11)-H(11A)	0.9900	C(42)-C(43)	1.372(5)
C(11)-H(11B)	0.9900	C(42)-H(42A)	0.9500
C(12)-H(12A)	0.9800	C(43)-C(44)	1.358(5)
C(12)-H(12B)	0.9800	C(43)-H(43A)	0.9500
C(12)-H(12C)	0.9800	C(44)-C(45)	1.398(4)
C(13)-H(13A)	0.9800	C(44)-H(44A)	0.9500
C(13)-H(13B)	0.9800	C(45)-C(51)	1.445(4)
C(13)-H(13C)	0.9800	C(51)-C(52)	1.366(4)
C(14)-H(14A)	0.9800	C(52)-C(53)	1.391(4)
C(14)-H(14B)	0.9800	C(52)-H(52A)	0.9500
C(14)-H(14C)	0.9800	C(53)-C(54)	1.413(4)
C(21)-H(21A)	0.9900	C(54)-C(55)	1.377(4)
C(21)-H(21B)	0.9900	C(54)-H(54A)	0.9500
C(22)-H(22A)	0.9800	C(55)-C(65)	1.462(4)
C(22)-H(22B)	0.9800	C(61)-C(62)	1.378(4)
C(22)-H(22C)	0.9800	C(61)-H(61A)	0.9500
C(23)-H(23A)	0.9800	C(62)-C(63)	1.389(5)
C(23)-H(23B)	0.9800	C(62)-H(62A)	0.9500
C(23)-H(23C)	0.9800	C(63)-C(64)	1.361(5)
C(24)-H(24A)	0.9800	C(63)-H(63A)	0.9500
C(24)-H(24B)	0.9800	C(64)-C(65)	1.387(4)
C(24)-H(24C)	0.9800	C(64)-H(64A)	0.9500
C(31)-C(53)	1.500(4)		
		C(55)-N(2)-V(1)	121.21(18)
N(2)-V(1)-C(21)	118.29(10)	C(51)-N(2)-V(1)	119.83(18)
N(2)-V(1)-C(11)	123.25(10)	C(61)-N(3)-C(65)	118.5(3)
C(21)-V(1)-C(11)	118.46(11)	C(61)-N(3)-V(1)	126.8(2)
N(2)-V(1)-N(3)	77.55(9)	C(65)-N(3)-V(1)	114.68(18)
C(21)-V(1)-N(3)	96.84(10)	C(11)-Si(1)-C(12)	110.07(16)
C(11)-V(1)-N(3)	96.43(11)	C(11)-Si(1)-C(14)	110.73(14)
N(2)-V(1)-N(1)	77.74(9)	C(12)-Si(1)-C(14)	107.7(2)
C(21)-V(1)-N(1)	97.43(10)	C(11)-Si(1)-C(13)	114.36(15)
C(11)-V(1)-N(1)	94.55(10)	C(12)-Si(1)-C(13)	106.9(2)
N(3)-V(1)-N(1)	155.11(9)	C(14)-Si(1)-C(13)	106.88(18)
C(41)-N(1)-C(45)	118.1(2)	C(21)-Si(2)-C(22)	112.39(15)
C(41)-N(1)-V(1)	126.9(2)	C(21)-Si(2)-C(24)	109.74(14)
C(45)-N(1)-V(1)	114.99(18)	C(22)-Si(2)-C(24)	107.98(18)
C(55)-N(2)-C(51)	118.6(2)	C(21)-Si(2)-C(23)	113.96(15)

C(22)-Si(2)-C(23)	105.58(17)	Si(2)-C(24)-H(24B)	109.5
C(24)-Si(2)-C(23)	106.85(15)	H(24A)-C(24)-H(24B)	109.5
C(32)-Si(3)-C(34)	108.2(2)	Si(2)-C(24)-H(24C)	109.5
C(32)-Si(3)-C(33)	109.8(2)	H(24A)-C(24)-H(24C)	109.5
C(34)-Si(3)-C(33)	110.7(2)	H(24B)-C(24)-H(24C)	109.5
C(32)-Si(3)-C(31)	111.0(2)	C(53)-C(31)-Si(3)	110.9(2)
C(34)-Si(3)-C(31)	109.42(17)	C(53)-C(31)-H(31A)	109.5
C(33)-Si(3)-C(31)	107.67(18)	Si(3)-C(31)-H(31A)	109.5
Si(1)-C(11)-V(1)	115.10(14)	C(53)-C(31)-H(31B)	109.5
Si(1)-C(11)-H(11A)	108.5	Si(3)-C(31)-H(31B)	109.5
V(1)-C(11)-H(11A)	108.5	H(31A)-C(31)-H(31B)	108.1
Si(1)-C(11)-H(11B)	108.5	Si(3)-C(32)-H(32A)	109.5
V(1)-C(11)-H(11B)	108.5	Si(3)-C(32)-H(32B)	109.5
H(11A)-C(11)-H(11B)	107.5	H(32A)-C(32)-H(32B)	109.5
Si(1)-C(12)-H(12A)	109.5	Si(3)-C(32)-H(32C)	109.5
Si(1)-C(12)-H(12B)	109.5	H(32A)-C(32)-H(32C)	109.5
H(12A)-C(12)-H(12B)	109.5	H(32B)-C(32)-H(32C)	109.5
Si(1)-C(12)-H(12C)	109.5	Si(3)-C(33)-H(33A)	109.5
H(12A)-C(12)-H(12C)	109.5	Si(3)-C(33)-H(33B)	109.5
H(12B)-C(12)-H(12C)	109.5	H(33A)-C(33)-H(33B)	109.5
Si(1)-C(13)-H(13A)	109.5	Si(3)-C(33)-H(33C)	109.5
Si(1)-C(13)-H(13B)	109.5	H(33A)-C(33)-H(33C)	109.5
H(13A)-C(13)-H(13B)	109.5	H(33B)-C(33)-H(33C)	109.5
Si(1)-C(13)-H(13C)	109.5	Si(3)-C(34)-H(34A)	109.5
H(13A)-C(13)-H(13C)	109.5	Si(3)-C(34)-H(34B)	109.5
H(13B)-C(13)-H(13C)	109.5	H(34A)-C(34)-H(34B)	109.5
Si(1)-C(14)-H(14A)	109.5	Si(3)-C(34)-H(34C)	109.5
Si(1)-C(14)-H(14B)	109.5	H(34A)-C(34)-H(34C)	109.5
H(14A)-C(14)-H(14B)	109.5	H(34B)-C(34)-H(34C)	109.5
Si(1)-C(14)-H(14C)	109.5	N(1)-C(41)-C(42)	123.0(3)
H(14A)-C(14)-H(14C)	109.5	N(1)-C(41)-H(41A)	118.5
H(14B)-C(14)-H(14C)	109.5	C(42)-C(41)-H(41A)	118.5
Si(2)-C(21)-V(1)	117.32(14)	C(41)-C(42)-C(43)	118.8(3)
Si(2)-C(21)-H(21A)	108.0	C(41)-C(42)-H(42A)	120.6
V(1)-C(21)-H(21A)	108.0	C(43)-C(42)-H(42A)	120.6
Si(2)-C(21)-H(21B)	108.0	C(44)-C(43)-C(42)	119.8(3)
V(1)-C(21)-H(21B)	108.0	C(44)-C(43)-H(43A)	120.1
H(21A)-C(21)-H(21B)	107.2	C(42)-C(43)-H(43A)	120.1
Si(2)-C(22)-H(22A)	109.5	C(43)-C(44)-C(45)	119.9(3)
Si(2)-C(22)-H(22B)	109.5	C(43)-C(44)-H(44A)	120.1
H(22A)-C(22)-H(22B)	109.5	C(45)-C(44)-H(44A)	120.1
Si(2)-C(22)-H(22C)	109.5	N(1)-C(45)-C(44)	120.4(3)
H(22A)-C(22)-H(22C)	109.5	N(1)-C(45)-C(51)	114.0(2)
H(22B)-C(22)-H(22C)	109.5	C(44)-C(45)-C(51)	125.5(3)
Si(2)-C(23)-H(23A)	109.5	C(52)-C(51)-N(2)	121.2(3)
Si(2)-C(23)-H(23B)	109.5	C(52)-C(51)-C(45)	125.6(3)
H(23A)-C(23)-H(23B)	109.5	N(2)-C(51)-C(45)	113.1(2)
Si(2)-C(23)-H(23C)	109.5	C(51)-C(52)-C(53)	121.1(3)
H(23A)-C(23)-H(23C)	109.5	C(51)-C(52)-H(52A)	119.4
H(23B)-C(23)-H(23C)	109.5	C(53)-C(52)-H(52A)	119.4
Si(2)-C(24)-H(24A)	109.5	C(52)-C(53)-C(54)	117.4(3)

C(52)-C(53)-C(31)	119.9(3)	C(61)-C(62)-H(62A)	120.7
C(54)-C(53)-C(31)	121.5(3)	C(63)-C(62)-H(62A)	120.7
C(55)-C(54)-C(53)	120.6(3)	C(64)-C(63)-C(62)	120.0(3)
C(55)-C(54)-H(54A)	119.7	C(64)-C(63)-H(63A)	120.0
C(53)-C(54)-H(54A)	119.7	C(62)-C(63)-H(63A)	120.0
N(2)-C(55)-C(54)	121.0(3)	C(63)-C(64)-C(65)	119.5(3)
N(2)-C(55)-C(65)	111.8(2)	C(63)-C(64)-H(64A)	120.3
C(54)-C(55)-C(65)	127.1(3)	C(65)-C(64)-H(64A)	120.3
N(3)-C(61)-C(62)	122.3(3)	N(3)-C(65)-C(64)	121.0(3)
N(3)-C(61)-H(61A)	118.8	N(3)-C(65)-C(55)	114.3(2)
C(62)-C(61)-H(61A)	118.8	C(64)-C(65)-C(55)	124.6(3)
C(61)-C(62)-C(63)	118.6(3)		

Table S4. Bond lengths [Å] and angles [°] for **2**.

V(1)-N(2)	1.9643(15)	N(1)-C(35)	1.364(2)
V(1)-C(21)	2.089(2)	C(31)-C(32)	1.370(3)
V(1)-C(11)	2.0895(18)	C(31)-H(31A)	0.9500
V(1)-N(3)	2.1133(16)	C(32)-C(33)	1.385(3)
V(1)-N(1)	2.1193(16)	C(32)-H(32A)	0.9500
C(11)-Si(1)	1.855(2)	C(33)-C(34)	1.380(3)
C(11)-H(11A)	0.9900	C(33)-H(33A)	0.9500
C(11)-H(11B)	0.9900	C(34)-C(35)	1.394(3)
Si(1)-C(14)	1.868(2)	C(34)-H(34A)	0.9500
Si(1)-C(12)	1.876(2)	C(35)-C(41)	1.461(3)
Si(1)-C(13)	1.881(2)	N(2)-C(41)	1.377(2)
C(12)-H(12A)	0.9800	N(2)-C(45)	1.380(2)
C(12)-H(12B)	0.9800	C(41)-C(42)	1.377(2)
C(12)-H(12C)	0.9800	C(42)-C(43)	1.407(3)
C(13)-H(13A)	0.9800	C(42)-H(42A)	0.9500
C(13)-H(13B)	0.9800	C(43)-C(44)	1.412(3)
C(13)-H(13C)	0.9800	C(43)-C(61)	1.480(3)
C(14)-H(14A)	0.9800	C(44)-C(45)	1.377(3)
C(14)-H(14B)	0.9800	C(44)-H(44A)	0.9500
C(14)-H(14C)	0.9800	C(45)-C(55)	1.462(3)
C(21)-Si(2)	1.8514(19)	N(3)-C(51)	1.358(2)
C(21)-H(21A)	0.9900	N(3)-C(55)	1.374(2)
C(21)-H(21B)	0.9900	C(51)-C(52)	1.374(3)
Si(2)-C(24)	1.869(2)	C(51)-H(51A)	0.9500
Si(2)-C(23)	1.870(2)	C(52)-C(53)	1.387(3)
Si(2)-C(22)	1.878(2)	C(52)-H(52A)	0.9500
C(22)-H(22A)	0.9800	C(53)-C(54)	1.380(3)
C(22)-H(22B)	0.9800	C(53)-H(53A)	0.9500
C(22)-H(22C)	0.9800	C(54)-C(55)	1.393(3)
C(23)-H(23A)	0.9800	C(54)-H(54A)	0.9500
C(23)-H(23B)	0.9800	C(61)-C(62)	1.388(3)
C(23)-H(23C)	0.9800	C(61)-C(66)	1.402(3)
C(24)-H(24A)	0.9800	C(62)-C(63)	1.384(3)
C(24)-H(24B)	0.9800	C(62)-H(62A)	0.9500
C(24)-H(24C)	0.9800	C(63)-C(64)	1.376(3)
N(1)-C(31)	1.349(2)	C(63)-H(63A)	0.9500

C(64)-C(65)	1.378(3)	C(65)-H(65A)	0.9500
C(64)-H(64A)	0.9500	C(66)-H(66A)	0.9500
C(65)-C(66)	1.380(3)		
N(2)-V(1)-C(21)	121.33(7)	C(21)-Si(2)-C(24)	112.68(10)
N(2)-V(1)-C(11)	120.95(7)	C(21)-Si(2)-C(23)	110.60(11)
C(21)-V(1)-C(11)	117.73(7)	C(24)-Si(2)-C(23)	106.60(12)
N(2)-V(1)-N(3)	77.54(6)	C(21)-Si(2)-C(22)	110.64(10)
C(21)-V(1)-N(3)	97.73(7)	C(24)-Si(2)-C(22)	107.02(11)
C(11)-V(1)-N(3)	95.48(7)	C(23)-Si(2)-C(22)	109.13(14)
N(2)-V(1)-N(1)	77.39(6)	Si(2)-C(22)-H(22A)	109.5
C(21)-V(1)-N(1)	96.06(7)	Si(2)-C(22)-H(22B)	109.5
C(11)-V(1)-N(1)	96.51(7)	H(22A)-C(22)-H(22B)	109.5
N(3)-V(1)-N(1)	154.91(6)	Si(2)-C(22)-H(22C)	109.5
Si(1)-C(11)-V(1)	116.06(9)	H(22A)-C(22)-H(22C)	109.5
Si(1)-C(11)-H(11A)	108.3	H(22B)-C(22)-H(22C)	109.5
V(1)-C(11)-H(11A)	108.3	Si(2)-C(23)-H(23A)	109.5
Si(1)-C(11)-H(11B)	108.3	Si(2)-C(23)-H(23B)	109.5
V(1)-C(11)-H(11B)	108.3	H(23A)-C(23)-H(23B)	109.5
H(11A)-C(11)-H(11B)	107.4	Si(2)-C(23)-H(23C)	109.5
C(11)-Si(1)-C(14)	110.82(10)	H(23A)-C(23)-H(23C)	109.5
C(11)-Si(1)-C(12)	112.13(10)	H(23B)-C(23)-H(23C)	109.5
C(14)-Si(1)-C(12)	107.23(12)	Si(2)-C(24)-H(24A)	109.5
C(11)-Si(1)-C(13)	111.18(9)	Si(2)-C(24)-H(24B)	109.5
C(14)-Si(1)-C(13)	107.23(12)	H(24A)-C(24)-H(24B)	109.5
C(12)-Si(1)-C(13)	108.04(11)	Si(2)-C(24)-H(24C)	109.5
Si(1)-C(12)-H(12A)	109.5	H(24A)-C(24)-H(24C)	109.5
Si(1)-C(12)-H(12B)	109.5	H(24B)-C(24)-H(24C)	109.5
H(12A)-C(12)-H(12B)	109.5	C(31)-N(1)-C(35)	118.08(16)
Si(1)-C(12)-H(12C)	109.5	C(31)-N(1)-V(1)	126.85(13)
H(12A)-C(12)-H(12C)	109.5	C(35)-N(1)-V(1)	115.07(12)
H(12B)-C(12)-H(12C)	109.5	N(1)-C(31)-C(32)	123.24(18)
Si(1)-C(13)-H(13A)	109.5	N(1)-C(31)-H(31A)	118.4
Si(1)-C(13)-H(13B)	109.5	C(32)-C(31)-H(31A)	118.4
H(13A)-C(13)-H(13B)	109.5	C(31)-C(32)-C(33)	118.83(18)
Si(1)-C(13)-H(13C)	109.5	C(31)-C(32)-H(32A)	120.6
H(13A)-C(13)-H(13C)	109.5	C(33)-C(32)-H(32A)	120.6
H(13B)-C(13)-H(13C)	109.5	C(34)-C(33)-C(32)	119.19(19)
Si(1)-C(14)-H(14A)	109.5	C(34)-C(33)-H(33A)	120.4
Si(1)-C(14)-H(14B)	109.5	C(32)-C(33)-H(33A)	120.4
H(14A)-C(14)-H(14B)	109.5	C(33)-C(34)-C(35)	119.55(18)
Si(1)-C(14)-H(14C)	109.5	C(33)-C(34)-H(34A)	120.2
H(14A)-C(14)-H(14C)	109.5	C(35)-C(34)-H(34A)	120.2
H(14B)-C(14)-H(14C)	109.5	N(1)-C(35)-C(34)	121.10(17)
Si(2)-C(21)-V(1)	115.64(9)	N(1)-C(35)-C(41)	113.96(16)
Si(2)-C(21)-H(21A)	108.4	C(34)-C(35)-C(41)	124.94(17)
V(1)-C(21)-H(21A)	108.4	C(41)-N(2)-C(45)	119.00(15)
Si(2)-C(21)-H(21B)	108.4	C(41)-N(2)-V(1)	120.45(12)
V(1)-C(21)-H(21B)	108.4	C(45)-N(2)-V(1)	120.55(12)
H(21A)-C(21)-H(21B)	107.4	N(2)-C(41)-C(42)	121.13(16)

N(2)-C(41)-C(35)	113.11(15)
C(42)-C(41)-C(35)	125.76(17)
C(41)-C(42)-C(43)	120.78(17)
C(41)-C(42)-H(42A)	119.6
C(43)-C(42)-H(42A)	119.6
C(42)-C(43)-C(44)	117.36(17)
C(42)-C(43)-C(61)	120.95(17)
C(44)-C(43)-C(61)	121.69(17)
C(45)-C(44)-C(43)	120.50(17)
C(45)-C(44)-H(44A)	119.8
C(43)-C(44)-H(44A)	119.8
C(44)-C(45)-N(2)	121.23(17)
C(44)-C(45)-C(55)	125.78(17)
N(2)-C(45)-C(55)	112.97(16)
C(51)-N(3)-C(55)	117.62(17)
C(51)-N(3)-V(1)	127.22(14)
C(55)-N(3)-V(1)	115.08(12)
N(3)-C(51)-C(52)	123.1(2)
N(3)-C(51)-H(51A)	118.5
C(52)-C(51)-H(51A)	118.5
C(51)-C(52)-C(53)	119.15(19)
C(51)-C(52)-H(52A)	120.4
C(53)-C(52)-H(52A)	120.4
C(54)-C(53)-C(52)	119.1(2)
C(54)-C(53)-H(53A)	120.4
C(52)-C(53)-H(53A)	120.4
C(53)-C(54)-C(55)	119.7(2)
C(53)-C(54)-H(54A)	120.2
C(55)-C(54)-H(54A)	120.2
N(3)-C(55)-C(54)	121.35(17)
N(3)-C(55)-C(45)	113.83(16)
C(54)-C(55)-C(45)	124.79(18)
C(62)-C(61)-C(66)	117.46(18)
C(62)-C(61)-C(43)	121.47(18)
C(66)-C(61)-C(43)	121.08(18)
C(63)-C(62)-C(61)	121.1(2)
C(63)-C(62)-H(62A)	119.4
C(61)-C(62)-H(62A)	119.4
C(64)-C(63)-C(62)	120.7(2)
C(64)-C(63)-H(63A)	119.6
C(62)-C(63)-H(63A)	119.6
C(63)-C(64)-C(65)	119.1(2)
C(63)-C(64)-H(64A)	120.5
C(65)-C(64)-H(64A)	120.5
C(64)-C(65)-C(66)	120.7(2)
C(64)-C(65)-H(65A)	119.6
C(66)-C(65)-H(65A)	119.6
C(65)-C(66)-C(61)	120.9(2)
C(65)-C(66)-H(66A)	119.5
C(61)-C(66)-H(66A)	119.5

Computational Details. Computational analysis for spin projection S_z of 3/2 and 1/2 was performed by using unabridged models with code Gaussian 09 (rev. E01),⁵ unrestricted density functional theory (UDFT)⁶ and the SMD polarizable continuum model (solvent = diethyl ether).⁷ Initial guess for a possible V^{II} (d^3) state was generated by using GaussView 5.0 Gaussian Fragment Option (Atom Groups Editor). Quartet (two α -spin electrons on the metal and one α -spin electron on the ligand, $|\uparrow\rangle_L|\uparrow\rangle_V$) was modeled by using standard Gaussian input parameters (charge = 0, multiplicity = 4) following Mulliken spin densities analysis. Initial guess for the doublet wavefunction (two α -spin electrons on the metal and one β -spin electron on the ligand, $|\downarrow\rangle_L|\uparrow\rangle_V$) was generated by using GaussView 5.0 Gaussian Fragment Option (Atom Groups Editor) within the broken-symmetry (BS) formalism⁸ as shown elsewhere.⁹ Wavefunctions were checked for the stabilities in each case. Doublet wavefunctions were found to be spin-contaminated (assuming that the “cutoff” for contamination is >30% contribution from quartet), and the Yamaguchi correction was applied for electronic energies:¹⁰

$${}^2E_{corr} = {}^2E + f({}^2E - {}^4E); \quad f = \frac{{}^2\langle S^2 \rangle}{{}^4\langle S^2 \rangle - {}^2\langle S^2 \rangle},$$

where $\langle S^2 \rangle$ is eigenvalue for the spin-squared operator \hat{S}^2 (expected eigenvalues for doublet and quartet are 0.75 and 3.75, respectively). Geometry optimization and frequency calculations for ${}^4\mathbf{1}$ and ${}^2\mathbf{1}$ were performed with an ultrafine integration grid and an increased integral accuracy (1×10^{-12}) and by using hybrid ω B97X-D functional¹¹ incorporating Grimme’s D2 dispersion model¹² and contacting 22.2% Hartee-Fock exchange term, as well as Minnesota hybrid M06 (27% Hartee-Fock exchange term), M062X (54% Hartee-Fock exchange term) and M06HF (100% Hartee-Fock exchange term) functionals¹³ corrected by Grimme’s D3 dispersion model,¹⁴ respectively. Basis sets def2-SVP (all atoms), def2-TZVP (all atoms), 6-311++G***(C,H,N, Si)/ECP10MDF(V)¹⁵ were used as specified. Ultrafine integration grid and standard integral accuracy was used for meta-GGA M06L¹⁶ functional. Mulliken spin density plots (difference between alpha- and beta-spin densities corresponding to the unpaired spin density at a given atom) were generated using the UCSF Chimera package¹⁷ with the optimized Cartesian coordinates of atoms as input data. Computational analysis presented in Scheme 4 and Scheme 9 was performed at the ω B97X-D/def2-SVP(Integral(UltraFineGrid))/SMD(diethyl ether) level. The final Gibbs free energies in continuum solvent, G (directly obtainable from output files under default $T = 298.15$ K, $C = 1$ atm with the harmonic approximation and a scaling factor = 1.0), were corrected to the standard state in solution (1 M), by adding 0.00301 Hartree. Tables S5–S7 contain additional information.

Table S5. Energy data for ${}^4\mathbf{1}$ vs ${}^2\mathbf{1}$ (Hartree).

M06L/def2svp Integral(UltraFineGrid) scrf=(smd,solvent=DiEthylEther)								
	$\langle S^2 \rangle$	E	G	v, cm ⁻¹	f	E_{corr}	$G - E$	G_{corr}
${}^4\mathbf{1}$	3.795	-3030.303106	-3029.753898					
${}^2\mathbf{1}$	1.79	-3030.297715	-3029.748326		0.894658	-3030.29289	0.549389	-3029.743502
wb97xd/def2svp integral=(ultrafinegrid,acc2e=12) scrf=(smd,solvent=DiEthylEther)								
	$\langle S^2 \rangle$	E	G	v, cm ⁻¹	f	E_{corr}	$G - E$	G_{corr}
${}^4\mathbf{1}$	3.799	-3030.108	-3029.55358					
${}^2\mathbf{1}$	1.79	-3030.10546	-3029.55026		0.890991	-3030.1032	0.555204	-3029.54799

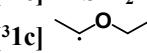
wb97xd/def2tzvp integral=(ultrafinegrid,acc2e=12) scrf=(smd,solvent=DiEthylEther)						
	<S ² >	E	G	f	E _{corr}	G – E
41	3.797	-3031.82908	-3031.27435	i14		
21	1.787	-3031.82637	-3031.27239		0.889055	-3031.82397
wb97xd/6-311++G** integral=(ultrafinegrid,acc2e=12) ECP10MDF scrf=(smd,solvent=DiEthylEther)						
	<S ² >	E	G	f	E _{corr}	G – E
41	3.797	-2159.36026	-2158.80835			
21	1.787	-2159.35796	-2158.80421		0.889055	-2159.35591
M06-D3/Def2SVP integral=(ultrafinegrid,acc2e=12) EmpiricalDispersion=GD3 scrf=(smd,solvent=DiEthylEther)						
	<S ² >	E	G	f	E _{corr}	G – E
41	3.813	-3029.44386	-3028.89882			
21	1.811	-3029.43776	-3028.89164		0.904595	-3029.43224
M062X-D3/Def2SVP integral=(ultrafinegrid,acc2e=12) EmpiricalDispersion=GD3 scrf=(smd,solvent=DiEthylEther)						
	<S ² >	E	G	f	E _{corr}	G – E
41	3.802	-3029.80009	-3029.25029			
21	1.789	-3029.79644	-3029.24232		0.888723	-3029.79319
M06HF-D3/Def2SVP integral=(ultrafinegrid,acc2e=12) EmpiricalDispersion=GD3 scrf=(smd,solvent=DiEthylEther)						
	<S ² >	E	G	f	E _{corr}	G – E
41	3.801	-3030.03698	-3029.4749			
21	1.789	-3030.0335	-3029.4703		0.889165	-3030.03041

Table S6. Energy data for Scheme 3 (Hartree) at the wb97xd/Def2SVP Integral(UltraFineGrid) scrf=(smd,solvent=DiEthylEther) level. G_{corr} = G (1 atm) – E + E_{corr} + 0.00301.

	<S ² >	E	G, 1 atm	G, 1 M	v, cm ⁻¹
A ³	2	-3066.037677	-3065.849377	-3065.846367	
A ¹	1	-3066.027175	-3065.837322	-3065.834312	
(CH ₃) ₃ SiCH ₂ Li		-455.8475387	-455.746994	-455.743984	
B:cation	2	-2582.226263	-2581.781787	-2581.778777	
B:anion		-448.3442185	-448.244168	-448.241158	
C ↓> _R ↑> _L ↑↑> _V	3.04	-3030.633101	-3030.072152	-3030.069142	
ts0a	2.8	-3030.630797	-3030.067731	-3030.064721	i292
C ↑> _R ↓> _L ↑↑> _V	3.05	-3030.630662	-3030.071194	-3030.068184	
ts0b	2.81	-3030.628881	-3030.066966	-3030.063956	i270
1H ³	2.02	-3030.702969	-3030.133796	-3030.130786	
1H ¹	1	-3030.68582	-3030.11529	-3030.11228	
4 ⁴	3.80	-2582.35572	-2581.917894	-2581.914884	
1 ⁴	3.799	-3030.108001	-3029.553574	-3029.550564	
ts1	3.79	-3478.972431	-3478.283431	-3478.280421	i925
ts2	3.88	-3478.916876	-3478.223411	-3478.220401	i1108

ts3	3.78	-3038.195717	-3037.634068	-3037.631058	i1114
D ⁴	3.79	-3038.243939	-3026.886982	-3037.673174	
(CH ₃) ₃ SiCH ₂	0.75	-448.2649725	-448.164003	-448.160993	
[(CH ₃) ₃ SiCH ₂] ₂		-896.500911	-896.447587	-896.444577	
(CH ₃) ₄ Si		-448.9397389	-448.824908	-448.821898	
LiH		-8.102796714	-8.11631	-8.1133	
LiCl		-467.6708962	-467.690442	-467.687432	

Table S7. Energy data for Scheme 9 (Hartree) at the wb97xd/Def2SVP Integral(UltraFineGrid) scrf=(smd,solvent=DiEthylEther) level. G_{corr} = G (1 atm) – E + E_{corr} + 0.00301.

	<S ² >	E	G, 1 atm	G, 1M	f	E _{corr}	G _{corr} , 1M
⁴1	3.799	-3030.108001	-3029.553574	-3029.550564			
pinBH		411.45988631	-411.301414	-411.298404			
pinBCH₂TMS		-859.2298168	-858.953905	-858.950895			
⁴1a	3.801	-2582.3414909	-2581.907358	-2581.904348			
²1a	1.77	-2582.3225688	-2581.888013	-2581.885003	0.87	-2582.30608	-2581.86851
⁴1b	3.804	-2134.574688	-2134.259917	-2134.256907			
²1b	1.655	-2134.563371	-2134.246295	-2134.243285	0.77	-2134.554656	-2134.23457
PhSiH₃		-522.6064871	-522.522989	-522.519979			
PhSiH₂CH₂Si(CH₃)₃		-859.2298168	-970.166554	-970.163544			
Et₂O		-233.4255753	-233.317913	-233.314903			
BpiBpin		-821.731291	-821.412741	-821.409731			
PhSiH₂PhSiH₂		-1044.033418	-1043.860435	-1043.857425			
[CH₃CHOCH₂CH₃]₂		-465.6622297	-465.446254	-465.443244			
³1c	2	-2135.167922	-2134.8397	-2134.83669			
[³1c]·Bpin	3.78	-2545.962113	-2545.466482	-2545.463472			
[³1c]·PhSiH₂	3.78	-2657.139613	-2656.715854	-2656.712844			
[³1c] 	3.78	-2367.946797	-2367.506933	-2367.503923			
⁴1d	3.79	-2546.050188	-2545.55056	-2545.54755			
⁴1e	3.79	-2546.053122	-2545.554149	-2545.551139			
⁴1f	3.79	-2657.187942	-2656.760224	-2656.757214			
⁴1g	3.79	-2657.200776	-2656.771368	-2656.768358			

Cartesian Coordinates for the optimized structures

⁴1 at M06L/def2svp			14	3.490599000	0.488847000	-2.223569000
23	1.796272000	-0.051825000	0.621003000	6	3.617653000	0.168630000
7	1.306037000	2.007548000	0.724129000	1	4.172161000	1.005771000
7	1.469111000	-2.063734000	0.040743000	1	4.215808000	-0.751154000
			6	2.586001000	-0.921532000	-3.090138000

1	1.517886000	-0.945599000	-2.820249000					
1	3.009266000	-1.907708000	-2.837664000					
1	2.636257000	-0.819639000	-4.186437000					
6	5.185182000	0.664690000	-3.043370000					
1	5.100468000	0.854073000	-4.126166000					
1	5.794807000	-0.244481000	-2.918299000					
1	5.761081000	1.498613000	-2.611094000					
6	2.534722000	2.079729000	-2.562721000					
1	1.466605000	1.975365000	-2.313084000					
1	2.587777000	2.362077000	-3.626780000					
1	2.924120000	2.932625000	-1.982766000					
14	0.110619000	-0.642809000	3.459467000					
6	1.784450000	-0.387123000	2.693157000					
1	2.407101000	-1.281720000	2.897804000					
1	2.275930000	0.474838000	3.187731000					
6	-0.732967000	-2.172660000	2.746957000					
1	-1.029855000	-2.024433000	1.696479000					
1	-1.650524000	-2.420333000	3.305421000					
1	-0.084351000	-3.063373000	2.780122000					
6	-1.022137000	0.830660000	3.130216000					
1	-1.313030000	0.889211000	2.068657000					
1	-0.551974000	1.792217000	3.394773000					
1	-1.955357000	0.756823000	3.712429000					
6	0.205169000	-0.873006000	5.333523000					
1	-0.791461000	-1.026370000	5.779279000					
1	0.652442000	0.003007000	5.829916000					
1	0.821410000	-1.744787000	5.605781000					
6	2.022369000	2.971897000	1.333494000					
1	2.950298000	2.644932000	1.813636000					
6	1.634654000	4.299576000	1.366906000					
1	2.257095000	5.036446000	1.876787000					
6	0.434707000	4.666521000	0.734897000					
1	0.095810000	5.704346000	0.740174000					
6	-0.314824000	3.686580000	0.103502000					
1	-1.251238000	3.942443000	-0.395441000					
6	0.132100000	2.358290000	0.104517000					
7	0.069204000	0.045428000	-0.374491000					
6	-0.574558000	1.249188000	-0.513752000					
6	-1.797396000	1.325523000	-1.169935000					
1	-2.304121000	2.288637000	-1.267431000					
6	-2.403310000	0.168972000	-1.695964000					
6	-1.715104000	-1.049452000	-1.546354000					
1	-2.154870000	-1.967634000	-1.943003000					
6	-0.489000000	-1.095933000	-0.892716000					
6	2.274577000	-3.111550000	0.299959000					
1	3.182207000	-2.885495000	0.868934000					
6	1.997703000	-4.402649000	-0.113049000					
1	2.689097000	-5.211850000	0.126720000					
6	0.817810000	-4.638515000	-0.838375000					
1	0.565021000	-5.643938000	-1.180807000					
6	-0.022903000	-3.571470000	-1.112931000					
1	-0.947409000	-3.725386000	-1.672411000					
6	0.314574000	-2.285969000	-0.668082000					
6	-3.765826000	0.219014000	-2.291537000					
1	-3.916704000	-0.606294000	-3.006441000					
1	-3.922787000	1.156914000	-2.850100000					
14	-5.136836000	0.104840000	-0.968458000					
6	-5.032192000	1.603478000	0.153981000					
1	-4.084229000	1.634216000	0.714039000					
1	-5.120074000	2.548848000	-0.404067000					
1	-5.842472000	1.592540000	0.899859000					
6	-4.875776000	-1.451333000	0.043360000					
1	-4.860668000	-2.358919000	-0.580274000					
1	-3.926681000	-1.417526000	0.602128000					
1	-5.679355000	-1.582155000	0.784934000					
6	-6.790950000	0.058872000	-1.847979000					
1	-7.626650000	-0.002208000	-1.133778000					
1	-6.951420000	0.959949000	-2.459881000					
1	-6.871852000	-0.810459000	-2.518594000					

²1 at M06L/def2svp

23	1.784483000	0.030502000	0.611357000
7	1.470935000	2.059725000	0.056465000
7	1.277893000	-2.035560000	0.680223000
14	3.513944000	-0.464496000	-2.185631000
6	3.621432000	-0.178685000	-0.349522000
1	4.224247000	0.734056000	-0.169311000
1	4.165262000	-1.028836000	0.109633000
6	2.545218000	-2.035567000	-2.571331000
1	1.475335000	-1.925131000	-2.332325000
1	2.918631000	-2.907150000	-2.009111000
1	2.608234000	-2.291017000	-3.641612000
6	5.224855000	-0.645773000	-2.966885000
1	5.162101000	-0.815077000	-4.054386000
1	5.780474000	-1.493995000	-2.536232000
1	5.841013000	0.254127000	-2.811572000
6	2.644486000	0.972778000	-3.041569000
1	1.573192000	1.010840000	-2.786535000
1	2.708698000	0.883610000	-4.138220000
1	3.080517000	1.948319000	-2.770704000
14	0.118122000	0.595098000	3.438641000
6	1.795891000	0.334040000	2.673608000
1	2.274707000	-0.539345000	3.160227000
1	2.422929000	1.220826000	2.896800000
6	-1.036892000	-0.851532000	3.075513000
1	-1.323190000	-0.886523000	2.011687000
1	-1.971500000	-0.769301000	3.654363000
1	-0.586463000	-1.826066000	3.326339000
6	-0.700687000	2.155792000	2.768519000
1	-1.001233000	2.042814000	1.714808000
1	-0.039379000	3.035615000	2.827725000
1	-1.614029000	2.399573000	3.335486000
6	0.229758000	0.773762000	5.316406000
1	-0.761758000	0.930874000	5.771894000
1	0.861522000	1.628260000	5.606774000
1	0.665963000	-0.122418000	5.785647000
6	2.281381000	3.097020000	0.334051000
1	3.186947000	2.856331000	0.900622000
6	2.013154000	4.397305000	-0.057681000
1	2.708431000	5.198811000	0.195979000
6	0.834534000	4.649895000	-0.780536000
1	0.587310000	5.662173000	-1.106654000
6	-0.011681000	3.593598000	-1.073915000
1	-0.934408000	3.763053000	-1.631794000
6	0.317202000	2.297110000	-0.650280000
7	0.065177000	-0.040777000	-0.393124000
6	-0.489439000	1.116268000	-0.892539000
6	-1.717722000	1.086751000	-1.541220000
1	-2.154260000	2.014522000	-1.919325000
6	-2.415731000	-0.125035000	-1.709284000
6	-1.813600000	-1.295795000	-1.206888000
1	-2.327870000	-2.253395000	-1.319860000
6	-0.589725000	-1.241213000	-0.552725000
6	1.983953000	-3.012764000	1.277299000
1	2.911523000	-2.699729000	1.767624000
6	1.587789000	-4.339167000	1.287668000
1	2.202059000	-5.088827000	1.788550000
6	0.388057000	-4.685489000	0.642943000
1	0.041590000	-5.720811000	0.629230000
6	-0.351704000	-3.691589000	0.024038000
1	-1.287280000	-3.934092000	-0.483076000
6	0.103706000	-2.364857000	0.047934000
6	-3.785453000	-0.154648000	-2.291325000
1	-3.952132000	-1.075656000	-2.875094000
1	-3.941317000	0.690617000	-2.981571000
14	-5.139435000	-0.075019000	-0.949000000
6	-4.847381000	1.436177000	0.121410000
1	-3.893406000	1.365408000	0.668350000
1	-4.825038000	2.368367000	-0.464561000

1	-5.641857000	1.547635000	0.875885000	6	0.064707000	3.692220000	-0.675946000
6	-5.040634000	-1.616113000	0.115875000	1	0.913631000	3.900578000	-1.327498000
1	-5.143389000	-2.539254000	-0.475891000	6	-0.279222000	2.366793000	-0.365922000
1	-4.088382000	-1.677464000	0.666128000	6	3.645009000	0.000335000	-2.499067000
1	-5.844363000	-1.624379000	0.868912000	1	3.800196000	0.887358000	-3.135995000
6	-6.805301000	0.022607000	-1.802510000	1	3.800198000	-0.886539000	-3.136204000
1	-7.630632000	0.064122000	-1.074940000	14	4.986591000	0.000191000	-1.141963000
1	-6.886041000	0.918120000	-2.437794000	6	4.785717000	-1.534352000	-0.073593000
1	-6.983538000	-0.852274000	-2.446736000	1	3.816553000	-1.536216000	0.451489000
				1	4.852977000	-2.458722000	-0.670874000
				1	5.577322000	-1.575140000	0.693134000
41 at wb97xd/def2svp				6	4.785617000	1.534445000	-0.073200000
23	-1.699480000	-0.000079000	0.743301000	1	4.852836000	2.458973000	-0.670242000
7	-1.341321000	-2.092647000	0.432411000	1	3.816441000	1.536122000	0.451862000
7	-1.341420000	2.092537000	0.432818000	1	5.577206000	1.575081000	0.693553000
14	-3.821599000	0.000201000	-1.813522000	6	6.674536000	0.000350000	-1.970504000
6	-3.675076000	-0.000004000	0.043077000	1	7.482703000	0.000270000	-1.220436000
1	-4.205953000	-0.892808000	0.432624000	1	6.807568000	-0.890310000	-2.606533000
1	-4.205940000	0.892716000	0.432833000	1	6.807517000	0.891191000	-2.606290000
6	-2.994604000	1.527435000	-2.562048000				
1	-1.899049000	1.478263000	-2.454512000				
1	-3.338149000	2.455649000	-0.2074855000				
1	-3.218618000	1.612182000	-3.638969000				
6	-5.629902000	0.000287000	-2.381442000				
1	-5.712663000	0.000402000	-3.481941000				
1	-6.163500000	0.889442000	-2.004656000				
1	-6.163525000	-0.888932000	-2.004841000				
6	-2.994658000	-1.526908000	-2.562336000				
1	-1.899100000	-1.477794000	-2.454826000				
1	-3.218679000	-1.611427000	-3.639304000				
1	-3.338232000	-2.455211000	-2.075363000				
14	0.432399000	-0.000461000	3.329961000				
6	-1.356008000	-0.000444000	2.807716000				
1	-1.843242000	0.892384000	3.251288000				
1	-1.843174000	-0.893460000	3.250984000				
6	1.342488000	1.523688000	2.678304000				
1	1.463764000	1.471616000	1.584718000				
1	2.349765000	1.601444000	3.121614000				
1	0.800613000	2.455497000	2.912284000				
6	1.342618000	-1.524281000	2.677712000				
1	1.463879000	-1.471774000	1.584144000				
1	0.800829000	-2.456228000	2.911340000				
1	2.349905000	-1.602115000	3.120986000				
6	0.608809000	-0.000815000	5.217030000				
1	1.667478000	-0.000829000	5.528680000				
1	0.128450000	-0.890046000	5.659565000				
1	0.128372000	0.888205000	5.659904000				
6	-2.065189000	-3.102692000	0.934889000				
1	-2.907114000	-2.818436000	1.571779000				
6	-1.781583000	-4.431948000	0.673468000				
1	-2.400466000	-5.219744000	1.104567000				
6	-0.689860000	-4.727612000	-0.154662000				
1	-0.436560000	-5.763683000	-0.388866000				
6	0.064778000	-3.692025000	-0.676810000				
1	0.913663000	-3.900204000	-1.328470000				
6	-0.279160000	-2.366691000	-0.366436000				
7	-0.144121000	0.000068000	-0.467457000				
6	0.439842000	-1.187603000	-0.841874000				
6	1.631317000	-1.202393000	-1.546879000				
1	2.100679000	-2.154197000	-1.803097000				
6	2.272136000	0.000265000	-1.900239000				
6	1.631290000	1.202810000	-1.546634000				
1	2.100620000	2.154683000	-1.802656000				
6	0.439806000	1.187848000	-0.841610000				
6	-2.065335000	3.102452000	0.935499000				
1	-2.907288000	2.818026000	1.572277000				
6	-1.781750000	4.431774000	0.674409000				
1	-2.400676000	5.219453000	1.105659000				
6	-0.689979000	4.727660000	-0.153593000				
1	-0.436687000	5.763793000	-0.387532000				

21 at wb97xd/def2svp

23	-1.785010000	0.030392000	0.582817000
7	-1.318824000	-2.087874000	0.391970000
7	-1.410121000	2.101570000	0.302993000
14	-3.477109000	-0.136491000	-2.272112000
6	-3.608410000	-0.098389000	-0.412157000
1	-4.154699000	-1.006075000	-0.084172000
1	-4.226045000	0.778356000	-0.128267000
6	-2.597356000	1.403658000	-2.922117000
1	-1.533434000	1.404420000	-2.634620000
1	-3.051098000	2.326919000	-2.524119000
1	-2.645112000	1.453564000	-4.023119000
6	-5.186181000	-0.211574000	-3.084713000
1	-5.113117000	-0.232682000	-4.185590000
6	-5.795990000	0.664223000	-2.805240000
1	-5.737244000	-1.113001000	-2.767085000
1	-2.505006000	-1.650989000	-2.853715000
1	-1.434883000	-1.555497000	-2.609280000
1	-2.583446000	-1.773806000	-3.947225000
1	-2.877133000	-2.578110000	-2.385826000
14	-0.213154000	0.068830000	3.503793000
6	-1.876706000	-0.001564000	2.661156000
1	-2.470674000	0.871181000	3.002155000
1	-2.402369000	-0.914385000	3.007565000
6	0.741475000	1.622678000	3.010306000
1	1.043167000	1.583305000	1.951214000
1	1.658381000	1.730762000	3.614274000
1	0.137165000	2.534532000	3.151211000
6	0.851183000	-1.425759000	3.044102000
1	1.187655000	-1.365593000	1.996723000
1	0.302355000	-2.374433000	3.168877000
1	1.753121000	-1.475387000	3.677500000
6	-0.393226000	0.079571000	5.389113000
1	0.588572000	0.123168000	5.891008000
1	-0.912288000	-0.826972000	5.743815000
1	-0.981290000	0.950262000	5.725387000
6	-2.067902000	-3.099125000	0.840507000
1	-2.997428000	-2.823402000	1.345228000
6	-1.700112000	-4.428310000	0.683184000
1	-2.341724000	-5.223162000	1.065351000
6	-0.499274000	-4.709281000	0.029912000
1	-0.173637000	-5.741577000	-0.113613000
6	0.281652000	-3.660689000	-0.437237000
1	1.223718000	-3.857977000	-0.948956000
6	-0.155849000	-2.347770000	-0.241208000
7	-0.047970000	0.023848000	-0.382566000
6	0.587322000	-1.147826000	-0.682588000
6	1.802690000	-1.168188000	-1.317456000
1	2.295351000	-2.114552000	-1.543648000

6	2.441556000	0.059976000	-1.674559000		1	2.453163000	5.201360000	0.997805000
6	1.780866000	1.240717000	-1.375435000		6	0.623772000	4.717619000	-0.058204000
1	2.246896000	2.195025000	-1.629442000		1	0.335492000	5.745976000	-0.235373000
6	0.529904000	1.229361000	-0.731054000		6	-0.169705000	3.689879000	-0.509242000
6	-2.199931000	3.111768000	0.700615000		1	-1.083947000	3.900403000	-1.046177000
1	-3.116842000	2.822080000	1.222139000		6	0.217473000	2.368133000	-0.273103000
6	-1.898382000	4.441224000	0.478760000		7	0.072914000	0.010502000	-0.373507000
1	-2.575166000	5.223912000	0.823105000		6	-0.534980000	1.199036000	-0.693476000
6	-0.700614000	4.746352000	-0.201491000		6	-1.755455000	1.219030000	-1.333959000
1	-0.427324000	5.785250000	-0.399032000		1	-2.229054000	2.164907000	-1.563688000
6	0.122906000	3.723901000	-0.617064000		6	-2.403045000	0.030238000	-1.677905000
1	1.050439000	3.942565000	-1.147402000		6	-1.757239000	-1.171984000	-1.356459000
6	-0.241675000	2.381773000	-0.357132000		1	-2.233904000	-2.111276000	-1.605168000
6	3.821662000	0.048416000	-2.255635000		6	-0.541107000	-1.166521000	-0.716786000
1	3.997916000	0.948550000	-2.867917000		6	2.113368000	-3.111600000	0.762290000
1	3.963806000	-0.823994000	-2.915882000		1	3.020293000	-2.841053000	1.289239000
14	5.165653000	-0.000584000	-0.903706000		6	1.779731000	-4.428010000	0.544016000
6	4.966723000	-1.560684000	0.127810000		1	2.425640000	-5.218375000	0.900156000
1	3.999989000	-1.573568000	0.656841000		6	0.599098000	-4.705240000	-0.143287000
1	5.028725000	-2.468879000	-0.494401000		1	0.303579000	-5.728512000	-0.337029000
1	5.762483000	-1.623451000	0.888732000		6	-0.189275000	-3.663769000	-0.575654000
6	4.975921000	1.512153000	0.195881000		1	-1.106422000	-3.858989000	-1.113318000
1	5.050888000	2.446111000	-0.385392000		6	0.207932000	-2.351164000	-0.317444000
1	4.003102000	1.511333000	0.714033000		6	-3.769500000	0.035657000	-2.282726000
1	5.764112000	1.534474000	0.966711000		1	-3.908292000	-0.833922000	-2.931916000
6	6.846946000	0.008437000	-1.745562000		1	-3.913508000	0.924779000	-2.903558000
1	7.661714000	-0.016834000	-1.003136000		14	-5.139864000	0.011571000	-0.970964000
1	6.967578000	-0.866418000	-2.405594000		6	-4.974885000	1.523859000	0.118505000
1	6.980869000	0.914346000	-2.359470000		1	-4.025518000	1.523102000	0.660074000
					1	-5.030680000	2.446616000	-0.465417000
					1	-5.777966000	1.552239000	0.860246000
					1	-4.971816000	-1.535231000	0.068870000
23	1.779013000	-0.000580000	0.615337000		6	-4.972484000	-5.026333000	-0.544667000
7	1.365275000	2.089703000	0.389248000		1	-5.774813000	-4.022484000	-1.550470000
7	1.356070000	-2.091135000	0.346690000		1	-6.792011000	-1.388186000	0.809336000
14	3.521381000	0.010094000	-2.239239000		6	-7.618074000	0.023694000	-1.850538000
6	3.623295000	-0.009051000	-0.391490000		1	-6.902599000	0.916889000	-2.471350000
1	4.201294000	0.869224000	-0.066820000		1	-6.900706000	-0.849730000	-2.499209000
1	4.186687000	-0.903031000	-0.085113000					
6	2.602611000	-1.501981000	-2.880769000					
1	1.540111000	-1.455128000	-2.629024000					
1	3.005240000	-2.426035000	-2.455641000					
1	2.681023000	-1.575005000	-3.969677000					
6	5.227438000	0.011996000	-3.043570000					
1	5.159820000	0.021672000	-4.135888000					
1	5.798631000	-0.874528000	-2.752154000					
1	5.804025000	0.889813000	-2.736883000					
6	2.612617000	1.540131000	-2.851185000					
1	1.550163000	1.496024000	-2.598897000					
1	2.690425000	1.633245000	-3.938610000					
1	3.022028000	2.453166000	-2.409091000					
14	0.122082000	-0.042119000	3.521908000					
6	1.788128000	-0.046048000	2.714743000					
1	2.329674000	-0.944670000	3.045954000					
1	2.349251000	0.827443000	3.079633000					
6	-0.885984000	-1.547156000	3.010720000					
1	-1.185623000	-1.483794000	1.961778000					
1	-1.797979000	-1.628348000	3.609881000					
1	-0.319474000	-2.473957000	3.139725000					
6	-0.860840000	1.492199000	3.050832000					
1	-1.161145000	1.462444000	2.000563000					
1	-0.278984000	2.405652000	3.204467000					
1	-1.771377000	1.572389000	3.652332000					
6	0.248545000	-0.067594000	5.403687000					
1	-0.739159000	-0.065762000	5.875104000					
1	0.795586000	0.805830000	5.771069000					
1	0.781810000	-0.958428000	5.748769000					
6	2.127869000	3.100180000	0.823336000					
1	3.032444000	2.815578000	1.347083000					
6	1.802992000	4.421115000	0.627438000					

21 at wb97xd/def2tzvp

23	-1.779435000	0.038081000	0.578523000
7	-1.316389000	-2.080851000	0.398544000
7	-1.388186000	2.102283000	0.281487000
14	-3.492216000	-0.132822000	-2.273322000
6	-3.605171000	-0.088873000	-0.423425000
1	-4.145822000	-0.986696000	-0.089734000
1	-4.211654000	0.783894000	-0.138378000
6	-2.623865000	1.398380000	-2.933748000
1	-1.565261000	1.401970000	-2.661591000
1	-3.070719000	2.314220000	-2.536287000
1	-2.685512000	1.443587000	-4.025216000
6	-5.197912000	-0.210671000	-3.071573000
1	-5.131190000	-0.235616000	-4.163605000
1	-5.800282000	0.659099000	-2.793312000
1	-5.741212000	-1.103964000	-2.749394000
6	-2.530564000	-1.642327000	-2.855617000
1	-1.467813000	-1.551005000	-2.618152000
1	-2.615475000	-1.763449000	-3.939693000
1	-2.900812000	-2.559930000	-2.389195000
14	-0.237330000	0.090045000	3.524709000
6	-1.878034000	0.020023000	2.662179000
1	-2.470268000	0.889477000	2.984788000
1	-2.406907000	-0.882361000	3.001885000
6	0.727826000	1.628023000	3.035681000
1	1.053326000	1.577918000	1.993546000
1	1.621887000	1.740064000	3.656508000
1	0.126255000	2.534141000	3.151122000
6	0.818016000	-1.408713000	3.096769000

1	1.161295000	-1.367610000	2.060119000	1	-3.431495000	-2.155806000	-2.259885000
1	0.265510000	-2.343353000	3.229603000	14	0.457519000	-0.409364000	3.289502000
1	1.705728000	-1.453797000	3.734842000	6	-1.325446000	-0.223541000	2.794144000
6	-0.438410000	0.119592000	5.398583000	1	-1.734251000	0.660710000	3.309980000
1	0.530032000	0.160789000	5.906570000	1	-1.873368000	-1.102261000	3.173431000
1	-0.963613000	-0.772854000	5.751501000	6	1.507186000	1.035586000	2.678185000
1	-1.019382000	0.990559000	5.715914000	1	1.627646000	0.999986000	1.591295000
6	-2.066009000	-3.089883000	0.841480000	1	2.508380000	1.004166000	3.123363000
1	-2.985368000	-2.812436000	1.342198000	1	1.058341000	2.001640000	2.934853000
6	-1.706955000	-4.411761000	0.680251000	6	1.205695000	-1.990099000	2.581398000
1	-2.346609000	-5.197772000	1.056782000	1	1.329291000	-1.921070000	1.496616000
6	-0.515551000	-4.694938000	0.026537000	1	0.575803000	-2.862405000	2.788844000
1	-0.199770000	-5.719635000	-0.122182000	1	2.193782000	-2.181833000	3.015493000
6	0.265875000	-3.654873000	-0.434392000	6	0.655130000	-0.487270000	5.169083000
1	1.195052000	-3.854704000	-0.948714000	1	1.705602000	-0.601665000	5.461499000
6	-0.158310000	-2.346880000	-0.232148000	1	0.097338000	-1.332549000	5.588116000
7	-0.041389000	0.016652000	-0.381530000	1	0.273957000	0.424927000	5.642287000
6	0.591598000	-1.155357000	-0.669554000	6	-2.125216000	-3.140976000	0.631198000
6	1.805553000	-1.183150000	-1.287365000	1	-2.958354000	-2.900260000	1.282772000
1	2.296810000	-2.123520000	-1.496257000	6	-1.860138000	-4.440510000	0.259097000
6	2.446458000	0.034395000	-1.649423000	1	-2.486956000	-5.247688000	0.616089000
1	1.792707000	1.212600000	-1.367717000	6	-0.768509000	-4.679046000	-0.584902000
1	2.260401000	2.154017000	-1.627040000	1	-0.528801000	-5.688087000	-0.900686000
6	0.544866000	1.212970000	-0.733609000	6	-0.000586000	-3.618876000	-1.013144000
6	-2.166307000	3.124576000	0.662105000	1	0.845586000	-3.784659000	-1.667637000
1	-3.080074000	2.850268000	1.176568000	6	-0.325804000	-2.320549000	-0.596291000
6	-1.852721000	4.439616000	0.429818000	7	-0.148815000	0.037884000	-0.477111000
1	-2.518136000	5.225093000	0.759331000	6	0.408991000	-1.123323000	-0.964906000
6	-0.653638000	4.725566000	-0.243459000	6	1.598298000	-1.093946000	-1.672825000
1	-0.372299000	5.751010000	-0.447834000	1	2.046046000	-2.020256000	-2.014539000
6	0.157418000	3.697770000	-0.641495000	6	2.255185000	0.114342000	-1.918108000
1	1.081793000	3.902661000	-1.163753000	6	1.638458000	1.295210000	-1.458754000
6	-0.216918000	2.367687000	-0.373248000	1	2.121506000	2.248747000	-1.637369000
6	3.820144000	0.012536000	-2.235232000	6	0.462787000	1.238359000	-0.748817000
1	3.989649000	0.896899000	-2.856186000	6	-1.961966000	3.040773000	1.237609000
1	3.953059000	-0.862853000	-2.878124000	1	-2.800911000	2.720574000	1.845696000
14	5.172266000	-0.016926000	-0.904570000	6	-1.636701000	4.375296000	1.108807000
6	4.974193000	-1.540854000	0.163824000	1	-2.222393000	5.129567000	1.618726000
1	4.021161000	-1.532157000	0.698801000	6	-0.543647000	4.716230000	0.309724000
1	5.021324000	-2.457487000	-0.430372000	1	-0.257643000	5.754138000	0.182625000
1	5.7711686000	-1.589348000	0.910691000	6	0.171537000	3.717754000	-0.320064000
6	5.013651000	1.517789000	0.153217000	1	1.020761000	3.963364000	-0.944481000
1	5.089379000	2.427722000	-0.448353000	6	-0.215486000	2.385981000	-0.146074000
1	4.055822000	1.540221000	0.679365000	6	3.628691000	0.148041000	-2.512295000
1	5.8060111000	1.550832000	0.906172000	1	3.776993000	1.053795000	-3.111097000
6	6.833772000	-0.045729000	-1.765868000	1	3.788766000	-0.708963000	-3.175592000
1	7.651806000	-0.057125000	-1.040467000	14	4.956977000	0.106622000	-1.147284000
1	6.936024000	-0.932547000	-2.397209000	6	4.688635000	-1.409915000	-0.074837000
1	6.964579000	0.834071000	-2.401662000	1	3.727919000	-1.361453000	0.448420000
1	-1.906124000	1.744434000	-2.296701000	1	4.707086000	-2.333363000	-0.663407000
1	-3.301618000	2.711974000	-1.800048000	1	5.474455000	-1.485718000	0.684727000
1	-3.234214000	2.023333000	-3.428936000	6	4.803740000	1.647385000	-0.085377000
6	-5.658384000	0.361601000	-2.308427000	1	4.896700000	2.561453000	-0.681609000
1	-5.7471111000	0.464891000	-3.396359000	1	3.842961000	1.678541000	0.438924000
1	-6.163219000	1.219079000	-1.848998000	1	5.592694000	1.666482000	0.674556000
1	-6.206700000	-0.540107000	-2.012721000	6	6.647562000	0.045868000	-1.960692000
6	-3.070439000	-1.201452000	-2.659241000	1	7.443919000	0.026450000	-1.208986000
1	-1.980354000	-1.190645000	-2.560475000	1	6.756126000	-0.847892000	-2.584207000
1	-3.306808000	-1.177448000	-3.729337000	1	6.812949000	0.920870000	-2.598261000

				⁴1 at M06/def2svp			
1	1.552066000	-1.327000000	-2.679365000	23	1.665442000	-0.055100000	0.768895000
1	3.046192000	-2.265434000	-2.573160000	7	1.189852000	2.010334000	0.808238000
1	2.680607000	-1.345400000	-4.040807000	7	1.452573000	-2.062696000	0.126598000
6	5.211959000	0.259947000	-3.034862000	14	3.854725000	0.501491000	-1.661660000
1	5.144297000	0.319461000	-4.127466000	6	3.656182000	0.178496000	0.159227000
1	5.807782000	-0.625059000	-2.784472000	1	4.113297000	1.027493000	0.711995000
1	5.765417000	1.139065000	-2.685654000	1	4.232545000	-0.737166000	0.413476000
6	2.550585000	1.714258000	-2.768393000	6	3.159475000	-0.921432000	-2.693860000
1	1.483604000	1.617125000	-2.544891000	1	2.056674000	-0.962482000	-2.641467000
1	2.647483000	1.878950000	-3.847649000	1	3.547588000	-1.900850000	-2.358474000
1	2.919725000	2.612262000	-2.260374000	1	3.432461000	-0.807001000	-3.758264000
14	0.184822000	-0.191749000	3.499857000	6	5.670740000	0.706873000	-2.154681000
6	1.850580000	-0.124779000	2.670724000	1	5.781027000	0.899524000	-3.237442000
1	2.420107000	-1.016806000	2.978623000	1	6.255044000	-0.199486000	-1.915449000
1	2.389660000	0.756094000	3.055323000	1	6.138793000	1.549951000	-1.615932000
6	-0.798802000	-1.700067000	2.940736000	6	2.957665000	2.082958000	-2.179168000
1	-1.100007000	-1.610342000	1.892334000	1	1.860497000	1.958489000	-2.142721000
1	-1.709834000	-1.815534000	3.539259000	1	3.221325000	2.367020000	-3.213724000
1	-0.215010000	-2.621850000	3.039944000	1	3.219285000	2.936204000	-1.526440000
6	-0.838217000	1.342353000	3.096224000	14	-0.562390000	-0.725651000	3.173506000
1	-1.168204000	1.334661000	2.052862000	6	1.231028000	-0.411677000	2.786590000
1	-0.268822000	2.263845000	3.261133000	1	1.808986000	-1.300789000	3.121137000
1	-1.735280000	1.388302000	3.724404000	1	1.569211000	0.457527000	3.391121000
6	0.346124000	-0.282963000	5.381043000	1	6.183964000	-2.314871000	2.359424000
1	-0.635360000	-0.323803000	5.867815000	1	-1.288185000	-2.210151000	1.264448000
1	0.878491000	0.590612000	5.774061000	1	-2.176609000	-2.593895000	2.757153000
1	0.906831000	-1.174370000	5.684269000	1	-0.503152000	-3.165245000	2.548204000
6	2.096474000	3.058894000	0.938056000	1	-0.503122800	0.687551000	2.581546000
1	3.006201000	2.757506000	1.445401000	6	-1.712457000	0.729520000	1.478018000
6	1.757798000	4.391785000	0.796251000	1	-1.315463000	1.671565000	2.939653000
1	2.404589000	5.162337000	1.196072000	1	-2.706214000	0.556915000	2.947420000
6	0.577143000	4.704898000	0.128989000	6	-0.854782000	-0.909838000	5.034329000
1	0.279080000	5.738207000	-0.007118000	1	-1.920026000	-1.093233000	5.264998000
6	-0.215316000	3.683029000	-0.362876000	1	-0.546856000	0.000616000	5.578809000
1	-1.133324000	3.906479000	-0.890374000	1	-0.272709000	-1.751960000	5.449209000
6	0.187860000	2.362475000	-0.176719000	6	1.800129000	2.956542000	1.538612000
7	0.055066000	-0.000475000	-0.385443000	1	2.624358000	2.615805000	2.176823000
6	-0.571163000	1.186971000	-0.647332000	6	1.430424000	4.289685000	1.505914000
6	-1.786339000	1.240056000	-1.268863000	1	1.962050000	5.020224000	2.119762000
1	-2.272788000	2.190468000	-1.451446000	6	0.367824000	4.668324000	0.673473000
6	-2.434772000	0.034982000	-1.668272000	1	0.048092000	5.712382000	0.618823000
6	-1.787719000	-1.158888000	-1.416810000	6	-0.275659000	3.700920000	-0.079268000
1	-2.260654000	-2.090997000	-1.705542000	1	-1.107811000	3.968656000	-0.735152000
6	-0.541740000	-1.184372000	-0.775284000	6	0.151028000	2.369113000	0.001357000
6	2.151309000	-3.149322000	0.597283000	7	0.160414000	0.061891000	-0.508111000
1	3.062783000	-2.891183000	1.126733000	6	-0.466103000	1.262004000	-0.715092000
6	1.831985000	-4.460134000	0.328805000	6	-1.627700000	1.332635000	-1.466962000
1	2.491630000	-5.258150000	0.644640000	1	-2.133833000	2.293069000	-1.607280000
6	0.634585000	-4.723796000	-0.362139000	1	-2.207160000	0.164234000	-1.995186000
1	0.349250000	-5.743957000	-0.593722000	6	-1.518759000	-1.047868000	-1.806473000
6	-0.170563000	-3.679500000	-0.742667000	1	-1.941651000	-1.975292000	-2.206842000
1	-1.093721000	-3.866587000	-1.276948000	6	-0.340372000	-1.080217000	-1.075619000
6	0.211150000	-2.356616000	-0.437897000	6	2.208212000	-3.105899000	0.503516000
6	-3.810831000	0.081394000	-2.255798000	1	3.007191000	-2.887013000	1.222268000
1	-3.980058000	-0.777898000	-2.914021000	6	2.010477000	-4.390375000	0.028496000
1	-3.942531000	0.983544000	-2.863958000	1	2.654913000	-5.204583000	0.367417000
14	-5.160989000	0.058256000	-0.915210000	6	0.975027000	-4.610829000	-0.891144000
6	-4.939390000	1.533449000	0.223921000	1	0.793023000	-5.610367000	-1.295037000
1	-3.978078000	1.492900000	0.746050000	6	0.184818000	-3.544425000	-1.284103000
1	-4.986600000	2.478624000	-0.327506000	1	-0.625557000	-3.685718000	-2.003667000
1	-5.728046000	1.554070000	0.983952000	6	0.435541000	-2.270534000	-0.757767000
6	-5.005597000	-1.530484000	0.070401000	6	-3.577768000	0.192493000	-2.571019000
1	-5.089618000	-2.411425000	-0.575104000	1	-3.758596000	-0.674593000	-3.231543000
1	-4.043650000	-1.583422000	0.590398000	1	-3.754415000	1.107487000	-3.166260000
1	-5.795343000	-1.596728000	0.826554000	14	-4.872192000	0.158452000	-1.163408000
6	-6.833115000	0.139563000	-1.764332000	6	-4.777063000	1.762103000	-0.188683000
1	-7.647498000	0.119996000	-1.032239000	1	-3.812880000	1.869075000	0.339649000
1	-6.935382000	1.058344000	-2.351597000	1	-4.914229000	2.647507000	-0.834131000

