

Supporting Information

Ligand-Controlled Nickel-Catalyzed C–O Bond Cleavage of Silyl Enol Ether for the Divergent Synthesis of Aryl Alkenes and Silicon-Containing Product

Shunqin Chang,^{‡a} Yueping Lin,^{‡a} Pei Gu,^b Changhui Lu,^a Minyan Wang,^{b,*} Liangbin Huang^{a,*}

^a State Key Laboratory of Pulp and Paper Engineering and Key Laboratory of Functional Molecular Engineering of Guangdong Province in School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, P. R. China.

^b State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, P. R. China

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I. General Information

Reagents

All compounds were used as received unless otherwise noted.

Metals and Ligand:

All metal catalysts and ligands, unless otherwise noted, were stored and handled in a nitrogen-filled glovebox. Ni(cod)₂ was purchased from *Energy Chemical* and used as received. Other catalyst in condition optimization table were Ni(acac)₂ (*Energy Chemical*), NiBr₂(dme) (*Energy Chemical*) and Ni(OTf)₂ (*Energy Chemical*). The ligands used were PCy₃ (*Laajoo*), PPh₃ (*Energy Chemical*), P^tBu₃ (*Energy Chemical*), Xantphos (*Bidepharm*), DPPF (*Bidepharm*), bpy (*Laajoo*), ICy-HCl (*Innochem*), IPr-HCl (*Energy Chemical*), **L13** (*Laajoo*), **L14** (*Innochem*), **L15** (*Bidepharm*).

Solvents:

The solvent 1,4-dioxane, CH₃CN, toluene, DMF and cyclopentyl methyl ether (CPME) were purchased from *Energy Chemical*. Tetrahydrofuran (THF) was distilled from sodium/benzophenone and stored under nitrogen before use.

Analytical Methods

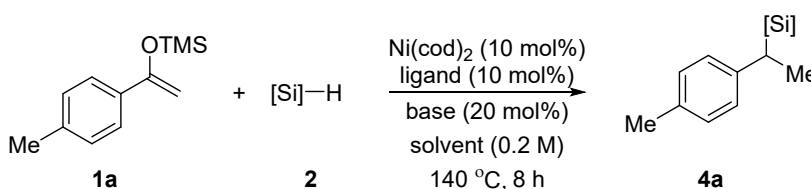
¹H nuclear magnetic resonance (NMR) spectroscopy chemical shifts are reported in ppm and referenced to TMS (tetramethylsilane) in CDCl₃ (δ = 0 ppm) or the residual solvent peak for CDCl₃ (δ = 7.26 ppm). For ¹³C NMR chemical shifts, the residual solvent peak (CDCl₃, δ = 77.00 ppm) were used as references. NMR spectra were recorded on Avance Bruker NMR spectrometers operating at either 400 MHz or 500 MHz and data analysis was performed using the MestReNova software. Chemical shifts are reported in parts per million (ppm), multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and br (broad). Coupling constants (J) are reported in Hertz. Melting points were measured using a melting point instrument. IR spectra were obtained with an infrared spectrometer on either potassium bromide

pellets or liquid films between two potassium bromide pellets. GC analyses were performed on an Agilent 7890B GC equipped with HP-5 columns (30 m × 320 μm × 0.25 μm), FID detectors, and hydrogen as the carrier gas. A sample volume of 1 μL was injected at a temperature of 250 °C and a 15:1 split ratio. The initial inlet pressure was 2.7 psi but varied as the column flow was held constant at 1 mL/min for the duration of the run. The initial oven temperature of 60 °C was held for 0 min followed by a temperature ramp of 50 °C/min up to 300 °C. The temperature was held at 300 °C for 6 min. The total run time was ~10.8 min and the FID temperature was 300 °C. GC/MS analyses were performed on a Shimadzu GCMS-QP2010SE equipped with an RTX-5MS column (30 m × 0.25 mm × 0.25 μm) with a quadrupole mass analyzer using helium as the carrier gas. The analysis method used in all cases was 5 μL injection of sample, an injection temp of 250 °C, and no split ratio. The initial inlet pressure was 7.8 psi, but varied as the column flow was held constant at 1.7 mL/min for the duration of the run. The interface temperature was held at 250 °C, and the ion source (EI+, 30 eV) was held at 250 °C. The initial oven temperature was held at 50 °C for 1 min with the detector off, followed by a temperature ramp, with the detector on, to 250 °C at 30 °C /min. The temperature was held at 250 °C for 0 min, then to 280 °C and held for 7 min. Total run time was 16.2 min. High resolution mass spectra (HRMS) was carried out on an electrospray (ESI+) ionization methods (ESI-quadrupole). Thin layer chromatography was performed on TLC Silica Gel 60 F254 plates. Visualization was accomplished with potassium permanganate after inspection under UV light. Flash chromatography was performed using silica gel 60, particle size 0.040-0.063 mm using standard flash techniques.

Procedure

All reactions were conducted in oven-dried Schlenk tubes. All the reaction temperatures reported are oil bath temperatures. Unless otherwise specified, all reactions are carried out in nitrogen atmosphere.

Table S3. Screening of reaction conditions for synthesis of benzylic silane silane^a



Entry	[Si]-H	Ligand	Base	Solvent	Yield (%) ^b
1	Et ₃ SiH	L5	LiO ^t Bu	1,4-dioxane	62
2	(EtO) ₃ SiH	L5	LiO ^t Bu	1,4-dioxane	n.d.
3	ⁱ Pr ₃ SiH	L5	LiO ^t Bu	1,4-dioxane	n.d.
4	(EtO) ₂ MeSiH	L5	LiO ^t Bu	1,4-dioxane	n.d.
5	Ph ₂ MeSiH	L5	LiO ^t Bu	1,4-dioxane	n.d.
6	PhSiH ₃	L5	LiO ^t Bu	1,4-dioxane	n.d.
7	Et ₃ SiH	L9	LiO ^t Bu	1,4-dioxane	45
8	Et ₃ SiH	L10	LiO ^t Bu	1,4-dioxane	n.d.
9	Et ₃ SiH	L11	LiO ^t Bu	1,4-dioxane	21
10	Et ₃ SiH	L12	LiO ^t Bu	1,4-dioxane	n.d.
11	Et ₃ SiH	L13	LiO ^t Bu	1,4-dioxane	trace
12	Et ₃ SiH	L14	LiO ^t Bu	1,4-dioxane	n.d.
13	Et ₃ SiH	L15	LiO ^t Bu	1,4-dioxane	n.d.
14	Et ₃ SiH	L5	KO ^t Bu	1,4-dioxane	trace
15	Et ₃ SiH	L5	NaO ^t Bu	1,4-dioxane	4
16	Et ₃ SiH	L5	Cs ₂ CO ₃	1,4-dioxane	6
17	Et ₃ SiH	L5	K ₃ PO ₄	1,4-dioxane	n.d.
18	Et ₃ SiH	L5	LiO ^t Bu	THF	35
19	Et ₃ SiH	L5	LiO ^t Bu	CPME	43
20	Et ₃ SiH	L5	LiO ^t Bu	toluene	15
21	Et ₃ SiH	L5	LiO ^t Bu	CH ₃ CN	trace
22	Et ₃ SiH	L5	LiO ^t Bu	DMF	trace
23 ^c	Et ₃ SiH	L5	LiO ^t Bu	1,4-dioxane	43

^aReaction conditions: **1a** (0.1 mmol), [Si]-H **2** (4 equiv), catalyst (10 mol%), ligand (10 mol%), base (20 mol%), solvent (0.5 mL). ^bDetermined by GC analysis with *n*-

dodecane as an internal standard. $c_{120}^{\circ}\text{C}$.

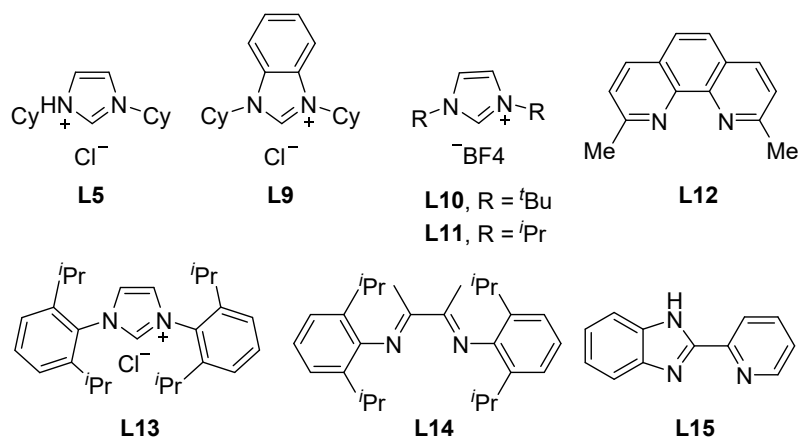
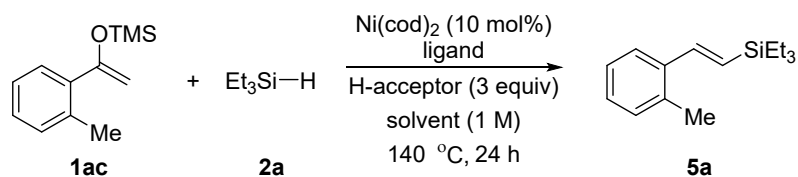


Table S4. Screening of reaction conditions for synthesis of vinyl silane^a



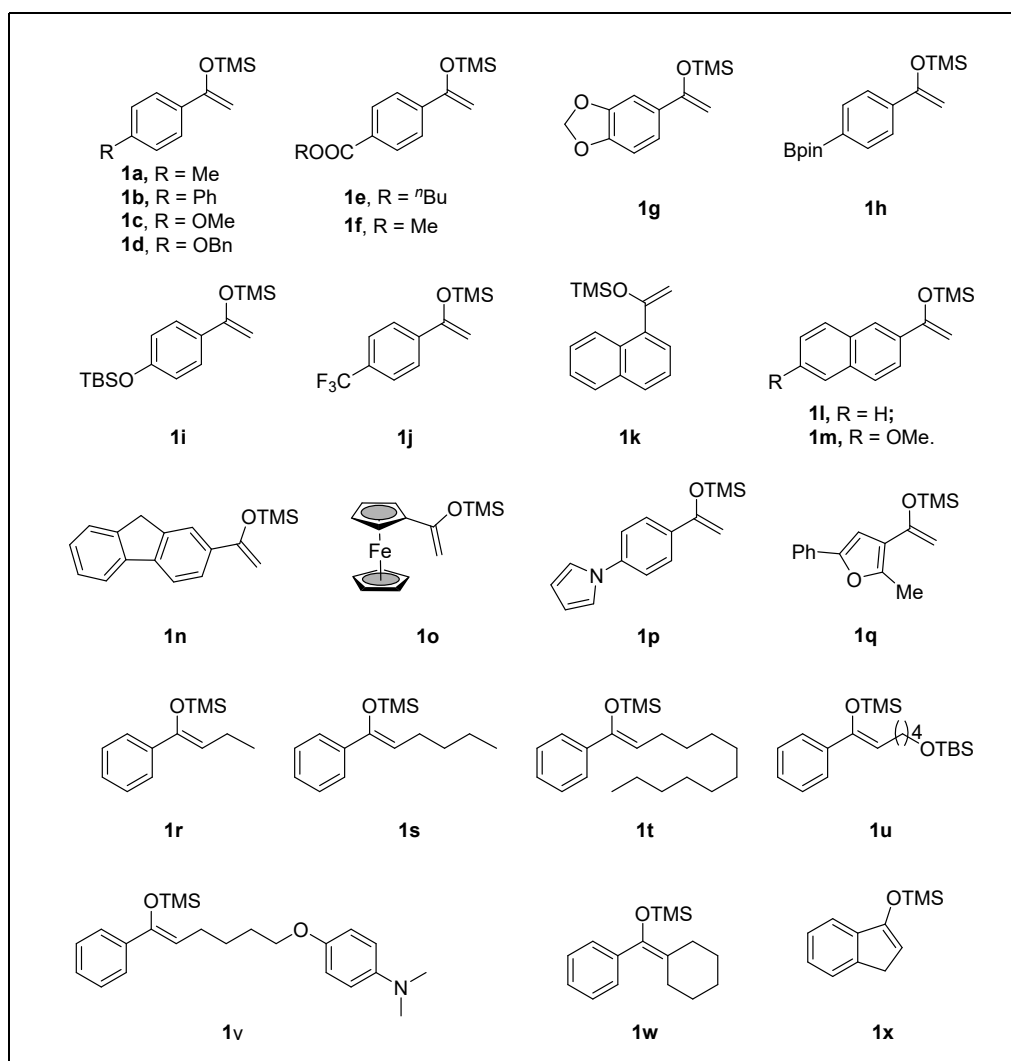
Entry	Ligand	H-acceptor (3 equiv)	Solvent (0.1 mL)	Yield (%) ^b
1	PCy ₃ (20 mol%)	1-octene	1,4-dioxane	3
2	PPh ₃ (20 mol%)	1-octene	1,4-dioxane	n.d.
3	P ^t Bu ₃ (20 mol%)	1-octene	1,4-dioxane	n.d.
4	dppe (10 mol%)	1-octene	1,4-dioxane	n.d.
5	ICy-HCl (10 mol%)	1-octene	1,4-dioxane	n.d.
6	PCy ₃ (20 mol%)	NBE	1,4-dioxane	39
7	PCy ₃ (20 mol%)	styrene	1,4-dioxane	n.d.
8	PCy ₃ (20 mol%)	1-octene	CPME	72(69) ^c
9	PCy ₃ (20 mol%)	1-octene	THF	10
10	PCy ₃ (20 mol%)	1-octene	toluene	n.d.

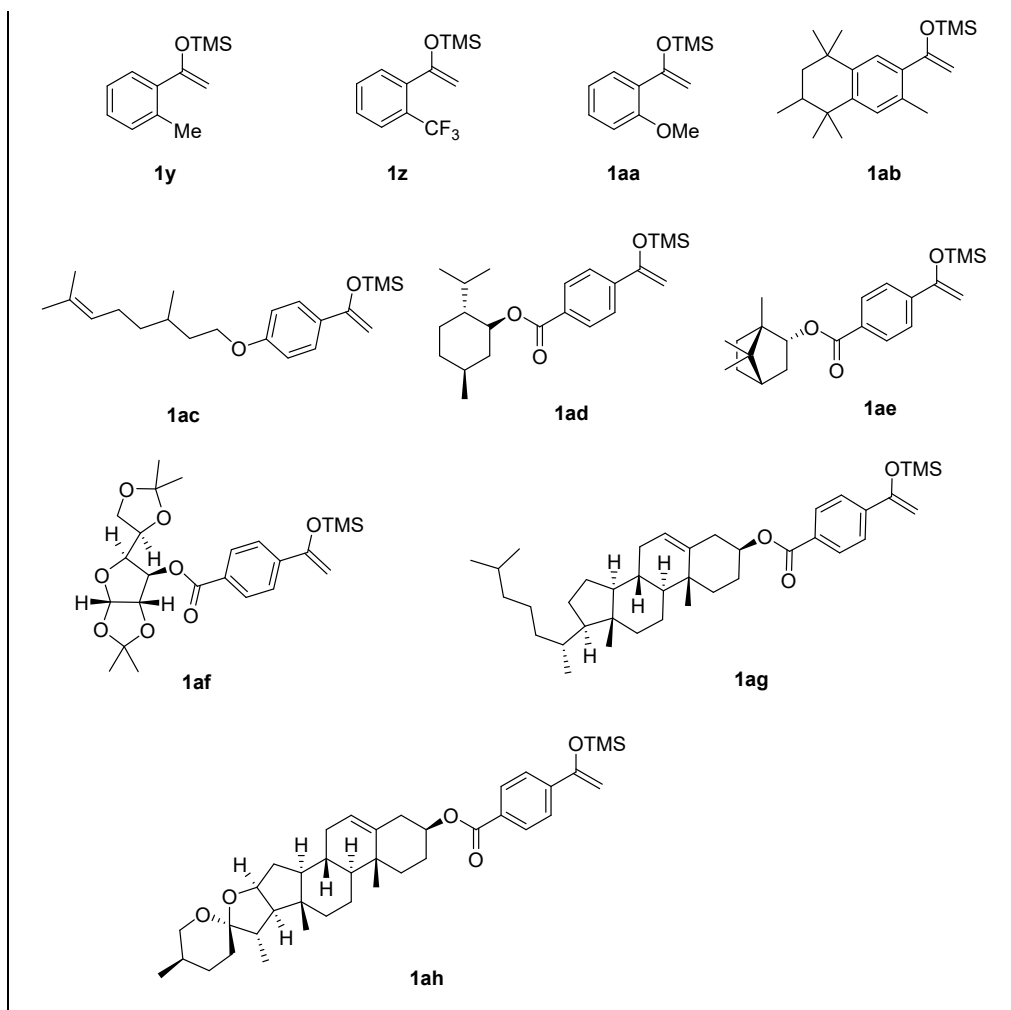
^aReaction conditions: **1ac** (0.1 mmol), **2a** (5 equiv), Ni(cod)₂ (10 mol%), ligand, H-acceptor (3 equiv), solvent (0.1 mL). ^bDetermined by GC analysis with *n*-dodecane as an internal standard. ^cIsolated yield.

III. Methods for the Synthesis.

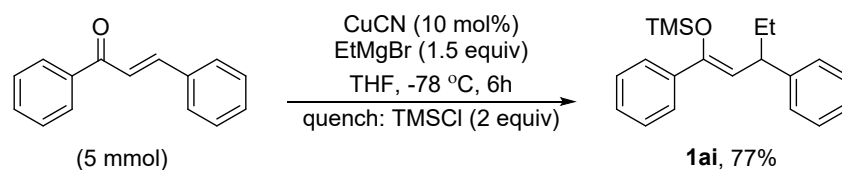
(1) General Procedure A: Synthesis of silyl enol ether **1**

The silyl enol ether compounds used here were synthesized according to known protocols.¹ A 100 mL round-bottom flask containing mixture of the corresponding ketone (25 mmol) and sodium iodide (30 mmol, 4.5 g) was evacuated and backfilled with argon three times. Dry acetonitrile (30 mL) was added and the mixture stirred for 5 min at room temperature. After this, triethylamine (30 mmol, 4.2 mL) and chlorotrimethylsilane (30 mmol, 3.82 mL) were added. The reaction mixture was stirred overnight at room temperature. After the reaction, the reaction liquid is evaporated and petroleum ether is added. The filtrate obtained by filtering is silyl enol ether after concentration, which can be used without purification.





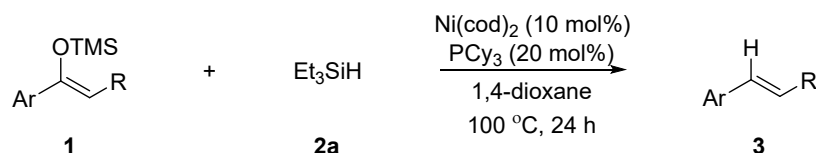
(2) Procedure B: Synthesis of silyl enol ethers **1ai**



Copper cyanide (0.5 mmol, 10 mol%, 44.5 mg) was added to a flame-dried Schlenk flask followed by anhydrous tetrahydrofuran (0.3 M) and the mixture was stirred at room temperature for 10 min. The mixture was cooled to -78°C and subsequently the appropriate Grignard reagent (7.5 mmol, 1.5 equiv) was added dropwise. The reaction mixture was stirred at -78°C for an additional 10 min. After this time, a solution of trans-chalcone (5 mmol, 1.0 equiv, 1.04g) in anhydrous tetrahydrofuran (1 M) was added dropwise over 1 h. The reaction mixture was stirred for 6 h and the resulting enolate was quenched by the addition of chlorotrimethylsilane (10 mmol, 2 equiv,

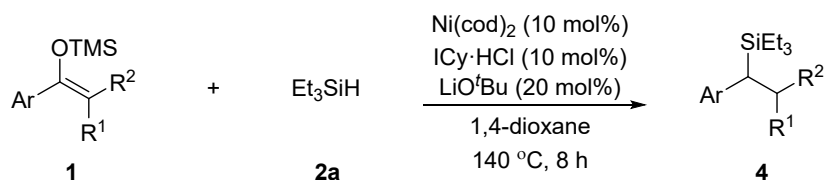
1.08 g), allowing the system to reach room temperature while stirring for additional 1 h. After this time, saturated aqueous solution of ammonium chloride was added to the reaction mixture and the layers were separated. The aqueous layer was extracted with ethyl acetate (three times). The combined organic layers were dried over magnesium sulfate, filtered and the solvent was evaporated under reduced pressure.

(3) General Procedure C: Synthesis of olefin from silyl enol ethers



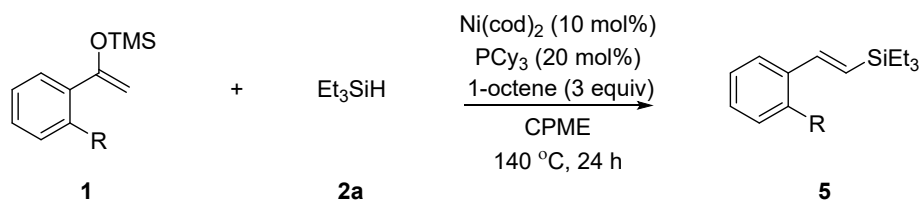
To an oven-dried 10-mL sealed tube equipped with a magnetic stir bar were subsequently added with Ni(cod)₂ (10 mol%), PCy₃ (20 mol%), Et₃SiH **2a** (1 mmol) and silyl enol ether **1** (0.5 mmol), then 1,4-dioxane (5 mL) was added, the mixture was stirred at 100 °C for 24 h. After the reaction, the reaction was quenched by ethyl acetate (1.5 mL) and evaporated. The desired products **3** were purified by flash chromatography on silica gel (petroleum ether/EtOAc = pure PE - 10:1).

(4) General Procedure D: Synthesis of benzyl silane from silyl enol ethers



To an oven-dried 10-mL sealed tube equipped with a magnetic stir bar were subsequently added with Ni(cod)₂ (10 mol%), ICy·HCl (10 mol%), LiO^tBu (20 mol%), 1,4-dioxane (2.5 mL) was added and the mixture was stirred at room temperature for 5min. Then Et₃SiH **2a** (2 mmol) and silyl enol ether **1** (0.5 mmol), the mixture was stirred at 140 °C for 8 h. After the reaction, the reaction was quenched by ethyl acetate (1.5 mL) and evaporated. The desired products **4** were purified by flash chromatography on silica gel (petroleum ether/EtOAc = pure PE - 10:1).

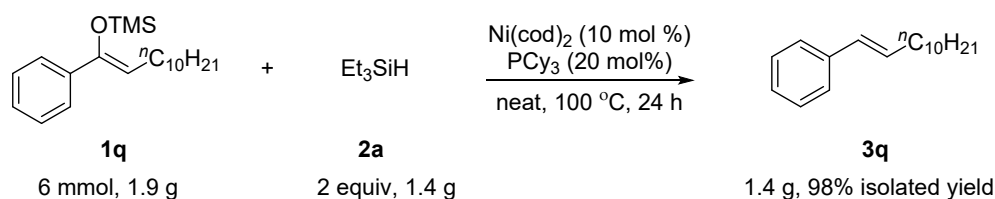
(5) General Procedure E: Synthesis of alkenyl silane from silyl enol ethers



To an oven-dried 10-mL sealed tube equipped with a magnetic stir bar were subsequently added with Ni(cod)₂ (10 mol%), PCy₃ (20 mol%), Et₃SiH **2a** (2.5 mmol), 1-octene (3 equiv) and silyl enol ether **1** (0.5 mmol), then CPME (cyclopentyl methyl ether) (0.5 mL) was added, the mixture was stirred at 140 °C for 24 h. After the reaction, the reaction was quenched by ethyl acetate (1 mL) and evaporated. The desired products **5** were purified by flash chromatography on silica gel (petroleum ether/EtOAc = PE - 20:1).

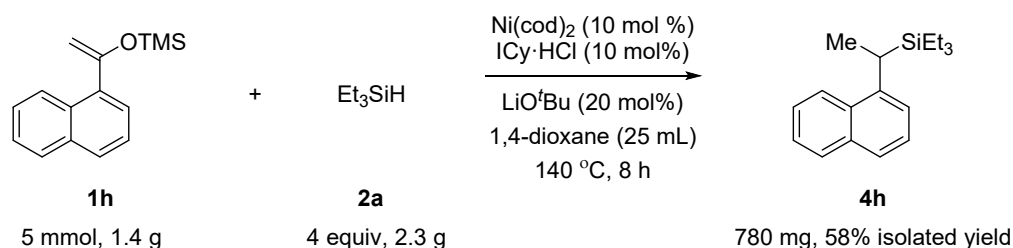
IV. Gram Scale Reactions

a) Hydrogenation of Silicon Enol Ether



To an oven-dried 10-mL sealed tube equipped with a magnetic stir bar were subsequently added with Ni(cod)₂ (10 mol%), PCy₃ (20 mol%), Et₃SiH (12 mmol) and **1q** (6 mmol), the mixture was stirred at 100 °C for 24 h. After the reaction, the reaction was quenched by ethyl acetate (3 mL) and evaporated. The desired products **3q** (1.4 g, 98% yield) were purified by flash chromatography on silica gel with petroleum ether.

b) Hydrosilylation of Silicon Enol Ether

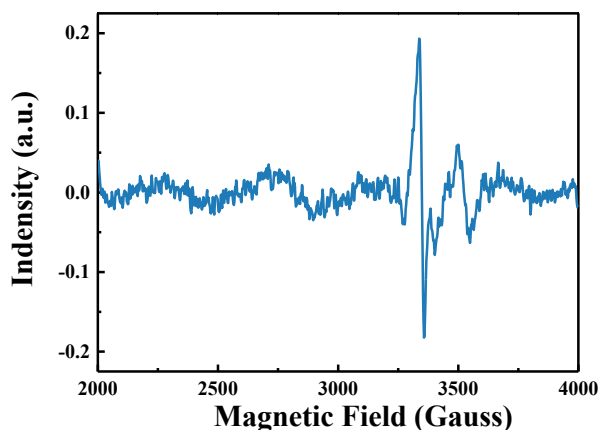


To an oven-dried 100-mL round bottom flask equipped with a magnetic stir bar were subsequently added with Ni(cod)₂ (10 mol%), ICy·HCl (10 mol%), LiO^tBu (20 mol%), 1,4-dioxane (25 mL) was added and the mixture was stirred at room temperature for 5 min. Then Et₃SiH (20 mmol) and **1h** (5 mmol), the mixture was stirred at 140 °C for 8 h. After the reaction, the reaction was quenched by ethyl acetate (10 mL) and evaporated. The desired products **4h** (780 mg, 58% yield) were purified by flash chromatography on silica gel with petroleum ether.

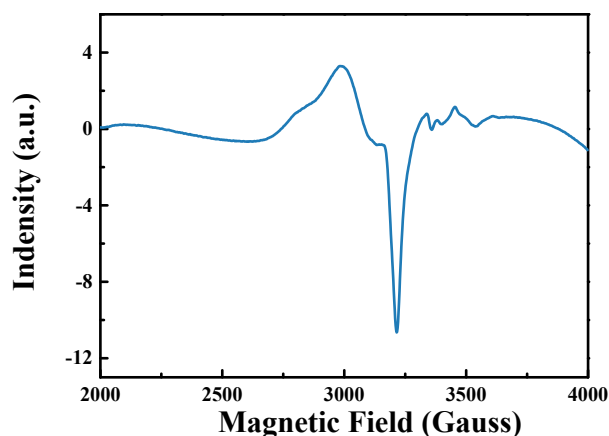
V. The Mechanism Researches and DFT Calculation

a) EPR experiments

To an oven-dried 10-mL sealed tube equipped with a magnetic stir bar were subsequently added with Ni(cod)₂ (10 mol%), PCy₃ (20 mol%), **1a** (0.5 mmol) and Et₃SiH (1.0 mmol), then 1,4-dioxane (0.5 mL) was added, the mixture was stirred at 100 °C for 3 h. After cooling, 0.2 mL of this solution was subjected to EPR measurements at 100 K under N₂.

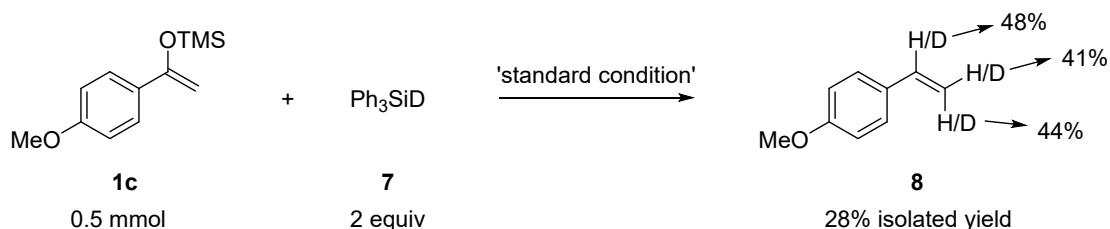


To an oven-dried 10-mL sealed tube equipped with a magnetic stir bar were subsequently added with Ni(cod)₂ (10 mol%), ICy·HCl (10 mol%), LiOtBu (20 mol%), **1a** (0.5 mmol) and Et₃SiH (2.0 mmol), then 1,4-dioxane (0.5 mL) was added, the mixture was stirred at 140 °C for 6 h. After cooling, 0.2 mL of this solution was subjected to EPR measurements at 100 K under N₂.

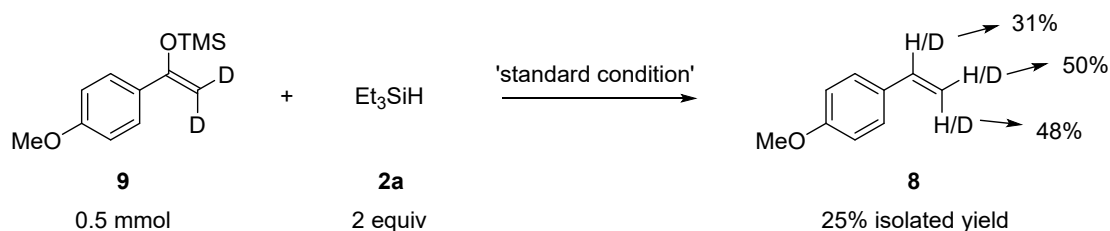


As shown in the figures, characteristic EPR spectra for Ni(I) species were obtained.

b) Deuterium-labeling experiment



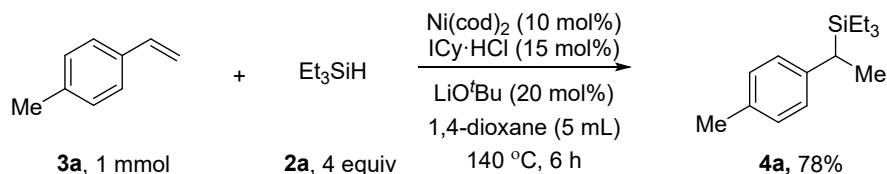
To an oven-dried 10-mL sealed tube equipped with a magnetic stir bar were subsequently added with Ni(cod)₂ (10 mol%), PCy₃ (20 mol%), **7** (1 mmol) and **1c** (0.5 mmol), then 1,4-dioxane (5 mL) was added, the mixture was stirred at 100 °C for 24 h. After the reaction, the reaction was quenched by ethyl acetate (2 mL) and evaporated. The desired products **8** were purified by flash chromatography on silica gel (petroleum ether/EtOAc = PE - 10:1).



To an oven-dried 10-mL sealed tube equipped with a magnetic stir bar were subsequently added with Ni(cod)₂ (10 mol%), PCy₃ (20 mol%), **2a** (1 mmol) and **9** (0.5 mmol), then 1,4-dioxane (5 mL) was added, the mixture was stirred at 100 °C for 24 h. After the reaction, the reaction was quenched by ethyl acetate (2 mL) and

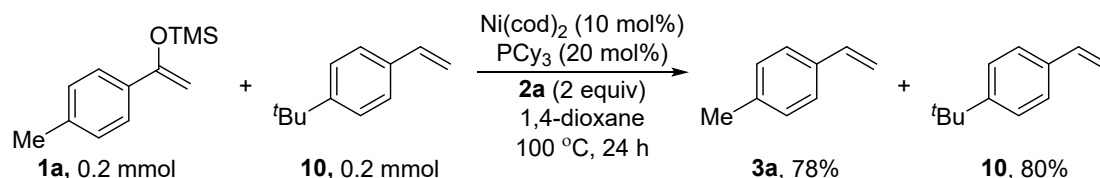
evaporated. The desired products **8** were purified by flash chromatography on silica gel (petroleum ether/EtOAc = pure PE - 10:1).

c) Hydrosilylation of styrene

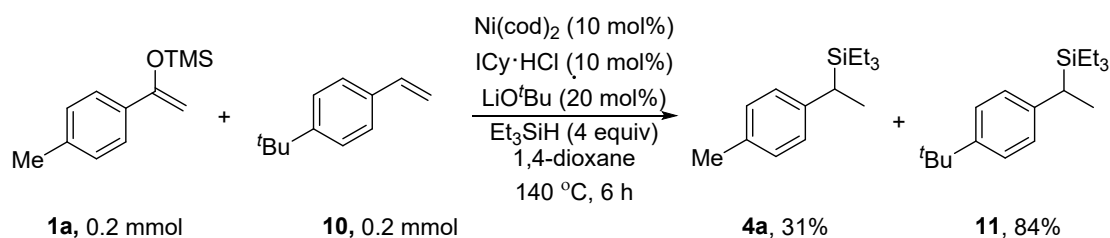


To an oven-dried 10-mL sealed tube equipped with a magnetic stir bar were subsequently added with $\text{Ni}(\text{cod})_2$ (10 mol%), $\text{ICy}\cdot\text{HCl}$ (15 mol%), LiO^tBu (20 mol%), 1,4-dioxane (5 mL) was added and the mixture was stirred at room temperature for 5min. Then **2a** (2 mmol) and **3a** (0.5 mmol) was added, the mixture was stirred at 140 °C for 8 h. After the reaction, the reaction was quenched by ethyl acetate (2 mL) and evaporated. The desired products **4a** were purified by flash chromatography on silica gel (petroleum ether/EtOAc = pure PE - 10:1).

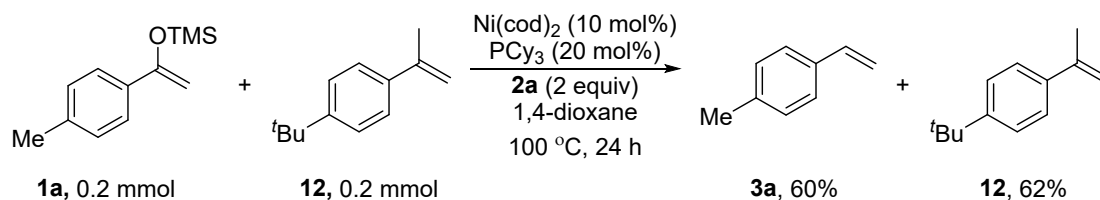
d) Competition experiment



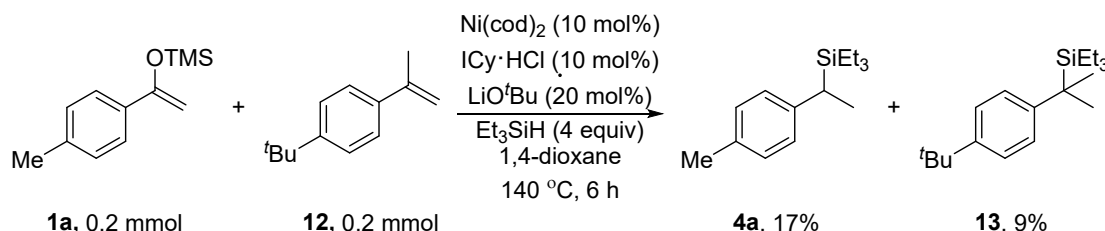
To an oven-dried 10-mL sealed tube equipped with a magnetic stir bar were subsequently added with $\text{Ni}(\text{cod})_2$ (10 mol%), PCy_3 (20 mol%), LiO^tBu (20 mol%), 1,4-dioxane (5 mL) was added and the mixture was stirred at room temperature for 5min. Then **1a** (0.2 mmol), **10** (0.2 mmol), and **2a** (0.4 mmol) was added, the mixture was stirred at 100 °C for 24 h. After the reaction, *n*-dodecane was added as internal standard and the products were determined by GC analysis.



To an oven-dried 10-mL sealed tube equipped with a magnetic stir bar were subsequently added with Ni(cod)₂ (10 mol%), ICy·HCl (15 mol%), LiO^tBu (20 mol%), 1,4-dioxane (5 mL) was added and the mixture was stirred at room temperature for 5min. Then **1a** (0.2 mmol), **10** (0.2 mmol), and **2a** (0.8 mmol) was added, the mixture was stirred at 140 °C for 6 h. After the reaction, *n*-dodecane was added as internal standard and the products were determined by GC analysis.



To an oven-dried 10-mL sealed tube equipped with a magnetic stir bar were subsequently added with Ni(cod)₂ (10 mol%), PCy₃ (20 mol%), LiO^tBu (20 mol%), 1,4-dioxane (5 mL) was added and the mixture was stirred at room temperature for 5min. Then **1a** (0.2 mmol), **12** (0.2 mmol), and **2a** (0.4 mmol) was added, the mixture was stirred at 100 °C for 24 h. After the reaction, *n*-dodecane was added as internal standard and the products were determined by GC analysis.



To an oven-dried 10-mL sealed tube equipped with a magnetic stir bar were subsequently added with Ni(cod)₂ (10 mol%), ICy·HCl (15 mol%), LiO^tBu (20 mol%), 1,4-dioxane (5 mL) was added and the mixture was stirred at room temperature for 5min. Then **1a** (0.2 mmol), **12** (0.2 mmol), and **2a** (0.8 mmol) was added, the mixture was stirred at 140 °C for 6 h. After the reaction, *n*-dodecane was added as internal standard and the products were determined by GC analysis.

e) Determination of the orders of the reaction

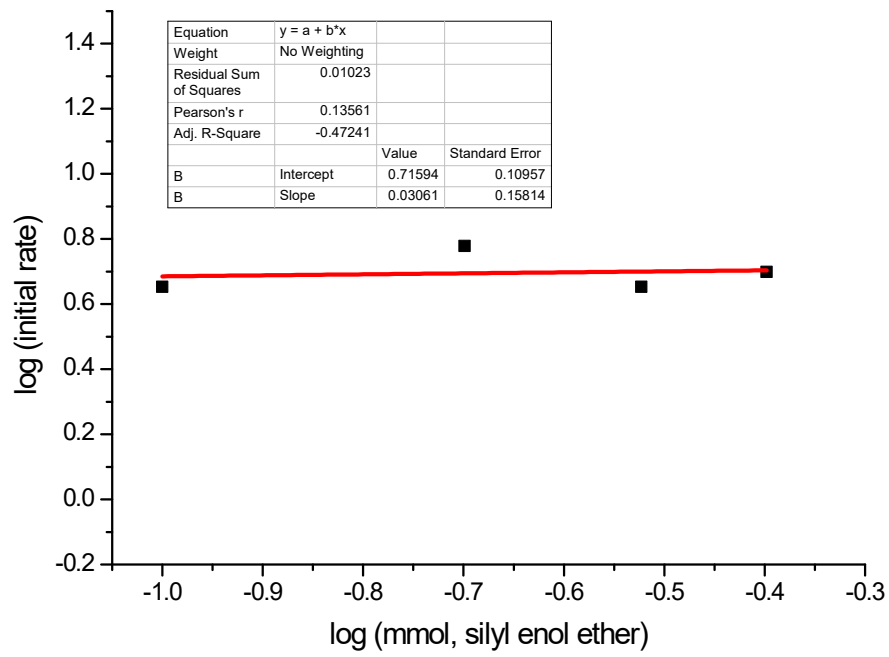
General procedure for kinetic experiments.

Kinetic experiments were run inside a N₂ filled glovebox. The data (product

yield versus time) was analyzed using the initial rates method. A significant enhancement on the initial rates with the concentration of catalyst and HSiEt_3 observed, therefore ruling out order 0 of these parameters. For silyl enol ether, it exhibits nearly zero-order dependence on their concentration. These kinetic results indicate that silyl enol ether is not involved in the rate determining step.

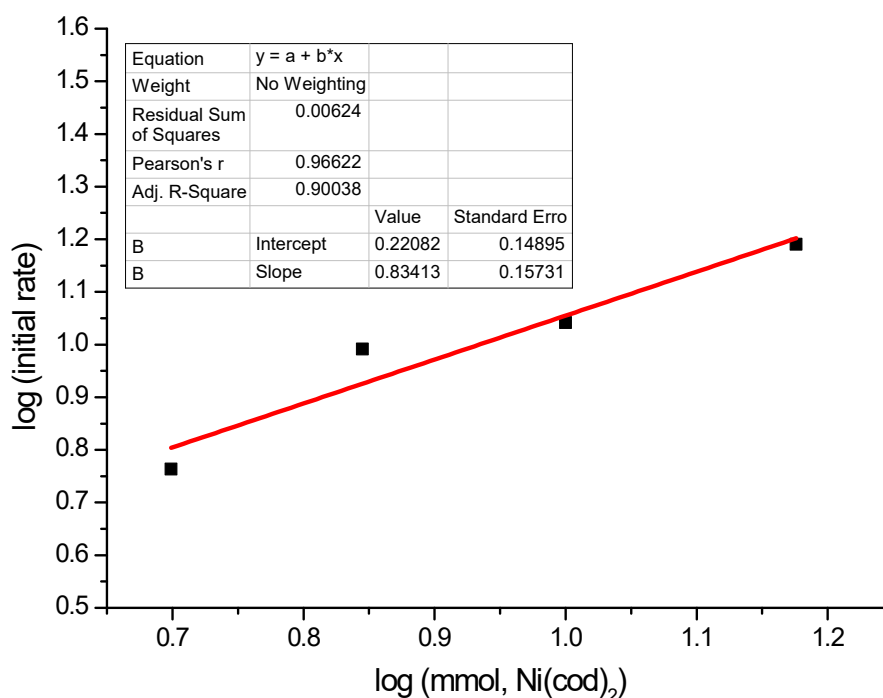
Investigate the reaction order of silyl enol ether

The order in silyl enol ether **1a** was determined by studying the initial rate of reactions with different **1a**. To an oven-dried 15 mL Schleck tube, equipped with a magnetic stir bar, was added silyl enol ether (0.2, 0.3, 0.4, 0.5 mmol), $\text{Ni}(\text{cod})_2$ (0.02 mmol), PCy_3 (0.04 mmol), Et_3SiH (47 mg, 0.4 mmol) and *n*-dodecane in 1,4-dioxane (2 mL), and the reaction was heated at 100 °C. Aliquots were taken out with a needle at 1 min, 1.5 min, 2 min, 2.5 min, 3 min, and 3.5 min, immediately filtered through a plug of SiO_2 washing with ethyl acetate. Product yield from the corresponding reaction was monitored by GC analysis using *n*-dodecane as internal standard in the indicated interval based on the amount of Et_3SiH . Using different amounts of silyl enol ether (0.2, 0.3, 0.4, 0.5 mmol). A log plot of initial rate versus $\log [\mathbf{1a}]$ gave a straight line ($R = -0.47241$), indicative of 0.03 order dependence on $[\mathbf{1a}]$. The results were shown in below.



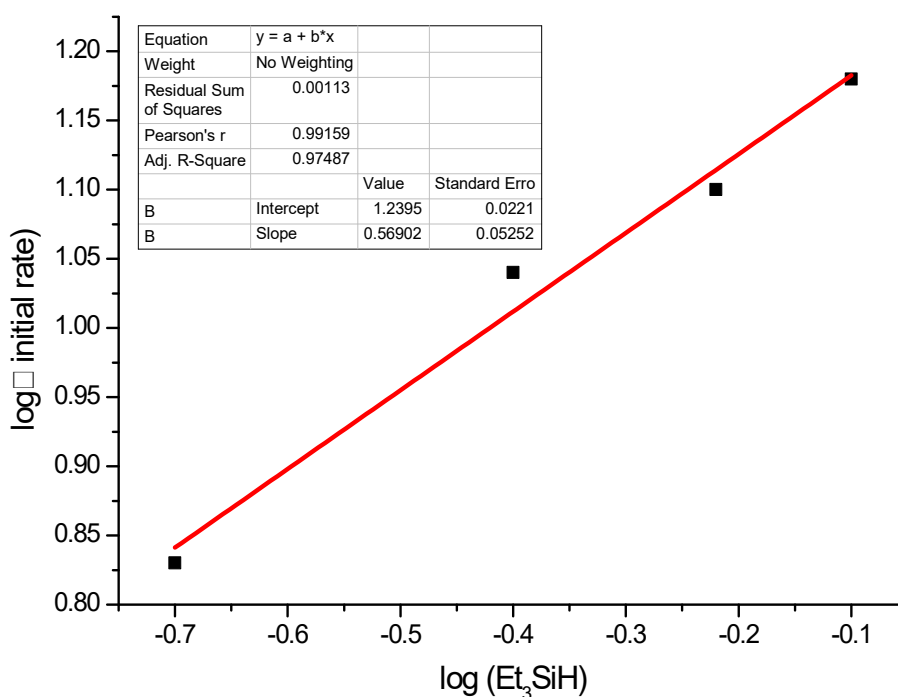
Investigate the reaction order of Ni(cod)₂

The order in Ni(cod)₂ was determined by studying the initial rate of reactions with different Ni(cod)₂. To an oven-dried 15 mL Schleck tube, equipped with a magnetic stir bar, was added silyl enol ether (0.2 mmol), Ni(cod)₂ (0.01, 0.02, 0.03, 0.04 mmol), PCy₃ (0.04 mmol), Et₃SiH (47 mg, 0.4 mmol) and *n*-dodecane in 1,4-dioxane (2 mL), and the reaction was heated at 100 °C. Aliquots were taken out with a needle at 1 min, 2 min, 3 min, 4 min, 5 min, and 6 min, immediately filtered through a plug of SiO₂ washing with ethyl acetate. Product yield from the corresponding reaction was monitored by GC analysis using *n*-dodecane as internal standard in the indicated interval based on the amount of silyl enol ether. Using different amounts of Ni(cod)₂ (0.01, 0.02, 0.03, 0.04 mmol). A log plot of initial rate versus log [Ni(cod)₂] gave a straight line (R = 0.90038), indicative of 0.83 order dependence on [Ni(cod)₂]. The results were shown in below.



Investigate the reaction order of Et₃SiH

The order in Et₃SiH was determined by studying the initial rate of reactions with different Et₃SiH. To an oven-dried 15 mL Schleck tube, equipped with a magnetic stir bar, was added silyl enol ether (0.2 mmol), Ni(cod)₂ (0.02 mmol), PCy₃ (0.04 mmol), Et₃SiH (0.2, 0.4, 0.6, 0.8 mmol) and *n*-dodecane in 1,4-dioxane (2 mL), and the reaction was heated at 100 °C. Aliquots were taken out with a needle at 1 min, 2 min, 3 min, 4 min, 5 min, and 6 min, immediately filtered through a plug of SiO₂ washing with ethyl acetate. Product yield from the corresponding reaction was monitored by GC analysis using *n*-dodecane as internal standard in the indicated interval based on the amount of silyl enol ether. Using different amounts of Et₃SiH (0.2, 0.4, 0.6, 0.8 mmol). A log plot of initial rate versus log [Et₃SiH] gave a straight line (R = 0.97487), indicative of 0.57 order dependence on [Et₃SiH]. The results were shown in below.



f) DFT calculation

Density functional theory (DFT) calculations were performed using the Gaussian 09 package² to elaborate the detailed reaction mechanism of the Nickel-catalyzed ligand-controlled C–O bond cleavage of silyl enol ether **1a**. Geometry optimizations were carried out at the B3LYP³ level of theory with Grimme D3 correction⁴ in the gas phase. A mixed basis set was used with LANL08⁵ for Ni atom and 6-31G(d)⁶ for all other atoms. Furthermore, the single-point solvation energies of all stationary points were calculated with B3LYP-D3 functional and a mixed basis set of 6-311++G(d,p)⁷ for all nonmetal atoms and the SDD⁸ for Ni with continuum model SMD⁹ (solvent = 1,4-dioxane). The calculated optimized structures are visualized utilizing CYLview program¹⁰.

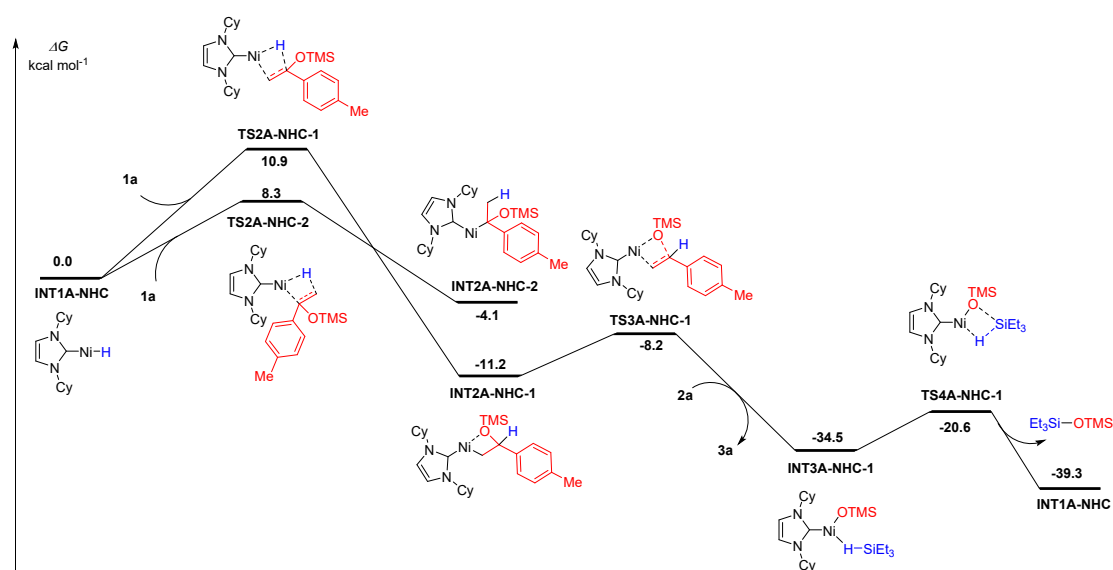


Fig. S1 The energy profile for the generation of **3a** in the presence of **INT1A-NHC**.

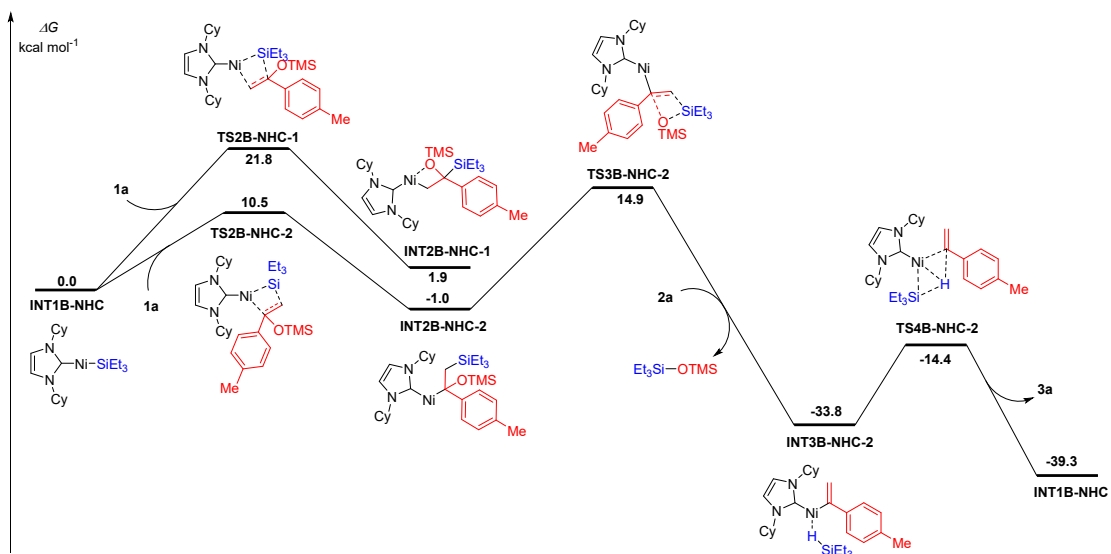


Fig. S2 The energy profile for the generation of 3a in the presence of INT1B-NHC.

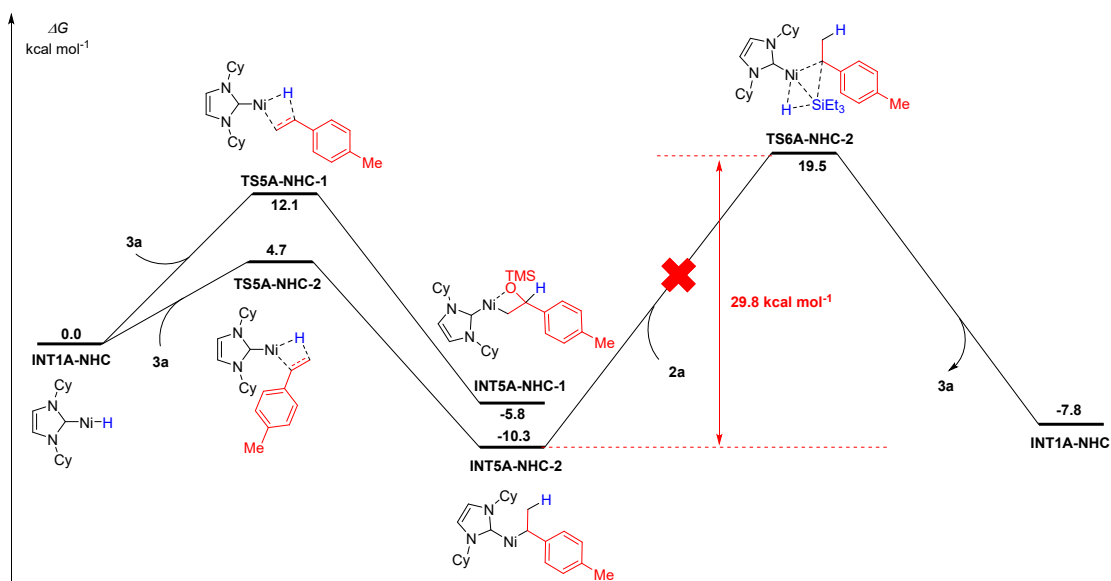
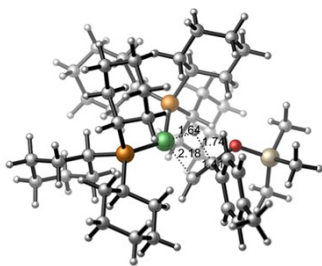
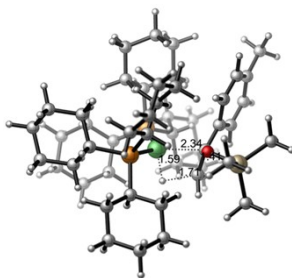


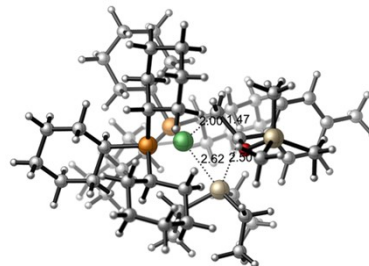
Fig. S3 The reaction between INT1A-NHC and 3a.



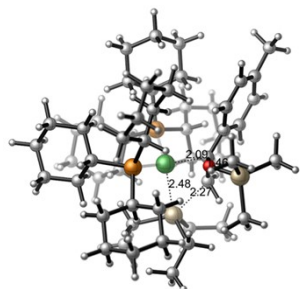
TS2A-1



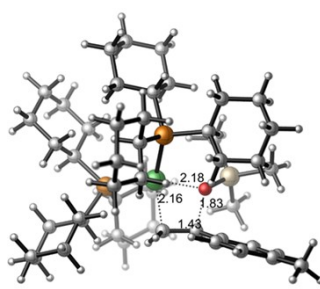
TS2A-2



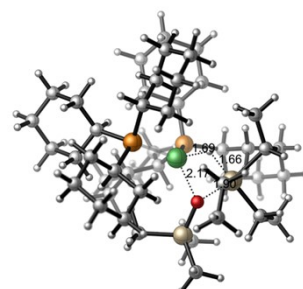
TS2B-1



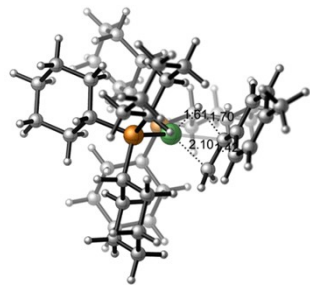
TS2B-2



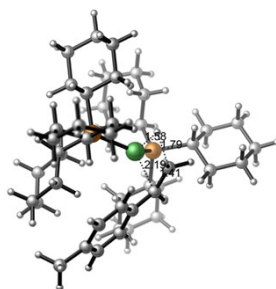
TS3A-1



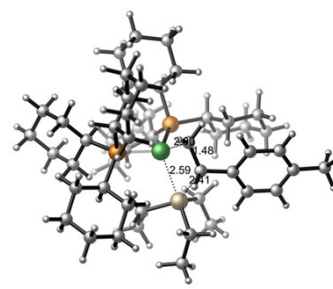
TS4A-1



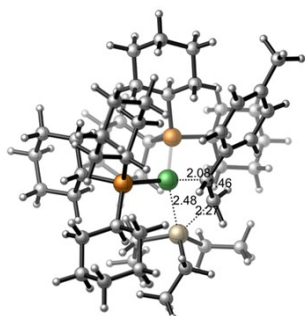
TS5A-1



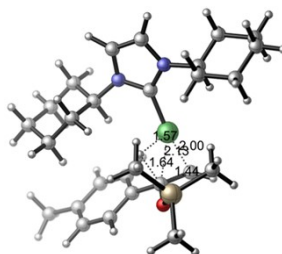
TS5A-2



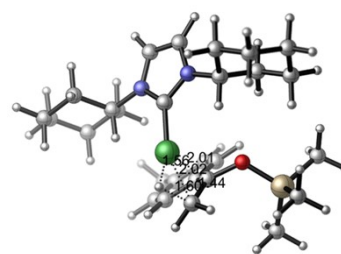
TS5B-1



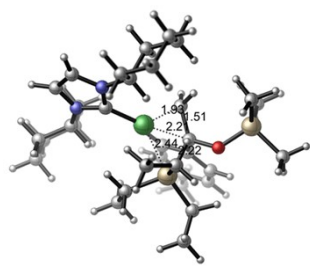
TS5B-2



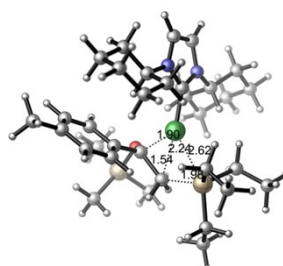
TS2A-NHC-1



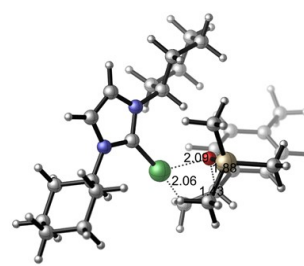
TS2A-NHC-2



TS2B-NHC-1



TS2B-NHC-2



TS3A-NHC-1

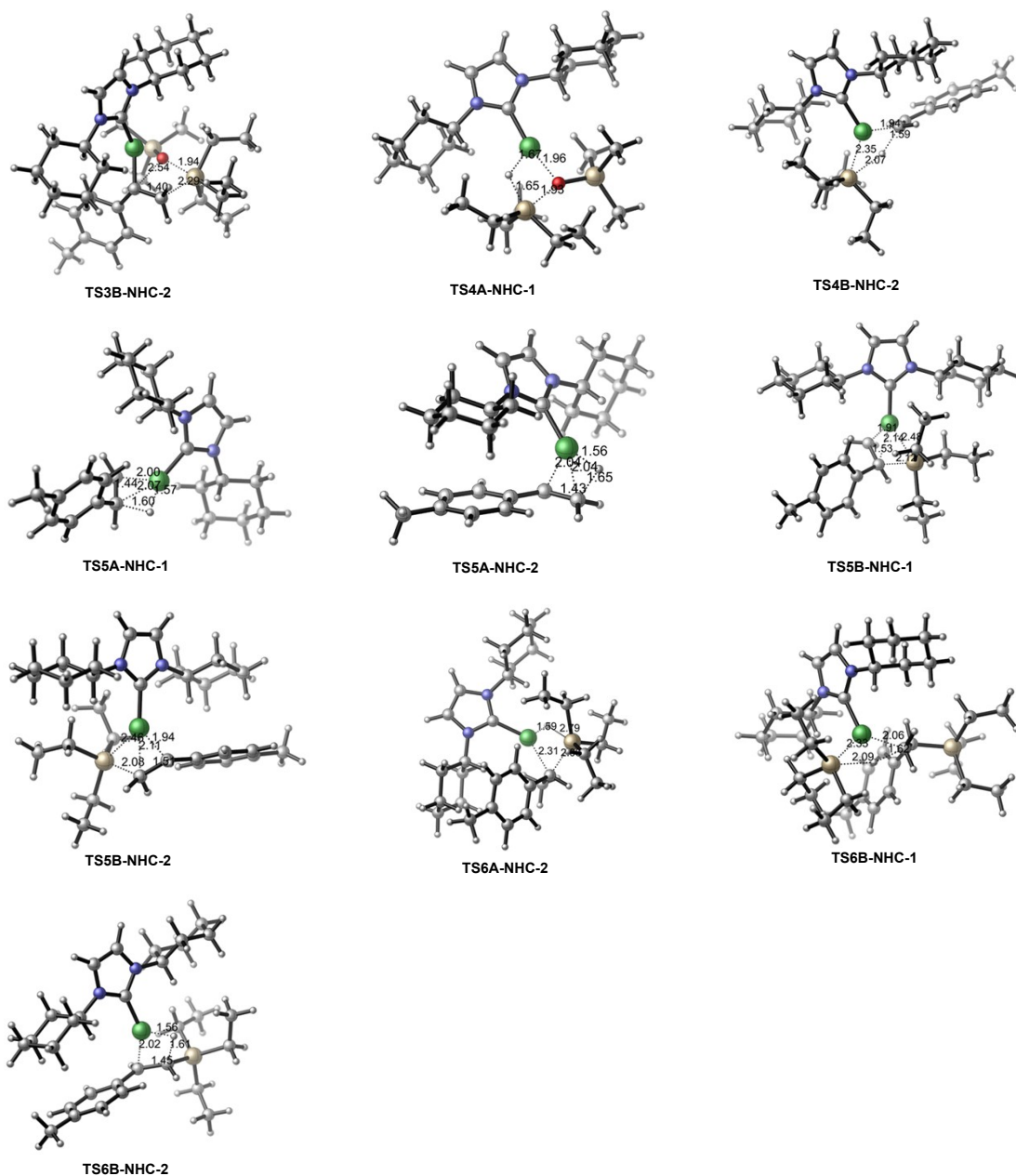


Fig. S4 Optimized structures of the key transition states. Distances are in Å.

Table S5. The calculated energies of stationary points (in Hartree/Particle), and vibrational frequencies of transitions states (in cm^{-1})

Structure	ZPE	H_{corr}	G_{corr}	E_{ele}	H_{sol}	G_{sol}
1a	0.267966	0.286336	0.220569	-833.108598	-832.822262	-832.888029
2a	0.207088	0.219394	0.169787	-527.908502	-527.689108	-527.738715
INT1A	0.983634	1.026970	0.907378	-2266.515848	-2265.488878	-2265.608470
INT1A-dimer	1.978482	2.063904	1.860310	-4533.090796	-4531.026892	-4531.230486
TS2A-1	1.257089	1.317588	1.162926	-3099.623292	-3098.305704	-3098.460366
INT2A-1	1.261147	1.322295	1.164553	-3099.666802	-3098.344507	-3098.502249
TS2A-2	1.257468	1.317669	1.165379	-3099.626844	-3098.309175	-3098.461465

INT2A-2	1.261834	1.322601	1.168512	-3099.668793	-3098.346192	-3098.500281
INT1B	1.179554	1.234390	1.091247	-2793.248684	-2792.014294	-2792.157437
TS2B-1	1.453796	1.524642	1.351957	-3626.314673	-3624.790031	-3624.962716
INT2B-1	1.453495	1.524934	1.349647	-3626.372078	-3624.847144	-3625.022431
TS2B-2	1.453919	1.524827	1.351653	-3626.339518	-3624.814691	-3624.987865
INT2B-2	1.453339	1.524966	1.349212	-3626.388945	-3624.863979	-3625.039733
TS3A-1	1.260245	1.320833	1.166158	-3099.652095	-3098.331262	-3098.485937
INT3A-1	1.306448	1.370958	1.207283	-3278.544060	-3277.173102	-3277.336777
3a	0.161346	0.170934	0.126441	-349.075034	-348.904100	-348.948593
TS4A-1	1.308264	1.370569	1.216850	-3278.514189	-3277.143620	-3277.297339
Et ₃ Si-OTMS	0.315944	0.337220	0.266791	-1012.007615	-1011.670395	-1011.740824
TS5A-1	1.148567	1.200599	1.063953	-2615.589944	-2614.389345	-2614.525991
INT5A-1	1.153561	1.205974	1.066639	-2615.626518	-2614.420544	-2614.559879
TS5A-2	1.149481	1.201440	1.065296	-2615.595378	-2614.393938	-2614.530082
INT5A-2	1.154645	1.206901	1.069478	-2615.629931	-2614.423030	-2614.560453
TS5B-1	1.346885	1.409082	1.252981	-3142.284772	-3140.875690	-3141.031791
INT5B-1	1.344106	1.407803	1.245301	-3142.354049	-3140.946246	-3141.108748
TS5B-2	1.347402	1.409568	1.253548	-3142.307875	-3140.898307	-3141.054327
INT5B-2	1.343388	1.407525	1.242065	-3142.357008	-3140.949483	-3141.114943
INT1A-NHC	0.383936	0.402394	0.336326	-867.350189	-866.947795	-867.013863
TS2A-NHC-1	0.653173	0.688988	0.585566	-1700.470017	-1699.781029	-1699.884451
INT2A-NHC-1	0.658634	0.694940	0.588451	-1700.508134	-1699.813194	-1699.919683
TS2A-NHC-2	0.653022	0.689373	0.583739	-1700.472331	-1699.782958	-1699.888592
INT2A-NHC-2	0.657101	0.694087	0.587386	-1700.495880	-1699.801793	-1699.908494
TS3A-NHC-1	0.656350	0.692747	0.584753	-1700.499643	-1699.806896	-1699.914890
INT3A-NHC-1	0.702097	0.742630	0.626723	-1879.373768	-1878.631138	-1878.747045
TS4A-NHC-1	0.702551	0.741360	0.631760	-1879.356672	-1878.615312	-1878.724912
INT1B-NHC	0.576760	0.607318	0.512603	-1394.079089	-1393.471771	-1393.566486
TS2B-NHC-1	0.846588	0.894070	0.764528	-2227.184253	-2226.290183	-2226.419725
INT2B-NHC-1	0.848573	0.895984	0.767706	-2227.219139	-2226.323155	-2226.451433
TS2B-NHC-2	0.846591	0.894403	0.762028	-2227.199857	-2226.305454	-2226.437829
INT2B-NHC-2	0.847543	0.895486	0.764928	-2227.220965	-2226.325479	-2226.456037
TS3B-NHC-2	0.846383	0.894071	0.763112	-2227.193841	-2226.299770	-2226.430729
INT3B-NHC-2	0.737827	0.777815	0.663879	-1743.170118	-1742.392303	-1742.506239
TS4B-NHC-2	0.735433	0.775216	0.660662	-1743.136009	-1742.360793	-1742.475347
TS5A-NHC-1	0.545964	0.573615	0.484639	-1216.427740	-1215.854125	-1215.943101
INT5A-NHC-1	0.551050	0.579309	0.485875	-1216.457529	-1215.878220	-1215.971654
TS5A-NHC-2	0.546803	0.574348	0.487433	-1216.442352	-1215.868004	-1215.954919
INT5A-NHC-2	0.551076	0.579119	0.490947	-1216.469820	-1215.890701	-1215.978873
TS6A-NHC-2	0.759202	0.798905	0.685625	-1744.355724	-1743.556819	-1743.670099
TS5B-NHC-1	0.739829	0.778646	0.666783	-1743.153047	-1742.374401	-1742.486264
INT5B-NHC-1	0.741173	0.780466	0.665988	-1743.186365	-1742.405899	-1742.520377
TS5B-NHC-2	0.741163	0.779492	0.670657	-1743.172911	-1742.393419	-1742.502254
INT5B-NHC-2	0.740744	0.780235	0.665660	-1743.189257	-1742.409022	-1742.523597
TS6B-NHC-1	0.948576	1.000383	0.859589	-2271.084528	-2270.084145	-2270.224939
4a	0.374975	0.396350	0.325756	-877.025543	-876.629193	-876.699787
TS6B-NHC-2	0.735698	0.775005	0.662723	-1743.171879	-1742.396874	-1742.509156
5a	0.350937	0.372286	0.297753	-875.797272	-875.424986	-875.499519

Notes: ZPE = zero-point vibrational energy in the gas phase; H_{corr} = thermal correction to enthalpy in the gas phase; G_{corr} = thermal correction to Gibbs free energy in the gas phase; E_{ele} = the electronic energies in solvent; H_{sol} = ethalpies in solvent; G_{sol} = Gibbs free energies in solvent.

DFT-Computed Energies and Cartesian Coordinate (unit: angstrom)

1a				H	-2.461178	2.796248	0.212735
C	3.497051	-0.984772	-0.164012	C	-3.110754	-0.026127	1.803072
C	2.170776	-1.403290	-0.185785	H	-4.176928	0.069864	2.042153
C	1.120312	-0.480387	-0.049166	H	-2.792913	-1.039430	2.069149
C	1.451700	0.876619	0.080194	H	-2.558474	0.673164	2.441520
C	2.782542	1.289218	0.099615	C	-3.848421	-0.751435	-1.132968
C	3.830653	0.368989	-0.014619	H	-4.912359	-0.511668	-1.011630
H	4.290126	-1.720525	-0.279788	H	-3.587924	-0.589370	-2.185419
H	1.949150	-2.455049	-0.338901	H	-3.722507	-1.818504	-0.920404
H	0.655493	1.607908	0.162787				
H	3.010581	2.347957	0.203488	2a			
C	5.273369	0.811970	0.037573	Si	0.001219	-0.000981	0.287604
H	5.383546	1.860448	-0.259279	H	0.003435	-0.000573	1.785590
H	5.680184	0.715631	1.053349	C	-1.039668	1.469420	-0.311194
H	5.904134	0.204941	-0.621561	C	-0.498510	2.849071	0.105815
C	-0.301577	-0.906898	-0.045331	H	-2.063750	1.343402	0.066960
C	-0.715032	-2.154075	0.239914	H	-1.118620	1.415658	-1.406999
H	-1.759455	-2.438110	0.196644	H	-1.147903	3.661163	-0.244170
H	-0.009359	-2.921563	0.530780	H	-0.423910	2.936761	1.196597
O	-1.151853	0.118022	-0.358243	H	0.501601	3.030421	-0.305821
Si	-2.793815	0.338816	-0.015834	C	1.793744	0.163041	-0.316019
C	-3.083376	2.149957	-0.416802	C	2.719906	-0.991438	0.107661
H	-2.835823	2.362440	-1.463021	H	2.196863	1.116116	0.053584
H	-4.131521	2.429421	-0.255099	H	1.783783	0.249591	-1.412497

H	3.746713	-0.837251	-0.246559	C	-2.536471	-2.075232	-1.682740
H	2.761494	-1.091338	1.199129	C	-4.626777	-1.218927	-0.521422
H	2.376424	-1.951432	-0.295772	H	-3.460793	-0.169088	-1.991432
C	-0.755635	-1.636219	-0.311342	C	-3.409203	-2.819204	-2.704379
C	-2.221787	-1.852741	0.105145	H	-2.293620	-2.754052	-0.852203
H	-0.137316	-2.462366	0.066182	H	-1.583194	-1.765962	-2.126492
H	-0.669304	-1.677110	-1.407140	C	-5.496937	-1.959170	-1.552591
H	-2.604646	-2.818456	-0.247720	H	-4.467507	-1.879536	0.341172
H	-2.334765	-1.834276	1.195986	H	-5.157273	-0.338174	-0.144825
H	-2.875466	-1.073384	-0.304198	C	-4.775847	-3.194835	-2.111969
				H	-2.887286	-3.716256	-3.061580
INT1A				H	-3.560497	-2.173049	-3.582089
C	-2.522316	-0.231017	1.716417	H	-6.453103	-2.247004	-1.096315
C	-2.077731	-1.683427	1.999205	H	-5.736279	-1.273243	-2.379003
C	-1.787056	0.739900	2.664283	H	-5.400180	-3.690385	-2.866466
H	-3.604339	-0.148430	1.886500	H	-4.627621	-3.921106	-1.298504
C	-2.250166	-2.067399	3.476205	C	-2.664940	1.967429	-0.292290
H	-1.020306	-1.782056	1.710784	C	-2.238754	2.478785	-1.685360
H	-2.632808	-2.385447	1.367891	C	-4.146569	2.285607	-0.023515
C	-1.938641	0.347994	4.142510	H	-2.059810	2.516315	0.443924
H	-0.720339	0.742771	2.393881	C	-2.511346	3.984105	-1.824940
H	-2.148926	1.765087	2.520754	H	-2.799561	1.939504	-2.462619
C	-1.495149	-1.099165	4.395631	H	-1.182326	2.245813	-1.857886
H	-1.903032	-3.096621	3.634460	C	-4.415667	3.794754	-0.160249
H	-3.319969	-2.052449	3.732635	H	-4.770601	1.747444	-0.750119
H	-1.360049	1.040855	4.767648	H	-4.446595	1.938356	0.973162
H	-2.991564	0.459756	4.441040	C	-3.983468	4.317670	-1.538700
H	-1.649112	-1.367512	5.448482	H	-2.230950	4.323848	-2.830049
H	-0.416580	-1.187948	4.201716	H	-1.871168	4.531988	-1.117065
C	-3.266043	-0.829475	-1.133091	H	-5.479282	4.003885	0.012851

H	-3.857482	4.330605	0.621956	H	2.646826	-2.089359	2.080698
H	-4.152455	5.400065	-1.604829	C	2.323565	0.406072	4.486411
H	-4.613161	3.852385	-2.311850	H	2.643940	2.507435	4.018200
P	-2.107080	0.192547	-0.063703	H	4.038864	1.472775	3.717248
C	2.905309	-1.825002	-0.728924	H	2.233669	-1.768853	4.512616
C	1.790024	-2.886402	-0.564647	H	3.795428	-1.108315	4.031074
C	3.423791	-1.851646	-2.181572	H	2.638725	0.497600	5.533569
H	3.742646	-2.077641	-0.060086	H	1.228574	0.509915	4.475308
C	2.266479	-4.290869	-0.963048	C	3.143073	1.135779	-1.200026
H	0.945319	-2.584656	-1.200174	C	2.365304	2.468557	-1.261357
H	1.409714	-2.895995	0.462604	C	4.624494	1.359472	-0.846375
C	3.898950	-3.257496	-2.586534	H	3.091635	0.719434	-2.213701
H	2.613919	-1.530651	-2.851219	C	3.034383	3.443411	-2.242717
H	4.250892	-1.144981	-2.313075	H	2.320361	2.932970	-0.267960
C	2.795763	-4.307720	-2.403093	H	1.333060	2.258711	-1.565855
H	1.443949	-5.008721	-0.847593	C	5.281302	2.340870	-1.832710
H	3.065279	-4.613760	-0.277829	H	4.706778	1.771499	0.168589
H	4.245501	-3.242917	-3.627994	H	5.169423	0.406434	-0.840712
H	4.767387	-3.534978	-1.969843	C	4.512907	3.670368	-1.891518
H	3.169464	-5.305759	-2.665800	H	2.492878	4.398200	-2.251770
H	1.968052	-4.085590	-3.092463	H	2.963528	3.030934	-3.260020
C	2.894867	0.016014	1.567614	H	6.327906	2.514603	-1.550492
C	2.537438	1.394812	2.160182	H	5.295108	1.887003	-2.834666
C	2.317538	-1.111661	2.449356	H	4.980456	4.347343	-2.617952
H	3.989834	-0.086773	1.539605	H	4.578598	4.166083	-0.911002
C	2.942658	1.522396	3.636833	P	2.223937	-0.146132	-0.187354
H	1.452324	1.547352	2.063794	Ni	0.051905	-0.018453	-0.560720
H	3.014286	2.193301	1.583153	H	0.123403	-0.029326	-2.163014
C	2.708975	-0.969847	3.928460				
H	1.221390	-1.096219	2.361185				

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C	3.934770	-0.352587	-2.647977	H	1.749135	-4.066611	-5.511165
C	3.256813	0.778943	-3.442918	H	0.985053	-4.507549	-3.984193
C	5.219320	0.161865	-1.971258	H	-0.719505	-3.551673	-5.525058
H	4.234108	-1.131287	-3.361876	H	0.252310	-2.093231	-5.728314
C	4.212634	1.460152	-4.433869	C	3.776245	-2.398811	-0.565960
H	2.859592	1.523048	-2.742023	C	2.979468	-3.245837	0.445352
H	2.396276	0.383755	-3.989385	C	4.677705	-3.317719	-1.414283
C	6.173249	0.818676	-2.982393	H	4.436992	-1.751901	0.029242
H	4.953755	0.901485	-1.211427	C	3.933324	-4.057094	1.342252
H	5.741042	-0.648791	-1.450469	H	2.314729	-3.936283	-0.094256
C	5.482692	1.963145	-3.736096	H	2.324379	-2.597525	1.038097
H	3.694127	2.286546	-4.937402	C	5.649257	-4.105231	-0.519266
H	4.494257	0.740394	-5.217075	H	4.051526	-4.034511	-1.960966
H	7.068217	1.185251	-2.462679	H	5.237964	-2.750570	-2.164992
H	6.515052	0.062237	-3.704631	C	4.884550	-4.936396	0.519149
H	6.168804	2.415088	-4.463746	H	3.364675	-4.678418	2.043123
H	5.213514	2.753441	-3.020093	H	4.524227	-3.362641	1.954881
C	1.586315	-2.142684	-2.595602	H	6.289603	-4.751683	-1.133537
C	0.321502	-1.363112	-3.007729	H	6.316650	-3.399298	-0.001895
C	2.240922	-2.748116	-3.856321	H	5.583977	-5.464667	1.179851
H	1.254018	-2.963953	-1.943696	H	4.298627	-5.708084	-0.002279
C	-0.662332	-2.256300	-3.774879	P	2.691637	-1.120872	-1.440804
H	0.606891	-0.518557	-3.647801	C	2.845882	3.098603	1.182930
H	-0.155857	-0.937475	-2.116276	C	3.208868	3.074469	-0.314837
C	1.258550	-3.652284	-4.620434	C	1.765620	4.171317	1.422818
H	2.552226	-1.936143	-4.528280	H	3.735535	3.389446	1.762257
H	3.145152	-3.310673	-3.611032	C	3.624093	4.449226	-0.856836
C	-0.012149	-2.886511	-5.012578	H	2.337315	2.695389	-0.861648
H	-1.552862	-1.678800	-4.057752	H	4.007699	2.353140	-0.496961
H	-1.008852	-3.055573	-3.106729	C	2.201060	5.552027	0.904897

H	0.849637	3.876219	0.899818	C	-0.753828	0.736565	4.508390
H	1.513441	4.252045	2.484873	H	0.924906	-0.430920	3.818033
C	2.548117	5.508561	-0.588168	H	-0.149095	0.063994	2.517967
H	3.829858	4.376525	-1.933228	C	0.731502	2.552256	5.462053
H	4.565119	4.759441	-0.377642	H	2.493891	1.462144	4.877260
H	1.401945	6.281841	1.092630	H	2.425423	3.087073	4.206713
H	3.079266	5.892611	1.473759	C	-0.137097	1.328263	5.783639
H	2.880948	6.494718	-0.936490	H	-1.330339	-0.163365	4.758050
H	1.643755	5.257923	-1.160844	H	-1.468505	1.456972	4.085703
C	3.971097	0.801153	2.581967	H	1.194328	2.945522	6.376722
C	3.812557	-0.611898	3.176374	H	0.094524	3.354837	5.061163
C	5.194220	0.843862	1.647822	H	-0.923493	1.594248	6.501922
H	4.154551	1.511698	3.400190	H	0.488350	0.563624	6.268603
C	5.097300	-1.114280	3.855494	P	2.378214	1.322600	1.703714
H	3.528239	-1.296640	2.368289	Ni	1.318689	0.020602	0.089027
H	2.990850	-0.634767	3.899487	H	-0.012722	1.085572	0.102158
C	6.475823	0.372429	2.352462	H	0.253510	-1.320336	0.160426
H	5.007292	0.192417	0.788064	C	-1.742621	-3.223344	1.776968
H	5.346652	1.854074	1.251364	C	-1.030057	-4.177189	0.797861
C	6.306920	-1.044881	2.913686	C	-0.740679	-2.765447	2.853152
H	4.948196	-2.141589	4.213169	H	-2.542010	-3.793010	2.272757
H	5.300445	-0.498078	4.744121	C	-0.454266	-5.391291	1.546473
H	7.319688	0.409840	1.650943	H	-0.233030	-3.622847	0.286151
H	6.716242	1.063826	3.173827	H	-1.718510	-4.535402	0.027354
H	7.217784	-1.366909	3.434349	C	-0.178032	-3.966205	3.627771
H	6.157699	-1.743548	2.077177	H	0.067833	-2.218669	2.353976
C	1.191989	1.625298	3.144608	H	-1.207503	-2.068539	3.556065
C	0.312136	0.401951	3.452047	C	0.489251	-4.969661	2.679706
C	1.816107	2.201771	4.429731	H	0.072144	-6.048480	0.841410
H	0.510849	2.379641	2.737622	H	-1.285347	-5.980423	1.963924

