Supporting Information for Syntheses, Characterization, and Reactivity of Diruthenium Hydrido Complexes

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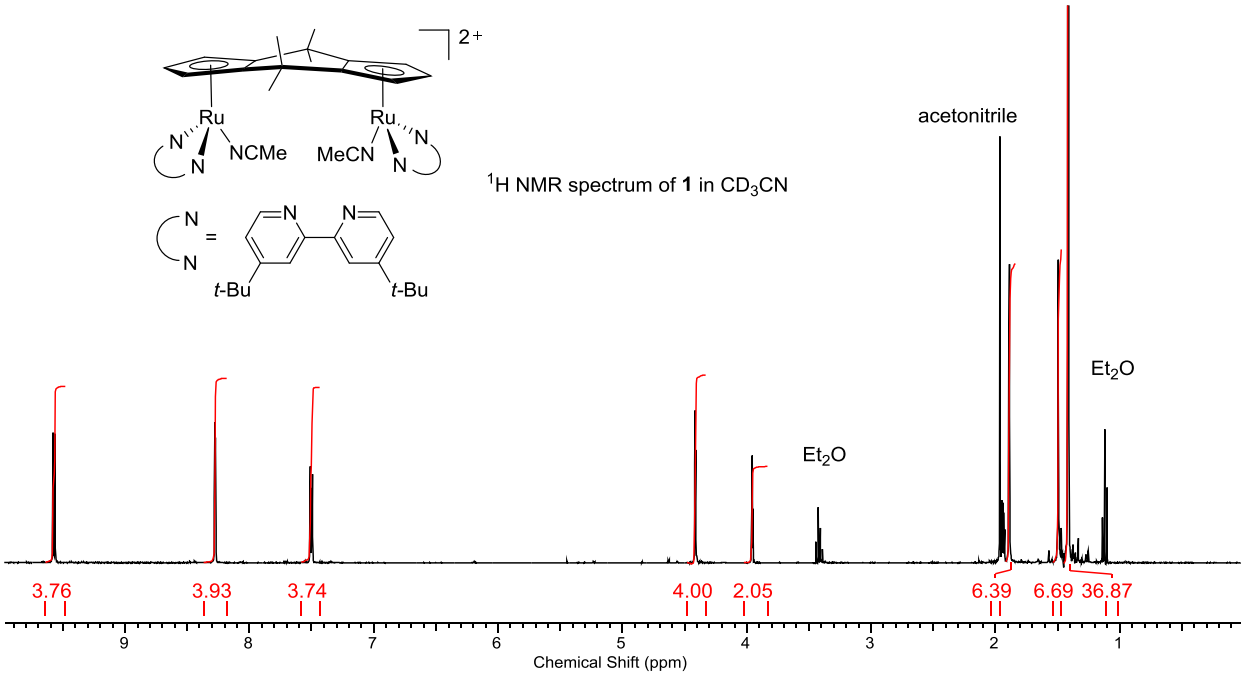

