Electronic Supplementary Information

Amido calcuim complexes coordinated by phenolate ligands for catalytic cross-dehydrogenative coupling amines with silanes

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Table S1. Crystal Data and Structures Refinement Details for Complexes **1**, **5**, **7**, **8**.

	1	**5**	**7**	**8**
Empirical formula	$C_{38}H_{61}CaN_3O_3Si_2$	$C_{55}H_{62}CaN_4O_2$	$C_{50}H_{70}CaN_2O_6$	$C_{54}H_{76}CaN_2O_6$
Formula Weight	704.15	851.16	835.16	889.24
T, K	100	100	100	100
Crystal System	Triclinic	Monoclinic	Triclinic	Triclinic
Space Group	*P-1*	*P2₁/c*	*P-1*	*P-1*
Unit Cell Dimensions	*a* = 10.7618(10) Å *b* = 12.4539(13) Å *c* = 15.7229(15) Å *α* = 74.996(2)° *β* = 86.375(2)° *γ* = 88.424(2)°	*a* = 19.4603(12) Å *b* = 14.0786(9) Å *c* = 17.4538(11) Å *α* = 90° *β* = 98.2580(10)° *γ* = 90°	*a* = 13.3721(7) Å *b* = 13.8868(7) Å *c* = 14.7330(8) Å *α* = 106.0090(10)° *β* = 105.5980(10)° *γ* = 100.5220(10)°	*a* = 11.8448(4) Å *b* = 14.0854(4) Å *c* =17.5399(6) Å *α* = 75.8870(10)° *β* = 89.098(2)° *γ* = 65.1700(10)°
V, Å^3	2031.2(3)	4732.3(5)	2433.5(2)	2563.15(14)
Z	2	4	2	2
d_{calc}, Mg/m^3	1.151	1.195	1.140	1.152
μ, mm^{-1}	0.250	0.178	0.176	0.171
F^{000}	764	1824	904	964
Crystal Size, mm	0.37 x 0.21 x 0.15	0.14 x 0.08 x 0.06	0.22 x 0.11 x 0.07	0.40 x 0.15 x 0.10
Θ Range for Data Collection, °	1.870–27.94	2.23–26.415	2.47–27.91	2.15–30.87
Index Ranges	–14 ≤ *h*≤ 14 –16 ≤*k*≤ 16 –20 ≤*l*≤ 20	–24 ≤ *h*≤ 24 –17 ≤*k*≤ 17 –21 ≤*l*≤ 21	–17 ≤ *h*≤ 17 –18 ≤*k*≤ 18 –19 ≤*l*≤ 19	–15 ≤ *h* ≤ 15 –20 ≤ *k* ≤ 20 –25 ≤ *l* ≤ 25
Reflns Collected	27526	47901	28391	35464
Independent Reflns (R_{int})	9719 (0.0402)	9686 (0.0924)	11492 (0.0719)	16082 (0.0333)
Completeness to θ, %	100.0	99.9	99.6	99.8
Data / Restraints / Parameters	9719 / 0 / 436	9686 / 109 / 613	11492 / 0 / 550	16082 / 57 / 604
GOF on F^2	1.015	1.017	1.0017	1.022
Final *R*Indices (*I*>2σ(*I*))	R_1 = 0.0488 wR_2 = 0.1130	R_1 = 0.0532 wR_2 = 0.1100	R_1 = 0.0610 wR_2 = 0.1125	R_1 = 0.0439 wR_2 = 0.1079
*R*Indices (all data)	R_1 = 0.0706 wR_2 = 0.1271	R_1 = 0.0896 wR_2 = 0.1242	R_1 = 0.1071 wR_2 = 0.1266	R_1 = 0.0591 wR_2 = 0.1158
Largest Diff Peak and Hole, e/Å^3	0.475 / –0.226	0.558 / –0.457	0.545 / –0.543	0.504 / –0.440

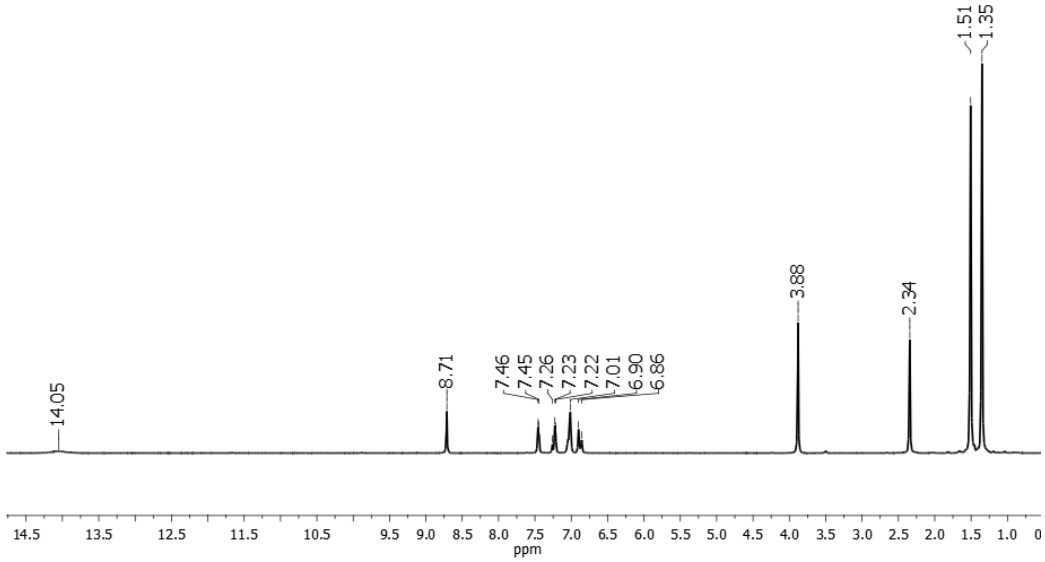

Figure S1 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **L^{4}H**.

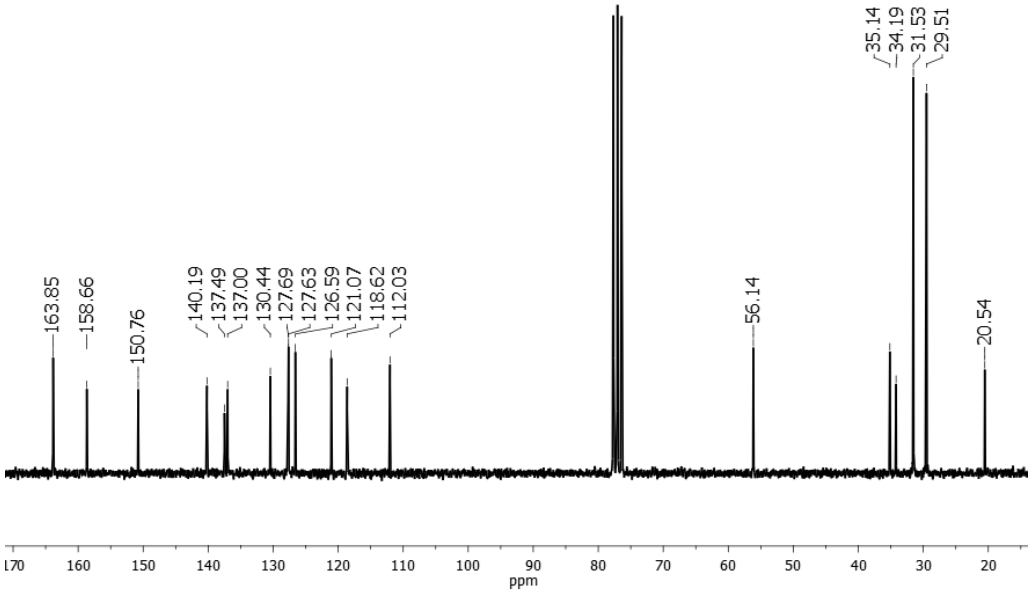

Figure S2 ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of **L^4H**.

