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Electronic Supplementary Information

Iron-Catalyzed *(E)*-Selective Hydrosilylation of Alkynes: Scope and Mechanistic Insights

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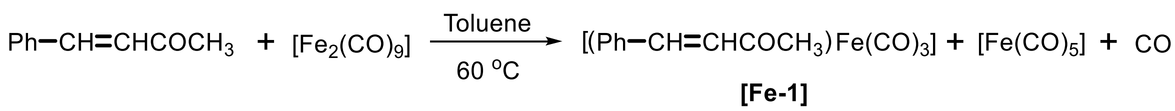
1. Methods and materials:

All manipulations were carried out under an inert atmosphere using standard Schlenk technique, cannula filtration or m-Braun glove box. Solvents were dried by standard procedures unless otherwise mentioned.[1a] THF was dried on sodium/benzophenone. Di-iron nonacarbonyl, organosilanes, diphenyl acetylene were purchased from Sigma-Aldrich. All other reagents/chemicals, solvents were purchased from local suppliers (Spectrochem Pvt. Ltd.; Avra Synthesis Pvt. Ltd.; Thomas Baker Pvt. Ltd. etc). Other alkynes (1b-1i) were prepared from literature procedure.[1b] Solution NMR spectra were recorded on a Bruker Avance 200, 400 and 500 MHz instruments at 298K unless mentioned otherwise. Chemical shifts are referenced to external reference TMS (^{1}H and ^{13}C) or or 85% H_3PO_4 (Ξ = 40.480747 MHz, ^{31}P). Coupling constants are given as absolute values. Multiplicities are given as follows s: singlet, d: doublet, t: triplet, m: multiplet, quat: quaternary carbon. Mass spectra were recorded on Thermo Scientific Q-Exactive mass spectrometer with Hypersil gold C18 column 150 x 4.6 mm diameter 8 μm particle size mobile phase used is 90% methanol + 10% water + 0.1% formic acid. The GC conversion of the products were determined by HP-5 column (30 m) on an Agilent 7890B GC system.

2. Synthesis of iron complex [Fe(CO)$_3$BDA] and [HFe(CO)$_4$SiPh$_3$]:

We began with the synthesis of [Fe(CO)$_3$(BDA)] complex by following a known literature procedure (scheme S1).[1c] 2.01 g (0.0137 mol) of benzylideneacetone, 5 g (0.0137 mol) of [$Fe_2(CO)_9$] were suspended in dry toluene (30 ml) in a Schlenk flask. The above suspension was heated at 60 °C for 5 hours, after which volatiles were evaporated under vacuum. Then the residue was purified by silica gel column chromatography, eluting with pet ether/ethyl acetate (99/1). The product [Fe-1] was obtained as orange red crystals (1.25 g, 32%). $Fe(CO)_5$ also formed as side product which is used in the synthesis of [Fe-3].



Scheme S1: Synthesis of [(Ph-CH=CHCOCH$_3$)Fe(CO)$_3$].

^{1}H NMR (500 MHz, CDCl$_3$): δ = 7.2 (m, 4H), 7.13 (m, 1H), 5.98 (d, J = 9.7 Hz, 1H, Ph-CH), 3.05 (d, J = 9.7 Hz, 1H, =CHCO), 2.48 (s, 3H, -CH$_3$).

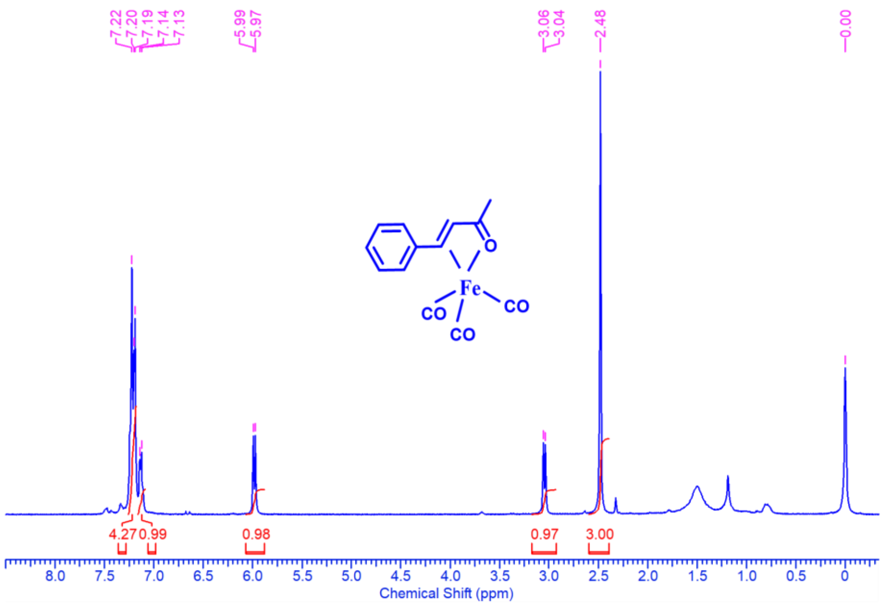


Figure S1: ^{1}H NMR spectrum of **[Fe(CO)$_3$BDA]**.

The iron catalyst [HFe(CO)$_4$SiPh$_3$] or [Fe-3] was prepared by a modified literature procedure.[2] [Fe(CO)$_5$] (3.63g, 2.5 mL, 0.018 mol) and [(C$_6$H$_5$)$_3$SiH] (4.3 g, 0.016 mol) were taken in a Schlenk tube, and 35 ml of n-heptane was added to it. The Schlenk tube was linked to a silicon oil bubbler, and the reaction mixture was exposed to UV radiation for eight hours while being constantly stirred at a temperature of 15-20 °C using a pyrex filtered medium pressure mercury vapour lamp (450 W) with a pyrex filter (hv > 300). Initially, the rate of evolution of carbon monoxide was rapid (i.e., one bubble/4 sec.). But it had nearly ceased at the end of the reaction. The reaction mixture was then run through a celite pad after that. Vacuum was used to evaporate the yellow filtrate, which decreased the volume of the solution to 10-15 ml. This concentrated filtrate was left overnight for crystallization at 0 °C. White coloured crystals were obtained (yield ~70 %) and separated with the help of cannula filtration and were washed with ice-cold pentane before drying under vacuum. The crystalline compound was characterized by ^{1}H NMR spectroscopy. The crystalline compound was stable only below 10 °C.

[HFe(CO)$_4$(SiPh$_3$)]

^{1}H NMR (500 MHz, C$_6$D$_6$): δ = 7.46 (m, 6H), 6.93 (m, 9H), -9.18 (s, 1H).

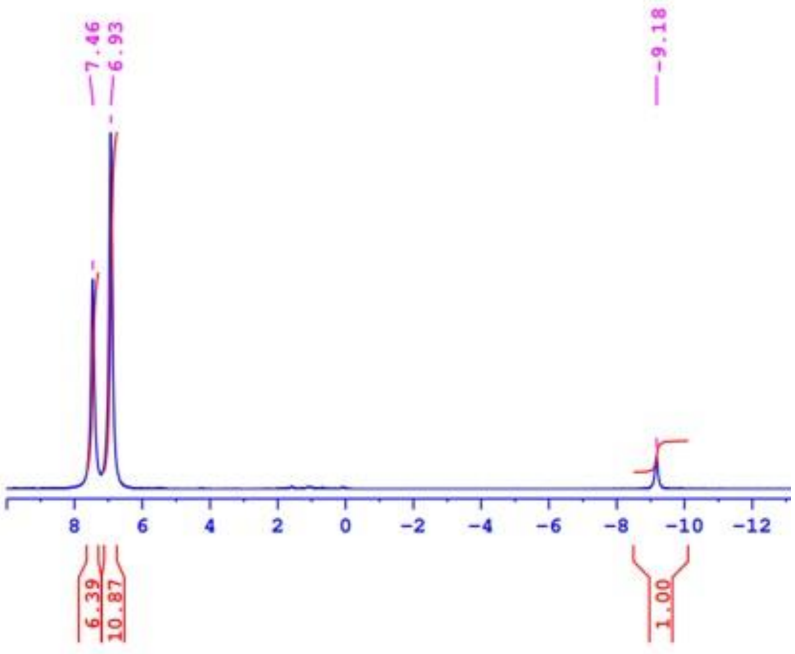
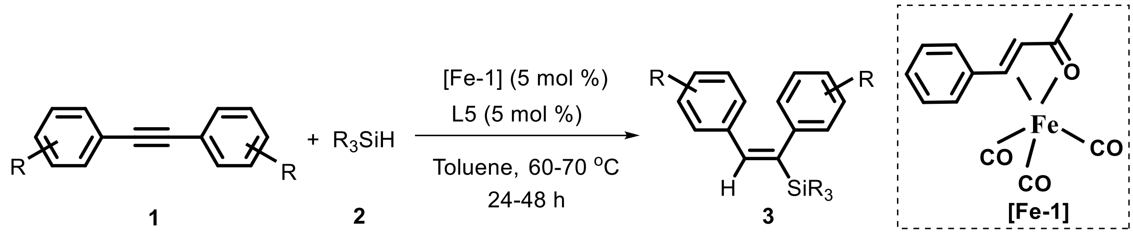


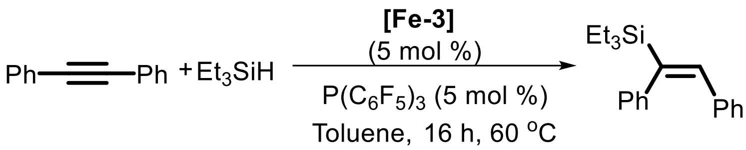
Figure S2. ^{1}H NMR spectrum of $[HFe(CO)_4(SiPh_3)]$.

3. General procedure for iron catalyzed hydrosilylation of alkynes:



Scheme S2: Fe-1 catalyzed Hydrosilylation of internal alkynes.

GP 1: Alkyne **1** (0.25 mmol), silane **2** (0.375 mmol), [Fe-1] (3.575 mg, 0.0125 mmol, 5 mol %), L5 (6.8 mg, 0.0125 mmol, 5 mol %) were introduced in a 10 mL teflon-valved flask equipped with a magnetic stir bar under argon atmosphere. Toluene (1 mL) was added to the reaction mixture. The reaction mixture was stirred at 60-70 °C for 24-48 h. The mixture was extracted with diethyl ether (3 × 10 mL). After that, the layers of mixed diethyl ether were dried over sodium sulphate and concentrated under vacuum. After evaporation of the solvent, the crude reaction mixture was purified by silica gel column chromatography (petroleum ether/EtOAc 50/1), yielding the hydrosilylated product. The conversion was determined by gas chromatography with respect to starting alkyne.



Scheme S3: [$HFe(CO)_4SiPh_3$] catalyzed hydrosilylation of Diphenylacetylene

GP 2: Alkyne **1a** (44.55 mg, 0.25 mmol), silane **2a** (40 mg, 0.375 mmol), [$HFe(CO)_4SiPh_3$] (5.35 mg, 0.0125 mmol, 5 mol %), L5 (6.8 mg, 0.0125 mmol, 5 mol %) were introduced in a 10 mL teflon-valved flask equipped with a magnetic stirrer under argon atmosphere. Toluene (1 mL) was added to the reaction mixture. The reaction mixture was stirred at 60 °C for 16 h. The mixture was extracted with diethyl ether (3 × 10 mL). After that, the layers of mixed diethyl ether were dried over sodium sulfate and concentrated under vacuum. After evaporation of the solvent, the crude reaction mixture was purified by silica gel column chromatography (petroleum ether/EtOAc 50/1), yielding (92%) the hydrosilylated product.

GC method 1: GC analysis was carried out on an Agilent 7890B GC system using HP-05 column (30 m × 320 µm × 0.25 µm), split ratio 30:1, column pressure 10 psi, injector temperature of 260 °C, detector temperature of 330 °C, argon carrier gas. Temperature program: Initial temperature 70 °C, hold for 1 min.; ramp 1: 4 °C/min. to 120 °C; ramp 2: 10 °C/min. to 250 °C; ramp 3: 20 °C/min. to 320 °C, hold for 2 min.

GC method 2: GC analysis was carried out on an Agilent 7890B GC system using HP-05 column (30 m × 320 µm × 0.25 µm), split ratio 30:1, column pressure 10 psi, injector temperature of 260 °C, detector temperature of 330 °C, argon carrier gas. Temperature program: Initial temperature 70 °C, hold for 1 min.; ramp 1: 4 °C/min. to 120 °C; ramp 2: 10 °C/min. to 250 °C, hold for 3 min; ramp 3: 20 °C/min. to 320 °C, hold for 5 min.

GC method 1 was applied for substrates 1a, 1b, 1c, 1d, 1e, 1f, 1g, 1j, 1k, 1l, 1m, 1n, 1o, 1p, 1q, 1r, 1s, 1t, 1u, 1v, 1w, 1x.

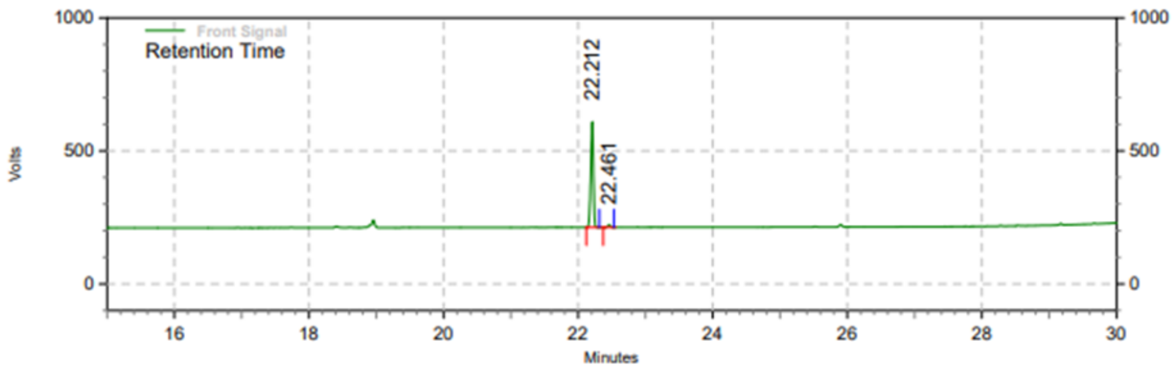
GC method 2 was applied for substrates 1h, 1i.

Table S1. GC retention time for alkynes, hydrosilylated products and conversion

Substrate	Retention time (min)	Product	Retention time (min)	Conversion (%)
1a	17.7	3a	22.2, 22.5	>99
1b	20.7	3b	23.8	80
1c	23.9	3c	26.3	87
1d	22.8	3d	24.5	88
1e	22.5	3e	25.5	>99
1f	24.09	3f	27.14	77
1g	17.3	3g	21.5	>99
1h	29.2	3h	30.3	64
1i	30.2	3i	31.6	41
1j	17.3	3j	20.4, 20.8	84
1k	20.7	3k	22.8, 23.1	61
1l	17.7	3l	21.1, 21.3	77
1m	17.7	3m	27.7, 28.0	38
1n	21.7	3n	28.3	79
1o	23.5	3o	29.7, 30.1	83
1p	18.3	3p	26.4, 26.6	91
1q	21.7	3q	29.2, 29.6	73
1r	3.7	3r	23.1, 23.3	97
1s	26.6	3s	29.6	92
1t	17.7	3t	28.2, 28.5	>99
1u	18.3	3u	27.2, 27.8	86

1v	20.7	3v	25.6, 25.7	90
1w	24.7	3w	28.7, 28.8	98
1x	21.6	3x	26.8, 26.9	87

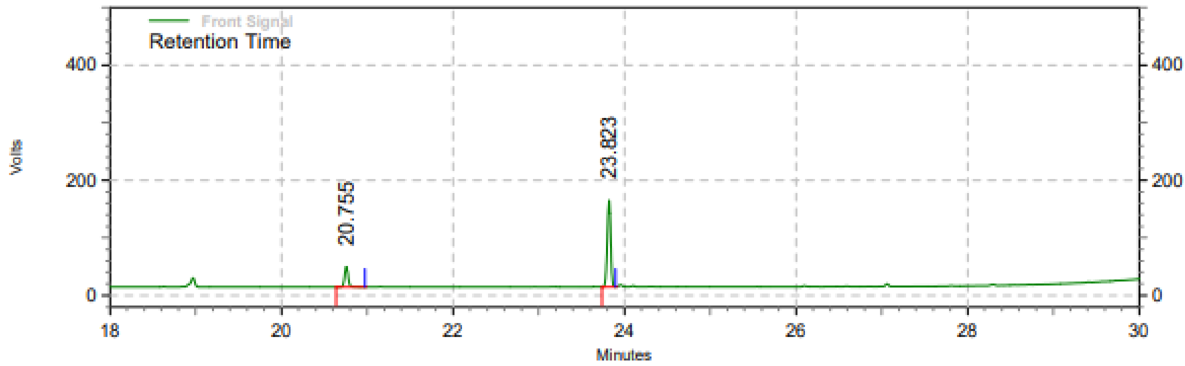
4. GC chromatogram for substrate scope of hydrosilylation of alkynes:



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
22.212	8344692	97.77	3055631	97.73
22.461	190173	2.23	70873	2.27
Totals	8534865	100.00	3126504	100.00

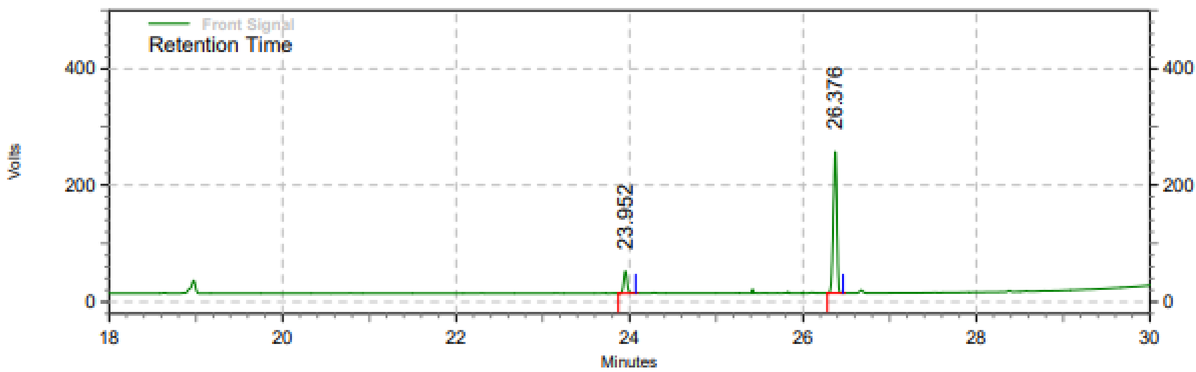
Figure S3. GC chromatogram of 3a (Table S1, under optimized condition).



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
20.755	761648	19.56	273978	19.20
23.823	3132564	80.44	1152919	80.80
Totals	3894212	100.00	1426897	100.00

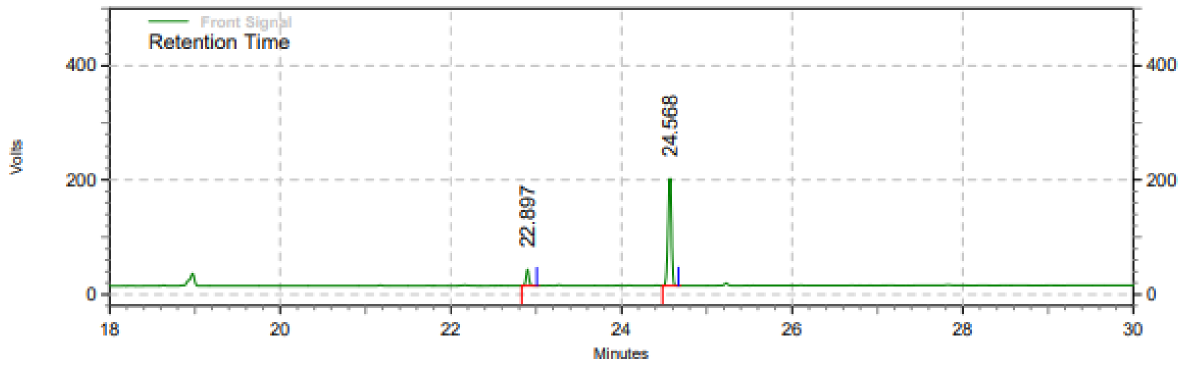
Figure S4. GC chromatogram of 3b.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
23.952	778761	12.86	290848	13.52
26.376	5277096	87.14	1860009	86.48
Totals	6055857	100.00	2150857	100.00

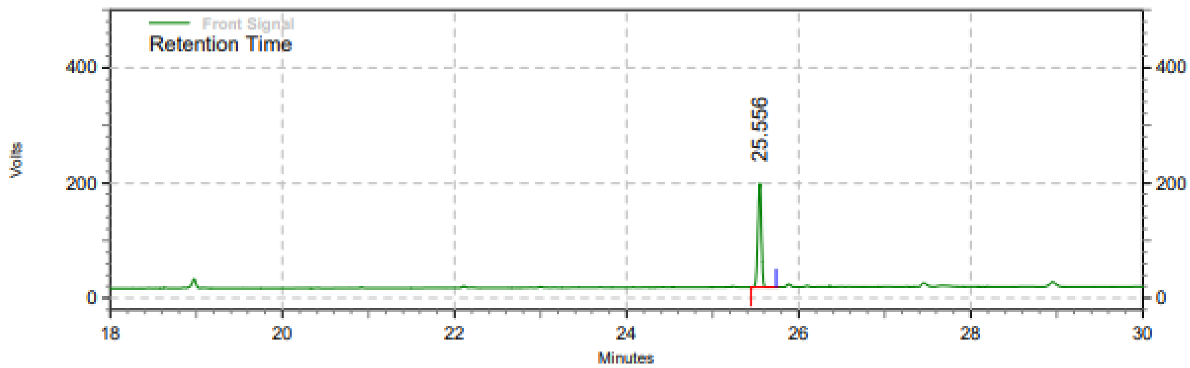
Figure S5. GC chromatogram of 3c.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
22.897	566007	12.36	222525	13.41
24.568	4013290	87.64	1436860	86.59
Totals	4579297	100.00	1659385	100.00

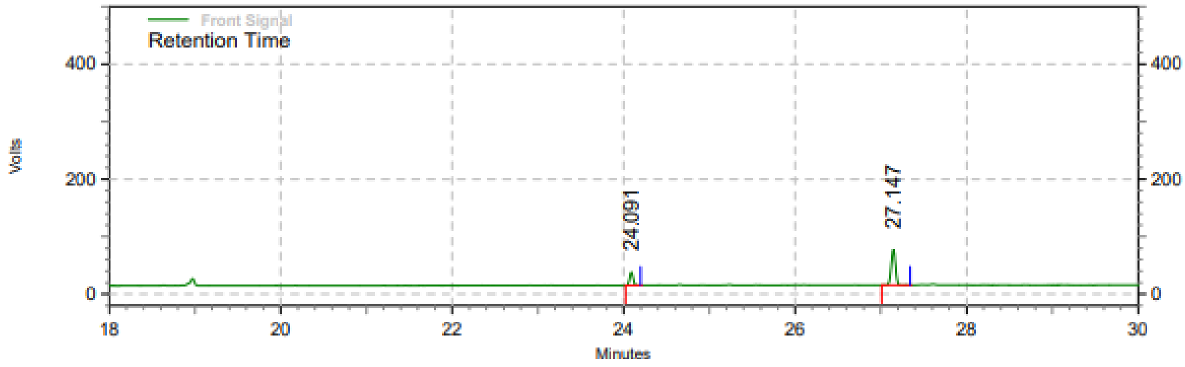
Figure S6. GC chromatogram of 3d.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
25.556	3977981	100.00	1394675	100.00
Totals	3977981	100.00	1394675	100.00

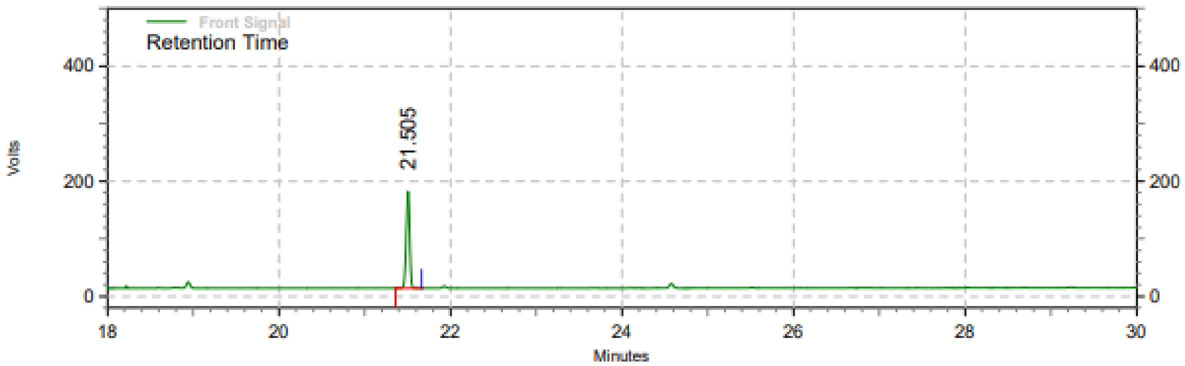
Figure S7. GC chromatogram of 3e.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
24.091	483260	23.42	171179	26.54
27.147	1579950	76.58	473798	73.46
Totals	2063210	100.00	644977	100.00

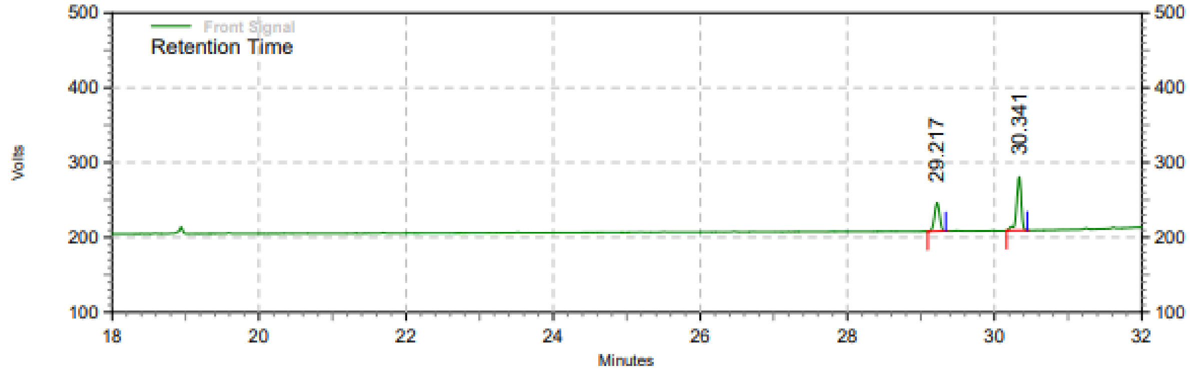
Figure S8. GC chromatogram of 3f.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
21.505	3572061	100.00	1291141	100.00
Totals	3572061	100.00	1291141	100.00

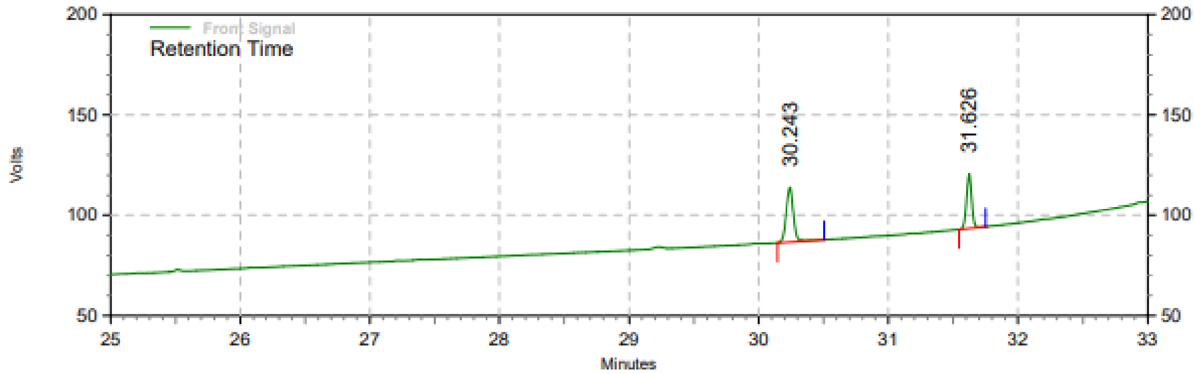
Figure S9. GC chromatogram of 3g.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
29.217	1374250	36.55	286564	34.26
30.341	2385578	63.45	549843	65.74
Totals	3759828	100.00	836407	100.00

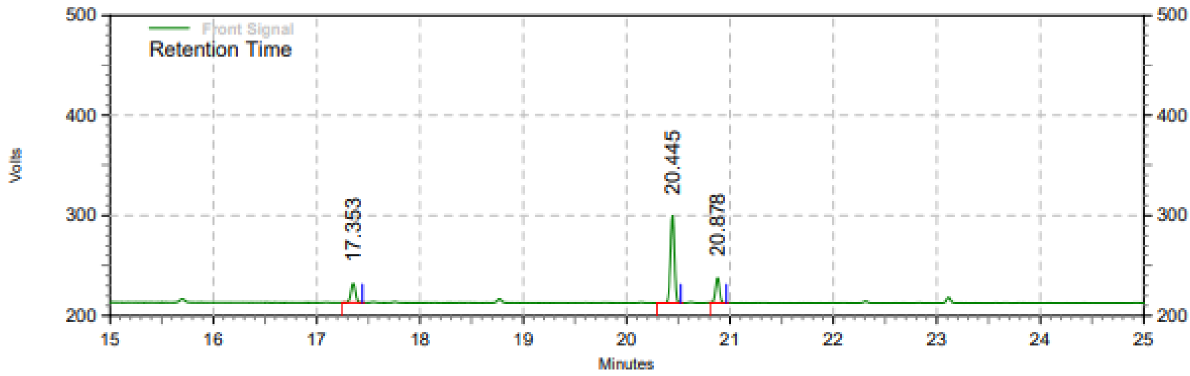
Figure S10. GC chromatogram of 3h.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
30.243	824164	58.88	209689	50.19
31.626	575464	41.12	208097	49.81
Totals	1399628	100.00	417786	100.00

Figure S11. GC chromatogram of 3i.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
17.353	452627	15.88	146983	14.58
20.445	1860525	65.29	669645	66.41
20.878	536430	18.82	191646	19.01
Totals	2849582	100.00	1008274	100.00

Figure S12A. GC chromatogram of 3j.

