

**Supporting Information for:**

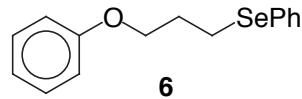
# **Dendrimeric Catalysts for the Activation of Hydrogen Peroxide. Increasing Activity per Catalytic Phenylseleno Group in Successive Generations**

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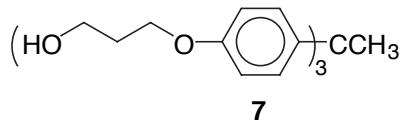
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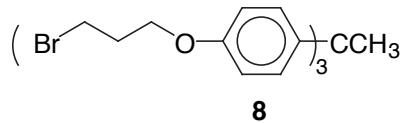
Spectral and analytical data for the compounds of this study.



For **6**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  7.52 (d, 2 H,  $J = 8$  Hz), 7.24-7.30 (m, 5 H), 6.95 (t, 1 H,  $J = 7$  Hz), 6.89 (d, 2 H,  $J = 8$  Hz), 4.06 (t, 2 H,  $J = 6$  Hz), 3.11 (t, 2 H,  $J = 6$  Hz), 2.18 (quint, 2 H,  $J = 5$  Hz);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  158.68, 132.37, 129.99, 129.33, 128.97, 126.70, 120.59, 114.36, 66.55, 29.64, 23.63; IR (NaCl) 3055, 2940, 1600, 1585, 1495, 1475, 1245, 1170, 1030, 755, 690  $\text{cm}^{-1}$ ; (+)FABMS,  $m/z$  292 ( $\text{C}_{15}\text{H}_{16}\text{O}^{80}\text{Se}$ ). **Anal.** Calcd for  $\text{C}_{15}\text{H}_{16}\text{OSe}$ : C, 61.86; H, 5.54. Found: C, 61.76; H, 5.49.

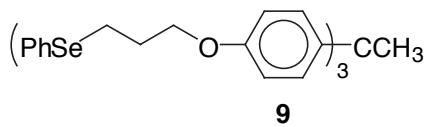


For **7**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  6.89 (d, 6 H,  $J = 9$  Hz), 6.80 (d, 6 H,  $J = 9$  Hz), 4.51 (t, 3 H,  $J = 5.1$  Hz,  $\text{D}_2\text{O}$ -exchangable), 3.98 (t, 6 H,  $J = 6$  Hz), 3.53 (quartet, 6 H,  $J = 6$  Hz), 2.01 (s, 3 H), 1.83 (quintet, 6 H,  $J = 6$  Hz);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  156.63, 141.25, 129.16, 113.65, 64.52, 57.38, 50.14, 32.22, 30.41; (+)FABMS,  $m/z$  481 ( $\text{C}_{29}\text{H}_{37}\text{O}_6$ , M + 1). **Anal.** Calc for  $\text{C}_{29}\text{H}_{36}\text{O}_6$ : C, 72.49; H, 7.55. Found: C, 72.07; H, 7.53.



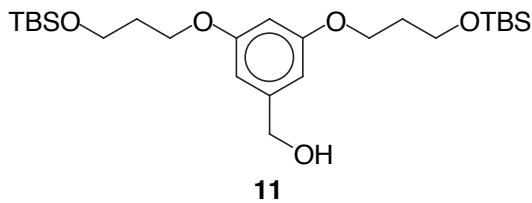
For **8**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  6.97 (d, 6 H,  $J = 9$  Hz), 6.77 (d, 6 H,  $J = 9$  Hz), 4.06 (t, 6 H,  $J = 6$  Hz), 3.58 (t, 6 H,  $J = 6$  Hz), 2.29 (quintet, 6 H,  $J = 6$  Hz), 2.08 (s, 3 H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  156.77, 142.09, 129.65, 113.81, 65.40, 50.72, 32.55, 30.79, 29.85; (+)FABMS,  $m/z$  673

$(C_{29}H_{34}O_3^{81}Br_3, M + 1)$ . **Anal.** Calc for  $C_{29}H_{33}O_3Br_3$ : C, 52.04; H, 4.97. Found: C, 52.17; H, 4.93.