1	-5.571308000	1.786761000	0.578151000	6	0.178233000	-3.379963000	-1.553888000
6	-4.498689000	-1.274446000	-0.009510000	1	-0.685766000	-3.497404000	-2.213754000
1	-4.435343000	-2.240100000	-0.541076000	6	0.430883000	-2.124858000	-0.961460000
1	-3.545741000	-1.118958000	0.527385000	6	-3.548775000	0.549451000	-2.532490000
1	-5.291545000	-1.368502000	0.753298000	1	-3.715604000	-0.232510000	-3.296212000
6	-6.571659000	-0.030661000	-1.935584000	1	-3.683335000	1.525945000	-3.035099000
1	-7.361042000	-0.040774000	-1.164180000	14	-4.893886000	0.379208000	-1.192309000
1	-6.793106000	0.799884000	-2.627999000	6	-4.762637000	1.817521000	0.010840000
1	-6.650656000	-0.972160000	-2.506139000	1	-3.797212000	1.822414000	0.546874000
				1	-4.872687000	2.789658000	-0.501661000
				1	-5.558974000	1.754378000	0.773427000
21 at M06/def2svp				6	-4.640171000	-1.232875000	-0.261479000
23	1.604764000	-0.150725000	0.857493000	1	-4.637714000	-2.105319000	-0.938633000
7	1.362790000	1.912261000	0.871949000	7	-3.686403000	-1.235291000	0.295289000
7	1.515200000	-1.950426000	-0.129915000	1	-5.449645000	-1.387467000	0.473570000
14	3.885340000	0.558080000	-1.503169000	6	-6.580030000	0.392562000	-2.019914000
6	3.608314000	0.087145000	0.281553000	1	-7.391773000	0.300937000	-1.277412000
1	4.067409000	0.864790000	0.927036000	1	-6.745600000	1.329426000	-2.579731000
1	4.140121000	-0.866639000	0.480007000	1	-6.684162000	-0.444621000	-2.731795000
6	3.223077000	-0.752812000	-2.687706000				
1	2.119219000	-0.787733000	-2.683994000				
1	3.591758000	-1.764764000	-2.440341000				
1	3.542150000	-0.530015000	-3.721848000				
6	5.731135000	0.762136000	-1.869418000				
1	5.907618000	1.042403000	-2.923866000				
1	6.285088000	-0.173819000	-1.676203000				
1	6.181814000	1.547053000	-1.236092000				
6	3.050025000	2.193302000	-1.941246000				
1	1.949646000	2.099092000	-1.957440000				
1	3.365616000	2.524893000	-2.946935000				
1	3.308359000	3.001383000	-1.232957000				
14	-0.818950000	-1.136562000	3.026834000				
6	0.961906000	-0.682892000	2.721139000				
1	1.654393000	-1.518246000	2.971528000				
1	1.270330000	0.197373000	3.328123000				
6	-1.280618000	-2.660805000	2.018885000				
1	-1.382928000	-2.421311000	0.945830000				
1	-2.243374000	-3.084187000	2.356782000				
1	-0.517436000	-3.455374000	2.110432000				
6	-1.944327000	0.292628000	2.533601000				
1	-1.937865000	0.432651000	1.438020000				
1	-1.622604000	1.243950000	2.995766000				
1	-2.988281000	0.109373000	2.846376000				
6	-1.135224000	-1.526223000	4.848443000				
1	-2.193168000	-1.790135000	5.027960000				
1	-0.893043000	-0.661926000	5.491938000				
1	-0.516950000	-2.375033000	5.190459000				
6	2.096547000	2.772302000	1.610570000				
1	2.972785000	2.349880000	2.116317000				
6	1.783920000	4.107205000	1.734943000				
1	2.413489000	4.761593000	2.341624000				
6	0.642949000	4.597375000	1.064687000				
1	0.366889000	5.652514000	1.141670000				
6	-0.123729000	3.731568000	0.316107000				
1	-1.020035000	4.080968000	-0.203215000				
6	0.249384000	2.377744000	0.219523000				
7	0.134218000	0.108337000	-0.343787000				
6	-0.440516000	1.361325000	-0.513776000				
6	-1.587175000	1.521211000	-1.272856000				
1	-2.038039000	2.516062000	-1.360334000				
6	-2.193584000	0.427342000	-1.918195000				
6	-1.519845000	-0.798620000	-1.853121000				
1	-1.921583000	-1.663858000	-2.392632000				
6	-0.353847000	-0.946699000	-1.109278000				
6	2.324075000	-3.007548000	0.117288000				
1	3.170989000	-2.820054000	0.787900000				
6	2.119483000	-4.252131000	-0.428179000				
1	2.804898000	-5.069775000	-0.194771000				
6	1.015722000	-4.438926000	-1.294484000				
1	0.830470000	-5.414745000	-1.751598000				

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23	-1.810046000	0.002435000	0.594838000
7	-1.362610000	-2.112881000	0.350530000
7	-1.360188000	2.116067000	0.345481000
14	-3.469871000	-0.002620000	-2.277304000
6	-3.652164000	0.001503000	-0.423961000
1	-4.237423000	-0.891060000	-0.127190000
1	-4.236282000	0.896111000	-0.131142000
6	-2.514387000	1.523234000	-2.862884000
1	-1.452592000	1.453590000	-2.575749000
1	-2.922833000	2.450135000	-2.427044000
1	-2.556332000	1.619999000	-3.959960000
6	-5.144265000	-0.004002000	-3.166303000
1	-5.022507000	-0.005756000	-4.261904000
1	-5.734892000	0.885276000	-2.892821000
1	-5.734917000	-0.892391000	-2.889992000
6	-2.515348000	-1.531494000	-2.856753000
1	-1.452667000	-1.459583000	-2.573510000
1	-2.560732000	-1.634686000	-3.953107000
1	-2.921871000	-2.456073000	-2.414215000
14	-0.238605000	0.003763000	3.514013000
6	-1.912425000	0.004041000	2.696644000
1	-2.468663000	0.898426000	3.039916000
1	-2.469819000	-0.888978000	3.041564000
6	0.765445000	1.526982000	3.007168000
1	1.081194000	1.453568000	1.953802000
1	1.676006000	1.620386000	3.621309000
1	0.184447000	2.457007000	3.122175000
6	0.762242000	-1.523273000	3.012316000
1	1.078382000	-1.453931000	1.958797000
1	0.179204000	-2.451655000	3.130211000
1	1.672473000	-1.616659000	3.626945000
6	-0.359855000	0.007179000	5.405964000
1	0.637369000	0.006973000	5.875747000
1	-0.904183000	-0.880454000	5.766810000
1	-0.902287000	0.897269000	5.763612000
6	-2.127628000	-3.130979000	0.765960000
1	-3.052688000	-2.857803000	1.280856000
6	-1.784944000	-4.458486000	0.564585000
1	-2.439370000	-5.253241000	0.920980000
6	-0.585258000	-4.739387000	-0.105933000
1	-0.281011000	-5.771299000	-0.287264000
6	0.211809000	-3.693804000	-0.538268000
1	1.145192000	-3.889335000	-1.064993000
6	-0.198504000	-2.372058000	-0.295380000
7	-0.053421000	0.000028000	-0.374450000
6	0.559474000	-1.185994000	-0.696806000
6	1.792327000	-1.204893000	-1.330966000
1	2.270326000	-2.157303000	-1.566437000

6	2.445409000	-0.002895000	-1.664176000		1	-2.311633000	-5.262265000	0.982152000
6	1.793844000	1.200348000	-1.334255000		6	-0.464980000	-4.716475000	-0.030238000
1	2.272909000	2.151598000	-1.572291000		1	-0.128773000	-5.742596000	-0.186097000
6	0.560750000	1.184728000	-0.699742000		6	0.310695000	-3.654176000	-0.475628000
6	-2.123830000	3.136204000	0.758658000		1	1.257806000	-3.832610000	-0.983363000
1	-3.049311000	2.865375000	1.274050000		6	-0.142040000	-2.347606000	-0.263470000
6	-1.779385000	4.462760000	0.554570000		7	-0.039961000	0.030726000	-0.381778000
1	-2.432764000	5.259137000	0.909248000		6	0.599653000	-1.137215000	-0.684750000
6	-0.579117000	4.740664000	-0.116446000		6	1.822895000	-1.153628000	-1.309558000
1	-0.273439000	5.771795000	-0.299809000		1	2.317964000	-2.098093000	-1.537309000
6	0.216525000	3.693204000	-0.546529000		6	2.461311000	0.077733000	-1.654532000
1	1.150297000	3.886438000	-1.073428000		6	1.797439000	1.257364000	-1.349560000
6	-0.195531000	2.372322000	-0.301041000		1	2.263459000	2.213734000	-1.594440000
6	3.821166000	-0.004743000	-2.252492000		6	0.541749000	1.237888000	-0.715247000
1	3.978689000	0.881855000	-2.887843000		6	-2.198247000	3.129599000	0.696726000
1	3.977621000	-0.893892000	-2.884531000		1	-3.123346000	2.844346000	1.206305000
14	5.162278000	-0.002893000	-0.894183000		6	-1.886331000	4.459520000	0.484222000
6	4.957878000	-1.536971000	0.175317000		1	-2.561931000	5.243545000	0.823682000
1	3.987038000	-1.537709000	0.695537000		6	-0.677751000	4.759321000	-0.181187000
1	5.029398000	-2.459246000	-0.422915000		1	-0.395189000	5.796019000	-0.371300000
1	5.747099000	-1.574670000	0.943072000		6	0.144425000	3.732911000	-0.591488000
6	4.962724000	1.538314000	0.165936000		1	1.079100000	3.945481000	-1.109969000
1	5.036663000	2.456636000	-0.438059000		6	-0.233165000	2.392366000	-0.340700000
1	3.992051000	1.545037000	0.686435000		6	3.841659000	0.072132000	-2.230607000
1	5.752277000	1.578514000	0.933219000		1	4.021565000	0.979822000	-2.828785000
6	6.849204000	-0.008315000	-1.726361000		1	3.988904000	-0.795565000	-2.894431000
1	7.657137000	-0.007172000	-0.977875000		14	5.170980000	0.010483000	-0.861746000
1	6.976106000	-0.901238000	-2.358336000		6	4.962428000	-1.562521000	0.149901000
1	6.979135000	0.879875000	-2.364351000		1	3.993855000	-1.579556000	0.673816000
					1	5.029251000	-2.461807000	-0.482908000
					1	5.754745000	-1.631063000	0.912439000
					6	4.963784000	1.511756000	0.251742000
23	-1.811751000	0.019816000	0.577168000		1	5.038535000	2.450438000	-0.320009000
7	-1.313345000	-2.108667000	0.362272000		1	3.988797000	1.498511000	0.763973000
7	-1.410301000	2.116834000	0.304301000		1	5.747990000	1.527432000	1.025305000
14	-3.450953000	-0.120317000	-2.282981000		6	6.863806000	0.032048000	-1.681808000
6	-3.638197000	-0.093347000	-0.425647000		1	7.665955000	0.000664000	-0.927742000
1	-4.189081000	-1.003805000	-0.118532000		1	6.992979000	-0.835240000	-2.348114000
1	-4.261171000	0.782219000	-0.156867000		1	7.001189000	0.944687000	-2.282621000
6	-2.561126000	1.432724000	-2.892085000					
1	-1.504090000	1.427156000	-2.580086000					
1	-3.025621000	2.348750000	-2.491249000					
1	-2.584707000	1.495524000	-3.992142000					
6	-5.130349000	-0.207865000	-3.154779000					
1	-5.015900000	-0.218825000	-4.251022000					
1	-5.756568000	0.658685000	-2.888208000					
1	-5.679084000	-1.117551000	-2.862195000					
6	-2.439561000	-1.619826000	-2.843478000					
1	-1.375563000	-1.497022000	-2.584400000					
1	-2.500266000	-1.744774000	-3.936834000					
1	-2.798988000	-2.552820000	-2.378453000					
14	-0.277947000	0.035986000	3.498495000					
6	-1.944939000	-0.019846000	2.658799000					
1	-2.531132000	0.852906000	3.007628000					
1	-2.472017000	-0.934092000	2.994842000					
6	0.676290000	1.594827000	3.013245000					
1	0.988999000	1.550268000	1.957349000					
1	1.585410000	1.705211000	3.626653000					
1	0.066885000	2.503959000	3.145499000					
6	0.784933000	-1.453951000	3.011564000					
1	1.138219000	-1.361225000	1.971883000					
1	0.229983000	-2.402496000	3.100461000					
1	1.675391000	-1.523952000	3.657459000					
6	-0.445232000	0.022876000	5.385360000					
1	0.540059000	0.060516000	5.877997000					
1	-0.961324000	-0.888208000	5.728593000					
1	-1.031330000	0.888503000	5.733593000					
6	-2.057328000	-3.132344000	0.790237000					
1	-2.994202000	-2.873137000	1.290311000					
6	-1.674917000	-4.456902000	0.617293000					

1	0.994849000	-1.826509000	1.959718000		1	-2.961289000	-2.900157000	-1.874772000
1	0.114953000	-2.649418000	3.279162000		14	0.197185000	0.528688000	3.336511000
1	1.679689000	-1.853123000	3.604709000		6	-1.561341000	0.215304000	2.768125000
6	-0.220318000	-0.031525000	5.344421000		1	-2.176970000	1.058805000	3.139419000
1	0.787829000	-0.075357000	5.784873000		1	-1.922696000	-0.704459000	3.261982000
1	-0.818009000	-0.859407000	5.756159000		6	0.857442000	2.180713000	2.674771000
1	-0.692273000	0.915885000	5.647408000		1	0.970409000	2.149279000	1.580302000
6	-2.164711000	-3.009399000	0.740451000		1	1.842625000	2.394299000	3.118043000
1	-3.074582000	-2.706201000	1.256326000		1	0.175207000	3.007101000	2.928693000
6	-1.852625000	-4.350438000	0.546721000		6	1.387228000	-0.832247000	2.749936000
1	-2.523715000	-5.122737000	0.914058000		1	1.514256000	-0.780943000	1.657718000
6	-0.672990000	-4.665393000	-0.123424000		1	1.016156000	-1.834477000	3.016850000
1	-0.395451000	-5.703298000	-0.297233000		1	2.374621000	-0.691386000	3.217228000
6	0.150967000	-3.639339000	-0.570674000		6	0.310130000	0.591324000	5.233677000
1	1.075100000	-3.856869000	-1.098752000		1	1.344146000	0.778829000	5.562000000
6	-0.234144000	-2.320953000	-0.331385000		1	-0.026610000	-0.362578000	5.668282000
7	-0.034679000	0.044992000	-0.448428000		1	-0.332361000	1.393705000	5.627842000
6	0.567893000	-1.133195000	-0.748078000		6	-1.942336000	-2.946657000	1.313152000
6	1.792988000	-1.192211000	-1.353687000		1	-2.821124000	-2.612402000	1.862534000
1	2.266315000	-2.146298000	-1.571795000		6	-1.572156000	-4.286645000	1.282181000
6	2.466459000	0.028683000	-1.690199000		1	-2.165457000	-5.026565000	1.813510000
6	1.833903000	1.218995000	-1.409353000		6	-0.436288000	-4.642889000	0.559738000
1	2.321941000	2.161136000	-1.651216000		1	-0.114361000	-5.681338000	0.510467000
6	0.567439000	1.228596000	-0.774236000		6	0.288327000	-3.656786000	-0.099798000
6	-2.073674000	3.189292000	0.730873000		1	1.178915000	-3.907808000	-0.668858000
1	-2.988368000	2.924801000	1.261926000		6	-0.151846000	-2.336835000	-0.017564000
6	-1.726193000	4.503627000	0.522472000		7	-0.079591000	-0.004671000	-0.461835000
1	-2.363918000	5.303780000	0.887804000		6	0.547895000	-1.186779000	-0.664478000
6	-0.524507000	4.773748000	-0.178103000		6	1.724481000	-1.280984000	-1.354241000
1	-0.218933000	5.801472000	-0.365124000		1	2.218830000	-2.237162000	-1.503401000
6	0.252147000	3.733177000	-0.621293000		6	2.331129000	-0.079615000	-1.859059000
1	1.174417000	3.919959000	-1.164959000		6	1.674384000	1.113718000	-1.676027000
6	-0.161781000	2.398768000	-0.371566000		1	2.113324000	2.036045000	-2.050879000
6	3.866978000	-0.016366000	-2.234995000		6	0.440998000	1.157901000	-0.969393000
1	4.058745000	0.843281000	-2.892881000		6	-2.214072000	3.180554000	0.425075000
1	4.032425000	-0.939657000	-2.807924000		1	-3.085820000	2.948439000	1.037840000
14	5.118563000	0.053853000	-0.788138000		6	-1.945145000	4.471624000	0.032942000
6	4.751733000	-1.326145000	0.446626000		1	-2.602654000	5.284144000	0.328573000
1	3.758106000	-1.188743000	0.898710000		6	-0.789786000	4.699052000	-0.758655000
1	4.791914000	-2.314805000	-0.034697000		1	-0.541441000	5.707033000	-1.085962000
1	5.503829000	-1.302305000	1.250173000		6	0.014438000	3.646097000	-1.110843000
6	4.970744000	1.724281000	0.079201000		1	0.903217000	3.805012000	-1.715634000
1	5.127716000	2.551270000	-0.629764000		6	-0.320553000	2.333171000	-0.677959000
1	3.982715000	1.838725000	0.548761000		6	3.709268000	-0.148167000	-2.452951000
1	5.736809000	1.794063000	0.866661000		1	3.902580000	0.724266000	-3.092767000
6	6.855177000	-0.151140000	-1.500601000		1	3.834439000	-1.061527000	-3.052668000
1	7.605330000	-0.102909000	-0.697033000		14	5.005776000	-0.152735000	-1.042267000
1	6.951955000	-1.121332000	-2.010354000		6	4.831487000	-1.717060000	0.003627000
1	7.069982000	0.648079000	-2.225733000		1	3.864638000	-1.739730000	0.527536000

#1 at M06HF/def2svp

23	-1.754822000	0.135867000	0.677034000		1	5.632856000	-1.732418000	0.758489000
7	-1.247717000	-2.005918000	0.677957000		6	4.738364000	1.363170000	0.049352000
7	-1.437910000	2.135997000	0.090294000		1	4.780823000	2.289577000	-0.543213000
14	-3.697335000	-0.491471000	-1.916225000		1	3.763624000	1.311643000	0.556995000
6	-3.683875000	-0.274071000	-0.055271000		1	5.527722000	1.406009000	0.815470000
1	-4.142637000	-1.169242000	0.400996000		6	6.722901000	-0.100604000	-1.826358000
1	-4.333698000	0.592058000	0.179457000		1	7.497907000	-0.105286000	-1.045168000
6	-2.965252000	1.025564000	-2.791843000		1	6.877682000	-0.974854000	-2.476233000
1	-1.895085000	1.133516000	-2.556082000		1	6.842825000	0.810822000	-2.430825000
1	-3.482922000	1.947268000	-2.483127000					
1	-3.069999000	0.917020000	-3.882530000					
6	-5.460831000	-0.739952000	-2.582088000					
1	-5.455768000	-0.859945000	-3.676523000					
1	-6.090200000	0.127111000	-2.328992000					
1	-5.915925000	-1.637015000	-2.134537000					
6	-2.679713000	-2.004882000	-2.450997000					
1	-1.603738000	-1.820134000	-2.311903000					
1	-2.854689000	-2.211246000	-3.518362000					

Scheme 4 computed at the ω B97X-D/def2-SVP/SMD (diethyl ether)/Ultrafinegrid level**A³**

23	-0.053097000	-0.056460000	0.840547000
17	1.400611000	1.826757000	0.775550000
17	-1.500078000	-1.922704000	0.541588000

7	-1.654279000	1.216549000	0.276132000		1	1.880445000	0.888539000	1.606201000
6	-2.447529000	1.782626000	1.187824000		14	0.096487000	0.000049000	0.065263000
1	-2.227953000	1.551789000	2.232080000		6	0.115788000	1.528889000	-1.063892000
6	-3.496646000	2.620954000	0.828100000		1	1.023105000	1.564671000	-1.690861000
1	-4.123341000	3.064679000	1.602242000		1	0.088906000	2.458475000	-0.469081000
6	-3.717456000	2.872122000	-0.521488000		1	-0.754843000	1.547991000	-1.742610000
1	-4.531430000	3.525898000	-0.840043000		6	-1.400977000	0.001223000	1.130208000
6	-2.886488000	2.279304000	-1.468392000		1	-1.389252000	0.890618000	1.794509000
1	-3.039673000	2.463664000	-2.531569000		1	-1.389356000	-0.886206000	1.797148000
6	-1.857280000	1.449890000	-1.033664000		1	-0.755329000	-1.550174000	-1.740131000
7	1.581936000	-1.282094000	0.266117000		6	0.115498000	-1.530398000	-1.061670000
6	2.333083000	-1.907812000	1.174439000		1	1.022634000	-1.567464000	-1.688812000
1	2.057081000	-1.755369000	2.219675000		1	0.088402000	-2.459078000	-0.465449000
6	3.408793000	-2.709616000	0.810308000		1	1.880958000	-0.888006000	1.605661000
1	3.999208000	-3.204298000	1.582057000		3	-3.105975000	-0.000610000	0.015274000
6	3.703072000	-2.857846000	-0.540411000					
1	4.540687000	-3.479245000	-0.862528000					
6	2.916096000	-2.202861000	-1.484023000					
1	3.129545000	-2.305751000	-2.547702000					
6	1.855224000	-1.416569000	-1.044946000					
7	0.004561000	0.024580000	-1.282992000					
6	-0.904611000	0.757700000	-1.930151000					
6	-0.907100000	0.825092000	-3.322423000					
1	-1.650032000	1.418447000	-3.854410000					
6	0.062568000	0.112515000	-4.021145000					
1	0.085194000	0.146468000	-5.111606000					
6	1.003186000	-0.644239000	-3.328882000					
1	1.766384000	-1.204845000	-3.867591000					
6	0.942195000	-0.666218000	-1.936364000					
17	-0.114742000	-0.150297000	3.127973000					
A¹								
23	-0.000137000	-0.944761000	0.000130000					
17	-0.000191000	-0.669794000	2.322803000					
17	0.000628000	-0.669864000	-2.322577000					
7	-2.091512000	-0.440494000	-0.0000331000					
6	-3.087286000	-1.324433000	-0.000579000					
1	-2.793621000	-2.376817000	-0.000877000					
6	-4.422825000	-0.932630000	-0.0000566000					
1	-5.210289000	-1.687217000	-0.000750000					
6	-4.716673000	0.426052000	-0.000212000					
1	-5.752009000	0.771946000	-0.0000173000					
6	-3.672512000	1.348411000	-0.0000066000					
1	-3.882416000	2.417827000	0.000066000					
6	-2.361144000	0.880796000	-0.000092000					
7	2.091531000	-0.440747000	0.000096000					
6	3.087177000	-1.324813000	0.000017000					
1	2.793403000	-2.377167000	0.000038000					
6	4.422773000	-0.933190000	-0.000220000					
1	5.210141000	-1.687877000	-0.000380000					
6	4.716790000	0.425454000	-0.000251000					
1	5.752170000	0.771215000	-0.000387000					
6	3.672745000	1.347950000	-0.000003000					
1	3.882797000	2.417336000	0.000050000					
6	2.361315000	0.880501000	0.000023000					
7	0.000094000	1.139397000	0.000100000					
6	-1.173111000	1.776195000	0.000049000					
6	-1.208416000	3.169899000	0.000057000					
1	-2.153329000	3.711992000	0.000041000					
6	0.000252000	3.861768000	0.000107000					
1	0.000319000	4.953173000	0.000134000					
6	1.208841000	3.169748000	0.000110000					
1	2.153813000	3.711735000	0.000084000					
6	1.173380000	1.776050000	0.000094000					
17	-0.000817000	-3.248005000	0.000320000					
(CH₃)₃SiCH₂Li								
1	2.625971000	0.000870000	0.252649000					
6	1.777269000	0.000437000	0.958898000					
Cation of B								
23	-0.004909000	0.003106000	-0.819199000					
14	1.111922000	-3.125994000	-1.042502000					
6	0.555479000	-1.594566000	-1.970601000					
1	-0.296959000	-1.880546000	-2.618903000					
1	1.384011000	-1.278708000	-2.635757000					
6	2.634978000	-2.750148000	0.009100000					
1	2.388910000	-2.092675000	0.858643000					
1	3.426424000	-2.258694000	-0.581105000					
1	3.059402000	-3.678633000	0.426317000					
6	1.542535000	-4.514911000	-2.242306000					
1	1.867484000	-5.421585000	-1.704742000					
1	2.358867000	-4.214065000	-2.919775000					
1	0.674562000	-4.785536000	-2.866105000					
6	-0.259716000	-3.726425000	0.109663000					
1	-0.424768000	-3.020911000	0.940735000					
1	-0.001913000	-4.702259000	0.554133000					
1	-1.216115000	-3.847247000	-0.426109000					
14	-1.090843000	3.132034000	-0.982447000					
6	-0.560687000	1.616190000	-1.951100000					
1	0.286307000	1.908227000	-2.603516000					
1	-1.400505000	1.321316000	-2.611364000					
6	0.306273000	3.712488000	0.148814000					
1	0.483358000	2.997203000	0.968695000					
1	0.060146000	4.684166000	0.608751000					
1	1.253287000	3.835881000	-0.402849000					
6	-2.589989000	2.741639000	0.098222000					
1	-2.325400000	2.069998000	0.931016000					
1	-3.396304000	2.261382000	-0.481054000					
1	-3.002103000	3.664180000	0.540220000					
6	-1.546499000	4.541928000	-2.148235000					
1	-1.857852000	5.439783000	-1.588303000					
1	-2.378240000	4.253604000	-2.812284000					
1	-0.692233000	4.822021000	-2.786625000					
7	-2.005134000	-0.652673000	-0.310032000					
6	-2.965740000	-0.933164000	-1.189690000					
1	-2.703179000	-0.831649000	-2.245379000					
6	-4.240004000	-1.333335000	-0.796109000					
1	-4.998924000	-1.552432000	-1.547669000					
6	-4.509676000	-1.441647000	0.562794000					
1	-5.496608000	-1.751023000	0.911553000					
6	-3.504079000	-1.150390000	1.483639000					
1	-3.700239000	-1.230492000	2.552430000					
6	-2.256820000	-0.756511000	1.011201000					
1	1.987129000	0.676191000	-0.301585000					
6	2.927605000	1.034430000	-1.174710000					
1	2.665060000	0.955244000	-2.232282000					
6	4.181235000	1.487835000	-0.772360000					
1	4.923198000	1.772226000	-1.519002000					
6	4.451401000	1.568324000	0.588410000					
1	5.420816000	1.922243000	0.943620000					
6	3.467907000	1.192543000	1.502442000					
1	3.661795000	1.252389000	2.572957000					

6	2.242127000	0.746724000	1.021143000		1	1.341065000	-5.265657000	1.125620000
7	-0.003882000	-0.016969000	1.258574000		6	1.008367000	-3.421822000	0.070005000
6	-1.111503000	-0.416347000	1.901498000		1	1.657693000	-3.685248000	-0.765026000
6	-1.123572000	-0.491732000	3.292185000		6	0.341800000	-2.186297000	0.084606000
1	-2.012121000	-0.812304000	3.834726000		7	-1.853149000	1.917375000	-0.086487000
6	0.036929000	-0.151214000	3.983349000		6	-2.687291000	2.870602000	0.350043000
1	0.054075000	-0.208824000	5.073011000		1	-3.196063000	2.665987000	1.295769000
6	1.176074000	0.259709000	3.295284000		6	-2.905233000	4.050250000	-0.341137000
1	2.083815000	0.521004000	3.837947000		1	-3.594174000	4.797891000	0.053577000
6	1.121086000	0.322412000	1.905219000		6	-2.221239000	4.247766000	-1.547415000
					1	-2.365871000	5.164578000	-2.122706000
					6	-1.357719000	3.268206000	-2.006411000
					1	-0.817678000	3.404178000	-2.943566000
Anion of B					6	-1.184980000	2.096775000	-1.252534000
1	1.431725000	-1.319287000	-1.461829000		7	-0.304191000	-0.044739000	-0.716484000
6	0.417853000	-1.470323000	-1.050579000		6	0.453633000	-1.169928000	-0.959213000
1	0.431139000	-2.417530000	-0.481954000		6	1.226443000	-1.270762000	-2.105291000
14	-0.143837000	-0.021265000	0.062909000		1	1.823576000	-2.164894000	-2.289685000
6	1.356483000	0.175834000	1.266952000		6	1.245234000	-0.212923000	-3.024497000
1	2.322735000	0.317591000	0.747184000		1	1.856331000	-0.274599000	-3.925490000
1	1.456768000	-0.714502000	1.914341000		6	0.460409000	0.922480000	-2.778289000
1	1.210061000	1.042230000	1.937519000		1	0.459099000	1.748789000	-3.489989000
6	-1.809269000	-0.279950000	0.695878000		6	-0.308240000	0.988499000	-1.628092000
1	-1.941767000	-1.205175000	1.293053000		14	4.802999000	-0.045168000	-1.030205000
1	-2.228077000	0.576414000	1.262687000		6	3.417499000	1.183536000	-0.891171000
1	-0.259231000	2.457591000	-0.397498000		1	2.432840000	0.934578000	-0.482802000
6	-0.026500000	1.562237000	-1.001661000		1	3.505593000	2.218671000	-1.247025000
1	0.983458000	1.706227000	-1.424927000		6	6.410395000	0.758179000	-0.461260000
1	-0.747000000	1.537910000	-1.837087000		1	6.649973000	1.644405000	-1.072146000
1	-0.277497000	-1.610546000	-1.895748000		1	7.254896000	0.053839000	-0.545675000
C ↓>_R ↑>_L ↑↑>_V					1	6.344084000	1.082766000	0.590066000
23	-1.443744000	0.054974000	0.900923000		6	4.436645000	-1.562819000	0.020576000
14	-3.965652000	-1.379795000	-0.756780000		1	5.175820000	-2.358106000	-0.173353000
6	-3.405038000	-0.662073000	0.867711000		1	3.436668000	-1.968013000	-0.201235000
1	-3.511666000	-1.443156000	1.648240000		1	4.466488000	-1.329865000	1.096556000
1	-4.091700000	0.166794000	1.135750000		6	5.019233000	-0.584227000	-2.828238000
6	-3.874766000	-0.090563000	-2.136568000		1	5.130393000	0.285312000	-3.496726000
1	-2.829313000	0.148804000	-2.389188000		1	4.156194000	-1.171446000	-3.179890000
1	-4.373761000	0.849374000	-1.846057000		1	5.920466000	-1.211073000	-2.938079000
1	-4.361723000	-0.457999000	-3.055739000					
6	-5.755930000	-1.994070000	-0.669737000					
1	-6.089140000	-2.418410000	-1.632419000					
1	-6.444573000	-1.172616000	-0.408584000					
1	-5.869207000	-2.776852000	0.099446000					
6	-2.887094000	-2.848829000	-1.260361000					
1	-1.877305000	-2.519912000	-1.553893000					
1	-3.323357000	-3.384467000	-2.120462000					
1	-2.778272000	-3.573128000	-0.435438000					
14	0.939986000	1.536142000	2.708639000					
6	-0.804318000	0.885471000	2.712767000					
1	-1.489537000	1.714542000	2.984023000					
1	-0.888339000	0.117498000	3.508944000					
6	1.149070000	2.891041000	1.407173000					
1	0.967755000	2.512982000	0.389411000					
1	2.169534000	3.309498000	1.429348000					
1	0.442211000	3.719541000	1.585025000					
6	2.161736000	0.141388000	2.347780000					
1	1.964013000	-0.327754000	1.372056000					
1	2.097638000	-0.649762000	3.114181000					
1	3.198459000	0.517650000	2.336903000					
6	1.430924000	2.290836000	4.375703000					
1	2.469294000	2.664541000	4.361960000					
1	1.352634000	1.547142000	5.186817000					
1	0.773494000	3.137088000	4.638010000					
7	-0.482190000	-1.854693000	1.109804000					
6	-0.650812000	-2.712905000	2.124966000					
1	-1.325656000	-2.386971000	2.920859000					
6	-0.018659000	-3.943313000	2.179895000					
1	-0.186150000	-4.608696000	3.027565000					
6	0.827831000	-4.301889000	1.122794000					

ts0a, i292 cm⁻¹

23	1.580190000	-0.018104000	0.864327000
14	3.842089000	1.510331000	-1.051868000
6	3.493500000	0.788679000	0.630624000
1	3.649286000	1.585679000	1.386539000
1	4.247985000	-0.000771000	0.828207000
6	3.653920000	0.205457000	-2.407397000
1	2.596647000	-0.071221000	-2.548382000
1	4.213995000	-0.714248000	-2.167864000
1	4.028519000	0.582563000	-3.374097000
6	5.604180000	2.197106000	-1.165680000
1	5.812024000	2.625008000	-2.161421000
1	6.350131000	1.406248000	-0.977688000
1	5.769426000	2.991120000	-0.417728000
6	2.653587000	2.926928000	-1.446473000
1	1.632898000	2.551862000	-1.624676000
1	2.970205000	3.467146000	-2.354744000
1	2.604453000	3.658614000	-0.622374000
14	-0.636891000	-1.614155000	2.772689000
6	1.078285000	-0.886494000	2.694984000
1	1.804809000	-1.690853000	2.931513000
1	1.163639000	-0.122533000	3.495114000
6	-0.844295000	-3.024248000	1.530530000
1	-0.839388000	-2.649662000	0.494890000
1	-1.802883000	-3.547254000	1.687602000
1	-0.037200000	-3.770779000	1.621330000
6	-1.956085000	-0.319112000	2.383737000
1	-1.890934000	0.009646000	1.335123000
1	-1.859053000	0.574774000	3.022722000

C ↑> _R ↓> _L ↑↑> _V				ts0b, i270 cm⁻¹			
1	-2.965129000	-0.735858000	2.540559000	14	0.914799000	1.513519000	2.721495000
6	-1.017781000	-2.314794000	4.491324000	6	-0.830570000	0.859116000	2.706700000
1	-2.033802000	-2.742679000	4.540718000	1	-1.517984000	1.686285000	2.977043000
1	-0.946140000	-1.530277000	5.263728000	1	-0.919456000	0.086695000	3.497895000
1	-0.304258000	-3.111386000	4.762434000	6	1.130067000	2.882113000	1.436394000
7	0.583677000	1.865179000	1.161603000	1	0.959949000	2.514127000	0.413038000
6	0.855019000	2.757323000	2.122407000	1	2.149055000	3.303106000	1.472817000
1	1.639766000	2.477326000	2.830055000	1	0.419175000	3.706610000	1.616507000
6	0.191760000	3.968972000	2.227246000	6	2.142123000	0.125486000	2.355970000
1	0.445206000	4.665902000	3.026844000	1	1.952428000	-0.335493000	1.374756000
6	-0.798909000	4.264632000	1.284550000	1	2.076016000	-0.672452000	3.115105000
1	-1.342792000	5.210408000	1.329802000	1	3.1774477000	0.505622000	2.355020000
6	-1.086083000	3.345388000	0.288632000	6	1.382957000	2.249250000	4.402553000
1	-1.851985000	3.561046000	-0.456402000	1	2.420167000	2.626242000	4.404562000
6	-0.375618000	2.137008000	0.246157000	1	1.298120000	1.495469000	5.203541000
7	1.986469000	-1.863996000	-0.164978000	1	0.719783000	3.090182000	4.667192000
6	2.935609000	-2.750963000	0.157145000	7	-0.469122000	-1.874756000	1.080912000
1	3.546200000	-2.505777000	1.030076000	6	-0.636137000	-2.741267000	2.088329000
6	3.145754000	-3.915974000	-0.563143000	1	-1.309957000	-2.422297000	2.887988000
1	3.931423000	-4.611091000	-0.265012000	6	-0.003976000	-3.972545000	2.131820000
6	2.328432000	-4.165379000	-1.670044000	1	-0.169998000	-4.645706000	2.973560000
1	2.462901000	-5.070755000	-2.265550000	6	0.840386000	-4.320943000	1.069352000
6	1.342561000	-3.251516000	-2.007308000	1	1.353322000	-5.284920000	1.062392000
1	0.697677000	-3.429355000	-2.867787000	6	1.019771000	-3.432254000	0.024193000
6	1.186928000	-2.095180000	-1.231326000	1	1.667735000	-3.689158000	-0.813938000
7	0.258456000	0.000801000	-0.591987000	6	0.353713000	-2.195301000	0.049675000
6	-0.593539000	1.076037000	-0.742143000	7	-1.846442000	1.912090000	-0.088479000
6	-1.569363000	1.081458000	-1.712155000	6	-2.683068000	2.859168000	0.354435000
1	-2.235496000	1.937154000	-1.823661000	1	-3.192863000	2.645445000	1.297636000
6	-1.756624000	-0.062164000	-2.523742000	6	-2.902947000	4.044480000	-0.327173000
1	-2.462808000	-0.033620000	-3.352423000	1	-3.594080000	4.787415000	0.072476000
6	-0.797068000	-1.102708000	-2.444146000	6	-2.216968000	4.252767000	-1.530599000
1	-0.864068000	-1.951980000	-3.124787000	1	-2.362445000	5.174100000	-2.098504000
6	0.175845000	-1.056315000	-1.472986000	6	-1.350908000	3.279294000	-1.996743000
14	-4.967355000	0.052852000	-1.037563000	1	-0.809926000	3.424441000	-2.931965000
6	-3.606125000	-1.196190000	-1.222248000	6	-1.176131000	2.100776000	-1.252715000
1	-2.922026000	-1.424992000	-0.395859000	7	-0.293480000	-0.044281000	-0.730084000
1	-3.697418000	-2.016991000	-1.946143000	6	0.464886000	-1.170415000	-0.983188000
6	-6.599307000	-0.809049000	-0.632306000	6	1.238310000	-1.259385000	-2.129580000
1	-6.885492000	-1.516084000	-1.428681000	1	1.835876000	-2.151664000	-2.321961000
1	-7.416456000	-0.075559000	-0.523828000	6	1.258602000	-0.192566000	-3.040107000
1	-6.527782000	-1.376756000	0.310010000	1	1.870412000	-0.246187000	-3.941076000
6	-4.575010000	1.267289000	0.348255000	6	0.470839000	0.941128000	-2.784852000
1	-5.327294000	2.073478000	0.378893000	1	0.469284000	1.772915000	-3.490303000
1	-3.584006000	1.731914000	0.227023000	6	-0.298583000	0.997737000	-1.635690000
1	-4.583791000	0.765687000	1.329053000	14	4.800823000	-0.020081000	-1.004881000
6	-5.211695000	0.994346000	-2.656551000	6	3.406672000	1.198428000	-0.864494000
1	-5.368735000	0.299548000	-3.498654000	1	2.415497000	0.934368000	-0.482175000
1	-4.345198000	1.629165000	-2.902492000	1	3.494879000	2.241207000	-1.197187000
1	-6.097397000	1.649065000	-2.597217000	6	6.396766000	0.783502000	-0.404641000
1	6.638219000	1.638219000	1.680754000	1	6.638219000	1.680754000	-0.998452000
1	7.246434000	0.085543000	-0.490211000	1	7.246434000	0.085543000	-0.490211000
1	6.316277000	1.090890000	0.650875000	1	6.316277000	1.090890000	0.650875000
6	4.430321000	-1.555268000	0.018681000	6	4.430321000	-1.555268000	0.018681000
1	5.175689000	-2.344002000	-0.178396000	1	5.175689000	-2.344002000	-0.178396000
1	3.435127000	-1.961267000	-0.222200000	1	3.435127000	-1.961267000	-0.222200000
1	4.445839000	-1.338784000	1.098392000	6	5.040380000	-0.531603000	-2.807903000
1	5.040380000	-0.531603000	-2.807903000	1	5.040380000	-0.531603000	-2.807903000
1	5.156330000	0.348241000	-3.461937000	1	5.156330000	0.348241000	-3.461937000
1	4.182528000	-1.115370000	-3.177576000	1	4.182528000	-1.115370000	-3.177576000
1	5.944544000	-1.154364000	-2.916913000	1	5.944544000	-1.154364000	-2.916913000
ts0b, i270 cm⁻¹				ts0b, i270 cm⁻¹			
23	1.576337000	-0.006329000	0.854319000	23	1.576337000	-0.006329000	0.854319000
14	3.845540000	1.505978000	-1.049493000	14	3.845540000	1.505978000	-1.049493000
6	3.486797000	0.793191000	0.636598000	6	3.486797000	0.793191000	0.636598000
1	3.638001000	1.595261000	1.387805000	1	3.638001000	1.595261000	1.387805000
1	4.240282000	0.005542000	0.842401000	1	4.240282000	0.005542000	0.842401000
6	3.668271000	0.193381000	-2.398254000	6	3.668271000	0.193381000	-2.398254000

1	2.612397000	-0.086345000	-2.543623000		1	-4.364385000	1.589217000	-2.900318000
1	4.229472000	-0.723626000	-2.151284000		1	-6.114967000	1.614989000	-2.585484000
1	4.047126000	0.566987000	-3.364631000					
6	5.608198000	2.191664000	-1.147519000					
1	5.825617000	2.615080000	-2.143074000					
1	6.352056000	1.401575000	-0.948697000		23	1.644898000	-0.024945000	0.811107000
1	5.765678000	2.989005000	-0.401524000		14	3.572555000	1.619476000	-1.367796000
6	2.658766000	2.918795000	-1.459976000		6	3.472068000	0.865510000	0.334227000
1	1.639277000	2.541759000	-1.640855000		1	3.695519000	1.662404000	1.073118000
1	2.980165000	3.451899000	-2.370737000		1	4.279342000	0.108862000	0.418297000
1	2.605106000	3.656807000	-0.641867000		6	3.286733000	0.322194000	-2.713245000
14	-0.614531000	-1.591792000	2.782262000		1	2.231998000	0.004510000	-2.740447000
6	1.100469000	-0.859962000	2.690244000		1	3.907283000	-0.575807000	-2.553418000
1	1.828705000	-1.661951000	2.928643000		1	3.535031000	0.726596000	-3.709163000
1	1.187453000	-0.090857000	3.485109000		6	5.272741000	2.396052000	-1.678166000
6	-0.823709000	-3.014659000	1.555810000		1	5.339820000	2.843625000	-2.684613000
1	-0.827467000	-2.650444000	0.516467000		1	6.074396000	1.642986000	-1.591477000
1	-1.779533000	-3.538965000	1.724794000		1	5.485490000	3.190375000	-0.942590000
1	-0.013603000	-3.757591000	1.648878000		6	2.278425000	2.978730000	-1.596572000
6	-1.939413000	-0.305118000	2.387454000		1	1.264489000	2.553402000	-1.668624000
1	-1.882683000	0.011093000	1.334514000		1	2.464185000	3.547239000	-2.523580000
1	-1.841670000	0.596450000	3.015360000		1	2.286707000	3.695838000	-0.758260000
1	-2.945771000	-0.723906000	2.555582000		14	-0.271438000	-1.658383000	2.973524000
6	-0.977392000	-2.274111000	4.511357000		6	1.408195000	-0.895131000	2.692602000
1	-1.991216000	-2.705423000	4.573292000		1	2.171903000	-1.687112000	2.836055000
1	-0.902892000	-1.480623000	5.274181000		1	1.576940000	-0.131086000	3.479036000
1	-0.258409000	-3.064735000	4.785249000		6	-0.606780000	-3.048332000	1.736540000
7	0.572556000	1.877874000	1.135297000		1	-0.757755000	-2.649313000	0.720786000
6	0.839978000	2.777417000	2.089776000		1	-1.516747000	-3.608643000	2.010747000
1	1.625038000	2.505029000	2.800092000		1	0.228432000	-3.767855000	1.696232000
6	0.172682000	3.987818000	2.185710000		6	-1.657031000	-0.383593000	2.796486000
1	0.422933000	4.691233000	2.980583000		1	-1.784225000	-0.076791000	1.746288000
6	-0.817891000	4.273238000	1.239436000		1	-1.458550000	0.523051000	3.392697000
1	-1.364834000	5.217609000	1.277375000		1	-2.617507000	-0.803823000	3.139978000
6	-1.101272000	3.346561000	0.249787000		6	-0.407876000	-2.402559000	4.711018000
1	-1.867051000	3.554335000	-0.497564000		1	-1.397648000	-2.859539000	4.882400000
6	-0.387323000	2.139084000	0.215927000		1	-0.255572000	-1.631824000	5.485634000
7	1.985916000	-1.860524000	-0.164010000		1	0.354570000	-3.184214000	4.868893000
6	2.938503000	-2.741108000	0.163783000		7	0.647488000	1.836174000	1.257546000
1	3.548482000	-2.487423000	1.034739000		6	1.024584000	2.735408000	2.171929000
6	3.152997000	-3.910641000	-0.548291000		1	1.896289000	2.472089000	2.776553000
1	3.941439000	-4.600643000	-0.245700000		6	0.358995000	3.939269000	2.351474000
6	2.335700000	-4.170693000	-1.652847000		1	0.699486000	4.647044000	3.108134000
1	2.473345000	-5.079763000	-2.242013000		6	-0.743366000	4.209582000	1.540182000
6	1.346220000	-3.263364000	-1.996273000		1	-1.293153000	5.147123000	1.645945000
1	0.701917000	-3.449856000	-2.855342000		6	-1.139114000	3.273427000	0.594275000
6	1.185807000	-2.101470000	-1.228582000		1	-1.997794000	3.468389000	-0.047832000
7	0.252383000	-0.003015000	-0.604215000		6	-0.419367000	2.081577000	0.471190000
6	-0.602208000	1.071057000	-0.763073000		7	2.013929000	-1.834073000	-0.301905000
6	-1.579320000	1.064742000	-1.732006000		6	3.043539000	-2.669361000	-0.129879000
1	-2.248417000	1.917441000	-1.849780000		1	3.727777000	-2.429324000	0.688019000
6	-1.764034000	-0.086131000	-2.534150000		6	3.246008000	-3.778463000	-0.937841000
1	-2.475968000	-0.069139000	-3.358177000		1	4.099729000	-4.434851000	-0.765351000
6	-0.802289000	-1.125111000	-2.446290000		6	2.333103000	-4.020216000	-1.965158000
1	-0.868506000	-1.980292000	-3.119648000		1	2.457423000	-4.880104000	-2.626723000
6	0.171814000	-1.068452000	-1.477254000		6	1.260032000	-3.156998000	-2.140277000
14	-4.978272000	0.032003000	-1.016385000		1	0.535247000	-3.328962000	-2.935644000
6	-3.624868000	-1.224434000	-1.196371000		6	1.121116000	-2.058874000	-1.286907000
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1	-3.716721000	-2.048525000	-1.916322000		6	-0.750141000	0.992596000	-0.482527000
6	-6.613526000	-0.814870000	-0.591610000		6	-1.819729000	0.999679000	-1.305429000
1	-6.909411000	-1.527997000	-1.379004000		1	-2.476036000	1.870051000	-1.343385000
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1	-5.313183000	2.074027000	0.376693000		1	-1.078524000	-1.956156000	-2.951249000
1	-3.574065000	1.710631000	0.224789000		6	0.014895000	-1.070773000	-1.360091000
1	-4.582157000	0.769489000	1.340869000		14	-4.977902000	0.040844000	-1.092884000
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6	-6.412981000	-1.170095000	-0.947198000		6	-0.750755000	0.992796000	-0.482059000
1	-6.586160000	-1.703409000	-1.896543000		6	-1.820808000	1.000474000	-1.304124000
1	-7.347373000	-0.649710000	-0.678545000		1	-2.476618000	1.871296000	-1.341713000
1	-6.215929000	-1.925965000	-0.168756000		6	-2.208397000	-0.214464000	-2.110219000
6	-4.804753000	0.955356000	0.545518000		1	-2.517113000	0.109088000	-3.121017000
1	-5.742815000	1.476615000	0.801134000		6	-1.025934000	-1.146959000	-2.219770000
1	-3.997125000	1.703333000	0.526550000		1	-1.081480000	-1.956066000	-2.951065000
1	-4.581138000	0.250261000	1.362989000		6	0.012880000	-1.071268000	-1.360467000
6	-5.333390000	1.263546000	-2.482392000		14	-4.979070000	0.041730000	-1.088731000
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1	-6.280565000	1.798769000	-2.301751000		1	-3.713142000	-1.783642000	-2.163284000
					6	-6.413685000	-1.169563000	-0.941383000
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1H¹					1	-7.347748000	-0.649539000	-0.670911000
23	1.641511000	-0.025718000	0.807675000		1	-6.215170000	-1.925817000	-0.163689000
14	3.565315000	1.615594000	-1.371203000		6	-4.804757000	0.956617000	0.549336000
6	3.465192000	0.860022000	0.330681000		1	-5.742653000	1.477940000	0.805426000
1	3.692052000	1.657476000	1.068171000		1	-3.997137000	1.704570000	0.529770000
1	4.273573000	0.104049000	0.411873000		1	-4.580743000	0.251606000	1.366763000
6	3.276890000	0.320622000	-2.718153000		6	-5.336057000	1.263933000	-2.478256000
1	2.221710000	0.004491000	-2.745404000		1	-5.426234000	0.746486000	-3.447927000
1	3.896290000	-0.578453000	-2.559994000		1	-4.541391000	2.021377000	-2.576485000
1	3.525339000	0.726255000	-3.713536000		1	-6.283254000	1.798856000	-2.296838000
6	5.267148000	2.388892000	-1.680214000					
1	5.335272000	2.837569000	-2.686089000		4⁴			
1	6.067136000	1.633970000	-1.594405000		23	0.000041000	0.000155000	-0.857924000
1	5.481473000	3.181844000	-0.943630000		14	-3.263461000	0.687861000	-0.901849000
6	2.273868000	2.977583000	-1.598107000		6	-1.751282000	0.365169000	-1.940464000
1	1.259275000	2.554263000	-1.672448000		1	-1.591609000	1.241923000	-2.601235000
1	2.461820000	3.547829000	-2.523605000		1	-1.959507000	-0.505907000	-2.595137000
1	2.282408000	3.692755000	-0.758168000		6	-3.650518000	-0.789736000	0.212728000
14	-0.270762000	-1.655372000	2.968889000		1	-2.898534000	-0.893610000	1.011462000
6	1.409191000	-0.892893000	2.684281000		1	-3.668139000	-1.734071000	-0.357199000
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6	-0.608662000	-3.045842000	1.733487000		1	-5.689748000	1.199989000	-1.355217000
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1	-0.247082000	-1.626568000	5.480757000		1	1.959141000	0.504333000	-2.596001000
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7	0.654503000	1.829120000	1.253377000		1	2.286306000	-1.994065000	1.004062000
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6	0.374224000	3.931203000	2.352578000		6	3.650675000	0.789950000	0.211618000
1	0.719354000	4.636574000	3.109415000		1	2.898615000	0.894692000	1.010162000
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6	3.044359000	-2.659034000	-0.126900000		7	0.431441000	2.050149000	-0.383231000
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6	3.249017000	-3.769954000	-0.931764000		1	0.575097000	2.754173000	-2.322026000
1	4.104412000	-4.423647000	-0.757195000		6	0.921364000	4.336247000	-0.887835000
6	2.336843000	-4.017442000	-1.958372000		1	1.082946000	5.105705000	-1.643609000
1	2.463320000	-4.879050000	-2.617259000		6	0.991694000	4.626690000	0.480939000
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1	-0.575691000	-2.753970000	-2.321845000		1	-2.100620000	-2.154683000	-1.802656000
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1⁴					6	-4.785617000	-1.534445000	-0.073200000
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7	1.341321000	2.092647000	0.432411000		1	-3.816441000	-1.536122000	0.451862000
7	1.341420000	-2.092537000	0.432818000		1	-5.577206000	-1.575081000	0.693553000
14	3.821599000	-0.000201000	-1.813522000		6	-6.674536000	-0.000350000	-1.970504000
6	3.675076000	0.000004000	0.043077000		1	-7.482703000	-0.000270000	-1.220436000
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1	1.899100000	1.477794000	-2.454826000					
1	3.218679000	1.611427000	-3.639304000					
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14	-0.432399000	0.000461000	3.329961000					
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6	-0.608809000	0.000815000	5.217030000					
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6	1.781583000	4.431948000	0.673468000					
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6	-0.439842000	1.187603000	-0.841874000					
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ts1, i925 cm⁻¹

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6	-0.558644000	2.690627000	2.594932000		6	2.416574000	-3.285279000	1.788743000
1	0.400516000	3.194518000	2.477305000		1	1.341097000	-3.100642000	1.636344000
6	-0.926201000	1.659323000	1.725831000		1	2.512943000	-4.007286000	2.617262000
7	-2.079814000	-1.557283000	-1.465809000		1	2.810412000	-3.767745000	0.878247000
6	-2.892896000	-2.438273000	-2.057555000		14	3.485647000	1.731356000	-2.577469000
1	-3.853065000	-2.614509000	-1.565797000		6	1.824714000	1.249612000	-1.881775000
6	-2.550201000	-3.098592000	-3.228337000		1	1.251679000	0.755788000	-2.693727000
1	-3.242674000	-3.810161000	-3.679539000		1	1.292977000	2.195619000	-1.656120000
6	-1.304984000	-2.828401000	-3.797638000		6	4.519437000	0.237019000	-3.100878000
1	-0.994640000	-3.330457000	-4.716382000		1	4.764971000	-0.406598000	-2.240219000
6	-0.457975000	-1.917054000	-3.182058000		1	5.472230000	0.564244000	-3.550391000
1	0.522996000	-1.700469000	-3.604292000		1	3.994643000	-0.374171000	-3.854265000
6	-0.875690000	-1.283929000	-2.007934000		6	4.505932000	2.717107000	-1.326828000
7	-0.702346000	0.154358000	-0.110736000		1	4.741840000	2.114977000	-0.433973000
6	-0.083124000	1.155780000	0.614393000		1	3.972772000	3.626140000	-1.000849000
6	1.163573000	1.603962000	0.334166000		1	5.463013000	3.039776000	-1.770415000
1	1.594327000	2.406640000	0.933217000		6	3.286520000	2.824581000	-4.111608000
6	2.018114000	0.927784000	-0.682351000		1	4.262508000	3.127421000	-4.528124000
1	2.666541000	0.130842000	-0.048067000		1	2.723481000	3.742705000	-3.872640000
6	1.186295000	0.085694000	-1.590711000		1	2.732101000	2.295648000	-4.905331000
1	1.643312000	-0.274738000	-2.513468000		7	1.319632000	-1.858456000	-1.191022000
6	-0.059872000	-0.308981000	-1.245600000		6	2.120004000	-2.435604000	-2.094559000
14	4.198597000	2.934320000	-0.433278000		1	3.017649000	-1.876879000	-2.366622000
6	3.042528000	1.797102000	-1.420203000		6	1.840891000	-3.669622000	-2.661312000
1	2.517167000	2.434977000	-2.156584000		1	2.523845000	-4.103320000	-3.392614000
1	3.688191000	1.131435000	-2.021179000		6	0.671776000	-4.326236000	-2.270645000
6	5.706914000	3.261398000	-1.511742000		1	0.413521000	-5.299170000	-2.693921000
1	6.265520000	2.332062000	-1.711415000		6	-0.162866000	-3.729773000	-1.337190000
1	6.397876000	3.969641000	-1.025206000		1	-1.079932000	-4.225592000	-1.019353000
1	5.414908000	3.693171000	-2.483561000		6	0.188854000	-2.485085000	-0.801135000
6	3.362224000	4.584515000	-0.069645000		7	1.261873000	1.558387000	1.287200000
1	4.067740000	5.273736000	0.424041000		6	2.023568000	2.627761000	1.543716000
1	2.484140000	4.481529000	0.587497000		1	2.902251000	2.755079000	0.907873000
1	3.022786000	5.066035000	-1.001763000		6	1.728980000	3.529544000	2.554920000
6	4.746083000	2.140763000	1.182645000		1	2.378866000	4.387621000	2.730119000
1	5.264651000	1.186122000	1.002756000		6	0.589991000	3.303268000	3.330665000
1	3.894630000	1.942309000	1.852950000		1	0.323855000	3.987322000	4.139109000
1	5.443809000	2.807602000	1.716579000		6	-0.205416000	2.198722000	3.063615000
6	3.123338000	-1.099317000	0.941770000		1	-1.100555000	2.005558000	3.654412000
1	2.086540000	-1.406260000	1.134543000		6	0.155000000	1.331748000	2.026115000
1	3.541203000	-0.505242000	1.765554000		7	-0.042089000	-0.556903000	0.585411000
14	4.224862000	-2.208256000	-0.062684000		6	-0.606217000	-1.760169000	0.208247000
6	3.310509000	-2.802631000	-1.600174000		6	-1.778159000	-2.208213000	0.743246000
1	3.175536000	-1.986554000	-2.327257000		1	-2.179527000	-3.178850000	0.451410000
1	2.314011000	-3.198574000	-1.343594000		6	-2.550242000	-1.341774000	1.611057000
1	3.874862000	-3.606436000	-2.102077000		1	-3.305758000	-1.816752000	2.240790000
6	4.742827000	-3.716149000	0.949018000		6	-1.780442000	-0.268353000	2.214640000
1	3.866468000	-4.312539000	1.251640000		1	-2.196284000	0.277939000	3.062534000
1	5.411875000	-4.371401000	0.365554000		6	-0.612821000	0.132651000	1.637495000
1	5.277388000	-3.417248000	1.865738000		14	-4.956215000	-1.528234000	-0.410299000
1	6.427193000	-1.889791000	-1.208593000		6	-3.797234000	-0.265228000	0.375507000
6	5.773829000	-1.264646000	-0.577202000		1	-2.896625000	0.048411000	-0.146890000
1	5.516826000	-0.359829000	-1.152259000		1	-4.119010000	0.372292000	1.200990000
1	6.362463000	-0.951779000	0.301107000		6	-6.703074000	-0.895920000	-0.742471000
					1	-7.129251000	-0.409434000	0.150943000
					1	-7.357495000	-1.746761000	-0.997162000
					1	-6.749357000	-0.177397000	-1.574057000
					6	-4.170619000	-2.103674000	-2.021823000
					1	-4.780116000	-2.884781000	-2.505781000
					1	-3.163220000	-2.515795000	-1.849516000
					1	-4.067287000	-1.268069000	-2.732865000
					6	-5.222445000	-3.020471000	0.723305000
					1	-5.654628000	-2.709420000	1.689610000
					1	-4.310405000	-3.598858000	0.934195000
					1	-5.944514000	-3.708980000	0.252732000
					6	-4.557767000	1.493345000	-0.893466000
					1	-5.572429000	1.629751000	-0.496751000

ts2, i1108 cm⁻¹

23	1.674183000	0.024801000	-0.184107000		1	-6.749357000	-0.177397000	-1.574057000
14	3.336332000	-1.682211000	2.183273000		6	-4.170619000	-2.103674000	-2.021823000
6	3.464626000	-0.580570000	0.683806000		1	-4.780116000	-2.884781000	-2.505781000
1	4.063019000	-1.122201000	-0.076835000		1	-3.163220000	-2.515795000	-1.849516000
1	4.043887000	0.317732000	0.979379000		1	-4.067287000	-1.268069000	-2.732865000
6	2.422557000	-0.820358000	3.595459000		6	-5.222445000	-3.020471000	0.723305000
1	1.343931000	-0.742811000	3.385121000		1	-5.654628000	-2.709420000	1.689610000
1	2.808664000	0.198403000	3.768464000		1	-4.310405000	-3.598858000	0.934195000
1	2.534239000	-1.383971000	4.537213000		1	-5.944514000	-3.708980000	0.252732000
6	5.055577000	-2.155407000	2.822635000		6	-4.557767000	1.493345000	-0.893466000
					1	-5.572429000	1.629751000	-0.496751000

1	-4.571004000	1.062364000	-1.904442000		6	-2.210051000	1.461153000	-2.797226000
14	-3.327444000	2.850101000	-0.552728000		1	-3.209067000	1.720263000	-2.437523000
6	-3.266388000	3.208437000	1.297881000		6	-1.805083000	1.775747000	-4.087205000
1	-4.265664000	3.461422000	1.690478000		1	-2.488258000	2.288512000	-4.765417000
1	-2.595155000	4.056422000	1.513114000		6	-0.513489000	1.424662000	-4.480302000
6	-3.842034000	4.438456000	-1.439819000		1	-0.154068000	1.661652000	-5.483712000
1	-4.836206000	4.780003000	-1.106626000		6	0.314516000	0.767972000	-3.579117000
1	-3.122840000	5.251815000	-1.242424000		1	1.328470000	0.485106000	-3.861666000
1	-3.888167000	4.288936000	-2.531338000		6	-0.167765000	0.482708000	-2.299902000
1	-0.889086000	3.177809000	-0.915334000		6	3.880062000	-1.966716000	-0.514666000
6	-1.606499000	2.374342000	-1.151732000		1	4.107079000	-2.341251000	-1.526176000
1	-1.587627000	2.223825000	-2.243980000		1	4.137095000	-2.780453000	0.183004000
1	-2.893417000	2.334070000	1.852816000		14	5.040630000	-0.499464000	-0.146482000
1	-1.232109000	1.450530000	-0.683998000		6	4.827098000	0.095769000	1.625255000

ts3, i1114 cm⁻¹

23	-1.879389000	0.407410000	0.163356000		6	4.704605000	0.929412000	-1.325064000
7	-1.410738000	-0.200892000	2.132585000		1	4.781258000	0.614365000	-2.378879000
7	-1.412820000	0.836516000	-1.925437000		1	3.701344000	1.356764000	-1.167853000
14	-2.896464000	-2.634335000	-0.736678000		1	5.439958000	1.735798000	-1.164527000
6	-3.445671000	-0.915321000	-0.306898000		6	6.800610000	-1.119110000	-0.396141000
1	-4.125172000	-0.976497000	0.568044000		1	7.533117000	-0.318735000	-0.199367000
1	-4.038035000	-0.520423000	-1.156760000		1	7.029571000	-1.956976000	0.283059000
6	-1.783033000	-2.672499000	-2.273943000		1	6.958377000	-1.471578000	-1.428896000
1	-0.830119000	-2.121821000	-2.203357000		1	1.861534000	-3.215818000	-1.016001000
1	-2.315134000	-2.212086000	-3.123514000		3	0.264752000	-2.895084000	-0.395437000
1	-1.550975000	-3.711294000	-2.564879000					
6	-4.318725000	-3.818673000	-1.113634000					
1	-3.956144000	-4.838818000	-1.325774000					
1	-4.893439000	-3.476491000	-1.990626000					
1	-5.017232000	-3.878409000	-0.262320000					
6	-1.928283000	-3.427113000	0.699149000					
1	-1.194542000	-2.762790000	1.187310000					
1	-1.439742000	-4.376086000	0.408939000					
1	-2.630600000	-3.686937000	1.507800000					
14	-0.766525000	3.472063000	0.861201000					
6	-2.279700000	2.422587000	0.567563000					
1	-2.862020000	2.881547000	-0.256835000					
1	-2.910533000	2.468272000	1.479745000					
6	0.322697000	3.548136000	-0.684010000					
1	0.829929000	2.585492000	-0.856865000					
1	1.105842000	4.317499000	-0.575273000					
1	-0.260694000	3.790797000	-1.588271000					
6	0.294247000	2.782583000	2.264481000					
1	0.760961000	1.827173000	1.974484000					
1	-0.299638000	2.600256000	3.175777000					
1	1.105036000	3.483487000	2.526392000					
6	-1.230320000	5.252414000	1.314995000					
1	-0.335968000	5.875064000	1.488988000					
1	-1.841995000	5.279931000	2.232791000					
1	-1.819002000	5.726980000	0.511526000					
6	-2.194448000	-0.086093000	3.218571000					
1	-3.181693000	0.353651000	3.047213000					
6	-1.807661000	-0.485372000	4.480873000					
1	-2.484972000	-0.367497000	5.327361000					
6	-0.516221000	-1.043785000	4.636953000					
1	-0.170288000	-1.367281000	5.621263000					
6	0.302286000	-1.173540000	3.539918000					
1	1.302437000	-1.596936000	3.642150000					
6	-0.152626000	-0.742873000	2.268246000					
7	-0.059068000	-0.306096000	-0.051823000					
6	0.600102000	-0.834391000	1.051168000					
6	1.855974000	-1.444318000	0.887459000					
1	2.359629000	-1.882642000	1.750003000					
6	2.416597000	-1.632507000	-0.399302000					
6	1.813155000	-0.821381000	-1.456614000					
1	2.303967000	-0.785511000	-2.429266000					
6	0.608140000	-0.228116000	-1.256919000					