H	0.541855	-3.620499	4.381856	H	-3.458055	-2.607857	3.848413
H	-0.995016	-4.461124	4.175277	C	-5.620599	0.108428	4.167449
H	0.844481	-5.849582	3.232177	H	-5.713977	1.705499	2.687070
H	1.369354	-4.491824	2.239469	H	-4.143985	1.530977	3.471488
C	-3.897696	-2.543335	-0.129158	H	-5.131266	-1.617800	5.397575
C	-3.323981	-2.808831	-1.537713	H	-3.785249	-0.511341	5.131612
C	-4.622822	-3.794527	0.407033	H	-5.930255	0.738411	5.011076
H	-4.650923	-1.748227	-0.230678	H	-6.532915	-0.367808	3.777721
C	-4.393736	-3.312439	-2.515644	P	-2.564709	-1.751187	0.944815
H	-2.533155	-3.564161	-1.472715	C	-4.237819	1.625765	-2.015679
H	-2.839665	-1.902128	-1.911072	C	-4.526793	0.256062	-2.659242
C	-5.700389	-4.277431	-0.579700	C	-5.460330	2.042881	-1.170581
H	-3.900703	-4.606632	0.561111	H	-4.150174	2.372659	-2.818871
H	-5.077423	-3.592591	1.382100	C	-5.790383	0.281722	-3.530305
C	-5.106717	-4.557178	-1.967812	H	-4.665940	-0.468593	-1.851303
H	-3.934488	-3.526364	-3.489728	H	-3.671657	-0.102067	-3.241906
H	-5.138986	-2.523637	-2.686225	C	-6.744916	2.065252	-2.020211
H	-6.192221	-5.175746	-0.184355	H	-5.596118	1.340719	-0.337842
H	-6.479833	-3.505359	-0.669672	H	-5.318379	3.035241	-0.730571
H	-5.891744	-4.887249	-2.660179	C	-7.007886	0.717611	-2.704843
H	-4.384942	-5.384355	-1.890137	H	-5.961675	-0.706527	-3.976175
C	-3.485908	-0.965547	2.394930	H	-5.642885	0.982904	-4.365383
C	-4.487950	0.091412	1.901244	H	-7.598327	2.348618	-1.390284
C	-4.149438	-1.847803	3.470357	H	-6.649045	2.846610	-2.788825
H	-2.673594	-0.412670	2.884635	H	-7.904720	0.776320	-3.334681
C	-4.992070	0.966041	3.058629	H	-7.209443	-0.045147	-1.937353
H	-5.348102	-0.404346	1.427296	C	-1.556100	2.441998	-2.546434
H	-4.017053	0.709177	1.134880	C	-0.076468	2.690785	-2.206804
C	-4.649965	-0.983129	4.642229	C	-1.658550	1.708733	-3.901456
H	-5.002920	-2.383593	3.035610	H	-2.044382	3.417480	-2.683062

C	0.623215	3.495484	-3.313429	P	-2.518148	1.581436	-1.152006
H	0.420478	1.727283	-2.048670	Ni	-1.137797	-0.209005	-0.031156
H	0.012196	3.215641	-1.250606				
C	-0.966632	2.511493	-5.017013	TS2A-1			
H	-1.197677	0.717856	-3.816973	C	3.436653	4.103798	-1.098824
H	-2.701274	1.550616	-4.190515	C	2.257065	3.421803	-1.402114
C	0.498401	2.810810	-4.680712	C	1.476350	2.848889	-0.390793
H	1.680681	3.638614	-3.057752	C	1.892537	3.013560	0.935847
H	0.177372	4.500623	-3.369639	C	3.069170	3.693266	1.237527
H	-1.037290	1.963233	-5.965751	C	3.871152	4.241229	0.224566
H	-1.508552	3.458607	-5.159807	H	4.030182	4.531080	-1.904523
H	0.954137	3.429897	-5.464627	H	1.938665	3.324863	-2.435836
H	1.056230	1.867122	-4.660619	H	1.290306	2.572748	1.724451
C	-2.762363	2.956360	0.141989	H	3.378180	3.795320	2.275904
C	-1.822616	2.827134	1.350246	C	5.178545	4.924384	0.549668
C	-2.765236	4.396283	-0.406411	H	5.438469	5.675395	-0.204347
H	-3.769800	2.758227	0.527321	H	5.141723	5.421158	1.525515
C	-2.150174	3.862406	2.435714	H	6.003222	4.199396	0.584582
H	-0.790118	2.939428	1.018002	C	0.178101	2.169504	-0.738410
H	-1.874946	1.809550	1.752341	O	-0.950100	2.892381	-0.326172
C	-3.106407	5.416536	0.691597	Si	-1.356797	4.457865	-0.805633
H	-1.772833	4.637857	-0.809581	C	-0.210271	5.744801	-0.041391
H	-3.474427	4.491503	-1.238853	H	0.804738	5.684503	-0.445993
C	-2.141202	5.292237	1.878350	H	-0.595290	6.756094	-0.227151
H	-1.434168	3.772205	3.262485	H	-0.141490	5.604228	1.043537
H	-3.143646	3.647669	2.857967	C	-3.098756	4.697111	-0.134277
H	-3.081498	6.433359	0.278337	H	-3.475893	5.698765	-0.374837
H	-4.135173	5.242953	1.042048	H	-3.794822	3.964423	-0.556756
H	-2.401516	6.014046	2.663056	H	-3.115457	4.583545	0.955367
H	-1.123254	5.542134	1.542746	C	-1.337902	4.584475	-2.686776

H	-2.006282	3.840093	-3.135272	C	6.198011	0.246709	-1.084466
H	-1.665260	5.578427	-3.017259	H	5.058124	1.883213	-1.959443
H	-0.332991	4.409131	-3.086256	H	4.957074	0.361661	-2.849634
C	2.169869	-1.903332	1.640072	H	6.911200	-1.648217	-0.279798
C	2.392400	-0.597639	2.432781	H	6.061387	-1.784027	-1.818472
C	1.014921	-2.716723	2.253753	H	7.123977	0.463231	-1.632735
H	3.082698	-2.509904	1.695673	H	6.278413	0.755962	-0.112109
C	2.626156	-0.870181	3.925516	C	1.482797	-3.150693	-0.951456
H	1.508923	0.039578	2.298899	C	1.026848	-2.948767	-2.411145
H	3.235454	-0.033716	2.015733	C	2.579600	-4.225478	-0.859342
C	1.220719	-2.966480	3.756599	H	0.613039	-3.525256	-0.397014
H	0.082624	-2.166192	2.087375	C	0.574705	-4.272882	-3.046296
H	0.908779	-3.681128	1.742154	H	1.854878	-2.531645	-3.003223
C	1.459169	-1.662744	4.530682	H	0.217917	-2.207509	-2.439640
H	2.762684	0.078431	4.461020	C	2.099978	-5.550321	-1.477386
H	3.558312	-1.441583	4.052355	H	3.475015	-3.890392	-1.399426
H	0.351516	-3.499341	4.164512	H	2.877494	-4.382637	0.184910
H	2.088092	-3.629656	3.894132	C	1.660812	-5.353462	-2.936122
H	1.648772	-1.879534	5.589869	H	0.298344	-4.111698	-4.096248
H	0.550839	-1.046899	4.490489	H	-0.331130	-4.622681	-2.532295
C	3.519991	-1.053406	-0.872268	H	2.894483	-6.305127	-1.414672
C	3.670070	0.456936	-1.112958	H	1.251580	-5.934965	-0.891459
C	4.747519	-1.593095	-0.107001	H	1.301252	-6.300528	-3.358355
H	3.511681	-1.536786	-1.861153	H	2.533282	-5.051969	-3.535014
C	4.980112	0.796134	-1.838179	P	1.812017	-1.479548	-0.154219
H	3.634771	0.994323	-0.156836	C	-2.756323	0.176952	1.874939
H	2.819194	0.819276	-1.689988	C	-1.788251	-0.286553	2.983966
C	6.054654	-1.263548	-0.848895	C	-2.809787	1.718552	1.891910
H	4.788705	-1.132676	0.888688	H	-3.762654	-0.212956	2.091541
H	4.674114	-2.673614	0.050359	C	-2.202888	0.241423	4.366265

H	-0.789741	0.087559	2.726795	C	-3.231516	-0.076030	-2.447051
H	-1.712732	-1.375266	3.022327	C	-4.866665	0.520418	-0.638487
C	-3.230672	2.260169	3.266812	H	-2.942050	1.444732	-0.967600
H	-1.820747	2.104136	1.626010	C	-3.930099	0.880320	-3.425646
H	-3.495813	2.101790	1.133579	H	-3.703243	-1.064687	-2.533235
C	-2.289970	1.772333	4.375233	H	-2.175460	-0.202231	-2.707253
H	-1.490945	-0.107341	5.125943	C	-5.603969	1.462153	-1.609088
H	-3.182295	-0.181023	4.637831	H	-5.320751	-0.478607	-0.702419
H	-3.251082	3.358100	3.237443	H	-5.017700	0.864175	0.389674
H	-4.257382	1.933547	3.492851	C	-5.417221	1.035721	-3.072650
H	-2.622378	2.136295	5.356104	H	-3.818661	0.517661	-4.455741
H	-1.286323	2.188835	4.203150	H	-3.436848	1.862905	-3.381534
C	-3.013828	-2.233775	0.124744	H	-6.671637	1.500622	-1.356488
C	-2.328803	-3.077837	-0.969181	H	-5.214829	2.482338	-1.478386
C	-3.009941	-3.028532	1.446247	H	-5.899750	1.757373	-3.744202
H	-4.065537	-2.090077	-0.160567	H	-5.922165	0.070982	-3.231520
C	-3.014510	-4.440231	-1.151471	P	-2.235046	-0.500230	0.187416
H	-1.286260	-3.232678	-0.672010	Ni	-0.039666	-0.135935	-0.336074
H	-2.293041	-2.543996	-1.922750	H	0.168451	1.143709	0.661892
C	-3.690343	-4.398480	1.280362	C	0.040654	1.382234	-1.900962
H	-1.973234	-3.185747	1.773607	H	-0.911479	1.418550	-2.416143
H	-3.516507	-2.470177	2.240327	H	0.911176	1.174143	-2.513705
C	-3.035716	-5.225866	0.166130				
H	-2.504196	-5.016952	-1.933560	INT2A-1			
H	-4.046213	-4.283867	-1.500547	C	-2.787220	1.018885	2.575439
H	-3.660676	-4.944227	2.232397	C	-2.453441	0.643081	1.272098
H	-4.752629	-4.244456	1.038647	C	-3.298831	-0.160087	0.502547
H	-3.558751	-6.182317	0.039478	C	-4.510445	-0.563346	1.087651
H	-2.001289	-5.466205	0.455644	C	-4.845194	-0.193634	2.388209
C	-3.368476	0.433496	-0.997147	C	-3.984770	0.600024	3.162985

H	-2.098405	1.641305	3.143985	C	3.461855	1.036854	3.566749
H	-1.505886	0.966182	0.852134	H	2.572842	-0.002450	1.884769
H	-5.191523	-1.174446	0.502970	H	3.956416	1.000082	1.461595
H	-5.788540	-0.529349	2.814999	C	2.239110	1.042816	4.494560
C	-4.325649	0.952541	4.592031	H	0.381409	2.145420	4.757197
H	-5.396376	1.152745	4.713650	H	1.760621	3.145273	4.301567
H	-4.071282	0.128922	5.273335	H	4.123524	0.195053	3.809517
H	-3.775716	1.837691	4.930271	H	4.045871	1.954063	3.733298
C	-2.932468	-0.688147	-0.889018	H	2.555967	1.140027	5.540506
O	-4.128673	-0.650999	-1.721741	H	1.714134	0.081362	4.410560
Si	-4.776593	0.689817	-2.476156	C	0.682043	3.512199	-0.526285
C	-4.681711	2.236925	-1.391105	C	-0.857274	3.470462	-0.443386
H	-3.644996	2.513681	-1.173449	C	1.210011	4.760550	0.213273
H	-5.161349	3.088686	-1.891029	H	0.941309	3.620380	-1.590843
H	-5.183678	2.074033	-0.431039	C	-1.485009	4.751788	-1.012199
C	-6.583607	0.242155	-2.780165	H	-1.170911	3.351213	0.602627
H	-7.106203	1.034137	-3.331433	H	-1.234164	2.596123	-0.977714
H	-6.665125	-0.683069	-3.362789	C	0.590883	6.045187	-0.365435
H	-7.110803	0.086581	-1.831456	H	0.943904	4.692785	1.276661
C	-3.934728	1.031471	-4.134721	H	2.301002	4.822576	0.167122
H	-3.956140	0.137417	-4.769705	C	-0.942894	6.003977	-0.309582
H	-4.438914	1.841656	-4.677983	H	-2.576698	4.699950	-0.921430
H	-2.885526	1.313428	-3.994754	H	-1.261421	4.812563	-2.087997
C	2.075672	2.084310	1.694834	H	0.972166	6.918273	0.179789
C	0.857162	2.085405	2.643596	H	0.914471	6.160744	-1.410652
C	3.055617	0.961460	2.086304	H	-1.366412	6.911628	-0.757641
H	2.595421	3.047319	1.784896	H	-1.262782	5.992256	0.743171
C	1.274013	2.175616	4.119018	C	3.024693	1.825898	-1.118831
H	0.289556	1.160800	2.483392	C	2.671910	1.411010	-2.563472
H	0.178990	2.910462	2.397893	C	3.928842	3.070359	-1.113355

H	3.608528	1.003852	-0.690796	H	-2.260142	-3.046441	4.889219
C	3.944100	1.165977	-3.390578	H	-2.380240	-1.686777	3.767245
H	2.077146	2.203697	-3.041242	C	2.527466	-2.735604	0.028110
H	2.040792	0.513615	-2.548236	C	3.405660	-1.768818	-0.786338
C	5.207060	2.811897	-1.930765	C	3.178568	-2.981622	1.404731
H	3.393123	3.920950	-1.555154	H	2.511267	-3.702981	-0.491970
H	4.191193	3.354752	-0.086537	C	4.845151	-2.278034	-0.941958
C	4.873400	2.388896	-3.369481	H	3.415524	-0.810117	-0.258727
H	3.676459	0.905662	-4.422413	H	2.964245	-1.571198	-1.768164
H	4.475858	0.297601	-2.973832	C	4.612815	-3.516426	1.249913
H	5.839610	3.708771	-1.932491	H	3.218741	-2.042841	1.971844
H	5.789399	2.015551	-1.443515	H	2.587044	-3.685353	2.000019
H	5.794170	2.178782	-3.928061	C	5.483862	-2.558121	0.425310
H	4.377305	3.225875	-3.883090	H	5.442007	-1.545205	-1.501515
P	1.473912	1.854999	-0.065645	H	4.841084	-3.201871	-1.539147
C	-0.031469	-2.819446	1.584816	H	5.056721	-3.680798	2.240266
C	0.232116	-1.854368	2.760564	H	4.580716	-4.496989	0.752183
C	-1.550604	-3.056902	1.469675	H	6.494833	-2.966806	0.302997
H	0.451490	-3.784507	1.795044	H	5.590286	-1.609278	0.973195
C	-0.354738	-2.370487	4.082702	C	0.001754	-3.157614	-1.360435
H	-0.234070	-0.892408	2.512984	C	0.549699	-2.729069	-2.736858
H	1.302614	-1.664730	2.880652	C	0.080580	-4.689284	-1.215270
C	-2.141941	-3.590999	2.784523	H	-1.054437	-2.862251	-1.339055
H	-2.035372	-2.107823	1.233635	C	-0.243073	-3.401232	-3.868099
H	-1.786212	-3.749858	0.656210	H	1.606888	-3.020830	-2.820584
C	-1.860240	-2.636595	3.952672	H	0.502363	-1.637831	-2.828617
H	-0.160041	-1.641485	4.881015	C	-0.714011	-5.375553	-2.341401
H	0.160465	-3.299091	4.371258	H	1.128342	-5.016664	-1.273310
H	-3.223197	-3.732383	2.663270	H	-0.294264	-5.017487	-0.239187
H	-1.712538	-4.580183	3.005515	C	-0.222535	-4.931445	-3.727838

H	0.163432	-3.102571	-4.843051	Si	-1.814745	-4.104821	-1.235692
H	-1.281676	-3.042258	-3.833954	C	-3.506374	-4.284083	-0.427219
H	-0.641046	-6.466400	-2.242196	H	-4.157593	-3.440776	-0.682294
H	-1.777899	-5.118689	-2.233746	H	-4.002485	-5.204603	-0.758609
H	-0.831698	-5.396344	-4.513377	H	-3.423309	-4.323060	0.664722
H	0.807592	-5.290544	-3.873959	C	-0.699050	-5.554043	-0.781646
P	0.731912	-2.106039	0.012600	H	0.312824	-5.413653	-1.177062
Ni	0.062878	0.038393	-0.527272	H	-0.608345	-5.668780	0.303551
H	-2.766687	-1.766377	-0.767702	H	-1.100070	-6.489137	-1.193905
C	-1.691964	-0.100111	-1.538090	C	-1.983335	-4.029634	-3.114205
H	-1.563938	-0.621139	-2.498210	H	-2.401809	-4.967730	-3.500357
H	-1.908131	0.948236	-1.807149	H	-2.641664	-3.212934	-3.430333
				H	-1.008350	-3.880455	-3.592207
TS2A-2				C	-2.522649	2.341529	0.933987
C	3.524738	-3.400893	-0.151310	C	-1.908789	2.507178	2.335658
C	2.469247	-2.822748	-0.848737	C	-2.116088	3.534746	0.046376
C	1.178151	-2.719921	-0.285115	H	-3.614575	2.349634	1.051645
C	1.003534	-3.294150	0.993632	C	-2.300613	3.851944	2.971600
C	2.064383	-3.876387	1.681980	H	-0.819522	2.448093	2.260623
C	3.354377	-3.928590	1.137104	H	-2.221460	1.692264	2.994911
H	4.503743	-3.455150	-0.625018	C	-2.511270	4.880286	0.674729
H	2.643318	-2.467027	-1.859059	H	-1.030673	3.502090	-0.089226
H	0.018801	-3.280141	1.444243	H	-2.549487	3.452459	-0.956879
H	1.885552	-4.295839	2.670349	C	-1.909829	5.036382	2.077588
C	4.517536	-4.508724	1.905027	H	-1.829829	3.944965	3.958959
H	4.180331	-5.207360	2.678767	H	-3.388097	3.869539	3.138419
H	5.209255	-5.045606	1.244975	H	-2.189377	5.704917	0.025494
H	5.098338	-3.722669	2.408175	H	-3.607907	4.941855	0.739964
C	0.043502	-2.127259	-1.005601	H	-2.230828	5.982864	2.530859
O	-1.219064	-2.643791	-0.636158	H	-0.813789	5.081463	1.995511

C	-2.759202	-0.614952	1.220740	H	-6.305935	2.079032	-2.512105
C	-1.686808	-1.048495	2.243698	H	-4.739419	2.186932	-3.312819
C	-4.114748	-0.372717	1.907077	H	-6.011509	0.260497	-4.230610
H	-2.866982	-1.462990	0.536975	H	-6.228145	-0.399021	-2.609677
C	-2.135939	-2.293767	3.019413	P	-2.081573	0.716318	0.083038
H	-1.484751	-0.239534	2.957424	C	2.687034	0.974199	1.571355
H	-0.747360	-1.243934	1.717436	C	1.536510	1.285508	2.549777
C	-4.557816	-1.621265	2.691299	C	3.170759	-0.473550	1.804814
H	-4.045391	0.479158	2.597203	H	3.518067	1.670874	1.754451
H	-4.880356	-0.113834	1.167987	C	1.893470	0.999991	4.015349
C	-3.491433	-2.064660	3.704442	H	0.673628	0.672053	2.259765
H	-1.373181	-2.571978	3.758873	H	1.220738	2.326251	2.451986
H	-2.220317	-3.136158	2.318142	C	3.530269	-0.754395	3.270618
H	-5.510466	-1.426541	3.201133	H	2.370428	-1.157037	1.506339
H	-4.741584	-2.440102	1.980265	H	4.030529	-0.714600	1.175264
H	-3.817544	-2.973945	4.225596	C	2.352581	-0.450226	4.203036
H	-3.378059	-1.284652	4.472528	H	1.024499	1.218068	4.650516
C	-3.265521	0.773161	-1.402961	H	2.697318	1.679730	4.336249
C	-3.500789	-0.635155	-1.979561	H	3.834491	-1.804171	3.366541
C	-4.622631	1.497261	-1.267087	H	4.395485	-0.141007	3.565273
H	-2.662387	1.323816	-2.139454	H	2.625462	-0.638654	5.249400
C	-4.204407	-0.573437	-3.343128	H	1.520482	-1.128211	3.960922
H	-4.132039	-1.206623	-1.284374	C	2.196387	3.000953	-0.644432
H	-2.555532	-1.170900	-2.048102	C	1.287968	3.304055	-1.857274
C	-5.339992	1.570255	-2.627562	C	1.888557	3.971082	0.511648
H	-5.261740	0.958190	-0.555346	H	3.237350	3.183116	-0.946836
H	-4.506404	2.511807	-0.875565	C	1.390509	4.772707	-2.296167
C	-5.538679	0.178717	-3.243574	H	0.253810	3.056327	-1.594143
H	-4.368592	-1.588550	-3.728472	H	1.533075	2.646182	-2.695269
H	-3.548510	-0.063573	-4.064328	C	1.994808	5.438647	0.065098

H	0.873584	3.787077	0.884453	H	1.102405	-1.336561	-2.700287
H	2.570903	3.795961	1.351363	H	-0.695041	-1.472050	-2.903214
C	1.087684	5.732280	-1.137358				
H	0.706981	4.957521	-3.135057	INT2A-2			
H	2.407020	4.969549	-2.669852	C	0.749916	-4.534344	-0.154953
H	1.744179	6.099477	0.905445	C	0.119131	-3.499749	-0.846979
H	3.038252	5.657262	-0.207060	C	-0.881750	-2.704215	-0.249510
H	1.206326	6.774875	-1.459078	C	-1.256067	-3.067974	1.065685
H	0.037763	5.613466	-0.834447	C	-0.632351	-4.107487	1.746587
C	3.528780	0.478236	-1.192004	C	0.403512	-4.853364	1.163460
C	3.332261	0.610965	-2.715401	H	1.520542	-5.115624	-0.660299
C	4.935486	0.987470	-0.814892	H	0.400293	-3.320314	-1.876845
H	3.488276	-0.589926	-0.955589	H	-2.056954	-2.519762	1.547368
C	4.393697	-0.201881	-3.474385	H	-0.955213	-4.346916	2.758880
H	3.430657	1.666235	-3.006306	C	1.127430	-5.929582	1.936700
H	2.321431	0.303154	-3.000213	H	1.932778	-5.507685	2.555797
C	6.015864	0.184118	-1.562174	H	0.450816	-6.464252	2.613818
H	5.032273	2.049480	-1.081444	H	1.586337	-6.667380	1.268531
H	5.111405	0.919335	0.263585	C	-1.491952	-1.524290	-0.935173
C	5.812084	0.240603	-3.083530	O	-2.852033	-1.318733	-0.438860
H	4.246693	-0.097483	-4.557225	Si	-4.217584	-2.225747	-0.786594
H	4.268535	-1.269672	-3.240533	C	-5.421819	-1.863913	0.621245
H	7.013726	0.557299	-1.297324	H	-5.525151	-0.783624	0.776835
H	5.971989	-0.863363	-1.228311	H	-6.417836	-2.267266	0.399846
H	6.562086	-0.377920	-3.592953	H	-5.083217	-2.306829	1.564582
H	5.969588	1.274017	-3.427075	C	-3.881474	-4.082112	-0.890032
P	2.073801	1.160254	-0.210005	H	-4.809495	-4.622064	-1.120840
Ni	0.044920	0.176934	-0.603227	H	-3.150571	-4.320793	-1.670654
C	0.137295	-1.407090	-2.213268	H	-3.481396	-4.467680	0.053129
H	-0.062469	0.290613	-2.189170	C	-5.036799	-1.669938	-2.402202

H	-5.953259	-2.248307	-2.578372	C	4.320261	-3.005721	-3.472340
H	-5.316101	-0.610769	-2.367767	H	2.336426	-2.883244	-4.363698
H	-4.380498	-1.814675	-3.266896	H	2.391912	-3.726398	-2.816329
C	3.480392	1.327166	-0.577424	H	6.072671	-2.941453	-2.184194
C	3.097522	1.983237	-1.922083	H	4.678994	-3.753277	-1.472024
C	3.554611	2.381990	0.541589	H	4.585299	-3.958164	-3.948313
H	4.485100	0.898964	-0.681194	H	4.712234	-2.208261	-4.121175
C	4.033732	3.146804	-2.283978	C	2.643588	-0.528220	1.587564
H	2.061149	2.341648	-1.861377	C	1.634509	-1.582598	2.076147
H	3.114831	1.238800	-2.725363	C	4.073905	-0.939585	1.981594
C	4.501141	3.534462	0.166900	H	2.401942	0.410709	2.107924
H	2.555074	2.782547	0.730592	C	1.747351	-1.816681	3.588289
H	3.893438	1.929977	1.479921	H	1.795369	-2.531167	1.549966
C	4.099971	4.190748	-1.161027	H	0.618517	-1.268517	1.826333
H	3.702832	3.610558	-3.221954	C	4.185907	-1.143816	3.502685
H	5.044028	2.751526	-2.467230	H	4.321412	-1.887895	1.487015
H	4.516349	4.278318	0.973727	H	4.810452	-0.200859	1.641898
H	5.525868	3.143110	0.082558	C	3.178446	-2.193800	3.995639
H	4.806320	4.989004	-1.421297	H	1.040410	-2.600701	3.886182
H	3.115320	4.665864	-1.046656	H	1.448757	-0.899667	4.118787
C	3.037957	-1.513416	-1.226389	H	5.209725	-1.440184	3.765193
C	2.404485	-1.572381	-2.632742	H	3.993872	-0.187154	4.011352
C	4.572354	-1.593718	-1.375575	H	3.252453	-2.313343	5.084046
H	2.691602	-2.403968	-0.682689	H	3.431817	-3.168576	3.551952
C	2.794817	-2.864471	-3.366642	P	2.304222	-0.098914	-0.209724
H	2.743470	-0.713708	-3.227895	C	-2.249592	2.421869	-1.316969
H	1.319444	-1.480517	-2.553601	C	-1.368460	2.289378	-2.582330
C	4.980008	-2.894833	-2.090610	C	-3.605874	1.729194	-1.543281
H	4.924452	-0.742563	-1.975586	H	-2.442987	3.490011	-1.136328
H	5.080836	-1.527514	-0.410923	C	-2.077577	2.805106	-3.843434

H	-1.110606	1.229770	-2.709571	C	-1.937277	0.268702	2.474656
H	-0.415902	2.814707	-2.447868	C	-3.439577	2.276975	2.065214
C	-4.309426	2.253987	-2.805065	H	-3.195333	0.542851	0.800557
H	-3.443012	0.652062	-1.627491	C	-3.019140	-0.359949	3.363654
H	-4.261753	1.876929	-0.678218	H	-1.229567	0.818093	3.108779
C	-3.425482	2.101780	-4.049289	H	-1.366181	-0.511893	1.966950
H	-1.430093	2.662314	-4.718510	C	-4.527615	1.634998	2.944178
H	-2.245761	3.888802	-3.748892	H	-2.824859	2.932894	2.697009
H	-5.260294	1.723648	-2.945425	H	-3.900298	2.920011	1.304330
H	-4.560487	3.316988	-2.668313	C	-3.913811	0.710281	4.006705
H	-3.935846	2.500059	-4.935564	H	-2.552437	-0.984871	4.136484
H	-3.250645	1.032207	-4.237270	H	-3.638607	-1.024479	2.748081
C	-0.676923	3.399944	0.899711	H	-5.134546	2.415410	3.421711
C	0.085665	3.200306	2.223859	H	-5.207366	1.051339	2.306864
C	0.156136	4.237966	-0.090051	H	-4.705879	0.239305	4.602883
H	-1.587670	3.975752	1.120892	H	-3.312114	1.314409	4.702821
C	0.545701	4.535596	2.832374	P	-1.274805	1.758196	0.164467
H	0.952297	2.548697	2.050462	Ni	-0.060012	-0.094585	-0.464779
H	-0.545263	2.680185	2.949456	C	-1.540110	-1.636883	-2.462873
C	0.617203	5.569019	0.528103	H	-0.546127	-1.585553	-2.915757
H	1.028645	3.658523	-0.411994	H	-2.006280	-2.572724	-2.817609
H	-0.423359	4.452737	-0.993829	H	-2.113576	-0.801465	-2.872659
C	1.378123	5.362461	1.844267				
H	1.115570	4.348332	3.751751	INT1B			
H	-0.342165	5.115075	3.126245	C	2.920055	1.594646	-0.684880
H	1.240145	6.115426	-0.192356	C	2.610721	1.579799	-2.197775
H	-0.265812	6.197107	0.718005	C	2.548744	2.956316	-0.069212
H	1.644257	6.331226	2.285990	H	4.001606	1.462435	-0.553736
H	2.323047	4.842302	1.640269	C	3.280363	2.750393	-2.934581
C	-2.562543	1.194959	1.410964	H	1.521796	1.625458	-2.337648

H	2.937290	0.633667	-2.643148	C	3.765494	0.655604	2.475411
C	3.239495	4.113835	-0.809281	H	1.751040	1.349367	2.157574
H	1.464922	3.094510	-0.122419	C	1.655258	-0.328022	4.305611
H	2.817697	2.991080	0.992359	H	2.194034	-1.630372	2.664395
C	2.907584	4.100506	-2.307711	H	0.631739	-0.857710	2.457980
H	3.001859	2.728536	-3.995830	C	3.773332	1.028448	3.968414
H	4.372432	2.623594	-2.892887	H	4.340368	-0.270173	2.339760
H	2.945545	5.070577	-0.359012	H	4.272112	1.431733	1.889512
H	4.328227	4.027308	-0.677936	C	3.077092	-0.047888	4.815515
H	3.427560	4.918399	-2.821994	H	1.194625	-1.139268	4.883304
H	1.830600	4.278508	-2.440401	H	1.028927	0.563632	4.459053
C	3.180808	-1.326422	-0.294494	H	4.804748	1.177774	4.312678
C	2.638047	-2.084266	-1.525539	H	3.254332	1.989538	4.101012
C	4.686316	-1.051134	-0.485708	H	3.054566	0.252617	5.870626
H	3.062712	-1.994286	0.572020	H	3.663951	-0.976991	4.764335
C	3.403219	-3.394878	-1.759062	P	2.064882	0.136211	0.142728
H	2.731941	-1.451478	-2.419026	C	-2.791253	0.567645	-1.810057
H	1.569873	-2.281040	-1.400938	C	-1.773410	0.215077	-2.921396
C	5.458162	-2.365549	-0.697270	C	-3.823739	-0.568778	-1.671964
H	4.829730	-0.416847	-1.371747	H	-3.331898	1.481538	-2.099833
H	5.107542	-0.504074	0.363052	C	-2.457788	-0.088676	-4.261197
C	4.912006	-3.147540	-1.900855	H	-1.209628	-0.668301	-2.590888
H	3.009842	-3.900218	-2.649800	H	-1.037694	1.017421	-3.047473
H	3.224042	-4.070280	-0.910107	C	-4.499536	-0.892163	-3.015495
H	6.526543	-2.152321	-0.831592	H	-3.318561	-1.464327	-1.292377
H	5.370501	-2.983143	0.208852	H	-4.595796	-0.302620	-0.941659
H	5.448444	-4.097929	-2.014593	C	-3.476239	-1.225358	-4.109662
H	5.097658	-2.567800	-2.817480	H	-1.701585	-0.348125	-5.013375
C	2.326050	0.427819	1.978668	H	-2.969396	0.815672	-4.625151
C	1.654051	-0.684631	2.811448	H	-5.200866	-1.725492	-2.880009

H	-5.098170	-0.025137	-3.333995	C	-4.490658	0.801573	3.753366
H	-3.985915	-1.417197	-5.062488	H	-2.759771	-0.249121	4.554871
H	-2.944230	-2.148498	-3.840326	H	-3.644426	-1.142881	3.320964
C	-1.815686	2.833176	-0.274945	H	-6.051088	1.702748	2.530364
C	-1.191730	3.433885	1.001152	H	-5.635629	0.049703	2.077685
C	-1.123294	3.378520	-1.540120	H	-5.189273	0.409908	4.503589
H	-2.867327	3.152670	-0.319012	H	-4.141963	1.776870	4.126046
C	-1.161541	4.970968	0.961463	P	-1.834610	0.942025	-0.218950
H	-0.173603	3.043147	1.127983	Ni	-0.140571	-0.624672	-0.108353
H	-1.751905	3.112298	1.884259	Si	-1.019483	-2.848837	0.121973
C	-1.092082	4.916022	-1.563542	C	-1.481289	-3.800940	-1.502707
H	-0.099948	2.988179	-1.594584	C	-0.438039	-3.756688	-2.628754
H	-1.638124	3.022084	-2.438311	H	-2.432970	-3.397102	-1.877032
C	-0.457220	5.499515	-0.294678	H	-1.693988	-4.850674	-1.253747
H	-0.674194	5.356623	1.866259	H	-0.768287	-4.299698	-3.525564
H	-2.195555	5.346472	0.977390	H	-0.217787	-2.725263	-2.933260
H	-0.552238	5.261056	-2.455194	H	0.510450	-4.207131	-2.309977
H	-2.121769	5.291952	-1.655840	C	0.396037	-3.904260	0.932972
H	-0.495074	6.595980	-0.320296	C	0.137920	-5.399073	1.185144
H	0.605108	5.224746	-0.259970	H	0.653867	-3.414769	1.884318
C	-3.042251	0.580710	1.175721	H	1.290604	-3.797855	0.304094
C	-2.314385	0.354406	2.517781	H	1.027571	-5.912932	1.577552
C	-4.242273	1.531196	1.336676	H	-0.667363	-5.547259	1.913724
H	-3.437866	-0.398743	0.889859	H	-0.156782	-5.918154	0.264728
C	-3.288005	-0.141385	3.598573	C	-2.561023	-3.133359	1.268326
H	-1.836171	1.281803	2.859416	C	-3.368371	-4.428682	1.067640
H	-1.514182	-0.377955	2.363651	H	-3.248111	-2.285825	1.155308
C	-5.210005	1.007346	2.411830	H	-2.203372	-3.076615	2.308206
H	-3.897099	2.530541	1.633763	H	-4.199187	-4.509147	1.783273
H	-4.769182	1.653494	0.381497	H	-3.801289	-4.470910	0.060931

H	-2.748088	-5.323264	1.185031	H	3.481649	-4.320288	3.007788
				H	3.481730	-2.550230	2.944443
				C	-2.104516	-2.271374	1.808802
TS2B-1				C	-1.067638	-3.406315	1.972761
C	5.352084	0.286723	1.774654	C	-1.982837	-1.218257	2.930460
C	4.024809	-0.106282	1.612229	H	-3.098279	-2.733654	1.872352
C	3.478476	-0.388273	0.345366	C	-1.039052	-3.977898	3.400033
C	4.357353	-0.275843	-0.741607	H	-0.071340	-3.051420	1.696863
C	5.679936	0.135079	-0.586238	H	-1.303964	-4.219323	1.281495
C	6.206092	0.433667	0.675207	C	-1.959517	-1.837336	4.334677
H	5.728050	0.486262	2.776330	H	-1.069555	-0.637851	2.765591
H	3.399670	-0.206829	2.491177	H	-2.812864	-0.506585	2.863541
H	4.016925	-0.513238	-1.735831	C	-0.846892	-2.884169	4.456401
H	6.314580	0.218047	-1.466059	H	-0.242613	-4.730292	3.471210
C	7.625105	0.920930	0.842111	H	-1.985558	-4.502652	3.600119
H	8.283748	0.516310	0.065807	H	-1.829234	-1.045432	5.083849
H	7.675374	2.016158	0.773433	H	-2.929060	-2.313958	4.545175
H	8.034889	0.637669	1.817919	H	-0.834474	-3.321245	5.462936
C	2.041766	-0.919505	0.261244	H	0.127715	-2.396371	4.307533
O	2.021396	-2.319833	0.016583	C	-2.108125	-2.800496	-1.130974
Si	2.950371	-3.540130	0.704575	C	-0.760041	-3.500233	-1.375518
C	4.720862	-3.539445	0.053449	C	-3.216194	-3.853632	-0.933537
H	4.730892	-3.459258	-1.039790	H	-2.339693	-2.252938	-2.053809
H	5.306725	-2.705751	0.452706	C	-0.829339	-4.392440	-2.621182
H	5.225162	-4.475373	0.327741	H	-0.501692	-4.127442	-0.520432
C	2.083365	-5.122670	0.159423	H	0.041957	-2.768482	-1.445388
H	2.692707	-6.002984	0.398458	C	-3.292700	-4.790173	-2.154830
H	1.116815	-5.235426	0.662630	H	-3.008226	-4.446945	-0.033106
H	1.901008	-5.120947	-0.921224	H	-4.190531	-3.381358	-0.776422
C	2.963641	-3.446698	2.590338	C	-1.937799	-5.445389	-2.466799
H	1.947217	-3.432647	2.998204				

H	0.140414	-4.878516	-2.789346	H	2.176496	2.233443	1.887617
H	-1.027479	-3.773836	-3.509316	C	2.917186	5.243722	-0.540790
H	-4.059156	-5.558764	-1.989765	H	1.862819	3.706561	-1.620122
H	-3.618471	-4.204806	-3.027910	H	0.853292	5.056727	-1.127153
H	-2.015756	-6.063356	-3.370429	C	4.090393	4.387776	-0.048135
H	-1.668913	-6.123299	-1.642957	H	4.507137	2.969521	1.548919
C	-3.700975	-0.563834	-0.040809	H	3.496525	4.336959	2.029712
C	-4.173654	-0.472428	-1.510938	H	3.186048	5.778643	-1.461091
C	-4.861803	-1.071441	0.843494	H	2.689598	6.011237	0.214513
H	-3.489526	0.461661	0.277052	H	4.971801	5.014814	0.138813
C	-5.411772	0.429403	-1.650305	H	4.371357	3.667256	-0.830341
H	-4.433911	-1.471892	-1.881590	C	-1.153782	2.938316	1.904670
H	-3.372211	-0.100087	-2.156475	C	-2.583658	2.379885	1.986421
C	-6.098641	-0.166165	0.703790	C	-0.340643	2.484457	3.134849
H	-5.133751	-2.096552	0.560806	H	-1.207117	4.036423	1.925180
H	-4.569727	-1.105408	1.897096	C	-3.283175	2.738701	3.306902
C	-6.559148	-0.056290	-0.755236	H	-2.524119	1.293058	1.886093
H	-5.729221	0.461872	-2.700680	H	-3.190699	2.740928	1.150469
H	-5.147577	1.458148	-1.370037	C	-1.039496	2.862279	4.451126
H	-6.910976	-0.547189	1.336043	H	-0.199223	1.398274	3.086926
H	-5.849228	0.837072	1.082083	H	0.656781	2.934486	3.124034
H	-7.421635	0.617379	-0.836783	C	-2.461278	2.292015	4.522661
H	-6.895865	-1.044628	-1.102291	H	-4.282378	2.283214	3.328559
P	-1.986993	-1.405897	0.131808	H	-3.433196	3.827874	3.351903
C	1.242373	3.596278	0.461037	H	-0.441365	2.508641	5.300893
C	2.437229	2.769569	0.972487	H	-1.085667	3.958827	4.532860
C	1.658527	4.394799	-0.794858	H	-2.954301	2.600998	5.453168
H	0.973703	4.332156	1.234267	H	-2.407915	1.195044	4.540947
C	3.690525	3.620619	1.216293	C	-1.297204	3.430979	-1.010873
H	2.666674	1.994089	0.238420	C	-2.454287	2.614414	-1.609023

C	-1.802491	4.828276	-0.598312	H	1.812980	-2.752493	-2.371682
H	-0.569962	3.561711	-1.824854	H	3.239818	-1.863129	-2.760353
C	-3.077494	3.333004	-2.814138	H	2.351310	-2.996714	-4.780927
H	-3.228224	2.451325	-0.851010	H	0.810299	-2.155734	-4.634232
H	-2.094144	1.626513	-1.897432	H	2.273774	-1.250925	-5.027368
C	-2.418720	5.562903	-1.801337	C	-0.394911	-0.278596	-2.971156
H	-2.569373	4.724296	0.181023	C	-0.471712	0.598730	-4.231969
H	-0.997721	5.430038	-0.160915	H	-1.189548	0.035235	-2.291244
C	-3.553471	4.743170	-2.435246	H	-0.636661	-1.315610	-3.230575
H	-3.911224	2.740381	-3.212048	H	-1.459489	0.520890	-4.707670
H	-2.328169	3.401002	-3.616487	H	-0.312045	1.657165	-3.995604
H	-2.787781	6.549068	-1.491207	H	0.275761	0.312851	-4.978864
H	-1.635483	5.741493	-2.553118				
H	-3.955591	5.262918	-3.313996	INT2B-1			
H	-4.379598	4.658767	-1.712873	C	1.020198	2.596052	2.546564
P	-0.297348	2.473449	0.277410	C	1.339912	1.961582	1.347137
Ni	-0.186776	0.158471	0.010897	C	2.294153	0.933596	1.290267
C	1.138751	-0.517897	1.354192	C	2.910018	0.571452	2.497875
H	0.806982	-1.363902	1.951551	C	2.567416	1.185929	3.702124
H	1.514278	0.277531	1.993669	C	1.612489	2.208899	3.753840
Si	1.337996	-0.329223	-2.059664	H	0.288586	3.402376	2.544364
C	2.254892	1.272372	-2.616938	H	0.835946	2.263332	0.439095
C	3.126479	1.212884	-3.883584	H	3.649611	-0.220525	2.493971
H	2.871377	1.627904	-1.786215	H	3.051494	0.860699	4.621110
H	1.479799	2.036175	-2.755553	C	1.205450	2.843419	5.062794
H	3.654392	2.161837	-4.049935	H	2.010957	2.792521	5.803724
H	3.888063	0.426221	-3.819344	H	0.933107	3.897149	4.932212
H	2.529990	1.010878	-4.779405	H	0.332560	2.335053	5.496007
C	2.155364	-1.868951	-2.917374	C	2.688331	0.292118	-0.034967
C	1.881050	-2.072096	-4.418953	O	3.184201	-1.035216	0.283810

Si	4.419581	-2.104649	0.011457	C	-1.636701	3.346097	-0.553536
C	4.568453	-2.670108	-1.795340	C	-0.534401	3.427616	-1.633501
H	3.695413	-2.375121	-2.384987	C	-2.656919	4.476822	-0.810799
H	5.453903	-2.260066	-2.290820	H	-1.164082	3.531514	0.423835
H	4.640869	-3.763919	-1.836320	C	0.166358	4.794452	-1.613184
C	3.991831	-3.602775	1.073515	H	-0.992065	3.272588	-2.621958
H	4.794596	-4.349665	1.024937	H	0.194428	2.623747	-1.507055
H	3.859557	-3.317700	2.123222	C	-1.969773	5.854291	-0.773517
H	3.067581	-4.082588	0.738113	H	-3.103726	4.340969	-1.805112
C	6.107995	-1.494295	0.609022	H	-3.478537	4.454211	-0.093853
H	6.070520	-1.189186	1.661669	C	-0.833167	5.942479	-1.801525
H	6.827040	-2.321074	0.531882	H	0.944993	4.826762	-2.384430
H	6.509431	-0.656175	0.032685	H	0.680417	4.914923	-0.648663
C	-3.543318	1.433403	-1.782241	H	-2.711505	6.643383	-0.952462
C	-2.871065	0.698845	-2.963948	H	-1.564338	6.026017	0.234847
C	-4.854723	0.734448	-1.372530	H	-0.323753	6.911516	-1.727383
H	-3.805196	2.446277	-2.111068	H	-1.260758	5.886702	-2.813790
C	-3.825729	0.499134	-4.149679	C	-3.236723	1.520295	1.226568
H	-2.514203	-0.275282	-2.609818	C	-2.268325	1.223653	2.387950
H	-1.974674	1.242725	-3.285943	C	-4.178105	2.674377	1.619451
C	-5.795600	0.529500	-2.571465	H	-3.860611	0.626915	1.092350
H	-4.629328	-0.241934	-0.930413	C	-3.024372	0.880945	3.679001
H	-5.373165	1.313396	-0.600512	H	-1.629936	2.097709	2.564623
C	-5.105650	-0.227274	-3.714020	H	-1.595553	0.409488	2.111700
H	-3.316077	-0.060838	-4.944205	C	-4.959490	2.317417	2.897119
H	-4.092950	1.478339	-4.574722	H	-3.584509	3.577709	1.812597
H	-6.695851	-0.006006	-2.243163	H	-4.875102	2.917519	0.809197
H	-6.129334	1.511014	-2.939791	C	-4.012795	1.992130	4.062061
H	-5.790978	-0.342403	-4.563122	H	-2.307836	0.704818	4.491645
H	-4.848981	-1.241853	-3.375041	H	-3.573823	-0.061058	3.533648

H	-5.628862	3.143965	3.168241	H	-3.643239	-1.903305	-1.315974
H	-5.600652	1.446531	2.693663	H	-3.098450	-3.499644	-1.792659
H	-4.587554	1.707656	4.952555	C	-5.628290	-2.833161	0.504586
H	-3.448191	2.898560	4.327060	H	-5.203538	-2.412318	2.597928
P	-2.273316	1.574492	-0.388168	H	-4.629760	-3.982586	2.039009
C	-0.383268	-3.251129	-1.503573	H	-5.573982	-3.406575	-1.594789
C	-0.628310	-2.498568	-2.831925	H	-4.866761	-4.588326	-0.494836
C	1.084957	-3.702454	-1.412500	H	-6.608195	-3.287816	0.697919
H	-1.005976	-4.158425	-1.497506	H	-5.813966	-1.774479	0.271583
C	-0.198797	-3.317435	-4.057572	C	0.087900	-2.717468	1.407811
H	-0.069830	-1.554168	-2.800624	C	0.067257	-1.688582	2.557443
H	-1.684100	-2.225158	-2.925883	C	-0.192698	-4.137105	1.938927
C	1.508900	-4.515663	-2.646587	H	1.105531	-2.674644	1.002446
H	1.725278	-2.822148	-1.305373	C	1.050437	-2.087088	3.667486
H	1.238267	-4.315230	-0.519128	H	-0.939550	-1.610759	2.988422
C	1.270260	-3.743630	-3.949614	H	0.329346	-0.701478	2.165235
H	-0.365532	-2.731978	-4.971274	C	0.781047	-4.528674	3.063779
H	-0.831363	-4.214784	-4.137690	H	-1.213983	-4.181439	2.341140
H	2.564484	-4.798059	-2.555302	H	-0.147575	-4.874624	1.127348
H	0.932031	-5.452653	-2.674323	C	0.760370	-3.496550	4.200699
H	1.562229	-4.351767	-4.815354	H	1.012893	-1.347572	4.476841
H	1.907165	-2.846815	-3.962250	H	2.069266	-2.049773	3.260843
C	-2.641604	-2.975978	0.275575	H	0.523779	-5.525690	3.445413
C	-3.344685	-2.331339	1.484097	H	1.797995	-4.598305	2.657407
C	-3.551862	-2.938520	-0.968953	H	1.486498	-3.771914	4.976605
H	-2.446674	-4.031875	0.510186	H	-0.231277	-3.506390	4.678794
C	-4.735931	-2.926990	1.748031	P	-0.962695	-2.163997	-0.059202
H	-3.444628	-1.256402	1.297862	Ni	-0.457484	0.046646	-0.489858
H	-2.729004	-2.430153	2.383375	C	1.513083	0.145705	-1.048044
C	-4.953052	-3.510112	-0.695042	H	1.492697	1.038234	-1.699878

H	1.813822	-0.659272	-1.732129	C	3.058684	-4.499112	0.681137
Si	4.055122	1.487037	-0.783167	H	4.209284	-3.862851	-1.026003
C	3.199538	3.099724	-1.343014	H	2.469075	-2.450102	-1.971704
C	4.095170	4.347895	-1.442740	H	-0.161097	-3.531807	1.237923
H	2.394564	3.311949	-0.633444	H	1.578587	-4.976308	2.175562
H	2.707410	2.921192	-2.308393	C	4.151094	-5.352233	1.279245
H	3.511876	5.229260	-1.740999	H	3.739383	-6.204175	1.832545
H	4.565354	4.580720	-0.480577	H	4.823549	-5.744952	0.507763
H	4.897664	4.224362	-2.177768	H	4.769531	-4.778243	1.984203
C	5.345926	1.949198	0.546980	C	-0.043450	-1.893296	-0.905083
C	6.736111	2.353236	0.025419	O	-1.350620	-2.423598	-0.680553
H	5.443477	1.116108	1.251054	Si	-2.003278	-3.835433	-1.330541
H	4.917106	2.769488	1.138721	C	-0.694584	-5.096287	-1.834634
H	7.421482	2.598581	0.847139	H	-0.135885	-5.483428	-0.977781
H	7.200639	1.546042	-0.554152	H	-1.172530	-5.938858	-2.351328
H	6.684775	3.230252	-0.629699	H	0.034572	-4.651603	-2.521642
C	4.872396	0.682878	-2.309771	C	-3.049915	-3.469621	-2.862260
C	5.463651	1.661517	-3.341633	H	-3.515583	-4.397822	-3.219555
H	4.112347	0.058722	-2.797250	H	-3.849768	-2.748983	-2.666177
H	5.661045	-0.004078	-1.983358	H	-2.439629	-3.071287	-3.680563
H	5.903560	1.125449	-4.192668	C	-3.115921	-4.492316	0.043379
H	4.698012	2.335674	-3.741450	H	-3.676271	-5.380478	-0.273032
H	6.252667	2.283430	-2.904252	H	-2.522698	-4.762307	0.924884
				H	-3.840644	-3.728638	0.350688
TS2B-2				C	-2.080872	2.165389	1.882302
C	3.261914	-3.769112	-0.496906	C	-1.084460	2.210470	3.051836
C	2.273978	-2.941260	-1.024835	C	-1.913729	3.456111	1.054214
C	1.025207	-2.769686	-0.388338	H	-3.091067	2.157992	2.310762
C	0.808238	-3.564303	0.760669	C	-1.288535	3.460028	3.925655
C	1.795132	-4.394688	1.281049	H	-0.069891	2.217043	2.645950

H	-1.166280	1.319277	3.678202	C	-4.753832	1.592432	0.414367
C	-2.147358	4.712752	1.907150	H	-3.333638	1.109248	-1.102362
H	-0.889216	3.484550	0.663839	C	-5.392157	-0.667129	-1.393846
H	-2.572444	3.468241	0.181445	H	-4.537981	-1.179969	0.507476
C	-1.188739	4.752146	3.104020	H	-3.408393	-1.355238	-0.825473
H	-0.550935	3.465190	4.738831	C	-5.940598	1.647764	-0.565105
H	-2.279832	3.408342	4.400235	H	-5.109502	1.212725	1.380790
H	-2.023381	5.610397	1.287491	H	-4.401421	2.611597	0.590609
H	-3.186652	4.719172	2.268209	C	-6.499502	0.251564	-0.864694
H	-1.393084	5.626375	3.735036	H	-5.778370	-1.682896	-1.551163
H	-0.159273	4.865580	2.732660	H	-5.059503	-0.302169	-2.374452
C	-2.263530	-0.809235	2.019916	H	-6.725472	2.297171	-0.155939
C	-0.990843	-1.312820	2.723526	H	-5.606023	2.112498	-1.504902
C	-3.395427	-0.602257	3.046070	H	-7.325797	0.315184	-1.584070
H	-2.550674	-1.616408	1.337986	H	-6.915931	-0.175744	0.059922
C	-1.269341	-2.615458	3.488576	P	-1.953968	0.605466	0.809606
H	-0.635449	-0.572036	3.447619	C	2.969196	0.355092	1.857931
H	-0.195249	-1.445313	1.985203	C	2.068313	0.712562	3.053158
C	-3.666441	-1.896512	3.834062	C	3.230769	-1.165835	1.860497
H	-3.118689	0.193342	3.751399	H	3.928027	0.880151	1.975759
H	-4.317157	-0.275450	2.556028	C	2.629209	0.208346	4.392648
C	-2.394224	-2.421194	4.514858	H	1.088569	0.263281	2.884918
H	-0.350662	-2.965520	3.977461	H	1.911131	1.789647	3.122045
H	-1.569897	-3.399873	2.779816	C	3.799438	-1.664439	3.196453
H	-4.456820	-1.724566	4.576306	H	2.289579	-1.685637	1.663818
H	-4.044638	-2.662159	3.140336	H	3.908757	-1.460423	1.057783
H	-2.603238	-3.361585	5.040620	C	2.878715	-1.303723	4.366663
H	-2.066886	-1.698343	5.277317	H	1.933087	0.472813	5.199863
C	-3.627605	0.687777	-0.136613	H	3.574711	0.727858	4.610477
C	-4.197543	-0.716980	-0.428094	H	3.942084	-2.750661	3.138130

H	4.792233	-1.219447	3.364964	C	5.752068	0.107866	-3.002763
H	3.306829	-1.641692	5.319176	H	4.106408	0.301251	-4.417355
H	1.919420	-1.828011	4.243433	H	4.008635	-1.118501	-3.379013
C	2.672434	2.762826	0.094092	H	7.032703	-0.131295	-1.259610
C	1.769669	3.459409	-0.938173	H	5.798290	-1.378254	-1.429943
C	2.648063	3.564896	1.409178	H	6.393253	-0.480971	-3.670930
H	3.704915	2.802862	-0.277645	H	6.043884	1.160938	-3.132259
C	2.188085	4.914229	-1.189306	P	2.239532	0.906994	0.190620
H	0.748392	3.453234	-0.547498	Ni	-0.052014	0.163928	-0.520626
H	1.735975	2.902773	-1.879300	C	0.118204	-1.164700	-2.158238
C	3.062991	5.029084	1.177606	H	1.135859	-1.122885	-2.529423
H	1.634479	3.547153	1.831166	H	-0.552864	-1.501384	-2.950151
H	3.315025	3.116206	2.152541	Si	-0.782929	0.819545	-2.794956
C	2.184237	5.712890	0.121167	C	0.352578	1.103539	-4.328388
H	1.512205	5.372424	-1.922365	H	-0.276834	1.702753	-5.002530
H	3.196421	4.935279	-1.629357	H	1.185298	1.767304	-4.062200
H	3.019320	5.578338	2.127062	C	-2.359776	0.039575	-3.575602
H	4.111959	5.055131	0.846964	H	-2.025221	-0.690930	-4.325608
H	2.522197	6.742715	-0.049794	H	-2.886223	-0.551311	-2.821492
H	1.152039	5.776966	0.497956	C	-1.301241	2.625553	-2.294373
C	3.578402	0.239464	-0.969373	H	-2.373344	2.596897	-2.067251
C	3.364052	0.709191	-2.417794	H	-0.818905	2.871382	-1.352837
C	5.055184	0.463372	-0.578049	C	0.888100	-0.100089	-5.120497
H	3.397172	-0.838475	-0.946984	H	1.364645	0.218938	-6.056767
C	4.276017	-0.051271	-3.392171	H	1.636439	-0.667892	-4.558749
H	3.587711	1.782822	-2.496450	H	0.086356	-0.799323	-5.388334
H	2.318604	0.587488	-2.698164	C	-3.335876	1.012336	-4.254778
C	5.985029	-0.299653	-1.540740	H	-2.837394	1.616592	-5.022667
H	5.299033	1.534339	-0.621529	H	-4.160445	0.478410	-4.745573
H	5.256579	0.138084	0.446458	H	-3.787115	1.709263	-3.538710

C	-1.035022	3.756821	-3.301265	H	-2.970754	3.992970	1.667072
H	-1.369621	4.724481	-2.902206	C	0.720620	5.335327	0.683985
H	0.031906	3.851625	-3.531364	H	0.726090	6.242403	1.302403
H	-1.560688	3.595571	-4.248959	H	1.743245	4.941895	0.672643
				H	0.460265	5.629470	-0.336205
INT2B-2				C	3.631447	-1.477574	0.013781
C	-4.154831	0.620327	2.709380	C	3.533015	-2.598198	1.065086
C	-3.464304	0.976509	1.546678	C	3.526680	-2.080877	-1.403071
C	-2.078771	1.233505	1.556888	H	4.621753	-1.017939	0.126758
C	-1.448759	1.141778	2.817612	C	4.583519	-3.695306	0.818518
C	-2.138156	0.805304	3.975441	H	2.531909	-3.039040	1.036313
C	-3.514332	0.525393	3.947856	H	3.673046	-2.193557	2.071433
H	-5.224312	0.424488	2.647588	C	4.583408	-3.166894	-1.648971
H	-4.025515	1.062803	0.622451	H	2.530981	-2.521126	-1.512546
H	-0.388643	1.343843	2.868361	H	3.604107	-1.306666	-2.174478
H	-1.596393	0.747644	4.918604	C	4.482755	-4.279109	-0.596750
C	-4.261493	0.160858	5.208994	H	4.470024	-4.487170	1.569966
H	-3.742863	-0.626016	5.771485	H	5.587657	-3.268576	0.960311
H	-4.360963	1.022289	5.883415	H	4.464410	-3.580361	-2.658760
H	-5.271416	-0.200148	4.986073	H	5.585747	-2.715323	-1.609477
C	-1.269037	1.547482	0.333082	H	5.262973	-5.033810	-0.756764
O	-0.282398	2.618760	0.647868	H	3.517226	-4.794416	-0.709399
Si	-0.485419	4.086959	1.437853	C	2.611660	0.660166	1.891132
C	0.019069	4.018757	3.265290	C	1.868497	-0.168587	2.965051
H	0.991038	3.523545	3.386027	C	4.054307	0.961760	2.336285
H	0.126131	5.042574	3.647369	H	2.066508	1.611167	1.801790
H	-0.707818	3.496270	3.892909	C	1.907796	0.513739	4.340056
C	-2.252678	4.740716	1.313664	H	2.321644	-1.161141	3.061035
H	-2.369908	5.642895	1.928071	H	0.832933	-0.330218	2.652263
H	-2.513505	5.001133	0.281573	C	4.080654	1.642243	3.716287

H	4.631012	0.026869	2.382492	H	-1.834364	-4.037162	0.962245
H	4.555325	1.604185	1.605944	C	-0.113905	-4.005013	3.231645
C	3.350239	0.806116	4.776130	H	0.475564	-2.331301	1.999306
H	1.400955	-0.120916	5.078853	H	0.638181	-3.889507	1.215180
H	1.346153	1.456508	4.299123	C	-2.411269	-3.040106	3.554159
H	5.118733	1.827953	4.020636	H	-1.878535	-1.321486	2.376531
H	3.594431	2.626072	3.636090	H	-3.296608	-2.157742	1.798014
H	3.360734	1.323610	5.743585	C	-1.032019	-3.239027	4.191449
H	3.886624	-0.144102	4.919666	H	0.891286	-4.115185	3.660328
C	3.117203	1.179784	-1.039943	H	-0.508266	-5.022585	3.089035
C	2.600507	2.600129	-0.742880	H	-3.062767	-2.457763	4.216125
C	4.647871	1.205345	-1.250221	H	-2.891945	-4.020276	3.411850
H	2.667004	0.865835	-1.992239	H	-1.115561	-3.767331	5.149897
C	2.996038	3.592072	-1.847875	H	-0.593500	-2.252640	4.405413
H	3.036033	2.947616	0.205184	C	-0.674360	-3.276792	-1.729662
H	1.518280	2.588771	-0.591474	C	-0.034080	-2.497703	-2.898841
C	5.032558	2.197530	-2.362483	C	0.244092	-4.433075	-1.291309
H	5.150008	1.499460	-0.320580	H	-1.602062	-3.737165	-2.098550
H	5.036312	0.218062	-1.516649	C	0.329990	-3.414960	-4.075137
C	4.513139	3.610266	-2.070114	H	0.863833	-1.986049	-2.533690
H	2.631410	4.593771	-1.591403	H	-0.701852	-1.708379	-3.248430
H	2.498122	3.312001	-2.786857	C	0.597264	-5.351101	-2.474263
H	6.123078	2.204271	-2.488083	H	1.172147	-4.031737	-0.866722
H	4.608526	1.846188	-3.315397	H	-0.235656	-5.023601	-0.502609
H	4.775620	4.292055	-2.889005	C	1.236916	-4.569939	-3.631132
H	5.007430	3.996520	-1.165968	H	0.813175	-2.826900	-4.866075
P	2.374135	-0.078348	0.177052	H	-0.593016	-3.827162	-4.509917
C	-1.383639	-3.064823	1.209683	H	1.268495	-6.150343	-2.133542
C	-0.010487	-3.303372	1.868582	H	-0.319667	-5.841435	-2.833689
C	-2.296094	-2.316967	2.205420	H	1.447263	-5.240876	-4.473594

H	2.204674	-4.165096	-3.302283	C	-0.015738	1.229127	-3.073540
C	-3.002040	-1.777157	-0.869869	H	0.948338	1.724626	-2.915031
C	-3.142447	-1.197854	-2.292983	H	-0.021329	0.377772	-2.375620
C	-3.961293	-2.979824	-0.733186	C	-4.011453	3.281517	-3.406773
H	-3.325109	-1.002560	-0.163848	H	-4.795518	3.245899	-4.174197
C	-4.582689	-0.729920	-2.555352	H	-4.458436	2.938852	-2.465865
H	-2.889809	-1.971975	-3.030551	H	-3.737206	4.335381	-3.270328
H	-2.439236	-0.376364	-2.448773	C	-0.131205	4.676761	-3.901733
C	-5.414465	-2.536079	-0.982746	H	-0.962624	4.765704	-4.611138
H	-3.689865	-3.754581	-1.464946	H	0.357636	5.657849	-3.844548
H	-3.891059	-3.446284	0.253374	H	0.595299	3.979419	-4.338967
C	-5.580596	-1.880475	-2.360942	C	-0.090748	0.718995	-4.521945
H	-4.666952	-0.320508	-3.569861	H	0.716053	0.007497	-4.743141
H	-4.827168	0.091194	-1.865837	H	-1.039494	0.207891	-4.723550
H	-6.091445	-3.394623	-0.885017	H	-0.011184	1.541477	-5.243354
H	-5.701089	-1.817341	-0.200702				
H	-6.609446	-1.522456	-2.492957	TS3A-1			
H	-5.407873	-2.637708	-3.140451	C	4.804733	-1.382516	2.391268
P	-1.202232	-2.051510	-0.375670	C	3.484815	-1.528578	1.972289
Ni	-0.026978	-0.071938	-0.031083	C	3.165548	-2.273444	0.826736
C	-2.135554	1.991690	-0.850645	C	4.222778	-2.895953	0.146367
H	-2.812344	1.166251	-1.094949	C	5.543172	-2.755189	0.568687
H	-2.804246	2.825247	-0.568691	C	5.861465	-1.982439	1.692406
Si	-1.369641	2.456177	-2.521145	H	5.019798	-0.790710	3.278739
C	-2.792454	2.423593	-3.791525	H	2.694448	-1.049136	2.540132
H	-2.400839	2.750583	-4.765015	H	4.007020	-3.496302	-0.733301
H	-3.112758	1.383628	-3.939466	H	6.338845	-3.249983	0.015781
C	-0.611835	4.194962	-2.522264	C	7.294507	-1.777610	2.122454
H	-1.329894	4.912177	-2.100587	H	7.935896	-2.602782	1.794367
H	0.231169	4.172115	-1.826137	H	7.705721	-0.853983	1.692380

H	7.380498	-1.693332	3.211684	H	-1.722510	5.529081	-1.617171
C	1.766916	-2.437273	0.335960	H	-2.810828	4.906584	-3.771237
O	1.701772	-1.214471	-1.019759	H	-3.072101	3.264458	-3.185233
Si	2.120693	-1.529340	-2.595844	C	2.313603	1.998348	-0.691555
C	1.000482	-0.524362	-3.747524	C	2.813035	3.374309	-1.176630
H	1.403335	0.482009	-3.907185	C	3.257631	1.443049	0.387804
H	0.903505	-1.001683	-4.731076	H	2.367490	1.303194	-1.539189
H	0.000146	-0.415975	-3.318262	C	4.269219	3.282837	-1.670324
C	1.923350	-3.369343	-3.028328	H	2.751980	4.105527	-0.358721
H	2.628284	-4.010922	-2.486132	H	2.192493	3.761396	-1.991973
H	0.913862	-3.735690	-2.815006	C	4.709287	1.354165	-0.098881
H	2.108510	-3.521154	-4.099603	H	3.228572	2.101471	1.266132
C	3.912661	-1.057378	-2.994459	H	2.908242	0.458375	0.696218
H	4.196319	-1.423410	-3.990329	C	5.208465	2.716814	-0.596122
H	4.041388	0.031368	-2.994319	H	4.611350	4.273245	-1.998555
H	4.616133	-1.475605	-2.266133	H	4.301278	2.630508	-2.556070
C	-0.318522	3.136001	-1.216188	H	5.343435	0.977112	0.712986
C	-0.371072	2.659259	-2.681785	H	4.772953	0.617764	-0.908126
C	-1.720761	3.550329	-0.742822	H	6.230332	2.636304	-0.989025
H	0.313867	4.031504	-1.169437	H	5.249954	3.419655	0.250249
C	-0.998765	3.709818	-3.610364	C	0.299225	2.516061	1.574814
H	-0.955356	1.730451	-2.731394	C	0.795346	1.566521	2.686031
H	0.632965	2.404185	-3.037121	C	0.789979	3.949711	1.853176
C	-2.332816	4.615131	-1.667958	H	-0.799119	2.519453	1.659702
H	-2.367158	2.668533	-0.730258	C	0.270669	2.022441	4.054481
H	-1.692623	3.935668	0.282540	H	1.890099	1.558334	2.713084
C	-2.392315	4.127416	-3.121681	H	0.485451	0.541779	2.462883
H	-1.051307	3.317042	-4.633859	C	0.295473	4.427483	3.231374
H	-0.347857	4.596306	-3.645900	H	1.888007	3.967639	1.833235
H	-3.334031	4.889535	-1.311401	H	0.451180	4.646683	1.077716

C	0.710858	3.464529	4.355240	H	-3.336307	1.750529	0.745280
H	0.625762	1.343778	4.841082	H	-4.291166	0.711615	1.779015
H	-0.828119	1.962395	4.059209	C	-5.212299	1.131029	-2.037999
H	0.671985	5.437809	3.437588	H	-3.055316	0.990735	-1.859067
H	-0.802374	4.500230	3.205998	H	-3.838308	-0.500528	-2.350325
H	0.298779	3.802053	5.314849	C	-5.458317	2.308372	-1.085686
H	1.806123	3.486419	4.457703	H	-5.607277	2.691353	1.050887
P	0.506412	1.810150	-0.156956	H	-6.341883	1.177266	0.528273
C	-2.637888	-2.576661	-0.921944	H	-5.150341	1.484616	-3.075553
C	-1.762634	-2.433736	-2.184767	H	-6.070079	0.443631	-1.990527
C	-2.389319	-3.963594	-0.294234	H	-6.401882	2.810169	-1.335301
H	-3.695703	-2.543783	-1.223841	H	-4.663208	3.052981	-1.217734
C	-2.014850	-3.556556	-3.201325	C	-2.704936	-1.725956	1.935483
H	-0.713948	-2.440673	-1.865622	C	-2.165296	-0.782145	3.029498
H	-1.922754	-1.461073	-2.661046	C	-4.151158	-2.159359	2.246327
C	-2.686040	-5.086265	-1.303539	H	-2.077834	-2.624201	1.984853
H	-1.341166	-4.039885	0.021196	C	-2.262444	-1.433845	4.417320
H	-3.003312	-4.114117	0.598908	H	-2.726293	0.161529	3.035249
C	-1.832235	-4.943369	-2.570149	H	-1.128330	-0.528698	2.801178
H	-1.341477	-3.434454	-4.059318	C	-4.234860	-2.820376	3.633384
H	-3.040711	-3.468788	-3.589958	H	-4.816950	-1.287230	2.236108
H	-2.512057	-6.062320	-0.832408	H	-4.528805	-2.844852	1.478136
H	-3.751877	-5.052937	-1.575371	C	-3.696969	-1.886431	4.728473
H	-2.081113	-5.730310	-3.293420	H	-1.905114	-0.734698	5.184545
H	-0.775154	-5.084821	-2.302696	H	-1.592810	-2.306129	4.448801
C	-3.933903	-0.110315	-0.206771	H	-5.271974	-3.107211	3.850695
C	-4.195970	1.070215	0.750467	H	-3.645058	-3.749108	3.627078
C	-3.933495	0.358166	-1.677203	H	-3.739271	-2.382095	5.706668
H	-4.764762	-0.822347	-0.089745	H	-4.347543	-1.001121	4.795202
C	-5.475068	1.837378	0.373996	P	-2.352999	-1.066374	0.205003

Ni	-0.083390	-0.453846	-0.021533	H	-2.395517	0.494768	-1.626705
H	1.656216	-3.302258	-0.313932	C	-3.461154	4.296382	-1.979972
C	0.624801	-2.128019	1.142237	H	-3.014573	3.844681	0.087258
H	-0.131228	-2.908895	1.142083	H	-1.713707	4.683749	-0.749387
H	0.815526	-1.753471	2.147361	C	-4.511743	3.201661	-2.219211
				H	-4.600346	1.071018	-2.664443
INT3A-1				H	-3.286463	1.922176	-3.467547
C	-1.013792	2.460198	1.729352	H	-3.947380	5.247927	-1.728805
C	-2.326394	1.758696	2.129045	H	-2.899615	4.464815	-2.911037
C	0.099130	2.084063	2.727643	H	-5.182829	3.492489	-3.037209
H	-1.174635	3.546865	1.758206	H	-5.136765	3.097989	-1.319353
C	-2.720242	2.058308	3.583794	C	0.999357	3.105160	-0.361817
H	-2.201561	0.677493	2.001488	C	1.233164	3.255308	-1.880228
H	-3.140926	2.057966	1.462670	C	1.056681	4.497112	0.300941
C	-0.289971	2.382864	4.181980	H	1.841488	2.520766	0.031061
H	0.302919	1.012399	2.611125	C	2.600560	3.895416	-2.161750
H	1.033768	2.601844	2.485451	H	0.451326	3.900723	-2.304465
C	-1.600131	1.681717	4.562628	H	1.148741	2.289016	-2.386445
H	-3.642314	1.516152	3.831157	C	2.422167	5.156298	0.032154
H	-2.947585	3.129931	3.686453	H	0.259928	5.135667	-0.103073
H	0.522029	2.071684	4.852655	H	0.891216	4.434572	1.380820
H	-0.405848	3.469376	4.310265	C	2.719915	5.262045	-1.471093
H	-1.887471	1.934682	5.590920	H	2.749751	3.999114	-3.244039
H	-1.448066	0.593529	4.533393	H	3.393220	3.227145	-1.796182
C	-1.813978	2.544201	-1.172311	H	2.456849	6.149000	0.498986
C	-2.877934	1.449746	-1.398114	H	3.205807	4.553382	0.515598
C	-2.473187	3.902312	-0.866801	H	3.717731	5.689093	-1.632575
H	-1.276879	2.644894	-2.125074	H	2.001215	5.957296	-1.929772
C	-3.843517	1.852717	-2.521388	P	-0.464570	1.968650	0.003148
H	-3.445829	1.290628	-0.475081	C	1.644588	-2.955728	0.792719

C	0.336932	-3.090431	1.606608	H	4.327157	-1.098495	4.367221
C	1.547518	-3.862984	-0.451373	H	4.491780	1.292934	5.040860
H	2.485799	-3.308501	1.409847	H	2.927591	1.629630	4.298146
C	0.104601	-4.545964	2.038323	C	3.086890	-1.188426	-1.092484
H	-0.490491	-2.745038	0.972890	C	3.176587	0.163208	-1.824519
H	0.344762	-2.438645	2.485766	C	4.485066	-1.798585	-0.896819
C	1.295765	-5.326368	-0.049548	H	2.514437	-1.844670	-1.760075
H	0.732531	-3.495638	-1.086013	C	3.890888	0.007483	-3.175204
H	2.466644	-3.820251	-1.044722	H	3.720727	0.897058	-1.216625
C	0.041375	-5.477246	0.820750	H	2.166901	0.557187	-1.966121
H	-0.816337	-4.621950	2.629316	C	5.200336	-1.958371	-2.249831
H	0.926258	-4.861424	2.699691	H	5.086783	-1.140438	-0.253881
H	1.208896	-5.943662	-0.953095	H	4.422125	-2.766937	-0.384914
H	2.169301	-5.701738	0.505619	C	5.282278	-0.620191	-3.000596
H	-0.081061	-6.520694	1.138855	H	3.968463	0.983201	-3.672403
H	-0.840685	-5.219496	0.221139	H	3.281629	-0.632797	-3.829554
C	3.118216	-0.663201	1.832697	H	6.205050	-2.373530	-2.098345
C	3.585579	0.800682	1.706583	H	4.646905	-2.684721	-2.862973
C	2.498067	-0.929754	3.221984	H	5.764592	-0.760159	-3.976139
H	3.999473	-1.314397	1.741222	H	5.919454	0.072191	-2.429668
C	4.497637	1.232596	2.865131	P	1.961803	-1.133689	0.413868
H	2.705174	1.452780	1.683653	Ni	-0.000066	-0.215352	-0.405820
H	4.110078	0.949673	0.757586	Si	-0.695304	-1.523892	-3.249076
C	3.419933	-0.476124	4.366227	C	-2.469545	-1.803289	-3.864791
H	1.538427	-0.404882	3.306392	H	-2.870115	-2.758496	-3.507555
H	2.282676	-1.996302	3.340557	H	-2.528297	-1.800791	-4.961088
C	3.824088	0.996150	4.222323	C	-0.113387	0.116118	-4.022145
H	4.769450	2.289544	2.745812	H	0.954313	0.289558	-3.844359
H	5.435142	0.658633	2.822875	H	-0.663840	0.955069	-3.578485
H	2.920576	-0.647739	5.328396	C	0.407936	-2.905781	-3.945656

H	0.113565	-3.883295	-3.543194	3a			
H	1.460317	-2.744596	-3.677468	C	0.945233	-1.190652	-0.009594
O	-0.653004	-1.495843	-1.619060	C	-0.436461	-1.047510	-0.005307
H	-0.278600	0.142682	-5.107312	C	-1.034045	0.227188	-0.000665
H	-3.130103	-1.009159	-3.493307	C	-0.180285	1.341492	-0.001956
H	0.348668	-2.961698	-5.040487	C	1.206161	1.194184	-0.006099
Si	-3.762210	-1.755983	0.841608	C	1.796204	-0.073481	-0.007685
H	-2.566450	-0.959188	0.461468	H	1.378007	-2.189019	-0.016097
C	-3.304736	-2.766349	2.384892	H	-1.059758	-1.937040	-0.009128
H	-2.626597	-3.573228	2.083442	H	-0.610853	2.340588	-0.002402
H	-4.210662	-3.259869	2.765989	H	1.838469	2.079280	-0.008913
C	-2.651411	-1.934748	3.502846	C	3.296018	-0.246703	0.012486
H	-2.397586	-2.548005	4.377200	H	3.812248	0.685356	-0.239461
H	-1.725250	-1.466155	3.150611	H	3.645787	-0.559649	1.005314
H	-3.312561	-1.130124	3.848980	H	3.619816	-1.015533	-0.698905
C	-5.212024	-0.602150	1.298341	C	-2.489964	0.437976	0.002147
H	-4.818026	0.257796	1.857666	C	-3.451147	-0.494721	0.008050
H	-5.847464	-1.149285	2.010452	H	-4.500253	-0.215090	0.010118
C	-6.077791	-0.109532	0.124437	H	-3.238922	-1.560590	0.011313
H	-6.526362	-0.949185	-0.419275	H	-2.794821	1.485052	-0.000105
H	-6.896881	0.535474	0.467595				
H	-5.491491	0.465518	-0.599448	TS4A-1			
C	-4.216423	-2.881007	-0.612994	C	-2.718998	0.175933	1.894892
H	-5.183091	-3.368508	-0.419262	C	-2.737675	-1.250851	2.475017
H	-4.368336	-2.240752	-1.492450	C	-1.802065	1.058769	2.763420
C	-3.135255	-3.932251	-0.923417	H	-3.740729	0.577516	1.925596
H	-3.026904	-4.644263	-0.096380	C	-3.153778	-1.264145	3.955126
H	-3.383530	-4.514825	-1.820176	H	-1.735072	-1.679100	2.372692
H	-2.165847	-3.449556	-1.091999	H	-3.420077	-1.889940	1.908485
				C	-2.217864	1.057813	4.241768

H	-0.779217	0.671810	2.667910	C	-2.871396	3.526797	-2.463942
H	-1.783297	2.088000	2.392771	H	-3.768519	1.584337	-2.226561
C	-2.249336	-0.366246	4.808460	H	-2.038552	1.525396	-2.538664
H	-3.130818	-2.295706	4.328822	C	-3.731661	4.218810	-0.188469
H	-4.195323	-0.919238	4.043221	H	-4.647542	2.281427	0.108193
H	-1.527894	1.686406	4.819994	H	-3.511952	2.736652	1.366705
H	-3.214844	1.514135	4.336466	C	-3.946284	4.316410	-1.704790
H	-2.589842	-0.357531	5.851595	H	-3.064467	3.555262	-3.544042
H	-1.230259	-0.776048	4.807314	H	-1.892297	4.002199	-2.307620
C	-3.362506	-0.837617	-0.855762	H	-4.528152	4.752016	0.346223
C	-2.990411	-2.330822	-0.858810	H	-2.786519	4.716654	0.077593
C	-4.852748	-0.652573	-0.508733	H	-3.950370	5.365909	-2.025068
H	-3.218179	-0.491417	-1.887579	H	-4.936215	3.905887	-1.953609
C	-3.865332	-3.109744	-1.851178	P	-2.130443	0.215281	0.105180
H	-3.142599	-2.758606	0.136277	C	3.695601	0.660323	0.383498
H	-1.927604	-2.447036	-1.076655	C	3.669631	-0.601025	1.263542
C	-5.743483	-1.451598	-1.477680	C	4.617978	0.409696	-0.826852
H	-5.036054	-0.996916	0.518012	H	4.144559	1.482882	0.960416
H	-5.136165	0.404306	-0.540929	C	5.074434	-0.990768	1.744070
C	-5.355135	-2.936941	-1.520140	H	3.243973	-1.414386	0.669117
H	-3.588754	-4.170900	-1.836747	H	2.995452	-0.477260	2.116099
H	-3.678352	-2.745928	-2.872605	C	6.038312	0.050980	-0.353479
H	-6.797909	-1.338409	-1.193865	H	4.218767	-0.413998	-1.430895
H	-5.642038	-1.023743	-2.486520	H	4.674947	1.286666	-1.479973
H	-5.977990	-3.470803	-2.249067	C	6.041076	-1.177458	0.565585
H	-5.558685	-3.391100	-0.538800	H	5.019784	-1.908859	2.342558
C	-2.562600	1.985235	-0.462046	H	5.458750	-0.203610	2.410823
C	-2.812241	2.067192	-1.984615	H	6.684499	-0.121558	-1.223865
C	-3.673717	2.755117	0.284976	H	6.460501	0.912387	0.185993
H	-1.627257	2.521738	-0.273027	H	7.056467	-1.377376	0.930940

H	5.734730	-2.057720	-0.014505	H	1.407950	1.972678	-4.379249
C	1.816172	2.629428	1.258525	H	3.559882	4.861401	-3.112027
C	0.538389	3.467713	1.091425	H	3.649515	3.189503	-3.663859
C	1.943286	2.121572	2.711272	H	1.815116	4.381712	-4.856859
H	2.682195	3.275800	1.054403	H	1.082448	4.833364	-3.318524
C	0.454464	4.613997	2.110789	P	1.912228	1.204669	0.019950
H	-0.323477	2.808629	1.219699	Ni	0.155619	-0.370402	0.041459
H	0.471630	3.874206	0.077214	Si	0.702232	-2.368503	-2.571755
C	1.850340	3.270351	3.728743	C	0.605030	-4.111228	-3.300257
H	1.152803	1.386655	2.909852	H	1.501845	-4.704846	-3.094053
H	2.894408	1.598872	2.854513	H	0.507568	-4.029044	-4.391350
C	0.567775	4.093139	3.549479	C	-0.706194	-1.352349	-3.334998
H	-0.487588	5.161016	1.971993	H	-0.956774	-0.510356	-2.681964
H	1.266355	5.331160	1.918644	H	-1.614618	-1.949993	-3.464709
H	1.907381	2.864978	4.746878	C	2.319138	-1.599910	-3.181921
H	2.721376	3.930937	3.603446	H	3.200488	-2.108527	-2.777958
H	0.544774	4.927290	4.261930	H	2.381506	-0.542352	-2.908178
H	-0.302255	3.460772	3.774707	O	0.554348	-2.278437	-0.919383
C	2.067160	2.074273	-1.644663	H	-0.423356	-0.949243	-4.315352
C	0.708339	2.220341	-2.350817	H	-0.259988	-4.671791	-2.931596
C	2.842839	3.404886	-1.666332	H	2.371549	-1.661554	-4.276904
H	2.643839	1.355464	-2.240035	Si	0.875915	-3.099483	0.761533
C	0.876974	2.733081	-3.787930	H	0.442459	-1.561593	1.200625
H	0.069332	2.915229	-1.794107	C	1.700707	-3.128514	2.552194
H	0.192396	1.255588	-2.344316	H	2.750976	-2.813931	2.508111
C	3.022912	3.904261	-3.110062	H	1.729323	-4.188669	2.848493
H	2.293388	4.166177	-1.097849	C	0.972682	-2.315682	3.625383
H	3.818818	3.296111	-1.178327	H	1.472250	-2.351773	4.604082
C	1.668783	4.049447	-3.821535	H	0.893520	-1.259625	3.331412
H	-0.107791	2.865437	-4.254474	H	-0.053397	-2.679640	3.770328