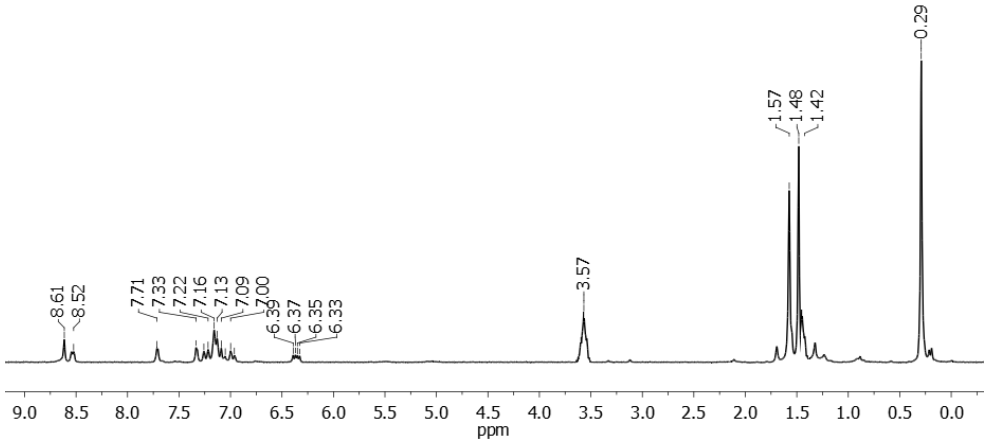

Figure S3 ^{1}H NMR spectrum (400 MHz, C_6D_6) of **1**.

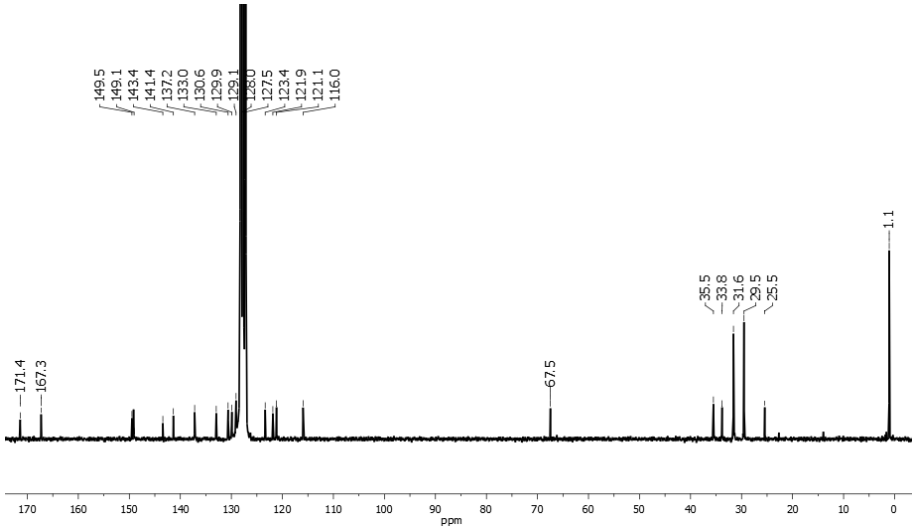

Figure S4 ^{13}C NMR spectrum (101 MHz, C_6D_6) of **1**.

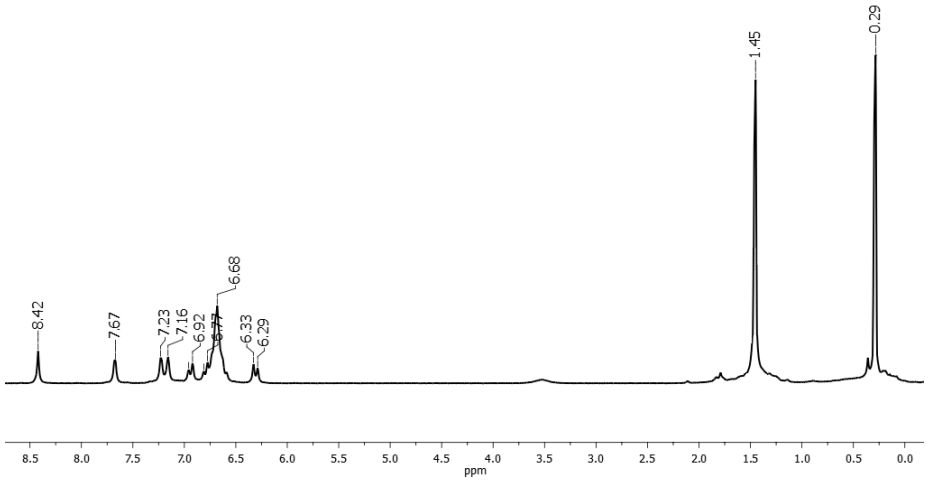

Figure S5 ^{1}H NMR spectrum (400 MHz, C_6D_6) of **2**.

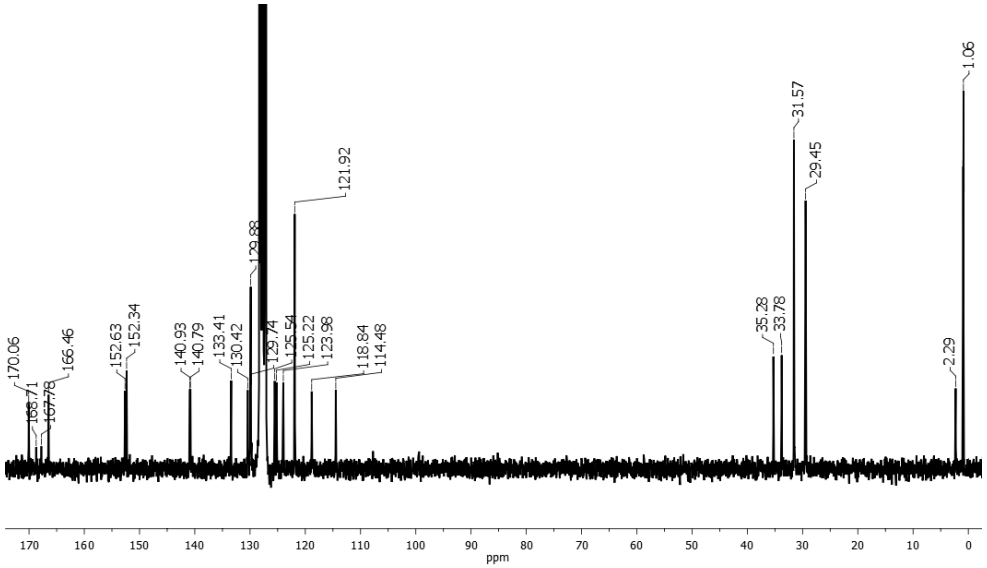

Figure S6 ^{13}C NMR spectrum (101 MHz, C_6D_6) of **2**.