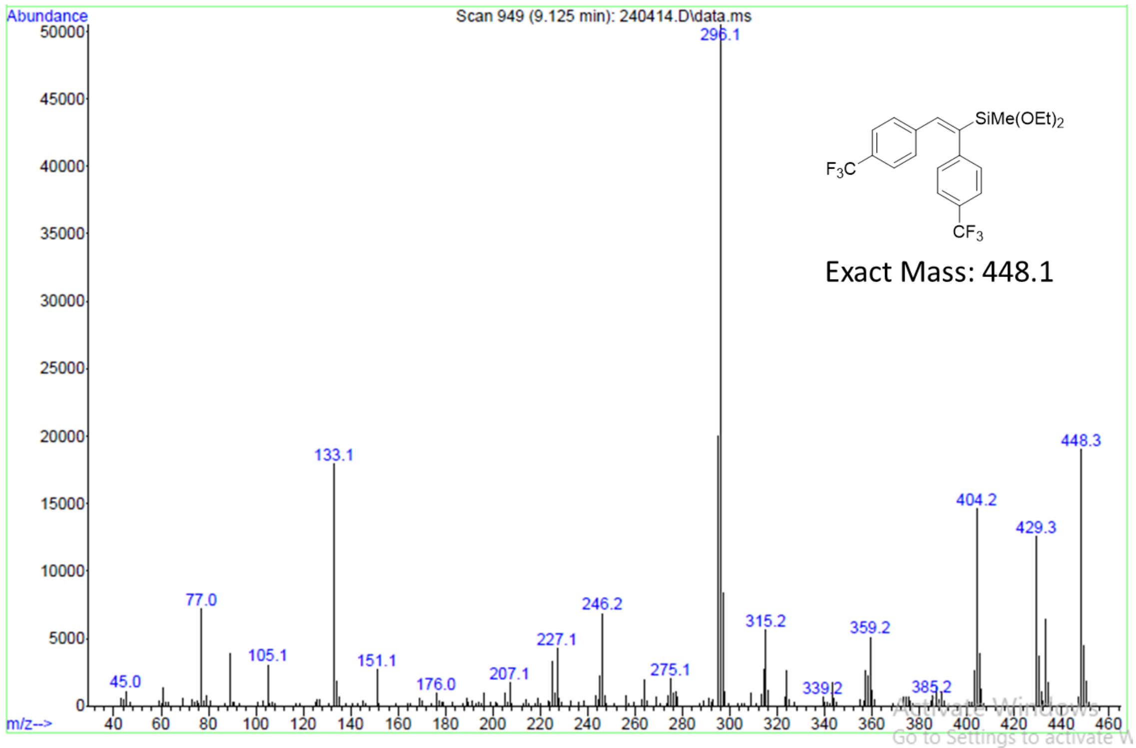
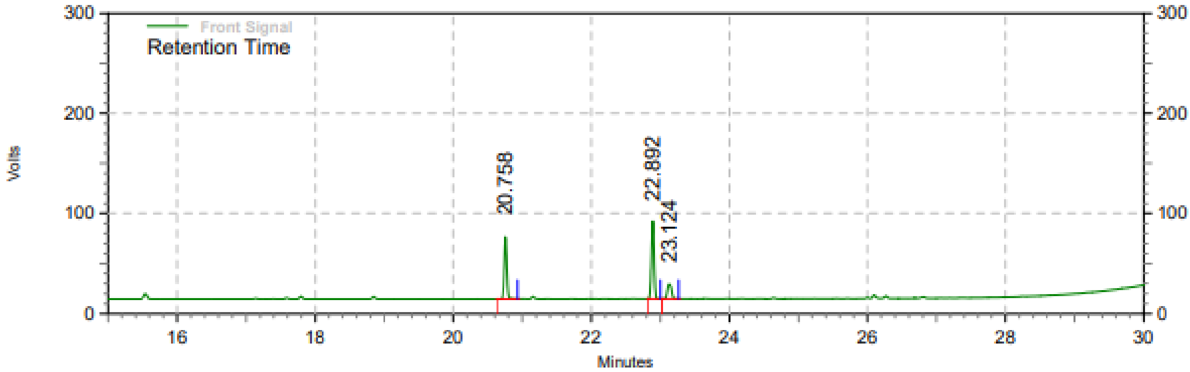


Figure S12B. GC-MS chromatogram of 3j.



Front Signal Results

Retention Time	Area	Area %	Height	Height %
20.758	1283624	38.61	475603	40.24
22.892	1584368	47.66	595043	50.35
23.124	456200	13.72	111175	9.41
Totals	3324192	100.00	1181821	100.00

Figure S13A. GC chromatogram of 3k.

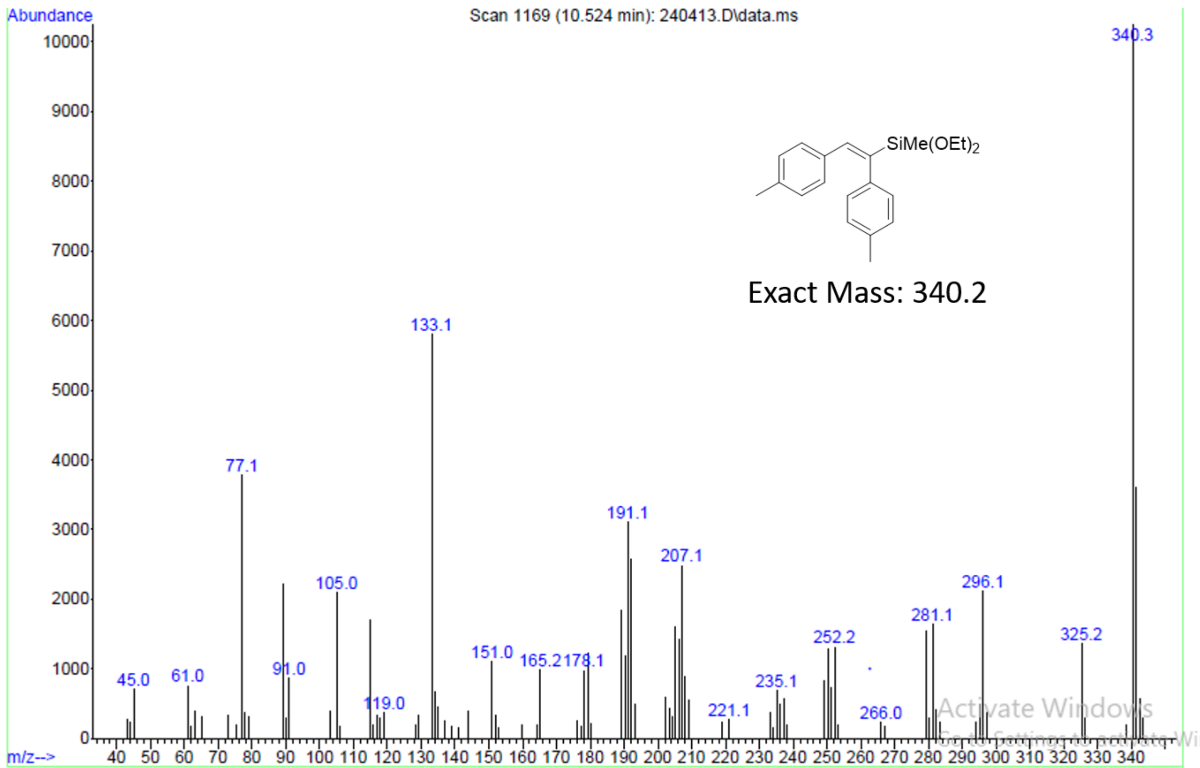
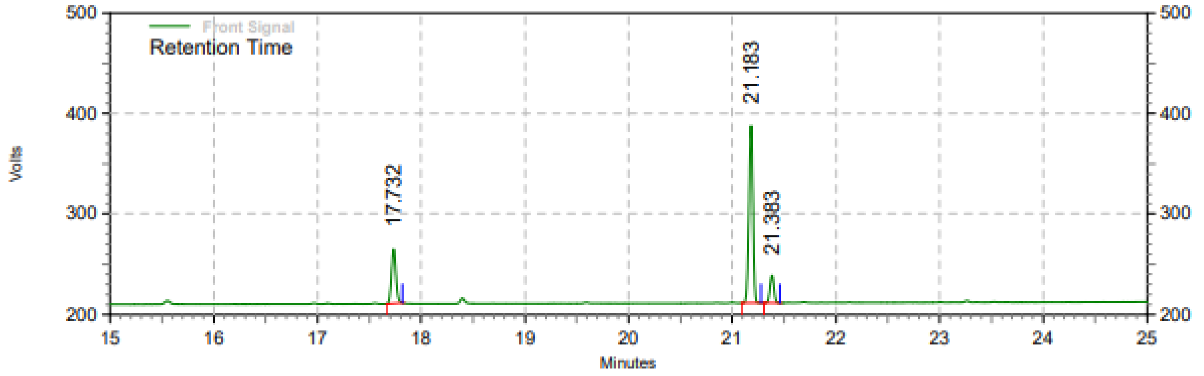


Figure S13B. GC-MS chromatogram of 3k.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
17.732	1216614	22.52	414453	20.95
21.183	3629051	67.17	1354301	68.47
21.383	557011	10.31	209193	10.58
Totals	5402676	100.00	1977947	100.00

Figure S14A. GC chromatogram of 3l.

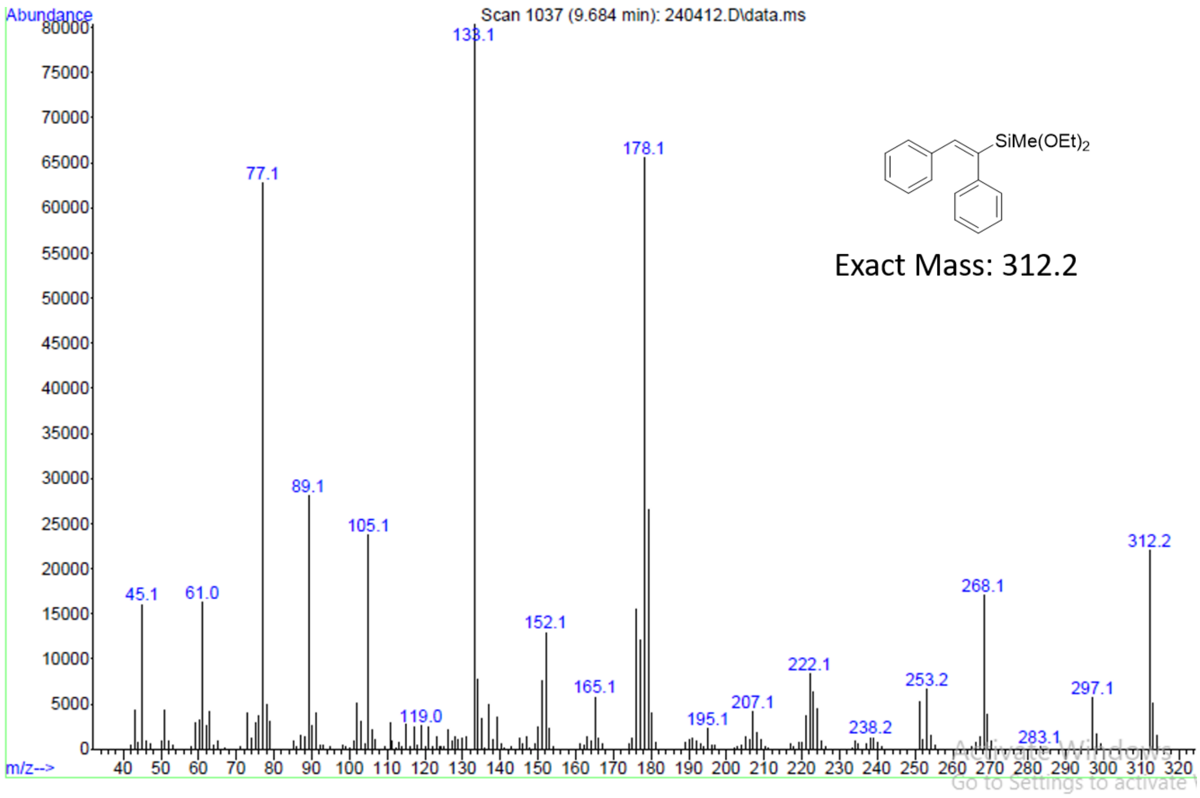
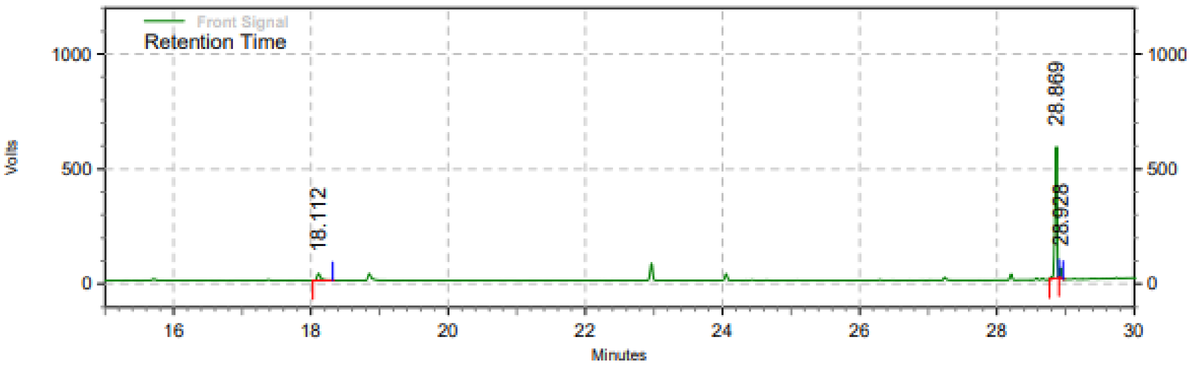


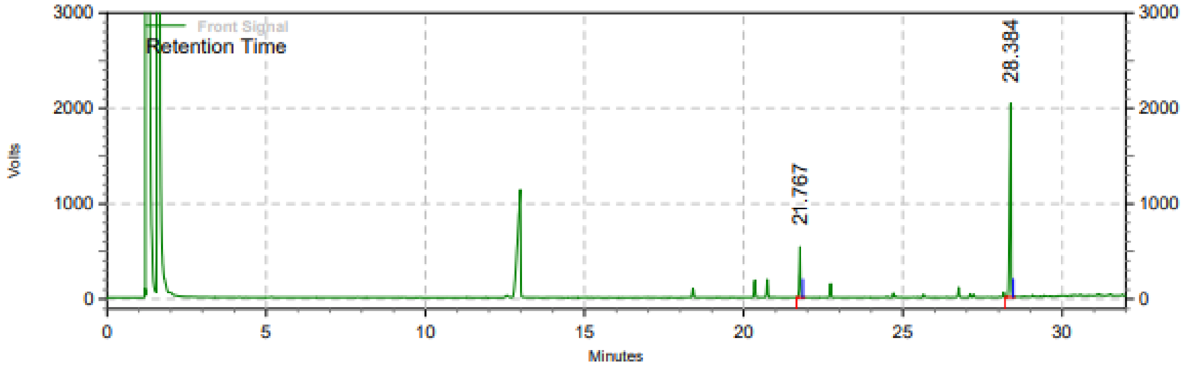
Figure S14B. GC-MS chromatogram of 3l.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
18.112	889930	8.40	252255	5.06
28.869	9170685	86.54	4381457	87.93
28.928	536650	5.06	348964	7.00
Totals	10597265	100.00	4982676	100.00

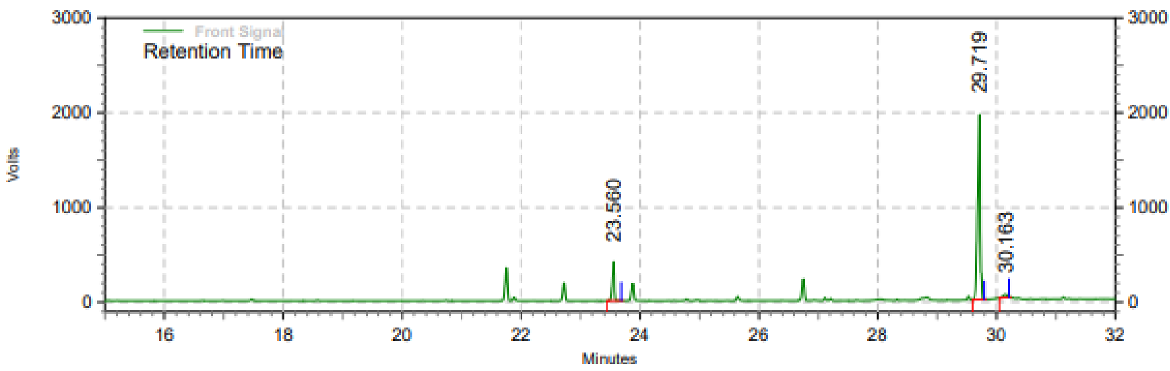
Figure S15. GC chromatogram of 3m.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
21.767	11234268	19.80	4100357	20.80
28.384	45504720	80.20	15615095	79.20
Totals	56738988	100.00	19715452	100.00

Figure S16. GC chromatogram of 3n.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
23.560	8962851	16.46	3131865	17.07
29.719	44232184	81.25	14982493	81.66
30.163	1242435	2.28	234011	1.28
Totals	54437470	100.00	18348369	100.00

Figure S17A. GC chromatogram of 3o.

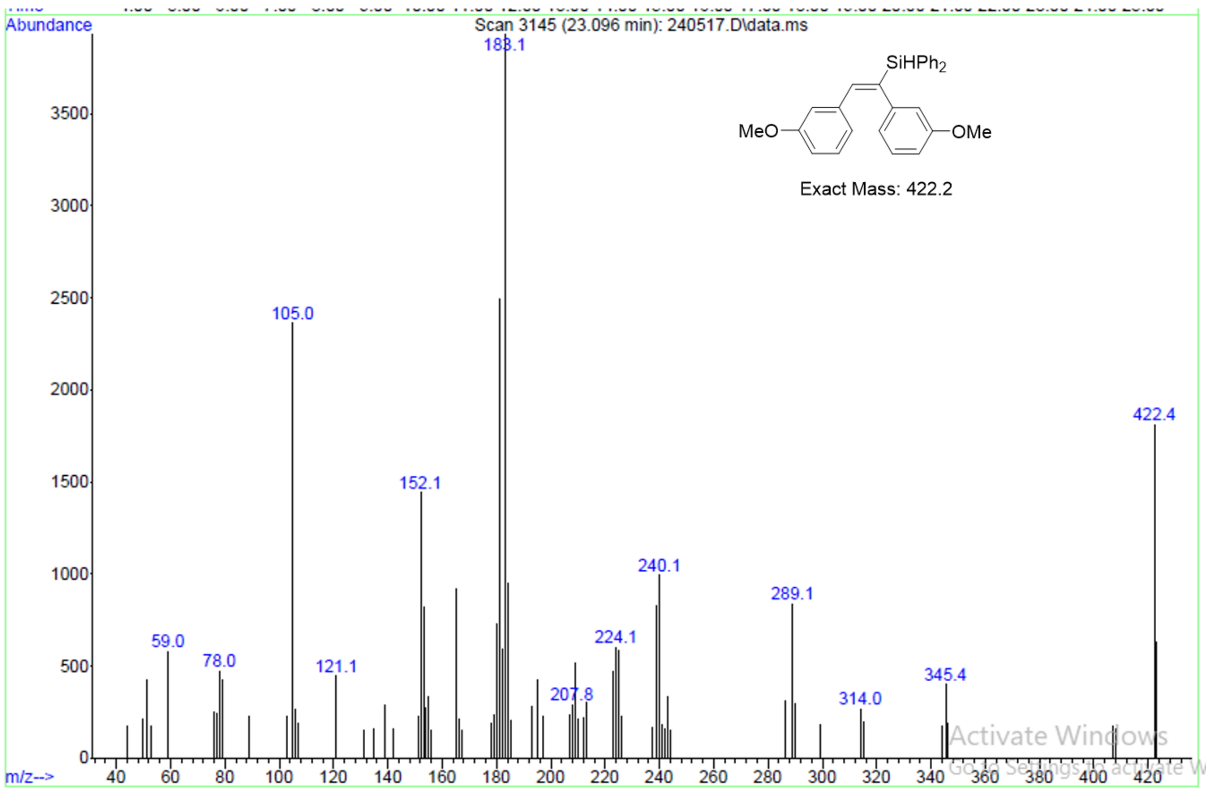
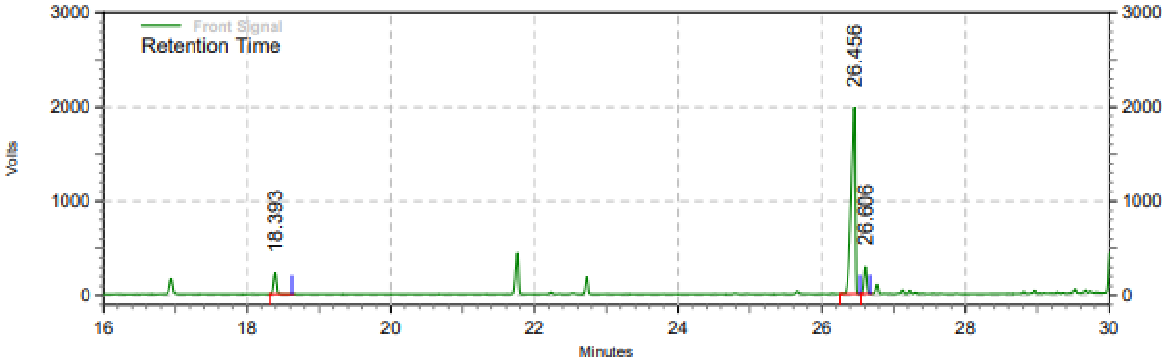


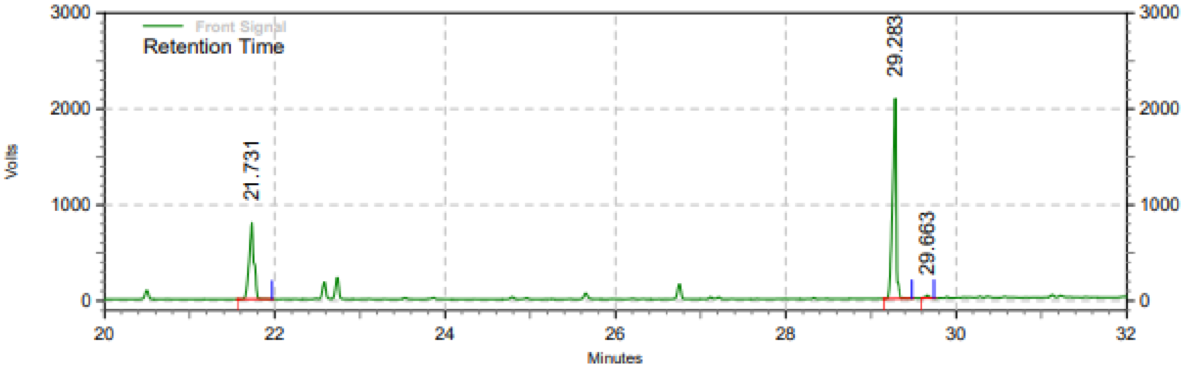
Figure S17B. GC-MS chromatogram of 3o.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
18.393	4858263	6.81	1675645	8.79
26.456	60574818	84.95	15179102	79.62
26.606	5870769	8.23	2209265	11.59
Totals	71303850	100.00	19064012	100.00

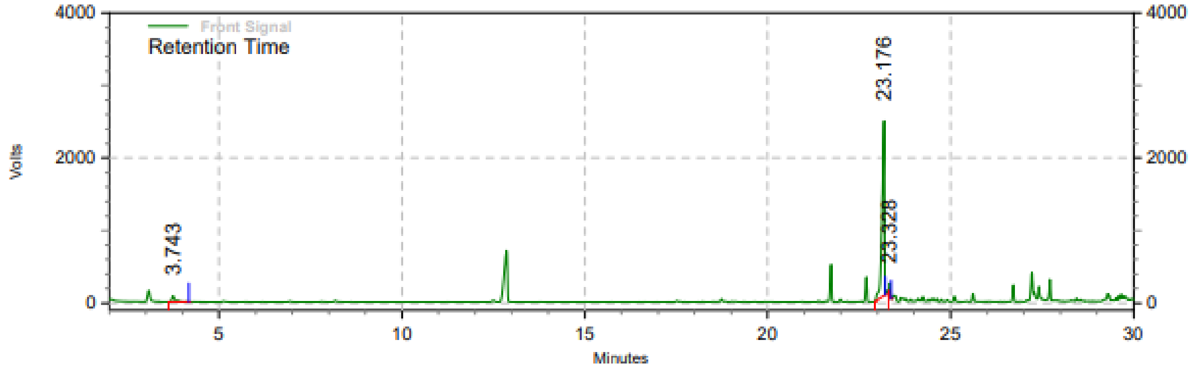
Figure S18. GC chromatogram of 3p.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
21.731	25269169	34.80	6126531	27.41
29.283	46704492	64.33	16012212	71.63
29.663	632435	0.87	215539	0.96
Totals	72606096	100.00	22354282	100.00

Figure S19. GC chromatogram of 3q.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
3.743	3859443	4.43	609212	3.02
23.176	80324021	92.26	18478537	91.61
23.328	2876191	3.30	1082556	5.37
Totals	87059655	100.00	20170305	100.00

Figure S20. GC chromatogram of 3r.