Figure S1. ^{1}H NMR spectrum of **1** in CD_3CN

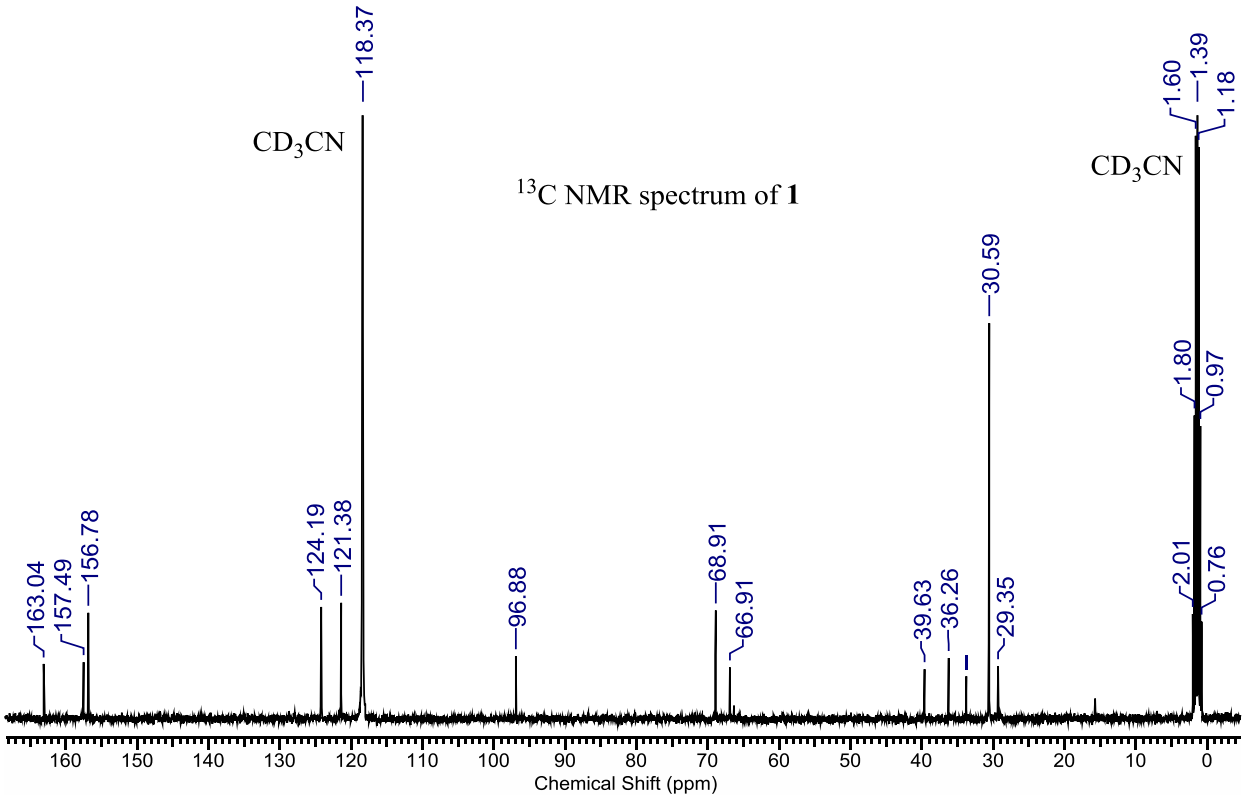

Figure S2. ^{13}C NMR spectrum of **1** in CD_3CN

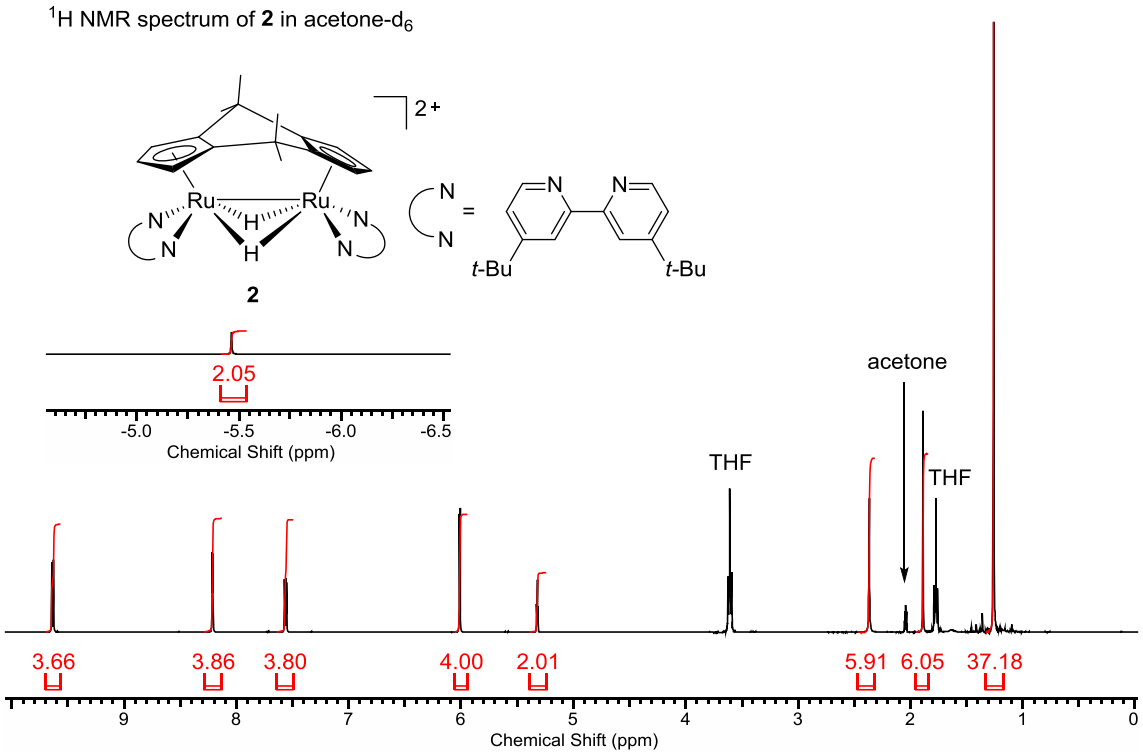

Figure S3. ^{1}H NMR spectrum of **2** in acetone-d$_6$

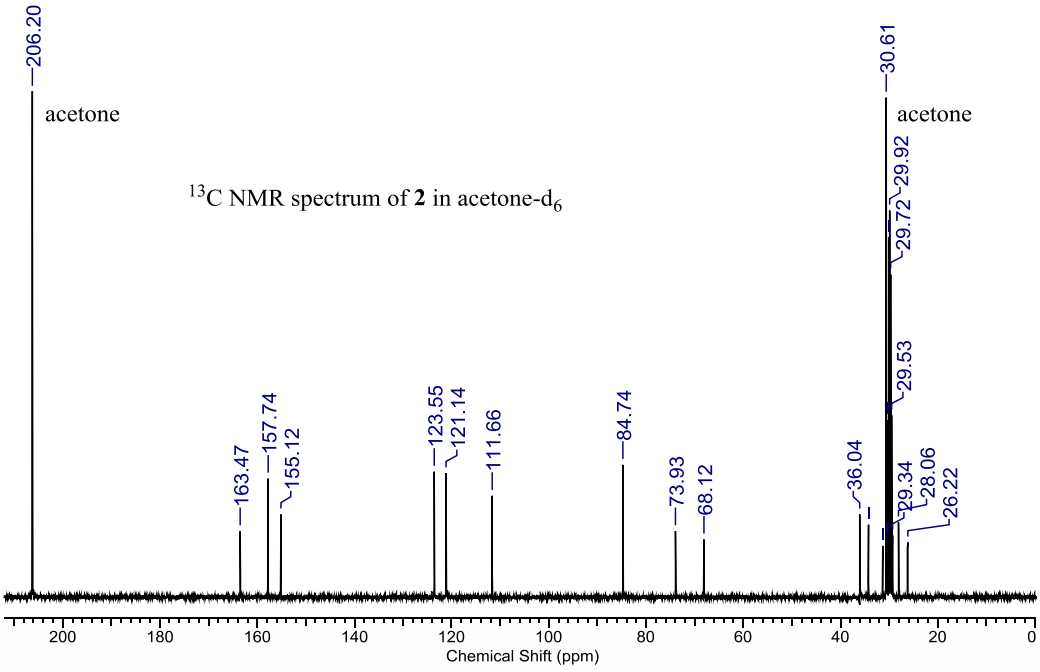

Figure S4. ^{13}C NMR spectrum of **2** in acetone-d$_6$

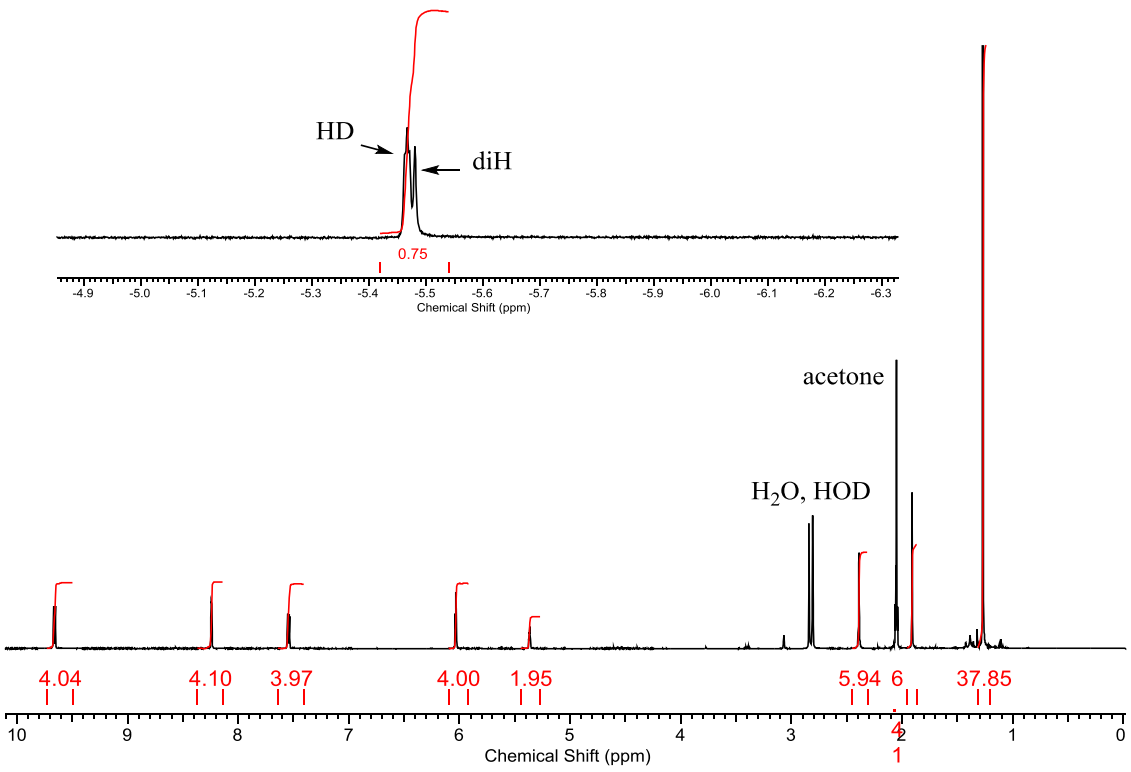

Figure S5. ^{1}H NMR spectrum of **2**-HD in acetone-d$_6$.

