Supporting Information

for

C(sp^3)–F, C(sp^2)–F and C(sp^3)–H bond activation at silicon(II) center

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Contents

❖ General Experimental Information

All manipulations were carried out in an inert atmosphere of argon using standard Schlenk techniques and in argon filled glove box. Solvents were purified by MBRAUN solvent purification system MB SPS-800.The starting material, [PhC(N*t*Bu)$_2$SiN(Si(CH$_3$)$_3$)$_2$] (**1**) was prepared by using literature procedure.[S1] Chemical purchased from Sigma Aldrich and TCI Chemicals were used without further purification. ^{1}H, ^{13}C, ^{29}Si and ^{19}F NMR spectra were recorded in $CDCl_3$ using a Bruker Avance DPX 200, Bruker Avance DPX 400 or a Bruker Avance DPX 500 spectrometer referenced to external $SiMe_4$, in the case of ^{1}H, ^{13}C and ^{29}Si NMR and $CFCl_3$ for the ^{19}F NMR spectra, respectively. Elemental analyses were performed by CSIR-National Chemical Laboratory, Pune. Melting points were measured in a sealed glass tube on a Stuart SMP-30 melting point apparatus. MALDI-TOF MS spectrum was recorded using DHB (2,5-dihydroxybenzoic acid) as the inert matrix on AB SCIEX MALDI TOF/TOF™ 5800.

❖ Synthesis of [PhC(N*t*Bu)$_2$]Si(F)N(Si(CH$_3$)$_3$)$_2$ (OC(Ph)=CF$_2$) (2)

A toluene (10 mL) solution of trifluoromethylacetophenone (0.083 g, 0.47 mmol) was added drop by drop to a toluene (10 mL) solution of **1** (0.2 g, 0.47 mmol) at room temperature and stirred overnight. The solvent was removed under reduced pressure and extracted with *n*-hexane (15 mL).The *n*-hexane was reduced *in vacuo* to about 5 mL and kept at room temperature for one day to obtain colourless crystals of **2**. Yield: 0.266 g (92.1 %). Mp: 128.9 °C Anal. Calcd. for $C_{29}H_{46}F_3N_3OSi_3$: C, 58.64; H, 7.81; N, 7.07. found: C, 56.83; H, 7.05; N, 6.90. Due to the sensitivity of the crystals the experimental values deviate from the calculated ones. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 0.10 (s, 18H, (Si*Me*$_3$)$_2$), 0.94 (s, 18H, *t*Bu), 7.14-7.38 (m, 10H, *Ph*) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$, 25 °C); δ 1.19 (Si*Me*$_3$), 5.64 (Si*Me*$_3$), 31.54 (*t*Bu), 54.27 (*t*Bu), 134.34 (*C*F$_2$), 114.69, 114.87, 115.05, 115.25, 127.68, 127.68, 128.09, 128.58, 129.90, 133.68, 151.25, 154.03 (*Ph*), 156.86 (*C*(O)Ph), 172.79 (N*C*N) ppm; ^{19}F NMR (376.63 MHz, $CDCl_3$, 25 °C) δ –93.76 (s, 1F, Si–*F*), –102.32 (d, , *J*= 75.32, 1F, C*F*$_2$), –117.76 (d, *J*=

75.32 Hz, 1F, CF_2) ppm; ^{29}Si{^{1}H}NMR (79.53 MHz, $CDCl_3$, 25 °C): δ 3.80 (SiN(*Si*Me$_3$)$_2$), –107.06 (d, *J*=236.71Hz, Si–F) ppm.

❖ **Synthesis of [PhC(N*t*Bu)$_2$]Si(H)N(Si(CH$_3$)$_3$)$_2$ (OC(Ph)=CH$_2$) (3)**

A toluene (10 mL) solution of acetophenone (0.057 g, 0.47 mmol) was added drop by drop to a toluene (10 mL) solution of **1** (0.2 g, 0.47 mmol) and stirred for 6 h. The solvent was removed under reduced pressure and the residue was extracted with *n*-hexane (10 mL) to yield **3** as a oily compound. Yield: 0.226 g (87.8 %). ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 0.19 (s, 18H, (Si*Me*$_3$)$_2$), 1.13 (s, 18H, *t*Bu), 4.44 (br, 1H, , C ═ C*H*$_2$), 4.75 (br, 1H, , C ═ C*H*$_2$), 5.17 (s, 1H, Si–*H*), 7.17-7.64 (m, 10H, *Ph*) ppm; ^{13}C NMR (125.76 MHz, $CDCl_3$, 25 °C); δ 5.08 (SiN(Si*Me*$_3$)$_2$), 32.02 (*t*Bu), 54.59 (*t*Bu), 88.95 (C=*C*H$_2$), 126.14, 127.59, 127.80, 128.32, 129.28, 129.44, 137.03, 139.87 (*Ph*), 157.44 (*C*(O)Ph), 166.63 (N*C*N) ppm; ^{13}C-DEPT NMR (125.76 MHz, $CDCl_3$, 25 °C); δ 4.73 (SiN(Si*Me*$_3$)$_2$), 31.82 (*t*Bu), –88.60 (C═*C*H$_2$), 125.79, 127.43, 127.53, 127.65, 127.71, 128.16, 129.12, 129.28 (*Ph*), ppm; ^{29}Si{^{1}H}NMR (79.53 MHz, $CDCl_3$, 25 °C): δ 2.59 (N(SiMe$_3$)$_2$),–81.12 (Si–H) ppm. HRMS (*m/z* %): 541.3 (100) [M]$^+$.

❖ **Synthesis of [PhC(NtBu)$_2$]Si(F)N(Si(CH$_3$)$_3$)$_2$ (C$_6$F$_5$) (4)**

A toluene (10 mL) solution of hexafluorobenzene (0.097 g, 0.52 mmol) was added drop by drop to a toluene (10 mL) solution of **1** (0.2 g, 0.47 mmol) and the resultant reaction mixture was stirred for 12h at 90 °C. The solvent was removed under reduced pressure and extracted with toluene (5 mL). Stored this solution at –30 °C in a freezer for 5 days afforded colourless crystals of **4**. Yield: 0.247g (85.4%). Mp: 148.3 °C. ^{1}H NMR (400 MHz, C_6D_6, 25 °C) δ 0.25 (s, 18H, (N(Si*Me*$_3$)$_2$), 0.86 (s, 9H, *t*Bu), 1.12 (s, 9H, *t*Bu), 7.24-7.30 (m, 5H, *Ph*) ppm; ^{13}C NMR (100.6 MHz, C_6D_6, 25 °C); δ 5.38 (N(Si*Me*$_3$)$_2$), 32.29, 32.32 (*t*Bu), 52.48, 55.46 (*t*Bu), 127.31, 127.95, 128.47, 129.35, 133.43, 136.23, 140.93, 153.04 (Ph), 166.45 (N*C*N) ppm; ^{19}F NMR (376.63 MHz, C_6D_6, 25 °C) δ –89.09 (s, 1F, Si–*F*), –125.53 (br, 2F, *o*-*F*),

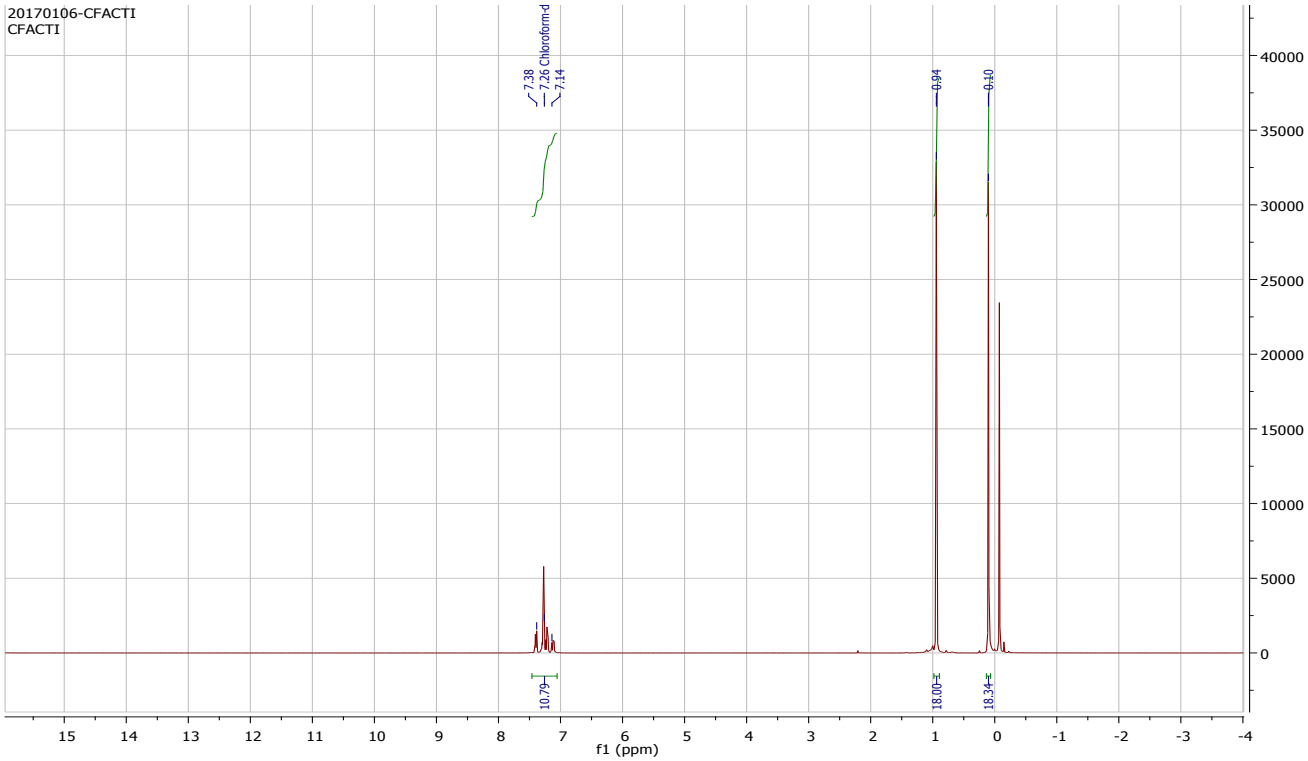
–154.97 (t, $^{3}J(^{19}F–^{19}F$=22.59 Hz, 1F, *p-F*), –162.19 (br, 2F, *m*-F) ppm; $^{29}Si\{^{1}H\}$NMR (79.53 MHz, C_6D_6, 25 °C): δ –16.77 ($SiN(SiMe_3)_2$), –62.17 (d, *J*=243.19 Hz, Si–F) ppm.

