Electronic Supplementary Information (ESI) for:

Synthesis of Structured Polysiloxazanes via Piers–Rubinsztajn Reaction

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Table of Contents

1. Experimental Section

General. All commercially available chemicals and reagents were used without further purification unless otherwise indicated. NMR spectroscopy was performed at 298 K using a Bruker AVANCE 400 spectrometer (400 MHz, ^{1}H, in $CDCl_3$; 126 MHz, ^{13}C, in $CDCl_3$) with solvent signal allotted as internal reference, and ^{29}Si NMR was recorded on a Bruker AVANCE II+ 400 spectrometer (79 MHz) in $CDCl_3$ used chromium acetylacetonate as a nonpolar paramagnetic relaxation agent, and ^{19}F NMR was recorded on AVANCE III 500WB spectrometer (470 MHz) in Toluene-d_8. MALDI-TOF spectra were recorded with Voyager-Elite (Matrix Assisted Laser Desorption/ Ionization Time of Flight) mass spectrometer (NaI were used as the salt and DT or 5-MSCA as the matrix). Single-crystal X-ray diffraction (XRD) data acquisition was performed on an ST Saturn 724+ diffractometer. All products were purified through column chromatography using neutral alumina with 200−300 mesh size using petroleum ether/ethyl acetate = 100 : 1 as an eluent unless otherwise stated.

Materials. 1,3-dimethoxy-1,1,3,3-tetraphenyldisilazane and 1, 3-dimethoxy-2, 4-dimethyl-2, 4-diphenyldisilazane were prepared according to the reported method[1, 2]. Triethylsilane, dimethylvinylsilane, and dimethylphenylsilane were used as received from Innochem. Trivinylsilane was obtained according to the literature[3]. Toluene was distilled from sodium under nitrogen before use.

General procedure.

(A) *P-R reaction of **1a** with Triethylsilane.* (Table 1, entry 1). $B(C_6F_5)_3$ (100 mg/mL in toluene, 0.16 mL, 0.031 mmol) was added dropwise to a solution of **1a** (0.88 g, 2.00 mmol), Et_3SiH (0.49 g, 4.2 mmol) in toluene (3 mL) under nitrogen. The reaction mixture was stirred at room temperature for 30 min. After concentration under reduced pressure, the resulting mixture was purified by alumina column chromatography to give 0.24g (0.23 mmol) of compound **4a** in 23% yield as a white solid, **5a** (0.12 mmol) in 18% yield, and the designed siloxazane **3a** (0.18 mmol) in 9% yield.

Entry 2~7 in Table 1 were performed in the same manner as described for entry 1 using respective dimethoxydisilazane and hydrosilane.

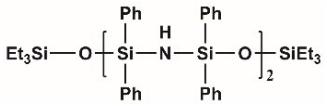
(B) *P-R reaction of **1a** with Si-H Terminated Oligosiloxane.* (Table 2, entry 1). To a solution of **1a** (0.88 g, 2.00 mmol), $B(C_6F_5)_3$ (5.12 mg, 0.01 mmol) in toluene (3 mL) was added dropwise oligosiloxane (1.07 g, 2.00 mmol) under nitrogen within 5 min. The reaction mixture was stirred at room temperature for 30 min. After concentration under reduced pressure, a large amount of hexane was added into the crude product. Then the precipitated catalyst was separated from the resulting mixture by centrifugation to produce polysiloxazane (1.78 g) in 93% yield as a pale yellow viscous liquid.

Entry 2~11 in Table 2 were performed in the same manner as described for entry 1 using respective

dimethoxydisilazane and oligosiloxane.

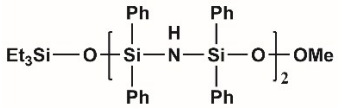
2. Characterization Data

1,1,3,3-tetraphenyl-N^1,N^3-bis(3,3,3-triethyl-1,1-diphenyldisiloxanyl)disiloxane-1,3-diamine (4a)



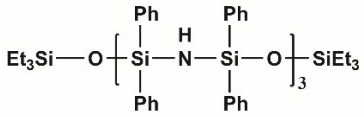
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 – 6.81 (m, 40H), 1.70 (s, 2H), 0.67 (t, *J* = 7.9 Hz, 18H), 0.31 (q, *J* = 7.8 Hz, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 136.95, 136.39, 134.93, 134.54, 129.37, 129.22, 127.30, 127.26, 6.84, 6.24. ^{29}Si NMR (79 MHz, $CDCl_3$) δ 11.27, -32.11, -34.84. HRMS (MOLDI-TOF) m/z: calcd. for $C_{60}H_{61}N_2O_3Si_6$ $[M + H]^+$: 1025.32978; found: 1025.329200.

N^1-(methoxydiphenylsilyl)-1,1,3,3-tetraphenyl-N^3-(3,3,3-triethyl-1,1-diphenyldisiloxanyl) disiloxane-1,3-diamine (2a)



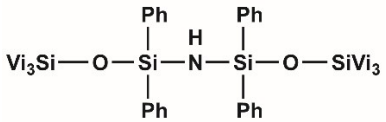
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 –7.00 (m, 40H), 3.28 (s, 3H), 1.96 (s, 1H), 1.80 (s, 1H), 0.76 (t, *J* = 7.9 Hz, 9H), 0.40 (q, *J* = 7.9 Hz, 6H).^{13}C NMR (126 MHz, $CDCl_3$) δ 136.97, 136.40, 136.21, 134.94, 134.85, 134.65, 134.57, 129.54, 129.39, 129.24, 127.50, 127.38, 127.32, 127.27, 50.61, 6.84, 6.25. HRMS (MOLDI-TOF) m/z: calcd. for $C_{55}H_{60}N_2NaO_3Si_5$ $[M + Na]^+$: 959.33480; found: 959.333974.

1,1,3,3-tetraphenyl-N^1-(1,1,3,3-tetraphenyl-3-((3,3,3-triethyl-1,1-diphenyldisiloxanyl)amino) disiloxanyl)-N^3-(3,3,3-triethyl-1,1-diphenyldisiloxanyl)disiloxane-1,3-diamine (5a)



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 – 6.80 (m, 60H), 1.68 (s, 1H), 1.58 (s, 1H), 1.46 (s, 1H), 0.66 (t, *J* = 8.0 Hz, 18H), 0.29 (q, *J* = 8.0 Hz, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 136.93, 136.29, 136.18, 134.94, 134.79, 134.51, 129.29, 129.27, 129.16, 127.28, 127.22, 6.82, 6.22. HRMS (MOLDI-TOF) m/z: calcd. for $C_{84}H_{94}N_3O_4Si_8$ $[M + H]^+$: 1432.53985; found: 1432.538936.

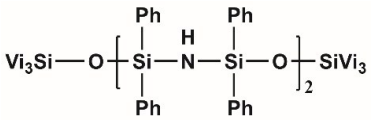
Bis(1,1-diphenyl-3,3,3-trivinyldisiloxanyl)amine



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.06 (m, 20H), 6.09 – 5.84 (m, 12H), 5.82 – 5.56 (m, 6H), 1.94 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 136.50, 135.28, 134.90, 134.70, 129.42, 127.34. ^{29}Si NMR (79 MHz, $CDCl_3$) δ -24.77, -31.36. HRMS (MOLDI-TOF) m/z: calcd. for $C_{36}H_{40}NO_2Si_4$ [M

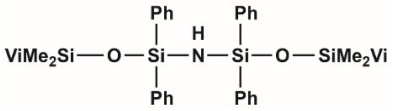
+ H]$^+$: 630.21361; found: 630.213671.

N^1,N^3-bis(1,1-diphenyl-3,3,3-trivinyldisiloxanyl)-1,1,3,3-tetraphenyldisiloxane-1,3-diamine



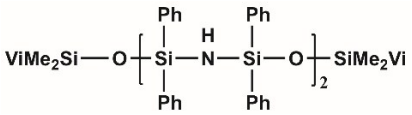
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 6.90 (m, 40H), 6.08 – 5.77 (m, 12H), 5.74 – 5.44 (m, 6H), 1.75 (s, 1H), 1.21 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 136.43, 136.26, 135.23, 134.98, 134.87, 134.73, 134.61, 129.39, 129.33, 127.34, 127.29. HRMS (MOLDI-TOF) m/z: calcd. for $C_{60}H_{73}N_2O_3Si_6$ [M+ H]$^+$: 1037.42368; found: 1037.423871.

Bis(3,3-dimethyl-1,1-diphenyl-3-vinyldisiloxanyl)amine



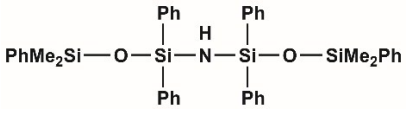
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 – 7.04 (m, 20H), 5.99 (dd, *J* = 20.3, 14.9 Hz, 2H), 5.81 (dd, *J* = 14.9, 4.0 Hz, 2H), 5.59 (dd, *J* = 20.3, 4.0 Hz, 2H), 1.86 (s, 1H), 0.00 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.96, 136.82, 134.32, 131.54, 129.13, 127.13, -0.00. ^{29}Si NMR (79 MHz, $CDCl_3$) δ -1.74, -31.92. HRMS (MOLDI-TOF) m/z: calcd. for $C_{32}H_{40}NO_2Si_4$ [M+ H]$^+$: 582.21361; found: 582.213002.

N^1,N^3-bis(3,3-dimethyl-1,1-diphenyl-3-vinyldisiloxanyl)-1,1,3,3-tetraphenyldisiloxane-1,3-diamine



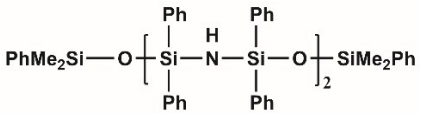
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 6.97 (m, 40H), 5.98 (dd, *J* = 20.2, 14.9 Hz, 2H), 5.83 (dd, *J* = 14.9, 4.0 Hz, 2H), 5.59 (dd, *J* = 20.2, 4.0 Hz, 2H), 1.80 (s, 1H), 1.29 (s, 1H), 0.00 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.96, 136.65, 136.22, 134.77, 134.30, 131.56, 129.19, 129.07, 127.11, -0.00. ^{29}Si NMR (79 MHz, $CDCl_3$) δ -2.81, -31.58, -33.35. HRMS (MOLDI-TOF) m/z: calcd. for $C_{56}H_{61}N_2O_3Si_6$ [M + H]$^+$: 977.32978; found: 977.329690.

Bis(3,3-dimethyl-1,1,3-triphenyldisiloxanyl)amine



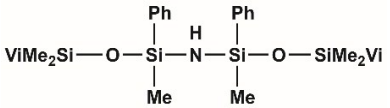
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 6.79 (m, 30H), 1.70 (s, 1H), 0.00 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.40, 136.79, 134.61, 133.18, 129.40, 129.20, 127.64 (d, *J* = 1.9 Hz), 127.41, 0.67. ^{29}Si NMR (79 MHz, $CDCl_3$) δ -1.34, -32.88. HRMS (MOLDI-TOF) m/z: calcd. for $C_{40}H_{44}NO_2Si_4$ [M+ H]$^+$:682.24491; found: 682.244418.

N^1,N^3-bis(3,3-dimethyl-1,1,3-triphenyldisiloxanyl)-1,1,3,3-tetraphenyldisiloxane-1,3-diamine

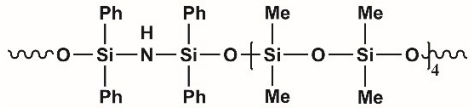


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 6.81 (m, 50H), 1.63 (s, 1H), 1.40 (s, 1H), 0.00 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 139.31, 136.64, 136.30, 134.93, 134.54, 133.16, 129.39, 129.30, 129.14, 127.58, 127.33, 0.65. ^{29}Si NMR (79 MHz, $CDCl_3$) δ -1.54, -32.05, -33.41. HRMS (MOLDI-TOF) m/z: calcd. for $C_{64}H_{65}N_2O_3Si_6$ $[M + H]^+$: 1077.36108; found: 1077.361040.

Bis(1,3,3-trimethyl-1-phenyl-3-vinyldisiloxanyl)amine



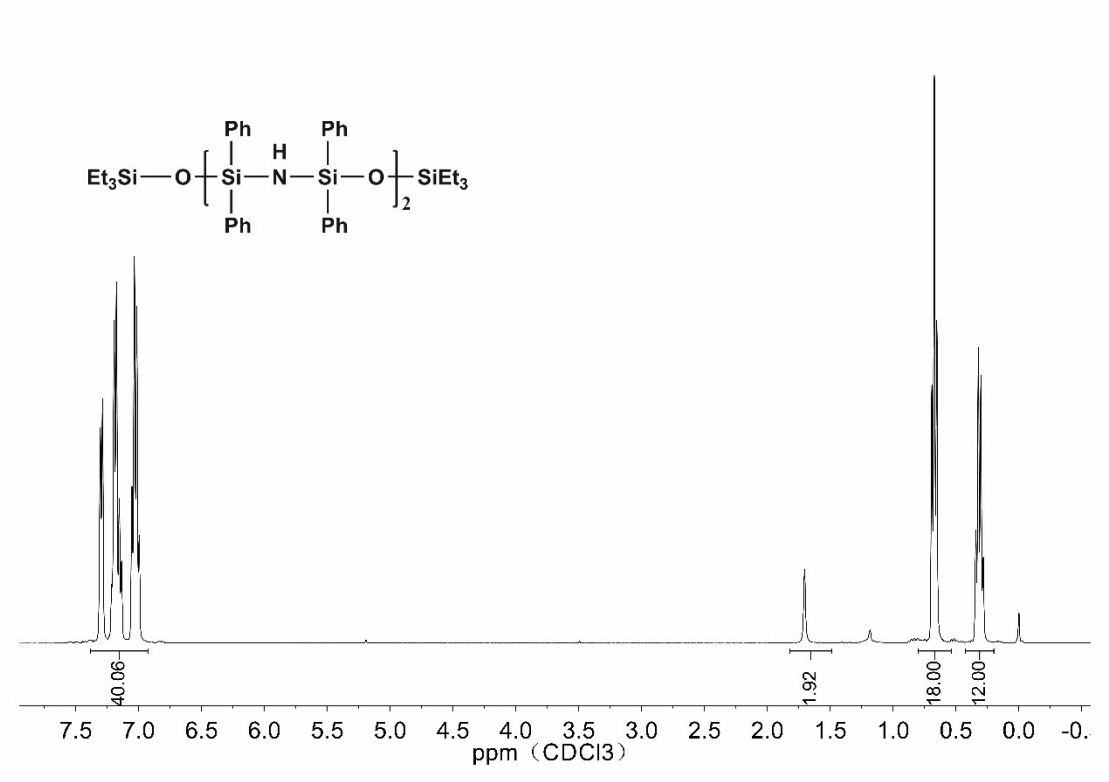
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.30 (m, 10H), 6.16 (dd, J = 20.3, 14.9 Hz, 2H), 5.97 (dd, J = 14.8, 3.9 Hz, 2H), 5.78 (dd, J = 20.3, 3.9 Hz, 2H), 0.37 (s, 6H), 0.21 (s, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.91, 133.35, 132.21, 129.92, 127.81, 0.26, -0.95. ^{29}Si NMR (79 MHz, $CDCl_3$) δ -2.42, -24.33. HRMS (ESI) m/z: calcd. for $C_{22}H_{36}NO_2Si_4$ $[M + H]^+$: 458.18176; found: 458.1812.



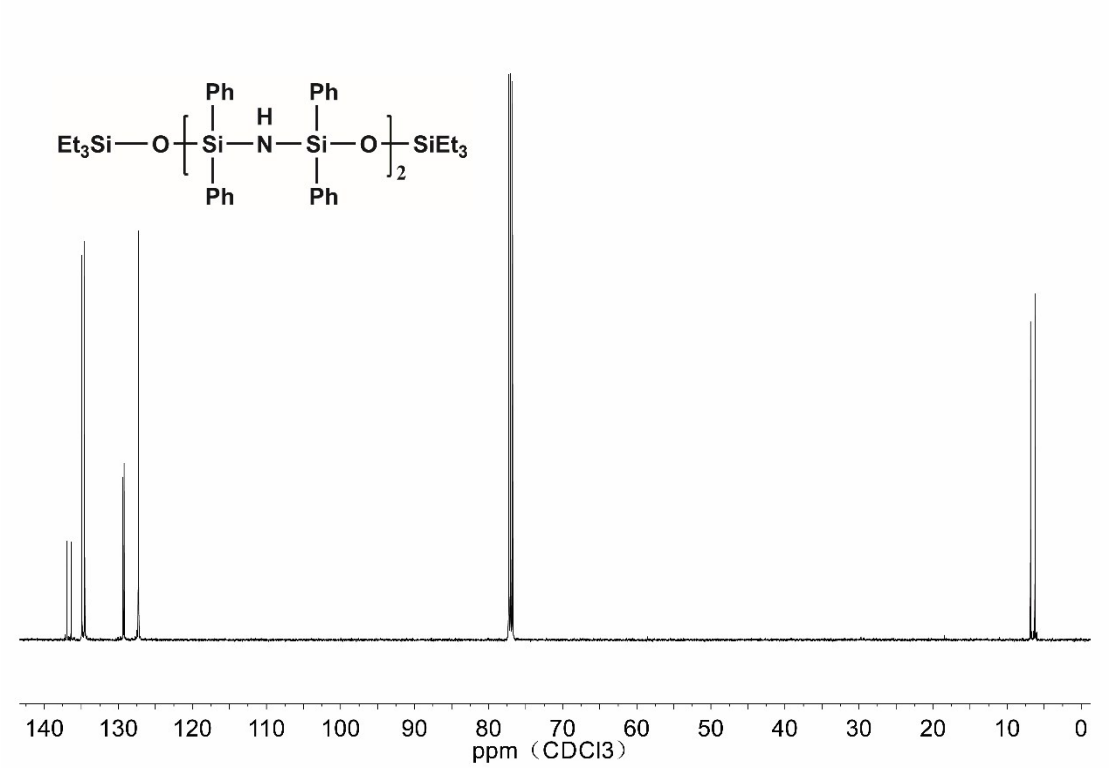
^{1}H NMR (400 MHz, Acetone-d_6) δ 7.79 – 6.92 (m, 20H), 1.30 (s, 1H), 0.23 – -0.15 (m, 48H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 136.83, 136.52, 134.99, 134.57, 129.28, 127.33, 1.07. ^{29}Si NMR (79 MHz, $CDCl_3$) δ -21.97, -31.70, -34.14.