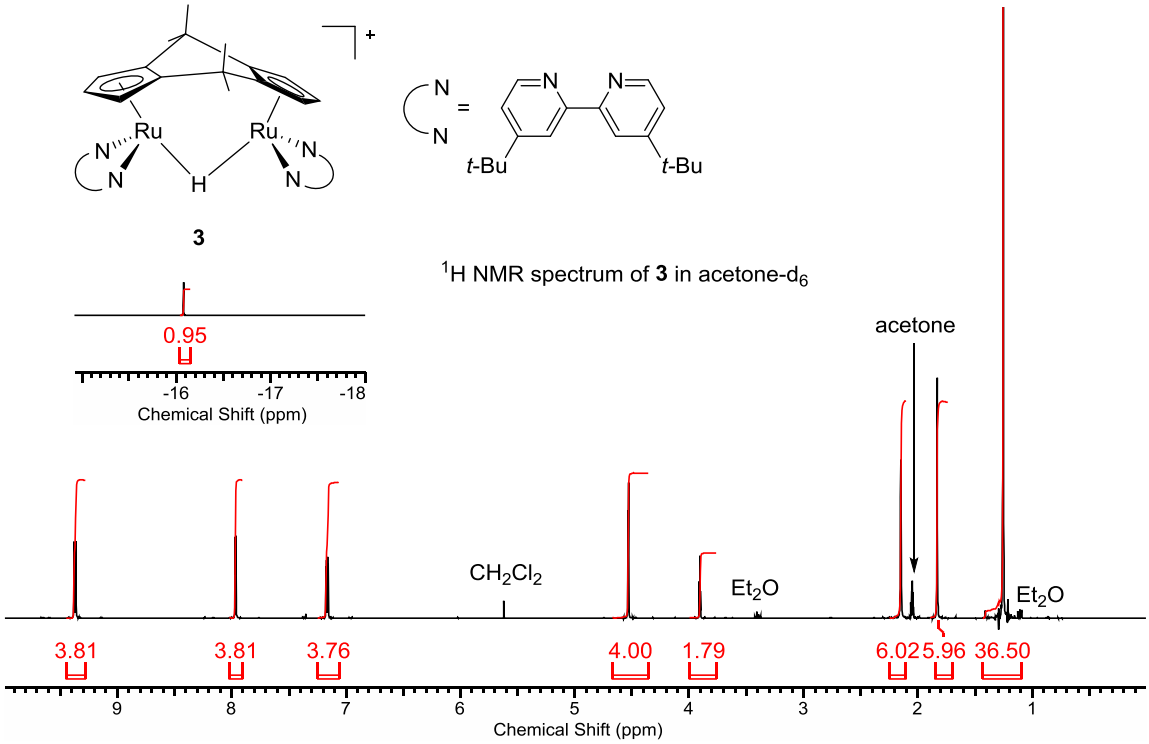

Figure S6. ^{1}H NMR spectrum of **3** in acetone-d$_6$

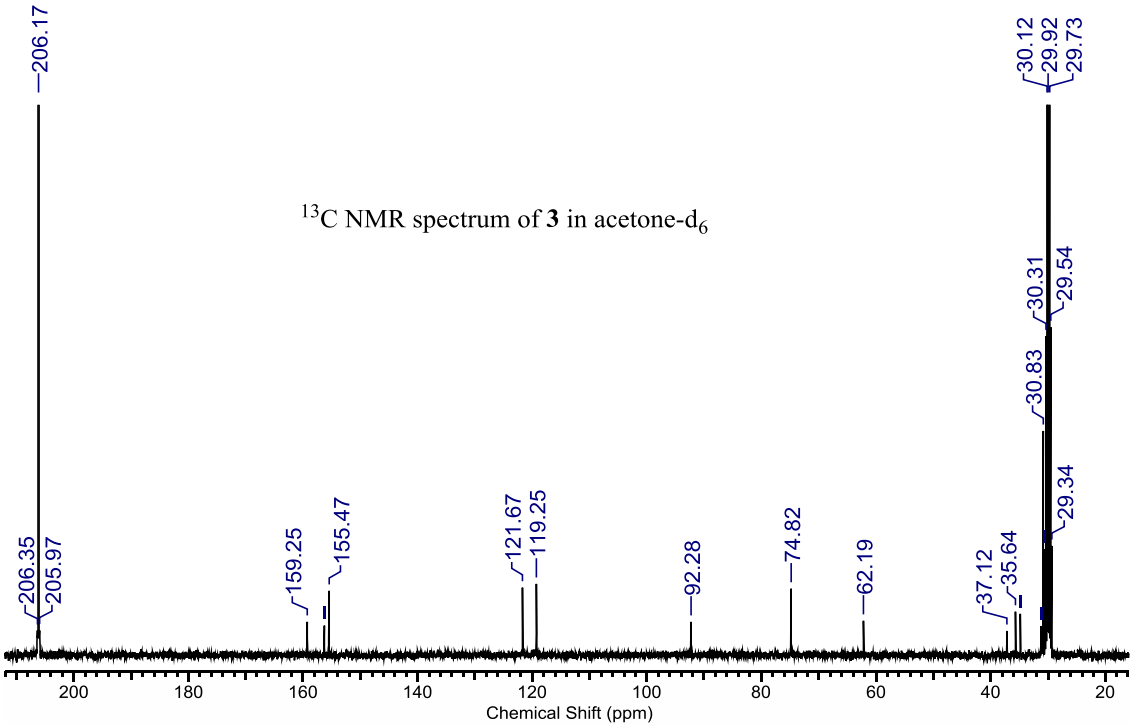

Figure S7. ^{13}C NMR spectrum of **3** in acetone-d$_6$

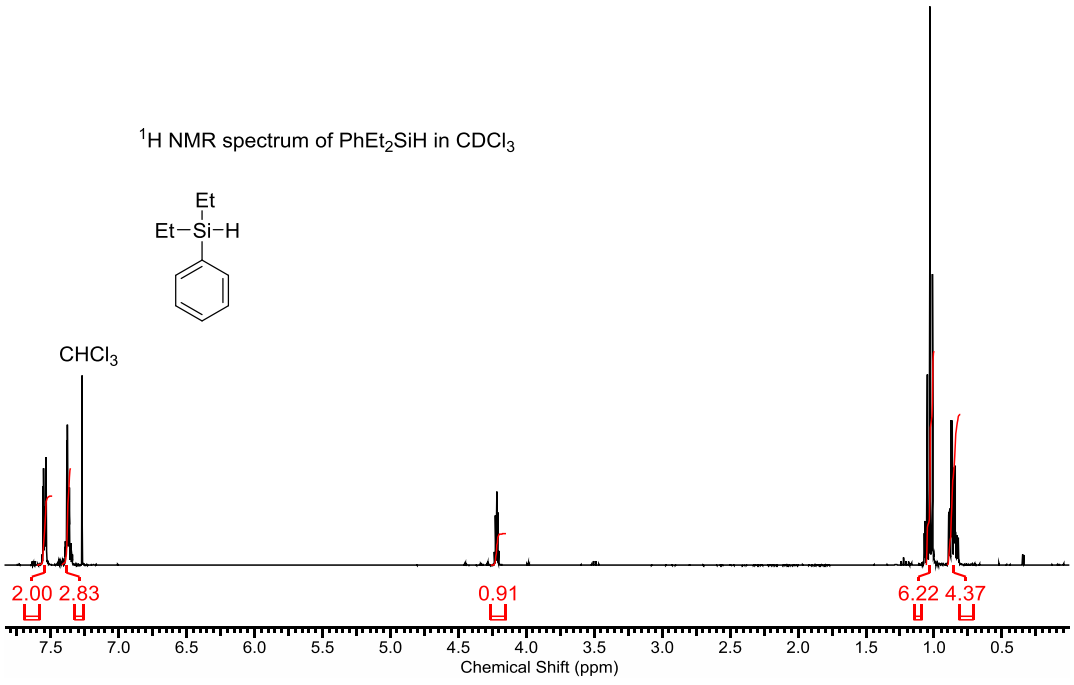

Figure S8. ^{1}H NMR spectrum of independently synthesized PhEt$_3$SiH in CDCl$_3$