❖ **Synthesis of $[PhC(N\mathit{t}Bu)_2]Si(F)N(Si(CH_3)_3)_2$ (4-$C_6F_4CF_3$) (5)**

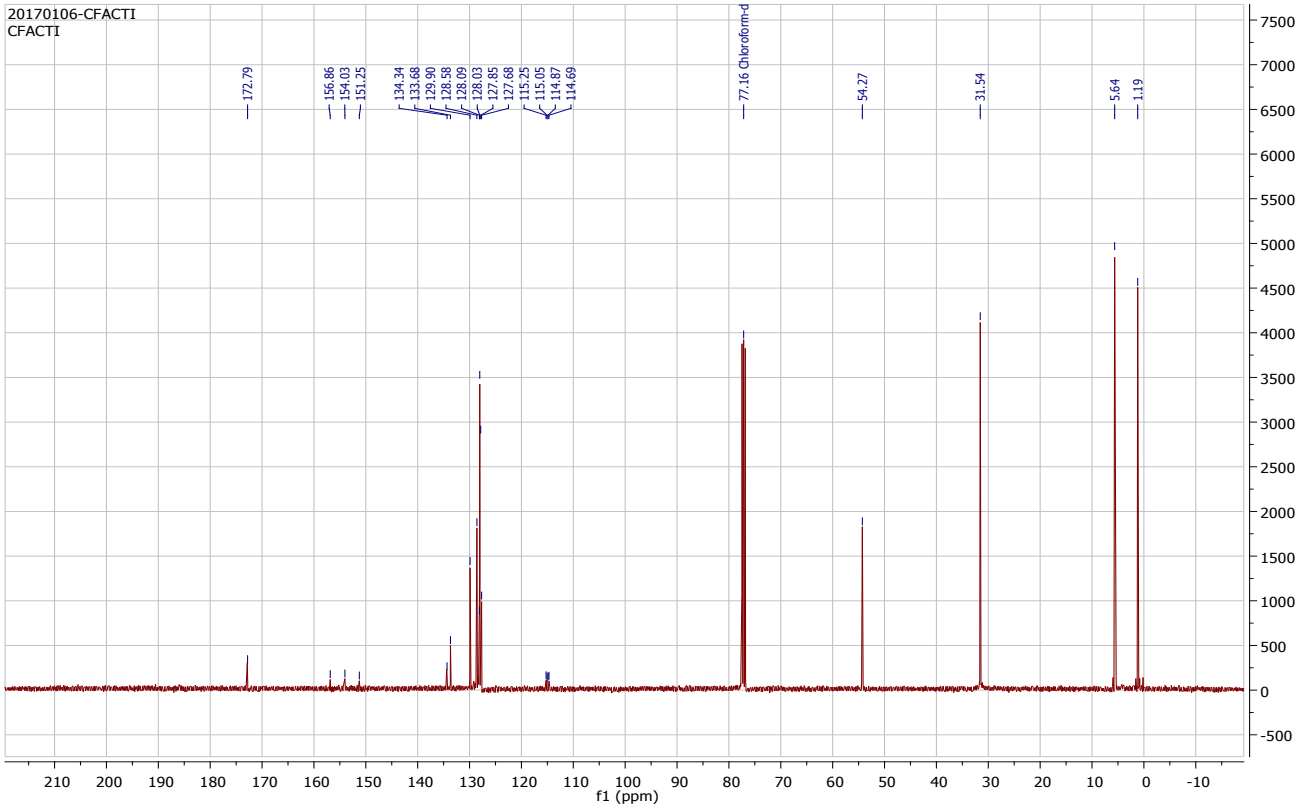
A toluene (10 mL) solution of octafluorotoluene (0.112 g, 0.47 mmol was added to a toluene (10 mL) solution of **1** (0.2 g, 0.47 mmol) at room temperature and stirred for 12h. Subsequently, all the volatiles were removed *in vacuo*, and the remaining residue was extracted with toluene (15 mL). The filtrate was reduced to 5 mL and stored at –30 °C in a freezer for one day to obtain colourless crystals of **5**. Yield: 0.248 g (79.3%). Mp: 97.4 °C Anal. Calcd. for $C_{28}H_{41}F_8N_3Si_3$: C, 51.27; H, 6.30; N, 6.41. found: C, 49.69; H, 6.13; N, 5.87. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) δ 0.36 (s, 18H, ($N(Si\mathit{Me}_3)_2$), 0.95 (s, 18H, *t*Bu), 7.26-7.36 (m, 5H, *Ph*) ppm; ^{13}C NMR (100.6 MHz, $CDCl_3$, 25 °C); δ 1.2 ($Si\mathit{Me}_3$), 5.16 ($Si\mathit{Me}_3$), 32.21 (*t*Bu), 55.45 (*t*Bu), 127.40, 127.80, 127.92, 128.33, 129.55, 135.35 (*Ph*), 167.63 (N*C*N) ppm; ^{19}F NMR (376.63 MHz, $CDCl_3$, 25 °C) δ –56.25 (t, $^{4}J(^{19}F–^{19}F$=22.59 Hz, 3F, CF_3), –85.09 (s, 1F, Si–F), –124.04 (br, 2F, *o*-F), –141.37 (br, 2F, *m*-F)ppm; $^{29}Si\{^{1}H\}$NMR (79.53 MHz, $CDCl_3$, 25 °C): δ –20.02 ($SiN(SiMe_3)_2$), –71.28 (d, *J*=245.02Hz, Si–F) ppm. MALDI-TOF-MS: [M+] calcd. for $C_{28}H_{41}F_8N_3Si_3$: 655.91, found for $C_{28}H_{41}F_7N_3Si_3$: 635.9.

❖ **Analytical data for compounds 2-5:**

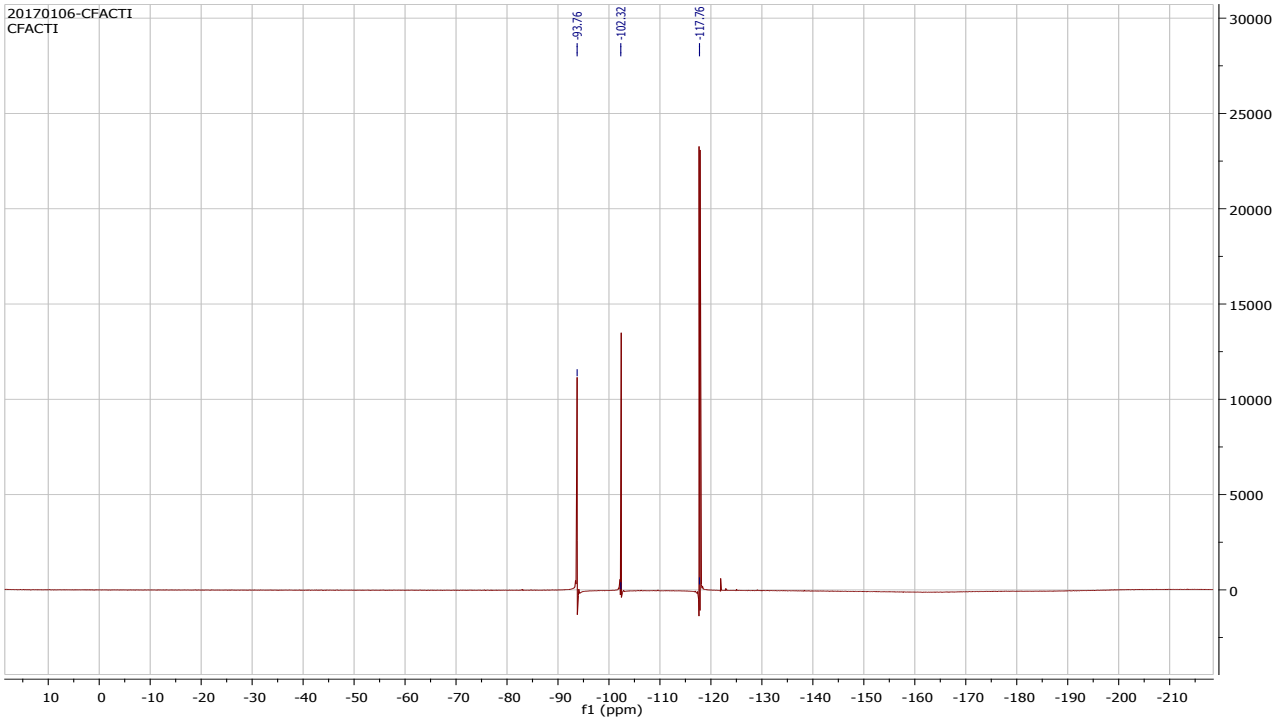
^{1}H NMR of 2:



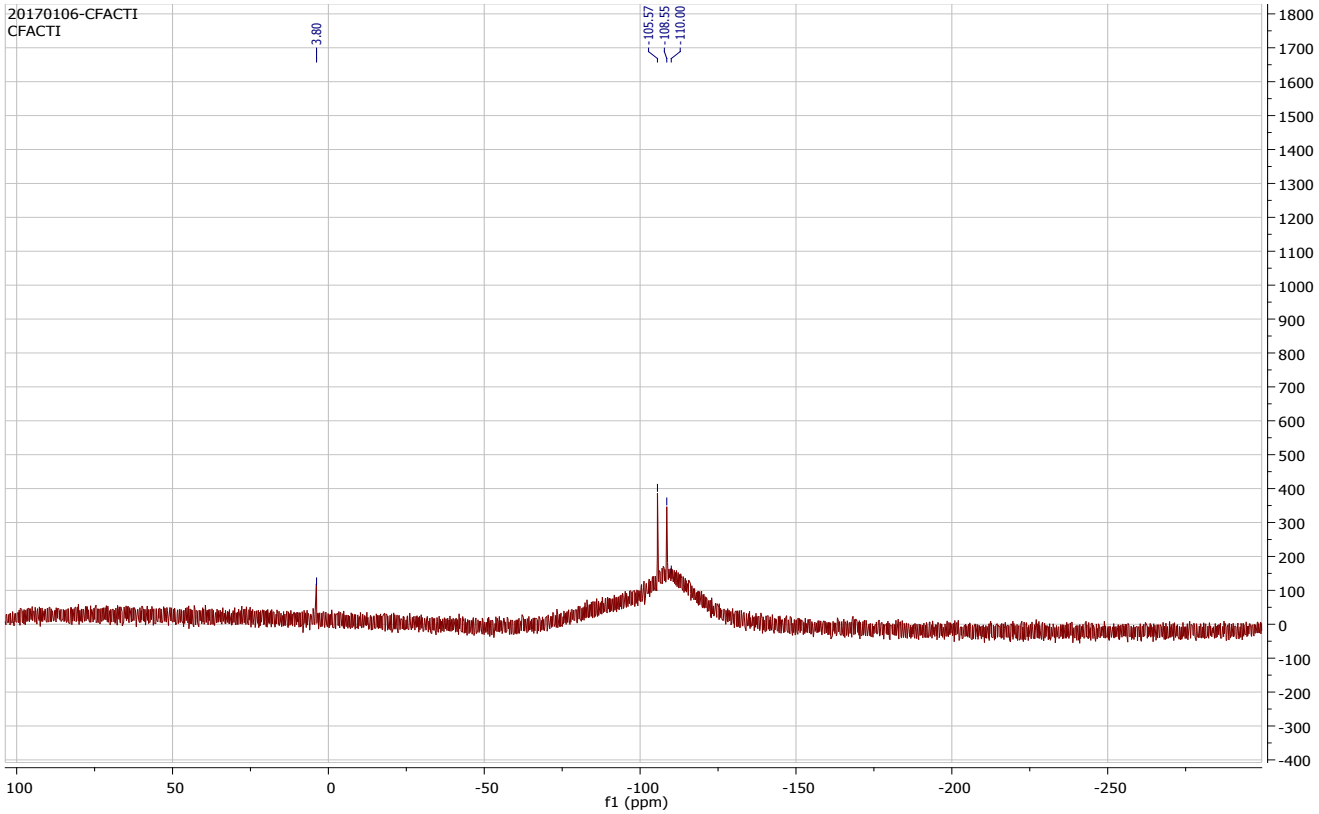
^{13}C NMR of 2:



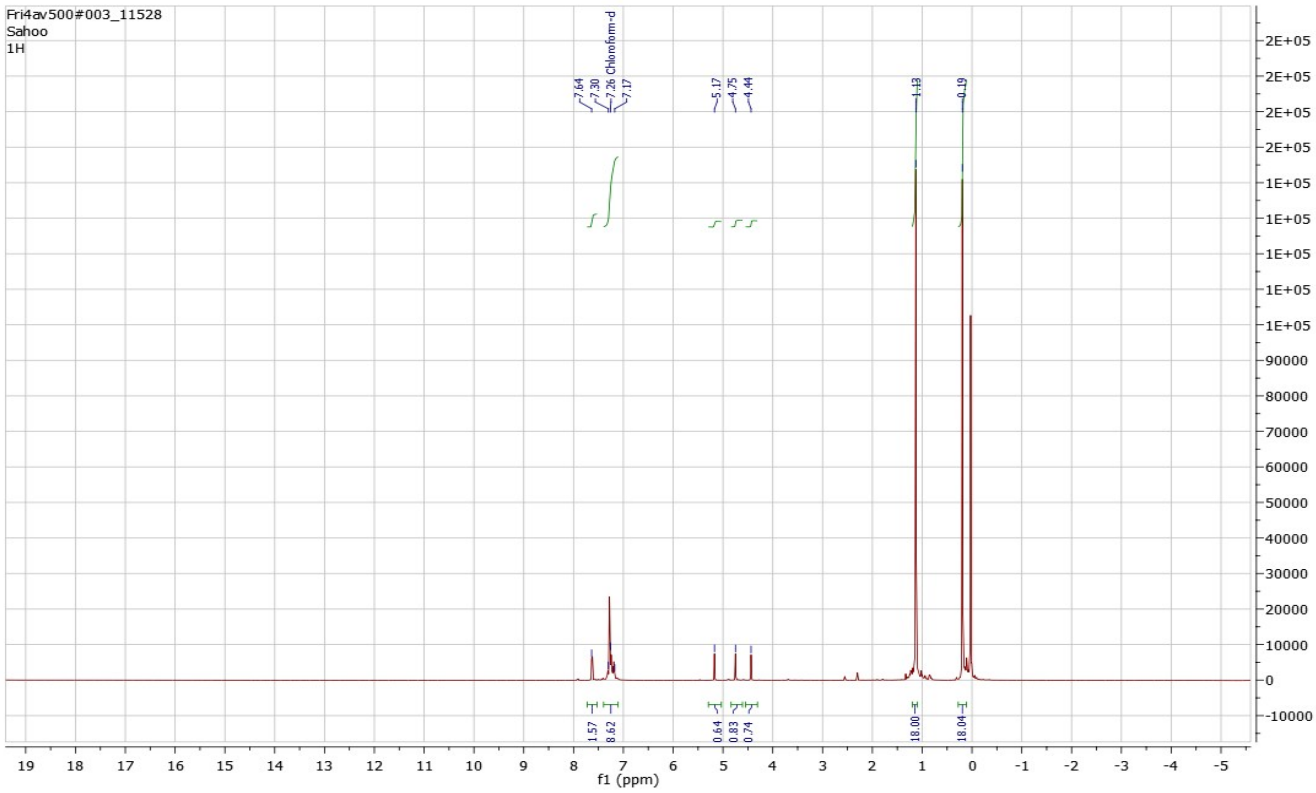
^{19} F NMR of 2:



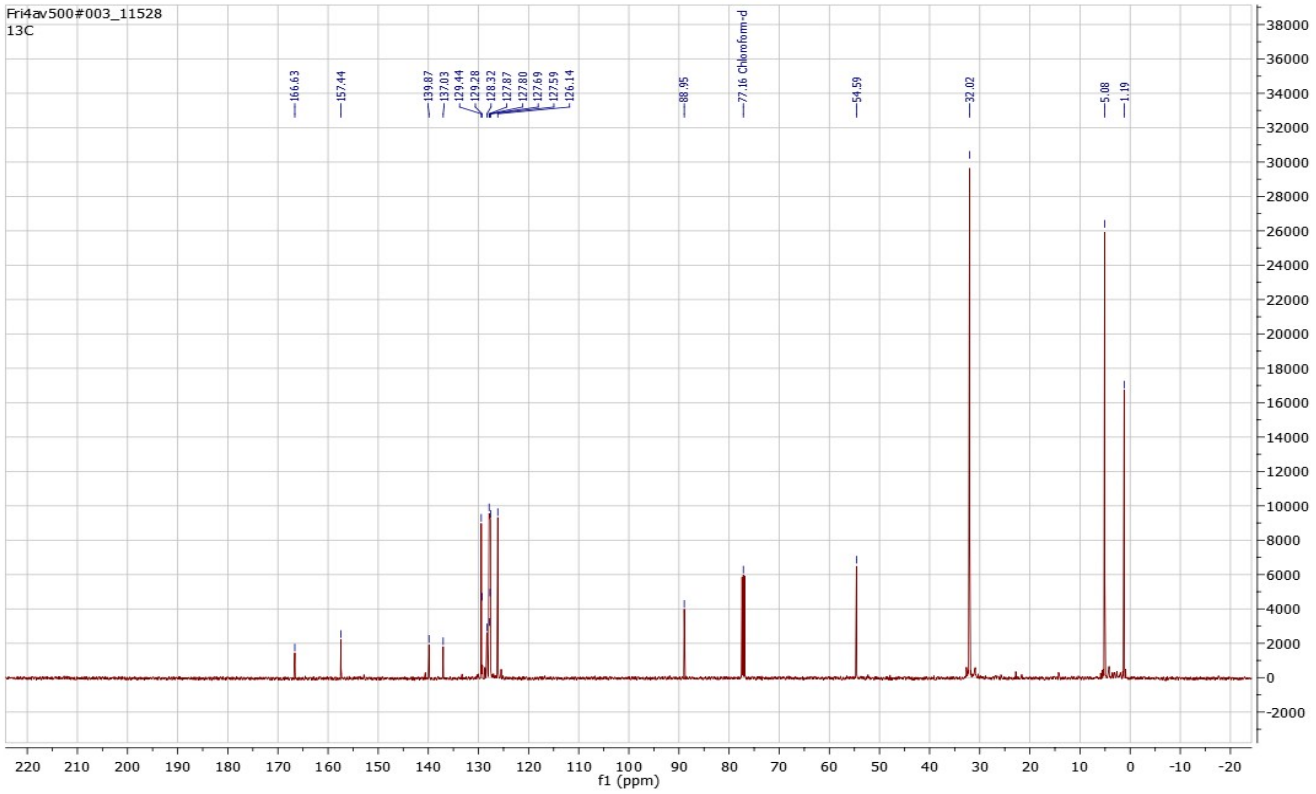
^{29}Si NMR of 2:



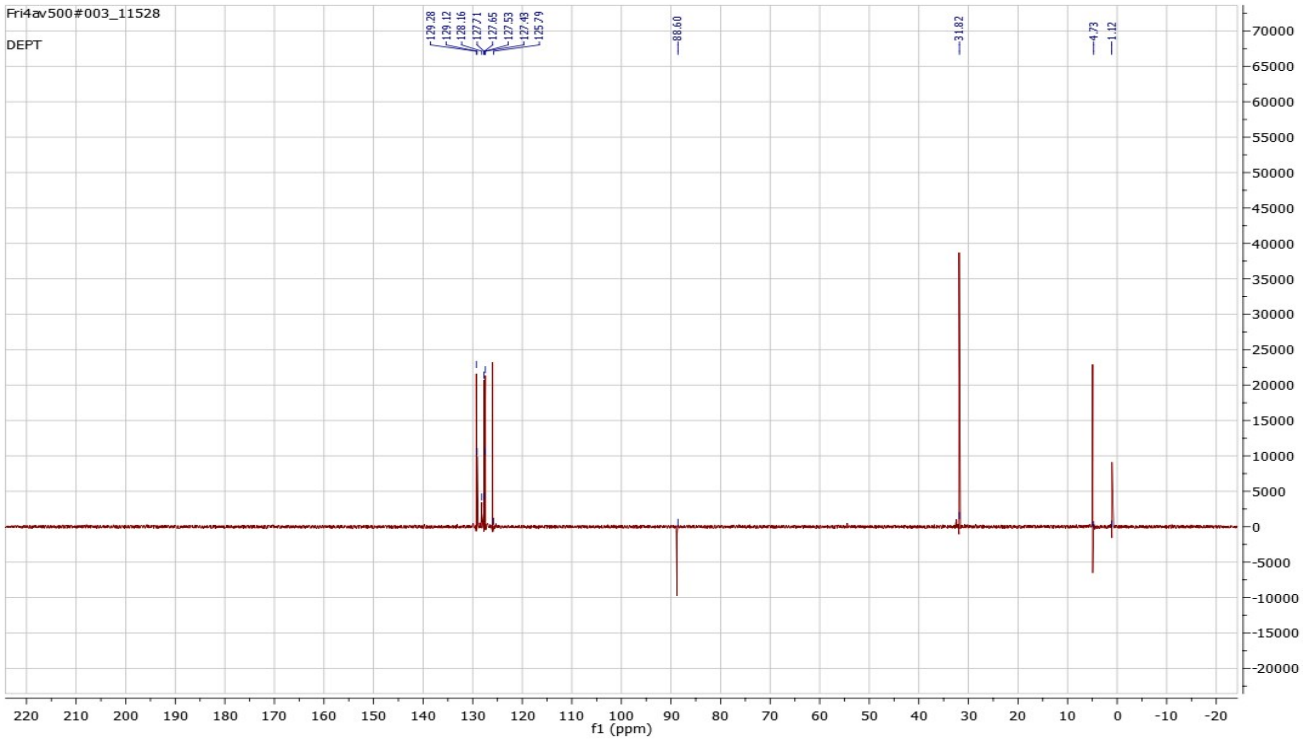
^{1}H NMR of 3:



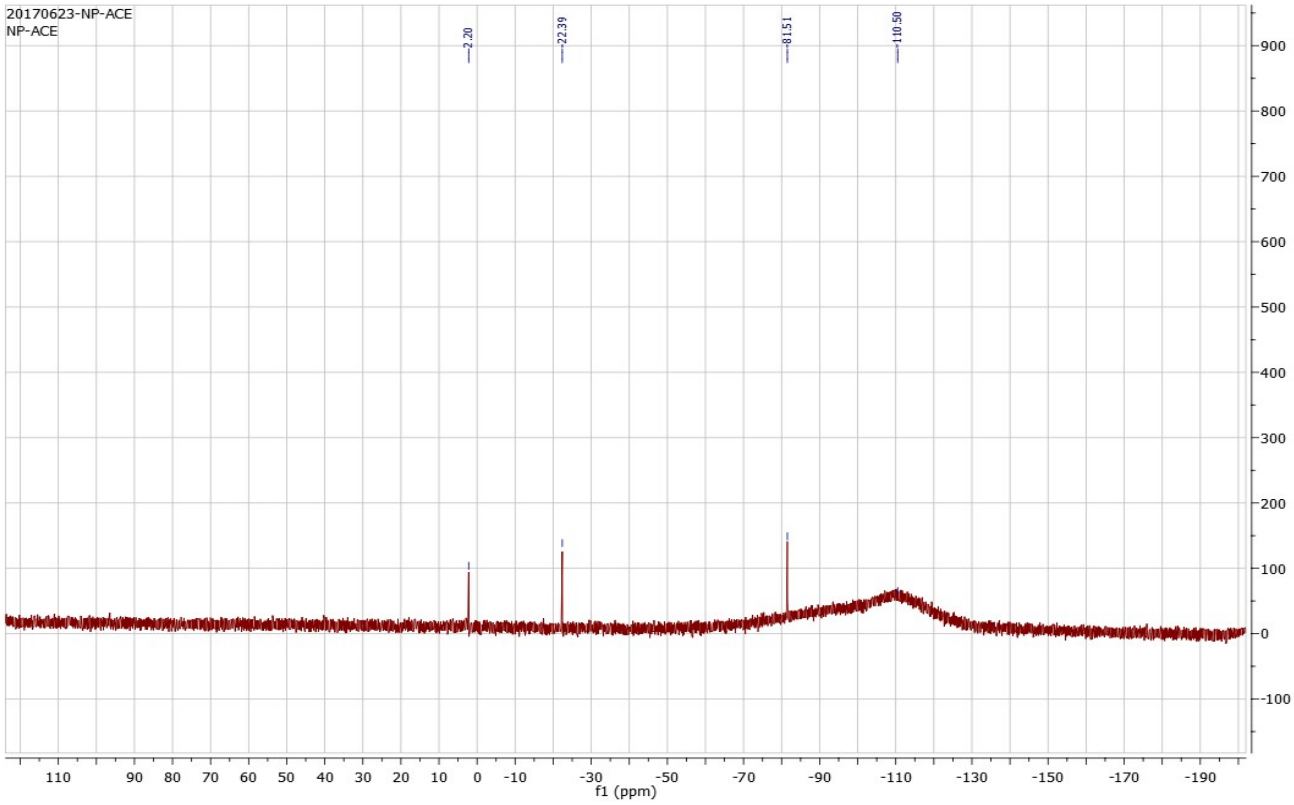
^{13} C NMR of 3:



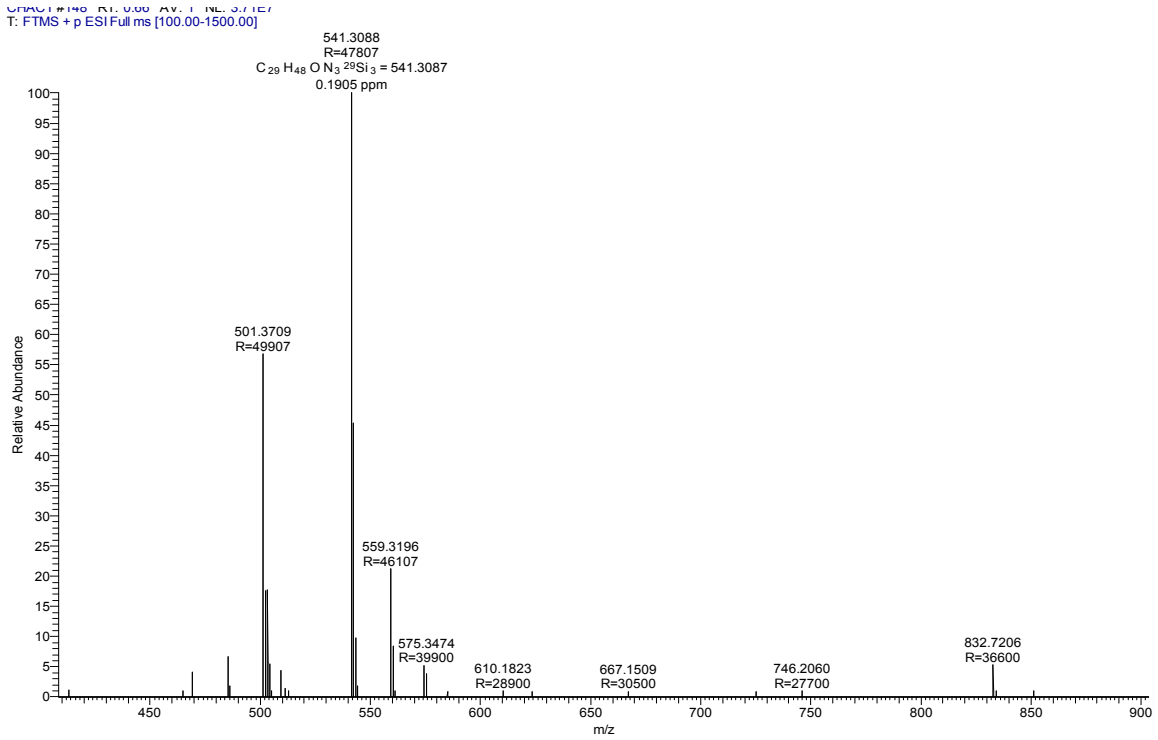
^{13}C-DEPT-135 NMR of 3:



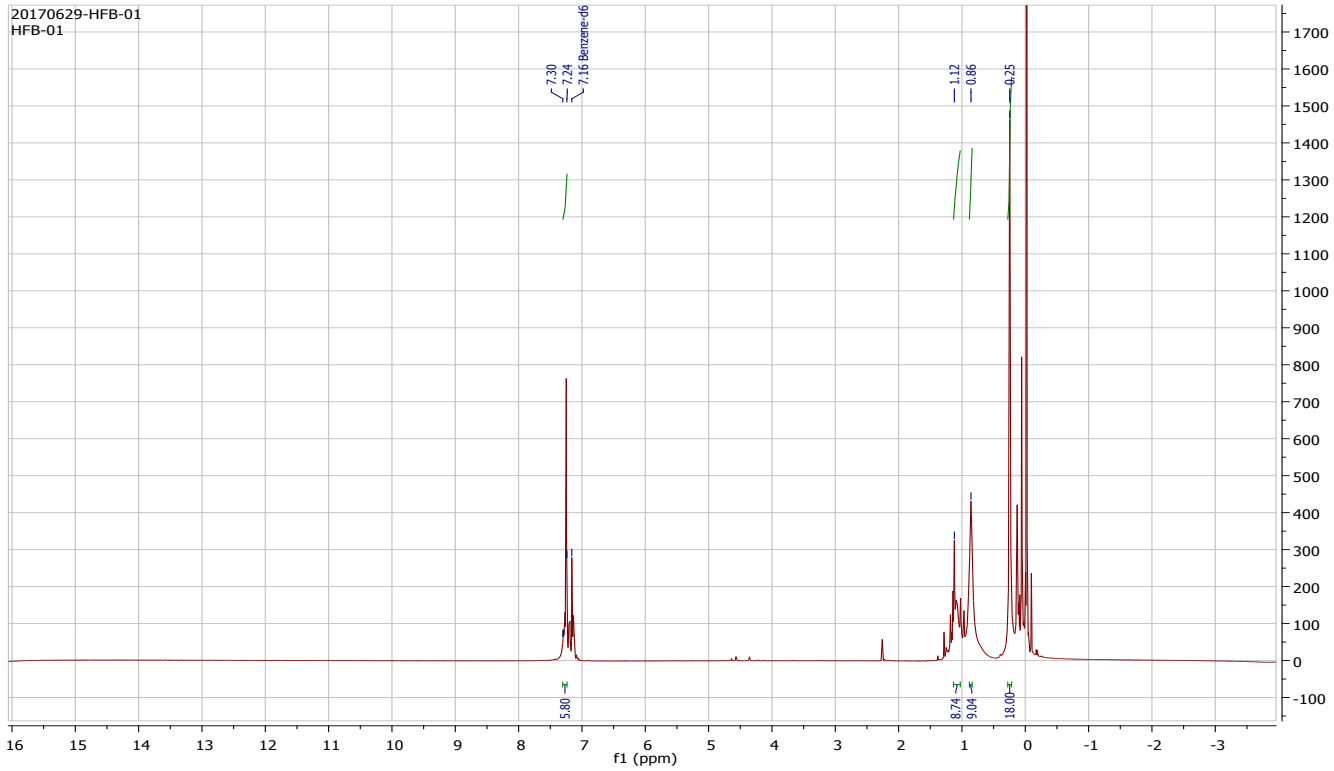
^{29}Si NMR of 3:



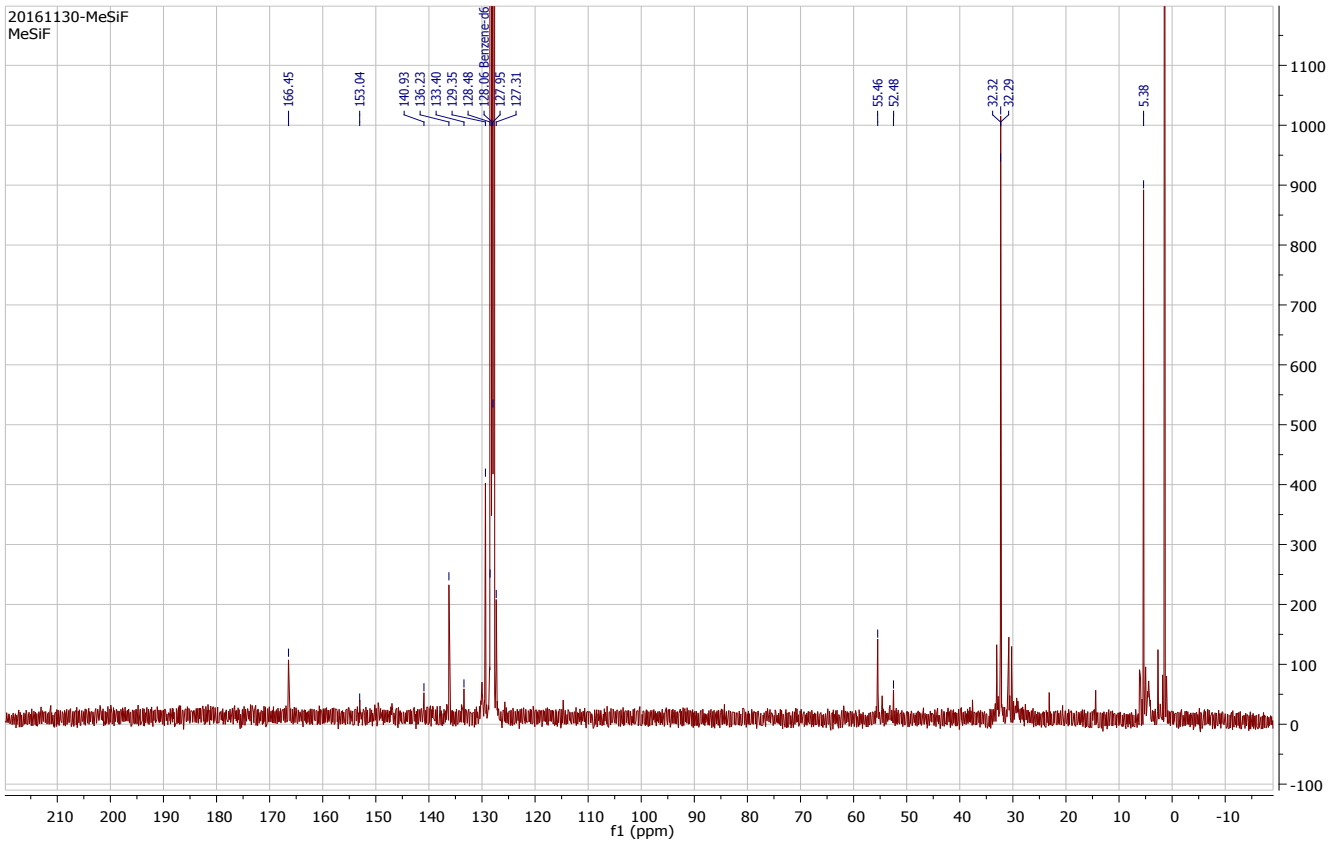
HRMS of 3:



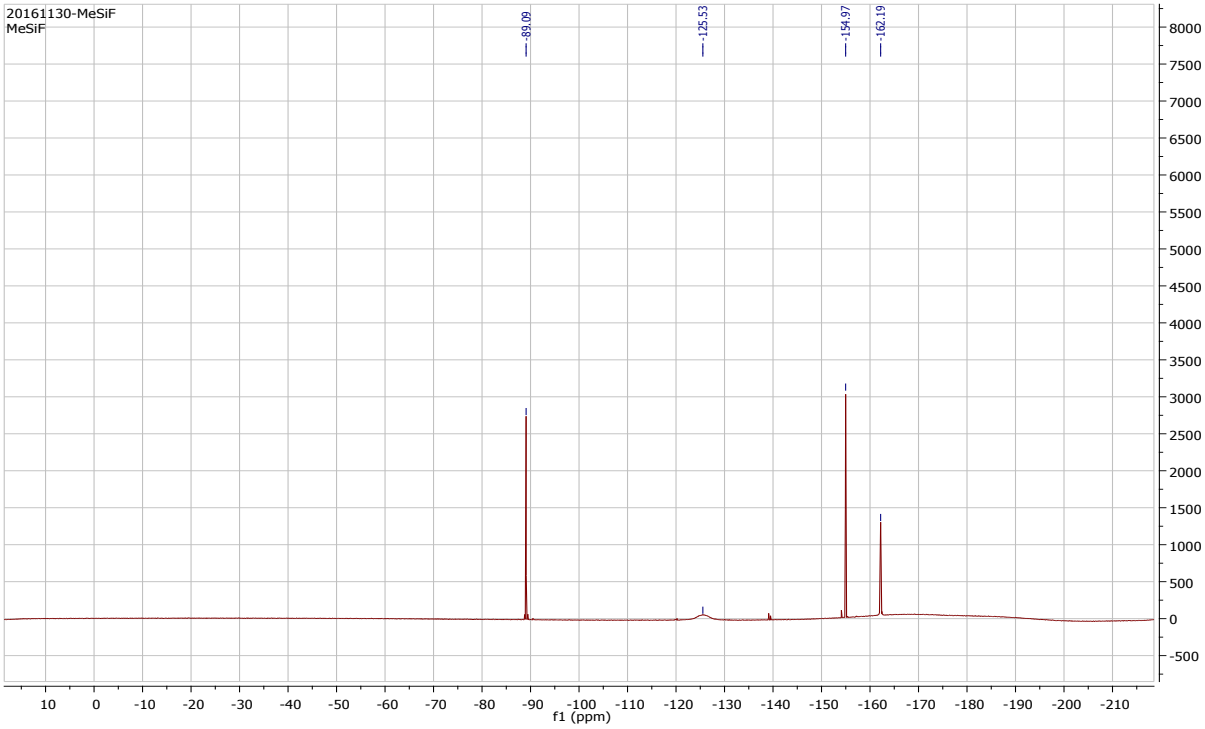
^{1}H NMR of 4:



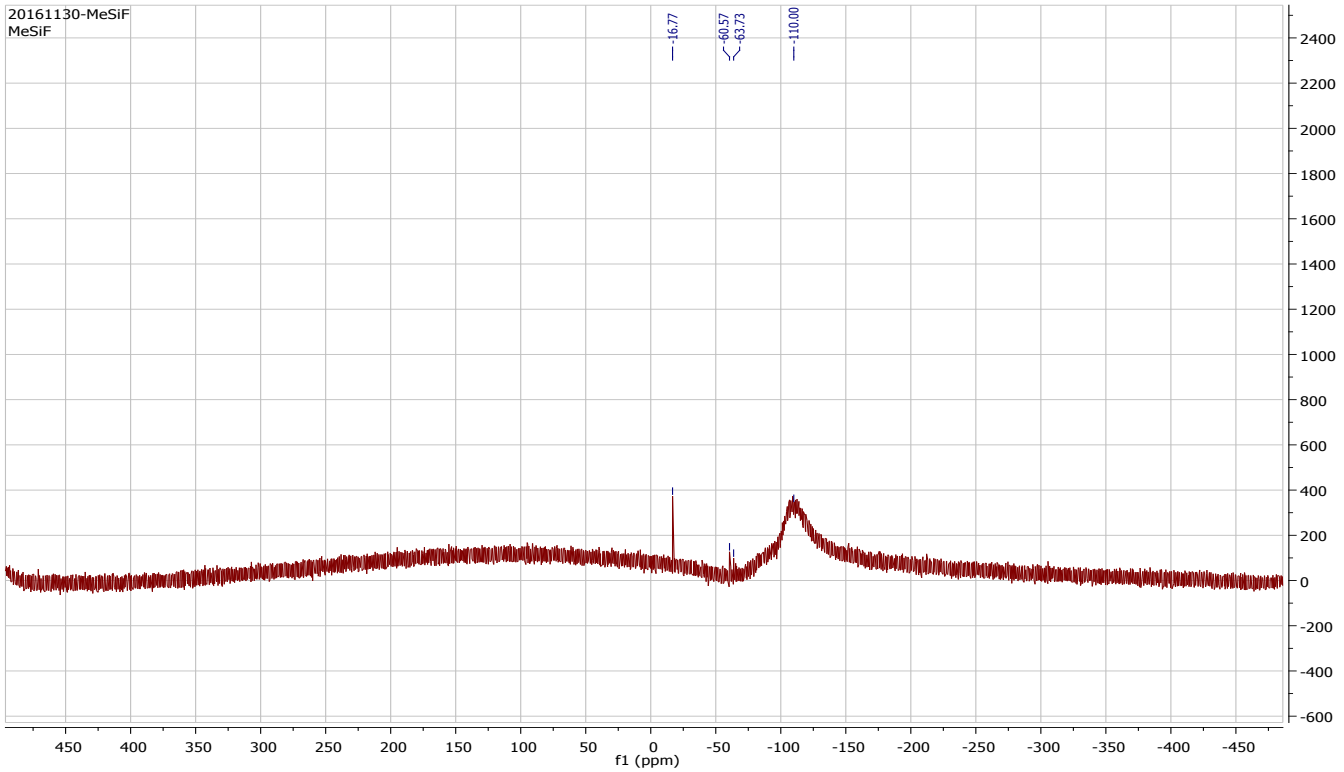
^{13}C NMR of 4:



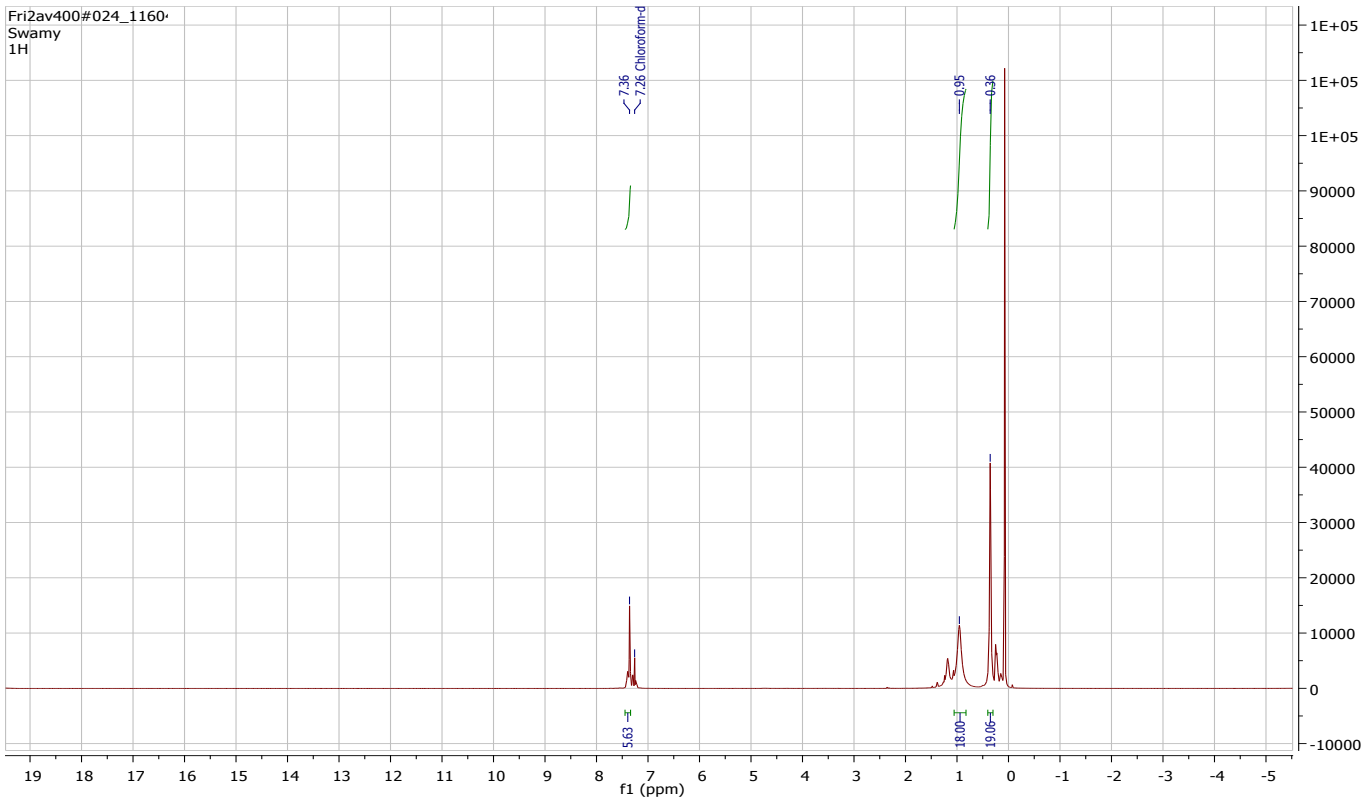
^{19}F NMR of 4:



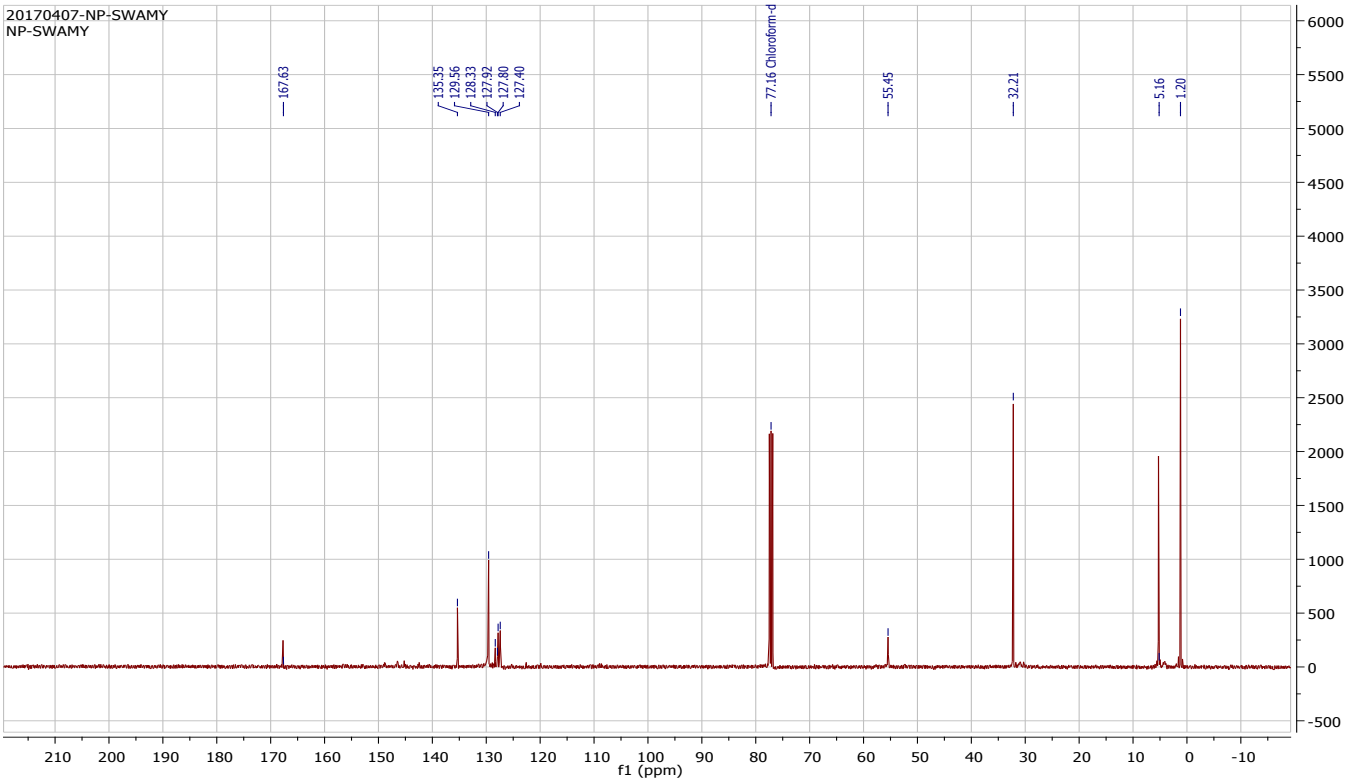
^{29}Si NMR of 4:



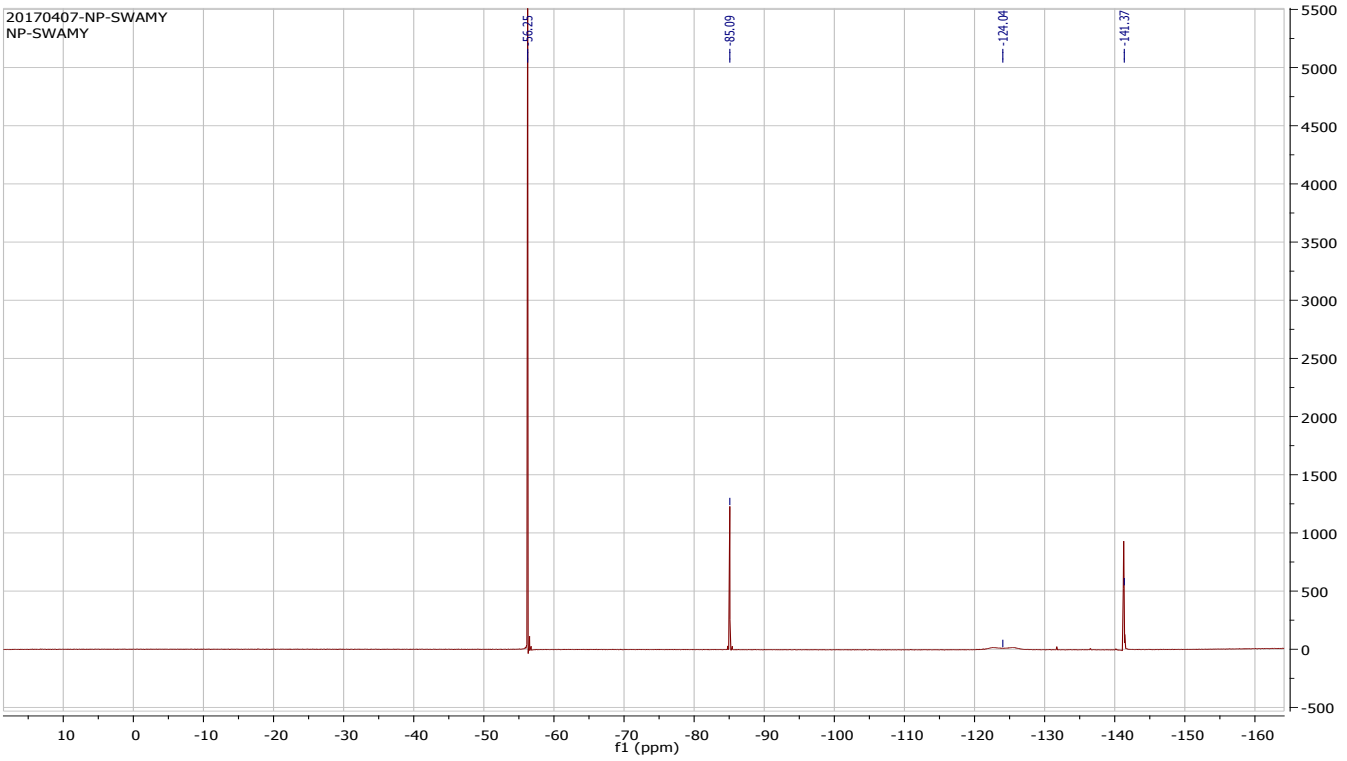
^{1}H NMR of 5:



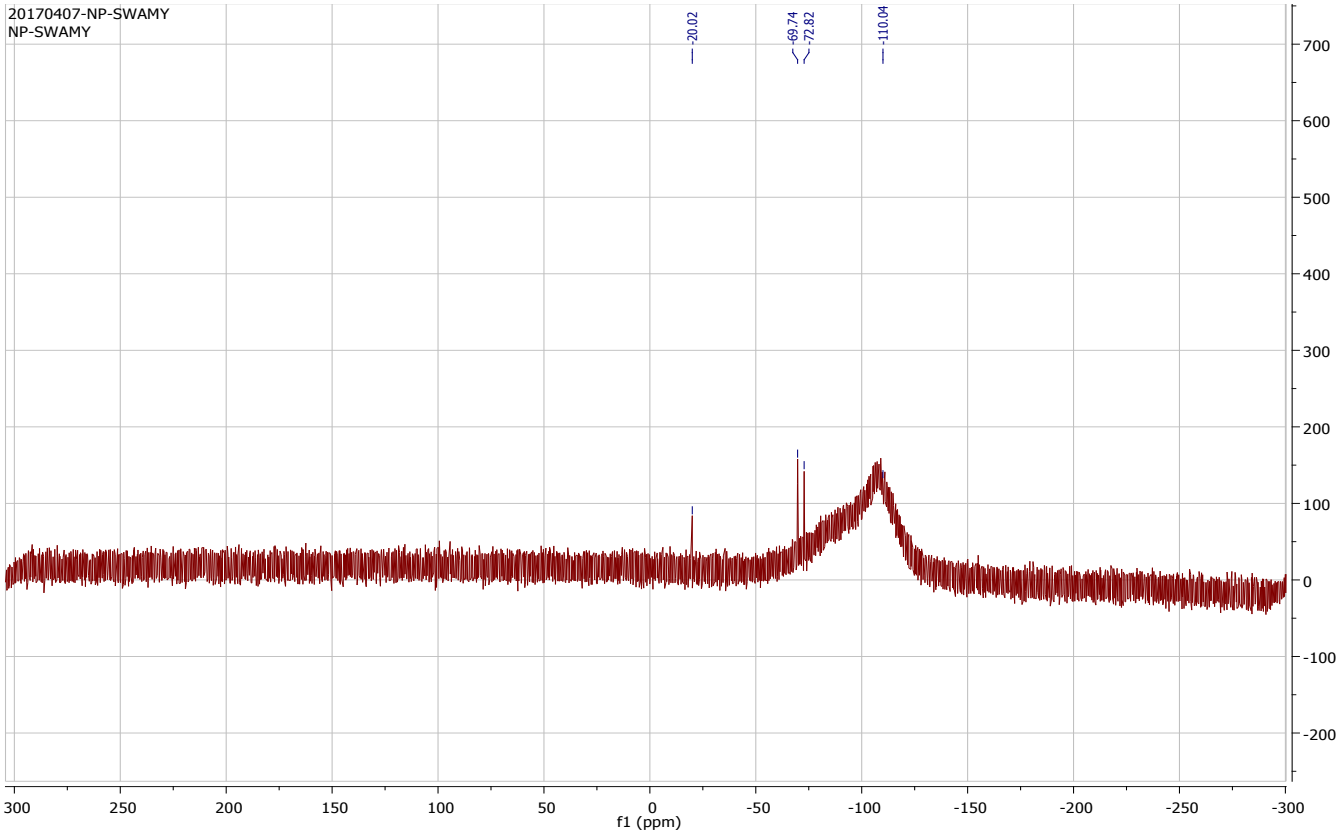
^{13}C NMR of 5:



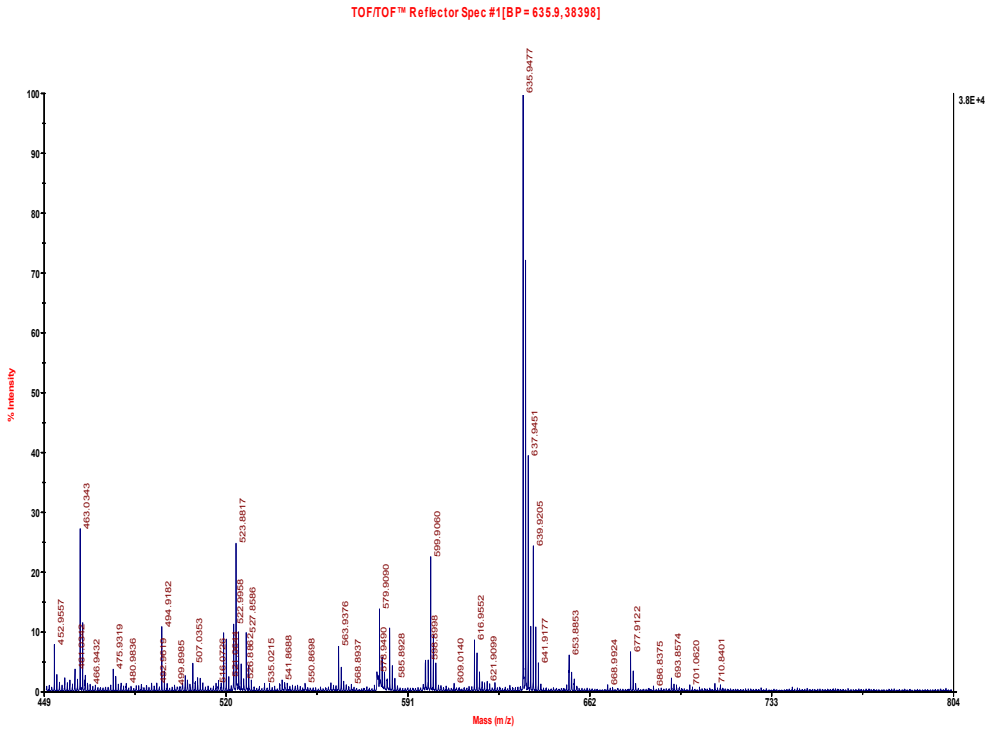
^{19}F NMR of 5:



^{29}Si NMR of 5:



MALDI-TOF-MS of 5



❖ **Crystallographic data for the structural analysis of compounds 2, 4 and 5.** X-ray intensity data measurements of compounds **2**, **4** and **5** were carried out on a Bruker SMART APEX II CCD diffractometer with graphite-monochromatized (MoKα= 0.71073Å) radiation. The X-ray generator was operated at 50 kV and 30 mA. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames. Data were collected with ω scan width of 0.5° at different settings of φ and 2θ keeping the sample-to-detector distance fixed at 5.00 cm. The X-ray data collection was monitored by APEX2 program (Bruker, 2006).[S2] All the data were corrected for Lorentzian, polarization, and absorption effects using SAINT and SADABS programs (Bruker, 2006). SHELX-97 was used for structure solution and full matrix least-squares refinement on $F2$.[S3] All the hydrogen atoms were placed in geometrically idealized position and constrained to ride on their parent atoms. An *ORTEP* III[S4] view of compounds **2**, **4** and **5** were drawn with 50% probability displacement ellipsoids and H atoms omitted for clarity.

Crystal Data for compound 2. $C_{29}H_{46}F_3N_3OSi_3$, M =593.96, colorless, 0.34 x 0.23 x 0.17 mm^3, orthorhombic, space group $P2_12_12_1$, a = 10.152 (3) Å, b = 10.449 (3) Å, c = 30.517 (9) Å, $\alpha=\beta=\gamma$ =90°, V = 3237.0 (17) Å^3, Z = 4, T = 296(2) K, $2\theta_{max}$=49.998°, D_{calc} (g cm^{-3}) = 1.219, $F(000)$ = 1272.0, μ (mm^{-1}) = 0.190, 46723 reflections collected, 5699 unique reflections (R_{int}= 0.1008), 4860 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.949, T_{max} = 0.968, 365, flack parameter x= 0.44(6), refined parameters, S = 1.162 , $R1$ = 0.0753, $wR2$ = 0.1793 (all data R = 0.0920, $wR2$ =0.1793), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.475, $\Delta\rho_{min}$= -0.397 (eÅ^{-3}).

Crystal Data for compound 4. $C_{27}H_{41}F_6N_3Si_3$, M =605.90, colorless, 0.38x 0.28 x 0.17 mm^3, monoclinic, space group $P2_1$/c, a = 14.962 (3) Å, b = 12.796 (3) Å, c = 17.935 (4) Å, $\alpha=\gamma$ 90°, β =113.789 (5) °, V =3141.9 (12) Å^3, Z = 4, T = 296(2) K, $2\theta_{max}$=49.996°, D_{calc} (g cm^{-3}) = 1.281, $F(000)$

= 1280.0, μ (mm^{-1}) = 0.208, 68453 reflections collected, 5530 unique reflections (R_{int}= 0.1653), 3387 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.932, T_{max} = 0.965, 365 refined parameters, S = 1.020, $R1$ = 0.0499, $wR2$ = 0.1152 (all data R = 0.1127, $wR2$ =0.1152), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.318, $\Delta\rho_{min}$= -0.305 (eÅ^{-3}).

Crystal Data for compound 5. $C_{28}H_{41}F_8N_3Si_3$, M =655.91, colorless, 0.38 x 0.27 x 0.22 mm^3, triclinic, space group P 1, a = 9.658 (2) Å, b = 9.771 (2) Å, c = 17.351 (4) Å, α=99.448 (6) °, β =91.554 (6) °,γ =94.467 (6) °, V = 1609.0 (7) Å^3, Z = 2, T = 296(2) K, $2\theta_{max}$=49.998°, D_{calc} (g cm^{-3}) = 1.354, $F(000)$ = 688.0, μ (mm^{-1}) = 0.217, 45397 reflections collected, 5670 unique reflections (R_{int}= 0.1746), 3256 observed ($I > 2\sigma(I)$) reflections, multi-scan absorption correction, T_{min} = 0.932, T_{max} = 0.953, 392 refined parameters, S = 1.038, $R1$ = 0.0713, $wR2$ = 0.1957 (all data R = 0.1457, $wR2$ =0.1957), maximum and minimum residual electron densities; $\Delta\rho_{max}$ = 0.429, $\Delta\rho_{min}$= -0.539 (eÅ^{-3}).