C	-0.713117	-4.125830	1.056782	H	-0.673123	-1.946944	2.478144
H	-1.547635	-3.457415	1.278880	C	-1.277901	1.078188	1.675595
H	-0.537498	-4.693720	1.981807	C	-0.833720	2.534854	1.450206
C	-1.121419	-5.102230	-0.055699	H	-0.632066	0.607912	2.430113
H	-0.342308	-5.850416	-0.240559	H	-2.292882	1.059134	2.098995
H	-2.043918	-5.644245	0.194597	H	-0.838662	3.111330	2.383472
H	-1.296009	-4.581248	-1.000954	H	0.181567	2.584224	1.038752
C	2.122293	-4.373535	-0.007808	H	-1.493914	3.050710	0.742931
H	2.113096	-5.223637	0.691450	O	0.270154	0.011206	-0.540558
H	1.711162	-4.760766	-0.945379	Si	1.913378	0.004300	-0.301814
C	3.580944	-3.952262	-0.233367	C	2.609622	-1.569163	-1.067597
H	4.063871	-3.660015	0.706030	H	2.367958	-1.625018	-2.135496
H	4.184703	-4.761195	-0.667889	H	3.701018	-1.615693	-0.966426
H	3.653080	-3.095891	-0.913842	H	2.190452	-2.460423	-0.585302
				C	2.627228	1.525689	-1.151487
Et ₃ Si-OTMS				H	2.221880	2.445022	-0.711747
Si	-1.256119	-0.001762	0.120183	H	3.719733	1.563369	-1.058963
C	-2.432675	0.685373	-1.187913	H	2.379395	1.530896	-2.219382
C	-2.375445	-0.054167	-2.536758	C	2.301670	0.054621	1.544734
H	-2.193504	1.747334	-1.339120	H	3.384350	0.025362	1.720009
H	-3.456820	0.662672	-0.786995	H	1.914430	0.969637	2.008235
H	-3.048043	0.397060	-3.276673	H	1.856515	-0.799390	2.068513
H	-1.361170	-0.034503	-2.950911				
H	-2.665605	-1.106621	-2.430767	TS5A-1			
C	-1.727528	-1.781336	0.559232	C	-4.804129	2.676111	0.790064
C	-0.762977	-2.488553	1.528361	C	-3.472486	2.403508	1.112307
H	-1.798141	-2.357265	-0.373964	C	-2.429865	2.750956	0.244203
H	-2.742537	-1.773280	0.983532	C	-2.776475	3.407621	-0.949506
H	-1.096618	-3.506657	1.764003	C	-4.099624	3.700386	-1.259404
H	0.243285	-2.567077	1.100101	C	-5.144960	3.328193	-0.399245

H	-5.589326	2.388181	1.486365	C	2.970533	4.781999	-0.584153
H	-3.243911	1.946054	2.068144	H	2.090006	3.492179	0.919922
H	-1.984787	3.683233	-1.643290	H	1.357908	3.332143	-0.671813
H	-4.331839	4.213481	-2.190476	C	5.255066	3.746406	-0.309560
C	-6.584859	3.588457	-0.772690	H	4.542543	2.431496	1.240347
H	-6.950088	2.834843	-1.484280	H	5.262169	1.587557	-0.125708
H	-7.241232	3.556141	0.103573	C	4.364967	4.948601	0.033228
H	-6.706277	4.567463	-1.250823	H	2.323862	5.625527	-0.310217
C	-0.989806	2.544721	0.573527	H	3.060462	4.797633	-1.681000
C	3.265108	-0.083927	1.386749	H	6.244435	3.854129	0.153840
C	2.797631	0.633069	2.671909	H	5.418255	3.714971	-1.397351
C	3.075357	-1.603334	1.543745	H	4.830022	5.881157	-0.310814
H	4.335759	0.107464	1.244607	H	4.270152	5.026438	1.126762
C	3.519805	0.103954	3.919539	C	2.846531	-0.455304	-1.533850
H	1.716850	0.475623	2.776569	C	2.139808	0.018548	-2.822199
H	2.940387	1.717517	2.585946	C	4.360196	-0.606211	-1.770956
C	3.791279	-2.142129	2.792834	H	2.438372	-1.446212	-1.291716
H	2.004159	-1.812477	1.626437	C	2.430610	-0.925016	-4.000207
H	3.435606	-2.136618	0.655946	H	2.490200	1.026878	-3.086400
C	3.331758	-1.412625	4.063014	H	1.061985	0.108251	-2.640064
H	3.147937	0.622030	4.812879	C	4.643131	-1.561992	-2.943160
H	4.593872	0.331816	3.846317	H	4.793093	0.376279	-2.003225
H	3.612342	-3.221481	2.884322	H	4.863970	-0.966710	-0.865670
H	4.877164	-2.011853	2.672889	C	3.940419	-1.094803	-4.226248
H	3.876428	-1.788152	4.938584	H	1.946722	-0.547315	-4.910062
H	2.266436	-1.627325	4.235703	H	1.986818	-1.909064	-3.794550
C	3.205375	2.244928	-0.466202	H	5.725224	-1.646112	-3.107412
C	2.313042	3.460462	-0.156435	H	4.285392	-2.568900	-2.679513
C	4.610289	2.425304	0.144497	H	4.127407	-1.803061	-5.043458
H	3.332629	2.221091	-1.557879	H	4.369438	-0.131180	-4.539571

P	2.307250	0.609179	-0.079942	H	-0.891761	-4.678889	-2.939420
C	-1.878171	-1.870386	1.808023	H	1.681396	-5.193014	-0.209612
C	-0.689939	-1.731713	2.788166	H	0.017733	-5.553790	-0.668992
C	-3.115017	-1.167617	2.405547	H	1.453786	-5.465434	-2.705083
H	-2.119519	-2.938746	1.696558	H	1.981824	-3.837154	-2.280767
C	-1.023844	-2.246591	4.196095	C	-3.036653	-0.843611	-0.726282
H	-0.405180	-0.673347	2.835581	C	-2.915494	-0.032380	-2.034694
H	0.188225	-2.260696	2.410657	C	-3.975053	-2.051363	-0.925415
C	-3.447913	-1.685480	3.814846	H	-3.505148	-0.161724	-0.004674
H	-2.923500	-0.089717	2.455615	C	-4.303102	0.408777	-2.526929
H	-3.991331	-1.298041	1.764175	H	-2.438287	-0.634213	-2.817252
C	-2.257108	-1.539767	4.769944	H	-2.269662	0.833824	-1.867070
H	-0.156492	-2.106053	4.854938	C	-5.362602	-1.594912	-1.406198
H	-1.213903	-3.329761	4.152909	H	-3.550400	-2.726628	-1.680836
H	-4.323189	-1.150172	4.205259	H	-4.069289	-2.638496	-0.003189
H	-3.731242	-2.746809	3.750005	C	-5.253830	-0.783705	-2.705223
H	-2.507115	-1.939795	5.760860	H	-4.203597	0.965463	-3.467951
H	-2.030707	-0.471755	4.905980	H	-4.731063	1.104544	-1.796335
C	-0.873816	-2.855778	-0.742280	H	-6.016673	-2.465356	-1.548199
C	-0.575430	-2.655111	-2.241197	H	-5.826943	-0.971991	-0.627127
C	0.335298	-3.503754	-0.042855	H	-6.246331	-0.438223	-3.023045
H	-1.726117	-3.542880	-0.643238	H	-4.876649	-1.438768	-3.505456
C	-0.079166	-3.937219	-2.929915	P	-1.377887	-1.223659	0.086670
H	0.179796	-1.867932	-2.345369	Ni	0.047234	0.580331	0.211679
H	-1.466526	-2.298492	-2.763317	C	-0.514513	1.898451	1.744013
C	0.807160	-4.790530	-0.737896	H	0.368620	2.304720	2.228340
H	1.160125	-2.783423	-0.033427	H	-1.217821	1.418307	2.417769
H	0.098986	-3.730051	1.001525	H	-0.378323	3.363617	0.210189
C	1.135574	-4.537437	-2.213322	H	-0.527019	1.678679	-0.819962
H	0.159243	-3.719490	-3.979196				

INT5A-1				H	5.055245	3.903644	-2.279605
C	-4.805701	-3.003234	-0.891857	H	3.321469	3.624443	-2.139616
C	-3.486891	-3.310565	-0.557898	C	3.034590	-2.254236	-0.527089
C	-2.905703	-2.836825	0.629078	C	2.413622	-2.666505	-1.881981
C	-3.712026	-2.062451	1.470677	C	4.567649	-2.397335	-0.606349
C	-5.029324	-1.743752	1.134972	H	2.668912	-2.973471	0.219443
C	-5.599318	-2.202122	-0.058053	C	2.782949	-4.116086	-2.230199
H	-5.227027	-3.386876	-1.819121	H	2.791480	-2.006135	-2.674447
H	-2.895443	-3.930676	-1.227328	H	1.329832	-2.535213	-1.853470
H	-3.297615	-1.709369	2.410855	C	4.958030	-3.845837	-0.952119
H	-5.622434	-1.131918	1.812860	H	4.959270	-1.730329	-1.387224
C	-7.008825	-1.819890	-0.445360	H	5.047992	-2.097509	0.329319
H	-7.659252	-1.736132	0.432796	C	4.306681	-4.310390	-2.263513
H	-7.030701	-0.848011	-0.957659	H	2.341891	-4.395827	-3.195633
H	-7.453014	-2.554790	-1.125773	H	2.342613	-4.785661	-1.476817
C	3.568238	0.642781	-0.532424	H	6.050556	-3.934055	-1.016642
C	3.445644	0.809555	-2.062116	H	4.636538	-4.506602	-0.133281
C	3.430043	2.008314	0.164126	H	4.558066	-5.360168	-2.462220
H	4.573177	0.256779	-0.314186	H	4.723438	-3.723445	-3.095955
C	4.445450	1.840408	-2.610472	C	2.619078	-0.613085	1.958528
H	2.419968	1.119027	-2.307192	C	1.739977	-1.659593	2.676929
H	3.604429	-0.149200	-2.565159	C	4.065239	-0.704202	2.484680
C	4.437808	3.031990	-0.383822	H	2.221448	0.373919	2.241947
H	2.413941	2.383467	0.006560	C	1.774680	-1.456831	4.199471
H	3.562598	1.909860	1.247451	H	2.101756	-2.669692	2.436551
C	4.305870	3.195204	-1.904314	H	0.711749	-1.607924	2.306948
H	4.305413	1.955271	-3.693059	C	4.104405	-0.475108	4.006103
H	5.467657	1.460789	-2.463681	H	4.465342	-1.703626	2.270870
H	4.300051	3.997423	0.120569	H	4.723532	0.014043	1.982377
H	5.457761	2.696924	-0.143666	C	3.210380	-1.482386	4.744640

H	1.165101	-2.224907	4.692597	H	-0.690078	3.577656	1.681089
H	1.312433	-0.486889	4.438469	C	0.515826	4.832393	-1.861489
H	5.137884	-0.542129	4.370137	H	1.016272	2.732400	-1.666710
H	3.758984	0.546870	4.223335	H	-0.435177	3.043609	-2.603306
H	3.215678	-1.279214	5.823220	C	1.217096	5.370172	-0.607899
H	3.626534	-2.492353	4.612521	H	0.867051	5.505140	1.535528
P	2.317854	-0.623328	0.094899	H	-0.570047	5.750019	0.545198
C	-2.275153	1.066675	-1.819813	H	1.160721	4.949008	-2.742273
C	-1.430169	0.375003	-2.918677	H	-0.387308	5.430890	-2.052571
C	-3.555759	0.248236	-1.567713	H	1.450657	6.435506	-0.729276
H	-2.565978	2.067395	-2.173938	H	2.176004	4.851862	-0.474493
C	-2.230144	0.158770	-4.211251	C	-2.393522	1.270752	1.182027
H	-1.097408	-0.599896	-2.532806	C	-1.639776	1.007416	2.507436
H	-0.518346	0.945158	-3.130056	C	-3.361889	2.463472	1.296368
C	-4.354267	0.019911	-2.860438	H	-2.992426	0.372679	0.995605
H	-3.282601	-0.722695	-1.141432	C	-2.602616	0.888344	3.700675
H	-4.199938	0.744104	-0.835169	H	-0.923453	1.812601	2.711543
C	-3.501197	-0.656369	-3.940207	H	-1.048616	0.088568	2.402393
H	-1.600296	-0.344559	-4.956260	C	-4.327870	2.275437	2.477789
H	-2.506974	1.134611	-4.638984	H	-2.804917	3.396400	1.451189
H	-5.236871	-0.590273	-2.634480	H	-3.923634	2.588923	0.362406
H	-4.721138	0.986008	-3.239799	C	-3.554893	2.089444	3.791689
H	-4.080449	-0.787832	-4.863233	H	-2.028093	0.780054	4.629717
H	-3.218532	-1.660545	-3.592250	H	-3.201966	-0.025356	3.595528
C	-0.733749	3.108034	-0.445118	H	-5.005892	3.135729	2.548995
C	-0.037238	3.672027	0.809513	H	-4.954961	1.390346	2.294715
C	0.114840	3.355595	-1.709145	H	-4.249968	1.960932	4.631097
H	-1.683318	3.649188	-0.572739	H	-2.974523	3.001376	3.998853
C	0.348148	5.150316	0.635770	P	-1.201293	1.284156	-0.274195
H	0.858710	3.079734	1.032792	Ni	0.019936	-0.694902	-0.107338

C	-0.415381	-2.675561	-0.017859	C	-3.755038	3.397659	1.116503
H	0.498761	-3.253708	0.186280	H	-1.912195	2.611691	0.302142
H	-0.728751	-3.000800	-1.026684	H	-3.287461	2.409762	-0.759414
C	-1.478245	-3.180516	0.991197	C	-3.322908	3.367927	2.589134
H	-1.267006	-2.784732	1.994764	H	-3.086290	1.930294	4.205331
H	-1.422909	-4.279227	1.089599	H	-4.510401	1.667389	3.200507
				H	-3.607004	4.399941	0.694089
				H	-4.832121	3.183332	1.047517
TS5A-2				H	-3.917443	4.077076	3.178985
C	4.010686	-2.750343	-1.253091	H	-2.276207	3.697457	2.662401
C	2.872828	-2.167875	-1.803556	C	-2.577243	-1.980079	0.489406
C	1.578425	-2.527392	-1.373146	C	-1.484613	-2.366838	1.508463
C	1.500294	-3.561352	-0.414292	C	-3.985294	-2.247379	1.053080
C	2.641648	-4.142291	0.131204	H	-2.436795	-2.651987	-0.368959
C	3.925513	-3.734274	-0.257557	C	-1.635388	-3.824464	1.965447
H	4.990844	-2.432157	-1.605297	H	-1.540321	-1.717055	2.390297
H	2.987709	-1.420306	-2.581959	H	-0.498254	-2.200784	1.061484
H	0.521518	-3.902995	-0.087567	C	-4.125851	-3.705695	1.525441
H	2.533995	-4.924410	0.880589	H	-4.182445	-1.576284	1.899465
C	5.164333	-4.308797	0.386856	H	-4.747844	-2.028381	0.297679
H	4.999373	-5.335208	0.733974	C	-3.036185	-4.081535	2.540839
H	6.012251	-4.320322	-0.307732	H	-0.861944	-4.064971	2.706558
H	5.471277	-3.717278	1.261336	H	-1.469583	-4.494042	1.107935
C	0.351892	-1.912619	-1.886768	H	-5.122749	-3.865432	1.956285
C	-3.140701	0.936738	0.859781	H	-4.049122	-4.372292	0.653400
C	-2.676441	0.919951	2.328476	H	-3.142198	-5.131424	2.841832
C	-2.978066	2.361669	0.290834	H	-3.166823	-3.476885	3.450897
H	-4.206169	0.670528	0.849464	C	-3.334982	-0.239252	-1.817451
C	-3.447961	1.952022	3.169138	C	-3.263969	-1.557035	-2.620568
H	-1.605834	1.143774	2.371827	C	-4.817797	0.173249	-1.678898
H	-2.806625	-0.073619	2.768206				

H	-2.827559	0.531063	-2.415477	H	2.187511	-2.289640	4.711969
C	-3.900474	-1.398953	-4.010928	H	1.300827	-2.454121	3.192606
H	-3.806514	-2.342894	-2.075955	C	1.415746	3.020054	0.283812
H	-2.233190	-1.901639	-2.724058	C	0.594345	3.540228	-0.917984
C	-5.475593	0.334906	-3.061608	C	0.761949	3.460472	1.606978
H	-5.364822	-0.589619	-1.108603	H	2.411299	3.483771	0.245185
H	-4.927606	1.111481	-1.128499	C	0.379800	5.060006	-0.852532
C	-5.361634	-0.943195	-3.902989	H	-0.369226	3.019470	-0.936371
H	-3.833506	-2.346416	-4.560838	H	1.077684	3.274124	-1.861623
H	-3.326199	-0.657772	-4.586272	C	0.548707	4.982094	1.663851
H	-6.528468	0.621061	-2.940314	H	-0.210164	2.963501	1.715578
H	-4.983764	1.163408	-3.592791	H	1.376675	3.148732	2.458767
H	-5.791474	-0.785541	-4.900304	C	-0.274125	5.482214	0.469558
H	-5.951349	-1.741269	-3.427343	H	-0.232564	5.383948	-1.704070
P	-2.239865	-0.283831	-0.255852	H	1.350818	5.568857	-0.951832
C	2.196591	0.500787	1.812014	H	0.057871	5.250362	2.608819
C	0.949356	0.274210	2.691318	H	1.527867	5.483811	1.663807
C	2.953062	-0.836132	1.630636	H	-0.388283	6.572908	0.513604
H	2.857680	1.229709	2.302764	H	-1.286319	5.056352	0.525351
C	1.252257	-0.452827	4.009448	C	3.315602	1.105863	-0.819784
H	0.232084	-0.314706	2.110110	C	3.204194	1.636541	-2.262857
H	0.456751	1.223085	2.913267	C	4.532630	1.753894	-0.127475
C	3.246962	-1.550890	2.957296	H	3.511788	0.031961	-0.895841
H	2.346341	-1.499511	1.005332	C	4.481187	1.323910	-3.060096
H	3.893558	-0.686914	1.093866	H	3.065622	2.726132	-2.243950
C	1.964716	-1.786562	3.762214	H	2.320655	1.216569	-2.753356
H	0.314808	-0.609202	4.560143	C	5.821753	1.445880	-0.911316
H	1.886907	0.183992	4.644079	H	4.397993	2.843735	-0.077917
H	3.748649	-2.503090	2.742529	H	4.640385	1.404414	0.904774
H	3.945798	-0.948456	3.557602	C	5.721437	1.912337	-2.371108

H	4.391923	1.712257	-4.082950	H	-2.016259	0.221717	5.663377
H	4.597828	0.233452	-3.145559	H	-0.809680	-0.448033	4.565468
H	6.683119	1.916000	-0.419072	C	-2.883310	1.485842	-0.916959
H	5.998943	0.360133	-0.887935	C	-3.215993	0.184417	-1.661614
H	6.631803	1.642767	-2.921756	C	-4.113693	1.968107	-0.120271
H	5.654071	3.010534	-2.391968	H	-2.667183	2.252593	-1.673610
P	1.677099	1.151466	0.108833	C	-4.430925	0.349433	-2.582473
Ni	-0.037157	-0.022261	-0.861908	H	-3.426883	-0.604092	-0.932100
C	0.285340	-0.881901	-2.846577	H	-2.343878	-0.158611	-2.229095
H	1.192278	-0.532071	-3.328693	C	-5.337971	2.130890	-1.038837
H	-0.591590	-0.811211	-3.480627	H	-4.357217	1.232729	0.657298
H	-0.546380	-2.500398	-1.713223	H	-3.908704	2.915133	0.391678
H	-0.091728	0.760678	-2.232375	C	-5.654681	0.831049	-1.792332
				H	-4.643360	-0.605058	-3.076255
INT5A-2				H	-4.198219	1.079374	-3.373319
C	-1.783801	1.315950	1.843197	H	-6.202921	2.455044	-0.445453
C	-2.279294	-0.101563	2.199546	H	-5.138088	2.931429	-1.767089
C	-0.677256	1.749482	2.822162	H	-6.515823	0.975663	-2.457157
H	-2.617184	2.019481	1.958113	H	-5.937782	0.051937	-1.068691
C	-2.753863	-0.193436	3.656127	C	-0.482265	3.002613	-0.251033
H	-1.451166	-0.802648	2.037494	C	-0.062551	3.154528	-1.730268
H	-3.075331	-0.425106	1.520562	C	-1.319581	4.219077	0.189983
C	-1.158977	1.666598	4.280354	H	0.436770	2.991155	0.349325
H	0.191707	1.095127	2.701289	C	0.700874	4.468555	-1.965737
H	-0.336753	2.768536	2.603250	H	-0.957035	3.153471	-2.368125
C	-1.653691	0.254934	4.628253	H	0.538699	2.292662	-2.043976
H	-3.068285	-1.221286	3.878150	C	-0.544454	5.529336	-0.031593
H	-3.640496	0.444069	3.791018	H	-2.248348	4.253655	-0.395170
H	-0.347104	1.966635	4.955499	H	-1.614253	4.130879	1.242261
H	-1.977815	2.385492	4.432143	C	-0.115676	5.682495	-1.498159

H	0.957151	4.564841	-3.028449	H	3.717360	1.538296	-1.646086
H	1.651063	4.442166	-1.414755	C	3.670479	2.846381	2.080542
H	-1.157087	6.385058	0.279780	H	1.771734	1.973983	1.556125
H	0.349412	5.531675	0.610424	H	2.777084	0.929145	2.544739
H	0.462310	6.605392	-1.632871	C	3.712651	3.871660	0.939380
H	-1.013595	5.777466	-2.126695	H	4.154294	3.938596	-1.190745
P	-1.251057	1.312083	0.038617	H	5.232962	2.905699	-0.255676
C	2.645882	-1.634784	1.505049	H	3.286545	3.309746	2.998674
C	1.365283	-1.732129	2.360699	H	4.692488	2.505375	2.302182
C	3.234495	-3.040308	1.265278	H	4.363808	4.715067	1.201475
H	3.397697	-1.076248	2.080845	H	2.703771	4.286573	0.793242
C	1.591851	-2.482877	3.678769	C	3.229714	-1.341465	-1.436792
H	0.591404	-2.237937	1.767898	C	2.651066	-0.927599	-2.807650
H	0.975764	-0.730487	2.565604	C	4.762991	-1.186514	-1.419644
C	3.472832	-3.773293	2.598420	H	3.011893	-2.410412	-1.325331
H	2.547879	-3.635426	0.657317	C	3.298021	-1.739395	-3.940575
H	4.177705	-2.976824	0.712821	H	2.828976	0.142279	-2.984147
C	2.184179	-3.875442	3.426456	H	1.565291	-1.070241	-2.799180
H	0.646104	-2.558579	4.231771	C	5.402725	-2.009670	-2.551500
H	2.281571	-1.904083	4.311875	H	5.038374	-0.132878	-1.555500
H	3.879753	-4.772963	2.399179	H	5.178027	-1.492553	-0.451953
H	4.234840	-3.233086	3.180455	C	4.829158	-1.614626	-3.920727
H	2.378646	-4.390212	4.375887	H	2.900651	-1.413747	-4.910517
H	1.450891	-4.484771	2.878109	H	3.018130	-2.796939	-3.824747
C	3.291873	0.953945	0.415614	H	6.492571	-1.878395	-2.540589
C	3.332488	1.986094	-0.725542	H	5.211441	-3.078038	-2.372097
C	2.801653	1.635617	1.707134	H	5.274570	-2.230719	-4.712174
H	4.314659	0.589990	0.594828	H	5.107950	-0.572284	-4.137875
C	4.183049	3.214968	-0.365681	P	2.252376	-0.567668	-0.024390
H	2.307975	2.301997	-0.942483	Ni	-0.037658	-0.653681	-0.531848

C	-0.427676	-2.507227	-1.355693	H	3.729852	-2.482186	-1.129969
H	-0.299433	-2.390780	-2.445541	H	6.084100	-2.628780	-0.614966
C	0.420677	-3.721000	-0.934398	C	7.325798	-2.426053	1.827061
H	1.469297	-3.591207	-1.218809	H	7.518442	-2.884203	2.803844
H	0.392582	-3.884024	0.149961	H	7.885826	-2.988909	1.072077
C	-1.876179	-2.799389	-1.104978	H	7.747443	-1.411808	1.856002
C	-2.809304	-2.945583	-2.150044	C	1.538779	-2.047780	0.696181
C	-2.382299	-2.949818	0.202135	C	-2.851627	-1.039163	2.144050
C	-4.164982	-3.162510	-1.904150	C	-2.554513	-2.418880	2.772663
H	-2.460359	-2.867558	-3.178179	C	-2.264277	0.092749	3.008669
C	-3.736592	-3.162927	0.450776	H	-3.944054	-0.937917	2.129248
H	-1.692459	-2.865112	1.038026	C	-3.002853	-2.476663	4.243141
C	-4.663241	-3.255155	-0.598090	H	-1.485228	-2.643941	2.714026
H	-4.852474	-3.258325	-2.743559	H	-3.070996	-3.206600	2.219502
H	-4.084478	-3.250359	1.479376	C	-2.698782	0.009121	4.477991
C	-6.141784	-3.419013	-0.331998	H	-1.171957	0.049753	2.932549
H	-6.657749	-2.448209	-0.308284	H	-2.560162	1.064151	2.601760
H	-6.626852	-4.019598	-1.110498	C	-2.364124	-1.360939	5.078881
H	-6.326864	-3.906705	0.632053	H	-2.756772	-3.461426	4.660517
H	0.072560	-4.657225	-1.403273	H	-4.098257	-2.379122	4.290651
				H	-2.216286	0.811224	5.051716
				H	-3.783931	0.179144	4.549223
TS5B-1				H	-2.703000	-1.419177	6.121036
C	4.890947	-2.237304	2.521209	H	-1.272469	-1.495464	5.089716
C	3.534508	-2.131042	2.222572	C	-2.929470	-2.331649	-0.541141
C	3.046386	-2.180825	0.899640	C	-1.991436	-3.544889	-0.385800
C	4.016383	-2.395931	-0.094529	C	-4.394981	-2.740267	-0.286636
C	5.377788	-2.485007	0.200495	H	-2.861237	-2.034336	-1.594951
C	5.849563	-2.391155	1.512447	C	-2.395495	-4.677681	-1.339839
H	5.209827	-2.192689	3.561158	H	-2.017603	-3.925043	0.640726
H	2.829162	-2.010673	3.036790				

H	-0.962997	-3.230582	-0.567765	C	3.420467	1.141126	1.108284
C	-4.804105	-3.892327	-1.223712	C	3.661153	2.527441	-0.989896
H	-4.524650	-3.057903	0.755420	H	2.814613	3.194320	0.855722
H	-5.070368	-1.891770	-0.437000	C	4.886079	1.410455	1.471912
C	-3.855194	-5.094742	-1.103501	H	3.358582	0.208470	0.544729
H	-1.723797	-5.535965	-1.210956	H	2.837917	0.971795	2.017334
H	-2.276014	-4.338677	-2.379634	C	5.130894	2.794594	-0.616659
H	-5.836957	-4.197985	-1.011895	H	3.622506	1.663351	-1.659920
H	-4.790808	-3.526607	-2.261395	H	3.281518	3.383194	-1.556692
H	-4.150095	-5.882221	-1.808536	C	5.726565	1.649890	0.213294
H	-3.945437	-5.524548	-0.094572	H	5.276223	0.558275	2.039807
C	-3.412267	0.585485	-0.282266	H	4.948324	2.294136	2.126137
C	-3.735368	0.459217	-1.788862	H	5.714730	2.954573	-1.532637
C	-4.703967	0.891038	0.505268	H	5.192479	3.728462	-0.037330
H	-2.771463	1.466306	-0.183621	H	6.768867	1.871535	0.477345
C	-4.428999	1.723834	-2.324201	H	5.738809	0.727523	-0.385655
H	-4.399129	-0.398280	-1.958992	C	0.250123	3.092741	1.266193
H	-2.826203	0.270158	-2.367382	C	-1.271939	3.279177	1.160849
C	-5.393504	2.157495	-0.032799	C	0.628765	2.669168	2.701206
H	-5.400290	0.044905	0.435492	H	0.728761	4.062531	1.065977
H	-4.490998	1.034255	1.569015	C	-1.808603	4.275159	2.200933
C	-5.702090	2.042357	-1.530861	H	-1.746259	2.306965	1.314227
H	-4.660617	1.594554	-3.389358	H	-1.557917	3.612078	0.158249
H	-3.736763	2.574749	-2.255361	C	0.091300	3.661153	3.746854
H	-6.312307	2.350209	0.535941	H	0.226701	1.667216	2.893043
H	-4.731948	3.020949	0.136340	H	1.715624	2.597207	2.809434
H	-6.164010	2.966642	-1.900387	C	-1.425558	3.858066	3.627127
H	-6.436045	1.237602	-1.686805	H	-2.899458	4.358634	2.103840
P	-2.264027	-0.811607	0.354827	H	-1.396199	5.273407	1.991526
C	2.797448	2.266698	0.264001	H	0.352961	3.312611	4.754307

H	0.591852	4.631573	3.610183	H	4.192344	-0.507052	-3.885667
H	-1.773309	4.605743	4.351358	H	3.895472	-2.151932	-3.315122
H	-1.932776	2.916592	3.877738	H	2.789238	-1.409125	-4.469767
C	0.607608	2.787107	-1.655578	C	1.458412	-3.618965	-1.977217
C	-0.706133	2.326303	-2.309822	C	1.355868	-4.128974	-3.426462
C	0.684598	4.326737	-1.639345	H	0.696263	-4.141543	-1.381570
H	1.415859	2.422698	-2.304280	H	2.411597	-3.943602	-1.547019
C	-0.855640	2.894409	-3.728406	H	1.487413	-5.218457	-3.472553
H	-1.558619	2.650003	-1.701497	H	0.378169	-3.905541	-3.867722
H	-0.736696	1.234932	-2.328793	H	2.117061	-3.682754	-4.074468
C	0.554579	4.893404	-3.063727	C	-0.394454	-1.431934	-2.804386
H	-0.131099	4.731779	-1.026843	C	-0.112145	-0.985055	-4.248485
H	1.617413	4.671750	-1.178726	H	-1.059847	-0.703751	-2.339296
C	-0.748285	4.426539	-3.731790	H	-0.955328	-2.374508	-2.817605
H	-1.812966	2.574501	-4.159855	H	-1.047317	-0.848969	-4.809888
H	-0.066019	2.472371	-4.367335	H	0.421582	-0.028626	-4.277869
H	0.598994	5.989852	-3.037622	H	0.493631	-1.714898	-4.794876
H	1.412132	4.556592	-3.664973	H	1.085014	-3.030847	0.566802
H	-0.812983	4.813858	-4.756395				
H	-1.603436	4.846980	-3.180891	INT5B-1			
P	0.943194	1.890391	-0.025028	C	2.024526	3.831674	0.495859
Ni	0.026800	-0.263409	0.141185	C	2.178058	2.576951	-0.096114
C	0.819906	-1.238573	1.698679	C	2.531411	1.444848	0.657783
H	0.106114	-1.789955	2.306967	C	2.716601	1.639756	2.037999
H	1.439886	-0.592622	2.318144	C	2.553231	2.890552	2.631505
Si	1.166804	-1.725847	-1.666463	C	2.198501	4.014259	1.873148
C	2.567946	-0.649530	-2.421744	H	1.753475	4.684026	-0.125435
C	3.402907	-1.209817	-3.585580	H	2.024143	2.473154	-1.163375
H	3.241226	-0.364159	-1.609398	H	2.996056	0.792076	2.658219
H	2.081658	0.282679	-2.737631	H	2.700548	2.995603	3.704970

C	1.960638	5.355662	2.525713	H	-2.934145	3.688967	-2.549971
H	2.614580	5.503984	3.392530	H	-2.881615	4.363565	-0.928051
H	2.134726	6.181073	1.826364	C	-0.669701	4.943000	-3.556981
H	0.925050	5.445130	2.883782	H	0.861184	3.504039	-4.129172
C	2.747051	0.095492	0.015898	H	1.043665	4.152359	-2.501501
C	-3.622745	1.206202	-1.209035	H	-2.253499	6.084872	-2.596810
C	-3.494630	0.406223	-2.524610	H	-0.880805	5.728844	-1.549471
C	-4.593544	0.510029	-0.237117	H	-0.120865	5.822887	-3.916021
H	-4.042465	2.193157	-1.441002	H	-1.333545	4.628996	-4.376357
C	-4.860761	0.125483	-3.167809	C	-2.195216	2.008853	1.283209
H	-2.983206	-0.542348	-2.310478	C	-0.855932	2.080429	2.040736
H	-2.853332	0.943208	-3.232994	C	-3.004362	3.297214	1.518004
C	-5.953358	0.220890	-0.893311	H	-2.761440	1.169016	1.713075
H	-4.148944	-0.429660	0.103343	C	-1.072176	2.321891	3.540533
H	-4.748323	1.123514	0.657036	H	-0.238722	2.887658	1.632087
C	-5.802264	-0.588485	-2.188535	H	-0.289112	1.159746	1.884432
H	-4.727181	-0.471994	-4.078658	C	-3.241621	3.525143	3.021032
H	-5.317630	1.076989	-3.478452	H	-2.440092	4.151122	1.120627
H	-6.601616	-0.308528	-0.182993	H	-3.961679	3.271553	0.982593
H	-6.451184	1.175055	-1.121459	C	-1.913312	3.582183	3.790954
H	-6.783648	-0.754059	-2.650679	H	-0.098630	2.402483	4.039213
H	-5.394164	-1.581824	-1.951389	H	-1.584614	1.450681	3.976843
C	-1.245433	2.970272	-1.392488	H	-3.813982	4.449163	3.174538
C	-0.434349	2.581568	-2.649741	H	-3.856756	2.703223	3.417201
C	-2.255140	4.072599	-1.775199	H	-2.099202	3.716153	4.864264
H	-0.531996	3.390522	-0.669285	H	-1.344549	4.463297	3.456714
C	0.301705	3.798837	-3.232189	P	-1.902377	1.447880	-0.483395
H	-1.114732	2.179317	-3.413707	C	-0.230147	-3.560738	-1.046351
H	0.273147	1.781795	-2.416797	C	-0.644885	-2.993256	-2.424206
C	-1.525224	5.306363	-2.335003	C	1.237602	-4.031579	-1.091038

H	-0.846516	-4.446805	-0.832537	H	-5.442525	-1.886966	1.253392
C	-0.407570	-3.999206	-3.559501	C	0.609197	-2.613099	1.656619
H	-0.062052	-2.080009	-2.606439	C	0.733789	-1.437064	2.647042
H	-1.696192	-2.683015	-2.411103	C	0.454733	-3.944381	2.416615
C	1.474875	-5.033187	-2.234011	H	1.558928	-2.645834	1.106259
H	1.894341	-3.166956	-1.232458	C	1.902029	-1.659869	3.619655
H	1.526310	-4.497876	-0.143597	H	-0.193875	-1.319652	3.221854
C	1.056721	-4.456365	-3.592780	H	0.877653	-0.505846	2.093292
H	-0.692784	-3.551118	-4.520204	C	1.635409	-4.166946	3.376910
H	-1.058122	-4.875231	-3.413657	H	-0.474520	-3.928149	3.002393
H	2.532765	-5.325613	-2.250361	H	0.368917	-4.787302	1.719796
H	0.897501	-5.949335	-2.037063	C	1.775311	-2.997496	4.363329
H	1.212690	-5.197041	-4.387533	H	1.957814	-0.826812	4.332191
H	1.696794	-3.593955	-3.830880	H	2.844689	-1.652391	3.052092
C	-2.239675	-3.007758	0.966595	H	1.506302	-5.112195	3.919867
C	-2.781050	-2.186129	2.153363	H	2.562238	-4.261936	2.791898
C	-3.314029	-3.164743	-0.129633	H	2.639288	-3.153902	5.021517
H	-1.998519	-4.016703	1.331728	H	0.885910	-2.966806	5.010552
C	-4.097181	-2.761254	2.701822	P	-0.635924	-2.268238	0.284852
H	-2.935057	-1.146713	1.834092	Ni	-0.225152	-0.173745	-0.556668
H	-2.040888	-2.150689	2.958807	C	1.722520	-0.260648	-1.098933
C	-4.636858	-3.718034	0.426796	H	1.855087	0.439369	-1.943642
H	-3.492394	-2.195028	-0.608408	H	2.002885	-1.231453	-1.529278
H	-2.958262	-3.834637	-0.919581	Si	4.562204	-0.062908	-0.592176
C	-5.163118	-2.888760	1.606231	C	4.763457	0.960005	-2.186140
H	-4.464197	-2.132136	3.523111	C	6.198386	1.358677	-2.575364
H	-3.900909	-3.755234	3.130887	H	4.159954	1.869236	-2.057231
H	-5.385186	-3.760271	-0.375576	H	4.290628	0.406219	-3.008953
H	-4.476096	-4.753579	0.761481	H	6.216004	1.955945	-3.496523
H	-6.076063	-3.342711	2.012362	H	6.671373	1.959318	-1.789412

H	6.835675	0.482757	-2.743717	H	-5.489847	4.411887	-2.826199
C	5.756538	0.558036	0.762011	H	-4.928344	4.914409	-1.229463
C	7.210867	0.060616	0.676976	C	-0.254240	0.838286	-2.339863
H	5.330223	0.262729	1.731972	C	2.704672	0.271892	1.974260
H	5.731908	1.656661	0.764673	C	1.784509	0.818792	3.079259
H	7.823597	0.455067	1.498402	C	2.884103	-1.243180	2.192922
H	7.261916	-1.033647	0.729945	H	3.682458	0.757980	2.081885
H	7.690877	0.362008	-0.260794	C	2.328085	0.507544	4.483874
C	4.897283	-1.915475	-0.914650	H	0.794972	0.365757	2.965984
C	6.022189	-2.240348	-1.914082	H	1.649028	1.898628	2.982066
H	3.961974	-2.367301	-1.269867	C	3.455846	-1.561017	3.582227
H	5.110535	-2.394188	0.053144	H	1.900873	-1.719973	2.104077
H	6.147118	-3.322938	-2.048619	H	3.511295	-1.691007	1.417061
H	5.809563	-1.810827	-2.900382	C	2.554512	-0.995915	4.687542
H	6.987409	-1.838184	-1.585928	H	1.634409	0.897537	5.240121
H	2.668205	-0.659523	0.810446	H	3.280834	1.038993	4.627002
				H	3.568863	-2.646893	3.695991
TS5B-2				H	4.462884	-1.126878	3.672033
C	-3.735678	2.383201	-2.631079	H	2.985373	-1.190417	5.677768
C	-2.709719	1.440046	-2.659970	H	1.584267	-1.514803	4.657382
C	-1.369192	1.788437	-2.378735	C	2.066531	2.546954	0.146108
C	-1.125485	3.166896	-2.179762	C	0.744643	3.159987	0.642872
C	-2.149814	4.104862	-2.148017	C	3.266487	3.274033	0.788801
C	-3.489163	3.731831	-2.347393	H	2.093986	2.735163	-0.935578
H	-4.753941	2.062663	-2.847582	C	0.693090	4.673452	0.382189
H	-2.952867	0.419353	-2.936519	H	0.644213	3.009458	1.721891
H	-0.098557	3.492814	-2.047389	H	-0.096548	2.648941	0.168061
H	-1.906862	5.151484	-1.971435	C	3.203896	4.793360	0.551621
C	-4.607477	4.743713	-2.267183	H	3.273216	3.084653	1.870806
H	-4.301283	5.716394	-2.670605	H	4.212662	2.888739	0.399338

C	1.878083	5.388739	1.043313	H	-0.789162	1.778528	2.199608
H	-0.259615	5.079185	0.745000	H	-1.316369	0.715645	3.484825
H	0.720278	4.865936	-0.698625	C	-3.800497	3.034669	1.484058
H	4.054253	5.280434	1.046267	H	-2.312014	2.227493	0.149358
H	3.309946	4.991862	-0.525458	H	-3.861368	1.439857	0.039510
H	1.842862	6.466167	0.838254	C	-2.835636	3.675850	2.486919
H	1.810916	5.271619	2.135583	H	-1.582526	3.067475	4.160866
C	3.677731	0.251841	-0.812353	H	-3.147817	2.260534	4.091153
C	3.769807	1.125206	-2.084467	H	-4.134568	3.772107	0.744409
C	5.050366	0.232803	-0.100378	H	-4.698735	2.685048	2.015964
H	3.486322	-0.772944	-1.146678	H	-3.322210	4.499784	3.024659
C	4.887118	0.652086	-3.029881	H	-1.987476	4.109428	1.938409
H	3.982035	2.164686	-1.803137	C	-1.876996	-2.132925	2.001942
H	2.810127	1.130799	-2.612567	C	-0.838822	-3.179117	1.559726
C	6.156306	-0.258535	-1.051450	C	-1.668922	-1.814075	3.494585
H	5.311622	1.237288	0.254281	H	-2.875030	-2.584113	1.914933
H	5.032675	-0.413501	0.781148	C	-0.906484	-4.460718	2.400227
C	6.242727	0.608144	-2.313594	H	0.154231	-2.733233	1.677146
H	4.933522	1.316149	-3.902611	H	-0.940506	-3.414079	0.496116
H	4.649541	-0.349649	-3.408155	C	-1.738502	-3.090400	4.352062
H	7.118728	-0.268432	-0.523649	H	-0.685562	-1.345287	3.636619
H	5.944434	-1.298833	-1.340337	H	-2.420496	-1.100213	3.847784
H	7.020207	0.228126	-2.988283	C	-0.722963	-4.144882	3.890773
H	6.540161	1.629215	-2.030880	H	-0.140539	-5.168272	2.058137
P	2.105160	0.651682	0.216059	H	-1.880788	-4.948345	2.246200
C	-2.629506	0.777119	1.733491	H	-1.574005	-2.834970	5.406886
C	-1.668770	1.432945	2.742326	H	-2.752647	-3.511542	4.284846
C	-3.146499	1.854008	0.752467	H	-0.815170	-5.055885	4.495338
H	-3.484592	0.373174	2.294492	H	0.295191	-3.759146	4.052668
C	-2.313436	2.623303	3.471900	C	-3.343992	-1.162849	-0.292563

C	-3.119119	-2.503480	-1.015582	H	1.558524	-2.741825	0.388856
C	-4.736161	-1.182795	0.374795	C	-0.999174	-3.506045	-3.932699
H	-3.357922	-0.379109	-1.056330	H	-1.431497	-4.453320	-4.281161
C	-4.197976	-2.744839	-2.082714	H	-1.831691	-2.816618	-3.764167
H	-3.154359	-3.328299	-0.289458	H	-0.406328	-3.099383	-4.761296
H	-2.128383	-2.526465	-1.466841	C	3.442413	-2.872081	-3.425954
C	-5.834238	-1.420045	-0.678802	H	3.164298	-3.932919	-3.445286
H	-4.779787	-1.984204	1.126176	H	4.069391	-2.684150	-4.307604
H	-4.948576	-0.248408	0.900897	H	4.075188	-2.721145	-2.543486
C	-5.602787	-2.717887	-1.465076	C	1.967841	-4.652999	-0.507022
H	-4.016601	-3.701092	-2.589306	H	2.584505	-5.005140	0.331651
H	-4.122102	-1.962580	-2.852899	H	0.965029	-5.073269	-0.371192
H	-6.819041	-1.436750	-0.194158	H	2.383304	-5.089373	-1.422416
H	-5.840572	-0.569102	-1.376101	H	0.683368	1.280035	-2.681279
H	-6.368294	-2.836335	-2.242465				
H	-5.710122	-3.574935	-0.783370	INT5B-2			
P	-1.860704	-0.670748	0.777643	C	-3.895741	-2.040526	2.062485
Ni	0.180774	-0.316439	-0.659868	C	-3.381338	-1.232278	1.048017
C	-0.432865	-0.572987	-2.658813	C	-2.480943	-0.176289	1.313807
H	-1.460169	-0.925345	-2.633382	C	-2.210972	0.056474	2.684332
H	0.033715	-0.907682	-3.586451	C	-2.721234	-0.752642	3.693279
Si	0.929648	-2.266215	-1.988463	C	-3.564903	-1.838095	3.406744
C	-0.146047	-3.713506	-2.670975	H	-4.581270	-2.845109	1.798775
H	0.590978	-4.501734	-2.883470	H	-3.699691	-1.421467	0.027756
H	-0.771165	-4.126266	-1.868068	H	-1.582156	0.900929	2.952422
C	2.202070	-1.964185	-3.408320	H	-2.471893	-0.530046	4.730118
H	1.664591	-2.101306	-4.357380	C	-4.088335	-2.739675	4.499924
H	2.508885	-0.912665	-3.405391	H	-3.367234	-3.527650	4.762306
C	1.934692	-3.116346	-0.558538	H	-4.296122	-2.179340	5.419633
H	2.962090	-2.739425	-0.626591	H	-5.015205	-3.240571	4.197449

C	-1.813321	0.630423	0.265975	H	-0.072336	2.294960	4.082430
C	3.855294	1.290102	0.075914	H	3.167182	4.294961	4.297628
C	4.307734	0.117629	0.967044	H	1.513549	4.373163	3.691576
C	4.340226	1.075815	-1.372326	H	1.571991	3.042099	5.790345
H	4.321033	2.209677	0.455228	H	2.800010	1.976459	5.108587
C	5.825668	-0.108255	0.898607	C	1.704613	2.966220	-1.011014
H	3.791917	-0.789821	0.637287	C	0.219098	3.374363	-1.052911
H	4.006289	0.281093	2.007216	C	2.588242	4.217545	-0.848635
C	5.858678	0.843739	-1.439405	H	1.933999	2.517058	-1.989368
H	3.828955	0.203676	-1.795248	C	-0.052206	4.389521	-2.174290
H	4.076395	1.931485	-2.003517	H	-0.068503	3.816304	-0.088259
C	6.291488	-0.326906	-0.546897	H	-0.410131	2.491649	-1.189984
H	6.099834	-0.966603	1.525194	C	2.332610	5.219979	-1.987919
H	6.343037	0.767233	1.318388	H	2.350070	4.705202	0.105489
H	6.157278	0.663952	-2.480320	H	3.651532	3.953986	-0.814302
H	6.378396	1.757571	-1.115494	C	0.852162	5.623745	-2.052886
H	7.380415	-0.455350	-0.585481	H	-1.109152	4.683827	-2.160475
H	5.849905	-1.257847	-0.932624	H	0.125964	3.902201	-3.144667
C	1.695864	2.227614	1.900932	H	2.966441	6.106045	-1.854765
C	1.293063	1.113885	2.894629	H	2.628040	4.761166	-2.943406
C	2.810138	3.095019	2.522578	H	0.679249	6.310154	-2.891216
H	0.807769	2.862048	1.758265	H	0.590204	6.173416	-1.136390
C	0.840093	1.700550	4.238954	P	1.985719	1.523418	0.171235
H	2.149332	0.448918	3.068792	C	0.773662	-3.155285	0.929701
H	0.499279	0.491928	2.468539	C	1.965876	-2.569043	1.715406
C	2.358032	3.690462	3.868010	C	-0.489809	-3.117383	1.819560
H	3.700105	2.474362	2.694623	H	0.999280	-4.196302	0.655969
H	3.117330	3.898761	1.847191	C	2.168311	-3.239516	3.082792
C	1.926337	2.594796	4.853223	H	1.780344	-1.498224	1.862198
H	0.570389	0.888444	4.926081	H	2.889391	-2.649579	1.138248

C	-0.280659	-3.794904	3.180306	H	-1.882370	-2.537999	-0.558579
H	-0.768741	-2.071635	1.987616	C	-2.975307	-2.720045	-3.032134
H	-1.343838	-3.579075	1.319578	H	-0.859572	-2.660518	-3.432051
C	0.896744	-3.170062	3.936335	H	-1.462988	-1.204166	-2.636705
H	3.010861	-2.761241	3.600361	C	-2.649492	-4.871936	-1.728630
H	2.448286	-4.293375	2.934279	H	-0.516993	-4.807431	-2.100330
H	-1.204548	-3.704495	3.763180	H	-0.944160	-4.879003	-0.394234
H	-0.092473	-4.870038	3.036768	C	-3.107006	-4.250277	-3.056726
H	1.051560	-3.670100	4.901070	H	-3.250595	-2.295243	-4.006111
H	0.661361	-2.117590	4.154474	H	-3.680694	-2.303890	-2.298445
C	1.685333	-2.684358	-1.957777	H	-2.698323	-5.967206	-1.783852
C	1.817691	-1.555200	-3.004797	H	-3.338305	-4.565059	-0.927851
C	3.079192	-3.096622	-1.450427	H	-4.141095	-4.543274	-3.278233
H	1.250065	-3.563047	-2.455081	H	-2.484512	-4.648912	-3.871940
C	2.753727	-1.946346	-4.159413	P	0.449123	-2.141361	-0.631044
H	2.196928	-0.658929	-2.499346	Ni	0.130644	0.046615	-0.090694
H	0.836958	-1.277574	-3.402450	C	-2.589481	0.815844	-1.057395
C	4.000902	-3.508755	-2.610475	H	-1.912634	1.193914	-1.839982
H	3.540561	-2.253119	-0.921296	H	-2.923640	-0.152863	-1.444503
H	2.998971	-3.920350	-0.731884	Si	-4.072810	2.004181	-1.012617
C	4.133090	-2.386185	-3.648971	C	-4.595081	2.371459	-2.810542
H	2.853634	-1.106112	-4.858756	H	-5.457698	3.052519	-2.811578
H	2.298827	-2.773252	-4.724886	H	-3.780586	2.923513	-3.303180
H	4.988349	-3.786743	-2.219260	C	-5.546284	1.244343	-0.078493
H	3.589916	-4.406008	-3.096290	H	-5.826708	0.309298	-0.585191
H	4.765313	-2.711377	-4.484882	H	-5.197611	0.938074	0.915818
H	4.641319	-1.526981	-3.187582	C	-3.533249	3.629980	-0.169049
C	-1.144643	-2.887344	-1.289328	H	-3.622485	3.493488	0.918205
C	-1.546939	-2.295497	-2.655771	H	-2.460080	3.764514	-0.358116
C	-1.225206	-4.425597	-1.350528	C	-4.929372	1.108106	-3.626117

H	-5.222228	1.347820	-4.656621	H	-2.537617	-0.001949	2.110578
H	-4.070817	0.426724	-3.679694	C	-5.396648	-0.500695	0.163303
H	-5.757832	0.548353	-3.174157	H	-5.297390	-0.624779	-2.009882
C	-6.779796	2.155921	0.050753	H	-4.721239	0.900050	-1.342607
H	-7.151655	2.480484	-0.929563	H	-5.046800	-0.197196	2.292416
H	-7.608512	1.649422	0.562407	H	-4.569490	1.160722	1.277461
H	-6.548432	3.060231	0.626551	H	-6.415448	-0.095063	0.181738
C	-4.287805	4.899967	-0.602378	H	-5.488497	-1.591270	0.276997
H	-3.923206	5.790748	-0.073900	C	2.471441	-0.137174	-0.044599
H	-4.169841	5.086309	-1.676888	C	3.131504	-0.451950	1.306445
H	-5.363550	4.822779	-0.406430	C	3.278598	-0.706413	-1.220577
H	-1.587204	1.622113	0.696092	H	2.410062	0.951188	-0.157021
				C	4.578760	0.062987	1.335482
INT1A-NHC				H	3.123934	-1.539826	1.467858
C	0.000012	0.245241	-0.098532	H	2.537587	-0.001734	2.110522
C	0.679040	-1.924583	-0.015713	C	4.725264	-0.187774	-1.182855
C	-0.678987	-1.924587	-0.015680	H	3.286336	-1.804539	-1.162935
H	1.380849	-2.742747	0.016029	H	2.787493	-0.436277	-2.162853
H	-1.380781	-2.742764	0.016028	C	5.396646	-0.500677	0.163344
N	-1.075333	-0.597045	-0.070313	H	5.046771	-0.196982	2.292423
N	1.075363	-0.597039	-0.070339	H	4.569482	1.160850	1.277341
C	-2.471423	-0.137206	-0.044557	H	5.297413	-0.624977	-2.009833
C	-3.278575	-0.706311	-1.220608	H	4.721269	0.899926	-1.342721
C	-3.131521	-0.452091	1.306449	H	6.415455	-0.095061	0.181753
H	-2.410033	0.951166	-0.156874	H	5.488471	-1.591241	0.277149
C	-4.725241	-0.187667	-1.182857	Ni	-0.000031	2.190807	-0.140307
H	-3.286334	-1.804443	-1.163084	H	-0.000020	3.735287	-0.169511
H	-2.787458	-0.436090	-2.162854				
C	-4.578772	0.062853	1.335504	TS2A-NHC-1			
H	-3.123956	-1.539980	1.467760	C	4.557030	1.637793	-0.042315

C	3.226190	2.060708	-0.070731	C	0.082679	1.787251	-2.141283
C	2.301220	1.456808	-0.929039	H	-0.697750	2.535878	-2.260382
C	2.755675	0.423659	-1.767198	H	0.609329	1.541814	-3.061888
C	4.083185	0.005947	-1.731776	C	-1.075060	-1.418837	-0.251968
C	5.010434	0.598065	-0.861379	C	-1.062964	-3.349883	0.944313
H	5.254362	2.123993	0.637024	C	-2.362633	-3.011460	0.735582
H	2.895786	2.865887	0.575435	H	-0.632784	-4.194423	1.458621
H	2.053412	-0.074779	-2.429043	H	-3.273173	-3.505608	1.034580
H	4.405752	-0.799005	-2.389581	N	-2.351689	-1.835860	-0.003251
C	6.434061	0.097737	-0.790663	N	-0.291320	-2.377219	0.328235
H	6.838170	-0.109810	-1.788514	C	-3.527482	-1.043322	-0.378514
H	7.092876	0.824920	-0.304265	C	-4.606752	-1.888645	-1.067073
H	6.496998	-0.837343	-0.216869	C	-4.089534	-0.282347	0.832545
C	0.855339	1.872793	-0.927681	H	-3.144167	-0.311093	-1.099728
O	0.607818	2.947865	-0.071394	C	-5.790291	-1.001801	-1.487111
Si	-0.659340	3.154269	1.015148	H	-4.967954	-2.664231	-0.376401
C	-2.321067	3.014610	0.134430	H	-4.173736	-2.403196	-1.933104
H	-2.384208	2.048270	-0.380605	C	-5.279043	0.595152	0.416130
H	-3.154747	3.079960	0.844994	H	-4.407396	-1.008058	1.595308
H	-2.446046	3.802681	-0.617122	H	-3.291119	0.324426	1.274258
C	-0.388603	4.893466	1.677681	C	-6.366290	-0.230681	-0.288864
H	-1.171671	5.168793	2.395128	H	-6.566717	-1.616814	-1.957797
H	0.578323	4.975454	2.187747	H	-5.449707	-0.286404	-2.249524
H	-0.401185	5.627729	0.864213	H	-5.692096	1.105130	1.294938
C	-0.592064	1.895105	2.419531	H	-4.919173	1.381457	-0.262232
H	0.428642	1.792104	2.806322	H	-7.185729	0.420663	-0.616681
H	-1.239923	2.207911	3.249466	H	-6.798476	-0.946349	0.426423
H	-0.916135	0.908101	2.075022	C	1.171247	-2.250626	0.419677
Ni	-0.458109	0.204851	-1.039233	C	1.583730	-1.677733	1.783310
H	0.451975	0.689725	0.140208	C	1.906312	-3.559441	0.110405

H	1.434662	-1.517675	-0.347542	C	-1.528461	1.871190	-1.256469
C	3.100404	-1.442237	1.824571	O	-1.176088	1.581803	0.174114
H	1.285769	-2.382129	2.574636	Si	-1.056727	2.806052	1.325279
H	1.040723	-0.741127	1.947268	C	0.179822	4.103294	0.745590
C	3.425858	-3.316747	0.142664	H	-0.154735	4.586464	-0.179804
H	1.645487	-4.324875	0.856140	H	0.343882	4.885053	1.497749
H	1.591633	-3.940544	-0.868974	H	1.137632	3.615826	0.528187
C	3.875702	-2.725678	1.488920	C	-0.437941	1.944994	2.881103
H	3.392521	-1.067425	2.813353	H	-0.172910	2.669161	3.661136
H	3.358083	-0.658651	1.101760	H	-1.198753	1.272156	3.292186
H	3.956900	-4.254258	-0.063352	H	0.453393	1.349849	2.650754
H	3.689282	-2.614734	-0.659898	C	-2.757751	3.572436	1.615614
H	4.953769	-2.521150	1.465524	H	-3.478634	2.804210	1.920501
H	3.712090	-3.470119	2.282861	H	-2.723972	4.336377	2.402780
				H	-3.144213	4.050734	0.707698
INT2A-NHC-1				Ni	0.764145	0.674003	-0.760615
C	-3.166847	-1.325798	-2.600593	H	-2.039952	2.847126	-1.246911
C	-2.204172	-0.364216	-2.298515	C	-0.215391	1.857689	-2.022757
C	-2.555396	0.822291	-1.641552	H	-0.357067	1.552925	-3.066521
C	-3.897363	1.003979	-1.288335	H	0.208749	2.872149	-2.037078
C	-4.859868	0.037225	-1.583706	C	1.588987	-0.591495	0.454962
C	-4.511721	-1.144113	-2.249474	C	1.859043	-2.302152	1.930841
H	-2.867794	-2.240676	-3.108959	C	3.084472	-2.010486	1.421909
H	-1.163076	-0.533707	-2.554888	H	1.563892	-3.038861	2.660361
H	-4.190524	1.912159	-0.765322	H	4.049776	-2.446299	1.624594
H	-5.895567	0.202769	-1.293771	N	2.903535	-0.960048	0.533396
C	-5.549180	-2.187656	-2.592963	N	0.962162	-1.423355	1.342569
H	-6.458776	-2.062794	-1.995624	C	3.947028	-0.371130	-0.313763
H	-5.840158	-2.128374	-3.650389	C	5.170139	0.076752	0.498134
H	-5.168843	-3.201571	-2.420654	C	4.337602	-1.328414	-1.450621

H	3.477054	0.517363	-0.752543	H	-2.901213	-3.622626	2.419963
C	6.217813	0.721627	-0.424070				
H	5.620184	-0.792214	0.999321	TS2A-NHC-2			
H	4.853002	0.773736	1.283092	C	2.926308	2.654252	0.164952
C	5.392942	-0.687296	-2.364089	C	1.834279	2.177558	0.881340
H	4.734860	-2.257633	-1.016590	C	0.608487	1.875322	0.241005
H	3.436666	-1.594221	-2.016421	C	0.563935	2.052400	-1.158402
C	6.620943	-0.227918	-1.563184	C	1.668806	2.522852	-1.865829
H	7.097328	1.016119	0.161110	C	2.874461	2.837386	-1.225752
H	5.800360	1.644644	-0.851790	H	3.845708	2.889968	0.698365
H	5.687193	-1.394177	-3.149094	H	1.931151	2.034542	1.953300
H	4.946338	0.179790	-2.872034	H	-0.349884	1.805055	-1.687257
H	7.345518	0.261720	-2.225305	H	1.591387	2.647277	-2.944714
H	7.126046	-1.108119	-1.137891	C	4.084532	3.310906	-1.995203
C	-0.501263	-1.437033	1.511439	H	4.600931	4.126753	-1.474693
C	-1.163854	-2.427353	0.542304	H	4.818147	2.503187	-2.129667
C	-0.919091	-1.706702	2.961662	H	3.810534	3.671003	-2.993015
H	-0.828624	-0.433005	1.232629	C	-0.553822	1.369449	0.974400
C	-2.691861	-2.352336	0.675522	O	-1.755269	1.273268	0.233469
H	-0.807108	-3.444944	0.762169	Si	-2.871898	2.532452	0.140473
H	-0.855505	-2.178212	-0.478848	C	-3.506975	2.533700	-1.633683
C	-2.448789	-1.616786	3.088669	H	-3.929055	1.559681	-1.904783
H	-0.600427	-2.714373	3.265839	H	-4.290444	3.288504	-1.775287
H	-0.425592	-0.993093	3.631320	H	-2.695274	2.755627	-2.336401
C	-3.143739	-2.590657	2.123710	C	-2.044780	4.170472	0.566618
H	-3.161782	-3.076140	-0.000319	H	-2.736668	5.009708	0.423571
H	-3.025571	-1.361147	0.344431	H	-1.705702	4.185631	1.608531
H	-2.748784	-1.817548	4.124565	H	-1.166529	4.334483	-0.067243
H	-2.768819	-0.590431	2.857790	C	-4.297553	2.183172	1.329349
H	-4.233130	-2.487199	2.203014	H	-5.089582	2.937020	1.235311

H	-4.745292	1.202182	1.130301	H	-4.919347	-3.224738	-1.803266
H	-3.957835	2.186068	2.372024	C	2.752078	-1.507476	0.186416
Ni	-0.078091	-0.432119	1.719830	C	3.555358	-2.668247	0.791351
C	-0.649017	1.374259	2.412577	C	3.537029	-0.772487	-0.909256
H	0.068159	1.966590	2.978208	H	2.511234	-0.790333	0.978539
H	-1.654632	1.442099	2.823273	C	4.907861	-2.171200	1.324485
H	-0.309490	0.022681	3.191496	H	3.723787	-3.433109	0.018896
C	0.258033	-1.620118	0.261564	H	2.966365	-3.138047	1.588175
C	1.257125	-2.785768	-1.411209	C	4.890136	-0.287604	-0.368544
C	-0.084787	-2.951778	-1.545811	H	3.709163	-1.453702	-1.755541
H	2.075064	-3.171820	-1.998270	H	2.941056	0.068581	-1.276640
H	-0.654257	-3.506724	-2.274315	C	5.705673	-1.442744	0.231845
N	-0.678525	-2.234203	-0.519740	H	5.483444	-3.014172	1.725849
N	1.447882	-1.967176	-0.308963	H	4.731325	-1.482338	2.163418
C	-2.124776	-2.088592	-0.313563	H	5.452545	0.207425	-1.169858
C	-2.790272	-1.397161	-1.511436	H	4.708456	0.473676	0.401501
C	-2.784349	-3.435241	0.014404	H	6.653488	-1.069358	0.639247
H	-2.215961	-1.425312	0.552432	H	5.963162	-2.157783	-0.563990
C	-4.295451	-1.224256	-1.259588				
H	-2.638042	-2.000857	-2.418153	INT2A-NHC-2			
H	-2.306520	-0.427751	-1.664904	C	-2.328710	-2.910846	0.873025
C	-4.288378	-3.247346	0.266184	C	-1.080996	-2.583621	1.374416
H	-2.637819	-4.129232	-0.826282	C	-0.047187	-2.057276	0.531877
H	-2.291794	-3.877884	0.888404	C	-0.401255	-1.871764	-0.843438
C	-4.973312	-2.562242	-0.926394	C	-1.672012	-2.217465	-1.322893
H	-4.770158	-0.760269	-2.133075	C	-2.660158	-2.742944	-0.489524
H	-4.434065	-0.529338	-0.419763	H	-3.074248	-3.326878	1.549510
H	-4.757100	-4.216628	0.475110	H	-0.872551	-2.749539	2.426430
H	-4.425234	-2.630054	1.166049	H	0.359225	-1.526955	-1.535524
H	-6.038425	-2.406601	-0.714481	H	-1.884437	-2.081857	-2.382464

C	-4.016132	-3.156199	-1.010617	N	-1.835874	2.158674	-0.256734
H	-4.833322	-2.702415	-0.433873	C	1.647424	2.771300	0.213560
H	-4.148635	-2.862174	-2.057950	C	2.356009	2.010814	-0.920592
H	-4.157899	-4.244528	-0.955932	C	2.284836	4.143350	0.451706
C	1.204046	-1.512973	1.051030	H	1.749685	2.174773	1.129168
O	2.245497	-1.362678	0.071885	C	3.849087	1.850821	-0.604451
Si	3.233396	-2.568214	-0.540051	H	2.217238	2.565708	-1.860114
C	3.648841	-2.014028	-2.294595	H	1.895621	1.024032	-1.033325
H	4.084977	-1.007734	-2.287130	C	3.776379	3.972067	0.788263
H	4.366760	-2.688212	-2.777807	H	2.193745	4.757361	-0.455926
H	2.745480	-1.980769	-2.915370	H	1.759909	4.670794	1.257921
C	2.348118	-4.235095	-0.550653	C	4.517609	3.204094	-0.318125
H	2.995717	-5.025299	-0.951380	H	4.350212	1.343329	-1.437625
H	2.044292	-4.529669	0.460579	H	3.948959	1.188375	0.266458
H	1.440313	-4.188841	-1.162093	H	4.235178	4.955315	0.948095
C	4.818730	-2.673205	0.482271	H	3.867578	3.422882	1.736471
H	5.527065	-3.398710	0.062120	H	5.568308	3.060666	-0.036908
H	5.318192	-1.697153	0.516998	H	4.517073	3.810573	-1.236260
H	4.601850	-2.972617	1.514173	C	-2.988051	1.241569	-0.202617
Ni	0.017462	0.048436	0.763036	C	-3.574143	1.171934	1.215421
C	1.734599	-1.934034	2.402557	C	-4.063000	1.587973	-1.236236
H	0.975918	-1.816505	3.183155	H	-2.573526	0.256385	-0.445710
H	2.082835	-2.982132	2.431359	C	-4.706622	0.135584	1.271320
H	2.583514	-1.296905	2.673317	H	-3.947945	2.166721	1.499684
C	-0.609011	1.764694	0.180798	H	-2.769807	0.906437	1.910907
C	-1.803266	3.464075	-0.725248	C	-5.183714	0.536385	-1.191064
C	-0.519525	3.895288	-0.589277	H	-4.491327	2.576586	-1.014857
H	-2.671784	3.971859	-1.111334	H	-3.618784	1.640454	-2.237996
H	-0.072943	4.844653	-0.835411	C	-5.787992	0.422607	0.217817
N	0.193926	2.848215	-0.024929	H	-5.146676	0.117154	2.275841

H	-4.274617	-0.858044	1.094608	H	0.785102	0.774666	3.284519
H	-5.960787	0.789942	-1.922363	H	-0.862569	0.635861	2.644573
H	-4.769401	-0.435432	-1.489107	C	1.854707	-2.324972	3.099353
H	-6.553315	-0.363427	0.235937	H	2.752307	-1.694950	3.091408
H	-6.297884	1.365149	0.467623	H	1.608468	-2.553841	4.144095
				H	2.114939	-3.270944	2.607595
TS3A-NHC-1				Ni	-0.536396	-0.669769	-0.806608
C	4.333819	-0.219135	-1.846241	H	1.409325	-3.133338	0.148969
C	3.042513	-0.684014	-1.625220	C	0.451106	-2.291982	-1.592619
C	2.811263	-1.788625	-0.789287	H	0.802410	-2.026787	-2.591405
C	3.912028	-2.394365	-0.173928	H	-0.232783	-3.144227	-1.592592
C	5.208004	-1.927712	-0.401914	C	-1.568096	0.868246	-0.256738
C	5.442793	-0.834610	-1.242234	C	-2.095092	2.936980	0.528861
H	4.488542	0.644977	-2.489333	C	-3.262549	2.303857	0.241506
H	2.192640	-0.179605	-2.076026	H	-1.917116	3.923344	0.924427
H	3.754115	-3.237454	0.494517	H	-4.284255	2.634071	0.342387
H	6.047632	-2.417813	0.086240	N	-2.922344	1.046540	-0.237822
C	6.841917	-0.331115	-1.508586	N	-1.074265	2.047375	0.229291
H	6.887895	0.763713	-1.466905	C	-3.875219	-0.004688	-0.608550
H	7.557953	-0.726786	-0.780570	C	-4.674437	-0.489170	0.610886
H	7.188536	-0.629326	-2.507250	C	-4.797241	0.438190	-1.752652
C	1.442057	-2.307317	-0.558573	H	-3.246999	-0.831235	-0.961599
O	0.885554	-1.013109	0.683296	C	-5.632830	-1.622703	0.214380
Si	0.423479	-1.457745	2.213239	H	-5.249090	0.352181	1.024942
C	-1.068764	-2.624474	2.135774	H	-3.976998	-0.817902	1.390438
H	-0.822318	-3.549792	1.599875	C	-5.752944	-0.699972	-2.144696
H	-1.447589	-2.900772	3.128032	H	-5.383562	1.312125	-1.433565
H	-1.876772	-2.134529	1.577692	H	-4.188497	0.754043	-2.608282
C	-0.069254	0.095881	3.174296	C	-6.559690	-1.196043	-0.934305
H	-0.436062	-0.148685	4.179363	H	-6.218997	-1.938094	1.085888

H	-5.042720	-2.495729	-0.100407	H	-2.670466	-0.205387	-2.293261
H	-6.424889	-0.364472	-2.943832	H	-2.128086	0.762448	-3.667818
H	-5.166384	-1.534504	-2.555910	C	-3.646561	2.146486	-0.210818
H	-7.209472	-2.029669	-1.227734	H	-3.455152	2.942665	0.519358
H	-7.220731	-0.388573	-0.585351	H	-3.599219	1.192768	0.330851
C	0.375791	2.296471	0.339970	O	-0.839760	2.051295	-1.058661
C	0.962884	2.726357	-1.013170	H	-3.832412	0.809964	-3.170511
C	0.709855	3.308830	1.440427	H	-1.876801	3.876152	-3.399968
H	0.810419	1.327851	0.605605	H	-4.672487	2.269300	-0.582371
C	2.483686	2.912713	-0.901083	Si	1.260946	2.059402	1.788485
H	0.483698	3.662846	-1.334927	H	1.094303	0.830932	0.914031
H	0.716299	1.957227	-1.755246	C	2.120165	1.355581	3.331415
C	2.234594	3.459814	1.560733	H	1.365248	0.881621	3.973415
H	0.279220	4.290552	1.194035	H	2.539703	2.185098	3.918988
H	0.271291	2.986525	2.391532	C	3.225429	0.337190	2.993690
C	2.853908	3.892944	0.222387	H	3.734589	-0.029872	3.893540
H	2.889721	3.256836	-1.860778	H	2.808603	-0.532249	2.470533
H	2.943958	1.938342	-0.694688	H	3.993020	0.773041	2.340649
H	2.475660	4.183610	2.348831	C	2.397042	3.232945	0.826748
H	2.667221	2.497261	1.868648	H	3.438288	3.031594	1.117711
H	3.944537	3.966880	0.316373	H	2.187285	4.261692	1.153364
H	2.489254	4.899252	-0.033217	C	2.239720	3.123793	-0.703014
				H	1.202057	3.277637	-1.014280
				H	2.883358	3.843766	-1.224354
INT3A-NHC-1				H	2.509668	2.117999	-1.048963
Ni	-0.083224	0.480370	-0.420404	C	-0.452282	2.761402	2.145978
Si	-2.366258	2.190716	-1.619076	H	-0.371716	3.607063	2.843899
C	-2.576653	3.823245	-2.556752	H	-0.817691	3.149821	1.188016
H	-2.369219	4.679353	-1.902391	C	-1.447211	1.713541	2.677406
H	-3.593021	3.942987	-2.954101	H	-1.115301	1.267714	3.623855
C	-2.799939	0.760753	-2.799892				

H	-2.438887	2.149869	2.845268	C	-4.522338	-2.339276	-0.443534
H	-1.568246	0.903801	1.946872	H	-2.983950	-3.866908	-0.490610
C	0.236262	-1.400385	-0.220720	H	-2.777723	-2.619178	-1.726603
C	-0.152905	-3.617430	0.096534	C	-3.955685	-1.759430	1.961984
C	1.184272	-3.463172	-0.092982	H	-2.374600	-3.248908	2.004845
H	-0.737496	-4.503904	0.284588	H	-1.811099	-1.606288	2.339251
H	1.975705	-4.194385	-0.105831	C	-4.923687	-2.505905	1.030650
N	1.405760	-2.104455	-0.275344	H	-5.199338	-2.907027	-1.092882
N	-0.714969	-2.351909	0.011503	H	-4.619858	-1.283158	-0.732130
C	2.686489	-1.438656	-0.561908	H	-4.226429	-1.924635	3.011789
C	3.889998	-2.210902	-0.013300	H	-4.039248	-0.678303	1.781861
C	2.834162	-1.148067	-2.063508	H	-5.948875	-2.148318	1.185765
H	2.627651	-0.478176	-0.039278	H	-4.919830	-3.575887	1.287423
C	5.181168	-1.417927	-0.273415				
H	3.967638	-3.186894	-0.513236	TS4A-NHC-1			
H	3.757678	-2.401779	1.058750	Ni	0.050628	0.173650	-0.172843
C	4.136542	-0.381584	-2.339405	Si	1.723934	2.618178	0.613899
H	2.828660	-2.100625	-2.612901	C	1.755800	4.414590	1.184895
H	1.962234	-0.569830	-2.391259	H	1.550648	5.109115	0.363663
C	5.358762	-1.118723	-1.770486	H	2.744328	4.659451	1.594989
H	6.042803	-1.975061	0.113355	C	2.223581	1.508963	2.067876
H	5.139397	-0.472239	0.286335	H	2.090564	0.448763	1.815634
H	4.251686	-0.218762	-3.417490	H	1.594581	1.710567	2.942610
H	4.068531	0.614124	-1.878619	C	2.963516	2.366418	-0.794528
H	6.268717	-0.528000	-1.932279	H	2.764406	3.052391	-1.626254
H	5.496761	-2.066255	-2.312200	H	2.881266	1.346022	-1.189798
C	-2.125347	-2.016686	0.244250	O	0.229331	2.112013	0.083853
C	-3.071444	-2.787730	-0.683885	H	3.271518	1.658456	2.357746
C	-2.501518	-2.193534	1.722243	H	1.014947	4.595730	1.972412
H	-2.195886	-0.950371	0.001107	H	3.999162	2.523206	-0.466635

Si	-1.622823	2.386032	-0.376001	C	-2.179791	-2.314513	-0.043467
H	-1.392995	0.798166	-0.748225	C	-3.069524	-3.295681	-0.815487
C	-3.036150	2.277762	-1.724561	C	-2.624970	-2.166771	1.419286
H	-2.608095	2.572087	-2.695184	H	-2.245349	-1.331990	-0.519806
H	-3.767419	3.063601	-1.478670	C	-4.537915	-2.844664	-0.743961
C	-3.749466	0.931248	-1.877345	H	-2.988091	-4.302034	-0.379649
H	-4.546698	0.958249	-2.633363	H	-2.730401	-3.363386	-1.856411
H	-3.042290	0.145199	-2.172779	C	-4.099244	-1.742974	1.497382
H	-4.210240	0.611016	-0.932956	H	-2.479690	-3.125999	1.938048
C	-2.507166	2.192101	1.303887	H	-1.980167	-1.426483	1.907030
H	-3.262413	1.403363	1.180619	C	-5.005273	-2.704851	0.713326
H	-3.068656	3.118425	1.495602	H	-5.170676	-3.559586	-1.283651
C	-1.622188	1.860897	2.514150	H	-4.642255	-1.878199	-1.255174
H	-0.888399	2.653392	2.703352	H	-4.414417	-1.683997	2.546065
H	-2.210896	1.727676	3.431918	H	-4.200305	-0.731322	1.081909
H	-1.052717	0.939171	2.339978	H	-6.045095	-2.357254	0.744995
C	-1.247833	4.260365	-0.650147	H	-4.987271	-3.694453	1.194389
H	-2.219153	4.769767	-0.733294	C	2.719887	-1.837109	-0.220949
H	-0.770285	4.662865	0.251300	C	3.569361	-2.135028	1.022716
C	-0.397736	4.606613	-1.883431	C	3.447310	-2.228335	-1.515097
H	-0.884719	4.277468	-2.810145	H	2.528319	-0.758935	-0.253240
H	-0.219166	5.686687	-1.978533	C	4.923560	-1.414055	0.926325
H	0.581482	4.115301	-1.845206	H	3.733557	-3.219363	1.101881
C	0.230099	-1.726650	-0.172786	H	3.022862	-1.824555	1.920994
C	1.132872	-3.810539	-0.061926	C	4.803584	-1.511269	-1.605493
C	-0.218829	-3.949135	-0.042148	H	3.601731	-3.316954	-1.529900
H	1.916617	-4.550863	-0.035811	H	2.812849	-1.979395	-2.373937
H	-0.828819	-4.836101	0.011335	C	5.667234	-1.788731	-0.365047
N	-0.753593	-2.671856	-0.121188	H	5.534223	-1.651333	1.805557
N	1.389745	-2.449747	-0.141246	H	4.750754	-0.328405	0.946189

H	5.328366	-1.819609	-2.517459	C	2.037762	-2.130360	-0.239047
H	4.630470	-0.428887	-1.691325	C	2.511398	-1.807107	1.186471
H	6.612987	-1.237288	-0.430499	C	2.842894	-3.279024	-0.856650
H	5.925900	-2.857688	-0.335915	H	2.180060	-1.234403	-0.855426
				C	4.010828	-1.475320	1.195032
INT1B-NHC				H	2.308185	-2.671754	1.834789
C	-0.309756	-1.351536	-0.364545	H	1.922772	-0.964058	1.567874
C	-0.056591	-3.589680	-0.080376	C	4.340657	-2.929150	-0.857894
C	-1.391254	-3.327420	-0.083595	H	2.696325	-4.194938	-0.266649
H	0.469348	-4.525477	0.015748	H	2.484847	-3.483876	-1.872877
H	-2.232582	-3.994626	0.009899	C	4.838787	-2.602842	0.559086
N	-1.525688	-1.960176	-0.270583	H	4.343537	-1.283485	2.221782
N	0.585440	-2.375176	-0.265449	H	4.171685	-0.542853	0.635943
C	-2.780967	-1.190264	-0.250122	H	4.913815	-3.760211	-1.285845
C	-3.933985	-1.927694	-0.940983	H	4.506692	-2.061173	-1.511941
C	-3.144930	-0.778731	1.185156	H	5.899779	-2.326597	0.531712
H	-2.556918	-0.280418	-0.819840	H	4.762959	-3.505550	1.183428
C	-5.199752	-1.054359	-0.934688	Ni	0.087044	0.581582	-0.363993
H	-4.151188	-2.863522	-0.406698	Si	0.563455	2.838506	-0.199073
H	-3.645189	-2.196439	-1.964294	C	1.609270	3.232896	1.376084
C	-4.423530	0.072563	1.199170	H	1.005169	2.987191	2.261905
H	-3.286606	-1.685597	1.790858	H	1.798915	4.315264	1.432406
H	-2.301745	-0.224153	1.614646	C	-1.007205	3.947266	-0.036762
C	-5.585639	-0.644504	0.495276	H	-1.501805	3.986424	-1.019031
H	-6.023301	-1.594515	-1.416707	H	-0.708033	4.980462	0.194134
H	-5.018559	-0.152322	-1.536527	C	1.561661	3.573234	-1.678693
H	-4.691923	0.321707	2.232500	H	2.469248	2.966218	-1.814995
H	-4.223013	1.025682	0.690621	H	0.968046	3.417347	-2.591824
H	-6.473882	-0.001500	0.477495	C	2.942518	2.470678	1.442859
H	-5.857938	-1.544508	1.066626	H	3.585017	2.714551	0.586495

H	3.515034	2.693860	2.354038	H	-2.823528	-3.375380	-2.465906
H	2.772945	1.385626	1.416259	H	-1.224603	-3.104672	-3.166176
C	1.949039	5.057423	-1.559989	H	-1.886864	-4.753739	-3.084378
H	2.506863	5.413453	-2.437694	C	-1.988377	-5.298758	0.154339
H	1.062423	5.695434	-1.456903	H	-1.932763	-6.293622	-0.304722
H	2.579538	5.236516	-0.680149	H	-1.581700	-5.372875	1.169961
C	-2.009689	3.455009	1.019547	H	-3.046811	-5.025507	0.240441
H	-1.559242	3.434277	2.020519	C	0.765647	-4.547207	-0.979540
H	-2.907940	4.085688	1.079450	H	1.252358	-4.474200	0.001003
H	-2.336287	2.429900	0.797318	H	0.845895	-5.588653	-1.316769
				H	1.328323	-3.923225	-1.681876
TS2B-NHC-1				Ni	0.468664	0.275623	-0.121871
C	-4.919718	-0.843144	-0.628179	C	-0.132846	-0.983189	-1.450080
C	-3.663359	-1.396459	-0.369392	H	0.594538	-1.788743	-1.577152
C	-2.489832	-0.668825	-0.603853	H	-0.581294	-0.696962	-2.404627
C	-2.629487	0.636442	-1.110328	Si	-0.660308	-0.762719	1.777121
C	-3.883086	1.184579	-1.364068	C	-0.617673	1.014521	2.545291
C	-5.057654	0.454427	-1.130638	C	-1.879715	1.852289	2.278357
H	-5.810470	-1.436811	-0.431262	H	0.277712	1.564639	2.234867
H	-3.590109	-2.398589	0.036701	H	-0.503126	0.861108	3.629628
H	-1.737833	1.227334	-1.299765	H	-1.821112	2.840304	2.755370
H	-3.950554	2.199140	-1.753281	H	-2.042565	2.005860	1.205910
C	-6.414740	1.042000	-1.439841	H	-2.779399	1.356550	2.660916
H	-7.209944	0.528451	-0.888484	C	-2.186552	-1.543848	2.621338
H	-6.460033	2.106903	-1.182792	C	-2.158071	-1.430943	4.156769
H	-6.652140	0.958445	-2.509335	H	-2.226197	-2.595943	2.324125
C	-1.115978	-1.247601	-0.338340	H	-3.102902	-1.082658	2.235392
O	-1.193032	-2.623735	0.087174	H	-2.992799	-1.980288	4.611348
Si	-1.043274	-4.013336	-0.850604	H	-1.232454	-1.841946	4.581157
C	-1.815004	-3.794664	-2.555208	H	-2.236135	-0.390081	4.492327