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23	-1.323346000	0.197993000	0.911745000					
7	-0.706311000	-1.748303000	1.404231000					
7	-1.267489000	2.046723000	-0.265858000					
14	-3.865932000	-0.857360000	-1.015142000					
6	-3.387769000	-0.062676000	0.583164000					
1	-3.757101000	-0.696503000	1.415343000					
1	-3.899108000	0.917321000	0.660507000					
6	-3.317779000	0.189965000	-2.508284000					
1	-2.246225000	0.433058000	-2.615505000					
1	-3.810101000	1.174567000	-2.435983000					
1	-3.654239000	-0.268266000	-3.453810000					
6	-5.717557000	-1.120849000	-1.258450000					
1	-5.936814000	-1.633159000	-2.210458000					
1	-6.254355000	-0.157540000	-1.261526000					
1	-6.135897000	-1.731629000	-0.441297000					
6	-3.064675000	-2.580832000	-1.171523000					
1	-2.041412000	-2.684668000	-0.766779000					
1	-3.097149000	-2.982628000	-2.200546000					
1	-3.653089000	-3.279909000	-0.555034000					
14	0.916165000	1.613304000	2.957684000					
6	-0.876093000	1.181871000	2.705935000					
1	-1.482744000	2.103803000	2.810279000					
1	-1.190770000	0.490657000	3.515203000					
6	1.392243000	3.056501000	1.829858000					
1	1.224470000	2.830959000	0.765588000					
1	2.453617000	3.331043000	1.950316000					
1	0.789312000	3.946400000	2.080057000					
6	2.001887000	0.108742000	2.604271000					
1	1.832325000	-0.277144000	1.587664000					
1	1.761275000	-0.709428000	3.304395000					
1	3.075479000	0.336586000	2.710658000					
6	1.290209000	2.167627000	4.730865000					
1	2.356250000	2.422918000	4.859767000					
1	1.047808000	1.370079000	5.453595000					
1	0.696664000	3.056068000	5.005777000					
6	-1.049805000	-2.459287000	2.492105000					
1	-1.727187000	-1.955565000	3.189818000					
6	-0.602536000	-3.736901000	2.750673000					
1	-0.918317000	-4.260786000	3.653481000					
6	0.284397000	-4.335708000	1.809102000					

1	0.675979000	-5.340961000	1.982951000		1	3.271759000	2.138904000	-0.889128000
6	0.653338000	-3.635916000	0.689752000		1	3.272072000	2.137865000	0.891412000
1	1.345913000	-4.070674000	-0.033155000		1	0.372471000	1.222118000	-0.878970000
6	0.155666000	-2.318621000	0.470907000		6	0.519791000	0.568177000	0.000475000
7	-0.106785000	-0.229413000	-0.588470000		1	0.372891000	1.222141000	0.879950000
6	0.459224000	-1.516064000	-0.671519000		1	2.432699000	-0.475151000	2.456175000
6	1.046336000	-1.940915000	-1.872633000		1	-2.058537000	1.960922000	1.540471000
1	1.419626000	-2.965974000	-1.935852000		6	-2.663167000	1.039254000	1.534437000
6	1.600240000	-0.945657000	-2.875014000		1	-3.723558000	1.338285000	1.582081000
6	0.921694000	0.390705000	-2.687554000		14	-2.322880000	0.000193000	0.000040000
1	1.093507000	1.155754000	-3.447762000		6	-2.662583000	1.033609000	-1.538301000
6	0.178078000	0.684701000	-1.594466000		1	-2.056713000	1.954428000	-1.548344000
6	-1.894338000	3.183497000	0.047305000		1	-3.722590000	1.333906000	-1.586572000
1	-2.533908000	3.153006000	0.932974000		1	-2.432464000	0.469068000	-2.457282000
6	-1.744979000	4.348967000	-0.692695000		6	-3.446758000	-1.511571000	0.002630000
1	-2.273425000	5.256468000	-0.398063000		1	-4.510145000	-1.219636000	0.001217000
6	-0.900963000	4.322410000	-1.801385000		1	-3.271341000	-2.140479000	-0.886047000
1	-0.744975000	5.220082000	-2.403255000		1	-3.272614000	-2.136329000	0.894486000
6	-0.252113000	3.138936000	-2.132192000		1	-0.372422000	-1.222990000	-0.877523000
1	0.418965000	3.098552000	-2.989791000		6	-0.519857000	-0.568156000	0.001217000
6	-0.461344000	2.004607000	-1.344737000		1	-0.372545000	-1.220978000	0.881471000
6	3.147480000	-0.826634000	-2.861373000		1	-2.431771000	0.478706000	2.455539000
1	3.455954000	-0.089472000	-3.628064000					
1	3.569468000	-1.789926000	-3.205660000					
14	4.071162000	-0.385221000	-1.263797000					
6	4.006539000	-1.779549000	-0.001123000					
1	2.994616000	-1.919738000	0.406897000					
1	4.327393000	-2.734355000	-0.450584000					
1	4.681788000	-1.564738000	0.844244000					
6	3.423604000	1.205883000	-0.499178000					
1	3.415107000	2.033064000	-1.228033000					
1	2.398682000	1.070955000	-0.127804000					
1	4.052803000	1.511732000	0.352828000					
6	5.873741000	-0.129867000	-1.763353000					
1	6.495549000	0.110380000	-0.884603000					
1	6.293633000	-1.036740000	-2.230118000					
1	5.980598000	0.698024000	-2.484090000					
1	1.350315000	-1.291861000	-3.896151000					
3	-1.179031000	-1.358820000	-2.130349000					

(CH₃)₃SiCH₂·

1	-1.580825000	0.579219000	-1.806926000	
6	-1.546221000	0.768001000	-0.721022000	
1	-2.459043000	0.337325000	-0.277011000	
14	-0.000035000	0.012881000	0.042110000	
6	0.003018000	-1.844981000	-0.290382000	
1	0.003169000	-2.044047000	-1.375452000	
1	-0.886822000	-2.330868000	0.142198000	
1	0.894634000	-2.327888000	0.141885000	
6	-0.000883000	0.328383000	1.875652000	
1	-0.921616000	0.404120000	2.469036000	
1	0.919344000	0.404053000	2.469835000	
1	2.458040000	0.346202000	-0.275078000	
6	1.544032000	0.772872000	-0.720510000	
1	1.580385000	0.582844000	-1.806141000	
1	1.572480000	1.864115000	-0.567570000	
1	-1.578926000	1.858936000	-0.566741000	

(CH₃)₃SiCH₂CH₂Si(CH₃)₃

1	2.058043000	-1.958586000	1.543640000	
6	2.663165000	-1.037259000	1.535789000	
1	3.723427000	-1.336800000	1.583226000	
14	2.322796000	-0.000240000	0.000032000	
6	2.662744000	-1.035574000	-1.536967000	
1	2.057524000	-1.956835000	-1.545586000	
1	3.722952000	-1.335173000	-1.585121000	
1	2.431951000	-0.472451000	-2.456648000	
6	3.446671000	1.511545000	0.000748000	
1	4.510052000	1.219580000	0.000379000	

(CH₃)₄Si

1	-0.494724000	2.351254000	-0.701338000	
6	-0.162747000	1.432042000	-1.212136000	
1	0.800222000	1.650832000	-1.702906000	
14	-0.000129000	-0.000108000	0.000113000	
6	1.263089000	0.440464000	1.325783000	
1	0.959012000	1.342346000	1.882725000	
1	2.253395000	0.638422000	0.882866000	
1	1.379870000	-0.379300000	2.054080000	
6	0.568914000	-1.540898000	-0.921288000	
1	1.545566000	-1.377496000	-1.406591000	
1	0.674438000	-2.398868000	-0.236583000	
1	-0.151767000	-1.825398000	-1.705959000	
1	-1.606653000	-1.167286000	1.524177000	
6	-1.669103000	-0.331497000	0.807502000	
1	-2.431490000	-0.592232000	0.054625000	
1	-0.897263000	1.204272000	-2.002498000	
1	-2.029712000	0.554301000	1.356656000	

LiH

1	0.000000000	0.000000000	-1.270676000	
3	0.000000000	0.000000000	0.423559000	
17	0.000000000	0.000000000	0.315570000	
3	0.000000000	0.000000000	-1.788232000	

LiCl

1	0.000458000	3.140010000	-0.000680000	
5	0.000459000	1.938046000	-0.000060000	
8	1.071393000	1.193975000	-0.386001000	
8	-1.071015000	1.194353000	0.385708000	
6	0.785929000	-0.183216000	-0.053234000	
6	-0.786052000	-0.182756000	0.053381000	
6	-1.478888000	-0.469635000	-1.277451000	
1	-1.366144000	-1.522664000	-1.572625000	

Scheme 9. Computed at the ω B97X-D/def2-SVP/SMD (diethyl ether)/Ultrafinegrid level

1	-2.552409000	-0.253863000	-1.175153000	8	0.781331000	0.918728000	-0.869104000
1	-1.082015000	0.163892000	-2.084503000	6	2.128419000	-0.747141000	0.086390000
6	-1.349390000	-1.082457000	1.141356000	6	1.935652000	0.811723000	-0.017212000
1	-1.068915000	-2.130929000	0.959638000	6	1.568991000	1.457589000	1.318643000
1	-0.992177000	-0.790827000	2.137458000	1	2.423932000	1.475415000	2.009939000
1	-2.447545000	-1.019937000	1.143520000	1	1.251799000	2.495290000	1.138727000
1	4.178947000	-0.469719000	1.277523000	1	0.737826000	0.927912000	1.807874000
1	2.552510000	-0.254301000	1.174969000	6	3.098319000	1.556217000	-0.653946000
1	1.082353000	0.164119000	2.084451000	1	4.019384000	1.411527000	-0.069180000
1	1.366008000	-1.522644000	1.573018000	1	3.279940000	1.222273000	-1.683730000
6	1.348807000	-1.083152000	-1.141157000	1	2.879277000	2.633908000	-0.681633000
1	2.446964000	-1.020858000	-1.143608000	6	2.994943000	-1.318796000	-1.035218000
1	1.068149000	-2.131527000	-0.959127000	1	2.915321000	-2.415771000	-1.023141000
1	0.991325000	-0.791707000	-2.137221000	1	2.661106000	-0.966618000	-2.022674000
1				1	4.053537000	-1.049671000	-0.908267000
PhSiH₃				6	2.631109000	-1.238257000	1.434935000
1	2.870783000	-0.055157000	1.403505000	1	2.737313000	-2.333029000	1.415696000
14	2.346178000	0.000098000	0.006479000	1	3.616712000	-0.805291000	1.663775000
1	2.860501000	1.245058000	-0.633113000	1	1.937815000	-0.981548000	2.246472000
PhSiH₂CH₂Si(CH₃)₃							
14	0.189357000	-0.360904000	-0.826711000				
6	-0.254985000	-1.204980000	-0.010920000	1	-0.016052000	-1.806545000	-1.147419000
6	-0.255602000	1.205332000	-0.010863000	1	-0.066471000	0.431354000	-2.069612000
6	-1.649581000	-1.207347000	0.003426000	6	1.990673000	-0.129801000	-0.324124000
6	-1.650456000	1.206771000	0.003350000	6	2.567896000	1.151037000	-0.299827000
6	-2.349148000	-0.0000405000	0.011097000	6	2.782405000	-1.217101000	0.077706000
1	0.275700000	-2.162075000	-0.021623000	6	3.886625000	1.340066000	0.111795000
1	0.274685000	2.162549000	-0.021439000	6	4.102953000	-1.033711000	0.491063000
1	-2.192941000	-2.155385000	0.006125000	6	4.656762000	0.245875000	0.508697000
1	-2.194325000	2.154517000	0.005789000	1	1.981673000	2.022333000	-0.610087000
1	-3.441897000	-0.000796000	0.020403000	1	2.365957000	-2.229121000	0.067379000
1				1	4.316717000	2.344686000	0.121187000
Et₂O				1	5.691002000	0.391462000	0.830322000
1	-0.891673000	2.364993000	1.056182000	1	4.702301000	-1.894288000	0.798590000
8	0.000000000	0.000000000	0.253545000	1	-4.859826000	0.563919000	1.574605000
6	0.000000000	-1.173510000	-0.511693000	6	-3.769379000	0.613629000	1.731393000
6	0.000000000	-2.372061000	0.411124000	1	-3.524035000	-0.027933000	2.593938000
1	0.888934000	-1.201303000	-1.175968000	14	-2.836885000	0.066982000	0.190896000
1	-0.888934000	-1.201303000	-1.175968000	6	-3.299951000	-1.709644000	-0.224880000
1	-0.891673000	-2.364993000	1.056182000	1	-4.391664000	-1.811523000	-0.342864000
1	0.000000000	-3.305581000	-0.171191000	1	-2.983379000	-2.402463000	0.572502000
1	0.891673000	-2.364993000	1.056182000	1	-2.831510000	-2.043582000	-1.165268000
6	0.000000000	1.173510000	-0.511693000	6	-0.981874000	0.184187000	0.529923000
6	0.000000000	2.372061000	0.411124000	1	-0.750468000	-0.411138000	1.432415000
1	-0.888934000	1.201303000	-1.175968000	1	-0.740861000	1.233200000	0.783554000
1	0.888934000	1.201303000	-1.175968000	1	-2.814066000	0.864876000	-2.187042000
1	0.891673000	2.364993000	1.056182000	6	-3.291951000	1.191014000	-1.248841000
1	0.000000000	3.305581000	-0.171191000	1	-4.382359000	1.193090000	-1.413614000
1				1	-2.980652000	2.231411000	-1.057280000
1				1	-3.515875000	1.651870000	2.002684000
pinBCH₂Si(CH₃)₃							
6	-2.450823000	1.785049000	0.485600000				
1	-1.449469000	1.983318000	0.899717000				
1	-3.196412000	2.077900000	1.243332000				
1	-2.582647000	2.442357000	-0.389736000	5	0.855825000	0.000025000	0.000110000
6	-2.356826000	-1.110260000	1.517511000	8	1.619198000	1.031620000	0.476703000
1	-3.103075000	-0.904565000	2.302765000	8	1.619130000	-1.031587000	-0.476637000
1	-2.427721000	-2.178968000	1.255845000	6	2.991407000	0.589594000	0.519437000
1	-1.356186000	-0.942978000	1.947445000	6	2.991350000	-0.589605000	-0.519457000
14	-2.640798000	-0.024848000	0.006308000	6	3.266019000	-0.129014000	-1.950348000
6	-4.372938000	-0.321204000	-0.667224000	1	4.317119000	0.163572000	-2.087213000
1	-5.139894000	-0.075034000	0.085981000	1	3.046703000	-0.957050000	-2.640255000
1	-4.512579000	-1.375941000	-0.956758000	1	2.626946000	0.721853000	-2.229488000
1	-4.564957000	0.299919000	-1.557820000	6	3.900840000	-1.754465000	-0.162101000
6	-1.364483000	-0.454768000	-1.321509000	1	4.948256000	-1.422575000	-0.097880000
1	-1.551841000	0.199659000	-2.189541000	1	3.618464000	-2.213772000	0.794063000
1	-1.534224000	-1.499973000	-1.629919000	1	3.836789000	-2.528602000	-0.941006000
5	0.085465000	-0.261400000	-0.788768000	6	3.266135000	0.128996000	1.950316000
8	0.790509000	-1.231994000	-0.123079000	1	3.046864000	0.957028000	2.640242000
1				1	2.627074000	-0.721865000	2.229492000

1	4.317238000	-0.163603000	2.087121000		1	-1.239409000	0.698880000	1.232149000
6	3.900935000	1.754406000	0.162042000		1	-2.685637000	1.309116000	-0.721507000
1	3.836975000	2.528541000	0.940958000		1	-3.054484000	2.340166000	0.685959000
1	4.948330000	1.422453000	0.097761000		1	-2.076158000	-2.980832000	0.659488000
1	3.618537000	2.213738000	-0.794105000		8	-0.041229000	-1.339361000	0.327299000
5	-0.855658000	0.000005000	0.000089000		6	1.146690000	-0.751090000	-0.164748000
8	-1.618936000	1.044486000	-0.447737000		6	2.328060000	-1.499732000	0.431545000
8	-1.618971000	-1.044478000	0.447861000		1	1.176721000	-0.848460000	-1.267316000
6	-2.991314000	0.604286000	-0.502390000		1	2.236768000	-2.572450000	0.207186000
6	-2.991352000	-0.604301000	0.502358000		1	3.286490000	-1.146316000	0.024970000
6	-3.267172000	-0.185357000	1.945791000		1	2.347921000	-1.381453000	1.526674000
1	-4.318450000	0.102869000	2.090312000		6	-1.028304000	-1.605565000	-0.639585000
1	-3.048163000	-1.032988000	2.611571000		6	-2.283388000	-2.084700000	0.054827000
1	-2.628510000	0.657137000	2.250015000		1	-0.668145000	-2.380631000	-1.346924000
6	-3.900130000	-1.758849000	0.111173000		1	-1.240254000	-0.697976000	-1.232318000
1	-4.947542000	-1.425532000	0.054746000		1	-2.687322000	-1.306945000	0.721026000
1	-3.616197000	-2.191199000	-0.857003000		1	-3.056399000	-2.338165000	-0.686211000
1	-3.837063000	-2.554525000	0.868150000					
6	-3.266984000	0.185441000	-1.945888000					
1	-3.047986000	1.033150000	-2.611157000					
1	-2.628223000	-0.656968000	-2.250143000					
1	-4.318227000	-0.102855000	-2.090534000					
6	-3.900123000	1.758803000	-0.111219000					
1	-3.836927000	2.554550000	-0.868111000					
1	-4.947553000	1.425505000	-0.054968000					
1	-3.616311000	2.191047000	0.857044000					
PhSiH₂SiH₂Ph								
14	-0.689279000	-0.008351000	0.951446000					
1	-0.403620000	-1.221701000	1.774798000					
1	-0.377605000	1.203028000	1.770293000					
6	-2.507179000	-0.000316000	0.456091000					
6	-3.130984000	1.188950000	0.043920000					
6	-3.258140000	-1.186303000	0.434914000					
6	-4.462476000	1.194387000	-0.370035000					
6	-4.590319000	-1.184284000	0.020372000					
6	-5.194373000	0.006431000	-0.382558000					
1	-2.572896000	2.130660000	0.047055000					
1	-2.801663000	-2.129502000	0.749996000					
1	-4.931577000	2.130104000	-0.683913000					
1	-5.159704000	-2.116966000	0.013622000					
1	-6.238010000	0.009414000	-0.706356000					
14	0.689265000	-0.008513000	-0.951404000					
1	0.403591000	-1.221988000	-1.774567000					
1	0.377605000	1.202728000	-1.770463000					
6	2.507173000	-0.000409000	-0.456071000					
6	3.130936000	1.188918000	-0.044001000					
6	3.258187000	-1.186356000	-0.434827000					
6	4.462435000	1.194446000	0.369918000					
6	4.590379000	-1.184247000	-0.020318000					
6	5.194389000	0.006523000	0.382509000					
1	2.572803000	2.130602000	-0.047190000					
1	2.801748000	-2.129601000	-0.749829000					
1	4.931505000	2.130206000	0.683717000					
1	6.238034000	0.009582000	0.706280000					
1	5.159802000	-2.116905000	-0.013517000					
[CH₃CHOCH₂CH₃]₂								
1	-2.073572000	2.982622000	-0.659335000					
8	-0.039671000	1.339845000	-0.327128000					
6	1.147577000	0.750240000	0.164868000					
6	2.329709000	1.497499000	-0.431643000					
1	1.177871000	0.847728000	1.267426000					
1	2.239675000	2.570325000	-0.207301000					
1	3.287726000	1.143006000	-0.025223000					
1	2.349244000	1.379187000	-1.526777000					
6	-1.026800000	1.606432000	0.639616000					
6	-2.281449000	2.086442000	-0.054962000					
1	-0.666325000	2.381172000	1.347159000					
⁴1a								
					23	1.822028000	0.000837000	-1.358969000
					7	1.404032000	-2.095332000	-1.129866000
					7	1.410318000	2.095378000	-1.127885000
					14	3.381337000	-0.005462000	1.618604000
					6	3.575563000	-0.007272000	-0.233570000
					1	4.161731000	-0.903629000	-0.523475000
					1	4.167962000	0.884712000	-0.524546000
					6	2.439181000	1.526194000	2.201640000
					1	1.378572000	1.475831000	1.907419000
					1	2.863333000	2.450576000	1.774405000
					1	2.474094000	1.618852000	3.300404000
					6	5.059419000	-0.009605000	2.498784000
					1	4.944773000	-0.008775000	3.596414000
					1	5.653857000	0.877882000	2.222646000
					1	5.649120000	-0.900501000	2.223470000
					6	2.430889000	-1.531409000	2.203318000
					1	1.370503000	-1.475532000	1.909303000
					1	2.465463000	-1.623123000	3.302173000
					1	2.849989000	-2.458527000	1.777016000
					1	1.945207000	-0.003751000	-3.102951000
					6	2.188615000	-3.106179000	-1.530046000
					1	3.103493000	-2.822795000	-2.057006000
					6	1.875411000	-4.434256000	-1.298039000
					1	2.546095000	-5.223311000	-1.640180000
					6	0.684728000	-4.727529000	-0.619604000
					1	0.403892000	-5.762822000	-0.415280000
					6	-0.134208000	-3.690632000	-0.207846000
					1	-1.061393000	-3.897566000	0.327052000
					6	0.247397000	-2.366345000	-0.475810000
					7	0.097640000	0.001820000	-0.408671000
					6	-0.513678000	-1.184154000	-0.075772000
					6	-1.730863000	-1.197823000	0.584083000
					1	-2.204938000	-2.149193000	0.832631000
					6	-2.375227000	0.005142000	0.931179000
					6	-1.728756000	1.205436000	0.584704000
					1	-2.200715000	2.157893000	0.833301000
					6	-0.510357000	1.189826000	-0.075416000
					6	2.197839000	3.104847000	-1.526866000
					1	3.112420000	2.819402000	-2.053284000
					6	1.888080000	4.433369000	-1.294593000
					1	2.561094000	5.220816000	-1.635841000
					6	0.697138000	4.729563000	-0.616827000
					1	0.418917000	5.765545000	-0.412382000
					6	-0.124711000	3.695007000	-0.206243000
					1	-1.051792000	3.904263000	0.327962000
					6	0.253287000	2.369144000	-0.474226000
					6	-3.733510000	0.005734000	1.563431000
					1	-3.866226000	0.893246000	2.204811000
					1	-3.864834000	-0.878537000	2.209593000
					14	-5.136185000	0.001566000	0.271999000

6	-4.986625000	-1.539362000	-0.794783000		1	5.034546000	-2.457972000	-0.166343000
1	-4.035329000	-1.551733000	-1.351261000		1	4.037857000	-1.558112000	-1.341409000
1	-5.038986000	-2.458153000	-0.187384000		1	5.807442000	-1.595879000	-1.517594000
1	-5.804430000	-1.581087000	-1.533340000		6	6.782808000	0.009063000	1.186755000
6	-4.986501000	1.536388000	-0.803438000		1	7.629315000	-0.004294000	0.480358000
1	-5.039267000	2.458560000	-0.201224000		1	6.8866686000	0.907550000	1.817193000
1	-4.034815000	1.545774000	-1.359310000		1	6.877856000	-0.873726000	1.840346000
1	-5.803842000	1.573871000	-1.542725000					
6	-6.779891000	0.003998000	1.184916000					
1	-7.625234000	0.001569000	0.477006000		4 1b			
1	-6.880143000	-0.884759000	1.829555000		7	-2.350753000	2.095606000	0.116182000
1	-6.880583000	0.896734000	1.823962000		7	-0.908553000	0.000300000	-0.269501000
					7	-2.354483000	-2.092377000	0.116113000
					6	-3.202497000	3.104926000	0.348187000
					1	-4.224033000	2.818636000	0.611577000
21a								
23	-1.833680000	0.007310000	-1.335145000		6	-2.826977000	4.434337000	0.264206000
7	-1.424363000	2.085772000	-1.126329000		1	-3.554618000	5.222512000	0.461038000
7	-1.391691000	-2.080885000	-1.137662000		6	-1.500139000	4.730467000	-0.075320000
14	-3.371401000	-0.033825000	1.631250000		1	-1.164813000	5.767103000	-0.148529000
6	-3.571576000	-0.042385000	-0.223060000		6	-0.614180000	3.694767000	-0.316862000
1	-4.178565000	0.839524000	-0.514880000		1	0.423104000	3.904871000	-0.578737000
1	-4.142399000	-0.948933000	-0.510829000		6	-1.065164000	2.368609000	-0.217576000
6	-2.400145000	-1.546820000	2.213000000		6	-0.237442000	-1.186652000	-0.444964000
1	-1.340698000	-1.476124000	1.918932000		6	1.102008000	-1.202456000	-0.799347000
1	-2.807340000	-2.479100000	1.786518000		6	1.811641000	-0.002052000	-0.985377000
1	-2.433006000	-1.639478000	3.311783000		6	1.104072000	1.199555000	-0.799520000
6	-5.051415000	-0.060429000	2.504552000		1	1.621597000	2.151053000	-0.934775000
1	-4.939376000	-0.056481000	3.602360000		6	-0.235420000	1.186086000	-0.445124000
1	-5.627479000	-0.959941000	2.228748000		6	-3.208070000	-3.100142000	0.347996000
1	-5.656962000	0.818457000	2.225475000		1	-4.229153000	-2.812012000	0.611131000
6	-2.449863000	1.511964000	2.205653000		6	-2.834920000	-4.430244000	0.264183000
1	-1.390418000	1.477195000	1.905084000		1	-3.564032000	-5.217097000	0.460855000
1	-2.480124000	1.605873000	3.304407000		6	-1.508531000	-4.728774000	-0.074934000
1	-2.890464000	2.428786000	1.778962000		1	-1.175022000	-5.766010000	-0.147950000
1	-2.040183000	-0.021784000	-3.055015000		6	-0.620658000	-3.694663000	-0.316320000
6	-2.220673000	3.089762000	-1.528292000		1	0.416336000	-3.906644000	-0.577812000
1	-3.132627000	2.794585000	-2.054069000		6	-1.069324000	-2.367710000	-0.217343000
6	-1.923479000	4.420518000	-1.301081000		1	1.617951000	-2.154824000	-0.934532000
1	-2.603950000	5.200440000	-1.644746000		23	-2.803518000	0.001975000	0.230899000
6	-0.731713000	4.730878000	-0.625211000		1	-4.015802000	0.002585000	-1.022209000
1	-0.463106000	5.770381000	-0.425577000		1	-3.195462000	0.001867000	1.926486000
6	0.099800000	3.707243000	-0.212993000		6	3.280610000	-0.003327000	-1.277824000
1	1.026247000	3.926876000	0.318459000		1	3.561416000	-0.890309000	-1.870226000
6	-0.264697000	2.373579000	-0.473831000		1	3.562640000	0.882108000	-1.871970000
7	-0.098449000	0.012039000	-0.405070000		14	4.333721000	-0.002416000	0.312238000
6	0.504439000	1.207008000	-0.075460000		6	3.929192000	-1.537767000	1.318964000
6	1.728717000	1.224018000	0.583957000		1	2.872362000	-1.546869000	1.631664000
1	2.197754000	2.178579000	0.831109000		1	4.124128000	-2.459593000	0.746182000
6	2.377641000	0.030692000	0.927582000		1	4.546188000	-1.576157000	2.232135000
6	1.737150000	-1.181220000	0.576864000		6	6.148069000	-0.006513000	-0.179838000
1	2.217230000	-2.130369000	0.821921000		1	6.798178000	-0.005727000	0.710752000
6	0.523137000	-1.169582000	-0.078347000		1	6.398453000	-0.899075000	-0.776594000
6	-2.172711000	-3.090402000	-1.547846000		1	6.401535000	0.882606000	-0.780418000
1	-3.086634000	-2.805305000	-2.075207000		6	3.934680000	1.537941000	1.313515000
6	-1.855596000	-4.419754000	-1.324571000		1	4.132410000	2.456957000	0.737177000
1	-2.523639000	-5.207833000	-1.674126000		1	2.878055000	1.551699000	1.626728000
6	-0.666257000	-4.715168000	-0.647376000		1	4.552258000	1.577668000	2.226235000
1	-0.382697000	-5.751137000	-0.450592000					
6	0.149970000	-3.677985000	-0.227091000		21b			
1	1.077550000	-3.885233000	0.307006000		7	2.463083000	-1.881169000	0.055707000
6	-0.235613000	-2.355091000	-0.485758000		7	0.819928000	0.008160000	-0.162471000
6	3.735915000	0.030229000	1.560402000		7	2.268356000	2.091585000	-0.002839000
1	3.861214000	-0.846931000	2.217588000		6	3.436417000	-2.816403000	0.174739000
1	3.873661000	0.924458000	2.191313000		1	4.433089000	-2.432403000	0.410727000
14	5.140204000	0.005526000	0.271514000		6	3.207771000	-4.161721000	0.019538000
6	4.998193000	1.531310000	-0.817588000		1	4.029105000	-4.871210000	0.125997000
1	4.046672000	1.539578000	-1.373763000		6	1.885536000	-4.596601000	-0.274345000
1	5.053596000	2.458215000	-0.222920000		1	1.669842000	-5.660189000	-0.396593000
1	5.816131000	1.559755000	-1.556597000		6	0.883187000	-3.667242000	-0.402249000
6	4.987440000	-1.544434000	-0.782063000		1	-0.138435000	-3.978716000	-0.626326000

6	1.170417000	-2.288325000	-0.242635000	6	-0.954321000	-1.249849000	0.381562000
6	0.127804000	1.139099000	-0.405165000	14	4.207414000	-1.177011000	-0.322489000
6	-1.194597000	1.122006000	-0.791033000	6	2.436524000	-1.854699000	-0.234314000
6	-1.854460000	-0.132554000	-0.953698000	1	1.957872000	-1.695004000	-1.217546000
6	-1.113994000	-1.284956000	-0.768612000	1	2.516012000	-2.951035000	-0.112005000
1	-1.581467000	-2.260279000	-0.920289000	6	5.254502000	-2.428352000	-1.262422000
6	0.249424000	-1.211596000	-0.389882000	1	5.290682000	-3.396773000	-0.736596000
6	3.138251000	3.100824000	0.122991000	1	6.290958000	-2.070856000	-1.380447000
1	4.173001000	2.820844000	0.333680000	1	4.846410000	-2.608868000	-2.270877000
6	2.752376000	4.429125000	-0.000434000	6	4.271748000	0.464029000	-1.245854000
1	3.491576000	5.223763000	0.105873000	1	5.314076000	0.806908000	-1.358198000
6	1.411174000	4.708873000	-0.255727000	1	3.709572000	1.258219000	-0.730565000
1	1.068981000	5.741220000	-0.352778000	1	3.843530000	0.359149000	-2.256545000
6	0.506766000	3.660324000	-0.385637000	6	4.897749000	-0.962539000	1.417451000
1	-0.547480000	3.856502000	-0.581175000	1	4.856779000	-1.909378000	1.981215000
6	0.966300000	2.350265000	-0.257749000	1	4.338252000	-0.206553000	1.992227000
1	-1.736614000	2.049066000	-0.982938000	1	5.951752000	-0.639816000	1.384253000
23	2.758717000	0.070447000	0.585424000				
1	4.494210000	0.232135000	0.932181000				
1	2.084658000	0.149447000	2.112719000				
6	-3.319434000	-0.176279000	-1.262643000	23	-1.467348000	0.232734000	2.295157000
1	-3.610788000	0.672007000	-1.904607000	1	-2.941063000	-0.492613000	1.771522000
1	-3.577329000	-1.099303000	-1.807847000	1	-1.251122000	0.727268000	3.932378000
14	-4.392096000	-0.123164000	0.313733000	7	-0.388190000	-1.624081000	2.440652000
6	-4.053732000	1.472310000	1.249097000	6	-0.713276000	-2.671373000	3.206558000
1	-3.003795000	1.528937000	1.579311000	1	-1.596444000	-2.550866000	3.838935000
1	-4.266126000	2.358256000	0.627917000	6	0.019583000	-3.848661000	3.203129000
1	-4.689167000	1.535291000	2.148206000	1	-0.278496000	-4.681984000	3.840358000
6	-6.197188000	-0.199510000	-0.206624000	6	1.134038000	-3.930160000	2.367218000
1	-6.861510000	-0.176148000	0.673119000	1	1.736541000	-4.840279000	2.334304000
1	-6.465321000	0.653411000	-0.851686000	6	1.471846000	-2.842822000	1.572667000
1	-6.413180000	-1.125516000	-0.764600000	1	2.336045000	-2.889417000	0.910319000
6	-3.961214000	-1.599604000	1.392702000	6	0.685405000	-1.688672000	1.627158000
1	-4.120555000	-2.550371000	0.857534000	7	-1.934144000	2.183856000	1.520581000
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6				6	-3.237816000	4.167393000	1.272686000
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31c				1	-2.499045000	5.602234000	-0.170179000
23	-2.562067000	1.062646000	-0.288719000	6	-1.241991000	3.858876000	-0.032330000
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1	-2.953949000	1.345254000	-1.943182000	6	-1.058979000	2.621830000	0.592066000
7	-1.153764000	2.679851000	-0.087194000	7	-0.042236000	0.507199000	1.035518000
6	-1.407339000	3.979618000	-0.273500000	6	0.921941000	-0.467592000	0.817461000
1	-2.429935000	4.234557000	-0.562891000	6	1.935864000	-0.323103000	-0.058832000
6	-0.435523000	4.955698000	-0.111606000	1	2.637487000	-1.144820000	-0.208555000
1	-0.680833000	6.006035000	-0.273168000	6	2.160200000	0.942172000	-0.847933000
6	0.848663000	4.552994000	0.256950000	1	2.168046000	0.681505000	-1.925431000
1	1.643256000	5.289851000	0.391864000	6	1.029393000	1.911102000	-0.602181000
6	1.112283000	3.203137000	0.447933000	1	1.045415000	2.844499000	-1.168497000
1	2.111724000	2.871012000	0.728833000	6	0.052450000	1.682213000	0.298692000
6	0.081296000	2.275197000	0.270984000	7	5.092174000	0.569104000	-0.864978000
7	-3.256717000	-0.973321000	-0.188140000	6	3.528747000	1.599206000	-0.544792000
6	-4.503923000	-1.399441000	-0.415756000	1	3.540216000	1.943723000	0.505056000
1	-5.231321000	-0.633456000	-0.696045000	1	3.619106000	2.511705000	-1.162755000
6	-4.864010000	-2.734020000	-0.304272000	6	6.527381000	1.761819000	-1.112295000
1	-5.892247000	-3.042522000	-0.496685000	1	6.362271000	2.411311000	-1.987780000
6	-3.879161000	-3.655132000	0.055367000	1	7.473589000	1.218261000	-1.270611000
1	-4.120872000	-4.715805000	0.151371000	6	6.659019000	2.412424000	-0.231714000
6	-2.583683000	-3.213377000	0.287964000	1	5.494754000	-0.550772000	0.595891000
1	-1.799434000	-3.918887000	0.561909000	6	6.446615000	-1.081443000	0.425811000
6	-2.294674000	-1.850854000	0.163228000	1	4.716440000	-1.308708000	0.775918000
7	-0.943810000	0.120262000	0.154250000	1	5.602122000	0.039036000	1.521347000
6	0.229656000	0.806236000	0.431244000	6	4.857808000	-0.466379000	-2.421331000
6	1.367861000	0.196019000	0.821280000	1	4.614353000	0.168632000	-3.289388000
1	2.243254000	0.794342000	1.078397000	1	4.045915000	-1.203439000	-2.308092000
6	1.501328000	-1.305596000	0.873599000	1	5.778559000	-1.022801000	-2.663704000
1	1.959052000	-1.585811000	1.841117000	5	-3.149012000	-1.894420000	-4.046318000
6	0.135866000	-1.941043000	0.774491000	8	-3.703221000	-0.799509000	-3.479676000

8	-2.221880000	-2.531214000	-3.296296000		14	-0.714377000	1.162294000	2.629994000
6	-3.259138000	-0.789065000	-2.087022000		1	-0.788397000	-0.325528000	2.679016000
6	-1.952313000	-1.660862000	-2.153963000		1	-1.745633000	1.782577000	1.755003000
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1	-0.418161000	-0.205794000	-1.660066000		6	1.168068000	2.947955000	1.442673000
1	0.122043000	-1.534837000	-2.716151000		6	2.144513000	1.090687000	2.636564000
1	-0.871413000	-0.216938000	-3.386638000		6	2.442068000	3.429343000	1.148294000
6	-1.702404000	-2.509694000	-0.921355000		6	3.418678000	1.573827000	2.346395000
1	-1.643363000	-1.864943000	-0.032040000		6	3.570530000	2.744635000	1.601064000
1	-2.501490000	-3.245132000	-0.762551000		1	0.294144000	3.496372000	1.078486000
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1	-5.306411000	-0.879614000	-1.435413000		1	4.299632000	1.033629000	2.701863000
1	-4.533941000	-2.479588000	-1.545185000		1	4.569509000	3.123721000	1.372620000
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6	-3.033781000	0.642932000	-1.639211000					
1	-3.990846000	1.184126000	-1.610419000					
1	-2.614236000	0.643387000	-0.622853000					
1	-2.351894000	1.183847000	-2.307875000					

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23	-3.183484000	-0.678925000	0.063136000		23	-2.579544000	0.778010000	-1.062181000
1	-4.382173000	-1.245981000	-1.037154000		1	-3.544859000	1.701586000	0.037158000
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7	-2.295570000	-2.606705000	0.415321000		7	-1.066777000	2.298005000	-1.285056000
6	-2.875770000	-3.648233000	1.021476000		6	-1.258755000	3.550675000	-1.715259000
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1	-2.732510000	-5.686644000	1.697915000		1	-0.421934000	5.484490000	-2.153071000
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6	-1.033297000	-2.710330000	-0.047666000		6	0.162399000	1.891942000	-0.910393000
7	-3.251560000	1.370119000	-0.597426000		7	-3.384452000	-1.127657000	-0.472384000
6	-4.281281000	2.212111000	-0.457898000		6	-4.668676000	-1.497412000	-0.529249000
1	-5.172294000	1.807237000	0.028450000		1	-4.447779000	-4.636481000	0.720629000
6	-4.229783000	3.526385000	-0.897719000		6	-2.816351000	-3.258582000	0.440186000
1	-5.089760000	4.183646000	-0.764214000		1	-2.060642000	-3.945778000	0.819685000
6	-3.055337000	3.973066000	-1.504982000		6	-2.454509000	-1.980188000	0.004517000
1	-2.973129000	5.001761000	-1.862296000		7	-1.000070000	-0.152614000	-0.489998000
6	-1.985839000	3.099289000	-1.648878000		6	0.231199000	0.488957000	-0.437669000
1	-1.057746000	3.433146000	-2.112577000		6	1.347965000	-0.092955000	0.039473000
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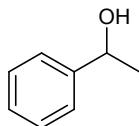
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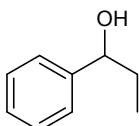
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Catalytic reaction details and characterization data



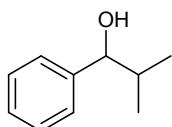
Chemical Formula: C₈H₁₀O
Molecular Weight: 122.1670

3a¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. Acetophenone (120.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **3a** was isolated. Yield: 117.0 mg (96%). ¹H NMR (400 MHz, CDCl₃) δ 7.33 – 7.20 (m, 4H), 7.20 – 7.11 (m, 1H), 4.78 (q, *J* = 6.5 Hz, 1H), 1.86 (br., 1H), 1.39 (d, *J* = 6.5 Hz, 3H) ppm; ¹³C NMR (101 MHz, CDCl₃) δ 145.9, 128.6, 127.6, 125.5, 70.5, 25.3 ppm.



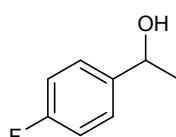
Chemical Formula: C₉H₁₂O
Molecular Weight: 136.1940

3b¹⁹: In a glovebox under N₂ atmosphere, catalyst **1/H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. Propiophenone (134.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **3b** was isolated. Yield: 129 mg (95%). ¹H NMR (500 MHz, CDCl₃) δ 7.34 – 7.22 (m, 4H), 7.22 – 7.17 (m, 1H), 4.53 (t, *J* = 6.6 Hz, 1H), 1.81 – 1.68 (m, 2H), 1.67 – 1.63 (br., 1H), 0.85 (t, *J* = 7.5, 3H) ppm; ¹³C NMR (126 MHz, CDCl₃) δ 144.7, 128.6, 127.7, 126.1, 76.2, 32.0, 10.3 ppm.



Chemical Formula: C₁₀H₁₄O
Molecular Weight: 150.2210

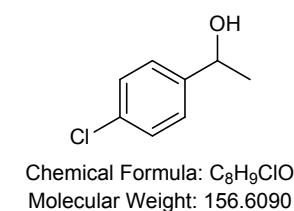
3c¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. Isobutyrophenone (148.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **3c** was isolated. Yield: 142.5 mg (95%). ¹H NMR (500 MHz, CDCl₃) δ 7.31 – 7.21 (m, 4H), 7.19 (td, *J* = 6.8, 1.6 Hz, 1H), 4.28 (d, *J* = 6.9 Hz, 1H), 1.88 (m, 1H), 1.79 (s, 1H), 0.93 (d, *J* = 6.8 Hz, 3H), 0.72 (d, *J* = 6.9 Hz, 3H) ppm; ¹³C NMR (126 MHz, CDCl₃) δ 143.7, 128.3, 127.5, 126.7, 80.2, 35.4, 19.1, 18.4 ppm.



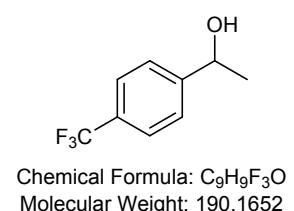
Chemical Formula: C₈H₉FO
Molecular Weight: 140.1574

3d¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 4-Fluoroacetophenone (138.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was

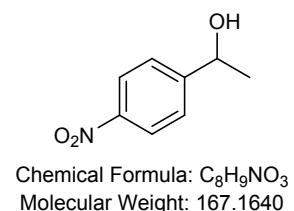
evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **3d** was isolated. Yield: 129 mg (92%). ¹H NMR (500 MHz, CDCl₃) δ 7.38 – 7.24 (m, 4H), 4.84 (d, *J* = 6.5 Hz, 1H), 2.50 (d, *J* = 1.8 Hz, 1H), 1.45 (d, *J* = 6.6, 3H). ppm; ¹³C NMR (126 MHz, CDCl₃) δ 144.3, 133.1, 128.6, 126.9, 69.7, 25.3 ppm.



then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **3e** was isolated. Yield: 147 mg (94%). ¹H NMR (600 MHz, CDCl₃) δ 7.31 (m, 4H), 4.86 (q, *J* = 6.5 Hz, 1H), 2.33 (d, *J* = 3.2 Hz, 1H), 1.47 (d, *J* = 6.5 Hz, 3H) ppm; ¹³C NMR (126 MHz, CDCl₃) δ 144.3, 133.1, 128.7, 126.9, 69.8, 25.3 ppm.



the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Yellowish oil of **3f** was isolated. Yield: 180 mg (95%). ¹H NMR (500 MHz, CDCl₃) δ 7.58 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 4.90 (q, *J* = 6.5 Hz, 1H), 2.59 (s, 1H), 1.46 (d, *J* = 6.6 Hz, 3H) ppm; ¹³C NMR (126 MHz, CDCl₃) δ 149.8, 129.67 (q, *J* = 32.2 Hz), 125.8, 125.5 (q, *J* = 3.8 Hz), 125.4, 123.2, 121.0, 69.9, 25.4 ppm.



the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Yellowish oil of **3g** was isolated. Yield: 155 mg (93%). ¹H NMR (600 MHz, CDCl₃) δ 8.16 (d, *J* = 9.3 Hz, 2H), 7.53 (d, *J* = 8.9 Hz, 2H), 5.01 (d, *J* = 6.7 Hz, 1H), 2.48 (s, 1H), 1.51 (d, *J* = 8.0 Hz, 2H) ppm; ¹³C NMR (151 MHz, CDCl₃) δ 153.2, 147.1, 126.1, 123.7, 69.4, 25.4 ppm.

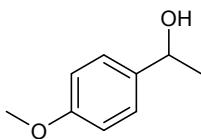
3e¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 4'-Chloroacetophenone (154.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and

3f²⁰: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 4'-Trifluoromethylacetophenone (188.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then

the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Yellowish oil of **3f** was isolated. Yield: 180 mg (95%). ¹H NMR (500 MHz, CDCl₃) δ 7.58 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 4.90 (q, *J* = 6.5 Hz, 1H), 2.59 (s, 1H), 1.46 (d, *J* = 6.6 Hz, 3H) ppm; ¹³C NMR (126 MHz, CDCl₃) δ 149.8, 129.67 (q, *J* = 32.2 Hz), 125.8, 125.5 (q, *J* = 3.8 Hz), 125.4, 123.2, 121.0, 69.9, 25.4 ppm.

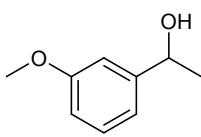
3g²⁰: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 4'-Nitroacetophenone (165.1 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then

the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Yellowish oil of **3g** was isolated. Yield: 155 mg (93%). ¹H NMR (600 MHz, CDCl₃) δ 8.16 (d, *J* = 9.3 Hz, 2H), 7.53 (d, *J* = 8.9 Hz, 2H), 5.01 (d, *J* = 6.7 Hz, 1H), 2.48 (s, 1H), 1.51 (d, *J* = 8.0 Hz, 2H) ppm; ¹³C NMR (151 MHz, CDCl₃) δ 153.2, 147.1, 126.1, 123.7, 69.4, 25.4 ppm.



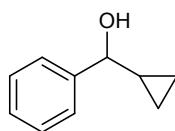
Chemical Formula: C₉H₁₂O₂
Molecular Weight: 152.1930

3h¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 4'-Methoxyacetophenone (150.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **3h** was isolated. Yield: 137 mg (90%). ¹H NMR (600 MHz, Chloroform-d) δ 7.30 (d, *J* = 8.4 Hz, 2H), 6.89 (d, *J* = 8.8 Hz, 2H), 4.86 (q, *J* = 6.4 Hz, 1H), 3.81 (s, 3H), 1.78 (s, 1H), 1.48 (d, *J* = 6.5 Hz, 3H) ppm; ¹³C NMR (151 MHz, CDCl₃) δ 159.1, 138.1, 126.8, 113.9, 70.1, 55.4, 25.2 ppm.



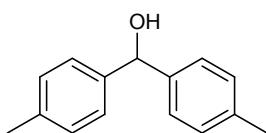
Chemical Formula: C₉H₁₂O₂
Molecular Weight: 152.1930

3i¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 3'-Methoxyacetophenone (150.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **3i** was isolated. Yield: 143 mg (94%). ¹H NMR (600 MHz, CDCl₃) δ 7.33 – 7.27 (m, 1H), 6.97 (dt, *J* = 6.5, 3.6 Hz, 2H), 6.84 (dd, *J* = 8.3, 2.7 Hz, 1H), 4.90 (q, *J* = 6.3 Hz, 1H), 3.84 (d, *J* = 1.9 Hz, 3H), 1.85 (s, 1H), 1.56 – 1.46 (m, 3H) ppm; ¹³C NMR (151 MHz, CDCl₃) δ 159.8, 147.6, 129.5, 117.7, 112.9, 110.9, 70.4, 55.2, 25.2 ppm.



Chemical Formula: C₁₀H₁₂O
Molecular Weight: 148.2050

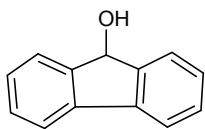
3j¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. Cyclopropyl phenyl ketone (146.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **3j** was isolated. Yield: 108 mg (73%). ¹H NMR (600 MHz, CDCl₃) δ 7.52 – 7.43 (m, 2H), 7.39 (dd, *J* = 9.0, 6.8 Hz, 2H), 7.34 – 7.30 (m, 1H), 4.02 (d, *J* = 8.6 Hz, 1H), 2.35 (s, 1H), 1.31 – 1.17 (m, 1H), 0.72 – 0.63 (m, 1H), 0.62 – 0.54 (m, 1H), 0.50 (dq, *J* = 9.9, 4.9 Hz, 1H), 0.40 (dq, *J* = 9.9, 5.0 Hz, 1H) ppm; ¹³C NMR (150 MHz, CDCl₃) δ 143.9, 128.4, 127.5, 126.1, 78.5, 19.2, 3.7, 2.8 ppm.



Chemical Formula: C₁₅H₁₆O
Molecular Weight: 212.2920

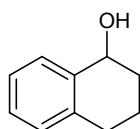
3k¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 4,4'-Dimethylbenzophenone (210.1 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was

evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. White solid of **3k** was isolated. Yield: 180 mg (85%). ¹H NMR (600 MHz, CDCl₃) δ 7.13 (d, *J* = 8.8 Hz, 4H), 7.02 (q, *J* = 8.9 Hz, 4H), 5.62 (s, 1H), 2.22 (s, 6H), 2.22 (s, 1H, overlapping) ppm; ¹³C NMR (151 MHz, CDCl₃) δ 141.2, 137.1, 129.2, 126.5, 75.9, 21.4 ppm.



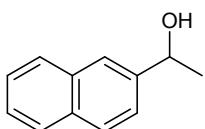
Chemical Formula: C₁₃H₁₀O
Molecular Weight: 182.2220

hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. White solid of **3l** was isolated. Yield: 176 mg (97%). ¹H NMR (600 MHz, CDCl₃) δ 7.64 (dd, *J* = 15.8, 7.7 Hz, 4H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.6 Hz, 2H), 5.54 (s, 1H), 2.08 (s, 1H) ppm; ¹³C NMR (151 MHz, CDCl₃) δ 145.7, 140.0, 129.1, 127.8, 125.2, 120.0, 75.2 ppm.



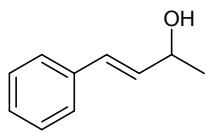
Chemical Formula: C₁₀H₁₂O
Molecular Weight: 148.2050

hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **3m** was isolated. Yield: 121 mg (82%). ¹H NMR (600 MHz, CDCl₃): δ 7.54 – 7.43 (m, 1H), 7.29 – 7.21 (m, 2H), 7.20 – 7.09 (m, 1H), 4.79 (dd, *J* = 6.0, 4.1 Hz, 1H), 2.86 (dt, *J* = 16.7, 5.5 Hz, 1H), 2.76 (ddd, *J* = 17.2, 8.2, 5.8 Hz, 1H), 2.07 (s, 1H), 2.01 (m, 2H), 1.96 – 1.88 (m, 1H), 1.81 (m, 1H) ppm. ¹³C NMR (151 MHz, CDCl₃): δ 138.9, 137.1, 129.0, 128.7, 127.6, 126.2, 68.1, 32.3, 29.3, 18.9 ppm.



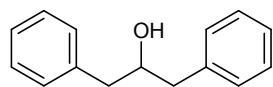
Chemical Formula: C₁₂H₁₂O
Molecular Weight: 172.2270

3l¹⁹: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 9-Fluorenone (180.2 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. White solid of **3l** was isolated. Yield: 176 mg (97%). ¹H NMR (600 MHz, CDCl₃) δ 7.64 (dd, *J* = 15.8, 7.7 Hz, 4H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.34 (t, *J* = 7.6 Hz, 2H), 5.54 (s, 1H), 2.08 (s, 1H) ppm; ¹³C NMR (151 MHz, CDCl₃) δ 145.7, 140.0, 129.1, 127.8, 125.2, 120.0, 75.2 ppm.



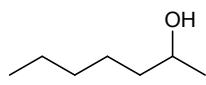
Chemical Formula: C₁₀H₁₂O
Molecular Weight: 148.2050

3o²¹: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 4-Phenyl-3-buten-2-one (146.2 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **3o** was isolated. Yield: 124 mg (84%). ¹H NMR (500 MHz, CDCl₃) δ 7.56 – 7.32 (m, 4H), 7.29 (t, J = 7.0 Hz, 1H), 6.59 (d, J = 15.9 Hz, 1H), 6.30 (dd, J = 16.0, 6.3 Hz, 1H), 4.51 (t, J = 6.4 Hz, 1H), 2.60 (s, 1H), 1.41 (d, J = 6.5 Hz, 3H) ppm; ¹³C NMR (126 MHz, CDCl₃) δ 136.9, 133.8, 129.4, 128.8, 127.8, 126.7, 69.0, 23.6 ppm.



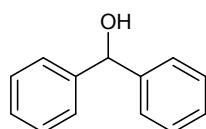
Chemical Formula: C₁₅H₁₆O
Molecular Weight: 212.2920

3p¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 1,3-Diphenylacetone (210.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. White solid of **3p** was isolated. Yield: 201.5 mg (95%). ¹H NMR (600 MHz, CDCl₃) δ 7.34 (t, J = 7.6 Hz, 4H), 7.32 – 7.22 (m, 6H), 4.16 – 4.06 (m, 1H), 2.90 (dd, J = 13.7, 4.7 Hz, 2H), 2.79 (dd, J = 13.7, 8.2 Hz, 2H), 1.63 (s, 1H) ppm; ¹³C NMR (150 MHz, CDCl₃) δ 138.4, 129.4, 128.6, 126.5, 73.6, 43.4 ppm.



Chemical Formula: C₇H₁₆O
Molecular Weight: 116.2040

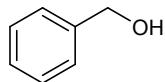
3q¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 2-Heptanone (114.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:40, v/v) as eluent. Colorless oil of **3q** was isolated. Yield: 100 mg (86%). ¹H NMR (500 MHz, CDCl₃) δ 3.74 (q, J = 6.0 Hz, 1H), 2.05 (s, 1H), 1.50 – 1.32 (m, 3H), 1.31 – 1.20 (m, 5H), 1.14 (dd, J = 6.3, 1.5 Hz, 3H), 0.85 (t, J = 6.8 Hz, 3H) ppm; ¹³C NMR (125 MHz, CDCl₃) δ 68.3, 39.6, 32.2, 25.8, 23.7, 22.3, 14.3 ppm.



Chemical Formula: C₁₃H₁₂O
Molecular Weight: 184.2380

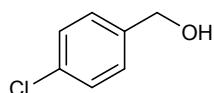
3s¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. Benzophenone (182.0 mg, 1.0 mmol) and phenylsilane (118.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The crude product was redissolved in methanol and 1 N NaOH (2 mL) was added. The solution was stirred for 30 min at room temperature and then extracted with CH₂Cl₂ (10 mL) for three times.

The combined organic phase was dried over anhydrous Na_2SO_4 and filtered. The solvent was removed under reduced pressure and the crude product was passed over a SiO_2 column using ethyl acetate/hexane (1:9, v/v) as an eluent. White solid of **3s** was isolated. Yield: 180 mg (98%).
 ^1H NMR (500 MHz, CDCl_3) δ 7.32 – 7.15 (m, 10H), 5.74 (s, 1H), 2.14 (s, 1H) ppm; ^{13}C NMR (126 MHz, CDCl_3) δ 143.8, 128.5, 127.6, 126.6, 76.3 ppm.



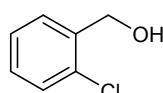
Chemical Formula: $\text{C}_7\text{H}_8\text{O}$
Molecular Weight: 108.1400

4a¹⁸: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in Et_2O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. Benzaldehyde (106.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO_2 using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **4a** was isolated. Yield: 100 mg (93%). ^1H NMR (600 MHz, Chloroform-*d*) δ 7.52 – 7.19 (m, 5H), 4.61 (s, 2H), 3.33 (br., 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 140.9, 128.5, 127.5, 127.0, 64.9 ppm.



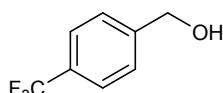
Chemical Formula: $\text{C}_7\text{H}_7\text{ClO}$
Molecular Weight: 142.5820

4b¹⁸: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in Et_2O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 4-Chlorobenzaldehyde (140.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO_2 using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **4b** was isolated. Yield: 135 mg (95%). ^1H NMR (600 MHz, CDCl_3) δ 7.45 – 7.29 (m, 2H), 7.27 – 7.10 (m, 2H), 4.58 (d, $J = 3.3$ Hz, 2H), 2.87 – 2.79 (br, 1H) ppm; ^{13}C NMR (150 MHz, CDCl_3) δ 139.2, 133.3, 128.6, 128.3, 64.3 ppm.



Chemical Formula: $\text{C}_7\text{H}_7\text{ClO}$
Molecular Weight: 142.5820

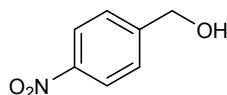
4c¹⁸: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in Et_2O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 2-Chlorobenzaldehyde (140.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO_2 using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **4c** was isolated. Yield: 131 mg (92%). ^1H NMR (600 MHz, CDCl_3) δ 7.56 – 7.42 (m, 1H), 7.42 – 7.32 (m, 1H), 7.29 (dd, $J = 8.3, 6.5$ Hz, 1H), 7.25 (td, $J = 7.6, 2.0$ Hz, 1H), 4.77 (s, 2H), 2.58 (s, 1H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 138.2, 132.7, 129.3, 128.8, 128.7, 127.0, 62.7 ppm.



Chemical Formula: $\text{C}_8\text{H}_7\text{F}_3\text{O}$
Molecular Weight: 176.1382

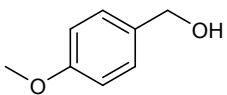
4d²⁰: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in Et_2O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 4-Trifluoromethylbenzaldehyde (174.1 mg, 1.0 mmol)

and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Yellowish oil of **4d** was isolated. Yield: 167 mg (95%). ¹H NMR (500 MHz, CDCl₃) δ 7.59 (d, *J* = 8.0 Hz, 2H), 7.43 (d, *J* = 7.9 Hz, 2H), 4.71 (s, 2H), 2.63 (s, 1H) ppm; ¹³C NMR (126 MHz, CDCl₃) δ 144.7, 129.8 (q, *J* = 32.4 Hz), 126.9, 125.53 (q, *J* = 3.8 Hz), 125.3, 123.2, 64.4 ppm.



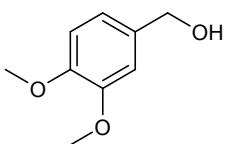
Chemical Formula: C₇H₇NO₃
Molecular Weight: 153.1370

4e¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/H** (0.54 mg, 1.0 μmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 4-Nitrobenzaldehyde (151.1 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Yellowish oil of **4e** was isolated. Yield: 130 mg (85%). ¹H NMR (500 MHz, CDCl₃) δ 8.18 (dd, *J* = 8.7, 1.9 Hz, 2H), 7.58 – 7.42 (m, 2H), 4.81 (s, 2H), 2.39 (s, 1H) ppm; ¹³C NMR (126 MHz, CDCl₃) δ 148.6, 147.5, 127.3, 124.0, 64.2 ppm.



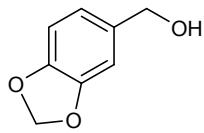
Chemical Formula: C₈H₁₀O₂
Molecular Weight: 138.1660

4f¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/H** (0.54 mg, 1.0 μmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 4-Methoxybenzaldehyde (136.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Yellowish oil of **4f** was isolated. Yield: 90 mg (65%). ¹H NMR (500 MHz, CDCl₃) δ 7.28 (d, *J* = 9.3 Hz, 2H), 6.89 (d, *J* = 9.0 Hz, 2H), 4.58 (d, *J* = 2.8 Hz, 2H), 3.88 – 3.72 (s, 3H), 2.41 (s, 1H) ppm; ¹³C NMR (126 MHz, CDCl₃) δ 159.1, 133.2, 128.6, 113.9, 64.8, 55.3 ppm.



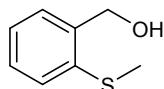
Chemical Formula: C₉H₁₂O₃
Molecular Weight: 168.1920

4g¹⁹: In a glovebox under N₂ atmosphere, catalyst **1/H** (0.54 mg, 1.0 μmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 3,4-Dimethoxybenzaldehyde (166.2 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **4g** was isolated. Yield: 136.2 mg (81%). ¹H NMR (500 MHz, CDCl₃) δ 6.83 (d, *J* = 1.8 Hz, 1H), 6.81 – 6.73 (m, 2H), 4.50 (d, *J* = 1.6 Hz, 2H), 3.79 (s, 3H), 3.78 (s, 3H), 2.83 (s, 1H) ppm; ¹³C NMR (126 MHz, CDCl₃) δ 149.0, 148.4, 133.8, 119.4, 111.0, 110.4, 65.0, 56.0, 55.8 ppm.



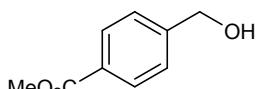
Chemical Formula: C₈H₈O₃
Molecular Weight: 152.1490

4h¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. Piperonal (150.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Yellowish oil of **4h** was isolated. Yield: 146 mg (96%). ¹H NMR (600 MHz, CDCl₃) δ 6.88 – 6.81 (m, 1H), 6.77 (m, 2H), 5.93 (s, 2H), 4.51 (s, 2H), 2.72 (s, 1H) ppm; ¹³C NMR (151 MHz, CDCl₃) δ 147.7, 147.0, 134.9, 120.5, 108.2, 107.9, 101.0, 65.0, 159.5, 133.5, 129.0, 114.3, 65.3, 55.6 ppm.



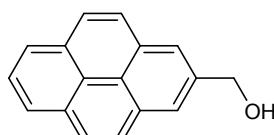
Chemical Formula: C₈H₁₀OS
Molecular Weight: 154.2270

4i¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 2-Methylthiobenzaldehyde (152.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **4i** was isolated. Yield: 140 mg (91%). ¹H NMR (500 MHz, CDCl₃) δ 7.46 – 7.37 (m, 1H), 7.36 – 7.29 (m, 2H), 7.25 – 7.19 (m, 1H), 4.79 (s, 2H), 2.52 (s, 3H), 2.02 (br., 1H) ppm; ¹³C NMR (125 MHz, CDCl₃) δ 138.9, 136.7, 128.4, 128.0, 126.6, 125.5, 63.6, 16.1 ppm.



Chemical Formula: C₉H₁₀O₃
Molecular Weight: 166.1760

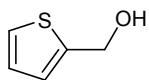
4j¹⁸: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. Methyl 4-formylbenzoate (164.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **4j** was isolated. Yield: 156 mg (94%). ¹H NMR (500 MHz, CDCl₃) δ 8.00 (dd, *J* = 8.3, 1.5 Hz, 2H), 7.45 – 7.35 (m, 2H), 4.74 (s, 2H), 3.90 (s, 3H), 2.22 (br., 1H) ppm; ¹³C NMR (126 MHz, CDCl₃) δ 167.1, 146.1, 129.8, 129.2, 126.5, 64.6, 52.2 ppm.



Chemical Formula: C₁₇H₁₂O
Molecular Weight: 232.2820

4k²²: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in Et₂O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. Pyrene-2-carbaldehyde (230.2 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:10, v/v) as eluent. Light yellow solid of **4k** was isolated. Yield: 216 mg (93%). ¹H NMR (600 MHz, CDCl₃) δ 8.26 (d, *J* = 9.1 Hz, 1H), 8.18 (d, *J* = 2.6 Hz, 1H), 8.17 (d,

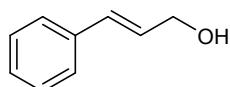
$J = 2.8$ Hz, 1H), 8.07 (t, $J = 8.3$ Hz, 2H), 8.05 – 7.98 (m, 3H), 7.96 (d, $J = 7.7$ Hz, 1H), 5.31 (s, 2H), 2.13 (s, 1H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 133.7, 131.2, 131.2, 130.7, 128.7, 127.8, 127.4, 127.4, 126.0, 125.9, 125.3, 125.2, 124.9, 124.7, 124.7, 122.9, 63.7 ppm.



Chemical Formula: $\text{C}_5\text{H}_6\text{OS}$
Molecular Weight: 114.1620

4l¹⁸: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in Et_2O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 2-Thiophenecarboxaldehyde (112.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of

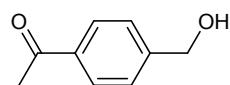
the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO_2 using ethyl acetate/hexane (1:10, v/v) as eluent. Yellow oil of **4l** was isolated. Yield: 91.2 mg (80%). ^1H NMR (600 MHz, CDCl_3) δ 7.30 (dd, $J = 5.0, 1.6$ Hz, 1H), 7.08 – 6.94 (m, 2H), 4.83 (s, 2H), 2.19 (s, 1H) ppm; ^{13}C NMR (150 MHz, CDCl_3) δ 144.0, 126.9, 125.6, 125.5, 60.0 ppm.



Chemical Formula: $\text{C}_9\text{H}_{10}\text{O}$
Molecular Weight: 134.1780

4m¹⁸: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in Et_2O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. *Trans*-cinnamaldehyde (132.0 mg, 1.0 mmol) and pinacolborane (256.0 mg, 2.0 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of

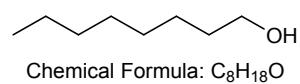
the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO_2 using ethyl acetate/hexane (1:10, v/v) as eluent. Yellowish oil of **4m** was isolated. Yield: 127.3 mg (95%). ^1H NMR (500 MHz, CDCl_3) δ 7.42 (d, $J = 8.3$ Hz, 2H), 7.38 – 7.32 (m, 2H), 7.30 (dd, $J = 7.2, 1.6$ Hz, 1H), 6.64 (d, $J = 16.0$ Hz, 1H), 6.44 – 6.33 (m, 1H), 4.33 (d, $J = 5.8$ Hz, 2H), 2.96 (s, 1H) ppm; ^{13}C NMR (125 MHz, CDCl_3) δ 136.9, 131.1, 128.8, 128.7, 127.8, 126.7, 63.6 ppm.