- **Details of the theoretical computational for compounds 2.** All the calculations in this study have been performed with density functional theory (DFT), with the aid of the Turbomole 7.1 suite of programs,[S5] using the PBE functional.[S6] The TZVP[S7] basis set has been employed. The resolution of identity (RI),[S8] along with the multipole accelerated resolution of identity (marij)[S9] approximations have been employed for an accurate and efficient treatment of the electronic Coulomb term in the DFT calculations. Solvent correction were incorporated with optimization calculations using the COSMO model,[S10] with toluene (ε = 2.374) as the solvent. The values reported are ΔG values, with zero point energy corrections, internal energy and entropic contributions included through frequency calculations on the optimized minima with the temperature taken to be 298.15 K. Harmonic frequency calculations were performed for all stationary points to confirm them as a local minima or transition state structures.

PBE/TZVP optimized geometries for all the compounds and transition states

1) **Rcts - Silylene complex**

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C	-1.077539	9.652311	9.595298
C	-0.492326	10.999203	9.344699
C	0.495029	11.501462	10.206477
H	0.820698	10.900200	11.057708
C	1.066087	12.753153	9.968352
H	1.835930	13.133876	10.642346
C	0.656190	13.514159	8.869165
H	1.105318	14.491320	8.681534
C	-0.330019	13.019989	8.009731
H	-0.656386	13.611379	7.152001
C	-0.903686	11.768565	8.245816
H	-1.678381	11.386295	7.578474
C	-3.116596	10.253051	11.037202
C	-2.401621	11.052714	12.140510
H	-1.884838	10.376429	12.836416
H	-3.138453	11.637082	12.711667
H	-1.666444	11.752319	11.721894
C	-3.833523	11.210404	10.065886
H	-3.136742	11.940480	9.633587
H	-4.620759	11.766341	10.596969
H	-4.299605	10.641342	9.248414
C	-4.159627	9.328656	11.686071
H	-4.693176	8.745524	10.920295

H	-4.896382	9.924367	12.243023
H	-3.680834	8.621733	12.377745
C	0.339747	8.203353	8.016969
C	0.543915	6.678914	8.039617
H	0.935113	6.351547	9.012700
H	1.254603	6.379415	7.256374
H	-0.407152	6.155313	7.861514
C	-0.178899	8.623196	6.627192
H	-1.153732	8.154404	6.428961
H	0.528962	8.310395	5.844659
H	-0.294882	9.713815	6.564686
C	1.684819	8.891616	8.305232
H	1.620582	9.981654	8.201432
H	2.437243	8.527225	7.590343
H	2.036170	8.659008	9.320894
N	-2.105520	6.392617	10.721866
Si	-0.907052	6.349770	12.043500
C	-1.753267	6.361875	13.748659
H	-2.380730	7.259745	13.854913
H	-0.987109	6.391806	14.539721
H	-2.386651	5.482677	13.921265
C	0.201341	4.807120	11.889196
H	-0.359310	3.862887	11.920141
H	0.934799	4.789600	12.710733

H	0.757252	4.835802	10.939635
C	0.278089	7.831272	12.065160
H	0.898185	7.883145	11.162547
H	0.940022	7.708164	12.936998
H	-0.258451	8.782675	12.171412
Si	-3.133886	4.959596	10.386251
C	-3.389843	3.859974	11.918812
H	-2.463572	3.489631	12.377060
H	-3.973965	2.983271	11.596027
H	-3.973818	4.383054	12.689595
C	-4.889156	5.459540	9.853815
H	-5.344941	6.127869	10.600172
H	-5.511084	4.552196	9.784182
H	-4.903785	5.971614	8.883142
C	-2.349594	3.898210	9.018688
H	-2.275809	4.473633	8.083309
H	-2.953925	2.999483	8.819570
H	-1.335719	3.577828	9.301414
N	-2.170065	9.366982	10.330352
N	-0.668977	8.488100	9.057925
Si	-2.370204	7.654471	9.464440

2) Rcts - PhCOCF$_3$

17

C	-1.796566	0.243333	-0.562927

O	-2.794565	-0.192765	-0.013287
C	-1.504401	0.093974	-2.006961
C	-0.334232	0.585611	-2.619230
C	-2.462075	-0.583417	-2.789547
C	-0.130181	0.396011	-3.985709
C	-2.252704	-0.767158	-4.152200
C	-1.084780	-0.278747	-4.752934
H	0.422657	1.112785	-2.040064
H	-3.365186	-0.957871	-2.305152
H	0.779058	0.777069	-4.453237
H	-2.998625	-1.291556	-4.751809
H	-0.919489	-0.424697	-5.822131
C	-0.759790	1.016098	0.331120
F	-0.600320	2.298304	-0.105058
F	-1.163485	1.062817	1.610380
F	0.463119	0.412813	0.301588

3) RC

85

O	-2.385264	1.893878	-2.216472
Si	-0.335533	-1.034813	-0.083449
N	0.862424	-0.202450	1.181369
C	1.651166	0.255122	0.187688
N	1.299132	-0.424139	-0.918187
N	-0.216262	-2.813672	0.177981

C	1.686274	-0.246008	-2.333243
C	3.210558	-0.135094	-2.508298
H	3.450963	-0.157855	-3.581268
H	3.727697	-0.974528	-2.022559
H	3.604427	0.800914	-2.094080
C	0.997266	0.992809	-2.937062
H	-0.092034	0.927439	-2.811101
H	1.352728	1.914833	-2.456389
H	1.220533	1.066706	-4.012319
C	1.185448	-1.503872	-3.063226
H	0.097714	-1.615579	-2.939551
H	1.668119	-2.408194	-2.666359
H	1.403317	-1.430475	-4.137929
Si	1.218371	-3.795387	0.590015
C	2.862467	-2.855065	0.500969
H	2.887335	-2.008614	1.198470
H	3.074245	-2.480811	-0.507284
H	3.659016	-3.561119	0.784127
H	1.536796	-4.870606	-1.649791
C	1.405527	-5.251133	-0.625343
H	0.546385	-5.935760	-0.629297
H	2.300739	-5.836941	-0.363721
C	1.104318	-4.456903	2.370846
H	1.042827	-3.619774	3.083140

H	0.231245	-5.102411	2.529902
H	2.008771	-5.037559	2.611936
H	-1.210158	-5.968152	0.718238
C	-1.996274	-5.216333	0.869103
H	-2.954366	-5.676153	0.578369
H	-2.049660	-4.982318	1.942393
Si	-1.775530	-3.631277	-0.162504
C	-3.267722	-2.542285	0.293344
C	-1.906143	-4.077046	-2.004203
H	-1.077235	-4.727671	-2.318495
H	-1.871200	-3.163718	-2.617174
H	-2.853616	-4.595811	-2.218133
H	-4.175178	-3.167755	0.275332
H	-3.405597	-1.710036	-0.408692
H	-3.158683	-2.124513	1.305474
C	-2.245710	2.792412	-1.400620
C	-2.669335	2.708656	0.010372
C	-3.143352	1.456740	0.457130
H	-3.142586	0.618365	-0.238415
H	-3.943772	0.330351	2.108471
C	-3.579200	1.302200	1.770659
C	-3.544133	2.387202	2.653364
H	-3.886701	2.264496	3.682826
C	-3.064745	3.630390	2.221659

H	-3.033275	4.474648	2.911952
C	-2.624837	3.794803	0.909663
H	-2.259021	4.770475	0.591309
C	-1.547979	4.108895	-1.898410
F	-0.459449	4.418836	-1.128004
F	-1.121772	3.984539	-3.165742
F	-2.398489	5.172479	-1.845186
C	2.655292	1.351985	0.274637
C	3.975182	1.060637	0.651769
H	4.254826	0.030108	0.878386
C	4.929248	2.078650	0.716671
H	5.954454	1.841323	1.007413
C	4.573947	3.395113	0.406440
H	5.321090	4.189616	0.454873
C	3.259101	3.690817	0.032434
H	2.973804	4.716619	-0.208955
H	1.276193	2.909704	-0.312361
C	2.303170	2.674998	-0.031620
C	0.705900	0.261679	2.574360
C	1.986940	-0.016739	3.380891
C	0.342978	1.756670	2.649785
C	-0.450788	-0.560300	3.167202
H	-0.604467	-0.288262	4.221055
H	-1.382971	-0.361551	2.617744

H	-0.239867	-1.637052	3.106969
H	-0.523563	1.971112	2.009577
H	0.081846	2.029089	3.683418
H	1.179603	2.392774	2.333116
H	1.832226	0.258624	4.434681
H	2.835066	0.566189	2.998171
H	2.247896	-1.084207	3.337770

4) TS_1

85

O	-1.971822	0.033091	-1.016234
Si	-0.182825	-0.828771	0.052811
N	0.996989	0.019265	1.278609
C	1.734607	0.506060	0.252336
N	1.335055	-0.170232	-0.849162
N	-0.244026	-2.590302	0.135232
C	1.884283	-0.191140	-2.227500
C	3.257326	-0.889358	-2.223233
H	3.651123	-0.937142	-3.249111
H	3.177793	-1.914912	-1.838352
H	3.981435	-0.337327	-1.608139
C	2.028211	1.212611	-2.840788
H	1.088189	1.771791	-2.774386
H	2.818577	1.793645	-2.349813
H	2.295537	1.110701	-3.902905

C	0.899969	-1.015799	-3.068181
H	-0.090216	-0.541904	-3.088739
H	0.792466	-2.030129	-2.659463
H	1.269828	-1.098028	-4.099424
Si	1.152882	-3.638593	0.583099
C	2.683601	-2.669902	1.139074
H	2.523622	-2.183575	2.108874
H	3.012292	-1.911413	0.419909
H	3.495858	-3.404860	1.257625
H	2.073945	-4.027783	-1.713527
C	1.685254	-4.679527	-0.916598
H	0.866173	-5.273526	-1.343613
H	2.490216	-5.371726	-0.624471
C	0.722790	-4.744508	2.067946
H	0.204570	-4.155932	2.840391
H	0.091062	-5.603603	1.812339
H	1.656846	-5.128069	2.507483
H	-1.001274	-5.815014	-0.395240
C	-1.855247	-5.224923	-0.039384
H	-2.752678	-5.602646	-0.555596
H	-1.989521	-5.411003	1.034871
Si	-1.783652	-3.365934	-0.432325
C	-3.299939	-2.618361	0.415949
C	-1.958421	-3.159683	-2.306161

H	-1.123838	-3.630751	-2.845926
H	-1.993780	-2.094396	-2.573428
H	-2.894609	-3.630277	-2.644906
H	-4.166033	-3.272800	0.230991
H	-3.527942	-1.626216	0.006669
H	-3.161403	-2.539626	1.504440
C	-2.318849	1.277017	-0.939074
C	-2.861873	1.830880	0.283178
C	-3.100604	0.936773	1.360195
H	-2.939187	-0.125195	1.196223
H	-3.736339	0.679176	3.400480
C	-3.556842	1.395817	2.595523
C	-3.790271	2.756776	2.802850
H	-4.161501	3.115765	3.764508
C	-3.545418	3.659881	1.754666
H	-3.713513	4.727983	1.909496
C	-3.084389	3.215577	0.520465
H	-2.889799	3.947926	-0.262449
C	-1.856660	2.191810	-2.045243
F	-0.755391	2.981897	-1.694676
F	-1.471988	1.506107	-3.152291
F	-2.818529	3.081743	-2.443299
C	2.676443	1.656003	0.284821
C	4.044227	1.451071	0.518781