3. Copies of NMR and MALDI-TOF Spectra of Siloxazanes

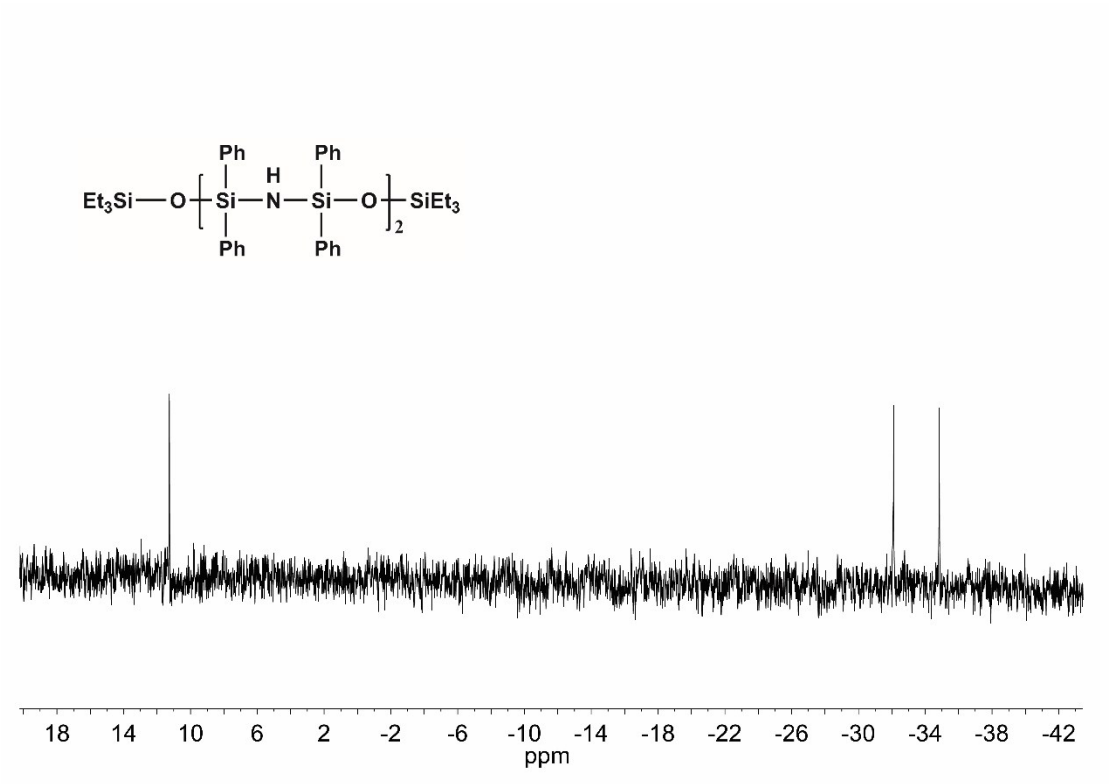
^{1}H NMR



^{13}C NMR

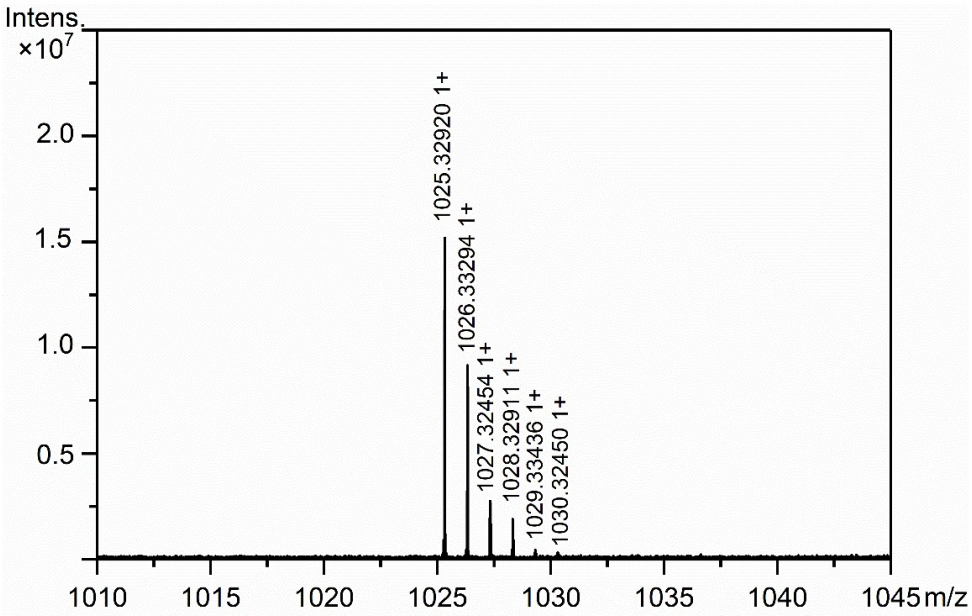


^{29}Si NMR

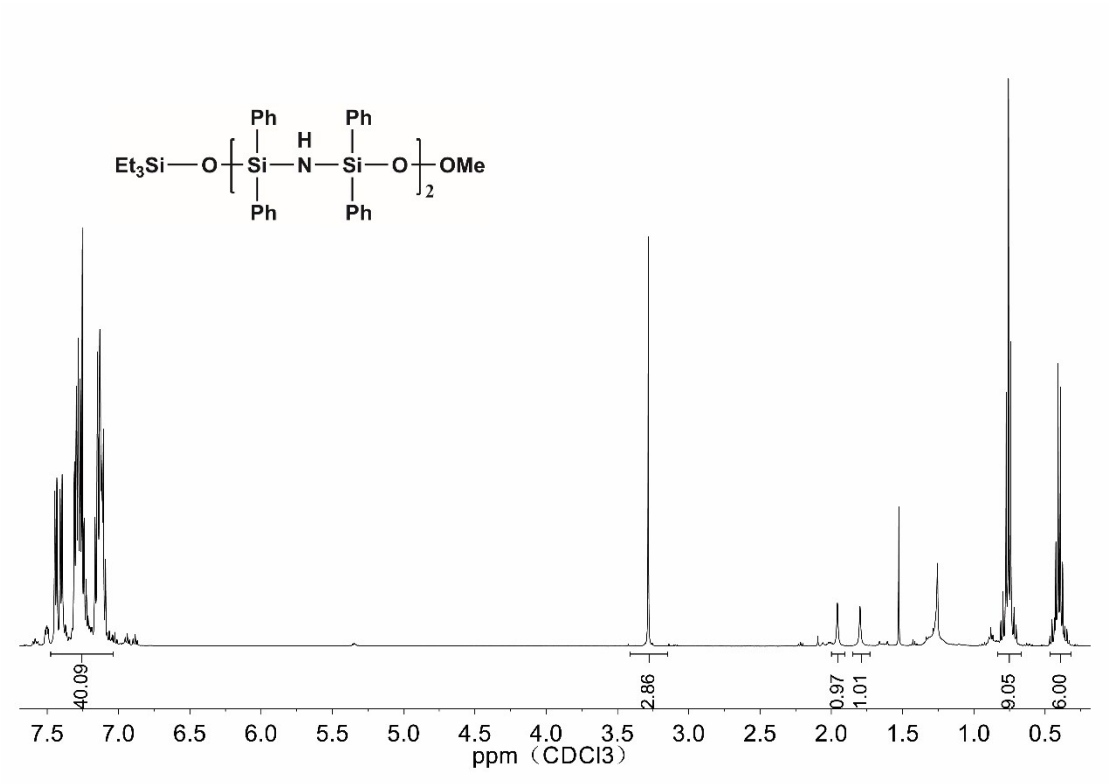


High-resolution MALDI-TOF-MS

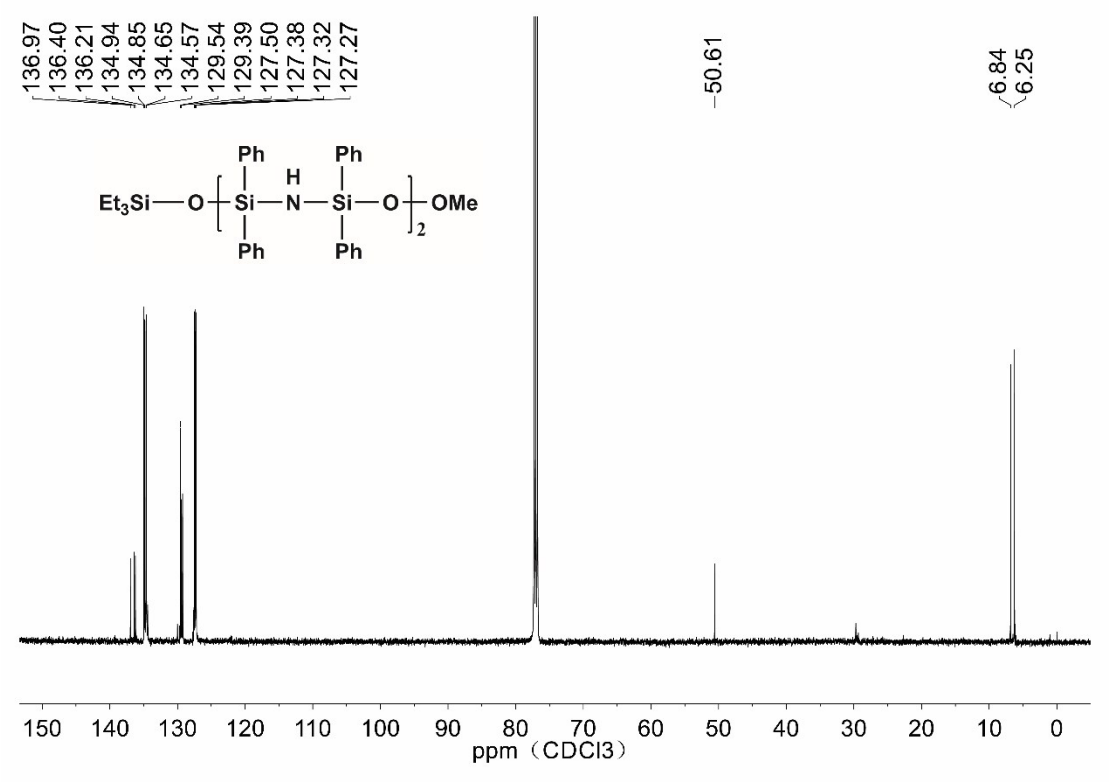
m/z: for $[M+H]^+$ = 1025.329200



^{1}H NMR

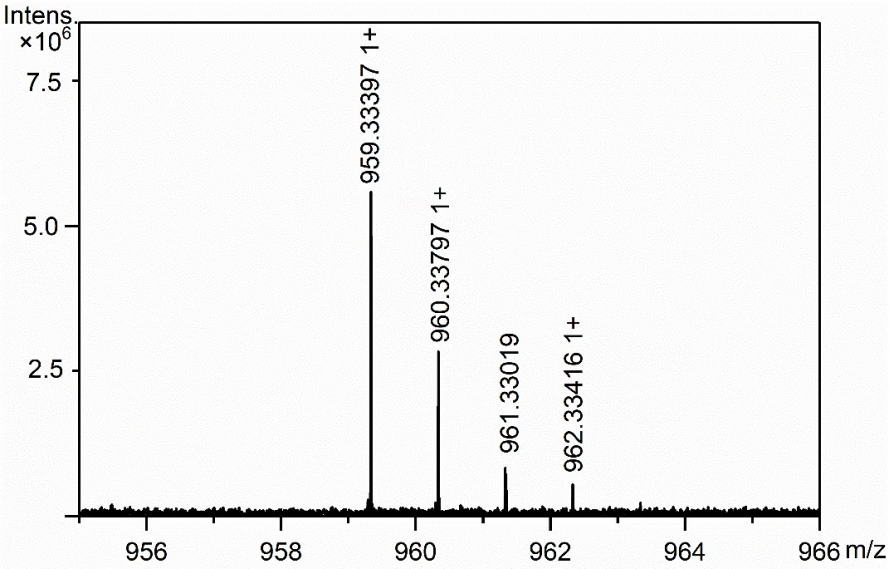


^{13}C NMR

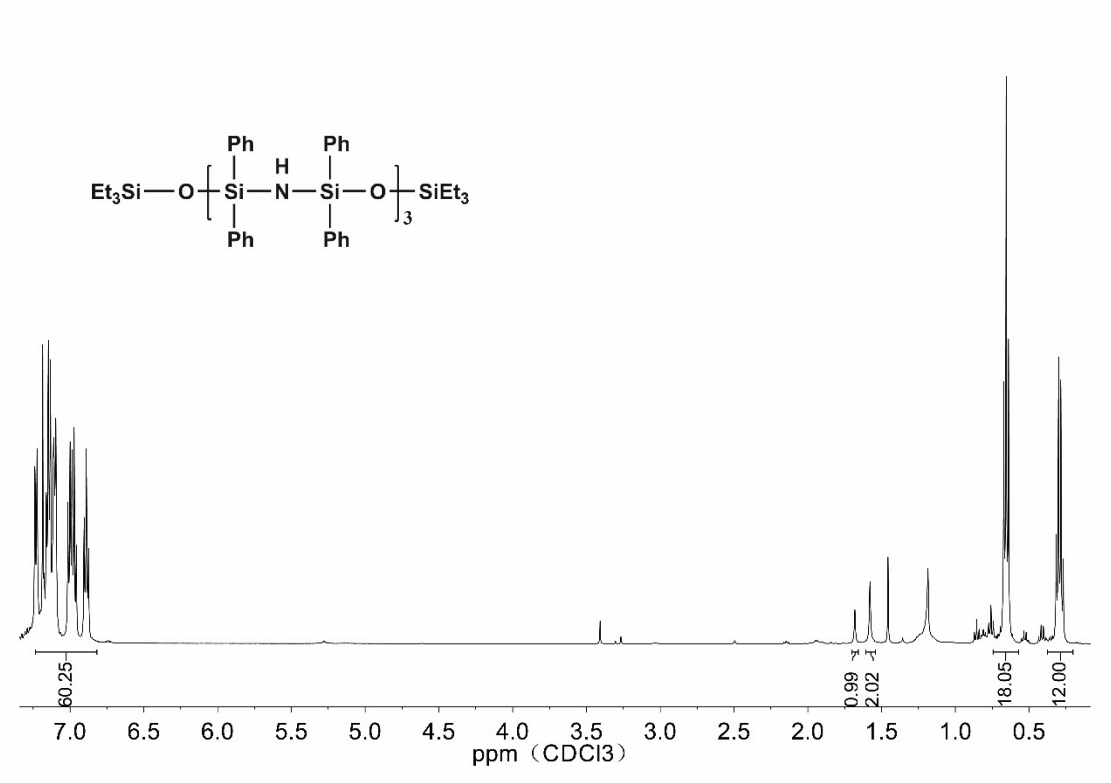


High-resolution MALDI-TOF-MS

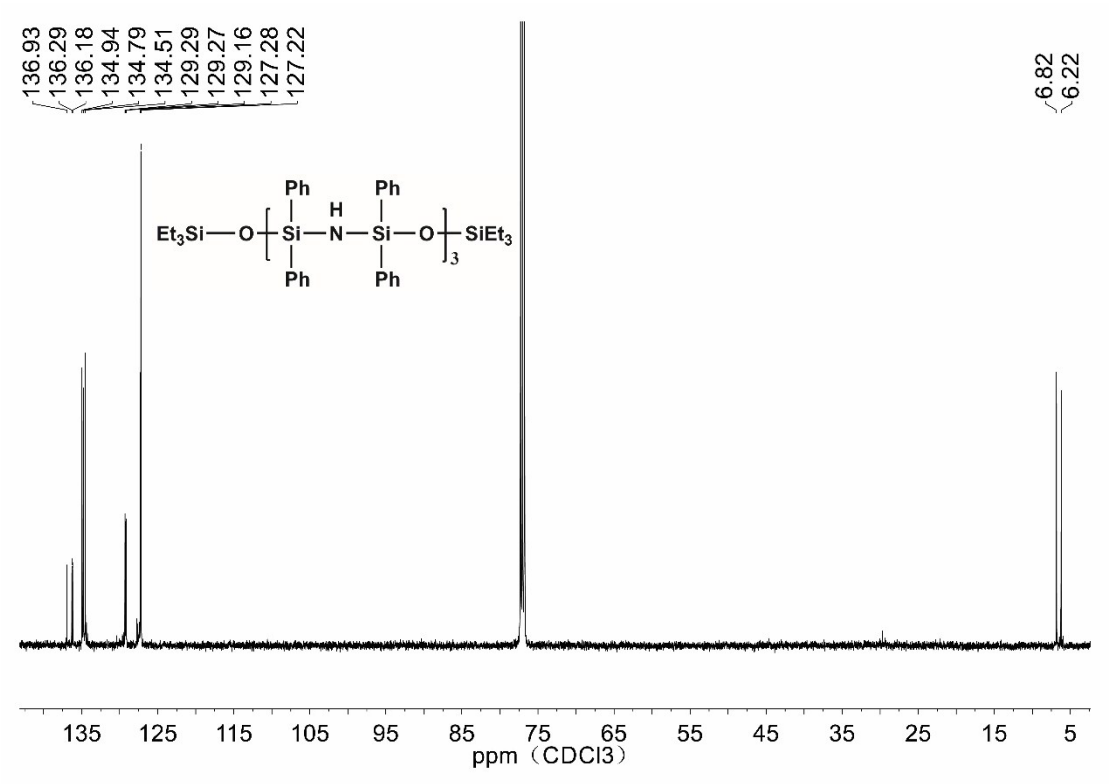
m/z: for $[M + Na]^+$ = 959.333974



^{1}H NMR

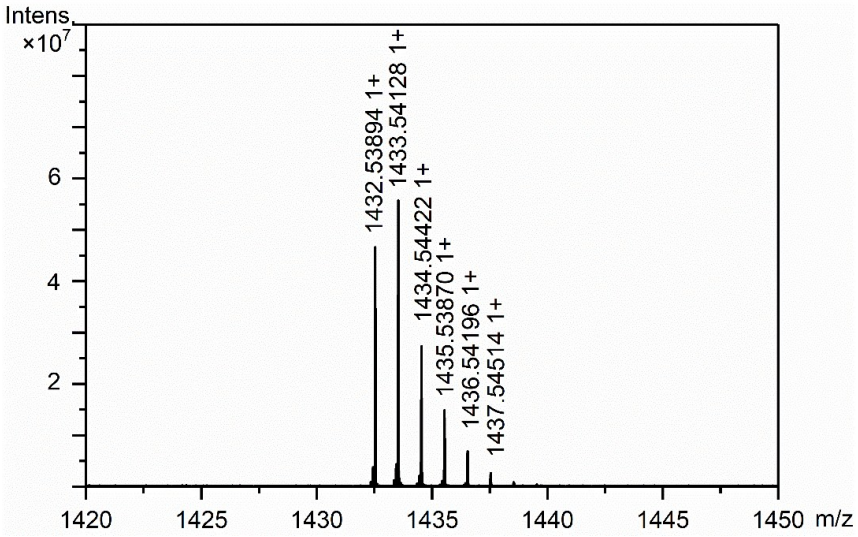


