Supplementary Information

Sodium Silylsilanolate as a Precursor of Silylcopper Species

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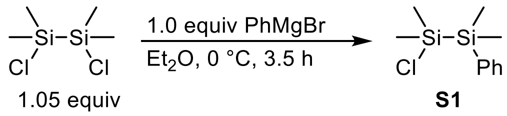
Instrumentation and Chemicals

^{1}H NMR (600 MHz), ^{13}C NMR (151 MHz), ^{19}F NMR (564 MHz) and ^{29}Si NMR (119 MHz) spectra were recorded on a JEOL ECZ-600 spectrometer. Chemical shifts in ^{1}H NMR spectra were recorded in delta (δ) units, parts per million (ppm) relative to residual $CHCl_3$ (δ = 7.26 ppm), C_6HD_5 (δ = 7.15 ppm) and $CHDCl_2$ (δ = 5.32 ppm). Chemical shifts in ^{13}C NMR spectra were recorded in delta (δ) units, parts per million (ppm) relative to $CDCl_3$ (δ = 77.00 ppm), C_6D_6 (δ = 128.00 ppm) and CD_2Cl_2 (δ = 53.800 ppm). For ^{19}F NMR spectra, fluorobenzene (^{19}F: δ = –113.50 ppm) was used as an external standard. For ^{29}Si NMR spectra, tetramethylsilane (^{29}Si: δ = 0.00 ppm) was used as an external standard. The following abbreviations are used for spin multiplicity: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. High resolution mass spectra (HRMS) were obtained on a Bruker micrOTOF II-KR spectrometer in Atmospheric Pressure Chemical Ionization (APCI or ESI) method using "LC/MS tuning mix, for APCI or ESI, low concentration" (Agilent Technologies, Inc.) as the internal standard. Melting points were determined on a Stanford Research Systems MPA100 melting point apparatus.

All non-aqueous reactions were carried out under an inert atmosphere of N_2 gas in oven-dried glassware unless otherwise noted. Dehydrated toluene, acetonitrile, hexane and benzene were purchased from FUJIFILM Wako Pure Chemical Corporation and stored under nitrogen atmosphere. Dehydrated THF and Et_2O was purchased from Kanto Chemical Co., Inc. and stored under nitrogen atmosphere. Dehydrated DCE was purchased from Sigma-Aldrich Co. LLC and stored under nitrogen atmosphere. CuCl was purchased from Wako Pure Chemical Industries, Ltd., and purified by washing with aqueous HCl and stored in a glove box after drying. NaH was purchased from Tokyo Chemical Industry Co., Ltd., and used after being washed with hexane and stored under nitrogen atmosphere. t*ert*-Butyl alcohol was purchased from Wako Pure Chemical Industries, Ltd., and used after being dried through storage over 4 Å molecular sieves. CuCl[P(OPh)$_3$][1], CuCl(bpy)[2], CuCl(dppe)[3], CuCl(IPr)[4], sodium trimethylsilyldimethylsilanolate (**1-Me**)[5], sodium benzyldimethylsilyldimethylsilanolate (**1-Benzyl**)[5], sodium allyldimethylsilyldimethylsilanolate (**1-Allyl**)[5], 1,2-bis(4-trifluoromethylphenyl)ethyne (**2b**)[6], 1,2-bis(4-cyanophenyl)ethyne (**2c**)[7], 1,2-bis(4-(*tert*-butoxycarbonyl)phenyl)ethyne (**2d**)[8], 1,2-bis(4-ethoxycarbonylphenyl)ethyne (**2h**)[9], 1,2-bis(4-fluorophenyl)ethyne (**2f**)[10], 1,2-bis(4-chlorophenyl)ethyne (**2g**)[10], 1,2-bis(4-methylphenyl)ethyne (**2h**)[6], 1,2-bis(2-methylphenyl)-ethyne (**2i**)[8], 1,2-bis(3-pyridinyl)ethyne (**2j**)[11], 1,2-bis(2-thiophenyl)ethyne (**2k**)[12], ((but-2-yn-1-yloxy)methyl)benzene (**2q**)[13], (1-(pent-3-yn-1-yloxy)methyl)benzene (**2r**)[14], and (methyl-1,2-propadienyl)cyclohexane (**2u**)[15] were prepared according to the literature. All other reagents were commercially available and used without further purification unless otherwise noted. Analytical thin layer chromatography (TLC) was performed on Merck precoated analytical plates, 0.25-mm thick, silica gel 60 F_{254}. Preparative flash chromatography was performed using Silica Gel (Wakosil® C-300 purchased from FUJIFILM Wako Pure Chemical Corporation). Preparative TLC was performed using silica gel (Merck 60P$F_{254+365}$). Preparative recycling gel permeation chromatography (GPC) was performed on a JAI LC-9260 II NEXT system using $CHCl_3$ as the eluent.

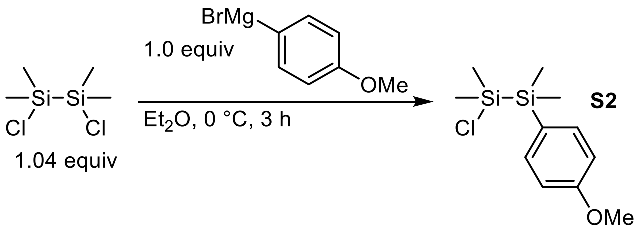
Preparation of Reagents and Substrates

Preparation of 1-chloro-2-phenyl-1,1,2,2-tetramethyldisilane (S1)



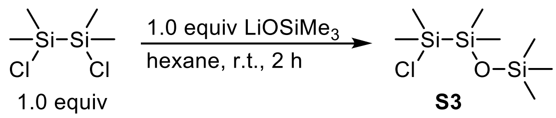
An oven-dried 500-mL round-bottomed flask equipped with a septum and a magnetic stir bar was charged with 1,2-dichloro-1,1,2,2-tetramethyldisilane (11.7 mL, 63.0 mmol) and Et_2O (150 mL). After the mixture was stirred at 0 °C for 10 min, phenylmagnesium bromide (0.67 M in THF, 89.6 mL, 60.0 mmol) was added dropwise to the flask over 15 min. After the reaction was stirred for 3.5 h, pentane (150 mL) was added to the reaction mixture. The resulting suspension was filtered through Na_2SO_4 and the filtrate was concentrated under reduced pressure. Distillation of the resulting residue under reduced pressure (56 °C/0.70 torr) provided **S1** (10.4 g, 45.3 mmol, 76%) as a colorless liquid.

Preparation of 1-chloro-2-(4-methoxyphenyl)-1,1,2,2-tetramethyldisilane (S2)



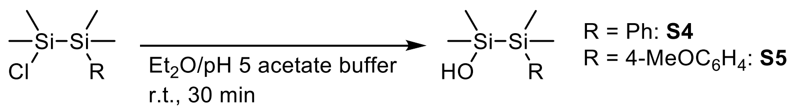
An oven-dried 500-mL round-bottomed flask equipped with a septum and a magnetic stir bar was charged with 1,2-dichloro-1,1,2,2-tetramethyldisilane (7.8 mL, 42.0 mmol) and Et_2O (100 mL). After the mixture was stirred at 0 °C for 10 min, 4-methoxyphenylmagnesium bromide (0.82 M in THF, 48.8 mL, 40.0 mmol) was added dropwise to the flask over 10 min. After the reaction was stirred for 3 h, pentane (150 mL) was added to the reaction mixture. The resulting suspension was filtered through Na_2SO_4 and the filtrate was concentrated under reduced pressure. Pentane (100 mL) was added to the residue and the filtration–concentration sequence was repeated again. Distillation of the resulting residue under reduced pressure (96–101 °C/0.90 torr) provided **S2** (8.40 g, 32.4 mmol, 81%) as a colorless liquid.

Preparation of 1-chloro-2-trimethylsiloxy-1,1,2,2-tetramethyldisilane (S3)



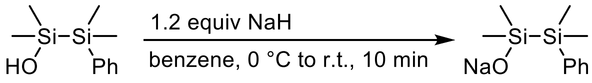
S3 was prepared according to the literature procedure with some modifications.[16] An oven-dried 500-mL round-bottomed flask equipped with a septum and a magnetic stir bar was charged with 1,2-dichloro-1,1,2,2-tetramethyldisilane (18.5 mL, 100 mmol) and hexane (400 mL). After lithium trimethylsilanolate (9.61 g, 100 mmol) was added to the flask at room temperature, the reaction mixture was stirred for 2 h. Hexane (100 mL) was added to the reaction mixture. The resulting suspension was filtered, and the filtrate was concentrated under reduced pressure. Distillation of the resulting residue under reduced pressure (55–58 °C/9 torr) provided **S3** (14.2 g, 59.1 mmol, 59%) as a colorless liquid.

Preparation of 2-phenyl-1,1,2,2-tetramethyldisilan-1-ol (S4) and 2-(4-methoxyphenyl)-1,1,2,2-tetramethyldisilan-1-ol (S5)



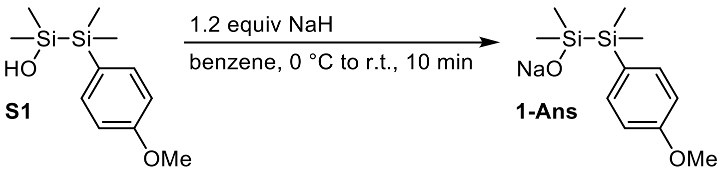
The synthesis of 2-phenyl-1,1,2,2-tetramethyldisilan-1-ol (**S4**) is representative. An open 300-mL round-bottomed flask equipped with a magnetic stir bar was charged with pH 5 acetate buffer (100 mL, 1.0 M) and Et_2O (20 mL) and the reaction mixture was stirred at room temperature under air. A solution of 1-chloro-2-phenyl-1,1,2,2-tetramethyldisilane (4.71 mL, 20.0 mmol) in Et_2O (16 mL) was added dropwise over 5 min. After 30 min, the mixture was poured into a separatory funnel with Et_2O (30 mL) and partitioned. The organic phase was collected, and the aqueous phase was extracted with Et_2O (30 mL). The combined organic extract was neutralized by washing with saturated $NaHCO_3$ aq. (30 mL). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure at 30 °C. The resulting residue was purified by column chromatography on silica gel (hexane/Et_2O = 4/1) to afford silanol **S4** (3.59 g, 17.1 mmol, 85%) as a colorless liquid.

Preparation of 1-Ph



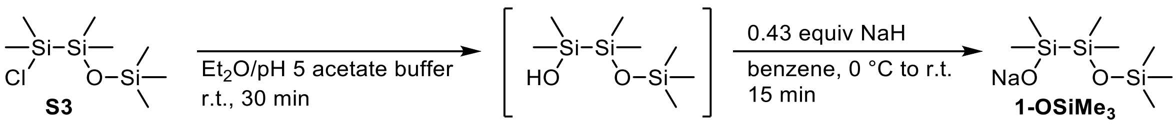
An oven-dried 50-mL round-bottomed flask equipped with a septum and a magnetic stir bar was charged with NaH (288 mg, 12.0 mmol) and benzene (5 mL). 2-phenyl-1,1,2,2-tetramethyldisilan-1-ol (**S4**, 2.20 mL, 10.0 mmol) was added dropwise at 0 °C to the mixture. The reaction mixture was warmed to room temperature over 5 min and stirring was continued for 10 min. The resulting suspension was filtered through a sintered glass filter under nitrogen atmosphere and the filtrate was concentrated under reduced pressure. The obtained powder was dissolved in hexane (6.0 mL) under nitrogen atmosphere and cooled to –78 °C to form the precipitate. The liquid phase was removed via cannulation and the remaining solid was dried under reduced pressure to provide **1-Ph** (1.80 g, 7.73 mmol, 77%) as a white powder.

Preparation of 1-Ans



An oven-dried 50-mL round-bottomed flask equipped with a septum and a magnetic stir bar was charged with NaH (288 mg, 12.0 mmol) and benzene (8 mL). 2-(4-Methoxyphenyl)-1,1,2,2-tetramethyldisilan-1-ol (**S5**, 2.40 mL, 10.0 mmol) was added dropwise at 0 °C to the mixture. The reaction mixture was warmed to room temperature over 5 min and stirring was continued for 10 min. The resulting suspension was filtered through a sintered glass filter under nitrogen atmosphere. The filtrate was concentrated under reduced pressure to provide **1-Ans** (2.30 g, 8.78 mmol, 88%) as a white powder.

Preparation of 1-OSiMe$_3$

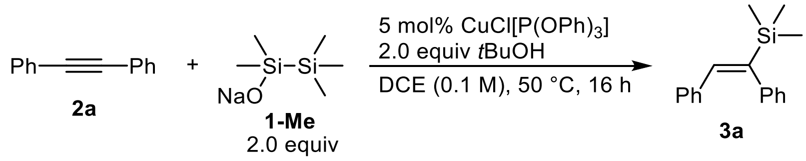


An open 200-mL round-bottomed flask equipped with a magnetic stir bar was charged with pH 5 acetate buffer (50 mL, 1.0 M) and Et_2O (12.5 mL) and the reaction mixture was stirred at room temperature under air. Solution of 1-chloro-2-trimethylsiloxy-1,1,2,2-tetramethyldisilane (**S3**, 2.70 mL, 10.0 mmol) in Et_2O (7 mL) was added dropwise over 5 min. After 30 min, the mixture was poured into a separatory funnel with Et_2O (20 mL) and partitioned. The organic phase was collected, and the aqueous phase was extracted with Et_2O (20 mL). The combined organic extract was neutralized by washing with saturated $NaHCO_3$ aq. (20 mL). The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure at room temperature. The resulting residue was immediately purified by column chromatography on silica gel (hexane/Et_2O = 4/1). The combined fractions were concentrated under reduced pressure at 35 °C to afford 2-trimethylsiloxy-1,1,2,2-tetramethyldisilan-1-ol (788 mg, 3.54 mmol).

An oven-dried 30-mL round-bottomed flask equipped with a septum and a magnetic stir bar was charged with NaH (101 mg, 4.25 mmol) and benzene (5 mL). The solution of 2-trimethylsiloxy-1,1,2,2-tetramethyldisilan-1-ol in benzene (2 mL) was added dropwise at 0 °C to the mixture. The reaction mixture was warmed to room temperature over 5 min and stirring was continued for 10 min. The resulting suspension was filtered through a sintered glass filter under nitrogen atmosphere. The filtrate was concentrated under reduced pressure to provide **1-OSiMe$_3$** (584 mg, 2.40 mmol, 24%) as a white powder.

Experimental Procedure

General Procedure for Copper-Catalyzed Hydrosilylation of Alkynes with 1-Me (Table 1, Scheme 1, Scheme 2)



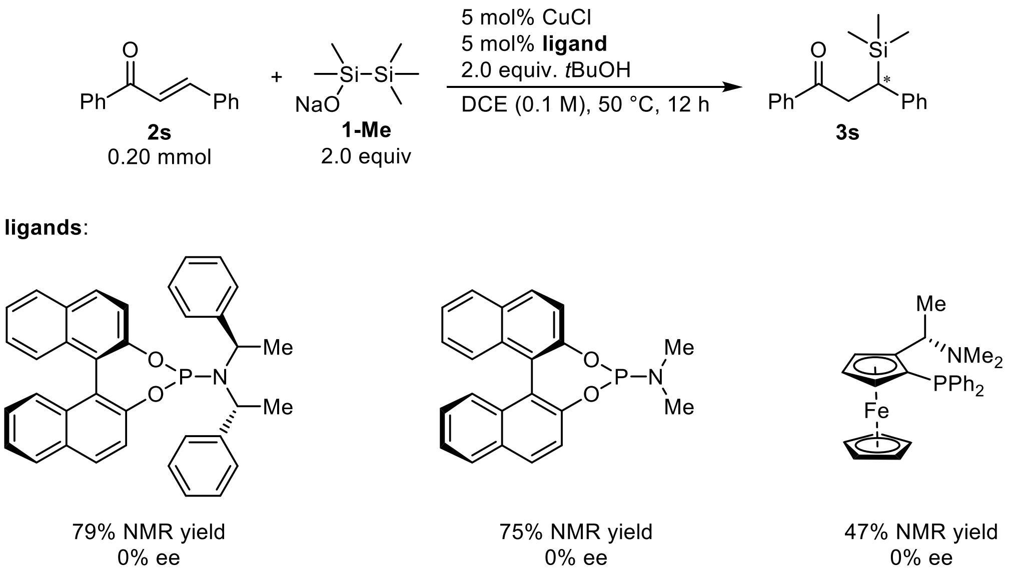
The silylation of diphenylacetylene (**2a**) is representative. An oven-dried 20-mL Schlenk tube equipped with a greaseless stopcock and a magnetic stir bar was charged with CuCl[P(OPh)$_3$] (10.2 mg, 0.0250 mmol), diphenylacetylene (**2a**, 89.0 mg, 0.499 mmol), **1-Me** (170 mg, 1.00 mmol), DCE (3.0 mL) and *t*BuOH (94.9 µL, 1.00 mmol). DCE (2.0 mL) was added to the mixture to rinse the inside wall of the tube. The resulting mixture was stirred at 50 °C. After 16 h, the reaction was quenched with saturated NH_4Cl aq. (10 mL). The mixture was poured into a separatory funnel with Et_2O (20 mL) and water (30 mL) and partitioned. The organic phase was collected, and the aqueous phase was extracted with Et_2O (20 mL × 2). The combined organic extract was washed with brine (10 mL), dried over Na_2SO_4 (ca. 10 g), filtered, and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (hexane only), and then GPC (eluent: $CHCl_3$) to give **3a** (107.3 mg, 0.425 mmol, 86%) as a colorless oil.

Stability Evaluation of Silylsilanolate under Air (toluene solution)[17]

A vial equipped with a septum and a magnetic stir bar was charged with sodium trimethylsilyldimethylsilanolate (**1-Me**, 34.1 mg, 0.200 mmol) and toluene (1.0 mL) under air. The vial was connected to a balloon filled with air through a needle. The mixture was stirred for a designated time at room temperature. The mixture was concentrated under reduced pressure and the yield of the recovered **1-Me** was analyzed by ^{1}H NMR analysis using 1,3,5-trimethoxybenzene as an internal standard.

Time	NMR Yield [%]
1 min	89
48 h	87

Reaction Using Chiral Phosphine Ligands for Enantioselective Hydrosilylation of 2s



An oven-dried 20-mL Schlenk tube equipped with a septum and a magnetic stir bar was charged with a chiral phosphine ligand (0.010 mmol), CuCl (27.5 mg, 0.010 mmol) and DCE (0.30 mL). The mixture was stirred at room temperature for 30 min to give a solution of the copper complex. Another oven-dried 20-mL Schlenk tube equipped with a septum and a magnetic stir bar was charged with **2s** (41.7 mg, 0.20 mmol), **1-Me** (68.1 mg, 0.40 mmol) and DCE (0.60 mL). The mixture was stirred at room temperature for 5 min. After the solution of the copper complex (0.30 mL) was added to the mixture, and the Schlenk tube that contained the copper complex was washed with DCE (0.20 mL× 3) and the solution was added to the reaction mixture. *t*BuOH (38.0 μL, 0.40 mmol) was added and the inside wall of the tube was rinsed with DCE (0.50mL). The resulting mixture was stirred at 50 °C. After 16 h, the reaction was quenched with saturated NH_4Cl aq. (5 mL). The mixture was poured into a separatory funnel with Et_2O (10mL) and water (15 mL) and partitioned. The organic phase was collected, and the aqueous phase was extracted with Et_2O (10 mL × 2). The combined organic extract was washed with brine (5 mL), dried over Na_2SO_4 (ca. 5 g), filtered, and concentrated under reduced pressure. The part of the residue was purified by preparative TLC (hexane/EtOAc = 10/1). The enantioselectivity of the obtained hydrosilylated product **3s** was analyzed by HPLC (HPLC: Column: DAICEL CHIRALPAK IA (4.6 mm × 250 mm), Eluent: hexane/*i*PrOH= 90:10, Flow rate: 1.0 ml/min, Detection: 254 nm, Retention time: t_1 = 3.95 min, t_2 = 4.35 min).

Computational Studies

General Computational Information

Preliminary structures of transition states were obtained at the level of B3LYP-D3BJ/def2-SVP[18,19,20] by using GRRM17 program[21] associated with Gaussian16 program.[22] All transition states and equilibrium structures were calculated at the level of B3LYP-D3BJ /def2-SVP in the gas-phase by using Gaussian16 program followed by frequency calculations to confirm their identity as either first-order saddle points or local minima. Intrinsic reaction coordinate (IRC) calculations were performed to ensure that the transition states found connected the corresponding reactants and products. Free energies at the optimized structures described in all energy diagrams were calculated at the level of ωB97X-D/def2-TZVP[23] with solvation effect of 1,2-dichloroethane (DCE) modeled by SMD[24] method at 323.15 K including a concentration correction (as the 1 mol L^{-1} standard state, 1.89 kcal mol^{-1} was added to every species). All geometries of equilibrium structures and transition states are contained in the XYZ file. To simplify the calculations, the ligand was modeled as 2,2'-bipyridyl and sodium trimethylsilanolate dimer was used as an activator. Images were generated by using CYLview.[25]

We independently tried to evaluate a pathway for the migration with the assistance of sodium trimethylsilanolate monomer. However, the transition state could not be located.

The relative energies of **INT-C1** and **INT-C2** are summarized in Figure S1. DFT calculations revealed that the sum of free energies of silylsilanolate-coordinated copper complex and sodium *tert*-butoxide is almost the same as that of *tert*-butoxide-coordinated copper complex and sodium trimethylsilyldimethylsilanolate. These results indicated that the ligand exchange between alkoxide and siloxide on the copper atom could be reversible in the current system.

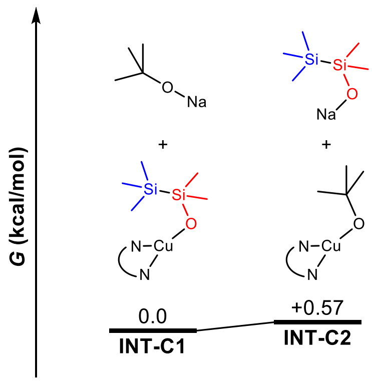


Figure S1. Free energies of INT-C1 and INT-C2

We hypothesized that copper *tert*-butoxide could react with sodium silylsilanolate to afford silylcopper without going through silylsilanolate-coordinated copper(I), accompanied with elimination of silanolate containing siloxane moiety. Thus, the pathway was calculated, but transition state could not be located (Figure S2).

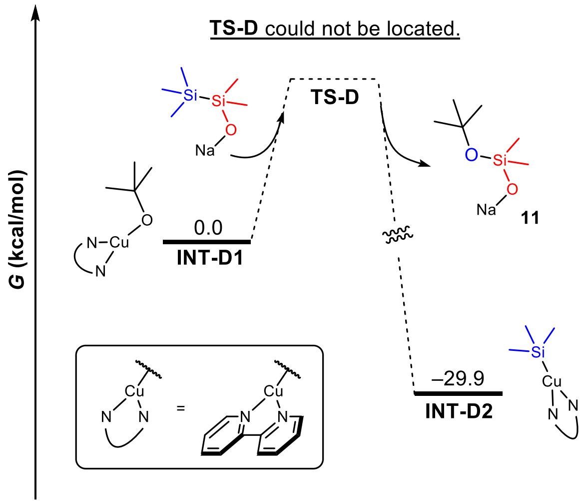


Figure S2. Energy profile of the transmetalation between copper *tert*-butoxide and sodium trimethylsilylsilanolate

We calculated a pathway for the migration of the silyl group with the assistance of sodium *tert*-butoxide dimer in place of sodium trimethylsilanolate dimer (Figure S3). The activation barrier required for this pathway is 28.4 kcal/mol, which is a little higher than that required for the migration pathway with the assist of sodium trimethylsilanolate dimer.

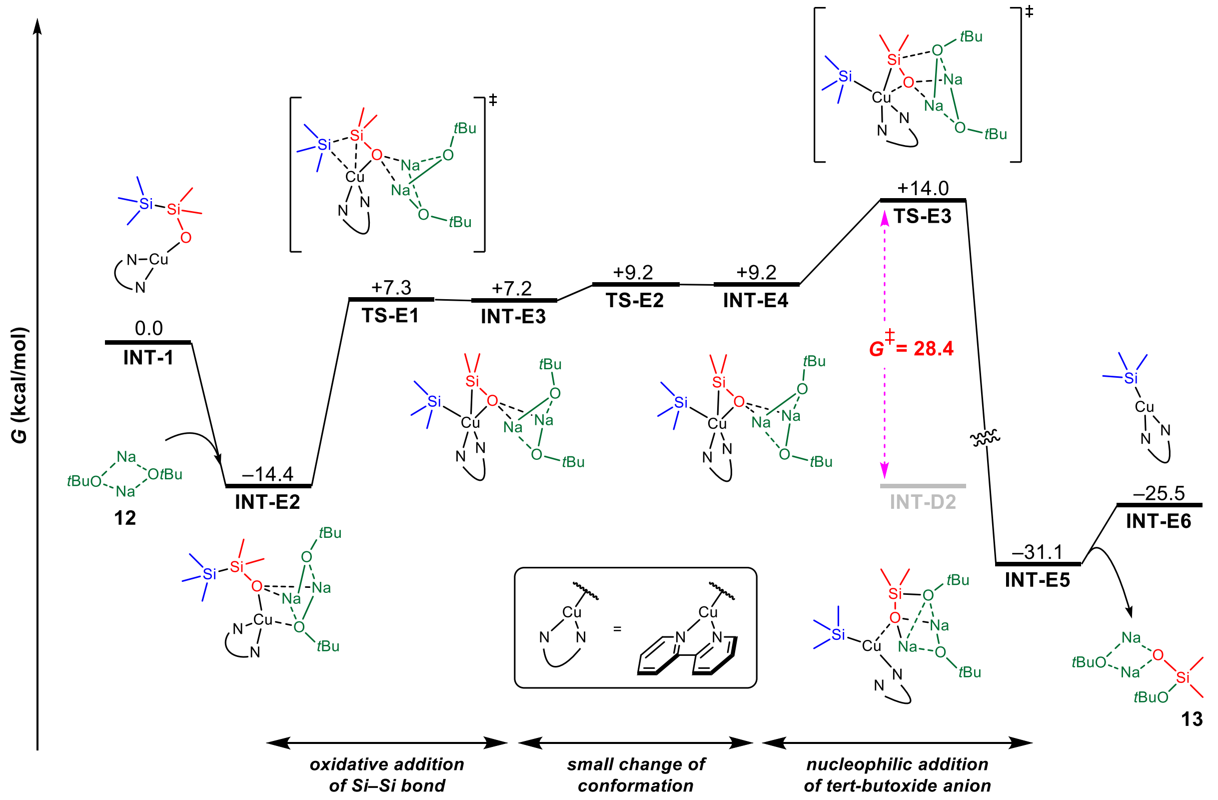


Figure S3. Energy profile of the migration pathway of the silyl group with the assist of sodium *tert*-butoxide dimer

Electronic Energy and Thermal Free Energies for Each Structure in Figure 4, S2, SX, and SX (in Hartree, B3LYP-D3BJ/def2-SVP level of theory)

Species	Electronic Energy	Thermal Free Energy
INT-1	–2989.048715	–2988.760059
TS-A1	–2989.027185	–2988.734556
INT-A2	–2989.027300	–2988.736299
dimethylsilanone	–444.384426	–444.338694
INT-B2	–4282.463371	–4281.972187
TS-B1	–4282.430114	–4281.933326
INT-B3	–4282.430426	–4281.934209
TS-B2	–4282.429138	–4281.933169
INT-B4	–4282.482380	–4281.988391
TS-B3	–4282.420847	–4281.927558
INT-B5	–4282.482380	–4281.988391
9	–1293.326337	–1293.154193
10	–1737.847217	–1737.597712
$CuSiMe_3$(bpy)	–2544.573764	–2544.355308
NaO*t*Bu	–395.183893	–395.093170
$NaOSi_2Me_5$	–1015.847701	–1015.703961
CuO*t*Bu(bpy)	–2368.383212	–2368.148972
11	–839.500819	–839.540940
INT-E2	–3779.608078	–3779.092421
TS-E1	–3779.567117	–3779.046697
INT-E3	–3779.567363	–3779.047970
TS-E2	–3779.566920	–3779.045882
INT-E4	–3779.566934	–3779.048060
TS-E3	-3779.561861	-3779.044007
INT-E5	-3779.626433	-3779.106703
12	–790.472915	–790.273911
13	–1234.991070	–1234.716252

Electronic Energy and Thermal Free Energies for Each Structure in Figure 4 and S2 (in Hartree, ωB97X-D/def2-TZVP/SMD (DCE)// B3LYP-D3BJ/def2-SVP level of theory)

Species	Electronic Energy	Thermal Free Energy	Corrected Thermal Free Energy
INT-1	–2989.971138	–2989.673785	–2989.670431
TS-A1	–2989.950617	–2989.649662	–2989.646308
INT-A2	–2989.950044	–2989.651153	–2989.647799
dimethylsilanone	–444.604938	–444.556313	–444.5529586
INT-B2	–4283.881006	–4283.372367	–4283.369013
TS-B1	–4283.855283	–4283.346593	–4283.343239
INT-B3	–4283.855464	–4283.346204	–4283.34285
TS-B2	–4283.854898	–4283.345100	–4283.341746
INT-B4	–4283.854842	–4283.348081	–4283.344727
TS-B3	–4283.838773	–4283.331320	–4283.327966
INT-B5	–4283.908390	–4283.401078	–4283.397724
9	–1293.866364	–1293.682650	–1293.679296
10	–1738.583598	–1738.324381	–1738.321027
$CuSiMe_3$(bpy)	–2545.297673	–2545.072751	–2545.069397
NaO*t*Bu	–395.415815	–395.323768	–395.3204136
$NaOSi_2Me_5$	–1016.265892	–1016.114737	–1016.111383
CuO*t*Bu(bpy)	–2369.121334	–2368.881906	–2368.878552
11	–839.932516	–839.971522	–839.9681676
INT-E2	–3780.909313	–3780.381300	–3780.377946
TS-E1	–3780.877239	–3780.346624	–3780.34327
INT-E3	–3780.877464	–3780.346638	–3780.343284
TS-E2	–3780.876632	–3780.343636	–3780.340282–
INT-E4	–3780.876386	–3780.343576	–3780.340222
TS-E3	–3780.864172	–3780.335972	–3780.332618
INT-E5	-3780.937151	-3780.407913	-3780.404559
12	–790.893047	–790.687886	–790.6845316
13	–1235.612200	–1235.329512	–1235.326158

Imaginary Frequencies for TSs in Figure 4 (B3LYP-D3BJ /def2-SVP level of theory)

non-assisted pathway		**silanolate dimer-assisted pathway**		***tert*-butoxide dimer-assisted pathway**	
TS-A1	–47.69*i* cm^{-1}	**TS-B1**	–54.83*i* cm^{-1}	**TS-D1**	–50.48*i* cm^{-1}
		TS-B2	–17.49*i* cm^{-1}	**TS-D2**	–15.47*i* cm^{-1}
		TS-B3	–96.50*i* cm^{-1}	**TS-D3**	–63.13*i* cm^{-1}

Cartesian Coordinates for Each Substrate

INT-1

Cu	-0.214248	-0.447563	-1.252463
N	-1.915864	-1.109500	-0.531490
N	-1.284399	1.487048	-0.763990
C	-0.713565	2.690690	-0.736008
C	-2.255395	1.186994	0.113233
C	-2.709640	2.119915	1.055536
C	-1.105207	3.681686	0.166981
C	-2.124685	3.386528	1.075807
H	0.093687	2.853006	-1.456635
H	-0.615629	4.657189	0.160504
H	-2.449357	4.129357	1.807709
C	-2.292437	-2.395432	-0.619105
C	-2.751858	-0.211677	0.045631
C	-3.996036	-0.605435	0.552657
C	-3.514882	-2.856193	-0.137245
C	-4.383539	-1.940806	0.461495
H	-1.575325	-3.075442	-1.084050
H	-3.772956	-3.912277	-0.229044
H	-5.353326	-2.261620	0.847649
H	-4.662235	0.135013	0.995680
H	-3.477716	1.854331	1.782815
O	1.512500	-0.131763	-1.782232
Si	2.762206	0.133918	-0.761081
C	4.353491	-0.671989	-1.401217
C	3.119354	1.992906	-0.555991
Si	2.241743	-0.739085	1.370313
C	3.705136	-0.742254	2.583777
C	1.605796	-2.521628	1.176781
C	0.829958	0.270717	2.158971
H	4.608637	-0.277417	-2.399863
H	4.228122	-1.763124	-1.496216
H	5.207447	-0.481878	-0.728856
H	3.305466	2.459942	-1.538893
H	4.003810	2.171929	0.079325
H	2.263735	2.511951	-0.092422
H	4.540421	-1.343770	2.188706
H	4.081635	0.281107	2.748424
H	2.398483	-3.188315	0.799518
H	1.121343	1.323937	2.304163
H	0.783177	-2.535870	0.442563
H	3.420866	-1.160047	3.564975
H	-0.056675	0.258093	1.506590
H	1.230999	-2.935635	2.128436
H	0.536183	-0.141648	3.139502

TS-A1

Cu	0.329339	0.018272	-0.650115
O	1.543711	0.328604	-2.242143
N	-1.218423	1.387506	-0.293564
Si	2.605515	0.293126	-1.028076
C	3.881962	-1.097964	-1.091249
C	3.465940	1.936984	-0.670793
Si	1.618033	-0.380955	1.386660
C	0.183352	0.232377	2.496579
C	1.704785	-2.268794	1.627668
C	3.151693	0.325314	2.280644
H	0.773777	-2.761643	1.305675
H	2.535413	-2.712218	1.056467
H	1.859214	-2.511775	2.693353
H	4.104263	0.015854	1.824739
H	3.129367	1.426422	2.298753
H	3.147618	-0.029557	3.326099
H	0.051952	1.323437	2.418494
H	-0.775734	-0.240540	2.235069
H	0.403939	-0.007077	3.552074
H	3.385895	-2.060022	-1.290416
H	4.571891	-0.895556	-1.929014
H	4.482181	-1.191787	-0.173151
H	3.934572	2.279899	-1.609643
H	2.738356	2.705516	-0.365440
H	4.247386	1.868950	0.100276
N	-1.280662	-1.246228	-0.536032
C	-1.223641	-2.573981	-0.696896
C	-2.445179	-0.665255	-0.172285
C	-3.594125	-1.435981	0.057383
C	-2.323438	-3.402859	-0.491027
C	-3.532244	-2.818376	-0.100564
H	-0.256089	-2.978133	-1.004434
H	-2.231492	-4.480682	-0.634329
H	-4.417754	-3.432524	0.075860
C	-1.088975	2.714830	-0.223372
C	-2.412444	0.813516	-0.047972
C	-3.529893	1.589884	0.293760
C	-2.150561	3.553635	0.110562
C	-3.394891	2.973756	0.376652
H	-0.094830	3.111963	-0.447131
H	-2.003915	4.633911	0.158945
H	-4.253143	3.594303	0.643036
H	-4.494623	1.123219	0.491219
H	-4.528881	-0.962543	0.356417

INT-A2

Cu	0.398149	0.001979	-0.591814
O	1.533573	0.158884	-2.300751
N	-1.177329	1.380853	-0.367027
Si	2.607207	0.208411	-1.103747
C	3.838279	-1.214825	-0.982564
C	3.490064	1.854075	-0.836776
Si	1.483366	-0.295068	1.480940
C	0.048090	0.333433	2.582619
C	1.630638	-2.162246	1.837316
C	3.016025	0.513800	2.281872
H	0.706604	-2.695147	1.559953
H	2.461979	-2.619743	1.278343
H	1.808026	-2.338971	2.912603
H	3.966671	0.180841	1.837940
H	2.974924	1.611847	2.201088
H	3.040096	0.255990	3.355121
H	-0.102769	1.418736	2.464134
H	-0.903280	-0.164561	2.336521
H	0.268786	0.136408	3.646801
H	3.324213	-2.176639	-1.128488
H	4.587402	-1.104731	-1.785943
H	4.375310	-1.241965	-0.021899
H	4.053697	2.091991	-1.755782
H	2.763881	2.665421	-0.673957
H	4.196929	1.839100	0.005560
N	-1.239277	-1.257629	-0.521456
C	-1.180297	-2.586713	-0.657487
C	-2.411502	-0.665295	-0.211350
C	-3.572658	-1.426306	-0.011782
C	-2.291430	-3.407834	-0.480207
C	-3.510867	-2.811382	-0.145504
H	-0.202068	-2.998502	-0.918246
H	-2.199963	-4.488361	-0.601741
H	-4.405599	-3.418796	0.006305
C	-1.043006	2.708261	-0.311844
C	-2.372241	0.815123	-0.108034
C	-3.484151	1.599289	0.233755
C	-2.099868	3.555390	0.016075
C	-3.344252	2.983590	0.298005

H	-0.047737	3.099579	-0.540305
H	-1.948915	4.635630	0.049641
H	-4.197982	3.610348	0.564375
H	-4.447408	1.137632	0.449312
H	-4.516438	-0.944081	0.241391

dimethylsilanone

O	0.000000	1.736562	0.000000
Si	0.000000	0.198079	0.000000
C	0.000000	-0.850225	-1.548496
C	0.000000	-0.850225	1.548496
H	0.000000	-0.218076	-2.447734
H	0.886571	-1.506687	-1.569900
H	-0.886571	-1.506687	-1.569900
H	0.000000	-0.218076	2.447734
H	-0.886571	-1.506687	1.569900
H	0.886571	-1.506687	1.569900

INT-B2

Cu	0.829047	-0.327490	0.300712
N	2.438979	-0.895148	-0.901794
N	2.388294	0.032410	1.591517
C	2.286001	0.725500	2.735122
C	3.610670	-0.146587	1.036308
C	4.768117	0.372988	1.632730
C	3.389123	1.263545	3.390294
C	4.657415	1.084094	2.824803
H	1.273905	0.854117	3.126423
H	3.255080	1.815466	4.322065
H	5.545062	1.505257	3.301404
C	2.329092	-1.599219	-2.036040
C	3.613345	-0.901994	-0.232273
C	4.724327	-1.612285	-0.709401
C	3.387124	-2.321897	-2.578525
C	4.611870	-2.326262	-1.899661
H	1.347137	-1.583706	-2.515554
H	3.253279	-2.871293	-3.511940
H	5.461414	-2.893204	-2.286043
H	5.653026	-1.629171	-0.137830
H	5.738105	0.244614	1.150984
C	-5.873912	1.495630	-0.306478
Si	-5.026018	-0.127067	0.183248
C	-6.180367	-1.558616	-0.276959
C	-4.880581	-0.128134	2.097703
O	-3.534193	-0.289201	-0.429975
Na	-1.650404	-0.083771	-1.367768
Na	-2.051642	-0.567835	1.177009
O	-0.556011	-1.680487	-0.257088
O	-0.639827	1.030719	0.545892
Si	-0.568223	-3.292535	0.044119
C	-1.162406	-4.250033	-1.470970
C	-1.774040	-3.613046	1.481201
C	1.141796	-3.923942	0.555173
Si	-0.530903	2.659807	0.339197
C	-2.266512	3.399141	0.182366
C	0.360667	3.536252	1.765361
Si	0.687020	2.993855	-1.652669
C	0.406110	4.683260	-2.467886
C	0.148226	1.644911	-2.898479
C	2.542319	2.743560	-1.343175
H	-5.985101	1.556381	-1.402643
H	-5.272313	2.362129	0.014229
H	-7.176058	-1.461595	0.188673
H	-5.850321	-0.008375	2.608993
H	-4.234016	0.701254	2.441894
H	-6.321861	-1.605572	-1.370095
H	-2.162139	-3.896622	-1.774160
H	-2.841514	3.219724	1.107344
H	-5.747826	-2.522798	0.040274
H	-4.450826	-1.081384	2.462124
H	-2.826058	2.920570	-0.637540
H	-0.476323	-4.090707	-2.320394
H	-2.242275	4.486326	-0.001157
H	-1.225171	-5.335763	-1.288204
H	-2.788955	-3.265680	1.217263
H	-0.129494	3.313244	2.729242
H	-1.854264	-4.680085	1.746145
H	0.345574	4.630460	1.625305
H	-1.448102	-3.083072	2.395966
H	1.412976	3.219313	1.836365
H	-0.661001	4.838804	-2.696861
H	1.117572	-4.986982	0.847942
H	1.864853	-3.818564	-0.269992
H	0.723717	5.498999	-1.797548
H	1.526908	-3.342905	1.409998
H	-0.936494	1.690940	-3.104372
H	2.936992	3.513471	-0.660352
H	0.418382	0.650466	-2.505221
H	0.974135	4.779812	-3.408829
H	2.706899	1.760080	-0.879212
H	0.661914	1.756447	-3.867343
H	3.124854	2.784720	-2.279009
H	-6.878767	1.592641	0.138896

TS-B1

Cu	1.592016	-0.175194	0.001289
N	1.424349	-1.990861	-0.900684
N	0.790675	-1.255648	1.605016
C	0.499665	-0.805468	2.831208
C	0.320645	-2.449782	1.194488
C	-0.446037	-3.247986	2.055435
C	-0.291917	-1.522010	3.726219
C	-0.766274	-2.774462	3.323751
H	0.914696	0.171480	3.098741
H	-0.520517	-1.112745	4.711368
H	-1.385820	-3.375509	3.992336
C	1.750967	-2.275070	-2.165970
C	0.671198	-2.856246	-0.192925
C	0.269081	-4.077242	-0.748067
C	1.361174	-3.453924	-2.796782
C	0.610267	-4.375380	-2.063277
H	2.350373	-1.526449	-2.690471
H	1.645787	-3.642868	-3.832978
H	0.286068	-5.315790	-2.513761
H	-0.332675	-4.776803	-0.172831
H	-0.816513	-4.217407	1.729666
C	-1.809685	4.494207	-1.028306
Si	-2.923214	3.233929	-0.141040
C	-4.702027	3.882932	-0.181782
C	-2.380862	3.237776	1.705056
O	-2.752207	1.735980	-0.728435
Na	-1.299794	0.568849	-1.846130
Na	-1.442314	0.644320	0.711608
O	-1.544427	-1.236185	-0.531860
O	0.347024	1.379008	-0.531313
Si	-3.062291	-1.820732	-0.418825
C	-4.161928	-1.161980	-1.813130
C	-3.842539	-1.258948	1.229804
C	-3.166762	-3.723352	-0.466636
Si	1.753952	2.188057	-0.297790
C	2.309978	3.095036	-1.855204
C	1.634760	3.384733	1.154679
Si	3.874027	0.834791	0.148942
C	4.879466	2.336997	0.752948
C	4.691656	0.245940	-1.462574
C	4.194104	-0.494409	1.482506
H	-2.108922	4.597553	-2.085546
H	-0.768845	4.131253	-1.012591

H	-4.787911	4.896224	0.246741
H	-2.531091	4.212338	2.198865
H	-1.306116	2.998820	1.811740
H	-5.073496	3.920961	-1.219786
H	-4.185611	-0.061666	-1.731567
H	1.552035	3.859951	-2.096202
H	-5.372592	3.213606	0.383135
H	-2.965123	2.493890	2.278725
H	2.368917	2.397386	-2.705423
H	-3.755861	-1.439249	-2.803091
H	3.282749	3.599210	-1.750475
H	-5.196729	-1.540738	-1.762840
H	-3.989820	-0.164517	1.207224
H	0.789118	4.066749	0.965891
H	-4.828551	-1.714269	1.421061
H	2.541593	3.990698	1.296321
H	-3.189957	-1.510505	2.085032
H	1.426069	2.847913	2.094189
H	4.812359	3.202616	0.076553
H	-4.220723	-4.049640	-0.472709
H	-2.689010	-4.122424	-1.376917
H	4.550676	2.661457	1.752484
H	-2.685282	-4.195146	0.405699
H	5.782330	0.149775	-1.325645
H	3.724482	-0.226311	2.442205
H	4.516661	0.954582	-2.287453
H	5.941576	2.045668	0.824425
H	3.813272	-1.483279	1.186927
H	4.307538	-0.738840	-1.771383
H	5.282165	-0.578180	1.652239
H	-1.835070	5.498307	-0.571668

INT-B3

Cu	1.703042	-0.072008	0.026717
N	1.451134	-1.857439	-0.947274
N	0.827919	-1.193496	1.572480
C	0.553583	-0.781870	2.816064
C	0.383001	-2.390304	1.143098
C	-0.334227	-3.234450	2.002599
C	-0.193157	-1.544679	3.711306
C	-0.636234	-2.802424	3.289843
H	0.946049	0.200203	3.097675
H	-0.410269	-1.166808	4.711424
H	-1.217531	-3.439905	3.959070
C	1.754207	-2.087448	-2.229367
C	0.708369	-2.747550	-0.263478
C	0.294003	-3.945557	-0.859048
C	1.350149	-3.238610	-2.900468
C	0.611954	-4.189445	-2.190406
H	2.348102	-1.318691	-2.730662
H	1.615495	-3.386269	-3.948429
H	0.277886	-5.110027	-2.673546
H	-0.304181	-4.663551	-0.303243
H	-0.679424	-4.207859	1.661422
C	-1.918887	4.422078	-1.043526
Si	-3.008844	3.156874	-0.133144
C	-4.794016	3.789190	-0.156713
C	-2.443205	3.181730	1.705712
O	-2.830982	1.656244	-0.711306
Na	-1.369943	0.508971	-1.842227
Na	-1.476613	0.593686	0.714006
O	-1.578697	-1.291867	-0.524658
O	0.262834	1.378985	-0.551780
Si	-3.082790	-1.897786	-0.351702
C	-4.244811	-1.268846	-1.707305
C	-3.806142	-1.333587	1.322439
C	-3.158898	-3.802621	-0.377676
Si	1.654963	2.195676	-0.305137
C	2.286440	3.074020	-1.845961
C	1.554965	3.386110	1.150229
Si	3.913441	0.757896	0.169142
C	4.778431	2.313035	0.847322
C	4.764225	0.334568	-1.477851
C	4.381864	-0.608415	1.419676
H	-2.232644	4.515607	-2.097483
H	-0.874497	4.068820	-1.039046
H	-4.884156	4.804935	0.265086
H	-2.598210	4.158475	2.193723
H	-1.364601	2.955690	1.800021
H	-5.178692	3.815630	-1.190261
H	-4.275886	-0.167945	-1.637765
H	1.571569	3.875744	-2.098817
H	-5.451171	3.118025	0.421617
H	-3.011119	2.435619	2.292600
H	2.329627	2.376194	-2.696313
H	-3.875840	-1.553577	-2.709430
H	3.279235	3.530728	-1.717166
H	-5.272327	-1.658136	-1.609833
H	-3.978188	-0.242825	1.296003
H	0.728381	4.089060	0.953271
H	-4.773411	-1.807198	1.559298
H	2.474811	3.968310	1.302579
H	-3.113590	-1.562719	2.152234
H	1.322062	2.850935	2.084254
H	4.652884	3.201250	0.209846
H	-4.206713	-4.145011	-0.330782
H	-2.720304	-4.203119	-1.306992
H	4.415441	2.565844	1.855835
H	-2.629353	-4.259914	0.474494
H	5.860551	0.320700	-1.352040
H	3.922310	-0.426207	2.404348
H	4.524415	1.068795	-2.262813
H	5.859837	2.105356	0.921457
H	4.056923	-1.602816	1.076963
H	4.458144	-0.660690	-1.837776
H	5.477648	-0.629698	1.556334
H	-1.948429	5.428940	-0.593181

TS-B2

Cu	-1.711416	-0.051672	0.009963
N	-1.453891	1.618788	-1.147649
N	-1.116655	1.312775	1.492914
C	-0.927877	1.051757	2.791510
C	-0.686888	2.475168	0.969148
C	-0.084530	3.446261	1.782196
C	-0.292697	1.944551	3.651726
C	0.127252	3.172475	3.128675
H	-1.301554	0.087350	3.149444
H	-0.144443	1.689504	4.702143
H	0.622291	3.908024	3.765956
C	-1.630323	1.684883	-2.471373
C	-0.895512	2.654488	-0.492501
C	-0.554994	3.831677	-1.170104
C	-1.278139	2.804819	-3.220683
C	-0.740216	3.904069	-2.546627
H	-2.075917	0.805646	-2.943984
H	-1.433168	2.815200	-4.300593
H	-0.459565	4.808599	-3.090268
H	-0.118519	4.672340	-0.636074
H	0.252537	4.390314	1.360361
C	2.440539	-3.753168	-1.693246
Si	3.311383	-3.012981	-0.161292
C	5.152646	-3.443897	-0.289295
C	2.608756	-3.926877	1.356169
O	3.022666	-1.420229	-0.074879
Na	1.500222	-0.550706	-1.428359
Na	1.516370	-0.405031	1.126989
O	1.495003	1.371106	-0.289533

O	-0.101986	-1.452046	-0.104911
Si	2.930302	2.140405	-0.187257
C	4.167471	1.458618	-1.448930
C	3.674119	1.875418	1.547691
C	2.826825	4.023319	-0.469870
Si	-1.471234	-2.323237	0.076066
C	-1.818548	-3.489158	-1.359541
C	-1.546748	-3.238411	1.720546
Si	-3.867131	-1.004991	-0.047274
C	-4.734702	-2.482226	0.783986
C	-4.472651	-0.962822	-1.849461
C	-4.608626	0.518976	0.834394
H	2.814878	-3.278097	-2.618736
H	1.353790	-3.568294	-1.629509
H	5.324414	-4.532163	-0.353316
H	2.757171	-5.019386	1.315844
H	1.524816	-3.735233	1.432978
H	5.599219	-2.975357	-1.182667
H	4.305945	0.385047	-1.235117
H	-1.049981	-4.280663	-1.358191
H	5.700523	-3.064039	0.589673
H	3.082616	-3.559451	2.283566
H	-1.746396	-2.949774	-2.316453
H	3.785081	1.572192	-2.479979
H	-2.806018	-3.971375	-1.303178
H	5.150109	1.957686	-1.404510
H	3.940138	0.810024	1.667427
H	-0.672787	-3.908995	1.778820
H	4.592024	2.461158	1.722521
H	-2.454671	-3.846262	1.840169
H	2.949000	2.151494	2.334563
H	-1.485263	-2.535662	2.566739
H	-4.460299	-3.456070	0.350984
H	3.837286	4.465900	-0.448066
H	2.385535	4.253569	-1.453854
H	-4.519116	-2.518326	1.863361
H	2.230406	4.538646	0.301086
H	-5.574104	-1.022421	-1.884581
H	-4.300812	0.560710	1.891431
H	-4.071009	-1.802367	-2.437992
H	-5.824748	-2.358721	0.663146
H	-4.291992	1.458658	0.356139
H	-4.175741	-0.025757	-2.346957
H	-5.711561	0.469003	0.803662
H	2.589390	-4.840898	-1.801977

INT-B4

Cu	1.733316	1.393021	0.619522
N	2.450021	-0.820381	-0.329547
N	1.542159	0.053191	2.170291
C	0.771929	0.438133	3.202330
C	1.658567	-1.267237	1.900272
C	0.988872	-2.237285	2.663932
C	0.063754	-0.460402	3.995584
C	0.172073	-1.831602	3.718592
H	0.706568	1.514170	3.376572
H	-0.557922	-0.093106	4.814020
H	-0.374996	-2.568388	4.310775
C	3.261457	-1.071452	-1.365531
C	2.510171	-1.631309	0.746152
C	3.372713	-2.736089	0.795034
C	4.146637	-2.147177	-1.400410
C	4.198439	-3.001220	-0.295470
H	3.197419	-0.376721	-2.208116
H	4.776081	-2.310236	-2.276704
H	4.881246	-3.853222	-0.278800
H	3.412477	-3.359475	1.689497
H	1.081838	-3.291493	2.400699
C	-3.431811	0.258792	-2.171307
Si	-4.184362	0.581349	-0.481660
C	-4.837500	-1.040874	0.218135
C	-5.536014	1.882545	-0.547724
O	-2.988340	1.077640	0.594456
Na	0.269850	0.059785	-1.345301
Na	-1.477144	-0.748611	0.934565
O	-0.911598	-1.688980	-0.907644
O	-0.379714	1.163514	0.474852
Si	-1.053779	-3.280856	-1.216546
C	-2.328739	-3.630053	-2.573157
C	-1.638411	-4.189378	0.356796
C	0.602243	-4.046664	-1.734526
Si	-1.654692	2.157646	0.601282
C	-1.832651	3.378589	-0.814636
C	-1.735994	3.058784	2.246648
Si	2.538593	2.755252	-1.028579
C	2.195551	4.637763	-0.937314
C	1.599034	2.237062	-2.659786
C	4.380506	2.636825	-1.549828
H	-2.609096	-0.468728	-2.057949
H	-3.041592	1.179130	-2.633343
H	-5.689236	-1.415549	-0.372561
H	-6.362645	1.566753	-1.205317
H	-5.140986	2.834633	-0.937465
H	-4.060017	-1.823516	0.186652
H	-3.319081	-3.240494	-2.282710
H	-2.765368	3.961439	-0.744941
H	-5.174217	-0.922560	1.261076
H	-5.949546	2.072221	0.455993
H	-1.816676	2.874127	-1.793034
H	-2.042154	-3.129845	-3.513675
H	-0.987418	4.084747	-0.796687
H	-2.436206	-4.707827	-2.782264
H	-2.622374	-3.809897	0.687196
H	-2.621557	3.710984	2.316431
H	-1.744739	-5.276968	0.207648
H	-0.837753	3.683569	2.383135
H	-0.925290	-4.037264	1.185830
H	-1.781412	2.338405	3.079613
H	1.128824	4.844236	-0.748334
H	0.522177	-5.127179	-1.941492
H	0.984273	-3.558303	-2.647437
H	2.764730	5.094696	-0.110198
H	1.359813	-3.905777	-0.946258
H	1.889341	2.867920	-3.518360
H	5.028818	3.050749	-0.758872
H	0.505191	2.349106	-2.545969
H	2.480759	5.156847	-1.870190
H	4.696674	1.591190	-1.705808
H	1.815633	1.195809	-2.971085
H	4.587123	3.195893	-2.480570
H	-4.178259	-0.171662	-2.859197

TS-B3

Cu	2.400273	-0.489744	0.102322
N	1.867180	-1.993890	-1.342060
N	1.398543	-2.000798	1.300950
C	1.241940	-1.973650	2.625237
C	0.468107	-2.590365	0.525696
C	-0.668936	-3.188001	1.086256
C	0.126174	-2.524741	3.261440
C	-0.843815	-3.145167	2.469226
H	2.031053	-1.475073	3.195941
H	0.026317	-2.468864	4.346837
H	-1.734594	-3.587378	2.920451
C	2.108971	-1.823605	-2.642534
C	0.678571	-2.489196	-0.944283
C	-0.331213	-2.796876	-1.864179
C	1.167046	-2.127458	-3.628509