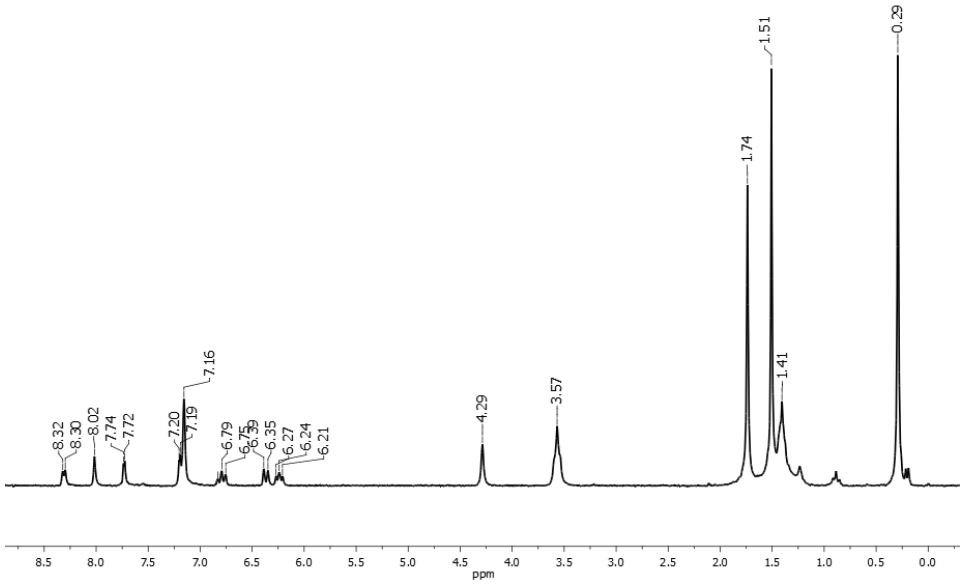

Figure S7 ^{1}H NMR spectrum (400 MHz, C_6D_6) of **3**.

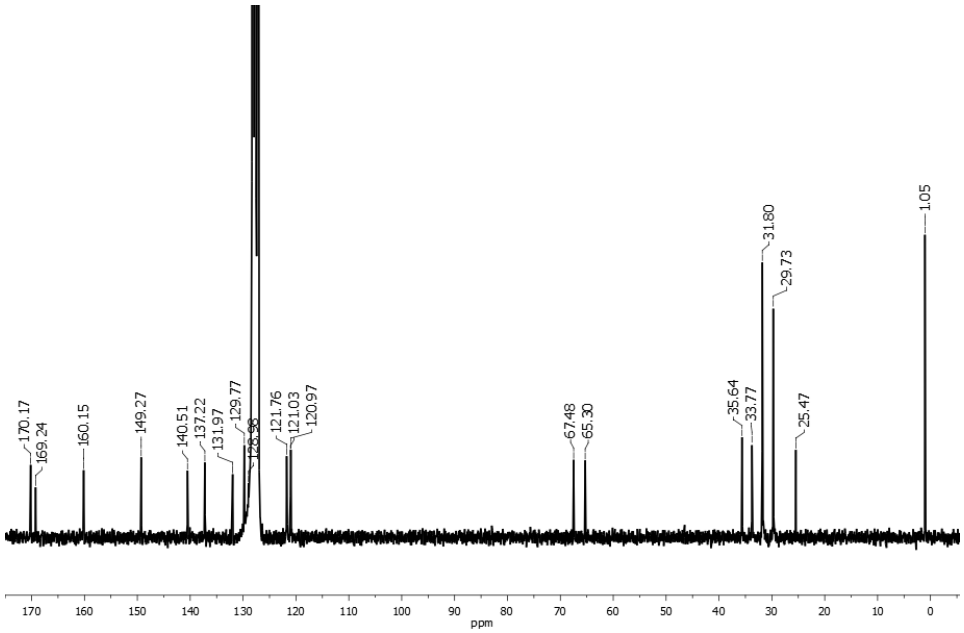

Figure S8 ^{13}C NMR spectrum (101 MHz, C_6D_6) of **3**.

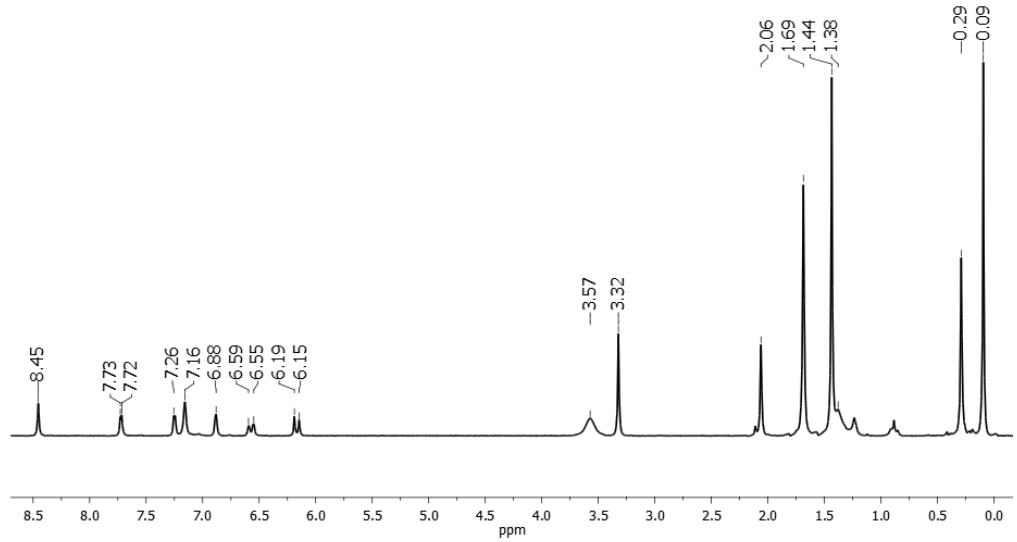

Figure S9 ^{1}H NMR spectrum (400 MHz, C_6D_6) of **4**.

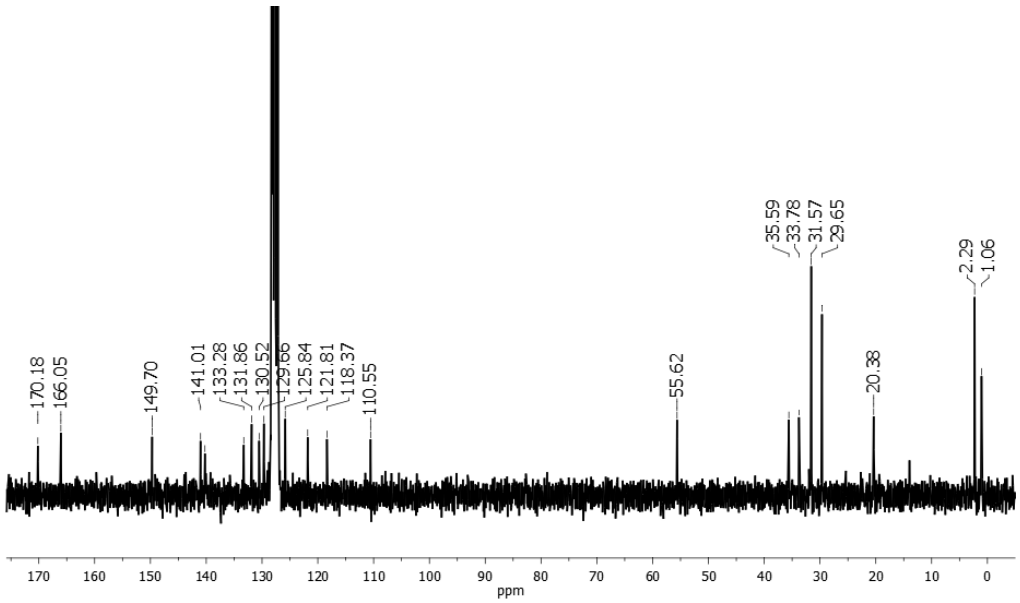

Figure S10 ^{13}C NMR spectrum (101 MHz, C_6D_6) of **4**.