^{13}C NMR

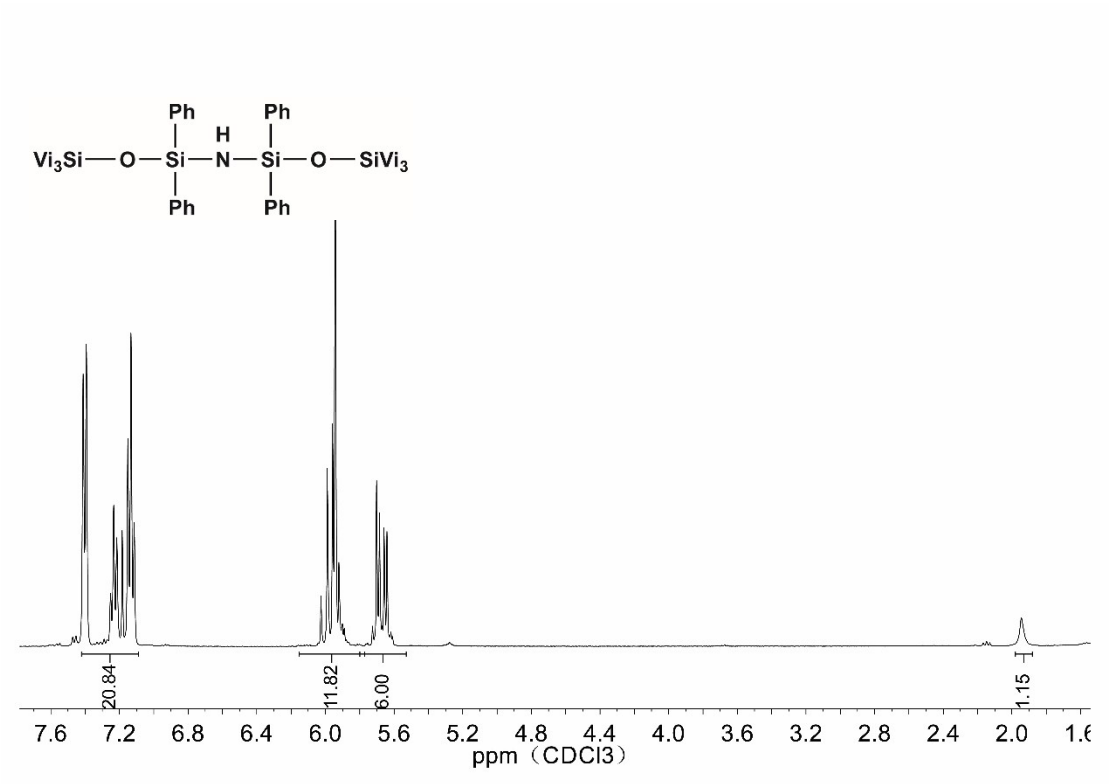


High-resolution MALDI-TOF-MS

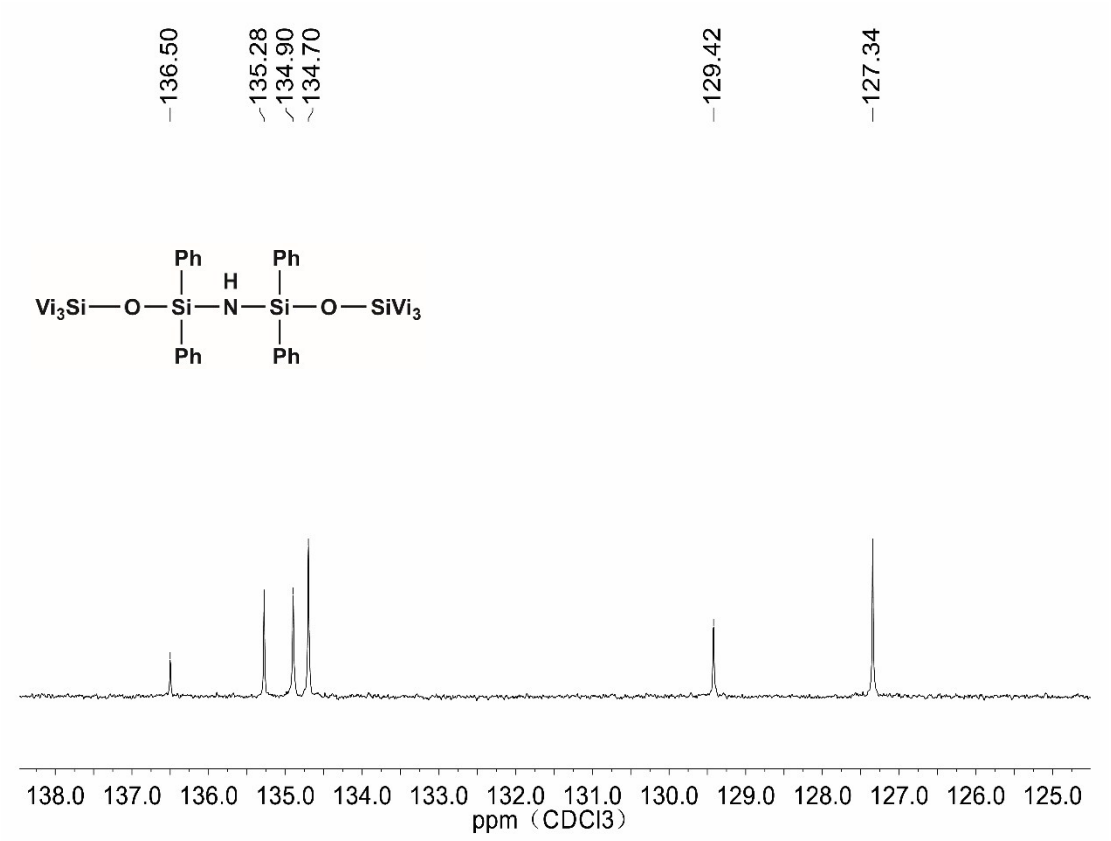
m/z: for $[M + H]^+$ = 1432.538936



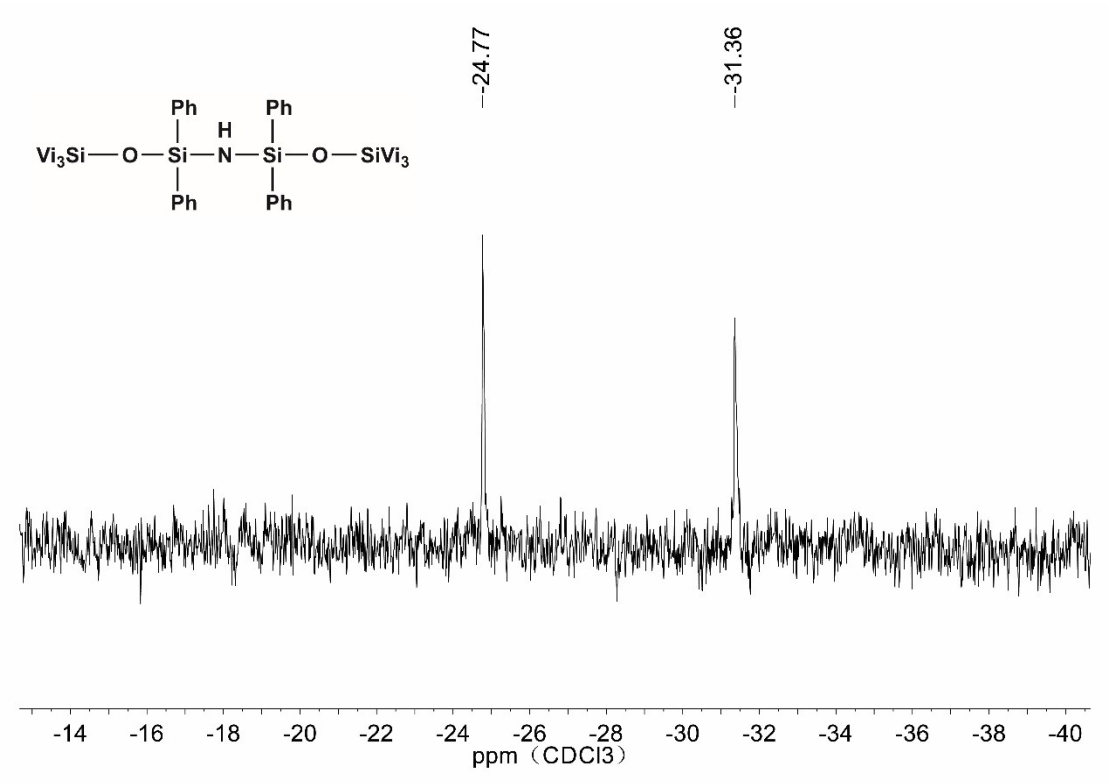
^{1}H NMR



^{13}C NMR

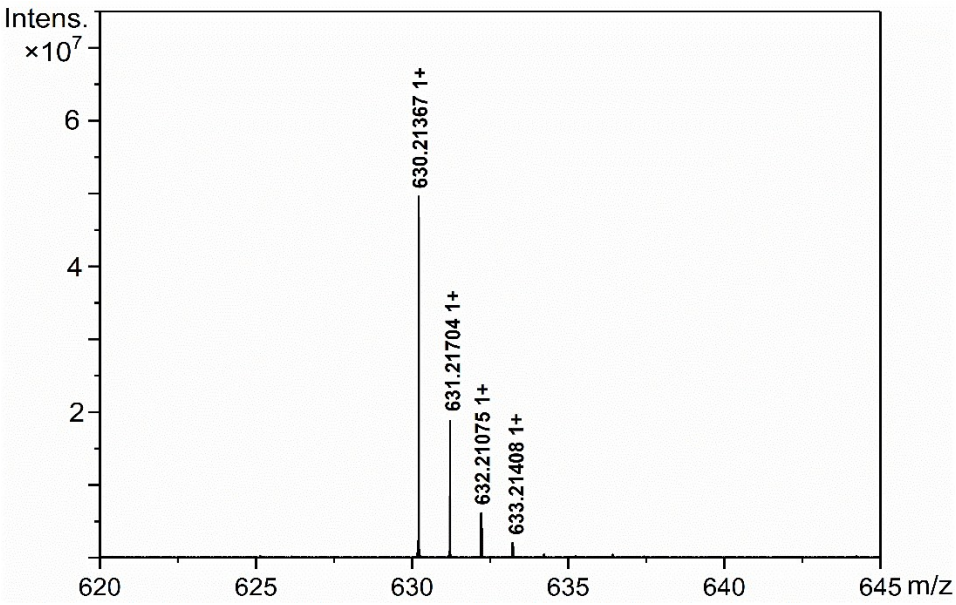


^{29}Si NMR

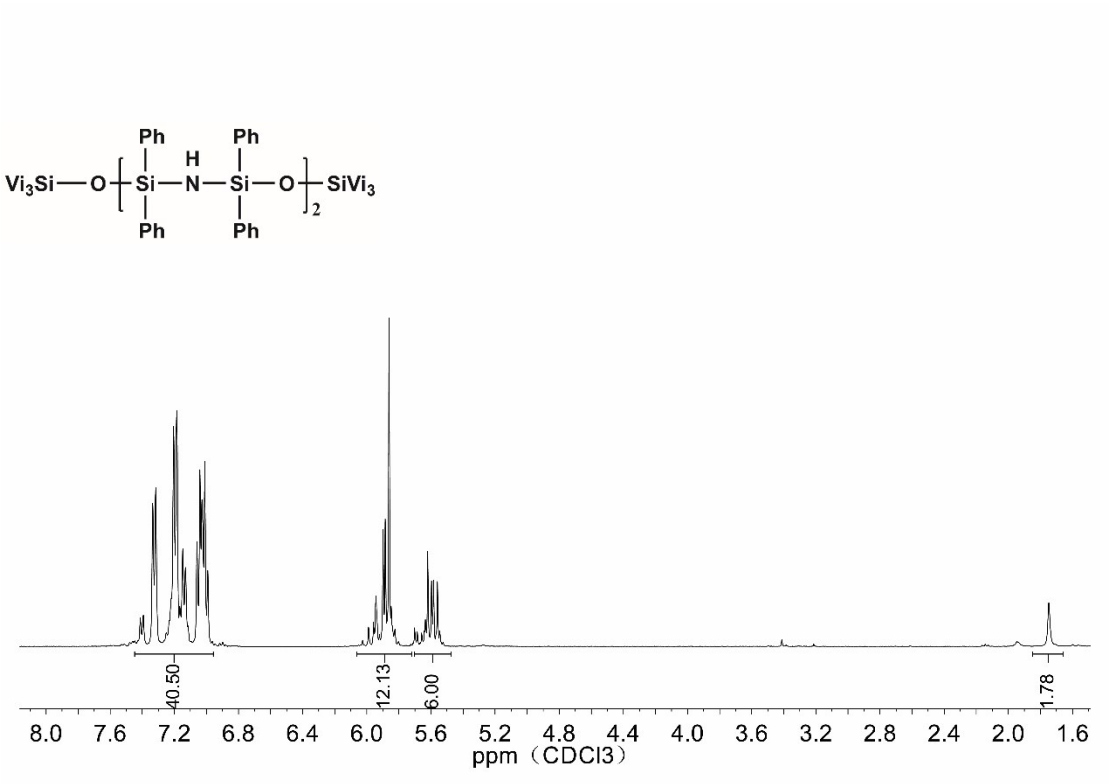


High-resolution MALDI-TOF-MS

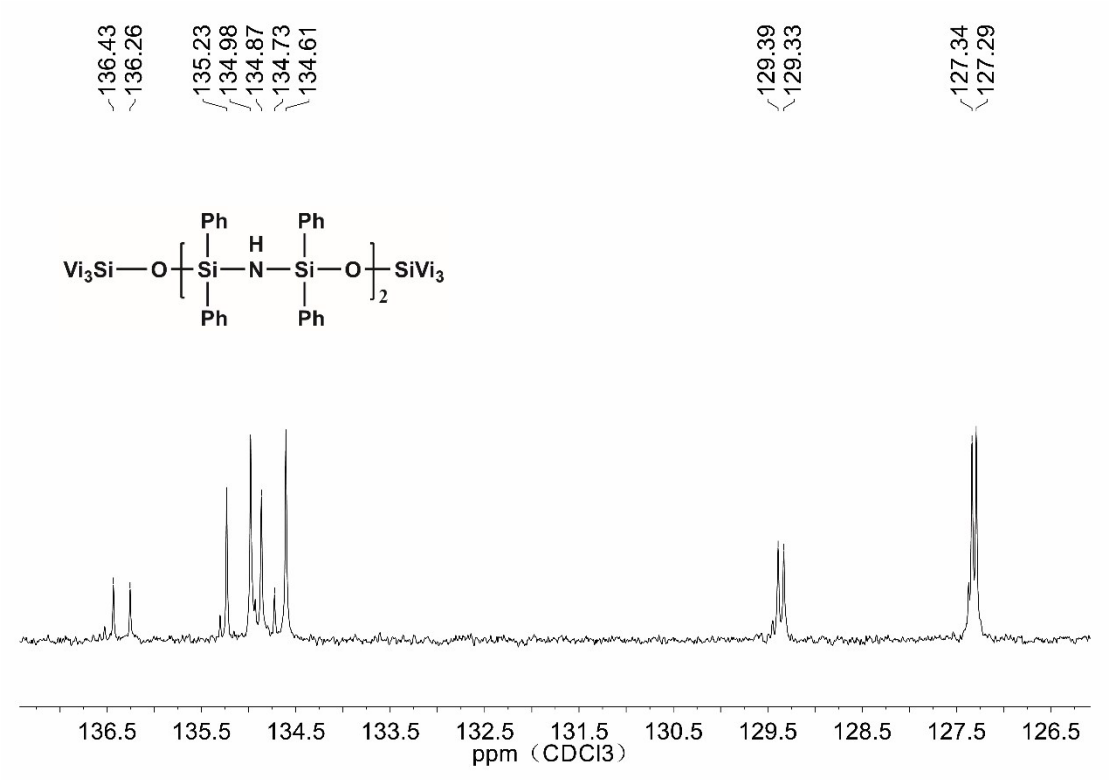
m/z: for $[M + H]^+$ = 630.213671



^{1}H NMR

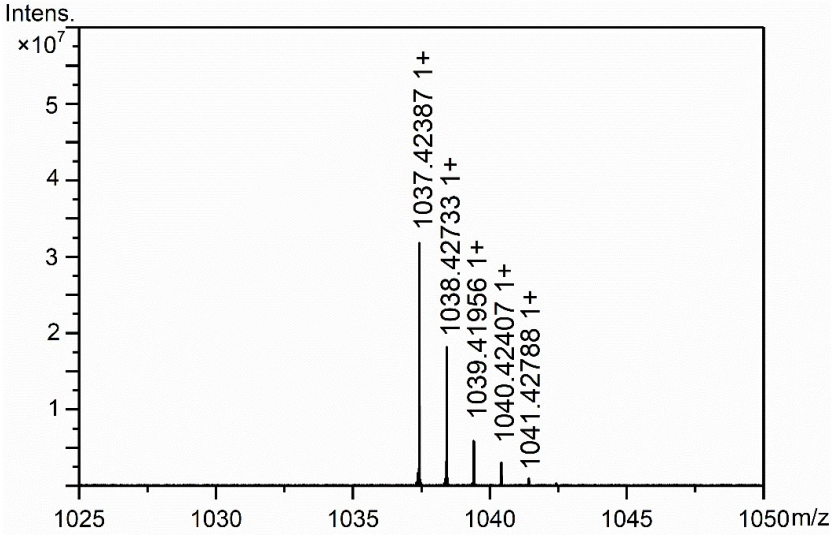


^{13}C NMR

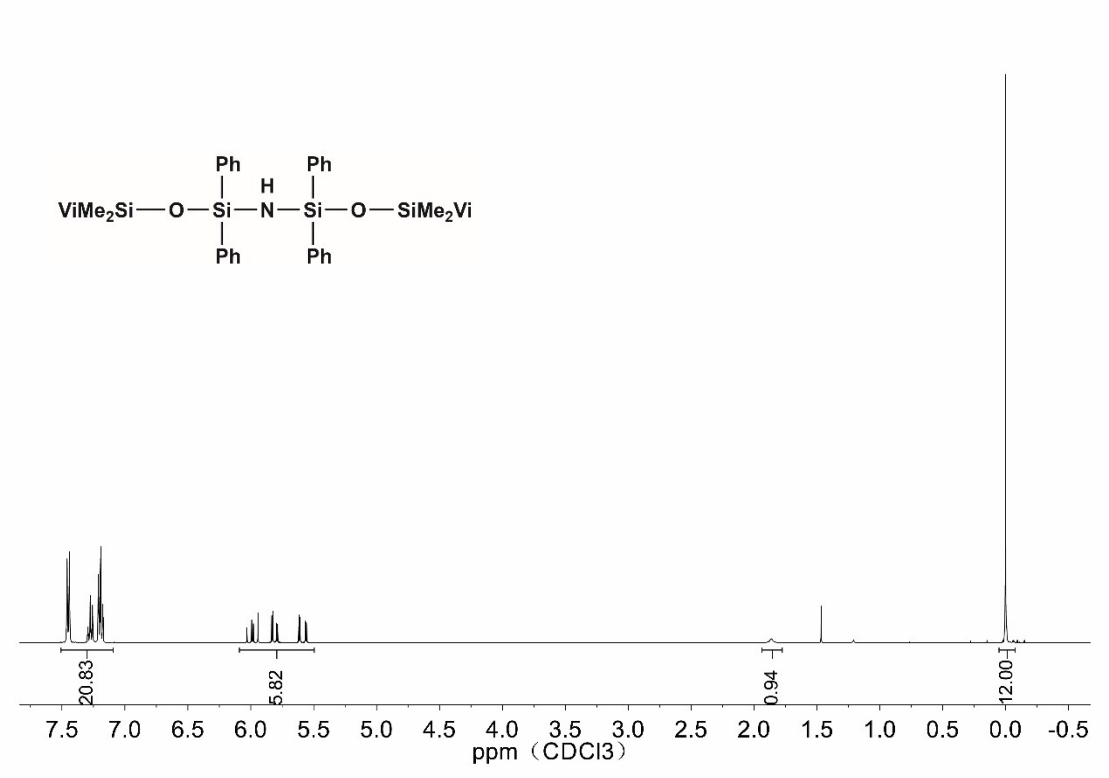


High-resolution MALDI-TOF-MS