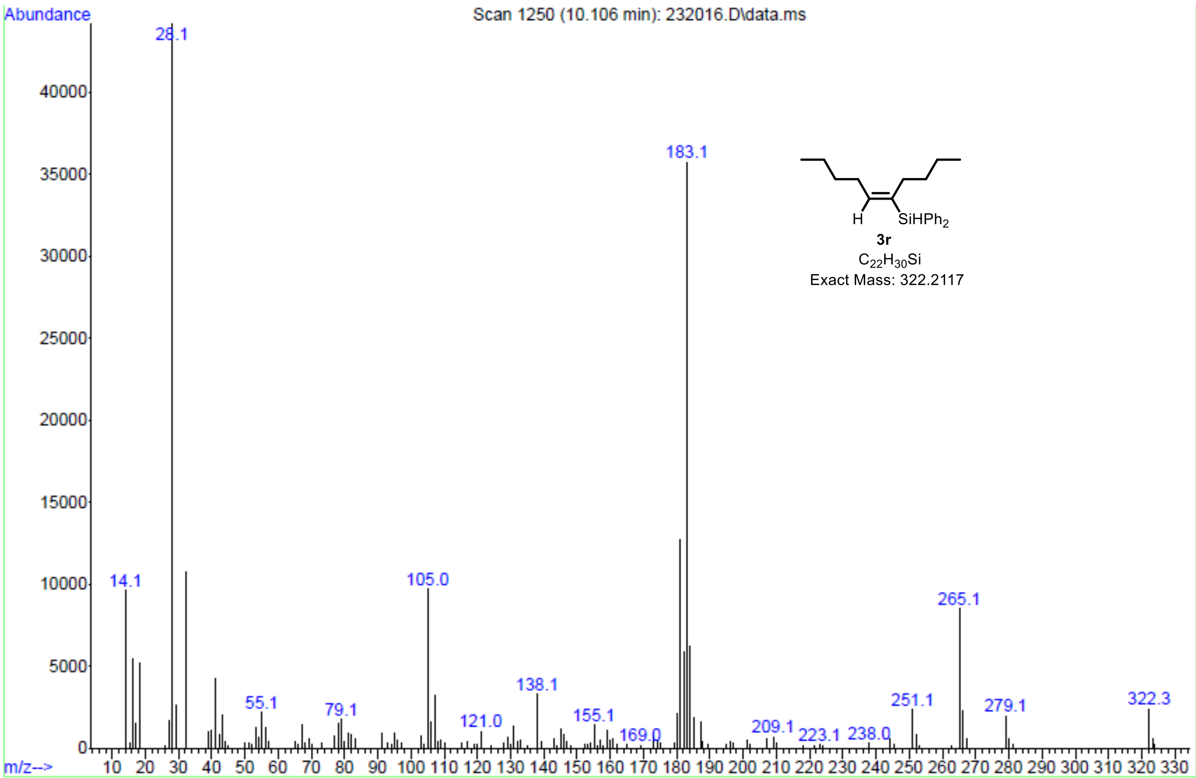
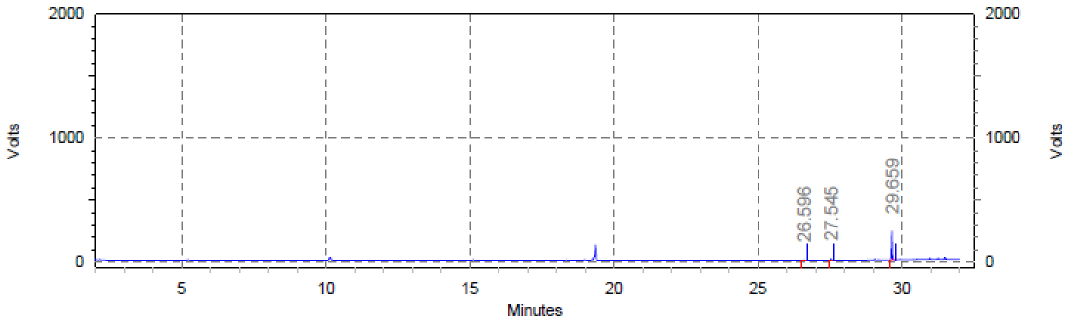


Figure.S21: GC-MS chromatogram of 3r



Front Signal Results

Retention Time	Area	Area %	Height	Height %
26.596	62909	1.82	24466	1.29
27.545	208623	6.04	98703	5.20
29.659	3184458	92.14	1774438	93.51
Totals	3455990	100.00	1897607	100.00

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Go to Settings to ac

Figure S22. GC chromatogram of 3s.

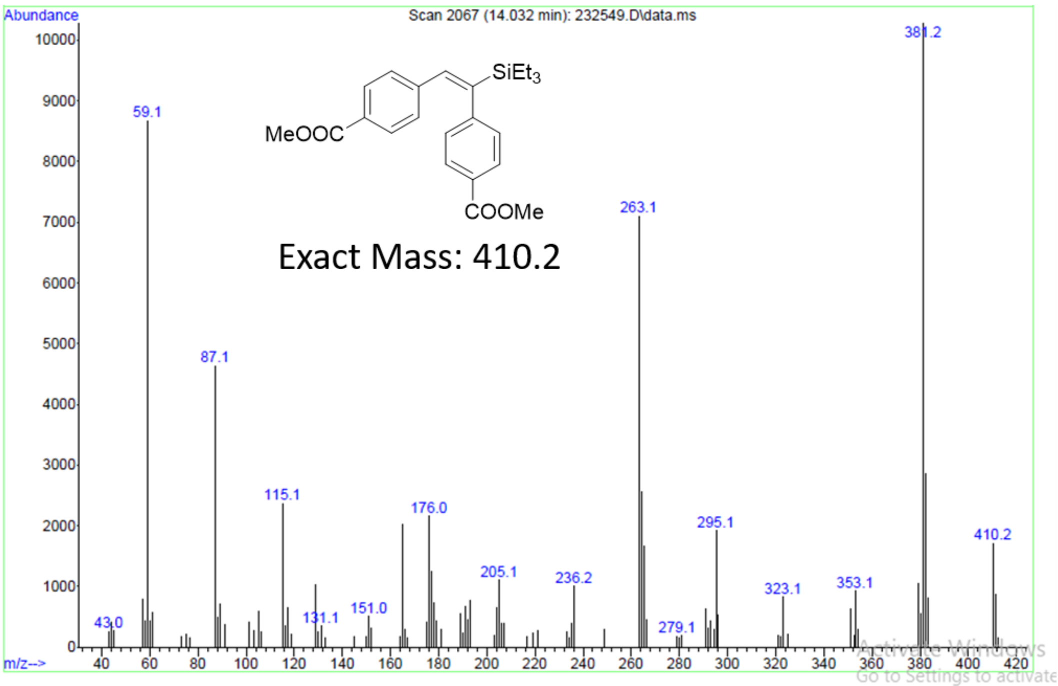
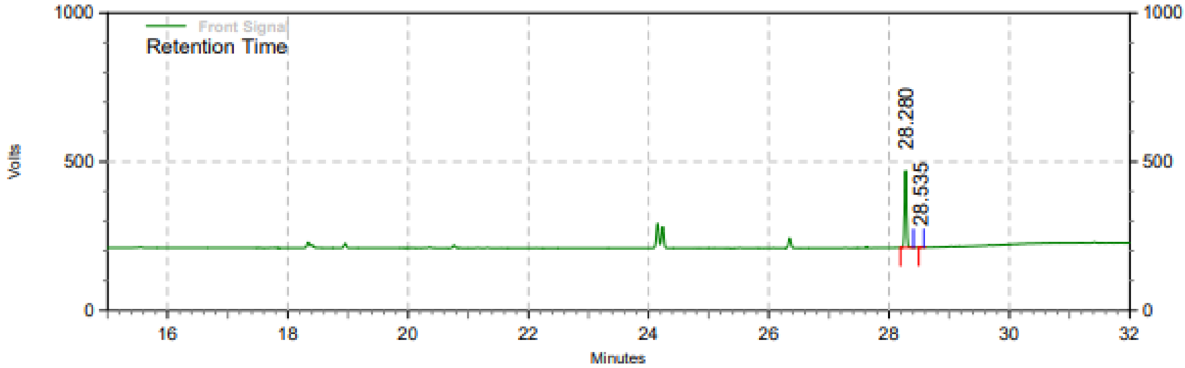


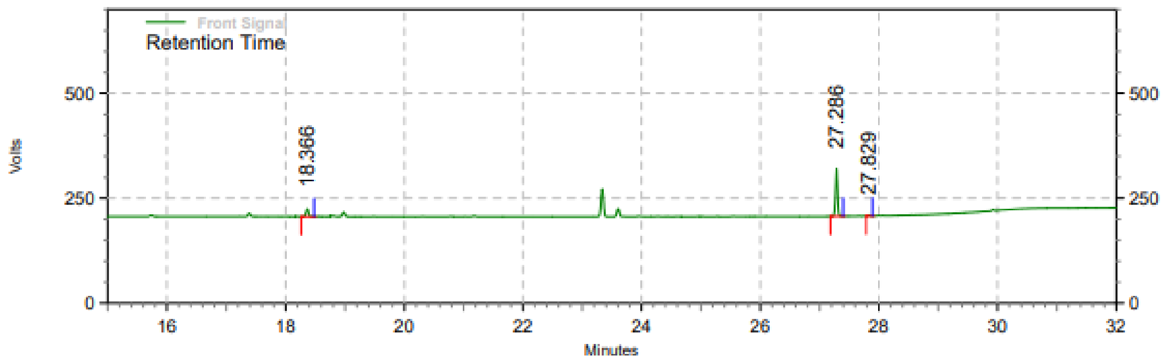
Figure S23. GC-MS chromatogram of 3s.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
28.280	4685663	99.67	1982270	99.61
28.535	15458	0.33	7666	0.39
Totals	4701121	100.00	1989936	100.00

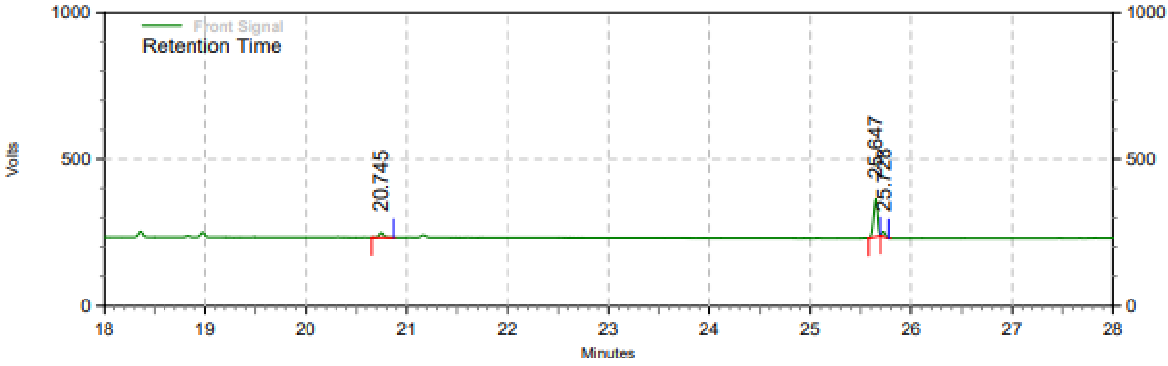
Figure S24. GC chromatogram of 3t.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
18.366	447061	16.15	148815	14.28
27.286	2284403	82.50	876724	84.11
27.829	37439	1.35	16806	1.61
Totals	2768903	100.00	1042345	100.00

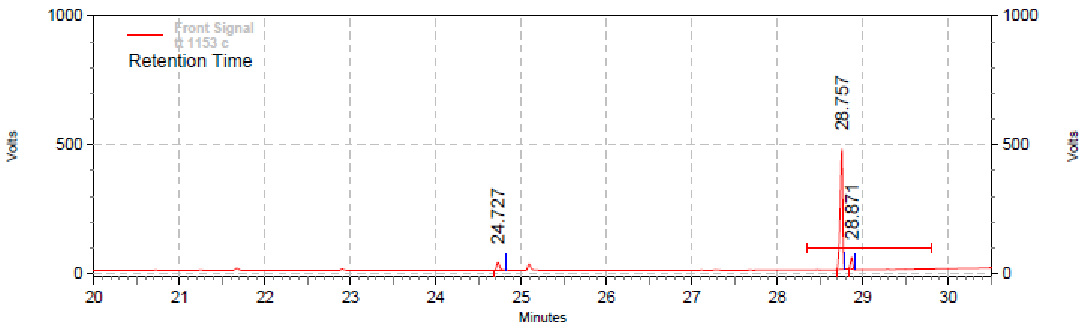
Figure S25. GC chromatogram of 3u.



Front Signal Results

Retention Time	Area	Area %	Height	Height %
20.745	344266	10.65	116848	9.50
25.647	2597133	80.34	987303	80.23
25.728	291156	9.01	126368	10.27
Totals	3232555	100.00	1230519	100.00

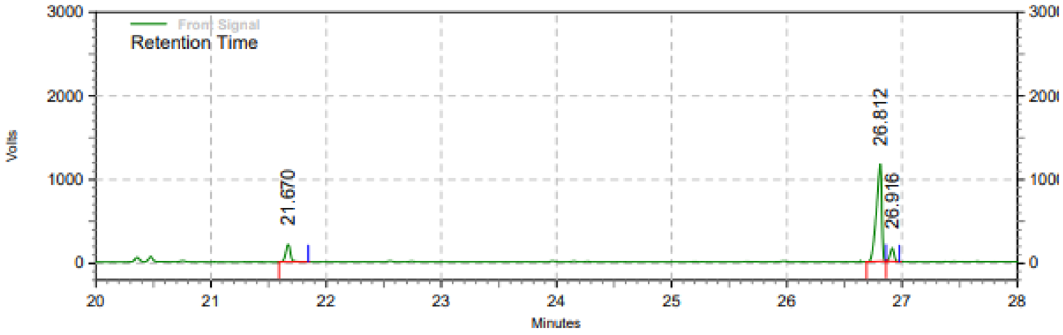
Figure S26. GC chromatogram of 3v.



Front Signal Results

Retention Time	Area	Area %
24.727	616817	7.10
28.757	7470597	85.96
28.871	603861	6.95
Totals	8691275	100.00

Figure S27. GC chromatogram of 3w.



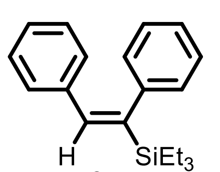
Front Signal
Results

Retention Time	Area	Area %	Height	Height %
21.670	4337355	12.01	1571458	13.43
26.812	28835540	79.82	8912854	76.16
26.916	2951957	8.17	1218936	10.42
Totals	36124852	100.00	11703248	100.00

Figure S28. GC chromatogram of 3x.

5. NMR of isolated compounds for hydrosilylation of alkynes:

Triethyl-[(Z)-(1,2-diphenylvinyl)]silane (3a)



3a

The desired product 3a was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (200 MHz, $CDCl_3$):** δ 7.32 (m, 2H), 7.22 (m, 1H), 7.11 (m, 3H), 7.03 (m, 2H), 6.98 (m, 2H), 6.8 (s, C=CH, 1H), 0.99 (t, J = 7.9 Hz, 9H), 0.68 (q, J = 7.9 Hz, 6H). This compound has been previously characterized.[3]

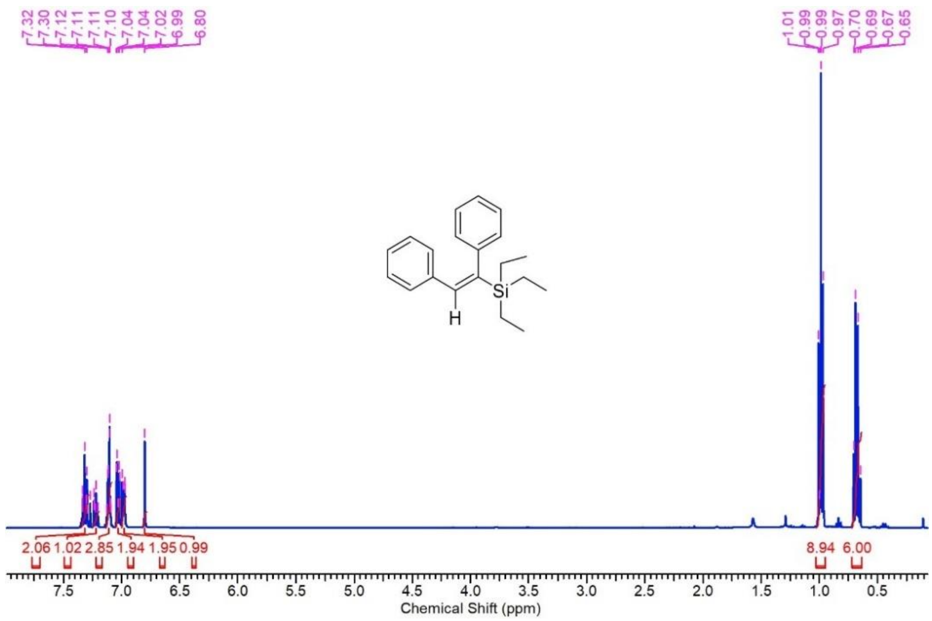
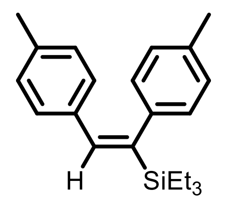


Figure S29: ^{1}H NMR of 3a in $CDCl_3$

(E)-(1,2-di-p-tolylvinyl)triethylsilane (3b)



3b

The desired product 3b was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (200 MHz, $CDCl_3$):** δ 7.14 (s, 1H), 7.12 (s, 1H), 6.92 (m, 6H), 6.75 (s, 1H), 2.38 (s, 3H, CH_3-Ar), 2.26 (s, 3H, CH_3-Ar), 0.98 (t, J = 8 Hz, 9H, -Si(CH_2CH_3)$_3$), 0.66 (q, J = 8 Hz, 6H, -Si(CH_2CH_3)$_3$). This compound has been previously characterized.[3]

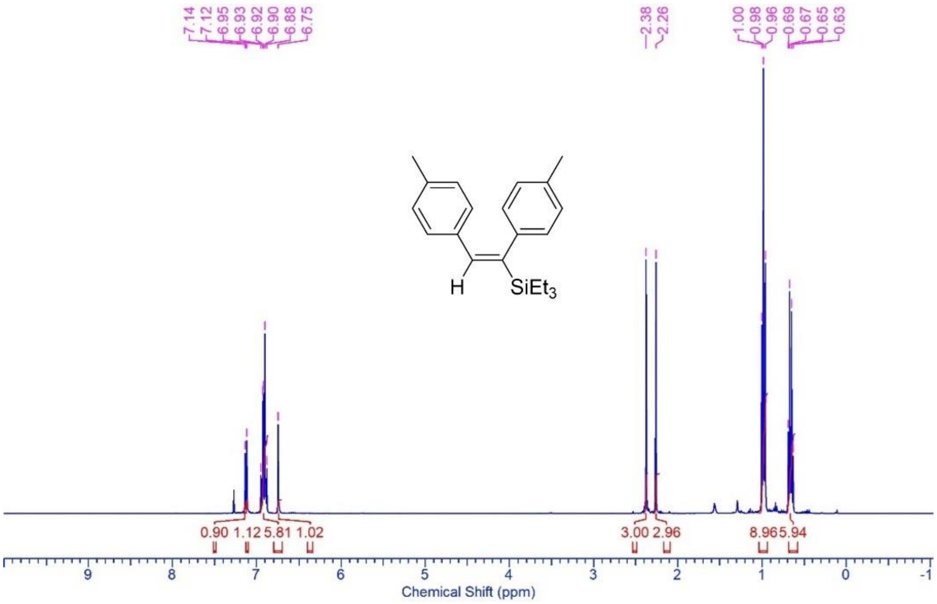
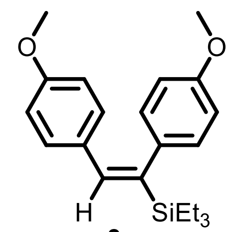


Figure S30: ^{1}H NMR of 3b in $CDCl_3$

(E)-(1,2-bis(4-methoxyphenyl)vinyl)triethylsilane (3c)



3c

The desired product 3c was obtained as a colorless oil by silica gel column chromatography. δ = 6.91-6.86 (m, 6H), 6.68-6.62 (m, 3H), 3.81 (s, 3H, -OCH_3), 3.71 (s, 3H, -OCH_3), 0.94 (t, J = 7.8 Hz, 9H, -Si-C-(CH_3)$_3$), 0.62 (q, J = 7.9 Hz, 6H, -Si(CH_2)$_3$). This compound has been previously characterized.[3]

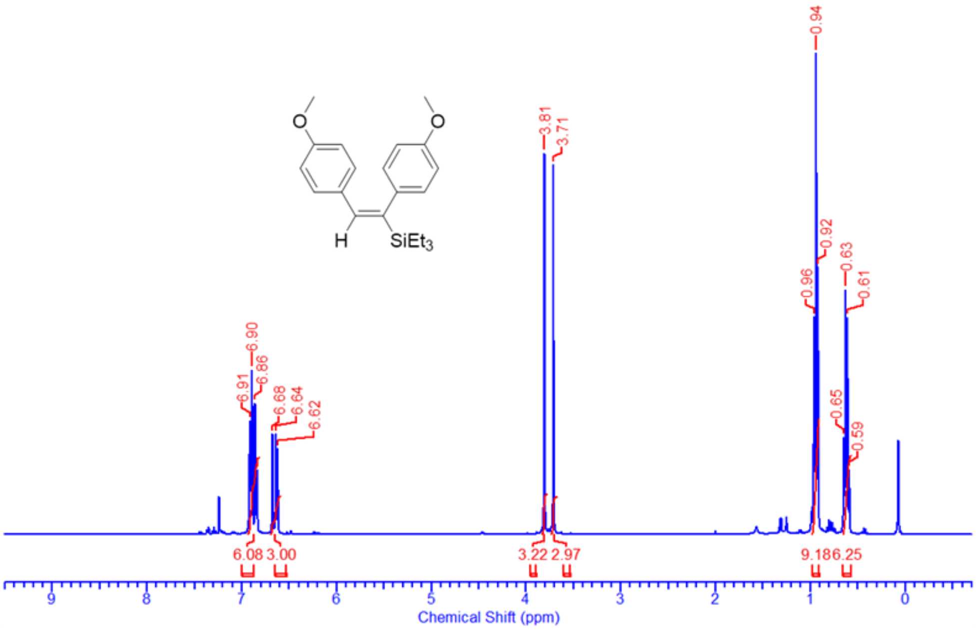
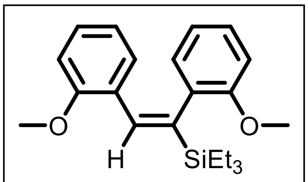


Figure S31: ^{1}H NMR of 3c in $CDCl_3$

(E)-(1,2-bis(2-methoxyphenyl)vinyl)triethylsilane (3d)



3d

The desired product 3d was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.15 (m, 2H), 7.06 (m, 1H), 6.83 (m, 2H), 6.79 (m, 3H), 6.56 (t, J = 5.6 Hz, 1H), 3.85 (s, 3H, $-OCH_3$), 3.75 (s, 3H, $-OCH_3$), 0.97 (t, J = 7.8 Hz, 9H, -Si-C-$(CH_3)_3$), 0.65 (q, J = 7.8 Hz, 6H, -Si$(CH_2)_3$). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 157.5, 156.5, 140.3, 134.3, 132.3, 129.6, 129.0, 128.1, 127.4, 126.9, 120.8, 120.0, 110.8, 110.2, 55.9, 55.1, 7.5, 3.6.