H	4.415135	0.442524	0.711694
C	4.927697	2.534102	0.507317
H	5.991629	2.366554	0.685441
C	4.450518	3.826536	0.269311
H	5.141836	4.671425	0.257194
C	3.085552	4.035316	0.044650
H	2.707471	5.042089	-0.142972
H	1.138462	3.114664	-0.145441
C	2.199868	2.956652	0.050202
C	0.846405	0.517095	2.668654
C	2.204588	0.508214	3.393469
C	0.243135	1.933214	2.712169
C	-0.100701	-0.473247	3.364809
H	-0.254093	-0.173154	4.410607
H	-1.080372	-0.487742	2.866192
H	0.315864	-1.490766	3.350988
H	-0.670516	1.987015	2.106465
H	-0.016515	2.195615	3.748382
H	0.960105	2.679427	2.345363
H	2.052787	0.785043	4.446921
H	2.904445	1.228918	2.951758
H	2.665471	-0.488875	3.363418

5) Int_1

85

O	-1.583322	-0.242465	-0.430912
Si	-0.079642	-0.803839	-0.040512
N	0.891008	0.239528	1.128203
C	1.681839	0.646586	0.107578
N	1.327976	-0.073971	-0.979445
N	-0.197322	-2.507840	0.093604
C	1.953885	-0.176760	-2.330943
C	3.369700	-0.768907	-2.214676
H	3.790388	-0.898611	-3.222047
H	3.353682	-1.751377	-1.723550
H	4.039693	-0.103985	-1.654696
C	2.014292	1.188336	-3.034377
H	1.029232	1.667808	-3.045105
H	2.727138	1.863128	-2.543724
H	2.351868	1.037044	-4.069990
C	1.069556	-1.136229	-3.138074
H	0.055271	-0.735129	-3.252261
H	1.010298	-2.121649	-2.654824
H	1.499498	-1.274425	-4.139305
Si	1.201593	-3.525802	0.617750
C	2.642690	-2.481356	1.269587
H	2.393877	-1.957864	2.201028
H	3.020922	-1.751446	0.543289
H	3.461571	-3.184913	1.487815

H	2.375512	-3.844868	-1.570285
C	1.888479	-4.515671	-0.847228
H	1.123250	-5.087478	-1.386866
H	2.649193	-5.224973	-0.485689
C	0.693259	-4.648946	2.056121
H	0.058226	-4.100295	2.767773
H	0.155306	-5.549631	1.736731
H	1.600712	-4.968938	2.590556
H	-0.767609	-5.661808	-0.787250
C	-1.649915	-5.191266	-0.337197
H	-2.532311	-5.567912	-0.879934
H	-1.741015	-5.528865	0.703462
Si	-1.751543	-3.299796	-0.483909
C	-3.235120	-2.806519	0.574642
C	-2.048765	-2.883119	-2.303294
H	-1.244999	-3.274853	-2.943421
H	-2.133474	-1.799813	-2.460346
H	-2.993719	-3.349926	-2.622320
H	-4.030771	-3.554248	0.431312
H	-3.629696	-1.824313	0.290060
H	-2.980413	-2.789744	1.644787
C	-2.147387	1.062622	-0.533031
C	-2.884379	1.565724	0.581776
C	-3.248771	0.709517	1.662965

H	-2.988983	-0.345000	1.606264
H	-4.188401	0.474467	3.578589
C	-3.936354	1.178635	2.780694
C	-4.309999	2.522445	2.889493
H	-4.852335	2.888661	3.762670
C	-3.969054	3.385428	1.835039
H	-4.238580	4.443568	1.892255
C	-3.275433	2.935047	0.717240
H	-3.012349	3.652559	-0.058716
C	-1.760829	1.799178	-1.685272
F	-0.508462	2.666176	-1.548829
F	-1.396893	1.020881	-2.762189
F	-2.654250	2.731551	-2.127937
C	2.727316	1.694702	0.170393
C	4.041952	1.363017	0.530335
H	4.297670	0.331521	0.778205
C	5.017239	2.360016	0.588865
H	6.039042	2.099086	0.869710
C	4.683569	3.685727	0.294696
H	5.447480	4.463920	0.343053
C	3.371982	4.013638	-0.061593
H	3.107993	5.046383	-0.295475
H	1.367777	3.263857	-0.426489
C	2.389444	3.023693	-0.128497

C	0.733091	0.771124	2.514668
C	2.089844	0.879137	3.231268
C	0.047452	2.146264	2.489865
C	-0.142155	-0.251853	3.253217
H	-0.326347	0.094688	4.278893
H	-1.119475	-0.359935	2.763536
H	0.349881	-1.234361	3.303110
H	-0.917109	2.103443	1.970727
H	-0.130802	2.483142	3.521314
H	0.684057	2.890975	1.993285
H	1.905950	1.117661	4.288437
H	2.714187	1.677216	2.813005
H	2.648981	-0.065583	3.187138

6) TS_2

85

C	-2.536070	0.184205	0.120761
C	-2.951131	-0.714393	-0.868436
F	-1.618305	-1.260639	-1.569862
Si	0.077658	-0.661125	0.100289
O	-1.360741	-0.230141	0.813779
F	-3.737981	-0.249428	-1.858225
F	-3.468369	-1.985713	-0.566775
C	-3.114980	1.442259	0.472841
C	-4.439673	1.825855	0.105219

C	-4.989957	3.029453	0.531181
C	-4.269772	3.916955	1.347286
C	-2.968235	3.560590	1.719782
C	-2.400546	2.360188	1.292923
H	-1.393535	2.092677	1.610622
H	-5.052111	1.151940	-0.494176
H	-6.016460	3.269307	0.240889
H	-4.721271	4.847257	1.695664
H	-2.382843	4.228099	2.358790
C	1.685181	0.726499	2.397350
C	3.207602	0.551246	2.542888
C	0.960474	-0.330114	3.245635
H	1.201492	-1.345878	2.902275
H	-0.128765	-0.194093	3.192651
H	1.274573	-0.238278	4.294011
C	1.279049	2.126612	2.885802
H	1.817719	2.921529	2.356072
H	0.200087	2.288397	2.765302
H	1.515816	2.212904	3.956165
H	3.487377	0.648309	3.601894
H	3.752823	1.320448	1.980321
H	3.530593	-0.438144	2.192759
C	2.100862	2.515458	-0.226255
C	3.498025	2.589558	-0.308001

C	4.123120	3.833921	-0.406218
C	3.358494	5.004492	-0.416540
C	1.964212	4.930033	-0.327992
C	1.331334	3.689495	-0.234513
H	0.243763	3.628022	-0.156297
H	1.364890	5.841901	-0.332229
H	3.850089	5.975966	-0.494587
H	5.210809	3.887364	-0.478975
H	4.092982	1.675623	-0.323709
C	1.414177	1.204937	-0.126665
N	1.274279	0.472425	0.988484
N	0.760172	0.557435	-1.123828
C	0.624573	0.909589	-2.574791
C	1.829004	1.714034	-3.096920
C	-0.668433	1.719103	-2.764079
C	0.568755	-0.398231	-3.386343
H	1.523383	-0.939662	-3.331063
H	0.388945	-0.147416	-4.441269
H	-0.826774	1.925661	-3.832631
H	-0.605012	2.679101	-2.233194
H	-1.536193	1.171116	-2.377697
H	1.750532	1.760054	-4.192132
H	1.854414	2.742765	-2.722598
H	2.781669	1.223898	-2.849720

H	-0.236460	-1.057552	-3.051466
C	3.346531	-1.398792	-0.928528
H	2.946114	-0.941116	-1.838918
H	4.313317	-1.862443	-1.180545
H	3.539809	-0.614090	-0.186946
Si	2.275885	-2.796867	-0.223190
C	2.233903	-4.157600	-1.540490
H	1.759877	-3.782623	-2.459669
H	3.264906	-4.458857	-1.781980
H	1.689953	-5.055561	-1.219173
H	-0.642546	-4.898233	-1.513524
C	-1.391436	-4.418465	-0.867376
H	-1.941558	-3.674247	-1.453467
H	-2.099216	-5.194317	-0.534860
H	1.120605	-5.546013	0.935940
C	0.366768	-5.029980	1.544029
H	-0.398518	-5.774344	1.816458
H	0.836625	-4.681348	2.474121
H	2.991527	-4.409335	1.608641
C	-1.833443	-3.050848	1.932517
H	-2.562798	-2.335392	1.544138
H	-1.324523	-2.598706	2.795782
H	-2.375440	-3.942699	2.285841
Si	-0.577602	-3.642330	0.651166

H	2.992973	-2.732055	2.189672
N	0.577799	-2.302055	0.171357
C	3.215068	-3.374258	1.325495
H	4.295278	-3.303680	1.124616

7) Pdt

85

Si	4.449362	4.723617	18.912177
Si	2.400679	2.521437	18.542520
Si	5.334318	1.815342	18.033504
F	3.066243	5.370349	18.147008
O	3.959125	5.307088	20.471998
F	4.208506	7.896616	19.483024
F	2.574690	8.632998	20.758446
N	6.327453	4.774030	19.651129
N	5.621498	5.650166	17.799137
N	4.143454	3.019123	18.624566
C	7.909321	6.397369	18.537309
C	6.666191	5.590790	18.658992
C	3.111235	6.303053	20.856586
C	3.279047	7.555239	20.387426
C	8.999872	8.556075	18.714371
H	8.950461	9.620921	18.948721
C	5.512694	6.171796	16.404873
C	7.851509	7.769024	18.827934

H	6.904955	8.213199	19.141563
C	6.936359	4.657054	21.004958
C	10.261437	6.616258	18.000028
H	11.199542	6.165199	17.671333
C	2.157243	5.975486	21.938162
C	4.728136	5.135923	15.576074
H	5.278490	4.186435	15.516373
H	4.591601	5.516729	14.553528
H	3.740992	4.941074	16.008578
C	9.120030	5.822975	18.125851
H	9.161479	4.757907	17.893235
C	10.205053	7.982481	18.296630
H	11.100018	8.599979	18.200627
C	1.314230	3.418153	19.802848
H	1.676933	3.284721	20.830488
H	0.304926	2.980995	19.739808
H	1.235883	4.493061	19.602553
C	4.748335	7.507232	16.423405
H	3.761136	7.378939	16.883614
H	4.616737	7.875829	15.395101
H	5.304474	8.263934	16.994085
C	1.660861	2.807087	16.817172
H	1.613849	3.884615	16.607369
H	0.636002	2.404896	16.783810

H	2.243249	2.323170	16.021766
C	6.219624	3.495513	21.710228
H	5.134003	3.641802	21.705129
H	6.565921	3.423430	22.750909
H	6.439910	2.544191	21.208726
C	6.742787	5.956866	21.811460
H	7.261268	6.797925	21.330410
H	7.164232	5.832982	22.820342
H	5.678809	6.203797	21.903835
C	8.438843	4.319545	20.949807
H	8.628262	3.449150	20.305650
H	8.782048	4.069155	21.964474
H	9.042375	5.161046	20.590719
C	0.912582	6.616159	22.078781
H	0.608687	7.380458	21.363385
C	2.209391	0.681368	18.995809
H	2.724359	-0.023140	18.330478
H	1.132435	0.453989	18.949382
H	2.543553	0.495384	20.026905
C	0.046962	6.263061	23.115573
H	-0.918369	6.765956	23.202812
C	6.876771	6.372101	15.725188
H	7.454910	7.192698	16.164918
H	6.696888	6.617052	14.668433

H	7.485091	5.457262	15.758983
C	1.632073	4.614108	23.889719
H	1.918616	3.827741	24.591227
C	0.400480	5.262717	24.027034
H	-0.281582	4.986655	24.833445
C	2.500270	4.963974	22.855604
H	3.455276	4.449998	22.746669
C	4.731751	1.028162	16.405582
H	3.773702	0.498512	16.483048
H	5.489781	0.299848	16.076838
H	4.634113	1.791777	15.619652
C	5.654275	0.422983	19.286374
H	6.104384	0.812751	20.209383
H	6.361650	-0.296512	18.844123
H	4.742375	-0.121789	19.559410
C	7.044782	2.510301	17.585919
H	6.990479	3.367383	16.902696
H	7.586985	1.701122	17.071940
H	7.621466	2.803822	18.4699

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