C	-0.078961	-2.610681	-3.223777
H	3.086036	-1.407071	-2.903756
H	1.403639	-1.969826	-4.682326
H	-0.857893	-2.828697	-3.958071
H	-1.320653	-3.089308	-1.520530
H	-1.420574	-3.652761	0.453982
C	-3.022449	3.190004	-1.952738
Si	-2.485075	3.345801	-0.124153
C	-4.053554	3.246033	0.936101
C	-1.729388	5.069370	0.103178
O	-1.438411	2.145365	0.212811
Na	-1.397698	0.562168	-1.453951
Na	-1.441723	0.136037	1.126770
O	-2.506159	-1.021706	-0.461884
O	0.423177	0.234083	-0.211708
Si	-4.002693	-1.390662	0.048081
C	-5.354542	-0.486086	-0.922937
C	-4.173928	-0.882551	1.886601
C	-4.373583	-3.253242	-0.039116
Si	1.251965	1.546252	0.243571
C	1.590183	2.890916	-1.010823
C	1.126022	2.132550	2.020403
Si	4.314365	0.755440	0.216607
C	4.616339	2.297310	1.297648
C	4.913722	1.207938	-1.538555
C	5.565022	-0.531884	0.879835
H	-3.550165	2.233828	-2.128004
H	-2.141465	3.229632	-2.620374
H	-4.771928	4.051126	0.707035
H	-2.456635	5.870611	-0.111039
H	-0.862270	5.219035	-0.562111
H	-4.566230	2.282688	0.777223
H	-5.206191	0.605201	-0.863365
H	0.734422	3.582598	-1.010859
H	-3.800678	3.316492	2.008042
H	-1.377065	5.203625	1.140103
H	1.697079	2.452632	-2.014779
H	-5.318183	-0.768594	-1.989111
H	2.503665	3.458198	-0.780362
H	-6.368469	-0.709627	-0.550556
H	-4.052572	0.209100	2.009829
H	0.240539	2.781351	2.095945
H	-5.155921	-1.141391	2.316091
H	2.020144	2.686704	2.337697
H	-3.411339	-1.388845	2.507994
H	1.001579	1.272600	2.698593
H	4.026399	3.172518	0.982831
H	-5.415018	-3.480309	0.244923
H	-4.217838	-3.634477	-1.063058
H	4.376510	2.094880	2.354373
H	-3.717359	-3.830062	0.635367
H	5.945709	1.599986	-1.514448
H	5.328277	-0.821071	1.917157
H	4.273646	1.971397	-2.008244
H	5.681831	2.581128	1.246141
H	5.557991	-1.449853	0.269941
H	4.910417	0.321450	-2.195093
H	6.590926	-0.121764	0.868968
H	-3.706576	3.992067	-2.276238

INT-B5

Cu	1.733316	1.393021	0.619522
N	2.450021	-0.820381	-0.329547
N	1.542159	0.053191	2.170291
C	0.771929	0.438133	3.202330
C	1.658567	-1.267237	1.900272
C	0.988872	-2.237285	2.663932
C	0.063754	-0.460402	3.995584
C	0.172073	-1.831602	3.718592
H	0.706568	1.514170	3.376572
H	-0.557922	-0.093106	4.814020
H	-0.374996	-2.568388	4.310775
C	3.261457	-1.071452	-1.365531
C	2.510171	-1.631309	0.746152
C	3.372713	-2.736089	0.795034
C	4.146637	-2.147177	-1.400410
C	4.198439	-3.001220	-0.295470
H	3.197419	-0.376721	-2.208116
H	4.776081	-2.310236	-2.276704
H	4.881246	-3.853222	-0.278800
H	3.412477	-3.359475	1.689497
H	1.081838	-3.291493	2.400699
C	-3.431811	0.258792	-2.171307
Si	-4.184362	0.581349	-0.481660
C	-4.837500	-1.040874	0.218135
C	-5.536014	1.882545	-0.547724
O	-2.988340	1.077640	0.594456
Na	0.269850	0.059785	-1.345301
Na	-1.477144	-0.748611	0.934565
O	-0.911598	-1.688980	-0.907644
O	-0.379714	1.163514	0.474852
Si	-1.053779	-3.280856	-1.216546
C	-2.328739	-3.630053	-2.573157
C	-1.638411	-4.189378	0.356796
C	0.602243	-4.046664	-1.734526
Si	-1.654692	2.157646	0.601282
C	-1.832651	3.378589	-0.814636
C	-1.735994	3.058784	2.246648
Si	2.538593	2.755252	-1.028579
C	2.195551	4.637763	-0.937314
C	1.599034	2.237062	-2.659786
C	4.380506	2.636825	-1.549828
H	-2.609096	-0.468728	-2.057949
H	-3.041592	1.179130	-2.633343
H	-5.689236	-1.415549	-0.372561
H	-6.362645	1.566753	-1.205317
H	-5.140986	2.834633	-0.937465
H	-4.060017	-1.823516	0.186652
H	-3.319081	-3.240494	-2.282710
H	-2.765368	3.961439	-0.744941
H	-5.174217	-0.922560	1.261076
H	-5.949546	2.072221	0.455993
H	-1.816676	2.874127	-1.793034
H	-2.042154	-3.129845	-3.513675
H	-0.987418	4.084747	-0.796687
H	-2.436206	-4.707827	-2.782264
H	-2.622374	-3.809897	0.687196
H	-2.621557	3.710984	2.316431
H	-1.744739	-5.276968	0.207648
H	-0.837753	3.683569	2.383135
H	-0.925290	-4.037264	1.185830
H	-1.781412	2.338405	3.079613
H	1.128824	4.844236	-0.748334
H	0.522177	-5.127179	-1.941492
H	0.984273	-3.558303	-2.647437
H	2.764730	5.094696	-0.110198
H	1.359813	-3.905777	-0.946258
H	1.889341	2.867920	-3.518360
H	5.028818	3.050749	-0.758872
H	0.505191	2.349106	-2.545969
H	2.480759	5.156847	-1.870190
H	4.696674	1.591190	-1.705808
H	1.815633	1.195809	-2.971085
H	4.587123	3.195893	-2.480570
H	-4.178259	-0.171662	-2.859197

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Na	-0.130027	-1.413614	0.000000

O	-1.585623	0.166441	-0.000001
Si	-3.212592	0.027496	0.000000
C	-3.689829	-1.816383	0.000005
C	-3.992825	0.822552	1.533324
C	-3.992827	0.822543	-1.533328
H	-3.587228	0.375184	2.456535
H	-3.776839	1.904443	1.566426
H	-5.089245	0.701448	1.551960
H	-3.287873	-2.326865	-0.894068
H	-3.287872	-2.326860	0.894082
H	-4.781451	-1.974441	0.000006
H	-3.776841	1.904434	-1.566437
H	-3.587231	0.375170	-2.456537
H	-5.089247	0.701439	-1.551961
Na	0.130026	1.413616	0.000000
O	1.585622	-0.166438	0.000002
Si	3.212592	-0.027496	0.000000
C	3.689832	1.816382	-0.000007
C	3.992826	-0.822544	1.533328
C	3.992823	-0.822555	-1.533323
H	3.776835	-1.904445	-1.566425
H	3.587226	-0.375187	-2.456535
H	5.089243	-0.701453	-1.551960
H	3.587231	-0.375169	2.456537
H	3.776838	-1.904434	1.566438
H	5.089247	-0.701442	1.551961
H	3.287876	2.326859	-0.894083
H	3.287878	2.326865	0.894067
H	4.781455	1.974438	-0.000009

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O	-1.035450	-2.176850	-0.121774
Si	-2.374945	-1.279850	-0.094420
C	-3.162010	-1.085767	1.609212
C	-3.690820	-1.784335	-1.337463
H	-3.513526	-2.067288	1.968285
H	-2.444194	-0.699203	2.350739
H	-4.030670	-0.407708	1.590225
H	-3.268431	-1.816445	-2.355499
H	-4.084618	-2.788336	-1.109202
H	-4.536157	-1.076709	-1.344059
Na	0.147652	-0.698492	-1.388611
O	1.915460	-0.827986	-0.183912
Si	3.313333	0.000077	-0.016323
C	3.144919	1.761784	-0.705861
C	3.781668	0.143312	1.819404
C	4.750409	-0.841065	-0.920302
H	2.984257	0.654746	2.385385
H	3.923972	-0.856696	2.267023
H	4.716911	0.707254	1.974534
H	2.874129	1.741703	-1.776376
H	2.357836	2.319536	-0.171809
H	4.082480	2.335853	-0.615448
H	4.912138	-1.862443	-0.535446
H	4.538827	-0.925112	-1.999905
H	5.695939	-0.284387	-0.804958
Na	0.795561	-2.249810	0.944220
O	-1.859314	0.282139	-0.629911
Si	-1.536800	1.772236	0.072714
C	-0.334874	1.518101	1.500080
C	-0.716730	2.802560	-1.271213
C	-3.126979	2.587440	0.648670
H	-3.842961	2.678322	-0.184201
H	-3.607338	2.001607	1.447909
H	-2.931303	3.598703	1.042145
H	0.239993	2.359305	-1.595057
H	-1.372369	2.890875	-2.152749
H	-0.490567	3.819961	-0.912285
H	-0.810987	0.975589	2.332540
H	0.531792	0.929270	1.155136
H	0.038212	2.477864	1.893391

CuSiMe$_3$(bpy)

Cu	0.713476	-0.383321	-0.145611
N	-1.162236	-1.297460	-0.061962
N	-0.673539	1.290281	-0.346305
C	-0.295042	2.568922	-0.374195
C	-1.937407	0.971976	-0.015042
C	-2.877246	1.959687	0.311471
C	-1.172491	3.614755	-0.080323
C	-2.486458	3.298277	0.273053
H	0.751346	2.753132	-0.635135
H	-0.828617	4.649725	-0.122236
H	-3.200122	4.085766	0.525145
C	-1.332877	-2.622734	-0.065080
C	-2.237145	-0.484749	-0.004217
C	-3.536374	-1.005633	0.062762
C	-2.593288	-3.217991	-0.007538
C	-3.714622	-2.388500	0.060952
H	-0.419309	-3.221748	-0.108653
H	-2.687846	-4.305093	-0.013709
H	-4.719859	-2.813081	0.107120
H	-4.399261	-0.340540	0.098380
H	-3.892210	1.692203	0.606642
Si	2.975035	-0.247742	0.085369
C	3.667983	-0.750086	1.801844
C	4.009344	-1.271873	-1.164383
C	3.605780	1.555138	-0.157823
H	3.217822	-0.145248	2.607562
H	3.449045	-1.808085	2.025795
H	4.763910	-0.614526	1.850807
H	3.803600	-2.351047	-1.061767
H	3.773514	-0.990917	-2.205011
H	5.093325	-1.119144	-1.011084
H	3.350224	1.933838	-1.163255
H	3.149768	2.238546	0.580113
H	4.702855	1.628025	-0.044172

NaO*t*Bu

Na	2.703067	0.000029	-0.000024
O	0.757800	0.000099	-0.000058
C	-0.617007	-0.000018	0.000006
C	-1.149324	0.977654	1.072728
C	-1.149430	0.440113	-1.383041
C	-1.149169	-1.417876	0.310377
H	-0.775410	1.993512	0.864072
H	-0.774895	0.676292	2.064845
H	-2.251953	1.013611	1.112651
H	-0.775180	1.450075	-1.618027
H	-2.252059	0.456500	-1.434076
H	-0.775397	-0.248417	-2.158504
H	-0.774711	-2.126342	-0.446699
H	-0.775166	-1.745068	1.294442
H	-2.251789	-1.470506	0.321605

NaOSi$_2$Me$_5$

Na	-1.343311	-2.690416	0.000038
O	-1.933022	-0.766426	0.000398
Si	-1.078783	0.611342	0.000044
C	-1.393761	1.703203	-1.522972
C	-1.393532	1.703874	1.522619
Si	1.244146	0.053329	-0.000010
C	2.189005	0.645581	1.539875
C	2.189256	0.646569	-1.539359
C	1.415926	-1.869126	-0.000587
H	-2.454584	2.005912	-1.562321
H	-1.166548	1.163156	-2.457198
H	-0.778928	2.619610	-1.503327

H	-2.454345	2.006615	1.561986
H	-0.778691	2.620266	1.502476
H	-1.166188	1.164233	2.457046
H	2.186151	1.746796	1.593386
H	1.714327	0.273904	2.463144
H	2.186416	1.747819	-1.592159
H	0.964243	-2.311245	0.908606
H	1.714728	0.275490	-2.462945
H	3.239998	0.309184	1.534602
H	0.963899	-2.310764	-0.909840
H	3.240248	0.310166	-1.534129
H	2.473417	-2.181151	-0.000854

CuO*t*Bu(bpy)

Cu	0.655733	-0.331138	-0.164828
N	-1.046553	-1.284948	-0.000360
N	-0.779584	1.339368	-0.326120
C	-0.475656	2.635107	-0.320927
C	-2.017033	0.924321	-0.020889
C	-3.034343	1.840136	0.287547
C	-1.430219	3.614187	-0.035748
C	-2.731215	3.202089	0.270190
H	0.570154	2.871498	-0.544170
H	-1.159472	4.671584	-0.048179
H	-3.503504	3.936899	0.508747
C	-1.131223	-2.626264	0.022030
C	-2.190549	-0.551578	-0.006662
C	-3.446031	-1.172034	0.008495
C	-2.345354	-3.306507	0.038150
C	-3.528451	-2.562432	0.030800
H	-0.181439	-3.164994	0.032670
H	-2.357467	-4.397428	0.057232
H	-4.501331	-3.058227	0.037203
H	-4.352910	-0.567700	-0.014369
H	-4.035798	1.503243	0.557521
O	2.286231	0.480499	-0.256980
C	3.505211	-0.082014	0.096100
C	4.592694	0.991734	-0.102021
C	3.485801	-0.526226	1.573021
C	3.817071	-1.299764	-0.797175
H	4.363042	1.866545	0.526758
H	4.592769	1.323866	-1.152136
H	5.601450	0.626780	0.154299
H	3.213072	0.330632	2.209435
H	4.455538	-0.927766	1.914452
H	2.716858	-1.305612	1.711423
H	3.034073	-2.064652	-0.656525
H	3.800735	-0.994225	-1.855360
H	4.796869	-1.756908	-0.575253

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Si	1.312604	0.280043	0.015008
O	-0.311565	-0.412319	-0.101804
C	-1.629229	0.122959	-0.022046
C	-1.733320	1.458528	-0.768266
C	-2.551659	-0.908476	-0.684880
C	-2.016728	0.301666	1.452322
H	-1.418055	1.340241	-1.815294
H	-1.093995	2.221731	-0.301527
H	-2.769085	1.831830	-0.755086
H	-2.250944	-1.066417	-1.732419
H	-3.603698	-0.584153	-0.669357
H	-2.492343	-1.874244	-0.153400
H	-1.916982	-0.655076	1.989825
H	-1.360930	1.034764	1.941593
H	-3.057857	0.647137	1.553768
C	1.347650	1.447671	1.498498
O	2.191677	-1.046849	0.143231
C	1.603488	1.288161	-1.554525
H	1.369271	0.687958	-2.449152
H	1.014357	2.217609	-1.599977
H	2.670352	1.561707	-1.611626
H	0.657989	2.302348	1.400983
H	1.108854	0.911354	2.430884
H	2.366839	1.855845	1.604950
Na	0.657969	-2.449359	0.008881

INT-E2

Cu	0.7112470	-0.6014910	0.426446
N	2.2290800	-0.9459280	-0.972112
N	2.3768730	-0.1672300	1.564725
C	2.3400900	0.4248890	2.766707
C	3.5407690	-0.1872440	0.875280
C	4.7066660	0.3970840	1.391678
C	3.4568750	1.0128880	3.351530
C	4.6660500	1.0004840	2.645862
H	1.3683260	0.4305220	3.266716
H	3.3779720	1.4781520	4.335437
H	5.5604870	1.4675260	3.063312
C	2.0779170	-1.5326290	-2.167573
C	3.4720970	-0.8398130	-0.446928
C	4.5973490	-1.3325430	-1.124411
C	3.1446580	-2.0338700	-2.906205
C	4.4339140	-1.9337430	-2.369121
H	1.0543680	-1.5977380	-2.544747
H	2.9678650	-2.4927440	-3.880437
H	5.2964550	-2.3283220	-2.910167
H	5.5856500	-1.2649790	-0.668617
H	5.6261070	0.4015770	0.805395
C	-5.2021470	0.5072930	-1.264839
C	-5.0507570	-0.1591610	0.124946
C	-5.8686150	-1.4691290	0.138967
C	-5.6151270	0.8020000	1.195375
O	-3.7229870	-0.4267490	0.373136
Na	-1.9617780	-0.3219790	-0.845321
Na	-2.0966360	-0.6526870	1.726347
O	-0.8111670	-1.8798220	0.302017
O	-0.6835660	0.8307020	0.805681
C	-0.8481020	-3.2711470	0.175886
C	-1.2210510	-3.6423370	-1.273754
C	-1.9342840	-3.8161260	1.125242
C	0.5136300	-3.8880870	0.535859
Si	-0.5239850	2.4445460	0.537202
C	-2.1948650	3.3081680	0.754934
C	0.7255690	3.2814890	1.694110
Si	0.2275660	2.7195150	-1.683435
C	-0.2858110	4.3694540	-2.467139
C	-0.5240310	1.3180720	-2.747478
C	2.1147810	2.5473810	-1.778537
H	-4.8129760	-0.1709520	-2.045268
H	-4.6136340	1.4405550	-1.293649
H	-6.9425760	-1.3128010	-0.063297
H	-6.6769710	1.0561030	1.033409
H	-5.0289270	1.7348970	1.200442
H	-5.4667070	-2.1621490	-0.618346
H	-2.2047630	-3.2127010	-1.527345
H	-2.5662530	3.1739210	1.785694
H	-5.7670770	-1.9550130	1.123221
H	-5.5217640	0.3377080	2.191767
H	-2.9486170	2.8693960	0.081604
H	-0.4717060	-3.2318760	-1.969811
H	-2.1333090	4.3902660	0.550826
H	-1.2754820	-4.7315650	-1.435488
H	-2.8993430	-3.3359120	0.895881
H	0.4527560	3.1226340	2.751840
H	-2.0592500	-4.9088790	1.048960
H	0.7561460	4.3696390	1.514038
H	-1.6658580	-3.5843140	2.171356

H	1.7415560	2.8848960	1.542971
H	-1.3823980	4.4825150	-2.464867
H	0.5000110	-4.9893560	0.482734
H	1.2929500	-3.5187210	-0.148326
H	0.1358620	5.2181570	-1.903559
H	0.7967010	-3.5926170	1.558950
H	-0.2113190	1.3930620	-3.801748
H	2.6083900	3.3766940	-1.246020
H	-1.6283770	1.3518440	-2.737465
H	0.0632780	4.4509260	-3.510651
H	2.4262880	1.6061200	-1.303078
H	-0.1734710	0.3404010	-2.376612
H	2.4786220	2.5455880	-2.819981
H	-6.2460900	0.7540630	-1.523352

TS-E1

Cu	1.408723	-0.069104	-0.017420
N	1.250466	-1.834833	-1.004435
N	0.720942	-1.250678	1.564278
C	0.465903	-0.867937	2.820654
C	0.285498	-2.445994	1.120648
C	-0.389448	-3.323016	1.983993
C	-0.242916	-1.661460	3.719472
C	-0.667584	-2.922270	3.285610
H	0.849067	0.115115	3.113128
H	-0.440061	-1.308323	4.732788
H	-1.215641	-3.585656	3.957796
C	1.555596	-2.058402	-2.286919
C	0.610200	-2.783360	-0.290659
C	0.325644	-4.032342	-0.858133
C	1.267070	-3.259119	-2.930593
C	0.650100	-4.269908	-2.189722
H	2.055998	-1.242037	-2.814050
H	1.530960	-3.397765	-3.980079
H	0.417952	-5.234054	-2.646836
H	-0.166175	-4.807079	-0.274095
H	-0.722995	-4.297889	1.634652
C	-2.473667	4.001257	-1.066514
C	-3.320744	3.082289	-0.151140
C	-4.819380	3.346724	-0.413897
C	-3.004322	3.450207	1.323354
O	-3.020013	1.760991	-0.383222
Na	-1.615352	0.657617	-1.641648
Na	-1.653803	0.633711	0.895993
O	-1.773966	-1.217177	-0.386268
O	0.081067	1.456313	-0.393533
C	-3.039427	-1.792782	-0.412979
C	-3.908067	-1.162153	-1.530289
C	-3.762370	-1.558884	0.938235
C	-2.947500	-3.311540	-0.672206
Si	1.467656	2.301180	-0.177905
C	1.921531	3.320516	-1.698262
C	1.369775	3.400510	1.351966
Si	3.657600	0.999651	0.091158
C	4.629513	2.506349	0.738842
C	4.424480	0.541884	-1.586715
C	4.093724	-0.388094	1.328614
H	-2.696934	3.772882	-2.122918
H	-1.405196	3.794558	-0.893705
H	-5.114436	4.395888	-0.235745
H	-3.252655	4.493511	1.584148
H	-1.925888	3.308981	1.520449
H	-5.056809	3.088537	-1.458541
H	-4.030650	-0.083356	-1.336395
H	1.120978	4.061240	-1.865848
H	-5.424983	2.694426	0.235795
H	-3.574101	2.785705	1.995882
H	1.975883	2.675143	-2.589067
H	-3.416439	-1.314357	-2.509787
H	2.874974	3.861778	-1.601251
H	-4.910671	-1.618026	-1.595874
H	-3.955254	-0.480933	1.072661
H	0.485250	4.051028	1.244174
H	-4.735407	-2.074768	1.004334
H	2.253479	4.039783	1.493722
H	-3.126728	-1.921430	1.763968
H	1.229488	2.796244	2.263153
H	4.497103	3.405923	0.118716
H	-3.941359	-3.782784	-0.754774
H	-2.396384	-3.494442	-1.607821
H	4.334681	2.758525	1.769388
H	-2.407324	-3.811785	0.145921
H	5.522644	0.476101	-1.500834
H	3.654877	-0.196834	2.320725
H	4.191024	1.294318	-2.356582
H	5.704590	2.256828	0.746529
H	3.741561	-1.374129	0.990865
H	4.059449	-0.434287	-1.942480
H	5.190717	-0.433536	1.448208
H	-2.658659	5.077466	-0.903336

INT-E3

Cu	1.494532	0.026325	0.018978
N	1.242141	-1.702730	-1.045304
N	0.726129	-1.199035	1.534834
C	0.498254	-0.863645	2.810068
C	0.317435	-2.394906	1.067011
C	-0.294392	-3.322667	1.924274
C	-0.153719	-1.708709	3.704727
C	-0.544307	-2.971653	3.245613
H	0.858198	0.122211	3.121368
H	-0.331235	-1.393365	4.733929
H	-1.043041	-3.676001	3.914563
C	1.519454	-1.866712	-2.342703
C	0.610246	-2.676955	-0.362901
C	0.312001	-3.900600	-0.977611
C	1.211371	-3.035577	-3.033745
C	0.608437	-4.078008	-2.324377
H	2.016628	-1.029493	-2.839649
H	1.452570	-3.128681	-4.093670
H	0.364508	-5.020393	-2.819292
H	-0.172948	-4.698032	-0.419343
H	-0.597874	-4.300363	1.556075
C	-2.586938	3.940026	-1.070767
C	-3.378323	3.017245	-0.110410
C	-4.890511	3.270773	-0.294524
C	-2.987409	3.391484	1.344877
O	-3.081124	1.697403	-0.354844
Na	-1.687712	0.608896	-1.642006
Na	-1.663218	0.596025	0.894314
O	-1.800304	-1.261732	-0.378876
O	0.011301	1.462820	-0.436806
C	-3.061551	-1.847591	-0.350817
C	-3.977557	-1.231771	-1.437665
C	-3.731688	-1.608756	1.026550
C	-2.969819	-3.367846	-0.602004
Si	1.394000	2.299970	-0.214204
C	1.955099	3.248029	-1.740835
C	1.315577	3.433039	1.288274
Si	3.694752	0.886493	0.126864
C	4.551904	2.430023	0.842527
C	4.499756	0.552267	-1.563210
C	4.234719	-0.520209	1.301572
H	-2.861994	3.705403	-2.113427
H	-1.509109	3.743503	-0.951534
H	-5.183149	4.318440	-0.103857
H	-3.229257	4.433660	1.616056
H	-1.899288	3.258563	1.485208

H	-5.180799	3.007597	-1.324427
H	-4.099376	-0.152252	-1.247606
H	1.214297	4.040397	-1.943733
H	-5.456481	2.616348	0.387985
H	-3.517266	2.725521	2.048195
H	1.987153	2.581052	-2.616037
H	-3.523585	-1.388569	-2.434325
H	2.941056	3.723230	-1.626556
H	-4.978435	-1.695623	-1.459540
H	-3.931235	-0.531822	1.159419
H	0.474925	4.131307	1.136746
H	-4.695834	-2.133714	1.135858
H	2.230144	4.022186	1.446054
H	-3.060175	-1.957954	1.829374
H	1.108611	2.857421	2.204540
H	4.385893	3.341952	0.249140
H	-3.963471	-3.845162	-0.636551
H	-2.461208	-3.555127	-1.560489
H	4.219138	2.631392	1.872917
H	-2.391146	-3.858607	0.195346
H	5.599622	0.550442	-1.472057
H	3.803945	-0.390585	2.307345
H	4.224583	1.317758	-2.305598
H	5.639375	2.243695	0.871002
H	3.919647	-1.506351	0.927155
H	4.196451	-0.429972	-1.959375
H	5.334649	-0.522482	1.401774
H	-2.773310	5.015182	-0.902024

TS-E2

Cu	-1.515007	-0.118126	-0.013712
N	-1.316163	1.603573	-1.091435
N	-0.883478	1.172137	1.518239
C	-0.667285	0.860113	2.801116
C	-0.517373	2.378587	1.045465
C	0.032632	3.343232	1.904300
C	-0.073176	1.743041	3.699505
C	0.269486	3.017982	3.234323
H	-0.988965	-0.137848	3.115642
H	0.096383	1.447074	4.735835
H	0.721974	3.750963	3.905404
C	-1.562584	1.740195	-2.398207
C	-0.785482	2.628162	-0.395245
C	-0.564351	3.868278	-1.009029
C	-1.323501	2.926332	-3.087423
C	-0.828396	4.015985	-2.366335
H	-1.976457	0.864882	-2.905699
H	-1.535648	2.994946	-4.155374
H	-0.643490	4.972652	-2.859399
H	-0.165454	4.704871	-0.439827
H	0.302827	4.328510	1.530541
C	3.675590	-3.353972	-1.614528
C	3.698117	-2.786190	-0.172947
C	5.155438	-2.789197	0.339354
C	2.844986	-3.717941	0.724155
O	3.190515	-1.508286	-0.158889
Na	1.718796	-0.561479	-1.499683
Na	1.692200	-0.495287	1.033329
O	1.706207	1.343365	-0.289760
O	0.076865	-1.494488	-0.272536
C	2.925202	2.013967	-0.292581
C	3.863001	1.443403	-1.385748
C	3.631905	1.843643	1.076103
C	2.727785	3.519742	-0.567547
Si	-1.270206	-2.388653	-0.051210
C	-1.675212	-3.511378	-1.506828
C	-1.240002	-3.362500	1.561858
Si	-3.667468	-1.091191	0.005468
C	-4.480810	-2.611877	0.814773
C	-4.370605	-0.970785	-1.757340
C	-4.368701	0.383363	0.997734
H	4.252797	-2.689130	-2.278486
H	2.634016	-3.391249	-1.981748
H	5.612127	-3.794597	0.347400
H	3.197392	-4.764143	0.735336
H	1.801675	-3.698593	0.371120
H	5.768852	-2.129281	-0.294786
H	4.060642	0.379061	-1.175896
H	-0.880572	-4.273354	-1.583268
H	5.182896	-2.385081	1.364716
H	2.858703	-3.344785	1.763899
H	-1.684414	-2.935617	-2.445024
H	3.381645	1.548627	-2.376319
H	-2.639256	-4.032387	-1.406157
H	4.829326	1.973586	-1.434406
H	3.899301	0.783561	1.223339
H	-0.329223	-3.984970	1.562461
H	4.562899	2.429896	1.158462
H	-2.110674	-4.020718	1.693271
H	2.953176	2.166631	1.884198
H	-1.182698	-2.686611	2.430046
H	-4.227166	-3.562249	0.321101
H	3.686507	4.062663	-0.616860
H	2.202498	3.656777	-1.525413
H	-4.201948	-2.697259	1.876818
H	2.121890	3.982761	0.226060
H	-5.472549	-1.028436	-1.736674
H	-4.002044	0.378073	2.036640
H	-4.002470	-1.784800	-2.401197
H	-5.576681	-2.491212	0.763635
H	-4.085346	1.347481	0.548071
H	-4.096670	-0.013955	-2.229958
H	-5.471301	0.324933	1.026337
H	4.096015	-4.371580	-1.693602

INT-E4

Cu	-1.524324	-0.128584	-0.020352
N	-1.347921	1.599190	-1.092049
N	-0.893375	1.161568	1.512395
C	-0.675055	0.850302	2.795052
C	-0.542056	2.373524	1.042057
C	-0.004384	3.343074	1.903075
C	-0.092532	1.738834	3.695570
C	0.235285	3.018427	3.232842
H	-0.985316	-0.151867	3.107779
H	0.079487	1.443195	4.731581
H	0.678027	3.755791	3.905613
C	-1.600148	1.736038	-2.397767
C	-0.814238	2.623429	-0.397861
C	-0.593857	3.863222	-1.012646
C	-1.363545	2.922205	-3.087683
C	-0.863692	4.011207	-2.368741
H	-2.016585	0.860853	-2.903424
H	-1.580680	2.991353	-4.154604
H	-0.679495	4.967569	-2.862663
H	-0.190510	4.699039	-0.445533
H	0.252822	4.332739	1.531682
C	3.974597	-3.245929	-1.611961
C	3.748671	-2.751153	-0.161933
C	5.109600	-2.721175	0.569073
C	2.815105	-3.760216	0.553149
O	3.186125	-1.496416	-0.171101
Na	1.730578	-0.541354	-1.520974
Na	1.675621	-0.490447	1.010288
O	1.693885	1.355570	-0.299122
O	0.077063	-1.481973	-0.321876
C	2.907392	2.035286	-0.284776
C	3.863153	1.474565	-1.367381

C	3.598116	1.866552	1.092326
C	2.701871	3.540338	-0.557907
Si	-1.252513	-2.396205	-0.079654
C	-1.671670	-3.517587	-1.532218
C	-1.174842	-3.376534	1.527781
Si	-3.663583	-1.129260	0.028091
C	-4.442942	-2.665331	0.841842
C	-4.397151	-1.005958	-1.722048
C	-4.367452	0.329858	1.041280
H	4.614492	-2.526722	-2.148892
H	3.005110	-3.303932	-2.138984
H	5.609300	-3.705364	0.600178
H	3.212457	-4.790099	0.571366
H	1.835267	-3.765889	0.049664
H	5.778443	-2.002301	0.069540
H	4.062957	0.410348	-1.158976
H	-0.871216	-4.271657	-1.624756
H	4.961224	-2.373758	1.605183
H	2.653744	-3.440433	1.598261
H	-1.702471	-2.938568	-2.467921
H	3.394895	1.581038	-2.364051
H	-2.628661	-4.048416	-1.416889
H	4.827375	2.009746	-1.400791
H	3.870658	0.807951	1.240850
H	-0.251276	-3.979484	1.507250
H	4.524109	2.458705	1.187886
H	-2.029490	-4.052902	1.672092
H	2.907140	2.182583	1.892625
H	-1.115328	-2.703661	2.398242
H	-4.185267	-3.609378	0.338251
H	3.656865	4.090716	-0.595975
H	2.185130	3.675755	-1.520686
H	-4.144281	-2.753135	1.898331
H	2.084361	3.996408	0.230730
H	-5.498164	-1.071803	-1.683480
H	-3.984560	0.322417	2.074307
H	-4.033747	-1.814050	-2.375958
H	-5.541070	-2.559225	0.810694
H	-4.103270	1.300391	0.593730
H	-4.137768	-0.044872	-2.194384
H	-5.468655	0.257302	1.086736
H	4.447646	-4.241751	-1.667332

TS-E3

Cu	2.134619	-0.528250	0.089583
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N	1.199814	-1.771422	1.602564
C	1.141744	-1.461309	2.898048
C	0.153444	-2.373814	1.006240
C	-1.012523	-2.677785	1.722939
C	0.015875	-1.722903	3.683257
C	-1.079702	-2.342026	3.075684
H	2.022899	-0.967413	3.318247
H	0.002177	-1.445000	4.738685
H	-1.987390	-2.554092	3.645218
C	1.577717	-2.292057	-2.356138
C	0.277206	-2.607542	-0.459079
C	-0.747679	-3.183459	-1.218293
C	0.607493	-2.862260	-3.183091
C	-0.578270	-3.307827	-2.596736
H	2.515004	-1.904675	-2.765549
H	0.778905	-2.942182	-4.258011
H	-1.374185	-3.741305	-3.206266
H	-1.679187	-3.490328	-0.753392
H	-1.870930	-3.118231	1.225233
C	-2.856740	3.666147	-1.657165
C	-2.405712	3.492348	-0.185855
C	-3.665748	3.392030	0.704509
C	-1.604880	4.744527	0.234421
O	-1.636438	2.350208	-0.059492
Na	-1.645216	0.556877	-1.412150
Na	-1.714064	0.505004	1.158239
O	-2.765999	-0.884688	-0.197393
O	0.172211	0.308558	-0.119329
C	-4.114402	-1.173095	-0.180691
C	-4.864876	-0.323356	-1.234438
C	-4.711629	-0.861201	1.214534
C	-4.361834	-2.666991	-0.497071
Si	1.166273	1.578485	0.015117
C	1.437939	2.654663	-1.492484
C	1.198896	2.480147	1.657019
Si	4.105623	0.618832	-0.102775
C	4.571313	2.295531	0.675725
C	4.619191	0.720452	-1.937568
C	5.305953	-0.624974	0.717238
H	-3.462782	2.796773	-1.968120
H	-1.970752	3.721825	-2.312255
H	-4.319763	4.278258	0.637073
H	-2.183676	5.677234	0.124866
H	-0.691398	4.833523	-0.374991
H	-4.255540	2.506638	0.417164
H	-4.706157	0.747442	-1.028203
H	0.572377	3.328757	-1.578263
H	-3.363039	3.271919	1.759215
H	-1.297467	4.657078	1.289239
H	1.494531	2.029810	-2.396996
H	-4.464031	-0.543058	-2.239681
H	2.356358	3.256124	-1.426824
H	-5.952111	-0.510259	-1.256628
H	-4.588378	0.211546	1.443150
H	0.265211	3.058676	1.721610
H	-5.785986	-1.098268	1.296773
H	2.055337	3.161984	1.751333
H	-4.174471	-1.442387	1.983873
H	1.235487	1.756966	2.486816
H	4.026886	3.146134	0.236652
H	-5.432175	-2.933130	-0.513074
H	-3.932064	-2.912200	-1.481949
H	4.378635	2.298882	1.760795
H	-3.871054	-3.303125	0.259143
H	5.671827	1.039240	-2.035132
H	5.108690	-0.716624	1.798128
H	3.996721	1.435667	-2.498002
H	5.649369	2.480168	0.526658
H	5.208388	-1.629948	0.275709
H	4.522567	-0.262586	-2.428597
H	6.353112	-0.295696	0.591588
H	-3.463699	4.571888	-1.825902

INT-E5

Cu	0.922574	1.493003	0.783844
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N	0.710338	-0.072344	2.100990
C	-0.440751	-0.176519	2.787891
C	1.429101	-1.193776	1.859084
C	0.996810	-2.455073	2.298651
C	-0.944572	-1.392009	3.240554
C	-0.208984	-2.560596	2.987956
H	-0.980671	0.756223	2.959735
H	-1.892292	-1.421991	3.780930
H	-0.576286	-3.535242	3.316197
C	3.777070	0.223719	-0.530569
C	2.674952	-1.006685	1.089715
C	3.834669	-1.746915	1.361154
C	4.967170	-0.471509	-0.330839
C	4.993277	-1.483430	0.635234
H	3.717378	1.032401	-1.264722
H	5.851734	-0.223621	-0.919907

H	5.908750	-2.045964	0.830178
H	3.830042	-2.501197	2.149281
H	1.581111	-3.342737	2.054894
C	-4.975802	-0.730068	-1.524360
C	-4.603163	-0.479976	-0.058017
C	-4.787203	-1.761707	0.762363
C	-5.456191	0.647398	0.533644
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Na	-1.340638	-1.510773	-0.094758
O	0.219131	-2.067610	-1.439276
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C	0.406207	-3.428633	-3.408163
C	-0.197013	-4.415864	-1.177072
C	2.120261	-3.531400	-1.570475
Si	-2.298916	1.290256	-0.206480
C	-2.782990	2.098609	-1.833584
C	-2.623872	2.462667	1.228718
Si	1.470888	3.355695	-0.424222
C	0.242674	4.828603	-0.420633
C	1.397393	2.773830	-2.285311
C	3.201635	4.169962	-0.296079
H	-4.327213	-1.510704	-1.952122
H	-4.847375	0.183423	-2.121987
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H	-5.336058	1.577579	-0.041475
H	-4.182495	-2.580598	0.337791
H	-0.656120	-3.254218	-3.643791
H	-3.830086	2.440385	-1.860824
H	-4.464077	-1.593790	1.801378
H	-5.166109	0.847574	1.575626
H	-2.623362	1.403699	-2.673933
H	0.995955	-2.654321	-3.927103
H	-2.140885	2.979400	-1.999304
H	0.698883	-4.412594	-3.812997
H	-1.270275	-4.285087	-1.402342
H	-3.524278	3.079993	1.085209
H	0.087917	-5.437168	-1.481371
H	-1.755995	3.134143	1.331869
H	-0.060610	-4.336602	-0.084309
H	-2.741804	1.910116	2.174333
H	-0.787695	4.488856	-0.619698
H	2.496503	-4.506327	-1.924520
H	2.722008	-2.737392	-2.043237
H	0.234068	5.329047	0.562478
H	2.287921	-3.468516	-0.484226
H	1.611195	3.599045	-2.987512
H	3.321651	4.667072	0.681529
H	0.389199	2.397269	-2.537749
H	0.500279	5.586475	-1.182489
H	4.009264	3.421635	-0.374073
H	2.135954	1.981758	-2.518862
H	3.366355	4.928854	-1.082584
H	-6.022718	-1.058608	-1.618596

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Na	-0.069018	1.419188	-0.000320
O	-1.576084	-0.092188	-0.000362
C	-2.957417	-0.014837	0.000041
C	-3.400885	1.467083	0.002546
C	-3.528647	-0.700438	-1.259294
C	-3.528139	-0.704498	1.257400
H	-3.109271	-0.226462	-2.161468
H	-3.234925	-1.763750	-1.269738
H	-4.629249	-0.649391	-1.315956
H	-3.003925	1.974274	0.899728
H	-3.004383	1.977175	-0.893199
H	-4.496324	1.594452	0.003012
H	-3.234489	-1.767868	1.264252
H	-3.108352	-0.233455	2.160919
H	-4.628712	-0.653607	1.314710
Na	0.069021	-1.419183	-0.000320
O	1.576084	0.092194	-0.000351
C	2.957417	0.014836	0.000045
C	3.400876	-1.467087	0.002429
C	3.528645	0.700532	-1.259242
C	3.528147	0.704398	1.257452
H	3.234516	1.767771	1.264378
H	3.108346	0.233301	2.160935
H	4.628719	0.653472	1.314761
H	3.109280	0.226616	-2.161452
H	3.234913	1.763843	-1.269606
H	4.629247	0.649510	-1.315903
H	3.003914	-1.974348	0.899570
H	3.004370	-1.977103	-0.893358
H	4.496315	-1.594464	0.002881

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O	-0.804405	-1.881372	0.018060
Si	-2.180668	-1.053921	-0.125052
C	-3.254752	-1.037612	1.425782
C	-3.243465	-1.580566	-1.585764
H	-3.535813	-2.080193	1.651699
H	-2.731387	-0.640733	2.309448
H	-4.186422	-0.465919	1.288851
H	-2.667540	-1.526436	-2.524736
H	-3.584934	-2.621985	-1.466547
H	-4.131128	-0.936726	-1.698631
Na	0.405911	-0.361815	-1.192590
O	2.133093	-0.550722	0.069768
C	3.369886	0.063249	-0.035691
C	3.405477	0.954413	-1.299389
C	3.631137	0.948671	1.201177
C	4.484678	-0.997897	-0.145160
H	2.842691	1.713393	1.288320
H	3.601795	0.330016	2.113734
H	4.608198	1.459518	1.164039
H	3.224173	0.338067	-2.197569
H	2.615621	1.723221	-1.237383
H	4.367745	1.474704	-1.438444
H	4.484361	-1.632651	0.757357
H	4.294153	-1.647120	-1.015178
H	5.490426	-0.557218	-0.251589
Na	1.002983	-2.001920	1.105722
O	-1.688719	0.542034	-0.601454
C	-1.496647	1.759596	0.126009
C	-0.608970	1.525512	1.359154
C	-0.794568	2.722717	-0.839850
C	-2.856895	2.339202	0.529843
H	-3.494465	2.453438	-0.359927
H	-3.371649	1.678611	1.240580
H	-2.739124	3.325247	1.005842
H	0.207657	2.350426	-1.112048
H	-1.387218	2.832235	-1.760333
H	-0.659584	3.716021	-0.385747
H	-1.100861	0.849474	2.073697
H	0.359206	1.081908	1.074003
H	-0.409426	2.475457	1.879197

Mass Spectroscopic Analysis of the Reaction

An oven-dried 20-mL Schlenk tube equipped with a greaseless stopcock and a magnetic stir bar was charged with CuCl[P(OPh)$_3$] (4.1 mg, 0.010 mmol), diphenylacetylene (**2a**, 35.6 mg, 0.200 mmol), **1-Me** (68.1 mg, 0.400 mmol), DCE (1.0 mL) and *t*BuOH (38.0 μL, 0.400 mmol). DCE (1.0 mL) was added to the mixture to rinse the inside wall of the tube. The resulting mixture was stirred at 50 °C. After 16 h, the reaction mixture was cooled to room temperature and the reaction mixture was directly analyzed by Low-resolution mass spectroscopy using positive APCI.

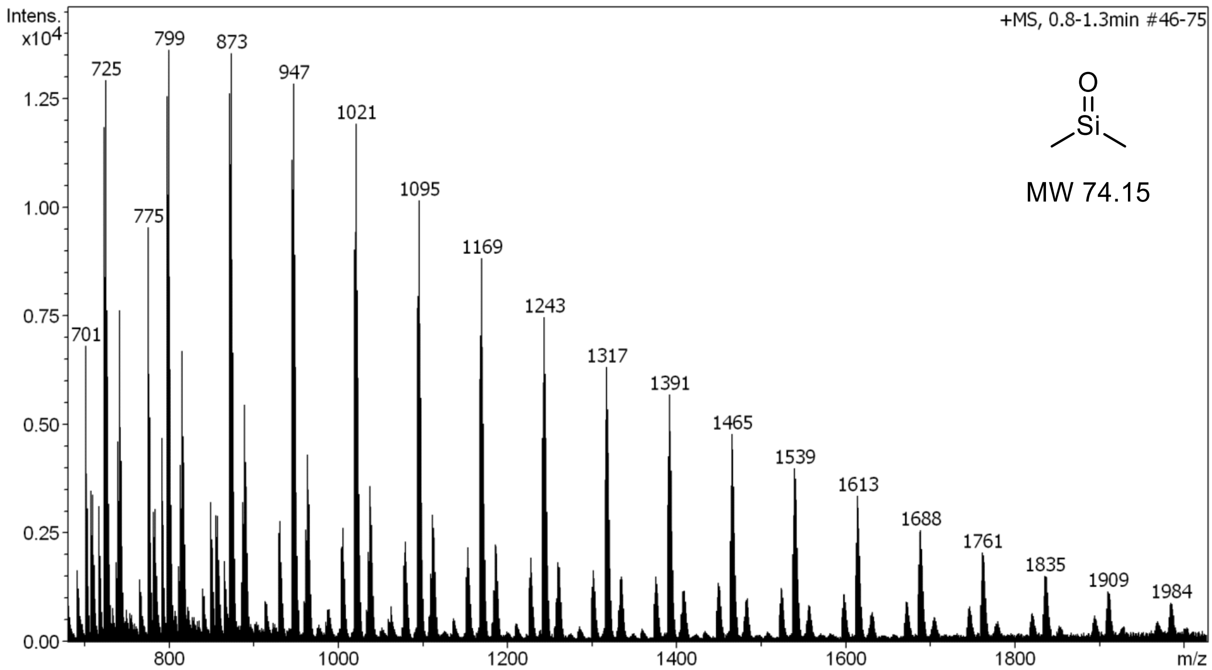


Figure S4. Positive APCI mass spectrum of the reaction mixture of 1a after completion of the reaction

The Low-resolution mass spectrum of the reaction mixture of **1a** after completion of the reaction is shown in Figure S4. The spectrum shows molecular weight distribution that fitted with the Gaussian distribution with interval of 74 mass units corresponding to the repeat unit of polydimethylsiloxane. Considering that the molecular weight of dimethylsilanone is 74.15, this result implies the formation of polydimethylsiloxane that is observed through a random cleavage during the ionization.

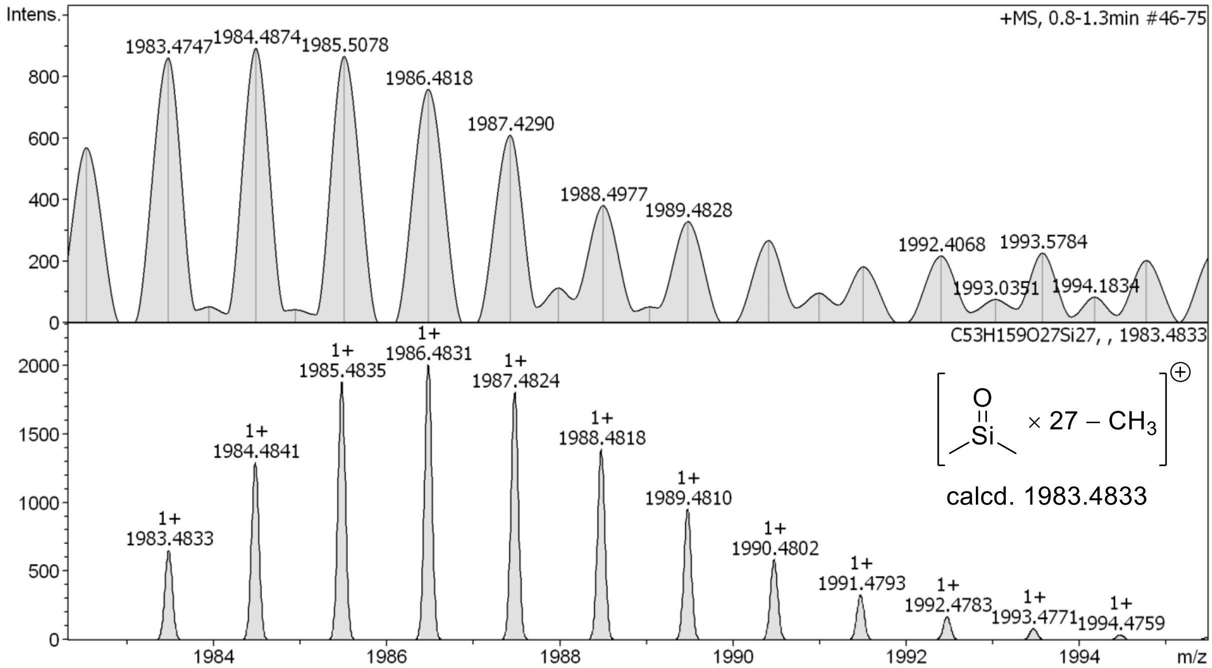
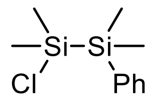


Figure S5. Observed (upper) and predicted (lower) HRMS spectra of the cationic species of dimethylsilanone 27-mer minus one methyl group

Figure 5 shows the HRMS spectrum around mass peak m/z 1984 of the reaction mixture after completion of the reaction. The upper spectrum is the observed HRMS spectrum and the lower one is the calculated mass values of cationic species of dimethylsilanone 27-mer minus one methyl group. These two spectra are in good agreement. This result suggested the formation of polydimethylsiloxane that is longer than 27-mer of dimethylsilanone during the reaction.

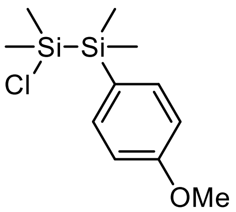
Characterization Data

1-chloro-2-phenyl-1,1,2,2-tetramethyldisilane (S1):



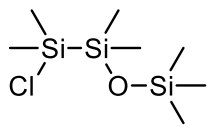
density: 0.97 g/cm^3. ^{1}H NMR (C_6D_6): δ 7.38 (m, 2H), 7.27–7.24 (m, 3H), 0.34 (s, 6H), 0.34 (s, 6H); ^{13}C NMR (C_6D_6): δ 136.8, 134.1, 129.3, 128.3, 2.0, –4.7; HRMS (APCI-MS, positive): *m/z* [M–Cl]$^+$ Calcd for $C_{10}H_{17}Si_2$ 193.0863, Found 193.0871.

1-chloro-2-(4-methoxyphenyl)-1,1,2,2-tetramethyldisilane (S2):



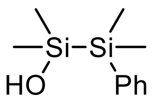
density: 1.01 g/cm^3. ^{1}H NMR (C_6D_6): δ 7.35 (d, J = 8.9 Hz, 2H), 6.82 (d, J = 8.9 Hz, 2H), 3.28 (s, 3H), 0.36 (s, 6H), 0.34 (s, 6H); ^{13}C NMR (C_6D_6): δ 161.2, 135.6, 127.1, 114.3, 54.5, 2.1, –4.4; HRMS (APCI-MS, positive): *m/z* [M–Cl]$^+$ Calcd for $C_{11}H_{19}OSi_2$ 223.0969, Found 223.0967.

1-chloro-2-trimethylsiloxy-1,1,2,2-tetramethyldisilane (S3):



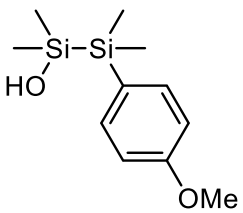
density: 0.89 g/cm^3. ^{1}H NMR (C_6D_6): δ 0.38 (s, 6H), 0.25 (s, 6H), 0.09 (s, 9H); ^{13}C NMR (C_6D_6): δ 2.0, 1.9, 1.3; HRMS (APCI-MS, positive): *m/z* [M–Cl]$^+$ Calcd for $C_7H_{21}OSi_3$ 205.0896, Found 205.0895.

2-phenyl-1,1,2,2-tetramethyldisilan-1-ol (S4):



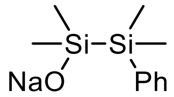
density: 0.89 g/cm^3. ^{1}H NMR (C_6D_6): δ 7.49 (dd, J = 8.2, 1.4 Hz, 2H), 7.22–7.17 (m, 3H), 0.74 (s, 1H), 0.32 (s, 6H), 0.16 (s, 6H); ^{13}C NMR (C_6D_6): δ 139.1, 134.2, 128.8, 128.2, 1.6, –3.8; ^{29}Si NMR (C_6D_6): δ 12.6, –24.8; HRMS (APCI-MS, positive): *m/z* [M–OH]$^+$ Calcd for $C_{10}H_{17}Si_2$ 193.0863, Found 193.0869.

2-(4-methoxyphenyl)-1,1,2,2-tetramethyldisilan-1-ol (S5):



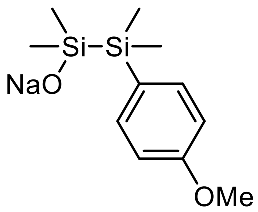
A colorless liquid (4.53 g, 18.1 mmol, 91%, density: 1.00 g/cm^3). ^{1}H NMR ($CDCl_3$): δ 7.41 (d, J = 8.9 Hz, 2H), 6.92 (d, J = 8.9 Hz, 2H), 3.81 (s, 3H), 0.35 (s, 6H), 0.24 (s, 6H); ^{13}C NMR ($CDCl_3$): δ 160.1, 135.1, 129.1, 113.7, 54.9, 1.4, –3.9; ^{29}Si NMR ($CDCl_3$): δ 13.9, –25.4; HRMS (APCI-MS, positive): *m/z* [M–OH]$^+$ Calcd for $C_{11}H_{19}OSi_2$ 223.0969, Found 223.0970.

Sodium (dimethylphenylsilyl)dimethylsilanolate (1-Ph):



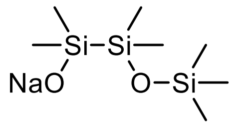
^{1}H NMR (C_6D_6): δ 7.51 (d, J = 7.5 Hz, 2H), 7.24 (dd, J = 7.5, 7.5 Hz, 2H), 7.17 (dd, J = 7.5, 7.5 Hz, 1H), 0.34 (s, 6H), 0.16 (s, 6H); ^{13}C NMR (C_6D_6): δ 143.4, 133.5, 128.9, 128.7, 5.8, –3.1; ^{29}Si NMR (C_6D_6): δ –12.4, –26.4; HRMS (ESI-MS, negative): *m/z* [M–Na]$^-$ Calcd for $C_{10}H_{17}OSi_2$ 209.0823; Found 209.0828.

Sodium (dimethyl(4-methoxyphenyl)silyl)dimethylsilanolate (1-Ans):



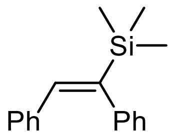
^{1}H NMR (C_6D_6): δ 7.49 (d, J = 8.2 Hz, 2H), 6.94 (d, J = 8.2 Hz, 2H), 3.38 (s, 3H), 0.39 (s, 6H), 0.19 (s, 6H); ^{13}C NMR (C_6D_6): δ 160.6, 134.9, 132.8, 114.9, 54.5, 5.7, –2.8; ^{29}Si NMR (C_6D_6) δ –12.0, –26.9; HRMS (ESI-MS, negative): *m/z* [M–Na]$^-$ Calcd for $C_{11}H_{19}OSi_2$ 239.0929, Found 239.0922.

Sodium (dimethyl(trimethyl)siloxysilyl)dimethylsilanolate (1-OSiMe$_3$):



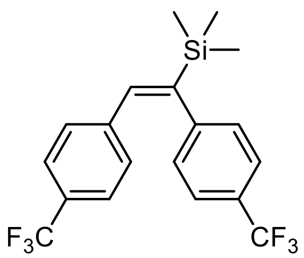
^{1}H NMR (C_6D_6): δ 0.25 (s, 6H), 0.21 (s, 6H), 0.13 (s, 9H); ^{13}C NMR (C_6D_6): δ 5.9, 3.1, 2.4; ^{29}Si NMR (C_6D_6): δ 13.9, 9.3, –15.4; HRMS (ESI-MS, negative): *m/z* [M–Na]$^-$ Calcd for $C_7H_{21}O_2Si_3$ 221.0855; Found 221.0845.