Chemical Formula: $\text{C}_9\text{H}_{10}\text{O}_2$
Molecular Weight: 150.1770

4n¹⁸: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in Et_2O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 4-Acetylbenzaldehyde (148.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was allowed to stir at room temperature for 2 h. At completion of

the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was analyzed by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO_2 using ethyl acetate/hexane (1:10, v/v) as eluent. Yellowish oil of **4n** was isolated. Yield: 121 mg (81%). ^1H NMR (600 MHz, CDCl_3) δ 7.91 (d, $J = 8.4$ Hz, 2H), 7.43 (d, $J = 8.2$ Hz, 2H), 4.75 (s, 2H), 2.70 (s, 1H), 2.58 (s, 3H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 198.2, 146.5, 136.2, 128.6, 126.6, 64.4, 26.6 ppm.

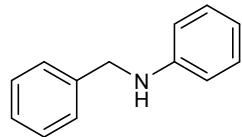


Chemical Formula: $\text{C}_8\text{H}_{18}\text{O}$
Molecular Weight: 130.2310

4o¹⁹: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in Et_2O (1.0 mL) in a 3.8 mL glass vial equipped with a stir bar. 1-Octanal (128.2 mg, 1.0 mmol) and pinacolborane (281.6 mg, 2.2 mmol) were then added. The reaction mixture was

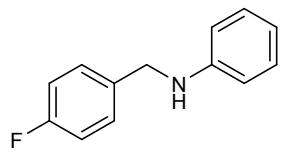
allowed to stir at room temperature for 2 h. At completion of the reaction, the reaction was

exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO_2 using ethyl acetate/hexane (1:10, v/v) as eluent. Colorless oil of **4o** was isolated. Yield: 110.5 mg (85%). ^1H NMR (500 MHz, CDCl_3) δ 3.59 (t, $J = 6.7$ Hz, 2H), 2.31 (s, 1H), 1.53 (t, $J = 7.0$ Hz, 2H), 1.27 (m, 10H), 0.85 (t, $J = 6.7$ Hz, 3H) ppm; ^{13}C NMR (126 MHz, CDCl_3) δ 63.2, 33.0, 32.1, 29.7, 29.6, 26.1, 22.9, 14.4 ppm.



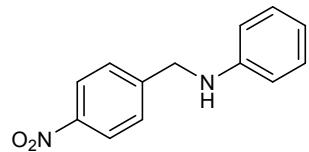
Chemical Formula: $\text{C}_{13}\text{H}_{13}\text{N}$
Molecular Weight: 183.2540

5a¹⁸: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped with a stir bar. Benzylideneaniline (181.0 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was sealed and allowed to heat to 50 °C for 16 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO_2 using ethyl acetate/hexane (1:5, v/v) as eluent. Colorless oil of **5a** was isolated. Yield: 165 mg (90%). ^1H NMR (600 MHz, CDCl_3) δ 7.69 – 7.43 (m, 4H), 7.39 (d, $J = 7.1$ Hz, 1H), 7.29 (dd, $J = 9.0, 7.2$ Hz, 2H), 6.84 (d, $J = 7.5$ Hz, 1H), 6.79 – 6.68 (m, 2H), 4.42 (s, 2H), 4.12 (br., 1H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 148.2, 139.5, 129.4, 128.7, 127.6, 127.3, 117.7, 112.9, 48.4 ppm.



Chemical Formula: $\text{C}_{13}\text{H}_{12}\text{FN}$
Molecular Weight: 201.2444

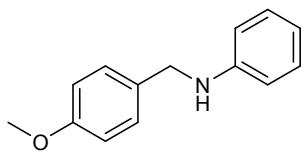
5b¹⁸: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped with a stir bar. 4-Fluorobenzylideneaniline (199.2 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was sealed and allowed to heat to 50 °C for 16 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO_2 using ethyl acetate/hexane (1:5, v/v) as eluent. Yellowish oil of **5b** was isolated. Yield: 169 mg (84%). ^1H NMR (600 MHz, CDCl_3) δ 7.36 (tt, $J = 5.5, 3.5$ Hz, 2H), 7.30 – 7.27 (m, 1H), 7.21 (td, $J = 7.5, 2.7$ Hz, 2H), 7.04 (ddt, $J = 8.7, 5.2, 3.1$ Hz, 2H), 6.80 (d, $J = 7.2$ Hz, 1H), 6.70 (dd, $J = 8.3, 5.1$ Hz, 2H), 4.33 (s, 2H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 163.9, 161.3, 129.32, 129.28, 129.23, 118.5, 115.5, 115.4, 113.6, 48.1 ppm.



Chemical Formula: $\text{C}_{13}\text{H}_{12}\text{N}_2\text{O}_2$
Molecular Weight: 228.2510

5c¹⁸: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped with a stir bar. 4-Nitrobenzylideneaniline (226.2 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was sealed and allowed to heat to 50 °C for 16 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO_2 using ethyl acetate/hexane (1:5, v/v) as eluent. Yellowish oil of **5c** was isolated. Yield: 164 mg (72%). ^1H NMR (600 MHz, CDCl_3) δ 8.21 (dd, $J = 8.6, 2.0$ Hz, 2H), 7.56 (d, $J = 8.5$ Hz, 2H), 7.20 (t, $J = 8.1$ Hz, 2H), 6.78 (t, $J = 7.3$ Hz, 1H), 6.62 (d, $J = 8.1$ Hz,

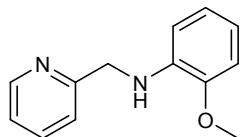
2H), 4.50 (s, 2H), 4.37 (s, 1H) ppm; ^{13}C NMR (151 MHz, CDCl_3) δ 147.5, 147.3, 129.4, 127.7, 123.9, 118.3, 113.0, 47.7 ppm.



Chemical Formula: $\text{C}_{14}\text{H}_{15}\text{NO}$
Molecular Weight: 213.2800

5d²³: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped with a stir bar. 4-Methoxybenzylideneaniline (211 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was sealed and allowed to heat to 50 °C for 16 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by

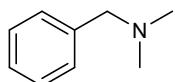
GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO_2 using ethyl acetate/hexane (1:5, v/v) as eluent. Yellowish oil of **5d** was isolated. Yield: 181mg (85%). ^1H NMR (600 MHz, CDCl_3) δ 7.29 (d, $J = 8.7$ Hz, 2H), 7.18 (dd, $J = 8.6, 7.3$ Hz, 2H), 6.88 (d, $J = 8.7$ Hz, 2H), 6.71 (s, 1H), 6.64 (dt, $J = 7.7, 1.1$ Hz, 2H), 4.25 (s, 2H), 3.96 (b, 1H), 3.81 (s, 3H) ppm; ^{13}C NMR (101 MHz, CDCl_3) δ 158.8, 148.2, 131.4, 129.3, 128.8, 117.5, 114.0, 112.8, 55.3, 47.8 ppm.



Chemical Formula: $\text{C}_{13}\text{H}_{14}\text{N}_2\text{O}$
Molecular Weight: 214.2680

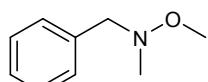
5e²³: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped with a stir bar. 2-Pyridylidene-o-anisidine (212 mg, 1.0 mmol) and pinacolborane (140.8 mg, 1.1 mmol) were then added. The reaction mixture was sealed and allowed to heat to 50 °C for 16 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The hydroborated product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO_2 using ethyl acetate/hexane (1:5, v/v) as eluent. Yellowish oil of **5e** was isolated. Yield: 173 mg (81%). ^1H

NMR (600 MHz, Chloroform-d) δ 8.60 (d, $J = 4.4$ Hz, 1H), 7.64 (td, $J = 7.7, 1.8$ Hz, 1H), 7.37 (d, $J = 7.9$ Hz, 1H), 7.24 – 7.13 (m, 1H), 6.92 – 6.74 (m, 2H), 6.69 (td, $J = 7.7, 1.6$ Hz, 1H), 6.54 (dd, $J = 7.8, 1.6$ Hz, 1H), 5.01 (br., 1H), 4.52 (s, 2H), 3.89 (s, 3H) ppm; ^{13}C NMR (151 MHz, Chloroform-d) δ 159.4, 149.4, 147.3, 138.1, 137.2, 122.4, 121.8, 121.5, 117.2, 110.5, 109.8, 55.8, 49.5 ppm. HR-MS [M + H $^+$]: 215.1181 (calc.: 215.1184).



Chemical Formula: $\text{C}_9\text{H}_{13}\text{N}$
Molecular Weight: 135.2100

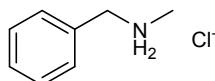
6a²⁴: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped with a stir bar. N,N-dimethylbenzamide (149 mg, 1.0 mmol) and pinacolborane (256 mg, 2.0 mmol) were then added. The reaction mixture was sealed and allowed to heat to 60 °C for 16 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The reduced product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO_2 using ethyl acetate/hexane (1:6, v/v) as an eluent. Colorless oil of **6a** was isolated. Yield: 122 mg (90%). ^1H NMR (600 MHz, Chloroform-d) δ 7.42–7.39 (m, 3H), 7.35 – 7.30 (m, 2H), 3.99 (s, 2H), 2.51 (s, 6H) ppm; ^{13}C NMR (151 MHz, Chloroform-d) δ 132.4, 131.4, 129.3, 128.6, 67.7, 49.8 ppm.



Chemical Formula: $\text{C}_9\text{H}_{13}\text{NO}$
Molecular Weight: 151.2090

6b: In a glovebox under N_2 atmosphere, catalyst **1/1H** (0.54 mg, 1.0 μmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped

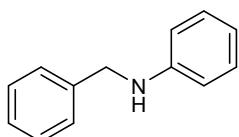
with a stir bar. N-methoxy-N-dimethylbenzamide (165 mg, 1.0 mmol) and pinacolborane (256 mg, 2.0 mmol) were then added. The reaction mixture was sealed and allowed to heat to 60 °C for 16 h. At completion of the reaction, the reaction was exposed to the air. The reduced product was analyzed by GC-MS and complete conversion to the reduced product **6b** was revealed. Then, to the reaction mixture was added a HCl solution (in Et₂O, 1 M, 2 mL). The white precipitate was collected and recrystallized by slowly diffusing Et₂O into a methanolic solution. Colorless crystals were collected and characterized by NMR as being identified as a **6c**·HCl salt. Yield: 134 mg (85%).



Chemical Formula: C₈H₁₂ClN⁻
Molecular Weight: 157.6415

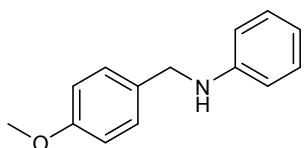
6c·HCl²⁴: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped with a stir bar. N-methylbenzamide (135 mg, 1.0 mmol) and pinacolborane (256 mg, 2.0 mmol) were then added. The reaction mixture was sealed and allowed to heat to 60 °C for 16 h. At completion

of the reaction, the reaction was exposed to the air and the solvent was evaporated. The reduced product was detected by GC-MS and 82% conversion of amide to **6c** was revealed. Then, to the reaction mixture was added a HCl solution (in Et₂O, 1 M, 2 mL). The white precipitate was collected and recrystallized by slowly diffusing Et₂O into a methanolic solution. Colorless crystals suitable for X-ray diffraction were isolated as a **6c**·HCl salt. Yield: 118 mg (75%). ¹H NMR (600 MHz, Chloroform-*d*) δ 9.85 (s, 2H), 7.57 – 7.49 (m, 2H), 7.43 – 7.32 (m, 3H), 4.02 (s, 2H), 2.48 (s, 3H) ppm; ¹³C NMR (151 MHz, Chloroform-*d*) δ 130.3, 129.8, 129.6, 129.2, 52.1, 31.2 ppm.



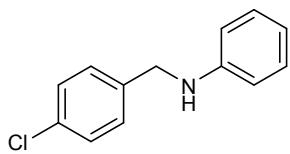
Chemical Formula: C₁₃H₁₃N
Molecular Weight: 183.2540

6d/5a: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped with a stir bar. N-phenylbenzamide (197 mg, 1.0 mmol) and pinacolborane (256 mg, 2.0 mmol) were then added. The reaction mixture was sealed and allowed to heat to 60 °C for 16 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The reduced product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:6, v/v) as eluent. Yellowish oil of **6d** was isolated. Yield: 119 mg (65%). NMR spectroscopic data is identical to that of **5a**.



Chemical Formula: C₁₄H₁₅NO
Molecular Weight: 213.2800

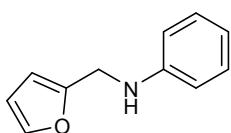
6e/5d: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped with a stir bar. N-phenyl-4-methoxybenzamide (227 mg, 1.0 mmol) and pinacolborane (256 mg, 2.0 mmol) were then added. The reaction mixture was sealed and allowed to heat to 60 °C for 16 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The reduced product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:6, v/v) as eluent. Yellowish oil of **6e** was isolated. Yield: 151 mg (71%). NMR spectroscopic data is identical to that of **5d**.



Chemical Formula: C₁₃H₁₂CIN
Molecular Weight: 217.6960

6f²³: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped with a stir bar. N-phenyl-4-chloroybenzamide (231 mg, 1.0 mmol) and pinacolborane (256 mg, 2.0 mmol) were then added. The reaction mixture was sealed and allowed to heat to 60 °C for 16 h. At completion of the reaction, the reaction was exposed to the air and the solvent was evaporated. The reduced product was detected by GC-MS,

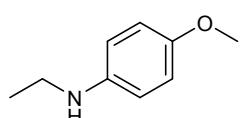
and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:6, v/v) as eluent. Yellowish oil of **6f** was isolated. Yield: 144 mg (66%). ¹H NMR (600 MHz, Chloroform-d) δ 7.31 (br. 4H), 7.18 (dd, *J* = 8.6, 7.2 Hz, 2H), 6.77 – 6.70 (m, 1H), 6.65 – 6.57 (m, 2H), 4.32 (s, 2H), 4.06 (br., 1H) ppm; ¹³C NMR (151 MHz, Chloroform-d) δ 147.8, 138.0, 132.9, 129.3, 128.8, 128.7, 117.8, 112.9, 47.6 ppm.



Chemical Formula: C₁₁H₁₁NO
Molecular Weight: 173.2150

6g²⁵: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped with a stir bar. N-phenyl-2-furamide (187 mg, 1.0 mmol) and pinacolborane (256 mg, 2.0 mmol) were then added. The reaction mixture was sealed and allowed to heat to 60 °C for 16 h. At completion of the reaction, the reaction was exposed to the air and the solvent was

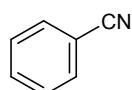
evaporated. The reduced product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:6, v/v) as eluent. Yellowish oil of **6g** was isolated. Yield: 125 mg (72%). ¹H NMR (600 MHz, Chloroform-d) δ 7.36 (dd, *J* = 1.8, 0.9 Hz, 1H), 7.23 – 7.17 (m, 2H), 6.77 (tt, *J* = 7.3, 1.1 Hz, 1H), 6.73 – 6.67 (m, 2H), 6.32 (d, *J* = 3.2 Hz, 1H), 6.26 – 6.22 (m, 1H), 4.84 (br., 1H), 4.32 (d, *J* = 0.8 Hz, 2H) ppm; ¹³C NMR (151 MHz, Chloroform-d) δ 152.4, 147.1, 142.1, 129.4, 118.6, 113.7, 110.5, 107.4, 41.8 ppm.



Chemical Formula: C₉H₁₃NO
Molecular Weight: 151.2090

6h²⁴: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped with a stir bar. N-(4-methoxyphenyl)acetamide (165 mg, 1.0 mmol) and pinacolborane (256 mg, 2.0 mmol) were then added. The reaction mixture was sealed and allowed to heat to 60 °C for 16 h. At completion of the reaction, the reaction was exposed to the air and the solvent was

evaporated. The reduced product was detected by GC-MS, and then the crude reaction mixture was purified through flash column chromatography with SiO₂ using ethyl acetate/hexane (1:6, v/v) as eluent. Colorless oil of **6h** was isolated. Yield: 106 mg (70%). ¹H NMR (600 MHz, Chloroform-d) δ 6.79 (d, *J* = 8.9 Hz, 2H), 6.59 (d, *J* = 8.9 Hz, 2H), 3.75 (s, 3H), 3.26 (br., 1H), 3.11 (d, *J* = 7.2 Hz, 2H), 1.24 (t, *J* = 7.2 Hz, 3H) ppm; ¹³C NMR (151 MHz, Chloroform-d) δ 152.0, 142.8, 114.9, 114.1, 55.8, 39.5, 15.0 ppm.



Chemical Formula: C₇H₅N
Molecular Weight: 103.1240

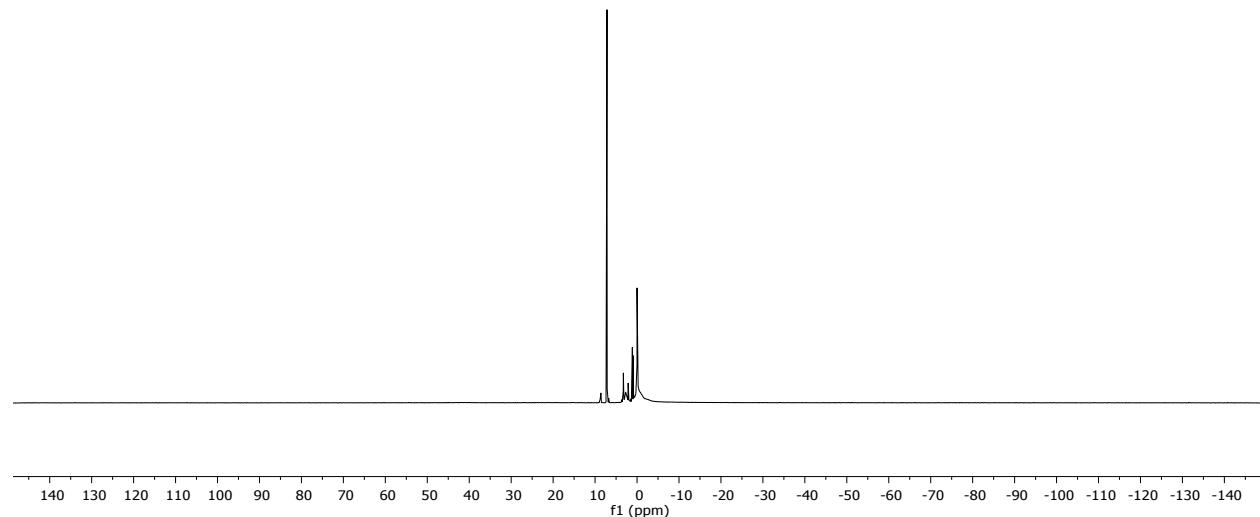
7: In a glovebox under N₂ atmosphere, catalyst **1/1H** (0.54 mg, 1.0 µmol) was dissolved in THF (1.0 mL) in a 20 mL Schlenk tube equipped with a stir bar. Benzamide (121 mg, 1.0 mmol) and pinacolborane (256 mg, 2.0 mmol) were then added. The reaction mixture was sealed and allowed to heat to 60 °C for 16 h. At completion of the reaction, the reaction was

exposed to the air and the product was analyzed by GC and identified as benzonitrile by comparison with authentic sample. GC-MS: 103 (calc. 103).

Copies of NMR spectra

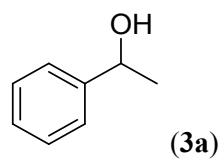
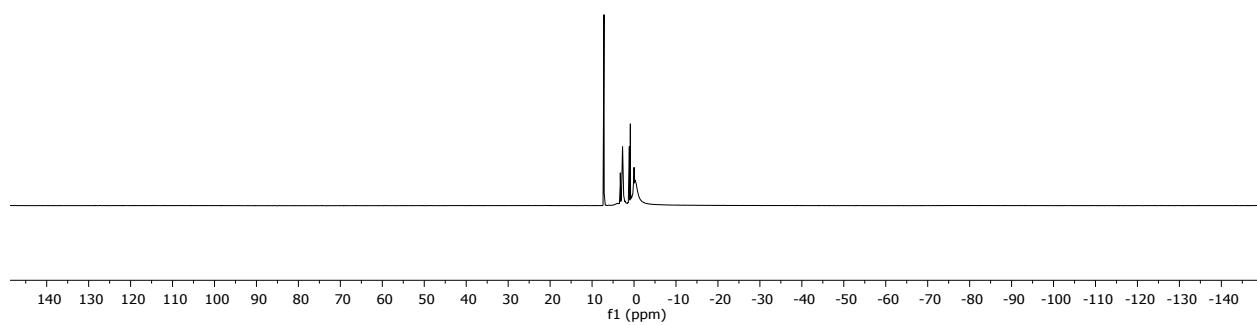
Vanadium complex 1/1H

^1H NMR (25 mg, C₆D₆, 400 MHz)

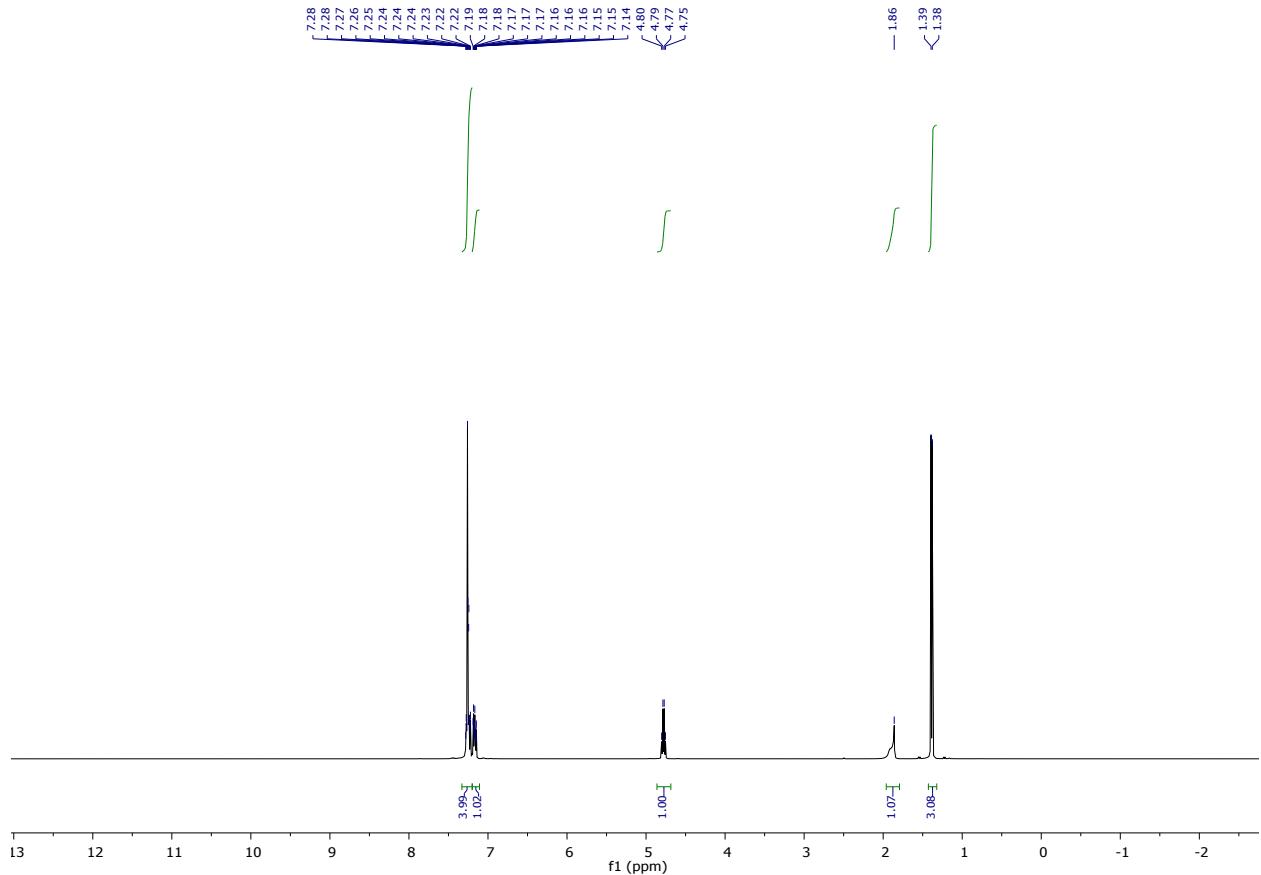


Vanadium complex 2

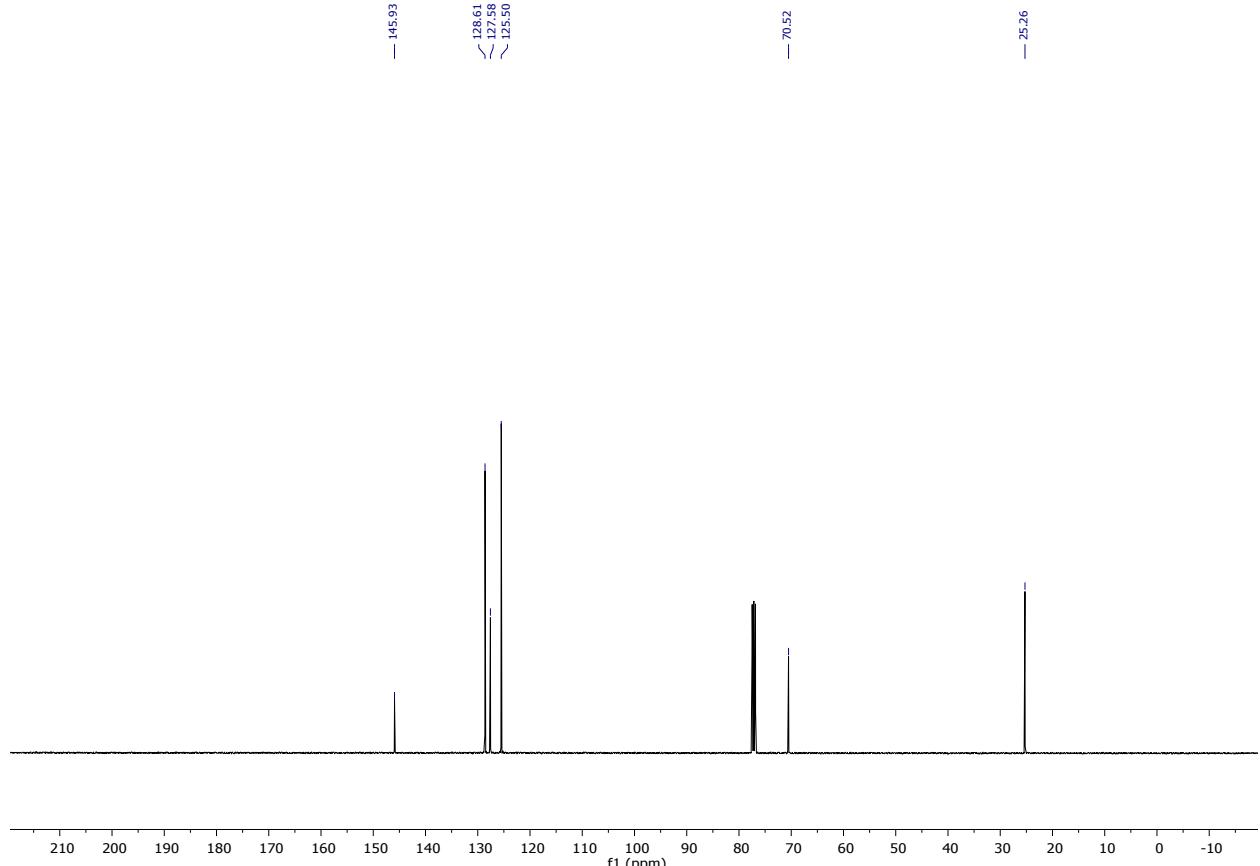
^1H NMR (22 mg, C₆D₆, 400 MHz)

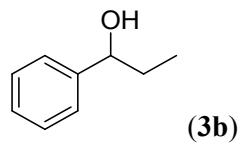


¹H NMR (400 MHz, CDCl₃):

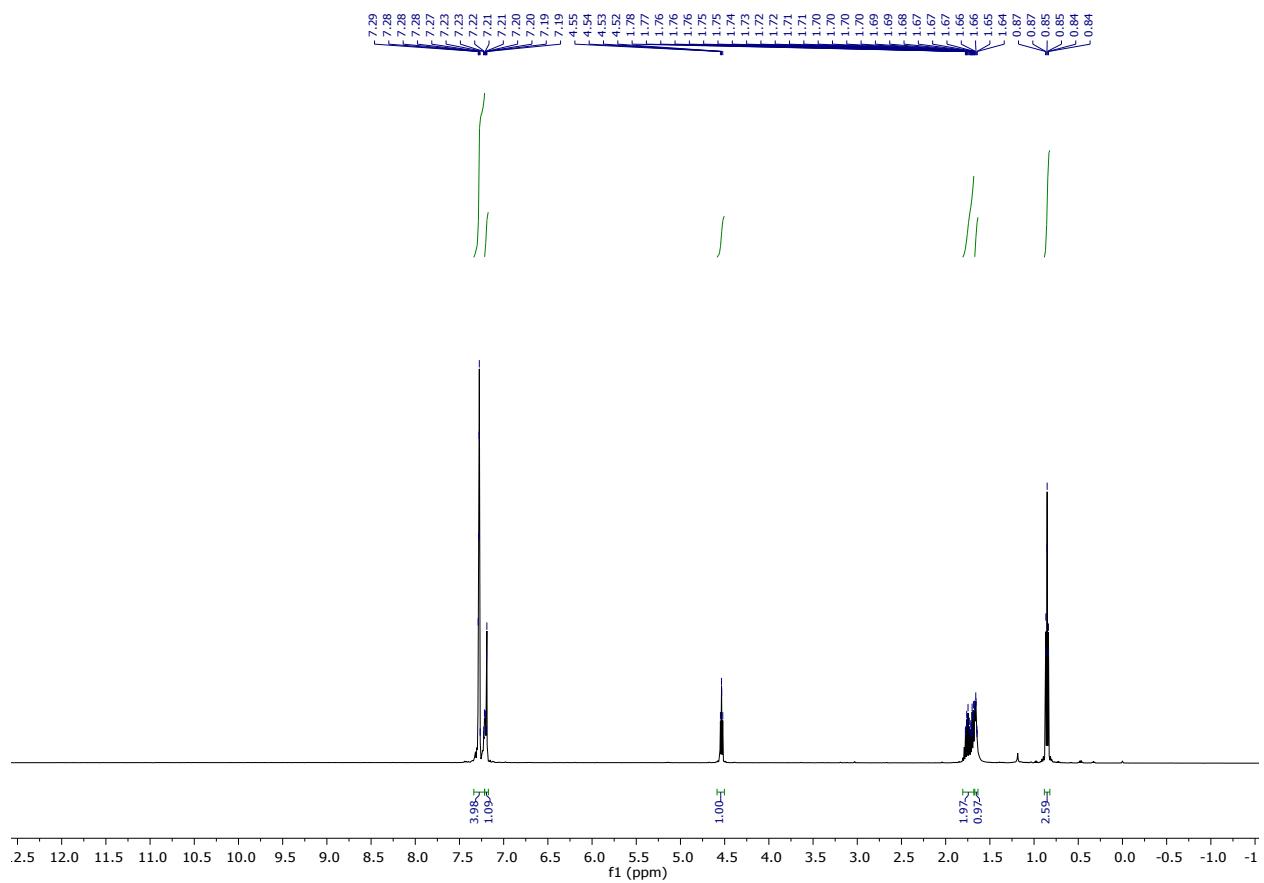


¹³C NMR (101 MHz, CDCl₃):

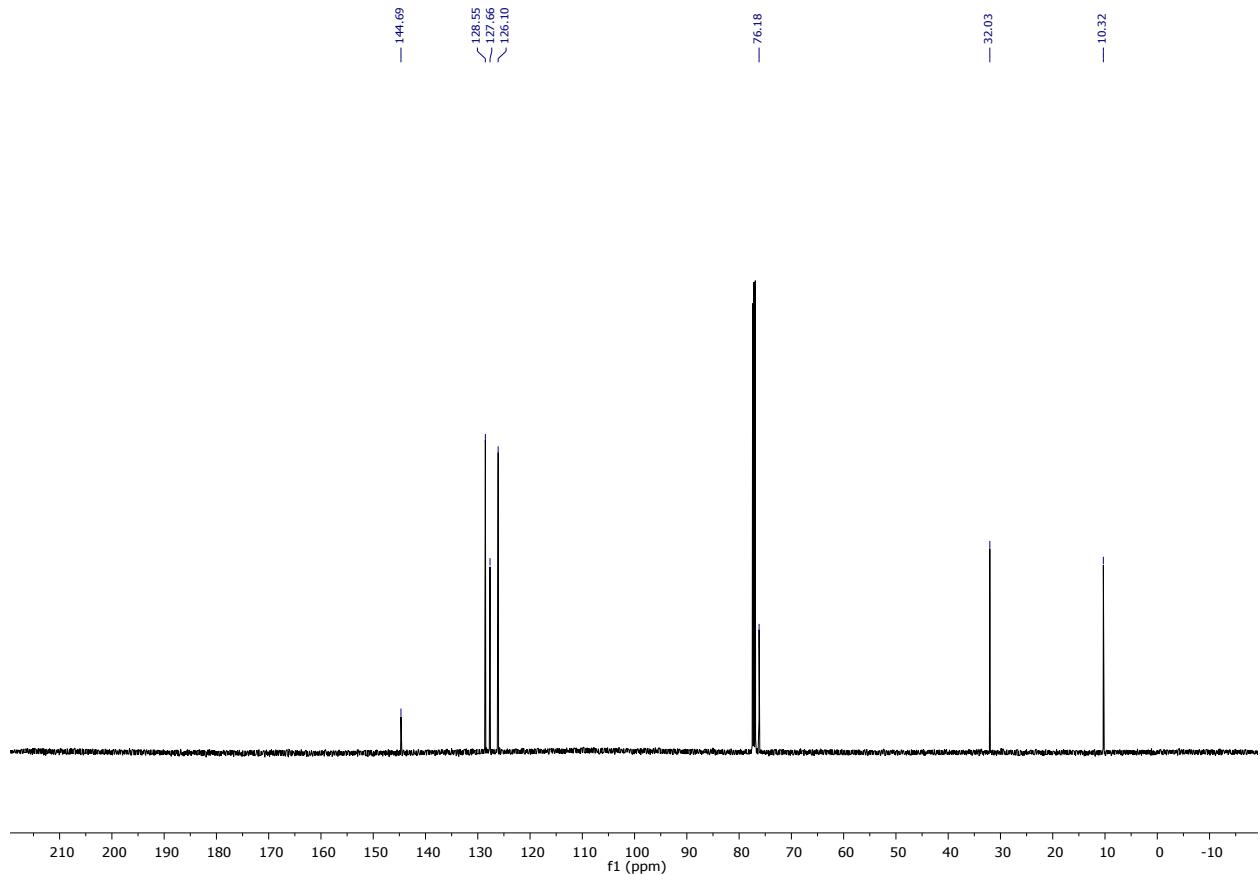


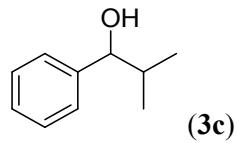


¹H NMR (500 MHz, CDCl₃):

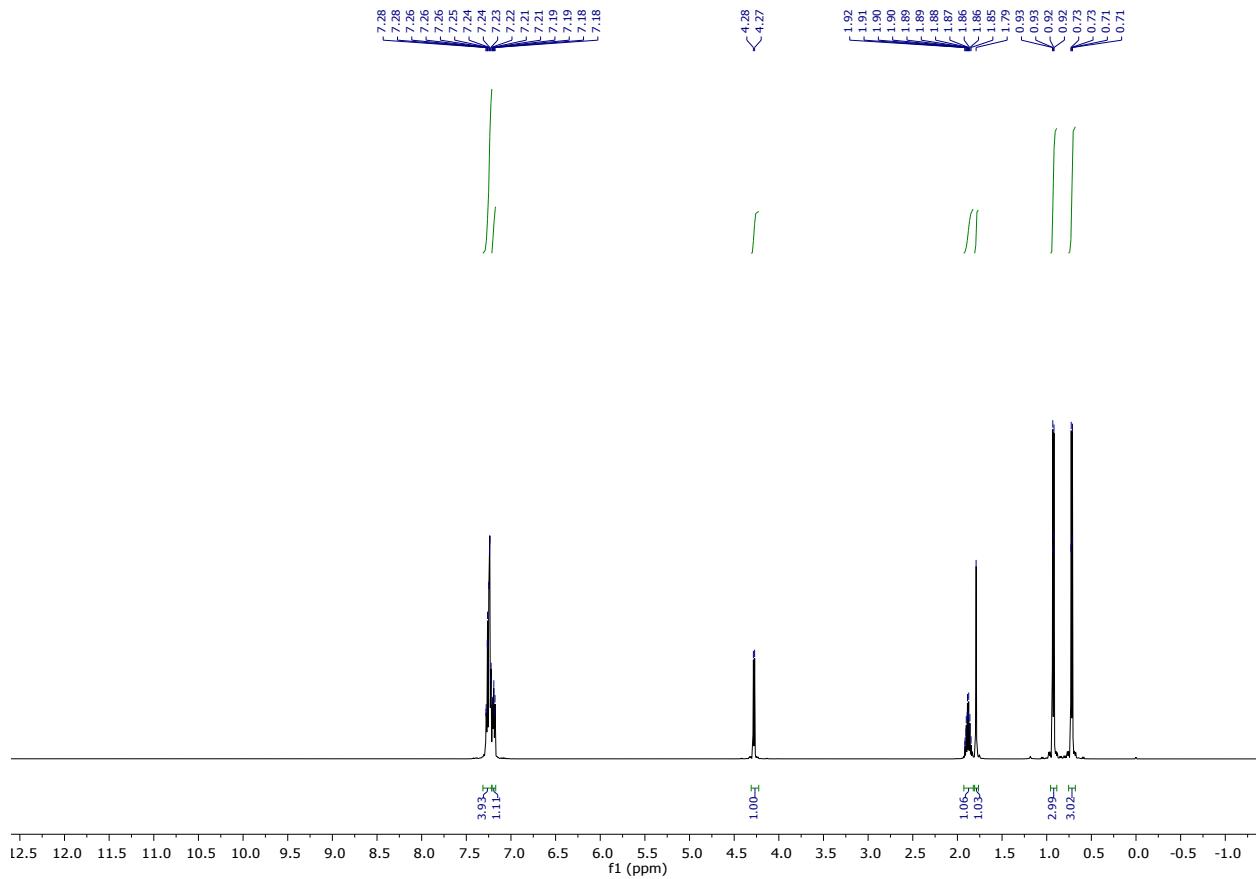


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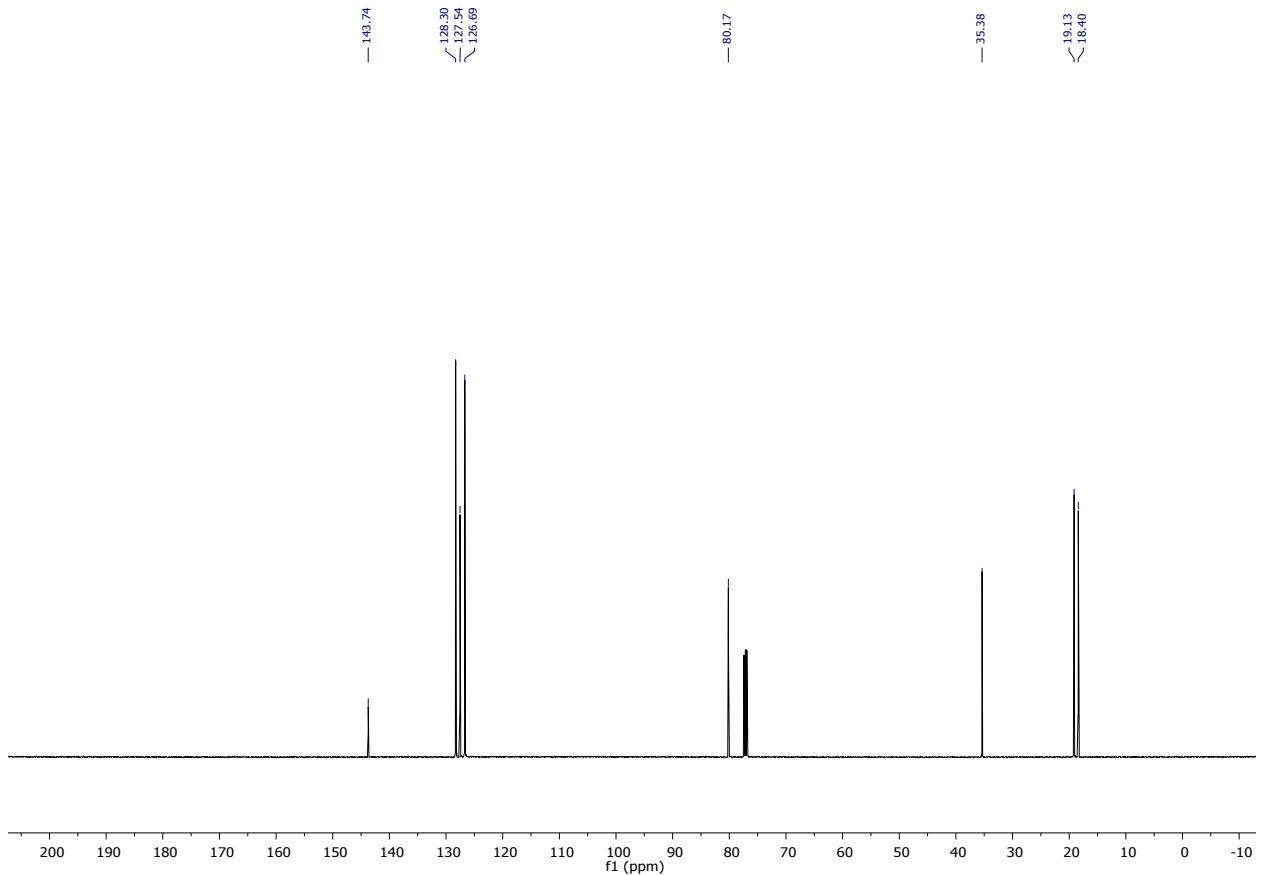


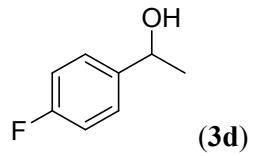


¹H NMR (500 MHz, CDCl₃):

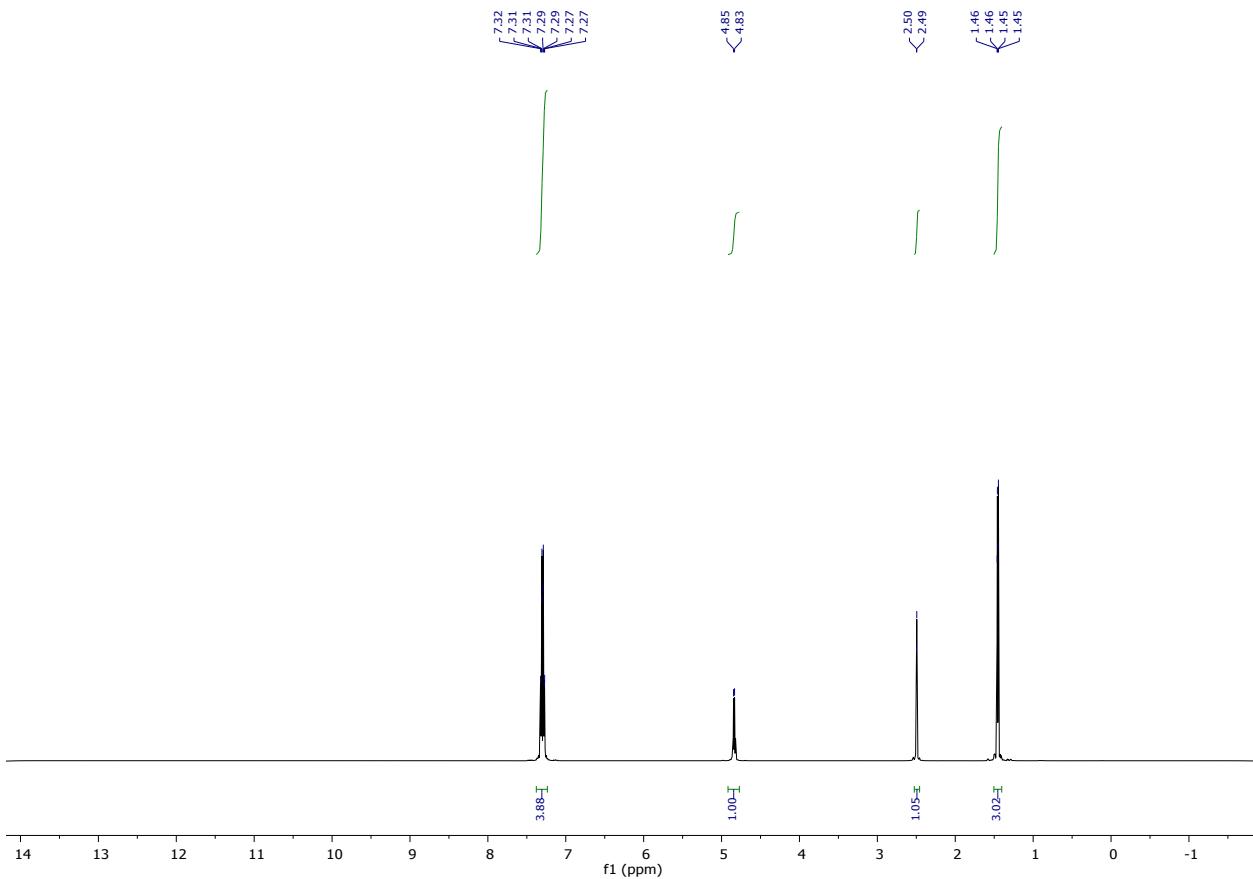


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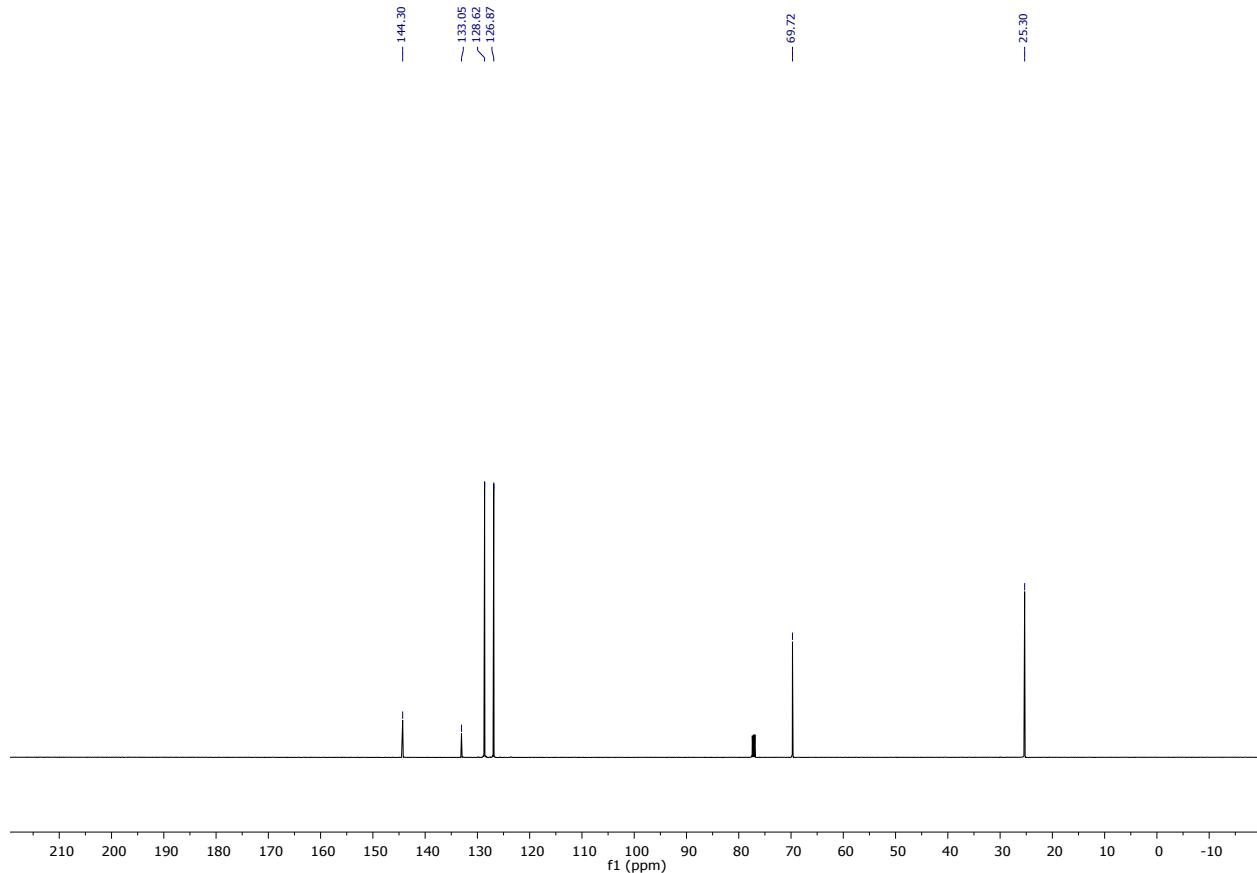


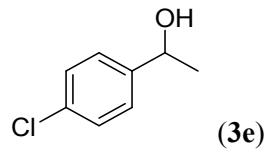


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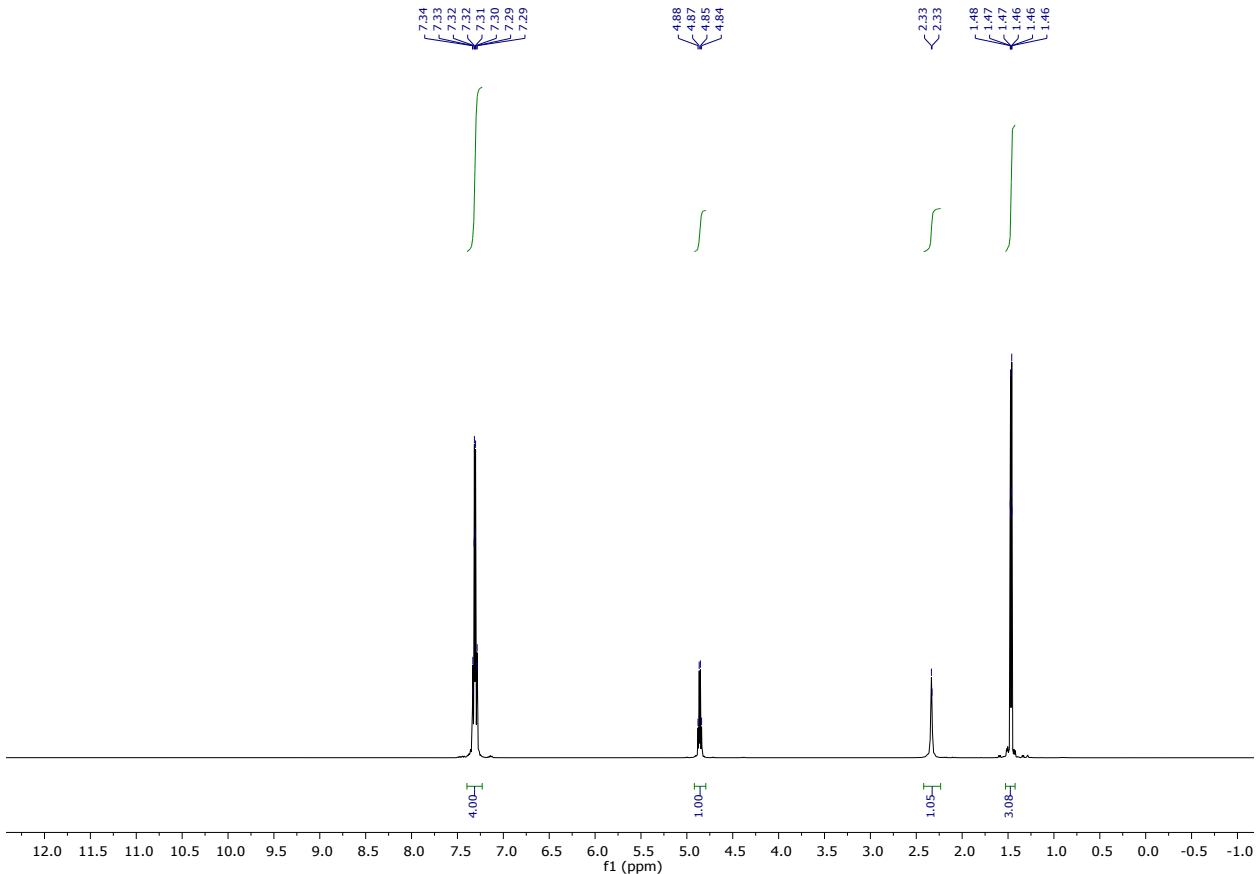


¹³C NMR (151 MHz, CDCl₃):

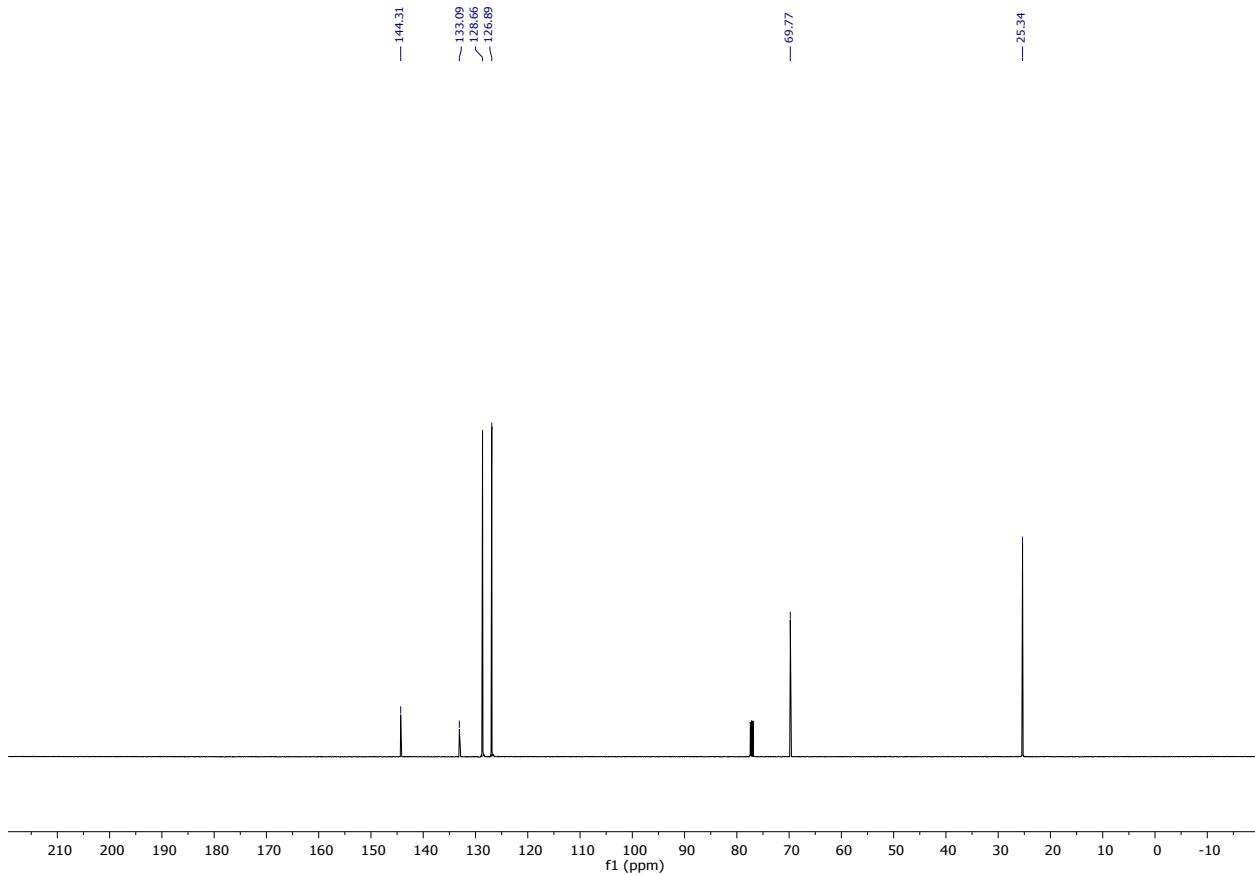


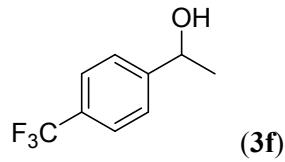


¹H NMR (500 MHz, CDCl₃):

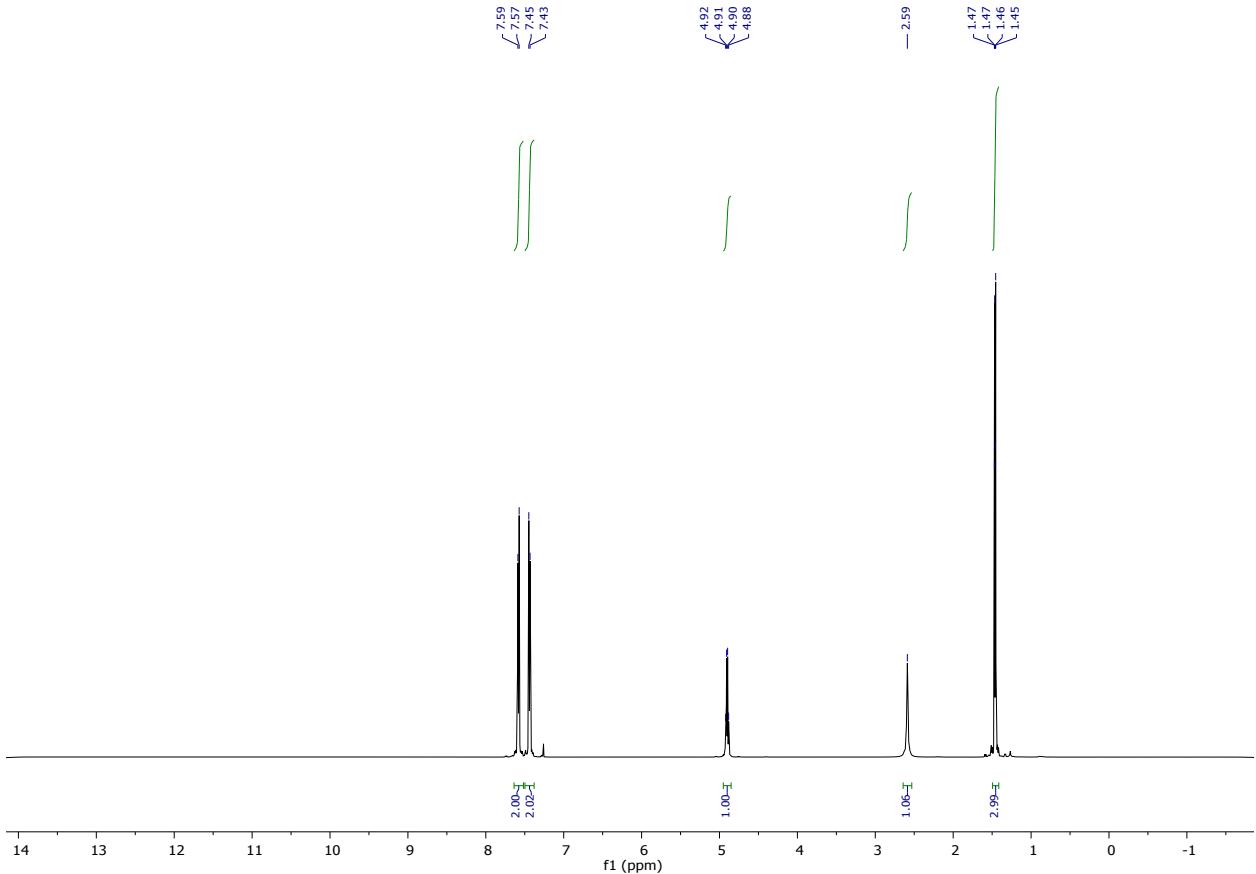


¹³C NMR (126 MHz, CDCl₃):

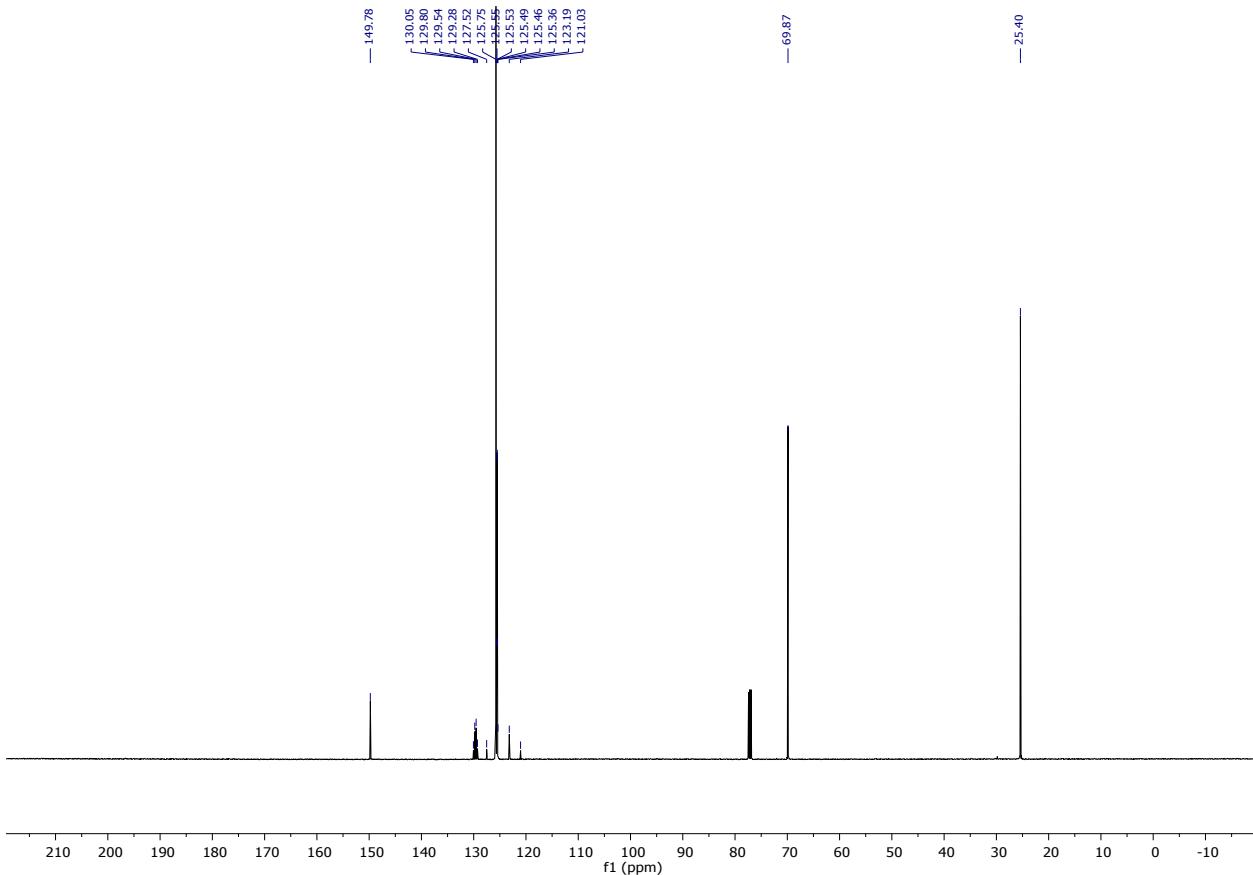


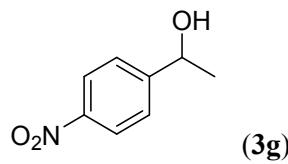


¹H NMR (500 MHz, CDCl₃):