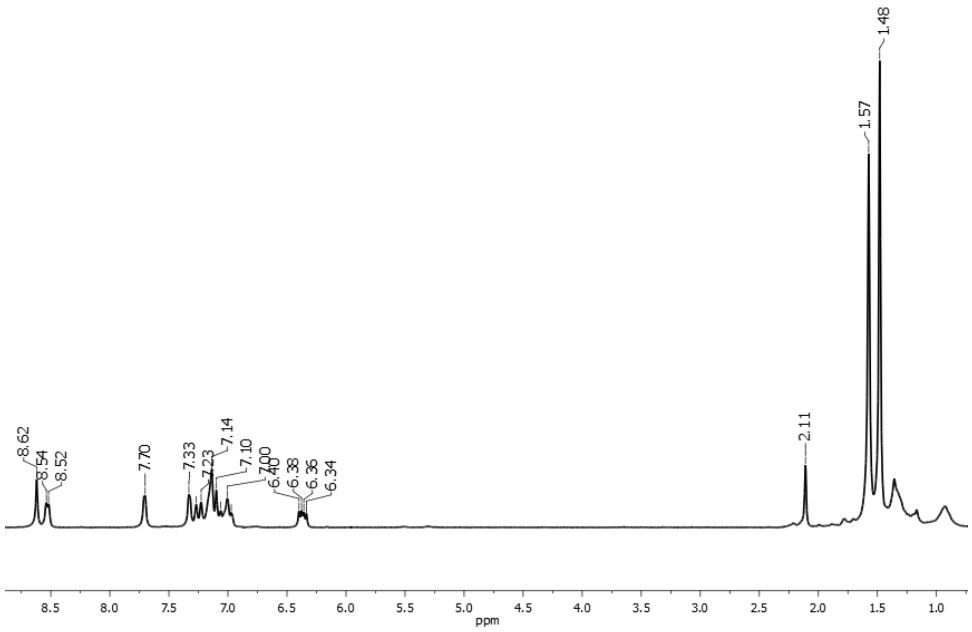

Figure S11 ^{1}H NMR spectrum (400 MHz, C_6D_6) of **5**.

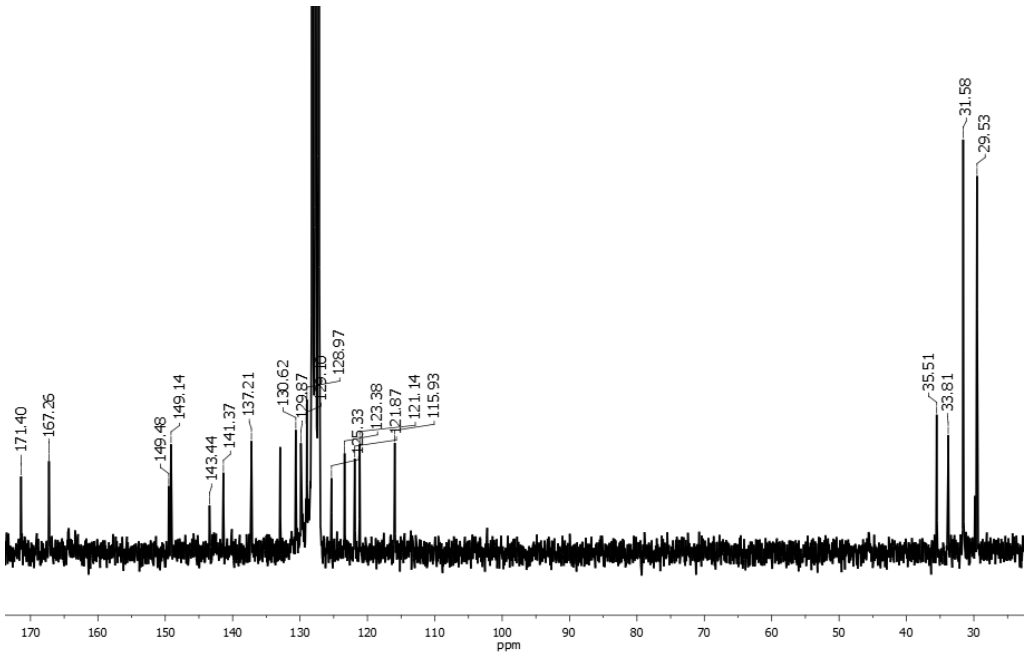

Figure S12 ^{13}C NMR spectrum (101 MHz, C_6D_6) of **5**.

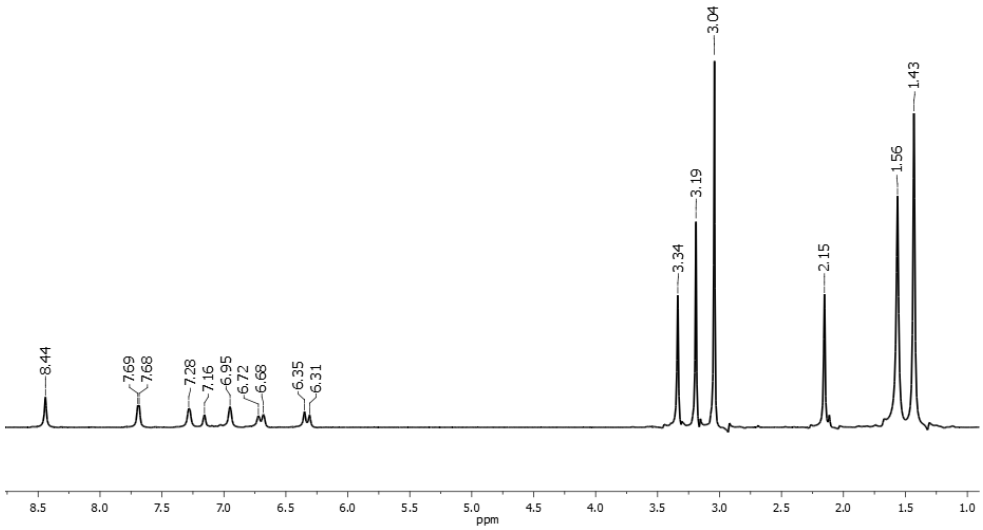

Figure S13 ^{1}H NMR spectrum (400 MHz, C_6D_6) of **7**.

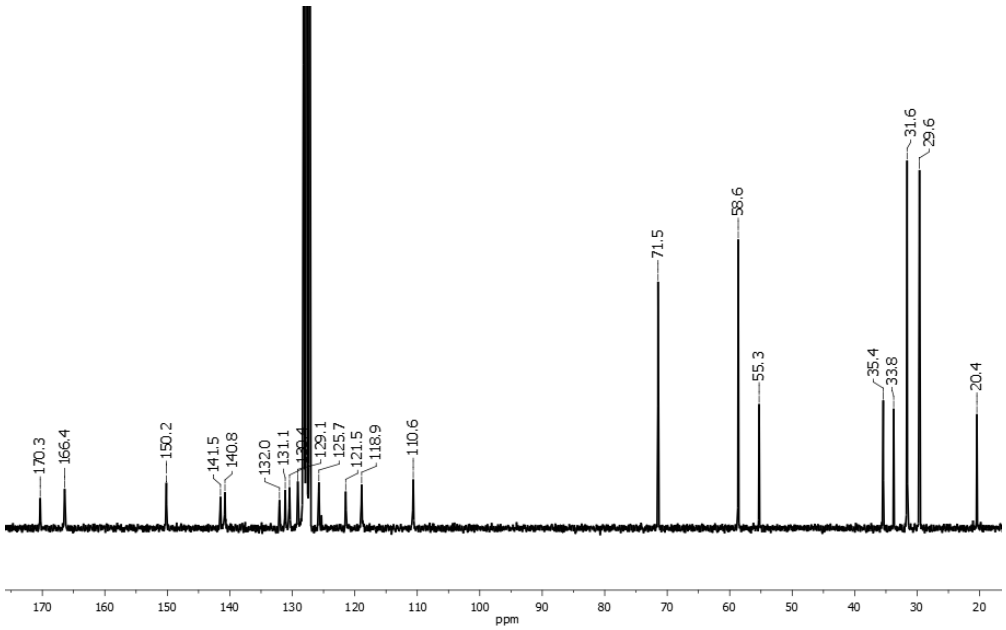

Figure S14 ^{13}C NMR spectrum (101 MHz, C_6D_6) of **7**.