(*E*)-(1,2-diphenylvinyl)trimethylsilane (3a):



R_f = 0.66 (hexane only). ^{1}H NMR ($CDCl_3$): δ 7.30 (dd, J = 7.6, 7.6 Hz, 2H), 7.21 (dd, J = 7.6, 7.6 Hz, 1H), 7.10–7.07 (m, 3H), 6.99 (d, J = 7.6 Hz, 2H), 6.96 (dd, J = 7.6, 2.1 Hz, 2H), 6.80 (s, 1H), 0.14 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 147.1, 142.7, 137.3, 137.3, 129.4, 128.6, 127.9, 127.4, 127.0, 125.6, –1.7; HRMS (APCI-MS, positive): *m/z* [M]$^+$ Calcd for $C_{17}H_{20}Si$ 252.1329, Found 252.1324. All the resonances in ^{1}H NMR spectrum were consistent with the reported values.[26] ^{1}H and ^{13}C NMR spectra are provided below.

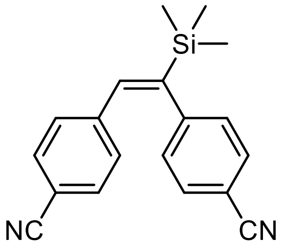
(*E*)-(1,2-di(4-trifluoromethylphenyl)vinyl)trimethylsilane (3b):



A white solid (174 mg, 0.449 mmol, 90%) from **2b** (157 mg, 0.501 mmol). Purification was done by GPC (eluent: $CHCl_3$). mp: 72.4–76.0 °C; R_f = 0.61 (hexane only); ^{1}H NMR ($CDCl_3$): δ 7.58 (d, J = 8.2 Hz, 2H), 7.36 (d, J = 8.2 Hz, 2H), 7.09 (d, J = 8.2 Hz, 2H), 7.02 (d, J = 8.2 Hz, 2H), 6.87 (s, 1H), 0.16 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 148.9, 146.3, 140.2, 136.7, 129.5, 129.0 (q, J = 31.9 Hz), 128.3 (q, J = 31.9 Hz), 127.6, 125.7

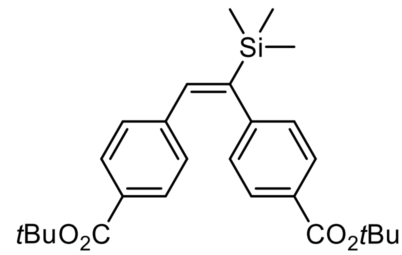
(q, J = 2.9 Hz), 125.0 (q, J = 2.9 Hz), 124.3 (q, J = 271.7 Hz), 124.0 (q, J = 271.7 Hz), –1.8; ^{19}F NMR ($CDCl_3$): –62.7, –63.0; HRMS (APCI-MS, positive): *m/z* $[M]^+$ Calcd for $C_{19}H_{18}F_6Si$ 388.1076, Found 388.1077.

(*E*)-(1,2-di(4-cyanophenyl)vinyl)trimethylsilane (3c):



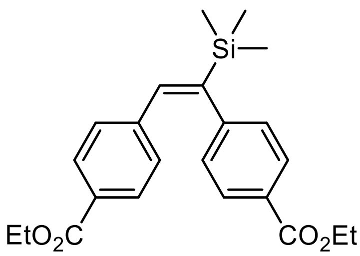
A white solid (115 mg, 0.380 mmol, 76%) from **2c** (113 mg, 0.497 mmol). Purification was done by column chromatography on silica gel (hexane/EtOAc = 10/1) and GPC (eluent: $CHCl_3$). mp: 132.8–135.3 °C; R_f = 0.25 (hexane/Etowah = 10/1); ^{1}H NMR ($CDCl_3$): δ 7.61 (d, J = 8.2 Hz, 2H), 7.40 (d, J = 8.2 Hz, 2H), 7.07 (d, J = 8.2 Hz, 2H), 6.99 (d, J = 8.2 Hz, 2H), 6.86 (s, 1H), 0.16 (s, 9H); ^{13}C NMR ($CDCl_3$) δ 149.9, 147.3, 140.8, 136.4, 132.5, 131.7, 129.6, 127.8, 118.7, 118.4, 110.6, 109.9, –2.0; HRMS (APCI-MS, positive): *m/z* $[M+H]^+$ Calcd for $C_{19}H_{19}N_2Si$ 303.1312, Found 303.1318.

(*E*)-(1,2-di(4-*tert*-butoxycarbonylphenyl)vinyl)trimethylsilane (3d):



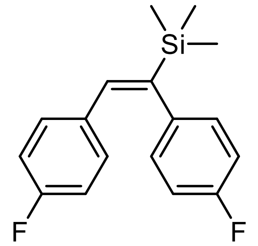
A pale yellow oil (225 mg, 0.497 mmol, 99%) from **2d** (190 mg, 0.500 mmol). Purification was done by GPC (eluent: $CHCl_3$). R_f = 0.22 (hexane/EtOAc = 20/1); ^{1}H NMR ($CDCl_3$): δ 7.93 (d, J = 8.2 Hz, 2H), 7.71 (d, J = 8.2 Hz, 2H), 7.02 (d, J = 8.2 Hz, 2H), 6.97 (d, J = 8.2 Hz, 2H), 6.86 (s, 1H), 1.61 (s, 9H), 1.54 (s, 9H), 0.14 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 165.6, 165.3, 149.0, 147.2, 140.9, 136.8, 130.3, 129.8, 129.5, 129.0, 127.1, 80.70, 80.65, 28.1, 28.0, –1.8 (one overlapped peak); HRMS (APCI-MS, positive): *m/z* $[M]^+$ Calcd for $C_{27}H_{36}O_4Si$ 452.2377, Found 452.2365.

(*E*)-(1,2-di(4-ethoxycarbonylphenyl)vinyl)trimethylsilane (3e):



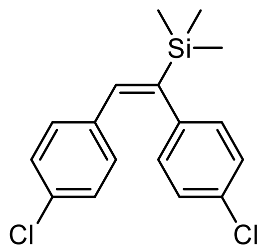
A colorless oil (113 mg, 0.284 mmol, 57%) from **2e** (161 mg, 0.500 mmol). Purification was done by column chromatography on silica gel (hexane/EtOAc = 20/1, then hexane/CH_2Cl_2 = 1/1), followed by GPC (eluent: $CHCl_3$). R_f = 0.47 (hexane/EtOAc = 10/1); ^{1}H NMR ($CDCl_3$): δ 7.99 (d, J = 8.2 Hz, 2H), 7.76 (d, J = 8.2 Hz, 2H), 7.05 (d, J = 8.2 Hz, 2H), 6.99 (d, J = 8.2 Hz, 2H), 6.87 (s, 1H), 4.38 (q, J = 7.2 Hz, 2H), 4.31 (q, J = 7.2 Hz, 2H), 1.40 (t, J = 7.2 Hz, 3H), 1.34 (t, J = 7.2 Hz, 3H), 0.15 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 166.5, 166.1, 149.3, 147.7, 141.2, 136.8, 130.0, 129.14, 129.12, 128.8, 128.0, 127.2, 60.8, 60.7, 14.3, 14.2, –1.8; HRMS (APCI-MS, positive): *m/z* $[M]^+$ Calcd for $C_{23}H_{28}O_4Si$ 396.1751, Found 396.1757.

(*E*)-(1,2-di(4-fluorophenyl)vinyl)trimethylsilane (3f):



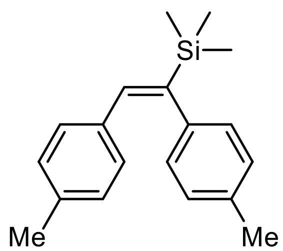
A white solid (110 mg, 0.380 mmol, 76%) from **2f** (108 mg, 0.502 mmol). Purification was done by column chromatography on silica gel (hexane only) and GPC (eluent: $CHCl_3$). mp: 92.6–93.9 °C; R_f = 0.67 (hexane only); ^{1}H NMR ($CDCl_3$): δ 7.01 (dd, J = 8.9, 8.9 Hz, 2H), 6.94–6.90 (m, 4H), 6.79 (dd, J = 8.9, 8.9 Hz, 2H), 6.77 (s, 1H), 0.13 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 161.6 (d, J = 249.0 Hz), 161.3 (d, J = 244.6 Hz), 145.7, 138.1 (d, J = 2.9 Hz), 136.7, 133.3 (d, J = 4.4 Hz), 131.0 (d, J = 8.6 Hz), 128.9 (d, J = 8.8 Hz), 115.7 (d, J = 20.2 Hz), 114.8 (d, J = 21.7 Hz), –1.8; ^{19}F NMR ($CDCl_3$): –114.7, –117.3; HRMS (APCI-MS, positive): *m/z* $[M]^+$ Calcd for $C_{17}H_{18}F_2Si$ 288.1140, Found 288.1136.

(*E*)-(1,2-di(4-chlorophenyl)vinyl)trimethylsilane (3g):



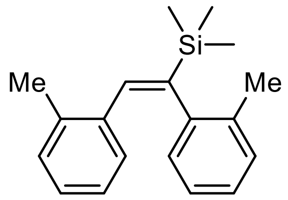
A yellow solid (137 mg, 0.426 mmol, 85%) from **2g** (124 mg, 0.501 mmol). Purification was done by GPC (eluent: $CHCl_3$). mp: 94.6–96.7 °C; R_f = 0.61 (hexane only); ^{1}H NMR ($CDCl_3$): δ 7.28 (d, J = 8.2 Hz, 2H), 7.08 (d, J = 8.2 Hz, 2H), 6.90 (d, J = 8.2 Hz, 2H), 6.88 (d, J = 8.2 Hz, 2H), 6.76 (s, 1H), 0.13 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 146.7, 140.8, 136.6, 135.4, 132.9, 131.7, 130.6, 129.0, 128.7, 128.2, –1.8; HRMS (APCI-MS, positive): *m/z* $[M]^+$ Calcd for $C_{17}H_{18}{}^{35}Cl_2Si$ 320.0549, Found 320.0554.

(*E*)-(1,2-di(4-methylphenyl)vinyl)trimethylsilane (3h):



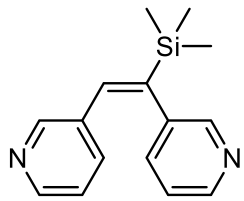
A white solid (131 mg, 0.467 mmol, 93%) from **2h** (103 mg, 0.500 mmol). Purification was done by column chromatography on silica gel (hexane only). mp: 78.3–83.7 °C; R_f = 0.54 (hexane only); ^{1}H NMR ($CDCl_3$): δ 7.11 (d, J = 7.6 Hz, 2H), 6.90 (d, J = 8.2 Hz, 2H), 6.87 (d, J = 7.6 Hz, 2H), 6.86 (d, J = 8.2 Hz, 2H), 6.74 (s, 1H), 2.35 (s, 3H), 2.23 (s, 3H), 0.11 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 145.9, 139.7, 137.1, 136.7, 134.8, 134.7, 129.4, 129.3, 128.6, 127.3, 21.2, 21.1, –1.6; HRMS (APCI-MS, positive): *m/z* $[M]^+$ Calcd for $C_{19}H_{24}Si$ 280.1642, Found 280.1649.

(*E*)-(1,2-di(2-methylphenyl)vinyl)trimethylsilane (3i):



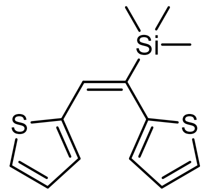
A colorless oil (113 mg, 0.402 mmol, 81%) from **2i** (103 mg, 0.499 mmol). 3.0 equiv **1-Me** and 3.0 equiv *t*BuOH were used. Purification was done by GPC (eluent: $CHCl_3$). R_f = 0.39 (hexane only); ^{1}H NMR ($CDCl_3$): δ 7.12 (ddd, J = 7.6, 7.6, 2.1 Hz, 1H), 7.08 (d, J = 7.6 Hz, 1H), 7.05 (ddd, J = 7.6, 7.6, 1.4 Hz, 3H), 7.037 (s, 1H), 7.036 (d, J = 7.6 Hz, 1H), 7.00–6.96 (m, 2H), 6.76 (dd, J = 7.6, 7.6 Hz, 1H), 6.70 (d, J = 7.6 Hz, 1H), 2.37 (s, 3H), 1.91 (s, 3H), 0.15 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 145.8, 141.2, 136.9, 136.7, 135.8, 134.0, 130.1, 129.8, 128.3, 128.1, 126.9, 125.5, 125.3, 125.2, 19.8, 19.7, –1.3; HRMS (APCI-MS, positive): *m/z* $[M]^+$ Calcd for $C_{19}H_{24}Si$ 280.1642, Found 280.1635.

(*E*)-(1,2-di(3-pyridinyl)vinyl)trimethylsilane (3k):



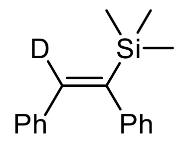
A colorless oil (105 mg, 0.411 mmol, 82%) from **2k** (90.3 mg, 0.501 mmol). Purification was done by column chromatography on silica gel (hexane/EtOAc = 8/1 to 0/1). R_f = 0.22 (hexane/EtOAc = 1/1); ^{1}H NMR ($CDCl_3$): δ 8.49 (dd, J = 4.8, 2.1 Hz, 1H), 8.33 (dd, J = 4.8, 2.1 Hz, 1H), 8.30 (d, J = 2.1 Hz, 1H), 8.25 (d, J = 2.1 Hz, 1H), 7.31 (ddd, J = 7.6, 2.1, 2.1 Hz,1H), 7.25 (dd, J = 7.6, 4.8 Hz, 2H), 7.09 (ddd, J = 8.2, 2.1, 2.1 Hz, 1H), 6.99 (dd, J = 8.2, 4.8 Hz, 1H), 6.90 (s, 1H), 0.17 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 150.6, 148.0, 147.9, 147.3, 146.0, 137.5, 135.6, 135.5, 134.7, 132.3, 123.4, 122.7, –2.0; HRMS (APCI-MS, positive): *m/z* $[M+H]^+$ Calcd for $C_{15}H_{19}N_2Si$ 255.1312, Found 255.1323.

(*E*)-(1,2-di(2-thiophenyl)vinyl)trimethylsilane (3l):



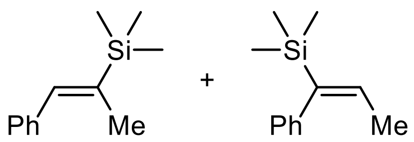
A white solid (107 mg, 0.406 mmol, 81%) from **2l** (95.5 mg, 0.502 mmol). Purification was done by GPC (eluent: $CHCl_3$). mp: 70.7–72.5 °C; R_f = 0.45 (hexane only); ^{1}H NMR ($CDCl_3$): δ 7.37 (dd, J = 4.8, 1.4 Hz, 1H), 7.12 (dd, J = 4.8, 1.4 Hz, 1H), 7.11 (s, 1H), 7.09 (dd, J = 5.5, 3.4 Hz, 1H), 6.97 (dd, J = 3.4, 1.4 Hz, 1H), 6.88 (dd, J = 5.5, 3.4 Hz, 1H), 6.68 (d, J = 3.4 Hz, 1H), 0.16 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 142.0, 140.5, 136.4, 134.4, 129.6, 127.74, 127.68, 125.8, 125.4, 124.6, –2.0; HRMS (APCI-MS, positive): *m/z* $[M]^+$ Calcd for $C_{13}H_{16}S_2Si$ 264.0457, Found 264.0459.

(*E*)-(1,2-diphenylvinyl-2-*d*)trimethylsilane (3m):



A colorless oil (73.4 mg, 0.290 mmol, 58%) from **2a** (88.6 mg, 0.497 mmol). Reaction time was 20 h. CH_3OD was used instead of *t*BuOH. Purification was done by GPC (eluent: $CHCl_3$) and column chromatography on silica gel (hexane only). R_f = 0.56 (hexane only); ^{1}H NMR ($CDCl_3$): δ 7.31 (t, J = 7.5 Hz, 2H), 7.23–7.20 (m, 1H), 7.12–7.07 (m, 3H), 6.99 (d, J = 7.5 Hz, 2H), 6.96–6.94 (m, 2H), 0.13 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 146.9, 142.7, 137.2, 136.8 (t, J = 23.2 Hz), 129.4, 128.6, 127.9, 127.3, 127.0, 125.6, –1.7; HRMS (APCI-MS, positive): *m/z* $[M]^+$ Calcd for $C_{17}H_{20}DSi$ 254.1470, Found 254.1476.

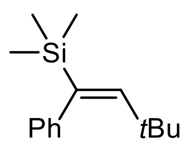
(*E*)-(1-phenylprop-1-en-2-yl)trimethylsilane and (*E*)-(1-phenylprop-1-en-1-yl)trimethylsilane (3n):



major minor

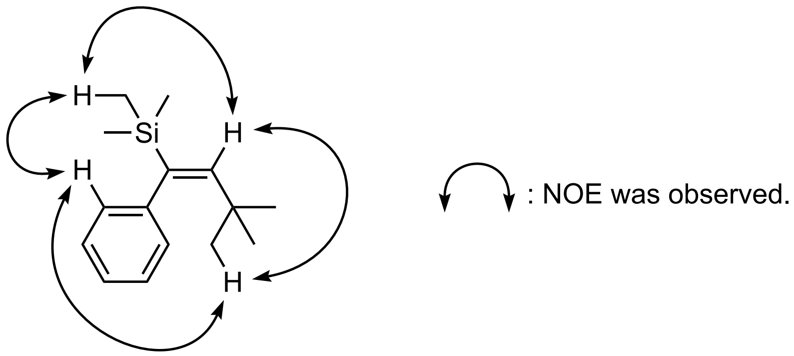
$P(OPh)_3$ as a ligand: A colorless oil (67.8 mg, 0.356 mmol, 70%, major:minor = 3.4:1 as an inseparable mixture) from **2n** (58.2 mg, 0.501 mmol). Purification was done by preparative TLC with an eluent (hexane only). R_f = 0.59 (hexane only); ^{1}H NMR ($CDCl_3$): δ 7.34 (major, dd, J = 7.6, 7.6 Hz, 2H), 7.31–7.29 (major, d, J = 7.6 Hz, 2H + minor, m, 2H), 7.21 (major, dd, J = 7.6, 7.6 Hz, 1H), 7.18 (minor, dd, J = 7.6, 7.6 Hz, 1H), 6.93 (minor, d, J = 7.6 Hz, 2H), 6.72 (s, 1H), 6.09 (minor, q, J = 6.6 Hz, 1H), 1.95 (major, s, 3H), 1.55 (minor, d, J = 6.6 Hz, 3H), 0.15 (major, s, 9H), 0.04 (minor, s, 9H); ^{13}C NMR ($CDCl_3$): δ 145.9, 142.4, 140.3 (major), 138.4 (major), 136.8 (major), 135.4, 129.0, 128.0, 127.8 (major), 126.4, 125.2 (major), 16.3 (major), 15.9, –1.6 (major), –2.1 (overlapped one peak); PCy_3 as a ligand: A colorless oil (54.5 mg, 0.286 mmol, 57%, major:minor = 25:1 as an inseparable mixture) from **2n** (58.2 mg, 0.501 mmol). Concentration of **2n**: 0.5 M. 5 mol% $[CuCl(PCy_3)]_2$ (10 mol% Cu), 3.0 equiv **1-Me**, and 3.0 equiv *t*BuOH were used. Purification was done by preparative TLC (hexane only) and GPC (eluent: $CHCl_3$). All the resonances in ^{1}H and ^{13}C NMR spectrum were consistent with the ones with $P(OPh)_3$ as a ligand. HRMS (APCI-MS, positive): *m/z* $[M–Me]^+$ Calcd for $C_{11}H_{15}Si$ 175.0938, Found 175.0935.

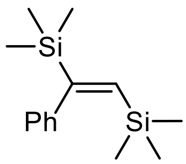
(*E*)-(3,3-dimethyl-1-phenylbut-1-en-1-yl)trimethylsilane (3o):



A white solid (46.2 mg, 0.199 mmol, 39%) from **2o** (79.9 mg, 0.505 mmol). The reaction temperature was 80 °C. Concentration of **2o**: 0.5 M. 10 mol% $CuCl[P(OPh)_3]$ was used. Purification was done by preparative TLC with an eluent (hexane only) and GPC (eluent: $CHCl_3$). mp: 40.6–41.9 °C; R_f = 0.79 (hexane only); ^{1}H NMR ($CDCl_3$): δ 7.22 (dd, J = 7.6, 7.6 Hz, 2H), 7.13 (dd, J = 7.6, 7.6 Hz, 1H), 6.92 (d, J = 7.6

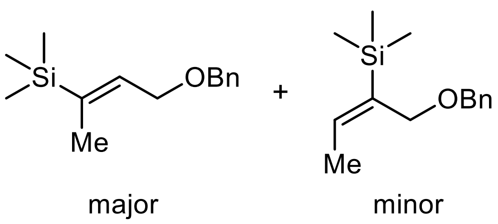
Hz, 2H), 5.83 (s, 1H), 0.86 (s, 9H), –0.01 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 149.0, 142.7, 141.8, 128.2, 127.3, 124.8, 35.9, 31.2, –1.8; HRMS (APCI-MS, positive): *m/z* $[M]^+$ Calcd for $C_{15}H_{24}Si$ 232.1642, Found 232.1649. The stereochemistry of the product was determined by analysis of NOE.



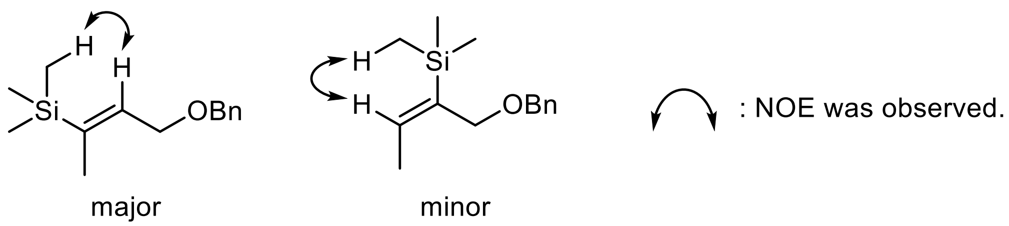


(*E*)-(1-phenylethene-1,2-diyl)bis(trimethylsilane) (3p): A colorless oil (114 mg, 0.459 mmol, 93%) from **2p** (86.3 mg, 0.495 mmol). Concentration of **2p**: 0.5 M. 10 mol% CuCl[P(OPh)$_3$] was used. Purification was done by preparative TLC with an eluent (hexane only). R_f = 0.72 (hexane only). All the resonances in ^{1}H and ^{13}C NMR spectrum (CD_2Cl_2) were consistent with the reported values.[27] ^{1}H and ^{13}C NMR spectra are provided below.

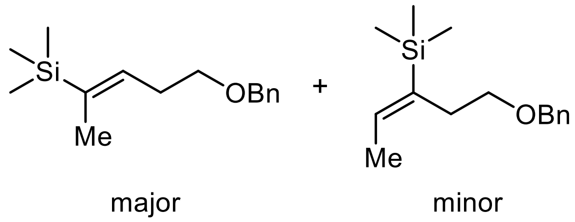
(*E*)-(4-(benzyloxy)but-2-en-2-yl)trimethylsilane and (*E*)-(1-(benzyloxy)but-2-en-2-yl)trimethylsilane (3q):



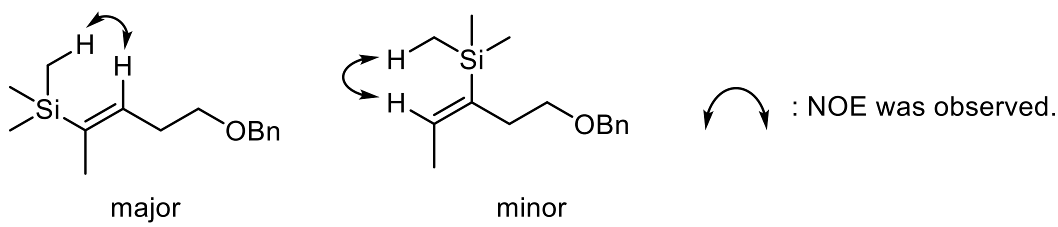
A colorless oil (93.7 mg, 0.400 mmol, 80%, major:minor = 7.4:1 as an inseparable mixture) from **2q** (80.1 mg, 0.500 mmol). Purification was done by column chromatography on silica gel (hexane/EtOAc = 1/0 to 40/1) and preparative TLC with an eluent (hexane/EtOAc = 20/1). R_f = 0.43 (hexane/EtOAc = 20/1); ^{1}H NMR ($CDCl_3$): δ 7.37–7.34 (major, m, 4H + minor, m, 4 H), 7.30–7.26 (major, m, 1H + minor, m, 1 H), 6.01 (minor, q, *J* = 6.6 Hz, 1H), 5.90–5.88 (major, m, 1H), 4.53 (major, s, 2H), 4.48 (minor, s, 2H), 4.18 (minor, s, 2H), 4.13 (major, d, *J* = 5.5 Hz, 2H), 1.72 (minor, d, *J* = 6.2 Hz, 3H), 1.67 (major, s, 3H), 0.09 (minor, s, 9H), 0.06 (major, s, 9H); ^{13}C NMR ($CDCl_3$): δ 140.0 (major), 139.2, 138.6, 138.3 (major), 137.2, 135.1 (major), 128.3 (major), 128.2, 127.8 (major), 127.7, 127.6 (major), 127.4, 72.5 (major), 72.4, 68.2, 67.0 (major), 14.8 (major), –1.1, –2.3 (major) (overlapped one peak); HRMS (APCI-MS, positive): *m/z* $[M+H]^+$ Calcd for $C_{14}H_{23}OSi$ 235.1513, Found 235.1521. The stereochemistry of the products was determined by analysis of NOE.



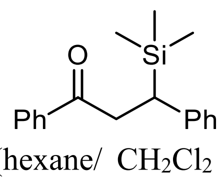
(*E*)-(5-(benzyloxy)pent-2-en-2-yl)trimethylsilane and (*E*)-(5-(benzyloxy)pent-2-en-3-yl)trimethylsilane (3r):



A colorless oil (83.9 mg, 0.338 mmol, 68%, major:minor = 3.1:1 as an inseparable mixture) from **2r** (87.1 mg, 0.500 mmol). Purification was done by column chromatography on silica gel (hexane/DCM = 10/1 to 2/1). R_f = 0.28 (hexane/DCM = 2/1); ^{1}H NMR ($CDCl_3$): δ 7.36–7.33 (major, d, J = 4.8 Hz, 4H + minor, m, 4H), 7.30–7.26 (major, m, 1H + minor, m, 1H), 5.93 (minor, q, J = 6.6 Hz, 1H), 5.72 (major, td, J = 6.5, 1.6 Hz, 1H), 4.53 (major, s, 2H), 4.52 (minor, s, 2H), 3.50 (major, t, J = 7.2 Hz, 2H), 3.38–3.35 (minor, m, 2H), 2.51 (minor, t, J = 8.2 Hz, 2H), 2.43 (major, q, J = 6.9 Hz, 2H), 1.70 (minor, d, J = 6.9 Hz, 3H), 1.68 (major, s, 3H), 0.04 (major. s, 9H), 0.03 (minor, s, 9H); ^{13}C NMR ($CDCl_3$): δ 138.51 (major), 138.46, 138.3 (major), 137.3, 136.6, 134.7 (major), 128.3 (major), 127.6 (major), 127.5 (major), 72.8 (major), 72.7, 69.5 (major), 69.3, 29.5, 29.0 (major), 14.5 (major), 14.4, –1.5, –2.2 (major) (overlapped three peaks); HRMS (APCI-MS, positive): *m/z* $[M–Me]^+$ Calcd for $C_{14}H_{21}OSi$ 233.1356, Found 233.1358. The stereochemistry of the products was determined by analysis of NOE.

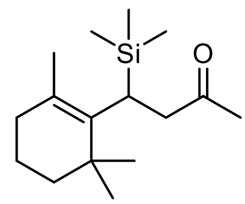


1,3-diphenyl-3-(trimethylsilyl)-1-propanone (3s):



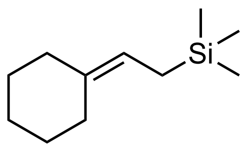
A colorless oil (92.2 mg, 0.326 mmol, 66%) from **2s** (104 mg, 0.497 mmol). Reaction time was 12 h. Purification was done by column chromatography on silica gel (hexane/CH_2Cl_2 = 1/1) and GPC (eluent: $CHCl_3$). R_f = 0.17 (hexane/ CH_2Cl_2 = 1/1). All the resonances in ^{1}H NMR and ^{13}C spectrum ($CDCl_3$) were consistent with the reported values.[28] ^{1}H and ^{13}C NMR spectra are provided below.

4-(2,6,6-trimethylcyclohex-1-en-1-yl)-4-(trimethylsilyl)butan-2-one (3t):



A colorless oil (118 mg, 0.443 mmol, 88%) from **2t** (96.3 mg, 0.501 mmol). Reaction time was 12 h. Purification was done by column chromatography on silica gel (hexane/CH_2Cl_2 = 3/1). R_f = 0.29 (hexane/CH_2Cl_2 = 3/1); ^{1}H NMR ($CDCl_3$): δ 3.05 (dd, J = 19.2, 11.0 Hz, 1H), 2.46 (dd, J = 19.2, 3.1 Hz, 1H), 2.27 (dd, J = 11.0, 3.1 Hz, 1H), 2.11 (s, 3H), 1.95–1.84 (m, 2H), 1.55–1.51 (m, 2H), 1.49 (s, 3H), 1.43–1.37 (m, 2H), 0.97 (s, 3H), 0.92 (s, 3H), 0.03 (s, 9H); ^{13}C NMR ($CDCl_3$): δ 208.5, 140.5, 126.3, 48.2, 39.8, 36.0, 33.1, 29.7, 28.5, 27.6, 22.9, 21.6, 19.5, –0.3; HRMS (APCI-MS, positive): *m/z* $[M+H]^+$ Calcd for $C_{16}H_{30}OSi$ 267.2139, Found 267.2140.

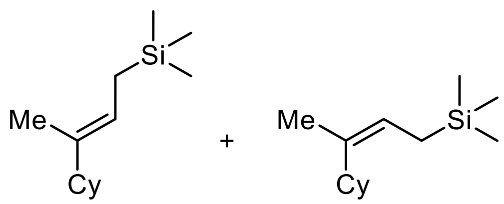
[2-(trimethylsilyl)ethylidene]cyclohexane (3u):



A colorless oil (65.7 mg, 0.360 mmol, 73%) from **2u** (53.4 mg, 0.494 mmol). Purification was done by column chromatography on silica gel (hexane only) and GPC (eluent: $CHCl_3$). R_f = 0.83 (hexane only); All the resonances in ^{1}H NMR and ^{13}C spectrum ($CDCl_3$) were consistent with the reported values.[29] ^{1}H and ^{13}C NMR spectra are provided below.

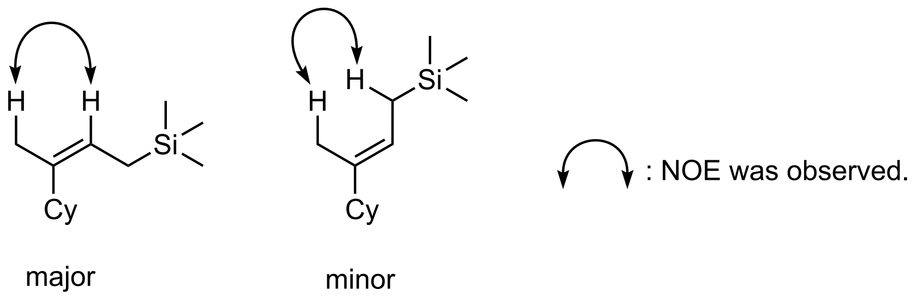
(*Z*)-(3-cyclohexylbut-2-en-1-yl)trimethylsilane (3v):

A colorless oil (69.1 mg, 0.328 mmol, 66%, *E*:*Z* = 1:3.1 as an inseparable mixture) from **2v**

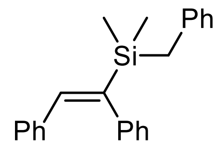


(*E*)-3v **(*Z*)-3v**

(67.5 mg, 0.495 mmol). Concentration of **2v**: 0.5 M and 10 mol% CuCl[P(OPh)$_3$] were used. Reaction time was 12 h. Purification was done by column chromatography on silica gel (hexane only) and GPC (eluent: $CHCl_3$). R_f = 0.85 (hexane only); ^{1}H NMR ($CDCl_3$): δ 5.17 (*E*, t, J = 8.2 Hz, 1H), 5.06 (*Z*, t, J = 8.2 Hz, 1H), 2.32 (*Z*, m, 1H), 1.82 (*E*, m, 1H), 1.78-1.61 (m, *Z*, 4H + *E*, 4H), 1.60 (*Z*, s, 3H), 1.52 (*E*, s, 3H), 1.46–1.11 (*Z*, m, 8H + *E*, m, 8H), –0.01 (*Z*, s, 9H), –0.03 (*E*, s, 9H); ^{13}C NMR ($CDCl_3$): δ 137.9, 137.7, 119.1, 117.9, 47.6, 39.2, 32.3, 31.0, 26.9, 26.8, 26.5, 26.3, 19.6, 18.3, 17.8, 14.2, –1.8 (overlapped one peak); HRMS (APCI-MS, positive): *m/z* $[M–Me]^+$ Calcd for $C_{12}H_{23}Si$ 195.1564, Found 195.1566. The stereochemistry of the products was determined by analysis of NOE.

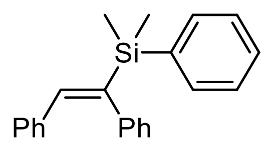


(*E*)-(1,2-diphenylvinyl)benzyldimethylsilane (3w):



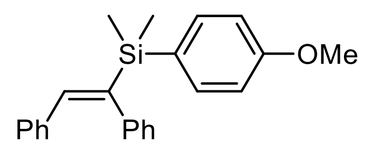
A white solid (152 mg, 0.465 mmol, 93%) from **2a** (89.5 mg, 0.502 mmol). Purification was done by column chromatography on silica gel (hexane only) and GPC (eluent: $CHCl_3$). mp: 81.7–83.5 °C; R_f = 0.24 (hexane only); ^{1}H NMR ($CDCl_3$): δ 7.32 (dd, *J* = 7.5, 7.5 Hz, 2H), 7.24–7.19 (m, 3H), 7.10–7.06 (m, 4H), 7.01–6.99 (m, 4H), 6.94 (dd, *J* = 6.2, 2.7 Hz, 2H), 6.78 (s, 1H), 2.20 (s, 2H), 0.09 (s, 6H): ^{13}C NMR ($CDCl_3$): δ 145.2, 142.4, 139.7, 138.6, 137.1, 129.5, 128.7, 128.4, 128.1, 127.9, 127.5, 127.1, 125.8, 124.1, 24.9, –3.6; HRMS (APCI-MS, positive): *m/z* $[M+H]^+$ Calcd for $C_{23}H_{25}Si$ 329.1720, Found 329.1716.

(*E*)-(1,2-diphenylvinyl)dimethylphenylsilane (3x):



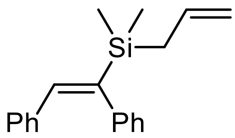
A colorless oil (150 mg, 0.476 mmol, 95%) from **2a** (89.0 mg, 0.499 mmol). Purification was done by column chromatography on silica gel (hexane only). R_f = 0.21 (hexane only); ^{1}H NMR ($CDCl_3$): δ 7.48 (dd, *J* = 7.6, 1.4 Hz, 2H), 7.39–7.34 (m, 3H), 7.23 (dd, *J* = 7.6, 7.6 Hz, 2H), 7.17 (dd, *J* = 7.6, 7.6 Hz, 1H), 7.09–7.06 (m, 3H), 6.94 (dd, *J* = 6.6, 3.0 Hz, 2H), 6.90 (d, *J* = 7.6 Hz, 2H), 6.82 (s, 1H), 0.39 (s, 6H); ^{13}C NMR ($CDCl_3$): δ 145.0, 142.3, 139.2, 137.6, 137.2, 134.3, 129.5, 129.1, 128.5, 127.9, 127.7, 127.6, 127.1, 125.7, –3.1; HRMS (APCI-MS, positive): *m/z* $[M]^+$ Calcd for $C_{22}H_{22}Si$ 314.1485, Found 314.1490.

(*E*)-(1,2-diphenylvinyl)dimethyl(4-methoxyphenyl)silane (3y):



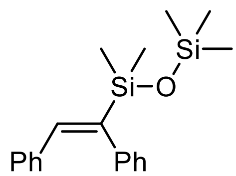
A colorless oil (158 mg, 0.458 mmol, 92%) from **2a** (89.0 mg, 0.499 mmol). Purification was done by column chromatography on silica gel (hexane/CH_2Cl_2 = 3/1) and preparative TLC with an eluent (hexane/CH_2Cl_2 = 3/1), followed by GPC (eluent: $CHCl_3$). R_f = 0.42 (hexane/CH_2Cl_2 = 3/1); ^{1}H NMR ($CDCl_3$): δ 7.47 (d, *J* = 9.0 Hz, 2H), 7.23 (dd, *J* = 7.6, 7.6 Hz, 2H), 7.16 (dd, *J* = 7.6, 7.6 Hz, 1H), 7.09–7.05 (m, 3H), 6.95–6.88 (m, 4H), 6.92 (d, *J* = 9.0 Hz, 2H), 6.80 (s, 1H), 3.83 (s, 3H), 0.36 (s, 6H); ^{13}C NMR ($CDCl_3$): δ 160.5, 145.4, 142.4, 138.9, 137.2, 135.7, 129.5, 128.5, 128.3, 127.8, 127.6, 127.1, 125.6, 113.5, 54.9, –3.0; HRMS (APCI-MS, positive): *m/z* $[M]^+$ Calcd for $C_{23}H_{24}OSi$ 344.1591, Found 344.1591.

(*E*)-(1,2-diphenylvinyl)allyldimethylsilane (3z):



A colorless oil (122 mg, 0.437 mmol, 87%) from **2a** (89.1 mg, 0.500 mmol). Purification was done by column chromatography on silica gel (hexane only) and GPC (eluent: $CHCl_3$). R_f = 0.40 (hexane only);[1]H NMR ($CDCl_3$): δ 7.31 (dd , J = 7.5, 7.5 Hz, 2H), 7.22 (dd, J = 7.5, 7.5 Hz, 1H), 7.10–7.08 (m, 3H), 7.00 (m, 2H), 6.96 (m, 2H), 6.81 (s, 1H), 5.77 (m, 1H), 4.894.83 (m, 2H), 1.63 (d, J = 8.2 Hz, 2H), 0.15 (s, 6H); [13]C NMR ($CDCl_3$): δ 145.3, 142.5, 138.3, 137.1, 134.6, 129.5, 128.7, 127.9, 127.4, 127.1, 125.7, 113.4, 22.6, –3.8; HRMS (APCI-MS, positive): *m/z* $[M+H]^+$ Calcd for $C_{19}H_{23}Si$ 279.1564, Found 279.1572.

(*E*)-(1,2-diphenylvinyl)dimethyltrimethylsiloxysilane (3aa):



A colorless oil (129 mg, 0.393 mmol, 79%) from **2a** (89.3 mg, 0.501 mmol). Purification was done by column chromatography on silica gel (hexane only) and GPC (eluent: $CHCl_3$). R_f = 0.38 (hexane only); [1]H NMR ($CDCl_3$): δ 7.29 (dd, J = 7.6, 7.6 Hz, 2H), 7.20 (dd, J = 7.6, 7.6 Hz, 1H), 7.11–7.09 (m, 3H), 7.03 (d, J = 6.6 Hz, 2H), 6.98 (m, 2H), 6.89 (s, 1H), 0.18 (s, 6H), 0.08 (s, 9H); [13]C NMR ($CDCl_3$): δ 146.4, 142.0, 137.7, 137.2, 129.6, 128.5, 127.9, 127.7, 127.1, 125.7, 1.9, 0.2; HRMS (APCI-MS, positive): *m/z* $[M+H]^+$ Calcd for $C_{19}H_{26}OSi_2$ 326.1517, Found 326.1523.

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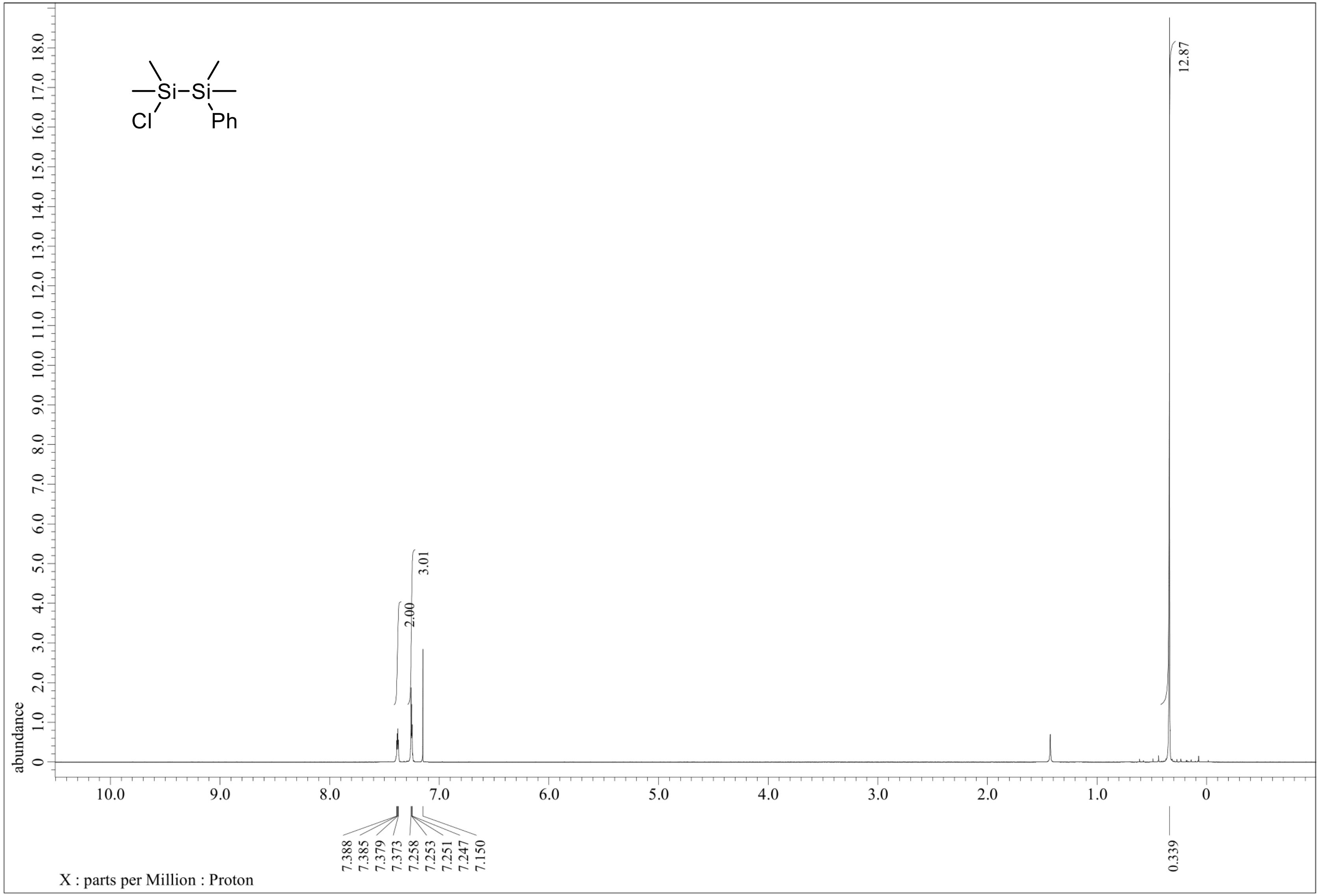