C	0.891104	-1.762879	2.295547	H	6.285029	-1.919528	-1.598754
C	1.996507	-0.942678	2.980307	C	0.616179	3.603350	-0.145383
H	1.279594	-2.234560	1.384046	C	0.717043	4.942198	0.591434
H	0.572295	-2.587585	2.948630	C	0.029346	3.768448	-1.555111
H	2.892180	-1.547217	3.178039	H	-0.057840	2.951431	0.417916
H	2.297819	-0.092014	2.357638	C	-0.672946	5.595208	0.674986
H	1.658058	-0.534051	3.940055	H	1.398473	5.616498	0.052865
C	1.927259	1.509017	-0.098592	H	1.136871	4.785285	1.592478
C	3.154214	3.398550	-0.392473	C	-1.357116	4.426240	-1.473318
C	4.013063	2.343440	-0.428004	H	0.707804	4.386386	-2.161035
H	3.342602	4.456461	-0.479997	H	-0.024613	2.779527	-2.025745
H	5.083559	2.318071	-0.553950	C	-1.297280	5.764749	-0.719520
N	3.251427	1.202340	-0.230783	H	-0.599154	6.564349	1.182746
N	1.889400	2.872501	-0.175801	H	-1.327127	4.962795	1.291751
C	3.713183	-0.191229	-0.297042	H	-1.764380	4.569439	-2.481382
C	3.753942	-0.685361	-1.749965	H	-2.043357	3.744714	-0.949783
C	5.045147	-0.410478	0.426795	H	-2.301573	6.197219	-0.633019
H	2.936389	-0.759231	0.224908	H	-0.694325	6.478937	-1.299844
C	4.143544	-2.170212	-1.792040				
H	4.482533	-0.086264	-2.315814	INT2B-NHC-1			
H	2.764911	-0.523607	-2.193062	C	2.936632	4.433909	0.087694
C	5.420322	-1.901528	0.384237	C	2.907096	3.069141	-0.216869
H	5.839390	0.172511	-0.061461	C	1.698806	2.370575	-0.296103
H	4.967665	-0.055847	1.461633	C	0.513954	3.097306	-0.066644
C	5.470131	-2.425809	-1.060008	C	0.545296	4.451563	0.242996
H	4.205462	-2.512817	-2.832003	C	1.761512	5.149409	0.328754
H	3.348281	-2.759310	-1.313944	H	3.895554	4.944585	0.148076
H	6.383543	-2.057586	0.884763	H	3.847625	2.554984	-0.385557
H	4.672007	-2.472568	0.952897	H	-0.434514	2.570223	-0.130284
H	5.707247	-3.496841	-1.064205	H	-0.388004	4.982451	0.424329

C	1.784558	6.624670	0.653769	H	5.748748	-1.198219	-2.271251
H	1.142870	6.855816	1.512788	C	4.337717	-0.003451	0.764840
H	2.797212	6.969176	0.888749	C	5.196381	-1.239623	1.092630
H	1.419311	7.224896	-0.190384	H	3.738159	0.254107	1.644393
C	1.595144	0.899251	-0.637334	H	4.995478	0.861235	0.602426
O	0.740327	0.234502	0.467289	H	5.822809	-1.071576	1.978211
Si	0.706246	0.311881	2.151610	H	4.571919	-2.117769	1.296336
C	-1.108128	0.457390	2.645883	H	5.865190	-1.501308	0.264830
H	-1.543557	1.347454	2.177332	C	2.540592	-1.980496	-0.860034
H	-1.693658	-0.408180	2.321999	C	3.467498	-2.973391	-1.583270
H	-1.212251	0.558481	3.733749	H	1.566805	-1.935010	-1.365176
C	1.628623	1.779549	2.897642	H	2.327156	-2.336522	0.157070
H	1.657689	1.665519	3.989577	H	3.025785	-3.977010	-1.641454
H	2.657375	1.875103	2.540129	H	3.672912	-2.650642	-2.610673
H	1.120467	2.720485	2.663999	H	4.433018	-3.076141	-1.074909
C	1.406673	-1.307332	2.832022	C	-2.339592	-1.024894	-0.224107
H	2.475394	-1.417379	2.618630	C	-3.653125	-2.579323	0.797953
H	1.272785	-1.370113	3.919540	C	-4.423519	-1.483421	0.568761
H	0.892120	-2.163191	2.382425	H	-3.898712	-3.521450	1.260801
Ni	-0.805168	-0.151308	-1.031659	H	-5.460025	-1.293138	0.798315
C	0.766171	0.687763	-1.910943	N	-3.607876	-0.548786	-0.052513
H	0.592161	1.634979	-2.433558	N	-2.385868	-2.279695	0.318632
H	1.247618	0.007006	-2.627665	C	-4.018869	0.796374	-0.470591
Si	3.176071	-0.186476	-0.745705	C	-5.063867	0.742265	-1.594114
C	4.132007	0.285521	-2.328543	C	-4.506392	1.639126	0.716687
C	5.619025	-0.113064	-2.355685	H	-3.100649	1.247466	-0.865635
H	4.036784	1.370280	-2.471887	C	-5.434220	2.160708	-2.054857
H	3.611799	-0.164442	-3.184121	H	-5.964047	0.225955	-1.229344
H	6.104245	0.201818	-3.288418	H	-4.666764	0.150382	-2.427486
H	6.175273	0.344975	-1.528953	C	-4.868494	3.057553	0.249698

H	-5.391748	1.165239	1.165282	C	-1.312599	-1.580944	-0.751299
H	-3.729663	1.663215	1.489013	C	-1.873081	-1.411397	-2.042978
C	-5.911937	3.025983	-0.878139	C	-3.232106	-1.586961	-2.274061
H	-6.204564	2.111151	-2.833764	C	-4.119333	-1.947304	-1.245296
H	-4.551395	2.628430	-2.514268	H	-4.228398	-2.391600	0.859741
H	-5.236470	3.647465	1.097784	H	-1.846650	-2.065439	1.296172
H	-3.958375	3.558370	-0.111784	H	-1.216884	-1.115110	-2.854653
H	-6.131541	4.044546	-1.220884	H	-3.620025	-1.441195	-3.281355
H	-6.854181	2.614740	-0.486013	C	-5.589167	-2.168443	-1.515346
C	-1.235496	-3.193876	0.257091	H	-6.185853	-2.053569	-0.602935
C	-1.108473	-4.069075	1.509551	H	-5.974407	-1.456678	-2.255763
C	-1.284730	-4.042016	-1.022638	H	-5.785838	-3.176819	-1.906810
H	-0.360990	-2.537123	0.199059	C	0.099432	-1.297436	-0.504965
C	0.147129	-4.951227	1.407312	O	0.931742	-1.338762	-1.659726
H	-1.989888	-4.719346	1.604426	Si	1.586039	-2.704464	-2.379285
H	-1.075280	-3.436848	2.404890	C	1.560107	-2.362686	-4.232134
C	-0.047895	-4.946693	-1.120929	H	2.061195	-1.412582	-4.454211
H	-2.201106	-4.650266	-1.012579	H	2.068492	-3.151614	-4.800126
H	-1.345430	-3.367133	-1.884375	H	0.529708	-2.290088	-4.599284
C	0.118519	-5.814295	0.136188	C	0.584463	-4.240417	-1.937338
H	0.231075	-5.581765	2.300565	H	0.979063	-5.132639	-2.439603
H	1.039078	-4.309235	1.388959	H	0.606790	-4.425435	-0.856789
H	-0.114544	-5.575859	-2.016671	H	-0.464522	-4.114958	-2.226669
H	0.840841	-4.314457	-1.243479	C	3.379566	-2.903925	-1.809987
H	1.035319	-6.412441	0.065741	H	3.901232	-3.677583	-2.387893
H	-0.718938	-6.524946	0.201771	H	3.927567	-1.962157	-1.938058
				H	3.443151	-3.183576	-0.751217
TS2B-NHC-2				Ni	0.186758	0.296379	0.519986
C	-3.573650	-2.114452	0.034727	C	0.754986	-1.854033	0.774195
C	-2.213835	-1.939463	0.282312	H	0.217889	-2.748061	1.129394

H	1.768930	-2.166492	0.509433	C	2.167227	2.591025	-0.721629
Si	1.183358	-1.045344	2.534458	C	2.414645	1.703510	-1.953108
C	1.760416	-2.613489	3.459270	C	3.086559	3.815805	-0.713506
H	2.047445	-2.302196	4.472783	H	2.376575	1.991130	0.170308
H	0.897250	-3.282397	3.588539	C	3.881713	1.255092	-1.995331
C	2.661618	0.167487	2.491821	H	2.169297	2.278612	-2.858476
H	3.304333	-0.100721	1.641308	H	1.748828	0.835704	-1.911911
H	2.268178	1.166075	2.260295	C	4.556499	3.360759	-0.748135
C	-0.282649	-0.308752	3.517930	H	2.886658	4.438813	-1.596965
H	-0.322223	0.765251	3.291656	H	2.888412	4.432381	0.172150
H	-1.217322	-0.722802	3.116947	C	4.839549	2.455898	-1.959387
C	2.922125	-3.386234	2.810077	H	4.060447	0.645346	-2.889620
H	3.258444	-4.217787	3.441909	H	4.077732	0.603976	-1.130185
H	2.631944	-3.813131	1.843034	H	5.216561	4.236626	-0.760015
H	3.790782	-2.739490	2.633265	H	4.780915	2.809186	0.176542
C	3.501799	0.232418	3.782894	H	5.882873	2.116809	-1.939417
H	3.965527	-0.733147	4.014068	H	4.715522	3.042356	-2.881899
H	4.308297	0.971819	3.698566	C	-2.635518	1.924417	0.006253
H	2.890241	0.516078	4.647928	C	-2.916621	2.044029	1.510874
C	-0.234050	-0.515677	5.044685	C	-3.830013	2.407708	-0.821490
H	-1.086914	-0.033599	5.538763	H	-2.461663	0.869049	-0.227733
H	-0.259797	-1.579147	5.307440	C	-4.165588	1.232400	1.883593
H	0.678264	-0.093637	5.483087	H	-3.056188	3.104677	1.767580
C	-0.159009	2.054135	-0.078056	H	-2.040974	1.682983	2.060176
C	-1.237506	3.803360	-1.041378	C	-5.079522	1.589063	-0.455269
C	0.097026	4.004105	-1.214071	H	-4.023766	3.470997	-0.615751
H	-2.076907	4.405302	-1.347647	H	-3.607657	2.311965	-1.891249
H	0.624322	4.809734	-1.698482	C	-5.381909	1.665086	1.049899
N	0.741745	2.935596	-0.610542	H	-4.375371	1.337699	2.955221
N	-1.378129	2.608134	-0.354226	H	-3.959758	0.169924	1.696341

H	-5.938184	1.946258	-1.037102	H	1.512172	-4.298489	-0.939229
H	-4.908497	0.543624	-0.739192	C	4.185669	-1.818458	-2.722011
H	-6.249743	1.038013	1.290152	H	4.578881	-2.446696	-3.531313
H	-5.654782	2.697860	1.314773	H	4.164377	-0.783425	-3.084946
				H	4.889098	-1.863012	-1.884781
INT2B-NHC-2				Ni	-0.382028	0.210907	-0.124172
C	-2.507734	-3.205817	-0.215006	C	1.452935	-1.795660	1.120286
C	-1.235087	-2.805041	0.181086	H	0.672845	-1.774715	1.895299
C	-0.431891	-1.959057	-0.634804	H	1.825283	-2.835960	1.094456
C	-1.020254	-1.550134	-1.872873	Si	2.813739	-0.645712	1.777284
C	-2.299308	-1.959317	-2.247360	C	3.137562	-1.115228	3.595733
C	-3.075041	-2.794908	-1.432345	H	3.888258	-0.431133	4.016274
H	-3.075027	-3.871644	0.433942	H	2.217995	-0.940581	4.173832
H	-0.837069	-3.162552	1.125117	C	4.433001	-0.841432	0.800956
H	-0.431836	-0.946004	-2.555752	H	4.555713	-1.911644	0.580113
H	-2.697575	-1.627447	-3.205001	H	4.281483	-0.360267	-0.172077
C	-4.449519	-3.248391	-1.866252	C	2.177629	1.148844	1.701078
H	-5.120631	-2.398408	-2.049162	H	2.088760	1.414315	0.637446
H	-4.408450	-3.827372	-2.798473	H	1.144663	1.143930	2.084342
H	-4.921024	-3.881811	-1.106725	C	3.602173	-2.571061	3.786569
C	0.835673	-1.342958	-0.192402	H	3.789135	-2.809111	4.841698
O	1.833608	-1.177513	-1.235151	H	2.852543	-3.281702	3.417802
Si	2.453499	-2.380850	-2.225454	H	4.531655	-2.768568	3.237725
C	1.459295	-2.587664	-3.823381	C	5.711935	-0.310259	1.471762
H	1.306367	-1.622385	-4.322270	H	5.900435	-0.803301	2.433292
H	2.006859	-3.236573	-4.519933	H	6.596144	-0.475465	0.842348
H	0.474786	-3.032510	-3.647427	H	5.652887	0.766475	1.668862
C	2.502814	-4.047255	-1.335997	C	3.011118	2.202738	2.450486
H	2.801065	-4.847183	-2.025691	H	2.553608	3.199255	2.406728
H	3.210442	-4.042007	-0.499287	H	3.126275	1.944941	3.510025

H	4.017691	2.293855	2.026408	H	-3.597857	1.026989	2.815690
C	-1.620237	1.683230	-0.121536	H	-2.103858	0.202750	2.335551
C	-3.505994	2.904064	0.209195	C	-5.613074	-1.001847	1.009182
C	-2.539539	3.757579	-0.223776	H	-5.553338	1.155912	1.058981
H	-4.536535	3.089969	0.464136	H	-5.270785	0.484361	-0.554525
H	-2.573095	4.818830	-0.411795	C	-5.285454	-1.229265	2.493264
N	-1.399540	2.993424	-0.427294	H	-3.551760	-1.256429	3.812721
N	-2.931766	1.642732	0.254182	H	-3.267877	-1.964865	2.221853
C	-0.081314	3.493742	-0.834075	H	-6.696633	-1.037599	0.843498
C	-0.146070	4.343252	-2.109903	H	-5.170043	-1.810348	0.414826
C	0.602639	4.246861	0.315397	H	-5.668960	-2.204307	2.818659
H	0.499227	2.588393	-1.049233	H	-5.800394	-0.468667	3.099216
C	1.267704	4.785948	-2.522624				
H	-0.766493	5.233237	-1.930308	TS3B-NHC-2			
H	-0.627637	3.768847	-2.910263	C	-4.538842	-2.357284	-0.347022
C	2.012648	4.692496	-0.098824	C	-3.481843	-1.879192	0.418439
H	-0.004137	5.124345	0.582813	C	-2.741585	-0.745265	0.018917
H	0.639273	3.593986	1.193887	C	-3.134512	-0.114402	-1.178384
C	1.976940	5.535191	-1.383358	C	-4.204279	-0.583377	-1.937226
H	1.213983	5.412849	-3.420716	C	-4.924003	-1.716670	-1.536725
H	1.855281	3.896655	-2.793008	H	-5.075747	-3.247829	-0.026030
H	2.483021	5.253003	0.717693	H	-3.205749	-2.406718	1.326154
H	2.633112	3.799885	-0.262732	H	-2.557136	0.745174	-1.510095
H	2.994779	5.808469	-1.687115	H	-4.477229	-0.075318	-2.859774
H	1.443353	6.476292	-1.183236	C	-6.091093	-2.231235	-2.344316
C	-3.543164	0.396999	0.749371	H	-6.075490	-1.842280	-3.367774
C	-3.195717	0.185559	2.232178	H	-6.089020	-3.326065	-2.396601
C	-5.055377	0.342277	0.511688	H	-7.046547	-1.932013	-1.892421
H	-3.071991	-0.402180	0.167558	C	-1.562980	-0.223574	0.728199
C	-3.772080	-1.141647	2.744360	O	0.331997	-1.557045	-0.316772

Si	0.415696	-2.180288	-1.865242	H	0.644550	-0.278438	4.168689
C	0.504773	-0.719276	-3.067587	C	-0.218963	-5.051200	2.073337
H	1.353283	-0.063350	-2.839725	H	-0.817172	-4.769942	2.946568
H	0.614900	-1.066554	-4.103544	H	-0.654446	-5.970356	1.659159
H	-0.405652	-0.111165	-3.005866	H	0.784748	-5.301530	2.436984
C	-1.109827	-3.196078	-2.315935	C	3.378253	-2.899033	1.996239
H	-1.093664	-3.449407	-3.384274	H	4.427420	-2.684998	1.748584
H	-1.175377	-4.130343	-1.749814	H	3.290521	-2.858935	3.086298
H	-2.020919	-2.620774	-2.118527	H	3.180470	-3.935079	1.692120
C	1.985656	-3.215008	-2.107443	C	0.763703	2.224252	-0.271714
H	1.983958	-3.690022	-3.096946	C	1.094990	4.452175	0.020668
H	2.883046	-2.586260	-2.044243	C	2.306810	3.892733	-0.240014
H	2.087795	-4.006748	-1.356873	H	0.825893	5.478333	0.212344
Ni	-0.033193	0.457238	-0.204292	H	3.284607	4.340388	-0.321364
C	-1.168935	-0.754371	1.963050	N	2.086174	2.533741	-0.412581
H	-0.553024	-0.102119	2.580151	N	0.165452	3.423480	-0.016099
H	-1.832485	-1.385700	2.565645	C	3.111749	1.525640	-0.707924
Si	0.526091	-2.215711	1.500851	C	3.707777	1.715759	-2.109762
C	0.569143	-2.364535	3.475585	C	4.201783	1.482083	0.372153
H	-0.435561	-2.572852	3.864641	H	2.576757	0.569414	-0.683795
H	1.150277	-3.279069	3.662748	C	4.715977	0.596920	-2.414949
C	-0.178703	-3.931836	1.021855	H	4.210217	2.692686	-2.161755
H	-1.193343	-3.740995	0.645517	H	2.899136	1.730289	-2.849960
H	0.382386	-4.284705	0.147403	C	5.216842	0.369968	0.062116
C	2.427901	-1.917010	1.288252	H	4.718691	2.451850	0.412851
H	2.660409	-1.906202	0.221347	H	3.733999	1.322143	1.350630
H	2.631127	-0.893234	1.639118	C	5.815612	0.530427	-1.343886
C	1.197806	-1.219251	4.281455	H	5.153719	0.748612	-3.408848
H	1.219487	-1.442865	5.357233	H	4.181924	-0.364237	-2.449628
H	2.231469	-1.021315	3.974214	H	6.009399	0.369536	0.819891

H	4.709969	-0.601369	0.135341	H	3.095394	-0.033508	2.350968
H	6.503531	-0.296436	-1.558453	H	4.264126	1.265842	2.084406
H	6.411016	1.454973	-1.382010	C	2.609195	3.388371	0.191327
C	-1.268220	3.510156	0.302405	H	3.341982	3.958900	0.779362
C	-1.516499	3.269924	1.798434	H	1.989855	4.125310	-0.333628
C	-1.907090	4.816011	-0.179395	C	3.330442	2.499811	-0.838558
H	-1.717422	2.672044	-0.239638	H	2.605614	1.910784	-1.414660
C	-3.024540	3.252016	2.085910	H	3.923836	3.092741	-1.545954
H	-1.023854	4.063389	2.379837	H	4.013870	1.794957	-0.348903
H	-1.060455	2.312938	2.071078	C	-0.159043	3.294908	1.719354
C	-3.418991	4.787553	0.102781	H	0.013277	4.105968	2.441740
H	-1.463302	5.670901	0.351341	H	-0.481197	3.758496	0.779593
H	-1.710407	4.958992	-1.249295	C	-1.261439	2.346432	2.221375
C	-3.706233	4.538115	1.592428	H	-0.963279	1.810914	3.132269
H	-3.199596	3.111349	3.159179	H	-2.190242	2.885112	2.446025
H	-3.466225	2.382794	1.577718	H	-1.492451	1.603670	1.450818
H	-3.876315	5.729007	-0.224921	C	0.604670	-1.402714	-0.020176
H	-3.879378	3.987231	-0.494423	C	0.311259	-3.491704	0.822995
H	-4.788534	4.486921	1.763783	C	1.639414	-3.336730	0.577122
H	-3.333454	5.392588	2.176995	H	-0.230875	-4.331759	1.225586
				H	2.459722	-4.020036	0.722613
				N	1.800487	-2.054759	0.070467
				N	-0.305203	-2.309644	0.441051
Ni	0.215769	0.404620	-0.656757	C	3.044396	-1.440599	-0.419934
Si	1.475659	2.417408	1.365295	C	4.292882	-2.016606	0.255372
H	1.201089	1.081119	0.708945	C	3.134629	-1.538885	-1.951614
C	2.368644	1.930715	2.971999	H	2.959217	-0.382616	-0.152007
H	1.622250	1.530722	3.672785	C	5.547754	-1.286671	-0.249828
H	2.770689	2.838144	3.445832	H	4.387129	-3.085021	0.013859
C	3.492776	0.897652	2.772480	H	4.203833	-1.934316	1.345206
H	3.991815	0.646661	3.716929				

C	4.403188	-0.845676	-2.471409	H	-1.036878	3.763840	-2.527838
H	3.137455	-2.600878	-2.237397	C	-2.142405	1.516225	-1.541747
H	2.235455	-1.082402	-2.382162	C	-2.597044	0.364674	-2.218388
C	5.666258	-1.381373	-1.779098	C	-3.099946	2.237204	-0.801764
H	6.439045	-1.705868	0.232205	C	-3.930076	-0.038019	-2.159109
H	5.495069	-0.230110	0.049833	H	-1.880027	-0.210124	-2.801901
H	4.477242	-0.974674	-3.557790	C	-4.428294	1.816350	-0.723801
H	4.319968	0.233931	-2.288974	H	-2.782615	3.132034	-0.273478
H	6.550747	-0.832488	-2.124868	C	-4.870708	0.668558	-1.394520
H	5.817029	-2.433944	-2.061473	H	-4.247730	-0.921403	-2.711126
C	-1.728464	-1.970726	0.607735	H	-5.137655	2.393274	-0.132379
C	-2.658102	-3.154043	0.314920	C	-6.296572	0.184363	-1.268089
C	-1.998132	-1.381691	1.999262	H	-6.399723	-0.555424	-0.461011
H	-1.923313	-1.189991	-0.135105	H	-6.982741	1.007959	-1.041074
C	-4.125435	-2.704114	0.423162	H	-6.641833	-0.297266	-2.190364
H	-2.476013	-3.961883	1.038609				
H	-2.447139	-3.556262	-0.683612	TS4B-NHC-2			
C	-3.457173	-0.912265	2.095359	Ni	-0.542488	-0.153286	0.773730
H	-1.792788	-2.147625	2.762059	Si	-2.080879	-1.575309	1.846032
H	-1.306471	-0.551735	2.173360	H	-0.072463	-1.462150	1.337756
C	-4.426720	-2.065495	1.788567	C	-2.943273	-2.619906	0.480695
H	-4.788292	-3.559967	0.245961	H	-3.637963	-1.971950	-0.073343
H	-4.326450	-1.971361	-0.367042	H	-3.569651	-3.391032	0.953019
H	-3.653273	-0.500321	3.092758	C	-1.954651	-3.274307	-0.498112
H	-3.618313	-0.097429	1.375975	H	-2.458173	-3.872595	-1.269471
H	-5.462933	-1.705130	1.810871	H	-1.348740	-2.511615	-1.004219
H	-4.340846	-2.830290	2.575247	H	-1.254589	-3.937441	0.025344
C	-0.701935	1.882494	-1.543820	C	-1.470063	-2.813208	3.180664
C	-0.329423	3.065741	-2.067467	H	-0.866424	-2.255277	3.911828
H	0.712032	3.384075	-2.076884	H	-0.767908	-3.508030	2.696007

C	-2.565325	-3.607678	3.911774	H	-5.264402	-0.365233	-1.418029
H	-3.179091	-4.185899	3.209667	H	-2.898782	-1.485657	-4.187319
H	-2.144210	-4.318033	4.635866	H	-3.317372	-1.775690	-2.502867
H	-3.241822	-2.943015	4.462569	H	-5.365096	-1.175317	-3.770311
C	-3.431096	-0.507331	2.707742	H	-4.612108	0.313889	-4.338877
H	-4.216406	-1.180645	3.082965	C	1.146459	2.714181	0.731614
H	-2.973448	-0.051313	3.597363	C	2.389964	2.325493	-0.083909
C	-4.064921	0.588602	1.838057	C	1.312557	4.081314	1.406475
H	-4.585222	0.159381	0.971681	H	0.994340	1.957218	1.508588
H	-4.802531	1.183466	2.393345	C	3.638255	2.331325	0.809760
H	-3.300069	1.274328	1.453523	H	2.515133	3.044064	-0.907271
C	-0.853249	1.526594	-0.148258	H	2.231381	1.335848	-0.523354
C	-0.459870	3.573564	-1.043432	C	2.564489	4.078794	2.300340
C	-1.534254	3.046115	-1.689364	H	1.423996	4.863563	0.642040
H	0.035592	4.522709	-1.169241	H	0.414437	4.321724	1.988248
H	-2.145102	3.453271	-2.478863	C	3.822075	3.687650	1.506951
N	-1.764278	1.801478	-1.125127	H	4.521995	2.069262	0.217108
N	-0.065087	2.639385	-0.099830	H	3.531958	1.543913	1.569833
C	-2.753601	0.815062	-1.582010	H	2.691250	5.064967	2.762932
C	-4.135496	1.437148	-1.810949	H	2.416615	3.362380	3.121483
C	-2.244115	0.069291	-2.825227	H	4.693859	3.661413	2.172247
H	-2.824747	0.099113	-0.758208	H	4.025362	4.459882	0.750106
C	-5.137016	0.353094	-2.240689	C	5.602967	-1.505927	-0.091176
H	-4.077453	2.199771	-2.600747	C	4.265572	-1.331140	0.244758
H	-4.468471	1.938574	-0.895264	C	3.232779	-1.742977	-0.622125
C	-3.255827	-0.996051	-3.273368	C	3.619356	-2.341308	-1.835138
H	-2.076149	0.794081	-3.635321	C	4.961684	-2.515168	-2.168709
H	-1.274693	-0.385163	-2.588082	C	5.981954	-2.102455	-1.304443
C	-4.650317	-0.390506	-3.494403	H	6.373991	-1.174550	0.602247
H	-6.119905	0.805882	-2.417666	H	4.015391	-0.869821	1.195591

H	2.848768	-2.670179	-2.529650	C	-5.687344	-1.509534	-1.249229
H	5.220886	-2.979662	-3.118188	H	-5.518487	0.517944	-0.529127
C	7.438471	-2.314974	-1.643668	H	-4.749823	0.269996	-2.103963
H	7.840591	-3.204762	-1.139851	C	-5.893450	-2.174806	0.121133
H	7.584237	-2.456345	-2.720161	H	-4.717474	-2.813840	1.839714
H	8.053186	-1.463183	-1.329142	H	-3.947554	-3.109957	0.283410
C	1.255759	-0.870516	0.699218	H	-6.652227	-1.327298	-1.737499
H	1.921100	-0.496406	1.487814	H	-5.125618	-2.191094	-1.903854
C	1.804904	-1.547025	-0.333461	H	-6.417312	-3.131068	0.001183
H	1.131408	-1.963936	-1.085539	H	-6.541217	-1.534351	0.738089
				C	0.403289	2.372301	0.236801
TS5A-NHC-1				C	1.131092	2.539425	-1.106116
C	0.594820	-1.199469	1.675329	C	0.571031	3.610022	1.125443
Ni	-0.304927	-0.851127	-0.078278	H	0.838016	1.510589	0.754123
C	1.060406	-2.185439	0.729232	C	2.621939	2.831944	-0.874045
H	0.708902	-3.205441	0.886749	H	0.666113	3.363131	-1.667139
C	-1.397244	0.708982	-0.131372	H	0.994371	1.624399	-1.694334
C	-2.090621	2.869210	-0.038178	C	2.064705	3.885633	1.364514
C	-3.190735	2.098021	-0.248913	H	0.125925	4.487505	0.634526
H	-1.998500	3.938342	0.061038	H	0.041511	3.462578	2.074427
H	-4.224999	2.377243	-0.364905	C	2.818880	4.054723	0.035941
N	-2.749381	0.785118	-0.313274	H	3.127173	2.982091	-1.835811
N	-1.007662	2.006888	0.040179	H	3.090362	1.955243	-0.405115
C	-3.572881	-0.429854	-0.420356	H	2.181815	4.778995	1.989671
C	-3.770583	-1.069562	0.963721	H	2.500255	3.046941	1.926173
C	-4.914218	-0.185696	-1.119783	H	3.886634	4.219381	0.225594
H	-2.976599	-1.120192	-1.030563	H	2.445962	4.953532	-0.477343
C	-4.554030	-2.383897	0.844279	H	-0.106219	-1.514907	2.448034
H	-4.312523	-0.360712	1.606845	C	2.487115	-2.118981	0.275360
H	-2.784742	-1.237532	1.412051	C	2.979050	-1.016879	-0.438136

C	3.385954	-3.139391	0.606746	C	-2.194223	4.611453	1.341741
C	4.324231	-0.928048	-0.788002	H	-3.837642	3.197163	1.287949
H	2.282776	-0.235392	-0.730214	H	-2.407700	2.583992	2.126311
C	4.733174	-3.051173	0.251967	C	-2.585994	5.425741	0.098962
H	3.031092	-4.006976	1.159016	H	-2.442364	5.296393	-2.071673
C	5.227946	-1.945018	-0.449563	H	-1.028402	4.692037	-1.212682
H	4.677042	-0.059841	-1.341949	H	-2.559196	5.099458	2.253283
H	5.411751	-3.856919	0.525114	H	-1.098244	4.574739	1.421248
C	6.679141	-1.866127	-0.864485	H	-2.158285	6.434053	0.155391
H	7.320290	-2.455042	-0.199215	H	-3.679335	5.547068	0.075215
H	6.825018	-2.252038	-1.882770	C	-2.349221	-2.449992	-0.022033
H	7.043686	-0.832437	-0.856087	C	-2.848131	-3.126134	1.263759
H	1.293014	-0.424512	1.989500	C	-2.764166	-3.234114	-1.275551
H	0.348840	-2.129167	-0.705643	H	-1.255019	-2.400110	0.014140
				C	-2.351774	-4.578354	1.338759
INT5A-NHC-1				H	-3.947722	-3.111555	1.277500
C	-1.929620	0.014264	-0.013643	H	-2.506063	-2.548086	2.130351
C	-4.102295	-0.631511	-0.208068	C	-2.265229	-4.685576	-1.192424
C	-4.081085	0.726538	-0.211206	H	-3.860311	-3.231336	-1.363172
H	-4.928246	-1.321097	-0.281044	H	-2.368368	-2.731866	-2.166178
H	-4.885195	1.441237	-0.286525	C	-2.758805	-5.374675	0.089257
N	-2.751382	1.102432	-0.095911	H	-2.740610	-5.057744	2.245012
N	-2.784885	-1.048097	-0.090525	H	-1.255925	-4.578127	1.428187
C	-2.272536	2.490285	-0.027739	H	-2.591286	-5.241682	-2.079428
C	-2.674766	3.292096	-1.274186	H	-1.165804	-4.688358	-1.205305
C	-2.738304	3.176542	1.265097	H	-2.365177	-6.396770	0.145715
H	-1.180055	2.406911	-0.003159	H	-3.855283	-5.459681	0.055011
C	-2.127119	4.725967	-1.189855	Ni	0.008399	-0.011821	0.229107
H	-3.771195	3.326457	-1.350483	C	6.359087	1.150651	-0.059537
H	-2.304758	2.781129	-2.170912	C	4.998287	1.148153	-0.365469

C	4.285247	-0.050258	-0.509413	C	-5.386063	-1.275621	-1.580208
C	4.994154	-1.247211	-0.338114	H	-5.380688	-0.589151	-2.435306
C	6.355204	-1.247142	-0.031935	H	-5.894560	-2.193625	-1.906520
C	7.063234	-0.047680	0.116689	H	-6.003735	-0.824696	-0.795015
H	6.886155	2.098311	0.038983	C	0.028319	-2.457355	0.263400
H	4.476070	2.093924	-0.499838	Ni	0.704156	-0.832897	1.305404
H	4.469050	-2.194189	-0.450929	C	0.385798	-2.824275	1.601990
H	6.878988	-2.194053	0.088519	H	-0.393991	-3.138593	2.293220
C	8.530398	-0.045052	0.481421	H	1.301923	-3.398336	1.730063
H	9.037040	-0.946907	0.119042	C	0.947065	0.756691	0.248255
H	9.048583	0.824058	0.059800	C	0.626503	2.613159	-1.013318
H	8.672688	-0.009133	1.570519	C	1.960154	2.346792	-1.016665
C	2.795415	-0.050060	-0.780013	H	0.076803	3.406005	-1.491776
H	2.536137	-0.937352	-1.373727	H	2.773071	2.866197	-1.496557
C	1.941769	-0.024414	0.515885	N	2.139678	1.218657	-0.233680
H	2.237524	-0.889791	1.135030	N	0.023209	1.632377	-0.243334
H	2.249334	0.856221	1.107413	C	3.395812	0.478349	-0.033942
H	2.542154	0.818240	-1.403818	C	3.514629	-0.664482	-1.054692
				C	4.631924	1.383567	-0.057298
TS5A-NHC-2				H	3.303264	0.033641	0.964264
C	-3.713664	-1.762294	0.271252	C	4.784028	-1.489393	-0.798380
C	-2.429265	-2.055906	0.726218	H	3.538312	-0.235922	-2.067300
C	-1.339816	-2.172762	-0.166756	H	2.616875	-1.287776	-0.980252
C	-1.622490	-1.956755	-1.534573	C	5.896968	0.551905	0.216376
C	-2.905069	-1.655505	-1.979151	H	4.730145	1.856216	-1.045025
C	-3.985853	-1.559424	-1.088113	H	4.523228	2.187945	0.680324
H	-4.525190	-1.685159	0.992990	C	6.037462	-0.600892	-0.790768
H	-2.264731	-2.181483	1.792237	H	4.876606	-2.278811	-1.553900
H	-0.807348	-2.020259	-2.252775	H	4.690460	-1.994213	0.174333
H	-3.076283	-1.494893	-3.042387	H	6.780287	1.200961	0.183580

H	5.844395	0.141722	1.235091	N	2.075055	-1.238147	0.372909
H	6.927875	-1.198258	-0.559388	C	-1.425838	-1.599071	-0.229102
H	6.190034	-0.182700	-1.796846	C	-1.607496	-1.606243	-1.756087
C	-1.417701	1.509884	0.063374	C	-2.310768	-2.648036	0.452068
C	-1.698528	1.906414	1.521570	H	-1.704465	-0.609891	0.149364
C	-2.287665	2.314191	-0.908282	C	-3.081149	-1.410075	-2.137810
H	-1.651114	0.449251	-0.059259	H	-1.235261	-2.562568	-2.152637
C	-3.185907	1.717859	1.853030	H	-0.985393	-0.808179	-2.179044
H	-1.403383	2.955919	1.668210	C	-3.783657	-2.414549	0.079227
H	-1.072732	1.292536	2.179915	H	-2.020217	-3.656667	0.123711
C	-3.775387	2.113283	-0.578330	H	-2.169675	-2.604050	1.538945
H	-2.049148	3.384696	-0.824003	C	-3.983926	-2.441894	-1.444195
H	-2.077846	2.007376	-1.940322	H	-3.194098	-1.470316	-3.227228
C	-4.083042	2.495233	0.877779	H	-3.387267	-0.399804	-1.838738
H	-3.378696	2.030550	2.886545	H	-4.412745	-3.170515	0.564786
H	-3.426118	0.648231	1.790224	H	-4.097051	-1.437667	0.466847
H	-4.388217	2.705130	-1.269389	H	-5.036145	-2.251595	-1.689859
H	-4.031505	1.059919	-0.739527	H	-3.747722	-3.447932	-1.822861
H	-5.140711	2.306363	1.100734	C	3.290859	-0.411205	0.396604
H	-3.918955	3.574883	1.013798	C	4.381956	-0.985502	1.306303
H	0.731516	-2.689084	-0.535437	C	3.814156	-0.167831	-1.028361
H	0.854306	-1.626659	2.636622	H	2.963101	0.552877	0.805687
				C	5.596713	-0.042714	1.333873
INT5A-NHC-2				H	4.705135	-1.964842	0.925441
C	0.851320	-0.690141	0.117197	H	3.983617	-1.143507	2.315907
C	1.992395	-2.617813	0.492785	C	5.038484	0.758867	-1.006749
C	0.682286	-2.943223	0.326954	H	4.076744	-1.135050	-1.480947
H	2.844445	-3.242773	0.704553	H	3.005193	0.266892	-1.628597
H	0.193888	-3.902972	0.367279	C	6.137722	0.214389	-0.081622
N	-0.000124	-1.755506	0.111088	H	6.379733	-0.467054	1.973620

H	5.300448	0.912986	1.789778	H	-1.759202	0.647760	-1.720505
H	5.423063	0.893375	-2.024647	C	-1.455888	3.757846	-1.630730
H	4.726376	1.752806	-0.654678	H	-0.890818	3.534163	-2.544474
H	6.982818	0.912430	-0.041853	H	-1.271502	4.821141	-1.415693
H	6.525669	-0.728412	-0.495237	C	-2.953665	3.536061	-1.903222
Ni	0.425906	1.145417	-0.275051	H	-3.298234	4.135479	-2.755911
C	-0.191350	3.009464	-0.620896	H	-3.145287	2.481082	-2.124857
H	0.377501	3.718277	-0.004829	H	-3.567881	3.815264	-1.038424
C	-1.372564	2.497538	0.092417	C	-2.161868	2.163607	0.944057
C	-2.599839	2.145223	-0.533409	H	-2.877078	1.606917	0.333873
C	-1.275866	2.175150	1.480118	H	-2.655261	3.112776	1.212516
C	-3.633328	1.534948	0.174077	C	-1.831129	1.392389	2.229630
H	-2.741612	2.374852	-1.585102	H	-1.108374	1.930953	2.854259
C	-2.313935	1.552726	2.169873	H	-2.728033	1.225560	2.841221
H	-0.373883	2.461145	2.018929	H	-1.403465	0.412041	1.993780
C	-3.519542	1.218484	1.536614	C	0.156290	3.964498	1.009584
H	-4.562690	1.303836	-0.345015	H	-0.661248	4.586204	1.405287
H	-2.189496	1.336228	3.229926	H	0.543852	3.407788	1.873300
C	-4.647974	0.569146	2.304000	C	1.263893	4.881072	0.465767
H	-4.343759	-0.389472	2.745857	H	0.950414	5.400989	-0.449127
H	-4.993410	1.204265	3.130657	H	1.544348	5.652466	1.194727
H	-5.510997	0.373544	1.657897	H	2.174962	4.317407	0.234126
C	-0.372367	3.515104	-2.045509	C	-0.681784	-1.519775	0.025478
H	-0.750191	2.729612	-2.713572	C	-0.252870	-3.694436	0.545187
H	0.590666	3.840009	-2.456309	C	-1.580647	-3.482310	0.740852
H	-1.069953	4.367575	-2.124807	H	0.342418	-4.583075	0.680997
				H	-2.356154	-4.150256	1.080899
TS6A-NHC-2				N	-1.821191	-2.152550	0.430484
Ni	-0.547218	0.266704	-0.768886	N	0.282976	-2.485093	0.123070
Si	-0.717141	2.737700	-0.194722	C	-3.139273	-1.507501	0.390339

C	-3.963368	-2.010373	-0.801958	H	3.342687	-1.371333	-2.384451
C	-3.899767	-1.645350	1.714449	H	5.282570	-2.819419	-1.807174
H	-2.916001	-0.454284	0.211883	H	4.202600	-4.171634	-1.470844
C	-5.298431	-1.254496	-0.876732	H	1.224800	3.005266	-1.286120
H	-4.146410	-3.090015	-0.694297	C	2.096761	1.517976	-0.064132
H	-3.378764	-1.856527	-1.715551	C	3.445990	1.717950	-0.405209
C	-5.228120	-0.875987	1.632551	C	1.838357	0.913881	1.174848
H	-4.106153	-2.706195	1.919866	C	4.480218	1.312963	0.436694
H	-3.280344	-1.269308	2.536518	H	3.690142	2.207646	-1.345106
C	-6.078401	-1.353341	0.444322	C	2.873145	0.505586	2.018969
H	-5.901488	-1.639126	-1.708189	H	0.811600	0.747057	1.485980
H	-5.090275	-0.198371	-1.099544	C	4.213470	0.689993	1.664497
H	-5.783024	-0.986231	2.572275	H	5.512304	1.485029	0.138101
H	-5.009862	0.195607	1.517305	H	2.629151	0.037649	2.970414
H	-7.005044	-0.769079	0.383880	C	5.333812	0.199357	2.550413
H	-6.375398	-2.399549	0.612928	H	5.635773	-0.819390	2.271088
C	1.652860	-2.274946	-0.362509	H	6.221803	0.835557	2.466942
C	2.711960	-2.892349	0.557860	H	5.032441	0.173315	3.603123
C	1.796513	-2.765275	-1.810828	C	1.096613	1.253914	-2.410528
H	1.791066	-1.190775	-0.351848	H	2.104544	1.391150	-2.824585
C	4.120540	-2.596807	0.015226	H	0.916339	0.168912	-2.377111
H	2.569593	-3.980800	0.617980	H	0.369561	1.674387	-3.108543
H	2.594978	-2.488679	1.570363	C	0.999841	1.960378	-1.025970
C	3.204385	-2.461622	-2.343448				
H	1.606980	-3.848054	-1.845362	TS5B-NHC-1			
H	1.026926	-2.281977	-2.424242	C	-1.001332	-0.218061	-2.135419
C	4.282246	-3.074747	-1.436048	Ni	0.201560	-0.006577	-0.661844
H	4.871595	-3.068981	0.660947	C	-1.232008	-1.470077	-1.285201
H	4.295276	-1.514427	0.061278	H	-1.135534	-2.357979	-1.919128
H	3.306061	-2.833042	-3.370297	Si	0.140460	-2.374189	0.060439

C	-0.700658	-4.103229	0.118476	C	4.351489	0.791703	1.412757
H	-0.155040	-4.666920	0.889165	H	2.851924	-0.192194	0.239818
H	-1.719167	-3.980412	0.508239	C	5.242807	-0.461428	-1.129597
C	1.842658	-2.703908	-0.764018	H	4.780326	1.660133	-1.232906
H	1.637094	-3.165436	-1.740476	H	3.544620	0.630071	-1.968181
H	2.348646	-1.761081	-0.998612	C	5.330699	-0.393322	1.404246
C	0.213971	-1.979971	1.945329	H	4.925198	1.729431	1.405346
H	-0.802128	-1.662636	2.218677	H	3.740166	0.791326	2.322351
H	0.364032	-2.948109	2.445885	C	6.153861	-0.425670	0.107022
C	-0.735361	-4.942075	-1.168235	H	5.840126	-0.439034	-2.049012
H	-1.204114	-5.919788	-0.997245	H	4.686085	-1.409027	-1.139242
H	-1.304893	-4.452624	-1.967344	H	5.990646	-0.338416	2.278321
H	0.273361	-5.128775	-1.556076	H	4.761590	-1.329863	1.496143
C	2.770829	-3.614657	0.058676	H	6.826986	-1.291807	0.107137
H	2.310507	-4.591876	0.246512	H	6.791388	0.470006	0.062990
H	3.725245	-3.794711	-0.453967	C	-0.890750	3.030203	-0.250182
H	3.003132	-3.173951	1.035950	C	-1.623332	3.141761	1.095111
C	1.232801	-0.969673	2.490753	C	-1.186095	4.232193	-1.155170
H	1.144956	-0.861754	3.579879	H	-1.233187	2.125009	-0.761586
H	2.262782	-1.282633	2.279263	C	-3.137870	3.267634	0.868562
H	1.092733	0.018402	2.040581	H	-1.248910	4.020206	1.641514
C	1.119033	1.568812	-0.125967	H	-1.389272	2.259839	1.703558
C	1.484668	3.779708	0.270272	C	-2.701733	4.347605	-1.386929
C	2.676262	3.141553	0.409223	H	-0.823159	5.158625	-0.686130
H	1.233252	4.822799	0.376854	H	-0.651807	4.115643	-2.105462
H	3.653862	3.527214	0.649972	C	-3.466279	4.449698	-0.057335
N	2.434829	1.795253	0.176970	H	-3.652946	3.378934	1.830851
N	0.548711	2.812254	-0.058659	H	-3.507362	2.336027	0.417958
C	3.439117	0.727516	0.181743	H	-2.917269	5.216346	-2.020739
C	4.243061	0.706448	-1.126484	H	-3.046408	3.460554	-1.937216

H	-4.546102	4.495931	-0.244809	H	-1.775981	-1.728561	0.483754
H	-3.191893	5.389753	0.444750	C	-4.022856	-2.782187	-0.677988
H	-0.561152	-0.431613	-3.115155	H	-2.424354	-4.043642	-1.407935
C	-2.557351	-1.480158	-0.565735	H	-2.238485	-2.345231	-1.860421
C	-2.838113	-0.554115	0.452649	C	-3.533734	-3.457735	1.716397
C	-3.573208	-2.380600	-0.916893	H	-1.884796	-4.725312	1.080340
C	-4.078544	-0.528348	1.087884	H	-1.406841	-3.451126	2.210687
H	-2.062161	0.151193	0.741779	C	-4.447200	-3.673281	0.499687
C	-4.813366	-2.356456	-0.277155	H	-4.657360	-2.971477	-1.552549
H	-3.393188	-3.105875	-1.706925	H	-4.158911	-1.726276	-0.408688
C	-5.090373	-1.432309	0.737971	H	-3.819313	-4.127621	2.536245
H	-4.262244	0.204913	1.871017	H	-3.661865	-2.430832	2.087493
H	-5.581003	-3.068196	-0.574776	H	-5.490859	-3.470839	0.769501
C	-6.421759	-1.429203	1.452964	H	-4.398971	-4.728836	0.192345
H	-6.397760	-2.068547	2.346186	C	3.166094	-1.797535	-0.112464
H	-6.696961	-0.421419	1.784413	C	4.282424	-2.675741	0.467360
H	-7.225054	-1.803183	0.808373	C	3.568529	-1.188457	-1.464569
H	-1.893583	0.406309	-2.237076	H	2.965581	-0.981017	0.590434
				C	5.576885	-1.857807	0.609987
				H	4.464767	-3.530376	-0.200043
INT5B-NHC-1				H	3.965354	-3.082182	1.435138
C	0.715493	-2.011173	0.267291	C	4.862819	-0.374287	-1.321787
C	1.683172	-3.699730	-0.906403	H	3.715648	-1.998304	-2.193935
C	0.349202	-3.954799	-0.852065	H	2.750471	-0.560805	-1.834694
H	2.485023	-4.251149	-1.371086	C	5.995215	-1.226292	-0.727574
H	-0.223316	-4.776208	-1.252025	H	6.378418	-2.495320	1.001762
N	-0.226329	-2.911561	-0.142982	H	5.415981	-1.062207	1.351777
N	1.888182	-2.514574	-0.216050	H	5.156466	0.033615	-2.296173
C	-1.656803	-2.773787	0.177643	H	4.669789	0.488604	-0.668564
C	-2.548445	-3.012304	-1.047602	H	6.897569	-0.617878	-0.591604
C	-2.055615	-3.674000	1.355330				

H	6.257092	-2.024891	-1.437711	H	-0.903212	1.075174	2.898399
Ni	0.382558	-0.369609	1.258068	C	-0.891410	4.311616	-2.083393
Si	0.669509	3.232038	0.141566	H	-1.750608	3.685775	-1.821015
C	1.505545	2.026681	-1.076442	H	-1.273154	5.200705	-2.602315
H	1.856647	1.161657	-0.496382	H	-0.286548	3.748325	-2.805172
H	0.753402	1.635330	-1.773825	C	2.674618	2.636629	-1.870142
C	2.020552	3.896946	1.307690	H	3.472192	2.990955	-1.206081
H	2.562558	3.037449	1.726938	H	3.125388	1.909178	-2.558505
H	2.754277	4.454123	0.707365	H	2.346820	3.493846	-2.471351
C	-0.067013	4.692566	-0.838579	C	1.504924	4.787932	2.452436
H	-0.693281	5.279571	-0.151135	H	2.324804	5.163451	3.078362
H	0.755495	5.361390	-1.132342	H	0.960784	5.661071	2.070491
C	-3.028393	0.682925	-1.282955	H	0.821083	4.233659	3.105669
C	-1.884699	1.041297	-0.574054				
C	-1.918206	2.014684	0.444089	TS5B-NHC-2			
C	-3.164713	2.600326	0.707907	C	0.696365	1.329665	-1.855629
C	-4.315713	2.236799	0.002323	Ni	-0.364619	0.422954	-0.504560
C	-4.272635	1.269622	-1.006077	C	-0.096981	2.412071	-1.155100
H	-2.953900	-0.056906	-2.078093	H	-0.863791	2.827651	-1.817131
H	-0.941638	0.564686	-0.825624	Si	-1.166057	2.460480	0.624222
H	-3.235799	3.359025	1.484385	C	-1.250062	4.369803	0.747264
H	-5.262831	2.716095	0.242647	H	-1.794082	4.586345	1.678273
C	-5.509166	0.858361	-1.771185	H	-0.231429	4.752333	0.908818
H	-6.367446	1.489091	-1.516665	C	-2.985728	1.858500	0.573295
H	-5.352478	0.928277	-2.855004	H	-3.331360	1.877685	-0.469670
H	-5.787479	-0.182096	-1.555363	H	-2.982204	0.804330	0.867872
C	-0.686889	2.430447	1.223351	C	-0.310512	1.930578	2.263377
H	-1.006066	3.282696	1.851527	H	0.733843	1.672876	2.044107
C	-0.124001	1.302110	2.147547	H	-0.275447	2.808531	2.925204
H	0.714257	1.719850	2.729895	C	-1.908395	5.124322	-0.419465

H	-2.013485	6.195124	-0.203286	H	-4.637585	-0.819683	-2.562084
H	-1.318392	5.036855	-1.338497	H	-6.101419	-1.313400	0.928294
H	-2.911221	4.735864	-0.637865	H	-5.222906	-0.153570	-0.065612
C	-3.971496	2.631677	1.469742	H	-6.784937	-1.465436	-1.492334
H	-4.066945	3.678188	1.161083	H	-6.077392	-2.975266	-0.921288
H	-4.974470	2.185493	1.438300	C	1.830621	-1.823799	0.638154
H	-3.648047	2.630372	2.517970	C	2.069476	-1.526423	2.125930
C	-0.981255	0.757438	3.000287	C	2.841572	-2.842722	0.095195
H	-0.431551	0.483116	3.909789	H	1.938648	-0.894047	0.072612
H	-2.007158	1.003785	3.299482	C	3.506945	-1.035228	2.353111
H	-1.029449	-0.129953	2.358980	H	1.886009	-2.440955	2.709863
C	-0.543191	-1.411231	-0.032312	H	1.344100	-0.776949	2.460356
C	-0.054593	-3.527088	0.638268	C	4.277444	-2.346724	0.325987
C	-1.377516	-3.497550	0.328446	H	2.711149	-3.808279	0.605430
H	0.561224	-4.337836	0.991965	H	2.654541	-3.008658	-0.972367
H	-2.124194	-4.275306	0.357085	C	4.535161	-2.038886	1.809158
N	-1.658831	-2.204412	-0.080778	H	3.673634	-0.852946	3.422065
N	0.441360	-2.254902	0.405041	H	3.635752	-0.075333	1.836842
C	-2.971192	-1.726432	-0.523746	H	4.988714	-3.098232	-0.038942
C	-3.447964	-2.449737	-1.791619	H	4.435790	-1.439257	-0.267126
C	-4.014949	-1.813534	0.599626	H	5.551383	-1.646174	1.939761
H	-2.807424	-0.673246	-0.773282	H	4.478036	-2.970961	2.392032
C	-4.790267	-1.866288	-2.260893	H	0.392450	1.121371	-2.882693
H	-3.565329	-3.522680	-1.581123	H	0.556500	3.232115	-0.830776
H	-2.683358	-2.354146	-2.571485	C	2.129187	1.208526	-1.619329
C	-5.354909	-1.227349	0.129662	C	2.781994	1.745743	-0.481797
H	-4.153625	-2.865790	0.887152	C	2.955647	0.507950	-2.533653
H	-3.643213	-1.286282	1.485988	C	4.156438	1.606968	-0.290889
C	-5.849323	-1.923192	-1.148572	H	2.203018	2.283630	0.263595
H	-5.139367	-2.401947	-3.151741	C	4.322688	0.369269	-2.331522

H	2.499854	0.081340	-3.425286	H	-5.415624	-1.852026	-2.180704
C	4.961807	0.917198	-1.204713	H	-3.987347	-2.371430	-1.285567
H	4.613783	2.046716	0.594456	H	-6.035013	-3.089078	-0.072001
H	4.916511	-0.170498	-3.067933	H	-6.645096	-1.435141	-0.066264
C	6.441472	0.724830	-0.971890	C	-0.266567	3.579834	-0.216123
H	6.658871	-0.258269	-0.528465	C	-0.380985	5.075835	-0.523748
H	7.008975	0.784345	-1.908560	C	0.656172	3.325560	0.987883
H	6.842523	1.482671	-0.289334	H	0.173541	3.077056	-1.087608
				C	1.014876	5.665081	-0.791515
				H	-0.825959	5.597359	0.335848
INT5B-NHC-2				H	-1.044550	5.235395	-1.382472
C	-1.721162	1.581343	-0.179184	C	2.048658	3.918888	0.732280
C	-2.749732	3.512370	0.430165	H	0.204977	3.777719	1.883038
C	-3.658844	2.507755	0.549899	H	0.722112	2.244942	1.159316
H	-2.847939	4.568367	0.621287	C	1.966884	5.414470	0.389260
H	-4.691090	2.533690	0.859420	H	0.929563	6.739206	-0.994996
N	-3.010439	1.337099	0.184804	H	1.431055	5.204108	-1.698804
N	-1.575117	2.931394	-0.024910	H	2.689398	3.757851	1.607313
C	-3.590514	-0.013258	0.131674	H	2.516415	3.375392	-0.101592
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H	6.351931	-2.557351	-2.692153	H	-3.895006	-0.936311	2.944308
H	6.775902	-1.934541	-1.093012	C	-2.621372	-2.263908	1.789876
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H	-2.412747	-0.762515	-0.699822	H	2.171653	5.974856	-1.634473
C	-4.961714	-1.658200	-1.326415	Si	3.878980	-0.790716	-0.129128
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H	-4.597833	0.410873	-0.725116	H	4.114631	-0.946217	2.341273
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H	-6.054040	-1.568795	-1.285405	C	4.415644	-1.906086	-1.578909
H	-4.639823	-2.048579	-0.352264	H	3.845261	-1.610094	-2.471884
H	-2.723785	-3.396561	-3.364152	H	5.465258	-1.676457	-1.812981
H	-2.595004	-3.148650	-1.626233	C	0.405237	-3.945655	0.939084
H	-4.961099	-3.634110	-2.232684	C	1.041846	-2.708156	1.017772
H	-4.962002	-2.306158	-3.392329	C	1.257453	-1.927485	-0.129026
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C	1.409163	3.286478	-1.299804	C	0.178194	-3.686470	-1.431900
C	-0.360252	5.043416	-0.828583	C	-0.049922	-4.455411	-0.283647
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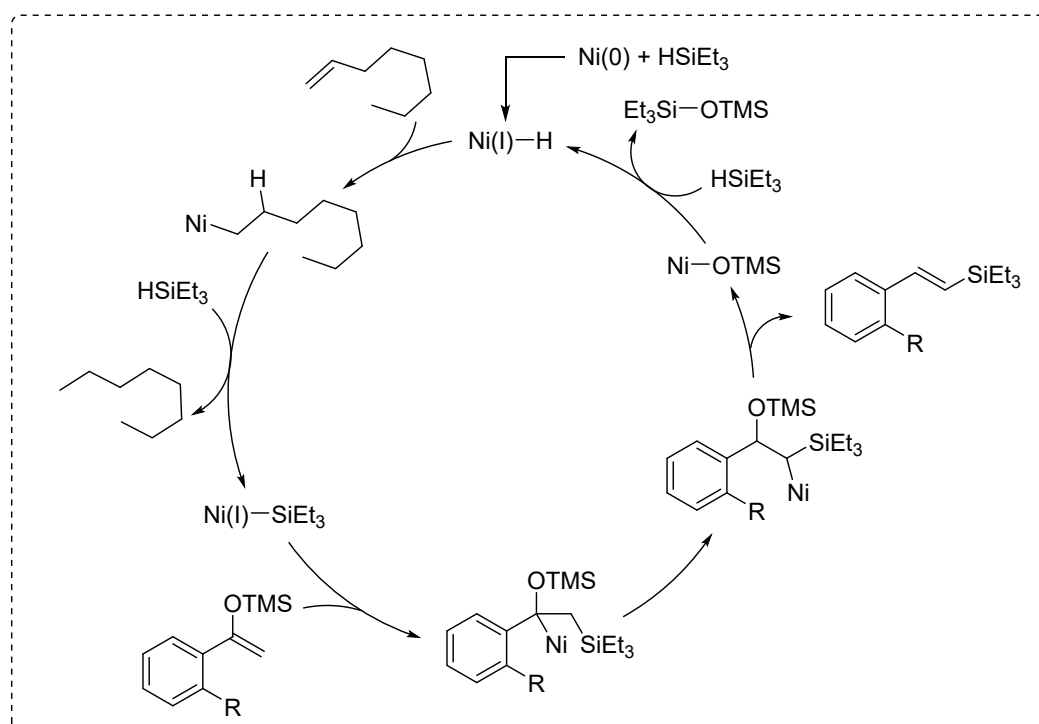
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H	-0.467769	-6.464652	0.414830	C	5.101634	-0.014437	0.319657
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H	1.935662	-0.107564	2.060879	H	5.741354	0.341631	-0.499287
H	1.908698	1.313949	1.038175	H	5.297754	0.626970	1.185994
C	4.267343	-3.422813	-1.347965	C	-0.971923	1.308959	-2.094123
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H	6.221484	-2.352260	2.554082	Si	-1.664309	-0.168645	0.325515
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C	1.518431	1.193407	-0.245924	H	0.911596	-1.484858	1.572297
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H	-4.850645	-1.322610	-1.559875	C	3.017974	-2.432945	1.237927
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C	-4.538438	-1.547897	1.487645	H	2.197032	1.776176	2.320444
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C	-5.440680	-2.023235	0.338474	H	1.558720	4.584290	1.440270
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H	4.699482	1.112278	-2.609966	C	2.372788	-1.097980 -0.025696
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H	4.474444	2.910396	2.284101	C	4.080224	1.095355 -0.013715
H	4.618375	1.218687	2.776260	C	4.632620	-0.189569 -0.020463
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C	1.663086	5.458673	-0.544640	H	1.722258	-1.967848 -0.033463
H	1.614504	6.501416	-0.206477	H	2.296739	2.293913 -0.007352
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C	-2.801017	2.163396	1.284442	H	6.429136	-1.184075 -0.708997
C	-3.779910	1.899311	-1.296267	C	0.363771	0.448544 -0.013862
H	-1.729235	1.778156	-1.915932	C	-0.640983	-0.450402 -0.023032
C	-4.171356	2.167722	1.050993	H	-0.376647	-1.511140 -0.033204
H	-2.429392	2.272246	2.301536	H	0.109079	1.510046 -0.002879
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C	-6.186628	1.968862	-0.483071	H	-3.003447	-1.504646 1.921588
H	-6.575146	0.948616	-0.349282	H	-4.256767	-0.297326 1.707400
H	-6.733273	2.614430	0.214325	H	-2.953437	0.095707 3.852819
H	-6.443936	2.280562	-1.501695	H	-1.464943	0.276307 2.910884
C	0.594548	2.115499	-0.501581	H	-2.763019	1.463639 2.750276
H	0.272751	2.522022	-1.464096	C	-2.707095	1.834965 -0.334281
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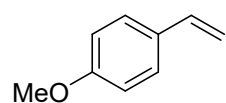
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H	-1.308526	2.055396	-2.007759
H	-2.977543	1.776799	-2.508138
C	-3.380130	-1.045416	-1.300071
C	-3.273337	-2.569552	-1.110104
H	-2.993454	-0.767955	-2.290273
H	-4.438157	-0.744581	-1.296234
H	-3.816443	-3.115601	-1.891473
H	-2.229752	-2.905576	-1.145017
H	-3.686421	-2.885184	-0.144421

g) Proposed mechanism for 5a-5c



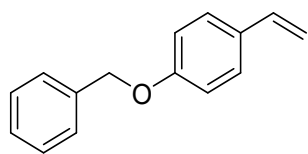
VI. Analysis Data for the Products

1-methoxy-4-vinylbenzene (**3c**)¹¹



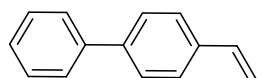
According to the general procedure B, the reaction gave **3c** in 75% yield (50 mg) as colorless liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.41 (d, *J* = 7.3 Hz, 2H), 6.92 (d, *J* = 7.3 Hz, 2H), 6.73 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.68 (d, *J* = 17.6 Hz, 1H), 5.19 (d, *J* = 10.9 Hz, 1H), 3.86 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 159.4, 136.2, 130.5, 127.4, 113.9, 111.6, 55.3.

1-(benzyloxy)-4-vinylbenzene (**3d**)¹¹



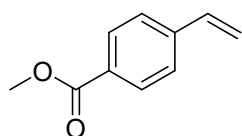
According to the general procedure B, the reaction gave **3d** in 91% yield (96 mg) as white solid. m.p. 62.2 – 62.8 °C. ¹H NMR (500 MHz, CDCl₃) δ 7.50 – 7.28 (m, 7H), 6.92 (dd, *J* = 8.7, 2.0 Hz, 2H), 6.65 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.60 (d, *J* = 17.5 Hz, 1H), 5.12 (d, *J* = 10.9 Hz, 1H), 5.06 (s, 2H). ¹³C NMR (126 MHz, CDCl₃) δ 158.6, 137.0, 136.2, 130.7, 128.6, 128.0, 127.5, 127.4, 114.9, 111.7, 70.0.

4-vinyl-1,1'-biphenyl (**3e**)¹²



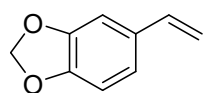
According to the general procedure B, the reaction gave **3e** in 73% yield (66 mg) as white solid. m.p. 118.8 – 119.4 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.62 (dd, *J* = 12.6, 8.0 Hz, 4H), 7.56 – 7.43 (m, 4H), 7.38 (t, *J* = 7.3 Hz, 1H), 6.80 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.83 (d, *J* = 17.6 Hz, 1H), 5.31 (d, *J* = 10.9 Hz, 1H). ¹³C NMR (126 MHz, CDCl₃) δ 140.8, 140.6, 136.7, 136.5, 128.8, 127.4, 127.3, 127.0, 126.7, 113.9.

Methyl 4-vinylbenzoate (**3f**)¹³



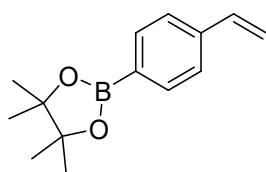
According to the general procedure B, the reaction gave **3f** in 62% yield (50 mg) as white solid. m.p. 32.1 – 32.7 °C. ¹H NMR (500 MHz, CDCl₃) δ 7.99 (d, *J* = 8.1 Hz, 2H), 7.46 (d, *J* = 8.0 Hz, 2H), 6.75 (dd, *J* = 17.6, 10.8 Hz, 1H), 5.86 (d, *J* = 17.6 Hz, 1H), 5.38 (d, *J* = 10.8 Hz, 1H), 3.91 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 166.9, 142.0, 136.0, 129.9, 129.3, 126.1, 116.5, 52.1.

5-vinylbenzo[d][1,3]dioxole (**3g**)¹⁴



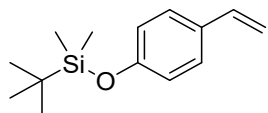
According to the general procedure B, the reaction gave **3g** in 98% yield (73 mg) as colorless liquid. ¹H NMR (400 MHz, CDCl₃) δ 6.99 (d, *J* = 1.6 Hz, 1H), 6.86 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.79 (d, *J* = 8.0 Hz, 1H), 6.65 (dd, *J* = 17.5, 10.8 Hz, 1H), 5.98 (s, 2H), 5.61 (dd, *J* = 17.5, 0.6 Hz, 1H), 5.16 (dd, *J* = 10.8, 0.5 Hz, 1H). ¹³C NMR (126 MHz, CDCl₃) δ 148.0, 147.4, 136.4, 132.2, 121.0, 112.0, 108.2, 105.4, 101.1.

4,4,5,5-tetramethyl-2-(4-vinylphenyl)-1,3,2-dioxaborolane (**3h**)¹⁵



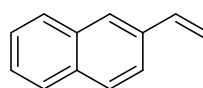
According to the general procedure B, the reaction gave **3h** in 57% yield (66 mg) as white solid. m.p. 31.4 – 31.9 °C. ¹H NMR (500 MHz, CDCl₃) δ 7.70 (d, *J* = 7.9 Hz, 2H), 7.33 (d, *J* = 7.8 Hz, 2H), 6.64 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.73 (d, *J* = 17.6 Hz, 1H), 5.20 (d, *J* = 10.8 Hz, 1H), 1.26 (s, 12H). ¹³C NMR (126 MHz, CDCl₃) δ 140.2, 136.9, 135.0, 134.7, 125.5, 114.8, 83.7, 24.8.

Tert-butyldimethyl(4-vinylphenoxy)silane (**3i**)¹⁶



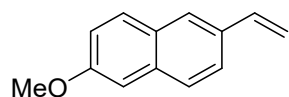
According to the general procedure B, the reaction gave **3i** in 60% yield (70 mg) as white solid. m.p. 39.0 – 39.6 °C. ¹H NMR (500 MHz, CDCl₃) δ 7.13 – 7.05 (m, 2H), 6.59 (d, *J* = 8.5 Hz, 2H), 6.46 (dd, *J* = 17.6, 10.8 Hz, 1H), 5.40 (dd, *J* = 17.6, 1.0 Hz, 1H), 4.92 (dd, *J* = 10.8, 1.1 Hz, 1H), 0.79 (s, 9H), -0.00 (s, 6H). ¹³C NMR (126 MHz, CDCl₃) δ 155.5, 136.4, 131.0, 127.3, 120.1, 111.7, 25.7, 18.2, -4.4.

2-vinylnaphthalene (**3j**)¹³



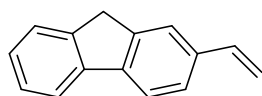
According to the general procedure B, the reaction gave **3j** in 49% yield (38 mg) as colorless liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.86 – 7.83 (m, 3H), 7.79 (d, *J* = 2.1 Hz, 1H), 7.68 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.52 – 7.45 (m, 2H), 6.93 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.91 (d, *J* = 17.6 Hz, 1H), 5.38 (d, *J* = 10.9 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 136.9, 135.0, 133.5, 133.1, 128.1, 128.0, 127.6, 126.3, 126.2, 125.9, 123.1, 114.1.

2-methoxy-6-vinylnaphthalene (**3k**)¹¹



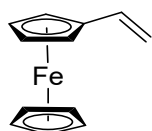
According to the general procedure B, the reaction gave **3k** in 57% yield (52 mg) as white solid. m.p. 88.8 – 89.7 °C. ¹H NMR (500 MHz, CDCl₃) δ 7.76 – 7.67 (m, 3H), 7.64 – 7.59 (m, 1H), 7.12 (t, *J* = 3.0 Hz, 2H), 6.86 (dd, *J* = 17.5, 10.8 Hz, 1H), 5.83 (d, *J* = 17.6 Hz, 1H), 5.29 (d, *J* = 10.8 Hz, 1H), 3.93 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 157.8, 137.0, 134.3, 133.0, 129.6, 129.0, 127.0, 126.2, 123.8, 119.0, 113.1, 105.9, 55.3.

2-vinyl-9H-fluorene (**3l**)¹⁷



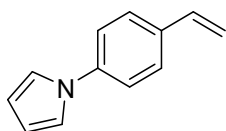
According to the general procedure B, the reaction gave **3l** in 45% yield (43 mg) as white solid. m.p. 38.3 – 38.8 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.76 (dd, *J* = 15.4, 7.7 Hz, 2H), 7.61 (s, 1H), 7.55 (d, *J* = 7.4 Hz, 1H), 7.43 (d, *J* = 8.6 Hz, 1H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.30 (td, *J* = 7.4, 1.1 Hz, 1H), 6.81 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.80 (dd, *J* = 17.6, 0.9 Hz, 1H), 5.26 (dd, *J* = 10.9, 0.9 Hz, 1H), 3.91 (s, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 143.6, 143.5, 141.5, 141.5, 137.2, 136.3, 126.8, 126.7, 125.4, 125.1, 122.6, 119.9, 119.9, 113.2, 36.9.

Vinylferrocene (**3m**)¹⁸



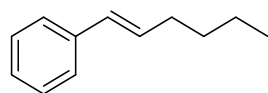
According to the general procedure B, the reaction gave **3m** in 62% yield (66 mg) as yellow oil. ¹H NMR (500 MHz, CDCl₃) δ 6.43 (d, *J* = 9.7 Hz, 1H), 5.32 (dd, *J* = 17.8, 7.3 Hz, 1H), 5.01 (s, 1H), 4.34 (d, *J* = 7.3 Hz, 2H), 4.19 (d, *J* = 7.2 Hz, 2H), 4.09 (d, *J* = 7.6 Hz, 5H). ¹³C NMR (126 MHz, CDCl₃) δ 134.7, 111.1, 83.6, 69.2, 68.7, 66.7.

1-(4-vinylphenyl)-1H-pyrrole (**3n**)¹⁸



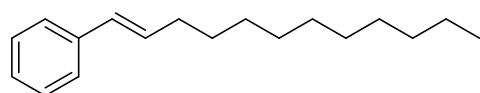
According to the general procedure B, the reaction gave **3n** in 53% yield (45 mg) as white solid. m.p. 41.2 – 41.7 °C. ¹H NMR (500 MHz, CDCl₃) δ 7.43 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 8.3 Hz, 2H), 7.07 (s, 2H), 6.70 (dd, *J* = 17.6, 10.9 Hz, 1H), 6.34 (s, 2H), 5.72 (d, *J* = 17.6 Hz, 1H), 5.24 (d, *J* = 10.9 Hz, 1H). ¹³C NMR (126 MHz, CDCl₃) δ 140.2, 135.9, 135.1, 127.4, 120.4, 119.2, 113.8, 110.6.

(E)-hex-1-en-1-ylbenzene (3p)¹⁹



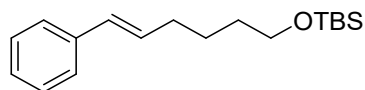
According to the general procedure B, the reaction gave **3p** in 98% yield (78 mg) as colorless liquid. ¹H NMR (500 MHz, CDCl₃) δ 7.26 (d, *J* = 7.5 Hz, 2H), 7.21 (t, *J* = 7.6 Hz, 2H), 7.11 (t, *J* = 7.2 Hz, 1H), 6.30 (d, *J* = 15.8 Hz, 1H), 6.15 (dt, *J* = 15.8, 6.9 Hz, 1H), 2.14 (q, *J* = 6.9 Hz, 2H), 1.41 – 1.36 (m, 2H), 1.34 – 1.28 (m, 2H), 0.85 (t, *J* = 7.3 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 138.0, 131.2, 129.7, 128.5, 126.8, 125.9, 32.7, 31.6, 22.3, 14.0.

(E)-dodec-1-en-1-ylbenzene (3q)²⁰



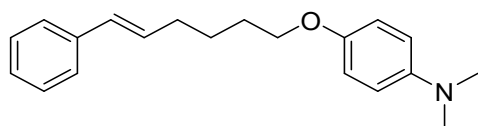
According to the general procedure B, the reaction gave **3q** in 99% yield (121 mg) as colorless liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.36 (d, *J* = 7.4 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.20 (t, *J* = 7.2 Hz, 1H), 6.40 (d, *J* = 15.8 Hz, 1H), 6.25 (dt, *J* = 15.8, 6.8 Hz, 1H), 2.22 (q, *J* = 7.0 Hz, 2H), 1.49 (p, *J* = 7.1 Hz, 2H), 1.31 (d, *J* = 15.9 Hz, 14H), 0.91 (t, *J* = 6.7 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 138.0, 131.2, 129.7, 128.4, 126.7, 125.9, 33.1, 31.9, 29.6, 29.5, 29.4, 29.4, 29.2, 22.7, 14.1.

(E)-tert-butyldimethyl((6-phenylhex-5-en-1-yl)oxy)silane (3r)²¹



According to the general procedure B, the reaction gave **3r** in 84% yield (121 mg) as colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 7.28 (d, *J* = 7.5 Hz, 2H), 7.22 (t, *J* = 7.6 Hz, 2H), 7.12 (t, *J* = 7.2 Hz, 1H), 6.32 (d, *J* = 15.8 Hz, 1H), 6.21 – 6.11 (m, 1H), 3.58 (t, *J* = 6.3 Hz, 2H), 2.17 (q, *J* = 7.0 Hz, 2H), 1.61 – 1.39 (m, 4H), 0.85 (s, 9H), 0.00 (s, 6H). ¹³C NMR (126 MHz, CDCl₃) δ 137.9, 130.9, 130.0, 128.5, 126.8, 126.0, 63.1, 32.8, 32.4, 26.0, 25.7, 18.4, -5.2.

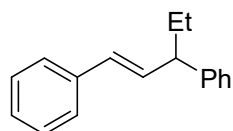
(E)-N,N-dimethyl-4-((6-phenylhex-5-en-1-yl)oxy)aniline (3s)



According to the general procedure B, the reaction gave **3s** in 79% yield (117 mg) as yellow oil. ¹H NMR (500 MHz, CDCl₃) δ 7.36 – 7.25 (m, 4H), 7.17 (t, *J* = 7.2 Hz, 1H), 6.83 (d, *J* = 8.8 Hz, 2H), 6.73 (d, *J* = 8.7

Hz, 2H), 6.39 (d, $J = 15.8$ Hz, 1H), 6.22 (dt, $J = 15.4, 6.8$ Hz, 1H), 3.92 (t, $J = 6.4$ Hz, 2H), 2.84 (s, 6H), 2.27 (q, $J = 7.0$ Hz, 2H), 1.80 (p, $J = 6.6$ Hz, 2H), 1.64 (p, $J = 7.4$ Hz, 2H). ^{13}C NMR (126 MHz, CDCl_3) δ 151.5, 145.8, 137.9, 130.6, 130.2, 128.5, 126.9, 126.0, 115.5, 115.0, 68.5, 41.9, 32.8, 29.0, 25.9. HRMS (ESI-quadrupole) m/z : $[\text{M}+\text{H}]^+$ Calcd. For $\text{C}_{20}\text{H}_{26}\text{NO}$ 296.2009; found: 296.2009.

(E)-pent-1-ene-1,3-diylidibenzene (3t)



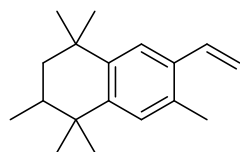
According to the general procedure B, the reaction gave **3t** in 70% yield (78 mg) as yellow oil. ^1H NMR (400 MHz, CDCl_3) δ 7.36

- 7.17 (m, 10H), 6.36 (dt, $J = 15.8, 11.6$ Hz, 2H), 3.32 (q, $J = 7.3$

Hz, 1H), 1.86 - 1.80 (m, 2H), 0.92 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3)

δ 144.6, 137.6, 134.3, 129.5, 128.5, 127.7, 127.0, 126.21, 126.15, 51.0, 28.8, 12.3.

1,1,2,4,4,7-hexamethyl-6-vinyl-1,2,3,4-tetrahydronaphthalene (3aa)²²



According to the general procedure B, the reaction gave **3aa** in 40% yield (24 mg) as colorless oil. ^1H NMR (500 MHz, CDCl_3)

δ 7.43 (s, 1H), 7.15 (s, 1H), 6.92 (dd, $J = 17.4, 11.0$ Hz, 1H),

5.62 (d, $J = 17.4$ Hz, 1H), 5.27 (d, $J = 11.0$ Hz, 1H), 2.34 (s, 3H), 1.90 (m, $J = 13.1,$

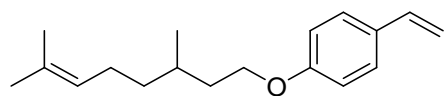
6.7, 2.6 Hz, 1H), 1.66 (t, $J = 13.2$ Hz, 1H), 1.39 (dd, $J = 13.5, 2.6$ Hz, 1H), 1.35 (s,

6H), 1.30 (s, 3H), 1.09 (s, 3H), 1.01 (d, $J = 6.8$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3)

δ 145.7, 142.5, 135.1, 134.2, 132.5, 128.7, 123.4, 114.3, 43.8, 37.5, 34.6, 34.1, 32.5,

32.1, 28.6, 24.9, 19.5, 16.8.

1-((3,7-dimethyloct-6-en-1-yl)oxy)-4-vinylbenzene (3ab)²³



According to the general procedure B, the reaction gave **3ab** in 62% yield (80 mg) as

colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 7.32 (d, $J = 8.7$ Hz, 2H), 6.94 - 6.80 (m,

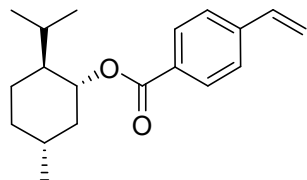
2H), 6.65 (dd, $J = 17.6, 10.9$ Hz, 1H), 5.59 (dd, $J = 17.6, 1.0$ Hz, 1H), 5.21 - 5.03 (m,

2H), 3.99 (q, $J = 6.6$ Hz, 2H), 2.01 (dq, $J = 15.9, 7.4$ Hz, 2H), 1.89-1.79 (m, 1H),

1.73-1.66 (m, 3H), 1.61 (s, 3H), 1.49-1.35 (m, 1H), 1.35-1.14 (m, 3H), 0.95 (d, $J =$

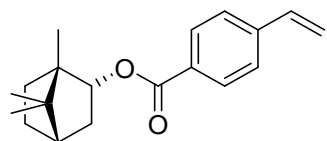
6.6 Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 159.0, 136.3, 131.3, 130.3, 127.4, 124.7, 114.5, 111.4, 66.4, 37.2, 36.2, 29.6, 25.7, 25.4, 19.6, 17.7.

(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 4-vinylbenzoate (3ac)



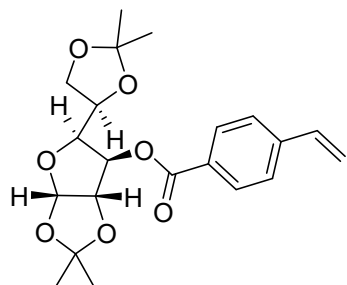
According to the general procedure C, the reaction gave **3ac** in 45% yield (64 mg) as colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 8.00 (d, $J = 8.4$ Hz, 2H), 7.46 (d, $J = 8.4$ Hz, 2H), 6.75 (dd, $J = 17.6, 10.9$ Hz, 1H), 5.85 (d, $J = 17.6$ Hz, 1H), 5.37 (d, $J = 10.9$ Hz, 1H), 4.93 (td, $J = 10.8, 4.4$ Hz, 1H), 2.13 (dd, $J = 12.1, 1.8$ Hz, 1H), 1.96 (td, $J = 7.0, 2.8$ Hz, 1H), 1.73 (dd, $J = 11.7, 2.7$ Hz, 2H), 1.60 – 1.49 (m, 2H), 1.25 (t, $J = 7.6$ Hz, 1H), 1.17 – 1.07 (m, 2H), 0.92 (t, $J = 6.4$ Hz, 6H), 0.79 (d, $J = 7.0$ Hz, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 165.8, 141.7, 136.1, 129.8, 127.8, 126.0, 116.3, 74.8, 47.3, 41.0, 34.3, 31.4, 26.5, 23.6, 22.0, 20.7, 16.5. HRMS (ESI-quadrupole) m/z : $[\text{M}+\text{H}]^+$ Calcd. For $\text{C}_{19}\text{H}_{27}\text{O}_2$ 287.2006; found: 287.1998.

(1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl 4-vinylbenzoate (3ad)



According to the general procedure B, the reaction gave **3ad** in 44% yield (62 mg) as yellow oil. ^1H NMR (500 MHz, CDCl_3) δ 7.93 (d, $J = 8.2$ Hz, 2H), 7.38 (d, $J = 8.3$ Hz, 2H), 6.67 (dd, $J = 17.6, 10.9$ Hz, 1H), 5.77 (d, $J = 17.6$ Hz, 1H), 5.29 (d, $J = 10.8$ Hz, 1H), 5.03 (m, $J = 9.9, 3.5, 2.2$ Hz, 1H), 2.44 – 2.35 (m, 1H), 2.05 (m, $J = 13.3, 9.5, 4.4$ Hz, 1H), 1.72 (m, $J = 12.2, 8.1, 4.0$ Hz, 1H), 1.65 (t, $J = 4.5$ Hz, 1H), 1.37 – 1.29 (m, 1H), 1.23 (m, $J = 12.4, 9.5, 4.5$ Hz, 1H), 1.04 (dd, $J = 13.8, 3.5$ Hz, 1H), 0.89 (s, 3H), 0.83 (s, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 166.5, 141.7, 136.0, 130.0, 129.8, 126.0, 116.3, 80.4, 49.1, 47.8, 45.0, 36.9, 28.1, 27.4, 19.7, 18.9. HRMS (ESI-quadrupole) m/z : $[\text{M}+\text{H}]^+$ Calcd. For $\text{C}_{19}\text{H}_{25}\text{O}_2$ 285.1849; found: 285.1847.

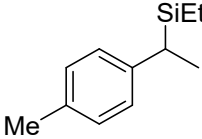
(3aS,5S,6R,6aS)-5-((R)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-d][1,3]dioxol-6-yl 4-vinylbenzoate (3ae)



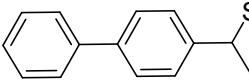
According to the general procedure C, the reaction gave **3ae** in 34% yield (66 mg) as colorless oil. ^1H NMR (400

MHz, CDCl₃) δ 8.00 (d, J = 8.3 Hz, 2H), 7.50 (d, J = 8.3 Hz, 2H), 6.78 (dd, J = 17.6, 10.9 Hz, 1H), 5.98 (d, J = 3.7 Hz, 1H), 5.90 (d, J = 17.6 Hz, 1H), 5.52 (d, J = 2.6 Hz, 1H), 5.43 (d, J = 10.9 Hz, 1H), 4.66 (d, J = 3.7 Hz, 1H), 4.41 – 4.34 (m, 2H), 4.16 – 4.09 (m, 2H), 1.58 (s, 3H), 1.44 (s, 3H), 1.35 (s, 3H), 1.29 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 164.9, 142.4, 135.8, 130.0, 128.5, 126.2, 116.9, 112.3, 109.3, 105.1, 83.3, 79.9, 72.5, 67.2, 26.8, 26.7, 26.1, 25.1. HRMS (ESI-quadrupole) m/z : [M+H]⁺ Calcd. For C₂₁H₂₇O₇ 391.1751; found: 391.1741.