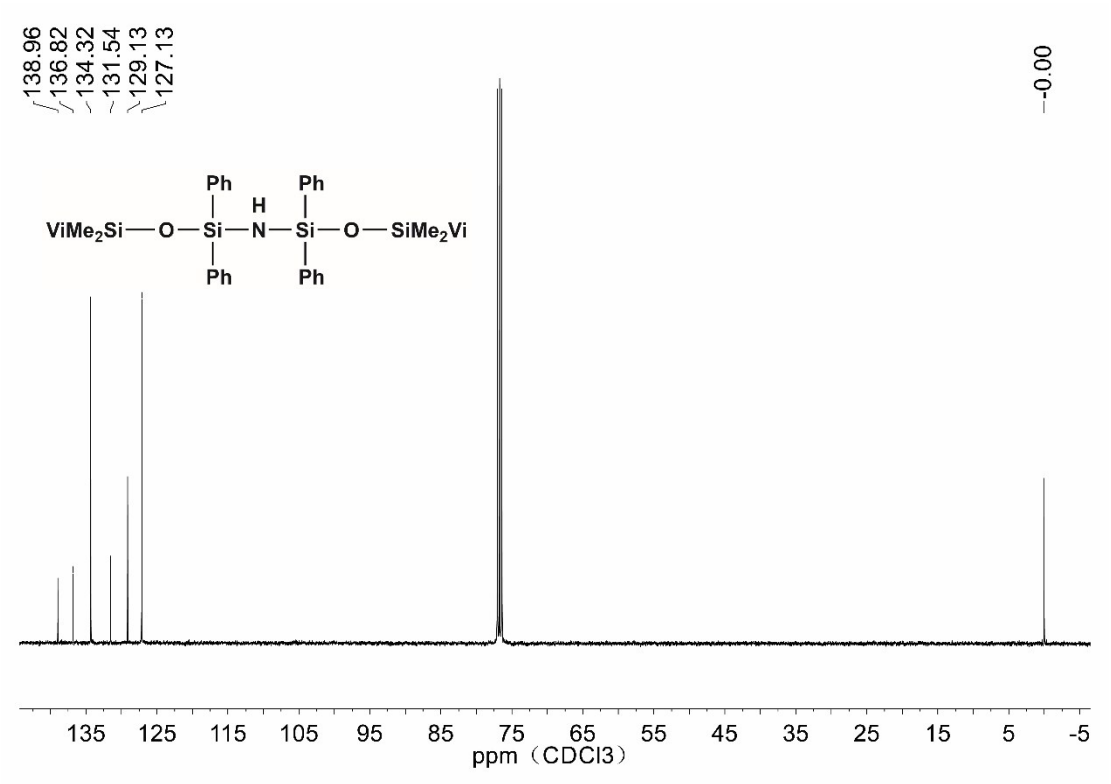
m/z: for $[M + H]^+$ = 1037.423871



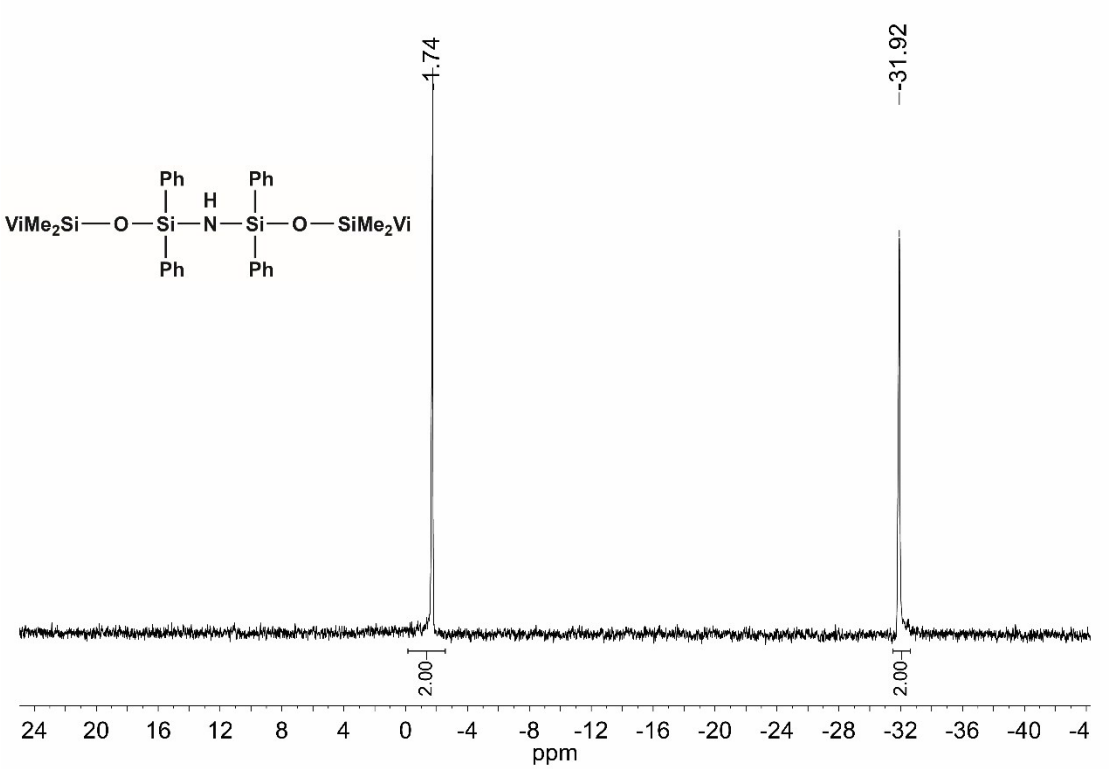
^{1}H NMR



^{13}C NMR

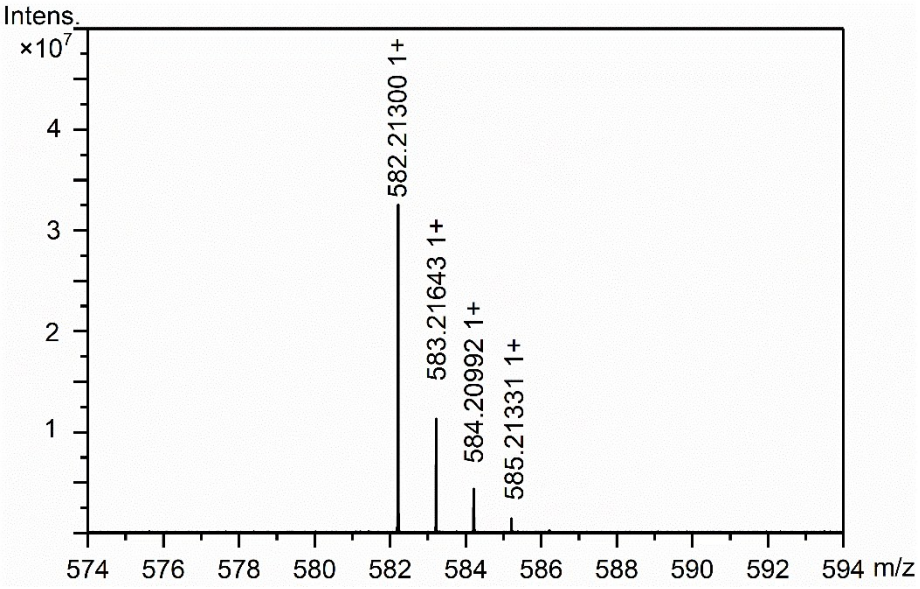


^{29}Si NMR

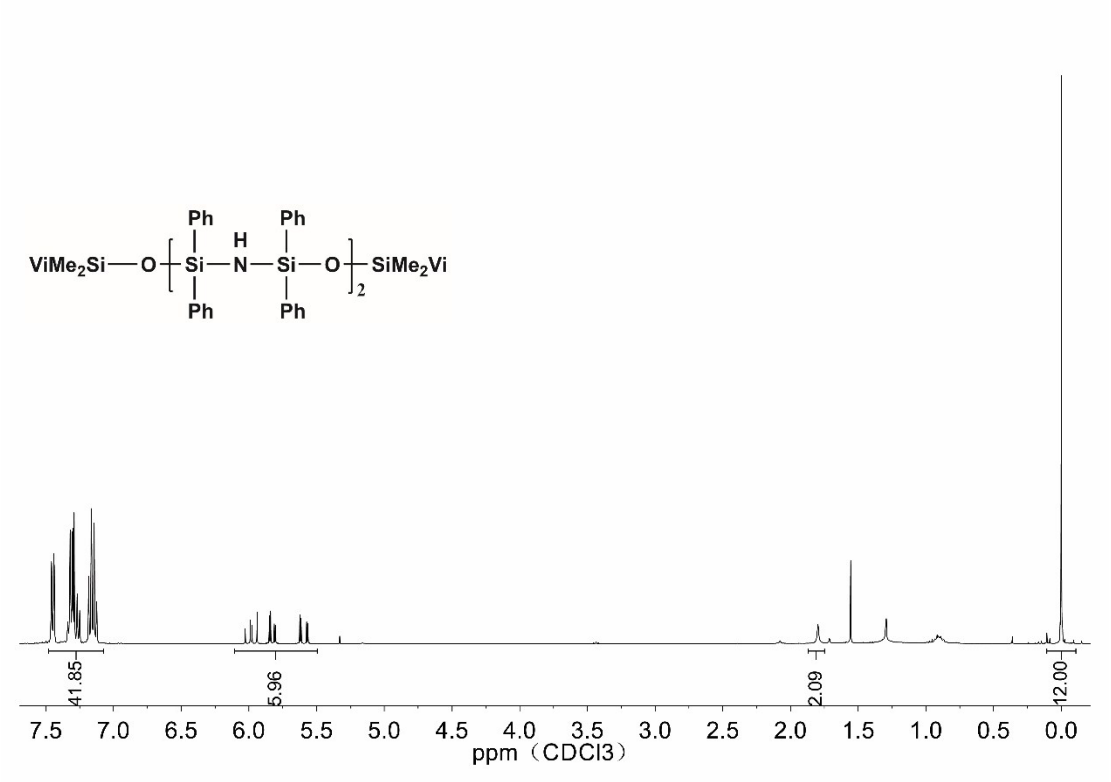


High-resolution MALDI-TOF-MS

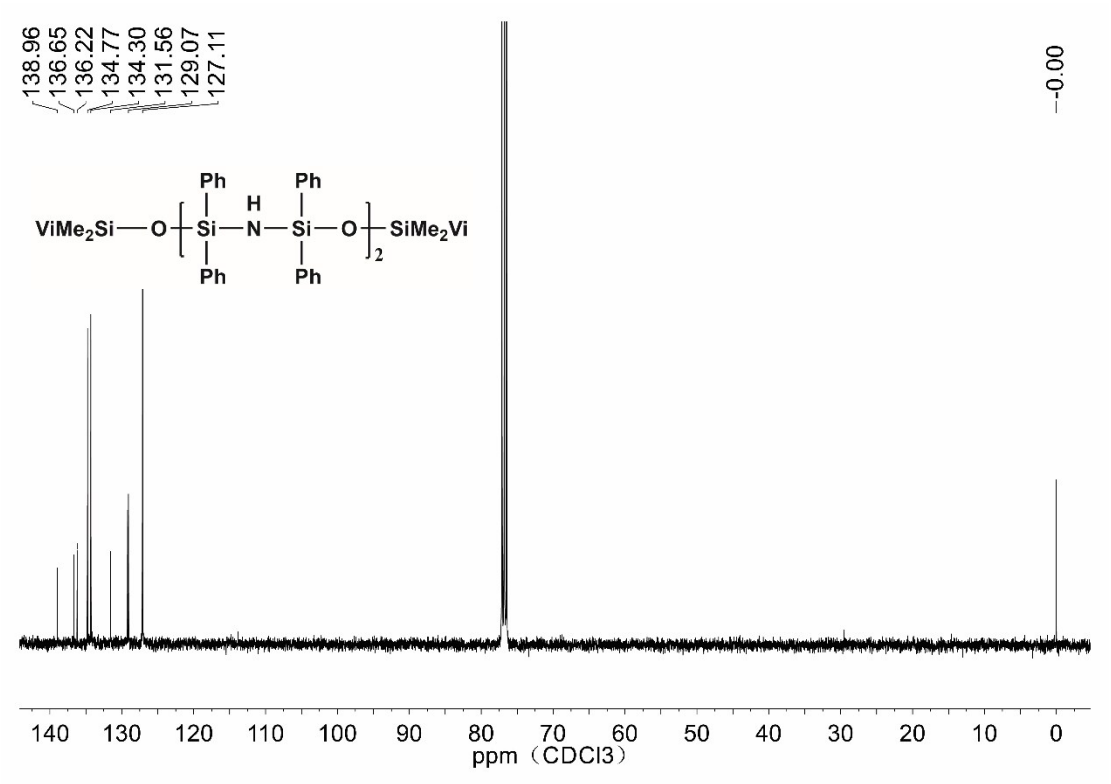
m/z: for $[M + H]^+$ = 582.213002



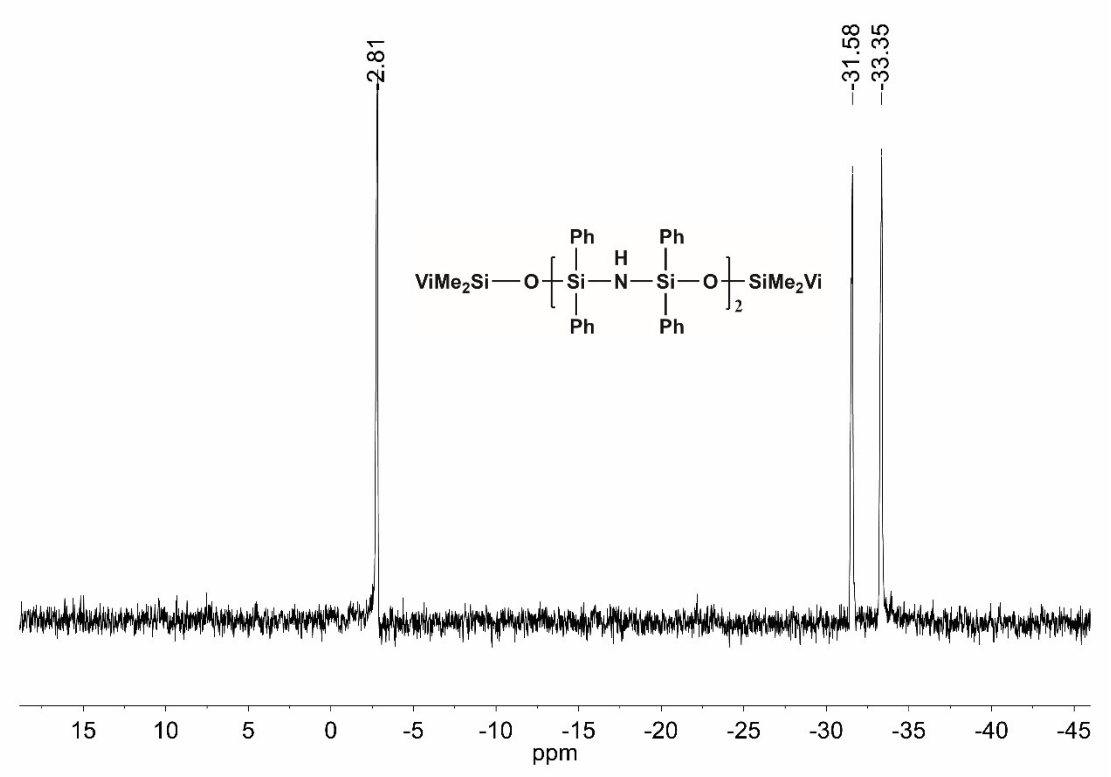
^{1}H NMR



^{13}C NMR

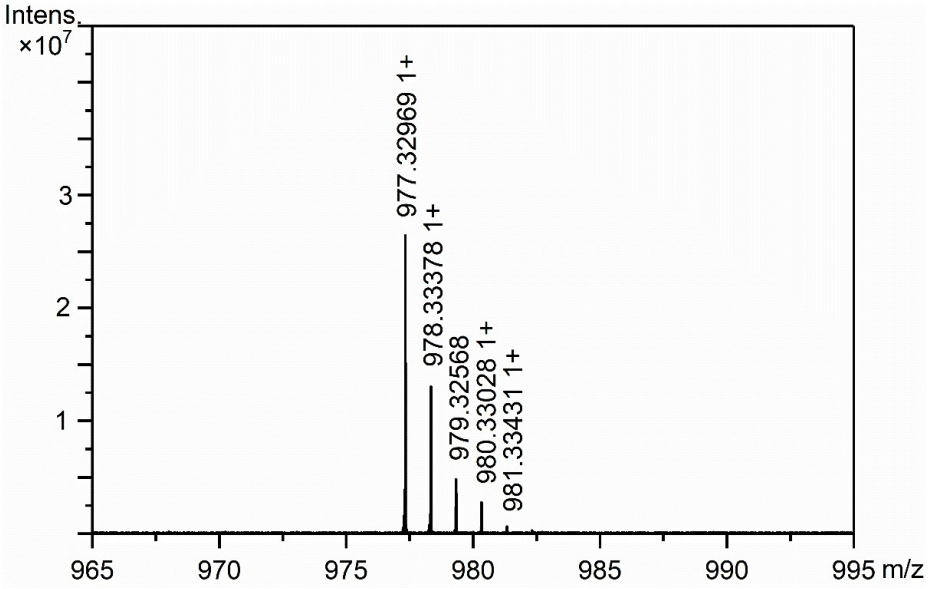


^{29}Si NMR

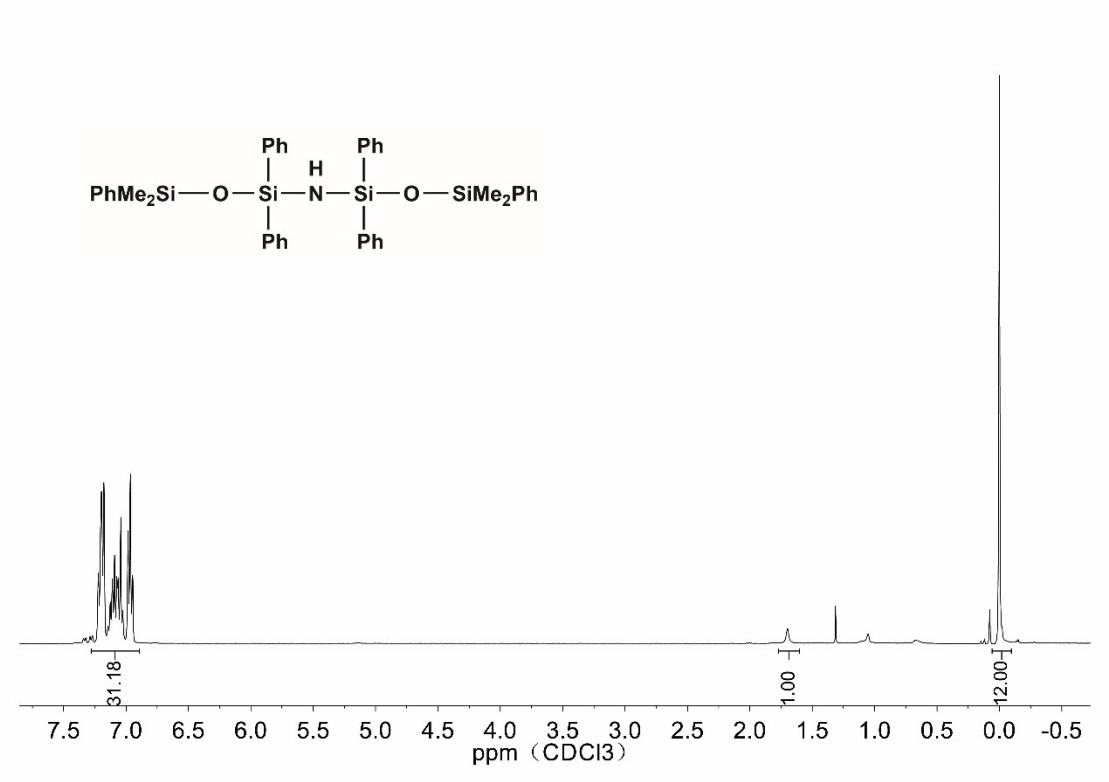


High-resolution MALDI-TOF-MS

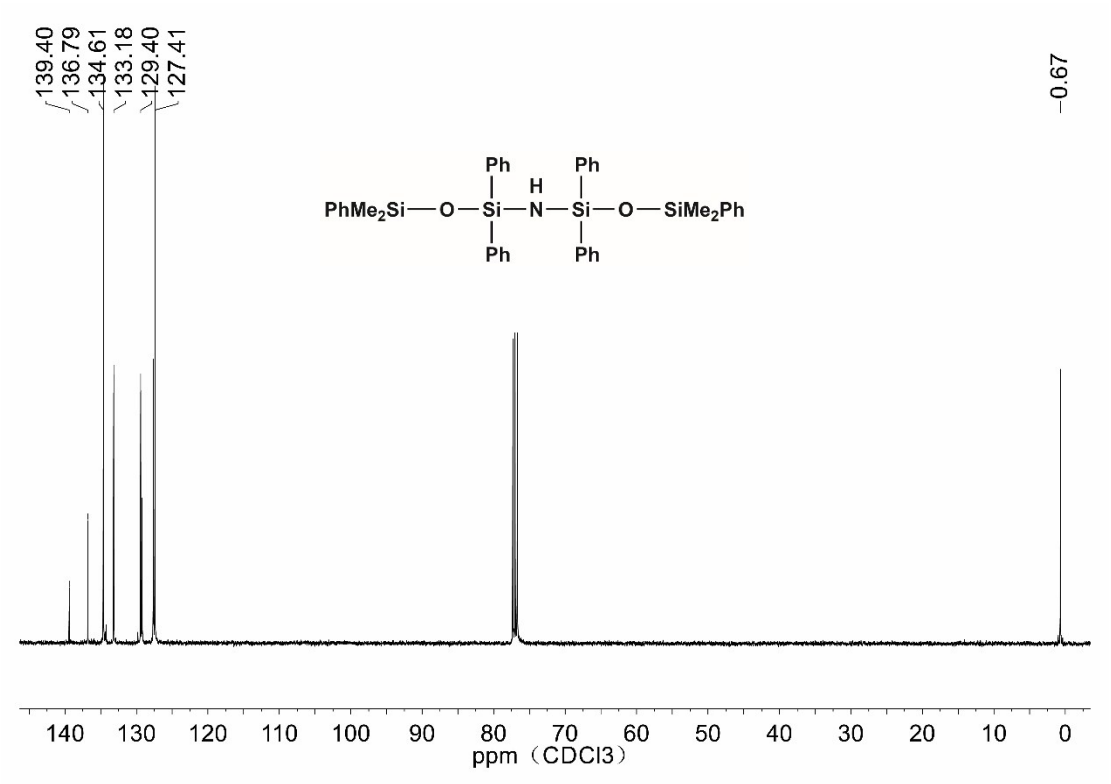