Figure S6. ^{1}H NMR (600 MHz, C_6D_6) spectrum of **S1**

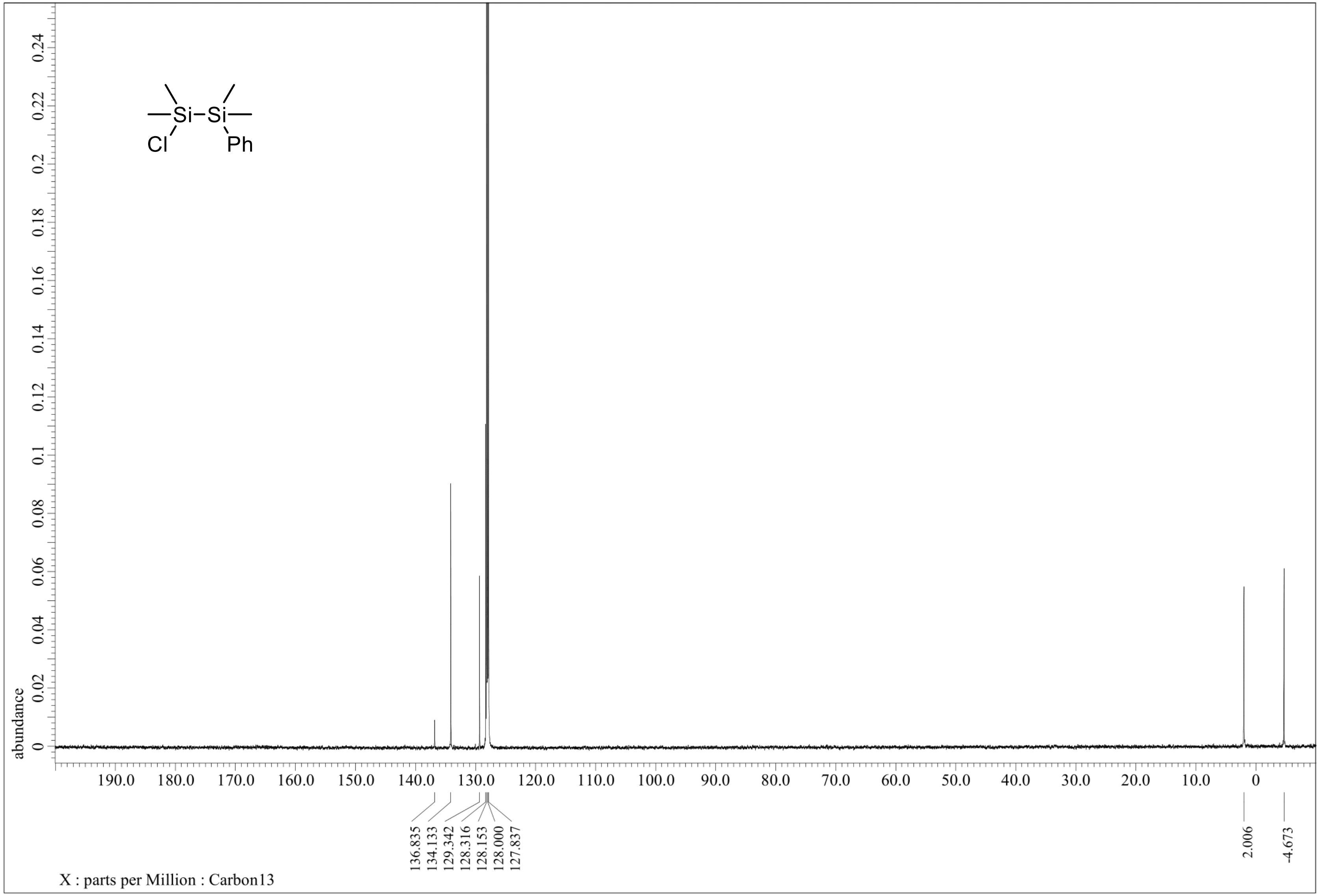

Figure S7. ^{13}C NMR (151 MHz, C_6D_6) spectrum of **S1**

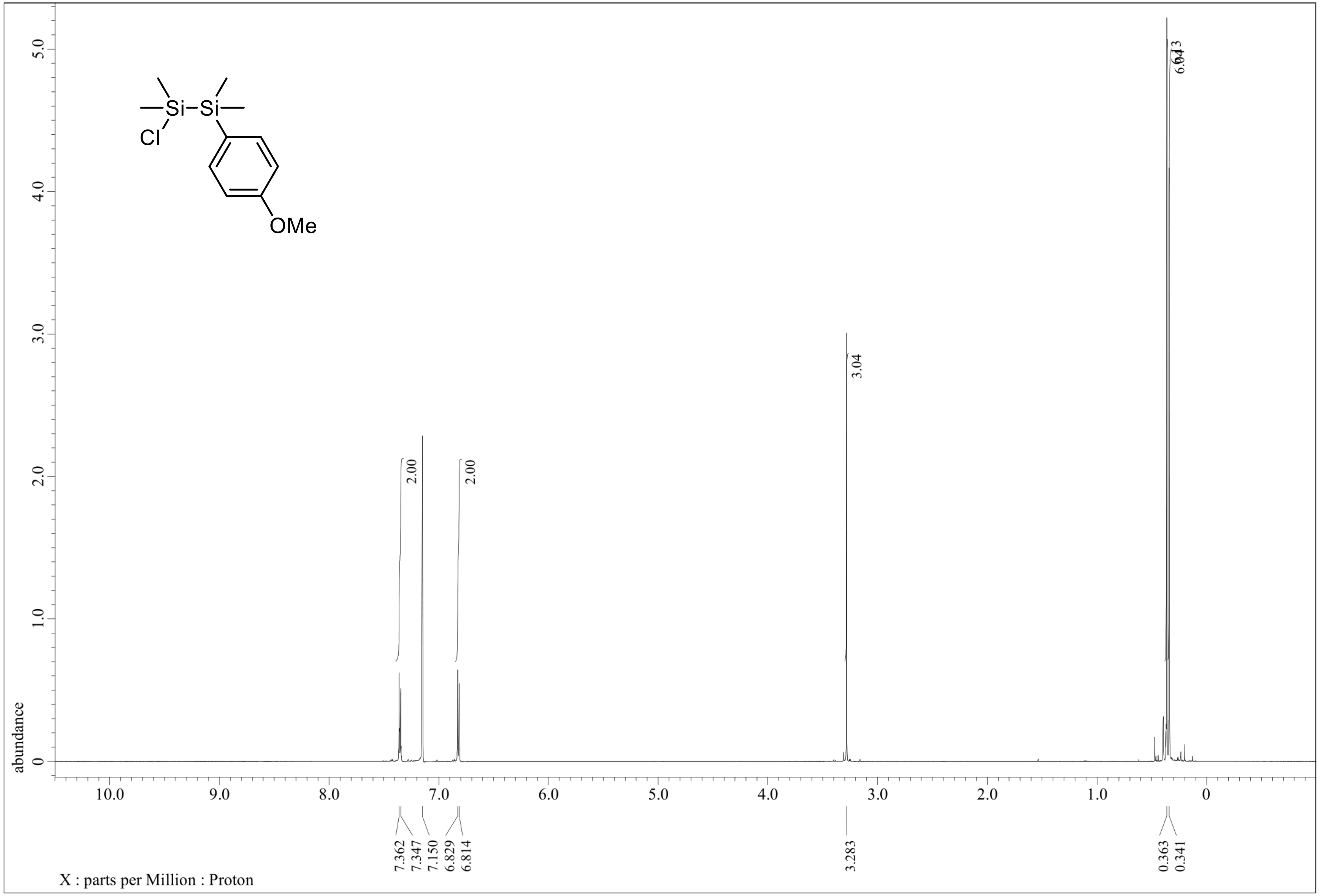

Figure S8. [1]H NMR (600 MHz, C_6D_6) spectrum of **S2**

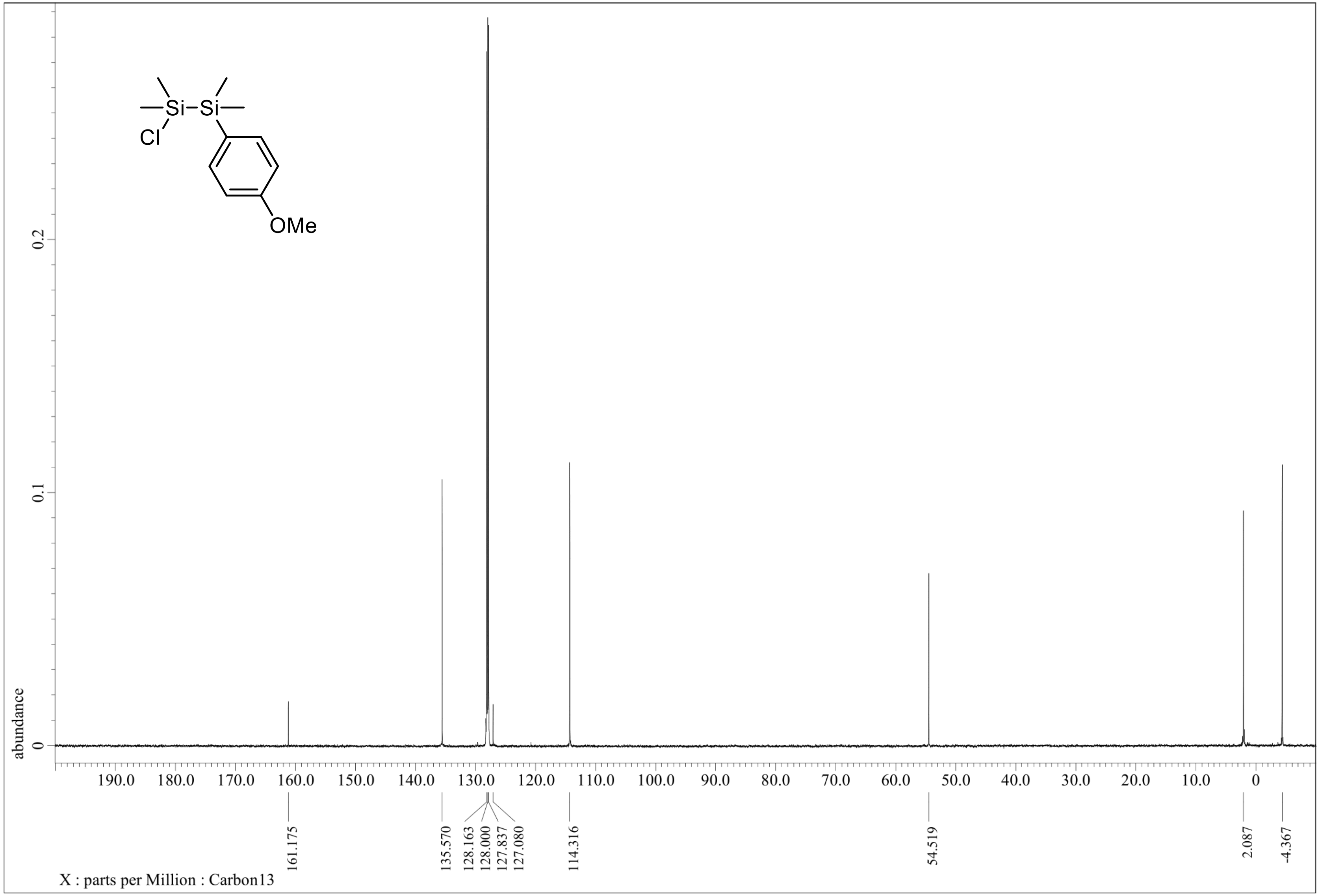

Figure S9. ^{13}C NMR (151 MHz, C_6D_6) spectrum of **S2**

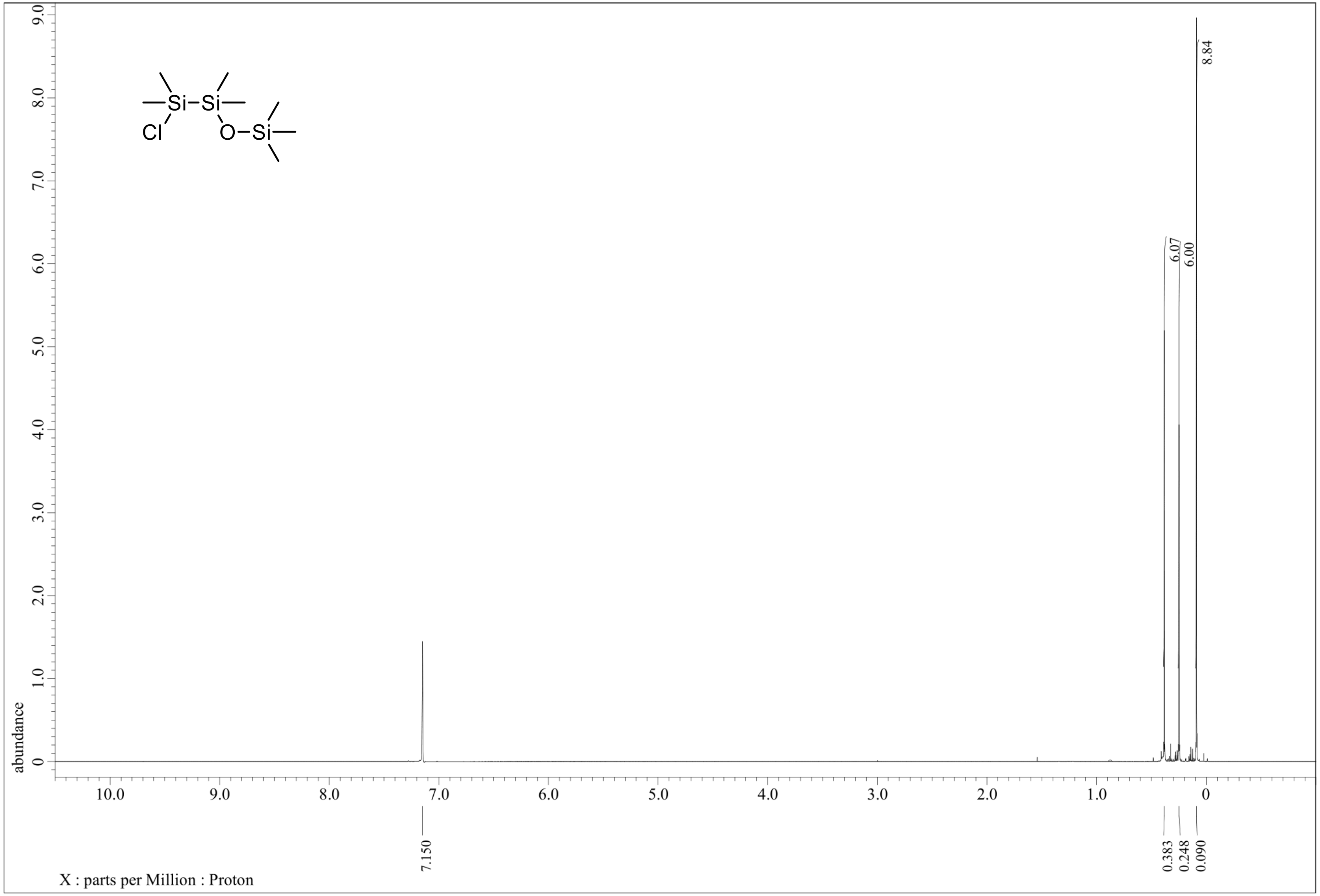

Figure S10. ^{1}H NMR (600 MHz, C_6D_6) spectrum of **S3**

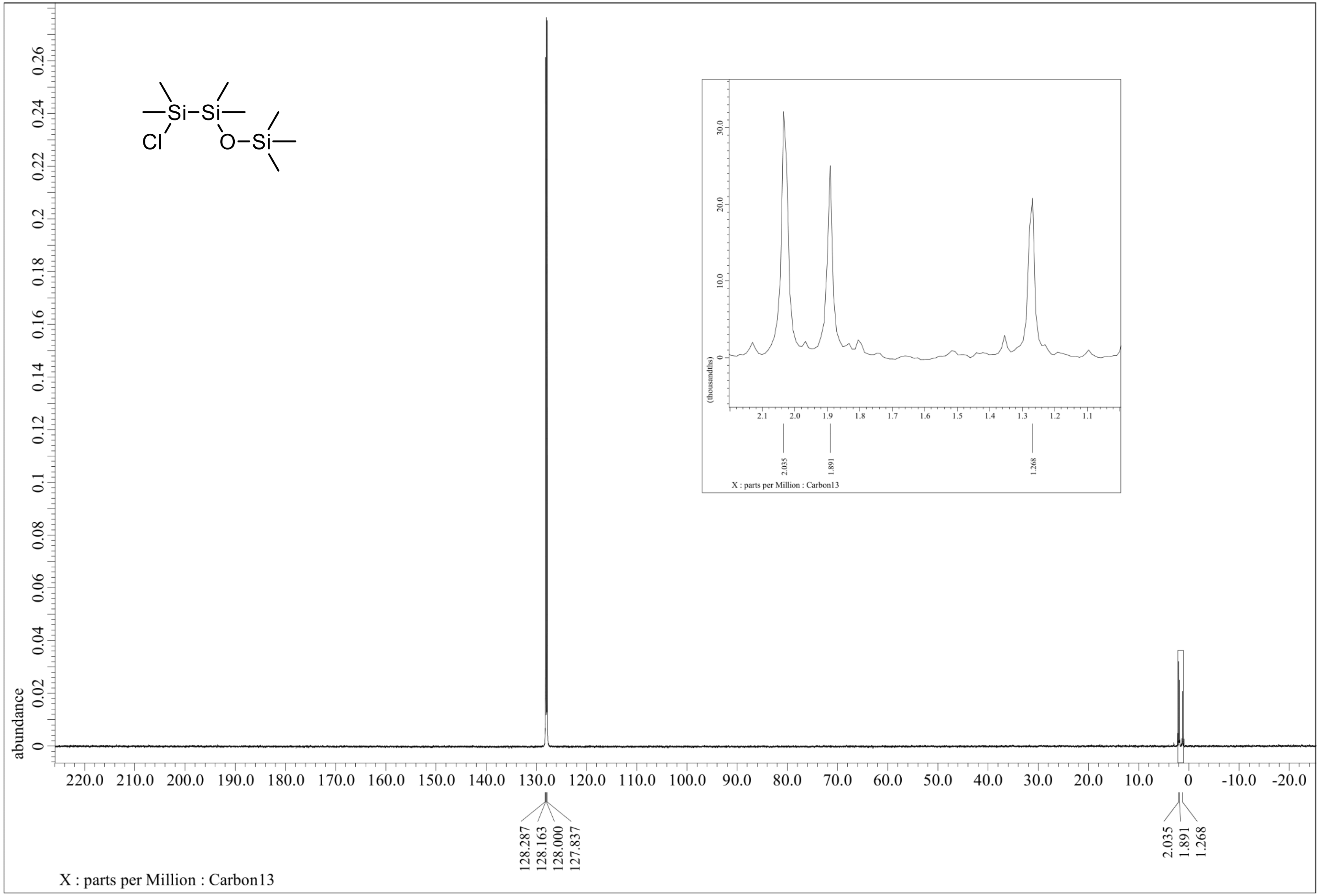

Figure S11. ^{13}C NMR (151 MHz, C_6D_6) spectrum of **S3**

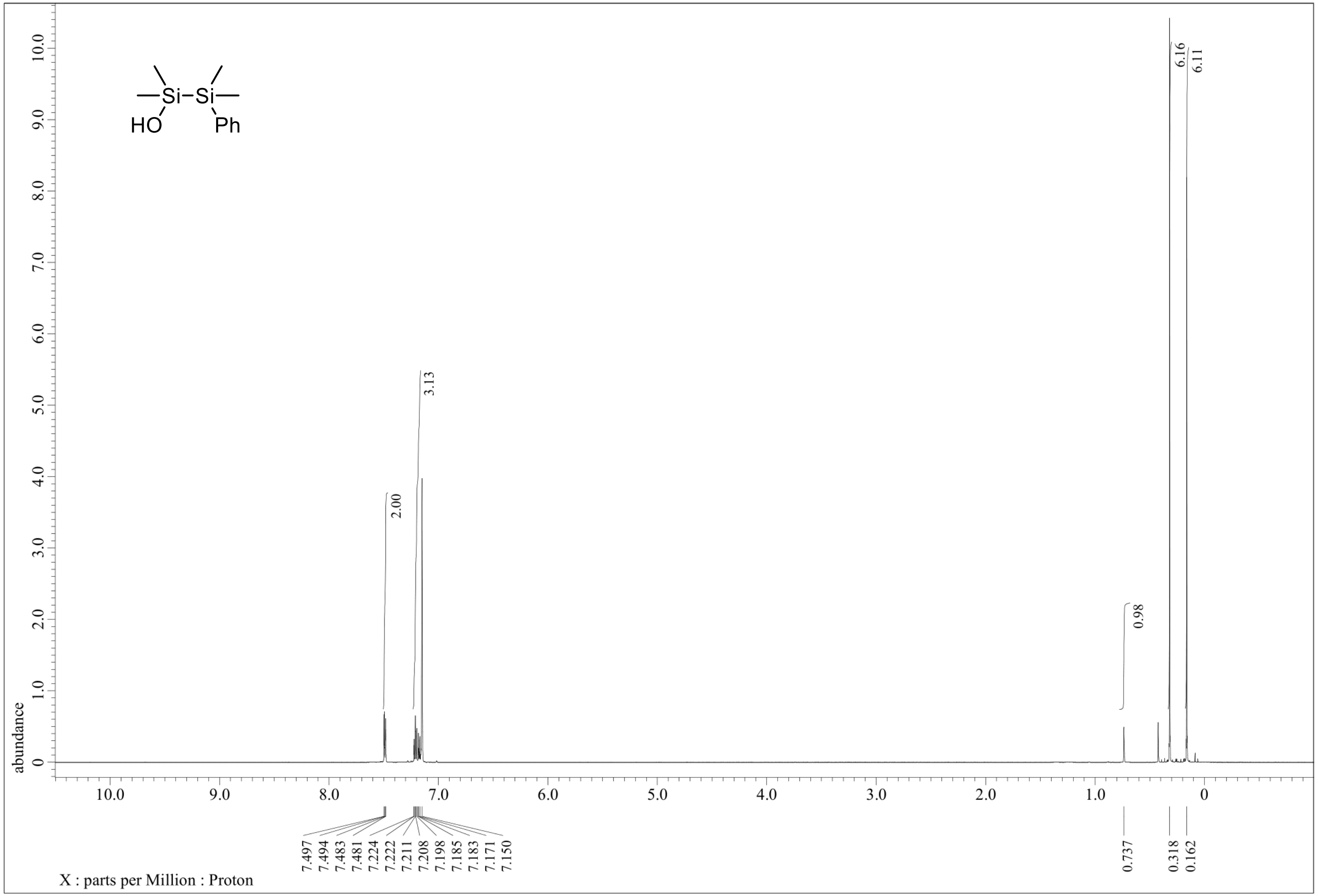

Figure S12. ^{1}H NMR (600 MHz, C_6D_6) spectrum of **S4**

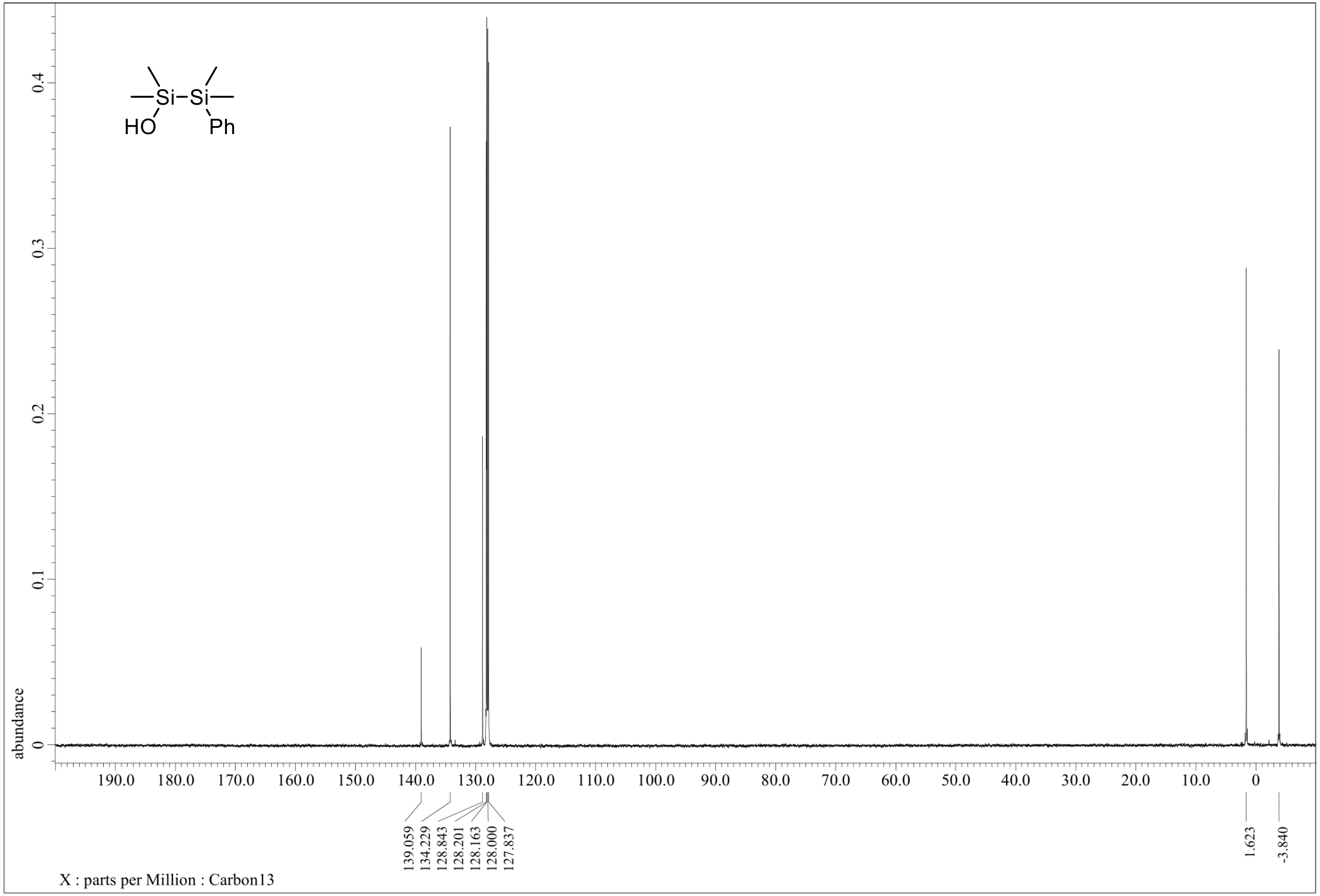

Figure S13. ^{13}C NMR (151 MHz, C_6D_6) spectrum of **S4**

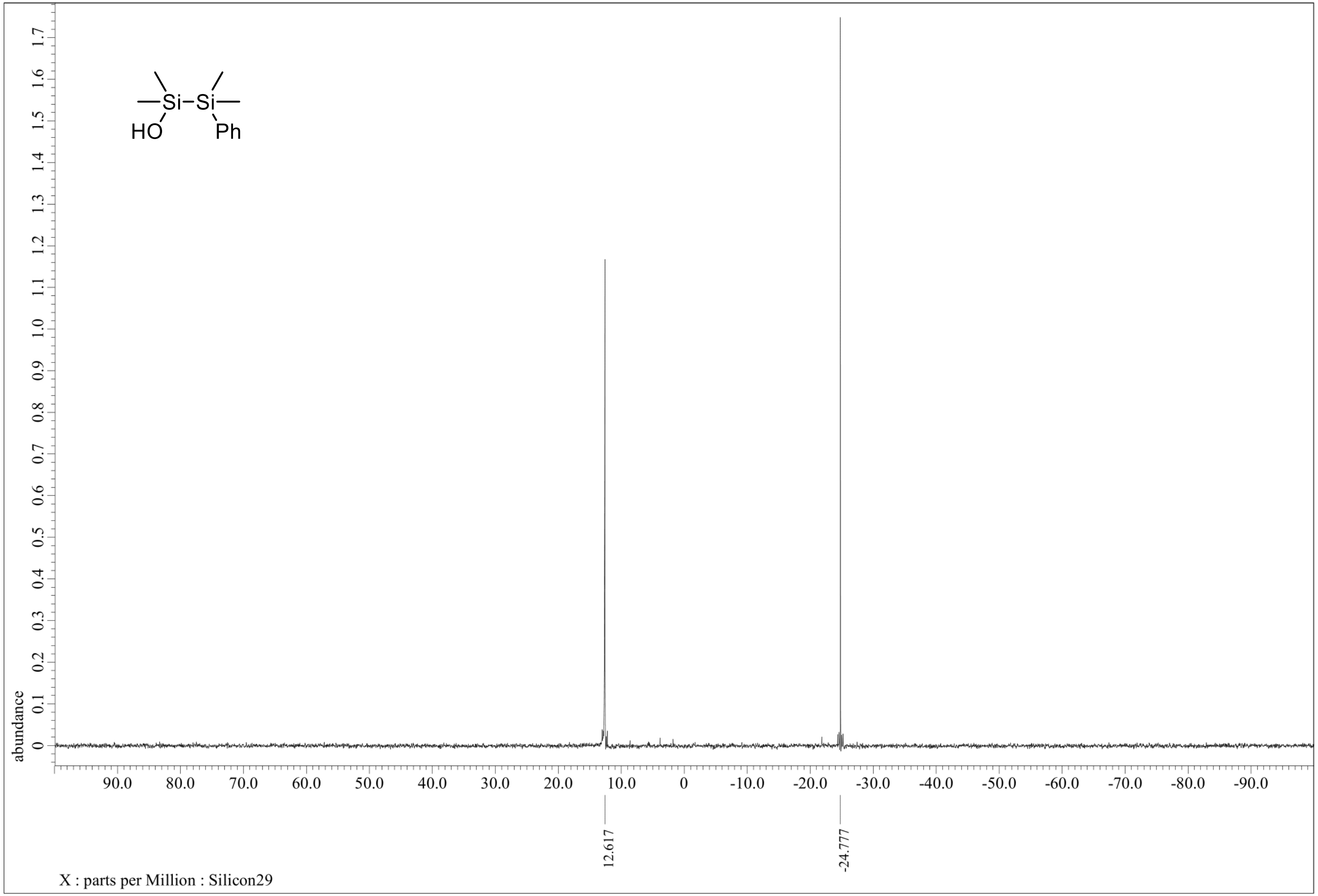

Figure S14. ^{29}Si NMR (119 MHz, C_6D_6) spectrum of **S4**

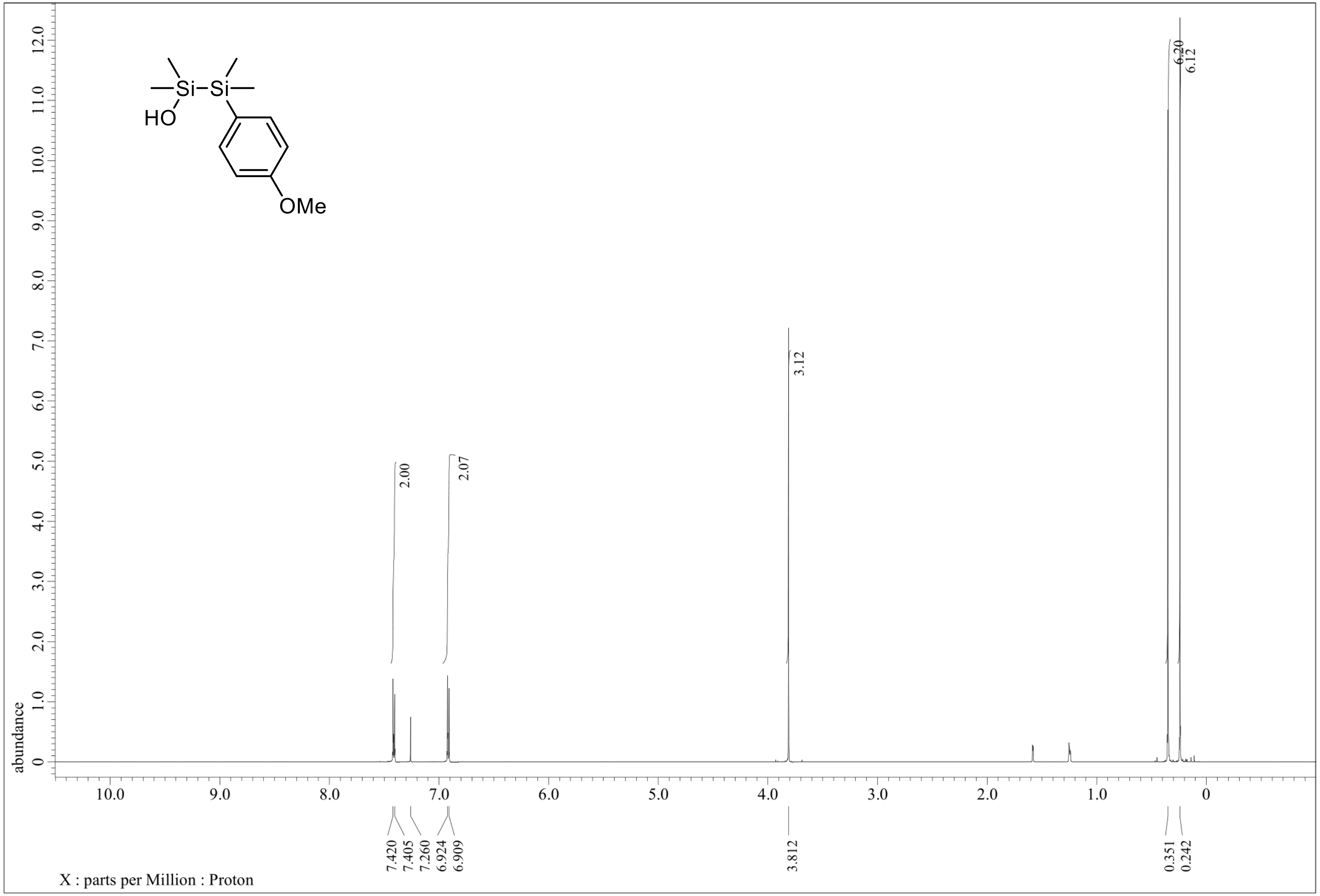

Figure S15. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **S5**

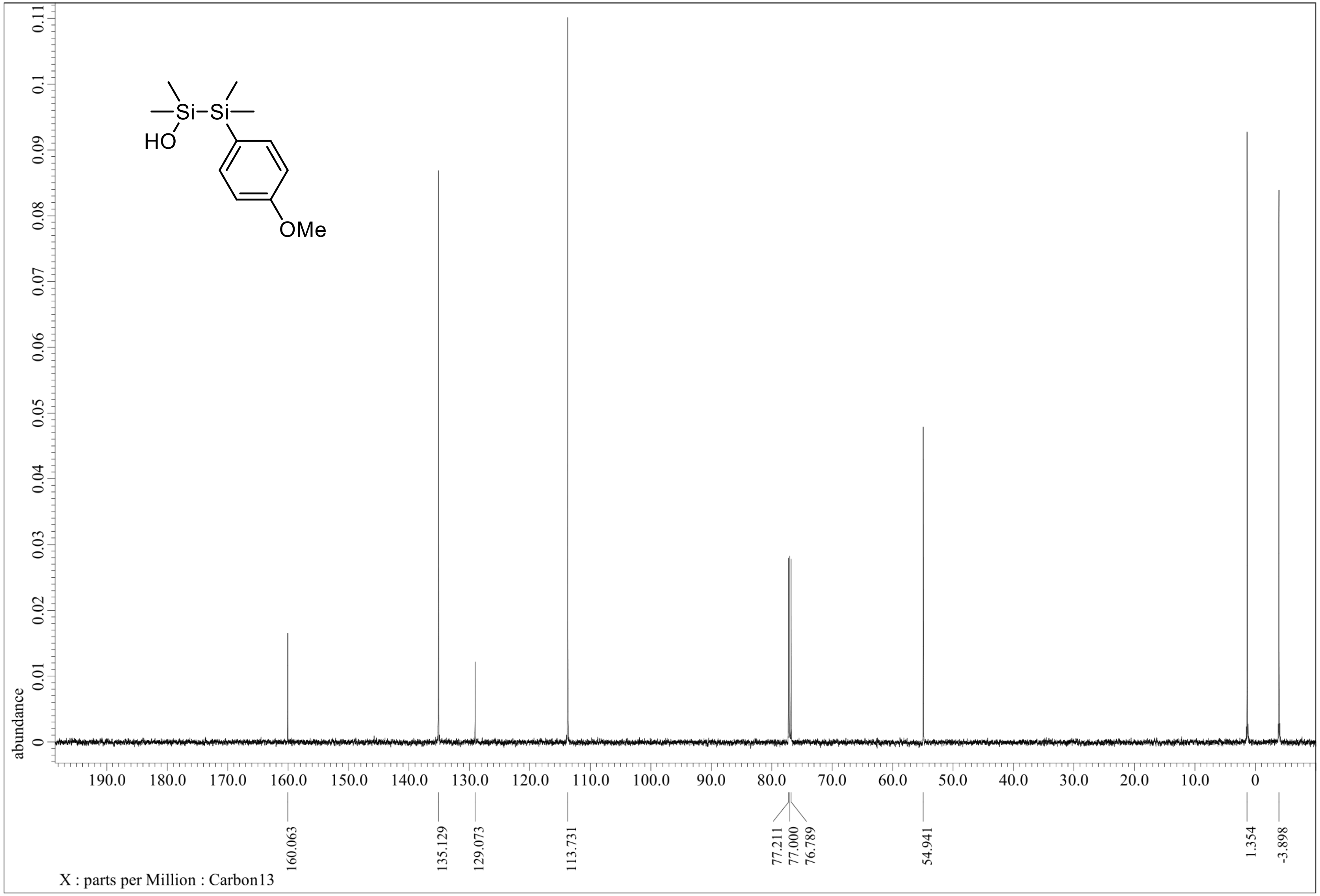

Figure S16. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **S5**

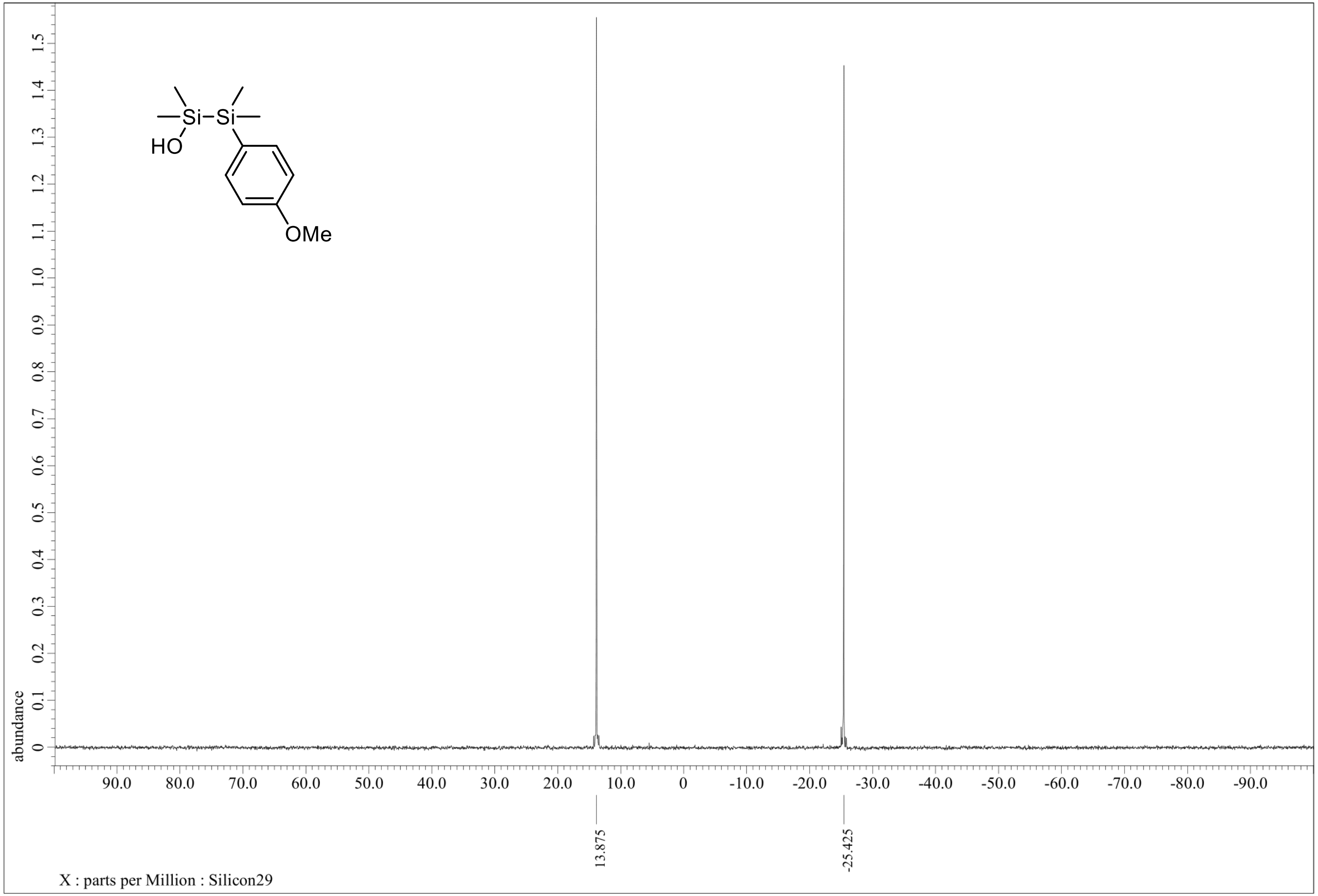

Figure S17. ^{29}Si NMR (119 MHz, $CDCl_3$) spectrum of **S5**

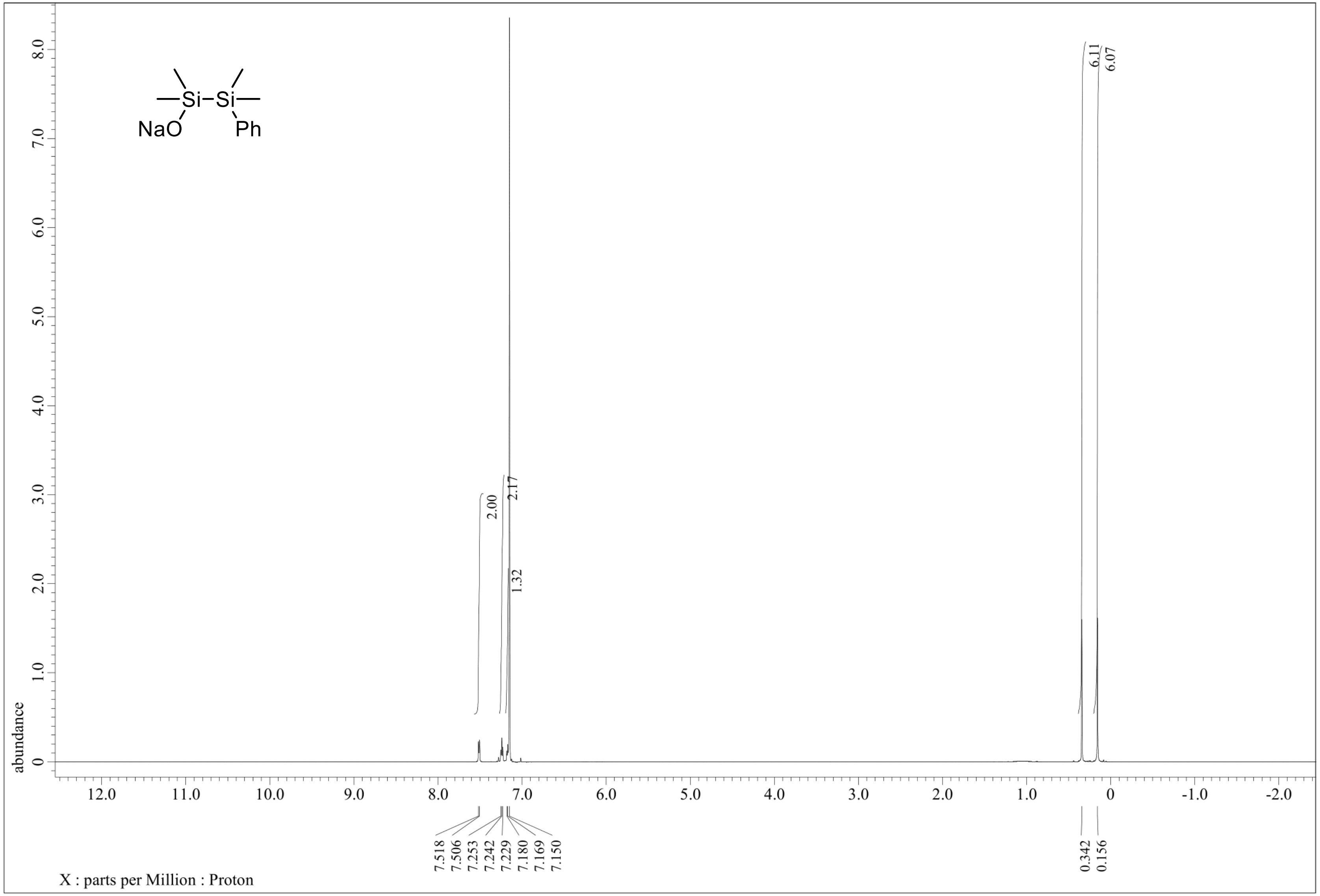

Figure S18. [1]H NMR (600 MHz, C_6D_6) spectrum of **1-Ph**

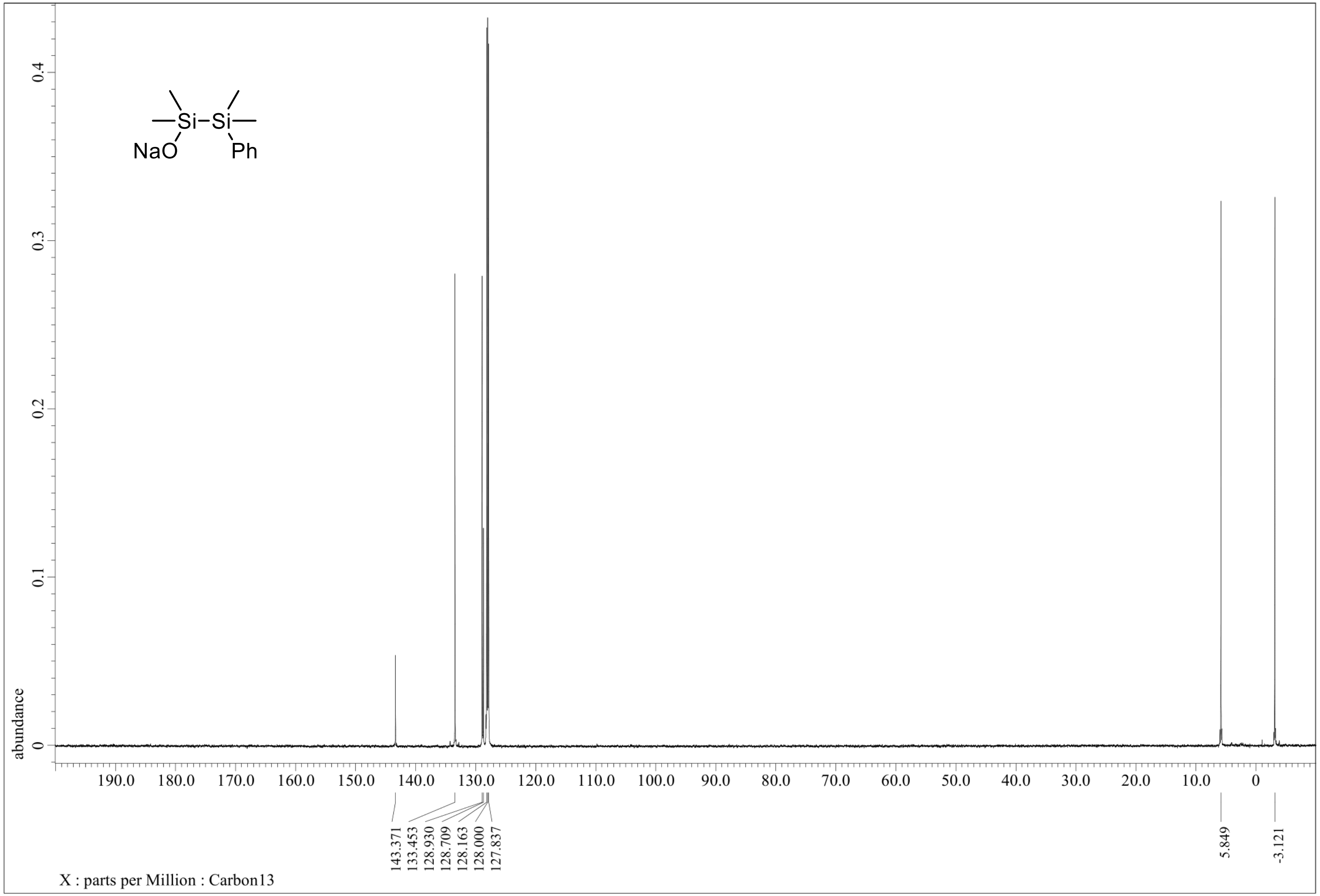

Figure S19. ^{13}C NMR (151 MHz, C_6D_6) spectrum of **1-Ph**

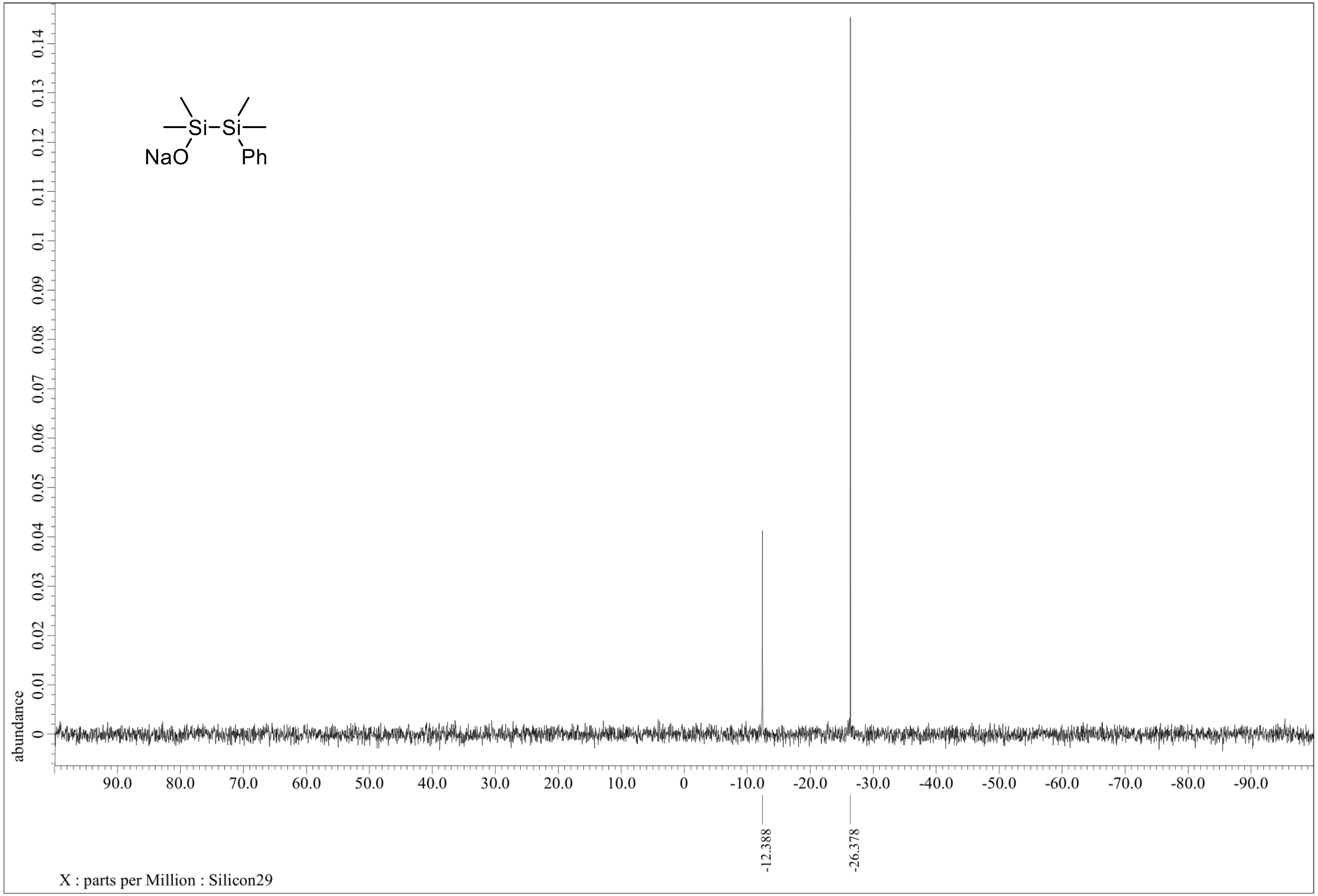

Figure S20. ^{29}Si NMR (119 MHz, C_6D_6) spectrum of **1-Ph**

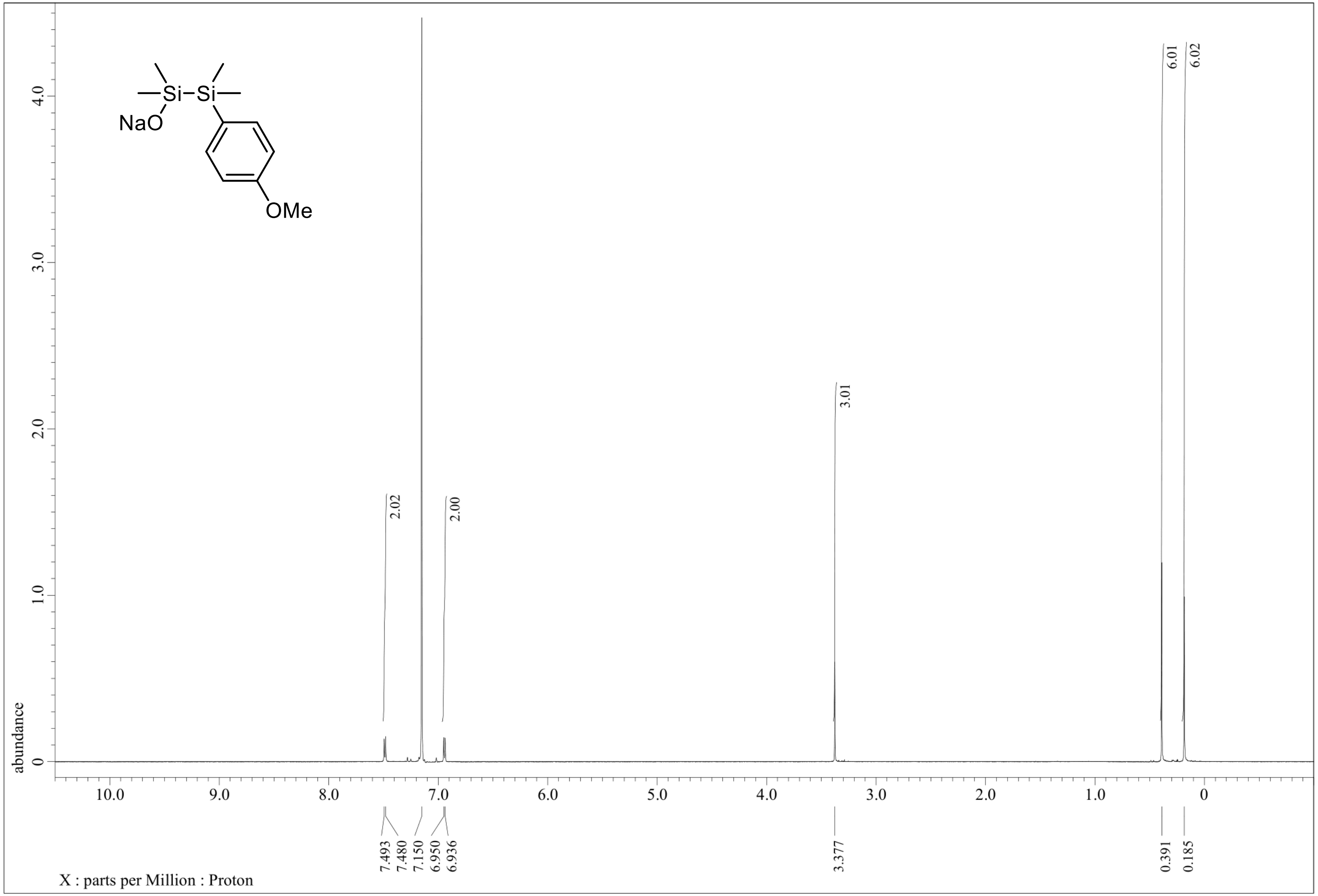

Figure S21. ^{1}H NMR (600 MHz, C_6D_6) spectrum of **1-Ans**

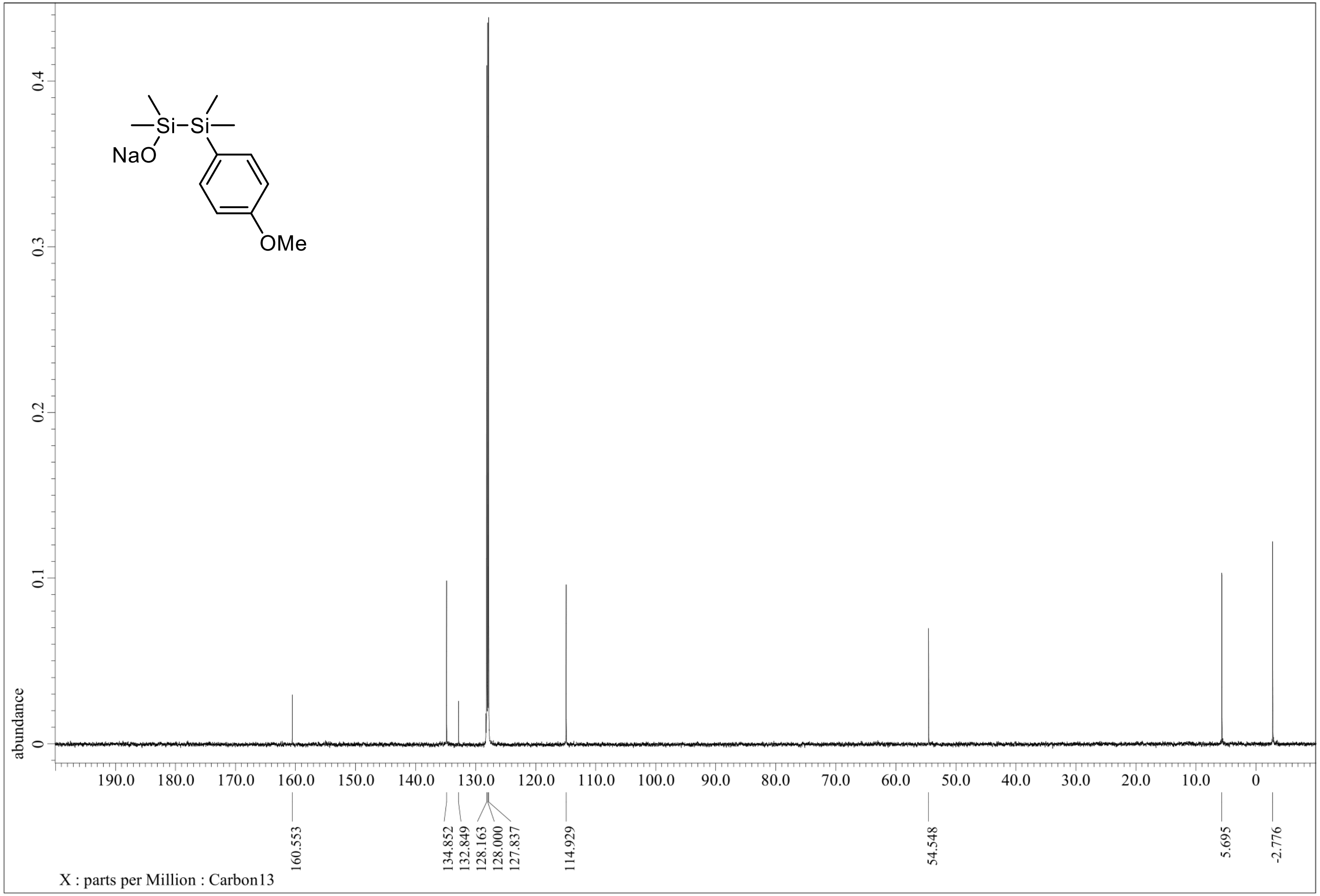

Figure S22. ^{13}C NMR (151 MHz, C_6D_6) spectrum of **1-Ans**

