Electronic Supplementary Information (ESI) for:

**Synthesis of Structured Polysiloxazanes via Piers–Rubinsztajn Reaction**

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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$_6$F$_5$)$_3$ (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$_3$SiH (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$_6$F$_5$)$_3$ (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
2. Characterization Data

1,1,3,3-tetraphenyl-N\textsuperscript{1},N\textsuperscript{3}-bis(3,3,3-triethyl-1,1-diphenyldisiloxanyl)disiloxane-1,3-diamine (4a)

\[ \text{Et}_3\text{Si} \overset{\text{O}}{\text{S}} \text{N} \overset{\text{O}}{\text{Si}} \text{Et}_3 \]

\(^1\text{H} \text{NMR (400 MHz, CDCl}_3) \) \( \delta \) 7.52 – 6.81 (m, 40H), 1.70 (s, 2H), 0.67 (t, \( J = 7.9 \text{ Hz}, 18\text{H} \)), 0.31 (q, \( J = 7.8 \text{ Hz}, 12\text{H} \)). \(^{13}\text{C} \text{NMR (126 MHz, CDCl}_3) \) \( \delta \) 136.95, 136.39, 134.93, 134.54, 129.37, 129.22, 127.30, 127.26, 6.84, 6.24. \(^{29}\text{Si} \text{NMR (79 MHz, CDCl}_3) \) \( \delta \) 11.27, -32.11, -34.84. HRMS (MOLDI-TOF) m/z: calcd. for C\textsubscript{60}H\textsubscript{61}N\textsubscript{2}O\textsubscript{3}Si\textsubscript{6}[M + H]\(^+\): 1025.32978; found: 1025.329200.

N\textsuperscript{1}-(methoxydiphenylsilyl)-1,1,3,3-tetraphenyl-N\textsuperscript{3}-(3,3,3-triethyl-1,1-diphenyldisiloxanyl)disiloxane-1,3-diamine (2a)

\[ \text{Et}_3\text{Si} \overset{\text{O}}{\text{S}} \text{N} \overset{\text{O}}{\text{Si}} \text{Et}_3 \]

\(^1\text{H} \text{NMR (400 MHz, CDCl}_3) \) \( \delta \) 7.60 – 7.00 (m, 40H), 3.28 (s, 3H), 1.96 (s, 1H), 1.80 (s, 1H), 0.76 (t, \( J = 7.9 \text{ Hz}, 9\text{H} \)), 0.40 (q, \( J = 7.9 \text{ Hz}, 6\text{H} \)). \(^{13}\text{C} \text{NMR (126 MHz, CDCl}_3) \) \( \delta \) 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\textsubscript{55}H\textsubscript{60}N\textsubscript{2}NaO\textsubscript{3}Si\textsubscript{5}[M + Na]\(^+\): 959.33480; found: 959.333974.

1,1,3,3-tetraphenyl-N\textsuperscript{1}-(1,1,3,3-tetraphenyl-3-((3,3,3-triethyl-1,1-diphenyldisiloxanyl)amino)disiloxanyl)-N\textsuperscript{3}-(3,3,3-triethyl-1,1-diphenyldisiloxanyl)disiloxane-1,3-diamine (5a)

\[ \text{Et}_3\text{Si} \overset{\text{O}}{\text{S}} \text{N} \overset{\text{O}}{\text{Si}} \text{Et}_3 \]

\(^1\text{H} \text{NMR (400 MHz, CDCl}_3) \) \( \delta \) 7.35 – 6.80 (m, 60H), 1.68 (s, 1H), 1.58 (s, 1H), 1.46 (s, 1H), 0.66 (t, \( J = 8.0 \text{ Hz}, 18\text{H} \)), 0.29 (q, \( J = 8.0 \text{ Hz}, 12\text{H} \)). \(^{13}\text{C} \text{NMR (126 MHz, CDCl}_3) \) \( \delta \) 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\textsubscript{84}H\textsubscript{94}N\textsubscript{3}O\textsubscript{4}Si\textsubscript{8}[M + H]\(^+\): 1432.53985; found: 1432.538936.