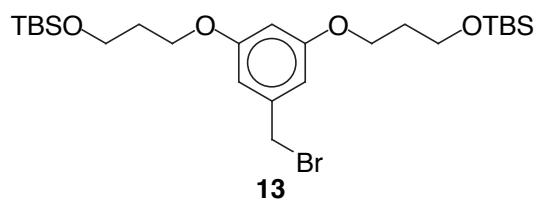


For **9**:  $^1H$  NMR ( $CDCl_3$ )  $\delta$  7.53 (d, 6 H,  $J = 7$  Hz), 7.23-7.28 (m, 9 H), 7.01 (d, 6 H,  $J = 9$  Hz), 6.79 (d, 6 H,  $J = 9$  Hz), 4.05 (t, 6 H,  $J = 6$  Hz), 3.12 (t, 6 H,  $J = 6$  Hz), 2.18 (quint, 6 H,  $J = 6$  Hz), 2.13 (s, 3 H);  $^{13}C$  NMR ( $CDCl_3$ )  $\delta$  156.76, 141.83, 132.50, 130.01, 129.57, 129.06, 126.81, 113.57, 66.67, 50.53, 30.73, 29.75, 24.10; (+)FABMS,  $m/z$  911 ( $C_{47}H_{49}O_3^{80}Se_3, M + 1$ ).

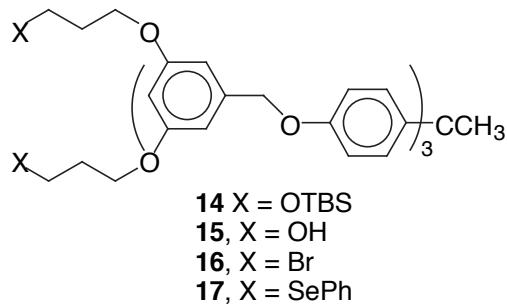
**Anal.** Calc for  $C_{47}H_{48}OSe_3$ : C, 62.88; H, 5.39. Found: C, 62.85; H, 5.25.



For **11**:  $^1H$  NMR ( $CDCl_3$ )  $\delta$  6.48 (d, 2 H,  $J = 1$  Hz), 6.37 (t, 1 H,  $J = 1$  Hz), 4.60 (d, 2 H,  $J = 6$  Hz), 4.02 (t, 4 H,  $J = 6$  Hz), 3.77 (t, 4 H,  $J = 6$  Hz), 1.95 (quintet, 4 H,  $J = 6$  Hz), 1.69 (t, 1 H,  $J = 6$  Hz, D<sub>2</sub>O-exchangable), 0.87 (s, 18 H), 0.02 (s, 12 H);  $^{13}C$  NMR ( $CDCl_3$ )  $\delta$  160.38, 143.16, 105.06, 100.49, 65.42, 64.49, 59.51, 32.37, 25.92, 18.31, -5.38; (+)FABMS,  $m/z$  485 ( $C_{25}H_{49}O_5Si_2, M + 1$ ). **Anal.** Calcd for  $C_{25}H_{48}O_5Si_2$ : C, 61.93; H, 9.98. Found: C, 61.76; H, 9.86.



For **13**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  6.50 (d, 2 H,  $J = 2$  Hz), 6.37 (t, 1 H,  $J = 2$  Hz), 4.39 (s, 2 H), 4.02 (t, 4 H,  $J = 6$  Hz), 3.77 (t, 4 H,  $J = 6$  Hz), 1.95 (quintet, 4 H,  $J = 6$  Hz), 0.87 (s, 18 H), 0.03 (s, 12 H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  160.33, 139.55, 107.47, 101.43, 64.58, 59.46, 33.73, 32.32, 25.90, 18.29, -5.41; (+)FABMS,  $m/z$  549 ( $\text{C}_{25}\text{H}_{48}^{81}\text{BrO}_4\text{Si}_2$ , M + 1). **Anal.** Calcd for  $\text{C}_{25}\text{H}_{47}\text{BrO}_4\text{Si}_2$ : C, 54.82; H, 8.65. Found: C, 54.54; H, 8.58.