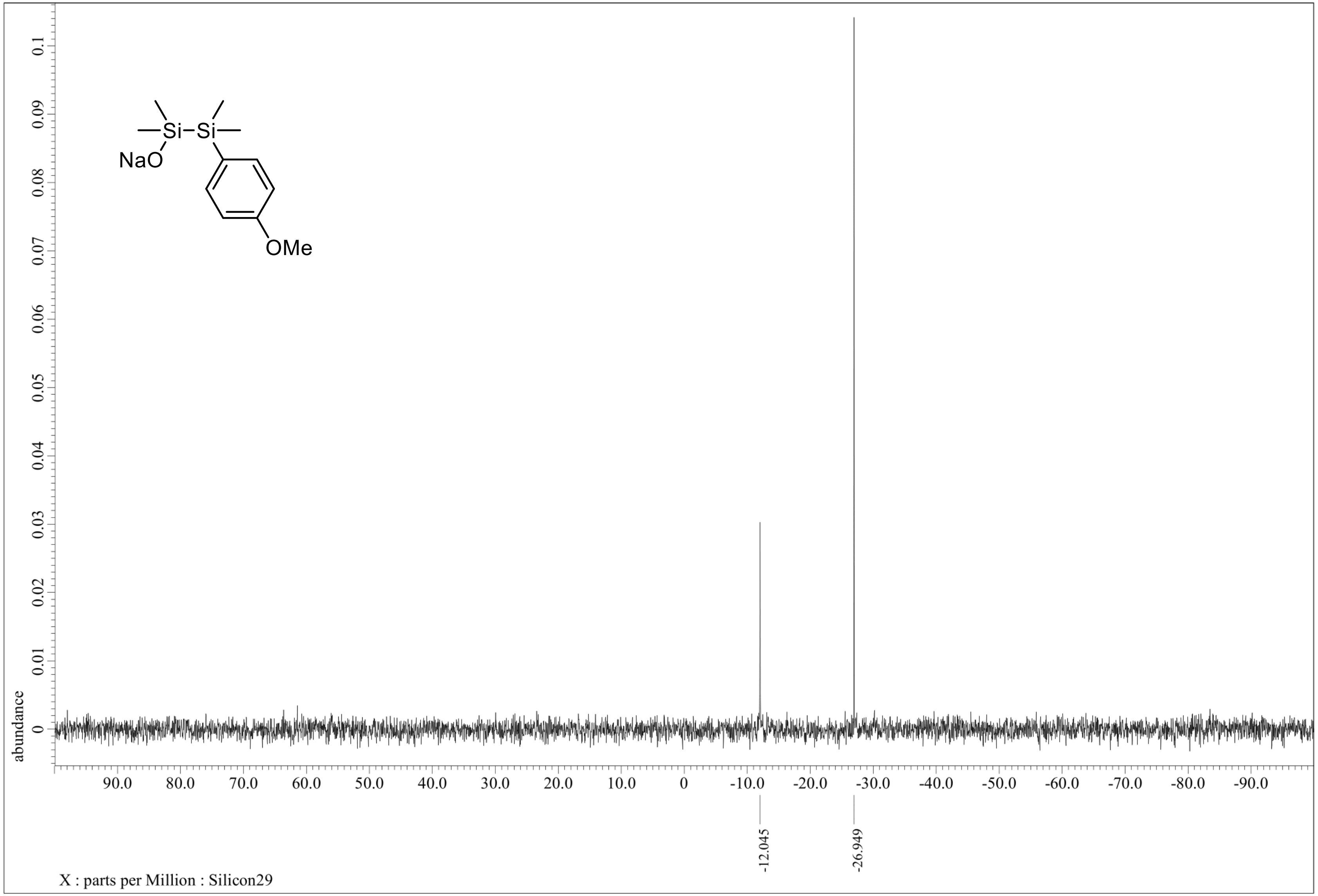

Figure S23. ^{29}Si NMR (119 MHz, C_6D_6) spectrum of **1-Ans**

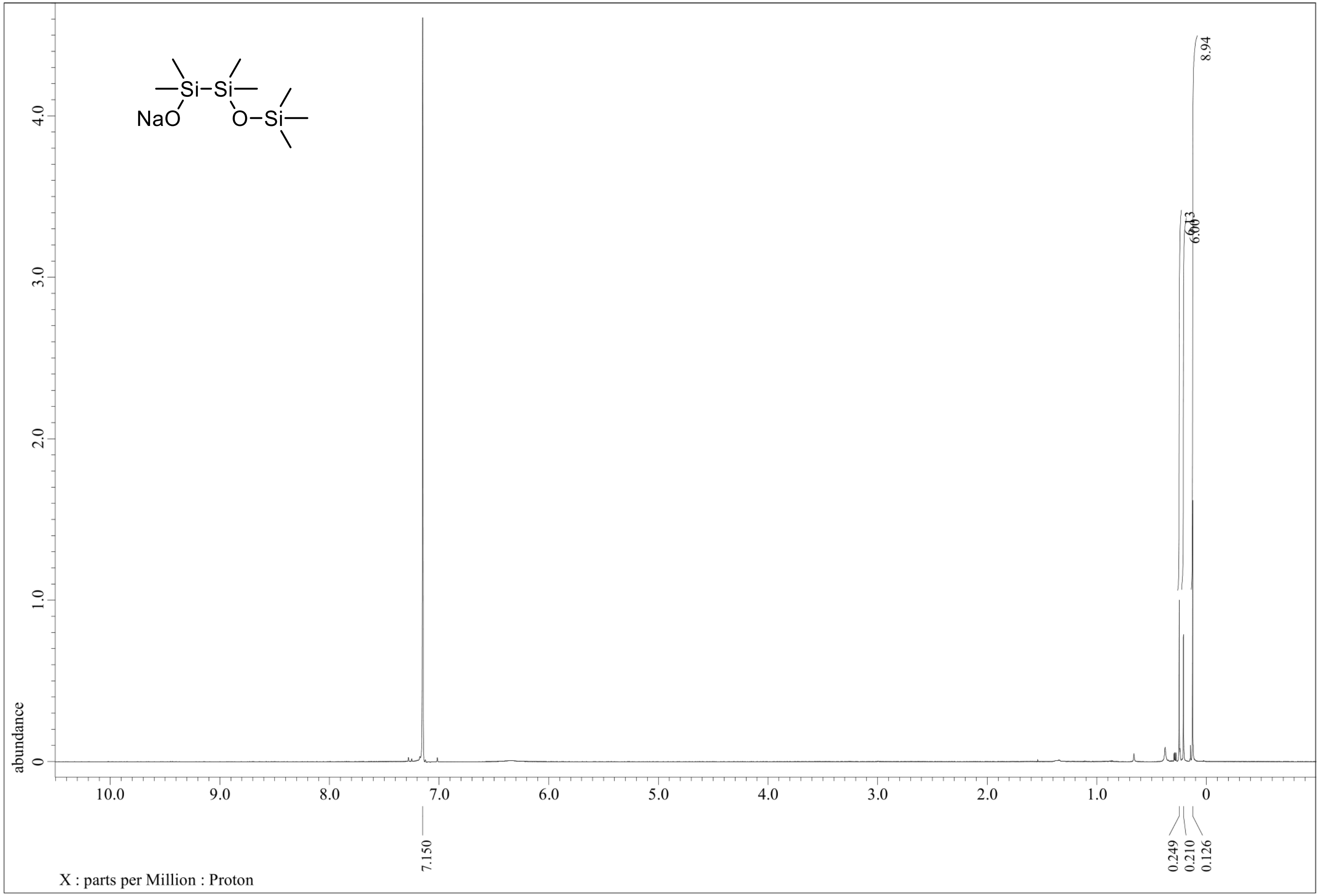

Figure S24. ^{1}H NMR (600 MHz, C_6D_6) spectrum of **1-OSiMe₃**

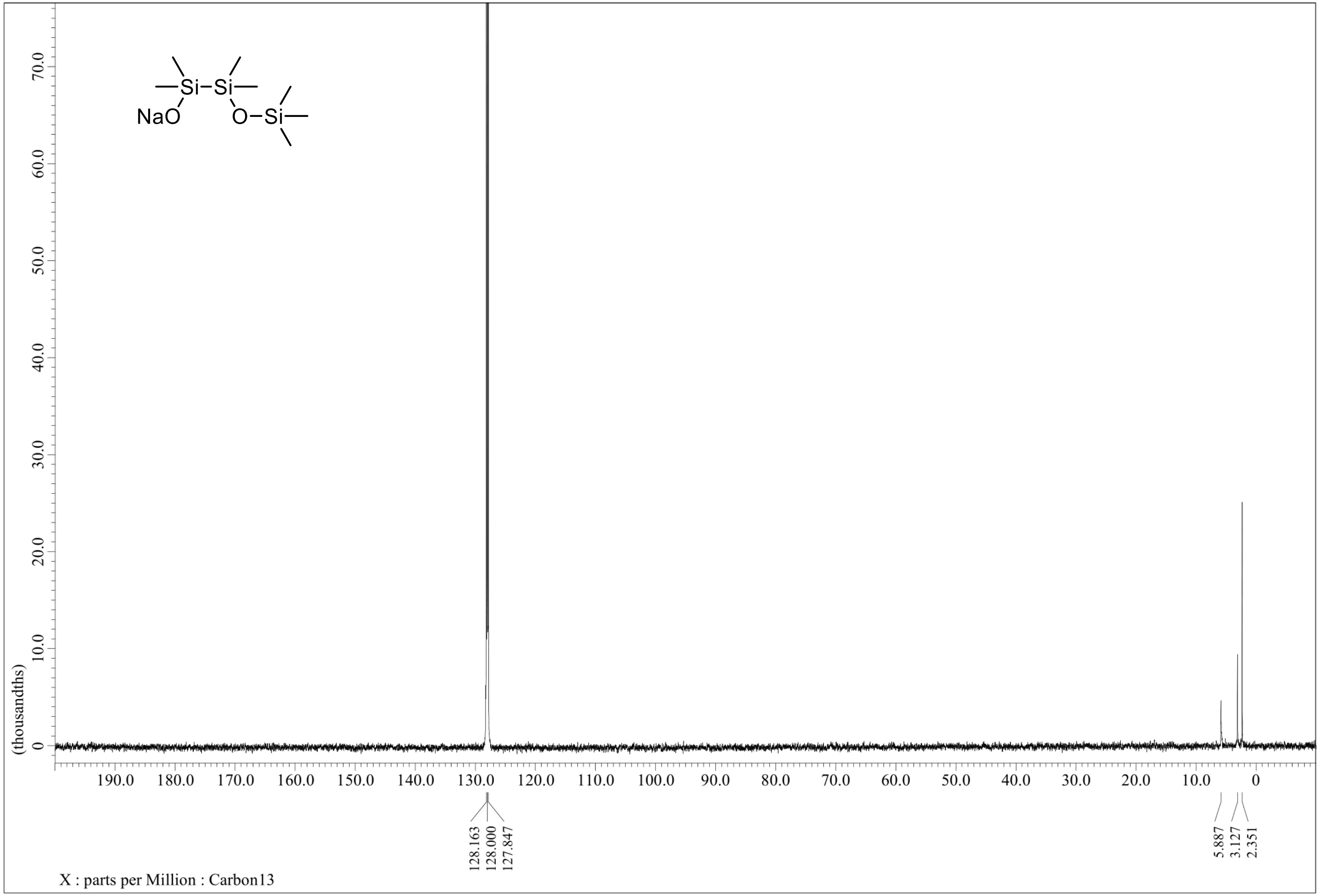

Figure S25. ^{13}C NMR (151 MHz, C_6D_6) spectrum of **1-OSiMe$_3$**

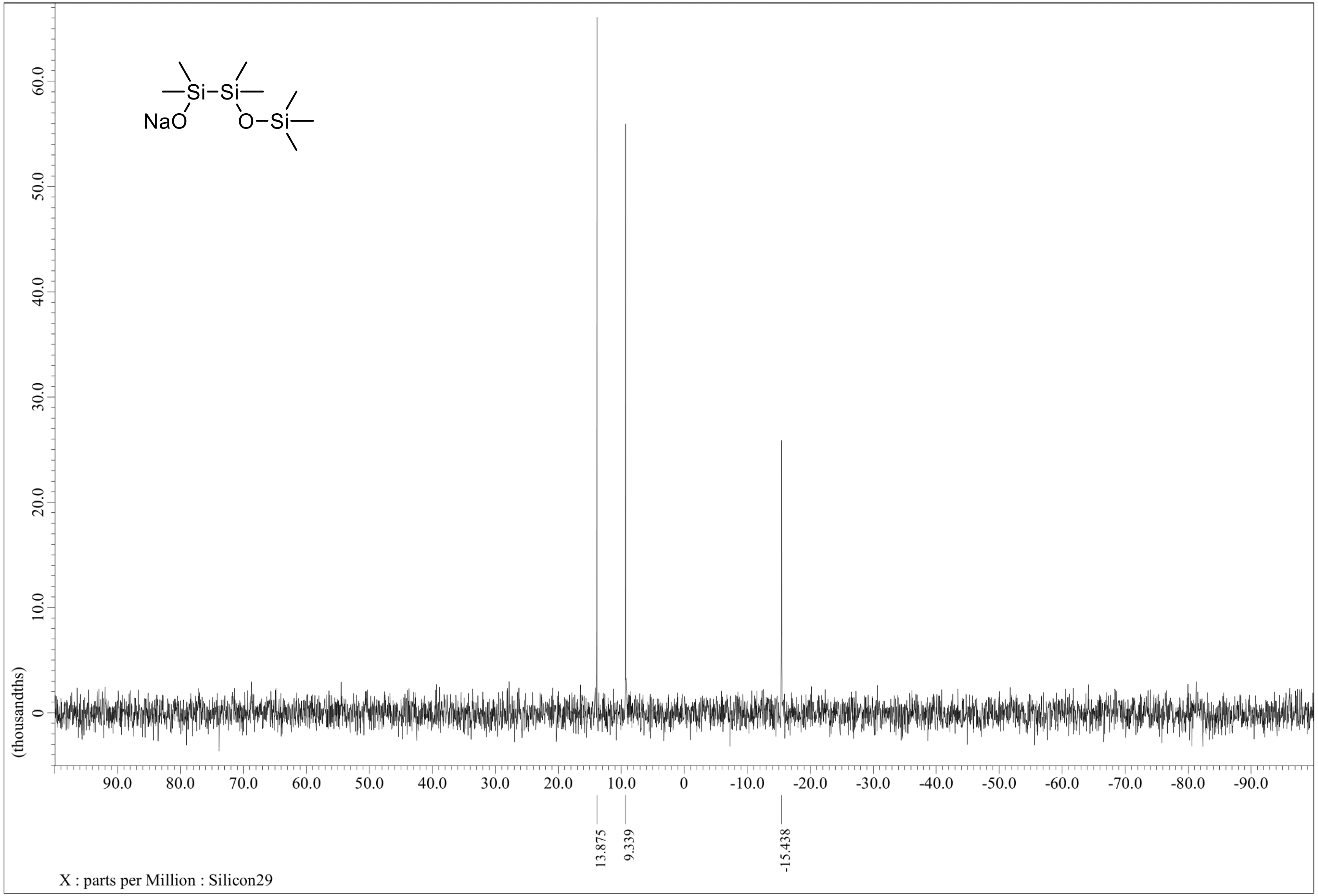

Figure S26. ^{29}Si NMR (119 MHz, C_6D_6) spectrum of **1-OSiMe$_3$**

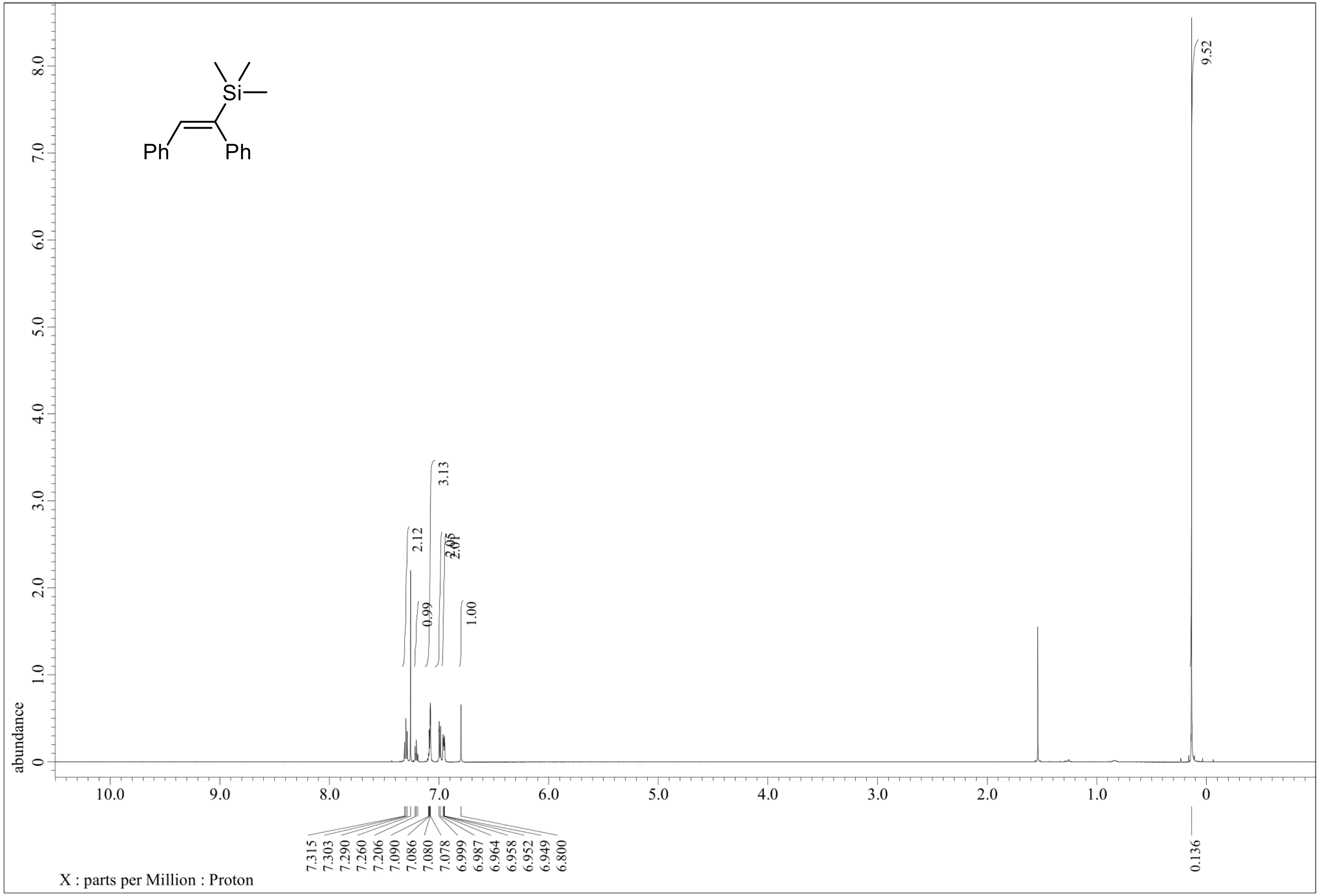

Figure S27. [1]H NMR (600 MHz, $CDCl_3$) spectrum of **3a**

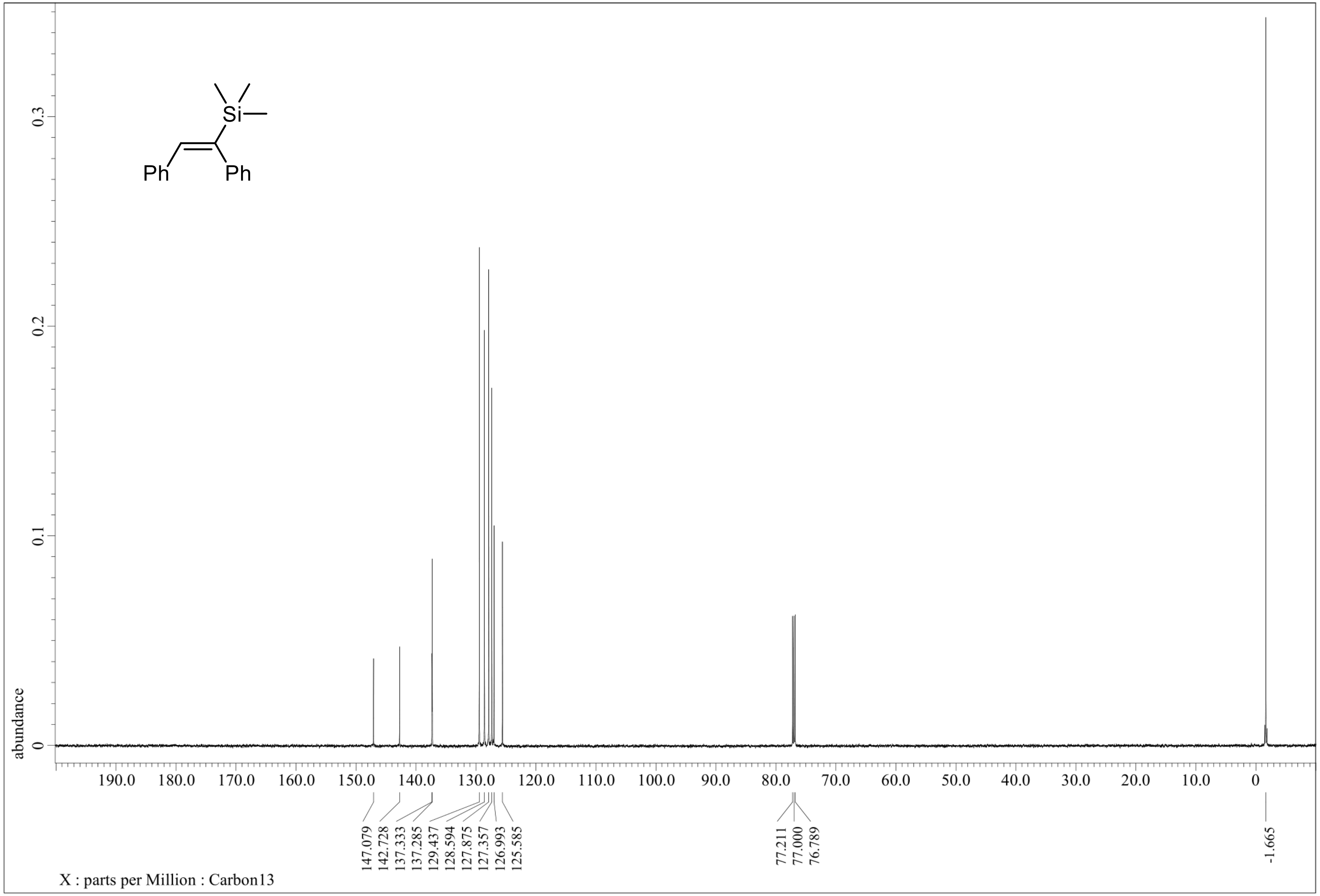

Figure S28. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3a**

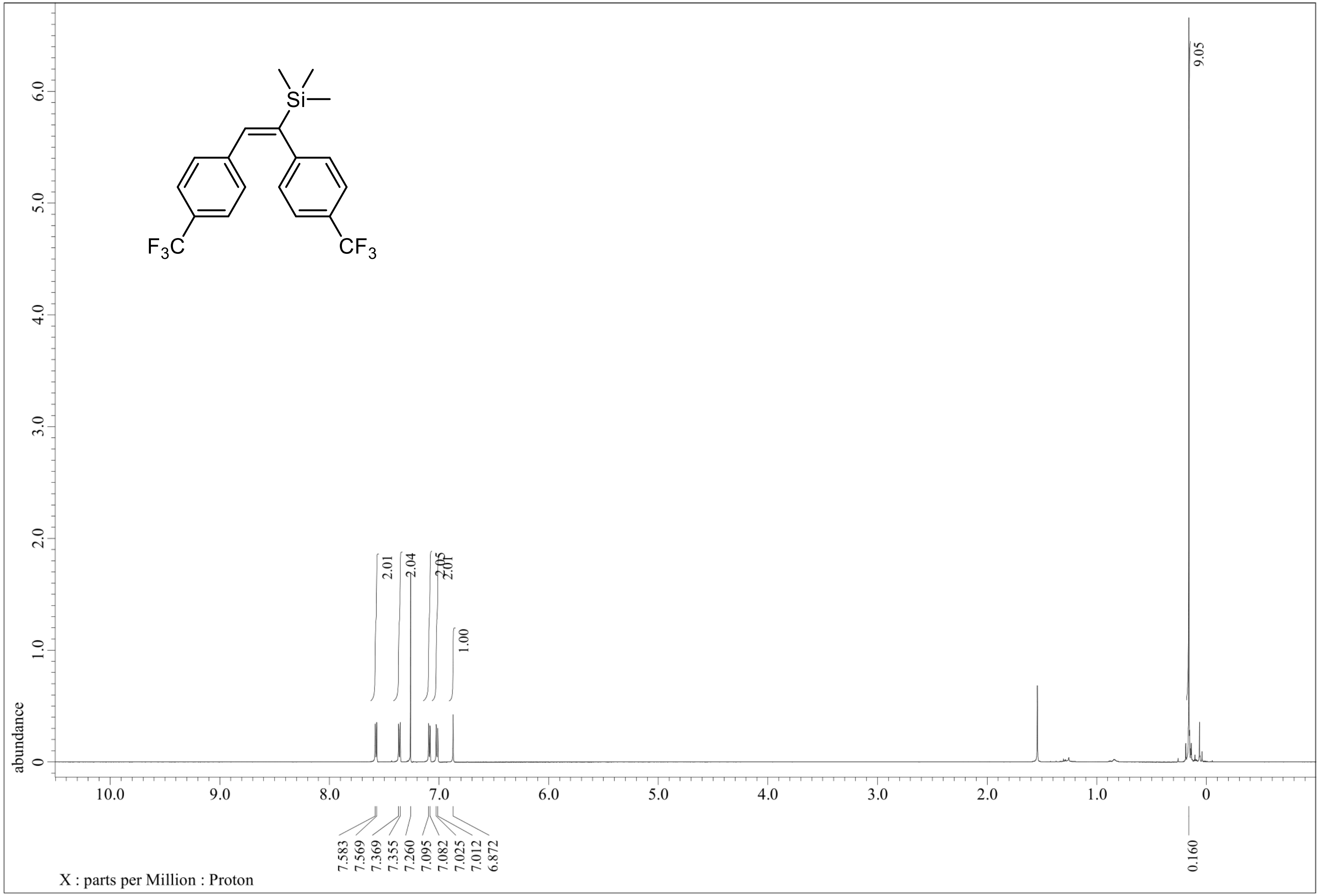

Figure S29. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3b**

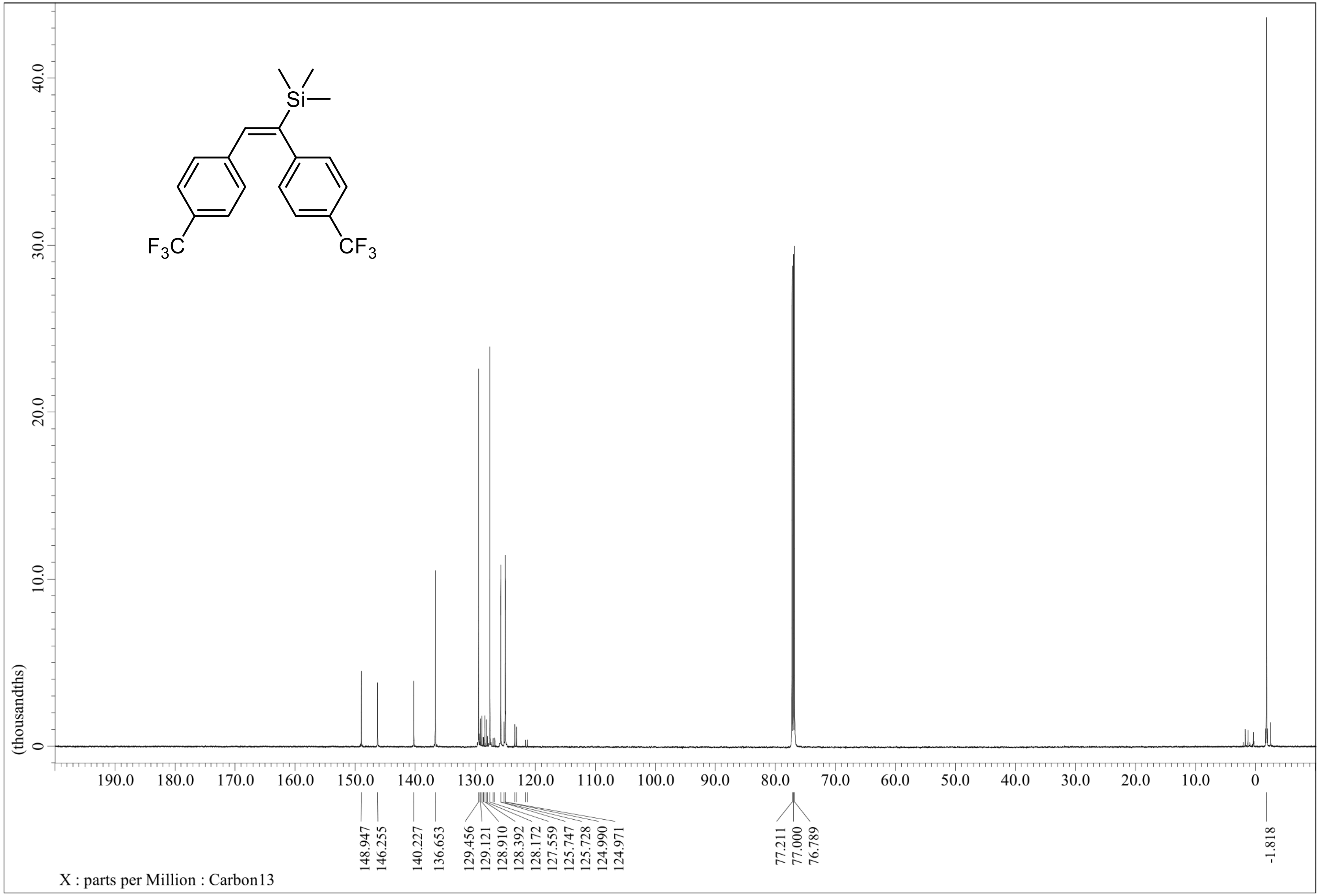

Figure S30. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3b**

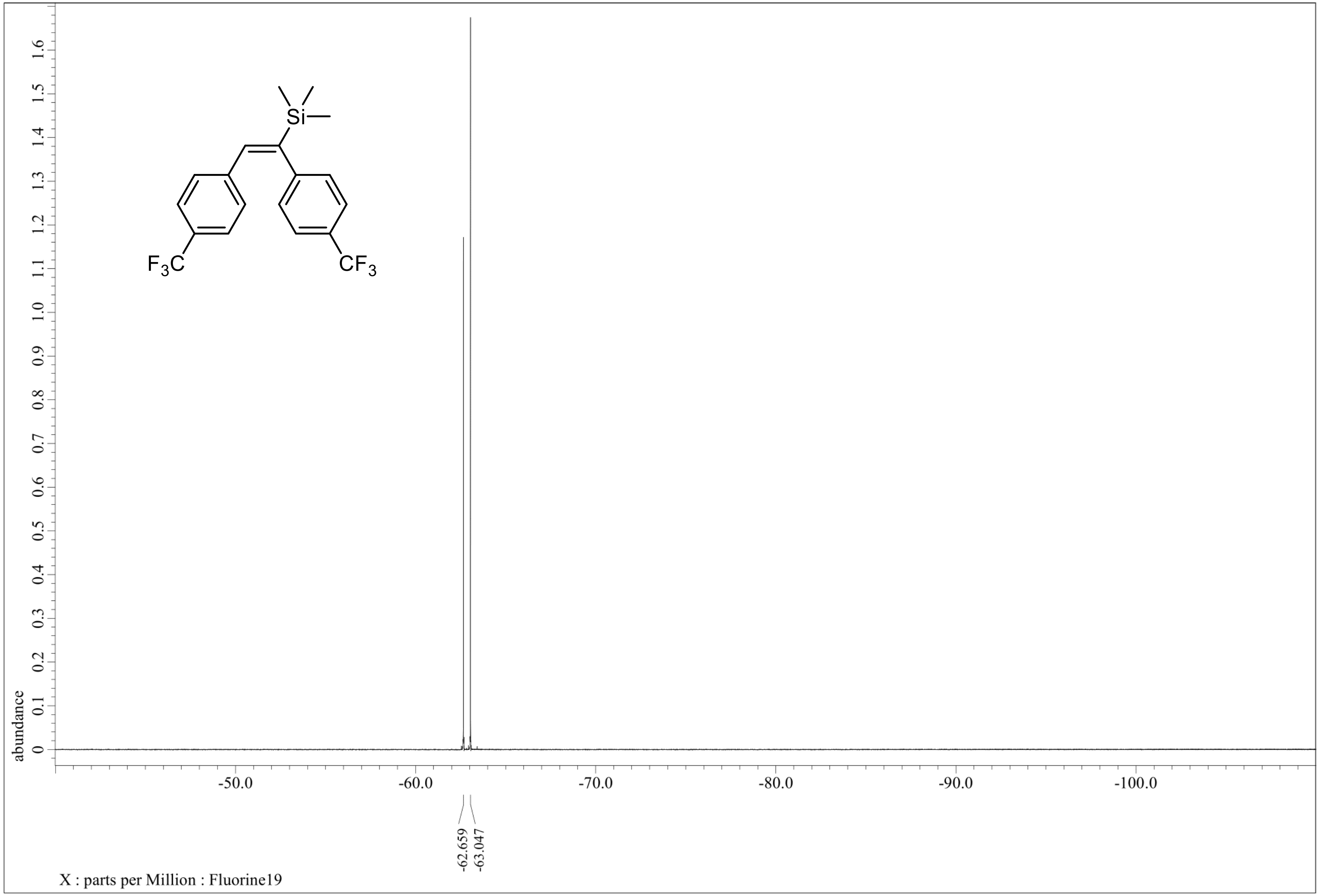

Figure S31. ^{19}F NMR (564 MHz, $CDCl_3$) spectrum of **3b**

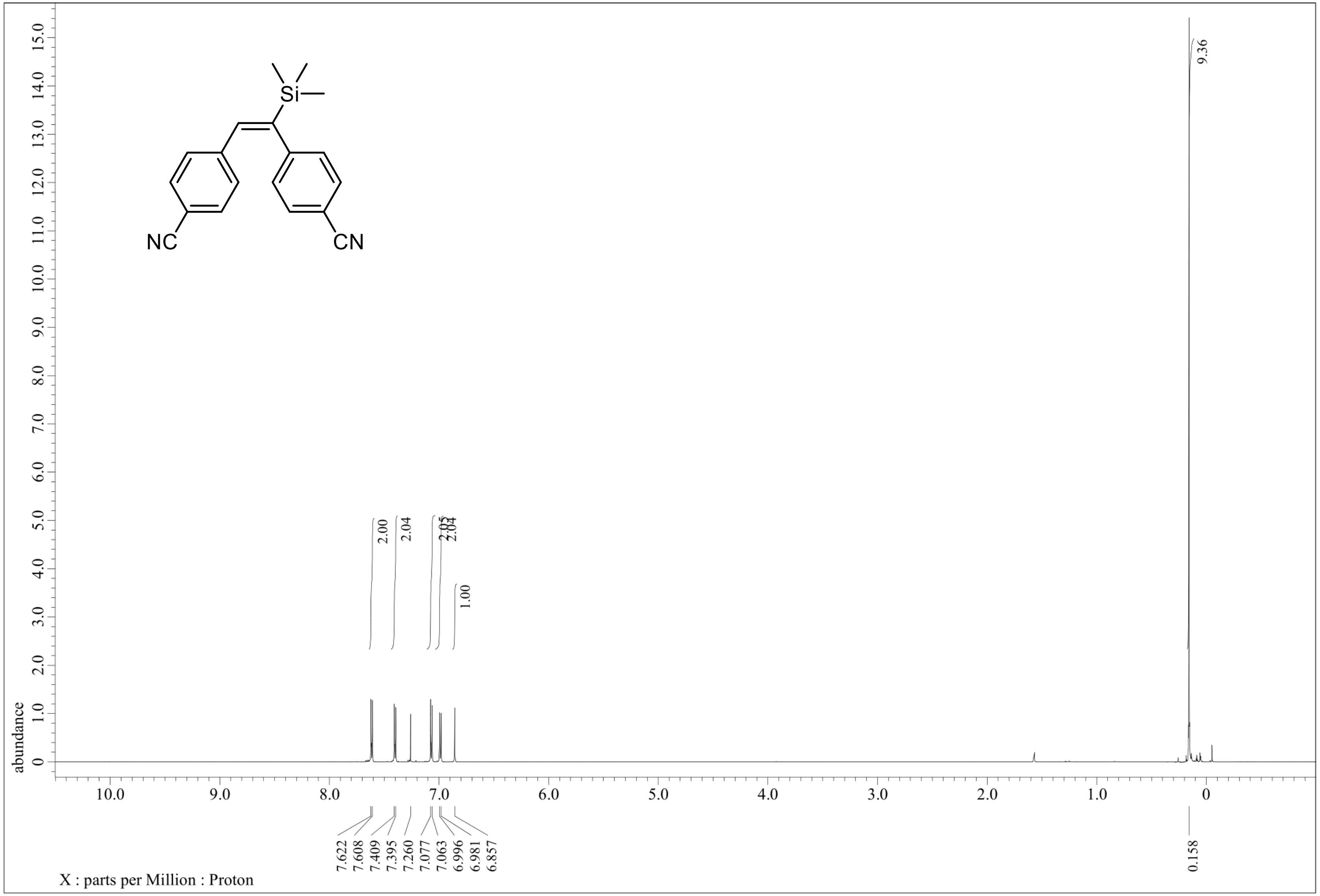

Figure S32. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3c**

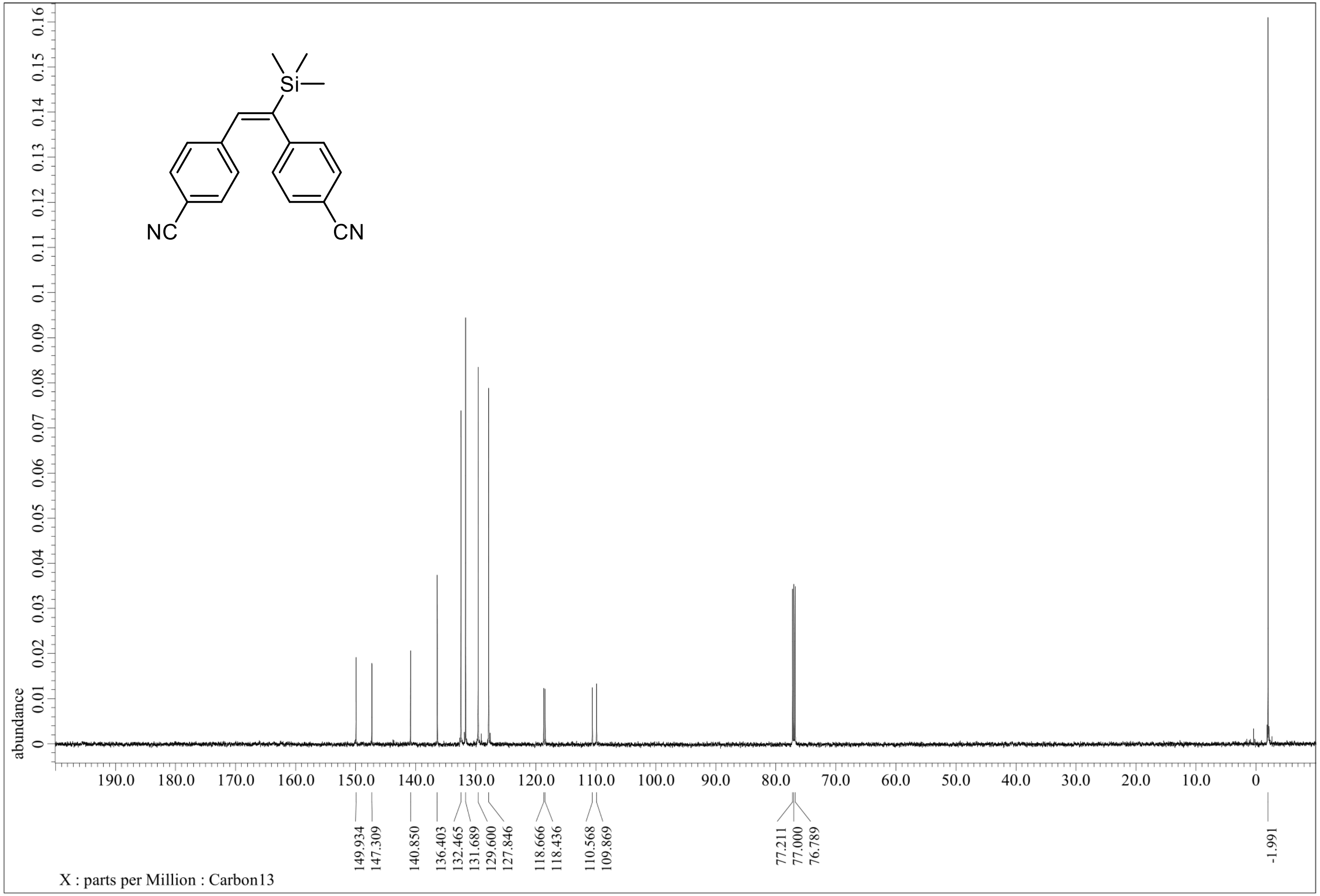

Figure S33. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3c**

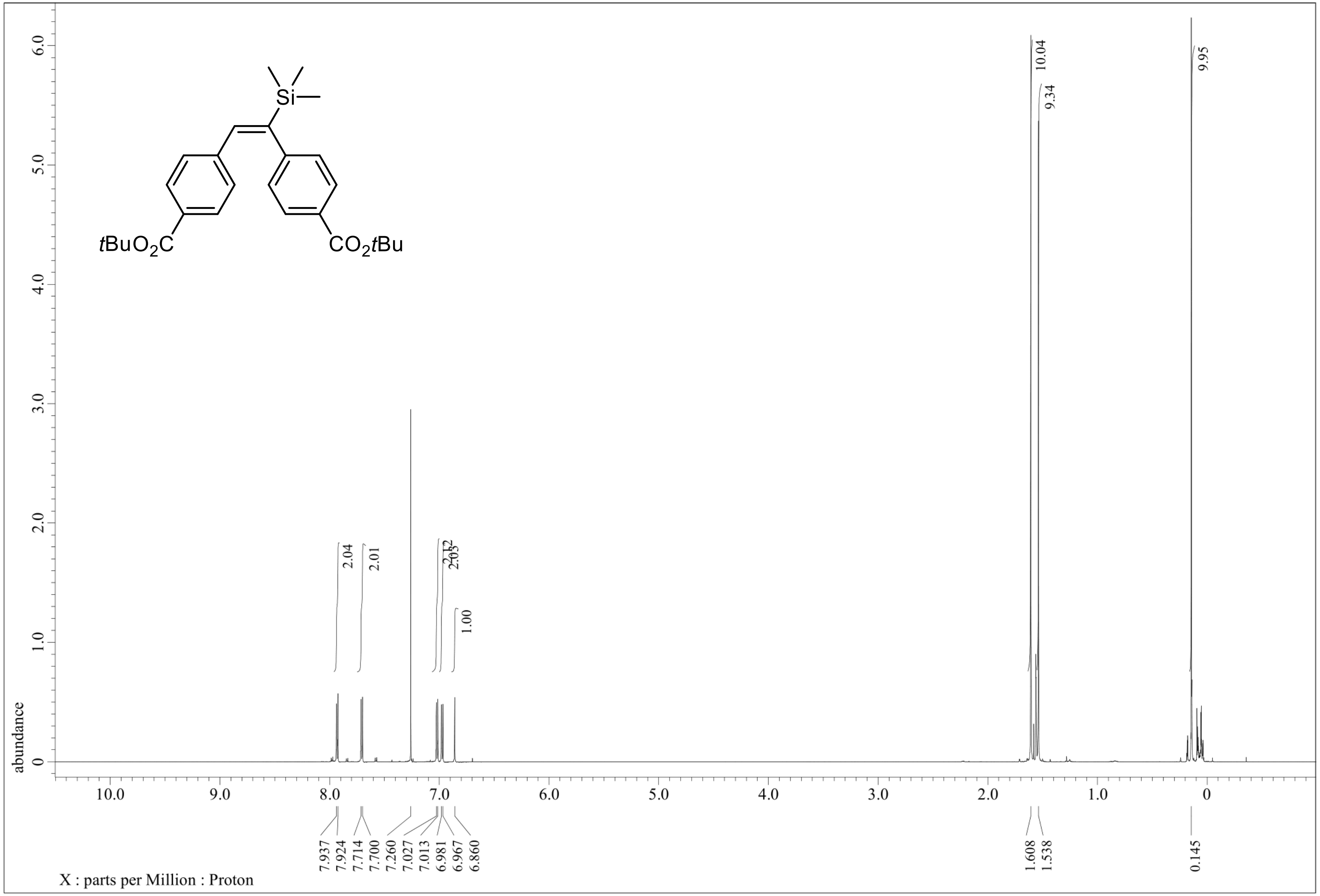

Figure S34. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3d**

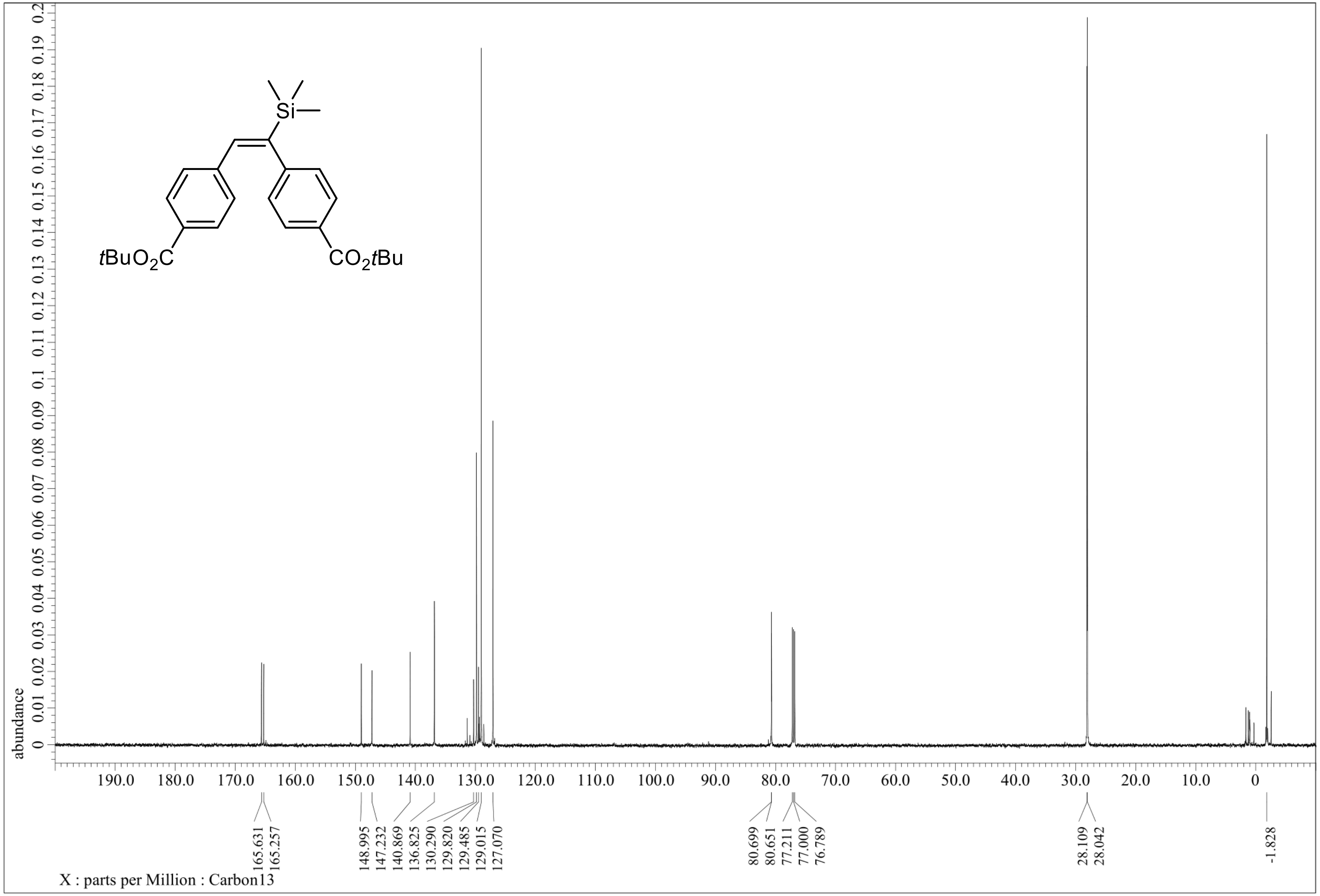

Figure S35. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3d**

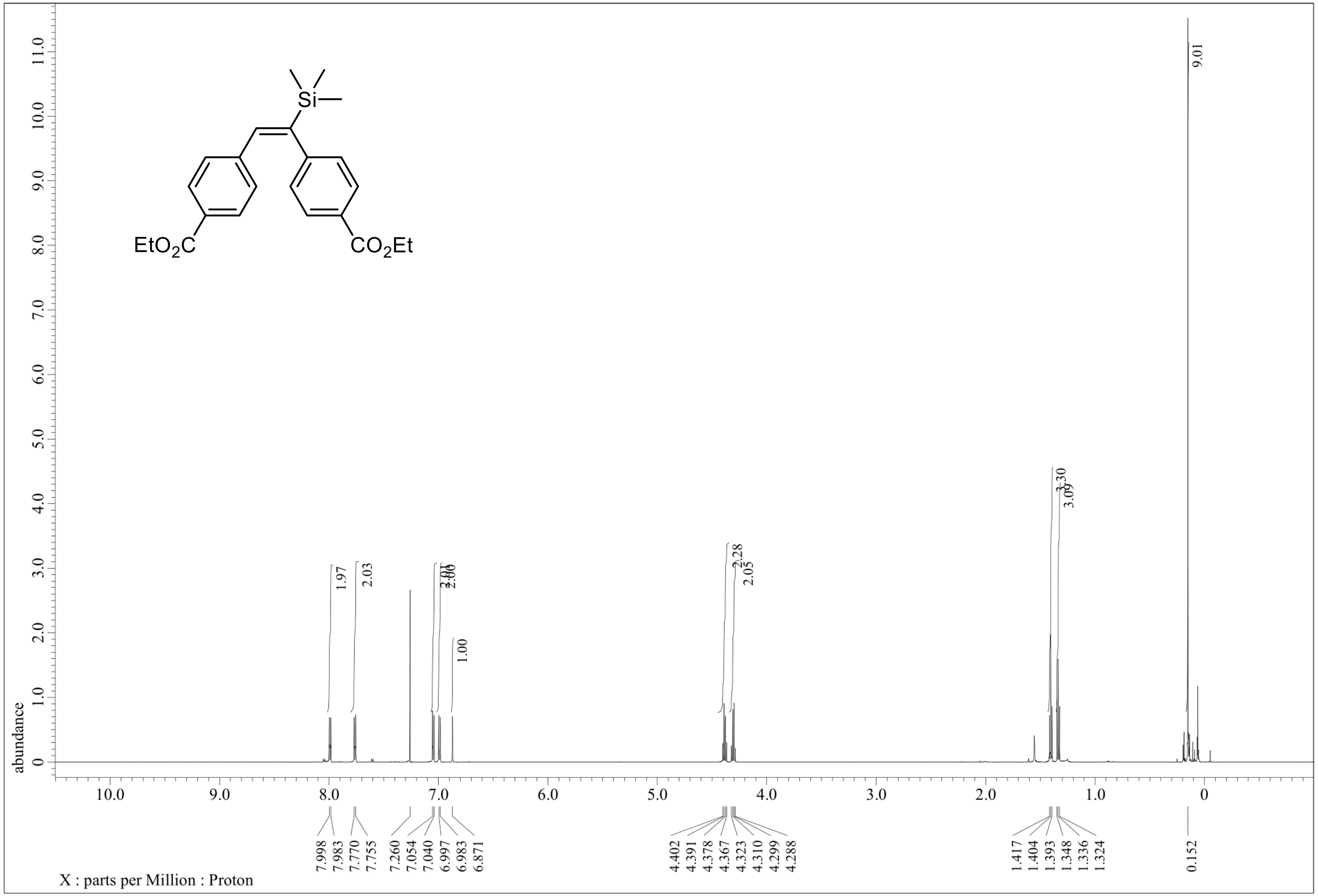

Figure S36. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3e**

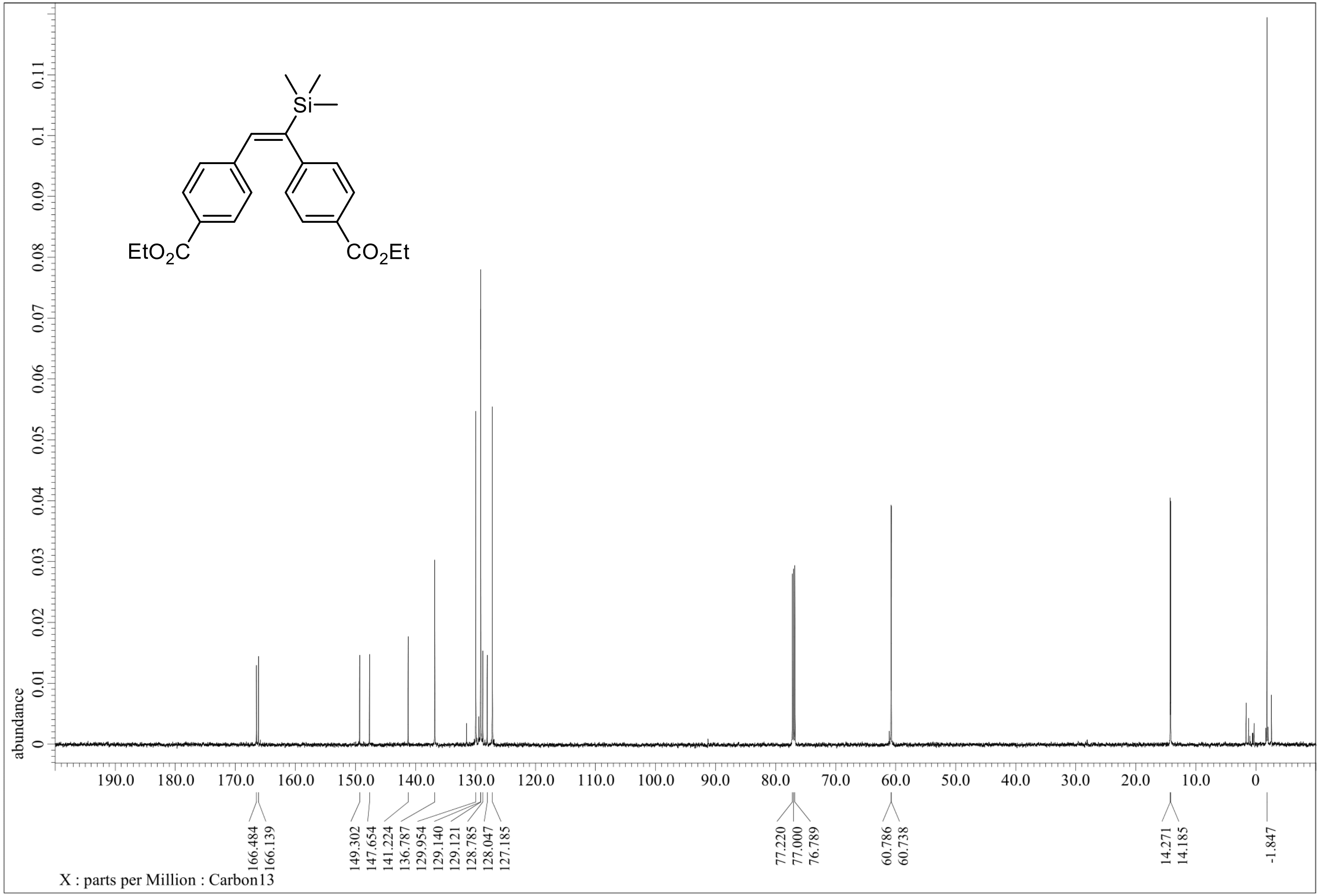

Figure S37. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3e**

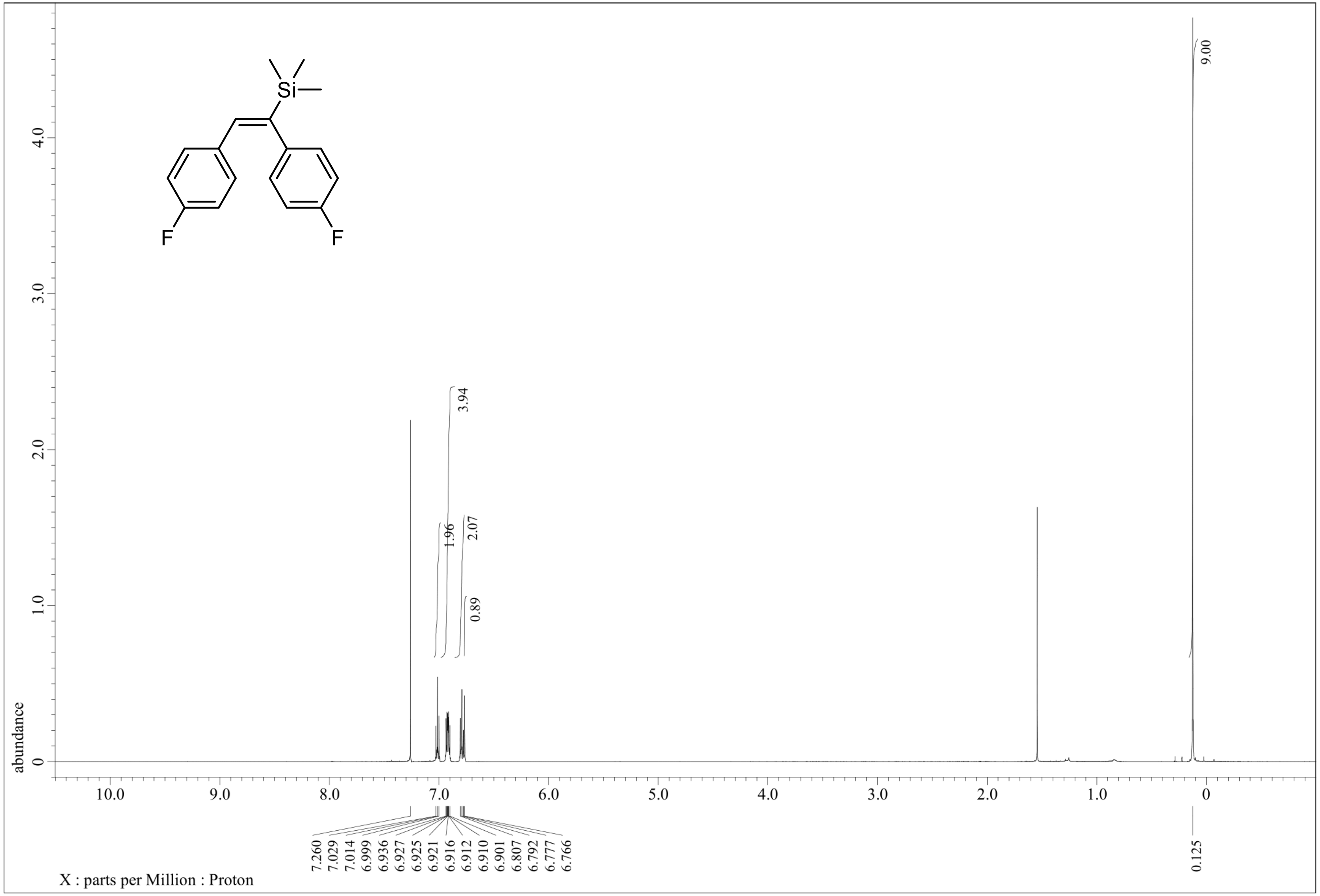