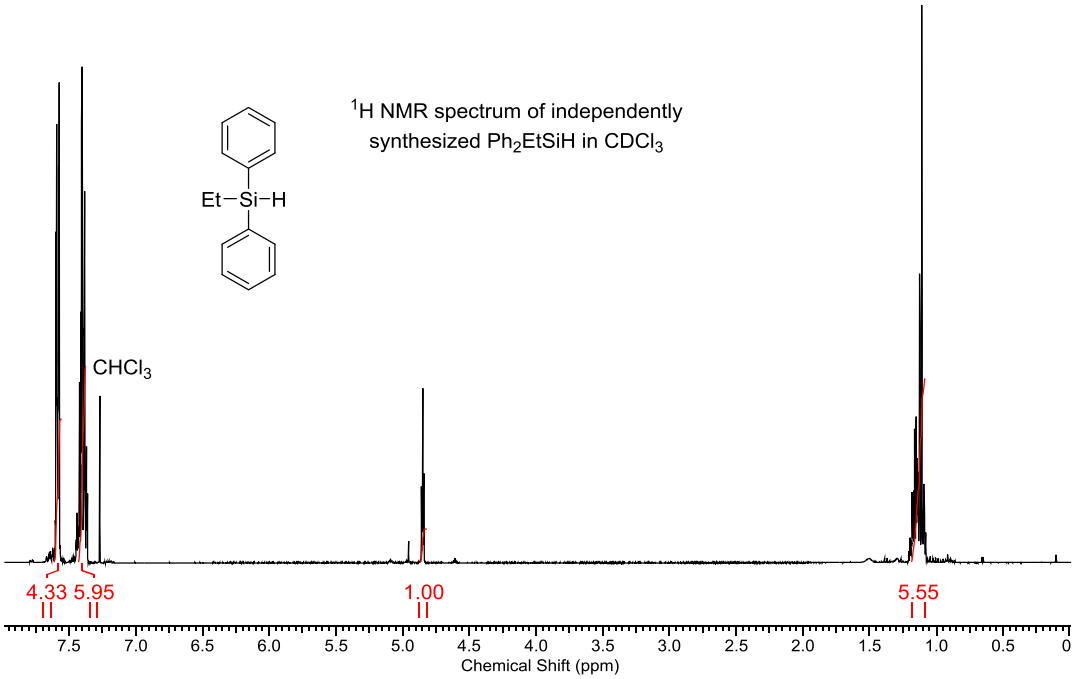

Figure S9. ^{1}H NMR spectrum of Ph_2EtSiH in $CDCl_3$

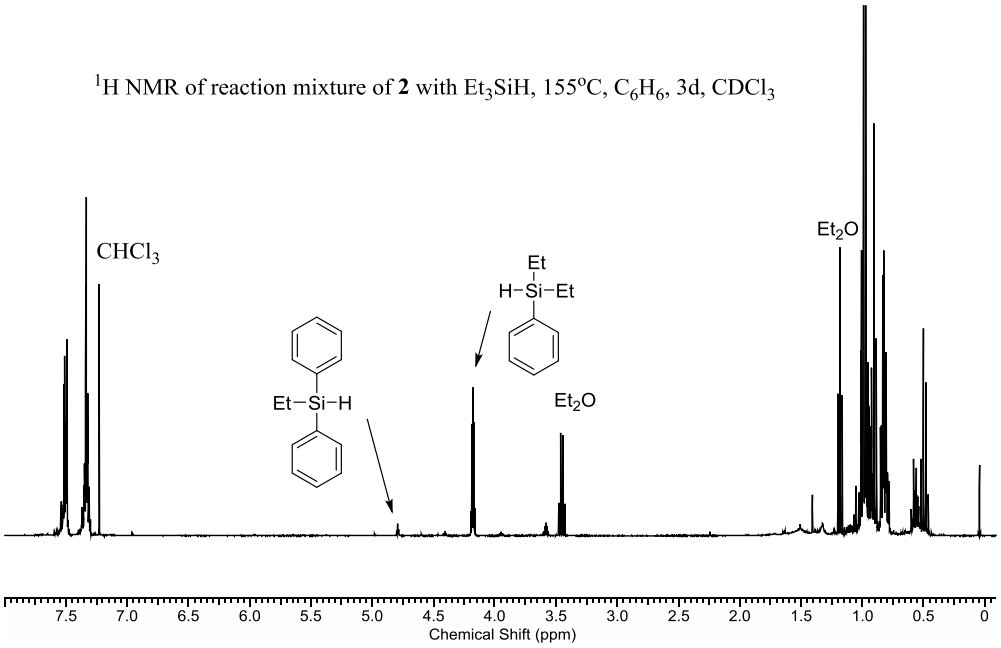

Figure S10.^{1}H NMR spectrum of a typical crude reaction mixture of **2** with C_6H_6 and Et_3SiH in $CDCl_3$

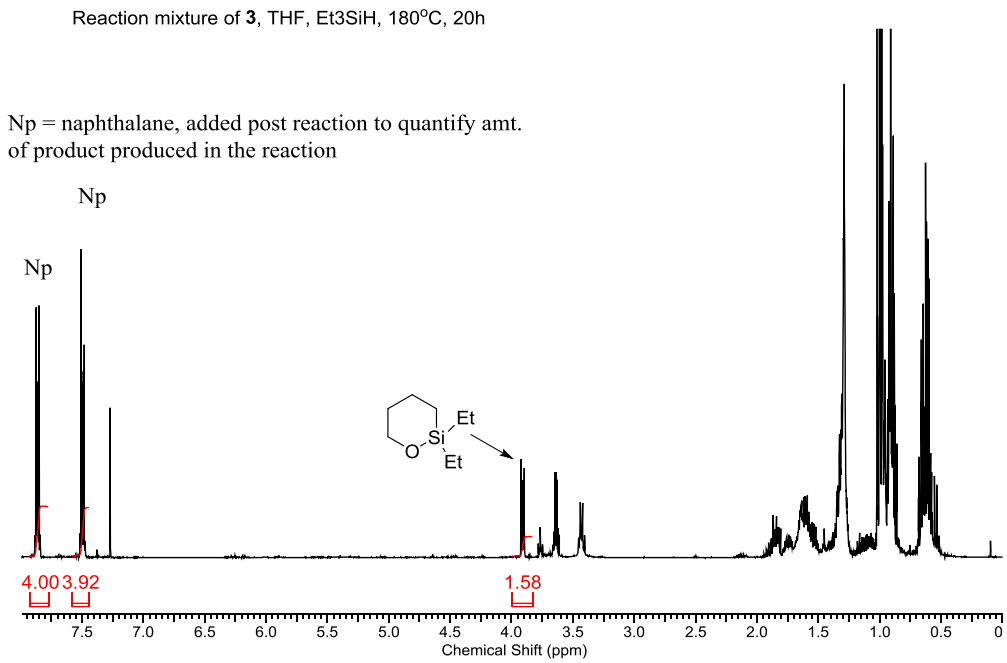

Figure S11. ^{1}H NMR spectrum of a typical crude reaction mixture of **3**, THF and Et_3SiH in $CDCl_3$