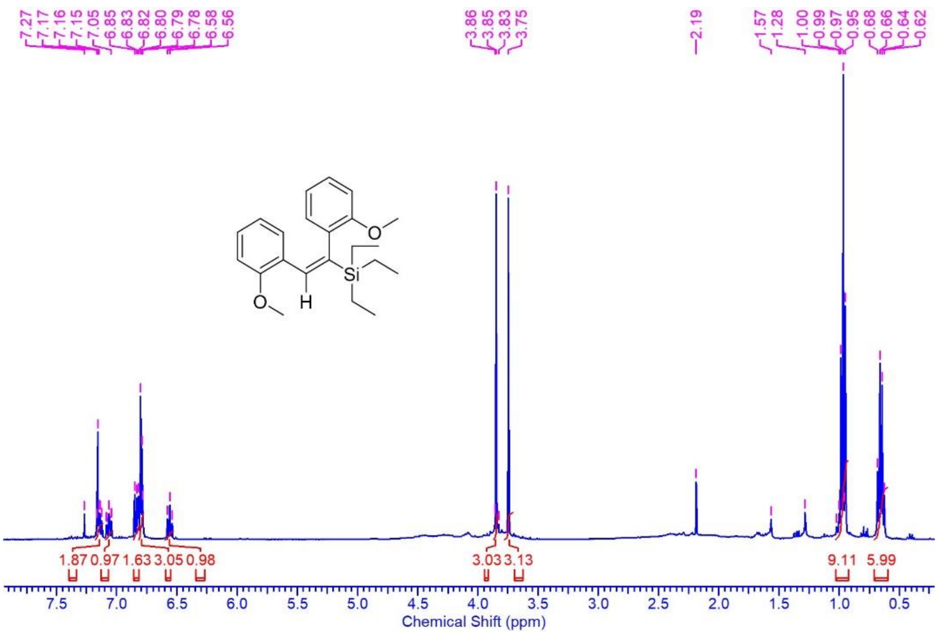


Figure S32: ^{1}H NMR of 3d in $CDCl_3$

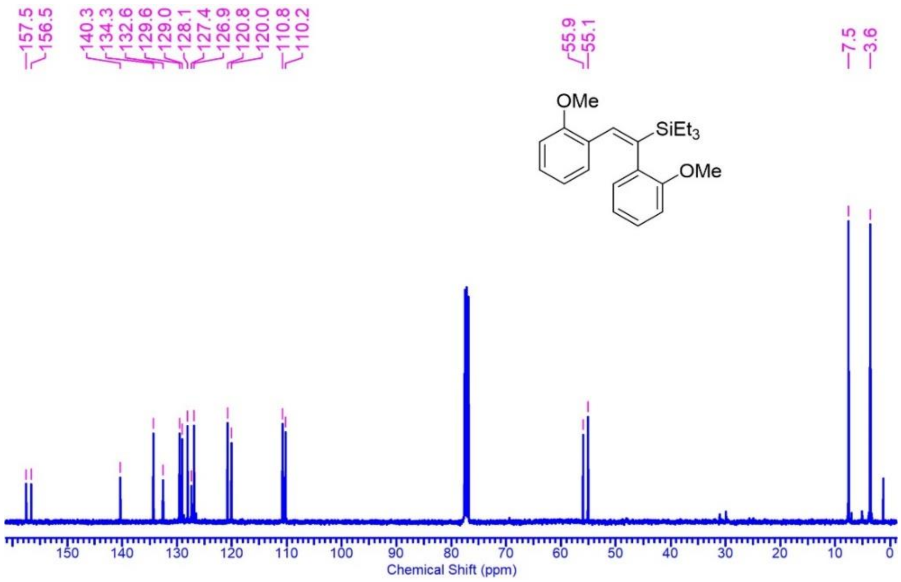
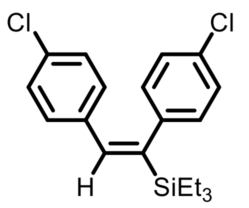


Figure S33: ^{13}C NMR of 3d in $CDCl_3$

(E)-(1,2-bis(4-chlorophenyl)vinyl)triethylsilane (3e)



3e

The desired product 3e was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.27 (d, J =8.38 Hz, 2H), 7.08 (d, J = 8.5 Hz, 2H), 6.92-6.86 (m, 4H), 6.73 (s, 1H, -C=CH), 0.95 (t, J = 8.0 Hz, 9H, -Si-C-$(CH_3)_3$), 0.63 (q, J = 7.75 Hz, 6H, -Si$(CH_2)_3$). The characterization of this compound has been previously reported.[3]

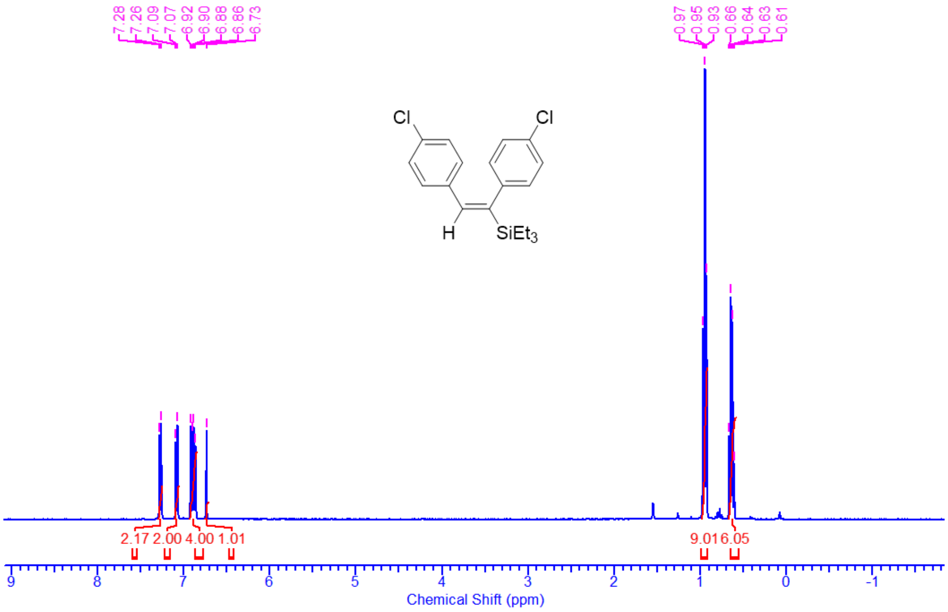
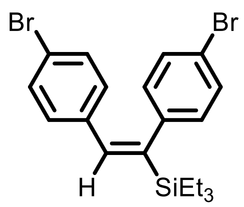


Figure S34: ^{1}H NMR of 3e in $CDCl_3$

(E)-(1,2-bis(4-bromophenyl)vinyl)triethylsilane (3f)



3f

The desired product 3f was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.45 (s, 1H), 7.43 (s, 1H), 7.27 (d, J = 3 Hz, 1H), 7.25 (s, 1H), 6.88 (s, 1H), 6.86 (s, 1H), 6.84 (s, 1H), 6.82 (s, 1H), 6.74 (s, 1H), 0.97 (t, J = 7.6 Hz, 9H, -Si-C-$(CH_3)_3$), 0.65 (q, J = 7.6 Hz, 6H, -Si$(CH_2)_3$). This compound has been previously characterized.[3]

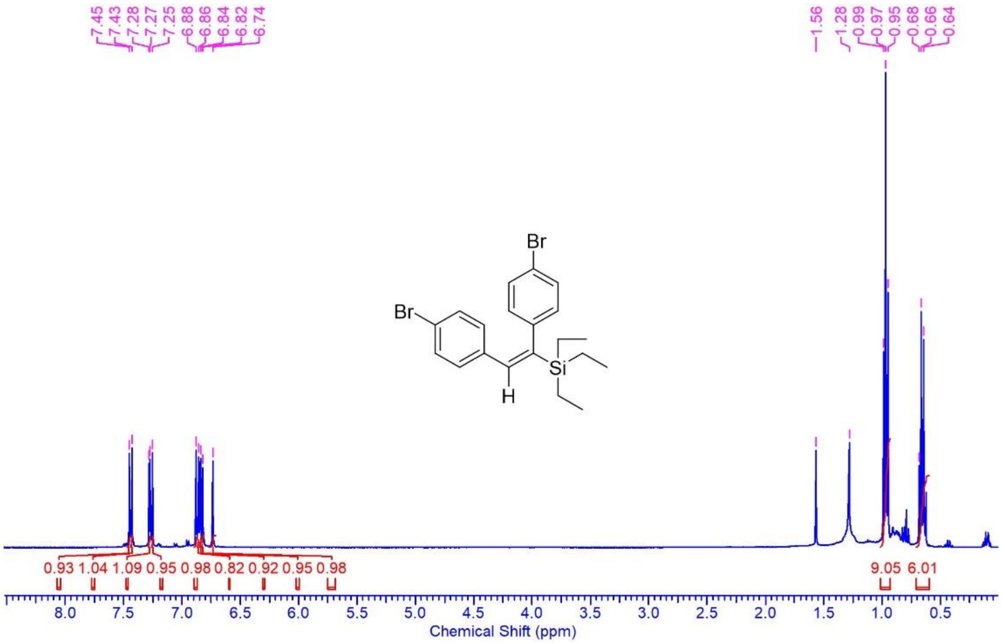
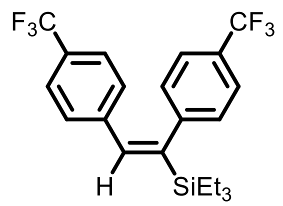


Figure S35: ^{1}H NMR of 3f in $CDCl_3$

(E)-(1,2-bis(4-(trifluoromethyl)phenyl)vinyl)triethylsilane (3g)



3g

The desired product 3g was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.58 (d, J = 8.3 Hz, 2H), 7.37 (d, J = 8.3 Hz, 2H), 7.11 (d, J = 8.3 Hz, 2H), 7.03 (d, J = 8.3 Hz, 2H), 6.87 (s, 1H, C=C-H), 0.98 (t, J = 7.6 Hz, 9H, -Si-C-$(CH_3)_3$), 0.68 (q, J = 7.6 Hz, 6H, -Si$(CH_2)_3$). **^{13}C NMR (125 MHz, $CDCl_3$):** δ = 146.9, 146.3, 140.4, 138.3, 129.7, 129.4, 129.0, 128.6, 128.3, 127.7, 125.9 (q, $^{3}J_{C-F}$ = 3.82 Hz), 125.1 (q, $^{3}J_{C-F}$ = 3.05 Hz), 123.1, 122.8, 7.4, 2.9.

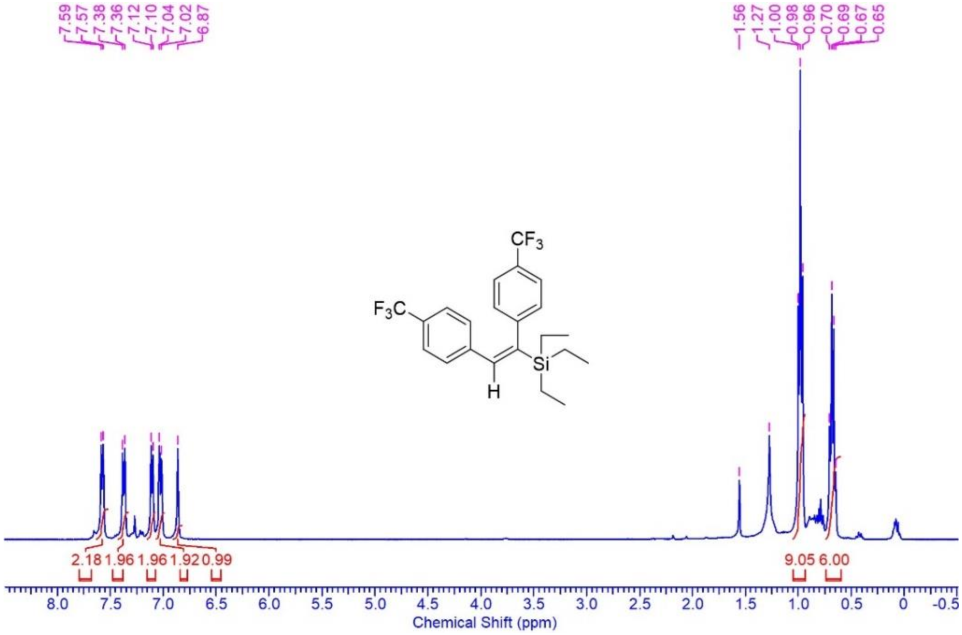


Figure S36: ^{1}H NMR of 3g in $CDCl_3$

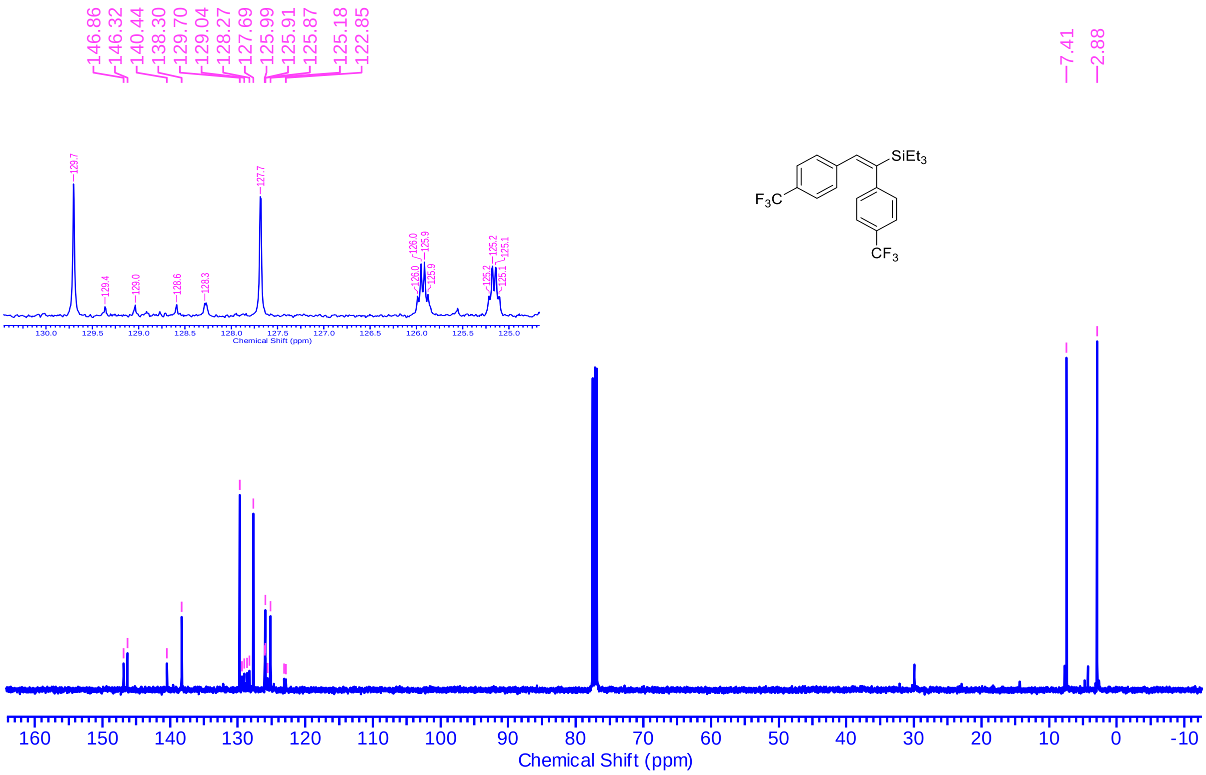
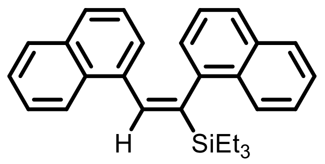


Figure S37: ^{13}C NMR of 3g in $CDCl_3$

(E)-(1,2-di(naphthalen-1-yl)vinyl)triethylsilane (3h)



3h

The desired product 3h was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (200 MHz, $CDCl_3$):** δ = 8.27 (d, J = 8.3 Hz, 1H), 7.95 (d, J = 8.3 Hz, 1H), 7.78 (m, 3H), 7.63 (m, 2H), 7.52 (m, 2H), 7.35 (m, 3H), 7.08 (m, 1H), 6.94 (m, 2H), 1.03(t, J = 7 Hz, 9H, -Si-C-$(CH_3)_3$), 0.76 (q, J = 7 Hz, 6H, -Si$(CH_2)_3$). This compound has been previously characterized.[3]

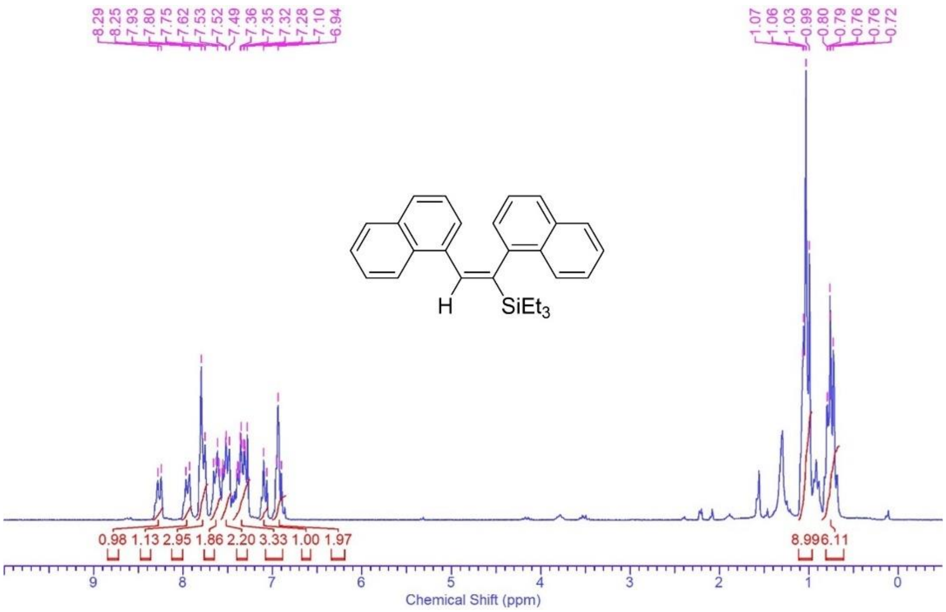
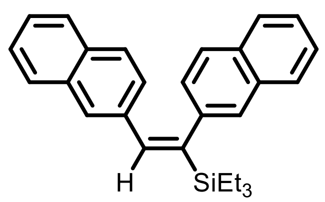


Figure S38: ^{1}H NMR of 3h in $CDCl_3$

(E)-(1,2-di(naphthalen-2-yl)vinyl)triethylsilane (3i)



3i

The desired product 3i was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.8 (m, 8H), 7.65 (m, 1H), 7.55 (m, 3H), 7.47 (m, 2H), 7.41 (d, J = 9.46 Hz, 1H), 7.36 (m, 2H), 7.2 (d, J = 8.35 Hz, 1H), 7.06 (s, 1H), 7.0 (d, J = 8.35 Hz, 1H), 1.03 (t, J = 7.8 Hz, 9H, -Si-C-$(CH_3)_3$), 0.73 (q, J = 7.8 Hz, 6H, -Si$(CH_2)_3$). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 144.5, 141.1, 139.3, 135.3, 134.0, 133.3, 132.5, 132.0, 129.5, 128.4, 128.2, 127.9, 127.6, 127.3, 127.2, 127.1, 126.1, 126.0, 125.4, 125.3, 7.8, 3.1.

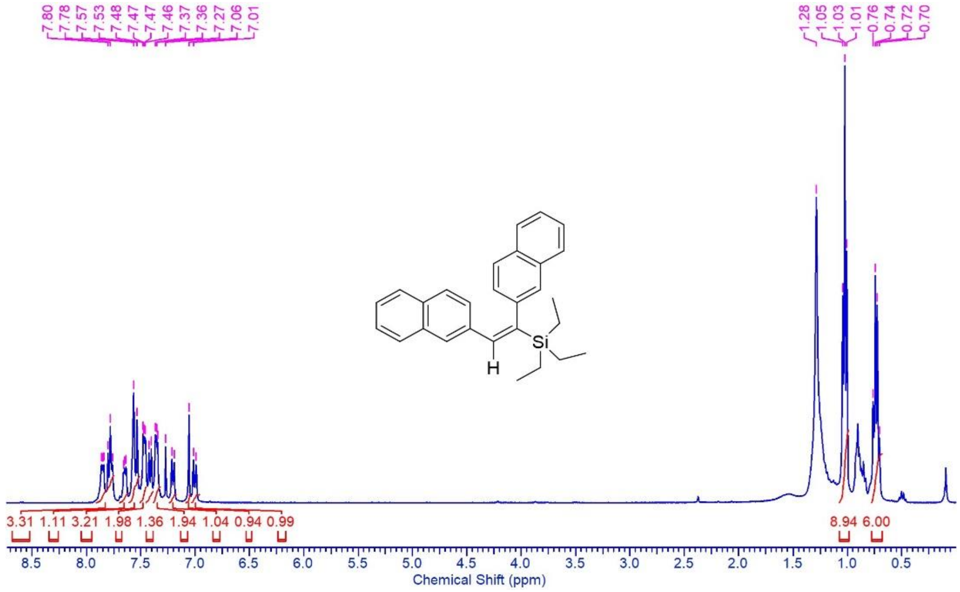


Figure S39: ^{1}H NMR of 3i in $CDCl_3$

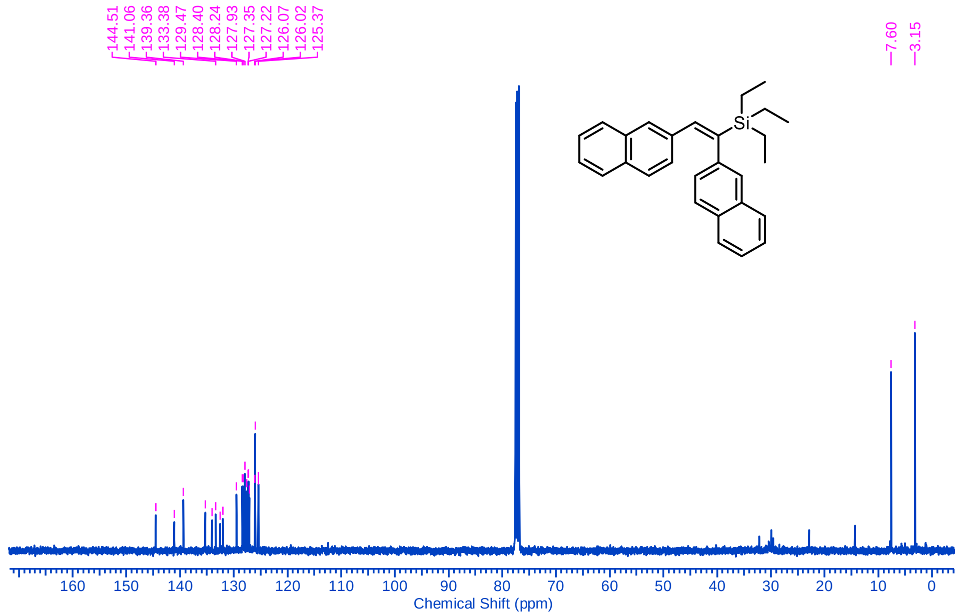
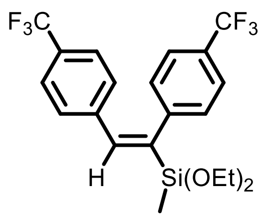


Figure S40: ^{13}C NMR of 3i in $CDCl_3$

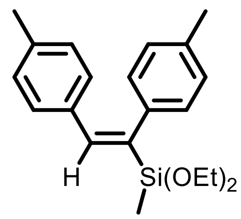
(E)-(1,2-bis(4-(trifluoromethyl)phenyl)vinyl)diethoxy(methyl)silane (3j)

Although GC analyses showed 80% conversion to product; however, concentration of the reaction mixture and attempts at purification of the resulting residue by column chromatography on silica gel or silica gel treated with NEt_3 resulted in decomposition of the product.



3j

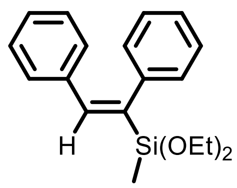
(E)-(1,2-di-p-tolylvinyl)diethoxy(methyl)silane (3k)



3k

Although GC analyses showed 61% conversion to product; however, concentration of the reaction mixture and attempts at purification of the resulting residue by column chromatography on silica gel or silica gel treated with NEt_3 resulted in decomposition of the product.

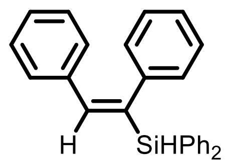
(E)-(1,2-diphenylvinyl)diethoxy(methyl)silane (3l)



3l

Although GC analyses showed 77% conversion to product; however, concentration of the reaction mixture and attempts at purification of the resulting residue by column chromatography on silica gel or silica gel treated with NEt3 resulted in decomposition of the product.

(E)-(1,2-diphenylvinyl)diphenylsilane (3m)



3m

The desired product 3m was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.6 (m, 2H), 7.58 (d, 2H) 7.42 (m, 2H), 7.38 (m, 4H), 7.19 (m, 3H), 7.12 (m, 3H), 7.03 (m, 5H), 5.31 (s, 1H). This compound has been previously characterized.[4]

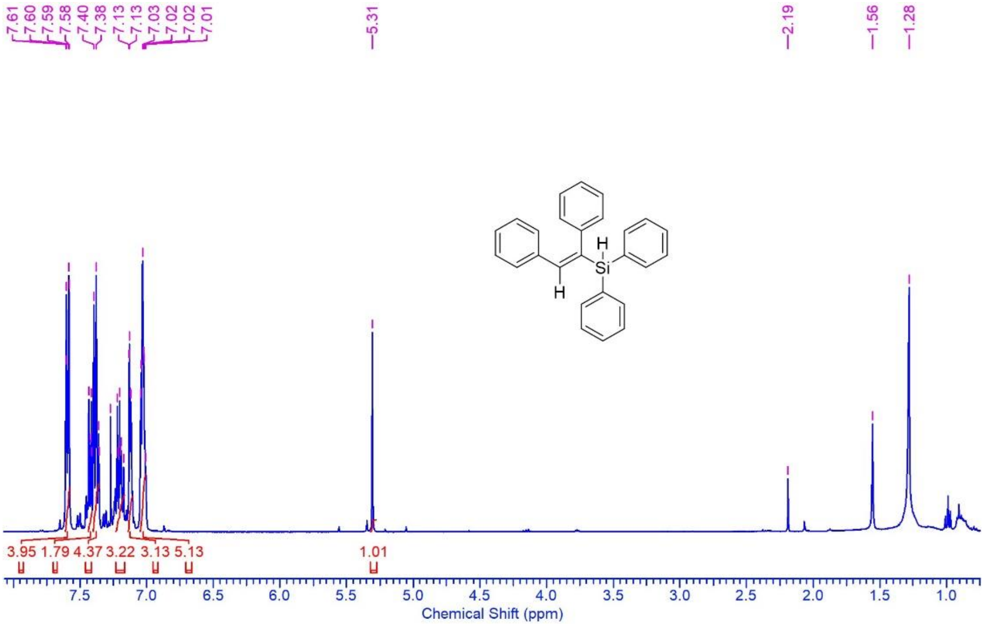
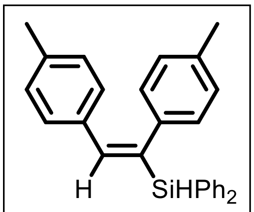


Figure S41: ^{1}H NMR of 3m in $CDCl_3$

(E)-(1,2-di-p-tolylvinyl)diphenylsilane (3n)



3n

The desired product 3n was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (200 MHz, $CDCl_3$):** δ = 7.54 (d, J = 2.2 Hz, 1H), 7.51 (d, J = 2.7 Hz, 2H) 7.36 (s, 1H), 7.33 (m, 3H), 7.30 (s, 1H), 6.99 (s, 1H), 6.95 (s, 2H), 6.87 (m, 8H), 5.22 (s, 1H, $-SiHPh_2$), 2.25 (s, 3H, CH_3-Ar), 2.19 (s, 3H, CH_3-Ar). This compound has been previously characterized.[4]

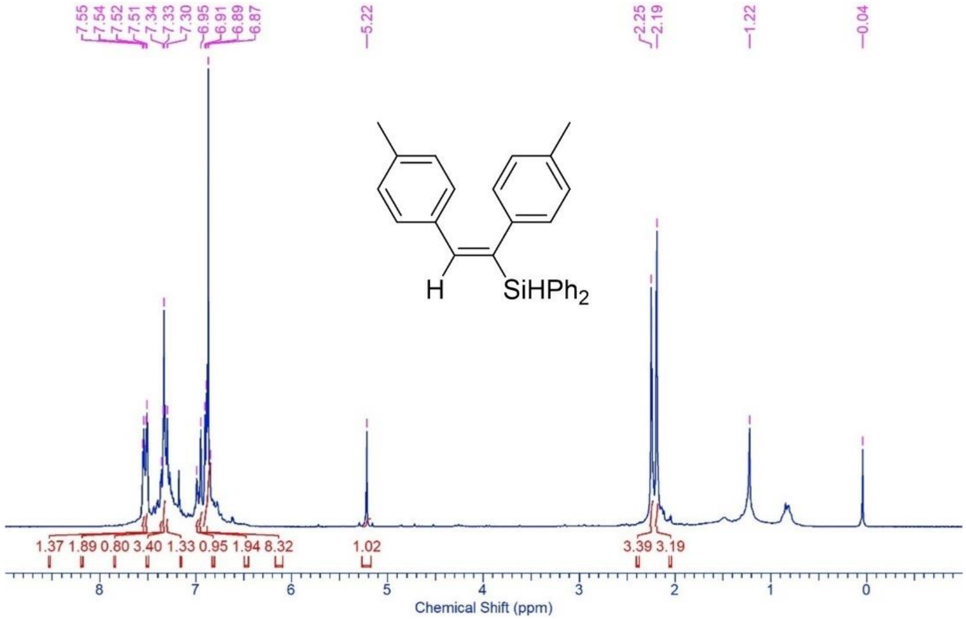
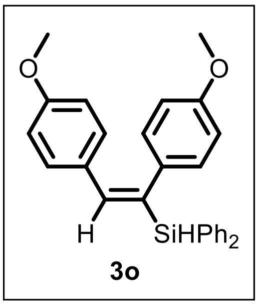
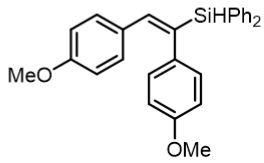


Figure S42A: ^{1}H NMR of 3n in $CDCl_3$

(E)-(1,2-bis(4-methoxyphenyl)vinyl)diphenylsilane (3o)