Figure S38. [1]H NMR (600 MHz, $CDCl_3$) spectrum of **3f**

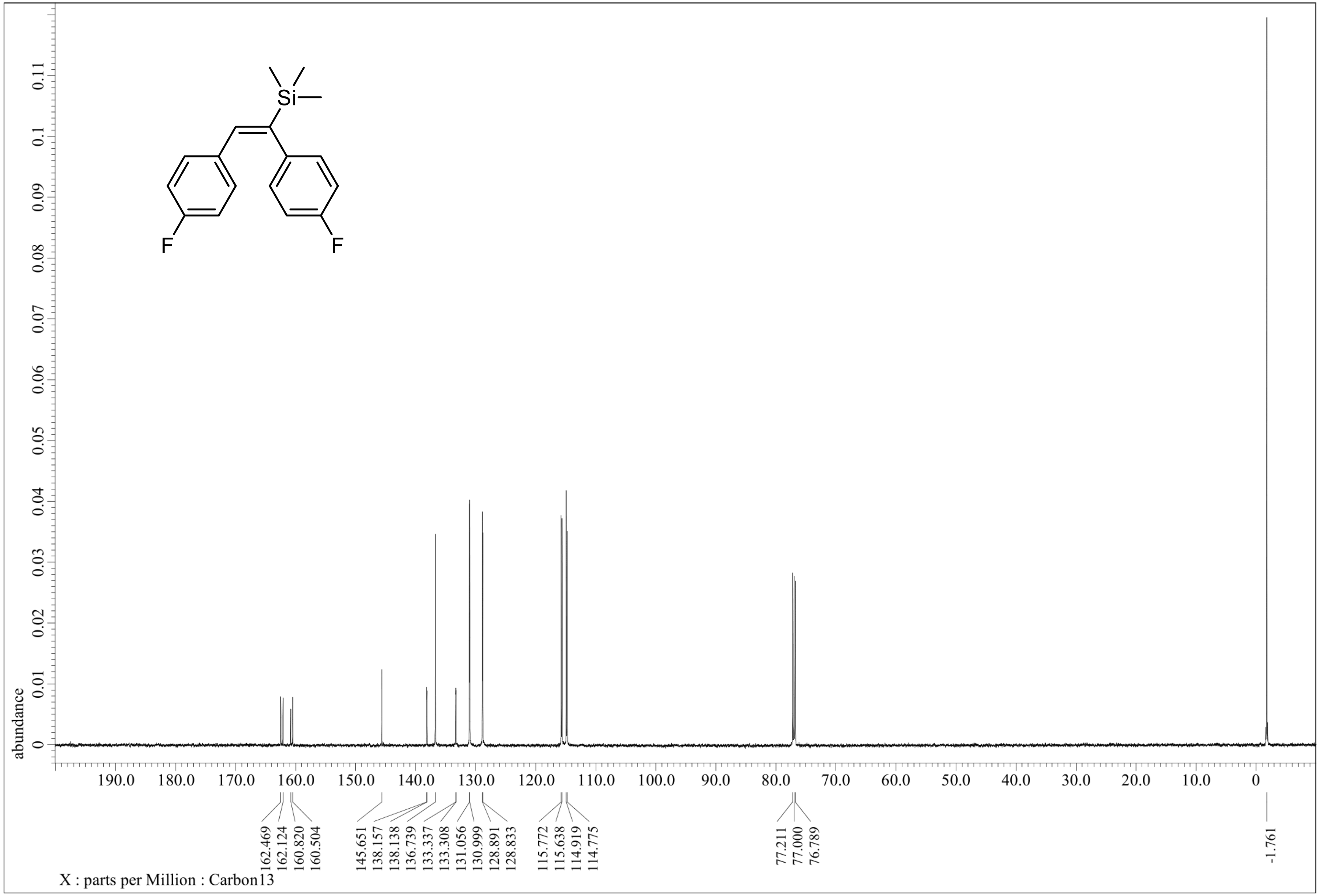

Figure S39. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3f**

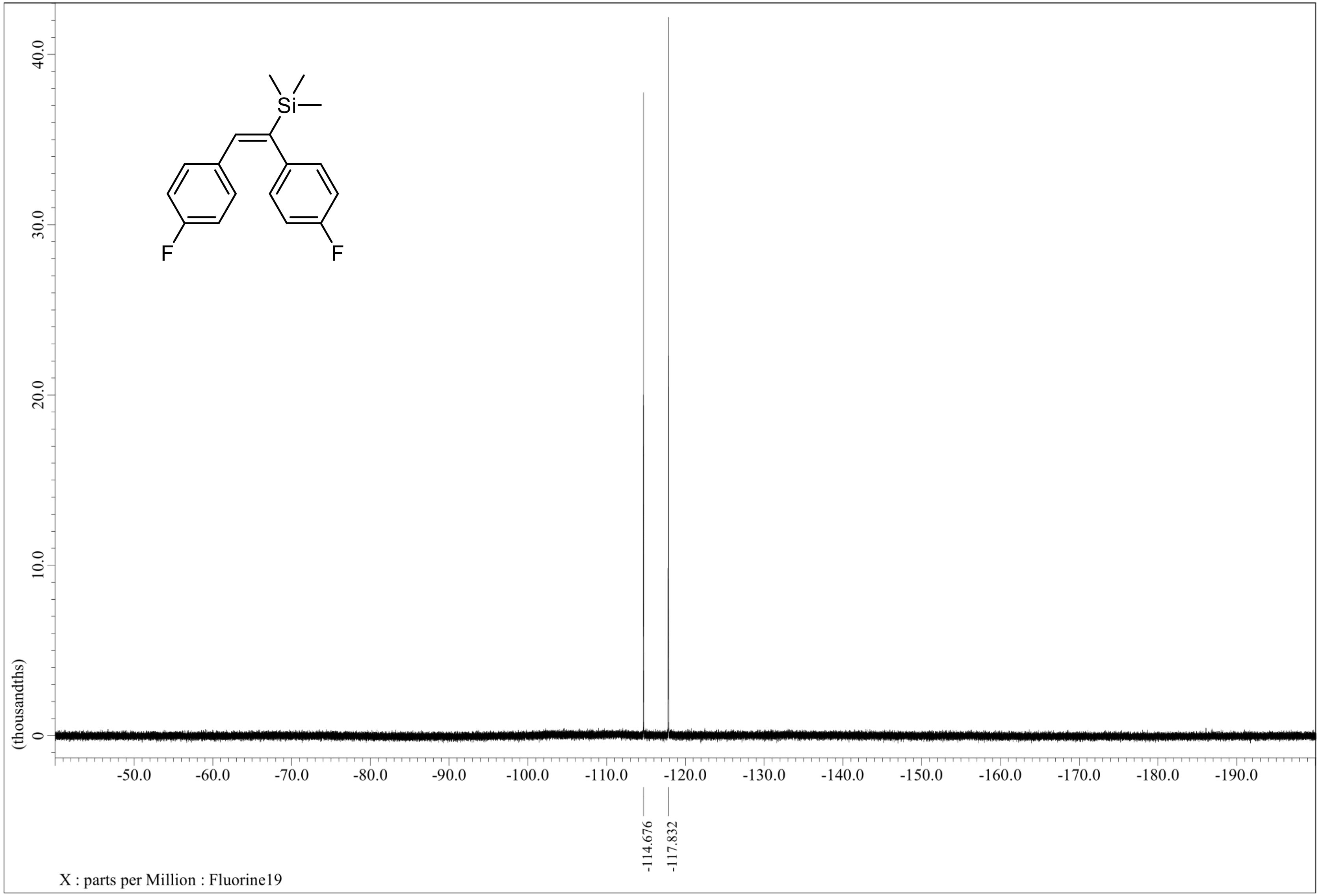

Figure S40. ^{19}F NMR (564 MHz, $CDCl_3$) spectrum of **3f**

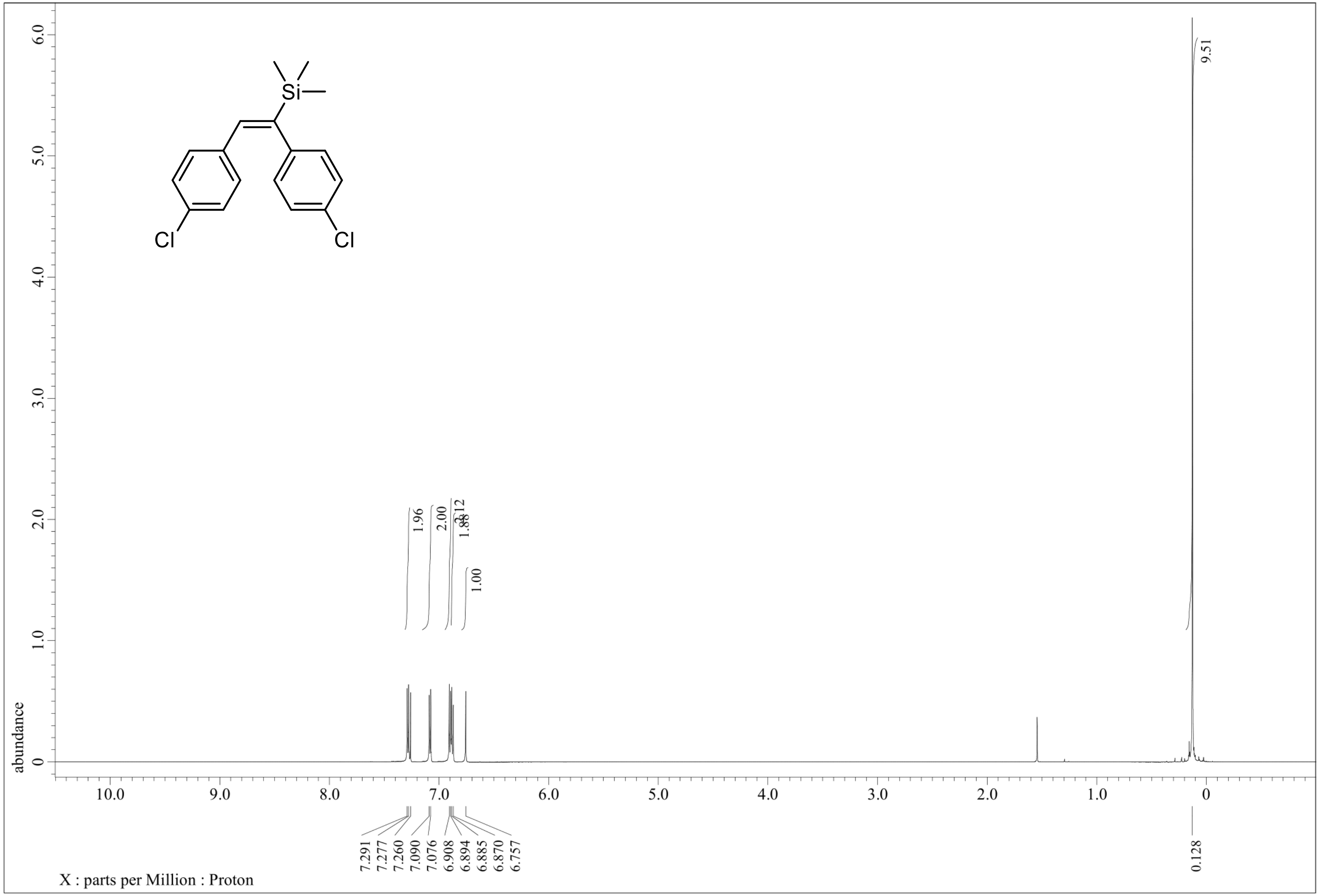

Figure S41. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3g**

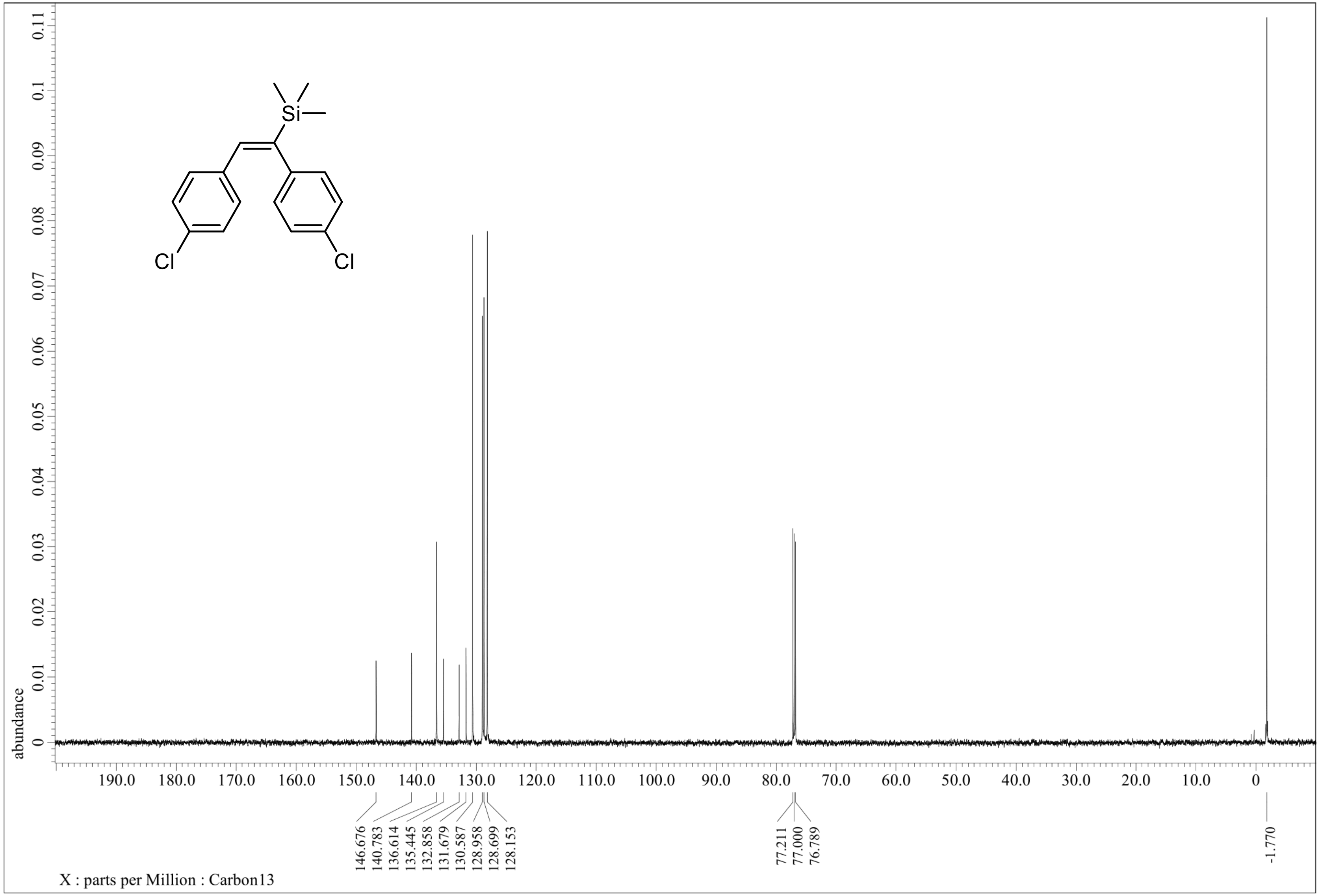

Figure S42. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3g**

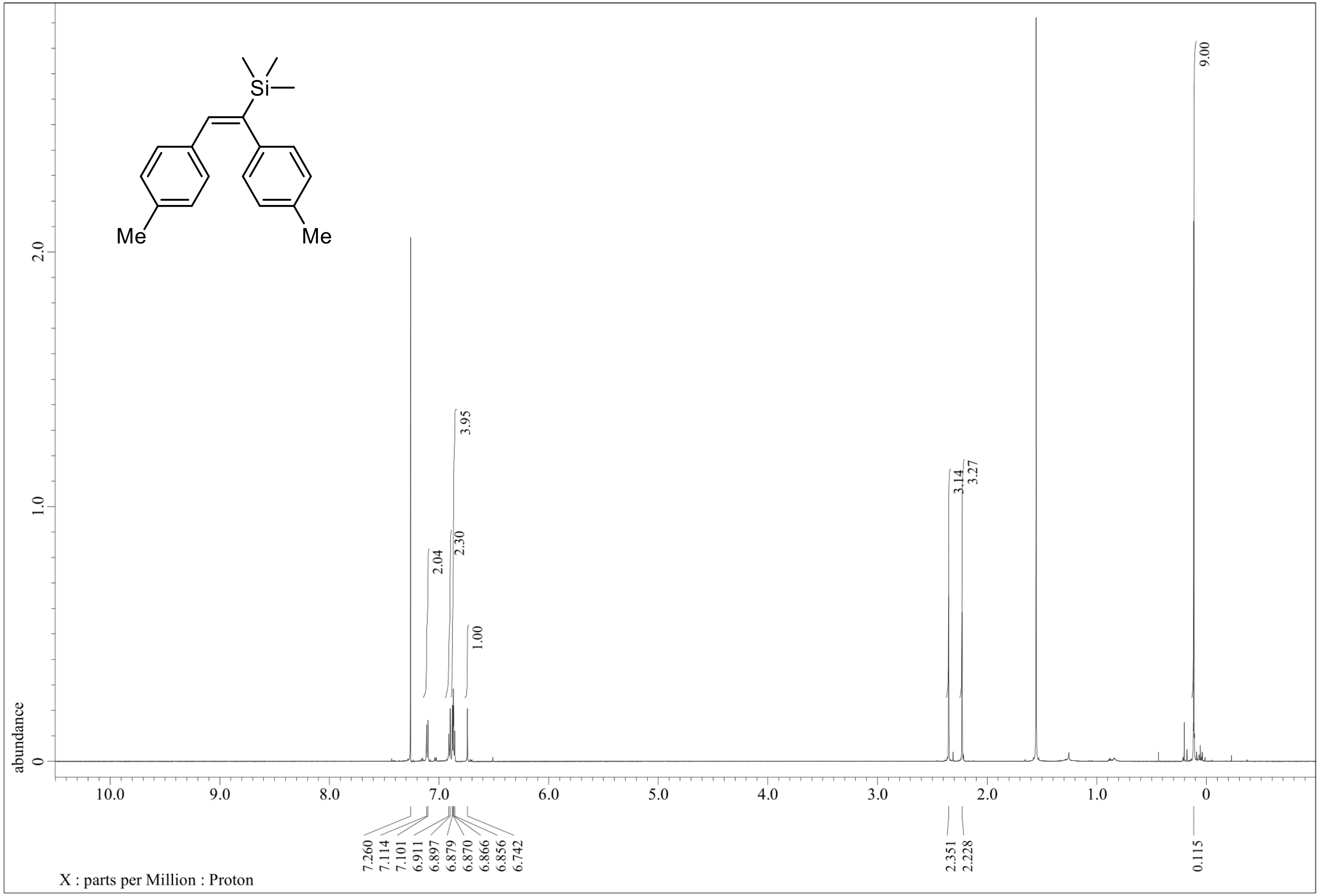

Figure S43. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3h**

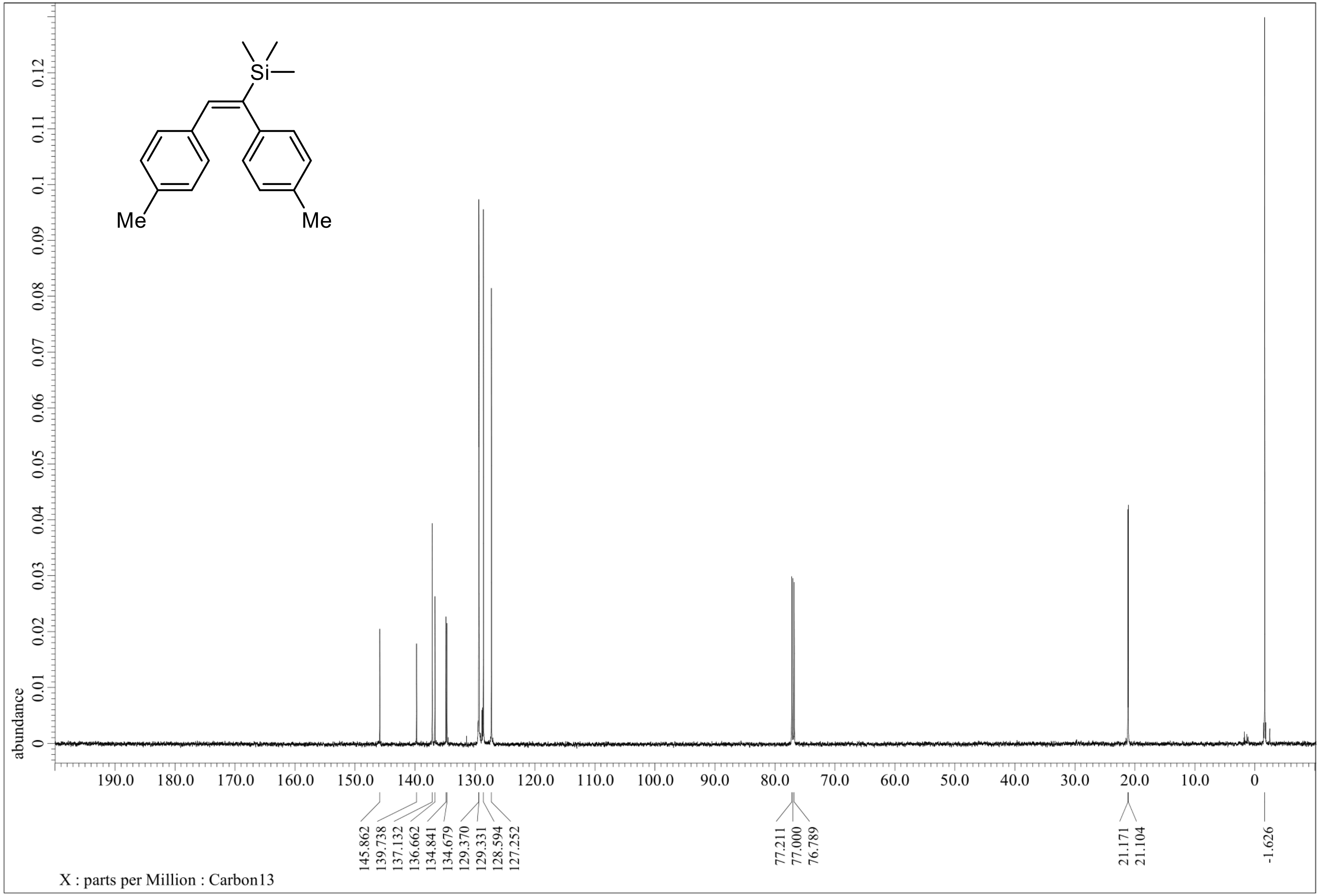

Figure S44. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3h**

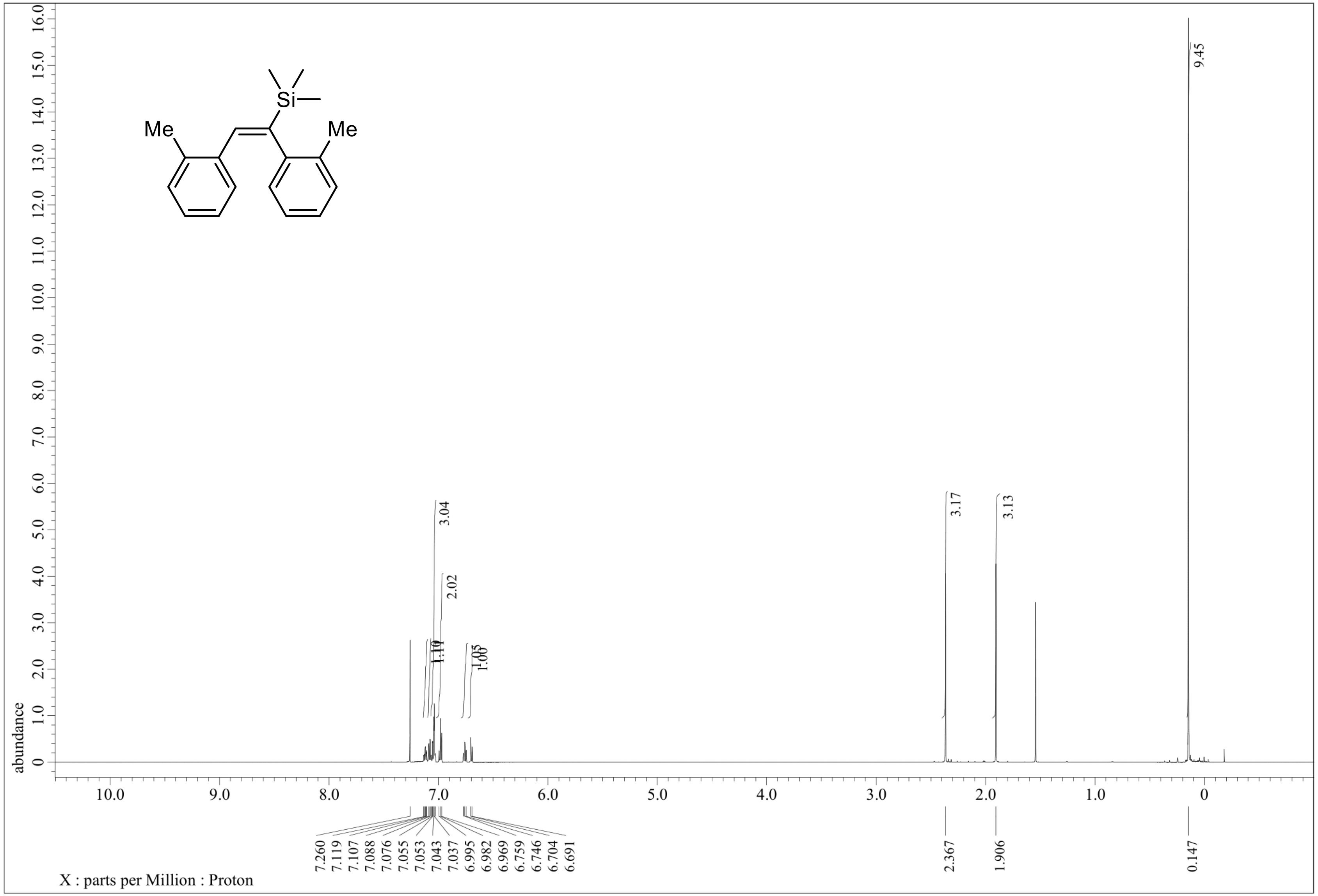

Figure S45. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3i**

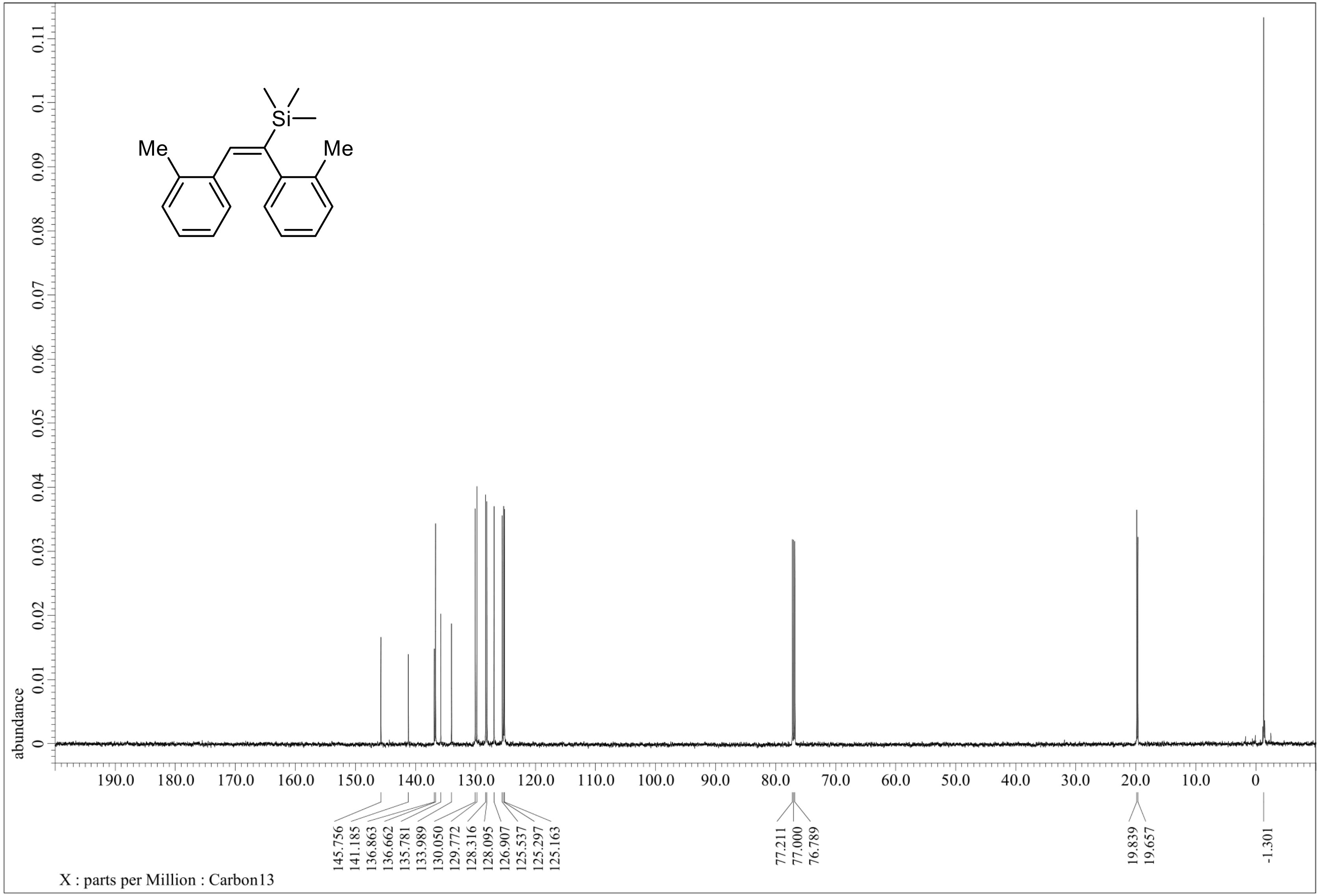

Figure S46. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3i**

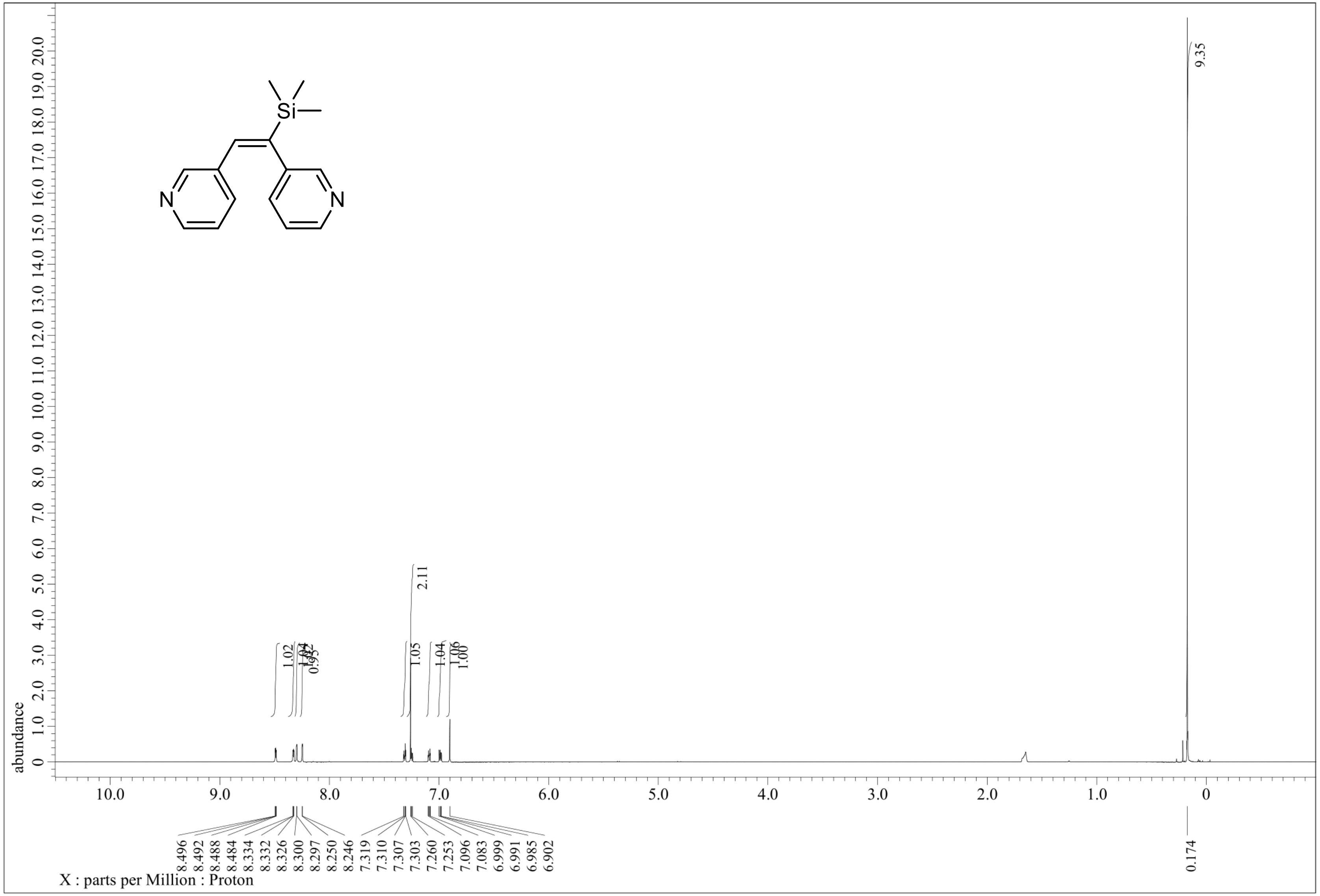

Figure S47. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3k**

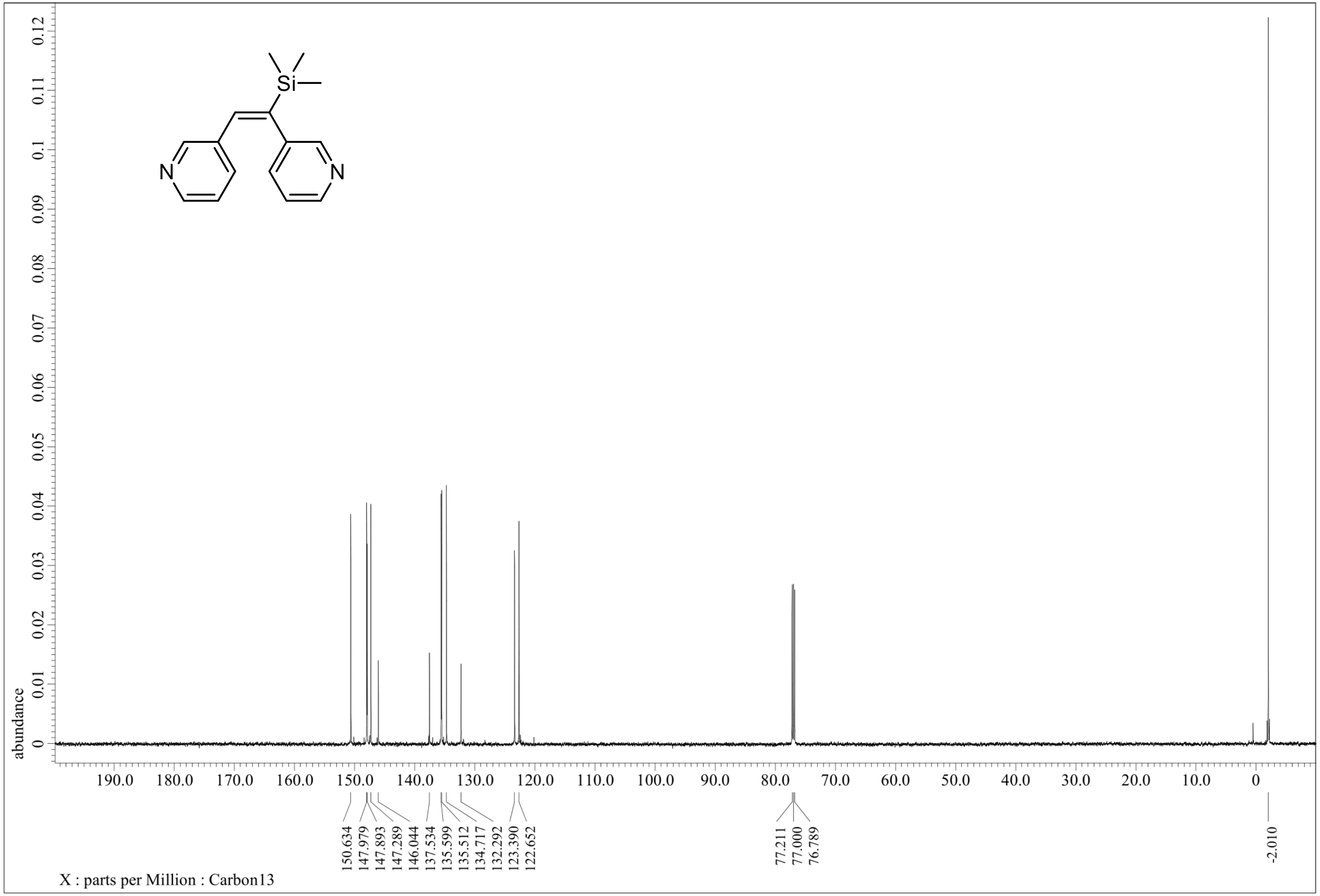

Figure S48. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3k**

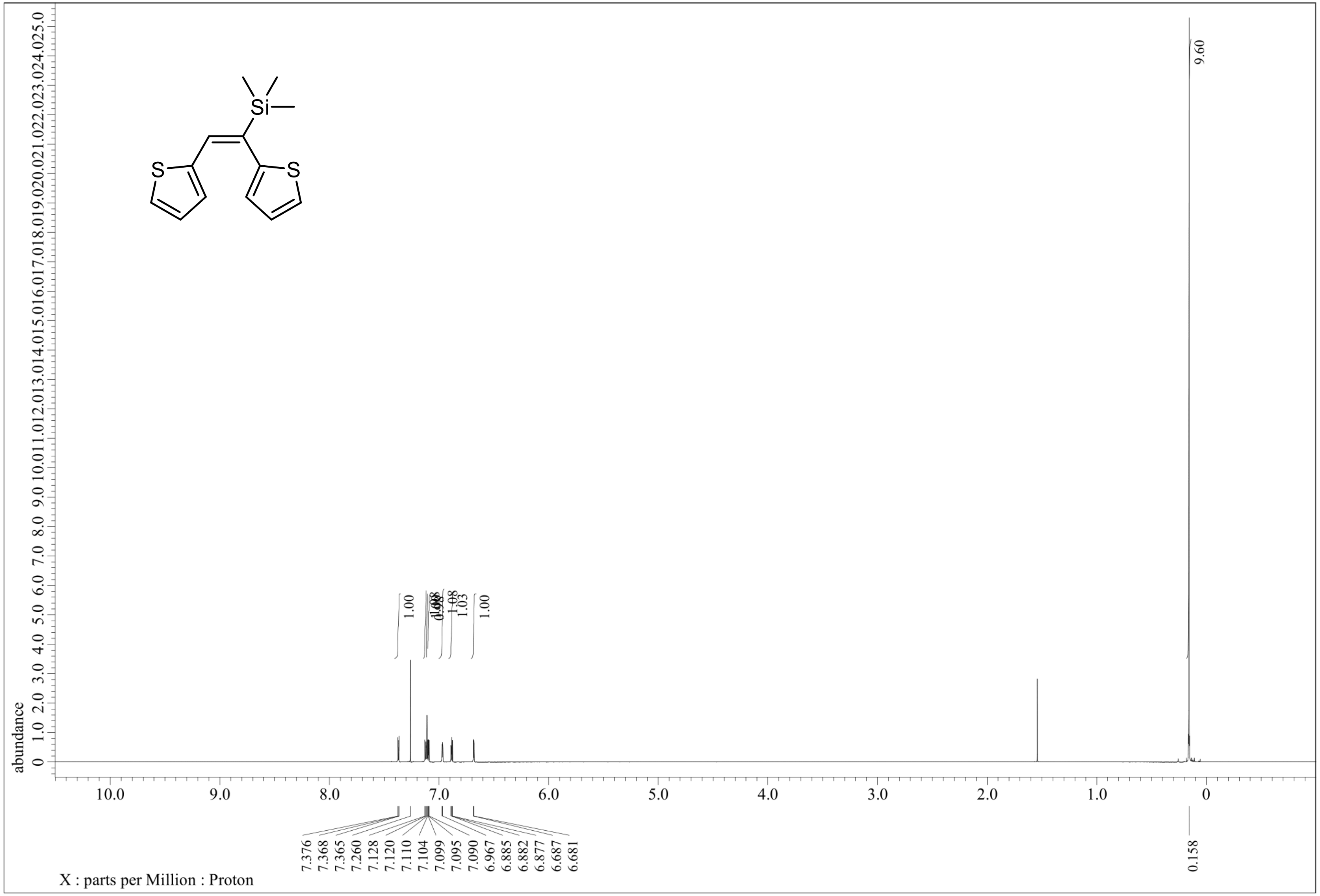

Figure S49. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3l**

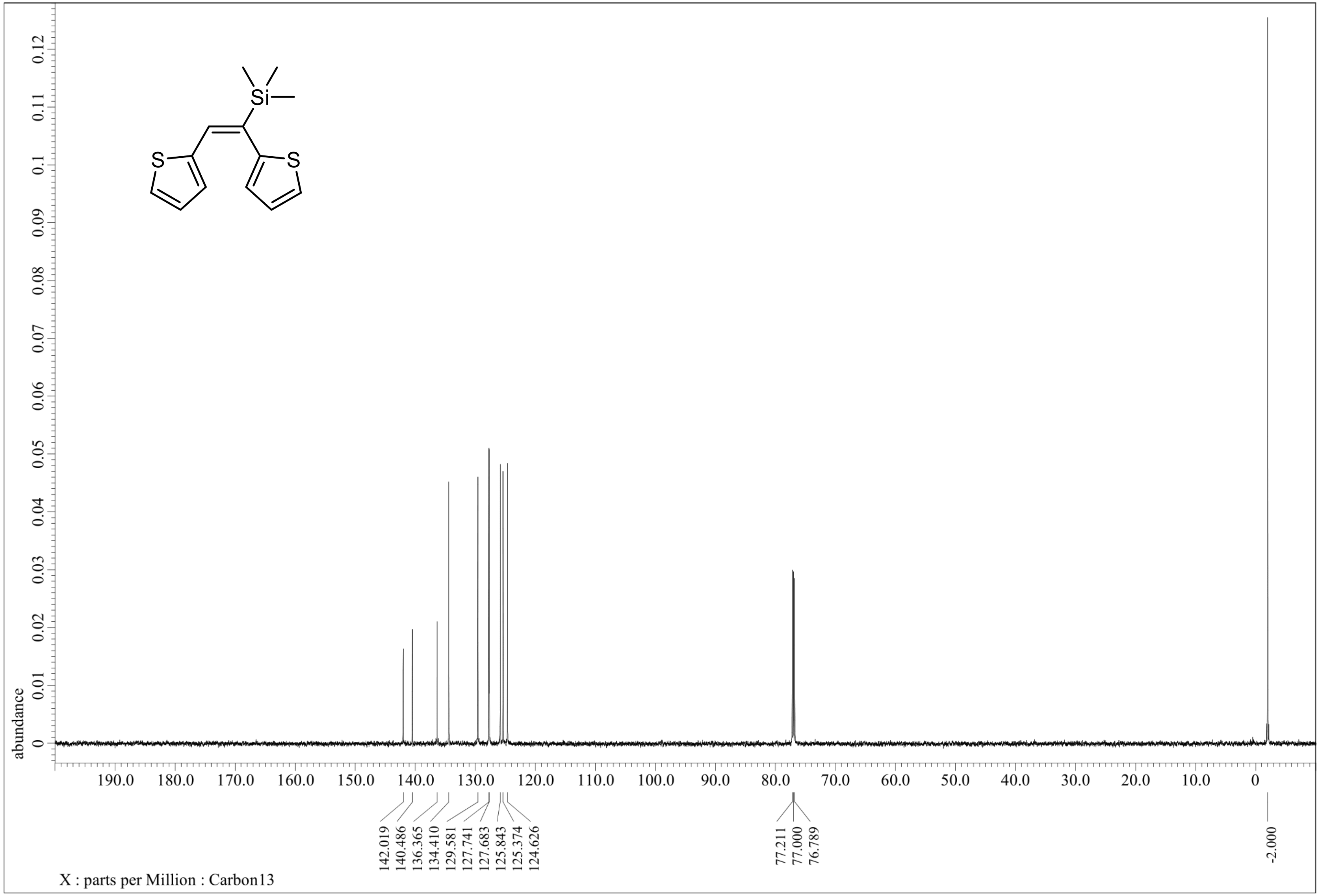

Figure S50. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3l**

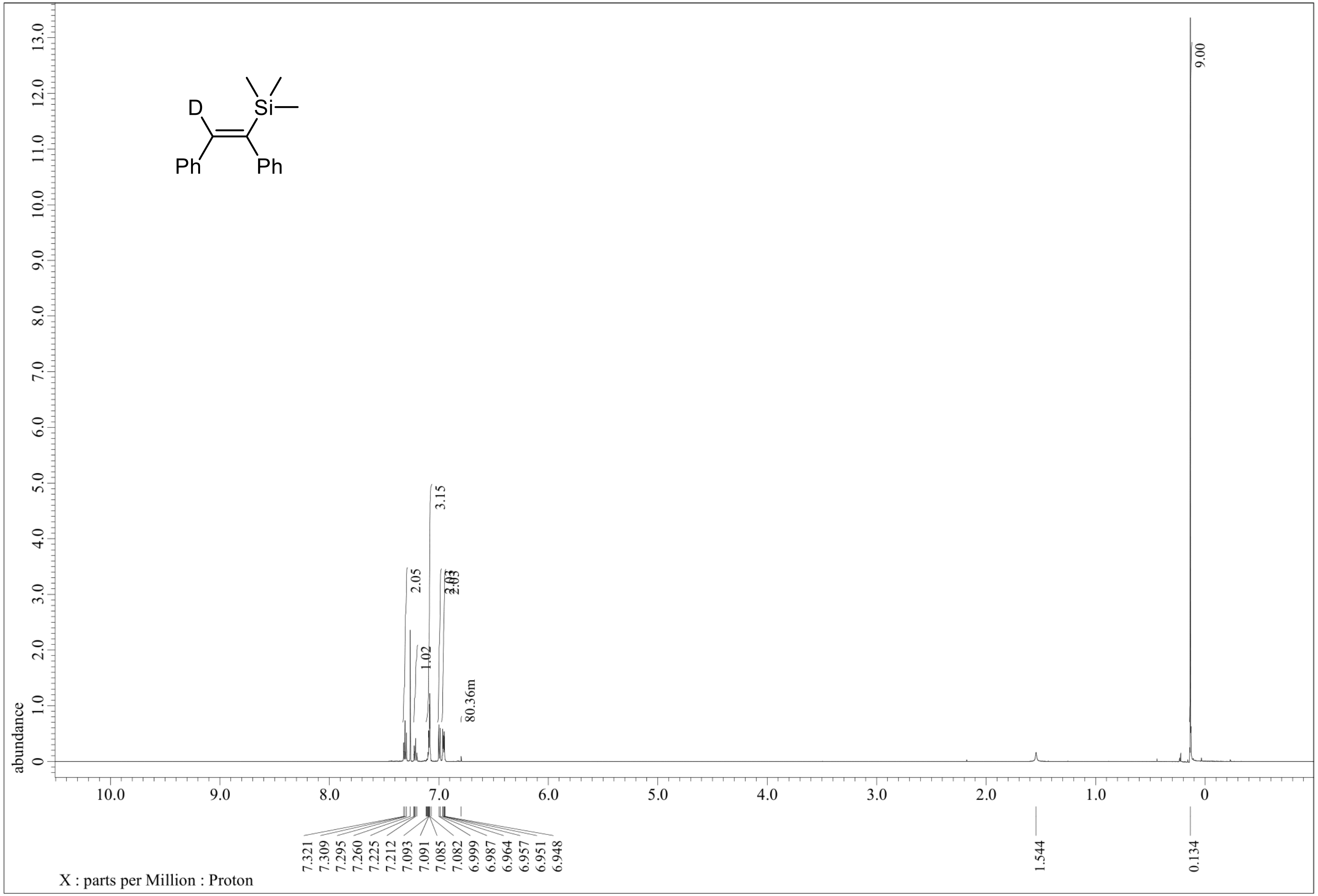

Figure S51. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3m**

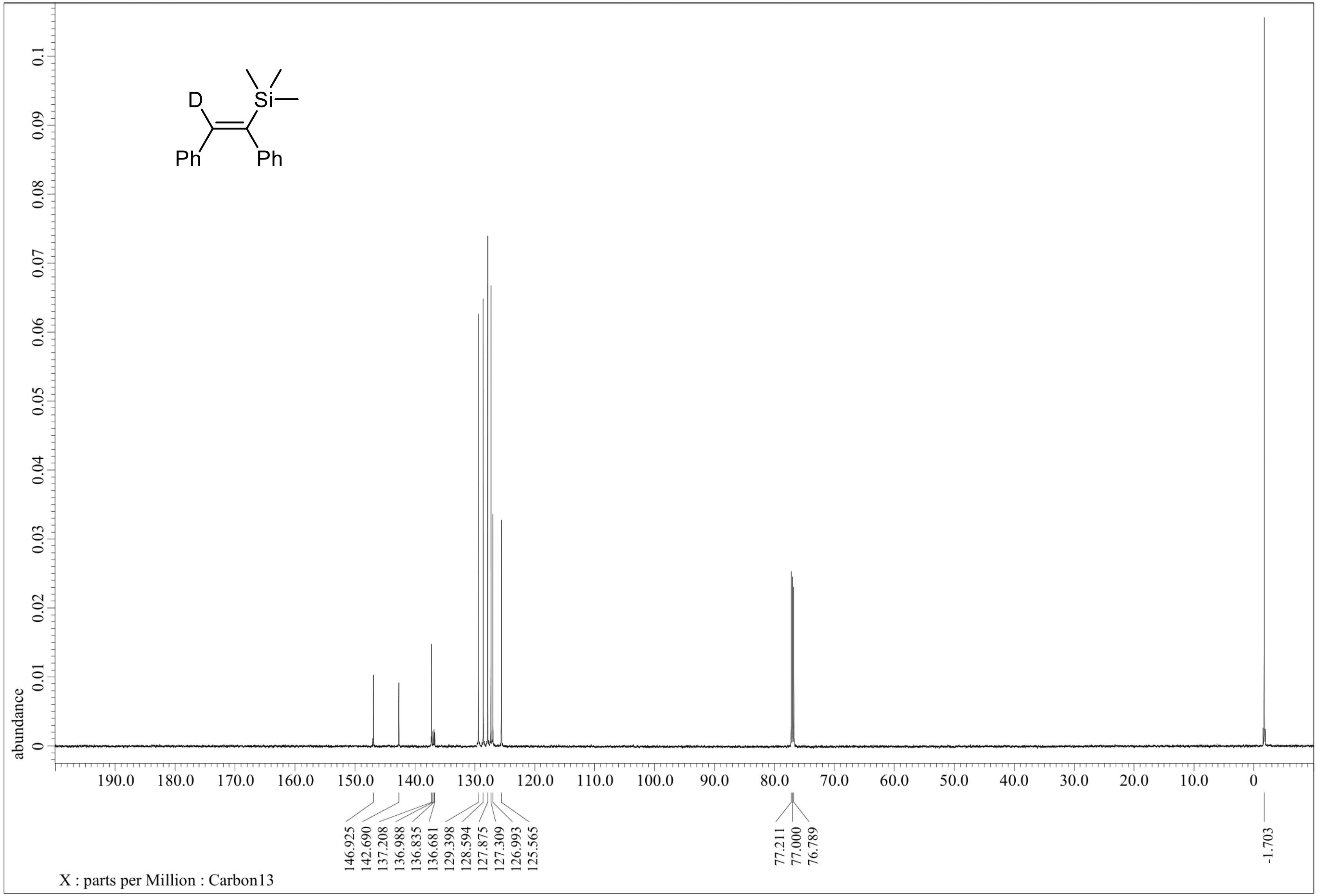

Figure S52. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3m**

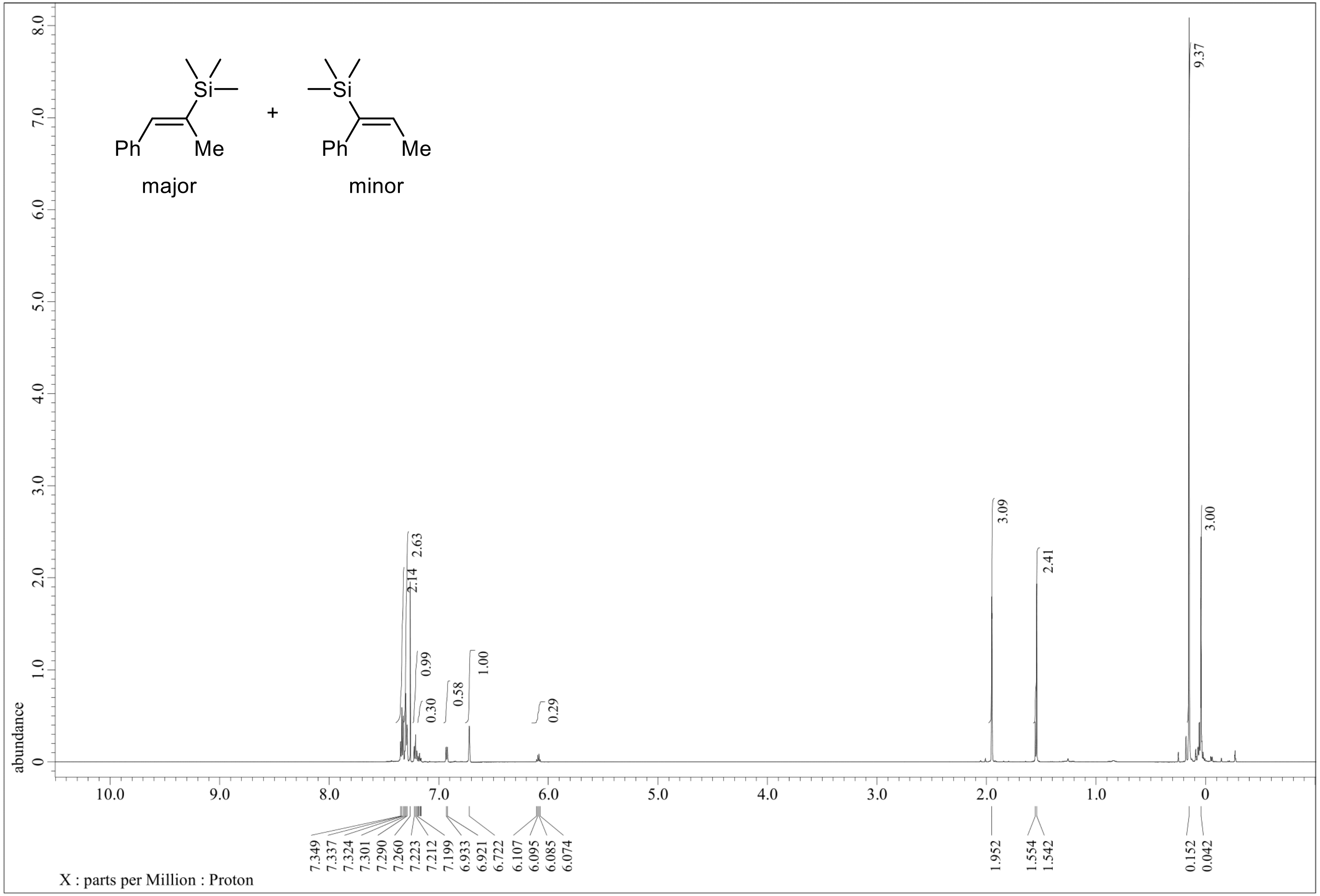

Figure S53. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3n** (using $P(OPh)_3$)