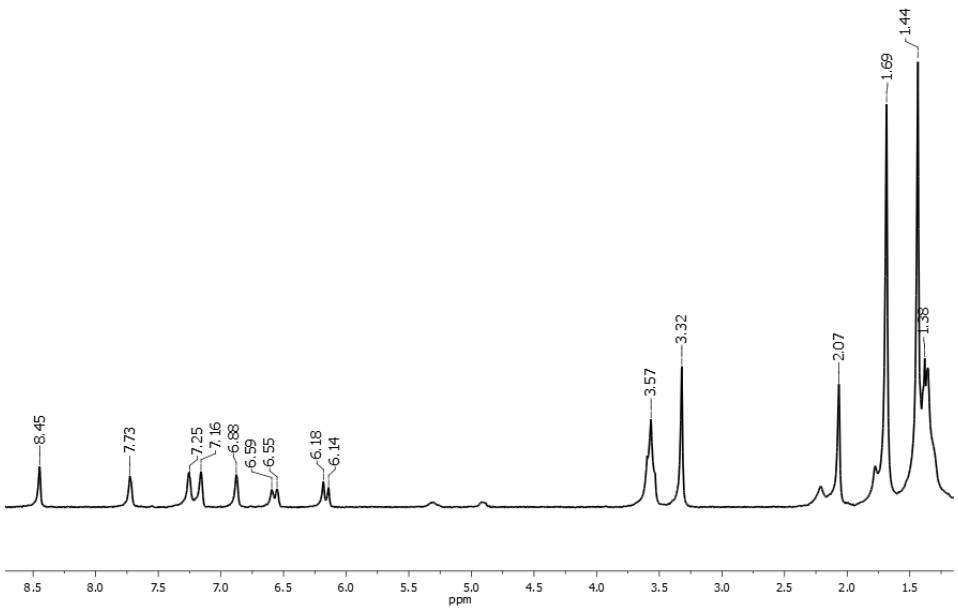

Figure S15 ^{1}H NMR spectrum (400 MHz, C_6D_6) of **8**.

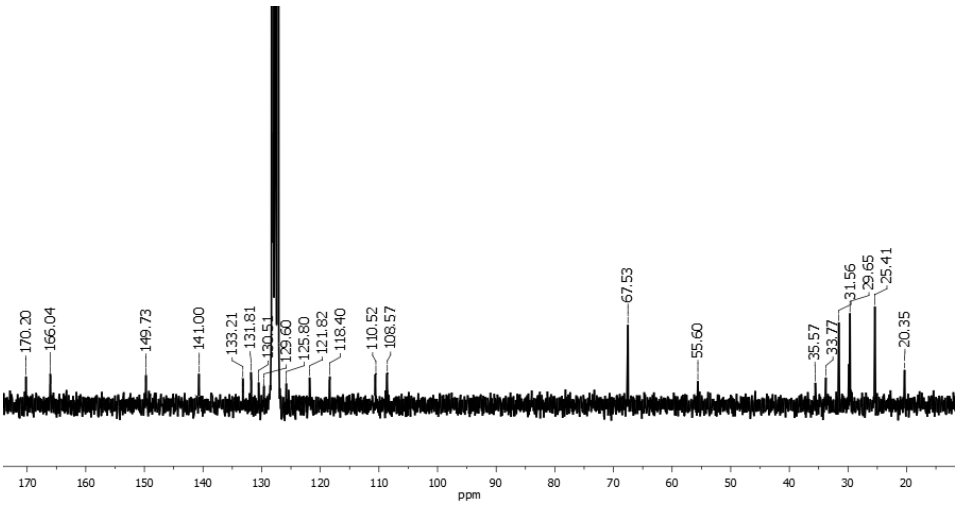

Figure S16 ^{13}C NMR spectrum (101 MHz, C_6D_6) of **8**.

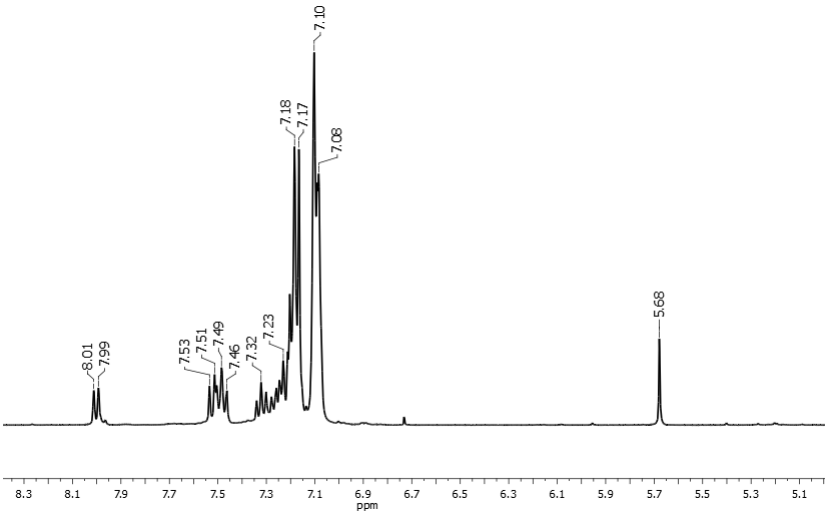

Figure S17 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **9-(phenylsilyl)-9H-carbazole**.

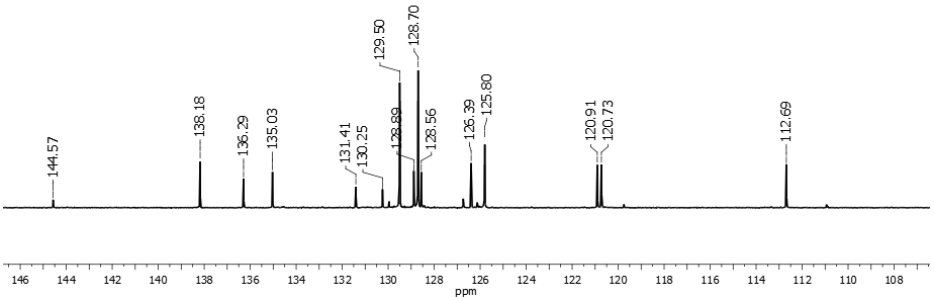

Figure S18 ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of **9-(phenylsilyl)-9H-carbazole**.

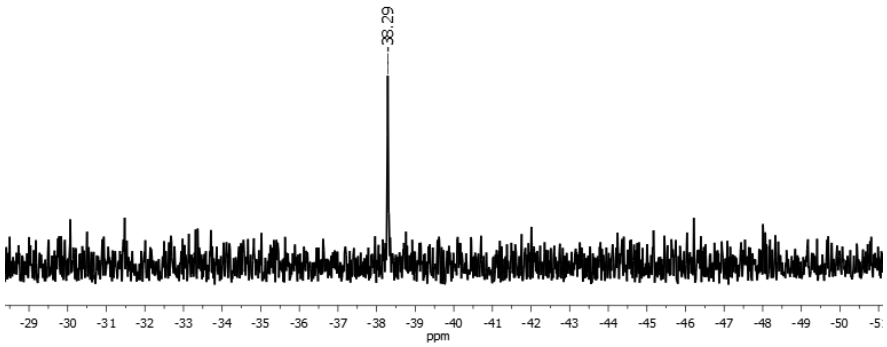

Figure S19 ^{29}Si NMR spectrum (79 MHz, $CDCl_3$) of **9-(phenylsilyl)-9H-carbazole**.