The desired product 3o was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (500 MHz, $CDCl_3$):** δ = 7.57 (d, J = 6.4 Hz, 4H), 7.44-7.36 (m, 6H), 6.98 (s, 1H), 6.96 (d, J = 2.5 Hz, 2H), 6.93 (d, *J*=3.5 Hz, 2 H), 6.76 (d, *J*=8.8 Hz, 2H), 6.65 (d, *J*=8.8 Hz, 2 H), 5.26 (s, 1 H), 3.78 (s, 3 H), 3.74 (s, 3 H). The characterization of this compound has been previously reported.[4]



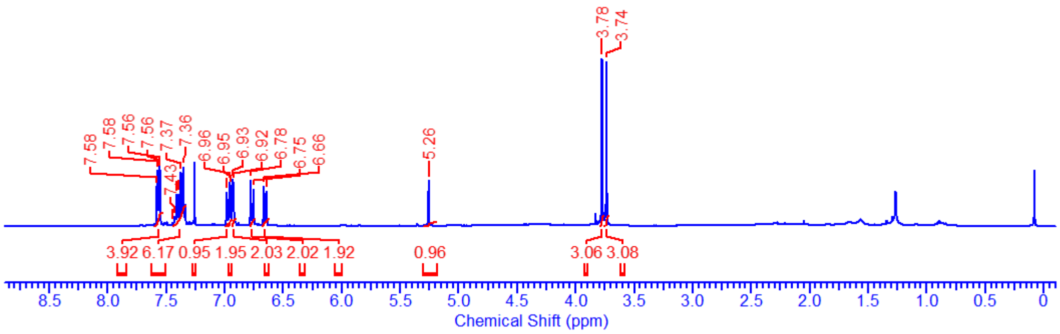
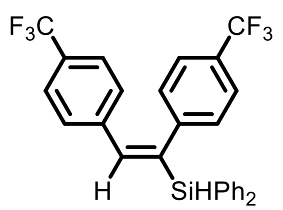


Figure S42B: ^{1}H NMR of 3o in $CDCl_3$

(E)-(1,2-bis(4-(trifluoromethyl)phenyl)vinyl)diphenylsilane (3p)



3p

The desired product 3p was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (200 MHz, $CDCl_3$):** δ = 7.56 (s, 2H), 7.54 (d, J = 1.4 Hz, 2H) 7.46 (s, 1H), 7.44 (s, 2H), 7.42 (s, 1H), 7.39 (s, 1H), 7.37 (s, 3H), 7.35 (m, 2H), 7.06 (m, 4H), 7.03 (s, 1H), 5.29 (s, 1H, -$SiHPh_2$). This compound has been previously characterized.[4]

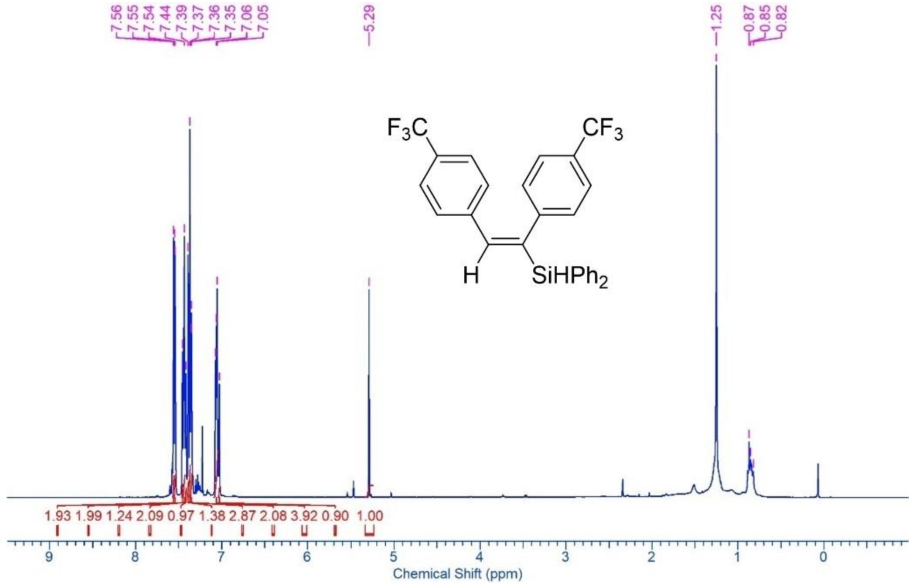
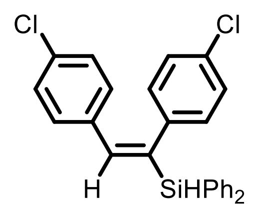


Figure S43: ^{1}H NMR of 3p in $CDCl_3$

(E)-(1,2-bis(4-chlorophenyl)vinyl)diphenylsilane (3q)



3q

The desired product 3q was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (200 MHz, $CDCl_3$):** δ = 7.49 (t, J = 1.7 Hz, 2H), 7.45 (d, J = 2.2 Hz, 2H) 7.40 (m, 1H), 7.36 (s, 1H), 7.33 (m, 3H), 7.29 (s, 1H), 7.17 (s, 1H), 7.12 (t, J = 2.2 Hz, 1H), 7.07 (m, 1H), 7.04 (m, 1H), 7.0 (m, 1H), 6.88 (s, 1H), 6.84 (d, J = 1.8 Hz, 2H), 6.80 (d, J = 1.6 Hz, 1H), 5.18 (s, 1H, -$SiHPh_2$). This compound has been previously characterized.[4]

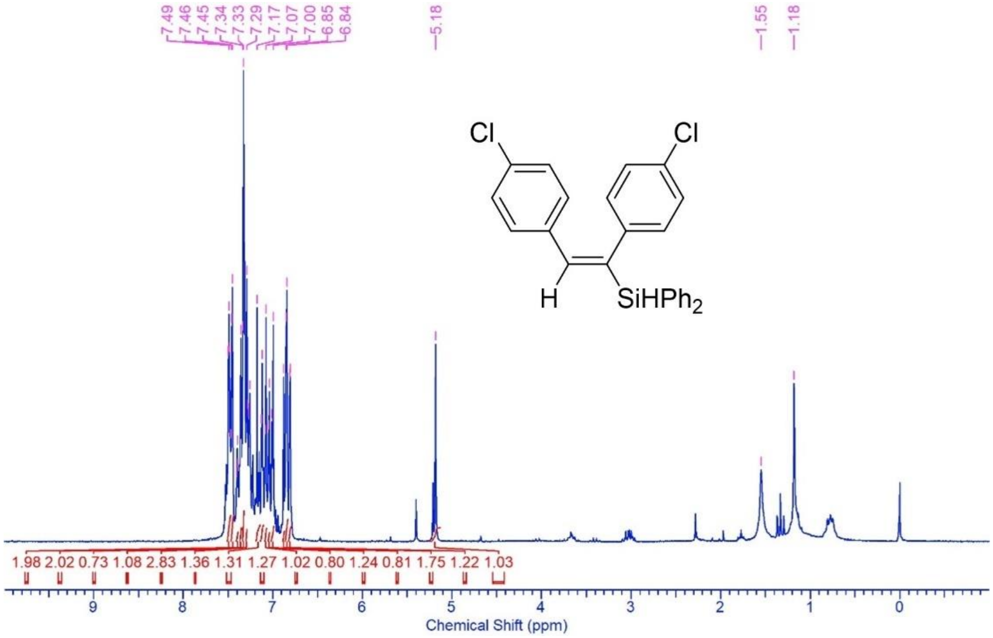
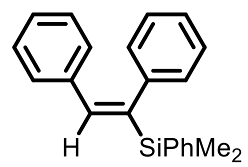


Figure S44: ^{1}H NMR of 3q in $CDCl_3$

(E)-(1,2-diphenylvinyl)dimethyl(phenyl)silane (3t)



3t

The desired product 3t was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (200 MHz, $CDCl_3$):** δ = 8.03 (br s, 1H), 7.86-7.69 (m, 9H), 7.59 (br s, 3H), 7.45-7.32 (m, 3H), 0.30 (s, 6H). This compound has been previously characterized.[5]

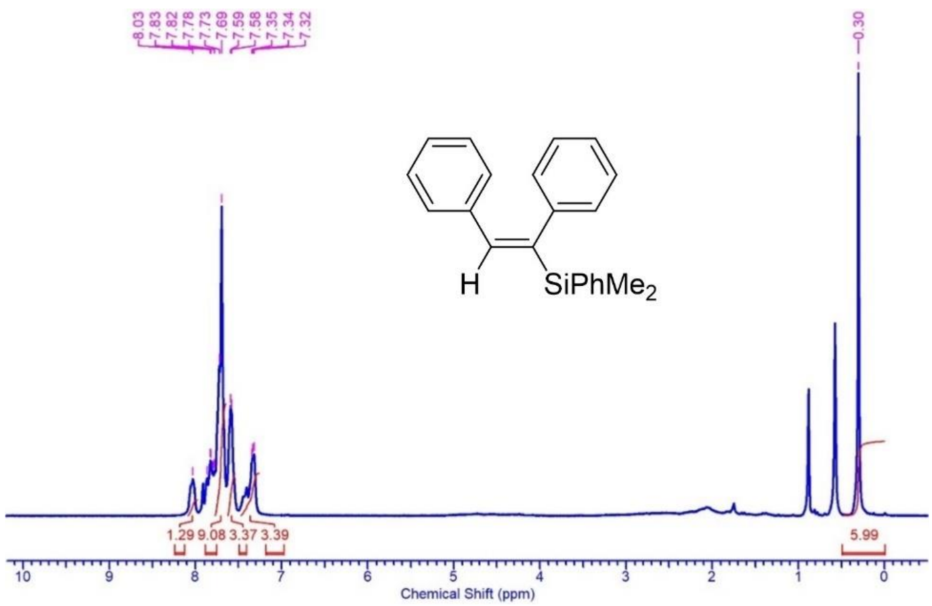
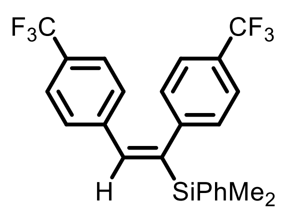


Figure S45: ^{1}H NMR of 3t in $CDCl_3$

(E)-(1,2-bis(4-(trifluoromethyl)phenyl)vinyl)dimethyl(phenyl)silane (3u)



3u

The desired product 3u was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (200 MHz, $CDCl_3$):** δ = 7.50-7.41 (m, 4H), 7.33-7.28 (m, 4H), 7.23-7.18 (m, 1H), 6.93-6.88 (m, 4H), 6.82 (s, 1H), 0.34 (s, 6H). This compound has been previously characterized.[5]

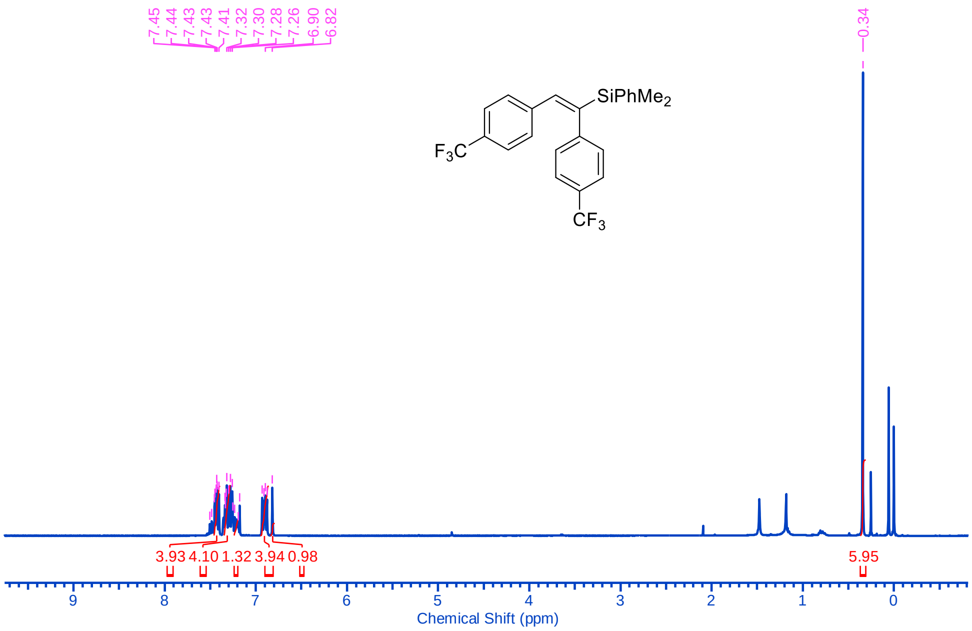
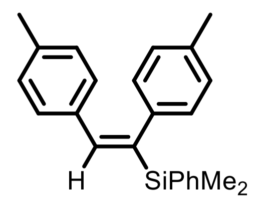


Figure S46: ^{1}H NMR of 3u in $CDCl_3$

(E)-(1,2-di-p-tolylvinyl)dimethyl(phenyl)silane (3v)



3v

The desired product 3v was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (200 MHz, $CDCl_3$):** δ = 7.85 (m, 1H), 7.65 (d, J = 2Hz, 1H) 7.63 (m, 1H), 7.50 (s, 2H), 7.40 (s, 1H), 7.35 (s, 1H), 7.31 (s, 1H), 7.16 (m, 3H), 7.11 (s, 1H), 7.07 (s, 1H), 7.03 (s, 1H), 2.61 (s, 3H, CH_3-Ar), 2.58 (s, 3H, CH_3-Ar), 0.67 (s, 3H, -$Si(CH_3)_2$), 0.11 (s, 3H, -$Si(CH_3)_2$). This compound has been previously characterized.[5]

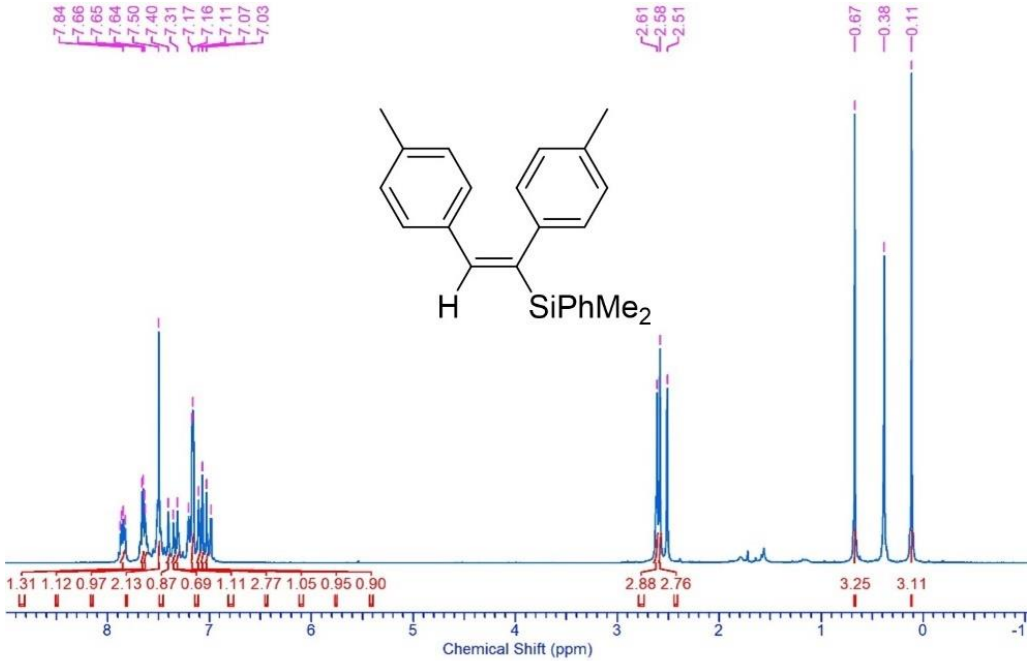
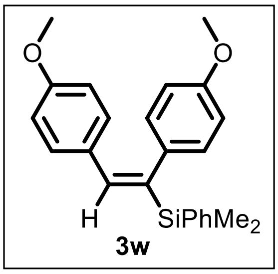


Figure S47: ^{1}H NMR of 3v in $CDCl_3$

(E)-(1,2-bis(4-methoxyphenyl)vinyl)dimethyl(phenyl)silane (3w)



The desired product 3w was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (200 MHz, $CDCl_3$):** δ = 7.84 (m, 1H), 7.65 (m, 3H), 7.51 (s, 3H), 7.11 (s, 3H), 7.05 (s, 1H), 7.0 (s, 1H), 6.96 (s, 2H), 4.10 (s, 3H), 4.08 (s, 3H), 0.67 (s, 3H, $-Si(CH_3)_2$), 0.14 (s, 3H, $-Si(CH_3)_2$). This compound has been previously characterized.[5]

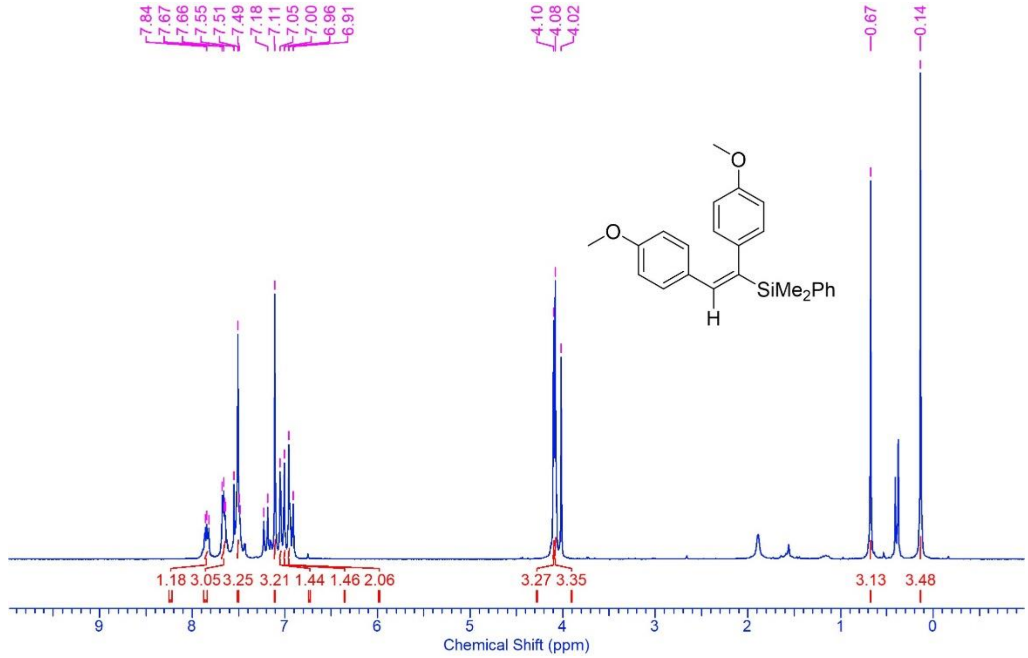
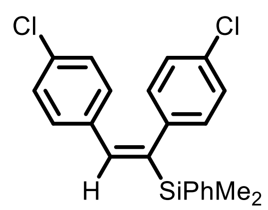


Figure S48: ^{1}H NMR of 3w in $CDCl_3$

(E)-(1,2-bis(4-chlorophenyl)vinyl)dimethyl(phenyl)silane (3x)



3x

The desired product 3x was obtained as a colorless oil by silica gel column chromatography. **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.55 (d, J = 2 Hz, 1H), 7.53 (m, 1H), 7.39 (d, J = 2 Hz, 2H), 7.37 (m, 1H), 7.24 (m, 1H), 7.20 (s, 1H), 7.11 (s, 1H), 7.06 (s,1H), 6.89 (s, 1H), 6.85 (s, 1H), 6.82 (s, 1H), 6.80 (s, 1H), 6.78 (s, 1H), 0.41 (s, 6H, -Si(CH_3)$_2$). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 145.0, 140.5, 138.6, 137.2, 135.6, 134.4, 133.3, 132.0, 130.9, 129.5, 129.2, 129.1, 128.4, 128.1, -3.1.

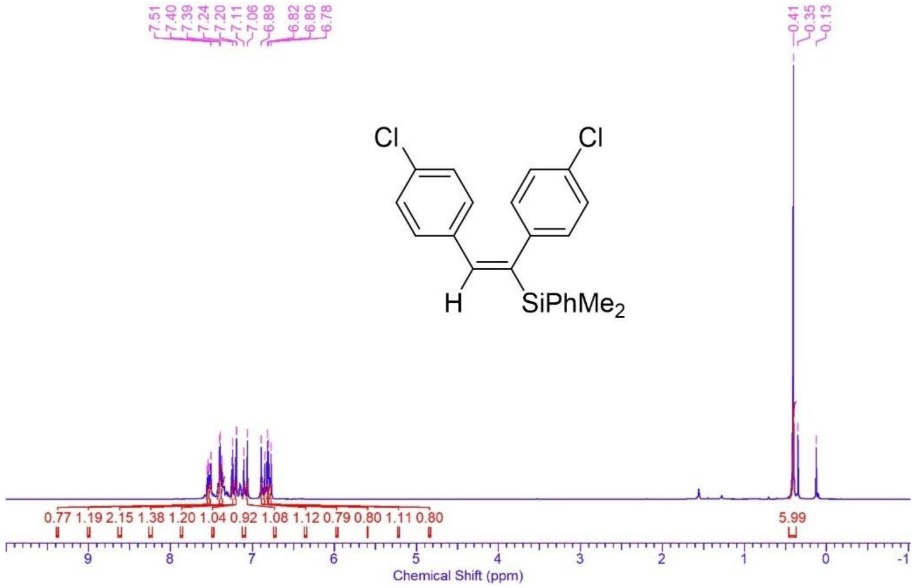


Figure S49: ^{1}H NMR of 3x in $CDCl_3$

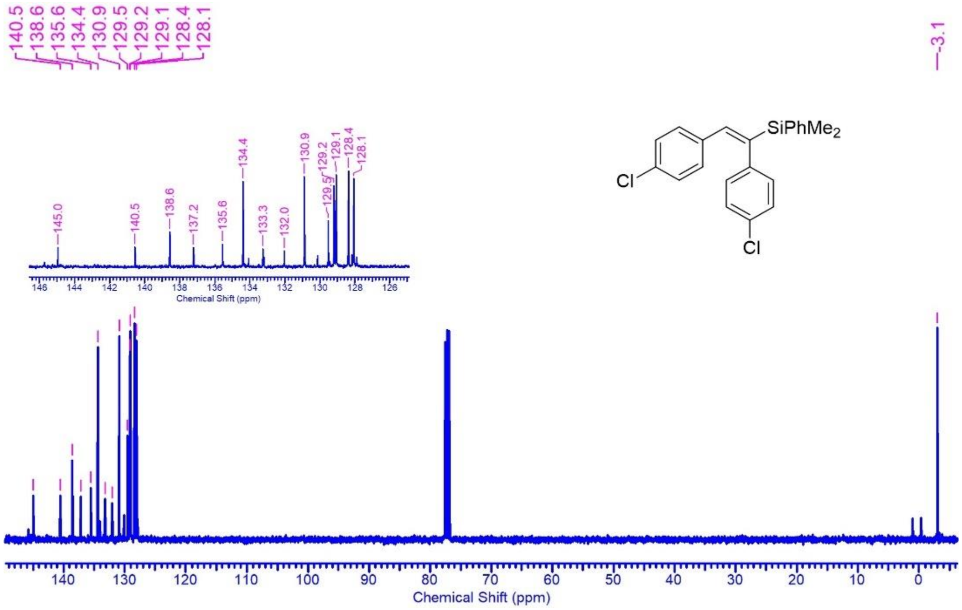
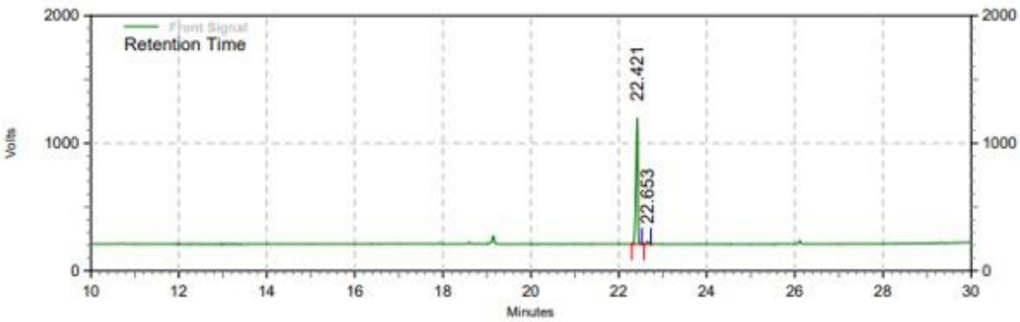


Figure S50: ^{13}C NMR of 3x in $CDCl_3$

6. Application:

6a. Gram scale synthesis:

Diphenylacetylene 1a (1 g, 5.62 mmol), triethylsilane 2a (980 mg, 8.43 mmol), [Fe-1] (80 mg, 0.281 mmol, 5 mol %), L5 (150 mg, 0.281 mmol, 5 mol %) were introduced in a 100 mL Schlenk flask equipped with a magnetic stir bar under argon atmosphere. Toluene (20 mL) was added to the reaction mixture. The reaction mixture was stirred at 70 °C for 24 h. The mixture was extracted with diethyl ether (3 × 20 mL). After that, the layers of mixed diethyl ether were dried over sodium sulfate and concentrated under vacuum. After evaporation of the solvent, the crude reaction mixture was purified by silica gel column chromatography (petroleum ether/EtOAc 50/1), yielding the hydrosilylated product. GC analysis showed full conversion with no starting alkyne (Rt = 17.7 min) with excellent E/Z ratio (98/2). The product was isolated in 90% yield (1.48 g).



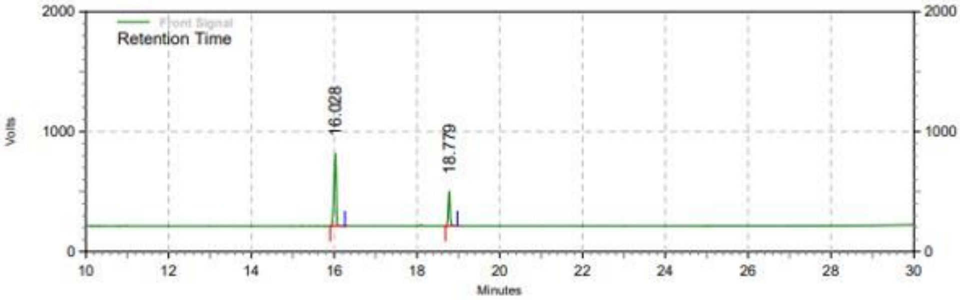
Front Signal
Results

Retention Time	Area	Area %	Height	Height %
22.421	22687095	97.93	7538810	97.65
22.653	480082	2.07	181419	2.35
Totals	23167177	100.00	7720229	100.00

Figure S51: GC chromatogram for gram scale reaction of 1a.

6b. Protodesilylation reaction:

3a (74 mg, 0.25 mmol), TBAF (1 M in THF, 1 mL, 1 mmol) were taken to a 10 mL teflon-valved flask equipped with a magnetic stir bar under argon atmosphere. THF (2 mL) was added to the reaction mixture. The reaction mixture was stirred at 80 °C for 24 h. The solvent was evaporated under vacuum. The residue was purified by silica gel column chromatography eluting with petroleum ether/EtOAc (v/v 50/1) to give a colourless viscous liquid (39 mg, 86%). GC analysis showed that it was Z/E mixture alkene in 71/29 ratio.