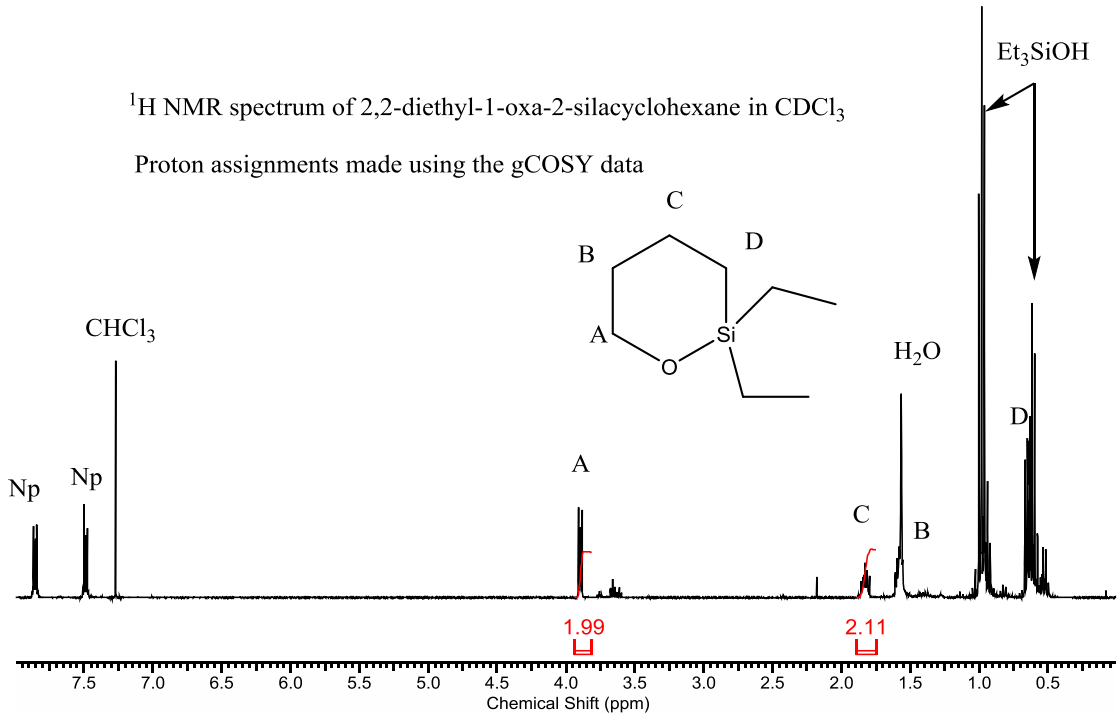

Figure S12. ^{1}H NMR spectrum of 2,2-diethyl-1-oxa-2-silacyclohexane after a vacuum transfer from the reaction mixture.