m/z: for $[M + H]^+$ = 977.32969



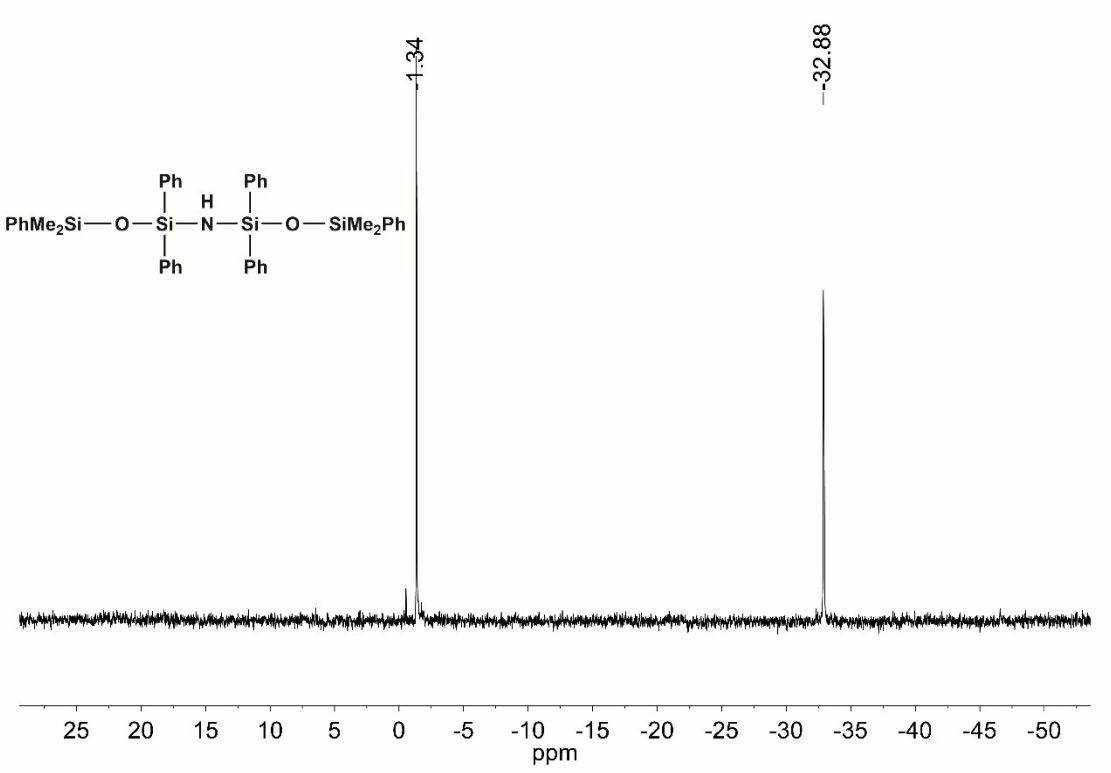
^{1}H NMR



^{13}C NMR

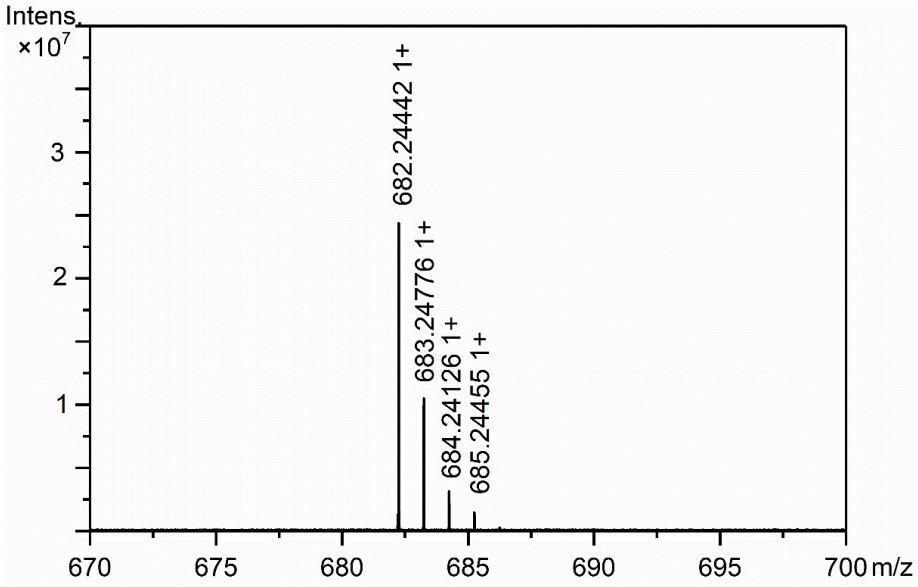


^{29}Si NMR

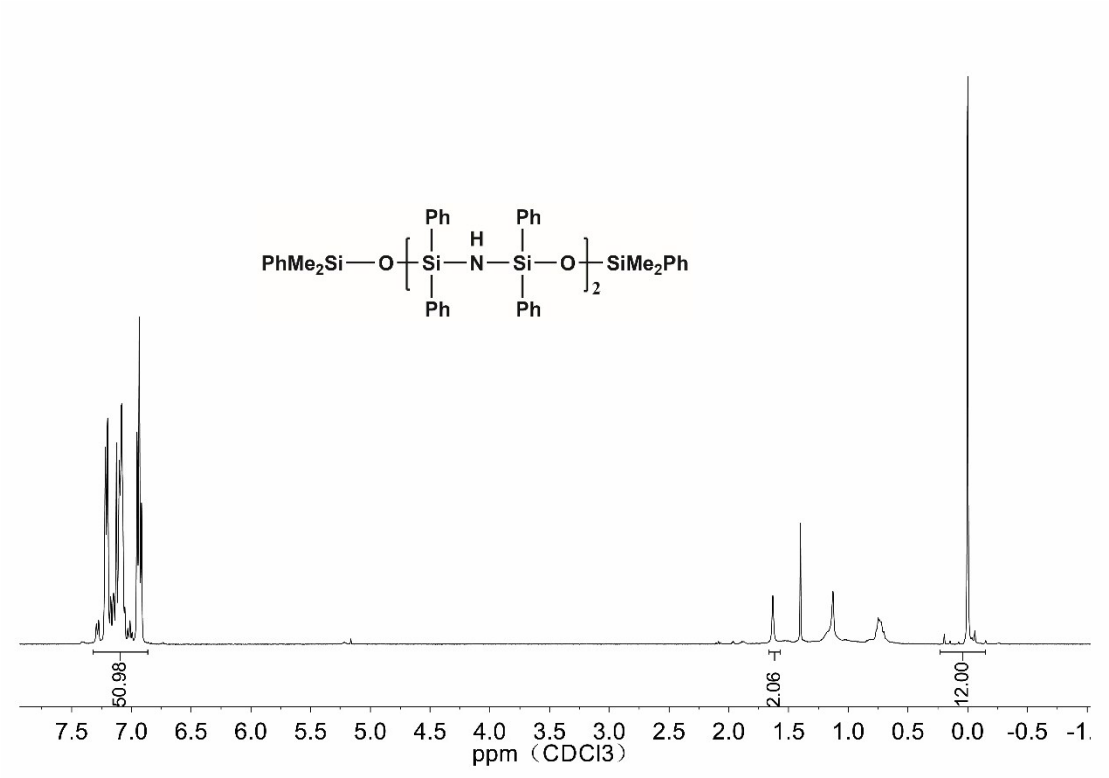


High-resolution MALDI-TOF-MS

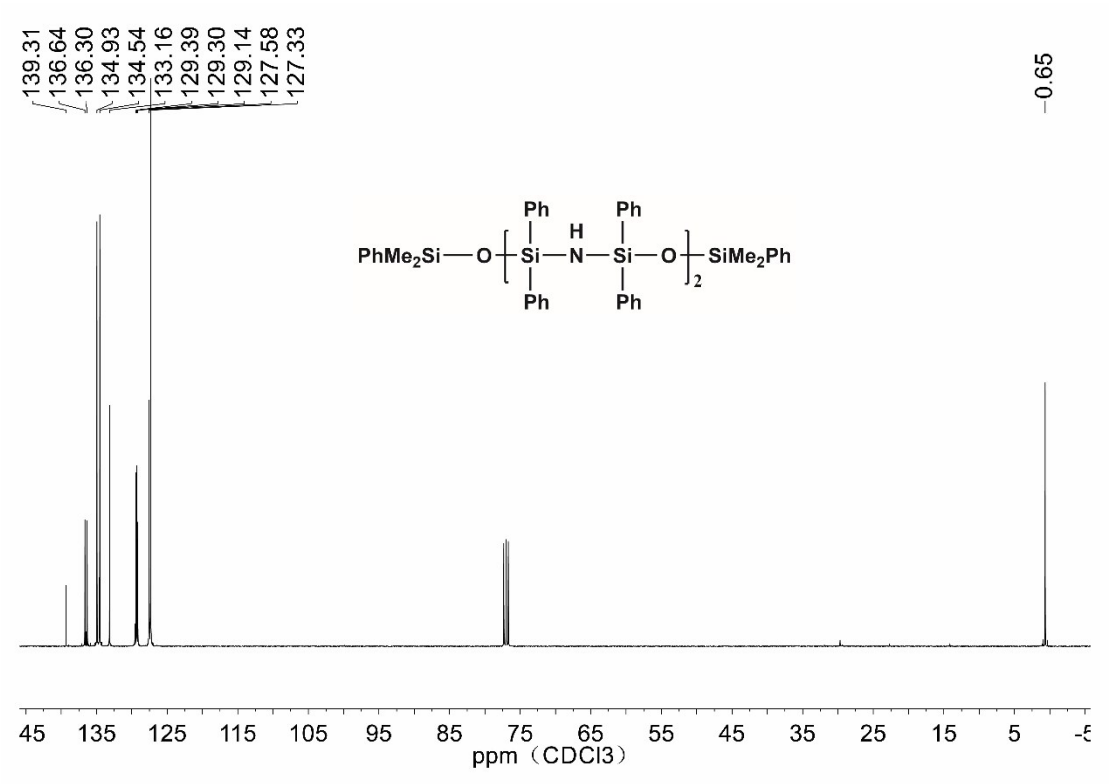
m/z: for $[M + H]^+$ = 682.244418



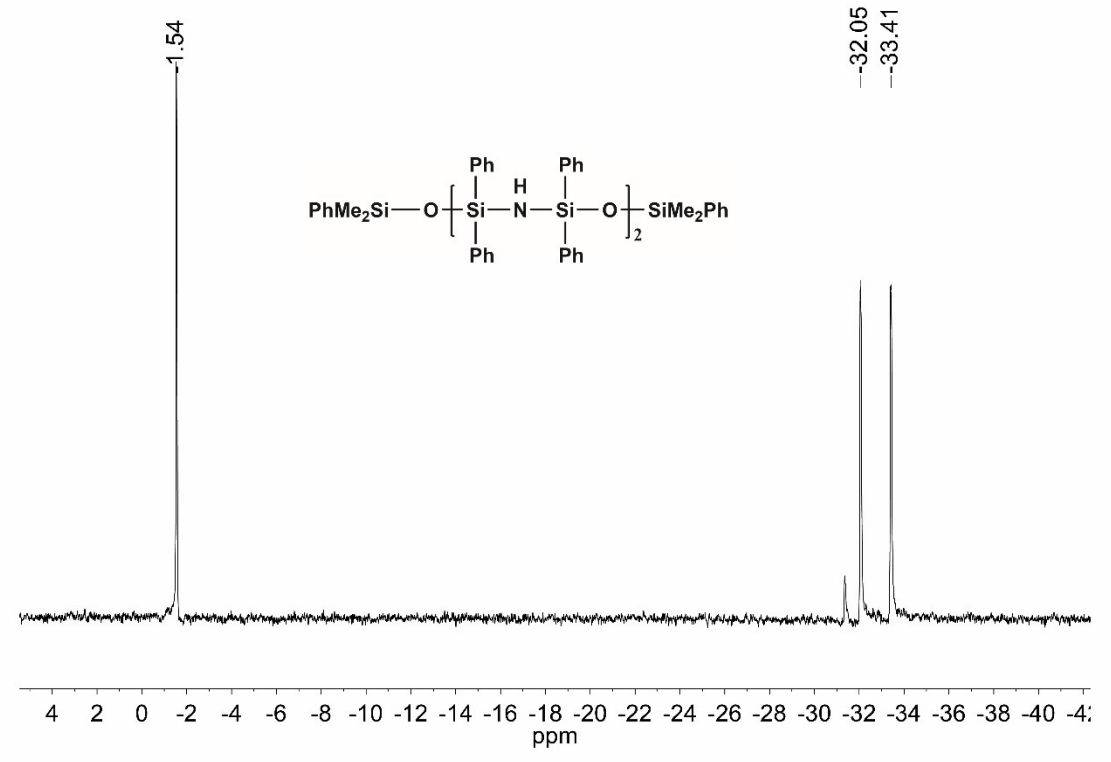
^{1}H NMR



^{13}C NMR

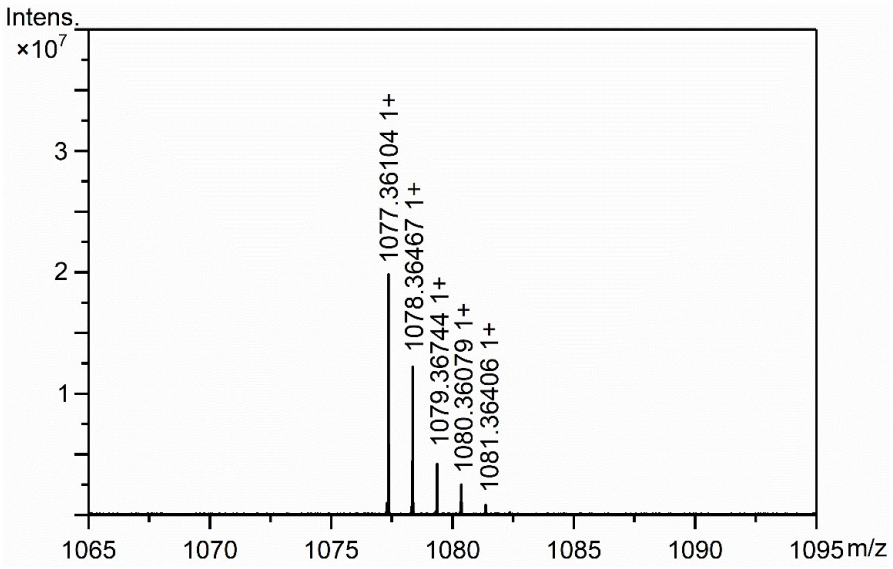


^{29}Si NMR

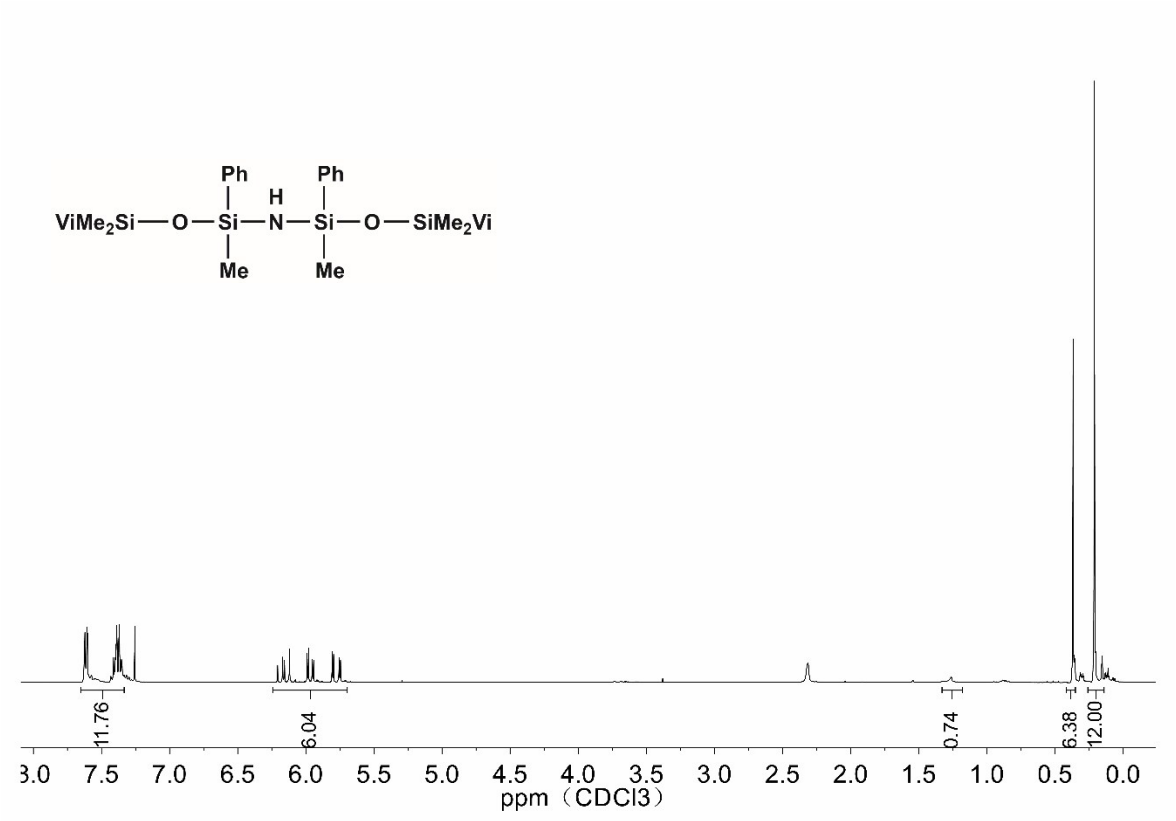


High-resolution MALDI-TOF-MS

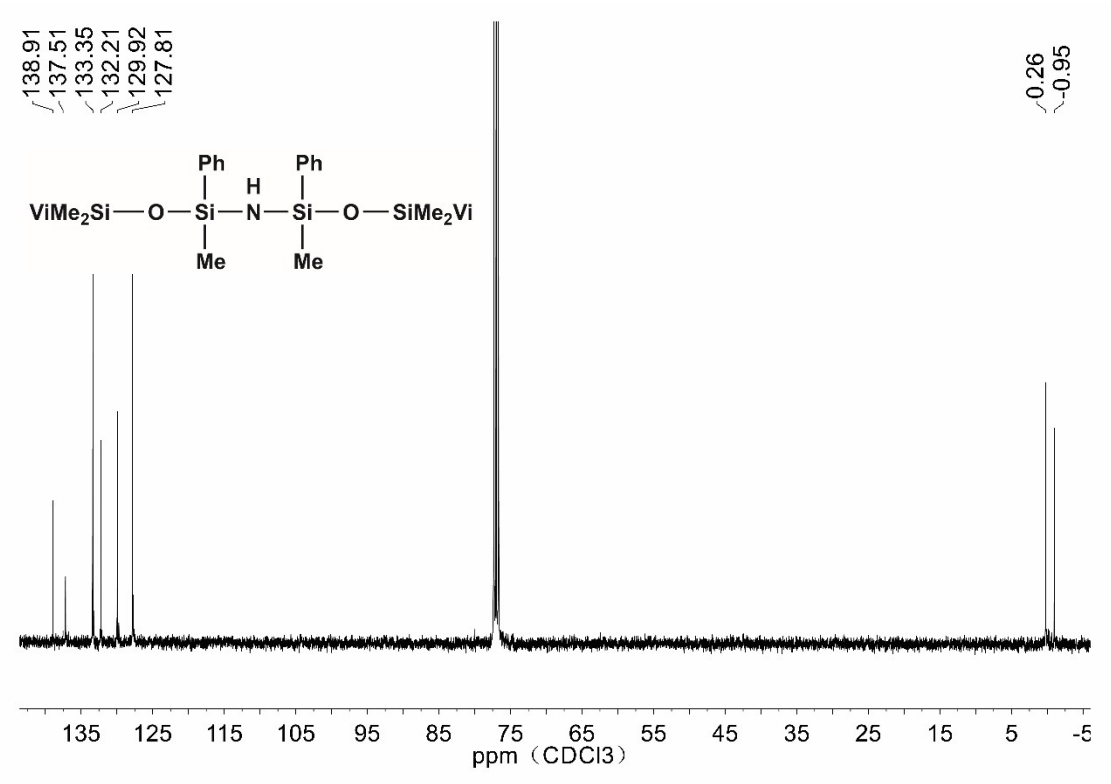
m/z: for $[M + H]^+$ = 1077.361040



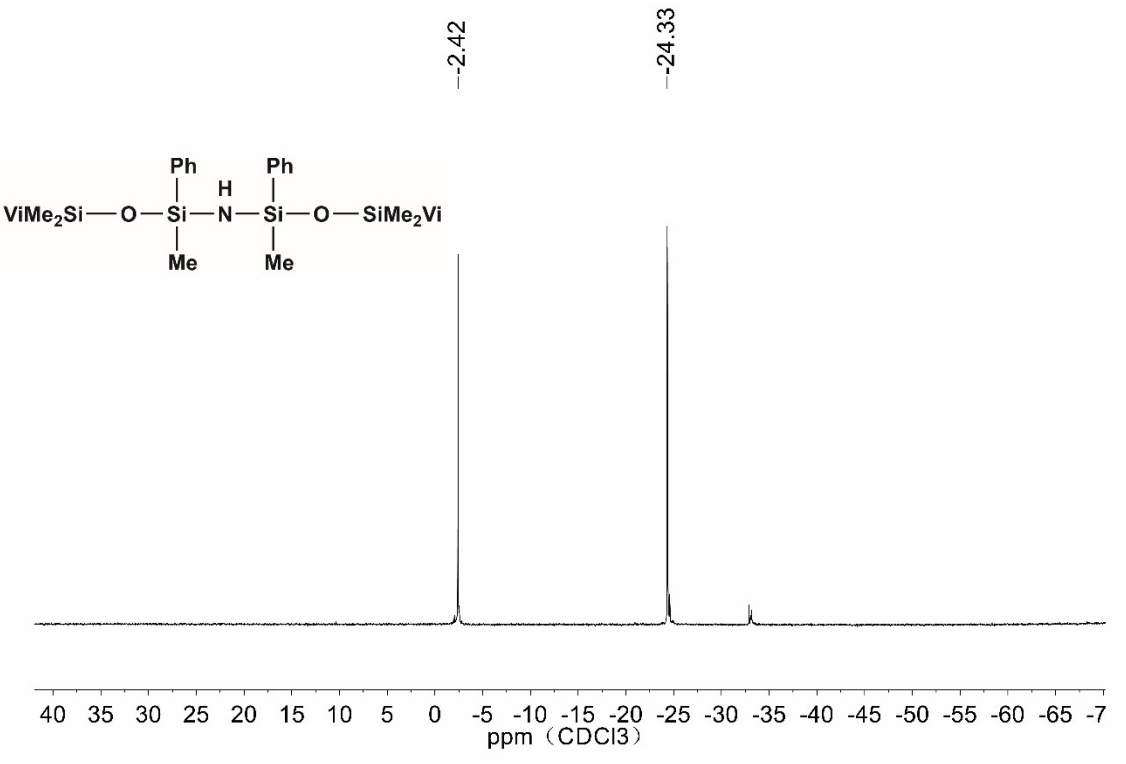