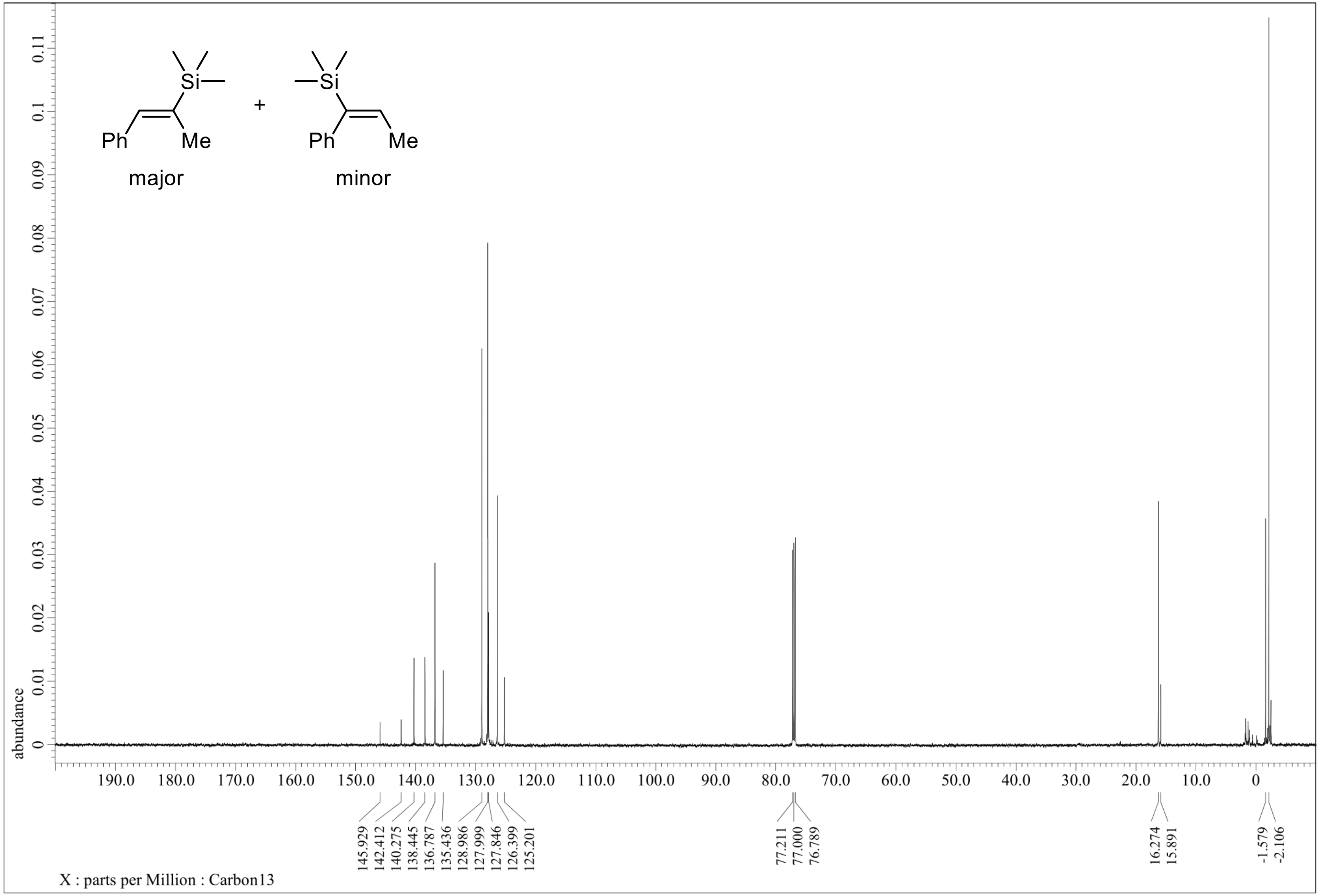

Figure S54. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3n** (using $P(OPh)_3$)

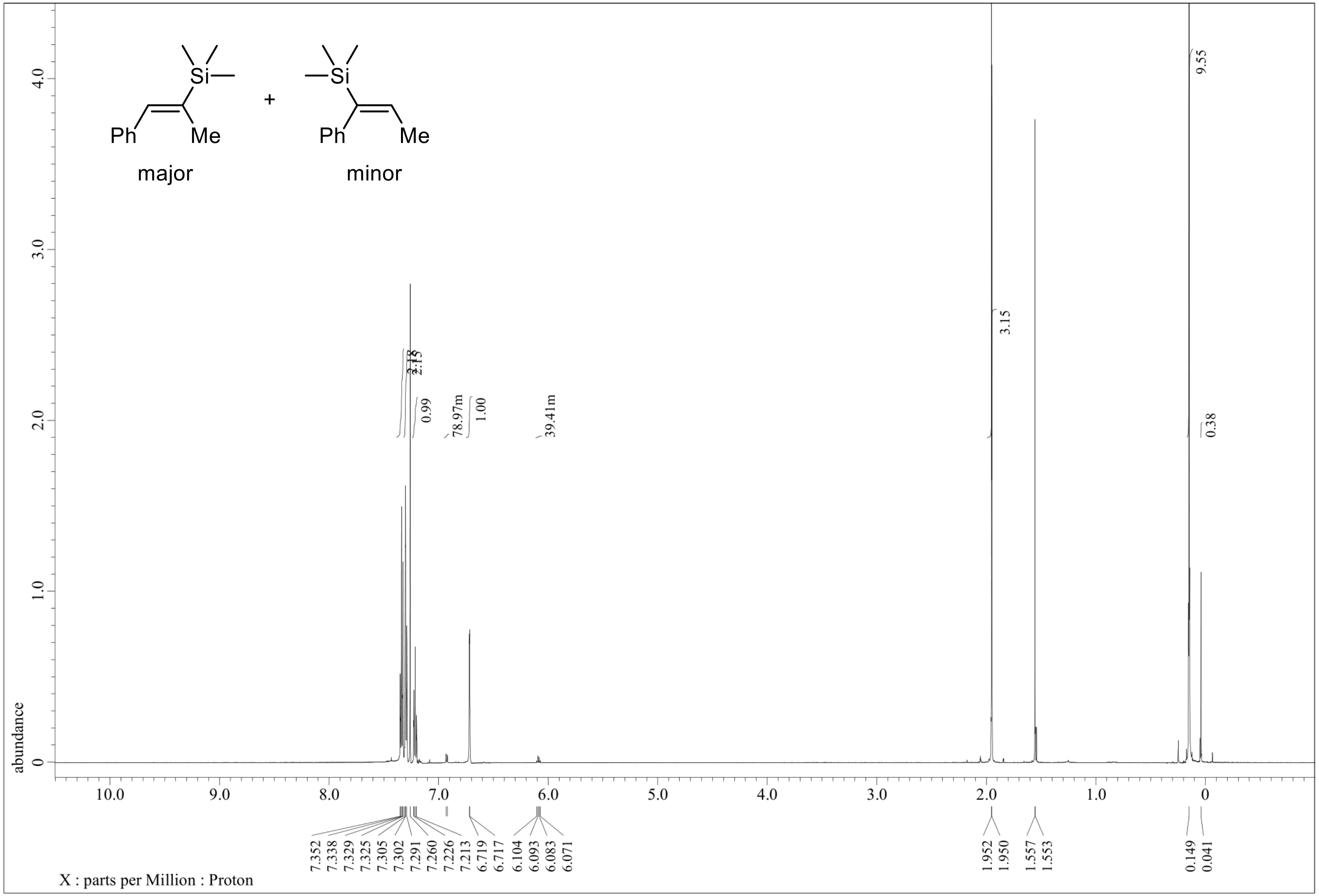

Figure S55. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3n** (using PCy_3)

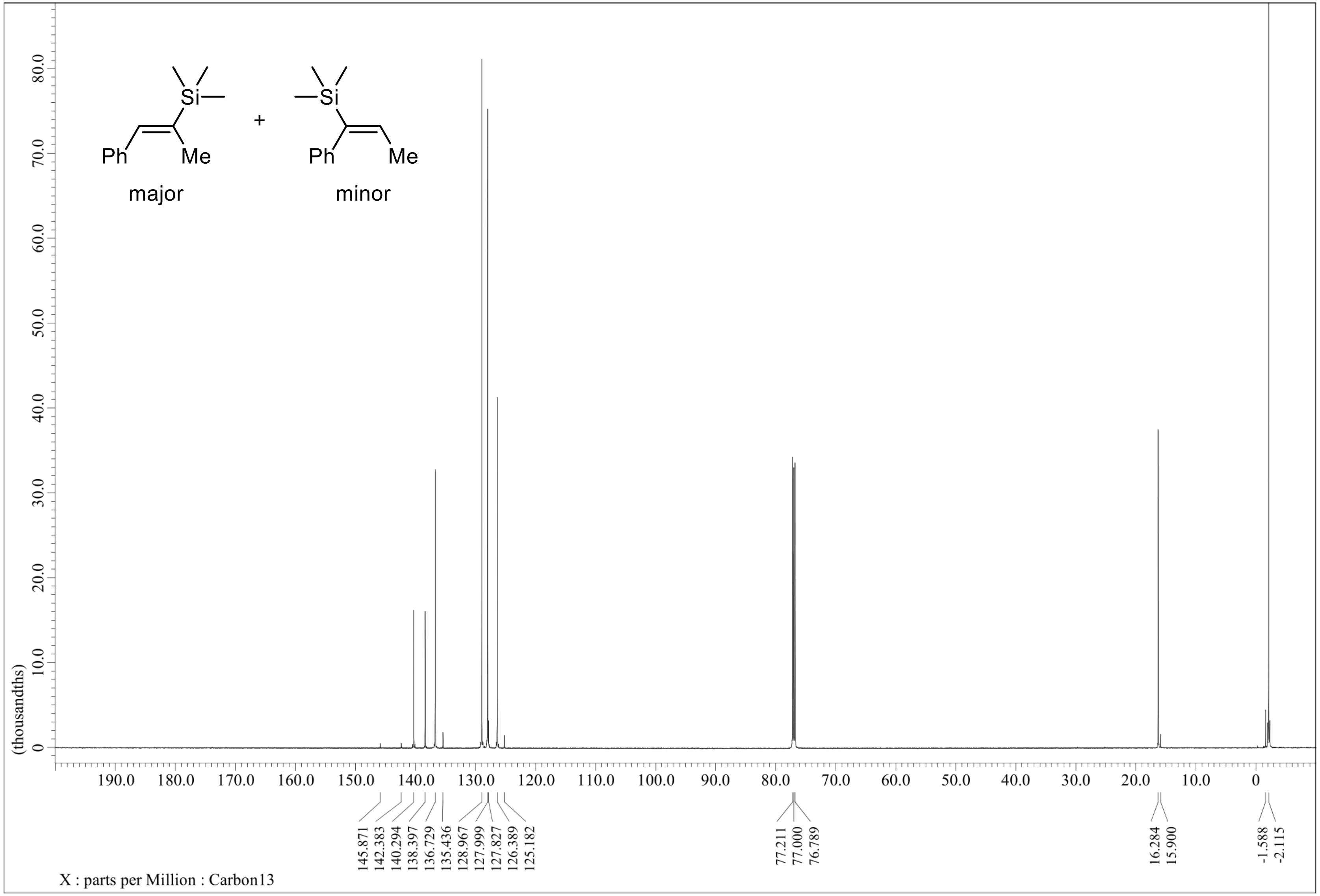

Figure S56. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3n** (using PCy_3)