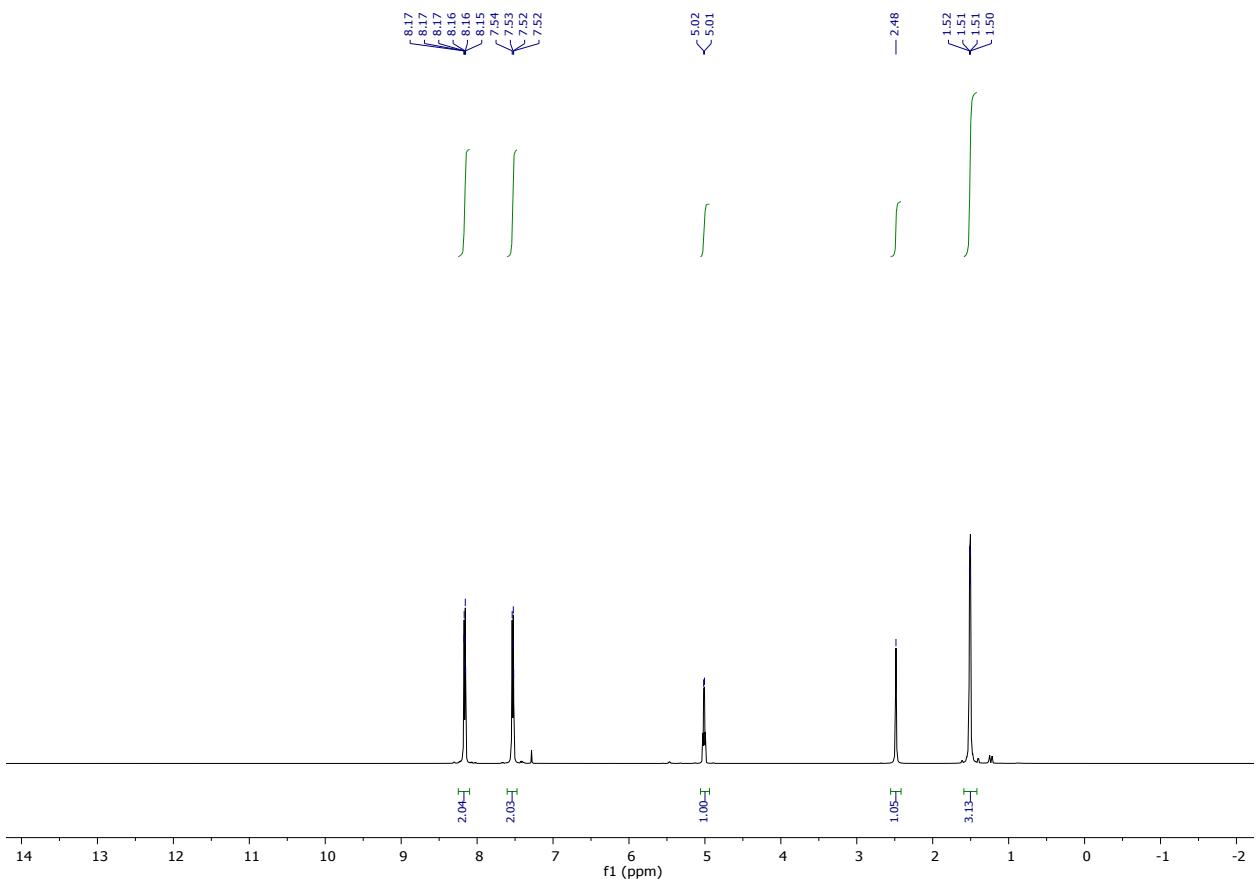


^{13}C NMR (126 MHz, CDCl_3):

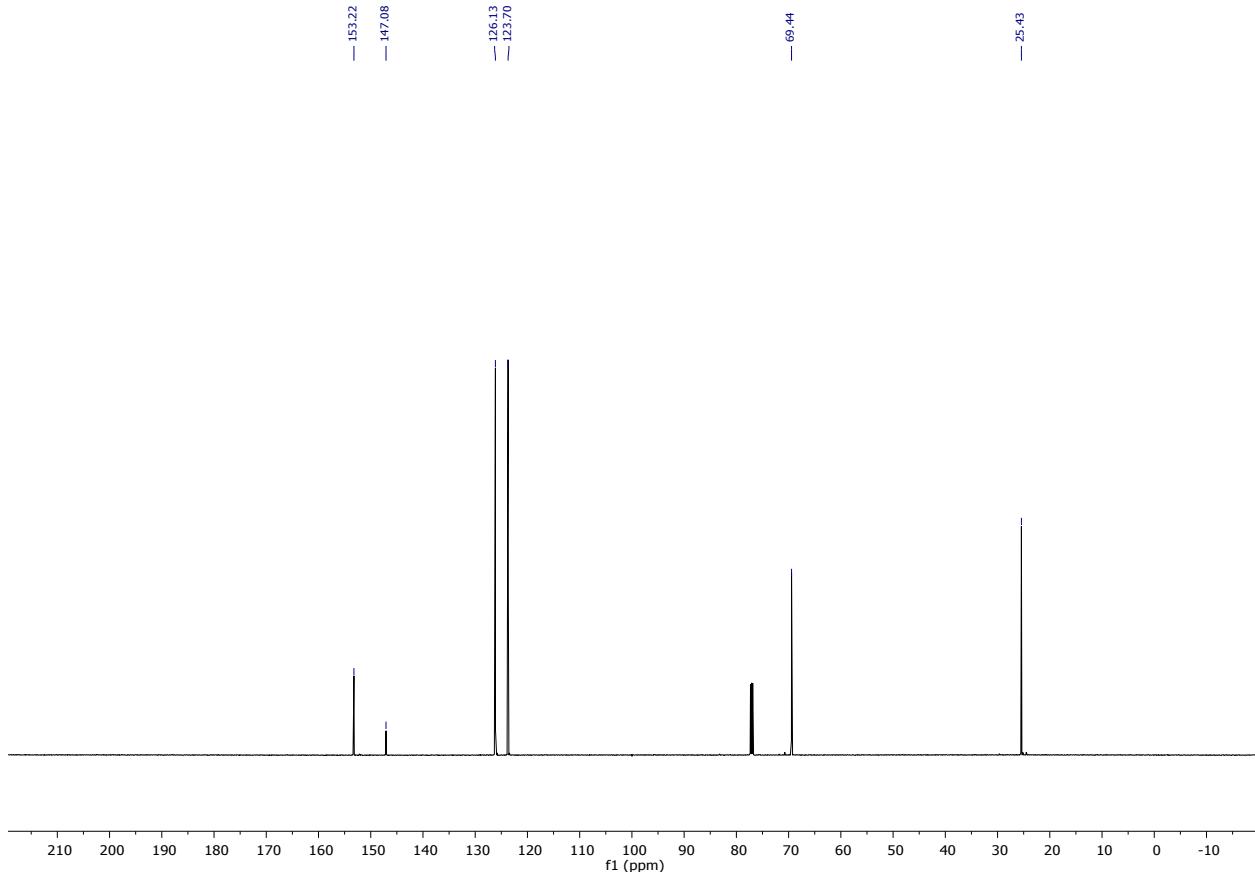


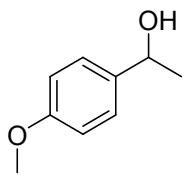


^1H NMR (600 MHz, CDCl_3):

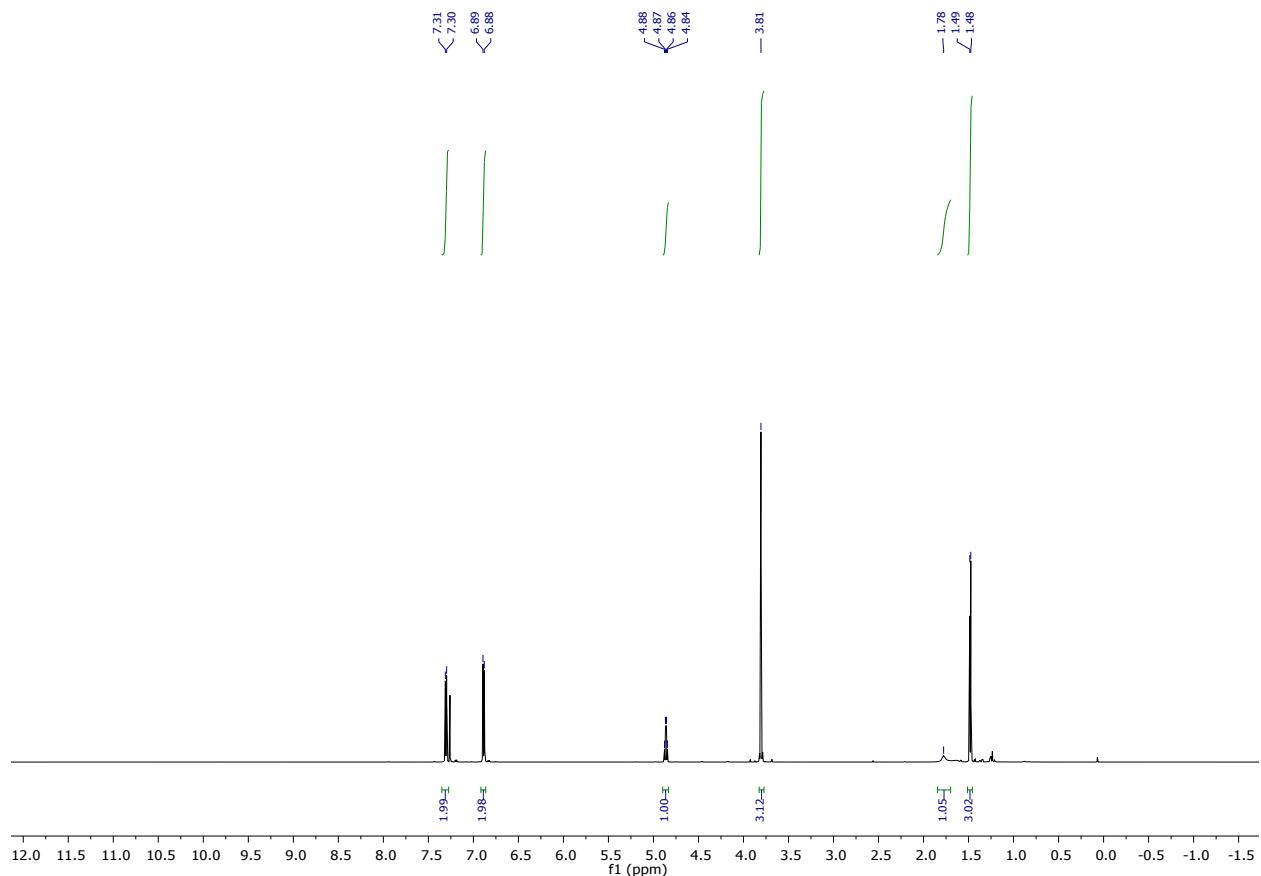


¹³C NMR (151 MHz, CDCl₃):

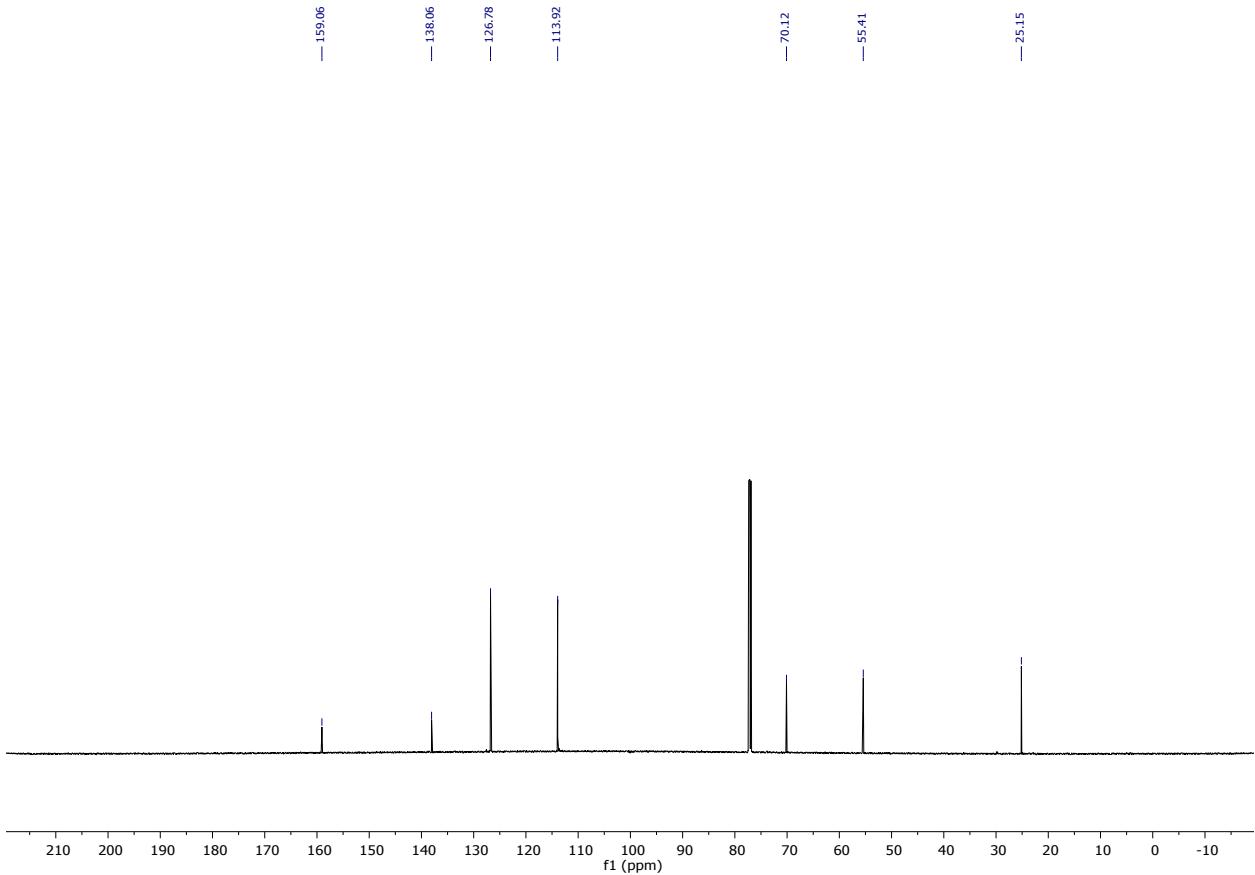


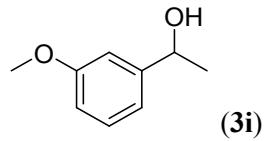


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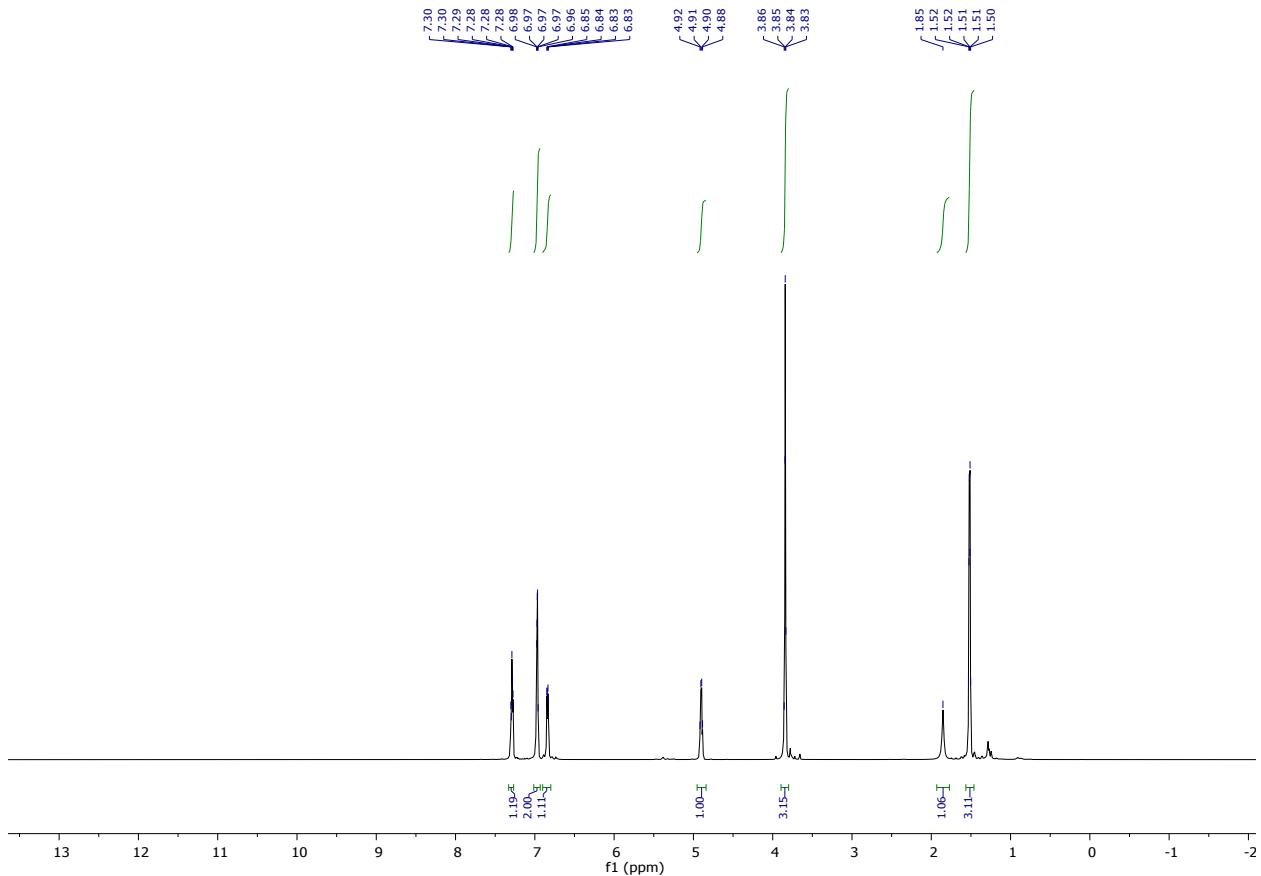


¹³C NMR (151 MHz, CDCl₃):

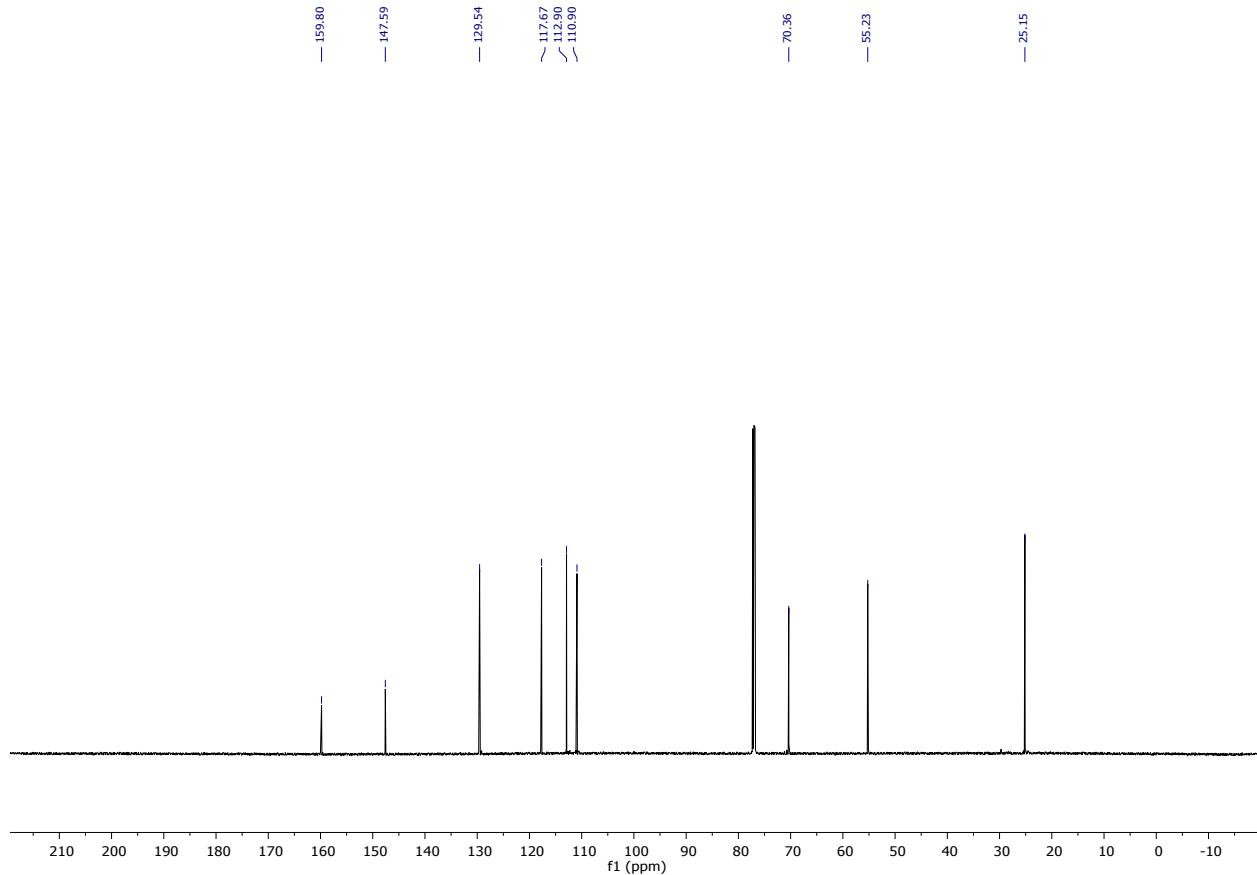


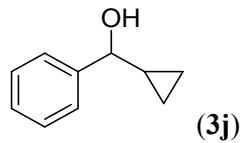


¹H NMR (600 MHz, CDCl₃):

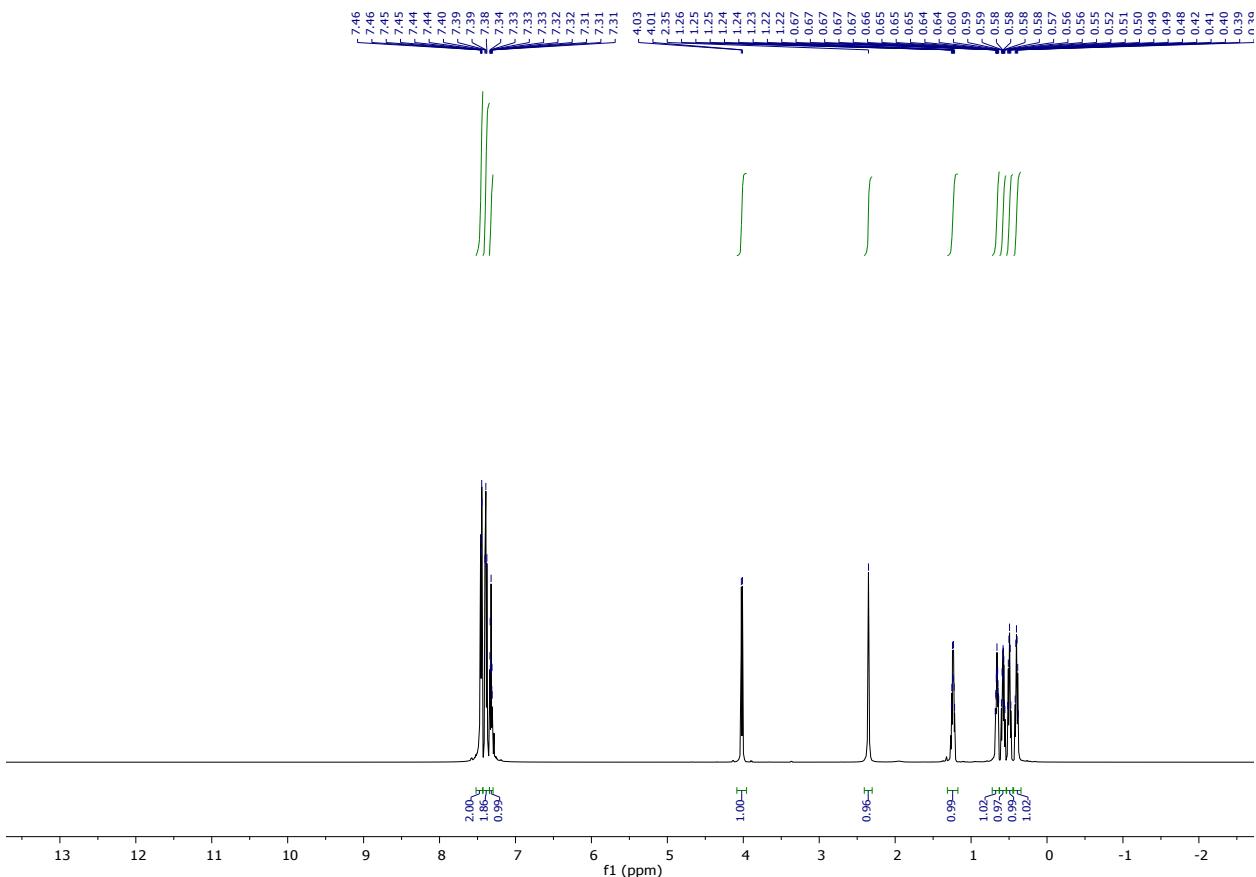


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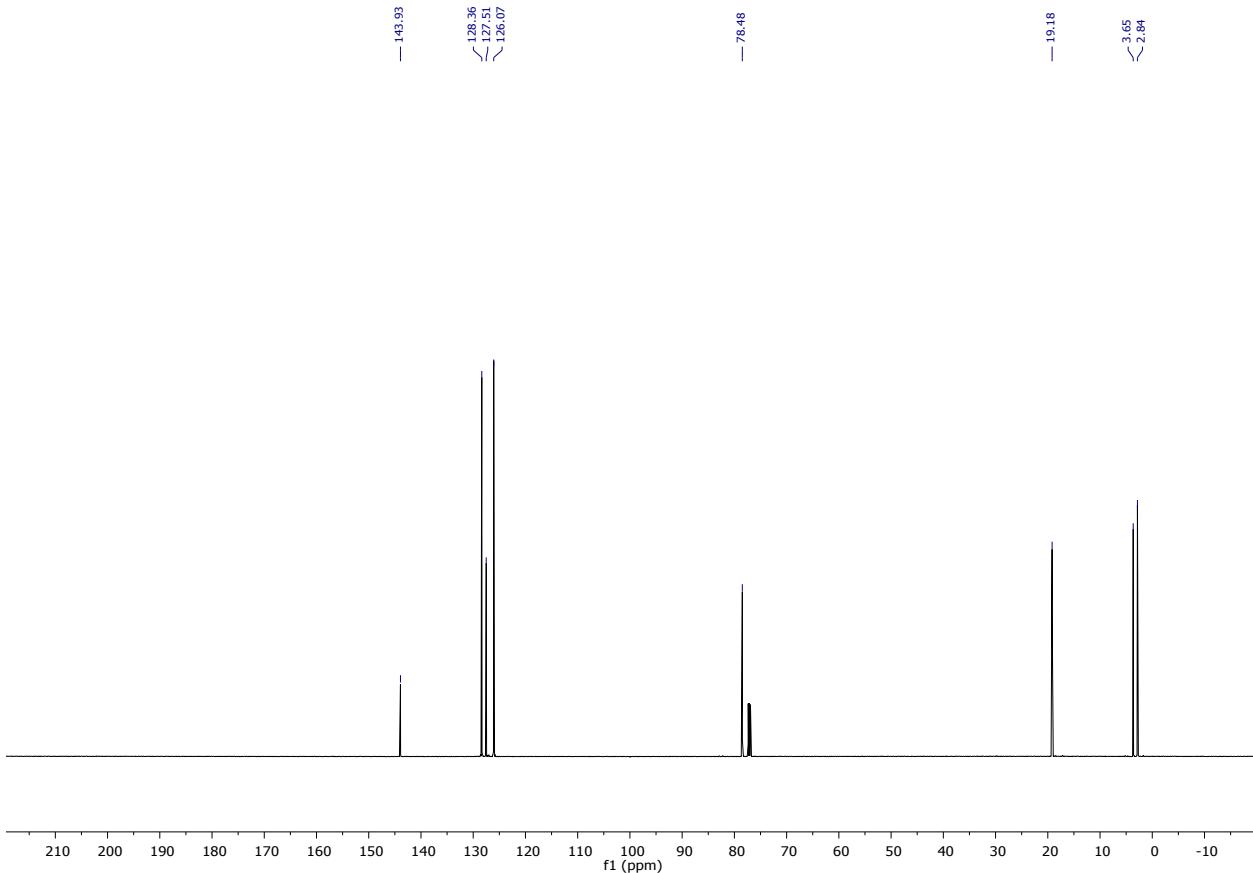


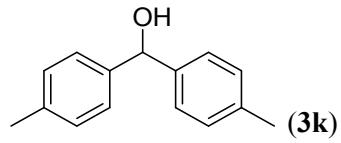


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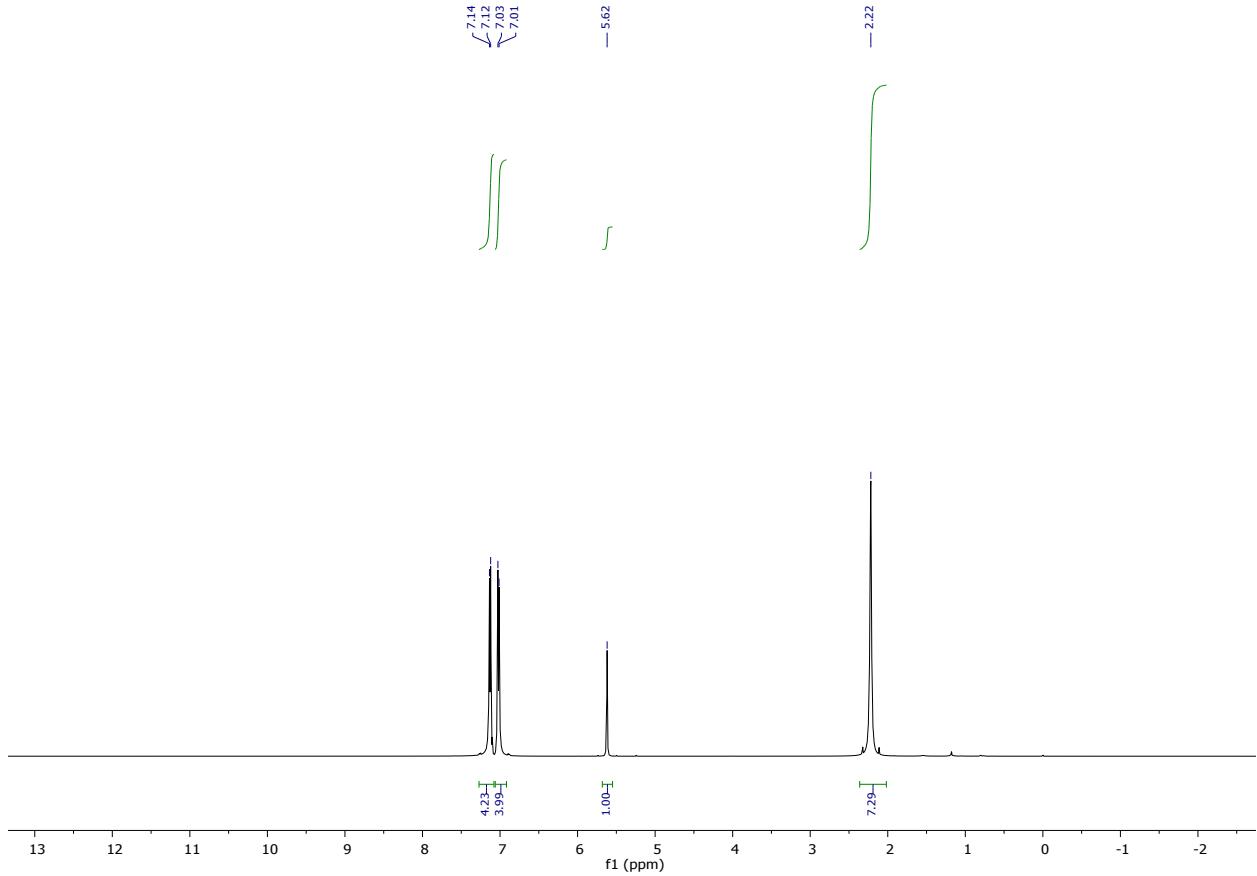


¹³C NMR (151 MHz, CDCl₃):

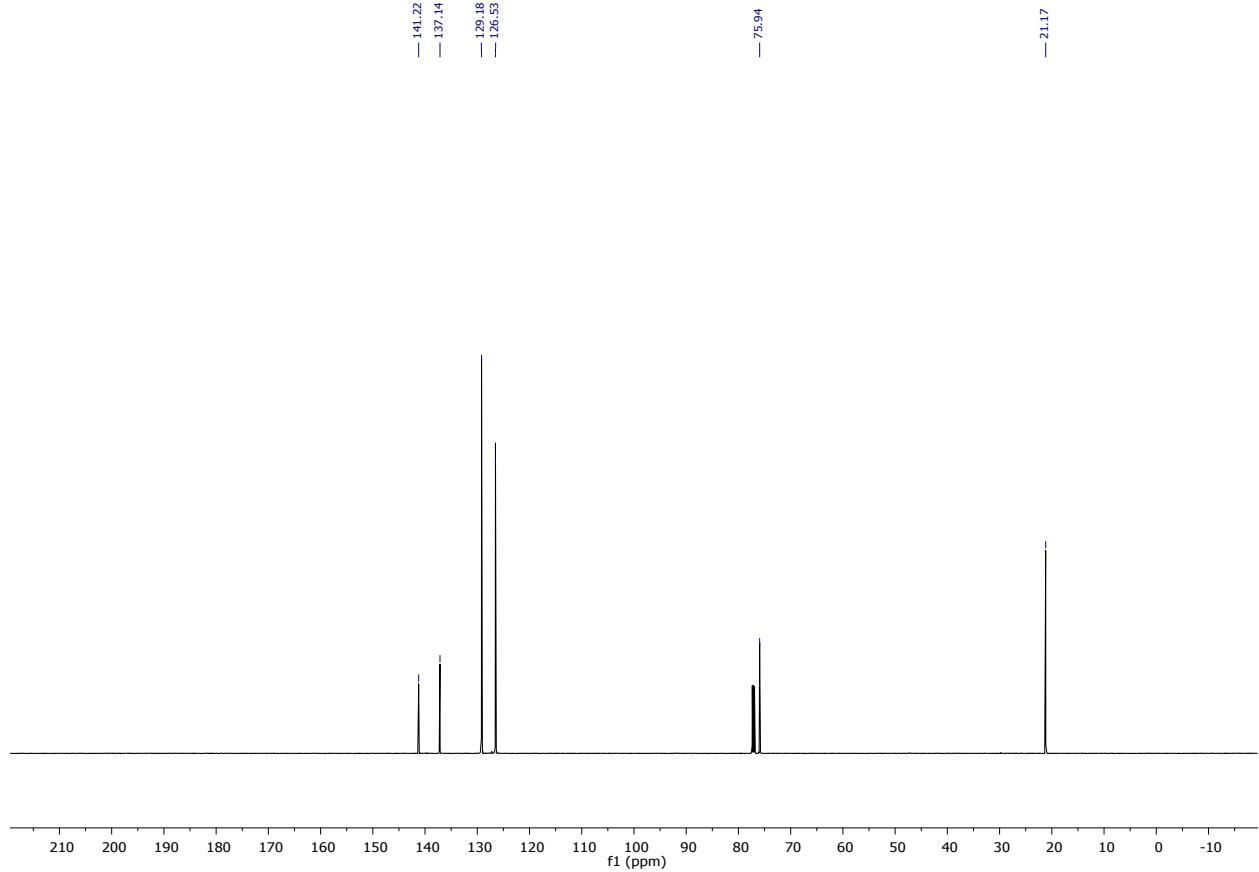


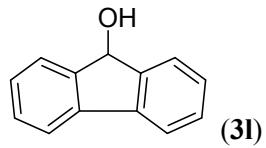


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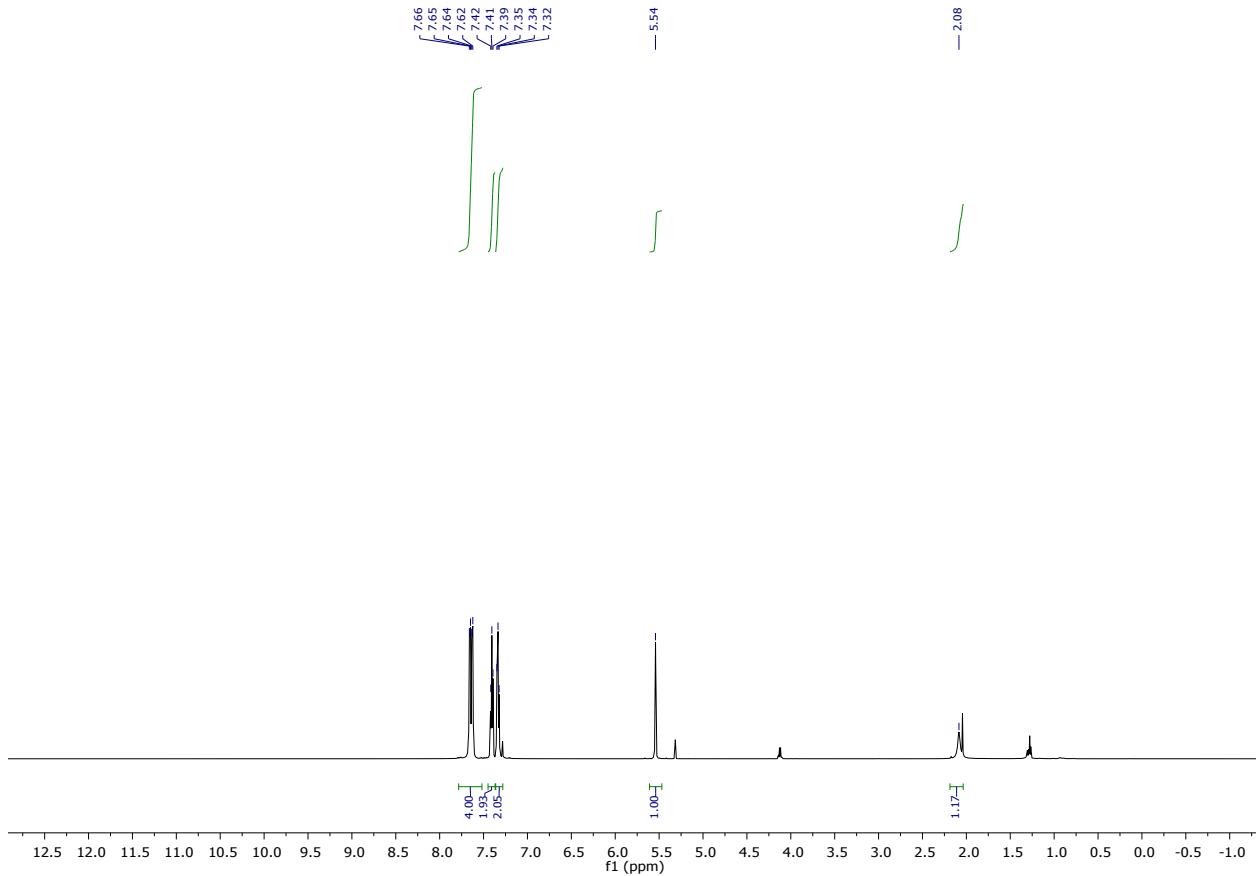


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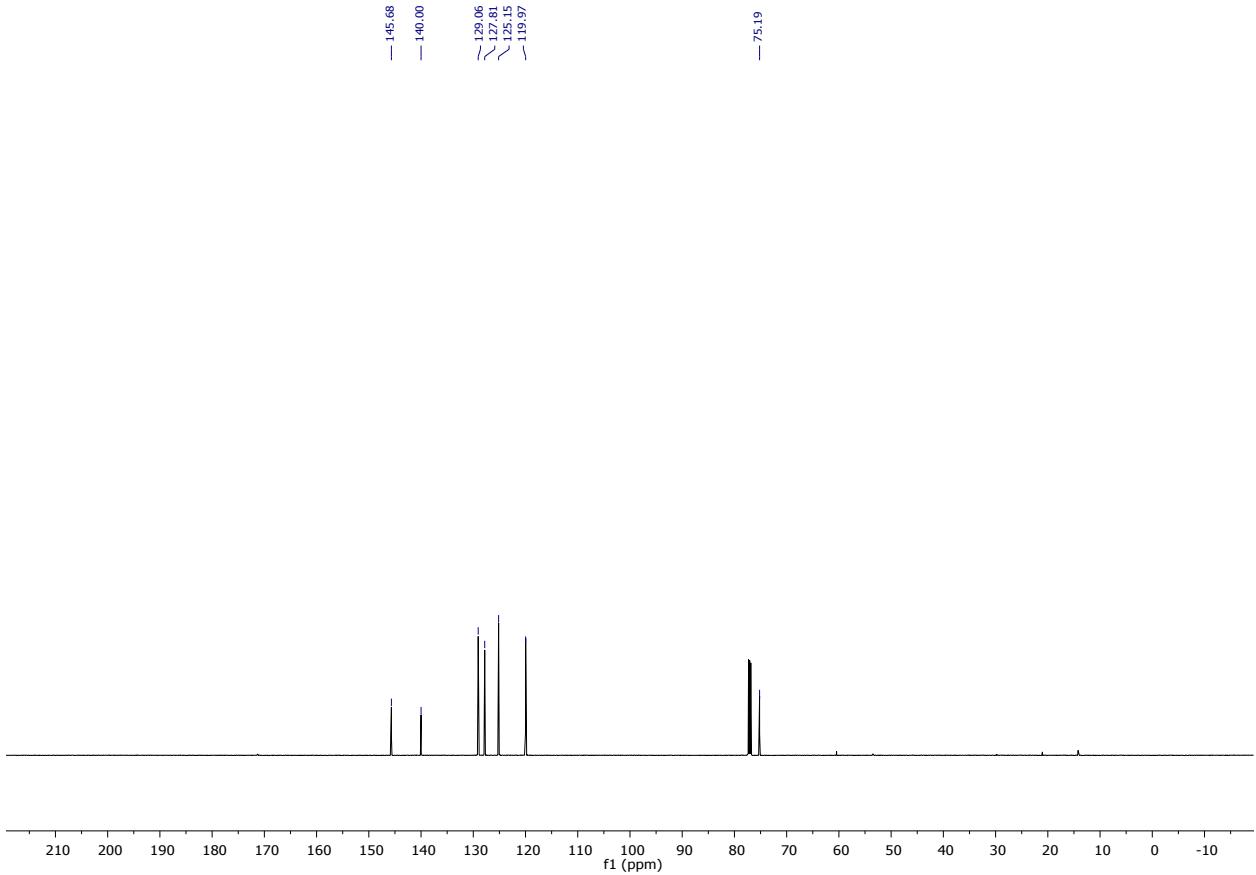


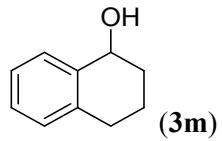


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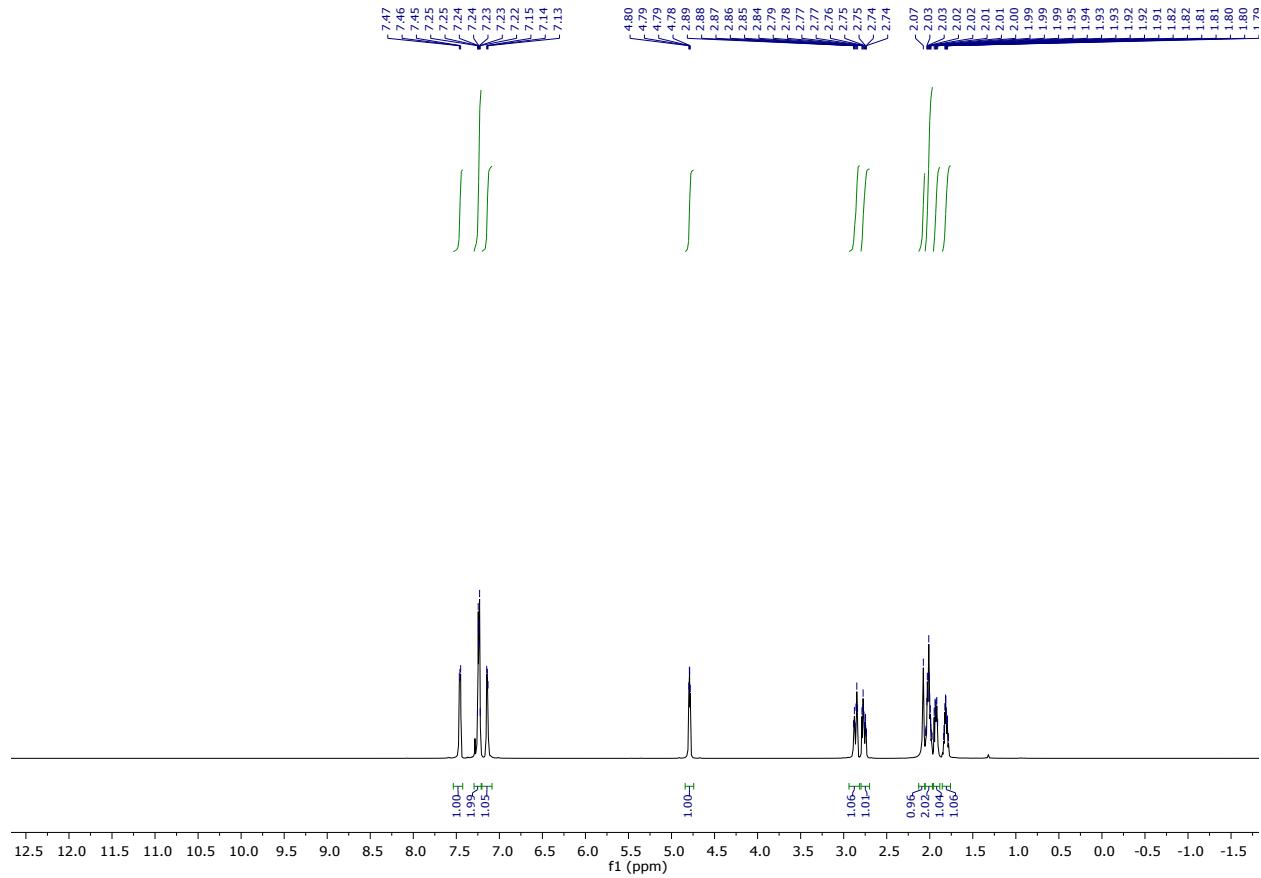


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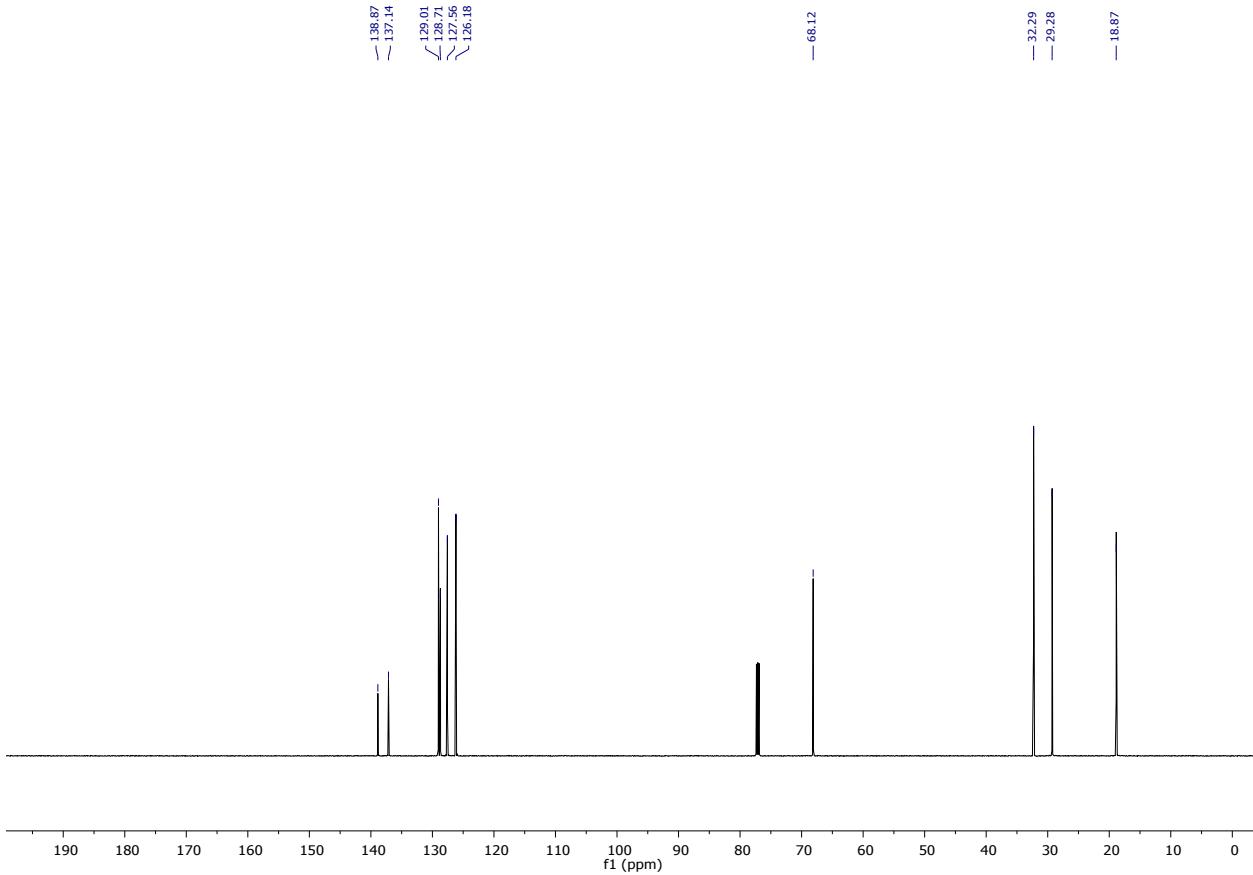


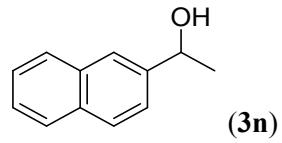


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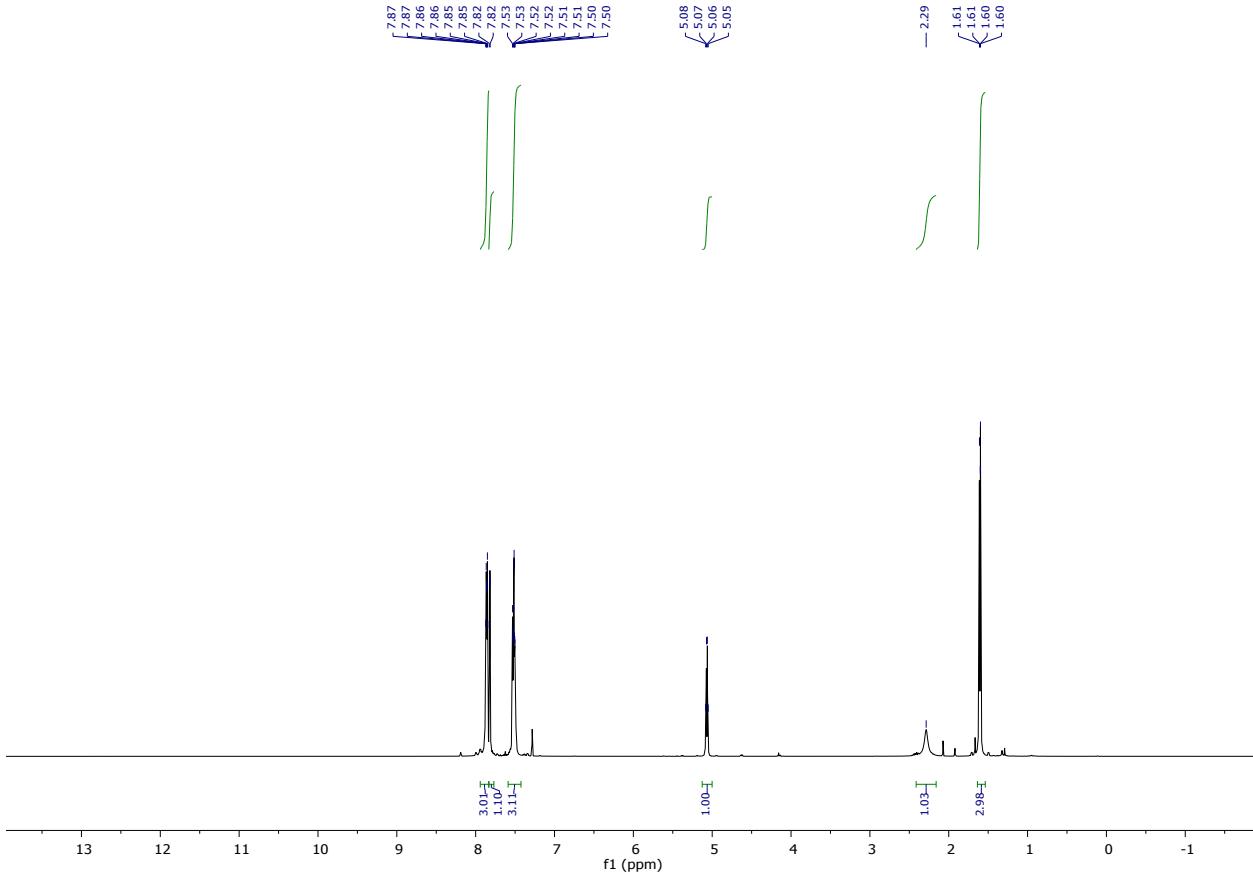


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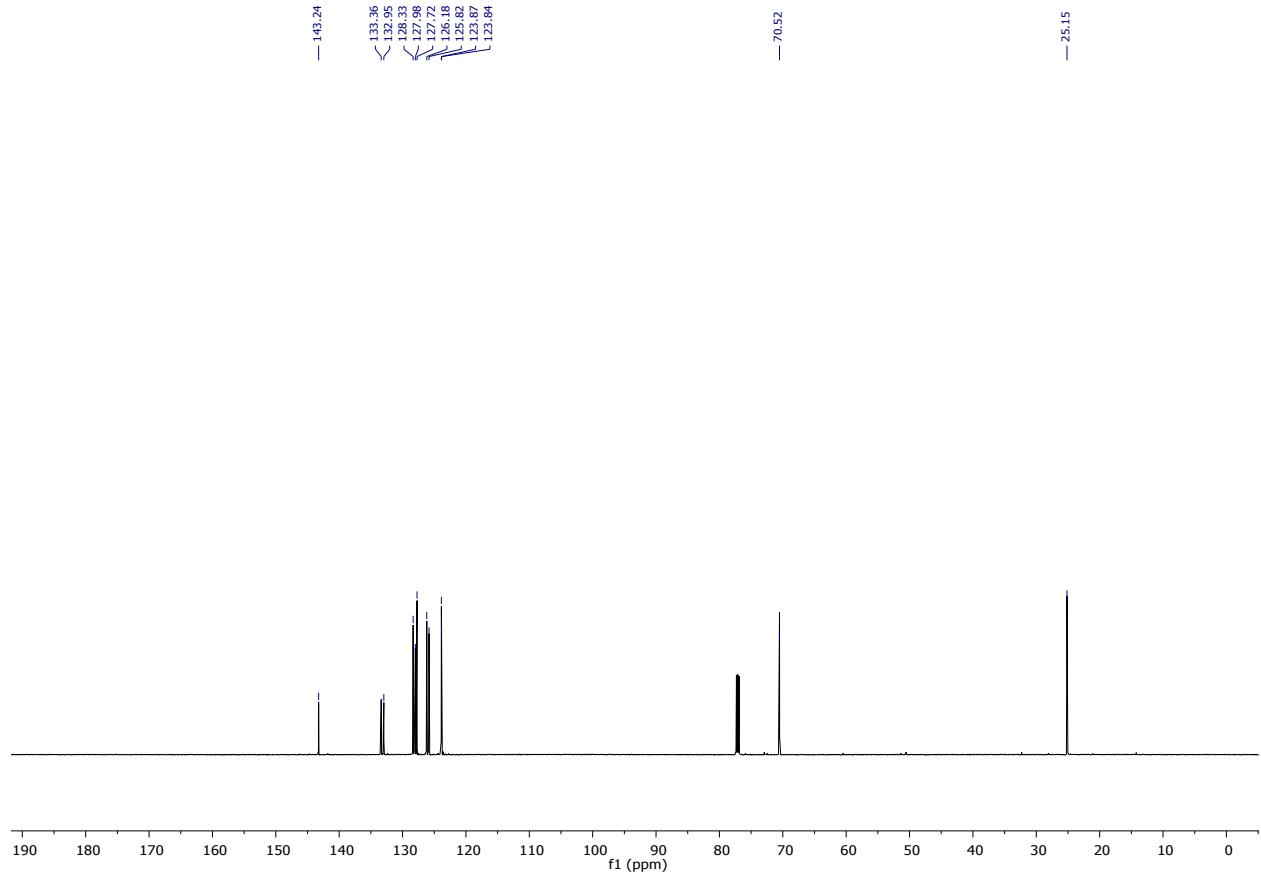


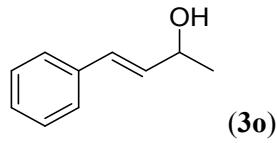


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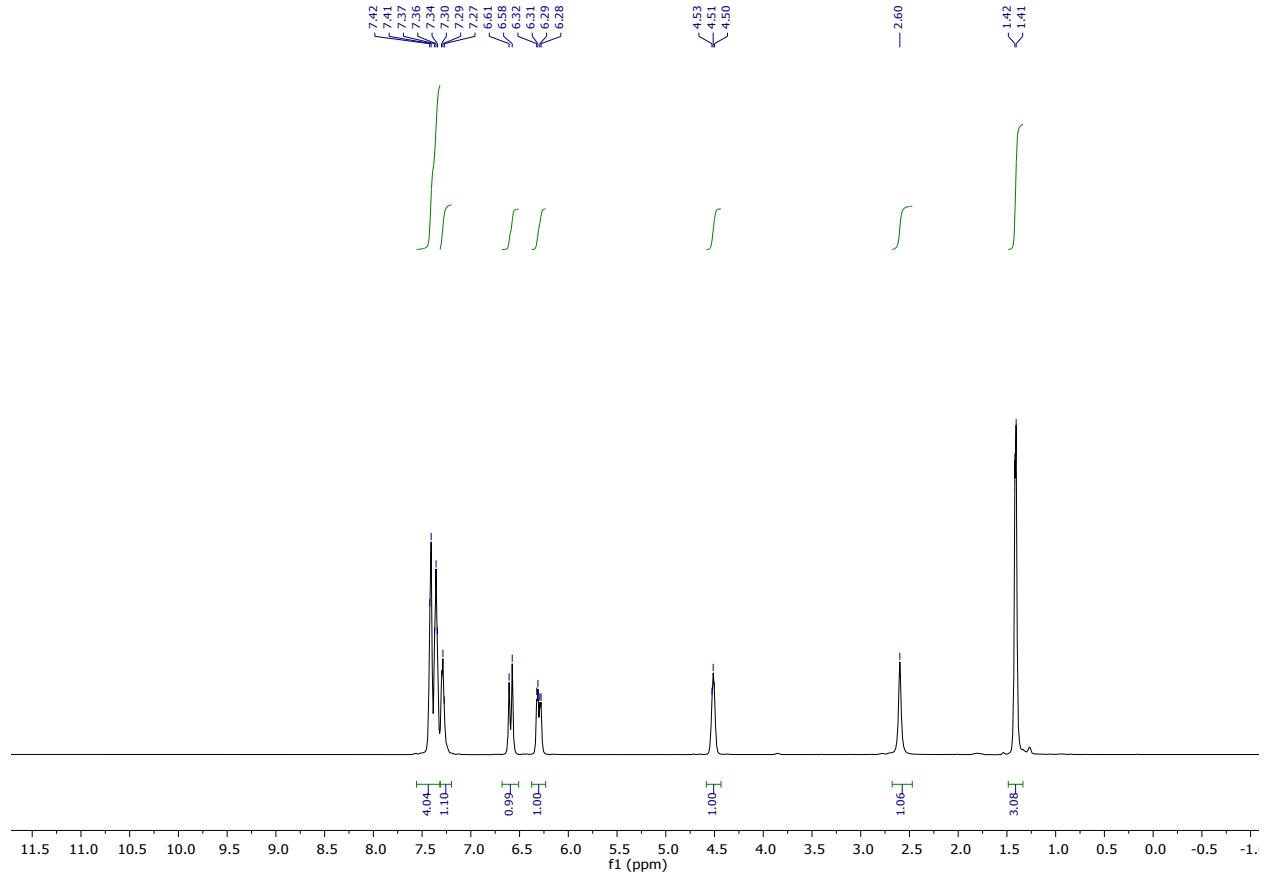


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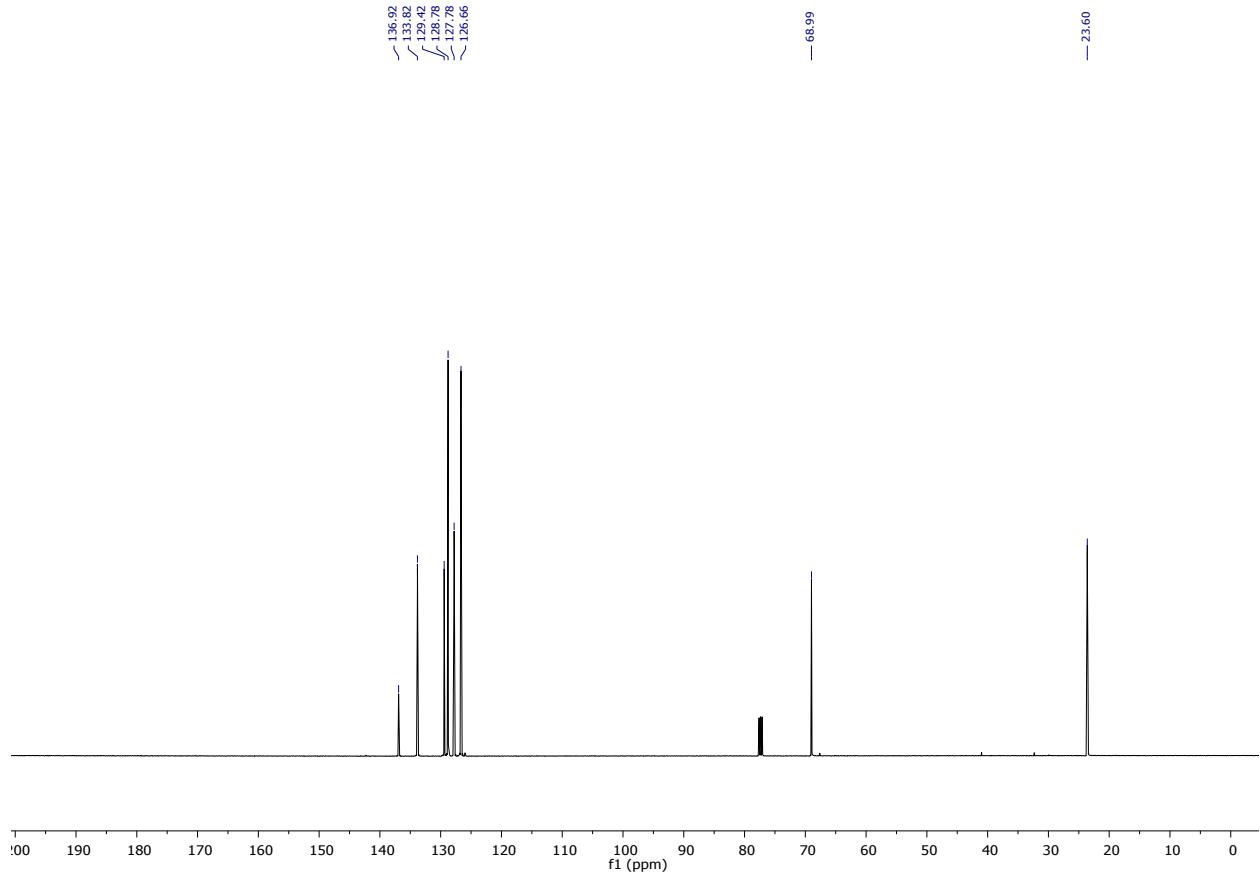


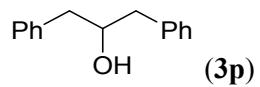


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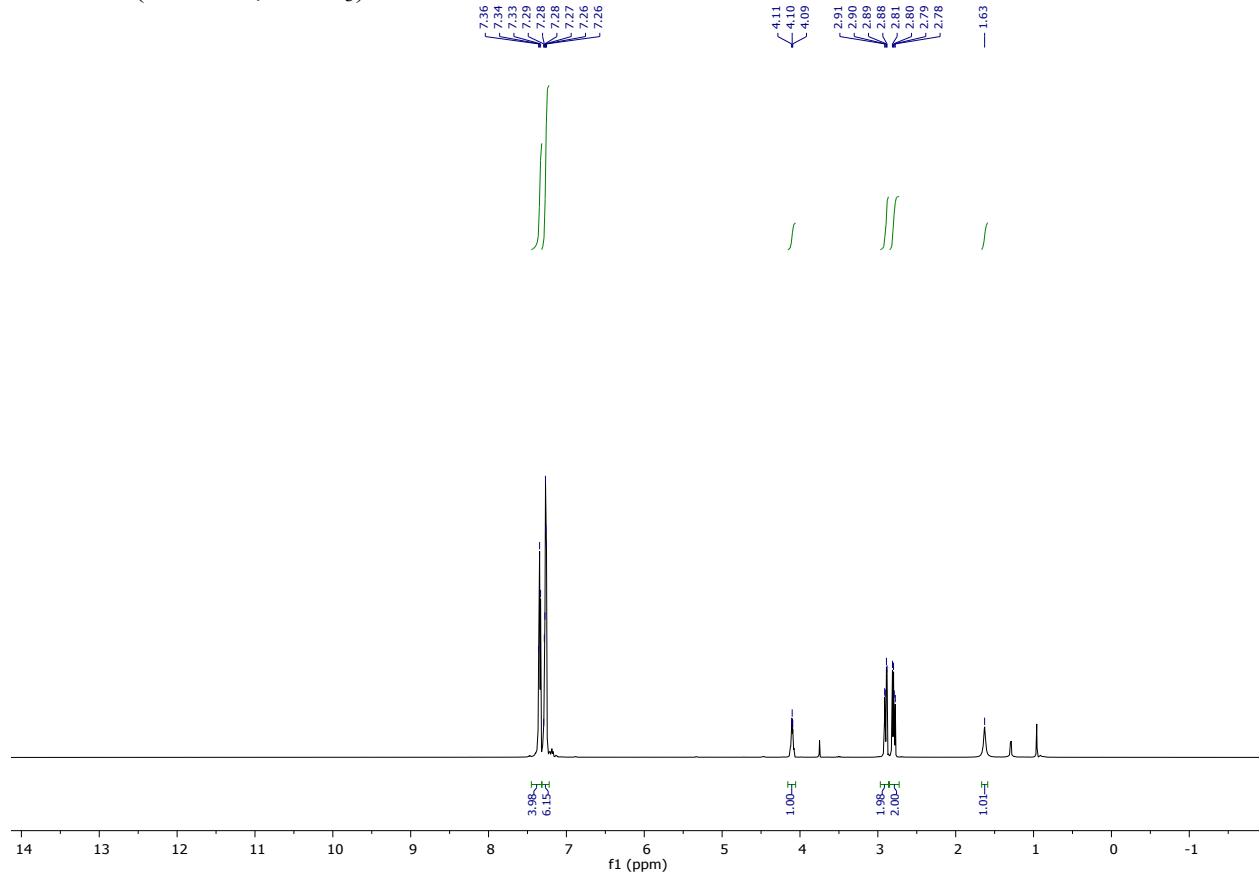