^{1}H NMR



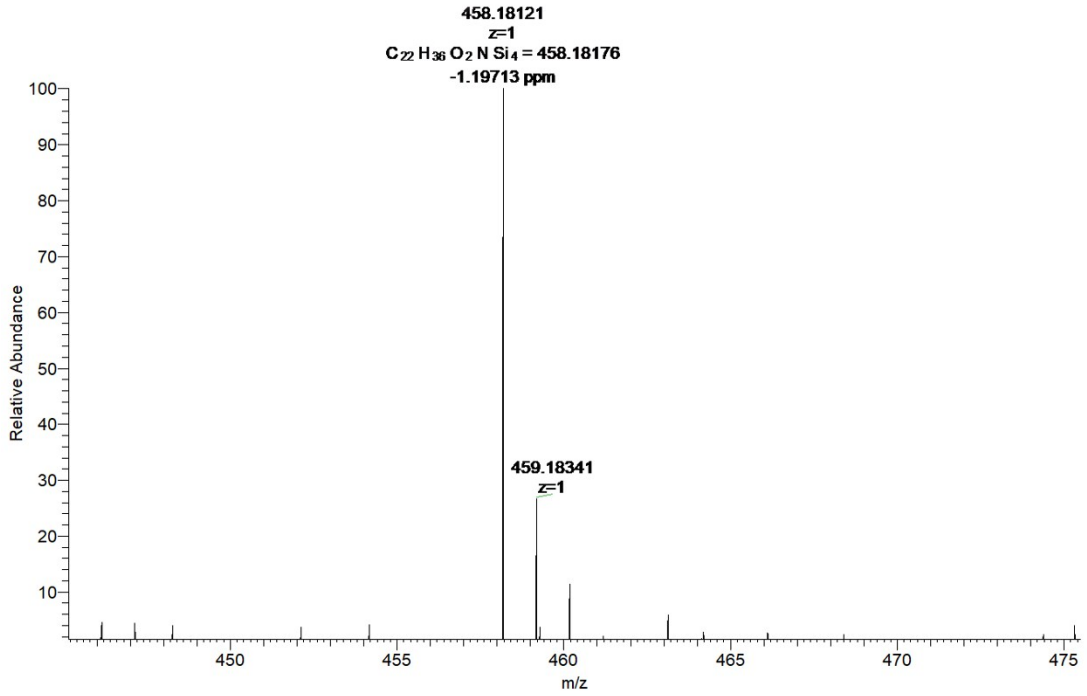
^{13}C NMR



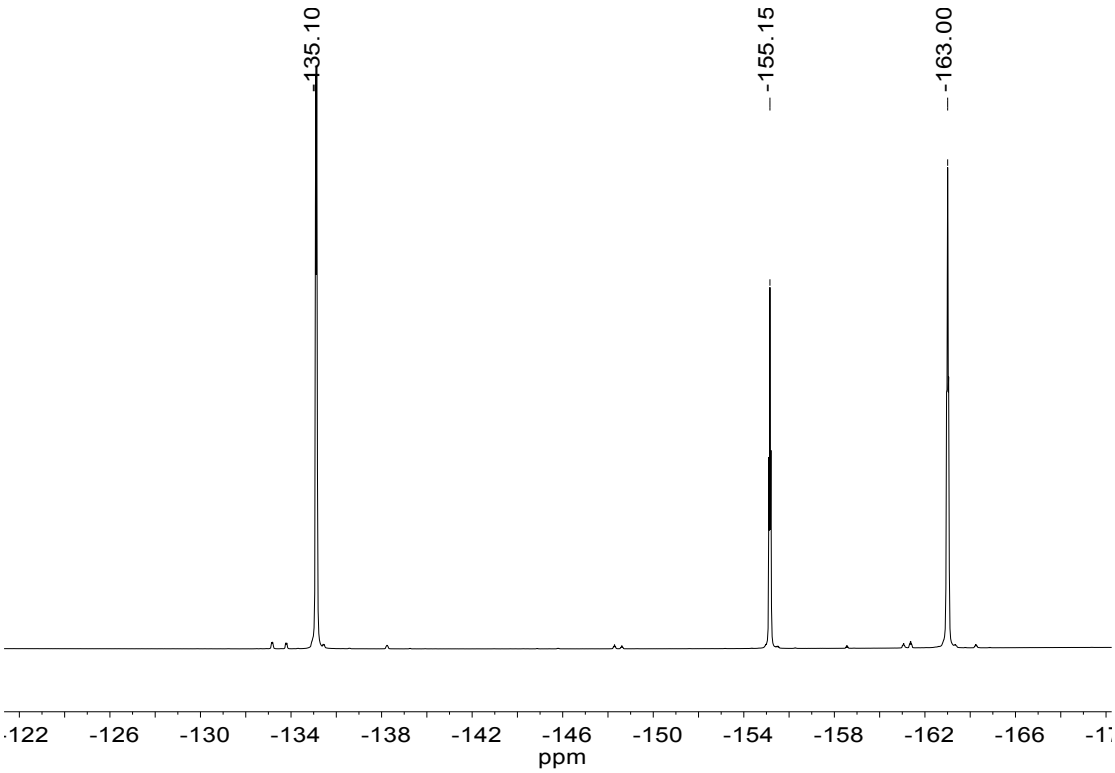
^{29}Si NMR



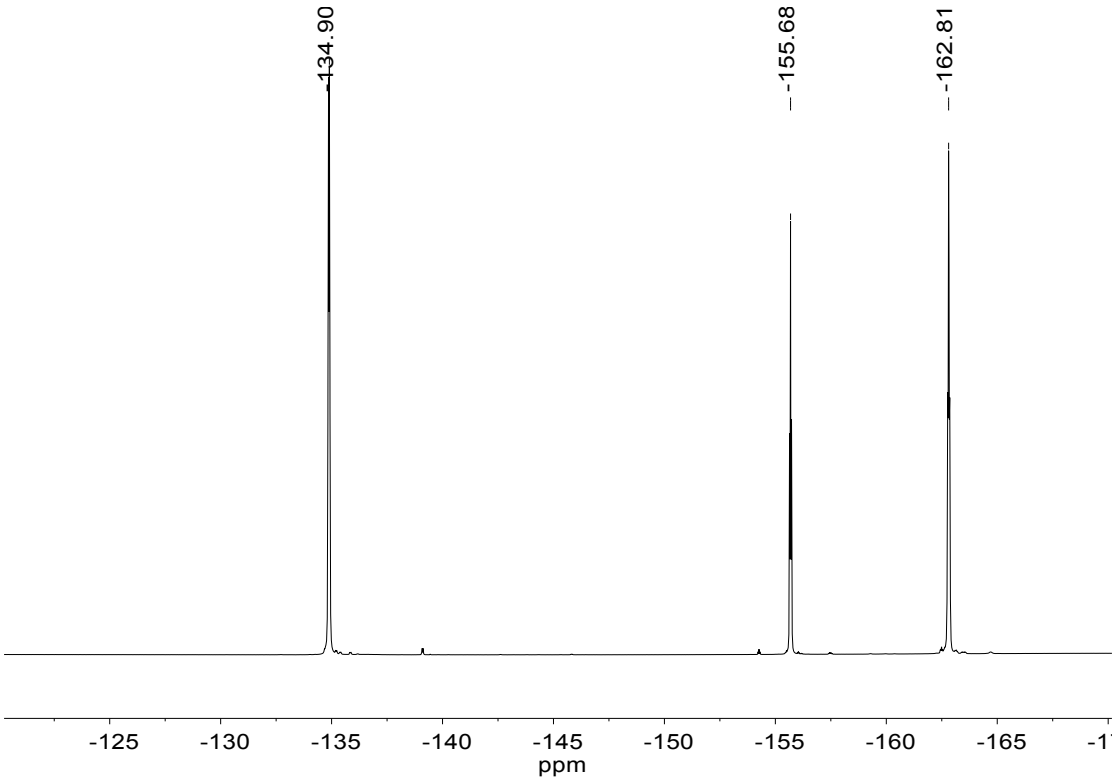
High-resolution ESI-MS
m/z: for $[M + H]^+$ = 458.18121



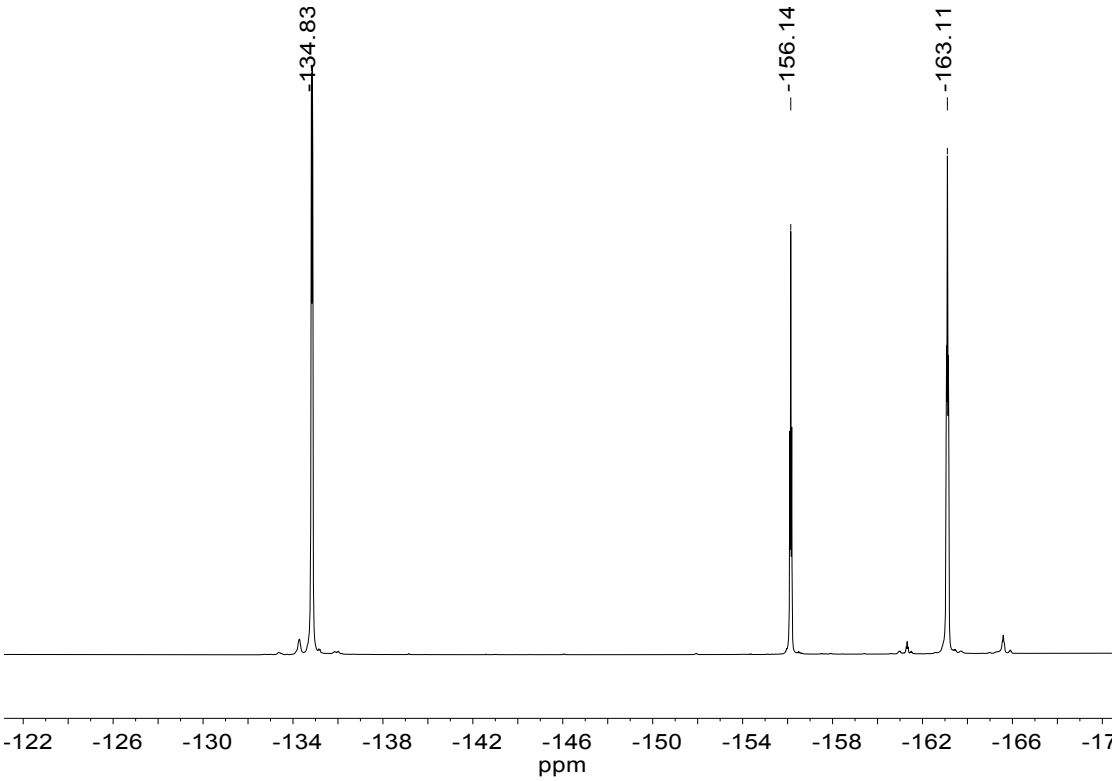
^{19}F NMR



Tris(pentaflouorphenyl)borane in toluene-d_8.



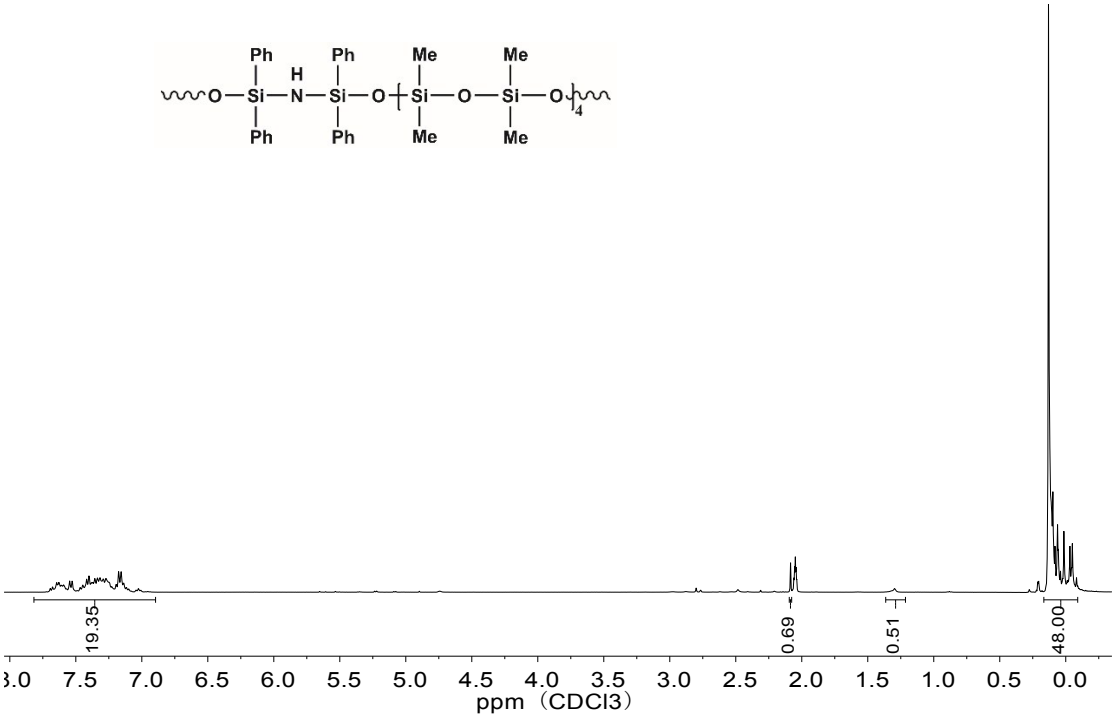
Solution of **1a** and tris(pentafluorophenyl)borane (0.5 equiv.) in toluene-d_8.



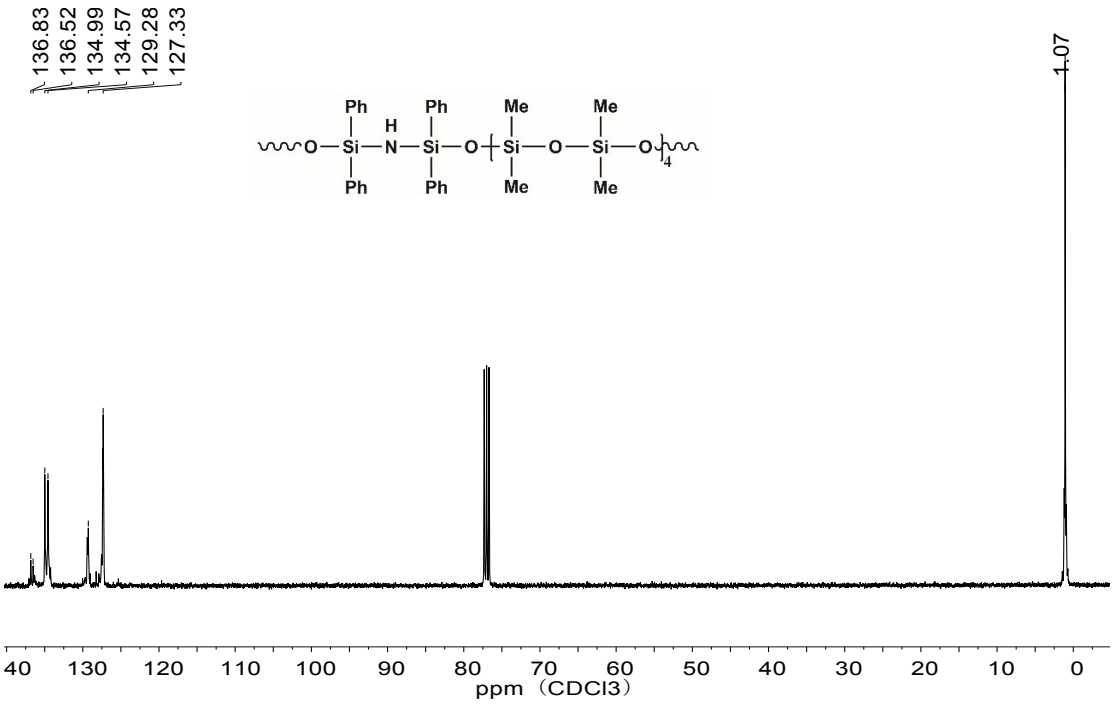
Solution of **1b** and tris(pentafluorophenyl)borane (0.5 equiv.) in toluene-d_8.