gCOSY spectrum for 2,2-diethyl-1-oxa-2-silacyclohexane, $CDCl_3$

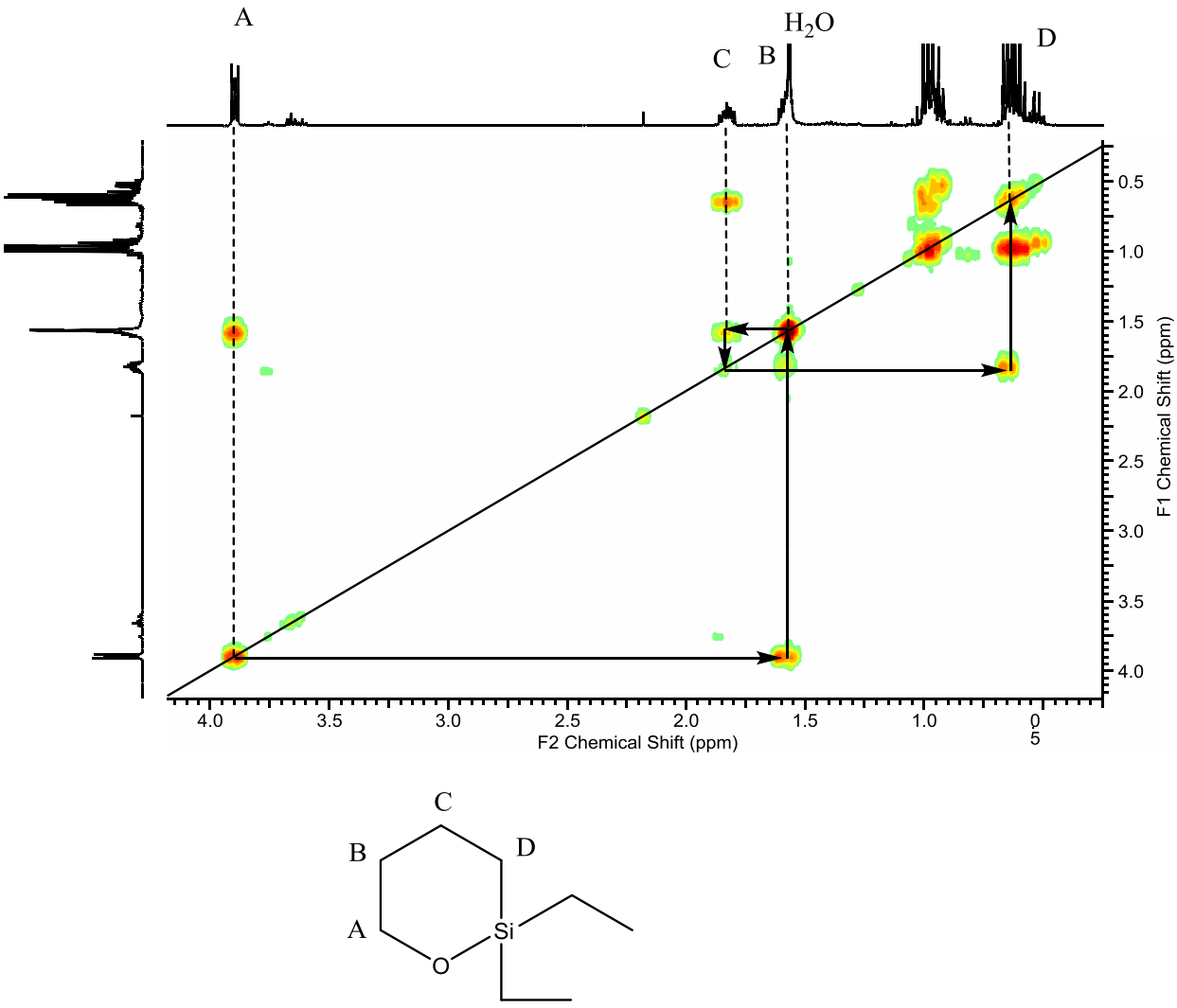

Figure S13. gCOSY spectrum of 2,2-diethyl-1-oxa-2-silacyclohexane, $CDCl_3$

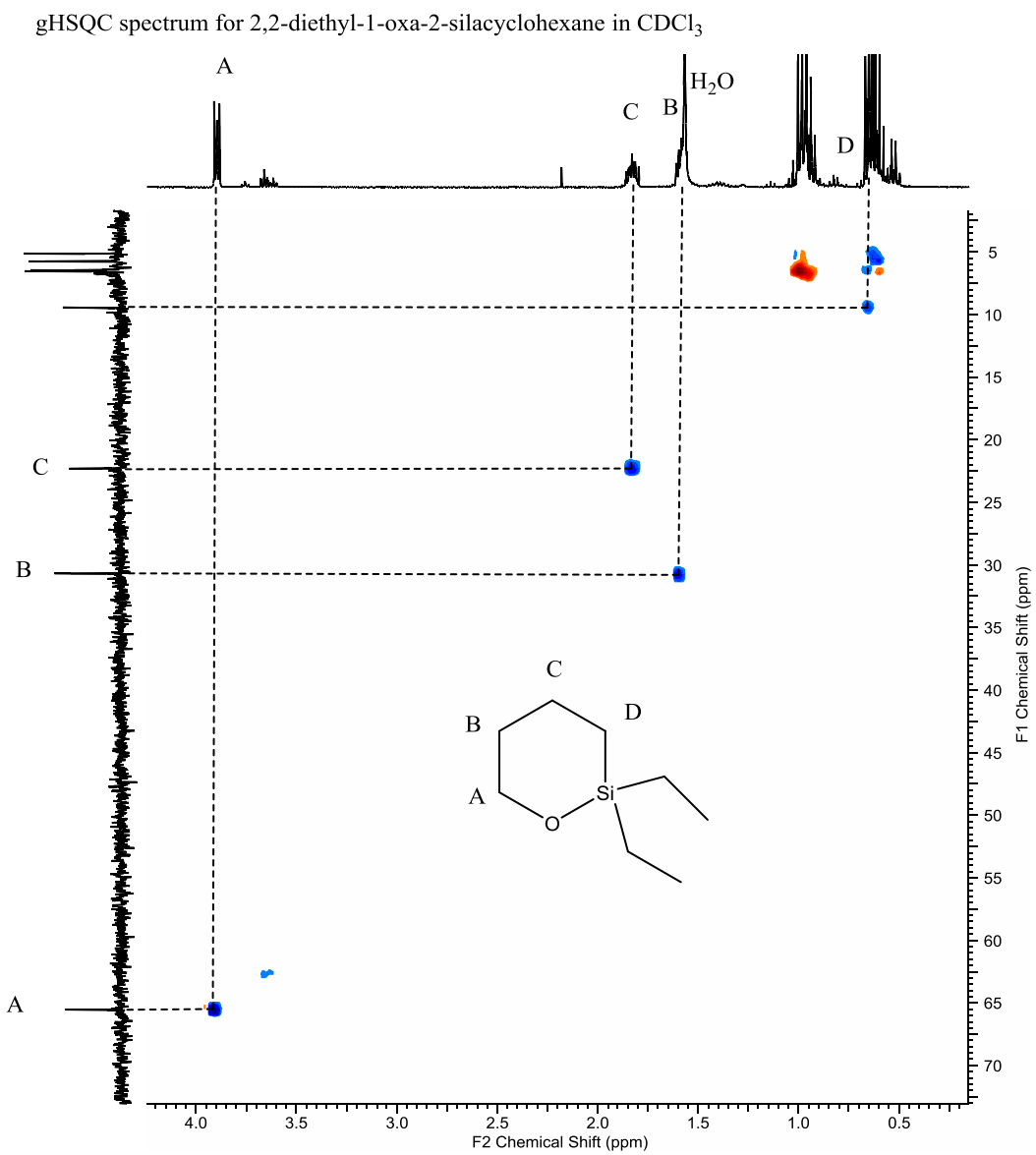

Figure S14. gHSQC spectrum of 2,2-diethyl-1-oxa-2-silacyclohexane, $CDCl_3$

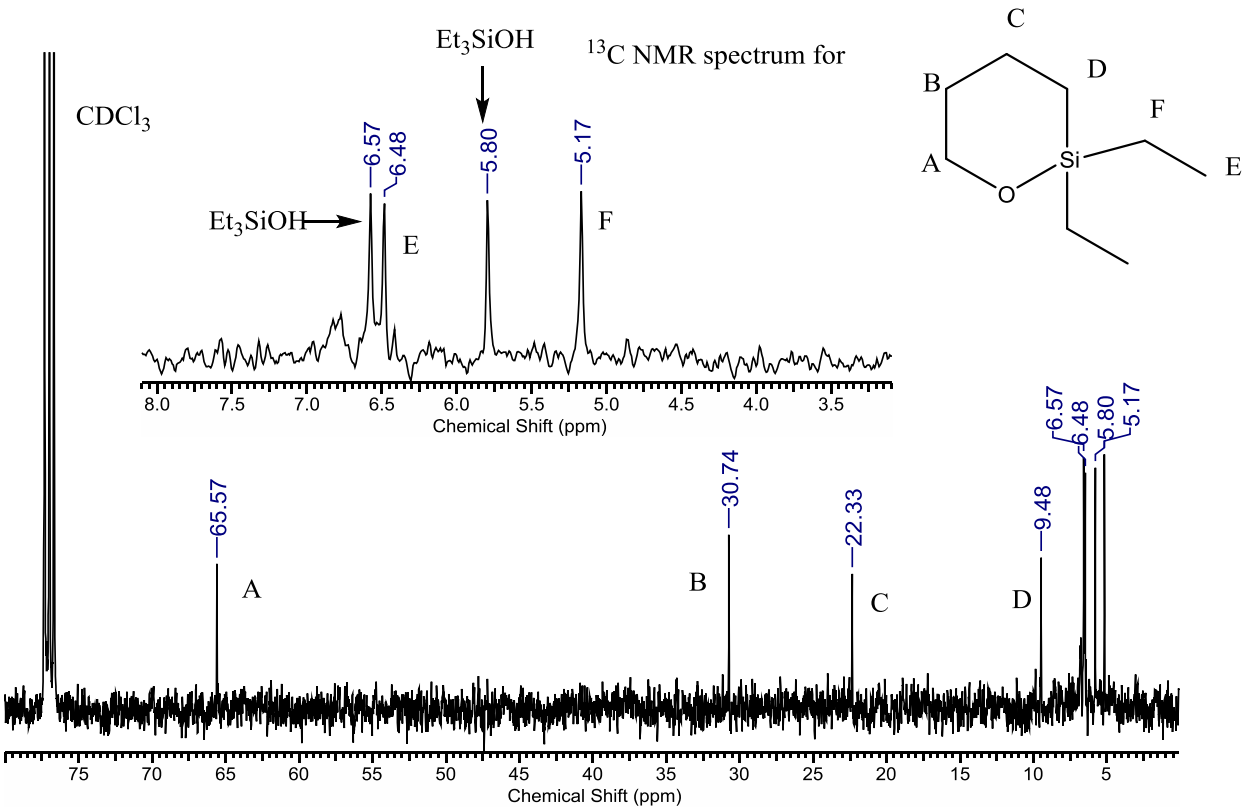

Figure S15. ^{13}C NMR spectrum for 2,2-diethyl-1-oxa-2-silacyclohexane, $CDCl_3$. Spectral data for Et_3SiOH (δ 6.57, 5.80) was obtained from the work of Nojima and co-workers.[1]