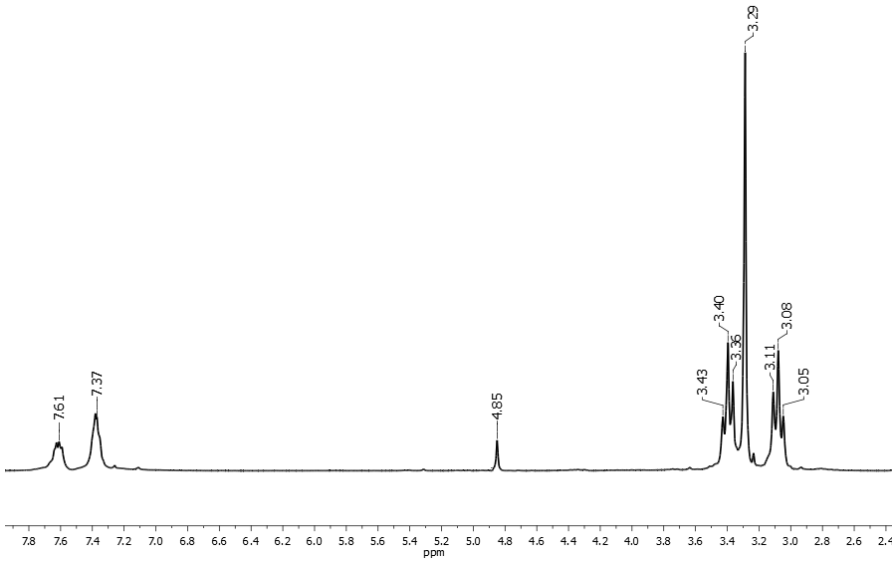

Figure S20 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **N,N-bis(2-methoxyethyl)-1-phenylsilanamine**.

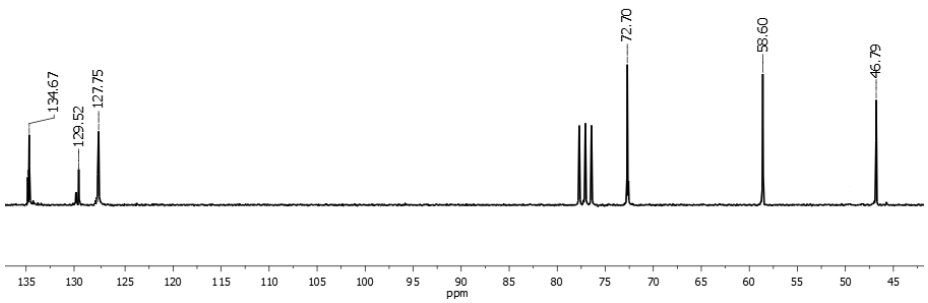

Figure S21 ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of **N,N-bis(2-methoxyethyl)-1-phenylsilanamine**.

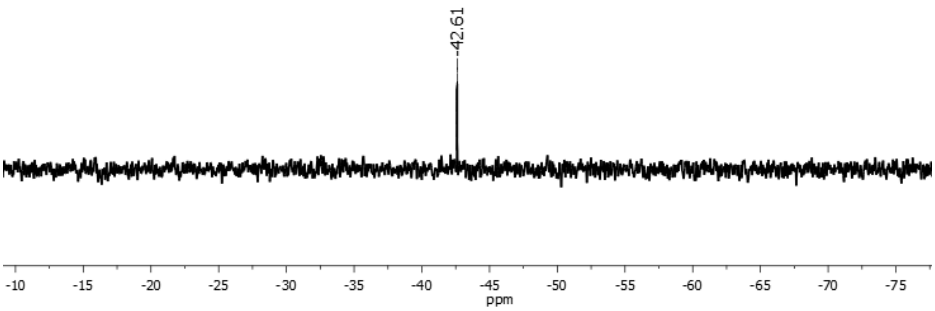

Figure S22 ^{29}Si NMR spectrum (79 MHz, $CDCl_3$) of **N,N-bis(2-methoxyethyl)-1-phenylsilanamine**

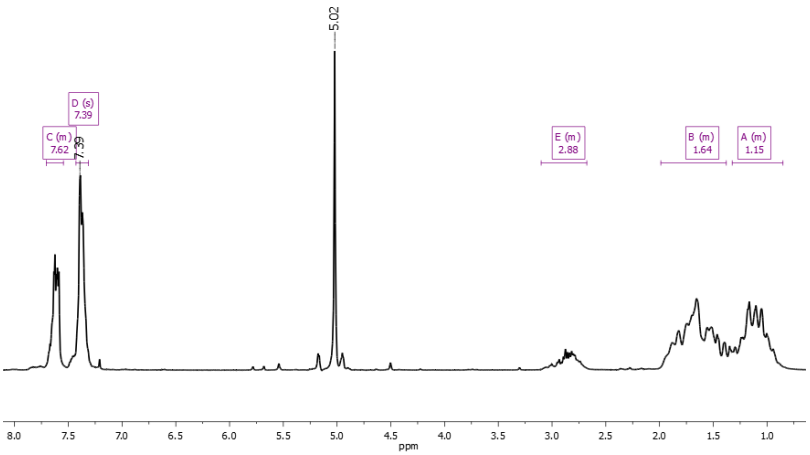

Figure S23 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **N-cyclohexyl-1-phenylsilanamine**.

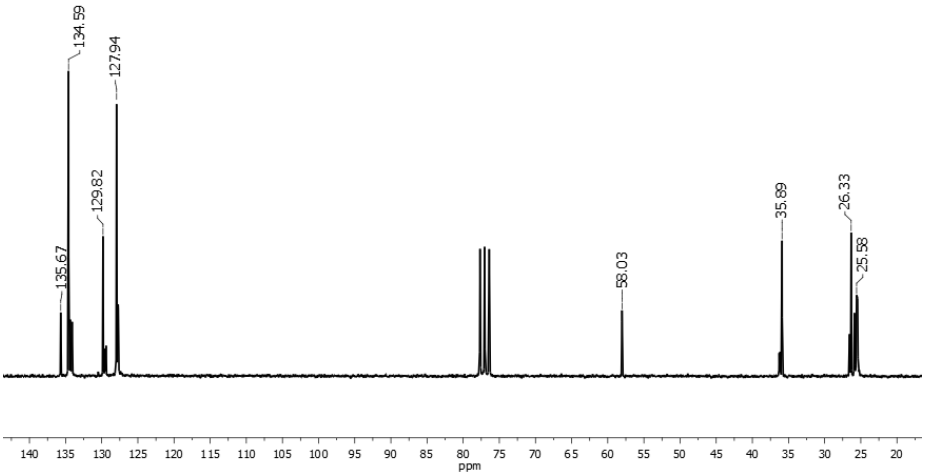

Figure S24 ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of **N-cyclohexyl-1-phenylsilanamine**.