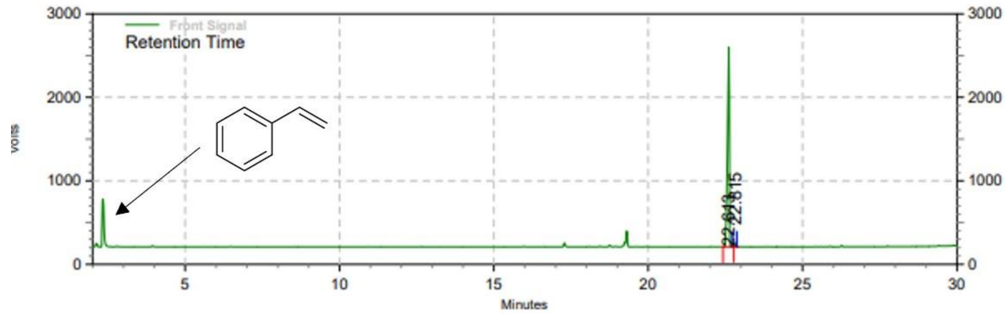


Front Signal
Results

Retention Time	Area	Area %	Height	Height %
16.028	16563078	71.26	4637054	67.71
18.779	6680885	28.74	2211359	32.29
Totals	23243963	100.00	6848413	100.00

Figure S52: GC chromatogram for protodesilylation reaction.

6c. Chemoselective hydrosilylation: Diphenylacetylene **1a** (44.55 mg, 0.25 mmol), triethylsilane **2a** (40 mg, 0.375 mmol), [Fe-1] (3.575 mg, 0.0125 mmol, 5 mol %), L5 (6.8 mg, 0.0125 mmol, 5 mol %) were introduced in a 10 mL teflon-valved flask equipped with a magnetic stir bar under argon atmosphere. Styrene (26 mg, 0.25 mmol) was also added to it under argon. Toluene (1 mL) was added to the reaction mixture. The reaction mixture was stirred at 60 °C for 24 h. The mixture was extracted with diethyl ether (10 mL) and passed through a short pad of silica and then injected in GC. GC analysis showed no presence of starting alkyne (R_t = 17.7 min). However, styrene (R_t = 2.2 min.) and hydrosilylated product of alkyne (R_t = 22.6, 22.8) were present there.



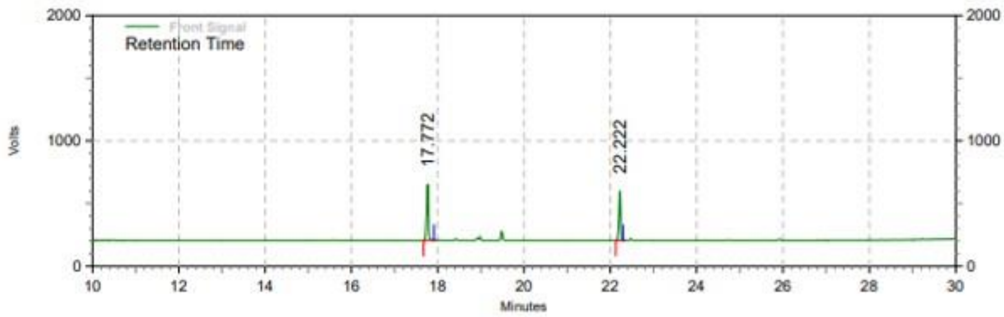
Front Signal
Results

Retention Time	Area	Area %	Height	Height %
22.613	74742941	98.84	18335524	98.04
22.815	877403	1.16	365607	1.95
Totals	75620344	100.00	18701131	100.00

Figure S53: GC chromatogram for chemoselective hydrosilylation reaction.

7. Mechanistic investigation:

7a. Test for homogeneity:
Diphenylacetylene **1a** (44.55 mg, 0.25 mmol), triethylsilane **2a** (40 mg, 0.375 mmol), [Fe-1] (3.575 mg, 0.0125 mmol, 5 mol %), L5 (6.8 mg, 0.0125 mmol, 5 mol %) were introduced in a 10 mL teflon-valved flask equipped with a magnetic stir bar under argon atmosphere. DCT (10.2 mg, 0.05 mmol) or [dppe (20 mg, 0.05 mmol) or bpy (7.8 mg, 0.05 mmol)] was also added to it under argon. Toluene (1 mL) was added to the reaction mixture. The reaction mixture was stirred at 60 °C for 16 h. The mixture was extracted with diethyl ether (10 mL) and passed through a short pad of silica and then injected in GC. GC analysis showed 45% conversion with respect to starting alkyne (R_t = 17.7 min) for DCT. However, in case of dppe or bpy, there was no conversion.

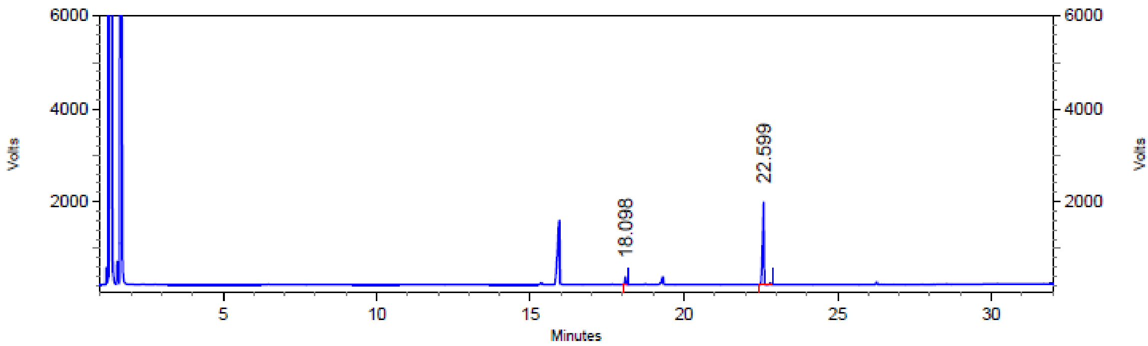


Front Signal
Results

Retention Time	Area	Area %	Height	Height %
17.772	10310793	55.49	3422937	53.27
22.222	8270680	44.51	3002608	46.73
Totals	18581473	100.00	6425545	100.00

Figure S54: GC chromatogram for hydrosilylation reaction of 1a in presence of DCT.

7b. Radical trap experiment: Diphenylacetylene **1a** (44.55 mg, 0.25 mmol), triethylsilane **2a** (40 mg, 0.375 mmol), [Fe-1] (3.575 mg, 0.0125 mmol, 5 mol %), L5 (6.8 mg, 0.0125 mmol, 5 mol %) were introduced in a 10 mL teflon-valved flask equipped with a magnetic stir bar under argon atmosphere. DPE (90 mg, 0.5 mmol) or [BHT (110 mg, 0.5 mmol)] was also added to it under argon. Toluene (1 mL) was added to the reaction mixture. The reaction mixture was stirred at 60 °C for 16 h. The mixture was extracted with diethyl ether (10 mL) and passed through a short pad of silica and then injected in GC. GC analysis showed 93% conversion (85% isolated yield) in presence of DPE whereas 78% conversion (72% isolated yield) in presence of BHT with respect to starting alkyne (R_t = 17.7 min).

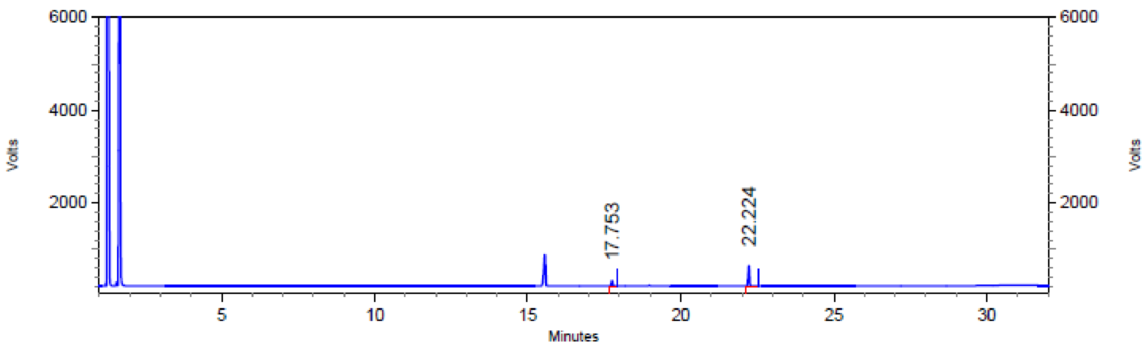


Front Signal
Results

Retention Time	Area	Area %	Height	Height %
18.098	3632258	6.91	1286700	8.64
22.599	48954345	93.09	13611135	91.36
Totals	52586603	100.00	14897835	100.00

Activate Wi

Figure S55: GC chromatogram for hydrosilylation reaction of 1a in presence of DPE.



Front Signal
Results

Retention Time	Area	Area %	Height	Height %
17.753	2710719	22.09	900129	20.92
22.224	9558372	77.91	3403286	79.08
Totals	12269091	100.00	4303415	100.00

Activate W

Figure S56: GC chromatogram for hydrosilylation reaction of 1a in presence of BHT.

7c. Procedure for XPS analysis:

Procedure for XPS analysis: X-ray photoemission spectroscopy (XPS) measurements were carried out using a Thermo Scientific Kalpha+ spectrometer using micro-focused and monochromatic Al Kα radiation with an energy of 1486.6 eV. The pass energy for the spectral acquisition was kept at 50 eV for individual core levels. The electron flood gun was utilized for providing charge compensation during data acquisition**.**The samples for XPS were prepared inside the glove box and transferred to a vacuum transfer module. By this way, the sample's exposure to the atmosphere was minimized.

Diphenylacetylene **1a** (44.55 mg, 0.25 mmol), triethylsilane **2a** (40 mg, 0.375 mmol), [Fe-1] (18 mg, 0.0625 mmol, 25 mol %), L5 (34 mg, 0.0625 mmol, 25 mol %) were introduced in a 10 mL teflon-valved flask equipped with a magnetic stir bar inside the glove-box. To the above mixture, toluene (1.0 mL) was added, and the resultant reaction mixture was stirred at 60 °C in a preheated oil bath for 12 min. After this, the reaction tube was transferred to the glove box. Inside the glove box, the sample for the XPS analysis was prepared. The sample was prepared before being moved to a vacuum transfer module, which was then evacuated in the glove box's antechamber. Using this vacuum transfer module, the samples were placed onto the spectrometer and then pumped down by turbo molecular pumps attached to the load lock chamber. Thus, samples were transferred effectively without being exposed to the atmosphere. The charge correction was done with C1s at 284.6 eV as standard. The same procedure was followed to perform other controlled XPS experiments, such as (i) [Fe-1], (ii) [Fe-1] + L5, (iii) [Fe-1] + L5 + Et_3SiH.

7d. Kinetic analysis:

Rate order determination

The initial rate method was used to determine the rate of the hydrosilylation reaction with different reaction components. Using MS Excel, the product concentration vs. time (min) plot data was linearly fitted. The reaction rate is represented by the slope of the linear fitting. The reaction rate is represented by the slope of the linear fitting. The log(rate) vs. log(conc) plot for each component was then used to determine the order of the reaction.

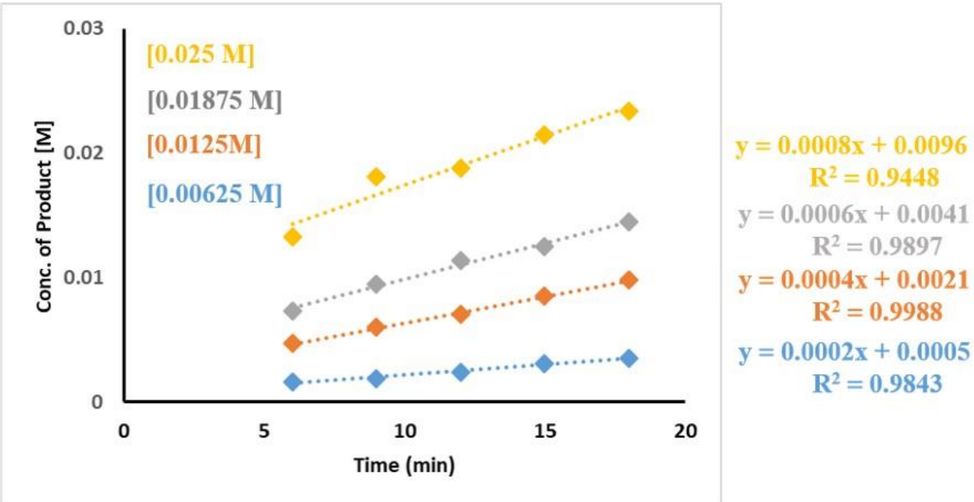
Rate order determination for [Fe-1]/L5:

To determine the order of the hydrosilylation reaction with respect to [Fe-1]/L5 catalyst system, the initial rates at different concentration of [Fe-1]/L5 were determined. In an oven dried teflon-screw capped tube, diphenylacetylene (0.25 mmol, 44.55 mg), triethylsilane (0.375 mmol, 40 mg) were taken under argon atmosphere. Specific amount of [Fe-1] and $P(C_6F_5)_3$ were added (as shown in table 2.3) to the tube. Dodecane (0.25 mmol, 42.6 mg, 57 µL) was added to the tube as an internal standard. The required amount of toluene was added to make the volume 1.0 mL. The tube was closed under argon and placed in a pre-heated oil bath at 60 °C. The aliquot was collected first after 6 min. Then it was collected at a constant interval of 3 min and the yield of the 3a (M) was determined with the help of GC. The data were collected till 18 min.

Table S2. Rate of hydrosilylation reaction at different initial concentration of catalyst

Entry	[Fe-1] (mg)	$P(C_6F_5)_3$ (mg)	Initial Conc. of [Fe-1]/L5 [M]	Initial rate (M/min)	R^2
1	1.8	3.4	0.00625	0.0002	0.9843
2	3.6	6.8	0.0125	0.0004	0.9988
3	5.4	10.2	0.01875	0.0006	0.9897
4	7.2	13.6	0.025	0.0008	0.9448

a)



b)

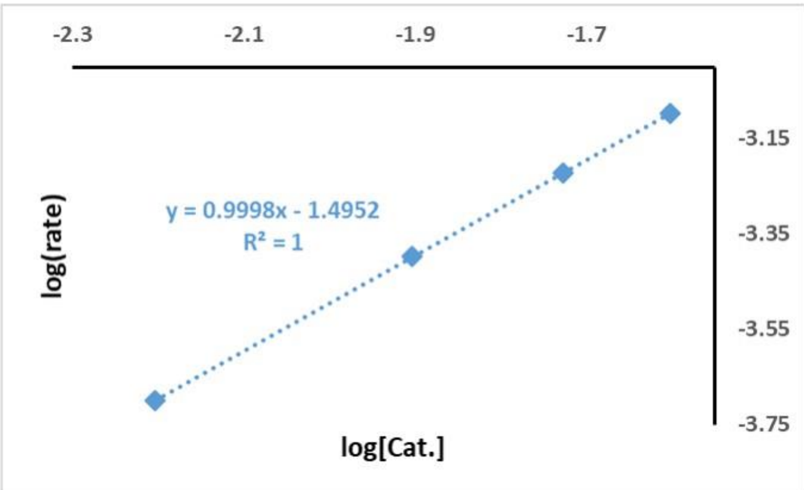


Figure S57: a) Time dependent formation of 3a at different concentration of catalyst. b) Plot of log(rate) vs. log[Cat.].

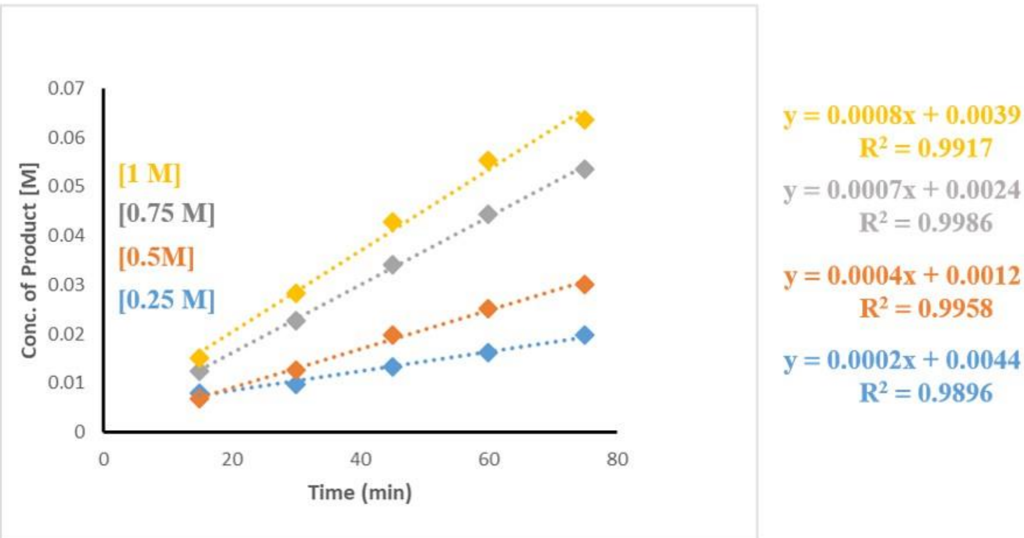
Rate order determination for triethylsilane:

To determine the order of the hydrosilylation reaction with respect to triethylsilane, the initial rates at different concentrations of triethylsilane were determined. In an oven dried teflon-screw capped tube, diphenylacetylene (0.25 mmol, 44.55 mg), [Fe-1] (0.00625 mmol,1.8 mg), $P(C_6F_5)_3$ (0.00625 mmol, 3.4 mg) were taken under argon atmosphere. Specific amount of triethylsilane was added (as shown in table 2.4) to the tube. Dodecane (0.25 mmol, 42.6 mg, 57 µL) was added to the tube as an internal standard. The required amount of toluene was added to make the volume 1.0 mL. The tube was closed under argon and placed in a pre-heated oil bath at 60 °C. The aliquot was collected at constant 15 minutes interval and the yield of the 3a (M) was determined with the help of GC. The data were collected till 75 min.

Table S3. Rate of hydrosilylation reaction at different initial concentration of silane

Entry	Et_3SiH (mg)	Initial Conc. of [Et_3SiH] [M]	Initial rate (M/min)	R^2
1	29	0.25	0.0002	0.9896
2	58	0.5	0.0004	0.9958
3	87	0.75	0.0007	0.9986
4	116	1.0	0.0008	0.9917

a)



b)

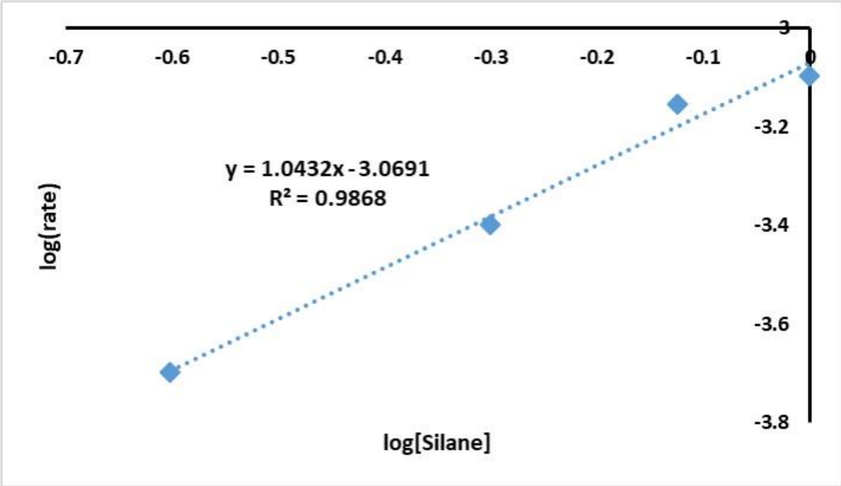


Figure S58: a) Time dependent formation of 3a at different concentration of Et_3SiH. b) Plot of log(rate) vs. log[Silane].

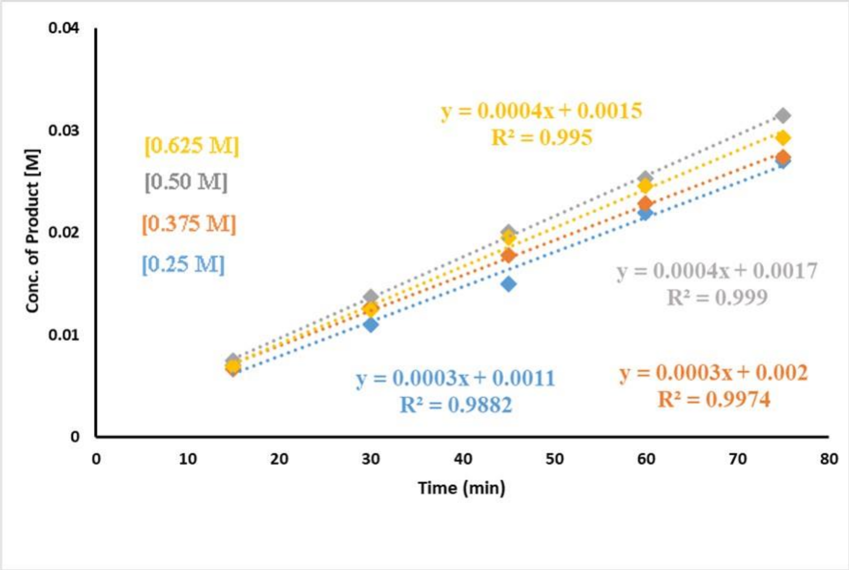
Rate order determination for diphenylacetylene:

To determine the order of the hydrosilylation reaction with respect to diphenylacetylene, the initial rates at different concentrations of diphenylacetylene were determined. In an oven dried teflon-screw capped tube, [Fe-1] (0.00625 mmol,1.8 mg), $P(C_6F_5)_3$ (0.00625 mmol, 3.4 mg), triethylsilane (0.375 mmol, 40 mg) were taken under argon atmosphere. Specific amount of diphenylacetylene was added (as shown in table 2.5) to the tube. Dodecane (0.25 mmol, 42.6 mg, 57 μL) was added to the tube as an internal standard. The required amount of toluene was added to make the volume 1.0 mL. The tube was closed under argon and placed in a pre-heated oil bath at 60 °C. The aliquot was collected at constant 15 min interval and the yield of the 3a (M) was determined with the help of GC. The data were collected till 75 minutes.

Table S4. Rate of hydrosilylation reaction at different initial concentration of alkyne

Entry	PhCCPh (mg)	Initial Conc. of [PhCCPh] [M]	Initial rate (M/min)	R^2
1	44.5	0.25	0.0003	0.9882
2	66.75	0.375	0.0003	0.9974
3	89	0.5	0.0004	0.999
4	111.25	0.625	0.0004	0.995

a)



b)

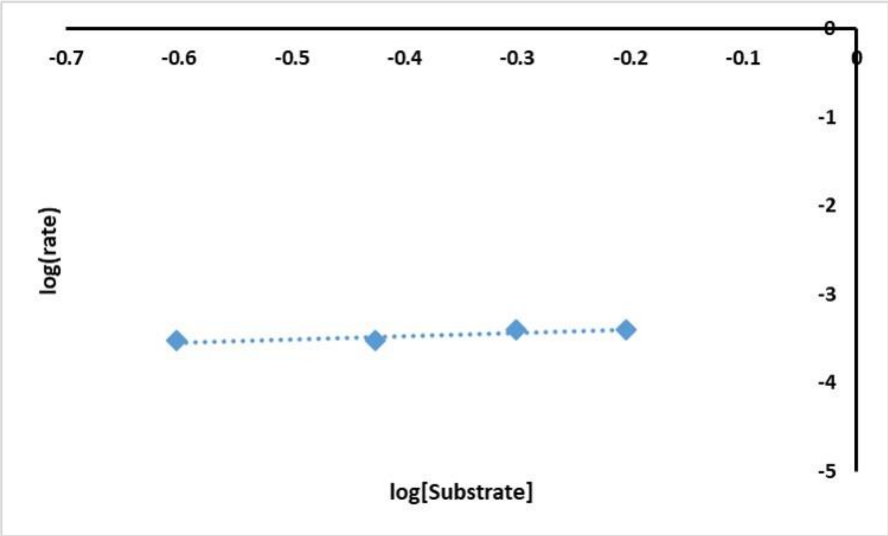
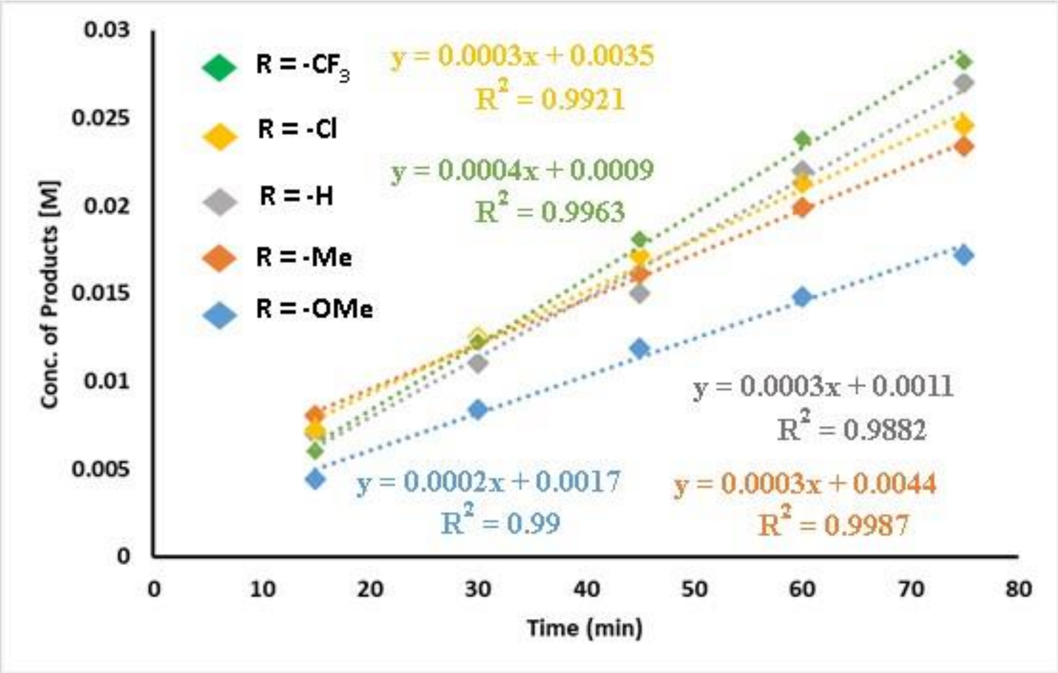


Figure S59. a) Time dependent formation of 3a at different concentration of diphenylacetylene. b) Plot of log(rate) vs. log[Substrate].

Rate determination for hydrosilylation of substituted alkynes with triethylsilane

As mentioned in the earlier section, representative procedure of rate measurement was followed by taking [Fe-1] (0.00625 mmol, 1.8 mg), $P(C_6F_5)_3$ (0.00625 mmol, 3.4 mg), triethylsilane (0.375 mmol, 40 mg) and 1,2-di-p-tolylethyne (0.25 mmol, 52 mg) or [1,2-bis(4-methoxyphenyl)ethyne (0.25 mmol, 59.57 mg); 1,2-diphenylethyne (0.25 mmol, 44.55 mg); 1,2-bis(4-chlorophenyl)ethyne (0.25 mmol; 61.8 mg); 1,2-bis(4-(trifluoromethyl)phenyl)ethyne (0.25 mmol, 78.55 mg)] under argon atmosphere. Dodecane (0.25 mmol, 42.6 mg, 57 µL) was added to the tube as an internal standard. The required amount of toluene was added to make the volume 1.0 mL. The tube was closed under argon and placed in a pre-heated oil bath at 60 °C. The aliquot was collected at constant 15 minutes interval and the yield of the 3a (M) was determined with the help of GC. The data were collected till 75 minutes. The initial rate for the coupling reactions are shown below (Figure S60). The Hammett plot was drawn from the correlation between the initial rates and the σ_p values, i.e $\log(k_R/k_H)$ vs. σ_p and slope obtained was 0.289 (Figure 4;manuscript).