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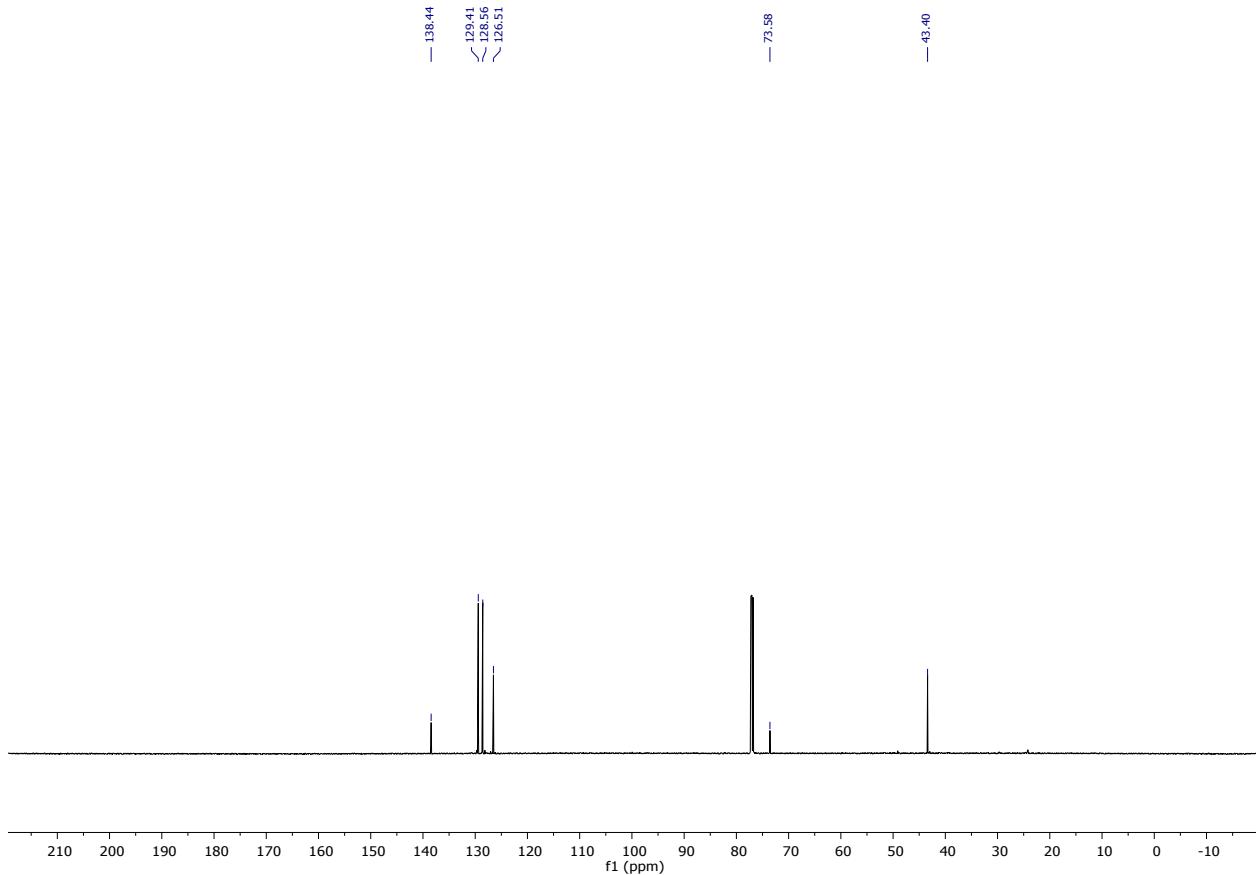


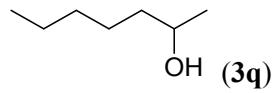


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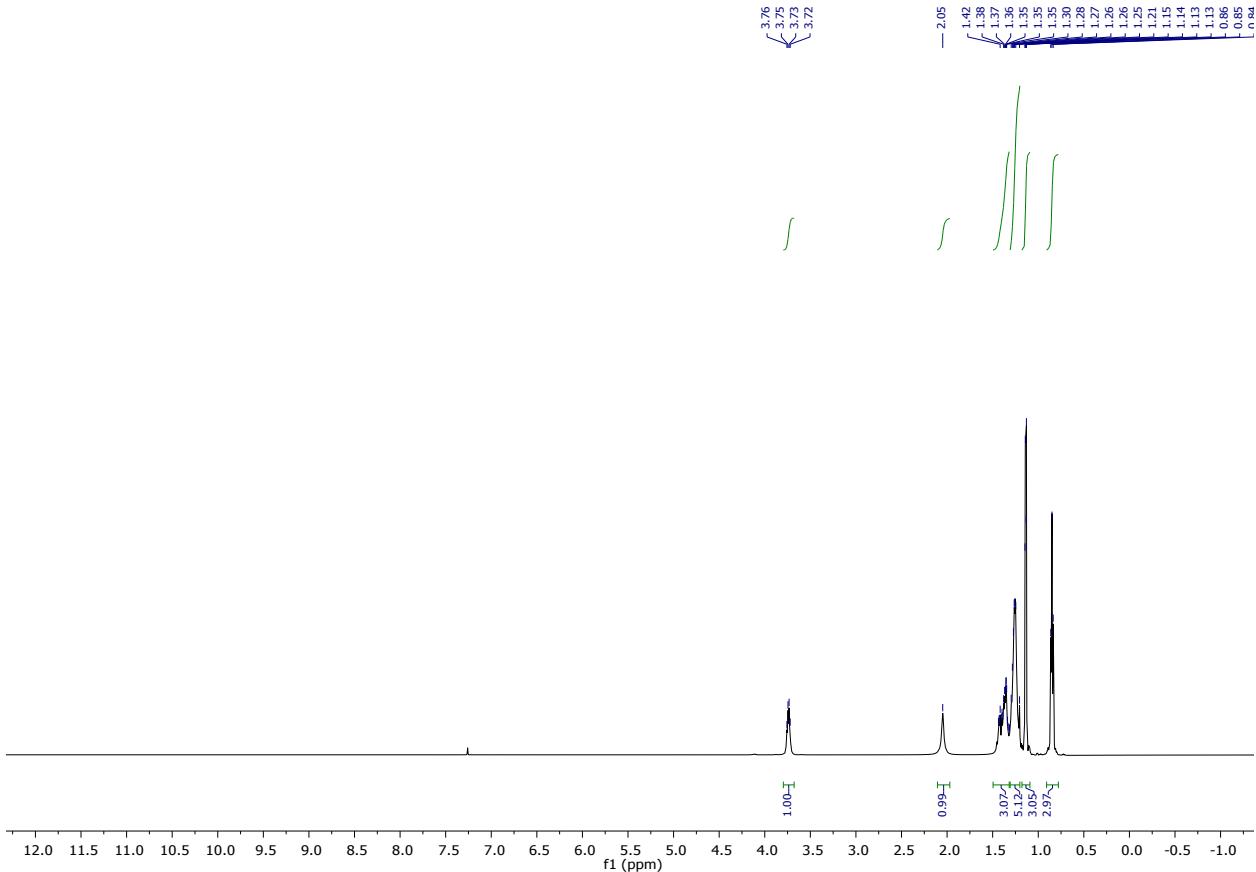


¹³C NMR (151 MHz, CDCl₃):

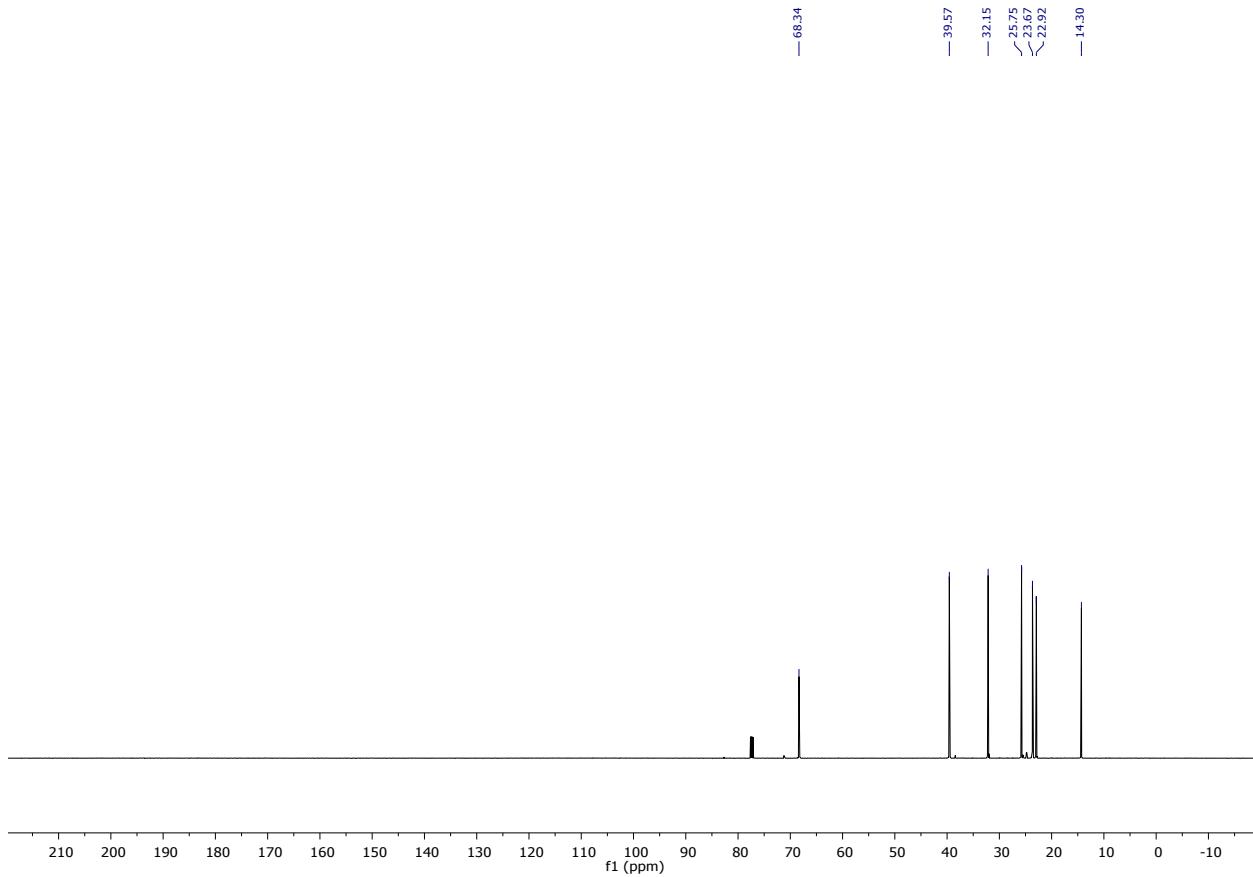


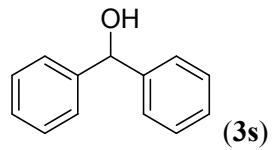


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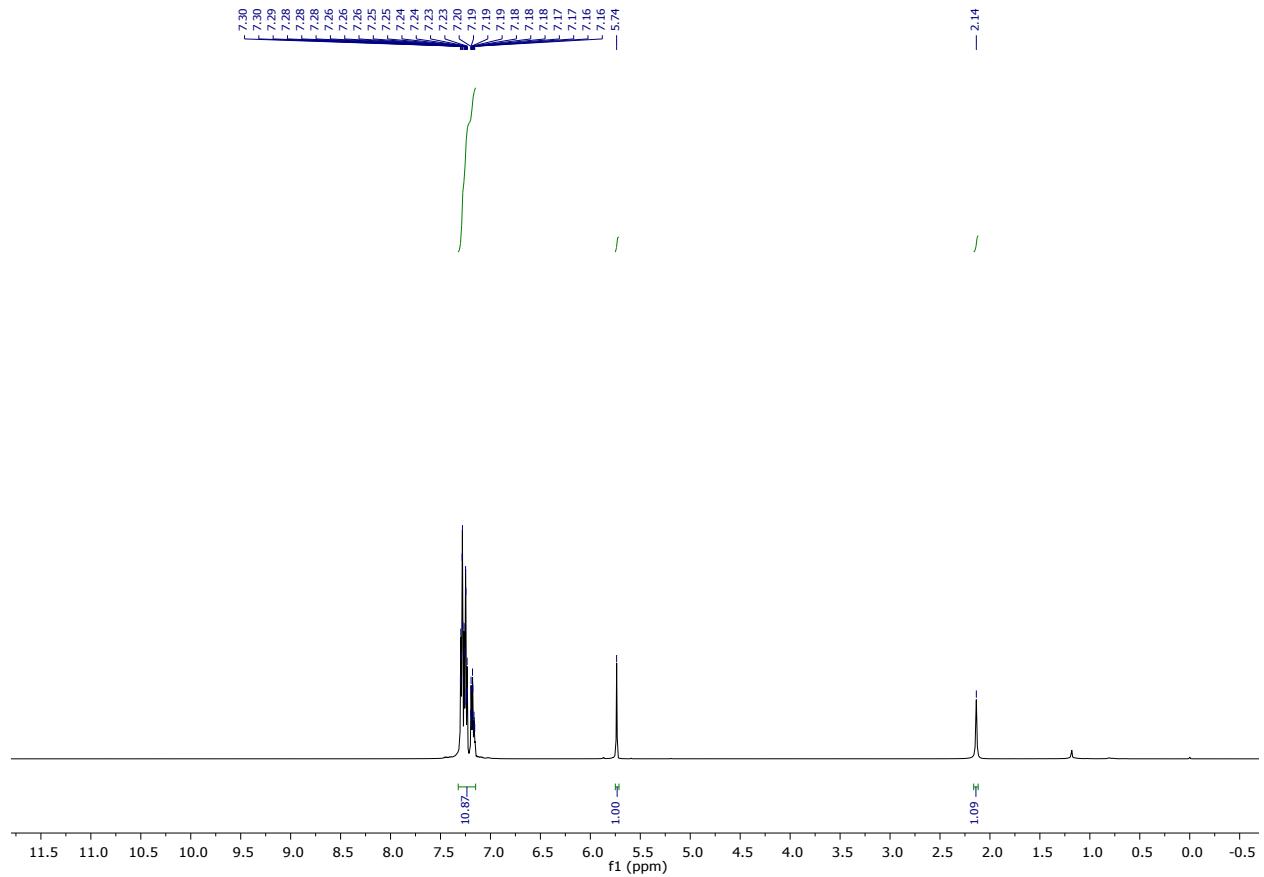


¹³C NMR (126 MHz, CDCl₃):

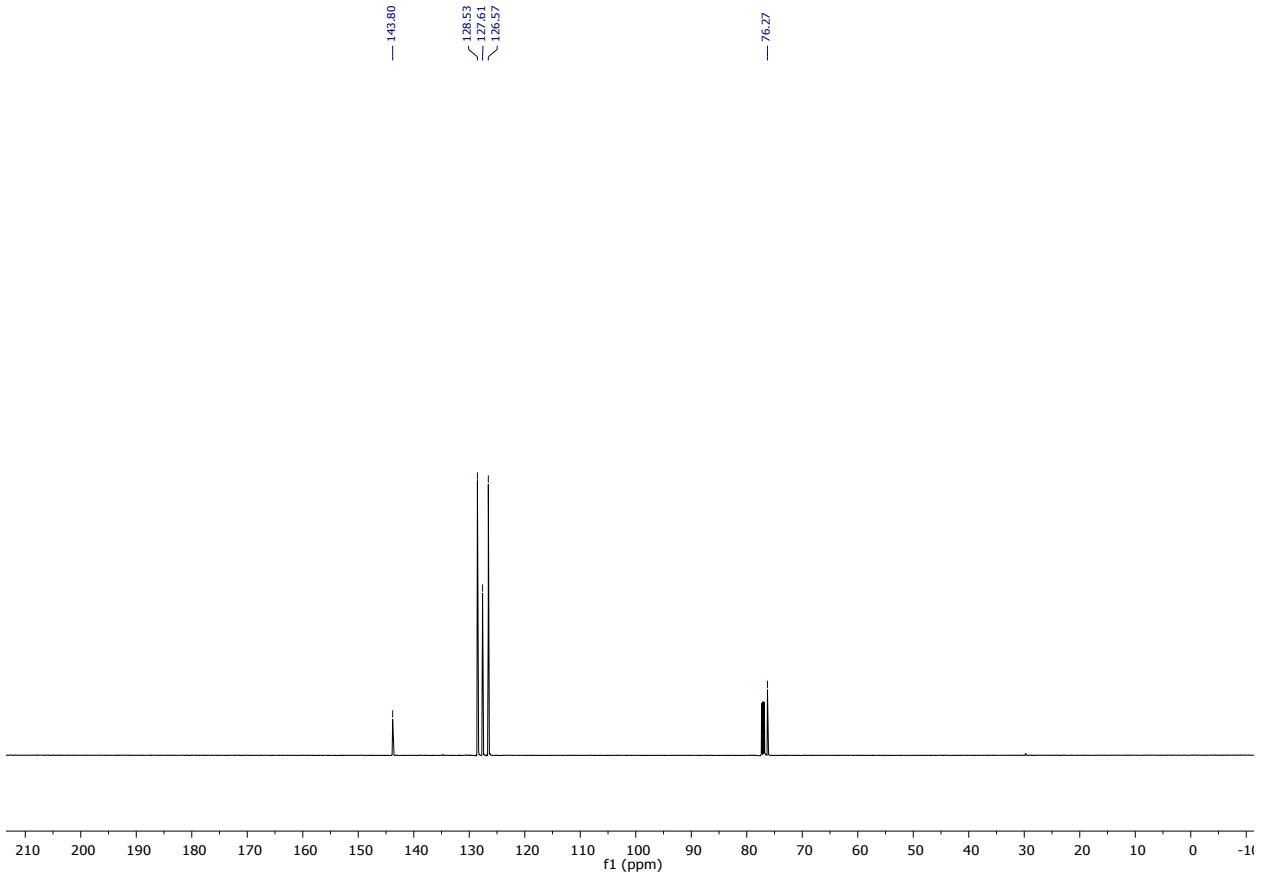


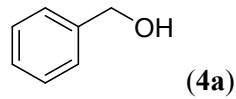


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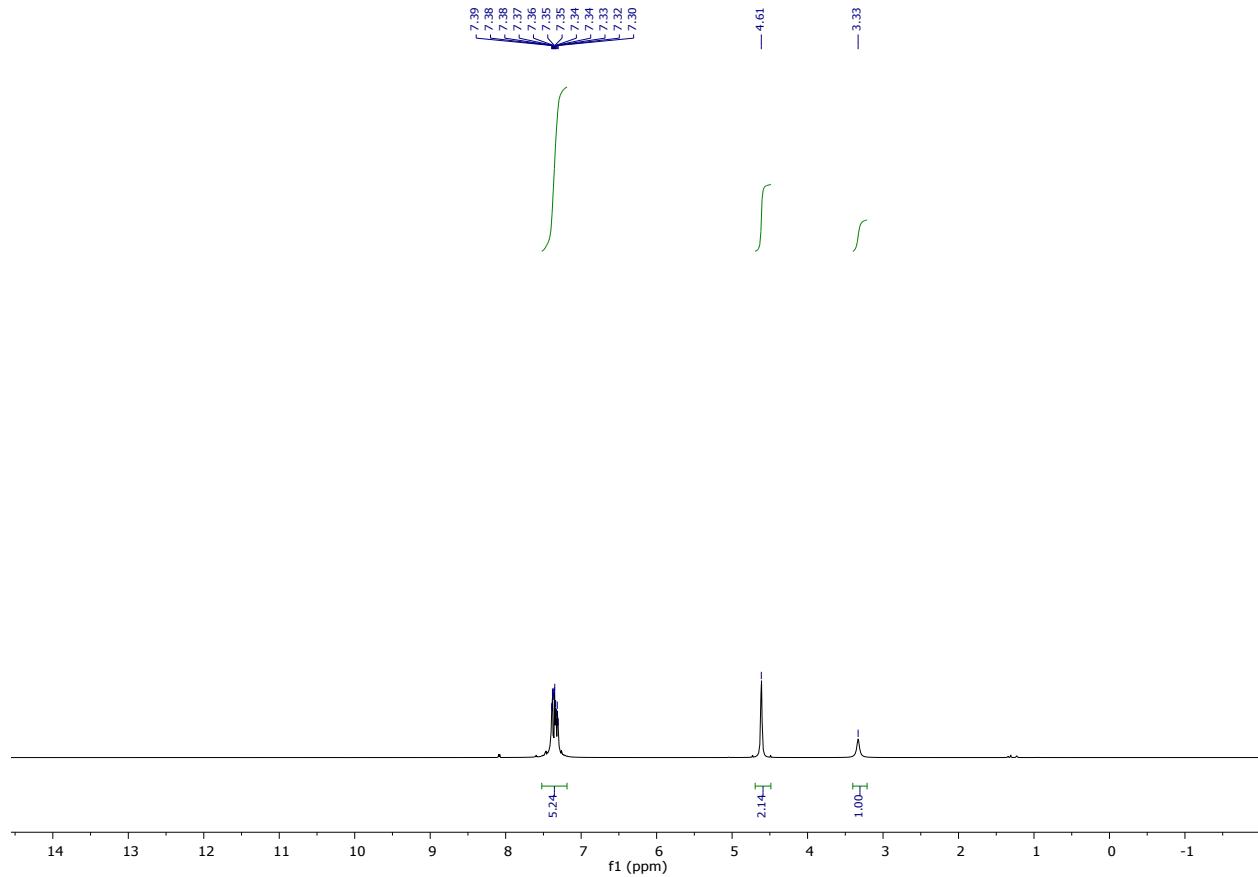


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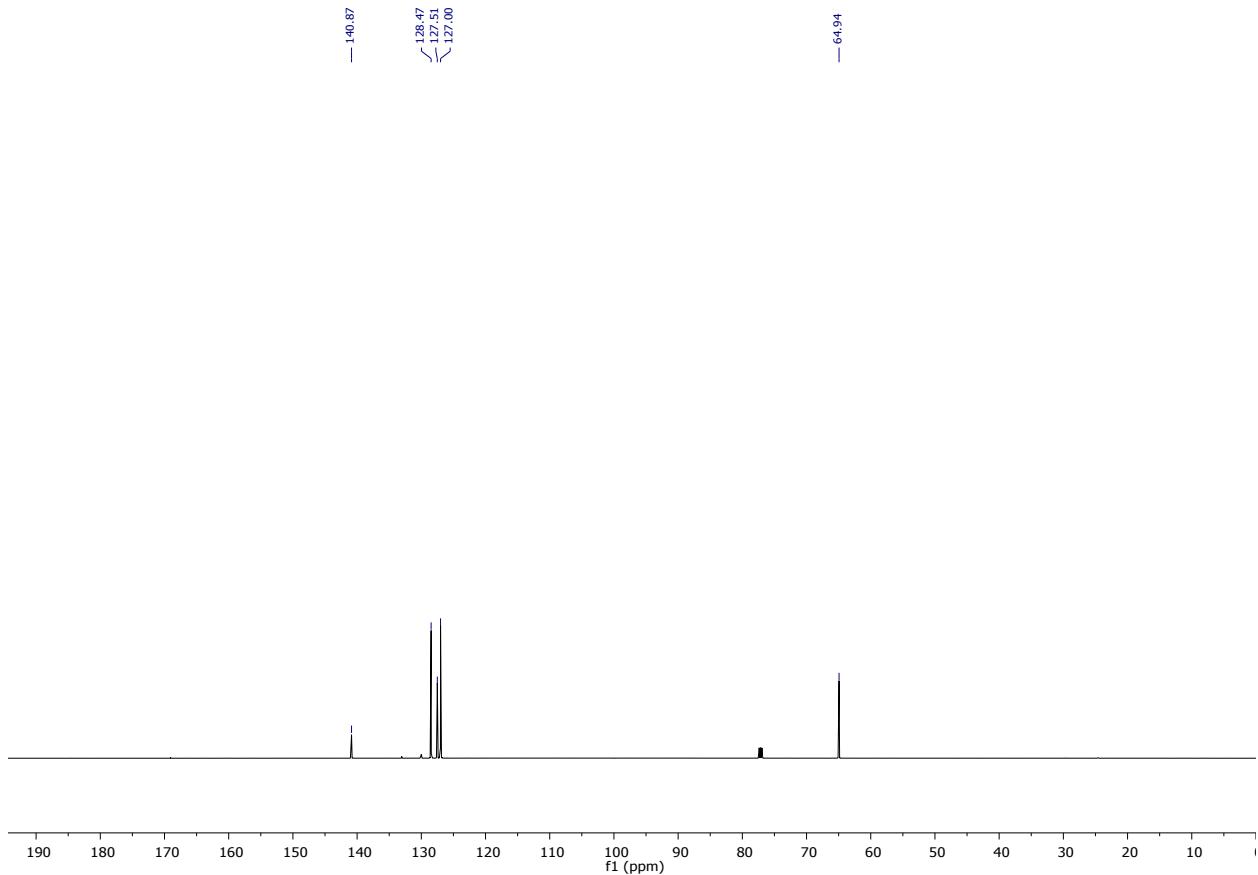


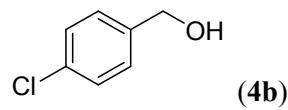


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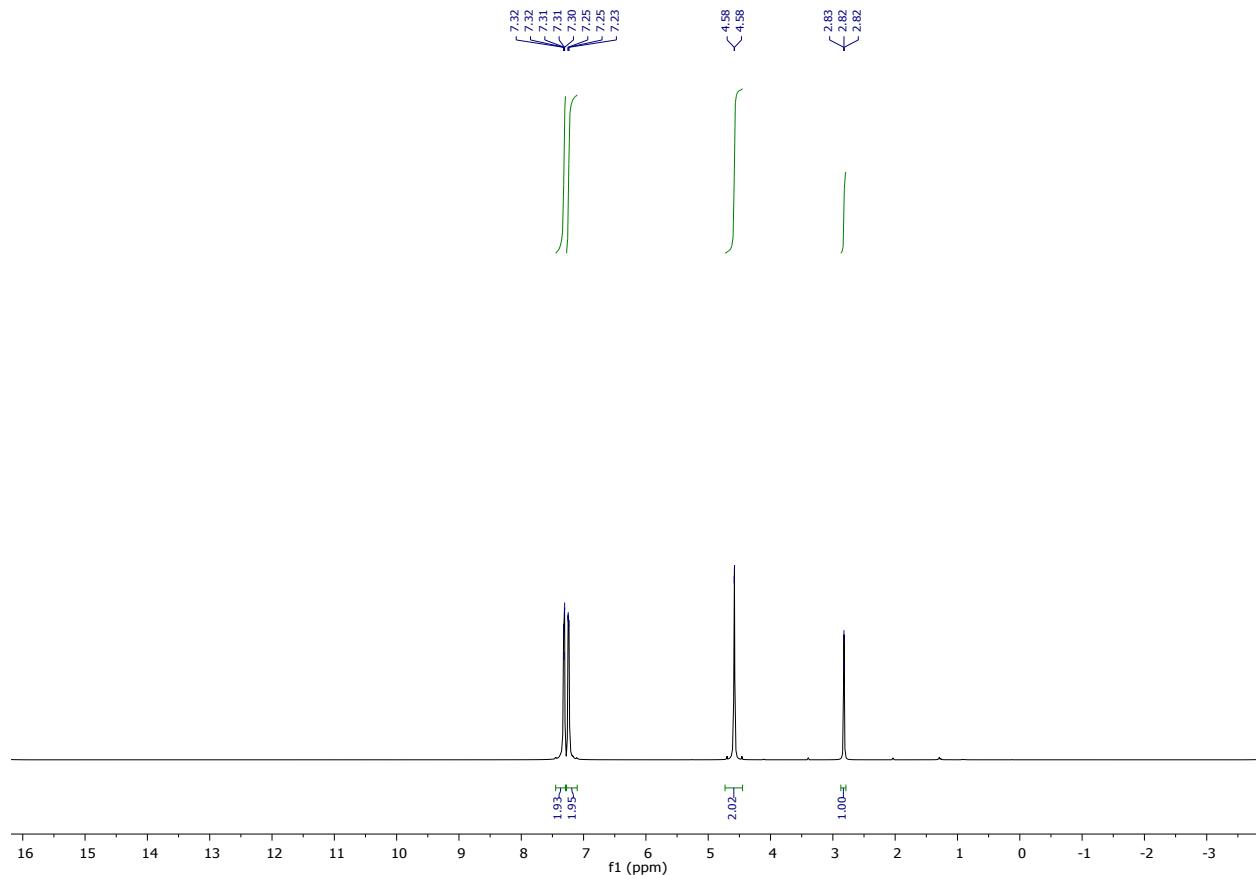


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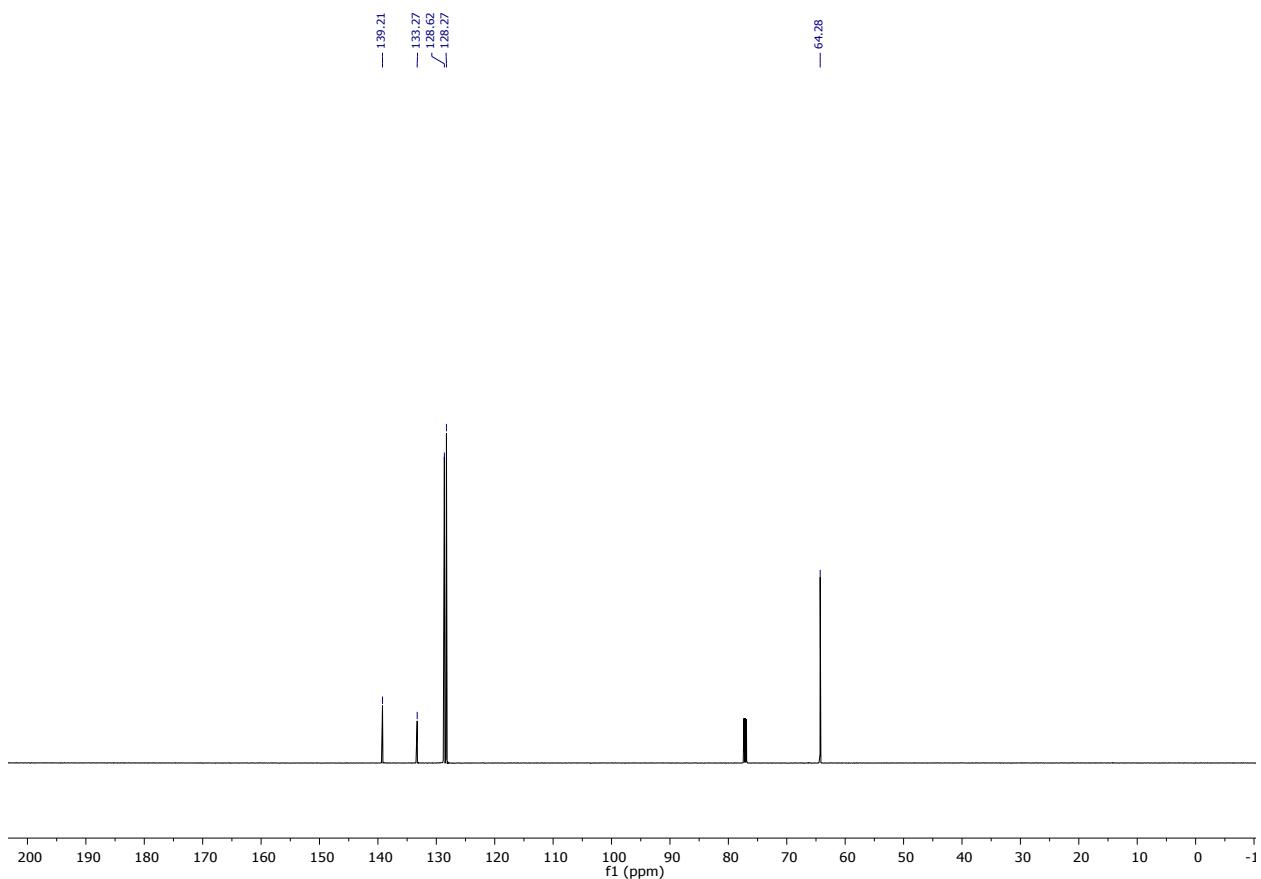


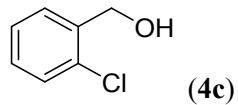


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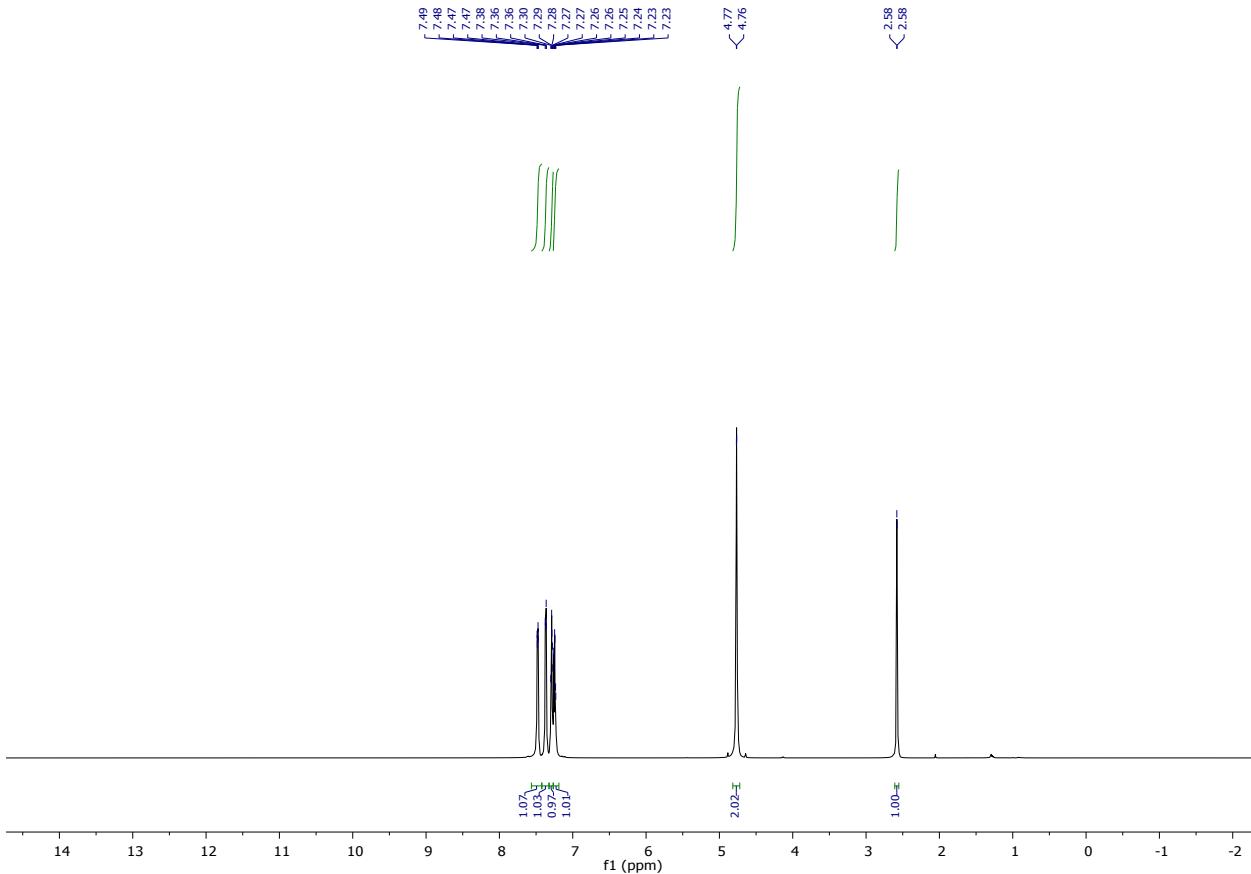


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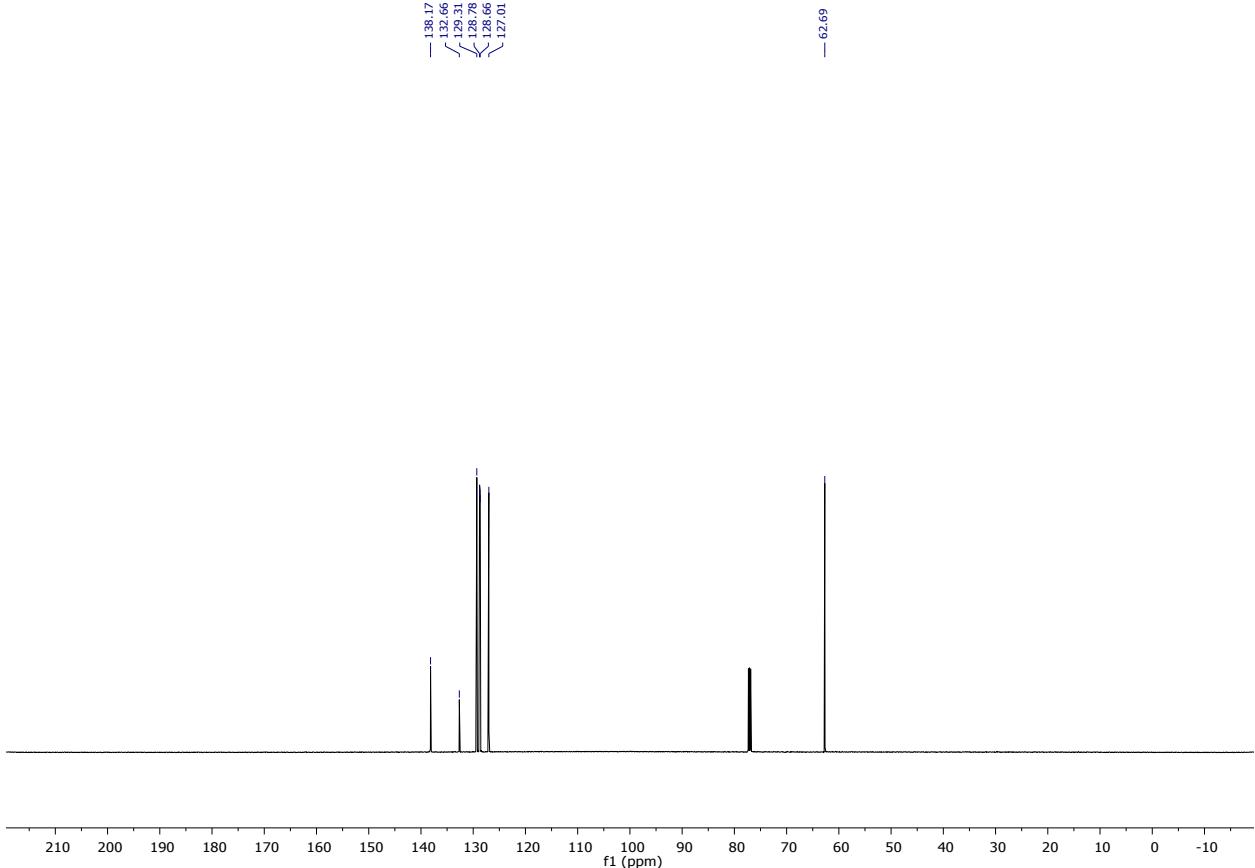


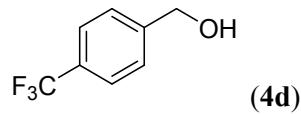


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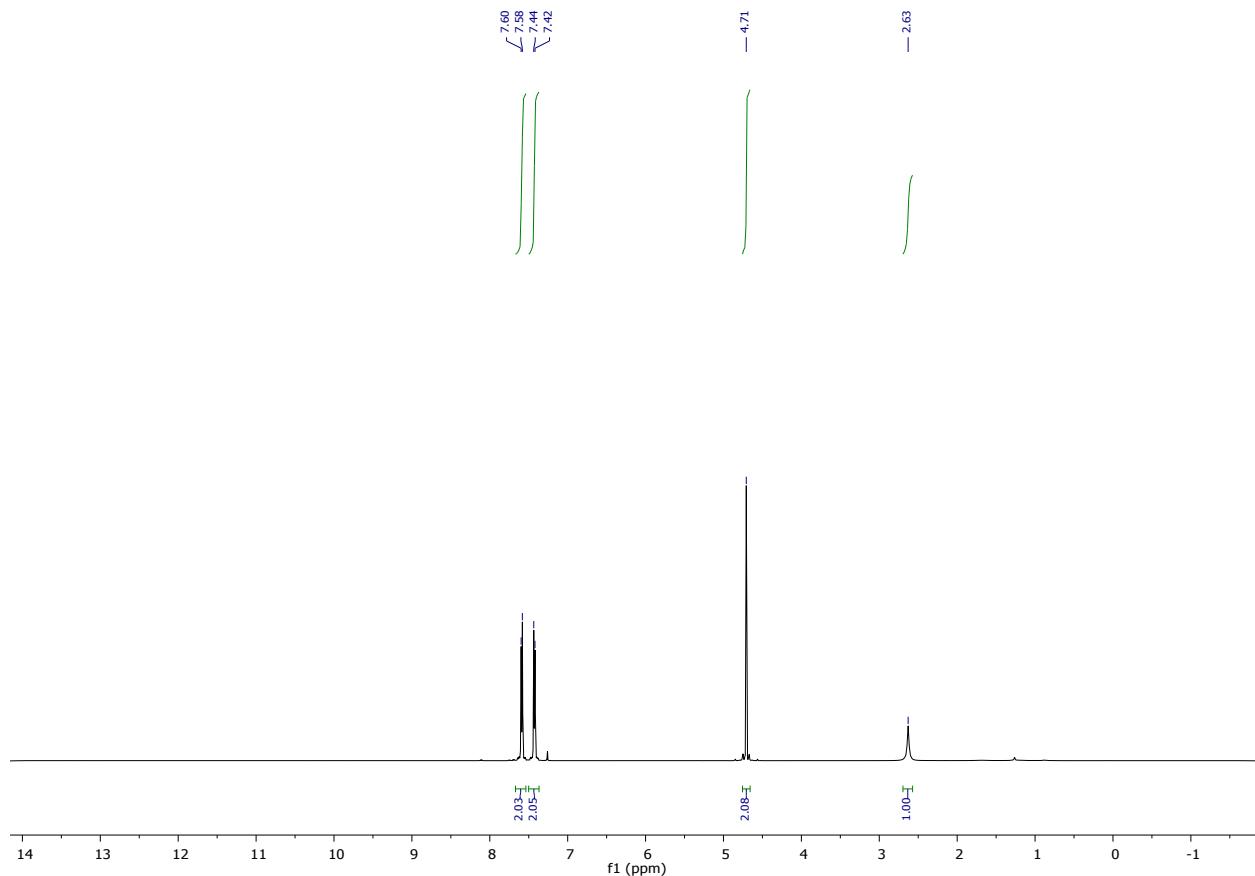


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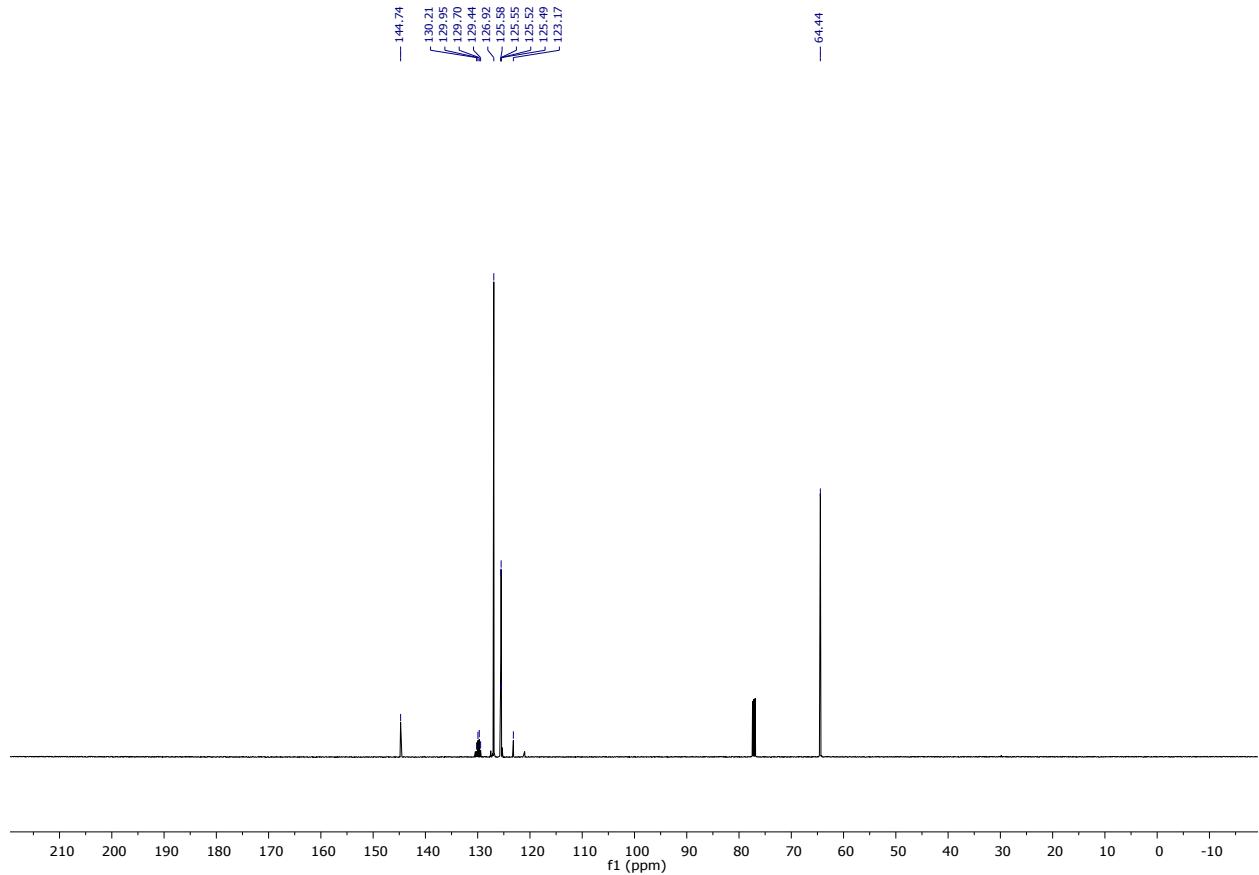


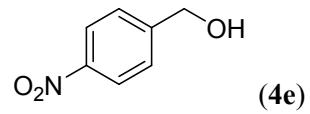


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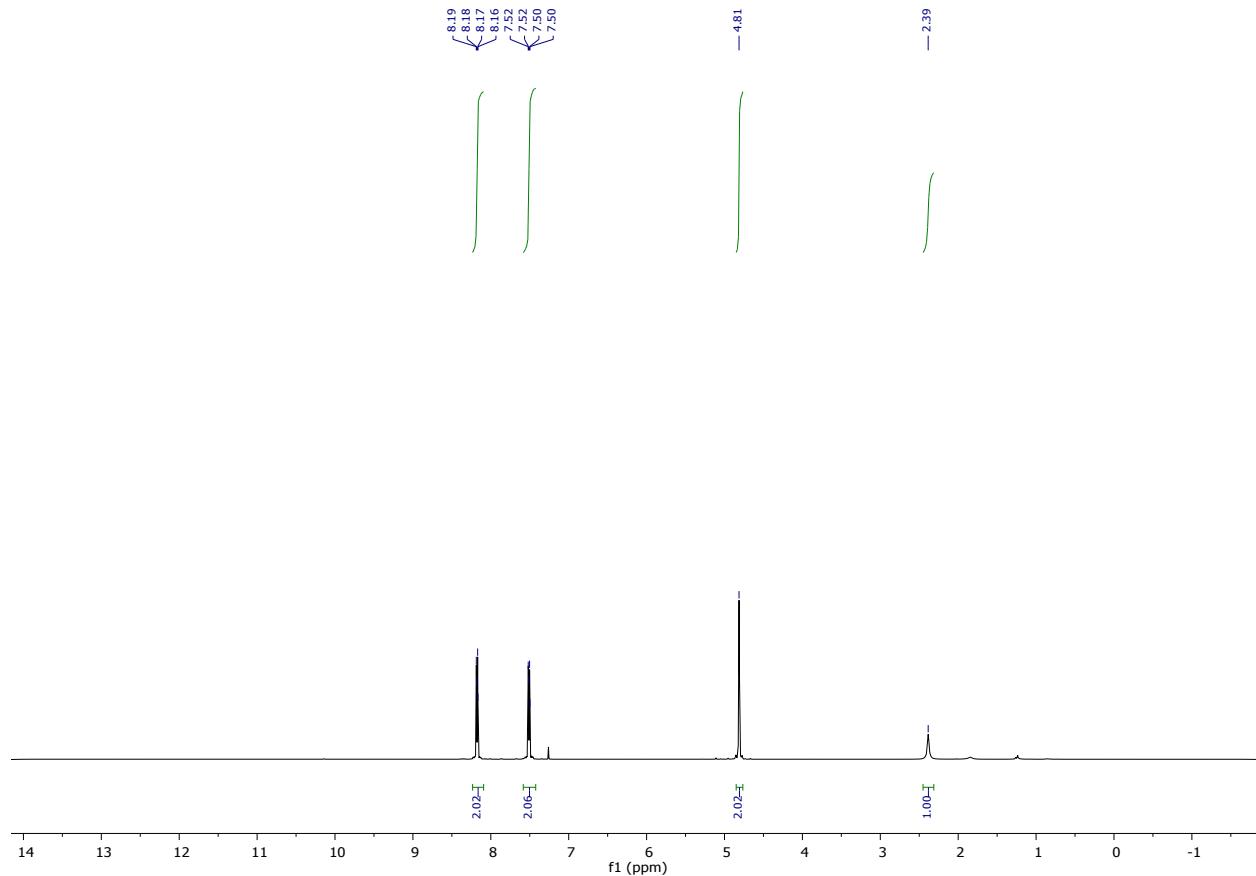


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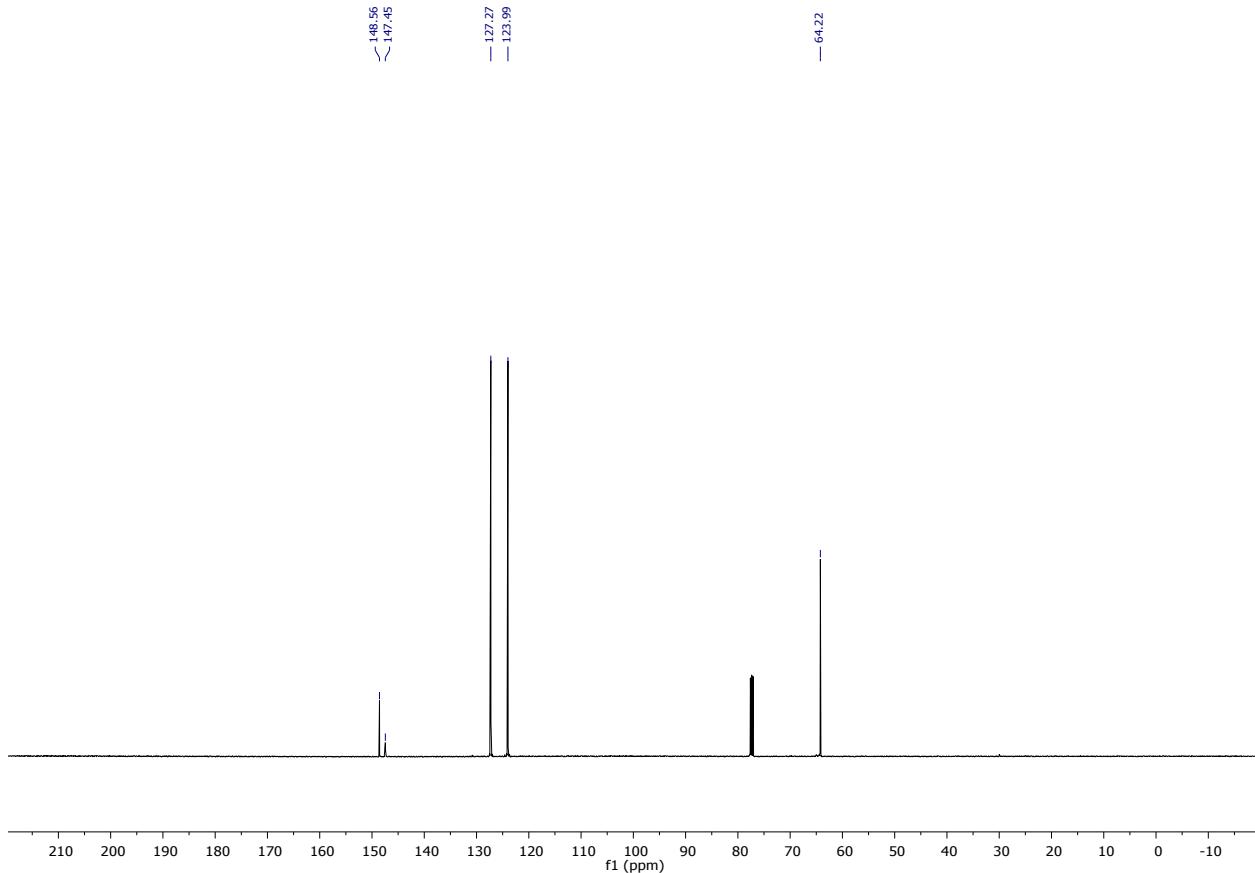


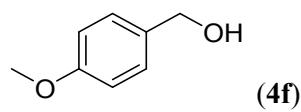


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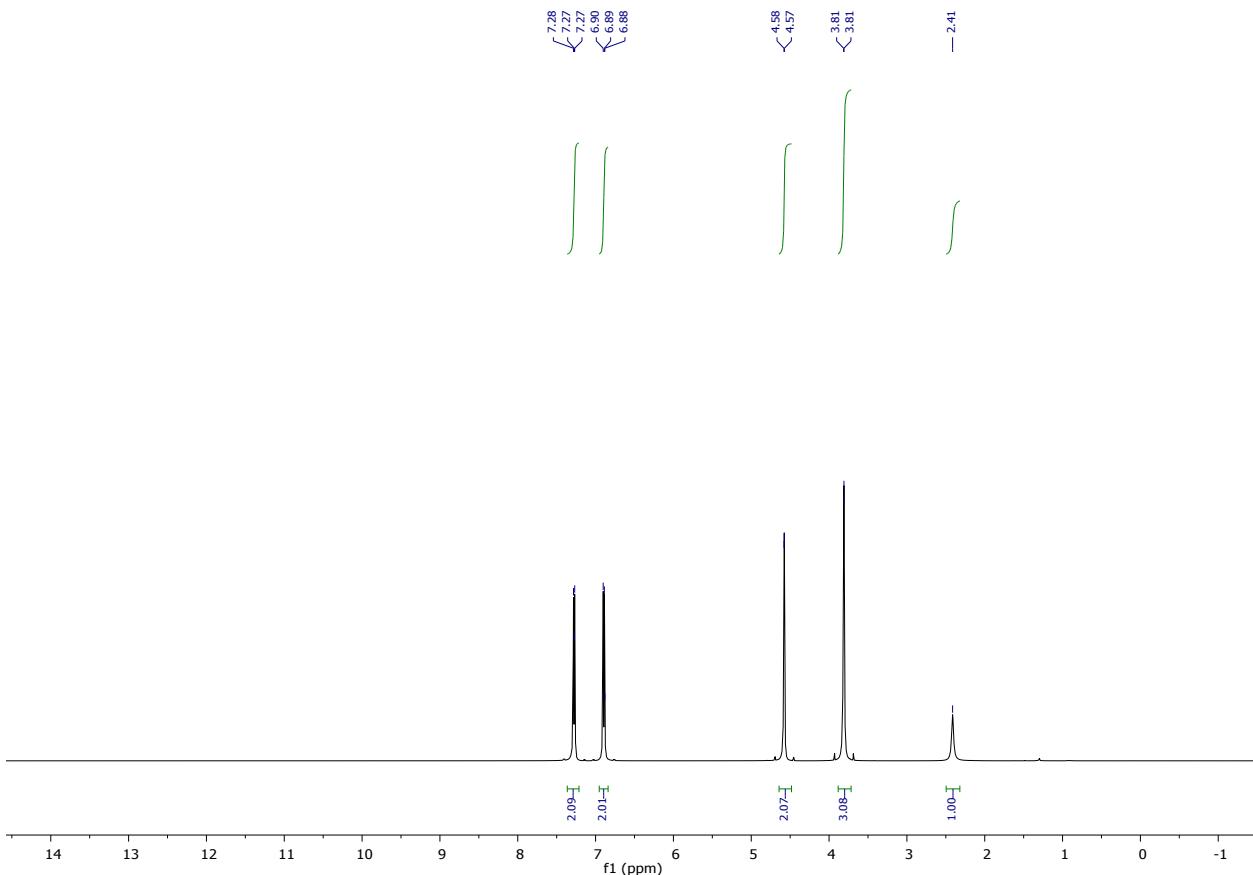


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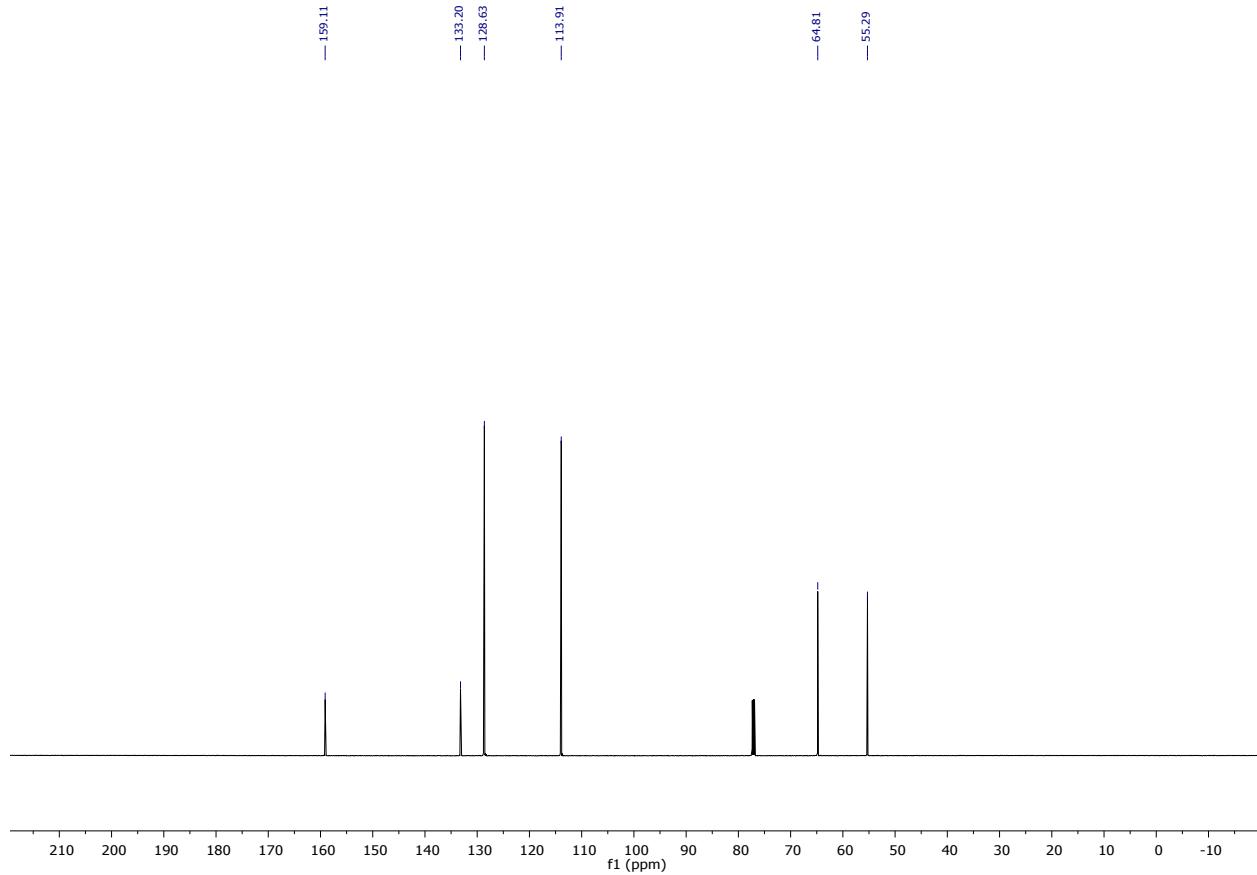


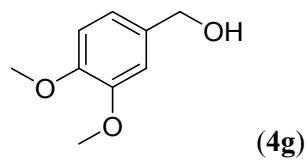


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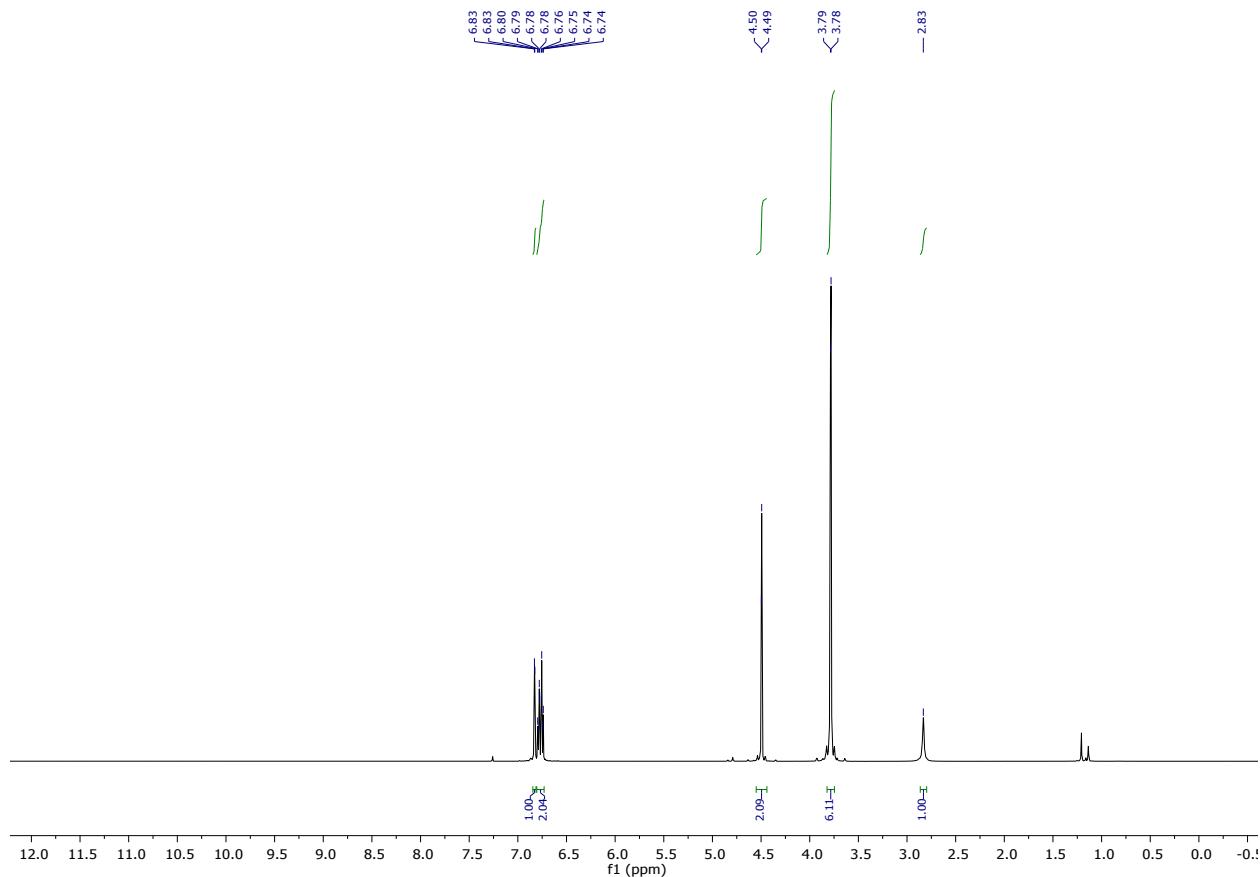