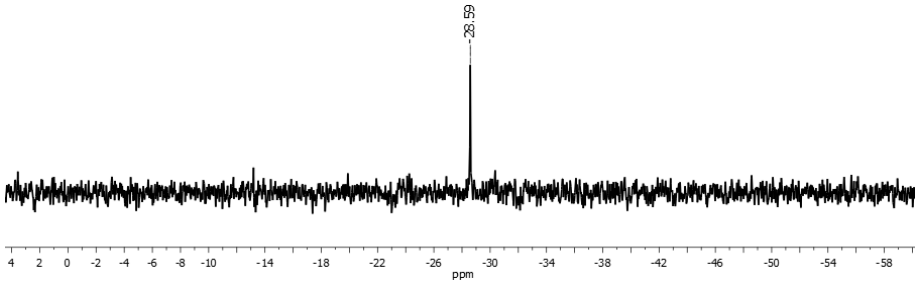

Figure S25 ^{29}Si NMR spectrum (79 MHz, $CDCl_3$) of **N-cyclohexyl-1-phenylsilanamine.**

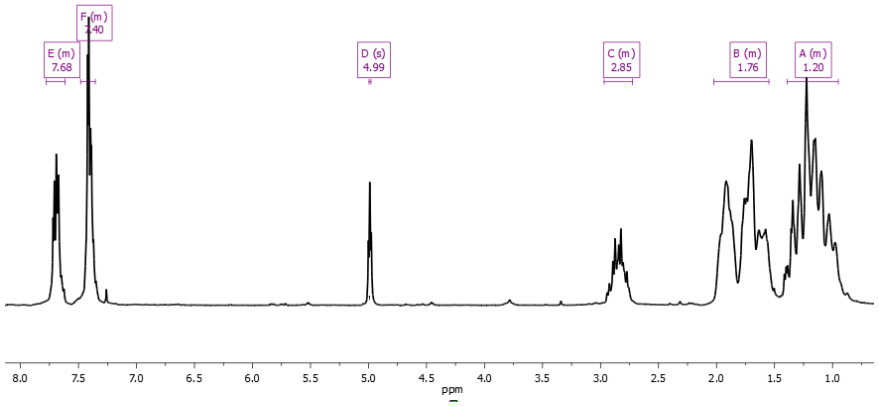

Figure S26 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **N,N-dicyclohexyl-1-phenylsilanamine**.

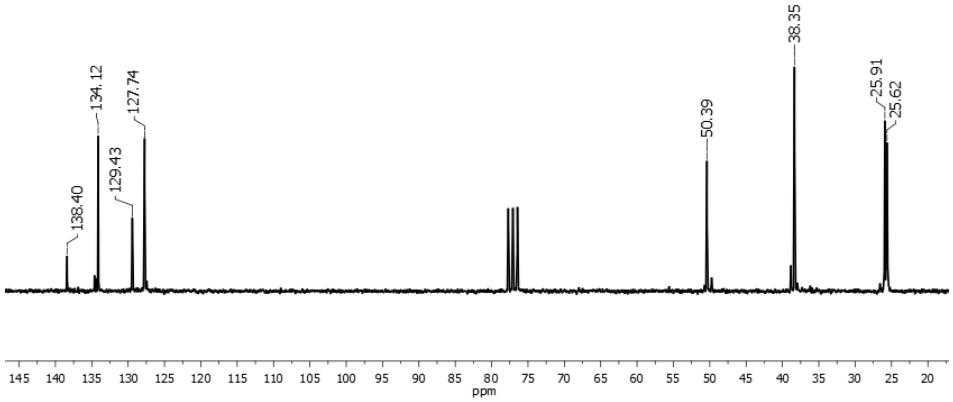

Figure S27 ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of **N,N-dicyclohexyl-1-phenylsilanamine**.

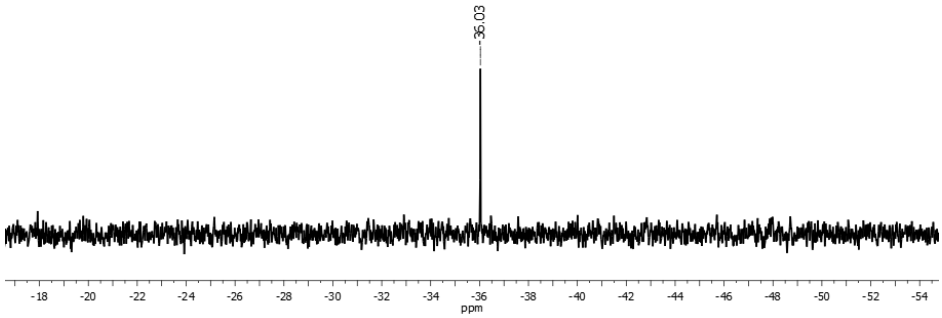

Figure S28 ^{29}Si NMR spectrum (79 MHz, $CDCl_3$) of **N,N-dicyclohexyl-1-phenylsilanamine.**

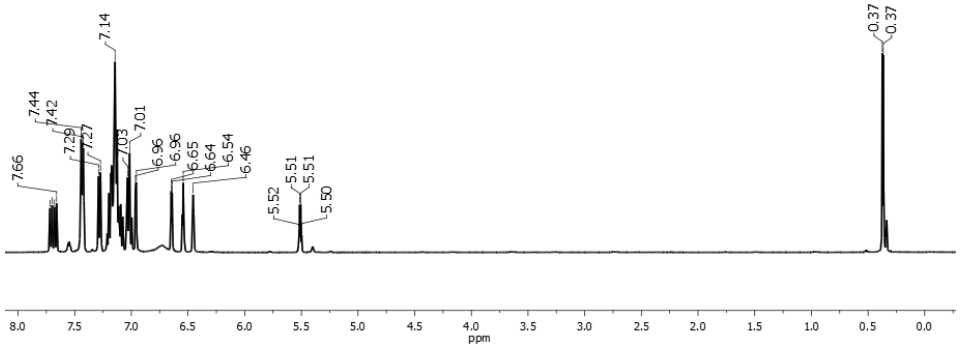

Figure S29 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **1-(methyl(phenyl)silyl)-1H-indole**.

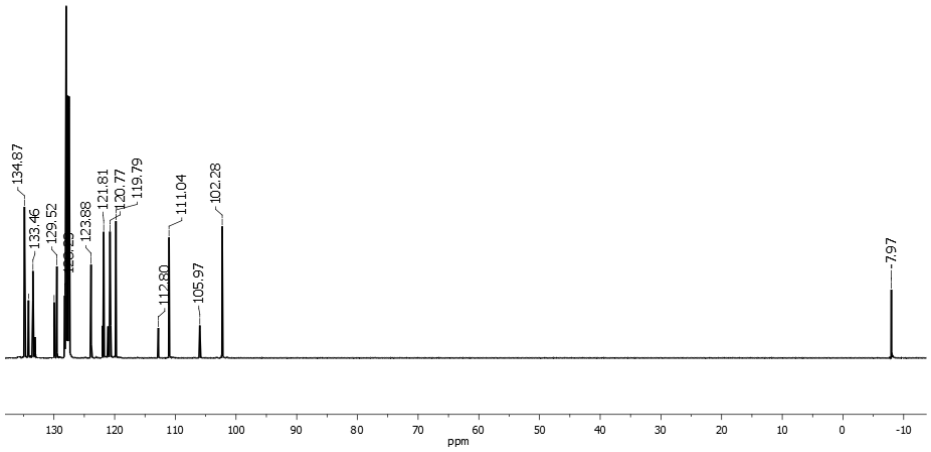

Figure S30 ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of **1-(methyl(phenyl)silyl)-1H-indole**.