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

\[ \text{Ph} \overset{\text{O}}{\text{Si}} \overset{\text{O}}{\text{S}} \text{N} \overset{\text{O}}{\text{Si}} \text{Et}_3 \]

\(^1\text{H} \text{NMR (400 MHz, CDCl}_3) \) \( \delta \) 7.56 – 7.06 (m, 20H), 6.09 – 5.84 (m, 12H), 5.82 – 5.56 (m, 6H), 1.94 (s, 1H). \(^{13}\text{C} \text{NMR (126 MHz, CDCl}_3) \) \( \delta \) 136.50, 135.28, 134.90, 134.70, 129.42, 127.34. \(^{29}\text{Si} \text{NMR (79 MHz, CDCl}_3) \) \( \delta \) -24.77, -31.36. HRMS (MOLDI-TOF) m/z: calcd. for C\textsubscript{36}H\textsubscript{46}NO\textsubscript{2}Si\textsubscript{4}[M + H]\(^+\): 695.333974; found: 695.333974.

dimethoxydisilazane and oligosiloxane.
\[ + \text{H}^+ \] found: 630.21361; found: 630.213671.

\[ \text{N}^1,\text{N}^3-\text{bis}(1,1-\text{diphenyl-3,3,3-trivinyldisiloxanyl}-1,1,3,3-\text{tetr phenyldisiloxane-1,3-diamine} \]

\[ \text{N}^1,\text{N}^3-\text{bis}(1,1-\text{diphenyl-3,3,3-trivinyldisiloxanyl}-1,1,3,3-\text{tetr phenyldisiloxane-1,3-diamine} \]

\[ \text{V}_{3}\text{Si} \equiv \text{O} \quad \text{Si} \quad \text{N} \quad \text{Si} \quad \text{O} \quad \text{SiV}_{3} \]

\[ ^1\text{H} \text{ NMR} (400 \text{ MHz, CDCl}_3) \delta 7.53 - 6.90 \text{ (m, 40H)}, 6.08 - 5.77 \text{ (m, 12H)}, 5.74 - 5.44 \text{ (m, 6H), 1.75 (s, 1H), 1.21 (s, 1H).} \quad ^{13}\text{C} \text{ NMR} (126 \text{ MHz, CDCl}_3) \delta 136.43, 136.26, 135.23, 134.98, 134.87, 134.73, 134.61, 129.39, 129.33, 127.34, 127.29. \text{ HRMS (MOLDI-TOF) m/z: calcd. for C}_{60}\text{H}_{73}\text{N}_{2}\text{O}_{3}\text{Si}_{6}[M+ \text{H}]^+: 1037.42368; \text{ found: 1037.423871.} \]

\[ \text{Bis}(3,3-\text{dimethyl-1,1-diphenyl-3-vinyl disiloxanyl)amine} \]

\[ \text{N}^1,\text{N}^3-\text{bis}(1,1-\text{diphenyl-3,3,3-trivinyldisiloxanyl)-1,1,3,3-tetraphen yldisiloxane-1,3-diamine} \]

\[ \text{V}_{3}\text{Si} \equiv \text{O} \quad \text{Si} \quad \text{N} \quad \text{Si} \quad \text{O} \quad \text{SiV}_{3} \]

\[ ^1\text{H} \text{ NMR} (400 \text{ MHz, CDCl}_3) \delta 7.56 - 7.04 \text{ (m, 20H)}, 5.99 (dd, \text{J} = 20.3, 14.9 \text{ Hz, 2H}), 5.81 (dd, \text{J} = 14.9, 4.0 \text{ Hz, 2H}), 5.59 (dd, \text{J} = 20.3, 4.0 \text{ Hz, 2H}), 1.86 (s, 1H), 0.00 (s, 12H). \quad ^{13}\text{C} \text{ NMR} (126 \text{ MHz, CDCl}_3) \delta 138.96, 136.82, 134.32, 131.54, 129.13, 127.13. \quad ^{29}\text{Si} \text{ NMR} (79 \text{ MHz, CDCl}_3) \delta -1.74, -31.92. \text{ HRMS (MOLDI-TOF) m/z: calcd. for C}_{32}\text{H}_{40}\text{NO}_{2}\text{Si}_{4}[M+ \text{H}]^+: 582.21361; \text{ found: 582.213002.} \]

\[ \text{N}^1,\text{N}^3-\text{bis}(3,3-\text{dimethyl-1,1,3-triphenyldisiloxanyl)-1,1,3,3-tetraphenyl disiloxane-1,3-diamine} \]

\[ \text{N}^1,\text{N}^3-\text{bis}(3,3-\text{dimethyl-1,1,3-triphenyldisiloxanyl)-1,1,3,3-tetraphenyl disiloxane-1,3-diamine} \]

\[ \text{V}_{3}\text{Si} \equiv \text{O} \quad \text{Si} \quad \text{N} \quad \text{Si} \quad \text{O} \quad \text{SiV}_{3} \]

\[ ^1\text{H} \text{ NMR} (400 \text{ MHz, CDCl}_3) \delta 7.36 - 6.79 \text{ (m, 30H)}, 1.70 (s, 1H), 0.00 (s, 12H). \quad ^{13}\text{C} \text{ NMR} (126 \text{ MHz, CDCl}_3) \delta 139.40, 136.79, 134.61, 133.18, 129.40, 129.20, 127.64 (d, \text{J} = 1.9 \text{ Hz}), 127.41, 0.67. \quad ^{29}\text{Si} \text{ NMR} (79 \text{ MHz, CDCl}_3) \delta -1.34, -32.88. \text{ HRMS (MOLDI-TOF) m/z: calcd. for C}_{40}\text{H}_{34}\text{NO}_{2}\text{Si}_{4}[M+ \text{H}]^+: 682.24491; \text{ found: 682.244418.} \]