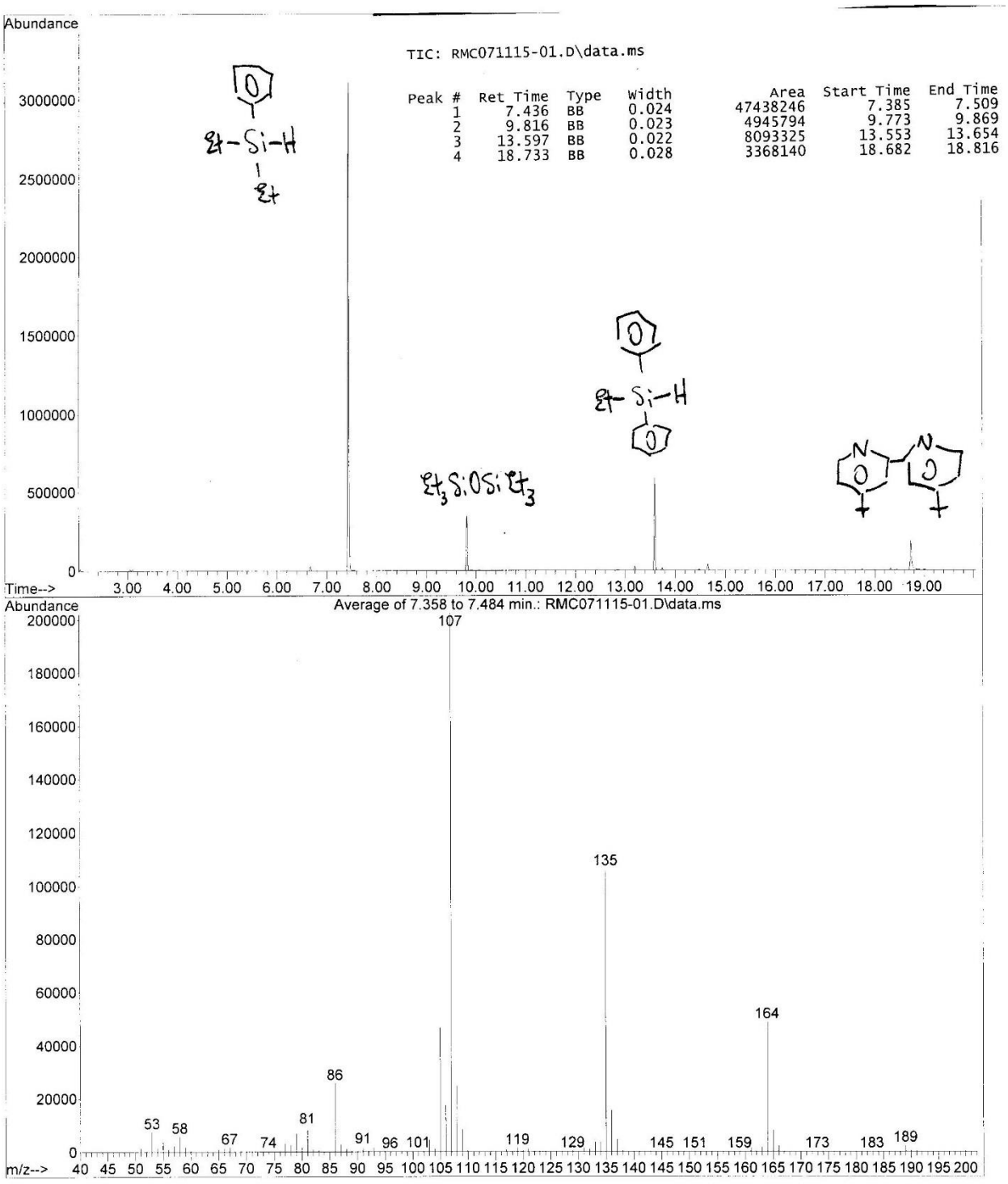

Figure S16. Typical GCMS trace for the crude reaction mixture of **3**, Et_3SiH and C_6H_6.