For **14**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  6.97 (d, 6 H,  $J = 9$  Hz), 6.83 (d, 6 H,  $J = 9$  Hz), 6.55 (d, 6 H,  $J = 2$  Hz), 6.39 (t, 3 H,  $J = 2$  Hz), 4.92 (s, 6 H), 4.02 (t, 12 H,  $J = 6$  Hz), 3.77 (t, 12 H,  $J = 6$  Hz), 2.08 (s, 3 H), 1.95 (quintet, 12 H,  $J = 6$  Hz), 0.86 (s, 54 H), 0.02 (s, 36 H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  160.32, 156.76, 141.93, 139.28, 129.55, 113.90, 105.66, 100.66, 69.92, 64.40, 59.43, 50.56, 32.33, 30.74, 25.90, 18.26, -5.40. **Anal.** Calcd for  $\text{C}_{95}\text{H}_{156}\text{O}_{15}\text{Si}_6$ : C, 66.85; H, 9.21. Found: C, 66.95; H, 9.26.

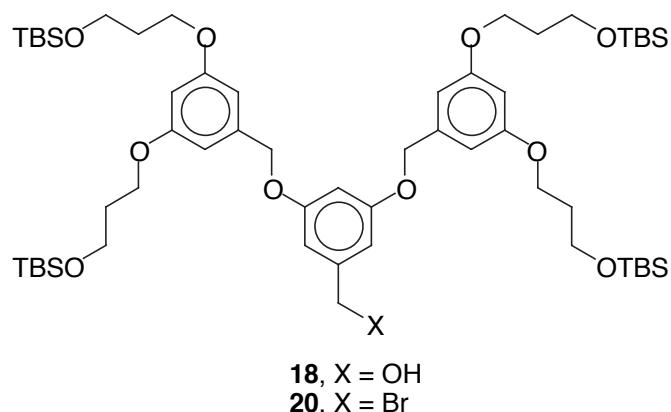
For **15**:  $^1\text{H}$  NMR ( $\text{DMSO}-d_6$ )  $\delta$  6.89 (s, 12 H), 6.56 (s, 6 H), 6.55 (d, 6 H,  $J = 2$  Hz), 6.41 (s, 3 H), 4.97 (s, 6 H), 3.98 (t, 12 H,  $J = 6$  Hz), 3.54 (t, 12 H,  $J = 6$  Hz), 2.01 (s, 3 H), 1.82 (quintet, 12 H,  $J = 6$  Hz);  $^{13}\text{C}$  NMR ( $\text{THF}-d_8$ )  $\delta$  161.58, 158.09, 142.89, 140.70, 130.40, 114.66, 106.29, 101.11, 70.57, 65.63, 59.08, 51.71, 33.62, 30.94.; (+)FABMS,  $m/z$  1021 ( $\text{C}_{59}\text{H}_{73}\text{O}_{15}$ , M + 1). **Anal.** Calcd for  $\text{C}_{59}\text{H}_{72}\text{O}_{15}$ : C, 69.39; H, 7.11. Found: C, 69.01; H, 7.12.

For **16**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  6.98 (d, 6 H,  $J = 9$  Hz), 6.85 (d, 6 H,  $J = 9$  Hz), 6.58 (s, 6 H), 6.41 (s, 3 H), 4.95 (s, 6 H), 4.08 (t, 12 H,  $J = 6$  Hz), 3.58 (t, 12 H,  $J = 6$  Hz), 2.29 (quintet, 12 H,

$J = 6$  Hz), 2.10 (s, 3 H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  159.99, 156.68, 142.01, 139.59, 129.59, 113.93, 105.96, 100.81, 69.83, 65.31, 50.60, 32.24, 30.72, 29.98. **Anal.** Calc for  $\text{C}_{59}\text{H}_{66}\text{Br}_6\text{O}_9$ : C, 50.67; H, 4.76. Found: C, 50.71; H, 4.81.