4. Copies of NMR and Gel Permeation Chromatography (GPC) Charts of Polymers

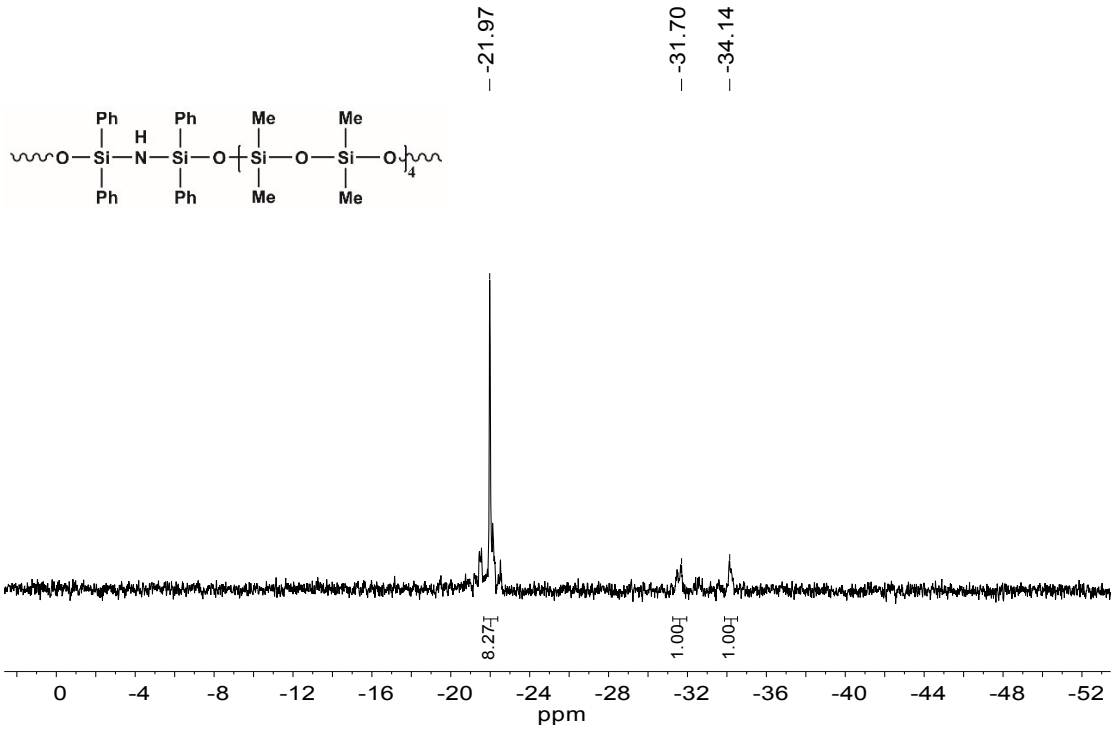
^{1}H NMR



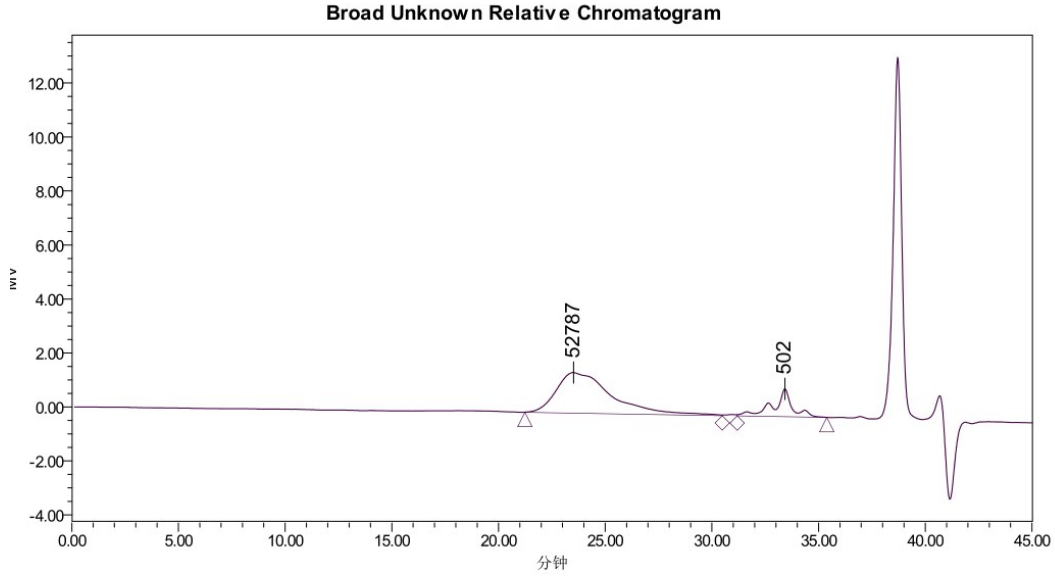
^{13}C NMR



^{29}Si NMR



Gel Permeation Chromatography (GPC) Charts of Polymers



Broad Unknown Relative Peak Table

	Distribution Name	Mn (Daltons)	Mw (Daltons)	MP (Daltons)	Mz (Daltons)	Mz+1 (Daltons)	Polydispersity	Mz/Mw	Mz+1/Mw
1		18051	44651	52787	75407	108216	2.473538	1.688819	2.423603

（Entry 8，Table 2）

5. X-ray Crystallographic Details

Crystallographic data for 4a:

Table1. Crystallographic data and refinement parameters for **4a** (see Figure 1 for structure).

Identification code	TX360
Empirical formula	$C_{60}H_{72}N_2O_3Si_6$
Formula weight	1037.73
Temperature/K	169.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.76140(10)
b/Å	13.3279(2)
c/Å	22.9045(3)
α/°	97.1130(10)
β/°	100.5090(10)
γ/°	97.9270(10)
Volume/Å^3	2867.71(7)
Z	2
ρ_{calc}g/cm^3	1.202
μ/mm^{-1}	1.710
F(000)	1108.0
Crystal size/mm^3	0.311 × 0.267 × 0.223
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.776 to 150.71
Index ranges	-12 ≤ h ≤ 12, -16 ≤ k ≤ 16, -28 ≤ l ≤ 25
Reflections collected	34331
Independent reflections	11438 [R_{int} = 0.0155, R_{sigma} = 0.0141]
Data/restraints/parameters	11438/1/665
Goodness-of-fit on F^2	1.052
Final R indexes [I>=2σ (I)]	R_1 = 0.0384, wR_2 = 0.1015
Final R indexes [all data]	R_1 = 0.0409, wR_2 = 0.1031
Largest diff. peak/hole / e Å^{-3}	0.80/-0.47

Table 2. Fractional atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å2x 10^3) for **4a**. U(eq) is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Si1	7137.6(5)	7816.0(3)	3752.2(2)	27.47(10)
Si2	3851.6(4)	7665.4(3)	3770.0(2)	22.88(9)
Si3	2744.7(4)	6221.0(3)	2527.5(2)	18.93(9)
Si4	2638.5(4)	3898.4(3)	2535.9(2)	19.98(9)
Si5	1233.5(4)	2354.0(3)	1334.5(2)	22.28(9)
Si6	3903.3(5)	2604.1(3)	738.5(2)	31.05(11)
O1	5410.9(12)	7629.6(9)	3632.1(5)	29.9(2)
O2	3262.6(11)	5104.5(8)	2532.9(5)	23.9(2)
O3	2728.6(12)	2269.6(9)	1136.2(5)	29.3(2)
N1	2674.3(15)	6797.3(11)	3228.8(6)	26.5(3)
N2	1411.5(15)	3374.2(10)	1896.1(6)	24.3(3)
C1	7588(3)	9877.1(18)	3510.5(12)	58.1(6)
C2	7754(2)	8785.7(16)	3296.8(9)	41.2(4)
C3	9456(2)	8481(2)	4748.3(12)	62.3(7)
C4	7847(2)	8269.2(16)	4568.8(8)	40.1(4)
C5	7497(4)	5735(2)	3831.1(15)	82.6(9)
C6	7737(3)	6593.6(18)	3496.9(11)	55.4(6)
C7	3356.8(17)	8968.6(12)	3768.2(7)	25.9(3)
C8	2121.3(18)	9145.4(14)	3409.7(8)	33.8(4)
C9	1735(2)	10111.4(15)	3439.9(9)	41.3(4)
C10	2582(2)	10927.3(14)	3832.1(9)	40.0(4)
C11	3814(2)	10775.1(14)	4190.9(8)	38.1(4)
C12	4193.9(18)	9812.4(13)	4158.4(8)	32.0(3)
C13	3792.5(16)	7304.4(12)	4530.9(7)	26.5(3)
C14	2937.1(19)	7732.0(16)	4886.9(8)	37.5(4)
C15	2897(2)	7477.8(17)	5454.5(9)	45.8(5)
C16	3711(2)	6789.2(15)	5676.9(8)	44.9(5)
C17	4570(2)	6357.1(15)	5335.7(8)	44.1(5)
C18	4606(2)	6611.3(13)	4767.1(8)	34.4(4)
C19	3966.2(15)	7064.0(11)	2188.4(6)	21.8(3)
C20	3781.5(18)	8082.3(12)	2173.3(7)	28.2(3)
C21	4564.6(19)	8717.6(13)	1875.5(8)	32.9(4)
C22	5559.5(18)	8347.6(13)	1586.0(8)	33.3(4)
C23	5784.4(19)	7352.4(15)	1605.7(8)	36.2(4)
C24	4991.9(18)	6712.6(13)	1902.1(7)	29.4(3)
C25	921.7(16)	6008.7(11)	2049.7(7)	23.5(3)
C26	-247.4(17)	5503.0(14)	2231.3(8)	32.8(4)

C27	-1581.7(19)	5314.1(16)	1862.4(10)	42.4(4)
C28	-1778.0(19)	5641.4(15)	1308.1(9)	41.4(4)
C29	-653(2)	6151.2(14)	1120.9(9)	39.5(4)
C30	686.6(18)	6328.6(13)	1487.8(7)	30.7(3)
C31	1792.0(16)	3831.0(11)	3204.5(7)	23.7(3)
C32	672(2)	3062.6(16)	3205.4(8)	40.8(4)
C33	76(2)	2996(2)	3708.1(9)	54.6(6)
C34	571(2)	3707.0(17)	4220.4(8)	45.0(5)
C35	1683(3)	4467.2(16)	4234.6(8)	48.5(5)
C36	2291(2)	4521.8(14)	3733.9(8)	39.4(4)
C37	4171.3(16)	3199.5(12)	2603.7(6)	24.0(3)
C38	5531.9(18)	3686.2(13)	2606.8(7)	31.0(3)
C39	6671(2)	3159.0(16)	2672.4(9)	41.5(4)
C40	6466(2)	2138.8(16)	2736.4(8)	42.1(4)
C41	5133(2)	1642.2(14)	2743.9(9)	41.1(4)
C42	3993.1(19)	2166.6(13)	2679.2(8)	33.8(4)
C43	629.9(17)	1096.8(12)	1567.9(7)	26.8(3)
C44	1272.0(19)	239.7(13)	1460.4(9)	36.5(4)
C45	749(2)	-701.2(15)	1607.5(10)	46.4(5)
C46	-412(2)	-801.4(15)	1868.1(9)	44.3(5)
C47	-1067(2)	35.3(15)	1982.7(8)	40.5(4)
C48	-560.3(19)	972.1(13)	1828.5(8)	33.2(4)
C49	-164.7(17)	2546.9(12)	697.8(7)	26.1(3)
C50	-1002(2)	1702.4(14)	310.4(8)	36.7(4)
C51	-2035(2)	1820.8(16)	-166.3(8)	41.9(4)
C52	-2269(2)	2782.7(16)	-266.5(8)	40.2(4)
C53	-1462(2)	3631.8(16)	110.0(9)	45.2(5)
C54	-424(2)	3511.6(13)	586.5(8)	36.3(4)
C55	3098(3)	2137.1(17)	-67.2(8)	51.9(5)
C56	2411(3)	1020.6(17)	-218.7(9)	52.2(5)
C57	5534(2)	2077.1(18)	1011.7(10)	49.5(5)
C58	5401(3)	943(2)	993.4(15)	72.0(8)
C59	4437(4)	4025.5(18)	866.3(11)	70.6(8)
C60	3429(5)	4640(2)	683.0(19)	69.9(14)
C60A	4513(9)	4588(6)	355(4)	53(3)

Table 3. Anisotropic Displacement Parameters (Å2×103) for **4a**. The Anisotropic displacement factor exponent takes the form: -2π2[h2a*2U11+2hka*b*U12+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1	25.8(2)	30.6(2)	26.4(2)	3.38(17)	5.01(17)	7.50(17)
Si2	24.3(2)	25.0(2)	17.10(19)	1.21(15)	3.12(15)	-0.60(15)
Si3	20.95(19)	17.82(18)	16.93(18)	3.03(14)	2.45(14)	1.03(14)
Si4	22.83(19)	18.03(18)	18.32(18)	3.29(14)	2.22(14)	2.89(14)
Si5	25.1(2)	19.94(19)	20.34(19)	0.75(15)	2.59(15)	3.39(15)
Si6	41.1(3)	28.5(2)	23.7(2)	4.54(17)	9.76(18)	1.36(18)
O1	27.7(6)	37.0(6)	24.7(5)	5.6(5)	6.0(4)	2.2(5)
O2	25.3(5)	19.5(5)	25.7(5)	5.1(4)	2.1(4)	2.0(4)
O3	30.6(6)	30.6(6)	27.8(6)	3.2(4)	8.0(5)	6.5(5)
N1	25.7(7)	29.6(7)	21.7(6)	-0.3(5)	7.5(5)	-4.3(5)
N2	24.0(6)	23.8(6)	23.7(6)	0.6(5)	1.0(5)	6.7(5)
C1	69.2(15)	49.0(12)	66.8(15)	27.7(11)	25.8(12)	13.6(11)
C2	35.0(9)	51.0(11)	38.2(10)	9.6(8)	12.9(8)	-0.7(8)
C3	41.2(12)	72.6(16)	60.6(14)	15.0(12)	-15.9(10)	-3.0(11)
C4	37.4(10)	47.9(11)	31.6(9)	5.0(8)	-0.7(7)	6.6(8)
C5	124(3)	50.3(15)	81(2)	9.6(14)	25.8(19)	33.5(16)
C6	67.6(15)	51.5(13)	51.2(12)	1.3(10)	11.1(11)	30.6(11)
C7	27.5(8)	28.9(8)	19.7(7)	1.8(6)	5.0(6)	1.0(6)
C8	32.4(9)	35.0(9)	29.2(8)	-1.6(7)	-0.2(7)	3.9(7)
C9	40.7(10)	43.2(10)	38.6(10)	4.8(8)	-0.2(8)	13.9(8)
C10	51.0(11)	30.7(9)	40.6(10)	5.1(7)	11.7(8)	11.4(8)
C11	42.5(10)	29.7(9)	37.7(9)	-3.4(7)	7.3(8)	-0.8(7)
C12	30.6(8)	32.2(8)	28.9(8)	-1.2(7)	1.4(7)	1.2(7)
C13	26.7(8)	28.6(8)	19.8(7)	0.6(6)	2.3(6)	-4.3(6)
C14	30.8(9)	53.5(11)	30.5(9)	9.7(8)	10.2(7)	6.4(8)
C15	47.0(11)	60.2(13)	33.0(10)	7.2(9)	20.8(8)	1.7(9)
C16	63.8(13)	44.6(11)	23.3(8)	8.0(7)	12.1(8)	-8.6(9)
C17	68.0(13)	33.4(9)	30.3(9)	11.2(7)	6.7(9)	5.4(9)
C18	49.8(10)	27.0(8)	26.7(8)	3.4(6)	11.2(7)	3.3(7)
C19	22.9(7)	22.3(7)	18.7(7)	3.4(5)	1.6(5)	1.4(5)
C20	33.1(8)	25.0(8)	29.6(8)	6.9(6)	11.5(7)	6.7(6)
C21	43.4(10)	22.6(8)	32.4(9)	8.0(6)	8.0(7)	1.2(7)
C22	34.1(9)	35.2(9)	29.3(8)	9.2(7)	8.6(7)	-6.1(7)
C23	34.8(9)	43.0(10)	36.0(9)	8.4(8)	17.8(7)	7.6(7)
C24	33.3(8)	27.5(8)	29.6(8)	5.6(6)	10.2(7)	6.7(6)
C25	24.8(7)	21.1(7)	23.3(7)	1.1(5)	2.3(6)	4.7(6)
C26	26.2(8)	39.0(9)	33.6(9)	7.7(7)	6.3(7)	4.6(7)

C27	23.4(8)	48.6(11)	53.0(12)	3.9(9)	7.1(8)	2.3(7)
C28	26.5(9)	41.7(10)	48.1(11)	-2.1(8)	-9.3(8)	8.7(7)
C29	40.6(10)	38.6(10)	34.2(9)	6.8(7)	-8.7(8)	10.1(8)
C30	31.8(8)	29.5(8)	27.9(8)	6.8(6)	-1.1(6)	2.5(6)
C31	26.1(7)	23.7(7)	21.2(7)	5.4(6)	2.8(6)	4.9(6)
C32	36.8(10)	50.1(11)	28.7(9)	-4.0(8)	9.6(7)	-11.3(8)
C33	42.4(11)	76.8(16)	36.3(10)	-1.0(10)	15.7(9)	-20.6(10)
C34	46.4(11)	62.8(13)	27.0(9)	6.7(8)	14.9(8)	3.5(9)
C35	72.5(14)	46.0(11)	22.0(8)	-0.3(8)	11.4(9)	-5.2(10)
C36	56.0(11)	33.2(9)	23.2(8)	3.7(7)	6.7(8)	-10.9(8)
C37	29.4(8)	24.9(7)	17.8(7)	3.8(5)	2.0(6)	7.6(6)
C38	30.7(8)	35.2(9)	30.9(8)	11.4(7)	8.9(7)	9.5(7)
C39	33.3(9)	56.0(12)	42.5(10)	17.6(9)	12.1(8)	17.4(8)
C40	45.4(11)	52.7(11)	34.4(9)	8.0(8)	6.1(8)	30.5(9)
C41	54.3(12)	29.7(9)	37.7(10)	3.8(7)	-3.1(8)	18.9(8)
C42	37.9(9)	25.8(8)	34.8(9)	6.0(7)	-1.6(7)	5.9(7)
C43	29.1(8)	23.7(7)	24.1(7)	2.2(6)	0.0(6)	1.5(6)
C44	33.6(9)	27.2(8)	49.1(11)	9.1(7)	6.4(8)	6.2(7)
C45	45.6(11)	28.4(9)	62.1(13)	13.5(9)	-2.2(9)	7.4(8)
C46	50.8(11)	32.4(9)	41.7(10)	15.3(8)	-5.2(9)	-9.7(8)
C47	43.8(10)	42.0(10)	29.7(9)	4.0(7)	6.6(8)	-11.6(8)
C48	35.9(9)	31.2(8)	28.7(8)	-1.1(7)	5.5(7)	-1.2(7)
C49	27.8(8)	27.8(8)	21.1(7)	0.5(6)	3.1(6)	4.3(6)
C50	42.4(10)	29.9(8)	31.7(9)	-1.2(7)	-2.2(7)	3.3(7)
C51	42.7(10)	45.2(11)	27.8(9)	-4.1(8)	-5.5(8)	-1.7(8)
C52	37.4(10)	56.3(12)	24.4(8)	7.7(8)	-1.8(7)	8.0(8)
C53	53.7(12)	39.2(10)	39.2(10)	10.6(8)	-5.8(9)	11.9(9)
C54	42.3(10)	28.5(8)	32.0(9)	1.8(7)	-4.7(7)	3.9(7)
C55	83.4(16)	46.1(11)	24.2(9)	7.2(8)	7.8(9)	6.2(11)
C56	63.2(14)	50.0(12)	34.3(10)	-10.6(9)	-0.4(9)	7.0(10)
C57	35.2(10)	67.2(14)	45.6(11)	0.6(10)	15.0(9)	4.6(9)
C58	55.1(15)	68.3(17)	93(2)	24.0(15)	-0.9(14)	23.4(13)
C59	112(2)	40.6(12)	47.9(13)	6.9(10)	8.8(14)	-17.5(13)
C60	81(3)	35.4(16)	78(3)	7.2(16)	-21(2)	6.4(16)
C60A	60(5)	42(4)	49(4)	22(3)	-3(4)	-12(3)