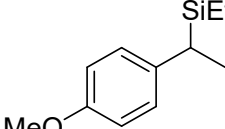
triethyl(1-(*p*-tolyl)ethyl)silane (**4a**)²⁴

 According to the general procedure C, the reaction gave **4a** in 68% yield (80 mg) as colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 7.06 (d, J = 7.9 Hz, 2H), 6.98 (d, J = 8.1 Hz, 2H), 2.31 (s, 3H), 2.28 (q, J = 7.7 Hz, 1H), 1.37 (d, J = 7.6 Hz, 3H), 0.92 (t, J = 8.0 Hz, 9H), 0.53 (q, J = 7.9 Hz, 6H). ¹³C NMR (126 MHz, CDCl₃) δ 143.1, 133.4, 128.7, 127.0, 26.3, 20.9, 15.6, 7.5, 2.1.

(1-([1,1'-biphenyl]-4-yl)ethyl)triethylsilane (**4b**)²⁴

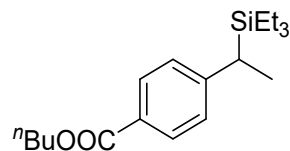
 According to the general procedure C, the reaction gave **4b** in 60% yield (89 mg) as white solid. m.p. 34.2 – 34.9 °C. ¹H NMR (500 MHz, CDCl₃) δ 7.63 (d, J = 7.2 Hz, 2H), 7.52 (d, J = 8.4 Hz, 2H), 7.45 (t, J = 7.7 Hz, 2H), 7.35 – 7.32 (m, 1H), 7.18 (d, J = 8.1 Hz, 2H), 2.40 (q, J = 7.6 Hz, 1H), 1.45 (d, J = 7.6 Hz, 3H), 0.95 (t, J = 8.0 Hz, 9H), 0.58 (q, J = 7.9 Hz, 6H). ¹³C NMR (126 MHz, CDCl₃) δ 145.5, 141.2, 137.0, 128.6, 127.5, 126.8, 126.7, 126.6, 26.6, 15.4, 7.5, 2.1.

Triethyl(1-(4-methoxyphenyl)ethyl)silane (**4c**)²⁴

 According to the general procedure C, the reaction gave **4c** in 50% yield (63 mg) as colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 6.98 (d, J = 8.6 Hz, 2H), 6.79 (d, J = 8.6 Hz, 2H), 3.77 (s, 3H), 2.24 (q, J = 7.6 Hz, 1H), 1.36 – 1.31 (m, 3H), 0.94 – 0.86 (m, 9H), 0.50 (q, J = 8.1 Hz, 6H). ¹³C NMR (126 MHz, CDCl₃) δ 156.7, 138.3, 127.8, 113.5, 55.2, 25.7, 15.7, 7.5,

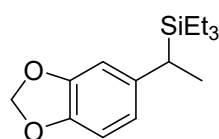
2.1. **HRMS** (ESI-quadrupole) m/z : $[M+H]^+$ Calcd. For $C_{15}H_{27}OSi$ 251.1826; found: 251.1827.

Butyl 4-(1-(triethylsilyl)ethyl)benzoate (4d)



According to the general procedure C, the reaction gave **4d** in 68% yield (109 mg) as colorless oil. **1H NMR** (500 MHz, $CDCl_3$) δ 7.90 (t, $J = 25.8$, 2H), 7.12 (d, $J = 8.3$ Hz, 2H), 4.30 (t, $J = 6.6$ Hz, 2H), 2.40 (q, $J = 7.4$ Hz, 1H), 1.77 – 1.71 (m, 2H), 1.48 (q, $J = 7.5$ Hz, 2H), 1.39 (dd, $J = 7.5$, 3.7 Hz, 3H), 0.98 (t, $J = 7.4$ Hz, 3H), 0.89 (t, $J = 7.9$ Hz, 9H), 0.51 (q, $J = 8.0$ Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 166.9, 152.3, 129.4, 126.9, 64.5, 30.8, 28.2, 27.7, 19.3, 15.1, 13.8, 7.4, 2.0. **HRMS** (ESI-quadrupole) m/z : $[M+H]^+$ Calcd. For $C_{19}H_{33}O_2Si$ 321.2244; found: 321.2245.

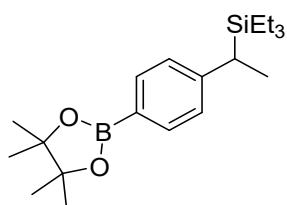
(1-(benzo[d][1,3]dioxol-5-yl)ethyl)triethylsilane (4e)



According to the general procedure C, the reaction gave **4e** in 51% yield (67 mg) as colorless oil. **1H NMR** (500 MHz, $CDCl_3$) δ 6.69 (d, $J = 8.0$ Hz, 1H), 6.58 (d, $J = 1.8$ Hz, 1H), 6.51 (dd, $J = 8.0$, 1.8 Hz, 1H), 5.89 (s, 2H), 2.22 (q, $J = 7.6$ Hz, 1H), 1.32 (d, $J = 7.6$ Hz, 3H), 0.90 (t, $J = 8.0$ Hz, 9H), 0.51 (q, $J = 7.9$ Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 147.3, 144.4, 140.3, 119.6, 107.9, 107.7, 100.5, 26.5, 15.9, 7.5, 2.1. **HRMS** (ESI-quadrupole) m/z : $[M+H]^+$ Calcd. For $C_{15}H_{25}O_2Si$ 265.1618; found: 165.1619.

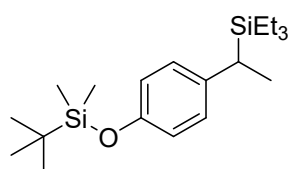
Triethyl(1-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)ethyl)silane

(4f)²⁴



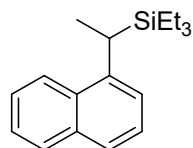
According to the general procedure C, the reaction gave **4f** in 50% yield (87 mg) as colorless oil. **1H NMR** (400 MHz, $CDCl_3$) δ 7.71 (d, $J = 8.0$ Hz, 2H), 7.11 (d, $J = 8.0$ Hz, 2H), 2.37 (q, $J = 7.5$ Hz, 1H), 1.40 (d, $J = 7.5$ Hz, 3H), 1.36 (s, 12H), 0.91 (t, $J = 7.9$ Hz, 9H), 0.53 (q, $J = 7.9$ Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 150.1, 134.6, 126.6, 83.5, 27.4, 24.86, 24.85, 15.2, 7.5, 2.0.

Tert-butyldimethyl(4-(1-(triethylsilyl)ethyl)phenoxy)silane (4g)



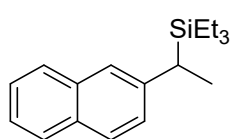
According to the general procedure C, the reaction gave **4g** in 57% yield (100 mg) as colorless liquid. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 6.74 (d, $J = 8.5$ Hz, 2H), 6.54 (d, $J = 8.5$ Hz, 2H), 2.05 (q, $J = 7.6$ Hz, 1H), 1.16 (d, $J = 7.7$ Hz, 3H), 0.81 (d, $J = 2.8$ Hz, 9H), 0.70 (t, $J = 8.0$ Hz, 9H), 0.32 (q, $J = 7.9$ Hz, 6H), -0.00 (s, 6H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 150.33, 136.71, 125.64, 117.53, 23.69, 23.64, 16.10, 13.53, 5.38, 0.00, -6.53. **HRMS** (ESI-quadrupole) m/z : $[\text{M}+\text{H}]^+$ Calcd. For $\text{C}_{20}\text{H}_{39}\text{OSi}_2$ 351.2534; found: 351.2537.

Triethyl(1-(naphthalen-1-yl)ethyl)silane (**4h**)



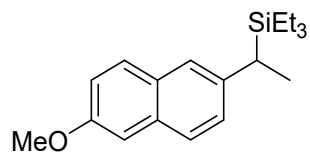
According to the general procedure C, the reaction gave **4h** in 93% yield (126 mg) as colorless liquid. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.14 (d, $J = 8.2$ Hz, 1H), 7.88 (dd, $J = 7.4, 2.0$ Hz, 1H), 7.66 (d, $J = 8.1$ Hz, 1H), 7.54–7.47 (m, 3H), 7.36 (d, $J = 7.2$ Hz, 1H), 3.29 (q, $J = 7.4$ Hz, 1H), 1.58 (dd, $J = 7.4, 1.8$ Hz, 3H), 0.89 (t, $J = 7.9$, 9H), 0.65–0.50 (m, 6H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 143.3, 133.9, 131.7, 128.9, 125.5, 125.2, 125.1, 124.7, 123.7, 123.6, 16.7, 7.5, 2.5. **HRMS** (ESI-quadrupole) m/z : $[\text{M}+\text{H}]^+$ Calcd. For $\text{C}_{18}\text{H}_{27}\text{Si}$ 271.1877; found: 271.1874.

Triethyl(1-(naphthalen-2-yl)ethyl)silane (**4i**)²⁴



According to the general procedure C, the reaction gave **4i** in 88% yield (119 mg) as colorless liquid. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.85–7.77 (m, 3H), 7.56 (s, 1H), 7.51 – 7.42 (m, 2H), 7.32 (d, $J = 8.5$ Hz, 1H), 2.56 (q, $J = 7.5$ Hz, 1H), 1.55 (d, $J = 7.6$ Hz, 3H), 0.98 (t, $J = 8.0$ Hz, 9H), 0.62 (q, $J = 8.0$ Hz, 6H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 144.1, 133.8, 131.3, 127.5, 127.3, 127.2, 127.1, 125.7, 124.4, 124.3, 27.1, 15.5, 7.5, 2.2.

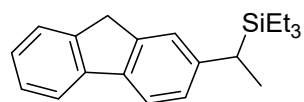
Triethyl(1-(6-methoxynaphthalen-2-yl)ethyl)silane (**4j**)²⁵



According to the general procedure C, the reaction gave **4j** in 57% yield (86 mg) as white solid. m.p. 52.4 – 52.9 °C. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.70 (dd, $J = 15.9, 8.6$ Hz, 2H),

7.49 (s, 1H), 7.29 (dd, $J = 8.4, 1.7$ Hz, 1H), 7.20 – 7.16 (m, 2H), 3.96 (s, 3H), 2.51 (q, $J = 7.6$, 1H), 1.54 (d, $J = 7.6$, 3H), 0.98 (t, $J = 7.9$, 9H), 0.62 (q, $J = 7.9$, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 156.7, 141.6, 132.1, 129.3, 128.7, 127.5, 126.2, 124.2, 118.4, 105.6, 55.3, 26.7, 15.6, 7.5, 2.2.

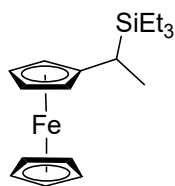
(1-(9H-fluoren-2-yl)ethyl)triethylsilane (4k)²⁶



According to the general procedure C, the reaction gave **4k** in 63% yield (97 mg) as white solid. m.p. 43.1 – 43.8 °C. ^1H

NMR (400 MHz, CDCl_3) δ 7.69 (d, $J = 7.5$ Hz, 1H), 7.62 (d, $J = 7.9$ Hz, 1H), 7.48 (d, $J = 7.4$ Hz, 1H), 7.31 (t, $J = 7.4$ Hz, 1H), 7.24 – 7.20 (m, 2H), 7.06 (d, $J = 7.9$ Hz, 1H), 3.83 (s, 2H), 2.37 (q, $J = 7.5$ Hz, 1H), 1.41 (d, $J = 7.5$ Hz, 3H), 0.88 (t, $J = 7.9$ Hz, 9H), 0.52 (q, $J = 7.9$ Hz, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 145.3, 143.3, 142.9, 142.0, 138.1, 126.6, 125.9, 125.8, 124.9, 123.6, 119.6, 119.3, 36.8, 27.1, 15.7, 7.5, 2.1.

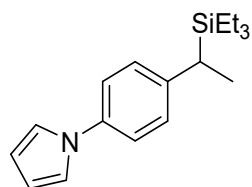
1-Ferrocenyl-1-(triethylsilyl)ethane (4l)²⁴



According to the general procedure C, the reaction gave **4l** in 51% yield (84 mg) as yellow oil. ^1H NMR (500 MHz, CDCl_3) δ 4.33 – 4.11 (m, 9H), 1.83 (s, 1H), 1.10 (s, 3H), 0.90 (d, $J = 12.3$ Hz, 9H),

0.56 – 0.50 (m, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 68.1, 67.3, 66.1, 18.7, 15.0, 7.5, 2.0.

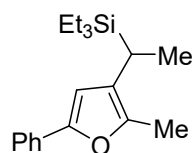
1-(4-(1-(triethylsilyl)ethyl)phenyl)-1H-pyrrole (4m)



According to the general procedure C, the reaction gave **4m** in 58% yield (83 mg) as colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 7.26 (d, $J = 8.3$ Hz, 2H), 7.10 (d, $J = 8.3$ Hz, 2H), 7.05 (s, 2H), 6.31 (s, 2H), 2.33 (q, $J = 7.6$ Hz, 1H), 1.39 (d, $J = 7.6$ Hz, 3H),

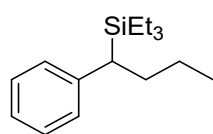
0.90 (t, $J = 8.0$ Hz, 9H), 0.53 (q, $J = 7.9$ Hz, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 143.9, 137.5, 127.9, 120.3, 119.3, 109.9, 26.4, 15.5, 7.5, 2.1. HRMS (ESI-quadrupole) m/z:[M+H]⁺ Calcd. For $\text{C}_{18}\text{H}_{28}\text{NSi}$ 286.1986; found: 286.1986.

Triethyl(1-(2-methyl-5-phenylfuran-3-yl)ethyl)silane (4n)



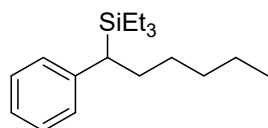
According to the general procedure C, the reaction gave **4n** in 40% yield (60 mg) as yellow oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.61 – 7.60 (m, 2H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.17 (t, *J* = 7.4, 1H), 6.43 (s, 1H), 2.26 (s, 3H), 2.04 (q, *J* = 7.6 Hz, 1H), 1.27 (d, *J* = 7.5 Hz, 3H), 0.94 (t, *J* = 7.9 Hz, 9H), 0.56 (q, *J* = 7.9, 6H). **¹³C NMR** (126 MHz, CDCl₃) δ 150.9, 145.0, 131.3, 128.5, 126.4, 124.7, 123.1, 106.4, 16.0, 15.8, 12.0, 7.5, 2.3. **HRMS** (ESI-quadrupole) *m/z*: [M+H]⁺ Calcd. For C₁₉H₂₉OSi 301.1982; found: 301.1982.

Triethyl(1-phenylbutyl)silane (**4o**)²⁷



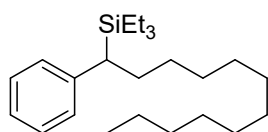
According to the general procedure C, the reaction gave **4o** in 86% yield (107 mg) as colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.22 (t, *J* = 7.3 Hz, 2H), 7.06 (t, *J* = 6.7 Hz, 3H), 2.17 (dd, *J* = 12.4, 3.2 Hz, 1H), 1.91 – 1.79 (m, 1H), 1.65 (m, *J* = 13.9, 7.1, 3.4 Hz, 1H), 1.32 (m, *J* = 13.9, 6.9, 3.4 Hz, 1H), 1.16 – 1.06 (m, 1H), 0.89 (t, *J* = 8.0 Hz, 9H), 0.84 (t, *J* = 7.3 Hz, 3H), 0.51 (q, *J* = 7.9 Hz, 6H). **¹³C NMR** (126 MHz, CDCl₃) δ 144.1, 128.0, 127.9, 124.1, 33.7, 32.0, 22.3, 13.9, 7.5, 2.3.

Triethyl(1-phenylhexyl)silane (**4p**)



According to the general procedure C, the reaction gave **4p** in 75% yield (104 mg) as colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.21 (t, *J* = 7.4 Hz, 2H), 7.05 (t, *J* = 8.1 Hz, 3H), 2.13 (dd, *J* = 12.6, 3.3 Hz, 1H), 1.88 – 1.77 (m, 1H), 1.70 – 1.64 (m, *J* = 9.3, 3.5 Hz, 1H), 1.35 – 1.05 (m, 6H), 0.88 (t, *J* = 7.9 Hz, 9H), 0.82 (t, *J* = 5.9 Hz, 3H), 0.49 (q, *J* = 7.9 Hz, 6H). **¹³C NMR** (126 MHz, CDCl₃) δ 144.1, 128.0, 127.9, 124.1, 34.1, 31.7, 29.7, 29.1, 22.5, 14.1, 7.5, 2.3.

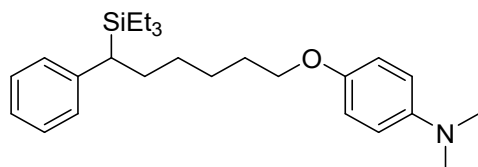
Triethyl(1-phenyldodecyl)silane (**4q**)



According to the general procedure C, the reaction gave **4q** in 59% yield (106 mg) as colorless oil. **¹H NMR** (500 MHz, CDCl₃) δ 7.21 (t, *J* = 7.5 Hz, 2H), 7.05 (t, *J* = 8.2 Hz, 3H), 2.13 (dd, *J* = 12.4, 3.2 Hz, 1H), 1.29 – 1.18 (m, 20H), 0.87 (t, *J* = 7.8 Hz, 12H), 0.49 (q, *J* = 7.9 Hz, 6H). **¹³C NMR** (126 MHz, CDCl₃) δ 144.1, 128.0, 127.9, 124.1, 34.1, 31.9,

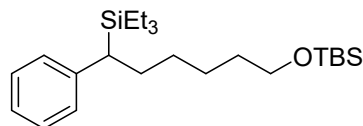
29.7, 29.7, 29.6, 29.6, 29.5, 29.4, 29.3, 26.2, 22.7, 14.1, 7.5, 2.3. **HRMS** (ESI-quadrupole) m/z : $[M+H]^+$ Calcd. For $C_{24}H_{45}Si$ 361.3285; found: 361.3286.

N,N-dimethyl-4-((6-phenyl-6-(triethylsilyl)hexyl)oxy)aniline (4r)



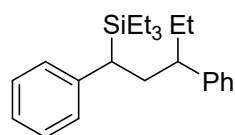
According to the general procedure C, the reaction gave **4r** in 54% yield (111 mg) as colorless oil. **1H NMR** (500 MHz, $CDCl_3$) δ 7.21 (t, $J = 7.6$ Hz, 2H), 7.05 (t, $J = 8.4$ Hz, 2H), 6.80 (d, $J = 8.5$ Hz, 2H), 6.72 (d, $J = 9.2$ Hz, 2H), 3.82 (t, $J = 6.5$ Hz, 2H), 2.84 (d, $J = 1.5$ Hz, 6H), 2.14 (dd, $J = 12.5, 3.2$ Hz, 1H), 1.85 (m 1H), 1.77 – 1.59 (m, 3H), 1.51 – 1.24 (m, 4H), 1.22 – 1.10 (m, 1H), 0.88 (t, $J = 7.9$ Hz, 9H), 0.49 (q, $J = 7.9$ Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 151.5, 145.6, 143.9, 128.0, 127.9, 124.2, 115.4, 114.9, 68.6, 41.8, 34.0, 29.6, 29.3, 29.1, 25.9, 7.5, 2.3. **HRMS** (ESI-quadrupole) m/z : $[M+H]^+$ Calcd. For $C_{26}H_{42}NOSi$ 412.3030; found: 412.3032.

Tert-butyldimethyl((6-phenyl-6-(triethylsilyl)hexyl)oxy)silane (4s)



According to the general procedure C, the reaction gave **4s** in 45% yield (92mg) as colorless oil. **1H NMR** (500 MHz, $CDCl_3$) δ 7.22 (t, $J = 7.5$ Hz, 2H), 7.11 – 7.02 (m, 2H), 3.54 (t, $J = 6.6$ Hz, 2H), 2.14 (dd, $J = 12.5, 3.2$ Hz, 1H), 1.84 (q, $J = 12.7$ Hz, 1H), 1.74 – 1.64 (m, 1H), 1.44 (dq, $J = 14.4, 7.1$ Hz, 2H), 1.37 – 1.19 (m, 4H), 1.13 – 1.08 (m, 1H), 0.91 – 0.86 (m, 18H), 0.50 (q, $J = 7.9$ Hz, 6H), 0.03 (s, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.0, 128.0, 127.9, 124.2, 63.3, 34.0, 32.7, 29.7, 29.1, 26.0, 25.6, 7.5, 2.3, -5.3. **HRMS** (ESI-quadrupole) m/z : $[M+H]^+$ Calcd. For $C_{24}H_{47}OSi_2$ 407.3160; found: 407.3160.

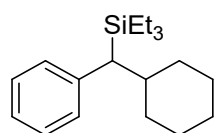
(1,3-diphenylpentyl)triethylsilane (4t)



According to the general procedure C, the reaction gave **4t** in 44% yield (74 mg) as yellow oil. **1H NMR** (400 MHz, $CDCl_3$) δ 7.34 – 7.09 (m, 8H), 7.03 (dd, $J = 13.0, 4.9$ Hz, 2H), 2.50 – 2.15 (m, 2H), 2.01 – 1.83 (m, 2H), 1.65 – 1.47 (m, 2H), 0.93 (t, $J = 7.9$ Hz, 3H), 0.81 (t, $J = 7.9$

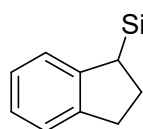
Hz, 6H), 0.71 (dt, $J = 23.0, 7.4$ Hz, 3H), 0.59 – 0.44 (m, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 146.7, 145.0, 143.7, 128.2, 128.1, 127.6, 125.9, 124.3, 46.1, 36.6, 31.3, 30.5, 12.3, 7.4, 2.3. HRMS (ESI-quadrupole) m/z : $[\text{M}+\text{H}]^+$ Calcd. For $\text{C}_{23}\text{H}_{35}\text{Si}$ 339.2503; found: 339.2497.

(cyclohexyl(phenyl)methyl)triethylsilane (4u)²⁷



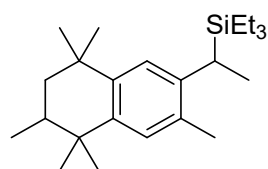
According to the general procedure C, the reaction gave **4u** in 68% yield (98 mg) as colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 7.21 (t, $J = 7.5$ Hz, 2H), 7.09 (t, $J = 7.4$ Hz, 1H), 7.03 (d, $J = 7.6$ Hz, 2H), 1.97 (t, $J = 10.2$ Hz, 2H), 1.89 – 1.72 (m, 2H), 1.38 – 1.22 (m, 2H), 1.19 – 1.03 (m, 3H), 1.02 – 0.92 (m, 2H), 0.89 (t, $J = 7.9$ Hz, 9H), 0.81 – 0.70 (m, 1H), 0.57 – 0.48 (m, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 144.2, 129.0, 127.9, 124.2, 41.7, 40.4, 33.9 (d, $J = 41.9$ Hz), 26.8 (d, $J = 20.8$ Hz), 26.5, 7.7, 4.1.

(2,3-dihydro-1H-inden-1-yl)triethylsilane (4v)²⁴



According to the general procedure C, the reaction gave **4v** in 45% yield (52 mg) as yellow oil. ^1H NMR (500 MHz, CDCl_3) δ 7.21 (d, $J = 7.1$ Hz, 1H), 7.15 – 7.06 (m, 3H), 2.97 – 2.93 (m, 2H), 2.70 (dd, $J = 9.7, 4.1$ Hz, 1H), 2.39 – 2.29 (m, 1H), 2.15 – 2.08 (m, 1H), 0.96 (t, $J = 8.0$ Hz, 9H), 0.64 (q, $J = 7.9$ Hz, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 146.7, 143.5, 125.8, 124.6, 124.3, 123.6, 33.0, 31.2, 27.4, 7.6, 2.8.

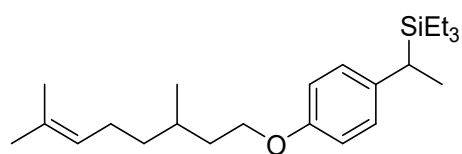
Triethyl(1-(3,5,5,6,8,8-hexamethyl-5,6,7,8-tetrahydronaphthalen-2-yl)ethyl)silane (4aa)



According to the general procedure C, the reaction gave **4aa** in 71% yield (127 mg) as colorless oil. ^1H NMR (500 MHz, CDCl_3) δ 7.07 (d, $J = 4.4$ Hz, 1H), 7.03 (s, 1H), 2.48 (qd, $J = 7.5, 1.6$ Hz, 1H), 2.26 (s, 3H), 1.92 – 1.84 (m, 1H), 1.65 (td, $J = 13.1, 4.7$ Hz, 1H), 1.40 – 1.25 (m, 13H), 1.03 (dd, $J = 27.6, 12.3$ Hz, 6H), 0.89 (td, $J = 7.9, 3.0$ Hz, 9H), 0.57 (tt, $J = 13.5, 6.9$ Hz, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 141.7, 141.4, 131.1, 129.7, 128.2, 124.7, 44.0, 37.1, 34.7, 32.3, 29.8, 28.9, 28.4, 26.7,

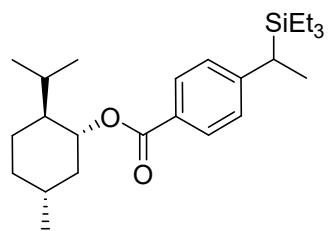
25.1, 21.2, 20.1, 16.9, 16.6, 7.5, 2.5. **HRMS** (ESI-quadrupole) m/z : $[M+H]^+$ Calcd. For $C_{24}H_{43}Si$ 359.3129; found: 359.3127.

(1-(4-((3,7-dimethyloct-6-en-1-yl)oxy)phenyl)ethyl)triethylsilane (4ab)



According to the general procedure C, the reaction gave **4ab** in 58% yield (108 mg) as colorless oil. **1H NMR** (500 MHz, $CDCl_3$) δ 6.98 (d, $J = 8.5$ Hz, 2H), 6.80 (d, $J = 8.7$ Hz, 2H), 5.12 (t, $J = 6.6$ Hz, 1H), 4.0 – 3.94 (m, 2H), 2.24 (q, $J = 7.6$ Hz, 1H), 2.06 – 1.98 (m, 2H), 1.85 – 1.81 (m, 1H), 1.70 (s, 3H), 1.62 (s, 3H), 1.43 – 1.39 (m, 1H), 1.35 (d, $J = 7.6$ Hz, 3H), 1.30 – 1.21 (m, 2H), 0.96 (d, $J = 6.8$ Hz, 3H), 0.90 (t, $J = 7.9$ Hz, 9H), 0.67 (t, $J = 8.0$ Hz, 1H), 0.52 (q, $J = 7.9$ Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 154.1, 136.0, 129.1, 125.7, 122.6, 112.1, 64.2, 35.1, 34.2, 27.5, 23.6, 23.6, 23.4, 17.5, 15.6, 13.6, 5.4, 0.0. **HRMS** (ESI-quadrupole) m/z : $[M+H]^+$ Calcd. For $C_{24}H_{43}OSi$ 375.3078; found: 375.3079.

(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 4-(1-(triethylsilyl)ethyl)benzoate (4ac)

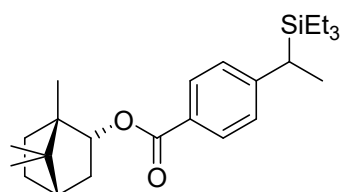


According to the general procedure C, the reaction gave **4ac** in 84% yield (168 mg) as yellow oil. **1H NMR** (500 MHz, $CDCl_3$) δ 7.91 (d, $J = 8.0$ Hz, 2H), 7.12 (d, $J = 8.1$ Hz, 2H), 4.91 (m, 1H), 2.40 (q, $J = 7.5$ Hz, 1H), 2.13 (d, $J = 12.3$ Hz, 1H), 1.99 (m, 1H), 1.73 (d, $J = 11.2$ Hz, 2H), 1.60 – 1.48 (m, 2H), 1.39 (d, $J = 7.5$ Hz, 3H), 1.18 – 1.04 (m, 2H), 0.95 – 0.83 (m, 16H), 0.80 (d, $J = 6.9$ Hz, 3H), 0.52 (q, $J = 7.9$ Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 166.3, 152.2, 129.4, 126.9, 126.8, 74.4, 47.3, 41.0, 34.4, 31.4, 27.6, 26.4, 23.6, 22.0, 20.8, 16.5, 15.1, 7.4, 2.0. **HRMS** (ESI-quadrupole) m/z : $[M+H]^+$ Calcd. For $C_{25}H_{43}O_2Si$ 403.3027; found: 403.3023.

(1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl

4-(1-

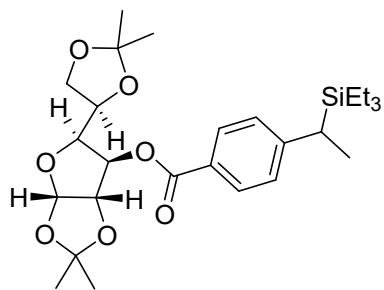
(triethylsilyl)ethyl)benzoate (4ad)



According to the general procedure C, the reaction gave **4ad** in 80% yield (160 mg) as white solid. m.p. 38.5 –

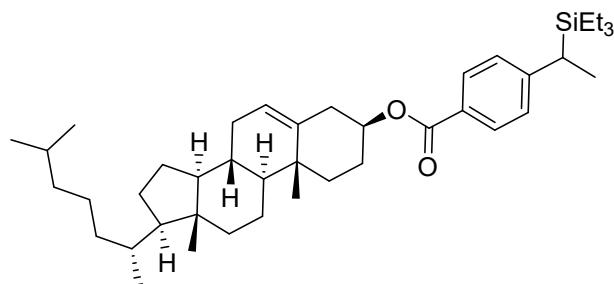
38.9 °C. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.95 (d, $J = 8.3$ Hz, 2H), 7.16 (d, $J = 8.3$ Hz, 2H), 5.13 – 5.09 (m, 1H), 2.52 – 2.40 (m, 2H), 2.21 – 2.14 (m, 1H), 1.84 – 1.79 (m, 1H), 1.75 (t, $J = 4.5$ Hz, 1H), 1.62 (s, 2H), 1.42 (d, $J = 7.5$ Hz, 3H), 1.13 (dd, $J = 13.8, 3.4$ Hz, 1H), 0.99 (s, 3H), 0.94 – 0.90 (m, 15H), 0.57 – 0.51 (m, 6H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 167.0, 152.3, 129.3, 126.9, 126.8, 80.1, 49.0, 47.8, 45.0, 36.9, 28.1, 27.6, 27.4, 19.7, 18.9, 15.1, 13.6, 7.5, 2.0. **HRMS** (ESI-quadrupole) m/z : $[\text{M}+\text{H}]^+$ Calcd. For $\text{C}_{25}\text{H}_{41}\text{O}_2\text{Si}$ 401.2870; found: 401.2879.

(3aS,5S,6R,6aS)-5-((R)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-d][1,3]dioxol-6-yl 4-(1-(triethylsilyl)ethyl)benzoate (4ae)



According to the general procedure C, the reaction gave **4ae** in 43% yield (109 mg) as yellow oil. $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.91 (d, $J = 8.3$ Hz, 2H), 7.16 (d, $J = 8.3$ Hz, 2H), 5.97 (d, $J = 3.6$ Hz, 1H), 5.50 (d, $J = 2.6$ Hz, 1H), 4.65 (d, $J = 3.7$ Hz, 1H), 4.43 – 4.35 (m, 2H), 4.14 (dd, $J = 11.3, 6.1$ Hz, 2H), 2.44 (q, $J = 7.4$ Hz, 1H), 1.59 (d, $J = 10.0$ Hz, 6H), 1.44 – 1.41 (m, 5H), 1.34 (s, 3H), 1.30 (s, 3H), 0.91 (t, $J = 7.9$ Hz, 8H), 0.53 (q, $J = 8.0$ Hz, 5H). $^{13}\text{C NMR}$ (126 MHz, CDCl_3) δ 165.1, 152.9, 129.7, 129.5, 127.1, 125.3, 12.3, 109.3, 105.1, 83.4, 79.9, 72.6, 70.1, 67.2, 26.8, 26.7, 26.2, 25.2, 7.4, 6.7, 4.7, 1.9. **HRMS** (ESI-quadrupole) m/z : $[\text{M}+\text{H}]^+$ Calcd. For $\text{C}_{27}\text{H}_{43}\text{O}_7\text{Si}$ 507.2773; found: 507.2782.

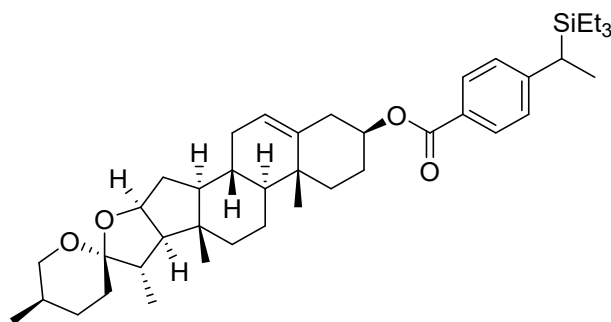
(3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 4-(1-(triethylsilyl)ethyl)benzoate (4af)



According to the general procedure C, the reaction gave **4af** in 53% yield (167 mg) as yellow oil. $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.92 (d,

$J = 7.9$ Hz, 2H), 7.32 (d, $J = 8.1$ Hz, 2H), 5.34 (d, $J = 5.0$ Hz, 1H), 4.83 (q, $J = 6.4$ Hz, 1H), 2.38 (d, $J = 8.2$ Hz, 2H), 2.25 – 2.13 (m, 1H), 1.93 (td, $J = 13.5, 12.8, 7.1$ Hz, 3H), 1.84 (d, $J = 13.7$ Hz, 1H), 1.79 – 1.74 (m, 1H), 1.51 (s, 3H), 1.42 (td, $J = 15.9, 14.9, 6.0$ Hz, 6H), 1.34 (d, $J = 6.4$ Hz, 3H), 1.27 (d, $J = 8.9$ Hz, 4H), 1.19 (d, $J = 9.3$ Hz, 3H), 1.10 – 1.03 (m, 4H), 0.99 (s, 3H), 0.93 (d, $J = 6.3$ Hz, 3H), 0.84 (d, $J = 8.2$ Hz, 9H), 0.79 (d, $J = 6.7$ Hz, 6H), 0.62 (s, 3H), 0.49 (p, $J = 7.4$ Hz, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 166.0, 152.0, 139.7, 129.5, 129.3, 125.0, 122.7, 74.4, 70.2, 56.7, 56.1, 50.0, 42.3, 39.7, 39.5, 38.2, 37.0, 36.6, 36.2, 31.9, 31.9, 28.2, 28.2, 28.0, 27.9, 27.1, 24.3, 23.8, 22.8, 22.6, 21.0, 19.4, 18.7, 11.8, 6.8, 4.8. HRMS (ESI-quadrupole) m/z : $[\text{M}+\text{H}]^+$ Calcd. For $\text{C}_{42}\text{H}_{69}\text{O}_2\text{Si}$ 633.5061; found: 633.5054.

(4S,5'R,6aR,6bS,8aS,8bR,9S,10R,11aS,12aS,12bS)-5',6a,8a,9-tetramethyl-1,3,3',4,4',5,5',6,6a,6b,6',7,8,8a,8b,9,11a,12,12a,12b-icosahydrospiro[naphtho[2',1':4,5]indeno[2,1-b]furan-10,2'-pyran]-4-yl 4-(1-(triethylsilyl)ethyl)benzoate (4ag)

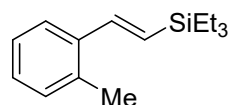


According to the general procedure C, the reaction gave **4ag** in 38% yield (125 mg) as white solid. m.p. 101.2 – 101.7 °C. ^1H NMR (500 MHz, CDCl_3) δ 7.91 (d, $J = 8.3$ Hz, 2H), 7.32 (d, $J = 8.3$ Hz, 2H), 5.37 –

5.31 (m, 1H), 4.82 (q, $J = 6.4$ Hz, 1H), 4.34 (q, $J = 7.5$ Hz, 1H), 3.40 (m, $J = 11.0, 4.5, 2.1$ Hz, 1H), 3.30 (t, $J = 10.9$ Hz, 1H), 2.38 (d, $J = 6.8$ Hz, 2H), 1.92 (m, $J = 12.3, 6.9, 5.6, 2.4$ Hz, 4H), 1.85 – 1.77 (m, 2H), 1.74 – 1.65 (m, 3H), 1.62 – 1.51 (m, 6H), 1.43 – 1.38 (m, 2H), 1.34 (d, $J = 6.4$ Hz, 3H), 1.22 – 1.11 (m, 4H), 1.11 – 1.02 (m, 2H), 1.01 (s, 3H), 0.90 (d, $J = 6.9$ Hz, 3H), 0.83 (t, $J = 7.9$ Hz, 9H), 0.73 – 0.70 (m, 6H), 0.49 (m, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 166.0, 152.0, 139.8, 129.5, 129.3, 125.1, 122.5, 109.3, 80.8, 74.3, 70.3, 66.9, 62.1, 56.5, 50.0, 41.6, 40.3, 39.8, 38.2, 37.0, 36.8, 32.1, 31.9, 31.5, 31.4, 30.3, 28.8, 27.9, 27.2, 20.9, 19.4, 17.2, 16.3, 14.6, 6.8, 4.8. HRMS (ESI-quadrupole) m/z : $[\text{M}+\text{H}]^+$ Calcd. For $\text{C}_{42}\text{H}_{65}\text{O}_4\text{Si}$ 661.4647; found:

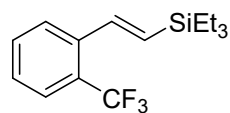
661.4645.

(E)-triethyl(2-methylstyryl)silane (5a)²⁸



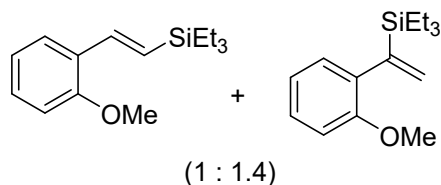
According to the general procedure D, the reaction gave **5a** in 69% yield (37 mg) as colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.60 – 7.52 (m, 1H), 7.23 – 7.16 (m, 4H), 6.36 (d, *J* = 19.2 Hz, 1H), 2.42 (s, 3H), 1.05 (t, *J* = 7.9 Hz, 9H), 0.68 (q, *J* = 7.9 Hz, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 142.8, 138.0, 135.1, 130.2, 127.8, 127.6, 126.1, 125.3, 19.6, 7.4, 3.6.

(E)-triethyl(2-(trifluoromethyl)styryl)silane (5b)²⁸



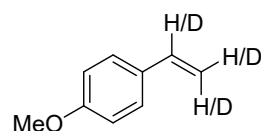
According to the general procedure D, the reaction gave **5b** in 26% yield (37 mg) as colorless oil. ¹H NMR (400 MHz, CDCl₃) δ 7.72 (d, *J* = 7.8 Hz, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.38 – 7.28 (m, 2H), 6.46 (d, *J* = 19.1 Hz, 1H), 1.02 (t, *J* = 7.9 Hz, 9H), 0.71 (q, *J* = 7.9 Hz, 6H). ¹³C NMR (126 MHz, CDCl₃) δ 148.9, 140.7, 138.1, 131.8, 131.8, 127.3, 127.2, 125.5, 125.5, 7.3, 3.4.

(E)-triethyl(2-methoxystyryl)silane (5c)²⁸



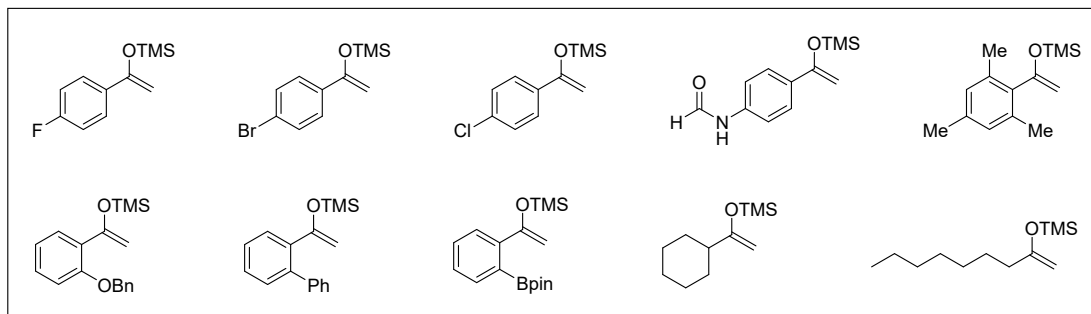
According to the general procedure D, the reaction gave **5c** in 50% yield (62 mg) as colorless oil. ¹H NMR (500 MHz, CDCl₃) δ 7.55 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.30 (d, *J* = 19.5 Hz, 1H), 7.25 – 7.15 (m, 2H), 6.97 (dd, *J* = 7.4, 1.8 Hz, 1H), 6.95 – 6.84 (m, 3H), 6.81 – 6.78 (m, 1H), 6.38 (d, *J* = 19.5 Hz, 1H), 5.79 (d, *J* = 3.3 Hz, 1H), 5.60 (d, *J* = 3.3 Hz, 1H), 3.84 (s, 3H), 3.76 (s, 4H), 0.99 (t, *J* = 7.9 Hz, 9H), 0.90 (t, *J* = 7.9 Hz, 13H), 0.66 (q, *J* = 7.9 Hz, 6H), 0.60 (q, *J* = 7.9 Hz, 9H). ¹³C NMR (126 MHz, CDCl₃) δ 156.6, 155.8, 149.1, 139.1, 135.3, 128.9, 128.8, 128.5, 127.4, 126.2, 126.1, 120.6, 120.6, 111.0, 109.8, 55.6, 54.8, 7.5, 7.4, 3.6, 3.5.

1-methoxy-4-(vinyl-d3)benzene (8)¹¹



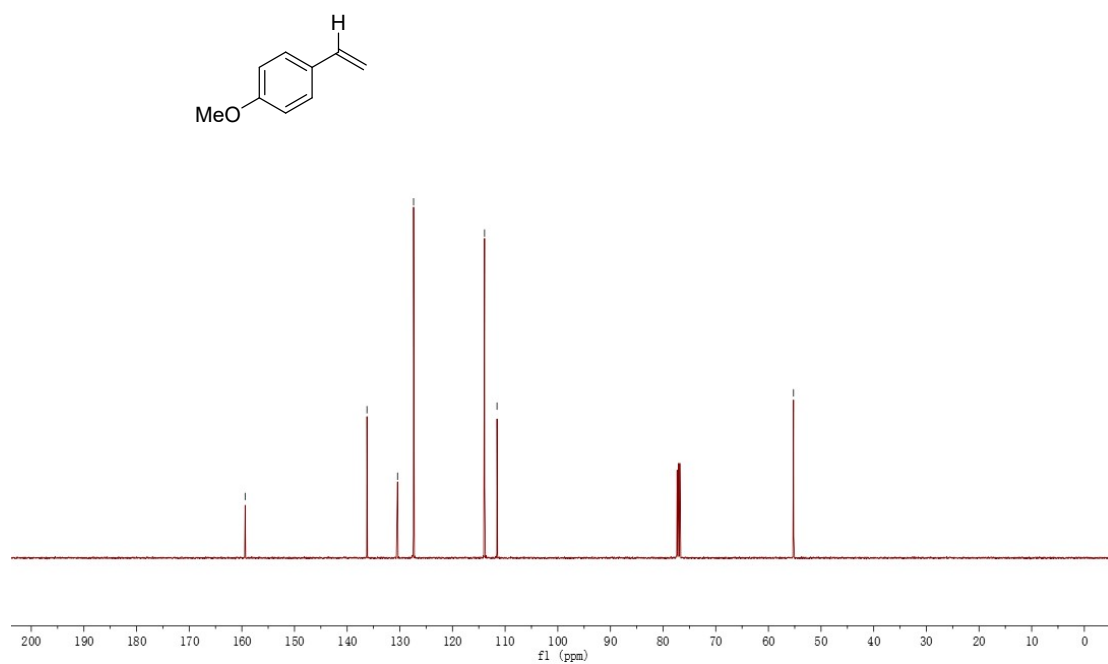
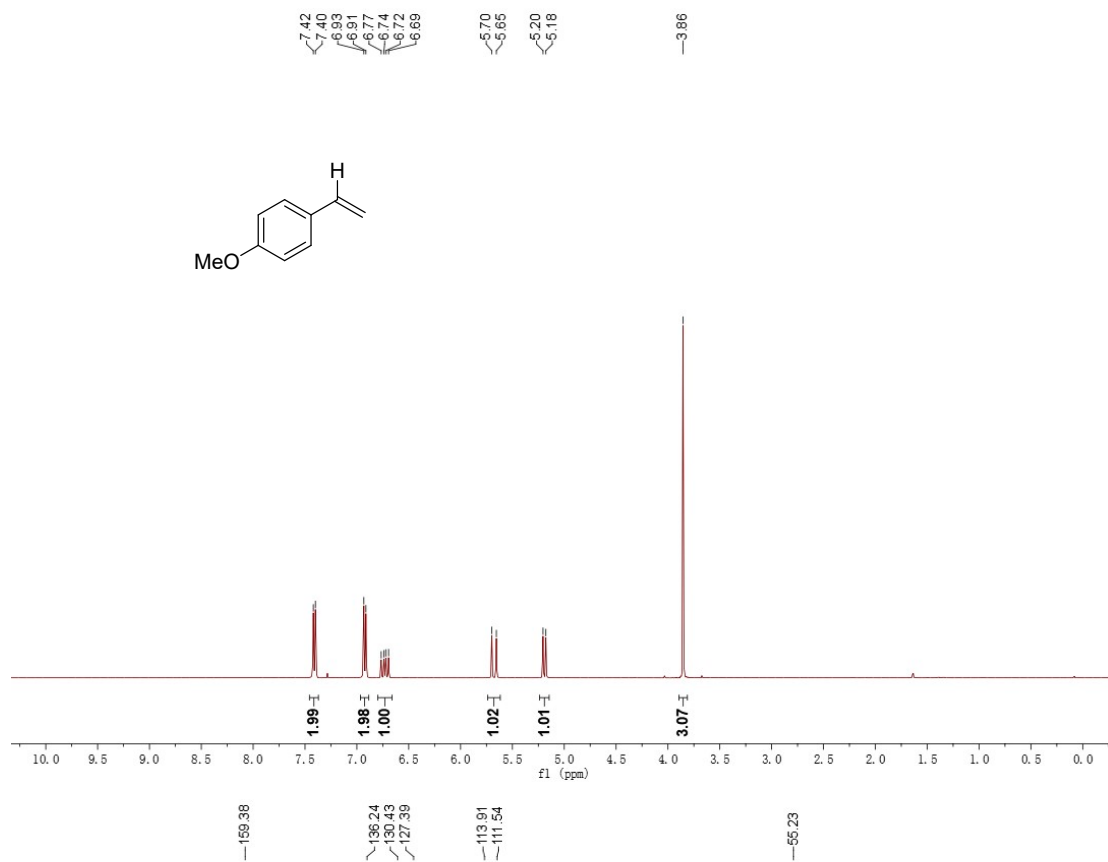
^1H NMR (500 MHz, CDCl_3) δ 7.26 (d, $J = 8.6$ Hz, 2H), 6.77 (d, $J = 8.7$ Hz, 2H), 6.62–6.52 (m, 0.52H), 5.57–5.45 (m, 0.59 H), 5.08–4.97 (m, 0.56H), 3.72 (s, 3H). **^{13}C NMR** (126 MHz, CDCl_3) δ 159.4, 136.2, 135.0, 129.7, 127.4, 113.9, 55.3.

VII. Unsuccessful substrate



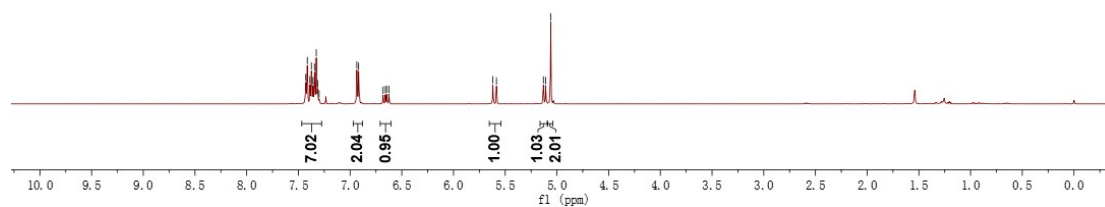
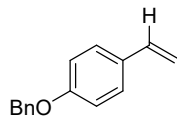
VIII. NMR Spectra of Compounds

1-methoxy-4-vinylbenzene (3c)

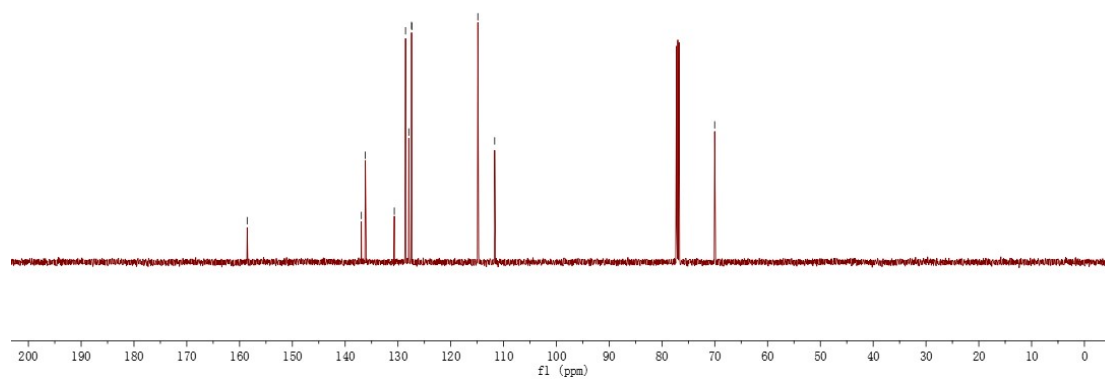
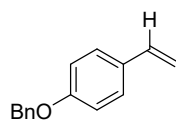


1-(benzyloxy)-4-vinylbenzene (3d)

7.43
7.41
7.39
7.37
7.36
7.34
7.33
7.31
6.93
6.92
6.66
6.65
6.62
5.62
5.56
5.13
5.06

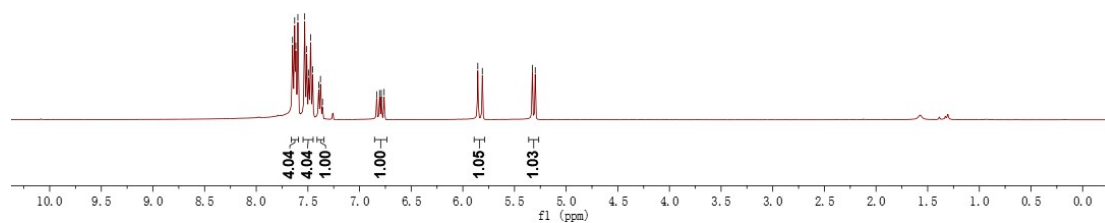
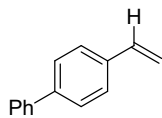


158.56
136.93
136.18
130.70
128.57
127.95
127.43
127.38
114.87
111.69
70.02

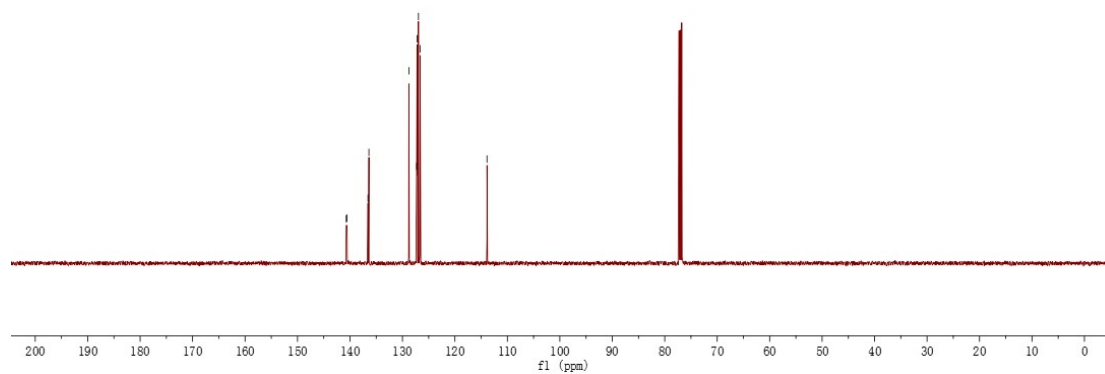
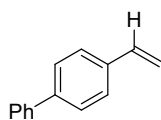


4-vinyl-1,1'-biphenyl (3e)

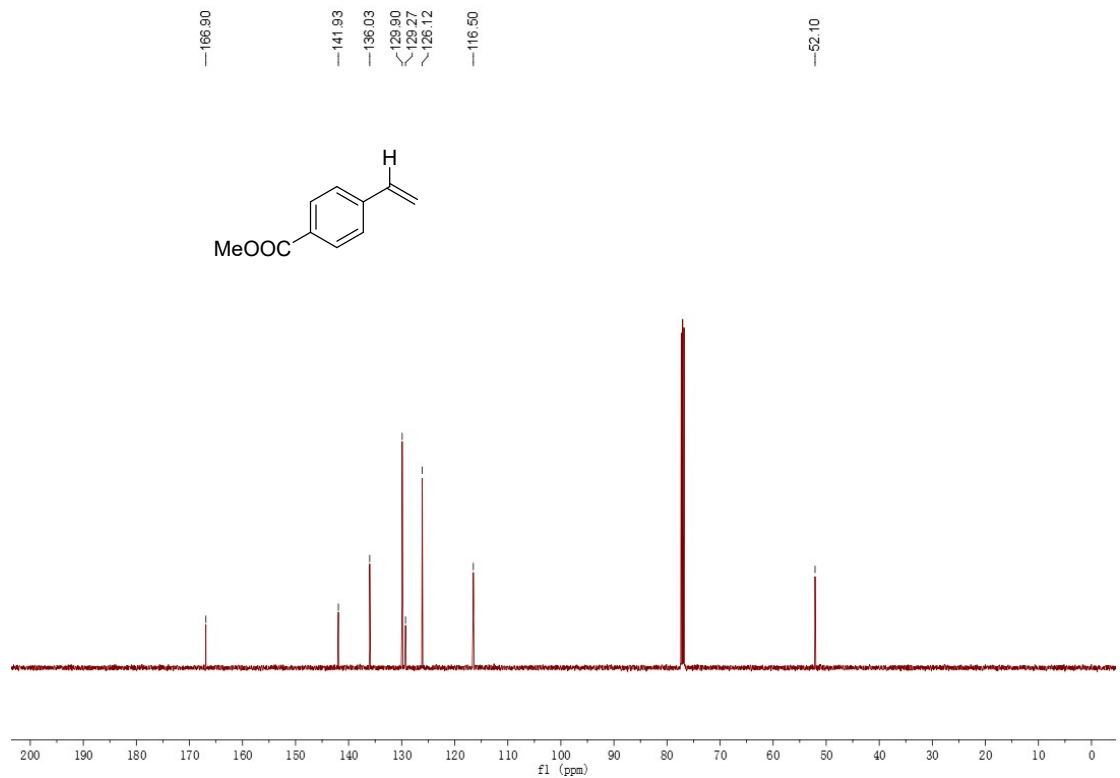
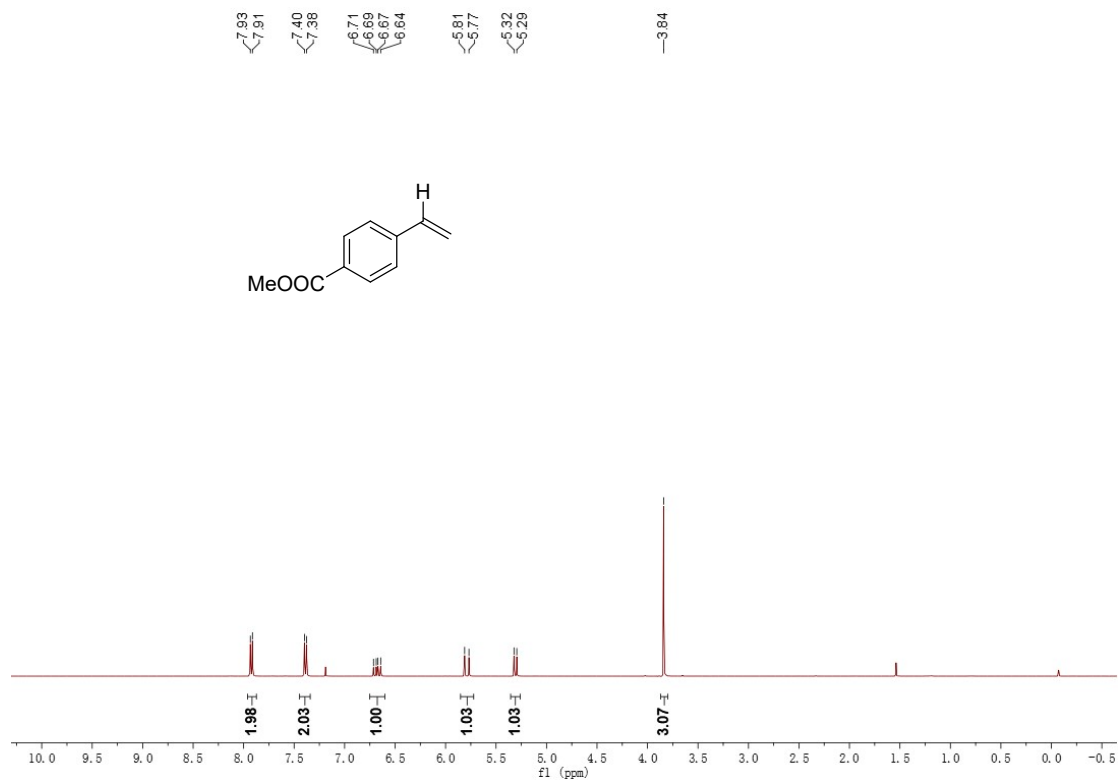
7.65
7.65
7.62
7.60
7.59
7.49
7.47
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6.83
6.81
6.79
5.86
5.81
5.33
5.30



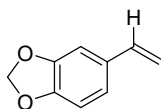
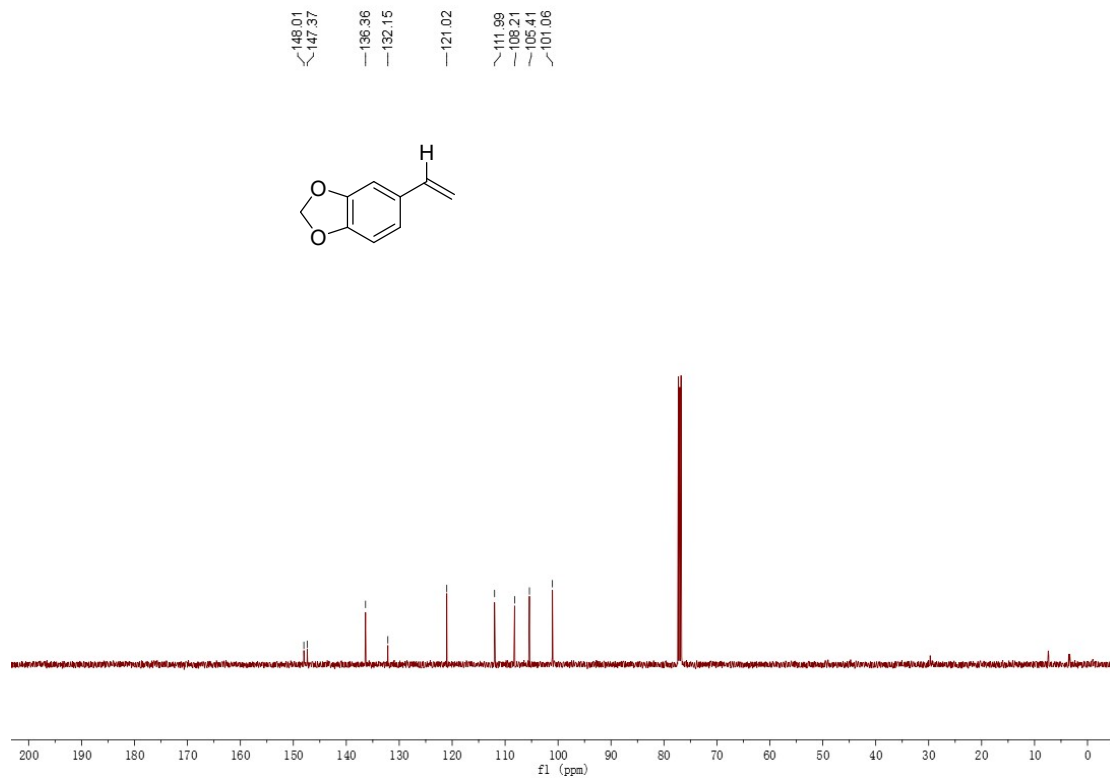
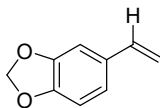
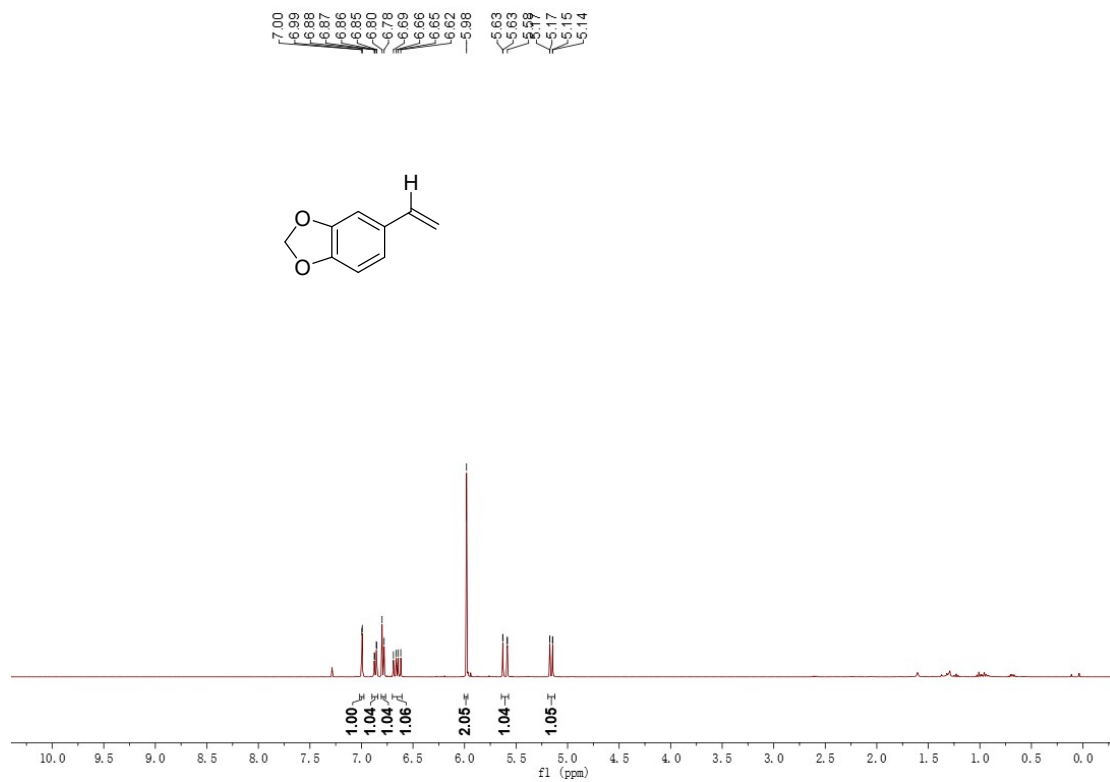
140.71
140.56
136.58
136.39
128.77
127.30
127.21
126.95
126.63
113.88



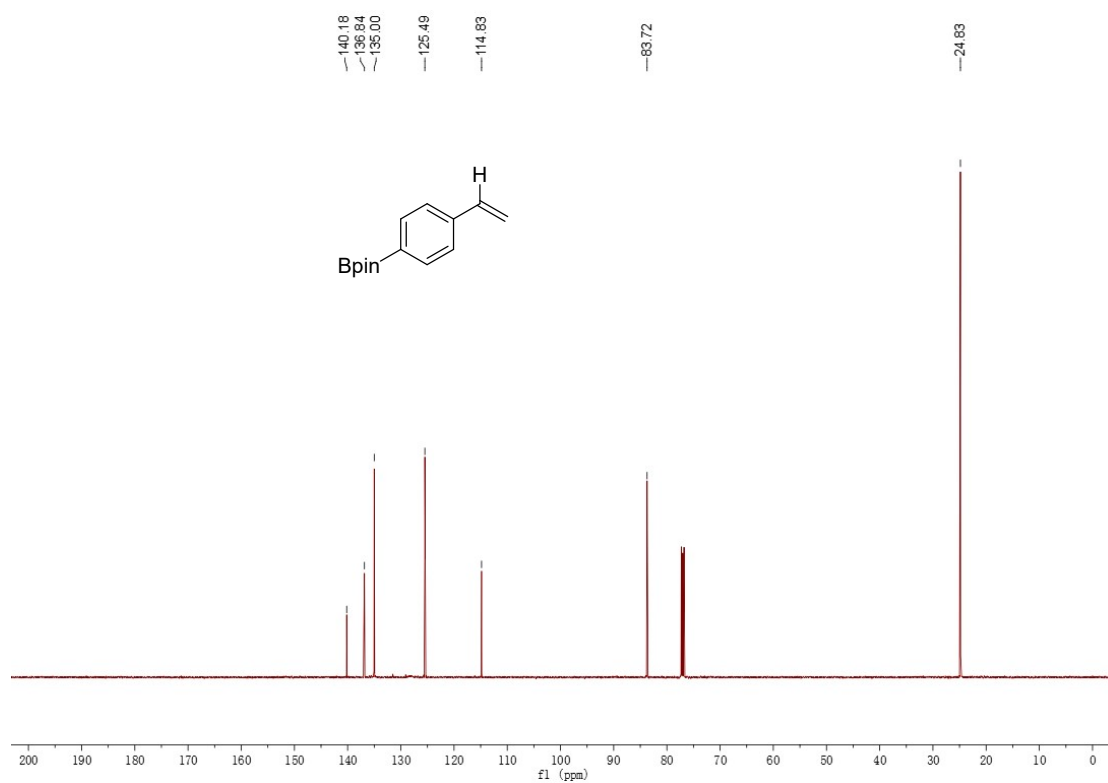
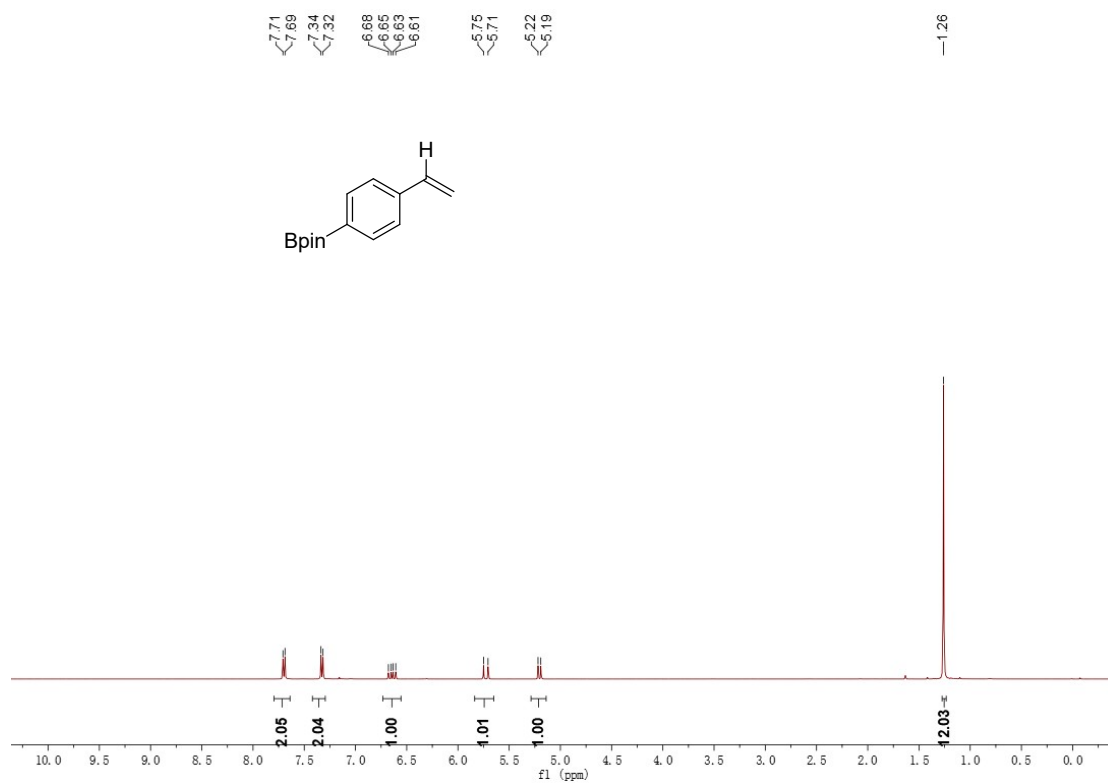
Methyl 4-vinylbenzoate (3f)



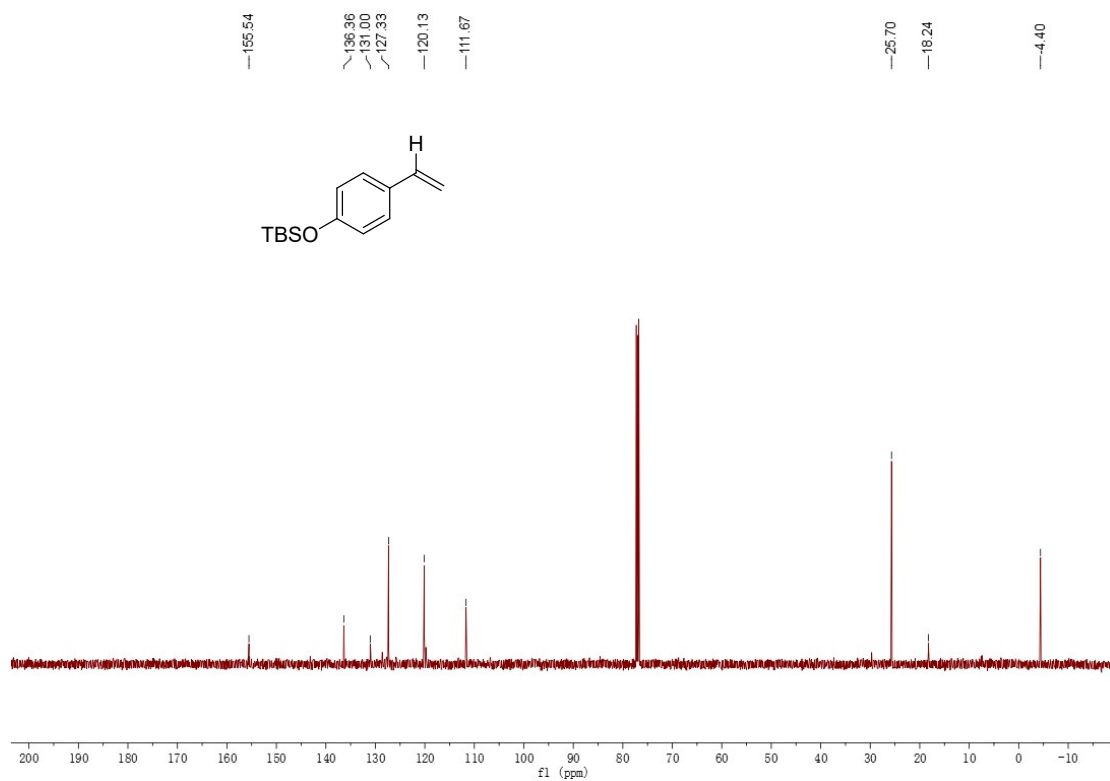
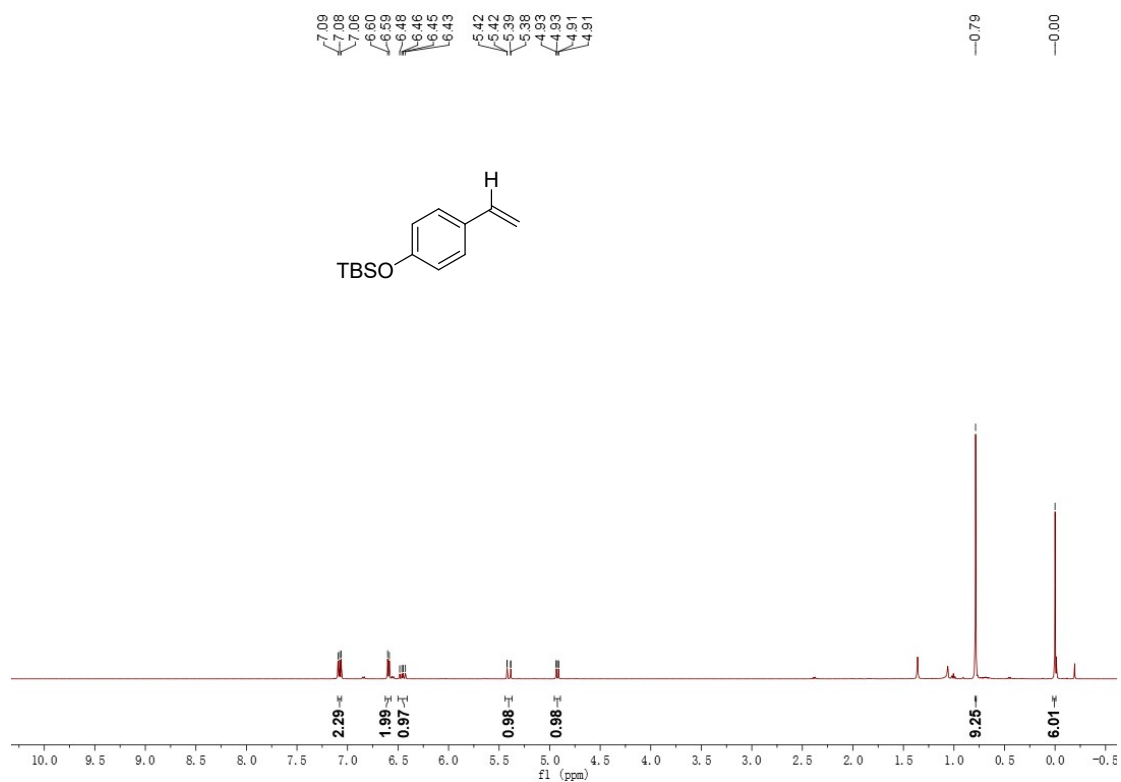
5-vinylbenzo[d][1,3]dioxole (3g)



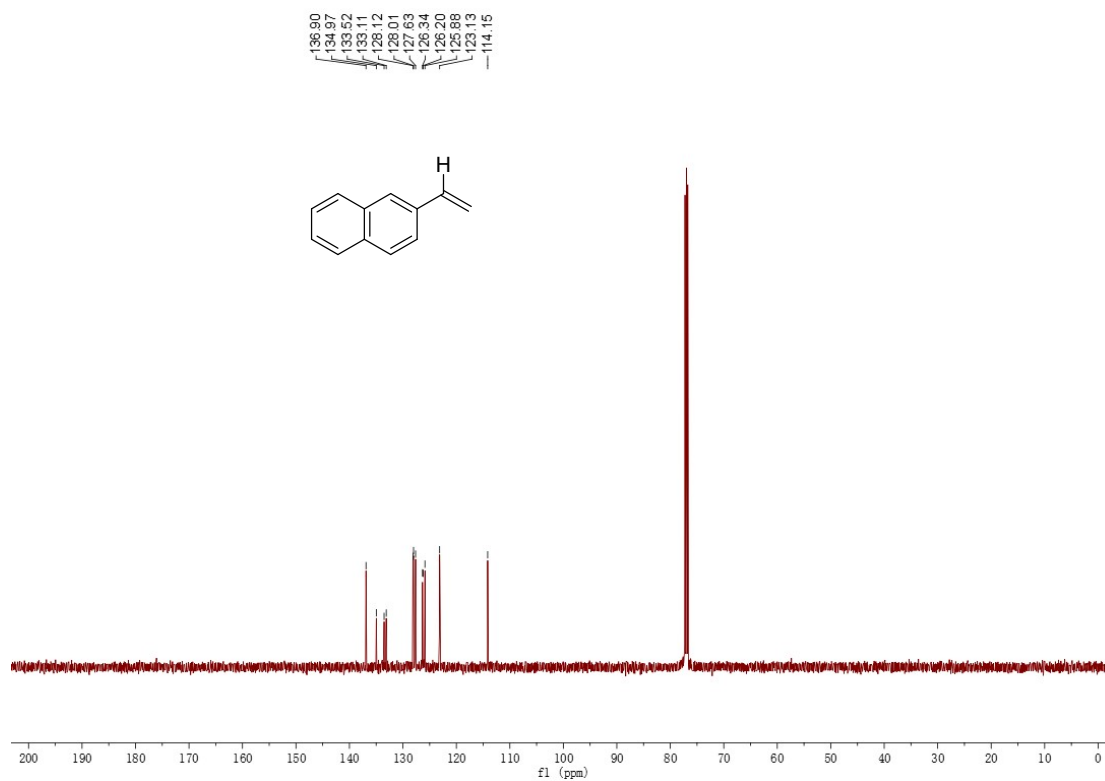
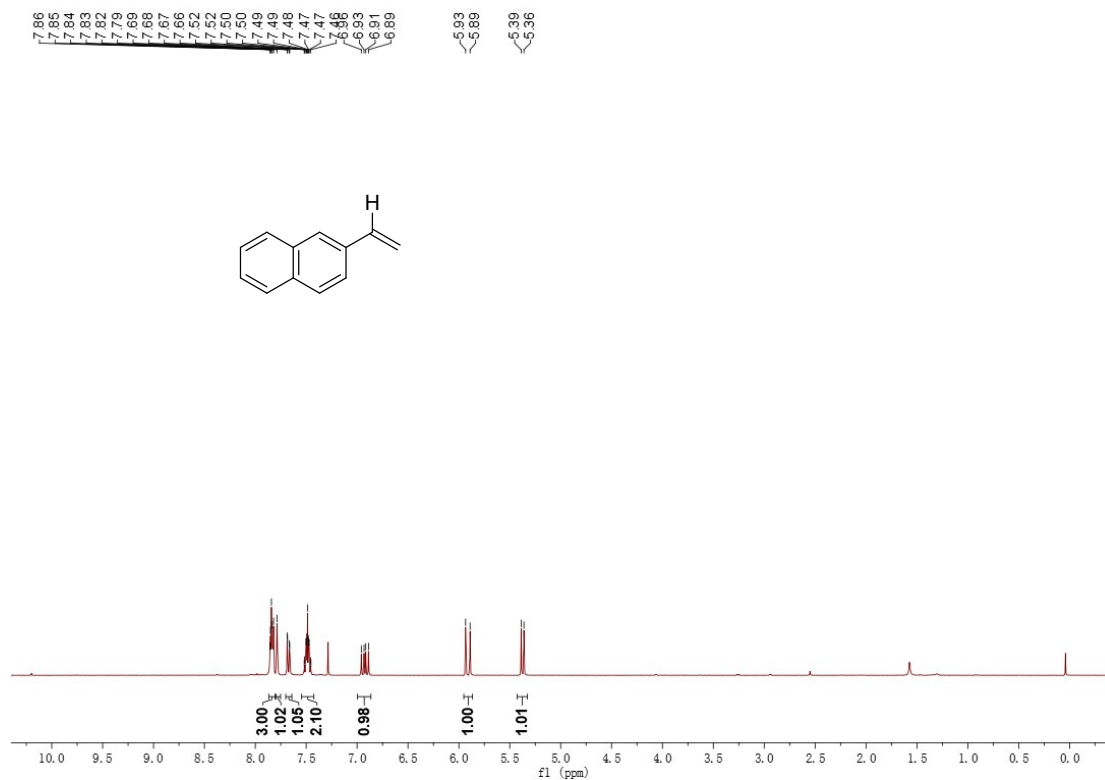
4,4,5,5-tetramethyl-2-(4-vinylphenyl)-1,3,2-dioxaborolane (3h)