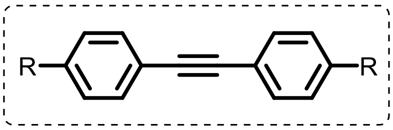


Figure S60. Time dependent formation of hydrosilylation products for the coupling of triethylsilane with different para-substituted alkynes.

Eyring analysis:

In an oven dried teflon-screw capped tube, diphenylacetylene (0.25 mmol, 44.55 mg), [Fe(BDA)(CO)$_3$] (2.5 mol %, 0.00625 mmol, 1.8 mg), $P(C_6F_5)_3$ (2.5 mol %, 0.00625 mmol, 3.4 mg), triethylsilane (0.375 mmol, 40 mg) were taken under argon atmosphere. Then internal standard dodecane (0.25 mmol, 42.6 mg, 57 µL) and 1 mL toluene were added to it under argon and transferred to a preheated oil bath set at different temperatures 45 °C, 50 °C, 55 °C, 60 °C. The aliquot was taken at 15-minute intervals, and GC was used to track the yield. The reaction rate is represented by the slope of the linear fitting.

Table S5. Rate of hydrosilylation reaction at different temperature

k [M/min]	T (K)	1/T	ln (k/T)	ln (k)
1.00E-04	318	0.003145	-14.972	-9.21
2.00E-04	323	0.003096	-14.295	-8.517
3.00E-04	328	0.003049	-13.905	-8.112
4.00E-04	333	0.003003	-13.632	-7.824

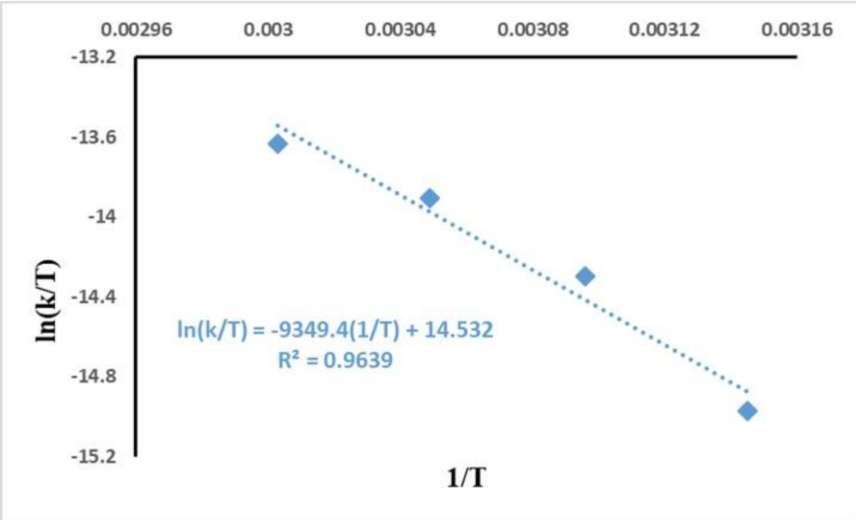


Figure S61. Eyring plot for [Fe-1] catalysed hydrosilylation of 1a with 2a in toluene.

Based on Eyring equation, activation thermodynamic parameters were calculated

Eyring equation

$$\ln(k/T) = -\Delta H^{\#}/RT + \ln(k_B/h) + \Delta S^{\#}/R$$

$$\Delta H^{\#} = 77.731 \text{ kJ mol}^{-1}$$

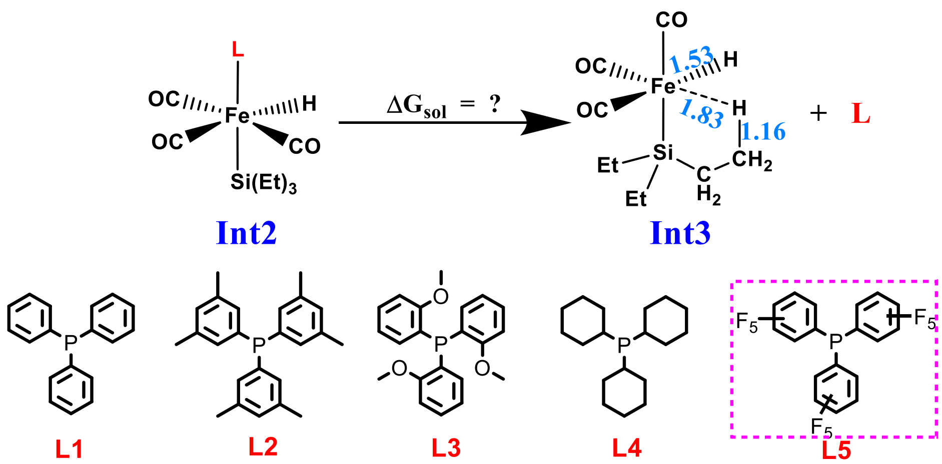
$$\Delta S^{\#} = -76.72 \text{ J K}^{-1} \text{ mol}^{-1}$$

$$\Delta G^{\#}_{(323\,K)} = 102.51 \text{ kJ mol}^{-1}$$

Supporting Information

8. Computational Details:

The density functional calculations were conducted using the Turbomole 7.5.0 suite of programs.[6] All geometries presented in the proposed mechanism were optimized using the B3LYP functional[7] and def2-TZVP basis set.[8] To account for long-range interactions, Grimme's dispersion correction (D3)[9] was employed. Accurate and efficient treatment of the electronic Coulomb term in the DFT calculations was achieved through the utilization of the resolution of identity (RI)[10] and multipole accelerated resolution of identity (marij)[11] approximations. The reported values correspond to ΔG values, which consider zero-point energy corrections, internal energy, and entropic contributions obtained through frequency calculations on the optimized minima at a temperature of 298.15 K. Solvent corrections were included in all calculations using the COSMO model[12] with an epsilon (∊) value of 2.38, representing toluene as the solvent utilized in the experimental studies. Harmonic frequency calculations were performed for all stationary points to confirm their classification as local minima. The absence of imaginary frequencies confirmed the minima, while the presence of a single imaginary frequency verified the transition states. Additionally, intrinsic reaction coordinate (IRC)[13] calculations were performed on all transition states to further validate their authenticity and confirm the correct determination of reactant and product structures.



L	ΔG_{sol} (kcal/mol)
L1	26.7
L2	25.9
L3	29.8
L4	34.5
L5	17.3

Figure S62. The Gibbs free energy (ΔG_{sol}) for the dissociation of all phosphine ligands (L1-L5) have been shown here. The DFT calculations have been done at the B3LYP-D3/def2-TZVP level of theory using toluene as solvent (ε=2.38). All the values are in kcal/mol.

XYZ Coordinates

Catalyst

Electronic Energy (-2065.920891Hartree)

Fe	-9.6229807	1.7728443	2.9757032
C	-8.8602069	0.3308585	2.1789393
C	-11.1145280	1.1232532	3.8023786
C	-8.7045697	1.6917809	4.5075329
O	-12.0545698	0.7049968	4.2909998
O	-8.3634061	-0.5538323	1.6622193
O	-8.1163236	1.6590248	5.4836243
C	-5.8587607	2.7512173	1.4982066
C	-4.5093529	2.8563868	1.8067536
C	-4.1086573	3.4673324	2.9918592
C	-5.0727183	3.9692583	3.8619349
C	-6.4223838	3.8610347	3.5532869
C	-6.8421777	3.2510668	2.3633263
H	-6.1629506	2.2721126	0.5746309
H	-3.7694818	2.4605822	1.1219288
H	-3.0569595	3.5504856	3.2355796
H	-4.7722971	4.4443453	4.7877846
H	-7.1520401	4.2493516	4.2520994
C	-8.2564883	3.1063157	1.9851078
H	-8.4196724	2.8138808	0.9540164
C	-9.3277093	3.8078403	2.6038994
H	-9.1831794	4.5365278	3.3887495
C	-10.6472158	3.4515374	2.2041240
O	-10.7428556	2.4436887	1.3974499
C	-11.8721099	4.1902387	2.6518387
H	-12.6909673	3.4947619	2.8312023
H	-11.6829346	4.7819524	3.5470469
H	-12.1770957	4.8670307	1.8488092

Int1

Electronic Energy (-4590.691617 Hartree)

P	-0.8317628	0.1650227	-0.2746398
C	-2.0322178	1.0553236	0.8612357
C	-1.8525192	1.4614139	2.1841668
C	-3.2811509	1.3546200	0.3113378
C	-2.8162166	2.1782588	2.8821351
C	-4.2649171	2.0565759	0.9863034
C	-4.0261607	2.4852118	2.2829774
C	-1.7057444	-1.4728544	-0.1775389
C	-2.1870487	-2.1237060	-1.3127141
C	-1.9895753	-2.0829630	1.0466754
C	-2.9119868	-3.3075365	-1.2345769
C	-2.7017553	-3.2629229	1.1524241
C	-3.1707474	-3.8794052	-0.0004289
C	0.6763713	-0.0721744	0.7757650
C	1.3522228	1.0664605	1.2139430

C	1.3090611	-1.2857825	1.0274042
C	2.5409879	1.0127179	1.9175885
C	2.4958766	-1.3717678	1.7441351
C	3.1132474	-0.2195029	2.2010832
F	-4.9574829	3.1606648	2.9502988
F	-2.5877442	2.5521955	4.1433072
F	-0.7518661	1.1525520	2.8797197
F	-3.5903142	0.9180224	-0.9177458
F	-5.4398708	2.3047399	0.4057136
F	0.8040981	-2.4447631	0.5799001
F	-1.9852584	-1.6392318	-2.5380201
F	-1.5457235	-1.5372823	2.1878852
F	-3.3633677	-3.8929987	-2.3445711
F	-3.8619360	-5.0115637	0.0819517
F	-2.9344686	-3.8146746	2.3447430
F	0.8374904	2.2798103	0.9745894
F	3.1461581	2.1342054	2.3144282
F	4.2565279	-0.2883386	2.8762475
F	3.0547861	-2.5635094	1.9741040
Fe	-0.2725209	1.1982030	-2.2174122
C	0.3127607	0.1164138	-3.5369408
C	-0.4434616	2.9778187	-2.0037860
C	-1.8454058	1.1871260	-3.0205567
O	0.7116265	-0.5352300	-4.3960236

O	-0.5514620	4.1167062	-1.8796042
O	-2.8202676	1.1996337	-3.6241323
C	6.5900635	0.6080111	-0.1169522
C	5.4639587	-0.1977274	-0.3542480
C	5.5252918	-1.5551305	-0.0033056
C	6.6732834	-2.0949625	0.5584579
C	7.7807185	-1.2843905	0.7844495
C	7.7343507	0.0684049	0.4459136
H	6.5622969	1.6626821	-0.3577936
H	4.6616338	-2.1865764	-0.1711629
H	6.7017928	-3.1435743	0.8249941
H	8.6760949	-1.7001558	1.2291501
H	8.5930674	0.7012671	0.6305241
C	4.2291018	0.3177048	-0.9175114
H	3.3809398	-0.3591009	-0.8864112
C	4.0149120	1.5190717	-1.4877154
H	4.8157987	2.2308946	-1.6412482
C	2.6993922	1.8825327	-1.9985621
O	1.7021024	1.2411656	-1.6311778
C	2.5907212	3.0290595	-2.9537505
H	1.8006958	2.8238936	-3.6751565
H	2.2968898	3.9234130	-2.3951699
H	3.5356275	3.2314772	-3.4549327

Int2

Electronic Energy (-4656.18161 Hartree)

P	-0.3132721	-0.0700325	0.0250708
C	-1.0359759	-0.2240271	-1.6795727
C	-1.8199316	0.7020900	-2.3693506
C	-0.7346109	-1.4005978	-2.3706294
C	-2.2230018	0.4978639	-3.6818473
C	-1.1321804	-1.6333629	-3.6762385
C	-1.8757367	-0.6702277	-4.3419069
C	-1.5100960	-1.1607468	0.9197199
C	-2.8888399	-1.0042212	0.7500310
C	-1.1105884	-2.1924365	1.7697765
C	-3.8185197	-1.8340154	1.3493697
C	-2.0238731	-3.0395155	2.3848577
C	-3.3813628	-2.8649707	2.1707241
C	-0.7345321	1.6288512	0.6080880
C	-1.2975953	1.9208040	1.8478750
C	-0.2622459	2.7197145	-0.1253080
C	-1.4173063	3.2225480	2.3184817
C	-0.3730281	4.0243238	0.3167231
C	-0.9576584	4.2794949	1.5510206
F	-2.2685152	-0.8747098	-5.5938532
F	-2.9621631	1.4154324	-4.3052188
F	-2.2501802	1.8272992	-1.7931197
F	-0.0498370	-2.3778952	-1.7607531
F	-0.8154735	-2.7737361	-4.2882594
F	0.3223410	2.5197127	-1.3132446
F	-3.3632452	0.0031131	0.0066616
F	0.1742353	-2.4119175	2.0520506
F	-5.1233139	-1.6437450	1.1575492
F	-4.2600295	-3.6702272	2.7541611
F	-1.5988584	-4.0160138	3.1849413
F	-1.7322123	0.9525078	2.6661888
F	-1.9666770	3.4539719	3.5107221
F	-1.0684343	5.5272897	1.9933571
F	0.0760062	5.0331746	-0.4290674
Fe	1.9194027	-0.3177759	0.1670601
H	2.0065054	1.1973064	0.2213671
Si	4.3261589	-0.1220559	0.3686283
C	1.9663383	-0.0294618	1.9287504
C	2.2356460	0.0299440	-1.5531847
C	2.1269946	-2.1128507	0.0867608
O	1.9873534	0.2543449	3.0373176
O	2.4181725	0.3140111	-2.6461260
O	2.3049193	-3.2377152	0.0084125
C	4.8671339	1.6918162	0.2889976
H	4.4221668	2.2036707	1.1488415
H	5.9496771	1.6946824	0.4675831
C	5.1906898	-1.1010964	-1.0137571

H 4.8606631 -0.7102941 -1.9801913

H 4.8379585 -2.1364675 -0.9775465

C 4.9922702 -0.7708366 2.0251260

H 6.0792008 -0.6384556 1.9714072

H 4.6552045 -0.1039550 2.8237965

C 4.6664882 -2.2248406 2.3841388

H 3.5942213 -2.3705274 2.5322778

H 4.9808270 -2.9160505 1.5984505

H 5.1640628 -2.5300427 3.3081479

C 4.5548725 2.4636576 -0.9977164

H 3.4785927 2.5564330 -1.1557386

H 4.9675374 3.4751268 -0.9657814

H 4.9717916 1.9679595 -1.8778390

C 6.7256364 -1.0723917 -0.9466725

H 7.1687080 -1.6251539 -1.7794383

H 7.1117951 -0.0510386 -0.9923727

H 7.0984375 -1.5217271 -0.0237045

Int2 with L1

Electronic Energy (-3167.54266 Hartree)

P -0.2732513 0.1068045 -0.0162615

C -0.9707310 0.0095960 -1.7103622

C -1.8567393 0.9551979 -2.2282446

C -0.6103519 -1.0871808 -2.5001150

C -2.3706576 0.8066684 -3.5137754

C -1.1312807 -1.2395835 -3.7770044

C -2.0125943 -0.2900243 -4.2885449

C -1.2844038 -1.1240086 0.8985481

C -2.5562133 -1.5036916 0.4580370

C -0.7959188 -1.6617070 2.0918766

C -3.3208927 -2.3983027 1.1981577

C -1.5635842 -2.5505869 2.8352347

C -2.8280251 -2.9217457 2.3894510

C -0.8789566 1.7175063 0.6202759

C -1.9393095 1.8185335 1.5228089

C -0.2542763 2.8883561 0.1771426

C -2.3643252 3.0650486 1.9744129

C -0.6882156 4.1311308 0.6175914

C -1.7435718 4.2227880 1.5218032

Fe 1.9748582 -0.1715500 0.1152367

H 2.1267795 1.3406068 0.0073594

Si 4.3765556 -0.2408271 0.3207303

C 2.0853773 0.3200050 1.8202436

C 2.3167215 0.0463304 -1.6151682

C 1.9537277 -1.9657622 0.1881944

O 2.1727691 0.7336942 2.8870766

O 2.5415965 0.2685560 -2.7167040

O 1.9499158 -3.1115734 0.1993019

C 5.1377248 1.4915328 0.1711474

H	4.7346861	2.0960130	0.9911725
H	6.2086365	1.3796497	0.3815130
C	5.1369056	-1.3708074	-1.0104669
H	4.8525726	-0.9873594	-1.9943994
H	4.6667931	-2.3565161	-0.9314318
C	4.9827113	-0.8811985	2.0072486
H	6.0772163	-0.8845944	1.9470844
H	4.7320602	-0.1362237	2.7680370
C	4.4861841	-2.2624128	2.4482372
H	3.4048146	-2.2672624	2.6017856
H	4.7093918	-3.0299606	1.7030898
H	4.9479244	-2.5745655	3.3888622
C	4.9470236	2.2270281	-1.1595288
H	3.8906309	2.4172564	-1.3601103
H	5.4595332	3.1927247	-1.1612421
H	5.3373261	1.6477629	-2.0001696
C	6.6645965	-1.5149597	-0.9373531
H	7.0445983	-2.1480413	-1.7441309
H	7.1641209	-0.5464832	-1.0211231
H	6.9830397	-1.9644876	0.0058314
H	0.1896367	-1.3908513	2.4437765
H	-1.1693793	-2.9573689	3.7579232
H	-3.4243928	-3.6189485	2.9647503
H	-4.3027478	-2.6852209	0.8426449
H	-3.1828100	3.1265982	2.6809063
H	-2.0753447	5.1916405	1.8737962
H	-0.1962853	5.0279137	0.2619948
H	0.5779627	2.8274778	-0.5118756
H	0.0829957	-1.8254702	-2.1161213
H	-0.8439544	-2.0947008	-4.3759040
H	-2.4137780	-0.4044099	-5.2878220
H	-3.0539692	1.5499765	-3.9054908
H	-2.1511854	1.8094223	-1.6339236
H	-2.9539399	-1.1033282	-0.4648087
H	-2.4380965	0.9290322	1.8819721

Int2 with L2

Electronic Energy (-3403.37680 Hartree)

P	-0.2724679	0.0755465	-0.0590200
C	-0.9626078	-0.0720182	-1.7536361
C	-1.9563820	0.7779097	-2.2388742
C	-0.5117392	-1.1226369	-2.5537241
C	-2.5032820	0.5862300	-3.5079638
C	-1.0423993	-1.3389354	-3.8227576
C	-2.0391673	-0.4767874	-4.2807497
C	-1.3552833	-1.0571655	0.8994125
C	-2.7279406	-1.1297221	0.6320810
C	-0.8219977	-1.8369372	1.9189966
C	-3.5574818	-1.9624458	1.3731204

C	-1.6311630	-2.6876664	2.6782127
C	-2.9910861	-2.7343819	2.3936933
C	-0.7677483	1.7509623	0.4887289
C	-1.5582288	1.9667821	1.6103122
C	-0.2563541	2.8490686	-0.2146086
C	-1.8493636	3.2669101	2.0420521
C	-0.5418871	4.1475940	0.1829464
C	-1.3399480	4.3376544	1.3184391
Fe	1.9655220	-0.2549361	0.1205960
H	2.1153272	1.2599835	0.1865974
Si	4.3532829	-0.3679899	0.4011559
C	2.0197696	0.0701223	1.8661378
C	2.3501794	0.1605355	-1.5621521
C	1.9425401	-2.0447901	-0.0043267
O	2.0736331	0.3808194	2.9701263
O	2.6000846	0.5136939	-2.6241582
O	1.9412486	-3.1856193	-0.1215344
C	5.1283607	1.3636130	0.4825071
H	4.7044958	1.8682539	1.3574799
H	6.1924128	1.2198743	0.7068826
C	5.1561282	-1.3381468	-1.0276641
H	4.8877477	-0.8531800	-1.9706815
H	4.6957722	-2.3309570	-1.0659357
C	4.8989692	-1.2113905	2.0188723
H	5.9949703	-1.2179248	1.9958219
H	4.6252992	-0.5616617	2.8554179
C	4.3816373	-2.6312211	2.2748372
H	3.2972565	-2.6427340	2.4054655
H	4.6128137	-3.3035387	1.4448200
H	4.8210024	-3.0627676	3.1781803
C	4.9765699	2.2550151	-0.7550771
H	3.9266129	2.4770521	-0.9562088
H	5.4945085	3.2097981	-0.6285912
H	5.3847874	1.7770070	-1.6492199
C	6.6833486	-1.4746146	-0.9372743
H	7.0878459	-2.0156935	-1.7974641
H	7.1719557	-0.4974775	-0.9083942
H	6.9880589	-2.0176783	-0.0396315
H	0.2371235	-1.7948665	2.1315209
H	-3.6317464	-3.3898572	2.9749314
H	-1.5611126	5.3498087	1.6414876
H	0.3727248	2.6870644	-1.0816430
H	0.2635090	-1.7846399	-2.1877836
H	-2.4643291	-0.6387476	-5.2662151
H	-2.3168281	1.5956251	-1.6279652
H	-3.1567298	-0.5324188	-0.1624938
H	-1.9558343	1.1275498	2.1663967
C	-2.6994927	3.4779925	3.2680184

H	-2.8331773	4.5382657	3.4841089
H	-3.6886401	3.0306516	3.1405013
H	-2.2444855	3.0083653	4.1437116
C	0.0069128	5.3328450	-0.5679524
H	-0.7877974	6.0352568	-0.8302785
H	0.7314912	5.8782314	0.0428068
H	0.5071125	5.0256230	-1.4866784
C	-5.0345332	-2.0447231	1.0874533
H	-5.3169361	-3.0536653	0.7756807
H	-5.6200987	-1.8065882	1.9790120
H	-5.3265550	-1.3542082	0.2959309
C	-1.0196267	-3.5449463	3.7550347
H	-0.4410840	-4.3618824	3.3147394
H	-0.3366799	-2.9653614	4.3794636
H	-1.7819358	-3.9850418	4.3986518
C	-3.5570376	1.5224586	-4.0397012
H	-3.1026127	2.3101853	-4.6477971
H	-4.2743410	0.9954064	-4.6713075
H	-4.1044056	2.0078471	-3.2304974
C	-0.5278444	-2.4550278	-4.6936178
H	-1.3208714	-2.8690764	-5.3187763
H	0.2587153	-2.0905570	-5.3609906
H	-0.1030507	-3.2631884	-4.0967899

Int2 with L3

Electronic Energy (-3511.09380 Hartree)

P	-0.3915510	-0.0027932	-0.0825772
C	-1.1185304	-0.2003631	-1.7607084
C	-1.8584839	0.8002599	-2.3843268
C	-0.9312235	-1.4157582	-2.4449634
C	-2.3774112	0.6334830	-3.6619442
C	-1.4446785	-1.5878160	-3.7322307
C	-2.1604529	-0.5609575	-4.3360261
C	-1.4554258	-1.1065706	0.9310747
C	-2.8662820	-1.0485594	0.8776969
C	-0.8684956	-2.0705182	1.7465306
C	-3.6342702	-1.9548886	1.6102695
C	-1.6287087	-2.9707532	2.4849547
C	-3.0124130	-2.9112102	2.4067933
C	-0.8370391	1.6914228	0.4660378
C	-1.5217281	1.9091967	1.6592711
C	-0.3357718	2.8112313	-0.2290999
C	-1.7277057	3.1919324	2.1566330
C	-0.5483661	4.0997496	0.2597085
C	-1.2428889	4.2840693	1.4511865
Fe	1.8760829	-0.2804196	0.1320049
H	1.9749691	1.2334712	0.2028912
Si	4.2522652	-0.1553469	0.3779450

C	1.8685287	0.0258249	1.8821090
C	2.1762590	0.1092970	-1.5770766
C	2.0282837	-2.0639934	0.0346326
O	1.8729308	0.3205906	2.9915635
O	2.3645287	0.4295571	-2.6613546
O	2.1853972	-3.1983896	-0.0393924
C	4.8688578	1.6426146	0.3586874
H	4.3989456	2.1542740	1.2054774
H	5.9423975	1.6139969	0.5825821
C	5.1389984	-1.1105252	-1.0133279
H	4.8085341	-0.7061506	-1.9746200
H	4.7846716	-2.1462933	-0.9929651
C	4.9022539	-0.8529712	2.0265123
H	5.9921357	-0.7381234	1.9964295
H	4.5588897	-0.1996089	2.8344377
C	4.5447456	-2.3080367	2.3492716
H	3.4665374	-2.4360902	2.4679730
H	4.8632293	-2.9882535	1.5552710
H	5.0156997	-2.6434968	3.2774902
C	4.6299301	2.4406114	-0.9275226
H	3.5636406	2.5354821	-1.1389070
H	5.0428576	3.4510716	-0.8592278
H	5.0896298	1.9567939	-1.7931668
C	6.6729234	-1.0830138	-0.9442269
H	7.1224415	-1.6294087	-1.7785984
H	7.0577743	-0.0605349	-0.9805236
H	7.0435485	-1.5366025	-0.0220598
H	0.2083295	-2.1196709	1.8008985
H	-1.1408152	-3.7088835	3.1076857
H	-3.6220355	-3.6068929	2.9703467
H	-4.7128996	-1.9171562	1.5686565
H	-1.8947781	1.0636543	2.2200594
H	-2.2610033	3.3303401	3.0880868
H	-1.3982230	5.2889157	1.8242219
H	-0.1707159	4.9570372	-0.2778783
H	-1.2943854	-2.5164369	-4.2625320
H	-2.5535772	-0.7046940	-5.3350761
H	-2.9467633	1.4304916	-4.1226862
H	-2.0482434	1.7230594	-1.8571195
O	-3.4015143	-0.0726397	0.1097843
O	-0.2572287	-2.3845103	-1.7762236
O	0.3400408	2.5458015	-1.3723261
C	0.9317292	3.6036221	-2.1148249
H	1.6528798	4.1584952	-1.5088011
H	1.4473315	3.1242422	-2.9429451
H	0.1723423	4.2889895	-2.5018590
C	-4.8119518	0.0256334	-0.0328019
H	-5.2333930	-0.8889824	-0.4588988

H -5.2945268 0.2403991 0.9250344

H -4.9800664 0.8538465 -0.7169054

C -0.0261788 -3.6417266 -2.4015165

H 0.5684317 -3.5274014 -3.3121269

H 0.5304726 -4.2306104 -1.6783457

H -0.9685906 -4.1434172 -2.6384352

Int2 with L4

Electronic Energy (-3178.38619 Hartree)