Table 4. Bond lengths [Å] and angles [°] for **4a**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Si1	O1	1.6361(12)	C19	C24	1.395(2)
Si1	C2	1.8625(19)	C20	C21	1.386(2)
Si1	C4	1.8641(19)	C21	C22	1.383(3)
Si1	C6	1.868(2)	C22	C23	1.379(3)
Si2	O1	1.6158(12)	C23	C24	1.393(2)
Si2	N1	1.7188(14)	C25	C26	1.400(2)
Si2	C7	1.8663(17)	C25	C30	1.395(2)
Si2	C13	1.8731(16)	C26	C27	1.389(2)
Si3	O2	1.6370(11)	C27	C28	1.382(3)
Si3	N1	1.7101(14)	C28	C29	1.374(3)
Si3	C19	1.8633(15)	C29	C30	1.392(2)
Si3	C25	1.8758(15)	C31	C32	1.392(2)
Si4	O2	1.6398(10)	C31	C36	1.393(2)
Si4	N2	1.7164(13)	C32	C33	1.389(3)
Si4	C31	1.8738(16)	C33	C34	1.379(3)
Si4	C37	1.8617(16)	C34	C35	1.372(3)
Si5	O3	1.6197(12)	C35	C36	1.389(3)
Si5	N2	1.7186(13)	C37	C38	1.394(2)
Si5	C43	1.8721(16)	C37	C42	1.400(2)
Si5	C49	1.8759(16)	C38	C39	1.390(2)
Si6	O3	1.6383(12)	C39	C40	1.377(3)
Si6	C55	1.861(2)	C40	C41	1.380(3)
Si6	C57	1.863(2)	C41	C42	1.389(3)
Si6	C59	1.866(2)	C43	C44	1.394(2)
C1	C2	1.517(3)	C43	C48	1.399(2)
C3	C4	1.526(3)	C44	C45	1.392(3)
C5	C6	1.469(4)	C45	C46	1.373(3)
C7	C8	1.396(2)	C46	C47	1.381(3)
C7	C12	1.401(2)	C47	C48	1.390(3)
C8	C9	1.388(3)	C49	C50	1.399(2)
C9	C10	1.383(3)	C49	C54	1.389(2)
C10	C11	1.382(3)	C50	C51	1.386(3)
C11	C12	1.381(3)	C51	C52	1.372(3)
C13	C14	1.397(2)	C52	C53	1.382(3)
C13	C18	1.395(2)	C53	C54	1.388(3)
C14	C15	1.389(3)	C55	C56	1.515(3)
C15	C16	1.379(3)	C57	C58	1.494(4)
C16	C17	1.381(3)	C59	C60	1.404(5)

C17	C18	1.391(2)	C59	C60A	1.474(7)
C19	C20	1.397(2)			

Table 5. Bond Angles for **4a**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Si1	C2	109.28(8)	C16	C15	C14	120.05(18)
O1	Si1	C4	108.74(8)	C15	C16	C17	119.87(17)
O1	Si1	C6	109.15(10)	C16	C17	C18	120.00(19)
C2	Si1	C4	110.61(9)	C17	C18	C13	121.32(17)
C2	Si1	C6	107.64(10)	C20	C19	Si3	118.91(11)
C4	Si1	C6	111.40(10)	C24	C19	Si3	123.37(12)
O1	Si2	N1	107.64(7)	C24	C19	C20	117.50(14)
O1	Si2	C7	112.28(7)	C21	C20	C19	121.55(15)
O1	Si2	C13	109.51(7)	C22	C21	C20	119.95(15)
N1	Si2	C7	109.96(7)	C23	C22	C21	119.62(15)
N1	Si2	C13	109.88(7)	C22	C23	C24	120.41(16)
C7	Si2	C13	107.57(7)	C23	C24	C19	120.95(15)
O2	Si3	N1	112.66(6)	C26	C25	Si3	121.87(12)
O2	Si3	C19	108.91(6)	C30	C25	Si3	120.83(12)
O2	Si3	C25	107.71(6)	C30	C25	C26	117.28(15)
N1	Si3	C19	110.02(7)	C27	C26	C25	121.26(17)
N1	Si3	C25	108.15(7)	C28	C27	C26	119.98(18)
C19	Si3	C25	109.32(7)	C29	C28	C27	120.06(16)
O2	Si4	N2	112.25(6)	C28	C29	C30	119.90(17)
O2	Si4	C31	107.89(6)	C29	C30	C25	121.51(16)
O2	Si4	C37	106.90(6)	C32	C31	Si4	121.64(12)
N2	Si4	C31	109.17(7)	C32	C31	C36	116.70(15)
N2	Si4	C37	110.14(7)	C36	C31	Si4	121.61(12)
C37	Si4	C31	110.45(7)	C33	C32	C31	121.52(17)
O3	Si5	N2	110.79(7)	C34	C33	C32	120.36(19)
O3	Si5	C43	106.55(7)	C35	C34	C33	119.39(17)
O3	Si5	C49	112.49(7)	C34	C35	C36	120.05(18)
N2	Si5	C43	112.75(7)	C35	C36	C31	121.95(17)
N2	Si5	C49	107.00(7)	C38	C37	Si4	121.86(12)
C43	Si5	C49	107.29(7)	C38	C37	C42	117.78(15)
O3	Si6	C55	107.88(9)	C42	C37	Si4	120.30(13)
O3	Si6	C57	108.62(8)	C39	C38	C37	121.13(17)
O3	Si6	C59	110.43(11)	C40	C39	C38	120.02(18)
C55	Si6	C57	113.73(11)	C39	C40	C41	120.04(17)
C55	Si6	C59	110.34(10)	C40	C41	C42	120.09(17)

C57	Si6	C59	105.84(13)	C41	C42	C37	120.92(17)
Si2	O1	Si1	158.40(8)	C44	C43	Si5	122.51(13)
Si3	O2	Si4	140.64(7)	C44	C43	C48	117.32(15)
Si5	O3	Si6	150.74(8)	C48	C43	Si5	120.06(12)
Si3	N1	Si2	133.44(9)	C45	C44	C43	121.23(18)
Si4	N2	Si5	135.85(9)	C46	C45	C44	120.34(19)
C1	C2	Si1	115.24(14)	C45	C46	C47	119.76(17)
C3	C4	Si1	114.63(16)	C46	C47	C48	120.05(18)
C5	C6	Si1	117.91(19)	C47	C48	C43	121.29(17)
C8	C7	Si2	122.59(12)	C50	C49	Si5	120.30(13)
C8	C7	C12	116.96(15)	C54	C49	Si5	122.72(12)
C12	C7	Si2	120.36(12)	C54	C49	C50	116.98(15)
C9	C8	C7	121.60(16)	C51	C50	C49	121.62(17)
C10	C9	C8	119.97(17)	C52	C51	C50	120.21(17)
C11	C10	C9	119.67(17)	C51	C52	C53	119.49(17)
C12	C11	C10	120.12(17)	C52	C53	C54	120.21(18)
C11	C12	C7	121.68(16)	C53	C54	C49	121.49(17)
C14	C13	Si2	120.90(13)	C56	C55	Si6	115.93(14)
C18	C13	Si2	121.66(12)	C58	C57	Si6	117.57(16)
C18	C13	C14	117.43(15)	C60	C59	Si6	119.1(2)
C15	C14	C13	121.34(18)	C60A	C59	Si6	120.5(4)

Table 6. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **4a**.

Atom	***x***	***y***	***z***	**U(eq)**
H1A	8003.94	10329.59	3272.22	87
H1B	8051.4	10072.34	3924.48	87
H1C	6601.94	9920.14	3470.09	87
H2A	8744.27	8771.19	3295.19	49
H2B	7236.23	8586.94	2885.42	49
H3A	9823.24	8992.34	4531.36	93
H3B	9821.19	7861.06	4654.51	93
H3C	9734.25	8722.89	5171.94	93
H4A	7489.47	8892.51	4683.93	48
H4B	7489.44	7756.47	4793.6	48
H5A	7932.92	5181.59	3680.32	124
H5B	6500.07	5506.24	3781.54	124
H5C	7900.38	5955.93	4249.68	124
H6A	7271.49	6362.76	3080.57	67
H6B	8741.96	6746.28	3506.59	67
H8	1543.09	8602.55	3144.29	41

H9	906.68	10210.04	3196.5	50
H10	2324.87	11575.06	3854.25	48
H11	4387.21	11321.99	4454.8	46
H12	5027.02	9721.97	4401.82	38
H14	2382.84	8196.34	4741.06	45
H15	2322.01	7772.25	5684.62	55
H16	3680.7	6616.08	6055.95	54
H17	5123.87	5896.09	5485.97	53
H18	5184.02	6313.23	4539.88	41
H20	3117.44	8339.84	2367.65	34
H21	4421.07	9392.16	1870.42	39
H22	6074	8767.57	1379.19	40
H23	6469.45	7106.99	1420	43
H24	5149.03	6041.24	1909.21	35
H26	-128.23	5289.37	2606.16	39
H27	-2342.82	4967.6	1988.28	51
H28	-2671.91	5516.49	1061.55	50
H29	-787.2	6377.29	749.6	47
H30	1442.51	6668.1	1355.34	37
H32	314.84	2582.88	2861.33	49
H33	-661.93	2467.79	3699.18	66
H34	155.18	3671.81	4553.32	54
H35	2029.79	4946.51	4579.62	58
H36	3054.45	5034.91	3752.74	47
H38	5680.48	4375.38	2564.24	37
H39	7571.69	3495.57	2673.1	50
H40	7225.68	1784.05	2774.54	51
H41	4997.74	955.39	2792.44	49
H42	3098.94	1826.85	2686.05	41
H44	2064.61	297.56	1287.23	44
H45	1189.01	-1264.95	1528.71	56
H46	-756.41	-1430.62	1967.22	53
H47	-1847.85	-28.2	2163.27	49
H48	-1021.24	1527.08	1899.95	40
H50	-860.73	1045.35	374.27	44
H51	-2572.23	1246.5	-419.16	50
H52	-2965.33	2862.65	-585.4	48
H53	-1613.82	4285.85	43.9	54
H54	109.06	4089.93	836.86	44
H55A	2391.81	2553.57	-194.74	62

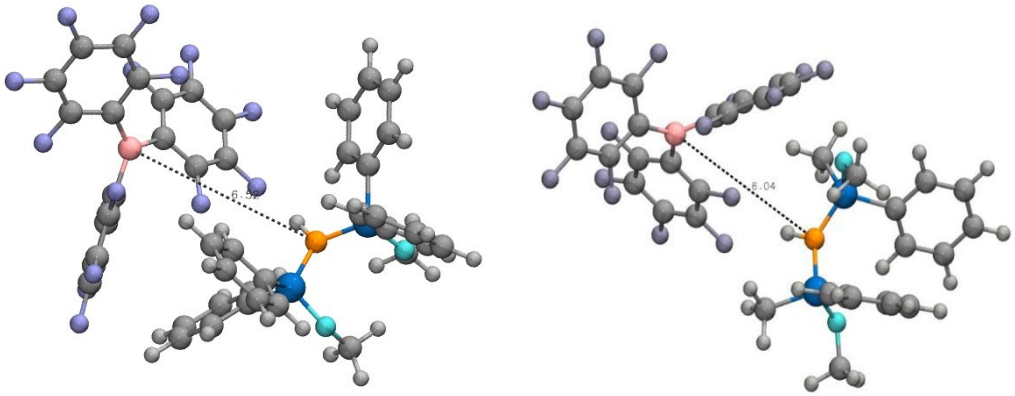
H55B	3826.61	2246.32	-300.17	62
H56A	1959.58	871.32	-635.87	78
H56B	1719.24	889.83	23.43	78
H56C	3117.74	593.46	-139.74	78
H57A	6224.16	2285.13	775.97	59
H57B	5914.17	2398.26	1423.99	59
H58A	5088.3	609.26	584.9	108
H58B	4726.56	719	1226.74	108
H58C	6301.65	772.17	1156.62	108
H59A	4801.17	4238.91	1293.55	85
H59B	5216.97	4181.41	665.77	85
H59C	3786.99	4313.04	1086.73	85
H59D	5361.76	4181.11	1130.24	85
H60A	2956.92	4385.83	275.04	105
H60B	3890.09	5333.13	710.34	105
H60C	2750.52	4619.62	938.34	105
H60D	5362.96	4505.45	212.87	79
H60E	4516.28	5302.47	482.11	79
H60F	3709.12	4322.46	37.59	79
H2	770(20)	3631(17)	1870(10)	37(6)
H1	2040(30)	6650(20)	3328(12)	54(8)

Table 7. Atomic Occupancy for **4a**

Atom	***Occupancy***	**Atom**	***Occupancy***	**Atom**	***Occupancy***
H59A	0.715(6)	H59B	0.715(6)	H59C	0.285(6)
H59D	0.285(6)	C60	0.715(6)	H60A	0.715(6)
H60B	0.715(6)	H60C	0.715(6)	C60A	0.285(6)
H60D	0.285(6)	H60E	0.285(6)	H60F	0.285(6)

6. Computational Details

All computations were performed using the hybrid density functional method B3LYP as implemented in the Gaussian16 program.[4] For all elements (B, C, H, N, O ,Si and F) the allelectron double-ζ basis set (6-31G*) was used.



The optimized structures of the 1a with $B(C_6F_5)_3$(right), and 1b with $B(C_6F_5)_3$(left).

Table 8. Cartesian coordinates of optimized ground state structures of **1a**, **1b** and $B(C_6F_5)_3$ at B3LYP/6-31G* level, respectively.

	1a+$B(C_6F_5)_3$				**1b**+$B(C_6F_5)_3$		
B	-3.255046	0.273185	-0.334455	B	-3.04162	0.063512	-0.364571
C	-2.391195	1.174094	-1.289913	C	-4.450793	0.340808	0.268923
C	-2.870544	2.371392	-1.842623	C	-5.241351	1.437418	-0.107852
C	-1.084092	0.828283	-1.662835	C	-5.012118	-0.493165	1.24793
C	-2.123485	3.166717	-2.704101	C	-6.497113	1.689864	0.430427
C	-0.308917	1.598433	-2.51808	C	-6.255512	-0.261331	1.822688
C	-0.829293	2.778239	-3.039477	C	-7.004394	0.835811	1.405909
C	-3.119321	-1.287862	-0.433233	C	-2.587575	-1.416949	-0.639081
C	-2.977699	-1.952135	-1.660213	C	-1.265545	-1.845292	-0.454356
C	-3.074791	-2.108841	0.702271	C	-3.474515	-2.405717	-1.090779
C	-2.798526	-3.325154	-1.762246	C	-0.845318	-3.146261	-0.69374
C	-2.871174	-3.481867	0.641567	C	-3.087295	-3.714664	-1.354387
C	-2.732121	-4.091599	-0.602226	C	-1.761948	-4.088984	-1.150374
C	-4.222033	0.91903	0.715833	C	-2.083405	1.252811	-0.717811
C	-3.929931	2.126766	1.370214	C	-1.234009	1.232834	-1.835561
C	-5.441833	0.323626	1.076154	C	-1.996716	2.408489	0.074646

C	-4.769743	2.701719	2.315657	C	-0.36706	2.268223	-2.156937
C	-6.315169	0.879868	2.002356	C	-1.123981	3.453493	-0.200596
C	-5.972552	2.074606	2.629671	C	-0.307615	3.382571	-1.325768
F	-2.779598	2.772903	1.118266	N	2.88095	-1.048198	-0.01754
F	-4.435897	3.84557	2.923479	H	2.048723	-1.583054	-0.262201
F	-6.793569	2.616732	3.527812	Si	3.253286	0.107156	-1.270911
F	-7.474813	0.281047	2.29644	Si	3.470709	-1.538427	1.541457
F	-5.831909	-0.825183	0.499283	C	4.174712	-0.110711	2.552114
F	-4.11662	2.790308	-1.566995	C	5.517286	0.291871	2.416716
F	-2.632847	4.295174	-3.209729	C	3.379056	0.580913	3.485607
F	-0.089759	3.534814	-3.852075	C	6.037359	1.349154	3.166647
F	0.939706	1.218501	-2.833234	H	6.165089	-0.224712	1.713264
F	-0.502934	-0.281441	-1.170183	C	3.893294	1.637477	4.239859
F	-2.520928	-5.405987	-0.685827	H	2.340006	0.2927	3.631047
F	-2.665534	-3.913993	-2.956627	C	5.225171	2.025394	4.079156
F	-3.026999	-1.259125	-2.811292	H	7.076372	1.643186	3.039769
F	-2.799726	-4.213706	1.758385	H	3.257087	2.155158	4.953723
F	-3.177498	-1.5672	1.931553	H	5.628787	2.847406	4.665145
Si	4.490707	1.083401	0.0865	C	5.113456	0.287819	-1.509009
N	3.258173	-0.054998	-0.395944	C	6.006959	-0.780091	-1.300459
H	2.480144	0.353495	-0.909608	C	5.641929	1.494854	-2.006538
Si	3.079884	-1.767768	-0.083769	C	7.37062	-0.645515	-1.573706
C	3.786858	2.811701	-0.211795	C	7.003886	1.634704	-2.279408
C	3.101231	3.137282	-1.398691	H	4.977983	2.338224	-2.182545
C	3.956361	3.83535	0.739073	C	7.871953	0.562428	-2.063026
C	2.59637	4.419499	-1.623083	H	8.04184	-1.484085	-1.4036
H	2.94881	2.381259	-2.164115	H	7.387482	2.578471	-2.659734
C	3.458401	5.12165	0.519462	H	8.933159	0.66766	-2.275529
H	4.479658	3.625411	1.668396	C	2.042468	-2.369022	2.445631
C	2.774546	5.41617	-0.661254	H	1.671775	-3.223799	1.866509
H	2.057167	4.633989	-2.542512	H	2.341056	-2.742017	3.43271
H	3.601122	5.892502	1.272804	H	1.198338	-1.684547	2.592045
H	2.381962	6.415695	-0.830821	O	4.704923	-2.644683	1.286274
C	5.047406	0.850539	1.860317	O	2.614211	1.633339	-1.016312
C	6.412596	0.841858	2.202401	C	2.40812	-0.480718	-2.841165

C	4.107992	0.731573	2.901938	H	1.319693	-0.542051	-2.726041
C	6.823311	0.717074	3.53068	H	2.609676	0.205872	-3.671065
H	7.157847	0.927796	1.416977	H	2.775686	-1.472297	-3.132387
C	4.514106	0.60858	4.231858	C	2.904106	2.478813	0.08905
H	3.044674	0.72284	2.67515	H	2.55885	3.488028	-0.159664
C	5.874061	0.601581	4.548264	H	2.381588	2.142878	0.993486
H	7.883668	0.70852	3.771418	H	3.978045	2.524908	0.30918
H	3.769826	0.511897	5.018233	C	5.346181	-3.358537	2.333832
H	6.192649	0.504252	5.583327	H	4.673616	-4.101393	2.785323
C	2.091636	-2.494918	-1.518803	H	6.204954	-3.889678	1.908891
C	2.108054	-1.92854	-2.807323	H	5.7125	-2.692482	3.127181
C	1.321602	-3.659454	-1.331274	H	5.63771	-1.722526	-0.904947
C	1.38434	-2.492914	-3.860176	F	-4.809294	2.29088	-1.051481
H	2.688149	-1.027804	-2.991858	F	-7.21865	2.74053	0.023364
C	0.593102	-4.22754	-2.377678	F	-8.20303	1.068324	1.939871
H	1.279539	-4.123952	-0.348949	F	-6.737284	-1.07814	2.766727
C	0.620855	-3.641822	-3.645768	F	-4.332253	-1.562528	1.69719
H	1.412018	-2.033306	-4.84525	F	-4.763834	-2.104301	-1.3188
H	-0.008711	-5.11551	-2.200381	F	-3.972269	-4.613224	-1.799651
H	0.04731	-4.077208	-4.459912	F	-1.37329	-5.33979	-1.391897
C	2.214499	-2.171534	1.537666	F	0.434602	-3.499282	-0.493402
C	2.84574	-2.911878	2.552987	F	-0.328714	-0.986603	-0.006442
C	0.888858	-1.752318	1.761251	F	-1.236594	0.174463	-2.668661
C	2.181575	-3.21932	3.742904	F	0.41167	2.197276	-3.23873
H	3.868831	-3.246391	2.40864	F	0.538751	4.376045	-1.59717
C	0.217258	-2.062102	2.945119	F	-1.05958	4.521861	0.603341
H	0.366293	-1.181163	0.997003	F	-2.751266	2.531574	1.18088
C	0.865544	-2.797858	3.940244				
H	2.691313	-3.79127	4.51454				
H	-0.812862	-1.743428	3.083105				
H	0.345169	-3.043446	4.8628				
O	5.910021	0.8948	-0.78172				
C	6.027162	1.101276	-2.181118				
H	5.348666	0.448564	-2.747818				
H	5.820594	2.144823	-2.453708				

H	7.055586	0.865628	-2.475434
O	4.569283	-2.48254	0.090298
C	5.558431	-2.609512	-0.925063
H	6.12633	-1.67872	-1.030354
H	6.244866	-3.409922	-0.628238
H	5.118184	-2.876564	-1.895197

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