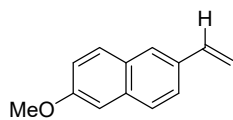
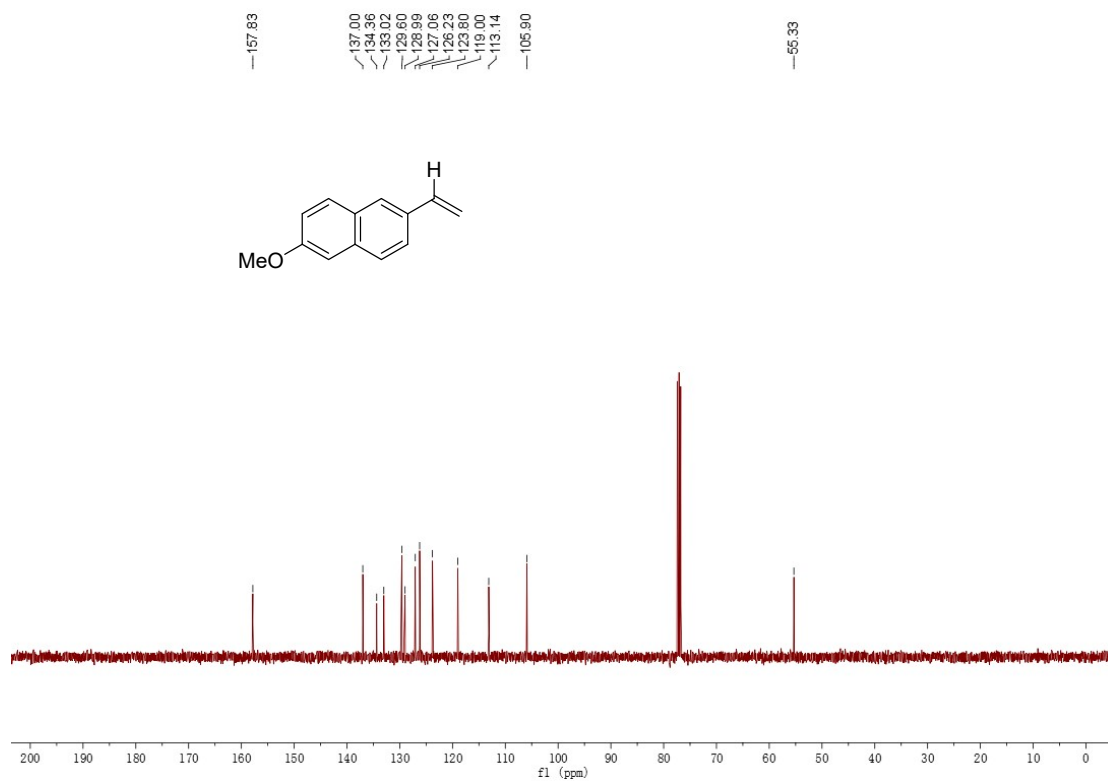
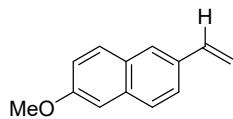
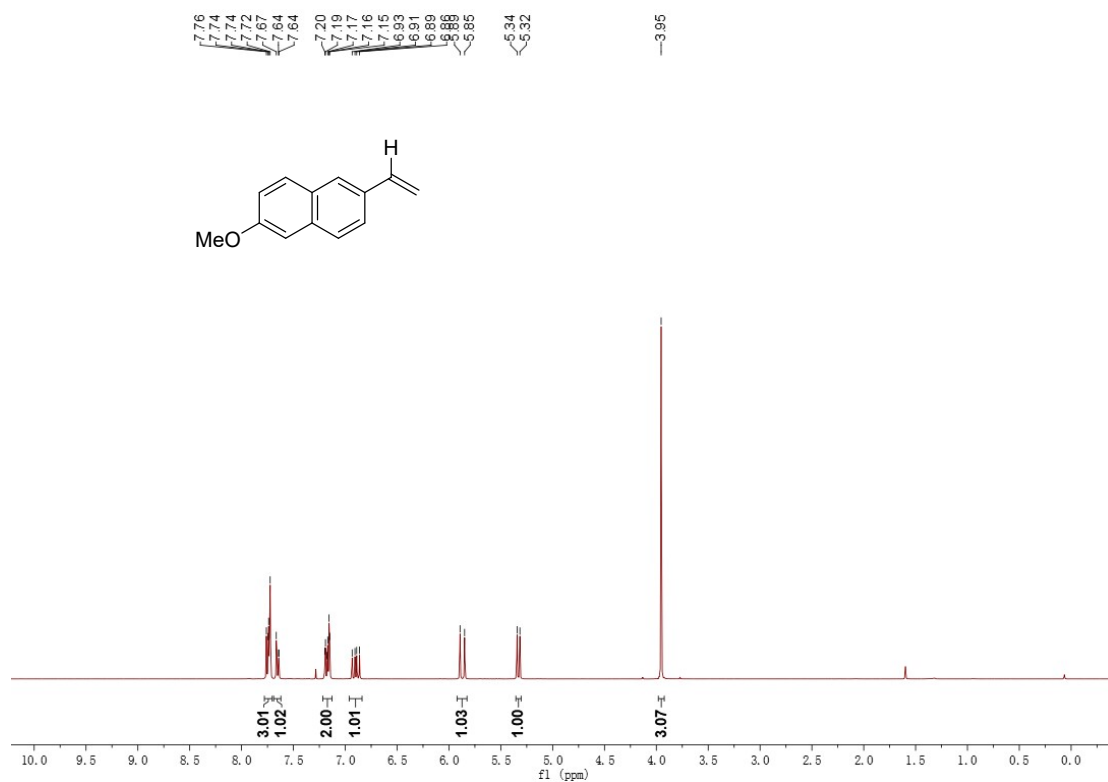
Tert-butyldimethyl(4-vinylphenoxy)silane (3i)



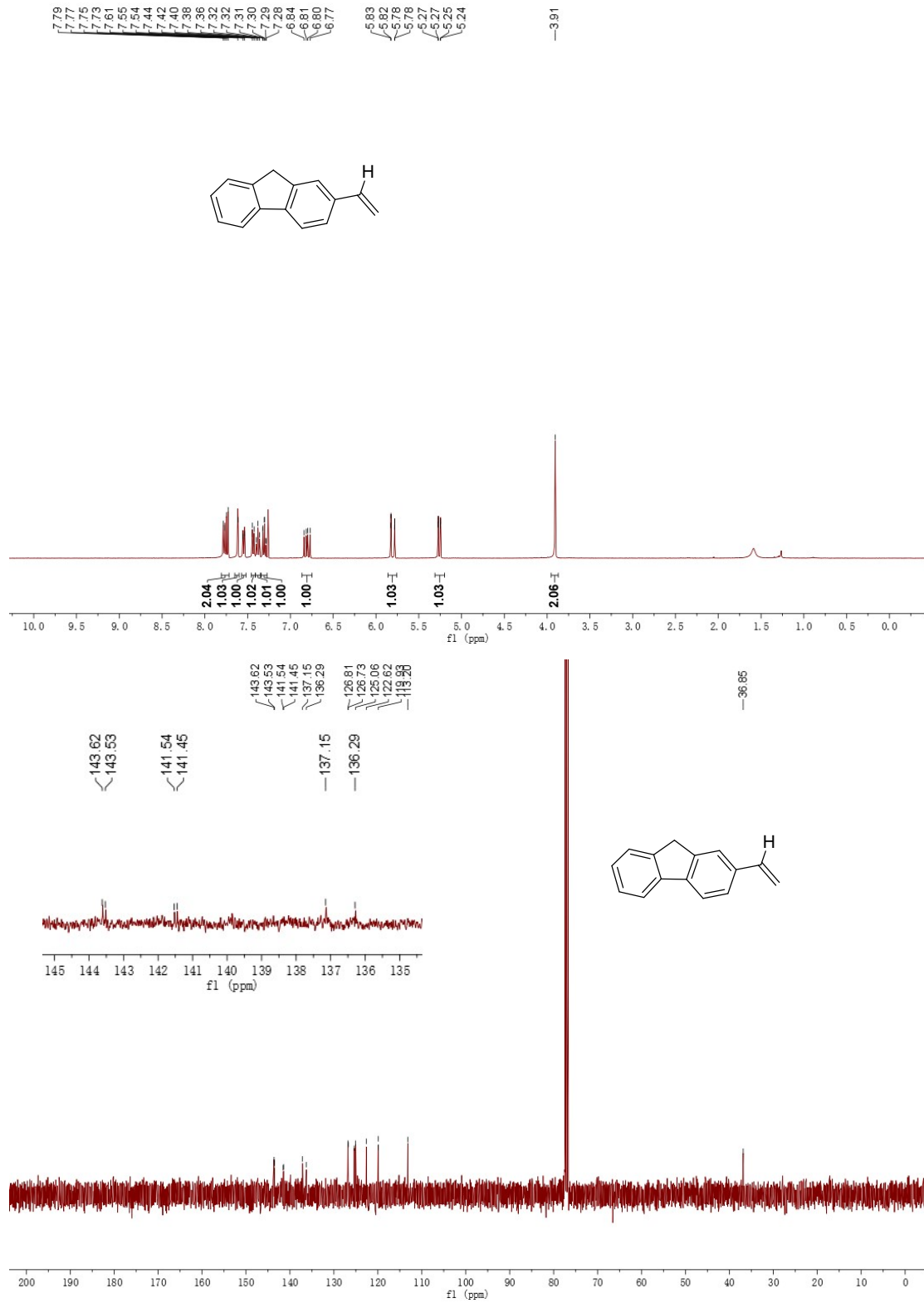
2-vinylnaphthalene (3j)



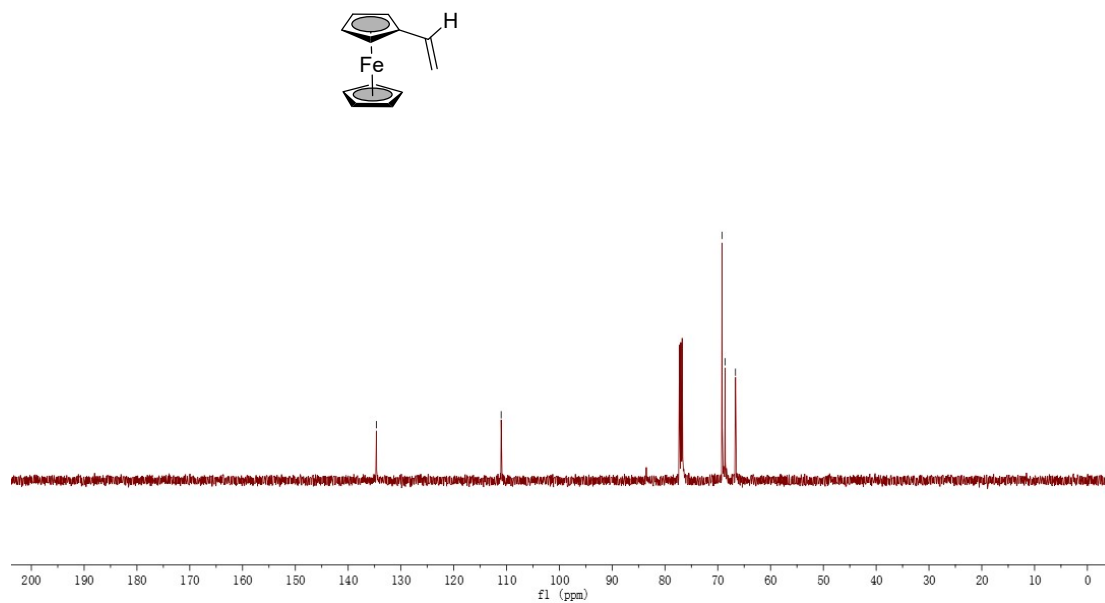
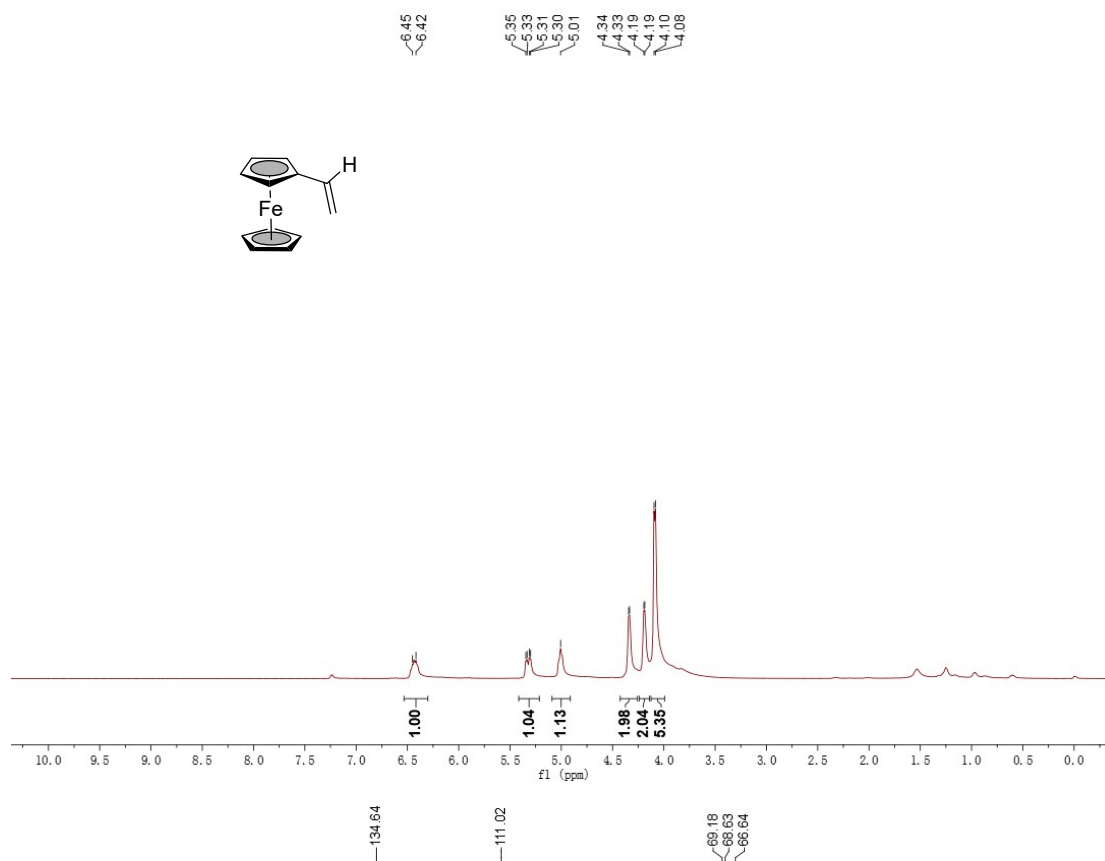
2-methoxy-6-vinylnaphthalene (3k)



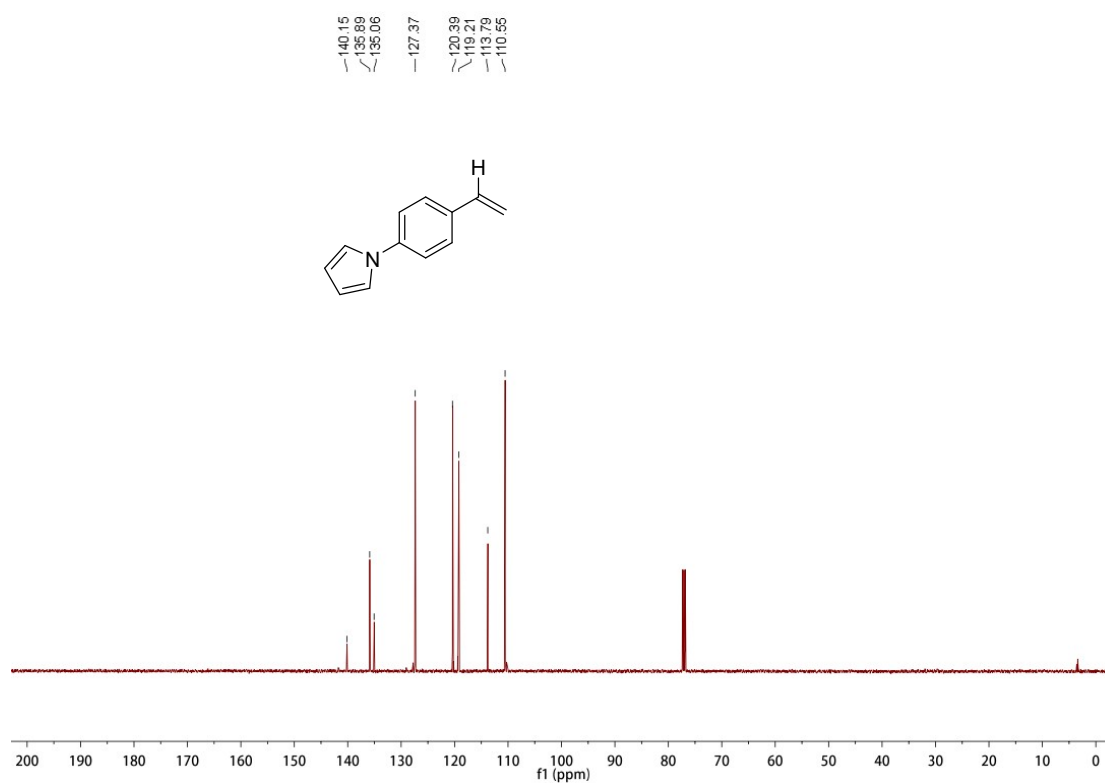
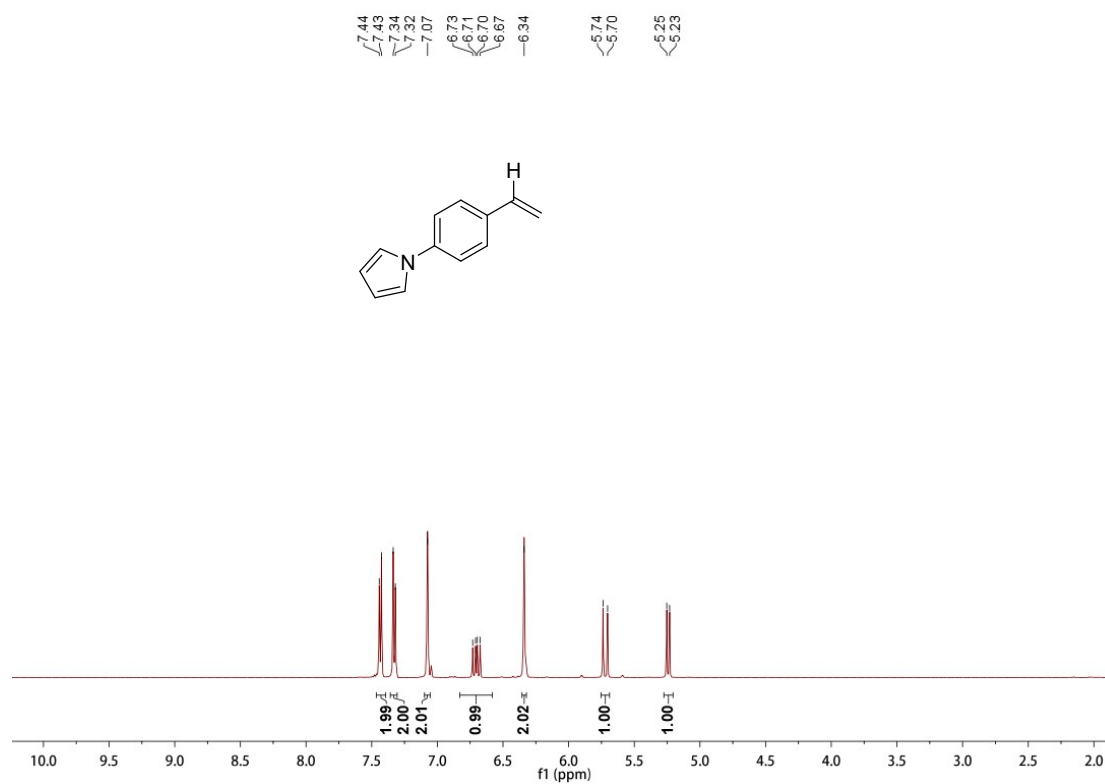
2-vinyl-9H-fluorene (3l)



Vinylferrocene (3m)



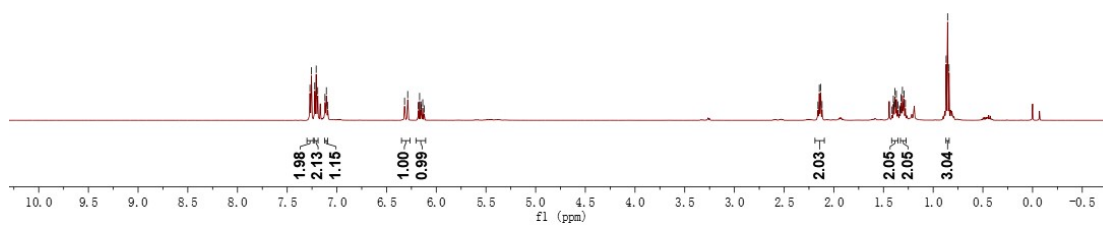
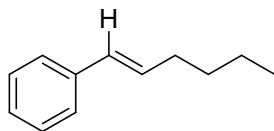
1-(4-vinylphenyl)-1H-pyrrole (3n)



(E)-hex-1-en-1-ylbenzene (3p)

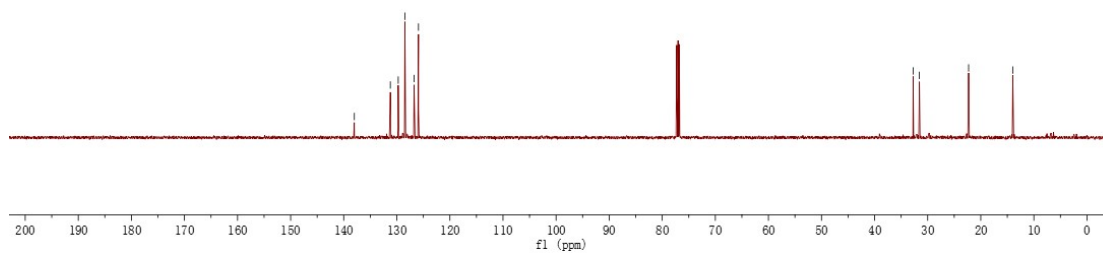
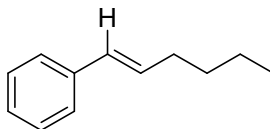
7.27
7.26
7.22
7.21
7.19
7.12
7.11
6.09
6.02
6.19
6.15
6.15
6.12

2.16
2.15
2.13
2.12
1.39
1.37
1.31
1.29
0.85
0.84

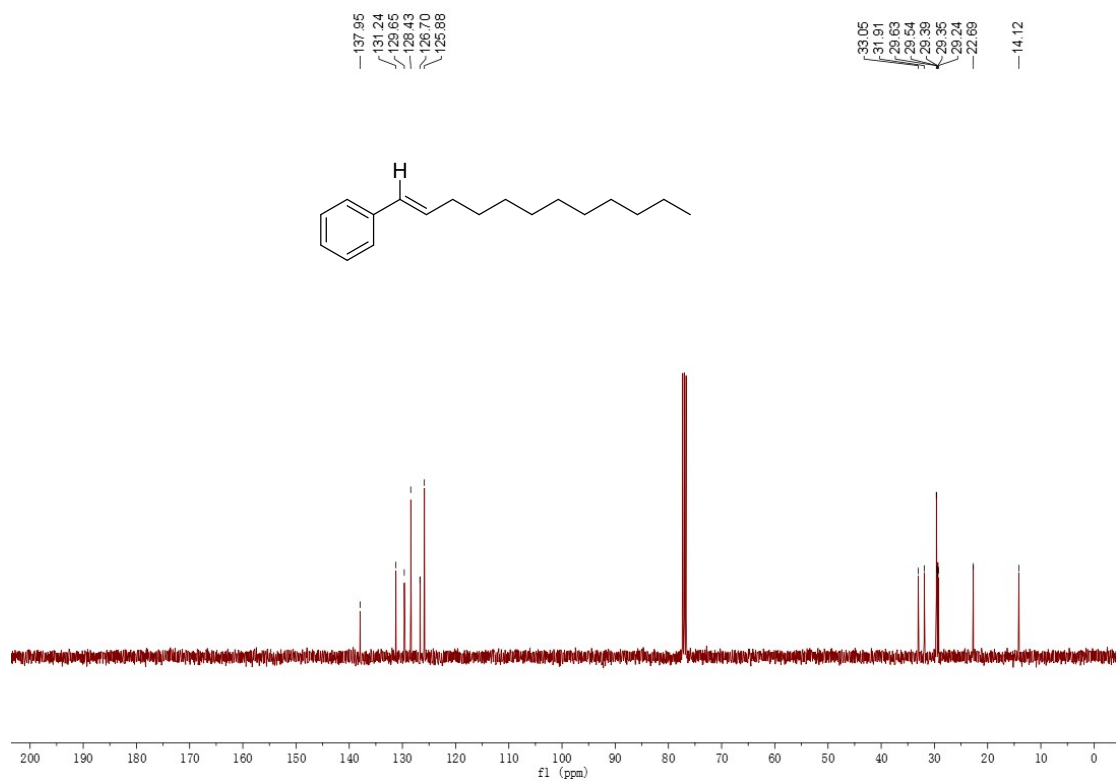
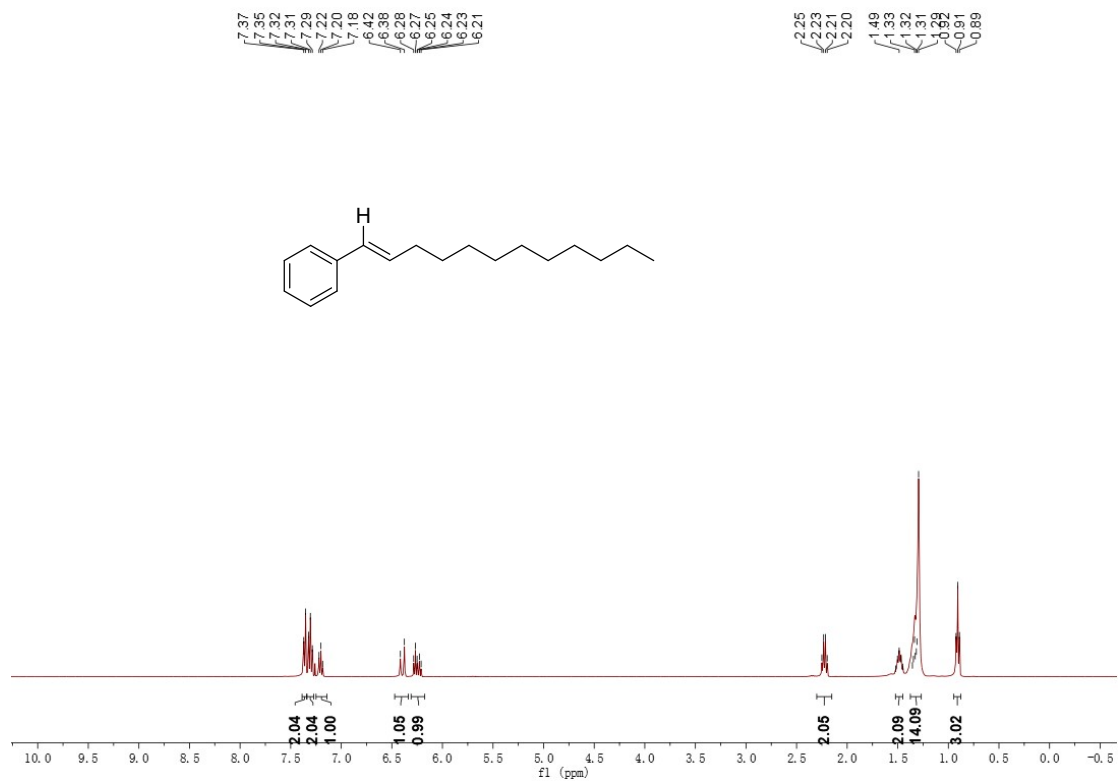


138.00
131.22
129.73
128.47
126.75
125.92

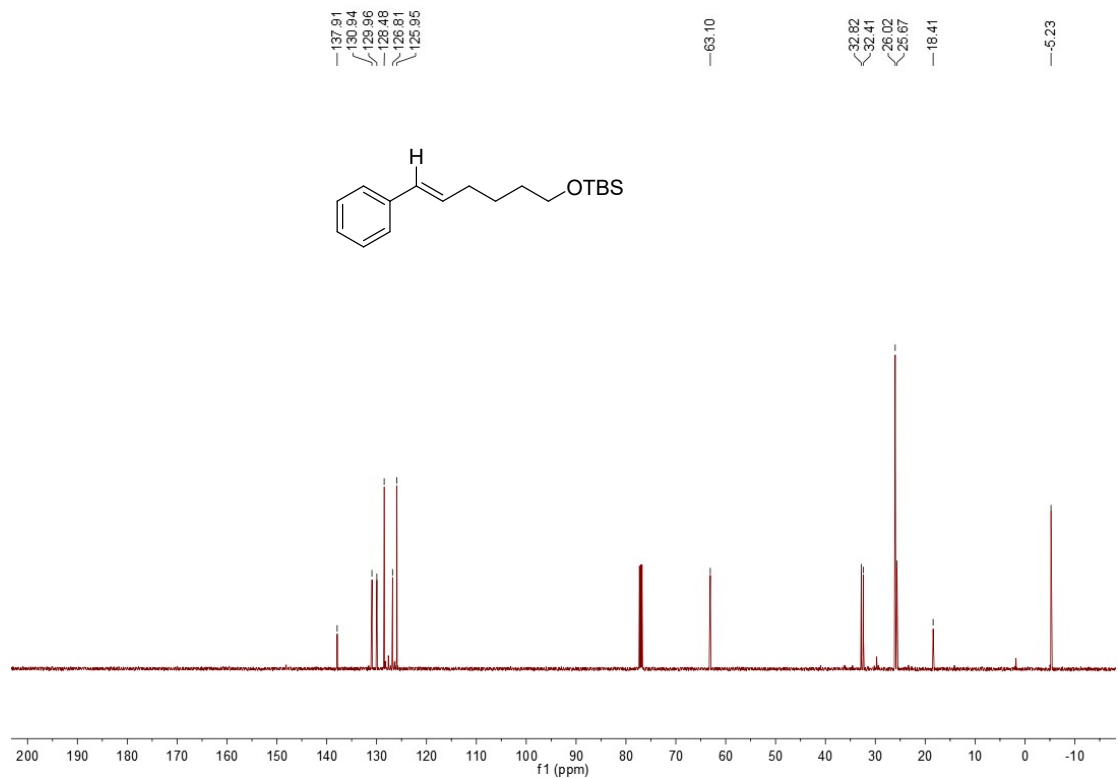
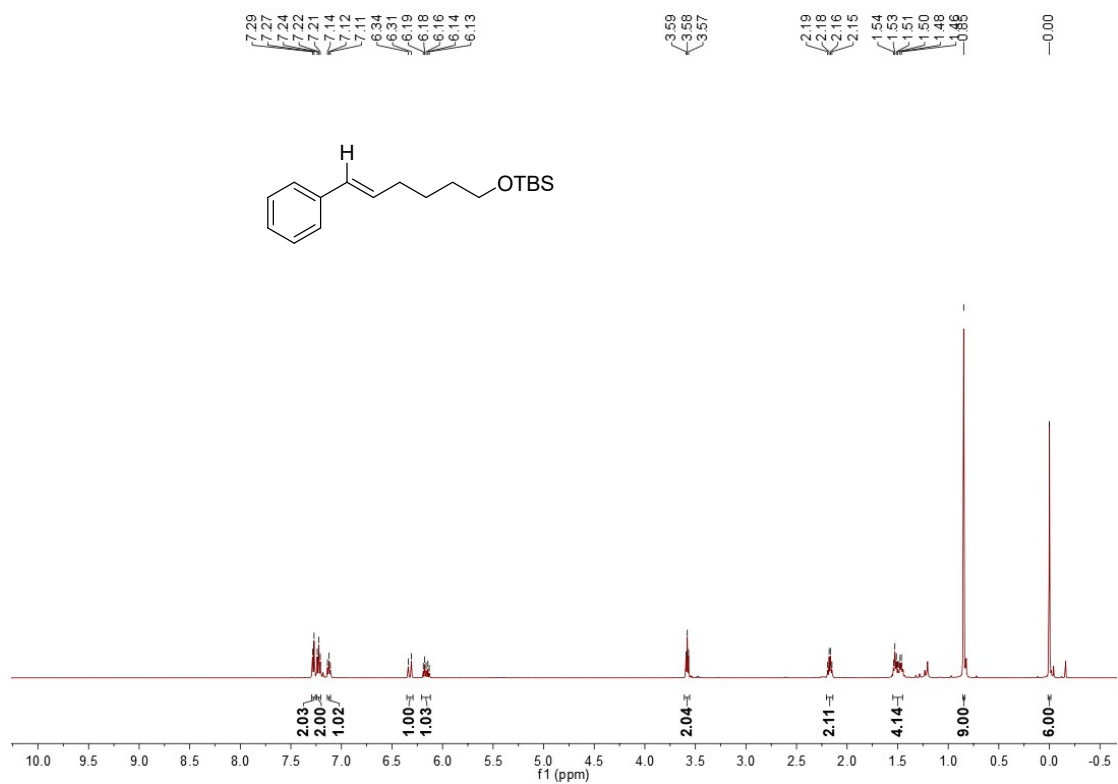
32.73
31.56
22.29
13.97



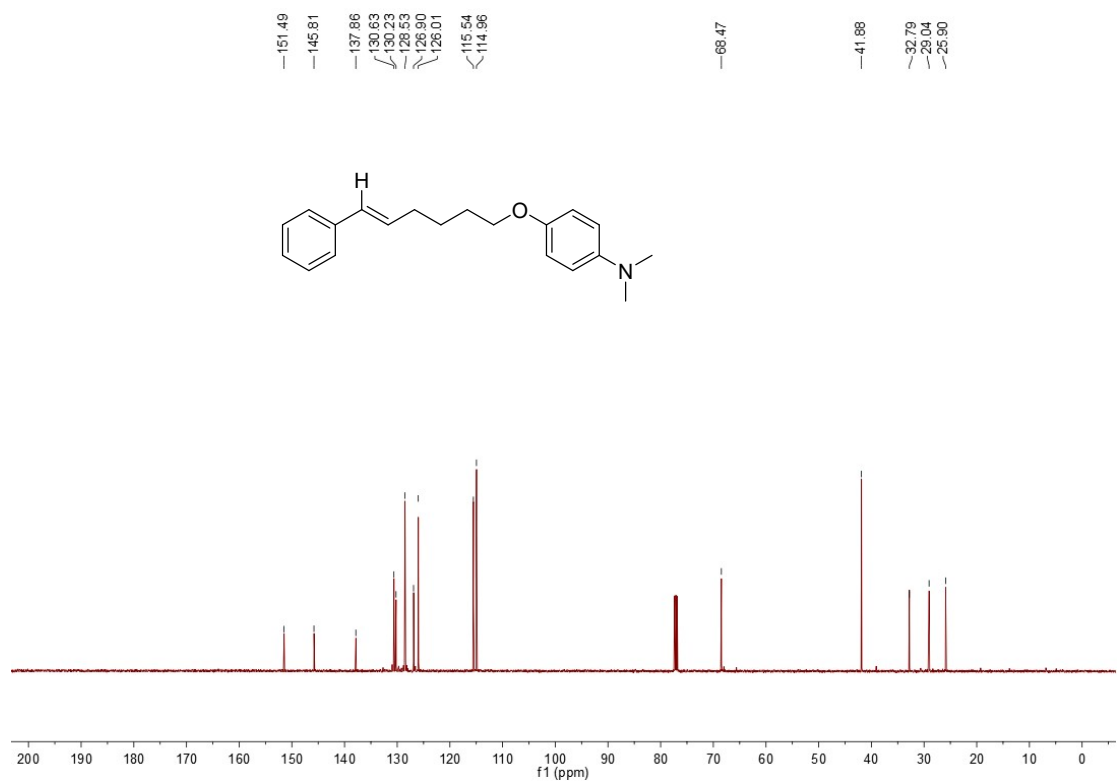
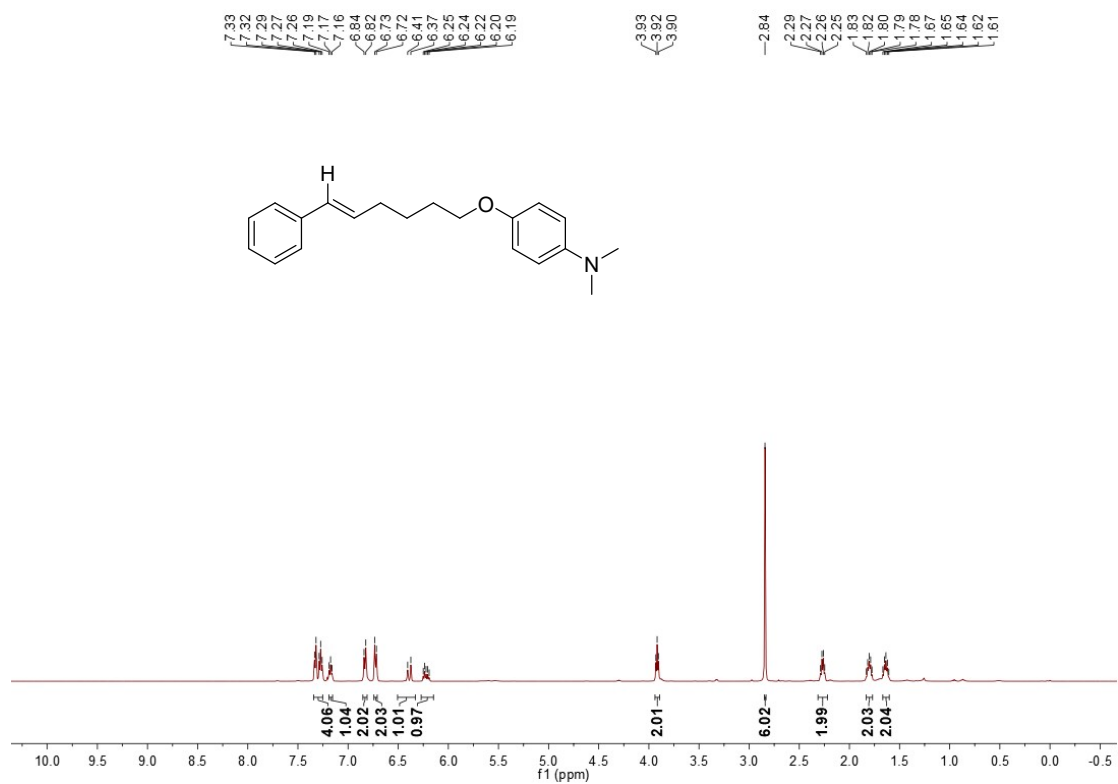
(E)-dodec-1-en-1-ylbenzene (3q)



(E)-tert-butyldimethyl((6-phenylhex-5-en-1-yl)oxy)silane (3r)



(E)-N,N-dimethyl-4-((6-phenylhex-5-en-1-yl)oxy)aniline (3s)

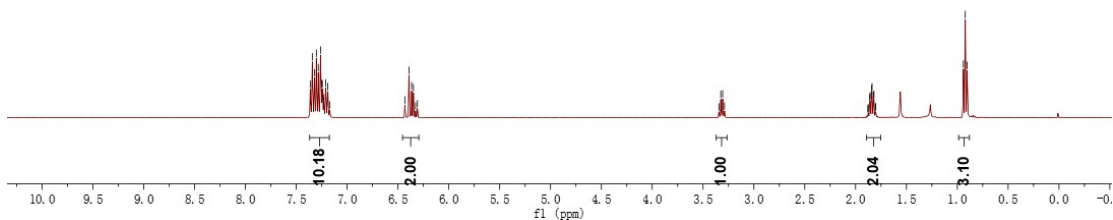
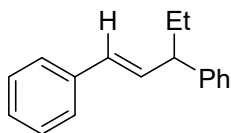


(E)-pent-1-ene-1,3-diylidibenzene (3t)

7.36
7.34
7.32
7.30
7.28
7.26
7.25
7.24
7.23
7.23
7.21
7.19
7.17
6.43
6.39
6.37
6.35
6.33
6.31

3.34
3.33
3.31
3.29

1.88
1.87
1.86
1.84
1.82
1.81
1.80
0.94
0.92
0.90

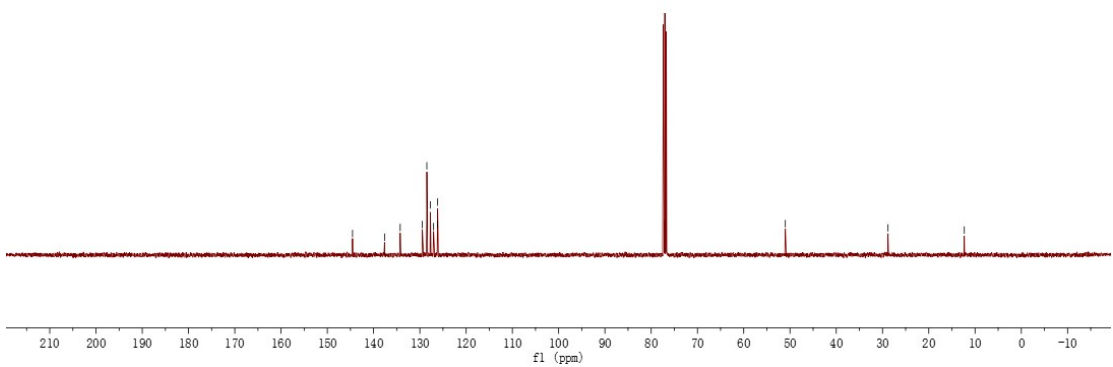
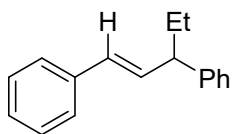


144.55
137.63
134.25
129.46
128.49
127.72
127.03
126.21
126.15

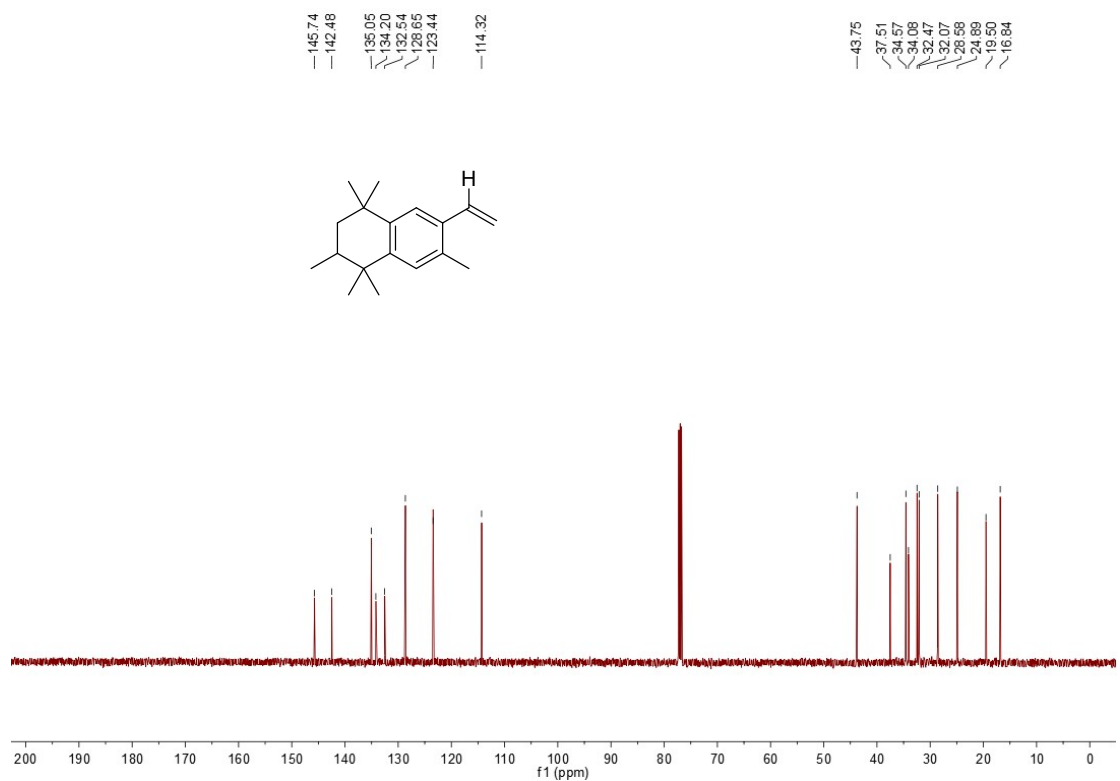
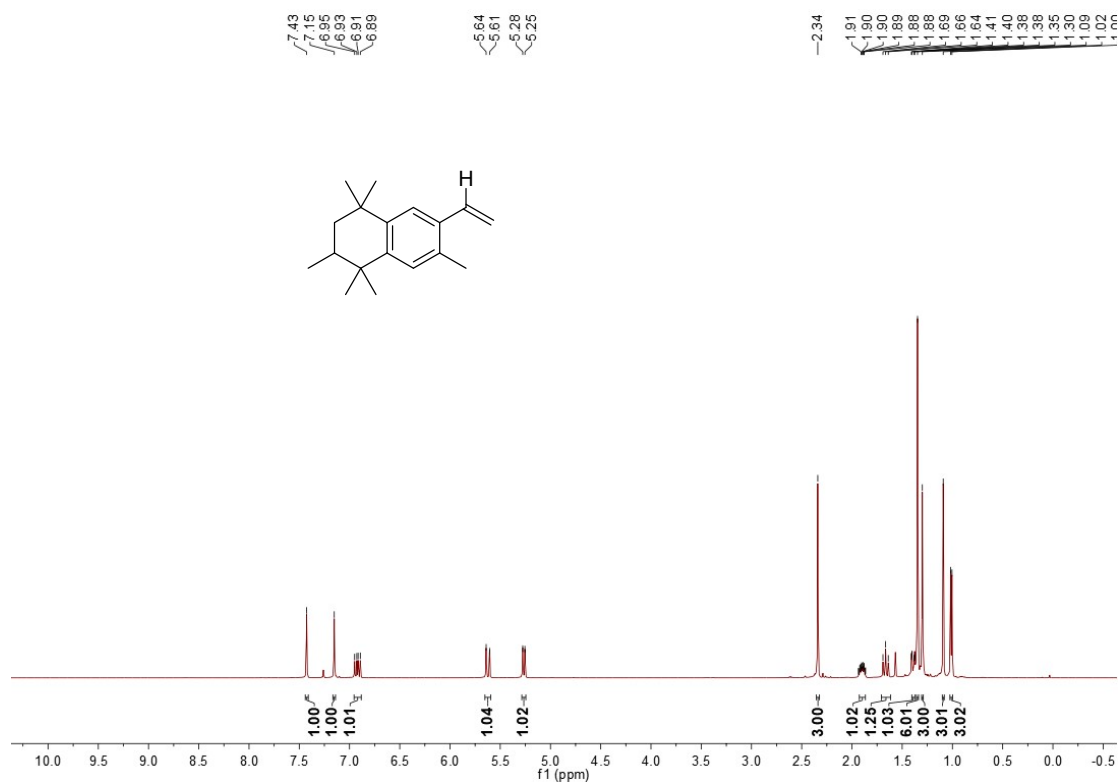
-51.00

-28.81

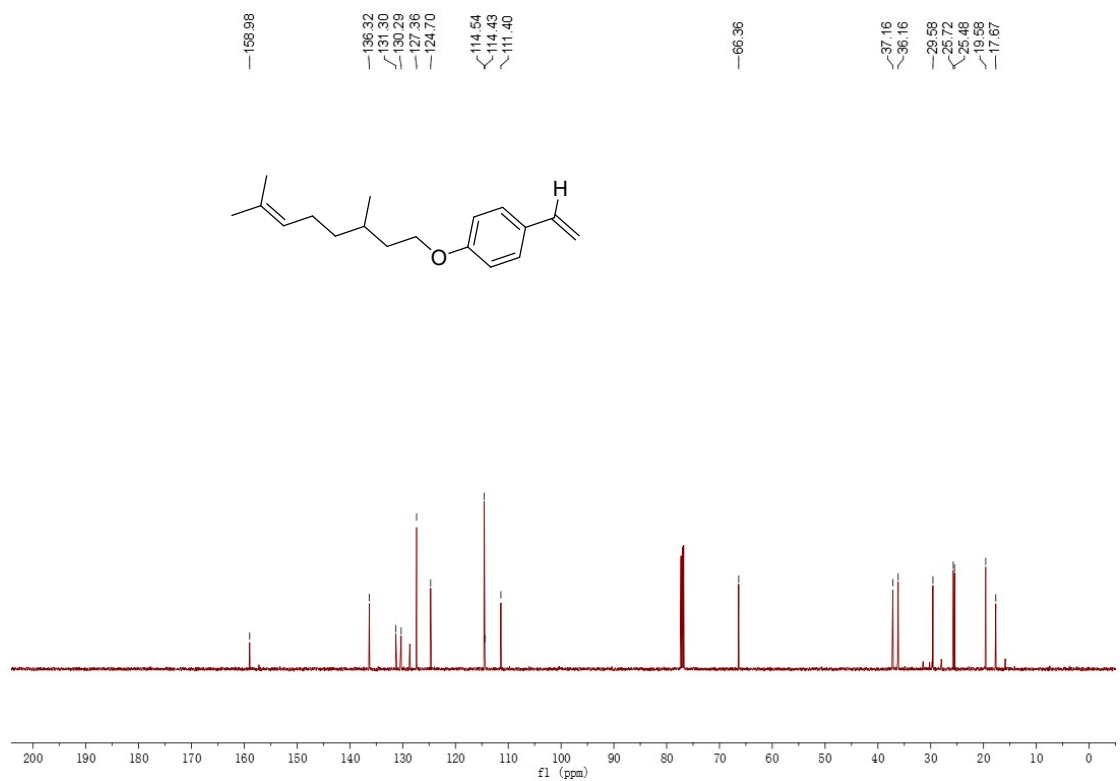
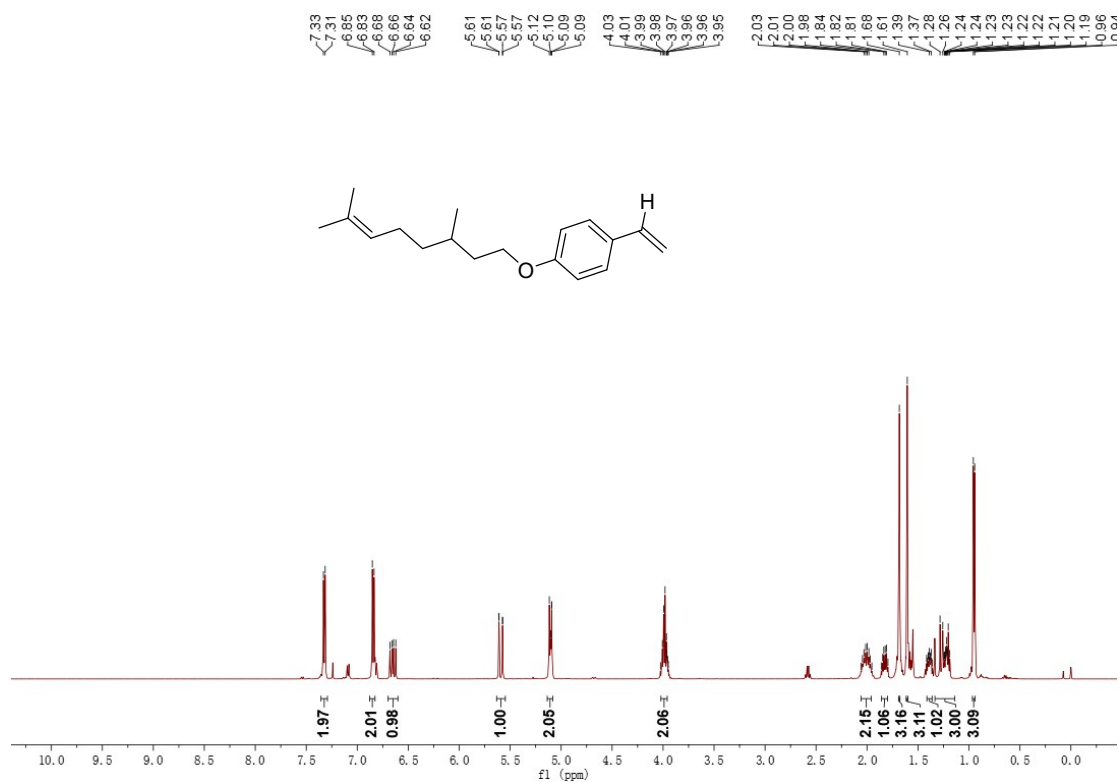
-12.32



1,1,2,4,4,7-hexamethyl-6-vinyl-1,2,3,4-tetrahydronaphthalene (3aa)

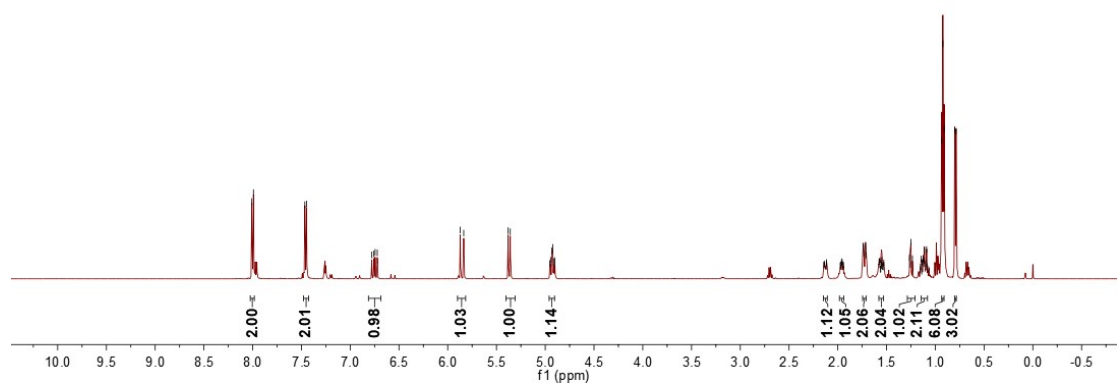
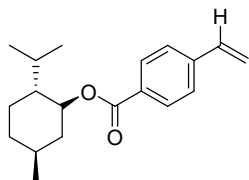


1-((3,7-dimethyloct-6-en-1-yl)oxy)-4-vinylbenzene (3ab)

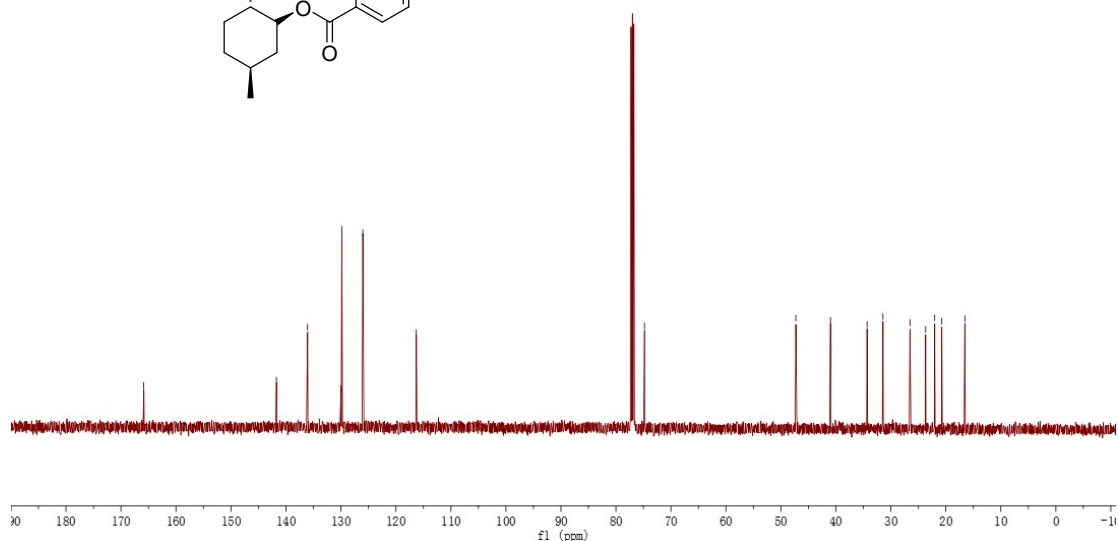
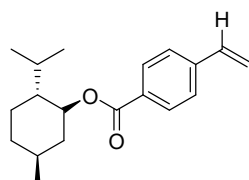


(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 4-vinylbenzoate (3ac)

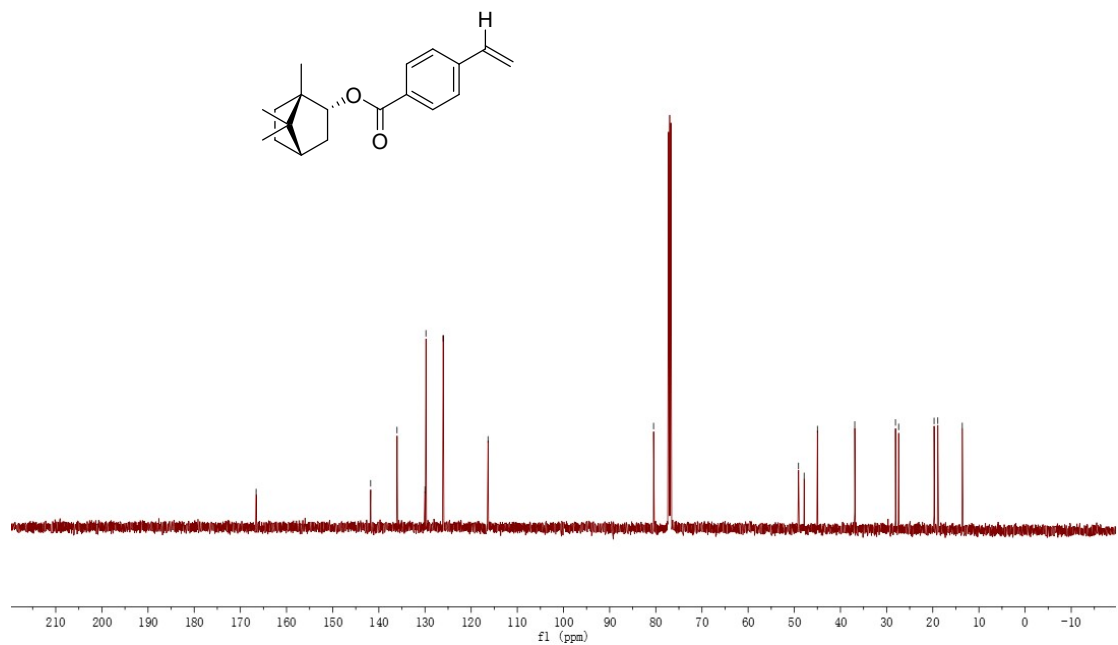
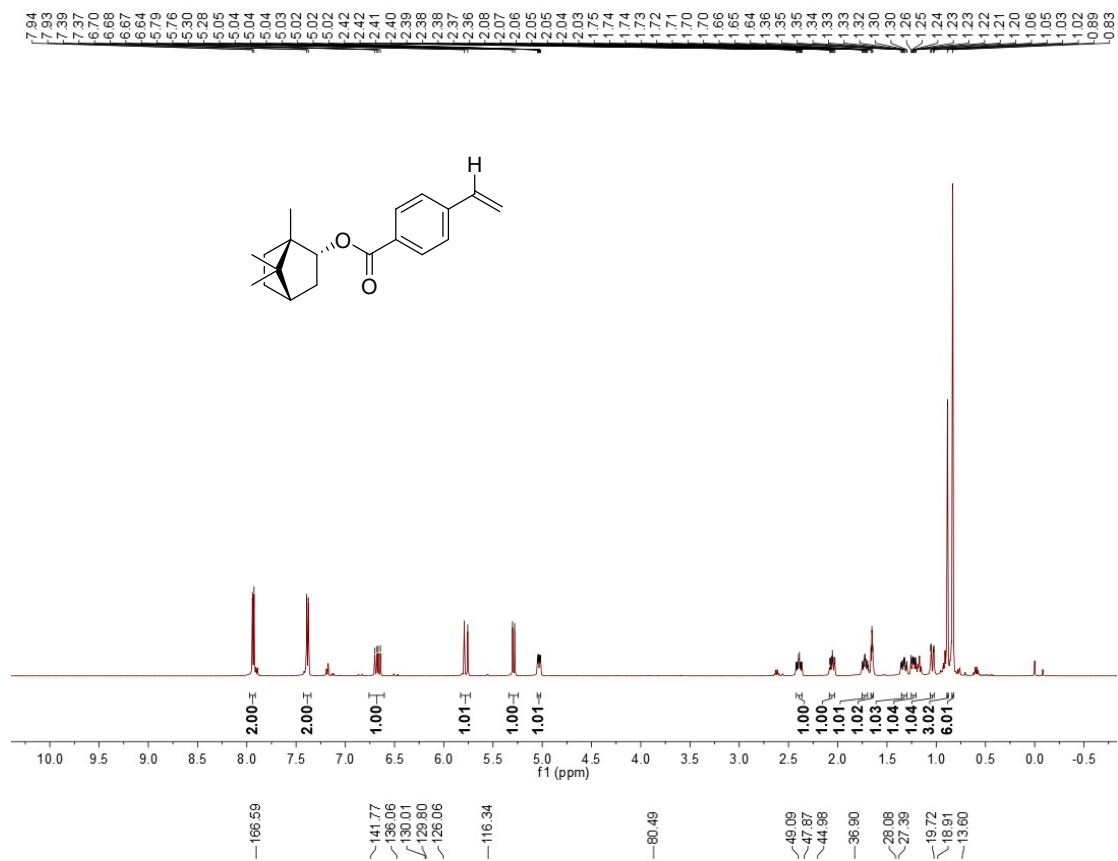
8.01, 7.99, 7.47, 7.45, 6.76, 6.74, 6.72, 5.87, 5.84, 5.38, 5.36, 4.95, 4.94, 4.93, 4.92, 4.91, 4.90, 2.14, 2.14, 2.12, 2.12, 2.11, 1.98, 1.97, 1.96, 1.96, 1.95, 1.94, 1.74, 1.73, 1.72, 1.71, 1.58, 1.57, 1.56, 1.56, 1.55, 1.55, 1.55, 1.54, 1.53, 1.53, 1.26, 1.26, 1.25, 1.23, 1.23, 1.15, 1.15, 1.14, 1.14, 1.12, 1.12, 1.11, 1.11, 1.10, 1.10, 1.09, 1.09, 1.08, 1.08, 0.93, 0.93, 0.81, 0.81, 0.80, 0.79



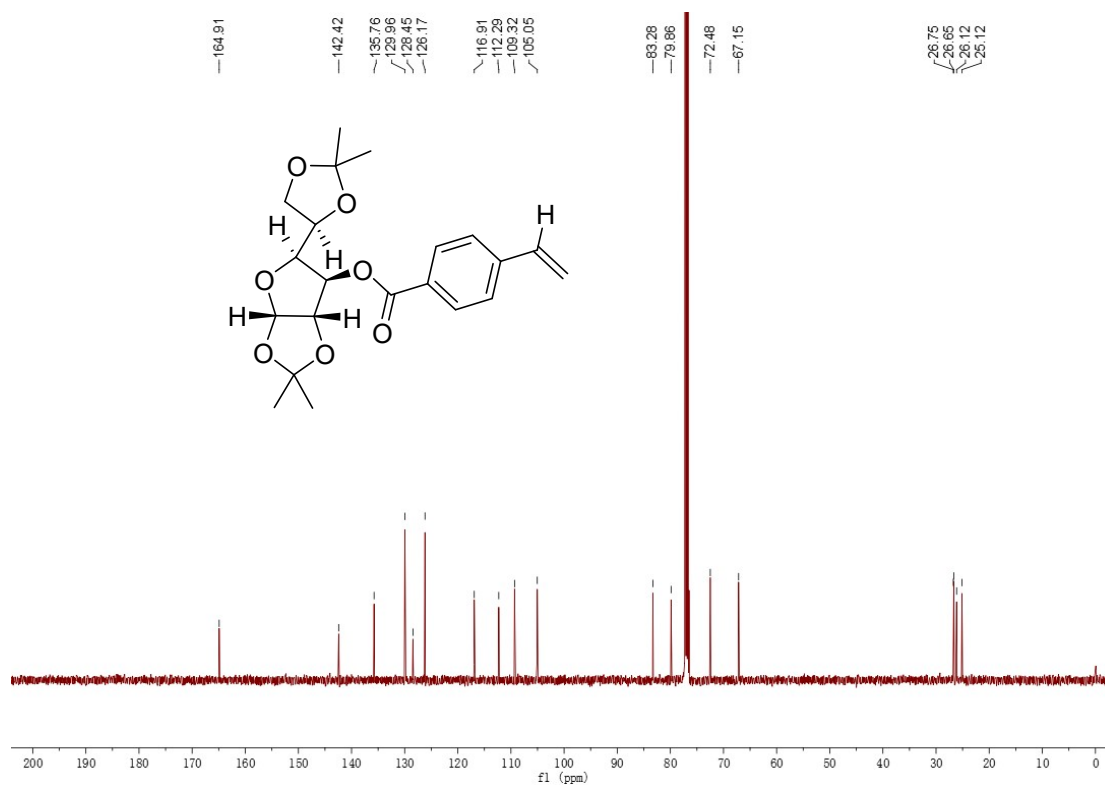
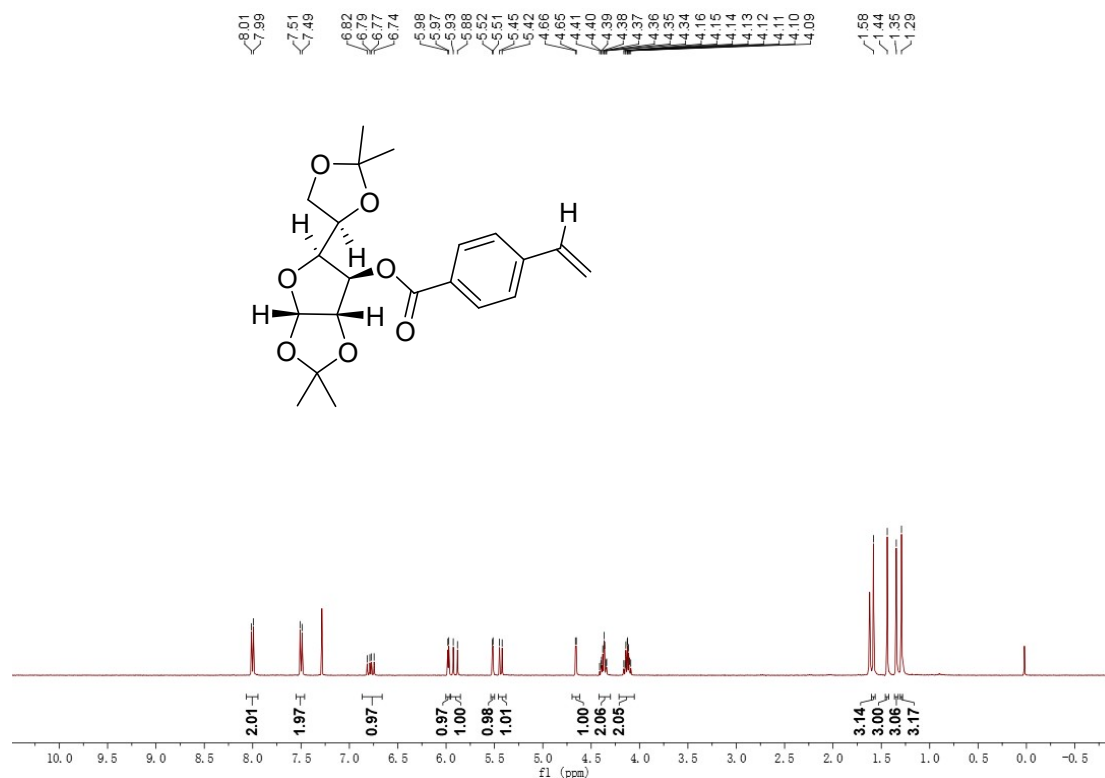
165.86, 141.74, 136.07, 130.00, 129.85, 126.03, 116.30, 74.80, 47.28, 40.98, 34.33, 31.44, 26.53, 23.68, 20.71, 16.55



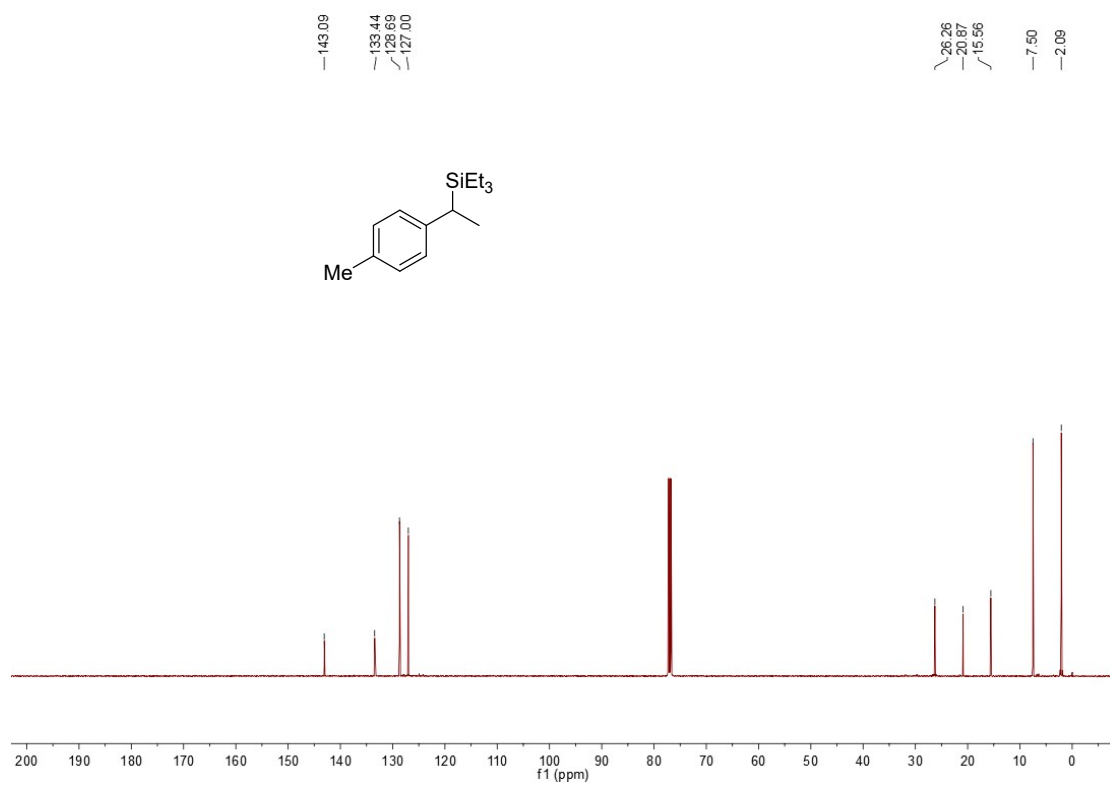
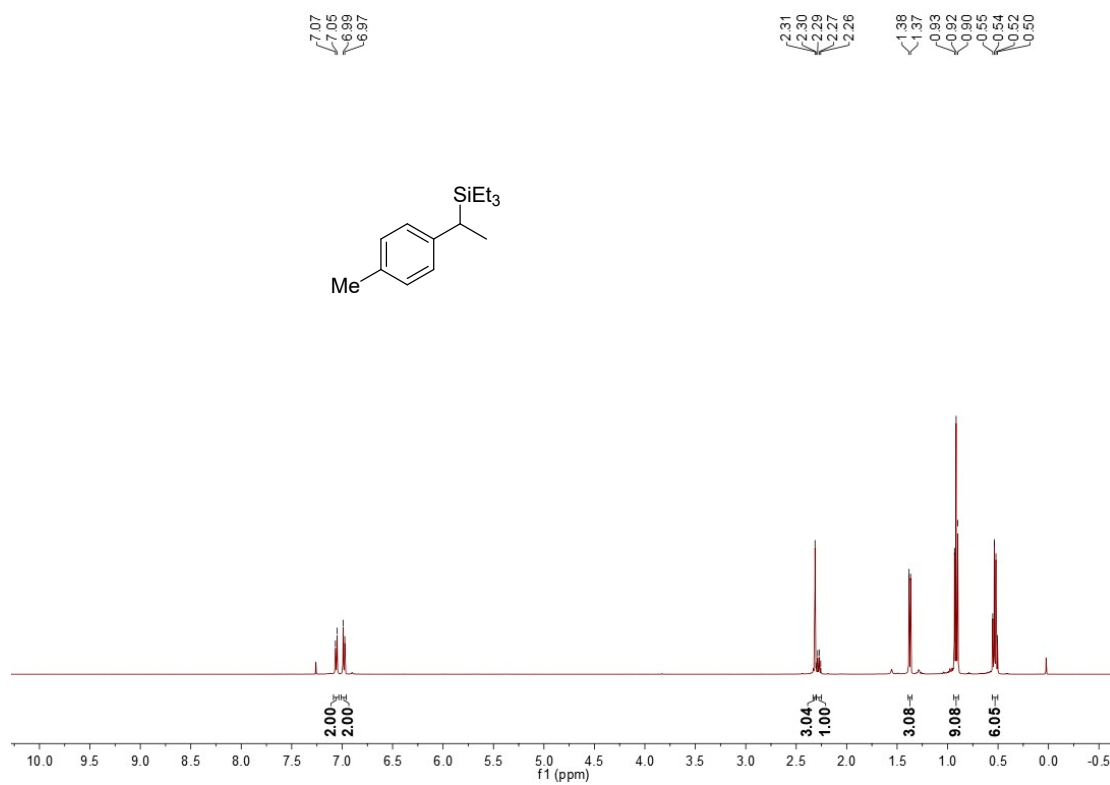
(1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl 4-vinylbenzoate (3ad)



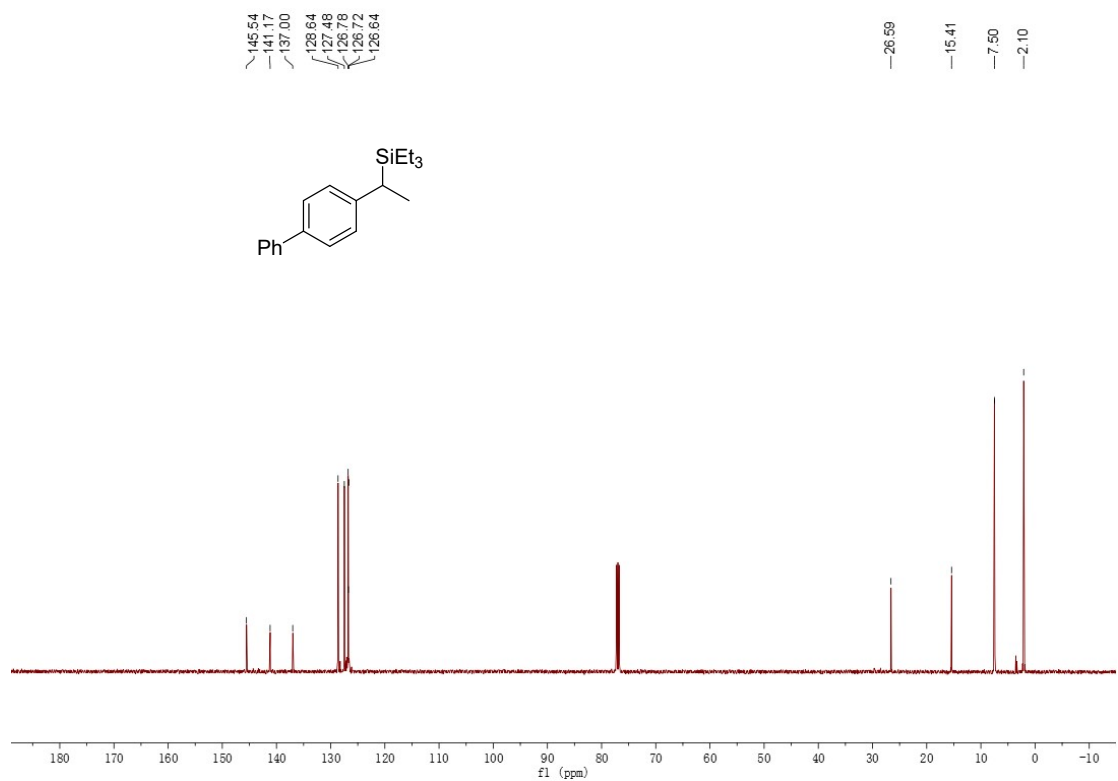
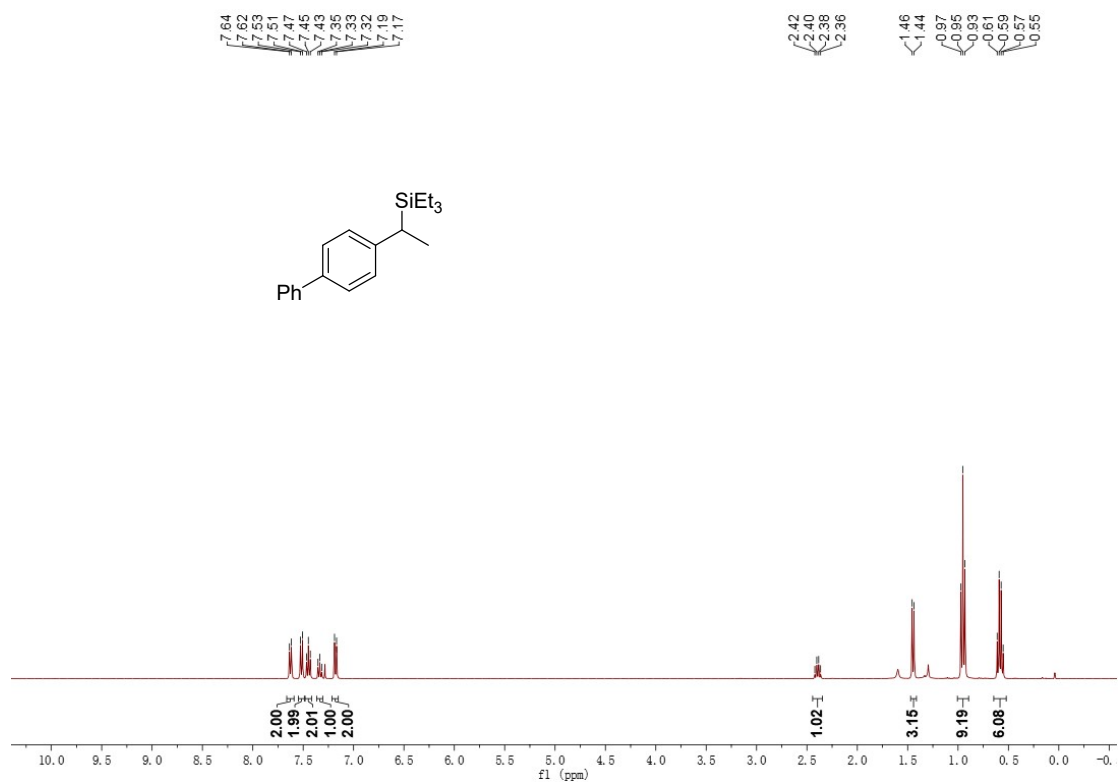
(3aS,5S,6R,6aS)-5-((R)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-d][1,3]dioxol-6-yl 4-vinylbenzoate (3ae)



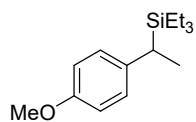
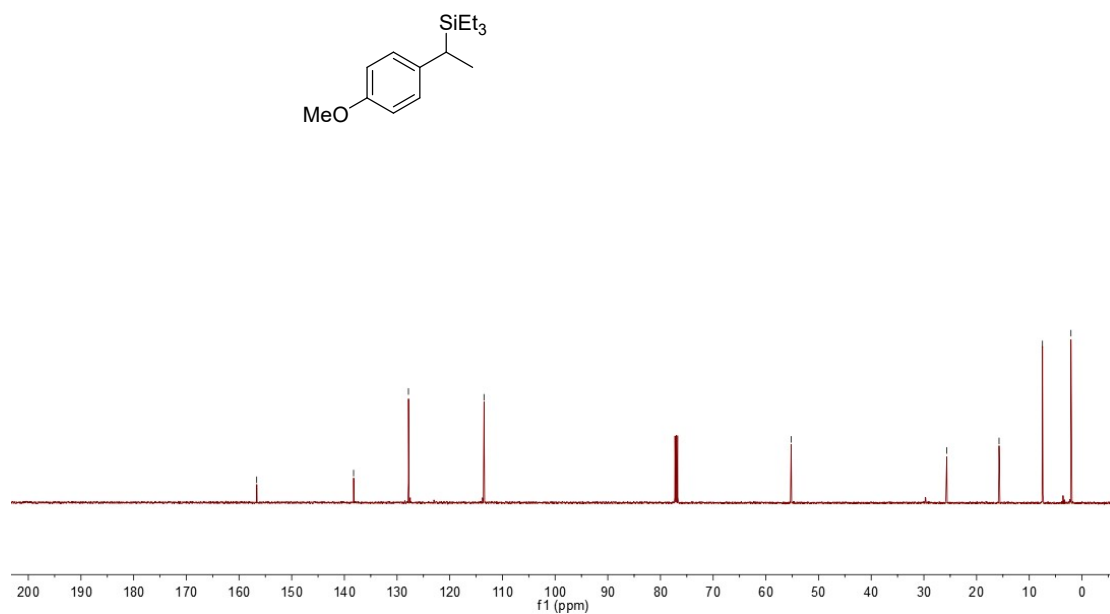
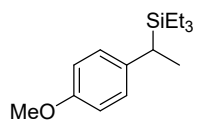
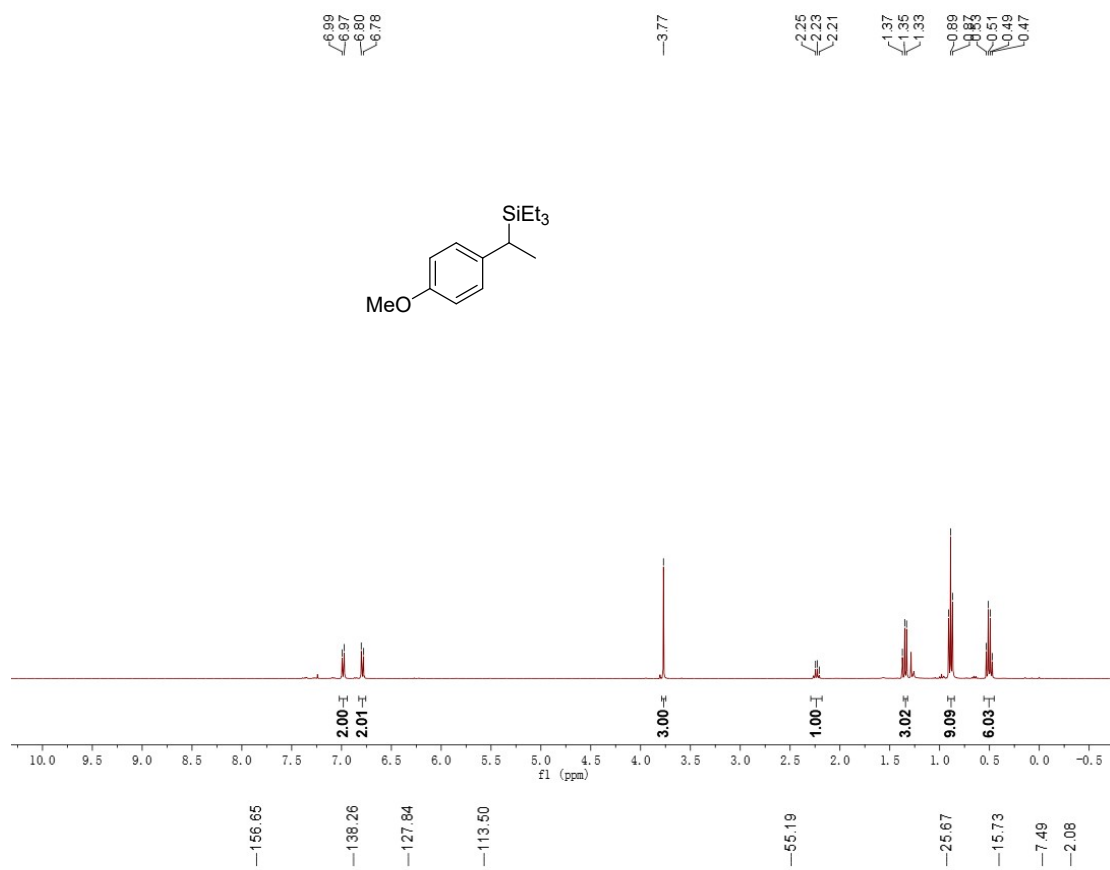
triethyl(1-(p-tolyl)ethyl)silane (4a)