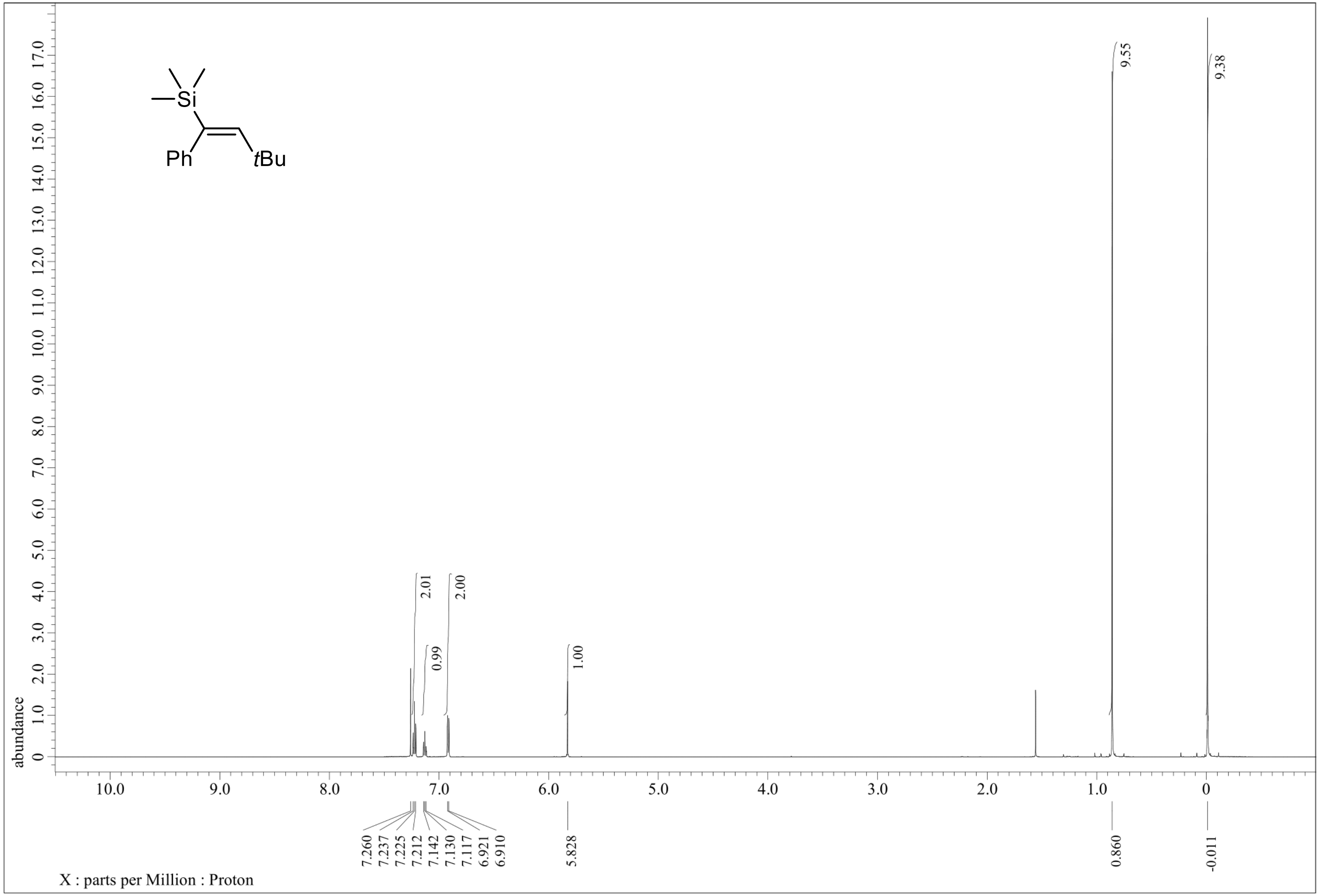

Figure S57. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3o**

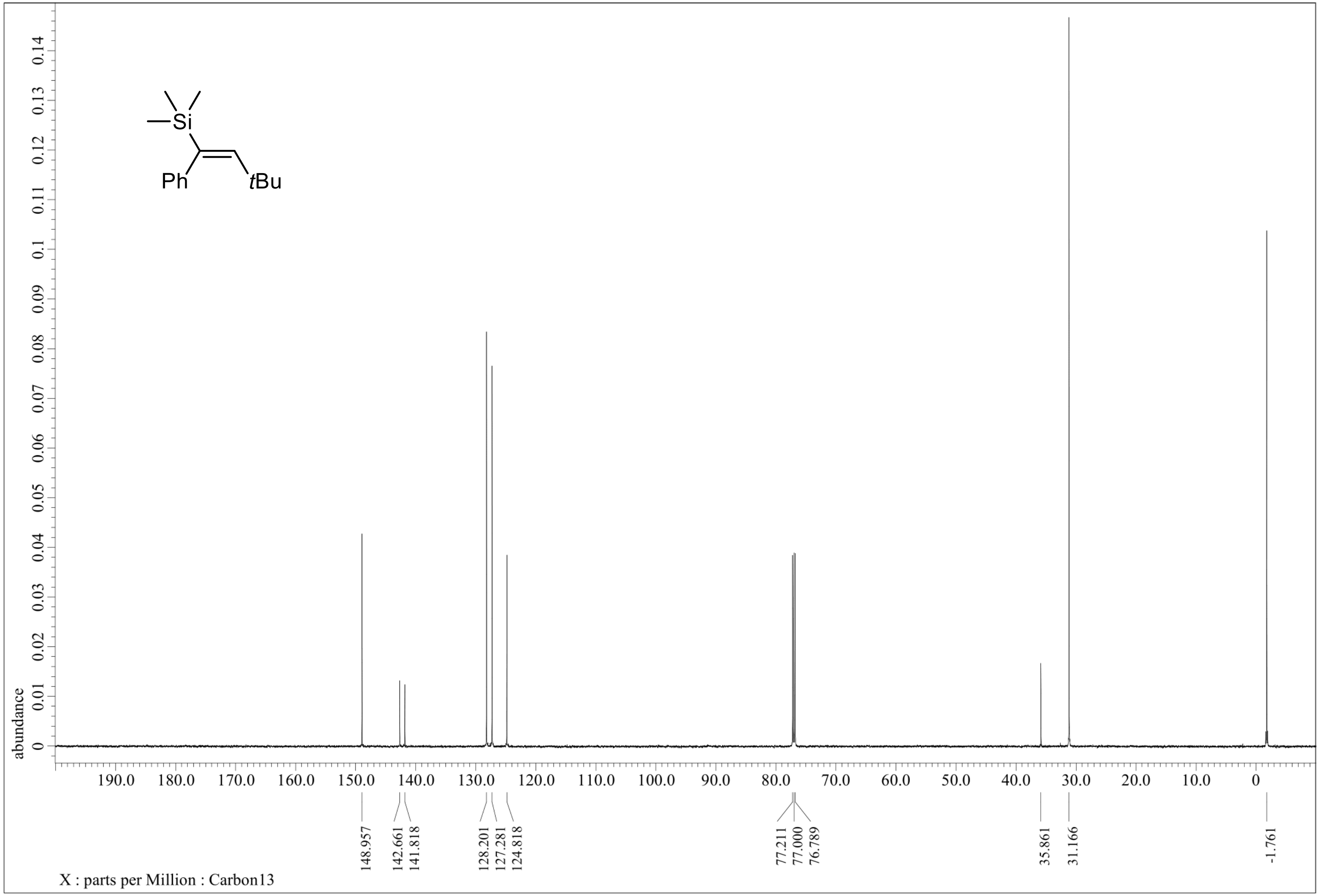

Figure S58. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3o**

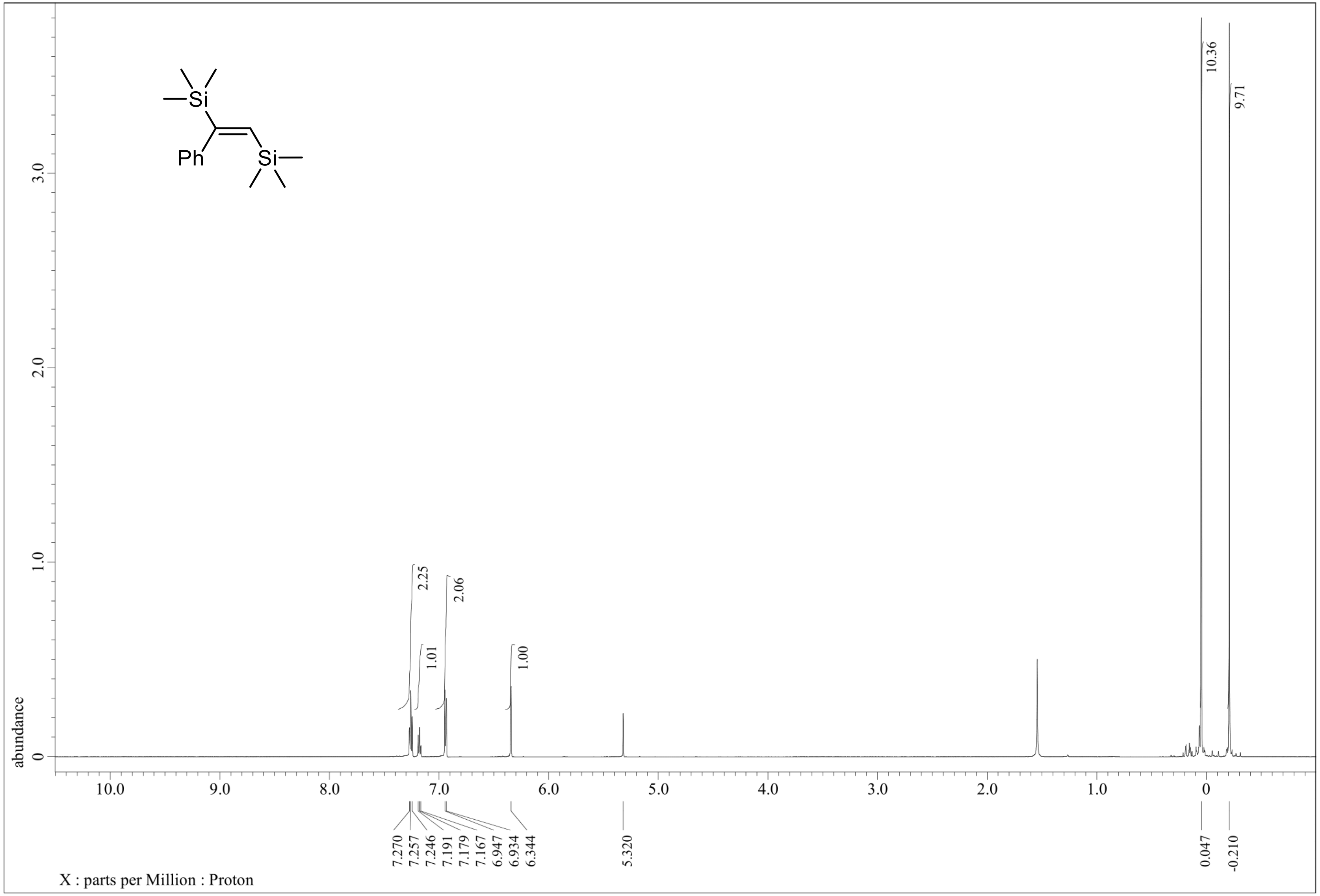

Figure S59. ^{1}H NMR (600 MHz, CD_2Cl_2) spectrum of **3p**

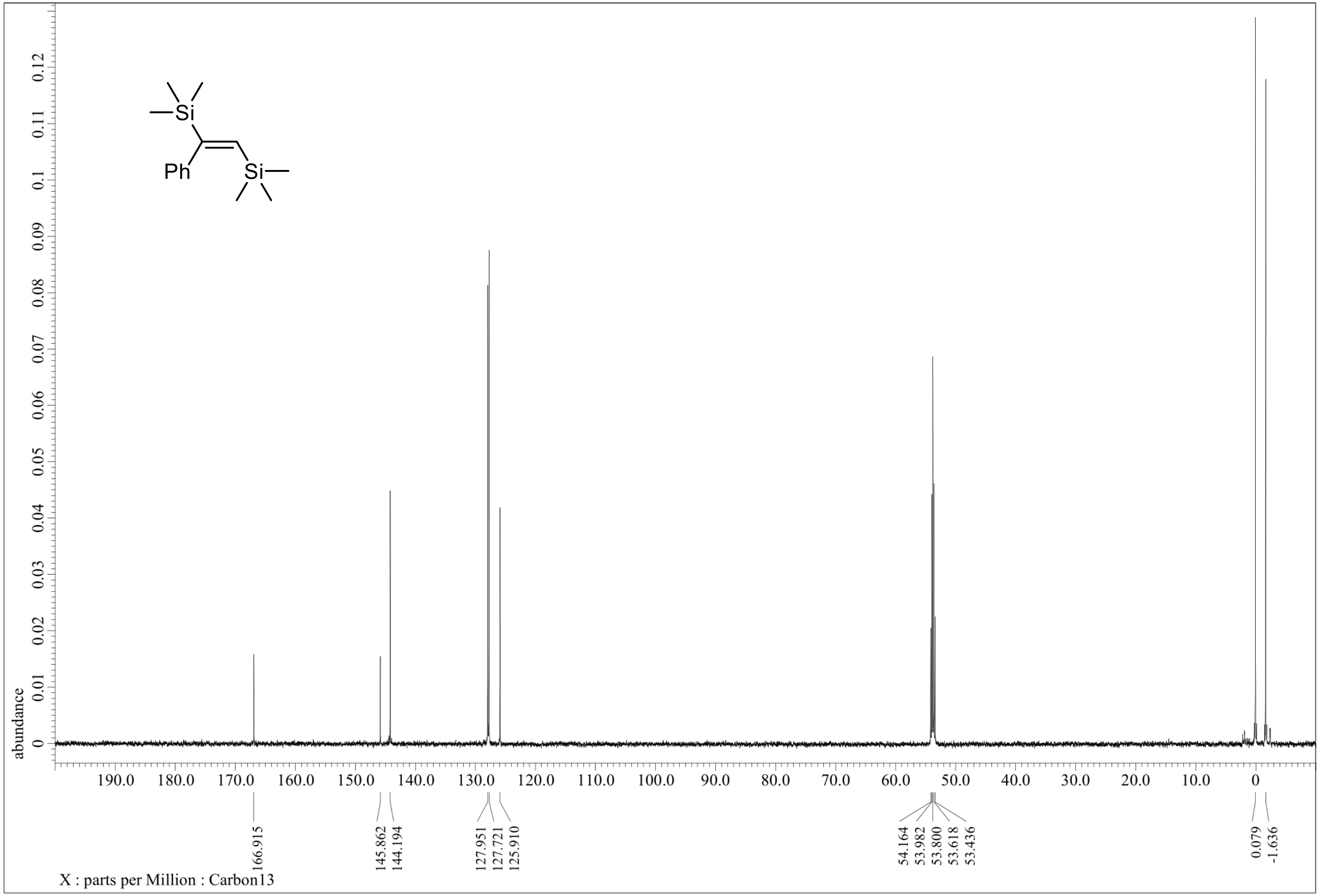

Figure S60. ^{13}C NMR (151 MHz, CD_2Cl_2) spectrum of **3p**

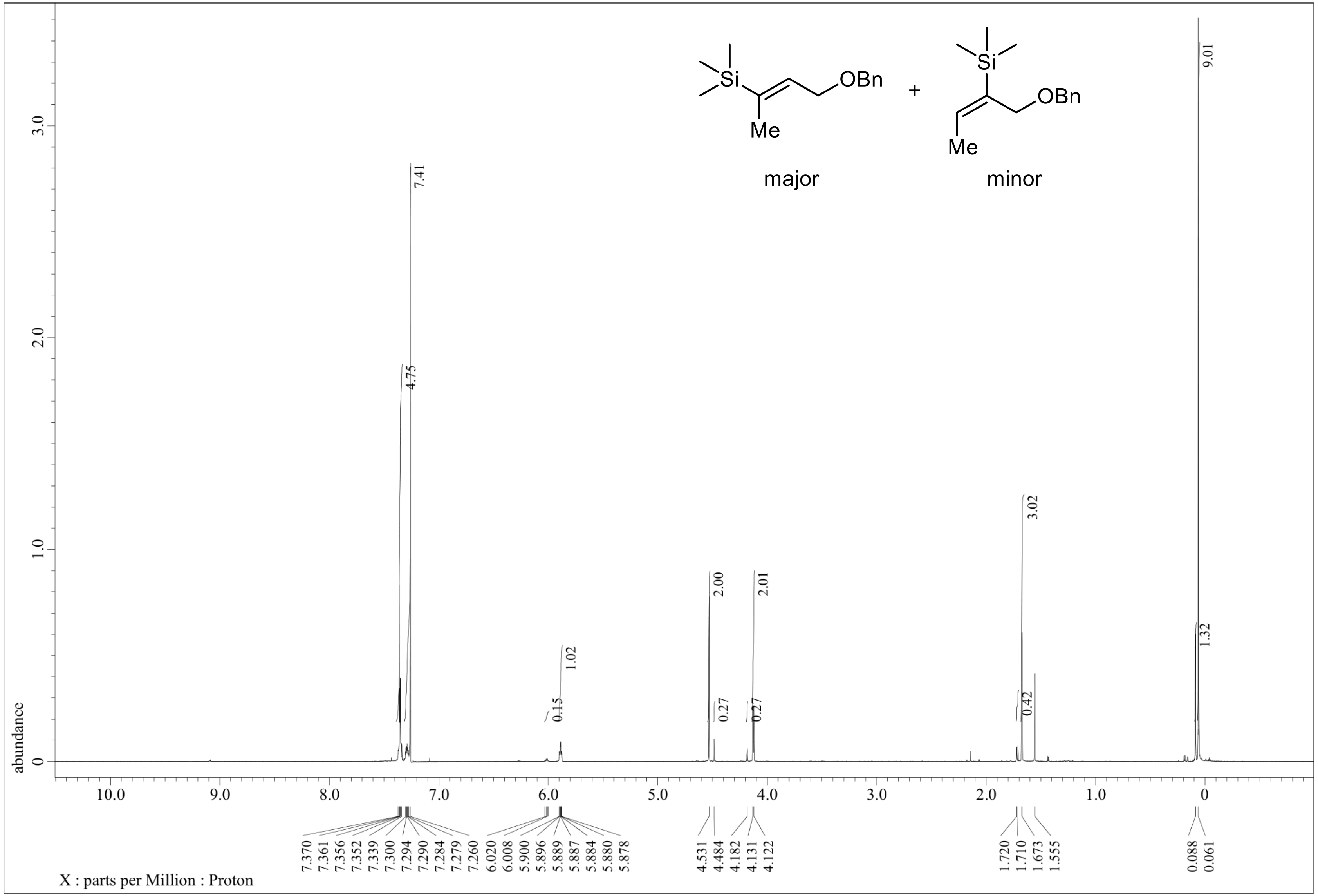

Figure S61. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3q**

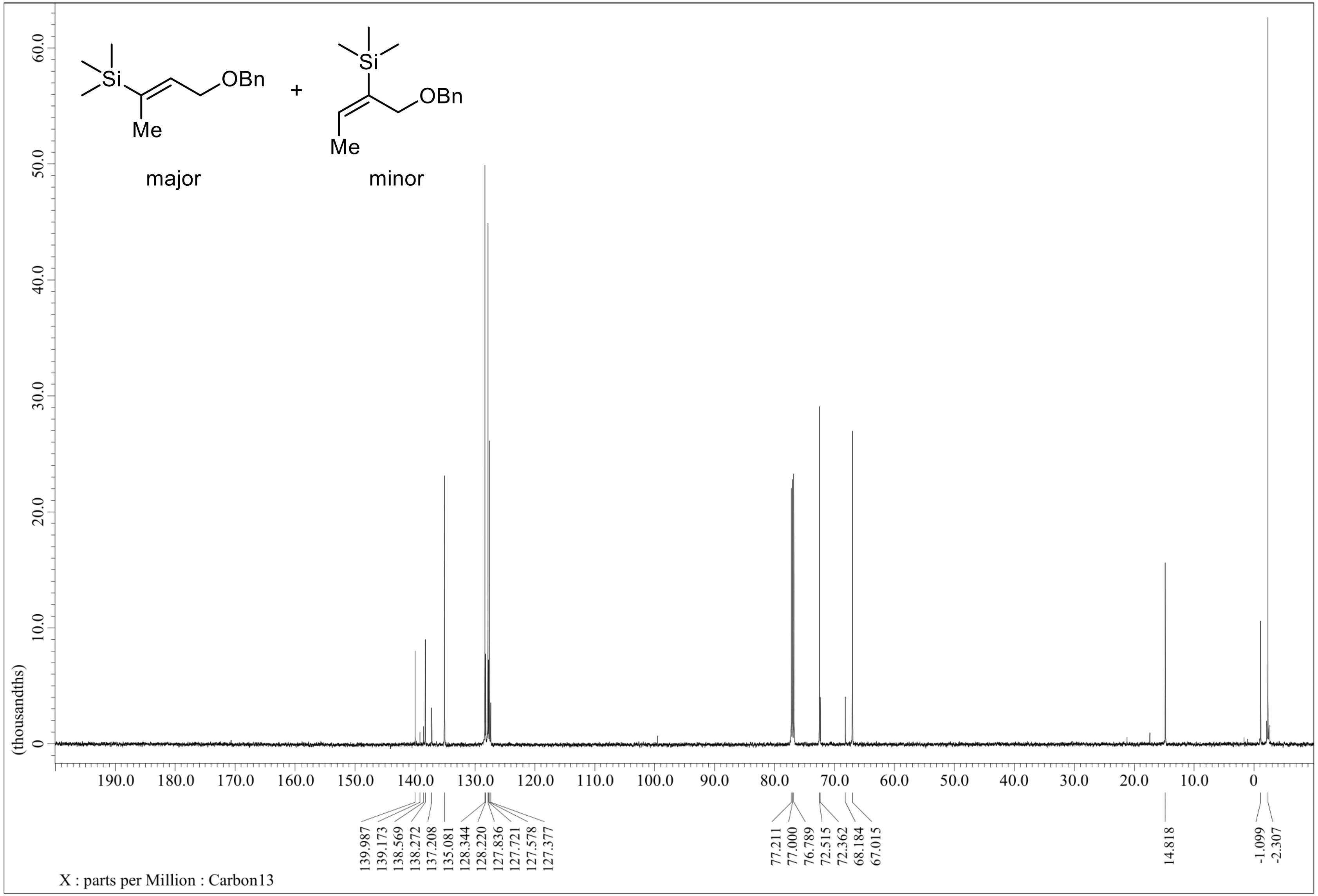

Figure S62. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3q**

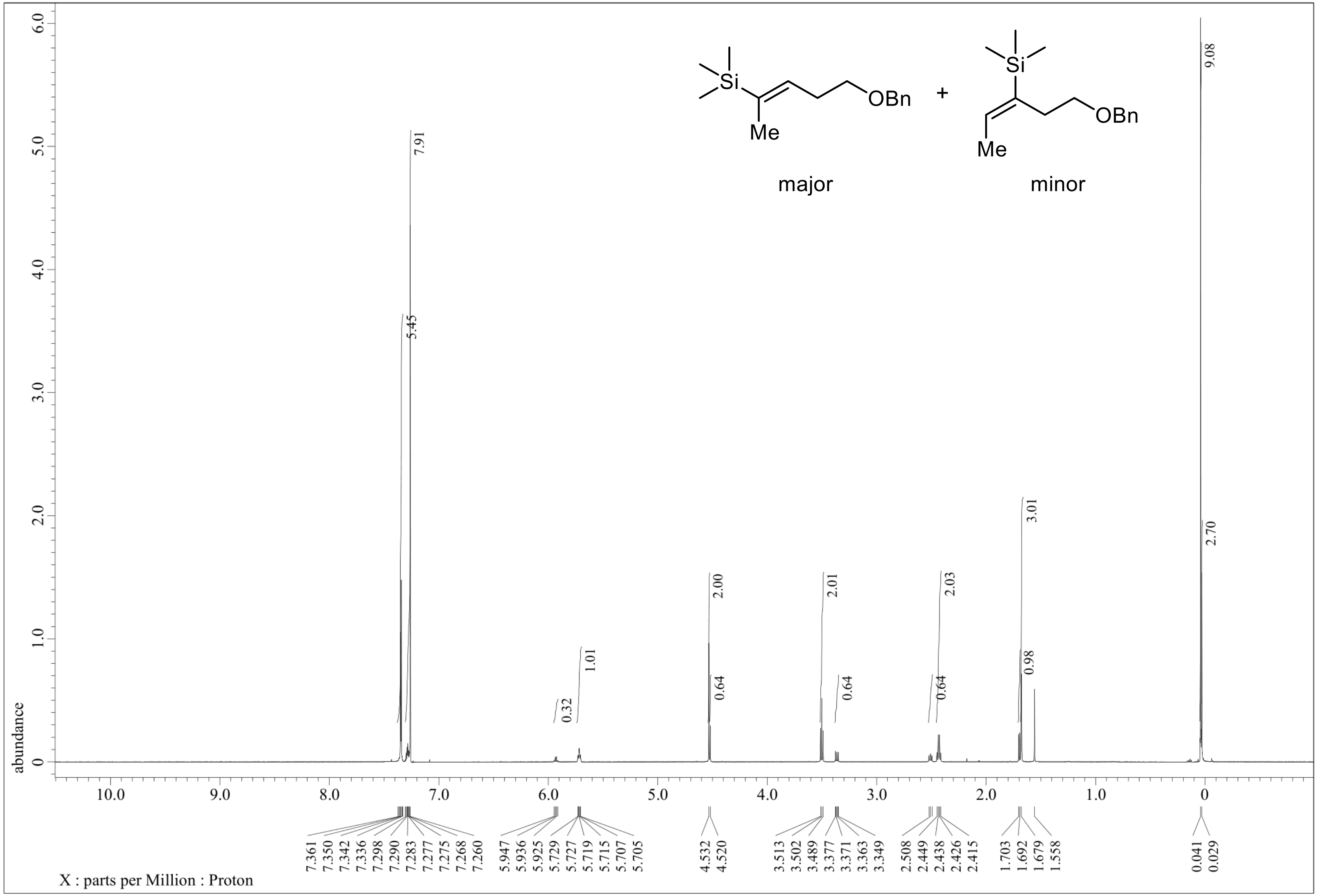

Figure S63. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3r**

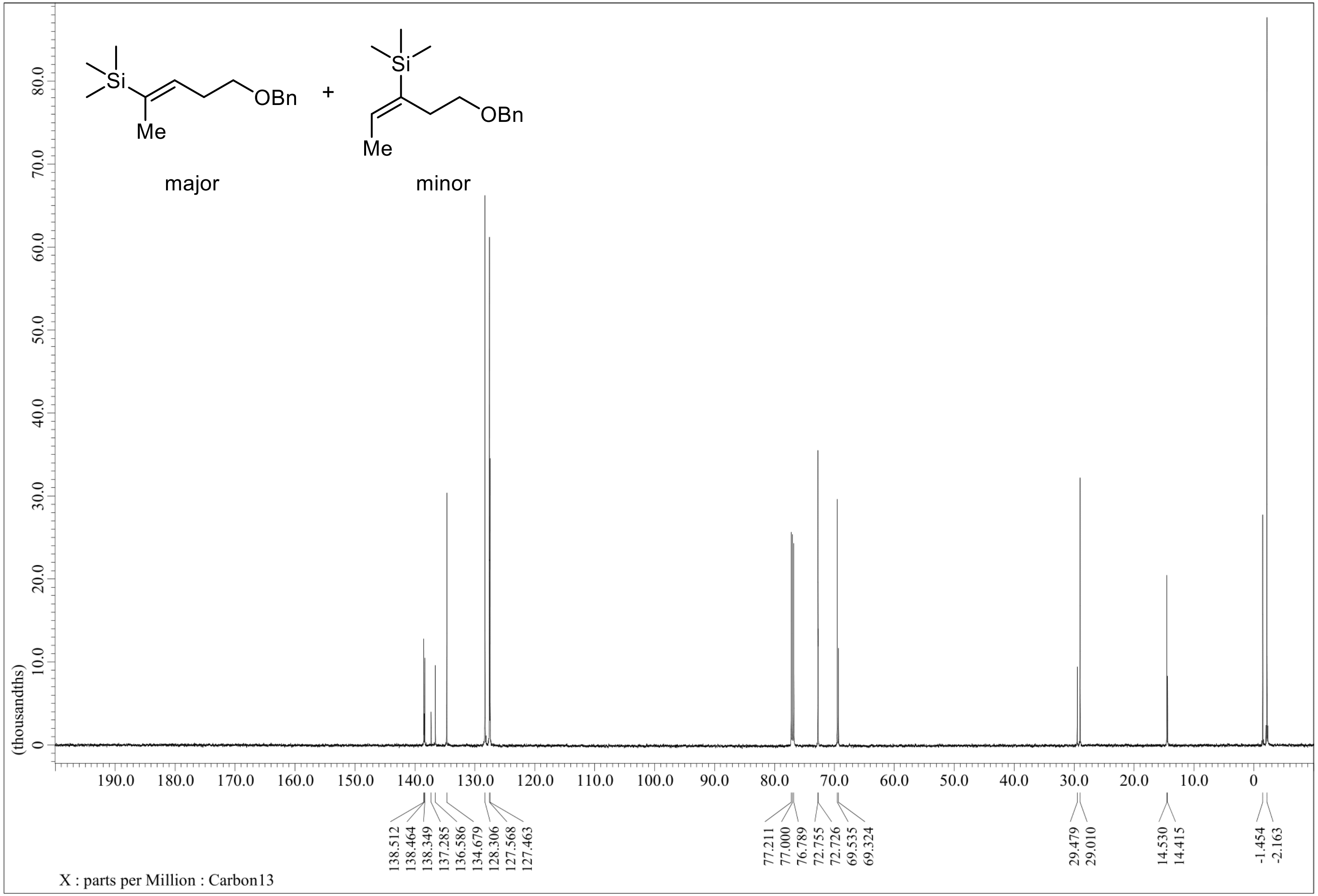

Figure S64. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3r**

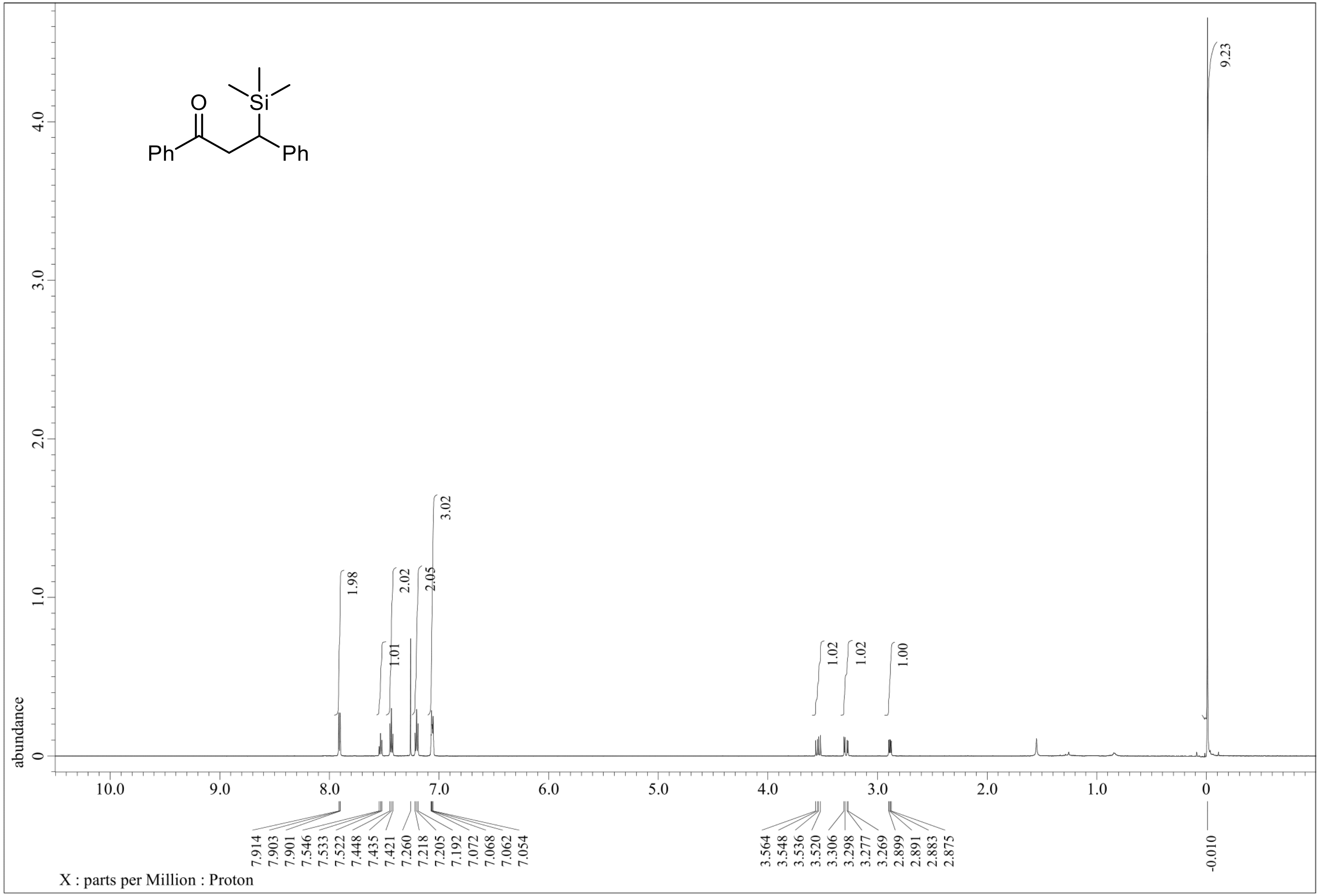

Figure S65. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3s**

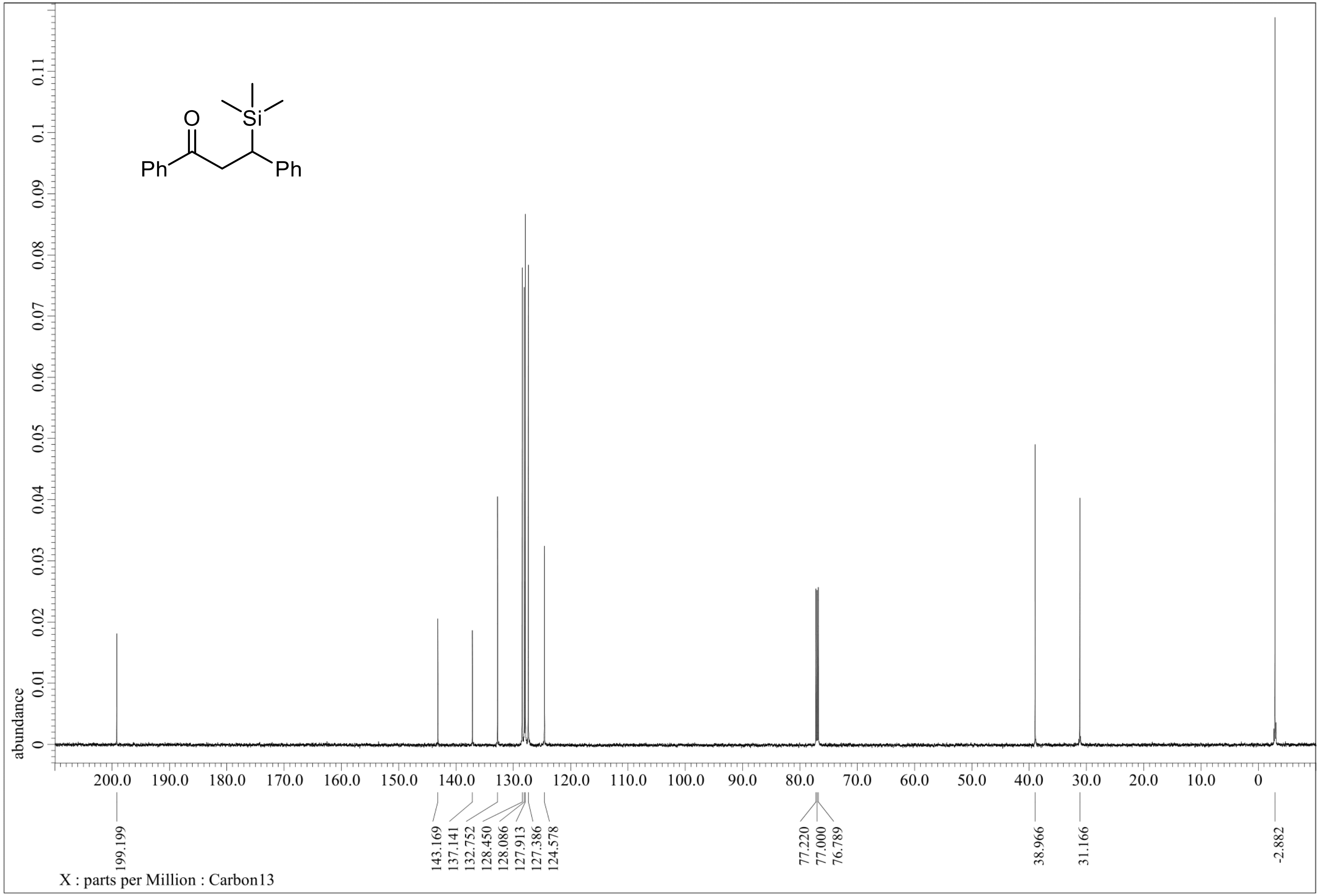

Figure S66. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3s**

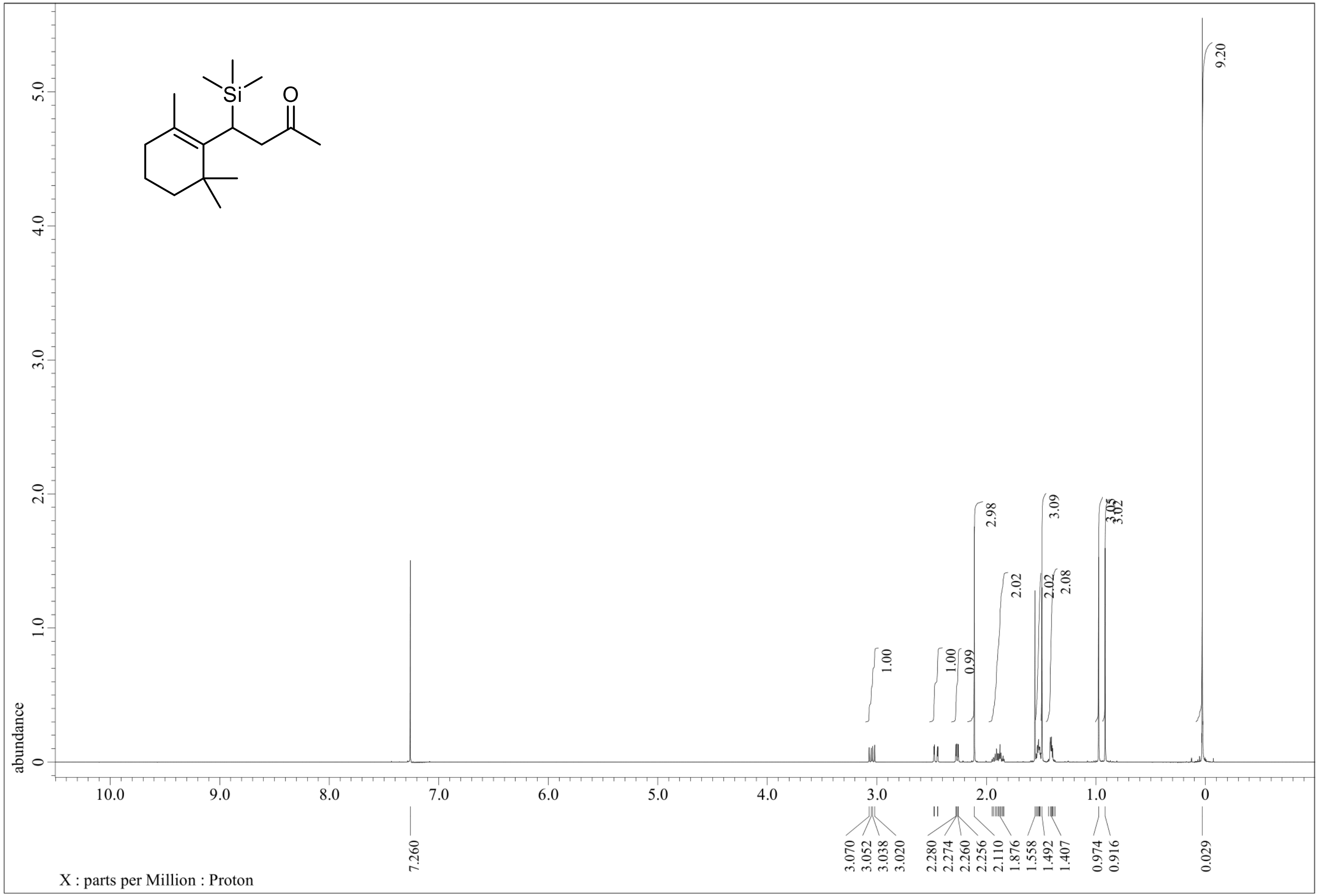

Figure S67. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3t**

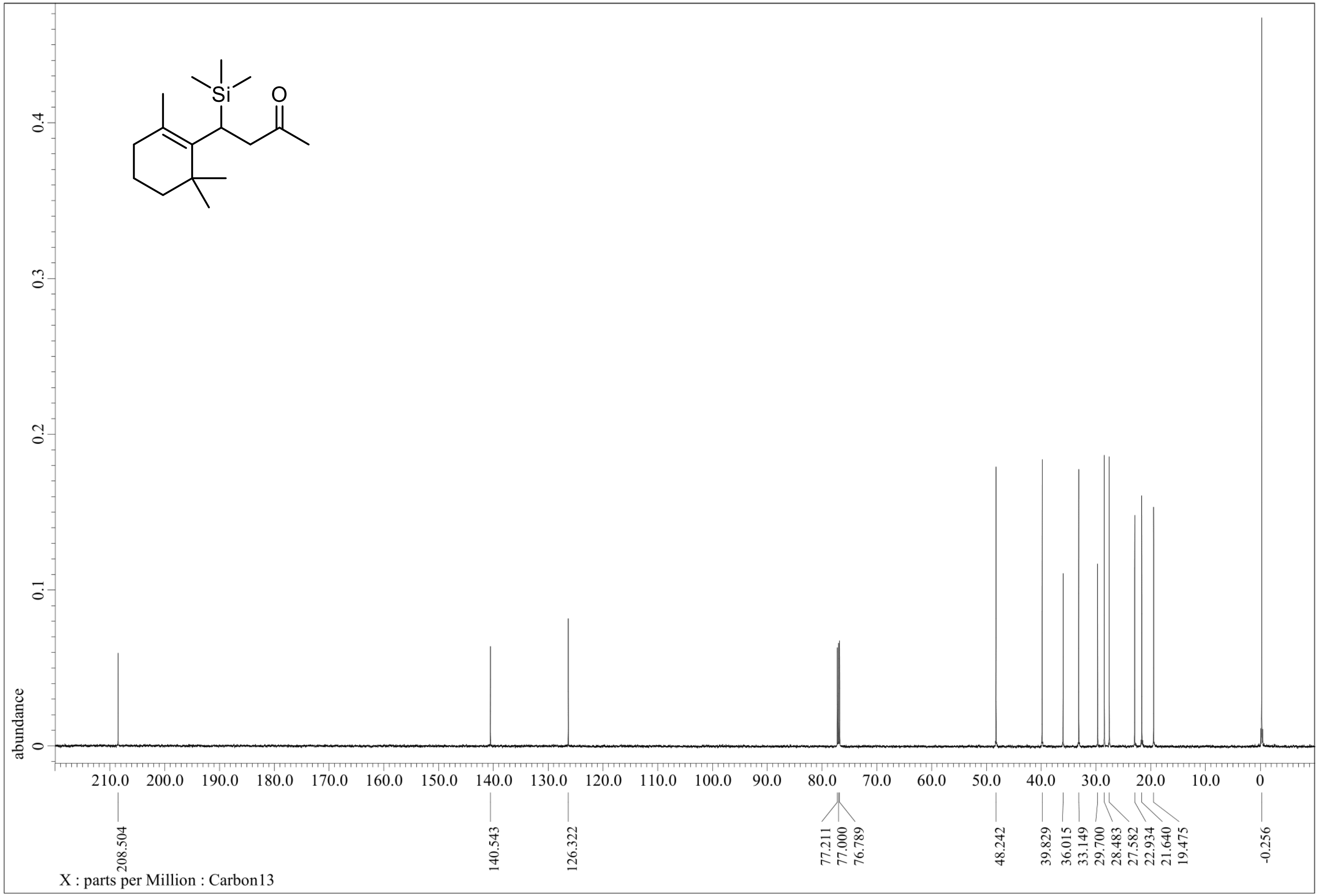

Figure S68. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3t**

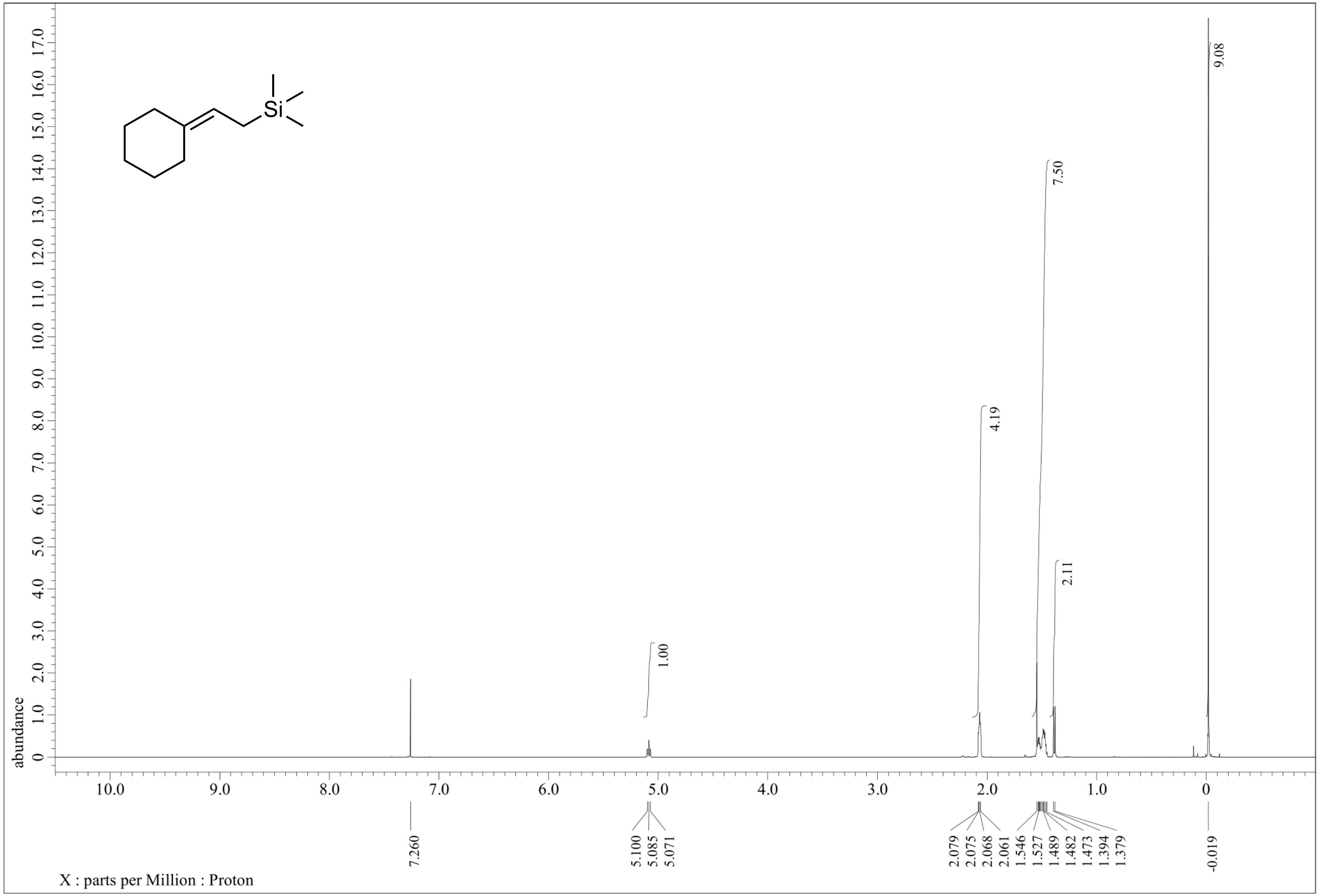

Figure S69. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3u**

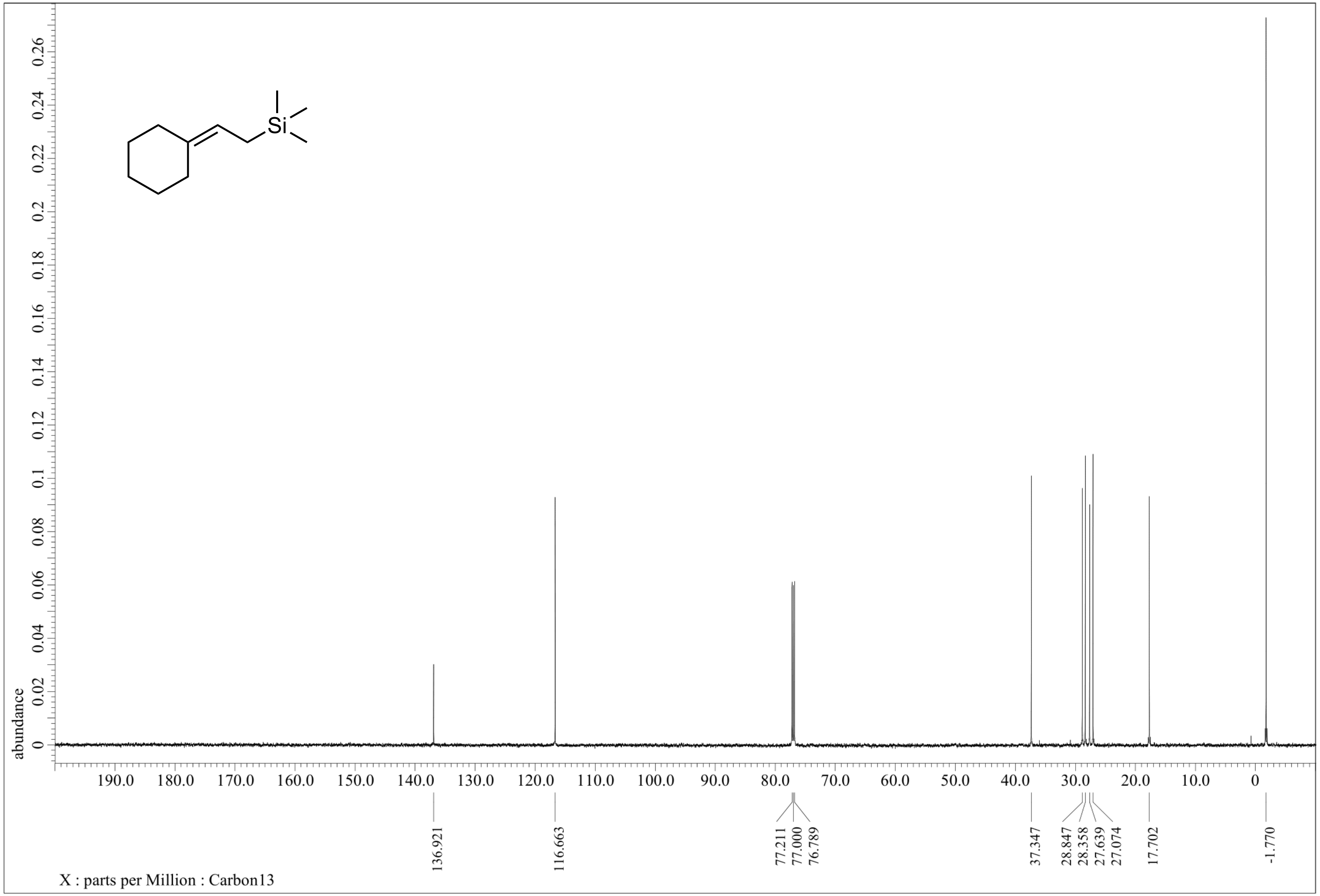

Figure S70. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3u**

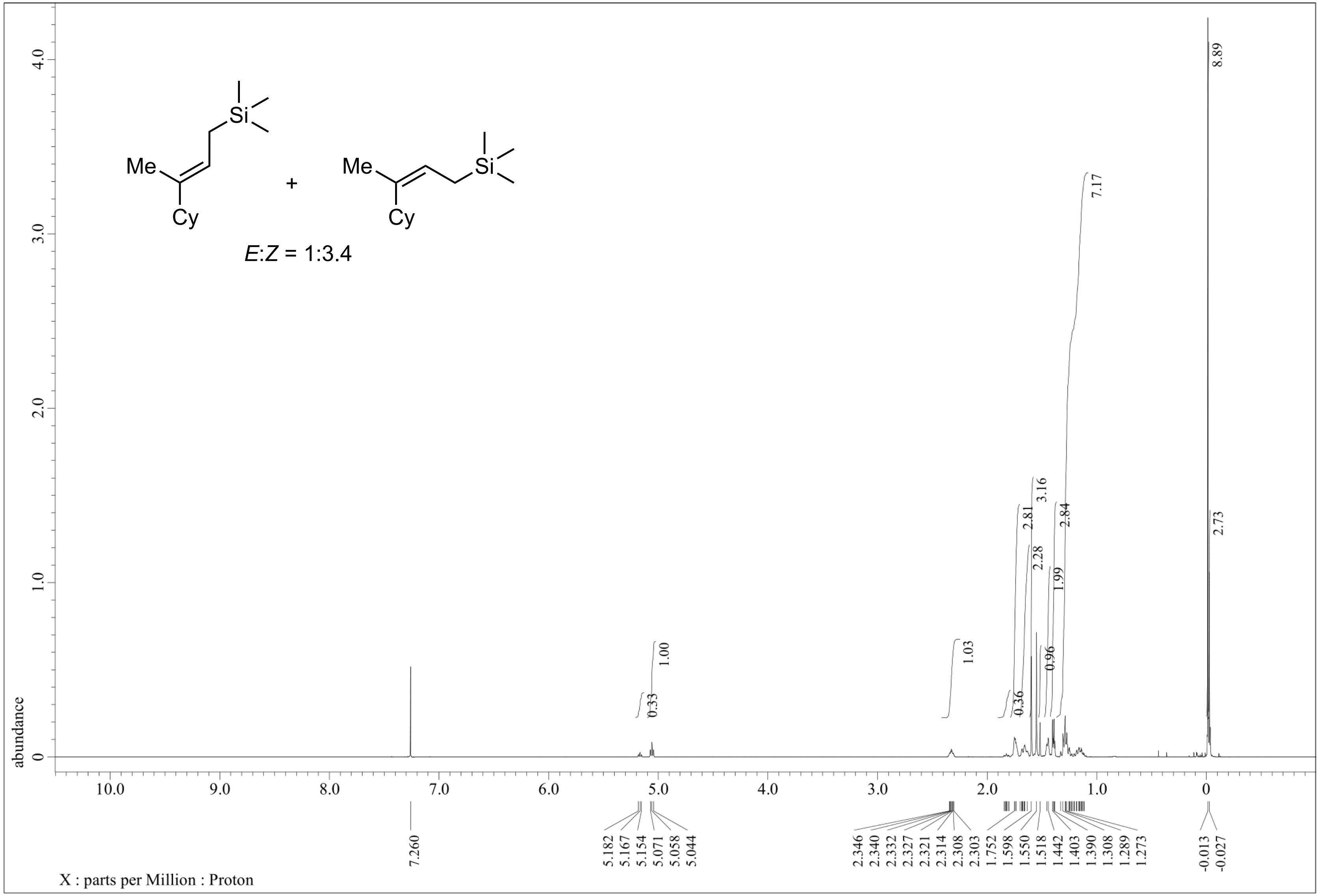

Figure S71. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3v**

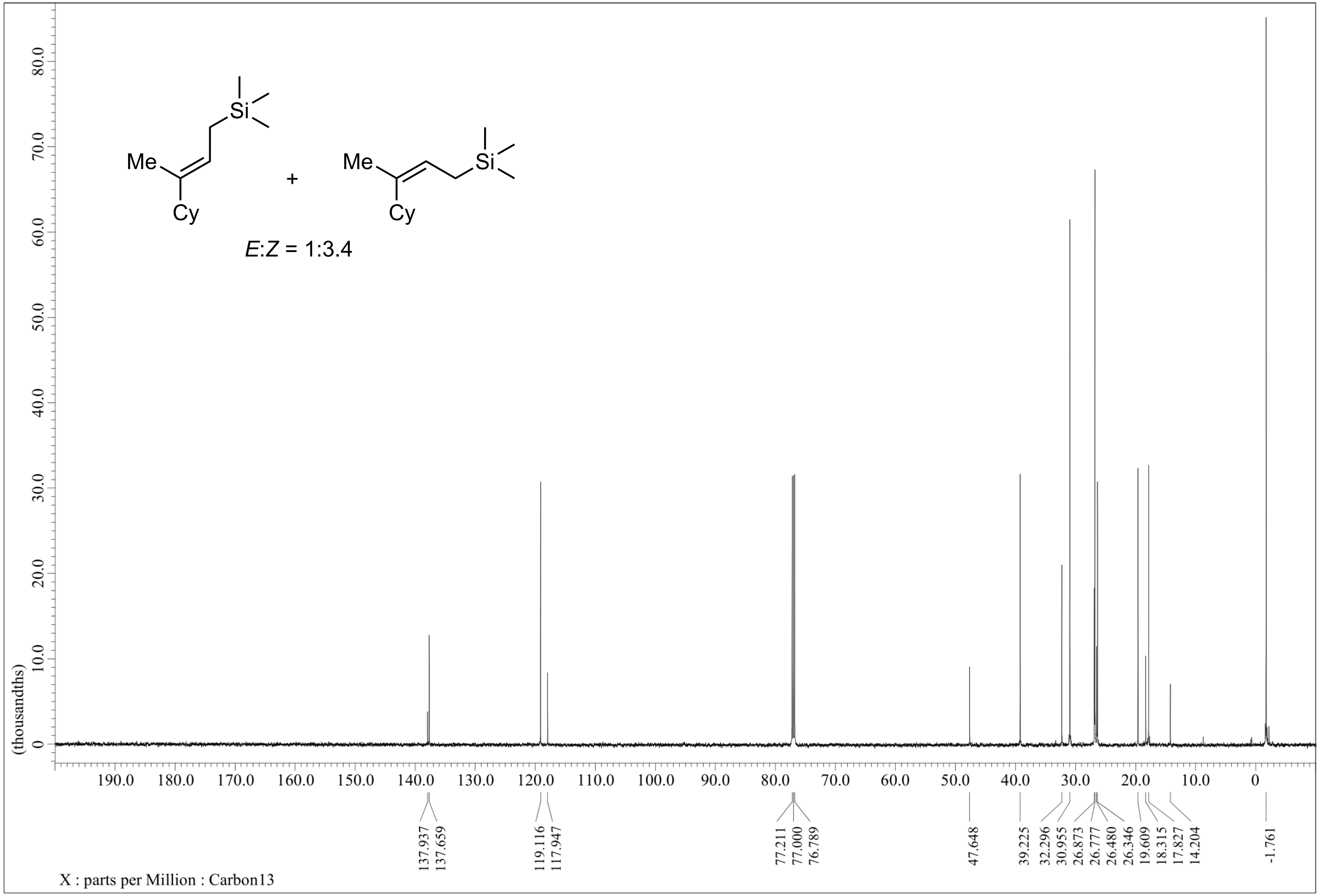

Figure S72. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3v**

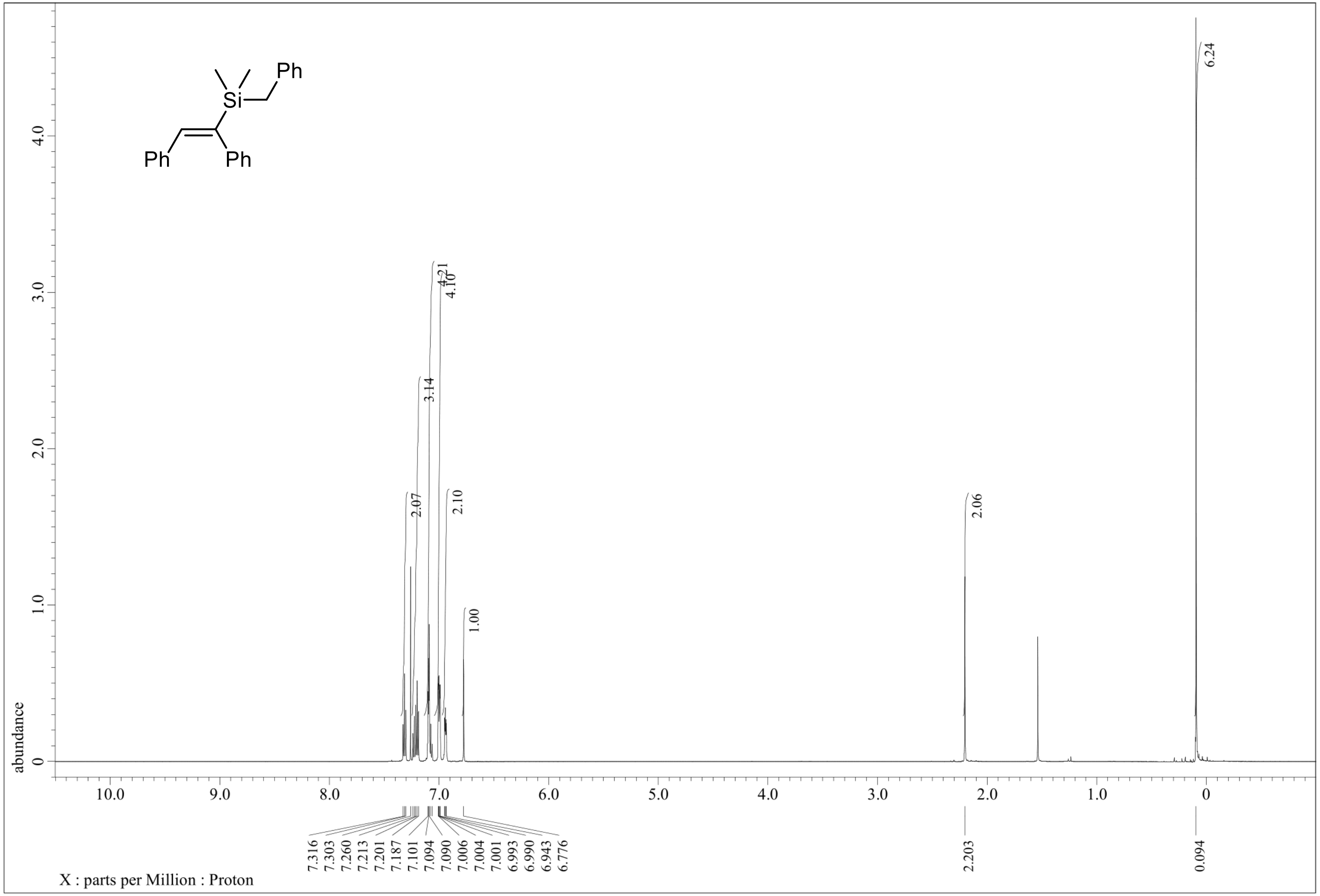

Figure S73. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3w**

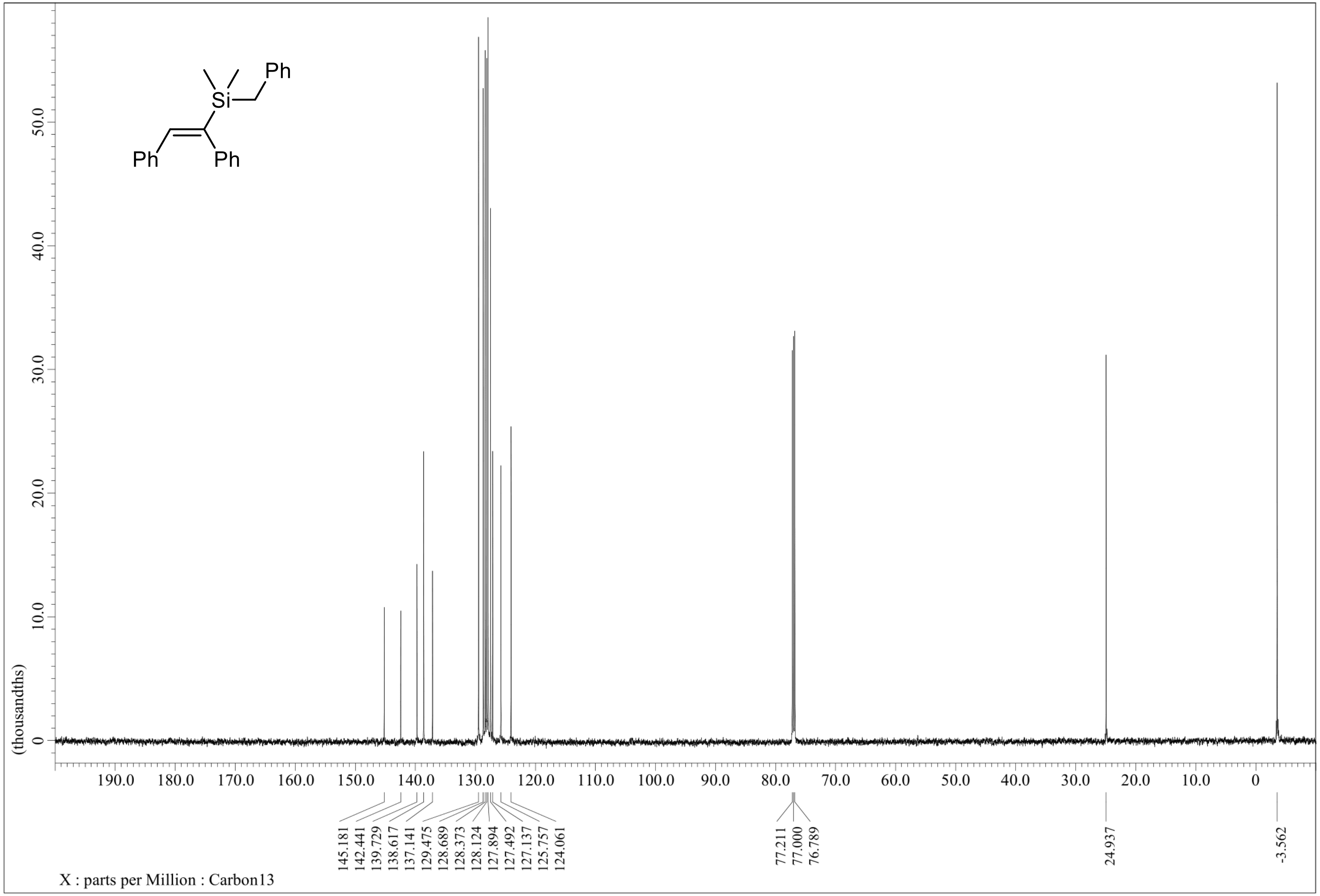

Figure S74. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3w**

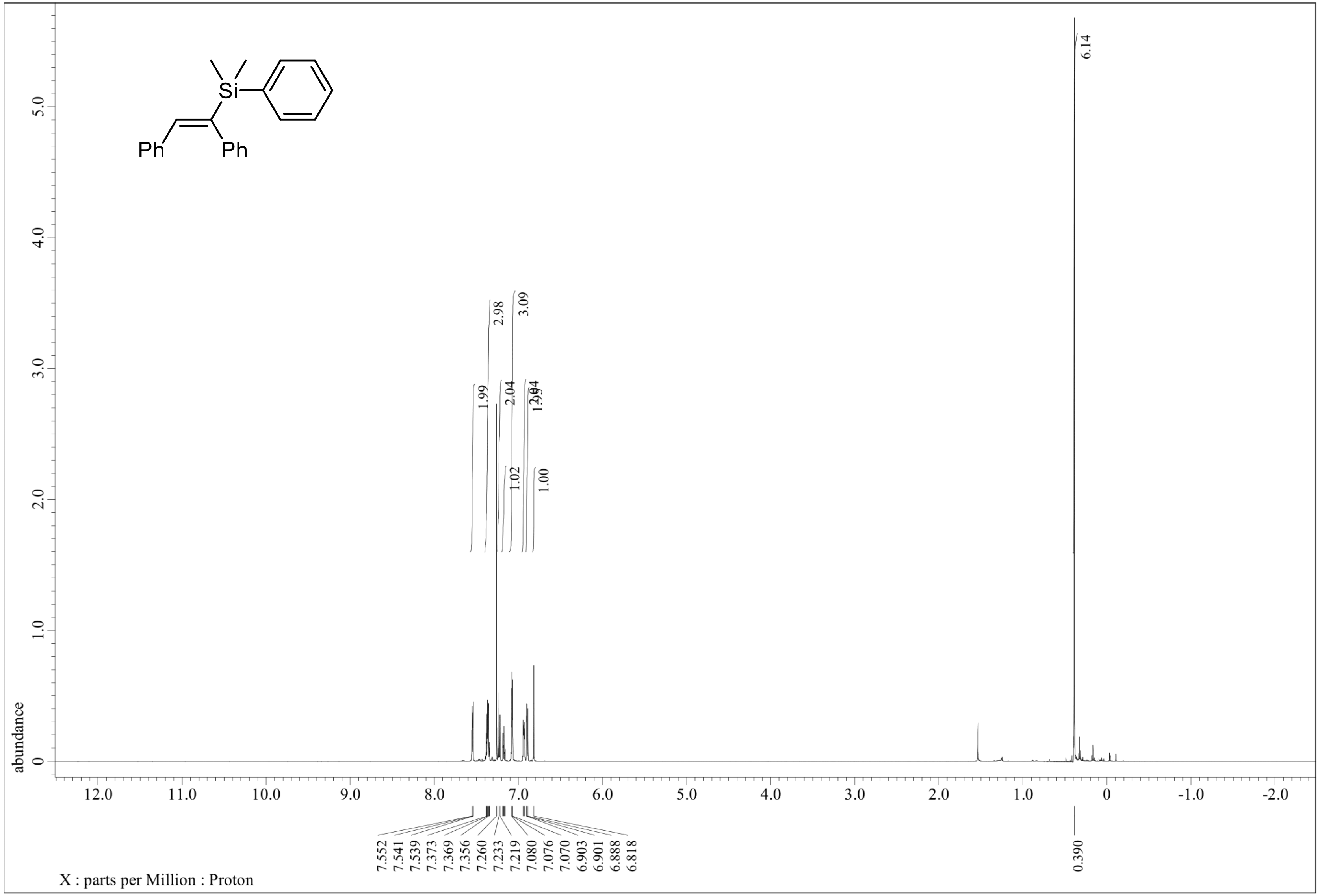

Figure S75. [1]H NMR (600 MHz, $CDCl_3$) spectrum of **3x**

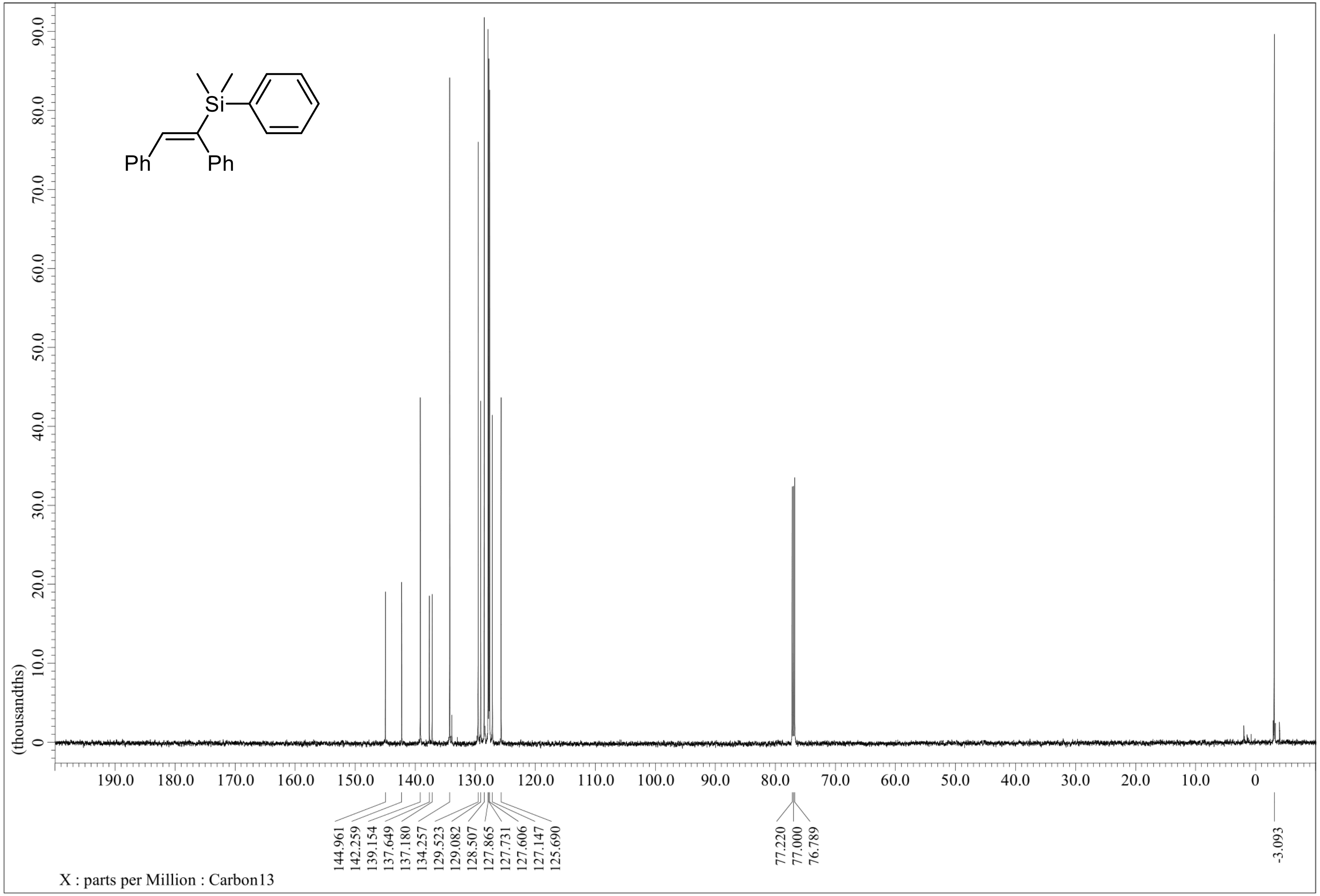

Figure S76. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3x**

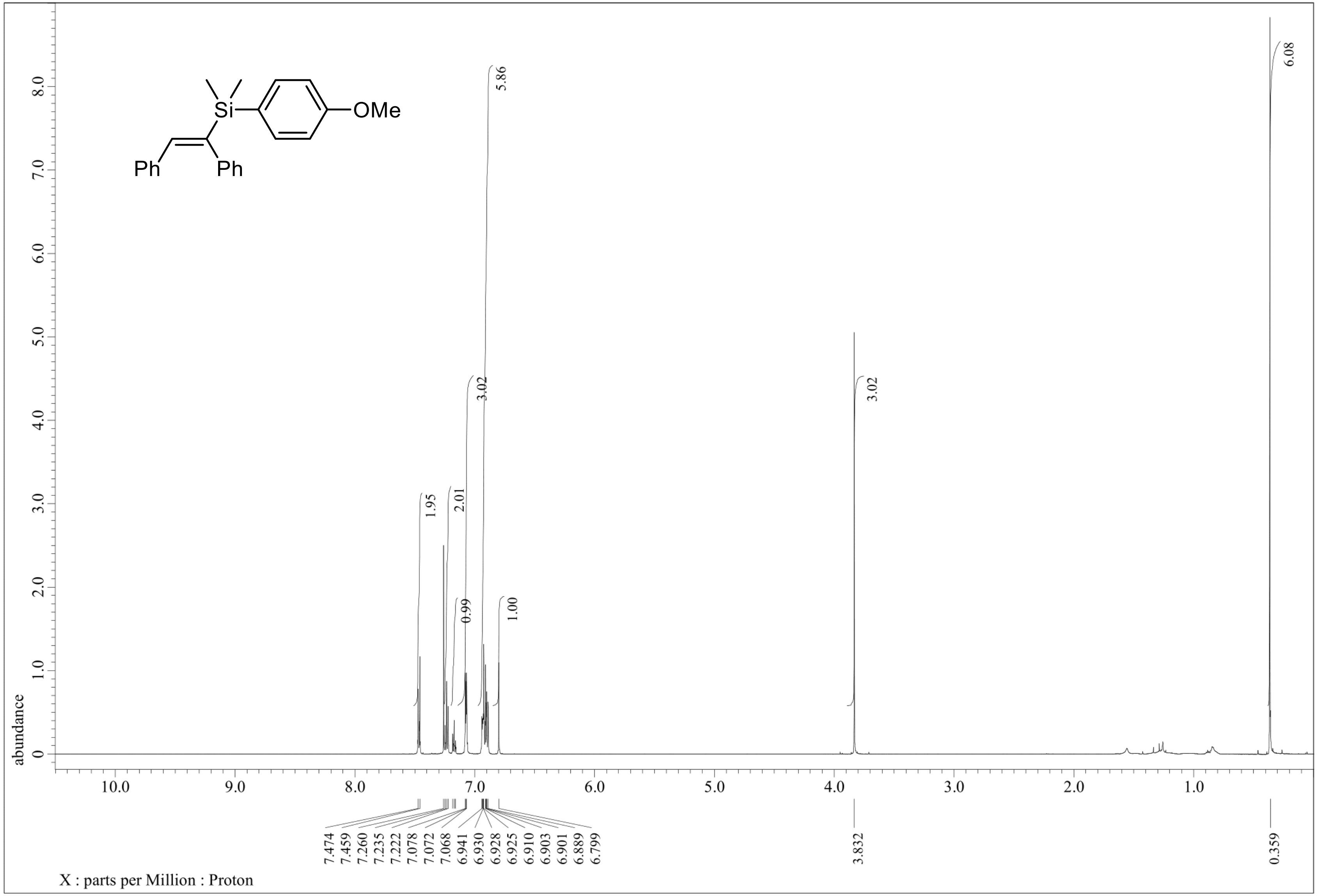

Figure S77. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3y**

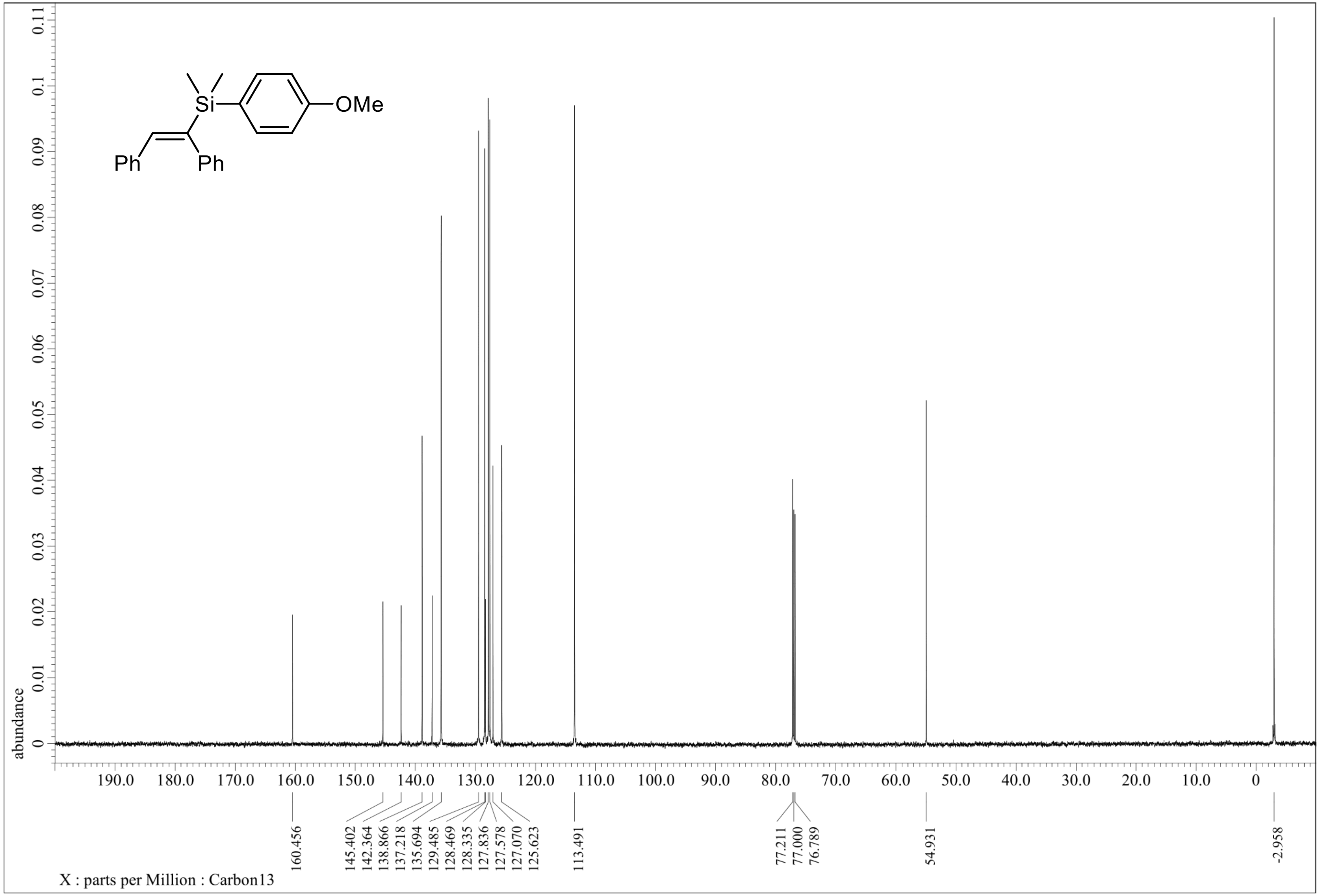

Figure S78. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3y**

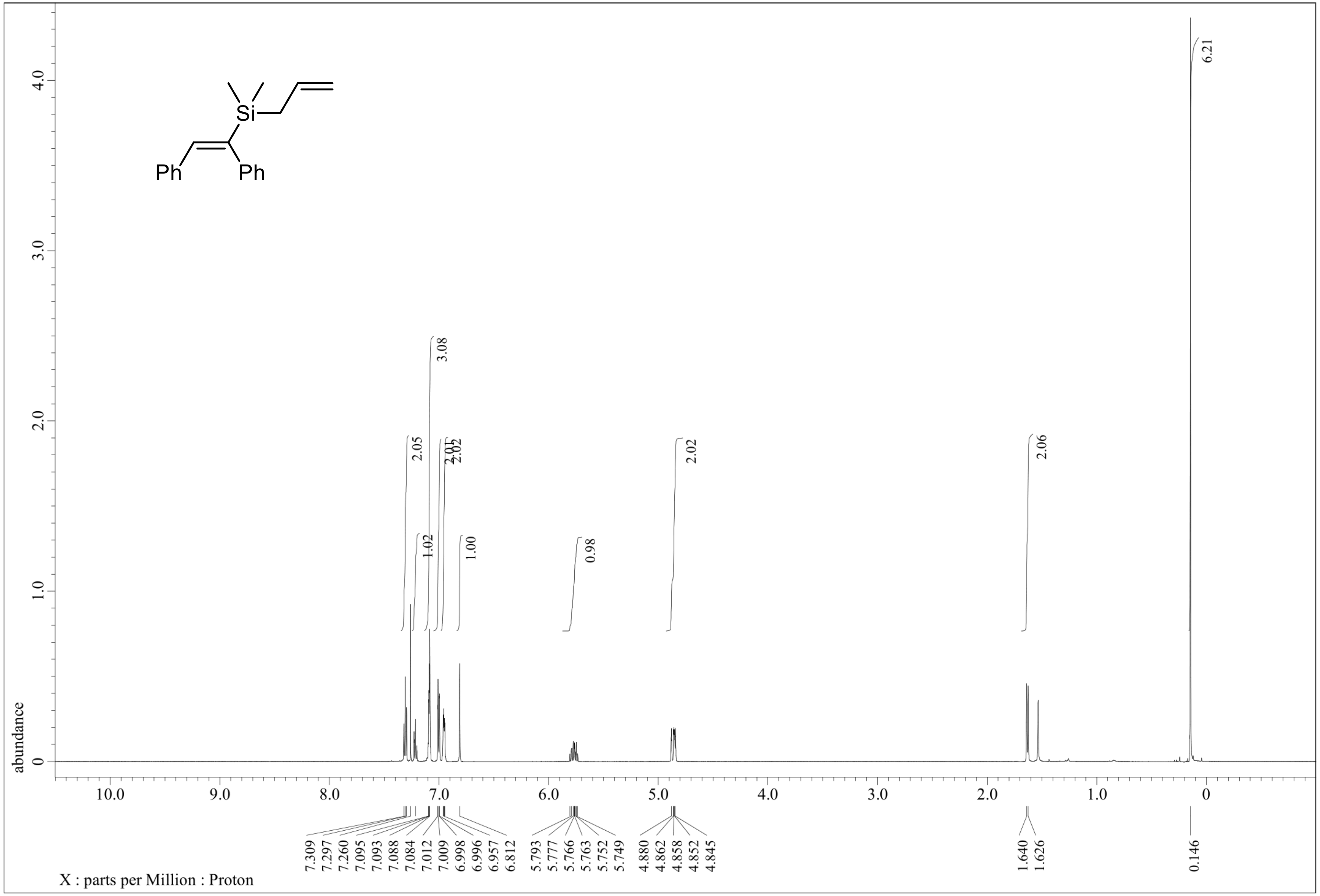

Figure S79. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3z**

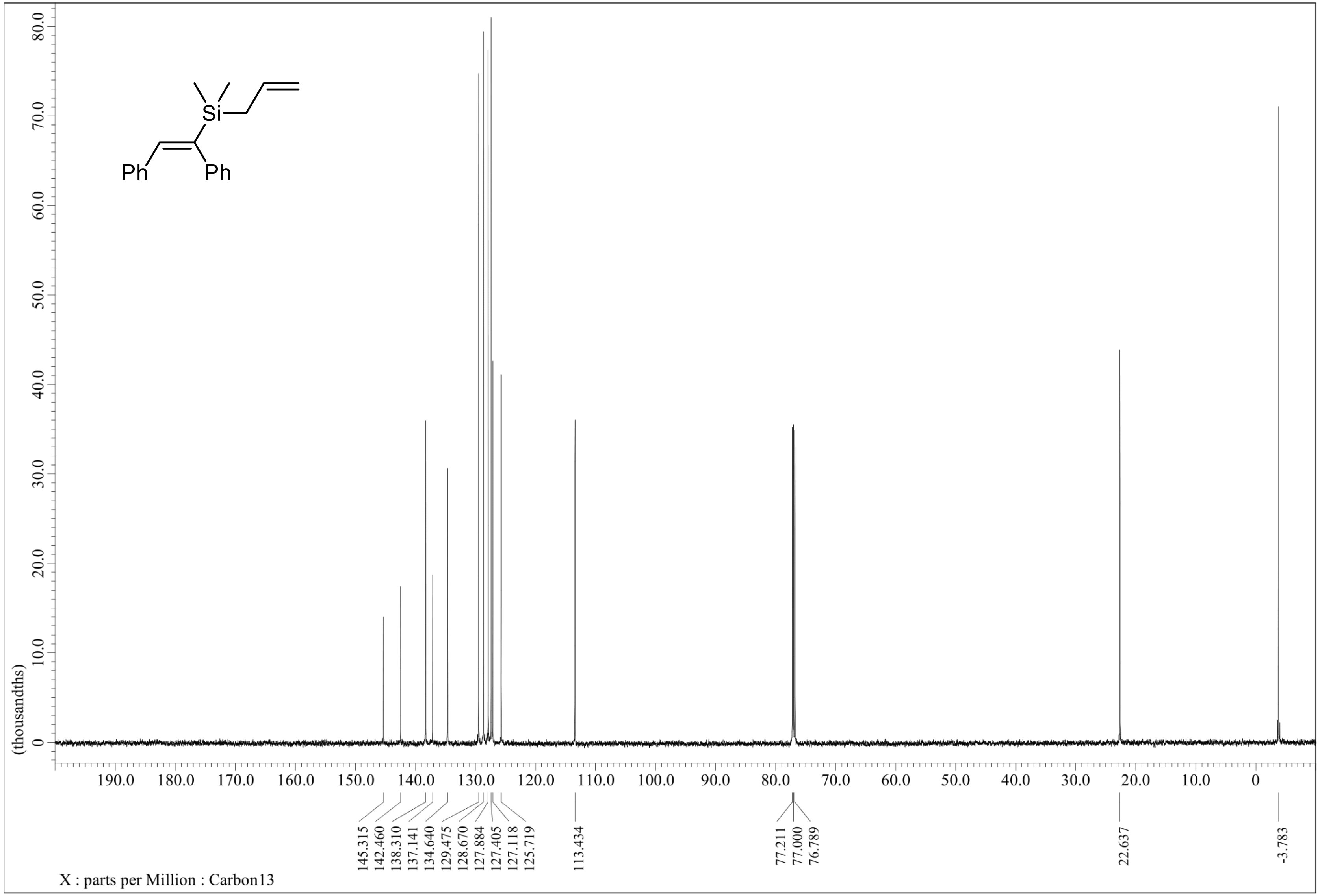

Figure S80. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3z**

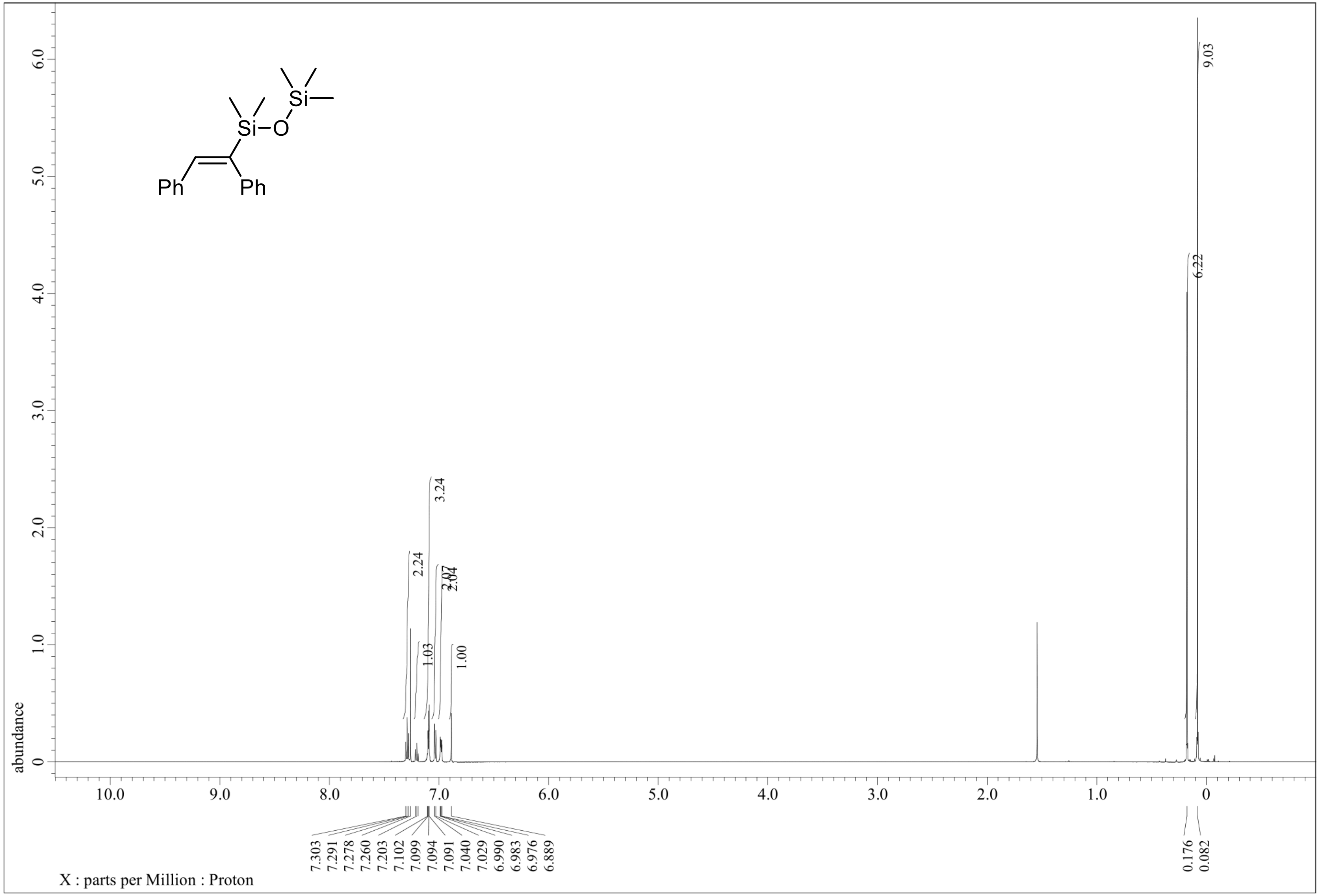

Figure S81. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of **3aa**

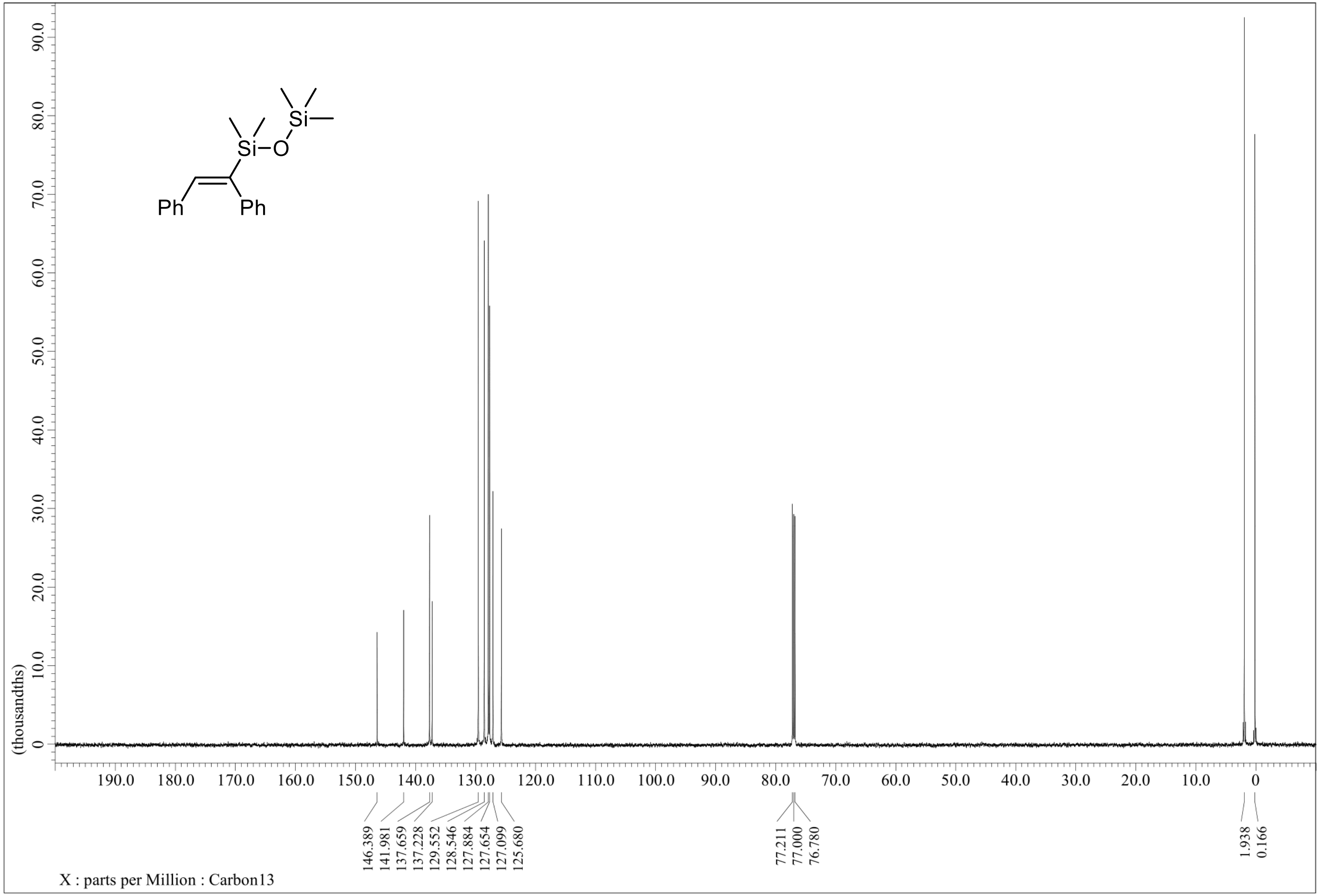

Figure S82. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of **3aa**