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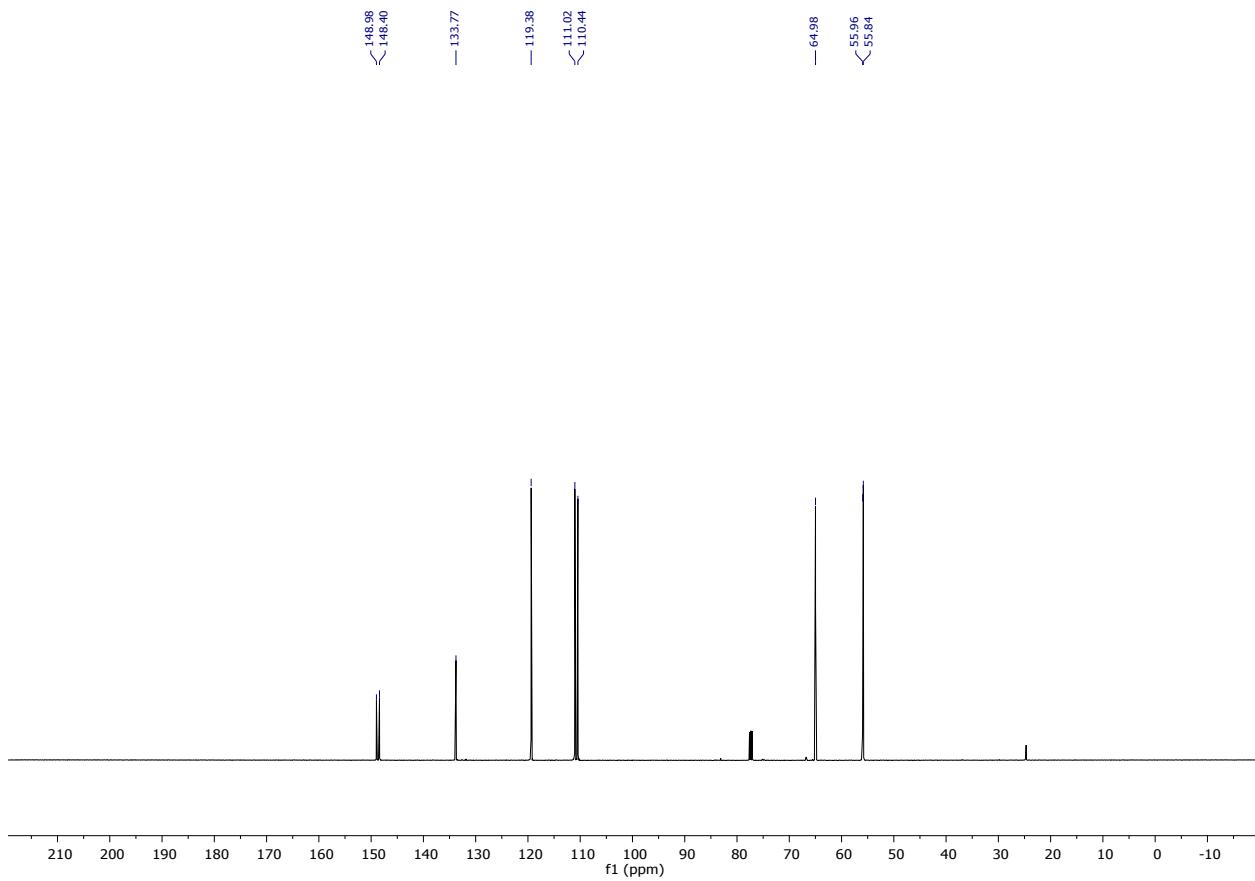


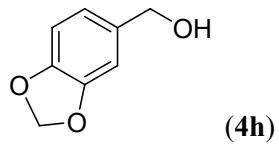


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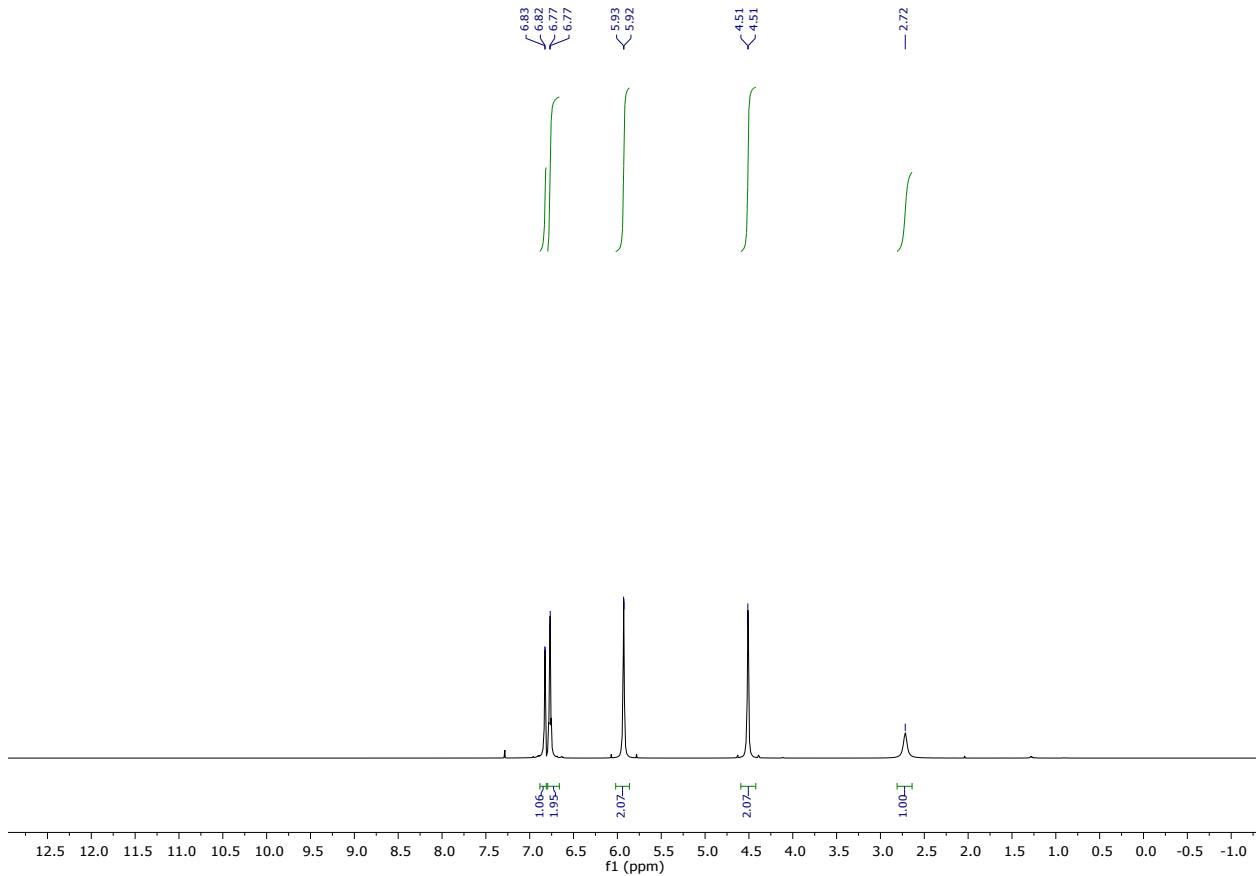


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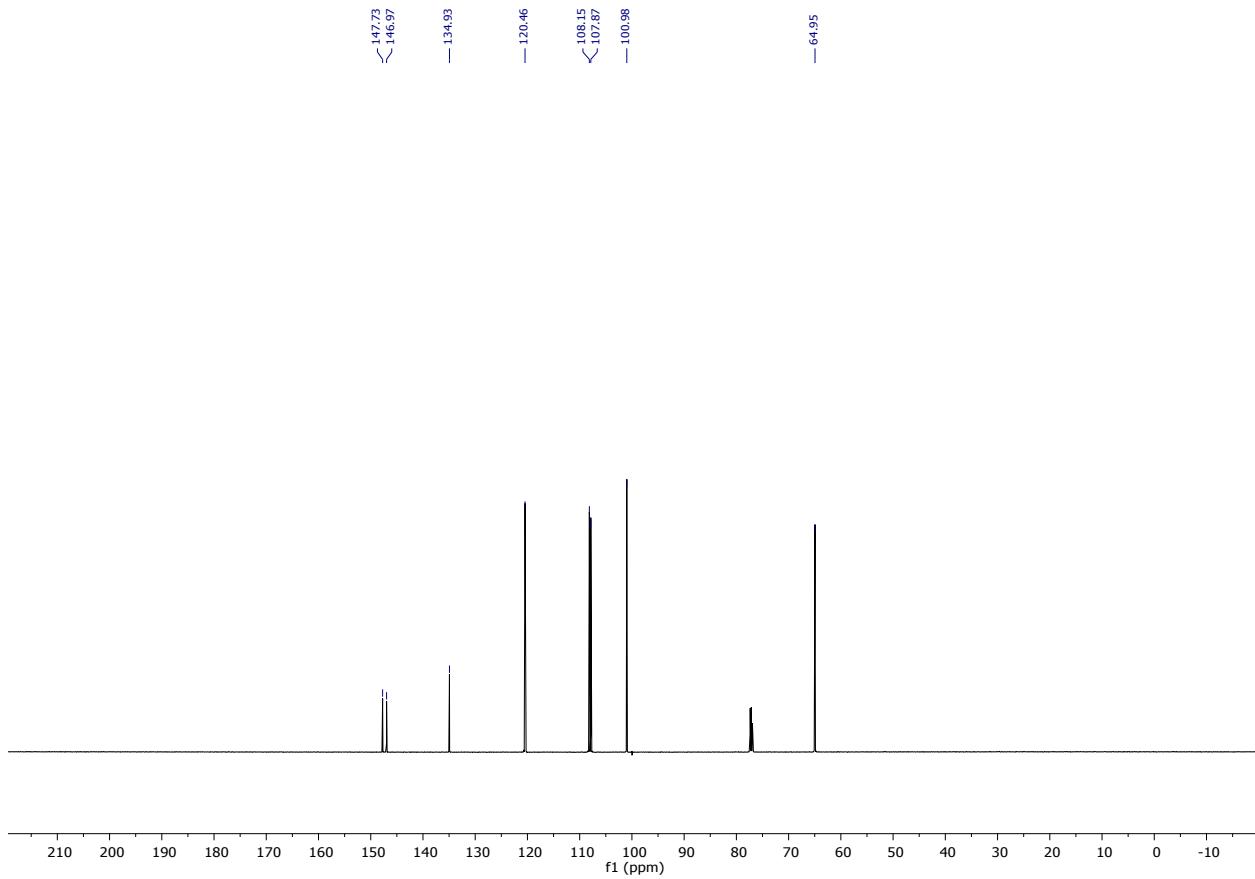


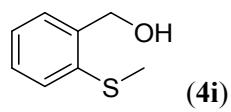


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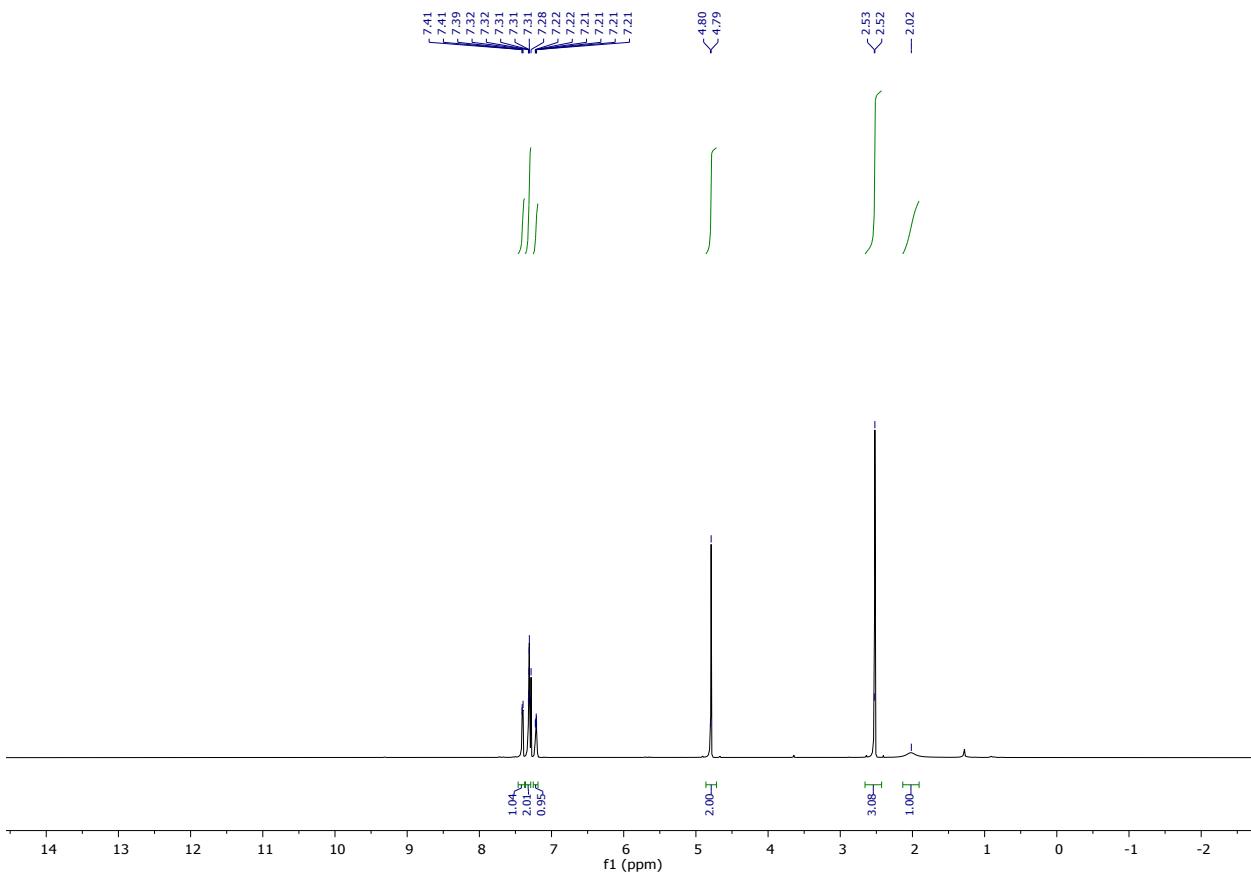


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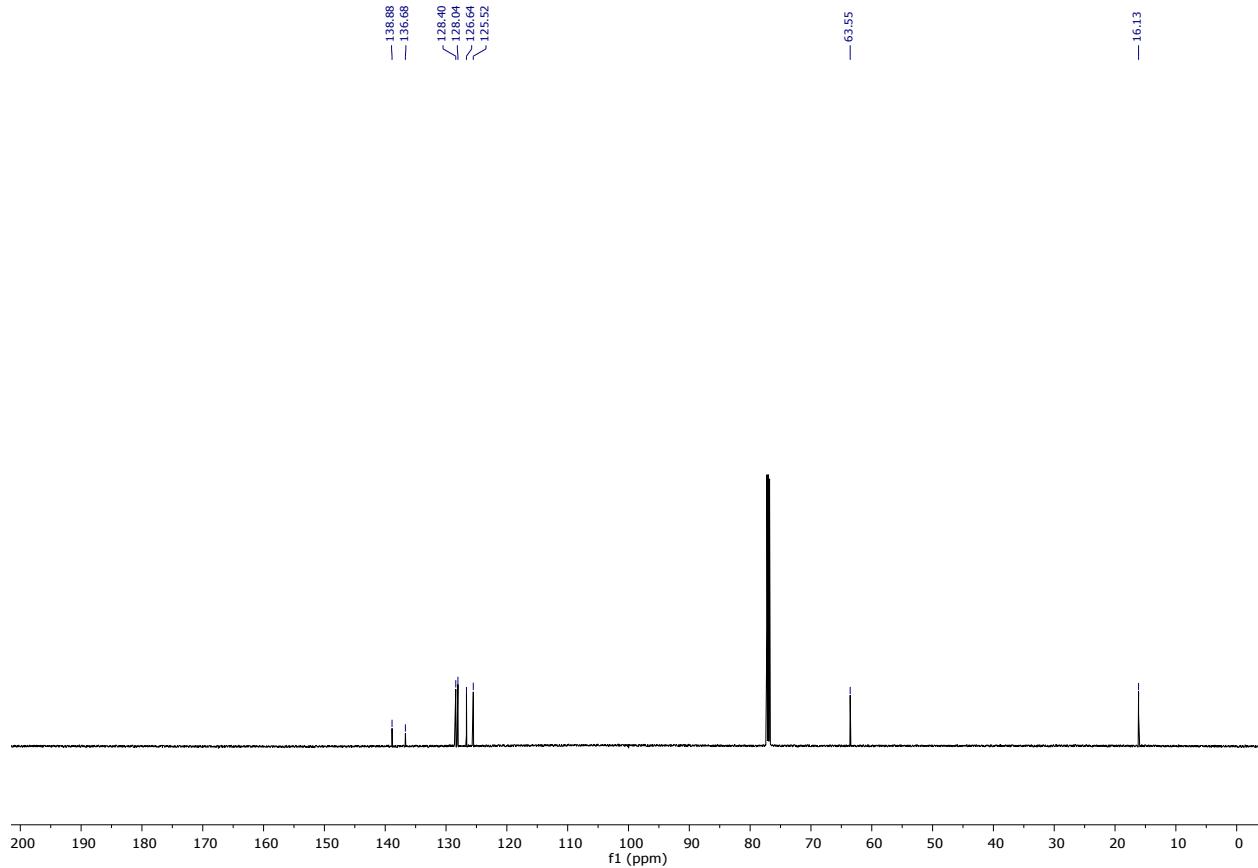


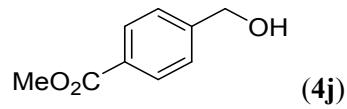


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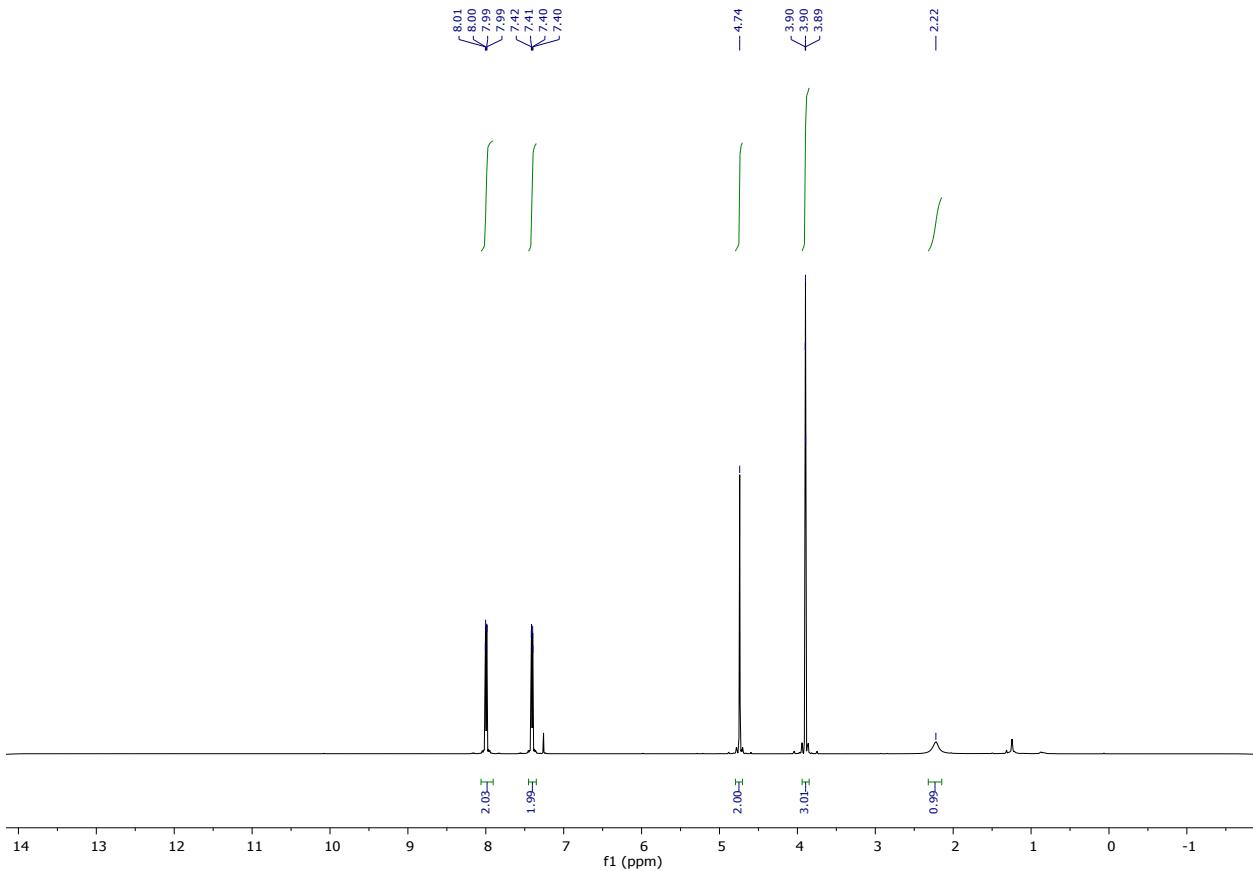


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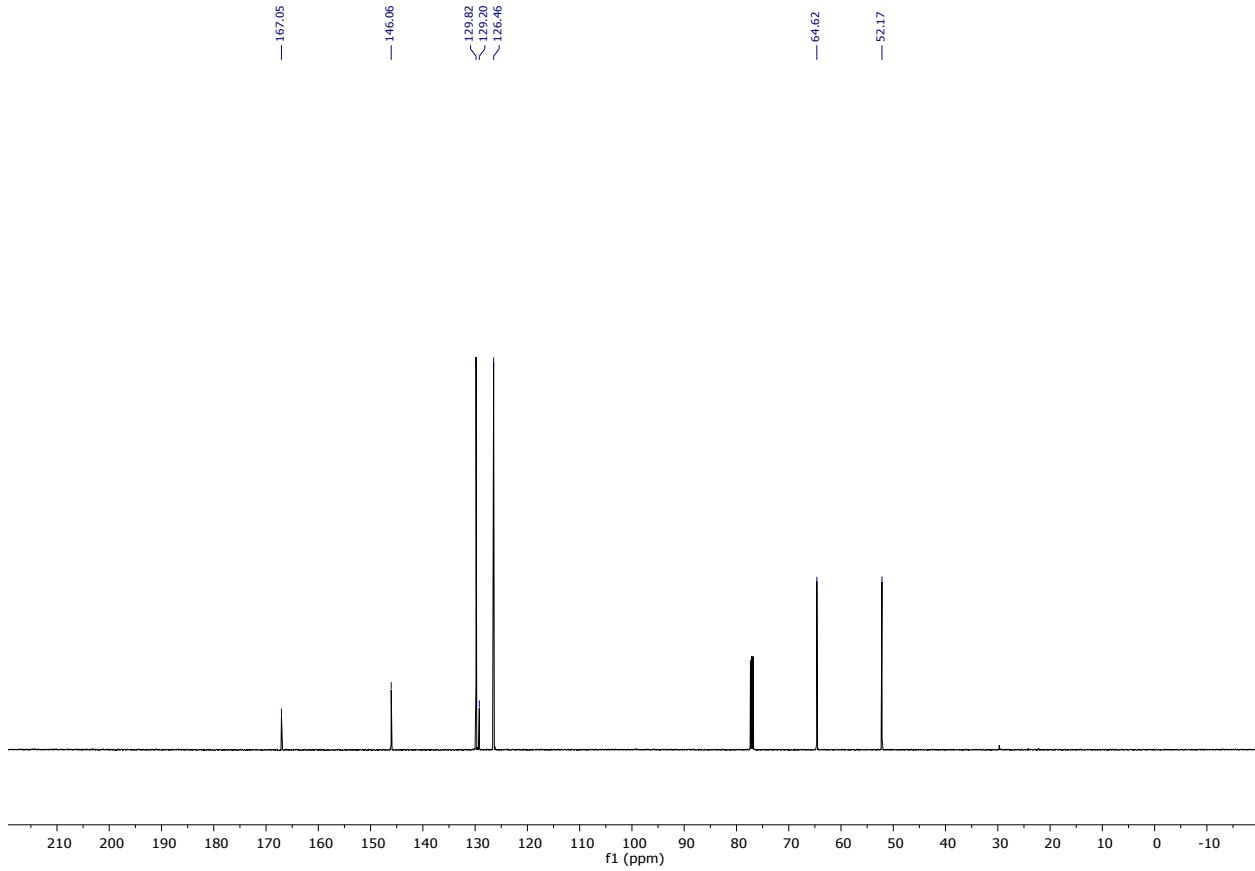


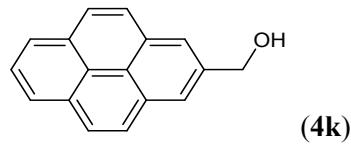


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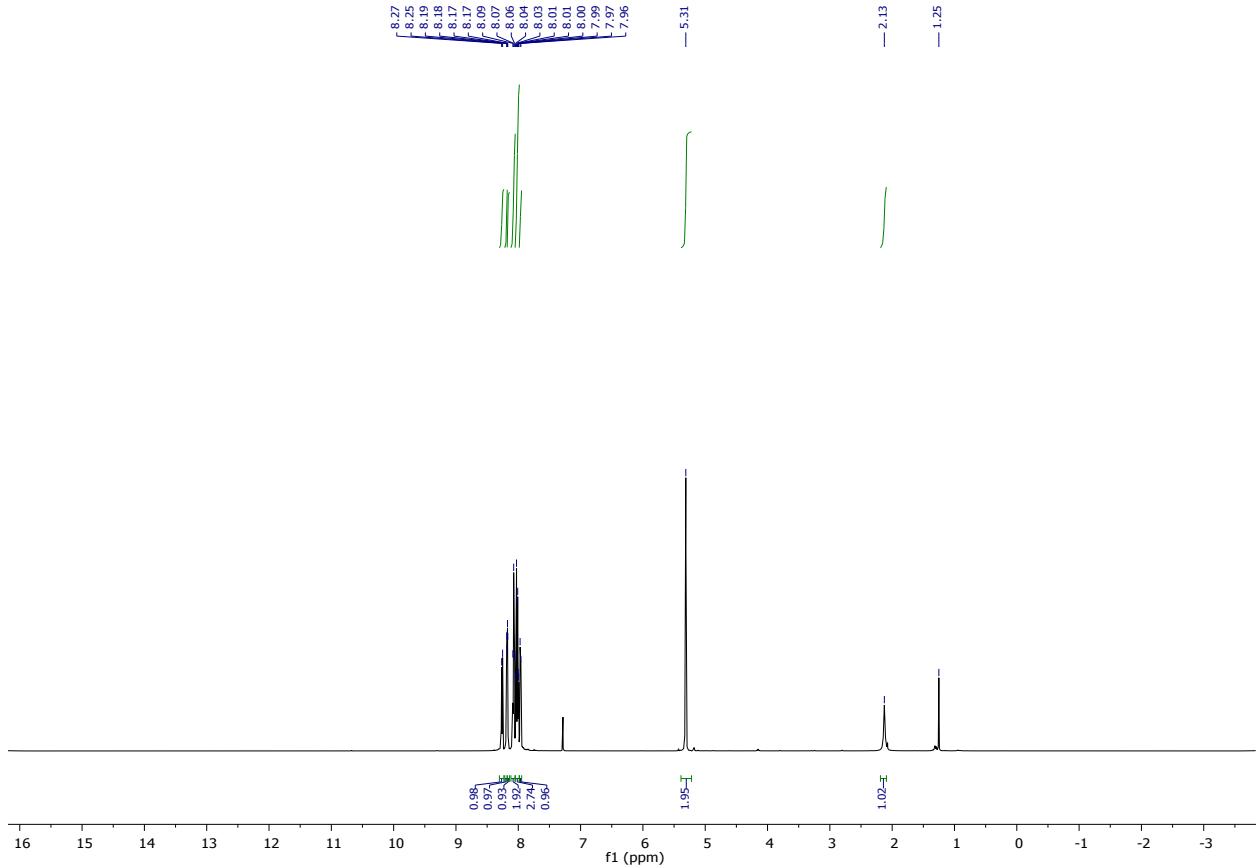


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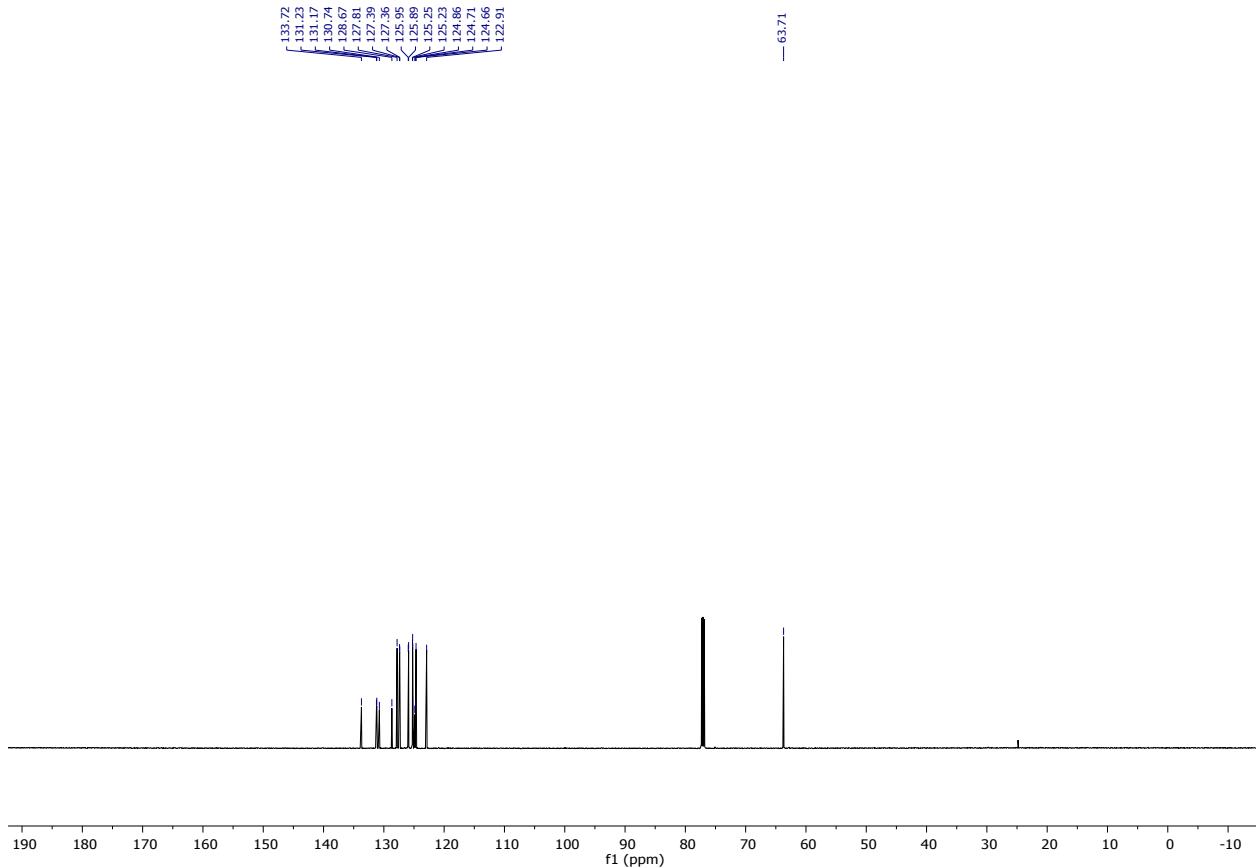


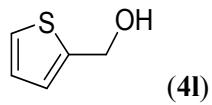


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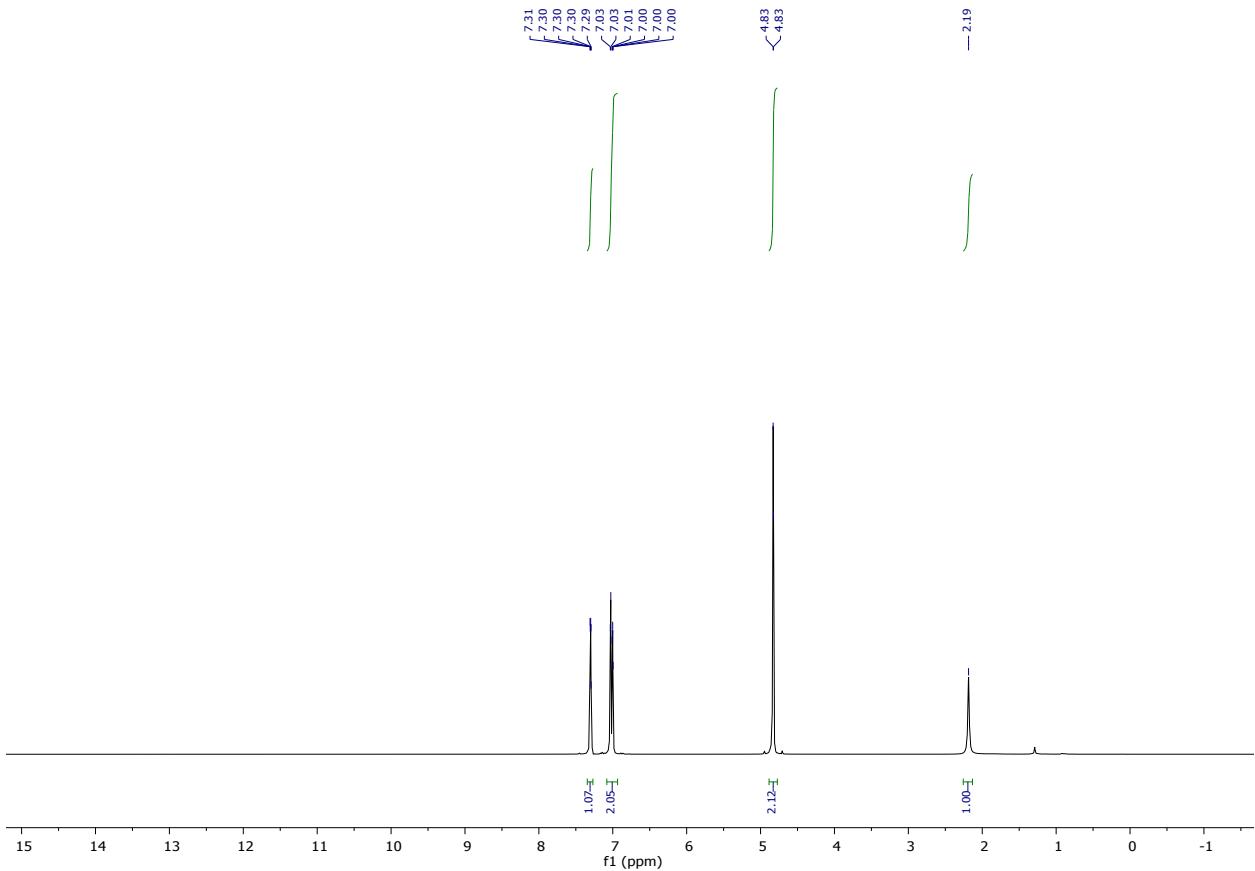


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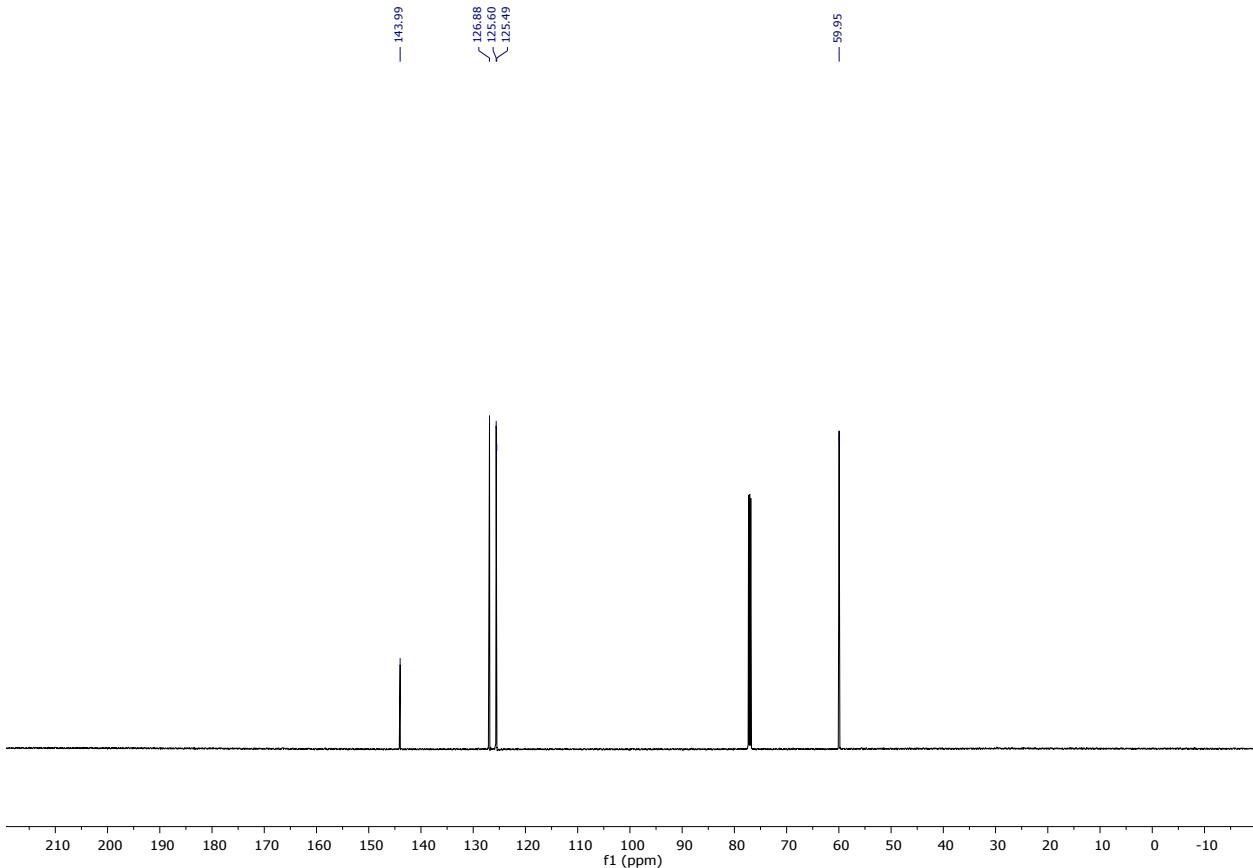


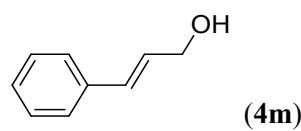


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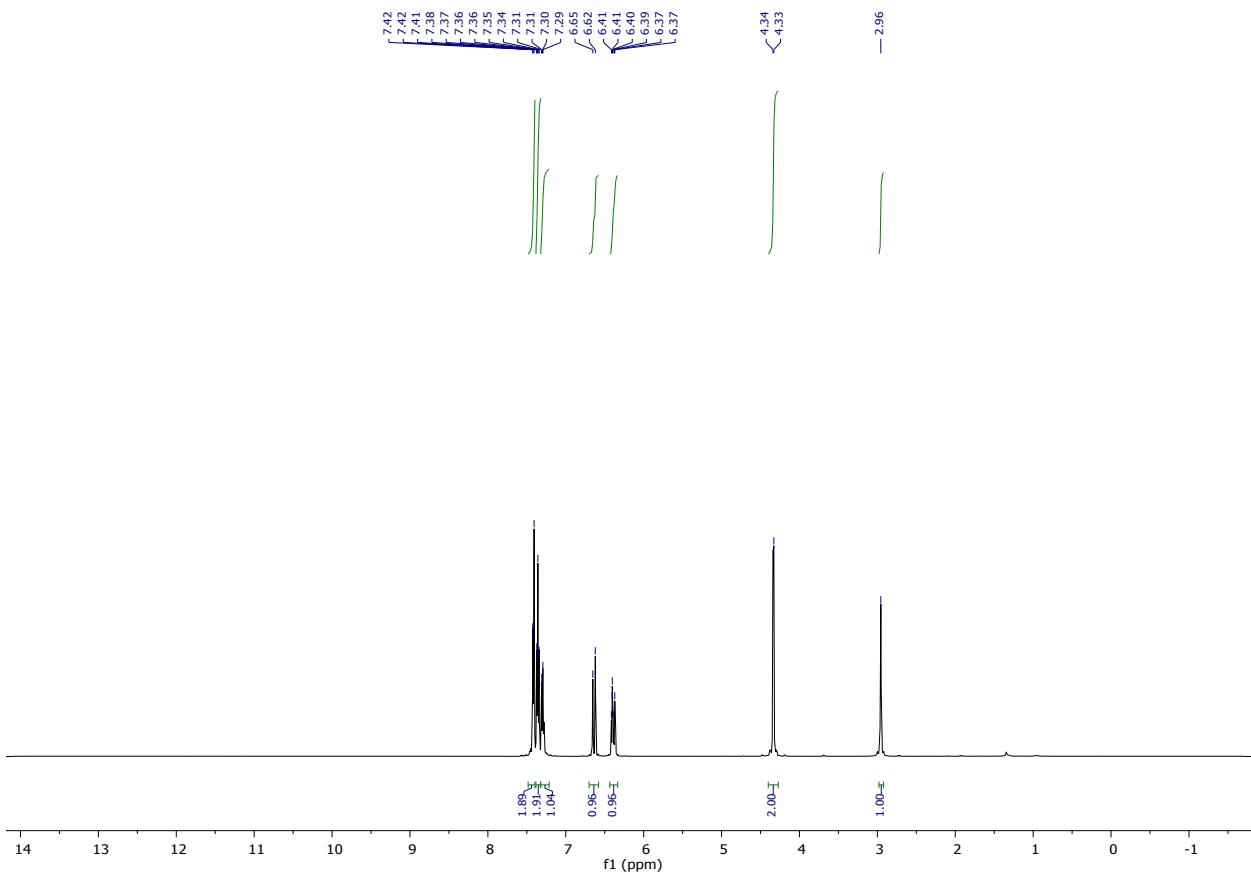


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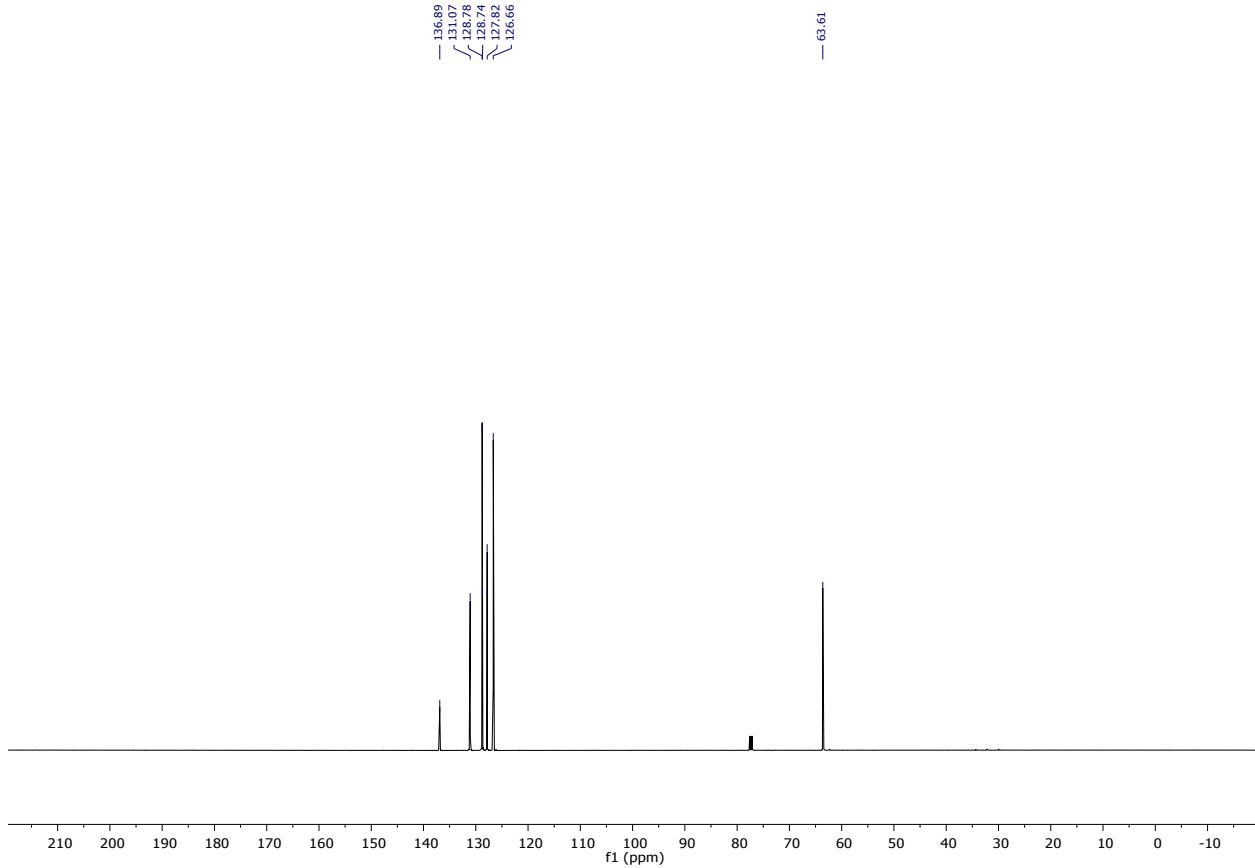


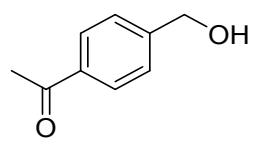


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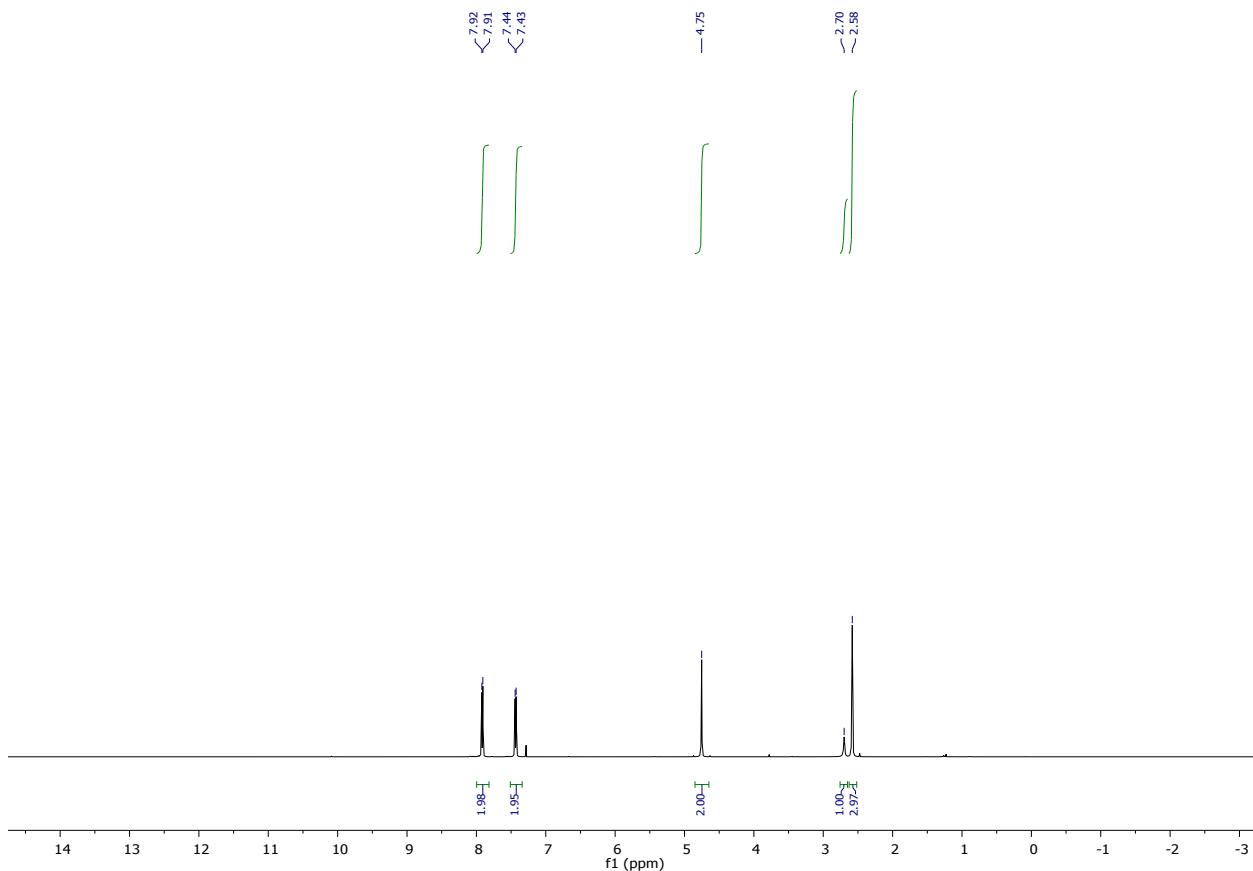


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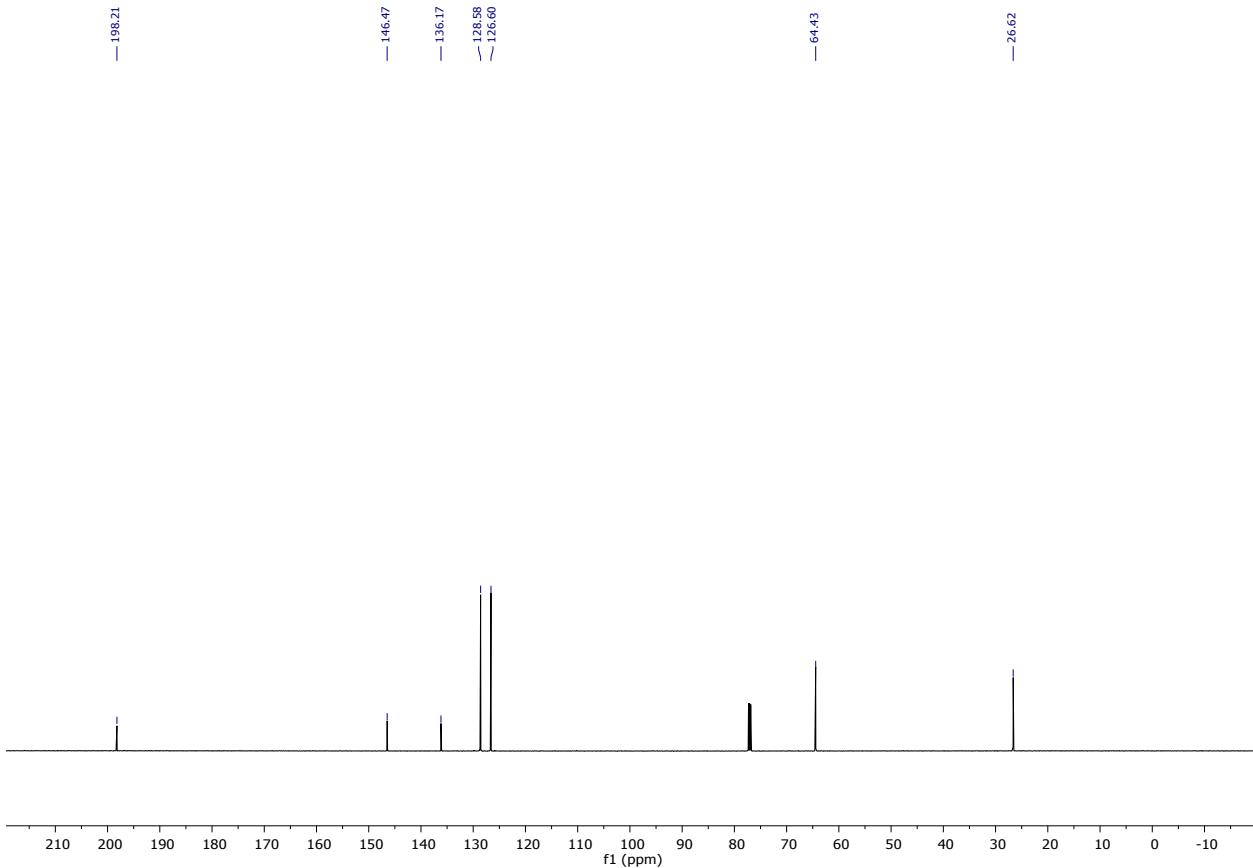


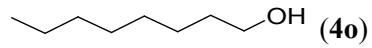


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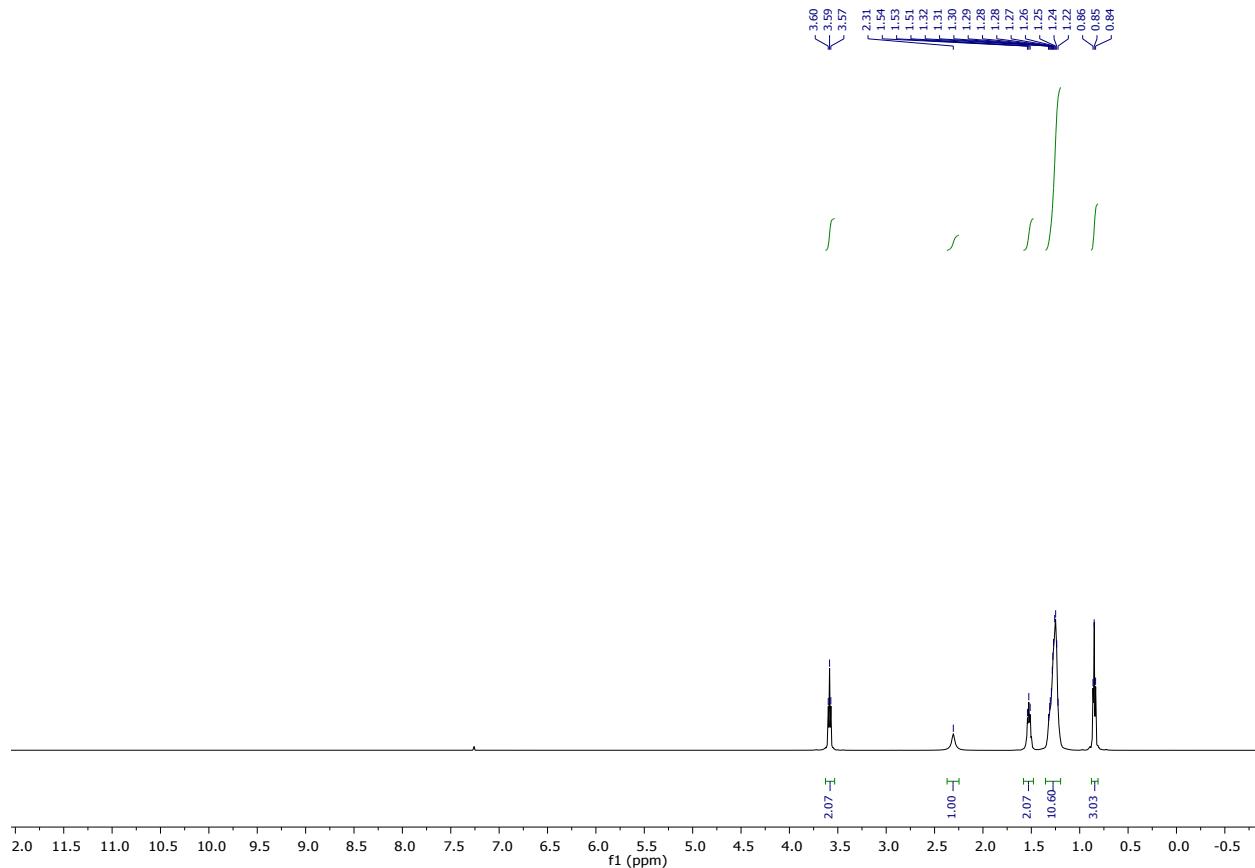


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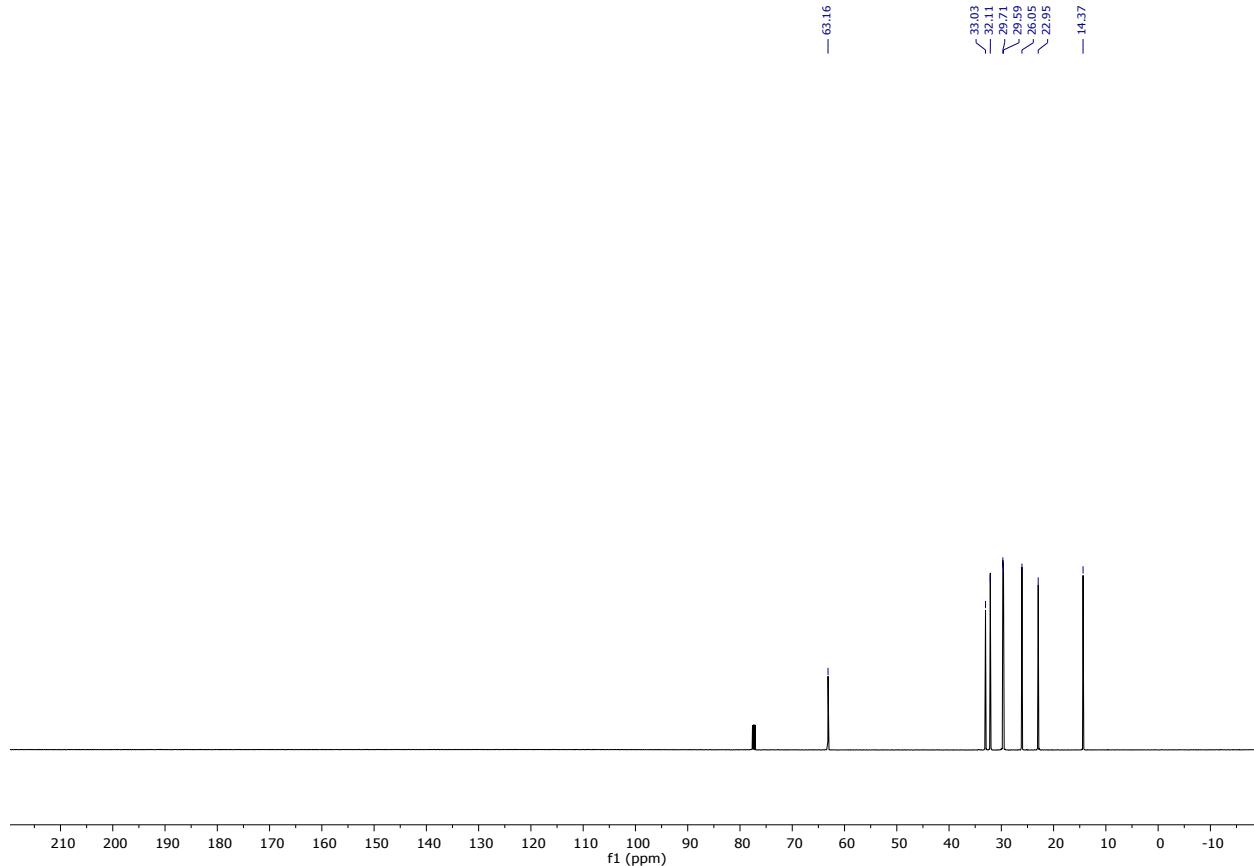


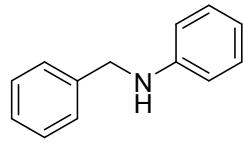


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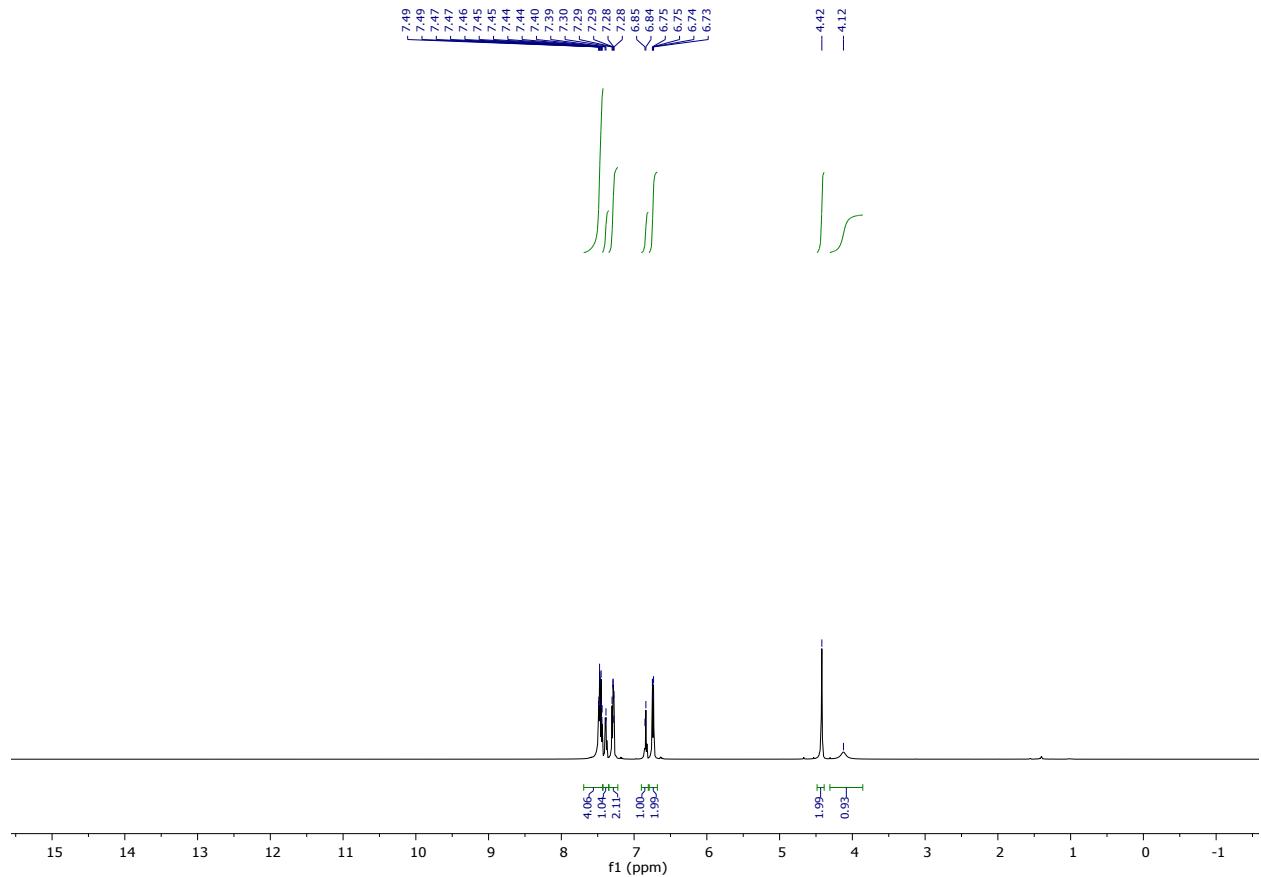


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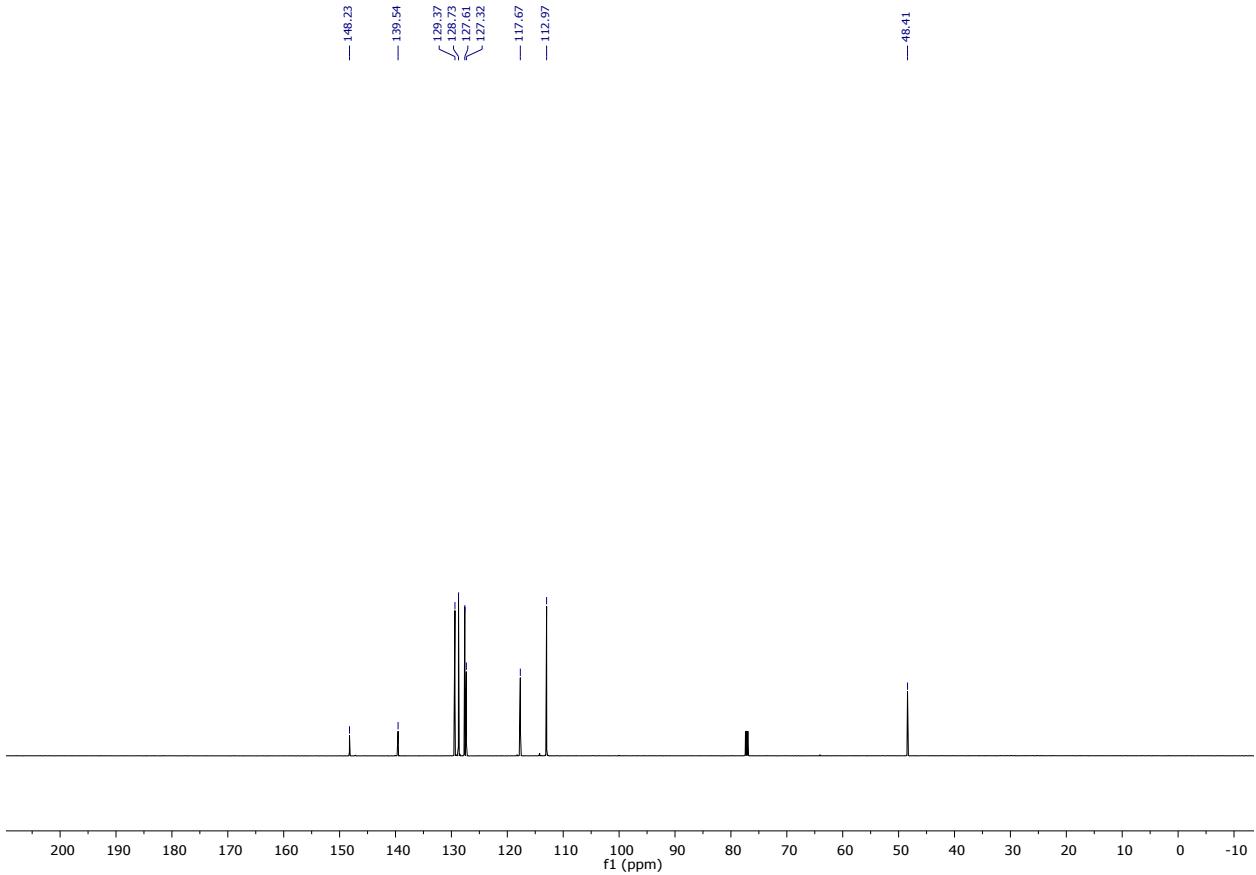