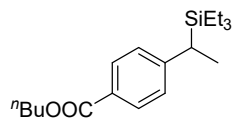
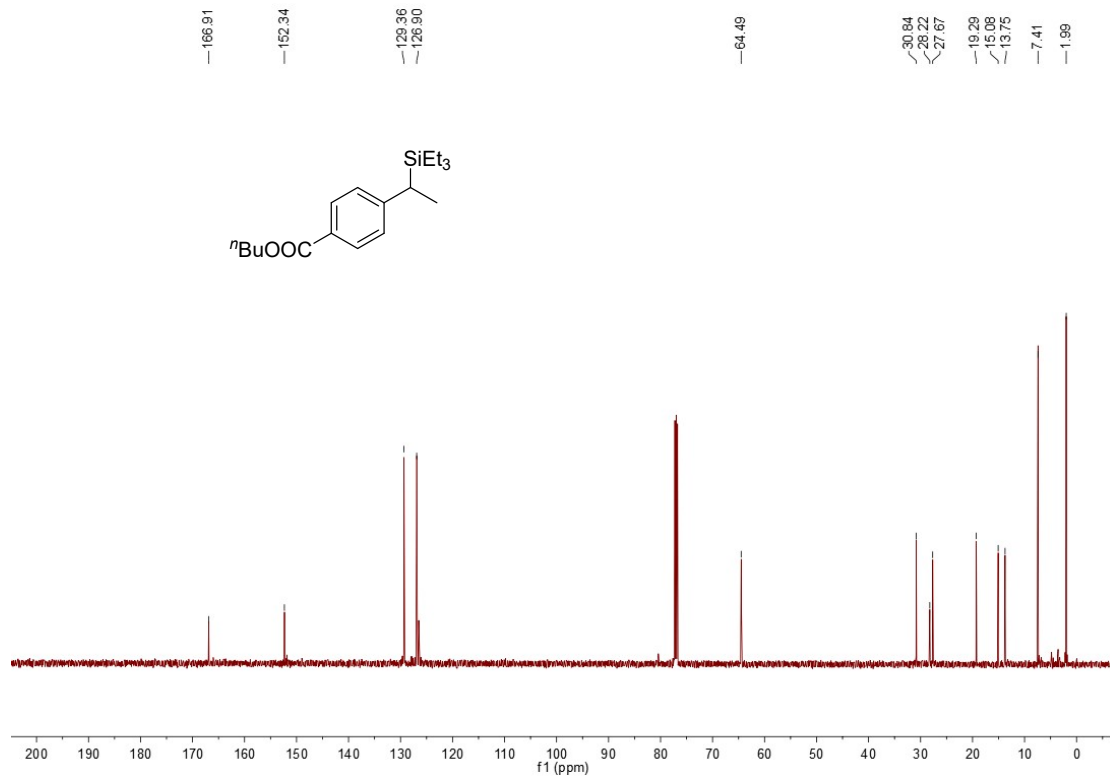
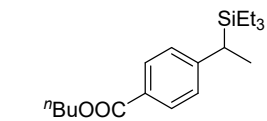
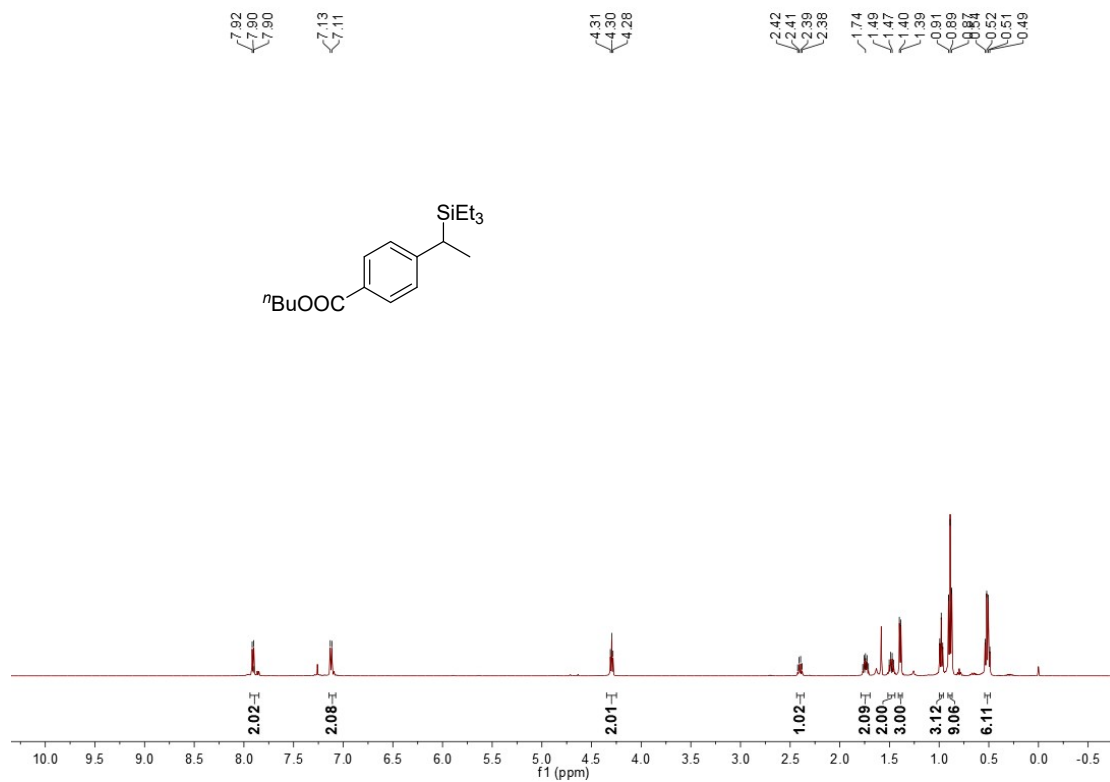
(1-([1,1'-biphenyl]-4-yl)ethyl)triethylsilane (4b)



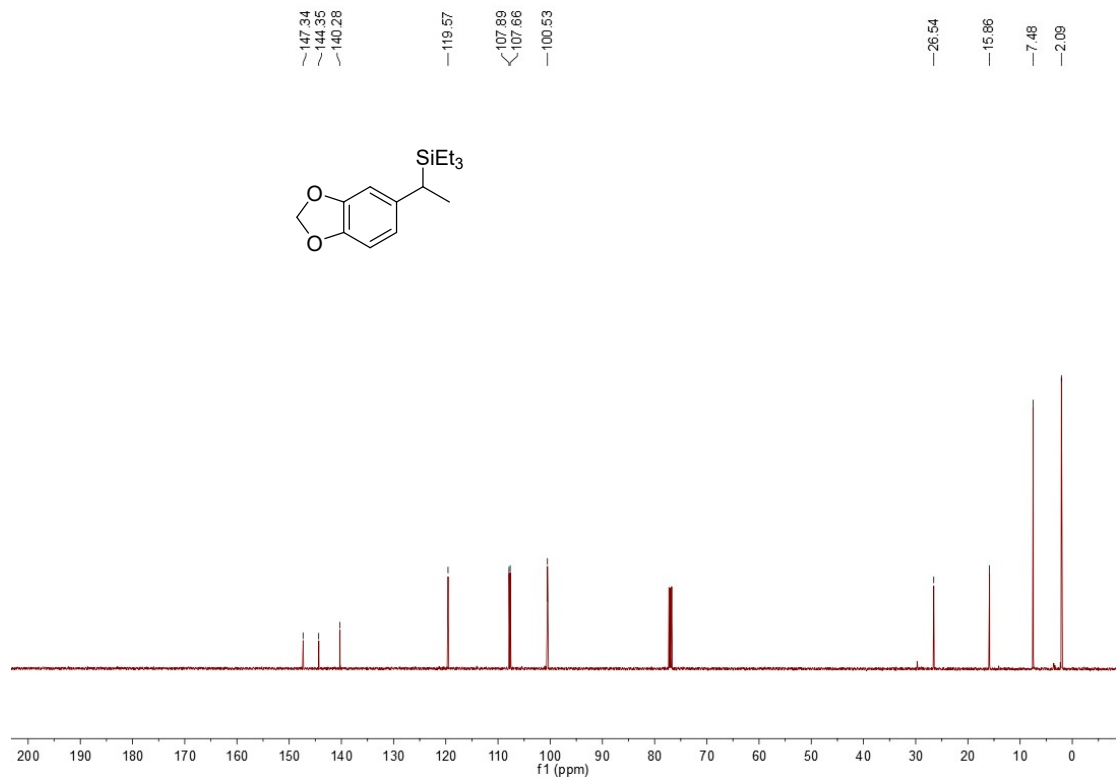
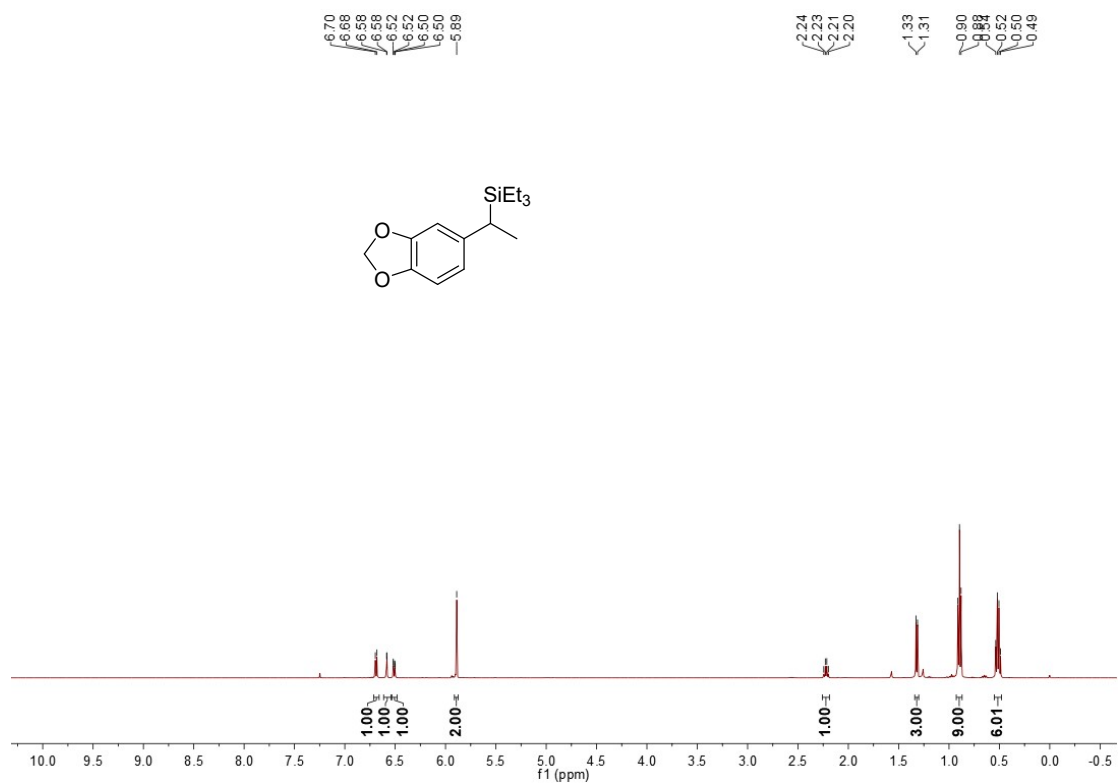
Triethyl(1-(4-methoxyphenyl)ethyl)silane (4c)



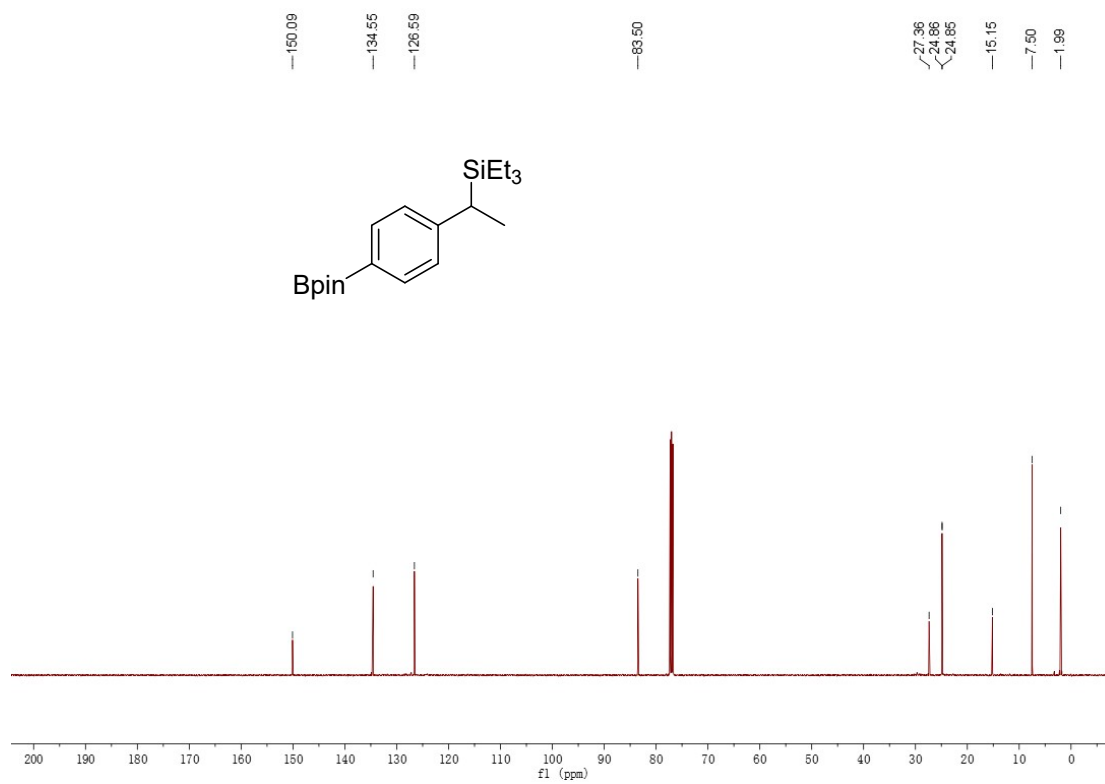
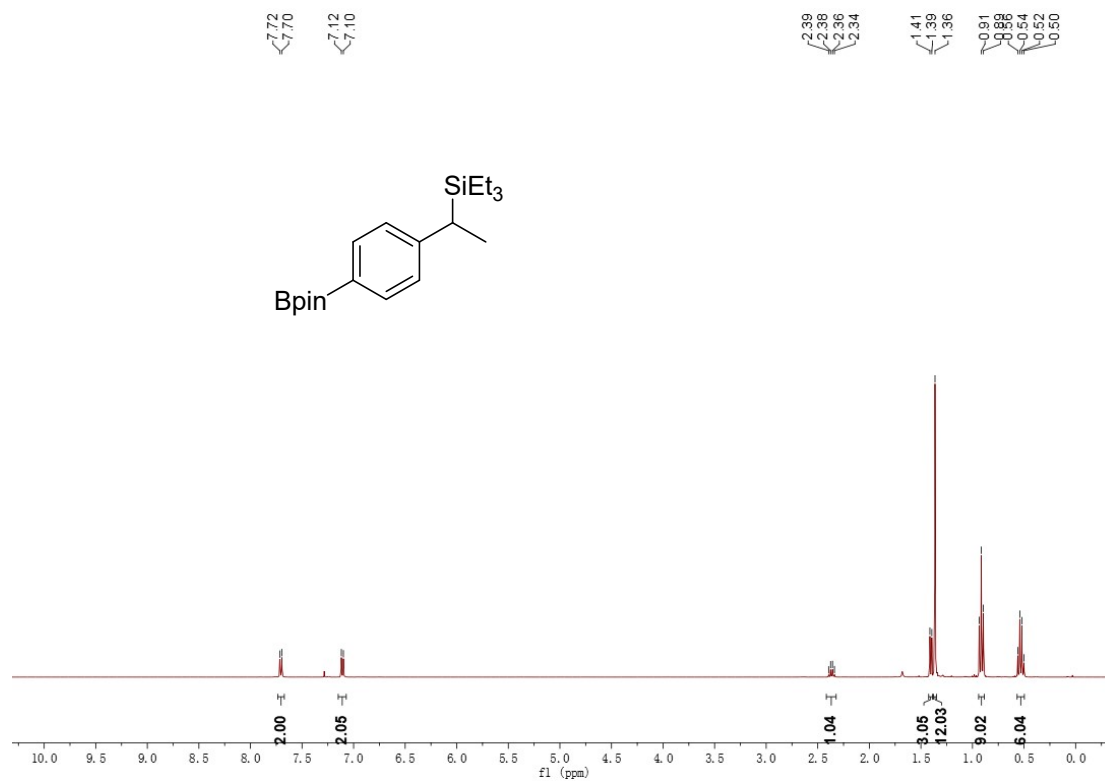
Butyl 4-(1-(triethylsilyl)ethyl)benzoate (4d)



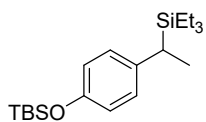
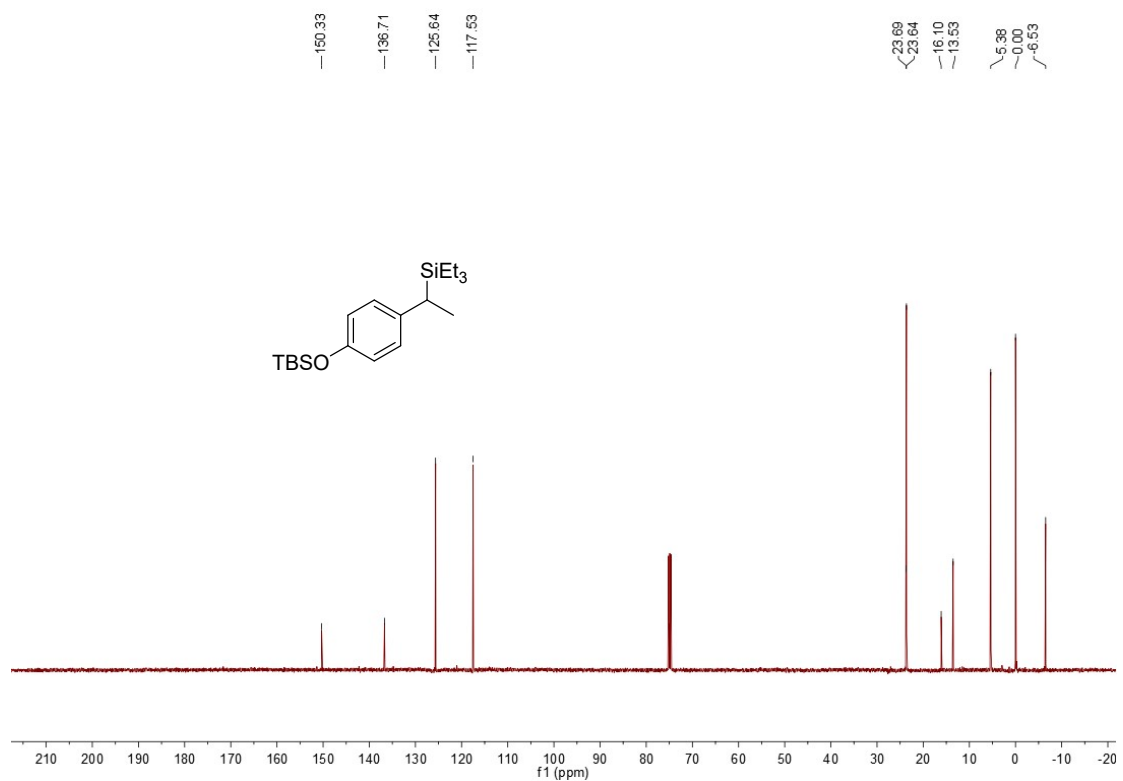
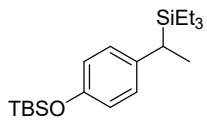
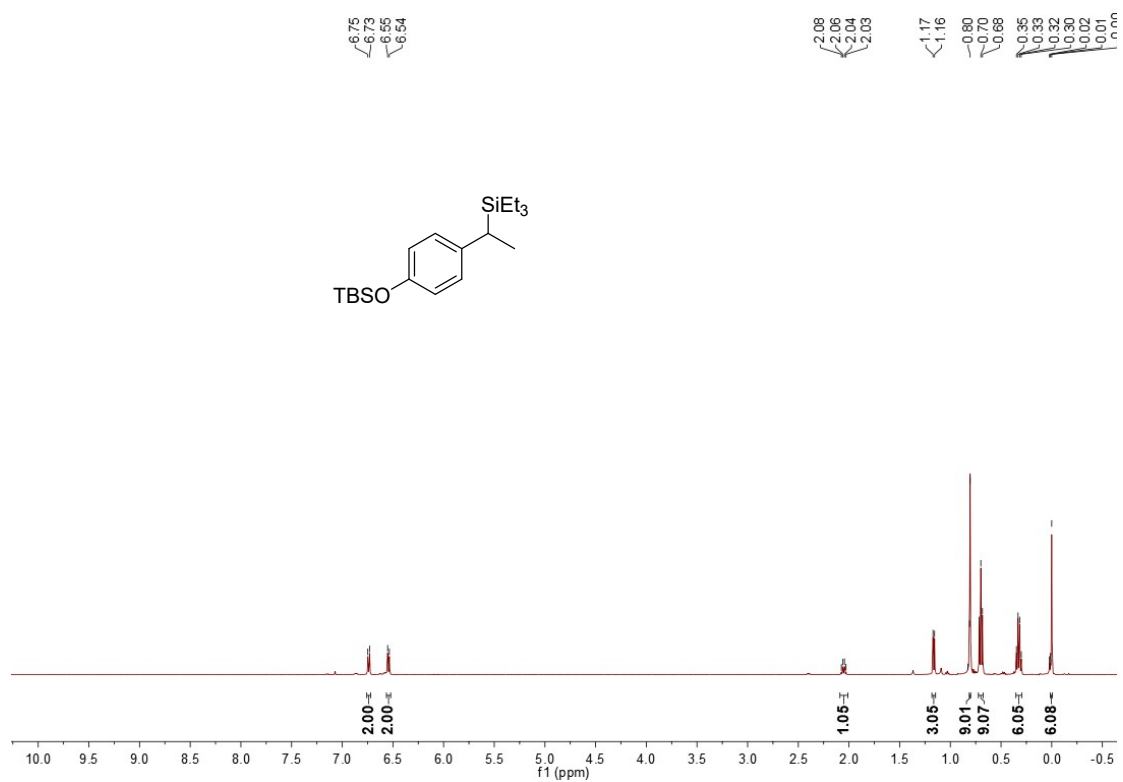
(1-(benzo[d][1,3]dioxol-5-yl)ethyl)triethylsilane (4e)



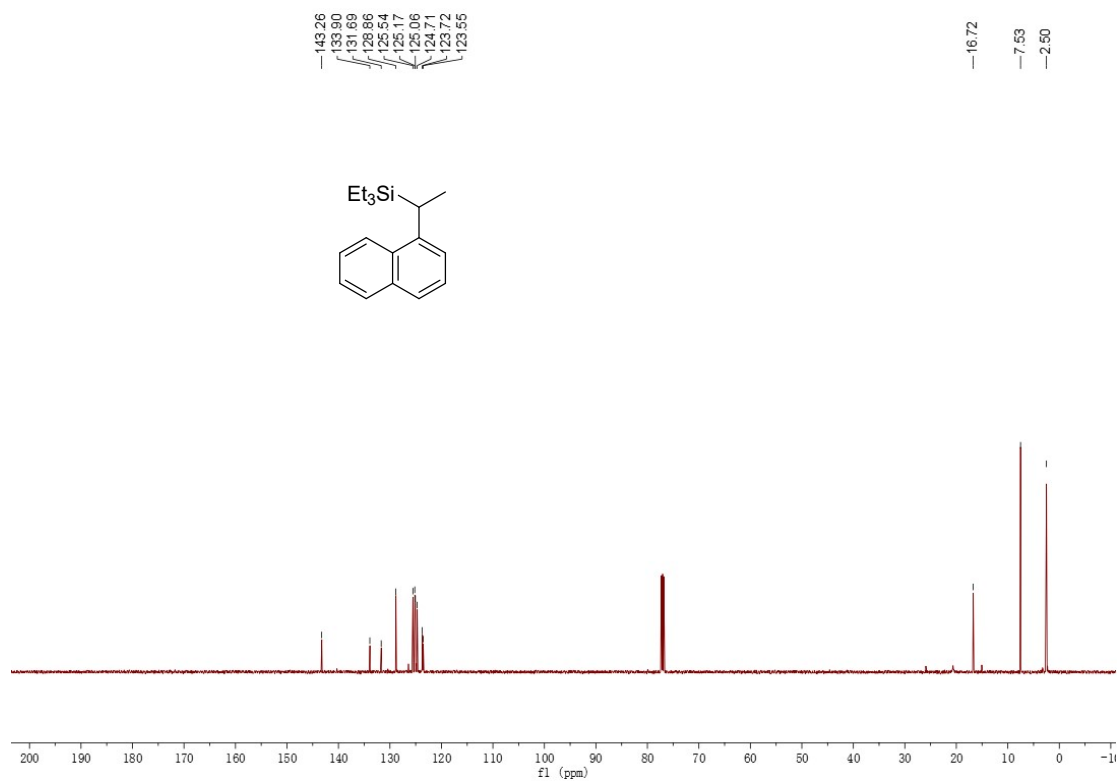
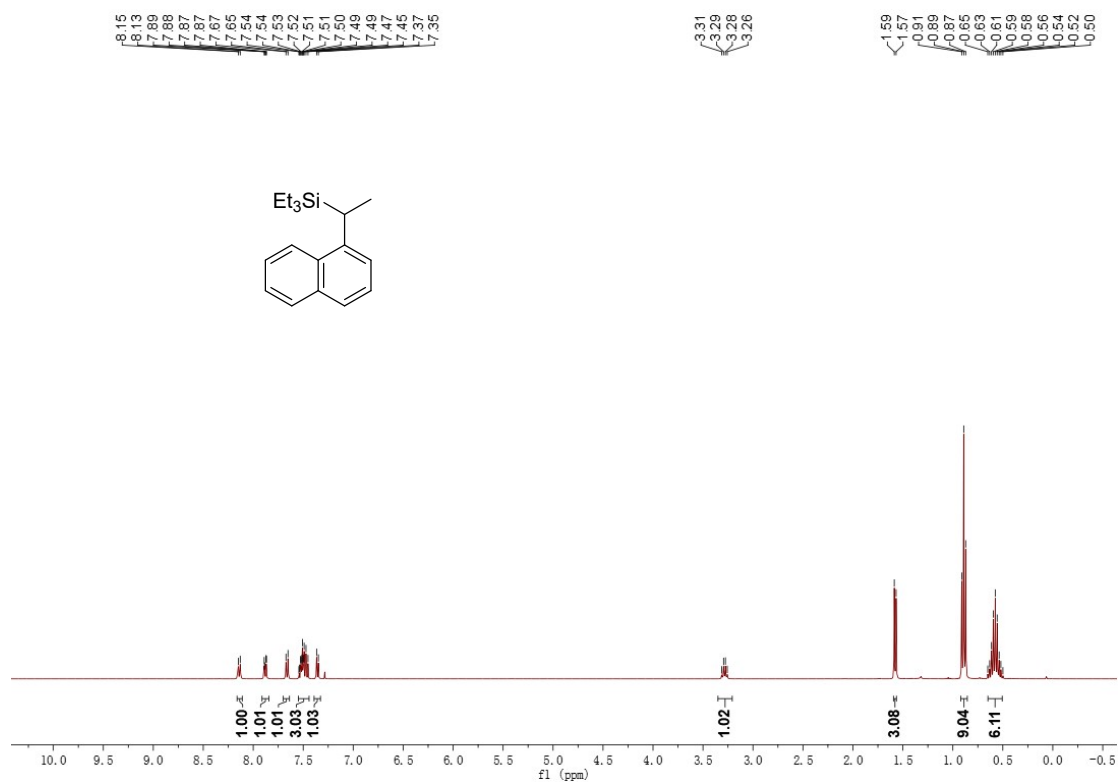
Triethyl(1-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)ethyl)silane (4f)



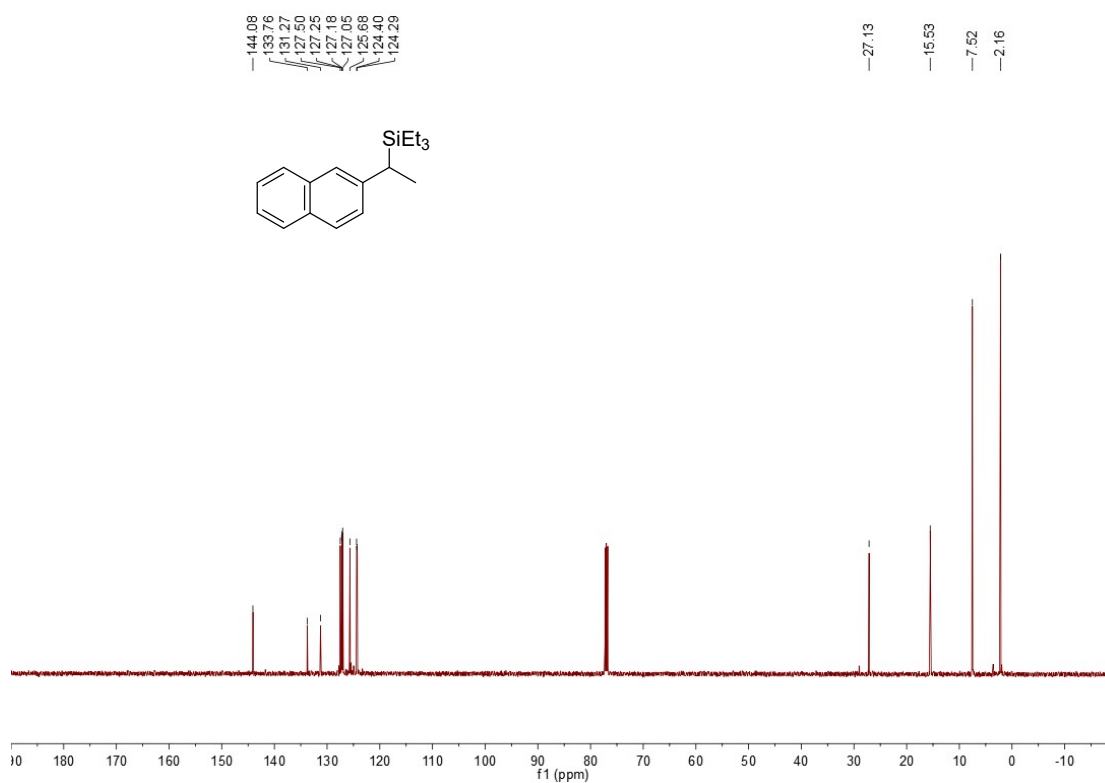
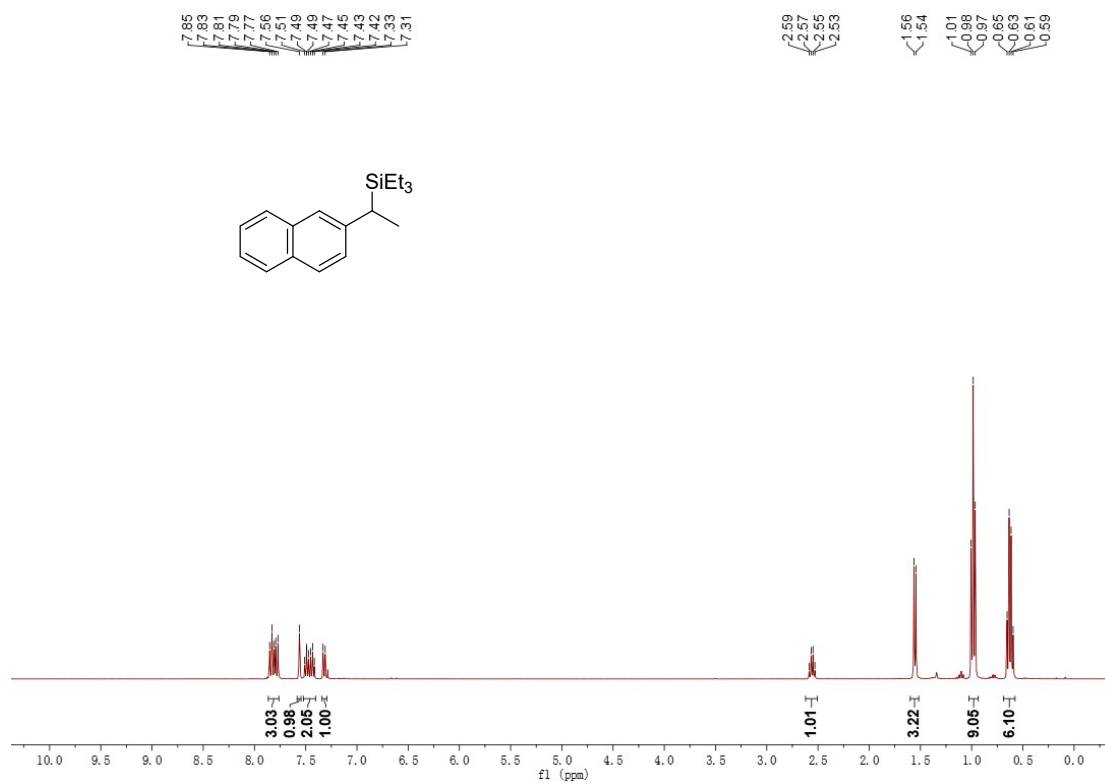
Tert-butyl dimethyl(4-(1-(triethylsilyl)ethyl)phenoxy)silane (4g)



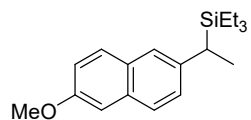
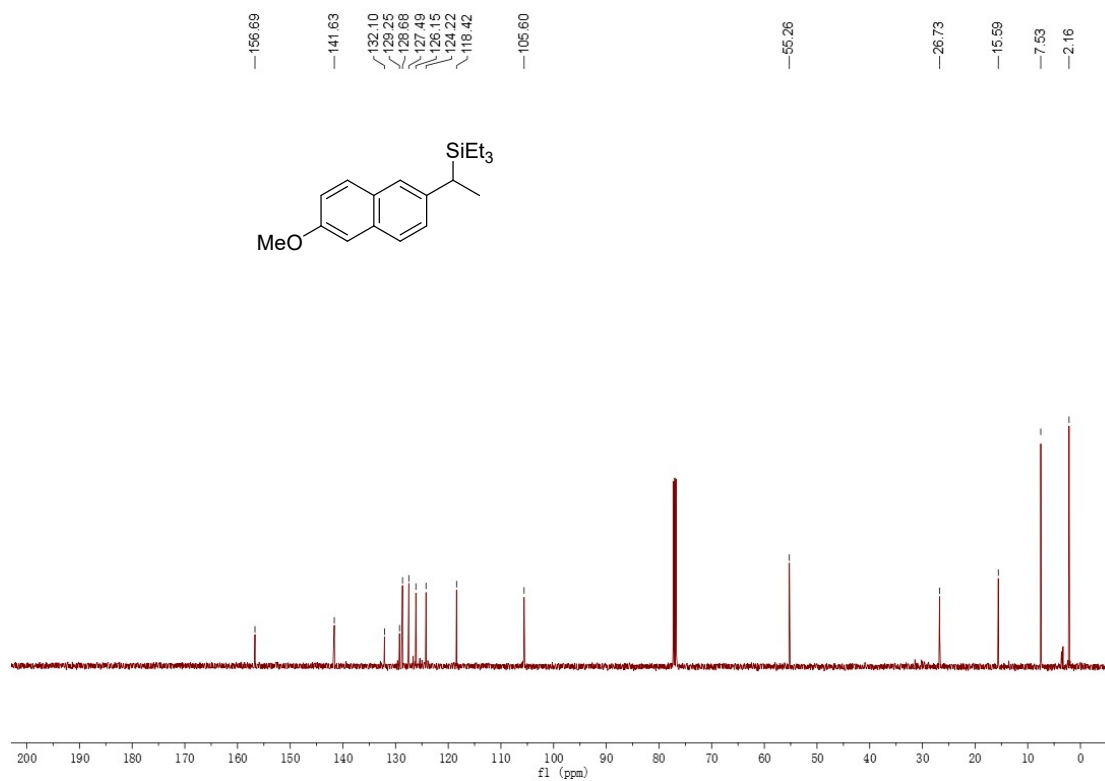
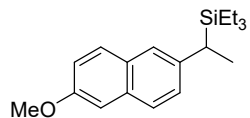
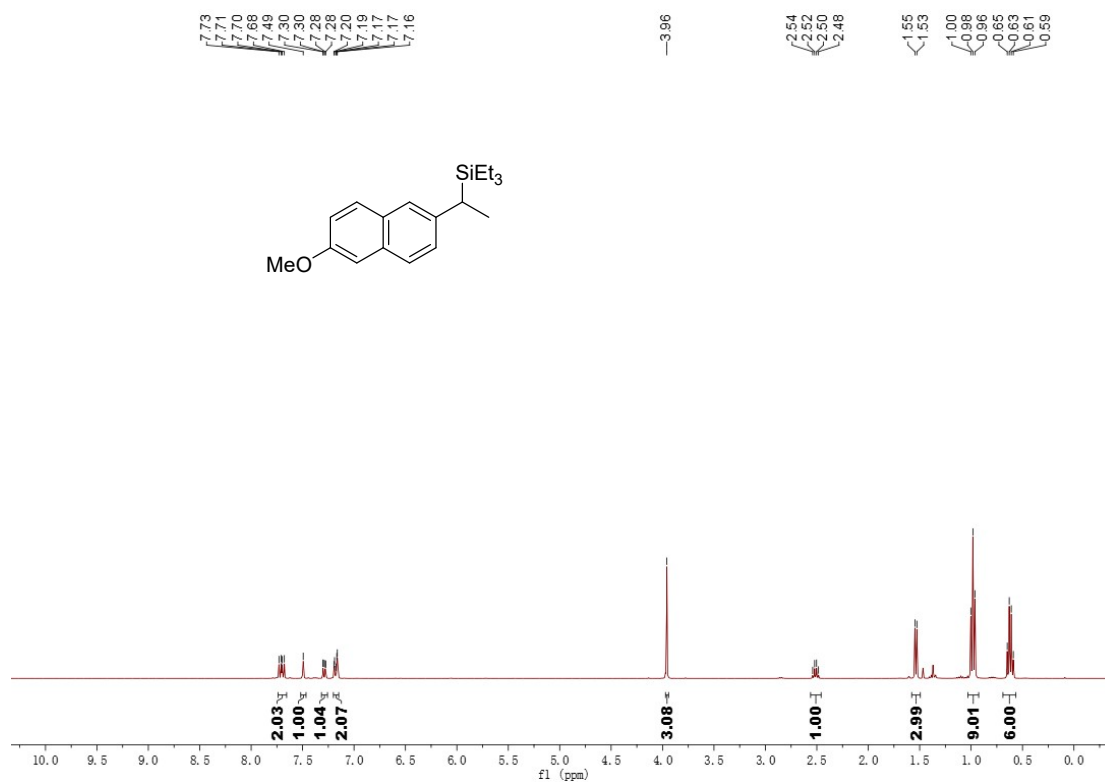
Triethyl(1-(naphthalen-1-yl)ethyl)silane (4h)



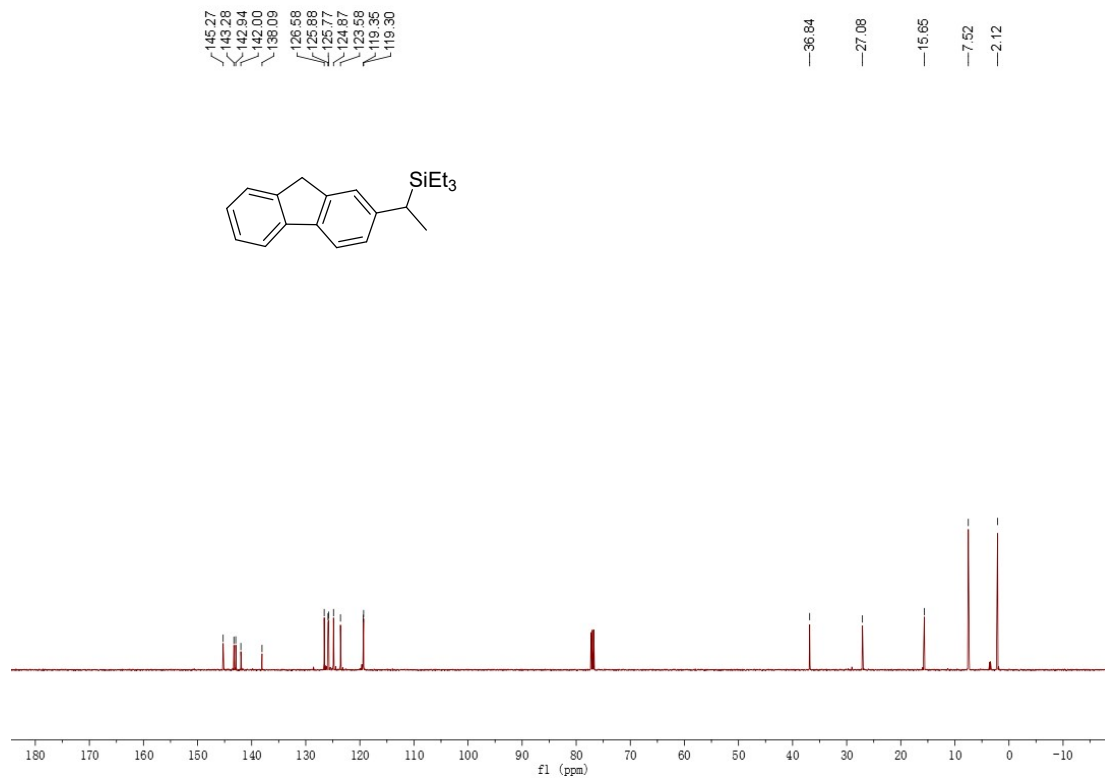
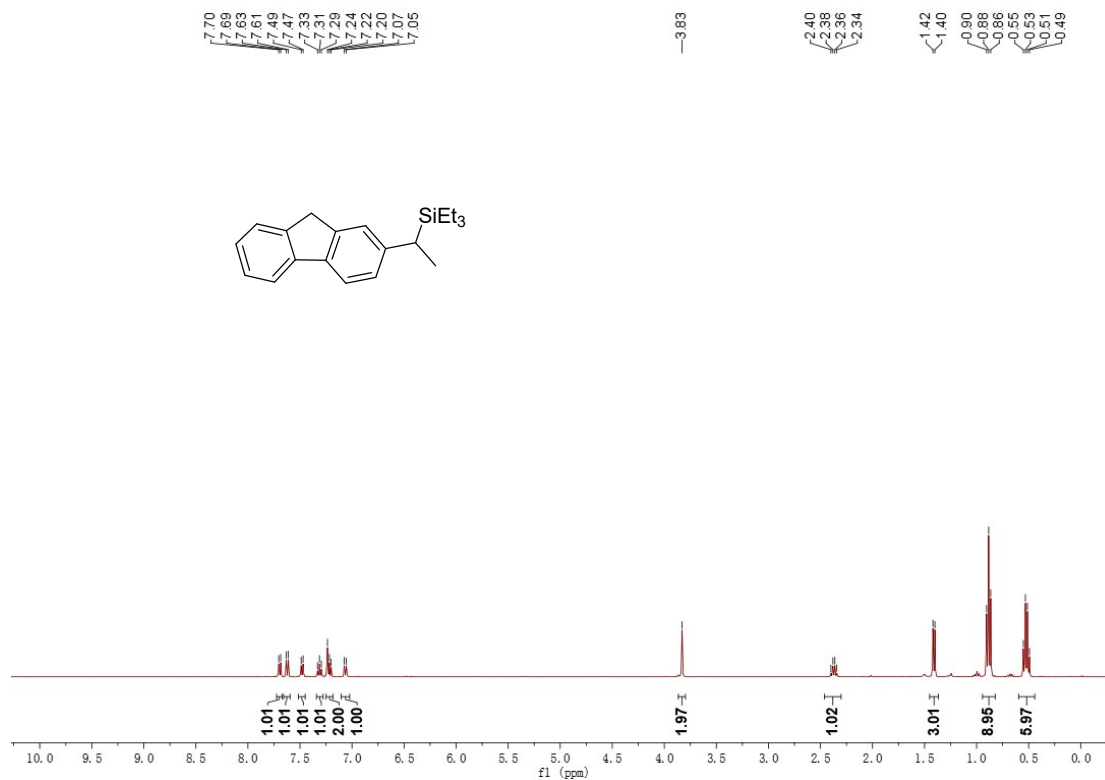
Triethyl(1-(naphthalen-2-yl)ethyl)silane (4i)



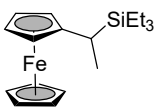
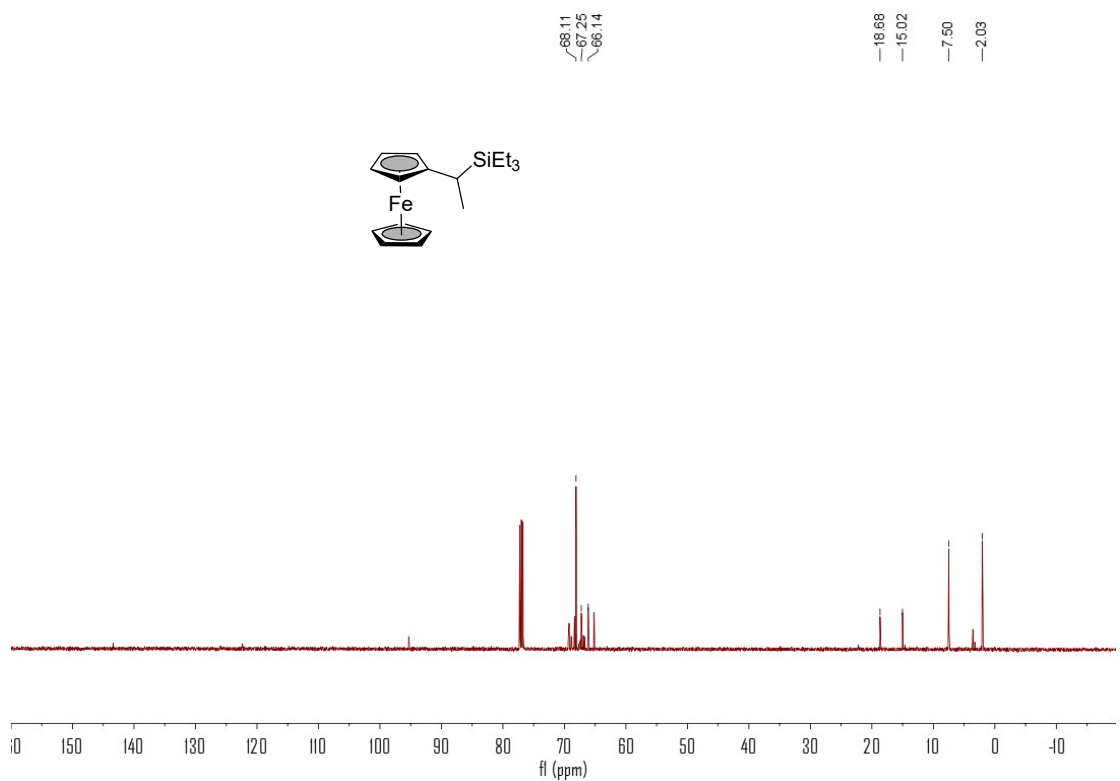
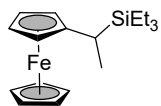
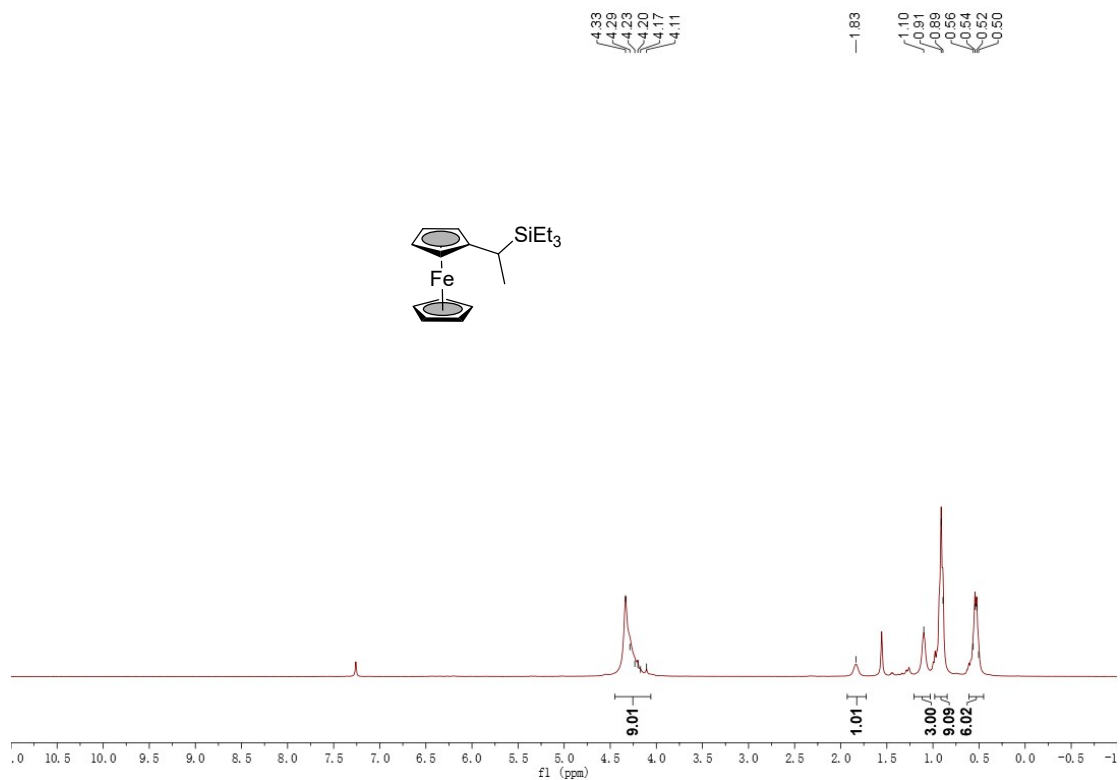
Triethyl(1-(6-methoxynaphthalen-2-yl)ethyl)silane (4j)



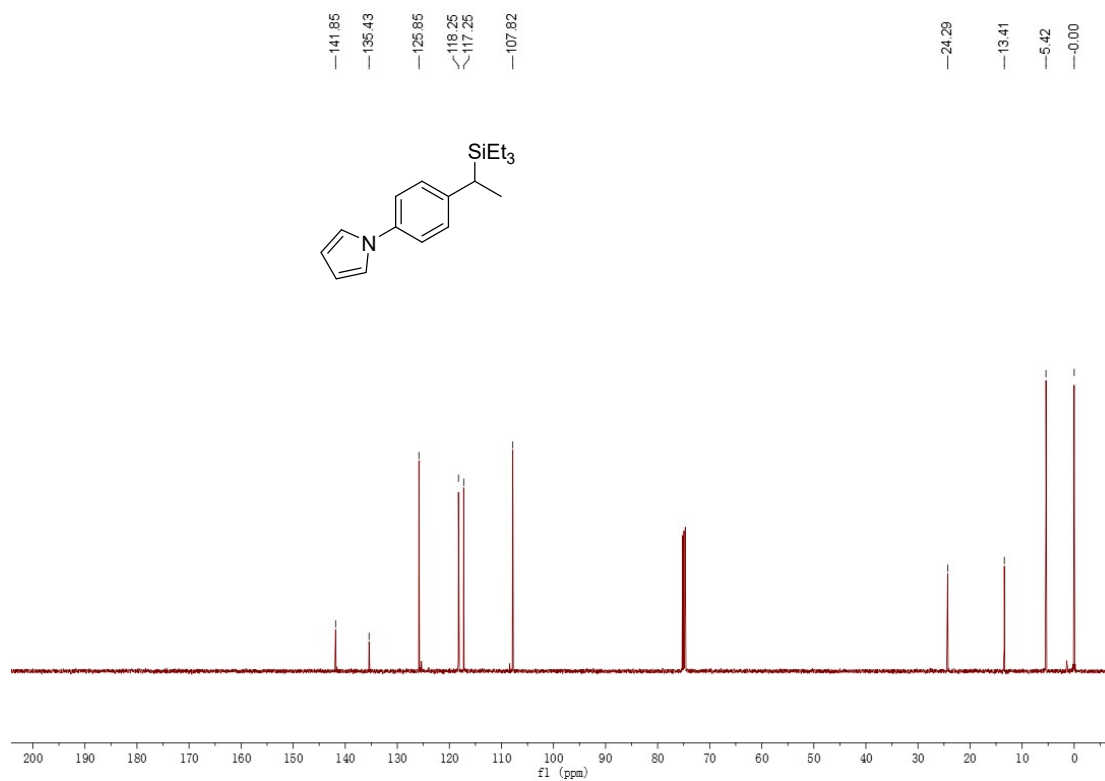
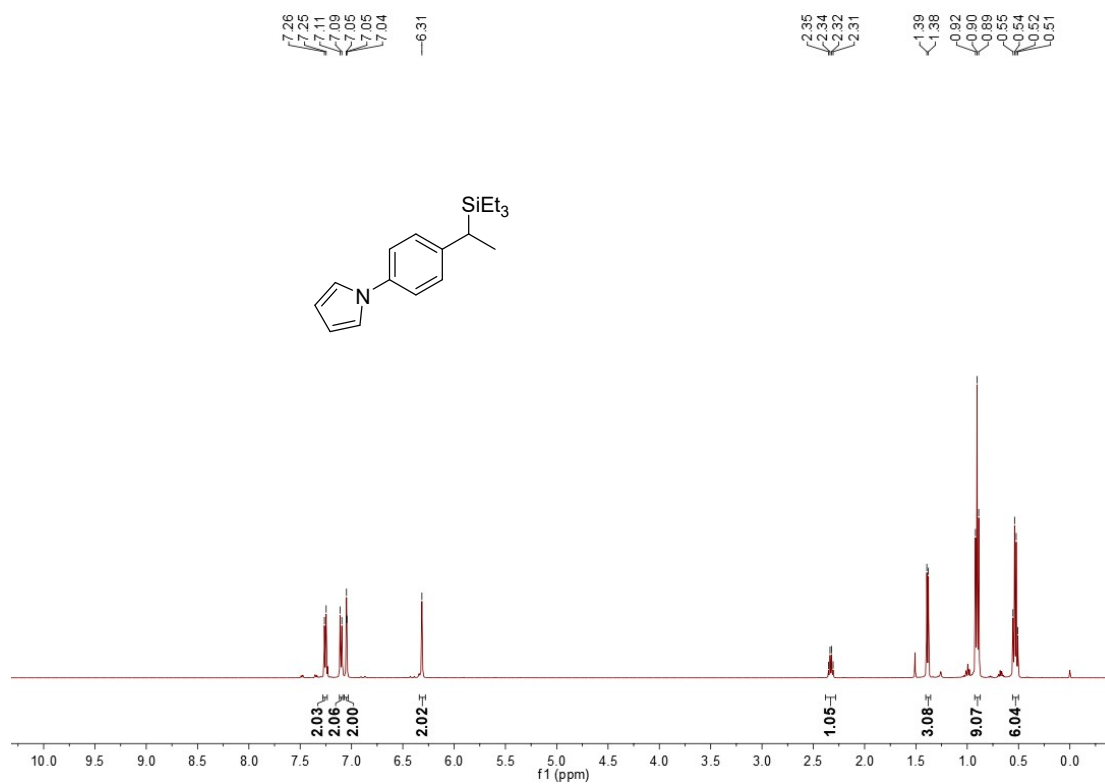
(1-(9H-fluoren-2-yl)ethyl)triethylsilane (4k)



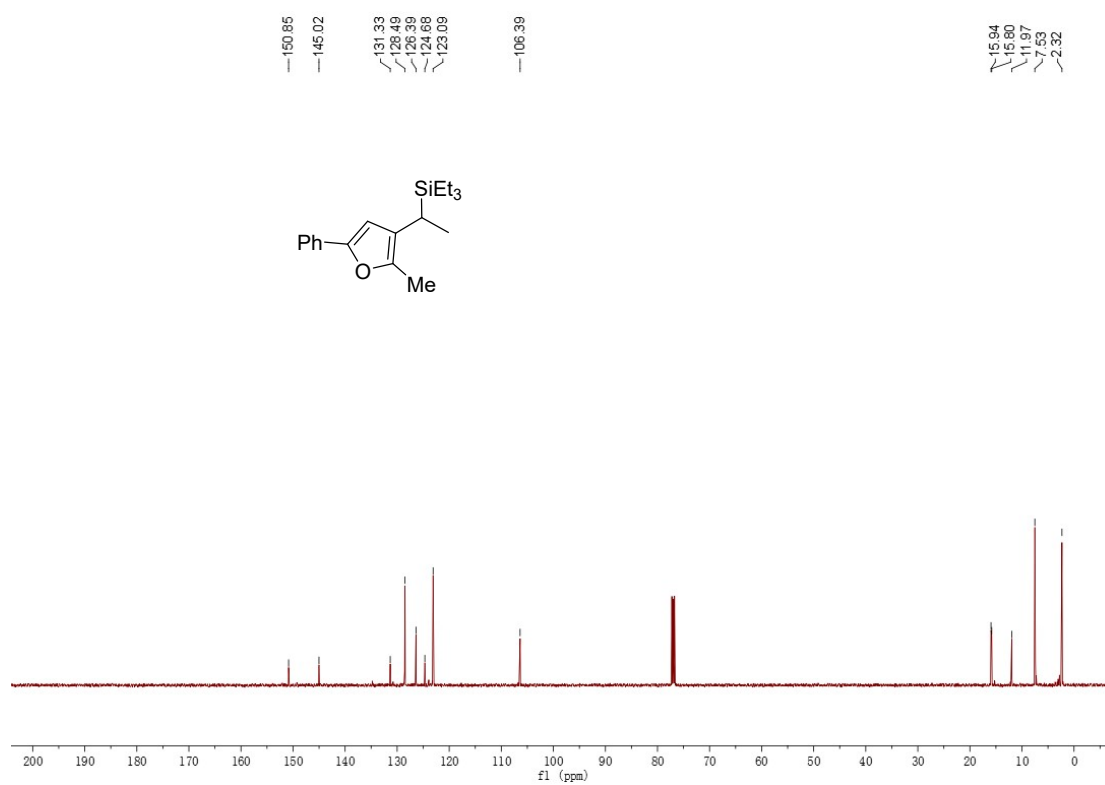
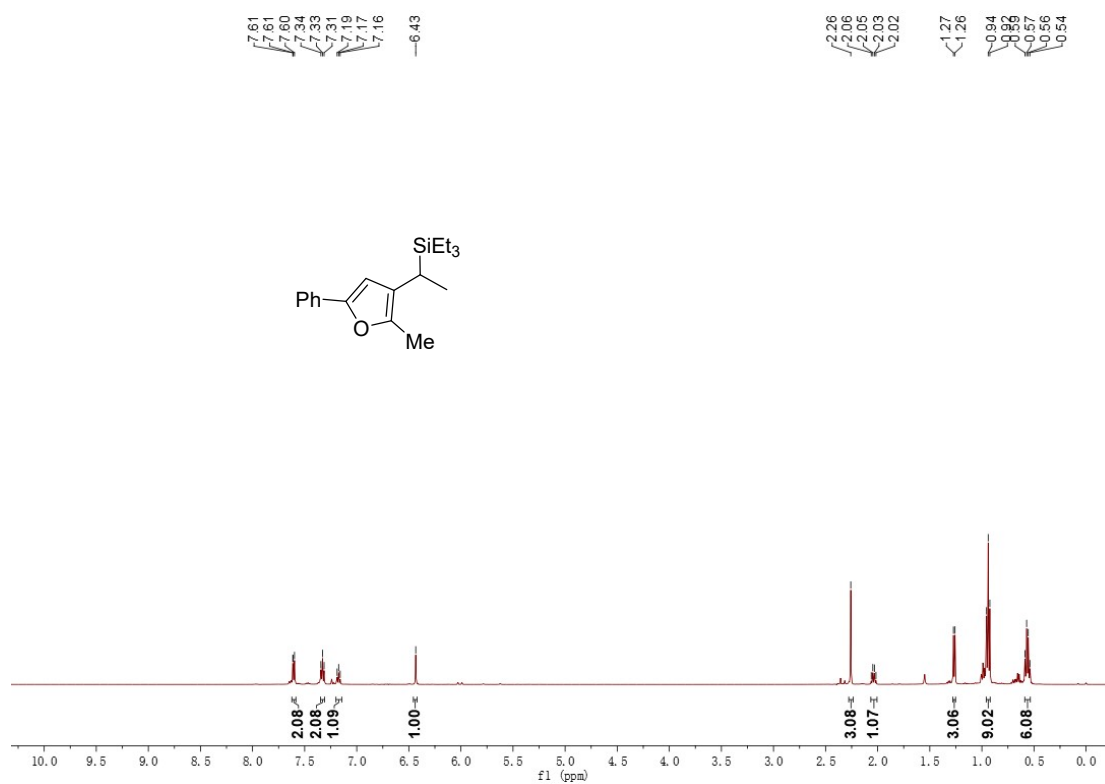
1-Ferrocenyl-1-(triethylsilyl)ethane (4l)



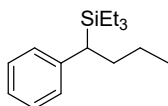
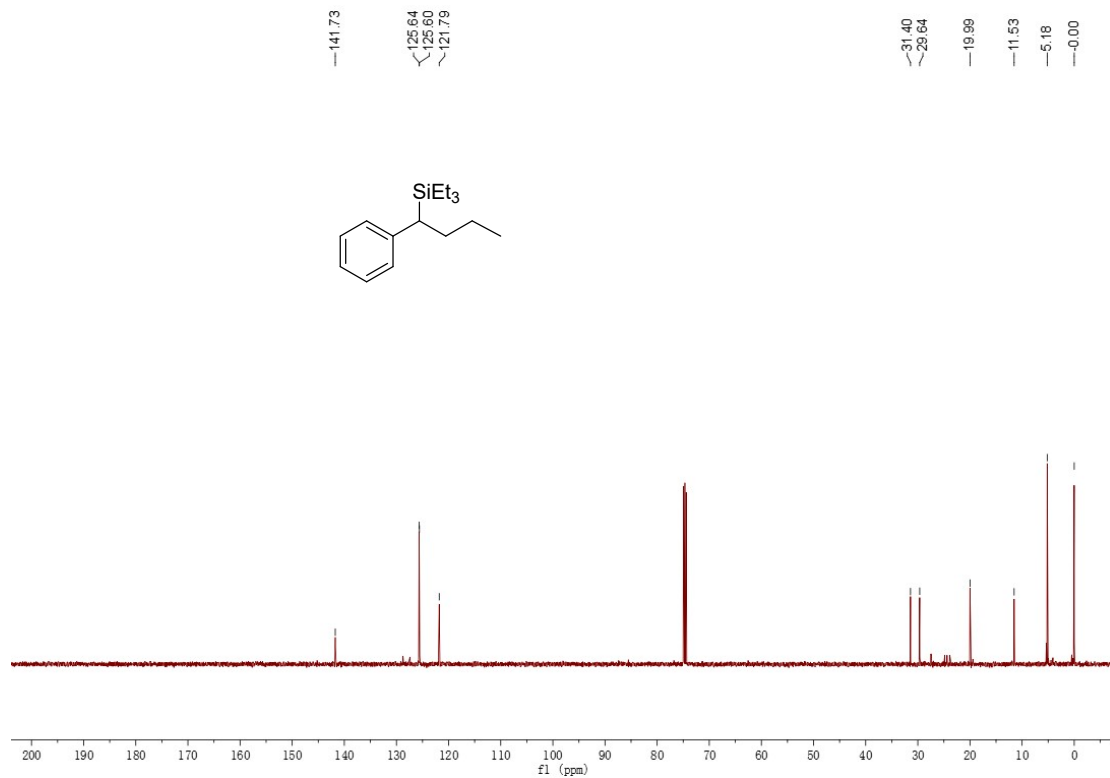
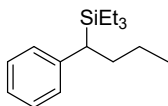
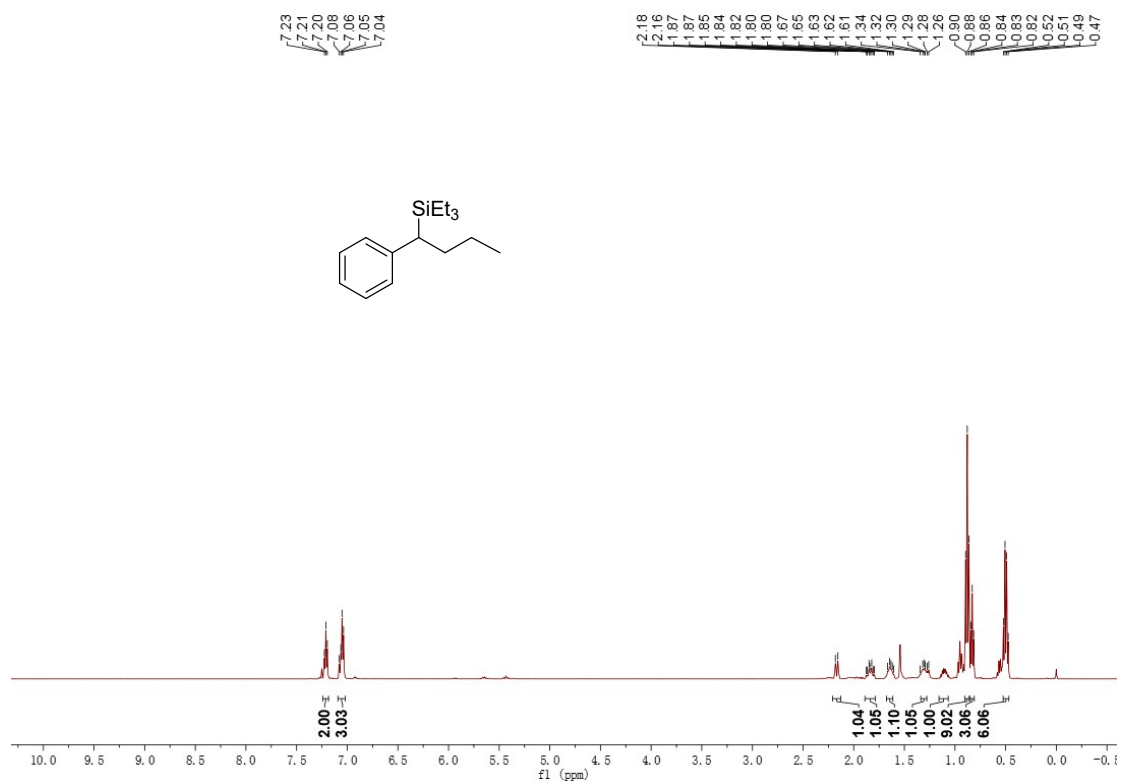
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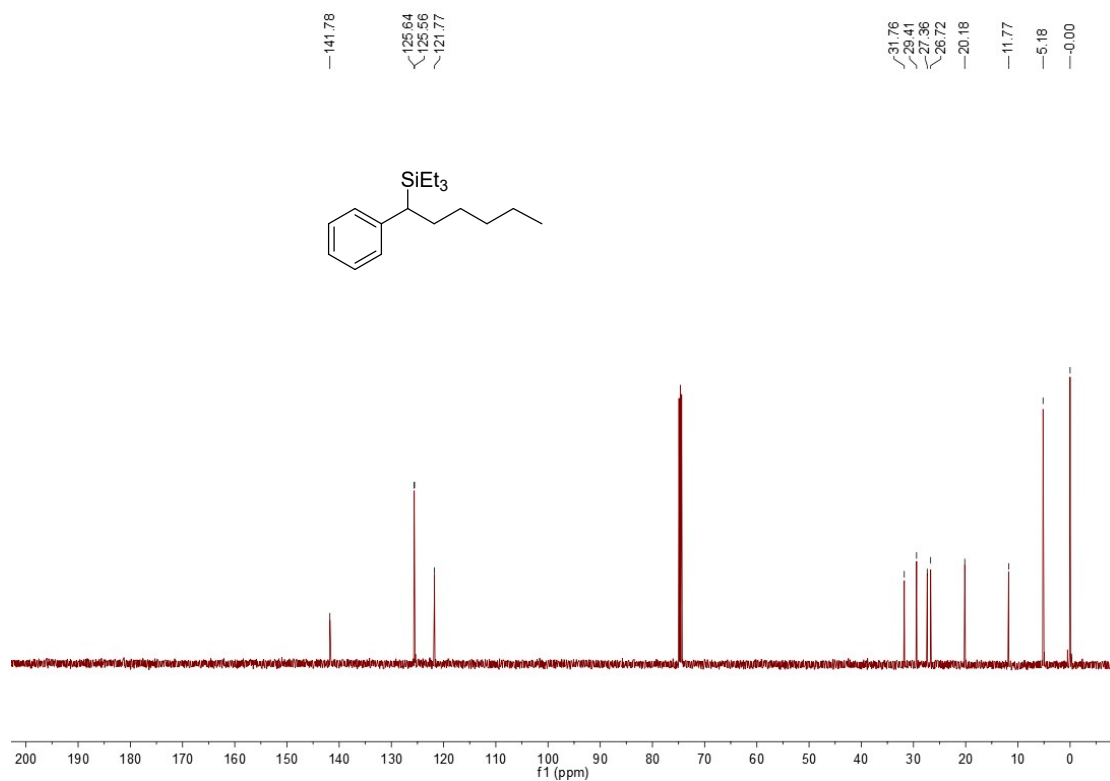
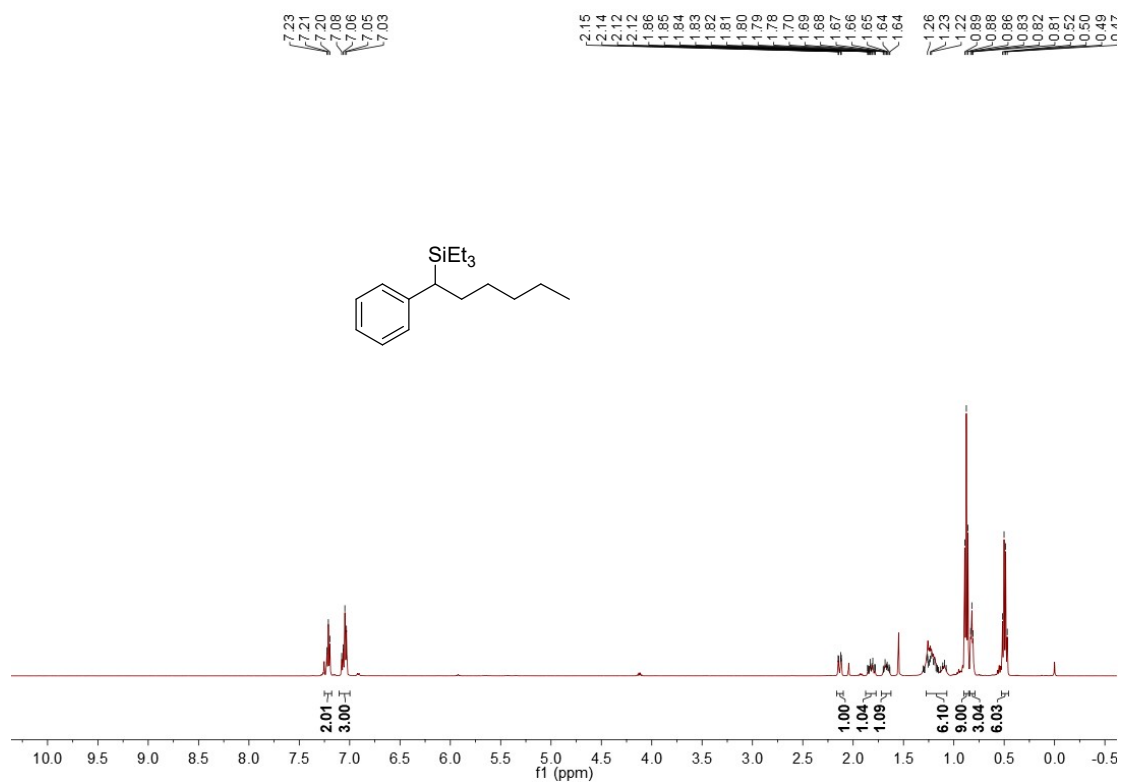
Triethyl(1-(2-methyl-5-phenylfuran-3-yl)ethyl)silane (4n)



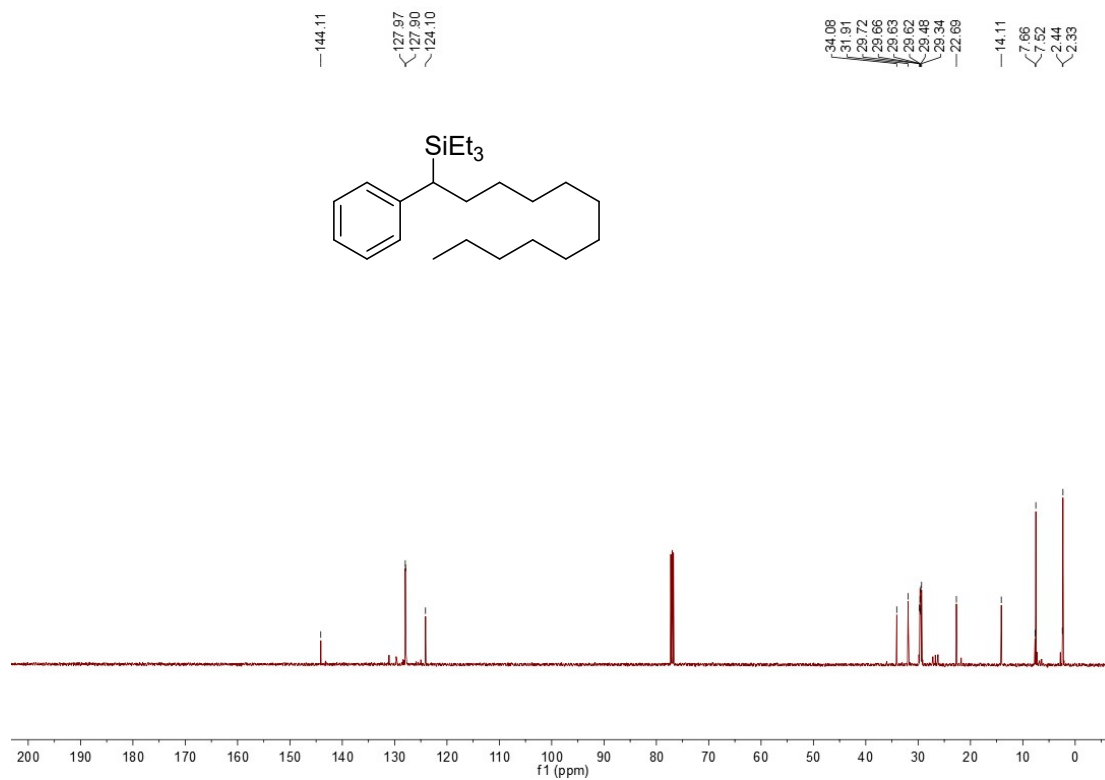
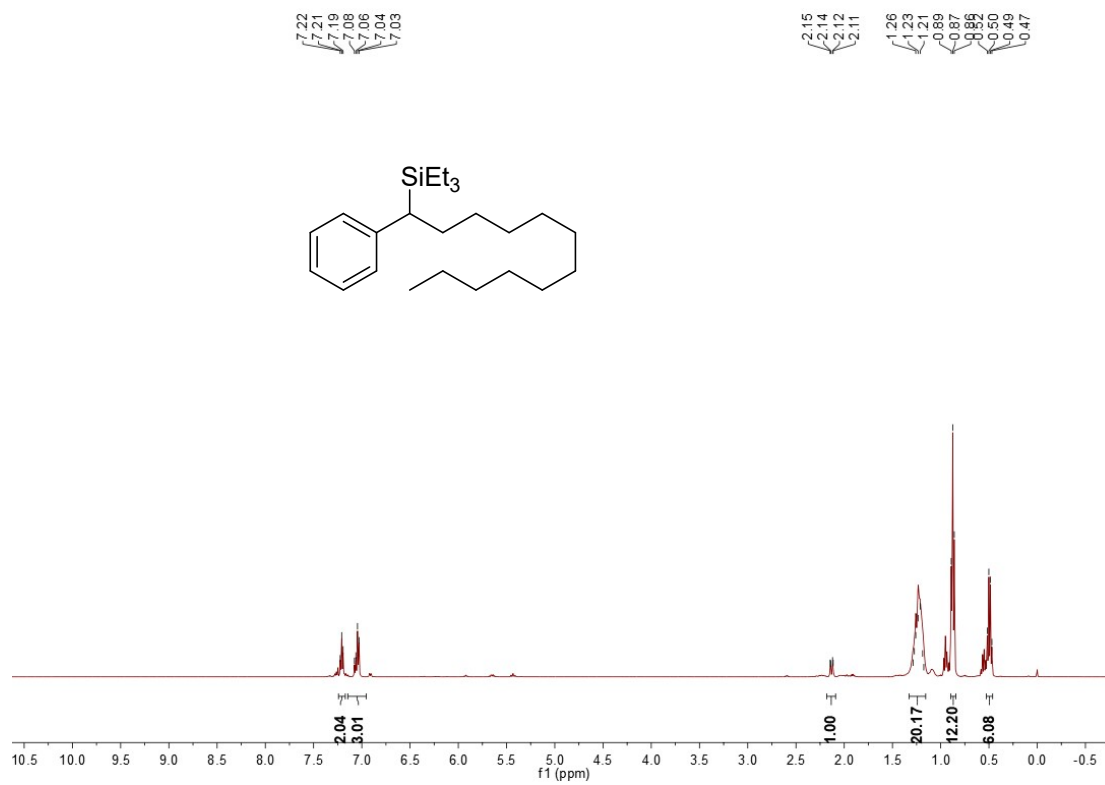
Triethyl(1-phenylbutyl)silane (4o)



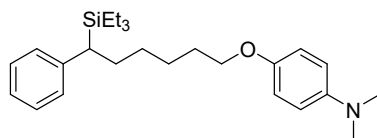
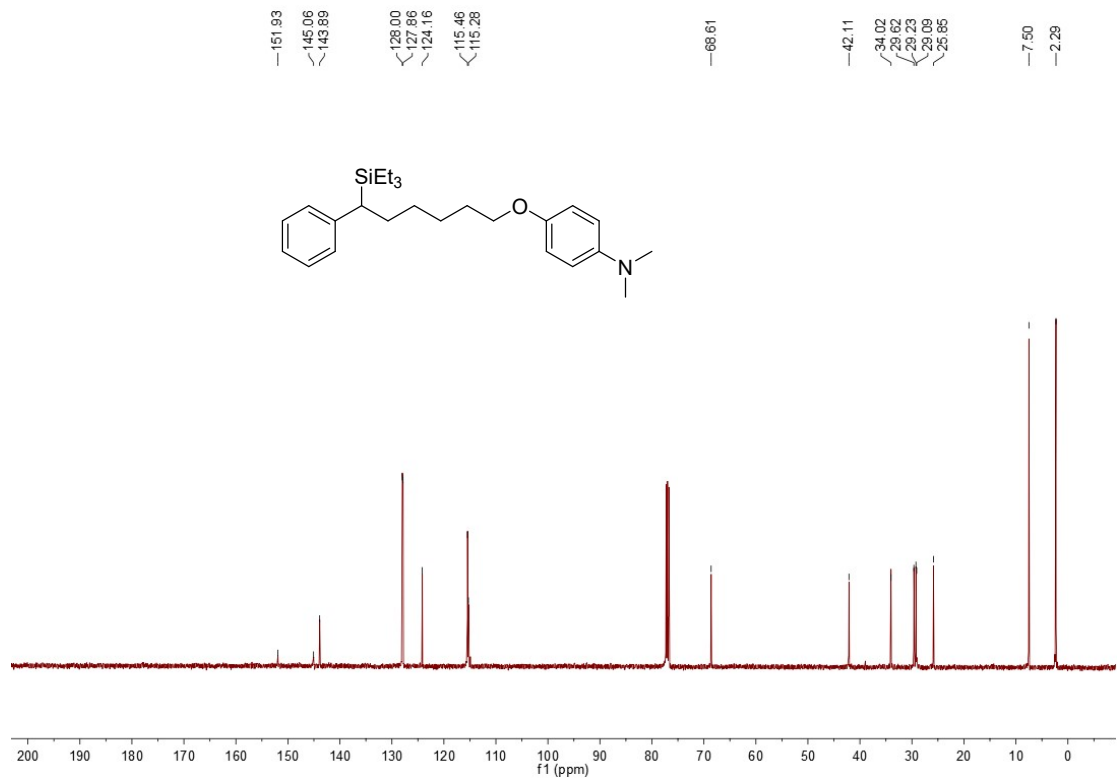
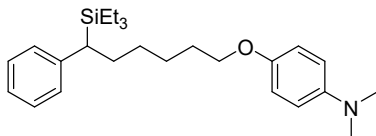
Triethyl(1-phenylhexyl)silane (4p)