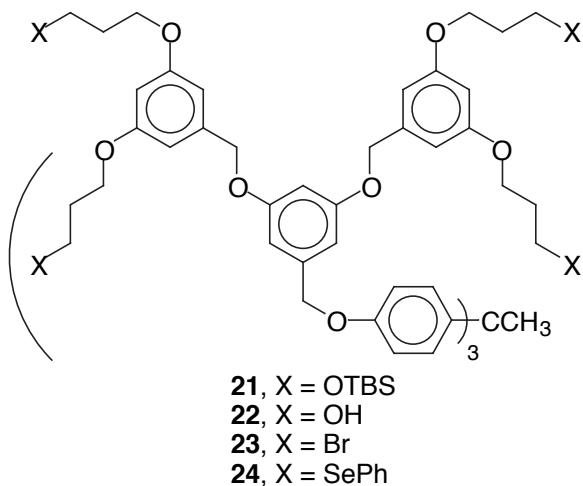
For **17**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  7.59 (d, 12 H,  $J = 7$  Hz), 7.29-7.33 (m, 18 H), 7.11 (d, 6 H,  $J = 9$  Hz), 6.96 (d, 6 H,  $J = 9$  Hz), 6.65 (s, 6 H), 6.46 (s, 3 H), 5.02 (s, 6 H), 4.10 (t, 12 H,  $J = 6$  Hz), 3.16 (t, 12 H,  $J = 7$  Hz), 2.21-2.24 (m, 15 H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  159.98, 156.63, 141.88, 139.33, 132.38, 129.86, 129.50, 128.96, 126.71, 113.85, 105.74, 100.62, 69.76, 66.76, 50.50, 30.66, 29.59, 23.95; ESMS, ion cluster  $m/z$  1840-1890 including  $m/z$  1876 for  $\text{C}_{95}\text{H}_{112}\text{O}_9\text{Se}_6$ .

**Anal.** Calc for  $\text{C}_{95}\text{H}_{112}\text{O}_9\text{Se}_6$ : C, 61.96; H, 6.13. Found: C, 61.58; H, 6.12.



For **18**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  6.59 (d, 2 H,  $J = 2$  Hz), 6.54 (d, 4 H,  $J = 2$  Hz), 6.52 (t, 1 H,  $J = 2$  Hz), 6.39 (t, 2 H,  $J = 2$  Hz), 4.94 (s, 4 H), 4.61 (d, 2 H,  $J = 7$  Hz), 4.02 (t, 8 H,  $J = 6$  Hz), 3.77 (t, 8 H,  $J = 6$  Hz), 1.95 (quintet, 8 H,  $J = 6$  Hz), 1.62 (t, 1 H,  $J = 7$  Hz,  $\text{D}_2\text{O}$ -exchangable), 0.86 (s, 36 H), 0.02 (s, 24 H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  160.41, 160.17, 143.36, 138.99, 105.74, 105.67, 101.28, 100.75, 70.03, 65.32, 64.52, 59.53, 32.35, 25.90, 18.28, -5.41; (+)FABMS,  $m/z$  1073 ( $\text{C}_{57}\text{H}_{101}\text{O}_{11}\text{Si}_4$ , M + 1). **Anal.** Calcd for  $\text{C}_{57}\text{H}_{100}\text{O}_{11}\text{Si}_4$ : C, 63.76; H, 9.39. Found: C, 63.34; H, 9.28.

For **20**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  6.60 (d, 2 H,  $J = 2$  Hz), 6.54 (d, 4 H,  $J = 2$  Hz), 6.52 (t, 1 H,  $J = 2$  Hz), 6.40 (t, 2 H,  $J = 2$  Hz), 4.93 (s, 4 H), 4.39 (s, 2 H), 4.02 (t, 8 H,  $J = 6$  Hz), 3.77 (t, 8 H,  $J = 6$  Hz), 1.95 (quintet, 8 H,  $J = 6$  Hz), 0.87 (s, 36 H), 0.02 (s, 24 H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  160.27, 159.86, 139.56, 138.67, 107.93, 105.58, 101.98, 100.66, 69.91, 64.32, 59.34, 33.38, 32.27, 25.85, 18.19, -5.45; (+)FABMS,  $m/z$  1137 ( $\text{C}_{57}\text{H}_{100}^{81}\text{BrO}_{10}\text{Si}_4$ , M + 1). **Anal.** Calcd for  $\text{C}_{57}\text{H}_{99}\text{BrO}_{10}\text{Si}_4$ : C, 60.23; H, 8.78. Found: C, 60.43; H, 8.76.