P -0.3562170 0.2745201 -0.2954174

Fe 1.8991123 -0.0753980 0.0061222

H 2.1343882 1.3666944 -0.4262602

Si 4.2631786 -0.2143971 0.4685492

C 1.9096149 0.7254564 1.5896834

C 2.4348581 -0.2548210 -1.6718385

C 1.7598566 -1.8137485 0.4131934

O 1.9319520 1.3283653 2.5676349

O 2.8222474 -0.3040536 -2.7529521

O 1.6876341 -2.9374659 0.6342164

C 5.1473482 1.4155182 0.0627814

H 4.7006408 2.1930265 0.6918846

H 6.1820210 1.3067182 0.4104376

C 5.0804935 -1.6247704 -0.5179951

H 4.9192234 -1.4422863 -1.5837324

H 4.5453962 -2.5536619 -0.2939464

C 4.6632936 -0.5348519 2.3028735

H 5.7551631 -0.6120750 2.3600550

H 4.4021005 0.3588696 2.8770690

C 4.0228311 -1.7702432 2.9453650

H 2.9350473 -1.6798007 2.9854761

H 4.2489109 -2.6813448 2.3857558

H 4.3729572 -1.9191737 3.9704230

C 5.1381139 1.8642905 -1.4026238

H 4.1208538 2.0505800 -1.7528766

H 5.7081397 2.7866524 -1.5435900

H 5.5732589 1.1067495 -2.0593490

C 6.5815677 -1.8118199 -0.2514323

H 7.0020206 -2.6058373 -0.8751898

H 7.1438309 -0.8991027 -0.4651130

H 6.7774766 -2.0789344 0.7894275

C -0.9889964 0.0884119 -2.0350248

C -0.4146422 1.1522254 -2.9883025

C -0.7479438 -1.3327183 -2.5751437

H -2.0707247 0.2454676 -1.9821397

C -0.9534869 0.9752117 -4.4119089

H 0.6737633 1.0856562 -3.0085874

H -0.6571887 2.1530006 -2.6301325

C -1.2742711 -1.4893465 -4.0059037

H 0.3223009 -1.5519342 -2.5620954

H	-1.2263118	-2.0729785	-1.9309781
C	-0.6822478	-0.4338204	-4.9416874
H	-0.5024502	1.7240651	-5.0683857
H	-2.0340577	1.1614559	-4.4158537
H	-1.0457359	-2.4948477	-4.3690684
H	-2.3667475	-1.3958738	-4.0012590
H	-1.0919095	-0.5471860	-5.9490089
H	0.4001126	-0.5865581	-5.0188219
C	-1.0145411	1.9247471	0.3077763
C	-0.0501487	3.1114216	0.1189082
C	-2.4105673	2.3131627	-0.2211718
H	-1.1011698	1.7576689	1.3880939
C	-0.5783831	4.3691621	0.8179670
H	0.0780691	3.3158524	-0.9481087
H	0.9375156	2.8696523	0.5024559
C	-2.9427346	3.5642734	0.4887215
H	-2.3469655	2.5207136	-1.2929752
H	-3.1227431	1.4988905	-0.1054694
C	-1.9814346	4.7440928	0.3381664
H	0.1161135	5.1970787	0.6521990
H	-0.6011747	4.1901226	1.8993721
H	-3.9279213	3.8198690	0.0885761
H	-3.0821640	3.3415634	1.5531818
H	-2.3540120	5.6120631	0.8887395
H	-1.9347780	5.0359762	-0.7175566
C	-1.3305764	-1.0130374	0.6590762
C	-1.0401961	-0.9722881	2.1704334
C	-2.8486396	-1.1058097	0.4284223
H	-0.8924598	-1.9422847	0.2793911
C	-1.6219789	-2.2021742	2.8770600
H	-1.4807600	-0.0681899	2.6039050
H	0.0317969	-0.9202103	2.3562747
C	-3.4242158	-2.3514243	1.1151527
H	-3.3386254	-0.2237563	0.8476486
H	-3.0880703	-1.1298107	-0.6358877
C	-3.1224779	-2.3506427	2.6156993
H	-1.4265453	-2.1344472	3.9505445
H	-1.0993402	-3.0951639	2.5167240
H	-4.5030338	-2.4000441	0.9432092
H	-2.9899456	-3.2471032	0.6564434
H	-3.4996536	-3.2658778	3.0796866
H	-3.6540621	-1.5157476	3.0874536

Int3

Electronic Energy (-2131.366288 Hartree)

Fe	0.8734366	0.2075392	-0.1313441
H	0.3788082	0.9979907	-1.3433864
C	1.3155244	-0.8065666	1.3116365
C	2.4985373	0.8287461	-0.6473178

C	0.5385137	-1.1341832	-1.1952722
O	1.5702093	-1.4760699	2.2013538
O	3.4986101	1.1964127	-1.0570871
O	0.2989691	-1.9889712	-1.9245568
Si	-1.3439990	0.3330847	0.3024395
C	-0.4295644	1.8040071	1.0898951
H	-0.5032088	1.7125434	2.1752880
H	0.6996627	1.7284435	0.9473162
C	-2.5932861	0.8316763	-1.0136171
H	-3.4323586	1.3198103	-0.5032300
H	-2.1282413	1.5939898	-1.6434997
C	-2.1054918	-0.8366515	1.5756781
H	-3.1403810	-0.5232073	1.7551477
H	-1.5705282	-0.6842633	2.5185261
C	-2.0679405	-2.3277050	1.2017302
H	-2.6106258	-2.5293773	0.2762710
H	-1.0423279	-2.6737834	1.0578263
H	-2.5159915	-2.9422897	1.9860718
C	-3.1177916	-0.3199398	-1.8863224
H	-2.3050439	-0.8263301	-2.4108461
H	-3.6429917	-1.0697918	-1.2912345
H	-3.8194828	0.0465798	-2.6393173
C	-0.8010764	3.2082674	0.5963958
H	-0.1660614	3.9726002	1.0502608
H	-0.6903988	3.2843478	-0.4857985
H	-1.8381808	3.4421088	0.8437602

Int4

Electronic Energy (-2670.721323 Hartree)

Fe	-0.0824562	0.8918283	-0.9438559
H	1.2900943	0.4628340	-1.4118247
C	-1.6018772	1.5581598	-0.2366005
C	-0.6527013	0.5255288	-2.6430266
C	0.6987580	2.4219951	-1.3202836
O	-2.5795907	1.9903775	0.1667948
O	-0.9776384	0.3434189	-3.7201620
O	1.2403259	3.3940156	-1.5935290
Si	0.9494420	1.4296877	1.2268308
C	0.2201213	0.3686639	2.6292385
H	0.4048725	-0.6815375	2.3857853
H	0.8605913	0.5872650	3.4935428
C	2.8059895	1.0212696	1.2605700
H	3.1462392	1.3453750	2.2525291
H	2.9246112	-0.0643787	1.2449343
C	0.8641850	3.2628588	1.7451861
H	1.6681770	3.7812701	1.2128392
H	1.1615515	3.2669409	2.8016447
C	-0.4375856	4.0546032	1.5753915
H	-0.7182750	4.1439734	0.5239548

H	-1.2757375	3.5856015	2.0927797
H	-0.3355393	5.0701246	1.9670085
C	3.6923969	1.6552046	0.1843642
H	4.7431044	1.3865792	0.3230619
H	3.4021537	1.3254301	-0.8149791
H	3.6291525	2.7456210	0.1951162
C	-1.2488855	0.5615357	3.0198278
H	-1.4599228	1.5953413	3.3002753
H	-1.9228428	0.2999818	2.2041376
H	-1.5183959	-0.0688268	3.8718694
C	0.4272904	-1.1579920	-0.3790022
C	-0.8089700	-1.0761674	-0.2884844
C	-2.1382594	-1.5422602	-0.0187536
C	-3.2425724	-1.1467018	-0.7843449
C	-2.3363000	-2.4408761	1.0428229
C	-4.5063749	-1.6468935	-0.5060090
H	-3.1052121	-0.4463976	-1.5964573
C	-3.6037132	-2.9304787	1.3209938
H	-1.4934715	-2.7360064	1.6531234
C	-4.6930597	-2.5374828	0.5475105
H	-5.3494175	-1.3345143	-1.1091917
H	-3.7428024	-3.6166787	2.1470042
H	-5.6821214	-2.9180886	0.7688606
C	1.6583430	-1.9006293	-0.2891129
C	2.7631945	-1.6628582	-1.1124283
C	1.7315449	-2.9346174	0.6585940
C	3.9068631	-2.4395266	-0.9991109
H	2.7204350	-0.8613361	-1.8367025
C	2.8803568	-3.7038807	0.7732673
H	0.8867905	-3.1221638	1.3077861
C	3.9728868	-3.4597833	-0.0544739
H	4.7526526	-2.2419135	-1.6455306
H	2.9239917	-4.4926820	1.5138027
H	4.8708913	-4.0573049	0.0388778

TS4a

Electronic Energy (-2670.72099 Hartree)

Imaginary frequency (1, -33.30 cm^{-1})

Fe	-0.1765057	0.9645982	-1.4574557
H	1.2164042	0.4863753	-1.7891711
C	-1.7015659	1.6908339	-0.8398479
C	-0.7046013	0.5731975	-3.1710811
C	0.6721290	2.4581494	-1.8410413
O	-2.6780691	2.1671263	-0.4844989
O	-1.0166137	0.3730063	-4.2483551
O	1.2657789	3.4008790	-2.1085751
Si	0.7378224	1.5007159	0.7602615
C	-0.1330800	0.5216360	2.1405404

H	-0.0257796	-0.5425030	1.9108223
H	0.4911996	0.6947854	3.0266008
C	2.5522763	0.9497521	0.9018116
H	2.8400369	1.1728811	1.9372495
H	2.5893829	-0.1388770	0.8120023
C	0.7460222	3.3480673	1.2257267
H	1.6006442	3.8027168	0.7148660
H	0.9953994	3.3712359	2.2942971
C	-0.5005803	4.2032576	0.9687212
H	-0.7276100	4.2692684	-0.0972887
H	-1.3862138	3.7989054	1.4606559
H	-0.3601025	5.2254455	1.3300839
C	3.5645804	1.5844636	-0.0566025
H	4.5731813	1.1990600	0.1156726
H	3.3143712	1.3795937	-1.0992581
H	3.6052602	2.6698659	0.0583461
C	-1.5940219	0.8356346	2.4791107
H	-1.7305564	1.8870957	2.7401077
H	-2.2606893	0.6150398	1.6459460
H	-1.9386582	0.2410709	3.3297178
C	0.3614083	-1.0879553	-0.9649051
C	-0.8630556	-0.9740061	-0.7612513
C	-2.1582543	-1.4404162	-0.3533698
C	-3.3321862	-1.0491579	-1.0101986
C	-2.2540135	-2.3262102	0.7323770
C	-4.5646848	-1.5355346	-0.5988804
H	-3.2724006	-0.3631974	-1.8439040
C	-3.4900377	-2.8012989	1.1450342
H	-1.3568925	-2.6195337	1.2604432
C	-4.6497920	-2.4091076	0.4816667
H	-5.4623939	-1.2248545	-1.1183266
H	-3.5490618	-3.4760059	1.9899507
H	-5.6139450	-2.7780395	0.8079864
C	1.5629130	-1.8832561	-1.0116276
C	2.6867642	-1.5478013	-1.7726163
C	1.5861685	-3.0739547	-0.2645424
C	3.8025977	-2.3726497	-1.7888825
H	2.6820595	-0.6337168	-2.3503537
C	2.7041571	-3.8942194	-0.2826817
H	0.7246821	-3.3458485	0.3303677
C	3.8186105	-3.5468798	-1.0428799
H	4.6635894	-2.0931971	-2.3827937
H	2.7078712	-4.8055282	0.3021311
H	4.6928611	-4.1853188	-1.0511511

Int4a

Electronic Energy (-5195.538338Hartree)

P	1.1404303	-0.2933264	0.5442649
C	2.9678705	0.0638389	0.6450434

C	3.9303932	-0.1144237	-0.3506305
C	3.4486387	0.4939081	1.8843237
C	5.2730747	0.1689002	-0.1403013
C	4.7817431	0.7821556	2.1207884
C	5.7029192	0.6227120	1.0969678
C	1.2887704	-2.0149106	1.2144034
C	1.8301974	-3.0693570	0.4722286
C	0.9912052	-2.2964195	2.5473375
C	1.9931334	-4.3411530	0.9909752
C	1.1564415	-3.5611059	3.0950980
C	1.6476061	-4.5912444	2.3124402
C	0.7745189	-0.4762530	-1.2547780
C	-0.0647036	-1.4516843	-1.7884447
C	1.1589231	0.5419160	-2.1264410
C	-0.4810122	-1.4285535	-3.1115048
C	0.7667999	0.5869855	-3.4514823
C	-0.0621578	-0.4075202	-3.9501458
F	6.9872791	0.8877767	1.3044868
F	6.1566978	-0.0065449	-1.1222867
F	3.6113162	-0.5808958	-1.5611070
F	2.6091142	0.6199207	2.9222106
F	5.1822320	1.1959886	3.3217024
F	1.9115434	1.5571212	-1.6740941
F	2.2358272	-2.8780958	-0.7885417
F	0.5473247	-1.3503532	3.3690232
F	2.4977693	-5.3193627	0.2384114
F	1.8039840	-5.8061117	2.8248022
F	0.8394985	-3.7872259	4.3681113
F	-0.4974565	-2.4737624	-1.0439955
F	-1.2829019	-2.3849837	-3.5790445
F	-0.4609206	-0.3753629	-5.2169062
F	1.1572250	1.5890508	-4.2373521
Fe	-0.3031332	1.4213006	1.3018352
H	-2.4780541	0.6900060	-0.8251901
Si	-1.8192657	3.3069708	1.9344426
C	1.0597012	2.5806024	1.3960358
C	-0.3002746	1.2186278	3.1019783
O	1.9340483	3.3143943	1.4254413
O	-0.2687812	1.1814459	4.2397309
C	-3.1903612	2.8497662	3.1652178
H	-2.7836699	2.2760014	4.0000682
H	-3.4716465	3.8196162	3.5961475
C	-2.7251371	4.1514673	0.4861383
H	-3.6036981	4.6065146	0.9590026
H	-3.1230844	3.4030399	-0.2024439
C	-0.8169963	4.6993473	2.7559814
H	-0.0893430	5.0914017	2.0399057
H	-1.5553534	5.5003928	2.8884761

C	-0.1285295	4.4200048	4.0963309
H	-0.8222542	4.0048932	4.8304811
H	0.6939582	3.7105014	3.9922042
H	0.2919866	5.3351016	4.5202682
C	-4.4420827	2.1722122	2.5914257
H	-4.9381594	2.8130722	1.8599515
H	-4.2027149	1.2379947	2.0863655
H	-5.1672828	1.9513409	3.3787571
C	-1.9578714	5.2395645	-0.2787095
H	-1.7122770	6.0797163	0.3729873
H	-1.0221671	4.8732603	-0.7028563
H	-2.5543608	5.6306869	-1.1068808
C	-2.6945539	0.0045416	-0.0163196
C	-1.9315458	0.0333180	1.0965443
C	-3.8399515	-0.8636557	-0.3685657
C	-4.7879505	-1.3429216	0.5463873
C	-4.0182626	-1.1912319	-1.7208629
C	-5.8471581	-2.1374340	0.1273972
H	-4.6983022	-1.0928895	1.5931062
C	-5.0683322	-1.9975957	-2.1407986
H	-3.3133916	-0.8135837	-2.4527903
C	-5.9892597	-2.4786822	-1.2152099
H	-6.5674956	-2.4915227	0.8550294
H	-5.1695253	-2.2459815	-3.1903583
H	-6.8125773	-3.1043452	-1.5367345
C	-2.1738063	-1.0098715	2.1356418
C	-2.0240672	-2.3646833	1.8045852
C	-2.5954363	-0.7158267	3.4365382
C	-2.2700169	-3.3714744	2.7283309
H	-1.7320280	-2.6283089	0.8005946
C	-2.8514004	-1.7193258	4.3623818
H	-2.7448296	0.3088506	3.7313140
C	-2.6833446	-3.0561712	4.0180657
H	-2.1426440	-4.4070190	2.4353951
H	-3.1826963	-1.4522792	5.3587235
H	-2.8734213	-3.8387322	4.7419061
C	-0.7159895	2.0452309	-0.3194272
O	-0.9458405	2.4608534	-1.3591053

TS4b

Electronic Energy (-2670.698137 Hartree)

Imaginary frequency (1, -112.44 cm^{-1})

Fe	-0.2762664	1.3207760	-1.5668277
H	1.0106658	0.8990208	-2.2791498
C	-1.9757609	1.7052922	-1.0043183
C	-0.6724601	1.1550023	-3.2846036
C	0.4938541	2.9446599	-1.6955852
O	-3.0946777	1.8627668	-0.8440196
O	-0.8690728	1.0340131	-4.4036707

O	0.9993691	3.9579443	-1.8409259
Si	0.2927224	1.4910136	1.0980599
C	-0.7922790	0.6566028	2.4192433
H	-0.2407334	-0.2048886	2.8011115
H	-0.8258115	1.3768207	3.2452365
C	2.1074383	1.4851131	1.6476070
H	2.1055292	2.0365854	2.5951463
H	2.4380957	0.4763473	1.8900468
C	-0.0827603	3.3649658	1.2982725
H	0.6926307	3.9350385	0.7842423
H	0.1429516	3.4703999	2.3677248
C	-1.4486184	3.9902121	1.0225228
H	-1.6500051	4.0698180	-0.0457898
H	-2.2637487	3.4189057	1.4702203
H	-1.4964099	5.0033806	1.4302621
C	3.0995426	2.1455660	0.6799812
H	4.1201080	2.0975989	1.0678013
H	3.0968822	1.6552192	-0.2944711
H	2.8639703	3.1984431	0.5132831
C	-2.2172753	0.2367320	2.0442575
H	-2.8362339	1.0930911	1.7733836
H	-2.2189437	-0.4495251	1.1952492
H	-2.7091164	-0.2698436	2.8784657
C	-0.6214820	-0.5674096	-1.0907820
C	0.2669194	-0.2647385	-0.1844726
C	1.3792542	-1.1411167	0.2650955
C	1.2040551	-2.0426992	1.3187834
C	2.5965089	-1.1308191	-0.4192718
C	2.2303014	-2.9053843	1.6872790
H	0.2558380	-2.0802669	1.8374479
C	3.6232051	-1.9892742	-0.0450902
H	2.7314397	-0.4460910	-1.2457326
C	3.4473699	-2.8762977	1.0133442
H	2.0767358	-3.6001789	2.5038381
H	4.5622431	-1.9664870	-0.5843634
H	4.2493486	-3.5419641	1.3066269
C	-1.2507526	-1.7221581	-1.6888174
C	-2.3263654	-1.5569964	-2.5740125
C	-0.8234035	-3.0318582	-1.3978929
C	-2.9523433	-2.6529318	-3.1526023
H	-2.6804797	-0.5592179	-2.7926934
C	-1.4401964	-4.1226195	-1.9902789
H	0.0040774	-3.1872261	-0.7217006
C	-2.5085420	-3.9397750	-2.8670793
H	-3.7849830	-2.5010125	-3.8277722
H	-1.0872352	-5.1220533	-1.7674400
H	-2.9907720	-4.7958733	-3.3221965

Int4b

Electronic Energy (-5195.519455 Hartree)

P	1.6851645	-0.2834226	1.2445652
C	1.0892713	1.2674440	0.4243917
C	0.7310556	2.4776809	1.0181412
C	1.0238635	1.2257141	-0.9709926
C	0.4090723	3.5992829	0.2657537
C	0.7029719	2.3273269	-1.7438797
C	0.4046549	3.5300048	-1.1188595
C	0.1339049	-1.2748307	1.0863370
C	-1.0970630	-0.7387366	1.4766600
C	0.1026828	-2.5640828	0.5566617
C	-2.2920889	-1.4172213	1.3215348
C	-1.0835082	-3.2669140	0.3889176
C	-2.2857545	-2.6907308	0.7669242
C	1.8001622	0.0679094	3.0506911
C	1.2880585	-0.7687411	4.0408887
C	2.6299405	1.1021364	3.4887628
C	1.5468961	-0.5640375	5.3899900
C	2.8961975	1.3337764	4.8251177
C	2.3478054	0.4943597	5.7863449
F	0.0876737	4.5974084	-1.8407594
F	0.0823710	4.7393855	0.8728275
F	0.6464668	2.6122927	2.3430105
F	1.2434493	0.0700739	-1.6133234
F	0.6604967	2.2346568	-3.0718333
F	3.2000971	1.9209965	2.5973306
F	-1.1518878	0.4666921	2.0557251
F	1.2211341	-3.1971843	0.1994232
F	-3.4411566	-0.8669481	1.7106692
F	-3.4242657	-3.3533843	0.6113409
F	-1.0685351	-4.4943441	-0.1271602
F	0.5370251	-1.8352215	3.7355911
F	1.0327854	-1.3881374	6.3016578
F	2.5963459	0.7016623	7.0739380
F	3.6736382	2.3502469	5.1936603
Fe	3.7460666	-0.9767252	0.5302694
H	4.3043721	-0.4102305	1.8276758
Si	6.0091111	-0.1184423	-2.7559202
C	4.2879160	0.6879029	0.1484962
C	3.3067818	-1.8179904	-1.0251049
O	4.6997458	1.7460176	0.0336470
O	3.0904377	-2.4086673	-1.9733352
C	7.2833832	1.2809376	-2.8805045
H	7.2378287	1.8517305	-1.9464884
H	8.2800230	0.8330573	-2.9050259
C	4.2938478	0.6869291	-2.9689616
H	4.3707062	1.6955861	-2.5529732

H	3.5347475	0.1845486	-2.3774939
C	6.3183439	-1.3176820	-4.1899723
H	6.1741086	-0.7508206	-5.1156636
H	7.3789166	-1.5825269	-4.1690408
C	5.4620563	-2.5905645	-4.2266068
H	5.5650877	-3.1715137	-3.3077568
H	4.4004889	-2.3613637	-4.3335079
H	5.7446073	-3.2382590	-5.0608814
C	7.1120430	2.2303719	-4.0757746
H	6.1567373	2.7585834	-4.0396353
H	7.9004190	2.9877886	-4.0965599
H	7.1535963	1.6934964	-5.0268816
C	3.7984542	0.7739519	-4.4226831
H	2.8567362	1.3261377	-4.4768455
H	4.5135414	1.2812523	-5.0722644
H	3.6211947	-0.2166474	-4.8451759
C	5.7323748	-1.3643074	-0.0091107
C	6.4156903	-1.0426179	-1.1265782
C	6.4155337	-2.1036760	1.0878048
C	6.6081314	-3.4849523	0.9940148
C	6.8622797	-1.4490997	2.2396619
C	7.2254862	-4.1913453	2.0195342
H	6.2685600	-4.0049387	0.1067570
C	7.4880498	-2.1509360	3.2613033
H	6.7166210	-0.3793759	2.3298744
C	7.6694963	-3.5281968	3.1587563
H	7.3629680	-5.2617545	1.9258361
H	7.8349691	-1.6224611	4.1412018
H	8.1514621	-4.0769107	3.9582205
C	7.8800861	-1.4150063	-1.1562378
C	8.3316372	-2.5727885	-1.7940660
C	8.8265686	-0.5934505	-0.5359458
C	9.6825559	-2.9029917	-1.8086135
H	7.6160647	-3.2297773	-2.2706034
C	10.1773795	-0.9183355	-0.5490297
H	8.4930089	0.3057930	-0.0336809
C	10.6125716	-2.0758726	-1.1875008
H	10.0076242	-3.8111443	-2.3024366
H	10.8908363	-0.2685502	-0.0561865
H	11.6650368	-2.3318432	-1.1974644
C	3.6537277	-2.4212408	1.6240275
O	3.5712305	-3.2426270	2.4072555

$Fe(CO)_3P(C_6F_5)_3$

Electronic Energy (-4128.447453 Hartree)

P	0.0561937	-0.0764282	-0.4119280
C	-0.5089818	1.6561889	-0.0538886
C	0.0680963	2.5751711	0.8237975
C	-1.6539763	2.0909532	-0.7288733

C	-0.4290767	3.8606347	0.9845415
C	-2.1691010	3.3686914	-0.5870595
C	-1.5491169	4.2627000	0.2732392
C	-1.1612516	-0.9676871	0.6354721
C	-1.9823487	-1.8859241	0.0021712
C	-1.3942887	-0.7388590	1.9877146
C	-2.9965063	-2.5674412	0.6500514
C	-2.3968606	-1.4030214	2.6749286
C	-3.2001721	-2.3187287	2.0018185
C	1.7001411	-0.2184910	0.3941369
C	2.7208719	0.6192815	-0.0523531
C	2.0747824	-1.2516803	1.2485068
C	4.0388793	0.4668070	0.3371733
C	3.3895243	-1.4297946	1.6555189
C	4.3763315	-0.5681213	1.2002778
F	-2.0372392	5.4880132	0.4294272
F	0.1532950	4.7065067	1.8350625
F	1.1253151	2.2520027	1.5756280
F	-2.3280788	1.2534603	-1.5269691
F	-3.2618528	3.7352187	-1.2562198
F	1.1747932	-2.1356546	1.7010579
F	-1.8030844	-2.1367985	-1.3238928
F	-0.6338123	0.1320123	2.6563897
F	-3.7656900	-3.4380473	0.0032122
F	-4.1643830	-2.9557997	2.6528894
F	-2.5995215	-1.1764550	3.9706535
F	2.4245804	1.6246156	-0.8906839
F	4.9788899	1.2995170	-0.1068648
F	5.6381092	-0.7341019	1.5838595
F	3.7084197	-2.4305721	2.4764380
Fe	-0.0602407	-1.1510686	-2.3467832
C	1.3263466	-0.3694892	-3.0910216
C	-1.1501240	-0.5716371	-3.6819683
C	0.8094397	-2.7353131	-2.3228673
O	2.2376453	0.1335426	-3.5700533
O	-1.8158520	-0.2182834	-4.5441524
O	1.3829727	-3.7289330	-2.3344760

Product

Electronic Energy (-1067.084237 Hartree)

C	0.5488354	-1.1770553	0.2984961
H	0.0756342	-2.1147888	0.6135571
C	-0.2759711	-0.1566558	-0.0465181
C	0.1920826	1.2133925	-0.3859585
C	0.0979230	1.7201342	-1.6953884
C	0.6963056	2.0590631	0.6208851
C	0.5174558	3.0198137	-1.9924955
H	-0.2830539	1.0775935	-2.4915892
C	1.1068865	3.3601011	0.3255311

H	0.7734227	1.6792291	1.6417968	H	-3.9801530	0.9438648	1.0956972
C	1.0221643	3.8462266	-0.9836971	C	-2.4586342	0.8076301	2.6530011
H	0.4499123	3.3876772	-3.0186628	H	-1.3629615	0.8193072	2.7603506
H	1.4986625	3.9972760	1.1214091	H	-2.8588545	1.6210592	3.2781703
H	1.3464183	4.8625130	-1.2158779	H	-2.8158931	-0.1411698	3.0821936
C	2.0186216	-1.2395963	0.3487901	C	-2.6044433	-2.1226329	0.6798011
C	2.8767870	-0.3796679	-0.3693897	H	-2.1474801	-2.8763925	0.0168836
C	2.6095259	-2.2441890	1.1452160	H	-2.1258628	-2.2539368	1.6646811
C	4.2622217	-0.5075982	-0.2705634	C	-4.1180524	-2.3698241	0.7933081
H	2.4547552	0.3873620	-1.0175218	H	-4.6182282	-2.2844717	-0.1836084
C	3.9955127	-2.3639378	1.2532831	H	-4.3364752	-3.3756189	1.1846350
H	1.9622027	-2.9337035	1.6938726	H	-4.5982924	-1.6453034	1.4693429
C	4.8301942	-1.4921004	0.5465675	C	-2.9221368	-0.1506961	-1.7192504
H	4.9053696	0.1658829	-0.8412570	H	-4.0194757	-0.2121089	-1.6160154
H	4.4261620	-3.1434219	1.8854067	H	-2.7127084	0.8808359	-2.0476498
H	5.9153288	-1.5842767	0.6235351	C	-2.4272982	-1.1618853	-2.7634495
Si	-2.1744498	-0.3825493	0.0228297	H	-2.6828477	-2.1943797	-2.4789140
C	-2.8802695	0.9577484	1.1837854	H	-2.8692790	-0.9775677	-3.7551447
H	-2.5570029	1.9368660	0.7921143	H	-1.3325564	-1.1229810	-2.8772865

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