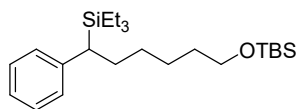
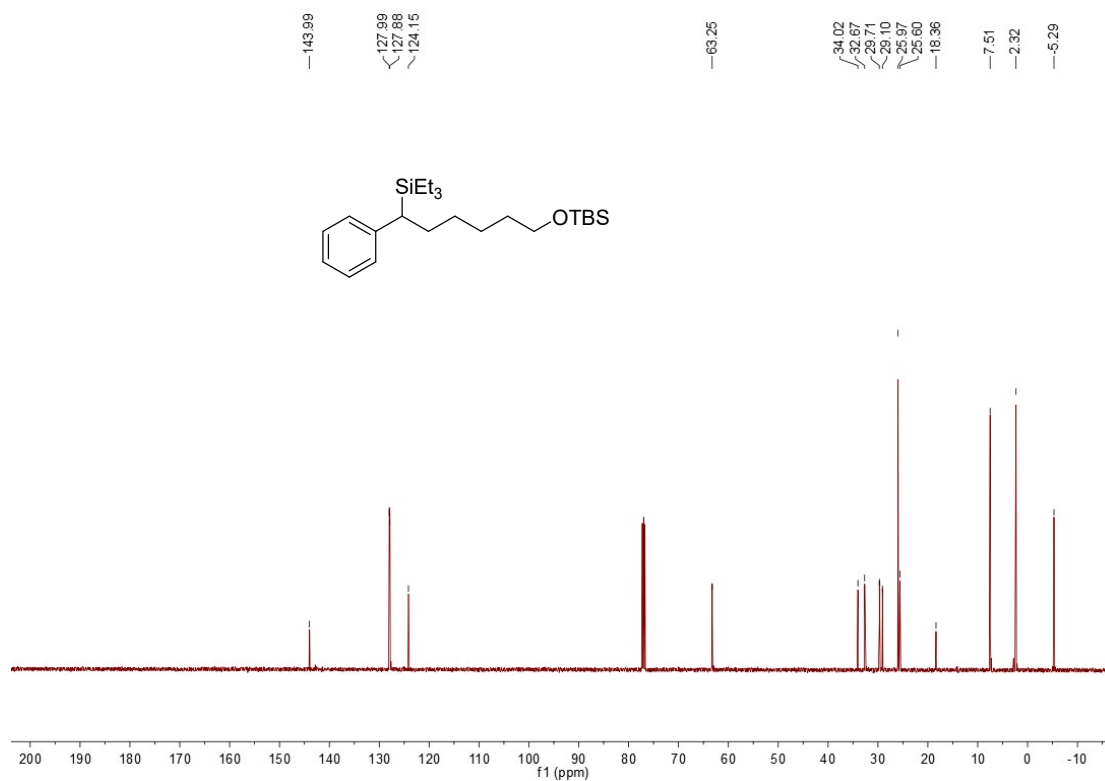
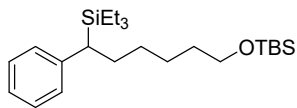
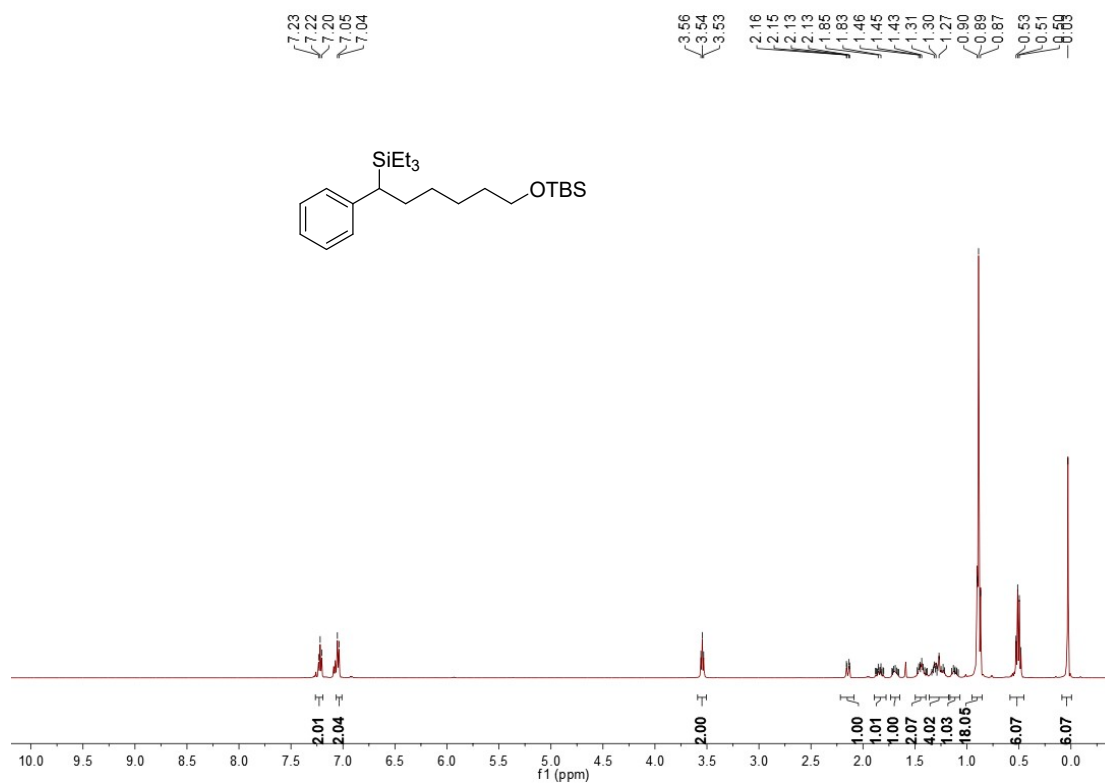
Triethyl(1-phenyldodecyl)silane (4q)



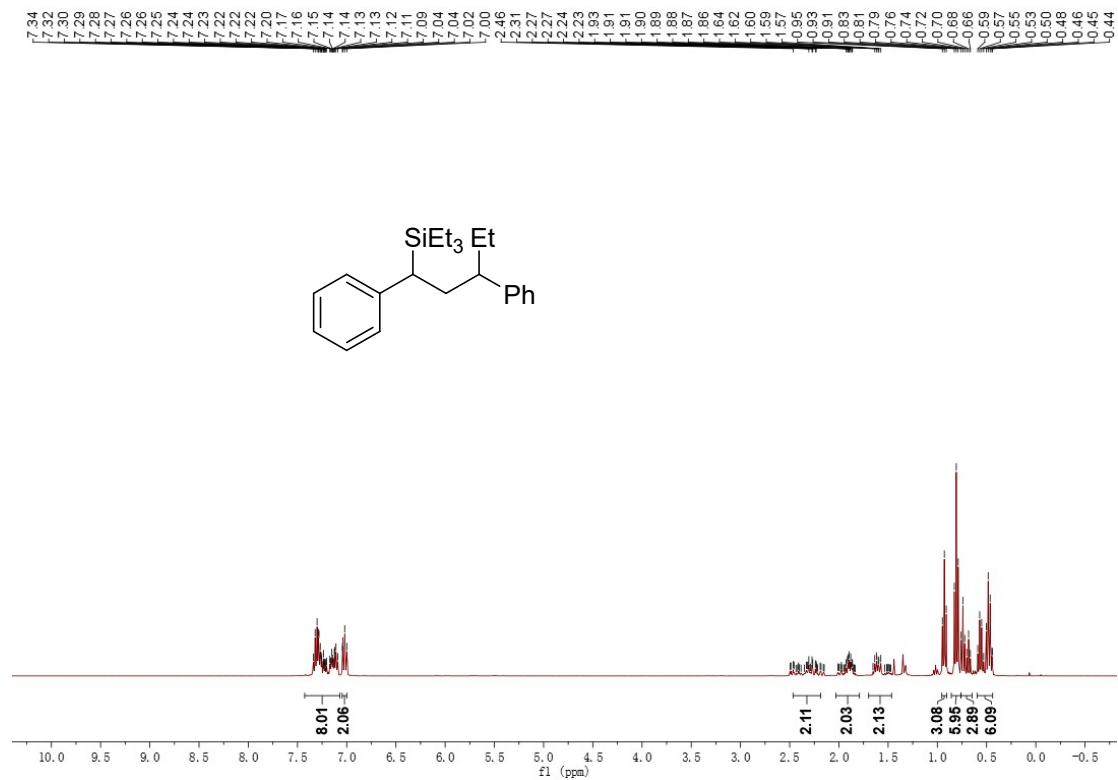
N,N-dimethyl-4-((6-phenyl-6-(triethylsilyl)hexyl)oxy)aniline (4r)



Tert-butyldimethyl((6-phenyl-6-(triethylsilyl)hexyl)oxy)silane (4s)



(1,3-diphenylpentyl)triethylsilane (4t)



146.74
145.03
143.70

28.18
28.12
27.64
25.89
24.25

-46.05

-36.64

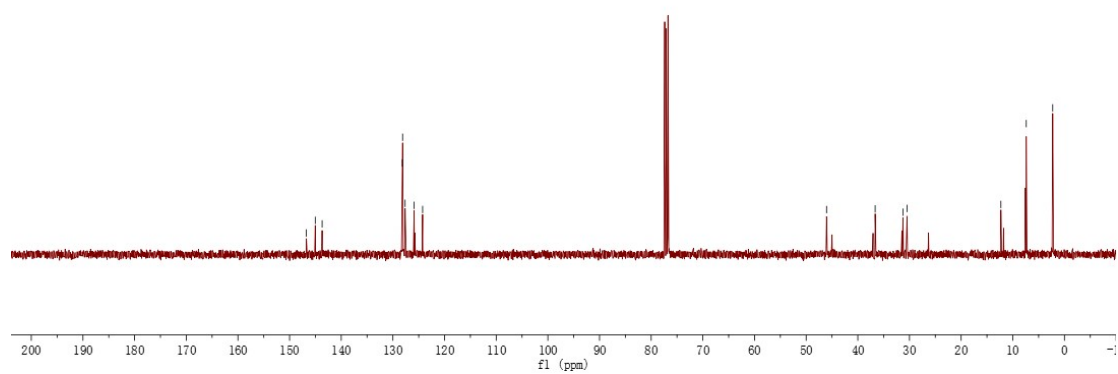
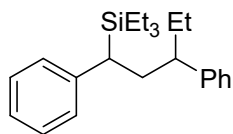
-31.25

-30.46

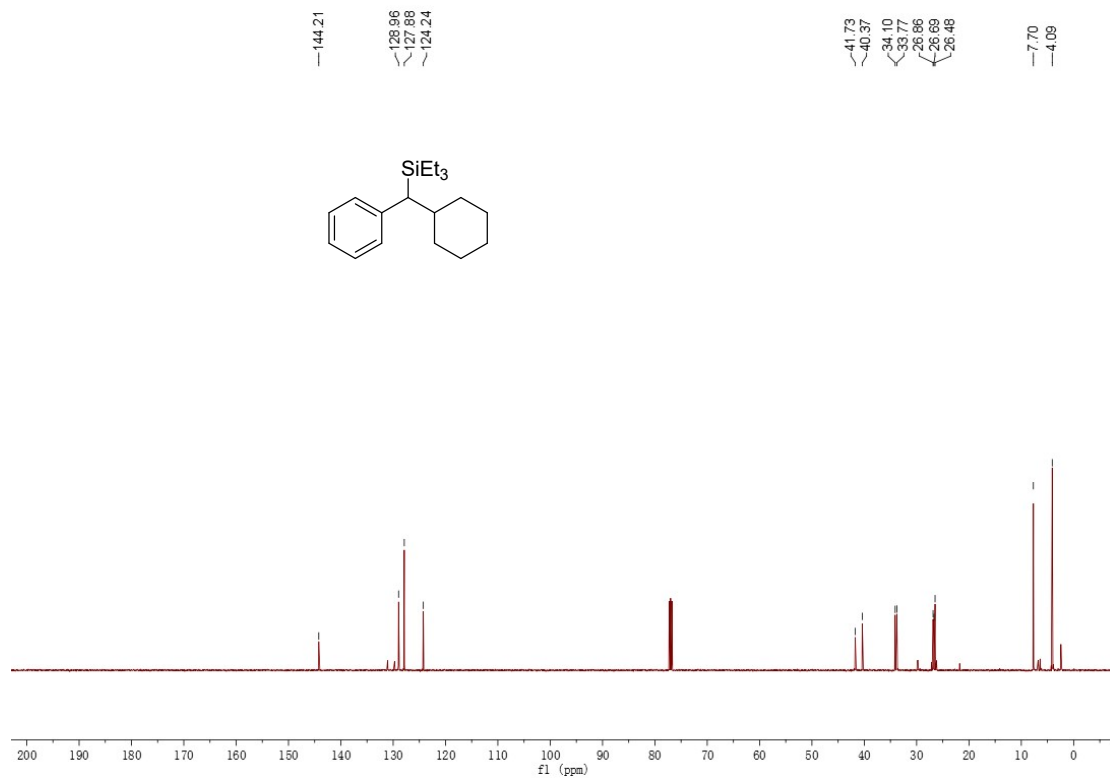
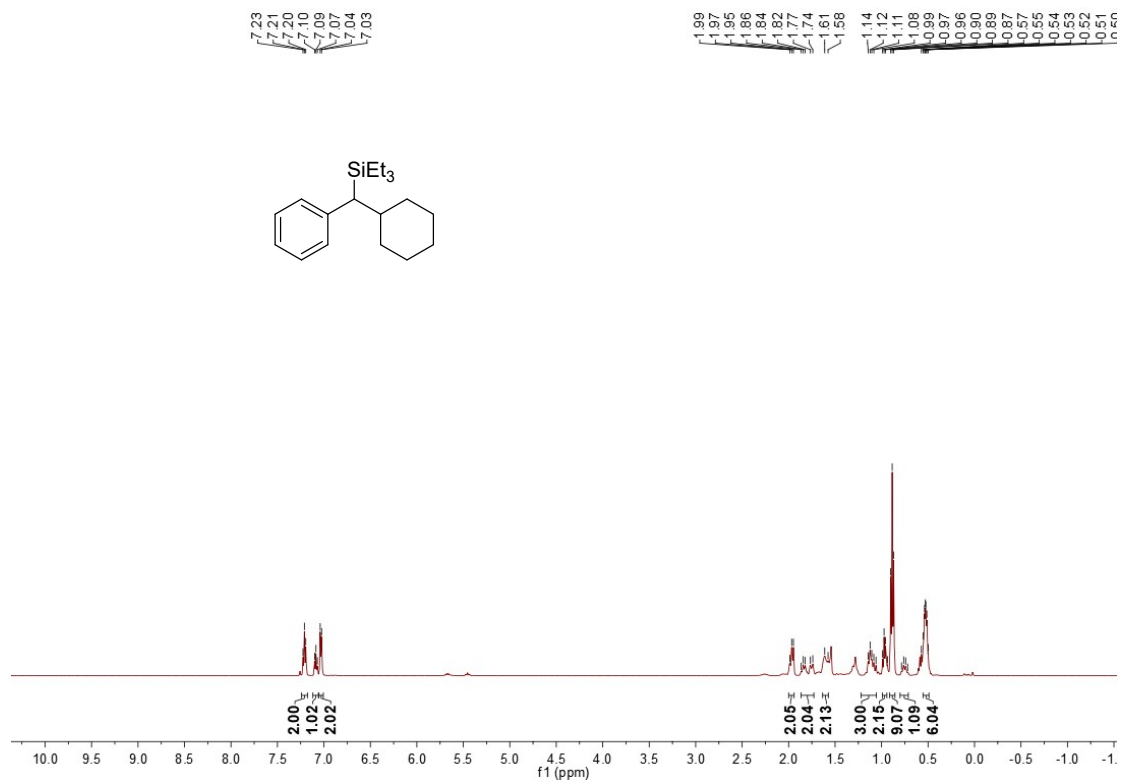
12.30

7.39

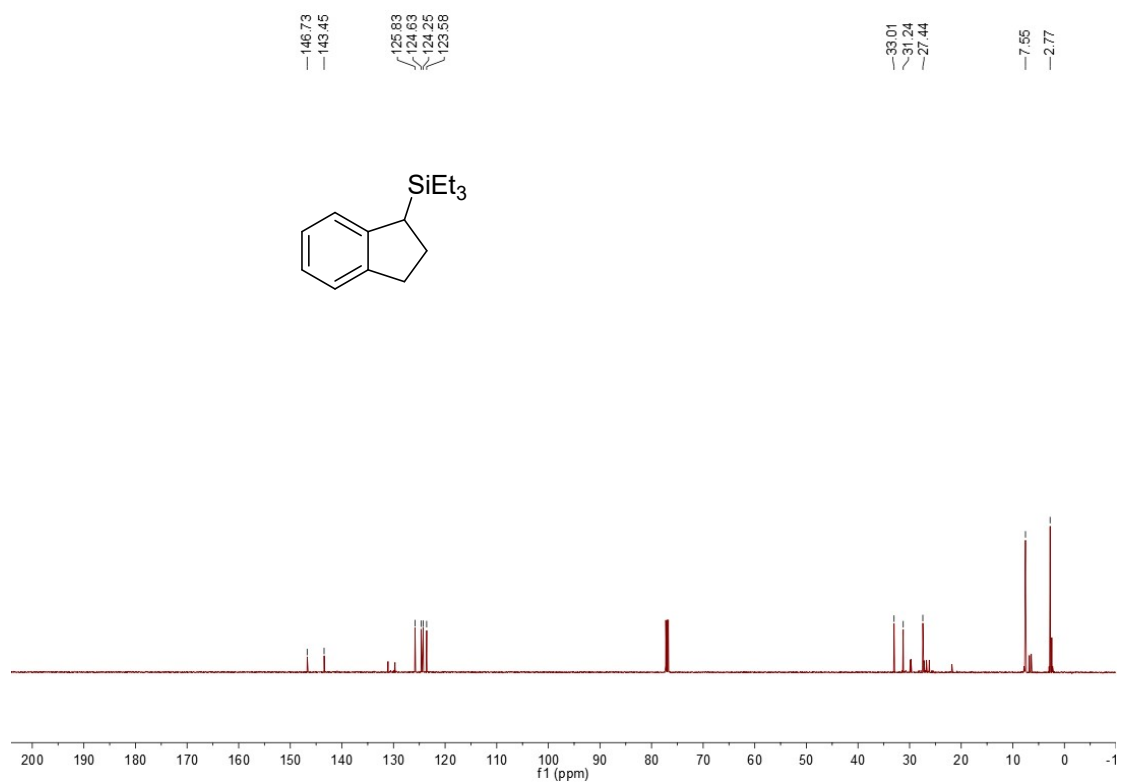
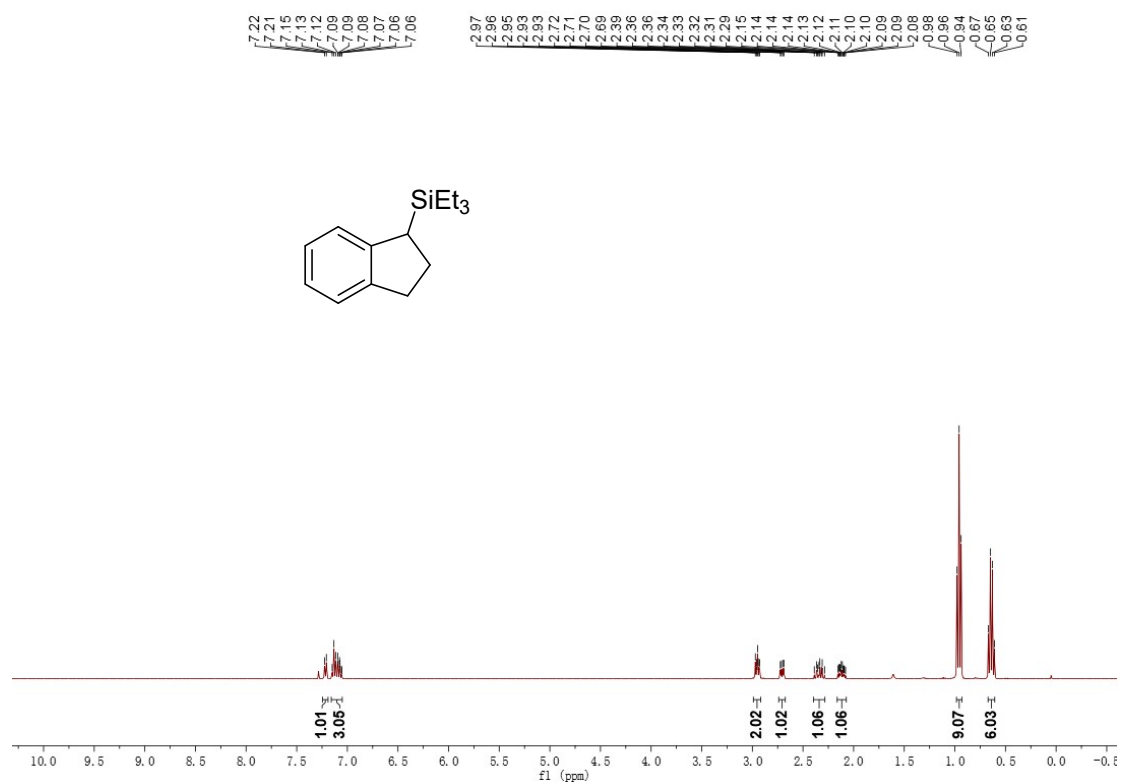
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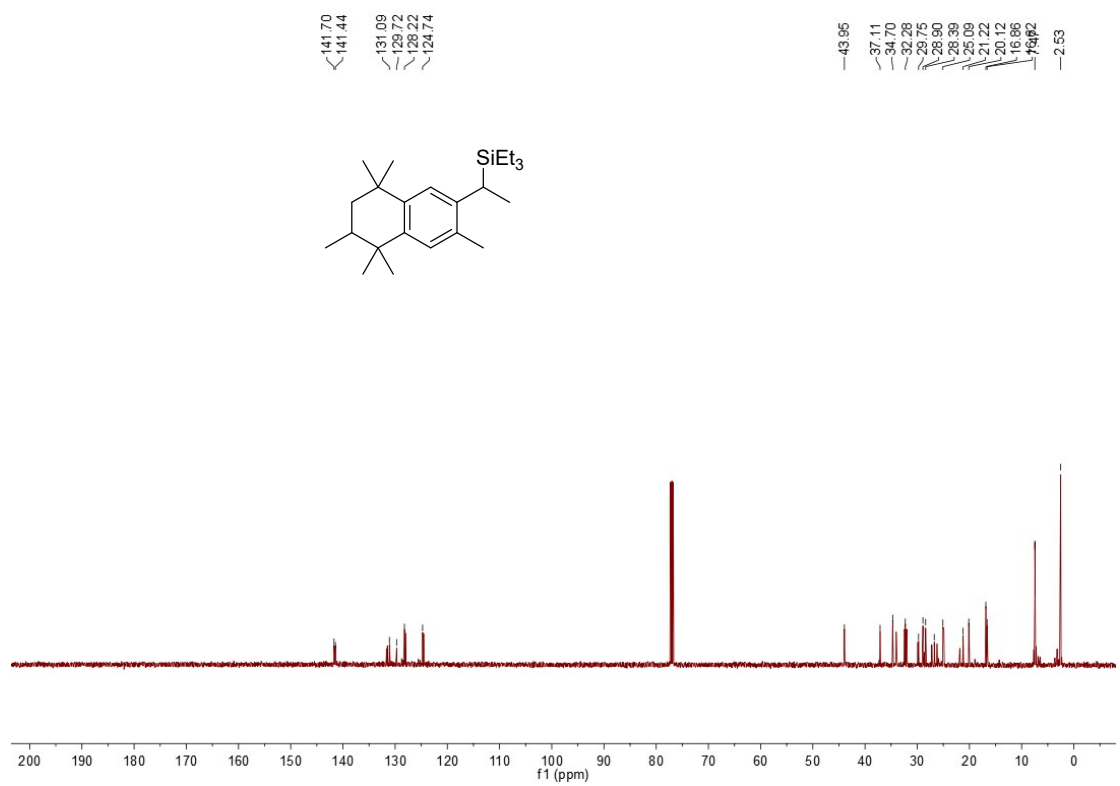
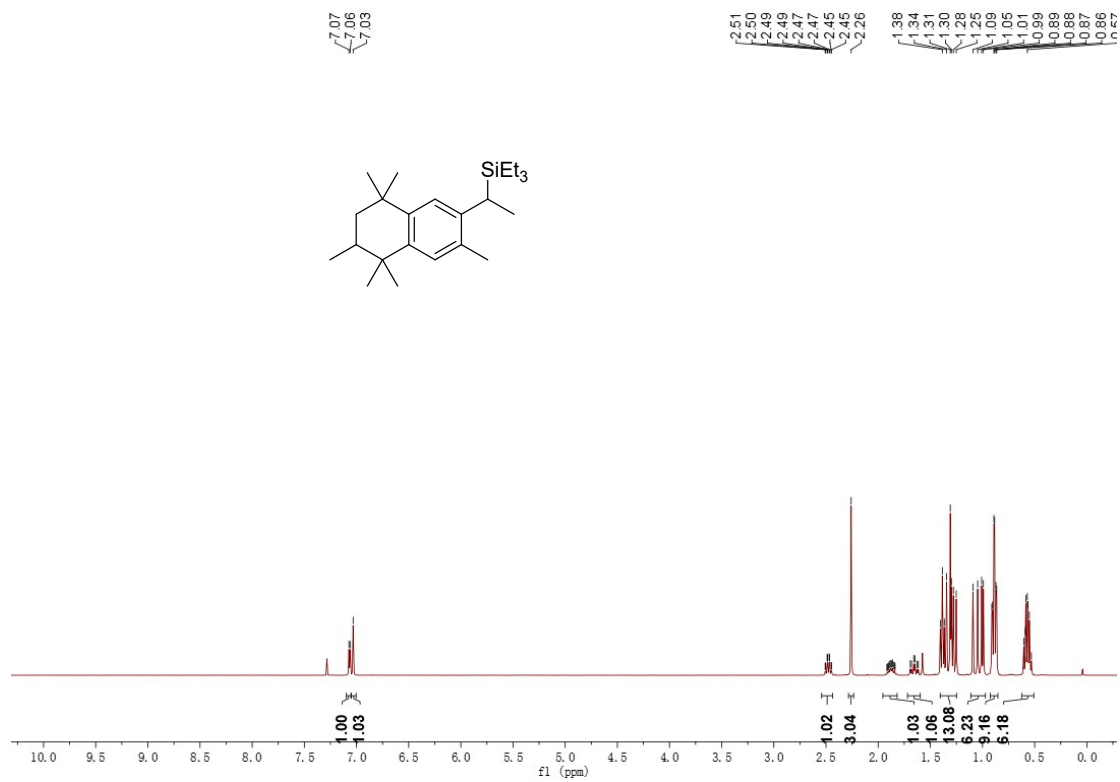
(cyclohexyl(phenyl)methyl)triethylsilane (4u)



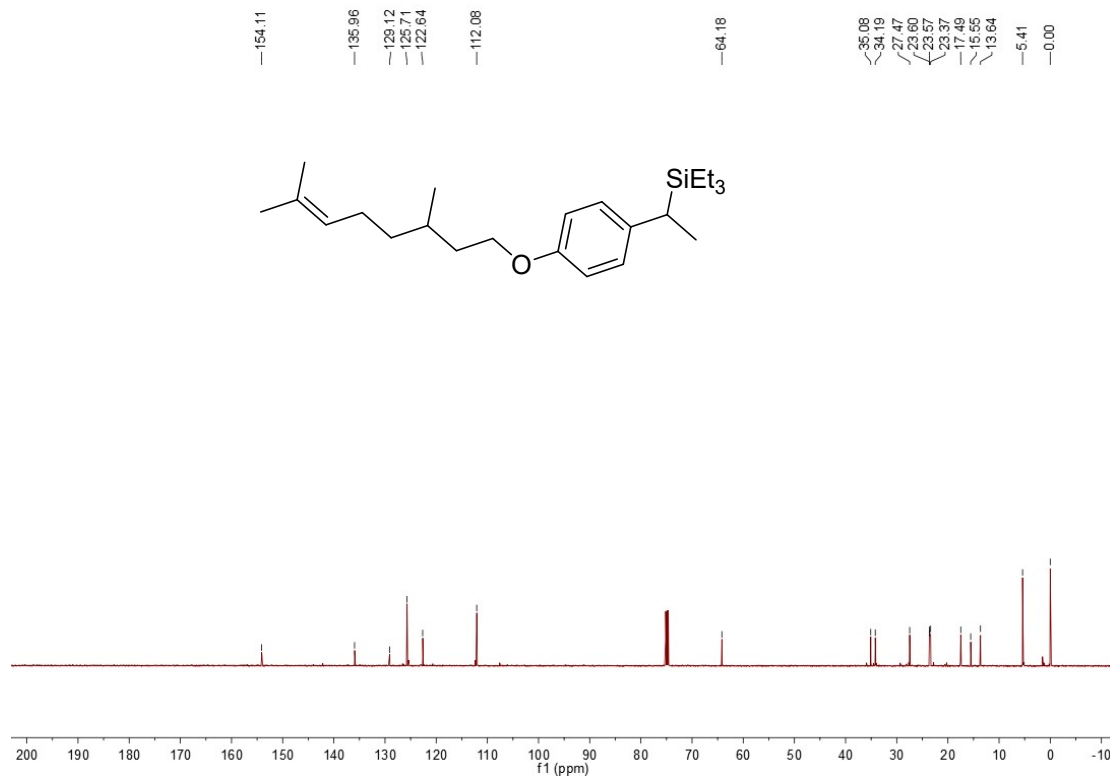
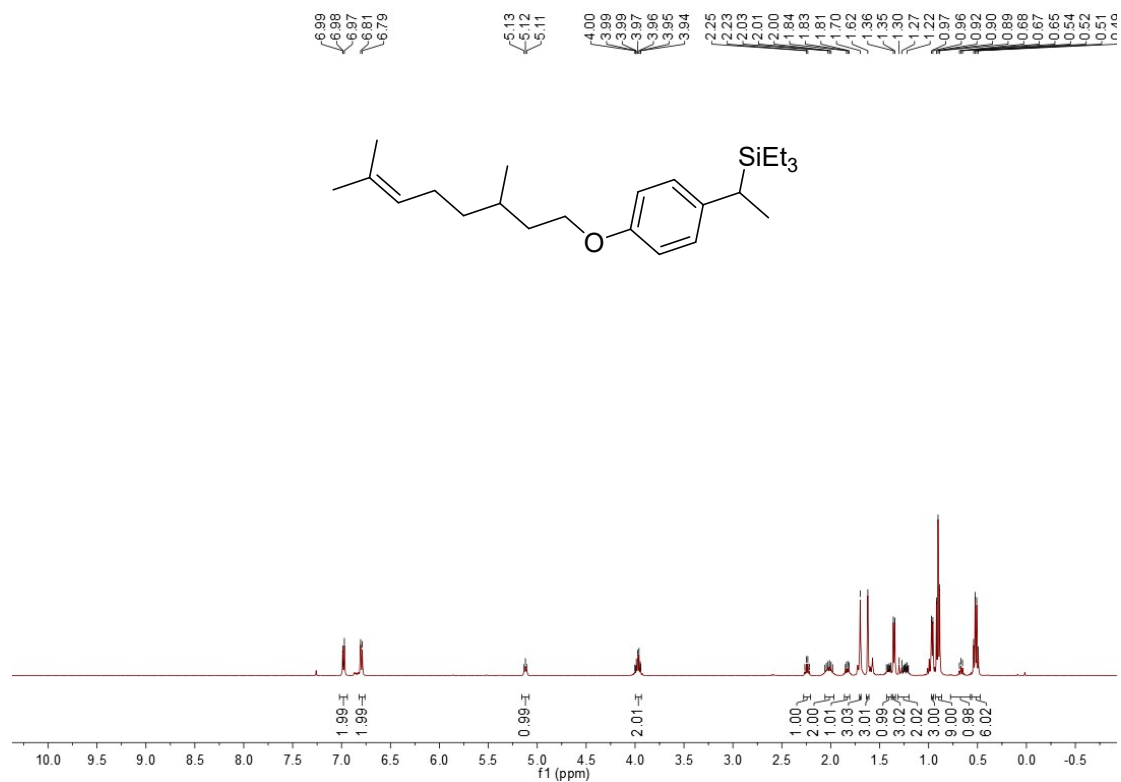
(2,3-dihydro-1H-inden-1-yl)triethylsilane (4v)



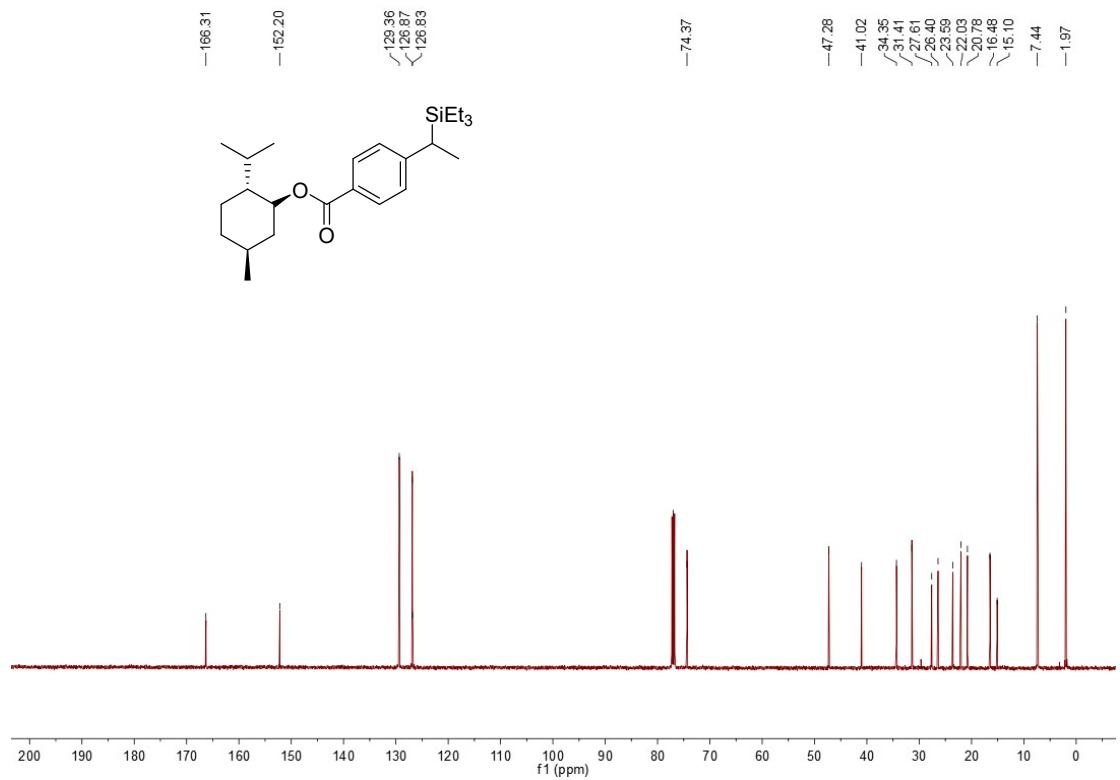
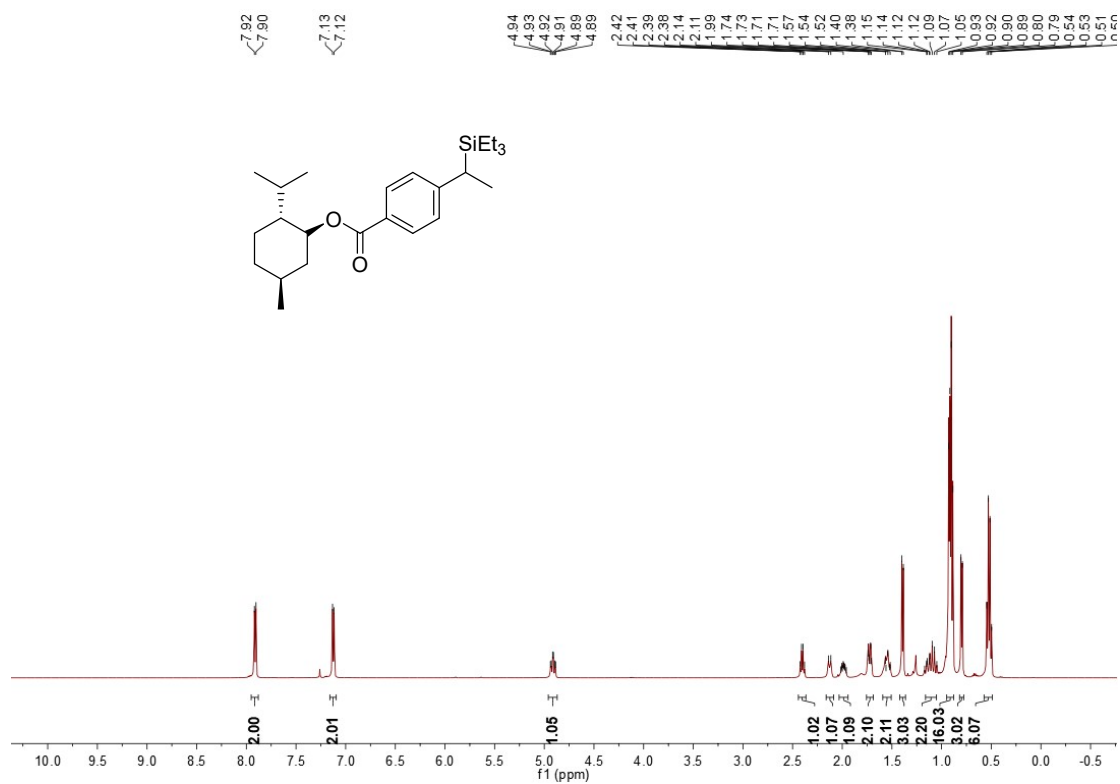
**Triethyl(1-(3,5,5,6,8,8-hexamethyl-5,6,7,8-tetrahydronaphthalen-2-yl)ethyl)silane
(4aa)**



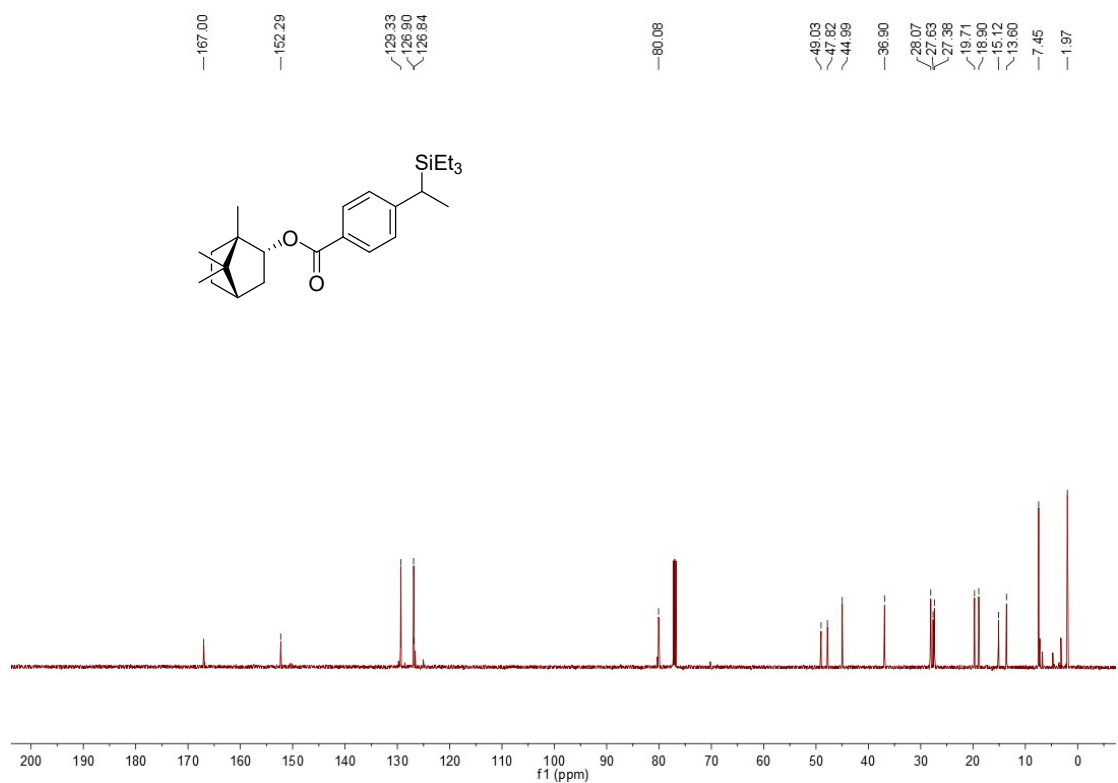
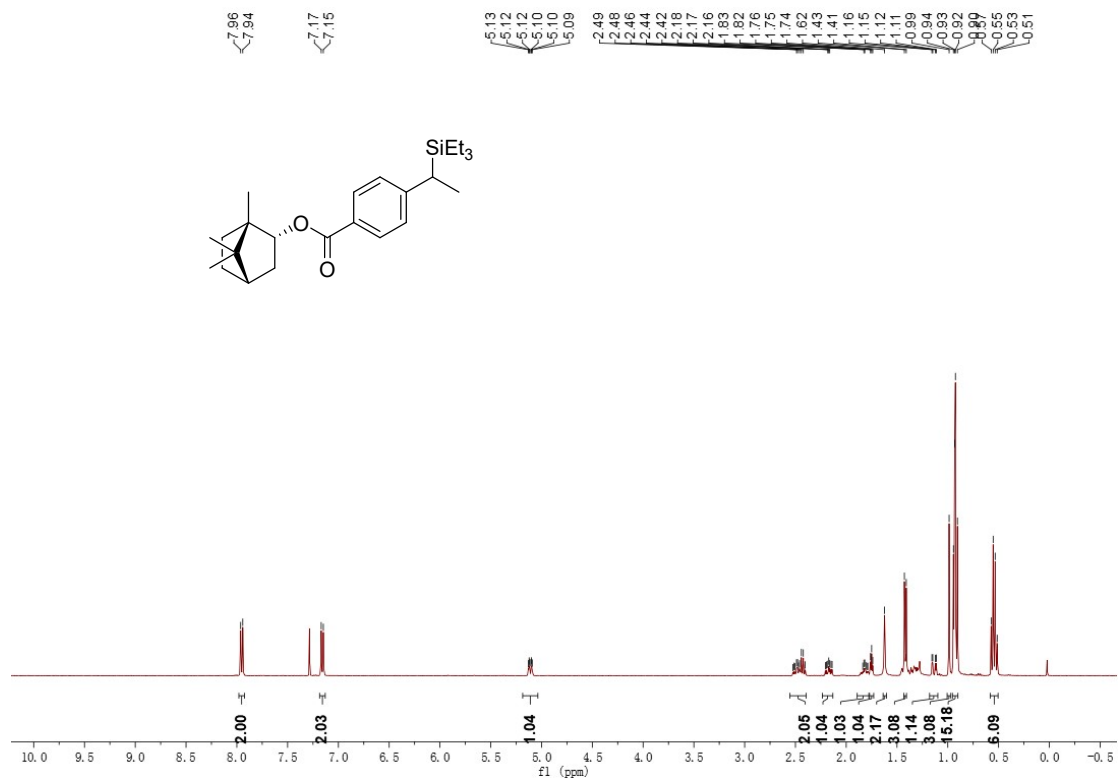
(1-(4-((3,7-dimethyloct-6-en-1-yl)oxy)phenyl)ethyl)triethylsilane (4ab)



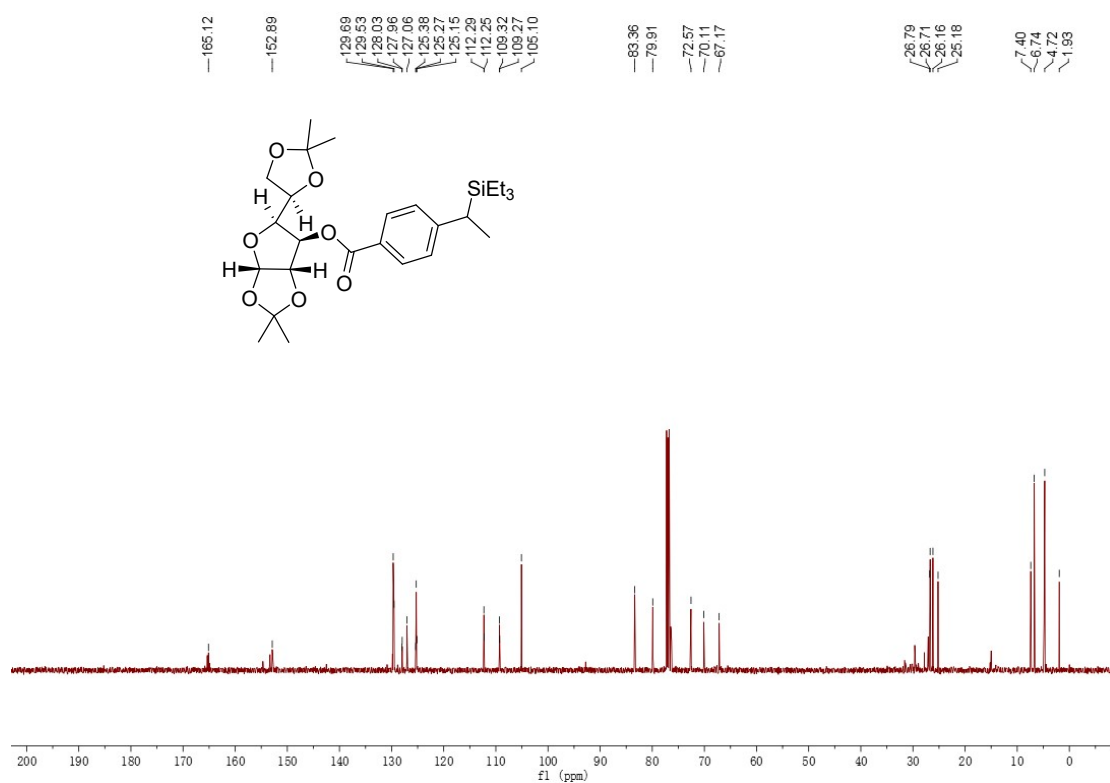
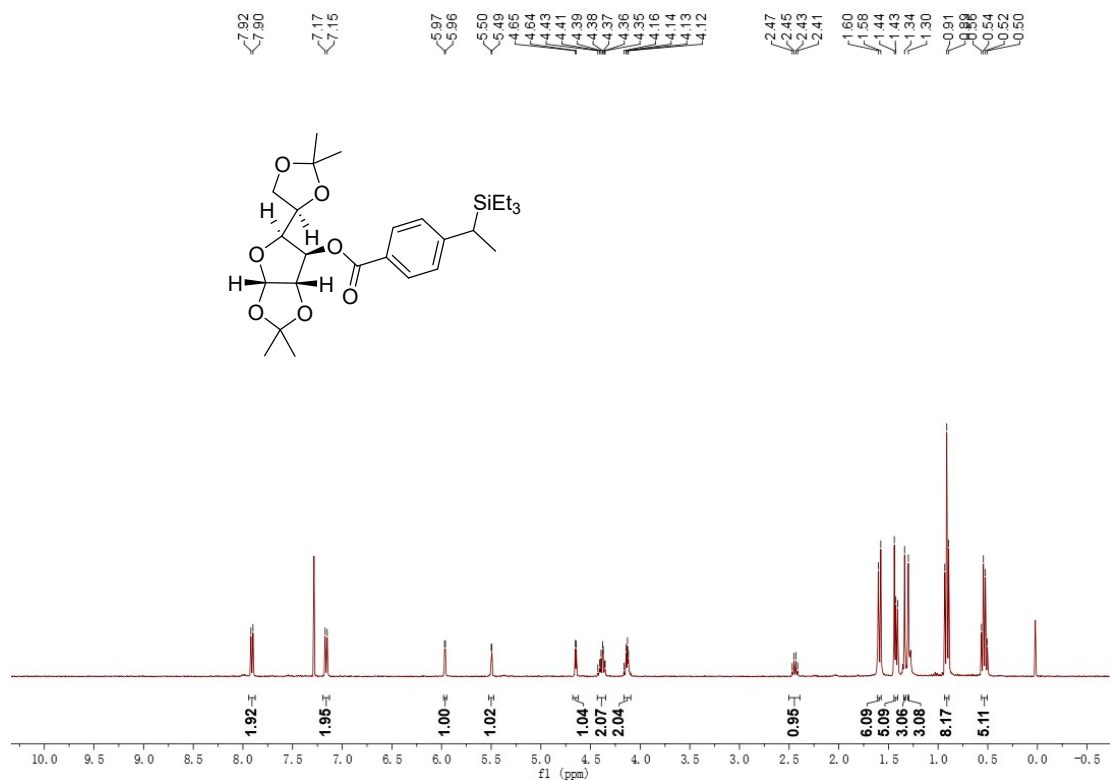
(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 4-(1-(triethylsilyl)ethyl)benzoate (4c)



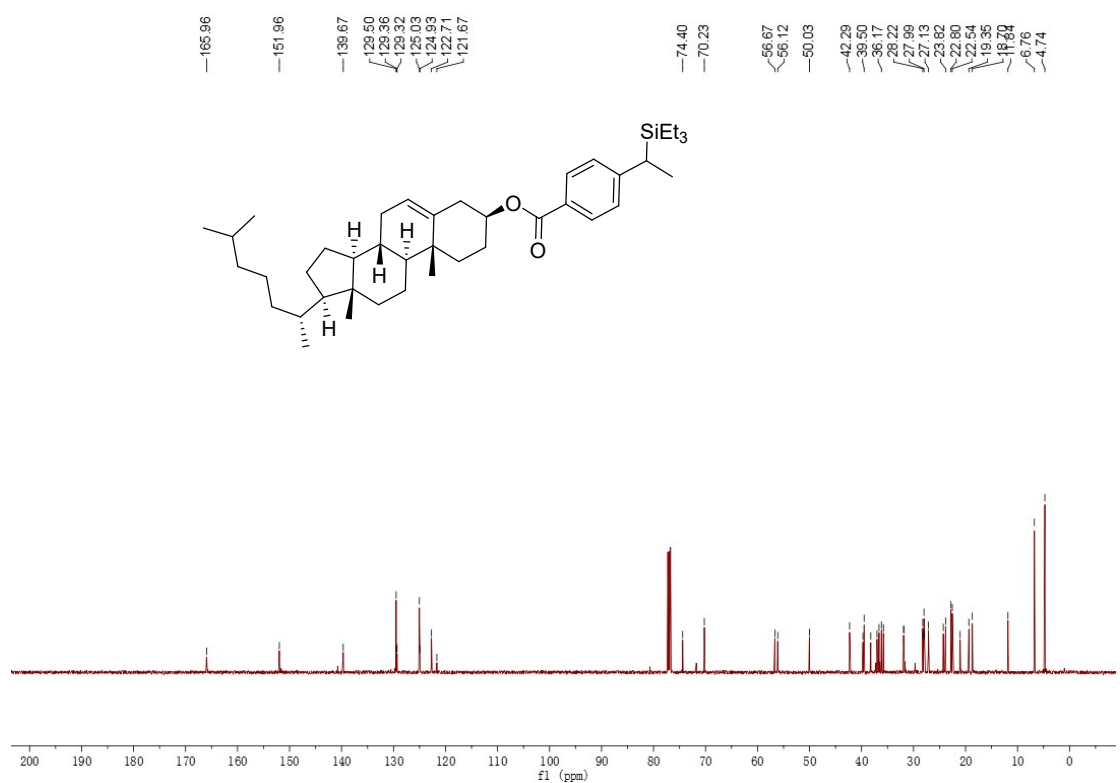
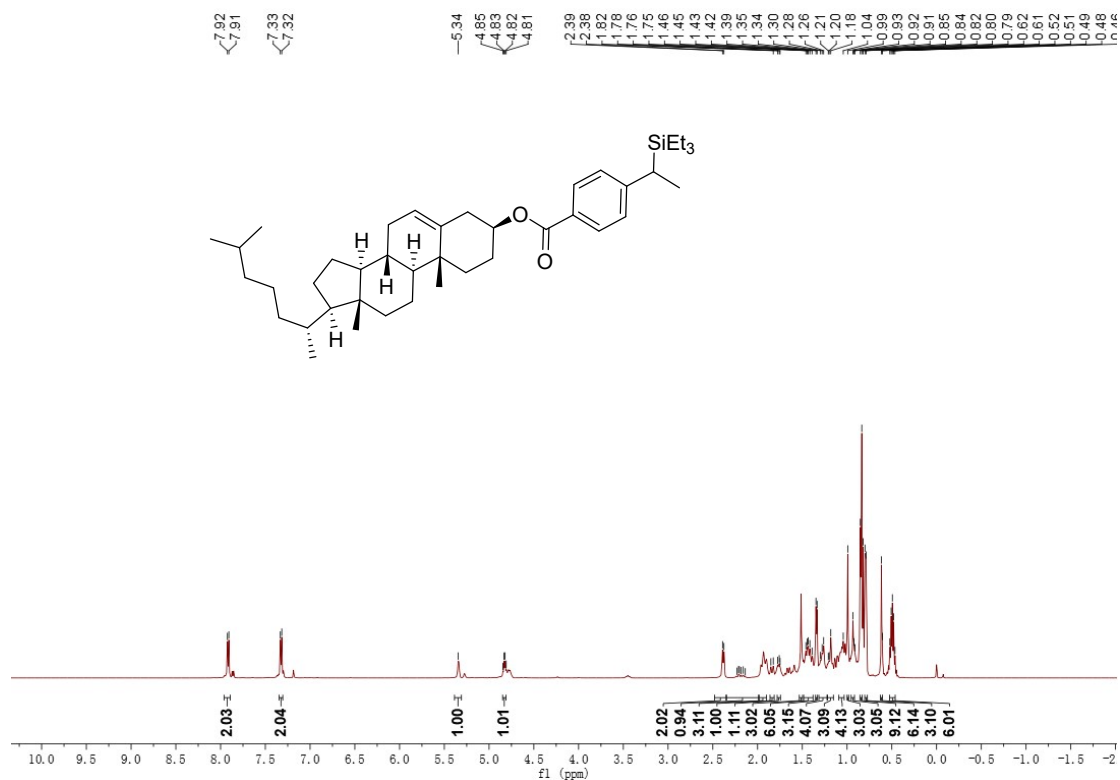
(1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl 4-(1-(triethylsilyl)ethyl)benzoate (4ad)



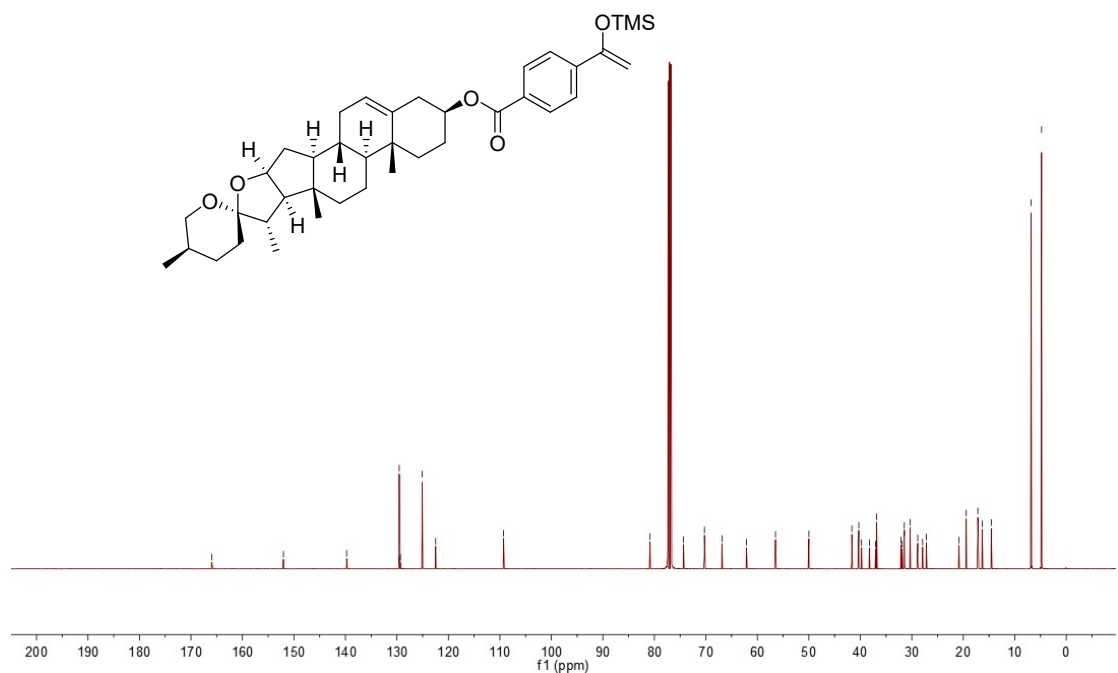
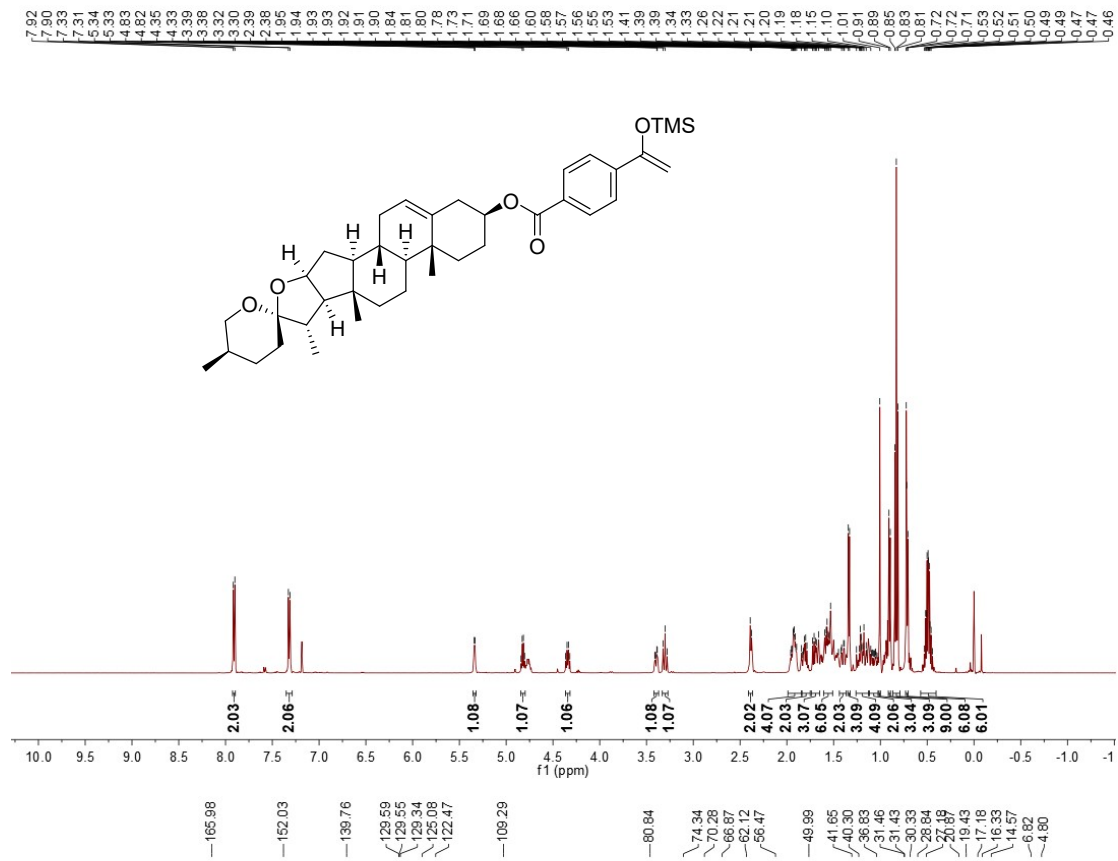
(3aS,5S,6R,6aS)-5-((R)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-d][1,3]dioxol-6-yl 4-(1-(triethylsilyl)ethyl)benzoate
(4ae)



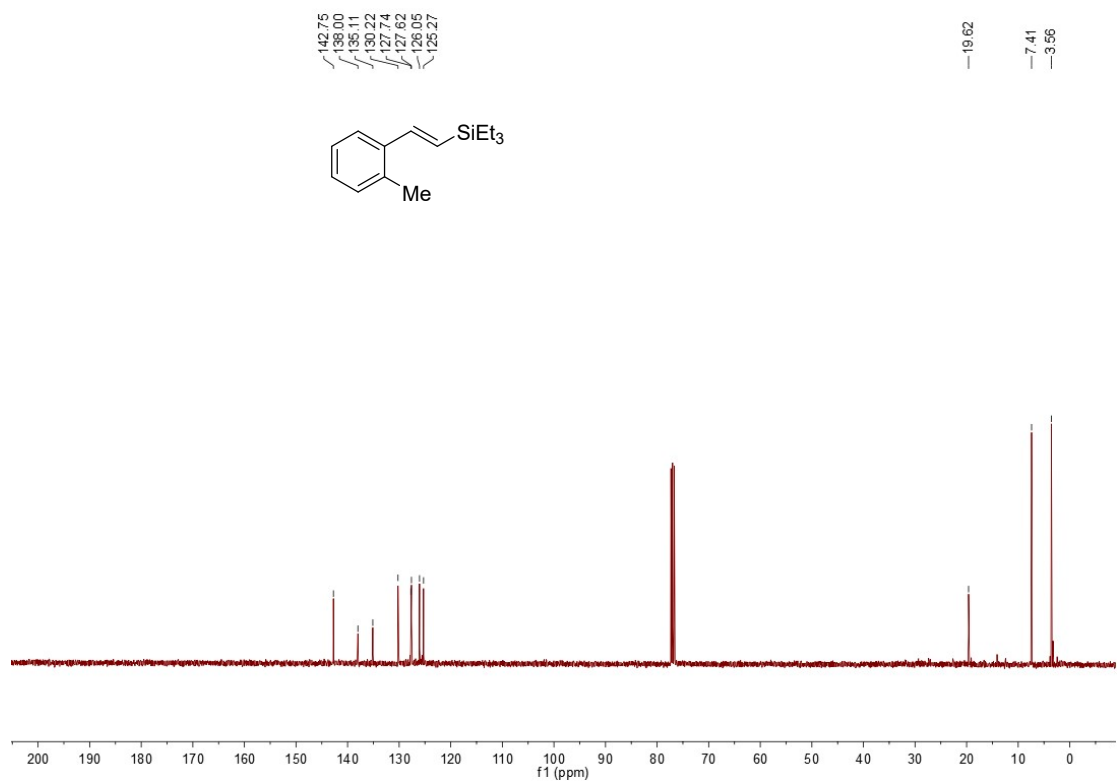
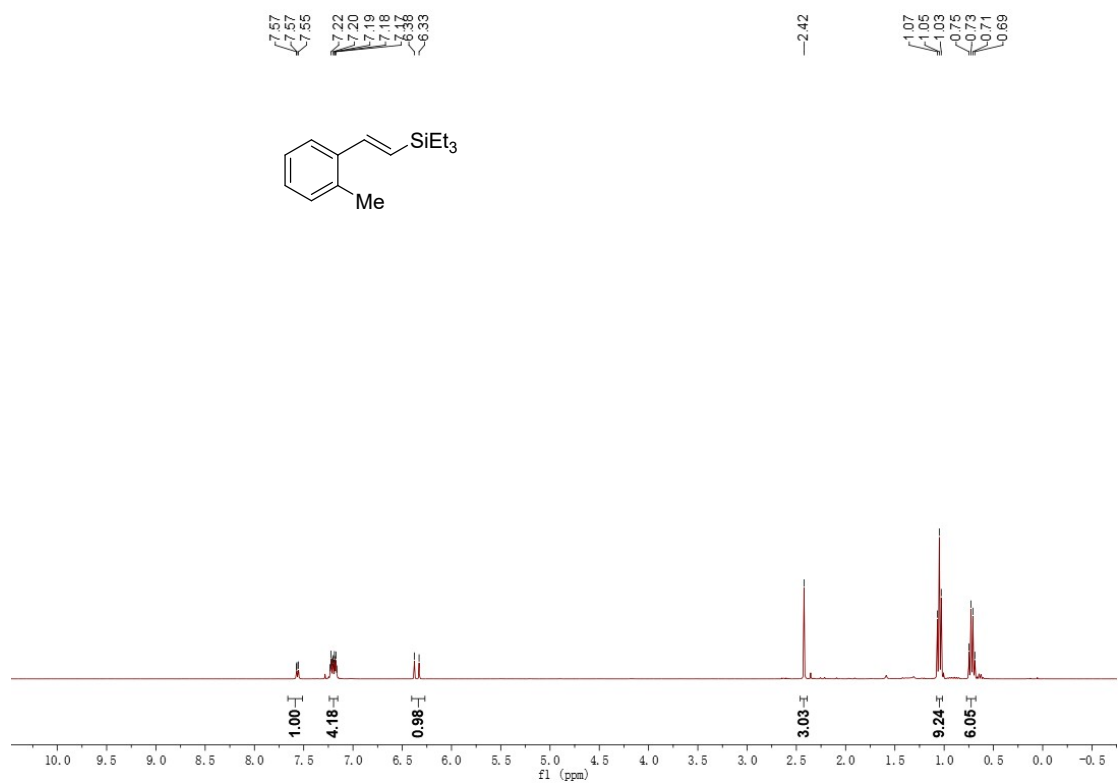
(3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-((R)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 4-(1-(triethylsilyl)ethyl)benzoate (4af)



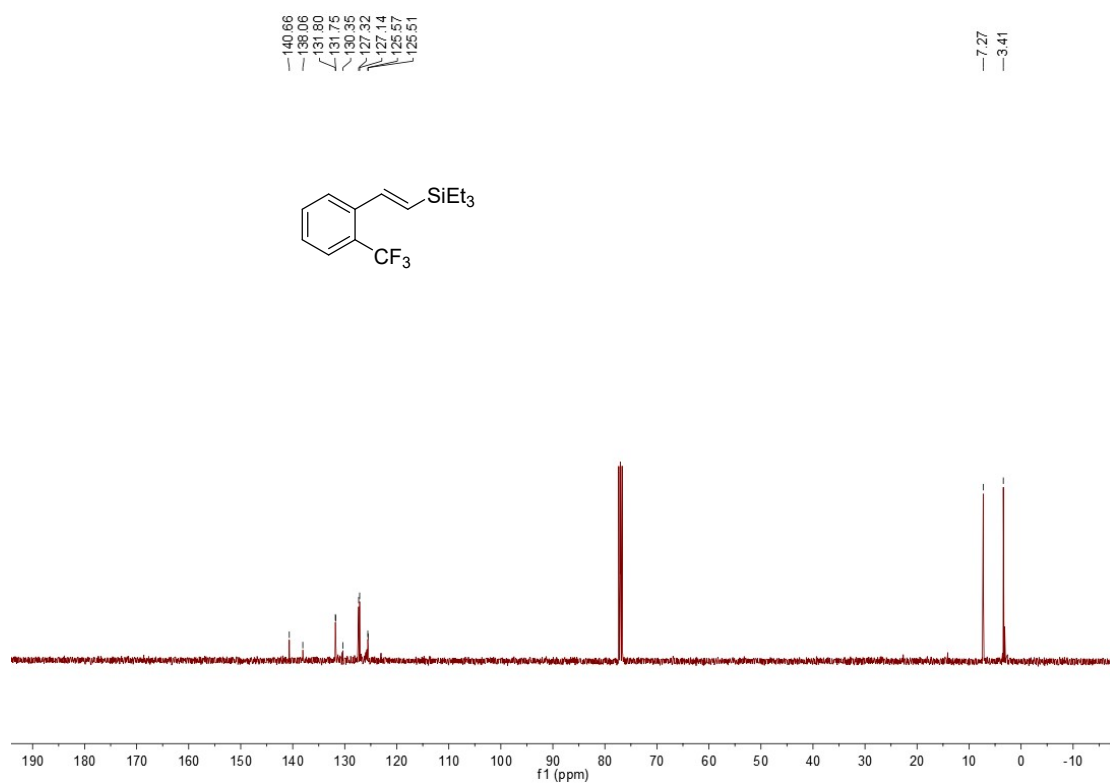
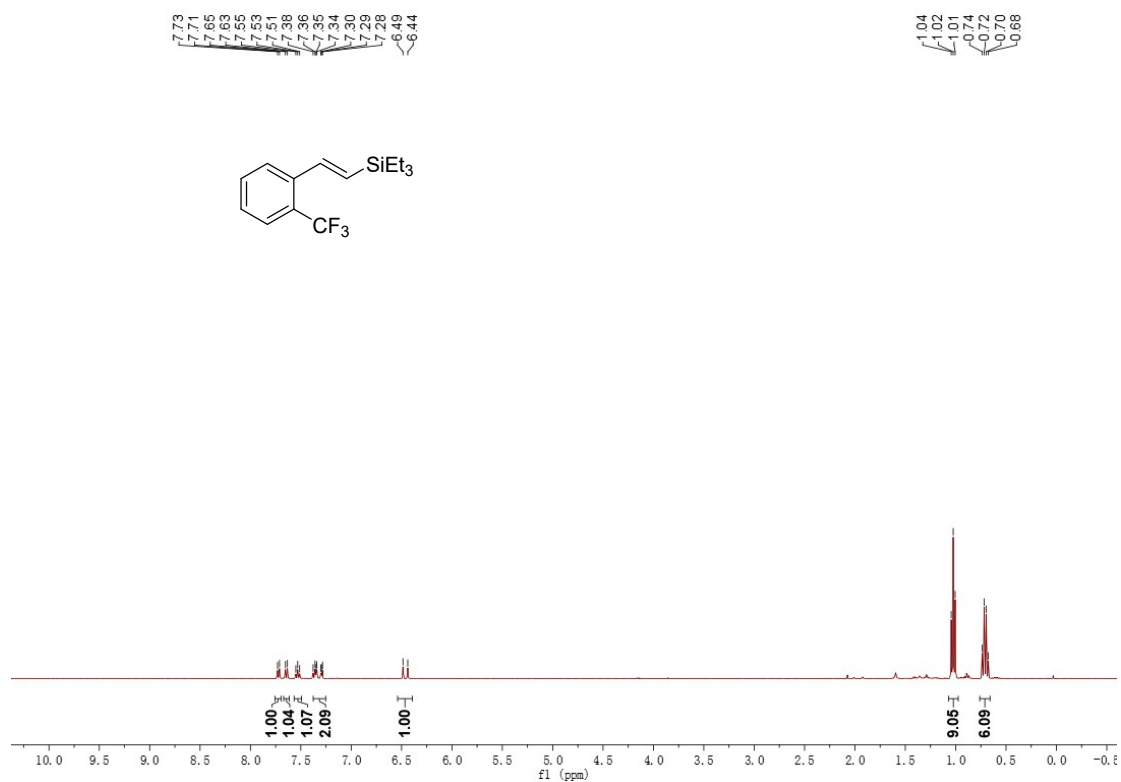
(4S,5'R,6aR,6bS,8aS,8bR,9S,10R,11aS,12aS,12bS)-5',6a,8a,9-tetramethyl-1,3,3',4,4',5,5',6,6a,6b,6',7,8,8a,8b,9,11a,12,12a,12b-icosahydrospiro[naphtho[2',1':4,5]indeno[2,1-b]furan-10,2'-pyran]-4-yl 4-(1-(triethylsilyl)ethyl)benzoate (4ag)



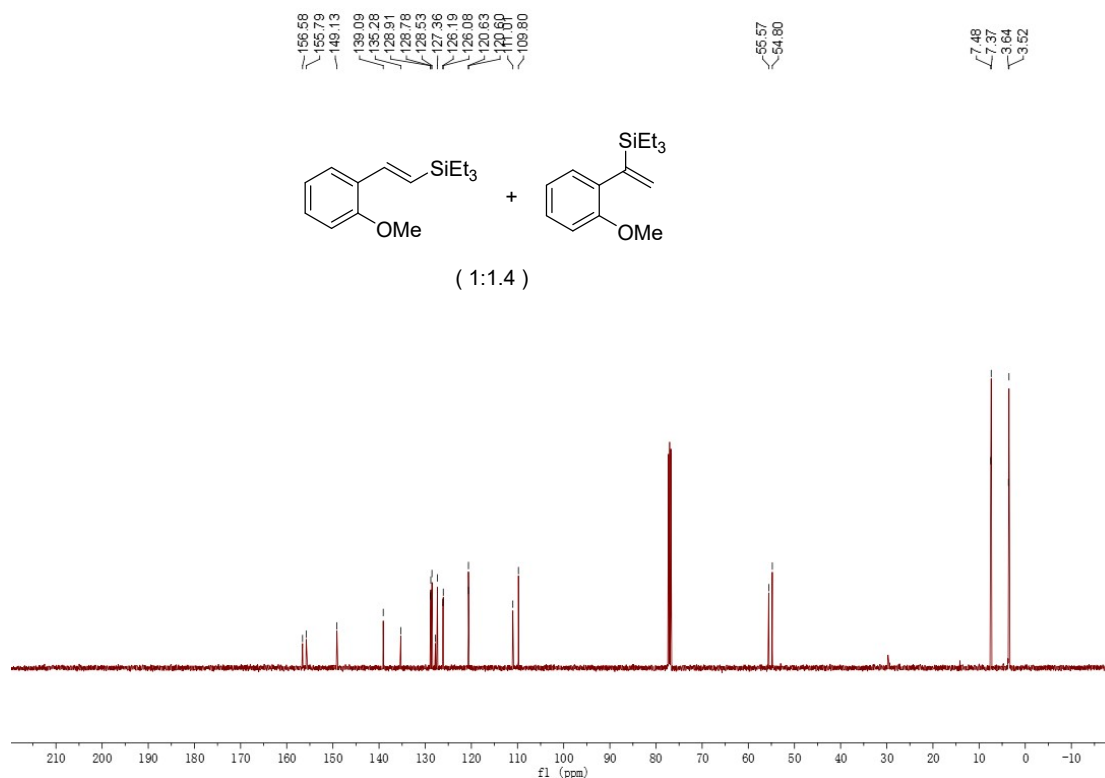
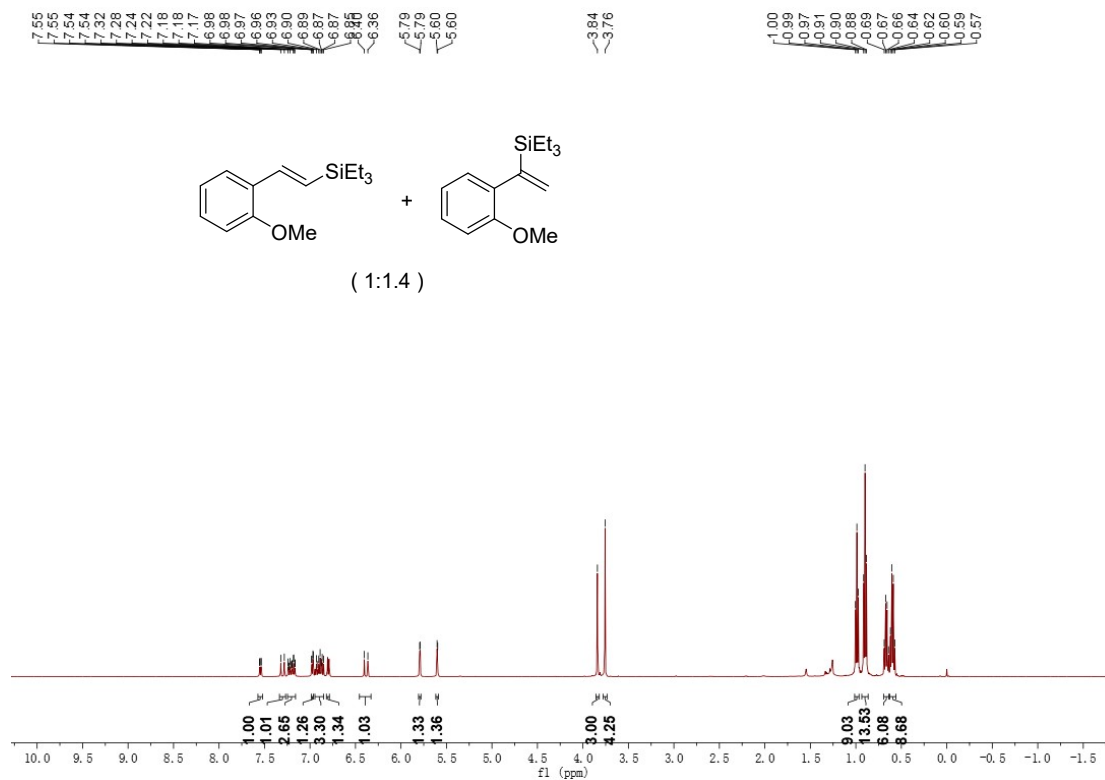
(E)-triethyl(2-methylstyryl)silane (5a)



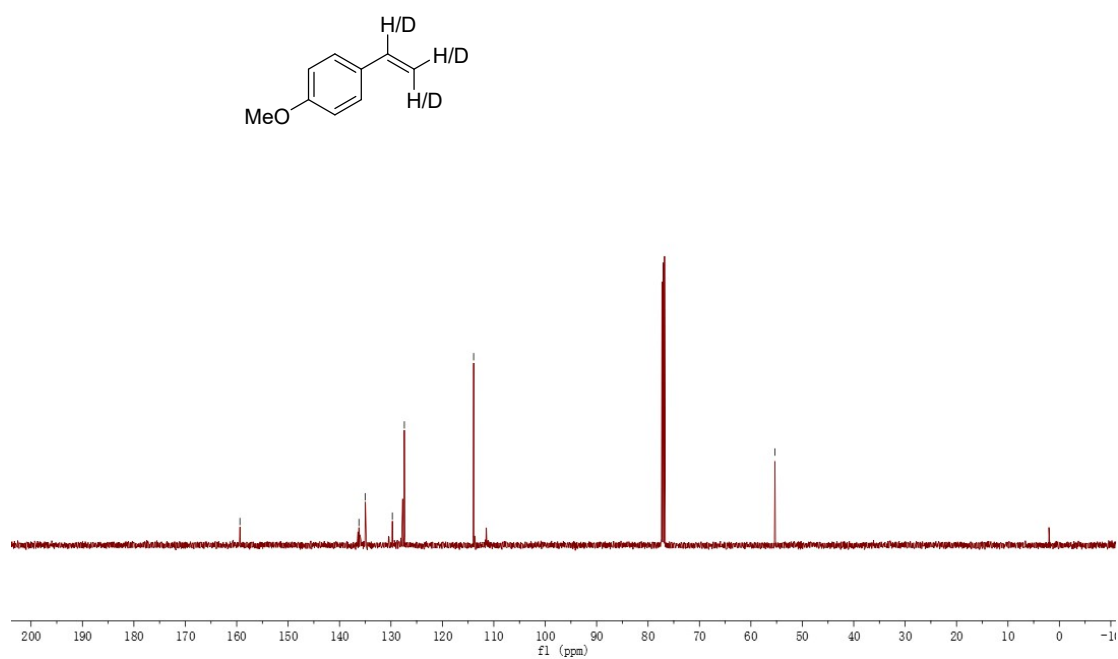
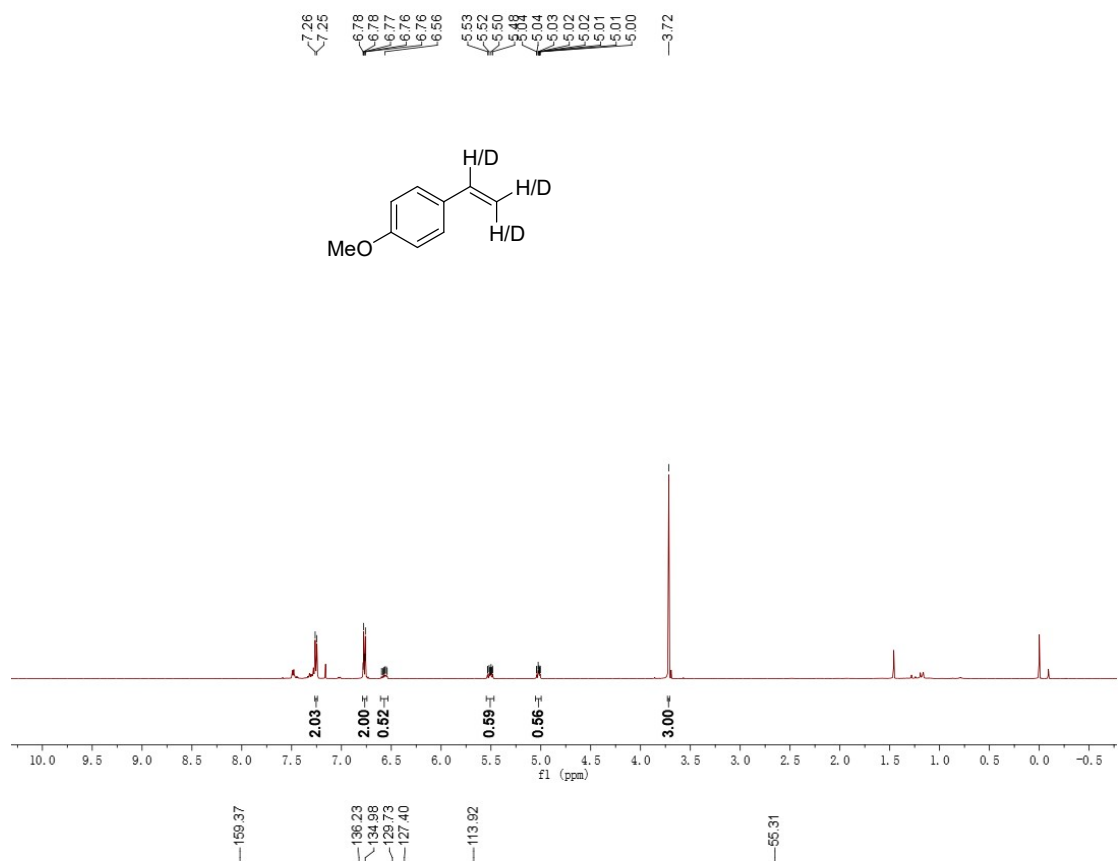
(E)-triethyl(2-(trifluoromethyl)styryl)silane (5b)



(E)-triethyl(2-methoxystyryl)silane (5c)



1-methoxy-4-(vinyl-d3)benzene (8)



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