For **21**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  6.99 (d, 6 H,  $J = 9$  Hz), 6.85 (d, 6 H,  $J = 9$  Hz), 6.66 (s, 6 H), 6.54 (s, 15 H), 6.39 (t, 6 H,  $J = 1$  Hz), 4.93 (s, 18 H), 4.01 (t, 24 H,  $J = 6$  Hz), 3.76 (t, 24 H,  $J = 6$  Hz), 2.09 (s, 3 H), 1.94 (quintet, 24 H,  $J = 6$  Hz), 0.85 (s, 108 H), 0.01 (s, 72 H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  160.41, 160.14, 156.76, 142.16, 139.37, 138.91, 129.67, 113.91, 106.45, 105.81, 102.70, 100.78, 70.08, 64.51, 59.50, 51.50, 32.35, 30.59, 25.90, 18.27, -5.41.

For **22**:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ )  $\delta$  6.96 (d, 6 H,  $J = 9$  Hz), 6.82 (d, 6 H,  $J = 9$  Hz), 6.66 (s, 6 H), 6.56 (s, 15 H), 6.40 (t, 6 H,  $J = 1$  Hz), 4.95 (s, 18 H), 4.03 (t, 24 H,  $J = 6$  Hz), 3.65 (t, 24 H,  $J = 6$  Hz), 3.59 (s, 12 H, D<sub>2</sub>O-exchangable), 2.06 (s, 3 H), 1.90 (quintet, 24 H,  $J = 6$  Hz);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ )  $\delta$  161.50, 161.20, 158.00, 142.92, 140.83, 140.36, 130.41, 114.71, 106.96, 106.35,

101.95, 101.25, 70.63, 65.63, 59.14, 51.46, 33.53, 30.59. **Anal.** Calc for C<sub>119</sub>H<sub>144</sub>O<sub>33</sub>: C, 67.98; H, 6.90. Found: C, 68.13; H, 6.85.

For **23**: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 6.98 (d, 6 H, *J* = 9 Hz), 6.83 (d, 6 H, *J* = 9 Hz), 6.65 (s, 6 H), 6.53-6.56 (overlapping peaks, 15 H), 6.39 (t, 6 H, *J* = 1 Hz), 4.94 (s, 18 H), 4.05 (t, 24 H, *J* = 6 Hz), 3.56 (t, 24 H, *J* = 6 Hz), 2.22 (quintet, 24 H, *J* = 6 Hz), 2.09 (s, 3 H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 160.02, 159.87, 156.74, 142.06, 140.83, 140.36, 129.62, 113.95, 106.45, 106.06, 101.49, 100.87, 69.86, 65.34, 63.26, 50.58, 32.17, 30.45, 29.96.

For **24**: <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 7.43-7.51 (m, 24 H), 7.16-7.24 (m, 36 H), 6.98 (d, 6 H, *J* = 9 Hz), 6.83 (d, 6 H, *J* = 9 Hz), 6.66 (d, 6 H, *J* = 2 Hz), 6.54 (t, 3 H, *J* = 2 Hz), 6.51 (d, 12 H, *J* = 2 Hz), 6.33 (t, 6 H, *J* = 2 Hz), 4.93 (s, 6 H), 4.91 (s, 12 H), 3.99 (t, 24 H, *J* = 6 Hz), 3.04 (24 H, *J* = 7 Hz), 2.11 (quint, 24 H, *J* = 6 Hz), 2.09 (s, 3 H); <sup>13</sup>C NMR (CDCl<sub>3</sub>) δ 160.16, 160.09, 156.78, 142.08, 139.52, 139.05, 132.56, 129.97, 129.66, 129.09, 126.86, 113.97, 106.43, 105.93, 101.53, 100.85, 70.01, 69.89, 66.90, 50.62, 30.20, 29.67, 24.05. **Anal.** Calc for C<sub>191</sub>H<sub>192</sub>O<sub>21</sub>Se<sub>12</sub>: C, 60.83; H, 5.13. Found: C, 60.39; H, 5.15.