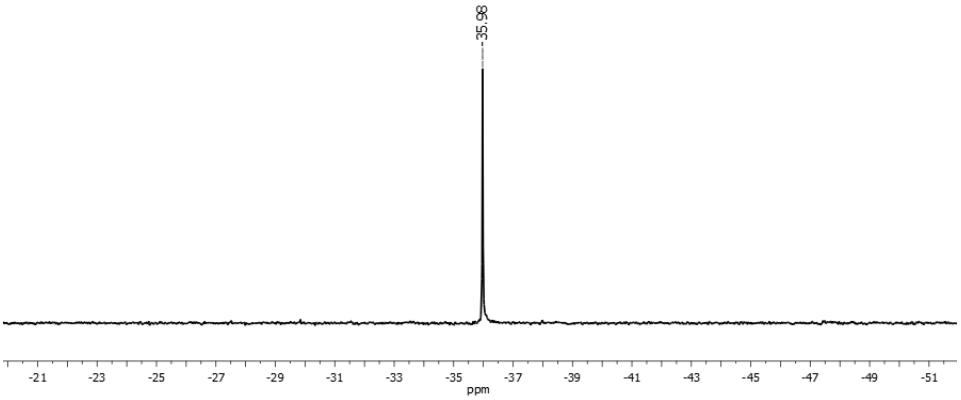

Figure S31 ^{29}Si NMR spectrum (79 MHz, $CDCl_3$) of **1-(methyl(phenyl)silyl)-1H-indole.**

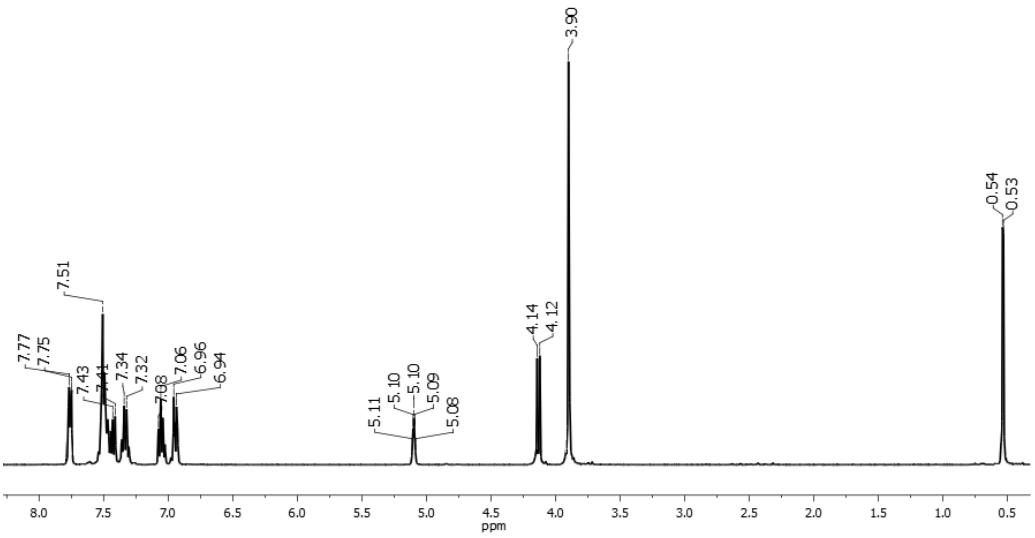

Figure S32 ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of **N-(2-methoxybenzyl)-1-methyl-1-phenylsilanamine**.

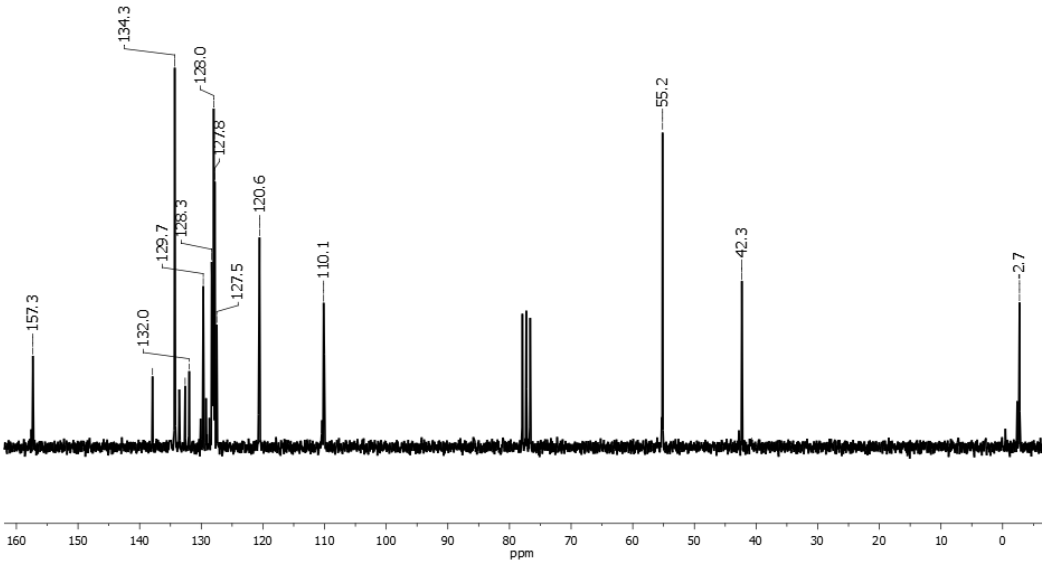

Figure S33 ^{13}C NMR spectrum (101 MHz, $CDCl_3$) of **N-(2-methoxybenzyl)-1-methyl-1-phenylsilanamine**.

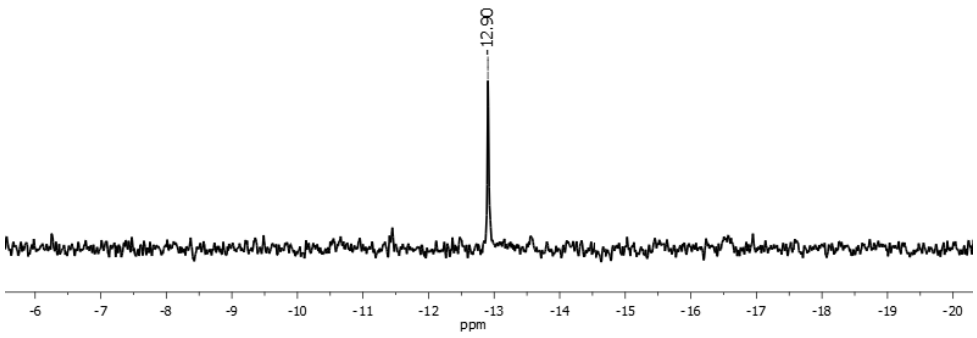

Figure S34 ^{29}Si NMR spectrum (79 MHz, $CDCl_3$) of **N-(2-methoxybenzyl)-1-methyl-1-phenylsilanamine.**

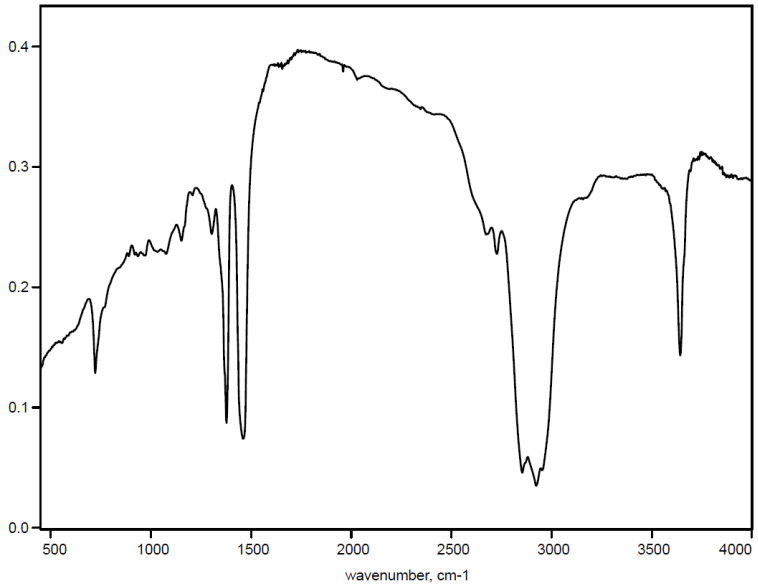

Figure S35 IR spectrum of CaH_2**.**