\[ \text{N}^1,\text{N}^3-\text{bis}(3,3-\text{dimethyl-1,1,3-triphenyldisiloxanyl)-1,1,3,3-tetraphenyl disiloxane-1,3-diamine} \]
$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.34 – 6.81 (m, 50H), 1.63 (s, 1H), 1.40 (s, 1H), 0.00 (s, 12H). $^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$ 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$_3$) $\delta$ -1.54, -32.05, -33.41. HRMS (MOLDI-TOF) m/z: calcd. for C$_{64}$H$_{65}$N$_2$O$_3$Si$_6$ [M + H]$^+$: 1077.36108; found: 1077.361040.

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

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 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$_3$) $\delta$ 138.91, 133.35, 132.21, 129.92, 127.81, 0.26, -0.95. $^{29}$Si NMR (79 MHz, CDCl$_3$) $\delta$ -2.42, -24.33. HRMS (ESI) m/z: calcd. for C$_{22}$H$_{36}$NO$_2$Si$_4$ [M + H]$^+$: 458.18176; found: 458.1812.

$^1$H NMR (400 MHz, Acetone-$d_6$) $\delta$ 7.79 – 6.92 (m, 20H), 1.30 (s, 1H), 0.23 – -0.15 (m, 48H). $^{13}$C NMR (126 MHz, CDCl$_3$) $\delta$ 136.83, 136.52, 134.99, 134.57, 129.28, 127.33, 1.07. $^{29}$Si NMR (79 MHz, CDCl$_3$) $\delta$ -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

$^1$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
$^{13}\text{C} \text{ NMR}$

$^{29}\text{Si} \text{ NMR}$
High-resolution MALDI-TOF-MS
m/z: for [M + H]$^+$ = 977.32969

$^1$H NMR

![NMR Spectrogram]
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
High-resolution ESI-MS

m/z: for [M + H]^+ = 458.18121

\[ C_{20}H_{30}O_2N_4S_4 \] = 458.18176

-1.19713 ppm

\[ 19F \text{NMR} \]

-135.1C
-155.15
-163.00
Tris(pentafluorophenyl)borane in toluene-d₈.

Solution of 1a and tris(pentafluorophenyl)borane (0.5 equiv.) in toluene-d₈.

Solution of 1b and tris(pentafluorophenyl)borane (0.5 equiv.) in toluene-d₈.
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

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<th>Distribution Name</th>
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<th>Mw (Daltons)</th>
<th>MP (Daltons)</th>
<th>Mz (Daltons)</th>
<th>Mz+1 (Daltons)</th>
<th>Polymersality</th>
<th>Mz/Mw</th>
<th>Mz+1/Mw</th>
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<td>1.88886</td>
<td>2.42903</td>
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(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).

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<th>Value</th>
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<td>Empirical formula</td>
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<td>Radiation</td>
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<td>2θ range for data collection/°</td>
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<tr>
<td>Index ranges</td>
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<td>Reflections collected</td>
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<tr>
<td>Independent reflections</td>
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<td>Goodness-of-fit on F²</td>
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<td>Final R indexes [I&gt;=2σ (I)]</td>
<td>R₁ = 0.0384, wR₂ = 0.1015</td>
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<td>Final R indexes [all data]</td>
<td>R₁ = 0.0409, wR₂ = 0.1031</td>
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<td>Largest diff. peak/hole / e Å⁻³</td>
<td>0.80/-0.47</td>
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Table 2. Fractional atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å² x 10^3) for 4a. U(eq) is defined as one-third of the trace of the orthogonalized Uᵢⱼ tensor.

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<th>Atom</th>
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<td>Si3</td>
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<td>1334.5(2)</td>
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<td>Si6</td>
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<td>2604.1(3)</td>
<td>738.5(2)</td>
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<td>3632.1(5)</td>
<td>29.9(2)</td>
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<td>5104.5(8)</td>
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<td>23.9(2)</td>
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Table 7. Atomic Occupancy for 4a
6. Computational Details

All computations were performed using the hybrid density functional method B3LYP as implemented in the Gaussian16 program. 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(C₆F₅)₃(right), and 1b with B(C₆F₅)₃(left).

Table 8. Cartesian coordinates of optimized ground state structures of 1a, 1b and B(C₆F₅)₃ at B3LYP/6-31G* level, respectively.

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7. References