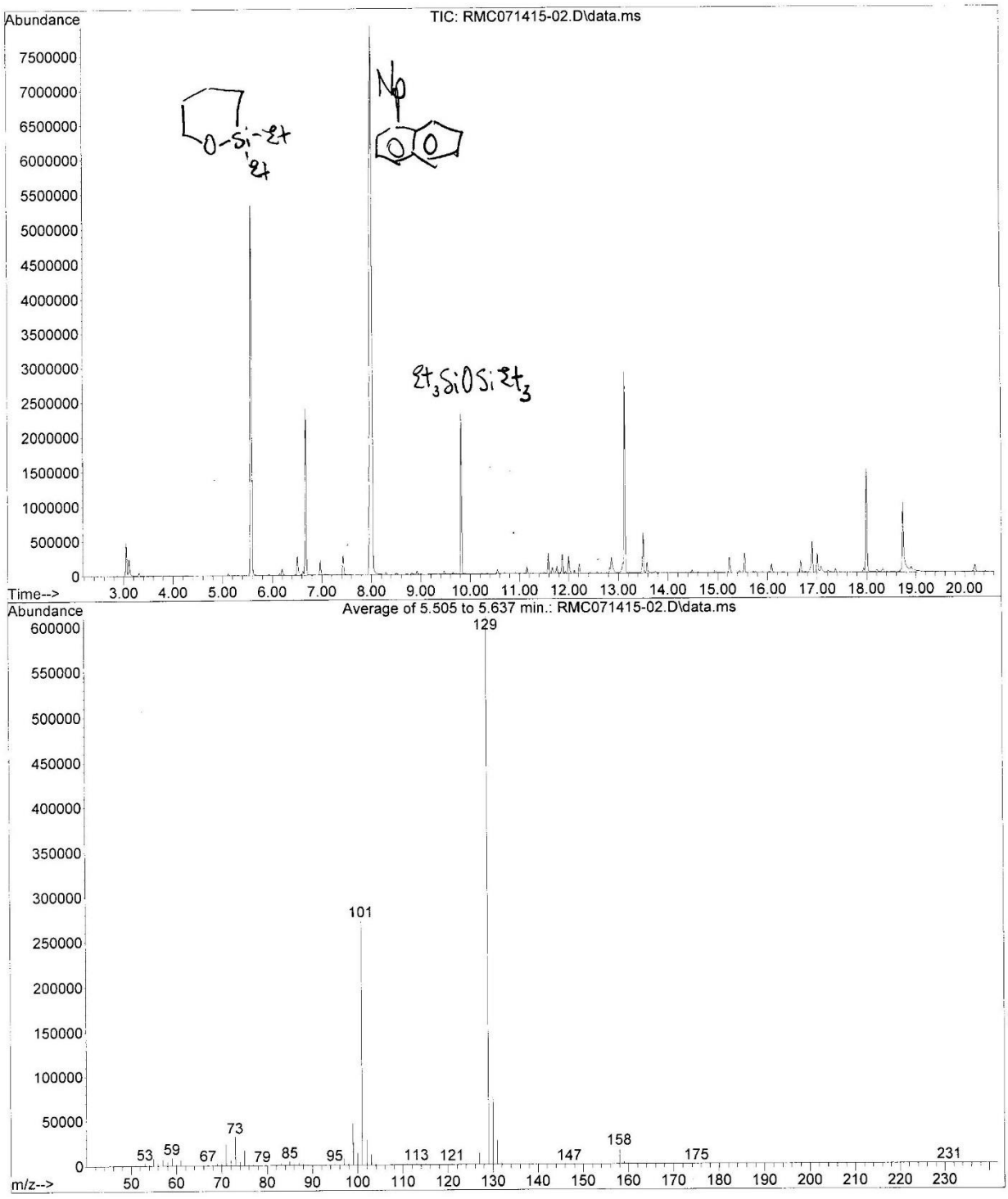

Figure S17. Typical GCMS trace for the reaction of **3**, THF and Et_3SiH

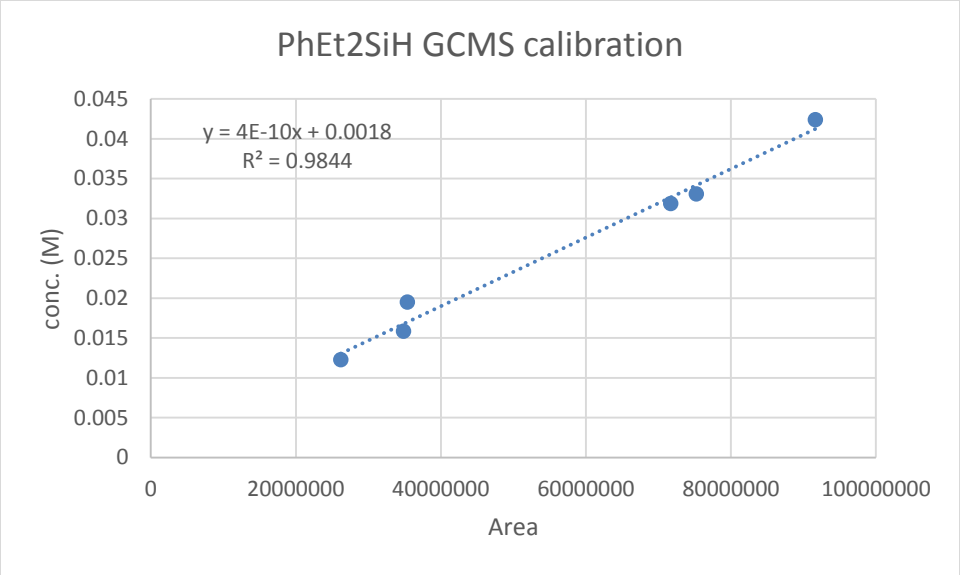

Table S1. GC/MS Calibration Curve for $PhEt_2SiH$

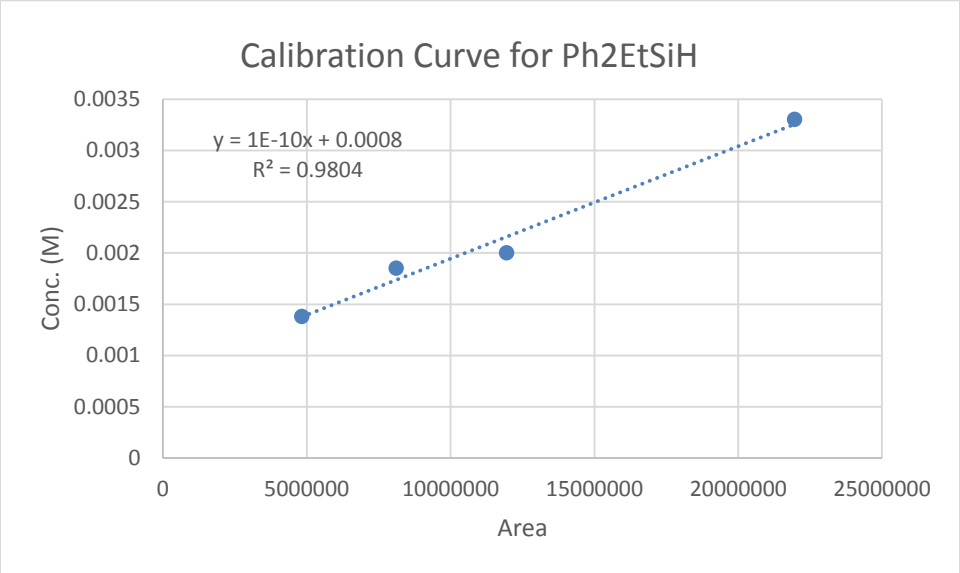

Table S2. GC/MS Calibration Curve for Ph_2EtSiH

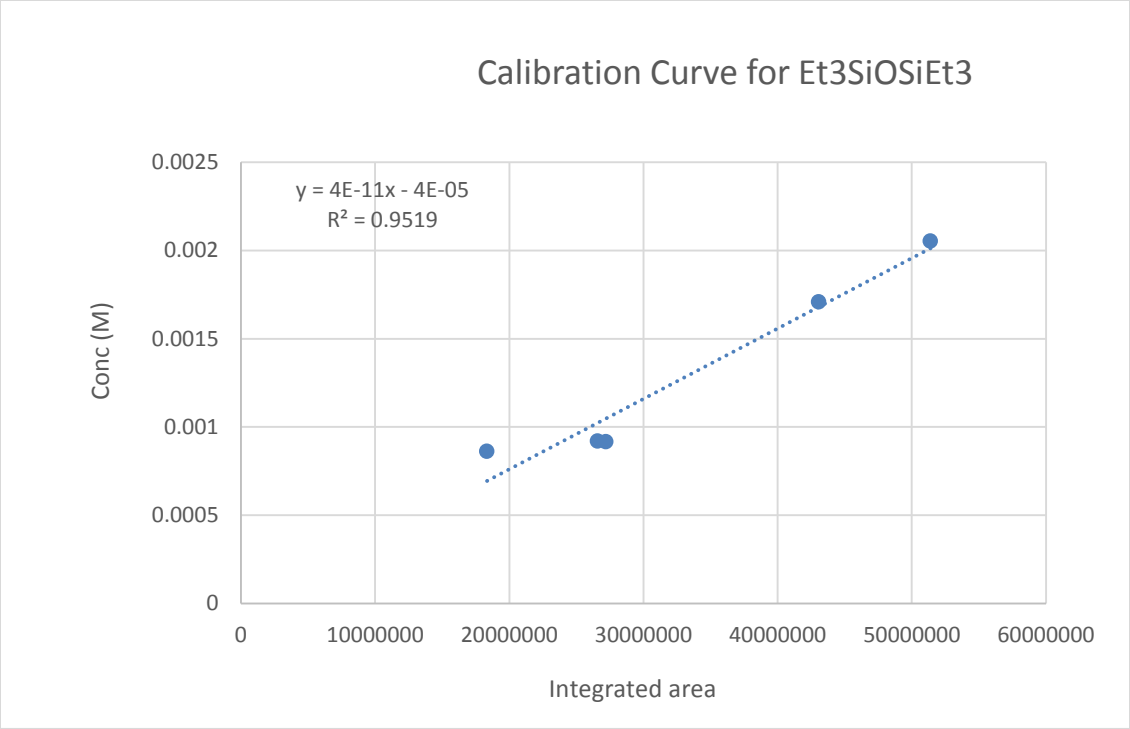

Table S3. GC/MS Calibration Curve for $Et_3SiOSiEt_3$.

Table S4: Crystal data summary for structures **1**, **2**, and **3**.

	1	**2**[a]	**3**
Formula	$C_{60}H_{75}F_6N_7O_6Ru_2S_2$	$C_{54}H_{68}F_6N_4O_6Ru_2S_2$	$C_{68}H_{82}F_3N_4O_3Ru_2S$
fw	1370.53	1249.38	1294.57
T (K)	173(2)	173(2)	100.0(5)
cryst syst	monoclinic	orthorhombic	*orthorhombic*
space group	$P2_1/n$	*Pnma*	*Fdd*2
a (Å)	16.5443(15)	17.5416(14)	38.385(4)
b (Å)	17.1285(15)	19.6877(15)	40.031(4)
c (Å)	22.7127(19)	18.0574(14)	16.3398(15)
α (deg)	90	90	90
β (deg)	103.0048(17)	90	90
γ (deg)	90	90	90
V (Å^3)	6271.2(9)	6236.2(8)	25107(4)
Z	4	4	16
ρ_{calcd} (g cm^{-3})	1.452	1.331	1.370
μ (mm^{-1})	0.620	0.615	0.572
color, shape	red, plate	orange, needle	purple, plate
reflns collected	221378	179041	144900
reflns independent	34762	12191	29710
R_{int}[b]	0.0637	0.0714	0.0891
reflns observed	23759	8101	21423
number of parameters	828	395	893
GOF[c] on F^2	1.011	1.025	0.989
$R1$ [$I > 2\sigma(I)$][d]	0.0412	0.0449	0.0504
$wR2$[e]	0.0989	0.1420	0.1124

[a]Due to the use of the SQUEEZE routine,[2] certain values in this column are known to be incorrect (see *Single crystal X-ray diffraction* and *Supporting Information*). [b]$R_{int} = \Sigma |F_o^2 - \langle F_o^2 \rangle| / \Sigma F_o^2$. [c]GOF = $S = [\Sigma w(F_o^2 - F_c^2)^2 / (m - n)]^{1/2}$, where $w = 1 / [\sigma^2(F_o^2) + (aP)^2 + bP]$, $P = 1/3 \max(0, F_o^2) + 2/3F_c^2$, m = number of independent reflections, and n = number of parameters. [d]$R1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$. [e]$wR2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma wF_o^2]^{1/2}$.

References

(1) Tokuyasu, T.; Kunikawa, S.; Masuyama, A.; Nojima, M., *Organic Letters* 2002, *4* (21), 3595-3598.
(2) Spek, A., *Acta Crystallographica Section D* 2009, *65* (2), 148-155.