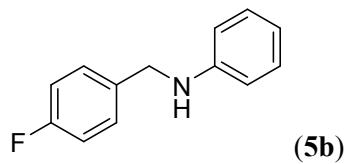


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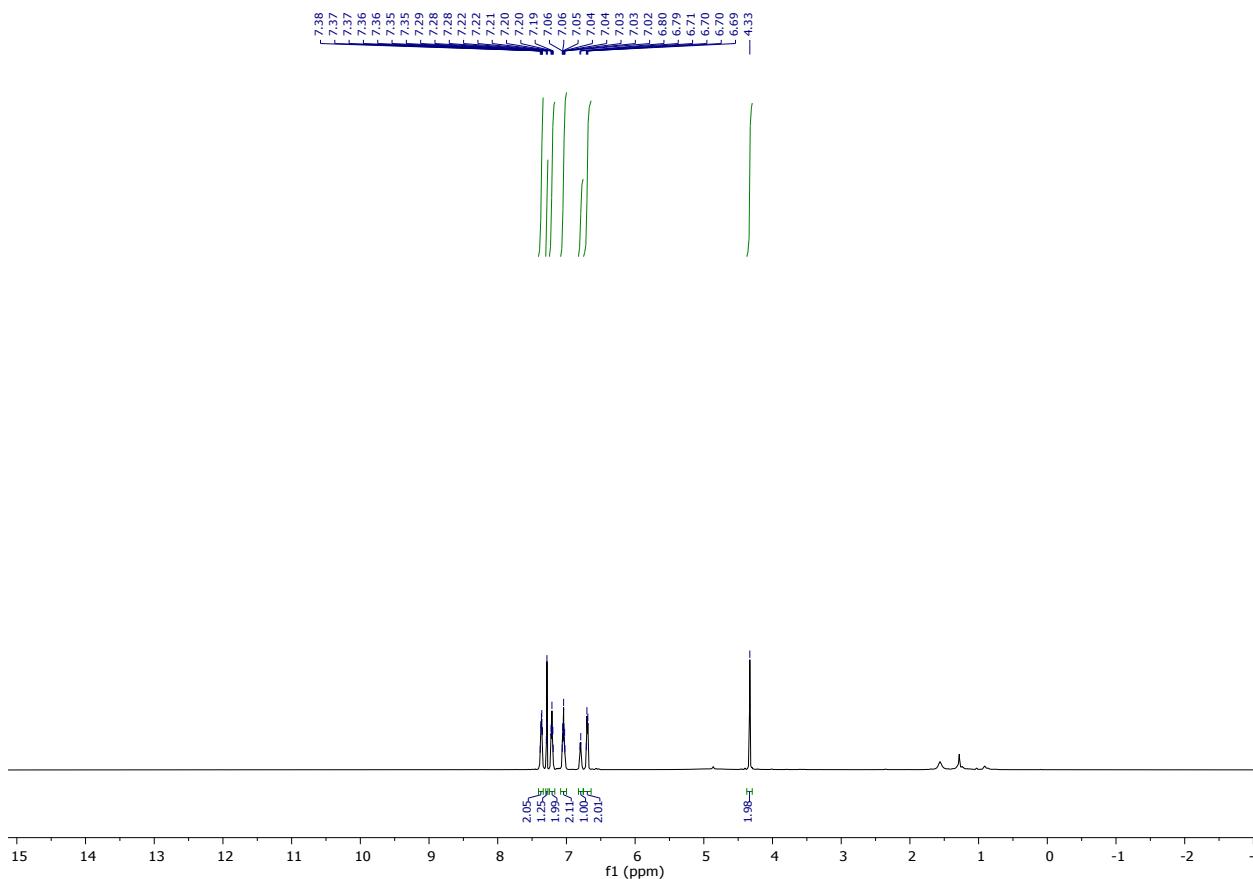


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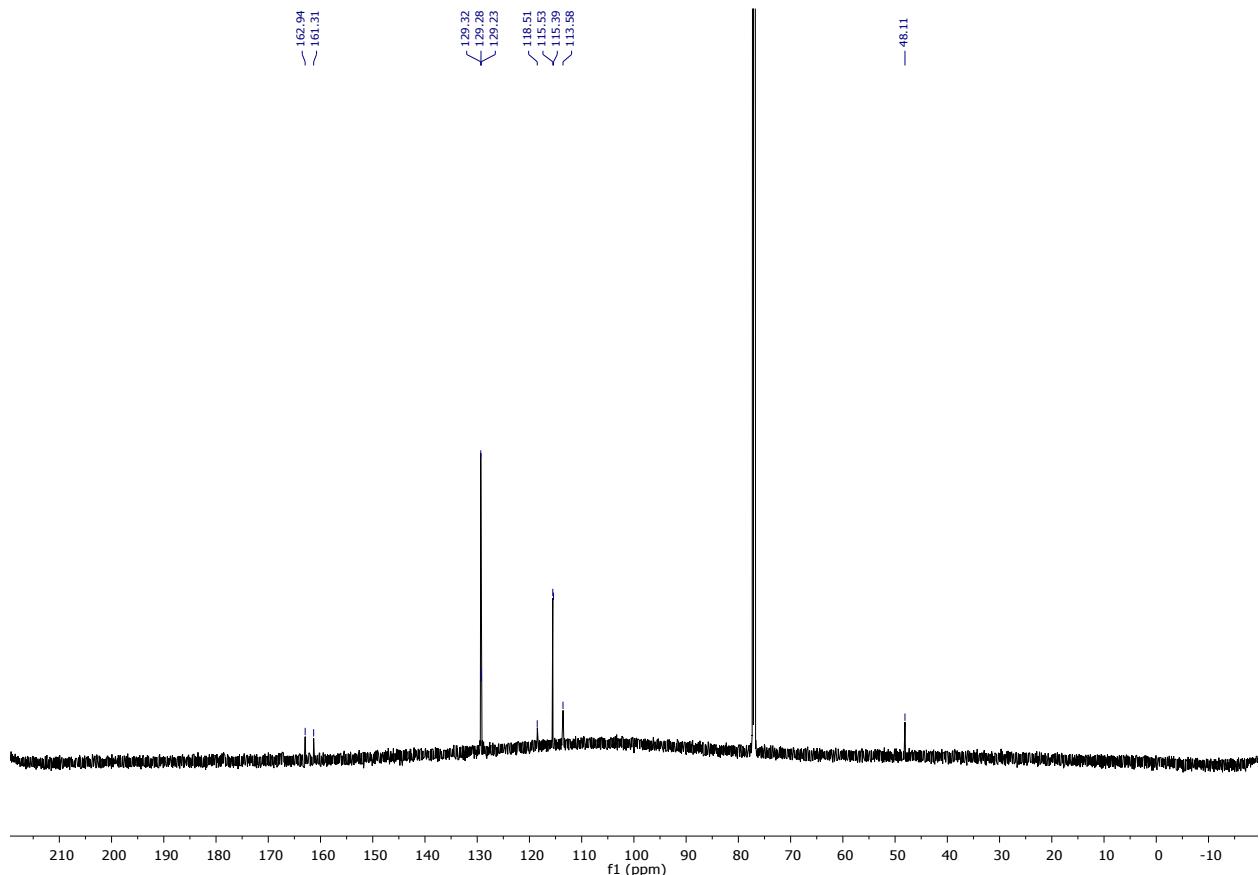


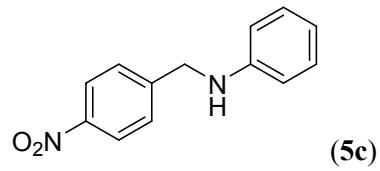


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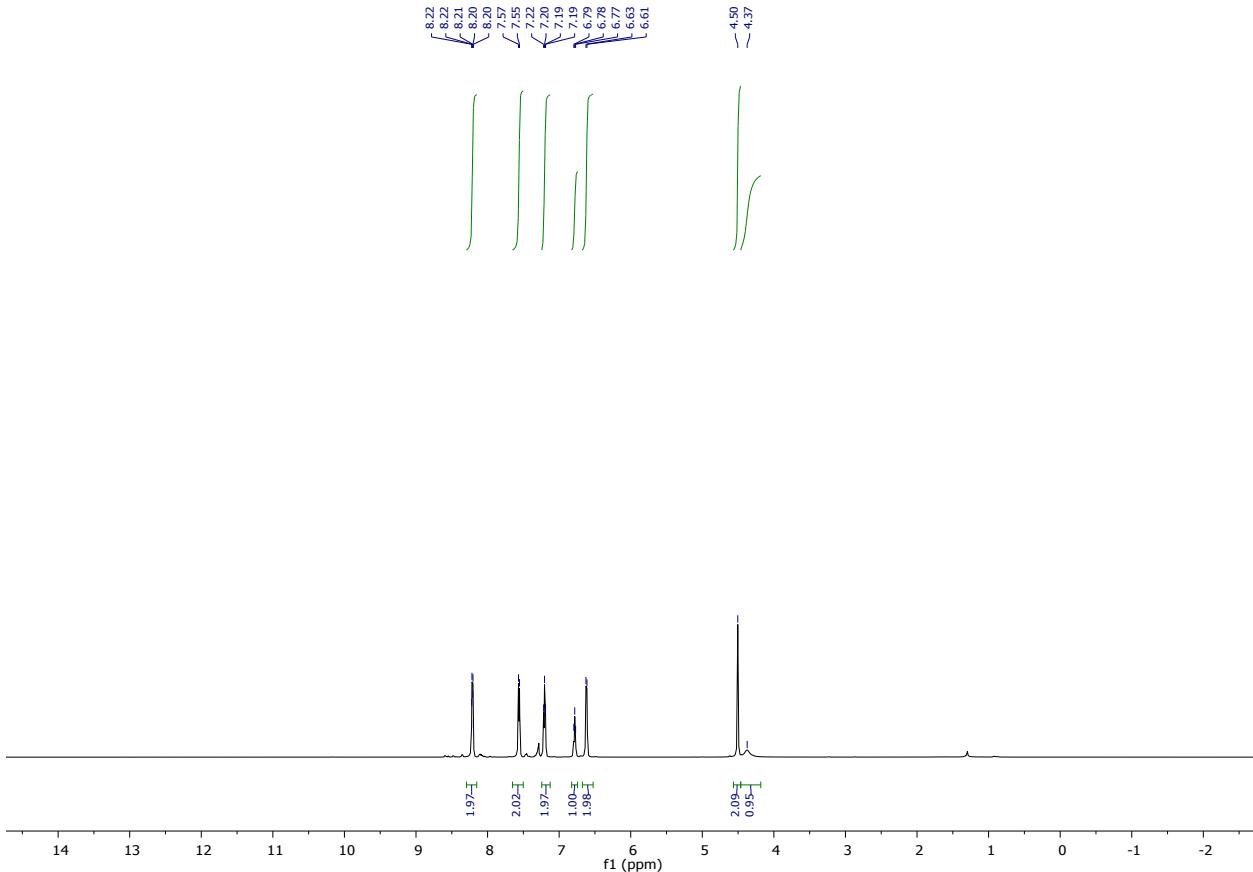


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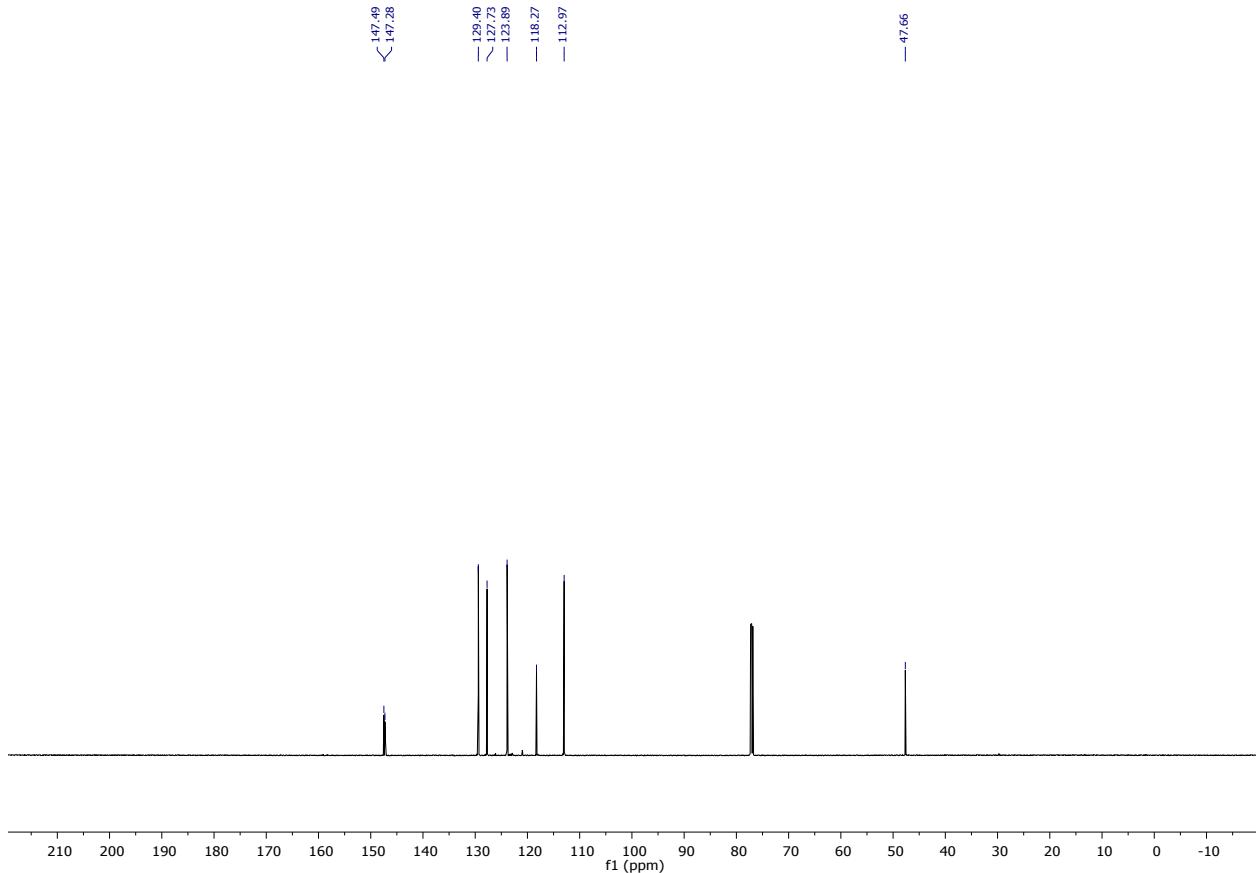


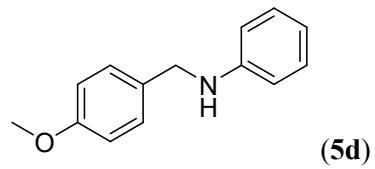


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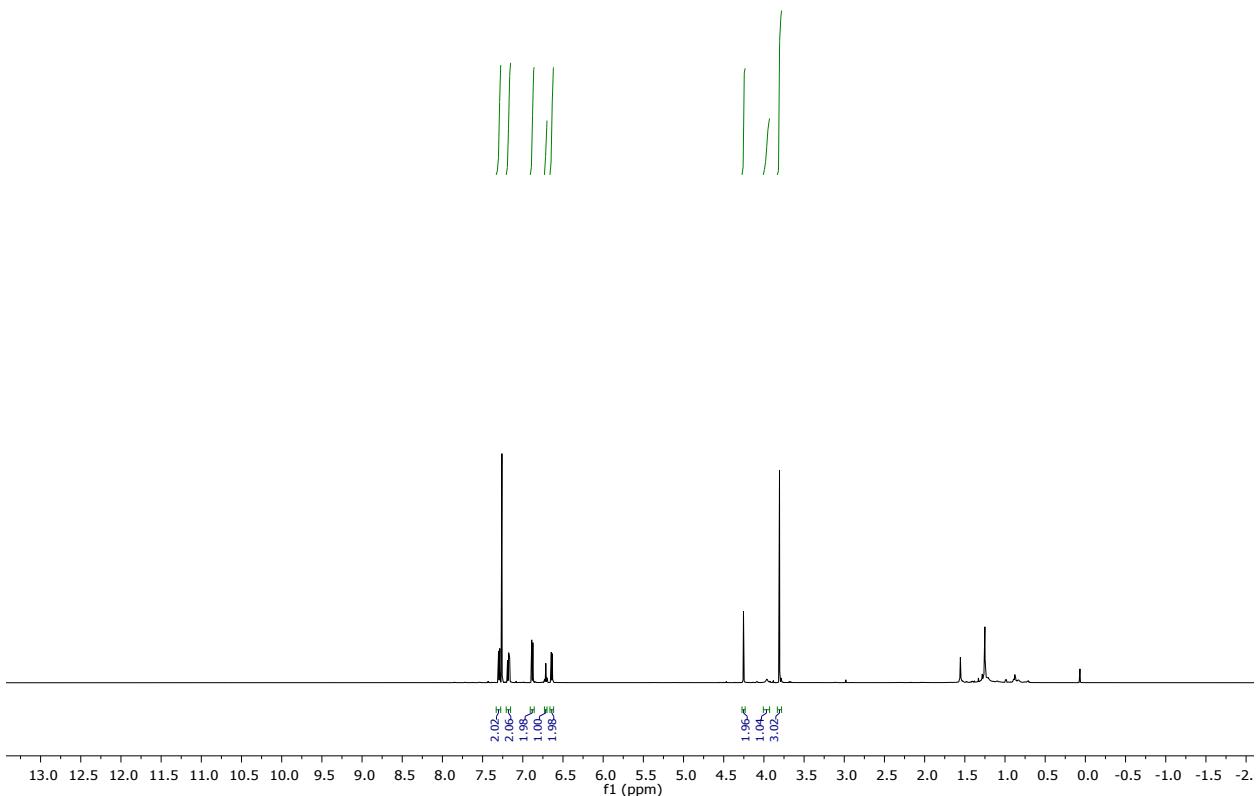


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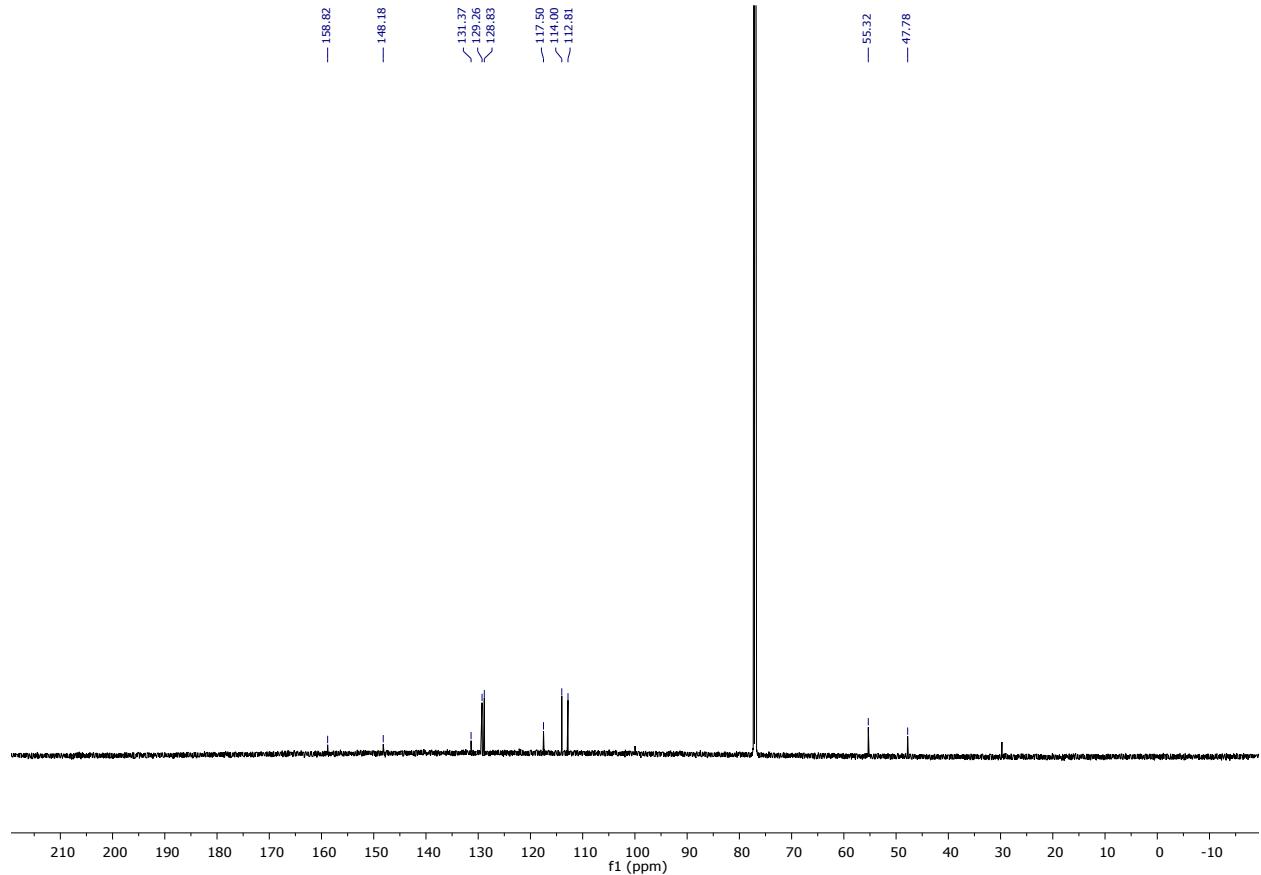


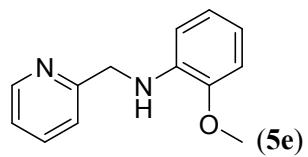


^1H NMR (600 MHz, CDCl_3):

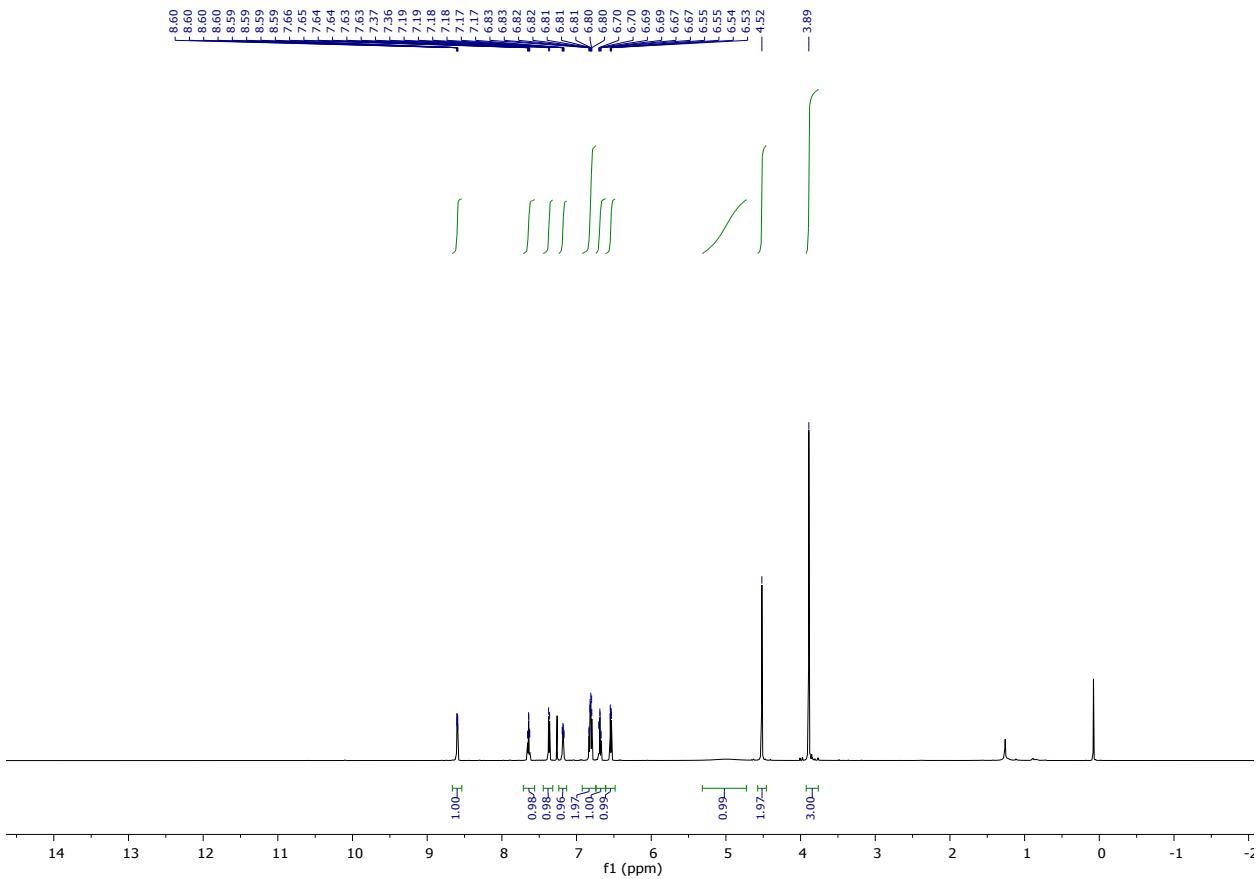


¹³C NMR (151 MHz, CDCl₃):

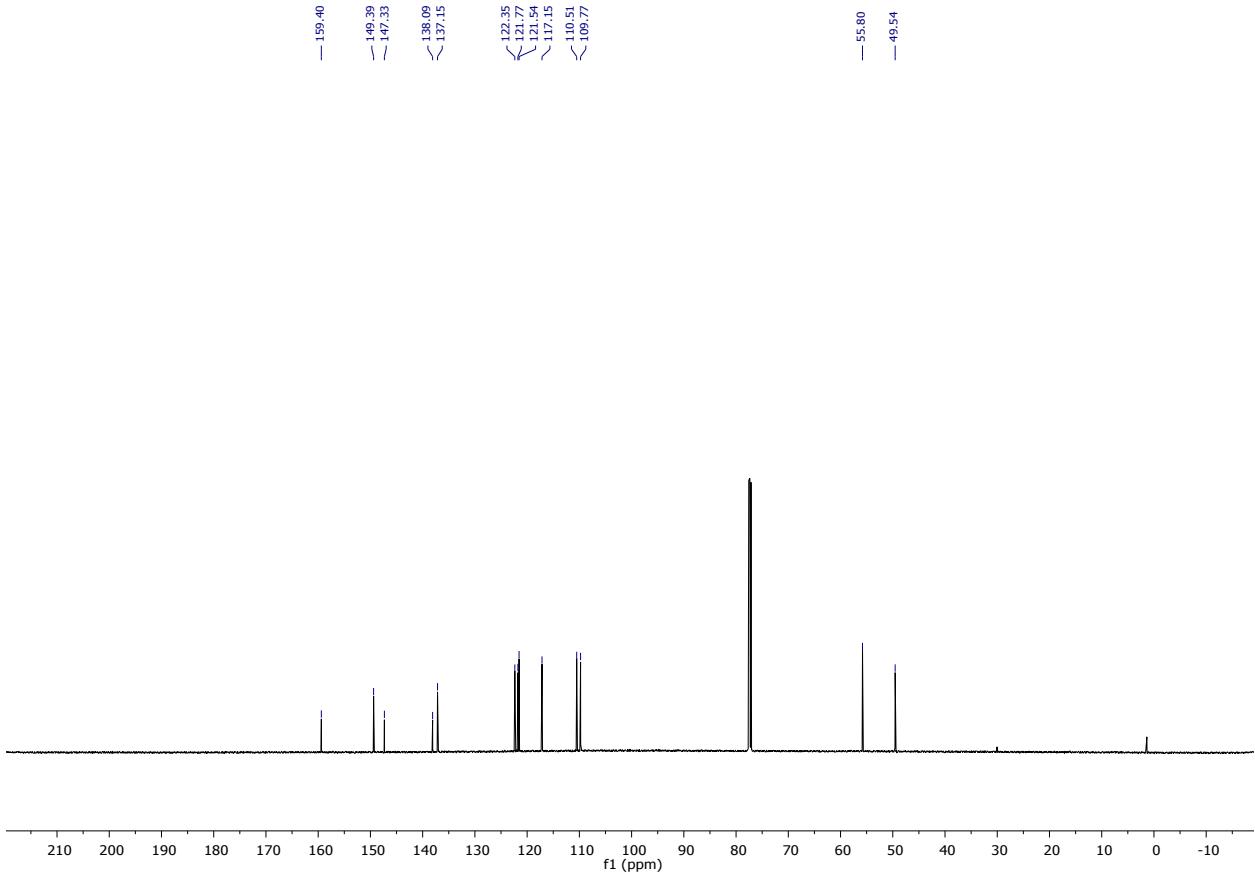


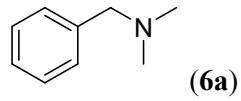


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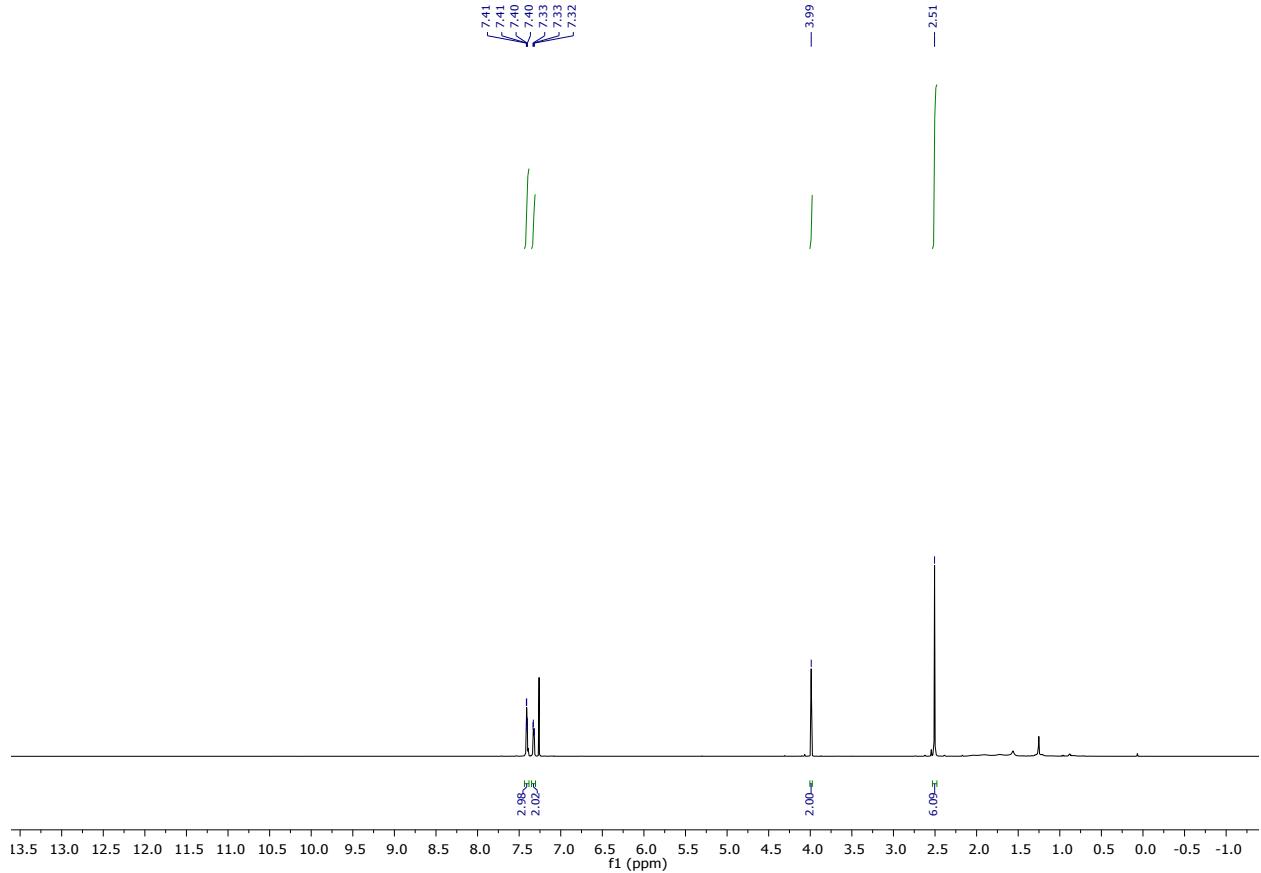


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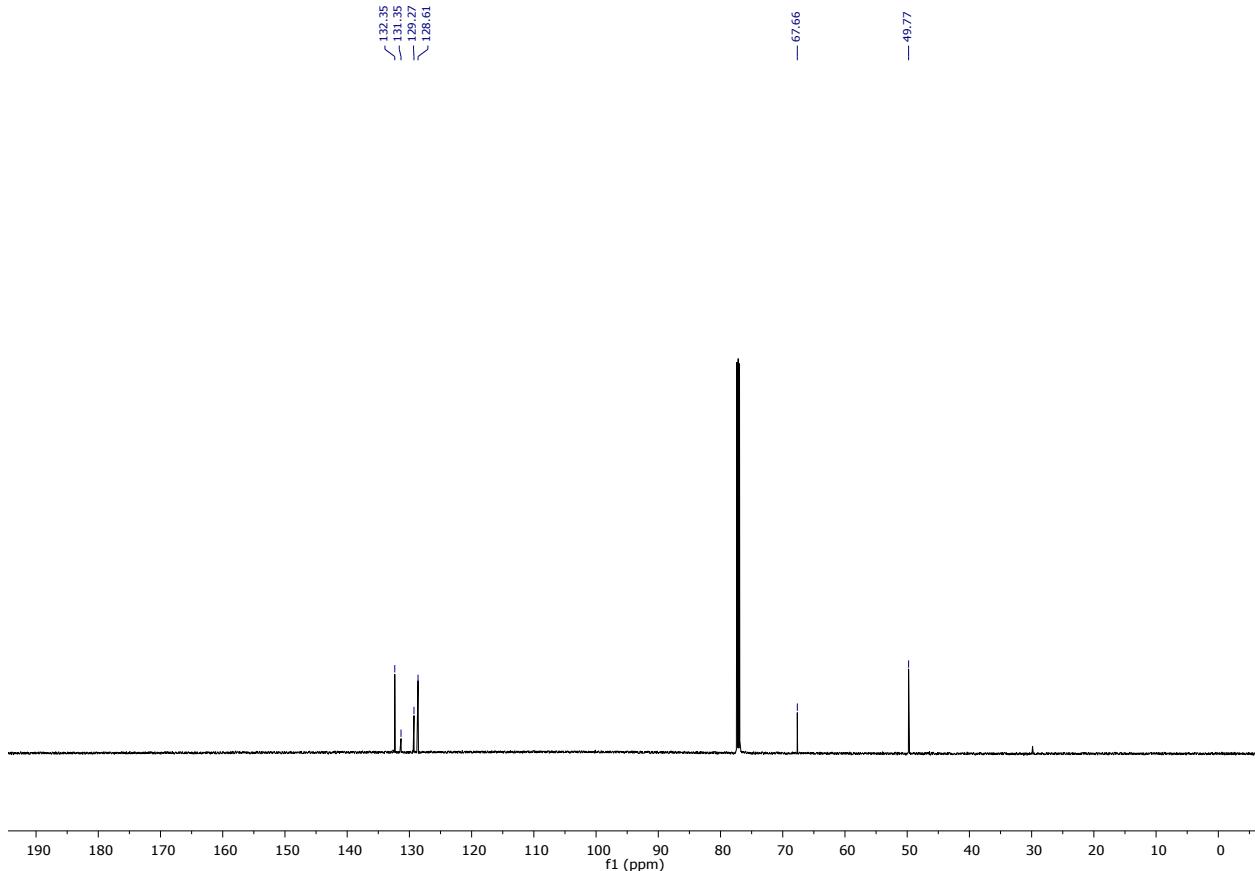


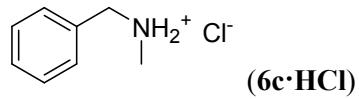


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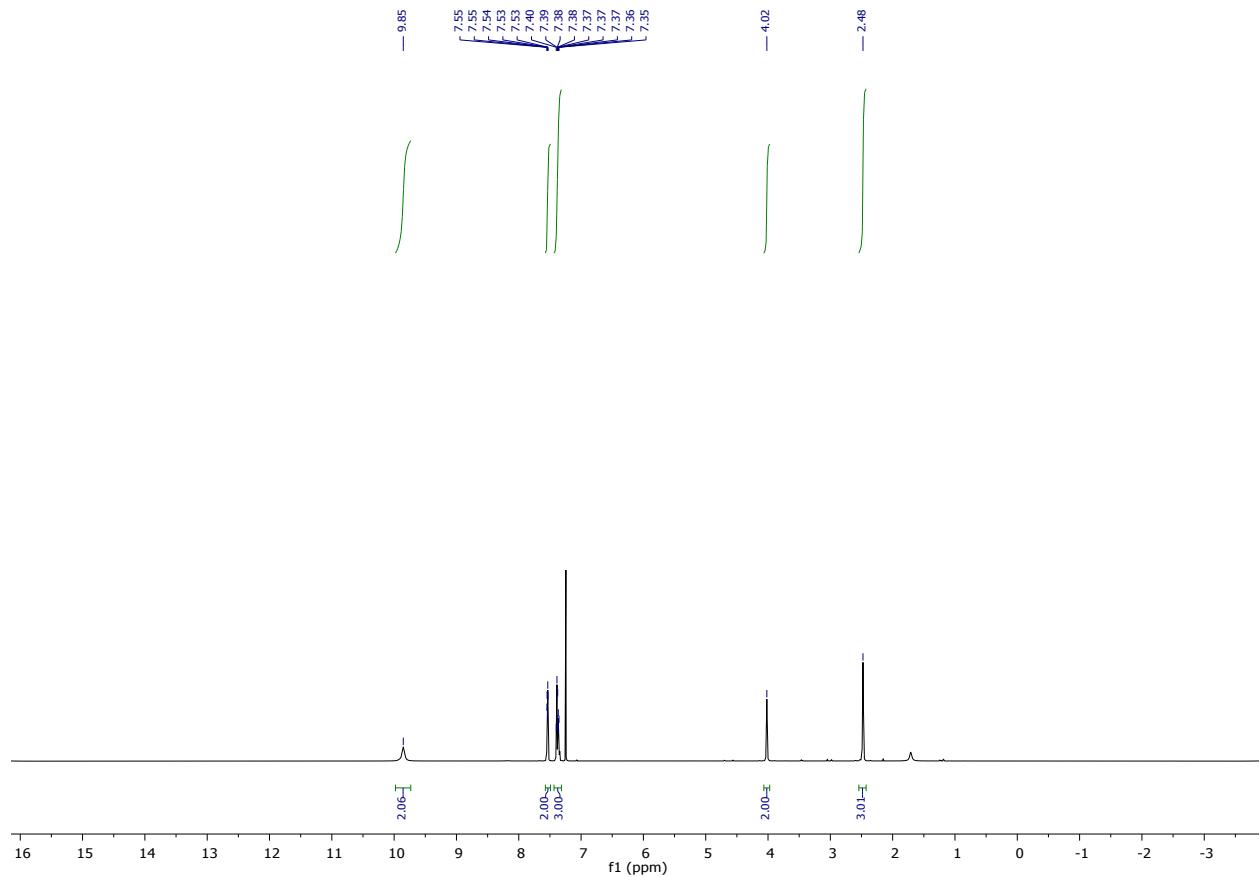


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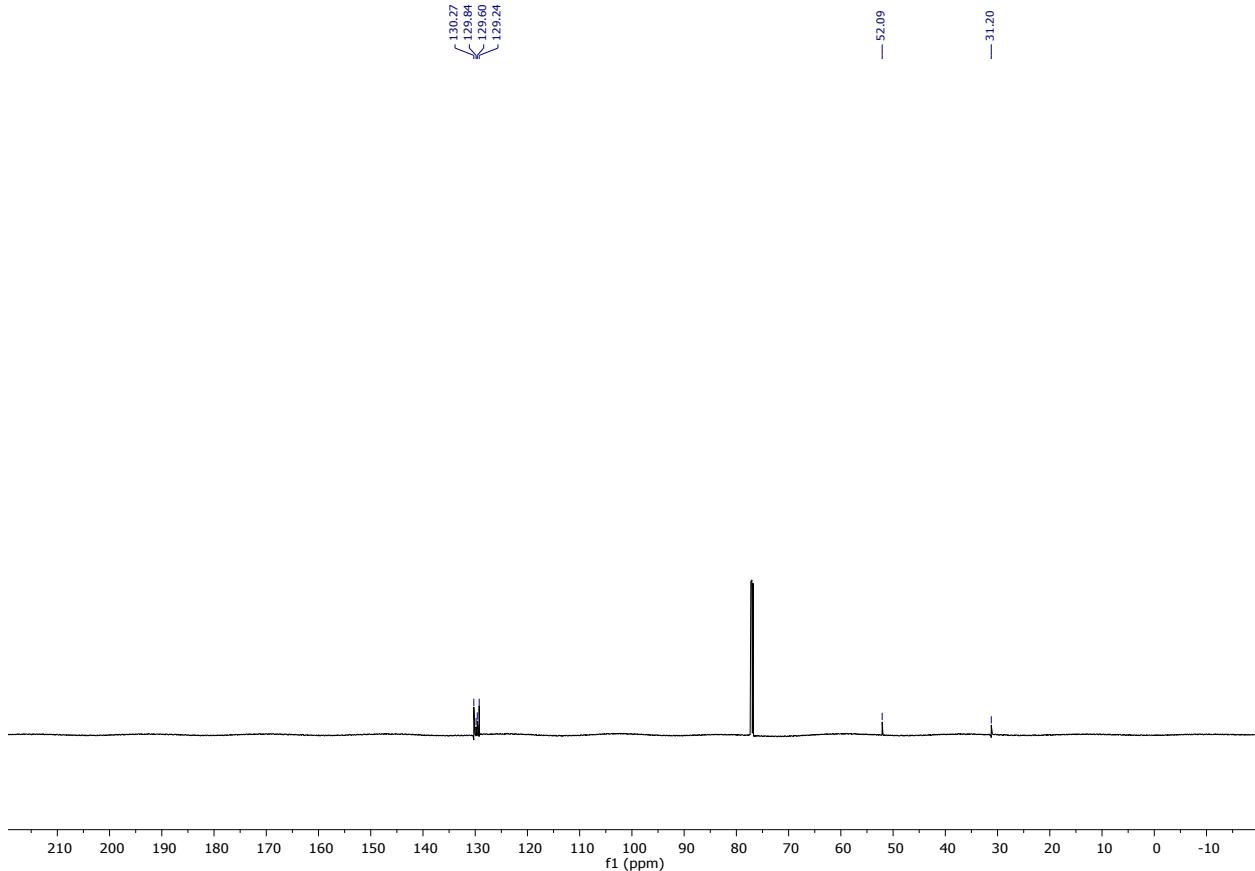


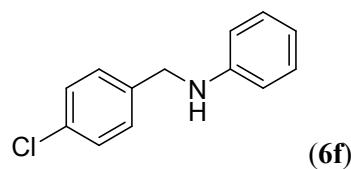


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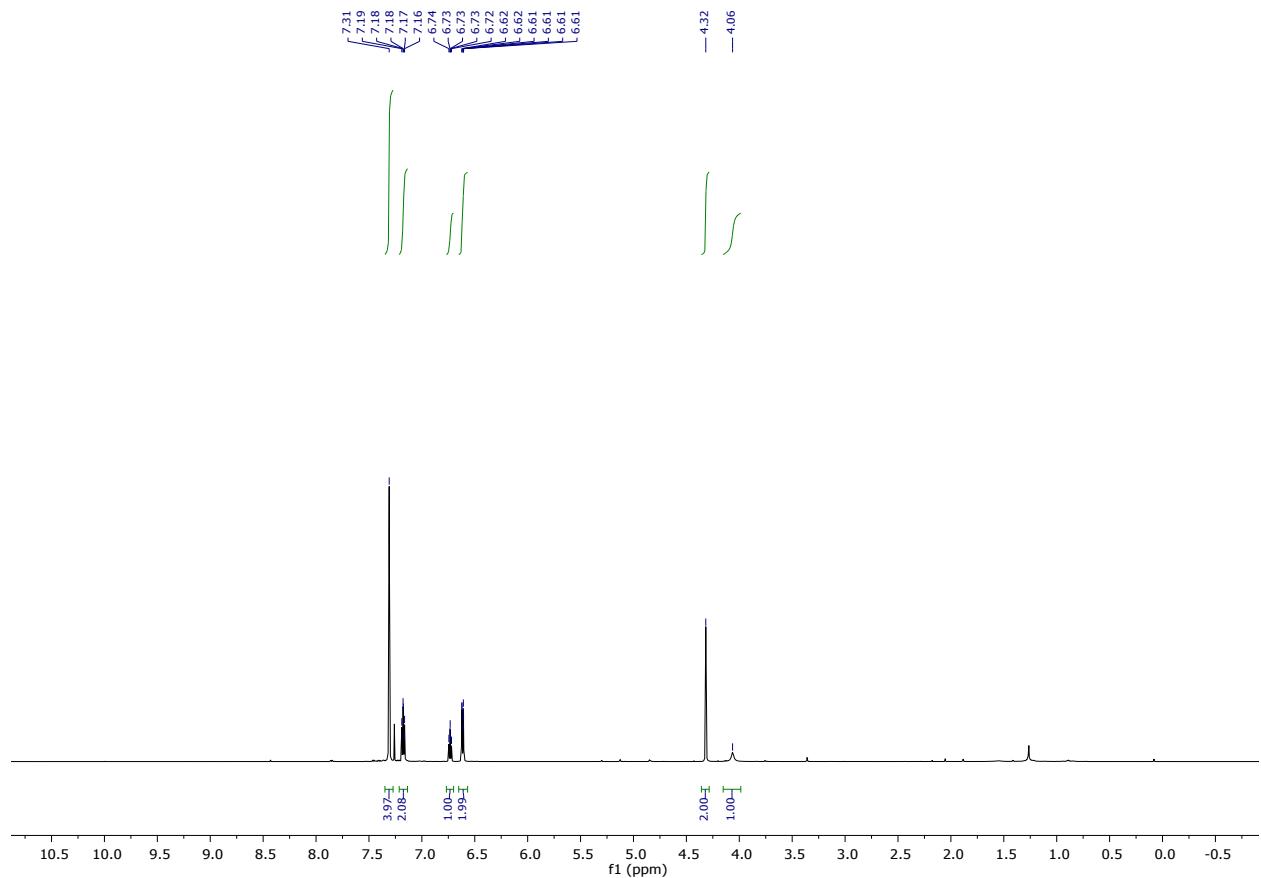


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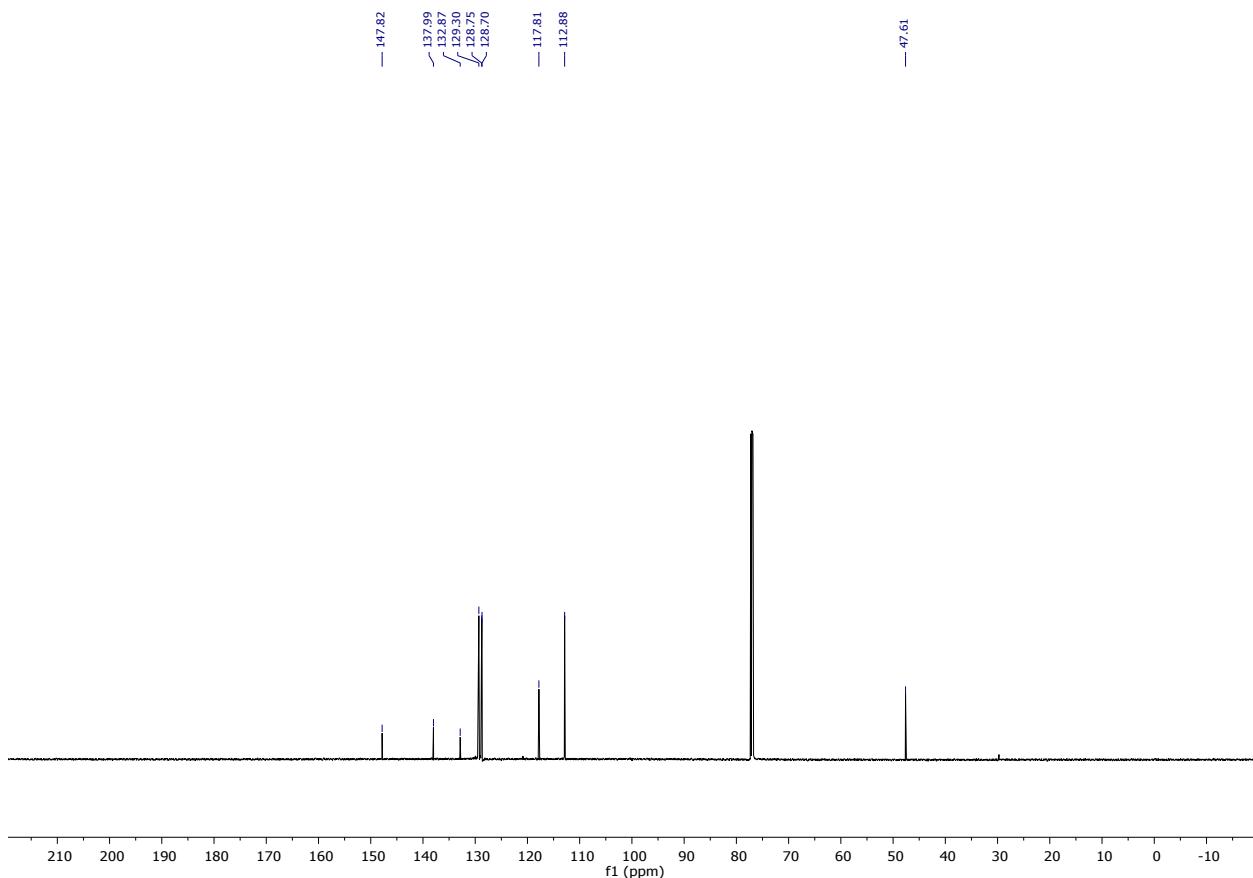


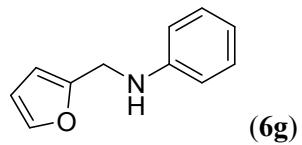


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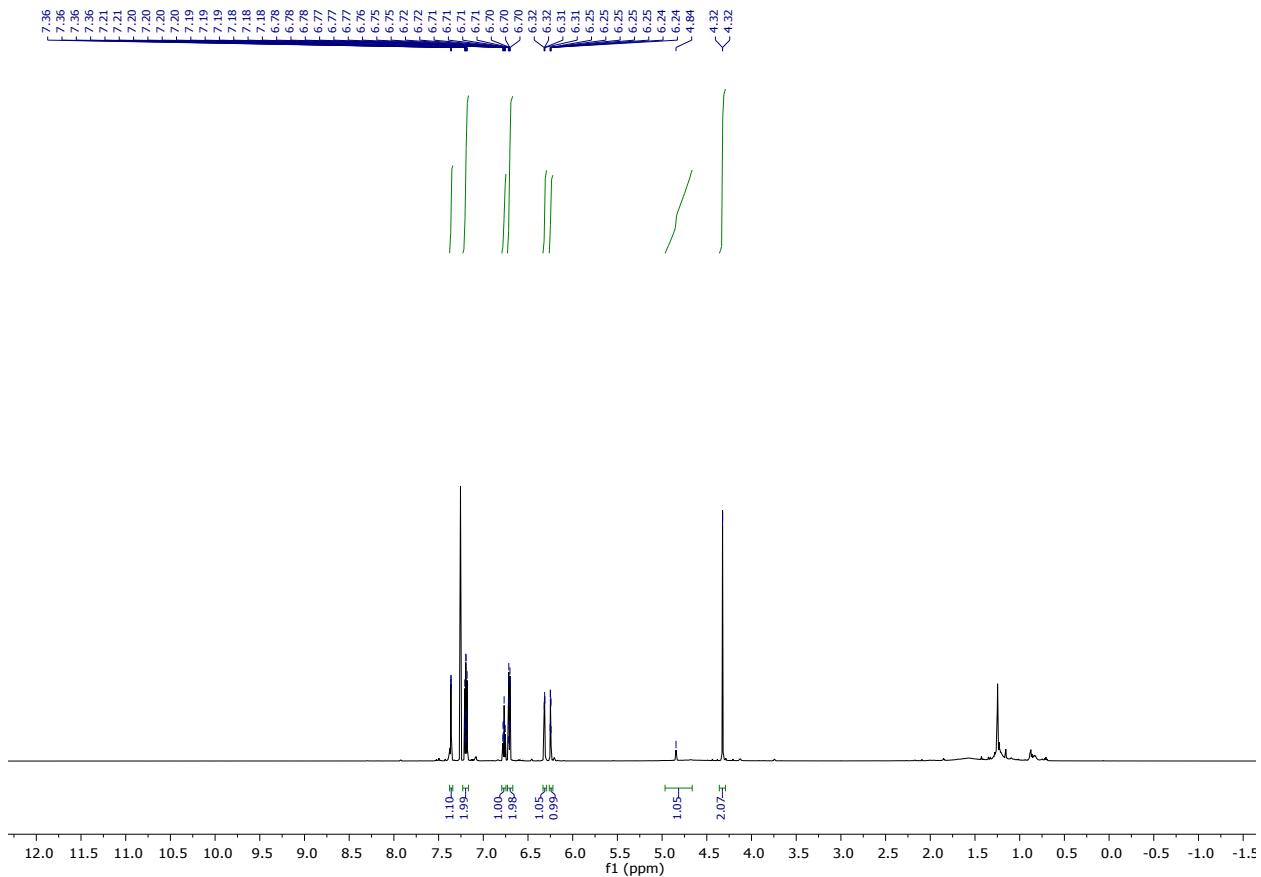


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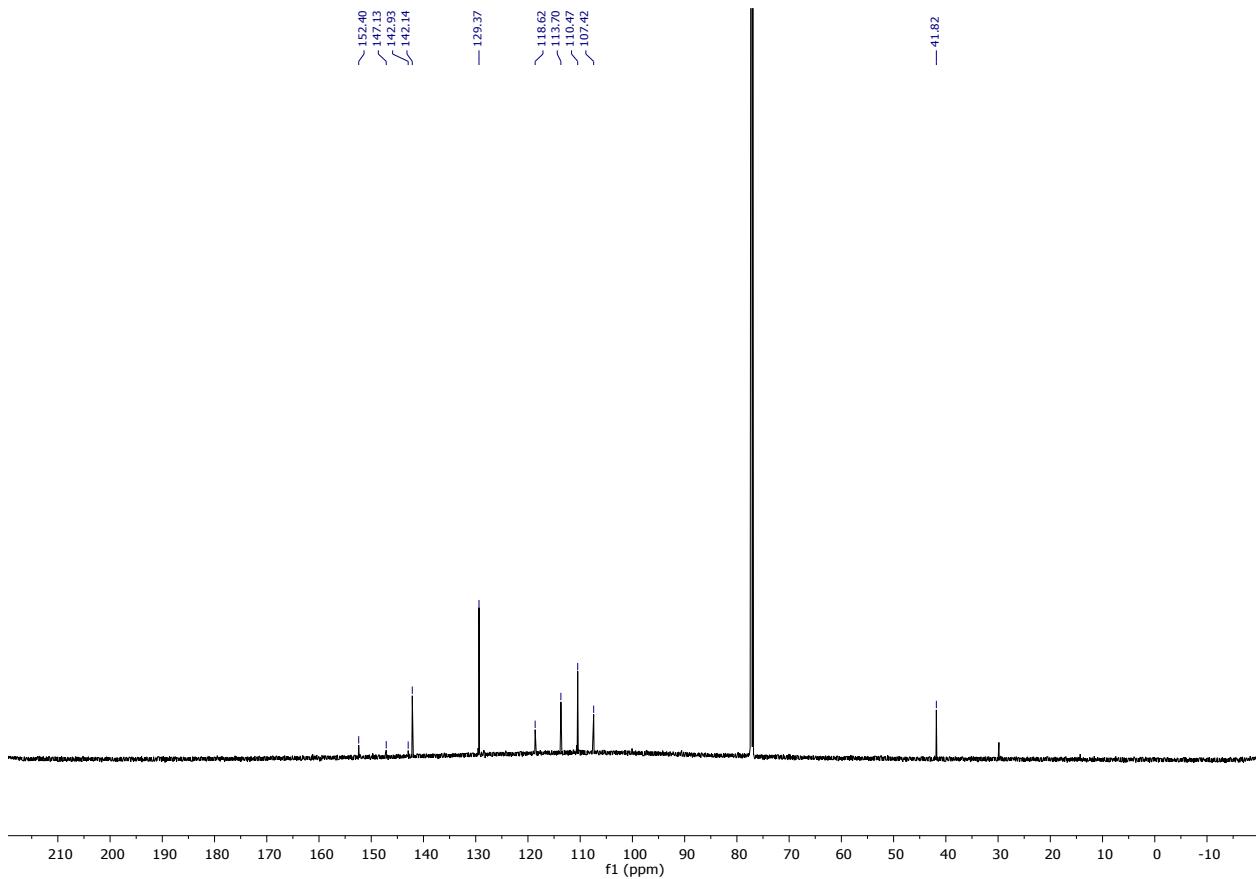


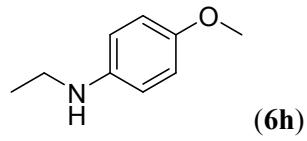


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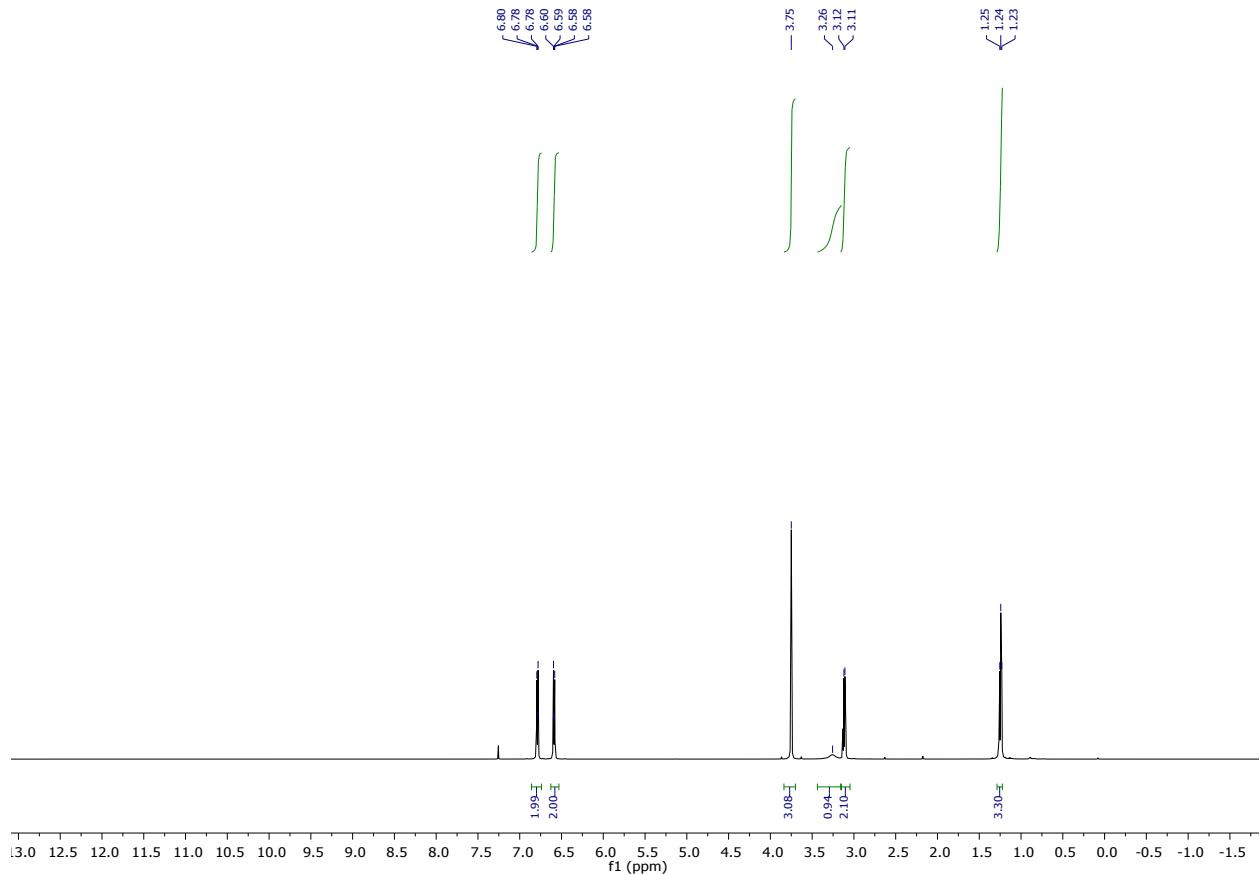


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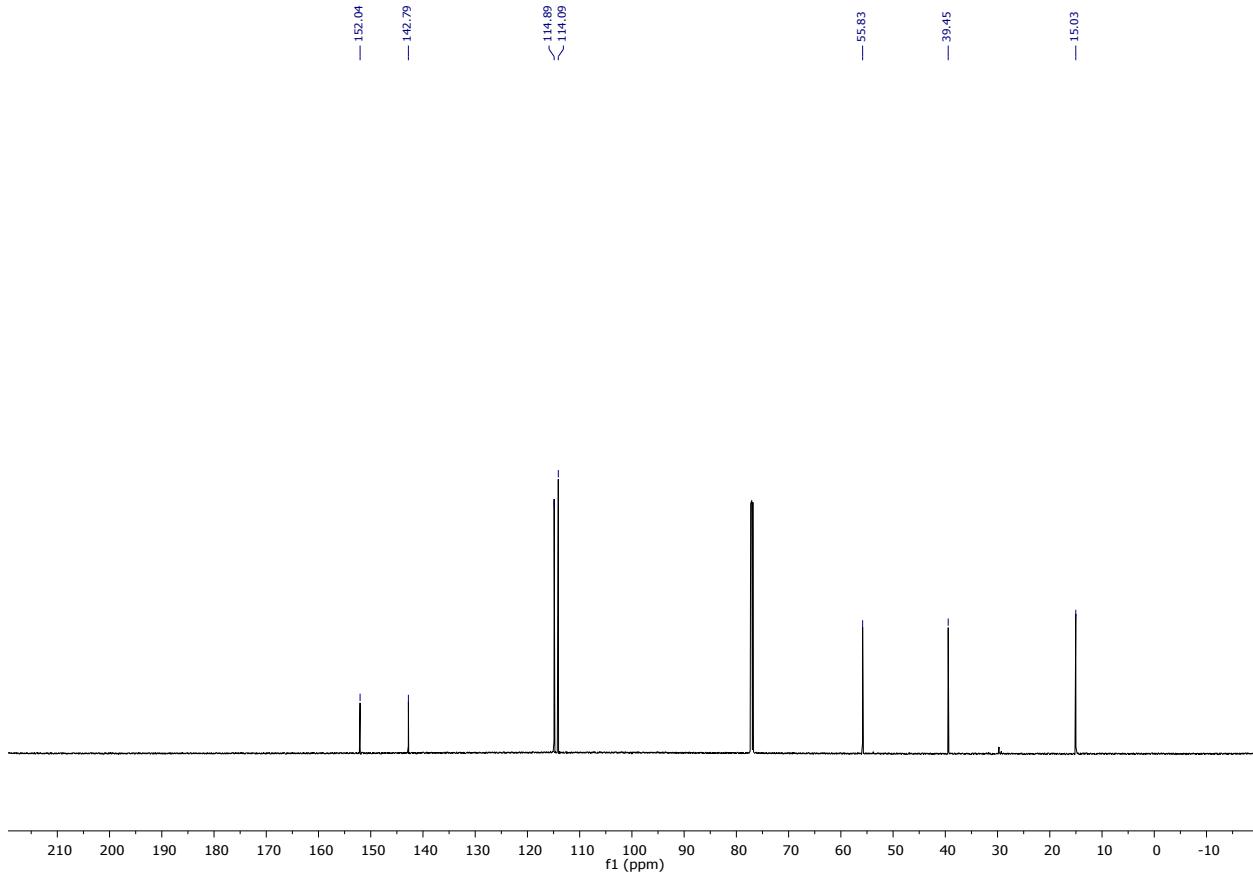




¹H NMR (600 MHz, CDCl₃):



¹³C NMR (151 MHz, CDCl₃):



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